

Supporting Information

Anion Binding, Electrochemistry and Solvatochromism of β -Pyrrole Brominated Oxoporphyrinogens

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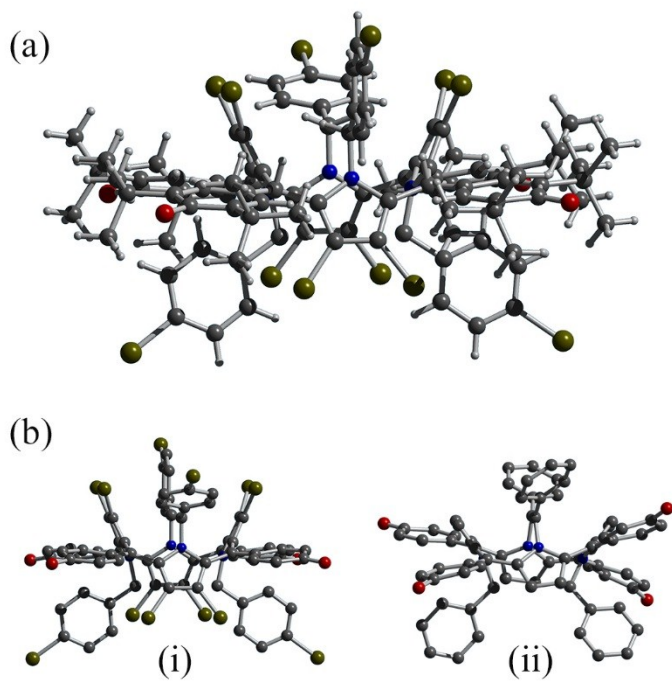


Figure S1. (a) X-ray crystal structure of β -Br₈OxPBz₄. (b) Comparison of the crystal structures of β -Br₈OxPBz₄ and its non-brominated analogue revealing higher symmetry of the former.

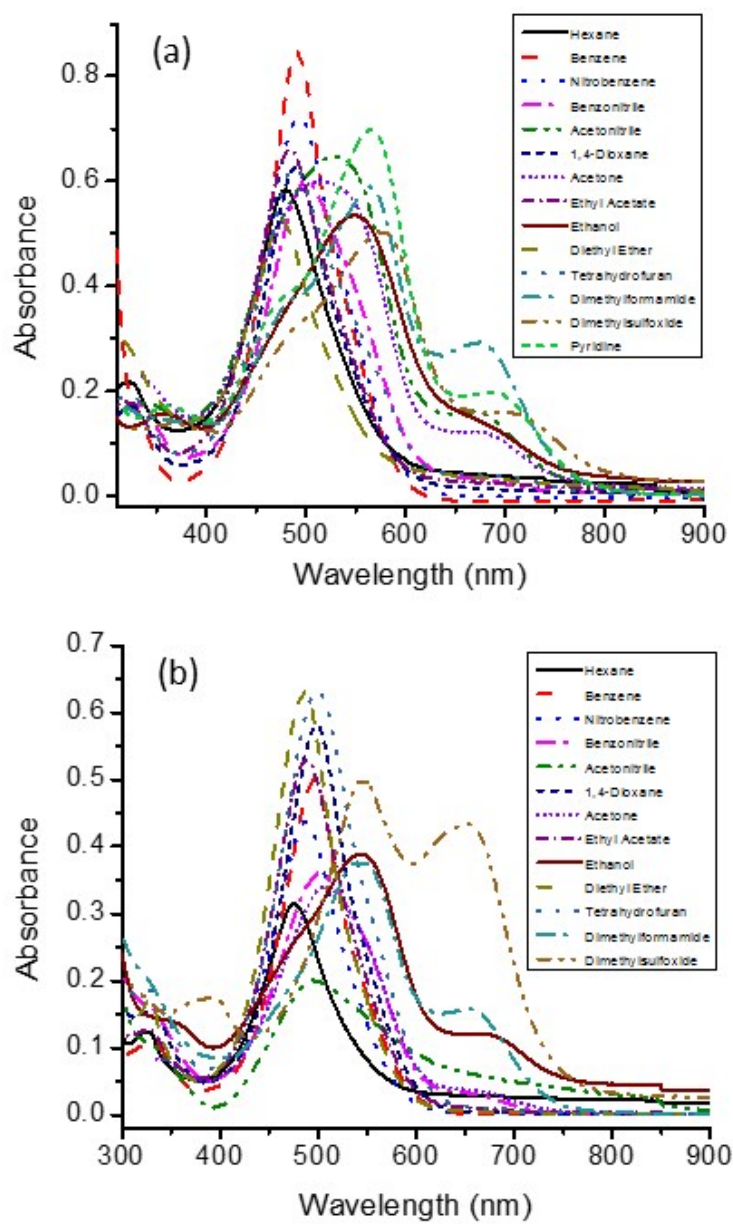


Figure S2. Absorption spectra of (a) β -Br₈OxP and (b) β -Br₈OxPBz₂ in different solvents.

