Supporting information for

1,3-Dipolar cycloadditions with *meso*-tetraarylchlorins – site selectivity and mixed bisadducts

J. Almeida, A. Aguiar, A. Leite, A. M. N. Silva, L. Cunha-Silva, B. de Castro, M. Rangel, G. Barone, A. C. Tomé* and A. M. G. Silva*

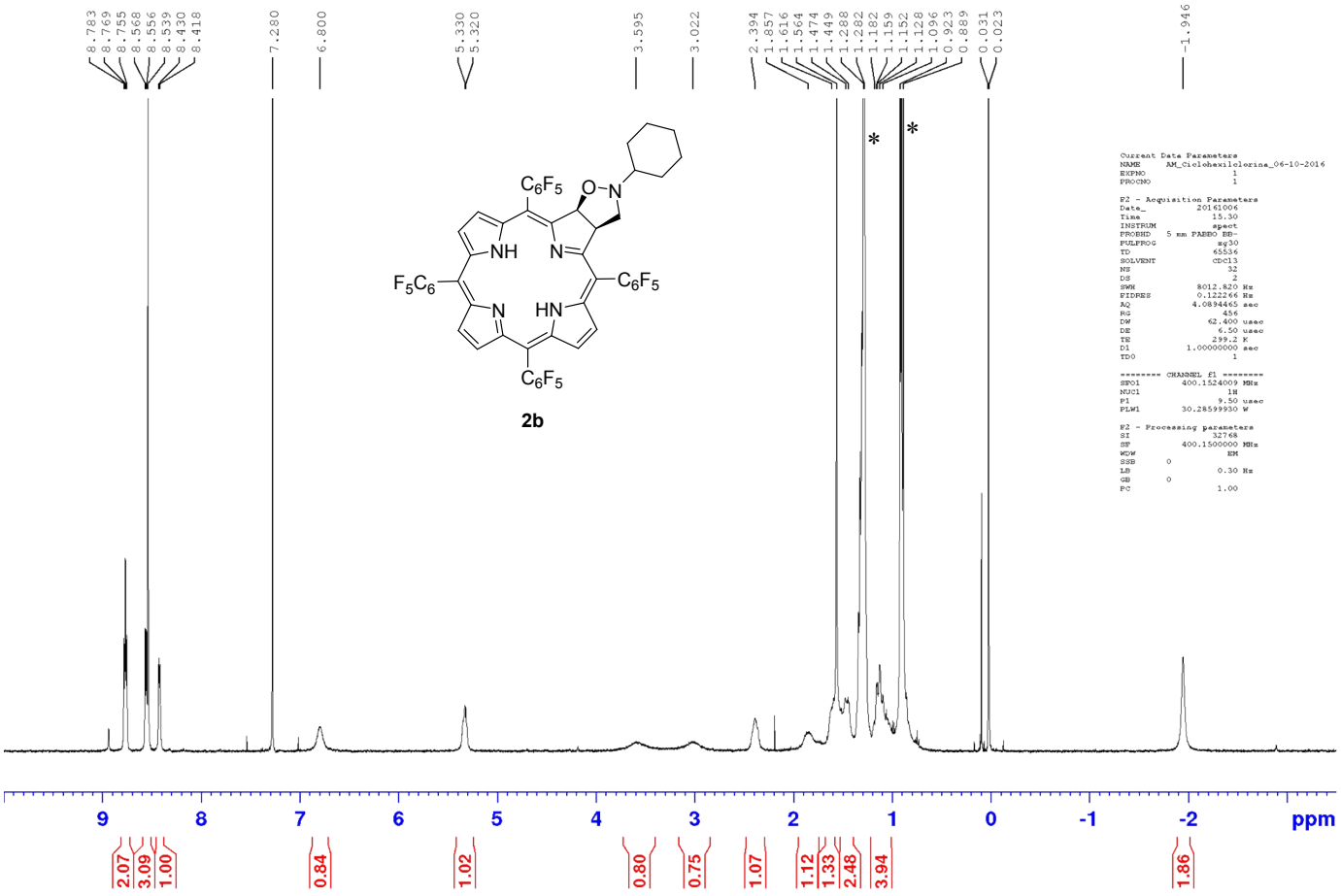
* Authors to whom correspondence should be addressed: Fax: (+351) 220402659; Tel: (+351) 220402585; e-mail: ana.silva@fc.up.pt or actome@ua.pt

Contents

Index of figures

Index of tables

NMR spectra of chlorin 2b



* Hexane used in the crystallization of the chlorin

Figure S1. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of **2b**.

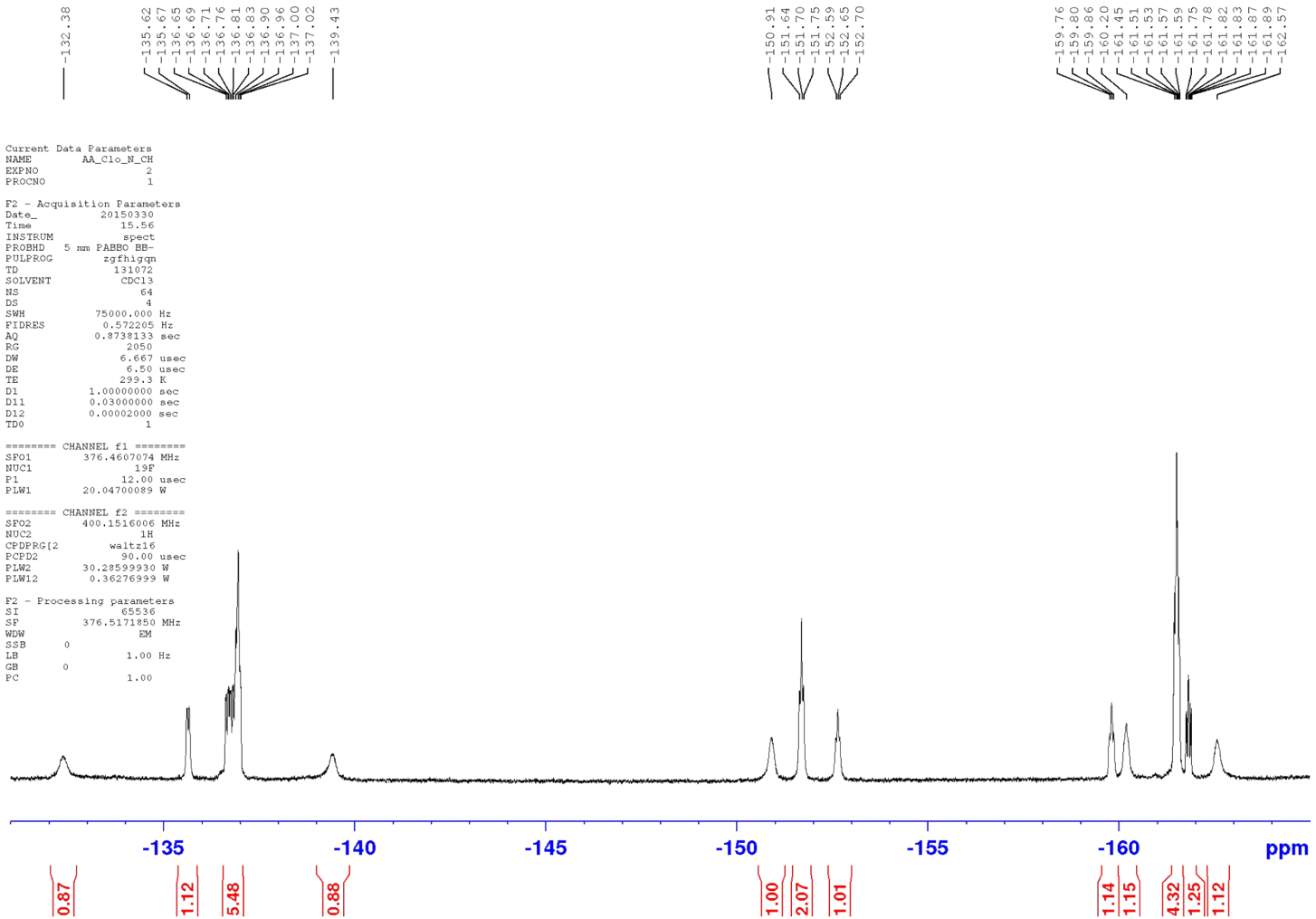
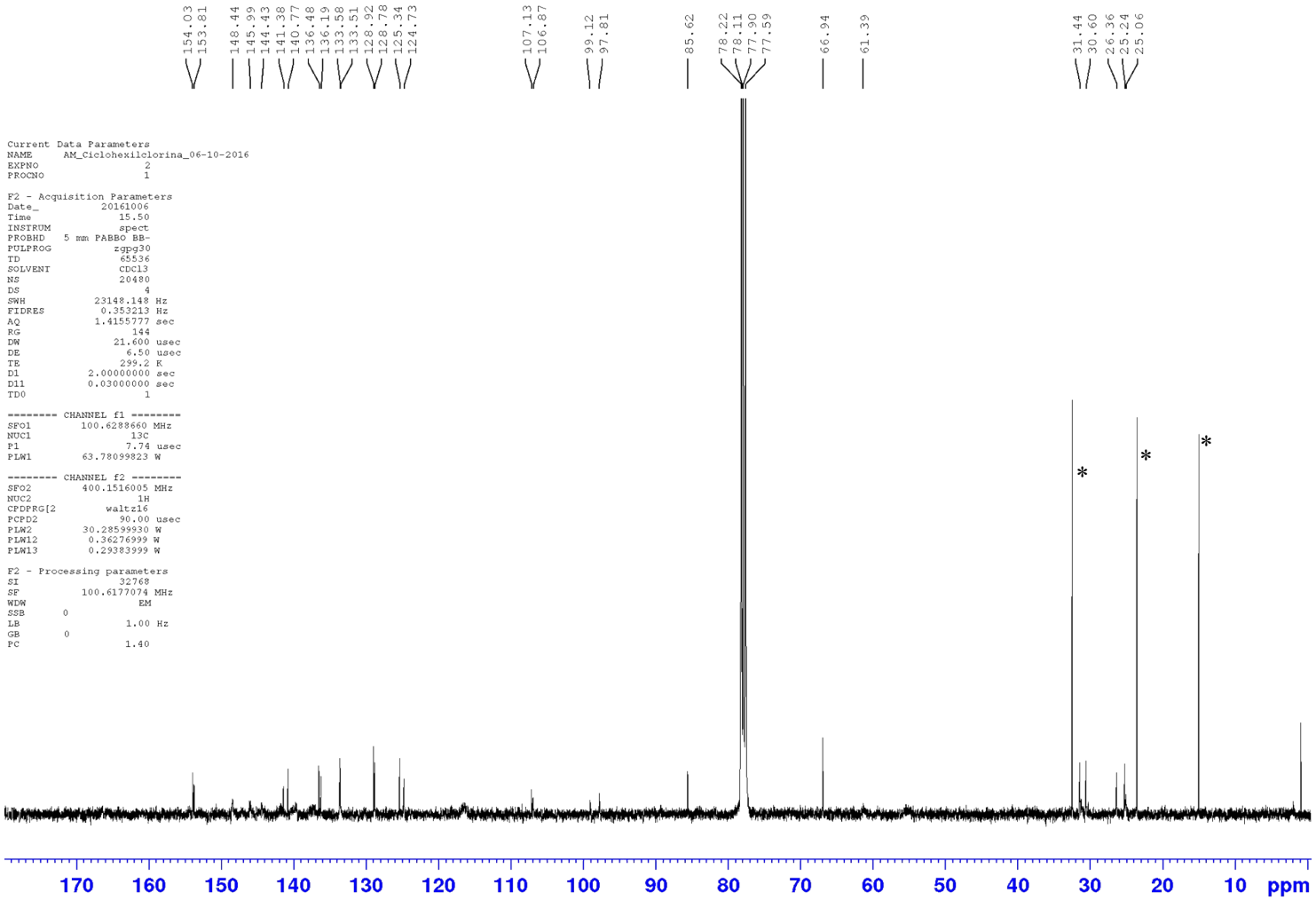


Figure S2. ^{19}F NMR spectrum (376.46 MHz, $CDCl_3$) of **2b**.



* Hexane used in the crystallization of the chlorin

Figure S3. ^{13}C NMR spectrum (100.63 MHz, $CDCl_3$) of **2b**.

NMR spectra of chlorin 2c

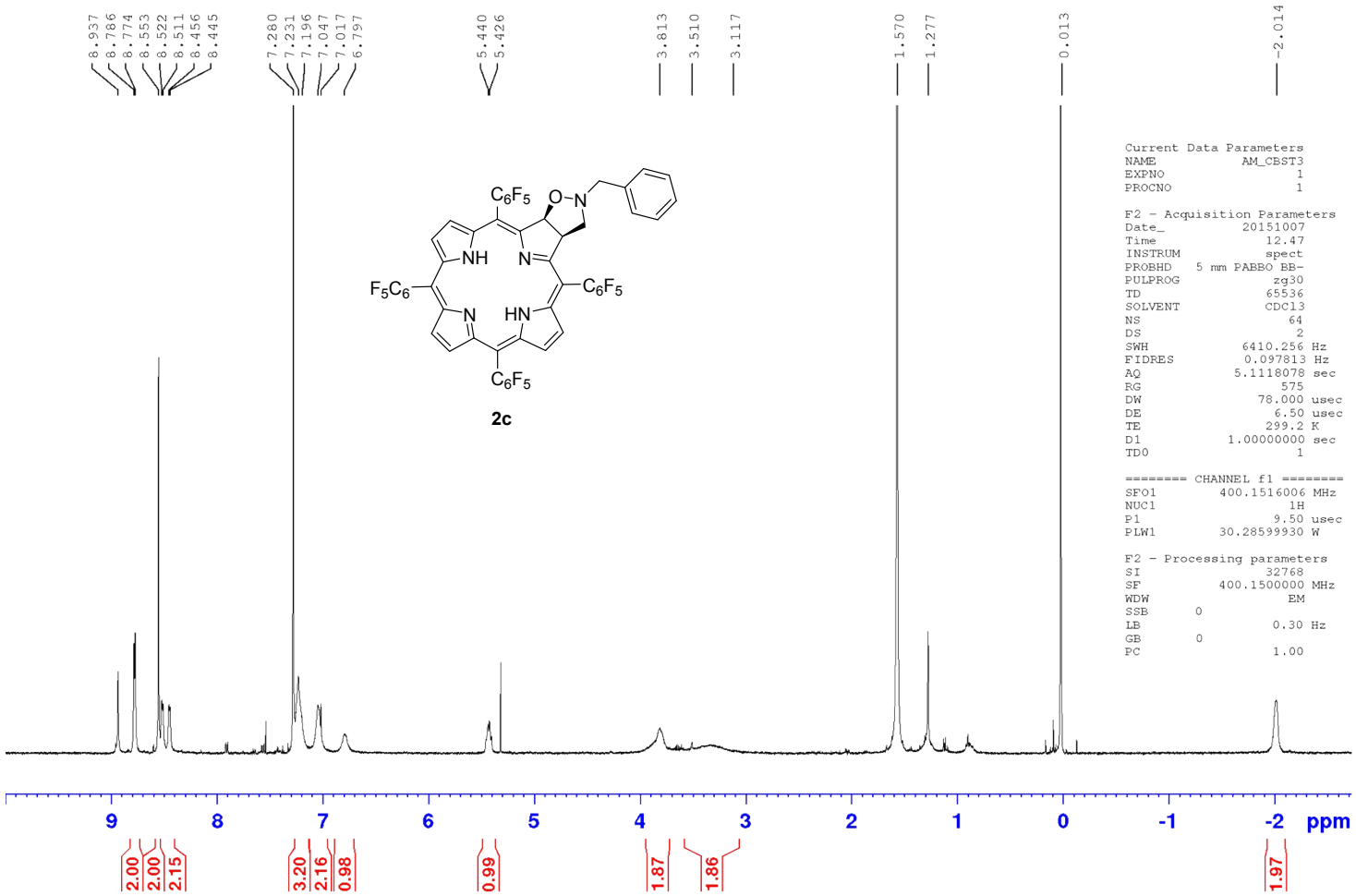


Figure S4. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of **2c**.

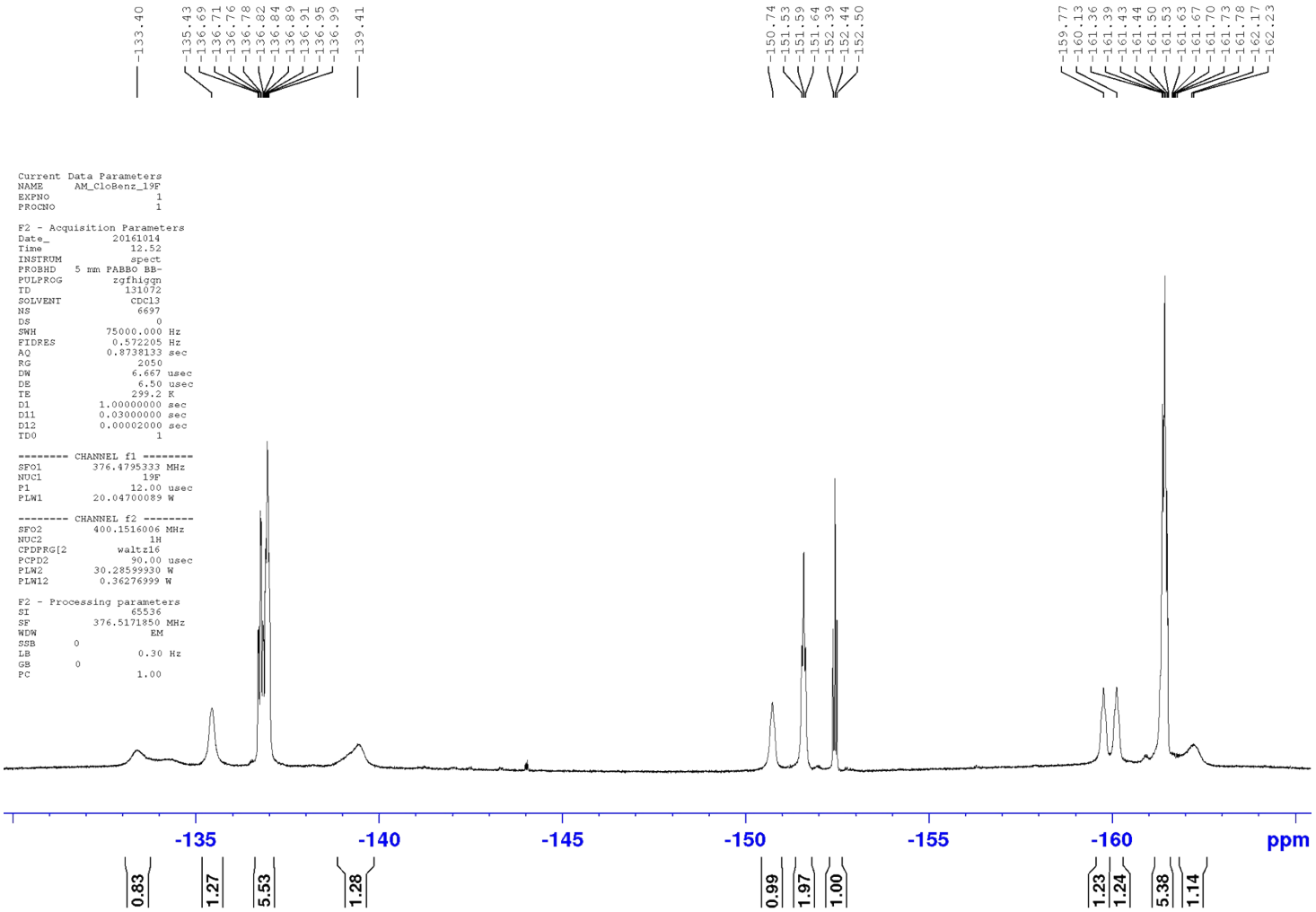


Figure S5. ^{19}F NMR spectrum (376.46 MHz, $CDCl_3$) of **2c**.

