

# Unveiling the photophysical properties of Boron-dipyrromethene dyes using a new accurate excited state coupled cluster method

Romain Berraud-Pache, Frank Neese, Giovanni Bistoni and Róbert Izsák\*

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm Platz 1., 45470 Mülheim an der Ruhr, Germany

## Computational details

The convergence criteria are defined as follows:

- For the optimization, the tightopt threshold was selected corresponding to: Energy change =  $1 \times 10^{-6}$  a.u., RMS gradient =  $3 \times 10^{-5}$  a.u., MAX gradient =  $1 \times 10^{-4}$  a.u., RMS step =  $6 \times 10^{-4}$  a.u., MAX step =  $1 \times 10^{-3}$  a.u.
- The GRID4 standard grid corresponds to a Lebedev angular grid with 302 points, a Gauss-Chebyshev radial grid with a radial integration accuracy (IntAcc) of 4.67.
- The TightPNO threshold corresponds to the following cutoff values:  $T_{\text{CutPairs}} = 10^{-5}$ ,  $T_{\text{CutDO}} = 5 \times 10^{-3}$ ,  $T_{\text{CutPNO}} = 1.00 \times 10^{-7}$ ,  $T_{\text{CutMKN}} = 10^{-3}$  and the MP2 pair treatment is full iterative.

In ESD calculations, the 0-0 energy is printed at the end of the calculation. It is computed using the following formula:

$$E^{0-0} = E^{\text{Adia}} + \Delta E^{\text{ZPE}}$$

with  $E^{\text{Adia}} = E^{\text{ES}}(R^{\text{ES}}) - E^{\text{GS}}(R^{\text{GS}})$ , the difference of the electronic energies computed for the GS and ES at their geometries and  $\Delta E^{\text{ZPE}} = E^{\text{ZPE}}(R^{\text{ES}}) - E^{\text{ZPE}}(R^{\text{GS}})$ , the difference of zero-point vibrational energy between the GS and ES. The computed 0-0 energies are very close to the energies of the most intense band of the absorption spectra.

**Table S1.** Comparison of geometries obtained with various methods for a more flexible dye, Bo.21. The geometries were optimized using the def2-TZVP basis set. Vertical absorption energies were computed using DLPNO-STEOM-CCSD, the def2-TZVP basis set and TIGHTPNO. The DLPNO-CCSD(T) calculations were carried out using the def2-TZVP basis set and TIGHTPNO. All values are relative to B3LYP results, the B3LYP vertical excitation energy being 16486 cm<sup>-1</sup>.

BODIPY 21	B3LYP	PBE0	M06-2X	$\omega$ B97XD	MP2
RMSD (Å)	0	0.14	0.24	0.42	0.24
Vertical excitation energies (cm <sup>-1</sup> )	0	-1	44	537	103
DLPNO-CCSD(T) energy (kcal)	0	1.385	5.678	-0.583	-1.949

**Table S2.** Parameters describing the solvent in calculations with the CPCM implicit solvent model.

Solvent	Dielectric constant ( $\epsilon$ )	Refractive Index
Chloroform	4.81	1.4458
Cyclohexane	2.02	1.4262
Dichloromethane	8.93	1.4241
Ethanol	24.5	1.3614
Ethyl Acetate	6.02	1.3724
Methanol	32.7	1.3284
N-Hexane	1.89	1.3758
Tetrahydrofuran	7.58	1.4072
Toluene	2.38	1.4969

**Table S3.** Experimental and computed excitation energies in eV for each BODIPY dye in the test set.

BODIPY number	STEOM	STEOM -CPCM	TDDFT-CPCM	TDDFT	Experiment Solvent
1	3.183	3.134	3.287	3.364	3.123 <sup>1</sup> CH <sub>2</sub> Cl <sub>2</sub>
2	2.900	2.845	3.105	3.123	2.774 <sup>1</sup> CH <sub>2</sub> Cl <sub>2</sub>
3	2.886	2.913	3.191	3.056	2.774 <sup>1</sup> CH <sub>2</sub> Cl <sub>2</sub>
4	2.166	2.19	2.455	2.43	2.206 <sup>2</sup> CH <sub>2</sub> Cl <sub>2</sub>
5	2.263	2.331	2.431	2.854	2.331 <sup>3</sup> THF
6	2.133	2.131	2.593	2.596	2.175 <sup>3</sup> CHCl <sub>3</sub>
7	2.026	2.043	2.417	2.448	2.050 <sup>3</sup> CHCl <sub>3</sub>
8	2.012	2.021	2.388	2.421	2.046 <sup>3</sup> CHCl <sub>3</sub>
9	2.140	2.148	2.578	2.608	2.172 <sup>3</sup> CHCl <sub>3</sub>
10	1.905	1.902	2.301	2.328	2.029 <sup>3</sup> CHCl <sub>3</sub>
11	1.836	1.775	2.216	2.243	1.922 <sup>3</sup> CHCl <sub>3</sub>
12	1.785	1.806	2.181	2.207	1.917 <sup>3</sup> CHCl <sub>3</sub>
13	2.463	2.455	3.08	3.129	2.460 <sup>4</sup> Cyclohexane
14	2.930	3.035	3.384	3.379	3.054 <sup>5</sup> Ethyl Acetate
15	2.417	2.434	2.843	2.872	2.357 <sup>6</sup> Cyclohexane
16	2.324	2.342	2.867	2.95	2.515 <sup>7-8</sup> Methanol
17	2.305	2.307	2.878	2.883	2.403 <sup>9</sup> CH <sub>2</sub> Cl <sub>2</sub>

18	2.113	2.184	2.509	2.535	2.175 <sup>9</sup> CH <sub>2</sub> Cl <sub>2</sub>
19	2.353	2.382	2.868	2.892	2.389 <sup>10</sup> CH <sub>2</sub> Cl <sub>2</sub>
20	2.204	2.192	2.61	2.641	2.234 <sup>11</sup> Toluene
21	2.020	2.044	2.446	2.441	2.199 <sup>12</sup> Methanol
22	1.848	1.851	2.219	2.24	1.934 <sup>13</sup> CH <sub>2</sub> Cl <sub>2</sub>
23	2.326	2.341	2.704	2.748	2.288 <sup>14</sup> CH <sub>2</sub> Cl <sub>2</sub>
24	2.03	2.018	2.36	2.387	2.026 <sup>14</sup> CH <sub>2</sub> Cl <sub>2</sub>
25	2.133	2.137	2.673	2.683	2.142 <sup>15</sup> CHCl <sub>3</sub>
26	3.125	3.223	3.315	3.306	3.139 <sup>16</sup> CH <sub>2</sub> Cl <sub>2</sub>
27	2.816	2.874	3.047	3.031	2.731 <sup>16</sup> CH <sub>2</sub> Cl <sub>2</sub>
28	2.894	2.918	2.741	3.143	2.756 <sup>17</sup> N-hexane
29	1.834	1.824	2.234	2.247	1.920 <sup>11</sup> Toluene
30	1.636	1.637	2.015	2.02	1.744 <sup>18</sup> CH <sub>2</sub> Cl <sub>2</sub>
31	3.147	3.146	3.044	3.187	3.077 <sup>19</sup> CH <sub>2</sub> Cl <sub>2</sub>
32	2.851	2.755	2.107	2.789	2.661 <sup>19</sup> CH <sub>2</sub> Cl <sub>2</sub>
33	2.866	2.864	2.784	2.873	2.904 <sup>19</sup> CH <sub>2</sub> Cl <sub>2</sub>
34	2.703	2.656	2.269	2.719	2.616 <sup>19</sup> CH <sub>2</sub> Cl <sub>2</sub>
35	1.602	1.625	1.866	1.866	1.636 <sup>20</sup> CHCl <sub>3</sub>
36	1.711	1.741	2.136	2.137	1.792 <sup>20</sup> CHCl <sub>3</sub>

37	2.387	2.333	2.795	2.857	$2.362^{21}$ Toluene
38	2.292	2.322	2.626	2.67	$2.344^{22}$ Cyclohexane
39	2.002	1.984	2.491	2.525	$2.088^{22}$ Cyclohexane
40	2.024	2.363	2.605	2.665	$2.242^{23}$ $\text{CH}_2\text{Cl}_2$
41	1.916	1.902	2.171	2.268	$1.953^{23}$ $\text{CH}_2\text{Cl}_2$
42	3.86	3.912	3.788	3.85	$3.713^7$ $\text{CH}_2\text{Cl}_2$
43	3.582	3.7	3.521	3.434	$3.493^7$ Ethanol
44	2.297	2.341	2.316	2.574	$2.385^{24}$ Toluene
45	2.215	2.228	2.559	2.6	$2.288^{24}$ Toluene
46	2.075	2.07	2.4	2.42	$2.036^{25}$ $\text{CH}_2\text{Cl}_2$
47	1.756	1.803	1.986	2.011	$1.824^{25}$ $\text{CH}_2\text{Cl}_2$

**Table S4.** Parameters used in the ESD calculation for the Bo.5 dye. The same parameters are used for all the three algorithms studied (VG, AHAS and AH).

Requested calculation:	absorption
Coordinate system:	Deloc. Internal (BAKER)
Lineshape function:	Gaussian
Homogeneous linewidth is:	50.00 cm <sup>-1</sup>
Inhomogeneous linewidth is:	250.00 cm <sup>-1</sup>
Number of points:	131072
Maximum time:	1592.65 fs
Spectral resolution:	3.33 cm <sup>-1</sup>
Temperature used:	298.15 K
Z value:	1.014323e-96
Cutoff for the correlation function:	1.00e-06
Last element of the correlation function:	0.000000,0.000000

The displacement vector can be defined as  $K = L_x^T(\bar{q}_0 - q_0)$  and the Duchinsky rotation matrix as  $J = L_x^T \bar{L}_x$  with  $L_x^T$  being the eigenvectors of the mass-weighted Hessian,  $\bar{L}_x$  the eigenvectors of the mass-weighted Hessian of the final geometry and  $\bar{q}_0(q_0)$  the mass-weighted Cartesian nuclear

coordinates of the final structure (initial structure). The displacement vectors are defined in mass weighted atomic units,  $a_0\sqrt{m_e}$  with  $a_0$  the bohr radius and  $m_e$  the mass of the electron.

It is sometimes also convenient to use dimensionless coordinates defined as  $Q_\alpha = \sqrt{\frac{\omega_\alpha}{\hbar}} q_\alpha$  with  $\omega_\alpha$  being the frequency of the mode  $\alpha$ . We will use dimensionless K vectors and K\*K (norm square of the displacement vector) values in the tables below.

**Table S5.** ESD parameters for Bo.5. K\*K (dimensionless) corresponds to the norm square of the displacement vector, the RMSD computed between the GS and 1<sup>st</sup> ES structures is also provided. The

diagonality index (DI) is computed for the Duchinsky J matrix J as:  $DI = \sqrt{\sum_i J_{ii}^2 / \sum_{ij} J_{ij}^2}$ .

BODIPY 5	AH	AHAS	VG
K*K	2.35	2.17	2.1
RMSD (Å)	0.2350	0.0516	0.0711
Diagonality index	0.620983	0.643773	0.999423
Maximum absorption (cm <sup>-1</sup> )	19599	18470	18636
Maximum fluorescence (cm <sup>-1</sup> )	18300	17695	17534

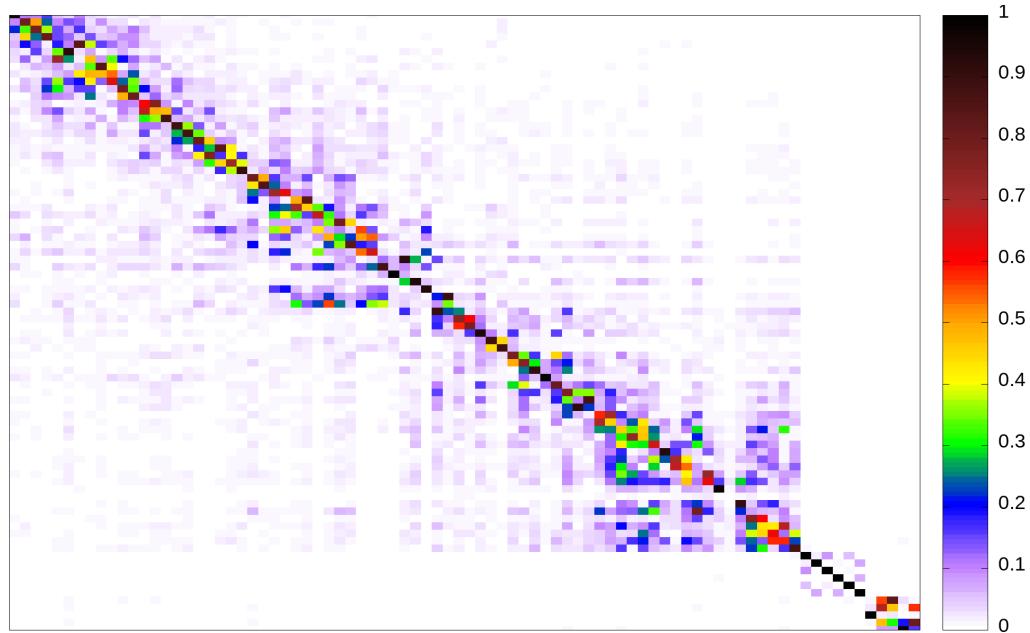
**Table S6.** Displacement vector K (dimensionless) for Bo.5 with the VG, AHAS or AH algorithms.

The K vector for VG (dimensionless) is:			The K vector for AHAS(dimensionless) is:		
mode	displacement	Qf corresp. mode	mode	displacement	Qf corresp. mode
1	-0.007402	1: 1.00;	1	-0.008768	1: 0.94;
2	0.002131	2: 1.00;	2	-0.001964	2: 0.62;
3	0.012622	3: 0.99;	3	0.007836	3: 0.62;
4	0.014483	4: 0.99;	4	0.014846	4: 0.66;
5	-0.000938	5: 1.00;	5	0.000108	7: 0.70;
6	-0.128950	6: 1.00;	6	-0.051723	6: 0.85;
7	-0.037671	7: 1.01;	7	-0.033395	5: 0.53;
8	-0.242364	8: 1.01;	8	-0.267629	9: 0.71;
9	-0.043366	9: 1.00;	9	-0.046932	
10	0.005992	10: 1.02;	10	0.004333	10: 0.41;
11	0.013429	11: 0.99;	11	0.023169	11: 0.62;
12	0.030195	12: 1.00;	12	0.036777	12: 0.65;
13	0.184157	13: 0.99;	13	0.178246	13: 0.36; 14: 0.58;
14	-0.022158	14: 1.01;	14	-0.042283	13: 0.44;
15	-0.042795	15: 1.02;	15	0.007171	15: 0.76;
16	0.187405	16: 0.98;	16	0.183804	16: 0.79;
17	0.246607	17: 1.00;	17	0.249953	17: 0.77;
18	0.011904	18: 1.00;	18	0.020054	18: 0.64;
19	0.230567	19: 1.00;	19	0.217860	20: 0.70;
20	-0.038128	20: 1.02;	20	-0.025353	19: 0.58;
21	0.092878	21: 1.01;	21	0.113338	21: 0.50;
22	-0.281111	22: 1.01;	22	-0.294140	22: 0.81;
23	0.415809	23: 0.98;	23	0.427007	23: 0.64;

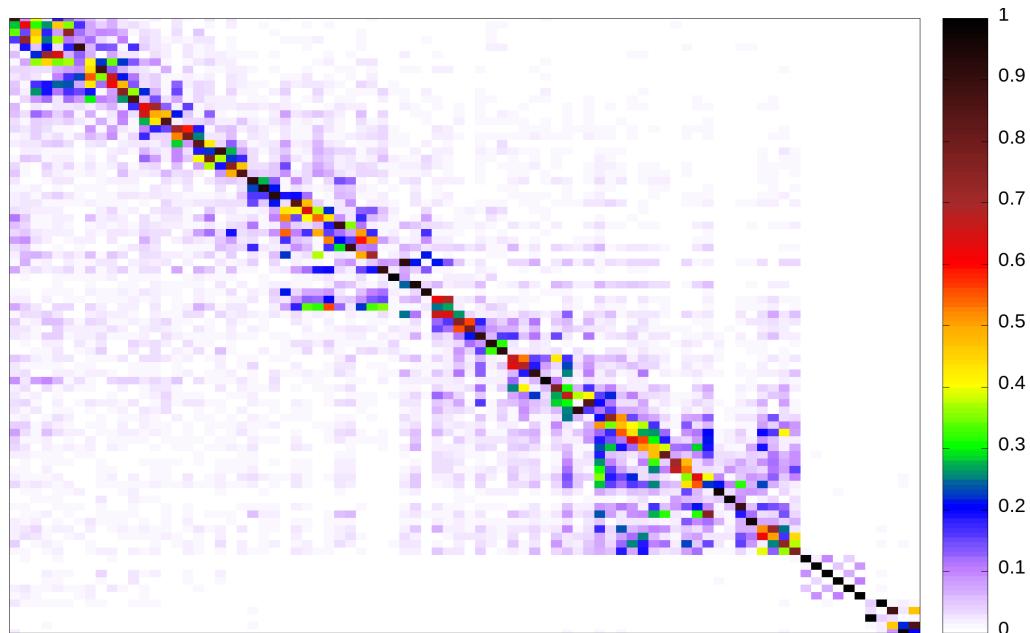
24	-0.182513	24: 1.00;	24	-0.189332	24: 0.73;
25	0.310388	25: 1.01;	25	0.345938	25: 0.51; 26: 0.39;
26	-0.056953	26: 1.01;	26	-0.026341	28: 0.70;
27	0.008612	27: 1.00;	27	0.008040	27: 0.49;
28	0.008963	28: 1.00;	28	0.009051	29: 0.44;
29	0.019842	29: 1.00;	29	0.021116	31: 0.63;
30	0.020916	30: 0.99;	30	0.017941	33: 0.31;
31	0.077178	31: 1.00;	31	0.068070	
32	-0.355837	32: 1.00;	32	-0.371104	32: 0.70;
33	-0.018419	33: 0.99;	33	-0.019088	34: 0.43;
34	-0.008749	34: 1.00;	34	-0.006299	37: 0.86;
35	0.011537	35: 1.00;	35	0.012865	35: 0.77;
36	0.000591	36: 1.01;	36	0.001779	36: 0.99;
37	-0.002686	37: 1.00;	37	-0.008605	38: 0.89;
38	-0.000598	38: 0.98;	38	0.000319	39: 0.87;
39	0.164413	39: 0.99;	39	0.153356	41: 0.80;
40	0.067256	40: 0.99;	40	0.063593	30: 0.31;
41	0.322075	41: 1.01;	41	0.354740	40: 0.81;
42	-0.139372	42: 1.00;	42	-0.132171	42: 0.56; 43: 0.37;
43	0.006325	43: 1.00;	43	-0.008076	42: 0.34; 43: 0.60;
44	-0.221323	44: 0.99;	44	-0.223899	44: 0.88;
45	0.004366	45: 1.00;	45	0.002404	45: 0.78;
46	0.001484	46: 1.00;	46	0.003482	46: 0.79;
47	0.050550	47: 1.00;	47	0.052644	47: 0.61;
48	0.120012	48: 1.00;	48	0.125854	48: 0.57;
49	0.190071	49: 1.00;	49	0.190581	49: 0.83;
50	-0.069815	50: 1.00;	50	-0.077347	50: 0.98;
51	-0.098938	51: 1.00;	51	-0.112042	51: 0.65;
52	-0.377937	52: 1.00;	52	-0.396040	52: 0.59;
53	0.201590	53: 1.00;	53	0.209739	54: 0.76;
54	-0.265746	54: 1.00;	54	-0.272872	53: 0.84;
55	0.024409	55: 1.00;	55	0.027844	55: 0.34; 56: 0.50;
56	-0.088996	56: 1.00;	56	-0.094975	55: 0.48;
57	-0.144314	57: 1.01;	57	-0.132794	
58	0.089495	58: 1.00;	58	0.095858	58: 0.54;
59	0.231439	59: 1.00;	59	0.232591	60: 0.43;
60	0.108122	60: 1.00;	60	0.104639	61: 0.86;
61	0.008322	61: 1.00;	61	0.005259	62: 0.49;
62	-0.046921	62: 1.00;	62	-0.046822	62: 0.45;
63	0.386523	63: 1.00;	63	0.388383	65: 0.53;
64	0.506479	64: 1.00;	64	0.500816	65: 0.39;
65	-0.150978	65: 1.00;	65	-0.149777	66: 0.97;
66	-0.023446	66: 1.00;	66	-0.022977	67: 1.00;
67	-0.213290	67: 1.00;	67	-0.210093	68: 0.81;
68	-0.025893	68: 1.01;	68	-0.022809	64: 0.62;
69	-0.060342	69: 1.00;	69	-0.063964	69: 0.57; 70: 0.37;
70	0.101960	70: 1.00;	70	0.103127	72: 0.47;
71	0.265707	71: 1.00;	71	0.256259	71: 0.39;
72	-0.250268	72: 0.99;	72	-0.240033	71: 0.34; 72: 0.34;
73	0.217717	73: 1.00;	73	0.218109	73: 0.75;
74	-0.019916	74: 1.00;	74	-0.020338	74: 0.99;
75	0.015711	75: 1.00;	75	0.015312	75: 0.99;
76	0.001566	76: 1.00;	76	0.000998	76: 0.99;
77	0.002457	77: 1.00;	77	0.004310	77: 1.00;
78	-0.001091	78: 1.00;	78	-0.002454	78: 1.00;
79	0.005819	79: 1.00;	79	0.006549	79: 0.99;

80	0.045873	80: 1.00;	80	0.043958	81: 0.31; 82: 0.69;
81	-0.035627	81: 1.00;	81	-0.033838	81: 0.46; 84: 0.33;
82	0.001653	82: 1.00;	82	0.001328	80: 1.00;
83	0.041720	83: 1.00;	83	0.036643	84: 0.65;
84	0.023141	84: 1.00;	84	0.019032	83: 0.96;
The K vector for AH (dimensionless) is:					
mode	displacement	Qf	corresp.	mode	
1	-0.009477	1:	0.77;		
2	0.007602	2:	0.38;		
3	0.032821	6:	0.55;		
4	0.024107	2:	0.54;		
5	-0.000594	7:	0.82;		
6	-0.603819	4:	0.52; 5:	0.41;	
7	-0.110922				
8	-0.394857	9:	0.77;		
9	-0.085479	8:	0.30; 10:	0.43;	
10	0.058111	10:	0.38;		
11	-0.043724	11:	0.57;		
12	-0.012015	12:	0.76;		
13	0.374264	13:	0.39; 14:	0.51;	
14	-0.012320	13:	0.43;		
15	-0.093012	15:	0.74;		
16	0.137606	16:	0.50; 17:	0.34;	
17	0.193850	17:	0.62;		
18	-0.061480	18:	0.70;		
19	0.338335	20:	0.80;		
20	-0.108511	19:	0.61;		
21	0.016517	21:	0.57;		
22	-0.350595	22:	0.73;		
23	0.422844	23:	0.84;		
24	-0.222624	24:	0.90;		
25	0.238171	25:	0.86;		
26	-0.184791	27:	0.71;		
27	0.003315	28:	0.41;		
28	-0.007485				
29	-0.034592	31:	0.79;		
30	0.032240				
31	0.126982	33:	0.35;		
32	-0.330092	32:	0.79;		
33	-0.020840	34:	0.50;		
34	0.004760	37:	0.85;		
35	-0.008665	35:	0.80;		
36	-0.003023	36:	1.00;		
37	0.015515	38:	0.91;		
38	-0.003628	39:	0.89;		
39	0.174225	40:	0.38; 41:	0.47;	
40	0.023236	30:	0.31;		
41	0.309268	40:	0.43; 41:	0.40;	
42	-0.143288	42:	0.57; 43:	0.32;	
43	-0.023673	42:	0.30; 43:	0.62;	
44	-0.238568	44:	0.82;		
45	0.046797	45:	0.87;		
46	0.050681	46:	0.85;		
47	0.002827	47:	0.45;		