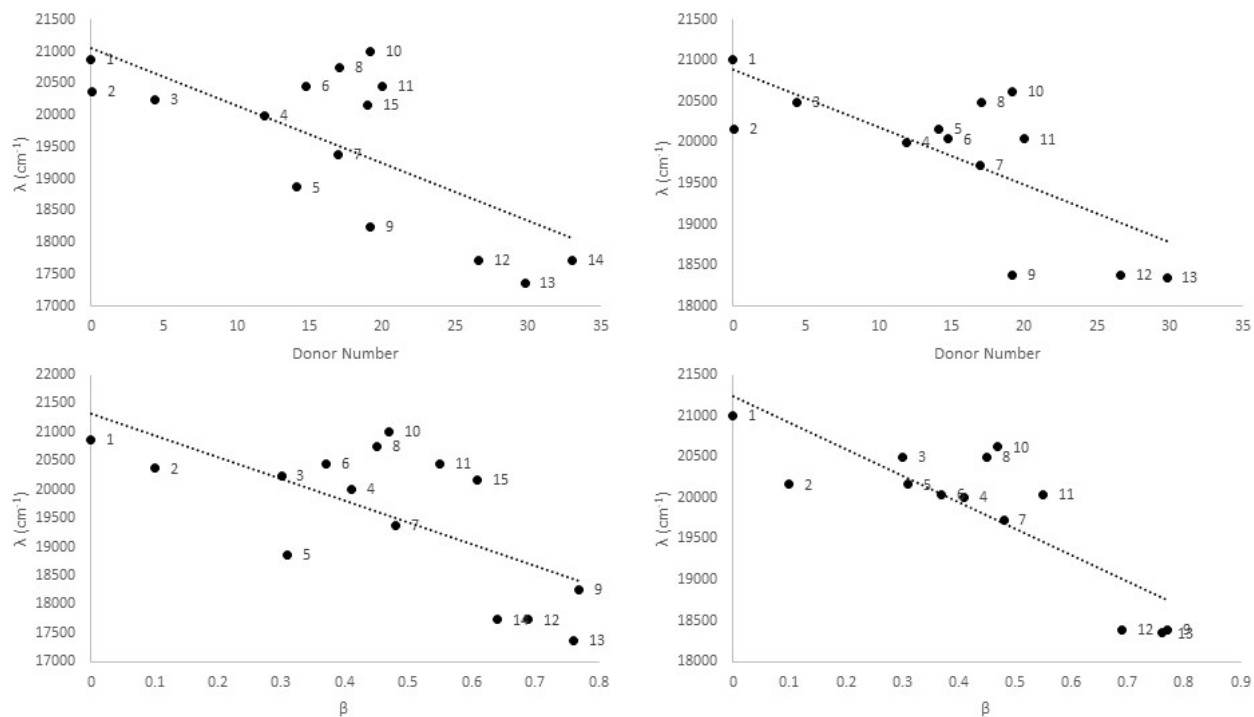


Figure S3. Plots of absorption peak maxima vs. donor number versus (a and b), and absorption peak maxima vs. β versus (c and d) for $\beta\text{-Br}_8\text{OxP}$ (plots a and c) and $\beta\text{-Br}_8\text{OxPBz}_2$ (plots b and d); Solvents: 1(hexane); 2(benzene); 3(nitrobenzene); 4(benzonitrile); 5(acetonitrile); 6(1,4-Dioxane); 7(acetone); 8(ethyl acetate); 9(ethanol); 10(diethyl ether); 11(tetrahydrofuran); 12(dimethylformamide); 13(dimethylsulfoxide); 14(pyridine).