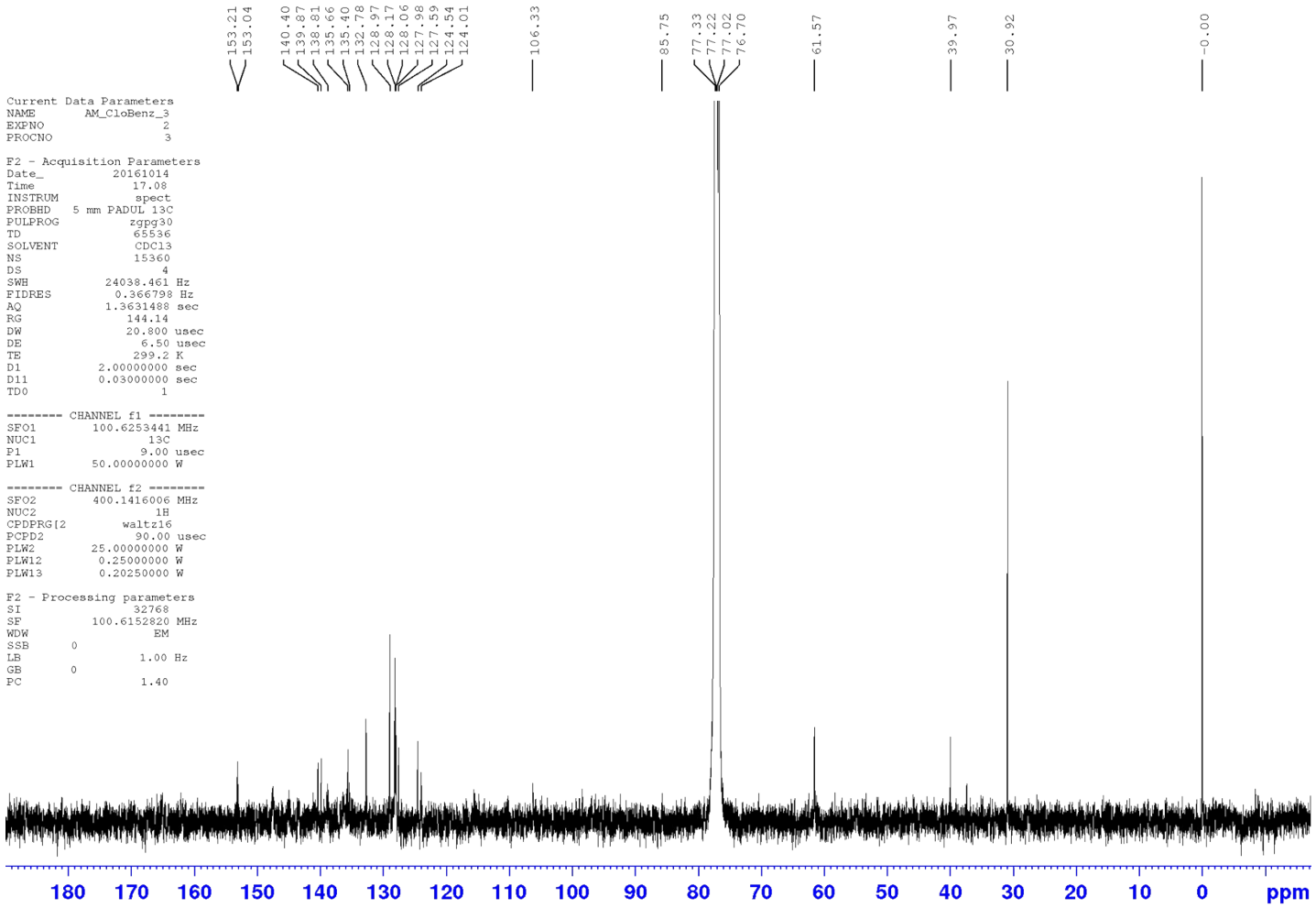


Figure S6. ^{13}C NMR spectrum (100.63 MHz, $CDCl_3$) of **2c**.

NMR spectra of BC *trans*-3c

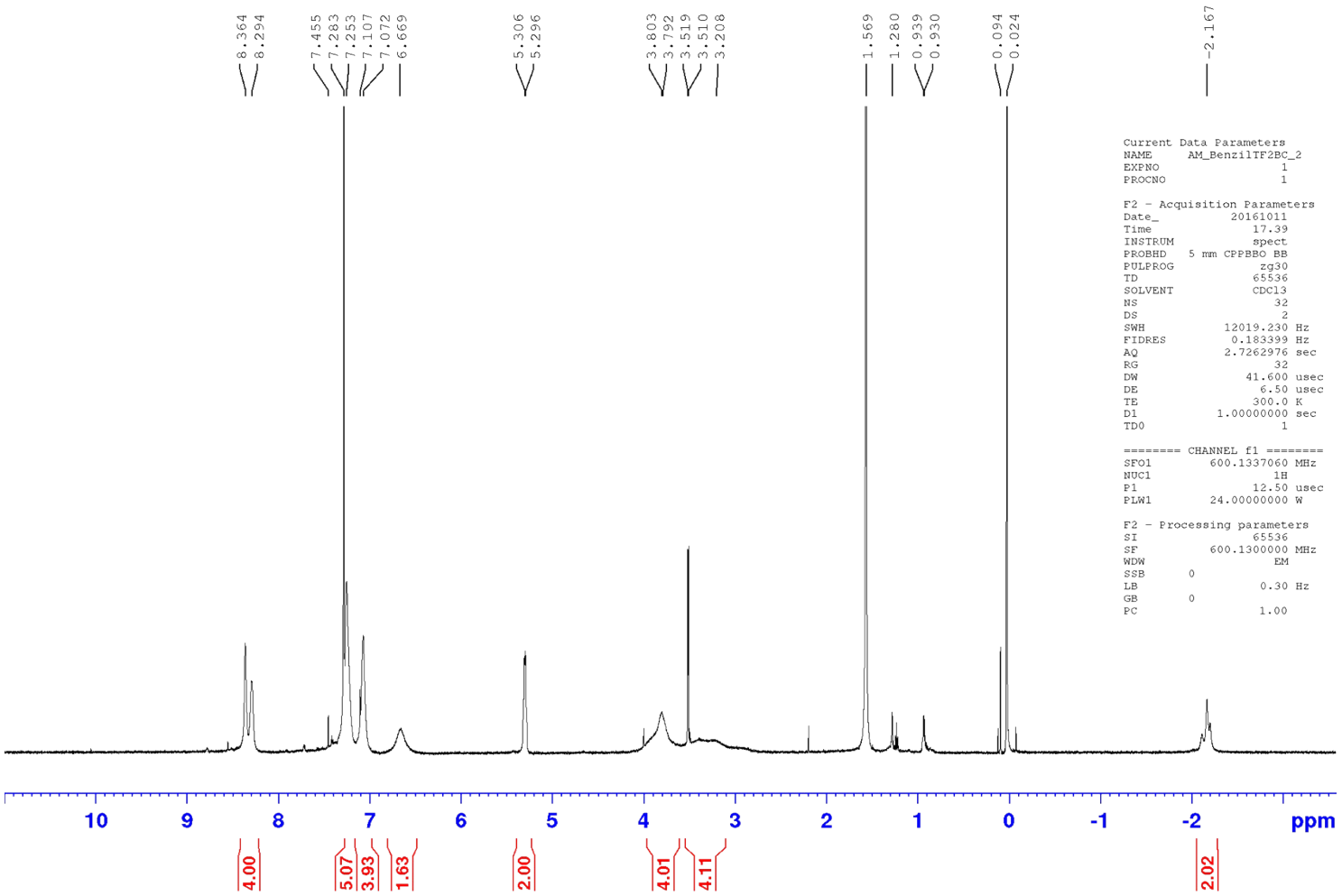


Figure S7. ^{1}H NMR spectrum (600.13 MHz, $CDCl_3$) of BC *trans*-**3c**.

Crystal and structure details for BC *trans*-3c.

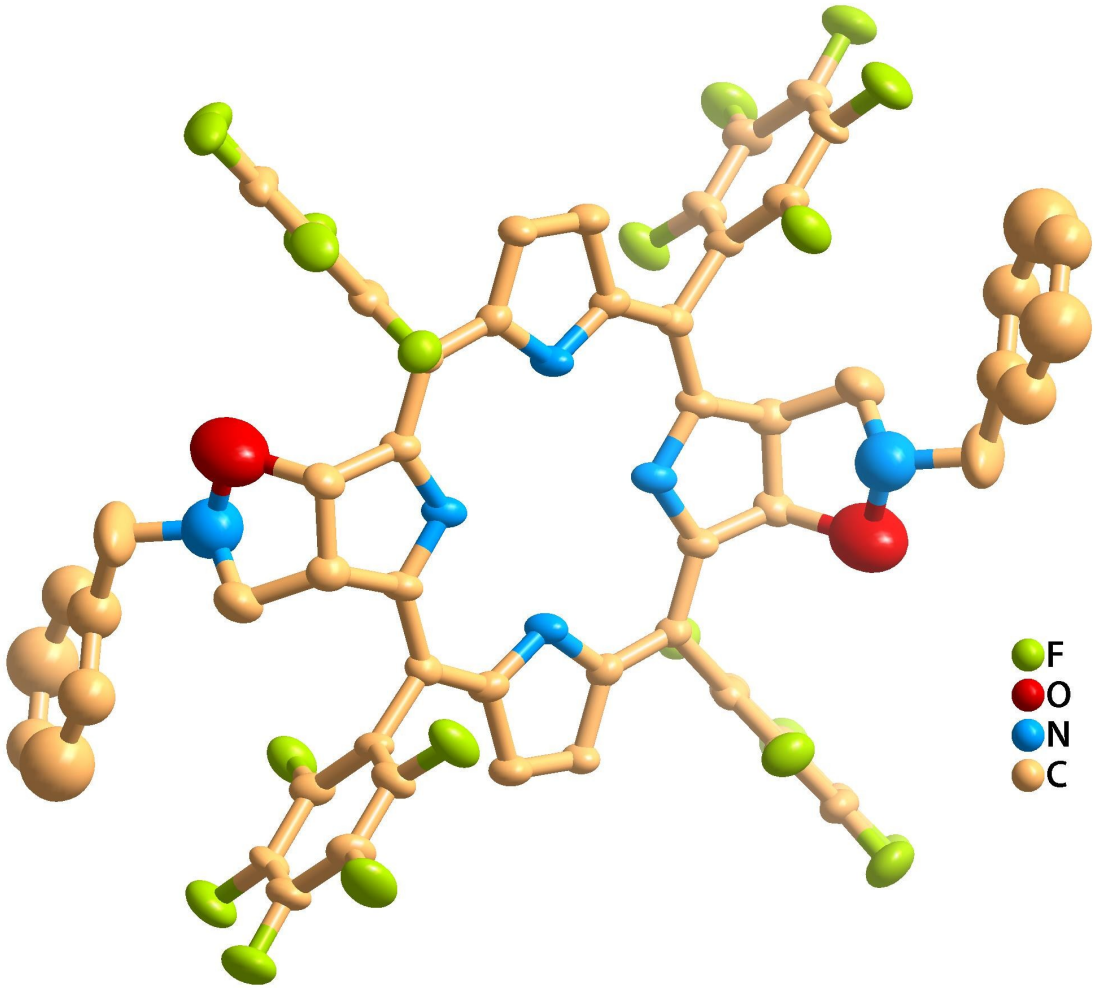


Figure S8. X-ray diffraction structure of BC *trans*-**3c**, with ellipsoids probability: 50%

Table S1. Crystal and structure refinement details for BC *trans*-**3c.**

Formula	$C_{60}H_{28}F_{20}N_6O_{44}$
Fw / g mol^{-1}	1244.88
Crystal type	Black prism
Crystal size / mm^3	0.18 × 0.16 × 0.10
Crystal system	Triclinic
Space group	*P*-1
a / Å	12.4994(13)
b / Å	13.1859(14)
c / Å	16.0253(17)
α / º	102.651(5)
β / º	95.439(6)
γ / º	92.898(10)
Volume / Å^3	92.290(6)
Z	2
Temparature / K	180(2)
D_c / g cm^{-3}	1.615
μ / mm^{-1}	0.150
θ range	3.638 – 25.027
Index ranges	−14 ≤ h ≤ 14 −15 ≤ k ≤ 15 −18 ≤ l ≤ 19
Collected reflection	51921
Independent reflections	8926 (R_{int} = 0.0620)
Data completeness	to θ = 25.03º, 99.1%
Final *R* indices [I>2σ(I)]	*R*1 = 0.1387 *wR*2 = 0.1059
Final *R* indices (all data)	*R*1 = 0.1877 *wR*2 = 0.4340
$(\Delta\rho)_{max,min}$ / e Å^{-3}	1.396 and −0.716

Table S2. C−H···F hydrogen bonds found in the crystal structure of BC *trans*-**3c**.

C–H···F	**H···A/Å**	**D···A/Å**	**<DHA/º**
C7–H7···F5	2.51	3.239(7)	129.5
C7–H7···F16	2.41	3.283(8)	145.1
C23–H23···F7^{i}	2.63	3.323(8)	126.7
C24–H24A···F10	2.60	3.547(10)	159.7
C33–H33···F3	2.61	3.209(8)	121.1

Symmetry transformations used to generate equivalent atoms: (*i*) *–x+1, –y+1, –z+1*;

NMR spectra of chlorin 2d

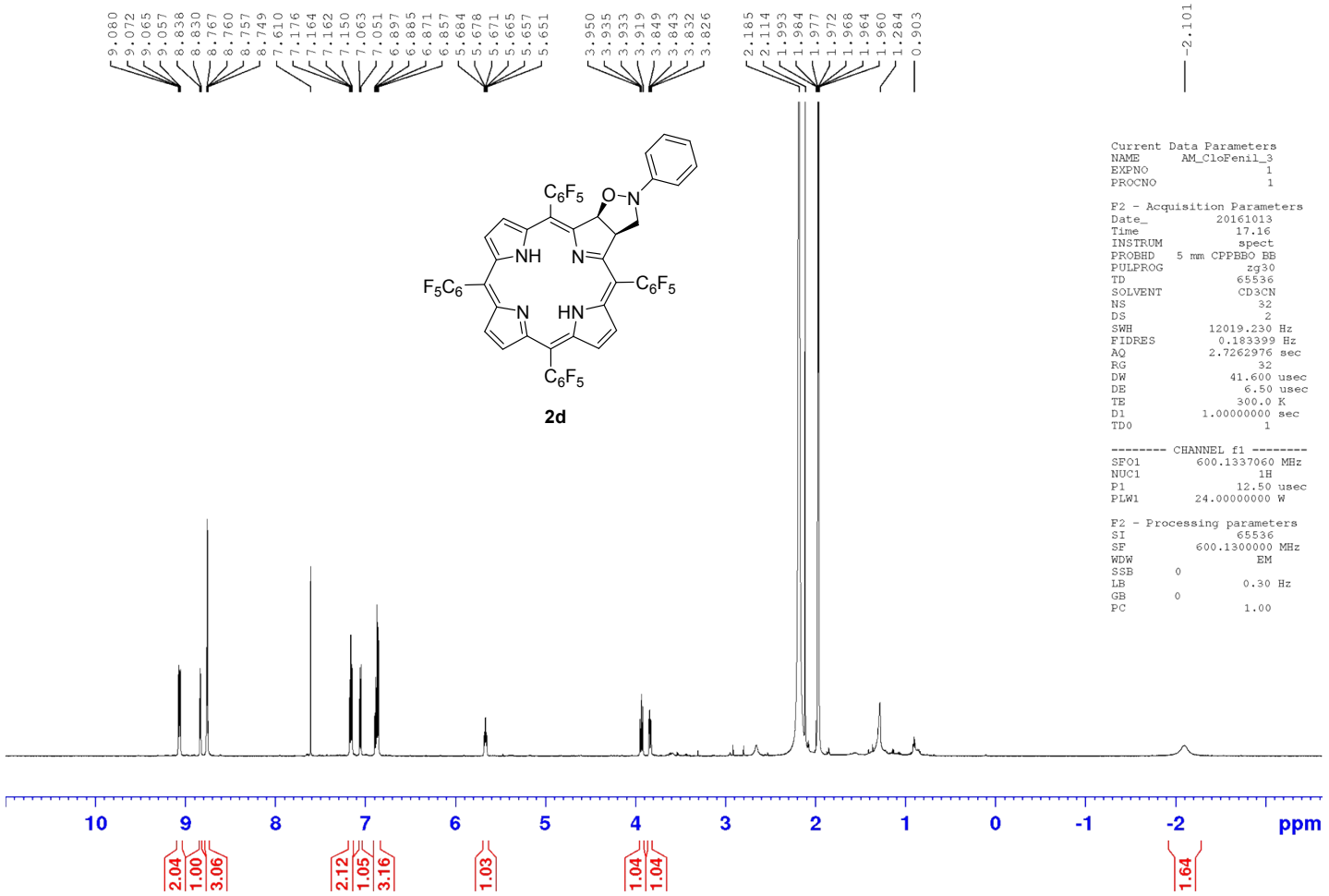


Figure S9. ^{1}H NMR spectrum (600.13 MHz, CD_3CN) of **2d**.

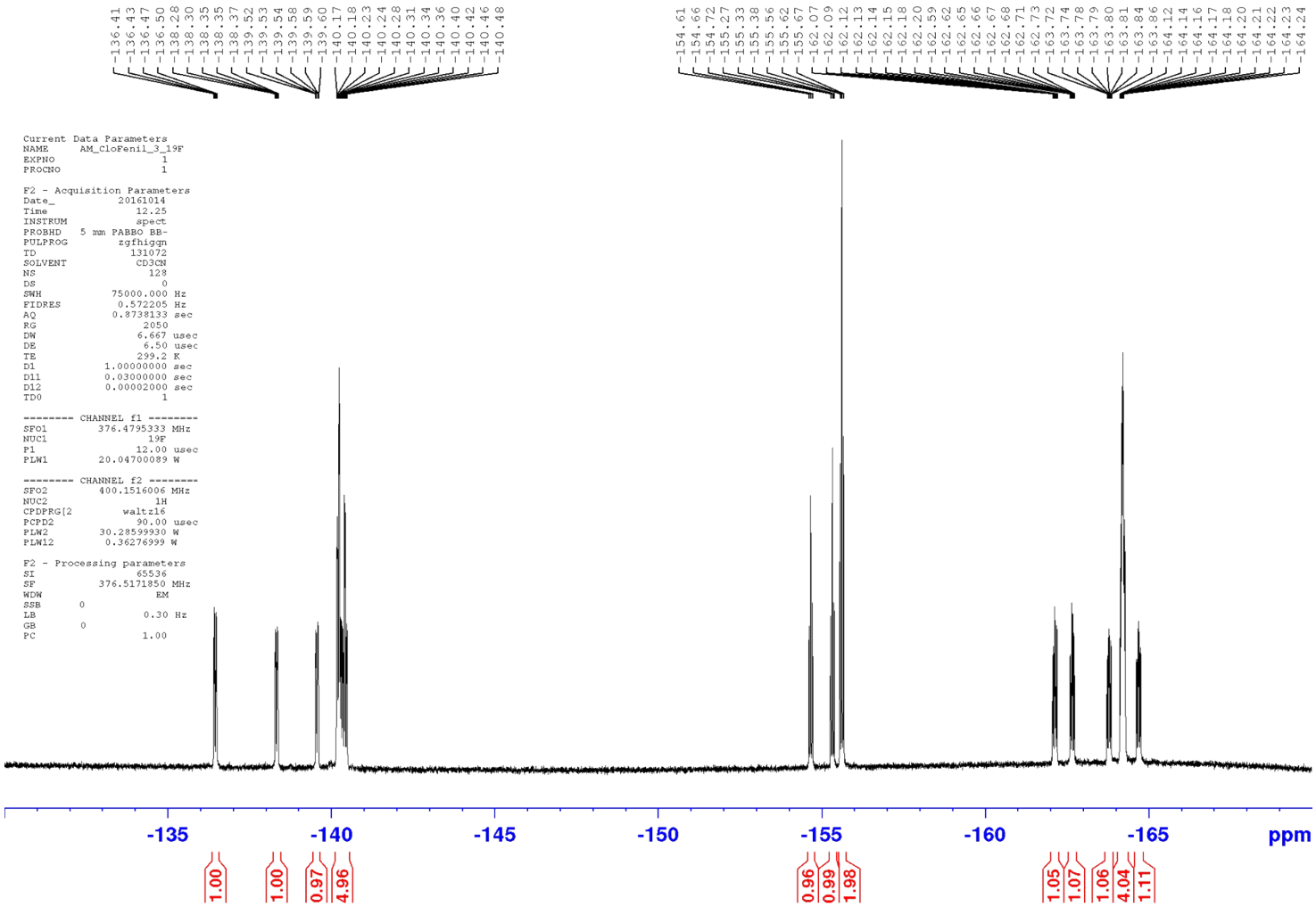


Figure S10. ^{19}F NMR spectrum (376.46 MHz, CD_3CN) of **2d**.