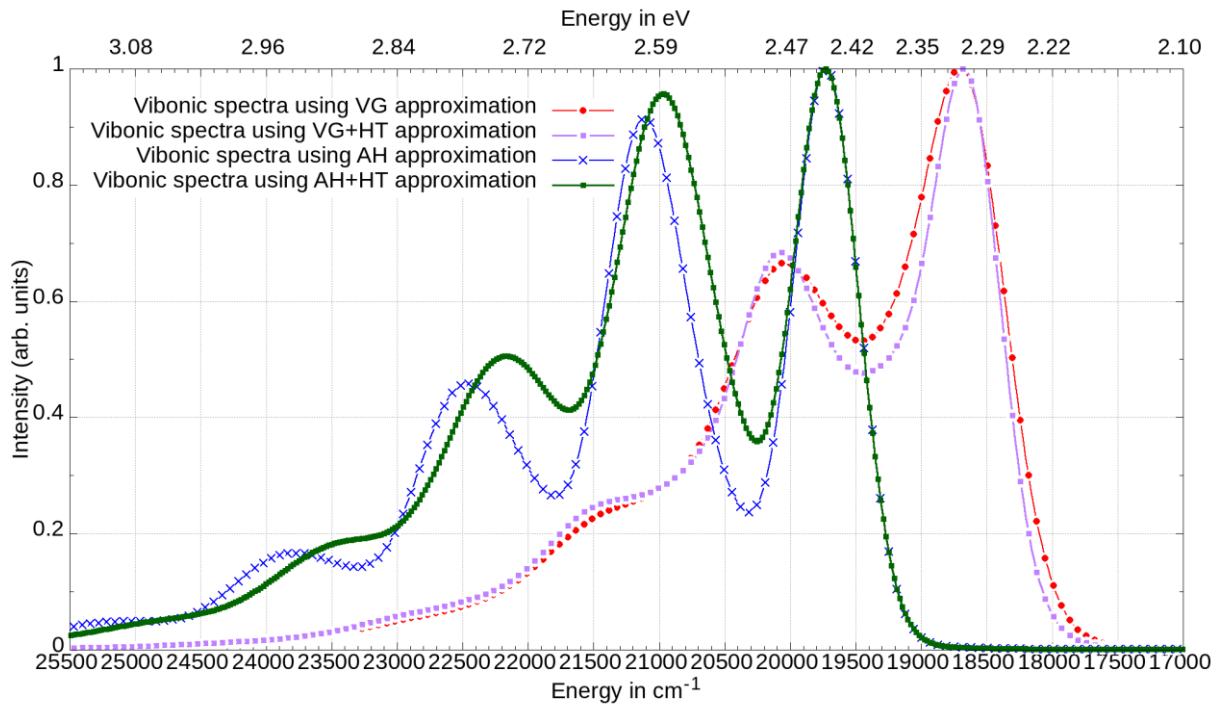
48	0.123266	47: 0.40; 48: 0.47;
49	0.280932	49: 0.83;
50	0.113703	50: 0.97;
51	-0.080812	51: 0.59;
52	-0.448940	52: 0.44;
53	0.344226	54: 0.71;
54	-0.315977	53: 0.84;
55	0.027118	56: 0.54;
56	-0.056440	
57	-0.371105	
58	0.117237	58: 0.41; 59: 0.32;
59	0.200677	
60	0.101031	61: 0.66;
61	-0.035646	62: 0.51;
62	-0.084478	62: 0.45;
63	0.485676	64: 0.41;
64	0.639086	
65	-0.184127	66: 0.94;
66	-0.063714	67: 0.98;
67	-0.246977	68: 0.79;
68	-0.070937	65: 0.57;
69	-0.074435	69: 0.94;
70	0.124248	71: 0.53;
71	0.358016	70: 0.38;
72	-0.365742	72: 0.54;
73	0.370878	73: 0.59;
74	-0.013836	74: 0.99;
75	0.020768	75: 0.99;
76	0.087332	76: 0.99;
77	-0.020926	77: 0.99;
78	-0.003186	78: 0.99;
79	0.007834	79: 0.98;
80	0.003709	81: 1.00;
81	-0.028002	82: 0.78;
82	-0.000602	80: 1.00;
83	0.032535	84: 0.74;
84	0.033313	83: 0.95;



**Figure S1.** Duschinsky matrix for the Bo.5 dye using the AHAS algorithm.



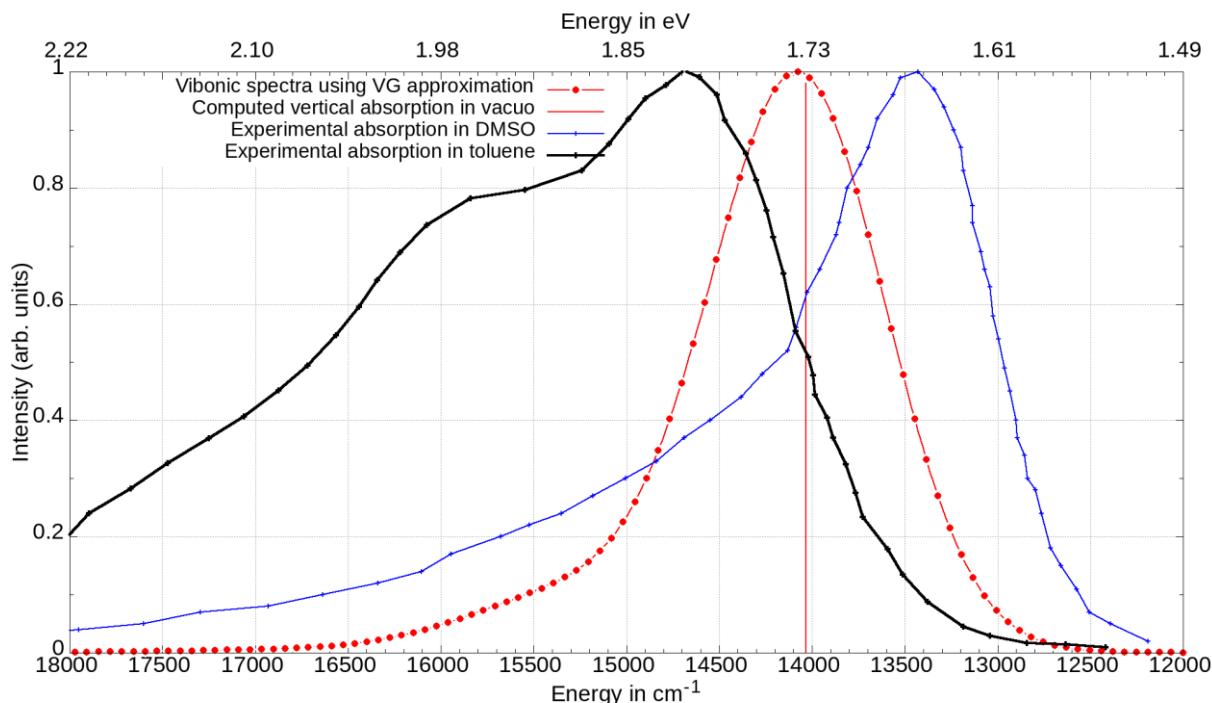
**Figure S2.** Duschinsky matrix for the Bo.5 dye using the AH algorithm.



**Figure S3.** Comparison between the computed vibronic spectra with and without the inclusion of Herzberg-Teller effects (HT) for the VG and AH algorithms. The Gaussian lineshape was used for the computed spectra with the default linewidth parameter of  $250 \text{ cm}^{-1}$ .

**Table S7.** The square norm of the displacement vector  $K^*K$  computed using the VG algorithm for all dyes in the test set. The value of  $K^*K$  is considered too large if it is above 8, in which case the calculation is aborted. The difference of vertical excitation energies ( $\lambda_{\text{vert}}$ ) and band maxima ( $\lambda_{\text{max}}$ ) are also provided in eV units. The MAE for the whole benchmark set is 0.00840 eV.

BODIPY	1	2	3	4	5	6	7	8	9
$K^*K$	3.220	1.490	1.651	1.152	2.100	0.932	0.783	0.772	0.824
$\lambda_{\text{max}} - \lambda_{\text{vert}}$ (eV)	0.00045	0.00120	0.00331	0.00438	-0.03794	0.00365	0.00335	0.00198	0.00483
BODIPY	10	11	12	13	14	15	16	17	18
$K^*K$	1.068	0.735	0.698	0.835	0.915	1.013	0.769	0.634	1.131
$\lambda_{\text{max}} - \lambda_{\text{vert}}$ (eV)	0.00672	0.06100	0.00404	-0.00353	0.00337	0.00968	0.00559	0.00424	0.00258
BODIPY	19	20	21	22	23	24	25	26	27
$K^*K$	2.878	2.468	1.837	0.970	0.900	0.787	0.544	1.765	1.391
$\lambda_{\text{max}} - \lambda_{\text{vert}}$ (eV)	0.00714	0.01276	0.00755	0.00318	0.00659	0.00238	0.00284	0.00494	0.00412
BODIPY	28	29	30	31	32	33	34	35	36
$K^*K$	1.245	0.954	0.746	2.589	3.155	3.666	2.437	1.380	0.759
$\lambda_{\text{max}} - \lambda_{\text{vert}}$ (eV)	-0.03988	0.00421	0.00424	0.00923	0.01589	0.01855	0.00841	0.00066	0.00411
BODIPY	37	38	39	40	41	42	43	44	45
$K^*K$	0.804	1.939	0.740	2.559	0.809	2.974	3.646	2.445	0.808
$\lambda_{\text{max}} - \lambda_{\text{vert}}$ (eV)	0.00161	0.00741	0.00262	0.02355	0.00152	0.00931	0.00317	0.00659	0.00273
BODIPY	46	47	SMcy7	PDT-1	BD-1	BOPHY-1			
$K^*K$	1.123	3.195	1.63	0.83	0.75	1.54			
$\lambda_{\text{max}} - \lambda_{\text{vert}}$ (eV)	0.00601	-0.01634	0.00511	-0.01423	-0.00190	0.00786			



**Figure S4.** Comparison between the computed vertical excitation energy, vibronic spectra and experimental absorption spectra of SMcy7. The vibronic spectrum has been computed using in vacuo structures and vertical energies while experimental data are measured in toluene and DMSO. The

shoulder observed in the experimental spectrum in toluene is much less prominent in the VG calculation. This might be due to neglecting mode mixing or solvent effects.

**Table S8.** Computed Mean Absolute Error in eV for the BODIPY dyes studied sorted according to the solvent model used. Calculations were carried out at the STEOM and STEOM-CPCM levels with the def2-TZVP basis set.

MAE	STEOM	STEOM-CPCM	Number of BODIPY
CH <sub>2</sub> Cl <sub>2</sub>	0.079	0.068	22
CHCl <sub>3</sub>	0.060	0.055	10
THF	0.068	0.000	1
Cyclohexane	0.050	0.052	4
Ethyl Acetate	0.124	0.019	1
Methanol	0.185	0.164	2
n-Hexane	0.138	0.162	1
Toluene	0.050	0.054	5
Ethanol	0.089	0.207	1
Apolar solvents	0.072	0.062	44
Polar solvents	0.153	0.178	3

**Table S9.** Computed vertical absorption energies in eV of 4 large BODIPY dyes obtained with DLPNO-STEOM-CCSD in gas phase and CPCM with the def2-SVP, def2-TZVP(-f) and def2-TZVP basis sets. The calculations times correspond to a parallel run on 8 cores of an Intel(R) Xeon(R) CPU E5-2640 v3 @ 2.60GHz) processor.

BODIPY	DLPNO-STEOM-CCSD			
	def2-SVP	def2-TZVP(-f)	def2-TZVP	Experiment
SMcy7 gas phase	1.74 (1d 17h)	1.71 (8d 1h)	1.74 (15d 7h)	1.82 (Toluene)
SMcy7 CPCM	1.44	1.45	1.48	
PDT-1 gas phase	1.80 (14h)	1.70 (2d 15h)	1.71 (4d 4h)	1.78 (CH <sub>2</sub> Cl <sub>2</sub> )
PDT-1 CPCM	1.78	1.69	1.70	
BD-1 gas phase	1.14 (2d 4h)	1.07 (6d 7h)	1.09 (16d 8h)	1.14 (CH <sub>2</sub> Cl <sub>2</sub> )
BD-1 CPCM	1.14	1.06	1.06	
BOPHY-1 gas phase	2.32 (3d 6h)	2.28 (8d 9h)	2.28 (26d 15h)	2.15 (CH <sub>2</sub> Cl <sub>2</sub> )
BOPHY-1 CPCM	2.33	2.27	2.27	

**Table S10.** Cartesian coordinates of the BODIPY dyes studied. Geometries were optimized at the DFT/D3-B3LYP level of theory with the def2-TZVP basis set.

45

BODIPY 1

F	0.10770619365186	-1.85288096847419	2.45515571705299
B	0.04910247232271	-1.86559936010254	1.06169743451927
F	1.07646146657718	-2.65064619954905	0.54644879604035
N	0.11406761459699	-0.44778033416080	0.47104077751374
C	-0.93086082550820	0.15030278631933	-0.12223319877478
C	-2.14170305475607	-0.48727327115017	-0.29588869124842
C	-2.34941382065409	-1.83166828113403	0.06884500040329
C	-3.57296652928046	-2.50166914984366	-0.17237844071299
C	-3.72545041662439	-3.81738223963290	0.16831852639229
C	-2.65798120912196	-4.50930291226727	0.76680609530170
C	-1.49342440697872	-3.82978986376016	0.99323372826448
N	-1.33790598214922	-2.52768546306715	0.66208578187669
C	-0.78261574434272	1.53897224904178	-0.63671342667625
C	-0.67563142511579	2.61828597557496	0.23848608511351
C	-0.55226723705966	3.90925264528249	-0.25609051699130
C	-0.52199497651225	4.13295207215464	-1.62824002088929
C	-0.63197807861733	3.06139767843312	-2.50481751334445
C	-0.77287409381502	1.77089986970742	-2.01078923657749
C	1.42119437436365	0.15654015146870	0.41943821934737
C	2.16926202347748	0.03072209791336	-0.76021086114247
C	3.43560655861973	0.60466669419898	-0.80700957766169
C	3.96237272721541	1.26121460628907	0.29440293980212
C	3.21657159395712	1.36034090953687	1.45609711958949
C	1.93668715717879	0.81269080986948	1.54243409674789
C	1.17349634106839	0.95913039231993	2.83085511843834
C	1.67521895931385	-0.73452480997959	-1.95724485571709
H	-2.95471184521179	0.05248711076443	-0.75379290318749
H	-4.37531531707443	-1.94476614797039	-0.63455392167128
H	-4.66270489277282	-4.32372233082296	-0.02307494902477
H	-2.74594166177058	-5.54579597419537	1.05481193578729
H	-0.63320050992798	-4.28964244319089	1.45629557285218
H	-0.69552447449351	2.44599636579976	1.30552559684791
H	-0.47651565376312	4.74213896230786	0.43036263896350
H	-0.41413597953496	5.13864546391307	-2.01290739835399
H	-0.60796840845008	3.22788151364272	-3.57420193266670
H	-0.86453998149715	0.93630500557712	-2.69201135204564
H	4.01748251091116	0.51778049195043	-1.71647624723475
H	4.95127745891466	1.69777089416075	0.24443329216612
H	3.62380583108039	1.87666003207600	2.31724698437559
H	0.14457118381101	0.62573244679113	2.74344393716623
H	1.63712258538885	0.35881347729549	3.61583887424377
H	1.18601214936570	2.00019847060376	3.16103264287907
H	0.59215194934038	-0.80926716014468	-2.00067761336696
H	2.06136733117239	-1.75577953899464	-1.92825557826503
H	2.02608904270462	-0.26290172455217	-2.87577167613233

51

## BODIPY 2

F	0.51130865936146	2.38698626223856	0.24885278524996
B	0.65095545049293	1.23812123369622	-0.52296324625539
F	0.51448414125646	1.55546005172838	-1.87686131540772
N	-0.43422584761233	0.20648331325870	-0.08872568838318
C	-0.20857713882707	-1.11128251027976	-0.13392711166370
C	1.07528315220574	-1.58927216288774	-0.32383065328930
C	2.20841888326510	-0.76435097843351	-0.34518748097800
C	3.49481283091436	-1.38450946603039	-0.32782711594208
C	4.61955723081505	-0.64032449644618	-0.30633172889949
C	4.53188314231213	0.77899374346929	-0.32520749575386
C	5.68956084813035	1.57594499447476	-0.33493176594789
C	5.60249142394342	2.94556627226281	-0.39345487663223
C	4.33732946728425	3.54144647537144	-0.45683854490493
C	3.18239622343473	2.78723104807636	-0.44620928340220
C	3.24800128486733	1.38313907803612	-0.36531105796351
N	2.09988721664918	0.58941073999191	-0.34844831876897
C	-1.28851460675704	-2.12183712721711	0.03975276314863
C	-1.42127819474518	-3.12066248525509	-0.92916155287747
C	-2.37011073959904	-4.12440832764723	-0.78729679271289
C	-3.18936835933153	-4.15331698039953	0.33469990094578
C	-3.06104342935064	-3.16723349638231	1.30563180817916
C	-2.12110932316429	-2.15668947031793	1.16004267724100
C	-1.76043461238770	0.69754117330242	0.18928168872282
C	-2.73034013037250	0.68859391313216	-0.81788031867860
C	-4.02224397679150	1.10008495196943	-0.48899541602695
C	-4.33994724847676	1.50677670934629	0.79534308777556
C	-3.35675282428645	1.52869965074679	1.77414053650811
C	-2.05317050751949	1.13574243777960	1.48829014644703
C	-1.01182106872843	1.15179738864744	2.57165787244310
C	-2.43463415069673	0.21997448067489	-2.21600625357599
H	1.23397611268048	-2.65492228173262	-0.32848038272277
H	3.529182072777643	-2.46491985562390	-0.31981839531139
H	5.59671876910425	-1.10715585412725	-0.28373645444545
H	6.65255038530559	1.08181836934146	-0.30067980794449
H	6.49600123885617	3.55474987656998	-0.40163699894238
H	4.25577882547702	4.61890214811982	-0.52129949927942
H	2.22694130125057	3.27771917667641	-0.49919085195116
H	-0.78408902118720	-3.09928691298477	-1.80306677687098
H	-2.46684858169290	-4.88491483419423	-1.55146502986392
H	-3.92372714241831	-4.93934578697587	0.45392835998635
H	-3.69114481914676	-3.18558149300889	2.18508064374863
H	-2.03353091991959	-1.40131827293019	1.92507390838594
H	-4.78399749011565	1.09423968064450	-1.25883698088614
H	-5.34886308579391	1.81658323663526	1.03521142855619
H	-3.59970268638991	1.85259877746809	2.77836613194336
H	-1.46926866380595	1.39244157383724	3.53071371823689
H	-0.50555743313809	0.18849079858625	2.66446567364747
H	-0.24077122207708	1.88994984163104	2.35701005264159
H	-3.14500901416669	0.65962085473736	-2.91500307713788
H	-2.53109004480619	-0.86707075554544	-2.28940467696955
H	-1.42994237707810	0.49339729596894	-2.52952823341771

63

## BODIPY 3

F	0.55398198217550	-2.12774873471710	0.56522501725151
B	0.90444719216213	-1.14677316845211	-0.36703510302255
F	0.75649300524201	-1.64616788836903	-1.65986306071700
N	-0.02157678877241	0.08127747738218	-0.15046102403576
C	0.42635446702100	1.27511818266801	0.25139961694116
C	1.79232757334599	1.51637604914751	0.30539810971185
C	2.76527564436249	0.53024189218197	0.10648816981376
C	4.14593868183410	0.88287571095073	0.22879443960002
C	5.10940803629763	-0.05793824235282	0.13751428038939
C	4.76071058301467	-1.41772025191007	-0.09494855477798
C	5.73776964468656	-2.42629911453811	-0.16188916578489
C	5.38294645999077	-3.73521108897906	-0.38133258256451
C	4.03038151437091	-4.05580151161351	-0.55150105733900
C	3.05015053549191	-3.08888640814806	-0.49731107030097
C	3.39154236702374	-1.74597664405832	-0.25513511922374
N	2.41921809368914	-0.75240705090721	-0.16012270899854
C	-0.47317489582015	2.36423264565270	0.72187870939671
C	-1.66588214649441	2.73491862124782	0.09700495833798
C	-2.43812796436766	3.76937439011039	0.60514258438588
C	-2.05060975466121	4.44343801956979	1.75621977246556
C	-0.87128492863147	4.08004648162624	2.39402138644105
C	-0.09409984028751	3.05265321148817	1.88082227345912
C	-1.42858325918629	-0.20102433900468	-0.29828423926965
C	-1.99362010291205	-0.12145591842522	-1.58251171077117
C	-3.35303012106434	-0.39541688561744	-1.71374181972586
C	-4.12650471646001	-0.73628143163481	-0.61516260225740
C	-3.54300419617566	-0.82663530759631	0.63715122859897
C	-2.18602105273017	-0.56958674592531	0.82199935907859
C	-1.58409898209213	-0.72081199920351	2.20666545882113
C	-1.74874478010142	-2.15717259308814	2.72188685236966
C	-2.17196095338642	0.28332238344140	3.20302836658398
C	-1.18287967616259	0.23834781436455	-2.81821255026419
C	-1.23297847215303	-0.89805487454796	-3.84693394210545
C	-1.61995898394133	1.56493709819199	-3.45593137731867
H	2.13509649647381	2.50831460110570	0.54492366993735
H	4.38363097767561	1.92000813511739	0.41742878594761
H	6.15470577009020	0.20519250656049	0.24493784913230
H	6.77606228568799	-2.14761020220335	-0.03074629722239
H	6.13668738658056	-4.50963995952908	-0.42437646809851
H	3.74071335909140	-5.08301012496888	-0.73056016223490
H	2.01984817798479	-3.36751123767137	-0.63234899380933
H	-1.99794232173598	2.22295905202295	-0.78757416114157
H	-3.35317228316223	4.04476468110161	0.09789560973763
H	-2.66419469811105	5.24059654011531	2.15491357706229
H	-0.55941602628761	4.58498775616703	3.29846602168789
H	0.80498824120510	2.75197294748139	2.39960976943380
H	-3.81327816635130	-0.34253955206640	-2.69192534378946
H	-5.18040359379608	-0.95094663148857	-0.73983930812508
H	-4.14702009878842	-1.11316398330185	1.48784894962373
H	-0.51685679445829	-0.52723909183296	2.12897406151020
H	-1.20622709890908	-2.28268391090759	3.66106745299100

H	-2.79822339092913	-2.39318686754874	2.91087500615564
H	-1.35558361213256	-2.87252387739991	2.00250664579839
H	-2.02426734329913	1.30949821757597	2.86853945461412
H	-3.24359691706078	0.12339873016251	3.34088040093919
H	-1.68967941248878	0.16841491379503	4.17617554424230
H	-0.14582652008992	0.35127369734016	-2.51541612165569
H	-2.23701160927824	-1.01597058664134	-4.25953051140511
H	-0.55552459080328	-0.68610622139927	-4.67606895744117
H	-0.93239928587498	-1.83993476899157	-3.39362597250905
H	-1.05291182285489	1.73995567453700	-4.37191334190587
H	-2.68024138268890	1.55792303861738	-3.71741156520430
H	-1.43904989099715	2.41236674531629	-2.79375848944005

33

## BODIPY 4

F	0.98948702500250	2.15108817988283	1.25803937407457
B	0.44044584112869	1.58097845347964	0.11279005637824
F	0.33463078655833	2.53645133523594	-0.89262072994246
N	1.31724923060721	0.38951380676446	-0.36765815014273
C	0.99293495145190	-0.96132386562950	-0.24219047659465
C	-0.23929509873660	-1.33841919639307	0.26792836435883
C	-1.20728583684771	-0.40063672278158	0.59652315288989
C	-2.55809686727021	-0.59830995591144	1.02655983466904
C	-3.22206116417669	-1.90868452689314	1.28762489864332
C	-3.09969974986791	0.67652725117315	1.09093681919322
C	-2.09525140483419	1.61167324532541	0.71680980149672
C	-2.53312455525670	2.95935855058779	0.72958961696557
C	-3.84183373087056	3.02978266274622	1.10359551559764
S	-4.58998865990519	1.49277762386898	1.45777156757521
N	-0.95391785929432	0.96051681526369	0.42838275555374
C	2.06381475795863	-1.76657350326770	-0.74676027612327
C	2.09042965198677	-3.25366689372340	-0.83681656840487
C	3.02069445838423	-0.86012357180886	-1.17164394038510
C	2.54055525146291	0.45474639446822	-0.91832395638430
C	3.44471745315666	1.47805497022323	-1.29713228500317
C	4.57101300461481	0.93508001781414	-1.83920819829456
S	4.58823669083988	-0.80847938644096	-1.91507240847202
H	-0.46416040327400	-2.38983205059013	0.38447695097104
H	-3.64666497081549	-2.32926804723622	0.37136564397553
H	-2.52418885179667	-2.63938109258069	1.69721521987757
H	-4.03943000084136	-1.79265271315098	1.99946051564380
H	-1.92478248239823	3.80896454671125	0.46429462498505
H	-4.44108083862210	3.92201213377367	1.19083884560114
H	1.38285028810489	-3.61901671313695	-1.58474995206370
H	1.82765297397063	-3.72034029161731	0.11456056924239
H	3.08046485136051	-3.60622883201929	-1.12387182396650
H	3.26729596629835	2.53490306355114	-1.17713930735161
H	5.42829029192103	1.47051231231144	-2.21467705456357

30

## BODIPY 5

F	1.08229686135815	1.25356458567903	1.73275383582622
B	0.52524662551724	1.10638810108515	0.46646402965977
F	0.41336051056291	2.34805929087109	-0.15626200429651
N	1.38280764510931	0.13499093335468	-0.39458758677515
C	0.89854832399599	-0.96603923298262	-1.09421023672653
C	-0.43146681357033	-1.35548639580995	-0.96103220361675
C	-1.30438199366779	-0.67560008912692	-0.14182997973022
C	-2.67793557444020	-0.91285600094000	0.15673155161170
C	-3.05898028892694	0.08752540693638	1.03127213818938
C	-1.93606270249467	0.91819010776358	1.26568875514508
N	-0.89209989276109	0.45326974852197	0.56816547222421
C	-1.84397747992563	2.12422102306458	2.12679063135720
C	-3.49958307779453	-2.04272312998255	-0.36383194031358
C	1.95011154360509	-1.57091936900831	-1.82672169448748
C	3.08071767255849	-0.82001862133390	-1.54849407955573
C	2.70410346818631	0.21983199391633	-0.65577723247087
C	3.78318395175038	1.04633239316702	-0.25350786350844
C	4.94103424070006	0.63176718955671	-0.84045637749634
S	4.77519153508748	-0.74813844274162	-1.89633409430220
H	-0.77770933758430	-2.22344922840516	-1.50561325719978
H	-4.03221164008707	0.22671687652456	1.47354013248569
H	-1.43664220495180	2.96340950035749	1.56126350695701
H	-1.15963936678148	1.94344984620936	2.95817103943384
H	-2.82160483585626	2.39096242461542	2.52292354020463
H	-3.50012632969011	-2.07246935391549	-1.45604071721098
H	-4.53178951153348	-1.95550223440122	-0.02767458934845
H	-3.11405204879620	-3.00302844148489	-0.01166784083772
H	1.85371102380169	-2.44562487949444	-2.44783139547915
H	3.70818059473803	1.87747637310980	0.42927666595421
H	5.91956710189073	1.06579862489390	-0.71086820569308

30

BODIPY 5, fully optimized 1<sup>st</sup> ES.

