

**Supporting Information for:**

**Accurate Prediction of the Excited States in the Fully Conjugated Porphyrin Tapes Across  
the Full Spectral Range: a Story of the Interplay Between  $\pi-\pi^*$  and Intramolecular  
Charge-Transfer Transitions in Soft Chromophores**

Rodion V. Belosludov,<sup>\*a</sup> Dustin E. Nevonen,<sup>b</sup> Victor N. Nemykin,<sup>\*b,c</sup>

<sup>a</sup> *Institute for Materials Research, Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai, 980-8577, Japan*

<sup>b</sup> *Department of Chemistry, University of Manitoba, Winnipeg, MB, R3T 2N2, Canada*

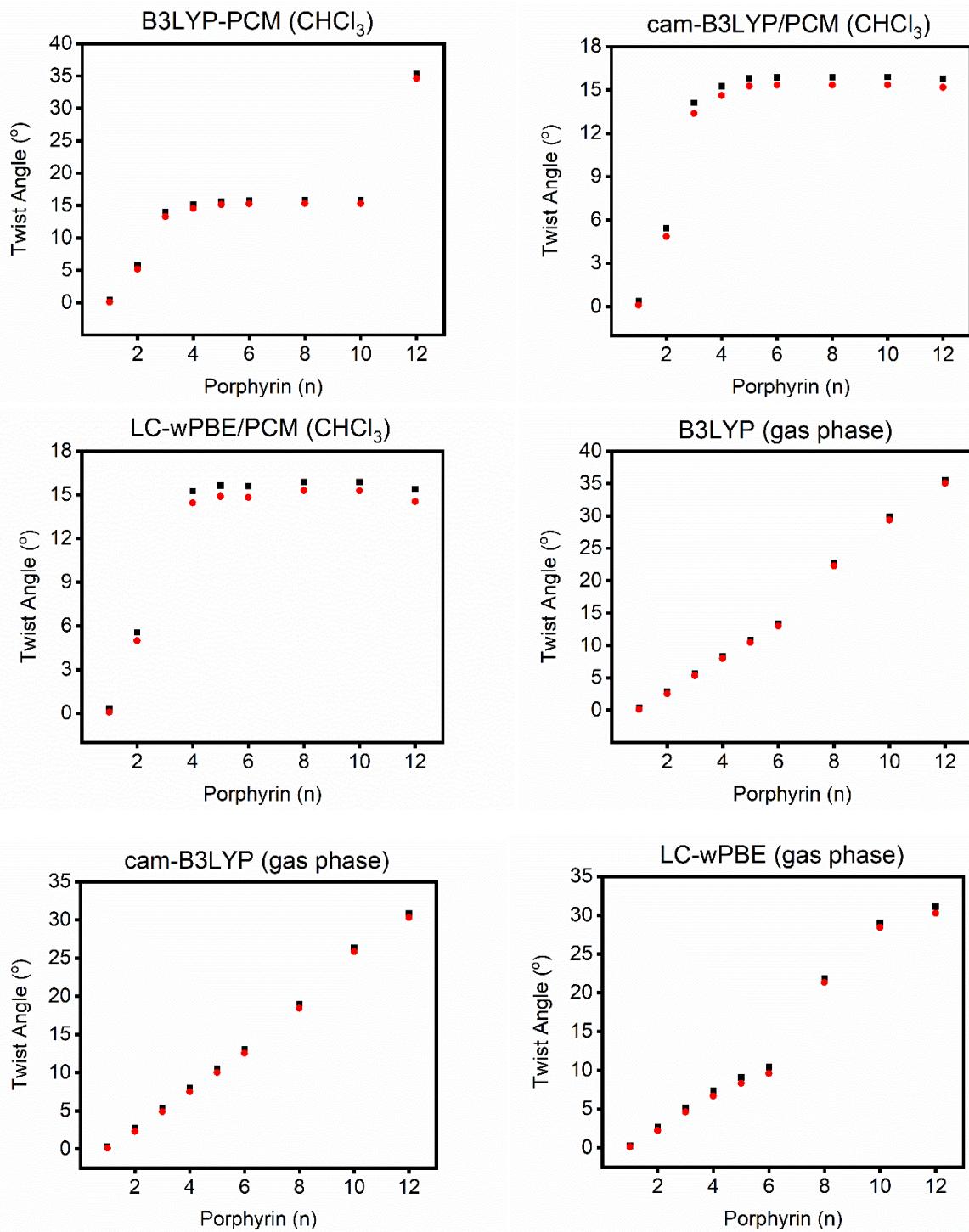
<sup>c</sup> *Department of Chemistry, University of Tennessee, Knoxville, TN 37996, USA*

Full Citation for Gaussian 09:

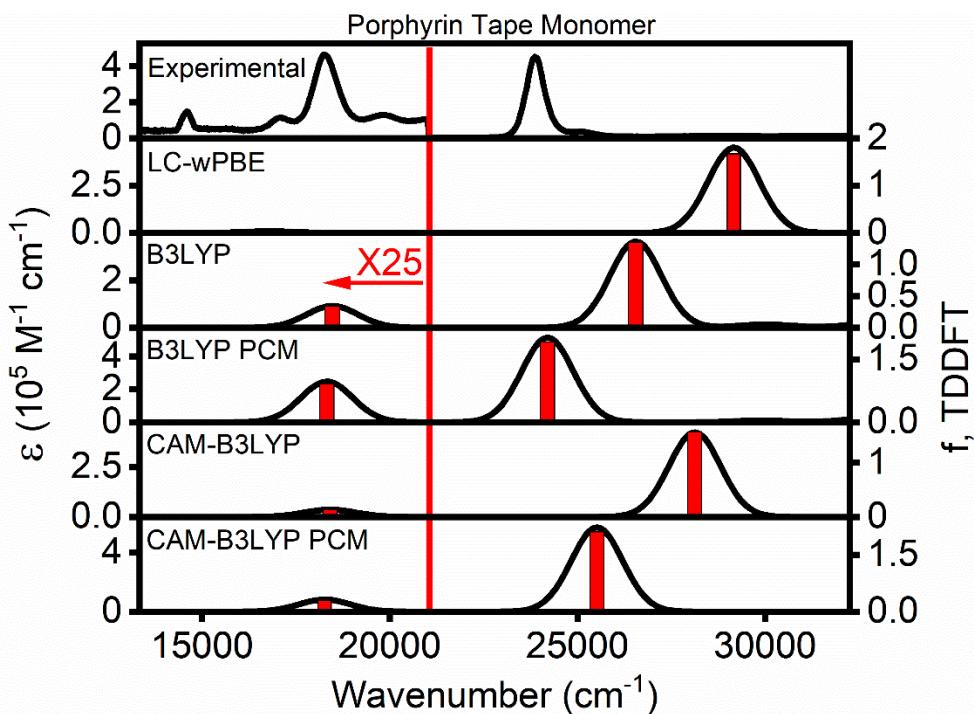
Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2009**.

Full citation for reference 31:

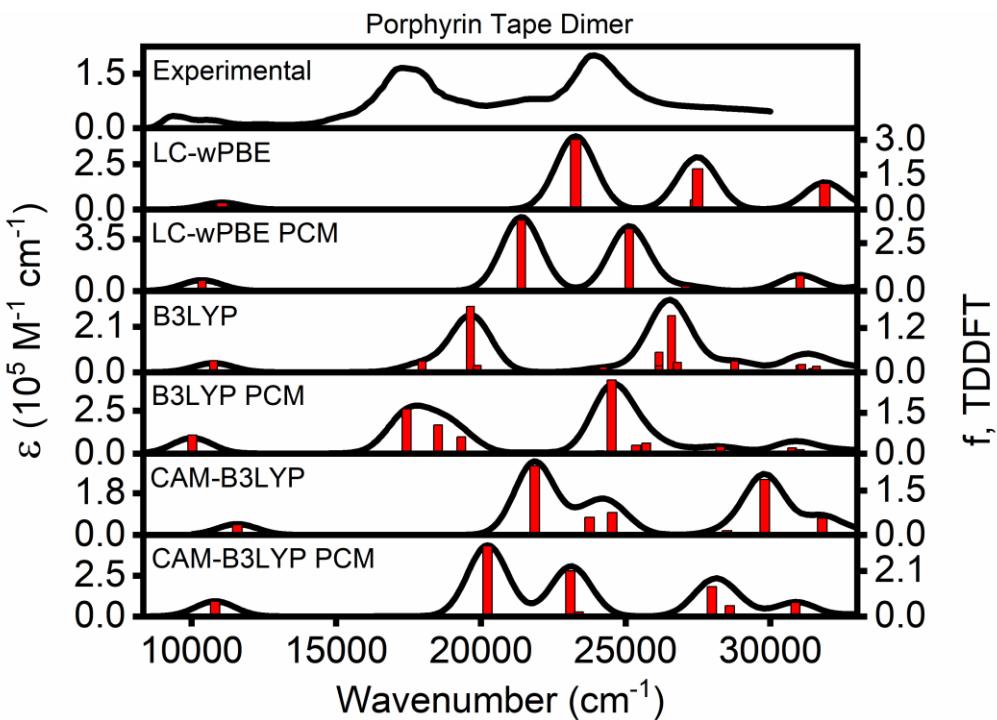
Agostinis, P.; Berg, K.; Cengel, K. A.; Foster, T. H.; Girotti, A. W.; Gollnick, S. O.; Hahn, S. M.; Hamblin, M. R.; Juzeniene, A.; Kessel, D.; Korbelik, M.; Moan, J.; Mroz, P.; Nowis, D.; Piette, J.; Wilson, B. C.; Golab, J. Photodynamic Therapy of Cancer: An Update. *Cancer J. Clin.* **2011**, *61*, 250– 281.



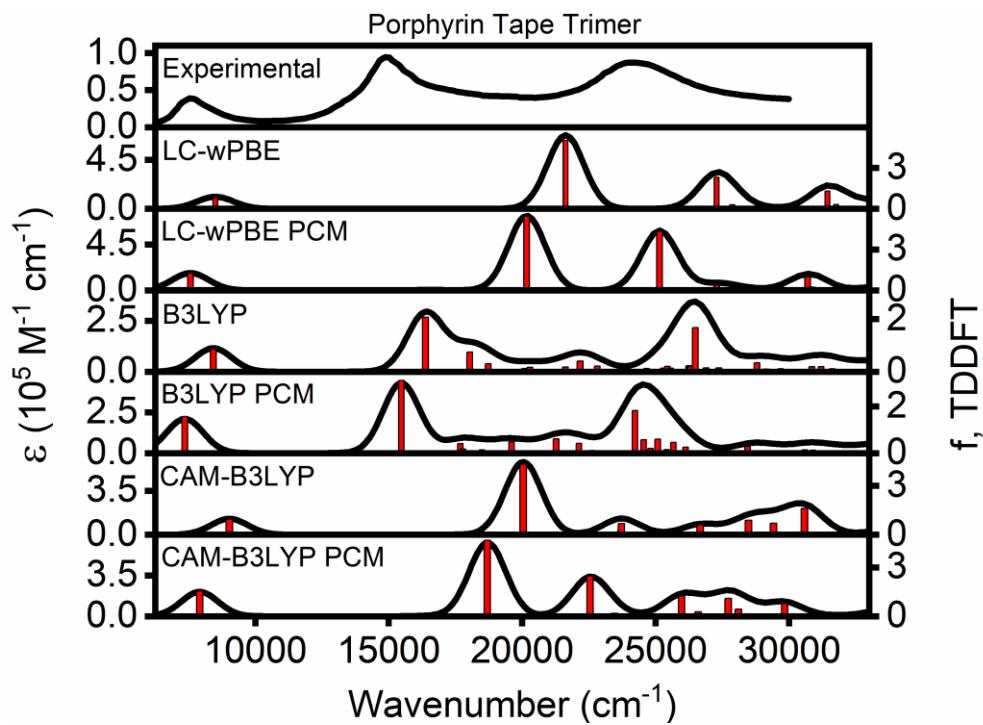
**Figure S1.**  $\alpha$  (black)- and  $\beta$  (red)-twist angle vs. number of porphyrin subunits in chain for three comparative exchange correlation functionals modelled with (PCM) and without (gas phase) solvent effects.



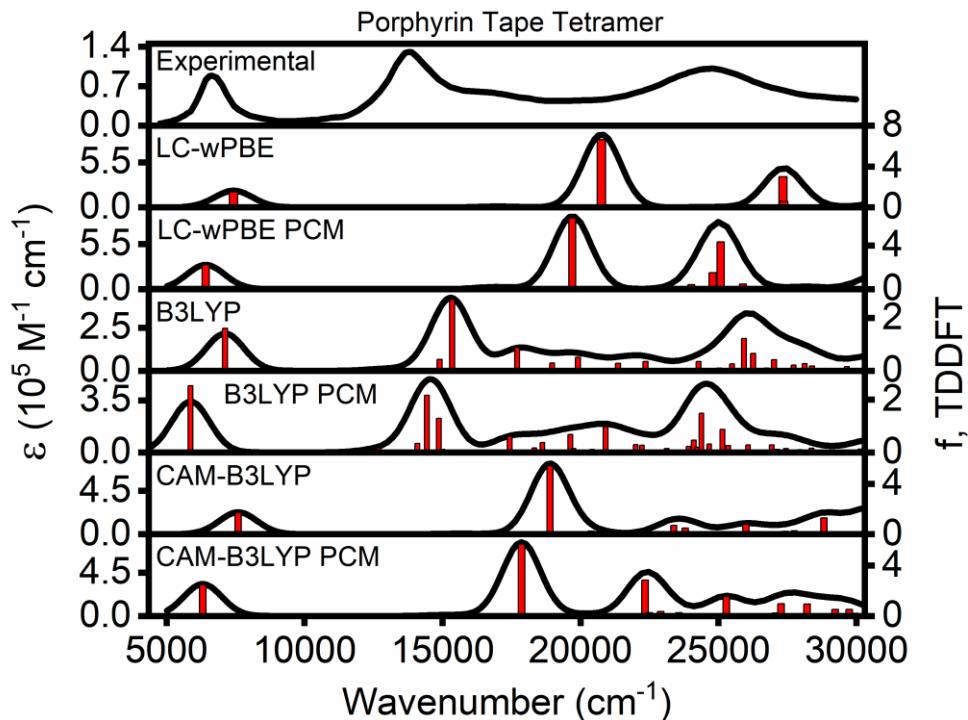
**Figure S2.** TDDFT-predicted UV-vis spectrum of **1** showing the exchange correlation functional comparison.



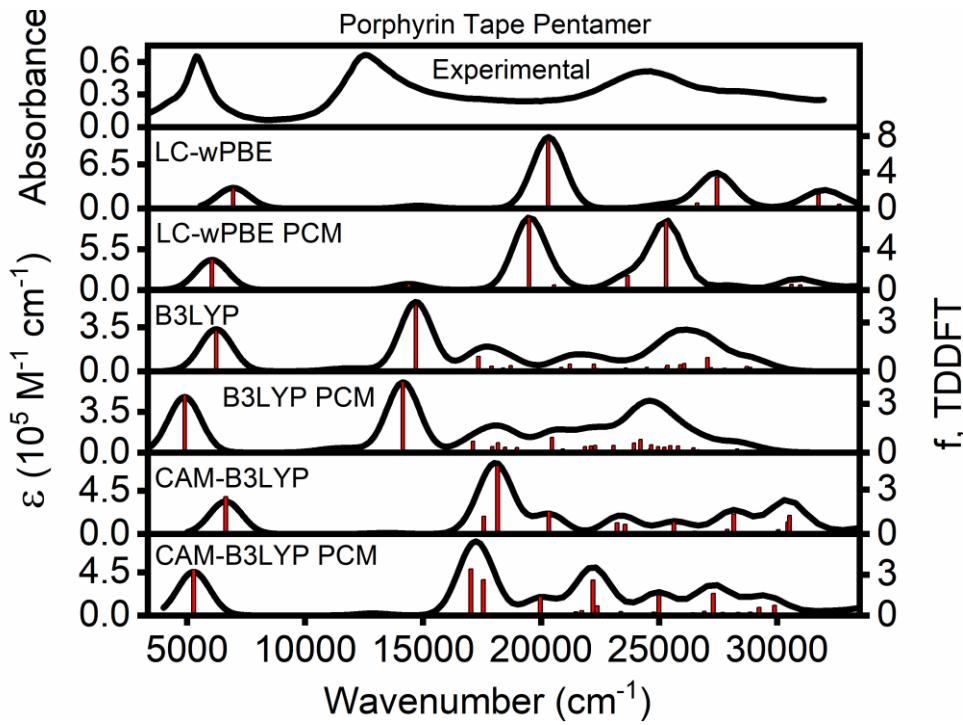
**Figure S3.** TDDFT-predicted UV-vis spectrum of **2** showing the exchange correlation functional comparison.



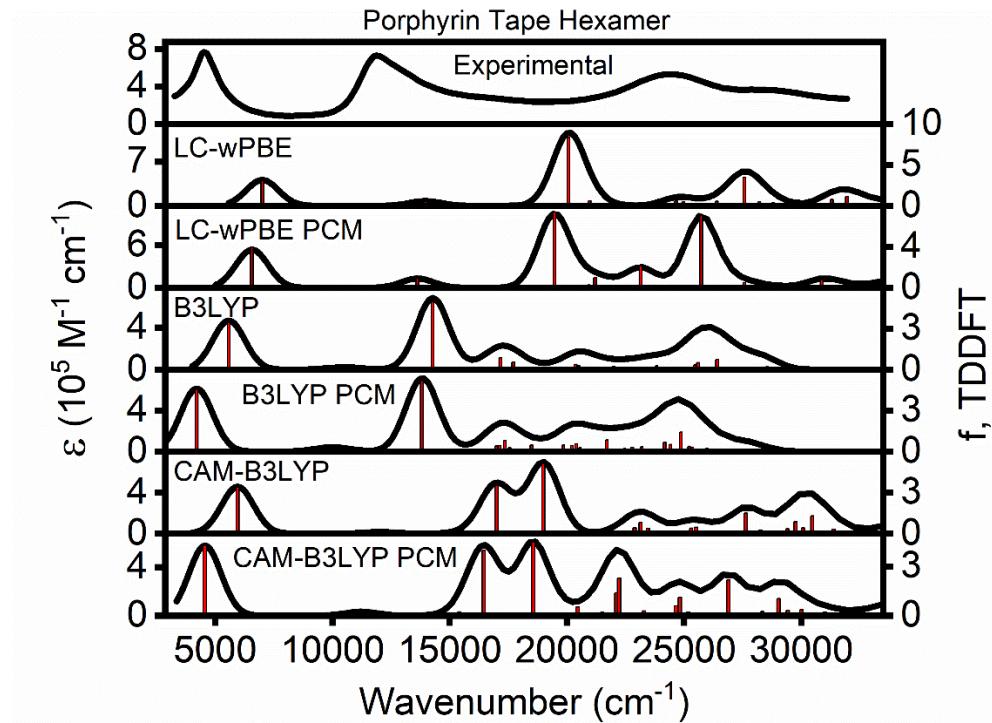
**Figure S4.** TDDFT-predicted UV-vis spectrum of **3** showing the exchange correlation functional comparison.



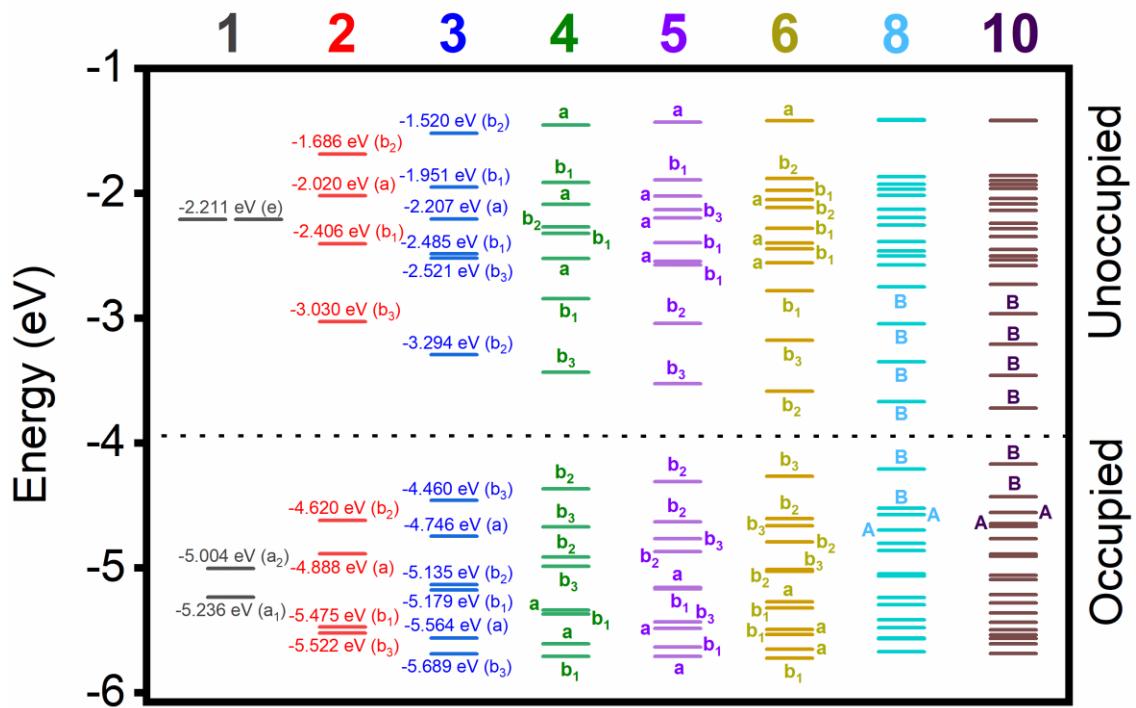
**Figure S5.** TDDFT-predicted UV-vis spectrum of **4** showing the exchange correlation functional comparison.



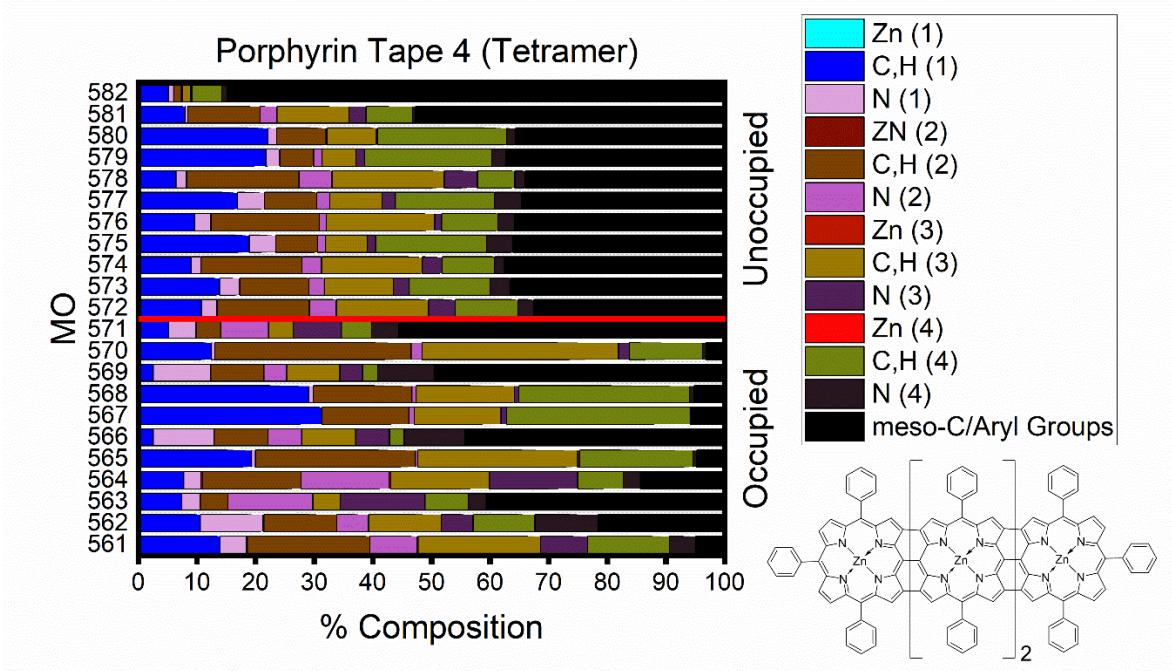
**Figure S6.** TDDFT-predicted UV-vis spectrum of **5** showing the exchange correlation functional comparison.



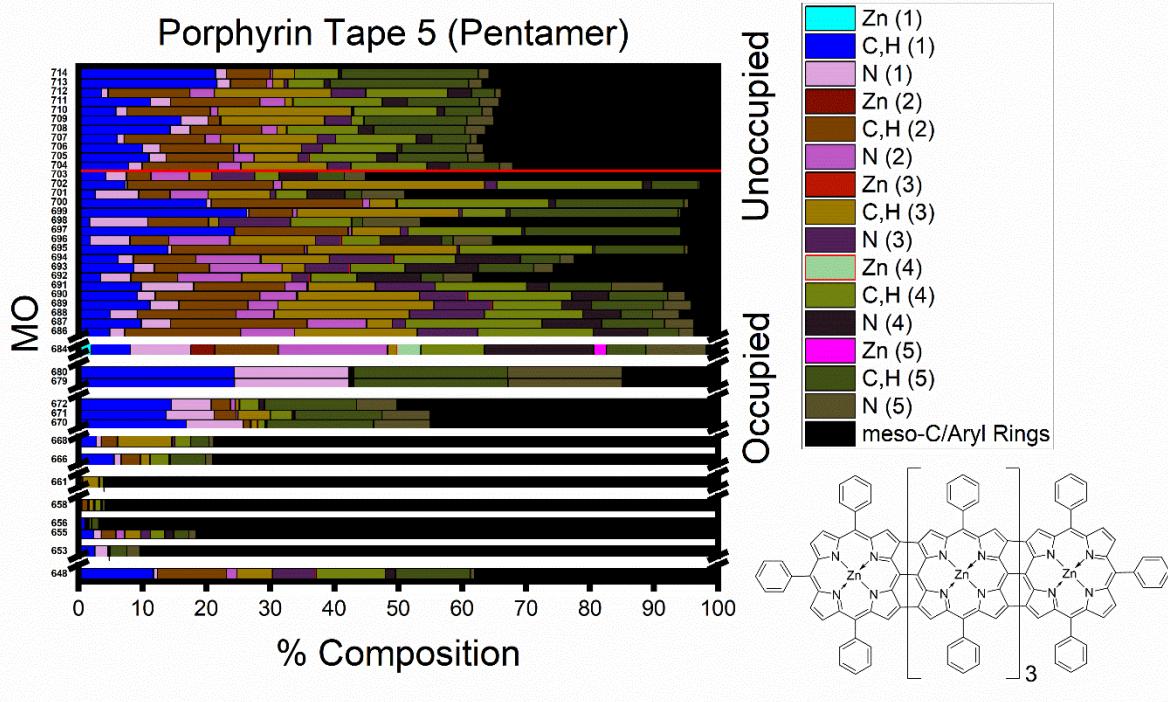
**Figure S7.** TDDFT-predicted UV-vis spectrum of **6** showing the exchange correlation functional comparison.



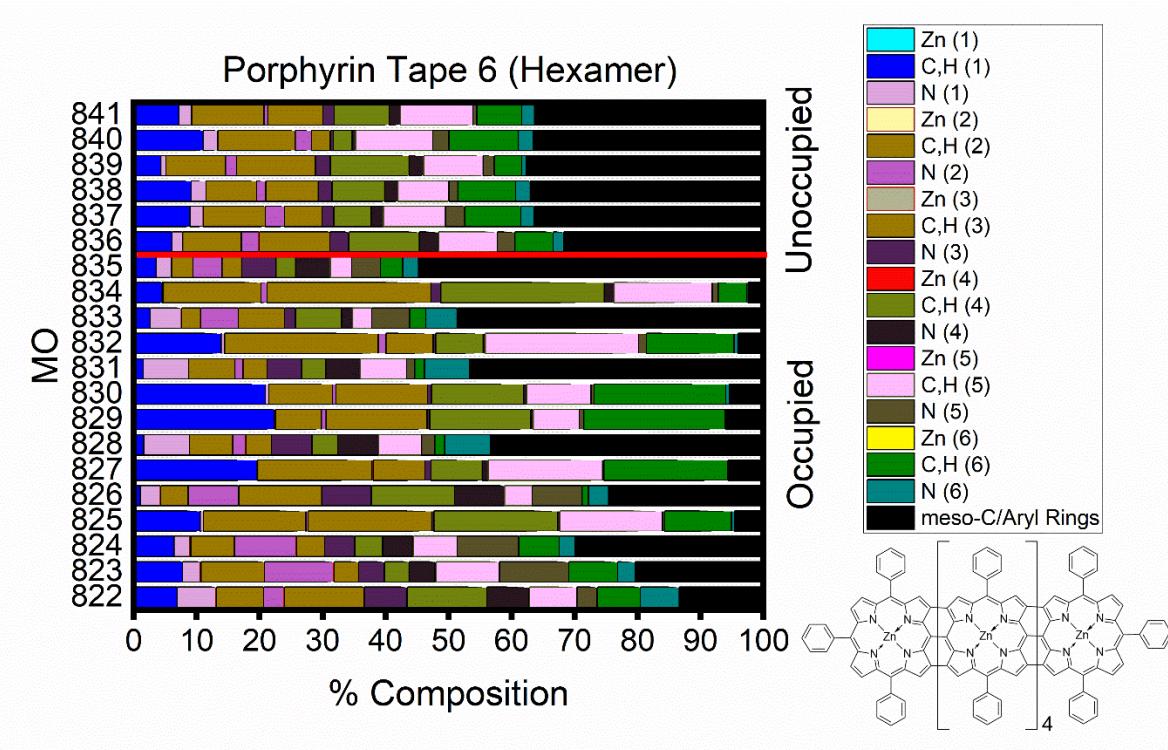
**Figure S8.** DFT-predicted energy level diagram for porphyrin tapes **1-10** (the 12-mer energy levels are not included due to program limitations associated with the large file size).



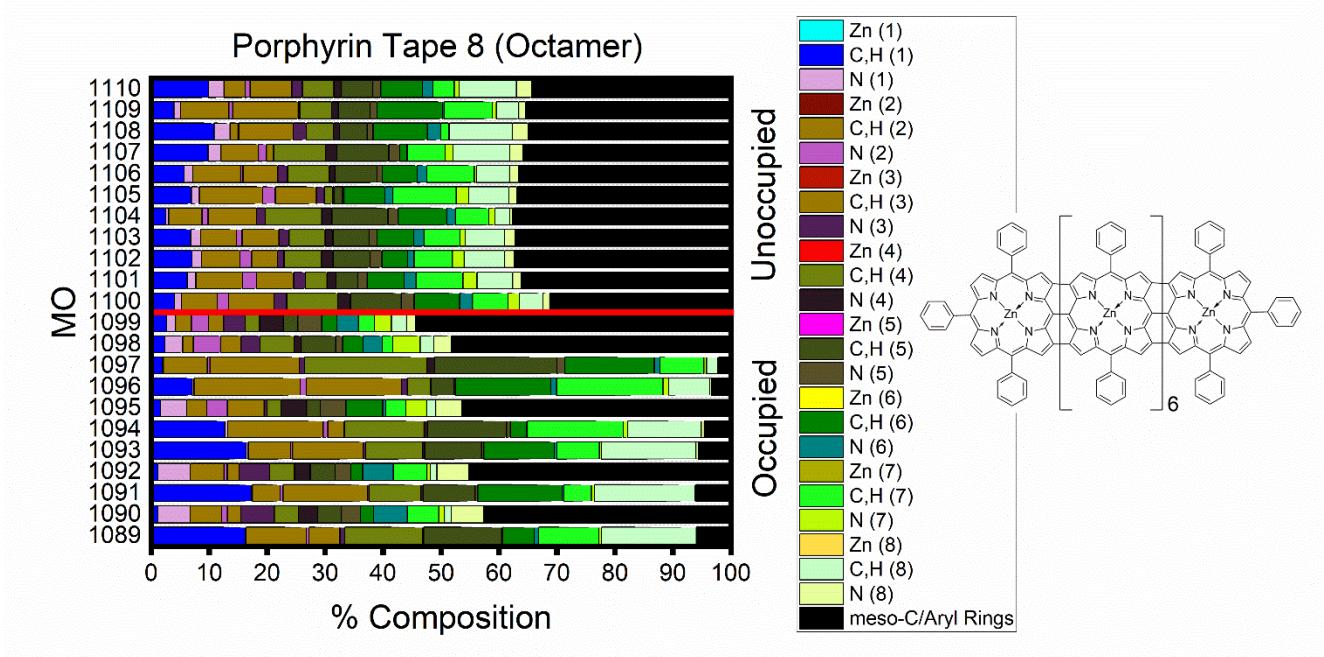
**Figure S9.** Molecular orbital percent composition diagram for tetramer **4**.



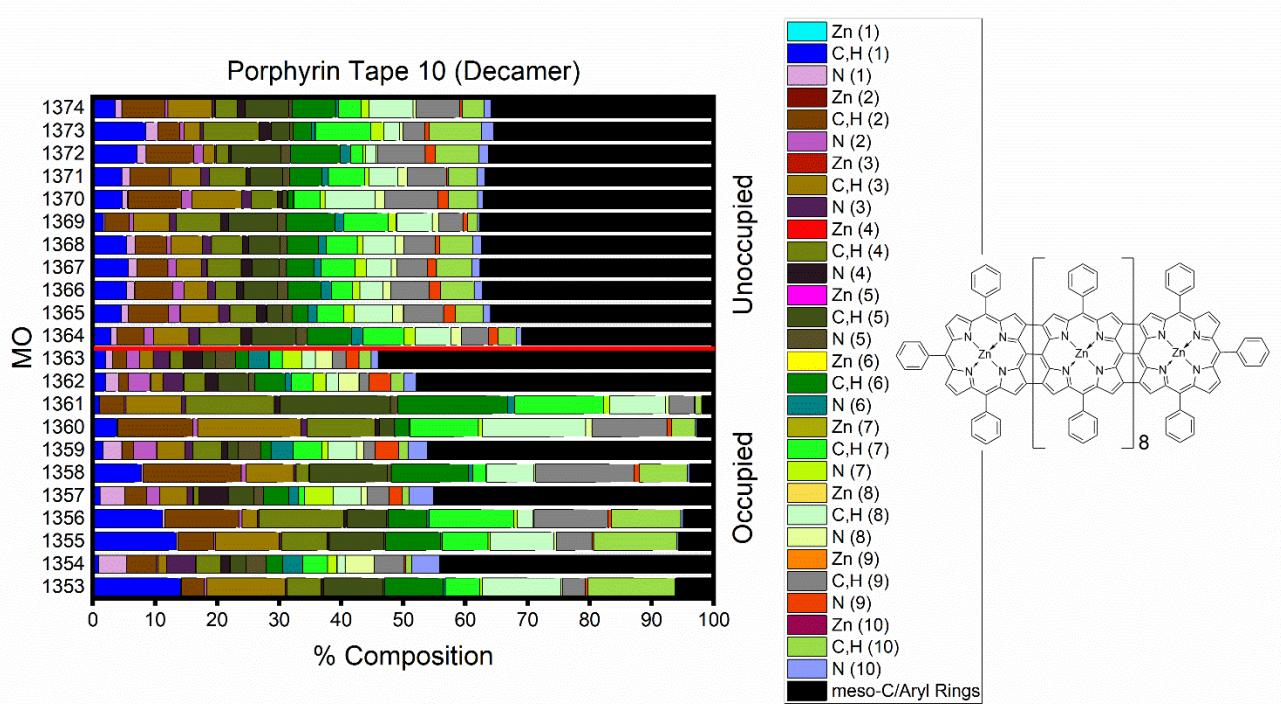
**Figure S10.** Molecular orbital percent composition diagram for pentamer **5**.



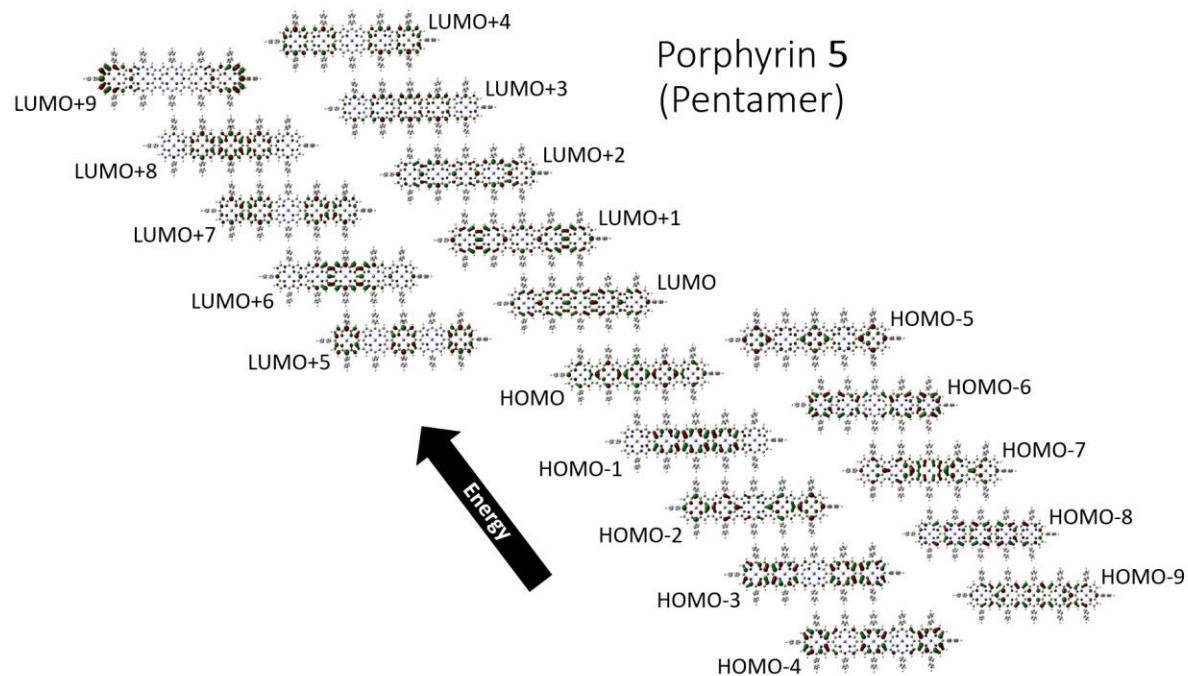
**Figure S11.** Molecular orbital percent composition diagram for hexamer **6**.



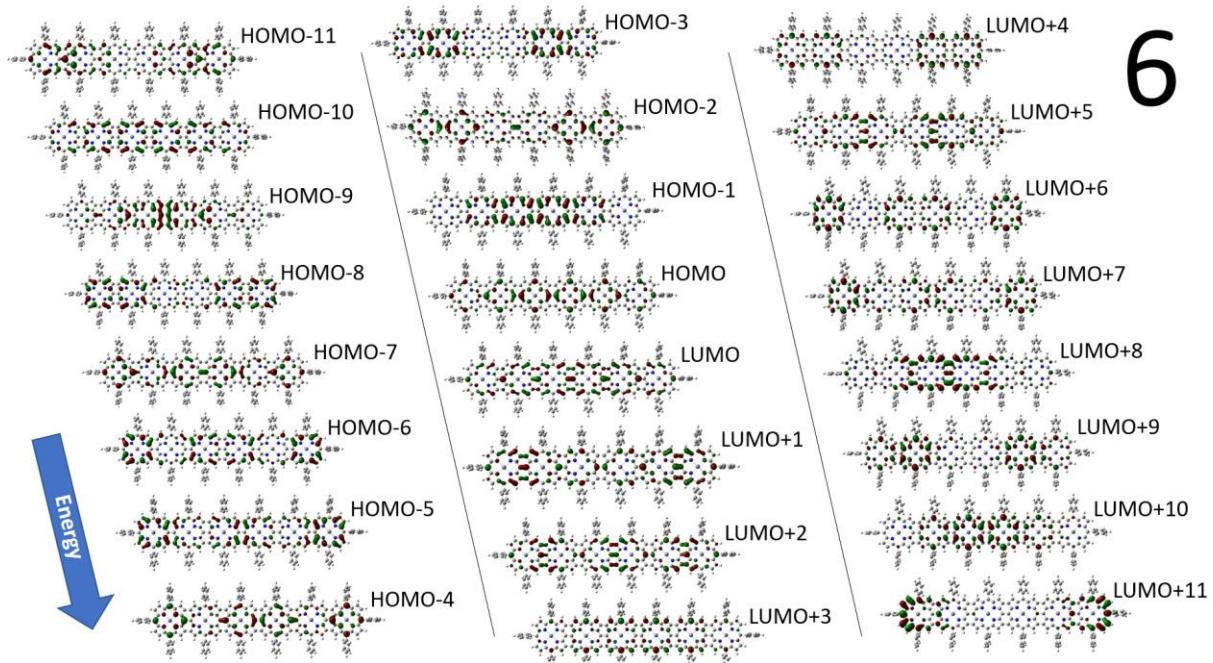
**Figure S12.** Molecular orbital percent composition diagram for octamer **8**.



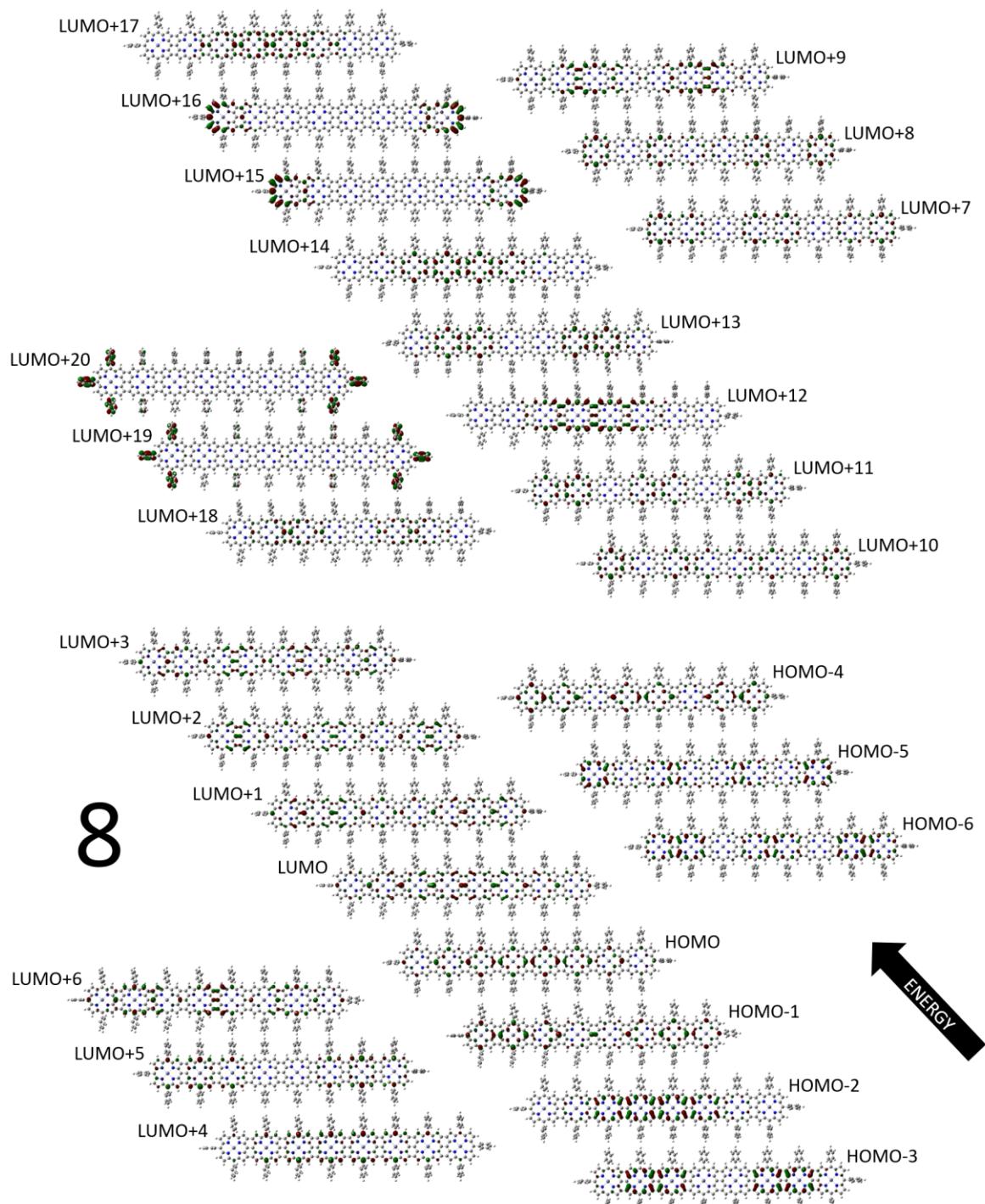
**Figure S13.** Molecular orbital percent composition diagram for decamer **10**.

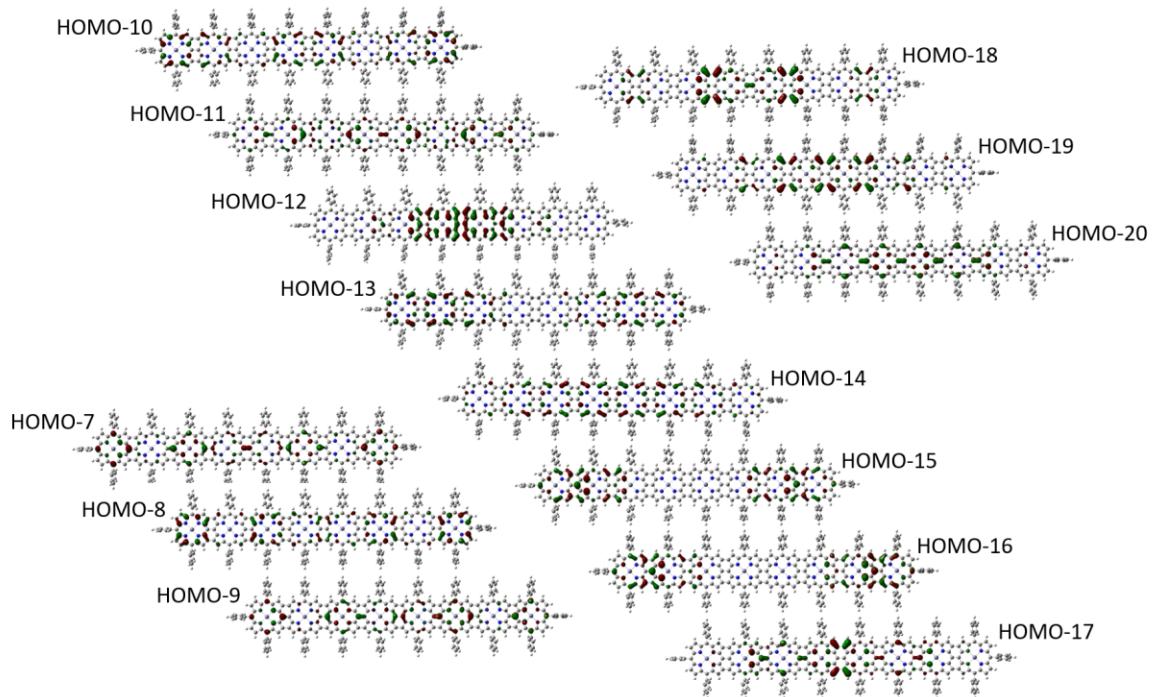


**Figure S14.** Selected DFT-predicted molecular orbitals for porphyrin tape 5.

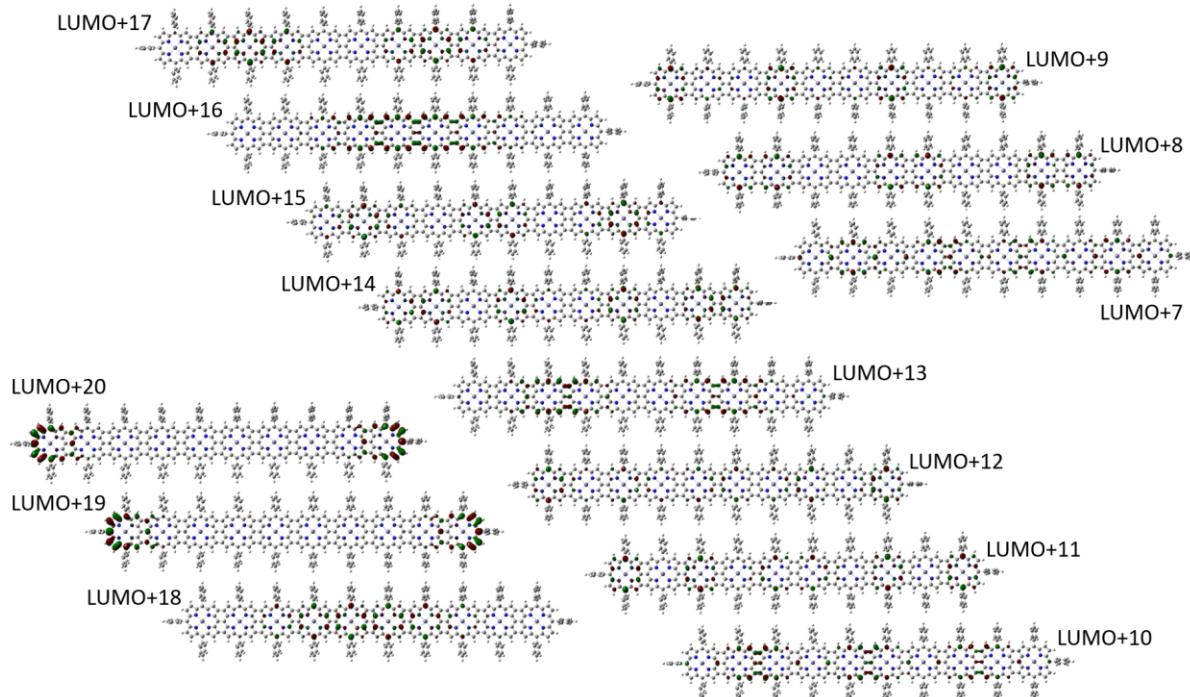


**Figure S15.** Selected DFT-predicted molecular orbitals for porphyrin tape 6.

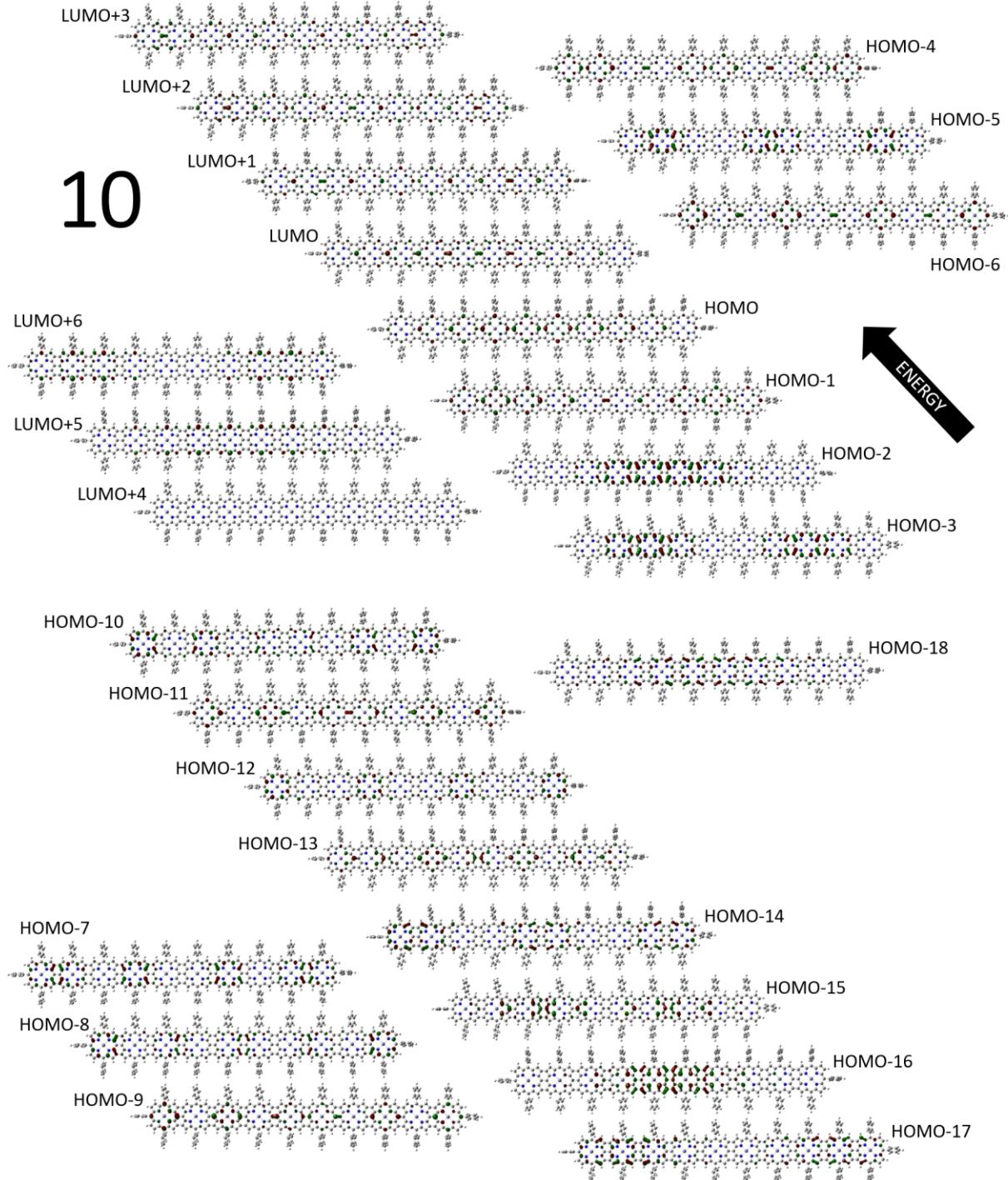




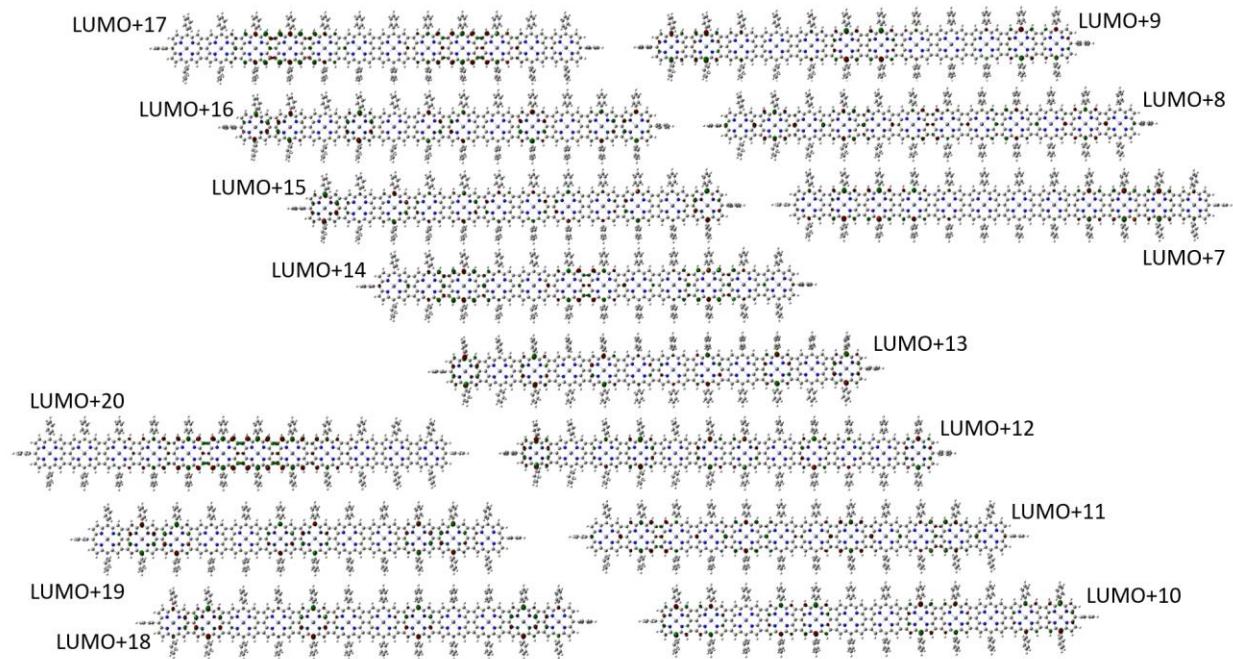
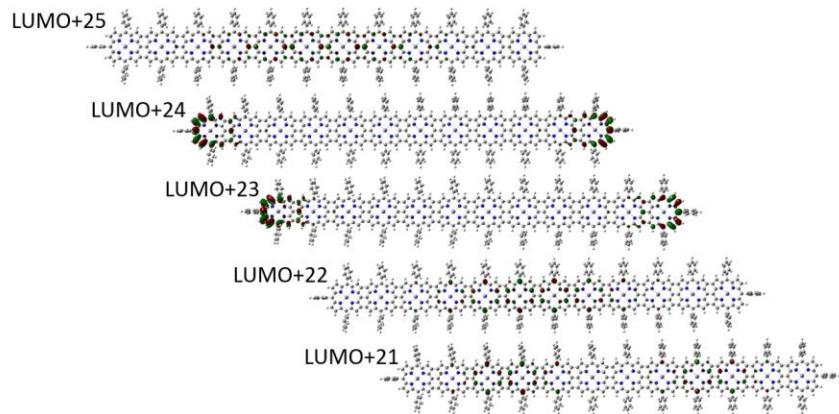
**Figure S16.** Selected DFT-predicted molecular orbitals for porphyrin tape **8**.

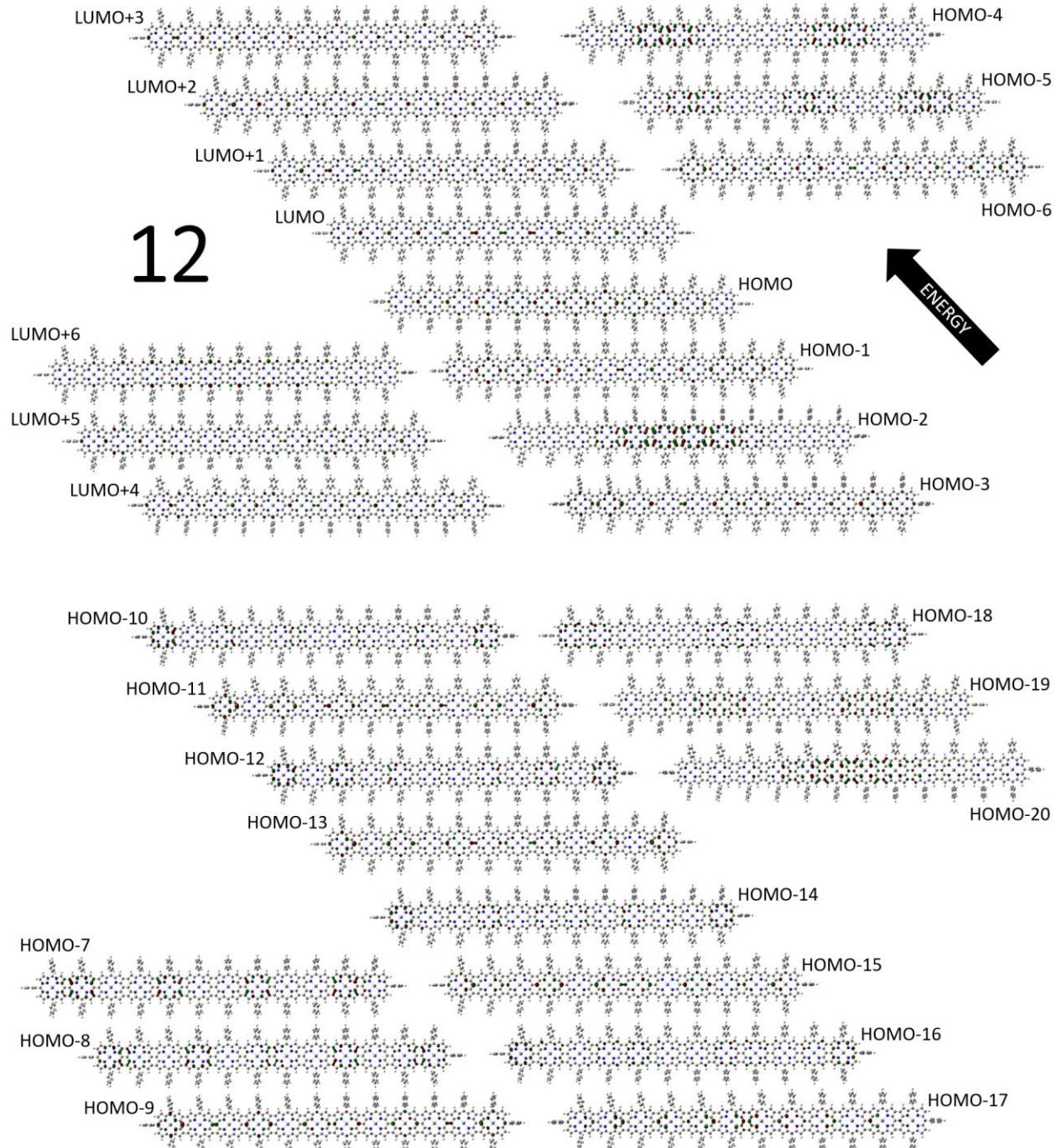


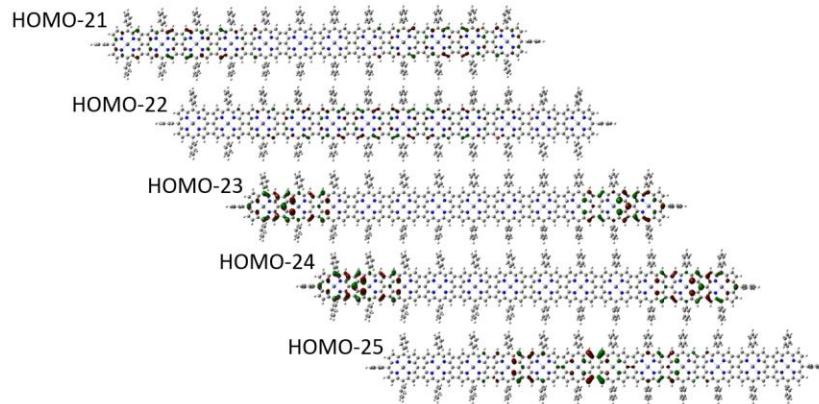
**10**



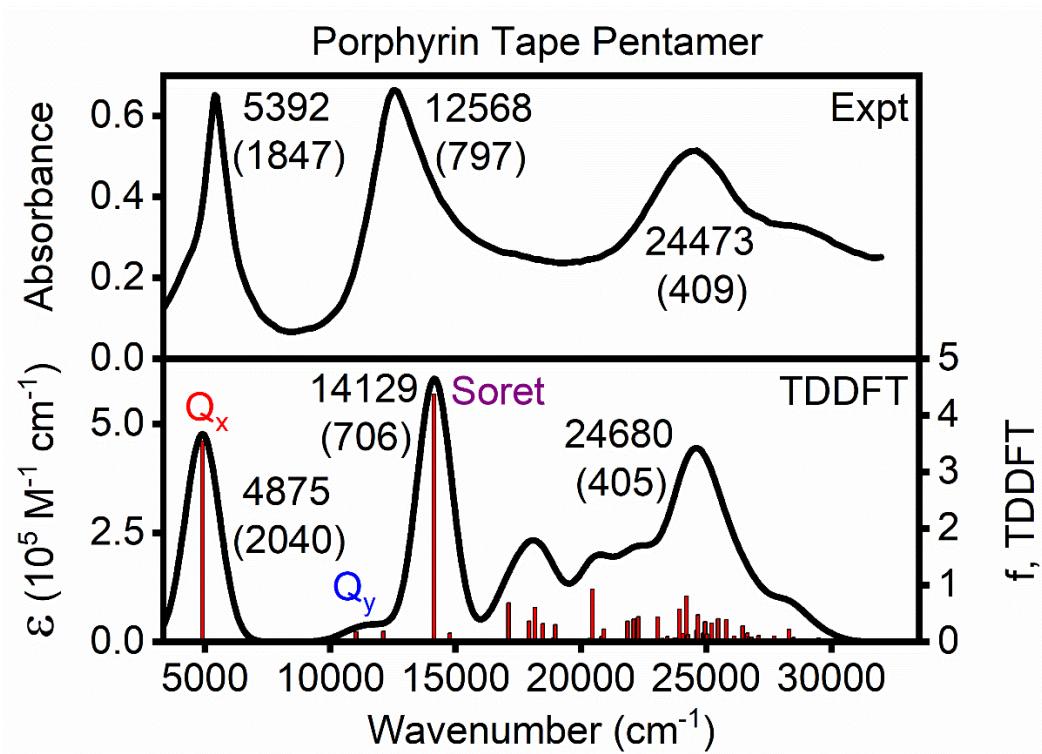
**Figure S17.** Selected DFT-predicted molecular orbitals for porphyrin tape **10**.



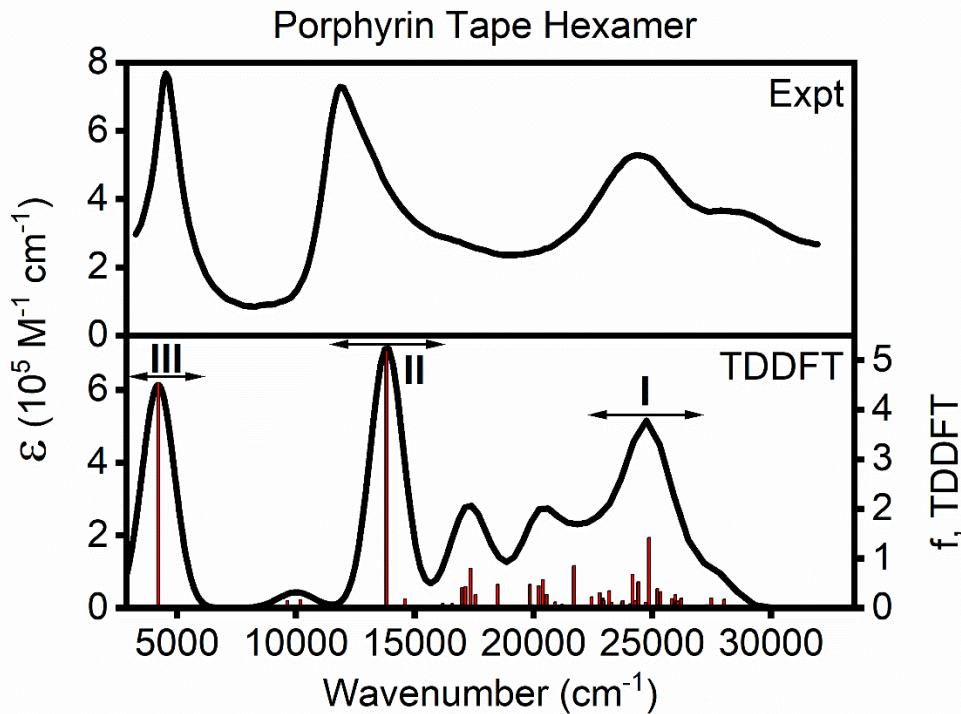




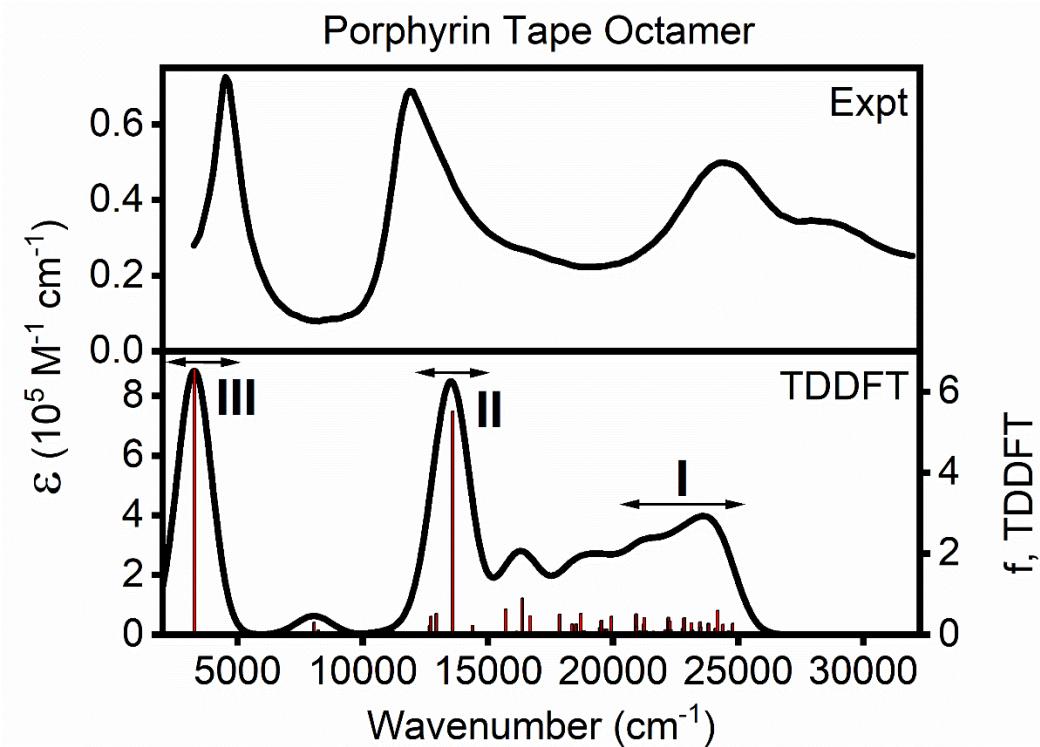
**Figure S18.** Selected DFT-predicted molecular orbitals for porphyrin tape **12**.



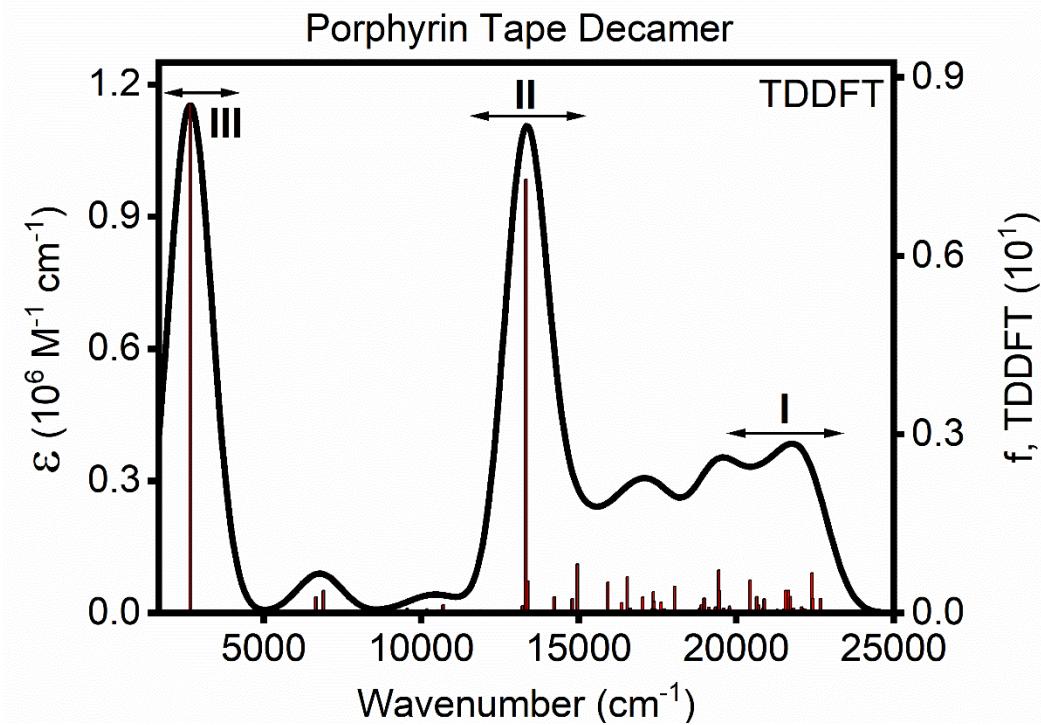
**Figure S19.** Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of pentamer **5**.



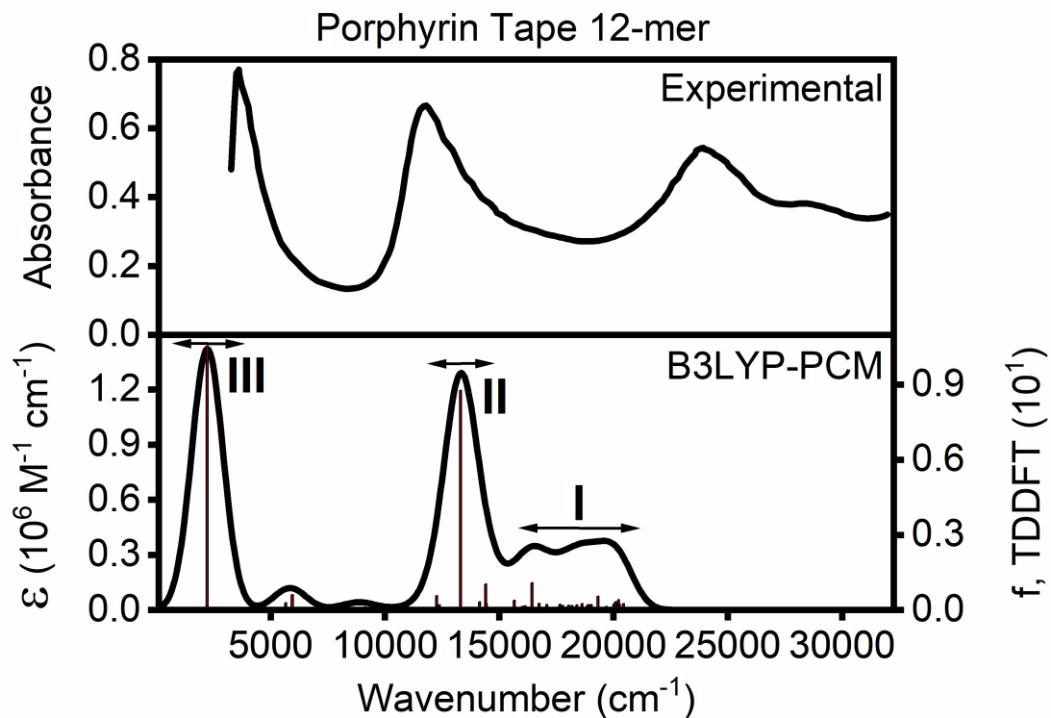
**Figure S20.** Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of hexamer **6**.



**Figure S21.** Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of octamer **8**.



**Figure S22.** TDDFT-predicted (bottom) UV-vis spectrum of decamer **10**.



**Figure S23.** Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of dodecamer **12**.

**Table S1.** TDDFT-predicted energies and compositions Q- and Soret-band assignments.<sup>a</sup>

<i>Cmpd.</i>	<i>Excited State</i>	<i>Assignment</i>	$\lambda/\text{nm}$	$E, \text{cm}^{-1}$	$f$	<i>Single-electron excitation contributions</i>
<b>1</b>	1,2	Q	546	18324	0.0368	H→L/L+1 (64%), H-1→L/L+1 (36%)
	3,4	Soret	413	24205	1.9080	H-1→L/L+1 (64%), H→L/L+1 (36%)
<b>2</b>	1	$Q_1$	997	10034	0.6740	H→L (94%), H-1→L+1 (5%)
	4	$Q_2$	620	16138	0.0174	H-2→L (65%), H→L+2 (33%)
	6	Soret-1	574	17434	1.6390	H-1→L+1 (91%), H-4→L (4%), H→L (4%)
	7	CT	540	18523	1.0460	H-4→L (93%), H-1→L+1 (3%), H→L (3%)
	8	Soret-type	517	19325	0.6133	H→L+2 (58%), H-2→L (27%), H-1→L+3 (11%), H-3→L+1 (4%)
	18	Soret-2	408	24518	2.7060	H-1→L+3 (59%), H-3→L+1 (24%), H→L+2 (8%), H-2→L (6%)
	22	CT	394	25362	0.3028	H→L+4 (37%), H-5→L+1 (33%), H-2→L+2 (26%), H-12→L (2%)
	23	CT	389	25715	0.3771	H-5→L+1 (58%), H→L+4 (29%), H-12→L (9%)
	42	Soret-type	354	28276	0.2657	H-3→L+3 (85%), H-2→L+2 (5%), H-18→L (2%)
	49	CT	325	30752	0.1397	H-25→L (62%), H-11→L+1 (29%), H-10→L+2 (3%)
<b>3</b>	50	CT	325	30753	0.2023	H-13→L+1 (80%), H-14→L+2 (7%), H-15→L+1 (4%), H-12→L+2 (2%)
	53	CT	322	31014	0.1444	H-11→L+1 (56%), H-25→L (30%), H-10→L+2 (4%)
	1	$Q_1$	1358	7363	1.5580	H→L (97%), H-1→L+2 (2%)
	6	Q-type	747	13388	0.0037	H→L+2 (96%)
	8	$Q_2$	649	15400	0.0645	H-4→L (76%), H→L+4 (20%), H-2→L+3 (2%)
	9	Soret-1	646	15475	3.1210	H-1→L+2 (90%), H-5→L (6%), H→L (3%)
	13	CT	565	17689	0.4068	H-7→L (66%), H-2→L+1 (22%), H-1→L+4 (4%), H-3→L+3 (2%)
	14	Q-type	562	17789	0.1775	H→L+4 (46%), H-3→L+1 (35%), H-4→L (16%)
	16	Q-type	541	18486	0.1366	H-2→L+1 (54%), H-7→L (30%), H-1→L+4 (7%), H-5→L (4%), H-3→L+3 (3%)
	21	Soret-type	510	19602	0.4884	H-3→L+1 (33%), H→L+4 (27%), H-9→L (25%), H-2→L+3 (7%), H-5→L+2 (4%)
25	Soret-type	470	21275	0.6094	H-2→L+3 (69%), H-1→L+5 (13%), H-3→L+1 (8%), H-4→L (3%)	
30	Soret-type	452	22133	0.4242	H-3→L+3 (48%), H-4→L+2 (45%)	
31	CT	442	22616	0.1127	H-6→L+1 (92%), H→L+5 (2%)	

	40	Soret-2	413	24226	1.8210	H-1→L+5 (46%), H-8→L+1 (16%), H-5→L+2 (11%), H-7→L+2 (10%), H-2→L+3 (5%)
	41	Soret-type	407	24548	0.5675	H-4→L+2 (28%), H→L+5 (22%), H-3→L+3 (13%), H-1→L+4 (9%), H-2→L+1 (7%), H-5→L (5%), H-30→L (4%), H-24→L (3%)
	46	CT	403	24810	0.2079	H-7→L+2 (45%), H-16→L (24%), H-6→L+3 (15%), H-5→L+2 (6%), H-1→L+5 (4%), H-8→L+1 (2%)
	48	CT	399	25082	0.5987	H-8→L+1 (68%), H-6→L+3 (9%), H-1→L+5 (8%), H-2→L+3 (4%), H-5→L+4 (3%), H-5→L+2 (2%)
	54	CT	394	25408	0.1447	H-9→L+2 (64%), H-21→L (25%), H-8→L+3 (3%), H-23→L (2%), H-19→L (2%)
	56	CT	390	25665	0.4594	H-6→L+3 (50%), H-7→L+2 (24%), H-8→L+1 (9%), H-7→L+4 (6%), H-5→L+4 (3%), H-1→L+5 (3%)
	60	Soret-type	383	26128	0.2541	H-4→L+4 (80%), H-9→L+2 (5%), H-8→L+3 (4%)
	85	Soret-type	352	28446	0.2923	H-2→L+6 (86%), H-11→L+1 (3%), H-5→L+5 (2%), H-4→L+4 (2%)
	100	CT	327	30586	0.1371	H-37→L (64%), H-16→L+2 (15%), H-5→L+5 (4%), H-17→L+3 (4%), H-6→L+6 (3%)
	104	CT	324	30890	0.1301	H-19→L+2 (46%), H-21→L+2 (14%), H-18→L+3 (9%), H-20→L+3 (9%), H-13→L+1 (5%), H-12→L+2 (4%), H-11→L+3 (3%)
<b>4</b>	1	Q <sub>1</sub>	1703	5871	2.5360	H→L (98%)
	10	Q-type	710	14091	0.3410	H→L+4 (38%), H-2→L+1 (34%), H-5→L (9%), H-7→L (7%), H-1→L+2 (6%), H-3→L+3 (2%)
	13	Soret-1	693	14439	2.1570	H-1→L+2 (43%), H→L+4 (39%), H-2→L+1 (14%)
	14	Soret-type	672	14872	1.2940	H-1→L+2 (45%), H-2→L+1 (39%), H→L+4 (12%)
	15	Q <sub>2</sub>	666	15006	0.1087	H-6→L (81%), H→L+6 (14%), H-2→L+5 (2%)
	24	CT	573	17438	0.6096	H-11→L (94%), H-9→L+1 (3%)
	30	Soret-type	537	18623	0.3683	H-4→L+1 (29%), H-12→L (28%), H→L+6 (27%), H-3→L+4 (9%)
	35	Soret-type	509	19632	0.6761	H-3→L+3 (83%), H-2→L+1 (2%), H→L+8 (2%), H-1→L+2 (2%)
	44	Soret-type	478	20916	0.9720	H-2→L+5 (66%), H-3→L+4 (12%), H-1→L+7 (4%), H-4→L+1 (4%), H-10→L+1 (3%), H-6→L (2%)
	51	CT	455	22000	0.2914	H-9→L+1 (40%), H→L+8 (38%), H-5→L+4 (7%), H-7→L+4 (2%)

52	Soret-type	450	22226	0.2735	H-5→L+3 (63%), H-10→L+1 (16%), H-1→L+7 (5%), H-2→L+5 (4%)		
68	CT	418	23926	0.2222	H-24→L (48%), H-4→L+5 (19%), H-6→L+3 (5%), H-5→L+4 (5%), H→L+8 (4%), H-26→L (3%), H-7→L+4 (2%), H-28→L (2%)		
71	Soret-type	415	24106	0.4672	H→L		
75	Soret-2	410	24385	1.4850	H-1→L+7 (30%), H-6→L+4 (14%), H-5→L+6 (13%), H-8→L+2 (11%), H-7→L+3 (10%), H-2→L+5 (4%)		
81	CT	405	24668	0.3100	H-9→L+2 (36%), H-6→L+4 (27%), H-8→L+2 (10%), H-7→L+3 (8%), H-5→L+6 (7%), H-1→L+7 (4%)		
89	CT	398	25144	0.8709	H-7→L+3 (43%), H-9→L+2 (24%), H-6→L+4 (12%), H-1→L+7 (8%), H-8→L+5 (3%)		
92	CT	394	25354	0.2540	H-13→L+2 (71%), H-7→L+4 (12%), H-12→L+3 (9%)		
107	Soret-type	384	26072	0.2753	H-2→L+7 (63%), H-42→L (12%), H-6→L+3 (4%), H-32→L (3%), H-4→L+5 (3%)		
121	Soret-type	371	26936	0.2849	H-6→L+6 (45%), H-12→L+3 (23%), H-10→L+5 (14%), H-13→L+5 (5%), H-13→L+2 (4%)		
5	1	Q <sub>1</sub>	2041	4899	3.5380	H→L (99%)	
	17	Soret-1	707	14141	4.3760	H-1→L+3 (91%), H-3→LUMO+4 (4%)	
	20	Q <sub>2</sub>	678	14758	0.1508	H-8→LUMO (83.5%), HOMO→L+8 (10.2%)	
	35	CT	584	17113	0.6864	H-15→L (88%), H-12→L+1 (5%), H-5→L+2 (2%)	
	44	Soret-type	550	18177	0.6039	H-3→L+4 (57%), H-5→L+2 (11%), H-1→L+8 (5%), H-2→L+6 (4%), H-1→L+3 (3%), H-9→L+1 (3%), H-4→L+5 (3%), H-7→L+1 (3%), H-15→L (3%), H-4→L+3 (2%)	
	63	Soret-type	489	20468	0.9282	H-2→L+7 (46%), H-3→L+6 (22%), H-13→L+1 (13%), H-5→L+8 (3%), H-4→L+2 (2%)	
	81	CT	452	22117	0.4041	H-16→L+1 (41%), H-5→L+5 (33%), H-13→L+1 (5%), H-1→L+9 (4%), H-7→L+4 (3%), H-24→L (2%)	
	82	Soret-type	449	22288	0.4433	H-4→L+5 (65%), H-8→L+3 (16%), H-6→L+4 (8%), H-6→L+7 (2%)	
	96	CT	443	23075	0.4360	H-10→L+3 (52%), H-9→L+4 (14%), H-1→L+9 (8%), H-7→L+4 (6%), H-8→L+2 (4%), H-24→L (2%), H-12→L+4 (2%)	
	107	Soret-type	418	23940	0.5761	H-5→L+8 (48%), H-1→L+9 (10%), H-6→L+6 (6%),	

					H-8→L+2 (6%), H-7→L+7 (5%), H-3→L+10 (3%), H-2→L+7 (3%), H-7→L+4 (2%), H-9→L+4 (2%)
113	Soret-2	413	24222	0.8048	H-1→L+9 (48%), H-6→L+6 (14%), H-11→L+3 (7%), H-7→L+4 (6%), H-5→L+8 (6%), H-8→L+2 (5%)
123	CT	405	24671	0.4728	H-11→L+3 (50%), H-15→L+3 (18%), H-7→L+4 (4%), H-6→L+6 (4%), H-11→L+5 (3%), H-9→L+4 (3%), H-7→L+7 (3%), H-10→L+5 (2%), H-42→L (2%), H-14→L+2 (2%)
150	CT	393	25473	0.4084	H-14→L+2 (67%), H-17→L+2 (11%), H-7→L+7 (3%), H-9→L+4 (3%), H-11→L+3 (2%)
<b>6</b>	1	Q <sub>1</sub>	2378	4205	H→L (99%)
	23	Soret-1	724	13815	H-1→L+3 (88%), H-3→L+4 (6%)
	27	Q <sub>2</sub>	685	14589	H-10→L (85%), H→L+10 (8%), H-8→L+1 (2%)
	47	CT	589	16992	H-18→L (74%), H-4→L+2 (9%), H-1→L+6 (7%), H-16→L+1 (4%), H-2→L+5 (2%)
	51	Soret-type	583	17142	H-1→L+6 (63%), H-3→L+4 (12%), H-13→L (11%), H-18→L (5%)
	53	Soret-type	576	17359	H-3→L+4 (64%), H-1→L+6 (14%), H-5→L+3 (8%), H-1→L+3 (6%)
	65	Soret-type	541	18492	H-6→L+2 (61%), H→L+10 (21%), H-2→L+9 (5%), H-4→L+4 (3%), H-4→L+7 (2%)
	80	CT	504	19856	H-15→L+1 (47%), H-2→L+9 (22%), H-5→L+5 (13%), H-10→L+2 (3%)
	86	CT	495	20219	H-16→L+1 (52%), H-3→L+7 (11%), H-14→L+1 (6%), H-18→L (5%), H-25→L (4%), H-7→L+5 (3%), H-5→L+6 (3%), H-13→L+2 (2%)
	90	Soret-type	490	20403	H-2→L+9 (33%), H-3→L+8 (24%), H-15→L+1 (19%), H-7→L+3 (4%), H-4→L+10 (2%)
109	Soret-type	461	21700	0.8562	H-4→L+7 (67%), H-10→L+2 (3%), H-1→L+11 (3%), H-3→L+8 (2%), H-21→L+1 (2%), H-7→L+6 (2%)
161	CT	414	24173	0.6758	H-1→L+11 (38%), H-6→L+8 (18%), H-14→L+3 (6%), H-12→L+3 (5%), H-9→L+4 (4%), H-3→L+12 (4%), H-17→L+2 (3%), H-8→L+5 (3%), H-12→L+6 (2%), H-4→L+7 (2%)
169	CT	410	24416	0.5232	H-16→L+3 (17%), H-20→L+2 (12%), H-17→L+2 (7%),

					H-13→L+4 (7%), H-7→L+6 (7%), H-1→L+11 (6%), H-6→L+8 (6%), H-9→L+7 (5%), H-14→L+3 (4%), H-7→L+9 (4%), H-12→L+6 (4%), H-4→L+10 (3%), H-18→L+4 (2%)
188	Soret-2	402	24862	1.4173	H-14→L+3 (32%), H-1→L+11 (14%), H-13→L+4 (11%), H-11→L+4 (10%), H-7→L+9 (6%), H-16→L+3 (5%)
<b>8</b>	1	Q <sub>1</sub>	3055	3274	6.5580 H→L (99%)
	30	Soret-type	786	12719	0.4475 H-4→L+2 (49%), H-12→L (17%), H→L+6 (11%), H-1→L+3 (7%), H-7→L+1 (6%), H-2→L+4 (3%)
	33	Soret-type	773	12935	0.5184 H-1→L+3 (66%), H-4→L+2 (15%), H→L+6 (9%), H-2→L+4 (4%)
	37	Soret-1	736	13593	5.5077 H-2→L+4 (74%), H-3→L+5 (9%), H-4→L+2 (8%)
	44	Q <sub>2</sub>	695	14384	0.2170 H-14→L (72%), H-6→L+2 (7%), H-8→L+1 (5%), H→L+14 (5%), H-13→L+1 (3%)
	62	Soret-type	636	15718	0.6282 H-2→L+7 (30%), H-3→L+5 (27%), H-17→L (8%), H-5→L+4 (7%), H-21→L (6%), H-11→L+1 (3%), H-16→L (2%), H→L+12 (2%)
	72	Soret-type	611	16368	0.9001 H-2→L+7 (41%), H-3→L+5 (24%), H-2→L+4 (11%), H-25→L (7%), H-5→L+4 (6%), H-3→L+8 (3%), H-7→L+3 (2%)
	78	CT	599	16694	0.4588 H-25→L (56%), H-9→L+2 (11%), H-23→L+1 (8%), H-21→L (7%), H-2→L+7 (6%), H-5→L+4 (5%)
	101	Soret-type	560	17868	0.4990 H-10→L+2 (60%), H→L+14 (22%), H-1→L+10 (6%)
	115	Soret-type	534	18712	0.5159 H-5→L+7 (39%), H-18→L+1 (29%), H-2→L+10 (4%), H-21→L (3%), H-3→L+8 (3%), H-3→L+5 (2%)
	147	Soret-type	502	19935	0.4488 H-1→L+13 (29%), H-14→L+2 (20%), H-5→L+9 (10%), H-3→L+12 (10%), H-7→L+7 (7%), H-11→L+4 (3%), H-9→L+5 (3%), H-24→L+1 (2%)
	171	Soret-type	478	20922	0.5058 H-4→L+11 (47%), H-13→L+3 (19%), H-7→L+13 (5%), H-14→L+2 (4%), H-10→L+6 (3%), H-1→L+13 (2%)
	178	Soret-type	471	21249	0.4190 H-13→L+3 (48%), H-4→L+11 (24%), H-4→L+14 (4%), H-22→L+2 (3%), H-14→L+2 (3%), H-10→L+6 (3%), H-3→L+12 (2%)
	208	Soret-type	450	22211	0.4272 H-7→L+10 (30%), H-43→L (14%), H-26→L+2 (11%), H-10→L+6 (8%), H-22→L+2 (5%), H-45→L (4%), H-4→L+14 (2%), H-9→L+8 (2%)
	227	Soret-type	438	22840	0.4189 H-9→L+8 (20%), H-8→L+9 (16%), H-15→L+4 (8%), H-10→L+6 (8%), H-11→L+7 (7%), H-16→L+5 (7%),

					H-7→L+10 (7%), H-6→L+12 (7%)
	277	Soret-2	414	24174	0.5980
<b>10</b>	1	Q <sub>1</sub>	3748	2668	8.5540
	54	Soret-1	750	13325	7.2832
	55	Soret-type	747	13390	0.5356
	65	Q <sub>2</sub>	703	14225	0.2703
	76	Soret-type	668	14963	0.8191
	98	Soret-type	628	15930	0.5227
	114	CT	604	16545	0.6096
	156	Soret-type	554	18043	0.4439
	206	Soret-type	514	19446	0.7194
	241	Soret-2	489	20444	0.5550
<b>12</b>	326	Soret-type	446	22404	0.6740
	1	Q <sub>1</sub>	4489	2228	10.550
	9	Soret-type	1681	5948	0.6014
	57	Soret-type	816	12259	0.5659
	73	Soret-1	752	13306	8.7710
	91	Q <sub>2</sub>	707	14138	0.3177
	94	Soret-type	694	14414	1.028
	156	CT	608	16438	1.080

284	Soret-2	518	19319	0.5391	H-10→L+8 (25%), H-1→L+21 (20%), H-21→L+3 (10.5%), H-8→L+11 (7%), H-2→L+1 (5%)
331	Soret-type	494	20224	0.4124	H-3→L+19 (26%), H-18→L+4 (20%), H-36→L+2 (19%), H-6→L+15 (7%), H-31→L+2 (3%), H-6→L+21 (2%)

<sup>a</sup> For compounds **2** and **3**, only excited states with  $f \geq 0.1$  are listed; for compound **4**, only excited states with  $f \geq 0.2$  are listed; for compounds **5-12**, only excited states with  $f \geq 0.4$  are listed; for all compounds, the additional excited states of lower than threshold intensities that are discussed specifically in the text (i.e.  $Q_2$ ) are also listed. For a complete description of the TDDFT-predicted excited states, see Supporting Information tables below.