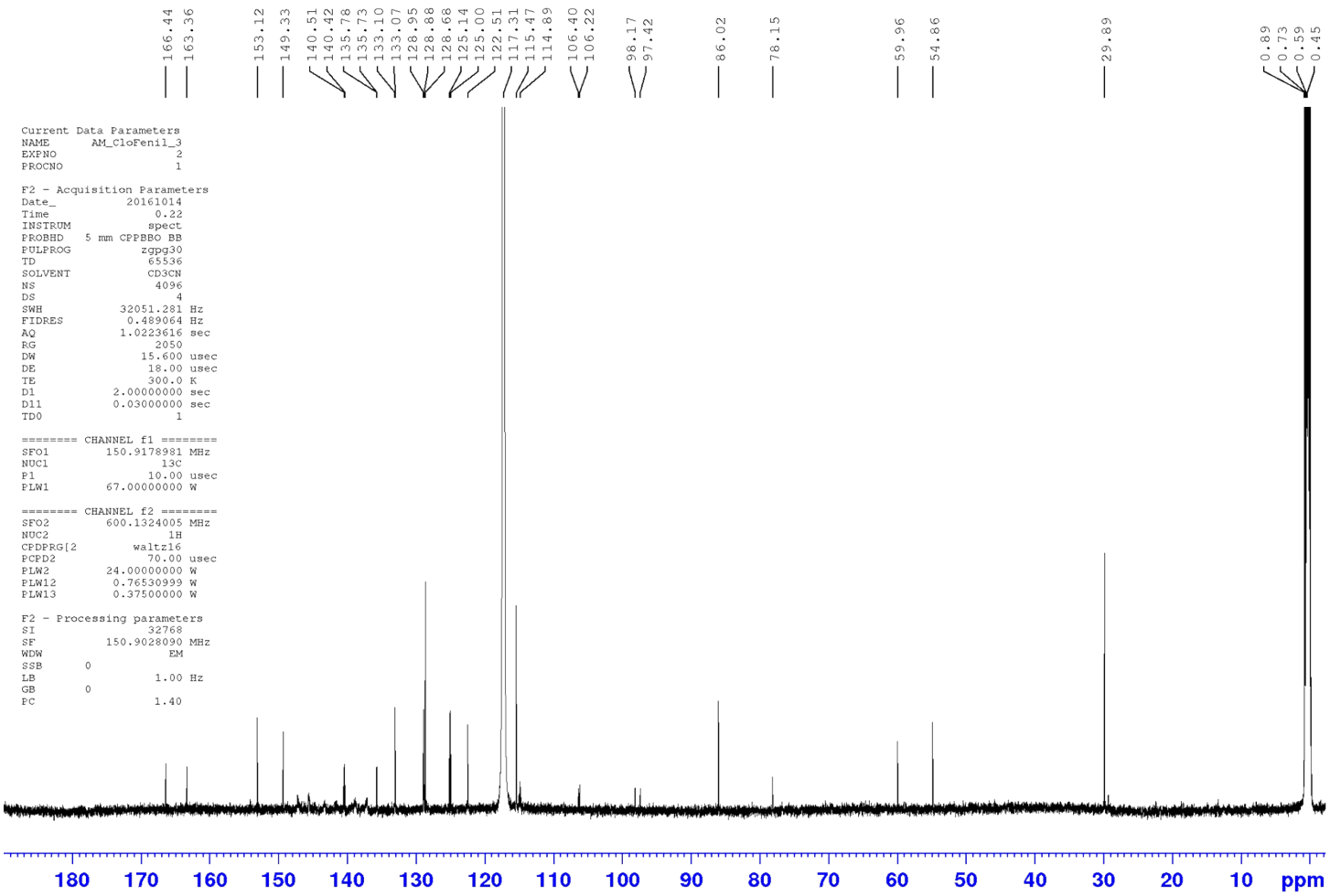


Figure S11. ^{13}C NMR spectrum (150.92 MHz, CD_3CN) of **2d**.

NMR spectra of chlorin 6a

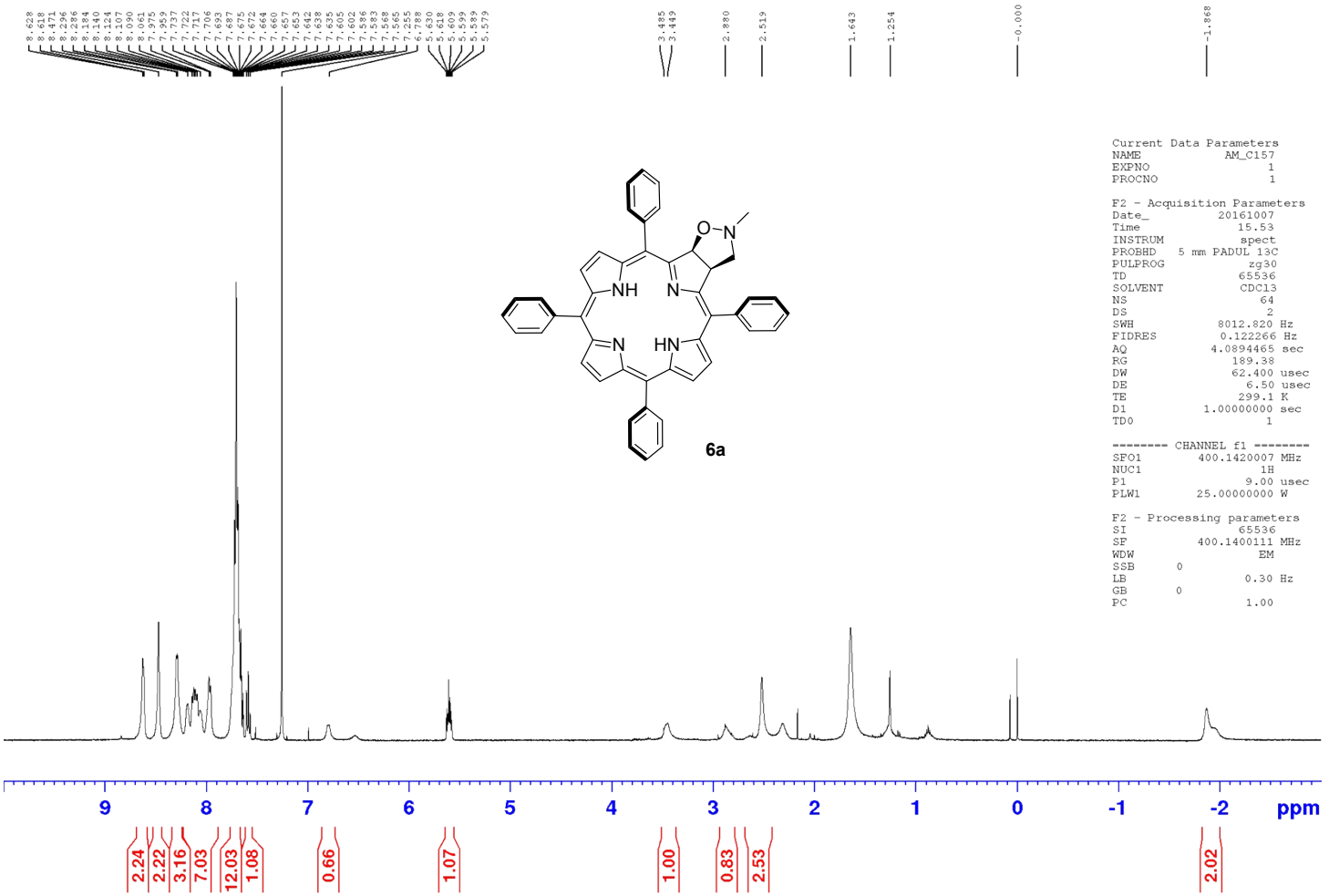


Figure S12. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of **6a**.

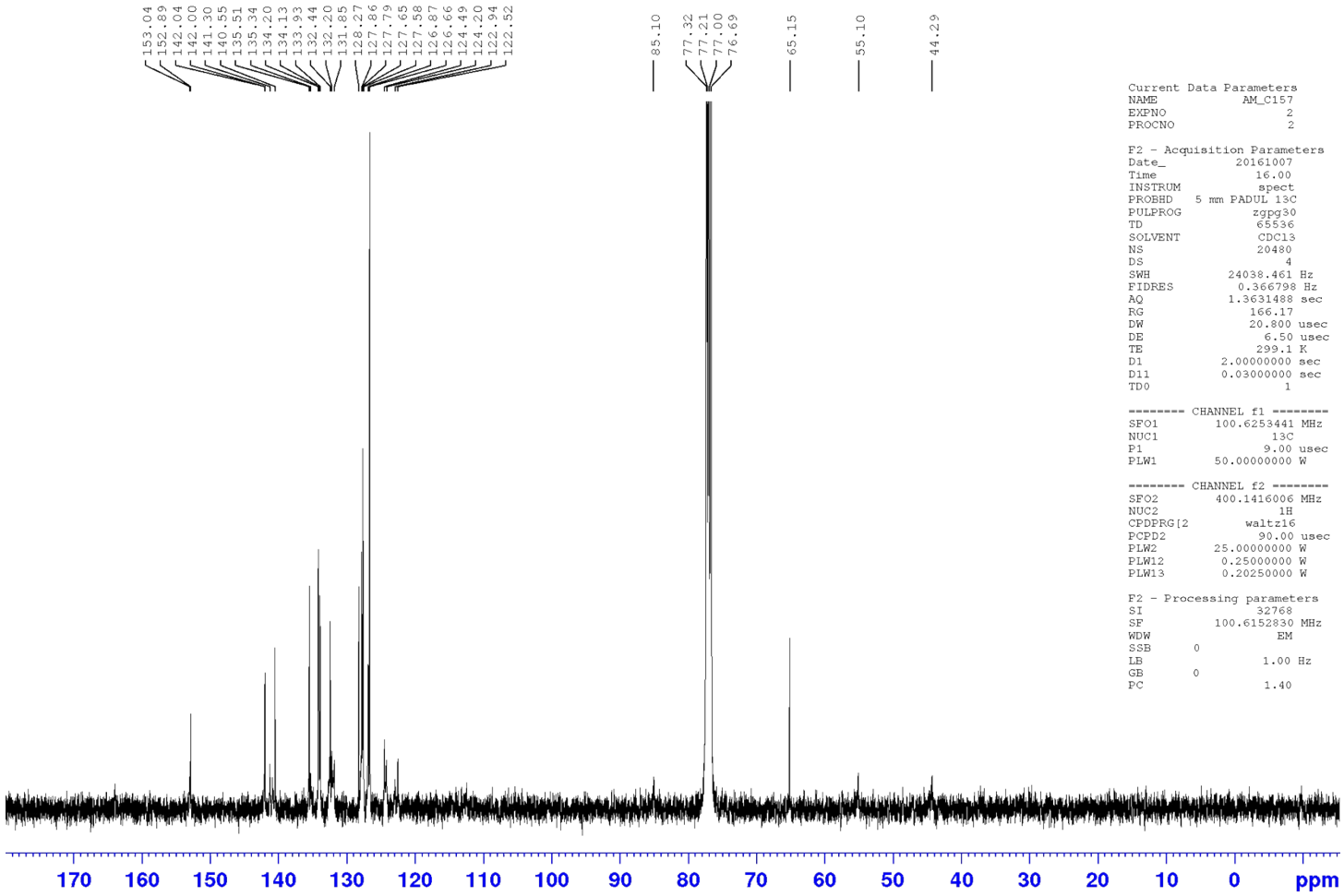


Figure S13. ^{13}C NMR spectrum (100.63 MHz, $CDCl_3$) of **6a**.

NMR spectra of chlorin 6b

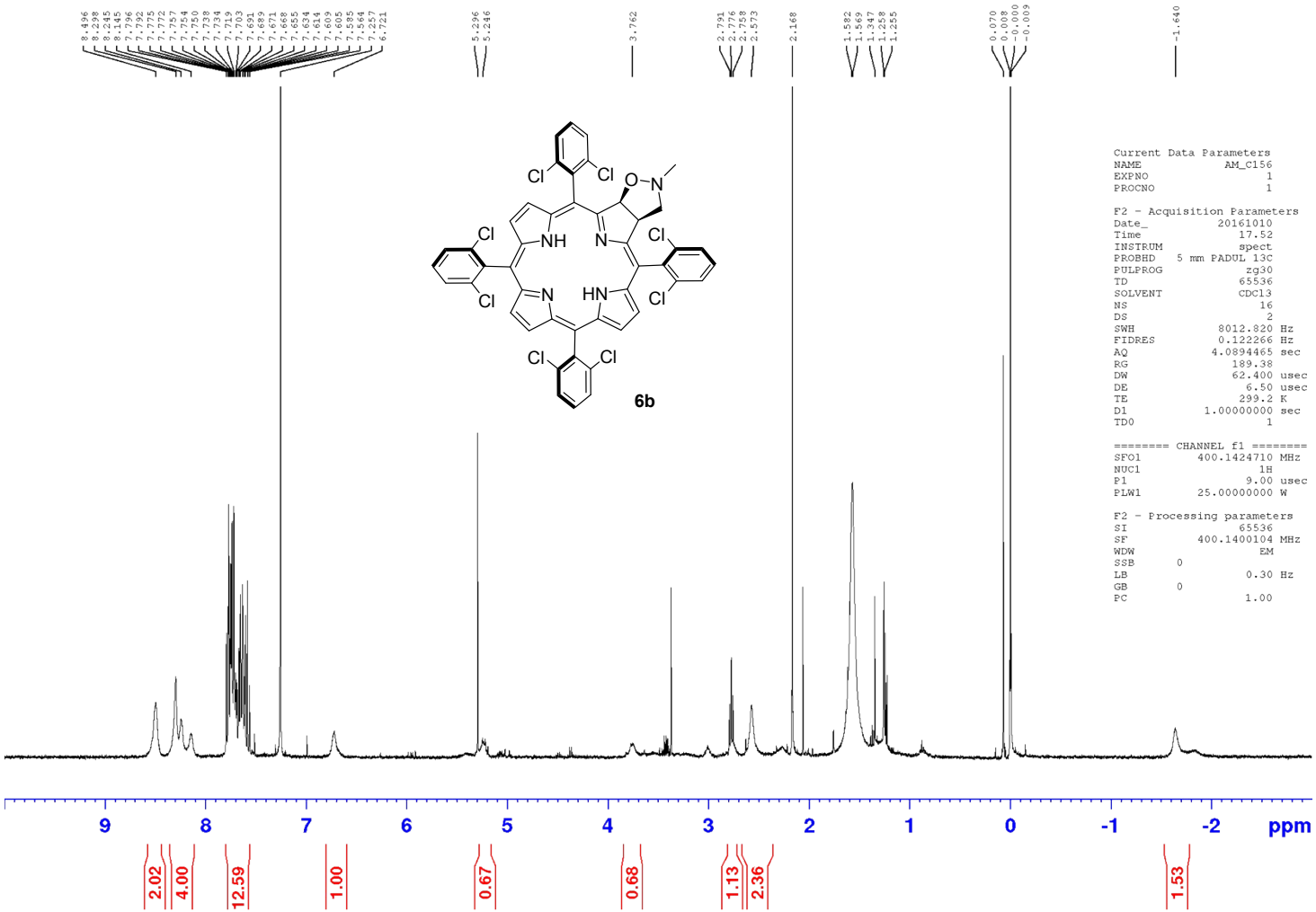


Figure S14. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of **6b**.

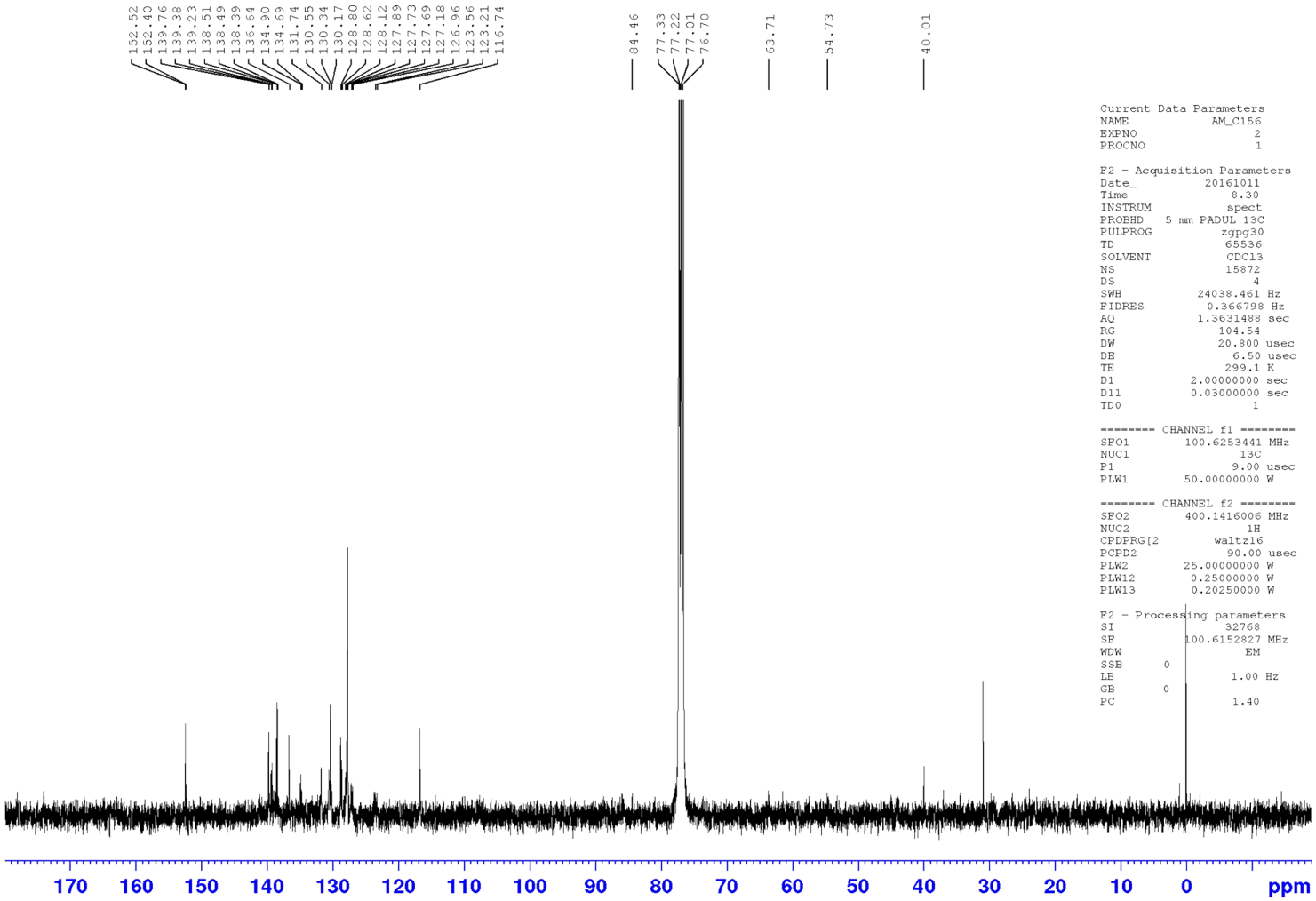


Figure S15. ^{13}C NMR spectrum (100.63 MHz, $CDCl_3$) of **6b**.