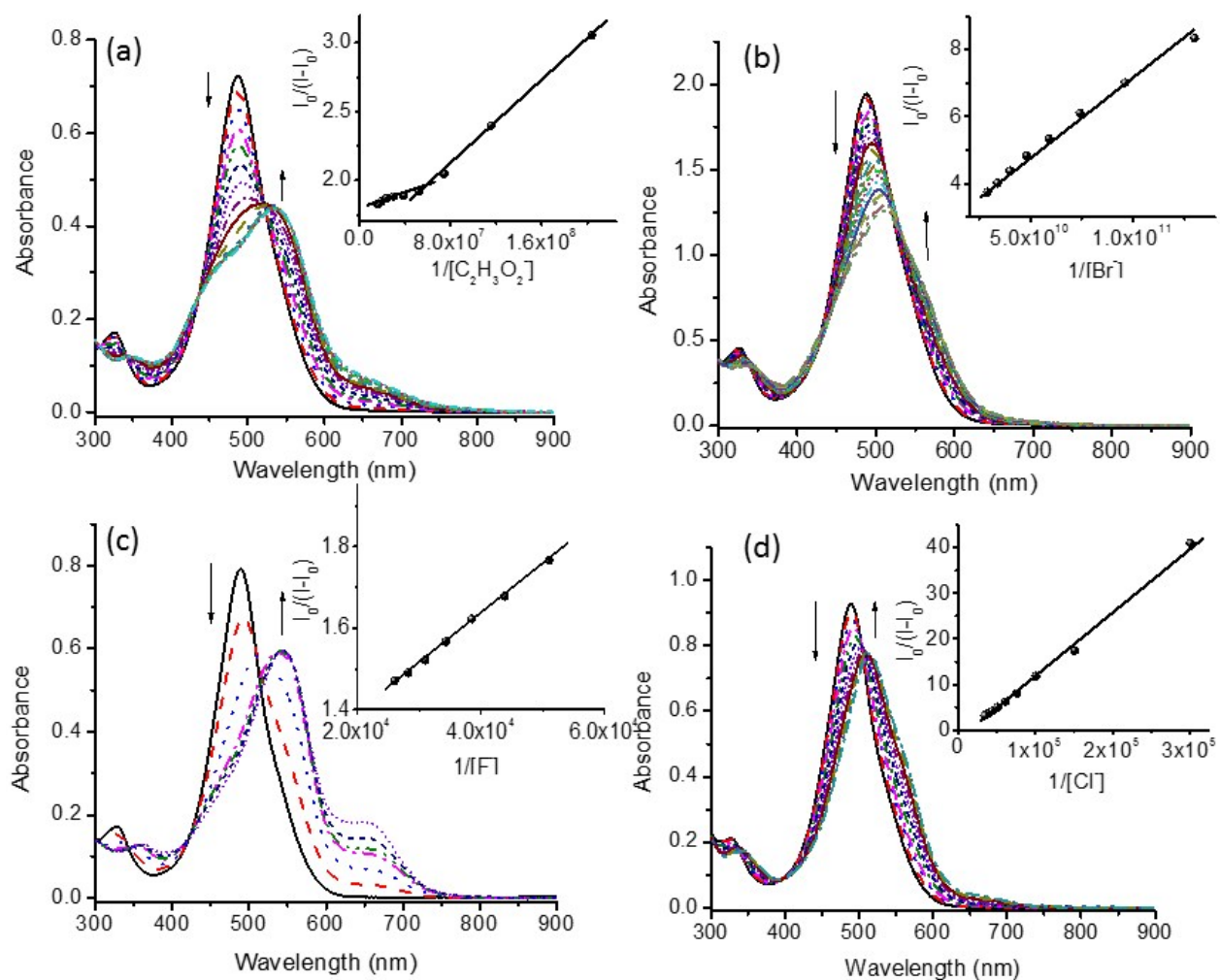


Figure S4. Spectral changes observed for (a) β -Br₈OxP during increased addition of acetate, (b) β -Br₈OxP during increased addition of bromide, (c) β -Br₈OxPBz₂ during increased addition of fluoride and (d) β -Br₈OxPBz₂ during increased addition of chloride in benzonitrile. Figure inset shows Benesi-Hildebrand plots constructed to obtain binding constants.

Table S1. Donor Numbers and β Values and Optical Absorption Spectral Data for β -Br₈OxP and β -Br₈OxPBz₂ in different solvents.

Solvent	Donor Number	β	β -Br ₈ OxP	β -Br ₈ OxPBz ₂
Hexane	0.0	0.00	323, 480	326, 475
Benzene	0.1	0.10	330, 492	333, 496
Nitrobenzene	4.4	0.30	493	488
Benzonitrile	11.9	0.41	333, 500	330(sh), 501, 661
Acetonitrile	14.1	0.31	338, 530, 674(sh)	331, 494
1,4-Dioxane	14.8	0.37	326, 489	333, 499, 665
Acetone	17.0	0.48	514, 679(sh)	342(sh), 509, 665(sh)
Ethyl Acetate	17.1	0.45	323, 484	329(sh), 487
Ethanol	19.2	0.77	359, 551, 667(sh)	356(sh), 542, 676(sh)
Diethyl Ether	19.2	0.47	321(sh), 476	329, 486
Tetrahydrofuran	20.0	0.55	325, 489, 696(sh)	328, 501
Dimethylformamide	26.6	0.69	486(sh), 564, 673(sh)	543, 660(sh)
Dimethylsulfoxide	29.8	0.76	365, 494(sh), 575, 711(sh)	393, 544, 654
Pyridine	33.1	0.64	360, 475(sh), 566, 693(sh)	