**Table S2.** Optimized coordinates for 1.

Zn 0.0000000000 0.0000000000 0.0000000000  
N 0.0000000000 2.0509880000 0.0000000000  
N 2.0509880000 0.0000000000 0.0000000000  
N -2.0509880000 0.0000000000 0.0000000000  
N 0.0000000000 -2.0509880000 0.0000000000  
C 1.1038440000 2.8705470000 0.0045110000  
C -1.1038440000 2.8705470000 -0.0045110000  
C 2.8705470000 1.1038440000 -0.0045110000  
C 2.8705470000 -1.1038440000 0.0045110000  
C -2.8705470000 1.1038440000 0.0045110000  
C -2.8705470000 -1.1038440000 -0.0045110000  
C 1.1038440000 -2.8705470000 -0.0045110000  
C -1.1038440000 -2.8705470000 0.0045110000  
C 2.4478980000 2.4478980000 0.0000000000  
C 0.6806860000 4.2542560000 -0.0023390000  
C -0.6806860000 4.2542560000 0.0023390000  
C 4.2542560000 0.6806860000 0.0023390000  
C 2.4478980000 -2.4478980000 0.0000000000  
C 4.2542560000 -0.6806860000 -0.0023390000  
C -2.4478980000 2.4478980000 0.0000000000  
C -4.2542560000 0.6806860000 -0.0023390000  
C -4.2542560000 -0.6806860000 0.0023390000  
C 0.6806860000 -4.2542560000 0.0023390000  
C -2.4478980000 -2.4478980000 0.0000000000  
C -0.6806860000 -4.2542560000 -0.0023390000  
H 5.1101940000 1.3396930000 0.0076810000  
H 5.1101940000 -1.3396930000 -0.0076810000  
H 1.3396930000 5.1101940000 -0.0076810000  
H -1.3396930000 5.1101940000 0.0076810000  
H -5.1101940000 1.3396930000 -0.0076810000  
H -5.1101940000 -1.3396930000 0.0076810000  
H -1.3396930000 -5.1101940000 -0.0076810000  
H 1.3396930000 -5.1101940000 0.0076810000  
C -3.5086390000 3.5086390000 0.0000000000  
C -4.2879200000 3.7445890000 1.1439740000  
C -3.7445890000 4.2879200000 -1.1439740000  
C -5.2754600000 4.7318790000 1.1445680000  
H -4.1122760000 3.1523820000 2.0378680000  
C -4.7318790000 5.2754600000 -1.1445680000  
H -3.1523820000 4.1122760000 -2.0378680000  
C -5.5005180000 5.5005180000 0.0000000000  
H -4.9020900000 5.8659580000 -2.0409240000  
C 3.5086390000 3.5086390000 0.0000000000  
C 3.7445890000 4.2879200000 1.1439740000  
C 4.2879200000 3.7445890000 -1.1439740000  
C 4.7318790000 5.2754600000 1.1445680000  
H 3.1523820000 4.1122760000 2.0378680000  
C 5.2754600000 4.7318790000 -1.1445680000  
H 4.1122760000 3.1523820000 -2.0378680000  
C 5.5005180000 5.5005180000 0.0000000000  
H 4.9020900000 5.8659580000 2.0409240000  
H 5.8659580000 4.9020900000 -2.0409240000  
C -3.5086390000 -3.5086390000 0.0000000000  
C -4.2879200000 -3.7445890000 -1.1439740000  
C -3.7445890000 -4.2879200000 1.1439740000  
C -5.2754600000 -4.7318790000 -1.1445680000  
H -4.1122760000 -3.1523820000 -2.0378680000  
C -4.7318790000 -5.2754600000 1.1445680000  
H -3.1523820000 -4.1122760000 2.0378680000  
C -5.5005180000 -5.5005180000 0.0000000000  
H -5.8659580000 -4.9020900000 -2.0409240000

H -4.9020900000 -5.8659580000 2.0409240000  
 C 3.5086390000 -3.5086390000 0.0000000000  
 C 3.7445890000 -4.2879200000 -1.1439740000  
 C 4.2879200000 -3.7445890000 1.1439740000  
 C 4.7318790000 -5.2754600000 -1.1445680000  
 H 3.1523820000 -4.1122760000 -2.0378680000  
 C 5.2754600000 -4.7318790000 1.1445680000  
 H 4.1122760000 -3.1523820000 2.0378680000  
 C 5.5005180000 -5.5005180000 0.0000000000  
 H 4.9020900000 -5.8659580000 -2.0409240000  
 H 5.8659580000 -4.9020900000 2.0409240000  
 H -5.8659580000 4.9020900000 2.0409240000  
 H 6.2688820000 6.2688820000 0.0000000000  
 H -6.2688820000 6.2688820000 0.0000000000  
 H -6.2688820000 -6.2688820000 0.0000000000  
 H 6.2688820000 -6.2688820000 0.0000000000

**Table S3.** Optimized coordinates for **2**.

C -0.1143410000 2.5269970000 7.7012460000  
 C -0.0627620000 1.2509230000 7.0236920000  
 N -0.0607050000 1.4532420000 5.6634080000  
 Zn 0.0000000000 0.0000000000 4.2210860000  
 N 0.0661100000 -1.4440330000 2.7707160000  
 C 0.0284950000 -1.2378130000 1.4217280000  
 C 0.0000000000 0.0000000000 0.7415400000  
 C -0.0284950000 1.2378130000 1.4217280000  
 N -0.0661100000 1.4440330000 2.7707160000  
 C -0.0890930000 2.8112100000 2.9582530000  
 C -0.1190610000 3.4631090000 4.2058990000  
 C -0.1080090000 2.8113950000 5.4603540000  
 C -0.1539160000 3.4889670000 6.7367420000  
 H -0.2065610000 4.5586850000 6.8770060000  
 C -0.0530240000 3.4811860000 1.6794480000  
 C -0.0217250000 2.5012890000 0.7188170000  
 C 0.0217250000 2.5012890000 -0.7188170000  
 C 0.0284950000 1.2378130000 -1.4217280000  
 N 0.0661100000 1.4440330000 -2.7707160000  
 Zn 0.0000000000 0.0000000000 -4.2210860000  
 N -0.0607050000 -1.4532420000 -5.6634080000  
 C -0.0627620000 -1.2509230000 -7.0236920000  
 C 0.0000000000 0.0000000000 -7.6728600000  
 C 0.0627620000 1.2509230000 -7.0236920000  
 N 0.0607050000 1.4532420000 -5.6634080000  
 C 0.1080090000 2.8113950000 -5.4603540000  
 C 0.1190610000 3.4631090000 -4.2058990000  
 C 0.0890930000 2.8112100000 -2.9582530000  
 C 0.0530240000 3.4811860000 -1.6794480000  
 H 0.0466060000 4.5511970000 -1.5316480000  
 C 0.1539160000 3.4889670000 -6.7367420000  
 C 0.1143410000 2.5269970000 -7.7012460000  
 H 0.1205900000 2.6685080000 -8.7721180000  
 H 0.2065610000 4.5586850000 -6.8770060000  
 C -0.1143410000 -2.5269970000 -7.7012460000  
 C -0.1539160000 -3.4889670000 -6.7367420000  
 C -0.1080090000 -2.8113950000 -5.4603540000  
 C -0.1190610000 -3.4631090000 -4.2058990000  
 C -0.0890930000 -2.8112100000 -2.9582530000  
 N -0.0661100000 -1.4440330000 -2.7707160000

C -0.0284950000 -1.2378130000 -1.4217280000  
 C -0.0217250000 -2.5012890000 -0.7188170000  
 C 0.0217250000 -2.5012890000 0.7188170000  
 C 0.0530240000 -3.4811860000 1.6794480000  
 C 0.0890930000 -2.8112100000 2.9582530000  
 C 0.1190610000 -3.4631090000 4.2058990000  
 C 0.1080090000 -2.8113950000 5.4603540000  
 N 0.0607050000 -1.4532420000 5.6634080000  
 C 0.0627620000 -1.2509230000 7.0236920000  
 C 0.1143410000 -2.5269970000 7.7012460000  
 C 0.1539160000 -3.4889670000 6.7367420000  
 H 0.2065610000 -4.5586850000 6.8770060000  
 C 0.0000000000 0.0000000000 7.6728600000  
 H 0.0466060000 -4.5511970000 1.5316480000  
 C -0.0530240000 -3.4811860000 -1.6794480000  
 H -0.0466060000 -4.5511970000 -1.5316480000  
 C 0.0000000000 0.0000000000 -0.7415400000  
 H -0.2065610000 -4.5586850000 -6.8770060000  
 H -0.1205900000 -2.6685080000 -8.7721180000  
 H -0.0466060000 4.5511970000 1.5316480000  
 H 0.1205900000 -2.6685080000 8.7721180000  
 H -0.1205900000 2.6685080000 8.7721180000  
 C 0.1631010000 4.9611570000 -4.2034820000  
 C -0.9354740000 5.7139450000 -4.6496350000  
 C 1.3047280000 5.6436940000 -3.7525630000  
 C -0.8939000000 7.1095010000 -4.6449650000  
 H -1.8278520000 5.1990370000 -4.9944890000  
 C 1.3474920000 7.0393330000 -3.7490270000  
 H 2.1638320000 5.0736460000 -3.4100530000  
 C 0.2481180000 7.7767190000 -4.1951050000  
 H -1.7559330000 7.6745890000 -4.9893680000  
 H 2.2416510000 7.5493090000 -3.4005700000  
 H 0.2808610000 8.8628200000 -4.1919820000  
 C -0.1631010000 4.9611570000 4.2034820000  
 C 0.9354740000 5.7139450000 4.6496350000  
 C -1.3047280000 5.6436940000 3.7525630000  
 C 0.8939000000 7.1095010000 4.6449650000  
 H 1.8278520000 5.1990370000 4.9944890000  
 C -1.3474920000 7.0393330000 3.7490270000  
 H -2.1638320000 5.0736460000 3.4100530000  
 C -0.2481180000 7.7767190000 4.1951050000  
 H 1.7559330000 7.6745890000 4.9893680000  
 H -2.2416510000 7.5493090000 3.4005700000  
 H -0.2808610000 8.8628200000 4.1919820000  
 C 0.1631010000 -4.9611570000 4.2034820000  
 C -0.9354740000 -5.7139450000 4.6496350000  
 C 1.3047280000 -5.6436940000 3.7525630000  
 C -0.8939000000 -7.1095010000 4.6449650000  
 H -1.8278520000 -5.1990370000 4.9944890000  
 C 1.3474920000 -7.0393330000 3.7490270000  
 H 2.1638320000 -5.0736460000 3.4100530000  
 C 0.2481180000 -7.7767190000 4.1951050000  
 H -1.7559330000 -7.6745890000 4.9893680000  
 H 2.2416510000 -7.5493090000 3.4005700000  
 H 0.2808610000 -8.8628200000 4.1919820000  
 C -0.1631010000 -4.9611570000 -4.2034820000  
 C 0.9354740000 -5.7139450000 -4.6496350000  
 C -1.3047280000 -5.6436940000 -3.7525630000  
 C 0.8939000000 -7.1095010000 -4.6449650000  
 H 1.8278520000 -5.1990370000 -4.9944890000  
 C -1.3474920000 -7.0393330000 -3.7490270000  
 H -2.1638320000 -5.0736460000 -3.4100530000  
 C -0.2481180000 -7.7767190000 -4.1951050000

```

H 1.7559330000 -7.6745890000 -4.9893680000
H -2.2416510000 -7.5493090000 -3.4005700000
H -0.2808610000 -8.8628200000 -4.1919820000
C 0.00000000000 0.00000000000 -9.1723590000
C 1.1561890000 0.3466450000 -9.8899790000
C -1.1561890000 -0.3466450000 -9.8899790000
C 1.1566960000 0.3463030000 -11.2863120000
H 2.0593440000 0.6114180000 -9.3471180000
C -1.1566960000 -0.3463030000 -11.2863120000
H -2.0593440000 -0.6114180000 -9.3471180000
C 0.00000000000 0.00000000000 -11.9889110000
H 2.0624680000 0.6133980000 -11.8241690000
H -2.0624680000 -0.6133980000 -11.8241690000
H 0.00000000000 0.00000000000 -13.0755090000
C 0.00000000000 0.00000000000 9.1723590000
C -1.1561890000 0.3466450000 9.8899790000
C 1.1561890000 -0.3466450000 9.8899790000
C -1.1566960000 0.3463030000 11.2863120000
H -2.0593440000 0.6114180000 9.3471180000
C 1.1566960000 -0.3463030000 11.2863120000
H 2.0593440000 -0.6114180000 9.3471180000
C 0.00000000000 0.00000000000 11.9889110000
H -2.0624680000 0.6133980000 11.8241690000
H 2.0624680000 -0.6133980000 11.8241690000
H 0.00000000000 0.00000000000 13.0755090000

```

**Table S4.** Optimized coordinates for **3**.

```

C -0.2929400000 2.5118230000 11.9077600000
C -0.1523990000 1.2431860000 11.2298530000
N -0.1623590000 1.4452580000 9.8692170000
Zn 0.00000000000 0.00000000000 8.4271250000
N -0.1620930000 1.4363150000 6.9780880000
C -0.1035950000 1.2349240000 5.6298870000
C 0.00000000000 0.00000000000 4.9485030000
C 0.1035950000 -1.2349240000 5.6298870000
N 0.1620930000 -1.4363150000 6.9780880000
C 0.2681050000 -2.8006470000 7.1658630000
C 0.3462230000 -3.4481640000 8.4126510000
C 0.2994560000 -2.7971160000 9.6674560000
N 0.1623590000 -1.4452580000 9.8692170000
C 0.1523990000 -1.2431860000 11.2298530000
C 0.00000000000 0.00000000000 11.8788620000
C 0.2929400000 -2.5118230000 11.9077600000
C 0.3948980000 -3.4695400000 10.9432910000
H 0.5202700000 -4.5331450000 11.0836210000
C 0.2624820000 -3.4727770000 5.8881810000
C 0.1661990000 -2.4973550000 4.9270650000
C 0.1099300000 -2.5005830000 3.4905050000
C 0.0344800000 -1.2407300000 2.7896050000
N -0.0058620000 -1.4485990000 1.4414870000
Zn 0.00000000000 0.00000000000 0.00000000000
N -0.0058620000 1.4485990000 -1.4414870000
C 0.0344800000 1.2407300000 -2.7896050000
C 0.00000000000 0.00000000000 -3.4698210000
C -0.0344800000 -1.2407300000 -2.7896050000
N 0.0058620000 -1.4485990000 -1.4414870000
C -0.0292000000 -2.8156520000 -1.2520790000
C 0.00000000000 -3.4682050000 0.00000000000

```

C 0.0292000000 -2.8156520000 1.2520790000  
 C 0.1137850000 -3.4821210000 2.5279400000  
 H 0.1726660000 -4.5503910000 2.6762920000  
 C -0.1137850000 -3.4821210000 -2.5279400000  
 C -0.1099300000 -2.5005830000 -3.4905050000  
 C -0.1661990000 -2.4973550000 -4.9270650000  
 C -0.1035950000 -1.2349240000 -5.6298870000  
 N -0.1620930000 -1.4363150000 -6.9780880000  
 Zn 0.0000000000 0.0000000000 -8.4271250000  
 N 0.1623590000 1.4452580000 -9.8692170000  
 C 0.1523990000 1.2431860000 -11.2298530000  
 C 0.0000000000 0.0000000000 -11.8788620000  
 C -0.1523990000 -1.2431860000 -11.2298530000  
 N -0.1623590000 -1.4452580000 -9.8692170000  
 C -0.2994560000 -2.7971160000 -9.6674560000  
 C -0.3462230000 -3.4481640000 -8.4126510000  
 C -0.2681050000 -2.8006470000 -7.1658630000  
 C -0.2624820000 -3.4727770000 -5.8881810000  
 H -0.3183170000 -4.5414080000 -5.7411120000  
 C -0.3948980000 -3.4695400000 -10.9432910000  
 C -0.2929400000 -2.5118230000 -11.9077600000  
 H -0.3111330000 -2.6519700000 -12.9786520000  
 H -0.5202700000 -4.5331450000 -11.0836210000  
 C 0.2929400000 2.5118230000 -11.9077600000  
 C 0.3948980000 3.4695400000 -10.9432910000  
 C 0.2994560000 2.7971160000 -9.6674560000  
 C 0.3462230000 3.4481640000 -8.4126510000  
 C 0.2681050000 2.8006470000 -7.1658630000  
 N 0.1620930000 1.4363150000 -6.9780880000  
 C 0.1035950000 1.2349240000 -5.6298870000  
 C 0.1661990000 2.4973550000 -4.9270650000  
 C 0.1099300000 2.5005830000 -3.4905050000  
 C 0.1137850000 3.4821210000 -2.5279400000  
 C 0.0292000000 2.8156520000 -1.2520790000  
 C 0.0000000000 3.4682050000 0.0000000000  
 C -0.0292000000 2.8156520000 1.2520790000  
 N 0.0058620000 1.4485990000 1.4414870000  
 C -0.0344800000 1.2407300000 2.7896050000  
 C -0.1099300000 2.5005830000 3.4905050000  
 C -0.1661990000 2.4973550000 4.9270650000  
 C -0.2624820000 3.4727770000 5.8881810000  
 C -0.2681050000 2.8006470000 7.1658630000  
 C -0.3462230000 3.4481640000 8.4126510000  
 C -0.2994560000 2.7971160000 9.6674560000  
 C -0.3948980000 3.4695400000 10.9432910000  
 H -0.5202700000 4.5331450000 11.0836210000  
 H -0.3183170000 4.5414080000 5.7411120000  
 C -0.1137850000 3.4821210000 2.5279400000  
 H -0.1726660000 4.5503910000 2.6762920000  
 C 0.0000000000 0.0000000000 3.4698210000  
 H 0.1726660000 4.5503910000 -2.6762920000  
 C 0.2624820000 3.4727770000 -5.8881810000  
 H 0.3183170000 4.5414080000 -5.7411120000  
 C 0.0000000000 0.0000000000 -4.9485030000  
 H 0.5202700000 4.5331450000 -11.0836210000  
 H 0.3111330000 2.6519700000 -12.9786520000  
 H -0.1726660000 -4.5503910000 -2.6762920000  
 H 0.3183170000 -4.5414080000 5.7411120000  
 H -0.3111330000 2.6519700000 12.9786520000  
 H 0.3111330000 -2.6519700000 12.9786520000  
 C 0.0000000000 4.9655020000 0.0000000000  
 C 1.0931460000 5.6835270000 0.5127170000  
 C -1.0931460000 5.6835270000 -0.5127170000

C 1.0939390000 7.0795790000 0.5111880000  
 H 1.9484110000 5.1409500000 0.9053910000  
 C -1.0939390000 7.0795790000 -0.5111880000  
 H -1.9484110000 5.1409500000 -0.9053910000  
 C 0.0000000000 7.7821340000 0.0000000000  
 H 1.9515140000 7.6173150000 0.9066070000  
 H -1.9515140000 7.6173150000 -0.9066070000  
 H 0.0000000000 8.8687210000 0.0000000000  
 C 0.4842690000 4.9402750000 -8.4109820000  
 C -0.5605230000 5.7597250000 -8.8688390000  
 C 1.6617430000 5.5504410000 -7.9486320000  
 C -0.4318090000 7.1498990000 -8.8641640000  
 H -1.4799060000 5.3013780000 -9.2224070000  
 C 1.7916730000 6.9406680000 -7.9454740000  
 H 2.4799600000 4.9282020000 -7.5970450000  
 C 0.7451210000 7.7448400000 -8.4029840000  
 H -1.2533430000 7.7674190000 -9.2173860000  
 H 2.7124080000 7.3940750000 -7.5881940000  
 H 0.8456910000 8.8267630000 -8.4000060000  
 C -0.4842690000 -4.9402750000 -8.4109820000  
 C 0.5605230000 -5.7597250000 -8.8688390000  
 C -1.6617430000 -5.5504410000 -7.9486320000  
 C 0.4318090000 -7.1498990000 -8.8641640000  
 H 1.4799060000 -5.3013780000 -9.2224070000  
 C -1.7916730000 -6.9406680000 -7.9454740000  
 H -2.4799600000 -4.9282020000 -7.5970450000  
 C -0.7451210000 -7.7448400000 -8.4029840000  
 H 1.2533430000 -7.7674190000 -9.2173860000  
 H -2.7124080000 -7.3940750000 -7.5881940000  
 H -0.8456910000 -8.8267630000 -8.4000060000  
 C 0.0000000000 -4.9655020000 0.0000000000  
 C -1.0931460000 -5.6835270000 0.5127170000  
 C 1.0931460000 -5.6835270000 -0.5127170000  
 C -1.0939390000 -7.0795790000 0.5111880000  
 H -1.9484110000 -5.1409500000 0.9053910000  
 C 1.0939390000 -7.0795790000 -0.5111880000  
 H 1.9484110000 -5.1409500000 -0.9053910000  
 C 0.0000000000 -7.7821340000 0.0000000000  
 H -1.9515140000 -7.6173150000 0.9066070000  
 H 1.9515140000 -7.6173150000 -0.9066070000  
 H 0.0000000000 -8.8687210000 0.0000000000  
 C 0.4842690000 -4.9402750000 8.4109820000  
 C -0.5605230000 -5.7597250000 8.8688390000  
 C 1.6617430000 -5.5504410000 7.9486320000  
 C -0.4318090000 -7.1498990000 8.8641640000  
 H -1.4799060000 -5.3013780000 9.2224070000  
 C 1.7916730000 -6.9406680000 7.9454740000  
 H 2.4799600000 -4.9282020000 7.5970450000  
 C 0.7451210000 -7.7448400000 8.4029840000  
 H -1.2533430000 -7.7674190000 9.2173860000  
 H 2.7124080000 -7.3940750000 7.5881940000  
 H 0.8456910000 -8.8267630000 8.4000060000  
 C -0.4842690000 4.9402750000 8.4109820000  
 C 0.5605230000 5.7597250000 8.8688390000  
 C -1.6617430000 5.5504410000 7.9486320000  
 C 0.4318090000 7.1498990000 8.8641640000  
 H 1.4799060000 5.3013780000 9.2224070000  
 C -1.7916730000 6.9406680000 7.9454740000  
 H -2.4799600000 4.9282020000 7.5970450000  
 C -0.7451210000 7.7448400000 8.4029840000  
 H 1.2533430000 7.7674190000 9.2173860000  
 H -2.7124080000 7.3940750000 7.5881940000  
 H -0.8456910000 8.8267630000 8.4000060000

```

C 0.00000000000 0.00000000000 -13.3782430000
C 1.1787370000 0.2603400000 -14.0956240000
C -1.1787370000 -0.2603400000 -14.0956240000
C 1.1791870000 0.2597320000 -15.4919420000
H 2.0989840000 0.4576950000 -13.5527820000
C -1.1791870000 -0.2597320000 -15.4919420000
H -2.0989840000 -0.4576950000 -13.5527820000
C 0.00000000000 0.00000000000 -16.1944930000
H 2.1022300000 0.4590130000 -16.0298070000
H -2.1022300000 -0.4590130000 -16.0298070000
H 0.00000000000 0.00000000000 -17.2810820000
C 0.00000000000 0.00000000000 13.3782430000
C -1.1787370000 0.2603400000 14.0956240000
C 1.1787370000 -0.2603400000 14.0956240000
C -1.1791870000 0.2597320000 15.4919420000
H -2.0989840000 0.4576950000 13.5527820000
C 1.1791870000 -0.2597320000 15.4919420000
H 2.0989840000 -0.4576950000 13.5527820000
C 0.00000000000 0.00000000000 16.1944930000
H -2.1022300000 0.4590130000 16.0298070000
H 2.1022300000 -0.4590130000 16.0298070000
H 0.00000000000 0.00000000000 17.2810820000

```

**Table S5.** Optimized coordinates for **4**.

```

Zn 0.00000000000 0.00000000000 12.6376340000
N -0.1875500000 1.4324580000 11.1885000000
C -0.1362330000 1.2319170000 9.8401650000
C 0.00000000000 0.00000000000 9.1580100000
C 0.1362330000 -1.2319170000 9.8401650000
N 0.1875500000 -1.4324580000 11.1885000000
C 0.3271080000 -2.7941450000 11.3765160000
C 0.4072130000 -3.4408240000 12.6231380000
C 0.3387710000 -2.7920350000 13.8784630000
N 0.1800310000 -1.4427570000 14.0802260000
C 0.1648710000 -1.2415500000 15.4410210000
C 0.00000000000 0.00000000000 16.0901160000
C -0.1648710000 1.2415500000 15.4410210000
N -0.1800310000 1.4427570000 14.0802260000
C -0.3387710000 2.7920350000 13.8784630000
C -0.4072130000 3.4408240000 12.6231380000
C -0.3271080000 2.7941450000 11.3765160000
C -0.3533170000 3.4649220000 10.0985130000
C -0.2413810000 2.4914220000 9.1371860000
C -0.2014730000 2.4949080000 7.7004030000
C -0.0843570000 1.2388560000 6.9995650000
N -0.0644060000 1.4471060000 5.6510610000
Zn 0.00000000000 0.00000000000 4.2076170000
N -0.0823070000 1.4463300000 2.7659890000
C -0.0337360000 1.2423040000 1.4186320000
C 0.00000000000 0.00000000000 0.7367810000
C 0.0337360000 -1.2423040000 1.4186320000
N 0.0823070000 -1.4463300000 2.7659890000
C 0.1167330000 -2.8145060000 2.9564800000
C 0.1683160000 -3.4638040000 4.2084780000
C 0.1568450000 -2.8113920000 5.4617700000
N 0.0644060000 -1.4471060000 5.6510610000
C 0.0843570000 -1.2388560000 6.9995650000
C 0.00000000000 0.00000000000 7.6803620000

```

C 0.2014730000 -2.4949080000 7.7004030000  
 C 0.2413810000 -2.4914220000 9.1371860000  
 C 0.3533170000 -3.4649220000 10.0985130000  
 H 0.4391330000 -4.5315310000 9.9513310000  
 C 0.2547470000 -3.4750120000 6.7372760000  
 H 0.3548130000 -4.5401360000 6.8859100000  
 C 0.0720850000 -3.4850010000 1.6814620000  
 C 0.0271750000 -2.5049520000 0.7178890000  
 C -0.0271750000 -2.5049520000 -0.7178890000  
 C -0.0337360000 -1.2423040000 -1.4186320000  
 N -0.0823070000 -1.4463300000 -2.7659890000  
 Zn 0.0000000000 0.0000000000 -4.2076170000  
 N 0.0644060000 1.4471060000 -5.6510610000  
 C 0.0843570000 1.2388560000 -6.9995650000  
 C 0.0000000000 0.0000000000 -7.6803620000  
 C -0.0843570000 -1.2388560000 -6.9995650000  
 N -0.0644060000 -1.4471060000 -5.6510610000  
 C -0.1568450000 -2.8113920000 -5.4617700000  
 C -0.1683160000 -3.4638040000 -4.2084780000  
 C -0.1167330000 -2.8145060000 -2.9564800000  
 C -0.0720850000 -3.4850010000 -1.6814620000  
 H -0.0692510000 -4.5549370000 -1.5336350000  
 C -0.2547470000 -3.4750120000 -6.7372760000  
 C -0.2014730000 -2.4949080000 -7.7004030000  
 C -0.2413810000 -2.4914220000 -9.1371860000  
 C -0.1362330000 -1.2319170000 -9.8401650000  
 N -0.1875500000 -1.4324580000 -11.1885000000  
 Zn 0.0000000000 0.0000000000 -12.6376340000  
 N 0.1800310000 1.4427570000 -14.0802260000  
 C 0.1648710000 1.2415500000 -15.4410210000  
 C 0.0000000000 0.0000000000 -16.0901160000  
 C -0.1648710000 -1.2415500000 -15.4410210000  
 N -0.1800310000 -1.4427570000 -14.0802260000  
 C -0.3387710000 -2.7920350000 -13.8784630000  
 C -0.4072130000 -3.4408240000 -12.6231380000  
 C -0.3271080000 -2.7941450000 -11.3765160000  
 C -0.3533170000 -3.4649220000 -10.0985130000  
 H -0.4391330000 -4.5315310000 -9.9513310000  
 C -0.4383270000 -3.4641070000 -15.1539560000  
 C -0.3197820000 -2.5084560000 -16.1187060000  
 H -0.3365520000 -2.6489620000 -17.1895610000  
 H -0.5781010000 -4.5259510000 -15.2939840000  
 C 0.3197820000 2.5084560000 -16.1187060000  
 C 0.4383270000 3.4641070000 -15.1539560000  
 C 0.3387710000 2.7920350000 -13.8784630000  
 C 0.4072130000 3.4408240000 -12.6231380000  
 C 0.3271080000 2.7941450000 -11.3765160000  
 N 0.1875500000 1.4324580000 -11.1885000000  
 C 0.1362330000 1.2319170000 -9.8401650000  
 C 0.2413810000 2.4914220000 -9.1371860000  
 C 0.2014730000 2.4949080000 -7.7004030000  
 C 0.2547470000 3.4750120000 -6.7372760000  
 C 0.1568450000 2.8113920000 -5.4617700000  
 C 0.1683160000 3.4638040000 -4.2084780000  
 C 0.1167330000 2.8145060000 -2.9564800000  
 N 0.0823070000 1.4463300000 -2.7659890000  
 C 0.0337360000 1.2423040000 -1.4186320000  
 C 0.0271750000 2.5049520000 -0.7178890000  
 C -0.0271750000 2.5049520000 0.7178890000  
 C -0.0720850000 3.4850010000 1.6814620000  
 C -0.1167330000 2.8145060000 2.9564800000  
 C -0.1683160000 3.4638040000 4.2084780000  
 C -0.1568450000 2.8113920000 5.4617700000

C -0.2547470000 3.4750120000 6.7372760000  
 H -0.3548130000 4.5401360000 6.8859100000  
 H -0.0692510000 4.5549370000 1.5336350000  
 C 0.0720850000 3.4850010000 -1.6814620000  
 H 0.0692510000 4.5549370000 -1.5336350000  
 C 0.0000000000 0.0000000000 -0.7367810000  
 H 0.3548130000 4.5401360000 -6.8859100000  
 C 0.3533170000 3.4649220000 -10.0985130000  
 H 0.4391330000 4.5315310000 -9.9513310000  
 C 0.0000000000 0.0000000000 -9.1580100000  
 H 0.5781010000 4.5259510000 -15.2939840000  
 H 0.3365520000 2.6489620000 -17.1895610000  
 H -0.3548130000 -4.5401360000 -6.8859100000  
 H 0.0692510000 -4.5549370000 1.5336350000  
 H -0.4391330000 4.5315310000 9.9513310000  
 C -0.4383270000 3.4641070000 15.1539560000  
 C -0.3197820000 2.5084560000 16.1187060000  
 C 0.3197820000 -2.5084560000 16.1187060000  
 C 0.4383270000 -3.4641070000 15.1539560000  
 H 0.5781010000 -4.5259510000 15.2939840000  
 H -0.5781010000 4.5259510000 15.2939840000  
 H -0.3365520000 2.6489620000 17.1895610000  
 H 0.3365520000 -2.6489620000 17.1895610000  
 C 0.5751040000 4.9299560000 -12.6220300000  
 C -0.4597470000 5.7702120000 -13.0643100000  
 C 1.7710570000 5.5160050000 -12.1764050000  
 C -0.3033990000 7.1575580000 -13.0605390000  
 H -1.3929750000 5.3304780000 -13.4050370000  
 C 1.9285480000 6.9033960000 -12.1742110000  
 H 2.5817240000 4.8772800000 -11.8370900000  
 C 0.8916520000 7.7285720000 -12.6160200000  
 H -1.1174880000 7.7915950000 -13.4015100000  
 H 2.8631340000 7.3381390000 -11.8299420000  
 H 1.0137190000 8.8082790000 -12.6137850000  
 C 0.2391200000 4.9595300000 -4.2090180000  
 C -0.8251510000 5.7286990000 -4.7079300000  
 C 1.3717180000 5.6242200000 -3.7104380000  
 C -0.7593910000 7.1231990000 -4.7066990000  
 H -1.7101590000 5.2275800000 -5.0896300000  
 C 1.4390060000 7.0186680000 -3.7125180000  
 H 2.2049030000 5.0413260000 -3.3282500000  
 C 0.3733080000 7.7726370000 -4.2098580000  
 H -1.5953900000 7.7012980000 -5.0911900000  
 H 2.3261640000 7.5148020000 -3.3281660000  
 H 0.4250690000 8.8579840000 -4.2102130000  
 C -0.2391200000 4.9595300000 4.2090180000  
 C 0.8251510000 5.7286990000 4.7079300000  
 C -1.3717180000 5.6242200000 3.7104380000  
 C 0.7593910000 7.1231990000 4.7066990000  
 H 1.7101590000 5.2275800000 5.0896300000  
 C -1.4390060000 7.0186680000 3.7125180000  
 H -2.2049030000 5.0413260000 3.3282500000  
 C -0.3733080000 7.7726370000 4.2098580000  
 H 1.5953900000 7.7012980000 5.0911900000  
 H -2.3261640000 7.5148020000 3.3281660000  
 H -0.4250690000 8.8579840000 4.2102130000  
 C -0.5751040000 4.9299560000 12.6220300000  
 C 0.4597470000 5.7702120000 13.0643100000  
 C -1.7710570000 5.5160050000 12.1764050000  
 C 0.3033990000 7.1575580000 13.0605390000  
 H 1.3929750000 5.3304780000 13.4050370000  
 C -1.9285480000 6.9033960000 12.1742110000  
 H -2.5817240000 4.8772800000 11.8370900000

C -0.8916520000 7.7285720000 12.6160200000  
 H 1.1174880000 7.7915950000 13.4015100000  
 H -2.8631340000 7.3381390000 11.8299420000  
 H -1.0137190000 8.8082790000 12.6137850000  
 C 0.5751040000 -4.9299560000 12.6220300000  
 C -0.4597470000 -5.7702120000 13.0643100000  
 C 1.7710570000 -5.5160050000 12.1764050000  
 C -0.3033990000 -7.1575580000 13.0605390000  
 H -1.3929750000 -5.3304780000 13.4050370000  
 C 1.9285480000 -6.9033960000 12.1742110000  
 H 2.5817240000 -4.8772800000 11.8370900000  
 C 0.8916520000 -7.7285720000 12.6160200000  
 H -1.1174880000 -7.7915950000 13.4015100000  
 H 2.8631340000 -7.3381390000 11.8299420000  
 H 1.0137190000 -8.8082790000 12.6137850000  
 C 0.0000000000 0.0000000000 17.5894040000  
 C 1.1809710000 -0.2502450000 18.3067230000  
 C -1.1809710000 0.2502450000 18.3067230000  
 C 1.1814050000 -0.2495030000 19.7030230000  
 H 2.1028840000 -0.4396630000 17.7639000000  
 C -1.1814050000 0.2495030000 19.7030230000  
 H -2.1028840000 0.4396630000 17.7639000000  
 C 0.0000000000 0.0000000000 20.4055510000  
 H 2.1061400000 -0.4407470000 20.2408830000  
 H -2.1061400000 0.4407470000 20.2408830000  
 H 0.0000000000 0.0000000000 21.4921340000  
 C 0.2391200000 -4.9595300000 4.2090180000  
 C -0.8251510000 -5.7286990000 4.7079300000  
 C 1.3717180000 -5.6242200000 3.7104380000  
 C -0.7593910000 -7.1231990000 4.7066990000  
 H -1.7101590000 -5.2275800000 5.0896300000  
 C 1.4390060000 -7.0186680000 3.7125180000  
 H 2.2049030000 -5.0413260000 3.3282500000  
 C 0.3733080000 -7.7726370000 4.2098580000  
 H -1.5953900000 -7.7012980000 5.0911900000  
 H 2.3261640000 -7.5148020000 3.3281660000  
 H 0.4250690000 -8.8579840000 4.2102130000  
 C -0.2391200000 -4.9595300000 -4.2090180000  
 C 0.8251510000 -5.7286990000 -4.7079300000  
 C -1.3717180000 -5.6242200000 -3.7104380000  
 C 0.7593910000 -7.1231990000 -4.7066990000  
 H 1.7101590000 -5.2275800000 -5.0896300000  
 C -1.4390060000 -7.0186680000 -3.7125180000  
 H -2.2049030000 -5.0413260000 -3.3282500000  
 C -0.3733080000 -7.7726370000 -4.2098580000  
 H 1.5953900000 -7.7012980000 -5.0911900000  
 H -2.3261640000 -7.5148020000 -3.3281660000  
 H -0.4250690000 -8.8579840000 -4.2102130000  
 C -0.5751040000 -4.9299560000 -12.6220300000  
 C 0.4597470000 -5.7702120000 -13.0643100000  
 C -1.7710570000 -5.5160050000 -12.1764050000  
 C 0.3033990000 -7.1575580000 -13.0605390000  
 H 1.3929750000 -5.3304780000 -13.4050370000  
 C -1.9285480000 -6.9033960000 -12.1742110000  
 H -2.5817240000 -4.8772800000 -11.8370900000  
 C -0.8916520000 -7.7285720000 -12.6160200000  
 H 1.1174880000 -7.7915950000 -13.4015100000  
 H -2.8631340000 -7.3381390000 -11.8299420000  
 H -1.0137190000 -8.8082790000 -12.6137850000  
 C 0.0000000000 0.0000000000 -17.5894040000  
 C 1.1809710000 0.2502450000 -18.3067230000  
 C -1.1809710000 -0.2502450000 -18.3067230000  
 C 1.1814050000 0.2495030000 -19.7030230000

H 2.1028840000 0.4396630000 -17.7639000000  
 C -1.1814050000 -0.2495030000 -19.7030230000  
 H -2.1028840000 -0.4396630000 -17.7639000000  
 C 0.0000000000 0.0000000000 -20.4055510000  
 H 2.1061400000 0.4407470000 -20.2408830000  
 H -2.1061400000 -0.4407470000 -20.2408830000  
 H 0.0000000000 0.0000000000 -21.4921340000

**Table S6.** Optimized coordinates for **5**.

Zn 0.0000000000 0.0000000000 8.4147170000  
 N -0.1561400000 1.4400870000 6.9745820000  
 C -0.0989140000 1.2391220000 5.6273250000  
 C 0.0000000000 0.0000000000 4.9448420000  
 C 0.0989140000 -1.2391220000 5.6273250000  
 N 0.1561400000 -1.4400870000 6.9745820000  
 C 0.2523230000 -2.8058590000 7.1648190000  
 C 0.3210110000 -3.4530840000 8.4164710000  
 C 0.2702620000 -2.8027260000 9.6700310000  
 N 0.1273810000 -1.4426900000 9.8587480000  
 C 0.1271570000 -1.2353540000 11.2076660000  
 C 0.0000000000 0.0000000000 11.8888250000  
 C -0.1271570000 1.2353540000 11.2076660000  
 N -0.1273810000 1.4426900000 9.8587480000  
 C -0.2702620000 2.8027260000 9.6700310000  
 C -0.3210110000 3.4530840000 8.4164710000  
 C -0.2523230000 2.8058590000 7.1648190000  
 C -0.2438260000 3.4773890000 5.8899020000  
 C -0.1550200000 2.5003390000 4.9262700000  
 C -0.1015880000 2.5028600000 3.4907320000  
 C -0.0307430000 1.2428070000 2.7903880000  
 N 0.0086020000 1.4484720000 1.4430890000  
 Zn 0.0000000000 0.0000000000 0.0000000000  
 N -0.0086020000 1.4484720000 -1.4430890000  
 C 0.0307430000 1.2428070000 -2.7903880000  
 C 0.0000000000 0.0000000000 -3.4729400000  
 C -0.0307430000 -1.2428070000 -2.7903880000  
 N 0.0086020000 -1.4484720000 -1.4430890000  
 C -0.0249620000 -2.8167310000 -1.2528110000  
 C 0.0000000000 -3.4678070000 0.0000000000  
 C 0.0249620000 -2.8167310000 1.2528110000  
 N -0.0086020000 -1.4484720000 1.4430890000  
 C 0.0307430000 -1.2428070000 2.7903880000  
 C 0.0000000000 0.0000000000 3.4729400000  
 C 0.1015880000 -2.5028600000 3.4907320000  
 C 0.1550200000 -2.5003390000 4.9262700000  
 C 0.2438260000 -3.4773890000 5.8899020000  
 H 0.2912530000 -4.5462700000 5.7421320000  
 C 0.1053000000 -3.4842170000 2.5266650000  
 H 0.1621570000 -4.5526140000 2.6744650000  
 C -0.1053000000 -3.4842170000 -2.5266650000  
 C -0.1015880000 -2.5028600000 -3.4907320000  
 C -0.1550200000 -2.5003390000 -4.9262700000  
 C -0.0989140000 -1.2391220000 -5.6273250000  
 N -0.1561400000 -1.4400870000 -6.9745820000  
 Zn 0.0000000000 0.0000000000 -8.4147170000  
 N 0.1273810000 1.4426900000 -9.8587480000  
 C 0.1271570000 1.2353540000 -11.2076660000  
 C 0.0000000000 0.0000000000 -11.8888250000  
 C -0.1271570000 -1.2353540000 -11.2076660000  
 N -0.1273810000 -1.4426900000 -9.8587480000  
 C -0.2702620000 -2.8027260000 -9.6700310000  
 C -0.3210110000 -3.4530840000 -8.4164710000

C -0.2523230000 -2.8058590000 -7.1648190000  
 C -0.2438260000 -3.4773890000 -5.8899020000  
 H -0.2912530000 -4.5462700000 -5.7421320000  
 C -0.3766900000 -3.4640100000 -10.9455870000  
 C -0.2786180000 -2.4873140000 -11.9087760000  
 C -0.3012850000 -2.4848670000 -13.3457490000  
 C -0.1608450000 -1.2288930000 -14.0487630000  
 N -0.2030180000 -1.4296260000 -15.3972230000  
 Zn 0.0000000000 0.0000000000 -16.8467810000  
 N 0.1894690000 1.4412060000 -18.2894750000  
 C 0.1705870000 1.2407300000 -19.6503510000  
 C 0.0000000000 0.0000000000 -20.2995090000  
 C -0.1705870000 -1.2407300000 -19.6503510000  
 N -0.1894690000 -1.4412060000 -18.2894750000  
 C -0.3619610000 -2.7886410000 -18.0875500000  
 C -0.4472570000 -3.4351600000 -16.8319280000  
 C -0.3682600000 -2.7886290000 -15.5854280000  
 C -0.4225600000 -3.4571250000 -14.3071640000  
 H -0.5318810000 -4.5215570000 -14.1598590000  
 C -0.4624660000 -3.4608250000 -19.3628200000  
 C -0.3331190000 -2.5067410000 -20.3278000000  
 H -0.3482100000 -2.6476410000 -21.3986240000  
 H -0.6106400000 -4.5215730000 -19.5025380000  
 C 0.3331190000 2.5067410000 -20.3278000000  
 C 0.4624660000 3.4608250000 -19.3628200000  
 C 0.3619610000 2.7886410000 -18.0875500000  
 C 0.4472570000 3.4351600000 -16.8319280000  
 C 0.3682600000 2.7886290000 -15.5854280000  
 N 0.2030180000 1.4296260000 -15.3972230000  
 C 0.1608450000 1.2288930000 -14.0487630000  
 C 0.3012850000 2.4848670000 -13.3457490000  
 C 0.2786180000 2.4873140000 -11.9087760000  
 C 0.3766900000 3.4640100000 -10.9455870000  
 C 0.2702620000 2.8027260000 -9.6700310000  
 C 0.3210110000 3.4530840000 -8.4164710000  
 C 0.2523230000 2.8058590000 -7.1648190000  
 N 0.1561400000 1.4400870000 -6.9745820000  
 C 0.0989140000 1.2391220000 -5.6273250000  
 C 0.1550200000 2.5003390000 -4.9262700000  
 C 0.1015880000 2.5028600000 -3.4907320000  
 C 0.1053000000 3.4842170000 -2.5266650000  
 C 0.0249620000 2.8167310000 -1.2528110000  
 C 0.0000000000 3.4678070000 0.0000000000  
 C -0.0249620000 2.8167310000 1.2528110000  
 C -0.1053000000 3.4842170000 2.5266650000  
 H -0.1621570000 4.5526140000 2.6744650000  
 H 0.1621570000 4.5526140000 -2.6744650000  
 C 0.2438260000 3.4773890000 -5.8899020000  
 H 0.2912530000 4.5462700000 -5.7421320000  
 C 0.0000000000 0.0000000000 -4.9448420000  
 H 0.5126310000 4.5250860000 -11.0945600000  
 C 0.4225600000 3.4571250000 -14.3071640000  
 H 0.5318810000 4.5215570000 -14.1598590000  
 C 0.0000000000 0.0000000000 -13.3660870000  
 H 0.6106400000 4.5215730000 -19.5025380000  
 H 0.3482100000 2.6476410000 -21.3986240000  
 H -0.5126310000 -4.5250860000 -11.0945600000  
 H -0.1621570000 -4.5526140000 -2.6744650000  
 H -0.2912530000 4.5462700000 5.7421320000  
 C -0.3766900000 3.4640100000 10.9455870000  
 C -0.2786180000 2.4873140000 11.9087760000  
 C -0.3012850000 2.4848670000 13.3457490000  
 C -0.1608450000 1.2288930000 14.0487630000

N -0.2030180000 1.4296260000 15.3972230000  
 Zn 0.0000000000 0.0000000000 16.8467810000  
 N -0.1894690000 1.4412060000 18.2894750000  
 C -0.1705870000 1.2407300000 19.6503510000  
 C -0.3331190000 2.5067410000 20.3278000000  
 C 0.0000000000 0.0000000000 20.2995090000  
 C 0.1705870000 -1.2407300000 19.6503510000  
 N 0.1894690000 -1.4412060000 18.2894750000  
 C 0.3619610000 -2.7886410000 18.0875500000  
 C 0.4472570000 -3.4351600000 16.8319280000  
 C 0.3682600000 -2.7886290000 15.5854280000  
 N 0.2030180000 -1.4296260000 15.3972230000  
 C 0.1608450000 -1.2288930000 14.0487630000  
 C 0.0000000000 0.0000000000 13.3660870000  
 C 0.3012850000 -2.4848670000 13.3457490000  
 C 0.2786180000 -2.4873140000 11.9087760000  
 C 0.3766900000 -3.4640100000 10.9455870000  
 H 0.5126310000 -4.5250860000 11.0945600000  
 C 0.4225600000 -3.4571250000 14.3071640000  
 H 0.5318810000 -4.5215570000 14.1598590000  
 C 0.4624660000 -3.4608250000 19.3628200000  
 C 0.3331190000 -2.5067410000 20.3278000000  
 H 0.6106400000 -4.5215730000 19.5025380000  
 C -0.4624660000 3.4608250000 19.3628200000  
 C -0.3619610000 2.7886410000 18.0875500000  
 C -0.4472570000 3.4351600000 16.8319280000  
 C -0.3682600000 2.7886290000 15.5854280000  
 C -0.4225600000 3.4571250000 14.3071640000  
 H -0.5318810000 4.5215570000 14.1598590000  
 H -0.6106400000 4.5215730000 19.5025380000  
 H -0.5126310000 4.5250860000 11.0945600000  
 H -0.3482100000 2.6476410000 21.3986240000  
 H 0.3482100000 -2.6476410000 21.3986240000  
 C 0.6362130000 4.9218950000 -16.8312900000  
 C -0.3931080000 5.7768730000 -17.2577680000  
 C 1.8466460000 5.4904620000 -16.4026460000  
 C -0.2173020000 7.1619090000 -17.2549470000  
 H -1.3371470000 5.3505530000 -17.5855480000  
 C 2.0235270000 6.8755330000 -16.4013900000  
 H 2.6531280000 4.8400400000 -16.0757840000  
 C 0.9919580000 7.7156160000 -16.8272850000  
 H -1.0272400000 7.8076720000 -17.5835590000  
 H 2.9689860000 7.2967980000 -16.0703110000  
 H 1.1291540000 8.7935030000 -16.8257960000  
 C 0.4534100000 4.9446410000 -8.4168440000  
 C -0.5843980000 5.7576590000 -8.9017010000  
 C 1.6184250000 5.5611690000 -7.9313800000  
 C -0.4612230000 7.1482550000 -8.8997020000  
 H -1.4939660000 5.2940550000 -9.2729410000  
 C 1.7429950000 6.9516850000 -7.9326750000  
 H 2.4313930000 4.9438290000 -7.5598850000  
 C 0.7032670000 7.7496800000 -8.4160610000  
 H -1.2773760000 7.7609030000 -9.2731640000  
 H 2.6543960000 7.4102430000 -7.5585350000  
 H 0.7996690000 8.8319710000 -8.4158010000  
 C 0.0000000000 4.9650550000 0.0000000000  
 C 1.0954840000 5.6826860000 0.5080940000  
 C -1.0954840000 5.6826860000 -0.5080940000  
 C 1.0963470000 7.0787090000 0.5061280000  
 H 1.9522640000 5.1400430000 0.8972610000  
 C -1.0963470000 7.0787090000 -0.5061280000  
 H -1.9522640000 5.1400430000 -0.8972610000  
 C 0.0000000000 7.7811750000 0.0000000000

H 1.9557260000 7.6164540000 0.8975480000  
 H -1.9557260000 7.6164540000 -0.8975480000  
 H 0.0000000000 8.8677550000 0.0000000000  
 C -0.4534100000 4.9446410000 8.4168440000  
 C 0.5843980000 5.7576590000 8.9017010000  
 C -1.6184250000 5.5611690000 7.9313800000  
 C 0.4612230000 7.1482550000 8.8997020000  
 H 1.4939660000 5.2940550000 9.2729410000  
 C -1.7429950000 6.9516850000 7.9326750000  
 H -2.4313930000 4.9438290000 7.5598850000  
 C -0.7032670000 7.7496800000 8.4160610000  
 H 1.2773760000 7.7609030000 9.2731640000  
 H -2.6543960000 7.4102430000 7.5585350000  
 H -0.7996690000 8.8319710000 8.4158010000  
 C 0.0000000000 0.0000000000 -21.7987840000  
 C -1.1821190000 -0.2449390000 -22.5160310000  
 C 1.1821190000 0.2449390000 -22.5160310000  
 C -1.1825430000 -0.2441170000 -23.9123260000  
 H -2.1048710000 -0.4302130000 -21.9732150000  
 C 1.1825430000 0.2441170000 -23.9123260000  
 H 2.1048710000 0.4302130000 -21.9732150000  
 C 0.0000000000 0.0000000000 -24.6148280000  
 H -2.1081310000 -0.4311360000 -24.4501940000  
 H 2.1081310000 0.4311360000 -24.4501940000  
 H 0.0000000000 0.0000000000 -25.7014090000  
 C -0.6362130000 -4.9218950000 -16.8312900000  
 C 0.3931080000 -5.7768730000 -17.2577680000  
 C -1.8466460000 -5.4904620000 -16.4026460000  
 C 0.2173020000 -7.1619090000 -17.2549470000  
 H 1.3371470000 -5.3505530000 -17.5855480000  
 C -2.0235270000 -6.8755330000 -16.4013900000  
 H -2.6531280000 -4.8400400000 -16.0757840000  
 C -0.9919580000 -7.7156160000 -16.8272850000  
 H 1.0272400000 -7.8076720000 -17.5835590000  
 H -2.9689860000 -7.2967980000 -16.0703110000  
 H -1.1291540000 -8.7935030000 -16.8257960000  
 C 0.0000000000 -4.9650550000 0.0000000000  
 C -1.0954840000 -5.6826860000 0.5080940000  
 C 1.0954840000 -5.6826860000 -0.5080940000  
 C -1.0963470000 -7.0787090000 0.5061280000  
 H -1.9522640000 -5.1400430000 0.8972610000  
 C 1.0963470000 -7.0787090000 -0.5061280000  
 H 1.9522640000 -5.1400430000 -0.8972610000  
 C 0.0000000000 -7.7811750000 0.0000000000  
 H -1.9557260000 -7.6164540000 0.8975480000  
 H 1.9557260000 -7.6164540000 -0.8975480000  
 H 0.0000000000 -8.8677550000 0.0000000000  
 C -0.4534100000 -4.9446410000 -8.4168440000  
 C 0.5843980000 -5.7576590000 -8.9017010000  
 C -1.6184250000 -5.5611690000 -7.9313800000  
 C 0.4612230000 -7.1482550000 -8.8997020000  
 H 1.4939660000 -5.2940550000 -9.2729410000  
 C -1.7429950000 -6.9516850000 -7.9326750000  
 H -2.4313930000 -4.9438290000 -7.5598850000  
 C -0.7032670000 -7.7496800000 -8.4160610000  
 H 1.2773760000 -7.7609030000 -9.2731640000  
 H -2.6543960000 -7.4102430000 -7.5585350000  
 H -0.7996690000 -8.8319710000 -8.4158010000  
 C 0.4534100000 -4.9446410000 8.4168440000  
 C -0.5843980000 -5.7576590000 8.9017010000  
 C 1.6184250000 -5.5611690000 7.9313800000  
 C -0.4612230000 -7.1482550000 8.8997020000  
 H -1.4939660000 -5.2940550000 9.2729410000

C 1.7429950000 -6.9516850000 7.9326750000  
 H 2.4313930000 -4.9438290000 7.5598850000  
 C 0.7032670000 -7.7496800000 8.4160610000  
 H -1.2773760000 -7.7609030000 9.2731640000  
 H 2.6543960000 -7.4102430000 7.5585350000  
 H 0.7996690000 -8.8319710000 8.4158010000  
 C 0.0000000000 0.0000000000 21.7987840000  
 C -1.1821190000 0.2449390000 22.5160310000  
 C 1.1821190000 -0.2449390000 22.5160310000  
 C -1.1825430000 0.2441170000 23.9123260000  
 H -2.1048710000 0.4302130000 21.9732150000  
 C 1.1825430000 -0.2441170000 23.9123260000  
 H 2.1048710000 -0.4302130000 21.9732150000  
 C 0.0000000000 0.0000000000 24.6148280000  
 H -2.1081310000 0.4311360000 24.4501940000  
 H 2.1081310000 -0.4311360000 24.4501940000  
 H 0.0000000000 0.0000000000 25.7014090000  
 C -0.6362130000 4.9218950000 16.8312900000  
 C 0.3931080000 5.7768730000 17.2577680000  
 C -1.8466460000 5.4904620000 16.4026460000  
 C 0.2173020000 7.1619090000 17.2549470000  
 H 1.3371470000 5.3505530000 17.5855480000  
 C -2.0235270000 6.8755330000 16.4013900000  
 H -2.6531280000 4.8400400000 16.0757840000  
 C -0.9919580000 7.7156160000 16.8272850000  
 H 1.0272400000 7.8076720000 17.5835590000  
 H -2.9689860000 7.2967980000 16.0703110000  
 H -1.1291540000 8.7935030000 16.8257960000  
 C 0.6362130000 -4.9218950000 16.8312900000  
 C -0.3931080000 -5.7768730000 17.2577680000  
 C 1.8466460000 -5.4904620000 16.4026460000  
 C -0.2173020000 -7.1619090000 17.2549470000  
 H -1.3371470000 -5.3505530000 17.5855480000  
 C 2.0235270000 -6.8755330000 16.4013900000  
 H 2.6531280000 -4.8400400000 16.0757840000  
 C 0.9919580000 -7.7156160000 16.8272850000  
 H -1.0272400000 -7.8076720000 17.5835590000  
 H 2.9689860000 -7.2967980000 16.0703110000  
 H 1.1291540000 -8.7935030000 16.8257960000

**Table S7.** Optimized coordinates for **7**.

Zn 0.0000000000 0.0000000000 4.2081980000  
 N -0.0806790000 1.4463700000 2.7650440000  
 C -0.0330720000 1.2433590000 1.4180990000  
 C 0.0000000000 0.0000000000 0.7349280000  
 C 0.0330720000 -1.2433590000 1.4180990000  
 N 0.0806790000 -1.4463700000 2.7650440000  
 C 0.1132500000 -2.8150790000 2.9556750000  
 C 0.1618250000 -3.4638860000 4.2084870000  
 C 0.1499370000 -2.8129910000 5.4619470000  
 N 0.0609600000 -1.4471850000 5.6522160000  
 C 0.0807690000 -1.2409080000 6.9997790000  
 C 0.0000000000 0.0000000000 7.6827680000  
 C -0.0807690000 1.2409080000 6.9997790000  
 N -0.0609600000 1.4471850000 5.6522160000  
 C -0.1499370000 2.8129910000 5.4619470000  
 C -0.1618250000 3.4638860000 4.2084870000  
 C -0.1132500000 2.8150790000 2.9556750000

C -0.0692760000 3.4857830000 1.6819920000  
 C -0.0262970000 2.5054200000 0.7176470000  
 C 0.0262970000 2.5054200000 -0.7176470000  
 C 0.0330720000 1.2433590000 -1.4180990000  
 N 0.0806790000 1.4463700000 -2.7650440000  
 Zn 0.0000000000 0.0000000000 -4.2081980000  
 N 0.0609600000 1.4471850000 -5.6522160000  
 C 0.0807690000 1.2409080000 -6.9997790000  
 C 0.0000000000 0.0000000000 -7.6827680000  
 C -0.0807690000 -1.2409080000 -6.9997790000  
 N -0.0609600000 -1.4471850000 -5.6522160000  
 C -0.1499370000 -2.8129910000 -5.4619470000  
 C -0.1618250000 -3.4638860000 -4.2084870000  
 C -0.1132500000 -2.8150790000 -2.9556750000  
 N -0.0806790000 -1.4463700000 -2.7650440000  
 C -0.0330720000 -1.2433590000 -1.4180990000  
 C 0.0000000000 0.0000000000 -0.7349280000  
 C -0.0262970000 -2.5054200000 -0.7176470000  
 C 0.0262970000 -2.5054200000 0.7176470000  
 C 0.0692760000 -3.4857830000 1.6819920000  
 H 0.0653540000 -4.5556980000 1.5342750000  
 C -0.0692760000 -3.4857830000 -1.6819920000  
 H -0.0653540000 -4.5556980000 -1.5342750000  
 C -0.2445120000 -3.4775960000 -6.7358400000  
 C -0.1931980000 -2.4975780000 -7.7002140000  
 C -0.2317570000 -2.4945110000 -9.1359780000  
 C -0.1325760000 -1.2360220000 -9.8371740000  
 N -0.1834380000 -1.4361100000 -11.1846360000  
 Zn 0.0000000000 0.0000000000 -12.6255300000  
 N 0.1520340000 1.4400570000 -14.0689250000  
 C 0.1428580000 1.2337100000 -15.4179760000  
 C 0.0000000000 0.0000000000 -16.0993180000  
 C -0.1428580000 -1.2337100000 -15.4179760000  
 N -0.1520340000 -1.4400570000 -14.0689250000  
 C -0.3163260000 -2.7976340000 -13.8802490000  
 C -0.3882440000 -3.4456330000 -12.6264260000  
 C -0.3152010000 -2.7992090000 -11.3749550000  
 C -0.3380520000 -3.4696020000 -10.0997880000  
 H -0.4166240000 -4.5366120000 -9.9518620000  
 C -0.4245190000 -3.4584510000 -15.1556750000  
 C -0.3072360000 -2.4839320000 -16.1190290000  
 C -0.3224740000 -2.4822650000 -17.5560430000  
 C -0.1693540000 -1.2277870000 -18.2590990000  
 N -0.2077780000 -1.4287410000 -19.6075230000  
 Zn 0.0000000000 0.0000000000 -21.0572040000  
 N 0.1921150000 1.4407570000 -22.4999420000  
 C 0.1718070000 1.2405730000 -23.8608540000  
 C 0.0000000000 0.0000000000 -24.5100220000  
 C -0.1718070000 -1.2405730000 -23.8608540000  
 N -0.1921150000 -1.4407570000 -22.4999420000  
 C -0.3685360000 -2.7875950000 -22.2979680000  
 C -0.4596510000 -3.4332940000 -21.0422080000  
 C -0.3816520000 -2.7867560000 -19.7958050000  
 C -0.4462840000 -3.4541840000 -18.5174610000  
 H -0.5635860000 -4.5177550000 -18.3701080000  
 C -0.4686040000 -3.4599600000 -23.5731190000  
 C -0.3359080000 -2.5063960000 -24.5382000000  
 H -0.3500450000 -2.6475180000 -25.6090030000  
 H -0.6189210000 -4.5204230000 -23.7127060000  
 C 0.3359080000 2.5063960000 -24.5382000000  
 C 0.4686040000 3.4599600000 -23.5731190000  
 C 0.3685360000 2.7875950000 -22.2979680000  
 C 0.4596510000 3.4332940000 -21.0422080000

C 0.3816520000 2.7867560000 -19.7958050000  
 N 0.2077780000 1.4287410000 -19.6075230000  
 C 0.1693540000 1.2277870000 -18.2590990000  
 C 0.3224740000 2.4822650000 -17.5560430000  
 C 0.3072360000 2.4839320000 -16.1190290000  
 C 0.4245190000 3.4584510000 -15.1556750000  
 C 0.3163260000 2.7976340000 -13.8802490000  
 C 0.3882440000 3.4456330000 -12.6264260000  
 C 0.3152010000 2.7992090000 -11.3749550000  
 N 0.1834380000 1.4361100000 -11.1846360000  
 C 0.1325760000 1.2360220000 -9.8371740000  
 C 0.2317570000 2.4945110000 -9.1359780000  
 C 0.1931980000 2.4975780000 -7.7002140000  
 C 0.2445120000 3.4775960000 -6.7358400000  
 C 0.1499370000 2.8129910000 -5.4619470000  
 C 0.1618250000 3.4638860000 -4.2084870000  
 C 0.1132500000 2.8150790000 -2.9556750000  
 C 0.0692760000 3.4857830000 -1.6819920000  
 H 0.0653540000 4.5556980000 -1.5342750000  
 H 0.3416860000 4.5430120000 -6.8839850000  
 C 0.3380520000 3.4696020000 -10.0997880000  
 H 0.4166240000 4.5366120000 -9.9518620000  
 C 0.0000000000 0.0000000000 -9.1540350000  
 H 0.5749990000 4.5175720000 -15.3045870000  
 C 0.4462840000 3.4541840000 -18.5174610000  
 H 0.5635860000 4.5177550000 -18.3701080000  
 C 0.0000000000 0.0000000000 -17.5762680000  
 H 0.6189210000 4.5204230000 -23.7127060000  
 H 0.3500450000 2.6475180000 -25.6090030000  
 H -0.5749990000 -4.5175720000 -15.3045870000  
 H -0.3416860000 -4.5430120000 -6.8839850000  
 H -0.0653540000 4.5556980000 1.5342750000  
 C -0.2445120000 3.4775960000 6.7358400000  
 C -0.1931980000 2.4975780000 7.7002140000  
 C -0.2317570000 2.4945110000 9.1359780000  
 C -0.1325760000 1.2360220000 9.8371740000  
 N -0.1834380000 1.4361100000 11.1846360000  
 Zn 0.0000000000 0.0000000000 12.6255300000  
 N -0.1520340000 1.4400570000 14.0689250000  
 C -0.1428580000 1.2337100000 15.4179760000  
 C -0.3072360000 2.4839320000 16.1190290000  
 C -0.3224740000 2.4822650000 17.5560430000  
 C -0.1693540000 1.2277870000 18.2590990000  
 N -0.2077780000 1.4287410000 19.6075230000  
 Zn 0.0000000000 0.0000000000 21.0572040000  
 N 0.2077780000 -1.4287410000 19.6075230000  
 C 0.1693540000 -1.2277870000 18.2590990000  
 C 0.0000000000 0.0000000000 17.5762680000  
 C 0.0000000000 0.0000000000 16.0993180000  
 C 0.1428580000 -1.2337100000 15.4179760000  
 N 0.1520340000 -1.4400570000 14.0689250000  
 C 0.3163260000 -2.7976340000 13.8802490000  
 C 0.3882440000 -3.4456330000 12.6264260000  
 C 0.3152010000 -2.7992090000 11.3749550000  
 N 0.1834380000 -1.4361100000 11.1846360000  
 C 0.1325760000 -1.2360220000 9.8371740000  
 C 0.0000000000 0.0000000000 9.1540350000  
 C 0.2317570000 -2.4945110000 9.1359780000  
 C 0.1931980000 -2.4975780000 7.7002140000  
 C 0.2445120000 -3.4775960000 6.7358400000  
 H 0.3416860000 -4.5430120000 6.8839850000  
 C 0.3380520000 -3.4696020000 10.0997880000  
 H 0.4166240000 -4.5366120000 9.9518620000

C 0.4245190000 -3.4584510000 15.1556750000  
 C 0.3072360000 -2.4839320000 16.1190290000  
 C 0.3224740000 -2.4822650000 17.5560430000  
 C 0.4462840000 -3.4541840000 18.5174610000  
 C 0.3816520000 -2.7867560000 19.7958050000  
 C 0.4596510000 -3.4332940000 21.0422080000  
 C 0.3685360000 -2.7875950000 22.2979680000  
 N 0.1921150000 -1.4407570000 22.4999420000  
 C 0.1718070000 -1.2405730000 23.8608540000  
 C 0.0000000000 0.0000000000 24.5100220000  
 C -0.1718070000 1.2405730000 23.8608540000  
 N -0.1921150000 1.4407570000 22.4999420000  
 C -0.3685360000 2.7875950000 22.2979680000  
 C -0.4596510000 3.4332940000 21.0422080000  
 C -0.3816520000 2.7867560000 19.7958050000  
 C -0.4462840000 3.4541840000 18.5174610000  
 H -0.5635860000 4.5177550000 18.3701080000  
 C -0.4686040000 3.4599600000 23.5731190000  
 C -0.3359080000 2.5063960000 24.5382000000  
 H -0.3500450000 2.6475180000 25.6090030000  
 H -0.6189210000 4.5204230000 23.7127060000  
 C 0.3359080000 -2.5063960000 24.5382000000  
 C 0.4686040000 -3.4599600000 23.5731190000  
 H 0.6189210000 -4.5204230000 23.7127060000  
 H 0.3500450000 -2.6475180000 25.6090030000  
 H 0.5635860000 -4.5177550000 18.3701080000  
 H 0.5749990000 -4.5175720000 15.3045870000  
 C -0.4245190000 3.4584510000 15.1556750000  
 C -0.3163260000 2.7976340000 13.8802490000  
 C -0.3882440000 3.4456330000 12.6264260000  
 C -0.3152010000 2.7992090000 11.3749550000  
 C -0.3380520000 3.4696020000 10.0997880000  
 H -0.4166240000 4.5366120000 9.9518620000  
 H -0.5749990000 4.5175720000 15.3045870000  
 H -0.3416860000 4.5430120000 6.8839850000  
 C 0.0000000000 0.0000000000 -26.0092700000  
 C 1.1821850000 0.2447220000 -26.7264830000  
 C -1.1821850000 -0.2447220000 -26.7264830000  
 C 1.1826030000 0.2438490000 -28.1227730000  
 H 2.1049750000 0.4298050000 -26.1836750000  
 C -1.1826030000 -0.2438490000 -28.1227730000  
 H -2.1049750000 -0.4298050000 -26.1836750000  
 C 0.0000000000 0.0000000000 -28.8252630000  
 H 2.1082300000 0.4306410000 -28.6606450000  
 H -2.1082300000 -0.4306410000 -28.6606450000  
 H 0.0000000000 0.0000000000 -29.9118410000  
 C 0.0000000000 0.0000000000 26.0092700000  
 C -1.1821850000 0.2447220000 26.7264830000  
 C 1.1821850000 -0.2447220000 26.7264830000  
 C -1.1826030000 0.2438490000 28.1227730000  
 H -2.1049750000 0.4298050000 26.1836750000  
 C 1.1826030000 -0.2438490000 28.1227730000  
 H 2.1049750000 -0.4298050000 26.1836750000  
 C 0.0000000000 0.0000000000 28.8252630000  
 H -2.1082300000 0.4306410000 28.6606450000  
 H 2.1082300000 -0.4306410000 28.6606450000  
 H 0.0000000000 0.0000000000 29.9118410000  
 C 0.6552680000 -4.9192110000 21.0417960000  
 C -0.3726400000 -5.7788360000 21.4622070000  
 C 1.8705950000 -5.4821370000 20.6197030000  
 C -0.1906940000 -7.1630850000 21.4597510000  
 H -1.3203210000 -5.3568110000 21.7850060000  
 C 2.0535840000 -6.8664230000 20.6188210000

H 2.6759990000 -4.8279990000 20.2976280000  
 C 1.0233660000 -7.7112330000 21.0385770000  
 H -0.9995640000 -7.8125780000 21.7835990000  
 H 3.0027150000 -7.2833680000 20.2928280000  
 H 1.1653280000 -8.7885010000 21.0373750000  
 C 0.5514000000 -4.9342900000 12.6270450000  
 C -0.4761340000 -5.7687680000 13.0969070000  
 C 1.7353270000 -5.5261180000 12.1570590000  
 C -0.3245250000 -7.1565680000 13.0952880000  
 H -1.3999190000 -5.3242670000 13.4562440000  
 C 1.8881910000 -6.9138330000 12.1586180000  
 H 2.5404760000 -4.8918070000 11.7972840000  
 C 0.8584740000 -7.7334790000 12.6269560000  
 H -1.1329720000 -7.7862210000 13.4570420000  
 H 2.8137490000 -7.3532430000 11.7964490000  
 H 0.9769620000 -8.8135740000 12.6269280000  
 C 0.2295370000 -4.9597130000 4.2084510000  
 C 1.3617290000 -5.6262180000 3.7114820000  
 C -0.8373530000 -5.7266210000 4.7051040000  
 C 1.4261630000 -7.0207730000 3.7133150000  
 H 2.1967270000 -5.0448530000 3.3309910000  
 C -0.7745520000 -7.1212400000 4.7029580000  
 H -1.7218610000 -5.2237860000 5.0856160000  
 C 0.3578290000 -7.7727140000 4.2080870000  
 H 2.3130680000 -7.5185720000 3.3305740000  
 H -1.6125140000 -7.6977920000 5.0854530000  
 H 0.4073290000 -8.8581610000 4.2079800000  
 C -0.2295370000 -4.9597130000 -4.2084510000  
 C 0.8373530000 -5.7266210000 -4.7051040000  
 C -1.3617290000 -5.6262180000 -3.7114820000  
 C 0.7745520000 -7.1212400000 -4.7029580000  
 H 1.7218610000 -5.2237860000 -5.0856160000  
 C -1.4261630000 -7.0207730000 -3.7133150000  
 H -2.1967270000 -5.0448530000 -3.3309910000  
 C -0.3578290000 -7.7727140000 -4.2080870000  
 H 1.6125140000 -7.6977920000 -5.0854530000  
 H -2.3130680000 -7.5185720000 -3.3305740000  
 H -0.4073290000 -8.8581610000 -4.2079800000  
 C -0.5514000000 -4.9342900000 -12.6270450000  
 C 0.4761340000 -5.7687680000 -13.0969070000  
 C -1.7353270000 -5.5261180000 -12.1570590000  
 C 0.3245250000 -7.1565680000 -13.0952880000  
 H 1.3999190000 -5.3242670000 -13.4562440000  
 C -1.8881910000 -6.9138330000 -12.1586180000  
 H -2.5404760000 -4.8918070000 -11.7972840000  
 C -0.8584740000 -7.7334790000 -12.6269560000  
 H 1.1329720000 -7.7862210000 -13.4570420000  
 H -2.8137490000 -7.3532430000 -11.7964490000  
 H -0.9769620000 -8.8135740000 -12.6269280000  
 C -0.6552680000 -4.9192110000 -21.0417960000  
 C 0.3726400000 -5.7788360000 -21.4622070000  
 C -1.8705950000 -5.4821370000 -20.6197030000  
 C 0.1906940000 -7.1630850000 -21.4597510000  
 H 1.3203210000 -5.3568110000 -21.7850060000  
 C -2.0535840000 -6.8664230000 -20.6188210000  
 H -2.6759990000 -4.8279990000 -20.2976280000  
 C -1.0233660000 -7.7112330000 -21.0385770000  
 H 0.9995640000 -7.8125780000 -21.7835990000  
 H -3.0027150000 -7.2833680000 -20.2928280000  
 H -1.1653280000 -8.7885010000 -21.0373750000  
 C 0.6552680000 4.9192110000 -21.0417960000  
 C -0.3726400000 5.7788360000 -21.4622070000  
 C 1.8705950000 5.4821370000 -20.6197030000

C -0.1906940000 7.1630850000 -21.4597510000  
 H -1.3203210000 5.3568110000 -21.7850060000  
 C 2.0535840000 6.8664230000 -20.6188210000  
 H 2.6759990000 4.8279990000 -20.2976280000  
 C 1.0233660000 7.7112330000 -21.0385770000  
 H -0.9995640000 7.8125780000 -21.7835990000  
 H 3.0027150000 7.2833680000 -20.2928280000  
 H 1.1653280000 8.7885010000 -21.0373750000  
 C -0.6552680000 4.9192110000 21.0417960000  
 C 0.3726400000 5.7788360000 21.4622070000  
 C -1.8705950000 5.4821370000 20.6197030000  
 C 0.1906940000 7.1630850000 21.4597510000  
 H 1.3203210000 5.3568110000 21.7850060000  
 C -2.0535840000 6.8664230000 20.6188210000  
 H -2.6759990000 4.8279990000 20.2976280000  
 C -1.0233660000 7.7112330000 21.0385770000  
 H 0.9995640000 7.8125780000 21.7835990000  
 H -3.0027150000 7.2833680000 20.2928280000  
 H -1.1653280000 8.7885010000 21.0373750000  
 C -0.5514000000 4.9342900000 12.6270450000  
 C 0.4761340000 5.7687680000 13.0969070000  
 C -1.7353270000 5.5261180000 12.1570590000  
 C 0.3245250000 7.1565680000 13.0952880000  
 H 1.3999190000 5.3242670000 13.4562440000  
 C -1.8881910000 6.9138330000 12.1586180000  
 H -2.5404760000 4.8918070000 11.7972840000  
 C -0.8584740000 7.7334790000 12.6269560000  
 H 1.1329720000 7.7862210000 13.4570420000  
 H -2.8137490000 7.3532430000 11.7964490000  
 H -0.9769620000 8.8135740000 12.6269280000  
 C -0.2295370000 4.9597130000 4.2084510000  
 C -1.3617290000 5.6262180000 3.7114820000  
 C 0.8373530000 5.7266210000 4.7051040000  
 C -1.4261630000 7.0207730000 3.7133150000  
 H -2.1967270000 5.0448530000 3.3309910000  
 C 0.7745520000 7.1212400000 4.7029580000  
 H 1.7218610000 5.2237860000 5.0856160000  
 C -0.3578290000 7.7727140000 4.2080870000  
 H -2.3130680000 7.5185720000 3.3305740000  
 H 1.6125140000 7.6977920000 5.0854530000  
 H -0.4073290000 8.8581610000 4.2079800000  
 C 0.2295370000 4.9597130000 -4.2084510000  
 C -0.8373530000 5.7266210000 -4.7051040000  
 C 1.3617290000 5.6262180000 -3.7114820000  
 C -0.7745520000 7.1212400000 -4.7029580000  
 H -1.7218610000 5.2237860000 -5.0856160000  
 C 1.4261630000 7.0207730000 -3.7133150000  
 H 2.1967270000 5.0448530000 -3.3309910000  
 C 0.3578290000 7.7727140000 -4.2080870000  
 H -1.6125140000 7.6977920000 -5.0854530000  
 H 2.3130680000 7.5185720000 -3.3305740000  
 H 0.4073290000 8.8581610000 -4.2079800000  
 C 0.5514000000 4.9342900000 -12.6270450000  
 C -0.4761340000 5.7687680000 -13.0969070000  
 C 1.7353270000 5.5261180000 -12.1570590000  
 C -0.3245250000 7.1565680000 -13.0952880000  
 H -1.3999190000 5.3242670000 -13.4562440000  
 C 1.8881910000 6.9138330000 -12.1586180000  
 H 2.5404760000 4.8918070000 -11.7972840000  
 C 0.8584740000 7.7334790000 -12.6269560000  
 H -1.1329720000 7.7862210000 -13.4570420000  
 H 2.8137490000 7.3532430000 -11.7964490000  
 H 0.9769620000 8.8135740000 -12.6269280000

**Table S8.** Optimized coordinates for **8**.

Zn 0.0000000000 0.0000000000 12.6257730000  
N 1.4362910000 0.1817660000 11.1833460000  
C 1.2369970000 0.1312730000 9.8361470000  
C 0.0000000000 0.0000000000 9.1519730000  
C -1.2369970000 -0.1312730000 9.8361470000  
N -1.4362910000 -0.1817660000 11.1833460000  
C -2.7999610000 -0.3108150000 11.3737390000  
C -3.4462480000 -0.3809520000 12.6261360000  
C -2.7997320000 -0.3092490000 13.8798540000  
N -1.4403070000 -0.1486110000 14.0695550000  
C -1.2358270000 -0.1394700000 15.4176030000  
C 0.0000000000 0.0000000000 16.1011400000  
C 1.2358270000 0.1394700000 15.4176030000  
N 1.4403070000 0.1486110000 14.0695550000  
C 2.7997320000 0.3092490000 13.8798540000  
C 3.4462480000 0.3809520000 12.6261360000  
C 2.7999610000 0.3108150000 11.3737390000  
C 3.4705990000 0.3330380000 10.0999040000  
C 2.4950760000 0.2287000000 9.1353400000  
C 2.4982680000 0.1907590000 7.6999700000  
C 1.2417170000 0.0796700000 6.9995640000  
N 1.4472150000 0.0597380000 5.6524870000  
Zn 0.0000000000 0.0000000000 4.2081490000  
N 1.4463980000 0.0804630000 2.7644070000  
C 1.2440060000 0.0329320000 1.4177850000  
C 0.0000000000 0.0000000000 0.7338010000  
C -1.2440060000 -0.0329320000 1.4177850000  
N -1.4463980000 -0.0804630000 2.7644070000  
C -2.8155030000 -0.1124370000 2.9552020000  
C -3.4639530000 -0.1600410000 4.2083970000  
C -2.8136710000 -0.1478800000 5.4619650000  
N -1.4472150000 -0.0597380000 5.6524870000  
C -1.2417170000 -0.0796700000 6.9995640000  
C 0.0000000000 0.0000000000 7.6835720000  
C -2.4982680000 -0.1907590000 7.6999700000  
C -2.4950760000 -0.2287000000 9.1353400000  
C -3.4705990000 -0.3330380000 10.0999040000  
H -4.5377430000 -0.4096700000 9.9521030000  
C -3.4784460000 -0.2416110000 6.7352030000  
H -4.5439090000 -0.3381170000 6.8833190000  
C -3.4863000000 -0.0684960000 1.6822650000  
C -2.5057780000 -0.0260380000 0.7174900000  
C -2.5057780000 0.0260670000 -0.7174910000  
C -1.2440050000 0.0329440000 -1.4177850000  
N -1.4463970000 0.0804770000 -2.7644070000  
Zn 0.0000000000 0.0000000000 -4.2081510000  
N 1.4472150000 -0.0597520000 -5.6524870000  
C 1.2417160000 -0.0796860000 -6.9995640000  
C 0.0000000000 0.0000000000 -7.6835720000  
C -1.2417160000 0.0796860000 -6.9995640000  
N -1.4472150000 0.0597520000 -5.6524870000  
C -2.8136690000 0.1479170000 -5.4619660000  
C -3.4639510000 0.1600850000 -4.2083980000  
C -2.8155020000 0.1124700000 -2.9552020000

C -3.4862990000 0.0685370000 -1.6822650000  
 H -4.5561990000 0.0641740000 -1.5345910000  
 C -3.4784420000 0.2416600000 -6.7352030000  
 C -2.4982650000 0.1907950000 -7.6999700000  
 C -2.4950720000 0.2287360000 -9.1353400000  
 C -1.2369950000 0.1312910000 -9.8361470000  
 N -1.4362880000 0.1817890000 -11.1833450000  
 Zn 0.0000000000 0.0000000000 -12.6257720000  
 N 1.4403060000 -0.1486220000 -14.0695550000  
 C 1.2358260000 -0.1394780000 -15.4176020000  
 C 0.0000000000 0.0000000000 -16.1011400000  
 C -1.2358260000 0.1394780000 -15.4176020000  
 N -1.4403060000 0.1486220000 -14.0695550000  
 C -2.7997290000 0.3092770000 -13.8798530000  
 C -3.4462430000 0.3809940000 -12.6261350000  
 C -2.7999570000 0.3108520000 -11.3737380000  
 C -3.4705940000 0.3330870000 -10.0999040000  
 H -4.5377370000 0.4097320000 -9.9521030000  
 C -3.4615310000 0.4143690000 -15.1538000000  
 C -2.4869420000 0.2993240000 -16.1183280000  
 H -4.5210890000 0.5619390000 -15.3022500000  
 C 2.4869420000 -0.2993240000 -16.1183280000  
 C 3.4615310000 -0.4143690000 -15.1538000000  
 C 2.7997290000 -0.3092770000 -13.8798530000  
 C 3.4462430000 -0.3809940000 -12.6261350000  
 C 2.7999570000 -0.3108520000 -11.3737380000  
 N 1.4362880000 -0.1817890000 -11.1833450000  
 C 1.2369950000 -0.1312910000 -9.8361470000  
 C 2.4950720000 -0.2287360000 -9.1353400000  
 C 2.4982650000 -0.1907950000 -7.6999700000  
 C 3.4784420000 -0.2416600000 -6.7352030000  
 C 2.8136690000 -0.1479170000 -5.4619660000  
 C 3.4639510000 -0.1600850000 -4.2083980000  
 C 2.8155020000 -0.1124700000 -2.9552020000  
 N 1.4463970000 -0.0804770000 -2.7644070000  
 C 1.2440050000 -0.0329440000 -1.4177850000  
 C 2.5057780000 -0.0260670000 -0.7174910000  
 C 2.5057780000 0.0260380000 0.7174900000  
 C 3.4863000000 0.0684960000 1.6822650000  
 C 2.8155030000 0.1124370000 2.9552020000  
 C 3.4639530000 0.1600410000 4.2083970000  
 C 2.8136710000 0.1478800000 5.4619650000  
 C 3.4784460000 0.2416110000 6.7352030000  
 H 4.5439090000 0.3381170000 6.8833190000  
 H 4.5562000000 0.0641220000 1.5345910000  
 C 3.4862990000 -0.0685370000 -1.6822650000  
 H 4.5561990000 -0.0641740000 -1.5345910000  
 C 0.0000000000 0.0000000000 -0.7338010000  
 H 4.5439040000 -0.3381810000 -6.8833190000  
 C 3.4705940000 -0.3330870000 -10.0999040000  
 H 4.5377370000 -0.4097320000 -9.9521030000  
 C 0.0000000000 0.0000000000 -9.1519720000  
 H 4.5210890000 -0.5619390000 -15.3022500000  
 H -4.5439040000 0.3381810000 -6.8833190000  
 H -4.5562000000 -0.0641220000 1.5345910000  
 H 4.5377430000 0.4096700000 9.9521030000  
 C 3.4615340000 0.4143450000 15.1538000000  
 C 2.4869430000 0.2993120000 16.1183280000  
 C 2.4855410000 0.3136750000 17.5543110000  
 C 1.2319030000 0.1661380000 18.2555860000  
 N 1.4323220000 0.2042540000 19.6031660000  
 Zn 0.0000000000 0.0000000000 21.0448300000  
 N 1.4380240000 0.1677050000 22.4879390000

C 1.2327300000 0.1518500000 23.8370390000  
 C 2.4817500000 0.3250180000 24.5378850000  
 C 2.4807390000 0.3350150000 25.9749190000  
 C 1.2271970000 0.1741970000 26.6780280000  
 N 1.4282520000 0.2102270000 28.0263560000  
 Zn 0.0000000000 0.0000000000 29.4761350000  
 N -1.4282520000 -0.2102270000 28.0263560000  
 C -1.2271970000 -0.1741970000 26.6780280000  
 C 0.0000000000 0.0000000000 25.9951100000  
 C 0.0000000000 0.0000000000 24.5185540000  
 C -1.2327300000 -0.1518500000 23.8370390000  
 N -1.4380240000 -0.1677050000 22.4879390000  
 C -2.7932860000 -0.3493520000 22.2990730000  
 C -3.4380940000 -0.4435070000 21.0449440000  
 C -2.7918300000 -0.3714660000 19.7936970000  
 N -1.4323220000 -0.2042540000 19.6031660000  
 C -1.2319030000 -0.1661380000 18.2555860000  
 C 0.0000000000 0.0000000000 17.5717580000  
 C -2.4855410000 -0.3136750000 17.5543110000  
 C -2.4869430000 -0.2993120000 16.1183280000  
 C -3.4615340000 -0.4143450000 15.1538000000  
 H -4.5210930000 -0.5619080000 15.3022500000  
 C -3.4590450000 -0.4327120000 18.5182450000  
 H -4.5231650000 -0.5434070000 18.3701100000  
 C -3.4542420000 -0.4572260000 23.5742640000  
 C -2.4817500000 -0.3250180000 24.5378850000  
 C -2.4807390000 -0.3350150000 25.9749190000  
 C -3.4524630000 -0.4601150000 26.9363350000  
 C -2.7857110000 -0.3891360000 28.2147330000  
 C -3.4322530000 -0.4663300000 29.4609950000  
 C -2.7870240000 -0.3718170000 30.7169260000  
 N -1.4405310000 -0.1935240000 30.9188950000  
 C -1.2405480000 -0.1722370000 32.2798470000  
 C 0.0000000000 0.0000000000 32.9290060000  
 C 1.2405480000 0.1722370000 32.2798470000  
 N 1.4405310000 0.1935240000 30.9188950000  
 C 2.7870240000 0.3718170000 30.7169260000  
 C 3.4322530000 0.4663300000 29.4609950000  
 C 2.7857110000 0.3891360000 28.2147330000  
 C 3.4524630000 0.4601150000 26.9363350000  
 H 4.5154960000 0.5821550000 26.7889730000  
 C 3.4595910000 0.4712200000 31.9919550000  
 C 2.5063080000 0.3367490000 32.9571180000  
 H 2.6476340000 0.3500810000 34.0278970000  
 H 4.5199400000 0.6223900000 32.1314550000  
 C -2.5063080000 -0.3367490000 32.9571180000  
 C -3.4595910000 -0.4712200000 31.9919550000  
 H -4.5199400000 -0.6223900000 32.1314550000  
 H -2.6476340000 -0.3500810000 34.0278970000  
 H -4.5154960000 -0.5821550000 26.7889730000  
 H -4.5118060000 -0.6185560000 23.7229330000  
 C 3.4542420000 0.4572260000 23.5742640000  
 C 2.7932860000 0.3493520000 22.2990730000  
 C 3.4380940000 0.4435070000 21.0449440000  
 C 2.7918300000 0.3714660000 19.7936970000  
 C 3.4590450000 0.4327120000 18.5182450000  
 H 4.5231650000 0.5434070000 18.3701100000  
 H 4.5118060000 0.6185560000 23.7229330000  
 H 4.5210930000 0.5619080000 15.3022500000  
 C 0.0000000000 0.0000000000 34.4282120000  
 C 0.2457170000 1.1820070000 35.1453910000  
 C -0.2457170000 -1.1820070000 35.1453910000  
 C 0.2447840000 1.1824180000 36.5416710000

H 0.4315400000 2.1046490000 34.6025960000  
 C -0.2447840000 -1.1824180000 36.5416710000  
 H -0.4315400000 -2.1046490000 34.6025960000  
 C 0.0000000000 0.0000000000 37.2441490000  
 H 0.4322860000 2.1078960000 37.0795430000  
 H -0.4322860000 -2.1078960000 37.0795430000  
 H 0.0000000000 0.0000000000 38.3307240000  
 C -4.9177060000 -0.6656410000 29.4607660000  
 C -5.7798810000 0.3617060000 29.8772400000  
 C -5.4774520000 -1.8838830000 29.0429410000  
 C -7.1636800000 0.1763660000 29.8750210000  
 H -5.3602530000 1.3115540000 30.1967840000  
 C -6.8612930000 -2.0702380000 29.0423280000  
 H -4.8212480000 -2.6888460000 28.7239780000  
 C -7.7087210000 -1.0405540000 29.4580840000  
 H -7.8152460000 0.9848030000 30.1957570000  
 H -7.2758320000 -3.0215530000 28.7196580000  
 H -8.7856370000 -1.1851420000 29.4570820000  
 C -4.9236330000 -0.6346250000 21.0461630000  
 C -5.7775960000 0.3862850000 21.4946570000  
 C -5.4923090000 -1.8384670000 20.5990410000  
 C -7.1623610000 0.2088390000 21.4942490000  
 H -5.3508490000 1.3249530000 21.8365840000  
 C -6.8769810000 -2.0170370000 20.6017640000  
 H -4.8424890000 -2.6385860000 20.2560770000  
 C -7.7163740000 -0.9937010000 21.0486100000  
 H -7.8075430000 1.0123190000 21.8393110000  
 H -7.2985440000 -2.9575470000 20.2573330000  
 H -8.7940760000 -1.1322600000 21.0495290000  
 C -4.9353070000 -0.5402040000 12.6259850000  
 C -5.5296870000 -1.7232740000 12.1571570000  
 C -5.7671590000 0.4903080000 13.0938330000  
 C -6.9177720000 -1.8725190000 12.1582650000  
 H -4.8972500000 -2.5305310000 11.7988600000  
 C -7.1553490000 0.3424020000 13.0911910000  
 H -5.3203860000 1.4132840000 13.4523460000  
 C -7.7349880000 -0.8398410000 12.6243560000  
 H -7.3593750000 -2.7975130000 11.7973470000  
 H -7.7831160000 1.1530640000 13.4512300000  
 H -8.8153880000 -0.9554840000 12.6237570000  
 C -4.9597670000 -0.2269160000 4.2082300000  
 C -5.6267160000 -1.3587800000 3.7111440000  
 C -5.7259750000 0.8404630000 4.7048720000  
 C -7.0212860000 -1.4224700000 3.7130690000  
 H -5.0457800000 -2.1940640000 3.3306680000  
 C -7.1206150000 0.7784690000 4.7024310000  
 H -5.2226570000 1.7246400000 5.0854670000  
 C -7.7726400000 -0.3536310000 4.2076490000  
 H -7.5195510000 -2.3091530000 3.3304440000  
 H -7.6967330000 1.6167930000 5.0847610000  
 H -8.8581100000 -0.4025310000 4.2074660000  
 C -4.9597640000 0.2269830000 -4.2082310000  
 C -5.7259880000 -0.8403840000 -4.7048740000  
 C -5.6266960000 1.3588560000 -3.7111440000  
 C -7.1206270000 -0.7783680000 -4.7024360000  
 H -5.2226830000 -1.7245680000 -5.0854700000  
 C -7.0212650000 1.4225680000 -3.7130700000  
 H -5.0457480000 2.1941310000 -3.3306660000  
 C -7.7726350000 0.3537410000 -4.2076520000  
 H -7.6967580000 -1.6166820000 -5.0847670000  
 H -7.5195160000 2.3092590000 -3.3304450000  
 H -8.8581040000 0.4026580000 -4.2074710000  
 C -4.9353010000 0.5402660000 -12.6259840000

C -5.7671670000 -0.4902340000 -13.0938320000  
 C -5.5296630000 1.7233460000 -12.1571580000  
 C -7.1553550000 -0.3423070000 -13.0911910000  
 H -5.3204080000 -1.4132170000 -13.4523440000  
 C -6.9177460000 1.8726110000 -12.1582660000  
 H -4.8972140000 2.5305930000 -11.7988600000  
 C -7.7349770000 0.8399440000 -12.6243560000  
 H -7.7831340000 -1.1529610000 -13.4512290000  
 H -7.3593350000 2.7976110000 -11.7973490000  
 H -8.8153760000 0.9556030000 -12.6237570000  
 C 4.9353010000 -0.5402660000 -12.6259840000  
 C 5.7671670000 0.4902340000 -13.0938320000  
 C 5.5296630000 -1.7233460000 -12.1571580000  
 C 7.1553550000 0.3423070000 -13.0911910000  
 H 5.3204080000 1.4132170000 -13.4523440000  
 C 6.9177460000 -1.8726110000 -12.1582660000  
 H 4.8972140000 -2.5305930000 -11.7988600000  
 C 7.7349770000 -0.8399440000 -12.6243560000  
 H 7.7831340000 1.1529610000 -13.4512290000  
 H 7.3593350000 -2.7976110000 -11.7973490000  
 H 8.8153760000 -0.9556030000 -12.6237570000  
 C 4.9177060000 0.6656410000 29.4607660000  
 C 5.7798810000 -0.3617060000 29.8772400000  
 C 5.4774520000 1.8838830000 29.0429410000  
 C 7.1636800000 -0.1763660000 29.8750210000  
 H 5.3602530000 -1.3115540000 30.1967840000  
 C 6.8612930000 2.0702380000 29.0423280000  
 H 4.8212480000 2.6888460000 28.7239780000  
 C 7.7087210000 1.0405540000 29.4580840000  
 H 7.8152460000 -0.9848030000 30.1957570000  
 H 7.2758320000 3.0215530000 28.7196580000  
 H 8.7856370000 1.1851420000 29.4570820000  
 C 4.9236330000 0.6346250000 21.0461630000  
 C 5.7775960000 -0.3862850000 21.4946570000  
 C 5.4923090000 1.8384670000 20.5990410000  
 C 7.1623610000 -0.2088390000 21.4942490000  
 H 5.3508490000 -1.3249530000 21.8365840000  
 C 6.8769810000 2.0170370000 20.6017640000  
 H 4.8424890000 2.6385860000 20.2560770000  
 C 7.7163740000 0.9937010000 21.0486100000  
 H 7.8075430000 -1.0123190000 21.8393110000  
 H 7.2985440000 2.9575470000 20.2573330000  
 H 8.7940760000 1.1322600000 21.0495290000  
 C 4.9353070000 0.5402040000 12.6259850000  
 C 5.5296870000 1.7232740000 12.1571570000  
 C 5.7671590000 -0.4903080000 13.0938330000  
 C 6.9177720000 1.8725190000 12.1582650000  
 H 4.8972500000 2.5305310000 11.7988600000  
 C 7.1553490000 -0.3424020000 13.0911910000  
 H 5.3203860000 -1.4132840000 13.4523460000  
 C 7.7349880000 0.8398410000 12.6243560000  
 H 7.3593750000 2.7975130000 11.7973470000  
 H 7.7831160000 -1.1530640000 13.4512300000  
 H 8.8153880000 0.9554840000 12.6237570000  
 C 4.9597670000 0.2269160000 4.2082300000  
 C 5.6267160000 1.3587800000 3.7111440000  
 C 5.7259750000 -0.8404630000 4.7048720000  
 C 7.0212860000 1.4224700000 3.7130690000  
 H 5.0457800000 2.1940640000 3.3306680000  
 C 7.1206150000 -0.7784690000 4.7024310000  
 H 5.2226570000 -1.7246400000 5.0854670000  
 C 7.7726400000 0.3536310000 4.2076490000  
 H 7.5195510000 2.3091530000 3.3304440000

H 7.6967330000 -1.6167930000 5.0847610000  
 H 8.8581100000 0.4025310000 4.2074660000  
 C 4.9597640000 -0.2269830000 -4.2082310000  
 C 5.7259880000 0.8403840000 -4.7048740000  
 C 5.6266960000 -1.3588560000 -3.7111440000  
 C 7.1206270000 0.7783680000 -4.7024360000  
 H 5.2226830000 1.7245680000 -5.0854700000  
 C 7.0212650000 -1.4225680000 -3.7130700000  
 H 5.0457480000 -2.1941310000 -3.3306660000  
 C 7.7726350000 -0.3537410000 -4.2076520000  
 H 7.6967580000 1.6166820000 -5.0847670000  
 H 7.5195160000 -2.3092590000 -3.3304450000  
 H 8.8581040000 -0.4026580000 -4.2074710000  
 C 2.5063170000 -0.3366890000 -32.9571180000  
 C 1.2405530000 -0.1722060000 -32.2798470000  
 N 1.4405350000 -0.1934880000 -30.9188950000  
 Zn 0.0000000000 0.0000000000 -29.4761350000  
 N 1.4282560000 -0.2101970000 -28.0263560000  
 C 1.2272010000 -0.1741720000 -26.6780280000  
 C 2.4807460000 -0.3349680000 -25.9749190000  
 C 2.4817550000 -0.3249790000 -24.5378850000  
 C 1.2327320000 -0.1518310000 -23.8370390000  
 N 1.4380260000 -0.1676850000 -22.4879380000  
 Zn 0.0000000000 0.0000000000 -21.0448300000  
 N -1.4380260000 0.1676850000 -22.4879380000  
 C -1.2327320000 0.1518310000 -23.8370390000  
 C 0.0000000000 0.0000000000 -24.5185540000  
 C 0.0000000000 0.0000000000 -25.9951100000  
 C -1.2272010000 0.1741720000 -26.6780280000  
 N -1.4282560000 0.2101970000 -28.0263560000  
 C -2.7857190000 0.3890780000 -28.2147330000  
 C -3.4322630000 0.4662560000 -29.4609950000  
 C -2.7870320000 0.3717520000 -30.7169260000  
 N -1.4405350000 0.1934880000 -30.9188950000  
 C -1.2405530000 0.1722060000 -32.2798470000  
 C 0.0000000000 0.0000000000 -32.9290070000  
 C -2.5063170000 0.3366890000 -32.9571180000  
 C -3.4596020000 0.4711370000 -31.9919540000  
 H -4.5199550000 0.6222840000 -32.1314540000  
 C -3.4524720000 0.4600470000 -26.9363350000  
 C -2.4807460000 0.3349680000 -25.9749190000  
 C -2.4817550000 0.3249790000 -24.5378850000  
 C -3.4542480000 0.4571790000 -23.5742640000  
 C -2.7932900000 0.3493210000 -22.2990730000  
 C -3.4380970000 0.4434800000 -21.0449430000  
 C -2.7918320000 0.3714510000 -19.7936970000  
 N -1.4323230000 0.2042500000 -19.6031660000  
 C -1.2319030000 0.1661370000 -18.2555860000  
 C 0.0000000000 0.0000000000 -17.5717580000  
 C 1.2319030000 -0.1661370000 -18.2555860000  
 N 1.4323230000 -0.2042500000 -19.6031660000  
 C 2.7918320000 -0.3714510000 -19.7936970000  
 C 3.4380970000 -0.4434800000 -21.0449430000  
 C 2.7932900000 -0.3493210000 -22.2990730000  
 C 3.4542480000 -0.4571790000 -23.5742640000  
 H 4.5118150000 -0.6184940000 -23.7229320000  
 C 3.4590460000 -0.4327050000 -18.5182450000  
 C 2.4855400000 -0.3136770000 -17.5543110000  
 H 4.5231660000 -0.5433980000 -18.3701100000  
 C -2.4855400000 0.3136770000 -17.5543110000  
 C -3.4590460000 0.4327050000 -18.5182450000  
 H -4.5231660000 0.5433980000 -18.3701100000  
 H -4.5118150000 0.6184940000 -23.7229320000

H -4.5155070000 0.5820670000 -26.7889730000  
 C 3.4524720000 -0.4600470000 -26.9363350000  
 C 2.7857190000 -0.3890780000 -28.2147330000  
 C 3.4322630000 -0.4662560000 -29.4609950000  
 C 2.7870320000 -0.3717520000 -30.7169260000  
 C 3.4596020000 -0.4711370000 -31.9919540000  
 H 4.5199550000 -0.6222840000 -32.1314540000  
 H 4.5155070000 -0.5820670000 -26.7889730000  
 C 0.0000000000 0.0000000000 -34.4282120000  
 C 0.2457520000 -1.1819990000 -35.1453910000  
 C -0.2457520000 1.1819990000 -35.1453910000  
 C 0.2448200000 -1.1824110000 -36.5416710000  
 H 0.4316030000 -2.1046370000 -34.6025960000  
 C -0.2448200000 1.1824110000 -36.5416710000  
 H -0.4316030000 2.1046370000 -34.6025960000  
 C 0.0000000000 0.0000000000 -37.2441490000  
 H 0.4323490000 -2.1078830000 -37.0795430000  
 H -0.4323490000 2.1078830000 -37.0795430000  
 H 0.0000000000 0.0000000000 -38.3307240000  
 C -4.9236380000 0.6345890000 -21.0461630000  
 C -5.4923190000 1.8384290000 -20.5990460000  
 C -5.7775960000 -0.3863280000 -21.4946510000  
 C -6.8769930000 2.0169920000 -20.6017680000  
 H -4.8425030000 2.6385530000 -20.2560850000  
 C -7.1623610000 -0.2088890000 -21.4942430000  
 H -5.3508430000 -1.3249950000 -21.8365740000  
 C -7.7163800000 0.9936500000 -21.0486090000  
 H -7.2985600000 2.9575020000 -20.2573410000  
 H -7.8075400000 -1.0123750000 -21.8393010000  
 H -8.7940830000 1.1322030000 -21.0495290000  
 C -4.9177200000 0.6655410000 -29.4607660000  
 C -5.4774850000 1.8837740000 -29.0429410000  
 C -5.7798770000 -0.3618210000 -29.8772380000  
 C -6.8613290000 2.0701060000 -29.0423280000  
 H -4.8212940000 2.6887480000 -28.7239780000  
 C -7.1636800000 -0.1765030000 -29.8750190000  
 H -5.3602340000 -1.3116620000 -30.1967820000  
 C -7.7087410000 1.0404080000 -29.4580830000  
 H -7.2758840000 3.0214150000 -28.7196580000  
 H -7.8152320000 -0.9849510000 -30.1957550000  
 H -8.7856590000 1.1849790000 -29.4570810000  
 C 4.9236380000 -0.6345890000 -21.0461630000  
 C 5.4923190000 -1.8384290000 -20.5990460000  
 C 5.7775960000 0.3863280000 -21.4946510000  
 C 6.8769930000 -2.0169920000 -20.6017680000  
 H 4.8425030000 -2.6385530000 -20.2560850000  
 C 7.1623610000 0.2088890000 -21.4942430000  
 H 5.3508430000 1.3249950000 -21.8365740000  
 C 7.7163800000 -0.9936500000 -21.0486090000  
 H 7.2985600000 -2.9575020000 -20.2573410000  
 H 7.8075400000 1.0123750000 -21.8393010000  
 H 8.7940830000 -1.1322030000 -21.0495290000  
 C 4.9177200000 -0.6655410000 -29.4607660000  
 C 5.4774850000 -1.8837740000 -29.0429410000  
 C 5.7798770000 0.3618210000 -29.8772380000  
 C 6.8613290000 -2.0701060000 -29.0423280000  
 H 4.8212940000 -2.6887480000 -28.7239780000  
 C 7.1636800000 0.1765030000 -29.8750190000  
 H 5.3602340000 1.3116620000 -30.1967820000  
 C 7.7087410000 -1.0404080000 -29.4580830000  
 H 7.2758840000 -3.0214150000 -28.7196580000  
 H 7.8152320000 0.9849510000 -30.1957550000  
 H 8.7856590000 -1.1849790000 -29.4570810000

H 2.6476420000 -0.3500180000 -34.0278970000  
H -2.6476420000 0.3500180000 -34.0278970000

**Table S9.** Optimized coordinates for **10**.

Zn 0.0000000000 0.0000000000 21.0446950000  
N 0.2029440000 -1.4325070000 19.6015650000  
C 0.1650890000 -1.2328700000 18.2542180000  
C 0.0000000000 0.0000000000 17.5693910000  
C -0.1650890000 1.2328700000 18.2542180000  
N -0.2029440000 1.4325070000 19.6015650000  
C -0.3676320000 2.7926200000 19.7921240000  
C -0.4368950000 3.4387900000 21.0443230000  
C -0.3429390000 2.7954440000 22.2982720000  
N -0.1648830000 1.4382390000 22.4881650000  
C -0.1488740000 1.2348210000 23.8362380000  
C 0.0000000000 0.0000000000 24.5199770000  
C 0.1488740000 -1.2348210000 23.8362380000  
N 0.1648830000 -1.4382390000 22.4881650000  
C 0.3429390000 -2.7954440000 22.2982720000  
C 0.4368950000 -3.4387900000 21.0443230000  
C 0.3676320000 -2.7926200000 19.7921240000  
C 0.4282340000 -3.4601050000 18.5180280000  
C 0.3109420000 -2.4861440000 17.5533410000  
C 0.2969320000 -2.4877410000 16.1177500000  
C 0.1384040000 -1.2366410000 15.4170180000  
N 0.1472630000 -1.4404100000 14.0694700000  
Zn 0.0000000000 0.0000000000 12.6254160000  
N 0.1812100000 -1.4363980000 11.1824480000  
C 0.1308530000 -1.2375970000 9.8354830000  
C 0.0000000000 0.0000000000 9.1506480000  
C -0.1308530000 1.2375970000 9.8354830000  
N -0.1812100000 1.4363980000 11.1824480000  
C -0.3094250000 2.8004310000 11.3729580000  
C -0.3786000000 3.4464970000 12.6258000000  
C -0.3069470000 2.8005810000 13.8795010000  
N -0.1472630000 1.4404100000 14.0694700000  
C -0.1384040000 1.2366410000 15.4170180000  
C 0.0000000000 0.0000000000 16.1015490000  
C -0.2969320000 2.4877410000 16.1177500000  
C -0.3109420000 2.4861440000 17.5533410000  
C -0.4282340000 3.4601050000 18.5180280000  
H -0.5371150000 4.5244050000 18.3699990000  
C -0.4113160000 3.4625370000 15.1528730000  
H -0.5581480000 4.5221880000 15.3012890000  
C -0.3314260000 3.4711640000 10.0998450000  
C -0.2277230000 2.4954400000 9.1348670000  
C -0.1900290000 2.4986690000 7.6997570000  
C -0.0793800000 1.2422300000 6.9994130000  
N -0.0594030000 1.4472090000 5.6526490000  
Zn 0.0000000000 0.0000000000 4.2080170000  
N 0.0804530000 -1.4464050000 2.7639380000  
C 0.0329090000 -1.2444670000 1.4175620000  
C 0.0000000000 0.0000000000 0.7329920000  
C -0.0329090000 1.2444670000 1.4175620000  
N -0.0804530000 1.4464050000 2.7639380000  
C -0.1122770000 2.8158150000 2.9548630000  
C -0.1595760000 3.4639570000 4.2082840000  
C -0.1473100000 2.8140720000 5.4619530000

