Supporting Information

Electron-Rich Dipyrrolonaphthyridinediones – Synthesis and Optical Properties

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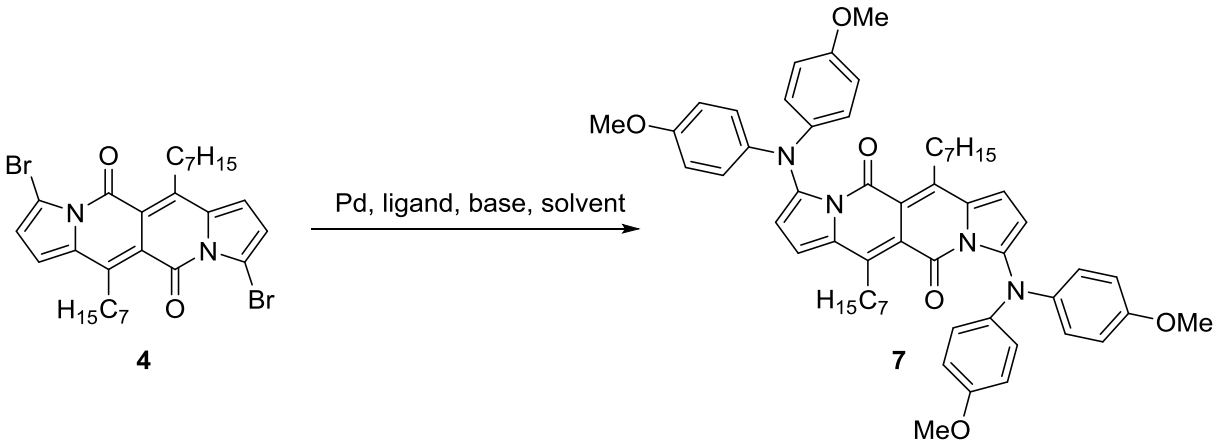
1. Screening of the Buchwald-Hartwig reaction conditions

Table S1. Screening of the Buchwald-Hartwig reaction conditions.



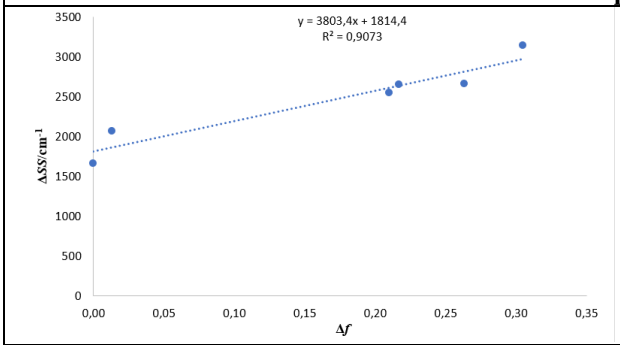
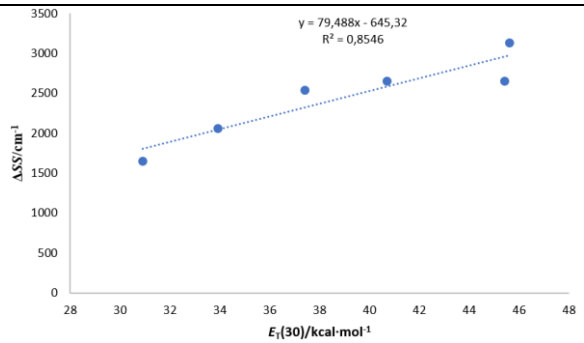
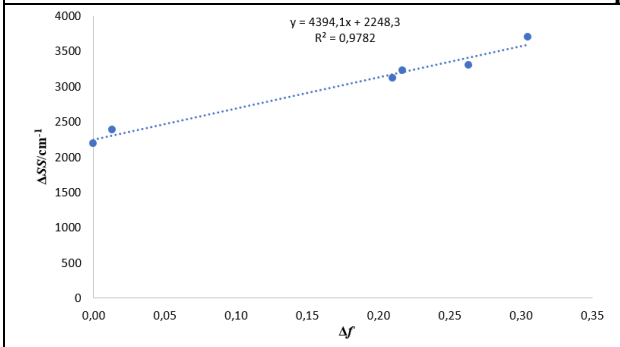
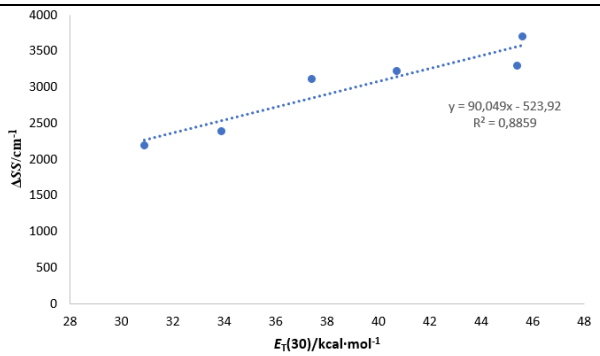
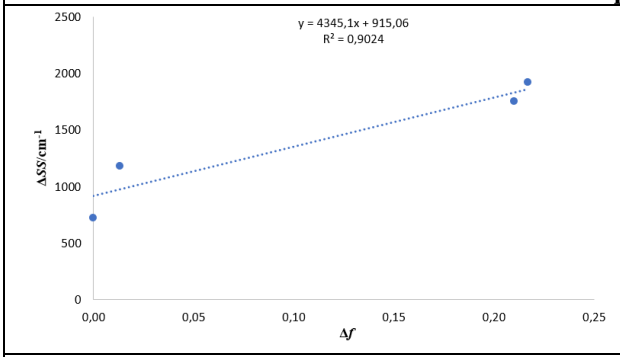
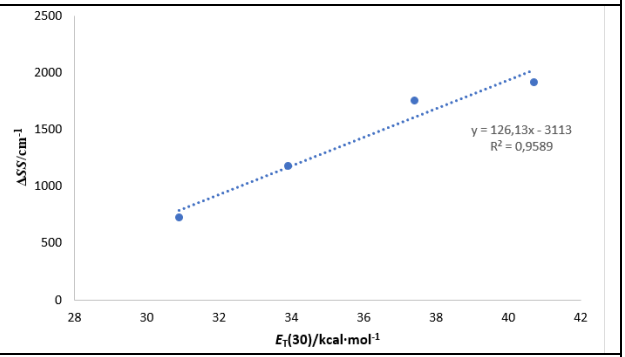
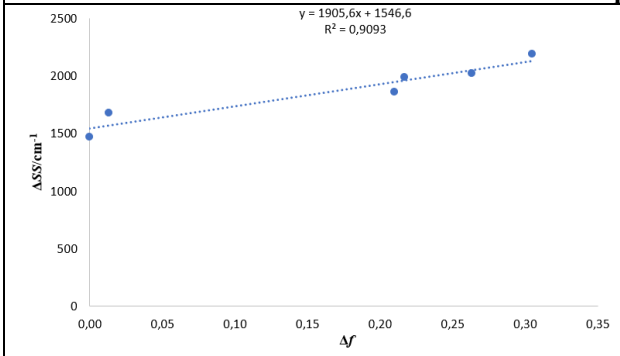
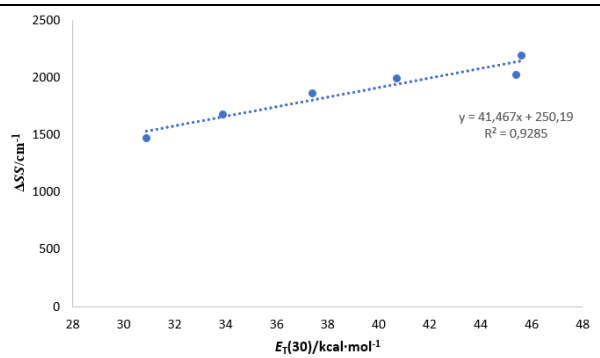
4 **7**

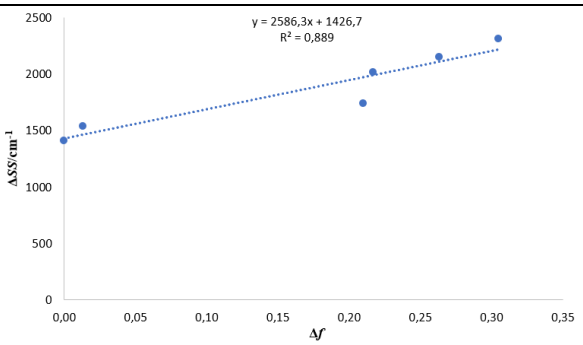
Entry	Reaction Conditions[a]					
	Catalyst	**Ligand**	**Base**	**Solvent**	**Temp.**	**Yields/%[d]**
1	$Pd_2(dba)_3$	XantPhos	Cs_2CO_3	PhMe	110	24
2	$Pd_2(dba)_3$	dppf	Cs_2CO_3	PhMe	110	30
3	$Pd_2(dba)_3$	BINAP	Cs_2CO_3	PhMe	110	37
4	$Pd_2(dba)_3$	XPhos	Cs_2CO_3	PhMe	110	31
5	$Pd_2(dba)_3$	*t*-BuXPhos	Cs_2CO_3	PhMe	110	traces
6[c]	**$Pd_2(dba)_3$**	**SPhos**	**Cs_2CO_3**	**PhMe**	**110**	**50**
7	$Pd_2(dba)_3$	RuPhos	Cs_2CO_3	PhMe	110	44
8	$Pd_2(dba)_3$	DavePhos	Cs_2CO_3	PhMe	110	0
9	$Pd_2(dba)_3$	P(*t*-Bu)$_3$	Cs_2CO_3	PhMe	110	traces
10	$Pd(OAc)_2$	SPhos	Cs_2CO_3	PhMe	110	25
11	$Pd_2(dba)_3$	SPhos	K_2CO_3	PhMe	110	10
12	$Pd_2(dba)_3$	SPhos	K_3PO_4	PhMe	110	13
13	$Pd_2(dba)_3$	SPhos	*t*-BuONa	PhMe	110	39
14	$Pd_2(dba)_3$	SPhos	Cs_2CO_3	dioxane	95	32
15[b]	$Pd_2(dba)_3$	SPhos	Cs_2CO_3	PhMe	110	41
16	RuPhos Pd G3	RuPhos	Cs_2CO_3	PhMe	110	43

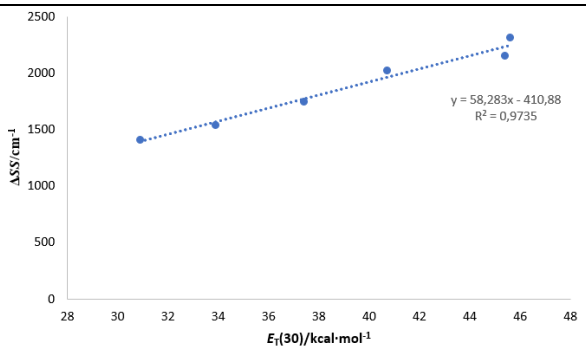
[a] Reaction conditions: **4** (0.05 mmol, 30.0 mg), aniline (3.0 eq, 34.5 mg), Pd source (10 $\%_{mol}$), ligand (20 $\%_{mol}$), base (4.0 eq), solvent (1 mL), 72h. [b] 5 $\%_{mol}$ of catalyst and 10 $\%_{mol}$ of ligand were used. [c] The bold entry signifies the optimal conditions. [d] Isolated yields.

2. Lippert-Mataga and $E_T(30)$ plots

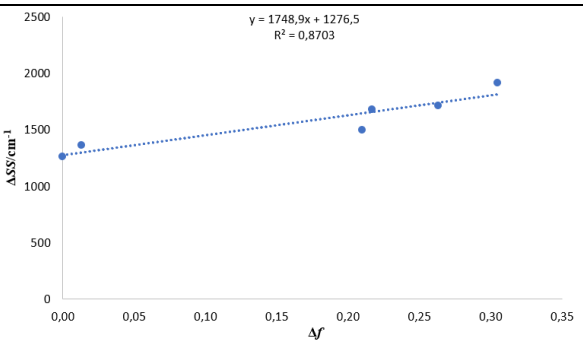
Table S2. Plots of Stokes shift (ΔSS) *versus* solvent orientation polarizability (Δf) or Reichhardt parameter ($E_T(30)$).

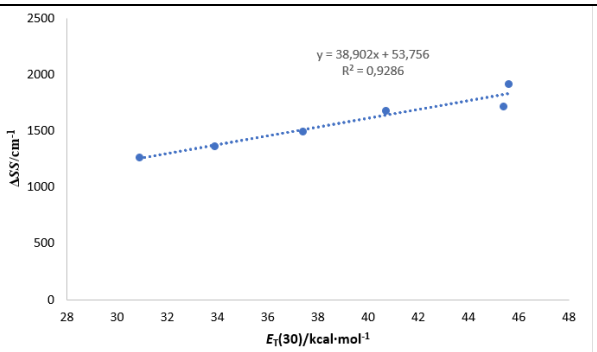
Lippert-Mataga plots	$E_T(30)$ plots
Compound 1	
	
Compound 2	
	
Compound 3	
	
Compound 5	
	
Compound 6	



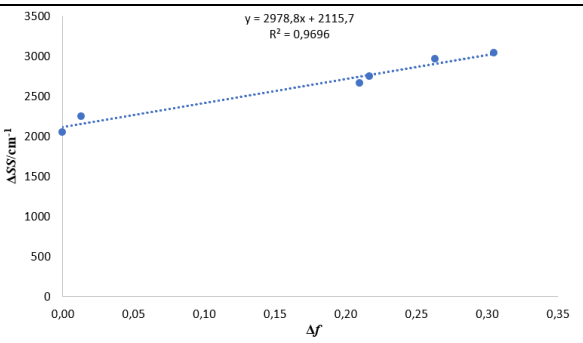


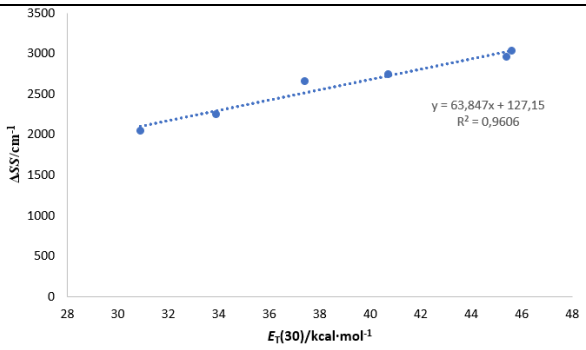
Compound 7



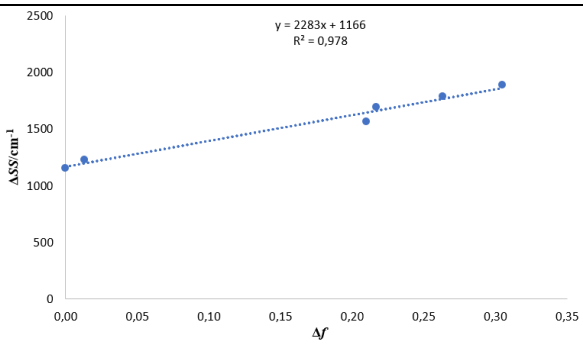


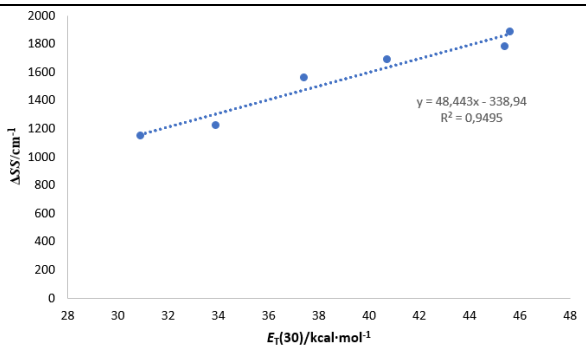
Compound 8





Compound 9



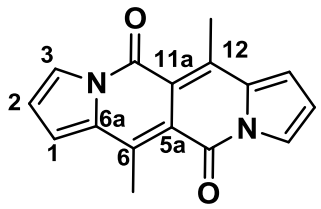


3. Computational details

Table S3. Theoretically and experimentally obtained vertical excitation energies in different solvents.

Solvent	λ_{abs}^{exp}/nm	λ_{abs}^{calc}/nm	f_{abs}	λ_{em}^{exp}/nm	λ_{em}^{calc}/nm	f_{em}
Compound 6						
Cyclohexane	608	512	0.8821	665	625	1.0067
Toluene	614	515	0.9033	678	634	1.0306
CH_2Cl_2	608	530	1.0066	693	684	1.1451
THF	608	529	0.9979	680	679	1.1356
DMSO	613	536	1.0443	706	707	1.1851
Compound 8						
Cyclohexane	565	478	0.8915	639	611	1.0379
Toluene	571	480	0.9124	655	619	1.0593
CH_2Cl_2	558	491	1.0184	659	662	1.1616
THF	560	491	1.0092	658	658	1.1531
DMSO	564	496	1.0391	677	683	1.1985

Table S4. Selected bond lengths in molecules **6** and **8** determined theoretically for both S_0 and S_1 states in various solvents.