NMR spectra of isobacteriochlorins 7 and 8

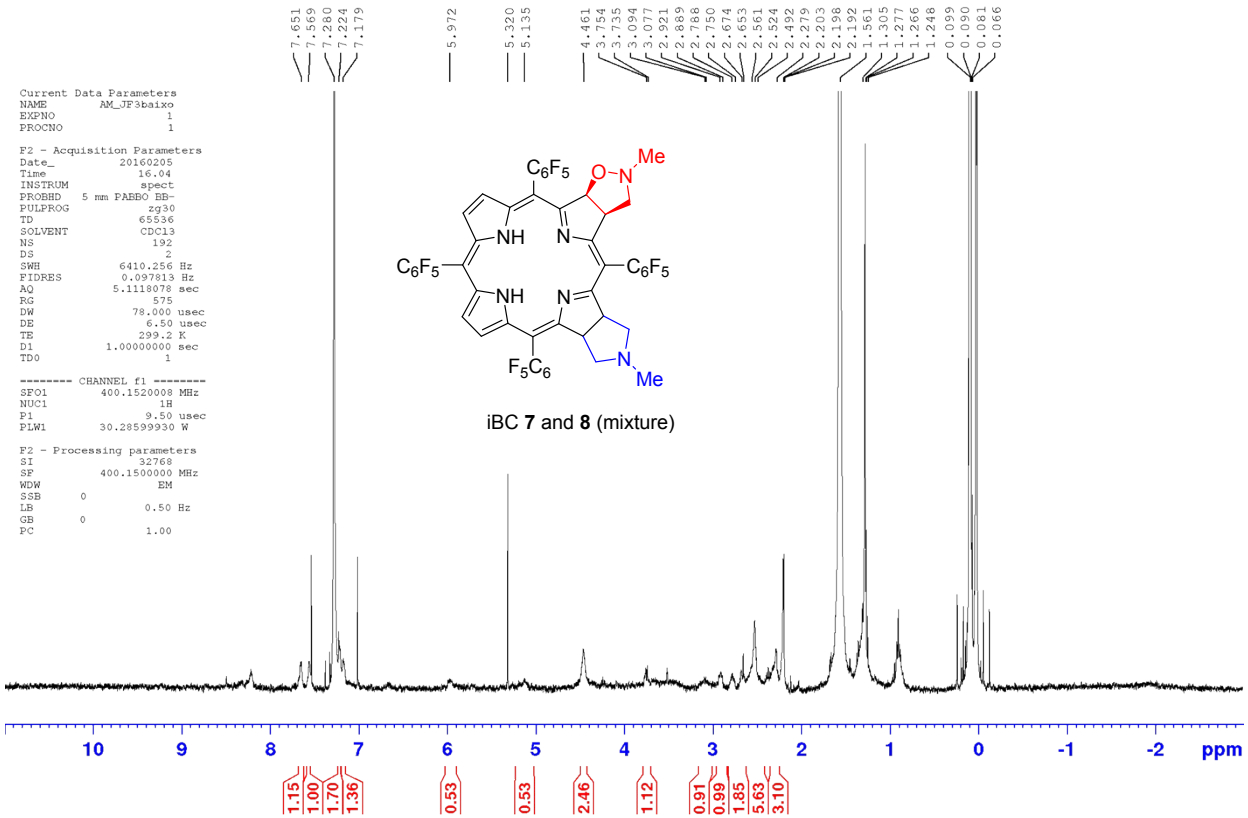


Figure S16. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of iBC **7** and **8**.

NMR spectra of bacteriochlorin *trans*-10

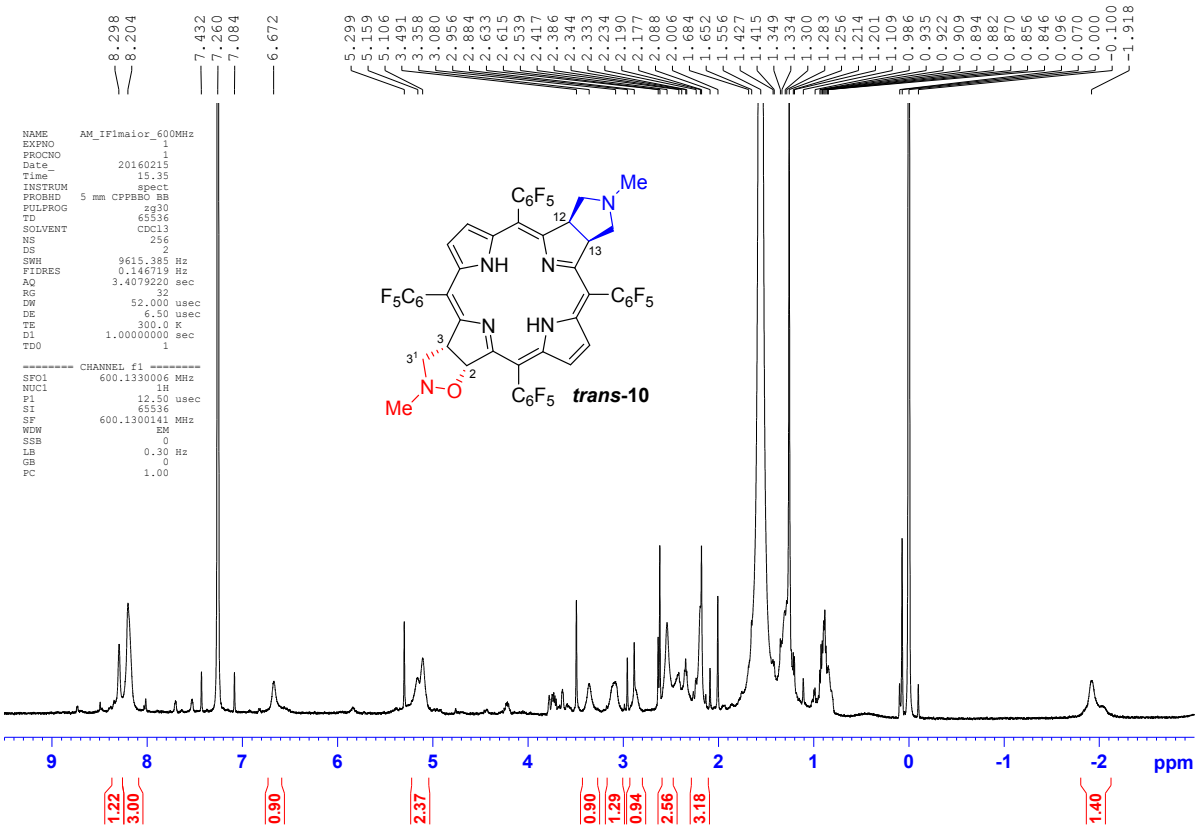


Figure S17. ^{1}H NMR spectrum (600.13 MHz, $CDCl_3$) of BC ***trans*-10**.

NMR spectra of bacteriochlorin *cis*-10

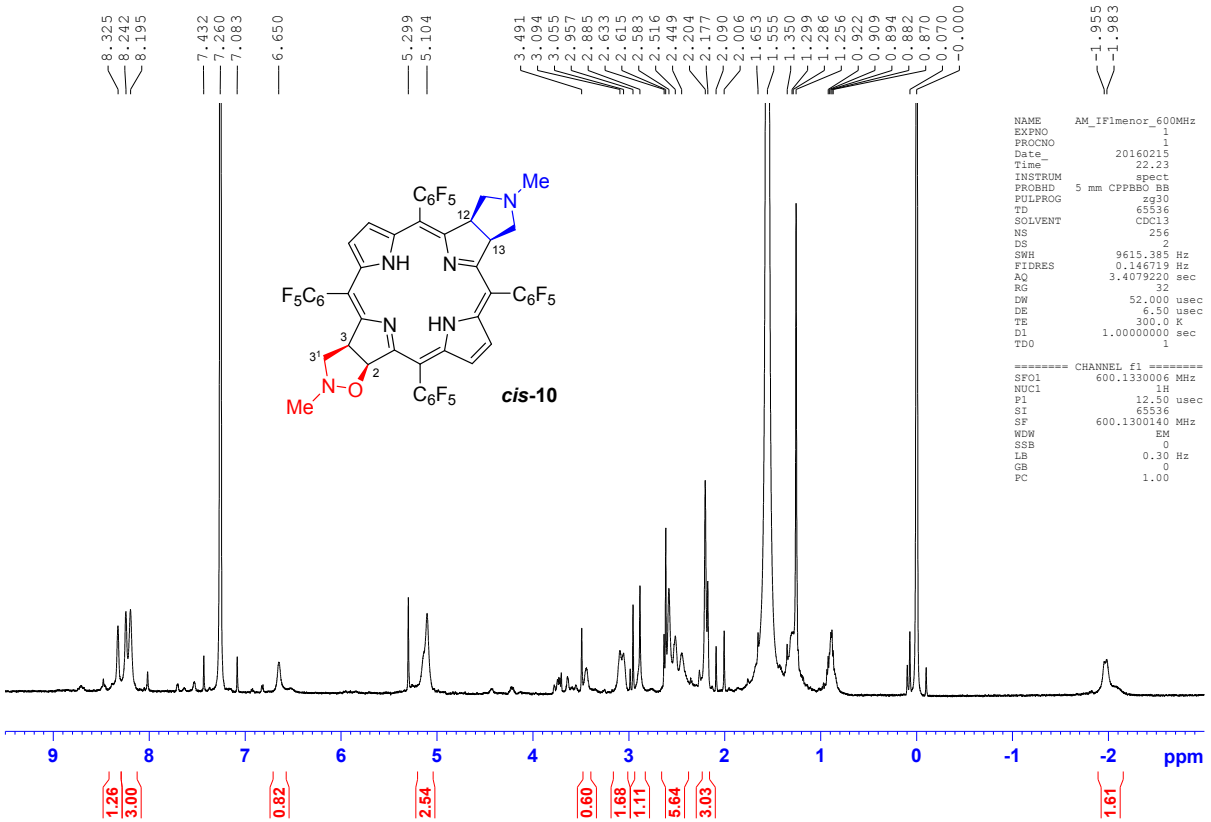


Figure S18. ^{1}H NMR spectrum (600.13 MHz, $CDCl_3$) of BC ***cis*-10**.

MS spectra

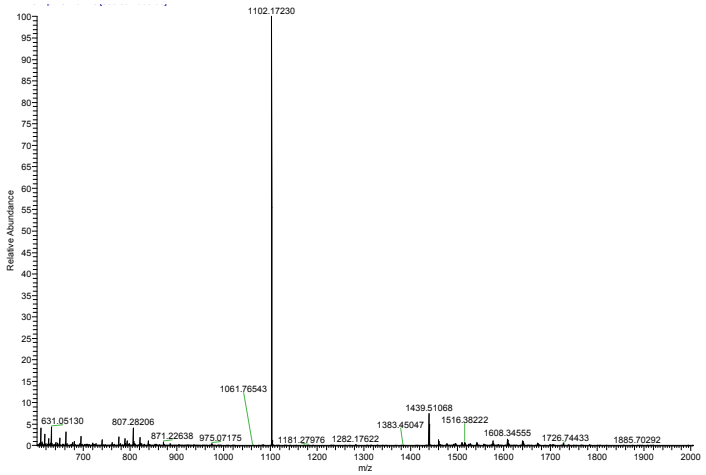


Figure S19. MS spectrum of chlorin **2b**.

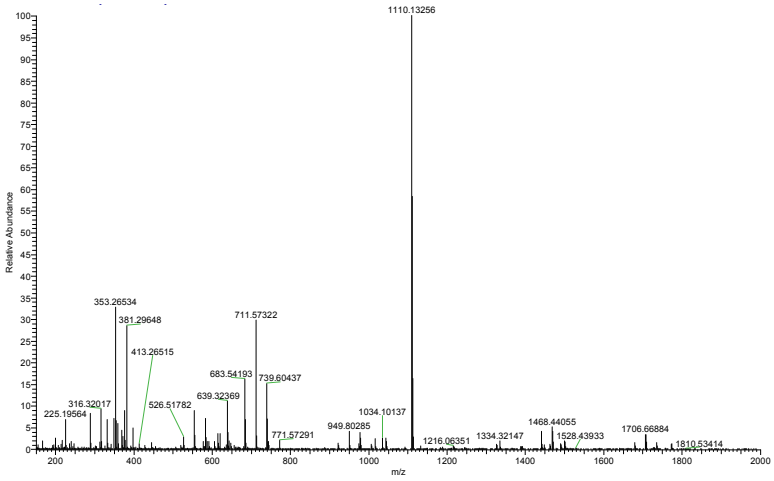


Figure S20. MS spectrum of chlorin **2c**.

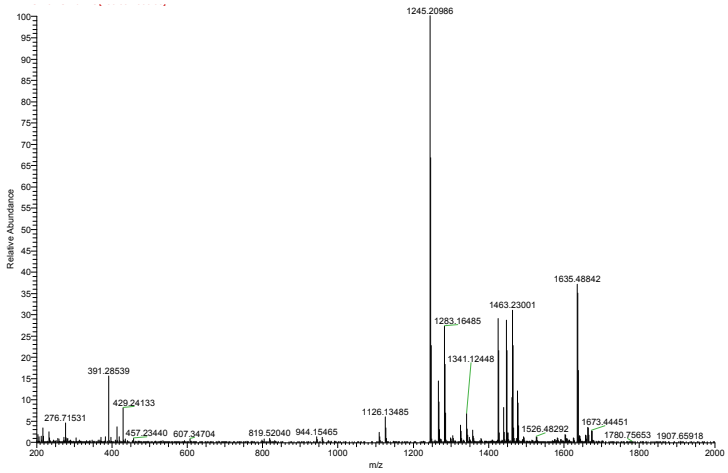


Figure S21. MS spectrum of BC *trans*-**3c**.

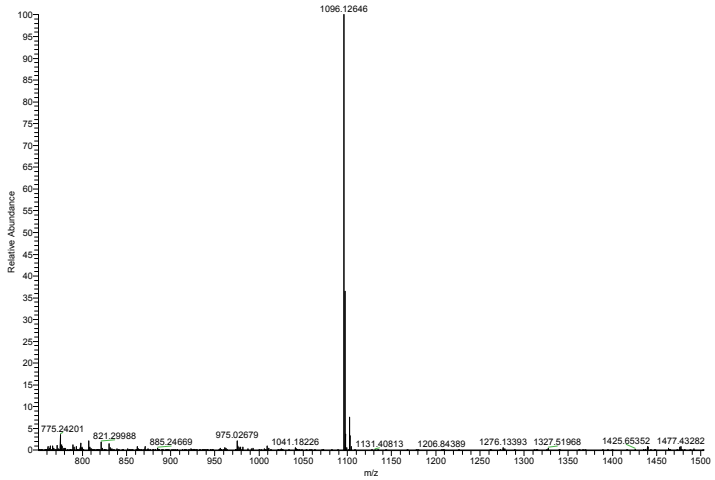


Figure S22. MS spectrum of chlorin **2d**.

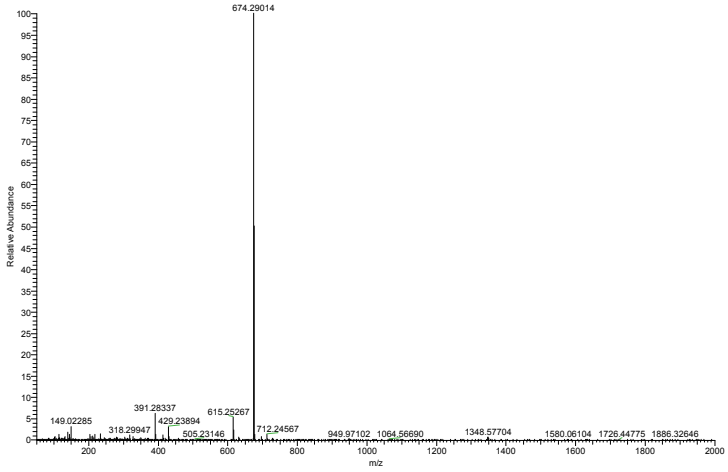


Figure S23. MS spectrum of chlorin **6a**.

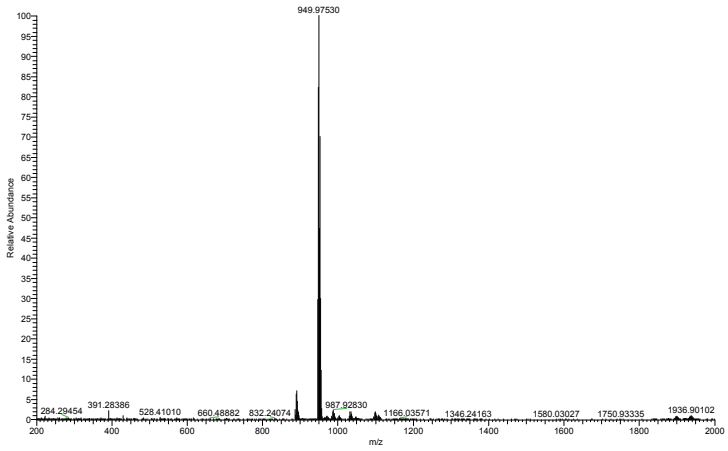


Figure S24. MS spectrum of chlorin **6b**.

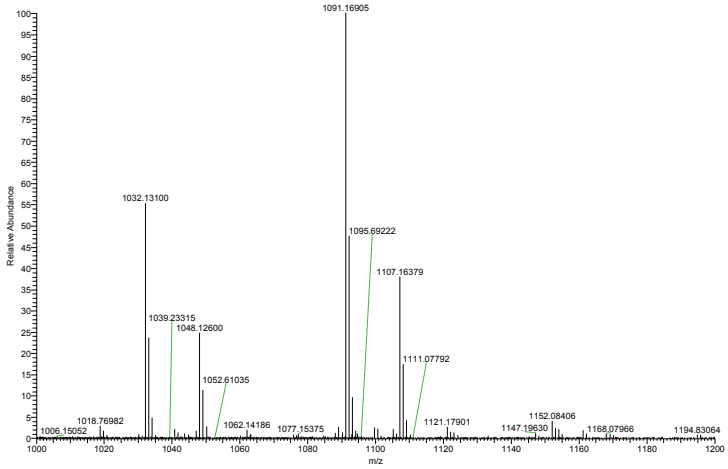


Figure S25. MS spectrum of iBC **7** and **8**.

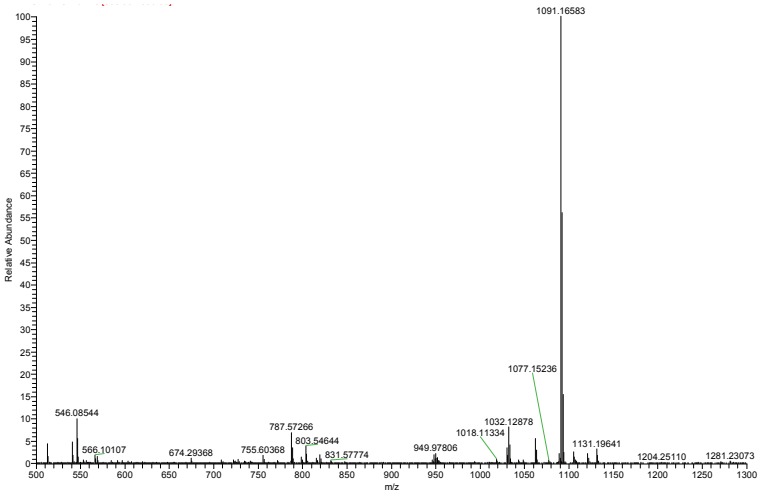


Figure S26. MS spectrum of BC *trans*-**10**.

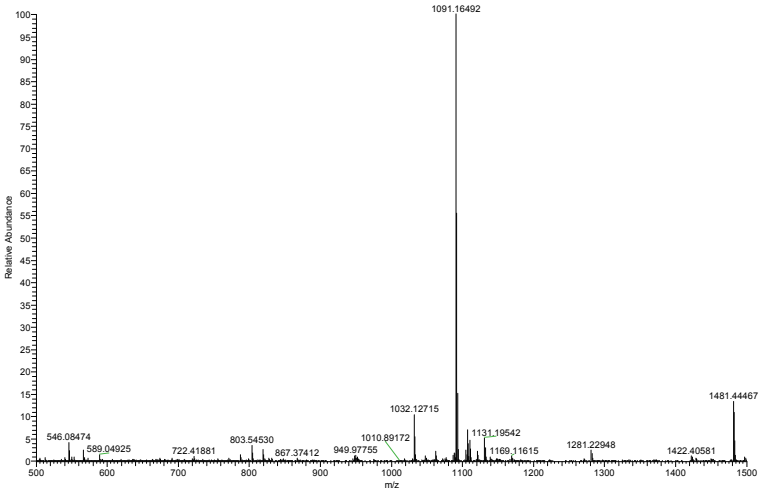


Figure S27. MS spectrum of BC *cis*-**10**.