C -0.2407310000 3.4789420000 6.7347050000  
 H -0.3370440000 4.5444190000 6.8827730000  
 C -0.0683930000 3.4866810000 1.6824520000  
 C -0.0260300000 2.5060610000 0.7173770000  
 C 0.0258660000 2.5060640000 -0.7173790000  
 C 0.0328170000 1.2444700000 -1.4175640000  
 N 0.0803430000 1.4464090000 -2.7639390000  
 Zn 0.0000000000 0.0000000000 -4.2080360000  
 N -0.0593100000 -1.4472140000 -5.6526500000  
 C -0.0793240000 -1.2422330000 -6.9994140000  
 C 0.0000000000 0.0000000000 -7.6840910000  
 C 0.0793240000 1.2422330000 -6.9994140000  
 N 0.0593100000 1.4472140000 -5.6526500000  
 C 0.1471620000 2.8140810000 -5.4619540000  
 C 0.1593680000 3.4639650000 -4.2082830000  
 C 0.1120910000 2.8158210000 -2.9548640000  
 C 0.0681710000 3.4866850000 -1.6824540000  
 H 0.0636390000 4.5565800000 -1.5348310000  
 C 0.2405740000 3.4789540000 -6.7347050000  
 C 0.1899350000 2.4986770000 -7.6997560000  
 H 0.3368410000 4.5444350000 -6.8827730000  
 C -0.1899350000 -2.4986770000 -7.6997560000  
 C -0.2405740000 -3.4789540000 -6.7347050000  
 C -0.1471620000 -2.8140810000 -5.4619540000  
 C -0.1593680000 -3.4639650000 -4.2082830000  
 C -0.1120910000 -2.8158210000 -2.9548640000  
 N -0.0803430000 -1.4464090000 -2.7639390000  
 C -0.0328170000 -1.2444700000 -1.4175640000  
 C -0.0258660000 -2.5060640000 -0.7173790000  
 C 0.0260300000 -2.5060610000 0.7173770000  
 C 0.0683930000 -3.4866810000 1.6824520000  
 C 0.1122770000 -2.8158150000 2.9548630000  
 C 0.1595760000 -3.4639570000 4.2082840000  
 C 0.1473100000 -2.8140720000 5.4619530000  
 N 0.0594030000 -1.4472090000 5.6526490000  
 C 0.0793800000 -1.2422300000 6.9994130000  
 C 0.1900290000 -2.4986690000 7.6997570000  
 C 0.2277230000 -2.4954400000 9.1348670000  
 C 0.3314260000 -3.4711640000 10.0998450000  
 C 0.3094250000 -2.8004310000 11.3729580000  
 C 0.3786000000 -3.4464970000 12.6258000000  
 C 0.3069470000 -2.8005810000 13.8795010000  
 C 0.4113160000 -3.4625370000 15.1528730000  
 H 0.5581480000 -4.5221880000 15.3012890000  
 H 0.4073980000 -4.5383470000 9.9520950000  
 C 0.2407310000 -3.4789420000 6.7347050000  
 H 0.3370440000 -4.5444190000 6.8827730000  
 C 0.0000000000 0.0000000000 7.6840910000  
 H 0.0639320000 -4.5565750000 1.5348280000  
 C -0.0681710000 -3.4866850000 -1.6824540000  
 H -0.0636390000 -4.5565800000 -1.5348310000  
 C 0.0000000000 0.0000000000 -0.7329930000  
 H -0.3368410000 -4.5444350000 -6.8827730000  
 H -0.0639320000 4.5565750000 1.5348280000  
 H -0.4073980000 4.5383470000 9.9520950000  
 H 0.5371150000 -4.5244050000 18.3699990000  
 C 0.4476490000 -3.4573670000 23.5719950000  
 C 0.3175530000 -2.4847700000 24.5367770000  
 C 0.3266350000 -2.4840000000 25.9727660000  
 C 0.1711600000 -1.2313160000 26.6740970000  
 N 0.2068950000 -1.4318410000 28.0215880000  
 Zn 0.0000000000 0.0000000000 29.4632970000  
 N 0.1695860000 -1.4377800000 30.9064700000

C 0.1528090000 -1.2326930000 32.2555750000  
 C 0.3270230000 -2.4815180000 32.9563450000  
 C 0.3363590000 -2.4806170000 34.3933630000  
 C 0.1746990000 -1.2271770000 35.0964920000  
 N 0.2104240000 -1.4281980000 36.4447620000  
 Zn 0.0000000000 0.0000000000 37.8945350000  
 N -0.2104240000 1.4281980000 36.4447620000  
 C -0.1746990000 1.2271770000 35.0964920000  
 C 0.0000000000 0.0000000000 34.4135250000  
 C 0.0000000000 0.0000000000 32.9371600000  
 C -0.1528090000 1.2326930000 32.2555750000  
 N -0.1695860000 1.4377800000 30.9064700000  
 C -0.3535310000 2.7926980000 30.7175850000  
 C -0.4510780000 3.4370120000 29.4633170000  
 C -0.3795250000 2.7907910000 28.2121820000  
 N -0.2068950000 1.4318410000 28.0215880000  
 C -0.1711600000 1.2313160000 26.6740970000  
 C 0.0000000000 0.0000000000 25.9901580000  
 C -0.3266350000 2.4840000000 25.9727660000  
 C -0.3175530000 2.4847700000 24.5367770000  
 C -0.4476490000 3.4573670000 23.5719950000  
 H -0.6061060000 4.5153940000 23.7202290000  
 C -0.4471980000 3.4573130000 26.9367080000  
 H -0.5628750000 4.5208920000 26.7885200000  
 C -0.4612330000 3.4537310000 31.9926460000  
 C -0.3270230000 2.4815180000 32.9563450000  
 C -0.3363590000 2.4806170000 34.3933630000  
 C -0.4615450000 3.4523240000 35.3547580000  
 C -0.3898780000 2.7856390000 36.6331750000  
 C -0.4669550000 3.4321620000 37.8793650000  
 C -0.3720630000 2.7869490000 39.1353950000  
 N -0.1935810000 1.4405330000 39.3373280000  
 C -0.1722320000 1.2405760000 40.6982980000  
 C 0.0000000000 0.0000000000 41.3474380000  
 C 0.1722320000 -1.2405760000 40.6982980000  
 N 0.1935810000 -1.4405330000 39.3373280000  
 C 0.3720630000 -2.7869490000 39.1353950000  
 C 0.4669550000 -3.4321620000 37.8793650000  
 C 0.3898780000 -2.7856390000 36.6331750000  
 C 0.4615450000 -3.4523240000 35.3547580000  
 H 0.5839950000 -4.5153050000 35.2073780000  
 C 0.4714030000 -3.4595590000 40.4103720000  
 C 0.3367490000 -2.5063050000 41.3755610000  
 H 0.3499510000 -2.6476790000 42.4463310000  
 H 0.6226640000 -4.5198910000 40.5498730000  
 C -0.3367490000 2.5063050000 41.3755610000  
 C -0.4714030000 3.4595590000 40.4103720000  
 H -0.6226640000 4.5198910000 40.5498730000  
 H -0.3499510000 2.6476790000 42.4463310000  
 H -0.5839950000 4.5153050000 35.2073780000  
 H -0.6239900000 4.5110810000 32.1412710000  
 C 0.4612330000 -3.4537310000 31.9926460000  
 C 0.3535310000 -2.7926980000 30.7175850000  
 C 0.4510780000 -3.4370120000 29.4633170000  
 C 0.3795250000 -2.7907910000 28.2121820000  
 C 0.4471980000 -3.4573130000 26.9367080000  
 H 0.5628750000 -4.5208920000 26.7885200000  
 H 0.6239900000 -4.5110810000 32.1412710000  
 H 0.6061060000 -4.5153940000 23.7202290000  
 C 0.0000000000 0.0000000000 42.8466220000  
 C 1.1819510000 -0.2460600000 43.5637780000  
 C -1.1819510000 0.2460600000 43.5637780000  
 C 1.1823560000 -0.2450990000 44.9600520000

H 2.1045450000 -0.4321310000 43.0209880000  
 C -1.1823560000 0.2450990000 44.9600520000  
 H -2.1045450000 0.4321310000 43.0209880000  
 C 0.0000000000 0.0000000000 45.6625230000  
 H 2.1077830000 -0.4328370000 45.4979240000  
 H -2.1077830000 0.4328370000 45.4979240000  
 H 0.0000000000 0.0000000000 46.7490950000  
 C -0.6667000000 4.9175350000 37.8792040000  
 C 0.3603900000 5.7799810000 38.2957470000  
 C -1.8851260000 5.4769110000 37.4614110000  
 C 0.1746280000 7.1637190000 38.2935710000  
 H 1.3103700000 5.3606380000 38.6152690000  
 C -2.0718980000 6.8606920000 37.4608840000  
 H -2.6898990000 4.8204780000 37.1424420000  
 C -1.0424620000 7.7084080000 37.8766670000  
 H 0.9828690000 7.8155120000 38.6143290000  
 H -3.0233420000 7.2749560000 37.1382490000  
 H -1.1873760000 8.7852770000 37.8757220000  
 C -0.6462730000 4.9220300000 29.4647260000  
 C 0.3737380000 5.7787910000 29.9098760000  
 C -1.8530660000 5.4872890000 29.0212960000  
 C 0.1925430000 7.1630680000 29.9097130000  
 H 1.3146050000 5.3546470000 30.2489910000  
 C -2.0353640000 6.8714770000 29.0243060000  
 H -2.6524990000 4.8352270000 28.6809970000  
 C -1.0128940000 7.7137210000 29.4677460000  
 H 0.9953460000 7.8104970000 30.2521250000  
 H -2.9780850000 7.2904240000 28.6827440000  
 H -1.1543600000 8.7910420000 29.4688730000  
 C -0.6241610000 4.9247900000 21.0447150000  
 C -1.8271250000 5.4960610000 20.5986380000  
 C 0.3996970000 5.7762040000 21.4912030000  
 C -2.0020910000 6.8811700000 20.6008120000  
 H -2.6293340000 4.8480800000 20.2571280000  
 C 0.2259240000 7.1614240000 21.4897080000  
 H 1.3375600000 5.3471700000 21.8323860000  
 C -0.9758400000 7.7181930000 21.0454480000  
 H -2.9420240000 7.3049330000 20.2575310000  
 H 1.0315920000 7.8047550000 21.8330970000  
 H -1.1115760000 8.7962520000 21.0457300000  
 C -0.5366650000 4.9356450000 12.6254560000  
 C -1.7192660000 5.5308020000 12.1564700000  
 C 0.4945650000 5.7665870000 13.0932930000  
 C -1.8674140000 6.9189880000 12.1576150000  
 H -2.5269860000 4.8989800000 11.7981690000  
 C 0.3478020000 7.1548880000 13.0903580000  
 H 1.4171070000 5.3190700000 13.4519480000  
 C -0.8340190000 7.7353960000 12.6235490000  
 H -2.7920870000 7.3613030000 11.7967680000  
 H 1.1589810000 7.7820390000 13.4502840000  
 H -0.9488010000 8.8158850000 12.6228570000  
 C -0.2262310000 4.9597570000 4.2080630000  
 C -1.3580280000 5.6267360000 3.7109050000  
 C 0.8413000000 5.7257160000 4.7047180000  
 C -1.4215420000 7.0213040000 3.7129220000  
 H -2.1933520000 5.0458960000 3.3303970000  
 C 0.7795250000 7.1203580000 4.7021040000  
 H 1.7253580000 5.2222640000 5.0853810000  
 C -0.3525380000 7.7724980000 4.2073920000  
 H -2.3081850000 7.5196880000 3.3303750000  
 H 1.6179540000 7.6963740000 5.0843380000  
 H -0.4012860000 8.8579710000 4.2071800000  
 C 0.2259320000 4.9597690000 -4.2080630000

C -0.8416410000 5.7256620000 -4.7047300000  
 C 1.3576810000 5.6268190000 -3.7108910000  
 C -0.7799540000 7.1203080000 -4.7021150000  
 H -1.7256640000 5.2221550000 -5.0854040000  
 C 1.4211080000 7.0213910000 -3.7129070000  
 H 2.1930360000 5.0460310000 -3.3303710000  
 C 0.3520630000 7.7725180000 -4.2073890000  
 H -1.6184140000 7.6962720000 -5.0843580000  
 H 2.3077150000 7.5198300000 -3.3303480000  
 H 0.4007430000 8.8579940000 -4.2071760000  
 C -0.2259320000 -4.9597690000 -4.2080630000  
 C 0.8416410000 -5.7256620000 -4.7047300000  
 C -1.3576810000 -5.6268190000 -3.7108910000  
 C 0.7799540000 -7.1203080000 -4.7021150000  
 H 1.7256640000 -5.2221550000 -5.0854040000  
 C -1.4211080000 -7.0213910000 -3.7129070000  
 H -2.1930360000 -5.0460310000 -3.3303710000  
 C -0.3520630000 -7.7725180000 -4.2073890000  
 H 1.6184140000 -7.6962720000 -5.0843580000  
 H -2.3077150000 -7.5198300000 -3.3303480000  
 H -0.4007430000 -8.8579940000 -4.2071760000  
 C 0.6667000000 -4.9175350000 37.8792040000  
 C -0.3603900000 -5.7799810000 38.2957470000  
 C 1.8851260000 -5.4769110000 37.4614110000  
 C -0.1746280000 -7.1637190000 38.2935710000  
 H -1.3103700000 -5.3606380000 38.6152690000  
 C 2.0718980000 -6.8606920000 37.4608840000  
 H 2.6898990000 -4.8204780000 37.1424420000  
 C 1.0424620000 -7.7084080000 37.8766670000  
 H -0.9828690000 -7.8155120000 38.6143290000  
 H 3.0233420000 -7.2749560000 37.1382490000  
 H 1.1873760000 -8.7852770000 37.8757220000  
 C 0.6462730000 -4.9220300000 29.4647260000  
 C -0.3737380000 -5.7787910000 29.9098760000  
 C 1.8530660000 -5.4872890000 29.0212960000  
 C -0.1925430000 -7.1630680000 29.9097130000  
 H -1.3146050000 -5.3546470000 30.2489910000  
 C 2.0353640000 -6.8714770000 29.0243060000  
 H 2.6524990000 -4.8352270000 28.6809970000  
 C 1.0128940000 -7.7137210000 29.4677460000  
 H -0.9953460000 -7.8104970000 30.2521250000  
 H 2.9780850000 -7.2904240000 28.6827440000  
 H 1.1543600000 -8.7910420000 29.4688730000  
 C 0.6241610000 -4.9247900000 21.0447150000  
 C 1.8271250000 -5.4960610000 20.5986380000  
 C -0.3996970000 -5.7762040000 21.4912030000  
 C 2.0020910000 -6.8811700000 20.6008120000  
 H 2.6293340000 -4.8480800000 20.2571280000  
 C -0.2259240000 -7.1614240000 21.4897080000  
 H -1.3375600000 -5.3471700000 21.8323860000  
 C 0.9758400000 -7.7181930000 21.0454480000  
 H 2.9420240000 -7.3049330000 20.2575310000  
 H -1.0315920000 -7.8047550000 21.8330970000  
 H 1.1115760000 -8.7962520000 21.0457300000  
 C 0.5366650000 -4.9356450000 12.6254560000  
 C 1.7192660000 -5.5308020000 12.1564700000  
 C -0.4945650000 -5.7665870000 13.0932930000  
 C 1.8674140000 -6.9189880000 12.1576150000  
 H 2.5269860000 -4.8989800000 11.7981690000  
 C -0.3478020000 -7.1548880000 13.0903580000  
 H -1.4171070000 -5.3190700000 13.4519480000  
 C 0.8340190000 -7.7353960000 12.6235490000  
 H 2.7920870000 -7.3613030000 11.7967680000

H -1.1589810000 -7.7820390000 13.4502840000  
 H 0.9488010000 -8.8158850000 12.6228570000  
 C 0.2262310000 -4.9597570000 4.2080630000  
 C 1.3580280000 -5.6267360000 3.7109050000  
 C -0.8413000000 -5.7257160000 4.7047180000  
 C 1.4215420000 -7.0213040000 3.7129220000  
 H 2.1933520000 -5.0458960000 3.3303970000  
 C -0.7795250000 -7.1203580000 4.7021040000  
 H -1.7253580000 -5.2222640000 5.0853810000  
 C 0.3525380000 -7.7724980000 4.2073920000  
 H 2.3081850000 -7.5196880000 3.3303750000  
 H -1.6179540000 -7.6963740000 5.0843380000  
 H 0.4012860000 -8.8579710000 4.2071800000  
 Zn 0.0000000000 0.0000000000 -29.4632990000  
 N -0.1696010000 -1.4377800000 -30.9064700000  
 C -0.1528340000 -1.2326910000 -32.2555750000  
 C 0.0000000000 0.0000000000 -32.9371590000  
 C 0.1528340000 1.2326910000 -32.2555750000  
 N 0.1696010000 1.4377800000 -30.9064700000  
 C 0.3536000000 2.7926920000 -30.7175860000  
 C 0.4511660000 3.4370030000 -29.4633170000  
 C 0.3796020000 2.7907820000 -28.2121820000  
 N 0.2069250000 1.4318360000 -28.0215890000  
 C 0.1711940000 1.2313110000 -26.6740980000  
 C 0.0000000000 0.0000000000 -25.9901600000  
 C -0.1711940000 -1.2313110000 -26.6740980000  
 N -0.2069250000 -1.4318360000 -28.0215890000  
 C -0.3796020000 -2.7907820000 -28.2121820000  
 C -0.4511660000 -3.4370030000 -29.4633170000  
 C -0.3536000000 -2.7926920000 -30.7175860000  
 C -0.4613280000 -3.4537200000 -31.9926470000  
 C -0.3270910000 -2.4815100000 -32.9563460000  
 C -0.3364200000 -2.4806080000 -34.3933630000  
 C -0.1747300000 -1.2271730000 -35.0964920000  
 N -0.2104560000 -1.4281940000 -36.4447630000  
 Zn 0.0000000000 0.0000000000 -37.8945340000  
 N -0.1935900000 -1.4405340000 -39.3373270000  
 C -0.1722500000 -1.2405740000 -40.6982980000  
 C 0.0000000000 0.0000000000 -41.3474390000  
 C 0.1722500000 1.2405740000 -40.6982980000  
 N 0.1935900000 1.4405340000 -39.3373270000  
 C 0.3721200000 2.7869430000 -39.1353950000  
 C 0.4670330000 3.4321530000 -37.8793650000  
 C 0.3899460000 2.7856300000 -36.6331750000  
 N 0.2104560000 1.4281940000 -36.4447630000  
 C 0.1747300000 1.2271730000 -35.0964920000  
 C 0.0000000000 0.0000000000 -34.4135250000  
 C 0.3364200000 2.4806080000 -34.3933630000  
 C 0.3270910000 2.4815100000 -32.9563460000  
 C 0.4613280000 3.4537200000 -31.9926470000  
 H 0.6241180000 4.5110630000 -32.1412730000  
 C 0.4616240000 3.4523130000 -35.3547580000  
 H 0.5840950000 4.5152910000 -35.2073810000  
 C 0.4715050000 3.4595460000 -40.4103710000  
 C 0.3368320000 2.5062920000 -41.3755600000  
 C -0.3368320000 -2.5062920000 -41.3755600000  
 C -0.4715050000 -3.4595460000 -40.4103710000  
 C -0.3721200000 -2.7869430000 -39.1353950000  
 C -0.4670330000 -3.4321530000 -37.8793650000  
 C -0.3899460000 -2.7856300000 -36.6331750000  
 C -0.4616240000 -3.4523130000 -35.3547580000  
 H -0.5840950000 -4.5152910000 -35.2073810000  
 H -0.6228070000 -4.5198730000 -40.5498640000

H 0.6228070000 4.5198730000 -40.5498640000  
 H -0.6241180000 -4.5110630000 -32.1412730000  
 C -0.4472960000 -3.4573020000 -26.9367070000  
 C -0.3267060000 -2.4839910000 -25.9727670000  
 C -0.3176220000 -2.4847600000 -24.5367780000  
 C -0.1489000000 -1.2348190000 -23.8362400000  
 N -0.1649190000 -1.4382340000 -22.4881660000  
 Zn 0.0000000000 0.0000000000 -21.0446990000  
 N -0.2029740000 -1.4325010000 -19.6015660000  
 C -0.1651080000 -1.2328670000 -18.2542200000  
 C -0.3109800000 -2.4861390000 -17.5533410000  
 C -0.2969510000 -2.4877370000 -16.1177510000  
 C -0.1383920000 -1.2366430000 -15.4170190000  
 N -0.1472210000 -1.4404140000 -14.0694720000  
 Zn 0.0000000000 0.0000000000 -12.6254140000  
 N 0.1472210000 1.4404140000 -14.0694720000  
 C 0.1383920000 1.2366430000 -15.4170190000  
 C 0.0000000000 0.0000000000 -16.1015500000  
 C 0.0000000000 0.0000000000 -17.5693920000  
 C 0.1651080000 1.2328670000 -18.2542200000  
 N 0.2029740000 1.4325010000 -19.6015660000  
 C 0.3677010000 2.7926110000 -19.7921240000  
 C 0.4369860000 3.4387770000 -21.0443230000  
 C 0.3430110000 2.7954360000 -22.2982740000  
 N 0.1649190000 1.4382340000 -22.4881660000  
 C 0.1489000000 1.2348190000 -23.8362400000  
 C 0.0000000000 0.0000000000 -24.5199800000  
 C 0.3176220000 2.4847600000 -24.5367780000  
 C 0.3267060000 2.4839910000 -25.9727670000  
 C 0.4472960000 3.4573020000 -26.9367070000  
 H 0.5629950000 4.5208770000 -26.7885190000  
 C 0.4477480000 3.4573530000 -23.5719960000  
 H 0.6062420000 4.5153740000 -23.7202310000  
 C 0.4282970000 3.4600960000 -18.5180290000  
 C 0.3109800000 2.4861390000 -17.5533410000  
 C 0.2969510000 2.4877370000 -16.1177510000  
 C 0.4113240000 3.4625340000 -15.1528740000  
 C 0.3069160000 2.8005850000 -13.8795020000  
 C 0.3785560000 3.4465020000 -12.6258000000  
 C 0.3093810000 2.8004360000 -11.3729580000  
 N 0.1811940000 1.4364000000 -11.1824470000  
 C 0.1308220000 1.2376010000 -9.8354820000  
 C 0.0000000000 0.0000000000 -9.1506480000  
 C -0.1308220000 -1.2376010000 -9.8354820000  
 N -0.1811940000 -1.4364000000 -11.1824470000  
 C -0.3093810000 -2.8004360000 -11.3729580000  
 C -0.3785560000 -3.4465020000 -12.6258000000  
 C -0.3069160000 -2.8005850000 -13.8795020000  
 C -0.4113240000 -3.4625340000 -15.1528740000  
 H -0.5581720000 -4.5221830000 -15.3012930000  
 C -0.3313320000 -3.4711710000 -10.0998450000  
 C -0.2276460000 -2.4954470000 -9.1348660000  
 H -0.4072660000 -4.5383580000 -9.9520940000  
 C 0.2276460000 2.4954470000 -9.1348660000  
 C 0.3313320000 3.4711710000 -10.0998450000  
 H 0.4072660000 4.5383580000 -9.9520940000  
 H 0.5581720000 4.5221830000 -15.3012930000  
 H 0.5371910000 4.5243940000 -18.3700020000  
 C -0.4282970000 -3.4600960000 -18.5180290000  
 C -0.3677010000 -2.7926110000 -19.7921240000  
 C -0.4369860000 -3.4387770000 -21.0443230000  
 C -0.3430110000 -2.7954360000 -22.2982740000  
 C -0.4477480000 -3.4573530000 -23.5719960000

H -0.6062420000 -4.5153740000 -23.7202310000  
 H -0.5371910000 -4.5243940000 -18.3700020000  
 H -0.5629950000 -4.5208770000 -26.7885190000  
 C 0.0000000000 0.0000000000 -42.8466230000  
 C -1.1819670000 -0.2459820000 -43.5637770000  
 C 1.1819670000 0.2459820000 -43.5637770000  
 C -1.1823720000 -0.2450210000 -44.9600520000  
 H -2.1045730000 -0.4319940000 -43.0209870000  
 C 1.1823720000 0.2450210000 -44.9600520000  
 H 2.1045730000 0.4319940000 -43.0209870000  
 C 0.0000000000 0.0000000000 -45.6625220000  
 H -2.1078100000 -0.4327010000 -45.4979250000  
 H 2.1078100000 0.4327010000 -45.4979250000  
 H 0.0000000000 0.0000000000 -46.7490940000  
 C 0.5366020000 4.9356510000 -12.6254550000  
 C 1.7191760000 5.5308220000 -12.1564160000  
 C -0.4946150000 5.7665820000 -13.0933390000  
 C 1.8673100000 6.9190100000 -12.1575590000  
 H 2.5268870000 4.8990100000 -11.7980780000  
 C -0.3478660000 7.1548850000 -13.0904020000  
 H -1.4171380000 5.3190560000 -13.4520320000  
 C 0.8339280000 7.7354060000 -12.6235420000  
 H 2.7919630000 7.3613360000 -11.7966730000  
 H -1.1590360000 7.7820270000 -13.4503640000  
 H 0.9486980000 8.8158960000 -12.6228480000  
 C 0.6242890000 4.9247730000 -21.0447130000  
 C 1.8272710000 5.4960080000 -20.5986350000  
 C -0.3995460000 5.7762170000 -21.4911950000  
 C 2.0022760000 6.8811120000 -20.6008060000  
 H 2.6294620000 4.8480040000 -20.2571290000  
 C -0.2257330000 7.1614330000 -21.4896960000  
 H -1.3374220000 5.3472110000 -21.8323760000  
 C 0.9760470000 7.7181660000 -21.0454370000  
 H 2.9422210000 7.3048480000 -20.2575250000  
 H -1.0313840000 7.8047870000 -21.8330800000  
 H 1.1118140000 8.7962210000 -21.0457160000  
 C 0.6463890000 4.9220170000 -29.4647290000  
 C -0.3735940000 5.7787950000 -29.9099090000  
 C 1.8531840000 5.4872560000 -29.0212750000  
 C -0.1923720000 7.1630690000 -29.9097500000  
 H -1.3144620000 5.3546690000 -30.2490420000  
 C 2.0355090000 6.8714400000 -29.0242890000  
 H 2.6525970000 4.8351800000 -28.6809540000  
 C 1.0130650000 7.7137010000 -29.4677570000  
 H -0.9951550000 7.8105110000 -30.2521830000  
 H 2.9782300000 7.2903700000 -28.6827090000  
 H 1.1545510000 8.7910200000 -29.4688880000  
 C 0.6668180000 4.9175200000 -37.8792010000  
 C -0.3602330000 5.7799970000 -38.2957740000  
 C 1.8852510000 5.4768590000 -37.4613730000  
 C -0.1744280000 7.1637290000 -38.2935950000  
 H -1.3102170000 5.3606820000 -38.6153240000  
 C 2.0720650000 6.8606340000 -37.4608420000  
 H 2.6899920000 4.8204020000 -37.1423790000  
 C 1.0426670000 7.7083810000 -37.8766570000  
 H -0.9826400000 7.8155460000 -38.6143760000  
 H 3.0235120000 7.2748700000 -37.1381810000  
 H 1.1876130000 8.7852460000 -37.8757090000  
 C -0.5366020000 -4.9356510000 -12.6254550000  
 C -1.7191760000 -5.5308220000 -12.1564160000  
 C 0.4946150000 -5.7665820000 -13.0933390000  
 C -1.8673100000 -6.9190100000 -12.1575590000  
 H -2.5268870000 -4.8990100000 -11.7980780000

C 0.3478660000 -7.1548850000 -13.0904020000  
 H 1.4171380000 -5.3190560000 -13.4520320000  
 C -0.8339280000 -7.7354060000 -12.6235420000  
 H -2.7919630000 -7.3613360000 -11.7966730000  
 H 1.1590360000 -7.7820270000 -13.4503640000  
 H -0.9486980000 -8.8158960000 -12.6228480000  
 C -0.6242890000 -4.9247730000 -21.0447130000  
 C -1.8272710000 -5.4960080000 -20.5986350000  
 C 0.3995460000 -5.7762170000 -21.4911950000  
 C -2.0022760000 -6.8811120000 -20.6008060000  
 H -2.6294620000 -4.8480040000 -20.2571290000  
 C 0.2257330000 -7.1614330000 -21.4896960000  
 H 1.3374220000 -5.3472110000 -21.8323760000  
 C -0.9760470000 -7.7181660000 -21.0454370000  
 H -2.9422210000 -7.3048480000 -20.2575250000  
 H 1.0313840000 -7.8047870000 -21.8330800000  
 H -1.1118140000 -8.7962210000 -21.0457160000  
 C -0.6463890000 -4.9220170000 -29.4647290000  
 C 0.3735940000 -5.7787950000 -29.9099090000  
 C -1.8531840000 -5.4872560000 -29.0212750000  
 C 0.1923720000 -7.1630690000 -29.9097500000  
 H 1.3144620000 -5.3546690000 -30.2490420000  
 C -2.0355090000 -6.8714400000 -29.0242890000  
 H -2.6525970000 -4.8351800000 -28.6809540000  
 C -1.0130650000 -7.7137010000 -29.4677570000  
 H 0.9951550000 -7.8105110000 -30.2521830000  
 H -2.9782300000 -7.2903700000 -28.6827090000  
 H -1.1545510000 -8.7910200000 -29.4688880000  
 C -0.6668180000 -4.9175200000 -37.8792010000  
 C 0.3602330000 -5.7799970000 -38.2957740000  
 C -1.8852510000 -5.4768590000 -37.4613730000  
 C 0.1744280000 -7.1637290000 -38.2935950000  
 H 1.3102170000 -5.3606820000 -38.6153240000  
 C -2.0720650000 -6.8606340000 -37.4608420000  
 H -2.6899920000 -4.8204020000 -37.1423790000  
 C -1.0426670000 -7.7083810000 -37.8766570000  
 H 0.9826400000 -7.8155460000 -38.6143760000  
 H -3.0235120000 -7.2748700000 -37.1381810000  
 H -1.1876130000 -8.7852460000 -37.8757090000  
 H -0.3500560000 -2.6476710000 -42.4463310000  
 H 0.3500560000 2.6476710000 -42.4463310000

**Table S10.** Optimized coordinates for **12**.

Zn 0.0000000000 0.0000000000 29.4630960000  
 N -0.2183250000 1.4299370000 28.0195090000  
 C -0.1768040000 1.2312690000 26.6722670000  
 C 0.0000000000 0.0000000000 25.9872400000  
 C 0.1768040000 -1.2312690000 26.6722670000  
 N 0.2183250000 -1.4299370000 28.0195090000  
 C 0.4088520000 -2.7868790000 28.2100970000  
 C 0.5071720000 -3.4291790000 29.4623050000  
 C 0.4150580000 -2.7853870000 30.7164130000  
 N 0.1931810000 -1.4346280000 30.9064420000  
 C 0.1919820000 -1.2288420000 32.2542010000  
 C 0.0000000000 0.0000000000 32.9379390000  
 C -0.1919820000 1.2288420000 32.2542010000  
 N -0.1931810000 1.4346280000 30.9064420000  
 C -0.4150580000 2.7853870000 30.7164130000

C -0.5071720000 3.4291790000 29.4623050000  
 C -0.4088520000 2.7868790000 28.2100970000  
 C -0.4749430000 3.4540030000 26.9361470000  
 C -0.3399450000 2.4823630000 25.9713910000  
 C -0.3267610000 2.4840630000 24.5358350000  
 C -0.1524350000 1.2350980000 23.8352540000  
 N -0.1666700000 1.4380240000 22.4877270000  
 Zn 0.0000000000 0.0000000000 21.0440830000  
 N -0.2040990000 1.4323770000 19.6003410000  
 C -0.1656410000 1.2333470000 18.2532190000  
 C 0.0000000000 0.0000000000 17.5677190000  
 C 0.1656410000 -1.2333470000 18.2532190000  
 N 0.2040990000 -1.4323770000 19.6003410000  
 C 0.3703670000 -2.7925910000 19.7909820000  
 C 0.4419890000 -3.4381950000 21.0436710000  
 C 0.3485690000 -2.7954010000 22.2975800000  
 N 0.1666700000 -1.4380240000 22.4877270000  
 C 0.1524350000 -1.2350980000 23.8352540000  
 C 0.0000000000 0.0000000000 24.5199850000  
 C 0.3267610000 -2.4840630000 24.5358350000  
 C 0.3399450000 -2.4823630000 25.9713910000  
 C 0.4749430000 -3.4540030000 26.9361470000  
 H 0.6011030000 -4.5163580000 26.7880680000  
 C 0.4580190000 -3.4566460000 23.5706890000  
 H 0.6201370000 -4.5141150000 23.7188430000  
 C 0.4306360000 -3.4602040000 18.5176480000  
 C 0.3120500000 -2.4862510000 17.5525370000  
 C 0.2977060000 -2.4879890000 16.1172170000  
 C 0.1387310000 -1.2370880000 15.4165210000  
 N 0.1473430000 -1.4403840000 14.0693080000  
 Zn 0.0000000000 0.0000000000 12.6250440000  
 N -0.1814720000 1.4363820000 11.1817080000  
 C -0.1308970000 1.2380180000 9.8349560000  
 C 0.0000000000 0.0000000000 9.1495860000  
 C 0.1308970000 -1.2380180000 9.8349560000  
 N 0.1814720000 -1.4363820000 11.1817080000  
 C 0.3097570000 -2.8006690000 11.3723150000  
 C 0.3790540000 -3.4464530000 12.6254230000  
 C 0.3074050000 -2.8009350000 13.8791620000  
 C 0.4121830000 -3.4628690000 15.1520800000  
 H 0.5594150000 -4.5224590000 15.3004620000  
 C 0.3315820000 -3.4714800000 10.0997340000  
 C 0.2277190000 -2.4956720000 9.1344610000  
 C 0.1900130000 -2.4989370000 7.6995620000  
 C 0.0793540000 -1.2426320000 6.9992750000  
 N 0.0591550000 -1.4472250000 5.6527670000  
 Zn 0.0000000000 0.0000000000 4.2079280000  
 N -0.0805710000 1.4464070000 2.7635360000  
 C -0.0328820000 1.24448520000 1.4173850000  
 C 0.0000000000 0.0000000000 0.7323160000  
 C 0.0328820000 -1.24448520000 1.4173850000  
 N 0.0805710000 -1.4464070000 2.7635360000  
 C 0.1122690000 -2.8160870000 2.9545770000  
 C 0.1594500000 -3.4639710000 4.2081630000  
 C 0.1471410000 -2.8143960000 5.4619380000  
 C 0.2406790000 -3.4792930000 6.7342790000  
 H 0.3370910000 -4.5447550000 6.8823170000  
 C 0.0682550000 -3.4869970000 1.6825980000  
 C 0.0259240000 -2.5062970000 0.7172810000  
 H 0.0636210000 -4.5568870000 1.5350090000  
 C -0.0259240000 2.5062970000 0.7172810000  
 C -0.0682550000 3.4869970000 1.6825980000  
 C -0.1122690000 2.8160870000 2.9545770000

C -0.1594500000 3.4639710000 4.2081630000  
 C -0.1471410000 2.8143960000 5.4619380000  
 N -0.0591550000 1.4472250000 5.6527670000  
 C -0.0793540000 1.2426320000 6.9992750000  
 C -0.1900130000 2.4989370000 7.6995620000  
 C -0.2277190000 2.4956720000 9.1344610000  
 C -0.3315820000 3.4714800000 10.0997340000  
 C -0.3097570000 2.8006690000 11.3723150000  
 C -0.3790540000 3.4464530000 12.6254230000  
 C -0.3074050000 2.8009350000 13.8791620000  
 N -0.1473430000 1.4403840000 14.0693080000  
 C -0.1387310000 1.2370880000 15.4165210000  
 C -0.2977060000 2.4879890000 16.1172170000  
 C -0.3120500000 2.4862510000 17.5525370000  
 C -0.4306360000 3.4602040000 18.5176480000  
 C -0.3703670000 2.7925910000 19.7909820000  
 C -0.4419890000 3.4381950000 21.0436710000  
 C -0.3485690000 2.7954010000 22.2975800000  
 C -0.4580190000 3.4566460000 23.5706890000  
 H -0.6201370000 4.5141150000 23.7188430000  
 H -0.5402720000 4.5244150000 18.3696570000  
 C -0.4121830000 3.4628690000 15.1520800000  
 H -0.5594150000 4.5224590000 15.3004620000  
 C 0.0000000000 0.0000000000 16.1017250000  
 H -0.4074680000 4.5386650000 9.9520260000  
 C -0.2406790000 3.4792930000 6.7342790000  
 H -0.3370910000 4.5447550000 6.8823170000  
 C 0.0000000000 0.0000000000 7.6844850000  
 H -0.0636210000 4.5568870000 1.5350090000  
 H 0.4074680000 -4.5386650000 9.9520260000  
 H 0.5402720000 -4.5244150000 18.3696570000  
 H -0.6011030000 4.5163580000 26.7880680000  
 C -0.5671900000 3.4394610000 31.9893060000  
 C -0.4206190000 2.4692900000 32.9543310000  
 C -0.4592000000 2.4629760000 34.3898990000  
 C -0.2429900000 1.2194080000 35.0911520000  
 N -0.3147660000 1.4129310000 36.4381900000  
 Zn 0.0000000000 0.0000000000 37.8783530000  
 N -0.2928680000 1.4175440000 39.3225800000  
 C -0.2841940000 1.2090090000 40.6712510000  
 C -0.6108010000 2.4270800000 41.3714170000  
 C -0.6567600000 2.4158960000 42.8078780000  
 C -0.3432070000 1.1915090000 43.5108430000  
 N -0.4333850000 1.3784620000 44.8583180000  
 Zn 0.0000000000 0.0000000000 46.3084180000  
 N 0.4333850000 -1.3784620000 44.8583180000  
 C 0.3432070000 -1.1915090000 43.5108430000  
 C 0.0000000000 0.0000000000 42.8285400000  
 C 0.0000000000 0.0000000000 41.3527880000  
 C 0.2841940000 -1.2090090000 40.6712510000  
 N 0.2928680000 -1.4175440000 39.3225800000  
 C 0.6118630000 -2.7473780000 39.1336320000  
 C 0.7346960000 -3.3886060000 37.8796640000  
 C 0.5812120000 -2.7566700000 36.6285380000  
 N 0.3147660000 -1.4129310000 36.4381900000  
 C 0.2429900000 -1.2194080000 35.0911520000  
 C 0.0000000000 0.0000000000 34.4075300000  
 C 0.4592000000 -2.4629760000 34.3898990000  
 C 0.4206190000 -2.4692900000 32.9543310000  
 C 0.5671900000 -3.4394610000 31.9893060000  
 H 0.7652820000 -4.4908780000 32.1368540000  
 C 0.6622970000 -3.4227940000 35.3536860000  
 H 0.8431170000 -4.4772620000 35.2056920000

C 0.8226750000 -3.3852720000 40.4075270000  
 C 0.6108010000 -2.4270800000 41.3714170000  
 C 0.6567600000 -2.4158960000 42.8078780000  
 C 0.9373350000 -3.3549020000 43.7691750000  
 C 0.8034900000 -2.6965210000 45.0471320000  
 C 0.9977360000 -3.3178470000 46.2936360000  
 C 0.8209750000 -2.6900560000 47.5501200000  
 N 0.4306280000 -1.3893230000 47.7525550000  
 C 0.3800220000 -1.1939730000 49.1133230000  
 C 0.0000000000 0.0000000000 49.7622210000  
 C -0.3800220000 1.1939730000 49.1133230000  
 N -0.4306280000 1.3893230000 47.7525550000  
 C -0.8209750000 2.6900560000 47.5501200000  
 C -0.9977360000 3.3178470000 46.2936360000  
 C -0.8034900000 2.6965210000 45.0471320000  
 C -0.9373350000 3.3549020000 43.7691750000  
 H -1.2020960000 4.3916930000 43.6221160000  
 C -1.0363870000 3.3348660000 48.8251650000  
 C -0.7527040000 2.4148640000 49.7903980000  
 H -0.7928930000 2.5513520000 50.8611040000  
 H -1.3585050000 4.3562670000 48.9650580000  
 C 0.7527040000 -2.4148640000 49.7903980000  
 C 1.0363870000 -3.3348660000 48.8251650000  
 H 1.3585050000 -4.3562670000 48.9650580000  
 H 0.7928930000 -2.5513520000 50.8611040000  
 H 1.2020960000 -4.3916930000 43.6221160000  
 H 1.0994660000 -4.4187470000 40.5553330000  
 C -0.8226750000 3.3852720000 40.4075270000  
 C -0.6118630000 2.7473780000 39.1336320000  
 C -0.7346960000 3.3886060000 37.8796640000  
 C -0.5812120000 2.7566700000 36.6285380000  
 C -0.6622970000 3.4227940000 35.3536860000  
 H -0.8431170000 4.4772620000 35.2056920000  
 H -1.0994660000 4.4187470000 40.5553330000  
 H -0.7652820000 4.4908780000 32.1368540000  
 C 0.0000000000 0.0000000000 51.2612790000  
 C -1.2060680000 0.0540290000 51.9785600000  
 C 1.2060680000 -0.0540290000 51.9785600000  
 C -1.2062930000 0.0531140000 53.3747990000  
 H -2.1465530000 0.0899970000 51.4358130000  
 C 1.2062930000 -0.0531140000 53.3747990000  
 H 2.1465530000 -0.0899970000 51.4358130000  
 C 0.0000000000 0.0000000000 54.0773150000  
 H -2.1498610000 0.0905100000 53.9126020000  
 H 2.1498610000 -0.0905100000 53.9126020000  
 H 0.0000000000 0.0000000000 55.1638810000  
 C 1.4209450000 -4.7553450000 46.2925340000  
 C 0.5495450000 -5.7617110000 46.7402500000  
 C 2.6982930000 -5.1253730000 45.8410830000  
 C 0.9441250000 -7.1008780000 46.7358130000  
 H -0.4441660000 -5.4902210000 47.0854820000  
 C 3.0940830000 -6.4643900000 45.8387420000  
 H 3.3841740000 -4.3560900000 45.4975480000  
 C 2.2180580000 -7.4563610000 46.2857080000  
 H 0.2539880000 -7.8662020000 47.0806990000  
 H 4.0882630000 -6.7308170000 45.4900800000  
 H 2.5255130000 -8.4985250000 46.2831210000  
 C 1.0547440000 -4.8513030000 37.8815980000  
 C 0.1318260000 -5.7868350000 38.3777520000  
 C 2.2842720000 -5.3175030000 37.3876770000  
 C 0.4292110000 -7.1507910000 38.3775190000  
 H -0.8256410000 -5.4403200000 38.7561940000  
 C 2.5831720000 -6.6811820000 37.3913080000

H 3.0099550000 -4.6038690000 37.0080910000  
 C 1.6562120000 -7.6022130000 37.8852060000  
 H -0.3000490000 -7.8602160000 38.7593330000  
 H 3.5420630000 -7.0224420000 37.0105810000  
 H 1.8882150000 -8.6637220000 37.8865010000  
 C 0.7312280000 -4.9098830000 29.4635440000  
 C 1.9377990000 -5.4535660000 28.9931240000  
 C -0.2611040000 -5.7842820000 29.9362760000  
 C 2.1468370000 -6.8338920000 28.9968540000  
 H 2.7162010000 -4.7876420000 28.6317200000  
 C -0.0534240000 -7.1647950000 29.9360890000  
 H -1.2013870000 -5.3768930000 30.2967290000  
 C 1.1515290000 -7.6938810000 29.4672900000  
 H 3.0891870000 -7.2359670000 28.6346410000  
 H -0.8352170000 -7.8261740000 30.2997500000  
 H 1.3137230000 -8.7682740000 29.4686740000  
 C 0.6318150000 -4.9238140000 21.0439090000  
 C 1.8344550000 -5.4930940000 20.5944230000  
 C -0.3893270000 -5.7767080000 21.4937550000  
 C 2.0117900000 -6.8778800000 20.5967210000  
 H 2.6345360000 -4.8438760000 20.2503310000  
 C -0.2132430000 -7.1616260000 21.4920400000  
 H -1.3268420000 -5.3491160000 21.8376340000  
 C 0.9881980000 -7.7164750000 21.0445330000  
 H 2.9514780000 -7.3001690000 20.2509800000  
 H -1.0168320000 -7.8062050000 21.8379270000  
 H 1.1257650000 -8.7942990000 21.0447810000  
 C 0.5373140000 -4.9355500000 12.6249790000  
 C 1.7197840000 -5.5304300000 12.1553250000  
 C -0.4935900000 -5.7665620000 13.0933680000  
 C 1.8681620000 -6.9185790000 12.1565150000  
 H 2.5271890000 -4.8984780000 11.7965740000  
 C -0.3466340000 -7.1548360000 13.0902290000  
 H -1.4159780000 -5.3191710000 13.4525410000  
 C 0.8350790000 -7.7351320000 12.6228950000  
 H 2.7927470000 -7.3607540000 11.7952860000  
 H -1.1575550000 -7.7821170000 13.4504940000  
 H 0.9500270000 -8.8156000000 12.6221450000  
 C 0.2260350000 -4.9597460000 4.2079150000  
 C 1.3576520000 -5.6266940000 3.7103240000  
 C -0.8413870000 -5.7255800000 4.7049770000  
 C 1.4211270000 -7.0212540000 3.7124350000  
 H 2.1928410000 -5.0458850000 3.3294970000  
 C -0.7796920000 -7.1202160000 4.7022350000  
 H -1.7252640000 -5.2220790000 5.0859700000  
 C 0.3522150000 -7.7723830000 4.2072060000  
 H 2.3076430000 -7.5196810000 3.3296640000  
 H -1.6180370000 -7.6962020000 5.0846850000  
 H 0.4009180000 -8.8578550000 4.2069830000  
 C -0.2260350000 4.9597460000 4.2079150000  
 C -1.3576520000 5.6266940000 3.7103240000  
 C 0.8413870000 5.7255800000 4.7049770000  
 C -1.4211270000 7.0212540000 3.7124350000  
 H -2.1928410000 5.0458850000 3.3294970000  
 C 0.7796920000 7.1202160000 4.7022350000  
 H 1.7252640000 5.2220790000 5.0859700000  
 C -0.3522150000 7.7723830000 4.2072060000  
 H -2.3076430000 7.5196810000 3.3296640000  
 H 1.6180370000 7.6962020000 5.0846850000  
 H -0.4009180000 8.8578550000 4.2069830000  
 C -1.4209450000 4.7553450000 46.2925340000  
 C -0.5495450000 5.7617110000 46.7402500000  
 C -2.6982930000 5.1253730000 45.8410830000

C -0.9441250000 7.1008780000 46.7358130000  
 H 0.4441660000 5.4902210000 47.0854820000  
 C -3.0940830000 6.4643900000 45.8387420000  
 H -3.3841740000 4.3560900000 45.4975480000  
 C -2.2180580000 7.4563610000 46.2857080000  
 H -0.2539880000 7.8662020000 47.0806990000  
 H -4.0882630000 6.7308170000 45.4900800000  
 H -2.5255130000 8.4985250000 46.2831210000  
 C -1.0547440000 4.8513030000 37.8815980000  
 C -0.1318260000 5.7868350000 38.3777520000  
 C -2.2842720000 5.3175030000 37.3876770000  
 C -0.4292110000 7.1507910000 38.3775190000  
 H 0.8256410000 5.4403200000 38.7561940000  
 C -2.5831720000 6.6811820000 37.3913080000  
 H -3.0099550000 4.6038690000 37.0080910000  
 C -1.6562120000 7.6022130000 37.8852060000  
 H 0.3000490000 7.8602160000 38.7593330000  
 H -3.5420630000 7.0224420000 37.0105810000  
 H -1.8882150000 8.6637220000 37.8865010000  
 C -0.7312280000 4.9098830000 29.4635440000  
 C -1.9377990000 5.4535660000 28.9931240000  
 C 0.2611040000 5.7842820000 29.9362760000  
 C -2.1468370000 6.8338920000 28.9968540000  
 H -2.7162010000 4.7876420000 28.6317200000  
 C 0.0534240000 7.1647950000 29.9360890000  
 H 1.2013870000 5.3768930000 30.2967290000  
 C -1.1515290000 7.6938810000 29.4672900000  
 H -3.0891870000 7.2359670000 28.6346410000  
 H 0.8352170000 7.8261740000 30.2997500000  
 H -1.3137230000 8.7682740000 29.4686740000  
 C -0.6318150000 4.9238140000 21.0439090000  
 C -1.8344550000 5.4930940000 20.5944230000  
 C 0.3893270000 5.7767080000 21.4937550000  
 C -2.0117900000 6.8777880000 20.5967210000  
 H -2.6345360000 4.8438760000 20.2503310000  
 C 0.2132430000 7.1616260000 21.4920400000  
 H 1.3268420000 5.3491160000 21.8376340000  
 C -0.9881980000 7.7164750000 21.0445330000  
 H -2.9514780000 7.3001690000 20.2509800000  
 H 1.0168320000 7.8062050000 21.8379270000  
 H -1.1257650000 8.7942990000 21.0447810000  
 C -0.5373140000 4.9355500000 12.6249790000  
 C -1.7197840000 5.5304300000 12.1553250000  
 C 0.4935900000 5.7665620000 13.0933680000  
 C -1.8681620000 6.9185790000 12.1565150000  
 H -2.5271890000 4.8984780000 11.7965740000  
 C 0.3466340000 7.1548360000 13.0902290000  
 H 1.4159780000 5.3191710000 13.4525410000  
 C -0.8350790000 7.7351320000 12.6228950000  
 H -2.7927470000 7.3607540000 11.7952860000  
 H 1.1575550000 7.7821170000 13.4504940000  
 H -0.9500270000 8.8156000000 12.6221450000  
 Zn 0.0000000000 0.0000000000 -21.0440830000  
 N 0.1666700000 1.4380240000 -22.4877270000  
 C 0.1524350000 1.2350980000 -23.8352540000  
 C 0.0000000000 0.0000000000 -24.5199850000  
 C -0.1524350000 -1.2350980000 -23.8352540000  
 N -0.1666700000 -1.4380240000 -22.4877270000  
 C -0.3485690000 -2.7954010000 -22.2975800000  
 C -0.4419890000 -3.4381950000 -21.0436710000  
 C -0.3703670000 -2.7925910000 -19.7909820000  
 N -0.2040990000 -1.4323770000 -19.6003410000  
 C -0.1656410000 -1.2333470000 -18.2532190000

C 0.00000000000 0.00000000000 -17.5677190000  
 C 0.1656410000 1.2333470000 -18.2532190000  
 N 0.2040990000 1.4323770000 -19.6003410000  
 C 0.3703670000 2.7925910000 -19.7909820000  
 C 0.4419890000 3.4381950000 -21.0436710000  
 C 0.3485690000 2.7954010000 -22.2975800000  
 C 0.4580190000 3.4566460000 -23.5706890000  
 C 0.3267610000 2.4840630000 -24.5358350000  
 C 0.3399450000 2.4823630000 -25.9713910000  
 C 0.1768040000 1.2312690000 -26.6722670000  
 N 0.2183250000 1.4299370000 -28.0195090000  
 Zn 0.0000000000 0.0000000000 -29.4630960000  
 N 0.1931810000 1.4346280000 -30.9064420000  
 C 0.1919820000 1.2288420000 -32.2542010000  
 C 0.0000000000 0.0000000000 -32.9379390000  
 C -0.1919820000 -1.2288420000 -32.2542010000  
 N -0.1931810000 -1.4346280000 -30.9064420000  
 C -0.4150580000 -2.7853870000 -30.7164130000  
 C -0.5071720000 -3.4291790000 -29.4623050000  
 C -0.4088520000 -2.7868790000 -28.2100970000  
 N -0.2183250000 -1.4299370000 -28.0195090000  
 C -0.1768040000 -1.2312690000 -26.6722670000  
 C 0.0000000000 0.0000000000 -25.9872400000  
 C -0.3399450000 -2.4823630000 -25.9713910000  
 C -0.3267610000 -2.4840630000 -24.5358350000  
 C -0.4580190000 -3.4566460000 -23.5706890000  
 H -0.6201370000 -4.5141150000 -23.7188430000  
 C -0.4749430000 -3.4540030000 -26.9361470000  
 H -0.6011030000 -4.5163580000 -26.7880680000  
 C -0.5671900000 -3.4394610000 -31.9893060000  
 C -0.4206190000 -2.4692900000 -32.9543310000  
 C -0.4592000000 -2.4629760000 -34.3898990000  
 C -0.2429900000 -1.2194080000 -35.0911520000  
 N -0.3147660000 -1.4129310000 -36.4381900000  
 Zn 0.0000000000 0.0000000000 -37.8783530000  
 N 0.2928680000 1.4175440000 -39.3225800000  
 C 0.2841940000 1.2090090000 -40.6712510000  
 C 0.0000000000 0.0000000000 -41.3527880000  
 C -0.2841940000 -1.2090090000 -40.6712510000  
 N -0.2928680000 -1.4175440000 -39.3225800000  
 C -0.6118630000 -2.7473780000 -39.1336320000  
 C -0.7346960000 -3.3886060000 -37.8796640000  
 C -0.5812120000 -2.7566700000 -36.6285380000  
 C -0.6622970000 -3.4227940000 -35.3536860000  
 H -0.8431170000 -4.4772620000 -35.2056920000  
 C -0.8226750000 -3.3852720000 -40.4075270000  
 C -0.6108010000 -2.4270800000 -41.3714170000  
 C -0.6567600000 -2.4158960000 -42.8078780000  
 C -0.3432070000 -1.1915090000 -43.5108430000  
 N -0.4333850000 -1.3784620000 -44.8583180000  
 Zn 0.0000000000 0.0000000000 -46.3084180000  
 N 0.4306280000 1.3893230000 -47.7525550000  
 C 0.3800220000 1.1939730000 -49.1133230000  
 C 0.0000000000 0.0000000000 -49.7622210000  
 C -0.3800220000 -1.1939730000 -49.1133230000  
 N -0.4306280000 -1.3893230000 -47.7525550000  
 C -0.8209750000 -2.6900560000 -47.5501200000  
 C -0.9977360000 -3.3178470000 -46.2936360000  
 C -0.8034900000 -2.6965210000 -45.0471320000  
 C -0.9373350000 -3.3549020000 -43.7691750000  
 H -1.2020960000 -4.3916930000 -43.6221160000  
 C -1.0363870000 -3.3348660000 -48.8251650000  
 C -0.7527040000 -2.4148640000 -49.7903980000

H -0.7928930000 -2.5513520000 -50.8611040000  
 H -1.3585050000 -4.3562670000 -48.9650580000  
 C 0.7527040000 2.4148640000 -49.7903980000  
 C 1.0363870000 3.3348660000 -48.8251650000  
 C 0.8209750000 2.6900560000 -47.5501200000  
 C 0.9977360000 3.3178470000 -46.2936360000  
 C 0.8034900000 2.6965210000 -45.0471320000  
 N 0.4333850000 1.3784620000 -44.8583180000  
 C 0.3432070000 1.1915090000 -43.5108430000  
 C 0.6567600000 2.4158960000 -42.8078780000  
 C 0.6108010000 2.4270800000 -41.3714170000  
 C 0.8226750000 3.3852720000 -40.4075270000  
 C 0.6118630000 2.7473780000 -39.1336320000  
 C 0.7346960000 3.3886060000 -37.8796640000  
 C 0.5812120000 2.7566700000 -36.6285380000  
 N 0.3147660000 1.4129310000 -36.4381900000  
 C 0.2429900000 1.2194080000 -35.0911520000  
 C 0.4592000000 2.4629760000 -34.3898990000  
 C 0.4206190000 2.4692900000 -32.9543310000  
 C 0.5671900000 3.4394610000 -31.9893060000  
 C 0.4150580000 2.7853870000 -30.7164130000  
 C 0.5071720000 3.4291790000 -29.4623050000  
 C 0.4088520000 2.7868790000 -28.2100970000  
 C 0.4749430000 3.4540030000 -26.9361470000  
 H 0.6011030000 4.5163580000 -26.7880680000  
 H 0.7652820000 4.4908780000 -32.1368540000  
 C 0.6622970000 3.4227940000 -35.3536860000  
 H 0.8431170000 4.4772620000 -35.2056920000  
 C 0.0000000000 0.0000000000 -34.4075300000  
 H 1.0994660000 4.4187470000 -40.5553330000  
 C 0.9373350000 3.3549020000 -43.7691750000  
 H 1.2020960000 4.3916930000 -43.6221160000  
 C 0.0000000000 0.0000000000 -42.8285400000  
 H 1.3585050000 4.3562670000 -48.9650580000  
 H 0.7928930000 2.5513520000 -50.8611040000  
 H -1.0994660000 -4.4187470000 -40.5553330000  
 H -0.7652820000 -4.4908780000 -32.1368540000  
 H 0.6201370000 4.5141150000 -23.7188430000  
 C 0.4306360000 3.4602040000 -18.5176480000  
 C 0.3120500000 2.4862510000 -17.5525370000  
 C 0.2977060000 2.4879890000 -16.1172170000  
 C 0.1387310000 1.2370880000 -15.4165210000  
 N 0.1473430000 1.4403840000 -14.0693080000  
 Zn 0.0000000000 0.0000000000 -12.6250440000  
 N 0.1814720000 1.4363820000 -11.1817080000  
 C 0.1308970000 1.2380180000 -9.8349560000  
 C 0.2277190000 2.4956720000 -9.1344610000  
 C 0.1900130000 2.4989370000 -7.6995620000  
 C 0.0793540000 1.2426320000 -6.9992750000  
 N 0.0591550000 1.4472250000 -5.6527670000  
 Zn 0.0000000000 0.0000000000 -4.2079280000  
 N -0.0591550000 -1.4472250000 -5.6527670000  
 C -0.0793540000 -1.2426320000 -6.9992750000  
 C 0.0000000000 0.0000000000 -7.6844850000  
 C 0.0000000000 0.0000000000 -9.1495860000  
 C -0.1308970000 -1.2380180000 -9.8349560000  
 N -0.1814720000 -1.4363820000 -11.1817080000  
 C -0.3097570000 -2.8006690000 -11.3723150000  
 C -0.3790540000 -3.4464530000 -12.6254230000  
 C -0.3074050000 -2.8009350000 -13.8791620000  
 N -0.1473430000 -1.4403840000 -14.0693080000  
 C -0.1387310000 -1.2370880000 -15.4165210000  
 C 0.0000000000 0.0000000000 -16.1017250000

C -0.2977060000 -2.4879890000 -16.1172170000  
 C -0.3120500000 -2.4862510000 -17.5525370000  
 C -0.4306360000 -3.4602040000 -18.5176480000  
 H -0.5402720000 -4.5244150000 -18.3696570000  
 C -0.4121830000 -3.4628690000 -15.1520800000  
 H -0.5594150000 -4.5224590000 -15.3004620000  
 C -0.3315820000 -3.4714800000 -10.0997340000  
 C -0.2277190000 -2.4956720000 -9.1344610000  
 C -0.1900130000 -2.4989370000 -7.6995620000  
 C -0.2406790000 -3.4792930000 -6.7342790000  
 C -0.1471410000 -2.8143960000 -5.4619380000  
 C -0.1594500000 -3.4639710000 -4.2081630000  
 C -0.1122690000 -2.8160870000 -2.9545770000  
 N -0.0805710000 -1.4464070000 -2.7635360000  
 C -0.0328820000 -1.2448520000 -1.4173850000  
 C 0.0000000000 0.0000000000 -0.7323160000  
 C 0.0328820000 1.2448520000 -1.4173850000  
 N 0.0805710000 1.4464070000 -2.7635360000  
 C 0.1122690000 2.8160870000 -2.9545770000  
 C 0.1594500000 3.4639710000 -4.2081630000  
 C 0.1471410000 2.8143960000 -5.4619380000  
 C 0.2406790000 3.4792930000 -6.7342790000  
 H 0.3370910000 4.5447550000 -6.8823170000  
 C 0.0682550000 3.4869970000 -1.6825980000  
 C 0.0259240000 2.5062970000 -0.7172810000  
 H 0.0636210000 4.5568870000 -1.5350090000  
 C -0.0259240000 -2.5062970000 -0.7172810000  
 C -0.0682550000 -3.4869970000 -1.6825980000  
 H -0.0636210000 -4.5568870000 -1.5350090000  
 H -0.3370910000 -4.5447550000 -6.8823170000  
 H -0.4074680000 -4.5386650000 -9.9520260000  
 C 0.3315820000 3.4714800000 -10.0997340000  
 C 0.3097570000 2.8006690000 -11.3723150000  
 C 0.3790540000 3.4464530000 -12.6254230000  
 C 0.3074050000 2.8009350000 -13.8791620000  
 C 0.4121830000 3.4628690000 -15.1520800000  
 H 0.5594150000 4.5224590000 -15.3004620000  
 H 0.4074680000 4.5386650000 -9.9520260000  
 H 0.5402720000 4.5244150000 -18.3696570000  
 C 0.0000000000 0.0000000000 -51.2612790000  
 C 1.2060680000 0.0540290000 -51.9785600000  
 C -1.2060680000 -0.0540290000 -51.9785600000  
 C 1.2062930000 0.0531140000 -53.3747990000  
 H 2.1465530000 0.0899970000 -51.4358130000  
 C -1.2062930000 -0.0531140000 -53.3747990000  
 H -2.1465530000 -0.0899970000 -51.4358130000  
 C 0.0000000000 0.0000000000 -54.0773150000  
 H 2.1498610000 0.0905100000 -53.9126020000  
 H -2.1498610000 -0.0905100000 -53.9126020000  
 H 0.0000000000 0.0000000000 -55.1638810000  
 C -0.2260350000 -4.9597460000 -4.2079150000  
 C -1.3576520000 -5.6266940000 -3.7103240000  
 C 0.8413870000 -5.7255800000 -4.7049770000  
 C -1.4211270000 -7.0212540000 -3.7124350000  
 H -2.1928410000 -5.0458850000 -3.3294970000  
 C 0.7796920000 -7.1202160000 -4.7022350000  
 H 1.7252640000 -5.2220790000 -5.0859700000  
 C -0.3522150000 -7.7723830000 -4.2072060000  
 H -2.3076430000 -7.5196810000 -3.3296640000  
 H 1.6180370000 -7.6962020000 -5.0846850000  
 H -0.4009180000 -8.8578550000 -4.2069830000  
 C -0.5373140000 -4.9355500000 -12.6249790000  
 C -1.7197840000 -5.5304300000 -12.1553250000

C 0.4935900000 -5.7665620000 -13.0933680000  
 C -1.8681620000 -6.9185790000 -12.1565150000  
 H -2.5271890000 -4.8984780000 -11.7965740000  
 C 0.3466340000 -7.1548360000 -13.0902290000  
 H 1.4159780000 -5.3191710000 -13.4525410000  
 C -0.8350790000 -7.7351320000 -12.6228950000  
 H -2.7927470000 -7.3607540000 -11.7952860000  
 H 1.1575550000 -7.7821170000 -13.4504940000  
 H -0.9500270000 -8.8156000000 -12.6221450000  
 C -0.6318150000 -4.9238140000 -21.0439090000  
 C 0.3893270000 -5.7767080000 -21.4937550000  
 C -1.8344550000 -5.4930940000 -20.5944230000  
 C 0.2132430000 -7.1616260000 -21.4920400000  
 H 1.3268420000 -5.3491160000 -21.8376340000  
 C -2.0117900000 -6.8778800000 -20.5967210000  
 H -2.6345360000 -4.8438760000 -20.2503310000  
 C -0.9881980000 -7.7164750000 -21.0445330000  
 H 1.0168320000 -7.8062050000 -21.8379270000  
 H -2.9514780000 -7.3001690000 -20.2509800000  
 H -1.1257650000 -8.7942990000 -21.0447810000  
 C -0.7312280000 -4.9098830000 -29.4635440000  
 C 0.2611040000 -5.7842820000 -29.9362760000  
 C -1.9377990000 -5.4535660000 -28.9931240000  
 C 0.0534240000 -7.1647950000 -29.9360890000  
 H 1.2013870000 -5.3768930000 -30.2967290000  
 C -2.1468370000 -6.8338920000 -28.9968540000  
 H -2.7162010000 -4.7876420000 -28.6317200000  
 C -1.1515290000 -7.6938810000 -29.4672900000  
 H 0.8352170000 -7.8261740000 -30.2997500000  
 H -3.0891870000 -7.2359670000 -28.6346410000  
 H -1.3137230000 -8.7682740000 -29.4686740000  
 C -1.0547440000 -4.8513030000 -37.8815980000  
 C -0.1318260000 -5.7868350000 -38.3777520000  
 C -2.2842720000 -5.3175030000 -37.3876770000  
 C -0.4292110000 -7.1507910000 -38.3775190000  
 H 0.8256410000 -5.4403200000 -38.7561940000  
 C -2.5831720000 -6.6811820000 -37.3913080000  
 H -3.0099550000 -4.6038690000 -37.0080910000  
 C -1.6562120000 -7.6022130000 -37.8852060000  
 H 0.3000490000 -7.8602160000 -38.7593330000  
 H -3.5420630000 -7.0224420000 -37.0105810000  
 H -1.8882150000 -8.6637220000 -37.8865010000  
 C -1.4209450000 -4.7553450000 -46.2925340000  
 C -0.5495450000 -5.7617110000 -46.7402500000  
 C -2.6982930000 -5.1253730000 -45.8410830000  
 C -0.9441250000 -7.1008780000 -46.7358130000  
 H 0.4441660000 -5.4902210000 -47.0854820000  
 C -3.0940830000 -6.4643900000 -45.8387420000  
 H -3.3841740000 -4.3560900000 -45.4975480000  
 C -2.2180580000 -7.4563610000 -46.2857080000  
 H -0.2539880000 -7.8662020000 -47.0806990000  
 H -4.0882630000 -6.7308170000 -45.4900800000  
 H -2.5255130000 -8.4985250000 -46.2831210000  
 C 1.4209450000 4.7553450000 -46.2925340000  
 C 0.5495450000 5.7617110000 -46.7402500000  
 C 2.6982930000 5.1253730000 -45.8410830000  
 C 0.9441250000 7.1008780000 -46.7358130000  
 H -0.4441660000 5.4902210000 -47.0854820000  
 C 3.0940830000 6.4643900000 -45.8387420000  
 H 3.3841740000 4.3560900000 -45.4975480000  
 C 2.2180580000 7.4563610000 -46.2857080000  
 H 0.2539880000 7.8662020000 -47.0806990000  
 H 4.0882630000 6.7308170000 -45.4900800000

H 2.5255130000 8.4985250000 -46.2831210000  
 C 0.2260350000 4.9597460000 -4.2079150000  
 C 1.3576520000 5.6266940000 -3.7103240000  
 C -0.8413870000 5.7255800000 -4.7049770000  
 C 1.4211270000 7.0212540000 -3.7124350000  
 H 2.1928410000 5.0458850000 -3.3294970000  
 C -0.7796920000 7.1202160000 -4.7022350000  
 H -1.7252640000 5.2220790000 -5.0859700000  
 C 0.3522150000 7.7723830000 -4.2072060000  
 H 2.3076430000 7.5196810000 -3.3296640000  
 H -1.6180370000 7.6962020000 -5.0846850000  
 H 0.4009180000 8.8578550000 -4.2069830000  
 C 0.5373140000 4.9355500000 -12.6249790000  
 C 1.7197840000 5.5304300000 -12.1553250000  
 C -0.4935900000 5.7665620000 -13.0933680000  
 C 1.8681620000 6.9185790000 -12.1565150000  
 H 2.5271890000 4.8984780000 -11.7965740000  
 C -0.3466340000 7.1548360000 -13.0902290000  
 H -1.4159780000 5.3191710000 -13.4525410000  
 C 0.8350790000 7.7351320000 -12.6228950000  
 H 2.7927470000 7.3607540000 -11.7952860000  
 H -1.1575550000 7.7821170000 -13.4504940000  
 H 0.9500270000 8.8156000000 -12.6221450000  
 C 0.6318150000 4.9238140000 -21.0439090000  
 C -0.3893270000 5.7767080000 -21.4937550000  
 C 1.8344550000 5.4930940000 -20.5944230000  
 C -0.2132430000 7.1616260000 -21.4920400000  
 H -1.3268420000 5.3491160000 -21.8376340000  
 C 2.0117900000 6.8778800000 -20.5967210000  
 H 2.6345360000 4.8438760000 -20.2503310000  
 C 0.9881980000 7.7164750000 -21.0445330000  
 H -1.0168320000 7.8062050000 -21.8379270000  
 H 2.9514780000 7.3001690000 -20.2509800000  
 H 1.1257650000 8.7942990000 -21.0447810000  
 C 0.7312280000 4.9098830000 -29.4635440000  
 C -0.2611040000 5.7842820000 -29.9362760000  
 C 1.9377990000 5.4535660000 -28.9931240000  
 C -0.0534240000 7.1647950000 -29.9360890000  
 H -1.2013870000 5.3768930000 -30.2967290000  
 C 2.1468370000 6.8338920000 -28.9968540000  
 H 2.7162010000 4.7876420000 -28.6317200000  
 C 1.1515290000 7.6938810000 -29.4672900000  
 H -0.8352170000 7.8261740000 -30.2997500000  
 H 3.0891870000 7.2359670000 -28.6346410000  
 H 1.3137230000 8.7682740000 -29.4686740000  
 C 1.0547440000 4.8513030000 -37.8815980000  
 C 0.1318260000 5.7868350000 -38.3777520000  
 C 2.2842720000 5.3175030000 -37.3876770000  
 C 0.4292110000 7.1507910000 -38.3775190000  
 H -0.8256410000 5.4403200000 -38.7561940000  
 C 2.5831720000 6.6811820000 -37.3913080000  
 H 3.0099550000 4.6038690000 -37.0080910000  
 C 1.6562120000 7.6022130000 -37.8852060000  
 H -0.3000490000 7.8602160000 -38.7593330000  
 H 3.5420630000 7.0224420000 -37.0105810000  
 H 1.8882150000 8.6637220000 -37.8865010000

**Table S11.** TDDFT-predicted band excitation data for **1**.

<i>Index</i>	<i>Energy (cm<sup>-1</sup>)</i>	$\lambda$ ( <i>nm</i> )	<i>Osc. Strength</i>	<i>Contributions</i>
0	18324	546	0.04	63.5% HOMO => L+1, 35.9% H-1 => LUMO
1	18324	546	0.04	63.5% HOMO => LUMO, 35.9% H-1 => L+1
2	24205	413	1.91	63.7% H-1 => LUMO, 35.9% HOMO => L+1
3	24205	413	1.91	63.7% H-1 => L+1, 35.9% HOMO => LUMO
4	27337	366	0.00	99.6% H-2 => L+1
5	27337	366	0.00	99.6% H-2 => LUMO
6	29230	342	0.00	47.9% H-4 => L+1, 47.9% H-5 => LUMO 46.8% H-4 => L+1, 46.8% H-5 => LUMO, 2.02%
7	29586	338	0.00	H-6 => L+1, 2.02% H-7 => LUMO
8	29907	334	0.04	94.9% H-3 => L+1
9	29907	334	0.04	94.9% H-3 => LUMO 47.1% H-4 => LUMO, 47.1% H-5 => L+1, 2.02%
10	30595	327	0.00	H-6 => LUMO, 2.02% H-7 => L+1
11	30960	323	0.00	48.9% H-4 => LUMO, 48.9% H-5 => L+1 88.8% HOMO => L+2, 3.42% H-6 => L+1, 3.42%
12	31244	320	0.00	H-7 => LUMO
13	31923	313	0.00	47.7% H-6 => LUMO, 47.7% H-7 => L+1 40.7% H-6 => L+1, 40.7% H-7 => LUMO, 6.86% HOMO => L+2, 2.82% H-10 => LUMO, 2.82% H-
14	31944	313	0.00	11 => L+1
15	32090	312	0.00	48.6% H-6 => L+1, 48.6% H-7 => LUMO
16	32327	309	0.03	56.1% H-9 => L+1, 39.0% H-8 => LUMO
17	32327	309	0.03	56.1% H-9 => LUMO, 39.0% H-8 => L+1 40.6% H-6 => LUMO, 40.6% H-7 => L+1, 14.0% H-1 => L+2, 2.15% H-4 => LUMO, 2.15% H-5 =>
18	32373	309	0.00	L+1 53.5% H-8 => LUMO, 27.9% H-9 => L+1, 16.0%
19	32844	304	0.01	H-14 => L+1 53.5% H-8 => L+1, 27.9% H-9 => LUMO, 16.0%
20	32844	304	0.01	H-14 => LUMO 34.1% H-10 => L+1, 34.1% H-11 => LUMO, 22.8% H-1 => L+2, 2.85% H-6 => LUMO, 2.85%
21	33340	300	0.00	H-7 => L+1 43.5% H-14 => L+1, 22.2% H-12 => LUMO, 18.1% H-13 => L+1, 9.34% H-9 => L+1, 4.69% H-
22	33375	300	0.07	8 => LUMO 43.5% H-14 => LUMO, 22.2% H-12 => L+1, 18.1% H-13 => LUMO, 9.34% H-9 => LUMO,
23	33375	300	0.07	4.69% H-8 => L+1
24	33460	299	0.00	48.8% H-10 => LUMO, 48.8% H-11 => L+1 57.6% H-1 => L+2, 15.1% H-10 => L+1, 15.1% H-
25	33678	297	0.00	11 => LUMO, 4.18% H-6 => LUMO, 4.18% H-7 => L+1
26	33682	297	0.15	35.6% H-14 => L+1, 31.3% H-13 => L+1, 26.3% H-12 => LUMO, 3.14% H-9 => L+1

				35.6% H-14 => LUMO, 31.3% H-13 => LUMO,
27	33682	297	0.15	26.3% H-12 => L+1, 3.14% H-9 => LUMO
				46.7% H-10 => LUMO, 46.7% H-11 => L+1,
28	33945	295	0.00	2.86% H-6 => L+1, 2.86% H-7 => LUMO
29	33951	295	0.00	48.5% H-10 => L+1, 48.5% H-11 => LUMO
30	34100	293	0.00	49.8% H-12 => LUMO, 48.1% H-13 => L+1
31	34100	293	0.00	49.8% H-12 => L+1, 48.1% H-13 => LUMO
32	34787	287	0.00	98.0% HOMO => L+3
33	34981	286	0.03	97.1% HOMO => L+5
34	34981	286	0.03	97.1% HOMO => L+4
35	35480	282	0.00	97.7% HOMO => L+6
36	35728	280	0.00	98.7% HOMO => L+8
37	35751	280	0.00	98.0% HOMO => L+7
38	36049	277	0.01	97.6% HOMO => L+9
39	36049	277	0.01	97.6% HOMO => L+10
40	36891	271	0.00	98.4% H-1 => L+3
41	37011	270	0.02	98.0% H-1 => L+4
42	37011	270	0.02	98.0% H-1 => L+5
43	37445	267	0.00	97.8% H-1 => L+6
44	37587	266	0.00	48.6% H-15 => LUMO, 48.6% H-16 => L+1
45	37765	265	0.00	99.5% H-1 => L+7
				94.9% H-1 => L+8, 2.04% H-15 => L+1, 2.04% H-
46	37841	264	0.00	16 => LUMO
47	38095	263	0.00	97.8% H-1 => L+10
48	38095	263	0.00	97.8% H-1 => L+9
				47.1% H-15 => L+1, 47.1% H-16 => LUMO,
49	38503	260	0.00	4.18% H-1 => L+8
				45.9% H-15 => L+1, 45.9% H-16 => LUMO,
50	39978	250	0.00	3.50% HOMO => L+12, 2.32% H-1 => L+2
				86.3% H-2 => L+2, 5.92% H-18 => L+1, 5.92% H-
51	40168	249	0.00	19 => LUMO
				44.4% H-15 => LUMO, 44.4% H-16 => L+1,
52	40859	245	0.00	3.20% H-1 => L+12
53	42855	233	0.00	96.4% H-3 => L+2
54	42933	233	0.06	96.8% H-4 => L+2
55	42933	233	0.06	96.8% H-5 => L+2
56	43706	229	0.00	96.2% HOMO => L+11
				9.02% H-8 => L+10, 8.81% H-12 => L+4, 8.30%
				H-7 => L+7, 8.02% H-6 => L+8, 7.66% H-11 =>
				L+3, 7.60% H-10 => L+6, 7.49% H-13 => L+5,
				6.98% H-9 => L+9, 6.20% H-6 => L+2, 4.41% H-
				11 => L+2, 3.43% H-3 => L+5, 3.18% H-4 => L+8,
57	44194	226	0.00	3.04% H-5 => L+7
				9.02% H-8 => L+9, 8.81% H-12 => L+5, 8.30% H-
				6 => L+7, 8.02% H-7 => L+8, 7.66% H-10 => L+3,
				7.60% H-11 => L+6, 7.49% H-13 => L+4, 6.98%
58	44194	226	0.00	H-9 => L+10, 6.20% H-7 => L+2, 4.41% H-10 =>

				L+2, 3.43% H-3 => L+4, 3.18% H-5 => L+8, 3.04% H-4 => L+7
59	44221	226	0.00	11.5% H-8 => L+8, 9.57% H-12 => L+3, 9.00% H-9 => L+7, 8.13% H-13 => L+6, 6.67% H-6 => L+4, 6.67% H-7 => L+5, 5.58% H-12 => L+2, 5.55% H-10 => L+5, 5.55% H-11 => L+4, 4.46% H-6 => L+10, 4.46% H-7 => L+9, 3.72% H-10 => L+9, 3.72% H-11 => L+10, 3.11% H-4 => L+10, 3.11% H-5 => L+9, 3.02% H-3 => L+6
60	44272	226	0.00	11.6% H-8 => L+7, 10.4% H-10 => L+4, 10.4% H-11 => L+5, 9.73% H-12 => L+6, 9.63% H-6 => L+9, 9.63% H-7 => L+10, 8.99% H-9 => L+8, 8.41% H-13 => L+3, 5.62% H-13 => L+2, 3.98% H-3 => L+3
61	44527	225	0.00	48.1% H-18 => L+1, 48.1% H-19 => LUMO
62	44792	223	0.00	48.1% H-18 => LUMO, 48.1% H-19 => L+1, 2.33% H-9 => L+2
63	44875	223	0.00	47.0% H-18 => LUMO, 47.0% H-19 => L+1, 3.15% HOMO => L+11
64	44949	222	0.03	87.5% H-6 => L+2, 2.63% H-11 => L+2
65	44949	222	0.03	87.5% H-7 => L+2, 2.63% H-10 => L+2
66	45158	221	0.00	40.8% H-18 => L+1, 40.8% H-19 => LUMO, 12.1% H-2 => L+2, 4.95% H-8 => L+2
67	45374	220	0.00	90.0% H-9 => L+2, 4.32% H-14 => L+2
68	45524	220	0.00	92.2% H-8 => L+2, 2.12% H-18 => L+1, 2.12% H-19 => LUMO
69	45901	218	0.00	99.7% H-1 => L+11
70	46273	216	0.00	72.7% HOMO => L+12, 12.2% H-12 => L+2, 4.89% H-2 => L+11, 2.58% H-3 => L+6
71	46294	216	0.00	82.0% H-14 => L+2, 4.54% H-9 => L+2, 3.94% H-1 => L+12, 2.27% H-4 => L+5, 2.27% H-5 => L+4
72	46427	215	0.07	90.9% H-17 => LUMO
73	46427	215	0.07	90.9% H-17 => L+1
74	46516	215	0.01	81.0% H-11 => L+2, 5.84% H-3 => L+5, 3.86% H-4 => L+3
75	46516	215	0.01	81.0% H-10 => L+2, 5.84% H-3 => L+4, 3.86% H-5 => L+3
76	46566	215	0.00	50.1% H-13 => L+2, 28.2% H-3 => L+3, 8.79% H-4 => L+5, 8.79% H-5 => L+4
77	46685	214	0.00	97.7% H-2 => L+3
78	46743	214	0.00	75.4% H-12 => L+2, 13.7% HOMO => L+12
79	46805	214	0.06	39.0% H-3 => L+5, 33.1% H-4 => L+3, 8.00% H-11 => L+2, 5.39% H-5 => L+6, 2.90% H-13 => L+5, 2.70% H-11 => L+3
80	46805	214	0.06	39.0% H-3 => L+4, 33.1% H-5 => L+3, 8.00% H-10 => L+2, 5.39% H-4 => L+6, 2.90% H-13 => L+4, 2.70% H-10 => L+3

				41.7% H-13 => L+2, 24.9% H-3 => L+3, 7.82% H-4 => L+5, 7.82% H-5 => L+4, 5.43% H-13 => L+3,
81	46845	213	0.00	2.05% H-10 => L+4, 2.05% H-11 => L+5
82	46883	213	0.01	97.0% H-2 => L+4
83	46883	213	0.01	97.0% H-2 => L+5
84	46979	213	0.00	35.6% H-3 => L+6, 24.7% H-4 => L+4, 24.7% H-5 => L+5, 4.31% H-12 => L+2, 2.53% H-13 => L+6
				31.1% H-4 => L+5, 31.1% H-5 => L+4, 15.7% H-3 => L+8, 5.57% H-14 => L+2, 5.02% H-14 => L+3,
85	47287	211	0.00	3.16% H-1 => L+12
				35.7% H-4 => L+4, 35.7% H-5 => L+5, 18.0% H-3 => L+7, 4.07% H-14 => L+6
86	47302	211	0.00	98.0% H-2 => L+6
87	47335	211	0.00	33.9% H-4 => L+3, 31.2% H-5 => L+6, 10.7% H-3 => L+5, 6.13% H-14 => L+5, 4.40% H-3 => L+9,
88	47432	211	0.03	3.87% H-5 => L+7, 2.71% H-4 => L+8
				33.9% H-5 => L+3, 31.2% H-4 => L+6, 10.7% H-3 => L+4, 6.13% H-14 => L+4, 4.40% H-3 => L+10,
89	47432	211	0.03	3.87% H-4 => L+7, 2.71% H-5 => L+8
				40.1% H-3 => L+9, 22.4% H-4 => L+8, 14.6% H-5 => L+7, 13.2% H-5 => L+6
90	47552	210	0.05	40.1% H-3 => L+10, 22.4% H-5 => L+8, 14.6% H-4 => L+7, 13.2% H-4 => L+6
91	47552	210	0.05	41.2% H-3 => L+8, 18.2% H-4 => L+9, 18.2% H-5 => L+10, 6.65% H-4 => L+5, 6.65% H-5 => L+4,
92	47565	210	0.00	3.52% H-14 => L+3
93	47642	210	0.00	99.3% H-2 => L+8
94	47652	210	0.00	99.1% H-2 => L+7
				41.3% H-3 => L+7, 17.8% H-4 => L+10, 17.8% H-5 => L+9, 6.04% H-4 => L+4, 6.04% H-5 => L+5,
95	47663	210	0.00	2.87% H-14 => L+6
96	47892	209	0.00	98.4% H-2 => L+10
97	47892	209	0.00	98.4% H-2 => L+9
				42.2% H-5 => L+7, 35.3% H-4 => L+8, 5.46% H-14 => L+9, 4.27% H-7 => L+7, 4.12% H-9 => L+9,
98	48129	208	0.01	4.07% H-6 => L+8
				42.2% H-4 => L+7, 35.3% H-5 => L+8, 5.46% H-14 => L+10, 4.27% H-6 => L+7, 4.12% H-9 =>
99	48129	208	0.01	L+10, 4.07% H-7 => L+8
				25.7% H-4 => L+9, 25.7% H-5 => L+10, 10.8% H-4 => L+5, 10.8% H-5 => L+4, 7.17% H-14 => L+8,
100	48169	208	0.00	7.13% H-3 => L+3, 4.71% H-9 => L+8, 2.95% H-6 => L+9, 2.95% H-7 => L+10
				29.5% H-4 => L+10, 29.5% H-5 => L+9, 6.89% H-14 => L+7, 5.87% H-4 => L+4, 5.87% H-5 => L+5,
101	48292	207	0.00	5.33% H-9 => L+7, 5.13% H-3 => L+6, 3.35% H-6 => L+10, 3.35% H-7 => L+9
				56.5% H-1 => L+12, 8.58% H-6 => L+5, 8.58% H-7 => L+4, 6.38% H-9 => L+3, 3.43% H-8 => L+6,
102	48699	205	0.00	2.08% H-4 => L+5, 2.08% H-5 => L+4

103	48825	205	0.00	31.2% H-3 => L+3, 19.5% H-4 => L+5, 19.5% H-5 => L+4, 12.7% H-4 => L+9, 12.7% H-5 => L+10 34.8% H-5 => L+6, 32.8% H-3 => L+5, 20.5% H-4 => L+3, 2.87% H-4 => L+8, 2.02% H-3 => L+9 34.8% H-4 => L+6, 32.8% H-3 => L+4, 20.5% H-5 => L+3, 2.87% H-5 => L+8, 2.02% H-3 => L+10 44.9% H-3 => L+6, 16.9% H-4 => L+4, 16.9% H-5 => L+5, 8.76% H-4 => L+10, 8.76% H-5 => L+9 25.5% H-3 => L+9, 15.5% H-4 => L+8, 14.9% H-5 => L+7, 11.7% H-6 => L+3, 4.98% H-7 => L+6, 4.14% H-5 => L+6, 4.14% H-9 => L+5, 3.84% H-8 => L+4, 2.16% H-6 => L+8, 2.13% H-7 => L+7, 2.13% H-11 => L+8, 2.08% H-10 => L+7 25.5% H-3 => L+10, 15.5% H-5 => L+8, 14.9% H-4 => L+7, 11.7% H-7 => L+3, 4.98% H-6 => L+6, 4.14% H-4 => L+6, 4.14% H-9 => L+4, 3.84% H-8 => L+5, 2.16% H-7 => L+8, 2.13% H-6 => L+7, 2.13% H-10 => L+8, 2.08% H-11 => L+7 33.7% H-3 => L+8, 24.8% H-4 => L+9, 24.8% H-5 => L+10, 5.61% H-1 => L+12, 2.39% H-4 => L+5, 2.39% H-5 => L+4 32.5% H-3 => L+7, 28.9% H-4 => L+10, 28.9% H-5 => L+9 23.4% H-6 => L+3, 19.0% H-3 => L+9, 10.0% H-5 => L+7, 9.49% H-4 => L+8, 5.00% H-9 => L+5, 3.72% H-8 => L+4, 3.28% H-7 => L+6, 2.83% H-13 => L+9, 2.82% H-3 => L+5, 2.71% H-10 => L+7, 2.58% H-12 => L+10, 2.58% H-11 => L+8, 2.27% H-16 => L+2 23.4% H-7 => L+3, 19.0% H-3 => L+10, 10.0% H-4 => L+7, 9.49% H-5 => L+8, 5.00% H-9 => L+4, 3.72% H-8 => L+5, 3.28% H-6 => L+6, 2.83% H-13 => L+10, 2.82% H-3 => L+4, 2.71% H-11 => L+7, 2.58% H-12 => L+9, 2.58% H-10 => L+8, 2.27% H-15 => L+2 15.4% H-6 => L+4, 15.4% H-7 => L+5, 12.7% H-8 => L+3, 7.38% H-12 => L+8, 7.22% H-13 => L+7, 6.16% H-9 => L+6, 4.72% H-6 => L+10, 4.72% H-7 => L+9, 3.86% H-10 => L+9, 3.86% H-11 => L+10, 3.54% H-3 => L+7, 2.98% H-10 => L+5, 2.98% H-11 => L+4, 2.14% H-4 => L+4, 2.14% H-5 => L+5, 2.11% H-14 => L+6 19.9% H-1 => L+12, 16.1% H-6 => L+5, 16.1% H-7 => L+4, 7.28% H-9 => L+3, 6.16% H-12 => L+7, 5.72% H-13 => L+8, 3.77% H-3 => L+8, 3.51% H-10 => L+10, 3.51% H-11 => L+9, 3.44% H-4 => L+9, 3.44% H-5 => L+10 80.3% H-20 => L+1, 11.0% HOMO => L+14 80.3% H-20 => LUMO, 11.0% HOMO => L+13 80.0% HOMO => L+14, 12.3% H-20 => L+1
104	48909	204	0.00	
105	48909	204	0.00	
106	49079	204	0.00	
107	49403	202	0.00	
108	49403	202	0.00	
109	49468	202	0.00	
110	49481	202	0.00	
111	49564	202	0.05	
112	49564	202	0.05	
113	49664	201	0.00	
114	49909	200	0.00	
115	50096	200	0.01	
116	50096	200	0.01	
117	50246	199	0.08	

118	50246	199	0.08	80.0% HOMO => L+13, 12.3% H-20 => LUMO 43.1% H-6 => L+5, 43.1% H-7 => L+4, 3.40% H-3 => L+3, 2.35% H-6 => L+9, 2.35% H-7 => L+10 38.8% H-6 => L+4, 38.8% H-7 => L+5, 5.50% H-3 => L+6, 3.94% H-6 => L+10, 3.94% H-7 => L+9, 2.23% H-10 => L+5, 2.23% H-11 => L+4
119	50310	199	0.01	38.8% H-6 => L+4, 38.8% H-7 => L+5, 5.50% H-3 => L+6, 3.94% H-6 => L+10, 3.94% H-7 => L+9, 2.23% H-10 => L+5, 2.23% H-11 => L+4 40.1% H-6 => L+3, 37.0% H-7 => L+6, 3.87% H-9 => L+5, 2.86% H-10 => L+6, 2.62% H-8 => L+4, 2.26% H-3 => L+5
120	50383	198	0.00	40.1% H-7 => L+3, 37.0% H-6 => L+6, 3.87% H-9 => L+4, 2.86% H-11 => L+6, 2.62% H-8 => L+5, 2.26% H-3 => L+4 40.4% H-8 => L+3, 15.8% H-6 => L+4, 15.8% H-7 => L+5, 6.10% H-6 => L+10, 6.10% H-7 => L+9, 4.62% H-14 => L+6
121	50428	198	0.00	61.4% H-9 => L+3, 9.10% H-6 => L+5, 9.10% H-7 => L+4, 8.26% H-8 => L+6, 4.38% H-14 => L+3 25.6% H-7 => L+7, 25.3% H-14 => L+5, 24.6% H-6 => L+8, 6.36% H-8 => L+4, 3.46% H-5 => L+6, 2.24% H-7 => L+6, 2.13% H-3 => L+9
122	50428	198	0.00	25.6% H-6 => L+7, 25.3% H-14 => L+4, 24.6% H-7 => L+8, 6.36% H-8 => L+5, 3.46% H-4 => L+6, 2.24% H-6 => L+6, 2.13% H-3 => L+10 29.6% H-9 => L+5, 29.6% H-8 => L+4, 15.7% H-7 => L+7, 5.94% H-6 => L+8, 4.09% H-14 => L+5, 2.87% H-7 => L+6, 2.12% H-8 => L+10
123	50784	197	0.00	29.6% H-9 => L+4, 29.6% H-8 => L+5, 15.7% H-6 => L+7, 5.94% H-7 => L+8, 4.09% H-14 => L+4, 2.87% H-6 => L+6, 2.12% H-8 => L+9
124	50786	197	0.00	74.3% H-14 => L+3, 4.43% H-9 => L+3, 2.54% H-4 => L+5, 2.54% H-5 => L+4 26.1% H-14 => L+5, 22.0% H-9 => L+5, 12.4% H-6 => L+8, 7.65% H-16 => L+2, 4.53% H-10 => L+7, 4.05% H-7 => L+7, 3.21% H-11 => L+8, 2.84% H-11 => L+3, 2.82% H-7 => L+6
125	50808	197	0.01	26.1% H-14 => L+4, 22.0% H-9 => L+4, 12.4% H-7 => L+8, 7.65% H-15 => L+2, 4.53% H-11 => L+7, 4.05% H-6 => L+7, 3.21% H-10 => L+8, 2.84% H-10 => L+3, 2.82% H-6 => L+6 31.1% H-9 => L+6, 23.5% H-8 => L+3, 15.6% H-6 => L+10, 15.6% H-7 => L+9, 4.33% H-6 => L+4, 4.33% H-7 => L+5
126	50808	197	0.01	35.0% H-6 => L+9, 35.0% H-7 => L+10, 8.58% H-8 => L+6, 2.87% H-10 => L+10, 2.87% H-11 => L+9, 2.75% H-3 => L+8, 2.21% H-9 => L+3 30.6% H-8 => L+4, 24.8% H-7 => L+6, 15.0% H-14 => L+5, 6.69% H-6 => L+3, 6.00% H-9 => L+5, 3.76% H-11 => L+3, 2.10% H-9 => L+9
127	50873	197	0.00	30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
128	50873	197	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
129	50927	196	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
130	50960	196	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
131	50960	196	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
132	50979	196	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
133	51107	196	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
134	51190	195	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10
135	51190	195	0.00	3.76% H-11 => L+3, 2.10% H-9 => L+9 30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10

136	51227	195	0.00	16.4% H-9 => L+6, 14.8% H-10 => L+5, 14.8% H-11 => L+4, 14.7% H-6 => L+10, 14.7% H-7 => L+9, 12.6% H-14 => L+6 28.0% H-8 => L+7, 27.4% H-14 => L+8, 23.1% H-9 => L+8, 5.30% H-4 => L+9, 5.30% H-5 => L+10,
137	51327	195	0.01	3.11% H-6 => L+9, 3.11% H-7 => L+10 29.5% H-8 => L+8, 29.0% H-9 => L+7, 26.0% H-14 => L+7, 4.75% H-4 => L+10, 4.75% H-5 =>
138	51347	195	0.00	L+9 28.2% H-16 => L+2, 15.7% H-14 => L+9, 15.1% H-6 => L+8, 9.21% H-7 => L+7, 5.49% H-8 => L+10, 4.25% H-11 => L+3, 3.68% H-11 => L+8, 2.22% H-7 => L+6, 2.19% H-5 => L+7, 2.06% H-10 => L+7
139	51409	195	0.01	

**Table S12.** TDDFT-predicted band excitation data for **2**.

Index	Energy ( $\text{cm}^{-1}$ )	$\lambda$ (nm)	Osc. Strength	Contributions
0	10034	997	0.67	93.9% HOMO => LUMO, 4.77% H-1 => L+1
1	10710	934	0.00	98.0% H-1 => LUMO
2	15028	665	0.00	94.1% HOMO => L+1, 3.56% H-5 => LUMO
3	16138	620	0.02	65.1% H-2 => LUMO, 32.6% HOMO => L+2 82.3% H-3 => LUMO, 13.8% H-1 => L+2, 3.49%
4	16742	597	0.00	H-2 => L+1 91.4% H-1 => L+1, 4.38% H-4 => LUMO, 3.89%
5	17434	574	1.64	HOMO => LUMO 93.4% H-4 => LUMO, 3.29% H-1 => L+1, 2.83%
6	18523	540	1.05	HOMO => LUMO 57.8% HOMO => L+2, 27.3% H-2 => LUMO,
7	19325	517	0.61	10.6% H-1 => L+3, 4.17% H-3 => L+1 56.7% HOMO => L+3, 34.4% H-1 => L+2, 6.40%
8	19602	510	0.00	H-3 => LUMO 93.0% H-5 => LUMO, 3.08% HOMO => L+1,
9	20645	484	0.00	2.56% H-3 => L+2 57.1% H-2 => L+1, 30.6% H-1 => L+2, 10.9%
10	21167	472	0.00	HOMO => L+3
11	21753	460	0.04	68.4% H-3 => L+1, 28.8% H-1 => L+3
12	21958	455	0.00	98.3% H-6 => LUMO
13	22992	435	0.00	97.9% H-7 => LUMO
14	23751	421	0.00	94.1% H-4 => L+1, 2.83% H-3 => L+2 64.0% H-2 => L+2, 25.6% HOMO => L+4, 4.81%
15	24104	415	0.10	H-3 => L+3, 4.23% H-5 => L+1 55.1% H-3 => L+2, 34.1% H-8 => LUMO, 4.00%
16	24448	409	0.00	H-2 => L+3, 3.36% H-1 => L+4 59.0% H-1 => L+3, 23.7% H-3 => L+1, 8.38%
17	24518	408	2.71	HOMO => L+2, 6.47% H-2 => LUMO

18	24760	404	0.00	35.8% H-2 => L+1, 30.1% HOMO => L+3, 18.6% H-1 => L+2, 10.0% H-3 => LUMO
19	24904	402	0.01	94.7% H-9 => LUMO, 2.41% H-4 => L+2 63.1% H-8 => LUMO, 26.6% H-3 => L+2, 3.23% H-2 => L+3, 2.81% H-4 => L+1, 2.30% H-1 => L+4
20	25081	399	0.00	37.2% HOMO => L+4, 33.1% H-5 => L+1, 25.5% H-2 => L+2, 2.24% H-12 => LUMO
21	25362	394	0.30	58.2% H-5 => L+1, 28.9% HOMO => L+4, 8.52% H-12 => LUMO
22	25715	389	0.38	77.0% H-10 => LUMO, 17.4% H-4 => L+2
23	25947	385	0.01	97.1% H-11 => LUMO
24	26144	383	0.00	94.4% H-13 => LUMO, 2.78% H-15 => LUMO
25	26249	381	0.00	74.2% H-12 => LUMO, 13.5% H-14 => LUMO,
26	26469	378	0.03	5.21% HOMO => L+4 57.0% H-4 => L+2, 20.5% H-6 => L+1, 15.8% H-10 => LUMO, 3.42% H-7 => L+2
27	26524	377	0.04	64.4% H-6 => L+1, 19.0% H-4 => L+2, 10.9% H-7 => L+2, 4.00% H-10 => LUMO
28	26613	376	0.00	83.8% H-14 => LUMO, 11.1% H-12 => LUMO
29	26767	374	0.06	93.4% H-15 => LUMO, 2.64% H-13 => LUMO
30	27044	370	0.00	70.3% H-7 => L+1, 28.2% H-6 => L+2
31	27187	368	0.00	95.6% H-16 => LUMO, 2.02% H-12 => LUMO
32	27202	368	0.06	73.7% H-1 => L+4, 22.5% H-2 => L+3
33	27440	364	0.00	91.5% H-17 => LUMO
34	27679	361	0.00	93.9% H-5 => L+2, 2.29% H-21 => LUMO
35	27914	358	0.00	95.2% H-18 => LUMO, 2.62% H-3 => L+3
36	27925	358	0.00	42.3% H-2 => L+3, 23.3% H-23 => LUMO, 16.6% H-20 => LUMO, 7.55% H-1 => L+4, 5.22% H-3 => L+2
37	27999	357	0.00	92.7% H-21 => LUMO, 2.07% H-17 => LUMO
38	28037	357	0.00	67.7% H-19 => LUMO, 30.3% H-22 => LUMO
39	28058	356	0.00	32.3% H-23 => LUMO, 25.8% H-20 => LUMO, 23.8% H-2 => L+3, 7.94% H-1 => L+4, 4.65% H-3 => L+2
40	28139	355	0.00	85.1% H-3 => L+3, 5.21% H-2 => L+2, 2.25% H-18 => LUMO
41	28276	354	0.27	65.7% H-22 => LUMO, 30.2% H-19 => LUMO
42	28294	353	0.00	55.6% H-20 => LUMO, 42.3% H-23 => LUMO
43	28316	353	0.00	90.4% H-24 => LUMO, 2.08% H-5 => L+3
44	29289	341	0.00	59.5% H-9 => L+1, 28.5% H-4 => L+3, 7.39% H-8 => L+2
45	29407	340	0.00	84.6% H-8 => L+1, 9.33% H-9 => L+2
46	29565	338	0.03	69.2% H-4 => L+3, 25.7% H-9 => L+1, 2.17% H-8 => L+2
47	30036	333	0.00	61.6% H-25 => LUMO, 28.9% H-11 => L+1, 2.84% H-10 => L+2
48	30752	325	0.14	