Solvent	Bonds														
	d(C_{11a}-C_{12})			d(C_{5a}-C_{11a})			d(C_6-C_{6a})			d(C_1-C_{6a})			d(C_{5a}-C_6)		
	S_0	S_1	d	S_0	S_1	d	S_0	S_1	d	S_0	S_1	d	S_0	S_1	d
Compound 6															
C_6H_{12}	1.378	1.418	0.039	1.466	1.430	-0.035	1.435	1.400	-0.035	1.385	1.413	0.0280	1.3781	1.4176	0.0395
PhMe	1.378	1.418	0.040	1.466	1.430	-0.036	1.435	1.400	-0.035	1.385	1.413	0.0284	1.3781	1.4182	0.0401
CH_2Cl_2	1.379	1.422	0.043	1.466	1.428	-0.038	1.435	1.396	-0.039	1.385	1.416	0.0308	1.3785	1.4217	0.0432
THF	1.378	1.421	0.043	1.466	1.428	-0.038	1.435	1.397	-0.038	1.385	1.415	0.0306	1.3784	1.4213	0.0429
DMSO	1.379	1.423	0.045	1.466	1.427	-0.039	1.435	1.395	-0.040	1.385	1.417	0.0318	1.3786	1.4231	0.0445
Compound 8															
C_6H_{12}	1.377	1.420	0.042	1.467	1.429	-0.038	1.438	1.400	-0.038	1.384	1.414	0.0294	1.3773	1.4196	0.0423
PhMe	1.377	1.420	0.043	1.467	1.429	-0.038	1.438	1.399	-0.039	1.384	1.414	0.0298	1.3773	1.4202	0.0429
CH_2Cl_2	1.377	1.423	0.046	1.467	1.426	-0.041	1.438	1.396	-0.042	1.384	1.416	0.0321	1.3773	1.4234	0.0461
THF	1.377	1.423	0.046	1.467	1.426	-0.040	1.438	1.396	-0.042	1.384	1.416	0.0319	1.3773	1.4231	0.0458
DMSO	1.377	1.425	0.047	1.467	1.425	-0.042	1.438	1.394	-0.043	1.384	1.417	0.0331	1.3774	1.4247	0.0473

Cartesian Coordinates

Compound **6**, S_0 state, cyclohexane:

Energy=-1909.4055

N	-2.37082	-0.47570	0.72588
C	-1.54897	-1.18846	1.59841
C	-0.11985	-1.10852	1.49640
C	0.42502	-0.34088	0.48995
C	-0.42499	0.34081	-0.49004
C	-1.89205	0.20639	-0.41389
C	-2.37081	-1.87570	2.47593
C	0.67396	-1.87463	2.51347
C	1.89207	-0.20647	0.41379
C	0.11987	1.10846	-1.49648
O	-2.67215	0.62198	-1.24139
N	2.37085	0.47568	-0.72594
C	1.54900	1.18842	-1.59848
C	3.69778	0.69546	-1.08276
C	3.70824	1.56104	-2.15557
C	2.37083	1.87568	-2.47600
C	-3.69775	-0.69546	1.08271
C	-3.70821	-1.56104	2.15552
H	1.44879	-2.48612	2.03514
H	1.21551	-1.18960	3.18039
H	0.02664	-2.51974	3.11649
N	-4.78323	-0.08894	0.45574
C	-5.76370	-0.91002	-0.15133
C	-4.90617	1.32007	0.50013
C	-5.45752	2.02637	-0.57564
C	-5.56831	3.40969	-0.51990
C	-5.11261	4.11654	0.59292
C	-4.54858	3.41750	1.65565
C	-4.45126	2.02895	1.61683
H	-5.78660	1.48349	-1.46169
H	-6.00148	3.94558	-1.36757
H	-5.19458	5.20460	0.62785
H	-4.18810	3.95479	2.53579
H	-4.02377	1.48659	2.46183
C	-7.12689	-0.61839	-0.01951
C	-8.07936	-1.44181	-0.61040
C	-7.69390	-2.57471	-1.32413
C	-6.33854	-2.87131	-1.44842
C	-5.37865	-2.04350	-0.87614
H	-7.43789	0.25757	0.55122
H	-9.13868	-1.19996	-0.49819
H	-8.44520	-3.22189	-1.78066
H	-6.01981	-3.75214	-2.01025
H	-4.31775	-2.26853	-0.99382
N	4.78327	0.08896	-0.45578
C	4.90630	-1.32004	-0.50029
C	5.76358	0.91004	0.15153
C	7.12681	0.61849	0.01993
C	8.07914	1.44192	0.61103
C	7.69350	2.57475	1.32478
C	6.33811	2.87128	1.44885
C	5.37835	2.04346	0.87635
H	7.43795	-0.25741	-0.55082
H	9.13850	1.20012	0.49899

H	8.44470	3.22194	1.78149
H	6.01924	3.75205	2.01069
H	4.31742	2.26843	0.99387
C	5.45758	-2.02641	0.57546
C	5.56845	-3.40973	0.51960
C	5.11290	-4.11649	-0.59334
C	4.54894	-3.41738	-1.65606
C	4.45154	-2.02883	-1.61710
H	5.78653	-1.48361	1.46160
H	6.00156	-3.94568	1.36726
H	5.19494	-5.20454	-0.62838
H	4.18858	-3.95459	-2.53629
H	4.02409	-1.48641	-2.46209
O	2.67218	-0.62210	1.24127
C	-0.67393	1.87456	-2.51357
H	-1.44881	2.48602	-2.03524
H	-0.02662	2.51971	-3.11655
H	-1.21544	1.18952	-3.18052
H	2.04209	2.51971	-3.28639
H	4.60688	1.90430	-2.66198
H	-4.60686	-1.90428	2.66195
H	-2.04207	-2.51974	3.28633

Compound **6**, S_1 state, cyclohexane:

Energy=-1909.3984

N	-0.70809	2.31839	-0.63791
C	-1.80939	1.50018	-0.92630
C	-1.76790	0.12443	-0.66791
C	-0.58168	-0.40406	-0.09945
C	0.58168	0.40406	0.09945
C	0.56372	1.81437	-0.30976
C	-2.80908	2.33381	-1.47545
C	-2.97152	-0.70101	-1.02263
C	-0.56372	-1.81437	0.30976
C	1.76790	-0.12443	0.66791
O	1.53910	2.54097	-0.37736
N	0.70809	-2.31839	0.63791
C	1.80939	-1.50018	0.92630
C	1.02878	-3.63178	0.96636
C	2.32288	-3.63625	1.49531
C	2.80908	-2.33381	1.47545
C	-1.02878	3.63178	-0.96636
C	-2.32288	3.63625	-1.49531
H	-2.68968	-1.60837	-1.57240
H	-3.49759	-1.05308	-0.12395
H	-3.67182	-0.12276	-1.63726
N	-0.21510	4.71833	-0.71779
C	-0.11039	5.72181	-1.71300
C	0.36473	4.89905	0.56032
C	1.63589	5.47215	0.68905
C	2.19458	5.64679	1.94703
C	1.50900	5.23730	3.09189
C	0.24984	4.65729	2.96301
C	-0.32632	4.49365	1.70698
H	2.18708	5.76042	-0.20628
H	3.18781	6.09248	2.03524
H	1.95666	5.36947	4.07881
H	-0.30045	4.33837	3.85093
H	-1.32215	4.05761	1.61131

C	-0.20931	7.07756	-1.37729
C	-0.11122	8.04834	-2.36806
C	0.07190	7.68468	-3.70082
C	0.16422	6.33465	-4.03579
C	0.08040	5.35736	-3.05137
H	-0.36724	7.36576	-0.33731
H	-0.19143	9.10271	-2.09470
H	0.14372	8.45049	-4.47553
H	0.31783	6.03726	-5.07537
H	0.17369	4.30115	-3.30760
N	0.21510	-4.71833	0.71779
C	-0.36473	-4.89905	-0.56032
C	0.11039	-5.72181	1.71300
C	0.20931	-7.07756	1.37729
C	0.11122	-8.04834	2.36806
C	-0.07190	-7.68468	3.70082
C	-0.16422	-6.33465	4.03579
C	-0.08040	-5.35736	3.05137
H	0.36724	-7.36576	0.33731
H	0.19143	-9.10271	2.09470
H	-0.14372	-8.45049	4.47553
H	-0.31783	-6.03726	5.07537
H	-0.17369	-4.30115	3.30760
C	-1.63589	-5.47215	-0.68905
C	-2.19458	-5.64679	-1.94703
C	-1.50900	-5.23730	-3.09189
C	-0.24984	-4.65729	-2.96301
C	0.32632	-4.49365	-1.70698
H	-2.18708	-5.76042	0.20628
H	-3.18781	-6.09248	-2.03524
H	-1.95666	-5.36947	-4.07881
H	0.30045	-4.33837	-3.85093
H	1.32215	-4.05761	-1.61131
O	-1.53910	-2.54097	0.37736
C	2.97152	0.70101	1.02263
H	2.68968	1.60837	1.57240
H	3.67182	0.12276	1.63726
H	3.49759	1.05308	0.12395
H	3.79706	-2.01004	1.78992
H	2.84907	-4.53186	1.81723
H	-2.84907	4.53186	-1.81723
H	-3.79706	2.01004	-1.78992

Compound **6**, S_0 state, toluene:

Energy=-1909.4065

N	-2.37137	-0.47425	0.72541
C	-1.55002	-1.18671	1.59874
C	-0.12084	-1.10776	1.49695
C	0.42475	-0.34101	0.49015
C	-0.42480	0.34090	-0.49017
C	-1.89190	0.20784	-0.41380
C	-2.37218	-1.87276	2.47686
C	0.67193	-1.87404	2.51467
C	1.89186	-0.20785	0.41383
C	0.12079	1.10758	-1.49702
O	-2.67183	0.62488	-1.24102
N	2.37132	0.47417	-0.72542
C	1.54997	1.18653	-1.59882
C	3.69845	0.69333	-1.08225

C	3.70937	1.55775	-2.15592
C	2.37213	1.87257	-2.47695
C	-3.69849	-0.69339	1.08225
C	-3.70942	-1.55786	2.15588
H	1.44572	-2.48709	2.03669
H	1.21415	-1.18908	3.18112
H	0.02390	-2.51779	3.11830
N	-4.78425	-0.08805	0.45428
C	-5.76370	-0.91124	-0.15190
C	-4.90949	1.32057	0.49852
C	-5.46855	2.02549	-0.57431
C	-5.58131	3.40874	-0.51882
C	-5.12031	4.11715	0.59087
C	-4.54889	3.41956	1.65069
C	-4.44930	2.03113	1.61212
H	-5.80265	1.48193	-1.45808
H	-6.02055	3.94325	-1.36423
H	-5.20395	5.20509	0.62564
H	-4.18416	3.95789	2.52844
H	-4.01585	1.49036	2.45509
C	-7.12753	-0.62407	-0.01676
C	-8.07872	-1.44972	-0.60672
C	-7.69116	-2.58052	-1.32277
C	-6.33510	-2.87280	-1.45029
C	-5.37659	-2.04264	-0.87892
H	-7.44023	0.25006	0.55586
H	-9.13856	-1.21137	-0.49190
H	-8.44141	-3.22949	-1.77852
H	-6.01479	-3.75198	-2.01379
H	-4.31525	-2.26445	-0.99891
N	4.78421	0.08806	-0.45423
C	4.90946	-1.32056	-0.49827
C	5.76374	0.91134	0.15172
C	7.12755	0.62427	0.01627
C	8.07882	1.45001	0.60599
C	7.69131	2.58079	1.32212
C	6.33527	2.87295	1.44995
C	5.37669	2.04270	0.87881
H	7.44018	-0.24983	-0.55642
H	9.13864	1.21175	0.49094
H	8.44161	3.22982	1.77770
H	6.01501	3.75211	2.01353
H	4.31536	2.26441	0.99905
C	5.46875	-2.02530	0.57457
C	5.58153	-3.40855	0.51928
C	5.12032	-4.11715	-0.59020
C	4.54868	-3.41975	-1.65003
C	4.44908	-2.03131	-1.61167
H	5.80303	-1.48159	1.45818
H	6.02094	-3.94293	1.36469
H	5.20397	-5.20510	-0.62481
H	4.18380	-3.95823	-2.52762
H	4.01546	-1.49070	-2.45464
O	2.67178	-0.62477	1.24111
C	-0.67201	1.87376	-2.51480
H	-1.44565	2.48701	-2.03681
H	-0.02398	2.51731	-3.11864
H	-1.21443	1.18875	-3.18102
H	2.04395	2.51606	-3.28801

H	4.60811	1.90025	-2.66270
H	-4.60816	-1.90037	2.66266
H	-2.04400	-2.51631	3.28787

Compound **6**, S_1 state, toluene:

Energy=-1909.3992

N	-0.70375	2.31883	-0.64109
C	-1.80484	1.50124	-0.93302
C	-1.76564	0.12613	-0.67436
C	-0.58149	-0.40354	-0.10117
C	0.58149	0.40354	0.10117
C	0.56630	1.81347	-0.30910
C	-2.80219	2.33584	-1.48603
C	-2.96851	-0.69839	-1.03407
C	-0.56630	-1.81347	0.30910
C	1.76564	-0.12613	0.67436
O	1.54305	2.53880	-0.37469
N	0.70375	-2.31883	0.64109
C	1.80484	-1.50124	0.93302
C	1.02256	-3.63248	0.97095
C	2.31503	-3.63758	1.50453
C	2.80219	-2.33584	1.48603
C	-1.02256	3.63248	-0.97095
C	-2.31503	3.63758	-1.50453
H	-2.68496	-1.60676	-1.58121
H	-3.50001	-1.04807	-0.13767
H	-3.66486	-0.12023	-1.65321
N	-0.20964	4.71886	-0.72096
C	-0.10970	5.72554	-1.71406
C	0.37040	4.90011	0.55701
C	1.63859	5.47994	0.68533
C	2.19758	5.65595	1.94308
C	1.51512	5.24161	3.08810
C	0.25876	4.65535	2.95959
C	-0.31767	4.49009	1.70385
H	2.18738	5.77301	-0.20995
H	3.18841	6.10702	2.03092
H	1.96289	5.37508	4.07479
H	-0.28926	4.33282	3.84762
H	-1.31149	4.04934	1.60895
C	-0.21894	7.07971	-1.37554
C	-0.12493	8.05335	-2.36400
C	0.06429	7.69370	-3.69704
C	0.16676	6.34504	-4.03480
C	0.08698	5.36508	-3.05260
H	-0.38156	7.36462	-0.33537
H	-0.21312	9.10656	-2.08864
H	0.13295	8.46165	-4.46991
H	0.32503	6.05100	-5.07461
H	0.18782	4.31007	-3.31094
N	0.20964	-4.71886	0.72096
C	-0.37040	-4.90011	-0.55701
C	0.10970	-5.72554	1.71406
C	0.21894	-7.07971	1.37554
C	0.12493	-8.05335	2.36400
C	-0.06429	-7.69370	3.69704
C	-0.16676	-6.34504	4.03480
C	-0.08698	-5.36508	3.05260
H	0.38156	-7.36462	0.33537

H	0.21312	-9.10656	2.08864
H	-0.13295	-8.46165	4.46991
H	-0.32503	-6.05100	5.07461
H	-0.18782	-4.31007	3.31094
C	-1.63859	-5.47994	-0.68533
C	-2.19758	-5.65595	-1.94308
C	-1.51512	-5.24161	-3.08810
C	-0.25876	-4.65535	-2.95959
C	0.31767	-4.49009	-1.70385
H	-2.18738	-5.77301	0.20995
H	-3.18841	-6.10702	-2.03092
H	-1.96289	-5.37508	-4.07479
H	0.28926	-4.33282	-3.84762
H	1.31149	-4.04934	-1.60895
O	-1.54305	-2.53880	0.37469
C	2.96851	0.69839	1.03407
H	2.68496	1.60676	1.58121
H	3.66486	0.12023	1.65321
H	3.50001	1.04807	0.13767
H	3.78947	-2.01290	1.80364
H	2.83964	-4.53342	1.82841
H	-2.83964	4.53342	-1.82841
H	-3.78947	2.01290	-1.80364

Compound **6**, S_0 state, THF:

Energy=-1909.4114

N	-2.37553	-0.45537	0.72437
C	-1.55957	-1.16832	1.60267
C	-0.12991	-1.10059	1.50159
C	0.42229	-0.34262	0.49133
C	-0.42229	0.34262	-0.49133
C	-1.89007	0.22321	-0.41281
C	-2.38622	-1.84473	2.48395
C	0.65455	-1.86933	2.52372
C	1.89007	-0.22321	0.41281
C	0.12991	1.10059	-1.50159
O	-2.66773	0.65042	-1.23857
N	2.37553	0.45537	-0.72437
C	1.55957	1.16832	-1.60267
C	3.70458	0.66634	-1.08091
C	3.72136	1.52416	-2.15930
C	2.38622	1.84473	-2.48395
C	-3.70458	-0.66634	1.08091
C	-3.72136	-1.52416	2.15930
H	1.41785	-2.49724	2.04821
H	1.20611	-1.18625	3.18431
H	-0.00009	-2.49975	3.13381
N	-4.78889	-0.06274	0.44700
C	-5.76180	-0.89224	-0.16275
C	-4.92084	1.34421	0.49260
C	-5.51062	2.04641	-0.56626
C	-5.62798	3.42968	-0.50999
C	-5.14281	4.14211	0.58689
C	-4.54214	3.44765	1.63303
C	-4.43648	2.05958	1.59359
H	-5.86816	1.50229	-1.44055
H	-6.09169	3.96047	-1.34463
H	-5.23070	5.22966	0.62262
H	-4.15815	3.98830	2.50109

H	-3.97907	1.52360	2.42679
C	-7.12861	-0.62316	-0.01993
C	-8.07201	-1.45575	-0.61321
C	-7.67292	-2.57595	-1.34023
C	-6.31369	-2.85087	-1.47492
C	-5.36326	-2.01327	-0.89991
H	-7.45072	0.24167	0.56155
H	-9.13425	-1.23171	-0.49226
H	-8.41687	-3.23046	-1.79840
H	-5.98467	-3.72194	-2.04593
H	-4.29977	-2.22267	-1.02428
N	4.78889	0.06274	-0.44700
C	4.92084	-1.34421	-0.49260
C	5.76180	0.89224	0.16275
C	7.12861	0.62316	0.01993
C	8.07201	1.45575	0.61321
C	7.67292	2.57595	1.34023
C	6.31369	2.85087	1.47492
C	5.36326	2.01327	0.89991
H	7.45072	-0.24167	-0.56155
H	9.13425	1.23171	0.49226
H	8.41687	3.23046	1.79840
H	5.98467	3.72194	2.04593
H	4.29977	2.22267	1.02428
C	5.51062	-2.04641	0.56626
C	5.62798	-3.42968	0.50999
C	5.14281	-4.14211	-0.58689
C	4.54214	-3.44765	-1.63303
C	4.43648	-2.05958	-1.59359
H	5.86816	-1.50229	1.44055
H	6.09169	-3.96047	1.34463
H	5.23070	-5.22966	-0.62262
H	4.15815	-3.98830	-2.50109
H	3.97907	-1.52360	-2.42679
O	2.66773	-0.65042	1.23857
C	-0.65455	1.86933	-2.52372
H	-1.41785	2.49724	-2.04821
H	0.00009	2.49975	-3.13381
H	-1.20611	1.18625	-3.18431
H	2.06352	2.48589	-3.29909
H	4.62193	1.85922	-2.66795
H	-4.62193	-1.85922	2.66795
H	-2.06352	-2.48589	3.29909

Compound **6**, S_1 state, THF:

Energy=-1909.403

N	-2.36839	-0.62648	0.53222
C	-1.57294	-1.43254	1.36091
C	-0.18044	-1.32879	1.33996
C	0.39779	-0.37397	0.46009
C	-0.39779	0.37397	-0.46009
C	-1.84634	0.14446	-0.52056
C	-2.45334	-2.25886	2.09922
C	0.61299	-2.24432	2.22854
C	1.84634	-0.14446	0.52056
C	0.18044	1.32879	-1.33996
O	-2.59027	0.56496	-1.39088
N	2.36839	0.62648	-0.53222
C	1.57294	1.43254	-1.36091