HPLC-DAD-MS analysis

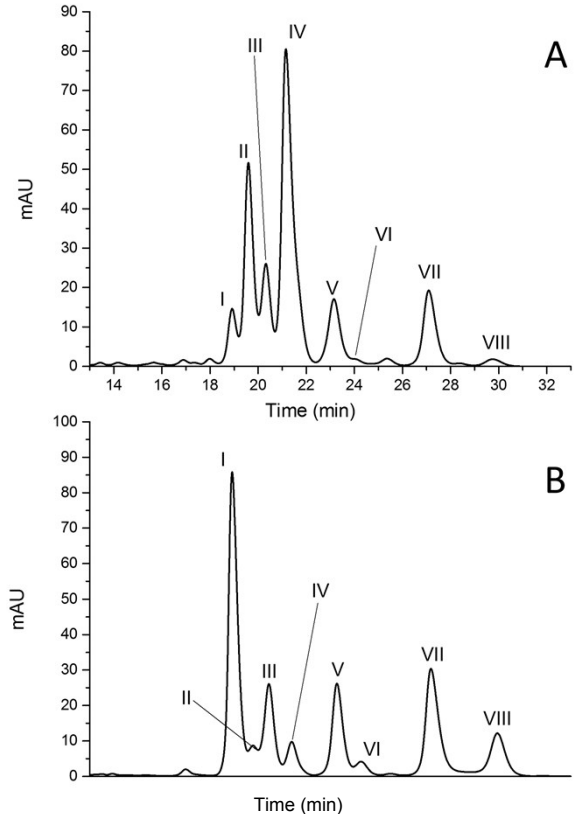
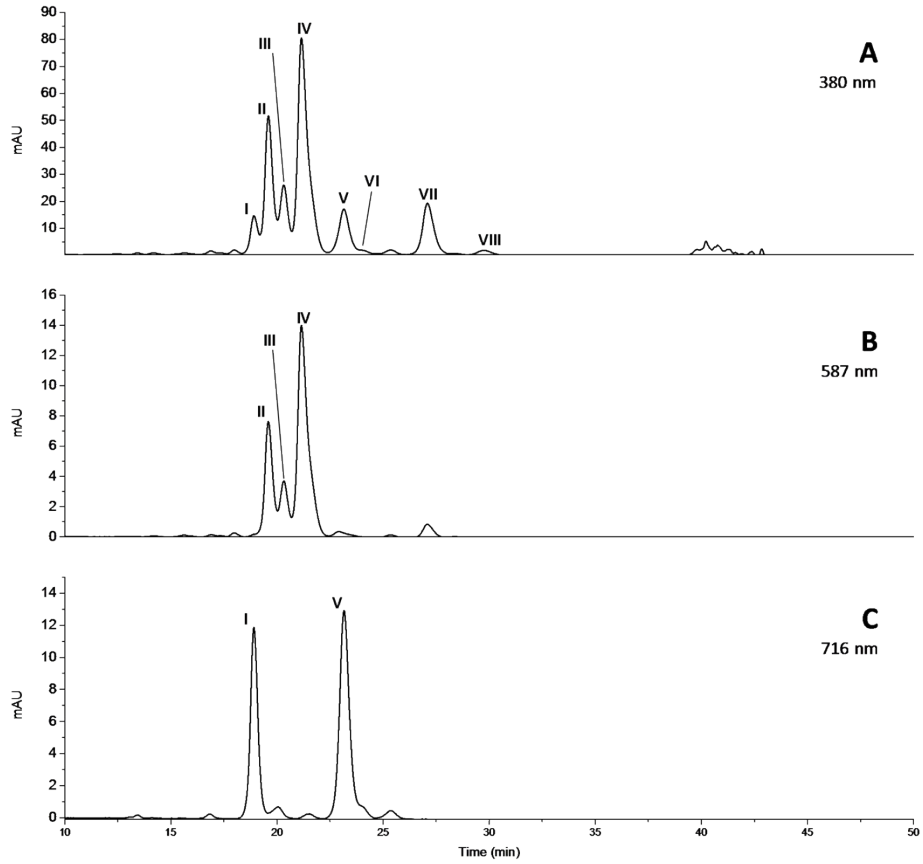
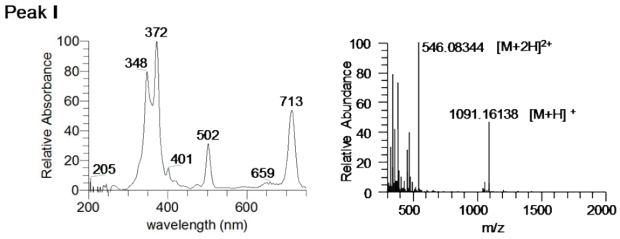
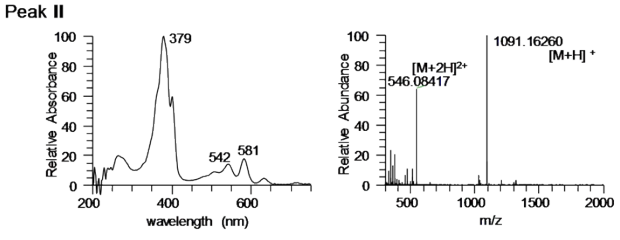


Figure S28. Chromatograms at λ = 380 nm obtained after HPLC-DAD-MS analysis of mixed bisadducts synthesized according to reaction route described in Scheme 3a (A) and Scheme 3b (B). Eight components were identified in both reactions: peaks I (retention time (RT) = 18.75 min) and V (RT = 22.97 min) correspond to BCs; peaks II, III and IV (RT = 19.44 min, 20.13 min and 21.01 min, respectively) correspond to iBCs; peak VII (RT = 26.95 min) to chlorin **9** and peaks VI (RT = 23.68 min) and VIII (RT = 30.01 min) to modified chlorins.

Figure S29 (Part 1)







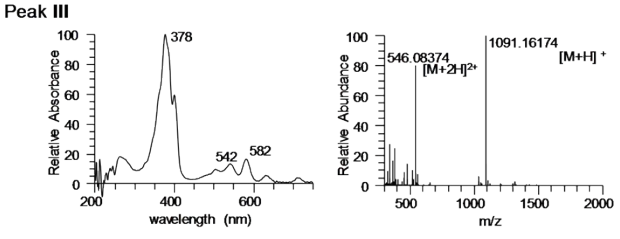
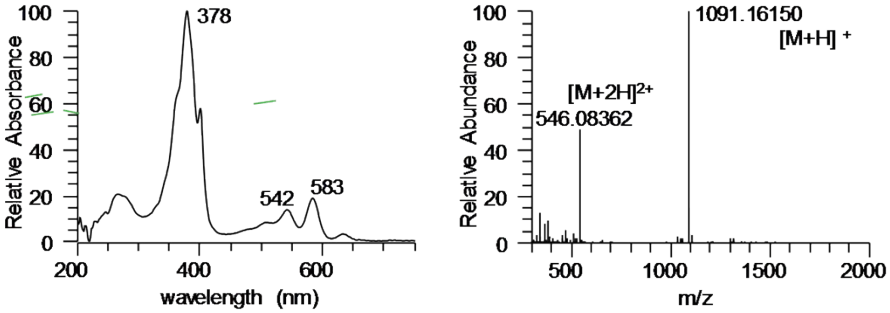
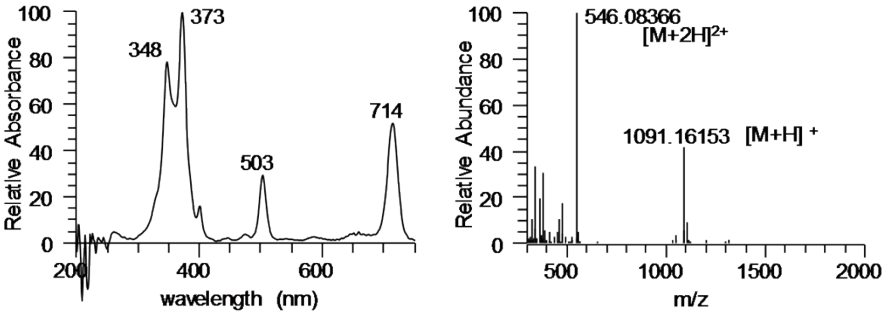


Figure S29 (Part 2)

Peak **IV**



Peak **V**



Peak **VII**

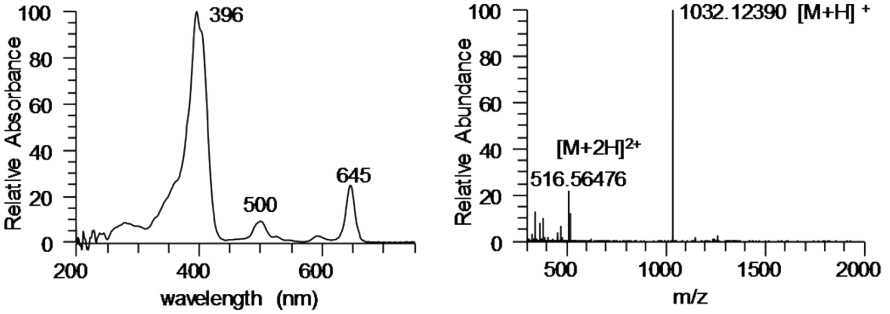


Figure S29 (Part 3)

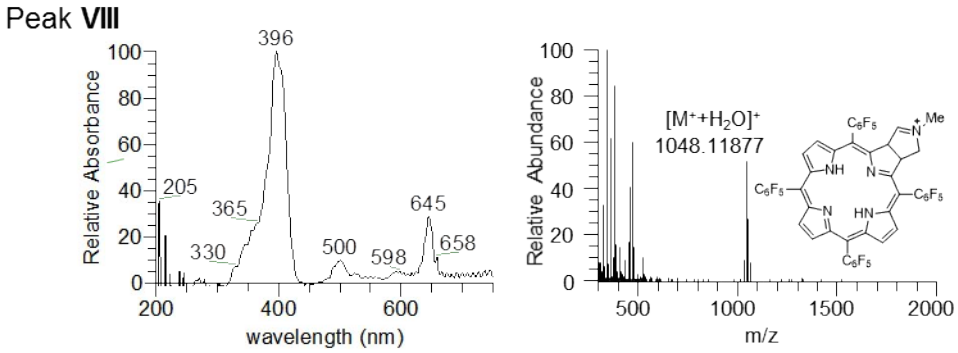
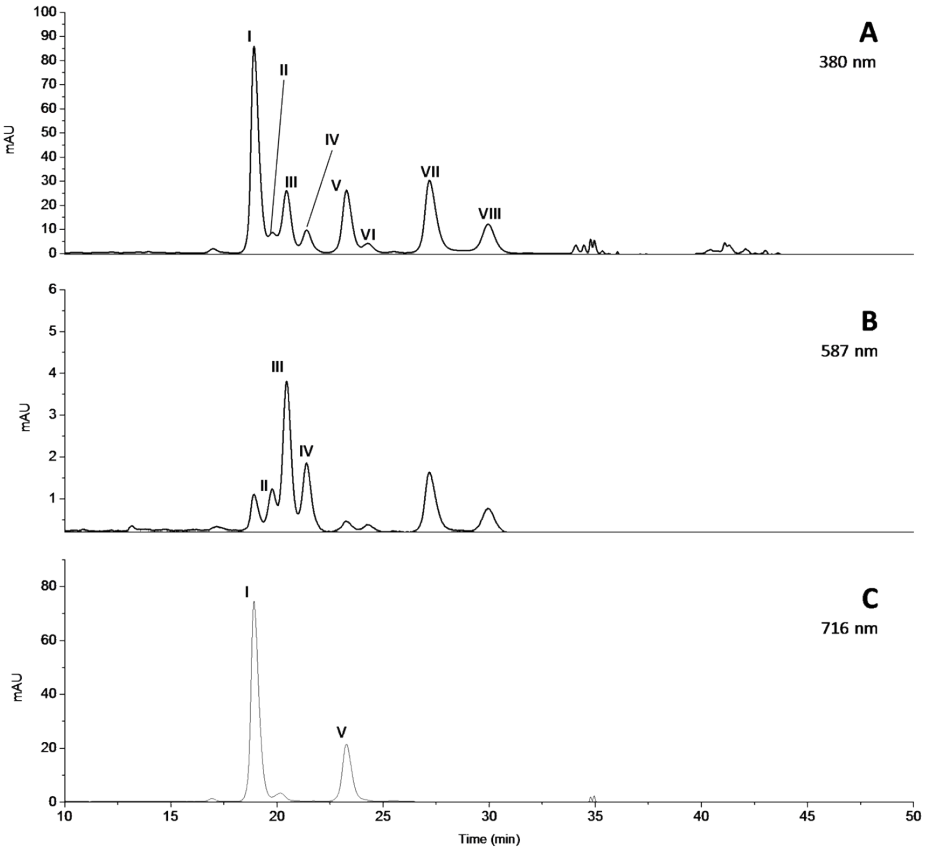
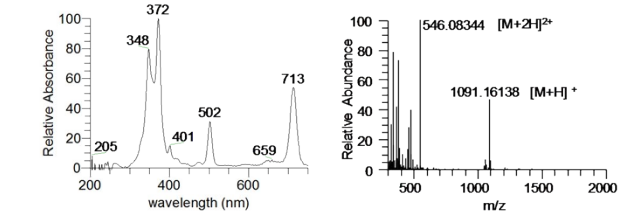


Figure S29. Results of HPLC-DAD-MS analysis of the mixture of bisadducts obtained following the synthetic route described in scheme 3a, aiming to obtain isobacteriochlorins (iBCs). **A**) Chromatogram at λ = 280 nm; **B**) chromatogram at λ = 582 nm (λ_{max} for iBCs); **C**) chromatogram at λ = 714 nm (λ_{max} for BCs). Electronic absorption (UV-visible) and mass spectra (MS) for individual peaks are given, except peak VI which provided very low intensity signals.

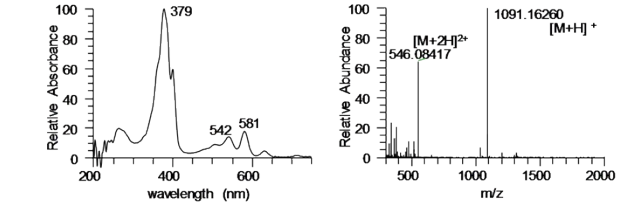
Figure S30 (Part 1)



Peak **I**



Peak **II**



Peak **III**

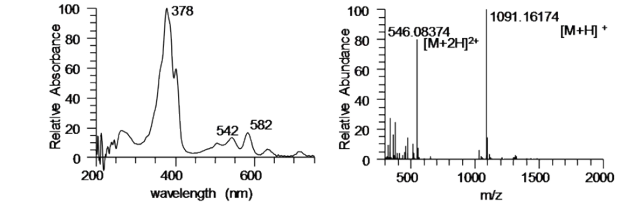
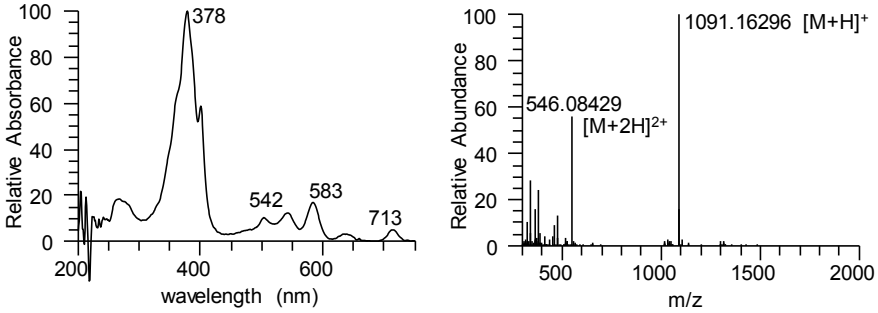
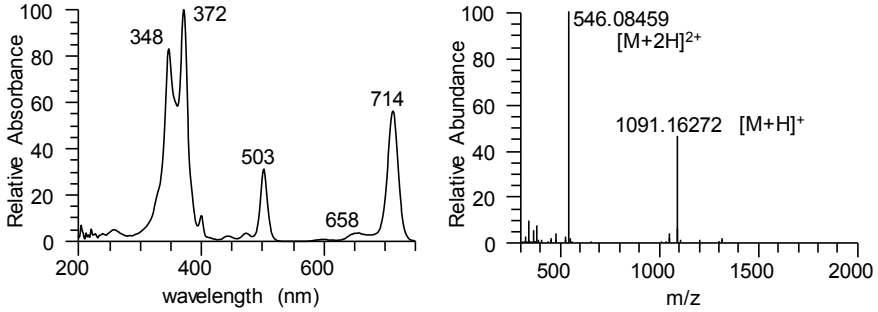


Figure S30 (Part 2)

Peak **IV**



Peak **V**



Peak **VI**

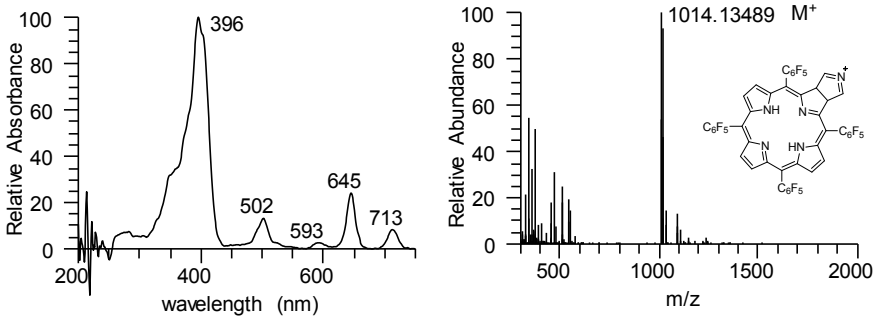


Figure S30 (Part 3):

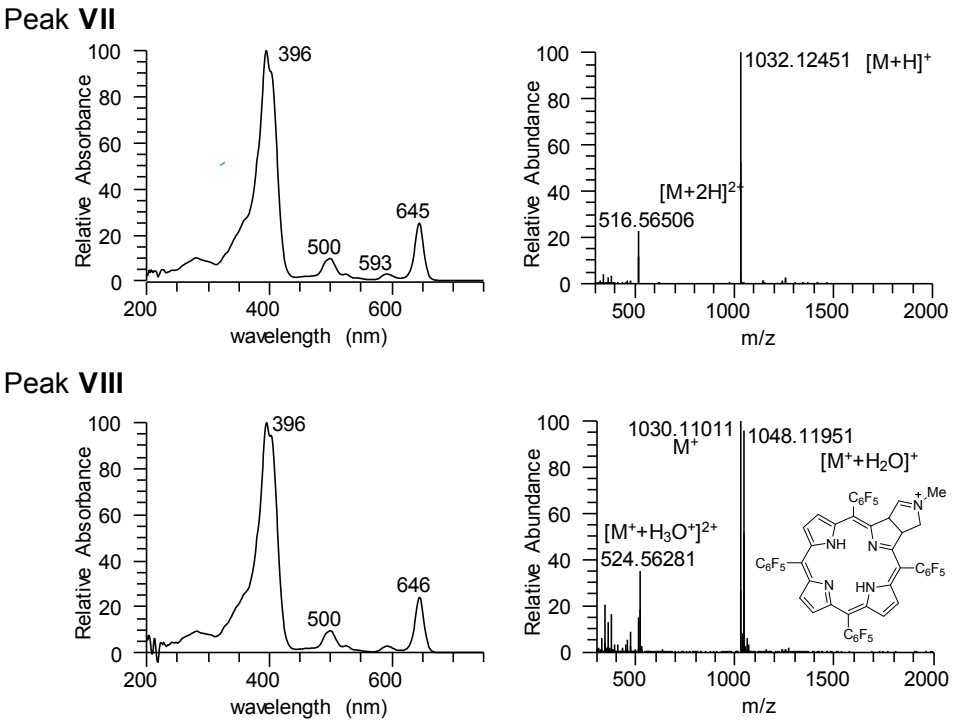


Figure S30. Results of HPLC-DAD-MS analysis of the mixture of bisadducts obtained following the synthetic route described in scheme 3b, aiming to obtain bacteriochlorins (BCs). **A**) Chromatogram at λ = 280 nm; **B**) chromatogram at λ = 714 nm (λ_{max} for BCs); **C**) chromatogram at λ = 582 nm (λ_{max} for iBCs). Electronic absorption (UV-visible) and mass spectra (MS) for individual peaks are given. The presence of a band at 713 nm in the UV-vis spectra of peaks II, III, IV and VI is due to the incomplete separation of the various iBCs from the more abundant BCs. A structure for the two modified chlorins is proposed.