F	1.13602946568688	1.00136420816377	1.78939103902416
B	0.53917589542901	0.98447316780177	0.53333662706533
F	0.56081316401232	2.26009461608749	-0.02264644315581
N	1.39264647038598	0.04120871409006	-0.38705953765955
C	0.92038730335965	-1.07818597893406	-1.08346144953449
C	-0.46400023159620	-1.45592980522651	-0.93639149947568
C	-1.30401966982550	-0.72168671247606	-0.13628069369559
C	-2.69600003448466	-0.89743275221653	0.14849965111911
C	-3.05718664866266	0.13651843495844	1.00330493465309
C	-1.92544793426166	0.92936705997604	1.25090195064798
N	-0.87140917585699	0.40747375130428	0.56862016796529
C	-1.80992980661153	2.14997662555045	2.08861141632065
C	-3.54210100078676	-2.00422295105311	-0.37285362710763
C	1.95328220134300	-1.62331675911445	-1.80869982717784
C	3.11011956767269	-0.79016605826874	-1.53900051474843
C	2.70642095014894	0.20459392409135	-0.65892384068636
C	3.74413119484930	1.10549843363018	-0.25744975784002
C	4.93050250279512	0.77184858773431	-0.84620247320676
S	4.75742605671271	-0.61877304206264	-1.88430450675111
H	-0.83126012143222	-2.31581321383276	-1.47257672579028
H	-4.03625409858970	0.31665945427234	1.41826069562138
H	-1.43761489437393	2.99102980364836	1.49866767541716
H	-1.10060666534383	2.00587763185862	2.90761649269048
H	-2.77925018312001	2.41678107244408	2.50553517757358
H	-3.63163091234460	-1.97249203517246	-1.46328342942855
H	-4.54602644149692	-1.95358071273445	0.04760390071346
H	-3.11989506998755	-2.98020902161473	-0.11501092998251
H	1.90053271498399	-2.49052760088154	-2.44385059229599
H	3.61038798813863	1.93034678820159	0.42518625992536
H	5.89057541325650	1.24932336977490	-0.75724014020046

44

## BODIPY 6

F	2.42369064389810	1.10050922195114	-1.34477554078423
B	1.86275719156445	0.67871628818758	-0.15386550420753
F	2.10493297811750	1.60622375204439	0.86122248679092
N	2.47332749383012	-0.69125566311727	0.25605195440558
C	1.75406236045318	-1.81775181021828	0.62996481078303
C	0.36788931939746	-1.79804837960101	0.58660743607439
C	-0.33110296380295	-0.69096661922158	0.15201397749774
C	-1.73282237541038	-0.56226740052969	-0.07655409078677
C	-1.90674658088962	0.65060843044170	-0.71410094996729
C	-0.63845638694287	1.27794886529808	-0.82926861519494
C	-0.42250766178095	2.60481884903473	-1.40246599167132
C	0.54271415898938	3.49590014212345	-0.91790597282611
C	0.67544295535549	4.75619532684824	-1.47917527175543
C	-0.13998730634305	5.15065872610327	-2.53317952909926
C	-1.10675495986067	4.27715229164583	-3.02015591895186
C	-1.25019037857963	3.01893070075594	-2.45748170833853
N	0.30650755987711	0.46278671003487	-0.30144986943358
C	-2.74431169126046	-1.53949401237443	0.33421176417567
C	-3.71302250275573	-2.00254697764470	-0.56189817204734
C	-4.64946363101380	-2.94802977855243	-0.16481936803807
C	-4.64334026251988	-3.43665683173193	1.13699743319750
C	-3.69643266248836	-2.97044451967797	2.04161713737666
C	-2.75281296459243	-2.03332451244743	1.64369903336813
C	2.64181885895445	-2.85874051947508	0.99925961827784
C	3.91409875001733	-2.33524444146895	0.84692971519459
C	3.78256673587597	-0.99577914461147	0.38462164347147
C	5.02343391979242	-0.34099221038831	0.18114404712654
C	6.05680961261971	-1.17553393712327	0.48580384055053
S	5.58152028065906	-2.76478321988784	1.02981046370415
H	-0.18401043702091	-2.68207181988095	0.87109474233593
H	-2.84339254728531	1.09676244492077	-1.00102072588202
H	1.17457370236911	3.20988776435490	-0.09336721215845
H	1.42127781853368	5.43525264327310	-1.08718177531838
H	-0.02287433042419	6.13279923351979	-2.97204080858864
H	-1.74447546330759	4.57477288461387	-3.84229828757546
H	-1.98972023665914	2.33610814085899	-2.85408800255396
H	-3.70964596788557	-1.63494404646630	-1.57951244956533
H	-5.38051744991748	-3.30955801650495	-0.87614271311299
H	-5.37386014829930	-4.17264347192113	1.44641103940972
H	-3.69456180147474	-3.33532935670456	3.06040857529192
H	-2.03021884880555	-1.65490258337327	2.35476452561648
H	2.34508247128292	-3.84144013920887	1.32456626593061
H	5.14060939216747	0.66963946737705	-0.17565489568524
H	7.10821235556567	-0.94332247125603	0.41960286296332

42

## BODIPY 7

F	1.25126198486302	0.61841629337150	1.91444235569150
B	1.54191004081261	0.42069829354856	0.56214025641018
F	1.08308258556376	1.49752942329480	-0.18636320166418
N	3.06946152984215	0.26798499879316	0.35622480172317
C	3.74361099118238	-0.93762199053921	0.22124921805825
C	3.01833917355586	-2.11035058090169	0.02309922985500
C	1.64397744023978	-2.10268006083697	-0.07556985209584
C	0.76066229911540	-3.14961250771418	-0.45547254271004
C	-0.49984472980570	-2.61551766510390	-0.52874023982871
C	-1.82149755818587	-3.20457551133539	-0.89532638635504
C	-2.68300367565034	-2.12227301564529	-1.55565681687143
C	-2.73596365752573	-0.85932817019084	-0.73038701238276
C	-3.89571017032417	-0.11413472177386	-0.66869454729877
C	-3.94419370350506	1.08727958401409	0.04470381115892
O	-5.12036310339582	1.75680310180322	-0.00223178997598
C	-5.20895585981190	3.01803083912424	0.64434417776925
C	-2.81726836005852	1.52135813377531	0.74286451158011
C	-1.65025936582999	0.77930270376990	0.68891509163914
C	-1.57431120300475	-0.40370596121382	-0.05391452418391
C	-0.39832115351752	-1.23841699313395	-0.14979550871203
N	0.89315711687415	-0.93584544795618	0.10048607409559
C	5.13946406522412	-0.70616182031362	0.17569269511511
C	5.29376654315707	0.67086225902672	0.25935607729290
C	4.00100337562932	1.24764983123554	0.37103630393892
C	4.00885721463602	2.66317510571510	0.44106994706869
C	5.28658550196950	3.13434665553626	0.37724844732438
S	6.51343246324280	1.90111555251291	0.24004486525925
H	3.54822384990013	-3.04167708397140	-0.12231297050493
H	1.06562719940733	-4.16099497756509	-0.67418331201573
H	-1.69680036481803	-4.05724791525366	-1.56416591265794
H	-2.32802643487971	-3.57460348754159	0.00265056908203
H	-3.69333063754540	-2.48886758004974	-1.73836251395513
H	-2.25022285024457	-1.88225097671800	-2.53351885876134
H	-4.78679833686533	-0.43882371149815	-1.18970940902039
H	-4.45303065162841	3.70920735070831	0.26406583639164
H	-6.19941347177858	3.40153199048629	0.41364138587288
H	-5.09852150185064	2.91863171318586	1.72779096628657
H	-2.83546077583505	2.42900833013122	1.32562493721480
H	-0.79482614540491	1.11801076964198	1.24880032050008
H	5.89423584338962	-1.46582270925980	0.05801311330837
H	3.13060295452506	3.28331528519894	0.51814109696090
H	5.59846153833588	4.16635467364242	0.40286030939652

52

## BODIPY 8

F	0.80947280095270	2.56972738938428	-1.20221929811850
B	-0.01136814494250	2.35112114896990	-0.10442367550752
F	0.58033474603531	2.87889701893065	1.04696736346536
N	-1.38623612902282	3.02212152956882	-0.33791564007393
C	-2.62135756078742	2.42735734824967	-0.13192656496871
C	-2.69201217442503	1.07086154345677	0.17358907465167
C	-1.56447234252055	0.28459612463177	0.24963794168577
C	-1.45608941417019	-1.12871362220772	0.45888330202356
C	-2.57175732484543	-2.06061657973934	0.64575197928363
C	-2.53273782483940	-3.01430812166900	1.66971261600941
C	-3.58549485246175	-3.89759136636081	1.86088950722939
C	-4.69932463684684	-3.84929127104853	1.03015573647076
C	-4.74624828802166	-2.91645173748151	0.00004852592949
C	-3.69470252450718	-2.03095846522801	-0.19148922326458
C	-0.10713756125451	-1.42435402708083	0.42504425941466
C	0.62010712812279	-2.72031773409847	0.54768139352091
C	1.85157796631050	-2.70406341726541	-0.36126006199407
C	2.66422758400437	-1.43579105052187	-0.23957327833363
C	4.03268532879816	-1.48305021426464	-0.48162924774643
C	4.80103335136116	-0.32024032477738	-0.45099115203003
O	6.12723836776467	-0.27255850650172	-0.71928052251061
C	6.80165556559069	-1.47479511973429	-1.05209172644095
C	4.19809975972792	0.89818412474605	-0.12788352133344
C	2.84640520072534	0.95358566005563	0.11712776780195
C	2.04246026966053	-0.19765208385927	0.03635518063987
C	0.60166473802027	-0.20859614085546	0.19162492071338
N	-0.27984457001675	0.81343580486190	0.09522909203418
C	-3.65344779798719	3.37046888589796	-0.34760867864104
C	-3.01297038491302	4.55105520729294	-0.69800018941651
C	-1.61388080437340	4.31053594667197	-0.67938791404198
C	-0.83258958688048	5.44567352682214	-1.01148656448740
C	-1.63736116258158	6.51296523303992	-1.27939304804366
S	-3.34725969149964	6.18738962591112	-1.15034575082910
H	-3.65931432379588	0.61827757788385	0.33283800053973
H	-1.67790138769210	-3.04373343470474	2.33170347785956
H	-3.54055182488412	-4.61852503242108	2.66687397019432
H	-5.52319223089338	-4.53367053554414	1.18491838178993
H	-5.60390535474836	-2.87817743967193	-0.65937958597366
H	-3.72876041519100	-1.32725186457726	-1.01243579657255
H	-0.03417036182941	-3.55431653473613	0.29139403518371
H	0.94013940358354	-2.87555121649919	1.58506574144301
H	2.48837474190788	-3.56446090536719	-0.15115107120372
H	1.51769779831954	-2.80340872212973	-1.40092449897855
H	4.48467444130710	-2.43641639413999	-0.71269331668685
H	7.82233026576505	-1.18653724227967	-1.28966755178788
H	6.80179670272528	-2.17359230034448	-0.21088876145483
H	6.34906956187847	-1.95723435659409	-1.92260276555152
H	4.81091690875738	1.78758634370446	-0.07964582601870
H	2.40603288051019	1.89832429682311	0.38231757566496
H	-4.70836662314777	3.17041498182187	-0.25937578516514
H	0.24482734829508	5.46702328462744	-1.05766459416363

H	-1.32036156104455	7.50292215835166	-1.56607523221011
---	-------------------	------------------	-------------------

40

## BODIPY 9

F	-1.30652845648576	-1.77421761514967	1.14282202124745
B	-1.29286156398516	-0.38686897276962	1.01030986249056
F	-0.57721930879731	0.19706375664343	2.05108319875037
N	-0.67644161089787	0.00699736127405	-0.36442876823991
C	-1.38753680382182	0.50295515490162	-1.45214564738349
C	-2.739907555831392	0.79827368885258	-1.33026185277677
C	-3.40982564843631	0.64606833118180	-0.13422021396533
C	-4.74032208855257	0.99703728092148	0.23167313038056
C	-4.84769660779087	0.73031984343365	1.58496138581771
C	-3.60634235058795	0.22488531560413	2.03601030778585
N	-2.75413858076219	0.16757823834440	1.00142641856154
C	-3.23148431101560	-0.15074846274186	3.42342134530124
C	-5.78852950389622	1.53449195902310	-0.68151735015133
C	-0.51312662032739	0.68766799625375	-2.55420899977163
C	0.73862606778861	0.30414647611186	-2.10968952816753
C	0.60881818177417	-0.12039653404231	-0.75767180430090
C	1.82033561113096	-0.54053379194403	-0.17395083852302
C	2.86825370248229	-0.43901298081965	-1.05540382196646
C	4.25956487588229	-0.79502139894143	-0.79838671108273
C	4.55795297698118	-1.78093823857362	0.15302116645768
C	5.87072444428135	-2.11857807529163	0.43678562266304
C	6.91681486881759	-1.48236380251718	-0.22419599474530
C	6.63521126498698	-0.51035786850171	-1.17844635347173
C	5.32104136469635	-0.16943049926470	-1.46604294989649
S	2.38267237383992	0.17820419068693	-2.63852208732533
H	-3.26754047910417	1.19256011702115	-2.18771210844998
H	-5.71237452508000	0.88941016837578	2.20907780189190
H	-2.41223828551949	0.47522771553349	3.77825900735962
H	-4.08562319451686	-0.03078723923265	4.08718709451597
H	-2.87612643559222	-1.18240328380355	3.46899722374426
H	-6.25225009526819	0.73586546070858	-1.26761065879063
H	-6.57684007196749	2.03096402981965	-0.11617321107051
H	-5.37404625130930	2.25608919297950	-1.38780187513811
H	-0.80297573600210	1.07188346924967	-3.51766468906607
H	1.92381414122110	-0.87183665390248	0.84656789611506
H	3.75078290507429	-2.29815693667820	0.65163137427515
H	6.07902948005061	-2.88716815560799	1.16951506844037
H	7.94112655849777	-1.74894167619332	0.00188265245385
H	7.44247837068696	-0.00903680049845	-1.69574247993651
H	5.11462789983835	0.60570723955347	-2.19303563403244

54

## BODIPY 10

F	0.56875877978582	-1.64568682750421	-0.06497642160247
B	0.16219941823744	-0.42763801186903	0.45036416414210
F	0.56573706786954	-0.29608326745091	1.78400725704992
N	0.77899417698526	0.71409423297657	-0.39567944874483
C	0.09773369566533	1.80620496221372	-0.91119046018758
C	-1.27261303287925	1.91241233434201	-0.72429777483211
C	-2.00242629058560	0.91898529423247	-0.09171333542311
C	-3.41927293909102	0.76031300911508	0.02227344777822
C	-3.62415687360473	-0.54705505840465	0.44363191777018
C	-2.36429259378714	-1.14892207593519	0.64966187438273
C	-2.13499320555937	-2.51799178135352	1.11368987476377
C	-2.90761120057254	-3.55327858906038	0.57244815801353
C	-2.69540918915383	-4.86834425377119	0.95996326056352
C	-1.72415789863940	-5.16679892025740	1.91029616623312
C	-0.97615789519442	-4.14062370667367	2.47578625362842
C	-1.17214210618505	-2.82704590900056	2.07978896614397
N	-1.39349386315502	-0.25780082630639	0.34244715009599
C	-4.44111463436509	1.78013667924909	-0.19432328099212
C	-5.73394702754871	1.41685508722124	-0.59397861014304
C	-6.72877370584277	2.37126913573353	-0.73661255690608
C	-6.45451844917204	3.71273394063125	-0.49343686174684
C	-5.17601497053584	4.09054664139771	-0.10297943180374
C	-4.18232835811802	3.13500661540917	0.05058214171954
C	1.00326224341306	2.63918992186878	-1.62702277984364
C	2.23770086940052	2.02486980730694	-1.52470526404546
C	2.06943563998947	0.83800719389748	-0.75803277141523
C	3.25237393534306	0.10690463749188	-0.55573551463409
C	4.33192530674885	0.71842077834838	-1.14528855289011
C	5.72221246647730	0.28570968873751	-1.08176987070469
C	6.72117317703821	0.87765115296091	-1.86633245307213
C	8.04365730666046	0.47230084483915	-1.75645691396037
C	8.39913020053014	-0.53200792952798	-0.86267835973253
C	7.41646340019621	-1.13614165347839	-0.08495155921253
C	6.09720861716187	-0.73166228113963	-0.18977957202551
S	3.89421333566836	2.20969243679021	-1.99682874525598
H	-1.79278372869649	2.76181434791100	-1.13937936522019
H	-4.56792117064889	-1.01143532370320	0.67299639806348
H	-3.64945216282147	-3.32448681058764	-0.18159054228476
H	-3.28188819830625	-5.66069715287288	0.51395803646978
H	-1.55109240918963	-6.19179700805145	2.21250131222468
H	-0.22796551544474	-4.36457881798559	3.22476717207245
H	-0.57954662520136	-2.03760012168890	2.51390548854878
H	-5.95145093934122	0.37790411830814	-0.80320169806117
H	-7.72059534185763	2.06760786113509	-1.04492249236699
H	-7.23353704262694	4.45574619172372	-0.60167043978600
H	-4.95467503435782	5.12932876320595	0.10564341422784
H	-3.21107584201430	3.43588822998634	0.41588618164548
H	0.74007585051591	3.55130790235002	-2.13503157929315
H	3.29854959683159	-0.82333988576824	-0.01486711931097
H	6.46260897045435	1.65803081107021	-2.57073746805318
H	8.79979424475894	0.94344590143076	-2.37024712266994

H	9.43074246302616	-0.84620065897084	-0.77237970595487
H	7.68074338005798	-1.92039401664436	0.61245015624475
H	5.35061610168075	-1.19466763387811	0.43854728039318

52

## BODIPY 11

F	0.23116059455973	0.64956389302902	0.54948032653751
B	0.19092093131448	-0.09363199997632	-0.62545448909033
F	-0.05813061682634	-1.43673912997251	-0.32844671233852
N	1.54966862431597	0.01832270490850	-1.38080018936566
C	1.69086411624787	0.22745115360633	-2.74685532627922
C	0.59030052692825	0.59094241549703	-3.50971401539872
C	-0.66061789575826	0.73794130437906	-2.95211320392299
C	-1.84971444162617	1.21963566156963	-3.55455986321673
C	-2.81983221791429	1.23393622784882	-2.58751856490367
C	-4.25288353461500	1.64648570793923	-2.64027703504370
C	-4.67802695935832	2.12004228721494	-1.24922013388825
C	-4.32285539225536	1.10088581688396	-0.19497417788159
C	-5.23613354598463	0.78395855033977	0.80074979302008
C	-4.90861102204600	-0.13818936186110	1.79541250981597
O	-5.75601743964059	-0.53543470424356	2.77549874612197
C	-7.09136919083947	-0.05687785375403	2.76343083655202
C	-3.63765055032779	-0.71685486706227	1.80695136467838
C	-2.72647457277881	-0.41147503410193	0.82002811084877
C	-3.05302095596468	0.47926193813120	-0.21724055017536
C	-2.23233991322794	0.72068652820977	-1.38605217670004
N	-0.92366777262234	0.44692891845326	-1.60992653079798
C	3.05054182897384	0.10363684421351	-3.12181390722837
C	3.73334799237463	-0.17086118265252	-1.95141084797829
C	2.79102160637165	-0.21769143436993	-0.88851260091640
C	3.37383825332994	-0.45199077773759	0.37433960807338
C	4.74262815497635	-0.57844914653545	0.28729563313677
C	5.70698042406150	-0.77239651747060	1.36220645807636
C	5.28548971319237	-0.98629922542839	2.68259695526389
C	6.20672206138655	-1.12409066756767	3.70762432270611
C	7.57156423505496	-1.06155740399500	3.44489821283903
C	8.00595511723352	-0.86695772549212	2.13911020604170
C	7.08661898888530	-0.72744994410794	1.11238528786696
S	5.33649778747733	-0.42950059085230	-1.37017368205107
H	0.72251254338947	0.80533718707755	-4.56121101775666
H	-1.93992876199871	1.52988238719058	-4.58371737037607
H	-4.40359676330168	2.43474920005571	-3.37972155612478
H	-4.87861468876955	0.80002083764570	-2.94570416476497
H	-5.74547911862470	2.33983829368166	-1.22095589133689
H	-4.15136176032006	3.05432759710826	-1.02413810041899
H	-6.20359872933719	1.26333731413102	0.78990433070181
H	-7.13060400432416	1.02607979636534	2.91496743059202
H	-7.59309588315733	-0.31399248784033	1.82627356716033
H	-7.59345494332586	-0.55484390737103	3.58830051772102
H	-3.39247710838123	-1.42289162144147	2.58818441745236
H	-1.76722623241821	-0.90083515748633	0.82594076488731
H	3.43736402676890	0.22965242454755	-4.11907165846099
H	2.81772148706588	-0.49311342127508	1.29608491511952
H	4.22984742003593	-1.04364529459049	2.90747511191844
H	5.85626238911675	-1.28389982737952	4.71877625863517
H	8.28761974759234	-1.16658780959031	4.24888564107997
H	9.06454457327908	-0.81945257088490	1.91775320219139

H	7.44729187181215	-0.56309832498668	0.10552623737800
---	------------------	-------------------	------------------

62

## BODIPY 12

F	0.95510243628582	-0.77588434328879	1.71800914347833
B	0.77891817949073	-0.23073831459451	0.44280978143801
F	1.08725325025070	-1.16996286739910	-0.53256181304912
N	1.69373855841802	1.01184592793389	0.28493634745511
C	1.27683252767375	2.32282953453775	0.46649568218442
C	-0.08127683644189	2.61234880776901	0.54144003647198
C	-1.04167944218488	1.63320054539219	0.40081561922310
C	-2.46368826058421	1.76267950650804	0.28805445231739
C	-3.23935516968984	3.00161611500506	0.38181790568174
C	-4.42156810589812	3.02799110052295	1.13283892990627
C	-5.16084494843379	4.19487479366137	1.25965186776635
C	-4.73590065112312	5.36324393110266	0.63777628117045
C	-3.57376969016489	5.34859972171845	-0.12517819464096
C	-2.83771067506002	4.17963025726091	-0.25920671278855
C	-2.95450355100742	0.48580325343163	0.09376065432290
C	-4.34123537305905	0.00266142546743	-0.17128726858464
C	-4.26571059673930	-1.23859156993774	-1.06251870881968
C	-3.31653351524076	-2.26113973440381	-0.49315059889092
C	-3.65846840038371	-3.60581764434128	-0.50600170690799
C	-2.78391523519536	-4.56425034577813	0.00460313680659
O	-3.06430015943930	-5.88996599624147	0.06355774008580
C	-4.36751009558380	-6.32239602534351	-0.30200531265312
C	-1.54401605648823	-4.16615731398115	0.51077466871336
C	-1.19826474725157	-2.83164216623145	0.53019642097521
C	-2.07589854255383	-1.84894139506307	0.04264204200275
C	-1.85261296733699	-0.41796198018027	0.12683935850369
N	-0.70498608777345	0.28001734168876	0.29598046620598
C	2.39569214760383	3.19345996655823	0.44052923635639
C	3.49466675626619	2.37996797399639	0.22864602115459
C	3.03905661294058	1.03689720944438	0.13955579503165
C	4.06653346326897	0.09874023499998	-0.08256603722084
C	5.29756513296733	0.70716051887266	-0.1746885849166
C	6.59619874117981	0.08167583767975	-0.39100754435172
C	6.70391688447086	-1.30788383017140	-0.55104829509716
C	7.93879369090765	-1.90758687383904	-0.73389112295816
C	9.09880027291860	-1.13954335568595	-0.76748019082455
C	9.00860296301619	0.23965051279494	-0.62111502799109
C	7.77396943934728	0.84200570954655	-0.43614468816999
S	5.20634138984336	2.46257258911273	0.01899946173490
H	-0.39184720856723	3.63772152260991	0.67325701270881
H	-4.74528581092976	2.13036770174665	1.64117997826371
H	-6.06670875990846	4.19413059498925	1.85156018529757
H	-5.30676369063104	6.27601359654853	0.74606735968404
H	-3.24111510557872	6.24822201690756	-0.62660244662723
H	-1.95789395891122	4.17143108885912	-0.88660321043850
H	-4.84276360106694	-0.26100767001240	0.76763279779493
H	-4.93811292647557	0.78467295267599	-0.64245736717542
H	-3.90946942527303	-0.93470445415725	-2.05340272593261
H	-5.25308518813800	-1.68067375468589	-1.19839586670274
H	-4.61284811099738	-3.89456638449150	-0.92088262774803
H	-5.13103643510063	-5.79591050546789	0.27542498253290

H	-4.55449256835047	-6.17535759784385	-1.36954779227725
H	-4.40585701924643	-7.38392659814871	-0.07013538321360
H	-0.87695692291021	-4.91962601309958	0.90571520287055
H	-0.25404385083577	-2.54098407170134	0.96050131465482
H	2.35692895644905	4.26475374083550	0.54713005095710
H	3.90095555641979	-0.96194677374703	-0.18034148028170
H	5.81547135360663	-1.92242070301467	-0.53079184908379
H	7.99699618843132	-2.98154177197372	-0.85540822185609
H	10.06161436290187	-1.61190604040216	-0.91024139179646
H	9.90179262684635	0.84999533885140	-0.64823164264579
H	7.72628719904967	1.91685572619700	-0.31630584653202

21

## BODIPY 13

B	3.30920022130760	2.66923905311263	6.90690451841702
N	2.25765413552505	3.41934812569229	6.01132667850010
N	2.93362987920653	3.02845778289759	8.39052166237048
F	4.58547012447055	3.12385240658977	6.61953323151572
F	3.20920551517546	1.30200279479063	6.71044724980207
C	2.18575599910223	3.39689137078942	4.67796008451257
H	2.88905529740791	2.82094524944644	4.09733297101931
C	1.11553048283243	4.19548509756896	4.23175287069161
H	0.83365578679639	4.35128602780161	3.20390227818427
C	0.51605814695847	4.72326280520697	5.36069732884603
H	-0.33720474999001	5.38099023363849	5.40725503105213
C	1.23415748902589	4.23541191996090	6.47828773300670
C	1.06079869290871	4.44460909681801	7.83774131807381
H	0.25449699952766	5.08493430335510	8.17202140172194
C	1.88836845865367	3.85672625107555	8.78176072488472
C	1.89008552851024	3.92919487600311	10.19528257269438
H	1.19376328387857	4.49786045019994	10.79071422644425
C	2.93761937199467	3.14309332179285	10.63994139694344
H	3.23897758308615	2.96352793450981	11.65831312367853
C	3.55521359670516	2.60653059785415	9.49439294866952
H	4.40659615691667	1.94737030089579	9.42989064897139

23

## BODIPY 14

B	3.35185709079135	2.67201170078999	6.89787358285596
N	2.28673646577063	3.38806972002752	6.00396593798779
N	2.95737221340765	3.02888257103591	8.36948801039121
F	4.62431554885785	3.13731639685818	6.60601266949094
F	3.28332737635961	1.29546752417741	6.72449401676502
C	2.30677473828016	3.47354735647453	4.66413933309063
H	3.13708206227390	3.07832637770866	4.10355130666844
C	1.14830772152403	4.11381686010968	4.20889367708283
H	0.89593557991316	4.32954975670868	3.18444453052880
C	0.39448638017868	4.42645786700341	5.33625802228955
H	-0.55479659975642	4.93759021424837	5.34613130388218
C	1.11396682193601	3.97044297445096	6.45228310769585
C	0.83057759288824	4.06340629902067	7.83310300526858
C	1.76868498944963	3.60316604820764	8.78228672172666
C	1.75946162644477	3.63421490554543	10.18740441347407
H	0.98194092908156	4.03168292699493	10.82013269147588
C	2.95854263712178	3.06871960900767	10.61346332560887
H	3.29397619031805	2.93270663921728	11.62772233533481
C	3.66707292318285	2.71100969845374	9.46136062038203
H	4.63308332876286	2.24467010015830	9.36702370315739
N	-0.32199942880038	4.62347147485025	8.24137961661867
H	-1.02104218320994	4.89969662168276	7.57765248165986
H	-0.55870400477603	4.65995635726803	9.21561558656393

44

## BODIPY 15

C	1.59675825599976	-4.19878353565780	4.11713463675454
C	0.33582448692536	-3.59311615901065	4.18889407025162
C	0.50831170632337	-2.23014748776456	3.90542120291310
C	1.89017727512612	-2.02817241217100	3.65608738770514
N	2.51744159231435	-3.26239412863636	3.79256419486742
C	2.62499744924922	-0.86887315333777	3.30268813952359
C	3.98401323692097	-0.94900654359151	3.03471187496215
C	4.97201200592971	-0.00202869878986	2.57254183612977
C	6.17295279865935	-0.67905887661068	2.44827062521450
C	5.92188020150502	-2.03022848271319	2.82425640617051
N	4.64124934867476	-2.18440745056174	3.16375325582739
B	4.01445163048323	-3.51711386545343	3.62287620564512
F	4.25510458806435	-4.50263043869520	2.64406094961809
C	1.96654976849434	-5.62418153732036	4.33466117362188
C	-0.62091541607277	-1.25019069548387	3.87050478668786
C	1.88373182548542	0.43470217434203	3.21623871101821
C	4.79965611265540	1.45184665841917	2.25235105410382
C	7.51697557056598	-0.19554428146062	2.01505019704740
N	6.82334913515604	-3.03151346468905	2.87143590900145
F	4.61265243325805	-3.92783574677204	4.81979905763743
H	1.12460867166590	-6.18260228104013	4.73917020711031
H	2.80574141702867	-5.70673308460975	5.02594155036383
H	2.27917044332479	-6.09324522146320	3.39956048274297
H	-1.56395768597825	-1.76277879225019	4.05341023743431
H	-0.70160928266421	-0.74381399727452	2.90706668861333
H	-0.52560769604505	-0.47165970582546	4.63090091379329
H	1.22060402920383	0.55357366066738	4.06947548858721
H	1.26285163022608	0.47321166728619	2.31783498315031
H	2.54852132899281	1.28611841534891	3.20205341870363
H	3.85879220107863	1.61210607078079	1.72602749292123
H	5.58073943921054	1.74490917781523	1.54878129182689
C	4.87842856015935	2.37115541002922	3.47921098646094
H	4.17199890705369	2.06885609897001	4.25186089310123
H	4.65835103215727	3.40331564631313	3.19849064312934
H	5.87537381180709	2.33899944038838	3.92133917137828
H	7.71286474547956	-2.89680339710907	2.42726248697376
H	6.48924572143852	-3.97685602771908	2.97355397332696
H	7.48700582918650	0.83324542923210	1.66000268722762
H	7.91735547439709	-0.80500874524367	1.19863711882638
H	8.24186539023855	-0.23883046321967	2.83421474112119
C	-0.96254609126876	-4.28166124507682	4.46864808597288
H	-0.80500823453721	-5.28804099988755	4.85462165728243
H	-1.57628820045591	-4.37163897408100	3.56738061362942
H	-1.55519544741754	-3.74144995607272	5.20923251162128

40

## BODIPY 16

C	1.55707378139849	-4.23615828551834	4.11241140070730
C	0.28645467446859	-3.61245338597032	4.18267378201513
C	0.40753352289280	-2.25398923701613	3.88562040762278
C	1.79399066243060	-2.06120482469058	3.62215491023709
N	2.44191561134797	-3.29492879248882	3.77741817404723
C	2.51074065543539	-0.91484480760893	3.25169006465357
C	3.90158365584299	-0.96682900605634	3.07950878522395
C	4.83566458131220	0.04710635853122	2.72669195407824
C	6.05315960745743	-0.61993632050131	2.58171700735236
C	5.88689719382487	-1.99329359707445	2.89195097428266
N	4.59820663468166	-2.18043736651770	3.18397745240141
B	3.95989029206022	-3.56132780544199	3.53691505074610
F	4.11217134369092	-4.44256317946563	2.47549726003063
C	1.90445253413490	-5.66271008816735	4.32598459550095
C	-0.68736425746987	-1.23988620616921	3.92785141718144
C	1.77489725668736	0.36307136306160	2.97093570538156
C	4.63380321046265	1.52382936573616	2.65227260195618
N	7.29019578627884	-0.03335094474443	2.15577332775478
C	6.90204568002299	-3.07377080715788	2.90129729252500
F	4.53663206853715	-4.06814527871358	4.69048188114614
H	1.17179640512111	-6.30306530168810	3.83808392738936
H	1.85705829976314	-5.89854420680195	5.39009036319466
H	2.89641013163285	-5.88581022935346	3.94882265458982
H	-1.54733723983750	-1.63554742369628	4.45672628527599
H	-1.03102754867778	-0.98658323670425	2.92128552015141
H	-0.36158790238225	-0.32240526206165	4.41179472549491
H	7.41295868426690	-3.11571280610651	1.93866972044298
H	6.45243551598033	-4.03481218041601	3.12218055039857
H	7.66888447031039	-2.84701773093881	3.64198798527454
N	-0.92321039566197	-4.31391378861026	4.50537933841288
O	-0.81986939474781	-5.36988053595732	5.12009922465451
O	-1.98936587162184	-3.82455661364161	4.14687575012224
O	7.24293916546488	1.04779557773538	1.57731345913543
O	8.32514061321478	-0.65452111649706	2.37187814538522
H	0.78205999893581	0.16363840298470	2.58745455489119
H	2.29683246416675	0.96090168141287	2.23383762348973
H	1.66802811772106	0.96461875716850	3.87766097530025
H	3.87909181061171	1.85756937096909	3.35809144071267
H	4.33274428878279	1.83801766030280	1.64952099493866
H	5.56559389145850	2.03865182787394	2.86682271590047

31

## BODIPY 17

C	1.50540350306627	-4.15594572420523	4.58893280585243
C	0.23757090108594	-3.56155196778556	4.73283731467628
C	0.35505438368997	-2.27939541544736	4.23150734509023
C	1.68514411344555	-2.11925180160527	3.77290809275911
N	2.37220985722825	-3.30464895415384	4.02614203654727
C	2.32036370662535	-1.02749506731505	3.17575321413046
C	3.68059294631286	-1.08780588404300	2.85924495488910
C	4.52089974951280	-0.14502785533121	2.21877715000358
C	5.78170271257035	-0.70201739579903	2.12944428655049
C	5.68573594268567	-1.98195127662115	2.70572925054131
N	4.44117738515231	-2.22027284657825	3.13878599741518
B	3.90093894794045	-3.55783568156581	3.76260827714307
F	4.53931082907492	-3.80114325247217	4.96222482704203
Cl	1.93592837680603	-5.73191567625521	5.06193672414186
Cl	6.94386976197348	-3.11623295612270	2.84753645504715
H	6.67346011715757	-0.27731307043286	1.70338096050694
H	4.21327016675747	0.82118593529837	1.85979800917388
C	1.55904510083716	0.19514008841644	2.85101868567116
H	-0.40986109765434	-1.52250407514076	4.20150516479800
H	-0.62607020958113	-4.03860834626014	5.16126646669313
C	2.00389764499452	1.44717567176725	3.28284323889247
C	1.32494194119486	2.60557034657871	2.93554718754446
C	0.19125523343903	2.51335885300791	2.13909337135633
C	-0.28095570331509	1.28170175489670	1.70841235807505
C	0.40179255254837	0.12856564402422	2.06991784842827
H	2.88346426011019	1.51292726186462	3.90722339616797
H	1.67573149122761	3.56768714311444	3.27972973982497
Br	-0.72126378141853	4.10369885392068	1.61975604887352
H	-1.16373592627221	1.22309618551233	1.08864162254418
H	0.05175750946693	-0.83080817803735	1.71456978196930
F	4.04657758333740	-4.58101231322970	2.84866738765082

38

## BODIPY 18

C	1.27700079638196	-4.30208452406353	4.48183296742564
C	0.04501767216682	-3.64077603023148	4.60661337133856
C	0.25539359763857	-2.34517647410335	4.16304139734382
C	1.60648870225097	-2.24745934953801	3.76256067501753
N	2.21312192593364	-3.47838375650536	3.98461174000169
C	2.33919683499319	-1.17411430121643	3.24262287578605
C	3.70869260590492	-1.30323774483120	3.01346488820053
C	4.60660843413305	-0.39319120264082	2.40042526820166
C	5.83593778592892	-1.00036673635115	2.35360081241289
C	5.70482965257324	-2.29107166597711	2.93494207152660
N	4.41565943417694	-2.46396225414736	3.32262189509909
B	3.74125522686794	-3.78501190820387	3.82715377273842
F	4.23468719355582	-4.13309378958087	5.08042475553932
Cl	1.60174907516985	-5.91972309326619	4.90496332240722
C	6.78668731231597	-3.23060994335487	3.08503026900711
H	6.75368439609904	-0.58518530004679	1.97313967259106
H	4.34944749995907	0.58518911116826	2.03586990728254
C	1.66535627228624	0.09316249944277	2.89512610095275
H	-0.46331881497038	-1.54416247701394	4.13743533092561
H	-0.86036354298029	-4.08172844412897	4.98498541579148
C	2.16242380046934	1.31674040518918	3.35205721421502
C	1.58205617384281	2.51388718870583	2.96134664613904
C	0.49210647403557	2.49164029836072	2.10192262738053
C	-0.04021510782214	1.29029889252671	1.65410800902420
C	0.54660108642136	0.09848086554660	2.05694238011933
H	3.00860767089982	1.32991635506667	4.02411563351751
H	1.97547455447562	3.45430700763724	3.31895656333921
Br	-0.27017302195501	4.13849040323634	1.51872347507124
H	-0.89033239396375	1.28378389957896	0.98731091211538
H	0.15547881269971	-0.83902230683488	1.68622435798382
F	3.92762596102408	-4.78558284517367	2.89246719671775
S	8.17955518389182	-3.05277543576060	2.04905951268399
C	8.99794452038687	-4.33649555722576	2.82634952619345
C	8.24762552779648	-4.88320835026541	3.83160518821955
C	6.98766370321551	-4.26145215042183	3.97938632339144
H	6.25695448559619	-4.53915571086941	4.71989395865108
H	9.97756141134617	-4.63365829096105	2.49029264605203
H	8.58706909725406	-5.70366728374538	4.44644131959585

33

## BODIPY 19

C	1.90877696498989	-4.06772821920634	4.53336014032923
C	0.60087222591279	-3.57240859247230	4.70868091651383
C	0.58761552479085	-2.29053429782378	4.19374837412496
C	1.89189322907257	-2.02394271767371	3.69871436332315
N	2.67195493165513	-3.14805764699937	3.94121554944116
C	2.43867527708830	-0.88491576214340	3.11421129888877
C	3.80988531861220	-0.84330036307782	2.79798059492594
C	4.58080882711541	0.19230536577800	2.21090666405777
C	5.87444722073689	-0.27400080220491	2.09862801748795
C	5.88039207545213	-1.59253507254201	2.59346953643090
N	4.63870004243435	-1.92584563861366	3.01750805852655
B	4.17137479537179	-3.32335451592629	3.54774287224384
F	4.91350575407945	-3.68494962037542	4.66018754305897
C	7.02628478564555	-2.50931694971506	2.63012118961714
H	6.73791355664877	0.23360991065746	1.70535512332792
H	4.20542017821682	1.15389803434488	1.90910619348492
C	1.57970499947559	0.27197073256715	2.80365826391626
H	-0.23535281016904	-1.59702676458905	4.18217345804600
H	-0.21563109904500	-4.10291244265024	5.16742318427406
C	1.90652006756117	1.55188163037918	3.25985983705780
C	1.10551814648033	2.63730078669766	2.93873834060742
C	-0.02256960998098	2.46357894544193	2.14428214230887
C	-0.35476370110307	1.19462894256011	1.68526990794092
C	0.43386337409670	0.10292359117248	2.01999284470968
H	2.77901670720365	1.68714642945632	3.88295443179728
H	1.36664646140486	3.61959154053632	3.30958353944953
H	-1.22572769204765	1.05380097538718	1.05928653979004
H	0.18514611755444	-0.88164882994951	1.64819672822550
F	4.27740827951635	-4.27276737865089	2.54258021347681
H	-0.63757533236795	3.31394547930028	1.88161212774080
H	2.31793465871720	-5.02559246287476	4.81046924617418
O	8.12462681049175	-2.17245593223631	2.24602692243569
H	6.83217391438879	-3.51762835455413	3.02570583626614

47

## BODIPY 20

C	1.70232661102332	-3.68575746721249	4.45999065879912
C	0.44529240503310	-3.06274501040218	4.63625267709444
C	0.59411410192735	-1.72759173177779	4.24803692082844
C	1.94820949569223	-1.57373800362411	3.81681771938958
N	2.59073596993890	-2.79375666979511	3.98343897178593
C	2.59007405381835	-0.51759331586401	3.19204524082191
C	3.90219181054191	-0.61235644047406	2.75400478664180
C	4.74015316712179	0.31724528832190	2.06973677121574
C	5.99980959599698	-0.28561830111364	1.94808341271676
C	5.90284865163154	-1.55994697423289	2.54876379689313
B	4.10153125706435	-3.04381655979695	3.67991084846887
F	4.79140602383025	-3.30041769017265	4.86404938250462
C	7.20602842495646	0.26832654384524	1.26171571113893
C	-0.42390041363218	-0.69938118358951	4.27828946633976
C	-0.77731394220833	-3.73593620874709	5.16621330493003
F	4.22922970967987	-4.11635619060806	2.79758046947168
C	2.03503461168231	-5.10542917920487	4.75162927399845
C	6.96062415953135	-2.59523151874532	2.68271366980846
H	7.88322822708691	-2.26797245595621	2.20906337878074
H	6.63842133449161	-3.53365970191668	2.22986014106071
H	7.15867479335435	-2.80518062698451	3.73535278245354
H	3.08318245698370	-5.32042381134296	4.57118818970475
H	1.43549653162416	-5.76709902569838	4.12213028986775
H	1.79403363794316	-5.34821918549399	5.78942848478073
H	-1.42916166011079	-3.02057961862527	5.66851901436421
H	-0.51865530134870	-4.51884289525166	5.87992598881136
H	-1.36050121348293	-4.20883401454709	4.36994592989623
H	6.91726339647280	1.00965063684268	0.51731739115407
H	7.76882298431849	-0.51550604293378	0.75359352077903
H	7.88903187810115	0.76052860896403	1.96071243337655
H	2.04712410214059	0.40120565339503	3.02842789578437
C	4.35120655937031	1.60737149054531	1.54126289457355
N	4.65120004370891	-1.74960895293371	3.01138589614153
S	2.82849572642927	1.83240454534515	0.72879305675075
C	3.17353979169890	3.47636932233230	0.38779800618739
C	4.40124782083123	3.84077694909918	0.86212455917510
C	5.07285455038995	2.77788766311108	1.51430605800792
C	-1.76151890303597	-0.80664995906263	3.97518475498965
C	-2.47333093404565	0.40996949040858	4.12175046937916
C	-1.68027911743026	1.43690582255598	4.54730183952067
S	-0.05978085555591	0.92486362777268	4.78242571967193
H	-2.20725422927702	-1.72553318362984	3.62628912467204
H	-3.52658509272573	0.52420550235596	3.91010917735460
H	-1.96262850889318	2.45872811365142	4.73992253626365
H	6.04533933562945	2.87225513429708	1.97309286134160
H	2.45719689046008	4.08505195235236	-0.13831852943321
H	4.81187006124157	4.83380557454152	0.75023305174194

61

## BODIPY 21

C	2.00070404783742	-3.97179366570947	4.64016436298528
C	0.77218465624935	-3.29563309224190	4.81155443348784
C	0.94224893926366	-1.97346195494903	4.42564488581151
C	2.28676579297822	-1.87799827758030	3.96312940623028
N	2.91696484829169	-3.10226858199077	4.14347537242233
C	2.88723629847194	-0.88250131862684	3.22081329161342
C	4.14596554122564	-1.02524945779371	2.67076599321894
C	4.88944190564003	-0.08267230739334	1.90738310371472
C	6.14815713225329	-0.63481697209442	1.74943165533996
C	6.16360984889858	-1.90583956933222	2.37099557435987
B	4.42690066091031	-3.36439315691633	3.78398774964350
F	5.17945295594225	-3.43136545923248	4.95708596515726
C	-0.03697496010724	-0.88951672522720	4.46263676390208
F	4.49754337828652	-4.55244097286041	3.06255571714059
C	2.22487997651659	-5.38655102372743	4.93429651512046
C	7.34900386237413	-2.76564620833711	2.38222831597499
H	2.34557264608187	0.03171277715336	3.03748431902664
C	4.39053189720608	1.19348748412828	1.39403578515160
N	4.93709305013881	-2.14491120593125	2.91446992926130
C	3.41444137888965	3.65805141020050	0.47201139587714
C	4.69891738348409	3.56432968785001	0.99549781343018
C	5.18176261328161	2.34686968203227	1.45179753907165
C	-1.39324711537304	-1.14883239550652	4.23084657407105
C	-2.32659211372602	-0.12326123985416	4.25331451489340
C	-1.92622919492429	1.18446489386044	4.50822394096896
H	-1.70769122682316	-2.15953627895355	4.00645876678121
H	-3.36886331180004	-0.34258344129605	4.06059627203628
H	6.17234689175322	2.28659046966211	1.88243821418798
H	5.32316040912595	4.44629979936018	1.05991615668111
C	1.20565167285265	-6.29674304939460	4.62490223682100
C	1.36589026956142	-7.65209278238676	4.86457246291699
C	2.54329674089392	-8.12269063525938	5.43474045332588
C	3.55122586907801	-7.22447486887511	5.76558854188308
C	3.40010311926220	-5.86924836064929	5.51832747087705
C	-0.58671559698515	1.45516340574300	4.75673431596394
H	-2.65441844955358	1.98473588821151	4.52064538306076
C	0.34731691239201	0.42934487172599	4.74129937646282
H	-0.26677249742450	2.46534168318241	4.97693676082258
H	1.37938647442587	0.64494207437359	4.97976614769611
C	3.11066624213771	1.29703455339197	0.83530064489711
C	2.62639565722947	2.51693651440567	0.38693774827507
H	3.03390856373330	4.60918527031840	0.12348771663482
H	2.50440126745593	0.40823861990042	0.72628777420914
H	1.63302524510423	2.57467436092076	-0.03791039385980
C	8.60218604345189	-2.13134650998845	2.37555554412915
C	9.77551537729910	-2.86426640623160	2.32339928110147
C	9.72727742949520	-4.25330220968827	2.27242973961758
C	8.49504874069335	-4.89433771633164	2.27692527493300
C	7.31524800860497	-4.16446659926779	2.33194253035125
H	0.29761913289917	-5.93545255069936	4.16103403012469
H	0.57522865573044	-8.34093324373093	4.59696487174761

H	2.67502417086929	-9.18053367359371	5.62252978761616
H	4.46688062187350	-7.58338410966623	6.21656396124471
H	4.19080969840224	-5.18269169370648	5.77539465959411
H	6.36900901253299	-4.67789390730246	2.32038786462952
H	8.65221463339046	-1.05250723510827	2.43376141436974
H	10.72797403815384	-2.35038977593115	2.32600498699914
H	10.64220805852888	-4.82934707697569	2.22660579685967
H	8.44627011084911	-5.97468912380806	2.22824999331100
H	-0.11253374352751	-3.73358535113791	5.24097997329312
H	6.95967032824249	-0.21950326113319	1.17833332252999

53

## BODIPY 22

C	2.01742514978591	-3.83157376452815	4.93112078681948
C	0.72242815468536	-3.24871116297624	5.10543646796779
C	0.80864487669820	-1.89883412595415	4.67047913579403
C	2.14441611256197	-1.70893804413252	4.21008112576757
N	2.83808462491680	-2.90181339076577	4.40115675436840
C	2.73021246871693	-0.64818101559672	3.55041013400406
C	3.97835340080158	-0.72881781695272	2.96673847454753
C	4.71499352794279	0.23831217426892	2.22607218830582
C	5.91528239737420	-0.39824321459035	1.81446390276729
C	5.87989418087312	-1.73351529070176	2.32166834234656
B	4.36087124338002	-3.07136143170098	4.01079560311198
F	5.15682944179993	-2.89342753564801	5.13646894632212
F	4.53366242001059	-4.31780152520613	3.44838422076467
C	2.39750442559418	-5.19629920374789	5.29017861262965
C	6.93562582896784	-2.72995644148446	2.13987020975219
H	2.17054641470954	0.27051054061111	3.44098613835529
C	4.45989464997308	1.56772539556167	1.87062743202940
N	4.72283960680563	-1.90970614672662	2.99607741277496
C	1.55403510681973	-6.25669033246205	4.93669824059740
C	1.88120419848606	-7.56125790738635	5.27523545886943
C	3.04848368318000	-7.82581795545207	5.98273172361502
C	3.88522309432348	-6.77708971995090	6.34752979918264
C	3.56750627083693	-5.47276756412035	6.00549606705985
C	8.26341505045902	-2.35436155334768	2.38157802008980
C	9.29769474244408	-3.26145085128996	2.21144215473334
C	9.02508415501700	-4.55430532113566	1.78101949933587
C	7.71392282628452	-4.92770871081932	1.50944253322033
C	6.67617755125920	-4.02481645970169	1.67999476292693
H	0.65911053840364	-6.05765051087058	4.36395217447674
H	1.22964122815564	-8.37196727865119	4.97659425724707
H	3.30815296650392	-8.84237953448912	6.24850332395403
H	4.79429461792377	-6.97611631134133	6.89878217117677
H	4.22430021154587	-4.66415195938521	6.28821874114278
H	5.66257903925964	-4.32120896146603	1.46357399255279
H	8.47548835834855	-1.35715859843956	2.74091587086257
H	10.31451065823559	-2.95947274434329	2.42572797692690
H	9.83042055470119	-5.26554566875132	1.65245915484400
H	7.49540511401512	-5.92768365562830	1.15882110965900
C	6.84232228019532	0.28610975904720	1.01425555504989
C	6.57453838683081	1.59344998228548	0.67033902089704
C	5.39168964009606	2.23140548730426	1.10020345395413
H	7.74411192399974	-0.20292402848883	0.67366044867770
H	7.27871139737298	2.14315840966284	0.06016894173944
H	5.21172687079456	3.25870734659672	0.81125040806446
H	3.55548858288932	2.06707457923672	2.19419472611044
C	-0.31044149369176	-1.06157535162794	4.73943576428294
C	-1.48871105014941	-1.57925741868344	5.23635545706372
C	-1.57459553454500	-2.91606979323394	5.67513595239390
C	-0.48016760286228	-3.75192293052470	5.62160937570971
H	-2.51209389386552	-3.28558814065101	6.06869309879678
H	-0.54808846364169	-4.77070218334465	5.97571254003230

H	-0.25718473299959	-0.03119407588101	4.41235443283756
H	-2.36526520222417	-0.94729804239498	5.2982579034879

27

## BODIPY 23

C	0.73814223941048	-3.21260331847515	4.79939760790038
C	0.81917807301338	-1.91052020043946	4.31593413437432
C	2.13624559278085	-1.72318510508005	3.85409425074077
N	2.84050880906487	-2.89621933800621	4.06995289136913
C	2.73826567364240	-0.65839290299159	3.18400845639405
C	4.00760197566600	-0.73922262749626	2.67194809942963
C	4.76327108510551	0.18406707716250	1.87885096264092
C	5.97239431098808	-0.46891839547784	1.52778470048492
C	5.91017505591672	-1.75441966748141	2.14435046229339
B	4.35428377835773	-3.10280570768719	3.79953694959900
F	5.08971113291095	-2.94935096718754	4.96360281141571
F	4.56339304110986	-4.32827621918061	3.20394952819744
H	2.17043230525710	0.24775326839082	3.02098902936070
C	4.52581664254483	1.49065294632781	1.44538191527263
N	4.77276292018558	-1.91002227098533	2.80985785207426
C	6.93447804684743	0.16138855742350	0.73331390831735
C	6.68026414148158	1.45075740024335	0.31109896532931
C	5.48607994605797	2.10754103140922	0.66630642943864
H	7.84987948662933	-0.34637158290736	0.46225905716000
H	7.40674933115118	1.97024175172061	-0.29899188105406
H	5.32020880798781	3.11962814491109	0.32113958094556
H	3.61837000522540	2.01294627124424	1.71979412898838
C	2.00436626587068	-3.78697211118723	4.63163967201081
Cl	7.12176017233830	-2.94051160908915	2.07031279672923
H	-0.12479653943384	-3.70228330603316	5.21682180268849
H	2.34620694209763	-4.77673607330398	4.88395344467754
H	0.03275075779218	-1.17459504582359	4.27118244322146

45

## BODIPY 24

C	1.26884432097849	-3.40334708788242	4.88009654149870
C	1.22466211139288	-2.21174837933957	4.16296899303339
C	2.55451629706944	-1.95967998221524	3.74177087908932
N	3.36679415538631	-2.99384690593852	4.19561704176469
C	3.09025154699702	-0.91524803131585	3.00361329495921
C	4.41770037213282	-0.88854441283839	2.63172044785064
C	5.14324412343279	0.03994167912285	1.81898606808681
C	6.44269480109693	-0.49812540891549	1.64881275965459
C	6.47593020226856	-1.73247895384047	2.37945631537131
B	4.90083570126174	-3.10397595024364	3.95677783288431
F	5.59476533050640	-2.92502874591952	5.14800380931754
F	5.20463933113095	-4.32830968296093	3.37814810007206
C	4.80579897303046	1.25610823467525	1.21910432810525
N	5.27528072428732	-1.93070538845384	2.95968333358263
C	7.39532560775078	0.15339378651805	0.86083239662768
C	7.04292831632119	1.34807298702213	0.26661054948571
C	5.75774285746258	1.89504026349452	0.44880303535865
C	2.59921152933653	-3.85939521633162	4.88888839799839
C	7.54024292332962	-2.62831302335038	2.45445071036958
C	3.15114322211269	-5.07904206503886	5.53439213804305
C	0.02977590012007	-1.36572618527398	3.87422497266233
C	8.45919634447453	-3.41371384298856	2.44872196297179
C	9.45464331354387	-4.41763982168402	2.44048736788746
C	10.79545337547744	-4.11316719511018	2.16517587362277
C	11.74717421634056	-5.12012576594159	2.15100493014869
C	11.37642041982877	-6.43769091892381	2.40087273820649
C	10.04748465571042	-6.74801446153009	2.67219684210933
C	9.08879204266361	-5.74894292314917	2.69709809721023
H	2.37713436717722	-5.58797736907496	6.10612733298517
H	3.97633121795135	-4.81950678562750	6.19993598270931
H	3.55390792856915	-5.76310732986355	4.78529574772075
H	0.27024931552116	-0.53774594879236	3.20831609226409
H	-0.38836666406509	-0.94173564077634	4.79071243007728
H	-0.75860102509682	-1.95453424958294	3.39973628581927
H	11.07599931922132	-3.08770769912428	1.96671007341957
H	9.75704940789918	-7.77213427278062	2.86651592423921
H	8.05302426925716	-5.97512975973184	2.91000282548882
H	12.78036049186734	-4.87800957180239	1.93908728243546
H	12.12211416162873	-7.22149275594450	2.38377728830008
H	8.38014597676155	-0.27223658654685	0.72168354977031
H	3.82535131414424	1.69321531611270	1.35895926299697
H	7.76018833634697	1.87702919014673	-0.34662477846062
H	5.51524870958971	2.83753411367822	-0.02427669163814
H	2.44586402207760	-0.10995095461674	2.67987049458122
H	0.44173613570446	-3.90632629731945	5.35503113931868

33

## BODIPY 25

C	1.08250774440266	-3.75250347933901	5.01476906039169
C	0.95675836871485	-2.51721944241062	4.42486638738856
C	2.28490905224891	-2.19821643456706	3.99249561816679
N	3.16132517970847	-3.22924654046657	4.34653500035613
C	2.74662857956644	-1.12054707499567	3.25161684954146
C	4.05914536863795	-1.05082402534121	2.80814136324907
C	4.68249920667052	-0.09225438076558	1.94724870522149
C	5.95682405935238	-0.57708163950166	1.77071845949754
C	6.11339657744745	-1.77216511789975	2.49817997961571
B	4.69410730293320	-3.25449094412508	4.09274672986014
F	5.38769468244324	-3.08418393786868	5.28896980074942
F	5.05007786924456	-4.45468614046602	3.48710012580103
N	4.96759808286015	-2.06543120610024	3.13047783965582
O	7.11343561247195	-0.27988788424635	1.10844794880242
C	2.42696798135419	-4.16723398353959	4.96020373214995
C	7.43819800119458	-2.22452063280419	2.27193142239844
H	2.05688948819691	-0.33545790568865	2.97363828338924
H	0.08616696085820	-1.90174719038980	4.27678177117515
C	2.49137715512089	-5.45080636990518	5.55791138465440
C	1.20649497915846	-5.73751318534388	5.92666661504423
O	0.32153065203458	-4.71771930693728	5.61077225361592
C	0.61434723799481	-6.92548405452336	6.57508272631969
H	1.39679162305580	-7.64171079897274	6.81797744630796
H	-0.11305056381126	-7.40769480875837	5.91712485400685
H	0.09263001510674	-6.64793704917548	7.49389333461250
H	4.20946324069343	0.78463016942696	1.53983922979472
C	7.99410554697681	-1.29871729605044	1.43469848402613
H	7.92694686945851	-3.10183231339582	2.65581094161851
H	3.34703928337633	-6.08857296779173	5.69310837543496
C	9.33931390173781	-1.21684868040419	0.83105198454820
H	9.78853066645300	-0.23834478089338	1.01767407615049
H	9.29497318660236	-1.36521218594038	-0.25221953001230
H	9.98266608773512	-1.98393841081907	1.25672874646767

29

## BODIPY 26

C	0.46941413928578	-3.78463240394182	5.08288450084464
C	0.61748989759035	-2.47984946051095	4.61750388507503
C	2.00454922225487	-2.34207730212054	4.15712782216499
N	2.65859663385269	-3.52186426776622	4.38886577831290
C	2.58339332060917	-1.27919393913322	3.53986358550180
C	3.90592014857291	-1.35571397554112	3.01369958178265
C	4.46215145056609	-0.31508282045534	2.24727651827723
C	5.71685473979997	-0.44821529141535	1.70188054381887
B	4.16646211102661	-3.70553021466439	4.18332549708588
F	4.87271877606710	-3.56165283745246	5.36735858559682
F	4.47641105678892	-4.87202323609581	3.51919824074180
N	4.64019576646446	-2.48176515879161	3.22075975508666
C	1.78754656833402	-4.47223541936209	4.96654532240415
H	2.01654857502328	-0.37810682472130	3.36483199856947
H	3.87418704449546	0.57711701801352	2.08621069651792
C	5.86213027606219	-2.61485263918172	2.67345041459210
C	6.43574664404032	-1.62923951722170	1.90952298916528
O	2.07862886142378	-5.59323330185261	5.29545063396203
C	-0.45111534948636	-1.59707844346943	4.63079417550210
C	-1.67382666114430	-2.06280273281673	5.10704564372109
C	-1.82202998408709	-3.37710035182057	5.55285000380670
C	-0.74200412437838	-4.25617397267452	5.54868350324106
H	-0.34892281587572	-0.57797791689871	4.28179972632727
H	-2.52556778775409	-1.39563336746081	5.12939365937693
H	-2.78550888536596	-3.71282787167381	5.91260793574576
H	-0.83841265404229	-5.27522933496504	5.89771062470614
H	6.35630864238044	-3.55299552568821	2.87742077336689
H	7.41775573448165	-1.77834084958251	1.48747615107905
H	6.14141865301414	0.35220195926508	1.11034145362677

35

## BODIPY 27

C	0.50722071357042	-3.84382879314285	5.09235140790198
C	0.67673561978393	-2.55484803042668	4.59162960867386
C	2.06255974765780	-2.45867013585490	4.12091651603027
N	2.69668115186401	-3.63450325255592	4.37848675962544
C	2.67309873614798	-1.42874896604163	3.48113201541565
C	4.01284373510326	-1.52601543563755	3.01246055789239
C	4.55035825350792	-0.42737390325374	2.28612607962024
C	5.80820242447879	-0.48040294895055	1.78682122652657
B	4.17621434928352	-3.91275766343595	4.07420146069067
F	4.91260557218178	-4.00352898935910	5.24473763339963
F	4.29906968055653	-5.03861843941535	3.28052279211394
N	4.75452330350809	-2.63244435029759	3.23147237540953
C	1.81106033941580	-4.56074205106682	4.97774179854412
H	2.13108851903019	-0.51942244418427	3.27398504263881
H	3.91848601781252	0.43589631440332	2.13496391580586
C	6.05151783922177	-2.70965873319077	2.74157137889383
C	6.60365905945014	-1.63144486753723	1.99793880805736
O	2.08098553466454	-5.68301218716665	5.31773518300570
C	-0.37049316543613	-1.64766210821133	4.59323706215645
C	-1.59827842022602	-2.07395451625434	5.09330889453879
C	-1.76930926155409	-3.37273068359988	5.57458940168314
C	-0.70859831296383	-4.27558694295384	5.58362486599738
H	-0.24810740751940	-0.64030853551038	4.21759498747532
H	-2.43537151921397	-1.38824190165496	5.10650341985704
H	-2.73586103686256	-3.67835198496029	5.95235685391078
H	-0.82418123640764	-5.28245486953324	5.96083630865386
C	7.91380008466405	-1.72425061289357	1.48844188678482
H	6.21898067545626	0.34859221033728	1.22407910563443
C	8.67035454940960	-2.84599529063247	1.70699828823284
C	8.12930798017127	-3.90439722419745	2.45416922660410
C	6.85493805299863	-3.84533317083720	2.96659897023764
H	8.72502119372451	-4.78898107633653	2.63625534880372
H	6.46770520260883	-4.67463305302555	3.53083590329020
H	8.30632923257938	-0.88942734161897	0.92122855342711
H	9.67232279133214	-2.91928802100307	1.30714636246651

26

## BODIPY 28

F	2.49200201080097	18.35920072504191	7.25114780316532
F	0.95785798181672	19.52811727899300	8.49004090358869
N	1.69631890740228	20.47898876998016	6.42202568819178
N	3.23392212308473	20.33380763608147	8.42604077624248
C	4.05889854506519	19.57551537688938	9.18944777095254
H	3.90771415551297	18.51017762748504	9.10369718189978
C	3.33089130150267	21.69673862289898	8.42251085471426
C	5.00432765349016	20.12467468297692	10.00701388148980
C	0.53800473809890	20.53949138379136	4.34282705380811
H	0.06258139008008	20.00615561074330	3.53404224318141
C	2.53068246161682	22.44346391067564	7.52060514471258
C	4.27503576787816	22.29982342876431	9.28944753271652
H	4.34668177628944	23.37773320956210	9.30391513482296
C	1.80161843025874	21.83939409434710	6.46400003276320
C	1.21035015504368	22.58420806643744	5.41517149011821
H	1.28067193600904	23.66151976317398	5.44830266450416
C	0.58675597027544	21.94514224482772	4.37830395909528
H	0.13861213742187	22.52390340166192	3.58166887347947
C	5.09684929685988	21.52729987979665	10.06336624235145
H	5.82456875378659	21.99886612641392	10.71052190690881
C	2.58355149121930	23.85389382549285	7.57542471333487
C	1.09588020503217	19.85201474478259	5.38160704839436
H	1.08495268528409	18.77440086167963	5.44602533699813
B	2.06832539621758	19.60814224744572	7.66705419712754
N	2.61921099333715	25.00909266632165	7.60879014287314
H	5.64546373661539	19.48882781373526	10.59807142256515

63

## BODIPY 29

C	1.86303277920036	-3.89491247125749	4.74925185745860
C	0.60948190523164	-3.24446901591155	4.85062730009639
C	0.76277271726092	-1.95023286400994	4.37008102561631
C	2.13234401145477	-1.82471198183845	3.99201485200130
N	2.78524727556073	-3.02866887737217	4.24532512067930
C	2.78385986979228	-0.76010778199258	3.39561890010095
C	4.13736136074995	-0.79085453189891	3.11850360822722
C	4.95555996092650	0.11227232535387	2.36976083165817
C	6.24276541889074	-0.41574791816047	2.40481054005165
C	6.20149578029135	-1.60062134788088	3.17996620392460
B	4.35599207902806	-3.09188024054981	4.32678537530612
F	4.70494054432611	-3.06952633811748	5.67866721466832
C	7.50869877244613	0.01735150069139	1.74448206270415
C	-0.26982688717091	-0.94023277199711	4.27567513671109
C	-0.56558624598179	-3.92277898980903	5.46943454954537
F	4.87437599215926	-4.21715651364649	3.69679737572163
C	1.98886734311427	-5.29920304343979	5.11926885524346
C	7.41231439477766	-2.35797571455783	3.45605524101338
H	2.20907548846663	0.11176108897379	3.12264583870061
C	4.53269985909565	1.31003231827379	1.67414100055494
N	4.92845553975927	-1.83132830363824	3.58712875322156
S	2.99297267450279	1.42893665679887	0.87100474538706
C	3.32322331910178	3.01736115087655	0.31560609266740
C	4.55979799080707	3.43956371750386	0.71175801847633
C	5.24792903028378	2.47009245720693	1.48103645028231
C	-1.58317755522098	-1.11172438703555	3.90691792723487
C	-2.33658986970736	0.08785617636323	3.93485940089602
C	-1.59836132228259	1.16459334324345	4.33576444660426
S	0.02039097525647	0.72168573639647	4.69265681163753
H	-1.97772809811033	-2.06660955871149	3.59344207117149
H	-3.37860279879475	0.15333966103594	3.65761312037453
H	-1.92047691722583	2.18712504114823	4.44385828110953
H	6.22778297806094	2.62638539521168	1.90569778586559
H	2.59355503010554	3.54869999677949	-0.27275523875745
H	4.96509041786366	4.40922276627153	0.46204648848183
C	8.33372830883394	-1.22500304343881	1.39127178964695
H	8.08994767436865	0.66239616706231	2.41477189316241
H	7.29414602081516	0.60331337797451	0.84966691899477
C	8.49808509674541	-2.14434604526911	2.57574319603534
H	9.31159048763924	-0.93807274643924	1.00215227876713
H	7.81693839399437	-1.76715856981560	0.59067352394614
C	9.69613278681359	-2.80667742756251	2.80785201156825
C	9.84454062258023	-3.65699961336495	3.89771451797743
C	8.78394241034221	-3.84960017436729	4.77362500781312
C	7.57510653042711	-3.20862498474293	4.55599960267605
H	6.76311385630278	-3.35101281537751	5.24996867026108
H	8.89847038316649	-4.49670552456191	5.63284625657469
C	0.99789705610824	-5.80447783086482	5.99548888110028
C	-0.04845247225055	-4.87516339913023	6.55235435784898
H	-1.12898505657356	-4.49223909616591	4.72042050080911
H	-1.24914082703684	-3.18475566576224	5.89200480125379

H	-0.86432984776540	-5.45053594133348	6.99072460141927
H	0.39718667261761	-4.27563267454827	7.35472561413194
C	2.94118232388842	-6.17719947624430	4.59060697782078
C	2.93313066107416	-7.51991091704615	4.93771881889749
C	1.97280350184560	-8.00993723400349	5.81364666016636
C	1.01008487558223	-7.15097514432544	6.33157265496233
H	3.67734738844752	-5.80788152225283	3.89838654270604
H	3.67502732810851	-8.18348613836967	4.51364248690716
H	1.96488159346627	-9.05703566918924	6.08791880363138
H	0.25027426772978	-7.53280795226655	7.00276447157781
H	10.52621923131067	-2.64600916512452	2.13019896065038
H	10.79007691739842	-4.15363745377362	4.07264115405708

61

## BODIPY 30

C	1.30534794341728	-1.50310506262165	3.31896908449026
N	2.01188938649081	-2.55962808968032	3.87896387958868
C	1.98624281781945	-0.36955493004755	2.87160718578807
C	3.37978436249610	-0.31438015807902	2.92978586384426
B	3.52421862385512	-2.69835201358163	3.94238999066254
N	4.09988295450160	-1.42378159305374	3.35167648000413
C	5.39436472743619	-1.35215415633902	2.99776455558692
C	5.61786985307803	-0.04509258243683	2.44765201360497
C	4.34461621465631	0.60633632476014	2.40055976945151
C	-0.07893337007354	-1.75739837584181	3.60137781221683
C	-0.13168146444969	-2.93173489924528	4.41761305328506
C	1.22056566722011	-3.37011548706245	4.60098186082616
C	1.22064415417196	0.78016456337533	2.32101365375060
C	0.80471432391154	1.81995515143155	3.15066036768833
C	0.07859723416334	2.88578622797398	2.63257110090897
C	-0.23291189737487	2.92392652218413	1.27804254408356
C	0.18303193506149	1.89205046613645	0.44480012837811
C	0.90255753649343	0.82240270838319	0.96420935015880
H	1.05186974027478	1.78904347212414	4.20357624961105
H	-0.24689082257983	3.68352021026532	3.28731873123323
H	-0.79641178819598	3.75393819722641	0.87245818284563
H	-0.05986893795340	1.91761832926406	-0.60962180749543
H	1.22724764450193	0.01662371071960	0.31895140290001
C	-1.26221837098293	-1.07939331283782	3.28038203164480
C	-2.45732058962176	-1.56704111018856	3.76969775929188
C	-2.50586208782171	-2.70809548253223	4.59150113916962
C	-1.35305673307367	-3.38824994108034	4.92582184464307
C	6.76076268652251	0.60660967512451	1.96884736482128
C	6.63563407237331	1.88886432426707	1.47526646953769
C	5.38479470515879	2.52904887757084	1.43262386509256
C	4.23883775907903	1.90087982625964	1.87756226140484
C	6.14914214610135	-2.58000045276860	2.99144824131619
C	1.85680861663515	-4.26157022090520	5.53677680172628
H	-1.24361120324085	-0.19424207533725	2.66267327317508
H	-3.37855807422137	-1.05767755570673	3.51808866687632
H	-3.45911143706419	-3.05382885116272	4.96861813955300
H	-1.39910195762070	-4.25203500977308	5.57253507910116
H	7.72753907974001	0.12653574039289	1.98809427077915
H	7.51147703620463	2.40939246150777	1.11137620531743
H	5.32015554496449	3.53429925446823	1.03777913578854
H	3.28459721452118	2.40326904546454	1.83106890522712
C	7.54154578498338	-2.64368093346234	2.83205063351294
C	8.18611388277146	-3.85436378275084	2.66742141167954
C	7.44156991488800	-5.03558997553323	2.63594876848325
C	6.06678577080879	-5.00691920555495	2.79110032700379
C	5.40531476676759	-3.79597087468542	2.99527574774788
C	1.21226200503545	-5.33990158409494	6.15821090989930
C	1.83398202229205	-6.05979183216978	7.16031760031401
C	3.11725883213456	-5.69849507389392	7.57448115476757
C	3.78353429601419	-4.64434207877980	6.97176822636362
C	3.18311583476594	-3.93112061620485	5.93567439977566

H	8.11633582285998	-1.72963822677136	2.85002568777988
H	9.26118051405484	-3.88563091303524	2.55287457603708
H	7.94239318197342	-5.98485640777123	2.49536180666337
H	5.47617348747132	-5.91271856768002	2.77851423321044
O	4.07240925990507	-3.80967226709601	3.15941977244142
H	0.22460190579413	-5.62326631627841	5.82448534467586
H	1.32764285549674	-6.89668403230052	7.62111760825109
H	3.60696083946928	-6.25796097287328	8.36086444244548
H	4.78327476938516	-4.36282020166235	7.27192167901115
O	3.86186900655323	-2.92668986601942	5.35231276205841

30

## BODIPY 31

C	1.05676157344097	-1.65750408411180	3.40258074194017
O	1.88558654883533	-2.57975998456195	3.84106157176067
C	1.50756911385560	-0.56233607646050	2.71256480760818
C	2.89548342660168	-0.33078712920070	2.54599728817981
B	3.27442243341245	-2.71184421417798	3.39278501890087
N	3.78786862360639	-1.25417719633043	2.97201601523300
F	3.36509101619027	-3.47878867186477	2.24374296983354
F	4.05195125953184	-3.17939204960635	4.42548407132480
C	5.10572185192347	-1.00264155565932	2.91147672975257
C	5.58465840608070	0.16984843463091	2.37326018841344
N	4.71793572339863	1.09561472661763	1.90050219703084
C	3.43326194034082	0.85587484200719	1.98982367341011
C	7.04986746529029	0.44236972120102	2.25535165765534
H	7.63080744829476	-0.23278579949106	2.88121576754318
H	7.26979183337286	1.47055163138446	2.54410384759793
H	7.37786233066948	0.30951386580086	1.22104864305730
C	-0.34723883418614	-1.87408933393407	3.78691609688004
C	-1.40535162456587	-1.18861657415751	3.17976576416147
C	-2.71320200408801	-1.43345746149851	3.57050284916461
C	-2.98325120847801	-2.35533992829357	4.57815552782102
C	-1.93659518875941	-3.03166203592851	5.19384651063627
C	-0.62946868995322	-2.80217181117724	4.79475171995739
H	0.18841774929943	-3.33052135222674	5.25993981430951
H	-1.21317518723720	-0.48349622677697	2.38240681827063
H	-3.52492287277183	-0.91002338473423	3.08346922284495
H	-4.00375430762151	-2.54660823243796	4.88397247508381
H	-2.13853639833462	-3.74268671600276	5.98403790061568
H	2.75228972404987	1.61302728323193	1.61677156385963
H	5.75101497772291	-1.77995811164059	3.29325902862254
H	0.82207287007809	0.19980742539951	2.38163951853068

38

## BODIPY 32

C	1.14843156713015	-1.49822889819573	3.41438142888198
O	1.95938372201244	-2.43905836752058	3.86110920463403
C	1.64272553109330	-0.42905406608381	2.70160901943798
C	3.03482884949157	-0.26385904252528	2.52262263149737
B	3.27785533101737	-2.67696212044195	3.27240874627929
N	3.88580833518561	-1.24655793751268	2.90468174436245
F	3.16586008029754	-3.37559930286517	2.07992022664080
F	4.10843099478004	-3.28884599192785	4.18119736676803
C	5.21503136104595	-1.05349405353408	2.86003963806491
C	5.74975614295399	0.11532890746719	2.37382839956456
N	4.92707746762842	1.09359364840515	1.92258703619189
C	3.63341337502254	0.91203734415825	1.99993946441418
C	7.22574913464804	0.34016537844083	2.29342414651518
H	7.77436760773608	-0.43304953946561	2.82910818013419
H	7.48617522053878	1.31129164714948	2.71711811839344
H	7.55764627161631	0.33746665688032	1.25284117488721
C	-0.24820331280448	-1.68270423639209	3.79028344898641
C	-1.30223748745658	-0.95412302095227	3.22562748392169
C	-2.61730826200204	-1.21559406633223	3.55599173549271
C	-2.94386502250927	-2.22924829894501	4.48275265767982
C	-1.87736715969742	-2.93167157683749	5.08116456611319
C	-0.57259898514019	-2.66767599566724	4.73336873639837
H	0.22712170768883	-3.22802968278128	5.19274311712097
H	-1.10108468955986	-0.19597626522439	2.48009116374665
H	-3.39731717605006	-0.65743998348764	3.06241924195542
N	-4.24361565450061	-2.54775096355827	4.79053632804258
H	-2.07718492130402	-3.68787779475032	5.82502527647099
H	2.99091533411093	1.71134814995218	1.64679630489260
H	5.81963509530870	-1.87484713642172	3.21515316296072
C	-5.33686878930299	-1.80655621950530	4.19927684727522
C	-4.53699399008888	-3.86401181507917	5.33548934832462
H	-5.45819472256439	-2.01495187251024	3.12710789872282
H	-5.18807832218699	-0.73373137128425	4.32921356605680
H	-6.26070558466640	-2.07261276934929	4.70758956989324
H	-4.34753642964891	-3.91890283245208	6.41226775942587
H	-3.93586042593978	-4.63344044842610	4.84555720535308
H	-5.58557808876657	-4.09462297789591	5.16067942607173
H	0.98949589488285	0.36083691547165	2.36969862842697

50

## BODIPY 33

C	1.63254467409749	-1.77330820980211	3.68910106611491
O	2.47563197738855	-2.11571018805438	4.63240338393598
C	2.06501935483612	-1.24693461128790	2.50131656257687
C	3.44642920908009	-1.03121359187659	2.26452572375952
B	3.91906602858873	-2.44034948187313	4.37565642208166
N	4.36770821286710	-1.51261588976559	3.12996236410282
C	4.05862295354361	-3.98264433475300	3.93285108759737
C	4.76788951390489	-1.98484931799201	5.66121042479259
C	5.67177951321026	-1.31039076250220	2.89488473204008
C	6.11030600771675	-0.62886554265142	1.78174345688117
N	5.21297593855207	-0.13462904733219	0.90028450324283
C	3.93833916335400	-0.32495132978492	1.13951793943048
C	7.56661503069870	-0.41108344501745	1.52366882133567
H	8.17814141198263	-1.00141019065945	2.20425446373985
H	7.82672955013484	0.64147455083591	1.66020546097916
H	7.81803969915800	-0.68542030220477	0.49829026226514
C	0.21606497795480	-1.99374783267988	4.02288868516075
C	-0.82796027310879	-1.35836939124948	3.34174651150464
C	-2.14698462641151	-1.62593656601159	3.67607641678030
C	-2.44334875124150	-2.53584967357708	4.68765222832695
C	-1.41130747508091	-3.16806858671036	5.37131074605542
C	-0.09183524863139	-2.89601112298495	5.04548944966561
H	0.71791268010240	-3.38264576395567	5.56683468222904
H	-0.61032389415246	-0.64174413283974	2.56138903775316
H	-2.94664533354202	-1.12313693391023	3.14868984745627
H	-1.63485059961938	-3.87540702358769	6.15899537507050
H	3.22693570168485	0.08336723611909	0.42994617718338
H	-3.47274116830738	-2.74844492384681	4.94662289794701
C	4.26093886464368	-4.40474403569123	2.61577260029420
C	4.34193318146238	-5.75337397554032	2.28067496372799
C	4.22298542985226	-6.72225414691169	3.26752109882104
C	4.00683212603248	-6.33072515995927	4.58505878478567
C	3.92351097786258	-4.98226564248499	4.90537382963223
H	3.76036382480439	-4.69354688458257	5.93702181814380
H	4.29661370453544	-7.77230340324065	3.01333856872741
H	3.90900989653375	-7.07841526821971	5.36262288389244
H	4.50222922699499	-6.04660190243348	1.25038474634546
C	4.38253139180710	-0.84858648507833	6.38107300212278
C	5.12718051346100	-0.37588520612993	7.45441266374756
C	6.29367875992755	-1.03258963480497	7.83271101154922
C	6.69524022815951	-2.16678911148433	7.13765563926961
H	3.47389685304754	-0.33095991601998	6.09806642908286
H	4.79966647884621	0.50406610196144	7.99414239855022
H	6.88006153550574	-0.66582791800960	8.66567645555151
C	5.94043593296114	-2.63037879767767	6.06432572723738
H	7.59555375520777	-2.69097425814122	7.43366873605085
H	6.26241026903462	-3.52092806663151	5.53715181538801
H	4.36182966986287	-3.67402749311102	1.82196424141639
H	6.35141183787918	-1.72296327443406	3.62499731476046
H	1.36475131281725	-0.95292911141934	1.73707654089380

58

## BODIPY 34

C	1.89295840435908	-1.53547929756676	3.80700443395445
O	2.74559415965811	-1.77139076898234	4.78699475569605
C	2.34464095301103	-1.06813202569960	2.59618076652937
C	3.72016795228816	-0.80872469363414	2.39316697883773
B	4.12955046863963	-2.24503228000347	4.46371763680763
N	4.63540148267094	-1.28311466145395	3.27326788604922
C	4.07766852299834	-3.75782253234056	3.90460939740726
C	5.09184881122025	-2.03465924925133	5.73661914568685
C	5.93644290208223	-1.01098527921917	3.09159196049497
C	6.37741455914613	-0.26203953149238	2.02393622865136
N	5.48741319106392	0.22482171230781	1.12962094052011
C	4.21706956800516	-0.04050655441864	1.31124994727853
C	7.82792379422944	0.04804045453423	1.83376809115083
H	8.44438759496989	-0.52353622415142	2.52607646468950
H	8.01984261978053	1.11023301579095	2.00541718321112
H	8.13820553776944	-0.18473452194909	0.81400369100780
C	0.48863657986700	-1.77432574085778	4.12132266195098
C	-0.50554510075432	-1.80815726569381	3.13626549380511
C	-1.81169005298992	-2.13012515376349	3.43753147596452
C	-2.20222831743910	-2.42901841766599	4.76108605079096
C	-1.20631519243315	-2.35809637762917	5.75829660296708
C	0.10014803459100	-2.05519282249486	5.43665119889079
H	0.85051163800536	-2.03386737403129	6.21375805362013
H	-0.25189837898339	-1.60928858979768	2.10414623913662
H	-2.53401113802949	-2.16207587486893	2.63668379366148
H	-1.45271895118262	-2.55904770877048	6.78937353683222
H	3.51126142005429	0.36439388882581	0.59389829983627
N	-3.49289009504572	-2.79143374192212	5.05965994262677
C	4.99388239839065	-4.27677567333989	2.98493612746530
C	4.96629639055845	-5.61345586153514	2.59907726256078
C	4.00891833413745	-6.46992919698390	3.12930698991535
C	3.08236424386914	-5.97728290275970	4.04206776851956
C	3.11920455055914	-4.63940004503449	4.41717416452883
H	2.39037929039879	-4.27027590913053	5.12844810796290
H	3.98159763409573	-7.50997633885096	2.82938944747558
H	2.33093021229873	-6.63558880341266	4.46084150475139
H	5.75221203430920	-3.63253647855960	2.55361752467614
H	5.69024717458471	-5.98626494210834	1.88469228671269
C	5.34229351919248	-0.75052458009697	6.23953532293156
C	6.22818046979039	-0.53551953676852	7.28755121774513
C	6.87578073381886	-1.61486030139655	7.88240362836533
C	6.63122985290801	-2.89913378661740	7.41477740961725
H	4.84652537767457	0.10192100937838	5.78753527881470
H	6.41599874112175	0.46943192817629	7.64644159493278
H	7.56390261445560	-1.45243653507068	8.70242476407458
C	5.75443766419698	-3.09927347935603	6.35167458328091
H	7.12723322136848	-3.74591747959965	7.87246348242255
H	5.58627841874296	-4.10435946243308	5.98686470053507
C	-4.51592919466878	-2.73840557337226	4.03502965288938
C	-3.91199118135936	-2.89798951322542	6.44357225254908
H	-4.24642447261343	-3.36167768842897	3.18008305717305

H	-4.69610426860339	-1.72006983789498	3.66919535323664
H	-5.44535997140162	-3.12454577103724	4.44563322549248
H	-3.89753645257084	-1.93129944025204	6.96087876155719
H	-3.26950770841830	-3.58654689809095	6.99348978927349
H	-4.92335324415105	-3.29494989770135	6.48041563132306
H	6.60998712260182	-1.41170884270550	3.83307248971099
H	1.65532552716068	-0.77833054559217	1.82056776145053

78

## BODIPY 35

C	-0.00413313217746	-2.86497620406442	3.10061042578476
N	0.75879474377856	-3.07729231023547	4.25085856825163
C	0.46085067643754	-2.08590370674477	2.07287979990288
C	1.72169245196530	-1.51002243019936	2.09650020160141
B	2.26487826195726	-2.59249923003539	4.40905536108553
C	3.76482771735187	-1.11652571187252	2.86075729581928
C	3.66475968680092	-0.48044571138739	1.60253249886766
C	2.36916281618621	-0.71338123190874	1.12931107463432
C	4.92213392079162	-1.13313660250846	3.79078019261576
H	4.71613591006435	-0.50772855809250	4.66297021403499
H	5.81398691894657	-0.75105519638632	3.29852296170013
H	5.11812186056509	-2.13998967932763	4.16008687625689
C	4.75423130526266	0.25457195528371	0.88409667312826
C	4.84367542455583	1.75229674597628	1.20303668813009
H	4.60491895363551	0.12887523462859	-0.19171326870853
H	5.71576222502362	-0.21494707130600	1.10485136297282
H	3.90519218218657	2.25728989117531	0.96815694417765
H	5.63264158198345	2.22805410398667	0.61842092256645
H	5.0586829317203	1.92090932556851	2.25987168502226
C	1.72778470406432	-0.17973694737320	-0.11047717356122
C	0.95982600718570	1.12855831920248	0.14784733966429
H	1.04017778815427	-0.92027245117956	-0.52753418645288
H	2.49020300080794	-0.00868579370962	-0.87296151278048
H	0.16036073791968	0.97046238882932	0.87313337390448
H	0.51417660813495	1.51252416538956	-0.77210732282506
H	1.62220535733102	1.89322304838868	0.55418681837732
F	2.39625134717017	-1.85015634057251	5.57772239188579
F	3.06072160256073	-3.73867886865981	4.46867884385211
C	-1.23179172262350	-3.57845805612549	3.25609553809762
C	-1.16599553053681	-4.20681596930648	4.54404213846921
C	0.09135504645566	-3.84315890348225	5.11711547027411
C	0.58331562224983	-4.19374551453676	6.47277688965193
H	0.07026872191168	-5.08019371527241	6.84203201013050
H	0.37914458470061	-3.37207182571527	7.16505338209269
H	1.65757170599648	-4.36788860757093	6.47600339745305
C	-2.33137908558417	-3.73880172060668	2.42820444691805
C	-3.36766074653880	-4.53324227710316	2.90769465990732
C	-2.19959337215752	-5.00783911836469	5.02037535233386
C	-4.63277473721056	-4.87876876288842	2.34152880635449
N	-5.29596531300013	-5.65271997221770	3.20264066973029
C	-4.52397786625115	-5.89085353059332	4.34180041125361
C	-3.29752230177209	-5.17240574848797	4.19078342946694
C	-5.13909633917641	-4.49715255624867	0.99943272506640
H	-4.61473667013658	-3.61483841223052	0.63615333924965
H	-6.20965809270401	-4.30167971468400	1.01568111375051
H	-4.96389821946539	-5.31125269189011	0.29064337574946
C	-4.97266351744510	-6.71840550466392	5.33963329542054
C	-6.22459185644118	-7.31495991573381	5.29713588085288
H	-4.32968410938364	-6.91440378176912	6.18600568829335
H	-2.38423246302309	-3.26866161314993	1.45513300046595
H	-2.14757830427941	-5.47651796692543	5.99418819596329

N	2.59489813976699	-1.73410465551563	3.15375629663811
N	-7.10806748870837	-7.05575499421643	4.25706686736434
C	-8.26555689789214	-7.70674987632254	4.52283208147493
C	-8.14712021048825	-8.40397022418891	5.74665604359669
C	-6.85252824225133	-8.17240009438759	6.22492497081180
C	-6.19614195805534	-8.75992076355724	7.43226055833437
C	-5.42170196373825	-10.04939523633873	7.10875617704970
H	-6.95086166402599	-8.97232472200131	8.19200177961853
H	-5.50992378231360	-8.03427848690642	7.87734246822358
H	-6.08203283255201	-10.80067260485684	6.67507074143491
H	-4.96449187204545	-10.46983767026793	8.00674730588170
H	-4.63055438349462	-9.85327109724867	6.38375623601611
C	-9.22227920111112	-9.18916519846125	6.43309482760798
C	-9.29510927379010	-10.67150706650836	6.04458386636942
H	-10.19090804603472	-8.72205659321601	6.23967023400464
H	-9.06896408769795	-9.11347208011802	7.51301323467570
H	-9.51046341334492	-10.79330431673625	4.98119204772501
H	-10.07761849261950	-11.18271213601536	6.60737103053010
H	-8.35041651863915	-11.17588789731015	6.25450053046186
C	-9.42641966657484	-7.66047435507578	3.59810339348427
H	-10.31328736347377	-8.07240790704354	4.07493770749819
H	-9.21677858388485	-8.24479661150584	2.69873321312992
H	-9.63385950113695	-6.64057713458285	3.27346000634002
B	-6.81165028541459	-6.10418821160453	3.06615334576786
F	-7.59097264403999	-4.94648905068640	3.13238334459741
F	-6.99691011148680	-6.74946768472418	1.84841945219198
H	-0.17262404035341	-1.92037858390156	1.21307397231650

78

## BODIPY 36

C	0.67460963495409	-3.86244273708301	4.57183185936034
C	0.58942161476393	-4.58373355543426	5.81407585602351
C	-0.38470804487857	-3.82119077847469	3.67550993734620
C	-1.53928444200029	-4.50390419530842	4.03266640478880
C	-0.56901156224806	-5.27312027404374	6.16244133061587
C	-2.80000986741082	-4.62786380334612	3.37234326776679
N	-3.61709425306709	-5.35354790908162	4.13095333836563
C	-2.96206195900863	-5.77115778280757	5.30143899325623
C	-1.63711407086939	-5.22788193277927	5.27142319175278
C	-3.15403552465545	-4.07827450346820	2.03971337585016
H	-2.54116468772852	-3.20596094120854	1.81658643323736
H	-4.20546374174710	-3.80621088148727	1.98224496428143
H	-2.96532733181307	-4.82988524725630	1.26822628683782
C	-3.60086545402188	-6.59239124021285	6.19940534155562
C	-4.90637669907767	-7.03542077918381	6.00917639935663
H	-3.06575906614756	-6.91593640623479	7.08133491122648
H	-0.31585535593360	-3.27198721149810	2.74579534220637
H	-0.64575397804327	-5.80731308324310	7.10078381531581
N	-5.64115866257448	-6.63111508196654	4.90070296489744
C	-6.86867311509181	-7.19277016670238	4.98001159694797
C	-6.95287992644029	-7.98198173978083	6.14750514323891
C	-5.71525278585478	-7.88921479917181	6.79454656346247
C	-5.28248817027377	-8.59268201868224	8.03861001464963
C	-4.64003536724397	-9.96291248197682	7.76158333501787
H	-6.14351551268545	-8.72478886758771	8.69791707048574
H	-4.57219212387660	-7.97013935800529	8.58816870099713
H	-5.34746183531764	-10.63346722713845	7.27355797702524
H	-4.30541987404628	-10.43242352679327	8.68845232749336
H	-3.77809552874209	-9.86037533809733	7.10054139995643
C	-8.15955649300473	-8.74592027459695	6.60155470229860
C	-8.27495005309609	-10.15896400772610	6.01080184596886
H	-9.06037332417392	-8.18051860895498	6.35109018671430
H	-8.14771577019264	-8.81544562731161	7.69236799875926
H	-8.32425029205293	-10.12879553327054	4.92071559027878
H	-9.17169547126313	-10.66278654751724	6.37726884587918
H	-7.41300917566293	-10.76831579104097	6.28605127334264
C	-7.91175110388256	-6.96600218435495	3.94632031762839
H	-8.87087367196240	-7.35752309020205	4.27894510677759
H	-7.63978865516840	-7.46302328856716	3.01238490913096
H	-8.01874065992558	-5.90428163111599	3.72067200427639
B	-5.15784374185835	-5.60071339362953	3.85162655619626
F	-5.82556114291666	-4.38378606794560	4.00393662027274
F	-5.31746527839346	-6.08341596050395	2.55750615444096
C	1.96021255207540	-3.24343803859194	4.53117665896521
N	2.61871261632623	-3.54512574356623	5.64583449350570
C	1.84297168263000	-4.36638661724723	6.47693313542232
C	2.52360948409274	-2.41096186365913	3.44015673612418
H	3.17663801741468	-1.63743301907571	3.83710455741576
H	1.72361798928244	-1.94912221356640	2.86297506306977
H	3.11965149872120	-3.03187318929624	2.76565187586492
N	4.38241351656008	-3.57291071705943	7.43426121580146

B	4.05717798272985	-3.02421184879506	6.02493762921160
F	4.02501193839912	-1.62695548184989	6.03887412993156
F	4.97510882769303	-3.47462470155269	5.07749962885112
C	2.31655744602339	-4.78147374221722	7.69951508310671
C	3.56230834702274	-4.40135615525702	8.20076012676944
H	1.67904403875857	-5.41278211849330	8.29612016395639
C	5.49856550854653	-3.29864195062518	8.14189241420020
C	4.22049505360748	-4.64733781743257	9.43684455613639
C	5.43888984618083	-3.95456871556320	9.38588101185647
C	6.57806082286116	-2.42203843624802	7.61314881289554
H	6.17667831133517	-1.67426634836765	6.93388672988473
H	7.31765562768931	-3.00915619232164	7.06210557302810
H	7.09156993459699	-1.91649651922565	8.42995941364654
C	3.77131010182120	-5.43309676283345	10.63923556359558
C	2.42259222813200	-6.14500513330124	10.59418964435919
H	3.77043199690169	-4.75446061249117	11.49877283686822
H	4.54475492123812	-6.17375474553397	10.86674503742248
H	1.59879783933667	-5.43841758324443	10.48206366496748
H	2.26279650265473	-6.68817528987988	11.52698027014297
H	2.37153410860846	-6.87298416937018	9.78302889560303
C	6.47450140413546	-3.86823779250345	10.47019906898978
C	7.89636061070529	-4.26940079908760	10.05558552081935
H	6.16496792141521	-4.49655264774151	11.30662239331257
H	6.50164913633200	-2.84595055749664	10.86486214629549
H	7.92542148822104	-5.29807551219667	9.69075765398295
H	8.57427709579733	-4.18443689801298	10.90737810605586
H	8.28596612678773	-3.63183419150343	9.26463993266005

28

## BODIPY 37

C	0.51184388715060	-4.38274309132954	4.67859431070486
C	0.54739113202177	-5.26142410190156	5.74709013037835
C	1.63177470460813	-3.54275235846422	4.80513755077464
N	2.33939811524090	-3.88206759667005	5.88674455067434
C	1.70609310041921	-4.95453538143527	6.50609044617097
N	4.09054928638787	-3.93814991895653	7.64296072038769
B	3.58261451097312	-3.10702623127932	6.42485947165460
F	3.20917105421409	-1.83199460832981	6.82672845920979
F	4.56763071596217	-3.05210175177351	5.45042102227505
C	2.24749402621157	-5.52680764114782	7.66919980870907
C	3.46168674822900	-5.04367062493174	8.19768919922806
C	1.56726039158437	-6.60159752286766	8.35332603917511
C	5.25246216115127	-3.74737217101657	8.28215405624618
C	4.30301397783344	-5.54585247733253	9.21921740638260
C	5.42125041309099	-4.72697746338729	9.27260350332450
H	1.94442421574273	-2.71999299948811	4.18313232728972
H	5.91066207340049	-2.94442689517202	7.99354205179150
H	-0.22736000646818	-4.33774829310219	3.89683695169348
H	-0.15276455385906	-6.04710314049421	5.96143124393810
H	4.12858874671971	-6.43360773338818	9.80022640414449
H	6.27422048296094	-4.82983526393667	9.92188838989512
C	1.47783034812504	-6.96052097076888	9.67267488126164
O	0.77063606672469	-7.44967082105499	7.61306003797308
C	0.20794956621435	-8.32212197847064	8.47262828067094
C	0.59768810553481	-8.07428030760434	9.75317667484251
Br	-0.91729494825758	-9.60925203968036	7.74013759583012
H	1.95118934037892	-6.45126627391601	10.49333641546474
H	0.28659633770467	-8.61062034209998	10.63184206990874

46

## BODIPY 38

C	-0.30063985306276	-4.55105369823246	4.59820527419426
C	-0.21220440675430	-5.38723778452270	5.68496590533491
C	0.88963888656580	-3.75746329356925	4.59502962058791
N	1.65318128889882	-4.09536166088450	5.65083716699280
C	1.01842570269997	-5.12282757690710	6.34643874755322
N	3.55411393997986	-4.23165771927360	7.23707628790317
B	2.98035113261400	-3.39483293101776	6.05679350011778
F	2.73944972122746	-2.08147710713353	6.44362983467786
F	3.82190372555798	-3.40480913422851	4.93218367063543
C	1.60907999121486	-5.70838424937628	7.44800772325181
C	2.87455804214415	-5.26552387200793	7.88420781505395
C	0.93475796774588	-6.82017399126177	8.15260467044814
C	4.74252526725307	-4.09157153557186	7.85978528153630
C	3.69321739301668	-5.75045087964644	8.91745010373225
C	4.87216564381369	-5.00981944224934	8.90435721676846
Cl	5.89676825822174	-2.93248706616148	7.37276796416844
H	-1.07771536201198	-4.51964839915491	3.85632580297073
H	-0.92577972591895	-6.13438138783594	5.98771676041551
C	0.54548309610450	-6.69516571932012	9.48745541275805
C	0.66517107187895	-8.01904063533027	7.49081754072982
C	0.02290236052534	-9.06034205111492	8.14645106471106
C	-0.37052852221003	-8.94020210699067	9.47836930999698
C	-0.10118928322946	-7.73779413937961	10.13340727968897
H	0.73122916988183	-5.76685863787659	10.01129931935430
C	-1.04362625454382	-10.07569352462635	10.19702650847746
H	-0.31545129588981	-10.66658842137325	10.76066663288460
H	-1.54292664170062	-10.74876573229443	9.49913316420015
H	-1.78452145334239	-9.70964107825404	10.90876434823257
N	1.32797696902053	-2.83910591663706	3.70837716047899
C	0.61166778069226	-2.20385220838581	2.68809263083886
C	-0.75770531091295	-1.95338798546626	2.77889071087980
C	-1.40811660240334	-1.29300484473851	1.74529556542752
C	-0.70795598229416	-0.86324014668521	0.62420659438883
C	0.66179677894203	-1.09313484946412	0.54728877606501
C	1.31868154683034	-1.76425991727765	1.56585337846216
H	-1.30021260978976	-2.23697430719563	3.66888171556627
H	-2.46834986863020	-1.09335281129640	1.83102213100267
H	-1.22037828833064	-0.34276524206147	-0.17310985774750
H	1.22310776717667	-0.75239534610966	-0.31277667534171
H	2.38200116999402	-1.95970884228074	1.49842770075931
H	2.31039594565957	-2.60917828546630	3.78799539146179
H	0.97711574926526	-8.13753841887345	6.46150155763235
H	-0.17453301878031	-9.98289985915141	7.61319336122410
H	-0.41471375923879	-7.61147384597843	11.16261972394950
H	3.44230318703315	-6.56261837106027	9.57815491565344
H	5.72994868508587	-5.10718502627601	9.54664129192173

58

## BODIPY 39

C	-0.08796594957701	-4.17330297497403	4.73861205763323
C	-0.02985937569066	-5.02220641288844	5.83020442457142
C	1.06024878335776	-3.34363540906320	4.81040196192014
N	1.77547469697904	-3.65686119011886	5.91230944247613
C	1.13813503120375	-4.71929579564737	6.56142113059616
N	3.59965376113020	-3.79230816971934	7.57471911031625
B	3.04478367414836	-2.94272849658936	6.41394365679818
F	2.77092089867439	-1.63437864789689	6.80697529418718
F	4.00385047533880	-2.88707678206377	5.36109887492534
C	1.70085664872459	-5.31587996943804	7.68712593316536
C	2.91117743422184	-4.84329330352399	8.19352948249705
C	1.11040920359911	-6.54425868471787	8.26444958345048
C	4.82277498927675	-3.69820185633928	8.14431332658445
C	3.74657275159281	-5.35864526555044	9.20676704801043
C	4.93253515522563	-4.64763358672683	9.19129552578760
N	5.75842514995542	-2.84747423058299	7.64496410753400
H	-0.82580588598369	-4.15733244122030	3.95658214061868
H	-0.73188298331402	-5.79782544350531	6.08523679855881
H	3.50049512571188	-6.19077037628657	9.84400245367666
H	5.80318929735926	-4.81092066536851	9.80006927757367
C	0.68271966422585	-6.61488376870909	9.58946776164666
C	1.06389645022927	-7.70535838559721	7.48945856331237
C	0.64004300994394	-8.90550456826039	8.03633600138412
C	0.24288859602563	-8.99075234728517	9.36985635085924
C	0.25766937338612	-7.82166883802053	10.13058190448939
H	0.69180104657951	-5.72123140083855	10.19973303498763
C	-0.19059656521928	-10.30948287870547	9.94864459927297
H	0.33314894087016	-11.13597513966660	9.46830856763844
H	-1.26195948643544	-10.47226161518507	9.79757853191699
H	0.00935248574023	-10.35957527995806	11.02011974175620
N	1.51028367541308	-2.40274013028524	3.94020414996690
C	0.82788990679498	-1.95188812578503	2.80017655856346
C	-0.51973240169848	-1.59529454048242	2.85874752391474
C	-1.16827966152466	-1.15271611179928	1.71510785947276
C	-0.48057532136320	-1.03259808713433	0.51252516030084
C	0.86898738893930	-1.36264332319509	0.46147962726769
C	1.52047458931810	-1.82710856230127	1.59475610432231
H	-1.04397617239392	-1.64567109365611	3.80285864295477
H	-2.21293173541696	-0.87608184598861	1.77146631828053
H	-0.98945227692313	-0.67968306147558	-0.37420818713723
H	1.41654868379047	-1.27223590227918	-0.46776456755756
H	2.56314555607491	-2.11577580816737	1.54807674840222
H	2.49008299411666	-2.17120652584276	4.02020036450577
H	1.40533449345839	-7.66821875232135	6.46381428168321
H	0.63993999709518	-9.79929320445494	7.42381689222673
H	-0.06168012589488	-7.85366625726756	11.16525876310846
C	7.05830957801647	-2.68356286361261	8.14943326309355
C	7.28676965911303	-2.51136531455860	9.51465445566819
C	8.14004099716717	-2.67275295793463	7.26684913972791
C	9.43170367736393	-2.50939350600817	7.74805914184190
C	9.66188601219968	-2.36782175495895	9.11137470363023

C	8.58295332802415	-2.36680803121444	9.98847753995432
H	7.96462792880973	-2.81679611772821	6.20780759086175
H	6.44709613776606	-2.47108789505145	10.19398413347466
H	8.74890185060726	-2.23397981737057	11.04996232514855
H	10.26248194460644	-2.51082299790810	7.05450246413712
H	10.66975780295521	-2.25231857440040	9.48674733390000
H	5.58230909630478	-2.52557491237030	6.70351498014095

59

## BODIPY 40

C	0.22367465972151	-5.11328562092133	4.77316825216346
C	0.30697871994301	-5.89853796253113	5.91236453384663
C	1.52016121376564	-4.57651567279920	4.55276334541594
N	2.36542480181657	-4.99663532515081	5.52041538881830
C	1.64751338408243	-5.82128292323124	6.36957341212140
N	4.27957843982914	-5.17060506011496	7.18577383314751
B	3.88897625549720	-4.59402378291997	5.74941037214877
F	3.98465569118529	-3.21952899407002	5.78100445190449
F	4.68259129249231	-5.22658835716504	4.83104663867646
C	2.23938819546163	-6.40368298589690	7.48181030454185
C	3.52671712012566	-6.10843096635781	7.87871903057419
C	5.40468319587654	-4.95931418086655	7.88458941112265
C	4.25794753040322	-6.51840233025576	9.02819864232981
C	5.43336634954414	-5.79045241420398	9.03876141950363
C	6.42360174295019	-3.95237525239391	7.47978172517641
C	1.97391933084325	-3.74332988403445	3.41549884473211
O	0.91925127406517	-3.15151835786807	2.80823803506357
O	3.11352666287608	-3.61838859378713	3.05677566959602
O	6.82370892214535	-3.26773083915681	8.57188224866923
O	6.83709677532301	-3.77105365370892	6.36923615690152
C	-1.04904238755665	-4.91770964195810	4.00925704765821
C	-2.09418549016724	-5.95857629959775	4.42517812033792
H	-0.86692593886695	-4.96337057190777	2.93545207135742
H	-1.43218476820723	-3.91032090724007	4.20371966381587
C	-2.17391023678679	-6.10166345788437	5.94428870449963
C	-0.85110482211044	-6.62275331011481	6.52084556930914
H	-0.76478641416263	-7.69709629158798	6.31822003392965
H	-0.84294558076571	-6.50731201184286	7.60813074612106
C	3.89391988418877	-7.52801210184182	10.06742427416666
C	5.15452372685638	-7.97888323344321	10.81888909216233
H	3.39026880830131	-8.38535940910886	9.61419666038041
H	3.18297963323847	-7.08790527900205	10.77669077101973
C	5.99931610935492	-6.78087452584388	11.25854322615091
C	6.51041828126743	-5.96041156661360	10.06521350203319
H	7.36412122002407	-6.47136066239904	9.60618571769470
H	6.88102689295345	-4.99155672266895	10.39890995006065
H	-1.83235123687213	-6.92899783241177	3.98997367156442
H	-3.06802387421192	-5.67882695547355	4.01891684350807
H	-2.40100816500352	-5.12627737845369	6.38532123795701
H	-2.98712099993144	-6.77292739367368	6.22531598206901
H	5.39286073240126	-6.13716988644751	11.90341127212740
H	6.84540856167878	-7.12121318180045	11.85849550821316
H	5.75046962013699	-8.62018753187697	10.16226272765446
H	4.87451154598910	-8.58211749221903	11.68416995093888
C	1.22678157664867	-2.33427790928156	1.65763024631329
C	7.78687383172356	-2.21542277606166	8.35085905868470
H	0.37402802601311	-1.66250184416735	1.57424273756168
C	1.40172778801697	-3.16858996190523	0.40388197750102
H	2.12391011792364	-1.75485924223998	1.87170057890838
H	0.50941356049297	-3.76413947293252	0.20413218468302
H	2.25791677734873	-3.83488792704108	0.49776905125582

H	1.57332722554055	-2.50886920875258	-0.44919738380888
C	8.08825837394010	-1.58997091790421	9.69510875056221
H	7.35564303179744	-1.49874242891789	7.65090948660779
H	8.67430032380497	-2.64582061663336	7.88459804701746
H	7.17890531152779	-1.19819372020408	10.15232322407033
H	8.78998728991848	-0.76382269870003	9.57164369893277
H	8.53516048861957	-2.31738277774364	10.37381836296350
H	1.65312961698781	-7.08723169466909	8.08184591756300

51

## BODIPY 41

C	0.17805821629208	-5.07168224593530	4.78609888088245
C	0.27002371799356	-5.91698462931743	5.92548253029124
C	1.48656823066009	-4.53926481150150	4.57299725336773
N	2.31833658374576	-4.99614998052945	5.53095650907697
C	1.62466461211566	-5.84548771562513	6.37304548255025
N	4.27075374684202	-5.19020061740162	7.19416621503238
B	3.85925123381771	-4.60414445923051	5.75482237799302
F	3.95096487869790	-3.23605798017221	5.79777253984474
F	4.62943519760289	-5.25206494767522	4.83492237134970
C	2.22780261534490	-6.42859137204011	7.47509039314729
C	3.51090098892465	-6.12712863361521	7.87889666974311
C	5.39835901877820	-4.94791992211677	7.87545954520930
C	4.24053727056572	-6.52999870217694	9.04213133408474
C	5.43586146542609	-5.76275895122784	9.04869048525401
C	6.43433446282431	-3.97439438017286	7.43923537148974
C	1.94497950077661	-3.68551088141429	3.45334351669730
O	0.89121978862547	-3.08810687847772	2.85237283216119
O	3.08682296579405	-3.55274346322188	3.10467387123338
O	6.96348255895410	-3.37485241162819	8.52614913942062
O	6.77156068635375	-3.75858852471097	6.30878446986665
C	-1.05330524447307	-4.90169164592747	4.13204702371439
C	-2.15572826540846	-5.55887089017766	4.63407062481920
C	-2.06036138932201	-6.39582814758710	5.76437210424768
C	-0.85773902781929	-6.58480594855726	6.41354268840586
C	3.98718141072868	-7.45647938982504	10.05659842728647
C	4.93141951724320	-7.60664208964249	11.05334681028793
C	6.11980302859172	-6.85010008529631	11.05902483128080
C	6.38242069633497	-5.92489945656081	10.07013432362294
C	1.19834591304896	-2.22822959173462	1.73135148479916
C	7.97087740172391	-2.37031759333428	8.27559190587174
H	0.34672003214118	-1.55190026398540	1.67639022921956
C	1.36903283560193	-3.01442578169044	0.44691909785882
H	2.09617797043959	-1.65854851528506	1.96678696872783
H	0.47203580854876	-3.59345194153142	0.22120070161792
H	2.21895141736270	-3.69167737648770	0.51615402151615
H	1.54873160510787	-2.32276550812867	-0.37861198140811
C	8.35642651111353	-1.77698286131672	9.61227923259426
H	7.55138432089224	-1.62476277076285	7.59940593189888
H	8.81503352843278	-2.84142278742678	7.76969678755322
H	7.48721605300631	-1.34146714440410	10.10631278145255
H	9.09697151161944	-0.98900022360400	9.46808950757460
H	8.78852795085936	-2.53402180786526	10.26774369593658
H	1.64696191502214	-7.11622648677157	8.07454560692446
H	6.83679658522717	-7.00331823266916	11.85469118105274
H	7.28878335449260	-5.33833438812723	10.07748426044962
H	3.08234066331286	-8.05017812331771	10.06141798515060
H	4.75783605093002	-8.32306233271803	11.84565562209166
H	-2.94802384801262	-6.89544269782682	6.12995902440448
H	-0.79753842498723	-7.22548169205990	7.28353045911156
H	-1.13185367137964	-4.25819216431290	3.27040615971846
H	-3.11683395051514	-5.42811055287408	4.15451071352219

30

## BODIPY 42

N	2.54847558774105	-4.67659209242540	5.71462193598233
C	2.01831491536881	-5.37782365440955	6.71616226770462
N	4.09383029071509	-4.92164643726409	7.50830339244838
B	4.06094962151407	-4.19480804843757	6.10419616506615
F	4.09600120716946	-2.82366799285834	6.20640441910845
F	4.97992723486684	-4.68211824442024	5.20483535127740
C	2.91066115897599	-5.53019999671233	7.81445285977257
C	4.89004468328111	-5.11457050402760	8.60484935471049
C	4.11916303735179	-5.82959687353358	9.52329678634085
N	2.87555133400160	-6.08665918977723	9.00443919537259
N	0.77299565961115	-5.73946875662247	6.39042752081125
C	0.48328538050301	-5.23808053036247	5.11588872704830
C	1.60682929243516	-4.57333630189002	4.70559488525067
H	0.16207792211250	-6.28276296266164	6.97629463852277
C	6.30102397017731	-4.64869091612501	8.69387243439345
C	4.47698225090326	-6.26639445724106	10.90349606122141
H	6.82125174953581	-4.81063799399891	7.74831380225775
H	6.83280888777995	-5.19714959166242	9.46933648338686
H	6.36807002544432	-3.58333314908562	8.93394321894350
H	5.52384407292886	-6.06117216237887	11.12834693757115
H	4.29290263838955	-7.33533733302854	11.03423008508024
H	3.86998476547256	-5.74240203875963	11.64449085621212
C	-0.83633309933269	-5.45537932430110	4.46835648648372
C	1.85978551359097	-3.83399658458501	3.44338557202112
H	2.87087793707655	-4.02964387503568	3.08529113249729
H	1.75916346471856	-2.75566419815619	3.59284293100843
H	1.15550759623938	-4.13903677132597	2.67136843992449
H	-1.01668190724285	-6.51077650678138	4.24578397126605
H	-0.88487821845470	-4.90490285920138	3.53186586598583
H	-1.65308697287446	-5.10044065293066	5.10173822232977

30

## BODIPY 43

N	2.76346374557552	-4.68816663020125	5.68240257018154
C	2.23548764583528	-5.39146810008084	6.68078502345181
N	4.31306989378232	-4.91275527513699	7.45513383777013
B	4.28141799065963	-4.19781469066584	6.05425990739799
F	4.30758091124270	-2.82867345257400	6.13799341269428
F	5.18730065244028	-4.69908829083091	5.15578263500364
C	3.14925067073525	-5.56680934084763	7.76524232812222
C	5.11638997949216	-5.10557908219530	8.54743579488648
C	4.35304163594178	-5.89845428080698	9.45847286438658
N	3.10649686134741	-6.16850008519440	8.92880017503860
N	0.95980347109330	-5.71802819801890	6.42223786080126
C	0.62606387039417	-5.17790339768623	5.17938032194688
C	1.78928700657973	-4.52689580857559	4.71490907174800
H	0.36273308783523	-6.23401121255652	7.04657683709679
C	6.40806450585900	-4.67886443270443	8.85462960189445
C	4.90131920718244	-6.27971159801012	10.68607427198594
C	-0.55537106103556	-5.18027510865100	4.45558611635398
C	1.79472015595234	-3.87009545100431	3.49064226009958
C	0.61277869882749	-3.87455438040591	2.76544895077918
C	-0.54227944641010	-4.51194253900618	3.23934707693447
H	2.68513367633921	-3.37552185381605	3.13045424292657
H	0.57787522682252	-3.37021616502053	1.80992435759681
H	-1.44572040279044	-5.67200768336376	4.82248144842620
H	-1.44424020951008	-4.48255727892857	2.64363168104885
C	6.92371866245507	-5.06705883909498	10.07733217711140
C	6.18459254631319	-5.86124460185568	10.97744408391104
H	6.97739780619124	-4.07298197861701	8.16371295301036
H	7.92000561587669	-4.75071314930804	10.35634532269582
H	4.32610852525010	-6.87986176398208	11.37817265395339
H	6.63641906972210	-6.14452533085995	11.91898016074575

## BODIPY 44

N	5.36959450111828	-4.40839727701271	7.39653340716735
N	7.29402113343824	-5.02809643090503	8.83106821988144
B	6.85136886568887	-4.04836844896787	7.70961515669817
F	6.94619960009896	-2.73755680403433	8.16720431975246
F	7.64619970233250	-4.22823410085550	6.58352826835808
C	6.49724350142662	-5.98697658143549	9.44503299799162
C	5.16386377373927	-6.18327949777948	9.04424586291090
C	4.61751927254109	-5.40837888603400	8.02568988943334
C	4.59896546133026	-3.78602894390942	6.49530146902663
C	3.31915878730444	-4.37372168657139	6.50102064174216
C	3.30992248905693	-5.38650296180598	7.44260635749035
C	8.50326904015827	-5.05326099954786	9.38570144031275
C	8.55012094028915	-6.03649487580682	10.39968226660431
C	7.27885797463631	-6.62236545811620	10.43102335141386
C	4.34227091771593	-7.22180632922716	9.74767814950753
C	5.08415934045050	-2.66123937649465	5.65656418382371
H	2.49316329426343	-4.07257183904899	5.87696696811433
C	2.13276554197463	-6.24875986504473	7.74837206476177
H	6.96826022122664	-7.41476742471659	11.08929798037729
H	9.28408540692661	-4.38417480623599	9.06442425733053
C	9.68949527249679	-6.30646537030760	11.18497692633658
H	5.85025192312374	-3.01013727747157	4.96153169970630
H	5.54499273810982	-1.89096139547167	6.27539402980121
H	4.26025580005102	-2.22977051169331	5.09076773476361
H	1.29144790735947	-5.96692719099479	7.11706615024346
H	1.81561395256397	-6.15101056988109	8.78914358892594
H	2.34318218178936	-7.30619442946608	7.56990479472003
H	4.93812882191937	-7.77974427921392	10.46333440876706
H	3.91218855173995	-7.93000654441270	9.04020967449869
H	3.51489338085336	-6.75544580998125	10.28515690425181
C	10.71152091093317	-6.45078165092357	11.81312617391661
C	11.94618982631325	-6.56732102250860	12.50684282413237
C	11.98866563791449	-6.66635035534511	13.90462575466789
C	13.20629632192649	-6.73040928654058	14.56521735691925
C	14.39763359385276	-6.69998127833012	13.84733247255603
C	14.36589585833637	-6.61159696265728	12.45921783069009
C	13.15353156131480	-6.54536989718153	11.79140379977837
H	11.06096097216469	-6.68279743533628	14.46013960549705
H	15.28886166217889	-6.58814082550742	11.89449339342991
H	13.12277093733252	-6.46820665321489	10.71279058059796
H	13.22703053411122	-6.80175644324631	15.64513052110696
H	15.34577188789748	-6.74600221676412	14.36677652199412

## BODIPY 45

N	5.70039196026296	-4.41171772328983	7.12937611833270
N	7.67283514383046	-4.87220449965552	8.56882960320999
B	7.24703613561183	-4.20528869329937	7.22365972276152
F	7.55058788587708	-2.84684391644370	7.24663183966524
F	7.86224404140705	-4.82690125713495	6.13956247149379
C	6.84941989721877	-5.63488416463876	9.37896509788625
C	5.48633829146792	-5.81328602575745	9.09728583835016
C	4.91815461118200	-5.18912196829648	7.99082145844211
C	4.91768102982295	-3.92052494039122	6.15877788678533
C	3.59375413216180	-4.35272733762408	6.37345150436336
C	3.57221627597648	-5.14644325813035	7.50640308993641
C	8.90559798162520	-4.83263801042335	9.13288332505371
C	8.89210859765567	-5.58573905686702	10.33104027437567
C	7.61479495763379	-6.08613985443107	10.48109110456240
C	4.66037696127652	-6.66099267706473	10.02043898278362
C	5.43112471838106	-3.08211406818135	5.04596619525711
H	2.74761844655386	-4.09395809503309	5.75726234640845
C	2.34743210959595	-5.79021465451109	8.06659290333692
H	7.25797969723697	-6.69524435862338	11.29350918111528
C	9.98719691017338	-4.13896620343934	8.58045026336289
H	6.03745535002194	-2.26201384478752	5.42890408882278
H	4.60409731929640	-2.68325584162964	4.46130920477775
H	6.07545401588898	-3.67727598291939	4.39462143193165
H	1.47197556862287	-5.45878339153864	7.51001172708283
H	2.19289365009923	-5.53644933346309	9.11689587161182
H	2.39075605811430	-6.88071709723244	7.99764167212789
H	5.28539212194258	-7.20593477035639	10.72106518779031
H	4.06791207372026	-7.38355463335198	9.46245254341686
H	3.96711991207328	-6.04500187903940	10.59688242961741
H	9.73819004585516	-5.71874305210427	10.98333561901853
C	10.92935091561756	-3.54669207168855	8.11083663192219
C	12.02482903697606	-2.85450461701464	7.54353841541203
C	13.33298509916234	-3.14435794056307	7.95852035066087
C	14.40901344048991	-2.48482414882642	7.38801443752407
C	14.19889988118849	-1.52146303835115	6.40565513093284
C	12.90355770836850	-1.22048868022248	5.99535155458768
C	11.81968669952103	-1.87816870700977	6.55629751054770
H	13.48807595707752	-3.89428074820250	8.72196667906495
H	12.73720206231838	-0.47077012969678	5.23286291068444
H	10.81016882879315	-1.65300329909811	6.24058760680899
H	15.41325980417172	-2.72408097152732	7.71305885605016
H	15.04046466572850	-1.00744505814032	5.96101093212315

41

## BODIPY 46

N	6.14880924805480	-4.56399475627791	7.47328640270364
N	8.13452984354062	-4.84054792453342	9.00533374273879
B	7.60651624944588	-4.14114172279293	7.69696199575224
F	7.65357745287514	-2.72944097489238	7.86168568844587
F	8.41817204278286	-4.49856825657739	6.63166781282000
C	7.32171245737830	-5.67079089151230	9.78782967619054
C	5.99653536326885	-5.86989865221319	9.49282064773193
C	5.39147696009887	-5.31194579797674	8.36729287322012
C	5.35237670850496	-4.19076913295136	6.44289284429727
C	4.06377022697023	-4.68923840459909	6.66925863693586
C	4.07217210861337	-5.39303912827601	7.87421438020159
C	9.39778837507800	-4.83916728663493	9.48742549951197
C	9.44734468436567	-5.71506393401474	10.63319963076935
C	8.14057488545935	-6.22866620751835	10.82095498533871
C	5.84380734255886	-3.39813181713219	5.28484218989625
H	3.21804044938711	-4.54466534023961	6.01582049167165
C	2.91845072550123	-6.09693018934690	8.50467573371718
H	6.51779820889119	-3.99527931484041	4.66640605820731
H	6.40348705529516	-2.52323681892622	5.61641246888082
H	5.00483929658402	-3.07031490559876	4.67304490329937
H	1.97799874036435	-5.70360080953963	8.11924243187731
H	2.91179766588280	-5.97474894038555	9.58959863646140
H	2.93745355270812	-7.16974972861753	8.28751089732789
H	5.41040800821749	-6.50192825144291	10.14593810484956
C	10.47395150468471	-6.06342854632304	11.51875411562552
C	10.19563669601709	-6.94915068548223	12.54116695823787
C	8.90244463283259	-7.47307686619195	12.71247829010959
C	7.86942683160223	-7.11286642597909	11.86925706351080
H	11.46245964204708	-5.64227112733298	11.41854000547940
H	10.98036407082308	-7.23743195155269	13.22775336133767
H	8.71377511804003	-8.16266105994917	13.52482496873483
H	6.87483695443713	-7.51129121750537	12.02172364198636
C	10.48931926890237	-4.07102536617927	8.97360959061370
N	10.34085785974050	-2.91193471596906	8.24442772077150
C	11.86557991319305	-4.29186190306761	9.09123367399006
C	12.52723621396551	-3.25325771599494	8.41453533982182
C	11.55072980771136	-2.41259330790181	7.90799536223209
H	12.32588330852292	-5.14012746738365	9.56399761069345
H	9.44325369660087	-2.51428769855738	7.99976580090167
H	13.58974590453643	-3.12289965147561	8.29789719698177
H	11.63850092451578	-1.49800510631371	7.34763256612524

71

## BODIPY 47

N	5.96182683479308	-3.74244562086110	7.01573359500377
N	8.09894960837740	-4.20378743354669	8.25136479389091
B	7.43423431243276	-3.33001050322928	7.14029868357997
F	7.46630450196689	-1.96270136587295	7.54029343384928
F	8.12826557012169	-3.48573874444041	5.94380162911941
C	7.36795797871463	-5.09342074217936	9.04472497924067
C	6.00664045095011	-5.23687471795852	8.89688338742872
C	5.29337963379148	-4.55855817501861	7.90662155853179
C	5.07351272286140	-3.26420086164164	6.09863772245286
C	3.79879339632467	-3.77717649592132	6.41355641113877
C	3.92045192925867	-4.57473326867260	7.54352557043650
C	9.41783670762082	-4.26626030951635	8.55829260965705
C	9.58657563575936	-5.24886941942082	9.59470812801616
C	8.29987806343382	-5.76279683069685	9.90351315429615
C	5.53605620867508	-2.39443729249007	5.06265588857665
H	2.88835822684224	-3.55649197855437	5.88107660561629
C	2.82387321944356	-5.30326797442028	8.24258757167040
H	1.85341152375152	-4.95317441671175	7.89219706032824
H	2.86363025717804	-5.14907620604829	9.32341220982856
H	2.87482047394464	-6.38012535353168	8.05460403978705
H	5.48294630507586	-5.92183403608350	9.54947507212504
C	10.70770620577587	-5.65733813617742	10.32539775251012
C	10.54529857170571	-6.61137630853385	11.30983805321062
C	9.27505473551946	-7.14520185114009	11.59288547266715
C	8.15001471972078	-6.72220193061741	10.91014655726144
H	11.67734797673321	-5.22578939122786	10.13146678125117
H	11.40142745037535	-6.94896673584205	11.87846122090639
H	9.17790947960485	-7.89091732273074	12.37131375476137
H	7.17689858673274	-7.12473027497818	11.15985566026773
C	10.41791365501696	-3.41761000743750	7.98048429783231
N	10.13612933884275	-2.10958442825817	7.63305666669400
C	11.74372970941109	-3.66092963809599	7.59768200528218
C	12.22324213367868	-2.46396761319219	7.01886438961351
C	11.20432934453645	-1.52470161925412	7.04690710536596
C	12.48956998588591	-4.95664072360260	7.62994631264729
H	9.21922478755643	-1.69426188529797	7.72619480504183
H	13.20266566504570	-2.31008757515066	6.59558490797297
C	11.13491519454191	-0.12549559831387	6.54276850338014
H	12.09839862995572	0.18415725923332	6.14077625444323
H	10.85293916845049	0.57362386113730	7.33442464295974
H	10.38906453410881	-0.02987392432964	5.74866603288132
H	11.81647177157257	-5.80652698811394	7.72697693983449
H	13.20875706381909	-5.00411533892009	8.45249643388643
H	13.05757124529412	-5.08362605785600	6.70686639014508
C	4.93436253378605	-2.03582897483175	3.91422311078705
C	5.62140657609479	-1.23879535878318	2.90591935813856
C	7.01435005083304	-1.09463528595379	2.92620257965845
C	7.68101724436004	-0.30865119632876	2.00498125681639
C	6.96252518904277	0.35628750729900	1.00962786076682
C	5.57782517562421	0.19600576649943	0.94189101908364
C	4.92524378103287	-0.59593189009265	1.87041729116444

H	6.53381668166619	-2.02306327775484	5.22932499469857
H	3.92092475284016	-2.35416992765883	3.69331212338728
H	7.60257375327103	-1.62853554083575	3.65886266100725
H	5.03466929281238	0.70140253705784	0.15510831115383
H	3.85022388610777	-0.71499506670833	1.80187750644654
H	8.75594097109482	-0.23911505854747	2.07191733452634
O	7.53235854809004	1.15787437571770	0.06261257830008
C	8.92081848396265	1.33561707572852	0.14149552953288
H	9.20039232260490	1.80832441661149	1.09050324510536
C	9.40327837025621	2.19343853174531	-1.01424937290995
H	9.44044625296499	0.37123010101065	0.08989154990901
O	8.71438556473978	2.58058760864962	-1.90887168860568
O	10.72553315150903	2.48960195193523	-1.00145674069916
C	11.59854698916229	2.13093899580934	0.08693164970512
C	13.02126890366283	2.25462163345157	-0.40950744673590
H	11.40308665974819	1.10986172681095	0.41942153206009
H	11.41341471715060	2.80965187932813	0.92368255210256
H	13.19697185051517	1.57080681152010	-1.23925138305500
H	13.71622231765203	2.00699038922690	0.39493097574351
H	13.22555246421279	3.26934424460961	-0.75125343347879

95

SMcy7

C	3.882828	-4.353488	8.324172
H	4.596321	-5.048204	8.417218
C	2.565736	-5.095286	8.393526
H	2.522466	-5.769078	7.669835
H	1.817268	-4.460206	8.270757
C	2.439883	-5.786864	9.750447
H	1.564675	-6.249311	9.806447
H	3.153188	-6.466933	9.845216
C	2.550726	-4.777223	10.872814
H	1.816335	-4.118079	10.797215
H	2.459655	-5.239670	11.742752
C	3.881805	-4.059489	10.818968
H	4.610441	-4.710263	10.978137
H	3.916572	-3.379420	11.538137
C	4.100263	-3.376281	9.467863
H	3.470998	-2.616696	9.377832
H	5.021720	-3.018460	9.425217
C	6.752189	-3.892087	4.381778
H	7.255187	-4.416263	5.067992
C	7.638615	-2.730739	4.069255
H	7.826665	-2.226441	4.899993
H	7.175080	-2.122862	3.439687
C	8.944561	-3.200509	3.451749
H	9.454675	-2.412676	3.135995
H	9.487631	-3.652494	4.146148
C	8.736409	-4.141097	2.306335
H	9.616512	-4.477993	1.998766
H	8.320760	-3.649355	1.555075
C	7.860962	-5.309769	2.676796
H	8.332184	-5.874750	3.338457
H	7.691301	-5.861149	1.871690
C	6.530382	-4.852554	3.260703
H	5.991252	-4.417310	2.554458
H	6.028010	-5.637249	3.592610
C	5.310750	-4.019731	6.332298
C	4.536718	-2.694119	4.391040
C	3.364846	-2.304911	5.167500
C	3.228657	-2.812347	6.457006
C	2.316164	-1.483597	4.636362
C	2.250016	-0.955235	3.339318
H	2.914776	-1.193783	2.703073
C	1.233584	-0.093117	2.968211
H	0.574567	0.104626	3.622764
C	1.090593	0.510575	1.718982
H	1.694775	0.267843	1.027383
C	0.113807	1.443839	1.439629
H	-0.513445	1.637397	2.125843
C	-0.027542	2.128093	0.231538
H	0.537377	1.881175	-0.491076
C	-0.937624	3.140873	0.026277
H	-1.561551	3.325014	0.719384

C	-1.003315	3.915105	-1.134429
H	-0.375721	3.717362	-1.819997
C	-1.896296	4.941486	-1.378890
C	-3.105826	5.369406	-0.553753
C	-3.732980	6.412528	-1.448459
C	-2.923680	6.630150	-2.552088
C	-3.210449	7.584339	-3.509256
H	-2.644189	7.722445	-4.258147
C	-4.365253	8.333461	-3.325533
H	-4.591201	9.000975	-3.963071
C	-5.189489	8.131533	-2.241289
H	-5.978674	8.650478	-2.147381
C	-4.874499	7.172112	-1.281752
H	-5.434698	7.041330	-0.525538
C	-2.678321	6.049475	0.764830
H	-2.044117	6.770348	0.568615
H	-2.252403	5.389285	1.350460
H	-3.467836	6.421944	1.210460
C	-4.067789	4.208058	-0.275907
H	-4.929283	4.562740	0.028000
H	-3.688608	3.629476	0.417846
H	-4.199264	3.689113	-1.096306
C	-0.712633	5.834992	-3.414056
H	0.115837	5.540993	-2.959380
H	-0.588718	6.778719	-3.685225
C	-0.919325	4.987521	-4.656824
H	-1.841260	5.116211	-4.994762
H	-0.807295	4.031240	-4.426147
C	0.087392	5.372545	-5.751838
H	1.004834	5.311862	-5.386761
H	0.014546	4.731188	-6.502452
C	-0.145947	6.740007	-6.256914
C	-0.380162	7.834395	-6.629959
H	-0.567627	8.715346	-6.931067
N	4.111913	-3.704284	6.985774
N	5.478096	-3.503925	5.062608
N	-1.819833	5.757569	-2.473473
O	6.141916	-4.713820	6.880020
O	4.744358	-2.359316	3.244334
O	2.240807	-2.500038	7.230666
O	1.281061	-1.222032	5.425961
B	1.333166	-1.412451	6.835436
F	1.870467	-0.246917	7.407497
F	0.124690	-1.668785	7.361620

57

## PDT-1

B	19.41965750596541	13.25538625917117	11.23112781957575
Br	19.33666446744866	16.95192070349123	2.68842249859101
Br	22.34624194105621	8.97232565344089	9.14607467754448
H	20.23993897213305	10.13175586671681	14.72950949652855
Br	18.13633702729357	19.75339119250620	17.76900918227074
C	20.19321196345757	15.68583885321558	3.78200172594863
C	21.37094679123954	15.03890133526739	3.52997806480244
H	21.95981460771049	15.19777016649800	2.63986352449565
C	21.71917907368370	14.15595756575061	4.57943951407152
H	22.62079407099463	13.56037796525561	4.58605806125502
C	20.81669695464538	14.15070841271328	5.61931855323792
C	20.84843326907895	13.36442296881723	6.82314639992201
C	20.27316570181169	13.64135684609500	8.04144163467736
H	19.75508022880735	14.56036664461567	8.26466616692869
C	20.48153426783754	12.58561206152095	8.95310121793724
C	21.21937924548712	11.50574563444358	8.40484254739455
C	21.32935096759587	10.53475203845951	9.37646661685112
C	20.65208770309553	11.03785908893880	10.53880163866382
C	20.52626570730441	10.52042738194679	11.83515249464198
C	20.08829062495527	11.34724281694665	12.86982699934052
C	20.02798377739289	11.08081147484186	14.26930352314955
C	19.70117218137300	12.28048489977616	14.86508319725798
C	19.52550215518049	13.25213011627721	13.83655085986279
C	19.20171393780602	14.53690287557875	14.31101115411944
H	19.03850690989159	15.39743942064321	13.68082204431382
C	19.13605007649024	14.55950784248116	15.68766105678487
C	18.86992195553857	15.67254893391815	16.55222850896381
C	18.75780125238978	15.67860088826370	17.92771453306574
C	18.44083360289049	17.92011358702987	17.50683705577022
C	20.91245161208419	9.11690157472264	12.10580648012487
C	22.04463476845444	8.82304289623502	12.86707471245403
H	22.60714690387775	9.62873827100275	13.31793581750509
C	22.48392962904265	7.51494856408921	12.98464574410393
H	23.38836588656978	7.28053851052036	13.52758924434600
C	21.78530435216703	6.47926204521814	12.36565477755180
C	20.61317449951128	6.76275991967144	11.66345669182492
H	20.06275478706829	5.96224213466938	11.19276824323324
C	20.18730848525654	8.07344800230983	11.52897615216758
H	19.30496551929654	8.29857813225184	10.94531910488829
C	22.36681395186917	5.11057166901068	12.42294869868646
C	22.09305745003424	2.85657051249857	11.78435017787818
H	22.95899058936456	2.83979968054074	11.12306440545775
H	21.29220686478456	2.24805094818378	11.37397791274080
H	22.39233290074079	2.49726987364611	12.76732477648552
F	18.04624228292252	13.22583898692647	11.01448336512184
F	19.90194321321199	14.55210244589709	11.10400270904178
N	20.16225595642104	12.31099997223232	10.23419924319214
N	19.74719993788360	12.67810139092560	12.63694448824931
O	23.45032013036510	4.85079114427580	12.88808630010666
O	21.56020031991942	4.18547375838355	11.86955862144602
S	19.49505570275357	15.23472959000660	5.29039673418121

S	21.68429139222183	11.80862132028069	6.77242897388460
S	19.46672462223757	12.98697671324596	16.42805339947753
S	18.66490016224893	17.28297918804017	15.92140634401973
C	18.51143576303929	16.95753944009808	18.47483750982829
H	18.85145658584990	14.78495807070792	18.52750015195420
H	18.39077879024845	17.16416574978817	19.52721445208102

94

BD-1

C	-4.26265108889794	5.03328676439349	-3.28911415542909
N	-5.06075189197238	4.30420789389914	-2.47117587899638
C	-2.92642994594015	4.74285228861730	-3.60102907839339
C	-2.38024081418005	3.53648988629605	-3.10704653068440
N	-3.11352854406203	2.76488664074962	-2.19833308164667
B	-4.52166069346738	3.12040741494178	-1.62142078935097
F	-4.42953438834268	3.54189711375522	-0.29321061616546
F	-5.36449401190323	2.01710420732041	-1.72668191186836
C	-4.98719175647327	6.15522571480914	-3.77118529479498
C	-6.27118132083091	6.07290637142269	-3.16683011255671
C	-6.28384498323768	4.93248842835182	-2.38016879096375
C	-1.19523562920987	2.82634823762594	-3.40306635760309
C	-1.21509811426638	1.65955603952749	-2.65731318156333
C	-2.41116237795114	1.64128435845305	-1.91841085813233
C	-7.40393196822392	4.36326250225610	-1.57722428415305
C	-8.26332347958443	3.38657092855935	-2.39458002448978
H	-8.02249528053267	5.18530847975677	-1.21248226893462
H	-6.99720976621362	3.85010910023691	-0.70647751471986
H	-8.74663704976372	3.90006060576607	-3.22764221294388
H	-9.03907390103877	2.94601808712436	-1.76600007846811
H	-7.64755145694639	2.58078173997825	-2.79173938967039
C	-2.85947194092843	0.56704710049043	-0.98494487915017
C	-2.83774027949531	0.96904780671324	0.49872434855524
H	-2.19697144990621	-0.28623631569179	-1.14099247545241
H	-3.86722767519480	0.25122542930690	-1.25674096180510
H	-1.84418170842491	1.31067730012943	0.79608911698752
H	-3.11001893267224	0.11189858167851	1.11678738805700
H	-3.54267534753279	1.77122202792816	0.69765581622094
C	-4.37468665905577	7.05774271298277	-4.65538007792744
C	-3.02612112422138	6.82567677396388	-5.00624793418441
C	-2.27111533871916	5.72814857860702	-4.42938472547831
C	-2.37674353990878	7.64242658688890	-5.95389401691286
C	-1.04672991531368	7.51487135767374	-6.30930847301053
C	-0.23886562142100	6.60157074890729	-5.51755977954149
C	-0.90705453123369	5.72176975143052	-4.64598959223816
C	-0.44247444299962	8.29638958581514	-7.36782256520488
C	1.16823357361571	6.55742901914257	-5.63771779167012
C	1.76288274625883	7.37618877310845	-6.61012210446279
C	0.95837292549612	8.20437406622129	-7.43719875853462
H	-7.09143612573578	6.76047772699687	-3.28504742516248
H	-0.44709476218808	3.09831228329227	-4.12529345477087
H	-0.47501820616235	0.87616276976485	-2.65419557107524
C	-5.13486058953216	8.21164433291433	-5.17398932395215
H	-0.30659466686264	5.01260477667528	-4.10621486857889
H	-2.95981689716808	8.42046078498146	-6.41184820453417
C	2.01050924839686	5.71202660781145	-4.76920144578568
C	-1.09338588354903	9.11610402230115	-8.31767210193396
N	-0.33041470164700	9.91605219792539	-9.17729278839908
B	1.22745524215816	9.93814242301146	-9.30688956105026
N	1.76098167005302	8.89809558629290	-8.28351442335893
C	3.07165978439905	8.55202451974787	-8.02514587604723

C	3.10669191300882	7.62154624152704	-7.00211657278289
C	4.19139969957138	9.16823786558268	-8.78995432875366
C	-2.45213251279958	9.32984593860950	-8.64762362541691
C	-2.49221602297638	10.27008694908679	-9.66260367954262
C	-1.16567790331965	10.62231281253496	-9.97184346430659
C	-0.70932899065873	11.63145406094174	-10.97054480883470
H	-1.46822350523371	11.69552928735133	-11.75358545013701
H	0.21332185227373	11.29297597675349	-11.43950538878718
C	-0.49086254787302	13.02409116530324	-10.35191386852991
H	-1.41069921552352	13.39997138958286	-9.89974637336893
H	-0.17158474688299	13.72741532995221	-11.12262065167123
H	0.27918372285170	12.98255588423310	-9.58433830390000
H	4.12040611136788	10.25388976721441	-8.67173014851882
H	4.02035396262761	8.97758647556300	-9.85358734263393
C	5.57827320632075	8.68234584584546	-8.38450257316954
H	5.78016303227689	8.88650843998106	-7.33115488396041
H	6.33910773919953	9.19393764197810	-8.97283237137992
H	5.69193329424788	7.60979924820699	-8.55618993482451
F	1.60656474145683	9.57189279442509	-10.60095554805419
F	1.71620188280602	11.20842410177166	-9.00380094871568
H	-3.30175358500953	8.82104127092838	-8.23050949928388
H	-3.36748523944424	10.65770086739721	-10.15733462072476
H	3.99118989273514	7.17994817310033	-6.58006767753930
C	-6.32354840138921	8.01142753409703	-5.88291714765412
C	-7.03894947688057	9.09411832388493	-6.37508767524802
C	-6.59142211272123	10.39187387921706	-6.15107199280920
C	-5.41864460690902	10.60226412004677	-5.43554270354082
C	-4.69394611127762	9.52023152383787	-4.95581047204981
C	2.93729880552861	4.82080902298878	-5.32208357617248
C	3.73384314615638	4.03254130223298	-4.50343025062778
C	3.63451990900157	4.13255202969901	-3.11946245062398
C	2.72842636151270	5.02437757935176	-2.55827736789512
C	1.92120369239907	5.80345371112256	-3.37503059757647
H	3.01781532281694	4.73383438993627	-6.39770480748254
H	4.43396918242776	3.33755281902772	-4.94835460161126
H	4.26105155797850	3.52110383993953	-2.48386695411945
H	2.64904264152796	5.11907875608952	-1.48297199765490
H	1.22805737407634	6.50603855761901	-2.93287150376035
H	-6.67101212641783	7.00228969758203	-6.06227700126110
H	-7.94852708524998	8.92434770880183	-6.93600116012704
H	-7.15363953103823	11.23312558346119	-6.53354400354905
H	-5.06386525483422	11.60722323748010	-5.24858070811667
H	-3.78461645519694	9.68494813486080	-4.39430604135302

98

## BOPHY-1

F 4.145387 2.486631 -4.239129  
F 5.769483 4.042372 -4.552767  
F 6.680987 0.216421 0.004858  
F 5.973552 -0.790276 -1.886840  
O 11.180321 -10.963052 5.946379  
O 5.271162 13.546926 -8.396888  
O 3.495823 11.654147 -7.102408  
O 11.033187 -6.438295 3.076116  
O 6.558585 16.879974 -8.435751  
N 4.559790 4.043580 -2.464931  
N 6.203981 2.281836 -3.004766  
N 8.074426 0.369001 -1.969728  
N 5.943137 1.629089 -1.783610  
C 4.470955 3.446099 -1.214476  
C 3.825063 4.328586 -0.314246  
C 3.553214 5.471717 -1.047486  
H 3.144215 6.258612 -0.708950  
C 3.979623 5.281054 -2.378855  
C 7.404402 2.073009 -3.534125  
H 7.619616 2.551954 -4.325053  
C 8.361721 1.222552 -3.033154  
C 9.705657 1.025489 -3.429377  
C 10.205724 0.055737 -2.595943  
H 11.095360 -0.275997 -2.608087  
C 9.185964 -0.369332 -1.718484  
C 5.093798 2.239520 -0.950328  
H 4.904764 1.815814 -0.121448  
C 3.495898 4.057134 1.111246  
H 4.247723 3.595880 1.539348  
H 2.696438 3.492974 1.159825  
H 3.326620 4.904588 1.575783  
C 10.416068 1.732229 -4.545177  
H 9.989792 1.506316 -5.398346  
H 11.355310 1.450637 -4.564912  
H 10.368987 2.700294 -4.402476  
C 3.888193 6.176048 -3.506800  
H 4.144208 5.854610 -4.363005  
C 3.457684 7.438727 -3.399015  
H 3.144129 7.702795 -2.541291  
C 3.413278 8.458268 -4.443464  
C 2.860659 9.706683 -4.141363  
H 2.465306 9.850210 -3.289712  
C 2.880975 10.734067 -5.062847  
H 2.487606 11.570324 -4.845760  
C 3.467031 10.553817 -6.295540  
C 3.990786 9.309502 -6.638630  
H 4.366647 9.166467 -7.499390  
C 4.069522 11.506004 -8.413283  
H 3.494111 10.930876 -8.978015  
H 4.966503 11.092276 -8.352559  
C 4.170014 12.880654 -9.003822

H	4.306918	12.821359	-9.981475
H	3.334621	13.384624	-8.835314
C	5.371715	14.894233	-8.800397
H	4.537371	15.378886	-8.577237
H	5.513557	14.946994	-9.778051
C	6.533912	15.511203	-8.077784
H	6.421394	15.412405	-7.098613
H	7.377744	15.068586	-8.344969
C	7.681012	17.570652	-7.907757
H	7.647588	18.510419	-8.185569
H	7.666196	17.519698	-6.928586
H	8.505769	17.160050	-8.243256
C	9.214311	-1.431689	-0.743867
H	8.476512	-1.527141	-0.153328
C	10.238372	-2.289256	-0.636082
H	10.943821	-2.172404	-1.261537
C	10.404911	-3.376195	0.315764
C	11.619052	-4.066975	0.330945
H	12.290882	-3.829091	-0.297547
C	11.874328	-5.082592	1.232693
H	12.711745	-5.530871	1.222067
C	10.907310	-5.440763	2.142032
C	9.680345	-4.786276	2.134442
H	9.005697	-5.043649	2.750788
C	9.437028	-3.766662	1.240284
H	8.596322	-3.323583	1.253947
C	12.318140	-7.030811	3.259350
H	12.901956	-6.406916	3.760322
H	12.733848	-7.200398	2.377337
C	11.002720	-11.188809	4.577057
H	10.114571	-10.826780	4.331125
H	10.960894	-12.168698	4.443464
C	3.956519	8.288797	-5.712592
H	4.315694	7.441644	-5.949415
C	12.147286	-11.744356	6.565761
H	12.195246	-11.512355	7.516089
H	11.911631	-12.690573	6.473158
H	13.017664	-11.581278	6.145249
C	12.199783	-8.304279	4.004735
H	13.066673	-8.524342	4.431320
H	11.518571	-8.214361	4.718240
O	11.832429	-9.324439	3.124240
C	11.976767	-10.655746	3.611548
H	12.873165	-10.722808	4.025988
H	11.976297	-11.259914	2.826693
B	5.127442	3.243696	-3.646464
B	6.676485	0.281585	-1.379948

1. Graser, M.; Kopacka, H.; Wurst, K.; Ruetz, M.; Kreutz, C. R.; Müller, T.; Hirtenlehner, C.; Monkowius, U.; Knör, G.; Bildstein, B., Efficient fluorophores based on pyridyl-enolato and enamido difluoroboron complexes: Simple alternatives to boron-dipyrromethene (bodipy) dyes. *Inorganica Chimica Acta* 2013, 405, 116-120.
2. Tanaka, K.; Yamane, H.; Yoshii, R.; Chujo, Y., Efficient light absorbers based on thiophene-fused boron dipyrromethene (BODIPY) dyes. *Bioorg Med Chem* 2013, 21 (10), 2715-9.
3. Jiang, X.-D.; Zhang, H.; Zhang, Y.; Zhao, W., Development of non-symmetric thiophene-fused BODIPYs. *Tetrahedron* 2012, 68 (47), 9795-9801.
4. Arroyo, I. J.; Hu, R.; Merino, G.; Tang, B. Z.; Pena-Cabrera, E., The smallest and one of the brightest. Efficient preparation and optical description of the parent borondipyrromethene system. *J Org Chem* 2009, 74 (15), 5719-22.
5. Banuelos, J.; Martin, V.; Gomez-Duran, C. F.; Arroyo Cordoba, I. J.; Pena-Cabrera, E.; Garcia-Moreno, I.; Costela, A.; Perez-Ojeda, M. E.; Arbeloa, T.; Lopez Arbeloa, I., New 8-amino-BODIPY derivatives: surpassing laser dyes at blue-edge wavelengths. *Chemistry* 2011, 17 (26), 7261-70.
6. Liras, M.; Prieto, J. B.; Pintado-Sierra, M.; Arbeloa, F. L.; Garcia-Moreno, I.; Costela, A.; Infantes, L.; Sastre, R.; Amat-Guerri, F., Synthesis, photophysical properties, and laser behavior of 3-amino and 3-acetamido BODIPY dyes. *Org Lett* 2007, 9 (21), 4183-6.
7. Loudet, A.; Burgess, K., BODIPY dyes and their derivatives: syntheses and spectroscopic properties. *Chem Rev* 2007, 107 (11), 4891-932.
8. Pavlopoulos, T. G.; Boyer, J. H.; Shah, M.; Thangaraj, K.; Soong, M. L., Laser action from 2,6,8-position trisubstituted 1,3,5,7-tetramethylpyrromethene-BF(2) complexes: part 1. *Appl Opt* 1990, 29 (27), 3885-6.
9. Rihn, S.; Retailleau, P.; Bugsaliewicz, N.; Nicola, A. D.; Ziessel, R., Versatile synthetic methods for the engineering of thiophene-substituted Bodipy dyes. *Tetrahedron Lett* 2009, 50 (50), 7008-7013.
10. Yu, C.; Jiao, L.; Yin, H.; Zhou, J.; Pang, W.; Wu, Y.; Wang, Z.; Yang, G.; Hao, E.,  $\alpha$ -/ $\beta$ -Formylated Boron-Dipyrin (BODIPY) Dyes: Regioselective Syntheses and Photophysical Properties. *Eur J Org Chem* 2011, 2011 (28), 5460-5468.
11. Leen, V.; Miscoria, D.; Yin, S.; Filarowski, A.; Ngongo, J. M.; Van der Auweraer, M.; Boens, N.; Dehaen, W., 1,7-Disubstituted boron dipyrromethene (BODIPY) dyes: synthesis and spectroscopic properties. *J Org Chem* 2011, 76 (20), 8168-76.
12. Wittmershaus, B. P.; Skibicki, J. J.; McLafferty, J. B.; Zhang, Y. Z.; Swan, S., Spectral properties of single BODIPY dyes in polystyrene microspheres and in solutions. *Journal of Fluorescence* 2001, 11 (2), 119-128.
13. Ulrich, G.; Goeb, S.; De Nicola, A.; Retailleau, P.; Ziessel, R., Chemistry at boron: synthesis and properties of red to near-IR fluorescent dyes based on boron-substituted diisoindolomethene frameworks. *J Org Chem* 2011, 76 (11), 4489-505.
14. Jiao, L.; Yu, C.; Liu, M.; Wu, Y.; Cong, K.; Meng, T.; Wang, Y.; Hao, E., Synthesis and functionalization of asymmetrical benzo-fused BODIPY dyes. *J Org Chem* 2010, 75 (17), 6035-8.
15. Umezawa, K.; Matsui, A.; Nakamura, Y.; Citterio, D.; Suzuki, K., Bright, color-tunable fluorescent dyes in the Vis/NIR region: establishment of new "tailor-made" multicolor fluorophores based on borondipyrromethene. *Chemistry* 2009, 15 (5), 1096-106.
16. Zhou, Y.; Xiao, Y.; Li, D.; Fu, M.; Qian, X., Novel fluorescent fluorine-boron complexes: synthesis, crystal structure, photoluminescence, and electrochemistry properties. *J Org Chem* 2008, 73 (4), 1571-4.
17. Kubota, Y.; Tsuzuki, T.; Funabiki, K.; Ebihara, M.; Matsui, M., Synthesis and fluorescence properties of a pyridomethene-BF<sub>2</sub> complex. *Org Lett* 2010, 12 (18), 4010-3.
18. Tomimori, Y.; Okujima, T.; Yano, T.; Mori, S.; Ono, N.; Yamada, H.; Uno, H., Synthesis of  $\pi$ -expanded O-chelated boron-dipyrromethene as an NIR dye. *Tetrahedron* 2011, 67 (18), 3187-3193.
19. Kubota, Y.; Hara, H.; Tanaka, S.; Funabiki, K.; Matsui, M., Synthesis and fluorescence properties of novel pyrazine-boron complexes bearing a beta-iminoketone ligand. *Org Lett* 2011, 13 (24), 6544-7.

20. Nakamura, M.; Tahara, H.; Takahashi, K.; Nagata, T.; Uoyama, H.; Kuzuhara, D.; Mori, S.; Okujima, T.; Yamada, H.; Uno, H., pi-Fused bis-BODIPY as a candidate for NIR dyes. *Org Biomol Chem* 2012, 10 (34), 6840-9.
21. Khan, T. K.; Ravikanth, M., 3-(Pyridine-4-thione)BODIPY as a chemodosimeter for detection of Hg(II) ions. *Dyes and Pigments* 2012, 95 (1), 89-95.
22. Rohand, T.; Baruah, M.; Qin, W.; Boens, N.; Dehaen, W., Functionalisation of fluorescent BODIPY dyes by nucleophilic substitution. *Chem Commun (Camb)* 2006, (3), 266-8.
23. Uppal, T.; Hu, X.; Fronczek, F. R.; Maschek, S.; Bobadova-Parvanova, P.; Vicente, M. G., Synthesis, computational modeling, and properties of benzo-appended BODIPYs. *Chemistry* 2012, 18 (13), 3893-905.
24. Leen, V.; Leemans, T.; Boens, N.; Dehaen, W., 2-and 3-Monohalogenated BODIPY Dyes and Their Functionalized Analogues: Synthesis and Spectroscopy. *Eur J Org Chem* 2011, (23), 4386-4396.
25. Yu, C.; Xu, Y.; Jiao, L.; Zhou, J.; Wang, Z.; Hao, E., Isoindole-BODIPY dyes as red to near-infrared fluorophores. *Chemistry* 2012, 18 (21), 6437-42.