C	3.70736	0.91935	-0.77684
C	3.75421	1.93747	-1.73599
C	2.45334	2.25886	-2.09922
C	-3.70736	-0.91935	0.77684
C	-3.75421	-1.93747	1.73599
H	1.43874	-2.71781	1.68206
H	1.08033	-1.69677	3.05910
H	-0.02604	-3.03218	2.64452
N	-4.77227	-0.25085	0.21216
C	-5.90986	-1.01107	-0.16729
C	-4.81225	1.16373	0.19564
C	-5.44044	1.84212	-0.85638
C	-5.47965	3.22958	-0.86383
C	-4.88066	3.96247	0.16232
C	-4.24965	3.28778	1.20457
C	-4.21982	1.89650	1.22968
H	-5.88416	1.27354	-1.67416
H	-5.97107	3.74746	-1.69037
H	-4.90748	5.05373	0.14811
H	-3.78477	3.84836	2.01851
H	-3.74286	1.37336	2.06013
C	-7.19622	-0.61605	0.21773
C	-8.29832	-1.37689	-0.15825
C	-8.13273	-2.54137	-0.90611
C	-6.85046	-2.93797	-1.28374
C	-5.74416	-2.17711	-0.92368
H	-7.32845	0.28659	0.81557
H	-9.29764	-1.06081	0.14860
H	-9.00041	-3.13773	-1.19468
H	-6.70923	-3.84362	-1.87739
H	-4.74138	-2.47421	-1.23436
N	4.77227	0.25085	-0.21216
C	4.81225	-1.16373	-0.19564
C	5.90986	1.01107	0.16729
C	7.19622	0.61605	-0.21773
C	8.29832	1.37689	0.15825
C	8.13273	2.54137	0.90611
C	6.85046	2.93797	1.28374
C	5.74416	2.17711	0.92368
H	7.32845	-0.28659	-0.81557
H	9.29764	1.06081	-0.14860
H	9.00041	3.13773	1.19468
H	6.70923	3.84362	1.87739
H	4.74138	2.47421	1.23436
C	5.44044	-1.84212	0.85638
C	5.47965	-3.22958	0.86383
C	4.88066	-3.96247	-0.16232
C	4.24965	-3.28778	-1.20457
C	4.21982	-1.89650	-1.22968
H	5.88416	-1.27354	1.67416
H	5.97107	-3.74746	1.69037
H	4.90748	-5.05373	-0.14811
H	3.78477	-3.84836	-2.01851
H	3.74286	-1.37336	-2.06013
O	2.59027	-0.56496	1.39088
C	-0.61299	2.24432	-2.22854
H	-1.43874	2.71781	-1.68206
H	0.02604	3.03218	-2.64452
H	-1.08033	1.69677	-3.05910

H	2.15532	2.98842	-2.84692
H	4.67313	2.35376	-2.14208
H	-4.67313	-2.35376	2.14208
H	-2.15532	-2.98842	2.84692

Compound **6**, S_0 state, dichloromethane:

Energy=-1909.4119

N	-2.37576	-0.45382	0.72460
C	-1.56011	-1.16659	1.60338
C	-0.13044	-1.09979	1.50214
C	0.42216	-0.34268	0.49142
C	-0.42216	0.34268	-0.49142
C	-1.88996	0.22433	-0.41250
C	-2.38698	-1.84196	2.48523
C	0.65345	-1.86861	2.52466
C	1.88996	-0.22433	0.41250
C	0.13044	1.09979	-1.50214
O	-2.66755	0.65232	-1.23811
N	2.37576	0.45382	-0.72460
C	1.56011	1.16659	-1.60338
C	3.70492	0.66405	-1.08138
C	3.72200	1.52099	-2.16040
C	2.38698	1.84196	-2.48523
C	-3.70492	-0.66405	1.08138
C	-3.72200	-1.52099	2.16040
H	1.41567	-2.49794	2.04930
H	1.20592	-1.18561	3.18456
H	-0.00168	-2.49777	3.13549
N	-4.78929	-0.06089	0.44695
C	-5.76123	-0.89133	-0.16326
C	-4.92228	1.34583	0.49259
C	-5.51600	2.04746	-0.56454
C	-5.63410	3.43072	-0.50834
C	-5.14600	4.14386	0.58679
C	-4.54159	3.45001	1.63124
C	-4.43499	2.06200	1.59186
H	-5.87637	1.50308	-1.43752
H	-6.10096	3.96087	-1.34163
H	-5.23457	5.23135	0.62252
H	-4.15526	3.99112	2.49797
H	-3.97451	1.52678	2.42384
C	-7.12844	-0.62483	-0.01930
C	-8.07073	-1.45838	-0.61306
C	-7.67004	-2.57702	-1.34167
C	-6.31039	-2.84945	-1.47742
C	-5.36110	-2.01083	-0.90192
H	-7.45180	0.23867	0.56345
H	-9.13329	-1.23638	-0.49121
H	-8.41310	-3.23231	-1.80017
H	-5.98017	-3.71932	-2.04955
H	-4.29732	-2.21839	-1.02698
N	4.78929	0.06089	-0.44695
C	4.92228	-1.34583	-0.49259
C	5.76123	0.89133	0.16326
C	7.12844	0.62483	0.01930
C	8.07073	1.45838	0.61306
C	7.67004	2.57702	1.34167
C	6.31039	2.84945	1.47742
C	5.36110	2.01083	0.90192

H	7.45180	-0.23867	-0.56345
H	9.13329	1.23638	0.49121
H	8.41310	3.23231	1.80017
H	5.98017	3.71932	2.04955
H	4.29732	2.21839	1.02698
C	5.51600	-2.04746	0.56454
C	5.63410	-3.43072	0.50834
C	5.14600	-4.14386	-0.58679
C	4.54159	-3.45001	-1.63124
C	4.43499	-2.06200	-1.59186
H	5.87637	-1.50308	1.43752
H	6.10096	-3.96087	1.34163
H	5.23457	-5.23135	-0.62252
H	4.15526	-3.99112	-2.49797
H	3.97451	-1.52678	-2.42384
O	2.66755	-0.65232	1.23811
C	-0.65345	1.86861	-2.52466
H	-1.41567	2.49794	-2.04930
H	0.00168	2.49777	-3.13549
H	-1.20592	1.18561	-3.18456
H	2.06462	2.48269	-3.30085
H	4.62263	1.85529	-2.66947
H	-4.62263	-1.85529	2.66947
H	-2.06462	-2.48269	3.30085

Compound **6**, S_1 state, dichloromethane:

Energy=-1909.4034

N	-2.36869	-0.62647	0.53067
C	-1.57364	-1.43341	1.35906
C	-0.18144	-1.33005	1.33882
C	0.39751	-0.37431	0.45990
C	-0.39751	0.37431	-0.45990
C	-1.84595	0.14482	-0.52132
C	-2.45469	-2.26037	2.09631
C	0.61141	-2.24707	2.22644
C	1.84595	-0.14482	0.52132
C	0.18144	1.33005	-1.33882
O	-2.58936	0.56574	-1.39210
N	2.36869	0.62647	-0.53067
C	1.57364	1.43341	-1.35906
C	3.70785	0.91938	-0.77458
C	3.75520	1.93849	-1.73280
C	2.45469	2.26037	-2.09631
C	-3.70785	-0.91938	0.77458
C	-3.75520	-1.93849	1.73280
H	1.43721	-2.71998	1.67954
H	1.07826	-1.70103	3.05827
H	-0.02792	-3.03551	2.64082
N	-4.77260	-0.25077	0.21006
C	-5.91093	-1.01121	-0.16753
C	-4.81295	1.16379	0.19297
C	-5.44397	1.84144	-0.85788
C	-5.48362	3.22893	-0.86607
C	-4.88245	3.96260	0.15827
C	-4.24891	3.28864	1.19950
C	-4.21852	1.89737	1.22532
H	-5.88993	1.27241	-1.67416
H	-5.97737	3.74616	-1.69163
H	-4.90972	5.05384	0.14357

H	-3.78248	3.84980	2.01215
H	-3.73959	1.37500	2.05511
C	-7.19640	-0.61762	0.22174
C	-8.29906	-1.37857	-0.15251
C	-8.13468	-2.54166	-0.90285
C	-6.85321	-2.93681	-1.28473
C	-5.74641	-2.17579	-0.92638
H	-7.32757	0.28387	0.82155
H	-9.29774	-1.06373	0.15764
H	-9.00275	-3.13811	-1.19003
H	-6.71303	-3.84139	-1.88025
H	-4.74428	-2.47185	-1.24019
N	4.77260	0.25077	-0.21006
C	4.81295	-1.16379	-0.19297
C	5.91093	1.01121	0.16753
C	7.19640	0.61762	-0.22174
C	8.29906	1.37857	0.15251
C	8.13468	2.54166	0.90285
C	6.85321	2.93681	1.28473
C	5.74641	2.17579	0.92638
H	7.32757	-0.28387	-0.82155
H	9.29774	1.06373	-0.15764
H	9.00275	3.13811	1.19003
H	6.71303	3.84139	1.88025
H	4.74428	2.47185	1.24019
C	5.44397	-1.84144	0.85788
C	5.48362	-3.22893	0.86607
C	4.88245	-3.96260	-0.15827
C	4.24891	-3.28864	-1.19950
C	4.21852	-1.89737	-1.22532
H	5.88993	-1.27241	1.67416
H	5.97737	-3.74616	1.69163
H	4.90972	-5.05384	-0.14357
H	3.78248	-3.84980	-2.01215
H	3.73959	-1.37500	-2.05511
O	2.58936	-0.56574	1.39210
C	-0.61141	2.24707	-2.22644
H	-1.43721	2.71998	-1.67954
H	0.02792	3.03551	-2.64082
H	-1.07826	1.70103	-3.05827
H	2.15720	2.99057	-2.84362
H	4.67431	2.35498	-2.13825
H	-4.67431	-2.35498	2.13825
H	-2.15720	-2.99057	2.84362

Compound **6**, S_0 state, DMSO:

Energy=-1909.4142

N	-2.37705	-0.44511	0.72589
C	-1.56310	-1.15689	1.60720
C	-0.13334	-1.09564	1.50488
C	0.42146	-0.34308	0.49182
C	-0.42146	0.34308	-0.49182
C	-1.88933	0.23059	-0.41089
C	-2.39109	-1.82603	2.49258
C	0.64745	-1.86546	2.52895
C	1.88933	-0.23059	0.41089
C	0.13334	1.09564	-1.50488
O	-2.66640	0.66267	-1.23581
N	2.37705	0.44511	-0.72589

C	1.56310	1.15689	-1.60720
C	3.70674	0.65067	-1.08447
C	3.72541	1.50260	-2.16711
C	2.39109	1.82603	-2.49258
C	-3.70674	-0.65067	1.08447
C	-3.72541	-1.50260	2.16711
H	1.40435	-2.50157	2.05413
H	1.20443	-1.18343	3.18602
H	-0.01022	-2.48875	3.14288
N	-4.79154	-0.04996	0.44747
C	-5.75781	-0.88585	-0.16568
C	-4.93026	1.35544	0.49240
C	-5.54726	2.05296	-0.55458
C	-5.66922	3.43620	-0.49976
C	-5.16320	4.15426	0.58399
C	-4.53671	3.46472	1.61852
C	-4.42517	2.07705	1.58055
H	-5.92449	1.50633	-1.41901
H	-6.15461	3.96206	-1.32515
H	-5.25534	5.24144	0.61887
H	-4.13614	4.00909	2.47668
H	-3.94652	1.54676	2.40534
C	-7.12714	-0.63614	-0.01258
C	-8.06294	-1.47517	-0.60915
C	-7.65288	-2.58282	-1.34958
C	-6.29086	-2.83893	-1.49416
C	-5.34831	-1.99438	-0.91569
H	-7.45763	0.21824	0.57959
H	-9.12734	-1.26656	-0.48015
H	-8.39070	-3.24257	-1.81014
H	-5.95368	-3.70032	-2.07495
H	-4.28281	-2.18937	-1.04687
N	4.79154	0.04996	-0.44747
C	4.93026	-1.35544	-0.49240
C	5.75781	0.88585	0.16568
C	7.12714	0.63614	0.01258
C	8.06294	1.47517	0.60915
C	7.65288	2.58282	1.34958
C	6.29086	2.83893	1.49416
C	5.34831	1.99438	0.91569
H	7.45763	-0.21824	-0.57959
H	9.12734	1.26656	0.48015
H	8.39070	3.24257	1.81014
H	5.95368	3.70032	2.07495
H	4.28281	2.18937	1.04687
C	5.54726	-2.05296	0.55458
C	5.66922	-3.43620	0.49976
C	5.16320	-4.15426	-0.58399
C	4.53671	-3.46472	-1.61852
C	4.42517	-2.07705	-1.58055
H	5.92449	-1.50633	1.41901
H	6.15461	-3.96206	1.32515
H	5.25534	-5.24144	-0.61887
H	4.13614	-4.00909	-2.47668
H	3.94652	-1.54676	-2.40534
O	2.66640	-0.66267	1.23581
C	-0.64745	1.86546	-2.52895
H	-1.40435	2.50157	-2.05413
H	0.01022	2.48875	-3.14288

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H      -1.20443      1.18343     -3.18602
H       2.07032      2.46420     -3.31083
H       4.62643      1.83234     -2.67853
H      -4.62643     -1.83234      2.67853
H      -2.07032     -2.46420      3.31083
```

Compound **6**, S_1 state, DMSO:

```
Energy=-1909.4053
N      -0.67285      2.32436     -0.65445
C      -1.77400      1.51275     -0.96994
C      -1.75157      0.14204     -0.71343
C      -0.58049     -0.39920     -0.11268
C       0.58049      0.39920      0.11268
C       0.58398      1.80759     -0.29931
C      -2.75559      2.35637     -1.54551
C      -2.95023     -0.67368     -1.10810
C      -0.58398     -1.80759      0.29931
C       1.75157     -0.14204      0.71343
O       1.57096      2.52425     -0.34876
N       0.67285     -2.32436      0.65445
C       1.77400     -1.51275      0.96994
C       0.97849     -3.64091      0.99063
C       2.26055     -3.65248      1.55325
C       2.75559     -2.35637      1.54551
C      -0.97849      3.64091     -0.99063
C      -2.26055      3.65248     -1.55325
H      -2.65693     -1.58313     -1.64796
H      -3.51440     -1.01537     -0.22881
H      -3.62264     -0.09143     -1.74903
N      -0.16965      4.72605     -0.73395
C      -0.10445      5.75091     -1.71668
C       0.41638      4.91408      0.54004
C       1.65574      5.55583      0.66072
C       2.22353      5.74244      1.91383
C       1.57784      5.28036      3.06211
C       0.34813      4.63725      2.94137
C      -0.23701      4.45983      1.69097
H       2.17620      5.89567     -0.23524
H       3.19060      6.24352      1.99473
H       2.03133      5.42353      4.04472
H      -0.17322      4.27975      3.83199
H      -1.21112      3.97540      1.60675
C      -0.30152      7.09140     -1.36692
C      -0.23786      8.08008     -2.34352
C       0.00796      7.74529     -3.67420
C       0.19734      6.40857     -4.02297
C       0.14779      5.41498     -3.05163
H      -0.50831      7.35501     -0.32888
H      -0.39448      9.12338     -2.06144
H       0.05245      8.52431     -4.43769
H       0.39864      6.13587     -5.06105
H       0.31377      4.36992     -3.31782
N       0.16965     -4.72605      0.73395
C      -0.41638     -4.91408     -0.54004
C       0.10445     -5.75091      1.71668
C       0.30152     -7.09140      1.36692
C       0.23786     -8.08008      2.34352
C      -0.00796     -7.74529      3.67420
C      -0.19734     -6.40857      4.02297
```

C	-0.14779	-5.41498	3.05163
H	0.50831	-7.35501	0.32888
H	0.39448	-9.12338	2.06144
H	-0.05245	-8.52431	4.43769
H	-0.39864	-6.13587	5.06105
H	-0.31377	-4.36992	3.31782
C	-1.65574	-5.55583	-0.66072
C	-2.22353	-5.74244	-1.91383
C	-1.57784	-5.28036	-3.06211
C	-0.34813	-4.63725	-2.94137
C	0.23701	-4.45983	-1.69097
H	-2.17620	-5.89567	0.23524
H	-3.19060	-6.24352	-1.99473
H	-2.03133	-5.42353	-4.04472
H	0.17322	-4.27975	-3.83199
H	1.21112	-3.97540	-1.60675
O	-1.57096	-2.52425	0.34876
C	2.95023	0.67368	1.10810
H	2.65693	1.58313	1.64796
H	3.62264	0.09143	1.74903
H	3.51440	1.01537	0.22881
H	3.73897	-2.04099	1.88288
H	2.77397	-4.55105	1.88734
H	-2.77397	4.55105	-1.88734
H	-3.73897	2.04099	-1.88288

Compound **8**, S_0 state, cyclohexane:

Energy=-2277.941

C	1.01730	-4.80818	-1.94154
C	0.21688	-5.07059	-0.82286
C	-1.05402	-5.63103	-1.01018
C	-1.50058	-5.94526	-2.28208
C	-0.69562	-5.68755	-3.40091
C	0.56565	-5.10979	-3.21770
N	0.68146	-4.73159	0.46597
C	0.34168	-5.47071	1.61484
C	0.20547	-6.86580	1.55814
C	-0.10717	-7.58879	2.69758
C	-0.27799	-6.93740	3.92628
C	-0.13030	-5.54622	3.98802
C	0.17108	-4.82252	2.84561
C	1.46129	-3.57834	0.60927
N	0.97894	-2.28995	0.40261
C	2.02741	-1.39092	0.57541
C	3.15408	-2.12096	0.91212
C	2.79620	-3.48727	0.92718
C	1.82688	0.02007	0.38588
C	0.56500	0.46383	0.05780
C	-0.56500	-0.46383	-0.05780
C	-0.36144	-1.90438	0.18489
C	0.36144	1.90438	-0.18489
N	-0.97894	2.28995	-0.40261
C	-2.02741	1.39092	-0.57541
C	-1.82688	-0.02007	-0.38588
C	-3.15408	2.12096	-0.91212
C	-2.79620	3.48727	-0.92718
C	-1.46129	3.57834	-0.60927
C	-3.02818	-0.90101	-0.55821
O	1.23860	2.73857	-0.21451

O	-1.23860	-2.73857	0.21451
C	3.02818	0.90101	0.55821
N	-0.68146	4.73159	-0.46597
C	-0.21688	5.07059	0.82286
C	1.05402	5.63103	1.01018
C	1.50058	5.94526	2.28208
C	0.69562	5.68755	3.40091
C	-0.56565	5.10979	3.21770
C	-1.01730	4.80818	1.94154
C	-0.34168	5.47071	-1.61484
C	-0.20547	6.86580	-1.55814
C	0.10717	7.58879	-2.69758
C	0.27799	6.93740	-3.92628
C	0.13030	5.54622	-3.98802
C	-0.17108	4.82252	-2.84561
H	-2.81774	-1.72809	-1.24753
H	-3.30074	-1.37767	0.39345
H	-3.88684	-0.33332	-0.93030
H	1.70233	5.80109	0.15164
H	2.49299	6.37764	2.41773
C	1.16330	6.00620	4.72054
H	-1.20032	4.90688	4.08148
H	-2.00657	4.36989	1.80673
H	-0.35654	7.38896	-0.61396
H	0.20582	8.67386	-2.64131
C	0.59704	7.68719	-5.10832
H	0.26519	5.02876	-4.93888
H	-0.26948	3.73879	-2.90448
H	0.35654	-7.38896	0.61396
H	-0.20582	-8.67386	2.64131
C	-0.59704	-7.68719	5.10832
H	-0.26519	-5.02876	4.93888
H	0.26948	-3.73879	2.90448
H	-1.70233	-5.80109	-0.15164
H	-2.49299	-6.37764	-2.41773
C	-1.16330	-6.00620	-4.72054
H	1.20032	-4.90688	-4.08148
H	2.00657	-4.36989	-1.80673
H	2.81774	1.72809	1.24753
H	3.88684	0.33332	0.93030
H	3.30074	1.37767	-0.39345
H	4.14307	-1.71762	1.10795
H	3.44380	-4.33668	1.13039
H	-3.44380	4.33668	-1.13039
H	-4.14307	1.71762	-1.10795
N	-1.53989	-6.26136	-5.78251
N	-0.85393	-8.29038	6.05957
N	0.85393	8.29038	-6.05957
N	1.53989	6.26136	5.78251

Compound **8**, S_1 state, cyclohexane:

Energy=-2277.9316

C	0.69224	-4.52276	-1.60755
C	-0.03866	-4.93835	-0.48804
C	-1.27091	-5.58163	-0.66788
C	-1.75486	-5.81557	-1.94182
C	-1.02514	-5.39570	-3.06499
C	0.20132	-4.74464	-2.88489
N	0.46000	-4.69018	0.80840

C	0.32671	-5.64532	1.84017
C	0.44497	-7.01551	1.56888
C	0.32477	-7.94236	2.59179
C	0.09597	-7.51790	3.90743
C	-0.01628	-6.14745	4.18000
C	0.09421	-5.22195	3.15576
C	1.20582	-3.55119	1.05751
N	0.82185	-2.26573	0.69166
C	1.86182	-1.38175	1.00627
C	2.88887	-2.14774	1.60334
C	2.47806	-3.47449	1.62996
C	1.74965	-0.01423	0.73020
C	0.55132	0.43878	0.11851
C	-0.55132	-0.43878	-0.11851
C	-0.45876	-1.84752	0.28828
C	0.45876	1.84752	-0.28828
N	-0.82185	2.26573	-0.69166
C	-1.86182	1.38175	-1.00627
C	-1.74965	0.01423	-0.73020
C	-2.88887	2.14774	-1.60334
C	-2.47806	3.47449	-1.62996
C	-1.20582	3.55119	-1.05751
C	-2.89214	-0.88163	-1.11181
O	1.38114	2.64252	-0.29285
O	-1.38114	-2.64252	0.29285
C	2.89214	0.88163	1.11181
N	-0.46000	4.69018	-0.80840
C	0.03866	4.93835	0.48804