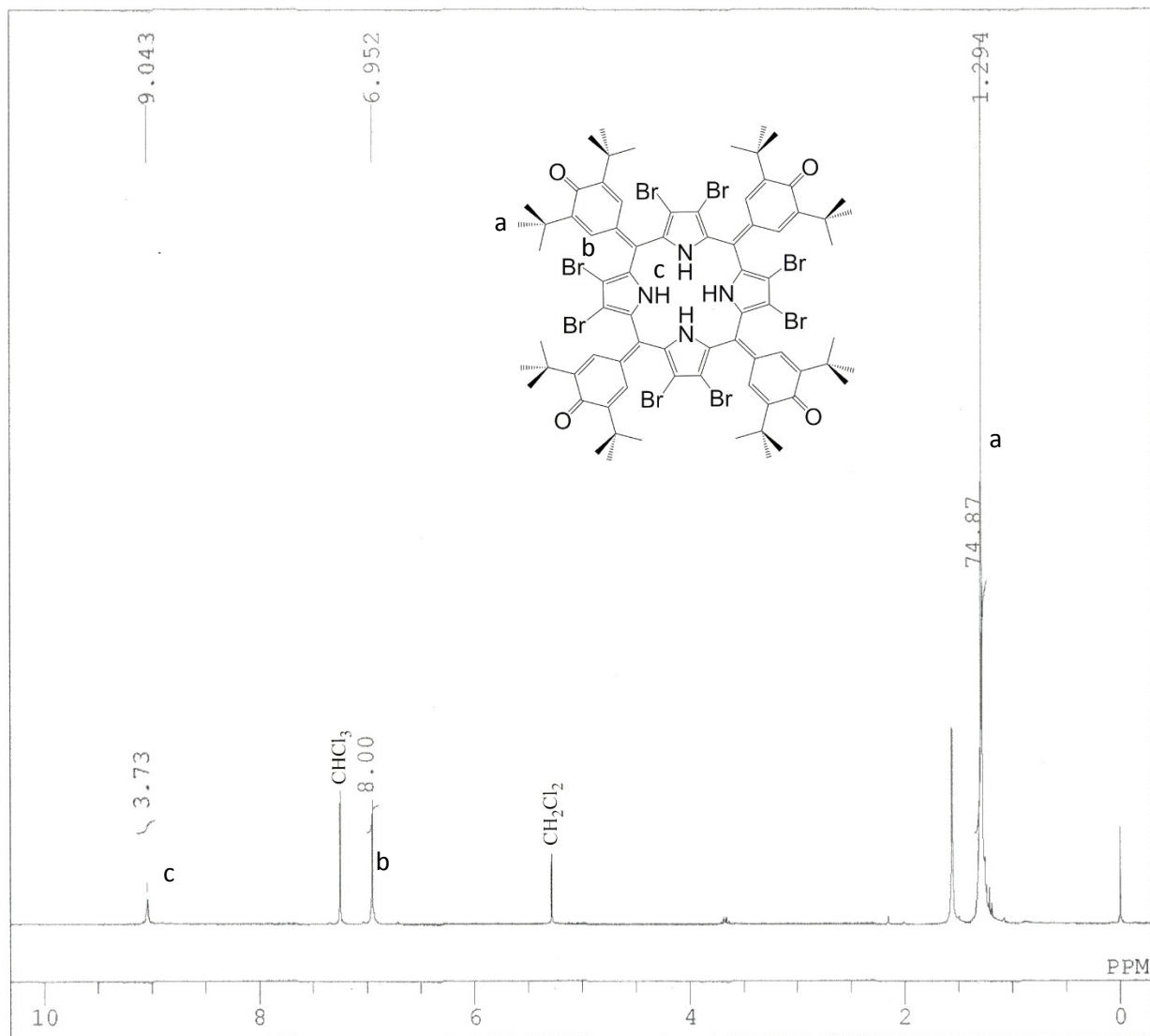


Figure S5. ^1H NMR spectrum of $\beta\text{-Br}_8\text{OxP}$.

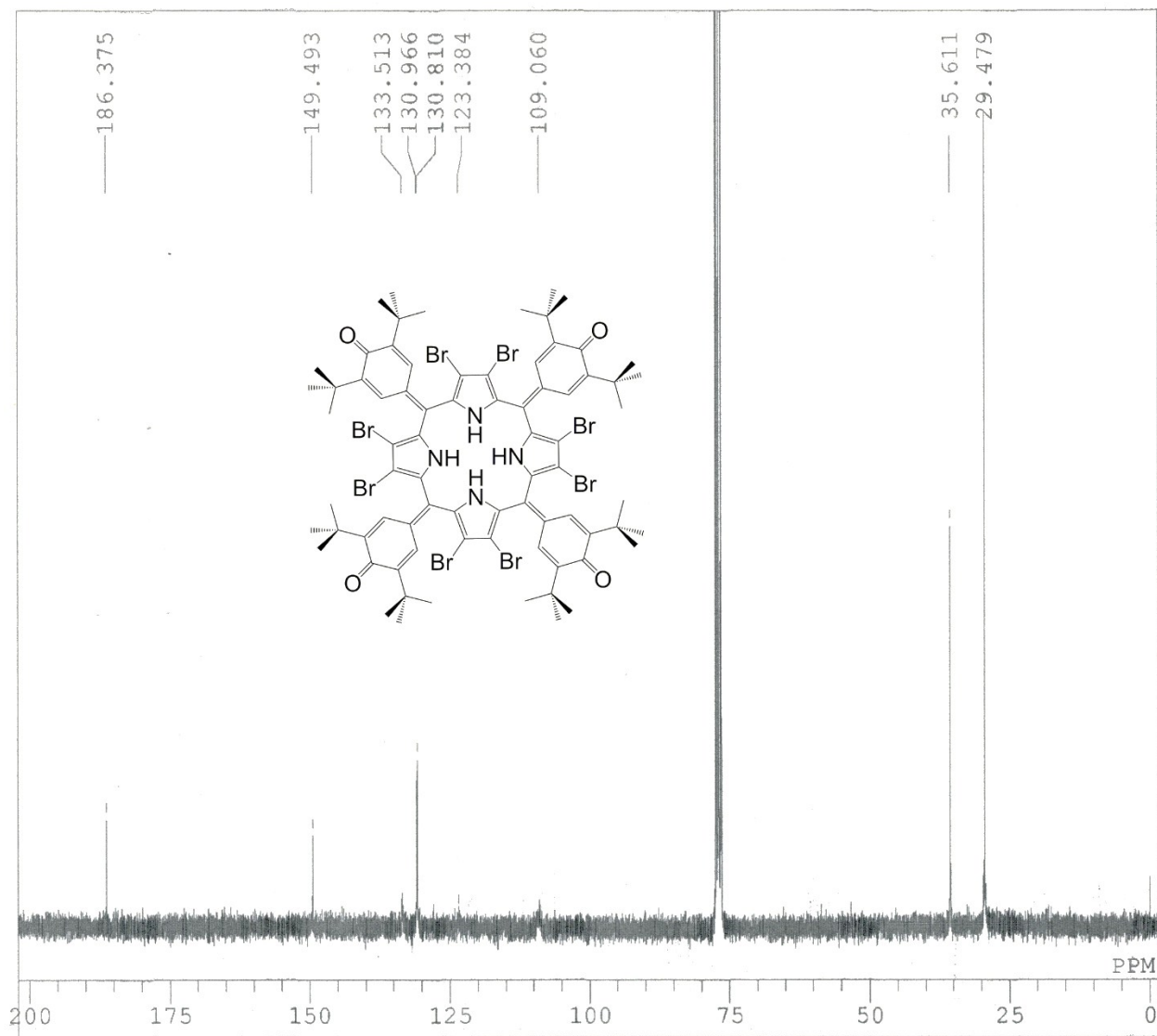


Figure S6. ¹³C NMR spectrum of β-Br₈OxP.

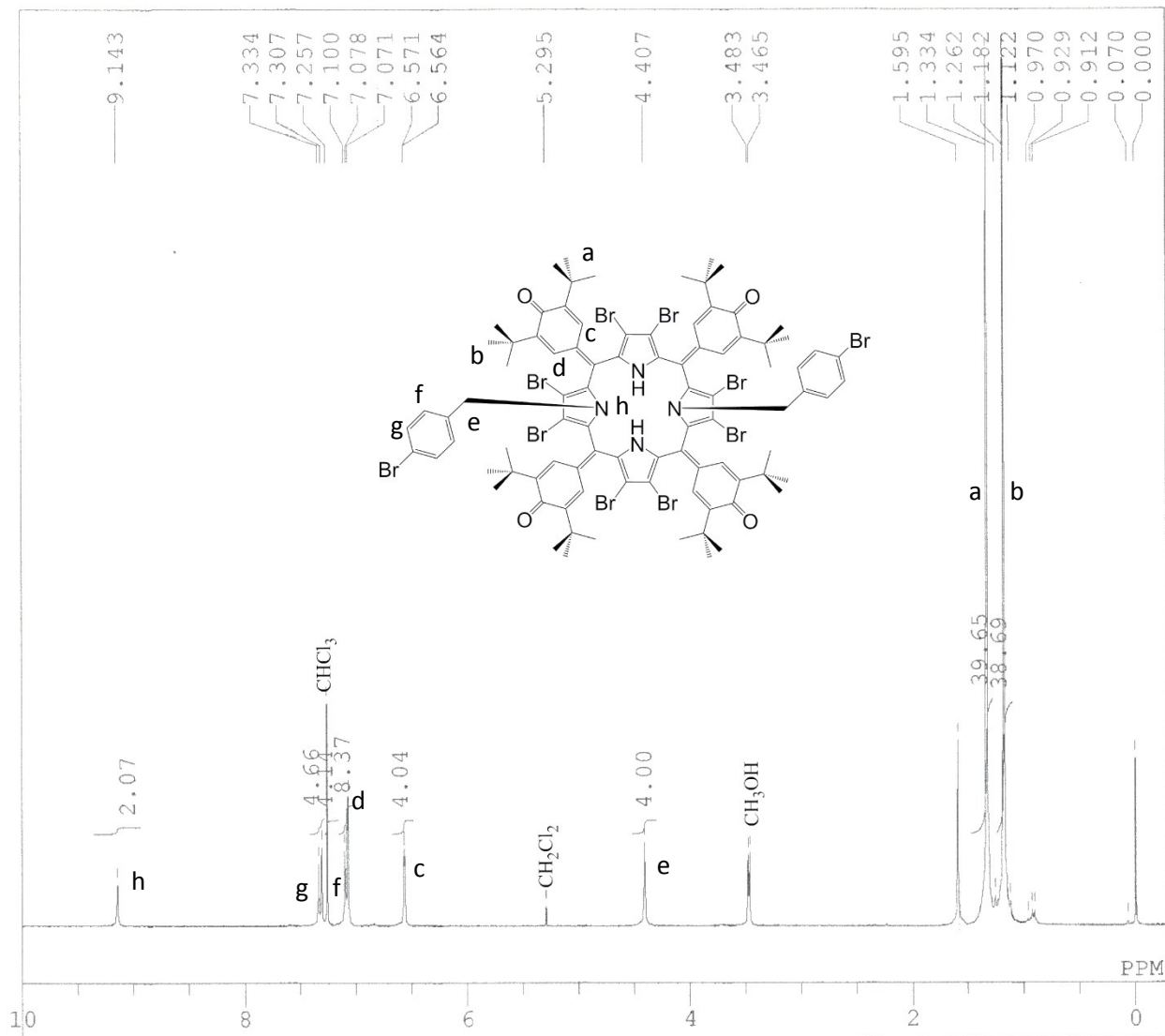


Figure S7. ¹H NMR spectrum of β -Br₈OxPBz₂

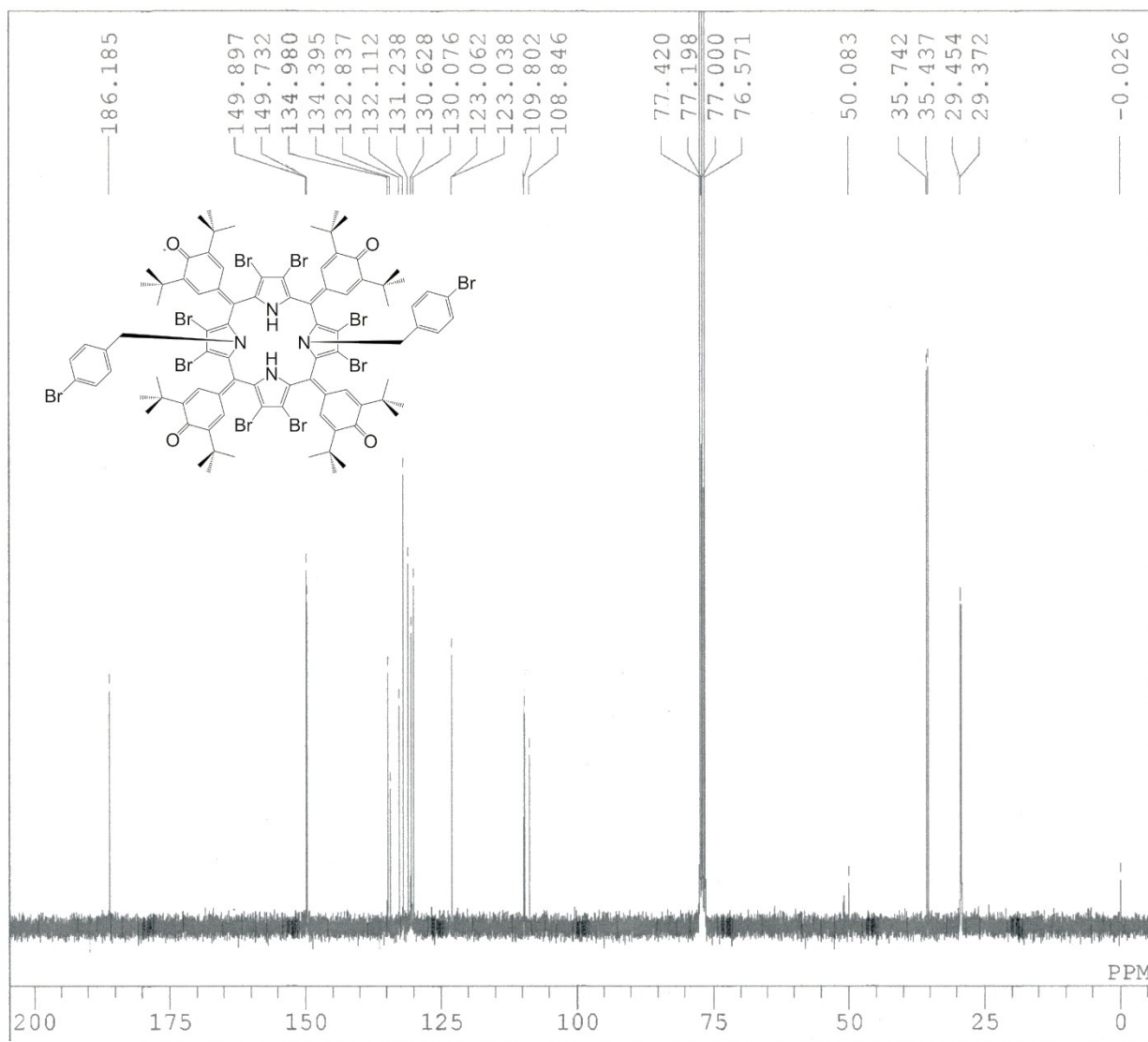


Figure S8. ¹³C NMR spectrum of β-Br₈OxPBz₂

Total energy and computed coordinates of brominated OxP derivatives

(a) Br₈OxP

Total Energy: -23003.60877555 A.U.

C	2.65411410	-2.28992468	-0.00802488
C	2.28993121	2.65410735	0.00798512
C	-2.65411487	2.28992600	-0.00792488
C	-2.28992572	-2.65411382	0.00797512
N	0.17507557	-2.36472518	0.15840513
C	1.33957521	-2.60893154	-0.55908493
C	-0.94585639	-2.77766144	-0.55093493
C	0.93111576	-3.12859250	-1.78812502
C	-0.47429990	-3.23251398	-1.78294502
C	2.77766798	-0.94586316	0.55088516
C	-2.60891853	-1.33957648	0.55906516
C	-3.19219670	-3.70272064	0.01309512
C	3.70272092	-3.19219566	-0.01316488
N	2.36471766	0.17507036	-0.15844490
C	3.23254863	-0.47430976	1.78288525
N	-2.36471842	-0.17506903	-0.15840490
C	-3.12857633	-0.93115295	1.78810525
C	-4.60117543	-3.48634354	0.30599514
C	-2.76880350	-5.06497137	-0.27484490
C	5.06498100	-2.76878215	0.27474514
C	3.48636568	-4.60116968	-0.30607491
C	3.12861309	0.93110745	1.78806525
C	2.60893807	1.33956845	0.55904516
C	-3.23250407	0.47427052	1.78295525

C	-2.77765624	0.94584887	0.55095516
C	-5.49739616	-4.49807728	0.30515514
C	-3.63503432	-6.10240626	-0.26469490
C	6.10243150	-3.63500046	0.26457514
C	4.49811502	-5.49737791	-0.30525491
C	-5.07131871	-5.88759993	0.02295512
C	5.88763925	-5.07128640	-0.02308489
C	-6.96803313	-4.31217187	0.56643516
C	-3.23223205	-7.52998318	-0.52047492
C	7.52999746	-3.23216852	0.52032516
C	4.31223148	-6.96801017	-0.56653492
C	0.94584783	2.77765652	-0.55090493
C	-1.33958377	2.60892661	-0.55901492
O	-5.88679982	-6.83580883	0.02719512
C	3.19218813	3.70271571	0.01310512
C	-3.70271543	3.19218918	-0.01302488
O	6.83585746	-5.88674716	-0.02735489
C	0.47427257	3.23253246	-1.78289502
N	-0.17507163	2.36470464	0.15845513
C	-0.93115089	3.12860473	-1.78804502
C	4.60117621	3.48635892	0.30597514
C	2.76876682	5.06496954	-0.27479490
C	-3.48634458	4.60117571	-0.30590491
C	-5.06497396	2.76878972	0.27490514
C	5.49738447	4.49810827	0.30513514
C	3.63497888	6.10242785	-0.26465490
C	-6.10241039	3.63500649	0.26478514
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C	5.07127888	5.88763401	0.02297512
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C	6.96802292	4.31221691	0.56637516

C	3.23213914	7.52998751	-0.52039492
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C	-7.52997481	3.23218861	0.52055516
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Br	-3.79861796	1.53518962	3.24707536
Br	-3.53215229	-2.05264905	3.26086537
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Br	3.53220781	2.05258015	3.26084536
Br	3.79868754	-1.53526007	3.24697536
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H	-7.55215269	-4.66875009	-0.28956491
H	4.66883781	-7.55213284	0.28944514
H	3.26362724	-7.20982803	-0.75729494
H	4.91505263	-7.27395706	-1.42932500
H	8.15588249	-3.49029890	-0.34151491

H	7.61258314	-2.16057753	0.71862517
H	7.92828198	-3.78869597	1.37647522
H	7.27400887	4.91506933	1.42912523
H	7.20983459	3.26362048	0.75716518
H	7.55211914	4.66877637	-0.28964491
H	3.78866189	7.92829394	-1.37653499
H	2.16053879	7.61255292	-0.71870494
H	3.49023985	8.15586164	0.34145514
H	-3.26359834	7.20984031	-0.75708494
H	-4.66874643	7.55213115	0.28972514
H	-4.91504719	7.27401458	-1.42903499
H	-7.61255425	2.16058981	0.71885517
H	-8.15586767	3.49031273	-0.34128491
H	-7.92824525	3.78871451	1.37671522
H	-0.15632095	2.06137002	1.12686520
H	0.15635145	-2.06140771	1.12681520
H	2.06137833	0.15634154	-1.12685497
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(b) Br₈OxPBz₂

Total Energy: -28663.78092458 A.U.

C	2.51373349	2.47054931	0.50998626
C	-2.51379023	2.47070459	0.50992626
C	-2.51373349	-2.47054931	0.50998626
C	2.51379023	-2.47070459	0.50992626
N	2.38914175	-0.00008527	0.63309627
C	2.82688842	1.14686797	-0.01515378
C	2.82698580	-1.14701393	-0.01515378

C	3.50719510	0.70388313	-1.15254387
C	3.50727026	-0.70395805	-1.15253387
C	1.14201097	2.63844157	1.00742630
C	1.14207066	-2.63857260	1.00739630
C	3.45600476	-3.47378958	0.64222627
C	3.45598037	3.47360584	0.64233627
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C	0.70339383	2.88639044	2.30542640
N	0.00002985	-2.46092194	0.22254624
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C	4.87989516	-3.21224319	0.49120626
C	3.05338227	4.83694299	0.95919629
C	4.87985222	3.21208185	0.49107626
C	-0.70345712	2.88650411	2.30540640
C	-1.14207066	2.63857260	1.00739630
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C	-1.14201097	-2.63844157	1.00742630
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C	0.00018031	-2.41825209	-1.27060388
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C	0.00004757	-3.80740301	-1.89161392
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C	1.20592880	-4.45828952	-2.18143395
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Br	4.21028820	1.78846253	-2.54041397
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H	7.51118458	2.90792994	0.28971624
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H	-4.05599692	7.59905229	2.30385640
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H	-3.94166206	7.92442735	0.57944627
H	-7.71473107	4.59593658	-0.25361380
H	-7.51124697	2.90801465	0.29031624
H	-7.78239972	4.22504632	1.46378633
H	-7.51118458	-2.90792994	0.28971624
H	-7.78259297	-4.22560001	1.46239633
H	-7.71433048	-4.59558102	-0.25517380
H	-2.49326190	-7.38234733	1.47131633
H	-3.93993356	-7.92401702	0.57739627

H	-4.05763036	-7.59988754	2.30181640
H	-1.92728135	0.00011910	1.53748634
H	1.92728135	-0.00011910	1.53748634

(c) Br₈OxPBz₄

Total Energy: -34323.93889516 A.U.

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C	-3.33787526	-1.23508555	-0.03016886
C	-1.23508320	3.33782612	0.02995114
C	3.33787076	1.23509740	-0.03008886
N	2.25322005	-1.04009712	-0.28584888
C	2.06392322	-2.20694017	0.46866118
C	3.02565530	-0.12243951	0.43882118
C	2.72489173	-2.00396887	1.67868127
C	3.31473003	-0.72748533	1.65976127
C	-0.12247282	-3.02566800	-0.43869889
C	2.20700211	2.06393354	-0.46860889
C	4.63728917	1.70989912	-0.05103886
C	1.70994707	-4.63722508	0.05115115
N	-1.04011037	-2.25317194	0.28593116
C	-0.72754494	-3.31486727	-1.65958899
N	1.04013139	2.25323622	0.28584116
C	2.00406609	2.72482955	-1.67867899
C	4.92374746	3.12941237	-0.20991887
C	5.77270973	0.80816397	0.08976115
C	0.80825304	-5.77269041	-0.08949886
C	3.12948622	-4.92359488	0.20991116

C	-2.00403686	-2.72503441	-1.67853899
C	-2.20696802	-2.06394429	-0.46856889
C	0.72755158	3.31462382	-1.65982899
C	0.12246716	3.02557169	-0.43890889
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C	3.60907959	-6.18718183	0.21771116
C	7.34619341	2.69546967	-0.08629887
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