Photophysical studies

Table S3. Absorption and emission spectra data for synthesized chlorins in methanol.

compound	Absorption λ_{max}[nm] (ε_{max} x 10^3 [M^{-1} cm^{-1}])					Emission	
	B(0,0)	Qy(1,0)	Qy(0,0)	Qx(1,0)	Qx(0,0)	λ_{max}[nm]	ϕ_F
chlorin 2a (ref S1)	398 (190)	499 (11)	525 (2.7)	594 (3.4)	646 (40)	650, 715	0.190
chlorin 2b	398 (140)	500 (13)	526 (3.7)	593 (3.8)	646 (32)	650, 709	0.135
chlorin 2c	398 (66)	500 (6.3)	524 (1.7)	591 (1.7)	645 (14)	648, 713	0.254
chlorin 2d	398 (380)	500 (37)	525 (1.2)	592 (11)	646 (86)	650, 705	0.054
chlorin 6a	408 (101)	513 (8.8)	540 (8.4)	589 (3.8)	642 (14.5)	644, 712	0.151
chlorin 6b	406 (90)	509 (8.6)	535 (4.8)	596 (2.8)	650 (20.8)	652, 719	0.020

Table S4. Absorption and emission spectra data for synthesized mixed BCs in methanol.

BC	Absorption λ_{max}[nm] (ε_{max} x 10^3 [M^{-1} cm^{-1}])			Emission	
	B(0,0)	Qy(1,0)	Qy(0,0)	λ_{max}[nm]	ϕ_F
***Trans*-10**	347 (130) 372 (140)	502 (52)	718 (85)	652, 722	0.145
***Cis*-10**	347 (130) 372 (150)	502 (51)	718 (84)	649, 713	0.156

Supplementary theoretical studies

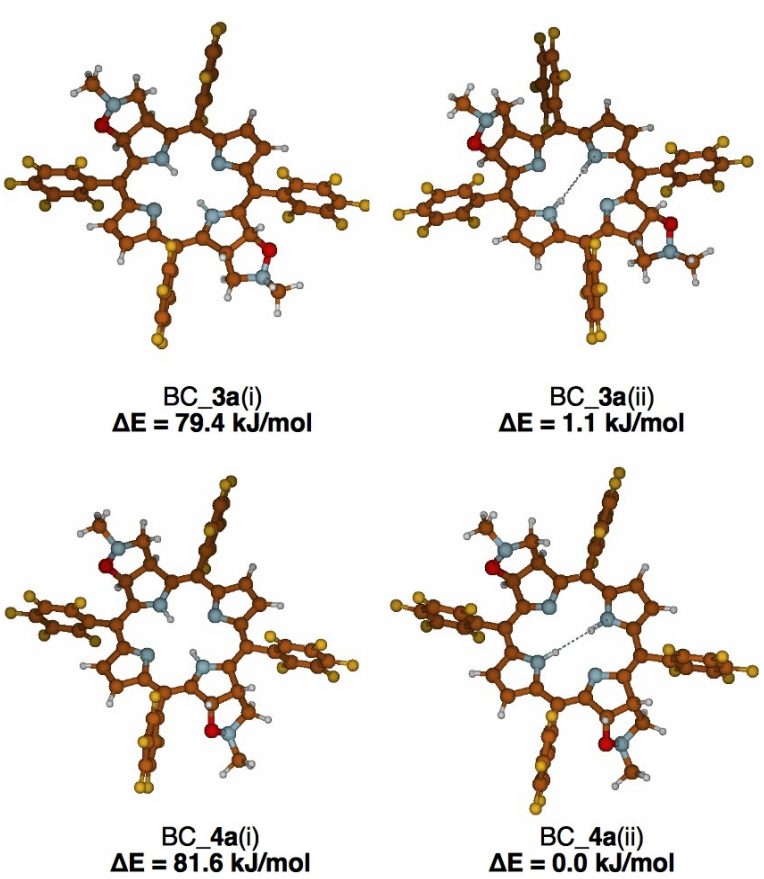


Figure S31. Optimized structures obtained by using semiempirical PM6 calculations for the *trans* isomers of BCs **3a** and **4a.** Two tautomers were considered for each isomer: (i) the inner hydrogens are connected to the β,β-saturated pyrrole rings or (ii) to the β,β-unsaturated pyrrole rings.

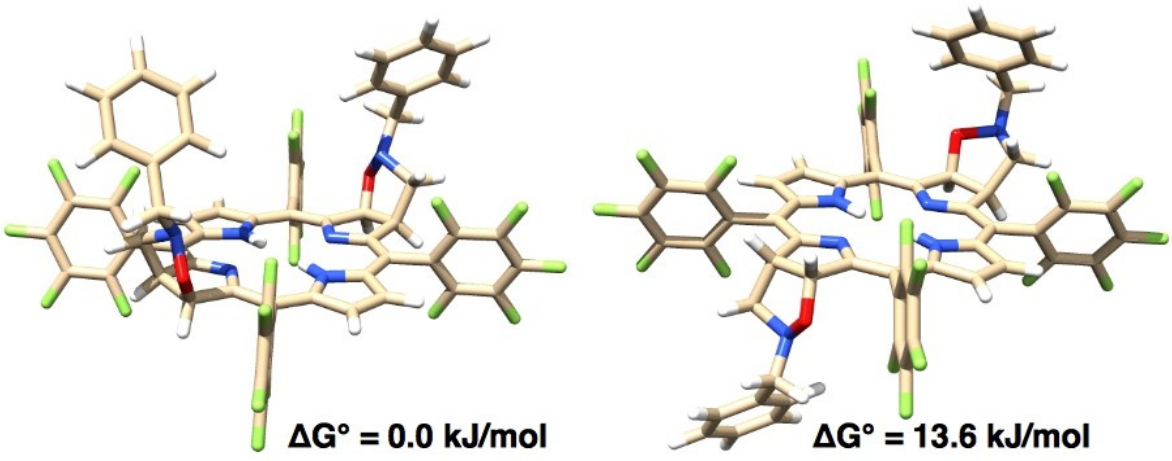


Figure S32. Optimized structures of BCs **3c** (*cis* and *trans*) obtained by DFT calculations.

Cartesian coordinates (in Å) and Sum of electronic and thermal Free Energies (in Hartree) of the compounds whose geometry was fully optimized by DFT calculations in the implicit toluene solvent

3a *cis*: -4316.086668

C	4.443294	0.450501	-0.141532
C	2.979409	0.886581	-0.232879
N	2.124710	-0.160258	-0.224273
C	2.829245	-1.312865	-0.133101
C	4.326336	-1.078398	0.015812
C	2.633248	2.238610	-0.311863
C	3.750259	3.237047	-0.360264
C	4.495474	3.448589	-1.522000
C	5.535696	4.371947	-1.581315
C	5.850078	5.120215	-0.450953
C	5.130413	4.931237	0.725998
C	4.101094	3.995593	0.759887
F	4.233448	2.724830	-2.623981
F	6.228440	4.545963	-2.714159
F	6.842134	6.014692	-0.493302
F	5.438003	5.644108	1.817161
F	3.437935	3.833156	1.912633
C	2.286799	-2.601933	-0.181345
C	3.236219	-3.762409	-0.152281
C	3.963490	-4.143248	-1.283814
C	4.827205	-5.234804	-1.280417
C	4.976158	-5.987169	-0.118390
C	4.273131	-5.633358	1.029996
C	3.417941	-4.535156	0.998232
F	3.857017	-3.429572	-2.415706
F	5.507629	-5.567856	-2.383565

F	5.800163	-7.038088	-0.102287
F	4.425283	-6.345539	2.152715
F	2.776268	-4.205108	2.130603
C	0.922752	-2.948984	-0.271700
C	0.382115	-4.265889	-0.388482
C	-0.986777	-4.164788	-0.428568
C	-1.333933	-2.782871	-0.335163
N	-0.149156	-2.086612	-0.251331
C	-2.633249	-2.238608	-0.311860
C	-2.979408	-0.886581	-0.232870
N	-2.124709	0.160259	-0.224258
C	-2.829244	1.312864	-0.133079
C	-4.326335	1.078396	0.015832
C	-4.443294	-0.450501	-0.141525
C	-2.286798	2.601934	-0.181328
C	-0.922752	2.948985	-0.271688
N	0.149156	2.086612	-0.251326
C	1.333933	2.782872	-0.335160
C	0.986777	4.164791	-0.428555
C	-0.382116	4.265890	-0.388473
C	-3.750260	-3.237045	-0.360264
C	-4.101087	-3.995601	0.759883
C	-5.130406	-4.931245	0.725993
C	-5.850079	-5.120212	-0.450955
C	-5.535704	-4.371933	-1.581312
C	-4.495482	-3.448576	-1.521996
F	-3.437919	-3.833175	1.912626
F	-4.233464	-2.724807	-2.623971
F	-6.228456	-4.545938	-2.714154
F	-6.842135	-6.014688	-0.493306
F	-5.437989	-5.644126	1.817150

C	-3.236218	3.762410	-0.152271
C	-3.963493	4.143238	-1.283806
C	-4.827208	5.234794	-1.280418
C	-4.976156	5.987172	-0.118399
C	-4.273124	5.633374	1.029989
C	-3.417934	4.535171	0.998234
F	-3.857025	3.429549	-2.415690
F	-5.507635	5.567835	-2.383566
F	-5.800160	7.038092	-0.102304
F	-4.425271	6.345568	2.152700
F	-2.776257	4.205136	2.130606
H	0.076262	1.081048	-0.188445
H	-0.076262	-1.081049	-0.188438
H	5.029259	0.774722	-1.003728
H	4.903243	-1.632795	-0.724827
H	0.967335	-5.171008	-0.442942
H	-1.695001	-4.973829	-0.520542
H	-5.029256	-0.774715	-1.003724
H	-4.903241	1.632800	-0.724804
H	-0.967336	5.171010	-0.442929
H	1.695001	4.973833	-0.520522
C	4.882834	-1.293290	1.442303
H	4.347827	-2.057813	2.009375
H	5.952653	-1.552872	1.396339
N	4.659267	0.014483	2.073771
C	5.521900	0.280302	3.214657
O	5.120301	0.930506	1.016972
H	5.352711	1.303478	3.557086
H	5.239090	-0.407386	4.016135
H	6.589394	0.146352	2.980178
C	-4.882834	1.293277	1.442324

N	-4.659272	-0.014502	2.073782
C	-5.521909	-0.280329	3.214663
O	-5.120304	-0.930515	1.016974
H	-5.352721	-1.303507	3.557086
H	-5.239101	0.407354	4.016147
H	-6.589401	-0.146377	2.980181
H	-5.952653	1.552861	1.396361
H	-4.347828	2.057793	2.009404

4a *cis*: -4316.085578

C	-4.399025	-0.751482	-0.108487
C	-2.907803	-1.082051	-0.203520
N	-2.130902	0.022561	-0.218224
C	-2.917023	1.124127	-0.147741
C	-4.393179	0.784645	0.010366
C	-2.465980	-2.407715	-0.269734
C	-3.507392	-3.485425	-0.287077
C	-4.264659	-3.758060	-1.428183
C	-5.233898	-4.756815	-1.457500
C	-5.461469	-5.521618	-0.317426
C	-4.727125	-5.274171	0.839412
C	-3.770443	-4.263725	0.843712
F	-4.086644	-3.022222	-2.539115
F	-5.940887	-4.987288	-2.571235
F	-6.384129	-6.488258	-0.331520
F	-4.950658	-6.003920	1.939708
F	-3.089575	-4.048426	1.977243
C	-2.469332	2.446870	-0.220112
C	-3.500880	3.535149	-0.228257
C	-4.248318	3.827296	-1.373045
C	-5.188237	4.853451	-1.406188

C	-5.396883	5.628924	-0.268779
C	-4.676067	5.362211	0.892012
C	-3.743917	4.328166	0.896922
F	-4.085297	3.088648	-2.481849
F	-5.885110	5.102216	-2.521238
F	-6.293847	6.618196	-0.287898
F	-4.883928	6.096249	1.991506
F	-3.084857	4.081815	2.040590
C	-1.131962	2.891868	-0.296925
C	-0.687125	4.241939	-0.421861
C	0.687137	4.241938	-0.421856
C	1.131971	2.891864	-0.296937
N	0.000004	2.110963	-0.237269
C	2.469340	2.446862	-0.220137
C	2.917029	1.124117	-0.147772
N	2.130905	0.022554	-0.218250
C	2.907804	-1.082061	-0.203537
C	4.399026	-0.751495	-0.108499
C	4.393184	0.784634	0.010340
C	2.465977	-2.407723	-0.269742
C	1.131619	-2.855002	-0.314405
N	-0.000001	-2.073622	-0.260523
C	-1.131624	-2.854997	-0.314400
C	-0.686014	-4.209158	-0.417152
C	0.686003	-4.209161	-0.417141
C	3.500891	3.535138	-0.228275
C	3.743937	4.328141	0.896912
C	4.676090	5.362183	0.892010
C	5.396900	5.628909	-0.268782
C	5.188246	4.853449	-1.406199
C	4.248324	3.827297	-1.373063

F	3.084883	4.081777	2.040581
F	4.085295	3.088664	-2.481876
F	5.885113	5.102226	-2.521250
F	6.293867	6.618178	-0.287894
F	4.883960	6.096208	1.991512
C	3.507384	-3.485438	-0.287073
C	4.264649	-3.758091	-1.428177
C	5.233882	-4.756851	-1.457483
C	5.461450	-5.521642	-0.317400
C	4.727108	-5.274179	0.839435
C	3.770431	-4.263728	0.843724
F	4.086636	-3.022266	-2.539118
F	5.940870	-4.987341	-2.571215
F	6.384105	-6.488287	-0.331484
F	4.950637	-6.003916	1.939739
F	3.089563	-4.048413	1.977253
H	0.000002	-1.064977	-0.204342
H	0.000001	1.103967	-0.157404
H	-4.965727	-1.138231	-0.957399
H	-5.009842	1.275761	-0.742852
H	-1.335066	5.100786	-0.506820
H	1.335079	5.100784	-0.506812
H	5.009849	1.275741	-0.742882
H	4.965733	-1.138253	-0.957403
H	1.335876	-5.067676	-0.489544
H	-1.335890	-5.067669	-0.489563
C	-4.963390	0.994586	1.431710
H	-4.488962	1.813251	1.976743
H	-6.050080	1.169424	1.381108
N	-4.640029	-0.274781	2.097546
C	-5.480594	-0.573132	3.246911

O	-5.030987	-1.251754	1.067068
H	-5.235154	-1.570412	3.618260
H	-5.251053	0.156385	4.028175
H	-6.554991	-0.526745	3.010353
O	5.030981	-1.251757	1.067065
N	4.640023	-0.274771	2.097531
C	5.480583	-0.573114	3.246902
C	4.963392	0.994587	1.431683
H	5.251046	0.156415	4.028157
H	5.235136	-1.570387	3.618264
H	6.554981	-0.526736	3.010345
H	6.050083	1.169419	1.381082
H	4.488966	1.813262	1.976705

7 *cis*: -4280.205600

C	-4.412849	-0.603337	-0.084394
C	-2.935548	-0.986437	-0.191872
N	-2.119254	0.089704	-0.197283
C	-2.864651	1.217766	-0.122074
C	-4.351314	0.931447	0.040972
C	-2.539354	-2.324197	-0.284440
C	-3.616631	-3.365091	-0.326560
C	-4.382483	-3.586511	-1.473092
C	-5.385624	-4.550326	-1.523906
C	-5.640178	-5.331308	-0.400585
C	-4.897996	-5.134979	0.760978
C	-3.906582	-4.158839	0.786890
F	-4.178511	-2.833551	-2.567823
F	-6.099770	-4.732075	-2.642173
F	-6.596163	-6.264570	-0.435247
F	-5.146963	-5.880707	1.845073

F	-3.218484	-3.993145	1.924362
C	-2.368398	2.522601	-0.206002
C	-3.357694	3.649116	-0.215007
C	-4.105269	3.960852	-1.354513
C	-5.006158	5.021457	-1.386252
C	-5.173653	5.812631	-0.252880
C	-4.451625	5.527452	0.902729
C	-3.559092	4.458979	0.906465
F	-3.981463	3.208517	-2.459282
F	-5.704514	5.288405	-2.496299
F	-6.033153	6.834799	-0.270739
F	-4.621083	6.276752	1.998625
F	-2.898989	4.195835	2.045657
C	-1.016319	2.914320	-0.300354
C	-0.522448	4.241182	-0.478390
C	0.850422	4.189195	-0.491755
C	1.246802	2.829117	-0.314129
N	0.086852	2.094512	-0.217891
C	2.566393	2.339428	-0.209286
C	2.965006	1.005661	-0.051962
N	2.144225	-0.068641	-0.117034
C	2.885014	-1.197333	-0.037446
C	4.366586	-0.920898	0.194375
C	4.423068	0.625860	0.182120
C	2.391891	-2.501757	-0.181340
C	1.042396	-2.894793	-0.298437
N	-0.062334	-2.077243	-0.232282
C	-1.220453	-2.815414	-0.335360
C	-0.820740	-4.177451	-0.490048
C	0.551040	-4.225678	-0.471855
C	3.636855	3.386370	-0.290332

C	3.880312	4.282195	0.755181
C	4.848547	5.278902	0.673100
C	5.607423	5.403015	-0.487351
C	5.399001	4.524035	-1.546521
C	4.421477	3.538984	-1.437574
F	3.185680	4.175558	1.899384
F	4.257661	2.701928	-2.474236
F	6.129889	4.637087	-2.662228
F	6.540040	6.354942	-0.579408
F	5.055716	6.112826	1.699434
C	3.384597	-3.624288	-0.237829
C	4.166951	-3.848981	-1.374760
C	5.071779	-4.903243	-1.460539
C	5.206038	-5.780530	-0.388028
C	4.447449	-5.585756	0.762844
C	3.553051	-4.520674	0.821850
F	4.074402	-3.015905	-2.423483
F	5.803410	-5.083726	-2.566867
F	6.068146	-6.798443	-0.458281
F	4.583833	-6.418258	1.802015
F	2.856766	-4.348984	1.956962
H	-0.027934	-1.072346	-0.136299
H	0.051310	1.091336	-0.106125
H	-5.001127	-0.965177	-0.929553
H	-4.953338	1.447653	-0.707265
H	-1.138905	5.119905	-0.590900
H	1.527890	5.019740	-0.616438
H	5.065302	1.020465	-0.607398
H	4.979370	-1.373466	-0.587377
H	1.168999	-5.104449	-0.573326
H	-1.498374	-5.009067	-0.608366

C	-4.906384	1.156033	1.465782
H	-4.400983	1.956556	2.010206
H	-5.986709	1.368311	1.422149
N	-4.622894	-0.125858	2.125804
C	-5.467134	-0.398951	3.278774
O	-5.052604	-1.086053	1.094851
H	-5.254336	-1.405310	3.645795
H	-5.208686	0.319742	4.061063
H	-6.540586	-0.315038	3.048197
C	4.870964	-1.314202	1.603842
N	4.573887	-0.136175	2.412026
C	5.174761	-0.148313	3.734187
C	4.958702	1.002559	1.584644
H	4.883116	0.752762	4.282584
H	4.817139	-1.016662	4.296139
H	6.280467	-0.189722	3.705235
H	6.058089	1.132416	1.535766
H	4.530779	1.924619	1.986690
H	5.957171	-1.528450	1.559638
H	4.373051	-2.194262	2.019230

8 *cis*: -4280.193868

C	2.106489	-3.454661	0.335251
C	0.980439	-2.407449	0.205793
N	1.466853	-1.157566	0.155655
C	2.831628	-1.193549	0.177754
C	3.385624	-2.604481	0.218163
C	-0.365658	-2.830424	0.163918
C	-0.564213	-4.321289	0.276884
C	-0.747935	-4.931467	1.520534
C	-0.909783	-6.307298	1.662084