C	1.27091	5.58163	0.66788
C	1.75486	5.81557	1.94182
C	1.02514	5.39570	3.06499
C	-0.20132	4.74464	2.88489
C	-0.69224	4.52276	1.60755
C	-0.32671	5.64532	-1.84017
C	-0.44497	7.01551	-1.56888
C	-0.32477	7.94236	-2.59179
C	-0.09597	7.51790	-3.90743
C	0.01628	6.14745	-4.18000
C	-0.09421	5.22195	-3.15576
H	-2.54527	-1.75721	-1.67585
H	-3.39929	-1.28484	-0.22422
H	-3.62509	-0.34161	-1.72198
H	1.85868	5.87606	-0.20116
H	2.71741	6.31098	2.07631
C	1.53212	5.63040	4.38722
H	-0.77822	4.42462	3.75365
H	-1.65772	4.03337	1.47328
H	-0.64113	7.35355	-0.55125
H	-0.42297	9.00701	-2.37540
C	0.02215	8.47955	-4.96721
H	0.20548	5.81091	-5.20025
H	0.01240	4.15745	-3.36543
H	0.64113	-7.35355	0.55125
H	0.42297	-9.00701	2.37540
C	-0.02215	-8.47955	4.96721
H	-0.20548	-5.81091	5.20025
H	-0.01240	-4.15745	3.36543
H	-1.85868	-5.87606	0.20116
H	-2.71741	-6.31098	-2.07631

C	-1.53212	-5.63040	-4.38722
H	0.77822	-4.42462	-3.75365
H	1.65772	-4.03337	-1.47328
H	2.54527	1.75721	1.67585
H	3.62509	0.34161	1.72198
H	3.39929	1.28484	0.22422
H	3.84380	-1.76282	1.94881
H	3.04288	-4.33195	1.98860
H	-3.04288	4.33195	-1.98860
H	-3.84380	1.76282	-1.94881
N	-1.93996	-5.81870	-5.45171
N	-0.11713	-9.25329	5.81970
N	0.11713	9.25329	-5.81970
N	1.93996	5.81870	5.45171

Compound **8**, S_0 state, toluene:

Energy=-2277.9434

C	1.01716	-4.80878	-1.94456
C	0.21720	-5.07301	-0.82584
C	-1.05234	-5.63671	-1.01326
C	-1.49799	-5.95243	-2.28509
C	-0.69323	-5.69309	-3.40374
C	0.56663	-5.11205	-3.22065
N	0.68073	-4.73240	0.46274
C	0.34060	-5.46969	1.61249
C	0.20328	-6.86484	1.55787
C	-0.10967	-7.58594	2.69835
C	-0.27979	-6.93235	3.92607
C	-0.13083	-5.54116	3.98600
C	0.17106	-4.81949	2.84247
C	1.46110	-3.57912	0.60506
N	0.97867	-2.29054	0.39975
C	2.02764	-1.39199	0.57184
C	3.15467	-2.12247	0.90628
C	2.79643	-3.48872	0.92105
C	1.82726	0.01926	0.38407
C	0.56513	0.46371	0.05780
C	-0.56513	-0.46371	-0.05780
C	-0.36150	-1.90453	0.18278
C	0.36150	1.90453	-0.18278
N	-0.97867	2.29054	-0.39975
C	-2.02764	1.39199	-0.57184
C	-1.82726	-0.01926	-0.38407
C	-3.15467	2.12247	-0.90628
C	-2.79643	3.48872	-0.92105
C	-1.46110	3.57912	-0.60506
C	-3.02909	-0.89944	-0.55635
O	1.23872	2.73895	-0.21123
O	-1.23872	-2.73895	0.21123
C	3.02909	0.89944	0.55635
N	-0.68073	4.73240	-0.46274
C	-0.21720	5.07301	0.82584
C	1.05234	5.63671	1.01326
C	1.49799	5.95243	2.28509
C	0.69323	5.69309	3.40374
C	-0.56663	5.11205	3.22065
C	-1.01716	4.80878	1.94456
C	-0.34060	5.46969	-1.61249
C	-0.20328	6.86484	-1.55787

C	0.10967	7.58594	-2.69835
C	0.27979	6.93235	-3.92607
C	0.13083	5.54116	-3.98600
C	-0.17106	4.81949	-2.84247
H	-2.81960	-1.72547	-1.24718
H	-3.30096	-1.37702	0.39504
H	-3.88789	-0.33092	-0.92678
H	1.70058	5.80863	0.15507
H	2.48933	6.38727	2.42047
C	1.15968	6.01363	4.72323
H	-1.20117	4.90774	4.08419
H	-2.00523	4.36783	1.80997
H	-0.35391	7.38978	-0.61463
H	0.20906	8.67100	-2.64343
C	0.59937	7.68005	-5.10915
H	0.26497	5.02195	-4.93599
H	-0.27076	3.73583	-2.90011
H	0.35391	-7.38978	0.61463
H	-0.20906	-8.67100	2.64343
C	-0.59937	-7.68005	5.10915
H	-0.26497	-5.02195	4.93599
H	0.27076	-3.73583	2.90011
H	-1.70058	-5.80863	-0.15507
H	-2.48933	-6.38727	-2.42047
C	-1.15968	-6.01363	-4.72323
H	1.20117	-4.90774	-4.08419
H	2.00523	-4.36783	-1.80997
H	2.81960	1.72547	1.24718
H	3.88789	0.33092	0.92678
H	3.30096	1.37702	-0.39504
H	4.14410	-1.71958	1.10091
H	3.44417	-4.33838	1.12274
H	-3.44417	4.33838	-1.12274
H	-4.14410	1.71958	-1.10091
N	-1.53527	-6.27059	-5.78519
N	-0.85667	-8.28168	6.06137
N	0.85667	8.28168	-6.06137
N	1.53527	6.27059	5.78519

Compound **8**, S_1 state, toluene:

Energy=-2277.934

C	0.68705	-4.52220	-1.60632
C	-0.04241	-4.94002	-0.48668
C	-1.27264	-5.58734	-0.66614
C	-1.75625	-5.82288	-1.93990
C	-1.02789	-5.40067	-3.06313
C	0.19661	-4.74568	-2.88353
N	0.45591	-4.69107	0.80972
C	0.32562	-5.64773	1.84074
C	0.44820	-7.01724	1.56806
C	0.33063	-7.94541	2.59005
C	0.10026	-7.52252	3.90595
C	-0.01617	-6.15268	4.18006
C	0.09174	-5.22603	3.15660
C	1.20159	-3.55226	1.05926
N	0.81892	-2.26649	0.69276
C	1.85890	-1.38312	1.00949
C	2.88459	-2.15015	1.60852
C	2.47292	-3.47636	1.63418

C	1.74838	-0.01598	0.73389
C	0.55114	0.43833	0.11967
C	-0.55114	-0.43833	-0.11967
C	-0.46030	-1.84722	0.28686
C	0.46030	1.84722	-0.28686
N	-0.81892	2.26649	-0.69276
C	-1.85890	1.38312	-1.00949
C	-1.74838	0.01598	-0.73389
C	-2.88459	2.15015	-1.60852
C	-2.47292	3.47636	-1.63418
C	-1.20159	3.55226	-1.05926
C	-2.89053	-0.87899	-1.11883
O	1.38348	2.64160	-0.28926
O	-1.38348	-2.64160	0.28926
C	2.89053	0.87899	1.11883
N	-0.45591	4.69107	-0.80972
C	0.04241	4.94002	0.48668
C	1.27264	5.58734	0.66614
C	1.75625	5.82288	1.93990
C	1.02789	5.40067	3.06313
C	-0.19661	4.74568	2.88353
C	-0.68705	4.52220	1.60632
C	-0.32562	5.64773	-1.84074
C	-0.44820	7.01724	-1.56806
C	-0.33063	7.94541	-2.59005
C	-0.10026	7.52252	-3.90595
C	0.01617	6.15268	-4.18006
C	-0.09174	5.22603	-3.15660
H	-2.54263	-1.75477	-1.68188
H	-3.40095	-1.28140	-0.23275
H	-3.62117	-0.33842	-1.73122
H	1.85913	5.88444	-0.20287
H	2.71713	6.32162	2.07389
C	1.53417	5.63736	4.38518
H	-0.77257	4.42392	3.75226
H	-1.65117	4.03005	1.47263
H	-0.64560	7.35393	-0.55025
H	-0.43215	9.00948	-2.37248
C	0.01531	8.48545	-4.96479
H	0.20645	5.81738	-5.20049
H	0.01791	4.16207	-3.36740
H	0.64560	-7.35393	0.55025
H	0.43215	-9.00948	2.37248
C	-0.01531	-8.48545	4.96479
H	-0.20645	-5.81738	5.20049
H	-0.01791	-4.16207	3.36740
H	-1.85913	-5.88444	0.20287
H	-2.71713	-6.32162	-2.07389
C	-1.53417	-5.63736	-4.38518
H	0.77257	-4.42392	-3.75226
H	1.65117	-4.03005	-1.47263
H	2.54263	1.75477	1.68188
H	3.62117	0.33842	1.73122
H	3.40095	1.28140	0.23275
H	3.83925	-1.76604	1.95565
H	3.03663	-4.33422	1.99363
H	-3.03663	4.33422	-1.99363
H	-3.83925	1.76604	-1.95565
N	-1.94143	-5.82744	-5.44964

N	-0.10832	-9.26026	5.81660
N	0.10832	9.26026	-5.81660
N	1.94143	5.82744	5.44964

Compound **8**, S_0 state, THF:

Energy=-2277.9546

C	1.00698	-4.80361	-1.95864
C	0.21416	-5.08654	-0.83863
C	-1.04366	-5.67734	-1.02585
C	-1.48449	-6.00076	-2.29728
C	-0.68581	-5.72317	-3.41614
C	0.56205	-5.11540	-3.23420
N	0.67163	-4.73750	0.44847
C	0.33241	-5.46801	1.60236
C	0.20148	-6.86445	1.55853
C	-0.11034	-7.57781	2.70392
C	-0.28586	-6.91386	3.92572
C	-0.14272	-5.52133	3.97589
C	0.15876	-4.80817	2.82712