				79.8% H-13 => L+1, 7.00% H-14 => L+2, 4.48%
49	30753	325	0.20	H-15 => L+1, 2.43% H-12 => L+2
50	30879	324	0.00	87.3% H-10 => L+1, 6.46% H-11 => L+2
				51.3% H-12 => L+1, 30.6% H-14 => L+1, 9.17%
51	30921	323	0.00	H-13 => L+2, 2.46% H-16 => L+1
				56.4% H-11 => L+1, 29.5% H-25 => LUMO,
52	31014	322	0.14	4.46% H-10 => L+2
				47.4% H-14 => L+1, 22.3% H-12 => L+1, 11.0%
				H-26 => LUMO, 5.81% H-16 => L+1, 3.56% H-6
53	31362	319	0.00	=> L+2
54	31376	319	0.07	93.2% H-5 => L+3, 2.21% H-24 => LUMO
				66.9% H-6 => L+2, 27.2% H-7 => L+1, 2.80% H-
55	31412	318	0.00	12 => L+1
				63.3% H-15 => L+1, 8.30% H-7 => L+2, 7.63% H-
56	31798	314	0.00	17 => L+1, 5.01% H-2 => L+4, 4.66% H-16 =>
				L+2, 3.28% H-13 => L+1
57	31948	313	0.00	78.1% H-16 => L+1, 6.29% H-15 => L+2, 5.86%
				H-12 => L+1
58	32045	312	0.00	74.5% H-7 => L+2, 12.5% H-6 => L+1, 7.42% H-
				15 => L+1, 3.27% H-2 => L+4
59	32063	312	0.00	78.7% H-26 => LUMO, 9.55% H-12 => L+1,
				4.40% H-14 => L+1
60	32197	311	0.00	82.3% H-3 => L+4, 12.6% HOMO => L+5
				82.4% H-2 => L+4, 5.47% H-15 => L+1, 2.33% H-
61	32318	309	0.04	17 => L+1, 2.25% H-21 => L+1
62	32355	309	0.00	82.5% HOMO => L+5, 11.3% H-3 => L+4
				57.4% H-17 => L+1, 9.09% H-21 => L+1, 8.83%
				HOMO => L+8, 7.83% H-15 => L+1, 4.94% H-12
63	32419	308	0.05	=> L+2, 2.14% H-14 => L+2
64	32526	307	0.00	91.2% HOMO => L+6, 5.91% HOMO => L+10
				44.9% HOMO => L+7, 44.2% H-18 => L+1, 2.15%
65	32632	306	0.00	H-17 => L+2
				61.0% H-21 => L+1, 16.1% H-17 => L+1, 7.84%
				HOMO => L+8, 5.66% H-18 => L+2, 2.49% H-2
66	32681	306	0.02	=> L+4
67	32694	306	0.00	48.2% HOMO => L+7, 43.1% H-18 => L+1
				64.8% H-19 => L+1, 23.4% H-22 => L+1, 4.68%
68	32753	305	0.00	H-23 => L+2
				57.5% H-23 => L+1, 31.0% H-20 => L+1, 5.03%
69	32774	305	0.01	H-19 => L+2
				77.3% HOMO => L+8, 11.3% H-21 => L+1, 3.00%
70	32850	304	0.00	H-17 => L+1
71	33020	303	0.00	89.1% H-6 => L+3, 6.41% H-7 => L+4
				84.0% HOMO => L+10, 5.36% HOMO => L+6,
72	33070	302	0.02	4.96% H-20 => L+1
				87.3% HOMO => L+9, 4.33% H-19 => L+1, 3.05%
73	33085	302	0.00	H-22 => L+1
				59.0% H-22 => L+1, 19.1% H-19 => L+1, 6.74%
				HOMO => L+9, 4.60% H-20 => L+2, 4.04% H-27
74	33266	301	0.00	=> LUMO

				52.6% H-20 => L+1, 30.8% H-23 => L+1, 5.58%
75	33293	300	0.01	H-22 => L+2, 4.97% HOMO => L+10
76	33301	300	0.00	97.1% HOMO => L+11
77	33398	299	0.00	95.6% HOMO => L+12
78	33440	299	0.00	79.1% H-8 => L+2, 9.26% H-9 => L+1, 6.63% H-27 => LUMO
79	33482	299	0.01	81.4% H-9 => L+2, 9.51% H-8 => L+1, 3.16% HOMO => L+15
80	33491	299	0.00	47.3% H-27 => LUMO, 36.7% HOMO => L+16, 3.86% H-8 => L+2, 2.14% H-24 => L+1
81	33634	297	0.02	92.1% HOMO => L+15, 2.85% H-9 => L+2, 2.05% H-20 => L+1
82	33683	297	0.00	59.1% H-7 => L+3, 21.0% HOMO => L+16, 9.10% H-6 => L+4, 4.37% H-27 => LUMO
83	33689	297	0.00	95.6% HOMO => L+13
84	33734	296	0.00	93.6% HOMO => L+14
85	33741	296	0.00	39.0% HOMO => L+16, 24.4% H-27 => LUMO, 22.2% H-7 => L+3, 3.39% H-6 => L+4
86	34400	291	0.02	54.9% H-10 => L+2, 34.9% H-4 => L+4, 5.57% H-11 => L+1
87	34457	290	0.00	55.3% H-11 => L+2, 31.1% H-24 => L+1, 4.67% H-10 => L+1, 2.76% H-27 => LUMO
88	34484	290	0.00	70.5% H-1 => L+5, 16.1% H-12 => L+2
89	34581	289	0.04	55.5% H-4 => L+4, 32.4% H-10 => L+2, 2.95% H-9 => L+2, 2.88% H-11 => L+1
90	34601	289	0.04	49.3% H-12 => L+2, 22.7% H-1 => L+5, 4.83% H-8 => L+3, 4.57% H-13 => L+1, 4.45% H-14 => L+2, 3.87% H-16 => L+2, 2.98% H-21 => L+1
91	34679	288	0.00	56.0% H-13 => L+2, 24.5% H-1 => L+6, 7.68% H-14 => L+1, 2.65% H-9 => L+3, 2.49% H-12 => L+1
92	34777	288	0.00	64.2% H-1 => L+6, 19.5% H-13 => L+2, 4.16% H-1 => L+10, 4.05% H-9 => L+3, 2.83% H-14 => L+1
93	34842	287	0.04	93.6% H-1 => L+7, 2.23% H-2 => L+8
94	34902	287	0.00	36.1% H-24 => L+1, 34.0% H-1 => L+8, 21.0% H-11 => L+2
95	34957	286	0.00	59.2% H-1 => L+8, 20.4% H-24 => L+1, 11.4% H-11 => L+2, 2.48% H-1 => L+14
96	35237	284	0.04	60.0% H-14 => L+2, 11.4% H-8 => L+3, 5.53% H-16 => L+2, 5.49% H-12 => L+2, 3.48% H-13 => L+1, 3.08% H-17 => L+1, 2.72% H-11 => L+3, 2.40% H-15 => L+1
97	35267	284	0.00	82.7% H-1 => L+10, 6.05% H-9 => L+3, 3.75% H-1 => L+6, 3.24% H-2 => L+9
98	35268	284	0.00	81.4% H-1 => L+9, 5.95% H-8 => L+3, 3.07% H-14 => L+2, 2.80% H-2 => L+10
99	35357	283	0.00	56.5% H-9 => L+3, 10.4% H-25 => L+1, 6.72% H-1 => L+10, 6.53% H-13 => L+2, 5.94% H-15 =>

				L+2, 3.94% H-8 => L+4, 2.59% H-1 => L+6, 2.49% H-5 => L+4
100	35396	283	0.00	57.9% H-8 => L+3, 10.8% H-1 => L+9, 9.07% H-14 => L+2, 7.21% H-16 => L+2, 5.89% H-12 => L+2, 3.71% H-9 => L+4
101	35512	282	0.00	95.9% H-1 => L+11
102	35586	281	0.00	97.0% H-1 => L+12
				40.6% H-25 => L+1, 17.4% H-17 => L+2, 15.6% H-1 => L+15, 11.8% H-21 => L+2, 5.48% H-9 => L+3, 2.22% H-13 => L+2
103	35597	281	0.00	69.2% H-15 => L+2, 9.91% H-9 => L+3, 9.78% H-17 => L+2, 4.18% H-16 => L+1
104	35639	281	0.00	53.0% H-16 => L+2, 15.3% H-1 => L+16, 7.41% H-14 => L+2, 6.63% H-8 => L+3, 5.16% H-18 => L+2, 4.62% H-15 => L+1, 4.43% H-12 => L+2
105	35713	280	0.00	81.2% H-1 => L+16, 11.7% H-16 => L+2
106	35822	279	0.00	79.8% H-1 => L+15, 8.74% H-25 => L+1, 4.12% H-17 => L+2, 2.18% H-21 => L+2
107	35842	279	0.00	92.5% H-1 => L+13, 3.51% H-2 => L+14
108	35937	278	0.00	91.1% H-1 => L+14, 3.75% H-2 => L+13, 3.05% H-1 => L+8
109	35958	278	0.00	62.0% H-5 => L+4, 21.1% H-17 => L+2, 4.76% H-25 => L+1, 4.31% H-15 => L+2, 2.67% H-9 => L+3
110	36223	276	0.00	34.3% H-17 => L+2, 27.7% H-5 => L+4, 10.9% H-21 => L+2, 7.80% H-15 => L+2, 6.03% H-25 => L+1, 4.25% H-10 => L+3, 3.68% H-18 => L+1
111	36349	275	0.00	67.7% H-19 => L+2, 22.2% H-22 => L+2, 5.35% H-23 => L+1, 2.06% H-20 => L+1
112	36355	275	0.00	84.4% H-18 => L+2, 3.86% H-21 => L+1, 3.84% H-16 => L+2, 3.43% H-17 => L+1, 2.05% H-12 => L+2
113	36358	275	0.00	54.6% H-23 => L+2, 33.7% H-20 => L+2, 5.75% H-19 => L+1, 2.33% H-12 => L+3
114	36381	275	0.00	62.6% H-21 => L+2, 19.9% H-25 => L+1, 8.48% H-10 => L+3, 2.31% H-5 => L+4
115	36405	275	0.00	43.6% H-28 => LUMO, 32.9% HOMO => L+17, 16.5% H-12 => L+3
116	36784	272	0.00	53.1% H-13 => L+3, 13.3% H-22 => L+2, 9.16% H-19 => L+2, 8.29% H-24 => L+2, 3.92% H-26 => L+1, 2.48% H-15 => L+3, 2.47% H-14 => L+4, 2.24% H-20 => L+1
117	36822	272	0.04	68.6% H-12 => L+3, 14.7% HOMO => L+17, 4.66% H-28 => LUMO, 2.81% H-20 => L+2, 2.17% H-13 => L+4
118	36935	271	0.00	52.4% H-20 => L+2, 34.2% H-23 => L+2, 6.02% H-22 => L+1
119	36988	270	0.00	53.6% H-22 => L+2, 20.6% H-13 => L+3, 13.7% H-19 => L+2, 4.57% H-26 => L+1, 2.90% H-20 => L+1
120	37006	270	0.01	

121	37034	270	0.01	71.5% H-29 => LUMO, 11.8% H-11 => L+3, 5.50% H-25 => L+2, 2.69% H-1 => L+17, 2.03% H-12 => L+2 80.5% H-10 => L+3, 4.47% H-17 => L+2, 4.07% H-21 => L+2, 3.04% H-5 => L+4, 2.91% H-25 => L+1
122	37160	269	0.00	75.3% H-11 => L+3, 14.8% H-29 => LUMO,
123	37167	269	0.05	2.40% H-27 => L+1, 2.03% H-10 => L+4 72.4% H-14 => L+3, 9.49% H-16 => L+3, 3.92% H-15 => L+4, 2.52% H-18 => L+3, 2.40% HOMO => L+17
124	37293	268	0.00	79.8% H-15 => L+3, 5.36% H-17 => L+3, 3.65% H-12 => L+4, 2.72% H-13 => L+3
125	37410	267	0.03	45.9% H-26 => L+1, 30.2% H-24 => L+2, 13.0%
126	37589	266	0.02	H-13 => L+3, 2.86% H-4 => L+4 49.9% H-31 => LUMO, 20.1% H-6 => L+4, 9.27% HOMO => L+17, 9.03% H-7 => L+3, 4.00% H-28 => LUMO, 2.81% H-16 => L+3
127	37887	264	0.00	54.9% H-24 => L+2, 39.2% H-26 => L+1
128	38019	263	0.02	78.5% H-16 => L+3, 12.1% H-14 => L+3 56.6% H-27 => L+1, 25.6% H-25 => L+2, 8.24%
129	38119	262	0.00	H-1 => L+17, 3.46% H-11 => L+3 33.3% H-28 => LUMO, 30.6% HOMO => L+17, 7.96% H-6 => L+4, 6.58% H-31 => LUMO, 5.66%
130	38298	261	0.12	H-26 => L+2, 3.29% H-18 => L+3 79.1% H-17 => L+3, 4.82% H-15 => L+3, 4.75%
131	38318	261	0.00	H-21 => L+3, 3.35% H-30 => LUMO 62.6% H-22 => L+3, 14.7% H-19 => L+3, 12.9%
132	38544	259	0.03	HOMO => L+18, 3.69% H-20 => L+4, 2.04% H-23 => L+4
133	38646	259	0.00	59.7% H-20 => L+3, 29.4% H-23 => L+3, 5.15%
134	38657	259	0.01	H-22 => L+4 80.5% HOMO => L+18, 10.1% H-22 => L+3,
135	38716	258	0.00	2.90% H-19 => L+3 58.2% H-18 => L+3, 21.4% H-6 => L+4, 10.8% H-
136	38915	257	0.00	31 => LUMO 34.4% H-6 => L+4, 28.9% H-18 => L+3, 27.0% H-
137	38946	257	0.00	31 => LUMO, 2.35% H-7 => L+3 84.8% H-32 => LUMO, 4.11% H-27 => L+1,
138	39014	256	0.00	3.56% H-25 => L+2 82.8% H-21 => L+3, 4.83% H-17 => L+3
139	39018	256	0.00	

**Table S13.** TDDFT-predicted band excitation data for **3**.

Index	Energy ( $\text{cm}^{-1}$ )	$\lambda$ (nm)	Osc. Strength	Contributions
0	7363	1358	1.56	97.2% HOMO => LUMO, 2.30% H-1 => L+2
1	8032	1245	0.00	98.4% H-1 => LUMO

2	11803	847	0.00	86.6% H-3 => LUMO, 9.80% H-1 => L+1 90.1% H-2 => LUMO, 3.41% H-6 => LUMO,
3	12019	832	0.00	2.99% H-1 => L+3 91.5% HOMO => L+1, 2.73% H-2 => LUMO,
4	12902	775	0.00	2.08% H-6 => LUMO
5	13388	747	0.00	96.4% HOMO => L+2
6	14502	690	0.00	88.2% H-1 => L+1, 10.1% H-3 => LUMO 75.8% H-4 => LUMO, 20.1% HOMO => L+4,
7	15400	649	0.06	2.17% H-2 => L+3 90.2% H-1 => L+2, 5.79% H-5 => LUMO, 2.96%
8	15475	646	3.12	HOMO => LUMO
9	15708	637	0.00	87.9% HOMO => L+3, 5.65% H-8 => LUMO
10	16417	609	0.00	85.7% H-6 => LUMO, 8.63% H-1 => L+3 78.4% H-5 => LUMO, 9.56% H-1 => L+4, 5.45%
11	16436	608	0.01	H-1 => L+2, 3.26% H-3 => L+3 66.4% H-7 => LUMO, 21.5% H-2 => L+1, 4.05%
12	17689	565	0.41	H-1 => L+4, 2.13% H-3 => L+3 45.5% HOMO => L+4, 34.6% H-3 => L+1, 16.2%
13	17789	562	0.18	H-4 => LUMO 65.4% H-2 => L+2, 25.8% H-8 => LUMO, 6.14%
14	18272	547	0.00	HOMO => L+3 53.5% H-2 => L+1, 30.3% H-7 => LUMO, 6.96%
15	18486	541	0.14	H-1 => L+4, 3.77% H-5 => LUMO, 2.61% H-3 => L+3 80.9% H-1 => L+3, 7.29% H-3 => L+2, 4.93% H-
16	18538	539	0.00	6 -> LUMO, 2.44% H-2 => LUMO, 2.20% HOMO => L+1 68.8% H-9 => LUMO, 18.0% H-3 => L+1, 6.08%
17	19027	526	0.08	H-2 => L+3, 3.05% HOMO => L+4, 2.00% HOMO => L+2
18	19038	525	0.00	65.0% H-8 => LUMO, 28.7% H-2 => L+2 84.6% H-3 => L+2, 3.13% HOMO => L+1, 2.97%
19	19595	510	0.00	H-2 => LUMO, 2.85% H-1 => L+3, 2.61% H-6 => LUMO 33.1% H-3 => L+1, 26.6% HOMO => L+4, 24.9%
20	19602	510	0.49	H-9 => LUMO, 6.87% H-2 => L+3, 4.29% H-5 => L+2 43.7% H-1 => L+4, 31.1% HOMO => L+5, 11.7%
21	20092	498	0.06	H-2 => L+1, 6.84% H-10 => LUMO, 2.72% H-5 => LUMO 87.6% H-10 => LUMO, 3.68% HOMO => L+5,
22	20292	493	0.01	2.97% H-12 => LUMO, 2.49% H-1 => L+4 33.2% HOMO => L+5, 25.2% H-3 => L+3, 19.5%
23	20891	479	0.04	H-1 => L+4, 19.0% H-4 => L+2 69.4% H-2 => L+3, 13.3% H-1 => L+5, 7.67% H-
24	21275	470	0.61	3 => L+1, 2.69% H-4 => LUMO 92.7% H-11 => LUMO, 3.64% H-10 => L+1,
25	21447	466	0.00	2.89% H-12 => L+1 66.7% H-4 => L+1, 23.9% H-2 => L+4, 2.94% H-
26	21679	461	0.00	6 => L+2, 2.69% H-5 => L+3

27	21864	457	0.00	91.4% H-12 => LUMO, 5.23% H-11 => L+1, 2.39% H-10 => LUMO
28	22066	453	0.00	43.5% H-5 => L+1, 28.7% H-3 => L+4, 10.6% HOMO => L+6, 9.84% H-4 => L+3
29	22133	452	0.42	47.6% H-3 => L+3, 45.1% H-4 => L+2
30	22616	442	0.11	92.4% H-6 => L+1, 2.16% HOMO => L+5 60.6% H-6 => L+2, 29.5% H-2 => L+4, 3.46% H-
31	22693	441	0.00	4 => L+1, 2.10% H-1 => L+6
32	22863	437	0.06	70.4% H-5 => L+2, 18.6% H-1 => L+5, 2.86% H- 2 => L+3, 2.08% H-14 => LUMO
33	22909	437	0.00	55.8% HOMO => L+6, 36.2% H-5 => L+1, 3.54% H-3 => L+4
34	23089	433	0.00	25.4% H-6 => L+2, 21.7% H-2 => L+4, 20.6% H- 4 => L+1, 10.4% H-13 => LUMO, 9.89% H-15 =>
35	23555	425	0.00	LUMO, 4.24% H-1 => L+6
36	23580	424	0.00	92.1% H-14 => LUMO, 2.53% H-13 => L+1 83.9% H-13 => LUMO, 3.99% H-2 => L+4, 3.08% H-15 => LUMO, 3.05% H-6 => L+2,
37	23952	417	0.00	2.33% H-14 => L+1 53.8% H-3 => L+4, 13.1% HOMO => L+6, 12.3% H-7 => L+1, 6.89% H-5 => L+1, 5.24% H-8 =>
38	23955	417	0.00	L+2, 2.82% H-4 => L+3
39	24226	413	1.82	82.0% H-15 => LUMO, 5.54% H-2 => L+4, 3.60% H-1 => L+6, 2.38% H-6 => L+2
40	24548	407	0.57	46.4% H-1 => L+5, 15.6% H-8 => L+1, 10.9% H- 5 => L+2, 10.2% H-7 => L+2, 5.20% H-2 => L+3, 2.39% H-4 => LUMO, 2.30% H-3 => L+1, 2.08%
41	24589	407	0.06	HOMO => L+4, 2.03% H-6 => L+3 27.6% H-4 => L+2, 22.2% HOMO => L+5, 12.9% H-3 => L+3, 9.48% H-1 => L+4, 7.42% H-2 =>
42	24604	406	0.00	L+1, 4.58% H-5 => LUMO, 3.86% H-30 =>
43	24647	406	0.00	LUMO, 3.42% H-24 => LUMO
44	24692	405	0.00	71.0% H-16 => LUMO, 12.7% H-7 => L+2, 8.77% H-6 => L+3
45	24810	403	0.21	60.3% H-18 => LUMO, 14.8% H-7 => L+1, 4.99% H-4 => L+3, 4.37% H-8 => L+2, 4.05% H- 5 => L+1, 3.64% H-22 => LUMO, 3.17% HOMO
46	24962	401	0.02	=> L+6
47	25082	399	0.60	94.8% H-17 => LUMO 54.4% H-4 => L+3, 32.7% H-7 => L+1, 4.17% H- 3 => L+4, 2.39% HOMO => L+6
				44.5% H-7 => L+2, 24.3% H-16 => LUMO, 14.6% H-6 => L+3, 5.84% H-5 => L+2, 4.34% H- 1 => L+5, 2.16% H-8 => L+1
				88.5% H-19 => LUMO, 3.63% H-23 => LUMO 67.5% H-8 => L+1, 8.67% H-6 => L+3, 8.06% H- 1 => L+5, 3.95% H-2 => L+3, 3.05% H-5 => L+4, 2.24% H-5 => L+2

				48.9% H-20 => LUMO, 19.8% H-18 => LUMO, 11.5% H-7 => L+1, 6.29% H-8 => L+2, 3.59% HOMO => L+6, 2.02% H-5 => L+1
48	25093	399	0.00	47.0% H-5 => L+3, 22.8% H-9 => L+1, 12.0% H- 1 => L+6, 6.71% H-2 => L+4, 5.49% H-6 => L+4 53.1% H-8 => L+2, 20.2% H-7 => L+1, 16.0% H- 4 => L+3, 2.76% H-18 => LUMO, 2.12% H-20 => LUMO
49	25114	398	0.00	54.6% H-21 => LUMO, 21.7% H-9 => L+2, 12.5% H-23 => LUMO, 2.51% H-8 => L+3, 2.35% H-4 => L+4
50	25223	396	0.00	65.4% H-9 => L+1, 20.5% H-1 => L+6, 5.40% H- 5 => L+3, 2.66% H-2 => L+4, 2.06% H-3 => L+5 63.8% H-9 => L+2, 24.5% H-21 => LUMO, 2.84% H-8 => L+3, 2.41% H-23 => LUMO,
51	25265	396	0.02	2.25% H-19 => LUMO 43.0% H-20 => LUMO, 21.6% H-8 => L+2, 12.1% H-18 => LUMO, 6.09% HOMO => L+6,
52	25344	395	0.00	4.22% H-7 => L+1, 4.12% H-2 => L+5 49.7% H-6 => L+3, 24.0% H-7 => L+2, 8.58% H- 8 => L+1, 5.83% H-7 => L+4, 3.31% H-5 => L+4, 2.56% H-1 => L+5
53	25408	394	0.14	92.0% H-22 => LUMO 76.5% H-23 => LUMO, 14.3% H-21 => LUMO, 4.53% H-19 => LUMO
54	25410	394	0.00	48.8% H-1 => L+6, 21.2% H-5 => L+3, 8.02% H- 9 => L+1, 5.09% H-6 => L+4, 3.43% H-7 => L+3 80.1% H-4 => L+4, 4.73% H-9 => L+2, 3.79% H- 8 => L+3
55	25665	390	0.46	69.3% H-26 => LUMO, 28.1% H-25 => LUMO 42.7% H-27 => LUMO, 32.3% H-10 => L+2, 11.3% H-29 => LUMO, 5.54% H-32 => LUMO,
56	25673	390	0.00	2.61% H-12 => L+4, 2.59% H-11 => L+3 47.2% H-10 => L+2, 24.9% H-27 => LUMO, 9.53% H-29 => LUMO, 5.22% H-32 => LUMO, 3.76% H-12 => L+4, 3.50% H-11 => L+3, 2.03%
57	25686	389	0.05	H-10 => L+4
58	25887	386	0.01	80.4% H-24 => LUMO, 7.83% H-30 => LUMO 40.2% H-6 => L+4, 31.9% H-7 => L+3, 12.1% H- 5 => L+3, 5.13% H-33 => LUMO, 3.48% H-1 =>
59	26128	383	0.25	L+6
60	26195	382	0.00	66.8% H-25 => LUMO, 29.1% H-26 => LUMO 83.6% H-30 => LUMO, 11.3% H-24 => LUMO
61	26228	381	0.00	71.6% H-28 => LUMO, 23.4% H-31 => LUMO 35.6% H-29 => LUMO, 31.1% H-32 => LUMO, 30.1% H-27 => LUMO
62	26257	381	0.04	51.8% H-32 => LUMO, 40.6% H-29 => LUMO, 2.46% H-5 => L+4
63	26274	381	0.01	70.3% H-31 => LUMO, 24.6% H-28 => LUMO
64	26316	380	0.00	
65	26406	379	0.00	
66	26495	377	0.01	
67	26542	377	0.00	
68	26551	377	0.01	
69	26807	373	0.00	
70	26820	373	0.00	

				79.4% H-10 => L+1, 7.87% H-2 => L+5, 7.77%
71	26849	372	0.00	H-12 => L+1 54.3% H-11 => L+2, 20.4% H-10 => L+3, 15.1%
72	26912	372	0.00	H-12 => L+3, 6.86% H-11 => L+4 68.7% H-2 => L+5, 7.90% H-10 => L+1, 6.19%
73	26944	371	0.00	H-34 => LUMO, 4.29% H-4 => L+3 51.6% H-5 => L+4, 17.6% H-12 => L+2, 11.0%
74	27054	370	0.02	H-11 => L+3, 4.82% H-10 => L+4, 2.90% H-32 => LUMO, 2.71% H-6 => L+3 37.0% H-12 => L+2, 27.9% H-5 => L+4, 18.5%
75	27232	367	0.01	H-11 => L+3, 9.74% H-10 => L+4 80.9% H-3 => L+5, 5.09% H-5 => L+3, 3.62% H-
76	27362	365	0.01	33 => LUMO 70.7% H-8 => L+3, 16.2% H-9 => L+4, 6.58% H-
77	27370	365	0.01	4 => L+4 84.1% H-33 => LUMO, 6.72% H-7 => L+3,
78	27437	364	0.00	2.94% H-3 => L+5 69.5% H-9 => L+3, 24.5% H-8 => L+4
79	27520	363	0.00	52.0% H-7 => L+3, 41.4% H-6 => L+4, 2.93% H-
80	28069	356	0.00	6 => L+2 87.4% H-11 => L+1, 4.41% H-12 => LUMO,
81	28354	353	0.01	2.66% H-2 => L+6, 2.12% H-10 => LUMO 70.3% H-35 => LUMO, 12.8% H-3 => L+6,
82	28395	352	0.00	5.41% H-7 => L+4, 3.30% H-4 => L+5 84.7% H-34 => LUMO, 3.26% H-2 => L+5
83	28438	352	0.00	86.0% H-2 => L+6, 2.73% H-11 => L+1, 2.44% H-5 => L+5, 2.26% H-4 => L+4
84	28446	352	0.29	84.5% H-12 => L+1, 6.82% H-10 => L+1, 4.92% H-11 => LUMO, 2.40% H-11 => L+5 74.7% H-7 => L+4, 12.3% H-35 => LUMO,
85	28643	349	0.00	3.96% H-6 => L+3, 3.31% H-3 => L+6 67.3% H-3 => L+6, 8.82% H-7 => L+4, 7.90% H-35 => LUMO, 4.53% H-5 => L+4, 2.70% H-4 =>
86	29019	345	0.10	L+5 64.9% H-13 => L+2, 18.2% H-14 => L+3, 4.60% H-8 => L+4, 2.10% H-9 => L+3 68.6% H-14 => L+2, 20.7% H-13 => L+3, 2.67% H-14 => L+4
87	29307	341	0.10	58.4% H-8 => L+4, 21.3% H-9 => L+3, 5.98% H-15 => L+2, 4.80% H-13 => L+2, 2.32% H-14 => L+3 69.3% H-15 => L+1, 10.7% H-13 => L+1, 5.22% H-23 => L+2, 2.64% H-21 => L+2, 2.07% H-30 => L+2
88	29441	340	0.00	78.6% H-9 => L+4, 16.2% H-8 => L+3, 2.63% H-9 => L+2 65.4% H-15 => L+2, 7.20% H-23 => L+1, 6.42% H-8 => L+4, 3.25% H-15 => L+4, 3.03% H-21 => L+1, 2.88% H-30 => L+1, 2.87% H-19 => L+1, 2.17% H-9 => L+3
89	29466	339	0.04	
90	29554	338	0.00	
91	29667	337	0.00	
92	29752	336	0.01	
93	29839	335	0.00	

94	29889	335	0.00	86.4% H-14 => L+1, 2.98% H-18 => L+2, 2.77% H-13 => LUMO
95	29901	334	0.02	77.2% H-13 => L+1, 8.22% H-15 => L+1, 3.65% H-19 => L+2, 2.60% H-14 => LUMO
96	30122	332	0.00	87.1% H-36 => LUMO, 2.09% H-35 => L+1
97	30273	330	0.02	84.8% H-4 => L+5, 6.59% H-3 => L+6 60.2% H-10 => L+3, 31.9% H-11 => L+2, 7.21%
98	30539	327	0.00	H-11 => L+4 64.3% H-37 => LUMO, 14.8% H-16 => L+2, 4.32% H-5 => L+5, 3.55% H-17 => L+3, 2.58%
99	30586	327	0.14	H-6 => L+6 52.6% H-16 => L+2, 14.2% H-37 => LUMO, 12.1% H-17 => L+3, 5.27% H-5 => L+5, 5.00%
100	30730	325	0.05	H-18 => L+1, 2.09% H-14 => L+2
101	30740	325	0.00	74.1% H-17 => L+2, 16.7% H-16 => L+3 53.1% H-18 => L+2, 13.5% H-20 => L+2, 11.5% H-19 => L+3, 6.46% H-14 => L+1, 3.50% H-21
102	30806	325	0.00	=> L+3, 2.39% H-22 => L+2 45.7% H-19 => L+2, 14.2% H-21 => L+2, 9.17% H-18 => L+3, 9.11% H-20 => L+3, 5.40% H-13
103	30890	324	0.13	=> L+1, 3.67% H-12 => L+2, 2.89% H-11 => L+3 32.9% H-12 => L+2, 32.8% H-11 => L+3, 9.46% H-10 => L+4, 7.74% H-10 => L+2, 7.22% H-12
104	30947	323	0.02	=> L+4, 4.06% H-19 => L+2, 2.26% H-21 => L+2 53.3% H-18 => L+1, 9.12% H-26 => L+1, 8.35% H-27 => L+2, 7.57% H-22 => L+1, 5.68% H-16 => L+2, 2.77% H-25 => L+1, 2.23% H-32 => L+2,
105	30964	323	0.00	2.18% H-29 => L+2 82.1% H-16 => L+1, 7.13% H-22 => L+2, 2.84%
106	31089	322	0.00	H-20 => L+2, 2.17% H-17 => LUMO
107	31112	321	0.02	88.5% H-17 => L+1, 3.77% H-23 => L+2 81.8% H-6 => L+5, 2.72% H-7 => L+6, 2.63% H-13 => L+2, 2.56% H-5 => L+6, 2.02% H-21 =>
108	31122	321	0.00	L+1 33.8% H-20 => L+2, 12.3% H-27 => L+1, 11.1% H-26 => L+2, 7.71% H-16 => L+1, 7.19% H-22 => L+2, 4.25% H-29 => L+1, 4.21% H-21 => L+3, 3.93% H-18 => L+2, 3.26% H-32 => L+1, 2.24%
109	31128	321	0.00	H-36 => LUMO
110	31243	320	0.06	71.0% H-5 => L+5, 10.6% H-37 => LUMO, 4.38% HOMO => L+7, 2.08% H-14 => L+2 64.3% H-19 => L+1, 7.37% HOMO => L+8, 7.18% HOMO => L+9, 6.86% H-15 => L+2,
111	31360	319	0.00	4.30% H-38 => LUMO, 3.93% H-23 => L+1 70.4% HOMO => L+7, 6.68% H-26 => L+1, 5.22% H-5 => L+5, 4.79% H-27 => L+2, 2.32%
112	31374	319	0.02	H-18 => L+1 59.7% H-12 => L+3, 13.0% H-11 => L+4, 11.8%
113	31436	318	0.00	H-10 => L+3, 10.7% H-11 => L+2

114	31452	318	0.00	42.6% HOMO => L+9, 34.1% HOMO => L+8, 15.8% H-19 => L+1, 3.78% H-21 => L+1 35.0% H-20 => L+1, 24.4% H-18 => L+1, 11.4% HOMO => L+7, 7.73% H-26 => L+1, 4.30% H-27 => L+2, 2.59% H-22 => L+1, 2.26% H-29 => L+2,
115	31469	318	0.00	2.07% H-5 => L+5 38.5% H-21 => L+2, 13.0% H-23 => L+2, 11.4% H-19 => L+2, 10.8% H-15 => L+1, 7.09% HOMO => L+10, 4.90% HOMO => L+12, 4.07% H-20 =>
116	31499	317	0.00	21.4% H-20 => L+2, 20.2% H-26 => L+2, 17.2% H-18 => L+2, 16.9% H-27 => L+1, 5.91% H-21 => L+3, 3.15% H-29 => L+1, 2.50% H-25 => L+2,
117	31599	316	0.00	2.28% H-32 => L+1 45.8% HOMO => L+10, 35.9% HOMO => L+12,
118	31633	316	0.01	8.78% H-21 => L+2, 3.09% H-19 => L+2 45.3% H-21 => L+1, 16.6% H-38 => LUMO, 7.88% H-23 => L+1, 5.97% H-15 => L+2, 3.19% H-30 => L+1, 2.85% HOMO => L+8, 2.80% H-6 => L+5, 2.24% HOMO => L+9, 2.19% H-33 =>
119	31662	316	0.00	L+2 46.9% H-10 => L+4, 17.4% H-12 => L+4, 8.57% H-10 => L+2, 8.30% H-23 => L+2, 4.99% H-11 => L+3, 3.33% H-12 => L+2, 2.97% HOMO =>
120	31699	315	0.01	L+12, 2.37% H-22 => L+3 47.6% HOMO => L+8, 38.6% HOMO => L+9,
121	31721	315	0.00	4.36% H-38 => LUMO, 4.26% HOMO => L+14, 2.31% H-2 => L+7 47.9% H-20 => L+1, 8.50% H-18 => L+1, 8.45%
122	31792	315	0.04	H-27 => L+2, 7.95% H-26 => L+1, 7.09% H-22 => L+1, 4.73% HOMO => L+7 46.6% H-22 => L+2, 13.9% HOMO => L+11,
123	31800	314	0.00	8.02% H-23 => L+3, 3.89% H-25 => L+2, 3.77% H-26 => L+2, 3.67% H-4 => L+6, 3.48% H-16 => L+1 35.8% H-23 => L+2, 13.1% HOMO => L+12, 9.67% H-22 => L+3, 9.03% H-10 => L+4, 5.56% H-21 => L+2, 3.83% H-17 => L+1, 3.62% HOMO => L+10, 3.24% H-24 => L+2, 2.94% H-12 =>
124	31861	314	0.01	L+4, 2.91% H-19 => L+2 58.3% H-38 => LUMO, 19.7% H-21 => L+1, 3.96% H-19 => L+1, 2.83% H-15 => L+2, 2.53%
125	31869	314	0.00	HOMO => L+9, 2.40% H-6 => L+5 74.7% HOMO => L+11, 7.23% H-22 => L+2,
126	31968	313	0.00	6.70% H-4 => L+6 36.8% HOMO => L+10, 31.1% HOMO => L+12,
127	31999	313	0.02	13.3% H-23 => L+2 66.4% H-23 => L+1, 12.1% H-21 => L+1, 5.22% H-19 => L+1, 3.60% H-15 => L+2, 2.93% H-38 => LUMO
128	32090	312	0.00	

				51.1% H-4 => L+6, 19.8% HOMO => L+15, 12.8% HOMO => L+17, 3.21% H-8 => L+5,
129	32181	311	0.00	2.54% H-22 => L+2, 2.05% H-25 => L+2 71.0% H-22 => L+1, 8.09% H-26 => L+1, 4.07%
130	32181	311	0.01	H-25 => L+1, 2.94% H-32 => L+2, 2.72% H-29 => L+2
131	32239	310	0.00	48.6% HOMO => L+15, 23.8% H-4 => L+6, 13.3% HOMO => L+17, 4.02% HOMO => L+11,
132	32279	310	0.00	2.35% HOMO => L+19 33.5% H-24 => L+2, 24.1% H-30 => L+2, 7.31%
133	32279	310	0.00	HOMO => L+12, 6.10% H-18 => L+3, 4.28% H- 33 => L+1, 3.93% H-20 => L+3, 2.29% HOMO
134	32323	309	0.00	=> L+10, 2.12% H-15 => L+1
135	32341	309	0.04	51.4% HOMO => L+13, 29.8% HOMO => L+18, 4.97% HOMO => L+21, 3.74% H-7 => L+5,
136	32426	308	0.03	3.07% H-6 => L+6 83.0% HOMO => L+14, 2.89% H-2 => L+13,
137	32465	308	0.00	2.35% HOMO => L+9 34.8% HOMO => L+13, 34.1% HOMO => L+18,
138	32468	308	0.00	7.09% H-7 => L+5, 5.41% H-6 => L+6, 5.24% H- 13 => L+3, 3.13% H-14 => L+2
139	32506	308	0.00	25.3% HOMO => L+18, 17.5% H-13 => L+3, 17.5% H-7 => L+5, 11.1% H-6 => L+6, 8.38% H- 14 => L+2, 3.24% H-14 => L+4, 2.93% H-20 =>
140	32521	307	0.00	L+1
141	32545	307	0.04	30.9% H-30 => L+2, 25.2% H-24 => L+2, 20.8%
142	32586	307	0.00	HOMO => L+16, 8.91% H-25 => L+3, 3.10% H- 28 => L+1, 3.01% H-26 => L+3
143	32588	307	0.01	49.6% H-25 => L+2, 10.8% H-26 => L+2, 9.44%
				HOMO => L+17, 8.60% H-24 => L+3, 4.20% H- 30 => L+3, 3.25% H-4 => L+6, 2.42% HOMO =>
				L+15
				28.7% H-14 => L+3, 15.3% H-28 => L+2, 13.5%
				H-24 => L+1, 9.67% H-13 => L+2, 5.94% H-21 => L+1, 5.41% H-31 => L+2, 5.06% HOMO =>
				L+14, 4.89% H-13 => L+4
				30.0% H-14 => L+3, 23.1% H-24 => L+1, 13.3%
				H-28 => L+2, 10.9% H-13 => L+2, 5.34% H-13 => L+4, 4.94% H-31 => L+2
				16.4% H-27 => L+2, 15.9% H-13 => L+3, 13.7%
				H-29 => L+2, 11.0% H-32 => L+2, 5.82% H-28 => L+3, 5.55% H-7 => L+5, 4.77% H-25 => L+1,
				4.48% H-14 => L+2, 4.23% H-22 => L+1, 3.66%
				HOMO => L+13, 3.22% H-6 => L+6, 2.73% H-14 => L+4, 2.15% H-31 => L+3, 2.05% H-26 => L+1
				75.3% HOMO => L+16, 9.43% H-30 => L+2,
				6.17% H-24 => L+2
				21.6% H-13 => L+3, 14.7% H-7 => L+5, 10.6%
				H-6 => L+6, 8.62% H-25 => L+1, 7.31% H-27 =>
				L+2, 6.74% HOMO => L+21, 5.86% H-14 =>

				L+2, 5.03% H-29 => L+2, 4.52% H-32 => L+2, 3.43% H-14 => L+4, 2.54% H-28 => L+3 58.2% HOMO => L+17, 24.9% HOMO => L+15,
144	32589	307	0.00	7.86% H-25 => L+2 26.3% H-30 => L+1, 21.2% H-24 => L+1, 19.8% H-28 => L+2, 7.34% HOMO => L+22, 5.02% H-
145	32658	306	0.00	23 => L+1, 4.84% H-31 => L+2 70.9% HOMO => L+21, 13.3% H-25 => L+1,
146	32744	305	0.01	5.38% HOMO => L+18
147	32847	304	0.00	78.8% HOMO => L+22, 12.2% H-30 => L+1 87.9% HOMO => L+19, 2.96% H-2 => L+20,
148	32920	304	0.00	2.67% HOMO => L+17 89.4% HOMO => L+20, 2.90% H-28 => L+1,
149	32923	304	0.00	2.86% H-2 => L+19 53.2% H-25 => L+1, 10.8% H-32 => L+2, 8.74%
				H-26 => L+1, 7.10% HOMO => L+21, 3.45% H-
150	32942	304	0.01	29 => L+2, 2.69% H-27 => L+2, 2.22% H-31 => L+3 41.5% H-30 => L+1, 25.1% H-24 => L+1, 12.2%
151	32975	303	0.00	H-31 => L+2, 5.85% HOMO => L+22, 2.88% H-
152	33009	303	0.00	28 => L+2, 2.69% H-32 => L+3 84.1% H-5 => L+6, 3.43% H-24 => L+1, 2.14%
				H-6 => L+5
153	33021	303	0.00	50.9% H-29 => L+1, 22.9% H-32 => L+1, 8.25%
154	33031	303	0.00	H-25 => L+2, 4.90% H-26 => L+2, 2.65% H-8 =>
155	33066	302	0.00	L+5, 2.56% H-27 => L+1 60.4% H-28 => L+1, 28.4% H-31 => L+1, 2.82%
				H-24 => L+2
156	33092	302	0.00	53.8% H-27 => L+1, 27.2% H-26 => L+2, 7.99%
				H-32 => L+1
157	33151	302	0.00	32.1% H-26 => L+1, 31.5% H-29 => L+2, 22.7%
				H-27 => L+2, 3.92% H-25 => L+1, 2.15% H-31
				=> L+3
158	33153	302	0.00	44.9% H-31 => L+2, 25.8% H-28 => L+2, 7.68%
159	33154	302	0.00	H-29 => L+3, 6.45% H-32 => L+3, 3.93% H-30
160	33211	301	0.00	=> L+1, 2.50% H-17 => L+2 42.4% H-32 => L+2, 17.0% H-29 => L+2, 12.0%
161	33217	301	0.00	H-26 => L+1, 9.33% H-27 => L+2, 8.12% H-31
162	33272	301	0.00	=> L+3, 3.96% H-28 => L+3 80.1% H-8 => L+5, 6.20% H-9 => L+6, 6.02% H-
163	33332	300	0.03	4 => L+6, 2.41% H-29 => L+1 63.0% H-31 => L+1, 27.8% H-28 => L+1 55.7% H-32 => L+1, 28.6% H-29 => L+1, 4.23%
				H-27 => L+1, 3.84% H-26 => L+2
				78.4% H-15 => L+3, 15.0% HOMO => L+23 58.2% HOMO => L+23, 15.9% H-15 => L+3,
				5.40% H-40 => LUMO, 3.74% H-17 => L+3, 2.58% H-27 => L+2, 2.57% HOMO => L+21

				61.5% H-9 => L+5, 9.85% H-18 => L+3, 7.05% H-8 => L+6, 6.23% H-33 => L+1, 3.90% H-19 => L+2, 2.48% H-1 => L+7
164	33412	299	0.08	59.9% H-16 => L+3, 16.5% H-17 => L+2, 10.8% H-17 => L+4, 4.60% H-31 => L+2, 3.68% H-33 => L+2
165	33521	298	0.00	58.0% H-17 => L+3, 16.7% H-16 => L+2, 10.3% H-16 => L+4, 3.10% H-32 => L+2, 2.29% H-15 => L+3
166	33536	298	0.00	57.3% H-1 => L+9, 37.7% H-1 => L+8
167	33543	298	0.00	66.2% H-1 => L+7, 17.0% H-39 => LUMO, 3.17% H-18 => L+3, 2.30% H-1 => L+13, 2.10% H-3 => L+8
168	33568	298	0.20	32.4% H-18 => L+3, 21.6% H-9 => L+5, 10.9% H-19 => L+2, 10.1% H-1 => L+7, 5.66% H-39 => LUMO, 4.24% H-19 => L+4, 4.15% H-30 => L+2, 2.00% H-20 => L+3
169	33693	297	0.00	52.1% H-19 => L+3, 10.3% H-18 => L+2, 10.2% H-18 => L+4, 7.85% H-20 => L+2, 3.86% H-1 => L+9, 3.30% H-34 => L+2, 2.51% H-26 => L+2
170	33756	296	0.00	50.8% H-1 => L+12, 41.7% H-1 => L+10
171	33763	296	0.04	49.7% H-6 => L+6, 40.1% H-7 => L+5, 3.00% H-34 => L+1
172	33836	296	0.00	53.8% H-33 => L+1, 8.33% H-39 => LUMO, 7.25% H-18 => L+3, 5.07% H-20 => L+3, 3.49% H-30 => L+2, 3.34% H-1 => L+7, 3.00% H-21 => L+2, 2.71% H-19 => L+2, 2.66% H-9 => L+5
173	33838	296	0.00	71.5% H-11 => L+4, 21.6% H-12 => L+3, 5.68% H-10 => L+3
174	33959	294	0.00	78.2% H-33 => L+2, 3.80% H-30 => L+1, 3.16% H-16 => L+3, 2.11% H-15 => L+4
175	34050	294	0.00	45.4% H-1 => L+8, 30.3% H-1 => L+9, 6.81% H-1 => L+14, 5.33% H-3 => L+7, 2.94% H-19 => L+3, 2.09% H-21 => L+3
176	34055	294	0.00	55.0% H-12 => L+4, 18.7% H-11 => L+3, 11.4% H-10 => L+4, 4.35% H-39 => LUMO, 2.94% H-20 => L+3, 2.31% H-33 => L+1
177	34079	293	0.00	24.2% H-39 => LUMO, 21.3% H-20 => L+3, 17.6% H-33 => L+1, 8.87% H-12 => L+4, 5.14% H-21 => L+2, 3.50% H-30 => L+2, 2.85% H-11 => L+3, 2.59% H-1 => L+7, 2.35% H-21 => L+4
178	34093	293	0.01	34.5% H-21 => L+3, 25.3% H-34 => L+2, 8.80% H-20 => L+2, 6.94% H-20 => L+4, 5.81% H-30 => L+3, 4.41% H-1 => L+8, 3.44% H-23 => L+3
179	34187	293	0.00	

**Table S14.** TDDFT-predicted band excitation data for **4**.

<i>Index</i>	<i>Energy (cm<sup>-1</sup>)</i>	$\lambda$ (nm)	<i>Osc. Strength</i>	<i>Contributions</i>
0	5871	1703	2.54	98.4% HOMO => LUMO
1	6707	1491	0.00	97.9% H-1 => LUMO
2	9452	1058	0.00	86.1% H-3 => LUMO, 11.4% H-1 => L+1
3	9738	1027	0.00	91.5% H-2 => LUMO, 5.29% HOMO => L+1 90.2% HOMO => L+1, 3.76% H-2 => LUMO,
4	10183	982	0.00	2.23% H-1 => L+3
5	11885	841	0.00	86.4% H-1 => L+1, 11.8% H-3 => LUMO 77.9% H-4 => LUMO, 11.1% H-3 => L+1, 4.04%
6	12386	807	0.00	H-1 => L+4, 2.50% HOMO => L+2
7	12583	795	0.00	94.3% HOMO => L+2, 2.41% H-4 => LUMO 82.1% H-5 => LUMO, 6.82% H-7 => LUMO,
8	12687	788	0.16	3.94% H-2 => L+1 37.8% HOMO => L+4, 33.9% H-2 => L+1, 8.55% H-5 => LUMO, 7.41% H-7 => LUMO, 6.40% H-1 => L+2, 2.34% H-3 => L+3
9	14091	710	0.34	92.1% HOMO => L+3, 2.56% H-2 => L+2, 2.37%
10	14305	699	0.01	H-12 => LUMO 70.0% H-3 => L+1, 15.5% H-4 => LUMO, 11.0%
11	14395	695	0.00	H-1 => L+4 42.5% H-1 => L+2, 38.8% HOMO => L+4, 13.9%
12	14439	693	2.16	H-2 => L+1 44.6% H-1 => L+2, 39.3% H-2 => L+1, 11.7%
13	14872	672	1.29	HOMO => L+4 81.0% H-6 => LUMO, 13.6% HOMO => L+6,
14	15006	666	0.11	2.13% H-2 => L+5 76.8% H-7 => LUMO, 5.70% H-1 => L+5, 5.38%
15	15730	636	0.00	HOMO => L+4, 3.59% H-3 => L+3, 2.19% H-5 => LUMO 68.1% HOMO => L+5, 10.7% H-10 => LUMO,
16	15935	628	0.00	8.65% H-1 => L+4, 3.08% H-6 => L+1, 2.23% H-2 => L+3
17	16099	621	0.00	88.0% H-8 => LUMO, 4.02% H-1 => L+6, 2.12% H-7 => L+1, 2.00% H-3 => L+5
18	16396	610	0.00	72.7% H-1 => L+4, 13.2% H-3 => L+1, 10.4% HOMO => L+5
19	16530	605	0.00	59.9% H-9 => LUMO, 25.9% H-1 => L+3, 3.54% H-1 => L+6, 3.15% H-3 => L+2, 3.13% H-5 =>
20	16737	597	0.00	L+1 HOMO => L-12 => LUMO 39.1% HOMO => L+6, 37.5% H-4 => L+1, 12.2%
21	17184	582	0.06	H-6 => LUMO, 5.73% H-3 => L+4, 2.02% H-12 => LUMO 64.5% H-1 => L+3, 16.7% H-9 => LUMO, 6.59% H-5 => L+1, 3.15% H-3 => L+5, 2.69% H-2 =>
22	17207	581	0.00	LUMO
23	17438	573	0.61	93.7% H-11 => LUMO, 2.67% H-9 => L+1

24	17747	563	0.00	66.5% H-10 => LUMO, 13.0% HOMO => L+5, 11.9% H-2 => L+3, 2.06% H-5 => L+2 63.8% H-3 => L+2, 18.5% H-5 => L+1, 4.78% H-1 => L+6, 2.80% H-1 => L+3, 2.74% H-4 => L+3, 2.59% H-2 => L+4
25	17780	562	0.00	45.4% H-5 => L+1, 27.7% H-3 => L+2, 16.5% H-9 => LUMO, 2.36% H-2 => L+4, 2.22% H-3 => L+5
26	18051	554	0.00	60.9% H-13 => LUMO, 22.6% H-2 => L+3, 9.32% H-10 => LUMO
27	18198	550	0.00	58.5% H-12 => LUMO, 22.3% H-4 => L+1, 6.64% HOMO => L+6, 3.50% H-2 => L+5, 3.43% H-2 => L+2
28	18330	546	0.17	29.2% H-4 => L+1, 28.3% H-12 => LUMO, 27.1% HOMO => L+6, 8.91% H-3 => L+4
29	18623	537	0.37	45.4% H-2 => L+3, 32.7% H-13 => LUMO, 8.48% H-10 => LUMO, 5.87% H-5 => L+2, 2.78% H-6 => L+1
30	18719	534	0.00	69.0% H-2 => L+4, 15.4% H-5 => L+1, 7.80% H-1 => L+6
31	18788	532	0.00	81.3% H-1 => L+5, 3.97% H-4 => L+2, 3.26% H-7 => LUMO, 2.59% H-8 => L+1
32	18898	529	0.02	92.8% H-14 => LUMO, 2.38% H-15 => L+1
33	19561	511	0.00	83.0% H-3 => L+3, 2.37% H-2 => L+1, 2.16% HOMO => L+8, 2.09% H-1 => L+2
34	19632	509	0.68	66.2% H-3 => L+4, 13.6% H-2 => L+5, 9.24% HOMO => L+6, 3.81% H-5 => L+3, 2.04% H-12 => LUMO
35	19743	507	0.14	74.1% H-6 => L+1, 9.28% H-2 => L+6, 5.75% H-2 => L+3, 2.68% H-5 => L+2, 2.25% HOMO => L+5
36	20005	500	0.00	50.2% H-7 => L+1, 16.6% H-1 => L+6, 12.2% HOMO => L+7, 9.03% H-2 => L+4, 3.89% H-8 => LUMO
37	20206	495	0.00	84.3% H-15 => LUMO, 7.55% H-17 => LUMO,
38	20286	493	0.00	5.31% H-14 => L+1
39	20310	492	0.00	80.2% H-5 => L+2, 6.30% H-2 => L+3, 3.14% H-6 => L+1, 2.82% H-7 => L+2, 2.11% H-5 => L+5
40	20333	492	0.00	42.9% H-1 => L+6, 31.6% H-7 => L+1, 6.49% H-6 => L+2, 5.04% H-4 => L+3, 4.47% H-2 => L+4, 2.51% H-3 => L+5, 2.07% HOMO => L+7
41	20419	490	0.11	44.8% H-4 => L+2, 38.2% H-8 => L+1, 3.74% H-3 => L+3, 2.99% H-6 => L+3
42	20862	479	0.04	39.1% H-4 => L+2, 31.6% H-8 => L+1, 10.8% H-3 => L+6, 5.90% H-1 => L+5, 4.64% H-4 => L+5
43	20916	478	0.97	66.4% H-2 => L+5, 11.8% H-3 => L+4, 4.12% H-1 => L+7, 3.59% H-4 => L+1, 3.26% H-10 => L+1, 2.16% H-6 => LUMO
44	20925	478	0.00	53.0% HOMO => L+7, 16.4% H-3 => L+5, 10.3% H-7 => L+1, 5.72% H-4 => L+3, 5.46% H-1 => L+6, 3.13% H-6 => L+2
45	21154	473	0.00	87.4% H-16 => LUMO, 5.20% H-15 => L+1, 4.41% H-17 => L+1

46	21343	469	0.00	84.2% H-17 => LUMO, 8.07% H-16 => L+1, 5.88% H-15 => LUMO
47	21538	464	0.00	62.5% H-2 => L+6, 13.2% H-4 => L+4, 10.3% H-6 => L+1, 3.01% H-5 => L+5, 2.53% H-1 => L+8 20.1% HOMO => L+8, 18.7% H-3 => L+6, 17.2% H-9 => L+1, 16.6% H-5 => L+4, 9.75% H-8 => L+1, 6.60% H-4 => L+5, 2.83% H-6 => L+3 56.2% H-3 => L+5, 17.3% H-6 => L+2, 14.5% H-4 => L+3, 6.36% HOMO => L+7
48	21600	463	0.08	40.0% H-9 => L+1, 38.2% HOMO => L+8, 7.40% H-5 => L+4, 2.15% H-7 => L+4
49	21711	461	0.00	63.1% H-5 => L+3, 15.9% H-10 => L+1, 4.53% H- 1 => L+7, 3.86% H-2 => L+5
50	22000	455	0.29	51.1% H-7 => L+2, 32.8% H-4 => L+4, 4.68% H-2 => L+6, 4.09% H-8 => L+3, 2.43% H-18 =>
51	22226	450	0.27	LUMO
52	22400	446	0.00	65.3% H-10 => L+1, 10.3% H-5 => L+3, 7.68% H- 13 => L+1, 6.85% H-1 => L+7, 2.20% H-7 => L+3, 2.08% H-8 => L+2
53	22547	444	0.05	90.0% H-11 => L+1, 3.48% H-4 => L+3 55.6% H-5 => L+4, 29.9% H-9 => L+1, 6.60% HOMO => L+8, 2.05% H-8 => L+1
54	22651	441	0.00	49.0% H-4 => L+3, 41.0% H-6 => L+2, 3.04% H- 11 => L+1, 2.21% H-6 => L+5
55	22666	441	0.01	44.2% H-18 => LUMO, 25.2% H-4 => L+4, 15.6% H-20 => LUMO, 5.80% H-7 => L+2
56	22714	440	0.00	70.8% H-19 => LUMO, 10.8% H-8 => L+2, 4.79% H-21 => LUMO, 4.60% H-7 => L+3, 3.46% H-18 => L+1
57	22830	438	0.00	45.9% H-18 => LUMO, 18.9% H-20 => LUMO, 15.5% H-7 => L+2, 7.81% H-4 => L+4, 2.22% H- 19 => L+1
58	22834	438	0.01	52.4% H-21 => LUMO, 23.0% H-13 => L+1, 9.04% H-19 => LUMO, 4.60% H-8 => L+2
59	22971	435	0.00	35.8% H-8 => L+2, 25.8% H-13 => L+1, 12.4% H- 19 => LUMO, 9.68% H-1 => L+7, 4.62% H-10 => L+1, 3.79% H-7 => L+3
60	23102	433	0.01	77.7% H-12 => L+1, 5.27% H-5 => L+5, 3.17% H- 2 => L+6, 2.56% H-4 => L+4
61	23120	433	0.14	57.9% H-3 => L+6, 10.6% HOMO => L+8, 8.52% H-6 => L+3, 4.30% H-4 => L+5, 3.40% H-10 => L+2, 3.14% H-9 => L+1, 3.01% H-4 => L+2, 2.29% H-8 => L+1
62	23138	432	0.00	59.6% H-20 => LUMO, 10.8% H-7 => L+2, 10.3% H-4 => L+4, 6.82% H-12 => L+1, 4.82% H-2 => L+6, 2.70% H-1 => L+8
63	23146	432	0.00	37.5% H-13 => L+1, 35.9% H-21 => LUMO, 13.1% H-8 => L+2, 3.59% H-7 => L+3, 2.89% H-9 => L+2
64	23247	430	0.00	
65	23315	429	0.05	

				56.9% H-5 => L+5, 9.90% H-1 => L+8, 6.99% H-11 => L+2, 5.33% H-12 => L+1, 4.87% H-2 => L+6, 4.59% H-9 => L+3, 3.42% H-3 => L+7
66	23800	420	0.00	48.0% H-24 => LUMO, 19.0% H-4 => L+5, 4.97% H-6 => L+3, 4.50% H-5 => L+4, 4.37% HOMO => L+8, 2.60% H-26 => LUMO, 2.05% H-7 => L+4, 2.03% H-28 => LUMO
67	23926	418	0.22	85.3% H-22 => LUMO, 3.21% H-23 => L+1, 2.19% H-9 => L+2
68	23971	417	0.00	92.1% H-23 => LUMO, 3.49% H-22 => L+1
69	23989	417	0.00	23.4% H-1 => L+7, 21.1% H-6 => L+4, 18.2% H-9 => L+2, 9.06% H-5 => L+3, 8.81% H-22 => LUMO, 4.77% H-7 => L+3, 3.88% H-10 => L+1, 2.22% H-5 => L+6
70	24106	415	0.47	49.9% H-25 => LUMO, 9.62% H-6 => L+2, 7.58% H-29 => LUMO, 5.82% HOMO => L+7, 3.01% H-4 => L+3, 2.92% H-27 => LUMO, 2.72% H-31 => LUMO, 2.66% H-39 => LUMO, 2.43% H-1 => L+6
71	24113	415	0.00	35.7% H-4 => L+5, 23.3% H-24 => LUMO, 13.5% H-28 => LUMO, 5.70% H-7 => L+4, 4.65% H-10 => L+2, 3.43% HOMO => L+8, 2.46% H-6 => L+6, 2.34% H-30 => LUMO
72	24223	413	0.19	35.9% H-25 => LUMO, 11.7% H-27 => LUMO, 10.4% H-6 => L+2, 9.35% HOMO => L+7, 5.64% H-4 => L+3, 4.36% H-3 => L+5, 3.64% H-39 => LUMO, 2.77% H-2 => L+4, 2.37% H-1 => L+6, 2.18% H-5 => L+1
73	24342	411	0.00	30.4% H-1 => L+7, 14.1% H-6 => L+4, 13.4% H-5 => L+6, 11.4% H-8 => L+2, 9.80% H-7 => L+3, 4.39% H-2 => L+5, 2.74% H-8 => L+5, 2.23% H-5 => L+3
74	24385	410	1.49	46.5% H-26 => LUMO, 18.0% H-28 => LUMO, 15.6% H-24 => LUMO, 4.97% H-30 => LUMO, 4.85% H-6 => L+3
75	24385	410	0.01	32.2% H-27 => LUMO, 21.3% H-4 => L+6, 8.38% H-6 => L+5, 6.47% H-8 => L+4, 3.75% H-29 => LUMO, 3.36% H-3 => L+5, 3.33% H-10 => L+3, 2.72% H-4 => L+3, 2.46% H-12 => L+2, 2.35% H-25 => LUMO
76	24503	408	0.00	33.2% H-6 => L+3, 22.3% H-28 => LUMO, 16.0% H-4 => L+5, 11.0% H-30 => LUMO, 4.99% H-7 => L+4, 2.80% H-10 => L+2
77	24514	408	0.04	28.7% H-8 => L+3, 28.4% H-11 => L+2, 20.4% H-1 => L+8, 7.80% H-7 => L+5, 2.83% H-9 => L+3, 2.32% H-2 => L+6, 2.17% H-3 => L+7
78	24614	406	0.00	39.9% H-26 => LUMO, 16.7% H-6 => L+3, 15.0% H-28 => LUMO, 8.55% H-30 => LUMO, 5.53% H-7 => L+4, 2.79% H-2 => L+7, 2.63% HOMO => L+8, 2.42% H-24 => LUMO
79	24636	406	0.00	

				36.2% H-9 => L+2, 27.1% H-6 => L+4, 10.4% H-8 => L+2, 8.30% H-7 => L+3, 7.20% H-5 => L+6, 3.87% H-1 => L+7
80	24668	405	0.31	42.0% H-27 => LUMO, 18.9% H-4 => L+6, 7.77% H-8 => L+4, 6.66% H-6 => L+5, 3.89% H-25 => LUMO, 3.16% HOMO => L+7, 3.02% H-2 => L+8, 2.73% H-6 => L+2, 2.56% H-12 => L+2
81	24735	404	0.00	85.3% H-14 => L+1, 4.06% H-15 => LUMO, 2.60% H-15 => L+4, 2.05% H-16 => L+1
82	24881	402	0.00	60.8% H-30 => LUMO, 19.6% H-28 => LUMO, 6.59% H-10 => L+2, 3.80% H-24 => LUMO,
83	24950	401	0.07	2.32% H-29 => L+1, 2.20% H-26 => LUMO, 83.2% H-29 => LUMO, 6.05% H-27 => LUMO,
84	24952	401	0.00	2.99% H-25 => LUMO, 47.2% H-1 => L+8, 18.3% H-5 => L+5, 15.5% H-11 => L+2, 3.04% H-8 => L+3, 2.48% H-9 => L+3,
85	24996	400	0.02	2.05% H-4 => L+4, 35.0% H-10 => L+2, 18.2% H-7 => L+4, 8.44% H-13 => L+2, 6.17% H-28 => LUMO, 5.97% H-2 => L+7, 3.67% H-5 => L+4, 3.44% H-30 => LUMO, 2.99% HOMO => L+8, 2.67% H-26 => LUMO,
86	25026	400	0.02	2.23% H-14 => L+1, 40.1% H-7 => L+4, 31.1% H-10 => L+2, 12.9% H-6 => L+3, 3.67% H-12 => L+3, 3.31% H-30 => LUMO, 2.06% H-13 => L+2
87	25071	399	0.07	42.5% H-7 => L+3, 24.2% H-9 => L+2, 11.5% H-6 => L+4, 7.65% H-1 => L+7, 2.63% H-8 => L+5
88	25144	398	0.87	65.3% H-12 => L+2, 16.9% H-4 => L+6, 7.23% H-13 => L+3, 4.23% H-10 => L+3
89	25284	396	0.00	93.8% H-33 => LUMO, 2.39% H-39 => LUMO
90	25337	395	0.00	70.7% H-13 => L+2, 12.1% H-7 => L+4, 8.76% H-12 => L+3
91	25354	394	0.25	45.3% H-5 => L+6, 16.7% H-6 => L+4, 8.42% H-34 => LUMO, 5.03% H-9 => L+5, 4.75% H-7 => L+3, 3.52% H-7 => L+6, 2.76% H-43 => LUMO, 2.54% H-9 => L+2
92	25374	394	0.00	71.9% H-36 => LUMO, 19.0% H-38 => LUMO, 3.50% H-41 => LUMO, 2.09% H-8 => L+3
93	25440	393	0.00	82.9% H-34 => LUMO, 4.04% H-5 => L+6, 3.05% H-37 => LUMO, 2.05% H-40 => LUMO
94	25443	393	0.03	47.5% H-35 => LUMO, 42.7% H-32 => LUMO, 2.62% H-13 => L+2, 2.29% H-2 => L+7
95	25449	393	0.00	74.8% H-15 => L+1, 11.0% H-17 => L+1, 6.34% H-14 => L+4, 2.62% H-14 => LUMO, 2.11% H-16 => LUMO
96	25533	392	0.00	67.2% H-31 => LUMO, 17.2% H-39 => LUMO
97	25548	391	0.00	37.3% H-11 => L+2, 28.3% H-8 => L+3, 11.2% H-7 => L+5, 5.17% H-1 => L+8, 3.04% H-11 => L+5,
98	25556	391	0.00	2.06% H-41 => LUMO
99	25690	389	0.01	47.2% H-35 => LUMO, 46.9% H-32 => LUMO

100	25724	389	0.00	54.6% H-39 => LUMO, 16.7% H-8 => L+4, 16.6% H-31 => LUMO, 3.93% H-33 => LUMO 58.1% H-8 => L+4, 14.9% H-39 => LUMO, 6.26% H-4 => L+6, 5.09% H-31 => LUMO, 4.57% H-12 => L+2
101	25773	388	0.00	57.4% H-37 => LUMO, 24.1% H-40 => LUMO, 5.80% H-34 => LUMO
102	25800	388	0.01	49.2% H-38 => LUMO, 23.1% H-36 => LUMO, 21.6% H-41 => LUMO
103	25815	387	0.00	20.5% H-37 => LUMO, 17.5% H-8 => L+5, 16.1% H-7 => L+6, 10.7% H-11 => L+3, 8.45% H-43 => LUMO, 6.16% H-5 => L+6, 4.56% H-40 => LUMO, 3.71% H-9 => L+5, 2.06% H-7 => L+3
104	25941	385	0.00	22.1% H-9 => L+3, 17.4% H-8 => L+3, 16.7% H-7 => L+5, 11.1% H-41 => LUMO, 8.66% H-38 => LUMO, 7.54% H-8 => L+6, 3.71% H-44 => LUMO, 2.70% H-11 => L+5
105	26003	385	0.00	63.4% H-2 => L+7, 12.3% H-42 => LUMO, 4.18% H-6 => L+3, 3.40% H-32 => LUMO, 3.15% H-4 => L+5
106	26072	384	0.28	56.8% H-41 => LUMO, 18.4% H-38 => LUMO, 7.56% H-9 => L+3, 5.78% H-7 => L+5
107	26098	383	0.00	62.2% H-40 => LUMO, 13.8% H-37 => LUMO, 4.21% H-14 => L+2, 4.09% H-8 => L+5, 3.71% H-7 => L+6, 2.58% H-11 => L+3
108	26106	383	0.00	69.0% H-14 => L+2, 9.15% H-15 => L+3, 3.82% H-17 => L+6, 2.96% H-16 => L+5, 2.80% H-14 => L+5, 2.35% H-40 => LUMO
109	26149	382	0.07	56.6% H-6 => L+5, 21.1% H-4 => L+6, 6.80% H-2 => L+8, 4.93% H-12 => L+2, 2.78% H-10 => L+6
110	26244	381	0.00	81.0% H-16 => L+1, 6.56% H-17 => LUMO, 4.03% H-15 => LUMO, 3.60% H-17 => L+4, 2.48% H-15 => L+4
111	26476	378	0.00	48.1% H-15 => L+2, 20.2% H-14 => L+3, 6.52% H-3 => L+7, 5.93% H-17 => L+5, 3.72% H-17 => L+2, 3.67% H-16 => L+3, 3.32% H-14 => L+6, 3.05% H-16 => L+6
112	26566	376	0.00	67.4% H-17 => L+1, 7.55% H-15 => L+1, 7.04% H-16 => LUMO, 5.91% H-16 => L+4, 4.91% H-2 => L+8, 3.66% H-9 => L+4
113	26608	376	0.00	79.7% H-43 => LUMO, 4.97% H-11 => L+3, 3.88% H-8 => L+5, 3.80% H-7 => L+6, 2.33% H-9 => L+5
114	26617	376	0.01	59.7% H-3 => L+7, 6.37% H-9 => L+3, 5.90% H-8 => L+3, 4.57% H-7 => L+5, 4.44% H-1 => L+8, 2.91% H-15 => L+2, 2.76% H-10 => L+4
115	26617	376	0.01	43.1% H-2 => L+8, 29.2% H-9 => L+4, 8.39% H-17 => L+1, 8.25% H-6 => L+5
116	26657	375	0.00	64.7% H-10 => L+3, 13.0% H-13 => L+3, 5.46% H-13 => L+6, 3.76% H-10 => L+6
117	26799	373	0.00	

				41.1% H-9 => L+3, 14.1% H-7 => L+5, 13.8% H-44 => LUMO, 13.7% H-3 => L+7, 3.85% H-7 => L+2, 2.31% H-11 => L+2
118	26870	372	0.01	59.1% H-9 => L+4, 24.6% H-2 => L+8, 6.28% H-6 => L+5, 2.34% H-4 => L+6
119	26872	372	0.00	44.8% H-6 => L+6, 22.5% H-12 => L+3, 13.9% H-10 => L+5, 4.83% H-13 => L+5, 4.39% H-13 => L+2
120	26936	371	0.28	41.4% H-44 => LUMO, 36.4% H-10 => L+4, 9.54% H-7 => L+5, 3.94% H-9 => L+3
121	27017	370	0.00	38.8% H-16 => L+2, 19.6% H-15 => L+3, 15.8% H-17 => L+3, 9.23% H-14 => L+5, 8.21% H-16 => L+5, 4.55% H-15 => L+6
122	27021	370	0.00	50.4% H-42 => LUMO, 29.5% H-11 => L+4, 3.32% H-6 => L+6, 3.12% H-2 => L+7, 2.82% H-10 => L+2
123	27128	369	0.11	42.4% H-17 => L+2, 28.6% H-16 => L+3, 15.7% H-15 => L+5, 9.14% H-14 => L+6
124	27167	368	0.00	31.5% H-3 => L+8, 28.3% H-11 => L+3, 14.6% H-8 => L+5, 8.03% H-5 => L+6, 4.09% H-9 => L+5, 2.96% H-4 => L+7
125	27234	367	0.07	42.9% H-10 => L+4, 26.6% H-44 => LUMO, 13.4% H-13 => L+4, 5.41% H-7 => L+5, 2.07% H-3 => L+7
126	27243	367	0.00	53.6% H-13 => L+3, 21.8% H-12 => L+5, 6.49% H-10 => L+6, 5.94% H-12 => L+2, 4.77% H-10 => L+3, 2.01% H-6 => L+5
127	27287	366	0.00	51.2% H-11 => L+4, 13.9% H-6 => L+6, 11.0% H-12 => L+3, 10.2% H-42 => LUMO, 3.39% H-13 => L+5
128	27443	364	0.09	40.1% H-3 => L+8, 21.0% H-11 => L+3, 13.2% H-8 => L+5, 9.20% H-45 => LUMO, 3.54% H-11 => L+6, 2.18% H-4 => L+7
129	27445	364	0.14	26.2% H-6 => L+6, 19.8% H-12 => L+3, 17.9% H-42 => LUMO, 13.4% H-11 => L+4, 5.38% H-13 => L+5, 4.30% H-4 => L+5, 2.19% H-10 => L+5, 2.14% H-12 => L+6, 2.02% H-2 => L+7
130	27548	363	0.02	50.9% H-18 => L+1, 36.4% H-12 => L+4, 2.60% H-19 => LUMO, 2.12% H-45 => LUMO, 2.10% H-19 => L+4
131	27745	360	0.02	71.2% H-19 => L+1, 16.0% H-13 => L+4, 3.70% H-18 => LUMO, 2.85% H-18 => L+4
132	27756	360	0.00	39.6% H-12 => L+4, 27.2% H-18 => L+1, 15.2% H-20 => L+1, 9.85% H-45 => LUMO
133	27791	360	0.00	65.1% H-13 => L+4, 16.0% H-19 => L+1, 9.06% H-10 => L+4
134	27859	359	0.00	70.9% H-20 => L+1, 10.6% H-18 => L+1, 8.83% H-12 => L+4
135	27947	358	0.10	31.4% H-9 => L+5, 21.4% H-8 => L+5, 19.6% H-7 => L+6, 15.5% H-11 => L+3, 2.52% H-11 => L+6, 2.39% H-5 => L+6
136	28016	357	0.02	

137	28024	357	0.00	89.0% H-21 => L+1, 2.21% H-20 => L+4 39.3% H-7 => L+6, 28.6% H-9 => L+5, 13.1% H-11 => L+6, 5.18% H-7 => L+3, 4.71% H-3 => L+8, 2.37% H-8 => L+5
138	28260	354	0.00	52.9% H-8 => L+6, 19.2% H-11 => L+5, 15.0% H-7 => L+5, 2.48% H-9 => L+6, 2.40% H-11 => L+2
139	28363	353	0.00	63.1% H-45 => LUMO, 8.11% H-12 => L+4, 6.57% H-3 => L+8, 5.44% H-20 => L+1, 4.17% H-8 => L+5, 2.05% H-44 => L+1, 2.01% H-9 => L+5
140	28375	352	0.15	37.4% H-10 => L+5, 28.3% H-12 => L+3, 18.4% H-12 => L+6, 6.47% H-13 => L+5, 3.39% H-10 => L+2, 2.63% H-13 => L+2
141	28585	350	0.00	33.0% H-9 => L+6, 30.5% H-11 => L+5, 22.1% H-8 => L+6, 2.31% H-4 => L+8
142	28677	349	0.00	39.7% H-12 => L+5, 15.7% H-13 => L+3, 12.9% H-13 => L+6, 10.5% H-10 => L+6, 6.69% H-10 => L+3, 6.59% H-12 => L+2, 3.47% H-46 => LUMO
143	28717	348	0.00	78.3% H-46 => LUMO, 2.78% H-10 => L+3, 2.06% H-2 => L+8
144	28823	347	0.00	85.3% H-22 => L+1, 3.75% H-23 => LUMO, 3.56% H-47 => LUMO, 2.45% H-23 => L+4
145	28893	346	0.00	90.0% H-23 => L+1, 3.77% H-22 => LUMO, 2.56% H-22 => L+4
146	28913	346	0.01	79.6% H-24 => L+1, 6.69% H-28 => L+1, 2.08% H-25 => LUMO
147	28938	346	0.00	63.5% H-25 => L+1, 10.2% H-29 => L+1, 7.98% H-20 => L+2, 2.54% H-27 => L+1, 2.43% H-39 => L+1, 2.35% H-31 => L+1
148	28980	345	0.00	43.8% H-28 => L+1, 23.3% H-30 => L+1, 11.8% H-21 => L+2, 6.42% H-26 => L+1, 2.27% H-24 => L+1
149	29075	344	0.00	39.4% H-27 => L+1, 15.8% H-18 => L+2, 8.97% H-19 => L+3, 8.81% H-25 => L+1, 5.27% H-29 => L+1, 4.80% H-20 => L+2, 2.94% H-39 => L+1, 2.19% H-18 => L+5, 2.15% H-26 => LUMO
150	29186	343	0.01	44.4% H-26 => L+1, 19.5% H-19 => L+2, 11.7% H-18 => L+3, 3.63% H-30 => L+1, 3.58% H-5 => L+7, 2.97% H-19 => L+5
151	29236	342	0.00	82.1% H-47 => LUMO, 5.11% H-22 => L+1, 3.35% H-45 => L+1
152	29271	342	0.00	82.4% H-4 => L+7, 3.91% H-6 => L+8, 3.82% H-3 => L+8
153	29332	341	0.06	54.1% H-13 => L+5, 31.1% H-10 => L+5, 4.55% H-12 => L+6, 2.98% H-13 => L+2, 2.10% H-6 => L+6
154	29338	341	0.01	81.7% H-14 => L+4, 4.34% H-16 => L+4, 4.00% H-15 => L+1, 2.91% H-5 => L+7, 2.11% H-17 => L+1
155	29409	340	0.00	68.9% H-5 => L+7, 12.6% H-26 => L+1, 3.24% H-2 => L+8, 3.18% H-14 => L+4
156	29455	340	0.00	

				35.8% H-18 => L+2, 19.2% H-19 => L+3, 13.3% H-25 => L+1, 7.65% H-27 => L+1, 4.62% H-18 => L+5, 4.39% H-20 => L+2, 4.20% H-29 => L+1 34.2% H-19 => L+2, 20.5% H-26 => L+1, 16.9% H-18 => L+3, 9.46% H-5 => L+7, 3.76% H-19 => L+5, 2.44% H-24 => L+1, 2.01% H-30 => L+1 51.1% H-10 => L+6, 25.0% H-13 => L+6, 6.45% H-13 => L+3, 5.33% H-10 => L+3 39.1% H-27 => L+1, 29.4% H-29 => L+1, 9.22% H-20 => L+2, 6.10% H-25 => L+1, 2.59% H-18 => L+2, 2.58% H-39 => L+1 40.8% H-30 => L+1, 35.4% H-28 => L+1, 4.25% H-24 => L+1, 4.01% H-26 => L+1, 2.71% H-35 => L+1, 2.19% H-29 => LUMO 38.5% H-33 => L+1, 26.3% H-29 => L+1, 12.1% H-20 => L+2, 7.70% H-39 => L+1, 2.11% H-28 => L+4, 2.06% H-36 => L+2 42.2% H-9 => L+6, 35.7% H-11 => L+5, 8.41% H-4 => L+8, 4.81% H-8 => L+6 45.0% H-14 => L+3, 21.1% H-15 => L+2, 20.7% H-34 => L+1, 3.01% H-15 => L+5 52.5% H-34 => L+1, 16.3% H-14 => L+3, 7.23% H-15 => L+2, 6.57% H-4 => L+8 64.3% H-36 => L+1, 18.1% H-38 => L+1, 5.10% H-33 => L+2, 4.11% H-41 => L+1, 2.57% H-34 => L+4 39.0% H-33 => L+1, 14.1% H-5 => L+8, 10.5% H-31 => L+1, 9.45% H-29 => L+1, 8.19% H-20 => L+2, 2.68% H-23 => L+2 35.9% H-35 => L+1, 20.4% H-32 => L+1, 13.3% H-30 => L+1, 8.27% HOMO => L+9, 7.95% H-21 => L+2, 2.07% H-22 => L+2, 2.05% H-34 => L+2 57.4% H-4 => L+8, 9.11% H-9 => L+6, 8.39% H-6 => L+7, 7.19% H-34 => L+1, 3.22% H-47 => LUMO, 2.48% H-11 => L+5 68.2% H-5 => L+8, 6.25% H-33 => L+1, 3.89% H-29 => L+1, 3.51% H-48 => LUMO, 3.44% H-20 => L+2, 2.63% H-8 => L+7, 2.20% H-2 => L+7 74.2% H-11 => L+6, 13.8% H-9 => L+5, 3.90% H-11 => L+3, 3.43% H-7 => L+6, 2.14% H-8 => L+5 68.4% H-15 => L+4, 22.2% H-17 => L+4, 3.33% H-14 => L+1 52.5% H-21 => L+2, 14.3% HOMO => L+9, 7.10% H-30 => L+1, 5.90% H-35 => L+1, 3.26% H-28 => L+1, 2.83% H-49 => LUMO, 2.35% H-20 => L+3 32.9% H-31 => L+1, 27.7% H-48 => LUMO, 20.8% H-20 => L+2, 5.24% H-39 => L+1, 2.02% H-29 => L+1 52.2% HOMO => L+9, 18.3% H-32 => L+1, 5.42% H-21 => L+2, 2.99% H-22 => L+2
157	29600	338	0.00	
158	29656	337	0.00	
159	29729	336	0.00	
160	29763	336	0.03	
161	29801	336	0.00	
162	29868	335	0.00	
163	29914	334	0.00	
164	30016	333	0.00	
165	30039	333	0.00	
166	30072	333	0.00	
167	30106	332	0.01	
168	30125	332	0.00	
169	30134	332	0.00	
170	30138	332	0.13	
171	30187	331	0.01	
172	30230	331	0.00	
173	30311	330	0.00	
174	30439	329	0.04	
175	30447	328	0.00	

				38.5% H-15 => L+3, 27.8% H-16 => L+2, 13.6% H-14 => L+2, 5.34% H-14 => L+5, 4.93% H-17 => L+3, 4.76% H-16 => L+5, 3.79% H-17 => L+6
176	30464	328	0.00	48.9% H-32 => L+1, 33.7% H-35 => L+1, 4.09% HOMO => L+9, 3.14% H-22 => L+2
177	30576	327	0.00	42.0% H-31 => L+1, 21.1% H-48 => LUMO, 19.5% H-39 => L+1, 2.49% H-23 => L+2
178	30576	327	0.07	58.4% H-37 => L+1, 22.2% H-40 => L+1, 4.15% H-34 => L+1, 2.30% H-26 => L+2
179	30676	326	0.00	42.1% H-38 => L+1, 22.9% H-41 => L+1, 22.0% H-36 => L+1, 3.21% H-27 => L+2, 2.17% H-37 => LUMO
180	30679	326	0.00	34.4% H-39 => L+1, 34.3% H-48 => LUMO, 10.9% H-20 => L+2, 4.44% H-23 => L+2, 2.13% H-22 => L+3
181	30724	325	0.16	28.8% H-24 => L+2, 16.3% H-25 => L+3, 12.9% H-26 => L+2, 6.46% H-17 => L+2, 4.79% H-27 => L+3, 4.02% H-37 => L+1, 2.47% H-26 => L+5,
182	30790	325	0.00	2.42% H-30 => L+2, 2.35% H-24 => L+5 42.0% H-25 => L+2, 14.5% H-24 => L+3, 9.82% H-26 => L+3, 6.23% H-27 => L+2, 3.98% H-38 => L+1, 3.33% H-25 => L+5, 2.37% H-27 => L+5, 2.27% H-29 => L+2, 2.24% H-41 => L+1, 2.20% H-36 => L+1
183	30799	325	0.15	48.6% H-23 => L+2, 20.6% H-22 => L+3, 13.3% H-39 => L+1, 3.91% H-23 => L+5, 2.37% H-29 => L+1
184	30814	325	0.00	50.9% H-22 => L+2, 21.4% H-23 => L+3, 7.02% H-35 => L+1, 4.00% H-22 => L+5, 2.90% HOMO => L+9, 2.07% H-30 => L+1
185	30819	324	0.00	29.1% H-17 => L+2, 11.2% H-16 => L+3, 7.78% H-15 => L+5, 6.28% H-28 => L+2, 5.93% H-15 => L+2, 5.85% H-24 => L+2, 5.44% H-37 => L+1, 5.05% H-17 => L+5, 4.24% H-14 => L+6, 2.20% H-43 => L+1
186	30840	324	0.00	49.0% H-40 => L+1, 19.1% H-37 => L+1, 3.57% H-17 => L+2, 3.06% H-43 => L+1, 2.48% H-26 => L+2, 2.46% H-28 => L+2, 2.08% H-24 => L+2
187	30935	323	0.00	60.2% H-41 => L+1, 25.2% H-38 => L+1, 3.56% H-25 => L+2, 2.48% H-40 => LUMO
188	30936	323	0.03	19.8% H-28 => L+2, 15.7% H-40 => L+1, 11.5% H-30 => L+2, 9.83% H-43 => L+1, 6.14% H-20 => L+4, 5.54% H-17 => L+2, 5.13% HOMO => L+13, 4.21% HOMO => L+15
189	30965	323	0.00	25.6% H-16 => L+2, 23.8% H-17 => L+3, 15.4% H-15 => L+6, 11.6% H-14 => L+5, 8.16% H-15 => L+3, 4.52% H-16 => L+5, 3.90% H-14 => L+2
190	30971	323	0.00	34.1% H-13 => L+6, 25.4% H-49 => LUMO, 20.5% H-12 => L+5, 8.93% H-10 => L+6
191	30990	323	0.00	68.4% H-12 => L+6, 20.1% H-13 => L+5, 7.74% H-10 => L+5
192	31014	322	0.00	

				48.8% H-49 => LUMO, 14.7% H-13 => L+6, 9.05% HOMO => L+11, 8.88% H-10 => L+6,
193	31025	322	0.00	7.11% H-12 => L+5, 2.64% H-7 => L+7
194	31060	322	0.00	55.2% HOMO => L+12, 39.1% HOMO => L+10 66.8% HOMO => L+11, 14.6% HOMO => L+16,
195	31068	322	0.00	9.81% H-49 => LUMO 28.5% H-27 => L+2, 12.0% H-29 => L+2, 7.05% HOMO => L+17, 6.39% H-21 => L+4, 5.42% H-26 => L+3, 5.19% H-39 => L+2, 3.73% H-44 => L+1, 3.24% HOMO => L+14, 2.93% H-25 => L+2,
196	31109	321	0.00	2.12% H-30 => L+3 42.4% HOMO => L+13, 40.9% HOMO => L+15,
197	31205	320	0.00	5.57% H-28 => L+2 39.0% H-26 => L+2, 25.2% H-24 => L+2, 10.5% H-27 => L+3, 4.95% H-30 => L+2, 3.39% H-34 =>
198	31298	320	0.00	L+1, 2.86% H-37 => L+1 50.3% HOMO => L+10, 38.2% HOMO => L+12,
199	31319	319	0.00	4.13% HOMO => L+18 62.2% HOMO => L+17, 22.1% HOMO => L+14,
200	31326	319	0.04	4.44% H-27 => L+2 43.7% H-14 => L+5, 20.4% H-17 => L+3, 16.2% H-16 => L+5, 6.66% H-14 => L+2, 6.06% H-17 =>
201	31382	319	0.00	L+6, 2.06% H-15 => L+6 80.6% H-16 => L+4, 5.18% H-17 => L+1, 4.40% H-14 => L+4, 3.12% H-15 => L+1, 2.52% H-15 =>
202	31451	318	0.00	L+7 35.5% HOMO => L+16, 24.9% H-7 => L+7, 10.8% HOMO => L+11, 10.5% HOMO => L+19, 6.31%
203	31525	317	0.00	H-8 => L+8 66.2% H-17 => L+4, 19.4% H-15 => L+4, 7.21%
204	31531	317	0.00	H-16 => L+1, 3.11% H-16 => L+7 67.9% H-6 => L+7, 13.6% H-4 => L+8, 8.13% H-
205	31556	317	0.00	43 => L+1, 2.91% H-30 => L+2 27.6% HOMO => L+15, 26.6% HOMO => L+13, 9.69% H-14 => L+6, 5.24% H-17 => L+5, 3.35%
				H-15 => L+5, 3.12% H-30 => L+2, 3.08% H-16 =>
206	31568	317	0.00	L+3, 2.24% H-2 => L+14, 2.22% HOMO => L+20, 2.19% H-15 => L+2, 2.15% H-29 => L+3 30.5% H-42 => L+1, 20.9% H-7 => L+7, 18.1%
207	31572	317	0.00	HOMO => L+16, 6.49% HOMO => L+19, 4.82% H-8 => L+8, 2.19% HOMO => L+11 61.6% HOMO => L+14, 21.1% HOMO => L+17,
208	31585	317	0.03	2.02% H-2 => L+13 23.8% H-14 => L+6, 14.8% HOMO => L+13, 14.3% HOMO => L+15, 12.5% H-17 => L+5, 8.16% H-15 => L+5, 7.72% H-16 => L+3, 5.17%
209	31602	316	0.00	H-15 => L+2, 3.40% H-16 => L+6, 2.21% H-17 => L+2 63.3% H-43 => L+1, 13.6% H-28 => L+2, 8.67%
210	31715	315	0.00	H-6 => L+7, 2.62% H-20 => L+4

				19.2% H-29 => L+2, 15.9% H-27 => L+2, 11.3% H-25 => L+2, 8.20% H-24 => L+3, 6.93% H-44 => L+1, 5.65% H-26 => L+3, 5.54% H-30 => L+3, 4.54% H-39 => L+2, 4.31% H-1 => L+9, 3.19% H-28 => L+3, 2.91% H-27 => L+5, 2.16% H-21 => L+4
211	31760	315	0.02	60.0% HOMO => L+20, 22.1% HOMO => L+22, 3.20% H-30 => L+2
212	31761	315	0.00	36.6% H-8 => L+7, 25.2% H-7 => L+8, 9.54% H-18 => L+2, 7.05% H-9 => L+7, 3.80% H-48 => LUMO, 2.94% H-19 => L+3
213	31802	314	0.01	19.8% HOMO => L+23, 16.5% H-29 => L+2, 12.5% H-44 => L+1, 10.2% HOMO => L+21, 5.11% H-39 => L+2, 4.23% H-30 => L+3, 4.11% H-28 => L+3, 3.70% H-31 => L+2, 3.22% H-50 => LUMO, 2.13% H-33 => L+2, 2.05% H-1 => L+9
214	31809	314	0.01	27.6% H-30 => L+2, 15.1% H-28 => L+2, 13.3% H-29 => L+3, 7.13% HOMO => L+20, 4.05% H-6 => L+7, 3.48% H-24 => L+2, 3.46% HOMO => L+13, 2.68% H-27 => L+3, 2.50% HOMO => L+15, 2.22% H-25 => L+3, 2.12% H-14 => L+6
215	31825	314	0.00	42.2% HOMO => L+23, 18.2% HOMO => L+21, 9.26% H-44 => L+1, 6.74% H-29 => L+2, 2.66% HOMO => L+14, 2.15% H-30 => L+3
216	31841	314	0.01	28.1% H-42 => L+1, 14.2% H-7 => L+7, 14.0% HOMO => L+29, 7.61% H-34 => L+2, 6.00% HOMO => L+27, 3.77% HOMO => L+19, 3.68% HOMO => L+16, 2.90% H-19 => L+2, 2.03% H-8 => L+8
217	31892	314	0.00	48.5% HOMO => L+18, 40.7% HOMO => L+26
218	31931	313	0.01	71.7% HOMO => L+19, 17.5% HOMO => L+16, 4.22% H-2 => L+18
219	31954	313	0.00	

**Table S15.** TDDFT-predicted band excitation data for **5**.

Index	Energy (cm <sup>-1</sup> )	$\lambda$ (nm)	Osc. Strength	Contributions
0	4899	2041	3.54	98.9% HOMO => LUMO
1	5948	1681	0.00	97.3% H-1 => LUMO
2	8001	1250	0.00	85.1% H-3 => LUMO, 12.5% H-1 => L+1
3	8126	1231	0.00	74.0% H-2 => LUMO, 24.2% HOMO => L+1
4	8558	1169	0.00	72.5% HOMO => L+1, 22.4% H-2 => LUMO
5	10296	971	0.00	84.9% H-1 => L+1, 12.8% H-3 => LUMO 78.5% H-4 => LUMO, 13.9% H-3 => L+1, 4.30%
6	10421	960	0.00	H-1 => L+2
7	11029	907	0.18	90.4% H-5 => LUMO, 2.39% H-2 => L+1
8	11810	847	0.03	70.0% HOMO => L+2, 21.1% H-2 => L+1

9	12086	827	0.00	83.3% HOMO => L+3, 8.93% H-3 => L+1, 3.05% H-4 => LUMO 68.9% H-2 => L+1, 24.5% HOMO => L+2, 2.11% H-5 => LUMO
10	12114	826	0.18	60.8% H-3 => L+1, 15.2% H-4 => LUMO, 13.5% HOMO => L+3, 7.32% H-1 => L+2
11	12290	814	0.00	75.4% H-6 => LUMO, 12.1% H-4 => L+1, 4.31% H-3 => L+2, 2.42% H-1 => L+6
12	12731	786	0.00	80.9% H-7 => LUMO, 7.04% H-9 => LUMO, 5.16% H-5 => L+1
13	12865	777	0.00	91.1% HOMO => L+4, 3.43% H-2 => L+3
14	13407	746	0.00	83.2% H-1 => L+2, 12.1% H-3 => L+1
15	14040	712	0.00	91.2% H-1 => L+3, 3.83% H-3 => L+4
16	14141	707	4.38	55.1% H-4 => L+1, 19.1% H-6 => LUMO, 14.4% H-3 => L+2, 5.40% H-1 => L+6
17	14475	691	0.00	30.1% HOMO => L+6, 20.7% H-9 => LUMO, 16.7% H-5 => L+1, 13.8% H-7 => LUMO, 13.2% H-2 => L+2, 2.06% H-10 => L+1
18	14724	679	0.00	83.5% H-8 => LUMO, 10.2% HOMO => L+8
19	14758	678	0.15	87.1% HOMO => L+5, 3.66% H-14 => LUMO, 3.29% H-2 => L+4
20	14944	669	0.00	65.6% H-5 => L+1, 24.0% HOMO => L+6, 4.23% H-9 => LUMO
21	15202	658	0.00	54.1% H-9 => LUMO, 21.5% HOMO => L+6, 5.01% H-1 => L+7, 4.41% H-1 => L+4, 4.09% H-2 => L+2, 2.47% H-3 => L+5
22	15520	644	0.00	80.8% H-10 => LUMO, 5.70% H-11 => LUMO, 3.88% H-9 => L+1, 2.59% H-1 => L+5
23	15631	640	0.00	87.5% H-2 => L+3, 4.17% HOMO => L+4
24	15665	638	0.00	71.7% H-2 => L+2, 18.8% HOMO => L+6, 4.48% H-5 => L+1
25	15800	633	0.00	26.5% H-3 => L+2, 21.0% HOMO => L+7, 18.5% H-4 => L+1, 10.8% H-1 => L+6, 10.5% H-13 => LUMO, 2.79% H-2 => L+3, 2.54% H-6 => L+2, 2.46% H-8 => L+1
26	15897	629	0.00	69.1% H-1 => L+4, 11.3% H-3 => L+3, 7.09% H-12 => LUMO, 4.55% H-9 => LUMO, 2.09% H-3 => L+5
27	16034	624	0.00	40.5% HOMO => L+7, 28.1% H-3 => L+2, 9.32% H-4 => L+1, 8.96% H-13 => LUMO, 3.52% H-1 => L+6, 2.48% H-8 => L+1
28	16153	619	0.00	71.7% H-11 => LUMO, 6.45% H-1 => L+8, 6.09% H-10 => LUMO, 5.58% H-7 => L+1, 2.29% H-3 => L+7
29	16246	616	0.03	73.6% H-12 => LUMO, 13.8% H-1 => L+4, 4.39% H-3 => L+3
30	16771	596	0.00	27.7% H-6 => L+1, 25.6% HOMO => L+8, 14.5% H-2 => L+4, 9.03% H-8 => LUMO, 7.52% H-14 => LUMO, 4.94% H-4 => L+2, 2.45% H-2 => L+7
31	16805	595	0.01	

				58.2% H-2 => L+4, 13.7% H-6 => L+1, 6.77% HOMO => L+8, 4.89% HOMO => L+5, 4.73% H-5 => L+3, 3.02% H-17 => LUMO
32	16857	593	0.00	77.6% H-3 => L+3, 9.06% H-12 => LUMO, 7.37% H-1 => L+4
33	16903	592	0.00	87.9% H-15 => LUMO, 5.08% H-12 => L+1, 2.24% H-5 => L+2
34	17113	584	0.69	69.2% H-13 => LUMO, 21.4% HOMO => L+7
35	17313	578	0.00	71.6% H-1 => L+6, 21.2% H-3 => L+2
36	17489	572	0.00	72.9% H-7 => L+1, 9.35% H-11 => LUMO, 3.07% H-1 => L+8, 2.98% H-5 => L+2, 2.78% H-3 => L+7, 2.75% H-1 => L+5
37	17516	571	0.00	54.0% H-14 => LUMO, 24.0% H-17 => LUMO, 8.27% H-6 => L+1, 3.59% HOMO => L+5, 3.12% H-2 => L+4
38	17684	565	0.04	80.9% H-1 => L+5, 3.75% H-11 => LUMO, 2.70% H-4 => L+3, 2.31% H-9 => L+1
39	17901	559	0.00	76.7% H-16 => LUMO, 10.2% H-2 => L+5, 2.38% H-8 => L+1
40	17937	558	0.00	37.7% H-6 => L+1, 28.4% HOMO => L+8, 16.2% H-17 => LUMO, 6.69% H-4 => L+2, 2.48% H-3 => L+6
41	17939	557	0.37	49.1% H-17 => LUMO, 24.9% H-14 => LUMO, 7.27% H-2 => L+4, 5.15% HOMO => L+8, 5.14% H-4 => L+2, 2.31% H-6 => L+1
42	18091	553	0.02	57.2% H-3 => L+4, 10.8% H-5 => L+2, 5.24% H-1 => L+8, 3.70% H-2 => L+6, 3.39% H-1 => L+3, 2.91% H-9 => L+1, 2.65% H-4 => L+5, 2.60% H-7 => L+1, 2.60% H-15 => LUMO, 2.06% H-4 => L+3
43	18177	550	0.60	42.9% H-2 => L+5, 19.6% H-8 => L+1, 13.7% H- 16 => LUMO, 7.45% HOMO => L+7, 5.48% H-5 => L+4, 3.93% H-13 => LUMO
44	18466	542	0.00	25.9% H-3 => L+4, 25.5% H-2 => L+6, 20.5% H-5 => L+2, 7.51% H-7 => L+1, 6.00% H-1 => L+8, 3.70% H-3 => L+7, 3.20% H-11 => LUMO, 2.49% H-9 => L+1
45	18475	541	0.32	68.0% H-5 => L+3, 9.85% H-4 => L+2, 6.79% H-2 => L+4, 3.27% HOMO => L+8, 2.90% H-2 => L+7, 2.11% H-5 => L+5, 2.10% H-17 => LUMO
46	18897	529	0.06	42.8% H-1 => L+7, 31.1% H-10 => L+1, 6.98% H- 9 => LUMO, 4.17% H-3 => L+5, 2.69% H-3 => L+8, 2.10% H-7 => L+2
47	18936	528	0.00	54.7% H-4 => L+2, 14.3% H-5 => L+3, 13.9% HOMO => L+8, 5.40% H-2 => L+7, 2.88% H-7 => L+4, 2.70% H-14 => LUMO
48	18978	527	0.30	43.6% H-9 => L+1, 33.4% H-4 => L+3, 9.42% H-5 => L+2, 2.77% H-10 => LUMO, 2.55% H-10 => L+2
49	19070	524	0.04	

50	19080	524	0.00	59.9% H-8 => L+1, 24.3% H-2 => L+5, 7.58% H-2 => L+8 77.4% H-18 => LUMO, 7.97% H-4 => L+3, 4.12% H-2 => L+6, 2.69% H-19 => L+1
51	19173	522	0.00	34.6% H-2 => L+6, 24.3% H-5 => L+2, 16.1% H-9 => L+1, 10.3% H-18 => LUMO, 3.40% H-4 => L+3, 2.90% H-1 => L+8
52	19230	520	0.01	41.3% H-4 => L+3, 18.4% H-9 => L+1, 14.3% H-5 => L+2, 11.5% H-2 => L+6, 2.95% H-1 => L+5,
53	19368	516	0.03	2.76% H-18 => LUMO 37.2% H-1 => L+7, 35.6% H-10 => L+1, 7.71% H-3 => L+5, 5.98% H-4 => L+4, 4.33% H-6 => L+3, 2.16% H-9 => L+2
54	19510	513	0.00	84.0% H-19 => LUMO, 6.47% H-18 => L+1, 4.05% H-21 => LUMO
55	19686	508	0.00	69.7% H-3 => L+5, 14.1% H-10 => L+1, 2.20% HOMO => L+10
56	19919	502	0.00	61.5% H-3 => L+6, 18.0% H-2 => L+7, 7.74% H-4 => L+2
57	19968	501	0.01	59.8% H-5 => L+4, 17.4% H-7 => L+3, 11.6% H-2 => L+5, 4.18% H-2 => L+8, 2.47% H-5 => L+7
58	20052	499	0.00	72.7% H-20 => LUMO, 12.5% H-22 => LUMO, 6.37% H-19 => L+1, 2.94% H-1 => L+8
59	20297	493	0.00	58.2% H-1 => L+8, 9.09% H-2 => L+6, 6.42% H-8 => L+3, 5.29% H-6 => L+4, 3.65% H-20 => LUMO, 3.11% H-4 => L+5, 2.88% HOMO => L+9, 2.65% H-5 => L+2, 2.03% H-4 => L+3
60	20323	492	0.06	57.9% H-4 => L+4, 11.1% H-7 => L+2, 4.63% HOMO => L+10, 3.81% H-6 => L+3, 3.72% H-3 => L+5, 3.49% H-10 => L+1, 2.89% H-11 => L+1, 2.72% H-5 => L+6
61	20458	489	0.00	46.3% H-2 => L+7, 22.0% H-3 => L+6, 12.8% H-13 => L+1, 2.70% H-5 => L+8, 2.20% H-4 => L+2
62	20468	489	0.93	37.5% H-11 => L+1, 18.3% H-7 => L+2, 11.2% H-4 => L+4, 10.4% H-3 => L+8, 6.00% H-1 => L+7, 5.97% H-4 => L+7
63	20499	488	0.00	45.5% H-2 => L+8, 29.6% H-6 => L+2, 7.20% H-8 => L+1, 5.58% H-4 => L+6, 3.84% H-5 => L+7
64	20585	486	0.00	48.5% HOMO => L+9, 15.6% H-3 => L+7, 15.2% H-12 => L+1, 3.09% H-4 => L+5, 3.09% H-2 =>
65	20827	480	0.10	L+10 68.9% H-12 => L+1, 8.64% HOMO => L+9, 5.06% H-3 => L+7, 4.04% H-15 => LUMO, 2.07% H-5 => L+2
66	20920	478	0.22	81.5% H-21 => LUMO, 6.58% H-20 => L+1, 5.60% H-22 => L+1, 2.87% H-19 => LUMO
67	20959	477	0.00	75.8% H-22 => LUMO, 10.4% H-21 => L+1,
68	21053	475	0.00	9.65% H-20 => LUMO
69	21144	473	0.04	73.0% H-13 => L+1, 13.3% H-2 => L+7, 3.63% H-5 => L+5

70	21151	473	0.00	63.6% H-7 => L+3, 17.7% H-5 => L+4, 5.05% H-9 => L+3, 3.46% H-7 => L+5, 2.44% H-6 => L+2 36.7% H-11 => L+1, 19.1% HOMO => L+10, 7.33% H-4 => L+4, 6.92% H-7 => L+2, 6.38% H-3 => L+8, 4.47% H-6 => L+3, 3.85% H-5 => L+6, 3.63% H-4 => L+7
71	21252	471	0.00	47.9% H-6 => L+3, 12.0% HOMO => L+10, 11.2% H-11 => L+1, 8.79% H-7 => L+2, 5.53% H-15 => L+1, 4.06% H-4 => L+4 45.6% H-6 => L+2, 20.0% H-2 => L+8, 14.5% H-14 => L+1, 4.94% H-5 => L+4, 3.36% H-17 => L+1
72	21345	469	0.00	22.7% H-7 => L+2, 19.5% H-6 => L+3, 18.7% HOMO => L+10, 14.3% H-3 => L+8, 8.58% H-15 => L+1, 2.78% H-4 => L+4, 2.73% H-4 => L+7 73.4% H-15 => L+1, 14.0% H-7 => L+2, 2.89% H-12 => L+2, 2.05% H-12 => LUMO
73	21362	468	0.01	54.0% H-3 => L+7, 13.7% HOMO => L+9, 9.99% H-6 => L+4, 8.74% H-8 => L+3, 5.27% H-4 => L+5 58.8% H-14 => L+1, 16.7% H-17 => L+1, 8.33% H-6 => L+2, 6.41% H-2 => L+8
74	21442	466	0.00	46.5% H-16 => L+1, 34.7% H-5 => L+5, 2.09% H-1 => L+9, 2.05% H-7 => L+7 69.8% H-17 => L+1, 16.8% H-14 => L+1, 3.32% H-16 => L+2, 2.90% H-16 => LUMO
75	21473	466	0.00	40.7% H-16 => L+1, 33.4% H-5 => L+5, 5.11% H-13 => L+1, 3.80% H-1 => L+9, 2.68% H-7 => L+4, 2.37% H-24 => LUMO
76	21479	466	0.01	65.2% H-4 => L+5, 15.9% H-8 => L+3, 8.41% H-6 => L+4, 2.31% H-6 => L+7 61.8% H-5 => L+6, 15.7% HOMO => L+10, 6.85% H-7 => L+2, 4.11% H-3 => L+8, 4.01% H-15 => L+1, 2.61% H-6 => L+3
77	21665	462	0.00	45.9% H-4 => L+6, 16.6% H-9 => L+3, 15.6% H-23 => LUMO, 5.03% H-10 => L+4, 3.44% H-6 => L+2, 2.93% H-2 => L+8, 2.81% H-27 => LUMO 34.9% H-8 => L+2, 18.3% H-24 => LUMO, 9.36% H-7 => L+4, 9.35% H-10 => L+3, 7.82% H-9 => L+4, 4.38% H-26 => LUMO, 2.77% H-11 => L+3, 2.34% H-5 => L+8
78	21867	457	0.37	61.4% H-23 => LUMO, 19.6% H-4 => L+6, 10.9% H-25 => LUMO, 3.75% H-24 => L+1 65.9% H-24 => LUMO, 14.9% H-8 => L+2, 5.66% H-7 => L+4, 4.03% H-23 => L+1, 3.35% H-5 => L+5 71.5% H-25 => LUMO, 11.1% H-27 => LUMO, 7.16% H-23 => LUMO, 3.23% H-9 => L+3
79	21979	455	0.00	50.3% H-3 => L+8, 13.4% H-5 => L+6, 6.51% H-6 => L+5, 5.82% H-6 => L+3, 5.72% H-8 => L+4,
80	22117	452	0.40	
81	22288	449	0.44	
82	22348	447	0.00	
83	22358	447	0.00	
84	22388	447	0.04	
85	22504	444	0.00	
86	22541	444	0.00	
87	22623	442	0.00	
88	22625	442	0.00	

				4.70% H-4 => L+7, 3.26% HOMO => L+10, 2.67% H-13 => L+3
89	22684	441	0.02	46.6% H-26 => LUMO, 23.2% H-8 => L+2, 15.9% H-7 => L+4, 2.52% H-5 => L+5
90	22750	440	0.00	72.3% H-27 => LUMO, 7.48% H-25 => LUMO, 5.45% H-23 => LUMO, 4.46% H-5 => L+7, 2.46% H-26 => L+1
91	22844	438	0.01	39.4% H-26 => LUMO, 35.4% H-7 => L+4, 5.82% H-8 => L+2, 3.36% H-5 => L+8, 2.98% H-5 => L+5, 2.26% H-24 => LUMO, 2.10% H-11 => L+3
92	22857	438	0.00	72.4% H-9 => L+2, 5.47% H-10 => L+1, 5.31% H-4 => L+7, 4.00% HOMO => L+10, 3.20% H-10 => L+6
93	22971	435	0.00	39.4% H-9 => L+3, 20.3% H-5 => L+7, 11.0% H-4 => L+6, 7.19% H-2 => L+8, 6.95% H-10 => L+4, 3.34% H-7 => L+5
94	22996	435	0.00	36.0% H-6 => L+4, 21.6% H-10 => L+2, 19.9% H-8 => L+3, 5.30% H-8 => L+5, 2.38% H-4 => L+8, 2.13% HOMO => L+9
95	23075	433	0.44	52.1% H-10 => L+3, 14.4% H-9 => L+4, 8.47% H-1 => L+9, 6.09% H-7 => L+4, 3.67% H-8 => L+2, 2.30% H-24 => LUMO, 2.07% H-12 => L+4
96	23144	432	0.01	33.1% H-5 => L+7, 10.4% H-1 => L+10, 9.63% H-9 => L+3, 8.14% H-4 => L+6, 6.19% H-7 => L+5, 5.69% H-27 => LUMO, 5.67% H-3 => L+9, 4.59% H-25 => LUMO, 2.82% H-7 => L+3, 2.30% H-23 => LUMO
97	23238	430	0.06	45.5% H-10 => L+2, 18.4% H-8 => L+3, 15.8% H-6 => L+4, 4.51% H-4 => L+8, 2.51% H-9 => L+6, 2.36% H-12 => L+1
98	23452	426	0.09	22.0% H-11 => L+2, 19.8% H-7 => L+6, 18.0% H-4 => L+8, 5.95% H-10 => L+2, 5.70% H-6 => L+7, 3.53% H-35 => LUMO, 2.79% H-8 => L+5, 2.03% H-15 => L+2
99	23545	425	0.00	48.4% H-30 => LUMO, 12.6% H-4 => L+7, 7.56% H-9 => L+2, 7.42% H-32 => LUMO, 3.98% H-34 => LUMO, 3.56% H-18 => L+1, 2.31% H-5 => L+6, 2.13% HOMO => L+10
100	23601	424	0.00	92.6% H-28 => LUMO, 5.06% H-29 => L+1
101	23603	424	0.00	91.9% H-29 => LUMO, 5.00% H-28 => L+1
102	23668	423	0.00	46.1% H-4 => L+7, 9.49% H-18 => L+1, 9.29% H-8 => L+4, 7.23% H-30 => LUMO, 4.77% H-34 => LUMO, 4.43% H-13 => L+3, 2.79% H-9 => L+2, 2.53% H-32 => LUMO, 2.36% H-6 => L+8
103	23672	422	0.00	73.5% H-18 => L+1, 8.42% H-30 => LUMO, 4.59% H-19 => LUMO, 2.78% H-4 => L+7, 2.54% H-19 => L+2
104	23746	421	0.06	64.5% H-31 => LUMO, 5.74% H-35 => LUMO, 3.47% H-8 => L+3, 3.04% H-10 => L+2, 2.51% H-6 => L+4, 2.00% H-48 => LUMO

				45.0% H-32 => LUMO, 21.9% H-34 => LUMO, 18.4% H-30 => LUMO, 6.80% H-36 => LUMO, 2.32% H-31 => L+1
105	23917	418	0.00	48.3% H-5 => L+8, 10.2% H-1 => L+9, 6.17% H-6 => L+6, 5.55% H-8 => L+2, 4.86% H-7 => L+7, 3.31% H-3 => L+10, 3.13% H-2 => L+7, 2.29% H-7 => L+4, 2.01% H-9 => L+4
106	23940	418	0.58	25.2% H-12 => L+3, 21.3% H-7 => L+5, 12.3% H-10 => L+4, 9.03% H-5 => L+7, 7.67% H-9 => L+5,
107	23987	417	0.00	4.78% H-11 => L+4, 2.88% H-7 => L+8 33.7% H-35 => LUMO, 20.9% H-33 => LUMO,
108	23994	417	0.00	16.2% H-31 => LUMO, 6.91% H-37 => LUMO, 3.06% H-8 => L+3, 2.58% HOMO => L+9 29.8% H-35 => LUMO, 19.4% H-37 => LUMO, 11.8% H-33 => LUMO, 5.11% H-8 => L+3, 4.08%
109	24075	415	0.15	HOMO => L+9, 3.23% H-31 => LUMO, 2.96% H-19 => L+1, 2.44% H-10 => L+2, 2.19% H-4 => L+8, 2.13% H-6 => L+4, 2.08% H-48 => LUMO 36.6% H-34 => LUMO, 17.5% H-32 => LUMO, 9.60% H-6 => L+5, 9.40% H-36 => LUMO, 5.24%
110	24114	415	0.00	H-8 => L+4, 3.09% H-2 => L+9, 2.57% H-30 => LUMO, 2.52% H-33 => L+1, 2.18% HOMO => L+10
111	24170	414	0.00	68.6% H-19 => L+1, 8.14% H-33 => LUMO, 5.34% H-18 => L+2, 4.54% H-20 => LUMO, 3.28% H-18 => LUMO, 3.25% H-21 => L+1
112	24222	413	0.80	48.3% H-1 => L+9, 13.9% H-6 => L+6, 6.74% H-11 => L+3, 5.75% H-7 => L+4, 5.71% H-5 => L+8, 5.48% H-8 => L+2, 2.61% H-5 => L+5 45.2% H-33 => LUMO, 9.07% H-8 => L+3, 7.17% HOMO => L+9, 3.71% H-6 => L+4, 3.27% H-7 => L+6, 2.39% H-19 => L+1, 2.28% H-4 => L+5, 2.26% H-3 => L+7, 2.18% H-31 => LUMO, 2.18% H-48 => LUMO, 2.15% H-5 => L+2, 2.13% H-32 => L+1
113	24272	412	0.13	26.1% H-6 => L+5, 18.2% H-32 => LUMO, 13.2% H-2 => L+9, 11.7% H-34 => LUMO, 6.75% HOMO => L+10, 5.02% H-8 => L+4, 3.20% H-30 => LUMO, 2.35% H-5 => L+6
114	24285	412	0.00	42.9% H-1 => L+10, 9.36% H-5 => L+7, 8.76% H-10 => L+4, 6.26% H-9 => L+3, 6.11% H-12 => L+3, 4.98% H-7 => L+5, 4.91% H-3 => L+9, 4.22% H-9 => L+5, 2.80% H-13 => L+2
115	24385	410	0.01	41.2% H-4 => L+8, 19.4% H-7 => L+6, 5.88% H-14 => L+3, 5.48% H-10 => L+2, 5.32% H-15 => L+2, 4.74% H-11 => L+2
116	24418	410	0.01	33.8% H-8 => L+4, 31.5% H-6 => L+5, 10.6% H-36 => LUMO, 4.49% H-13 => L+3, 3.18% H-8 => L+7, 2.08% H-4 => L+7
117	24493	408	0.00	

				62.6% H-37 => LUMO, 21.7% H-35 => LUMO, 3.98% H-33 => LUMO, 3.64% H-36 => L+1, 3.24% H-31 => LUMO
118	24524	408	0.04	63.5% H-36 => LUMO, 12.5% H-34 => LUMO, 9.28% H-8 => L+4, 2.38% H-37 => L+1, 2.19% H- 6 => L+5
119	24525	408	0.00	22.8% H-9 => L+4, 20.0% H-10 => L+3, 15.4% H- 11 => L+3, 13.0% H-5 => L+8, 8.60% H-10 => L+5, 4.78% H-6 => L+6, 4.58% H-15 => L+3,
120	24627	406	0.21	3.27% H-1 => L+9 40.2% H-7 => L+5, 16.5% H-1 => L+10, 13.8% H- 13 => L+2, 7.94% H-12 => L+3, 5.49% H-10 => L+4
121	24641	406	0.01	49.7% H-11 => L+3, 17.6% H-15 => L+3, 3.83% H-7 => L+4, 3.63% H-6 => L+6, 3.20% H-11 => L+5, 3.16% H-9 => L+4, 2.56% H-7 => L+7, 2.32% H-10 => L+5, 2.16% H-42 => LUMO,
122	24671	405	0.47	2.08% H-14 => L+2 67.2% H-20 => L+1, 15.2% H-22 => L+1, 5.82%
123	24697	405	0.00	H-19 => L+2, 4.10% H-19 => LUMO 39.8% H-12 => L+2, 16.4% H-40 => LUMO, 8.47% H-13 => L+3, 7.75% H-2 => L+9, 6.56% H- 44 => LUMO, 4.36% H-39 => LUMO, 2.97% H-8
124	24778	404	0.00	=> L+4 44.3% H-11 => L+2, 11.0% H-2 => L+10, 8.28% H-7 => L+6, 6.36% H-48 => LUMO, 5.12% H-14
125	24814	403	0.01	=> L+3, 4.07% H-6 => L+7, 2.99% H-38 => LUMO, 2.27% H-41 => LUMO
126	24831	403	0.00	73.2% H-40 => LUMO, 10.1% H-12 => L+2, 7.19% H-13 => L+3, 3.29% H-8 => L+4
127	24889	402	0.15	34.6% H-6 => L+6, 31.3% H-42 => LUMO, 10.5% H-45 => LUMO, 4.67% H-15 => L+3, 3.85% H-5 => L+8, 3.64% H-9 => L+4, 2.41% H-1 => L+9 50.4% H-42 => LUMO, 27.7% H-6 => L+6, 6.26% H-9 => L+4, 3.20% H-5 => L+8, 2.97% H-45 =>
128	24929	401	0.06	LUMO 53.9% H-13 => L+3, 14.6% H-12 => L+2, 7.21% H-8 => L+4, 4.34% H-39 => LUMO, 3.73% H-16
129	24932	401	0.00	=> L+3, 3.39% H-40 => LUMO, 2.01% H-14 => L+4
130	24937	401	0.00	59.9% H-13 => L+2, 10.0% H-43 => LUMO, 6.70% H-12 => L+3, 6.03% H-1 => L+10, 2.39% H-7 => L+5, 2.37% H-5 => L+7
131	24948	401	0.00	75.2% H-41 => LUMO, 5.49% H-38 => LUMO, 4.06% H-11 => L+2, 3.98% H-48 => LUMO, 2.76% H-7 => L+6
132	24961	401	0.35	20.9% H-15 => L+3, 16.6% H-9 => L+4, 14.9% H- 12 => L+4, 14.8% H-45 => LUMO, 7.26% H-11 => L+3, 5.74% H-7 => L+7, 3.13% H-1 => L+9, 2.92% H-47 => LUMO, 2.18% H-5 => L+8

133	25011	400	0.00	77.0% H-43 => LUMO, 7.48% H-46 => LUMO, 4.44% H-13 => L+2, 2.52% H-49 => LUMO 26.5% H-7 => L+6, 11.4% H-14 => L+3, 10.6% H- 11 => L+2, 9.07% H-2 => L+10, 6.79% H-8 => L+5, 6.27% H-41 => LUMO, 5.75% H-4 => L+8, 4.26% H-13 => L+4, 4.00% H-6 => L+7, 3.69% H- 38 => LUMO, 2.06% H-9 => L+6
134	25019	400	0.01	50.6% H-45 => LUMO, 13.3% H-42 => LUMO, 12.1% H-47 => LUMO, 3.44% H-15 => L+3, 3.22% H-9 => L+4, 2.64% H-50 => LUMO, 2.29% H-12 => L+4
135	25024	400	0.13	39.8% H-39 => LUMO, 29.9% H-44 => LUMO,
136	25033	399	0.00	16.7% H-12 => L+2, 2.93% H-40 => LUMO 50.4% H-38 => LUMO, 17.6% H-48 => LUMO, 4.12% H-14 => L+3, 2.70% H-11 => L+2, 2.63%
137	25130	398	0.02	H-13 => L+4 46.2% H-17 => L+3, 19.0% H-14 => L+3, 9.28% H-6 => L+7, 6.21% H-4 => L+8, 3.46% H-16 => L+4, 2.41% H-14 => L+5
138	25227	396	0.33	33.2% H-12 => L+3, 21.3% H-10 => L+4, 12.3% H-9 => L+5, 5.99% H-1 => L+10, 5.30% H-13 => L+2, 4.18% H-15 => L+4
139	25243	396	0.00	50.8% H-44 => LUMO, 26.8% H-39 => LUMO,
140	25252	396	0.00	5.60% H-16 => L+3, 3.06% H-2 => L+9 56.9% H-48 => LUMO, 24.8% H-38 => LUMO,
141	25291	395	0.01	10.4% H-41 => LUMO 47.3% H-16 => L+3, 11.4% H-39 => LUMO, 9.99% H-14 => L+4, 8.52% H-17 => L+4, 4.21% H-44 => LUMO, 2.90% H-12 => L+2, 2.41% H-13 => L+5
142	25302	395	0.00	35.5% H-15 => L+2, 17.3% H-17 => L+3, 15.3% H-6 => L+7, 6.47% H-16 => L+4, 5.18% H-14 => L+3, 4.80% H-4 => L+8, 4.29% H-8 => L+5
143	25359	394	0.01	54.1% H-47 => LUMO, 20.5% H-50 => LUMO, 16.1% H-45 => LUMO, 2.69% H-46 => L+1, 2.43% H-14 => L+2
144	25377	394	0.00	62.8% H-46 => LUMO, 18.6% H-49 => LUMO,
145	25382	394	0.00	9.10% H-43 => LUMO, 2.28% H-47 => L+1 70.0% H-21 => L+1, 8.01% H-22 => LUMO, 5.41% H-20 => LUMO, 4.62% H-22 => L+2,
146	25390	394	0.00	3.88% H-20 => L+2 41.5% H-15 => L+2, 16.3% H-14 => L+3, 11.0% H-17 => L+3, 7.06% H-16 => L+4, 6.10% H-2 =>
147	25446	393	0.04	L+10, 4.44% H-6 => L+7, 3.12% H-7 => L+6 67.2% H-22 => L+1, 10.9% H-21 => LUMO,
148	25465	393	0.00	9.46% H-20 => L+1, 8.63% H-21 => L+2 66.8% H-14 => L+2, 11.1% H-17 => L+2, 2.93% H-7 => L+7, 2.56% H-9 => L+4, 2.22% H-11 =>
149	25473	393	0.41	L+3 41.7% H-2 => L+9, 14.2% H-51 => LUMO, 10.8% H-16 => L+3, 5.55% H-39 => LUMO, 3.14% H-6
150	25498	392	0.00	

				=> L+5, 2.78% H-8 => L+4, 2.47% H-17 => L+4, 2.42% H-4 => L+7, 2.09% H-13 => L+3 21.5% H-49 => LUMO, 12.8% H-52 => LUMO, 11.6% H-46 => LUMO, 8.96% H-7 => L+8, 5.64% H-15 => L+4, 5.50% H-12 => L+5, 5.34% H-9 => L+8, 5.18% H-10 => L+7, 4.10% H-7 => L+5, 3.53% H-11 => L+7, 3.31% H-16 => L+2 52.6% H-50 => LUMO, 21.0% H-47 => LUMO, 4.23% H-9 => L+7, 3.27% H-10 => L+5, 2.96% H- 15 => L+3, 2.47% H-49 => L+1, 2.04% H-53 => LUMO, 2.00% H-17 => L+2
151	25590	391	0.00	42.1% H-49 => LUMO, 12.1% H-16 => L+2, 11.5% H-46 => LUMO, 6.55% H-7 => L+8, 2.79% H-11 => L+4, 2.29% H-7 => L+5, 2.08% H-11 => L+7 49.3% H-17 => L+2, 9.13% H-50 => LUMO, 6.86% H-9 => L+7, 5.88% H-10 => L+5, 5.44% H- 15 => L+3, 5.00% H-14 => L+2, 2.84% H-47 => LUMO, 2.33% H-16 => L+1, 2.26% H-16 => L+6 62.2% H-16 => L+2, 8.79% H-52 => LUMO, 4.44% H-10 => L+4, 3.48% H-7 => L+8, 2.10% H- 49 => LUMO, 2.02% H-3 => L+9
152	25601	391	0.00	26.2% H-17 => L+2, 16.5% H-15 => L+3, 12.6% H-7 => L+7, 6.58% H-9 => L+7, 6.12% H-53 => LUMO, 4.91% H-10 => L+5, 4.43% H-50 => LUMO, 2.90% H-5 => L+8, 2.89% H-15 => L+5 47.5% H-2 => L+10, 21.4% H-6 => L+7, 6.04% H- 15 => L+2, 4.04% H-14 => L+3, 3.58% H-55 => LUMO
153	25633	390	0.00	14.6% H-10 => L+4, 12.6% H-9 => L+5, 12.6% H- 10 => L+7, 11.9% H-11 => L+4, 8.99% H-8 => L+6, 8.44% H-52 => LUMO, 5.30% H-49 => LUMO, 3.19% H-7 => L+8, 2.36% H-9 => L+3, 2.23% H-9 => L+8 42.8% H-7 => L+7, 6.32% H-14 => L+2, 6.04% H- 10 => L+5, 5.99% H-3 => L+10, 5.51% H-5 => L+8, 4.57% H-9 => L+4, 3.83% H-50 => LUMO, 3.70% H-9 => L+7, 2.37% H-15 => L+3, 2.26% H- 53 => LUMO, 2.05% H-4 => L+9
154	25678	389	0.01	49.4% H-6 => L+8, 18.0% H-8 => L+7, 5.42% H-2 => L+9, 3.98% H-13 => L+5, 3.84% H-16 => L+3, 3.39% H-17 => L+4, 2.55% H-14 => L+4 64.0% H-8 => L+5, 12.4% H-6 => L+7, 7.04% H-2 => L+10, 4.34% H-8 => L+8 32.3% H-3 => L+9, 21.5% H-11 => L+4, 7.43% H- 52 => LUMO, 6.51% H-9 => L+5, 6.22% H-1 => L+10, 5.93% H-10 => L+4, 3.44% H-8 => L+6,
155	25730	389	0.00	2.54% H-12 => L+3 66.8% H-18 => L+3, 13.0% H-19 => L+4, 4.28% H-20 => L+5, 3.04% H-22 => L+8, 2.95% H-18 => L+5, 2.15% H-21 => L+7
156	25797	388	0.02	
157	25809	387	0.39	
158	25831	387	0.00	
159	25865	387	0.01	
160	25962	385	0.00	
161	25995	385	0.00	
162	26054	384	0.00	
163	26118	383	0.10	

				37.9% H-8 => L+6, 23.3% H-11 => L+4, 15.6% H-52 => LUMO, 3.78% H-12 => L+5, 3.05% H-19 => L+3, 2.27% H-7 => L+8
164	26157	382	0.00	24.6% H-3 => L+9, 24.4% H-52 => LUMO, 6.25% H-16 => L+2, 6.10% H-11 => L+4, 3.90% H-9 => L+5, 3.59% H-54 => LUMO, 3.51% H-19 => L+3, 3.21% H-10 => L+7, 3.04% H-15 => L+4, 2.42%
165	26230	381	0.01	H-8 => L+6, 2.00% H-24 => L+1 26.7% H-8 => L+6, 15.1% H-19 => L+3, 10.7% H-52 => LUMO, 7.21% H-9 => L+5, 7.03% H-18 => L+4, 4.72% H-3 => L+9, 3.66% H-15 => L+4, 3.55% H-7 => L+8, 2.68% H-12 => L+5, 2.59% H-20 => L+4, 2.51% H-9 => L+8
166	26415	379	0.00	26.7% H-19 => L+3, 13.0% H-11 => L+4, 12.5% H-18 => L+4, 9.37% H-3 => L+9, 5.13% H-8 => L+6, 4.52% H-9 => L+5, 3.31% H-20 => L+4, 2.42% H-52 => LUMO, 2.30% H-12 => L+5,
167	26424	378	0.01	2.12% H-22 => L+7 70.3% H-53 => LUMO, 5.56% H-23 => L+1, 4.35% H-10 => L+5, 2.65% H-27 => L+1, 2.59%
168	26442	378	0.02	H-3 => L+10, 2.08% H-52 => L+1 53.8% H-3 => L+10, 16.0% H-23 => L+1, 4.84% H-7 => L+7, 4.10% H-1 => L+9, 3.81% H-4 =>
169	26462	378	0.28	L+9, 2.90% H-12 => L+4 63.3% H-13 => L+4, 6.28% H-16 => L+4, 5.86% H-14 => L+3, 4.50% H-14 => L+5, 2.45% H-17 =>
170	26470	378	0.00	L+8, 2.38% H-13 => L+7, 2.02% H-17 => L+5 69.2% H-51 => LUMO, 5.01% H-2 => L+9, 3.99%
171	26506	377	0.00	H-13 => L+3, 2.43% H-8 => L+4 79.0% H-24 => L+1, 5.58% H-23 => LUMO,
172	26536	377	0.00	4.33% H-23 => L+2, 4.24% H-9 => L+5 59.7% H-23 => L+1, 6.01% H-3 => L+10, 5.55%
173	26557	377	0.03	H-12 => L+4, 3.98% H-24 => LUMO, 3.77% H-25 => L+1, 3.59% H-53 => LUMO, 3.12% H-24 =>
174	26647	375	0.01	L+2, 3.10% H-7 => L+7 69.2% H-25 => L+1, 9.99% H-27 => L+1, 6.83%
175	26653	375	0.15	H-12 => L+4 81.5% H-9 => L+6, 5.84% H-7 => L+6, 3.13% H-10 => L+2
176	26712	374	0.08	19.2% H-20 => L+3, 14.0% H-12 => L+4, 11.3% H-10 => L+5, 10.7% H-19 => L+4, 10.2% H-25 => L+1, 4.98% H-18 => L+5, 3.44% H-3 => L+10, 3.34% H-22 => L+5, 2.63% H-22 => L+3, 2.00% H-21 => L+7
177	26791	373	0.00	50.0% H-26 => L+1, 23.7% H-54 => LUMO, 6.56% H-7 => L+8, 6.56% H-9 => L+5, 2.22% H-11 => L+4 24.1% H-12 => L+4, 20.1% H-20 => L+3, 8.68% H-19 => L+4, 8.14% H-10 => L+5, 5.72% H-18 =>
178	26799	373	0.08	L+5, 3.47% H-22 => L+5, 3.23% H-15 => L+3,

				2.52% H-22 => L+3, 2.46% H-3 => L+10, 2.42% H-15 => L+5
179	26876	372	0.00	75.9% H-27 => L+1, 8.69% H-25 => L+1, 3.70% H-53 => LUMO, 3.24% H-26 => L+2
180	26903	372	0.00	31.6% H-14 => L+4, 31.5% H-17 => L+4, 5.99% H-13 => L+5, 4.91% H-13 => L+8, 4.89% H-8 => L+7, 4.51% H-6 => L+8, 2.45% H-51 => LUMO, 2.13% H-17 => L+7
181	26919	371	0.00	26.2% H-7 => L+8, 26.0% H-26 => L+1, 10.9% H-15 => L+4, 10.1% H-9 => L+5, 7.68% H-54 => LUMO, 3.80% H-12 => L+5, 2.25% H-10 => L+7, 2.07% H-8 => L+6
182	27031	370	0.00	28.5% H-10 => L+6, 15.1% H-6 => L+8, 9.73% H-16 => L+5, 9.36% H-16 => L+3, 9.05% H-14 => L+4, 4.99% H-8 => L+7, 4.59% H-13 => L+5, 4.34% H-17 => L+4, 3.77% H-14 => L+7
183	27082	369	0.00	24.0% H-21 => L+3, 13.9% H-20 => L+4, 13.0% H-54 => LUMO, 12.8% H-22 => L+4, 8.08% H-19 => L+5, 7.26% H-21 => L+5, 4.46% H-18 => L+7, 4.38% H-20 => L+7, 2.72% H-19 => L+8, 2.16% H-26 => L+1
184	27091	369	0.11	31.1% H-16 => L+4, 14.3% H-14 => L+5, 13.7% H-17 => L+5, 9.64% H-17 => L+3, 7.53% H-13 => L+7, 5.66% H-14 => L+3, 5.44% H-8 => L+8, 4.53% H-16 => L+7
185	27102	369	0.00	34.1% H-54 => LUMO, 15.4% H-7 => L+8, 9.82% H-15 => L+4, 9.52% H-26 => L+1, 6.40% H-21 => L+3, 3.54% H-20 => L+4, 3.36% H-22 => L+4, 2.05% H-19 => L+5
186	27103	369	0.00	56.9% H-10 => L+6, 6.82% H-16 => L+5, 6.76% H-17 => L+4, 6.22% H-8 => L+7, 4.02% H-14 => L+4, 2.60% H-16 => L+3, 2.13% H-14 => L+7
187	27169	368	0.00	34.9% H-22 => L+3, 27.7% H-21 => L+4, 16.3% H-20 => L+5, 10.5% H-19 => L+7, 6.68% H-18 => L+8
188	27387	365	0.00	30.4% H-9 => L+7, 25.7% H-10 => L+5, 18.4% H-10 => L+8, 4.62% H-15 => L+3, 4.43% H-9 => L+4, 3.88% H-12 => L+4, 2.95% H-15 => L+5
189	27446	364	0.00	39.7% H-15 => L+4, 17.0% H-10 => L+7, 13.2% H-9 => L+8, 7.80% H-12 => L+3, 6.06% H-9 => L+5, 4.03% H-54 => LUMO, 2.40% H-15 => L+7
190	27468	364	0.00	50.4% H-8 => L+7, 16.3% H-6 => L+8, 13.1% H-17 => L+4, 5.54% H-16 => L+5, 3.92% H-16 => L+3, 3.62% H-14 => L+4, 2.61% H-6 => L+5
191	27474	364	0.00	83.7% H-18 => L+2, 5.53% H-19 => L+1, 4.53% H-19 => L+6
192	27563	363	0.03	60.4% H-11 => L+5, 11.3% H-29 => L+1, 5.74% H-12 => L+7, 2.80% H-15 => L+8, 2.65% H-3 => L+10

				71.7% H-29 => L+1, 12.0% H-11 => L+5, 4.69%
193	27627	362	0.01	H-28 => LUMO, 3.34% H-28 => L+2, 2.10% H-56 => LUMO
194	27629	362	0.00	85.8% H-28 => L+1, 5.50% H-29 => LUMO, 3.99% H-29 => L+2
195	27662	362	0.03	51.3% H-30 => L+1, 13.0% H-55 => LUMO, 8.70% H-32 => L+1, 7.69% H-34 => L+1, 2.58% H-8 => L+8
196	27720	361	0.10	45.3% H-55 => LUMO, 26.7% H-30 => L+1, 9.00% H-8 => L+8
197	27761	360	0.00	68.2% H-31 => L+1, 14.2% H-35 => L+1, 3.06% H-11 => L+6, 2.89% H-30 => LUMO, 2.28% H-30 => L+2
198	27839	359	0.00	44.0% H-19 => L+2, 29.2% H-11 => L+6, 4.97% H-18 => L+6, 4.24% H-21 => L+2, 2.59% H-20 => L+1
199	27883	359	0.02	34.7% H-8 => L+8, 19.9% H-55 => LUMO, 8.57% H-16 => L+4, 6.39% H-34 => L+1, 5.04% H-32 => L+1, 4.89% H-6 => L+7, 2.52% H-14 => L+5, 2.32% H-14 => L+3
200	27912	358	0.00	19.9% H-19 => L+2, 19.1% H-11 => L+6, 17.8% H-35 => L+1, 12.3% H-31 => L+1, 6.17% H-37 => L+1, 4.42% H-33 => L+1
201	27940	358	0.02	38.5% H-32 => L+1, 19.6% H-34 => L+1, 14.0% H-8 => L+8, 7.29% H-30 => L+1, 4.80% H-36 => L+1
202	27994	357	0.04	66.2% H-56 => LUMO, 11.0% H-4 => L+9, 4.53% H-3 => L+10, 4.30% H-29 => L+1, 3.04% H-54 => L+1
				24.2% H-35 => L+1, 17.7% H-13 => L+5, 12.9% H-11 => L+6, 8.76% H-14 => L+4, 6.65% H-33 => L+1, 5.48% H-37 => L+1, 4.04% H-14 => L+7, 4.03% H-19 => L+2, 2.35% H-31 => L+1, 2.23% H-16 => L+8, 2.09% H-13 => L+3
203	28003	357	0.00	27.2% H-13 => L+5, 23.9% H-11 => L+6, 13.3% H-14 => L+4, 7.85% H-35 => L+1, 4.77% H-14 => L+7, 3.48% H-19 => L+2, 2.97% H-13 => L+3, 2.72% H-16 => L+8, 2.36% H-33 => L+1
204	28048	357	0.00	41.2% H-12 => L+5, 12.5% H-9 => L+8, 9.99% H-15 => L+7, 7.04% H-11 => L+7, 6.48% H-10 => L+7, 4.81% H-4 => L+10, 3.71% H-12 => L+8, 2.05% H-15 => L+4, 2.00% H-10 => L+4
205	28107	356	0.00	40.0% H-34 => L+1, 33.5% H-32 => L+1, 9.37% H-36 => L+1, 4.39% H-33 => LUMO, 3.64% H-33 => L+2
206	28138	355	0.00	64.0% H-33 => L+1, 14.9% H-37 => L+1, 5.99% H-35 => L+1, 2.40% H-34 => L+2, 2.30% H-32 => LUMO, 2.15% H-34 => LUMO
207	28140	355	0.00	30.2% H-15 => L+5, 20.7% H-13 => L+6, 17.3% H-12 => L+7, 10.3% H-9 => L+7, 6.53% H-11 =>
208	28227	354	0.01	

				L+8, 2.39% H-15 => L+3, 2.34% H-16 => L+6, 2.33% H-56 => LUMO
				18.6% H-16 => L+7, 18.4% H-14 => L+5, 13.2% H-16 => L+4, 12.8% H-8 => L+8, 4.61% H-13 => L+4, 4.60% H-14 => L+3, 4.60% H-13 => L+7, 4.56% H-17 => L+8, 4.13% H-17 => L+5, 3.55%
209	28246	354	0.00	H-14 => L+8, 2.74% H-17 => L+3 78.6% H-5 => L+9, 4.38% H-7 => L+10, 3.62% H- 2 => L+10, 3.07% H-55 => LUMO
210	28313	353	0.22	45.4% H-13 => L+6, 26.2% H-4 => L+9, 5.89% H- 15 => L+5, 5.72% H-56 => LUMO, 2.07% H-3 => L+10
211	28389	352	0.05	28.4% H-16 => L+5, 15.8% H-17 => L+4, 13.0% H-13 => L+5, 7.87% H-17 => L+7, 7.69% H-16 => L+3, 7.15% H-13 => L+8, 6.62% H-14 => L+7, 5.14% H-5 => L+10
212	28438	352	0.00	73.1% H-12 => L+6, 6.52% H-36 => L+1, 2.76% H-15 => L+2
213	28460	351	0.04	42.6% H-4 => L+9, 19.3% H-13 => L+6, 8.67% H- 9 => L+7, 6.71% H-56 => LUMO, 6.30% H-15 => L+5, 2.81% H-16 => L+6, 2.17% H-12 => L+7, 2.12% H-6 => L+10
214	28481	351	0.07	58.4% H-37 => L+1, 19.0% H-35 => L+1, 6.36% H-33 => L+1, 3.85% H-31 => L+1, 3.79% H-36 => LUMO, 3.39% H-36 => L+2
215	28505	351	0.00	63.0% H-36 => L+1, 13.4% H-34 => L+1, 8.32% H-12 => L+6, 2.77% H-37 => LUMO, 2.31% H-37 => L+2
216	28514	351	0.02	70.7% H-5 => L+10, 6.20% H-7 => L+9, 5.00% H- 58 => LUMO, 3.97% H-2 => L+9, 2.39% H-17 => L+4
217	28555	350	0.00	33.9% H-4 => L+10, 33.3% H-57 => LUMO, 8.25% H-12 => L+5, 4.93% H-10 => L+7, 4.80% H-6 => L+9, 3.26% H-3 => L+9, 2.54% H-56 => L+1
218	28579	350	0.00	32.7% H-17 => L+5, 19.4% H-14 => L+5, 8.12% H-14 => L+8, 7.26% H-16 => L+4, 5.44% H-17 => L+3, 4.92% H-12 => L+6, 4.33% H-13 => L+4, 4.24% H-17 => L+8, 3.14% H-8 => L+8, 2.74% H- 40 => L+1
219	28586	350	0.01	65.2% H-20 => L+2, 20.9% H-22 => L+2, 4.61% H-19 => L+6, 2.67% H-19 => L+1
220	28645	349	0.00	76.6% H-40 => L+1, 8.27% H-44 => L+1, 3.25% H-39 => L+1
221	28738	348	0.00	26.3% H-42 => L+1, 26.1% H-14 => L+6, 17.8% H-17 => L+6, 3.51% H-4 => L+10, 3.43% H-12 => L+8, 3.27% H-9 => L+8, 2.95% H-10 => L+7,
222	28745	348	0.00	2.70% H-11 => L+7, 2.41% H-45 => L+1
223	28788	347	0.00	34.0% H-42 => L+1, 12.7% H-57 => LUMO, 9.56% H-10 => L+7, 7.25% H-45 => L+1, 6.89%

				H-9 => L+8, 6.60% H-12 => L+8, 4.88% H-12 => L+5, 4.72% H-11 => L+7 31.2% H-41 => L+1, 24.5% H-48 => L+1, 17.2% H-15 => L+6, 4.29% H-38 => L+1, 3.11% H-25 => L+3, 2.94% H-58 => LUMO
224	28800	347	0.00	28.0% H-14 => L+6, 15.5% H-42 => L+1, 12.7% H-17 => L+6, 12.2% H-57 => LUMO, 6.86% H-45 => L+1, 5.32% H-9 => L+8, 4.86% H-10 => L+7, 2.63% H-4 => L+10, 2.46% H-12 => L+8 27.2% H-4 => L+10, 23.5% H-57 => LUMO,
225	28841	347	0.00	17.9% H-9 => L+8, 4.97% H-17 => L+6, 4.60% H- 10 => L+7, 2.86% H-9 => L+5, 2.56% H-12 => L+8, 2.43% H-7 => L+8 52.3% H-15 => L+6, 30.0% H-41 => L+1, 2.99%
226	28917	346	0.00	H-38 => L+1, 2.14% H-5 => L+10 83.6% H-43 => L+1, 6.24% H-46 => L+1, 2.17%
227	28950	345	0.00	H-45 => L+2, 2.14% H-49 => L+1 41.4% H-39 => L+1, 31.5% H-44 => L+1, 12.2%
228	28981	345	0.00	H-40 => L+1 57.4% H-45 => L+1, 17.0% H-42 => L+1, 11.8%
229	28986	345	0.01	H-47 => L+1, 3.21% H-43 => L+2, 2.66% H-50 => L+1 42.7% H-38 => L+1, 14.9% H-41 => L+1, 14.7%
230	28987	345	0.00	H-15 => L+6, 10.3% H-48 => L+1, 3.59% H-58 => LUMO 54.7% H-11 => L+7, 8.87% H-10 => L+7, 8.27%
231	29001	345	0.00	H-9 => L+8, 6.71% H-12 => L+5, 5.48% H-4 => L+10, 2.87% H-7 => L+8, 2.33% H-12 => L+8 36.4% H-12 => L+7, 22.8% H-15 => L+5, 19.7%
232	29146	343	0.00	H-15 => L+8, 6.49% H-11 => L+5, 5.24% H-12 => L+4, 3.79% H-10 => L+5 65.9% H-58 => LUMO, 8.42% H-38 => L+1,
233	29158	343	0.04	3.66% H-60 => LUMO, 2.98% H-41 => L+1, 2.90% H-5 => L+10 39.3% H-39 => L+1, 38.8% H-44 => L+1, 4.20%
234	29170	343	0.00	HOMO => L+11, 2.49% H-38 => LUMO, 2.41% H-24 => L+3, 2.17% H-23 => L+4 40.2% H-48 => L+1, 25.3% H-38 => L+1, 10.9%
235	29228	342	0.00	H-41 => L+1, 5.58% H-58 => LUMO 65.0% H-10 => L+8, 15.7% H-9 => L+7, 5.13% H- 15 => L+5, 5.08% H-11 => L+8, 2.02% H-10 =>
236	29267	342	0.00	L+5 69.8% H-21 => L+2, 7.06% H-19 => L+2, 6.95% H-22 => L+1, 5.18% H-20 => L+1, 3.54% H-22 =>
237	29292	341	0.00	L+6, 3.47% H-20 => L+6 62.3% H-46 => L+1, 19.3% H-49 => L+1, 8.34% H-43 => L+1, 2.73% H-47 => LUMO, 2.00% H-47
238	29330	341	0.00	=> L+2 52.7% H-47 => L+1, 20.0% H-50 => L+1, 16.5%
239	29376	340	0.00	H-45 => L+1, 3.14% H-46 => LUMO, 2.31% H-46
240	29377	340	0.00	=> L+2

				53.7% H-22 => L+2, 15.3% H-20 => L+2, 8.93% H-21 => L+1, 6.61% H-21 => L+6, 3.92% H-13 => L+7
241	29380	340	0.00	37.0% H-13 => L+7, 11.7% H-17 => L+5, 11.1% HOMO => L+11, 6.41% H-16 => L+7, 6.22% H-22 => L+2, 4.61% H-14 => L+8, 3.86% H-17 => L+8, 2.73% H-44 => L+1, 2.20% H-13 => L+4, 2.13% H-8 => L+8
242	29386	340	0.00	55.2% H-17 => L+6, 35.4% H-14 => L+6, 3.57% H-16 => L+2
243	29476	339	0.00	85.5% H-16 => L+6, 6.23% H-13 => L+6, 2.40% H-17 => L+2
244	29479	339	0.07	34.0% H-24 => L+3, 27.4% H-23 => L+4, 9.47% H-24 => L+5, 4.75% H-13 => L+7, 3.92% HOMO => L+11, 3.76% H-44 => L+1, 3.51% H-39 => L+1, 2.58% H-23 => L+7
245	29529	339	0.03	39.3% H-23 => L+3, 31.2% H-24 => L+4, 10.5% H-23 => L+5, 3.58% H-38 => L+1, 2.78% H-24 => L+7, 2.27% H-48 => L+1
246	29542	338	0.00	47.9% HOMO => L+11, 8.98% H-51 => L+1, 7.30% H-13 => L+7, 5.24% H-24 => L+3, 3.79% H-23 => L+4, 3.76% H-14 => L+5, 2.29% H-44 => L+1, 2.09% H-26 => L+3
247	29576	338	0.00	63.2% H-50 => L+1, 21.8% H-47 => L+1, 3.38% H-49 => LUMO, 2.52% H-49 => L+2
248	29587	338	0.00	68.2% H-49 => L+1, 21.5% H-46 => L+1, 3.55% H-50 => LUMO, 2.62% H-50 => L+2
249	29588	338	0.00	33.1% H-13 => L+8, 22.1% H-17 => L+7, 14.2% H-14 => L+7, 6.61% H-16 => L+8, 5.27% H-16 => L+5, 3.58% H-17 => L+4, 3.32% H-14 => L+4,
250	29622	338	0.00	2.30% H-8 => L+7, 2.14% H-13 => L+5 37.8% H-15 => L+7, 18.9% H-12 => L+8, 12.8% H-11 => L+7, 10.2% H-9 => L+8, 6.04% H-10 => L+7, 4.46% H-15 => L+4, 3.73% H-50 => L+1, 2.44% H-12 => L+5
251	29629	338	0.00	58.7% H-11 => L+8, 7.37% H-15 => L+5, 6.81% H-52 => L+1, 6.76% H-15 => L+8, 4.74% H-11 => L+5, 2.30% H-7 => L+7
252	29697	337	0.00	59.6% H-18 => L+4, 27.4% H-19 => L+3, 5.43% H-19 => L+5, 3.35% H-20 => L+4
253	29747	336	0.00	51.0% H-26 => L+3, 8.95% H-27 => L+4, 7.48% H-51 => L+1, 5.55% H-25 => L+4, 3.07% H-13 => L+7, 2.34% HOMO => L+11
254	29937	334	0.00	21.1% H-16 => L+5, 15.1% H-16 => L+8, 14.8% H-25 => L+3, 11.3% H-17 => L+7, 9.50% H-14 => L+7, 6.77% H-13 => L+5, 3.72% H-27 => L+3, 3.51% H-26 => L+4, 2.70% H-48 => L+1, 2.63% H-17 => L+4
255	29944	334	0.00	29.4% H-16 => L+7, 20.9% H-14 => L+5, 17.1% H-17 => L+8, 12.6% H-17 => L+5, 4.68% H-16 => L+4, 4.01% H-51 => L+1, 3.12% H-14 => L+8
256	30000	333	0.01	

				21.3% H-25 => L+3, 18.7% H-27 => L+3, 11.9% H-16 => L+5, 10.2% H-26 => L+4, 9.11% H-14 => L+7, 4.80% H-48 => L+1, 4.36% H-16 => L+8, 2.14% H-17 => L+7
257	30043	333	0.00	41.8% H-26 => L+2, 17.4% H-52 => L+1, 6.84% H-11 => L+8, 4.70% H-37 => L+3, 4.19% H-24 => L+2, 2.68% H-35 => L+3, 2.10% H-27 => L+6, 2.07% H-25 => L+6
258	30105	332	0.01	29.4% H-25 => L+2, 26.7% H-27 => L+2, 6.64% H-34 => L+3, 5.01% H-26 => L+6, 4.48% H-23 => L+2, 3.68% H-36 => L+3, 3.60% H-53 => L+1, 3.10% H-26 => L+1, 2.04% H-37 => L+4
259	30106	332	0.00	

**Table S16.** TDDFT-predicted band excitation data for **6**.

Index	Energy (cm <sup>-1</sup> )	$\lambda$ (nm)	Osc.Strength	Contributions
0	4205	2378	4.55	99.0% HOMO => LUMO
1	5464	1830	0.00	96.5% H-1 => LUMO, 2.18% H-3 => L+1
2	6961	1436	0.00	62.8% H-2 => LUMO, 35.4% HOMO => L+1
3	7054	1418	0.00	84.3% H-3 => LUMO, 13.0% H-1 => L+1
4	7434	1345	0.00	62.1% HOMO => L+1, 34.3% H-2 => LUMO 76.7% H-5 => LUMO, 15.6% H-3 => L+1, 4.89%
5	9016	1109	0.00	H-1 => L+2
6	9237	1083	0.00	83.8% H-1 => L+1, 13.3% H-3 => LUMO
7	9646	1037	0.14	91.2% H-4 => LUMO, 4.01% HOMO => L+2
8	10195	981	0.16	84.1% HOMO => L+2, 7.56% H-2 => L+1 86.0% H-2 => L+1, 7.64% HOMO => L+2, 2.09%
9	10396	962	0.04	H-4 => LUMO 67.3% H-3 => L+1, 20.0% H-5 => LUMO, 8.22%
10	10793	927	0.00	H-1 => L+2 73.2% H-6 => LUMO, 15.1% H-5 => L+1, 5.38%
11	11084	902	0.00	H-3 => L+2, 2.28% H-1 => L+5 83.5% H-7 => LUMO, 5.99% H-4 => L+1, 2.34%
12	11739	852	0.00	H-12 => LUMO, 2.29% H-9 => L+1
13	11818	846	0.00	96.2% HOMO => L+3
14	12445	804	0.00	82.8% H-1 => L+2, 11.8% H-3 => L+1 44.7% H-5 => L+1, 19.2% H-6 => LUMO, 18.8% HOMO => L+4, 9.11% H-3 => L+2, 2.86% H-1 => L+5
15	12628	792	0.00	46.7% HOMO => L+5, 18.3% H-2 => L+2, 18.2% H-4 => L+1, 6.93% H-7 => LUMO, 2.21% H-12 => LUMO
16	12827	780	0.00	83.9% H-9 => LUMO, 5.29% H-7 => L+1, 3.59%
17	12834	779	0.04	H-11 => LUMO 73.6% HOMO => L+4, 12.4% H-5 => L+1, 3.92% H-6 => LUMO, 3.22% H-3 => L+2, 3.12% H-2 => L+3
18	12876	777	0.00	

				72.4% H-8 => LUMO, 12.5% H-6 => L+1, 4.75% H-5 => L+2, 2.39% H-3 => L+5, 2.10% H-15 => LUMO
19	12947	772	0.00	63.5% H-4 => L+1, 29.3% HOMO => L+5, 3.26% H-7 => LUMO
20	13115	762	0.00	73.3% H-2 => L+2, 18.1% HOMO => L+5, 4.98% H-4 => L+1
21	13528	739	0.00	87.9% H-1 => L+3, 6.16% H-3 => L+4
22	13815	724	5.21	61.1% H-3 => L+2, 23.2% H-5 => L+1, 10.7% H-1 => L+5
23	14049	712	0.00	80.2% HOMO => L+6, 4.31% H-6 => L+1, 4.20% H-2 => L+4, 3.14% H-8 => LUMO
24	14081	710	0.00	40.8% H-6 => L+1, 19.5% H-8 => LUMO, 13.8% H-5 => L+2, 8.88% HOMO => L+6, 6.76% H-3 => L+5, 3.36% H-1 => L+8, 2.79% H-10 => L+1
25	14556	687	0.00	84.7% H-10 => LUMO, 7.85% HOMO => L+10, 2.26% H-8 => L+1
26	14589	685	0.18	88.4% H-2 => L+3, 4.76% HOMO => L+4
27	14927	670	0.00	43.7% H-11 => LUMO, 16.7% HOMO => L+8, 10.9% H-9 => LUMO, 9.93% H-7 => L+1, 6.68% H-2 => L+5, 5.20% H-4 => L+2, 3.93% H-12 => L+1
28	15016	666	0.00	52.8% H-12 => LUMO, 23.2% H-1 => L+4, 10.1% H-3 => L+3, 3.16% H-11 => L+1, 2.66% H-14 => LUMO, 2.50% H-1 => L+7
29	15183	659	0.00	71.5% HOMO => L+7, 6.38% H-1 => L+5, 5.59% H-17 => LUMO, 3.42% H-2 => L+6, 2.73% H-2 => L+3
30	15322	653	0.00	59.0% H-7 => L+1, 18.3% H-11 => LUMO, 4.71% H-13 => LUMO, 3.24% H-4 => L+2, 2.38% H-1 => L+9, 2.25% HOMO => L+8
31	15385	650	0.00	45.0% H-1 => L+4, 26.7% H-12 => LUMO, 14.9% H-3 => L+3, 3.26% H-3 => L+6
32	15446	647	0.00	71.3% H-1 => L+5, 14.6% H-3 => L+2, 7.33% HOMO => L+7, 2.03% H-3 => L+8
33	15515	645	0.00	49.3% HOMO => L+8, 23.1% H-11 => LUMO, 8.68% H-2 => L+5, 4.72% H-7 => L+1, 3.28% H-4 => L+2
34	15658	639	0.01	31.1% H-6 => L+1, 21.4% H-5 => L+2, 11.0% H- 15 => LUMO, 9.50% HOMO => L+9, 8.25% H-3 => L+5, 5.88% H-1 => L+8, 3.07% H-8 => L+2, 2.33% H-10 => L+1
35	15743	635	0.00	68.4% H-2 => L+4, 6.07% H-4 => L+3, 5.57% HOMO => L+6, 5.07% H-5 => L+2, 2.23% HOMO => L+9
36	15873	630	0.00	70.4% H-13 => LUMO, 7.29% H-7 => L+1, 6.49% H-1 => L+6, 4.14% H-3 => L+4, 2.74% H-2 => L+5
37	15970	626	0.04	

				34.7% HOMO => L+9, 18.9% H-15 => LUMO, 17.0% H-5 => L+2, 9.90% H-2 => L+4, 4.27% H-6 => L+1, 4.08% H-10 => L+1
38	16088	622	0.00	73.8% H-14 => LUMO, 5.77% H-9 => L+1, 4.96% H-12 => LUMO, 4.95% H-1 => L+10, 2.10% H-3 => L+9
39	16116	621	0.00	56.9% H-4 => L+2, 19.1% HOMO => L+8, 6.32% H-7 => L+1, 6.04% H-2 => L+5, 3.81% H-18 => LUMO
40	16186	618	0.09	68.6% H-3 => L+3, 25.2% H-1 => L+4, 2.46% H-5 => L+4
41	16341	612	0.00	43.4% H-8 => L+1, 25.8% HOMO => L+10, 9.49% H-10 => LUMO, 6.22% H-17 => LUMO, 6.21% H- 6 => L+2, 2.14% H-2 => L+9, 2.07% H-5 => L+5
42	16561	604	0.00	65.7% H-2 => L+5, 12.5% H-4 => L+2, 8.52% HOMO => L+8, 4.83% H-18 => LUMO, 2.62% H- 13 => LUMO
43	16570	604	0.09	85.2% H-16 => LUMO, 4.96% H-13 => L+1, 3.12% H-18 => L+1
44	16663	600	0.00	32.3% H-3 => L+5, 29.1% H-5 => L+2, 12.8% HOMO => L+9, 9.90% H-1 => L+8, 8.47% H-15 => LUMO
45	16991	589	0.00	74.1% H-18 => LUMO, 8.50% H-4 => L+2, 7.32% H-1 => L+6, 4.35% H-16 => L+1, 2.37% H-2 => L+5
46	16992	589	0.41	43.4% H-2 => L+6, 20.9% H-17 => LUMO, 12.7% HOMO => L+7, 6.49% H-4 => L+4, 4.86% H-8 => L+1, 3.10% H-20 => LUMO
47	16995	588	0.02	81.9% H-9 => L+1, 9.54% H-14 => LUMO
48	17025	587	0.00	51.7% H-15 => LUMO, 17.0% HOMO => L+9, 13.3% H-3 => L+5, 7.71% H-1 => L+8, 2.68% H-5 => L+2
49	17027	587	0.00	63.0% H-1 => L+6, 12.3% H-3 => L+4, 10.7% H- 13 => LUMO, 5.32% H-18 => LUMO
50	17142	583	0.43	56.8% H-19 => LUMO, 16.5% H-4 => L+3, 15.9% H-21 => LUMO
51	17350	576	0.00	64.3% H-3 => L+4, 14.1% H-1 => L+6, 7.64% H-5 => L+3, 5.78% H-1 => L+3
52	17359	576	0.80	41.2% H-17 => LUMO, 21.4% H-20 => LUMO, 20.0% H-2 => L+6, 7.65% H-8 => L+1, 2.32% HOMO => L+7
53	17434	574	0.05	33.5% HOMO => L+10, 32.3% H-8 => L+1, 11.4% H-6 => L+2, 6.57% H-17 => LUMO, 4.93% H-5 => L+5, 3.89% H-20 => LUMO, 2.16% H-3 => L+8
54	17559	570	0.27	64.9% H-21 => LUMO, 15.9% H-19 => LUMO, 3.88% H-10 => L+1, 3.38% H-20 => L+1, 2.87% H-2 => L+7, 2.50% H-2 => L+4
55	17745	564	0.00	63.6% H-20 => LUMO, 16.2% H-2 => L+6, 10.6% H-17 => LUMO, 2.13% H-21 => L+1
56	17857	560	0.00	

				60.4% H-4 => L+3, 9.91% H-21 => LUMO, 7.44% H-19 => LUMO, 7.14% H-2 => L+4, 4.03% H-2 => L+7, 2.86% H-10 => L+1
57	17869	560	0.00	25.3% H-11 => L+1, 16.6% H-7 => L+2, 9.21% H-4 => L+5, 6.95% H-1 => L+10, 6.69% H-1 => L+7, 6.18% H-3 => L+9, 5.61% H-12 => LUMO, 5.28% H-2 => L+8, 3.55% H-3 => L+6, 3.01% H-5 => L+7, 2.01% H-14 => LUMO
58	17981	556	0.00	48.5% H-10 => L+1, 15.6% H-1 => L+8, 10.4% HOMO => L+9, 5.53% H-2 => L+7, 5.31% H-19 => LUMO, 2.88% H-4 => L+3, 2.68% H-3 => L+5
59	18087	553	0.00	79.8% H-5 => L+3, 6.57% H-3 => L+4, 2.71% H-12 => L+1, 2.44% H-6 => L+4
60	18211	549	0.00	45.7% H-1 => L+8, 24.5% H-3 => L+5, 5.68% HOMO => L+9, 5.27% H-4 => L+3, 4.19% H-19 => LUMO, 2.84% H-2 => L+7, 2.81% H-10 => L+1
61	18245	548	0.00	38.9% H-1 => L+7, 11.2% H-7 => L+2, 10.6% H-11 => L+1, 9.61% H-2 => L+8, 5.80% H-4 => L+5, 5.31% H-1 => L+10, 2.58% H-3 => L+6, 2.22% H-12 => LUMO, 2.19% H-9 => L+1
62	18253	548	0.00	67.0% H-12 => L+1, 8.02% H-11 => LUMO, 5.13% H-11 => L+2, 4.46% H-5 => L+3, 4.01% H-1 => L+9, 2.79% H-3 => L+7
63	18385	544	0.03	61.3% H-6 => L+2, 21.4% HOMO => L+10, 4.53% H-2 => L+9, 3.00% H-4 => L+4, 2.42% H-4 => L+7
64	18492	541	0.47	36.6% H-1 => L+7, 25.8% H-11 => L+1, 8.52% H-3 => L+6, 7.05% H-5 => L+4, 4.49% H-7 => L+2, 3.83% H-6 => L+3, 2.50% H-2 => L+8
65	18660	536	0.00	55.4% H-2 => L+7, 20.7% H-10 => L+1, 6.86% H-2 => L+10, 3.47% H-4 => L+6, 2.05% H-1 => L+8, 2.01% H-19 => LUMO
66	18710	534	0.00	66.7% H-4 => L+4, 9.89% H-7 => L+3, 9.71% H-2 => L+6, 3.89% H-6 => L+2
67	18748	533	0.01	57.6% H-3 => L+6, 14.6% H-11 => L+1, 8.24% H-7 => L+2, 3.73% H-2 => L+8, 2.81% H-22 => LUMO, 2.27% H-1 => L+4
68	18765	533	0.00	42.2% H-7 => L+2, 28.0% H-2 => L+8, 9.38% H-4 => L+5, 7.86% H-3 => L+6, 2.65% H-1 => L+10
69	18931	528	0.00	86.2% H-22 => LUMO, 3.88% H-23 => L+1, 3.42% H-3 => L+6
70	18940	528	0.00	66.4% H-5 => L+4, 4.39% H-3 => L+6, 4.08% H-1 => L+7, 3.23% H-2 => L+8, 3.02% H-3 => L+3, 2.90% H-11 => L+1, 2.83% H-6 => L+3, 2.45% H-4 => L+5
71	19251	519	0.00	37.2% H-1 => L+9, 17.8% H-9 => L+2, 9.52% H-14 => L+1, 8.72% H-12 => L+1, 4.52% H-3 => L+10, 3.31% H-13 => LUMO, 2.55% H-7 => L+5, 2.22% H-3 => L+7
72	19261	519	0.00	

				81.6% H-23 => LUMO, 7.19% H-22 => L+1, 2.72% H-25 => LUMO, 2.57% H-24 => L+1, 2.06% H-1 => L+9
73	19309	518	0.00	57.4% H-5 => L+5, 14.3% H-2 => L+9, 8.02% H-6 => L+2, 4.64% HOMO => L+10, 4.15% H-3 => L+8
74	19311	518	0.02	53.6% H-4 => L+5, 30.9% H-2 => L+8, 3.42% H-5 => L+4, 2.18% H-7 => L+2
75	19452	514	0.00	46.0% H-24 => LUMO, 31.3% H-13 => L+1, 4.78% H-23 => L+1, 3.89% H-26 => LUMO,
76	19775	506	0.00	2.36% H-5 => L+4 46.6% H-13 => L+1, 33.5% H-24 => LUMO, 3.20% H-23 => L+1, 2.63% H-16 => LUMO,
77	19832	504	0.00	2.38% H-26 => LUMO 33.0% H-1 => L+9, 32.6% H-9 => L+2, 17.4% H- 14 => L+1, 2.01% H-8 => L+3
78	19836	504	0.01	46.6% H-15 => L+1, 22.4% H-2 => L+9, 13.3% H- 5 => L+5, 3.08% H-10 => L+2
79	19856	504	0.47	39.0% H-2 => L+10, 23.2% H-8 => L+2, 11.8% H- 4 => L+6, 7.10% H-4 => L+9, 2.91% H-7 => L+4, 2.91% H-6 => L+5, 2.85% H-10 => L+1, 2.29% H- 2 => L+7
80	19857	504	0.00	35.3% H-4 => L+6, 24.2% H-8 => L+2, 14.4% H-2 => L+7, 7.62% H-7 => L+4, 5.08% H-9 => L+3, 2.44% H-6 => L+5, 2.40% H-10 => L+1
81	19889	503	0.00	48.0% H-3 => L+7, 20.1% H-14 => L+1, 8.27% H- 5 => L+6, 3.71% H-3 => L+10, 3.63% HOMO => L+12, 2.39% H-12 => L+1, 2.27% H-9 => L+2
82	19946	501	0.06	46.9% H-7 => L+3, 24.3% H-3 => L+8, 10.8% H-4 => L+4, 5.44% H-5 => L+5, 2.11% H-9 => L+4
83	20082	498	0.00	45.9% H-6 => L+3, 26.9% H-1 => L+10, 6.56% H- 5 => L+4, 4.65% H-2 => L+8, 3.42% H-6 => L+6, 2.78% H-10 => L+3
84	20108	497	0.00	51.9% H-16 => L+1, 10.5% H-3 => L+7, 5.58% H- 14 => L+1, 5.20% H-18 => LUMO, 3.93% H-25 => LUMO, 3.27% H-7 => L+5, 3.07% H-5 => L+6, 2.18% H-13 => L+2
85	20219	495	0.44	64.2% H-25 => LUMO, 17.8% H-27 => LUMO, 6.82% H-24 => L+1, 4.10% H-16 => L+1
86	20289	493	0.03	32.2% H-3 => L+8, 23.9% H-7 => L+3, 20.8% H- 15 => L+1, 6.81% H-5 => L+5, 6.61% H-2 => L+9
87	20343	492	0.01	21.8% H-14 => L+1, 19.4% H-3 => L+7, 18.6% H- 16 => L+1, 16.6% H-9 => L+2, 5.09% H-5 => L+6, 4.16% H-6 => L+4, 3.92% H-1 => L+9
88	20368	491	0.00	33.3% H-2 => L+9, 24.4% H-3 => L+8, 19.3% H- 15 => L+1, 3.70% H-7 => L+3, 2.02% H-4 => L+10
89	20403	490	0.57	35.4% H-1 => L+10, 34.2% H-6 => L+3, 7.63% H- 8 => L+4, 3.21% H-10 => L+3, 3.10% H-2 => L+8, 2.23% H-13 => L+1
90	20421	490	0.00	

				36.7% H-17 => L+1, 22.3% H-8 => L+2, 18.5% H-2 => L+10, 3.37% H-4 => L+6, 3.28% H-20 => L+1, 2.24% H-9 => L+3
91	20529	487	0.00	47.2% H-5 => L+6, 13.7% H-14 => L+1, 13.6% H-9 => L+2, 7.55% HOMO => L+12, 2.86% H-6 => L+4
92	20554	487	0.27	81.6% H-18 => L+1, 4.19% HOMO => L+11, 3.50% H-16 => L+2, 3.15% H-16 => LUMO
93	20701	483	0.00	41.8% H-17 => L+1, 16.8% H-8 => L+2, 12.2% H-2 => L+10, 8.12% H-4 => L+6, 5.61% H-20 => L+1, 4.52% H-6 => L+5
94	20745	482	0.00	45.1% HOMO => L+11, 20.9% H-3 => L+9, 6.88% H-18 => L+1, 3.97% H-5 => L+7, 3.59% H-2 => L+12, 3.18% H-4 => L+5, 2.63% H-5 => L+10, 2.18% H-1 => L+7
95	20785	481	0.00	75.4% H-26 => LUMO, 7.59% H-25 => L+1, 6.60% H-27 => L+1, 4.36% H-24 => LUMO
96	20828	480	0.00	70.3% H-19 => L+1, 21.0% H-21 => L+1, 66.4% H-27 => LUMO, 13.8% H-25 => LUMO, 12.3% H-26 => L+1, 2.60% H-25 => L+2
97	20859	479	0.00	35.0% H-9 => L+3, 25.3% H-7 => L+4, 19.0% H-4 => L+6, 4.70% H-17 => L+1, 2.97% H-20 => L+1, 2.67% H-7 => L+7
99	20905	478	0.00	22.5% HOMO => L+12, 16.4% H-3 => L+10, 8.04% H-5 => L+9, 7.51% H-5 => L+6, 7.00% H-4 => L+8, 5.16% H-7 => L+5, 4.21% H-14 => L+1, 4.14% H-9 => L+2, 3.89% H-11 => L+2, 2.87% H-8 => L+6, 2.77% H-2 => L+11, 2.54% H-6 => L+7, 2.10% H-1 => L+9
100	20910	478	0.12	47.0% H-6 => L+4, 12.0% H-5 => L+6, 10.4% H-8 => L+3, 6.52% H-3 => L+10, 3.33% HOMO => L+12, 3.26% H-6 => L+7, 2.64% H-7 => L+5, 2.12% H-5 => L+9, 2.09% H-14 => L+1, 64.4% H-21 => L+1, 16.7% H-19 => L+1, 4.45% H-20 => L+2, 4.31% H-20 => LUMO, 2.89% H-4 => L+7
101	21062	475	0.06	72.7% H-20 => L+1, 5.00% H-17 => L+1, 4.98% H-4 => L+6, 3.57% H-21 => L+2, 2.76% H-21 => LUMO, 2.50% H-6 => L+5
102	21187	472	0.07	77.2% H-10 => L+2, 4.13% H-2 => L+9, 2.43% H-8 => L+5
103	21220	471	0.00	48.6% H-3 => L+9, 20.2% HOMO => L+11, 5.53% H-8 => L+4, 5.11% H-6 => L+6, 4.70% H-10 => L+3, 3.04% H-1 => L+10, 2.24% H-5 => L+7
104	21269	470	0.00	55.3% H-6 => L+5, 12.3% H-9 => L+3, 8.15% H-2 => L+10, 4.52% H-11 => L+3, 3.26% H-9 => L+6, 3.08% H-20 => L+1, 2.70% H-7 => L+4
105	21333	469	0.00	35.9% H-7 => L+5, 32.9% HOMO => L+12, 7.70% H-4 => L+8, 6.52% H-6 => L+4, 5.38% H-11 => L+2, 2.64% H-9 => L+2
106	21433	467	0.00	
107	21580	463	0.05	

				67.2% H-4 => L+7, 3.31% H-10 => L+2, 2.78% H-1 => L+11, 2.48% H-3 => L+8, 2.35% H-21 => L+1, 2.08% H-7 => L+6
108	21700	461	0.86	68.6% H-11 => L+2, 5.43% H-7 => L+5, 5.24% H-12 => L+5, 5.04% H-12 => L+1, 4.79% H-4 => L+8, 2.65% H-16 => L+1
109	21711	461	0.03	75.8% H-12 => L+2, 5.53% H-11 => L+1, 5.28% H-11 => L+5, 3.16% HOMO => L+11, 2.61% H-13 => L+1
110	21755	460	0.00	42.9% H-7 => L+4, 24.0% H-9 => L+3, 13.5% H-6 => L+5, 4.11% H-9 => L+6, 2.92% H-2 => L+10, 2.34% H-4 => L+3
111	21771	459	0.00	39.7% H-8 => L+3, 21.1% H-6 => L+4, 18.0% H-3 => L+10, 7.33% H-7 => L+5, 5.81% H-10 => L+4
112	21820	458	0.00	67.3% H-5 => L+7, 9.26% H-10 => L+3, 7.15% H-8 => L+4, 2.25% H-6 => L+9, 2.25% HOMO => L+11
113	22036	454	0.00	57.0% H-4 => L+8, 19.5% H-7 => L+5, 5.35% H-8 => L+3, 3.39% HOMO => L+12, 2.90% H-9 => L+8, 2.37% H-13 => L+2
114	22046	454	0.04	36.1% H-28 => LUMO, 24.7% H-5 => L+8, 9.27% H-4 => L+9, 7.16% H-32 => LUMO, 4.49% H-6 => L+5, 3.08% H-29 => L+1, 2.93% H-2 => L+10, 2.20% H-7 => L+7
115	22178	451	0.00	46.4% H-5 => L+8, 20.5% H-28 => LUMO, 16.0% H-30 => LUMO, 4.28% H-4 => L+9, 2.08% H-11 => L+3
116	22242	450	0.00	74.3% H-29 => LUMO, 9.08% H-31 => LUMO, 5.91% H-28 => L+1, 2.07% H-4 => L+7
117	22242	450	0.01	39.4% H-3 => L+10, 22.3% H-8 => L+3, 7.88% H-4 => L+8, 6.87% H-5 => L+9, 5.49% H-8 => L+6, 5.44% H-6 => L+7
118	22336	448	0.00	66.3% H-30 => LUMO, 14.0% H-28 => LUMO, 6.33% H-5 => L+8, 2.20% H-2 => L+10
119	22347	447	0.00	56.0% H-31 => LUMO, 23.3% H-33 => LUMO, 9.29% H-29 => LUMO, 3.41% H-7 => L+6
120	22367	447	0.01	27.7% H-9 => L+5, 25.7% H-14 => L+2, 10.8% H-5 => L+10, 5.61% H-7 => L+8, 3.99% H-8 => L+7, 3.65% H-6 => L+9, 2.90% H-10 => L+6, 2.72% H-3 => L+9, 2.49% H-1 => L+10, 2.48% H-5 => L+7
121	22389	447	0.00	32.9% H-4 => L+9, 19.1% H-32 => LUMO, 18.0% H-28 => LUMO, 5.48% H-30 => LUMO, 2.85% H-11 => L+3, 2.20% H-7 => L+10
122	22393	447	0.00	31.6% H-33 => LUMO, 15.2% H-31 => LUMO, 15.2% H-7 => L+6, 14.1% H-9 => L+4, 4.08% H-12 => L+3, 2.85% H-32 => L+1, 2.44% H-11 => L+4
123	22449	445	0.22	61.6% H-32 => LUMO, 13.6% H-4 => L+9, 5.16% H-30 => LUMO, 3.62% H-11 => L+3, 2.17% H-12 => L+4, 2.11% H-33 => L+1
124	22591	443	0.00	

				34.1% H-33 => LUMO, 21.4% H-9 => L+4, 11.1% H-7 => L+6, 6.76% H-31 => LUMO, 4.71% H-4 => L+7, 4.61% H-12 => L+3, 3.07% H-4 => L+10, 2.14% H-14 => L+3
125	22623	442	0.03	68.2% H-6 => L+6, 11.4% H-10 => L+3, 6.29% H-8 => L+4, 2.26% H-14 => L+2, 2.10% H-5 => L+4
126	22719	440	0.00	26.2% H-7 => L+6, 23.6% H-12 => L+3, 11.8% H-11 => L+4, 6.92% H-8 => L+5, 4.08% H-31 => LUMO, 3.20% H-29 => LUMO, 2.88% H-10 => L+2, 2.64% H-1 => L+11, 2.48% H-4 => L+7,
127	22788	439	0.30	2.34% H-9 => L+7, 2.23% H-6 => L+8
128	22846	438	0.00	84.6% H-22 => L+1, 6.14% H-23 => LUMO, 3.52% H-23 => L+2, 2.03% H-24 => L+1
129	22915	436	0.19	31.7% H-4 => L+10, 31.0% H-8 => L+5, 7.23% H-7 => L+6, 4.05% H-10 => L+2, 3.93% H-6 => L+8, 3.34% H-7 => L+9, 3.31% H-9 => L+4, 2.21% H-2 => L+9
130	22947	436	0.16	66.0% H-13 => L+2, 6.27% H-5 => L+9, 3.79% H-7 => L+5, 2.85% H-16 => L+1, 2.09% H-8 => L+3
131	23021	434	0.01	39.0% H-11 => L+3, 22.5% H-12 => L+4, 6.34% H-15 => L+2, 4.32% H-5 => L+8, 2.68% H-13 => L+3, 2.56% H-1 => L+12, 2.45% H-32 => LUMO, 2.27% H-9 => L+3
132	23127	432	0.00	50.7% H-5 => L+9, 7.06% H-36 => LUMO, 6.68% H-13 => L+2, 4.92% HOMO => L+12, 4.58% H-8 => L+3, 3.73% H-11 => L+2, 2.87% H-10 => L+4, 2.49% H-6 => L+10
133	23183	431	0.34	34.4% H-9 => L+4, 17.7% H-12 => L+3, 11.6% H-7 => L+6, 8.07% H-11 => L+4, 4.71% H-4 => L+10, 3.94% H-9 => L+7, 2.76% H-13 => L+4
134	23222	431	0.00	69.1% H-23 => L+1, 6.00% H-24 => LUMO, 5.94% H-22 => L+2, 4.41% H-22 => LUMO, 3.06% H-25 => L+1, 2.09% H-14 => L+2
135	23293	429	0.11	47.8% H-36 => LUMO, 21.4% H-38 => LUMO, 5.07% H-5 => L+9, 3.57% H-13 => L+2, 3.54% H-40 => LUMO, 2.65% H-10 => L+4, 2.39% H-8 => L+6, 2.08% H-6 => L+7
136	23316	429	0.00	41.4% H-9 => L+5, 27.1% H-14 => L+2, 9.08% H-10 => L+3, 4.95% H-8 => L+4, 2.56% H-23 => L+1
137	23341	428	0.00	71.0% H-35 => LUMO, 13.6% H-15 => L+2, 4.99% H-34 => L+1
138	23342	428	0.00	43.3% H-8 => L+4, 21.1% H-10 => L+3, 14.1% H-5 => L+10, 6.75% H-9 => L+5, 2.87% H-6 => L+3, 2.17% H-10 => L+6
139	23344	428	0.00	87.6% H-34 => LUMO, 6.14% H-35 => L+1
140	23367	428	0.00	56.9% H-15 => L+2, 19.3% H-35 => LUMO, 4.12% H-1 => L+12, 3.38% H-11 => L+3, 2.24% H-3 => L+11

				62.4% H-37 => LUMO, 7.65% H-41 => LUMO, 3.86% H-39 => LUMO, 3.47% H-14 => L+2, 2.92% H-10 => L+3, 2.77% H-36 => L+1 42.4% H-8 => L+5, 27.3% H-4 => L+10, 6.41% H- 1 => L+11, 3.63% H-34 => LUMO, 3.21% H-3 => L+12, 2.41% H-17 => L+2, 2.30% H-12 => L+3 34.1% H-16 => L+2, 21.9% H-5 => L+10, 9.17% H-14 => L+2, 5.13% H-8 => L+4, 3.67% H-9 => L+5, 2.90% H-37 => LUMO, 2.54% H-6 => L+9, 2.16% H-2 => L+12, 2.12% H-18 => L+1 41.1% H-38 => LUMO, 15.5% H-36 => LUMO, 13.1% H-40 => LUMO, 12.5% H-42 => LUMO,
141	23426	427	0.00	
142	23463	426	0.06	
143	23519	425	0.00	
144	23547	425	0.01	3.10% H-18 => L+2, 2.43% H-37 => L+1 25.6% H-7 => L+7, 17.8% H-9 => L+6, 11.3% H-4 => L+9, 6.29% H-15 => L+2, 6.16% H-13 => L+3, 4.35% H-1 => L+12, 2.70% H-9 => L+3, 2.26% H- 10 => L+5, 2.20% H-19 => L+2, 2.07% H-14 => L+4
145	23608	424	0.00	53.8% H-41 => LUMO, 14.1% H-39 => LUMO, 8.29% H-43 => LUMO, 5.32% H-37 => LUMO, 3.14% H-5 => L+10, 2.84% H-16 => L+2, 2.39% H-14 => L+2
146	23672	422	0.00	67.2% H-24 => L+1, 6.14% H-23 => L+2, 5.24% H-23 => LUMO, 4.87% H-26 => L+1, 4.83% H-25 => LUMO
147	23687	422	0.00	63.2% H-42 => LUMO, 15.5% H-44 => LUMO,
148	23722	422	0.11	7.96% H-38 => LUMO, 4.09% H-6 => L+7 23.7% H-6 => L+7, 12.7% H-2 => L+11, 12.2% H- 36 => LUMO, 11.3% H-40 => LUMO, 7.38% HOMO => L+12, 4.45% H-8 => L+6, 4.10% H-38 => LUMO
149	23750	421	0.14	39.4% H-16 => L+2, 12.5% H-37 => LUMO, 10.7% H-39 => LUMO, 7.72% H-14 => L+2, 6.27% H-2 => L+12, 4.68% H-5 => L+10, 3.04% HOMO => L+11
150	23776	421	0.00	69.0% H-17 => L+2, 6.08% H-1 => L+11, 4.31% H-4 => L+10, 3.83% H-20 => L+2, 2.04% H-15 => L+5
151	23855	419	0.00	23.3% H-39 => LUMO, 16.3% H-41 => LUMO, 10.6% H-10 => L+3, 8.26% H-43 => LUMO, 7.67% H-14 => L+2, 5.66% H-5 => L+10, 4.10% H-57 => LUMO, 3.03% H-16 => L+2, 2.87% H-40 => L+1
152	23858	419	0.00	28.9% H-7 => L+7, 14.9% H-13 => L+3, 8.46% H- 11 => L+3, 6.73% H-10 => L+5, 5.34% H-9 => L+6, 5.12% H-9 => L+9, 3.62% H-11 => L+6, 3.07% H-4 => L+9, 2.91% H-15 => L+2, 2.69% H- 18 => L+3, 2.64% H-12 => L+4, 2.54% H-7 => L+4, 2.27% H-19 => L+2
153	23859	419	0.00	

				47.9% H-18 => L+2, 25.7% H-40 => LUMO, 2.73% H-2 => L+11, 2.64% H-16 => L+5, 2.32% H-6 => L+7
154	23926	418	0.01	27.6% H-18 => L+2, 26.1% H-40 => LUMO, 11.0% H-6 => L+7, 10.4% H-38 => LUMO, 7.00% H-44 => LUMO, 4.04% H-42 => LUMO, 2.42% H- 39 => L+1
155	23942	418	0.04	36.0% H-39 => LUMO, 11.6% H-10 => L+3, 7.94% HOMO => L+11, 6.18% H-2 => L+12, 3.25% H-57 => LUMO, 2.67% H-41 => LUMO, 2.59% H-6 => L+6, 2.55% H-8 => L+4, 2.29% H-5 => L+7, 2.03% H-14 => L+2
156	24008	417	0.00	24.3% H-6 => L+7, 23.2% H-10 => L+4, 13.1% H- 2 => L+11, 12.7% H-8 => L+6, 3.76% HOMO => L+12, 3.30% H-15 => L+3, 3.25% H-38 => LUMO, 2.86% H-40 => LUMO
157	24064	416	0.08	64.3% H-19 => L+2, 15.4% H-21 => L+2, 6.88% H-1 => L+12, 2.02% H-4 => L+9
158	24104	415	0.00	61.2% H-25 => L+1, 20.2% H-27 => L+1, 6.44% H-24 => L+2, 4.90% H-24 => LUMO
159	24110	415	0.00	38.4% H-1 => L+11, 18.4% H-6 => L+8, 5.70% H- 14 => L+3, 4.74% H-12 => L+3, 4.36% H-9 => L+4, 3.94% H-3 => L+12, 3.08% H-17 => L+2, 3.02% H-8 => L+5, 2.27% H-12 => L+6, 2.09% H- 4 => L+7
160	24173	414	0.68	20.5% H-5 => L+10, 9.65% H-7 => L+8, 9.17% H- 6 => L+9, 7.72% H-8 => L+7, 7.37% H-43 => LUMO, 6.07% H-10 => L+6, 5.61% H-2 => L+12, 4.16% H-17 => L+3, 3.61% H-15 => L+4, 3.08% H-9 => L+5, 2.67% H-8 => L+4
161	24212	413	0.00	65.1% H-44 => LUMO, 14.5% H-42 => LUMO, 8.26% H-40 => LUMO, 4.46% H-43 => L+1,
162	24249	412	0.05	2.22% H-36 => LUMO
163	24254	412	0.00	65.2% H-43 => LUMO, 10.6% H-41 => LUMO, 3.49% H-44 => L+1, 2.63% H-2 => L+12, 2.44% H-7 => L+8, 2.39% H-37 => LUMO, 2.21% H-5 => L+10
164	24276	412	0.14	50.8% H-6 => L+8, 20.2% H-20 => L+2, 5.29% H- 4 => L+10, 4.57% H-12 => L+3, 4.37% H-1 => L+11
165	24299	412	0.01	34.0% H-21 => L+2, 20.1% H-1 => L+12, 14.9% H-10 => L+5, 8.27% H-9 => L+6, 3.09% H-3 => L+11, 2.23% H-20 => L+5, 2.11% H-20 => L+1, 2.10% H-11 => L+3
166	24364	410	0.00	43.3% H-20 => L+2, 9.13% H-16 => L+3, 8.97% H-12 => L+6, 6.82% H-12 => L+3, 5.76% H-6 => L+8, 5.61% H-11 => L+4, 2.67% H-4 => L+10, 2.62% H-21 => L+1, 2.27% H-11 => L+7, 2.27% H-13 => L+4, 2.15% H-21 => L+5
167	24385	410	0.00	30.7% H-10 => L+5, 30.4% H-21 => L+2, 9.04% H-19 => L+2, 4.13% H-13 => L+3, 2.53% H-20 =>

				L+5, 2.42% H-15 => L+2, 2.39% H-1 => L+12, 2.37% H-20 => L+1
168	24416	410	0.52	16.6% H-16 => L+3, 11.8% H-20 => L+2, 7.35% H-17 => L+2, 7.26% H-13 => L+4, 6.85% H-7 => L+6, 5.75% H-1 => L+11, 5.71% H-6 => L+8, 5.31% H-9 => L+7, 4.37% H-14 => L+3, 3.72% H- 7 => L+9, 3.60% H-12 => L+6, 2.73% H-4 => L+10, 2.33% H-18 => L+4 18.2% H-10 => L+5, 18.0% H-1 => L+12, 9.43% H-7 => L+7, 8.19% H-9 => L+6, 6.74% H-18 => L+3, 6.06% H-11 => L+3, 5.64% H-19 => L+2, 5.16% H-11 => L+6, 2.83% H-4 => L+9, 2.77% H- 12 => L+7, 2.11% H-16 => L+4
169	24447	409	0.01	36.7% H-8 => L+6, 27.2% H-10 => L+4, 6.96% H- 10 => L+7, 4.40% H-6 => L+7, 4.03% H-48 => LUMO, 2.79% H-15 => L+3, 2.37% H-6 => L+4 45.5% H-7 => L+8, 14.9% H-47 => LUMO, 8.83% H-11 => L+5, 4.86% H-6 => L+9, 4.15% H-9 => L+5, 3.61% H-50 => LUMO
170	24458	409	0.00	72.9% H-47 => LUMO, 9.91% H-7 => L+8, 3.36% H-45 => LUMO, 2.21% H-50 => LUMO
171	24463	409	0.00	25.1% H-9 => L+6, 19.8% H-13 => L+3, 9.43% H- 1 => L+12, 7.25% H-21 => L+2, 6.41% H-16 => L+4, 3.94% H-10 => L+5, 3.53% H-11 => L+3, 3.19% H-12 => L+4, 2.54% H-9 => L+9, 2.43% H- 19 => L+2, 2.31% H-7 => L+10
172	24485	408	0.00	63.8% H-48 => LUMO, 11.3% H-54 => LUMO, 5.64% H-8 => L+6, 4.27% H-46 => LUMO, 3.89% H-2 => L+11
173	24553	407	0.01	88.5% H-49 => LUMO, 3.31% H-52 => LUMO, 2.11% H-14 => L+3
174	24568	407	0.00	76.3% H-51 => LUMO, 19.5% H-53 => LUMO 63.9% H-50 => LUMO, 12.3% H-57 => LUMO,
175	24590	407	0.00	5.45% H-11 => L+5, 4.00% H-47 => LUMO 42.4% H-26 => L+1, 7.78% H-46 => LUMO, 6.54% H-27 => LUMO, 5.07% H-48 => LUMO, 4.79% H-25 => LUMO, 3.94% H-54 => LUMO, 3.69% H-2 => L+11, 3.67% H-27 => L+2, 3.53%
176	24610	406	0.00	H-12 => L+5, 3.16% H-25 => L+2 22.8% H-26 => L+1, 19.6% H-48 => LUMO, 15.7% H-46 => LUMO, 5.70% H-2 => L+11, 5.46% H-54 => LUMO, 3.38% H-27 => LUMO,
177	24670	405	0.00	2.40% H-25 => LUMO, 2.38% H-12 => L+5 56.4% H-27 => L+1, 13.6% H-26 => LUMO,
178	24670	405	0.00	10.9% H-25 => L+1, 9.61% H-26 => L+2 55.9% H-52 => LUMO, 13.3% H-14 => L+3, 5.69% H-7 => L+9, 5.58% H-55 => LUMO, 2.49% H-13 => L+4, 2.18% H-58 => LUMO
179	24682	405	0.00	32.9% H-45 => LUMO, 15.3% H-2 => L+12, 10.5% H-57 => LUMO, 10.0% H-11 => L+5,
180	24714	405	0.00	
181	24728	404	0.11	
182	24737	404	0.00	

				6.87% H-50 => LUMO, 3.51% H-47 => LUMO, 3.37% H-6 => L+9, 3.07% H-7 => L+8
				22.4% H-52 => LUMO, 20.3% H-7 => L+9, 10.9% H-14 => L+3, 6.17% H-49 => LUMO, 3.52% H-11 => L+4, 3.31% H-12 => L+6, 3.00% H-12 => L+3, 2.80% H-20 => L+2, 2.74% H-9 => L+7, 2.28% H-9 => L+10, 2.22% H-9 => L+4
183	24740	404	0.02	63.8% H-53 => LUMO, 17.3% H-51 => LUMO, 9.40% H-56 => LUMO, 3.26% H-52 => L+1, 2.44% H-59 => LUMO
184	24742	404	0.00	30.6% H-12 => L+5, 14.7% H-46 => LUMO, 14.7% H-15 => L+3, 7.49% H-10 => L+4, 4.77% H-54 => LUMO, 2.82% H-13 => L+2, 2.80% H-11 => L+8, 2.30% H-9 => L+8, 2.27% H-21 => L+3
185	24767	404	0.02	16.4% H-6 => L+10, 10.2% H-54 => LUMO, 9.25% H-19 => L+3, 7.96% H-46 => LUMO, 7.23% H-9 => L+8, 6.41% H-8 => L+6, 5.52% H-8 => L+9, 4.47% H-14 => L+5, 4.01% H-60 => LUMO, 4.00% H-15 => L+6, 3.43% H-17 => L+4,
186	24853	402	0.00	2.58% H-10 => L+7, 2.43% H-18 => L+2 31.9% H-14 => L+3, 14.0% H-1 => L+11, 10.7% H-13 => L+4, 10.1% H-11 => L+4, 6.35% H-7 => L+9, 4.99% H-16 => L+3, 3.70% H-9 => L+7,
187	24862	402	1.42	2.93% H-52 => LUMO, 2.28% H-17 => L+2 46.5% H-15 => L+3, 21.2% H-12 => L+5, 6.22% H-10 => L+4, 5.03% H-17 => L+4, 2.57% H-13 =>
188	24864	402	0.03	L+2, 2.40% H-8 => L+6, 2.15% H-9 => L+8 27.0% H-13 => L+3, 12.8% H-18 => L+3, 10.0% H-11 => L+6, 9.28% H-12 => L+4, 7.52% H-1 => L+12, 4.21% H-7 => L+7, 3.13% H-10 => L+5, 2.89% H-12 => L+7, 2.85% H-9 => L+6, 2.65% H-13 => L+6, 2.42% H-11 => L+3
189	24885	402	0.00	26.3% H-45 => LUMO, 18.4% H-11 => L+5, 12.3% H-2 => L+12, 7.74% H-7 => L+8, 5.02% H-57 => LUMO, 3.92% H-17 => L+3, 2.58% H-15 =>
190	24915	401	0.00	L+4, 2.38% H-10 => L+3 27.7% H-6 => L+9, 24.1% H-17 => L+3, 18.3% H-11 => L+5, 6.67% H-15 => L+4, 3.45% H-57 =>
191	24957	401	0.00	LUMO, 2.56% H-19 => L+4, 2.26% H-10 => L+6 54.6% H-54 => LUMO, 29.7% H-46 => LUMO, 2.38% H-48 => LUMO, 2.21% H-45 => L+1,
192	24980	400	0.02	2.15% H-2 => L+11 50.1% H-57 => LUMO, 20.1% H-45 => LUMO, 13.5% H-50 => LUMO, 2.60% H-54 => L+1,
193	25007	400	0.00	2.55% H-11 => L+5 20.8% H-11 => L+4, 18.6% H-7 => L+9, 10.8% H-14 => L+3, 8.97% H-12 => L+3, 8.41% H-9 =>
194	25010	400	0.02	L+10, 5.20% H-61 => LUMO, 3.47% H-9 => L+7, 2.99% H-13 => L+4, 2.64% H-13 => L+7, 2.36% H-6 => L+8

195	25101	398	0.02	62.7% H-55 => LUMO, 17.5% H-58 => LUMO, 9.64% H-52 => LUMO, 3.40% H-56 => L+1 59.8% H-56 => LUMO, 16.3% H-59 => LUMO,
196	25102	398	0.00	10.8% H-53 => LUMO, 3.49% H-55 => L+1 21.1% H-2 => L+11, 17.8% H-19 => L+3, 11.6% H-60 => LUMO, 9.44% H-21 => L+3, 7.96% H-46 => LUMO, 4.31% H-9 => L+8, 2.87% H-17 =>
197	25123	398	0.03	L+4, 2.40% H-10 => L+4, 2.26% H-15 => L+3 27.0% H-18 => L+3, 16.6% H-16 => L+4, 15.6% H-12 => L+4, 8.62% H-7 => L+7, 7.32% H-9 => L+6, 5.13% H-11 => L+3, 2.52% H-56 => LUMO,
198	25161	397	0.00	2.13% H-14 => L+4 23.6% H-19 => L+3, 22.1% H-6 => L+10, 9.50% H-2 => L+11, 8.65% H-21 => L+3, 4.36% H-12 => L+5, 4.12% H-60 => LUMO, 4.10% H-8 => L+9, 3.04% H-10 => L+4, 2.08% H-9 => L+8, 2.02% H-
199	25215	397	0.39	46 => LUMO 25.9% H-20 => L+3, 16.2% H-17 => L+3, 14.1% H-6 => L+9, 8.92% H-21 => L+4, 8.74% H-2 => L+12, 3.12% H-7 => L+8, 2.84% H-64 => LUMO,
200	25256	396	0.00	2.20% H-15 => L+4 31.8% H-58 => LUMO, 14.4% H-55 => LUMO, 10.2% H-9 => L+7, 7.61% H-61 => LUMO, 7.43% H-16 => L+3, 4.74% H-18 => L+4, 4.45% H-11 =>
201	25311	395	0.03	L+4, 2.36% H-9 => L+10 67.8% H-59 => LUMO, 20.0% H-56 => LUMO,
202	25325	395	0.00	3.71% H-58 => L+1 33.5% H-58 => LUMO, 16.8% H-16 => L+3, 13.5% H-9 => L+7, 6.89% H-55 => LUMO, 5.57% H-18 => L+4, 3.54% H-61 => LUMO, 2.48% H-9
203	25329	395	0.06	=> L+10, 2.46% H-7 => L+9 44.0% H-21 => L+3, 26.4% H-20 => L+4, 8.07% H-19 => L+3, 5.86% H-6 => L+10, 3.82% H-17 =>
204	25356	394	0.33	L+4, 2.32% H-12 => L+5, 2.22% H-19 => L+6 38.7% H-7 => L+10, 7.76% H-12 => L+4, 7.36% H-9 => L+9, 5.74% H-10 => L+5, 4.82% H-62 => LUMO, 4.48% H-13 => L+3, 2.77% H-9 => L+6, 2.51% H-4 => L+9, 2.43% H-8 => L+8, 2.36% H- 18 => L+3, 2.15% H-11 => L+3, 2.11% H-33 =>
205	25385	394	0.00	L+1 28.9% H-20 => L+3, 12.8% H-2 => L+12, 12.3% H-21 => L+4, 11.1% H-11 => L+5, 7.94% H-17 => L+3, 7.25% H-19 => L+4, 2.73% H-64 => LUMO,
206	25395	394	0.00	2.56% H-15 => L+4 32.3% H-10 => L+6, 25.4% H-8 => L+7, 7.17% H- 2 => L+12, 6.38% H-6 => L+9, 4.56% H-17 => L+3, 3.59% H-19 => L+4, 2.62% H-20 => L+3,
207	25460	393	0.00	2.30% H-64 => LUMO, 2.28% H-11 => L+5 15.9% H-28 => L+1, 12.0% H-11 => L+7, 9.42% H-61 => LUMO, 8.31% H-12 => L+6, 7.42% H-16
208	25546	391	0.00	=> L+3, 7.34% H-12 => L+9, 6.83% H-58 =>

				LUMO, 4.04% H-11 => L+4, 2.78% H-3 => L+12, 2.59% H-16 => L+6, 2.33% H-13 => L+7, 2.24% H-29 => LUMO
209	25576	391	0.00	18.6% H-29 => L+1, 10.4% H-12 => L+7, 8.40% H-18 => L+3, 7.96% H-3 => L+11, 7.72% H-11 => L+6, 7.37% H-12 => L+4, 5.35% H-62 => LUMO, 4.90% H-11 => L+9, 4.22% H-59 => LUMO, 3.01% H-1 => L+12, 2.43% H-28 => LUMO, 2.29% H-11 => L+3
210	25705	389	0.00	52.0% H-29 => L+1, 19.1% H-3 => L+11, 4.82% H-28 => LUMO, 4.74% H-1 => L+12, 3.59% H-28 => L+2, 2.17% H-11 => L+6, 2.07% H-5 => L+12 49.5% H-9 => L+8, 12.6% H-12 => L+5, 9.78% H- 6 => L+10, 8.37% H-19 => L+3, 3.34% H-14 => L+5, 2.29% H-17 => L+4
211	25710	389	0.02	60.9% H-28 => L+1, 9.75% H-61 => LUMO, 5.42% H-29 => LUMO, 4.08% H-29 => L+2, 4.02% H-3 => L+12, 2.34% H-32 => L+1, 2.04% H-12 => L+6
212	25718	389	0.01	40.4% H-8 => L+7, 38.4% H-10 => L+6, 7.55% H- 10 => L+9, 3.25% H-6 => L+9, 2.59% H-6 => L+6, 2.37% H-8 => L+4
213	25769	388	0.00	21.9% H-14 => L+4, 14.1% H-3 => L+11, 13.2% H-62 => LUMO, 7.68% H-8 => L+8, 6.31% H-29 => L+1, 4.77% H-31 => L+1, 4.12% H-13 => L+6, 3.60% H-1 => L+12, 2.62% H-11 => L+9, 2.39% H-12 => L+7
214	25823	387	0.00	62.7% H-30 => L+1, 11.0% H-61 => LUMO,
215	25823	387	0.19	7.44% H-3 => L+12 30.9% H-61 => LUMO, 25.7% H-30 => L+1, 13.7% H-3 => L+12, 7.25% H-32 => L+1, 2.72%
216	25847	387	0.02	H-7 => L+9, 2.49% H-63 => LUMO 64.4% H-31 => L+1, 20.1% H-33 => L+1, 3.97%
217	25893	386	0.00	H-62 => LUMO 22.6% H-3 => L+11, 19.5% H-14 => L+4, 17.2% H-11 => L+6, 7.40% H-33 => L+1, 4.17% H-62 => LUMO, 3.80% H-18 => L+3, 3.37% H-12 => L+7, 2.91% H-29 => L+1
218	25931	386	0.01	35.0% H-3 => L+12, 10.8% H-9 => L+7, 10.7% H- 61 => LUMO, 4.56% H-1 => L+11, 4.23% H-12 => L+6, 3.44% H-28 => L+1, 3.38% H-63 => LUMO, 2.57% H-16 => L+6, 2.56% H-11 => L+7, 2.42% H-5 => L+11, 2.36% H-16 => L+3, 2.31% H-12 => L+9, 2.22% H-13 => L+7
219	25970	385	0.26	66.1% H-60 => LUMO, 4.89% H-2 => L+11, 4.32% H-15 => L+3, 2.79% H-14 => L+5, 2.15% H-10 => L+4
220	26021	384	0.13	29.3% H-8 => L+8, 19.6% H-62 => LUMO, 15.3% H-14 => L+4, 4.10% H-11 => L+6, 3.44% H-12 => L+7, 3.05% H-13 => L+6, 2.68% H-31 => L+1,
221	26049	384	0.00	

				2.44% H-12 => L+4, 2.32% H-23 => L+3, 2.00% H-65 => LUMO
222	26063	384	0.01	57.0% H-32 => L+1, 7.89% H-12 => L+6, 5.14% H-7 => L+9, 4.30% H-63 => LUMO, 3.66% H-30 => L+1, 3.39% H-11 => L+4, 2.31% H-33 => L+2 54.3% H-22 => L+3, 13.4% H-23 => L+4, 5.07% H-13 => L+4, 4.89% H-24 => L+6, 2.89% H-22 => L+6, 2.24% H-25 => L+7, 2.19% H-9 => L+7, 2.15% H-27 => L+10
223	26086	383	0.14	85.9% H-13 => L+5, 2.27% H-16 => L+2, 2.25% H-18 => L+5
224	26094	383	0.00	56.9% H-33 => L+1, 14.1% H-31 => L+1, 9.29% H-62 => LUMO, 3.72% H-32 => L+2, 2.99% H-14 => L+4, 2.59% H-32 => LUMO, 2.39% H-3 => L+11
225	26120	383	0.00	82.5% H-22 => L+2, 5.75% H-23 => L+1, 3.91% H-23 => L+5, 2.50% H-22 => LUMO
226	26125	383	0.00	33.5% H-13 => L+4, 15.1% H-9 => L+7, 6.93% H-18 => L+4, 4.36% H-7 => L+9, 4.36% H-22 => L+3, 3.48% H-14 => L+3, 2.86% H-16 => L+3, 2.80% H-32 => L+1, 2.48% H-15 => L+5, 2.46% H-23 => L+4, 2.25% H-13 => L+7, 2.24% H-12 => L+3
227	26169	382	0.03	44.8% H-8 => L+8, 21.4% H-7 => L+10, 14.4% H-62 => LUMO, 4.89% H-14 => L+4, 2.14% H-11 => L+6
228	26203	382	0.00	34.6% H-8 => L+9, 22.6% H-6 => L+10, 15.3% H-10 => L+7, 5.76% H-10 => L+10, 2.70% H-15 => L+6, 2.52% H-19 => L+3, 2.12% H-6 => L+7, 2.01% H-5 => L+9
229	26221	381	0.19	55.1% H-15 => L+4, 8.73% H-19 => L+4, 8.60% H-17 => L+3, 3.27% H-17 => L+6, 3.15% H-15 => L+7, 2.71% H-19 => L+7
230	26252	381	0.00	16.1% H-12 => L+6, 15.5% H-63 => LUMO, 12.3% H-32 => L+1, 9.69% H-13 => L+4, 7.94% H-16 => L+6, 7.24% H-15 => L+5, 3.96% H-7 => L+9, 3.74% H-11 => L+4, 2.30% H-12 => L+9, 2.15% H-16 => L+3, 2.07% H-12 => L+3 28.8% H-23 => L+3, 14.5% H-22 => L+4, 5.06% H-24 => L+4, 5.02% H-62 => LUMO, 5.01% H-13 => L+6, 4.05% H-11 => L+6, 2.85% H-16 => L+4, 2.62% H-14 => L+4, 2.29% H-11 => L+9, 2.02% H-22 => L+7, 2.00% H-25 => L+6
231	26269	381	0.03	12.4% H-11 => L+6, 11.6% H-23 => L+3, 8.18% H-14 => L+4, 7.08% H-62 => LUMO, 5.86% H-22 => L+4, 5.52% H-18 => L+3, 5.01% H-16 => L+4, 4.35% H-7 => L+10, 4.21% H-18 => L+6, 3.99% H-13 => L+6, 3.74% H-11 => L+9, 3.28% H-9 => L+9, 3.27% H-24 => L+4, 3.18% H-8 => L+8, 2.55% H-12 => L+4
232	26289	380	0.00	
233	26316	380	0.00	

				35.7% H-63 => LUMO, 14.7% H-15 => L+5, 7.04% H-9 => L+7, 6.74% H-16 => L+6, 5.23% H- 18 => L+4, 4.49% H-61 => LUMO, 2.99% H-9 => L+10, 2.64% H-12 => L+9, 2.06% H-7 => L+9 64.0% H-14 => L+5, 9.50% H-23 => L+2, 8.75% H-9 => L+8, 2.56% H-60 => LUMO
234	26389	379	0.04	62.9% H-23 => L+2, 10.7% H-14 => L+5, 5.46% H-22 => L+5, 5.03% H-24 => L+1, 3.44% H-22 => L+1, 2.56% H-24 => L+5
235	26397	379	0.00	55.1% H-15 => L+5, 17.2% H-63 => LUMO, 3.56% H-12 => L+6, 2.60% H-13 => L+4, 2.53% H-32 => L+1, 2.17% H-10 => L+8, 2.01% H-7 => L+9
236	26490	378	0.00	19.5% H-8 => L+10, 14.7% H-17 => L+6, 14.3% H-19 => L+4, 9.13% H-21 => L+4, 7.86% H-10 => L+9, 5.93% H-15 => L+7, 4.04% H-15 => L+4, 3.59% H-17 => L+3, 2.22% H-6 => L+9
237	26495	377	0.01	37.9% H-24 => L+3, 17.4% H-23 => L+4, 12.2% H-22 => L+6, 5.22% H-25 => L+4, 4.27% H-27 => L+7, 3.05% H-26 => L+3, 2.98% H-22 => L+9, 2.21% H-23 => L+10, 2.09% H-26 => L+9, 2.03% H-27 => L+4
238	26534	377	0.00	34.2% H-17 => L+4, 14.2% H-15 => L+6, 9.90% H-20 => L+4, 9.47% H-8 => L+9, 5.03% H-21 => L+6, 4.31% H-19 => L+3, 2.88% H-10 => L+10, 2.56% H-15 => L+3, 2.31% H-15 => L+9 68.2% H-34 => L+1, 9.45% H-65 => LUMO,
240	26675	375	0.01	6.35% H-35 => LUMO, 4.30% H-35 => L+2 41.4% H-36 => L+1, 13.4% H-38 => L+1, 12.5% H-18 => L+5, 8.09% H-64 => LUMO, 2.61% H-40 => L+1, 2.03% H-4 => L+11
241	26757	374	0.00	83.2% H-35 => L+1, 7.19% H-34 => LUMO, 5.20% H-34 => L+2
242	26766	374	0.00	68.1% H-16 => L+5, 11.3% H-37 => L+1, 2.64% H-18 => L+2, 2.28% H-13 => L+8, 2.25% H-9 => L+8, 2.15% H-18 => L+8
243	26774	373	0.00	37.2% H-9 => L+9, 20.8% H-17 => L+5, 4.91% H- 7 => L+10, 3.61% H-20 => L+5, 3.55% H-65 => LUMO, 3.15% H-7 => L+7, 2.76% H-25 => L+3, 2.32% H-14 => L+10, 2.21% H-11 => L+6, 2.19% H-34 => L+1, 2.00% H-14 => L+4
244	26774	373	0.01	29.1% H-25 => L+3, 15.6% H-24 => L+4, 9.62% H-23 => L+6, 6.78% H-27 => L+6, 5.79% H-22 => L+7, 4.46% H-27 => L+3, 3.60% H-26 => L+7, 3.54% H-17 => L+5, 3.06% H-22 => L+10, 2.98% H-65 => LUMO, 2.49% H-25 => L+9, 2.16% H-26 => L+4
245	26836	373	0.00	47.6% H-65 => LUMO, 17.1% H-17 => L+5, 13.7% H-34 => L+1, 2.86% H-16 => L+4, 2.59% H-63 => L+1
246	26882	372	0.00	
247	26887	372	0.00	

				23.6% H-36 => L+1, 20.9% H-24 => L+2, 20.2% H-64 => LUMO, 4.01% H-18 => L+5, 3.49% H-19 => L+4, 2.44% H-23 => L+5, 2.24% H-26 => L+2, 2.17% H-21 => L+4
248	26900	372	0.00	45.0% H-24 => L+2, 9.07% H-64 => LUMO, 6.71% H-36 => L+1, 5.20% H-23 => L+5, 4.71% H-26 => L+2, 2.90% H-25 => L+1, 2.62% H-23 => L+1, 2.35% H-19 => L+4, 2.14% H-21 => L+4
249	26925	371	0.00	35.5% H-10 => L+7, 20.5% H-37 => L+1, 13.7% H-8 => L+9, 4.92% H-10 => L+10, 3.18% H-41 => L+1, 3.16% H-16 => L+5, 3.00% H-8 => L+6
250	26928	371	0.05	34.8% H-16 => L+4, 15.5% H-17 => L+5, 10.4% H-9 => L+9, 7.54% H-13 => L+3, 7.22% H-18 => L+3, 4.17% H-11 => L+9, 4.08% H-12 => L+7, 3.85% H-18 => L+6
251	26941	371	0.00	44.2% H-37 => L+1, 18.1% H-10 => L+7, 10.1% H-16 => L+5, 3.78% H-8 => L+9, 3.50% H-41 => L+1, 2.25% H-36 => LUMO, 2.00% H-36 => L+2
252	26949	371	0.01	17.5% H-11 => L+7, 13.8% H-12 => L+6, 10.6% H-9 => L+10, 9.56% H-12 => L+9, 9.11% H-10 => L+8, 4.42% H-15 => L+5, 4.23% H-63 => LUMO, 3.03% H-16 => L+3, 3.00% H-7 => L+9, 2.42% H-11 => L+4
253	26959	371	0.02	18.4% H-18 => L+5, 15.2% H-38 => L+1, 13.2% H-21 => L+4, 7.02% H-64 => LUMO, 6.99% H-20 => L+6, 4.81% H-19 => L+4, 4.68% H-20 => L+3, 4.13% H-40 => L+1, 3.55% H-42 => L+1, 3.31% H-8 => L+10, 3.17% H-10 => L+9, 3.02% H-19 => L+7
254	26979	371	0.00	32.1% H-38 => L+1, 13.5% H-42 => L+1, 8.04% H-36 => L+1, 7.64% H-21 => L+4, 7.10% H-40 => L+1, 6.23% H-20 => L+6, 4.52% H-20 => L+3, 2.42% H-10 => L+9, 2.21% H-8 => L+10, 2.09% H-19 => L+7
255	27042	370	0.00	27.0% H-14 => L+6, 20.7% H-19 => L+5, 14.0% H-21 => L+5, 5.24% H-18 => L+4, 4.95% H-10 => L+8, 4.14% H-9 => L+10, 3.39% H-13 => L+7
256	27081	369	0.00	17.2% H-17 => L+5, 16.0% H-65 => LUMO, 12.3% H-9 => L+9, 5.78% H-20 => L+5, 5.63% H-12 => L+7, 5.43% H-11 => L+9, 4.09% H-11 => L+6, 2.86% H-26 => L+4, 2.83% H-16 => L+4, 2.57% H-18 => L+3, 2.47% H-27 => L+3, 2.05% H-5 => L+12
257	27091	369	0.00	28.6% H-41 => L+1, 14.3% H-39 => L+1, 6.28% H-21 => L+6, 5.97% H-20 => L+4, 5.96% H-21 => L+3, 5.33% H-37 => L+1, 4.01% H-19 => L+6, 3.03% H-43 => L+1, 2.88% H-20 => L+7, 2.73% H-19 => L+3, 2.39% H-10 => L+7, 2.27% H-17 => L+7, 2.08% H-17 => L+4
258	27109	369	0.02	20.9% H-26 => L+3, 13.8% H-27 => L+4, 12.8% H-25 => L+4, 10.1% H-10 => L+8, 8.50% H-26 =>
259	27115	369	0.00	

				L+6, 8.36% H-24 => L+6, 5.32% H-23 => L+7, 5.30% H-25 => L+7, 3.49% H-24 => L+9, 3.22% H-22 => L+9, 2.25% H-23 => L+10 39.1% H-18 => L+5, 19.5% H-64 => LUMO, 3.86% H-4 => L+11, 3.74% H-20 => L+6, 3.72% H-36 => L+1, 3.64% H-38 => L+1, 3.21% H-20 => L+3, 2.22% H-16 => L+8, 2.03% H-19 => L+4 30.8% H-10 => L+8, 24.8% H-19 => L+5, 13.0% H-18 => L+4, 4.32% H-16 => L+3, 3.81% H-21 =>
260	27135	369	0.00	
261	27152	368	0.01	20.9% H-41 => L+1, 11.9% H-39 => L+1, 10.8% H-20 => L+4, 9.39% H-21 => L+6, 8.54% H-21 => L+3, 5.11% H-19 => L+6, 4.84% H-10 => L+7, 4.76% H-19 => L+3, 3.53% H-20 => L+7, 2.97% H-17 => L+7, 2.40% H-37 => L+1, 2.03% H-17 => L+4
262	27157	368	0.02	52.0% H-42 => L+1, 15.1% H-38 => L+1, 8.65% H-44 => L+1, 5.41% H-18 => L+5, 3.90% H-40 => L+1
263	27175	368	0.00	27.2% H-27 => L+3, 23.1% H-26 => L+4, 14.7% H-25 => L+6, 9.76% H-24 => L+7, 6.84% H-23 =>
264	27180	368	0.00	L+9, 4.80% H-22 => L+10, 3.21% H-9 => L+9 22.5% H-8 => L+10, 16.2% H-19 => L+4, 7.77% H-4 => L+11, 7.20% H-20 => L+6, 5.92% H-64 => LUMO, 5.59% H-17 => L+3, 5.36% H-20 => L+3, 5.22% H-42 => L+1, 4.95% H-10 => L+9, 3.13% H-21 => L+7
265	27218	367	0.00	21.8% H-14 => L+6, 21.5% H-18 => L+4, 13.2% H-9 => L+10, 8.49% H-19 => L+5, 6.62% H-13 => L+7, 4.81% H-16 => L+3, 3.53% H-10 => L+8,
266	27280	367	0.06	2.96% H-11 => L+10, 2.40% H-12 => L+9 52.7% H-39 => L+1, 21.4% H-41 => L+1, 9.03% H-43 => L+1, 5.03% H-40 => LUMO, 4.10% H-40
267	27320	366	0.00	=> L+2
268	27321	366	0.03	29.4% H-10 => L+8, 15.3% H-9 => L+10, 14.1% H-19 => L+5, 12.5% H-14 => L+6, 6.86% H-18 =>
269	27327	366	0.00	L+4, 4.86% H-21 => L+5 60.2% H-40 => L+1, 10.7% H-44 => L+1, 7.28% H-38 => L+1, 4.73% H-39 => LUMO, 4.00% H-42
270	27374	365	0.00	=> L+1, 3.48% H-39 => L+2 52.6% H-13 => L+6, 4.23% H-11 => L+9, 3.71% H-18 => L+6, 3.64% H-16 => L+4, 3.43% H-14 =>
271	27445	364	0.00	L+4, 3.25% H-20 => L+5, 2.57% H-12 => L+10, 2.55% H-17 => L+5, 2.32% H-14 => L+7, 2.31% H-18 => L+9, 2.18% H-9 => L+9, 2.18% H-13 =>
272	27448	364	0.01	L+3, 2.13% H-12 => L+4, 2.08% H-5 => L+12 59.6% H-25 => L+2, 23.4% H-27 => L+2, 4.34% H-24 => L+5, 3.90% H-24 => L+1 55.5% H-21 => L+5, 19.4% H-19 => L+5, 6.48% H-5 => L+11, 4.90% H-20 => L+2, 4.87% H-20 => L+8

273	27454	364	0.00	63.6% H-4 => L+11, 9.67% H-64 => LUMO, 4.53% H-7 => L+12 67.6% H-20 => L+5, 6.58% H-17 => L+5, 5.78% H-5 => L+12, 3.92% H-21 => L+8, 3.48% H-21 =>
274	27468	364	0.00	L+2 70.3% H-4 => L+12, 6.18% H-7 => L+11, 5.79%
275	27487	364	0.20	H-67 => LUMO, 4.48% H-2 => L+11 50.8% H-5 => L+11, 17.3% H-66 => LUMO, 7.63% H-3 => L+12, 5.00% H-6 => L+12, 4.82%
276	27556	363	0.02	H-14 => L+6, 4.57% H-21 => L+5 48.8% H-15 => L+6, 23.9% H-17 => L+4, 8.10%
277	27578	363	0.00	H-15 => L+3, 7.47% H-17 => L+7 71.6% H-43 => L+1, 9.61% H-41 => L+1, 4.76%
278	27645	362	0.02	H-44 => LUMO, 3.80% H-44 => L+2, 2.30% H-39 => L+1, 2.22% H-37 => L+1 65.3% H-44 => L+1, 12.4% H-42 => L+1, 6.70%
279	27648	362	0.00	H-40 => L+1, 5.35% H-43 => LUMO, 4.31% H-43 => L+2 57.5% H-5 => L+12, 6.13% H-6 => L+11, 5.82%
280	27754	360	0.00	H-68 => LUMO, 5.79% H-3 => L+11, 4.65% H-13 => L+6, 3.27% H-20 => L+5 25.9% H-16 => L+6, 19.8% H-11 => L+7, 12.4%
281	27795	360	0.00	H-9 => L+10, 8.15% H-18 => L+4, 7.52% H-18 => L+7, 7.34% H-14 => L+6, 4.58% H-13 => L+7, 3.78% H-16 => L+3, 2.26% H-12 => L+6, 2.14% H-13 => L+4 28.4% H-17 => L+6, 10.4% H-19 => L+4, 9.70%
				H-17 => L+3, 8.78% H-19 => L+7, 8.15% H-8 => L+10, 7.15% H-15 => L+4, 6.18% H-20 => L+9, 5.27% H-15 => L+7, 3.39% H-21 => L+10, 2.68%
282	27822	359	0.00	H-21 => L+4, 2.15% HOMO => L+13 30.7% H-12 => L+7, 23.4% H-18 => L+6, 12.0%
283	27852	359	0.00	H-16 => L+7, 6.61% H-12 => L+10, 5.75% H-18 => L+3, 5.26% H-11 => L+6, 4.70% H-16 => L+4 71.3% H-11 => L+8, 6.90% H-47 => L+1, 3.80%
284	27863	359	0.02	H-12 => L+5, 3.16% H-9 => L+8, 2.61% H-4 => L+12, 2.51% H-50 => L+1, 2.22% H-67 => LUMO 69.8% H-47 => L+1, 9.86% H-11 => L+8, 8.37%
285	27870	359	0.01	H-50 => L+1, 2.30% H-45 => L+1 69.1% H-12 => L+8, 8.65% H-48 => L+1, 3.81%
286	27953	358	0.00	H-11 => L+5, 2.94% H-54 => L+1, 2.15% H-18 => L+5 56.5% H-26 => L+2, 7.68% H-27 => L+1, 6.27%
				H-24 => L+2, 6.12% H-25 => L+1, 4.78% H-48 => L+1, 4.63% H-25 => L+5, 4.59% H-27 => L+5, 3.78% H-12 => L+8
287	27975	357	0.00	91.1% H-49 => L+1, 3.24% H-52 => L+1 16.9% H-20 => L+4, 12.5% H-19 => L+6, 6.91%
288	27977	357	0.00	H-19 => L+3, 6.50% H-10 => L+10, 5.92% H-17 => L+7, 5.89% H-20 => L+7, 4.84% H-15 => L+9, 4.57% H-27 => L+2, 4.06% H-57 => L+1, 3.68%
289	27991	357	0.07	

				H-21 => L+3, 3.32% H-67 => LUMO, 3.23% H-50 => L+1, 3.12% H-21 => L+9, 2.13% H-15 => L+6 57.5% H-48 => L+1, 10.6% H-54 => L+1, 10.1% H-12 => L+8, 5.70% H-26 => L+2, 3.60% H-46 =>
290	27996	357	0.00	L+1 60.3% H-51 => L+1, 13.8% H-53 => L+1, 13.0%
291	27999	357	0.05	H-66 => LUMO, 3.22% H-5 => L+11 44.4% H-27 => L+2, 13.9% H-25 => L+2, 10.9% H-26 => L+1, 8.08% H-26 => L+5, 2.91% H-20 =>
292	28006	357	0.00	L+4, 2.27% H-19 => L+6 46.3% H-66 => LUMO, 15.8% H-51 => L+1, 11.7% H-5 => L+11, 4.13% H-53 => L+1, 2.99% H-65 => L+1, 2.66% H-11 => L+7, 2.03% H-19 =>
293	28017	357	0.17	L+5 27.7% H-57 => L+1, 22.4% H-50 => L+1, 9.51% H-45 => L+1, 7.89% H-47 => L+1, 3.16% H-67 =>
294	28033	357	0.00	LUMO, 2.72% H-27 => L+2, 2.58% H-20 => L+4 29.5% H-10 => L+9, 16.9% H-21 => L+4, 8.74% H-17 => L+6, 8.25% H-20 => L+3, 6.41% H-8 => L+10, 6.31% H-20 => L+6, 5.56% H-15 => L+10, 4.08% H-17 => L+9, 3.28% H-21 => L+7, 2.39% H-8 => L+7
295	28043	357	0.00	35.3% H-45 => L+1, 33.9% H-50 => L+1, 7.30% H-47 => L+1, 6.81% H-67 => LUMO, 2.74% H-46 => LUMO, 2.21% H-46 => L+2
296	28160	355	0.00	42.1% H-46 => L+1, 18.1% H-54 => L+1, 12.1% H-48 => L+1, 2.80% H-10 => L+9, 2.58% H-20 =>
297	28169	355	0.00	L+6, 2.28% H-45 => LUMO, 2.01% H-45 => L+2 26.4% H-10 => L+9, 12.0% H-8 => L+10, 10.6% H-20 => L+6, 7.93% H-21 => L+7, 7.09% H-46 => L+1, 4.75% H-21 => L+4, 4.39% H-20 => L+3, 4.37% H-48 => L+1, 3.27% H-17 => L+9, 2.80% H-19 => L+4, 2.62% H-19 => L+10, 2.14% H-8 => L+7
298	28183	355	0.00	78.1% H-52 => L+1, 6.55% H-55 => L+1, 3.12% H-53 => L+2, 3.05% H-49 => L+1, 2.49% H-53 => LUMO
299	28189	355	0.00	

**Table S17.** TDDFT-predicted band excitation data for **8**.

Index	Energy (cm <sup>-1</sup> )	$\lambda$ (nm)	Osc. Strength	Contributions
0	3274	3055	6.56	98.8% HOMO => LUMO
1	4898	2042	0.00	94.8% H-2 => LUMO, 3.00% H-3 => L+1
2	5416	1846	0.00	54.1% H-1 => LUMO, 43.7% HOMO => L+1
3	5924	1688	0.00	54.3% HOMO => L+1, 43.7% H-1 => LUMO
4	5930	1686	0.00	82.9% H-3 => LUMO, 13.3% H-2 => L+1

				74.9% H-5 => LUMO, 16.5% H-3 => L+1, 5.41%
5	7269	1376	0.00	H-2 => L+2
6	7634	1310	0.06	75.0% H-4 => LUMO, 22.5% HOMO => L+2 82.2% H-2 => L+1, 13.5% H-3 => LUMO, 2.26%
7	7929	1261	0.00	H-3 => L+2 65.2% HOMO => L+2, 18.7% H-4 => LUMO,
8	8059	1241	0.31	12.0% H-1 => L+1 83.1% H-1 => L+1, 9.01% HOMO => L+2, 2.40%
9	8225	1216	0.11	H-4 => LUMO 69.0% H-6 => LUMO, 18.0% H-5 => L+1, 7.01%
10	8789	1138	0.00	H-3 => L+2, 2.83% H-2 => L+3 65.0% H-3 => L+1, 21.1% H-5 => LUMO, 8.23%
11	8973	1114	0.00	H-2 => L+2, 2.31% H-2 => LUMO 88.0% H-7 => LUMO, 3.63% H-4 => L+1, 3.56%
12	9597	1042	0.00	HOMO => L+3
13	10190	981	0.00	80.9% HOMO => L+3, 9.84% H-1 => L+2 54.1% H-5 => L+1, 27.0% H-6 => LUMO, 10.6%
14	10309	970	0.00	H-3 => L+2, 3.00% H-2 => L+3 84.3% H-4 => L+1, 4.87% H-7 => LUMO, 3.55%
15	10329	968	0.00	H-1 => L+2, 2.30% H-1 => LUMO 63.7% H-8 => LUMO, 17.1% H-6 => L+1, 7.93%
16	10371	964	0.00	H-5 => L+2, 2.87% H-2 => L+2, 2.29% H-3 => L+3 77.9% H-2 => L+2, 11.3% H-3 => L+1, 3.38% H-3 => L+3, 2.54% H-8 => LUMO, 2.27% H-2 =>
17	10445	957	0.00	LUMO 80.7% H-1 => L+2, 9.41% HOMO => L+3, 5.35%
18	10559	947	0.00	H-4 => L+1, 2.01% HOMO => L+1
19	11209	892	0.09	81.7% H-9 => LUMO, 7.81% H-7 => L+1
20	11453	873	0.00	95.5% HOMO => L+4 62.7% H-3 => L+2, 21.7% H-5 => L+1, 9.23% H-2 => L+3
21	11520	868	0.00	46.1% H-6 => L+1, 29.6% H-8 => LUMO, 12.3% H-5 => L+2, 4.62% H-3 => L+3
22	11777	849	0.00	65.9% H-10 => LUMO, 15.3% H-8 => L+1, 6.38% H-6 => L+2, 3.28% H-5 => L+3
23	11896	841	0.00	H-6 => L+2, 3.28% H-5 => L+3
24	12114	826	0.00	90.0% HOMO => L+5, 5.24% H-1 => L+4 44.0% HOMO => L+6, 15.1% H-1 => L+3, 11.8% H-7 => L+1, 11.6% H-4 => L+2, 5.67% H-9 =>
25	12166	822	0.02	LUMO, 2.50% H-12 => LUMO 76.5% H-11 => LUMO, 7.67% H-9 => L+1, 4.11% H-12 => L+1, 2.90% H-15 => LUMO, 2.18% H-7 => L+2
26	12316	812	0.00	61.4% H-7 => L+1, 23.8% HOMO => L+6, 6.31% H-9 => LUMO, 2.59% H-1 => L+3
27	12345	810	0.00	66.3% H-12 => LUMO, 7.78% H-4 => L+2, 7.16% HOMO => L+6, 4.63% H-11 => L+1, 4.59% H-7 =>
28	12668	789	0.23	L+1, 2.08% H-9 => L+2 48.5% H-4 => L+2, 17.0% H-12 => LUMO, 10.6% HOMO => L+6, 7.09% H-1 => L+3, 5.65% H-7 =>
29	12719	786	0.45	L+1, 2.82% H-2 => L+4

30	12836	779	0.00	50.8% H-5 => L+2, 29.1% H-6 => L+1, 10.0% H-3 => L+3, 3.43% H-2 => L+6 78.8% H-2 => L+3, 13.5% H-3 => L+2, 2.39% H-2 => L+1, 2.28% H-3 => L+6 66.1% H-1 => L+3, 14.9% H-4 => L+2, 9.26% HOMO => L+6, 3.71% H-2 => L+4
31	12840	779	0.00	66.1% H-1 => L+3, 14.9% H-4 => L+2, 9.26% HOMO => L+6, 3.71% H-2 => L+4 86.2% HOMO => L+7, 5.47% H-1 => L+5 66.9% H-13 => LUMO, 12.7% H-10 => L+1, 5.16% H-8 => L+2, 2.71% H-6 => L+3, 2.66% H-19 => LUMO
32	12935	773	0.52	40.7% H-8 => L+1, 28.1% H-10 => LUMO, 12.9% H-6 => L+2, 5.81% H-5 => L+3, 2.87% H-3 => L+6 74.4% H-2 => L+4, 8.83% H-3 => L+5, 7.81% H-4 => L+2
33	13028	768	0.00	59.3% H-3 => L+3, 22.5% H-5 => L+2, 10.4% H-2 => L+6 26.3% H-9 => L+1, 16.8% HOMO => L+9, 16.1% H-11 => LUMO, 9.70% H-7 => L+2, 7.30% H-4 => L+3, 7.11% H-1 => L+6, 6.28% H-15 => LUMO, 2.01% H-16 => L+1
34	13196	758	0.00	74.4% H-1 => L+4, 11.4% HOMO => L+8, 5.71% HOMO => L+5, 3.74% H-1 => L+7 70.8% HOMO => L+8, 14.7% H-1 => L+4, 3.18% H-1 => L+7, 2.93% H-4 => L+5
35	13239	755	0.00	46.4% H-9 => L+1, 29.3% HOMO => L+9, 8.26% H-1 => L+6, 2.66% H-4 => L+3, 2.53% H-15 => LUMO, 2.41% H-2 => L+5 32.9% H-8 => L+1, 28.9% H-6 => L+2, 14.0% H-14 => LUMO, 10.0% H-5 => L+3, 4.06% H-3 => L+6, 2.03% H-2 => L+9
36	13593	736	5.51	71.9% H-14 => LUMO, 7.20% H-6 => L+2, 4.92% H-8 => L+1, 4.81% HOMO => L+14, 3.01% H-13 => L+1
37	13886	720	0.00	39.3% H-2 => L+5, 27.6% H-3 => L+4, 11.0% HOMO => L+9, 9.29% H-7 => L+2, 2.19% H-5 => L+5 30.3% H-10 => L+1, 24.4% H-13 => LUMO, 11.3% H-8 => L+2, 6.15% H-6 => L+3, 5.59% HOMO => L+10, 5.25% H-14 => L+1, 4.06% H-5 => L+6, 3.12% H-19 => LUMO, 2.30% H-3 => L+9
38	13937	718	0.00	76.0% H-1 => L+5, 7.42% H-4 => L+4, 6.72% HOMO => L+7, 2.10% HOMO => L+4 41.3% H-7 => L+2, 16.7% HOMO => L+9, 10.8% H-9 => L+1, 10.7% H-2 => L+5, 7.59% H-4 => L+3, 5.93% H-3 => L+4, 2.51% H-1 => L+6
39	13961	716	0.00	64.1% H-16 => LUMO, 7.30% H-15 => L+1, 5.71% H-17 => LUMO, 5.22% H-11 => L+1, 3.11% H-12 => LUMO 40.5% H-15 => LUMO, 18.0% HOMO => L+9, 17.9% H-7 => L+2, 7.56% H-1 => L+6, 5.25% H-4 => L+3, 2.64% H-16 => L+1
40	14084	710	0.00	
41	14182	705	0.00	
42	14275	701	0.02	
43	14384	695	0.22	
44	14438	693	0.00	
45	14492	690	0.00	
46	14609	685	0.00	
47	14813	675	0.00	
48	14960	668	0.04	
49	15027	665	0.00	

				65.8% HOMO => L+10, 6.22% H-2 => L+6, 3.98% H-1 => L+8, 3.87% H-24 => LUMO, 2.85% H-1 => L+5
50	15043	665	0.00	30.2% H-15 => LUMO, 22.3% H-4 => L+3, 19.7% H-1 => L+6, 10.8% H-7 => L+2, 3.11% H-18 => LUMO
51	15088	663	0.00	68.3% H-2 => L+6, 14.4% H-3 => L+3, 6.39% HOMO => L+10, 2.40% H-2 => L+2
52	15139	661	0.00	39.1% H-5 => L+3, 36.1% H-6 => L+2, 12.2% H-3 => L+6, 4.98% H-2 => L+9
53	15231	657	0.00	44.9% H-4 => L+3, 43.2% H-1 => L+6
54	15291	654	0.00	55.9% H-11 => L+1, 13.1% H-16 => LUMO, 7.70% H-17 => LUMO, 4.58% H-9 => L+2, 4.37% H-12 => LUMO
55	15370	651	0.07	59.9% H-1 => L+7, 8.08% HOMO => L+8, 8.05% HOMO => L+11, 6.99% H-4 => L+5, 4.06% H-1 => L+10, 2.07% H-7 => L+4, 2.04% H-22 => LUMO
56	15475	646	0.00	56.1% H-17 => LUMO, 8.56% HOMO => L+12, 5.72% H-2 => L+7, 4.85% H-3 => L+5, 3.73% H-11 => L+1, 3.57% H-21 => LUMO, 2.26% H-12 => LUMO
57	15550	643	0.07	41.3% H-10 => L+1, 17.2% H-19 => LUMO, 6.47% HOMO => L+13, 5.75% H-8 => L+2, 4.39% H-6 => L+3, 4.15% H-13 => L+2, 3.17% H-14 => L+1, 2.93% H-5 => L+6, 2.62% H-3 => L+9
58	15567	642	0.00	76.1% H-18 => LUMO, 2.97% H-1 => L+6, 2.39% H-15 => LUMO, 2.37% H-3 => L+7, 2.08% H-2 => L+8
59	15589	641	0.00	47.8% HOMO => L+11, 14.4% H-1 => L+7, 10.4% H-22 => LUMO, 7.88% H-13 => L+1, 2.81% H-1 => L+10, 2.40% H-4 => L+8, 2.00% H-14 => L+2
60	15683	638	0.00	30.4% H-2 => L+7, 27.1% H-3 => L+5, 8.34% H-17 => LUMO, 7.39% H-5 => L+4, 5.93% H-21 => LUMO, 2.71% H-11 => L+1, 2.48% H-16 => LUMO, 2.21% HOMO => L+12
61	15718	636	0.63	54.3% H-3 => L+4, 37.2% H-2 => L+5, 3.44% H-5 => L+5, 2.45% H-3 => L+7
62	15775	634	0.00	24.7% H-19 => LUMO, 22.7% H-8 => L+2, 18.0% HOMO => L+13, 8.13% H-10 => L+1, 5.99% H-6 => L+3, 4.35% H-14 => L+1, 2.59% H-1 => L+11, 2.47% H-5 => L+6
63	15923	628	0.00	47.5% HOMO => L+12, 11.8% H-11 => L+1, 10.1% H-1 => L+9, 8.56% H-17 => LUMO, 5.02% H-4 => L+6, 2.93% H-7 => L+3, 2.80% H-16 => LUMO
64	15953	627	0.01	44.1% H-12 => L+1, 36.1% H-20 => LUMO, 3.13% H-2 => L+14, 2.72% H-11 => L+2, 2.31% H-15 => LUMO
65	16000	625	0.00	43.2% H-12 => L+1, 41.3% H-20 => LUMO, 4.69% H-17 => L+1, 2.91% H-18 => LUMO
66	16135	620	0.00	25.6% H-3 => L+6, 21.1% H-13 => L+1, 19.7% H-5 => L+3, 7.48% H-2 => L+9, 5.27% HOMO =>
67	16143	619	0.01	

				L+14, 5.09% H-22 => LUMO, 3.69% H-14 => LUMO, 2.63% H-10 => L+2 58.7% H-21 => LUMO, 10.8% H-9 => L+2, 4.93% HOMO => L+12, 4.24% H-2 => L+7, 4.20% H-18 => L+1, 2.65% H-3 => L+5, 2.64% H-25 => LUMO 24.0% H-3 => L+6, 23.5% H-13 => L+1, 10.9% H-5 => L+3, 10.7% HOMO => L+14, 8.25% H-22 => LUMO, 4.39% H-14 => LUMO, 3.96% H-2 => L+9, 2.91% HOMO => L+11, 2.66% H-10 => L+2 78.3% H-4 => L+4, 7.84% H-1 => L+5, 3.74% H-27 => LUMO, 2.20% H-7 => L+5 41.3% H-2 => L+7, 23.7% H-3 => L+5, 11.1% H-2 => L+4, 6.61% H-25 => LUMO, 6.03% H-5 => L+4, 2.63% H-3 => L+8, 2.46% H-7 => L+3 49.6% H-1 => L+8, 10.2% HOMO => L+10, 6.56% H-4 => L+7, 5.60% H-24 => LUMO, 4.50% H-8 => L+2, 3.78% H-19 => LUMO, 3.22% H-27 => LUMO, 3.00% H-7 => L+5 33.3% H-9 => L+2, 13.6% HOMO => L+12, 11.6% H-25 => LUMO, 10.9% H-21 => LUMO, 10.7% H-7 => L+3, 5.65% H-3 => L+5, 5.21% H-11 => L+1 81.6% H-23 => LUMO, 6.24% H-21 => L+1, 5.14% H-25 => L+1 39.4% H-19 => LUMO, 14.7% HOMO => L+13, 13.4% H-14 => L+1, 6.92% H-8 => L+2, 5.54% H-6 => L+3, 3.13% H-5 => L+6, 2.52% H-2 => L+12, 2.33% H-3 => L+9, 2.16% H-10 => L+3 35.2% H-8 => L+2, 16.8% H-6 => L+3, 10.1% HOMO => L+13, 7.68% H-1 => L+8, 7.27% H-5 => L+6, 5.26% H-14 => L+1, 4.64% H-3 => L+9, 3.05% H-2 => L+12, 2.38% H-19 => LUMO 56.0% H-25 => LUMO, 10.8% H-9 => L+2, 7.85% H-23 => L+1, 7.08% H-21 => LUMO, 6.09% H-2 => L+7, 5.11% H-5 => L+4 44.6% H-22 => LUMO, 29.5% HOMO => L+11, 12.1% H-13 => L+1, 2.71% H-4 => L+5 52.2% H-4 => L+5, 16.0% H-26 => LUMO, 11.7% H-1 => L+7, 8.04% H-7 => L+4 18.7% H-1 => L+9, 17.1% H-9 => L+2, 16.6% H-4 => L+6, 12.7% HOMO => L+12, 10.9% H-7 => L+3, 9.92% H-5 => L+4, 5.41% H-25 => LUMO 61.9% H-24 => LUMO, 14.8% H-27 => LUMO, 6.77% H-1 => L+8, 3.31% H-14 => L+1, 2.97% HOMO => L+10 58.4% H-5 => L+4, 13.8% H-3 => L+5, 6.26% H-9 => L+2, 4.96% H-4 => L+6, 3.29% H-2 => L+4, 2.89% H-1 => L+9, 2.80% H-6 => L+5 26.7% HOMO => L+14, 14.0% H-13 => L+1, 12.6% H-10 => L+2, 11.8% H-22 => LUMO, 10.2% H-26 => LUMO, 5.47% H-4 => L+5, 5.13% H-8 => L+3, 2.84% H-6 => L+6
68	16149	619	0.08	
69	16237	616	0.01	
70	16259	615	0.00	
71	16368	611	0.90	
72	16446	608	0.00	
73	16527	605	0.00	
74	16571	603	0.00	
75	16628	601	0.00	
76	16650	601	0.00	
77	16694	599	0.46	
78	16813	595	0.07	
79	16853	593	0.01	
80	16972	589	0.01	
81	17015	588	0.00	
82	17017	588	0.00	
83	17057	586	0.07	

84	17072	586	0.00	40.9% H-3 => L+7, 34.7% H-2 => L+8, 6.10% H-18 => LUMO, 5.22% H-5 => L+5 44.9% H-26 => LUMO, 11.3% H-29 => LUMO, 7.17% H-1 => L+10, 6.86% H-4 => L+5, 6.29% HOMO => L+14, 6.06% H-13 => L+1, 3.44% H-10 => L+2
85	17113	584	0.03	51.3% H-27 => LUMO, 23.9% H-28 => LUMO, 6.31% H-24 => LUMO, 3.77% H-4 => L+7, 2.65% H-4 => L+4
86	17184	582	0.00	62.7% H-2 => L+9, 19.3% H-3 => L+6, 5.06% H-29 => LUMO, 3.89% H-3 => L+12, 2.76% H-2 => L+3
87	17281	579	0.00	30.8% H-1 => L+9, 28.1% H-7 => L+3, 18.0% H-15 => L+1, 3.64% H-16 => LUMO, 2.78% H-9 => L+2, 2.57% H-16 => L+2, 2.53% H-25 => LUMO, 2.06% HOMO => L+12
88	17318	577	0.00	42.2% H-2 => L+8, 19.3% H-3 => L+7, 18.0% H-5 => L+5, 5.15% H-6 => L+4, 3.93% H-2 => L+5, 3.13% H-3 => L+10, 2.30% H-16 => L+1
89	17348	576	0.00	29.9% H-14 => L+1, 14.0% H-6 => L+3, 12.0% HOMO => L+13, 11.9% H-28 => LUMO, 8.38% H-5 => L+6, 7.87% H-2 => L+12, 6.31% H-3 => L+9
90	17378	575	0.00	46.3% H-15 => L+1, 17.3% H-7 => L+3, 9.33% H-1 => L+9, 7.42% H-16 => LUMO, 6.02% H-16 =>
91	17414	574	0.00	L+2 32.5% H-6 => L+3, 15.0% H-28 => LUMO, 10.5% H-5 => L+6, 9.08% HOMO => L+13, 7.95% H-14 => L+1, 6.49% H-3 => L+9, 4.89% H-27 => LUMO, 3.64% H-2 => L+12
92	17439	573	0.00	64.0% H-29 => LUMO, 9.53% H-1 => L+10, 5.32% H-28 => L+1, 3.44% H-2 => L+9, 3.13% H-4 =>
93	17439	573	0.00	L+8, 3.11% H-26 => LUMO 60.5% H-16 => L+1, 9.71% H-15 => LUMO, 7.85%
94	17466	573	0.00	H-15 => L+2, 3.90% H-2 => L+8 28.0% H-28 => LUMO, 15.2% HOMO => L+13, 14.4% H-27 => LUMO, 12.0% H-14 => L+1, 8.17% H-1 => L+8, 5.54% H-24 => LUMO, 2.87% H-4 =>
95	17481	572	0.00	L+7, 2.86% H-29 => L+1, 2.71% H-6 => L+3 60.4% H-4 => L+6, 17.3% H-1 => L+9, 14.1% H-7 => L+3
96	17569	569	0.00	43.6% H-1 => L+10, 13.6% H-26 => LUMO, 6.44% H-22 => LUMO, 6.09% H-29 => LUMO, 4.33% H-10 => L+2, 3.97% H-4 => L+5, 3.96% HOMO => L+11, 3.77% H-4 => L+8, 2.60% HOMO => L+14
97	17679	566	0.01	48.8% H-5 => L+5, 24.0% H-3 => L+7, 5.97% H-6 => L+4, 4.82% H-2 => L+8, 3.76% H-3 => L+4, 2.08% H-2 => L+5, 2.02% H-11 => L+2
98	17695	565	0.00	42.4% H-11 => L+2, 8.30% H-20 => LUMO, 7.51% H-9 => L+3, 5.68% H-2 => L+14, 4.01% H-16 => L+1, 3.96% H-7 => L+6, 3.81% H-17 => L+1, 3.16% H-1 => L+12, 3.00% H-4 => L+9, 2.87% H-3 => L+13, 2.77% H-5 => L+5
99	17734	564	0.00	

				60.2% H-10 => L+2, 22.2% HOMO => L+14, 5.86%
100	17868	560	0.50	H-1 => L+10 56.5% H-4 => L+7, 9.19% H-1 => L+8, 8.86% H-28 => LUMO, 8.35% H-7 => L+5, 3.60% H-24 =>
101	17879	559	0.00	LUMO, 3.00% H-9 => L+4 33.0% H-2 => L+10, 23.3% H-3 => L+8, 16.0% H-12 => L+2, 4.73% H-17 => LUMO, 4.56% H-15 =>
102	18111	552	0.01	L+1, 2.64% H-20 => L+1, 2.43% H-2 => L+13 39.3% H-5 => L+6, 13.4% H-3 => L+9, 11.8% H-1 => L+11, 11.4% H-2 => L+12, 4.31% HOMO =>
103	18203	549	0.00	L+13, 3.05% H-6 => L+9, 2.51% H-13 => L+2 53.4% H-12 => L+2, 12.4% H-2 => L+10, 6.77% H-18 => L+1, 6.25% H-3 => L+8, 3.04% H-11 => L+3
104	18280	547	0.02	33.5% H-11 => L+2, 21.4% H-1 => L+12, 9.90% H-4 => L+9, 6.69% H-7 => L+6, 5.54% H-2 => L+14, 3.65% H-9 => L+3, 3.47% H-6 => L+4
105	18304	546	0.00	27.0% H-5 => L+7, 21.4% H-2 => L+10, 17.5% H-3 => L+8, 11.4% H-18 => L+1, 6.26% H-6 => L+5
106	18354	545	0.26	78.9% H-7 => L+4, 9.14% H-4 => L+5, 3.51% H-9 => L+5, 2.07% H-26 => LUMO
107	18401	543	0.00	30.8% H-1 => L+11, 14.0% H-13 => L+2, 12.6% H-3 => L+9, 9.70% H-5 => L+6, 5.77% H-14 => L+1, 5.45% H-2 => L+12, 3.85% H-4 => L+10, 2.81% H-1 => L+14
108	18403	543	0.00	72.5% H-6 => L+4, 10.1% H-5 => L+5, 3.14% H-8 => L+5, 2.25% H-3 => L+4, 2.09% H-1 => L+12
109	18491	541	0.00	53.9% H-8 => L+3, 12.4% HOMO => L+14, 8.32% H-1 => L+13, 6.11% H-6 => L+6, 4.25% H-10 => L+2, 2.88% H-4 => L+11
110	18518	540	0.26	70.3% H-17 => L+1, 6.33% H-30 => LUMO, 3.12% H-20 => LUMO, 2.24% H-11 => L+2
111	18606	537	0.00	34.3% H-3 => L+8, 28.1% H-18 => L+1, 9.95% H-2 => L+10, 6.93% H-5 => L+7, 2.72% H-2 => L+7, 2.60% H-20 => L+1, 2.35% H-21 => LUMO, 2.06% H-5 => L+10
112	18629	537	0.06	81.7% H-30 => LUMO, 5.68% H-17 => L+1, 5.22% H-31 => L+1
113	18669	536	0.00	38.6% H-5 => L+7, 29.3% H-18 => L+1, 4.12% H-2 => L+10, 3.06% H-21 => LUMO, 2.72% H-3 =>
114	18712	534	0.52	L+8, 2.24% H-3 => L+5 36.1% H-19 => L+1, 22.5% H-4 => L+8, 11.6% H-1 => L+10, 5.23% H-7 => L+7, 5.22% H-14 => L+2, 2.94% H-22 => LUMO, 2.47% H-9 => L+5
115	18740	534	0.01	33.4% H-19 => L+1, 24.4% H-4 => L+8, 8.97% H-8 => L+3, 7.72% H-1 => L+13, 5.20% H-1 => L+10, 4.08% H-7 => L+7, 2.06% H-4 => L+11
116	18839	531	0.09	18.9% H-2 => L+11, 17.4% H-1 => L+12, 16.9% H-9 => L+3, 14.2% H-21 => L+1, 5.99% H-3 => L+10, 4.17% H-16 => L+1, 2.82% H-23 => LUMO, 2.20% H-11 => L+2
117	18861	530	0.00	

118	18882	530	0.00	44.5% H-13 => L+2, 19.6% H-1 => L+14, 14.9% H-1 => L+11, 2.26% H-10 => L+3 80.0% H-31 => LUMO, 8.51% H-30 => L+1, 3.62% H-32 => L+1
119	18884	530	0.00	48.0% H-7 => L+5, 13.7% H-4 => L+7, 10.4% H-9 => L+4, 7.45% H-2 => L+12, 5.86% H-3 => L+9, 2.03% H-4 => L+4
120	18952	528	0.00	27.9% H-2 => L+11, 18.7% H-9 => L+3, 13.6% H-3 => L+10, 11.3% H-1 => L+12, 3.82% H-21 => L+1, 3.11% H-4 => L+9
121	19043	525	0.00	32.4% H-2 => L+12, 28.0% H-3 => L+9, 11.4% H-7 => L+5, 6.25% H-22 => L+1, 6.13% H-13 => L+2, 3.65% H-5 => L+12, 2.67% H-2 => L+6
122	19112	523	0.00	33.0% H-6 => L+5, 18.1% H-20 => L+1, 6.92% H-12 => L+2, 6.28% H-5 => L+7, 5.98% H-2 => L+13, 3.83% H-8 => L+4, 3.19% H-3 => L+14, 2.84% H-15 => L+1, 2.31% H-5 => L+4, 2.09% H-2 => L+10
123	19119	523	0.04	37.0% H-20 => L+1, 27.0% H-6 => L+5, 7.87% H-18 => L+1, 6.82% H-12 => L+2, 4.76% H-5 => L+7, 3.49% H-8 => L+4
124	19143	522	0.00	57.2% H-21 => L+1, 13.3% H-9 => L+3, 6.43% H-1 => L+12, 2.67% H-23 => LUMO, 2.27% H-18 => L+2, 2.12% H-7 => L+6, 2.04% H-11 => L+2
125	19185	521	0.00	33.5% H-6 => L+6, 18.7% H-8 => L+3, 9.74% H-1 => L+13, 8.99% H-19 => L+1, 8.63% H-5 => L+9, 5.38% H-4 => L+8, 2.74% H-14 => L+2
126	19190	521	0.00	76.6% H-32 => LUMO, 8.97% H-31 => L+1, 3.24% H-34 => LUMO, 2.86% H-33 => L+1, 2.42% H-30 => L+2
127	19214	520	0.00	45.5% H-22 => L+1, 19.0% H-1 => L+14, 6.28% H-26 => L+1, 5.29% H-2 => L+12, 4.05% H-4 => L+13, 2.34% H-19 => L+2, 2.13% H-3 => L+9, 2.07% H-7 => L+5, 2.05% H-4 => L+10
128	19365	516	0.00	23.5% H-9 => L+3, 22.6% H-7 => L+6, 15.5% H-1 => L+12, 7.70% H-4 => L+9, 7.57% H-2 => L+11, 4.66% H-5 => L+8, 2.88% H-6 => L+7, 2.33% H-25 => L+1
129	19392	516	0.00	35.7% H-3 => L+10, 13.5% H-5 => L+8, 12.9% H-2 => L+11, 8.61% H-7 => L+6, 3.50% H-4 => L+9, 3.50% H-1 => L+12, 2.47% H-2 => L+8, 2.38% H-17 => L+1
130	19448	514	0.00	63.5% H-23 => L+1, 8.13% H-25 => LUMO, 4.07% H-21 => L+2, 3.56% H-25 => L+2, 2.89% H-20 => L+1, 2.86% H-21 => LUMO, 2.31% H-2 => L+13
131	19462	514	0.18	25.0% H-22 => L+1, 20.1% H-1 => L+14, 18.2% H-1 => L+11, 8.34% H-13 => L+2, 6.12% H-4 => L+10, 3.61% H-4 => L+13, 2.64% H-7 => L+8
132	19473	514	0.00	39.7% H-14 => L+2, 19.9% H-6 => L+6, 11.9% H-1 => L+13, 8.94% H-19 => L+1, 2.59% H-13 => L+1, 2.43% H-4 => L+14, 2.23% H-13 => L+3
133	19532	512	0.35	

				74.3% H-33 => LUMO, 9.83% H-32 => L+1, 5.26% H-35 => LUMO, 2.69% H-31 => L+2, 2.12% H-34 => L+1
134	19571	511	0.00	37.8% H-25 => L+1, 33.2% H-4 => L+9, 7.70% H-7 => L+6, 5.98% H-1 => L+12, 3.85% H-23 => LUMO, 2.75% H-23 => L+2
135	19620	510	0.00	18.1% H-2 => L+13, 14.4% H-20 => L+1, 9.81% H-23 => L+1, 8.94% H-3 => L+11, 8.21% H-6 => L+5, 4.22% H-16 => L+2, 3.90% H-15 => L+1, 3.45% H-12 => L+2, 3.15% H-4 => L+12, 3.05% HOMO => L+16, 2.03% H-7 => L+9, 2.03% H-5 => L+10, 2.00% H-11 => L+3
136	19630	509	0.13	63.4% H-24 => L+1, 17.9% H-27 => L+1, 3.14% H-22 => L+2, 2.89% H-14 => L+2, 2.18% H-22 => LUMO
137	19642	509	0.01	40.3% H-5 => L+8, 19.8% H-3 => L+10, 8.58% H-7 => L+6, 7.48% H-6 => L+7, 5.05% H-2 => L+11, 2.29% H-2 => L+8
138	19703	508	0.00	29.4% H-10 => L+3, 21.4% H-4 => L+10, 9.33% H-13 => L+2, 6.09% H-8 => L+6, 5.84% H-1 => L+11, 5.27% H-2 => L+12, 4.64% H-7 => L+8, 2.39% H-9 => L+7
139	19719	507	0.00	20.8% H-4 => L+8, 15.9% H-7 => L+7, 15.0% H-6 => L+6, 9.91% H-14 => L+2, 9.65% H-1 => L+13, 6.74% H-5 => L+9, 5.58% H-9 => L+5, 3.08% H-11 => L+4
140	19753	506	0.12	41.2% H-25 => L+1, 21.1% H-4 => L+9, 20.4% H-7 => L+6, 2.53% H-23 => L+2, 2.45% H-23 => LUMO
141	19794	505	0.00	68.3% H-26 => L+1, 12.2% H-29 => L+1, 2.98% H-24 => L+2, 2.73% H-7 => L+5, 2.66% H-22 => L+1, 2.31% H-24 => LUMO
142	19840	504	0.00	64.4% H-27 => L+1, 11.7% H-28 => L+1, 9.34% H-24 => L+1, 3.10% H-26 => L+2, 2.71% H-6 => L+6
143	19861	504	0.02	60.9% H-34 => LUMO, 9.08% H-36 => LUMO, 8.41% H-33 => L+1, 8.12% H-15 => L+2, 2.39% H-32 => L+2
144	19924	502	0.00	25.5% H-16 => L+2, 24.0% H-2 => L+13, 10.2% H-8 => L+4, 5.44% H-15 => L+1, 3.47% H-5 => L+10, 3.27% H-15 => L+3, 2.95% H-11 => L+3, 2.92% H-8 => L+7, 2.63% H-6 => L+8, 2.63% H-6 => L+5, 2.49% H-2 => L+10
145	19924	502	0.00	28.6% H-1 => L+13, 20.2% H-14 => L+2, 10.3% H-5 => L+9, 9.82% H-3 => L+12, 7.13% H-7 => L+7, 3.09% H-11 => L+4, 2.81% H-9 => L+5, 2.29% H-24 => L+1
146	19935	502	0.45	54.9% H-15 => L+2, 9.09% H-16 => L+1, 8.72% H-34 => LUMO, 6.01% H-16 => L+3, 4.19% H-5 => L+8
147	19957	501	0.00	37.6% H-5 => L+9, 22.7% H-7 => L+7, 7.17% H-6 => L+6, 5.17% H-4 => L+8, 4.09% H-3 => L+12,
148	19990	500	0.06	

				3.23% H-14 => L+2, 2.92% H-24 => L+1, 2.78% H-9 => L+5
149	20014	500	0.00	48.7% H-8 => L+4, 18.2% H-16 => L+2, 4.43% H-6 => L+5, 4.12% H-10 => L+5, 3.58% H-11 => L+3, 2.69% H-15 => L+3, 2.64% H-3 => L+11, 2.14% H-15 => L+1
150	20033	499	0.00	34.1% H-6 => L+7, 16.1% H-5 => L+8, 14.6% H-2 => L+14, 7.25% H-8 => L+5, 3.49% H-15 => L+2, 3.37% H-6 => L+10, 2.91% H-2 => L+11
151	20162	496	0.01	37.2% H-11 => L+3, 9.00% H-3 => L+11, 6.94% H-2 => L+13, 6.75% H-16 => L+2, 6.63% H-8 => L+4, 4.60% H-9 => L+6, 2.50% H-17 => L+2, 2.22% H-20 => L+1, 2.08% H-7 => L+9
152	20164	496	0.00	46.9% H-9 => L+4, 16.4% H-29 => L+1, 8.07% H-7 => L+5, 6.36% H-26 => L+1, 4.49% H-11 => L+5, 2.66% H-10 => L+3, 2.45% H-28 => LUMO
153	20211	495	0.00	36.5% H-2 => L+14, 17.1% H-6 => L+7, 8.75% H-12 => L+3, 4.16% H-8 => L+8, 3.48% H-1 => L+12, 2.50% H-18 => L+2, 2.09% H-14 => L+4
154	20217	495	0.07	64.9% H-28 => L+1, 7.12% H-29 => LUMO, 6.30% H-27 => L+1, 6.20% H-29 => L+2, 4.44% H-24 => L+1, 2.23% H-1 => L+13
155	20242	494	0.00	50.3% H-29 => L+1, 19.4% H-9 => L+4, 5.14% H-7 => L+5, 4.75% H-28 => LUMO, 4.51% H-28 => L+2, 4.18% H-26 => L+1, 2.39% H-4 => L+10
156	20247	494	0.00	54.3% H-35 => LUMO, 30.1% H-37 => LUMO, 7.43% H-34 => L+1, 2.12% H-33 => L+2
157	20331	492	0.01	44.5% H-10 => L+3, 24.9% H-4 => L+10, 12.2% H-1 => L+14, 3.65% H-9 => L+4
158	20350	491	0.01	32.2% H-3 => L+11, 12.3% H-16 => L+2, 11.4% H-8 => L+4, 10.0% H-5 => L+10, 8.05% H-2 => L+13, 5.95% H-3 => L+14, 3.79% HOMO => L+16, 2.47% H-20 => L+1
159	20504	488	0.02	58.7% H-3 => L+12, 19.9% H-5 => L+9, 6.05% H-7 => L+7, 4.98% H-2 => L+9, 2.74% H-6 => L+12
160	20532	487	0.00	24.6% H-8 => L+5, 18.4% H-12 => L+3, 18.1% H-6 => L+7, 6.97% H-10 => L+4, 5.20% H-18 => L+2, 4.65% HOMO => L+15, 2.44% H-3 => L+13
161	20552	487	0.06	20.4% H-3 => L+11, 19.6% H-5 => L+10, 13.0% H-6 => L+8, 8.21% H-17 => L+2, 6.57% H-5 => L+13, 6.23% HOMO => L+16, 5.19% H-8 => L+7, 2.88% H-2 => L+10, 2.75% H-2 => L+13
162	20657	484	0.00	65.7% H-36 => LUMO, 9.26% H-35 => L+1, 8.04% H-37 => L+1, 7.16% H-34 => LUMO, 2.78% H-36 => L+2, 2.19% H-34 => L+2
163	20665	484	0.00	24.4% H-4 => L+10, 14.9% H-12 => L+4, 14.5% H-7 => L+8, 9.30% H-11 => L+5, 8.71% H-9 => L+7, 8.47% H-8 => L+6, 3.15% H-6 => L+9, 2.76% H-10 => L+3, 2.64% H-7 => L+11, 2.16% H-2 => L+12

				49.6% H-37 => LUMO, 19.9% H-35 => LUMO, 14.5% H-36 => L+1, 3.49% H-35 => L+2, 2.38% H- 33 => LUMO, 2.17% H-34 => L+1 24.8% H-11 => L+3, 12.0% H-4 => L+12, 11.6% HOMO => L+16, 7.74% H-3 => L+14, 6.36% H-2 => L+13, 5.58% H-7 => L+9, 5.42% H-5 => L+13, 3.56% H-16 => L+2, 3.15% H-9 => L+6, 3.02% H-5 => L+10
164	20668	484	0.00	
165	20678	484	0.01	21.9% H-3 => L+13, 19.4% H-8 => L+5, 15.8% HOMO => L+15, 5.21% H-5 => L+14, 5.16% H-2 => L+11, 3.93% H-5 => L+11, 2.11% H-10 => L+7, 2.03% H-6 => L+13 35.8% H-9 => L+5, 23.2% H-7 => L+7, 19.6% H-11 => L+4, 5.67% H-3 => L+12, 3.17% H-12 => L+5, 2.14% H-7 => L+4
166	20748	482	0.00	31.6% HOMO => L+15, 28.5% H-12 => L+3, 7.69% H-8 => L+5, 5.48% H-2 => L+14, 3.48% H-1 => L+16, 3.34% H-15 => L+2, 3.21% H-18 => L+2, 2.30% H-10 => L+7
167	20760	482	0.00	52.9% H-8 => L+6, 10.3% H-1 => L+14, 8.48% H- 12 => L+4, 5.57% H-4 => L+13, 2.24% H-10 => L+3, 2.24% H-6 => L+9 46.8% H-4 => L+11, 19.1% H-13 => L+3, 4.69% H- 7 => L+13, 3.54% H-14 => L+2, 2.82% H-10 => L+6, 2.19% H-1 => L+13
168	20825	480	0.00	40.9% H-5 => L+10, 11.3% H-6 => L+8, 8.11% H-8 => L+7, 6.55% H-17 => L+2, 5.38% H-6 => L+11, 4.17% H-3 => L+14, 3.94% H-10 => L+5, 3.79% H- 3 => L+11, 2.90% H-3 => L+8, 2.09% H-9 => L+6, 2.02% H-13 => L+4
169	20903	478	0.01	36.3% HOMO => L+16, 15.0% H-17 => L+2, 10.3% H-9 => L+6, 6.45% H-4 => L+12, 4.26% H-21 => L+2, 3.58% H-5 => L+10, 3.09% H-1 => L+15, 2.25% H-2 => L+13, 2.19% H-7 => L+9
170	20922	478	0.51	61.2% H-18 => L+2, 17.5% H-12 => L+3, 3.04% H- 21 => L+1, 2.80% H-3 => L+13 30.8% H-3 => L+13, 15.4% H-8 => L+5, 12.8% HOMO => L+15, 6.51% H-2 => L+14, 5.68% H-10 => L+4, 4.75% H-18 => L+2, 3.37% H-13 => L+5, 3.17% H-12 => L+3, 2.12% H-2 => L+11 39.5% H-17 => L+2, 16.6% H-6 => L+8, 13.3% H-9 => L+6, 6.42% H-11 => L+3, 4.73% HOMO => L+16, 2.92% H-3 => L+14
171	20948	477	0.19	28.4% H-19 => L+2, 21.6% H-7 => L+8, 10.2% H-4 => L+13, 6.56% H-8 => L+6, 5.21% H-14 => L+3, 3.58% H-6 => L+9, 3.17% H-22 => L+1, 2.64% H-9 => L+10, 2.55% H-12 => L+4
172	21066	475	0.09	48.2% H-13 => L+3, 24.0% H-4 => L+11, 3.91% H- 4 => L+14, 3.31% H-22 => L+2, 2.70% H-14 => L+2, 2.68% H-10 => L+6, 2.30% H-3 => L+12
173	21074	475	0.00	
174	21161	473	0.00	
175	21217	471	0.26	
176	21244	471	0.00	
177	21249	471	0.42	

178	21316	469	0.00	28.0% H-12 => L+4, 20.6% H-7 => L+8, 13.4% H-4 => L+13, 8.93% H-19 => L+2, 5.29% H-11 => L+5, 3.34% H-14 => L+3 34.9% H-4 => L+12, 8.97% H-9 => L+6, 7.35% H-7 => L+9, 7.00% H-17 => L+2, 6.78% H-21 => L+2, 5.12% H-8 => L+7, 4.39% HOMO => L+16, 4.08% H-3 => L+14, 2.61% H-10 => L+5, 2.08% H-6 => L+8
179	21322	469	0.09	36.9% H-6 => L+8, 15.9% H-9 => L+6, 11.7% H-3 => L+14, 4.97% H-4 => L+12, 4.67% H-8 => L+7, 4.50% H-10 => L+5, 3.53% H-13 => L+4, 2.14% H-21 => L+2, 2.01% H-7 => L+9 38.7% H-6 => L+9, 17.1% H-19 => L+2, 11.3% H-8 => L+6, 7.94% H-5 => L+12, 6.71% H-4 => L+13, 3.75% H-7 => L+8, 3.39% H-1 => L+14
180	21445	466	0.05	40.8% H-10 => L+4, 27.2% H-20 => L+2, 4.39% H-12 => L+3, 3.57% H-18 => L+2, 3.41% H-8 => L+5, 2.99% H-17 => L+3, 2.29% H-11 => L+6, 2.25% H-13 => L+5 39.4% H-11 => L+4, 31.1% H-9 => L+5, 9.69% H-12 => L+5, 3.95% H-7 => L+4, 3.08% H-12 => L+8, 2.92% H-11 => L+7
181	21449	466	0.00	26.6% H-20 => L+2, 19.7% H-10 => L+4, 14.5% H-3 => L+13, 5.83% H-2 => L+14, 4.46% H-6 => L+13, 4.43% H-5 => L+11, 3.37% H-8 => L+5, 2.93% H-12 => L+3, 2.83% H-17 => L+3, 2.39% H-5 => L+14 34.4% H-21 => L+2, 22.5% H-7 => L+9, 14.5% H-4 => L+12, 5.61% H-17 => L+2, 4.57% H-25 => L+2, 2.31% H-18 => L+3
182	21478	466	0.00	28.3% H-19 => L+2, 18.2% H-4 => L+13, 12.0% H-7 => L+8, 11.6% H-6 => L+9, 6.75% H-5 => L+12 61.3% H-5 => L+11, 5.61% H-10 => L+4, 4.95% HOMO => L+15, 3.61% H-14 => L+4, 3.44% H-10 => L+7, 3.00% H-5 => L+14, 2.23% H-3 => L+10, 2.22% H-13 => L+5, 2.18% H-2 => L+14 25.5% H-8 => L+7, 18.7% H-3 => L+14, 14.8% H-21 => L+2, 6.31% H-7 => L+9, 5.85% H-4 => L+12, 5.54% H-9 => L+6, 2.12% H-8 => L+10
183	21491	465	0.00	27.9% H-7 => L+9, 15.5% H-9 => L+6, 13.1% H-3 => L+14, 12.3% H-21 => L+2, 9.05% H-8 => L+7 31.7% H-4 => L+14, 15.9% H-22 => L+2, 13.9% H-13 => L+3, 6.90% H-41 => LUMO, 4.63% H-10 => L+6, 2.57% H-1 => L+13, 2.47% H-8 => L+9, 2.17% H-26 => L+2, 2.10% H-7 => L+13 41.8% H-22 => L+2, 12.2% H-7 => L+10, 8.36% H-4 => L+11, 4.46% H-41 => LUMO, 3.63% H-9 => L+8, 3.59% H-39 => LUMO, 3.14% H-38 => LUMO, 2.15% H-4 => L+14
184	21611	463	0.00	81.1% H-30 => L+1, 6.98% H-31 => LUMO, 4.40% H-31 => L+2, 2.78% H-32 => L+1
185	21616	463	0.08	
186	21622	462	0.01	
187	21698	461	0.00	
188	21737	460	0.03	
189	21771	459	0.02	
190	21783	459	0.03	
191	21829	458	0.04	
192	21831	458	0.00	

				52.5% H-5 => L+12, 16.9% H-6 => L+9, 5.69% H-14 => L+3, 3.59% H-42 => LUMO, 2.50% H-3 => L+9, 2.32% H-40 => LUMO, 2.10% H-8 => L+12
193	21890	457	0.00	46.3% H-40 => LUMO, 12.9% H-9 => L+7, 8.77% H-38 => LUMO, 7.67% H-39 => LUMO, 3.67% H-14 => L+3, 2.40% H-24 => L+2
194	21926	456	0.00	27.5% H-38 => LUMO, 24.1% H-39 => LUMO, 13.0% H-40 => LUMO, 8.06% H-5 => L+12, 4.11% H-14 => L+3, 3.72% H-4 => L+13, 3.33% H-6 => L+9, 2.89% H-39 => L+1, 2.53% H-38 => L+1
195	21960	455	0.00	37.4% H-39 => LUMO, 32.7% H-38 => LUMO, 6.24% H-41 => LUMO, 4.37% H-4 => L+14, 3.86% H-38 => L+1, 3.37% H-39 => L+1, 2.56% H-22 => L+2, 2.17% H-43 => LUMO
196	21967	455	0.00	30.5% H-14 => L+3, 23.6% H-42 => LUMO, 20.3% H-40 => LUMO, 3.67% H-9 => L+7, 3.35% H-4 => L+13, 2.45% H-44 => LUMO, 2.35% H-24 => L+2
197	21996	455	0.00	25.5% H-10 => L+5, 24.9% H-8 => L+7, 9.36% H-5 => L+13, 8.65% H-13 => L+4, 6.66% H-3 => L+14, 2.99% H-10 => L+8, 2.53% H-6 => L+11, 2.45% H-8 => L+4
198	22013	454	0.01	23.5% H-9 => L+7, 22.6% H-14 => L+3, 6.27% H-44 => LUMO, 6.22% H-38 => LUMO, 5.44% H-39 => LUMO, 4.47% H-5 => L+12, 4.17% H-42 => LUMO, 4.16% H-12 => L+4, 2.41% H-24 => L+2, 2.27% H-19 => L+2
199	22014	454	0.00	66.1% H-23 => L+2, 6.20% H-25 => L+1, 3.54% H-25 => L+3, 3.34% H-20 => L+2, 3.23% H-21 => L+1, 3.04% H-21 => L+3
200	22036	454	0.00	38.9% H-41 => LUMO, 32.3% H-43 => LUMO, 5.37% H-10 => L+6, 3.38% H-45 => LUMO, 2.91% H-22 => L+2, 2.90% H-4 => L+14
201	22057	453	0.00	67.5% H-31 => L+1, 7.60% H-32 => LUMO, 7.28% H-30 => L+2, 5.70% H-30 => LUMO, 3.48% H-33 => L+1, 2.48% H-32 => L+2
202	22079	453	0.00	28.6% H-43 => LUMO, 26.5% H-41 => LUMO, 20.6% H-45 => LUMO, 8.18% H-7 => L+10, 2.66% H-42 => L+1
203	22083	453	0.12	45.1% H-42 => LUMO, 11.3% H-40 => LUMO, 9.16% H-9 => L+7, 4.85% H-44 => LUMO, 4.39% H-12 => L+4, 3.97% H-24 => L+2, 2.83% H-4 => L+13, 2.30% H-41 => L+1, 2.11% H-6 => L+9
204	22126	452	0.00	66.1% H-24 => L+2, 7.08% H-9 => L+7, 3.39% H-28 => L+2, 2.72% H-22 => L+3, 2.21% H-22 => L+1
205	22193	451	0.00	20.4% H-6 => L+10, 12.6% H-20 => L+2, 12.0% H-11 => L+6, 7.55% H-23 => L+2, 5.15% H-16 => L+3, 4.52% HOMO => L+15, 4.24% H-9 => L+9, 3.37% H-5 => L+11, 3.17% H-8 => L+11, 2.56% H-15 => L+2, 2.53% H-14 => L+4, 2.45% H-7 => L+12, 2.22% H-5 => L+14
206	22204	450	0.00	

				29.9% H-7 => L+10, 14.4% H-43 => LUMO, 10.5% H-26 => L+2, 8.18% H-10 => L+6, 5.44% H-22 => L+2, 4.43% H-45 => LUMO, 2.36% H-4 => L+14, 2.21% H-9 => L+8
207	22211	450	0.43	67.8% H-25 => L+2, 6.31% H-15 => L+3, 5.20% H-23 => L+3, 4.68% H-23 => L+1, 4.31% H-7 => L+9
208	22217	450	0.00	54.0% H-45 => LUMO, 10.1% H-43 => LUMO, 6.27% H-7 => L+10, 6.03% H-44 => L+1, 5.78% H-26 => L+2, 2.95% H-22 => L+2, 2.01% H-41 => LUMO
209	22267	449	0.33	67.5% H-44 => LUMO, 8.34% H-42 => LUMO, 6.08% H-45 => L+1, 2.82% H-9 => L+7
210	22268	449	0.00	48.1% H-6 => L+10, 10.1% H-20 => L+2, 6.67% H-5 => L+14, 4.88% H-11 => L+6, 4.12% H-6 => L+13, 2.96% H-14 => L+4, 2.96% H-9 => L+9, 2.73% H-13 => L+5, 2.51% H-7 => L+12, 2.03% H-5 => L+8
211	22285	449	0.00	23.6% H-10 => L+6, 23.4% H-26 => L+2, 14.2% H-4 => L+14, 7.03% H-7 => L+10, 5.21% H-29 => L+2, 3.74% H-41 => LUMO, 2.67% H-22 => L+2
212	22310	448	0.12	38.7% H-15 => L+3, 12.7% H-10 => L+5, 9.13% H-16 => L+2, 8.42% H-25 => L+2, 4.45% H-16 => L+6, 3.89% H-5 => L+13, 3.80% HOMO => L+16, 3.69% H-32 => L+1
213	22347	447	0.00	33.1% H-26 => L+2, 16.1% H-10 => L+6, 9.55% H-4 => L+14, 6.46% H-29 => L+2, 4.56% H-15 => L+4, 4.02% H-12 => L+5, 4.01% H-16 => L+5, 2.01% H-11 => L+7
214	22381	447	0.04	72.9% H-27 => L+2, 7.08% H-28 => L+2, 3.04% H-44 => LUMO, 2.76% H-11 => L+5
215	22396	447	0.00	61.3% H-32 => L+1, 7.39% H-33 => LUMO, 7.05% H-31 => L+2, 6.81% H-31 => LUMO, 4.17% H-34 => L+1, 3.12% H-15 => L+3
216	22402	446	0.00	53.3% H-16 => L+3, 11.2% H-11 => L+6, 7.55% H-15 => L+2, 7.45% H-15 => L+6, 4.12% H-18 => L+2, 2.83% H-23 => L+2
217	22442	446	0.00	37.4% H-5 => L+13, 14.4% H-15 => L+3, 14.2% H-10 => L+5, 3.39% H-14 => L+5, 3.22% H-6 => L+14, 3.13% H-12 => L+6, 2.90% H-10 => L+8
218	22464	445	0.00	39.9% H-11 => L+5, 10.0% H-12 => L+7, 7.63% H-9 => L+4, 6.47% H-9 => L+7, 6.39% H-27 => L+2, 5.72% H-12 => L+4, 4.72% H-42 => LUMO, 4.58% H-14 => L+3, 3.48% H-17 => L+4
219	22508	444	0.00	56.9% H-28 => L+2, 7.30% H-29 => L+1, 6.24% H-29 => L+3, 5.33% H-27 => L+2, 4.79% H-7 => L+11, 2.71% H-4 => L+13
220	22640	442	0.00	61.9% H-29 => L+2, 9.52% H-26 => L+2, 7.36% H-28 => L+1, 6.80% H-28 => L+3, 2.51% H-7 => L+10
221	22659	441	0.03	36.4% H-13 => L+4, 11.9% H-5 => L+13, 11.5% H-10 => L+5, 5.60% H-12 => L+6, 5.13% H-6 =>
222	22721	440	0.04	

				L+11, 3.78% H-13 => L+7, 3.17% H-8 => L+10, 2.39% H-50 => LUMO, 2.30% H-48 => LUMO 32.3% H-33 => L+1, 17.8% H-8 => L+8, 12.2% H-5 => L+14, 4.14% H-32 => LUMO, 3.92% H-32 => L+2, 3.61% H-34 => LUMO, 2.87% H-11 => L+6, 2.85% H-35 => L+1, 2.64% H-6 => L+10, 2.39% H- 14 => L+4
223	22738	440	0.00	30.3% H-33 => L+1, 25.0% H-8 => L+8, 9.06% H-5 => L+14, 3.79% H-32 => L+2, 3.54% H-32 => LUMO, 3.30% H-34 => LUMO, 2.86% H-6 => L+10, 2.86% H-14 => L+4, 2.81% H-35 => L+1, 2.35% H-11 => L+6
224	22746	440	0.00	20.9% H-12 => L+5, 14.0% H-11 => L+7, 13.4% H- 10 => L+6, 6.24% H-7 => L+10, 5.54% H-11 => L+4, 5.21% H-9 => L+8, 4.85% H-15 => L+4, 4.34% H-16 => L+5, 3.01% H-29 => L+2, 2.96% H- 45 => LUMO, 2.39% H-4 => L+14, 2.15% H-6 => L+12
225	22770	439	0.15	20.1% H-9 => L+8, 15.5% H-8 => L+9, 8.44% H-15 => L+4, 7.76% H-10 => L+6, 7.14% H-11 => L+7, 7.13% H-16 => L+5, 6.88% H-7 => L+10, 6.75% H- 6 => L+12
226	22840	438	0.42	41.6% H-7 => L+11, 10.0% H-28 => L+2, 9.90% H- 4 => L+13, 7.30% H-9 => L+10, 4.66% H-24 => L+2, 3.59% H-11 => L+8, 2.04% H-15 => L+5
227	22840	438	0.00	29.4% H-8 => L+8, 24.7% H-5 => L+14, 18.9% H- 11 => L+6, 3.09% H-16 => L+3, 2.89% H-13 => L+5, 2.12% H-10 => L+4
228	22844	438	0.00	30.8% H-50 => LUMO, 21.7% H-12 => L+6, 12.4% H-48 => LUMO, 3.78% H-5 => L+13, 2.92% H-11 => L+9, 2.49% H-52 => LUMO, 2.37% H-10 => L+5, 2.35% H-20 => L+3, 2.05% H-3 => L+14
229	22871	437	0.00	27.1% H-48 => LUMO, 17.7% H-13 => L+4, 17.2% H-12 => L+6, 11.3% H-50 => LUMO, 2.32% H-18 => L+3, 2.25% H-54 => LUMO, 2.03% HOMO => L+16
230	22909	437	0.00	26.5% H-15 => L+5, 25.9% H-16 => L+4, 7.91% H- 16 => L+7, 7.81% H-11 => L+5, 3.60% H-13 => L+6, 3.54% H-14 => L+3, 2.68% H-3 => L+15,
231	22984	435	0.01	2.40% H-2 => L+16 52.2% H-46 => LUMO, 34.9% H-47 => LUMO,
232	23029	434	0.01	4.91% H-47 => L+1, 3.37% H-46 => L+1 52.2% H-47 => LUMO, 34.9% H-46 => LUMO,
233	23030	434	0.00	4.88% H-46 => L+1, 3.34% H-47 => L+1 49.6% H-49 => LUMO, 20.5% H-51 => LUMO, 8.44% H-53 => LUMO, 3.34% H-48 => L+1, 2.05% H-10 => L+7, 2.03% H-13 => L+5, 2.02% H-16 =>
234	23049	434	0.00	L+3 60.1% H-34 => L+1, 7.79% H-33 => L+2, 7.55% H- 36 => L+1, 7.50% H-33 => LUMO, 4.60% H-35 =>
235	23073	433	0.00	LUMO, 2.27% H-37 => L+2

				33.4% H-6 => L+11, 9.30% H-12 => L+6, 9.00% H-50 => LUMO, 5.78% H-15 => L+3, 5.41% H-1 => L+15, 4.53% H-13 => L+4, 4.01% HOMO => L+16, 3.18% H-18 => L+3, 3.10% H-48 => LUMO
236	23122	432	0.03	36.0% H-8 => L+9, 10.6% H-16 => L+5, 8.87% H-9 => L+8, 8.48% H-15 => L+4, 5.10% H-6 => L+12, 3.69% H-4 => L+14, 3.14% H-15 => L+7, 2.26% H-18 => L+4
237	23128	432	0.29	29.0% H-7 => L+12, 10.0% H-5 => L+14, 9.14% H-9 => L+9, 8.95% H-11 => L+6, 8.59% H-10 => L+7, 4.93% H-49 => LUMO, 4.79% H-1 => L+16, 2.51% HOMO => L+15, 2.19% H-13 => L+8
238	23148	432	0.00	31.1% H-12 => L+5, 15.3% H-9 => L+8, 9.73% H-11 => L+4, 6.50% H-16 => L+5, 5.53% H-12 => L+8, 5.07% H-18 => L+4, 3.25% H-8 => L+9, 3.03% H-15 => L+4, 2.55% H-15 => L+7, 2.42% H-11 => L+10, 2.07% H-7 => L+10
239	23180	431	0.11	18.0% H-55 => LUMO, 15.4% H-17 => L+3, 15.1% H-53 => LUMO, 8.37% H-51 => LUMO, 6.96% H-49 => LUMO, 5.19% H-11 => L+6, 4.11% H-10 => L+7, 4.01% H-6 => L+13, 2.25% H-7 => L+12
240	23181	431	0.00	28.3% H-48 => LUMO, 20.9% H-50 => LUMO, 12.2% H-54 => LUMO, 9.54% H-6 => L+11, 3.77% H-49 => L+1, 3.74% H-12 => L+6, 3.74% H-52 => LUMO, 3.70% H-1 => L+15, 2.87% H-13 => L+4, 2.12% HOMO => L+16
241	23186	431	0.02	49.5% H-10 => L+7, 7.17% H-11 => L+6, 5.25% H-17 => L+3, 4.95% H-9 => L+9, 4.68% H-5 => L+14, 3.49% H-14 => L+4, 3.08% H-6 => L+13, 2.53% H-8 => L+5, 2.10% H-13 => L+5
242	23260	430	0.00	19.5% H-17 => L+3, 19.3% H-51 => LUMO, 12.4% H-49 => LUMO, 11.1% H-53 => LUMO, 7.23% H-7 => L+12, 4.07% H-10 => L+7, 2.74% H-13 => L+5, 2.58% H-11 => L+6, 2.20% H-55 => LUMO, 2.20% H-50 => L+1
243	23278	430	0.00	32.3% H-56 => LUMO, 32.2% H-54 => LUMO, 7.50% H-48 => LUMO, 5.50% H-52 => LUMO, 4.80% H-1 => L+15, 3.46% H-12 => L+6, 3.32% H-50 => LUMO
244	23303	429	0.01	31.5% H-11 => L+7, 18.7% H-9 => L+8, 7.96% H-8 => L+9, 5.47% H-15 => L+4, 5.38% H-12 => L+8, 4.08% H-9 => L+5, 2.99% H-18 => L+4, 2.99% H-11 => L+4, 2.38% H-12 => L+11, 2.26% H-11 => L+10
245	23313	429	0.06	38.6% H-35 => L+1, 22.1% H-37 => L+1, 8.70% H-55 => LUMO, 5.72% H-34 => L+2, 4.65% H-34 => LUMO, 3.32% H-51 => LUMO, 2.34% H-49 => LUMO
246	23329	429	0.00	31.3% H-56 => LUMO, 11.7% H-6 => L+11, 9.04% H-18 => L+3, 7.09% H-1 => L+15, 2.93% H-58 => LUMO, 2.76% H-52 => LUMO, 2.65% H-13 =>
247	23341	428	0.05	

				L+7, 2.32% H-48 => LUMO, 2.26% H-10 => L+8, 2.21% H-50 => LUMO
248	23366	428	0.00	14.4% H-1 => L+16, 12.6% H-55 => LUMO, 9.36% H-35 => L+1, 6.81% H-49 => LUMO, 5.87% H-37 => L+1, 5.80% HOMO => L+15, 5.30% H-13 => L+5, 5.22% H-14 => L+4, 4.03% H-51 => LUMO, 3.93% H-17 => L+3, 3.91% H-7 => L+12, 2.01% H- 4 => L+15
249	23369	428	0.01	35.0% H-6 => L+12, 21.1% H-7 => L+13, 6.22% H- 8 => L+9, 5.53% H-19 => L+3, 3.33% H-14 => L+6, 2.85% H-9 => L+14, 2.81% H-10 => L+12, 2.52% H-4 => L+11, 2.02% H-9 => L+11
250	23392	428	0.04	19.7% H-54 => LUMO, 15.9% H-1 => L+15, 8.66% H-6 => L+11, 7.58% H-56 => LUMO, 6.59% H-58 => LUMO, 5.97% H-50 => LUMO, 4.66% H-8 => L+10, 3.82% HOMO => L+16, 3.55% H-10 => L+8, 2.74% H-13 => L+7, 2.48% H-52 => LUMO, 2.04% H-4 => L+16, 2.00% H-18 => L+3
251	23414	427	0.00	38.4% H-55 => LUMO, 12.7% H-1 => L+16, 7.34% H-57 => LUMO, 6.28% H-7 => L+12, 5.13% H-51 => LUMO, 3.64% H-6 => L+13, 3.48% HOMO => L+15
252	23418	427	0.00	47.7% H-13 => L+6, 5.81% H-7 => L+14, 5.80% H- 14 => L+3, 4.80% H-10 => L+9, 3.87% H-16 => L+4, 3.42% H-2 => L+16, 2.66% H-9 => L+13, 2.47% H-3 => L+15, 2.31% H-11 => L+8
253	23468	426	0.31	46.9% H-18 => L+3, 15.0% H-56 => LUMO, 4.31% H-21 => L+2, 3.81% H-11 => L+9, 3.64% H-52 => LUMO, 2.51% H-20 => L+3
254	23497	426	0.18	34.6% H-6 => L+12, 23.1% H-7 => L+13, 9.05% H- 8 => L+9, 5.49% H-19 => L+3, 4.34% H-4 => L+14, 3.96% H-9 => L+11, 2.87% H-14 => L+6
255	23584	424	0.00	43.5% H-52 => LUMO, 13.1% H-54 => LUMO, 6.58% H-58 => LUMO, 4.60% H-20 => L+3, 4.24% H-1 => L+15, 3.81% H-50 => LUMO, 3.28% H-6 => L+14, 3.04% H-53 => L+1, 2.76% H-12 => L+6, 2.48% H-51 => L+1
256	23586	424	0.00	31.2% H-53 => LUMO, 19.7% H-51 => LUMO, 14.6% H-9 => L+9, 8.36% H-7 => L+12, 4.72% H- 57 => LUMO, 4.08% H-52 => L+1, 2.69% H-17 => L+3, 2.02% H-1 => L+16
257	23593	424	0.00	17.5% H-52 => LUMO, 16.1% H-20 => L+3, 14.3% H-6 => L+14, 13.2% H-12 => L+6, 5.88% H-18 => L+3, 4.71% H-8 => L+13, 2.53% H-5 => L+13, 2.23% H-17 => L+6
258	23594	424	0.00	38.2% H-9 => L+9, 13.0% H-53 => LUMO, 10.9% H-7 => L+12, 7.49% H-51 => LUMO, 3.94% H-17 => L+3, 3.56% H-1 => L+16, 3.23% H-21 => L+3, 2.49% H-11 => L+12, 2.33% H-57 => LUMO

259	23665	423	0.00	21.2% H-7 => L+11, 18.8% H-9 => L+10, 14.4% H-12 => L+7, 9.36% H-11 => L+8, 8.58% H-13 => L+6, 6.23% H-12 => L+4, 3.05% H-11 => L+5 30.3% H-13 => L+5, 19.7% H-6 => L+13, 12.5% H-17 => L+3, 9.68% H-14 => L+4, 4.07% H-10 => L+4, 3.71% H-5 => L+14, 3.66% H-14 => L+7, 2.55% H-8 => L+11
260	23674	422	0.00	53.7% H-36 => L+1, 12.5% H-37 => LUMO, 10.6% H-35 => LUMO, 6.72% H-37 => L+2, 5.77% H-35 => L+2, 3.77% H-34 => L+1, 2.07% H-36 => L+3 42.6% H-37 => L+1, 19.9% H-36 => LUMO, 15.0% H-35 => L+1, 11.7% H-36 => L+2, 2.71% H-34 => LUMO, 2.33% H-35 => L+3
261	23776	421	0.00	56.7% H-8 => L+10, 9.72% H-14 => L+5, 7.25% H-13 => L+7, 3.50% H-1 => L+15, 3.17% H-19 => L+4, 2.87% H-6 => L+8, 2.62% H-10 => L+11, 2.40% H-18 => L+3, 2.18% H-13 => L+4 59.3% H-19 => L+3, 8.58% H-7 => L+13, 5.49% H-2 => L+15, 3.47% H-3 => L+16, 3.15% H-22 => L+2, 3.11% H-11 => L+7, 2.40% H-14 => L+6
262	23784	420	0.00	33.2% H-14 => L+4, 13.0% H-17 => L+3, 8.51% H-75 => LUMO, 5.48% H-68 => LUMO, 4.17% H-13 => L+5, 3.64% H-6 => L+13, 2.52% H-14 => L+7, 2.36% H-7 => L+12
263	23805	420	0.28	15.7% H-12 => L+7, 12.4% H-7 => L+14, 7.16% H-12 => L+10, 5.61% H-13 => L+6, 4.99% H-11 => L+5, 4.45% H-18 => L+5, 4.23% H-21 => L+4, 3.39% H-22 => L+3, 3.19% H-12 => L+4, 3.00% H-9 => L+10, 2.30% H-17 => L+4, 2.29% H-17 => L+7, 2.21% H-2 => L+16, 2.10% H-11 => L+11 68.6% H-58 => LUMO, 7.59% H-54 => LUMO, 6.22% H-57 => L+1, 5.27% H-56 => LUMO, 3.57% H-52 => LUMO, 2.59% H-48 => LUMO
264	23831	420	0.26	67.6% H-57 => LUMO, 8.22% H-55 => LUMO, 6.98% H-53 => LUMO, 5.90% H-58 => L+1, 2.94% H-49 => LUMO
265	23834	420	0.00	30.8% H-7 => L+14, 14.2% H-9 => L+10, 7.77% H-12 => L+7, 6.74% H-17 => L+4, 6.07% H-11 => L+5, 5.98% H-13 => L+6, 3.78% H-9 => L+13, 2.56% H-12 => L+4 21.1% H-6 => L+13, 14.6% H-21 => L+3, 11.2% H-13 => L+5, 9.01% H-1 => L+16, 6.53% H-75 => LUMO, 2.77% H-60 => LUMO, 2.52% H-19 => L+5, 2.21% H-13 => L+8
266	23883	419	0.01	16.3% H-9 => L+10, 14.1% H-11 => L+8, 11.0% H-21 => L+4, 4.31% H-18 => L+5, 4.15% H-13 => L+6, 3.98% H-16 => L+4, 3.89% H-16 => L+7, 3.82% H-11 => L+11, 3.80% H-12 => L+7, 3.80% H-15 => L+8, 3.57% H-9 => L+7, 2.34% H-12 => L+13, 2.28% H-17 => L+7, 2.27% H-25 => L+4 87.2% H-59 => LUMO, 5.45% H-63 => LUMO
267	23898	418	0.04	
268	23900	418	0.00	
269	23955	417	0.00	
270	23972	417	0.00	
271	24071	415	0.00	
272	24078	415	0.00	

				15.1% H-14 => L+6, 14.3% H-18 => L+4, 11.5% H-11 => L+7, 11.3% H-12 => L+5, 8.92% H-19 => L+3, 8.06% H-15 => L+4, 3.93% H-15 => L+7, 3.28% H-21 => L+5, 2.27% H-2 => L+15
273	24085	415	0.16	50.7% H-21 => L+3, 9.14% H-6 => L+13, 4.26% H-25 => L+3, 4.12% H-9 => L+9, 2.58% H-18 => L+6, 2.39% H-7 => L+12, 2.09% H-8 => L+11
274	24096	415	0.00	54.2% H-62 => LUMO, 21.1% H-64 => LUMO, 7.09% H-20 => L+3, 6.50% H-6 => L+14
275	24131	414	0.00	36.1% H-2 => L+15, 9.64% H-15 => L+4, 8.61% H-3 => L+16, 5.55% H-67 => LUMO, 5.39% H-7 => L+13, 5.22% H-19 => L+3, 4.29% H-18 => L+4, 2.68% H-15 => L+7, 2.60% H-12 => L+5, 2.46% H-14 => L+6
276	24174	414	0.60	29.1% H-62 => LUMO, 16.9% H-6 => L+14, 16.1% H-20 => L+3, 4.61% H-10 => L+8, 4.34% H-72 => LUMO, 3.97% H-64 => LUMO, 3.58% H-61 => LUMO, 2.10% H-13 => L+7, 2.06% H-18 => L+3
277	24188	413	0.00	31.7% H-2 => L+16, 16.9% H-22 => L+3, 7.94% H-3 => L+15, 6.75% H-13 => L+6, 5.78% H-10 => L+9, 4.76% H-7 => L+14, 2.70% H-9 => L+10, 2.69% H-66 => LUMO, 2.16% H-8 => L+12, 2.03% H-11 => L+8
278	24198	413	0.01	85.0% H-65 => LUMO, 5.66% H-67 => LUMO
279	24201	413	0.01	66.3% H-63 => LUMO, 14.1% H-68 => LUMO, 5.52% H-59 => LUMO, 3.02% H-60 => LUMO,
280	24202	413	0.00	2.35% H-62 => L+1 17.2% H-64 => LUMO, 16.3% H-6 => L+14, 12.8% H-72 => LUMO, 11.4% H-61 => LUMO, 7.74% H-23 => L+3, 6.40% H-1 => L+15, 3.92% H-10 => L+8
281	24204	413	0.00	59.6% H-66 => LUMO, 34.9% H-69 => LUMO
282	24214	413	0.00	50.6% H-10 => L+8, 14.3% H-14 => L+5, 4.75% H-64 => LUMO, 4.03% H-13 => L+10, 3.99% H-8 => L+10, 3.48% H-62 => LUMO, 2.88% H-8 => L+7, 2.87% H-19 => L+4, 2.11% H-13 => L+4
283	24231	413	0.00	74.7% H-67 => LUMO, 9.51% H-70 => LUMO,
284	24264	412	0.02	7.43% H-65 => LUMO 49.1% H-69 => LUMO, 28.2% H-66 => LUMO, 11.7% H-71 => LUMO, 3.06% H-22 => L+3, 2.95% H-67 => L+1
285	24264	412	0.00	49.6% H-22 => L+3, 8.63% H-2 => L+16, 6.05% H-71 => LUMO, 3.35% H-12 => L+7, 2.91% H-26 => L+3, 2.59% H-9 => L+10, 2.33% H-19 => L+6, 2.26% H-17 => L+4
286	24332	411	0.00	39.5% H-64 => LUMO, 17.0% H-61 => LUMO, 7.33% H-62 => LUMO, 6.67% H-13 => L+7, 5.10% H-20 => L+3, 2.06% H-60 => L+1
287	24347	411	0.00	

				40.8% H-68 => LUMO, 19.5% H-63 => LUMO, 18.4% H-60 => LUMO, 2.69% H-64 => L+1, 2.15% H-75 => LUMO
288	24358	411	0.00	15.8% H-75 => LUMO, 14.5% H-8 => L+11, 9.59% H-60 => LUMO, 8.54% H-15 => L+6, 6.89% H-68 => LUMO, 5.16% H-30 => L+2, 4.92% H-10 => L+10, 3.73% H-1 => L+16, 2.81% H-16 => L+3, 2.81% H-6 => L+13, 2.38% H-13 => L+8 42.8% H-14 => L+6, 6.49% H-7 => L+13, 6.40% H- 24 => L+3, 5.27% H-2 => L+15, 4.38% H-18 => L+4, 3.72% H-21 => L+5, 2.32% H-15 => L+4, 2.24% H-23 => L+4, 2.12% H-15 => L+7 51.6% H-71 => LUMO, 8.58% H-10 => L+9, 7.94% H-69 => LUMO, 4.94% H-74 => LUMO, 4.53% H- 70 => L+1, 2.73% H-17 => L+4, 2.44% H-7 => L+14, 2.33% H-66 => LUMO
289	24372	410	0.00	70.2% H-70 => LUMO, 7.80% H-67 => LUMO, 6.65% H-73 => LUMO, 5.34% H-71 => L+1 72.8% H-30 => L+2, 5.89% H-31 => L+1, 4.09% H- 31 => L+3, 3.58% H-30 => LUMO
290	24383	410	0.25	20.1% H-10 => L+9, 12.8% H-71 => LUMO, 11.7% H-16 => L+4, 7.49% H-7 => L+14, 4.66% H-16 => L+7, 3.66% H-2 => L+16, 3.25% H-15 => L+8, 2.93% H-11 => L+8, 2.74% H-17 => L+4, 2.61% H- 8 => L+12, 2.32% H-69 => LUMO
291	24406	410	0.00	27.7% H-23 => L+3, 12.9% H-61 => LUMO, 12.8% H-13 => L+7, 5.99% H-11 => L+9, 4.77% H-20 => L+3, 4.20% H-14 => L+5, 4.06% H-72 => LUMO, 2.99% H-21 => L+6, 2.69% H-18 => L+3, 2.47% H- 25 => L+2
292	24413	410	0.01	23.6% H-13 => L+7, 22.1% H-20 => L+3, 10.4% H- 14 => L+5, 7.83% H-11 => L+9, 5.40% H-14 => L+8, 4.55% H-10 => L+8, 2.45% H-9 => L+12, 2.21% H-10 => L+5
293	24414	410	0.00	30.5% H-24 => L+3, 14.3% H-9 => L+11, 5.69% H- 7 => L+13, 4.87% H-14 => L+6, 4.64% H-12 => L+8, 2.50% H-11 => L+10, 2.46% H-7 => L+10, 2.22% H-38 => L+1, 2.14% H-17 => L+5, 2.03% H- 11 => L+7
294	24453	409	0.00	12.7% H-9 => L+11, 9.83% H-11 => L+10, 9.24% H-18 => L+4, 8.53% H-23 => L+4, 6.34% H-20 => L+4, 5.92% H-11 => L+7, 4.90% H-2 => L+15, 4.37% H-14 => L+6, 3.89% H-24 => L+3, 3.83% H- 17 => L+5, 2.75% H-25 => L+5, 2.67% H-12 => L+8, 2.01% H-17 => L+8
295	24482	408	0.00	25.0% H-60 => LUMO, 10.9% H-75 => LUMO, 10.4% H-8 => L+11, 5.76% H-25 => L+3, 5.34% H- 1 => L+16, 4.20% H-15 => L+6, 3.69% H-13 => L+5, 2.82% H-22 => L+4
296	24510	408	0.00	37.3% H-17 => L+4, 13.3% H-26 => L+3, 11.5% H- 10 => L+9, 6.03% H-12 => L+7, 5.04% H-20 =>
297	24517	408	0.03	
298	24539	408	0.01	
299	24558	407	0.00	
300	24559	407	0.00	

				L+5, 3.64% H-18 => L+5, 2.86% H-7 => L+14, 2.42% H-29 => L+3 37.5% H-25 => L+3, 5.96% H-12 => L+9, 5.54% H- 21 => L+3, 4.60% H-8 => L+11, 4.14% H-23 => L+2, 4.01% H-23 => L+6, 3.83% H-7 => L+12, 3.53% H-22 => L+4, 3.23% H-26 => L+4, 2.36% H- 1 => L+16, 2.26% H-14 => L+7, 2.01% H-19 => L+5
301	24570	407	0.00	17.9% H-39 => L+1, 15.7% H-38 => L+1, 9.61% H- 10 => L+9, 6.23% H-11 => L+8, 5.26% H-17 => L+4, 4.90% H-2 => L+16, 3.11% H-38 => LUMO, 2.70% H-39 => LUMO, 2.60% H-26 => L+3, 2.41% H-12 => L+7, 2.04% H-8 => L+12
302	24582	407	0.00	19.8% H-38 => L+1, 17.4% H-39 => L+1, 15.8% H- 24 => L+3, 4.47% H-23 => L+4, 4.30% H-18 => L+4, 3.79% H-27 => L+3, 3.31% H-39 => LUMO, 2.89% H-38 => LUMO, 2.70% H-18 => L+7, 2.15% H-39 => L+2, 2.07% H-16 => L+8
303	24585	407	0.00	20.0% H-23 => L+3, 19.9% H-11 => L+9, 14.4% H- 16 => L+6, 5.62% H-72 => LUMO, 4.88% H-9 => L+12, 4.04% H-15 => L+9, 2.93% H-18 => L+3, 2.53% H-12 => L+6, 2.19% H-78 => LUMO
304	24603	406	0.07	31.6% H-72 => LUMO, 11.3% H-78 => LUMO, 10.8% H-1 => L+15, 7.61% H-31 => L+2, 5.32% H- 23 => L+3, 4.29% H-13 => L+7, 3.80% H-14 => L+5
305	24608	406	0.09	39.9% H-75 => LUMO, 24.2% H-60 => LUMO, 20.9% H-68 => LUMO, 4.12% H-72 => L+1, 2.17% H-61 => L+1
306	24644	406	0.00	28.8% H-31 => L+2, 19.8% H-72 => LUMO, 19.1% H-61 => LUMO, 3.19% H-32 => L+1, 2.86% H-30 => L+3, 2.77% H-14 => L+5, 2.54% H-64 => LUMO, 2.48% H-11 => L+9, 2.14% H-30 => L+1
307	24650	406	0.01	30.8% H-31 => L+2, 19.8% H-61 => LUMO, 6.11% H-1 => L+15, 3.97% H-14 => L+5, 3.45% H-78 => LUMO, 3.30% H-72 => LUMO, 3.19% H-30 => L+3, 3.10% H-32 => L+1, 2.08% H-13 => L+7, 2.03% H-11 => L+9
308	24657	406	0.04	19.0% H-39 => L+1, 16.6% H-38 => L+1, 11.1% H- 11 => L+8, 6.59% H-16 => L+4, 5.70% H-10 => L+9, 5.28% H-21 => L+4, 4.33% H-16 => L+7, 2.87% H-23 => L+5, 2.50% H-74 => LUMO, 2.34% H-38 => LUMO, 2.04% H-39 => LUMO
309	24680	405	0.00	15.3% H-16 => L+6, 15.3% H-14 => L+5, 10.8% H- 6 => L+14, 6.39% H-8 => L+13, 5.85% H-13 => L+7, 3.81% H-19 => L+4, 3.67% H-10 => L+11, 3.66% H-19 => L+7, 3.38% H-23 => L+3, 3.05% H- 24 => L+4, 2.81% H-13 => L+10, 2.70% H-15 => L+3, 2.11% H-15 => L+9, 2.02% H-13 => L+4
310	24686	405	0.00	16.1% H-38 => L+1, 14.1% H-39 => L+1, 12.8% H- 27 => L+3, 5.24% H-23 => L+4, 5.03% H-24 =>
311	24687	405	0.03	

				L+3, 3.83% H-12 => L+8, 3.51% H-21 => L+5, 2.85% H-9 => L+11, 2.47% H-18 => L+7, 2.30% H- 40 => L+1, 2.10% H-15 => L+4 27.3% H-15 => L+6, 17.5% H-8 => L+11, 9.21% H- 25 => L+3, 5.25% H-16 => L+3, 4.85% H-14 => L+7, 4.74% H-22 => L+4, 2.95% H-16 => L+9, 2.90% H-75 => LUMO, 2.86% H-12 => L+9, 2.34% H-19 => L+5, 2.06% H-13 => L+8, 2.06% H-1 =>
312	24710	405	0.00	L+16 54.6% H-73 => LUMO, 11.2% H-76 => LUMO, 8.25% H-27 => L+3, 7.52% H-70 => LUMO, 4.30% H-74 => L+1, 2.89% H-74 => LUMO 55.5% H-74 => LUMO, 11.1% H-77 => LUMO, 7.61% H-71 => LUMO, 4.36% H-73 => L+1, 4.19%
313	24750	404	0.00	H-26 => L+3, 2.94% H-73 => LUMO 42.1% H-27 => L+3, 18.9% H-40 => L+1, 6.00% H- 42 => L+1, 4.24% H-28 => L+3, 3.41% H-20 =>
314	24753	404	0.00	L+4 52.7% H-19 => L+4, 9.52% H-22 => L+5, 5.19% H- 14 => L+5, 4.50% H-16 => L+6, 3.27% H-78 =>
315	24760	404	0.02	LUMO, 3.19% H-24 => L+7, 2.48% H-8 => L+13, 2.38% H-13 => L+4, 2.06% H-13 => L+7 48.2% H-40 => L+1, 6.25% H-44 => L+1, 4.97% H- 9 => L+11, 4.08% H-18 => L+4, 3.32% H-11 =>
316	24779	404	0.00	L+13, 2.59% H-12 => L+8, 2.05% H-79 => LUMO 49.9% H-26 => L+3, 9.61% H-17 => L+4, 5.60% H- 29 => L+3, 5.15% H-2 => L+16, 2.74% H-7 =>
317	24780	404	0.27	L+14, 2.21% H-74 => LUMO 17.1% H-40 => L+1, 15.6% H-12 => L+8, 13.5% H- 42 => L+1, 10.8% H-27 => L+3, 4.93% H-44 =>
318	24798	403	0.01	L+1, 3.72% H-73 => LUMO, 2.37% H-28 => L+3,
319	24806	403	0.00	2.05% H-11 => L+13

**Table S18.** TDDFT-predicted band excitation data for **10**.

Index	Energy (cm <sup>-1</sup> )	$\lambda$ (nm)	Osc. Strength	Contributions
0	2668	3748	8.55	98.5% HOMO => LUMO, 2.16% H-1 => L+1
1	4430	2258	0.00	50.5% H-1 => LUMO, 46.7% HOMO => L+1
2	4584	2181	0.00	93.3% H-2 => LUMO, 3.72% H-3 => L+1
3	4933	2027	0.00	51.4% HOMO => L+1, 47.2% H-1 => LUMO 81.8% H-3 => LUMO, 13.2% H-2 => L+1, 2.33%
4	5307	1884	0.00	H-5 => L+1 74.0% H-5 => LUMO, 16.4% H-3 => L+1, 5.56%
5	6274	1594	0.00	H-2 => L+2
6	6293	1589	0.03	62.8% H-4 => LUMO, 34.4% HOMO => L+2

				42.4% HOMO => L+2, 30.9% H-1 => L+1, 22.6%
7	6658	1502	0.27	H-4 => LUMO 64.4% H-1 => L+1, 20.2% HOMO => L+2, 11.1%
8	6897	1450	0.38	H-4 => LUMO 80.8% H-2 => L+1, 13.3% H-3 => LUMO, 2.66%
9	7148	1399	0.00	H-3 => L+2 67.5% H-7 => LUMO, 18.1% H-5 => L+1, 7.69%
10	7408	1350	0.00	H-3 => L+2, 2.99% H-2 => L+3 63.2% H-3 => L+1, 20.9% H-5 => LUMO, 8.54%
11	7899	1266	0.00	H-2 => L+2, 2.85% H-2 => LUMO 78.3% H-6 => LUMO, 15.1% HOMO => L+3,
12	8019	1247	0.00	2.11% H-4 => L+1 67.8% HOMO => L+3, 16.4% H-6 => LUMO,
13	8461	1182	0.00	11.1% H-4 => L+1 80.7% H-4 => L+1, 12.8% HOMO => L+3, 2.26%
14	8626	1159	0.00	H-1 => LUMO 62.7% H-8 => LUMO, 19.2% H-7 => L+1, 8.77%
15	8646	1157	0.00	H-5 => L+2, 3.87% H-3 => L+3
16	8720	1147	0.00	93.2% H-1 => L+2, 2.52% HOMO => L+1 53.0% H-5 => L+1, 27.5% H-7 => LUMO, 9.96%
17	8886	1125	0.00	H-3 => L+2, 2.94% H-2 => L+3, 2.60% H-3 => LUMO 78.8% H-2 => L+2, 11.7% H-3 => L+1, 3.20% H-2 => LUMO, 2.99% H-3 => L+3
18	9238	1082	0.00	84.7% H-9 => LUMO, 6.23% H-6 => L+1, 3.10% HOMO => L+4
19	9561	1046	0.07	57.5% H-10 => LUMO, 18.3% H-8 => L+1, 9.77%
20	9925	1008	0.00	H-7 => L+2, 3.35% H-5 => L+3, 2.54% H-3 => L+2 59.6% H-3 => L+2, 20.0% H-5 => L+1, 8.29% H-2 => L+3, 2.89% H-10 => LUMO, 2.69% H-5 => L+3
21	10011	999	0.00	44.5% H-7 => L+1, 32.5% H-8 => LUMO, 11.3% H-5 => L+2, 4.15% H-3 => L+3, 2.15% H-5 => LUMO
22	10021	998	0.00	77.4% HOMO => L+4, 10.8% H-1 => L+3, 2.88% H-9 => LUMO
23	10175	983	0.07	73.2% H-6 => L+1, 12.1% H-4 => L+2, 6.68% H-9 => LUMO, 2.48% H-4 => LUMO
24	10287	972	0.02	43.5% H-4 => L+2, 29.2% H-1 => L+3, 11.8% HOMO => L+4, 10.0% H-6 => L+1
25	10529	950	0.05	52.5% H-1 => L+3, 35.9% H-4 => L+2, 3.03% HOMO => L+4, 2.72% H-6 => L+1
26	10695	935	0.14	79.7% H-11 => LUMO, 9.11% H-9 => L+1, 2.10% H-13 => L+1, 2.01% H-6 => L+2
27	10872	920	0.00	50.3% H-5 => L+2, 28.4% H-7 => L+1, 9.01% H-3 => L+3, 2.97% H-2 => L+4, 2.28% H-3 => L+1
28	10980	911	0.00	58.9% H-12 => LUMO, 16.9% H-10 => L+1, 7.69% H-8 => L+2, 4.53% H-7 => L+3, 2.58% HOMO => L+5, 2.32% H-5 => L+4
29	11189	894	0.00	71.0% H-2 => L+3, 11.3% H-3 => L+2, 3.58% H-10 => LUMO, 2.98% H-2 => L+1, 2.79% H-8 => L+1, 2.31% H-5 => L+3
30	11210	892	0.00	

				35.2% H-8 => L+1, 31.4% H-10 => LUMO, 10.8% H-7 => L+2, 6.57% H-2 => L+3, 3.90% H-3 => L+4,
31	11229	891	0.00	3.74% H-5 => L+3
32	11251	889	0.00	90.9% HOMO => L+5, 2.16% H-1 => L+6
33	11704	854	0.00	88.8% HOMO => L+6, 6.13% H-1 => L+5 43.8% HOMO => L+7, 13.4% H-1 => L+4, 9.61%
34	11772	849	0.00	H-4 => L+3, 8.70% H-9 => L+1, 7.91% H-6 => L+2, 4.59% H-11 => LUMO, 2.16% H-15 => LUMO 73.1% H-13 => LUMO, 9.16% H-11 => L+1, 2.86%
35	11869	843	0.05	H-9 => L+2, 2.69% H-16 => LUMO, 2.33% H-15 => L+1 57.2% H-9 => L+1, 19.8% HOMO => L+7, 9.04%
36	11873	842	0.00	H-11 => LUMO, 5.16% H-6 => L+2, 3.82% H-1 => L+4, 2.21% H-6 => LUMO 60.6% H-3 => L+3, 20.4% H-5 => L+2, 9.40% H-2
37	11962	836	0.00	=> L+4, 2.10% H-2 => L+2 40.0% H-7 => L+2, 35.2% H-8 => L+1, 10.9% H-5
38	12120	825	0.00	=> L+3, 4.04% H-3 => L+4 38.6% H-6 => L+2, 18.9% HOMO => L+7, 15.6%
39	12241	817	0.00	H-9 => L+1, 15.4% H-4 => L+3, 3.70% H-1 => L+4 62.8% H-14 => LUMO, 15.2% H-12 => L+1, 6.63%
40	12357	809	0.00	H-10 => L+2, 3.88% H-8 => L+3, 2.11% H-7 => L+4 79.8% HOMO => L+8, 6.01% H-1 => L+6, 3.63%
41	12362	809	0.00	H-12 => LUMO 59.6% H-15 => LUMO, 14.2% H-6 => L+2, 5.93%
42	12435	804	0.00	H-13 => L+1, 4.59% H-16 => L+1, 2.51% H-1 => L+4, 2.16% HOMO => L+7, 2.00% H-9 => L+3 33.2% H-10 => L+1, 30.7% H-12 => LUMO, 11.0%
43	12442	804	0.00	H-8 => L+2, 7.30% HOMO => L+8, 5.45% H-7 => L+3, 3.01% H-5 => L+4 29.2% H-1 => L+4, 21.5% H-6 => L+2, 18.2% H-4 => L+3, 12.1% H-15 => LUMO, 8.59% HOMO => L+7
44	12464	802	0.00	82.9% H-16 => LUMO, 7.88% H-15 => L+1
45	12523	799	0.01	48.7% H-4 => L+3, 40.5% H-1 => L+4, 3.20% H-6 => L+2 46.7% H-5 => L+3, 31.0% H-7 => L+2, 10.8% H-3 => L+4, 3.65% H-2 => L+7
46	12619	792	0.00	74.2% H-2 => L+4, 13.4% H-3 => L+3, 3.26% H-2 => L+2, 2.24% H-3 => L+7 81.9% HOMO => L+9, 8.16% H-1 => L+8
47	12972	771	0.00	32.5% H-11 => L+1, 16.9% H-13 => LUMO, 11.5% HOMO => L+10, 10.5% H-9 => L+2, 5.38% H-6 => L+3, 4.73% H-4 => L+4, 4.31% H-1 => L+7, 2.01%
48	13116	762	0.00	H-19 => LUMO 25.1% H-10 => L+1, 20.5% H-17 => LUMO, 19.9%
49	13165	760	0.00	H-8 => L+2, 7.46% H-7 => L+3, 5.90% H-12 => L+2, 4.97% H-14 => L+1, 3.20% H-5 => L+4, 2.20% H-3 => L+7
50	13216	757	0.12	
51	13319	751	0.00	

				43.9% H-17 => LUMO, 13.9% H-10 => L+1, 10.8% H-8 => L+2, 8.28% H-14 => L+1, 4.00% H-7 => L+3, 3.28% H-10 => L+3
52	13323	751	0.00	63.8% H-2 => L+5, 12.1% H-3 => L+6, 4.49% H-6 => L+3, 3.26% H-5 => L+8, 2.99% H-2 => L+8, 2.88% HOMO => L+10
53	13325	750	7.28	36.3% HOMO => L+10, 33.7% H-11 => L+1, 11.5% H-1 => L+7, 5.04% H-2 => L+5, 4.69% H-4 => L+4
54	13390	747	0.54	85.4% H-1 => L+5, 5.29% HOMO => L+6, 4.00% H-4 => L+6, 2.36% HOMO => L+9
55	13394	747	0.00	32.9% H-12 => L+1, 30.7% H-14 => LUMO, 12.0% H-10 => L+2, 6.41% H-8 => L+3, 4.04% H-7 => L+4, 2.11% H-5 => L+7
56	13574	737	0.00	70.1% H-1 => L+6, 7.75% H-4 => L+5, 7.25% HOMO => L+8, 5.05% HOMO => L+11, 3.72% H-1 => L+9, 2.71% HOMO => L+5
57	13832	723	0.00	45.2% H-9 => L+2, 19.1% HOMO => L+10, 14.5% H-11 => L+1, 11.9% H-6 => L+3, 2.58% H-4 => L+4
58	13840	723	0.02	55.9% H-3 => L+4, 24.4% H-5 => L+3, 9.92% H-2 => L+7, 2.04% H-2 => L+3
59	13874	721	0.00	74.1% HOMO => L+11, 6.56% H-1 => L+6, 5.38% H-1 => L+9, 2.93% H-4 => L+8
60	14028	713	0.00	44.0% H-2 => L+6, 38.4% H-3 => L+5, 4.93% H-5 => L+6, 2.39% H-3 => L+8, 2.13% H-2 => L+9
61	14046	712	0.00	39.8% H-8 => L+2, 33.7% H-7 => L+3, 9.83% H-5 => L+4, 4.40% H-3 => L+7, 2.22% HOMO => L+11, 2.04% H-2 => L+10
62	14089	710	0.00	26.0% H-9 => L+2, 21.7% H-4 => L+4, 20.7% HOMO => L+10, 17.3% H-1 => L+7, 7.76% H-6 => L+3
63	14151	707	0.03	83.8% H-18 => LUMO, 4.66% H-17 => L+1, 3.62% HOMO => L+18, 2.08% H-12 => L+1
64	14225	703	0.27	41.3% H-13 => L+1, 17.0% H-15 => LUMO, 8.73% H-20 => LUMO, 7.03% H-11 => L+2, 3.39% HOMO => L+13, 3.33% H-9 => L+3, 2.70% H-19 => L+1, 2.58% H-11 => LUMO, 2.02% H-6 => L+4
65	14359	696	0.00	42.3% H-1 => L+7, 39.5% H-6 => L+3, 6.09% H-9 => L+2, 3.36% HOMO => L+10, 2.55% H-2 => L+5
66	14389	695	0.01	40.8% H-1 => L+8, 14.2% H-12 => L+1, 8.99% H-10 => L+2, 7.27% HOMO => L+9, 4.73% H-4 => L+6, 4.29% H-8 => L+3, 2.68% HOMO => L+12, 2.38% H-1 => L+11, 2.26% H-7 => L+4
67	14455	692	0.01	26.9% H-17 => LUMO, 22.9% H-14 => L+1, 9.91% H-12 => L+2, 8.32% H-18 => L+1, 5.91% H-10 => L+3, 5.24% H-24 => LUMO, 4.86% H-8 => L+4, 2.89% H-7 => L+7, 2.11% H-5 => L+10
68	14481	691	0.00	55.5% H-4 => L+4, 21.4% H-6 => L+3, 14.8% H-1 => L+7
69	14526	688	0.04	29.1% H-1 => L+8, 26.0% H-12 => L+1, 14.4% H-10 => L+2, 6.71% H-8 => L+3, 3.83% H-7 => L+4,
70	14529	688	0.01	

				3.07% H-4 => L+6, 2.51% H-5 => L+7, 2.18% HOMO => L+9
71	14668	682	0.00	30.4% H-13 => L+1, 22.0% HOMO => L+13, 21.0% H-20 => LUMO, 7.94% H-1 => L+10, 4.22% H-4 => L+7, 3.60% H-16 => L+1, 2.37% H-19 => L+1 58.3% H-19 => LUMO, 6.58% H-20 => L+1, 4.77%
72	14799	676	0.24	H-2 => L+8, 4.22% H-3 => L+6, 2.95% H-15 => L+1, 2.75% H-22 => LUMO, 2.58% H-5 => L+5, 2.09% H-4 => L+4
73	14825	675	0.00	70.5% HOMO => L+12, 5.72% H-1 => L+11, 3.55% H-1 => L+8, 3.54% H-2 => L+7, 3.28% H-31 =>
74	14848	673	0.00	LUMO, 2.70% H-4 => L+9, 2.07% H-12 => L+1 41.0% H-5 => L+4, 33.7% H-7 => L+3, 11.1% H-3 => L+7, 4.30% H-2 => L+10
75	14963	668	0.82	28.8% H-2 => L+8, 26.7% H-3 => L+6, 14.1% H-5 => L+5, 6.93% H-15 => L+1, 4.46% H-22 => LUMO, 4.28% H-19 => LUMO
76	14970	668	0.00	69.4% H-2 => L+7, 14.6% H-3 => L+4, 4.14% HOMO => L+12, 3.33% H-2 => L+3, 3.05% H-3 => L+10
77	15018	666	0.00	43.7% H-20 => LUMO, 12.3% HOMO => L+13, 10.7% H-21 => LUMO, 4.47% H-16 => L+1, 4.19% H-19 => L+1, 3.35% H-11 => L+2, 2.40% H-1 =>
78	15170	659	0.02	L+10, 2.09% H-9 => L+3 61.0% H-15 => L+1, 12.6% H-19 => LUMO, 6.72% H-16 => LUMO, 4.56% H-13 => L+2, 2.10% H-2 => L+8
79	15220	657	0.00	41.6% H-1 => L+9, 9.48% HOMO => L+11, 9.23% HOMO => L+14, 7.48% H-4 => L+8, 5.46% H-14 => L+1, 4.70% H-1 => L+12, 3.94% H-4 => L+5, 2.46% H-24 => LUMO
80	15229	657	0.00	51.7% H-21 => LUMO, 13.6% H-11 => L+2, 7.71% H-13 => L+1, 4.22% H-9 => L+3, 3.34% H-20 => LUMO, 2.20% H-16 => L+1, 2.17% HOMO => L+13
81	15262	655	0.00	49.8% H-10 => L+2, 20.2% H-8 => L+3, 10.1% H-7 => L+4, 5.14% H-5 => L+7, 3.18% H-3 => L+10 30.0% H-11 => L+2, 24.1% HOMO => L+13, 19.8% H-21 => LUMO, 4.05% H-9 => L+3, 3.99% H-13 => L+1, 3.79% H-20 => LUMO, 2.74% H-1 =>
82	15269	655	0.00	L+10, 2.41% H-25 => LUMO 43.0% H-4 => L+5, 10.7% H-14 => L+1, 9.16% HOMO => L+14, 6.17% H-24 => LUMO, 5.94% H-
83	15323	653	0.00	1 => L+6, 4.36% H-1 => L+9, 2.43% H-17 => L+2 72.0% H-22 => LUMO, 4.88% H-23 => LUMO,
84	15337	652	0.03	2.86% H-19 => LUMO, 2.44% H-25 => L+1 32.8% H-4 => L+5, 18.7% H-1 => L+9, 13.2% H-14 => L+1, 7.51% H-24 => LUMO, 4.02% H-6 => L+6, 2.63% H-1 => L+6, 2.22% HOMO => L+14, 2.13% H-17 => L+2
85	15385	650	0.00	

				71.8% H-16 => L+1, 8.55% H-11 => L+2, 6.66% HOMO => L+13, 2.54% H-15 => LUMO, 2.51% H- 15 => L+2
86	15451	647	0.00	44.1% H-3 => L+5, 43.3% H-2 => L+6, 4.58% H-5 => L+6, 3.62% H-3 => L+8
87	15500	645	0.00	40.9% HOMO => L+14, 12.6% H-14 => L+1, 10.3% H-29 => LUMO, 6.04% H-24 => LUMO, 4.45% HOMO => L+17, 3.99% H-1 => L+9, 3.15% H-1 => L+12, 2.96% H-5 => L+4
88	15530	644	0.00	28.4% HOMO => L+15, 24.3% H-17 => L+1, 13.8% H-27 => LUMO, 5.21% H-1 => L+14, 3.86% H-18 => L+2, 3.20% H-8 => L+3, 2.40% H-18 => LUMO, 2.13% H-14 => L+2
89	15636	640	0.02	67.4% H-23 => LUMO, 5.74% H-21 => L+1, 5.45% H-22 => LUMO, 3.96% H-26 => L+1, 3.51% HOMO => L+16
90	15680	638	0.03	39.4% H-25 => LUMO, 11.2% H-3 => L+8, 7.37% H-9 => L+3, 7.34% H-2 => L+9, 4.78% H-5 => L+6, 3.24% H-22 => L+1, 2.87% H-26 => LUMO, 2.60% H-6 => L+4, 2.18% H-21 => LUMO, 2.01% H-30 => LUMO
91	15688	637	0.00	21.6% H-11 => L+2, 14.0% HOMO => L+13, 12.3% H-9 => L+3, 12.3% H-4 => L+7, 11.8% H-6 => L+4, 6.23% H-25 => LUMO, 6.03% H-1 => L+10, 2.20% H-16 => L+1, 2.03% H-2 => L+9
92	15721	636	0.00	48.4% H-3 => L+7, 25.7% H-5 => L+4, 9.61% H-2 => L+10, 2.86% HOMO => L+14
93	15725	636	0.00	67.1% H-4 => L+6, 11.0% H-1 => L+8, 8.32% H-6 => L+5, 3.68% H-1 => L+5, 2.34% H-4 => L+9
94	15760	635	0.00	24.0% H-12 => L+2, 23.9% H-24 => LUMO, 13.0% H-14 => L+1, 8.56% HOMO => L+17, 7.38% H-10 => L+3, 3.68% H-8 => L+4, 3.22% H-18 => L+1
95	15812	632	0.00	25.6% H-17 => L+1, 20.0% H-8 => L+3, 17.2% H- 27 => LUMO, 5.54% HOMO => L+18, 4.67% H-18 => LUMO, 3.99% H-7 => L+4, 3.19% H-5 => L+7, 3.11% H-14 => L+2, 2.33% H-24 => L+1, 2.10% H- 3 => L+10
96	15912	628	0.02	47.9% H-2 => L+8, 18.8% H-3 => L+6, 14.6% H-2 => L+5, 9.19% H-5 => L+5, 3.91% H-3 => L+9
97	15930	628	0.52	23.6% H-1 => L+10, 20.9% H-9 => L+3, 17.9% H- 26 => LUMO, 8.15% H-25 => LUMO, 6.34% HOMO => L+13, 6.12% H-4 => L+7, 2.42% H-11 => L+2
98	15960	627	0.00	32.8% H-26 => LUMO, 18.5% H-9 => L+3, 9.54% H-25 => LUMO, 7.84% H-1 => L+10, 4.60% H-3 => L+8, 3.93% H-2 => L+9, 2.94% H-23 => L+1,
99	15995	625	0.00	2.10% H-5 => L+6, 2.02% H-4 => L+7 25.5% H-8 => L+3, 17.8% H-7 => L+4, 8.15% H-17 => L+1, 7.34% H-27 => LUMO, 7.31% H-5 => L+7, 6.85% H-1 => L+11, 3.61% HOMO => L+18, 2.97%
100	16022	624	0.01	

				H-3 => L+10, 2.57% HOMO => L+12, 2.20% HOMO => L+15
101	16032	624	0.00	46.6% HOMO => L+16, 9.09% H-1 => L+13, 6.43% H-15 => L+1, 5.75% H-13 => L+2, 4.97% H-4 => L+10, 3.78% H-6 => L+7, 3.78% H-11 => L+3, 3.34% H-9 => L+4
102	16112	621	0.00	50.2% H-1 => L+11, 8.51% HOMO => L+12, 7.00% H-4 => L+9, 4.88% H-27 => LUMO, 3.56% H-7 => L+4, 3.18% H-6 => L+8, 2.30% HOMO => L+15, 2.29% H-8 => L+3
103	16142	620	0.00	21.0% H-26 => LUMO, 20.7% H-3 => L+8, 12.3% H-25 => LUMO, 11.8% H-2 => L+9, 8.36% H-5 => L+6, 3.67% H-1 => L+10, 3.37% H-30 => LUMO, 2.29% H-7 => L+5, 2.23% H-23 => L+1
104	16156	619	0.01	71.5% H-28 => LUMO, 6.89% H-32 => LUMO, 5.35% H-25 => L+1, 2.70% HOMO => L+16
105	16202	617	0.00	42.5% H-6 => L+4, 26.3% H-1 => L+10, 15.1% H-9 => L+3, 4.55% H-4 => L+7
106	16274	614	0.00	35.7% H-18 => L+1, 34.6% H-24 => LUMO, 11.7% HOMO => L+17, 3.78% H-17 => LUMO, 3.52% H- 17 => L+2
107	16351	612	0.00	52.6% H-4 => L+7, 20.0% H-6 => L+4, 10.1% H-1 => L+10, 3.93% H-30 => LUMO, 2.01% H-25 => LUMO
108	16367	611	0.17	56.1% H-5 => L+5, 18.8% H-3 => L+6, 7.17% H-2 => L+5, 4.35% H-7 => L+6, 2.29% H-28 => LUMO 55.8% H-4 => L+8, 13.6% H-1 => L+9, 7.10% H-6 => L+6, 3.04% H-33 => LUMO, 3.02% H-1 => L+6,
109	16374	611	0.00	2.78% H-35 => LUMO, 2.70% H-9 => L+5 49.0% H-12 => L+2, 10.5% H-10 => L+3, 8.07% H- 8 => L+4, 5.77% H-7 => L+7, 4.09% H-5 => L+10, 3.36% HOMO => L+14, 3.12% H-3 => L+13, 2.75%
110	16417	609	0.00	H-2 => L+16, 2.28% H-29 => LUMO 45.0% H-13 => L+2, 18.9% HOMO => L+16, 6.64% H-11 => L+3, 5.31% H-32 => LUMO, 3.74% H-23 => LUMO, 3.65% H-15 => L+1, 2.45% H-9 => L+4,
111	16453	608	0.04	2.12% H-5 => L+5, 2.01% H-16 => L+2 63.8% H-30 => LUMO, 5.92% H-6 => L+4, 5.70% H-32 => L+1, 5.65% H-28 => L+1, 4.54% H-4 =>
112	16526	605	0.00	L+7 66.9% H-32 => LUMO, 10.3% H-30 => L+1, 5.86% H-13 => L+2, 3.75% H-28 => LUMO, 2.65% H-3
113	16545	604	0.61	=> L+6, 2.60% H-28 => L+2 44.9% H-29 => LUMO, 17.8% HOMO => L+14, 6.89% H-1 => L+12, 5.39% H-18 => L+1, 2.90% H- 31 => L+1, 2.45% H-33 => LUMO, 2.30% H-10 =>
114	16617	602	0.00	L+3 53.8% H-2 => L+9, 16.1% H-5 => L+6, 7.11% H-7 => L+5, 4.94% H-30 => LUMO, 3.41% H-2 => L+6, 3.32% H-3 => L+11, 2.81% H-3 => L+5, 2.70% H-3
115	16634	601	0.00	=> L+8

				33.3% HOMO => L+15, 22.5% H-27 => LUMO, 17.0% H-17 => L+1, 8.39% H-31 => LUMO, 2.82%
116	16641	601	0.08	HOMO => L+18, 2.01% H-29 => L+1 43.5% H-7 => L+4, 29.0% H-5 => L+7, 10.5% H-3 => L+10, 5.00% H-2 => L+13
117	16687	599	0.00	68.3% H-2 => L+10, 17.8% H-3 => L+7, 3.78% H-2 => L+4, 3.51% H-3 => L+13
118	16707	599	0.00	22.6% H-31 => LUMO, 15.9% H-27 => LUMO, 13.8% HOMO => L+18, 11.9% HOMO => L+15, 8.67% H-14 => L+2, 4.86% H-34 => LUMO, 2.83%
119	16736	598	0.00	H-12 => L+3 25.1% H-34 => LUMO, 14.3% H-31 => LUMO, 11.5% HOMO => L+18, 9.79% H-14 => L+2, 6.84% H-17 => L+1, 5.14% H-6 => L+5, 3.21% H-12 =>
120	16783	596	0.01	L+3, 2.24% H-4 => L+9 50.9% H-33 => LUMO, 17.7% H-1 => L+12, 12.9% H-29 => LUMO, 2.17% H-4 => L+8, 2.07% HOMO
121	16806	595	0.00	=> L+11 33.3% H-3 => L+8, 20.1% H-5 => L+6, 16.3% H-19 => L+1, 4.35% H-2 => L+9, 4.32% H-7 => L+5, 4.14% H-2 => L+6, 3.51% H-20 => LUMO, 3.10% H-5 => L+9, 2.83% H-20 => L+2, 2.76% H-3 =>
122	16862	593	0.00	L+5 59.0% H-20 => L+1, 12.2% H-19 => LUMO, 10.1% H-19 => L+2
123	16884	592	0.01	45.8% H-19 => L+1, 11.0% H-5 => L+6, 8.93% H- 20 => LUMO, 8.24% H-3 => L+8, 7.58% H-20 =>
124	16886	592	0.00	L+2 28.2% H-31 => LUMO, 22.3% H-34 => LUMO, 11.1% H-6 => L+5, 7.18% H-37 => LUMO, 4.16% H-36 => LUMO, 3.03% H-1 => L+11, 2.52% H-33 => L+1, 2.15% H-1 => L+14
125	16928	591	0.00	82.8% H-35 => LUMO, 3.03% H-6 => L+6, 2.80% H-1 => L+9, 2.23% H-34 => L+1
126	16954	590	0.00	38.5% H-3 => L+9, 20.7% H-2 => L+11, 17.6% H-5 => L+8, 4.42% H-23 => LUMO, 3.07% H-22 =>
127	17024	587	0.27	LUMO, 2.59% H-7 => L+6 21.8% HOMO => L+17, 20.4% H-18 => L+1, 14.4% H-10 => L+3, 5.60% H-1 => L+12, 5.28% H-33 => LUMO, 4.27% H-2 => L+16, 3.20% H-3 => L+13, 3.00% H-5 => L+10, 2.39% H-12 => L+4, 2.39% H- 7 => L+7
128	17043	587	0.00	19.4% H-13 => L+2, 15.5% HOMO => L+16, 13.4% H-11 => L+3, 9.81% H-9 => L+4, 8.57% H-6 => L+7, 7.96% H-4 => L+10, 6.93% H-1 => L+13, 3.77% H-20 => L+1
129	17051	586	0.00	20.3% H-1 => L+12, 19.3% H-10 => L+3, 12.0% H- 36 => LUMO, 7.97% H-33 => LUMO, 6.97% H-37 => LUMO, 4.41% H-29 => LUMO, 4.08% H-4 =>
130	17126	584	0.00	L+11, 3.09% H-8 => L+4, 2.61% H-7 => L+7

				23.7% H-4 => L+9, 17.0% H-37 => LUMO, 11.4% H-1 => L+11, 10.1% H-6 => L+5, 9.87% H-36 => LUMO, 4.41% H-4 => L+6, 3.33% H-9 => L+6, 3.03% H-1 => L+8, 2.85% H-34 => LUMO, 2.69% H-36 => L+1, 2.64% H-6 => L+8
131	17134	584	0.00	27.1% H-10 => L+3, 25.8% HOMO => L+17, 12.1% H-18 => L+1, 5.36% H-29 => LUMO, 4.89% H-36 => LUMO, 3.33% H-8 => L+4, 2.84% H-37 => LUMO, 2.67% H-1 => L+12, 2.13% H-7 => L+7
132	17157	583	0.00	67.5% H-15 => L+2, 4.57% H-13 => L+3, 3.69% H-26 => LUMO, 3.20% H-16 => L+3, 2.18% H-22 => L+1, 2.12% H-13 => L+1
133	17232	580	0.00	50.0% H-6 => L+5, 30.1% H-34 => LUMO, 4.05%
134	17249	580	0.00	H-1 => L+11, 3.59% H-4 => L+6
				32.3% H-36 => LUMO, 18.7% H-37 => LUMO,
				12.4% H-33 => LUMO, 10.1% H-1 => L+12, 7.30%
				H-4 => L+8, 4.00% H-37 => L+1, 2.84% H-29 =>
135	17319	577	0.00	LUMO, 2.32% H-36 => L+1
136	17330	577	0.07	61.6% H-16 => L+2, 4.75% H-1 => L+13, 4.09% H-15 => L+3, 3.30% H-5 => L+8
				32.8% H-2 => L+11, 25.0% H-5 => L+8, 11.1% H-7 => L+6, 7.55% H-16 => L+2, 4.62% H-8 => L+5,
137	17372	576	0.36	3.76% H-3 => L+6
				28.3% H-14 => L+2, 12.2% H-37 => LUMO, 11.2%
				H-4 => L+9, 9.25% HOMO => L+18, 7.06% H-36 => LUMO, 6.54% H-1 => L+14, 2.36% H-4 =>
138	17381	575	0.16	L+12, 2.16% HOMO => L+15
				25.9% H-14 => L+2, 15.5% HOMO => L+18, 12.8%
				H-37 => LUMO, 10.4% H-4 => L+9, 7.45% H-36 => LUMO, 4.15% H-5 => L+7, 2.79% H-3 => L+10,
139	17395	575	0.19	2.77% H-31 => LUMO
				46.0% H-11 => L+3, 21.0% H-1 => L+13, 5.84% H-4 => L+10, 4.34% HOMO => L+16, 3.90% H-5 =>
140	17426	574	0.06	L+8, 3.68% H-16 => L+2
				31.7% H-3 => L+10, 30.2% H-5 => L+7, 10.1% H-2 => L+13, 4.06% H-4 => L+9, 3.75% H-37 =>
				LUMO, 2.17% H-36 => LUMO, 2.09% H-3 => L+4,
141	17450	573	0.00	2.09% H-6 => L+5
				69.6% H-7 => L+5, 15.3% H-5 => L+6, 4.71% H-3 => L+5, 4.32% H-8 => L+6
142	17480	572	0.00	61.0% H-6 => L+6, 10.1% H-4 => L+8, 8.28% H-9 => L+5, 4.03% H-33 => LUMO, 3.65% H-35 =>
				LUMO, 3.13% H-4 => L+5, 2.03% H-1 => L+12
143	17609	568	0.00	38.6% H-3 => L+9, 24.3% H-2 => L+11, 9.09% H-5 => L+8, 7.21% H-2 => L+8, 4.01% H-9 => L+4,
				2.43% H-1 => L+13, 2.24% H-3 => L+12, 2.04% H-21 => L+1
144	17611	568	0.17	40.9% H-1 => L+14, 8.14% H-4 => L+9, 6.10% HOMO => L+15, 5.87% H-4 => L+12, 4.50% H-14 => L+2, 4.06% H-31 => LUMO, 3.86% H-6 =>
145	17722	564	0.07	L+11, 3.43% H-18 => L+2, 3.27% H-24 => L+1,

				2.91% H-27 => LUMO, 2.74% H-3 => L+10, 2.10% H-1 => L+17 60.5% H-8 => L+4, 6.43% H-5 => L+10, 6.04% H-3 => L+13, 5.66% H-2 => L+16, 5.20% H-7 => L+7, 3.52% HOMO => L+17, 2.91% H-10 => L+7, 2.42% H-7 => L+3 29.8% H-1 => L+13, 22.0% H-9 => L+4, 11.6% H-11 => L+3, 9.79% H-6 => L+7, 9.39% H-21 => L+1, 2.69% H-3 => L+9, 2.21% H-7 => L+6 61.5% H-21 => L+1, 6.80% H-23 => LUMO, 3.88% H-6 => L+7, 3.02% H-5 => L+8, 2.85% H-2 => L+11, 2.75% H-11 => L+3, 2.71% H-9 => L+4, 2.59% H-23 => L+2 18.5% H-23 => L+1, 13.8% H-3 => L+11, 11.9% H-22 => L+1, 7.91% H-2 => L+12, 7.09% H-5 => L+9, 6.36% H-26 => LUMO, 4.47% H-21 => LUMO, 4.06% H-13 => L+3, 2.16% H-15 => L+2 25.5% H-22 => L+1, 10.1% H-15 => L+2, 9.09% H-1 => L+16, 4.96% H-2 => L+18, 4.24% H-4 => L+13, 3.85% H-11 => L+4, 3.77% H-9 => L+7, 3.76% H-6 => L+10, 3.39% H-3 => L+17, 3.36% H-26 => LUMO, 3.05% H-3 => L+11, 2.90% H-5 => L+9, 2.87% H-13 => L+3, 2.23% H-19 => L+1, 2.20% H-25 => LUMO 42.9% H-7 => L+6, 10.7% H-5 => L+8, 7.29% H-8 => L+5, 6.03% H-9 => L+4, 5.29% H-6 => L+7, 4.63% H-5 => L+5, 4.23% H-4 => L+10, 3.58% H-1 => L+13, 2.53% H-2 => L+11, 2.08% H-3 => L+6 45.2% H-17 => L+2, 13.1% H-1 => L+15, 8.82% HOMO => L+17, 5.54% H-18 => L+1, 4.02% H-14 => L+3, 2.95% H-4 => L+14, 2.93% H-7 => L+7 34.5% H-22 => L+1, 18.7% H-2 => L+12, 16.7% H-3 => L+11, 3.92% H-13 => L+3, 2.57% H-25 => LUMO, 2.44% H-5 => L+9 33.7% H-4 => L+10, 29.4% H-9 => L+4, 8.86% H-7 => L+6, 7.60% H-5 => L+8, 7.37% H-1 => L+13, 2.49% H-6 => L+7 53.2% H-12 => L+3, 15.2% H-24 => L+1, 12.8% HOMO => L+18, 3.50% H-10 => L+4, 2.75% H-14 => L+2, 2.10% H-10 => L+2 44.0% H-4 => L+11, 17.3% H-1 => L+12, 8.86% H-6 => L+9, 4.50% H-17 => L+2, 4.03% H-9 => L+8, 2.83% H-4 => L+14, 2.49% H-1 => L+15 54.6% H-24 => L+1, 8.36% H-12 => L+3, 6.68% H-1 => L+17, 6.58% H-1 => L+14, 4.10% HOMO => L+18, 3.84% H-18 => L+2, 2.12% H-29 => L+1 52.6% H-6 => L+7, 28.9% H-4 => L+10, 8.00% H-9 => L+4 21.9% H-2 => L+12, 17.3% H-5 => L+9, 15.1% H-7 => L+8, 9.52% H-23 => L+1, 8.62% H-22 => L+1, 5.73% H-8 => L+6, 2.30% H-10 => L+5
146	17722	564	0.00	
147	17754	563	0.00	
148	17777	563	0.01	
149	17796	562	0.00	
150	17860	560	0.00	
151	17914	558	0.03	
152	17919	558	0.00	
153	17943	557	0.00	
154	18010	555	0.00	
155	18043	554	0.44	
156	18054	554	0.00	
157	18124	552	0.03	
158	18151	551	0.00	
159	18169	550	0.00	

				43.4% H-6 => L+8, 13.9% H-4 => L+9, 12.5% H-2 => L+13, 7.66% H-9 => L+6, 4.56% H-3 => L+10, 3.49% H-11 => L+5, 2.14% H-4 => L+6
160	18207	549	0.00	43.6% H-2 => L+13, 21.2% H-3 => L+10, 14.5% H-6 => L+8, 4.42% H-3 => L+16, 3.59% H-2 => L+7, 2.59% H-4 => L+9
161	18301	546	0.01	30.1% H-23 => L+1, 16.1% H-5 => L+9, 14.4% H-1 => L+16, 7.63% H-3 => L+11, 3.79% H-4 => L+13, 2.70% H-2 => L+12, 2.23% H-2 => L+15, 2.14% H-7 => L+8, 2.06% H-2 => L+18
162	18306	546	0.00	39.1% H-7 => L+7, 10.4% H-17 => L+2, 7.55% H-27 => L+1, 7.35% H-1 => L+15, 6.01% H-2 => L+16, 5.44% H-3 => L+13, 4.18% H-4 => L+11, 2.53% H-8 => L+10, 2.51% H-5 => L+10
163	18320	546	0.00	67.8% H-25 => L+1, 6.83% H-28 => LUMO, 4.26% H-26 => L+1, 2.94% H-22 => L+2, 2.34% H-22 => LUMO, 2.08% H-28 => L+2
164	18338	545	0.02	20.5% H-7 => L+7, 19.7% H-27 => L+1, 16.7% H-1 => L+15, 8.80% H-1 => L+18, 6.76% H-17 => L+2, 5.57% H-5 => L+10, 3.35% H-3 => L+13, 3.14% H-2 => L+16, 2.32% H-24 => L+2
165	18425	543	0.00	35.9% H-3 => L+11, 23.9% H-2 => L+12, 14.5% H-5 => L+9, 6.65% H-2 => L+9, 2.90% H-13 => L+3, 2.49% H-5 => L+12, 2.15% H-23 => L+1, 2.14% H-3 => L+14, 2.02% H-7 => L+8
166	18477	541	0.00	50.0% H-26 => L+1, 5.76% H-16 => L+2, 4.97% H-21 => L+1, 4.49% H-15 => L+3, 3.79% H-25 => L+1, 3.14% H-23 => LUMO, 2.45% H-13 => L+4, 2.41% H-23 => L+2, 2.21% H-3 => L+18, 2.04% H-20 => L+1, 2.02% H-19 => L+2
167	18504	540	0.00	83.8% H-38 => LUMO, 6.53% H-39 => L+1
168	18522	540	0.00	21.2% H-10 => L+4, 16.1% H-12 => L+3, 15.0% H-18 => L+2, 13.7% H-1 => L+17, 7.52% H-8 => L+7, 4.71% H-24 => L+1, 3.07% H-7 => L+10, 2.34%
169	18529	540	0.01	HOMO => L+18, 2.31% H-4 => L+15 34.6% H-13 => L+3, 23.0% H-1 => L+16, 6.57% H-23 => L+1, 3.98% H-5 => L+9, 3.63% H-11 => L+4, 2.73% H-28 => L+1, 2.54% H-4 => L+13, 2.51% H-2 => L+12, 2.38% H-3 => L+11, 2.16% H-15 => L+2
170	18565	539	0.00	44.0% H-18 => L+2, 12.0% H-1 => L+14, 6.62% H-24 => L+1, 5.97% H-10 => L+4, 5.40% H-4 => L+12, 3.41% HOMO => L+18, 2.28% H-17 => L+3, 2.17% H-12 => L+3, 2.07% H-6 => L+11
171	18594	538	0.03	26.4% H-2 => L+14, 19.9% H-3 => L+12, 9.22% H-8 => L+5, 8.23% H-20 => L+1, 5.73% H-19 => L+2, 5.03% H-5 => L+11, 2.54% H-7 => L+6
172	18610	537	0.01	46.4% H-27 => L+1, 11.8% H-1 => L+18, 10.2% H-1 => L+15, 7.26% H-4 => L+11, 5.59% H-31 => L+1, 3.83% H-17 => L+2, 2.43% H-24 => L+2
173	18626	537	0.00	

				24.0% H-28 => L+1, 19.4% H-7 => L+8, 14.4% H-13 => L+3, 9.30% H-5 => L+9, 2.72% H-30 => LUMO, 2.11% H-23 => L+1
174	18641	536	0.00	75.7% H-39 => LUMO, 9.03% H-38 => L+1, 4.25% H-40 => L+1
175	18661	536	0.00	35.5% H-28 => L+1, 22.6% H-7 => L+8, 11.7% H-5 => L+9, 4.39% H-8 => L+6, 3.76% H-30 => LUMO, 2.27% H-25 => L+2
176	18666	536	0.00	59.2% H-8 => L+5, 9.54% H-7 => L+6, 5.55% H-3 => L+12, 4.51% H-10 => L+6, 2.89% H-5 => L+11, 2.47% H-5 => L+5
177	18714	534	0.00	56.6% H-9 => L+5, 10.1% H-6 => L+6, 5.86% H-5 => L+10, 4.22% H-11 => L+6, 3.92% H-1 => L+18
178	18758	533	0.00	24.6% H-1 => L+18, 13.4% H-9 => L+5, 13.3% H-14 => L+3, 10.1% H-5 => L+10, 6.19% H-17 => L+2, 3.85% H-12 => L+4, 3.41% H-4 => L+17,
179	18802	532	0.00	2.61% HOMO => L+17, 2.05% H-4 => L+11 24.8% H-20 => L+2, 10.9% H-19 => L+1, 6.75% H-28 => L+1, 5.48% H-19 => L+3, 4.88% H-40 => LUMO, 4.83% H-7 => L+8, 4.19% H-13 => L+3, 3.89% H-2 => L+15, 3.44% H-3 => L+14, 2.08% H-5 => L+12, 2.08% H-16 => L+3
180	18826	531	0.00	31.6% H-29 => L+1, 17.0% H-4 => L+12, 11.5% H-1 => L+14, 11.0% H-10 => L+4, 3.89% H-6 => L+11, 2.75% H-18 => L+2, 2.49% H-27 => LUMO
181	18833	531	0.07	18.6% H-19 => L+2, 16.0% H-2 => L+14, 9.54% H-26 => L+1, 5.98% H-20 => L+1, 5.63% H-7 => L+9, 5.10% H-30 => L+1, 4.09% H-2 => L+17, 3.58% H-8 => L+8, 3.00% H-10 => L+6, 2.96% H-25 => L+1, 2.93% H-20 => L+3, 2.59% H-3 => L+12
182	18890	529	0.11	37.3% H-29 => L+1, 16.9% H-10 => L+4, 11.4% H-33 => L+1, 9.19% H-4 => L+12, 4.62% H-1 => L+17, 2.41% H-27 => L+2, 2.14% H-18 => L+2
183	18891	529	0.14	71.0% H-40 => LUMO, 8.85% H-39 => L+1, 3.72% H-41 => L+1, 2.77% H-38 => L+2, 2.19% H-42 => LUMO
184	18895	529	0.00	24.5% H-6 => L+9, 23.1% H-31 => L+1, 14.3% H-4 => L+11, 7.00% H-34 => L+1, 5.40% H-9 => L+8, 4.89% H-5 => L+10, 3.22% H-11 => L+6
185	18948	528	0.00	56.3% H-30 => L+1, 9.51% H-32 => LUMO, 7.63% H-19 => L+2, 4.62% H-32 => L+2, 4.05% H-28 => LUMO, 3.75% H-28 => L+2, 2.06% H-15 => L+3, 2.01% H-2 => L+14
186	18981	527	0.25	34.3% H-15 => L+3, 17.0% H-19 => L+2, 5.99% H-26 => L+1, 5.38% H-30 => L+1, 4.20% H-5 => L+11, 2.93% H-13 => L+4, 2.47% H-16 => L+4, 2.17% H-20 => L+3, 2.17% H-7 => L+9, 2.07% H-16 => L+2
187	19025	526	0.00	37.9% H-32 => L+1, 8.16% H-8 => L+6, 7.88% H-1 => L+16, 5.55% H-9 => L+7, 5.47% H-20 => L+2, 5.39% H-11 => L+4, 4.55% H-30 => LUMO, 3.02%
188	19027	526	0.00	

				H-13 => L+3, 2.85% H-30 => L+2, 2.84% H-28 => L+1 27.3% H-5 => L+10, 17.5% H-14 => L+3, 14.0% H-2 => L+16, 9.13% H-3 => L+13, 6.86% H-6 => L+9, 4.10% H-17 => L+2, 2.19% H-31 => L+1, 2.07% H-4 => L+11, 2.05% H-12 => L+4 25.2% H-16 => L+3, 23.2% H-20 => L+2, 11.9% H-2 => L+15, 4.37% H-3 => L+14, 3.41% H-4 => L+13, 2.60% H-15 => L+4, 2.54% H-19 => L+3, 2.16% H-19 => L+1
189	19034	525	0.00	25.2% H-16 => L+3, 23.2% H-20 => L+2, 11.9% H-2 => L+15, 4.37% H-3 => L+14, 3.41% H-4 => L+13, 2.60% H-15 => L+4, 2.54% H-19 => L+3, 2.16% H-19 => L+1
190	19081	524	0.00	35.7% H-33 => L+1, 20.2% H-9 => L+6, 10.3% H-6 => L+8, 6.86% H-35 => L+1, 5.43% H-11 => L+5, 2.56% H-31 => LUMO, 2.24% H-31 => L+2, 2.06% H-29 => L+1
191	19118	523	0.00	38.5% H-31 => L+1, 13.3% H-6 => L+9, 11.4% H-34 => L+1, 6.37% H-5 => L+10, 3.46% H-3 => L+13, 2.99% H-27 => L+1, 2.81% H-29 => L+2, 2.69% H-4 => L+11
192	19119	523	0.00	37.3% H-32 => L+1, 11.7% H-1 => L+16, 9.39% H-11 => L+4, 7.22% H-8 => L+6, 5.04% H-13 => L+3, 4.94% H-30 => LUMO, 4.70% H-30 => L+2, 2.40% H-6 => L+10
193	19119	523	0.00	27.1% H-5 => L+11, 8.32% H-7 => L+9, 7.71% H-41 => LUMO, 7.45% H-15 => L+3, 7.36% H-26 => L+1, 6.22% H-2 => L+14, 6.16% H-3 => L+12, 5.36% H-19 => L+2, 2.73% H-8 => L+5, 2.20% H-3 => L+15
194	19136	523	0.10	47.1% H-35 => L+1, 8.38% H-8 => L+7, 7.55% H-9 => L+6, 6.82% H-10 => L+4, 6.04% H-4 => L+12, 2.49% H-1 => L+17, 2.17% H-34 => L+2
195	19144	522	0.00	65.5% H-41 => LUMO, 9.40% H-40 => L+1, 3.38% H-5 => L+11, 3.20% H-43 => LUMO, 2.88% H-39 => L+2, 2.69% H-42 => L+1
196	19154	522	0.01	37.3% H-8 => L+6, 10.2% H-7 => L+8, 8.03% H-1 => L+16, 7.45% H-16 => L+3, 5.46% H-10 => L+5, 4.62% H-13 => L+3, 3.16% H-7 => L+5, 2.46% H-20 => L+2
197	19164	522	0.00	21.6% H-1 => L+15, 20.8% H-14 => L+3, 12.2% H-1 => L+18, 12.1% H-34 => L+1, 6.28% H-4 => L+14, 4.12% H-4 => L+17, 2.65% H-5 => L+10, 2.40% H-6 => L+12
198	19172	522	0.00	17.7% H-10 => L+4, 12.5% H-35 => L+1, 10.1% H-9 => L+6, 9.63% H-8 => L+7, 8.87% H-33 => L+1, 7.85% H-4 => L+12, 5.69% H-7 => L+10, 5.50% H-1 => L+17, 3.46% H-18 => L+2, 2.93% H-6 => L+8, 2.17% H-5 => L+13, 2.07% H-11 => L+5
199	19175	522	0.01	48.3% H-34 => L+1, 8.74% H-31 => L+1, 5.89% H-37 => L+1, 4.07% H-1 => L+18, 3.92% H-1 => L+15, 3.55% H-33 => L+2, 3.41% H-36 => L+1, 3.38% H-14 => L+3, 2.09% H-9 => L+5, 2.03% H-33 => LUMO, 2.00% H-35 => L+2
200	19299	518	0.00	

201	19304	518	0.03	41.3% H-3 => L+12, 19.8% H-2 => L+14, 9.77% H-5 => L+11, 6.79% H-7 => L+9, 6.57% H-2 => L+11, 3.33% H-5 => L+14
202	19343	517	0.10	20.0% H-33 => L+1, 18.9% H-35 => L+1, 16.9% H-9 => L+6, 6.31% H-1 => L+17, 5.75% H-4 => L+12, 4.39% H-29 => L+1, 2.93% H-34 => L+2, 2.81% H-11 => L+5, 2.80% H-6 => L+8, 2.68% H-18 => L+2
203	19412	515	0.00	46.7% H-11 => L+4, 19.7% H-4 => L+13, 7.45% H-1 => L+16, 6.68% H-6 => L+10, 5.65% H-16 => L+3
204	19440	514	0.00	70.5% H-42 => LUMO, 10.9% H-41 => L+1, 4.93% H-44 => LUMO, 3.48% H-40 => L+2, 2.35% H-43 => L+1
205	19446	514	0.72	33.2% H-8 => L+7, 25.6% H-1 => L+17, 5.25% H-36 => L+1, 3.08% H-4 => L+12, 3.04% H-37 => L+1, 2.84% H-18 => L+2, 2.25% H-4 => L+18
206	19461	514	0.37	33.1% H-7 => L+9, 29.0% H-5 => L+11, 8.71% H-8 => L+8, 3.62% H-3 => L+12, 3.46% H-3 => L+9, 3.09% H-7 => L+12, 2.53% H-5 => L+8, 2.20% H-2 => L+14
207	19507	513	0.00	25.3% H-3 => L+13, 11.2% H-14 => L+3, 10.2% H-2 => L+16, 5.63% H-5 => L+16, 5.57% H-37 => L+1, 4.81% H-4 => L+14, 4.69% H-6 => L+9, 4.13% H-2 => L+10, 3.23% H-36 => L+1, 2.50% H-12 => L+4, 2.05% H-9 => L+11
208	19521	512	0.00	33.0% H-16 => L+3, 22.7% H-2 => L+15, 9.46% H-3 => L+14, 3.69% H-10 => L+8, 3.37% H-11 => L+4, 3.16% H-8 => L+6, 2.08% H-8 => L+9
209	19600	510	0.08	33.3% H-36 => L+1, 19.2% H-37 => L+1, 5.85% H-37 => LUMO, 5.42% H-33 => L+1, 5.24% H-1 => L+17, 4.28% H-37 => L+2, 3.40% H-36 => LUMO, 2.92% H-35 => L+1, 2.49% H-36 => L+2, 2.42% H-8 => L+7, 2.17% H-4 => L+12
210	19606	510	0.04	18.8% H-15 => L+3, 15.1% H-2 => L+17, 7.25% H-22 => L+2, 6.76% H-4 => L+16, 5.28% H-3 => L+15, 5.02% H-19 => L+2, 4.14% H-3 => L+18, 3.74% H-6 => L+13, 2.91% H-9 => L+10, 2.69% H-26 => L+1, 2.61% H-7 => L+9, 2.05% H-16 => L+4
211	19615	510	0.00	33.2% H-37 => L+1, 19.2% H-36 => L+1, 5.45% H-36 => LUMO, 5.19% H-3 => L+13, 4.70% H-2 => L+16, 4.36% H-34 => L+1, 4.14% H-36 => L+2, 3.16% H-37 => LUMO, 2.86% H-31 => L+1, 2.55% H-4 => L+14, 2.41% H-37 => L+2
212	19677	508	0.00	37.4% H-4 => L+13, 29.8% H-9 => L+7, 5.71% H-21 => L+2, 5.71% H-11 => L+4, 4.88% H-6 => L+10, 3.22% H-3 => L+14
213	19729	507	0.01	66.8% H-43 => LUMO, 10.8% H-42 => L+1, 7.06% H-45 => LUMO, 3.43% H-41 => L+2
214	19732	507	0.00	40.8% H-21 => L+2, 9.42% H-5 => L+12, 6.16% H-7 => L+11, 4.04% H-16 => L+3, 3.92% H-10 => L+5, 3.67% H-23 => L+1, 3.55% H-8 => L+6.

				2.70% H-8 => L+9, 2.45% H-20 => L+2, 2.40% H-2 => L+15
215	19740	507	0.06	20.9% H-7 => L+10, 18.9% H-8 => L+7, 10.3% H-5 => L+13, 9.01% H-4 => L+12, 5.61% H-3 => L+16, 5.46% H-6 => L+11, 3.04% H-9 => L+9, 2.45% H-2 => L+13, 2.35% H-10 => L+10
216	19744	506	0.00	20.5% H-2 => L+16, 19.7% H-12 => L+4, 14.4% H-14 => L+3, 13.0% H-4 => L+14, 9.04% H-3 => L+13, 4.66% H-10 => L+7, 2.49% H-1 => L+15
217	19787	505	0.12	31.8% H-8 => L+8, 23.3% H-7 => L+9, 12.5% H-22 => L+2, 8.14% H-10 => L+6, 3.16% H-8 => L+11, 3.05% H-12 => L+5, 2.44% H-5 => L+8, 2.15% H-7 => L+6
218	19798	505	0.00	19.2% H-9 => L+7, 17.5% H-3 => L+14, 15.4% H-21 => L+2, 9.60% H-5 => L+12, 6.53% H-2 => L+15, 3.73% H-2 => L+12, 3.48% H-6 => L+10, 3.07% H-10 => L+5, 2.08% H-7 => L+11
219	19801	505	0.08	20.1% H-7 => L+10, 19.7% H-6 => L+11, 13.4% H-4 => L+12, 6.85% H-17 => L+3, 5.88% H-9 => L+9, 3.94% H-8 => L+7, 3.40% H-5 => L+13, 3.10% H-11 => L+8, 2.78% H-36 => L+1
220	19843	504	0.00	40.5% H-9 => L+8, 22.4% H-6 => L+9, 9.65% H-11 => L+6, 5.40% H-13 => L+5, 2.69% H-3 => L+13, 2.64% H-6 => L+6, 2.39% H-2 => L+16
221	19887	503	0.00	54.2% H-6 => L+10, 14.9% H-9 => L+7, 8.16% H-4 => L+13, 5.47% H-21 => L+2, 4.17% H-3 => L+14
222	19950	501	0.00	48.8% H-10 => L+5, 7.96% H-5 => L+12, 7.10% H-8 => L+6, 6.95% H-2 => L+18, 5.21% H-7 => L+11, 4.69% H-12 => L+6
223	19985	500	0.01	49.4% H-22 => L+2, 18.5% H-8 => L+8, 4.29% H-15 => L+3, 2.47% H-25 => L+1, 2.25% H-2 => L+14, 2.09% H-4 => L+16
224	19986	500	0.00	62.9% H-44 => LUMO, 13.6% H-46 => LUMO, 10.1% H-43 => L+1, 3.21% H-42 => L+2, 3.11% H-47 => L+1
225	19990	500	0.01	54.2% H-17 => L+3, 7.01% H-6 => L+11, 5.60% H-4 => L+15, 4.61% H-1 => L+17, 2.97% H-14 => L+4, 2.91% H-18 => L+2, 2.38% H-18 => L+4,
226	20053	499	0.01	2.22% H-6 => L+17, 2.00% H-14 => L+2
227	20096	498	0.01	33.7% H-12 => L+4, 31.3% H-4 => L+14, 9.47% H-24 => L+2, 7.38% H-1 => L+18
228	20121	497	0.00	22.7% H-2 => L+17, 15.2% H-13 => L+4, 11.0% H-23 => L+2, 4.97% H-8 => L+8, 4.64% H-3 => L+15, 4.14% H-15 => L+3, 3.94% H-11 => L+7, 2.47% H-9 => L+10
				21.2% H-3 => L+14, 19.3% H-2 => L+15, 16.6% H-10 => L+5, 5.90% H-21 => L+2, 5.45% H-2 => L+18, 5.23% H-5 => L+12, 4.24% H-7 => L+11, 2.98% H-3 => L+17, 2.49% H-2 => L+12

				24.2% H-2 => L+18, 18.5% H-5 => L+12, 12.1% H-3 => L+14, 3.06% H-2 => L+15, 2.89% H-25 => L+2, 2.71% H-7 => L+14, 2.55% H-3 => L+17
229	20161	496	0.00	44.0% H-24 => L+2, 10.7% H-18 => L+3, 9.91% H-12 => L+4, 6.33% H-4 => L+17, 3.03% H-27 => L+1, 2.95% H-1 => L+18, 2.93% H-9 => L+8
230	20181	496	0.00	36.6% H-11 => L+5, 17.9% H-5 => L+13, 12.7% H-7 => L+10, 9.53% H-9 => L+6, 3.86% H-13 => L+6, 3.77% H-3 => L+16, 2.08% H-3 => L+10, 2.03% H-6 => L+5
231	20183	495	0.01	46.2% H-45 => LUMO, 36.4% H-47 => LUMO,
232	20208	495	0.00	7.04% H-44 => L+1, 2.22% H-43 => L+2
233	20249	494	0.00	25.2% H-11 => L+5, 17.1% H-7 => L+10, 15.9% H-5 => L+13, 12.1% H-3 => L+16, 6.13% H-6 => L+11, 6.02% H-9 => L+6, 2.16% H-2 => L+13
234	20264	493	0.01	15.4% H-23 => L+2, 11.9% H-5 => L+14, 8.12% H-3 => L+15, 7.41% H-3 => L+18, 7.14% HOMO => L+20, 7.01% H-7 => L+12, 5.76% H-2 => L+17, 3.72% H-8 => L+8, 3.34% H-10 => L+6, 3.27% H-8 => L+11, 2.67% H-10 => L+9, 2.35% H-26 => L+1, 2.20% H-19 => L+2, 2.11% H-21 => L+3, 2.08% H-2 => L+14
235	20305	492	0.00	23.5% H-5 => L+12, 22.0% H-7 => L+11, 9.95% H-25 => L+2, 8.75% H-8 => L+9, 3.29% HOMO => L+19, 3.17% H-10 => L+8, 2.72% H-15 => L+4, 2.50% H-16 => L+3, 2.26% H-22 => L+3
236	20336	492	0.01	28.6% H-23 => L+2, 22.6% H-3 => L+15, 9.94% H-4 => L+16, 4.71% H-2 => L+14, 3.95% H-5 => L+14, 3.45% H-3 => L+18, 2.36% H-6 => L+13
237	20415	490	0.00	59.0% H-25 => L+2, 5.77% H-28 => L+1, 5.42% H-7 => L+11, 3.43% H-22 => L+3, 3.29% H-2 => L+18, 2.92% H-26 => L+2
238	20416	490	0.00	47.4% H-10 => L+6, 9.60% H-8 => L+8, 6.92% H-12 => L+5, 5.69% HOMO => L+20, 4.30% H-2 => L+17, 3.96% H-8 => L+5, 3.69% H-12 => L+8
239	20441	489	0.00	21.4% H-24 => L+2, 13.4% H-4 => L+14, 8.97% H-18 => L+3, 7.83% H-6 => L+12, 4.94% H-10 => L+7, 4.37% H-4 => L+17, 3.92% H-9 => L+11, 3.81% H-11 => L+9, 3.49% H-6 => L+15, 3.24% H-16 => L+5, 3.11% H-12 => L+4, 2.12% H-2 => L+16
240	20444	489	0.56	31.2% H-27 => L+2, 30.2% H-4 => L+15, 6.13% H-17 => L+3, 4.30% H-6 => L+11, 2.52% H-24 => L+3, 2.43% H-29 => L+1, 2.11% H-24 => L+1
241	20471	488	0.00	26.6% H-10 => L+7, 17.2% H-18 => L+3, 10.2% H-12 => L+4, 8.54% H-4 => L+17, 6.10% H-8 => L+10, 5.75% H-24 => L+2, 3.04% H-1 => L+18, 2.56% H-4 => L+14, 2.43% H-7 => L+13, 2.02% H-2 => L+16
242	20498	488	0.00	23.6% H-26 => L+2, 15.5% H-7 => L+11, 6.46% H-3 => L+17, 4.63% HOMO => L+19, 3.62% H-2 =>

				L+15, 3.30% H-2 => L+18, 3.23% H-15 => L+4, 2.70% H-5 => L+18, 2.48% H-23 => L+1, 2.07% H- 10 => L+8
243	20541	487	0.00	45.7% H-13 => L+4, 15.4% H-4 => L+16, 10.6% H- 23 => L+2, 3.80% H-2 => L+17, 3.67% HOMO => L+20, 2.63% H-6 => L+13
244	20549	487	0.00	27.0% H-6 => L+11, 13.7% H-5 => L+13, 13.1% H- 9 => L+9, 7.28% H-11 => L+8, 7.26% H-13 => L+6, 7.12% H-15 => L+5, 4.69% H-3 => L+16, 2.22% H- 27 => L+2, 2.01% H-16 => L+6
245	20556	486	0.00	56.9% H-46 => LUMO, 9.87% H-45 => L+1, 8.92% H-47 => L+1, 8.58% H-44 => LUMO, 3.96% H-46 => L+2, 2.58% H-44 => L+2
246	20559	486	0.00	39.4% H-47 => LUMO, 22.7% H-45 => LUMO, 15.9% H-46 => L+1, 4.07% H-45 => L+2, 3.83% H- 43 => LUMO, 3.32% H-44 => L+1
247	20611	485	0.00	22.3% H-11 => L+6, 14.3% H-9 => L+8, 13.0% H- 18 => L+3, 12.3% H-13 => L+5, 10.7% H-10 => L+7, 2.56% H-11 => L+9, 2.27% H-16 => L+8
248	20636	485	0.00	19.3% H-18 => L+3, 12.7% H-11 => L+6, 12.3% H- 9 => L+8, 6.00% H-6 => L+12, 5.50% H-10 => L+7, 4.69% H-1 => L+18, 4.43% H-13 => L+5, 4.15% H- 15 => L+6, 3.79% H-4 => L+17, 3.68% H-16 => L+5, 3.35% H-13 => L+8, 2.62% H-4 => L+14,
249	20636	485	0.00	2.18% H-9 => L+11, 2.07% H-6 => L+15 20.4% H-7 => L+11, 20.3% H-8 => L+9, 12.7% H- 26 => L+2, 7.71% HOMO => L+19, 6.35% H-10 => L+8, 3.31% H-2 => L+18, 3.10% H-3 => L+17,
250	20646	484	0.01	2.84% H-2 => L+15, 2.80% H-10 => L+11 31.5% H-3 => L+16, 18.5% H-5 => L+13, 7.33% H- 4 => L+18, 6.72% H-9 => L+9, 4.54% H-6 => L+11, 4.12% H-2 => L+13, 3.78% H-7 => L+16, 2.85% H- 11 => L+8, 2.61% H-1 => L+17, 2.61% H-27 => L+2
251	20653	484	0.28	48.4% H-28 => L+2, 5.25% H-30 => L+1, 4.74% H- 11 => L+7, 3.95% H-25 => L+3, 3.84% H-32 => L+2, 2.96% H-4 => L+16, 2.74% H-3 => L+15, 2.20% H-25 => L+1
252	20711	483	0.00	25.9% HOMO => L+19, 11.5% H-8 => L+9, 7.71% H-26 => L+2, 7.06% H-19 => L+3, 4.16% H-3 => L+17, 4.14% H-5 => L+15, 3.53% H-1 => L+20, 3.06% H-15 => L+4, 2.79% H-20 => L+2
253	20712	483	0.13	30.3% H-27 => L+2, 21.2% H-4 => L+15, 8.61% H- 3 => L+16, 8.00% H-17 => L+3, 6.66% H-14 => L+4, 2.17% H-12 => L+7, 2.02% H-6 => L+17 25.2% H-3 => L+15, 10.6% H-2 => L+17, 7.72% H- 23 => L+2, 7.60% H-28 => L+2, 7.46% H-5 => L+14, 5.37% H-5 => L+17, 4.75% H-7 => L+12, 4.04% HOMO => L+20, 3.53% H-2 => L+14, 2.72%
254	20743	482	0.05	H-8 => L+11, 2.02% H-4 => L+16

				24.9% H-4 => L+16, 14.2% H-20 => L+3, 6.96% HOMO => L+20, 5.75% H-3 => L+18, 4.93% H-5 => L+17, 3.95% H-7 => L+15, 3.49% H-19 => L+2, 3.40% H-10 => L+6, 2.62% H-19 => L+4, 2.30% H-7 => L+12, 2.28% H-22 => L+2, 2.27% H-23 => L+2
255	20856	479	0.08	30.8% H-14 => L+4, 17.5% H-4 => L+15, 9.82% H-4 => L+18, 8.27% H-27 => L+2, 7.85% H-3 => L+16, 4.38% H-12 => L+7, 3.11% H-17 => L+3
256	20896	479	0.23	38.6% H-29 => L+2, 15.4% H-4 => L+17, 10.3% H-10 => L+7, 5.57% H-18 => L+3, 2.55% H-31 => L+1, 2.49% H-8 => L+10, 2.26% H-27 => L+3,
257	20899	478	0.00	2.21% H-27 => L+1, 2.02% H-1 => L+18
258	20933	478	0.00	42.5% H-19 => L+3, 10.2% H-26 => L+2, 9.38% H-20 => L+2, 7.46% H-15 => L+4, 6.66% H-20 => L+4, 3.92% HOMO => L+19, 2.86% H-3 => L+17, 2.21% H-21 => L+2
259	20937	478	0.00	27.5% HOMO => L+20, 25.7% H-5 => L+14, 14.8% H-20 => L+3, 3.81% H-19 => L+2, 2.96% H-10 => L+6, 2.62% H-1 => L+19, 2.09% H-19 => L+4, 2.08% H-4 => L+16
260	20956	477	0.00	29.6% H-29 => L+2, 19.7% H-10 => L+7, 17.6% H-8 => L+10, 6.44% H-7 => L+13, 4.01% H-4 => L+17, 3.57% H-33 => L+2, 2.47% H-5 => L+16
261	20969	477	0.00	31.7% H-8 => L+9, 17.5% H-10 => L+8, 10.8% H-3 => L+17, 6.86% H-12 => L+6, 5.19% H-15 => L+4, 3.77% H-14 => L+5, 2.97% H-2 => L+15, 2.54% H-2 => L+18, 2.39% H-7 => L+8
262	21001	476	0.02	23.2% H-20 => L+3, 22.0% H-5 => L+14, 6.56% H-3 => L+18, 5.46% H-19 => L+2, 4.05% H-2 => L+17, 3.91% H-7 => L+15, 3.71% H-11 => L+7, 3.29% H-19 => L+4, 3.14% HOMO => L+20, 3.12% H-8 => L+11, 2.34% H-3 => L+15, 2.32% H-10 => L+9, 2.22% H-23 => L+2
263	21029	476	0.01	15.6% H-9 => L+10, 15.3% H-11 => L+7, 11.0% H-32 => L+2, 9.13% H-4 => L+16, 8.67% H-13 => L+4, 5.31% H-28 => L+2, 5.31% HOMO => L+20, 5.27% H-20 => L+3, 5.15% H-6 => L+13, 3.59% H-16 => L+4
264	21044	475	0.00	18.2% H-15 => L+4, 15.0% HOMO => L+19, 13.4% H-26 => L+2, 13.1% H-19 => L+3, 9.39% H-30 => L+2, 3.65% H-20 => L+2, 2.96% H-13 => L+7, 2.77% H-3 => L+17, 2.76% H-25 => L+2
265	21068	475	0.00	38.6% H-6 => L+12, 25.5% H-16 => L+5, 7.95% H-15 => L+6, 4.44% H-13 => L+8, 2.71% H-33 => L+2, 2.42% H-9 => L+14, 2.12% H-16 => L+8
266	21093	474	0.00	54.6% H-31 => L+2, 5.82% H-14 => L+4, 5.49% H-4 => L+18, 4.54% H-9 => L+9, 3.49% H-29 => L+1, 2.97% H-34 => L+2, 2.95% H-29 => L+3, 2.17% H-15 => L+5

				20.3% H-8 => L+10, 14.4% H-4 => L+17, 9.42% H-6 => L+12, 7.39% H-16 => L+5, 5.77% H-33 => L+2, 5.36% H-7 => L+13, 5.14% H-29 => L+2, 4.80% H-5 => L+16, 2.90% H-15 => L+6, 2.84% H-18 => L+3, 2.15% H-6 => L+18
267	21107	474	0.01	60.1% H-30 => L+2, 7.51% H-15 => L+4, 7.21% H-32 => L+1, 4.52% H-32 => L+3, 3.98% H-28 => L+1, 3.71% H-28 => L+3, 2.66% H-26 => L+2
268	21112	474	0.00	37.8% H-32 => L+2, 12.9% H-12 => L+5, 10.4% H-11 => L+7, 6.48% H-30 => L+3, 5.80% H-28 => L+2, 5.11% H-30 => L+1, 2.43% H-20 => L+3, 2.34% H-10 => L+6
269	21144	473	0.01	41.6% H-9 => L+9, 15.1% H-15 => L+5, 8.59% H-31 => L+2, 7.29% H-13 => L+6, 5.50% H-11 => L+8, 4.89% H-16 => L+6, 2.20% H-11 => L+11, 2.10% H-6 => L+8
270	21155	473	0.03	26.0% H-16 => L+4, 25.8% H-12 => L+5, 13.5% H-32 => L+2, 6.33% H-10 => L+6, 2.33% H-30 => L+1, 2.06% H-14 => L+6, 2.05% H-22 => L+2
271	21159	473	0.00	27.0% H-10 => L+8, 24.0% H-3 => L+17, 13.7% H-2 => L+18, 7.24% H-15 => L+4, 2.77% HOMO => L+19, 2.23% H-2 => L+15
272	21200	472	0.00	25.1% H-38 => L+1, 20.7% H-12 => L+5, 16.5% H-16 => L+4, 5.46% H-11 => L+7, 3.64% H-2 =>
273	21204	472	0.02	L+17, 2.50% H-39 => LUMO, 2.10% H-3 => L+15 51.9% H-38 => L+1, 8.69% H-16 => L+4, 6.97% H-12 => L+5, 4.71% H-39 => LUMO, 3.92% H-11 =>
274	21221	471	0.02	L+7, 3.39% H-39 => L+2, 2.63% H-40 => L+1 62.3% H-33 => L+2, 4.42% H-6 => L+12, 3.42% H-31 => L+1, 3.18% H-4 => L+17, 3.06% H-31 =>
275	21276	470	0.00	L+3, 2.99% H-36 => L+2 43.0% H-7 => L+12, 8.50% H-6 => L+13, 7.65% H-3 => L+18, 5.42% H-32 => L+2, 5.30% H-11 => L+7, 4.26% H-4 => L+16, 3.14% HOMO => L+20,
276	21287	470	0.02	2.55% H-5 => L+11, 2.04% H-2 => L+17 30.6% H-34 => L+2, 24.2% H-4 => L+18, 17.0% H-14 => L+4, 5.05% H-31 => L+2, 3.08% H-3 =>
277	21291	470	0.06	L+16 72.7% H-35 => L+2, 4.12% H-13 => L+5, 3.63% H-34 => L+1, 3.18% H-34 => L+3
278	21317	469	0.00	43.4% H-34 => L+2, 11.6% H-14 => L+4, 11.3% H-4 => L+18, 7.17% H-31 => L+2, 3.46% H-33 => L+1, 3.28% H-37 => L+2, 2.54% H-33 => L+3, 2.00% H-35 => L+1
279	21318	469	0.01	27.4% H-6 => L+13, 15.7% H-11 => L+7, 11.0% H-7 => L+12, 10.8% H-16 => L+4, 6.43% H-9 => L+10, 3.81% H-4 => L+16, 3.76% H-3 => L+18
280	21326	469	0.01	32.2% H-13 => L+5, 25.3% H-11 => L+6, 8.41% H-35 => L+2, 5.78% H-15 => L+6, 4.38% H-9 => L+5, 3.09% H-13 => L+8, 3.01% H-16 => L+8, 2.29% H-5 => L+16
281	21358	468	0.00	

				64.6% H-39 => L+1, 8.48% H-38 => L+2, 7.88% H-40 => LUMO, 6.72% H-38 => LUMO, 4.46% H-41 => L+1, 2.60% H-40 => L+2
282	21396	467	0.00	30.7% H-8 => L+10, 27.9% H-7 => L+13, 22.5% H-5 => L+16, 2.66% H-10 => L+13, 2.19% H-2 => L+16
283	21409	467	0.00	44.4% H-5 => L+15, 10.7% H-10 => L+8, 5.73% H-3 => L+17, 5.51% H-12 => L+6, 4.90% H-3 => L+14, 2.98% H-14 => L+8, 2.56% H-17 => L+6, 2.52% H-7 => L+17, 2.17% HOMO => L+19, 2.06% H-7 => L+14
284	21454	466	0.00	24.3% H-9 => L+10, 15.5% H-3 => L+18, 12.3% H-6 => L+13, 9.97% H-8 => L+11, 4.27% H-32 => L+2, 4.00% H-21 => L+3, 3.52% H-7 => L+12, 2.29% H-8 => L+14
285	21510	465	0.06	28.7% H-9 => L+10, 14.7% H-6 => L+13, 14.1% H-3 => L+18, 7.16% H-8 => L+11, 4.93% H-11 => L+7, 4.16% H-10 => L+9, 3.10% H-16 => L+4, 2.89% H-7 => L+12
286	21549	464	0.02	22.6% H-6 => L+14, 16.5% H-37 => L+2, 9.60% H-36 => L+2, 4.94% H-11 => L+8, 3.59% H-12 => L+7, 3.41% H-14 => L+4, 3.24% H-36 => L+1, 2.89% H-4 => L+18, 2.57% H-36 => L+3, 2.47% H-34 => L+2, 2.20% H-9 => L+12
287	21575	464	0.38	36.4% H-12 => L+6, 12.5% H-5 => L+15, 12.3% H-10 => L+8, 8.53% H-14 => L+5, 4.33% H-22 => L+3, 3.99% H-5 => L+18, 3.95% H-2 => L+18, 2.97% H-12 => L+9, 2.57% H-10 => L+5
288	21585	463	0.00	36.3% H-36 => L+2, 21.0% H-37 => L+2, 6.92% H-37 => L+1, 5.69% H-9 => L+11, 5.14% H-37 => L+3, 4.55% H-33 => L+2, 4.01% H-36 => L+1, 2.98% H-36 => L+3, 2.11% H-6 => L+12
289	21603	463	0.00	59.4% H-40 => L+1, 8.87% H-41 => LUMO, 8.49% H-39 => LUMO, 8.26% H-39 => L+2, 5.12% H-42 => L+1, 2.26% H-41 => L+2, 2.13% H-38 => L+3
290	21633	462	0.00	18.6% H-11 => L+8, 15.4% H-37 => L+2, 8.89% H-36 => L+2, 8.46% H-15 => L+5, 8.03% H-12 => L+7, 4.46% H-16 => L+6, 2.71% H-36 => L+1, 2.64% H-14 => L+4, 2.22% H-10 => L+10, 2.01% H-36 => L+3
291	21633	462	0.00	30.7% H-6 => L+14, 9.70% H-11 => L+8, 8.58% H-37 => L+2, 4.97% H-36 => L+2, 3.82% H-15 => L+5, 2.65% H-55 => LUMO, 2.46% H-48 => LUMO, 2.44% H-49 => LUMO
292	21661	462	0.38	26.0% H-5 => L+16, 15.7% H-7 => L+13, 15.0% H-9 => L+11, 2.99% H-49 => LUMO, 2.98% H-48 => LUMO, 2.87% H-8 => L+16, 2.69% H-36 => L+2, 2.56% H-16 => L+5, 2.46% H-6 => L+12
293	21687	461	0.00	20.9% H-15 => L+4, 9.70% H-6 => L+16, 7.67% H-13 => L+7, 7.28% H-5 => L+18, 7.12% H-9 => L+13, 6.99% H-11 => L+10, 5.33% H-22 => L+3,
294	21704	461	0.00	

				4.38% H-26 => L+2, 3.88% H-7 => L+17, 2.55% H-2 => L+18, 2.44% HOMO => L+19
295	21721	460	0.00	20.1% H-7 => L+13, 15.6% H-5 => L+16, 15.4% H-9 => L+11, 8.95% H-49 => LUMO, 8.94% H-48 => LUMO, 6.24% H-50 => LUMO
296	21725	460	0.27	47.1% H-8 => L+11, 8.21% H-21 => L+3, 4.36% H-12 => L+8, 4.29% H-5 => L+17, 3.29% H-14 => L+6, 3.16% H-10 => L+12, 2.88% H-17 => L+5, 2.62% H-7 => L+9, 2.03% H-3 => L+18
297	21754	460	0.00	28.4% H-50 => LUMO, 13.0% H-9 => L+11, 9.03% H-52 => LUMO, 6.17% H-48 => LUMO, 6.15% H-49 => LUMO, 5.44% H-16 => L+5, 4.91% H-6 => L+15, 4.46% H-17 => L+4, 3.51% H-4 => L+17
298	21758	460	0.00	52.2% H-50 => LUMO, 10.3% H-48 => LUMO, 10.3% H-49 => LUMO, 5.24% H-17 => L+4, 3.01% H-9 => L+11
299	21769	459	0.00	27.8% H-12 => L+7, 25.4% H-51 => LUMO, 7.62% H-11 => L+8, 6.79% H-49 => LUMO, 6.79% H-48 => LUMO, 3.66% H-10 => L+10, 3.27% H-4 => L+18, 2.24% H-14 => L+4
300	21782	459	0.06	24.6% H-48 => LUMO, 24.6% H-49 => LUMO, 20.4% H-51 => LUMO, 8.08% H-53 => LUMO, 5.56% H-6 => L+14, 3.04% H-49 => L+1, 3.01% H-48 => L+1
301	21826	458	0.08	23.0% H-51 => LUMO, 21.6% H-53 => LUMO, 9.26% H-12 => L+7, 6.53% H-11 => L+8, 6.30% H-6 => L+14, 4.62% H-48 => LUMO, 4.57% H-49 => LUMO, 3.12% H-4 => L+18, 2.78% H-13 => L+6, 2.06% H-55 => LUMO
302	21836	458	0.00	56.4% H-22 => L+3, 7.58% H-13 => L+7, 7.32% H-25 => L+2, 3.19% H-12 => L+6, 2.33% H-7 => L+14
303	21837	458	0.00	37.3% H-17 => L+4, 11.8% H-49 => LUMO, 11.7% H-48 => LUMO, 4.61% H-52 => LUMO, 4.36% H-18 => L+3, 3.49% H-14 => L+7, 2.96% H-9 => L+11, 2.44% H-5 => L+16, 2.19% H-6 => L+15
304	21867	457	0.00	44.3% H-52 => LUMO, 27.3% H-54 => LUMO, 7.84% H-17 => L+4, 2.92% H-50 => LUMO, 2.13% H-51 => L+1
305	21875	457	0.00	61.6% H-21 => L+3, 7.05% H-5 => L+17, 3.05% H-3 => L+18, 2.71% H-10 => L+9
306	21891	457	0.00	56.2% H-41 => L+1, 9.33% H-40 => LUMO, 8.43% H-40 => L+2, 8.39% H-42 => LUMO, 5.50% H-43 => L+1, 2.18% H-39 => L+3
307	21904	457	0.01	55.8% H-55 => LUMO, 11.7% H-53 => LUMO, 6.54% H-11 => L+8, 6.15% H-51 => LUMO, 2.94% H-57 => LUMO, 2.47% H-12 => L+7
308	21940	456	0.00	43.7% H-54 => LUMO, 24.2% H-52 => LUMO, 11.9% H-56 => LUMO, 4.99% H-53 => L+1
309	21943	456	0.02	36.2% H-53 => LUMO, 16.9% H-55 => LUMO, 14.6% H-57 => LUMO, 10.9% H-51 => LUMO,

				3.50% H-54 => L+1, 3.21% H-52 => L+1, 2.41% H-12 => L+7 58.8% H-7 => L+14, 8.70% H-5 => L+15, 3.79% H-5 => L+12, 3.30% H-8 => L+12, 3.19% H-22 => L+3, 2.74% H-18 => L+5, 2.64% H-8 => L+15, 2.48% H-17 => L+6 33.5% H-10 => L+9, 21.4% H-5 => L+17, 4.18% H-7 => L+18, 4.17% H-25 => L+3, 2.75% H-10 => L+12, 2.54% H-8 => L+11, 2.43% HOMO => L+20, 2.41% H-3 => L+15, 2.12% H-18 => L+6, 2.04% H-16 => L+4 41.6% H-56 => LUMO, 14.7% H-6 => L+15, 6.00% H-57 => L+1, 5.28% H-17 => L+4, 4.58% H-9 => L+11, 2.45% H-4 => L+17, 2.19% H-9 => L+14
310	21966	455	0.00	37.5% H-24 => L+3, 18.0% H-18 => L+4, 7.67% H-57 => LUMO, 4.58% H-6 => L+17, 2.97% H-12 => L+7, 2.80% H-17 => L+7, 2.41% H-27 => L+2 52.2% H-57 => LUMO, 10.2% H-55 => LUMO, 7.92% H-56 => L+1, 6.72% H-53 => LUMO, 3.38% H-24 => L+3 35.5% H-23 => L+3, 15.9% H-6 => L+16, 6.19% H-14 => L+5, 3.47% H-13 => L+7, 2.84% H-15 => L+10, 2.82% H-21 => L+4, 2.69% H-26 => L+4, 2.29% H-5 => L+15, 2.09% H-9 => L+13, 2.04% H-3 => L+17, 2.02% H-12 => L+6 29.0% H-14 => L+5, 18.9% H-5 => L+18, 18.5% H-12 => L+6, 7.13% H-13 => L+7, 4.20% H-3 => L+17, 2.90% H-10 => L+5, 2.41% H-17 => L+6, 2.16% H-18 => L+8 56.1% H-42 => L+1, 9.50% H-41 => LUMO, 8.69% H-41 => L+2, 7.66% H-43 => LUMO, 6.83% H-44 => L+1, 2.32% H-40 => L+3 27.8% H-6 => L+15, 23.1% H-56 => LUMO, 9.94% H-54 => LUMO, 3.27% H-17 => L+4, 3.26% H-9 => L+14, 3.17% H-57 => L+1, 2.58% H-4 => L+17 31.1% H-13 => L+6, 8.23% H-24 => L+3, 7.92% H-11 => L+5, 7.29% H-12 => L+7, 5.37% H-15 => L+8, 4.74% H-15 => L+5, 4.72% H-16 => L+9, 4.34% H-10 => L+10, 3.66% H-16 => L+6, 2.78% H-57 => LUMO, 2.76% H-8 => L+13, 2.43% H-21 => L+5 27.8% H-10 => L+9, 16.4% H-25 => L+3, 11.7% H-12 => L+8, 6.27% H-14 => L+6, 4.25% H-12 => L+11, 2.84% H-3 => L+18, 2.79% H-7 => L+15, 2.24% H-17 => L+5, 2.18% H-62 => LUMO 26.2% H-25 => L+3, 22.6% H-5 => L+17, 7.61% H-12 => L+8, 4.57% H-21 => L+3, 3.20% H-3 => L+18, 2.46% H-22 => L+4 27.3% H-10 => L+10, 12.9% H-8 => L+13, 11.1% H-12 => L+7, 7.33% H-7 => L+16, 6.72% H-13 =>
311	21987	455	0.01	
312	22061	453	0.00	
313	22075	453	0.10	
314	22115	452	0.07	
315	22129	452	0.00	
316	22165	451	0.00	
317	22167	451	0.00	
318	22173	451	0.00	
319	22183	451	0.00	
320	22192	451	0.06	
321	22256	449	0.03	
322	22266	449	0.00	

				L+6, 4.18% H-18 => L+4, 3.65% H-4 => L+18, 2.59% H-15 => L+5, 2.13% H-11 => L+5 46.1% H-11 => L+9, 9.35% H-13 => L+8, 9.12% H- 9 => L+11, 7.34% H-16 => L+5, 4.77% H-56 => LUMO, 2.93% H-16 => L+8, 2.51% H-9 => L+8 32.5% H-8 => L+12, 12.0% H-23 => L+3, 7.61% H- 13 => L+7, 7.49% H-14 => L+5, 5.98% H-7 => L+14, 3.71% H-5 => L+18, 3.45% H-10 => L+11, 3.31% H-17 => L+6, 2.86% H-7 => L+11 33.3% H-9 => L+12, 9.55% H-11 => L+11, 8.90% H-6 => L+14, 5.09% H-15 => L+8, 4.73% H-13 => L+9, 4.64% H-10 => L+10, 3.30% H-18 => L+4, 3.13% H-24 => L+3, 2.21% H-6 => L+17 24.0% H-26 => L+3, 16.6% H-25 => L+3, 5.39% H- 5 => L+17, 4.65% H-23 => L+4, 4.31% H-28 => L+2, 3.77% H-15 => L+7, 3.63% H-13 => L+10, 3.37% H-3 => L+18, 2.92% H-8 => L+17, 2.35% H- 12 => L+8 30.9% H-18 => L+4, 29.6% H-24 => L+3, 5.58% H- 9 => L+12, 4.36% H-6 => L+17, 3.46% H-13 => L+6, 2.24% H-17 => L+3, 2.12% H-17 => L+7 54.6% H-43 => L+1, 9.38% H-42 => LUMO, 8.84% H-42 => L+2, 8.43% H-45 => L+1, 6.55% H-44 => LUMO, 2.33% H-41 => L+3 27.2% H-8 => L+12, 26.3% H-13 => L+7, 15.2% H- 23 => L+3, 6.93% H-6 => L+16, 3.14% H-7 => L+14, 3.03% H-14 => L+5 31.0% H-12 => L+8, 15.9% H-7 => L+15, 6.25% H- 26 => L+3, 6.07% HOMO => L+20, 4.34% H-1 => L+19, 4.16% H-20 => L+3, 3.21% H-19 => L+4, 2.79% H-60 => LUMO, 2.31% H-8 => L+14 34.6% H-5 => L+18, 16.4% H-6 => L+16, 14.8% H- 14 => L+5, 4.89% H-8 => L+12, 4.56% H-9 => L+13, 4.23% H-13 => L+7, 2.38% H-3 => L+17 26.8% H-27 => L+3, 15.5% H-14 => L+7, 10.4% H- 17 => L+4, 7.31% H-6 => L+18, 5.48% H-12 => L+10, 2.69% H-10 => L+13, 2.56% H-18 => L+7, 2.14% H-4 => L+17, 2.06% H-24 => L+4 26.8% H-7 => L+16, 21.6% H-10 => L+10, 11.1% H-6 => L+17, 8.40% H-8 => L+13, 6.74% H-18 => L+4, 2.44% H-19 => L+6 24.6% H-27 => L+3, 7.13% H-20 => L+6, 6.59% H- 11 => L+9, 6.19% H-13 => L+8, 6.03% H-16 => L+8, 5.12% H-19 => L+5, 4.83% H-13 => L+5, 4.81% H-15 => L+6, 4.25% H-17 => L+4, 3.69% H- 14 => L+7, 3.51% H-19 => L+8, 2.32% H-16 => L+5 40.6% H-62 => LUMO, 19.9% H-60 => LUMO, 15.1% H-7 => L+15, 3.06% H-12 => L+8, 2.36% H- 15 => L+7
323	22303	448	0.00	
324	22367	447	0.00	
325	22404	446	0.67	
326	22415	446	0.16	
327	22435	446	0.24	
328	22441	446	0.00	
329	22485	445	0.00	
330	22509	444	0.00	
331	22523	444	0.00	
332	22576	443	0.00	
333	22583	443	0.01	
334	22617	442	0.00	
335	22639	442	0.02	

				11.1% H-1 => L+20, 10.7% H-6 => L+16, 7.95% HOMO => L+19, 7.38% H-20 => L+4, 5.69% H-19 => L+3, 4.36% H-61 => LUMO, 4.13% H-28 => L+3, 3.97% H-7 => L+17, 3.73% H-22 => L+3, 3.11% H-23 => L+3, 3.00% H-14 => L+5, 2.85% H-4 => L+19, 2.37% H-13 => L+7, 2.01% H-19 => L+7
336	22644	442	0.00	28.1% H-6 => L+17, 14.1% H-10 => L+10, 9.30% H-8 => L+13, 5.70% H-7 => L+16, 5.61% H-18 => L+4, 4.38% H-4 => L+18, 4.17% H-29 => L+3, 3.54% H-9 => L+12, 2.92% H-9 => L+15, 2.59% H-19 => L+6, 2.37% H-13 => L+6
337	22676	441	0.24	53.5% H-44 => L+1, 9.39% H-43 => LUMO, 9.36% H-46 => L+1, 9.07% H-43 => L+2, 3.86% H-45 => LUMO, 3.41% H-47 => L+2, 2.40% H-47 => LUMO, 2.39% H-42 => L+3
338	22677	441	0.00	19.8% H-27 => L+3, 13.6% H-11 => L+9, 13.6% H-13 => L+8, 9.67% H-14 => L+7, 7.88% H-6 => L+18, 3.86% H-15 => L+6, 2.42% H-16 => L+8, 2.40% H-11 => L+6, 2.29% H-6 => L+15
339	22681	441	0.00	

**Table S19.** TDDFT-predicted band excitation data for **12**.

Index	Energy (cm <sup>-1</sup> )	$\lambda$ (nm)	Osc. Strength	Contributions
0	2228	4489	10.55	98.2% HOMO => LUMO, 2.46% H-1 => L+1
1	3722	2687	0.00	48.4% HOMO => L+1, 48.4% H-1 => LUMO
2	4216	2372	0.00	49.6% HOMO => L+1, 49.3% H-1 => LUMO
3	4385	2280	0.00	91.9% H-2 => LUMO, 4.26% H-4 => L+1 80.8% H-4 => LUMO, 13.0% H-2 => L+1, 2.86%
4	4923	2031	0.00	H-5 => L+1
5	5332	1875	0.02	55.6% H-3 => LUMO, 41.2% HOMO => L+2 73.4% H-5 => LUMO, 16.0% H-4 => L+1, 5.55%
6	5656	1768	0.00	H-2 => L+2, 2.02% H-7 => L+1 37.1% H-1 => L+1, 33.3% HOMO => L+2, 24.9%
7	5662	1766	0.29	H-3 => LUMO 58.0% H-1 => L+1, 22.5% HOMO => L+2, 16.0%
8	5948	1681	0.60	H-3 => LUMO 66.5% H-7 => LUMO, 18.7% H-5 => L+1, 6.41%
9	6528	1532	0.00	H-4 => L+2, 3.39% H-2 => L+3 78.9% H-2 => L+1, 13.2% H-4 => LUMO, 4.52%
10	6620	1511	0.00	H-4 => L+2
11	6848	1460	0.00	67.6% H-6 => LUMO, 25.8% HOMO => L+3 61.8% H-4 => L+1, 20.4% H-5 => LUMO, 8.98%
12	7198	1389	0.00	H-2 => L+2, 3.17% H-2 => LUMO

13	7215	1386	0.00	52.5% HOMO => L+3, 23.5% H-6 => LUMO, 17.3% H-3 => L+1
14	7384	1354	0.00	52.1% H-3 => L+1, 31.5% H-1 => L+2, 10.1% HOMO => L+3
15	7505	1332	0.00	61.7% H-8 => LUMO, 18.9% H-7 => L+1, 9.18% H-5 => L+2, 4.17% H-4 => L+3
16	7512	1331	0.00	59.2% H-1 => L+2, 22.7% H-3 => L+1, 7.78% HOMO => L+3, 4.42% H-6 => LUMO
				52.2% H-5 => L+1, 26.9% H-7 => LUMO, 9.80% H-4 => L+2, 3.16% H-4 => LUMO, 3.00% H-2 =>
17	7957	1257	0.00	L+3 78.6% H-9 => LUMO, 10.9% HOMO => L+4,
18	8251	1212	0.05	4.77% H-6 => L+1 76.9% H-2 => L+2, 11.7% H-4 => L+1, 4.05% H-2
19	8425	1187	0.00	=> LUMO, 3.28% H-4 => L+3 57.6% H-10 => LUMO, 19.5% H-8 => L+1, 10.1%
20	8547	1170	0.00	H-7 => L+2, 4.81% H-5 => L+3, 2.55% H-4 => L+4 66.0% HOMO => L+4, 15.0% H-9 => LUMO,
21	8711	1148	0.07	10.4% H-6 => L+1, 2.32% H-1 => L+3 44.0% H-7 => L+1, 32.5% H-8 => LUMO, 10.6%
				H-5 => L+2, 4.00% H-4 => L+3, 2.74% H-5 =>
22	8850	1130	0.00	LUMO 71.5% H-6 => L+1, 16.2% HOMO => L+4, 4.07%
23	8883	1126	0.10	H-3 => L+2, 2.39% H-3 => LUMO
24	9008	1110	0.00	47.2% H-3 => L+2, 44.2% H-1 => L+3 61.0% H-4 => L+2, 20.3% H-5 => L+1, 8.59% H-2
25	9009	1110	0.00	=> L+3, 2.45% H-2 => L+1, 2.08% H-5 => L+3 45.3% H-1 => L+3, 41.5% H-3 => L+2, 5.74% H-6
26	9124	1096	0.12	=> L+1 81.8% H-11 => LUMO, 7.96% H-9 => L+1, 2.81%
27	9521	1050	0.00	HOMO => L+5, 2.12% H-13 => L+1 54.3% H-12 => LUMO, 19.0% H-10 => L+1, 10.8%
28	9619	1040	0.00	H-8 => L+2, 4.67% H-7 => L+3, 2.75% H-5 => L+4 50.2% H-5 => L+2, 27.1% H-7 => L+1, 8.56% H-4
				=> L+3, 2.76% H-2 => L+4, 2.72% H-4 => L+1, 2.16% H-7 => L+3
29	9766	1024	0.00	37.1% H-8 => L+1, 36.8% H-10 => LUMO, 11.3% H-7 => L+2, 4.91% H-5 => L+3, 2.21% H-7 =>
30	9829	1017	0.00	LUMO, 2.01% H-12 => L+1, 2.01% H-4 => L+4 75.9% H-2 => L+3, 12.3% H-4 => L+2, 3.98% H-2
31	10109	989	0.00	=> L+1, 3.33% H-4 => L+4 69.6% HOMO => L+5, 10.9% H-1 => L+4, 6.10%
32	10145	986	0.00	H-9 => L+1, 5.11% H-11 => LUMO 61.0% H-9 => L+1, 13.6% H-6 => L+2, 6.86% H-11
				=> LUMO, 4.92% HOMO => L+5, 4.09% H-3 =>
33	10244	976	0.00	L+3, 2.46% H-6 => LUMO 32.9% H-6 => L+2, 23.7% H-3 => L+3, 13.6% H-1
34	10486	954	0.00	=> L+4, 12.5% H-9 => L+1, 11.2% HOMO => L+5 77.7% H-13 => LUMO, 10.0% H-11 => L+1, 2.64%
35	10628	941	0.06	H-9 => L+2, 2.22% H-15 => L+1

36	10639	940	0.00	40.9% H-6 => L+2, 32.1% H-1 => L+4, 10.3% H-3 => L+3, 5.76% HOMO => L+5, 4.55% H-9 => L+1 34.5% H-7 => L+2, 29.4% H-8 => L+1, 8.67% H-5 => L+3, 7.56% H-14 => LUMO, 5.51% H-10 => L+2, 3.40% H-4 => L+4, 3.16% H-12 => L+1 59.9% H-4 => L+3, 19.1% H-5 => L+2, 9.06% H-2 => L+4, 2.44% H-2 => L+2, 2.14% H-4 => L+1 48.0% H-14 => LUMO, 15.1% H-12 => L+1, 6.85% H-7 => L+2, 6.33% H-8 => L+3, 5.53% H-10 => L+2, 5.20% H-8 => L+1, 3.07% H-7 => L+4 53.0% H-3 => L+3, 35.3% H-1 => L+4, 4.21% H-6 => L+2
37	10647	939	0.00	L+2, 3.40% H-4 => L+4, 3.16% H-12 => L+1 59.9% H-4 => L+3, 19.1% H-5 => L+2, 9.06% H-2 => L+4, 2.44% H-2 => L+2, 2.14% H-4 => L+1 48.0% H-14 => LUMO, 15.1% H-12 => L+1, 6.85% H-7 => L+2, 6.33% H-8 => L+3, 5.53% H-10 => L+2, 5.20% H-8 => L+1, 3.07% H-7 => L+4
38	10679	936	0.00	53.0% H-3 => L+3, 35.3% H-1 => L+4, 4.21% H-6 => L+2
39	10698	935	0.00	38.7% H-12 => LUMO, 32.0% H-10 => L+1, 11.6% H-8 => L+2, 5.24% H-7 => L+3, 3.11% H-5 => L+4, 2.08% H-14 => L+1
40	10763	929	0.00	93.0% HOMO => L+6, 2.81% H-1 => L+7 80.3% HOMO => L+7, 6.20% H-1 => L+6, 5.16% H-5 => L+3
41	10850	922	0.00	43.4% H-5 => L+3, 27.2% H-7 => L+2, 9.08% H-4 => L+4, 7.94% HOMO => L+7, 2.95% H-2 => L+5, 2.02% H-4 => L+2
42	11103	901	0.00	46.5% HOMO => L+8, 12.6% H-1 => L+5, 8.37% H-3 => L+4, 6.19% H-6 => L+3, 5.63% H-11 => L+1, 5.22% H-9 => L+2, 3.27% H-13 => LUMO, 2.16% H-17 => LUMO
43	11438	874	0.00	71.9% H-15 => LUMO, 10.2% H-13 => L+1, 3.40% H-11 => L+2, 2.45% H-19 => LUMO, 2.39% H-17 => L+1
44	11461	873	0.00	54.7% H-11 => L+1, 14.7% HOMO => L+8, 11.8% H-13 => LUMO, 8.14% H-9 => L+2, 3.76% H-1 => L+5, 2.52% H-9 => LUMO
45	11496	870	0.03	37.9% H-10 => L+1, 30.1% H-8 => L+2, 9.88% H-7 => L+3, 5.07% H-5 => L+4, 2.86% H-12 => L+2, 2.73% H-2 => L+4
46	11522	868	0.00	55.2% H-16 => LUMO, 16.0% H-14 => L+1, 7.27% H-12 => L+2, 5.06% H-10 => L+3, 2.82% H-8 => L+4
47	11538	867	0.00	70.3% H-2 => L+4, 12.4% H-4 => L+3, 4.26% H-4 => L+5, 3.66% H-2 => L+2
48	11621	861	0.00	38.8% H-14 => LUMO, 29.0% H-12 => L+1, 11.8% H-10 => L+2, 6.04% H-8 => L+3, 3.65% H-7 => L+4, 2.17% H-16 => L+1
49	11714	854	0.00	32.2% H-9 => L+2, 19.2% H-11 => L+1, 16.6% HOMO => L+8, 16.5% H-6 => L+3, 6.41% H-3 => L+4
50	11748	851	0.00	83.7% HOMO => L+9, 6.74% H-1 => L+7 34.8% H-9 => L+2, 13.4% H-17 => LUMO, 12.7% H-1 => L+5, 12.0% H-3 => L+4, 11.2% HOMO => L+8, 3.62% H-6 => L+3, 2.11% H-11 => L+3
51	11872	842	0.00	83.7% HOMO => L+9, 6.74% H-1 => L+7 34.8% H-9 => L+2, 13.4% H-17 => LUMO, 12.7% H-1 => L+5, 12.0% H-3 => L+4, 11.2% HOMO => L+8, 3.62% H-6 => L+3, 2.11% H-11 => L+3
52	11897	841	0.03	83.7% HOMO => L+9, 6.74% H-1 => L+7 34.8% H-9 => L+2, 13.4% H-17 => LUMO, 12.7% H-1 => L+5, 12.0% H-3 => L+4, 11.2% HOMO => L+8, 3.62% H-6 => L+3, 2.11% H-11 => L+3
53	11941	837	0.00	83.7% HOMO => L+9, 6.74% H-1 => L+7 34.8% H-9 => L+2, 13.4% H-17 => LUMO, 12.7% H-1 => L+5, 12.0% H-3 => L+4, 11.2% HOMO => L+8, 3.62% H-6 => L+3, 2.11% H-11 => L+3
54	12092	827	0.09	83.7% HOMO => L+9, 6.74% H-1 => L+7 34.8% H-9 => L+2, 13.4% H-17 => LUMO, 12.7% H-1 => L+5, 12.0% H-3 => L+4, 11.2% HOMO => L+8, 3.62% H-6 => L+3, 2.11% H-11 => L+3

				51.5% H-17 => LUMO, 7.06% H-15 => L+1, 7.02% H-20 => LUMO, 6.21% H-3 => L+4, 5.99% H-1 => L+5, 3.80% H-6 => L+3, 2.57% H-13 => L+2, 2.22% H-9 => L+2, 2.12% HOMO => L+8
55	12130	824	0.00	46.7% H-6 => L+3, 34.5% H-1 => L+5, 6.26% H-9 => L+2, 3.24% HOMO => L+8
56	12259	816	0.57	56.9% H-4 => L+4, 22.1% H-5 => L+3, 9.34% H-2 => L+5, 2.41% H-2 => L+3, 2.17% H-4 => L+2
57	12317	812	0.00	38.7% H-7 => L+3, 36.9% H-8 => L+2, 9.68% H-5 => L+4, 4.03% H-4 => L+5, 2.09% H-5 => L+2
58	12344	810	0.00	58.6% H-3 => L+4, 22.1% H-1 => L+5, 11.0% H-6 => L+3
59	12380	808	0.20	71.5% H-19 => LUMO, 7.72% H-20 => L+1, 6.99% H-17 => L+1, 2.40% H-15 => LUMO
60	12389	807	0.00	75.7% H-20 => LUMO, 10.7% H-19 => L+1, 3.77% H-17 => LUMO, 2.49% H-17 => L+2
61	12427	805	0.01	68.7% HOMO => L+10, 8.38% H-12 => L+1, 7.10% H-1 => L+9, 3.99% H-10 => L+2
62	12535	798	0.00	47.2% H-18 => LUMO, 12.4% H-16 => L+1, 8.93% H-14 => L+2, 7.96% H-12 => L+1, 4.30% H-10 => L+2, 2.36% H-12 => L+3, 2.06% H-8 => L+3
63	12636	791	0.00	28.0% H-12 => L+1, 17.6% H-10 => L+2, 14.1% HOMO => L+10, 12.5% H-18 => LUMO, 7.56% H-8 => L+3, 3.68% H-7 => L+4, 2.39% H-16 => L+1, 2.27% H-5 => L+5
64	12681	789	0.00	43.7% H-13 => L+1, 17.1% H-15 => LUMO, 10.7% H-11 => L+2, 4.78% H-9 => L+3, 3.90% HOMO => L+11, 2.61% H-6 => L+4, 2.36% H-11 => LUMO
65	12713	787	0.00	45.3% HOMO => L+11, 18.3% H-13 => L+1, 14.9% H-1 => L+8, 7.53% H-3 => L+5, 3.58% H-6 => L+4
66	12826	780	0.00	36.3% H-16 => LUMO, 27.5% H-14 => L+1, 11.7% H-12 => L+2, 6.33% H-10 => L+3, 4.34% H-8 => L+4, 2.15% H-18 => L+1, 2.14% H-7 => L+5
67	12856	778	0.00	84.3% H-1 => L+6, 5.96% HOMO => L+7, 4.33% H-3 => L+7
68	12980	770	0.00	45.5% H-5 => L+4, 29.4% H-7 => L+3, 10.3% H-4 => L+5, 3.59% H-2 => L+8, 2.32% H-4 => L+3
69	13072	765	0.00	40.2% H-11 => L+2, 18.2% H-13 => L+1, 15.9% HOMO => L+11, 13.5% H-9 => L+3, 4.77% H-6 => L+4
70	13227	756	0.00	62.3% HOMO => L+12, 12.9% H-1 => L+7, 10.4% H-1 => L+10, 3.18% HOMO => L+9
71	13231	756	0.00	63.1% H-2 => L+6, 14.9% H-4 => L+7, 4.88% H-5 => L+9, 4.64% H-2 => L+9, 3.79% H-6 => L+3
72	13306	752	8.77	43.1% H-10 => L+2, 26.3% H-8 => L+3, 10.0% H-7 => L+4, 5.32% H-5 => L+5, 3.65% H-2 => L+5
73	13315	751	0.00	69.7% H-2 => L+5, 13.2% H-4 => L+4, 4.86% H-4 => L+8, 3.97% H-2 => L+3
74	13328	750	0.00	61.1% H-1 => L+7, 16.1% HOMO => L+12, 7.25% H-3 => L+6, 4.42% HOMO => L+9, 3.07% H-3 => L+9, 2.64% HOMO => L+6
75	13336	750	0.00	

				60.6% H-21 => LUMO, 13.3% H-18 => L+1, 6.27% H-16 => L+2, 3.42% H-28 => LUMO, 3.22% H-14 => L+3, 2.04% H-12 => L+4
76	13400	746	0.01	29.2% H-11 => L+2, 13.4% HOMO => L+11, 13.4% H-9 => L+3, 13.3% H-6 => L+4, 6.37% H-3 => L+5, 5.54% H-4 => L+6, 5.12% H-2 => L+7, 2.77% H-1 => L+8
77	13460	743	0.00	26.1% H-1 => L+8, 16.0% H-9 => L+3, 15.6% H-3 => L+5, 13.9% HOMO => L+11, 8.82% H-4 => L+6, 8.44% H-2 => L+7
78	13632	734	0.00	44.0% H-14 => L+1, 19.9% H-12 => L+2, 10.4% H-10 => L+3, 6.00% H-8 => L+4, 4.18% H-7 => L+5, 2.49% HOMO => L+12, 2.08% H-16 => L+2
79	13667	732	0.00	47.8% H-15 => L+1, 19.3% H-17 => LUMO, 8.78% H-13 => L+2, 3.62% H-11 => L+3, 2.96% H-13 => LUMO
80	13715	729	0.00	30.8% H-18 => LUMO, 23.9% H-16 => L+1, 10.7% H-14 => L+2, 5.78% H-12 => L+3, 4.45% H-10 => L+4, 3.18% HOMO => L+13, 2.42% H-8 => L+5, 2.25% H-22 => LUMO
81	13751	727	0.00	64.2% H-1 => L+9, 9.06% HOMO => L+10, 7.36% H-3 => L+7, 3.92% H-1 => L+12, 3.52% HOMO => L+13, 2.98% HOMO => L+7, 2.44% H-6 => L+6
82	13788	725	0.00	35.0% H-9 => L+3, 15.9% H-4 => L+6, 15.5% H-2 => L+7, 10.2% H-6 => L+4, 5.97% H-11 => L+2, 3.11% H-1 => L+8, 2.80% H-5 => L+7, 2.37% H-3 => L+5
83	13849	722	0.00	40.9% H-1 => L+8, 26.0% H-6 => L+4, 15.1% H-3 => L+5, 6.29% H-9 => L+3
84	13865	721	0.00	53.6% H-4 => L+5, 23.8% H-5 => L+4, 9.64% H-2 => L+8, 2.39% H-2 => L+4, 2.27% H-4 => L+3
85	13902	719	0.00	30.2% H-8 => L+3, 25.3% H-7 => L+4, 15.3% HOMO => L+13, 8.80% H-5 => L+5, 3.80% H-4 => L+8
86	13981	715	0.00	56.1% HOMO => L+13, 9.90% H-8 => L+3, 6.99% H-7 => L+4, 5.19% H-1 => L+9, 4.76% H-1 => L+12, 2.80% H-3 => L+10, 2.27% H-5 => L+5
87	13987	715	0.00	33.3% HOMO => L+14, 19.7% H-15 => L+1, 12.3% H-1 => L+11, 7.38% H-3 => L+8, 5.17% H-23 => LUMO, 4.89% H-6 => L+5, 3.23% H-19 => L+1, 2.94% H-9 => L+4
88	13987	715	0.00	42.1% H-3 => L+5, 30.7% H-6 => L+4, 7.86% H-2 => L+7, 7.23% H-4 => L+6, 2.64% H-1 => L+8
89	14019	713	0.00	83.0% H-22 => LUMO, 6.05% H-21 => L+1, 2.92% HOMO => L+22
90	14138	707	0.32	46.3% H-12 => L+2, 15.6% H-10 => L+3, 8.65% H-8 => L+4, 4.81% H-7 => L+5, 4.18% H-14 => L+3, 3.27% H-21 => LUMO, 2.99% H-5 => L+8
91	14312	699	0.00	61.3% H-1 => L+10, 11.1% HOMO => L+12, 9.62% H-3 => L+9, 4.07% H-1 => L+13, 3.03% HOMO => L+15, 2.01% HOMO => L+9
92	14404	694	0.00	

93	14414	694	1.03	24.7% H-2 => L+9, 21.7% H-4 => L+7, 17.1% H-5 => L+6, 16.6% H-13 => L+2, 3.34% H-15 => L+1, 2.49% H-7 => L+7 44.7% H-17 => L+1, 16.2% H-19 => LUMO, 8.34% H-24 => LUMO, 5.29% H-15 => L+2, 3.38% H-19 => L+2, 3.33% H-15 => LUMO, 2.23% H-23 => L+1, 2.08% H-20 => L+1, 2.04% H-13 => L+3 31.7% H-13 => L+2, 19.5% HOMO => L+14, 11.9% H-11 => L+3, 10.5% H-15 => L+1, 4.48% H-2 => L+9, 4.02% H-4 => L+7, 3.79% H-9 => L+4, 3.05% H-5 => L+6																							
94	14429	693	0.00	24.6% H-21 => LUMO, 14.5% H-18 => L+1, 9.36% H-22 => L+1, 7.58% H-16 => L+2, 5.53% H-28 => LUMO, 4.75% H-12 => L+4, 4.74% H-12 => L+2, 4.41% H-10 => L+3, 3.30% H-14 => L+3, 2.97% H-10 => L+5, 2.15% H-8 => L+8 37.2% H-16 => L+1, 11.6% H-14 => L+2, 7.18% H-12 => L+3, 7.12% H-7 => L+4, 6.47% H-5 => L+5, 5.69% H-8 => L+5, 4.90% H-10 => L+4, 2.25% H-4 => L+8																							
95	14436	693	0.24	59.6% HOMO => L+15, 11.6% H-3 => L+6, 5.94% H-1 => L+13, 3.10% H-3 => L+12, 2.56% H-1 => L+10, 2.49% H-1 => L+7, 2.12% H-37 => LUMO 33.1% H-5 => L+5, 28.6% H-7 => L+4, 8.09% H-4 => L+8, 7.45% H-16 => L+1, 4.21% H-14 => L+2, 2.87% H-2 => L+11, 2.61% H-7 => L+8 41.3% H-24 => LUMO, 25.6% H-17 => L+1, 11.3% H-20 => L+1, 5.24% H-23 => L+1, 3.78% HOMO => L+17																							
96	14436	693	0.00	66.3% H-3 => L+6, 9.79% HOMO => L+15, 7.05% H-1 => L+7, 5.00% H-6 => L+7, 3.74% H-1 => L+10 25.2% H-23 => LUMO, 23.3% HOMO => L+14, 14.2% H-19 => L+1, 12.5% H-13 => L+2, 3.26% H-20 => LUMO, 3.13% H-24 => L+1, 2.10% H-2 => L+9, 2.04% H-4 => L+7 43.0% H-23 => LUMO, 16.3% H-19 => L+1, 6.60% H-13 => L+2, 6.37% H-11 => L+3, 4.70% H-24 => L+1, 4.45% H-9 => L+4, 2.98% H-6 => L+5, 2.02% H-3 => L+8																							
97	14611	684	0.01	49.0% H-20 => L+1, 20.9% H-24 => LUMO, 4.99% H-19 => LUMO, 4.53% H-26 => LUMO, 2.18% H-23 => L+1 69.4% H-2 => L+8, 14.7% H-4 => L+5, 4.45% H-2 => L+4, 2.79% H-4 => L+11 36.9% H-19 => L+1, 9.99% H-11 => L+3, 6.97% H-9 => L+4, 6.71% H-13 => L+2, 5.93% H-20 => LUMO, 5.26% H-6 => L+5, 4.70% H-3 => L+8, 3.76% HOMO => L+14, 2.91% H-1 => L+11, 2.27% H-17 => L+2																							
98	14653	682	0.00	101	14708	680	0.00	102	14759	678	0.02	103	14838	674	0.02	104	14844	674	0.00	105	14862	673	0.00	106	14894	671	0.02

107	14945	669	0.00	48.8% H-10 => L+3, 21.5% H-8 => L+4, 9.11% H-7 => L+5, 4.63% H-5 => L+8, 3.55% H-4 => L+11 58.6% H-3 => L+7, 10.1% H-1 => L+9, 8.11% H-1 => L+12, 7.73% H-6 => L+6, 4.73% H-3 => L+10,
108	14967	668	0.00	4.40% H-1 => L+6, 2.45% HOMO => L+13 68.9% H-25 => LUMO, 6.13% H-11 => L+3, 5.08% H-1 => L+11, 3.09% H-27 => L+1
109	15031	665	0.00	33.5% H-11 => L+3, 17.1% H-1 => L+11, 11.2% H-25 => LUMO, 10.4% H-3 => L+8, 9.89% HOMO => L+14, 4.31% H-6 => L+5, 3.02% H-13 => L+2
110	15071	664	0.00	64.9% H-26 => LUMO, 5.89% H-20 => L+1, 5.44% H-27 => LUMO
111	15076	663	0.00	40.2% H-1 => L+12, 11.6% HOMO => L+16, 9.41% HOMO => L+13, 7.73% H-3 => L+7, 6.24% H-1 => L+15, 5.35% H-3 => L+10, 3.96% H-6 => L+9, 2.24% HOMO => L+10
112	15100	662	0.00	40.3% H-18 => L+1, 19.0% H-28 => LUMO, 7.44% H-21 => L+2, 5.30% HOMO => L+18, 3.76% H-22 => L+1, 2.26% H-16 => LUMO
113	15214	657	0.00	20.6% H-4 => L+9, 16.6% H-2 => L+10, 13.3% H-27 => LUMO, 13.2% H-5 => L+7, 6.72% H-7 => L+6, 6.17% HOMO => L+17, 4.86% H-26 => LUMO, 2.26% H-20 => L+1, 2.10% H-33 => LUMO
114	15225	657	0.00	48.1% HOMO => L+16, 13.1% H-1 => L+12, 6.64% H-14 => L+2, 4.48% H-36 => LUMO, 3.20% H-1 => L+15, 3.15% H-3 => L+13, 2.27% H-3 => L+7 34.8% H-1 => L+11, 28.3% H-9 => L+4, 15.3% H-11 => L+3, 10.6% H-6 => L+5
115	15255	656	0.00	47.3% H-14 => L+2, 7.04% H-12 => L+3, 5.96% HOMO => L+16, 5.11% H-10 => L+4, 3.74% H-7 => L+8, 3.58% H-8 => L+5, 3.21% H-31 => LUMO, 2.91% H-4 => L+8, 2.65% H-5 => L+5
116	15269	655	0.02	34.3% H-27 => LUMO, 16.8% H-15 => L+2, 4.73% H-5 => L+7, 4.72% H-4 => L+9, 4.62% H-2 => L+10, 4.40% H-25 => L+1, 4.02% HOMO => L+17, 3.62% H-17 => L+1
117	15299	654	0.01	43.4% H-2 => L+7, 39.9% H-4 => L+6, 8.04% H-4 => L+9, 3.85% H-5 => L+7
118	15319	653	0.00	25.4% HOMO => L+17, 12.7% H-20 => L+1, 8.40% H-26 => LUMO, 6.90% H-15 => L+2, 5.99% H-1 => L+14, 5.93% H-24 => LUMO, 3.85% H-13 => L+3, 3.25% H-3 => L+11, 2.83% H-11 => L+4, 2.64% H-6 => L+8, 2.62% H-17 => L+1, 2.53% H-9 => L+5
119	15354	651	0.00	28.8% H-3 => L+8, 28.0% H-9 => L+4, 14.1% H-1 => L+11, 6.17% H-6 => L+5, 5.54% H-29 => LUMO, 2.45% H-30 => LUMO
120	15387	650	0.00	46.3% H-4 => L+8, 24.5% H-5 => L+5, 9.32% H-2 => L+11, 2.86% H-14 => L+2, 2.79% H-5 => L+11,
121	15412	649	0.06	
122	15446	647	0.00	

				2.25% H-4 => L+4, 2.10% HOMO => L+16, 2.10% H-2 => L+5
123	15464	647	0.00	58.8% H-3 => L+9, 13.5% H-1 => L+10, 6.96% H-6 => L+7, 3.47% H-1 => L+7, 2.68% H-9 => L+6, 2.43% H-3 => L+12
124	15495	645	0.00	32.5% H-6 => L+5, 25.7% H-29 => LUMO, 8.89% H-30 => LUMO, 8.44% H-9 => L+4, 3.66% H-3 => L+8
125	15520	644	0.00	38.7% H-8 => L+4, 18.3% H-7 => L+5, 8.11% H-5 => L+8, 5.14% HOMO => L+18, 4.33% H-34 => LUMO, 4.24% H-4 => L+11, 2.59% H-3 => L+9, 2.23% H-2 => L+14
126	15526	644	0.05	40.9% H-21 => L+1, 14.3% HOMO => L+19, 7.60% H-31 => LUMO, 5.04% H-22 => LUMO, 4.56% H-22 => L+2, 3.64% H-18 => L+2, 3.24% H-18 => LUMO, 3.21% H-12 => L+3, 3.13% H-1 => L+18
127	15551	643	0.03	31.7% H-3 => L+8, 25.8% H-29 => LUMO, 20.3% H-6 => L+5, 3.06% H-1 => L+11, 2.61% H-30 => LUMO
128	15562	643	0.00	30.6% H-15 => L+2, 23.3% H-27 => LUMO, 18.0% HOMO => L+17, 6.13% H-13 => L+3, 3.34% H-17 => L+1, 2.50% H-1 => L+14
129	15628	640	0.00	22.1% HOMO => L+18, 15.5% H-34 => LUMO, 12.0% H-28 => LUMO, 7.99% H-7 => L+5, 5.42% HOMO => L+21, 5.07% H-1 => L+16, 4.70% H-8 => L+4, 3.38% HOMO => L+15, 3.33% H-1 => L+13
130	15665	638	0.39	45.0% H-2 => L+9, 15.7% H-2 => L+6, 11.9% H-4 => L+7, 11.8% H-5 => L+6, 3.90% H-4 => L+10, 2.65% H-9 => L+4
131	15709	637	0.01	48.9% H-30 => LUMO, 15.9% H-29 => LUMO, 4.68% H-27 => L+1, 2.29% H-33 => L+1, 2.16% H-32 => L+1, 2.08% H-26 => L+1, 2.02% H-4 => L+10
132	15725	636	0.00	21.6% H-16 => L+2, 18.4% H-18 => L+1, 16.2% H-28 => LUMO, 9.77% HOMO => L+18, 6.66% H-14 => L+3, 3.47% H-12 => L+4, 2.32% HOMO => L+21
133	15757	635	0.03	37.2% H-31 => LUMO, 17.7% H-21 => L+1, 13.7% H-12 => L+3, 5.07% HOMO => L+22, 4.31% H-28 => L+1, 3.92% HOMO => L+19, 3.59% H-22 => LUMO, 2.18% H-18 => L+2
134	15829	632	0.00	51.0% H-1 => L+13, 9.87% HOMO => L+15, 7.92% H-3 => L+12, 5.21% HOMO => L+18, 4.09% H-6 => L+10, 2.79% H-34 => LUMO, 2.67% H-3 => L+9, 2.22% HOMO => L+12
135	15839	631	0.00	50.0% H-32 => LUMO, 9.22% H-33 => LUMO, 8.26% H-15 => L+2, 6.19% H-29 => L+1, 6.14% H-13 => L+3
136	15959	627	0.00	48.7% H-33 => LUMO, 20.1% H-32 => LUMO, 7.27% H-30 => L+1, 3.02% H-13 => L+3

137	15966	626	0.01	46.8% H-12 => L+3, 14.2% H-10 => L+4, 8.54% H-8 => L+5, 5.90% H-31 => LUMO, 4.86% H-7 => L+8, 3.11% H-5 => L+11 24.9% HOMO => L+20, 23.3% H-17 => L+2, 7.72% H-20 => L+2, 5.44% H-19 => L+1, 5.35% H-15 => L+3, 5.00% H-1 => L+17, 3.28% H-13 => L+4, 2.85% H-3 => L+14, 2.53% H-20 => LUMO, 2.42% H-11 => L+5, 2.24% H-6 => L+11, 2.14% H-9 => L+8
138	15974	626	0.00	45.1% H-22 => L+1, 29.4% H-28 => LUMO, 6.31% HOMO => L+21, 4.87% H-21 => LUMO, 3.91% H-21 => L+2 47.0% H-5 => L+6, 22.9% H-4 => L+7, 10.8% H-2 => L+6, 4.35% H-5 => L+9, 4.26% H-7 => L+7, 3.03% H-35 => LUMO
139	15982	626	0.00	14.6% HOMO => L+17, 12.0% H-15 => L+2, 11.9% H-11 => L+4, 11.0% H-33 => LUMO, 9.47% H-13 => L+3, 7.95% H-9 => L+5, 6.66% H-32 => LUMO, 5.43% H-38 => LUMO, 3.91% H-6 => L+8, 3.35% H-3 => L+11, 2.34% H-2 => L+10 50.1% H-3 => L+10, 16.4% H-1 => L+12, 9.90% H-6 => L+9, 3.16% H-6 => L+6, 2.50% H-3 => L+13, 2.04% H-1 => L+9
140	16013	625	0.14	47.5% H-35 => LUMO, 10.0% H-4 => L+10, 5.94% H-5 => L+9, 5.84% H-2 => L+12, 4.42% H-7 => L+7, 3.32% H-4 => L+7, 3.17% H-40 => LUMO, 2.65% H-33 => L+1 47.1% H-2 => L+10, 14.7% H-5 => L+7, 7.45% H-7 => L+6, 6.39% H-4 => L+6, 5.11% H-2 => L+7, 4.35% H-4 => L+12, 2.99% H-13 => L+3 36.6% H-7 => L+5, 30.1% H-5 => L+8, 10.2% H-4 => L+11, 4.40% H-2 => L+14, 4.32% H-16 => L+2, 3.49% H-8 => L+8, 2.30% H-5 => L+4 67.1% H-6 => L+6, 10.0% H-3 => L+7, 6.14% H-9 => L+7, 3.35% H-42 => LUMO, 2.54% H-3 => L+10 19.8% H-35 => LUMO, 17.7% H-4 => L+10, 13.4% H-5 => L+9, 8.40% H-2 => L+12, 6.85% H-40 => LUMO, 6.12% H-30 => LUMO, 3.92% HOMO => L+20, 3.76% H-7 => L+7, 3.13% H-29 => LUMO, 2.30% H-33 => L+1 47.1% H-16 => L+2, 7.50% H-14 => L+3, 5.98% H-12 => L+4, 4.78% H-10 => L+5, 4.12% H-7 => L+11, 3.66% HOMO => L+18, 3.37% H-7 => L+5, 2.92% H-5 => L+8, 2.56% H-8 => L+8, 2.49% H-5 => L+14, 2.08% H-4 => L+17 38.4% HOMO => L+20, 35.2% H-17 => L+2, 4.66% H-1 => L+17, 2.80% H-30 => LUMO
141	16045	623	0.00	31.1% H-13 => L+3, 20.3% H-1 => L+14, 13.8% HOMO => L+17, 10.3% H-3 => L+11, 6.19% H-6 => L+8
142	16071	622	0.00	14.6% HOMO => L+17, 12.0% H-15 => L+2, 11.9% H-11 => L+4, 11.0% H-33 => LUMO, 9.47% H-13 => L+3, 7.95% H-9 => L+5, 6.66% H-32 => LUMO, 5.43% H-38 => LUMO, 3.91% H-6 => L+8, 3.35% H-3 => L+11, 2.34% H-2 => L+10 50.1% H-3 => L+10, 16.4% H-1 => L+12, 9.90% H-6 => L+9, 3.16% H-6 => L+6, 2.50% H-3 => L+13, 2.04% H-1 => L+9
143	16124	620	0.16	47.5% H-35 => LUMO, 10.0% H-4 => L+10, 5.94% H-5 => L+9, 5.84% H-2 => L+12, 4.42% H-7 => L+7, 3.32% H-4 => L+7, 3.17% H-40 => LUMO, 2.65% H-33 => L+1 47.1% H-2 => L+10, 14.7% H-5 => L+7, 7.45% H-7 => L+6, 6.39% H-4 => L+6, 5.11% H-2 => L+7, 4.35% H-4 => L+12, 2.99% H-13 => L+3 36.6% H-7 => L+5, 30.1% H-5 => L+8, 10.2% H-4 => L+11, 4.40% H-2 => L+14, 4.32% H-16 => L+2, 3.49% H-8 => L+8, 2.30% H-5 => L+4 67.1% H-6 => L+6, 10.0% H-3 => L+7, 6.14% H-9 => L+7, 3.35% H-42 => LUMO, 2.54% H-3 => L+10 19.8% H-35 => LUMO, 17.7% H-4 => L+10, 13.4% H-5 => L+9, 8.40% H-2 => L+12, 6.85% H-40 => LUMO, 6.12% H-30 => LUMO, 3.92% HOMO => L+20, 3.76% H-7 => L+7, 3.13% H-29 => LUMO, 2.30% H-33 => L+1 47.1% H-16 => L+2, 7.50% H-14 => L+3, 5.98% H-12 => L+4, 4.78% H-10 => L+5, 4.12% H-7 => L+11, 3.66% HOMO => L+18, 3.37% H-7 => L+5, 2.92% H-5 => L+8, 2.56% H-8 => L+8, 2.49% H-5 => L+14, 2.08% H-4 => L+17 38.4% HOMO => L+20, 35.2% H-17 => L+2, 4.66% H-1 => L+17, 2.80% H-30 => LUMO
144	16154	619	0.00	31.1% H-13 => L+3, 20.3% H-1 => L+14, 13.8% HOMO => L+17, 10.3% H-3 => L+11, 6.19% H-6 => L+8
145	16184	618	0.00	14.6% HOMO => L+17, 12.0% H-15 => L+2, 11.9% H-11 => L+4, 11.0% H-33 => LUMO, 9.47% H-13 => L+3, 7.95% H-9 => L+5, 6.66% H-32 => LUMO, 5.43% H-38 => LUMO, 3.91% H-6 => L+8, 3.35% H-3 => L+11, 2.34% H-2 => L+10 50.1% H-3 => L+10, 16.4% H-1 => L+12, 9.90% H-6 => L+9, 3.16% H-6 => L+6, 2.50% H-3 => L+13, 2.04% H-1 => L+9
146	16224	616	0.00	47.5% H-35 => LUMO, 10.0% H-4 => L+10, 5.94% H-5 => L+9, 5.84% H-2 => L+12, 4.42% H-7 => L+7, 3.32% H-4 => L+7, 3.17% H-40 => LUMO, 2.65% H-33 => L+1 47.1% H-2 => L+10, 14.7% H-5 => L+7, 7.45% H-7 => L+6, 6.39% H-4 => L+6, 5.11% H-2 => L+7, 4.35% H-4 => L+12, 2.99% H-13 => L+3 36.6% H-7 => L+5, 30.1% H-5 => L+8, 10.2% H-4 => L+11, 4.40% H-2 => L+14, 4.32% H-16 => L+2, 3.49% H-8 => L+8, 2.30% H-5 => L+4 67.1% H-6 => L+6, 10.0% H-3 => L+7, 6.14% H-9 => L+7, 3.35% H-42 => LUMO, 2.54% H-3 => L+10 19.8% H-35 => LUMO, 17.7% H-4 => L+10, 13.4% H-5 => L+9, 8.40% H-2 => L+12, 6.85% H-40 => LUMO, 6.12% H-30 => LUMO, 3.92% HOMO => L+20, 3.76% H-7 => L+7, 3.13% H-29 => LUMO, 2.30% H-33 => L+1 47.1% H-16 => L+2, 7.50% H-14 => L+3, 5.98% H-12 => L+4, 4.78% H-10 => L+5, 4.12% H-7 => L+11, 3.66% HOMO => L+18, 3.37% H-7 => L+5, 2.92% H-5 => L+8, 2.56% H-8 => L+8, 2.49% H-5 => L+14, 2.08% H-4 => L+17 38.4% HOMO => L+20, 35.2% H-17 => L+2, 4.66% H-1 => L+17, 2.80% H-30 => LUMO
147	16230	616	0.11	31.1% H-13 => L+3, 20.3% H-1 => L+14, 13.8% HOMO => L+17, 10.3% H-3 => L+11, 6.19% H-6 => L+8
148	16274	614	0.00	14.6% HOMO => L+17, 12.0% H-15 => L+2, 11.9% H-11 => L+4, 11.0% H-33 => LUMO, 9.47% H-13 => L+3, 7.95% H-9 => L+5, 6.66% H-32 => LUMO, 5.43% H-38 => LUMO, 3.91% H-6 => L+8, 3.35% H-3 => L+11, 2.34% H-2 => L+10 50.1% H-3 => L+10, 16.4% H-1 => L+12, 9.90% H-6 => L+9, 3.16% H-6 => L+6, 2.50% H-3 => L+13, 2.04% H-1 => L+9
149	16292	614	0.00	47.5% H-35 => LUMO, 10.0% H-4 => L+10, 5.94% H-5 => L+9, 5.84% H-2 => L+12, 4.42% H-7 => L+7, 3.32% H-4 => L+7, 3.17% H-40 => LUMO, 2.65% H-33 => L+1 47.1% H-2 => L+10, 14.7% H-5 => L+7, 7.45% H-7 => L+6, 6.39% H-4 => L+6, 5.11% H-2 => L+7, 4.35% H-4 => L+12, 2.99% H-13 => L+3 36.6% H-7 => L+5, 30.1% H-5 => L+8, 10.2% H-4 => L+11, 4.40% H-2 => L+14, 4.32% H-16 => L+2, 3.49% H-8 => L+8, 2.30% H-5 => L+4 67.1% H-6 => L+6, 10.0% H-3 => L+7, 6.14% H-9 => L+7, 3.35% H-42 => LUMO, 2.54% H-3 => L+10 19.8% H-35 => LUMO, 17.7% H-4 => L+10, 13.4% H-5 => L+9, 8.40% H-2 => L+12, 6.85% H-40 => LUMO, 6.12% H-30 => LUMO, 3.92% HOMO => L+20, 3.76% H-7 => L+7, 3.13% H-29 => LUMO, 2.30% H-33 => L+1 47.1% H-16 => L+2, 7.50% H-14 => L+3, 5.98% H-12 => L+4, 4.78% H-10 => L+5, 4.12% H-7 => L+11, 3.66% HOMO => L+18, 3.37% H-7 => L+5, 2.92% H-5 => L+8, 2.56% H-8 => L+8, 2.49% H-5 => L+14, 2.08% H-4 => L+17 38.4% HOMO => L+20, 35.2% H-17 => L+2, 4.66% H-1 => L+17, 2.80% H-30 => LUMO
150	16307	613	0.00	31.1% H-13 => L+3, 20.3% H-1 => L+14, 13.8% HOMO => L+17, 10.3% H-3 => L+11, 6.19% H-6 => L+8

151	16326	613	0.00	63.5% H-2 => L+11, 17.0% H-4 => L+8, 4.75% H-2 => L+5, 3.34% H-4 => L+14 22.5% H-1 => L+15, 18.5% H-36 => LUMO, 15.6% HOMO => L+16, 4.32% H-3 => L+13, 4.29% H-39 => LUMO, 3.38% H-2 => L+11, 2.84% H-31 => LUMO, 2.64% H-37 => L+1, 2.58% H-6 => L+12, 2.35% H-10 => L+4, 2.23% H-21 => L+1, 2.09% HOMO => L+13, 2.07% H-34 => L+1
152	16367	611	0.01	40.6% H-4 => L+9, 20.4% H-5 => L+7, 7.79% H-7 => L+6, 7.24% H-2 => L+7, 4.78% H-38 => LUMO, 3.47% H-4 => L+6, 3.18% H-5 => L+10, 2.03% H-2 => L+10
153	16378	611	0.00	45.6% H-38 => LUMO, 9.03% H-13 => L+3, 7.30% H-2 => L+10, 5.99% H-40 => L+1, 5.91% H-35 => L+1, 4.52% H-4 => L+9, 3.92% H-33 => LUMO, 2.28% H-11 => L+4
154	16396	610	0.00	63.7% H-40 => LUMO, 13.0% H-38 => L+1, 5.84% H-35 => LUMO, 2.98% H-35 => L+2
155	16438	608	1.08	46.9% H-34 => LUMO, 27.2% HOMO => L+18, 4.72% H-22 => L+1, 2.77% H-6 => L+7, 2.49% H-36 => L+1
156	16468	607	0.00	41.7% H-6 => L+7, 8.89% H-3 => L+9, 8.64% H-43 => LUMO, 7.67% H-9 => L+6, 6.66% H-37 => LUMO, 4.22% H-34 => LUMO, 3.43% H-3 => L+6, 3.13% H-41 => LUMO, 2.88% H-6 => L+10
157	16478	607	0.00	19.9% H-18 => L+2, 15.9% H-21 => L+1, 12.8% HOMO => L+22, 8.71% H-1 => L+15, 7.46% H-36 => LUMO, 5.78% H-16 => L+3, 5.48% HOMO => L+19, 2.73% H-39 => LUMO, 2.71% H-14 => L+4, 2.49% H-1 => L+21
158	16483	607	0.00	47.5% H-23 => L+1, 11.6% H-24 => LUMO, 10.4% H-19 => L+2, 9.25% H-24 => L+2, 3.14% H-38 => LUMO, 2.31% H-23 => L+3
159	16498	606	0.00	50.3% H-24 => L+1, 12.6% H-23 => LUMO, 9.81% H-23 => L+2, 9.23% H-20 => L+2, 2.31% H-24 => L+3
160	16509	606	0.03	51.3% H-10 => L+4, 11.5% H-8 => L+5, 9.28% H-7 => L+8, 5.69% H-5 => L+11, 4.07% H-4 => L+14, 3.97% H-31 => LUMO, 2.44% H-2 => L+17
161	16515	606	0.00	38.2% HOMO => L+19, 22.6% H-31 => LUMO, 8.20% HOMO => L+22, 4.57% H-18 => L+2, 4.07% H-1 => L+15, 3.31% H-10 => L+4, 2.53% H-22 => L+2, 2.19% H-39 => LUMO
162	16593	603	0.04	41.4% H-37 => LUMO, 8.67% H-41 => LUMO, 8.56% H-6 => L+7, 8.27% H-3 => L+12, 8.18% H-1 => L+13, 3.29% H-43 => LUMO, 2.70% H-9 => L+9, 2.11% HOMO => L+15
163	16606	602	0.00	33.0% H-1 => L+14, 22.3% H-11 => L+4, 10.9% H-13 => L+3, 10.7% H-38 => LUMO, 7.46% H-9 => L+5, 3.62% H-6 => L+8
164	16610	602	0.00	

				35.1% H-36 => LUMO, 26.2% H-39 => LUMO, 5.16% HOMO => L+19, 5.10% H-1 => L+15, 4.12% H-21 => L+1, 2.93% H-18 => L+2, 2.67% HOMO => L+16, 2.64% H-3 => L+10, 2.05% H-1 => L+18 57.6% H-20 => L+2, 8.13% H-24 => L+1, 6.74% H- 17 => L+2, 5.32% H-19 => L+3, 4.14% H-19 => L+1, 3.04% HOMO => L+20
165	16632	601	0.00	
166	16665	600	0.01	61.6% H-19 => L+2, 10.9% H-23 => L+1, 3.84% H- 20 => L+3, 2.61% H-17 => L+1, 2.48% H-20 => L+1, 2.32% H-17 => L+3, 2.17% H-24 => LUMO 35.8% H-2 => L+12, 20.2% H-5 => L+9, 12.0% H-7 => L+7, 6.11% H-8 => L+6, 5.60% H-4 => L+7, 5.28% H-4 => L+10, 2.03% H-4 => L+13
167	16675	600	0.00	21.4% H-41 => LUMO, 21.1% H-37 => LUMO, 15.3% H-3 => L+12, 12.2% H-43 => LUMO, 5.52% H-1 => L+16, 4.28% H-45 => LUMO, 2.32% H-39 => L+1, 2.30% H-3 => L+15
168	16744	597	0.26	37.4% H-11 => L+4, 17.1% H-1 => L+14, 12.8% H- 3 => L+11, 11.9% H-6 => L+8, 6.81% H-9 => L+5 17.1% H-14 => L+3, 15.0% H-41 => LUMO, 13.1% HOMO => L+21, 10.4% H-22 => L+1, 3.97% H-3 => L+12, 3.47% H-1 => L+13, 2.86% H-2 => L+20, 2.60% H-16 => L+4, 2.15% H-7 => L+11
169	16746	597	0.00	49.2% H-42 => LUMO, 19.0% H-39 => LUMO, 4.91% H-36 => LUMO, 4.72% H-6 => L+6, 4.12% H-1 => L+15, 3.50% H-3 => L+10, 2.70% H-3 => L+13, 2.24% H-43 => L+1
170	16780	596	0.00	26.1% H-43 => LUMO, 10.9% H-3 => L+12, 8.48% H-14 => L+3, 7.65% H-41 => LUMO, 5.56% H-1 => L+13, 3.85% H-45 => LUMO, 3.68% H-6 => L+10, 3.35% HOMO => L+21, 2.99% H-3 => L+9, 2.14% H-22 => L+1
171	16826	594	0.00	56.2% H-7 => L+6, 18.5% H-5 => L+7, 6.96% H-4 => L+6, 5.07% H-8 => L+7, 2.45% H-7 => L+9 18.1% H-4 => L+11, 14.3% H-41 => LUMO, 13.6% H-5 => L+8, 13.3% H-43 => LUMO, 7.42% H-14 => L+3, 4.60% H-2 => L+14, 3.46% H-1 => L+13, 2.97% H-6 => L+7, 2.77% H-3 => L+12, 2.57% H-5 => L+14
172	16832	594	0.00	28.7% H-42 => LUMO, 15.4% H-39 => LUMO, 10.6% H-1 => L+15, 8.13% H-36 => LUMO, 6.87% H-44 => LUMO, 5.59% H-6 => L+9, 3.63% H-3 => L+10, 2.25% H-41 => L+1
173	16862	593	0.00	20.0% H-4 => L+11, 17.9% H-43 => LUMO, 15.0% H-5 => L+8, 13.0% H-41 => LUMO, 6.32% H-6 => L+7, 5.72% H-2 => L+14, 3.80% H-45 => LUMO, 2.93% H-1 => L+13, 2.26% H-42 => L+1
174	16863	593	0.00	33.9% H-9 => L+5, 32.2% H-3 => L+11, 5.40% H- 11 => L+4, 4.77% H-4 => L+12, 4.33% H-5 => L+10, 2.55% H-1 => L+14, 2.34% H-2 => L+13
175	16884	592	0.00	
176	16888	592	0.00	
177	16909	591	0.00	
178	16925	591	0.00	

				32.0% H-14 => L+3, 31.7% HOMO => L+21, 10.4% H-22 => L+1, 2.48% H-12 => L+4, 2.39% H-10 => L+5, 2.05% H-34 => LUMO
179	16947	590	0.01	21.0% H-4 => L+10, 17.0% H-15 => L+3, 12.6% H-2 => L+12, 6.22% H-17 => L+2, 5.58% HOMO => L+20, 5.29% H-2 => L+9, 4.63% H-13 => L+4, 3.52% H-11 => L+5, 2.12% H-9 => L+8
180	16969	589	0.03	21.2% H-4 => L+10, 15.2% H-2 => L+12, 11.4% H-15 => L+3, 6.25% H-2 => L+9, 5.63% H-5 => L+9, 5.50% H-13 => L+4, 4.97% HOMO => L+20, 4.80% H-17 => L+2, 2.52% H-11 => L+5, 2.10% H-30 => LUMO, 2.10% H-9 => L+8
181	16978	589	0.10	22.0% H-4 => L+12, 18.0% H-5 => L+10, 10.2% H-2 => L+13, 9.44% H-9 => L+5, 7.56% H-3 => L+11, 6.13% H-7 => L+9, 5.96% H-27 => LUMO, 2.57% H-25 => L+1, 2.25% H-6 => L+8
182	17001	588	0.00	31.7% H-6 => L+9, 20.8% H-44 => LUMO, 11.2% H-3 => L+10, 8.63% H-8 => L+5, 3.63% H-45 => L+1, 3.36% H-3 => L+7, 3.16% H-39 => LUMO, 3.15% H-9 => L+7, 2.30% H-7 => L+8
183	17049	587	0.00	37.6% H-8 => L+5, 10.4% H-18 => L+2, 9.48% H-7 => L+8, 8.16% HOMO => L+22, 5.66% H-5 => L+11, 4.75% H-44 => LUMO, 3.68% H-6 => L+9, 3.43% H-4 => L+14, 2.86% H-10 => L+8
184	17064	586	0.07	55.1% H-6 => L+8, 16.1% H-3 => L+11, 15.3% H-9 => L+5, 2.35% H-7 => L+6
185	17068	586	0.00	38.7% H-18 => L+2, 17.2% HOMO => L+22, 10.5% H-8 => L+5, 3.03% HOMO => L+19, 2.85% H-7 => L+8, 2.31% H-21 => L+3, 2.25% H-6 => L+9
186	17084	585	0.21	50.0% H-45 => LUMO, 16.3% H-1 => L+16, 7.35% H-44 => L+1, 4.37% H-3 => L+15, 2.03% HOMO => L+18
187	17176	582	0.00	41.9% H-7 => L+7, 25.1% H-5 => L+9, 10.1% H-8 => L+6, 7.04% H-5 => L+6, 4.67% H-4 => L+7, 2.53% H-7 => L+10
188	17186	582	0.06	40.7% H-44 => LUMO, 16.6% H-6 => L+9, 10.8% H-39 => LUMO, 6.74% H-1 => L+15, 6.38% H-45 => L+1, 2.31% H-9 => L+7
189	17195	582	0.01	24.2% H-1 => L+16, 15.9% H-3 => L+12, 15.6% H-45 => LUMO, 9.46% H-37 => LUMO, 5.38% HOMO => L+18, 3.56% H-34 => LUMO, 3.00% H-43 => LUMO, 2.43% H-44 => L+1, 2.31% HOMO => L+21, 2.30% H-6 => L+13, 2.14% H-3 => L+15
190	17259	579	0.00	65.4% H-25 => L+1, 5.34% H-27 => LUMO, 4.56% H-5 => L+10, 3.55% H-17 => L+3, 2.67% H-29 => L+1, 2.14% H-27 => L+2, 2.02% H-7 => L+9
191	17274	579	0.00	45.3% H-26 => L+1, 12.1% H-15 => L+3, 7.02% H-1 => L+17, 6.43% H-29 => LUMO, 3.51% H-3 => L+14, 3.04% H-27 => L+1, 2.89% HOMO => L+20, 2.27% H-6 => L+11
192	17293	578	0.00	

193	17370	576	0.00	29.0% H-2 => L+13, 19.1% H-7 => L+9, 11.6% H-4 => L+12, 9.97% H-5 => L+10, 8.91% H-8 => L+7, 4.41% H-10 => L+6, 2.38% H-5 => L+7, 2.25% H-4 => L+9 29.8% H-26 => L+1, 15.6% H-15 => L+3, 13.2% H-1 => L+17, 7.87% HOMO => L+20, 4.81% H-3 => L+14, 3.52% H-6 => L+11, 3.23% H-27 => L+1, 2.52% H-29 => LUMO, 2.21% H-9 => L+8
194	17389	575	0.01	14.8% H-28 => L+1, 13.1% H-1 => L+18, 11.0% H-3 => L+13, 9.22% HOMO => L+19, 7.16% H-22 => L+2, 6.30% H-1 => L+15, 6.04% H-3 => L+16, 4.78% H-7 => L+8, 4.61% H-44 => LUMO, 2.90% H-6 => L+12, 2.22% H-31 => LUMO 67.1% H-12 => L+4, 4.27% H-7 => L+11, 4.25% H-5 => L+14, 3.74% H-2 => L+20, 3.57% H-4 => L+17, 3.29% H-8 => L+8, 2.61% H-14 => L+5,
195	17454	573	0.03	2.57% H-10 => L+3, 2.25% HOMO => L+21 38.4% H-27 => L+1, 7.67% H-15 => L+3, 6.45% H-30 => LUMO, 6.44% H-25 => LUMO, 6.24% H-5 => L+12, 6.16% H-4 => L+13, 3.16% H-7 => L+10, 2.88% H-2 => L+15, 2.78% H-30 => L+2
196	17459	573	0.00	55.9% H-21 => L+2, 12.1% HOMO => L+21, 5.46% H-1 => L+16, 3.76% H-1 => L+19, 3.58% H-22 => L+1, 2.50% H-18 => L+3, 2.19% H-22 => L+3 18.4% H-29 => L+1, 9.99% H-17 => L+3, 8.86% H-32 => LUMO, 6.51% H-25 => L+1, 4.55% H-15 => L+4, 4.35% H-2 => L+22, 3.96% H-4 => L+21, 3.92% H-19 => L+2, 3.85% H-1 => L+20, 3.34% H-13 => L+5, 3.00% H-33 => LUMO, 2.77% H-30 => L+1, 2.62% H-11 => L+8, 2.42% H-5 => L+19, 2.40% H-3 => L+17, 2.26% H-26 => L+2, 2.24% H-9 => L+11, 2.12% H-6 => L+14
197	17487	572	0.01	35.7% H-28 => L+1, 24.2% H-3 => L+13, 6.91% H-1 => L+15, 4.01% H-6 => L+12, 2.91% H-22 => L+2, 2.35% H-44 => LUMO, 2.23% H-16 => L+3 39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15
198	17514	571	0.01	39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4 29.3% H-2 => L+14, 22.0% H-6 => L+10, 9.31% H-4 => L+11, 8.51% H-3 => L+12, 5.95% H-9 => L+9, 3.80% H-9 => L+6, 2.96% H-2 => L+8, 2.52% H-4 => L+17, 2.38% H-1 => L+16
199	17575	569	0.00	39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15 39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4
200	17589	569	0.07	39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15 39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4 29.3% H-2 => L+14, 22.0% H-6 => L+10, 9.31% H-4 => L+11, 8.51% H-3 => L+12, 5.95% H-9 => L+9, 3.80% H-9 => L+6, 2.96% H-2 => L+8, 2.52% H-4 => L+17, 2.38% H-1 => L+16
201	17642	567	0.03	39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4 39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15 39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4
202	17659	566	0.23	39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15 39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4 29.3% H-2 => L+14, 22.0% H-6 => L+10, 9.31% H-4 => L+11, 8.51% H-3 => L+12, 5.95% H-9 => L+9, 3.80% H-9 => L+6, 2.96% H-2 => L+8, 2.52% H-4 => L+17, 2.38% H-1 => L+16
203	17665	566	0.00	39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15 39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4 29.3% H-2 => L+14, 22.0% H-6 => L+10, 9.31% H-4 => L+11, 8.51% H-3 => L+12, 5.95% H-9 => L+9, 3.80% H-9 => L+6, 2.96% H-2 => L+8, 2.52% H-4 => L+17, 2.38% H-1 => L+16

				38.9% H-4 => L+12, 31.6% H-2 => L+13, 9.77% H-2 => L+10, 8.30% H-5 => L+10, 2.84% H-5 => L+13, 2.83% H-4 => L+15
204	17699	565	0.00	28.8% H-1 => L+17, 27.0% H-13 => L+4, 10.6% H-15 => L+3, 7.45% H-11 => L+5, 3.31% H-8 => L+6, 2.45% H-9 => L+8
205	17701	565	0.01	34.3% H-9 => L+6, 21.5% H-2 => L+14, 9.74% H-6 => L+10, 9.18% H-4 => L+11, 4.80% H-6 => L+7, 3.96% H-9 => L+9, 2.44% H-3 => L+12, 2.02% H-2 => L+8
206	17714	565	0.00	34.0% H-5 => L+10, 24.3% H-7 => L+9, 7.44% H-2 => L+13, 5.28% H-8 => L+7, 4.22% H-30 => L+1, 4.16% H-4 => L+9, 3.52% H-29 => L+1, 3.20% H-5 => L+7, 2.62% H-7 => L+12
207	17732	564	0.00	35.4% H-9 => L+6, 20.6% H-6 => L+10, 8.98% H-2 => L+14, 6.76% H-11 => L+7, 6.05% H-6 => L+7, 5.48% H-3 => L+12, 2.82% H-4 => L+11, 2.26% H-3 => L+9
208	17737	564	0.00	21.5% H-28 => L+1, 20.8% H-16 => L+3, 15.9% H-1 => L+18, 9.91% HOMO => L+22, 5.09% H-3 => L+13, 3.85% H-1 => L+21, 3.11% H-22 => L+2, 2.17% H-34 => L+1
209	17784	562	0.18	38.0% H-29 => L+1, 12.9% H-30 => L+1, 6.75% H-7 => L+9, 4.00% H-33 => LUMO, 2.61% H-15 => L+4, 2.52% H-20 => L+3, 2.32% H-17 => L+3, 2.22% H-27 => L+2, 2.01% H-5 => L+10
210	17785	562	0.00	22.4% H-4 => L+13, 17.7% H-27 => L+1, 17.7% H-2 => L+15, 11.6% H-5 => L+12, 3.41% H-24 => L+1, 2.73% H-15 => L+3, 2.28% H-25 => L+2,
211	17832	561	0.00	2.09% H-23 => L+2
				59.5% H-8 => L+6, 14.9% H-7 => L+7, 4.81% H-10 => L+7, 4.71% H-5 => L+6, 2.63% H-8 => L+9,
212	17835	561	0.01	2.02% H-1 => L+17
				35.3% H-30 => L+1, 15.2% H-17 => L+3, 10.8% H-20 => L+3, 3.06% H-33 => LUMO, 2.92% H-27 => L+2, 2.86% H-27 => LUMO, 2.85% H-29 => L+1,
213	17895	559	0.00	2.57% H-1 => L+20, 2.34% H-26 => LUMO
				37.5% H-10 => L+5, 20.5% H-31 => L+1, 7.96% H-1 => L+19, 2.82% HOMO => L+21, 2.65% H-21 =>
214	17912	558	0.00	L+2, 2.62% H-2 => L+20, 2.37% H-12 => L+8
				44.7% H-31 => L+1, 22.9% H-10 => L+5, 4.48% H-28 => L+2, 2.60% H-36 => L+1, 2.49% H-34 =>
215	17972	556	0.00	LUMO, 2.30% H-4 => L+17
				52.1% H-22 => L+2, 12.0% H-1 => L+18, 4.94% H-1 => L+21, 4.70% H-28 => L+1, 3.43% H-34 =>
216	17984	556	0.00	L+1, 2.71% H-5 => L+11, 2.61% H-21 => L+1
				25.0% H-13 => L+4, 17.6% H-1 => L+17, 8.80% H-32 => L+1, 6.95% H-9 => L+8, 6.18% H-6 => L+11,
217	17993	556	0.03	5.39% H-3 => L+14, 4.37% H-11 => L+5
				56.4% H-9 => L+7, 13.8% H-6 => L+9, 10.1% H-11 => L+6, 4.63% H-6 => L+6

				13.9% H-19 => L+3, 12.6% H-33 => L+1, 12.0% H-7 => L+10, 5.91% H-2 => L+15, 5.80% H-27 => L+1, 5.58% H-32 => L+1, 5.29% H-5 => L+12, 4.66% H-8 => L+9, 3.02% H-20 => L+2, 2.87% H-26 => L+1, 2.31% H-17 => L+4, 2.26% H-10 => L+7
219	18038	554	0.18	15.3% H-32 => L+1, 10.3% H-7 => L+10, 8.38% H-2 => L+15, 6.97% H-19 => L+3, 6.57% H-13 => L+4, 5.59% H-5 => L+12, 4.97% H-8 => L+9, 3.25% H-6 => L+11, 3.04% H-3 => L+14, 2.94% H-26 => L+1, 2.93% H-1 => L+17, 2.59% H-10 => L+7, 2.58% H-4 => L+13, 2.26% H-9 => L+8
220	18059	554	0.09	39.7% H-17 => L+3, 20.3% H-1 => L+20, 5.35% H-3 => L+17, 4.03% H-24 => L+2, 3.19% H-19 => L+4, 2.79% H-6 => L+14, 2.76% H-25 => L+1, 2.27% H-19 => L+2
221	18079	553	0.00	16.5% H-1 => L+19, 15.5% H-3 => L+15, 14.0% H-1 => L+16, 8.66% H-10 => L+5, 6.93% H-3 => L+18, 4.55% H-6 => L+13, 4.32% H-21 => L+2, 3.71% H-1 => L+22, 2.59% H-9 => L+12, 2.11% H-18 => L+3, 2.09% H-8 => L+8
222	18081	553	0.00	31.6% H-8 => L+7, 13.3% H-24 => L+2, 12.9% H-7 => L+9, 7.40% H-23 => L+1, 7.04% H-10 => L+6, 4.18% H-7 => L+6, 3.09% H-23 => L+3, 2.25% H-1 => L+20, 2.20% H-5 => L+7, 2.09% H-2 => L+16
223	18136	551	0.00	34.8% H-33 => L+1, 17.7% H-32 => L+1, 6.19% H-13 => L+4, 5.41% H-35 => LUMO, 3.14% H-7 => L+10, 2.92% H-30 => L+2, 2.74% H-30 => LUMO,
224	18138	551	0.06	2.26% H-2 => L+15, 2.25% H-23 => L+2
				23.7% H-24 => L+2, 17.7% H-8 => L+7, 13.0% H-23 => L+1, 6.52% H-1 => L+20, 5.72% H-7 => L+9, 5.16% H-23 => L+3, 2.99% H-10 => L+6, 2.75% H-7 => L+6
225	18161	551	0.00	34.4% H-14 => L+4, 11.8% H-16 => L+3, 10.5% HOMO => L+22, 8.60% H-1 => L+21, 8.30% H-12 => L+5, 3.16% H-3 => L+19, 3.15% H-10 => L+8, 2.77% H-34 => L+1
226	18180	550	0.18	19.6% H-3 => L+14, 16.0% H-23 => L+2, 15.9% H-11 => L+5, 11.8% H-5 => L+12, 5.77% H-24 => L+1, 5.14% H-1 => L+17, 3.10% H-24 => L+3, 2.86% H-6 => L+11, 2.29% H-4 => L+13, 2.16% H-13 => L+4
227	18215	549	0.03	26.8% H-23 => L+2, 17.4% H-11 => L+5, 12.5% H-3 => L+14, 9.57% H-24 => L+1, 5.32% H-24 => L+3, 5.25% H-19 => L+3, 2.82% H-13 => L+4, 2.40% H-33 => L+1, 2.02% H-9 => L+8
228	18235	548	0.11	33.4% H-5 => L+11, 22.9% H-4 => L+14, 11.4% H-2 => L+17, 11.0% H-34 => L+1, 3.30% H-4 => L+8
229	18259	548	0.00	44.5% H-20 => L+3, 8.85% H-29 => L+1, 8.30% H-30 => L+1, 4.51% H-35 => L+1, 3.91% H-19 => L+2, 3.46% H-19 => L+4
230	18279	547	0.00	

				33.3% H-34 => L+1, 12.0% H-3 => L+13, 10.0% H-6 => L+12, 6.71% H-5 => L+11, 3.49% H-4 => L+14, 3.10% H-1 => L+18, 2.80% H-9 => L+10, 2.74% H-31 => L+2, 2.19% H-22 => L+2
231	18290	547	0.03	23.4% H-3 => L+15, 15.2% H-18 => L+3, 9.10% H-21 => L+2, 7.34% H-1 => L+16, 5.52% H-8 => L+8, 4.37% H-1 => L+19, 3.88% H-36 => L+1, 3.54% H-16 => L+4, 3.52% H-31 => L+1, 3.26% H-6 => L+13, 2.05% HOMO => L+21
232	18297	547	0.00	30.3% H-19 => L+3, 25.8% H-32 => L+1, 14.9% H-33 => L+1, 3.12% H-20 => L+4
233	18344	545	0.00	64.3% H-35 => L+1, 4.94% H-33 => LUMO, 4.84% H-38 => LUMO, 4.02% H-33 => L+2, 3.59% H-20 => L+3, 3.52% H-40 => L+1
234	18372	544	0.00	35.9% H-1 => L+22, 14.6% H-18 => L+3, 11.1% H-36 => L+1, 7.10% H-1 => L+19, 3.64% H-3 => L+21, 2.43% HOMO => L+21, 2.24% H-16 => L+4, 2.02% H-8 => L+8, 2.02% H-3 => L+15
235	18373	544	0.00	28.9% H-6 => L+12, 16.6% H-34 => L+1, 11.3% H-3 => L+13, 10.3% H-37 => L+1, 6.75% H-9 => L+10, 4.01% H-1 => L+18, 2.73% H-11 => L+9
236	18376	544	0.01	21.3% H-9 => L+8, 18.6% H-3 => L+14, 13.2% H-5 => L+12, 9.07% H-7 => L+10, 6.96% H-4 => L+13, 6.34% H-6 => L+11, 6.20% H-11 => L+5, 2.51% H-4 => L+10
237	18393	544	0.20	35.6% H-2 => L+15, 32.7% H-4 => L+13, 8.18% H-2 => L+12, 4.75% H-7 => L+10, 3.16% H-3 => L+14, 3.01% H-4 => L+16, 2.60% H-5 => L+15
238	18432	543	0.05	83.5% H-46 => LUMO, 7.25% H-47 => L+1, 2.04% H-48 => L+2
239	18439	542	0.00	24.2% H-5 => L+12, 14.4% H-11 => L+5, 13.4% H-6 => L+11, 9.81% H-7 => L+10, 6.89% H-8 => L+9, 5.03% H-3 => L+14, 2.93% H-9 => L+8, 2.87% H-4 => L+10, 2.49% H-2 => L+15, 2.01% H-4 => L+13
240	18442	542	0.08	38.2% H-8 => L+8, 12.7% H-9 => L+9, 11.1% H-18 => L+3, 6.22% H-6 => L+10, 5.24% H-2 => L+20, 4.38% H-4 => L+17, 3.32% H-5 => L+14, 2.24% H-11 => L+7, 2.06% H-7 => L+5
241	18463	542	0.00	23.6% H-9 => L+9, 15.4% H-36 => L+1, 14.1% H-8 => L+8, 11.4% H-6 => L+10, 4.48% H-11 => L+7,
242	18481	541	0.00	2.97% H-1 => L+22, 2.20% H-13 => L+6
243	18496	541	0.00	22.0% H-2 => L+16, 21.4% H-4 => L+15, 10.8% H-20 => L+3, 7.29% H-5 => L+13, 4.75% H-24 => L+2, 4.33% H-1 => L+20, 2.29% H-26 => L+2, 2.19% H-10 => L+9
244	18522	540	0.00	33.9% H-36 => L+1, 16.5% H-39 => L+1, 12.3% H-9 => L+9, 4.24% H-3 => L+15, 3.93% H-1 => L+22, 3.13% H-6 => L+10, 2.89% H-8 => L+8, 2.87% H-34 => L+2, 2.19% H-11 => L+7

				38.8% H-6 => L+11, 35.3% H-9 => L+8, 4.22% H-11 => L+5, 3.49% H-3 => L+14, 2.89% H-38 => L+1
245	18530	540	0.02	76.4% H-47 => LUMO, 9.22% H-46 => L+1, 4.99% H-48 => L+1
246	18538	539	0.00	32.8% H-14 => L+4, 14.1% H-1 => L+21, 12.3% H-1 => L+18, 4.99% H-3 => L+16, 3.69% H-37 => L+1, 3.62% H-3 => L+19, 2.88% H-12 => L+5, 2.72% H-10 => L+8
247	18558	539	0.09	53.3% H-38 => L+1, 11.5% H-40 => LUMO, 6.23% H-40 => L+2, 4.36% H-6 => L+11, 4.30% H-35 => LUMO, 4.18% H-11 => L+5, 3.73% H-35 => L+2, 2.69% H-8 => L+9
248	18625	537	0.25	50.0% H-40 => L+1, 9.82% H-38 => LUMO, 7.24% H-1 => L+20, 6.49% H-38 => L+2, 3.70% H-24 => L+2, 2.98% H-15 => L+4, 2.78% H-17 => L+3, 2.05% H-11 => L+8, 2.02% H-13 => L+5 43.9% H-37 => L+1, 25.6% H-41 => L+1, 4.14% H-14 => L+4, 4.12% H-36 => L+2, 3.75% H-6 =>
249	18635	537	0.00	L+12, 3.37% H-34 => L+1, 2.46% H-36 => LUMO 19.3% H-15 => L+4, 17.8% H-1 => L+20, 17.7% H-40 => L+1, 8.20% H-17 => L+3, 4.58% H-13 => L+5, 4.02% H-38 => LUMO, 3.96% H-24 => L+2, 3.29% H-30 => L+1, 2.99% H-38 => L+2
250	18639	536	0.00	37.9% H-8 => L+9, 24.6% H-7 => L+10, 6.95% H-10 => L+7, 3.87% H-7 => L+7, 3.63% H-38 => L+1, 3.03% H-5 => L+9, 2.95% H-9 => L+8, 2.56% H-8 => L+12, 2.27% H-12 => L+6
251	18675	535	0.00	33.2% H-43 => L+1, 31.0% H-41 => L+1, 8.22% H-37 => L+1, 4.62% H-12 => L+5, 2.86% H-3 =>
252	18682	535	0.02	L+16, 2.83% H-39 => L+2, 2.51% H-39 => LUMO 42.6% H-39 => L+1, 26.6% H-42 => L+1, 6.80% H-36 => L+1, 4.19% H-37 => L+2, 3.24% H-37 => LUMO
253	18706	535	0.01	65.1% H-48 => LUMO, 7.69% H-47 => L+1, 4.46% H-49 => L+1, 3.10% H-7 => L+12, 2.72% H-46 =>
254	18710	534	0.00	L+2 24.6% H-18 => L+3, 17.5% H-1 => L+22, 14.4% H-1 => L+19, 7.60% H-7 => L+11, 5.88% H-8 => L+8, 4.69% H-3 => L+21, 4.10% H-3 => L+15, 2.79% H-42 => L+1
255	18716	534	0.00	19.2% H-7 => L+12, 14.7% H-5 => L+13, 9.57% H-48 => LUMO, 9.47% H-8 => L+10, 8.79% H-2 => L+16, 5.24% H-10 => L+6, 5.08% H-10 => L+9, 3.21% H-8 => L+7, 2.31% H-2 => L+19
256	18738	534	0.01	14.6% H-3 => L+16, 14.3% H-43 => L+1, 8.13% H-4 => L+14, 6.95% H-2 => L+17, 6.33% H-12 => L+5, 5.33% H-1 => L+18, 3.67% H-14 => L+4, 3.32% H-6 => L+15, 3.23% H-6 => L+12, 3.08% H-21 => L+3, 2.88% H-22 => L+2, 2.63% H-9 => L+13
257	18760	533	0.00	
258	18792	532	0.00	

				28.8% H-25 => L+2, 11.3% H-2 => L+18, 9.68% H-4 => L+16, 5.23% H-32 => L+1, 4.26% H-5 => L+15, 4.09% H-2 => L+21, 3.28% H-17 => L+4, 2.31% H-3 => L+20, 2.05% H-33 => L+1, 2.03% H-25 => LUMO
259	18839	531	0.00	22.9% H-43 => L+1, 14.1% H-2 => L+17, 13.4% H-4 => L+14, 8.55% H-41 => L+1, 5.86% H-12 => L+5, 3.77% H-42 => L+2, 3.20% H-1 => L+21, 3.06% H-2 => L+11, 2.83% H-4 => L+20, 2.71% H-42 => LUMO
260	18858	530	0.17	58.0% H-10 => L+6, 10.8% H-8 => L+7, 7.08% H-12 => L+7, 4.76% H-7 => L+12, 3.16% H-7 => L+6, 2.03% H-8 => L+10
261	18874	530	0.00	44.4% H-42 => L+1, 10.5% H-39 => L+1, 4.97% H-44 => L+1, 4.27% H-43 => L+2, 3.53% H-7 => L+11, 3.31% H-41 => LUMO, 3.05% H-41 => L+2, 2.87% H-9 => L+9, 2.80% H-43 => LUMO
262	18881	530	0.00	17.0% H-12 => L+5, 12.7% H-41 => L+1, 9.87% H-43 => L+1, 6.07% H-1 => L+21, 5.24% H-37 => L+1, 5.23% H-2 => L+17, 4.68% H-45 => L+1, 4.30% H-4 => L+14, 3.37% H-3 => L+16, 3.01% H-11 => L+6, 2.95% H-9 => L+7, 2.88% H-1 => L+18, 2.29% H-42 => L+2
263	18912	529	0.22	71.3% H-49 => LUMO, 10.7% H-48 => L+1, 4.11% H-50 => L+1, 3.38% H-47 => L+2, 2.18% H-51 => LUMO
264	18919	529	0.00	42.8% H-26 => L+2, 10.3% H-15 => L+4, 7.04% H-5 => L+13, 3.92% H-4 => L+15, 3.83% H-1 => L+20, 3.67% H-2 => L+16, 2.64% H-29 => L+1
265	18962	527	0.00	41.5% H-7 => L+11, 8.65% H-6 => L+13, 7.10% H-3 => L+15, 5.40% H-2 => L+20, 5.18% H-4 => L+17, 3.15% H-44 => L+1, 2.86% H-5 => L+14, 2.65% H-5 => L+8, 2.60% H-9 => L+12, 2.04% H-8 => L+14
266	18979	527	0.00	17.5% H-21 => L+3, 14.6% H-12 => L+5, 11.2% H-2 => L+17, 8.53% H-1 => L+21, 6.84% H-3 => L+16, 6.06% H-22 => L+2, 3.81% H-4 => L+14, 3.41% H-6 => L+12, 3.08% H-18 => L+4, 2.81% H-11 => L+6, 2.33% H-9 => L+10
267	19023	526	0.21	27.0% H-15 => L+4, 11.0% H-3 => L+17, 10.2% H-4 => L+15, 7.54% H-1 => L+20, 7.12% H-26 => L+2, 5.99% H-6 => L+14, 4.14% H-9 => L+11, 2.33% H-5 => L+16, 2.10% H-2 => L+19, 2.01% H-2 => L+13
268	19028	526	0.00	16.6% H-6 => L+13, 15.9% H-3 => L+15, 10.2% H-7 => L+11, 8.22% H-1 => L+19, 6.31% H-39 => L+1, 5.36% H-9 => L+12, 3.31% H-42 => L+1, 2.89% H-6 => L+16, 2.53% H-11 => L+10, 2.38% H-22 => L+3, 2.12% H-1 => L+22
269	19029	526	0.00	16.1% H-25 => L+2, 15.7% H-2 => L+18, 11.3% H-4 => L+16, 6.60% H-8 => L+9, 4.43% H-27 => L+1,
270	19034	525	0.02	

				4.06% H-10 => L+7, 3.80% H-17 => L+4, 3.27% H-10 => L+10, 2.68% H-5 => L+15, 2.68% H-19 => L+3, 2.63% H-23 => L+2 56.8% H-11 => L+6, 8.41% H-9 => L+7, 3.85% H-11 => L+9, 3.34% H-41 => L+1, 2.89% H-13 => L+7, 2.52% H-6 => L+6, 2.36% H-9 => L+10, 2.16% H-2 => L+17, 2.16% H-6 => L+12, 2.03% H-4 => L+14 25.2% H-50 => LUMO, 17.6% H-5 => L+13, 9.56% H-2 => L+16, 7.99% H-7 => L+12, 4.94% H-26 => L+2, 4.50% H-8 => L+10, 4.22% H-49 => L+1, 2.23% H-4 => L+12, 2.19% H-4 => L+18 29.9% H-9 => L+10, 21.5% H-6 => L+12, 6.72% H-12 => L+5, 5.53% H-13 => L+7, 5.50% H-11 => L+9, 4.92% H-11 => L+6, 2.78% H-6 => L+9, 2.00% H-21 => L+3 26.7% H-16 => L+4, 16.4% H-44 => L+1, 8.37% H-18 => L+3, 5.45% H-14 => L+5, 4.35% H-45 => LUMO, 3.37% H-1 => L+19, 2.95% H-45 => L+2, 2.54% H-3 => L+18, 2.42% H-7 => L+11, 2.07% H-4 => L+17 25.0% H-4 => L+15, 23.0% H-5 => L+13, 14.8% H-50 => LUMO, 4.40% H-2 => L+16, 3.79% H-2 => L+13, 3.01% H-4 => L+12, 2.38% H-49 => L+1, 2.29% H-7 => L+12, 2.09% H-8 => L+10, 2.09% H-7 => L+15 13.4% H-25 => L+2, 10.8% H-19 => L+3, 7.09% H-17 => L+4, 5.39% H-23 => L+2, 5.24% H-15 => L+5, 4.62% H-2 => L+21, 3.81% H-13 => L+8, 3.71% H-4 => L+22, 3.65% H-10 => L+7, 3.61% H-3 => L+20, 3.22% H-11 => L+11, 3.04% H-6 => L+17, 2.91% H-9 => L+14, 2.27% H-7 => L+13 28.5% H-50 => LUMO, 15.4% H-2 => L+16, 10.1% H-26 => L+2, 8.25% H-4 => L+15, 4.48% H-49 => L+1, 4.26% H-4 => L+18, 4.22% H-7 => L+12, 2.47% H-10 => L+6 56.5% H-45 => L+1, 13.4% H-44 => LUMO, 8.71% H-44 => L+2, 3.62% H-12 => L+5 41.3% H-10 => L+7, 12.1% H-8 => L+9, 10.1% H-25 => L+2, 7.30% H-12 => L+6, 5.27% H-8 => L+6, 3.66% H-12 => L+9, 2.63% H-4 => L+16 38.6% H-44 => L+1, 12.2% H-16 => L+4, 8.31% H-45 => LUMO, 5.59% H-45 => L+2, 4.83% H-6 => L+13, 3.75% H-1 => L+19, 2.64% H-3 => L+15, 2.35% H-18 => L+3, 2.05% H-3 => L+18 33.3% H-21 => L+3, 15.5% H-3 => L+16, 9.79% H-12 => L+5, 7.91% H-10 => L+8, 7.34% H-9 => L+10, 2.66% H-8 => L+11 20.3% H-7 => L+12, 9.84% H-2 => L+19, 5.23% H-4 => L+18, 4.15% H-10 => L+9, 3.90% H-20 => L+3, 3.77% H-19 => L+4, 3.35% H-8 => L+10,
271	19061	525	0.01	
272	19132	523	0.00	
273	19134	523	0.01	
274	19137	523	0.00	
275	19145	522	0.00	
276	19154	522	0.00	
277	19171	522	0.00	
278	19190	521	0.00	
279	19192	521	0.00	
280	19220	520	0.00	
281	19240	520	0.00	
282	19265	519	0.00	

				3.11% H-26 => L+2, 3.07% H-2 => L+22, 3.05% H-15 => L+4, 2.92% H-13 => L+5, 2.75% H-1 => L+20, 2.32% H-5 => L+10, 2.31% H-32 => L+2, 2.11% H-17 => L+5, 2.03% H-5 => L+16
283	19319	518	0.54	24.8% H-10 => L+8, 20.4% H-1 => L+21, 10.5% H-21 => L+3, 7.08% H-8 => L+11, 4.51% H-2 => L+17, 4.36% H-3 => L+16, 4.34% H-12 => L+5, 2.94% H-7 => L+14, 2.19% H-3 => L+19
284	19345	517	0.00	17.4% H-7 => L+12, 14.9% H-8 => L+10, 12.0% H-27 => L+2, 9.22% H-13 => L+5, 5.96% H-3 => L+17, 5.69% H-26 => L+2, 2.35% H-11 => L+8, 2.32% H-30 => L+1, 2.12% H-7 => L+9
285	19354	517	0.00	40.6% H-11 => L+7, 16.2% H-9 => L+9, 10.5% H-13 => L+6, 7.58% H-5 => L+14, 3.82% H-9 => L+6, 3.12% H-44 => L+1
286	19388	516	0.00	47.0% H-28 => L+2, 13.2% H-22 => L+3, 5.47% H-3 => L+18, 5.31% H-31 => L+1, 5.13% H-6 => L+13, 4.53% H-1 => L+19, 2.45% H-31 => L+3, 2.17% H-21 => L+4
287	19389	516	0.00	66.8% H-51 => LUMO, 11.4% H-50 => L+1, 4.26% H-53 => LUMO, 3.98% H-49 => L+2, 2.80% H-52 => L+1
288	19410	515	0.00	54.8% H-27 => L+2, 9.52% H-8 => L+10, 5.46% H-15 => L+4, 5.18% H-30 => L+1, 5.00% H-25 => L+3, 4.11% H-3 => L+17
289	19434	515	0.00	27.4% H-13 => L+5, 20.0% H-3 => L+17, 9.50% H-8 => L+10, 4.84% H-1 => L+20, 3.37% H-15 => L+4, 2.80% H-2 => L+16, 2.27% H-19 => L+4, 2.21% H-15 => L+8
290	19437	514	0.00	35.6% H-5 => L+14, 9.90% H-2 => L+20, 9.31% H-16 => L+4, 8.69% H-11 => L+7, 4.65% H-7 => L+17, 4.10% H-6 => L+13, 3.56% H-4 => L+11, 3.05% H-3 => L+18
291	19449	514	0.04	19.4% H-5 => L+15, 17.5% H-7 => L+13, 11.4% H-2 => L+18, 7.42% H-8 => L+12, 5.61% H-30 => L+2, 3.82% H-25 => L+2, 3.19% H-10 => L+7, 2.25% H-4 => L+16
292	19514	512	0.00	52.4% H-29 => L+2, 7.84% H-30 => L+2, 4.87% H-17 => L+4, 3.86% H-26 => L+3, 2.99% H-32 => L+1, 2.60% H-33 => L+1, 2.34% H-4 => L+16
293	19573	511	0.01	20.4% H-16 => L+4, 15.1% H-3 => L+18, 11.5% H-5 => L+14, 7.55% H-22 => L+3, 7.53% H-4 => L+17, 6.52% H-6 => L+13, 3.65% H-2 => L+20, 3.04% H-1 => L+22, 2.37% H-14 => L+5
294	19592	510	0.00	43.8% H-22 => L+3, 26.5% H-28 => L+2, 3.27% H-4 => L+17, 3.05% H-21 => L+2, 2.67% H-5 => L+14, 2.53% H-21 => L+4, 2.33% H-3 => L+18
295	19615	510	0.00	26.9% H-10 => L+8, 8.64% H-31 => L+2, 8.46% H-3 => L+16, 8.04% H-8 => L+11, 5.33% H-6 => L+15, 4.81% H-7 => L+14, 3.52% H-5 => L+17,

				3.50% H-3 => L+19, 2.93% H-2 => L+17, 2.61% H-6 => L+18, 2.34% H-12 => L+11
296	19621	510	0.00	18.3% H-3 => L+17, 17.0% H-52 => LUMO, 14.7% H-13 => L+5, 9.32% H-9 => L+11, 5.29% H-11 => L+8, 5.09% H-6 => L+14, 4.84% H-8 => L+10, 4.71% H-10 => L+9, 2.96% H-51 => L+1
297	19627	510	0.00	48.9% H-52 => LUMO, 8.78% H-51 => L+1, 5.67% H-13 => L+5, 5.63% H-3 => L+17, 4.01% H-54 => LUMO, 3.51% H-9 => L+11, 3.08% H-50 => L+2, 2.03% H-6 => L+14, 2.01% H-11 => L+8
298	19678	508	0.00	33.9% H-17 => L+4, 8.61% H-3 => L+20, 8.56% H-30 => L+2, 3.76% H-2 => L+21, 3.06% H-6 => L+17, 2.99% H-4 => L+19, 2.86% H-2 => L+18, 2.63% H-29 => L+2, 2.31% H-24 => L+3, 2.19% H-10 => L+7, 2.13% H-19 => L+5
299	19682	508	0.00	29.2% H-10 => L+9, 15.2% H-8 => L+10, 8.20% H-13 => L+5, 5.91% H-12 => L+7, 5.68% H-11 => L+8, 3.44% H-19 => L+4, 2.85% H-8 => L+7, 2.49% H-10 => L+12, 2.28% H-14 => L+6, 2.21% H-2 => L+19, 2.12% H-2 => L+16
300	19688	508	0.14	23.3% H-31 => L+2, 14.6% H-8 => L+11, 10.8% H-10 => L+8, 6.54% H-7 => L+14, 5.92% H-9 => L+10, 3.63% H-6 => L+15, 2.87% H-3 => L+16, 2.51% H-5 => L+17, 2.15% H-11 => L+12, 2.13% H-11 => L+9
301	19694	508	0.05	18.6% H-4 => L+16, 14.2% H-30 => L+2, 11.3% H-20 => L+4, 7.65% H-7 => L+13, 6.69% H-8 => L+12, 4.97% H-17 => L+4, 4.47% H-25 => L+2, 4.35% H-2 => L+15, 3.23% H-10 => L+10, 3.16% H-2 => L+18, 2.21% H-27 => L+1
302	19744	506	0.01	29.4% H-31 => L+2, 17.8% H-6 => L+15, 11.6% H-3 => L+16, 5.08% H-9 => L+13, 2.95% H-34 => L+1, 2.90% H-21 => L+3, 2.48% H-11 => L+12, 2.14% H-28 => L+1
303	19750	506	0.00	17.0% H-30 => L+2, 14.9% H-2 => L+18, 14.7% H-4 => L+16, 9.10% H-29 => L+2, 6.10% H-17 => L+4, 4.84% H-12 => L+6, 4.42% H-2 => L+15, 4.20% H-10 => L+7, 2.41% H-20 => L+4, 2.33% H-5 => L+15
304	19778	506	0.00	23.4% H-6 => L+13, 23.3% H-9 => L+12, 8.10% H-11 => L+10, 5.31% H-13 => L+9, 3.54% H-3 => L+18, 3.36% H-4 => L+17, 3.11% H-2 => L+20, 2.95% H-17 => L+6, 2.70% H-15 => L+7, 2.42% H-22 => L+3, 2.17% H-14 => L+5
305	19826	504	0.00	37.1% H-6 => L+14, 32.1% H-11 => L+8, 5.96% H-32 => L+2, 3.45% H-3 => L+17, 3.34% H-33 => L+2, 2.07% H-23 => L+3
306	19828	504	0.07	37.4% H-5 => L+15, 9.84% H-4 => L+16, 7.21% H-8 => L+12, 5.00% H-4 => L+13, 3.76% H-7 => L+13, 3.53% H-10 => L+10, 3.45% H-29 => L+2,

				3.09% H-30 => L+2, 3.08% H-24 => L+3, 2.84% H-7 => L+16
				20.5% H-32 => L+2, 9.54% H-4 => L+18, 9.19% H-23 => L+3, 9.12% H-19 => L+4, 8.47% H-5 => L+16, 5.88% H-24 => L+2, 3.27% H-7 => L+15, 2.47% H-9 => L+11, 2.26% H-2 => L+19, 2.25% H-6 => L+14, 2.22% H-10 => L+9, 2.19% H-29 => L+3
307	19836	504	0.00	36.7% H-11 => L+9, 23.1% H-9 => L+10, 8.85% H-13 => L+7, 5.30% H-15 => L+6, 3.15% H-9 => L+7, 2.67% H-31 => L+2, 2.56% H-8 => L+11
308	19844	504	0.03	62.6% H-53 => LUMO, 11.1% H-52 => L+1, 5.00% H-55 => LUMO, 3.92% H-51 => L+2, 2.52% H-54 => L+1, 2.47% H-57 => LUMO, 2.05% H-56 => L+1
309	19848	504	0.00	14.1% H-23 => L+3, 13.3% H-2 => L+19, 8.00% H-24 => L+2, 7.56% H-19 => L+4, 7.23% H-11 => L+8, 5.20% H-33 => L+2, 3.88% H-7 => L+15, 3.39% H-24 => L+4, 3.23% H-8 => L+13, 2.39% H-10 => L+9, 2.37% H-12 => L+10, 2.01% H-10 => L+12
310	19859	504	0.00	42.0% H-14 => L+5, 14.4% H-3 => L+18, 6.97% H-34 => L+2, 5.87% H-1 => L+22, 5.55% H-12 => L+8, 5.11% H-16 => L+4, 3.08% H-3 => L+21
311	19866	503	0.01	16.2% H-32 => L+2, 15.1% H-19 => L+4, 12.9% H-33 => L+2, 6.25% H-10 => L+9, 4.85% H-11 => L+8, 3.69% H-2 => L+19, 3.57% H-23 => L+3,
312	19896	503	0.00	2.93% H-35 => L+1, 2.46% H-6 => L+14 33.4% H-24 => L+3, 12.6% H-23 => L+2, 10.3% H-12 => L+6, 6.58% H-23 => L+4, 5.79% H-5 => L+15, 3.75% H-2 => L+21, 3.08% H-3 => L+20,
313	19915	502	0.01	2.27% H-10 => L+7 28.4% H-4 => L+17, 16.1% H-2 => L+20, 8.43% H-9 => L+12, 7.36% H-5 => L+20, 7.13% H-2 => L+14, 4.90% H-3 => L+18, 4.46% H-3 => L+21, 3.05% H-6 => L+13, 2.18% H-6 => L+19, 2.11% H-34 => L+2
314	19915	502	0.00	25.5% H-18 => L+4, 10.2% H-3 => L+19, 8.18% H-21 => L+3, 6.45% H-1 => L+21, 6.34% H-3 => L+22, 5.60% H-16 => L+5, 5.17% H-8 => L+11, 4.13% H-6 => L+21, 2.33% H-14 => L+8, 2.31% H-31 => L+2, 2.03% H-6 => L+15
315	19948	501	0.02	21.8% H-33 => L+2, 19.0% H-23 => L+3, 5.04% H-4 => L+18, 4.97% H-9 => L+11, 4.84% H-24 => L+2, 4.49% H-6 => L+14, 3.91% H-5 => L+16, 3.51% H-24 => L+4, 3.22% H-19 => L+4, 2.61% H-30 => L+3, 2.58% H-2 => L+22
316	19949	501	0.00	20.8% H-12 => L+6, 18.5% H-20 => L+4, 8.32% H-7 => L+13, 6.75% H-24 => L+3, 5.78% H-30 => L+2, 5.03% H-29 => L+2, 2.41% H-10 => L+7, 2.23% H-4 => L+16, 2.11% H-23 => L+2
317	19953	501	0.02	

318	19968	501	0.04	27.6% H-12 => L+6, 16.9% H-7 => L+13, 16.7% H-20 => L+4, 5.03% H-14 => L+7, 4.72% H-2 => L+18, 4.66% H-10 => L+7, 2.77% H-4 => L+16, 2.15% H-5 => L+12
319	19979	501	0.00	49.7% H-9 => L+11, 13.1% H-6 => L+14, 11.1% H-11 => L+8, 9.47% H-33 => L+2
320	20018	500	0.23	17.2% H-7 => L+13, 16.7% H-20 => L+4, 11.9% H-8 => L+12, 6.85% H-3 => L+20, 5.34% H-10 => L+10, 3.50% H-2 => L+18, 3.16% H-35 => L+2, 2.74% H-2 => L+21, 2.55% H-12 => L+9, 2.42% H-8 => L+15, 2.19% H-5 => L+12
321	20024	499	0.00	62.5% H-54 => LUMO, 10.5% H-53 => L+1, 10.4% H-56 => LUMO, 3.56% H-52 => L+2, 2.98% H-57 => L+1
322	20057	499	0.00	35.7% H-8 => L+11, 21.0% H-7 => L+14, 10.8% H-5 => L+17, 7.85% H-18 => L+4, 5.51% H-4 => L+20, 2.17% H-10 => L+14
323	20083	498	0.00	59.7% H-34 => L+2, 12.2% H-3 => L+18, 3.81% H-31 => L+3, 3.45% H-31 => L+1, 2.82% H-14 => L+5, 2.80% H-36 => L+1, 2.16% H-36 => L+3
324	20085	498	0.32	48.9% H-35 => L+2, 4.49% H-40 => L+2, 4.43% H-38 => L+1, 4.35% H-33 => L+3, 4.04% H-2 => L+21, 2.90% H-33 => L+1, 2.03% H-13 => L+8
325	20115	497	0.00	12.6% H-10 => L+9, 12.3% H-19 => L+4, 10.6% H-32 => L+2, 9.83% H-12 => L+7, 7.41% H-2 => L+19, 6.06% H-4 => L+18, 5.67% H-5 => L+16, 4.20% H-23 => L+3, 3.50% H-14 => L+6, 2.88% H-2 => L+16, 2.71% H-33 => L+2, 2.63% H-4 => L+21
326	20178	496	0.00	27.9% H-2 => L+22, 12.2% H-32 => L+2, 9.32% H-4 => L+21, 7.60% H-33 => L+2, 2.71% H-8 => L+13, 2.27% H-7 => L+15, 2.20% H-6 => L+14, 2.11% H-10 => L+12, 2.06% H-12 => L+7
327	20180	496	0.01	56.0% H-55 => LUMO, 17.3% H-57 => LUMO, 6.38% H-54 => L+1, 2.13% H-8 => L+12, 2.06% H-53 => L+2
328	20187	495	0.11	19.9% H-8 => L+12, 12.3% H-2 => L+21, 9.02% H-4 => L+19, 6.82% H-3 => L+20, 6.81% H-35 => L+2, 6.29% H-55 => LUMO, 3.24% H-7 => L+13, 3.06% H-5 => L+18
329	20192	495	0.00	29.2% H-3 => L+21, 9.99% H-1 => L+22, 7.89% H-22 => L+3, 7.86% H-6 => L+19, 6.34% H-2 => L+20, 6.16% H-4 => L+17, 3.80% H-6 => L+16, 3.39% H-3 => L+18, 2.31% H-9 => L+12
330	20224	494	0.41	26.1% H-3 => L+19, 19.6% H-18 => L+4, 19.2% H-36 => L+2, 6.70% H-6 => L+15, 3.13% H-31 => L+2, 2.28% H-6 => L+21
331	20245	494	0.00	38.9% H-13 => L+6, 11.1% H-11 => L+7, 8.25% H-14 => L+5, 5.72% H-12 => L+8, 4.11% H-15 => L+7, 3.16% H-37 => L+2, 2.85% H-9 => L+6, 2.11% H-13 => L+9, 2.05% H-10 => L+11

332	20261	494	0.22	45.4% H-36 => L+2, 10.5% H-3 => L+19, 8.64% H-6 => L+15, 5.85% H-39 => L+2, 3.43% H-34 => L+1, 3.35% H-34 => L+3, 2.47% H-18 => L+4, 2.19% H-3 => L+22 21.4% H-12 => L+8, 17.6% H-14 => L+5, 17.3% H-13 => L+6, 6.88% H-10 => L+11, 5.55% H-2 => L+20, 4.14% H-11 => L+7, 3.33% H-3 => L+18, 2.90% H-8 => L+14, 2.32% H-6 => L+16
333	20281	493	0.00	36.4% H-12 => L+7, 15.9% H-2 => L+19, 10.0% H-4 => L+18, 4.64% H-10 => L+9, 4.44% H-10 => L+6, 4.37% H-14 => L+6, 2.81% H-2 => L+16, 2.31% H-4 => L+21 25.2% H-3 => L+20, 22.3% H-15 => L+5, 8.29% H-17 => L+4, 4.80% H-13 => L+8, 4.45% H-24 => L+3, 3.76% H-30 => L+2, 3.31% H-40 => L+2, 2.94% H-11 => L+11
334	20292	493	0.00	16.3% H-8 => L+12, 11.8% H-10 => L+10, 10.0% H-4 => L+19, 9.06% H-5 => L+18, 6.58% H-4 => L+22, 4.82% H-2 => L+18, 4.65% H-7 => L+16, 4.22% H-12 => L+9, 3.56% H-10 => L+13, 2.45% HOMO => L+24 25.4% H-4 => L+18, 8.71% H-2 => L+22, 8.69% H-7 => L+15, 8.07% H-5 => L+16, 5.09% H-19 => L+4, 4.49% H-23 => L+3, 4.24% H-2 => L+16, 4.12% H-5 => L+19, 3.55% H-12 => L+7, 3.33%
335	20299	493	0.00	HOMO => L+23, 2.97% H-8 => L+13 21.5% H-7 => L+14, 16.2% H-6 => L+15, 7.84% H-4 => L+20, 5.01% H-36 => L+2, 4.88% H-9 => L+13, 4.42% H-18 => L+4, 3.67% H-2 => L+17, 3.62% H-5 => L+17, 3.41% H-13 => L+10, 3.17% H-11 => L+12, 2.96% H-8 => L+17, 2.91% H-19 => L+6
336	20312	492	0.04	24.4% H-9 => L+12, 19.9% H-37 => L+2, 12.9% H-11 => L+10, 5.65% H-15 => L+7, 5.35% H-13 => L+9, 4.36% H-43 => L+2, 3.79% H-17 => L+6 17.5% H-10 => L+10, 14.1% HOMO => L+24, 7.74% H-2 => L+21, 5.20% H-8 => L+12, 5.19% H-15 => L+5, 5.10% H-3 => L+20, 4.20% H-20 => L+4, 3.25% H-4 => L+22, 3.17% H-12 => L+9, 2.79% H-12 => L+12, 2.73% H-1 => L+23, 2.71% H-24 => L+3, 2.61% H-7 => L+16, 2.31% H-5 => L+18
337	20345	492	0.00	56.9% H-38 => L+2, 10.00% H-40 => L+1, 6.52% H-40 => L+3, 5.86% H-5 => L+16, 4.53% H-35 => L+1, 3.33% H-35 => L+3 43.1% H-37 => L+2, 7.72% H-11 => L+10, 7.67% H-9 => L+12, 6.42% H-12 => L+8, 6.13% H-41 => L+2, 3.18% H-13 => L+9, 2.40% H-36 => L+3, 2.06% H-6 => L+16
338	20379	491	0.01	20.6% H-3 => L+22, 11.0% H-3 => L+19, 10.7% H-7 => L+14, 9.16% H-6 => L+15, 7.16% H-9 =>
339	20381	491	0.00	
340	20397	490	0.01	
341	20416	490	0.00	
342	20428	490	0.00	
343	20441	489	0.24	

				L+13, 5.55% H-4 => L+20, 3.70% H-11 => L+12, 2.27% H-18 => L+4, 2.26% H-1 => L+21, 2.11% H- 15 => L+9 62.0% H-40 => L+2, 12.0% H-38 => L+1, 9.84% H- 38 => L+3, 3.09% H-15 => L+5, 2.32% H-35 => L+2															
344	20451	489	0.01	33.8% H-5 => L+16, 7.31% H-38 => L+2, 6.24% H- 25 => L+3, 5.45% H-8 => L+13, 5.25% HOMO => L+23, 3.98% H-4 => L+15, 3.85% H-10 => L+12, 2.81% H-7 => L+15, 2.34% H-19 => L+4, 2.25% H- 7 => L+18, 2.07% H-12 => L+10 16.6% H-5 => L+17, 15.5% H-13 => L+7, 15.2% H- 11 => L+9, 8.78% H-15 => L+6, 7.38% H-7 => L+14, 5.28% H-42 => L+2, 2.44% H-13 => L+10, 2.29% H-4 => L+14, 2.27% H-3 => L+22, 2.22% H- 39 => L+2, 2.19% H-18 => L+4 57.1% H-39 => L+2, 10.9% H-42 => L+2, 3.67% H- 37 => L+1, 2.92% H-37 => L+3, 2.54% H-18 => L+4, 2.33% H-5 => L+17 53.3% H-56 => LUMO, 14.7% H-57 => L+1, 5.86% H-54 => LUMO, 5.84% H-56 => L+2, 4.99% H-55 => L+1, 2.29% H-52 => LUMO, 2.03% H-54 => L+2															
345	20466	489	0.00	45.7% H-57 => LUMO, 17.8% H-56 => L+1, 10.3% H-55 => LUMO, 4.42% H-57 => L+2, 3.82% H-53 => LUMO, 2.69% H-54 => L+1, 2.53% H-55 => L+2															
346	20509	488	0.00	349	20561	486	0.00	15.9% H-5 => L+17, 11.2% H-13 => L+7, 7.02% H- 3 => L+22, 6.87% H-39 => L+2, 6.72% H-18 => L+4, 6.58% H-11 => L+9, 6.24% H-42 => L+2, 4.46% H-16 => L+5, 3.67% H-15 => L+6, 2.00% H- 11 => L+6 16.0% H-15 => L+5, 11.0% H-26 => L+3, 10.8% H- 10 => L+10, 7.24% H-3 => L+20, 4.80% H-5 => L+21, 3.66% H-29 => L+2, 3.29% HOMO => L+24, 3.25% H-6 => L+17, 3.05% H-7 => L+19, 3.04% H- 9 => L+14, 2.40% H-12 => L+12, 2.06% H-4 => L+22 23.8% HOMO => L+23, 9.39% H-25 => L+3, 5.57% H-7 => L+15, 4.24% H-4 => L+21, 4.05% H-5 => L+19, 3.78% H-1 => L+24, 3.31% H-2 => L+19, 3.11% H-5 => L+22, 2.81% H-17 => L+5, 2.68% H- 7 => L+21, 2.65% H-27 => L+2, 2.62% H-7 => L+18, 2.30% H-8 => L+19 62.8% H-41 => L+2, 10.4% H-43 => L+2, 3.32% H- 12 => L+8, 2.81% H-39 => L+1, 2.40% H-39 => L+3, 2.23% H-9 => L+12 52.1% H-43 => L+2, 6.79% H-6 => L+16, 6.71% H- 12 => L+8, 6.17% H-42 => L+1, 4.97% H-42 => L+3, 2.87% H-41 => L+2, 2.47% H-45 => L+2, 2.23% H-21 => L+4											
350	20566	486	0.05	351	20570	486	0.02	352	20575	486	0.00	353	20578	486	0.00	354	20598	485	0.00

355	20611	485	0.02	51.4% H-42 => L+2, 6.06% H-13 => L+7, 4.83% H-43 => L+1, 4.00% H-43 => L+3, 3.59% H-39 => L+2, 3.44% H-11 => L+9, 3.01% H-41 => L+1, 2.80% H-15 => L+6, 2.72% H-44 => L+2, 2.60% H-41 => L+3 14.8% H-6 => L+16, 14.3% H-12 => L+8, 10.2% H-43 => L+2, 9.01% H-21 => L+4, 6.06% H-37 => L+2, 4.17% H-3 => L+21, 3.74% H-41 => L+2, 3.25% H-22 => L+3, 2.03% H-18 => L+5, 2.02% H-34 => L+2
356	20620	485	0.01	32.6% H-7 => L+15, 31.5% H-25 => L+3, 6.43% H-5 => L+16, 3.01% H-27 => L+2, 2.93% H-5 => L+13, 2.35% H-17 => L+5, 2.06% HOMO => L+23
357	20667	484	0.00	16.6% H-10 => L+10, 14.8% HOMO => L+24, 14.0% H-4 => L+19, 9.37% H-12 => L+9, 4.93% H-2 => L+18, 3.35% H-14 => L+7, 3.31% H-2 => L+21, 2.80% H-26 => L+3, 2.76% H-5 => L+21, 2.43% H-14 => L+10
358	20678	484	0.00	16.9% H-10 => L+11, 16.8% H-21 => L+4, 16.7% H-12 => L+8, 8.87% H-8 => L+14, 6.09% H-6 => L+16, 3.48% H-7 => L+17, 2.80% H-2 => L+20,
359	20725	483	0.00	2.15% H-14 => L+11