C	-0.887313	-7.117140	0.530908
C	-0.705981	-6.544305	-0.724830
C	-0.549033	-5.166346	-0.835044
F	-0.769587	-4.180302	2.635185
F	-1.086599	-6.853113	2.873239
F	-1.041821	-8.439957	0.649697
F	-0.680452	-7.321903	-1.816257
F	-0.390431	-4.653975	-2.064534
C	3.649286	-0.071227	0.151380
C	5.133905	-0.246353	0.201661
C	5.795080	-0.572955	1.389752
C	7.178368	-0.712965	1.458391
C	7.945724	-0.511929	0.314305
C	7.322406	-0.190554	-0.888400
C	5.936695	-0.063620	-0.928752
F	5.086986	-0.787798	2.510156
F	7.773776	-1.029701	2.614502
F	9.274336	-0.638697	0.368115
F	8.054639	-0.012579	-1.994635
F	5.366042	0.218658	-2.111187
C	3.180569	1.267093	0.085249
C	3.942672	2.466111	0.012722
C	3.060277	3.519549	-0.039353
C	1.730360	3.003332	0.011397
N	1.858448	1.622467	0.079619
C	0.554737	3.770355	0.019460
C	-0.781432	3.349481	0.070183
N	-1.282233	2.053726	0.054556
C	-2.648007	2.070068	0.148828
C	-3.050693	3.433733	0.234538
C	-1.917871	4.208482	0.182461

C	-3.467223	0.913184	0.154712
C	-2.992659	-0.394484	0.103007
N	-1.670668	-0.729944	0.068327
C	-1.555137	-2.072186	0.070160
C	-2.912089	-2.765586	-0.028607
C	-3.911383	-1.599623	0.076402
C	0.756855	5.256237	-0.015059
C	0.576297	5.987243	-1.192525
C	0.757133	7.367025	-1.238379
C	1.129685	8.049410	-0.083302
C	1.318151	7.349492	1.105544
C	1.129894	5.970177	1.127084
F	0.218539	5.360992	-2.321817
F	1.317516	5.326583	2.287525
F	1.673769	8.003967	2.217236
F	1.305778	9.372745	-0.115497
F	0.577799	8.038077	-2.382001
C	-4.941281	1.149754	0.219699
C	-5.687758	0.870704	1.368898
C	-7.060815	1.089846	1.436725
C	-7.726061	1.621123	0.335211
C	-7.015712	1.914143	-0.825871
C	-5.645236	1.674325	-0.869959
F	-5.083693	0.351244	2.450357
F	-7.740586	0.805714	2.554474
F	-9.042327	1.843157	0.389960
F	-7.653680	2.414881	-1.890752
F	-4.996779	1.948144	-2.012315
H	-0.811881	1.155175	-0.035469
H	1.157163	0.887406	0.145537
H	2.022555	-4.025132	1.263100

H	4.076264	-2.744076	1.050888
H	5.020525	2.519129	0.001664
H	3.309748	4.567027	-0.111140
H	-1.869270	5.285185	0.237531
H	-4.069207	3.776034	0.335843
H	-4.509083	-1.646738	0.990162
H	-3.041470	-3.500485	0.768492
C	3.990612	-3.113523	-1.111225
H	4.431584	-2.322664	-1.721206
H	4.747714	-3.888565	-0.911329
N	2.815696	-3.655250	-1.806251
C	3.119480	-4.645944	-2.827034
O	2.165653	-4.406037	-0.721020
H	2.180815	-5.059952	-3.200729
H	3.631603	-4.136758	-3.647840
H	3.756145	-5.462066	-2.451213
C	-3.249309	-3.408880	-1.421561
H	-3.078665	-4.485451	-1.453358
N	-4.658063	-3.105396	-1.685558
H	-2.628927	-2.945714	-2.197399
C	-5.571459	-4.046795	-1.031342
C	-4.817754	-1.731726	-1.198020
H	-6.603163	-3.771771	-1.268942
H	-5.394656	-5.052288	-1.424003
H	-5.477309	-4.090167	0.068176
H	-5.868683	-1.512911	-0.998730
H	-4.469705	-1.033081	-1.968142

10 *cis*: -4280.192951

C	1.707971	-3.701956	-0.162963
C	0.707579	-2.544103	-0.079723

N	1.317360	-1.350063	0.003343
C	2.665459	-1.535131	0.093065
C	3.072198	-2.997839	0.020467
C	-0.685279	-2.805081	-0.050081
C	-1.058630	-4.266197	0.012846
C	-1.067196	-4.948350	1.235486
C	-1.404243	-6.294677	1.341310
C	-1.751662	-7.007120	0.196624
C	-1.751473	-6.366576	-1.038612
C	-1.411742	-5.017767	-1.110010
F	-0.721457	-4.301739	2.359928
F	-1.398045	-6.906480	2.531669
F	-2.078989	-8.299163	0.284049
F	-2.083856	-7.043101	-2.144798
F	-1.424031	-4.440105	-2.326790
C	3.587630	-0.504816	0.254548
C	5.025631	-0.835051	0.496908
C	5.452692	-1.399565	1.703549
C	6.790571	-1.682862	1.963849
C	7.753967	-1.385280	1.004371
C	7.367867	-0.824593	-0.210050
C	6.021887	-0.560947	-0.446576
F	4.553957	-1.707555	2.653105
F	7.155703	-2.225258	3.131976
F	9.042262	-1.645931	1.243087
F	8.288767	-0.551795	-1.142554
F	5.684479	-0.047661	-1.640355
C	3.265970	0.877261	0.224663
C	4.145564	1.989097	0.360066
C	3.400135	3.133739	0.212990
C	2.036151	2.766087	0.004952

N	2.007381	1.377485	0.021915
C	0.962655	3.660453	-0.119895
C	-0.414448	3.392897	-0.134681
N	-1.050678	2.165213	-0.015490
C	-2.408104	2.335669	0.033981
C	-2.664971	3.731039	-0.074700
C	-1.454062	4.370747	-0.190095
C	-3.338522	1.275675	0.186013
C	-2.996184	-0.069443	0.200917
N	-1.732871	-0.562621	0.051560
C	-1.775049	-1.907594	0.023766
C	-3.213470	-2.431586	0.076146
C	-4.029996	-1.170752	0.360366
C	1.342584	5.108402	-0.204353
C	1.859009	5.653881	-1.383352
C	2.223068	6.994418	-1.477368
C	2.072660	7.825910	-0.370831
C	1.560931	7.313099	0.818234
C	1.205706	5.968782	0.888868
F	2.015265	4.881049	-2.466658
F	0.718960	5.506128	2.048711
F	1.419128	8.110511	1.883468
F	2.418120	9.113227	-0.450260
F	2.712598	7.487368	-2.620883
C	-4.775815	1.660279	0.321633
C	-5.464388	1.525869	1.529564
C	-6.807846	1.864452	1.662608
C	-7.498898	2.368391	0.565080
C	-6.843671	2.518775	-0.654192
C	-5.504148	2.158980	-0.762772
F	-4.833439	1.030424	2.609074

F	-7.433632	1.717628	2.837845
F	-8.787025	2.706338	0.680965
F	-7.507722	2.997473	-1.714000
F	-4.909006	2.308926	-1.954710
H	-0.674542	1.222016	0.050651
H	1.241143	0.724997	-0.128994
H	1.510659	-4.445121	0.610856
H	3.588295	-3.303828	0.933177
H	5.205395	1.925230	0.552399
H	3.758730	4.149864	0.273253
H	-1.293286	5.432288	-0.299106
H	-3.643243	4.186190	-0.063126
H	-4.490445	-1.155597	1.353452
H	-3.338949	-3.202604	0.837412
C	3.878121	-3.371829	-1.243445
H	4.563718	-2.588936	-1.576428
H	4.475286	-4.283856	-1.044376
N	2.840735	-3.596598	-2.242841
C	3.314016	-4.193055	-3.479678
C	1.813112	-4.373522	-1.557761
H	2.480716	-4.304788	-4.180247
H	4.060829	-3.541554	-3.943863
H	3.772455	-5.189379	-3.330021
C	-3.824285	-2.884274	-1.288137
H	-3.842051	-3.965548	-1.422870
N	-5.192530	-2.367881	-1.297466
H	-3.272019	-2.433893	-2.116885
C	-6.133786	-3.171089	-0.510037
O	-5.058830	-1.078023	-0.662133
H	-7.091526	-2.648404	-0.484886
H	-6.273402	-4.127132	-1.022668

H	-5.809016	-3.366587	0.523340
H	2.110676	-5.432948	-1.426730
H	0.885516	-4.354607	-2.131590

3c *cis*: -4778.057821

O	4.996336	1.641524	0.197869
C	4.341228	1.045497	-0.917452
C	4.440005	-0.479906	-0.718864
C	5.055186	-0.577843	0.697898
N	4.683027	0.714064	1.294806
C	2.828429	1.276804	-0.952870
N	2.127472	0.121876	-0.908758
C	2.986638	-0.921107	-0.822405
C	2.297529	2.567340	-1.025260
C	3.265393	3.710124	-1.120163
C	3.756750	4.356416	0.017116
C	4.647035	5.422318	-0.068438
C	5.067571	5.869725	-1.318234
C	4.599393	5.246149	-2.470728
C	3.708662	4.181594	-2.357900
C	2.625573	-2.273066	-0.838223
C	3.723557	-3.293319	-0.791119
C	4.486954	-3.602104	-1.920764
C	5.491085	-4.565737	-1.899509
C	5.749266	-5.260290	-0.720676
C	5.013457	-4.974750	0.426145
C	4.016886	-4.003635	0.376577
F	3.377734	3.952784	1.236751
F	5.102693	6.019255	1.040703
F	5.920886	6.894319	-1.410041
F	5.003558	5.671865	-3.674746

F	3.282990	3.594779	-3.488067
F	4.276413	-2.938484	-3.068660
F	6.202493	-4.831837	-3.001363
F	6.708116	-6.189347	-0.687325
F	5.268359	-5.630785	1.564133
F	3.343925	-3.735355	1.506449
C	5.525715	1.149781	2.410602
C	0.937257	2.932988	-1.010903
C	0.411386	4.259834	-1.062391
C	-0.958305	4.180208	-1.003759
C	-1.320454	2.801295	-0.917588
N	-0.145079	2.086090	-0.928187
C	-2.625559	2.273099	-0.838199
C	-3.723543	3.293351	-0.791077
C	-4.486919	3.602180	-1.920723
C	-5.491050	4.565815	-1.899448
C	-5.749250	5.260323	-0.720594
C	-5.013460	4.974739	0.426228
C	-4.016890	4.003625	0.376641
F	-4.276361	2.938604	-3.068640
F	-6.202439	4.831957	-3.001305
F	-6.708099	6.189381	-0.687224
F	-5.268381	5.630732	1.564237
F	-3.343950	3.735300	1.506515
C	-2.986624	0.921139	-0.822438
N	-2.127454	-0.121838	-0.908823
C	-2.828409	-1.276765	-0.952992
C	-4.341208	-1.045464	-0.917581
C	-4.439991	0.479930	-0.718929
C	-5.055186	0.577802	0.697831
N	-4.683030	-0.714130	1.294687

O	-4.996324	-1.641544	0.197707
C	-2.297511	-2.567298	-1.025401
C	-0.937240	-2.932951	-1.011019
N	0.145095	-2.086055	-0.928255
C	1.320470	-2.801260	-0.917652
C	0.958322	-4.180171	-1.003867
C	-0.411368	-4.259796	-1.062526
C	-5.525728	-1.149900	2.410454
C	-3.265380	-3.710074	-1.120344
C	-3.708589	-4.181554	-2.358098
C	-4.599326	-5.246101	-2.470962
C	-5.067575	-5.869655	-1.318485
C	-4.647108	-5.422232	-0.068672
C	-3.756815	-4.356339	0.016917
F	-3.282849	-3.594757	-3.488250
F	-5.003430	-5.671827	-3.674996
F	-5.920899	-6.894239	-1.410325
F	-5.102841	-6.019143	1.040453
F	-3.377876	-3.952682	1.236568
H	0.090941	-1.078137	-0.888082
H	-0.090925	1.078171	-0.888036
H	-4.843141	-1.426613	-1.809931
H	-5.070728	0.970941	-1.460279
H	-1.657120	5.002303	-1.025679
H	1.008355	5.156104	-1.133075
H	4.843173	1.426682	-1.809780
H	5.070749	-0.970888	-1.460228
H	1.657138	-5.002266	-1.025795
H	-1.008335	-5.156064	-1.133245
H	-4.636858	1.384646	1.301101
H	-6.147713	0.699940	0.629031

H	6.147712	-0.699982	0.629104
H	4.636848	-1.384713	1.301128
H	6.595300	1.090016	2.152583
C	5.232467	0.337560	3.654320
H	5.280849	2.204613	2.575072
C	6.256627	-0.342110	4.322473
C	5.988920	-1.069572	5.484920
C	4.688644	-1.131267	5.986320
C	3.657775	-0.460807	5.321477
C	3.928127	0.269816	4.165415
H	7.270565	-0.299006	3.933210
H	6.795407	-1.589409	5.993867
H	4.477718	-1.698266	6.888271
H	2.643088	-0.505676	5.706388
H	3.128070	0.788409	3.645771
H	-5.280856	-2.204737	2.574883
H	-6.595311	-1.090131	2.152425
C	-5.232502	-0.337729	3.654210
C	-6.256677	0.341898	4.322383
C	-5.988992	1.069313	5.484865
C	-4.688721	1.131000	5.986282
C	-3.657837	0.460583	5.321419
C	-3.928168	-0.269991	4.165321
H	-7.270611	0.298800	3.933107
H	-6.795490	1.589117	5.993827
H	-4.477812	1.697962	6.888259
H	-2.643155	0.505448	5.706342
H	-3.128099	-0.788552	3.645663

3a *trans:* -4316.083058

C	4.416315	0.947957	-0.097554

C	2.920576	1.232579	-0.104686
N	2.171943	0.103995	-0.113384
C	2.986701	-0.972575	-0.171962
C	4.466239	-0.585571	-0.252564
C	2.420607	2.539116	-0.101411
C	3.409289	3.666051	-0.153843
C	4.011661	4.051885	-1.354844
C	4.909102	5.113396	-1.428958
C	5.220472	5.829600	-0.276216
C	4.645406	5.468718	0.939268
C	3.752175	4.401758	0.983717
F	3.746262	3.372634	-2.481317
F	5.467356	5.452246	-2.596856
F	6.077497	6.852089	-0.334292
F	4.953259	6.145446	2.051920
F	3.234798	4.063848	2.176465
C	2.589745	-2.312782	-0.161229
C	3.662826	-3.356652	-0.261774
C	4.070431	-3.856623	-1.500475
C	5.058372	-4.831114	-1.618251
C	5.663449	-5.332013	-0.469649
C	5.280478	-4.853548	0.780776
C	4.291426	-3.879184	0.871283
F	3.512535	-3.385740	-2.627242
F	5.424813	-5.288105	-2.822831
F	6.612048	-6.268649	-0.565853
F	5.866959	-5.332754	1.885703
F	3.950930	-3.441852	2.090332
C	1.276542	-2.811004	-0.060993
C	0.890675	-4.184506	0.013770
C	-0.477165	-4.239799	0.112104

C	-0.979820	-2.902441	0.091332
N	0.114790	-2.074365	-0.006923
C	-2.332165	-2.508327	0.146902
C	-2.831180	-1.199844	0.140854
N	-2.084223	-0.072458	0.089521
C	-2.902141	1.006971	0.106717
C	-4.370195	0.615076	0.141611
C	-4.326902	-0.913014	0.163479
C	-2.509913	2.347994	0.069721
C	-1.193259	2.847763	0.013561
N	-0.032006	2.108390	-0.016324
C	1.066871	2.934572	-0.070829
C	0.568980	4.273048	-0.080105
C	-0.801990	4.220078	-0.024576
C	-3.324610	-3.629644	0.204866
C	-4.013460	-3.945971	1.379438
C	-4.930931	-4.990597	1.445517
C	-5.171936	-5.763949	0.313039
C	-4.504742	-5.477657	-0.875090
C	-3.598682	-4.421206	-0.915493
F	-3.817226	-3.212408	2.487048
F	-2.987169	-4.162129	-2.080793
F	-4.740805	-6.213171	-1.967518
F	-6.045241	-6.772834	0.364552
F	-5.573674	-5.260343	2.587837
C	-3.593146	3.384205	0.078465
C	-3.945504	4.078923	-1.082279
C	-4.947375	5.045030	-1.089852
C	-5.636361	5.330692	0.085731
C	-5.317087	4.650542	1.257296
C	-4.303516	3.696882	1.239633

F	-3.304903	3.829764	-2.231691
F	-5.255728	5.695905	-2.218252
F	-6.602506	6.253784	0.088854
F	-5.979320	4.919459	2.389793
F	-4.033772	3.045325	2.384018
H	0.009673	1.099239	0.005801
H	0.068618	-1.066016	-0.048013
H	4.937747	1.480505	-0.893553
H	4.937434	-0.940222	-1.172378
H	1.575945	-5.018145	0.003566
H	-1.085292	-5.126849	0.200790
H	-4.800226	-1.332364	1.052918
H	-4.903613	1.054777	0.988913
H	-1.482826	5.057099	-0.007240
H	1.181859	5.160051	-0.126112
O	5.261478	-1.074236	0.821796
N	4.926126	-0.153834	1.919431
C	5.883218	-0.450337	2.973614
C	5.116782	1.149195	1.268139
H	5.689729	0.232298	3.805399
H	5.719679	-1.474738	3.314576
H	6.927865	-0.336067	2.644453
O	-5.015692	0.985049	-1.109659
N	-5.877657	-0.103038	-1.504665
C	-7.144287	0.016384	-0.774242
C	-5.099122	-1.290534	-1.139780
H	-7.814311	-0.770857	-1.130963
H	-7.049499	-0.070967	0.319137
H	-7.587597	0.984355	-1.014229
H	-4.393158	-1.510829	-1.945466
H	-5.764016	-2.146824	-1.013177

H	6.182571	1.383711	1.116417
H	4.658218	1.924711	1.884475

4a *trans:* -4316.083093

C	-4.455082	-0.659035	-0.267238
C	-2.968881	-1.021530	-0.197289
N	-2.172965	0.067657	-0.119070
C	-2.941359	1.182682	-0.085198
C	-4.431768	0.871232	-0.077358
C	-2.548448	-2.354718	-0.209166
C	-3.601287	-3.416438	-0.332372
C	-3.996712	-3.900184	-1.581393
C	-4.964826	-4.891745	-1.719954
C	-5.561512	-5.427007	-0.582537
C	-5.190319	-4.965362	0.677748
C	-4.221138	-3.973413	0.789072
F	-3.446242	-3.396723	-2.697618
F	-5.320252	-5.332374	-2.933872
F	-6.490930	-6.380470	-0.698811
F	-5.768935	-5.477573	1.771968
F	-3.891409	-3.552883	2.016998
C	-2.464545	2.497375	-0.062234
C	-3.474044	3.606947	-0.083755
C	-4.089762	4.009646	-1.272355
C	-5.006493	5.056202	-1.317196
C	-5.324310	5.739724	-0.146501
C	-4.736122	5.361208	1.057287
C	-3.823600	4.309828	1.072334
F	-3.818031	3.361961	-2.415810
F	-5.577019	5.411984	-2.474095
F	-6.199978	6.747525	-0.176326

F	-5.049737	6.006484	2.186906
F	-3.293598	3.953995	2.254279
C	-1.118039	2.918351	-0.042603
C	-0.647345	4.266022	-0.044473
C	0.725622	4.240157	-0.015378
C	1.145099	2.875970	0.000593
N	-0.001317	2.113962	-0.015417
C	2.474044	2.402754	0.029749
C	2.896590	1.069887	0.077193
N	2.084882	-0.014994	0.080531
C	2.838041	-1.136286	0.159856
C	4.326617	-0.829182	0.205457
C	4.372155	0.696301	0.110804
C	2.368296	-2.454084	0.171284
C	1.027349	-2.875895	0.084985
N	-0.082320	-2.069353	-0.025786
C	-1.226968	-2.828931	-0.104555
C	-0.813974	-4.195563	-0.039329
C	0.552411	-4.223743	0.082955
C	3.530107	3.466075	0.006559
C	4.264214	3.805505	1.146639
C	5.240714	4.797341	1.135008
C	5.496206	5.493768	-0.043274
C	4.783342	5.183946	-1.198496
C	3.818477	4.180715	-1.160917
F	4.054471	3.145122	2.297181
F	3.160359	3.899390	-2.295093
F	5.031576	5.846467	-2.334156
F	6.426313	6.451674	-0.066705
F	5.926474	5.089851	2.246261
C	3.386724	-3.549590	0.263083