C	1.45507	-3.58467	0.58728
N	0.97399	-2.29463	0.38724
C	2.02613	-1.39948	0.55745
C	3.15338	-2.13322	0.88352
C	2.79186	-3.49877	0.89637
C	1.82852	0.01309	0.37753
C	0.56618	0.46246	0.05868
C	-0.56618	-0.46246	-0.05868
C	-0.36410	-1.90494	0.17112
C	0.36410	1.90494	-0.17112
N	-0.97399	2.29463	-0.38724
C	-2.02613	1.39948	-0.55745
C	-1.82852	-0.01309	-0.37753
C	-3.15338	2.13322	-0.88352
C	-2.79186	3.49877	-0.89637
C	-1.45507	3.58467	-0.58728
C	-3.03398	-0.88801	-0.55016
O	1.24267	2.73955	-0.19106
O	-1.24267	-2.73955	0.19106
C	3.03398	0.88801	0.55016
N	-0.67163	4.73750	-0.44847
C	-0.21416	5.08654	0.83863
C	1.04366	5.67734	1.02585
C	1.48449	6.00076	2.29728
C	0.68581	5.72317	3.41614
C	-0.56205	5.11540	3.23420
C	-1.00698	4.80361	1.95864
C	-0.33241	5.46801	-1.60236
C	-0.20148	6.86445	-1.55853
C	0.11034	7.57781	-2.70392
C	0.28586	6.91386	-3.92572
C	0.14272	5.52133	-3.97589
C	-0.15876	4.80817	-2.82712
H	-2.83087	-1.70716	-1.25099
H	-3.30135	-1.37249	0.39897
H	-3.89348	-0.31376	-0.90952
H	1.68804	5.86718	0.16860
H	2.46651	6.45674	2.43052
C	1.14595	6.05313	4.73484
H	-1.19215	4.89614	4.09724

H	-1.98550	4.34166	1.82616
H	-0.35706	7.39741	-0.62076
H	0.20416	8.66363	-2.65645
C	0.60474	7.65307	-5.11368
H	0.28031	4.99390	-4.92079
H	-0.25536	3.72391	-2.87760
H	0.35706	-7.39741	0.62076
H	-0.20416	-8.66363	2.65645
C	-0.60474	-7.65307	5.11368
H	-0.28031	-4.99390	4.92079
H	0.25536	-3.72391	2.87760
H	-1.68804	-5.86718	-0.16860
H	-2.46651	-6.45674	-2.43052
C	-1.14595	-6.05313	-4.73484
H	1.19215	-4.89614	-4.09724
H	1.98550	-4.34166	-1.82616
H	2.83087	1.70716	1.25099
H	3.89348	0.31376	0.90952
H	3.30135	1.37249	-0.39897
H	4.14488	-1.73361	1.07436
H	3.43901	-4.35034	1.09187
H	-3.43901	4.35034	-1.09187
H	-4.14488	1.73361	-1.07436
N	-1.51650	-6.31861	-5.79686
N	-0.86161	-8.24834	6.07042
N	0.86161	8.24834	-6.07042
N	1.51650	6.31861	5.79686

Compound **8**, S_1 state, THF:

Energy=-2277.944

C	0.66024	-4.51833	-1.60613
C	-0.05858	-4.95003	-0.48468
C	-1.27691	-5.62093	-0.66081
C	-1.76008	-5.86512	-1.93308
C	-1.04210	-5.42843	-3.05763
C	0.17071	-4.75041	-2.88197
N	0.43885	-4.69619	0.81070
C	0.32107	-5.65798	1.84000
C	0.46935	-7.02414	1.56458
C	0.36220	-7.95635	2.58396
C	0.11691	-7.53849	3.89896
C	-0.02453	-6.17149	4.17643
C	0.07318	-5.24166	3.15486
C	1.18408	-3.55818	1.06186
N	0.80670	-2.27068	0.69391
C	1.84614	-1.39000	1.02194
C	2.86584	-2.16217	1.62912
C	2.45086	-3.48611	1.64851
C	1.74232	-0.02443	0.75115
C	0.54984	0.43642	0.12590
C	-0.54984	-0.43642	-0.12590
C	-0.46595	-1.84657	0.27674
C	0.46595	1.84657	-0.27674
N	-0.80670	2.27068	-0.69391
C	-1.84614	1.39000	-1.02194
C	-1.74232	0.02443	-0.75115
C	-2.86584	2.16217	-1.62912
C	-2.45086	3.48611	-1.64851
C	-1.18408	3.55818	-1.06186

C	-2.88187	-0.86646	-1.15390
O	1.39239	2.63881	-0.26718
O	-1.39239	-2.63881	0.26718
C	2.88187	0.86646	1.15390
N	-0.43885	4.69619	-0.81070
C	0.05858	4.95003	0.48468
C	1.27691	5.62093	0.66081
C	1.76008	5.86512	1.93308
C	1.04210	5.42843	3.05763
C	-0.17071	4.75041	2.88197
C	-0.66024	4.51833	1.60613
C	-0.32107	5.65798	-1.84000
C	-0.46935	7.02414	-1.56458
C	-0.36220	7.95635	-2.58396
C	-0.11691	7.53849	-3.89896
C	0.02453	6.17149	-4.17643
C	-0.07318	5.24166	-3.15486
H	-2.52838	-1.74069	-1.71568
H	-3.40669	-1.26846	-0.27613
H	-3.60248	-0.32196	-1.77446
H	1.85432	5.93389	-0.20875
H	2.71103	6.38336	2.06333
C	1.54650	5.67574	4.37798
H	-0.73916	4.41746	3.75132
H	-1.61597	4.00934	1.47664
H	-0.67868	7.35589	-0.54763
H	-0.48361	9.01773	-2.36397
C	-0.01117	8.50504	-4.95517
H	0.22568	5.84044	-5.19606
H	0.05500	4.18016	-3.36774
H	0.67868	-7.35589	0.54763
H	0.48361	-9.01773	2.36397
C	0.01117	-8.50504	4.95517
H	-0.22568	-5.84044	5.19606
H	-0.05500	-4.18016	3.36774
H	-1.85432	-5.93389	0.20875
H	-2.71103	-6.38336	-2.06333
C	-1.54650	-5.67574	-4.37798
H	0.73916	-4.41746	-3.75132
H	1.61597	-4.00934	-1.47664
H	2.52838	1.74069	1.71568
H	3.60248	0.32196	1.77446
H	3.40669	1.26846	0.27613
H	3.81910	-1.78180	1.98451
H	3.00978	-4.34599	2.01063
H	-3.00978	4.34599	-2.01063
H	-3.81910	1.78180	-1.98451
N	-1.95246	-5.87507	-5.44156
N	-0.07443	-9.28295	5.80529
N	0.07443	9.28295	-5.80529
N	1.95246	5.87507	5.44156

Compound **8**, S_0 state, dichloromethane:

Energy=-2277.9556

C	1.00535	-4.80250	-1.96027
C	0.21367	-5.08808	-0.84003
C	-1.04253	-5.68251	-1.02717
C	-1.48282	-6.00678	-2.29856
C	-0.68519	-5.72656	-3.41753

C	0.56100	-5.11522	-3.23577
N	0.67046	-4.73809	0.44687
C	0.33137	-5.46789	1.60124
C	0.20188	-6.86452	1.55874
C	-0.10978	-7.57702	2.70470
C	-0.28657	-6.91188	3.92570
C	-0.14482	-5.51913	3.97463
C	0.15655	-4.80690	2.82525
C	1.45423	-3.58533	0.58537
N	0.97339	-2.29511	0.38585
C	2.02589	-1.40037	0.55591
C	3.15308	-2.13452	0.88124
C	2.79115	-3.49996	0.89385
C	1.82865	0.01233	0.37677
C	0.56631	0.46229	0.05877
C	-0.56631	-0.46229	-0.05877
C	-0.36444	-1.90497	0.16974
C	0.36444	1.90497	-0.16974
N	-0.97339	2.29511	-0.38585
C	-2.02589	1.40037	-0.55591
C	-1.82865	-0.01233	-0.37677
C	-3.15308	2.13452	-0.88124
C	-2.79115	3.49996	-0.89385
C	-1.45423	3.58533	-0.58537
C	-3.03457	-0.88664	-0.54928
O	1.24319	2.73958	-0.18860
O	-1.24319	-2.73958	0.18860
C	3.03457	0.88664	0.54928
N	-0.67046	4.73809	-0.44687
C	-0.21367	5.08808	0.84003
C	1.04253	5.68251	1.02717
C	1.48282	6.00678	2.29856
C	0.68519	5.72656	3.41753
C	-0.56100	5.11522	3.23577
C	-1.00535	4.80250	1.96027
C	-0.33137	5.46789	-1.60124
C	-0.20188	6.86452	-1.55874
C	0.10978	7.57702	-2.70470
C	0.28657	6.91188	-3.92570
C	0.14482	5.51913	-3.97463
C	-0.15655	4.80690	-2.82525
H	-2.83245	-1.70472	-1.25164
H	-3.30102	-1.37228	0.39950
H	-3.89431	-0.31163	-0.90682
H	1.68620	5.87487	0.16997
H	2.46354	6.46564	2.43151
C	1.14466	6.05754	4.73613
H	-1.19032	4.89381	4.09882
H	-1.98257	4.33777	1.82810
H	-0.35855	7.39838	-0.62168
H	0.20241	8.66299	-2.65820
C	0.60530	7.65016	-5.11422
H	0.28333	4.99076	-4.91886
H	-0.25220	3.72251	-2.87478
H	0.35855	-7.39838	0.62168
H	-0.20241	-8.66299	2.65820
C	-0.60530	-7.65016	5.11422
H	-0.28333	-4.99076	4.91886
H	0.25220	-3.72251	2.87478

H	-1.68620	-5.87487	-0.16997
H	-2.46354	-6.46564	-2.43151
C	-1.14466	-6.05754	-4.73613
H	1.19032	-4.89381	-4.09882
H	1.98257	-4.33777	-1.82810
H	2.83245	1.70472	1.25164
H	3.89431	0.31163	0.90682
H	3.30102	1.37228	-0.39950
H	4.14480	-1.73530	1.07180
