Supporting Information for

Self-assembly of (Boron-dipyrromethane)-diphenylalanine Conjugates Forming Chiral Supramolecular Materials

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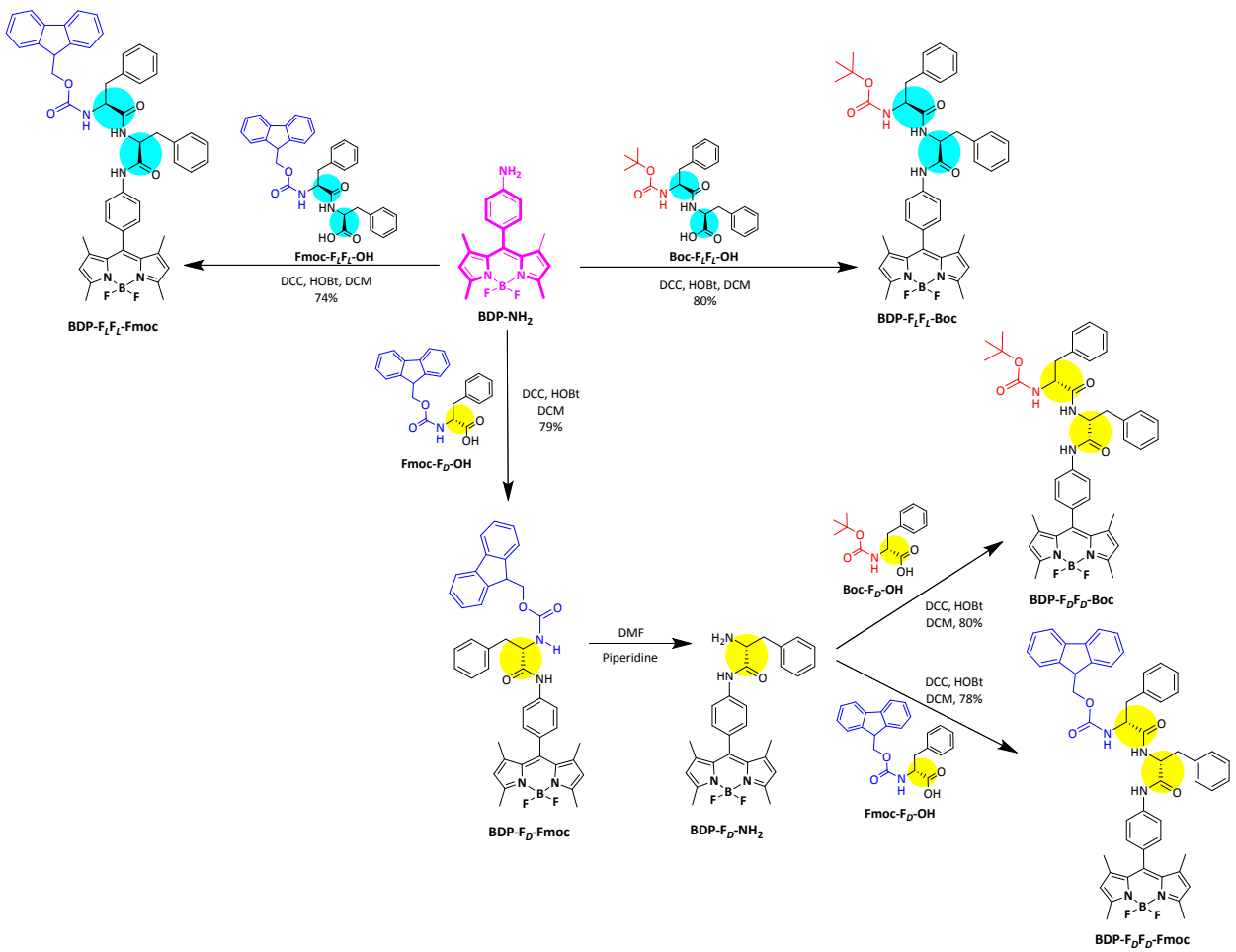


Scheme S1. Reaction conditions for the preparation of compounds **BDP-F$_L$F$_L$-Boc**, **BDP-F$_L$F$_L$-Fmoc**, **BDP-F$_D$F$_D$-Boc** and **BDP-F$_D$F$_D$-Fmoc**.

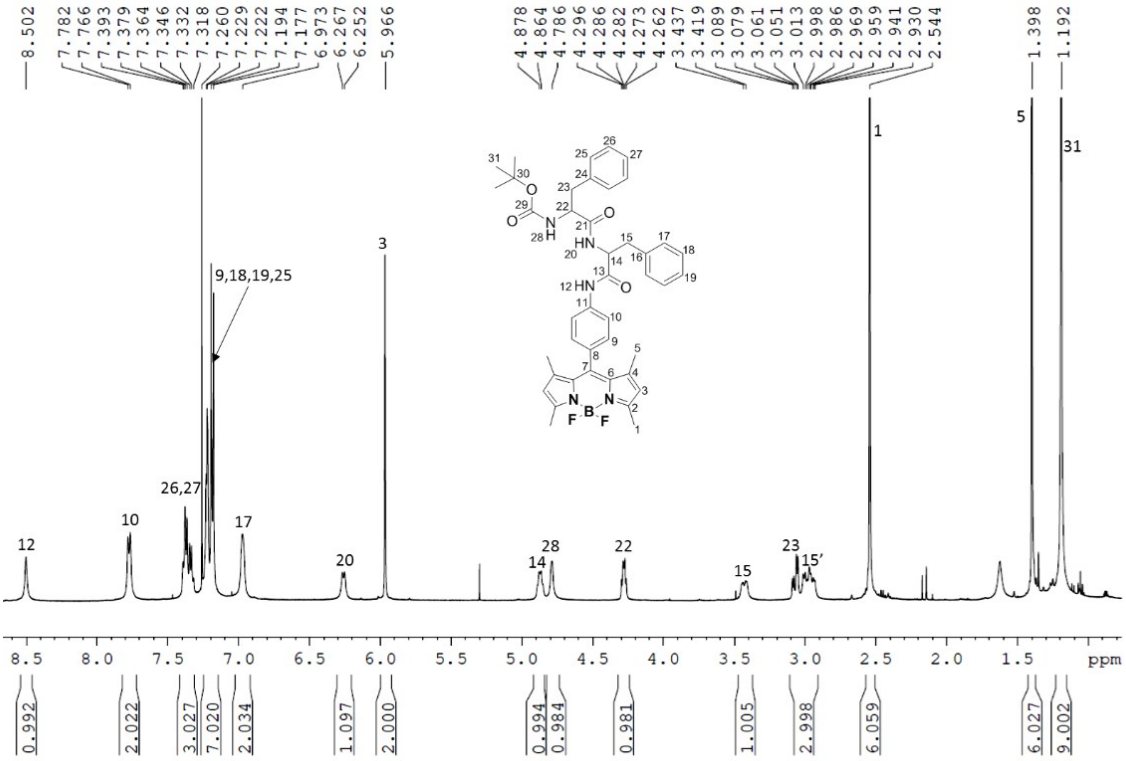


Figure S1. ^{1}H NMR spectrum of **BDP-F$_L$F$_L$-Boc** in $CDCl_3$.

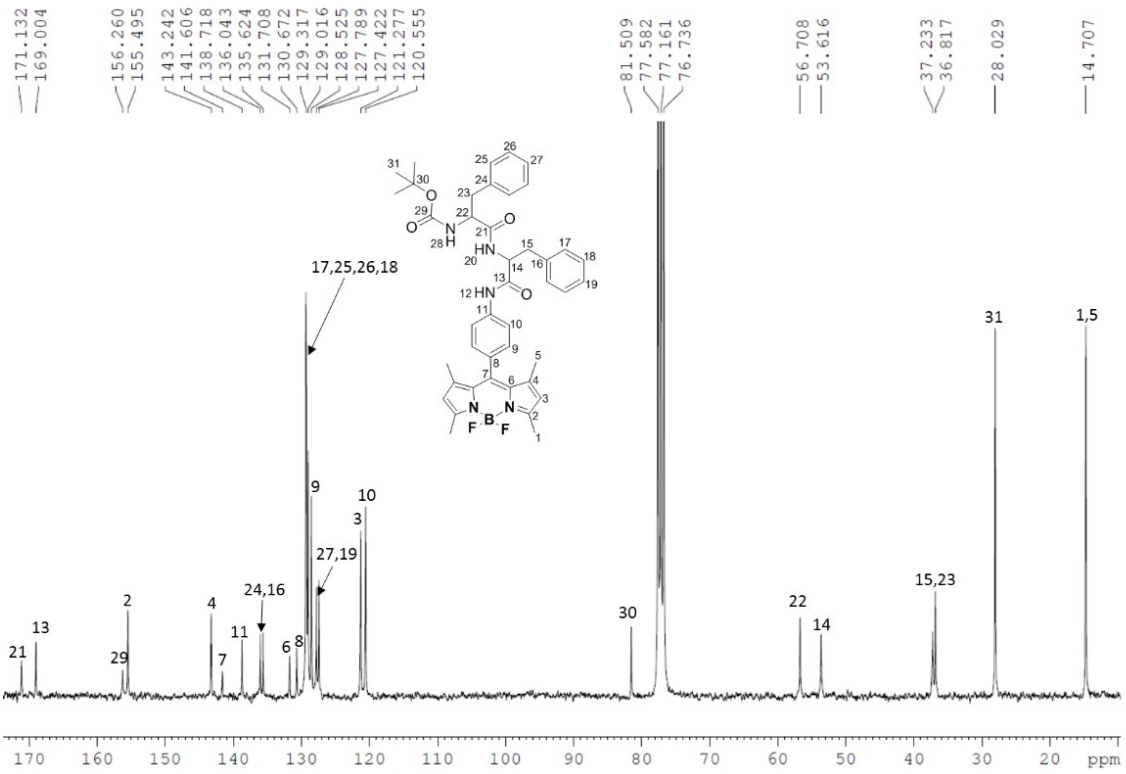


Figure S2. ^{13}C NMR spectrum of **BDP-F$_L$F$_L$-Boc** in $CDCl_3$.

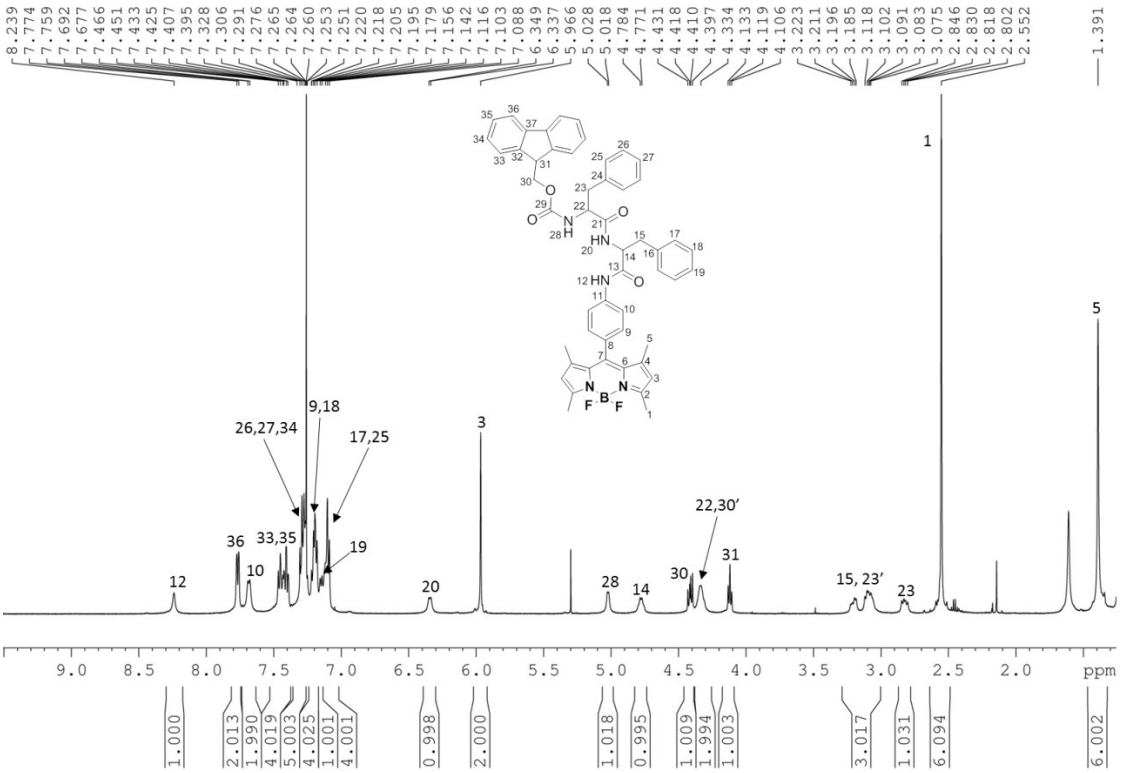


Figure S3. ^{1}H NMR spectrum of **BDP-F$_L$F$_L$-Fmoc** in $CDCl_3$.

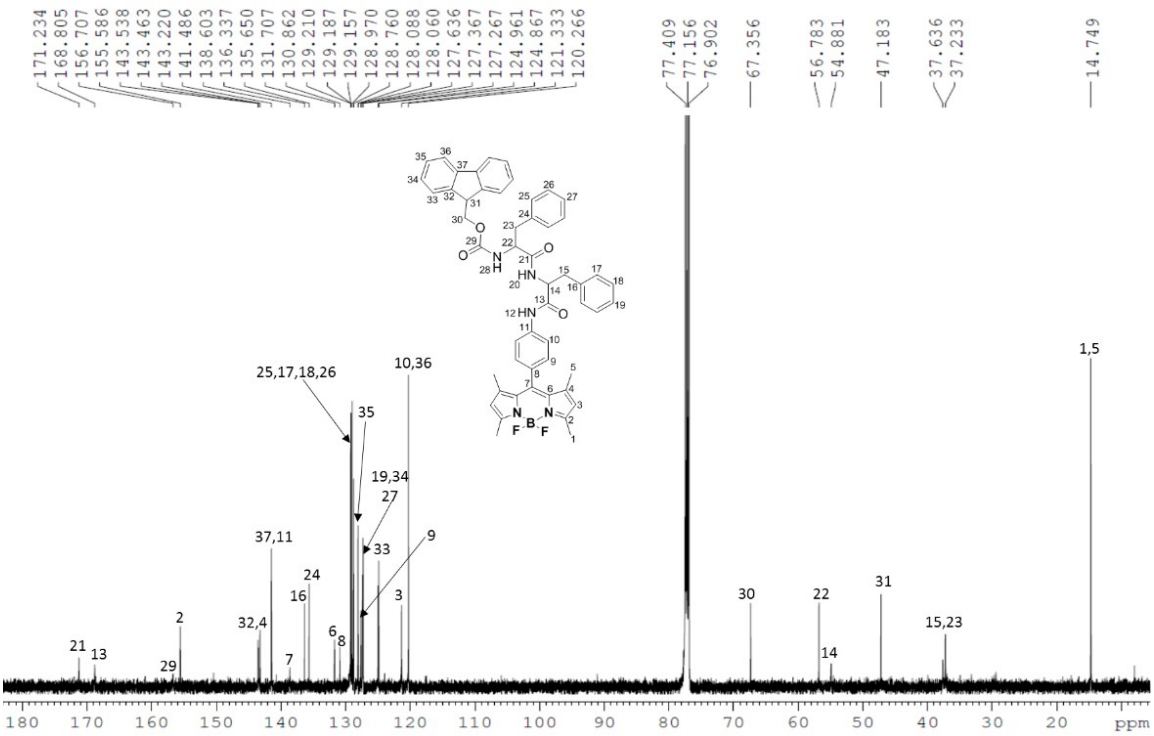


Figure S4. ^{13}C NMR spectrum of **BDP-F$_L$F$_L$-Fmoc** in $CDCl_3$.

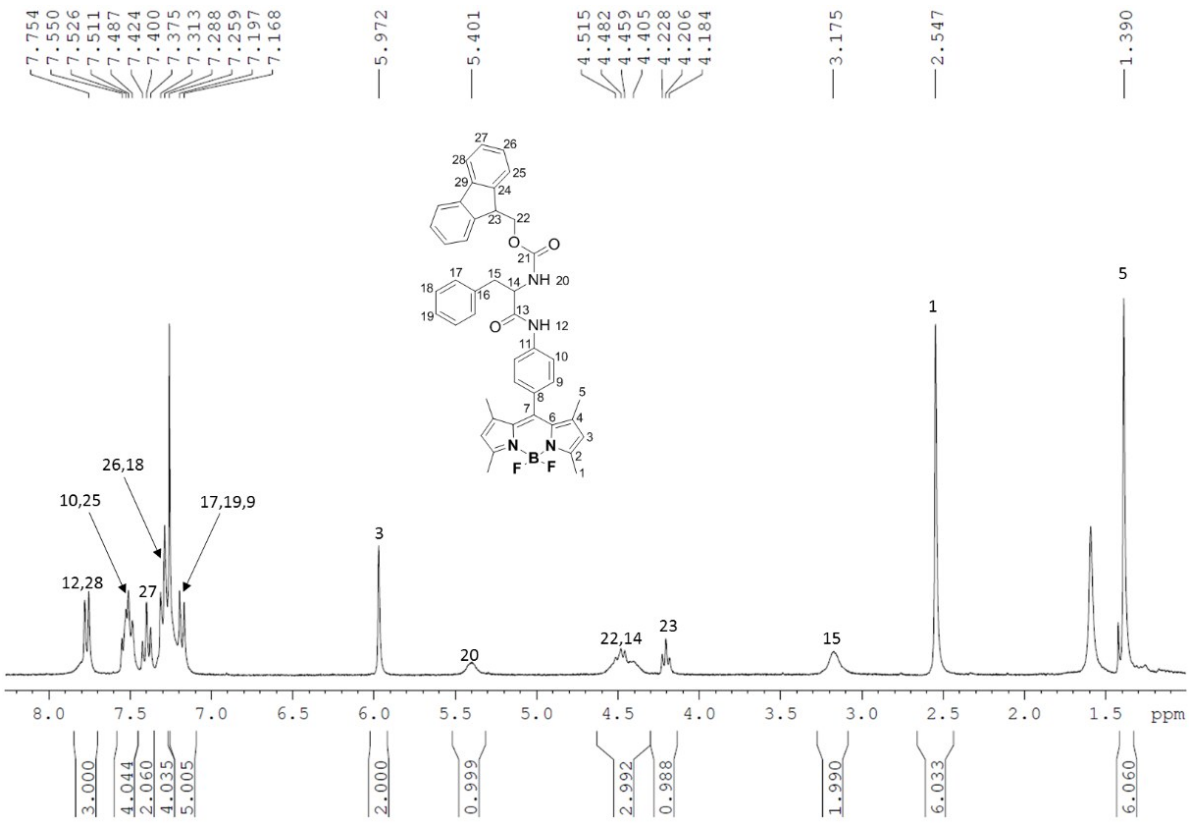


Figure S5. ^{1}H NMR spectrum of **BDP-F$_D$-Fmoc** in $CDCl_3$.

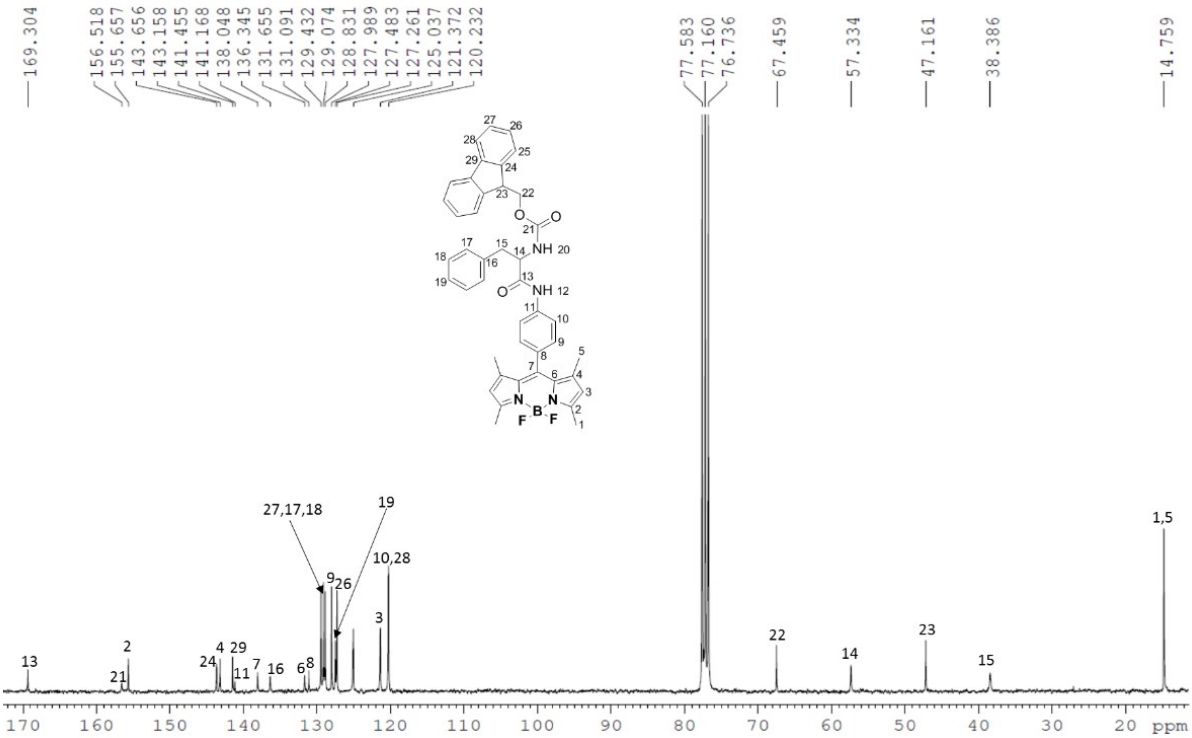


Figure S6. ^{13}C NMR spectrum of **BDP-F$_D$-Fmoc** in $CDCl_3$.