C	3.721866	-4.328782	-0.848187
C	4.662576	-5.351872	-0.776643
C	5.307304	-5.610315	0.429977
C	5.004933	-4.846387	1.553351
C	4.052248	-3.836349	1.457071
F	3.123820	-4.106812	-2.025778
F	4.955379	-6.083269	-1.858940
F	6.214466	-6.588290	0.508972
F	5.624697	-5.089542	2.715367
F	3.797948	-3.105772	2.556439
H	-0.059356	-1.059792	-0.052702
H	-0.019721	1.103933	-0.005630
H	-4.922046	-1.001011	-1.193999
H	-4.966901	1.412415	-0.858278
H	-1.278375	5.141090	-0.067798
H	1.388643	5.091370	0.001311
H	4.881305	1.152924	0.960773
H	4.809702	-1.230524	1.100990
H	1.178448	-5.098265	0.171168
H	-1.481878	-5.042667	-0.071067
C	-5.129309	1.028432	1.295792
H	-4.681003	1.796895	1.928355
H	-6.199474	1.248691	1.153752
N	-4.914353	-0.286205	1.915371
C	-5.862332	-0.623127	2.965654
O	-5.238865	-1.185825	0.797421
H	-5.680386	-1.652231	3.282181
H	-5.677119	0.043326	3.812321
H	-6.909965	-0.518783	2.642775
O	4.984960	-1.335087	-0.990863
N	5.891236	-0.317894	-1.467670

C	7.142493	-0.416683	-0.708496
C	5.152251	0.923481	-1.221755
H	7.845731	0.312011	-1.121324
H	7.034775	-0.229963	0.371049
H	7.553516	-1.417015	-0.854863
H	4.451742	1.085331	-2.045986
H	5.844081	1.766693	-1.178483

7 *trans:* -4280.202641

C	4.473232	0.720425	0.154796
C	2.994437	1.067873	0.020503
N	2.197584	-0.025196	-0.024220
C	2.968910	-1.136507	-0.008105
C	4.455556	-0.826921	0.132090
C	2.556559	2.395888	-0.069788
C	3.597991	3.471155	-0.166906
C	4.316950	3.682260	-1.347444
C	5.266164	4.692908	-1.471764
C	5.511643	5.539189	-0.394042
C	4.818153	5.356919	0.799184
C	3.877659	4.335298	0.895875
F	4.117235	2.877478	-2.403145
F	5.934797	4.860974	-2.618951
F	6.416941	6.515510	-0.500514
F	5.060464	6.159541	1.842538
F	3.246313	4.173572	2.070050
C	2.499963	-2.452374	-0.125513
C	3.515733	-3.547456	-0.262506
C	4.218929	-3.739426	-1.455888
C	5.145225	-4.765705	-1.618832
C	5.382734	-5.647932	-0.568525

C	4.704871	-5.485618	0.636494
C	3.787434	-4.447590	0.772169
F	4.026720	-2.900212	-2.485854
F	5.799119	-4.914397	-2.777136
F	6.265857	-6.639657	-0.712235
F	4.940343	-6.322766	1.653954
F	3.172049	-4.306137	1.957458
C	1.155857	-2.880480	-0.140172
C	0.689679	-4.229062	-0.218830
C	-0.679904	-4.215246	-0.131940
C	-1.105162	-2.857174	-0.016989
N	0.037088	-2.087256	-0.030442
C	-2.431575	-2.395681	0.090983
C	-2.858531	-1.065304	0.147680
N	-2.070931	0.033362	0.083742
C	-2.846668	1.142615	0.113445
C	-4.332563	0.817232	0.190576
C	-4.334449	-0.711560	0.242901
C	-2.382101	2.460804	0.044281
C	-1.040461	2.888991	-0.028036
N	0.082107	2.091087	-0.020954
C	1.223172	2.857029	-0.097638
C	0.792934	4.217046	-0.170017
C	-0.578865	4.236631	-0.118039
C	-3.486235	-3.459967	0.130629
C	-4.144481	-3.795957	1.315544
C	-5.133249	-4.774240	1.365463
C	-5.480231	-5.455321	0.202488
C	-4.844051	-5.145639	-0.996586
C	-3.867090	-4.154830	-1.020795
F	-3.847464	-3.144202	2.453240

F	-3.278848	-3.881595	-2.192662
F	-5.180263	-5.796638	-2.117141
F	-6.422277	-6.402653	0.236191
F	-5.744918	-5.066043	2.520678
C	-3.404232	3.556954	0.040344
C	-3.713930	4.263631	-1.126253
C	-4.647638	5.296470	-1.143442
C	-5.307391	5.644305	0.032369
C	-5.031014	4.955503	1.210412
C	-4.085983	3.933580	1.201005
F	-3.108826	3.944450	-2.279988
F	-4.917082	5.950909	-2.279028
F	-6.207268	6.631057	0.028954
F	-5.666556	5.284025	2.341363
F	-3.855793	3.281257	2.352207
H	0.068903	1.082064	0.024303
H	0.052858	-1.079069	0.029490
H	5.052832	1.149323	-0.664791
H	5.023859	-1.244789	-0.701047
H	1.321792	-5.096977	-0.324197
H	-1.338277	-5.070125	-0.143524
H	-4.804125	-1.123748	1.140982
H	-4.792174	1.268062	1.071896
H	-1.214110	5.108773	-0.134661
H	1.448380	5.070340	-0.249119
C	5.066987	-1.238530	1.493223
H	4.625781	-2.142104	1.921239
H	6.153317	-1.417951	1.368368
N	4.793744	-0.089562	2.350019
C	5.485014	-0.116064	3.627179
C	5.091120	1.078640	1.528143

H	5.209349	0.763980	4.216469
H	5.189459	-1.006483	4.190672
H	6.586748	-0.126868	3.521425
C	-5.156273	1.107058	-1.103394
N	-5.938706	-0.105561	-1.358945
C	-7.163567	-0.193131	-0.556784
O	-5.044510	-1.160709	-0.946217
H	-7.607456	-1.177407	-0.715647
H	-7.010916	-0.040715	0.522720
H	-7.861015	0.565866	-0.922100
H	-4.483495	1.276855	-1.948798
H	-5.822594	1.966186	-1.007117
H	6.180971	1.240026	1.409560
H	4.667309	1.977919	1.982120

8 *trans:* -4280.196150

C	-1.685734	-3.703946	0.295795
C	-0.696771	-2.548475	0.123126
N	-1.311123	-1.358694	0.023626
C	-2.659916	-1.549426	-0.001010
C	-3.059380	-3.004837	0.176185
C	0.692995	-2.802947	0.048953
C	1.084451	-4.257395	-0.010875
C	1.634323	-4.933943	1.079582
C	2.030023	-6.266821	1.017666
C	1.879346	-6.967892	-0.174705
C	1.330764	-6.330495	-1.284107
C	0.952739	-4.994759	-1.191497
F	1.801509	-4.287173	2.249693
F	2.552947	-6.873343	2.091721
F	2.250960	-8.249605	-0.252000

F	1.178317	-7.003606	-2.431734
F	0.413152	-4.421565	-2.277295
C	-3.587255	-0.529155	-0.195098
C	-5.032525	-0.871722	-0.362649
C	-5.988427	-0.543930	0.605013
C	-7.341832	-0.825648	0.443203
C	-7.776139	-1.459071	-0.717981
C	-6.853470	-1.810569	-1.699144
C	-5.507151	-1.509026	-1.514114
F	-5.602578	0.040783	1.750172
F	-8.223570	-0.500579	1.396674
F	-9.071887	-1.737776	-0.885156
F	-7.266445	-2.423215	-2.815375
F	-4.647515	-1.871809	-2.479961
C	-3.262428	0.850369	-0.260175
C	-4.137488	1.950828	-0.489773
C	-3.393567	3.102743	-0.407547
C	-2.036432	2.750742	-0.134613
N	-2.007655	1.363744	-0.066425
C	-0.974024	3.651566	0.026908
C	0.396866	3.386009	0.173619
N	1.046501	2.162044	0.091560
C	2.397348	2.328725	0.239822
C	2.631663	3.715737	0.451488
C	1.415524	4.356782	0.411872
C	3.347827	1.275950	0.160297
C	3.019561	-0.069409	0.043331
N	1.743411	-0.554333	0.040410
C	1.772379	-1.897045	-0.006925
C	3.205290	-2.426683	-0.109516
C	4.059975	-1.161590	-0.112397

C	-1.354723	5.100822	0.039213
C	-1.093650	5.936032	-1.051304
C	-1.443846	7.283535	-1.048510
C	-2.074844	7.826576	0.067516
C	-2.349636	7.021216	1.169549
C	-1.989066	5.676794	1.144256
F	-0.491752	5.444932	-2.143040
F	-2.264848	4.930881	2.222662
F	-2.952907	7.543000	2.243933
F	-2.416281	9.117319	0.081088
F	-1.183271	8.055344	-2.110048
C	4.785369	1.679548	0.192350
C	5.622706	1.374556	1.270924
C	6.960701	1.756150	1.308280
C	7.496268	2.484382	0.249652
C	6.693142	2.811246	-0.839579
C	5.361305	2.406465	-0.856964
F	5.146936	0.667882	2.310149
F	7.729099	1.438631	2.357396
F	8.776894	2.863078	0.276111
F	7.206541	3.503874	-1.863334
F	4.622878	2.730459	-1.928593
H	0.684853	1.228187	-0.088774
H	-1.241729	0.725576	0.136193
H	-1.536358	-4.469203	-0.466431
H	-3.643657	-3.358007	-0.675849
H	-5.193297	1.872267	-0.698857
H	-3.749238	4.112477	-0.544559
H	1.237057	5.412159	0.550484
H	3.598068	4.164098	0.624868
H	4.789874	-1.147919	0.697516

H	3.454803	-3.115619	0.701444
C	-3.767453	-3.306088	1.516778
H	-4.390779	-4.215663	1.408590
H	-4.414583	-2.495586	1.862776
N	-2.658245	-3.503849	2.443870
C	-3.044223	-4.040794	3.736992
C	-1.693385	-4.323415	1.716606
H	-2.161841	-4.136335	4.377300
H	-3.525040	-5.035138	3.665321
H	-3.745675	-3.358871	4.227625
O	3.413387	-3.065955	-1.399955
N	4.688233	-2.628928	-1.919658
C	5.741701	-3.455985	-1.321697
C	4.743326	-1.221847	-1.512518
H	6.695137	-3.162663	-1.769972
H	5.544576	-4.498633	-1.576998
H	5.824483	-3.366351	-0.227639
H	5.777776	-0.873102	-1.504388
H	4.176588	-0.626516	-2.233878
H	-2.011310	-5.382596	1.650734
H	-0.721583	-4.295584	2.215228

10 *trans:* -4280.196235

C	1.789756	-3.658049	0.304959
C	0.769564	-2.532602	0.107431
N	1.349447	-1.325095	0.027029
C	2.704385	-1.474362	0.035925
C	3.143443	-2.916131	0.228073
C	-0.610664	-2.830666	-0.002115
C	-0.943245	-4.296333	-0.115027
C	-1.484117	-5.034691	0.940835

C	-1.802225	-6.385363	0.831113
C	-1.576968	-7.044967	-0.373863
C	-1.036697	-6.346954	-1.450715
C	-0.735538	-4.995119	-1.309446
F	-1.720227	-4.433376	2.121687
F	-2.319434	-7.049890	1.871562
F	-1.874457	-8.341450	-0.495752
F	-0.815879	-6.976524	-2.610946
F	-0.213175	-4.357133	-2.369699
C	3.605030	-0.429206	-0.145271
C	5.063686	-0.730371	-0.273454
C	5.981632	-0.376736	0.721338
C	7.346655	-0.619330	0.598035
C	7.831766	-1.237152	-0.551364
C	6.948014	-1.612890	-1.559044
C	5.588788	-1.350996	-1.411887
F	5.546259	0.194289	1.855512
F	8.191267	-0.271199	1.576567
F	9.139167	-1.478136	-0.682087
F	7.410337	-2.211147	-2.663738
F	4.767319	-1.736923	-2.401821
C	3.242576	0.939665	-0.236803
C	4.089184	2.060269	-0.473104
C	3.310170	3.191265	-0.428975
C	1.959907	2.805219	-0.169815
N	1.970550	1.419633	-0.073281
C	0.870115	3.677496	-0.033529
C	-0.491330	3.373782	0.123958
N	-1.102948	2.128975	0.076999
C	-2.455771	2.256567	0.247695
C	-2.730475	3.639823	0.434858

C	-1.536662	4.317562	0.358627
C	-3.371195	1.172937	0.210465
C	-2.999832	-0.158759	0.085502
N	-1.716008	-0.617284	0.046006
C	-1.721201	-1.959308	-0.039625
C	-3.140289	-2.520778	-0.167953
C	-4.015657	-1.275923	-0.044570
C	1.206591	5.137564	-0.054093
C	0.923849	5.938124	-1.164962
C	1.232114	7.295604	-1.193018
C	1.841577	7.884375	-0.088283
C	2.136761	7.114276	1.033513
C	1.817949	5.759153	1.039104
F	0.342096	5.402756	-2.246623
F	2.112315	5.048122	2.136076
F	2.719083	7.679645	2.097386
F	2.142799	9.185081	-0.104534
F	0.951787	8.033595	-2.273311
C	-4.821694	1.520299	0.287492
C	-5.606064	1.192177	1.397170
C	-6.959655	1.506606	1.472575
C	-7.565041	2.185376	0.419256
C	-6.814416	2.532637	-0.700562
C	-5.465641	2.194253	-0.756196
F	-5.061112	0.526711	2.430849
F	-7.677142	1.169971	2.552262
F	-8.862113	2.501022	0.482000
F	-7.394973	3.181180	-1.717829
F	-4.778242	2.540777	-1.853045
H	-0.715425	1.205624	-0.102780
H	1.218746	0.763501	0.123547

H	1.689657	-4.426234	-0.462377
H	3.765951	-3.251442	-0.603802
H	5.150562	2.008673	-0.661599
H	3.638627	4.208073	-0.580600
H	-1.389033	5.380672	0.472195
H	-3.708037	4.059867	0.616013
H	-4.718259	-1.311621	0.792176
H	-3.355955	-3.253089	0.609940
C	3.817586	-3.193965	1.591118
H	4.474765	-4.081668	1.503683
H	4.424978	-2.361838	1.957333
N	2.686483	-3.430231	2.482230
C	3.048988	-3.954832	3.787216
C	1.774462	-4.281395	1.724058
H	2.150763	-4.078726	4.400044
H	3.563723	-4.933029	3.731300
H	3.712499	-3.250664	4.298666
C	-3.517394	-3.052301	-1.585700
H	-3.586692	-4.140284	-1.633543
N	-4.818078	-2.456440	-1.905403
H	-2.783061	-2.714551	-2.322559
C	-5.952214	-3.169931	-1.308396
O	-4.733655	-1.146503	-1.304046
H	-6.857765	-2.589684	-1.493910
H	-6.047942	-4.134663	-1.814528
H	-5.858457	-3.347574	-0.225982
H	0.786933	-4.289625	2.191735
H	2.132100	-5.328466	1.666450

3c *trans:* -4778.052625

C	5.422689	0.802139	0.158426

C	4.314958	0.456987	1.181568
C	4.202594	-1.070507	1.059097
O	5.031543	-1.441797	-0.045335
N	6.139884	-0.477121	0.028522
C	2.905947	0.916497	0.824882
N	2.071521	-0.115227	0.560933
C	2.742042	-1.284195	0.695888
C	2.557897	2.272854	0.782776
C	3.623123	3.272568	1.115148
C	4.066620	3.469156	2.426221
C	5.053102	4.397312	2.746896
C	5.618480	5.172489	1.737965
C	5.201456	5.004352	0.420208
C	4.218551	4.063088	0.126378
C	2.226972	-2.568060	0.502756
C	3.165200	-3.721001	0.703722
C	3.781260	-4.360158	-0.374828
C	4.653984	-5.429964	-0.201922
C	4.932587	-5.887017	1.083378
C	4.341679	-5.268464	2.181313
C	3.469284	-4.202532	1.979018
F	3.553542	2.729835	3.423096
F	5.453018	4.555150	4.014054
F	6.562038	6.070372	2.032562
F	5.749250	5.742060	-0.552771
F	3.851938	3.916935	-1.155342
F	3.542241	-3.941743	-1.627855
F	5.225405	-6.020102	-1.259044
F	5.768248	-6.914030	1.262388
F	4.610790	-5.702377	3.418900
F	2.929940	-3.616497	3.060014

C	6.931868	-0.658683	-1.200749
C	1.301407	2.816721	0.448513
C	0.948124	4.201069	0.420092
C	-0.362119	4.300172	0.024553
C	-0.862771	2.979886	-0.194828
N	0.175868	2.117826	0.076212
C	-2.166504	2.635159	-0.599888
C	-3.076121	3.796001	-0.877016
C	-3.165619	4.354200	-2.154078
C	-3.994014	5.438199	-2.433404
C	-4.759728	5.993409	-1.412748
C	-4.695826	5.458300	-0.128686
C	-3.860693	4.374439	0.123842
F	-2.447737	3.834090	-3.162467
F	-4.054853	5.948458	-3.670286
F	-5.557252	7.035763	-1.664868
F	-5.438199	5.988283	0.852223
F	-3.827768	3.885381	1.370585
C	-2.690954	1.349893	-0.764449
N	-2.028756	0.185229	-0.589398
C	-2.876962	-0.849352	-0.801398
C	-4.298540	-0.393729	-1.100453
C	-4.150174	1.138495	-1.177709
O	-5.102022	1.682793	-0.269114
N	-5.118334	0.693929	0.818787
C	-5.298537	-0.558762	0.069141
C	-2.532082	-2.204368	-0.757713
C	-1.266766	-2.750508	-0.455325
N	-0.131705	-2.052517	-0.112576
C	0.913462	-2.915693	0.128814
C	0.407069	-4.234224	-0.076481

C	-0.915045	-4.134190	-0.434948
C	-6.250110	1.081213	1.664127
C	-3.599698	-3.208969	-1.073162
C	-4.009279	-3.454213	-2.387077
C	-4.980056	-4.401563	-2.699257
C	-5.565414	-5.145167	-1.677977
C	-5.186966	-4.923908	-0.356600
C	-4.216109	-3.967013	-0.073331
F	-3.478895	-2.742310	-3.394287
F	-5.347854	-4.606296	-3.969585
F	-6.495735	-6.059488	-1.964345
F	-5.757434	-5.626933	0.628606
F	-3.893372	-3.760295	1.213108
H	-0.080742	-1.046015	-0.041744
H	0.128844	1.111478	0.000881
H	-4.684594	-0.835747	-2.019267
H	-4.372621	1.574375	-2.154526
H	-0.937393	5.205012	-0.097286
H	1.609895	5.013263	0.678881
H	4.588481	0.765101	2.192641
H	4.511936	-1.598984	1.967536
H	0.982071	-5.140357	0.036863
H	-1.585838	-4.946332	-0.669581
H	4.984074	1.141078	-0.789654
H	6.121025	1.559274	0.522694
H	-6.323574	-0.661904	-0.320527
H	-5.071849	-1.401994	0.722763
H	-7.198850	1.046683	1.104921
H	-6.067240	2.122946	1.948445
C	-6.325711	0.202081	2.894426
C	-5.234960	0.117738	3.772000

C	-5.306282	-0.675451	4.916087
C	-6.471177	-1.393795	5.201402
C	-7.560674	-1.316549	4.333700
C	-7.484930	-0.525509	3.184433
H	-4.329770	0.673822	3.547055
H	-4.454485	-0.731895	5.587651
H	-6.527160	-2.009523	6.094275
H	-8.468689	-1.873084	4.546866
H	-8.334891	-0.469671	2.509148
C	6.274403	-0.328831	-2.529985
H	7.264989	-1.701002	-1.184608
H	7.820615	-0.033540	-1.062286
C	6.622929	0.841810	-3.217128
C	6.034191	1.158250	-4.443308
C	5.082532	0.302858	-4.999564
C	4.726685	-0.867353	-4.324078
C	5.318188	-1.183232	-3.100836
H	7.368346	1.509330	-2.790772
H	6.320523	2.068655	-4.961958
H	4.623110	0.543662	-5.953823
H	3.988401	-1.538696	-4.753385
H	5.031286	-2.091329	-2.582200

References:

S1. A. Aguiar, A. Leite, A. M. N. Silva, A. C. Tomé, L. Cunha-Silva, B. Castro, M. Rangel and A. M. G. Silva, *Org. Biomol. Chem*., **2015**, *13*, 7131–7135.