H	3.43817	-4.35177	1.08875
H	-3.43817	4.35177	-1.08875
H	-4.14480	1.73530	-1.07180
N	-1.51471	-6.32394	-5.79814
N	-0.86208	-8.24475	6.07144
N	0.86208	8.24475	-6.07144
N	1.51471	6.32394	5.79814

Compound **8**, S_1 state, dichloromethane:

Energy=-2277.945

C	0.65694	-4.51749	-1.60618
C	-0.06038	-4.95109	-0.48448
C	-1.27721	-5.62489	-0.66019
C	-1.76047	-5.86991	-1.93226
C	-1.04400	-5.43122	-3.05702
C	0.16735	-4.75042	-2.88183
N	0.43701	-4.69674	0.81074
C	0.32057	-5.65907	1.83989
C	0.47240	-7.02476	1.56432
C	0.36639	-7.95738	2.58345
C	0.11871	-7.54012	3.89821
C	-0.02622	-6.17351	4.17587
C	0.07038	-5.24336	3.15448
C	1.18217	-3.55881	1.06215
N	0.80536	-2.27112	0.69406
C	1.84468	-1.39072	1.02345
C	2.86367	-2.16342	1.63160
C	2.44837	-3.48714	1.65021
C	1.74155	-0.02530	0.75320
C	0.54968	0.43623	0.12664
C	-0.54968	-0.43623	-0.12664
C	-0.46655	-1.84651	0.27559
C	0.46655	1.84651	-0.27559
N	-0.80536	2.27112	-0.69406
C	-1.84468	1.39072	-1.02345
C	-1.74155	0.02530	-0.75320
C	-2.86367	2.16342	-1.63160
C	-2.44837	3.48714	-1.65021
C	-1.18217	3.55881	-1.06215
C	-2.88072	-0.86516	-1.15804
O	1.39333	2.63853	-0.26466
O	-1.39333	-2.63853	0.26466
C	2.88072	0.86516	1.15804
N	-0.43701	4.69674	-0.81074
C	0.06038	4.95109	0.48448
C	1.27721	5.62489	0.66019
C	1.76047	5.86991	1.93226
C	1.04400	5.43122	3.05702
C	-0.16735	4.75042	2.88183
C	-0.65694	4.51749	1.60618

C	-0.32057	5.65907	-1.83989
C	-0.47240	7.02476	-1.56432
C	-0.36639	7.95738	-2.58345
C	-0.11871	7.54012	-3.89821
C	0.02622	6.17351	-4.17587
C	-0.07038	5.24336	-3.15448
H	-2.52653	-1.73910	-1.71982
H	-3.40708	-1.26729	-0.28125
H	-3.60027	-0.32019	-1.77941
H	1.85334	5.93991	-0.20947
H	2.71018	6.39053	2.06206
C	1.54840	5.67952	4.37713
H	-0.73471	4.41592	3.75129
H	-1.61158	4.00635	1.47722
H	-0.68366	7.35587	-0.54757
H	-0.49058	9.01841	-2.36336
C	-0.01406	8.50703	-4.95416
H	0.22915	5.84300	-5.19531
H	0.06040	4.18218	-3.36742
H	0.68366	-7.35587	0.54757
H	0.49058	-9.01841	2.36336
C	0.01406	-8.50703	4.95416
H	-0.22915	-5.84300	5.19531
H	-0.06040	-4.18218	3.36742
H	-1.85334	-5.93991	0.20947
H	-2.71018	-6.39053	-2.06206
C	-1.54840	-5.67952	-4.37713
H	0.73471	-4.41592	-3.75129
H	1.61158	-4.00635	-1.47722
H	2.52653	1.73910	1.71982
H	3.60027	0.32019	1.77941
H	3.40708	1.26729	0.28125
H	3.81671	-1.78342	1.98801
H	3.00674	-4.34723	2.01266
H	-3.00674	4.34723	-2.01266
H	-3.81671	1.78342	-1.98801
N	-1.95443	-5.87969	-5.44056
N	-0.07073	-9.28524	5.80413
N	0.07073	9.28524	-5.80413
N	1.95443	5.87969	5.44056

Compound **8**, S_0 state, DMSO:

Energy=-2277.9602

C	0.99638	-4.79565	-1.96870
C	0.21119	-5.09548	-0.84716
C	-1.03631	-5.70889	-1.03381
C	-1.47402	-6.03722	-2.30501
C	-0.68248	-5.74272	-3.42472
C	0.55477	-5.11276	-3.24384
N	0.66474	-4.74095	0.43875
C	0.32615	-5.46711	1.59565
C	0.20519	-6.86476	1.56030
C	-0.10584	-7.57277	2.70913
C	-0.29051	-6.90139	3.92573
C	-0.15708	-5.50747	3.96790
C	0.14391	-4.80007	2.81545
C	1.45008	-3.58857	0.57589
N	0.97052	-2.29751	0.37855
C	2.02479	-1.40475	0.54812

C	3.15151	-2.14084	0.87047
C	2.78748	-3.50578	0.88210
C	1.82944	0.00855	0.37246
C	0.56696	0.46149	0.05917
C	-0.56696	-0.46149	-0.05917
C	-0.36598	-1.90518	0.16230
C	0.36598	1.90518	-0.16230
N	-0.97052	2.29751	-0.37855
C	-2.02479	1.40475	-0.54812
C	-1.82944	-0.00855	-0.37246
C	-3.15151	2.14084	-0.87047
C	-2.78748	3.50578	-0.88210
C	-1.45008	3.58857	-0.57589
C	-3.03768	-0.87987	-0.54354
O	1.24548	2.73989	-0.17496
O	-1.24548	-2.73989	0.17496
C	3.03768	0.87987	0.54354
N	-0.66474	4.74095	-0.43875
C	-0.21119	5.09548	0.84716
C	1.03631	5.70889	1.03381
C	1.47402	6.03722	2.30501
C	0.68248	5.74272	3.42472
C	-0.55477	5.11276	3.24384
C	-0.99638	4.79565	1.96870
C	-0.32615	5.46711	-1.59565
C	-0.20519	6.86476	-1.56030
C	0.10584	7.57277	-2.70913
C	0.29051	6.90139	-3.92573
C	0.15708	5.50747	-3.96790
C	-0.14391	4.80007	-2.81545
H	-2.84175	-1.69108	-1.25567
H	-3.29721	-1.37342	0.40297
H	-3.89954	-0.30078	-0.88888
H	1.67586	5.91477	0.17669
H	2.44771	6.51118	2.43652
C	1.13882	6.07855	4.74285
H	-1.17955	4.87973	4.10710
H	-1.96668	4.31643	1.83813
H	-0.36853	7.40321	-0.62707
H	0.19157	8.65947	-2.66797
C	0.60869	7.63493	-5.11709
H	0.30141	4.97425	-4.90850
H	-0.23367	3.71492	-2.85961
H	0.36853	-7.40321	0.62707
H	-0.19157	-8.65947	2.66797
C	-0.60869	-7.63493	5.11709
H	-0.30141	-4.97425	4.90850
H	0.23367	-3.71492	2.85961
H	-1.67586	-5.91477	-0.17669
H	-2.44771	-6.51118	-2.43652
C	-1.13882	-6.07855	-4.74285
H	1.17955	-4.87973	-4.10710
H	1.96668	-4.31643	-1.83813
H	2.84175	1.69108	1.25567
H	3.89954	0.30078	0.88888
H	3.29721	1.37342	-0.40297
H	4.14419	-1.74360	1.06023
H	3.43367	-4.35877	1.07453
H	-3.43367	4.35877	-1.07453

H	-4.14419	1.74360	-1.06023
N	-1.50651	-6.34932	-5.80474
N	-0.86516	-8.22598	6.07674
N	0.86516	8.22598	-6.07674
N	1.50651	6.34932	5.80474

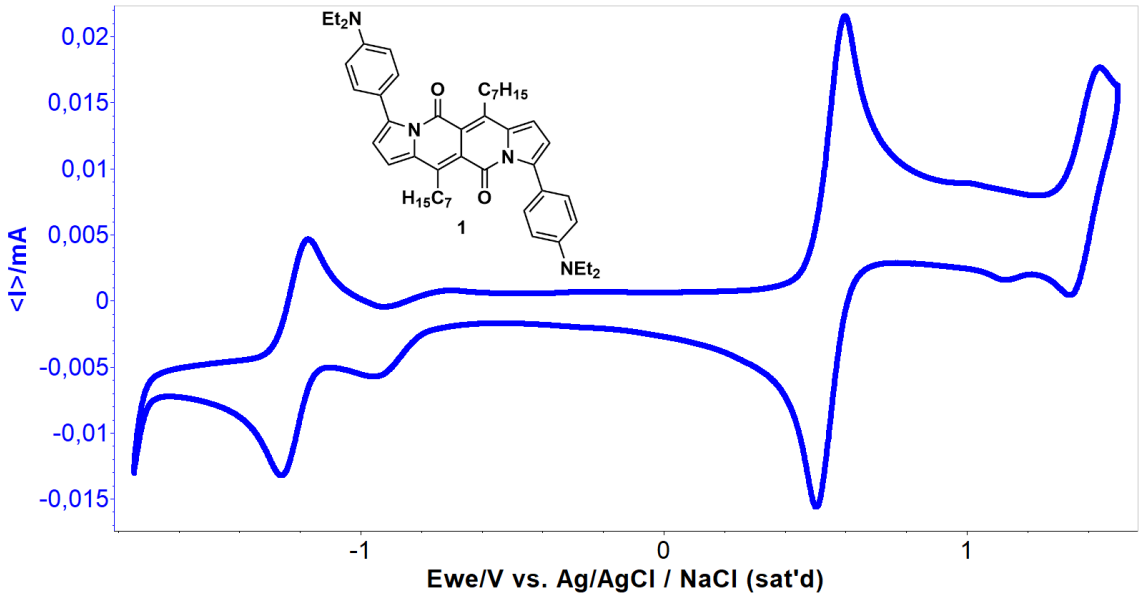
Compound **8**, S_1 state, DMSO:

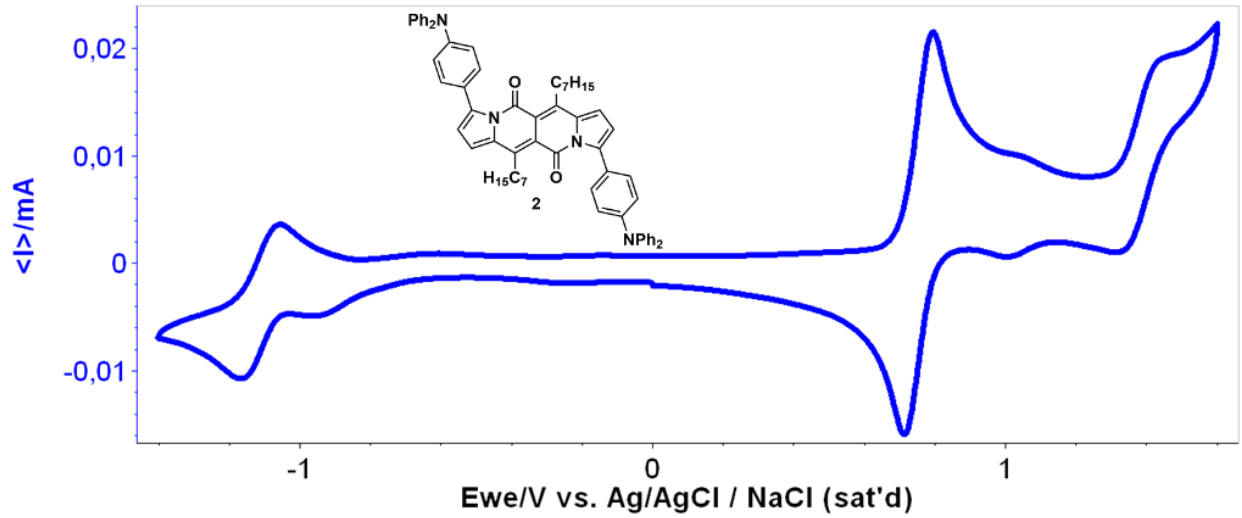
Energy=-2277.945

C	0.65694	-4.51749	-1.60618
C	-0.06038	-4.95109	-0.48448
C	-1.27721	-5.62489	-0.66019
C	-1.76047	-5.86991	-1.93226
C	-1.04400	-5.43122	-3.05702
C	0.16735	-4.75042	-2.88183
N	0.43701	-4.69674	0.81074
C	0.32057	-5.65907	1.83989
C	0.47240	-7.02476	1.56432
C	0.36639	-7.95738	2.58345
C	0.11871	-7.54012	3.89821
C	-0.02622	-6.17351	4.17587
C	0.07038	-5.24336	3.15448
C	1.18217	-3.55881	1.06215
N	0.80536	-2.27112	0.69406
C	1.84468	-1.39072	1.02345
C	2.86367	-2.16342	1.63160
C	2.44837	-3.48714	1.65021
C	1.74155	-0.02530	0.75320
C	0.54968	0.43623	0.12664
C	-0.54968	-0.43623	-0.12664
C	-0.46655	-1.84651	0.27559
C	0.46655	1.84651	-0.27559
N	-0.80536	2.27112	-0.69406
C	-1.84468	1.39072	-1.02345
C	-1.74155	0.02530	-0.75320
C	-2.86367	2.16342	-1.63160
C	-2.44837	3.48714	-1.65021
C	-1.18217	3.55881	-1.06215
C	-2.88072	-0.86516	-1.15804
O	1.39333	2.63853	-0.26466
O	-1.39333	-2.63853	0.26466
C	2.88072	0.86516	1.15804
N	-0.43701	4.69674	-0.81074
C	0.06038	4.95109	0.48448
C	1.27721	5.62489	0.66019
C	1.76047	5.86991	1.93226
C	1.04400	5.43122	3.05702
C	-0.16735	4.75042	2.88183
C	-0.65694	4.51749	1.60618
C	-0.32057	5.65907	-1.83989
C	-0.47240	7.02476	-1.56432
C	-0.36639	7.95738	-2.58345
C	-0.11871	7.54012	-3.89821
C	0.02622	6.17351	-4.17587
C	-0.07038	5.24336	-3.15448
H	-2.52653	-1.73910	-1.71982
H	-3.40708	-1.26729	-0.28125