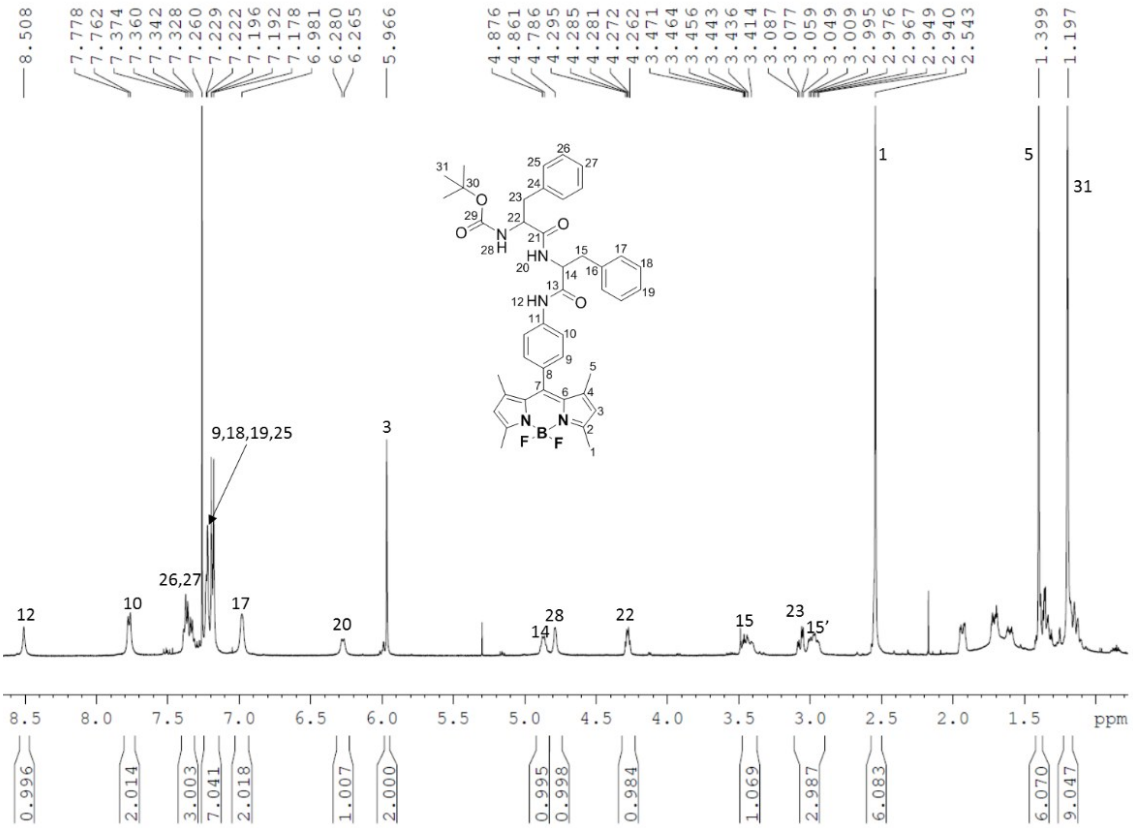


Figure S7. ^{1}H NMR spectrum of **BDP-F$_D$F$_D$-Boc** in $CDCl_3$.

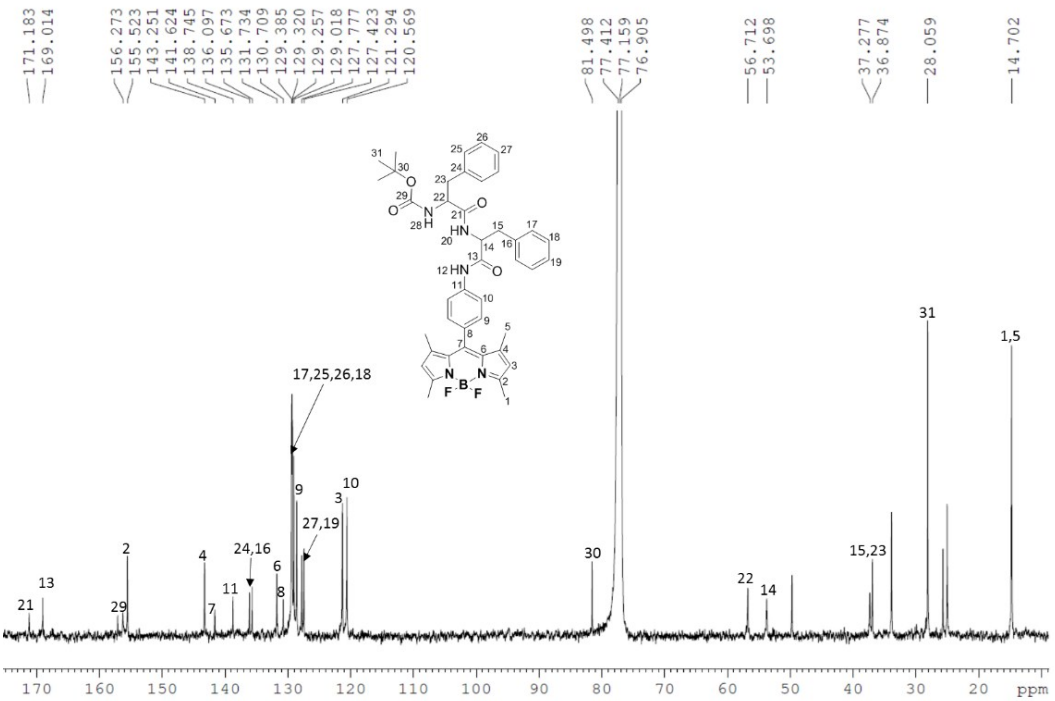


Figure S8. ^{13}C NMR spectrum of **BDP-F$_D$F$_D$-Boc** in $CDCl_3$.

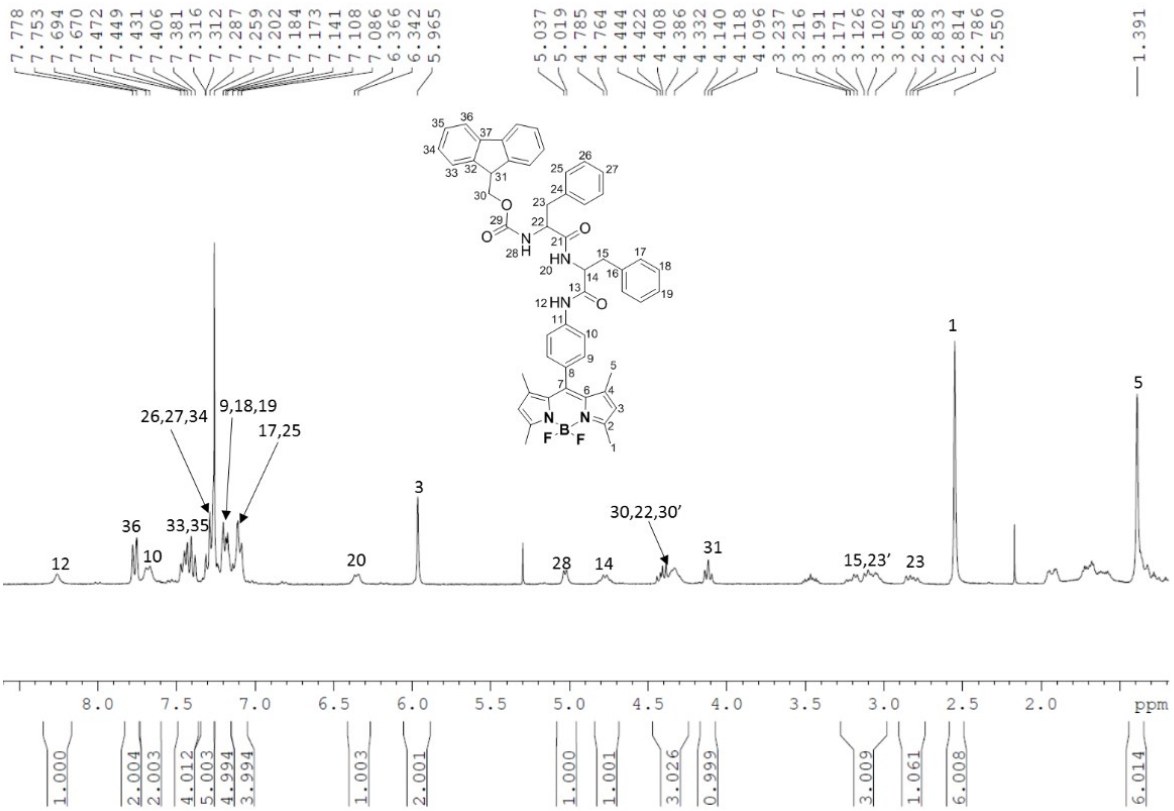


Figure S9. ^{1}H NMR spectrum of **BDP-F$_D$F$_D$-Fmoc** in $CDCl_3$.

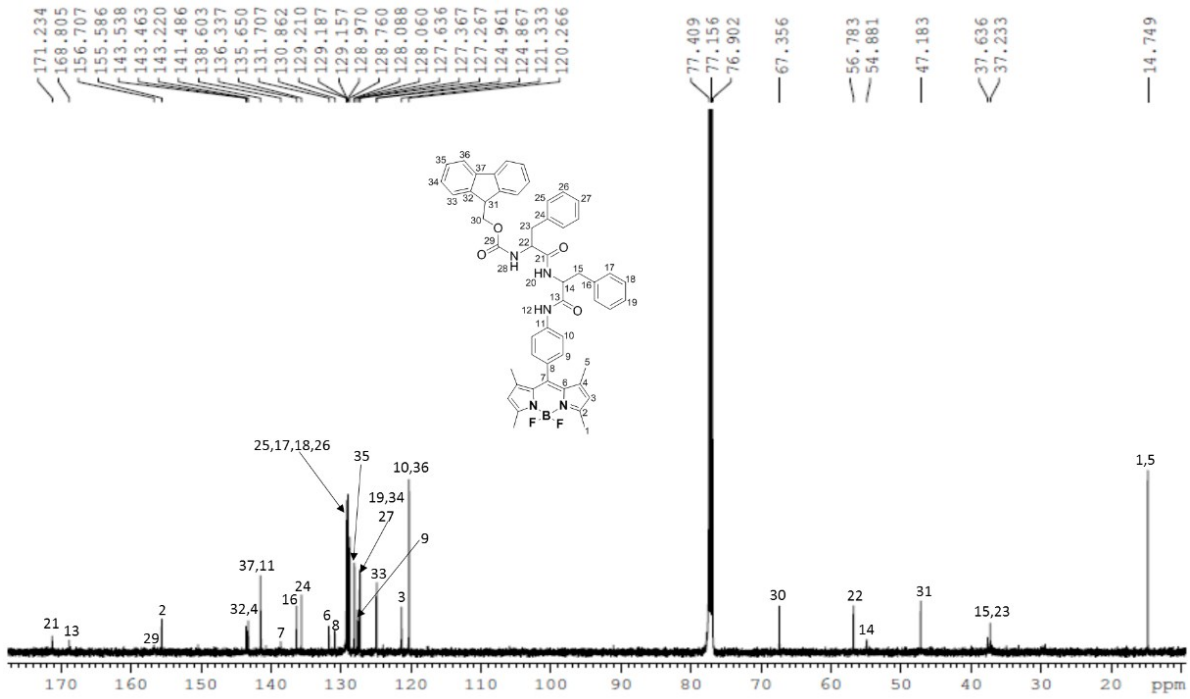


Figure S10. ^{13}C NMR spectrum of **BDP-F$_D$F$_D$-Fmoc** in $CDCl_3$.

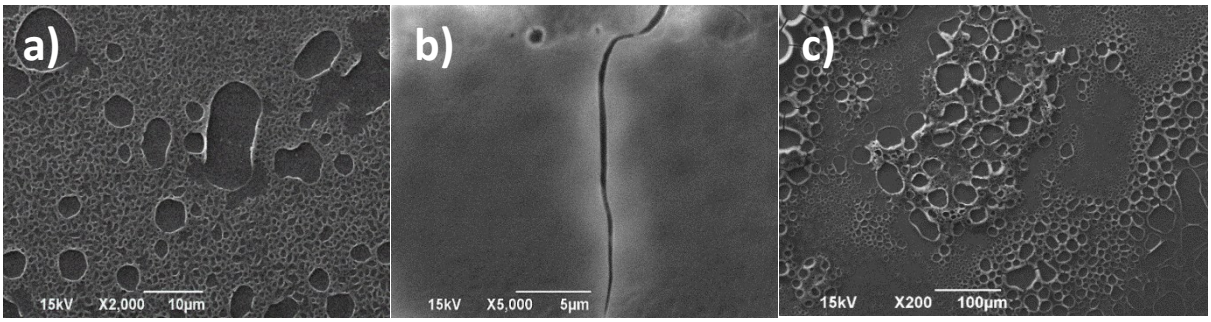


Figure S11. SEM images of a) **BDP-NH_2** in 1:1 DCM/heptane 1 mM, b) **BDP-F_LF_L-Boc** in DCM 1 mM, c) **BDP-F_LF_L-Fmoc** in DCM 1 mM.

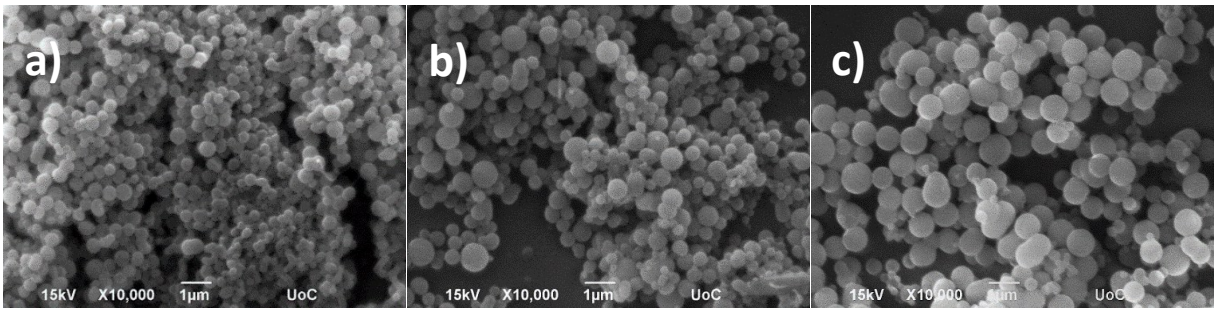


Figure S12. SEM images of **BDP-F_LF_L-Boc** in DCM/heptane 1:1 a) 1 mM, b) 2 mM, c) 4 mM.

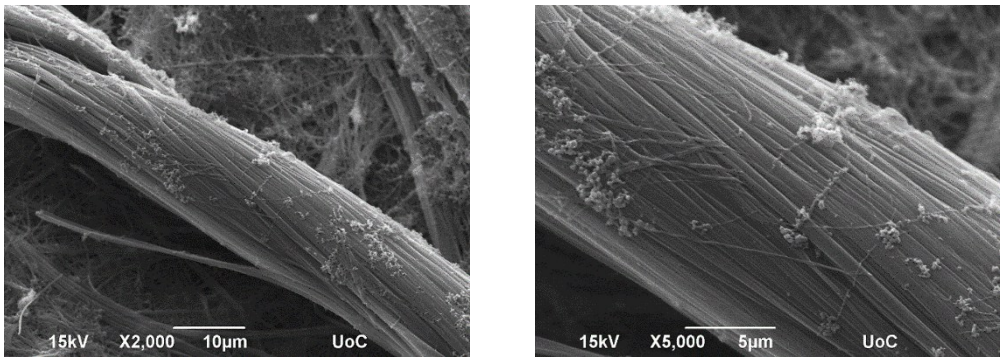


Figure S13. SEM images of **BDP-F_LF_L-Boc** in dry DCM/dry heptane 2:8 1 mM.

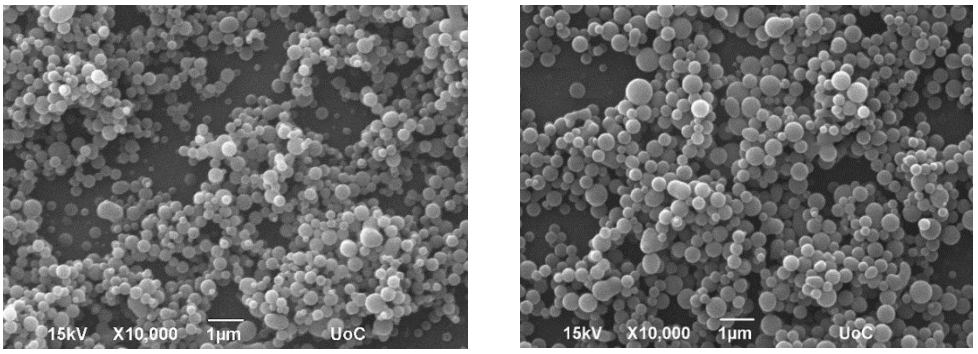


Figure S14. SEM images of a) **BDP-F$_L$F$_L$-Boc** and b) **BDP-F$_L$F$_L$-Fmoc** in dry DCM/dry heptane 1:1 1 mM.

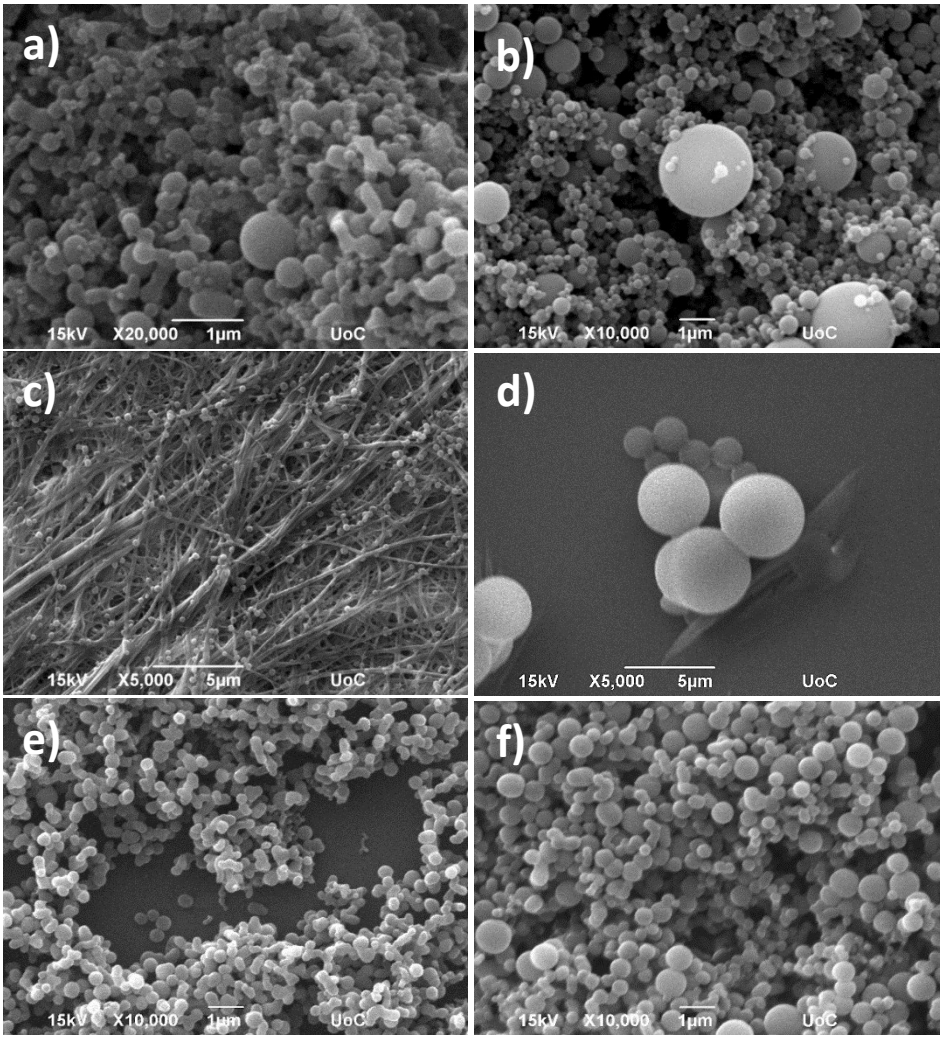


Figure S15. SEM images of a) **BDP-F$_D$F$_D$-Boc** in acetonitrile/water 1:60, b) **BDP-F$_D$F$_D$-Fmoc** in acetonitrile/water 1:60, c) **BDP-F$_D$F$_D$-Boc** in dry DCM/dry heptane 2:8, d) **BDP-F$_D$F$_D$-Fmoc** in dry DCM/dry heptane, e) **BDP-F$_D$F$_D$-Boc** in dry DCM/dry heptane 1:1, f) **BDP-F$_D$F$_D$-Fmoc** in dry DCM/dry heptane 1:1. In all the above studies the concentration was 1 mM.

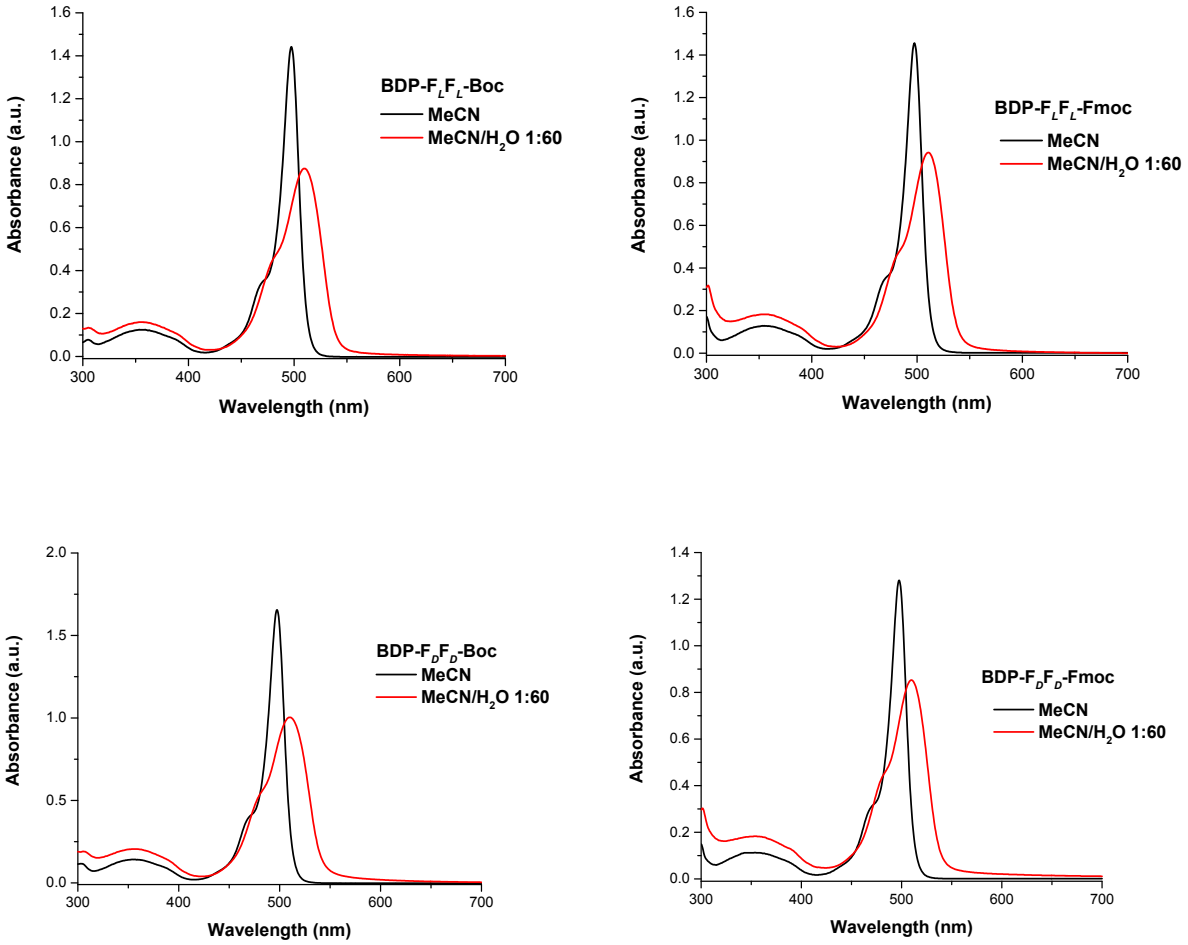


Figure S16. Absorption spectra of **BDP-F$_L$F$_L$-Boc**, **BDP-F$_L$F$_L$-Fmoc**, **BDP- F$_D$F$_D$-Boc** and **BDP- F$_D$F$_D$-Fmoc** in MeCN solution and MeCN/water 1:60 with 1.8x10^{-5} M concentration.

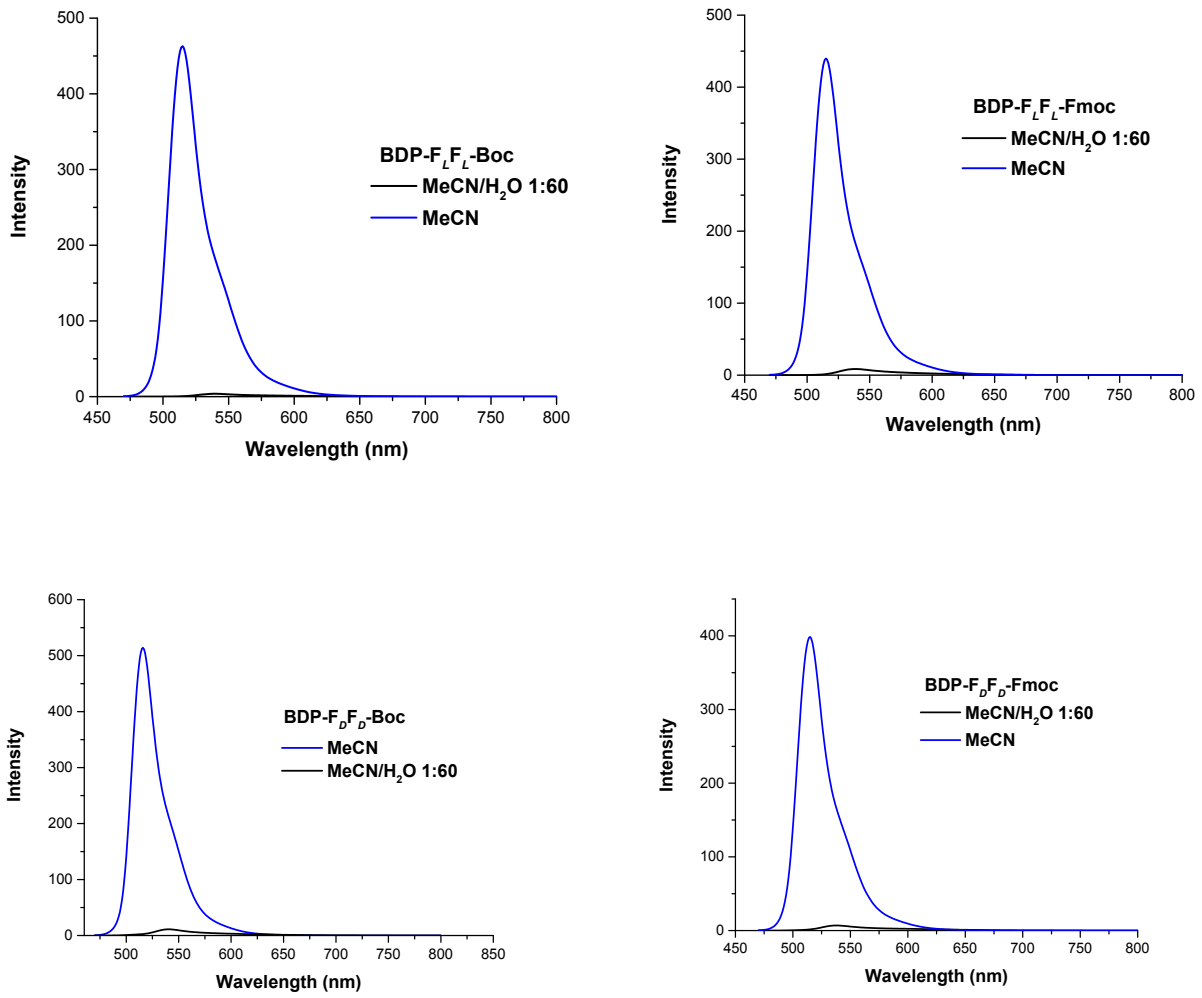


Figure S17. Emission spectra of **BDP-F$_L$F$_L$-Boc**, **BDP-F$_D$F$_D$-Boc**, **BDP-F$_L$F$_L$-Fmoc** and **BDP-F$_D$F$_D$-Fmoc** in MeCN and MeCN/water 1:60 solutions with 1.8x10^{-5} M concentration upon excitation at 460 nm.

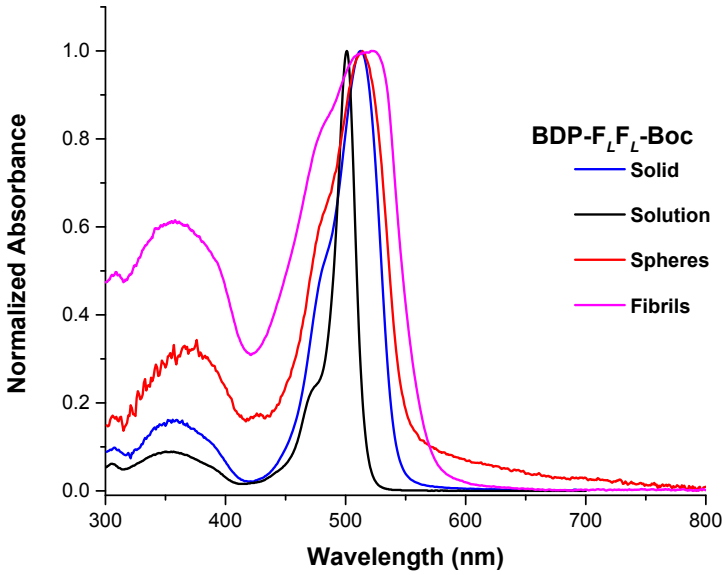


Figure S18. Normalized Absorption spectra of **BDP-F$_L$F$_L$-Boc** in DCM solution (black line), as self-assembled spheres (red line), as self-assembled fibrils (magenta line) and as the solid (blue line).

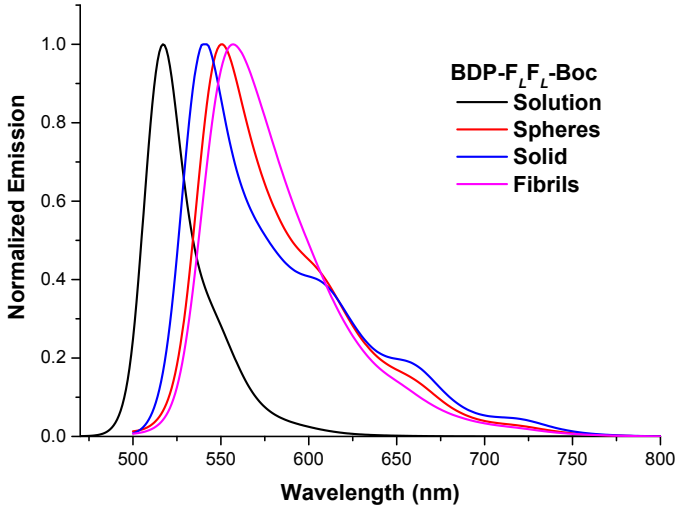


Figure S19. Normalized emission spectra of **BDP-F$_L$F$_L$-Boc** in DCM solution (λ_{ex}= 465 nm) (black line), as self-assembled spheres (λ_{ex}= 485 nm) (red line), as self-assembled fibrils (λ_{ex}= 485 nm) (magenta line) and as the solid (λ_{ex}= 485 nm) (blue line).

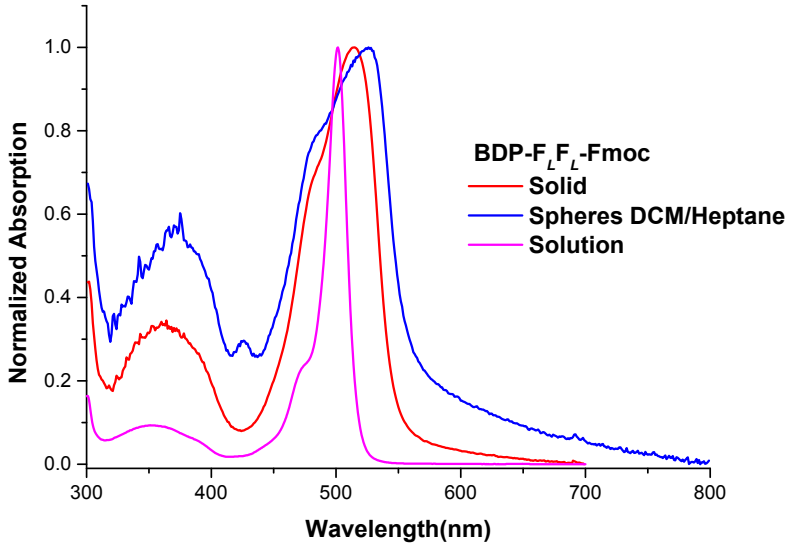


Figure S20. Normalized Absorption spectra of **BDP-F$_L$F$_L$-Fmoc** in DCM solution (magenta line), as self-assembled spheres (blue line) and as the solid (red line).

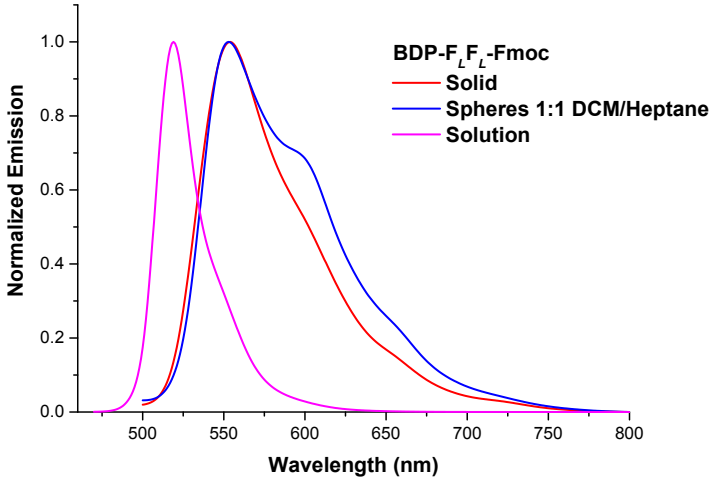


Figure S21. Normalized emission spectra of **BDP-F$_L$F$_L$-Fmoc** in DCM solution (λ_{ex}= 465 nm) (magenta line), as self-assembled spheres (λ_{ex}= 485 nm) (blue line) and as the solid (λ_{ex}= 485 nm) (red line).

Table S1. Summary of Spectroscopic Data for **BDP-F$_L$F$_L$-Boc** and **BDP-F$_L$F$_L$-Fmoc** in MeCN and MeCN/H_2O solutions.

Compound	Absorption		Emission					
	λ_{max}/nm		λ_{max}/nm		Φ		Stokes Shift /cm^{-1}	
Solvent	MeCN	MeCN / H_2O 1:60	MeCN	MeCN / H_2O 1:60	MeCN	MeCN / H_2O 1:60	MeCN	MeCN / H_2O 1:60
BDP-F$_L$F$_L$-Boc	497	510	515	540	0.25	0.00062	703	1089
BDP-F$_L$F$_L$-Fmoc	498	511	515	538	0.24	0.00144	663	982

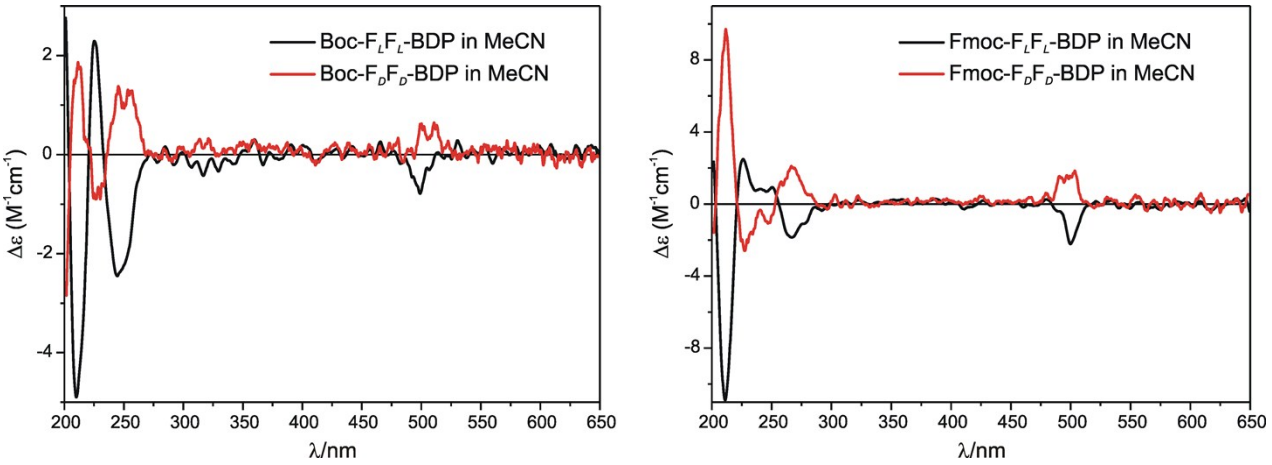
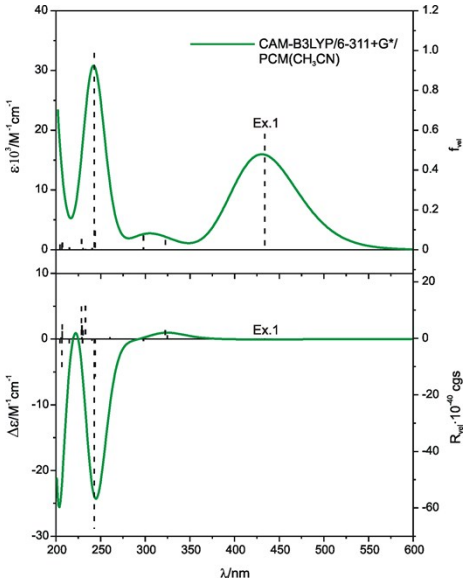
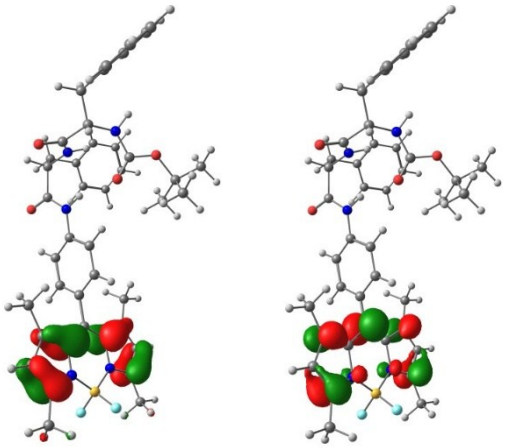


Figure S22. ECD spectra of **BDP-F$_L$F$_L$-Boc** and **BDP-F$_D$F$_D$-Boc** (left part), **BDP-F$_L$F$_L$-Fmoc** and **BDP-F$_D$F$_D$-Fmoc** (right part) in MeCN solution.

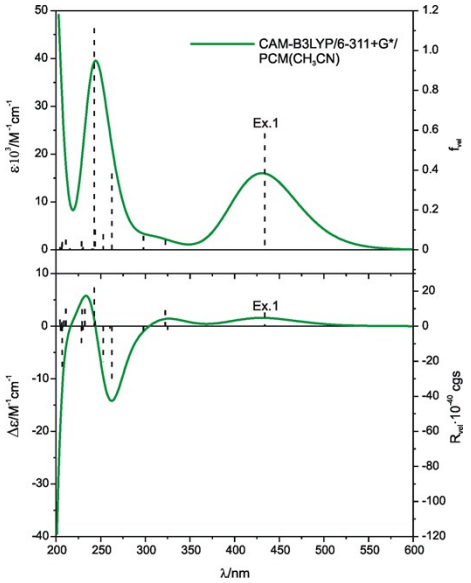


Ex.1 MO 194 → MO 195

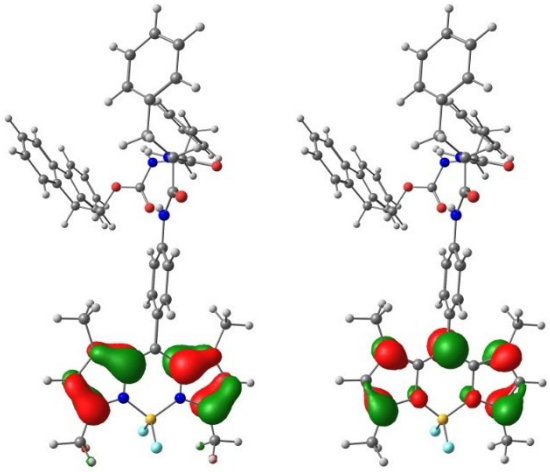


MO194 MO195

Figure S23. Computed UV (top) and ECD (bottom) spectra of the lowest energy conformer **1**(1) of compound **BDP-F$_L$F$_L$-Boc** and visualization of molecular orbitals in HOMO-LUMO electron transition.



Ex.1 MO 225 → MO 226



MO225 MO226

Figure S24. Computed UV (top) and ECD (bottom) spectra of the lowest energy conformer **2**(1) of compound **BDP-F$_L$F$_L$-Fmoc** and visualization of molecular orbitals in HOMO-LUMO electron transition.

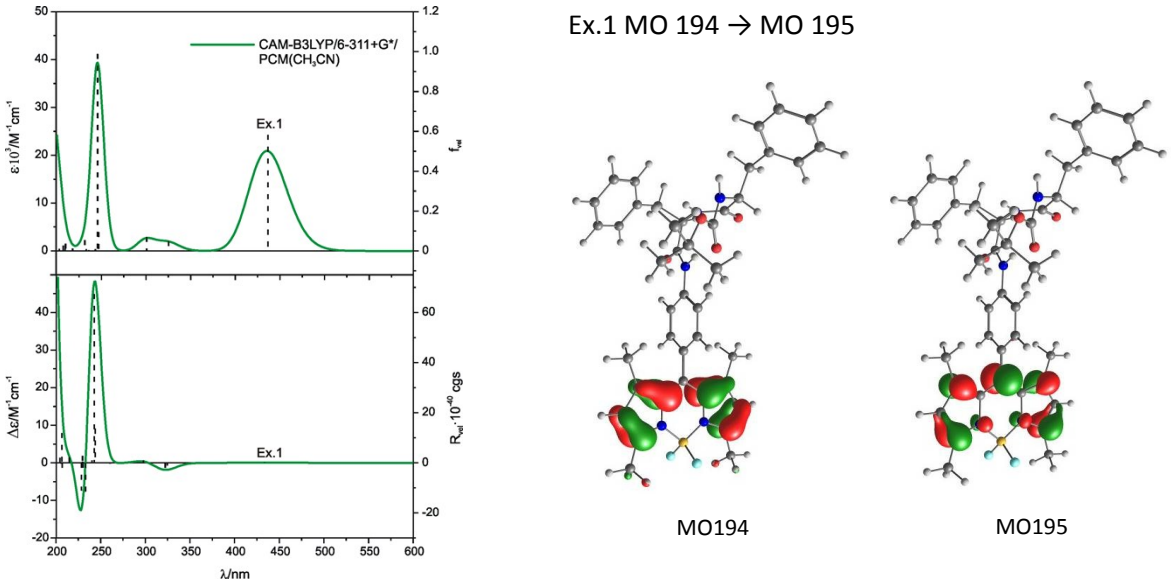


Figure S25. Computed UV (top) and ECD (bottom) spectra of the lowest energy conformer **3**(1) of compound **BDP-F$_D$F$_D$-Boc** and visualization of molecular orbitals in HOMO-LUMO electron transition.

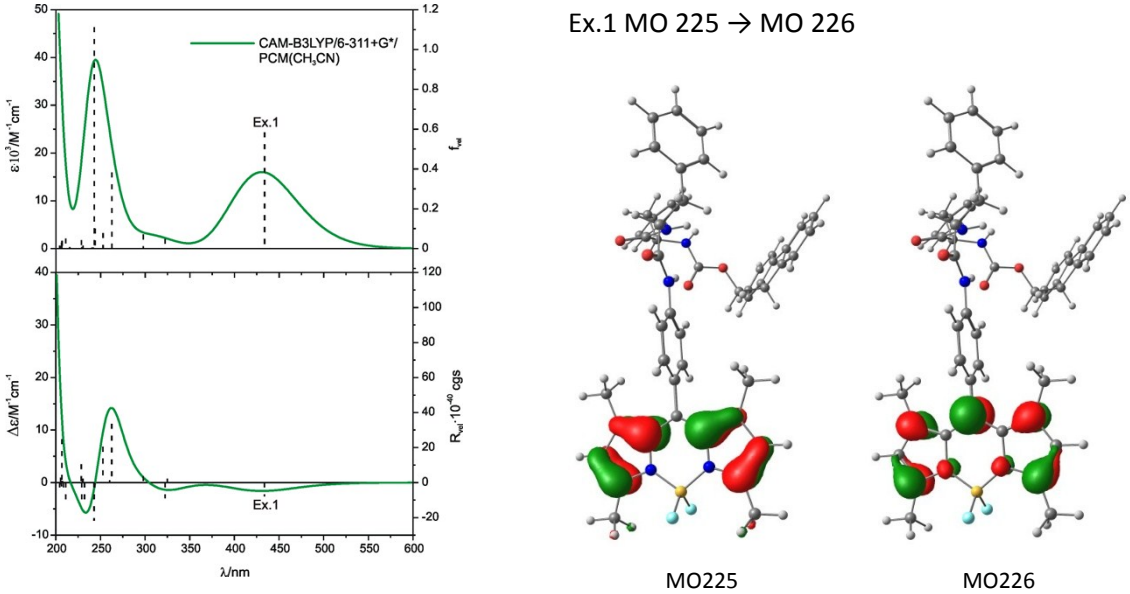


Figure S26. Computed UV (top) and ECD (bottom) spectra of the lowest energy conformer **4**(1) of compound **BDP-F$_D$F$_D$-Fmoc** and visualization of molecular orbitals in HOMO-LUMO electron transition.

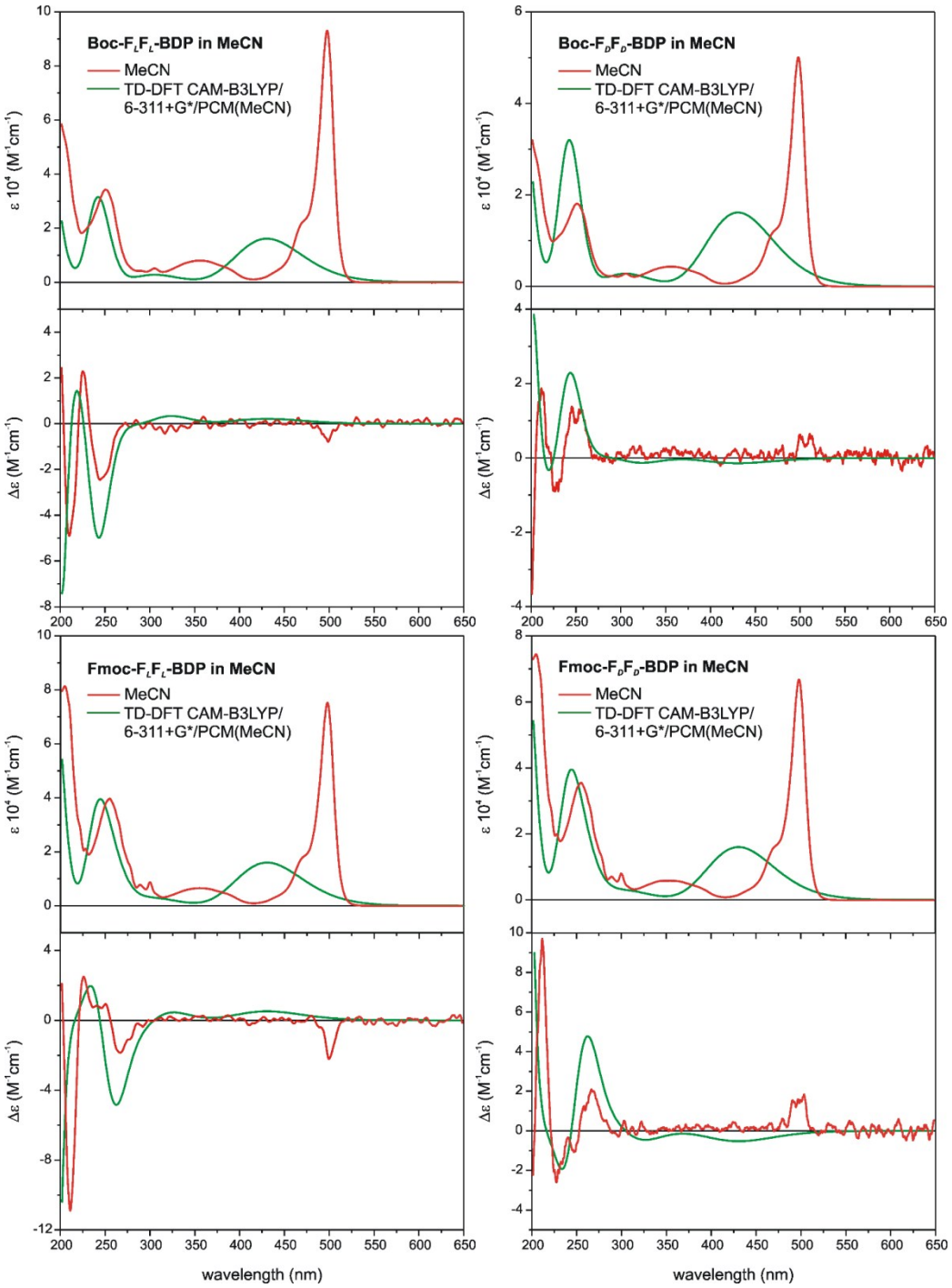


Figure S27. Comparison of experimental UV (top) and ECD (bottom) spectra of compounds **BDP-F$_L$F$_L$-Boc, BDP-F$_L$F$_L$-Fmoc , BDP-F$_D$F$_D$-Boc** and **BDP-F$_D$F$_D$-Fmoc** in MeCN solution with the simulated curves calculated at CAM-B3LYP/6-311+G*/PCM(MeCN) level of theory.

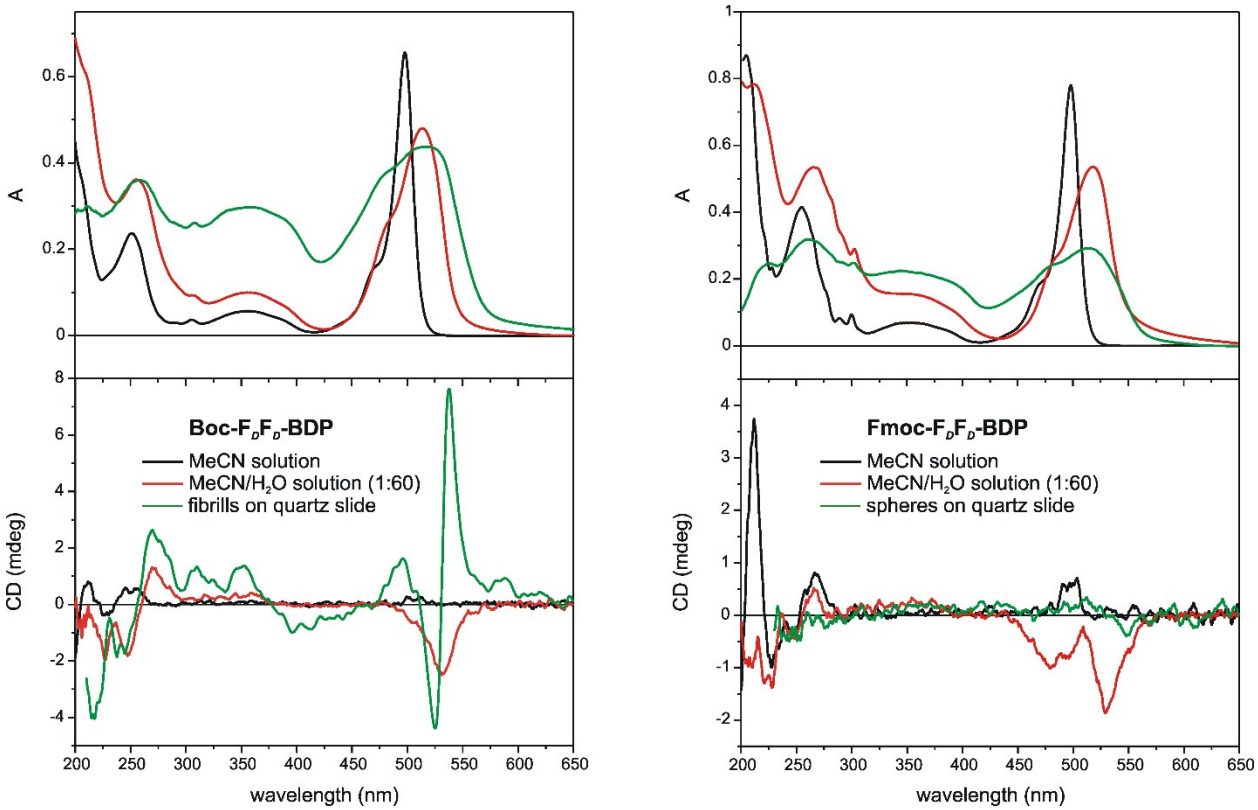


Figure S28. UV-Vis and ECD spectra of **BDP-F$_D$F$_D$-Boc** (left) and **BDP-F$_D$F$_D$-Fmoc** (right) dissolved in MeCN (black traces), in MeCN/H_2O 1:60 mixture (red traces) and nanostructures obtained from dry DCM/heptane 2:8 solution placed on quartz slide (green traces).

Table S2. Calculated at B3LYP/6-311+G*/PCM(CH_3CN) level of theory relative energies and conformer distribution at 25° C for **BDP-F_LF_L-Boc**.

Conf.	*ΔG* [kcal mol^{-1}]	Pop. [%]
1(1)	0.00	46.4
1(2)	0.50	19.9
1(3)	0.51	19.7
1(4)	1.03	8.2
1(5)	1.52	3.5
1(6)	1.77	2.3

Table S3. Cartesian coordinates for individual conformers of compound **BDP-F_LF_L-Boc**.

Input orientation of compound **BDP-F_LF_L-Boc** conf. 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.187165	0.073278	-0.604712
2	6	0	2.875593	0.993967	-1.606319
3	1	0	3.672983	1.521885	-2.119167
4	6	0	1.555819	1.255209	-1.968905
5	1	0	1.339947	1.969388	-2.747850
6	6	0	0.510548	0.582212	-1.321854
7	6	0	0.817912	-0.341382	-0.310772
8	1	0	0.015896	-0.863472	0.198626
9	6	0	2.138200	-0.589407	0.040648
10	1	0	2.352461	-1.309616	0.823325
11	7	0	-0.857047	0.778570	-1.620259
12	1	0	-1.504076	0.279383	-1.017030
13	6	0	-1.402314	1.489399	-2.644714
14	6	0	-2.943336	1.446219	-2.775005
15	8	0	-0.760161	2.129264	-3.471641
16	7	0	-3.614841	0.625070	-1.783740
17	1	0	-3.115931	0.979996	-3.748020
18	6	0	-3.548302	2.871595	-2.826902
19	1	0	-3.947943	1.060054	-0.932829
20	1	0	-2.988213	3.428481	-3.579945
21	1	0	-4.572485	2.775177	-3.194614
22	6	0	-3.545769	3.618117	-1.509080
23	6	0	-4.696114	3.660950	-0.710612
24	6	0	-2.397255	4.283411	-1.056286
25	1	0	-5.604765	3.173561	-1.052815
26	6	0	-4.699678	4.339725	0.509393
27	6	0	-2.397511	4.962476	0.160820
28	1	0	-1.499912	4.281184	-1.667088
29	1	0	-5.603747	4.364579	1.109229
30	6	0	-3.548703	4.990686	0.950002
31	1	0	-1.500022	5.476086	0.490414
32	1	0	-3.549702	5.523057	1.895496
33	6	0	-3.888023	-0.688383	-1.968757
34	6	0	-4.647254	-1.395887	-0.834399
35	8	0	-3.572349	-1.313818	-2.977226
36	7	0	-4.596587	-0.683326	0.437946
37	1	0	-4.158877	-2.369335	-0.731877
38	6	0	-6.115695	-1.615317	-1.267732

39	1	0	-5.459514	-0.589849	0.955777
40	1	0	-6.599414	-0.642538	-1.397217
41	1	0	-6.088122	-2.090018	-2.250983
42	6	0	-6.913187	-2.464888	-0.300617
43	6	0	-6.660770	-3.838372	-0.179747
44	6	0	-7.915689	-1.898431	0.494331
45	1	0	-5.895702	-4.302196	-0.795963
46	6	0	-7.386461	-4.620909	0.715474
47	6	0	-8.645011	-2.679695	1.393480
48	1	0	-8.139337	-0.839092	0.403773
49	1	0	-7.179873	-5.683591	0.791984
50	6	0	-8.380943	-4.042877	1.507793
51	1	0	-9.419890	-2.221350	1.999414
52	1	0	-8.947074	-4.652874	2.204032
53	6	0	-3.446347	-0.660992	1.182312
54	8	0	-2.344759	-0.919656	0.716410
55	8	0	-3.714430	-0.292486	2.441433
56	6	0	-2.651895	-0.096911	3.466850
57	6	0	-3.459077	0.324807	4.692922
58	1	0	-4.169646	-0.453988	4.978812
59	1	0	-2.788327	0.501914	5.536484
60	1	0	-4.013506	1.245444	4.497422
61	6	0	-1.929194	-1.419296	3.720725
62	1	0	-2.644325	-2.206522	3.972371
63	1	0	-1.348809	-1.735345	2.855334
64	1	0	-1.247947	-1.301916	4.567351
65	6	0	-1.706324	1.020177	3.028230
66	1	0	-1.118483	0.735138	2.157087
67	1	0	-2.265586	1.929739	2.795551
68	1	0	-1.016927	1.250084	3.844582
69	9	0	7.876304	-1.698869	1.519702
70	9	0	8.612861	-0.177316	-0.030705
71	7	0	6.547029	0.302024	1.154924
72	7	0	6.644965	-1.498533	-0.564910
73	6	0	6.885559	1.157841	2.144554
74	6	0	5.781745	1.978957	2.433381
75	6	0	4.728216	1.620771	1.598634
76	6	0	5.215859	0.550106	0.782640
77	6	0	4.606617	-0.203094	-0.231938
78	6	0	5.310922	-1.215515	-0.900244
79	6	0	4.927561	-2.109342	-1.951402
80	6	0	6.043316	-2.897980	-2.211643
81	6	0	7.083315	-2.506961	-1.350526
82	5	0	7.457514	-0.775607	0.529591
83	1	0	5.767956	2.757558	3.183473
84	1	0	6.112746	-3.684400	-2.950321
85	6	0	3.621007	-2.233100	-2.674142
86	1	0	2.795032	-2.461011	-1.996773
87	1	0	3.352663	-1.313335	-3.198796
88	1	0	3.682820	-3.035247	-3.411935
89	6	0	3.381238	2.276936	1.611172
90	1	0	3.134345	2.727574	0.647239
91	1	0	2.581027	1.570215	1.842034
92	1	0	3.362294	3.065373	2.365911
93	6	0	8.228388	1.186649	2.794112
94	1	0	8.465583	0.227156	3.260631
95	1	0	9.017873	1.391793	2.066783
96	1	0	8.256162	1.960122	3.561725

97	6	0	8.459156	-3.079107	-1.276490
98	1	0	9.217255	-2.320393	-1.486562
99	1	0	8.671856	-3.475802	-0.280646
100	1	0	8.568468	-3.886285	-2.000964

Input orientation of **BDP-F_LF_L-Boc** conf. 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.298340	0.075634	-0.281674
2	6	0	2.872266	0.900578	0.760778
3	1	0	3.572415	1.191082	1.537220
4	6	0	1.561197	1.366463	0.830594
5	1	0	1.254308	2.003007	1.645990
6	6	0	0.641147	1.005050	-0.162791
7	6	0	1.064621	0.174639	-1.211921
8	1	0	0.364194	-0.112366	-1.989958
9	6	0	2.374330	-0.282300	-1.268719
10	1	0	2.678179	-0.922187	-2.090372
11	7	0	-0.699218	1.440785	-0.186995
12	1	0	-1.264757	1.081430	-0.950617
13	6	0	-1.385919	2.165742	0.745666
14	6	0	-2.869257	2.391596	0.355204
15	8	0	-0.915758	2.587498	1.792629
16	7	0	-3.652479	1.187316	0.656015
17	1	0	-2.927550	2.532693	-0.725728
18	6	0	-3.479438	3.610744	1.062456
19	1	0	-4.130617	1.139001	1.544925
20	1	0	-4.561205	3.567052	0.904981
21	1	0	-3.302694	3.528707	2.137084
22	6	0	-2.949027	4.933327	0.546008
23	6	0	-2.050720	5.699114	1.296706
24	6	0	-3.361908	5.421361	-0.701112
25	1	0	-1.718916	5.335215	2.263283
26	6	0	-1.574257	6.919259	0.815024
27	6	0	-2.886008	6.638001	-1.187593
28	1	0	-4.069965	4.849958	-1.295221
29	1	0	-0.879558	7.499815	1.413760
30	6	0	-1.988492	7.391805	-0.429808
31	1	0	-3.220504	6.999887	-2.154642
32	1	0	-1.618934	8.340541	-0.805307
33	6	0	-3.753550	0.154149	-0.204167
34	6	0	-4.648943	-1.012445	0.230287
35	8	0	-3.153802	0.122641	-1.283246
36	7	0	-5.325135	-1.496442	-0.958406
37	1	0	-5.411845	-0.661090	0.926286
38	6	0	-3.820417	-2.139632	0.914085
39	1	0	-4.820565	-1.467098	-1.832663
40	1	0	-4.504724	-2.982979	1.041479
41	1	0	-3.040104	-2.463574	0.220295
42	6	0	-3.219195	-1.759451	2.248705
43	6	0	-1.841588	-1.559125	2.391117
44	6	0	-4.035925	-1.600342	3.377053
45	1	0	-1.190278	-1.685289	1.531374
46	6	0	-1.292123	-1.206323	3.624387
47	6	0	-3.491666	-1.244240	4.610091
48	1	0	-5.106420	-1.766688	3.294372

49	1	0	-0.220658	-1.059006	3.713995
50	6	0	-2.116011	-1.045000	4.737582
51	1	0	-4.140531	-1.129102	5.472466
52	1	0	-1.690513	-0.771144	5.697513
53	6	0	-6.557499	-2.070100	-0.920737
54	8	0	-7.231387	-2.186465	0.092066
55	8	0	-6.909201	-2.472884	-2.160418
56	6	0	-8.210541	-3.124533	-2.442904
57	6	0	-8.129798	-3.379119	-3.947524
58	1	0	-7.284220	-4.027702	-4.188015
59	1	0	-9.044063	-3.866641	-4.293375
60	1	0	-8.013713	-2.441337	-4.495769
61	6	0	-8.313182	-4.444492	-1.677831
62	1	0	-7.450161	-5.080454	-1.891518
63	1	0	-8.372694	-4.282967	-0.602655
64	1	0	-9.211441	-4.980111	-1.996075
65	6	0	-9.357979	-2.166927	-2.119311
66	1	0	-9.434882	-1.977309	-1.049794
67	1	0	-9.220782	-1.214142	-2.637301
68	1	0	-10.301236	-2.601355	-2.460659
69	9	0	8.087882	-2.223207	-1.488761
70	9	0	8.575785	-1.106607	0.454499
71	7	0	6.370819	-2.100937	0.226057
72	7	0	7.006066	-0.084149	-1.092522
73	6	0	6.429077	-3.275095	0.892652
74	6	0	5.148730	-3.582961	1.384735
75	6	0	4.271621	-2.569881	1.011952
76	6	0	5.051025	-1.623405	0.272341
77	6	0	4.708948	-0.410913	-0.344458
78	6	0	5.673208	0.352084	-1.019567
79	6	0	5.585094	1.599851	-1.716716
80	6	0	6.866848	1.870659	-2.184078
81	6	0	7.721059	0.826013	-1.790153
82	5	0	7.547263	-1.391526	-0.476782
83	1	0	4.900538	-4.465665	1.957644
84	1	0	7.169773	2.736646	-2.756176
85	6	0	4.400644	2.489611	-1.941130
86	1	0	3.601714	1.982083	-2.486400
87	1	0	3.966480	2.841670	-1.002689
88	1	0	4.701236	3.363883	-2.521544
89	6	0	2.813815	-2.547473	1.356860
90	1	0	2.545353	-1.672276	1.952842
91	1	0	2.180441	-2.528787	0.467145
92	1	0	2.557939	-3.438417	1.933274
93	6	0	7.676447	-4.077739	1.052984
94	1	0	8.091194	-4.366668	0.084011
95	1	0	8.450625	-3.509797	1.575061
96	1	0	7.468336	-4.983013	1.623458
97	6	0	9.180836	0.697526	-2.070090
98	1	0	9.760716	0.652331	-1.144777
99	1	0	9.400012	-0.215657	-2.629009
100	1	0	9.526726	1.551183	-2.653128

Input orientation of compound **BDP-F_LF_L-Boc** conf. 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.658069	0.458754	-0.278183
2	6	0	3.196840	1.351381	0.690870
3	1	0	3.887779	1.751661	1.425613
4	6	0	1.861461	1.745692	0.740421
5	1	0	1.527727	2.437186	1.498462
6	6	0	0.952197	1.241593	-0.199402
7	6	0	1.411738	0.343780	-1.175655
8	1	0	0.720465	-0.053370	-1.912354
9	6	0	2.745031	-0.040990	-1.212466
10	1	0	3.076236	-0.735602	-1.977111
11	7	0	-0.414094	1.585873	-0.235671
12	1	0	-0.971520	1.108586	-0.940222
13	6	0	-1.117235	2.410654	0.595358
14	6	0	-2.620347	2.497837	0.221010
15	8	0	-0.640869	3.031834	1.535459
16	7	0	-3.318150	1.252483	0.559262
17	1	0	-2.689389	2.604028	-0.864150
18	6	0	-3.294407	3.701507	0.894897
19	1	0	-3.803090	1.206178	1.444480
20	1	0	-3.249703	3.579790	1.980045
21	1	0	-2.689990	4.582265	0.664693
22	6	0	-4.723391	3.921155	0.444255
23	6	0	-4.998606	4.417922	-0.836973
24	6	0	-5.798966	3.637970	1.292718
25	1	0	-4.179338	4.659609	-1.508605
26	6	0	-6.311278	4.617295	-1.260376
27	6	0	-7.115783	3.836274	0.873196
28	1	0	-5.608815	3.266735	2.295728
29	1	0	-6.503203	5.006280	-2.255281
30	6	0	-7.376082	4.324498	-0.406070
31	1	0	-7.935468	3.611516	1.548103
32	1	0	-8.398497	4.481268	-0.734080
33	6	0	-3.357308	0.185717	-0.262412
34	6	0	-4.183673	-1.014880	0.213252
35	8	0	-2.748652	0.147943	-1.337354
36	7	0	-4.793422	-1.605415	-0.962653
37	1	0	-4.985761	-0.680305	0.872674
38	6	0	-3.299214	-2.045141	0.976777
39	1	0	-4.278392	-1.566696	-1.830435
40	1	0	-3.928105	-2.925904	1.132574
41	1	0	-2.479412	-2.349767	0.320788
42	6	0	-2.763761	-1.554396	2.303229
43	6	0	-1.410034	-1.239180	2.465624
44	6	0	-3.620106	-1.401844	3.402664
45	1	0	-0.728465	-1.357073	1.628497
46	6	0	-0.922613	-0.781013	3.690275
47	6	0	-3.138114	-0.940900	4.626927
48	1	0	-4.671893	-1.656022	3.304595
49	1	0	0.131452	-0.545419	3.796100
50	6	0	-1.785917	-0.627820	4.774465
51	1	0	-3.816675	-0.832878	5.467063
52	1	0	-1.408515	-0.272158	5.727656
53	6	0	-5.978171	-2.271200	-0.919886
54	8	0	-6.658925	-2.399434	0.086856
55	8	0	-6.275212	-2.749665	-2.146848
56	6	0	-7.513858	-3.516975	-2.420023
57	6	0	-7.386377	-3.823726	-3.911631
58	1	0	-6.486579	-4.409609	-4.113174

59	1	0	-8.251544	-4.398024	-4.250378
60	1	0	-7.337315	-2.901983	-4.495982
61	6	0	-7.520967	-4.809362	-1.602590
62	1	0	-6.604185	-5.378772	-1.776398
63	1	0	-7.614175	-4.610748	-0.535992
64	1	0	-8.365375	-5.430767	-1.912176
65	6	0	-8.741420	-2.645445	-2.151898
66	1	0	-8.851916	-2.420598	-1.092186
67	1	0	-8.673871	-1.705807	-2.706354
68	1	0	-9.639892	-3.169565	-2.488276
69	9	0	8.999420	-0.377263	0.482638
70	9	0	8.556288	-1.660802	-1.365874
71	7	0	7.363300	0.441254	-1.116177
72	7	0	6.849534	-1.502414	0.356063
73	6	0	8.021205	1.331690	-1.891136
74	6	0	7.106985	2.292737	-2.356597
75	6	0	5.845638	1.988938	-1.855211
76	6	0	6.008615	0.807517	-1.062511
77	6	0	5.093215	0.047595	-0.319417
78	6	0	5.506463	-1.093235	0.384442
79	6	0	4.786931	-2.019182	1.206224
80	6	0	5.720920	-2.953155	1.642083
81	6	0	6.977550	-2.617333	1.109008
82	5	0	7.979848	-0.785581	-0.411847
83	1	0	7.356834	3.125706	-2.999054
84	1	0	5.526697	-3.800631	2.284761
85	6	0	3.334211	-2.046073	1.571723
86	1	0	3.022986	-1.135975	2.089337
87	1	0	2.690758	-2.145137	0.694576
88	1	0	3.136029	-2.893046	2.231148
89	6	0	4.611270	2.790239	-2.136752
90	1	0	3.831155	2.192194	-2.612925
91	1	0	4.175666	3.208130	-1.226262
92	1	0	4.854446	3.619378	-2.803816
93	6	0	9.484273	1.263933	-2.174826
94	1	0	10.071178	1.357483	-1.257345
95	1	0	9.757787	0.310452	-2.632959
96	1	0	9.771950	2.069008	-2.851115
97	6	0	8.267423	-3.339225	1.311033
98	1	0	8.686475	-3.678717	0.360484
99	1	0	9.015889	-2.693675	1.777358
100	1	0	8.113633	-4.208213	1.950954

Input orientation of compound **BDP-F_LF_L-Boc** conf. 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.959276	-0.462532	-0.127251
2	6	0	3.367916	-0.581352	-1.386101
3	1	0	3.969193	-0.439197	-2.278160
4	6	0	2.014879	-0.881189	-1.529176
5	1	0	1.579888	-0.968499	-2.512757
6	6	0	1.219417	-1.067971	-0.390318
7	6	0	1.810442	-0.949821	0.877509
8	1	0	1.207535	-1.091408	1.768946
9	6	0	3.160367	-0.652417	1.004986
10	1	0	3.593790	-0.565932	1.995733

11	7	0	-0.154171	-1.380805	-0.432247
12	1	0	-0.612650	-1.489069	0.470711
13	6	0	-0.985035	-1.458330	-1.513344
14	6	0	-2.453851	-1.776986	-1.122102
15	8	0	-0.637997	-1.301625	-2.676251
16	7	0	-3.063259	-0.639065	-0.429865
17	1	0	-2.437155	-2.605517	-0.409144
18	6	0	-3.276995	-2.175630	-2.355538
19	1	0	-3.611682	0.022550	-0.963017
20	1	0	-3.341438	-1.321914	-3.035196
21	1	0	-2.710094	-2.941814	-2.889271
22	6	0	-4.660440	-2.696401	-2.028374
23	6	0	-4.828617	-3.983550	-1.500252
24	6	0	-5.800375	-1.919038	-2.259656
25	1	0	-3.958792	-4.611142	-1.326609
26	6	0	-6.098453	-4.477135	-1.206953
27	6	0	-7.074584	-2.408831	-1.967276
28	1	0	-5.696186	-0.924369	-2.683563
29	1	0	-6.207294	-5.478748	-0.803265
30	6	0	-7.227522	-3.689551	-1.438911
31	1	0	-7.945878	-1.790257	-2.157385
32	1	0	-8.217092	-4.073797	-1.214006
33	6	0	-2.917857	-0.405427	0.888273
34	6	0	-3.613252	0.848872	1.447647
35	8	0	-2.218264	-1.113267	1.621496
36	7	0	-4.532714	1.458709	0.501647
37	1	0	-2.804615	1.570220	1.592727
38	6	0	-4.254221	0.592202	2.835809
39	1	0	-5.467297	1.077239	0.438018
40	1	0	-3.494347	0.122806	3.462776
41	1	0	-4.471613	1.570419	3.271471
42	6	0	-5.513221	-0.248519	2.818781
43	6	0	-6.775786	0.358589	2.787972
44	6	0	-5.449823	-1.649090	2.838567
45	1	0	-6.849365	1.442362	2.794690
46	6	0	-7.942092	-0.408027	2.770111
47	6	0	-6.612818	-2.417633	2.822588
48	1	0	-4.482502	-2.139389	2.875935
49	1	0	-8.909559	0.083528	2.751196
50	6	0	-7.863774	-1.799773	2.786433
51	1	0	-6.542228	-3.500397	2.844476
52	1	0	-8.768822	-2.398373	2.777975
53	6	0	-4.383230	2.759632	0.084232
54	8	0	-3.379607	3.426695	0.264341
55	8	0	-5.495202	3.150360	-0.563279
56	6	0	-5.619620	4.490186	-1.194336
57	6	0	-7.020791	4.436062	-1.800609
58	1	0	-7.774461	4.273945	-1.026639
59	1	0	-7.245160	5.378811	-2.304413
60	1	0	-7.097628	3.629677	-2.533534
61	6	0	-5.533832	5.579109	-0.124925
62	1	0	-6.262505	5.396680	0.669095
63	1	0	-4.539669	5.633866	0.316013
64	1	0	-5.764155	6.548087	-0.575338
65	6	0	-4.562856	4.652773	-2.286727
66	1	0	-3.556683	4.694795	-1.872327
67	1	0	-4.616543	3.826813	-3.000612
68	1	0	-4.747873	5.580899	-2.833643

69	9	0	9.245014	0.693524	-0.790148
70	9	0	9.038391	0.690547	1.494177
71	7	0	7.716882	-0.901980	0.221214
72	7	0	7.178805	1.530856	0.175622
73	6	0	8.392562	-2.071047	0.277904
74	6	0	7.475111	-3.131849	0.182852
75	6	0	6.193461	-2.604636	0.064010
76	6	0	6.346872	-1.181224	0.089684
77	6	0	5.411004	-0.139475	0.008179
78	6	0	5.819182	1.201789	0.052318
79	6	0	5.078538	2.426054	-0.004123
80	6	0	6.017671	3.448196	0.085406
81	6	0	7.297471	2.876917	0.194606
82	5	0	8.332869	0.511694	0.278764
83	1	0	7.736460	-4.180828	0.199763
84	1	0	5.811450	4.509521	0.074839
85	6	0	3.601895	2.646287	-0.130449
86	1	0	3.201909	2.231572	-1.058512
87	1	0	3.044894	2.182734	0.686803
88	1	0	3.386609	3.716381	-0.120395
89	6	0	4.950281	-3.431221	-0.063502
90	1	0	4.257167	-3.262270	0.763828
91	1	0	4.402340	-3.212047	-0.982570
92	1	0	5.211769	-4.491028	-0.071427
93	6	0	9.874540	-2.167908	0.420247
94	1	0	10.387625	-1.667039	-0.404438
95	1	0	10.216979	-1.694447	1.343934
96	1	0	10.181522	-3.213809	0.434198
97	6	0	8.600418	3.593721	0.313949
98	1	0	9.117877	3.327352	1.238957
99	1	0	9.270658	3.340239	-0.511304
100	1	0	8.436838	4.671421	0.307450

Input orientation of compound **BDP-F$_L$F$_L$-Boc** conf. 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.383703	0.203144	0.420558
2	6	0	-2.473404	-0.327229	-0.499145
3	1	0	-2.831364	-0.780344	-1.417490
4	6	0	-1.108208	-0.282068	-0.250988
5	1	0	-0.419619	-0.704511	-0.976104
6	6	0	-0.615786	0.297394	0.927557
7	6	0	-1.521173	0.827911	1.855837
8	1	0	-1.159593	1.274582	2.769006
9	6	0	-2.888350	0.775576	1.593442
10	1	0	-3.576971	1.191696	2.321448
11	7	0	0.784038	0.316333	1.100947
12	1	0	1.326355	-0.084091	0.346305
13	6	0	1.516779	0.788512	2.144780
14	6	0	3.049382	0.673624	1.997183
15	8	0	1.049489	1.285043	3.163916
16	7	0	3.496268	-0.054289	0.814421
17	1	0	3.368927	0.093222	2.865309
18	6	0	3.717195	2.070874	2.093929
19	1	0	3.784313	0.487851	0.009472
20	1	0	3.389281	2.512765	3.036356

21	1	0	4.794717	1.908658	2.174421
22	6	0	3.416362	3.011955	0.945261
23	6	0	4.267282	3.085783	-0.165763
24	6	0	2.277935	3.830363	0.967554
25	1	0	5.165494	2.476272	-0.200707
26	6	0	3.982316	3.943110	-1.230234
27	6	0	1.993040	4.689190	-0.092758
28	1	0	1.614975	3.802679	1.826614
29	1	0	4.655846	3.986876	-2.080202
30	6	0	2.843557	4.746367	-1.198000
31	1	0	1.109919	5.318844	-0.052957
32	1	0	2.623993	5.417252	-2.022168
33	6	0	3.907543	-1.354300	0.872184
34	6	0	4.621041	-1.866721	-0.398318
35	8	0	3.760968	-2.060329	1.862474
36	7	0	6.061908	-1.791318	-0.188897
37	1	0	4.389922	-1.209967	-1.237829
38	6	0	4.215543	-3.309018	-0.747287
39	1	0	6.520751	-2.530119	0.324008
40	1	0	4.878192	-3.639219	-1.552494
41	1	0	4.411412	-3.949842	0.115924
42	6	0	2.771572	-3.452633	-1.181096
43	6	0	1.818892	-4.042855	-0.343199
44	6	0	2.363125	-3.009334	-2.446538
45	1	0	2.116902	-4.394251	0.639550
46	6	0	0.494101	-4.190212	-0.757030
47	6	0	1.040318	-3.151663	-2.862742
48	1	0	3.088651	-2.560223	-3.119299
49	1	0	-0.228343	-4.655397	-0.093976
50	6	0	0.100350	-3.744259	-2.017937
51	1	0	0.745402	-2.807136	-3.848840
52	1	0	-0.928616	-3.860663	-2.342302
53	6	0	6.791413	-0.681704	-0.499457
54	8	0	6.322305	0.319490	-1.020722
55	8	0	8.079357	-0.873050	-0.156829
56	6	0	9.128590	0.149073	-0.400098
57	6	0	10.382141	-0.534112	0.144052
58	1	0	10.583075	-1.464387	-0.392182
59	1	0	11.246354	0.123164	0.024971
60	1	0	10.270791	-0.763661	1.206270
61	6	0	9.263278	0.411243	-1.900211
62	1	0	9.428866	-0.524296	-2.440731
63	1	0	8.377897	0.899096	-2.305135
64	1	0	10.125200	1.059192	-2.079271
65	6	0	8.817290	1.417833	0.393770
66	1	0	7.928854	1.921729	0.016531
67	1	0	8.668070	1.183094	1.450809
68	1	0	9.661719	2.107943	0.319432
69	9	0	-8.816853	0.591174	0.466440
70	9	0	-8.438443	-0.495465	-1.517559
71	7	0	-6.985905	-1.002476	0.363058
72	7	0	-6.838909	1.190964	-0.810424
73	6	0	-7.463148	-2.150345	0.893091
74	6	0	-6.400263	-2.854463	1.485290
75	6	0	-5.230371	-2.121094	1.317847
76	6	0	-5.603500	-0.938476	0.601713
77	6	0	-4.852298	0.157781	0.152998
78	6	0	-5.460247	1.212100	-0.544499

79	6	0	-4.929047	2.421640	-1.097173
80	6	0	-6.005532	3.084842	-1.676913
81	6	0	-7.165286	2.312832	-1.489540
82	5	0	-7.808534	0.069737	-0.381719
83	1	0	-6.491289	-3.808705	1.985390
84	1	0	-5.970562	4.036433	-2.189017
85	6	0	-3.522877	2.939004	-1.093673
86	1	0	-3.136860	3.075082	-0.080977
87	1	0	-2.833913	2.262849	-1.604928
88	1	0	-3.484412	3.904667	-1.601206
89	6	0	-3.885827	-2.552856	1.818566
90	1	0	-3.156028	-2.647719	1.011476
91	1	0	-3.468482	-1.845283	2.538603
92	1	0	-3.970668	-3.522966	2.311751
93	6	0	-8.896561	-2.559678	0.833509
94	1	0	-9.541113	-1.823063	1.319702
95	1	0	-9.241315	-2.653309	-0.199349
96	1	0	-9.032525	-3.519732	1.331603
97	6	0	-8.548598	2.633548	-1.947087
98	1	0	-8.923488	1.875747	-2.639872
99	1	0	-9.247138	2.672102	-1.107645
100	1	0	-8.561180	3.599213	-2.452665

Input orientation of compound **BDP-F_LF_L-Boc** conf. 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.818848	0.552326	0.086727
2	6	0	-3.225520	0.910294	-1.125011
3	1	0	-3.807243	0.872894	-2.040285
4	6	0	-1.894959	1.318095	-1.191433
5	1	0	-1.457743	1.590644	-2.139483
6	6	0	-1.124797	1.373322	-0.021604
7	6	0	-1.717957	1.014679	1.199169
8	1	0	-1.135033	1.053276	2.114061
9	6	0	-3.045031	0.610617	1.250389
10	1	0	-3.480601	0.338445	2.205987
11	7	0	0.225133	1.775157	0.013597
12	1	0	0.677743	1.728058	0.924053
13	6	0	1.043334	2.139828	-1.018396
14	6	0	2.487257	2.458722	-0.551210
15	8	0	0.700560	2.213532	-2.190944
16	7	0	3.176322	1.233413	-0.138535
17	1	0	2.416700	3.093187	0.335813
18	6	0	3.277129	3.194840	-1.642787
19	1	0	3.749150	0.730144	-0.814235
20	1	0	3.384700	2.543804	-2.513812
21	1	0	2.667662	4.040557	-1.971306
22	6	0	4.633308	3.686367	-1.180496
23	6	0	4.735537	4.752455	-0.276301
24	6	0	5.812839	3.098509	-1.649459
25	1	0	3.834436	5.235799	0.091202
26	6	0	5.979638	5.211531	0.152436
27	6	0	7.061676	3.555712	-1.224273
28	1	0	5.758423	2.278849	-2.359851
29	1	0	6.036652	6.040655	0.850579
30	6	0	7.149121	4.612646	-0.319786

31	1	0	7.964182	3.086220	-1.602557
32	1	0	8.118503	4.970957	0.011143
33	6	0	3.075716	0.724217	1.103961
34	6	0	3.940456	-0.510371	1.435419
35	8	0	2.354885	1.222990	1.977402
36	7	0	3.720415	-1.652837	0.544852
37	1	0	3.564989	-0.838270	2.403622
38	6	0	5.428986	-0.109370	1.610323
39	1	0	3.321059	-2.481787	0.957452
40	1	0	5.842735	0.188711	0.646588
41	1	0	5.446706	0.776707	2.252449
42	6	0	6.268766	-1.205818	2.227280
43	6	0	6.215017	-1.455642	3.605045
44	6	0	7.108122	-2.000600	1.438913
45	1	0	5.579341	-0.842482	4.238088
46	6	0	6.975026	-2.473931	4.178230
47	6	0	7.871355	-3.021255	2.008318
48	1	0	7.173251	-1.815687	0.370827
49	1	0	6.923227	-2.648392	5.248259
50	6	0	7.805595	-3.262502	3.379974
51	1	0	8.518671	-3.624646	1.379852
52	1	0	8.399803	-4.053956	3.825085
53	6	0	4.156398	-1.773679	-0.737930
54	8	0	4.654108	-0.858267	-1.387332
55	8	0	3.949350	-3.024131	-1.179116
56	6	0	4.211726	-3.430909	-2.586288
57	6	0	3.784272	-4.897414	-2.583960
58	1	0	2.728562	-4.995892	-2.321198
59	1	0	3.932014	-5.329571	-3.576082
60	1	0	4.374949	-5.474109	-1.868570
61	6	0	3.337517	-2.612041	-3.535691
62	1	0	2.285947	-2.678937	-3.245376
63	1	0	3.631782	-1.563711	-3.553745
64	1	0	3.431512	-3.011488	-4.548747
65	6	0	5.702624	-3.301633	-2.897017
66	1	0	6.023980	-2.261448	-2.904939
67	1	0	6.297540	-3.849510	-2.161928
68	1	0	5.905272	-3.732489	-3.880966
69	9	0	-8.833190	-1.155656	1.402213
70	9	0	-8.997332	-0.848464	-0.864794
71	7	0	-6.895686	-1.675217	0.031016
72	7	0	-7.602504	0.685324	0.402286
73	6	0	-6.920769	-3.014959	-0.144488
74	6	0	-5.603221	-3.477389	-0.306637
75	6	0	-4.736435	-2.392300	-0.229625
76	6	0	-5.560843	-1.241421	-0.014513
77	6	0	-5.246314	0.116808	0.140552
78	6	0	-6.253398	1.071265	0.346438
79	6	0	-6.198866	2.490324	0.530244
80	6	0	-7.515777	2.908288	0.690968
81	6	0	-8.358611	1.786189	0.608950
82	5	0	-8.119600	-0.759950	0.244253
83	1	0	-5.323699	-4.509792	-0.464624
84	1	0	-7.849800	3.923901	0.852135
85	6	0	-5.014010	3.407107	0.555842
86	1	0	-4.314817	3.154170	1.356098
87	1	0	-4.448232	3.374675	-0.377941
88	1	0	-5.346593	4.434940	0.712489

89	6	0	-3.246947	-2.492416	-0.357246
90	1	0	-2.866301	-1.911427	-1.200314
91	1	0	-2.731744	-2.127745	0.534223
92	1	0	-2.959586	-3.534458	-0.509575
93	6	0	-8.171809	-3.827664	-0.155152
94	1	0	-8.705273	-3.748600	0.795564
95	1	0	-8.858593	-3.491006	-0.935631
96	1	0	-7.934909	-4.876982	-0.331596
97	6	0	-9.845713	1.761783	0.726005
98	1	0	-10.308860	1.338766	-0.168764
99	1	0	-10.167477	1.149152	1.572103
100	1	0	-10.226799	2.773168	0.867947

Table S4. Calculated at B3LYP/6-311+G*/PCM(CH_3CN) level of theory relative energies and conformer distribution at 25° C for **BDP-F_LF_L-Fmoc**.

Conf.	*ΔG* [kcal mol^{-1}]	Pop. [%]
2(1)	0.00	95.3
2(2)	2.10	2.8
2(3)	2.67	1.0
2(4)	2.75	0.9

Table S5. Cartesian coordinates for individual conformers of compound **BDP-F_LF_L-Fmoc**.

Input orientation of **BDP-F_LF_L-Fmoc** conf. 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.317504	-0.715681	-0.100115
2	6	0	3.213726	0.016699	0.348533
3	1	0	3.358288	0.993173	0.798920
4	6	0	1.927053	-0.491379	0.227907
5	1	0	1.081691	0.088136	0.581724
6	6	0	1.709813	-1.753197	-0.347356
7	6	0	2.810273	-2.491527	-0.803572
8	1	0	2.663277	-3.462673	-1.249391
9	6	0	4.095068	-1.967643	-0.675521
10	1	0	4.936252	-2.553284	-1.031886
11	7	0	0.371843	-2.200808	-0.429814
12	1	0	-0.319368	-1.557875	-0.055473
13	6	0	-0.093521	-3.394531	-0.889341
14	6	0	-1.624494	-3.606710	-0.837156
15	8	0	0.607470	-4.293505	-1.342419
16	7	0	-2.354232	-2.588074	-0.101428
17	1	0	-1.754449	-4.554960	-0.311055
18	6	0	-2.175893	-3.745745	-2.274778
19	1	0	-2.843798	-1.866727	-0.613121
20	1	0	-2.070932	-2.787612	-2.794187
21	1	0	-1.531266	-4.456679	-2.795210
22	6	0	-3.615528	-4.210462	-2.327337
23	6	0	-3.949312	-5.532122	-2.002397
24	6	0	-4.642267	-3.336709	-2.700192
25	1	0	-3.166953	-6.231750	-1.721559
26	6	0	-5.273028	-5.965528	-2.042993

27	6	0	-5.969993	-3.766741	-2.743165
28	1	0	-4.404366	-2.311359	-2.968682
29	1	0	-5.511029	-6.994153	-1.791540
30	6	0	-6.289620	-5.082415	-2.412583
31	1	0	-6.751324	-3.073344	-3.037504
32	1	0	-7.320349	-5.419926	-2.446653
33	6	0	-2.505064	-2.614710	1.244126
34	6	0	-3.341812	-1.482881	1.864249
35	8	0	-2.017215	-3.481144	1.963373
36	7	0	-3.497080	-0.325750	0.987711
37	1	0	-2.795719	-1.188848	2.765121
38	6	0	-4.726232	-2.035073	2.274931
39	1	0	-4.421406	0.068317	0.877799
40	1	0	-5.268973	-2.345222	1.377225
41	1	0	-4.544182	-2.937027	2.863365
42	6	0	-5.557995	-1.051965	3.071878
43	6	0	-5.207355	-0.723833	4.388709
44	6	0	-6.690167	-0.449308	2.512830
45	1	0	-4.339717	-1.189640	4.847496
46	6	0	-5.964100	0.186729	5.122508
47	6	0	-7.450751	0.464957	3.245171
48	1	0	-6.990525	-0.703303	1.500128
49	1	0	-5.679719	0.425152	6.142355
50	6	0	-7.088588	0.786860	4.551385
51	1	0	-8.326332	0.920233	2.793840
52	1	0	-7.678619	1.495341	5.123437
53	6	0	-2.448448	0.506117	0.733343
54	8	0	-1.279113	0.227215	0.958527
55	8	0	-2.864392	1.652741	0.169184
56	6	0	-1.837567	2.593503	-0.224024
57	1	0	-1.271358	2.890627	0.659899
58	1	0	-1.154977	2.104402	-0.920626
59	6	0	-2.512263	3.798438	-0.873803
60	6	0	-3.508355	4.532479	0.011424
61	1	0	-1.692158	4.476024	-1.147851
62	6	0	-3.346486	3.479872	-2.105464
63	6	0	-3.324369	5.079787	1.274751
64	6	0	-4.753987	4.631663	-0.636753
65	6	0	-2.976861	2.819359	-3.270086
66	6	0	-4.653630	3.978516	-1.949832
67	6	0	-4.397917	5.727176	1.895783
68	1	0	-2.365642	5.013773	1.780563
69	6	0	-5.823544	5.280951	-0.017888
70	6	0	-3.925015	2.653006	-4.285404
71	1	0	-1.969091	2.436739	-3.401651
72	6	0	-5.598204	3.814747	-2.964476
73	6	0	-5.635978	5.825865	1.253475
74	1	0	-4.267874	6.158164	2.883083
75	1	0	-6.787210	5.365252	-0.510338
76	6	0	-5.224144	3.146783	-4.131767
77	1	0	-3.649139	2.138914	-5.200300
78	1	0	-6.607917	4.197917	-2.855515
79	1	0	-6.458454	6.332693	1.747774
80	1	0	-5.947896	3.011297	-4.928959
81	9	0	8.842101	2.177705	0.858494
82	9	0	9.680306	0.259756	-0.079003
83	7	0	7.555369	1.103922	-0.900656
84	7	0	7.733011	0.075181	1.361939

85	6	0	7.841297	1.787224	-2.031047
86	6	0	6.731764	1.726762	-2.892055
87	6	0	5.729285	0.983925	-2.277073
88	6	0	6.254593	0.585420	-1.006198
89	6	0	5.701596	-0.172124	0.037018
90	6	0	6.430490	-0.426834	1.208075
91	6	0	6.103559	-1.159221	2.394522
92	6	0	7.219235	-1.071191	3.220479
93	6	0	8.205174	-0.310825	2.567883
94	5	0	8.488931	0.918294	0.313820
95	1	0	6.679257	2.186735	-3.869131
96	1	0	7.324453	-1.510316	4.202861
97	6	0	4.847758	-1.895310	2.749626
98	1	0	3.978334	-1.234670	2.780856
99	1	0	4.616358	-2.685457	2.031922
100	1	0	4.955900	-2.355106	3.733750
101	6	0	4.391335	0.702877	-2.890180
102	1	0	4.217047	-0.367105	-3.024588
103	1	0	3.569990	1.080771	-2.277259
104	1	0	4.327649	1.179641	-3.870122
105	6	0	9.140980	2.477166	-2.277657
106	1	0	9.340036	3.235285	-1.516122
107	1	0	9.976169	1.772564	-2.252654
108	1	0	9.127987	2.962453	-3.253685
109	6	0	9.562464	0.039371	3.078653
110	1	0	10.346124	-0.337225	2.416527
111	1	0	9.694678	1.122158	3.146357
112	1	0	9.711677	-0.389422	4.069685

Input orientation of **BDP-F$_L$F$_L$-Fmoc** conf. 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.301621	0.280197	0.159124
2	6	0	4.615228	0.712759	-0.980181
3	1	0	5.103057	0.690474	-1.948917
4	6	0	3.308473	1.171901	-0.888213
5	1	0	2.793789	1.501940	-1.785070
6	6	0	2.648890	1.212304	0.350331
7	6	0	3.331657	0.782393	1.496378
8	1	0	2.842616	0.806424	2.457898
9	6	0	4.642678	0.323093	1.388912
10	1	0	5.156295	-0.006837	2.286050
11	7	0	1.325267	1.696470	0.357293
12	1	0	0.944121	1.955640	-0.550490
13	6	0	0.443083	1.774022	1.397095
14	6	0	-0.947742	2.315195	0.967335
15	8	0	0.693170	1.459607	2.552859
16	7	0	-1.647515	1.332250	0.136200
17	1	0	-0.785339	3.196083	0.341047
18	6	0	-1.790368	2.702380	2.191081
19	1	0	-2.293756	0.691450	0.576781
20	1	0	-2.000032	1.806860	2.781863
21	1	0	-1.168215	3.339938	2.823629
22	6	0	-3.077671	3.421444	1.846639
23	6	0	-3.052997	4.749580	1.399700
24	6	0	-4.318150	2.789103	1.982375

25	1	0	-2.102389	5.266478	1.300197
26	6	0	-4.233296	5.423949	1.092775
27	6	0	-5.503283	3.460218	1.675262
28	1	0	-4.363420	1.765317	2.342327
29	1	0	-4.192620	6.453998	0.753069
30	6	0	-5.464475	4.779957	1.228831
31	1	0	-6.455045	2.951434	1.790071
32	1	0	-6.384450	5.304771	0.992812
33	6	0	-1.448212	1.204884	-1.189438
34	6	0	-2.237592	0.093689	-1.905405
35	8	0	-0.632697	1.891442	-1.814463
36	7	0	-3.269726	-0.501779	-1.071658
37	1	0	-1.500639	-0.693135	-2.086385
38	6	0	-2.772268	0.550501	-3.286716
39	1	0	-4.163676	-0.031323	-1.014850
40	1	0	-1.936001	0.998144	-3.826050
41	1	0	-3.060255	-0.352018	-3.831121
42	6	0	-3.941413	1.511174	-3.237474
43	6	0	-5.257434	1.037582	-3.322788
44	6	0	-3.739097	2.892549	-3.107955
45	1	0	-5.437309	-0.026674	-3.444942
46	6	0	-6.341682	1.915233	-3.273566
47	6	0	-4.819782	3.771779	-3.060474
48	1	0	-2.727630	3.281700	-3.053195
49	1	0	-7.352476	1.526774	-3.345875
50	6	0	-6.125704	3.286014	-3.141177
51	1	0	-4.641673	4.838110	-2.965641
52	1	0	-6.966553	3.971108	-3.107742
53	6	0	-3.266252	-1.832693	-0.758371
54	8	0	-2.334568	-2.597169	-0.934219
55	8	0	-4.443084	-2.179359	-0.196336
56	6	0	-4.575021	-3.553672	0.229325
57	1	0	-4.415003	-4.210009	-0.627438
58	1	0	-3.808319	-3.771356	0.974912
59	6	0	-5.973412	-3.746368	0.811057
60	6	0	-7.115065	-3.439102	-0.146387
61	1	0	-6.018725	-4.801561	1.113472
62	6	0	-6.301733	-2.858602	2.001971
63	6	0	-7.365207	-3.957335	-1.410623
64	6	0	-7.992749	-2.500384	0.428225
65	6	0	-5.618895	-2.711249	3.202592
66	6	0	-7.488190	-2.140326	1.761099
67	6	0	-8.500333	-3.528320	-2.106928
68	1	0	-6.697406	-4.686454	-1.859746
69	6	0	-9.126861	-2.075222	-0.265829
70	6	0	-6.125400	-1.833709	4.167430
71	1	0	-4.706438	-3.266023	3.400213
72	6	0	-7.994664	-1.267460	2.725556
73	6	0	-9.372384	-2.595066	-1.537851
74	1	0	-8.706858	-3.924984	-3.095605
75	1	0	-9.811172	-1.353783	0.169539
76	6	0	-7.303212	-1.118697	3.929010
77	1	0	-5.601369	-1.709061	5.109413
78	1	0	-8.910261	-0.711320	2.550646
79	1	0	-10.249607	-2.273492	-2.089919
80	1	0	-7.684474	-0.443313	4.688084
81	9	0	10.298016	-1.331201	-1.327600
82	9	0	10.334145	-1.658358	0.942319

83	7	0	8.254917	-2.074878	-0.243533
84	7	0	9.099743	0.247361	0.077887
85	6	0	8.202652	-3.410513	-0.442794
86	6	0	6.856132	-3.812454	-0.481139
87	6	0	6.050528	-2.693105	-0.300226
88	6	0	6.942841	-1.583544	-0.147698
89	6	0	6.706432	-0.216597	0.059988
90	6	0	7.770557	0.690318	0.173392
91	6	0	7.797952	2.106178	0.385370
92	6	0	9.141424	2.465784	0.408244
93	6	0	9.920941	1.311530	0.217902
94	5	0	9.533532	-1.217294	-0.140433
95	1	0	6.516415	-4.828212	-0.628709
96	1	0	9.534565	3.463094	0.548951
97	6	0	6.663911	3.069981	0.558676
98	1	0	6.008846	3.096510	-0.315094
99	1	0	6.035438	2.816321	1.415289
100	1	0	7.056300	4.076528	0.715148
101	6	0	4.552678	-2.726400	-0.282687
102	1	0	4.144416	-2.379885	0.669414
103	1	0	4.117429	-2.094488	-1.060081
104	1	0	4.204924	-3.748243	-0.445545
105	6	0	9.408918	-4.275682	-0.592146
106	1	0	10.020432	-3.962610	-1.442075
107	1	0	10.045999	-4.226783	0.294580
108	1	0	9.109182	-5.312527	-0.745114
109	6	0	11.409481	1.223727	0.168047
110	1	0	11.794578	0.545059	0.933004
111	1	0	11.752705	0.843873	-0.797710
112	1	0	11.848318	2.208922	0.326613

Input orientation of **BDP-F$_L$F$_L$-Fmoc** conf. 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.943914	-0.876631	-0.456972
2	6	0	-3.622319	-1.952156	-1.290989
3	1	0	-4.401719	-2.455917	-1.852553
4	6	0	-2.309318	-2.386491	-1.411209
5	1	0	-2.081245	-3.222950	-2.064623
6	6	0	-1.280842	-1.754098	-0.697887
7	6	0	-1.593757	-0.676279	0.139931
8	1	0	-0.814566	-0.176698	0.694289
9	6	0	-2.916037	-0.251795	0.251109
10	1	0	-3.143180	0.584984	0.903347
11	7	0	0.028502	-2.253174	-0.878301
12	1	0	0.100198	-3.035696	-1.513559
13	6	0	1.193433	-1.840331	-0.306842
14	6	0	2.430863	-2.666101	-0.693409
15	8	0	1.297076	-0.899669	0.472801
16	7	0	3.518278	-1.729691	-0.931084
17	1	0	2.265566	-3.210150	-1.624141
18	6	0	2.803950	-3.674342	0.430006
19	1	0	3.567774	-0.911176	-0.339221
20	1	0	3.753087	-4.129495	0.135118
21	1	0	2.990838	-3.109402	1.347031
22	6	0	1.765772	-4.747104	0.672900

23	6	0	1.653425	-5.839115	-0.198237
24	6	0	0.891570	-4.672001	1.763524
25	1	0	2.330865	-5.923904	-1.043409
26	6	0	0.690907	-6.825680	0.011479
27	6	0	-0.072050	-5.658205	1.978127
28	1	0	0.967764	-3.838312	2.455494
29	1	0	0.622541	-7.665979	-0.672010
30	6	0	-0.176560	-6.737541	1.101343
31	1	0	-0.737718	-5.584019	2.832084
32	1	0	-0.923598	-7.506712	1.268132
33	6	0	4.412102	-1.866149	-1.930788
34	6	0	5.443476	-0.728563	-2.087929
35	8	0	4.419470	-2.812964	-2.717345
36	7	0	5.338458	0.305483	-1.069609
37	1	0	5.191339	-0.256213	-3.040070
38	6	0	6.888369	-1.277858	-2.208293
39	1	0	5.865326	0.190963	-0.213805
40	1	0	6.874890	-2.051359	-2.977966
41	1	0	7.514452	-0.463116	-2.579825
42	6	0	7.470047	-1.825632	-0.921906
43	6	0	8.283642	-1.026406	-0.107699
44	6	0	7.205727	-3.140007	-0.510762
45	1	0	8.522954	-0.013164	-0.418052
46	6	0	8.809528	-1.519286	1.087938
47	6	0	7.730957	-3.635905	0.681391
48	1	0	6.592041	-3.782245	-1.134299
49	1	0	9.440283	-0.883691	1.701114
50	6	0	8.532549	-2.825726	1.487332
51	1	0	7.519125	-4.658076	0.978555
52	1	0	8.943663	-3.212982	2.413886
53	6	0	4.903378	1.566375	-1.353522
54	8	0	4.383922	1.915931	-2.398113
55	8	0	5.119815	2.379753	-0.291510
56	6	0	4.651107	3.742614	-0.394681
57	1	0	5.324084	4.316344	0.241498
58	1	0	4.757909	4.075732	-1.425664
59	6	0	3.195727	3.888054	0.075675
60	6	0	2.709895	5.320566	-0.083886
61	1	0	2.579319	3.206349	-0.522390
62	6	0	2.988736	3.641053	1.562347
63	6	0	2.634131	6.098970	-1.232891
64	6	0	2.305118	5.841078	1.160274
65	6	0	3.224872	2.492796	2.310275
66	6	0	2.476732	4.799100	2.181403
67	6	0	2.151970	7.408552	-1.133948
68	1	0	2.934595	5.704030	-2.198563
69	6	0	1.824109	7.147795	1.257465
70	6	0	2.955503	2.508597	3.683039
71	1	0	3.611405	1.594196	1.842738
72	6	0	2.207166	4.812917	3.550845
73	6	0	1.752384	7.927001	0.101550
74	1	0	2.085417	8.025743	-2.023876
75	1	0	1.507555	7.557599	2.211427
76	6	0	2.452403	3.659412	4.297143
77	1	0	3.136226	1.617901	4.276042
78	1	0	1.810301	5.700609	4.033331
79	1	0	1.380227	8.944617	0.161794
80	1	0	2.247000	3.654420	5.362767

81	9	0	-9.316058	-0.039916	-0.756135
82	9	0	-8.667507	1.600423	0.709924
83	7	0	-7.163550	1.029725	-1.110755
84	7	0	-7.514080	-0.536240	0.795918
85	6	0	-7.368466	1.968893	-2.060622
86	6	0	-6.179837	2.145090	-2.790261
87	6	0	-5.210224	1.289764	-2.277774
88	6	0	-5.837672	0.576929	-1.205850
89	6	0	-5.356260	-0.407576	-0.330521
90	6	0	-6.182050	-0.959519	0.659826
91	6	0	-5.937714	-1.955689	1.659101
92	6	0	-7.130042	-2.096654	2.361175
93	6	0	-8.081821	-1.217620	1.815519
94	5	0	-8.202417	0.525846	-0.086886
95	1	0	-6.053579	2.836229	-3.612054
96	1	0	-7.308980	-2.766899	3.190462
97	6	0	-4.689530	-2.730760	1.952698
98	1	0	-4.362278	-3.324506	1.096249
99	1	0	-3.854632	-2.079989	2.222215
100	1	0	-4.866973	-3.412516	2.786527
101	6	0	-3.808896	1.195395	-2.799737
102	1	0	-3.067421	1.437753	-2.035132
103	1	0	-3.570815	0.192964	-3.162660
104	1	0	-3.677090	1.893040	-3.628856
105	6	0	-8.666364	2.676323	-2.262466
106	1	0	-9.472065	1.973014	-2.487504
107	1	0	-8.963466	3.225909	-1.365749
108	1	0	-8.583201	3.382386	-3.088786
109	6	0	-9.494801	-1.028942	2.255609
110	1	0	-9.668289	-0.008406	2.606915
111	1	0	-10.195233	-1.207909	1.436339
112	1	0	-9.728510	-1.716885	3.068260

Input orientation of **BDP-F$_L$F$_L$-Fmoc** conf. 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.530345	0.316479	-0.328988
2	6	0	-3.869012	0.120547	-1.542568
3	1	0	-4.363804	-0.418875	-2.343633
4	6	0	-2.580063	0.604785	-1.755328
5	1	0	-2.088933	0.441946	-2.702215
6	6	0	-1.922568	1.304998	-0.734578
7	6	0	-2.583824	1.503445	0.487632
8	1	0	-2.087482	2.042929	1.288051
9	6	0	-3.868619	1.016402	0.685185
10	1	0	-4.358574	1.182671	1.638715
11	7	0	-0.625704	1.842239	-0.857820
12	1	0	-0.268861	2.331625	-0.039100
13	6	0	0.260468	1.721993	-1.889885
14	6	0	1.609473	2.436000	-1.607681
15	8	0	0.041289	1.127100	-2.936658
16	7	0	2.354879	1.745235	-0.553423
17	1	0	1.382346	3.434397	-1.225194
18	6	0	2.452647	2.555950	-2.885472
19	1	0	3.031262	1.042751	-0.819944
20	1	0	2.701845	1.555320	-3.248094

21	1	0	1.817784	3.005502	-3.652896
22	6	0	3.710265	3.380097	-2.705312
23	6	0	3.635245	4.770768	-2.548841
24	6	0	4.973140	2.778071	-2.698113
25	1	0	2.666790	5.263047	-2.566983
26	6	0	4.787912	5.535761	-2.380182
27	6	0	6.130957	3.540186	-2.530497
28	1	0	5.057183	1.703587	-2.833957
29	1	0	4.708152	6.611939	-2.264169
30	6	0	6.041817	4.921723	-2.368362
31	1	0	7.100854	3.053025	-2.530363
32	1	0	6.940228	5.516549	-2.239659
33	6	0	2.163904	1.970939	0.762668
34	6	0	3.129131	1.260651	1.728082
35	8	0	1.283644	2.720955	1.193369
36	7	0	3.670564	0.026516	1.173108
37	1	0	2.536230	1.021767	2.612724
38	6	0	4.311591	2.177950	2.136176
39	1	0	4.660932	-0.036491	0.983882
40	1	0	4.964040	1.571992	2.772679
41	1	0	4.888642	2.432793	1.242450
42	6	0	3.926423	3.440367	2.874948
43	6	0	4.000362	4.689441	2.250753
44	6	0	3.509825	3.383818	4.211091
45	1	0	4.329438	4.754221	1.217790
46	6	0	3.657402	5.854502	2.938353
47	6	0	3.163841	4.544128	4.900921
48	1	0	3.458672	2.424802	4.719220
49	1	0	3.722292	6.814883	2.436895
50	6	0	3.235259	5.785125	4.265225
51	1	0	2.843905	4.480627	5.936096
52	1	0	2.969004	6.689723	4.802269
53	6	0	2.967502	-1.141308	1.215461
54	8	0	1.804590	-1.239837	1.565111
55	8	0	3.734033	-2.169830	0.796382
56	6	0	3.105790	-3.470379	0.761077
57	1	0	2.834475	-3.762438	1.777187
58	1	0	2.192674	-3.411449	0.167158
59	6	0	4.090418	-4.464818	0.150855
60	6	0	5.413795	-4.596287	0.889591
61	1	0	3.567491	-5.430955	0.154978
62	6	0	4.540783	-4.132533	-1.263762
63	6	0	5.648649	-4.897682	2.225048
64	6	0	6.487889	-4.377768	0.006273
65	6	0	3.773820	-3.901417	-2.398622
66	6	0	5.946290	-4.090286	-1.329679
67	6	0	6.969212	-4.975540	2.680513
68	1	0	4.826885	-5.073641	2.912841
69	6	0	7.805261	-4.458886	0.460720
70	6	0	4.419504	-3.622059	-3.608020
71	1	0	2.689135	-3.936665	-2.359177
72	6	0	6.589832	-3.814765	-2.537374
73	6	0	8.037032	-4.757580	1.804442
74	1	0	7.166288	-5.209204	3.721688
75	1	0	8.640275	-4.293972	-0.212954
76	6	0	5.815575	-3.579614	-3.674850
77	1	0	3.831976	-3.439373	-4.501816
78	1	0	7.673081	-3.783043	-2.599166

79	1	0	9.055775	-4.822871	2.172694
80	1	0	6.301597	-3.363501	-4.620784
81	9	0	-9.462274	-1.144446	1.494672
82	9	0	-9.467903	-1.967548	-0.646032
83	7	0	-7.380459	-2.018692	0.596812
84	7	0	-8.323666	0.134804	-0.228835
85	6	0	-7.271126	-3.273285	1.087105
86	6	0	-5.908641	-3.597995	1.206651
87	6	0	-5.151555	-2.512812	0.777740
88	6	0	-6.090462	-1.504263	0.388083
89	6	0	-5.912521	-0.207824	-0.117019
90	6	0	-7.014552	0.604205	-0.423582
91	6	0	-7.102591	1.936220	-0.941551
92	6	0	-8.460387	2.221988	-1.039361
93	6	0	-9.189779	1.104547	-0.597432
94	5	0	-8.694614	-1.262758	0.309820
95	1	0	-5.525838	-4.540192	1.573683
96	1	0	-8.895766	3.145621	-1.394795
97	6	0	-6.011104	2.888692	-1.324168
98	1	0	-5.365191	3.135514	-0.478487
99	1	0	-5.364857	2.482402	-2.105391
100	1	0	-6.446691	3.817774	-1.696623
101	6	0	-3.653656	-2.484538	0.758620
102	1	0	-3.257972	-2.339765	-0.249219
103	1	0	-3.248597	-1.678221	1.374066
104	1	0	-3.262307	-3.429139	1.140965
105	6	0	-8.439644	-4.134854	1.430627
106	1	0	-9.069614	-3.666360	2.190856
107	1	0	-9.072360	-4.313461	0.557521
108	1	0	-8.096434	-5.097082	1.810874
109	6	0	-10.673283	0.963188	-0.526302
110	1	0	-11.022519	0.121881	-1.130004
111	1	0	-11.006211	0.780465	0.498576
112	1	0	-11.154009	1.872036	-0.888488

Table S6. Calculated at B3LYP/6-311+G*/PCM(CH_3CN) level of theory relative energies and conformer distribution at 25° C for **BDP-F_DF_D-Boc**.

Conf.	*ΔG* [kcal mol^{-1}]	Pop. [%]
3(1)	0.00	46.4
3(2)	0.10	39.0
3(3)	1.04	8.1
3(4)	1.49	3.7
3(5)	1.66	2.8

Table S7. Cartesian coordinates for individual conformers of **BDP-F_DF_D-Boc**.

Input orientation of **BDP-F_DF_D-Boc** conf. 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.187053	0.073419	-0.604697
2	6	0	-2.875478	0.994498	-1.605942
3	1	0	-3.672851	1.522676	-2.118540

4	6	0	-1.555700	1.255798	-1.968490
5	1	0	-1.339822	1.970274	-2.747161
6	6	0	-0.510445	0.582442	-1.321787
7	6	0	-0.817822	-0.341547	-0.311077
8	1	0	-0.015816	-0.863921	0.198045
9	6	0	-2.138113	-0.589614	0.040330
10	1	0	-2.352367	-1.310143	0.822710
11	7	0	0.857143	0.778839	-1.620172
12	1	0	1.504189	0.279655	-1.016962
13	6	0	1.402410	1.489665	-2.644644
14	6	0	2.943431	1.446550	-2.774852
15	8	0	0.760258	2.129404	-3.471661
16	7	0	3.614899	0.625292	-1.783641
17	1	0	3.116108	0.980444	-3.747907
18	6	0	3.548355	2.871949	-2.826533
19	1	0	3.947936	1.060163	-0.932647
20	1	0	4.572585	2.775603	-3.194135
21	1	0	2.988348	3.428897	-3.579592
22	6	0	3.545620	3.618360	-1.508648
23	6	0	2.397030	4.283625	-1.056004
24	6	0	4.695823	3.661130	-0.709975
25	1	0	1.499795	4.281450	-1.666963
26	6	0	2.397071	4.962590	0.161158
27	6	0	4.699171	4.339803	0.510086
28	1	0	5.604543	3.173784	-1.052054
29	1	0	1.499524	5.476177	0.490629
30	6	0	3.548121	4.990732	0.950547
31	1	0	5.603137	4.364604	1.110080
32	1	0	3.548955	5.523023	1.896086
33	6	0	3.887976	-0.688168	-1.968749
34	6	0	4.647266	-1.395775	-0.834510
35	8	0	3.572252	-1.313498	-2.977270
36	7	0	4.596515	-0.683402	0.437949
37	1	0	4.159036	-2.369313	-0.732156
38	6	0	6.115752	-1.614941	-1.267863
39	1	0	5.459385	-0.590285	0.955945
40	1	0	6.088266	-2.089481	-2.251195
41	1	0	6.599346	-0.642077	-1.397165
42	6	0	6.913314	-2.464592	-0.300873
43	6	0	7.915636	-1.898148	0.494308
44	6	0	6.661124	-3.838149	-0.180351
45	1	0	8.139136	-0.838758	0.403995
46	6	0	8.644990	-2.679491	1.393361
47	6	0	7.386849	-4.620765	0.714774
48	1	0	5.896213	-4.301972	-0.796763
49	1	0	9.419728	-2.221151	1.999480
50	6	0	8.381140	-4.042743	1.507338
51	1	0	7.180437	-5.683500	0.791013
52	1	0	8.947295	-4.652800	2.203505
53	6	0	3.446210	-0.661274	1.182252
54	8	0	2.344639	-0.919690	0.716181
55	8	0	3.714228	-0.293274	2.441529
56	6	0	2.651586	-0.097721	3.466847
57	6	0	3.458685	0.323483	4.693147
58	1	0	4.013347	1.244052	4.497979
59	1	0	2.787857	0.500511	5.536665
60	1	0	4.169044	-0.455541	4.978932
61	6	0	1.706331	1.019689	3.028387

62	1	0	2.265819	1.929186	2.796003
63	1	0	1.118516	0.735011	2.157108
64	1	0	1.016892	1.249554	3.844718
65	6	0	1.928563	-1.420019	3.720229
66	1	0	1.348263	-1.735704	2.854646
67	1	0	2.643483	-2.207468	3.971776
68	1	0	1.247190	-1.302742	4.566768
69	9	0	-8.612730	-0.177188	-0.030594
70	9	0	-7.876196	-1.699259	1.519298
71	7	0	-6.546846	0.301703	1.155121
72	7	0	-6.644884	-1.498303	-0.565270
73	6	0	-6.885312	1.157174	2.145089
74	6	0	-5.781443	1.978123	2.434174
75	6	0	-4.727957	1.620194	1.599263
76	6	0	-5.215691	0.549849	0.782894
77	6	0	-4.606508	-0.203019	-0.231966
78	6	0	-5.310871	-1.215195	-0.900586
79	6	0	-4.927567	-2.108684	-1.952050
80	6	0	-6.043367	-2.897183	-2.212531
81	6	0	-7.083316	-2.506445	-1.351226
82	5	0	-7.457390	-0.775697	0.529476
83	1	0	-5.767595	2.756452	3.184549
84	1	0	-6.112854	-3.683348	-2.951477
85	6	0	-3.621046	-2.232253	-2.674872
86	1	0	-3.352575	-1.312261	-3.199061
87	1	0	-2.795088	-2.460621	-1.997632
88	1	0	-3.682973	-3.034019	-3.413071
89	6	0	-3.380960	2.276301	1.611985
90	1	0	-2.580765	1.569466	1.842559
91	1	0	-3.134081	2.727279	0.648206
92	1	0	-3.361950	3.064464	2.367009
93	6	0	-8.228138	1.185846	2.794639
94	1	0	-9.017572	1.391554	2.067408
95	1	0	-8.465528	0.226137	3.260610
96	1	0	-8.255797	1.958896	3.562683
97	6	0	-8.459128	-3.078647	-1.277254
98	1	0	-8.671372	-3.476535	-0.281780
99	1	0	-9.217330	-2.319698	-1.486070
100	1	0	-8.568768	-3.884992	-2.002607

Input orientation of **BDP-F$_D$F$_D$-Boc** conf. 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.661094	0.465069	-0.275380
2	6	0	-2.741025	-0.058143	-1.189689
3	1	0	-3.066992	-0.769978	-1.940625
4	6	0	-1.407106	0.324175	-1.149712
5	1	0	-0.710195	-0.092025	-1.870419
6	6	0	-0.954167	1.243682	-0.190723
7	6	0	-1.870733	1.772188	0.728394
8	1	0	-1.542302	2.480915	1.472733
9	6	0	-3.206476	1.379401	0.676399
10	1	0	-3.903107	1.798613	1.395026
11	7	0	0.412766	1.585692	-0.223995
12	1	0	0.971266	1.106794	-0.926722
13	6	0	1.115914	2.406240	0.611203

14	6	0	2.620030	2.491968	0.240290
15	8	0	0.638714	3.025677	1.552016
16	7	0	3.315020	1.242461	0.569218
17	1	0	2.690712	2.606993	-0.843904
18	6	0	3.295988	3.688263	0.925367
19	1	0	3.802047	1.189766	1.452898
20	1	0	2.695023	4.572699	0.700310
21	1	0	3.247636	3.558112	2.009390
22	6	0	4.727119	3.906943	0.481071
23	6	0	5.798723	3.618368	1.332738
24	6	0	5.008452	4.408550	-0.796938
25	1	0	5.603867	3.243638	2.333549
26	6	0	7.117605	3.815895	0.919358
27	6	0	6.323194	4.607175	-1.214196
28	1	0	4.192429	4.654692	-1.470890
29	1	0	7.934115	3.586880	1.596677
30	6	0	7.383996	4.308802	-0.356834
31	1	0	6.519862	4.999918	-2.206693
32	1	0	8.408021	4.464943	-0.680081
33	6	0	3.353940	0.182451	-0.261068
34	6	0	4.182683	-1.021147	0.202909
35	8	0	2.743492	0.152907	-1.335318
36	7	0	4.789649	-1.601636	-0.979445
37	1	0	4.986451	-0.691023	0.862541
38	6	0	3.301669	-2.058356	0.960835
39	1	0	4.272378	-1.556121	-1.845558
40	1	0	2.479153	-2.357444	0.305685
41	1	0	3.931394	-2.940339	1.106109
42	6	0	2.771778	-1.579653	2.293920
43	6	0	3.633302	-1.433840	3.390229
44	6	0	1.418086	-1.269491	2.465802
45	1	0	4.685245	-1.684397	3.284848
46	6	0	3.156322	-0.984258	4.620657
47	6	0	0.935669	-0.822688	3.696623
48	1	0	0.732590	-1.382561	1.631223
49	1	0	3.838858	-0.881333	5.458205
50	6	0	1.804072	-0.676033	4.777626
51	1	0	-0.118483	-0.590928	3.809761
52	1	0	1.430584	-0.329227	5.735608
53	6	0	5.976767	-2.263698	-0.945929
54	8	0	6.660987	-2.398157	0.057640
55	8	0	6.271793	-2.730683	-2.177787
56	6	0	7.512314	-3.491353	-2.460913
57	6	0	7.381689	-3.786027	-3.954665
58	1	0	7.327814	-2.859609	-4.531154
59	1	0	8.247884	-4.354438	-4.300650
60	1	0	6.483368	-4.373336	-4.158657
61	6	0	8.737615	-2.617853	-2.188944
62	1	0	8.665352	-1.673880	-2.735392
63	1	0	8.850333	-2.401443	-1.127704
64	1	0	9.636918	-3.136097	-2.532141
65	6	0	7.526296	-4.790477	-1.654366
66	1	0	7.621834	-4.600445	-0.586405
67	1	0	6.611065	-5.361712	-1.830361
68	1	0	8.372038	-5.406236	-1.971517
69	9	0	-9.002552	-0.301143	0.466118
70	9	0	-8.573017	-1.680507	-1.315206
71	7	0	-6.867016	-1.458157	0.400762

72	7	0	-7.353348	0.415845	-1.167762
73	6	0	-7.007756	-2.541088	1.196856
74	6	0	-5.758153	-2.860326	1.756012
75	6	0	-4.815669	-1.948268	1.292915
76	6	0	-5.522716	-1.052930	0.427528
77	6	0	-5.096647	0.055542	-0.319050
78	6	0	-5.999271	0.783441	-1.108400
79	6	0	-5.822142	1.928638	-1.949714
80	6	0	-7.074528	2.209594	-2.485694
81	6	0	-7.997173	1.270184	-1.993458
82	5	0	-7.986597	-0.766849	-0.405287
83	1	0	-5.574164	-3.682590	2.433512
84	1	0	-7.312912	3.013270	-3.168550
85	6	0	-4.582983	2.717817	-2.244146
86	1	0	-4.152068	3.159071	-1.342557
87	1	0	-3.801821	2.104129	-2.698327
88	1	0	-4.818348	3.528784	-2.935892
89	6	0	-3.366504	-1.967403	1.672659
90	1	0	-2.714835	-2.089636	0.804589
91	1	0	-3.059115	-1.044536	2.169649
92	1	0	-3.175746	-2.797061	2.355856
93	6	0	-8.302773	-3.249161	1.414127
94	1	0	-9.056463	-2.579902	1.836536
95	1	0	-8.708110	-3.633922	0.474934
96	1	0	-8.161460	-4.086136	2.098096
97	6	0	-9.453817	1.185330	-2.304218
98	1	0	-9.701582	0.236702	-2.787472
99	1	0	-10.059734	1.249243	-1.397149
100	1	0	-9.742022	1.997743	-2.971436

Input orientation of **BDP-F$_D$F$_D$-Boc** conf. 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.959279	-0.462416	-0.127759
2	6	0	-3.160580	-0.653401	1.004455
3	1	0	-3.594201	-0.567820	1.995198
4	6	0	-1.810630	-0.950652	0.876942
5	1	0	-1.207858	-1.093041	1.768351
6	6	0	-1.219368	-1.067689	-0.390897
7	6	0	-2.014647	-0.879833	-1.529725
8	1	0	-1.579470	-0.966278	-2.513307
9	6	0	-3.367693	-0.580024	-1.386620
10	1	0	-3.968815	-0.436995	-2.278646
11	7	0	0.154209	-1.380472	-0.432813
12	1	0	0.612596	-1.489120	0.470166
13	6	0	0.985166	-1.457911	-1.513829
14	6	0	2.453954	-1.776764	-1.122491
15	8	0	0.638330	-1.300844	-2.676757
16	7	0	3.063478	-0.639190	-0.429781
17	1	0	2.437080	-2.605605	-0.409879
18	6	0	3.277190	-2.174982	-2.356012
19	1	0	3.611917	0.022590	-0.962728
20	1	0	2.710281	-2.940912	-2.890096
21	1	0	3.341770	-1.320987	-3.035311
22	6	0	4.660565	-2.696013	-2.028940
23	6	0	5.800563	-1.918529	-2.259565

24	6	0	4.828627	-3.983503	-1.501601
25	1	0	5.696457	-0.923593	-2.682877
26	6	0	7.074717	-2.408532	-1.967285
27	6	0	6.098409	-4.477296	-1.208398
28	1	0	3.958749	-4.611178	-1.328494
29	1	0	7.946064	-1.789866	-2.156882
30	6	0	7.227539	-3.689589	-1.439686
31	1	0	6.207170	-5.479165	-0.805312
32	1	0	8.217068	-4.074002	-1.214865
33	6	0	2.917822	-0.405706	0.888325
34	6	0	3.613149	0.848484	1.448022
35	8	0	2.217963	-1.113539	1.621344
36	7	0	4.532637	1.458553	0.502197
37	1	0	2.804479	1.569760	1.593293
38	6	0	4.254086	0.591481	2.836153
39	1	0	5.467323	1.077288	0.438789
40	1	0	4.471231	1.569603	3.272153
41	1	0	3.494272	0.121684	3.462893
42	6	0	5.513287	-0.248940	2.818929
43	6	0	5.450194	-1.649538	2.838289
44	6	0	6.775723	0.358465	2.788387
45	1	0	4.482968	-2.140053	2.875463
46	6	0	6.613361	-2.417822	2.822119
47	6	0	7.942205	-0.407894	2.770337
48	1	0	6.849064	1.442257	2.795495
49	1	0	6.543020	-3.500614	2.843670
50	6	0	7.864188	-1.799667	2.786210
51	1	0	8.909571	0.083877	2.751639
52	1	0	8.769372	-2.398070	2.777611
53	6	0	4.382993	2.759505	0.084901
54	8	0	3.379235	3.426377	0.264961
55	8	0	5.494961	3.150460	-0.562468
56	6	0	5.619324	4.490438	-1.193224
57	6	0	7.020684	4.436659	-1.799114
58	1	0	7.097818	3.630445	-2.532195
59	1	0	7.245045	5.379565	-2.302629
60	1	0	7.774134	4.274465	-1.024945
61	6	0	4.562827	4.653099	-2.285888
62	1	0	4.616822	3.827267	-2.999899
63	1	0	3.556549	4.694916	-1.871725
64	1	0	4.747900	5.581355	-2.832568
65	6	0	5.533038	5.579133	-0.123594
66	1	0	4.538740	5.633544	0.317087
67	1	0	6.261556	5.396679	0.670561
68	1	0	5.763251	6.548251	-0.573762
69	9	0	-9.037095	0.690769	1.495674
70	9	0	-9.246085	0.692619	-0.788453
71	7	0	-7.716702	-0.902195	0.222120
72	7	0	-7.178994	1.530717	0.174795
73	6	0	-8.392236	-2.071322	0.279356
74	6	0	-7.474737	-3.132052	0.183940
75	6	0	-6.193191	-2.604723	0.064390
76	6	0	-6.346723	-1.181324	0.089974
77	6	0	-5.411023	-0.139474	0.007801
78	6	0	-5.819341	1.201750	0.051460
79	6	0	-5.078835	2.426078	-0.005518
80	6	0	-6.018081	3.448155	0.083628
81	6	0	-7.297809	2.876769	0.193186

82	5	0	-8.332816	0.511434	0.279581
83	1	0	-7.735983	-4.181062	0.201035
84	1	0	-5.811981	4.509506	0.072623
85	6	0	-3.602207	2.646412	-0.132015
86	1	0	-3.044866	2.181201	0.684043
87	1	0	-3.202748	2.233470	-1.061112
88	1	0	-3.386841	3.716472	-0.120057
89	6	0	-4.950024	-3.431257	-0.063762
90	1	0	-4.401501	-3.210705	-0.982142
91	1	0	-4.257407	-3.263664	0.764276
92	1	0	-5.211653	-4.491015	-0.073434
93	6	0	-9.874160	-2.168283	0.422417
94	1	0	-10.216272	-1.693989	1.345796
95	1	0	-10.387635	-1.668241	-0.402533
96	1	0	-10.180967	-3.214219	0.437451
97	6	0	-8.600862	3.593482	0.312224
98	1	0	-9.270345	3.340873	-0.513927
99	1	0	-9.119162	3.326101	1.236457
100	1	0	-8.437252	4.671183	0.306964

Input orientation of **BDP-F$_D$F$_D$-Boc** conf. 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.383779	0.202951	0.420826
2	6	0	2.473436	-0.326359	-0.499442
3	1	0	2.831336	-0.778501	-1.418292
4	6	0	1.108246	-0.281224	-0.251294
5	1	0	0.419596	-0.702751	-0.976886
6	6	0	0.615907	0.297039	0.927867
7	6	0	1.521335	0.826399	1.856764
8	1	0	1.159788	1.272152	2.770391
9	6	0	2.888505	0.774139	1.594341
10	1	0	3.577168	1.189389	2.322809
11	7	0	-0.783933	0.315822	1.101299
12	1	0	-1.326194	-0.084799	0.346723
13	6	0	-1.516765	0.788778	2.144713
14	6	0	-3.049366	0.673839	1.997039
15	8	0	-1.049581	1.285949	3.163589
16	7	0	-3.496180	-0.054187	0.814324
17	1	0	-3.368963	0.093511	2.865197
18	6	0	-3.717223	2.071070	2.093559
19	1	0	-3.783905	0.487886	0.009215
20	1	0	-4.794742	1.908812	2.174008
21	1	0	-3.389397	2.513148	3.035932
22	6	0	-3.416369	3.011932	0.944721
23	6	0	-2.277935	3.830334	0.966853
24	6	0	-4.267261	3.085506	-0.166336
25	1	0	-1.614986	3.802842	1.825928
26	6	0	-1.993029	4.688937	-0.093637
27	6	0	-3.982282	3.942605	-1.230988
28	1	0	-5.165444	2.475943	-0.201182
29	1	0	-1.109907	5.318601	-0.053956
30	6	0	-2.843528	4.745875	-1.198905
31	1	0	-4.655789	3.986170	-2.080987
32	1	0	-2.623950	5.416582	-2.023217
33	6	0	-3.907759	-1.354096	0.872216

34	6	0	-4.621122	-1.866582	-0.398332
35	8	0	-3.761617	-2.059974	1.862679
36	7	0	-6.062010	-1.791238	-0.189060
37	1	0	-4.389968	-1.209869	-1.237864
38	6	0	-4.215557	-3.308889	-0.747173
39	1	0	-6.520780	-2.529802	0.324258
40	1	0	-4.411560	-3.949684	0.116031
41	1	0	-4.878100	-3.639142	-1.552455
42	6	0	-2.771523	-3.452549	-1.180753
43	6	0	-2.362730	-3.008777	-2.445916
44	6	0	-1.819140	-4.043366	-0.342940
45	1	0	-3.088015	-2.559202	-3.118629
46	6	0	-1.039879	-3.151240	-2.861937
47	6	0	-0.494306	-4.190858	-0.756587
48	1	0	-2.117407	-4.395125	0.639603
49	1	0	-0.744697	-2.806340	-3.847826
50	6	0	-0.100215	-3.744445	-2.017224
51	1	0	0.227901	-4.656510	-0.093601
52	1	0	0.928784	-3.860955	-2.341452
53	6	0	-6.791535	-0.681670	-0.499787
54	8	0	-6.322477	0.319424	-1.021281
55	8	0	-8.079435	-0.872936	-0.156952
56	6	0	-9.128634	0.149221	-0.400167
57	6	0	-10.382115	-0.533733	0.144425
58	1	0	-10.270546	-0.763060	1.206671
59	1	0	-11.246309	0.123585	0.025402
60	1	0	-10.583259	-1.464112	-0.391554
61	6	0	-8.817020	1.418110	0.393363
62	1	0	-8.667550	1.183571	1.450415
63	1	0	-7.928633	1.921860	0.015802
64	1	0	-9.661405	2.108284	0.319106
65	6	0	-9.263661	0.411107	-1.900295
66	1	0	-8.378322	0.898778	-2.305539
67	1	0	-9.429489	-0.524521	-2.440591
68	1	0	-10.125552	1.059121	-2.079278
69	9	0	8.816127	0.591233	0.468556
70	9	0	8.439787	-0.493539	-1.516851
71	7	0	6.839032	1.191596	-0.809343
72	7	0	6.985878	-1.002995	0.362038
73	6	0	7.165393	2.314004	-1.487560
74	6	0	6.005663	3.086236	-1.674245
75	6	0	4.929195	2.422576	-1.095035
76	6	0	5.460361	1.212584	-0.543345
77	6	0	4.852382	0.157671	0.153223
78	6	0	5.603464	-0.939106	0.600802
79	6	0	5.230203	-2.122510	1.315538
80	6	0	6.399993	-2.856210	1.482171
81	6	0	7.462948	-2.151536	0.890729
82	5	0	7.808725	0.070260	-0.381035
83	1	0	5.970682	4.038267	-2.185540
84	1	0	6.490900	-3.811012	1.981223
85	6	0	3.885575	-2.554626	1.815716
86	1	0	3.468181	-1.847665	2.536324
87	1	0	3.155883	-2.648703	1.008432
88	1	0	3.970264	-3.525193	2.308033
89	6	0	3.523015	2.939896	-1.091083
90	1	0	2.834157	2.264333	-1.603277
91	1	0	3.136832	3.074691	-0.078277

92	1	0	3.484566	3.906179	-1.597437
93	6	0	8.548629	2.634858	-1.945220
94	1	0	9.248246	2.668721	-1.106508
95	1	0	8.921572	1.879574	-2.641841
96	1	0	8.561938	3.602653	-2.446690
97	6	0	8.896227	-2.561192	0.830211
98	1	0	9.238961	-2.658918	-0.202978
99	1	0	9.541814	-1.822796	1.312232
100	1	0	9.032989	-3.519411	1.331608

Input orientation of **BDP-F_DF_D-Boc** conf. 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.818691	0.551850	0.087842
2	6	0	3.224501	0.908147	-1.123969
3	1	0	3.805538	0.869387	-2.039621
4	6	0	1.893898	1.315875	-1.190014
5	1	0	1.455998	1.587075	-2.138137
6	6	0	1.124608	1.372849	-0.019696
7	6	0	1.718628	1.015883	1.201152
8	1	0	1.136375	1.055846	2.116416
9	6	0	3.045708	0.611781	1.251975
10	1	0	3.481945	0.340927	2.207641
11	7	0	-0.225351	1.774540	0.015888
12	1	0	-0.677897	1.726753	0.926331
13	6	0	-1.043388	2.140902	-1.015635
14	6	0	-2.487281	2.459423	-0.548085
15	8	0	-0.700518	2.216201	-2.188054
16	7	0	-3.176572	1.233676	-0.137175
17	1	0	-2.416678	3.092651	0.339817
18	6	0	-3.276944	3.197260	-1.638680
19	1	0	-3.749192	0.731267	-0.813690
20	1	0	-2.667328	4.043380	-1.965858
21	1	0	-3.384513	2.547520	-2.510672
22	6	0	-4.633065	3.688286	-1.175713
23	6	0	-5.812654	3.099981	-1.643975
24	6	0	-4.735153	4.754282	-0.271393
25	1	0	-5.758378	2.280386	-2.354453
26	6	0	-7.061403	3.556666	-1.217980
27	6	0	-5.979168	5.212842	0.158151
28	1	0	-3.834000	5.237947	0.095566
29	1	0	-7.963962	3.086848	-1.595735
30	6	0	-7.148703	4.613517	-0.313378
31	1	0	-6.036081	6.041909	0.856370
32	1	0	-8.118023	4.971427	0.018168
33	6	0	-3.076131	0.722748	1.104624
34	6	0	-3.940917	-0.512299	1.434265
35	8	0	-2.355430	1.220304	1.978863
36	7	0	-3.720738	-1.653586	0.542209
37	1	0	-3.565607	-0.841466	2.402102
38	6	0	-5.429484	-0.111584	1.609461
39	1	0	-3.321203	-2.483014	0.953682
40	1	0	-5.447332	0.773741	2.252619
41	1	0	-5.843155	0.187606	0.646032
42	6	0	-6.269238	-1.208802	2.225077
43	6	0	-7.108219	-2.002966	1.435688

44	6	0	-6.215796	-1.459995	3.602603
45	1	0	-7.173125	-1.816981	0.367775
46	6	0	-7.871385	-3.024351	2.003870
47	6	0	-6.975741	-2.479020	4.174570
48	1	0	-5.580391	-0.847343	4.236412
49	1	0	-8.518413	-3.627250	1.374632
50	6	0	-7.805930	-3.266964	3.375302
51	1	0	-6.924187	-2.654547	5.244436
52	1	0	-8.400089	-4.058992	3.819460
53	6	0	-4.156220	-1.772618	-0.740902
54	8	0	-4.653941	-0.856355	-1.389118
55	8	0	-3.948701	-3.022347	-1.183880
56	6	0	-4.210828	-3.427201	-2.591660
57	6	0	-3.782951	-4.893581	-2.591370
58	1	0	-4.373541	-5.471469	-1.876872
59	1	0	-3.930462	-5.324362	-3.584126
60	1	0	-2.727241	-4.992128	-2.328637
61	6	0	-5.701731	-3.297915	-2.902343
62	1	0	-6.296561	-3.846988	-2.168078
63	1	0	-6.023387	-2.257811	-2.908854
64	1	0	-5.904154	-3.727460	-3.886914
65	6	0	-3.336771	-2.606730	-3.539819
66	1	0	-3.631341	-1.558462	-3.556398
67	1	0	-2.285207	-2.673741	-3.249510
68	1	0	-3.430572	-3.004758	-4.553452
69	9	0	8.834115	-1.153239	1.402282
70	9	0	8.996321	-0.851387	-0.865579
71	7	0	7.602670	0.685463	0.399110
72	7	0	6.895397	-1.675907	0.033948
73	6	0	8.359000	1.786791	0.602512
74	6	0	7.516256	2.909062	0.683004
75	6	0	6.199171	2.490744	0.524661
76	6	0	6.253511	1.071292	0.343847
77	6	0	5.246179	0.116402	0.141216
78	6	0	5.560512	-1.242188	-0.011093
79	6	0	4.735860	-2.393482	-0.222920
80	6	0	5.602536	-3.478767	-0.298538
81	6	0	6.920259	-3.016026	-0.138751
82	5	0	8.119565	-0.760217	0.243999
83	1	0	7.850442	3.925026	0.841619
84	1	0	5.322807	-4.511484	-0.454095
85	6	0	3.246236	-2.493831	-0.348763
86	1	0	2.732071	-2.128386	0.543000
87	1	0	2.864542	-1.913629	-1.191890
88	1	0	2.958780	-3.536040	-0.499763
89	6	0	5.014352	3.407587	0.549681
90	1	0	4.447813	3.373583	-0.383585
91	1	0	4.315804	3.156014	1.350934
92	1	0	5.347087	4.435678	0.704302
93	6	0	9.846233	1.762626	0.717895
94	1	0	10.169038	1.150643	1.564050
95	1	0	10.308377	1.339016	-0.177124
96	1	0	10.227384	2.774160	0.858602
97	6	0	8.171288	-3.828750	-0.149252
98	1	0	8.856564	-3.494469	-0.932084
99	1	0	8.706576	-3.746776	0.800181
100	1	0	7.934073	-4.878600	-0.322076

Table S8. Calculated at B3LYP/6-311+G*/PCM(CH_3CN) level of theory relative energies and conformer distribution at 25° C for **BDP-F_DF_D-Fmoc.**

Conf.	*ΔG* [kcal mol^{-1}]	Pop. [%]
4(1)	0.00	98.4
4(2)	2.64	1.1
4(3)	3.16	0.5

Table S9. Cartesian coordinates for individual conformers of **BDP-F_DF_D-Fmoc**.

Input orientation of **BDP-F_DF_D-Fmoc** conf. 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.317197	-0.716105	-0.099660
2	6	0	-4.094678	-1.968036	-0.675088
3	1	0	-4.935811	-2.553690	-1.031547
4	6	0	-2.809866	-2.491919	-0.802977
5	1	0	-2.662820	-3.463072	-1.248756
6	6	0	-1.709469	-1.753569	-0.346657
7	6	0	-1.926787	-0.491781	0.228630
8	1	0	-1.081476	0.087729	0.582576
9	6	0	-3.213482	0.016260	0.349166
10	1	0	-3.358107	0.992702	0.799597
11	7	0	-0.371475	-2.201148	-0.428979
12	1	0	0.319661	-1.558242	-0.054466
13	6	0	0.094019	-3.394689	-0.888844
14	6	0	1.625015	-3.606691	-0.836760
15	8	0	-0.606879	-4.293611	-1.342165
16	7	0	2.354709	-2.587977	-0.101109
17	1	0	1.755141	-4.554907	-0.310649
18	6	0	2.176320	-3.745700	-2.274433
19	1	0	2.843818	-1.866351	-0.612844
20	1	0	1.531684	-4.456656	-2.794820
21	1	0	2.071271	-2.787565	-2.793821
22	6	0	3.615968	-4.210350	-2.327106
23	6	0	4.642647	-3.336544	-2.699989
24	6	0	3.949826	-5.532013	-2.002256
25	1	0	4.404688	-2.311194	-2.968418
26	6	0	5.970385	-3.766522	-2.743074
27	6	0	5.273555	-5.965364	-2.042962
28	1	0	3.167517	-6.231689	-1.721408
29	1	0	6.751666	-3.073081	-3.037435
30	6	0	6.290087	-5.082196	-2.412577
31	1	0	5.511609	-6.993993	-1.791581
32	1	0	7.320826	-5.419663	-2.446728
33	6	0	2.505928	-2.614696	1.244397
34	6	0	3.342560	-1.482701	1.864386
35	8	0	2.018545	-3.481349	1.963699
36	7	0	3.497306	-0.325464	0.987877
37	1	0	2.796611	-1.188845	2.765397
38	6	0	4.727210	-2.034558	2.274705
39	1	0	4.421504	0.068843	0.877743
40	1	0	4.545535	-2.936556	2.863187

41	1	0	5.269791	-2.344585	1.376861
42	6	0	5.558945	-1.051226	3.071402
43	6	0	6.690826	-0.448330	2.512036
44	6	0	5.208560	-0.723101	4.388304
45	1	0	6.990989	-0.702316	1.499276
46	6	0	7.451373	0.466167	3.244128
47	6	0	5.965270	0.187684	5.121854
48	1	0	4.341162	-1.189100	4.847342
49	1	0	8.326724	0.921628	2.792542
50	6	0	7.089463	0.788061	4.550409
51	1	0	5.681096	0.426093	6.141760
52	1	0	7.679455	1.496730	5.122263
53	6	0	2.448385	0.506223	0.734025
54	8	0	1.279205	0.227005	0.959608
55	8	0	2.863859	1.653008	0.169877
56	6	0	1.836694	2.593659	-0.222742
57	1	0	1.153632	2.104413	-0.918774
58	1	0	1.271107	2.890868	0.661552
59	6	0	2.510861	3.798516	-0.873206
60	6	0	3.344230	3.479761	-2.105398
61	1	0	1.690524	4.475999	-1.146805
62	6	0	3.507528	4.532809	0.011160
63	6	0	2.973822	2.818978	-3.269616
64	6	0	4.651442	3.978541	-1.950804
65	6	0	3.324393	5.080387	1.274492
66	6	0	4.752685	4.631966	-0.637929
67	6	0	3.921257	2.652487	-4.285576
68	1	0	1.965987	2.436260	-3.400384
69	6	0	5.595299	3.814634	-2.966092
70	6	0	4.398322	5.728008	1.894614
71	1	0	2.366031	5.014421	1.780996
72	6	0	5.822623	5.281485	-0.019970
73	6	0	5.220455	3.146398	-4.132972
74	1	0	3.644767	2.138184	-5.200165
75	1	0	6.605055	4.197911	-2.857947
76	6	0	5.635916	5.826660	1.251406
77	1	0	4.268943	6.159206	2.881907
78	1	0	6.785931	5.365768	-0.513120
79	1	0	5.943645	3.010804	-4.930652
80	1	0	6.458698	6.333669	1.745006
81	9	0	-8.841663	2.177706	0.857892
82	9	0	-9.680072	0.259316	-0.078512
83	7	0	-7.732588	0.075430	1.362311
84	7	0	-7.555210	1.102909	-0.900871
85	6	0	-8.204674	-0.310061	2.568450
86	6	0	-7.218729	-1.070225	3.221267
87	6	0	-6.103121	-1.158642	2.395260
88	6	0	-6.430099	-0.426691	1.208558
89	6	0	-5.701298	-0.172542	0.037319
90	6	0	-6.254405	0.584460	-1.006234
91	6	0	-5.729164	0.982476	-2.277293
92	6	0	-6.731733	1.724944	-2.892567
93	6	0	-7.841248	1.785676	-2.031555
94	5	0	-8.488621	0.917992	0.313833
95	1	0	-7.323907	-1.508971	4.203820
96	1	0	-6.679295	2.184510	-3.869836
97	6	0	-4.391206	0.701302	-2.890315
98	1	0	-3.569830	1.078756	-2.277178

99	1	0	-4.217198	-0.368686	-3.025070
100	1	0	-4.327280	1.178353	-3.870101
101	6	0	-4.847334	-1.894658	2.750549
102	1	0	-4.615537	-2.684534	2.032686
103	1	0	-3.978035	-1.233870	2.782298
104	1	0	-4.955720	-2.354763	3.734502
105	6	0	-9.561839	0.040542	3.079258
106	1	0	-9.693432	1.123371	3.147635
107	1	0	-10.345644	-0.335175	2.416823
108	1	0	-9.711392	-0.388744	4.070025
109	6	0	-9.141077	2.475205	-2.278505
110	1	0	-9.975861	1.770044	-2.255156
111	1	0	-9.341328	3.232247	-1.516235
112	1	0	-9.127499	2.961630	-3.253957

Input orientation of **BDP-F$_D$F$_D$-Fmoc** conf. 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.301419	0.280252	0.159125
2	6	0	-4.642615	0.323697	1.388983
3	1	0	-5.156374	-0.005815	2.286193
4	6	0	-3.331605	0.782992	1.496385
5	1	0	-2.842657	0.807446	2.457944
6	6	0	-2.648682	1.212390	0.350225
7	6	0	-3.308116	1.171460	-0.888371
8	1	0	-2.793335	1.501093	-1.785320
9	6	0	-4.614868	0.712282	-0.980287
10	1	0	-5.102573	0.689588	-1.949077
11	7	0	-1.325077	1.696585	0.357205
12	1	0	-0.943902	1.955621	-0.550608
13	6	0	-0.442866	1.774139	1.396982
14	6	0	0.947946	2.315284	0.967164
15	8	0	-0.692917	1.459728	2.552755
16	7	0	1.647648	1.332321	0.135981
17	1	0	0.785519	3.196165	0.340875
18	6	0	1.790643	2.702422	2.190859
19	1	0	2.293917	0.691527	0.576532
20	1	0	1.168532	3.339952	2.823474
21	1	0	2.000351	1.806874	2.781575
22	6	0	3.077954	3.421484	1.846420
23	6	0	4.318450	2.789317	1.982800
24	6	0	3.053291	4.749438	1.398926
25	1	0	4.363672	1.765672	2.343148
26	6	0	5.503621	3.460422	1.675797
27	6	0	4.233624	5.423792	1.092109
28	1	0	2.102670	5.266211	1.298912
29	1	0	6.455392	2.951773	1.791110
30	6	0	5.464825	4.779978	1.228824
31	1	0	4.192955	6.453696	0.751962
32	1	0	6.384822	5.304784	0.992881
33	6	0	1.448187	1.204902	-1.189626
34	6	0	2.237528	0.093725	-1.905682
35	8	0	0.632608	1.891427	-1.814592
36	7	0	3.269688	-0.501828	-1.072051
37	1	0	1.500536	-0.693049	-2.086707
38	6	0	2.772152	0.550603	-3.286988

39	1	0	4.163685	-0.031466	-1.015304
40	1	0	3.060120	-0.351890	-3.831439
41	1	0	1.935858	0.998284	-3.826240
42	6	0	3.941309	1.511268	-3.237777
43	6	0	3.739002	2.892643	-3.108205
44	6	0	5.257326	1.037678	-3.323181
45	1	0	2.727535	3.281791	-3.053392
46	6	0	4.819690	3.771872	-3.060756
47	6	0	6.341577	1.915328	-3.273995
48	1	0	5.437191	-0.026574	-3.445376
49	1	0	4.641588	4.838199	-2.965879
50	6	0	6.125605	3.286106	-3.141546
51	1	0	7.352365	1.526874	-3.346375
52	1	0	6.966459	3.971195	-3.108134
53	6	0	3.265947	-1.832630	-0.758352
54	8	0	2.334094	-2.596969	-0.933919
55	8	0	4.442722	-2.179366	-0.196241
56	6	0	4.574433	-3.553588	0.229766
57	1	0	3.807695	-3.770960	0.975401
58	1	0	4.414333	-4.210109	-0.626838
59	6	0	5.972792	-3.746379	0.811552
60	6	0	6.301271	-2.858408	2.002277
61	1	0	6.017904	-4.801509	1.114196
62	6	0	7.114508	-3.439528	-0.145956
63	6	0	5.618457	-2.710671	3.202866
64	6	0	7.487863	-2.140400	1.761250
65	6	0	7.364550	-3.958066	-1.410084
66	6	0	7.992366	-2.500849	0.428457
67	6	0	6.125116	-1.833005	4.167514
68	1	0	4.705904	-3.265243	3.400598
69	6	0	7.994483	-1.267407	2.725515
70	6	0	8.499759	-3.529413	-2.106480
71	1	0	6.696593	-4.687137	-1.859052
72	6	0	9.126560	-2.076048	-0.265682
73	6	0	7.303054	-1.118253	3.928934
74	1	0	5.601112	-1.708053	5.109469
75	1	0	8.910177	-0.711466	2.550473
76	6	0	9.371989	-2.596210	-1.537594
77	1	0	8.706211	-3.926319	-3.095073
78	1	0	9.810999	-1.354646	0.169544
79	1	0	7.684429	-0.442768	4.687860
80	1	0	10.249276	-2.274923	-2.089729
81	9	0	-10.298318	-1.331140	-1.326928
82	9	0	-10.333506	-1.658573	0.942956
83	7	0	-9.099566	0.247337	0.078246
84	7	0	-8.254716	-2.074804	-0.243771
85	6	0	-9.920764	1.311504	0.218300
86	6	0	-9.141246	2.465776	0.408520
87	6	0	-7.797772	2.106195	0.385525
88	6	0	-7.770375	0.690320	0.173610
89	6	0	-6.706239	-0.216557	0.060028
90	6	0	-6.942642	-1.583474	-0.147846
91	6	0	-6.050316	-2.693021	-0.300448
92	6	0	-6.855912	-3.812345	-0.481552
93	6	0	-8.202432	-3.410413	-0.443215
94	5	0	-9.533343	-1.217316	-0.140085
95	1	0	-9.534393	3.463084	0.549231
96	1	0	-6.516187	-4.828085	-0.629220

97	6	0	-4.552461	-2.726324	-0.282830
98	1	0	-4.117212	-2.094840	-1.060569
99	1	0	-4.144209	-2.379280	0.669078
100	1	0	-4.204717	-3.748251	-0.445140
101	6	0	-6.663722	3.070042	0.558587
102	1	0	-6.035498	2.816841	1.415518
103	1	0	-6.008425	3.096020	-0.315017
104	1	0	-7.056101	4.076692	0.714386
105	6	0	-11.409312	1.223713	0.168469
106	1	0	-11.752581	0.845590	-0.797960
107	1	0	-11.794315	0.543646	0.932207
108	1	0	-11.848175	2.208610	0.328786
109	6	0	-9.408684	-4.275566	-0.592824
110	1	0	-10.046619	-4.225677	0.293215
111	1	0	-10.019323	-3.963233	-1.443666
112	1	0	-9.108953	-5.312594	-0.744527

Input orientation of **BDP-F$_D$F$_D$-Fmoc** conf. 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.944712	-0.876297	-0.456965
2	6	0	2.916797	-0.251699	0.251279
3	1	0	3.143862	0.585072	0.903551
4	6	0	1.594585	-0.676428	0.140237
5	1	0	0.815381	-0.177016	0.694726
6	6	0	1.281760	-1.754248	-0.697613
7	6	0	2.310274	-2.386412	-1.411078
8	1	0	2.082290	-3.222891	-2.064495
9	6	0	3.623210	-1.951841	-1.290993
10	1	0	4.402626	-2.455438	-1.852675
11	7	0	-0.027514	-2.253560	-0.877881
12	1	0	-0.099102	-3.036224	-1.512975
13	6	0	-1.192539	-1.840596	-0.306697
14	6	0	-2.429869	-2.666538	-0.693186
15	8	0	-1.296327	-0.899669	0.472601
16	7	0	-3.517398	-1.730280	-0.930872
17	1	0	-2.264504	-3.210609	-1.623892
18	6	0	-2.802859	-3.674792	0.430261
19	1	0	-3.566777	-0.911603	-0.339230
20	1	0	-2.989707	-3.109858	1.347295
21	1	0	-3.751996	-4.129949	0.135392
22	6	0	-1.764676	-4.747557	0.673112
23	6	0	-1.652368	-5.839559	-0.198047
24	6	0	-0.890442	-4.672491	1.763715
25	1	0	-2.329828	-5.924311	-1.043202
26	6	0	-0.689866	-6.826146	0.011628
27	6	0	0.073161	-5.658721	1.978276
28	1	0	-0.966597	-3.838814	2.455698
29	1	0	-0.621538	-7.666433	-0.671877
30	6	0	0.177628	-6.738046	1.101472
31	1	0	0.738848	-5.584558	2.832217
32	1	0	0.924650	-7.507234	1.268229
33	6	0	-4.411348	-1.867018	-1.930435
34	6	0	-5.442808	-0.729530	-2.087687
35	8	0	-4.418731	-2.814005	-2.716775
36	7	0	-5.338169	0.304312	-1.069139

37	1	0	-5.190353	-0.256893	-3.039602
38	6	0	-6.887588	-1.278977	-2.208713
39	1	0	-5.864214	0.188943	-0.212946
40	1	0	-7.513649	-0.464222	-2.580243
41	1	0	-6.873718	-2.052299	-2.978545
42	6	0	-7.469599	-1.827139	-0.922643
43	6	0	-7.205597	-3.141725	-0.511959
44	6	0	-8.283161	-1.028070	-0.108240
45	1	0	-6.591890	-3.783811	-1.135625
46	6	0	-7.731122	-3.637988	0.679918
47	6	0	-8.809335	-1.521316	1.087114
48	1	0	-8.522199	-0.014655	-0.418225
49	1	0	-7.519527	-4.660313	0.976710
50	6	0	-8.532687	-2.827973	1.486042
51	1	0	-9.440061	-0.885835	1.700437
52	1	0	-8.944030	-3.215505	2.412376
53	6	0	-4.904533	1.565726	-1.352906
54	8	0	-4.386228	1.916204	-2.397754
55	8	0	-5.120793	2.378448	-0.290356
56	6	0	-4.653397	3.741779	-0.393344
57	1	0	-4.761140	4.075131	-1.424149
58	1	0	-5.326476	4.314681	0.243464
59	6	0	-3.197845	3.888295	0.076122
60	6	0	-2.989703	3.641154	1.562623
61	1	0	-2.581294	3.207168	-0.522457
62	6	0	-2.713134	5.321177	-0.083479
63	6	0	-3.224578	2.492604	2.310498
64	6	0	-2.478087	4.799440	2.181553
65	6	0	-2.638644	6.099833	-1.232398
66	6	0	-2.307854	5.841727	1.160501
67	6	0	-2.954349	2.508348	3.683093
68	1	0	-3.610779	1.593827	1.843035
69	6	0	-2.207663	4.813198	3.550827
70	6	0	-2.157255	7.409705	-1.133551
71	1	0	-2.939494	5.704858	-2.197934
72	6	0	-1.827605	7.148730	1.257594
73	6	0	-2.451647	3.659398	4.297080
74	1	0	-3.134091	1.617432	4.276057
75	1	0	-1.811102	5.701076	4.033213
76	6	0	-1.757159	7.928188	0.101767
77	1	0	-2.091699	8.027100	-2.023408
78	1	0	-1.510642	7.558561	2.211406
79	1	0	-2.245587	3.654364	5.362576
80	1	0	-1.385605	8.946025	0.161938
81	9	0	8.667835	1.601775	0.709608
82	9	0	9.316689	-0.038308	-0.756609
83	7	0	7.163858	1.030787	-1.110981
84	7	0	7.514937	-0.535191	0.795542
85	6	0	7.368474	1.970081	-2.060804
86	6	0	6.179728	2.146054	-2.790302
87	6	0	5.210355	1.290482	-2.277787
88	6	0	5.838077	0.577715	-1.205961
89	6	0	5.356971	-0.406956	-0.330652
90	6	0	6.183003	-0.958772	0.659567
91	6	0	5.939001	-1.955071	1.658811
92	6	0	7.131449	-2.095817	2.360717
93	6	0	8.082969	-1.216528	1.815026
94	5	0	8.202901	0.527105	-0.087243

95	1	0	6.053252	2.837218	-3.612039
96	1	0	7.310653	-2.766080	3.189930
97	6	0	4.691027	-2.730442	1.952486
98	1	0	3.855992	-2.079881	2.222071
99	1	0	4.363858	-3.324247	1.096050
100	1	0	4.868683	-3.412176	2.786283
101	6	0	3.808996	1.195828	-2.799610
102	1	0	3.571086	0.193360	-3.162533
103	1	0	3.067551	1.438004	-2.034919
104	1	0	3.676946	1.893465	-3.628690
105	6	0	8.666176	2.677830	-2.262745
106	1	0	8.963207	3.227496	-1.366054
107	1	0	9.472044	1.974724	-2.487805
108	1	0	8.582780	3.383855	-3.089065
109	6	0	9.495939	-1.027560	2.254999
110	1	0	10.196332	-1.206098	1.435605
111	1	0	9.669175	-0.007060	2.606529
112	1	0	9.729931	-1.715632	3.067450