H	-3.60027	-0.32019	-1.77941
H	1.85334	5.93991	-0.20947
H	2.71018	6.39053	2.06206

C	1.54840	5.67952	4.37713
H	-0.73471	4.41592	3.75129
H	-1.61158	4.00635	1.47722
H	-0.68366	7.35587	-0.54757
H	-0.49058	9.01841	-2.36336
C	-0.01406	8.50703	-4.95416
H	0.22915	5.84300	-5.19531
H	0.06040	4.18218	-3.36742
H	0.68366	-7.35587	0.54757
H	0.49058	-9.01841	2.36336
C	0.01406	-8.50703	4.95416
H	-0.22915	-5.84300	5.19531
H	-0.06040	-4.18218	3.36742
H	-1.85334	-5.93991	0.20947
H	-2.71018	-6.39053	-2.06206
C	-1.54840	-5.67952	-4.37713
H	0.73471	-4.41592	-3.75129
H	1.61158	-4.00635	-1.47722
H	2.52653	1.73910	1.71982
H	3.60027	0.32019	1.77941
H	3.40708	1.26729	0.28125
H	3.81671	-1.78342	1.98801
H	3.00674	-4.34723	2.01266
H	-3.00674	4.34723	-2.01266
H	-3.81671	1.78342	-1.98801
N	-1.95443	-5.87969	-5.44056
N	-0.07073	-9.28524	5.80413
N	0.07073	9.28524	-5.80413
N	1.95443	5.87969	5.44056

4. CV measurements

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H15C7
NPh2
2
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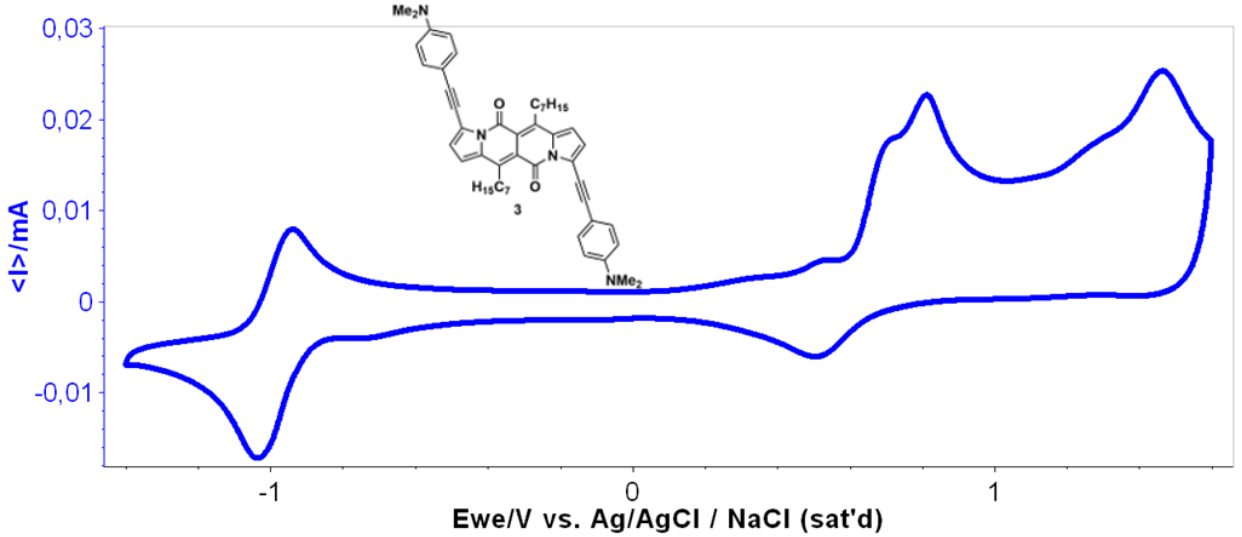
0,01
0
-0,01
<I>/mA
-1
0
1
Ewe/V vs. Ag/AgCl / NaCl (sat'd)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C7H15
H15C7
NMe2
3
0,03
0,02
0,01
0
-0,01
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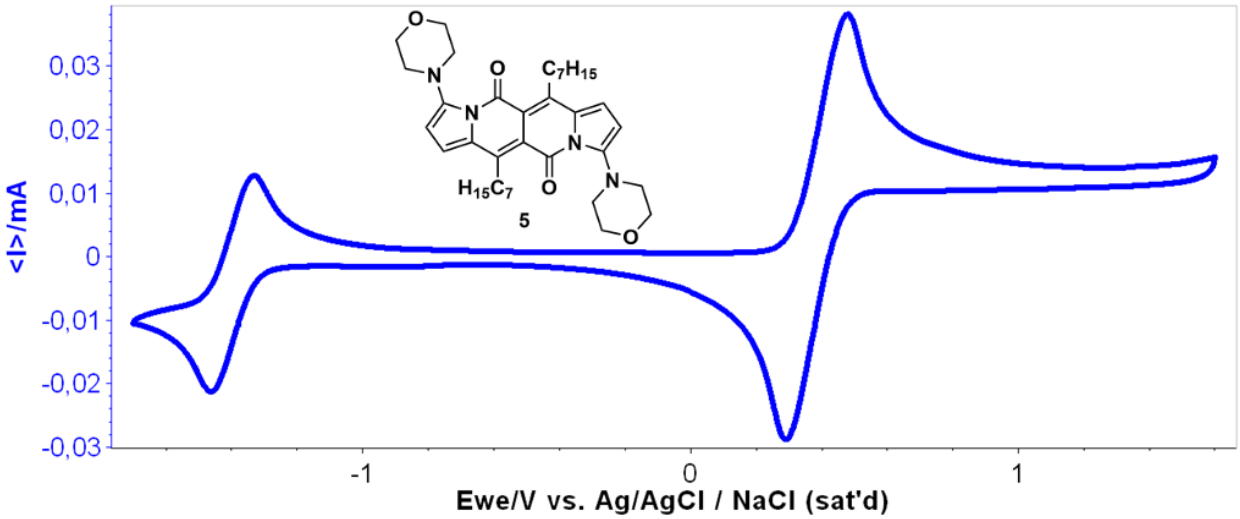
-1
0
1
Ewe/V vs. Ag/AgCl / NaCl (sat'd)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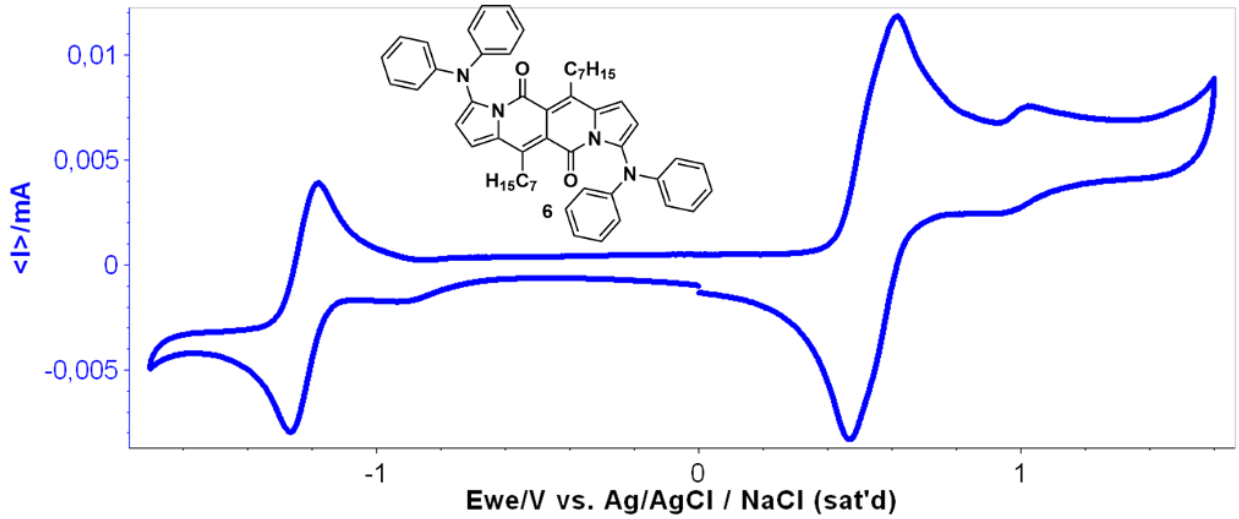
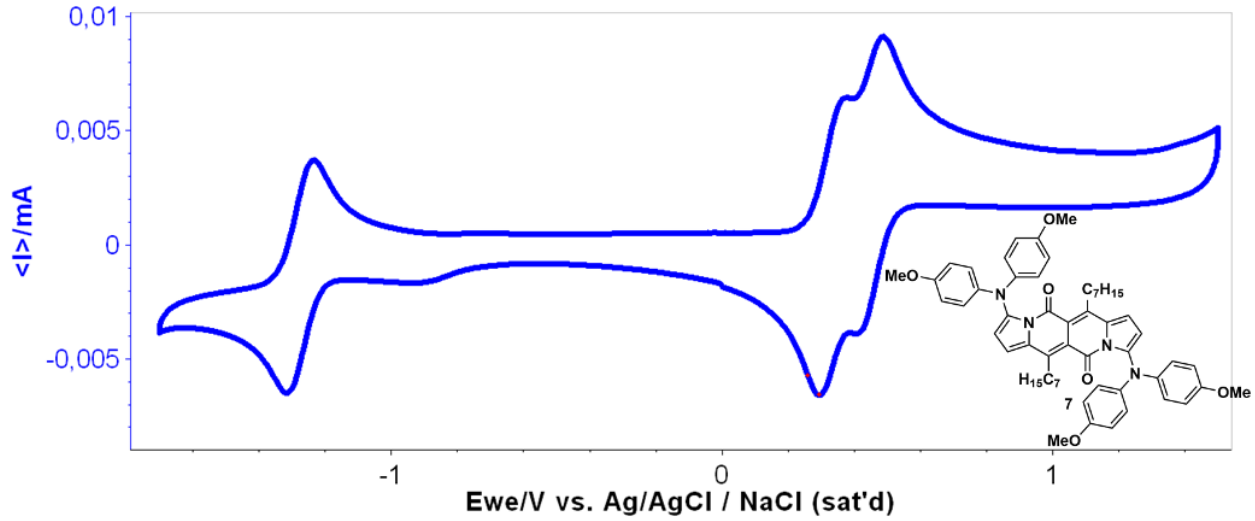
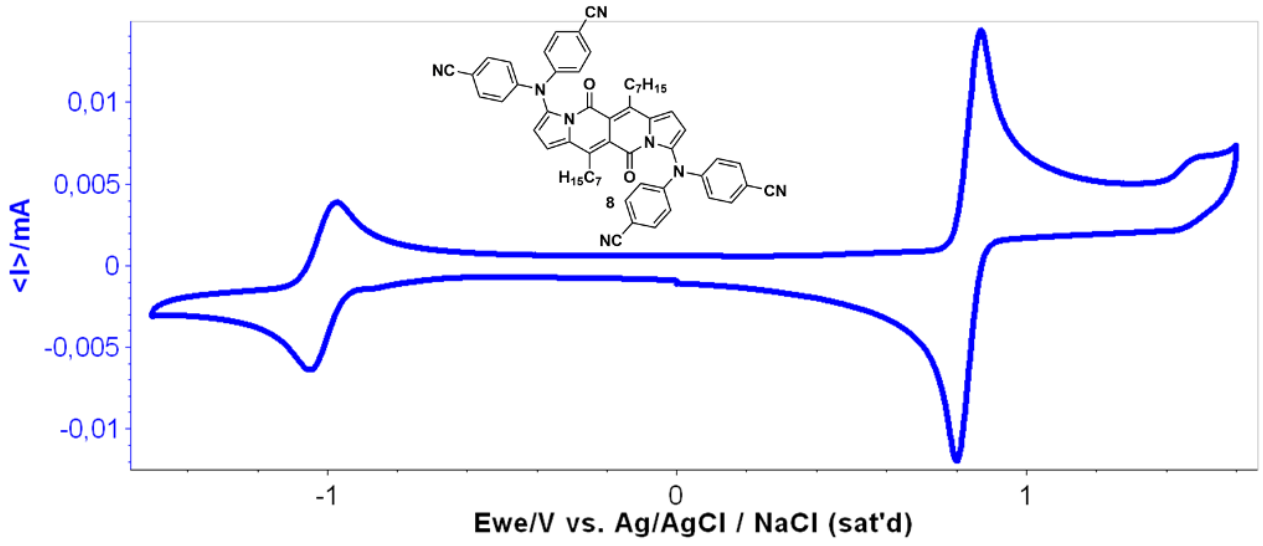
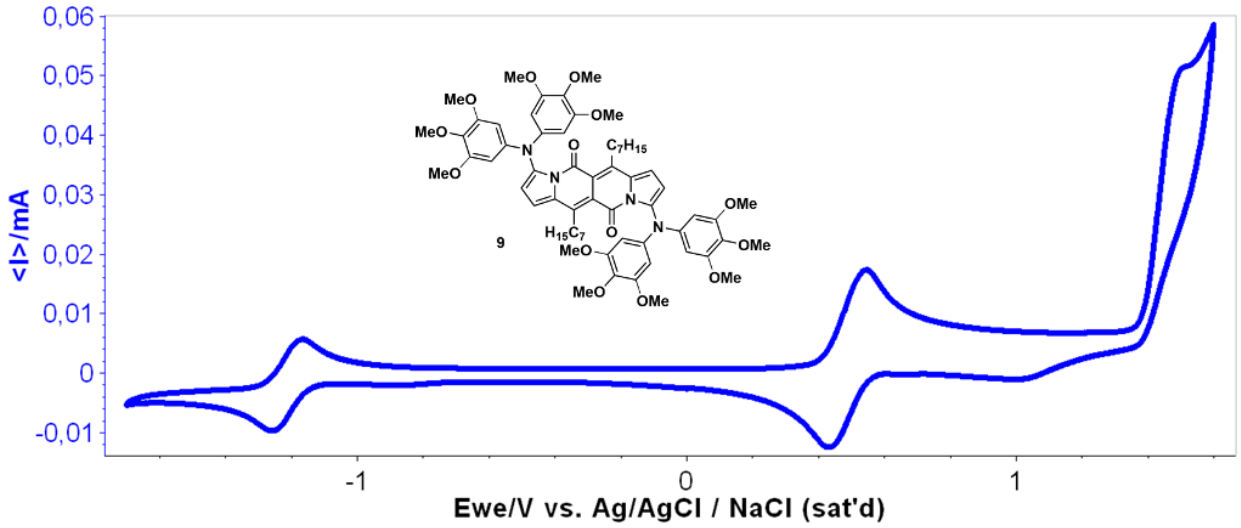
H15C7
5
0,03
0,02
0,01
0
-0,01
-0,02
-0,03
<I>/mA
-1
0
1
Ewe/V vs. Ag/AgCl / NaCl (sat'd)


0,01
0,005
0
-0,005
<I>/mA
-1
0
1
Ewe/V vs. Ag/AgCl / NaCl (sat'd)
6


0,01
0,005
0
-0,005
<I>/mA
-1
0
1
Ewe/V vs. Ag/AgCl / NaCl (sat'd)
7


0,01
0,005
0
-0,005
-0,01
<I>/mA
-1
0
1
Ewe/V vs. Ag/AgCl / NaCl (sat'd)
8



5. Photostability studies

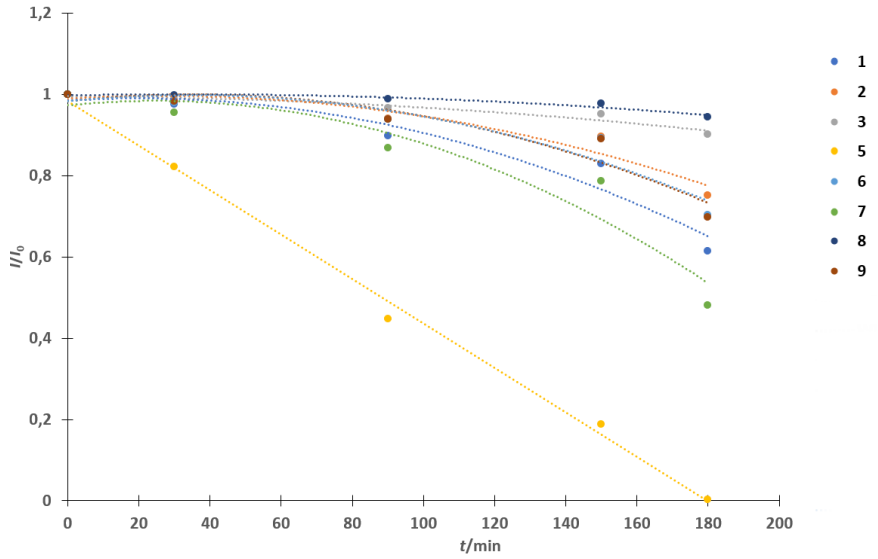
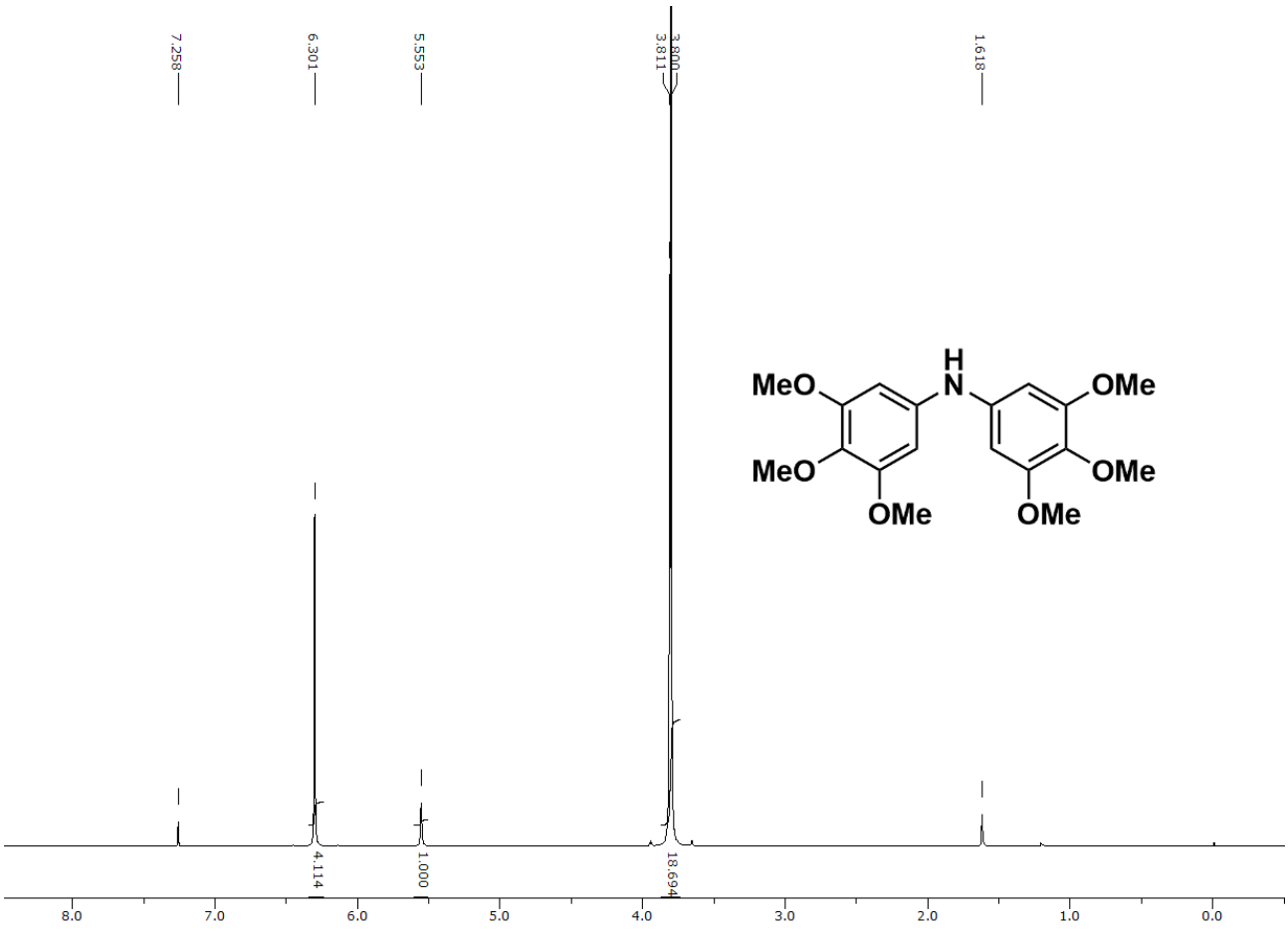


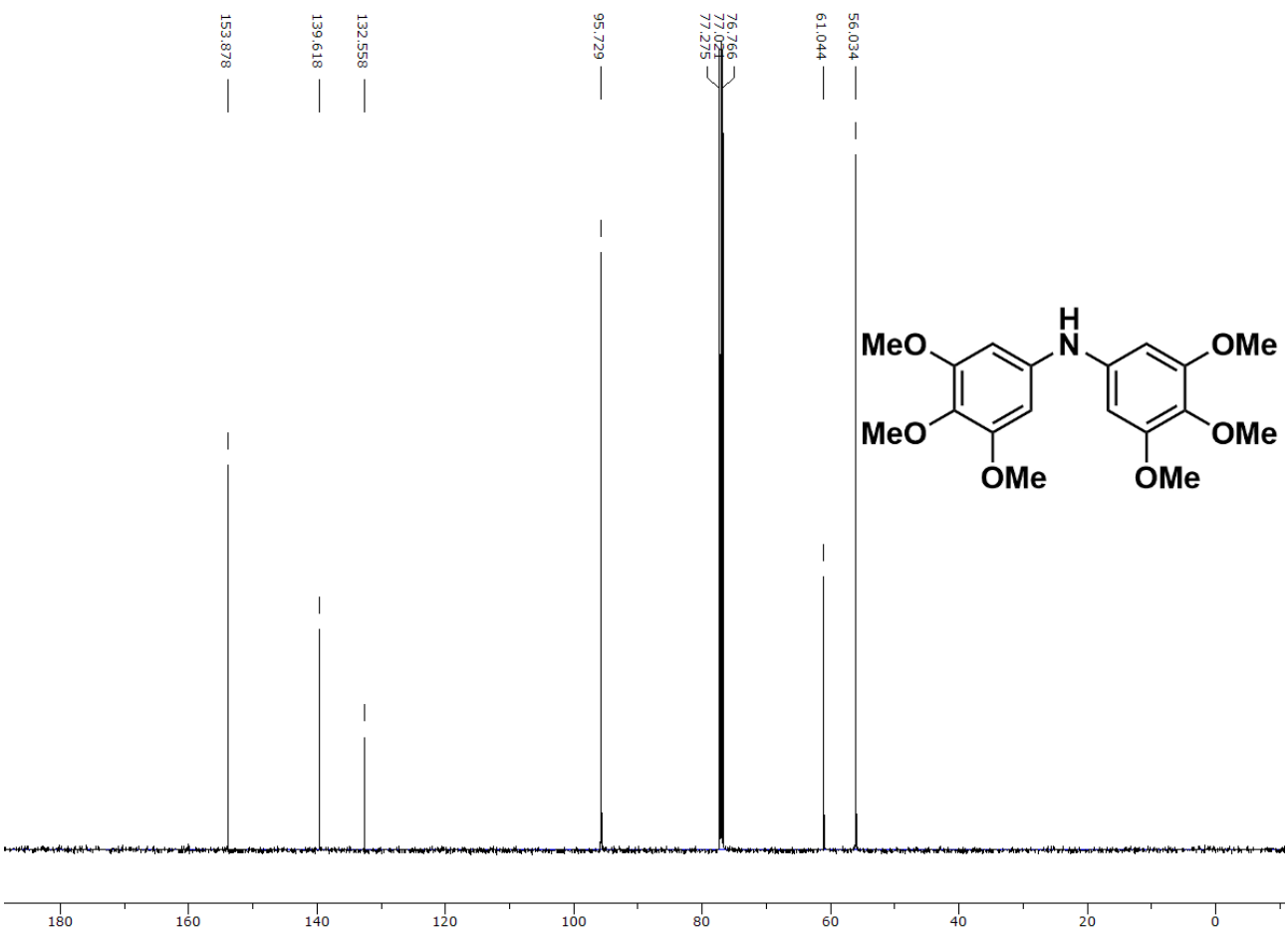
Table S5. Half-life times ($t_{1/2}$) for all considered dyes.

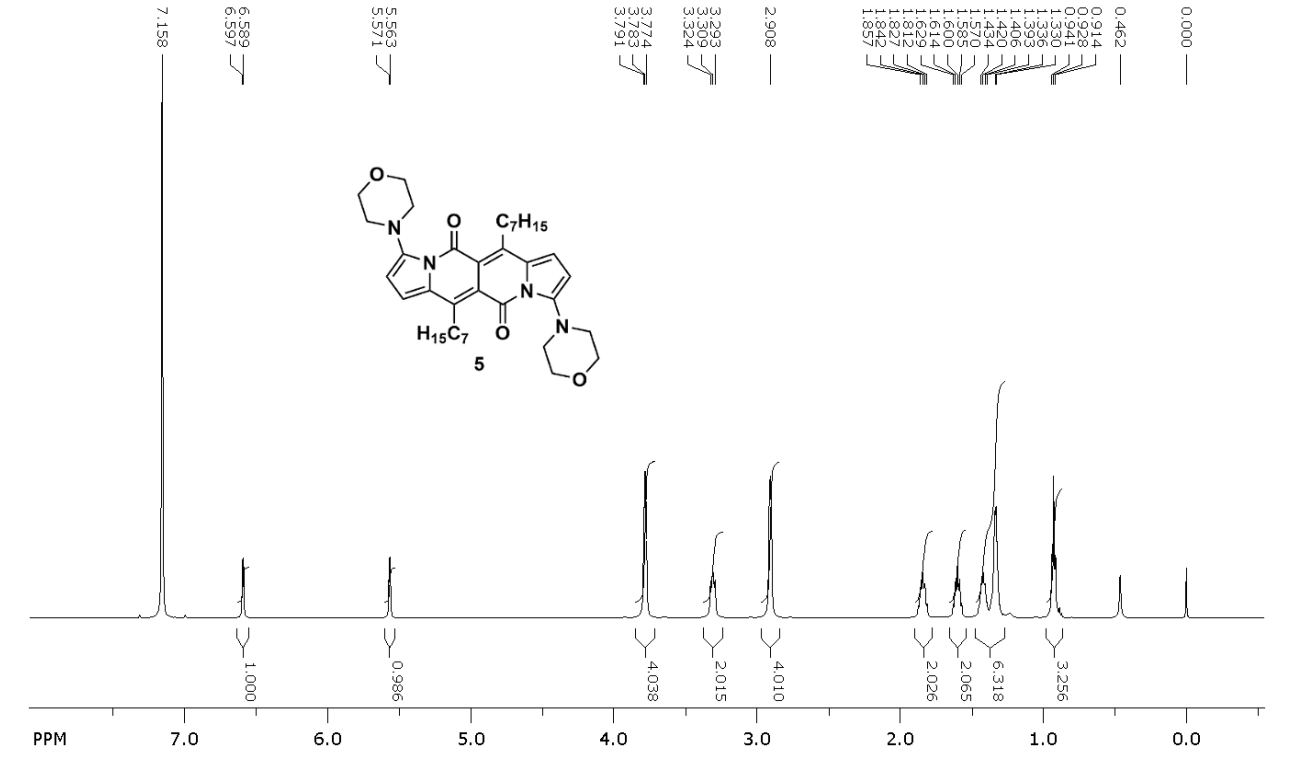
Compound	$t_{1/2}$/min
1	247
2	263
3	488
5	88
6	273
7	178
8	503
9	270

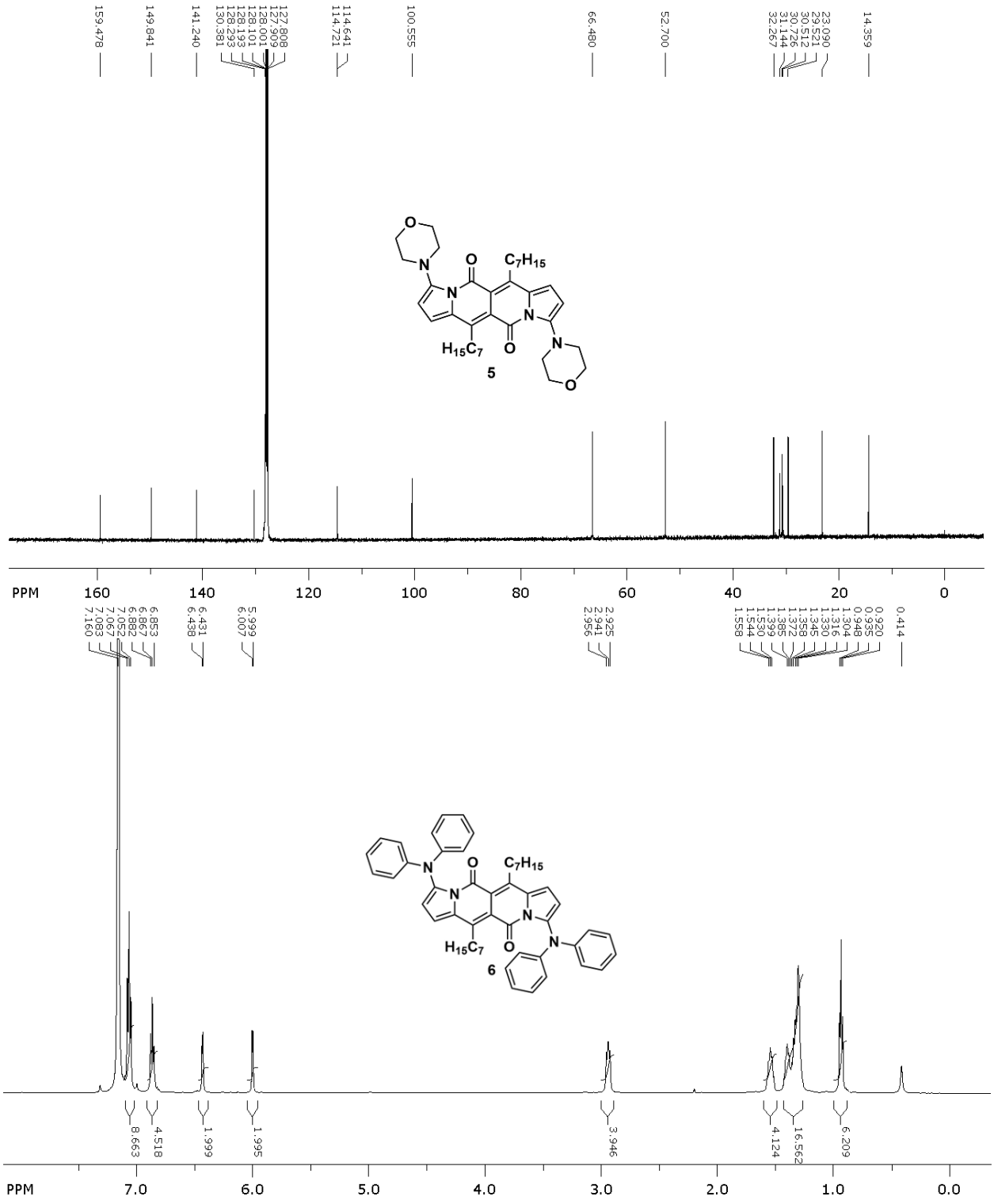
6. ^{1}H and ^{13}C NMR spectra of all new compounds.

Note: despite the fact that the samples were dried overnight under high vacuum at 70 °C there are traces of solvents.




153.878
139.618
132.558
95.729
77.275
61.044
56.034
MeO
MeO
OMe
H
N
OMe
OMe
OMe


7.158
6.589
6.587
5.563
5.571
3.774
3.783
3.791
3.293
3.309
3.324
2.908
1.857
1.842
1.827
1.812
1.629
1.614
1.600
1.585
1.570
1.454
1.420
1.406
1.393
1.330
0.941
0.928
0.914
0.462
0.000
C_7H_{15}
$H_{15}C_7$
5
1.000
0.986
4.038
2.015
4.010
2.026
2.065
6.318
3.256
PPM
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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149.841
141.240
130.381
128.293
128.193
128.101
128.001
127.909
127.808
114.721
114.641
100.555
66.480
52.700
32.267
31.144
30.726
30.512
29.521
23.090
14.359
5
PPM
160
140
120
100
80
60
40
20
0
7.160
7.083
7.067
7.052
6.882
6.867
6.853
6.438
6.431
6.007
5.999
2.956
2.941
2.925
1.558
1.544
1.530
1.385
1.372
1.358
1.345
1.330
1.316
1.304
0.948
0.935
0.920
0.414
6
8.663
4.518
1.999
1.995
3.946
4.124
16.562
6.209
PPM
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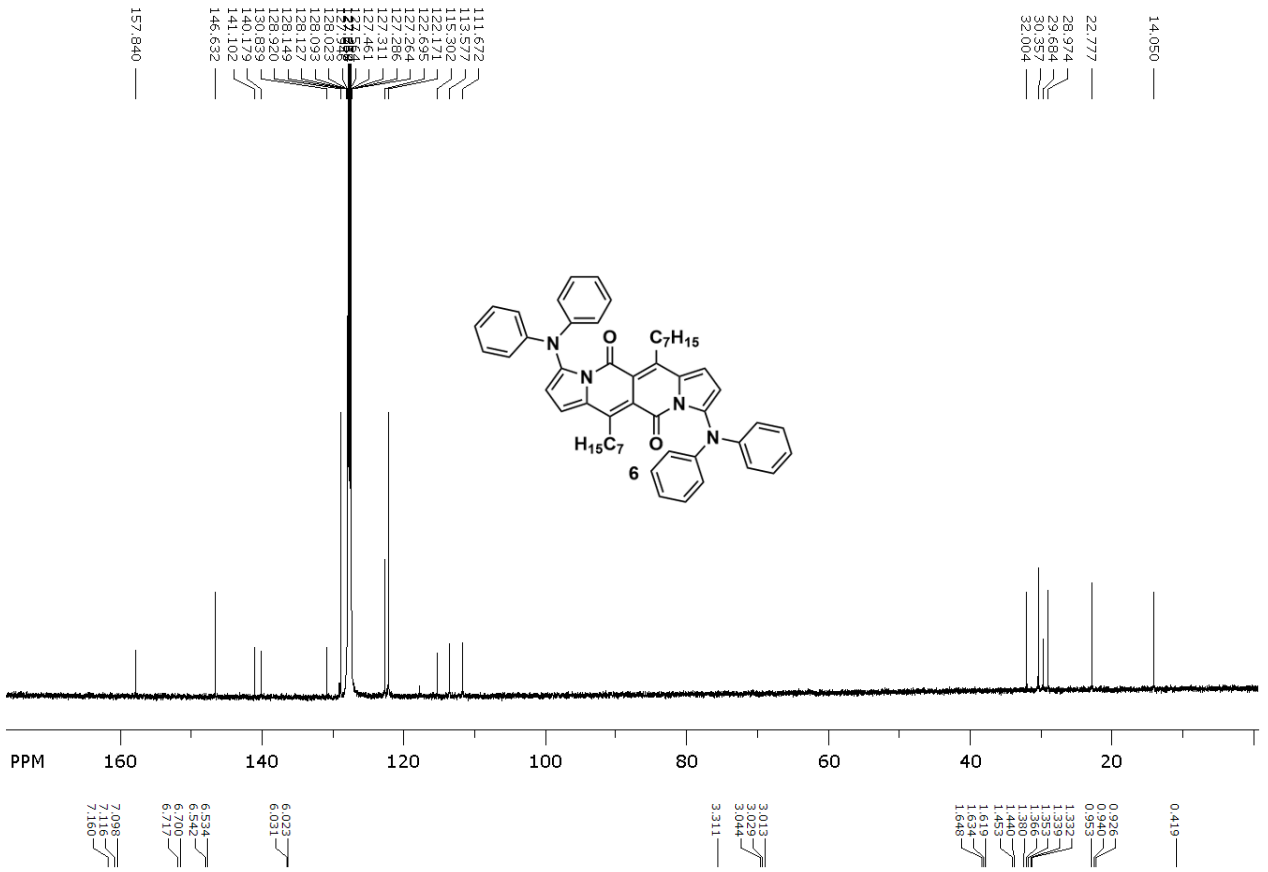
6.0
5.0
4.0
3.0
2.0
1.0
0.0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140.179
130.839
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128.093
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127.286
127.264
122.695
122.171
115.302
113.577
111.672
32.004
30.357
29.684
28.974
22.777
14.050
PPM
160
140
120
100
80
60
40
20
7.160
7.116
7.098
6.717
6.700
6.542
6.534
6.031
6.023
3.311
3.044
3.029
3.013
1.648
1.634
1.619
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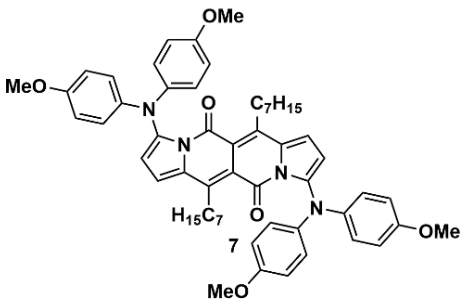
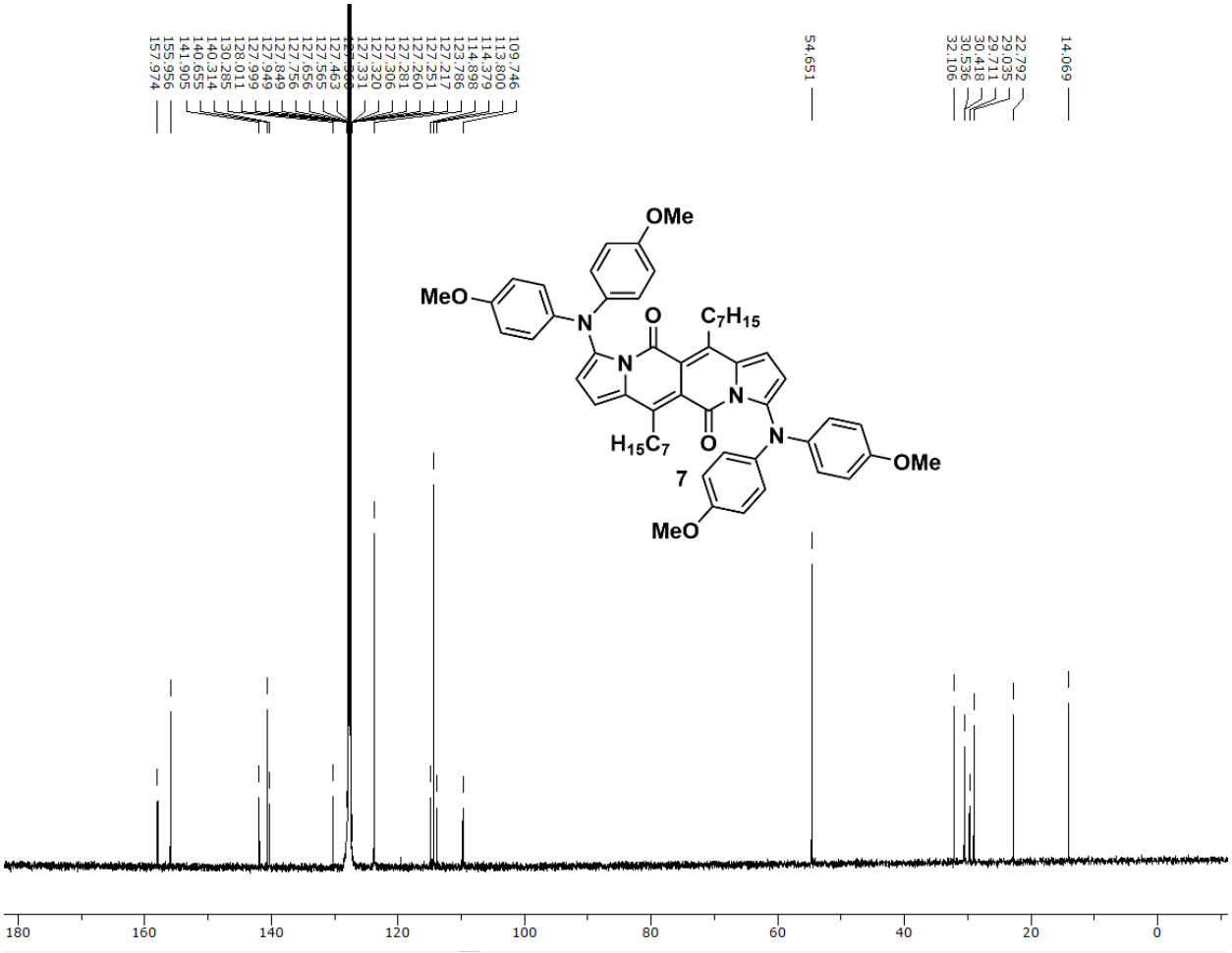
1.440
1.380
1.366
1.353
1.332
0.953
0.940
0.926
0.419


OMe
MeO
N
O
C_7H_{15}
N
O
$H_{15}C_7$
N
OMe
7
MeO

8.400
8.157
2.120
2.000
12.288
3.983
4.172
4.472
12.332
6.284
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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141.905
140.655
140.254
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127.756
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127.585
127.463
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127.320
127.306
127.281
127.260
127.251
127.217
123.766
114.898
114.379
113.800
109.746
54.651
32.106
30.536
30.418
29.711
29.035
22.792
14.069
OMe
MeO
N
O
C7H15
N
N
H15C7
O
N
OMe
7
MeO
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140
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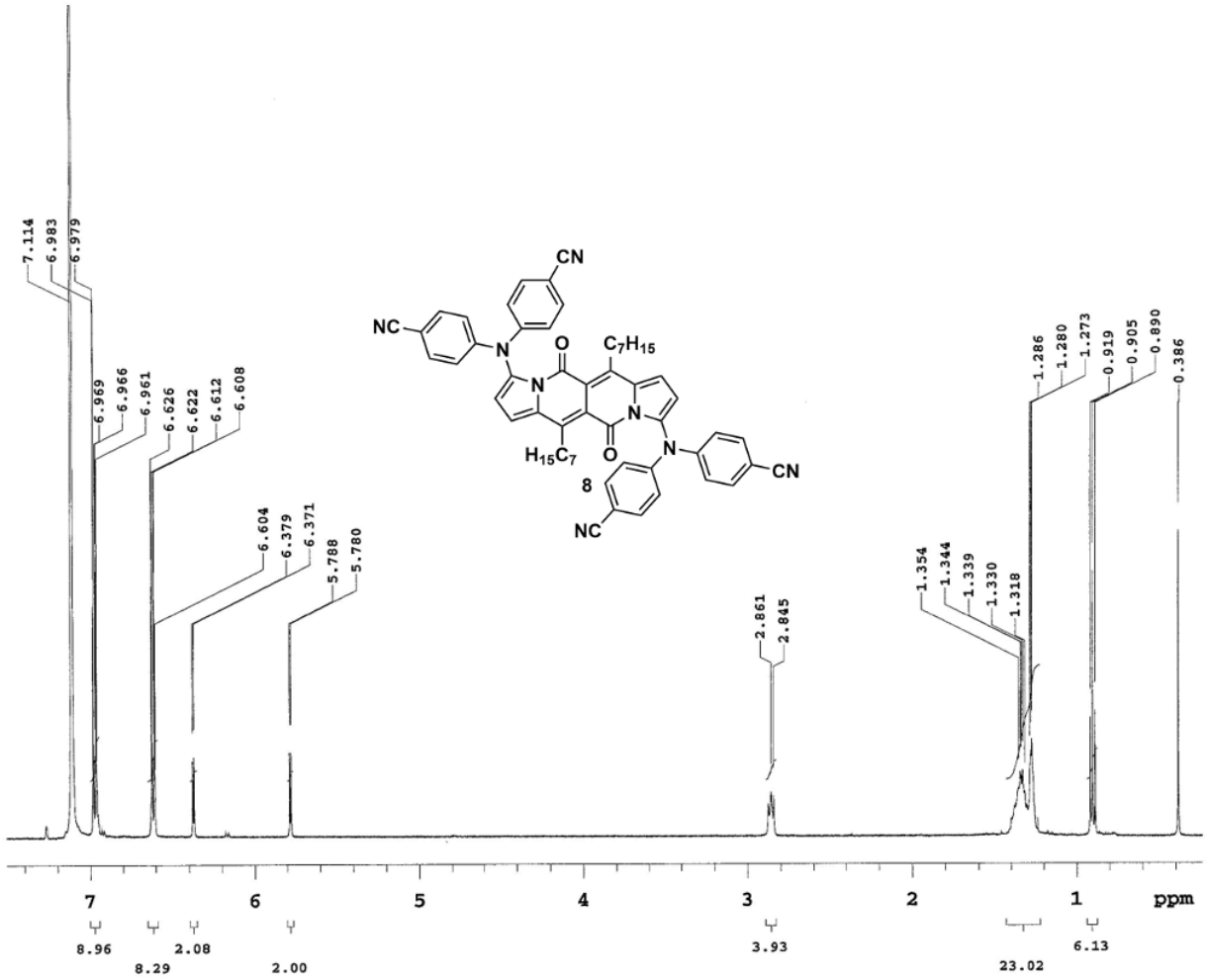
80
60
40
20
0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6.966
6.961
6.626
6.622
6.612
6.608
6.604
6.379
6.371
5.788
5.780
2.861
2.845
1.354
1.344
1.339
1.330
1.318
1.286
1.280
1.273
0.919
0.905
0.890
0.386
CN
NC
N
O
C_7H_{15}
$H_{15}C_7$
8
7
6
5
4
3
2
1
ppm
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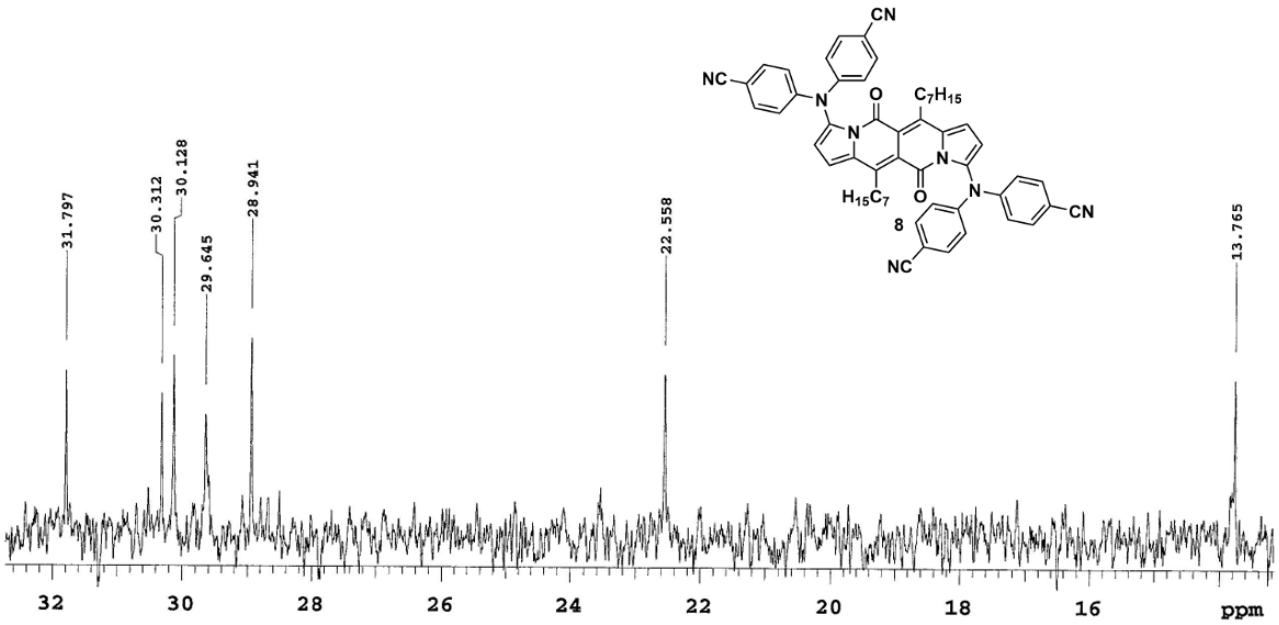
2.08
2.00
3.93
23.02
6.13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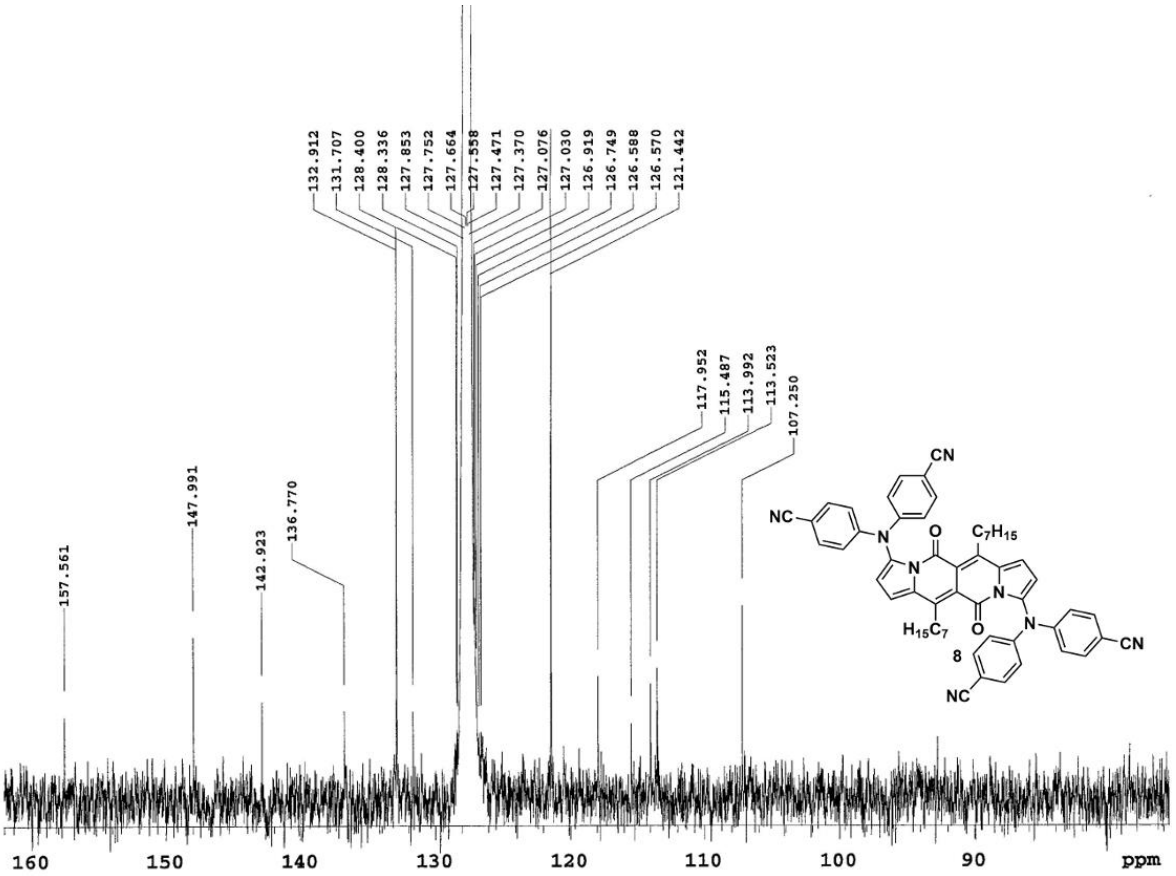
30.312
30.128
29.645
28.941
22.558
13.765
CN
NC
N
O
C_7H_{15}
$H_{15}C_7$
8
32
30
28
26
24
22
20
18
16
ppm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126.749
126.588
126.570
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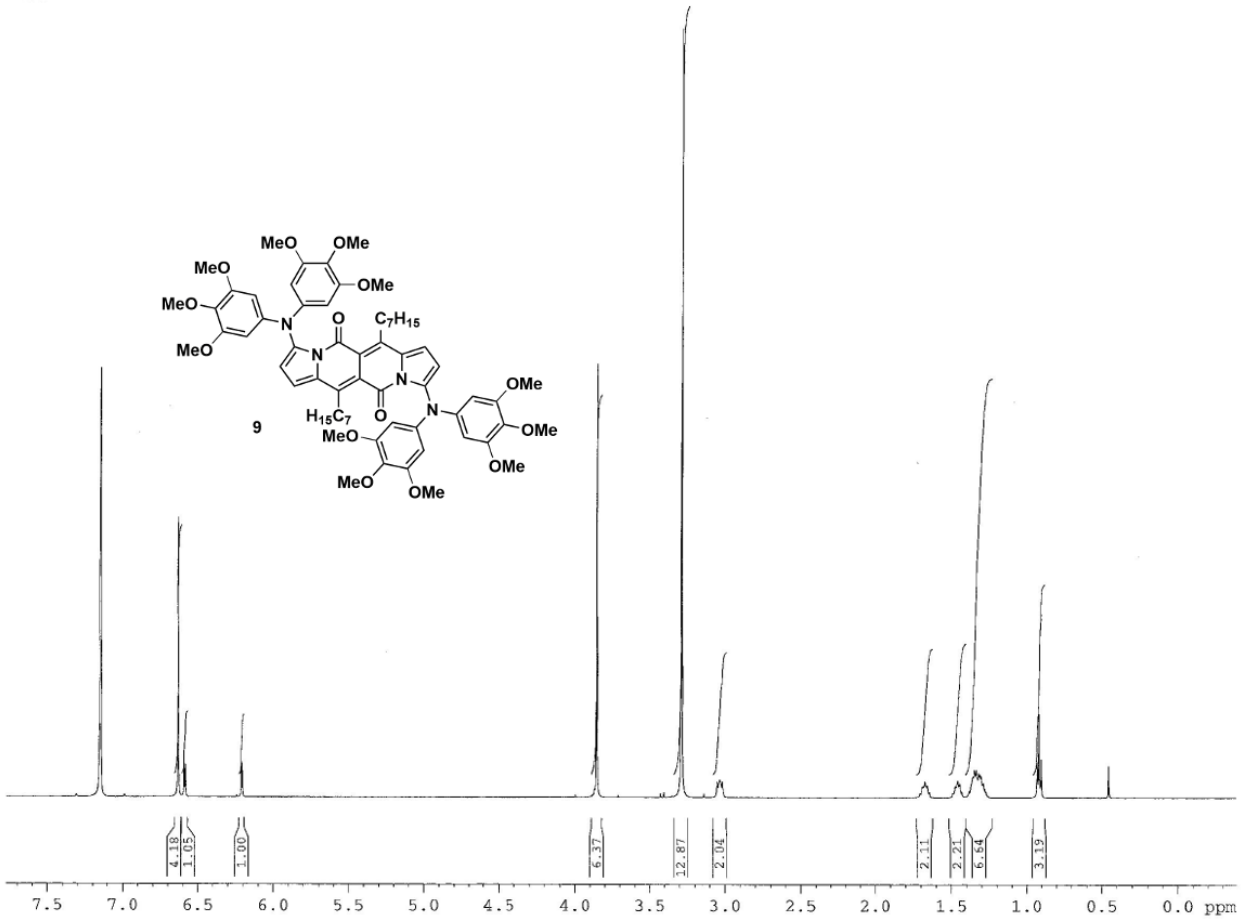
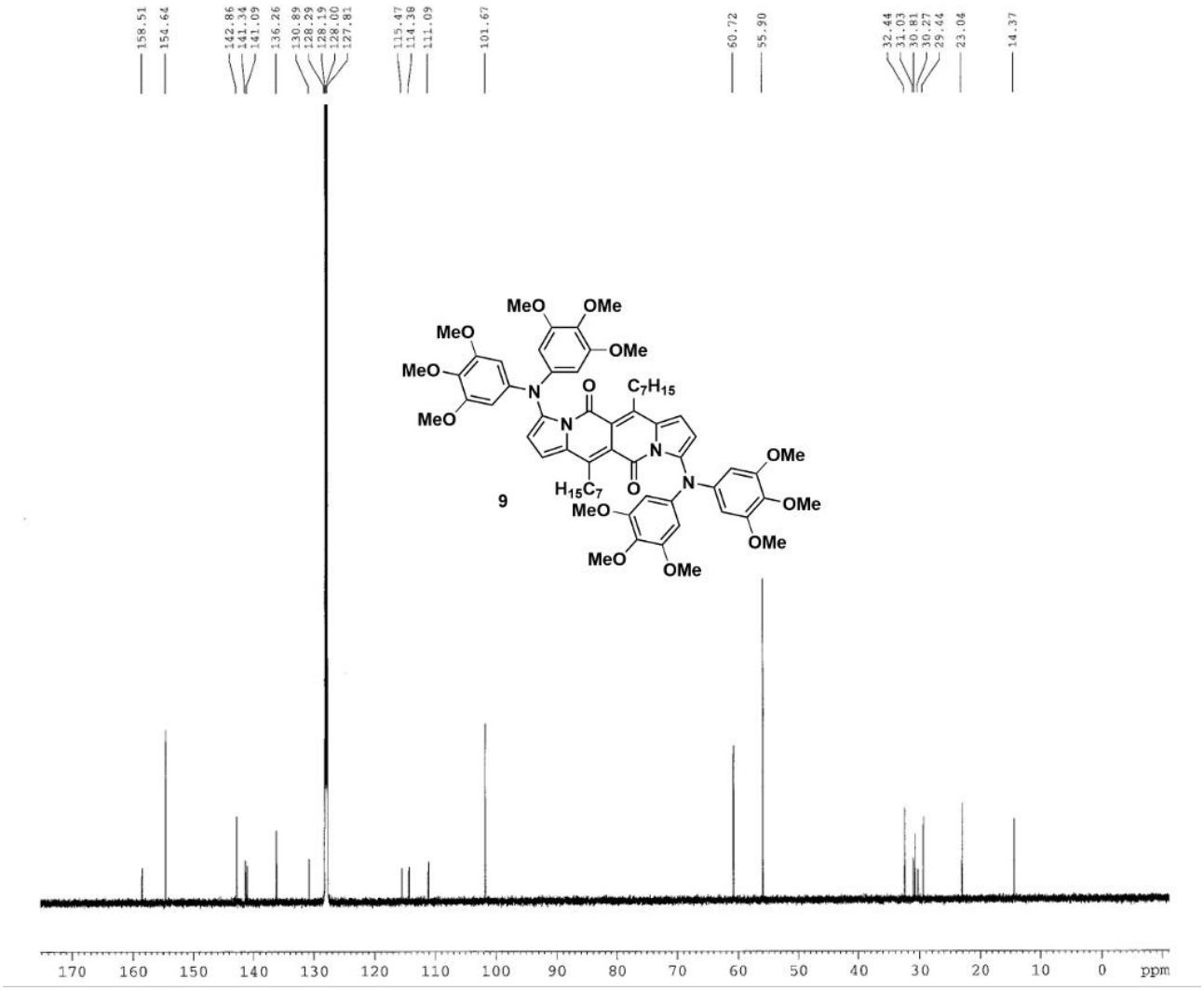
115.487
113.992
113.523
107.250
157.561
147.991
142.923
136.770
CN
NC
N
O
C_7H_{15}
$H_{15}C_7$
8
160
150
140
130
120
110
100
90
ppm


MeO
OMe
N
O
C_7H_{15}
$H_{15}C_7$
9
4.18
1.05
1.00
6.37
12.87
2.04
2.11
2.21
6.64
3.19
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm


158.51
154.64
142.86
141.34
141.09
136.26
130.89
128.29
128.19
128.00
127.81
115.47
114.38
111.09
101.67
60.72
55.90
32.44
31.03
30.81
30.27
29.44
23.04
14.37
MeO
OMe
MeO
OMe
MeO
N
O
C_7H_{15}
N
N
O
OMe
$H_{15}C_7$
O
N
OMe
MeO
OMe
MeO
OMe
9
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm