

SUPPORTING INFORMATION

Synthesis and electronic properties of A₃B-thienyl porphyrins: Experimental and computational investigations

Poomani Ram Kumar,^a Neethinathan Johnnee Britto,^b Arunkumar Kathiravan,^c Antonia Neels,^d Madhavan Jaccob^b and E. M. Mothi^{a*}

^a Centre for Scientific and Applied Research, PSN College of Engineering and Technology, Melathediyoore, Tirunelveli 627 152, India.

^b Department of Chemistry & Computational Chemistry Laboratory, Loyola Institute of Frontier Energy (LIFE), Loyola College, Chennai – 600 034, India.

^c Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology, Adavi, Chennai 600 062, India.

^d Center for X-ray Analytics, Empa - Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland.

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Table S1. Crystallographic data for **1** and **3**

<i>Compounds</i>	1	3
<i>CCDC number</i>	1574876	1574875
<i>Empirical formula</i>	C ₃₈ H ₂₄ N ₄ O S ₃	[(C ₄₁ H ₃₀ S ₃ N ₄ O ₃)(C ₆ H ₁₄) _{0.64}]
<i>Formula weight</i>	648.79	761.92
<i>Crystal system</i>	Monoclinic	Monoclinic
<i>Space group</i>	P2 ₁ /c	P2 ₁ /c
<i>a</i> (Å)	6.6311(3)	12.3276(11)
<i>b</i> (Å)	11.1557(5)	13.0193(7)
<i>c</i> (Å)	21.0852(9)	23.939(2)
<i>β</i> (°)	93.419(4)	93.247(7)
<i>V</i> (Å ³)	1556.99(12)	3836.0(5)
<i>Z</i>	2	4
<i>Absorption coefficient</i> (mm ⁻¹)	0.277	0.240
<i>Collected reflections</i>	14651	48920
<i>Independent reflections</i>	2775	6839
<i>R</i> _(int)	0.091	0.061
<i>R</i> ₁ (Observed data)	0.0835	0.0377
<i>wR</i> ₂ (all data)	0.2002	0.1090

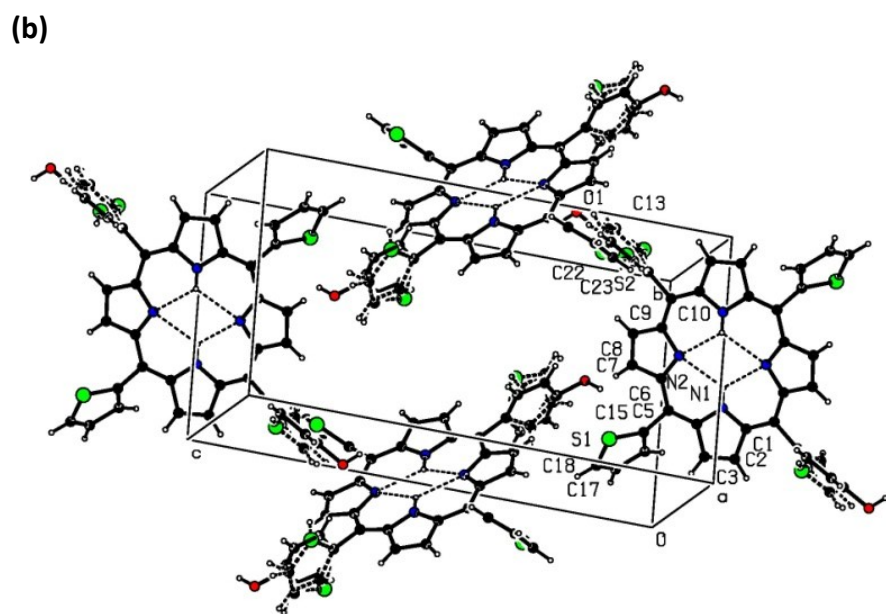
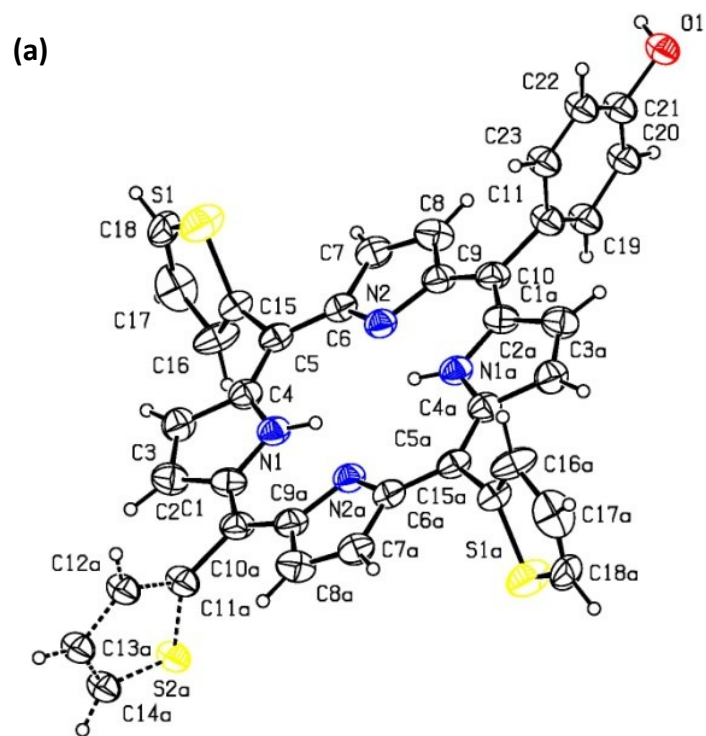
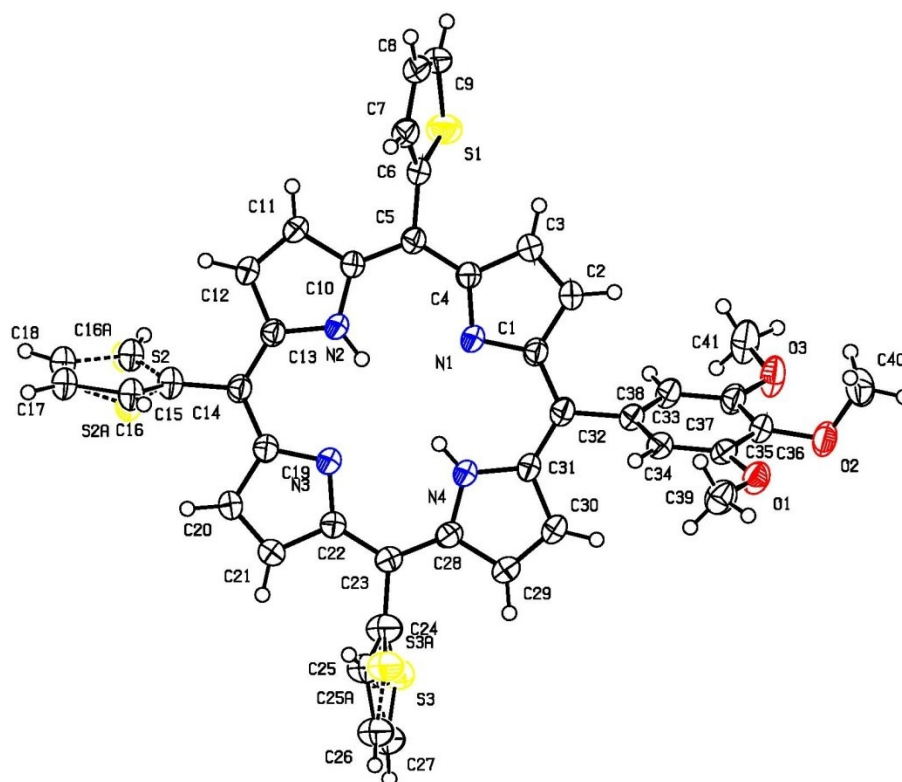
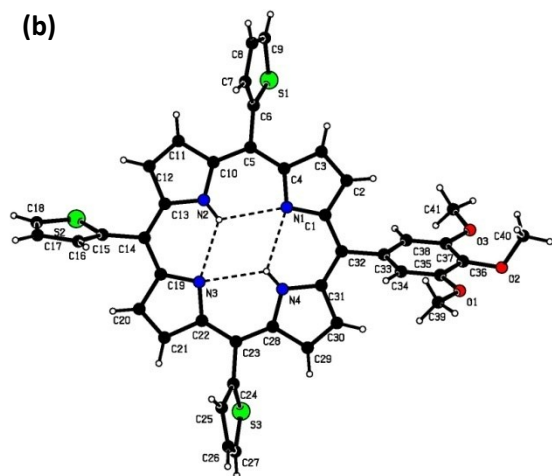


Fig. S1 (a) ORTEP molecular view (b) Packing diagram of porphyrin **1**

(a)



(b)



(c)

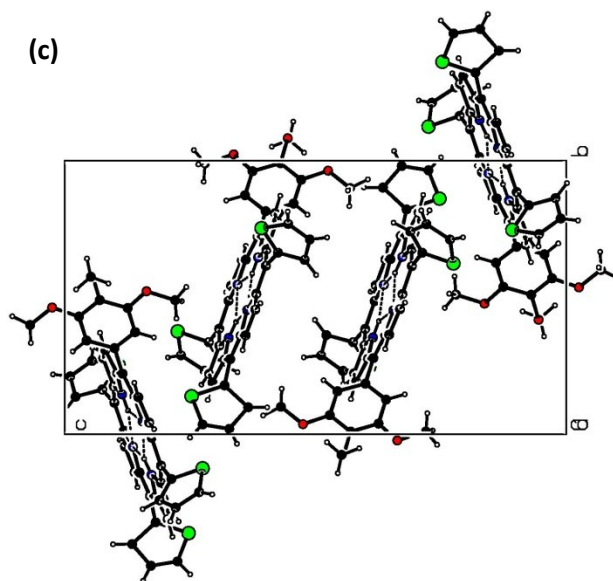


Fig. S2 (a) ORTEP molecular view (b) intramolecular NH bonding (c) Packing diagram of porphyrin **3**

Structural characterizations of porphyrins 5-1

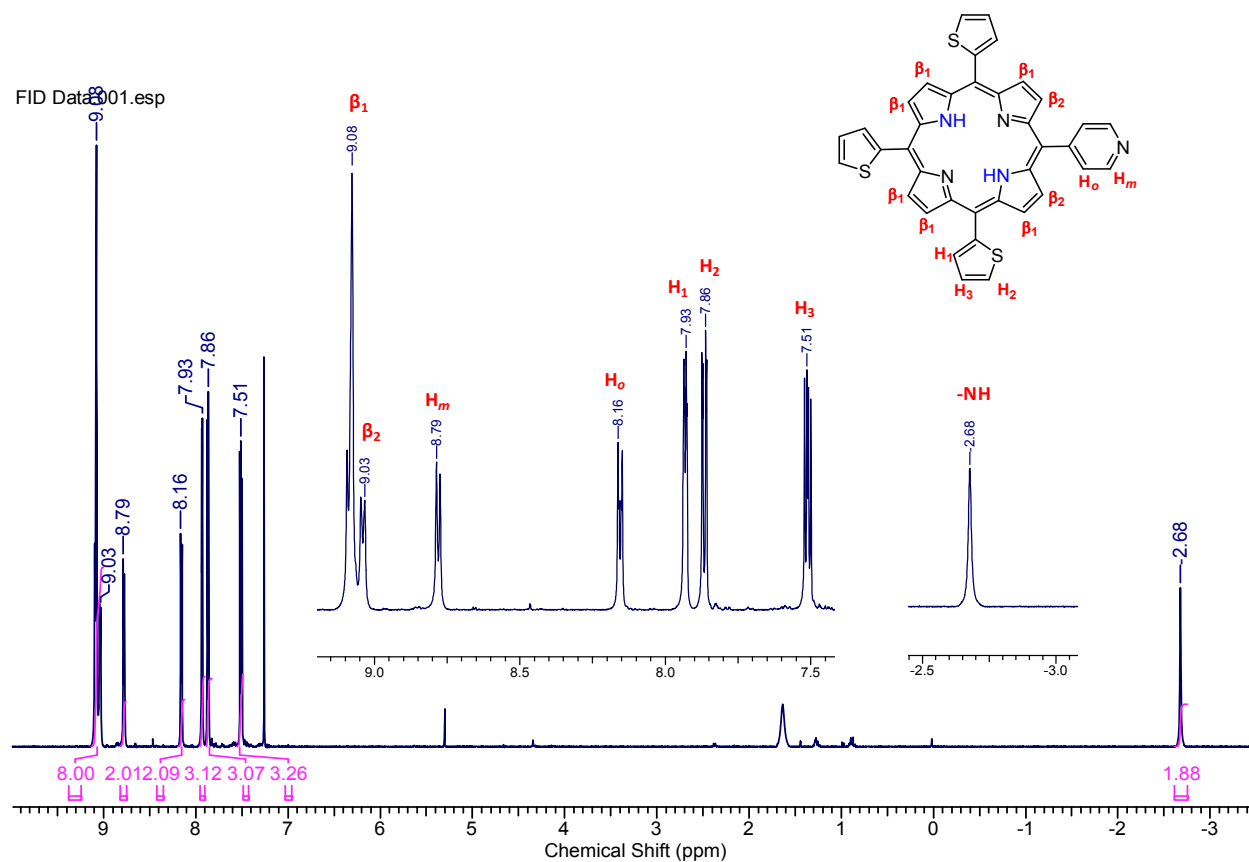


Fig. S3 ^1H -NMR (400MHz, CDCl_3) spectrum of porphyrin **5**

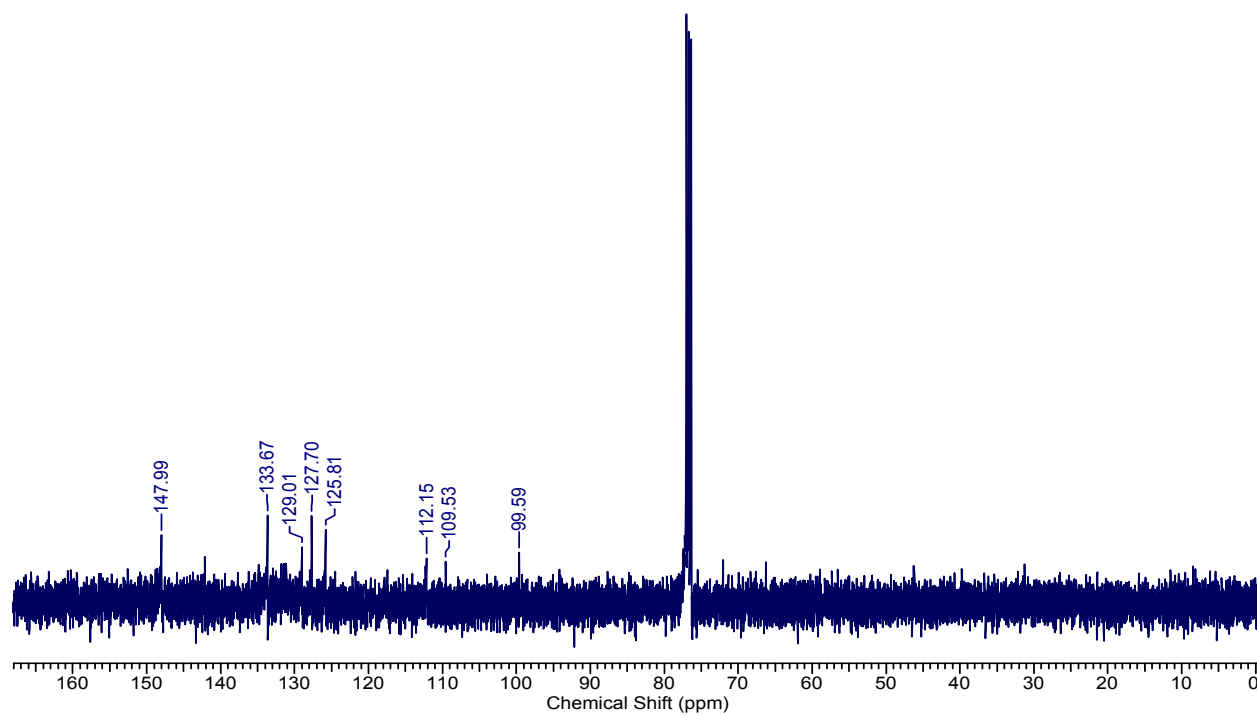


Fig. S4 ^{13}C – NMR (400MHz, CDCl_3) spectrum of porphyrin **5**

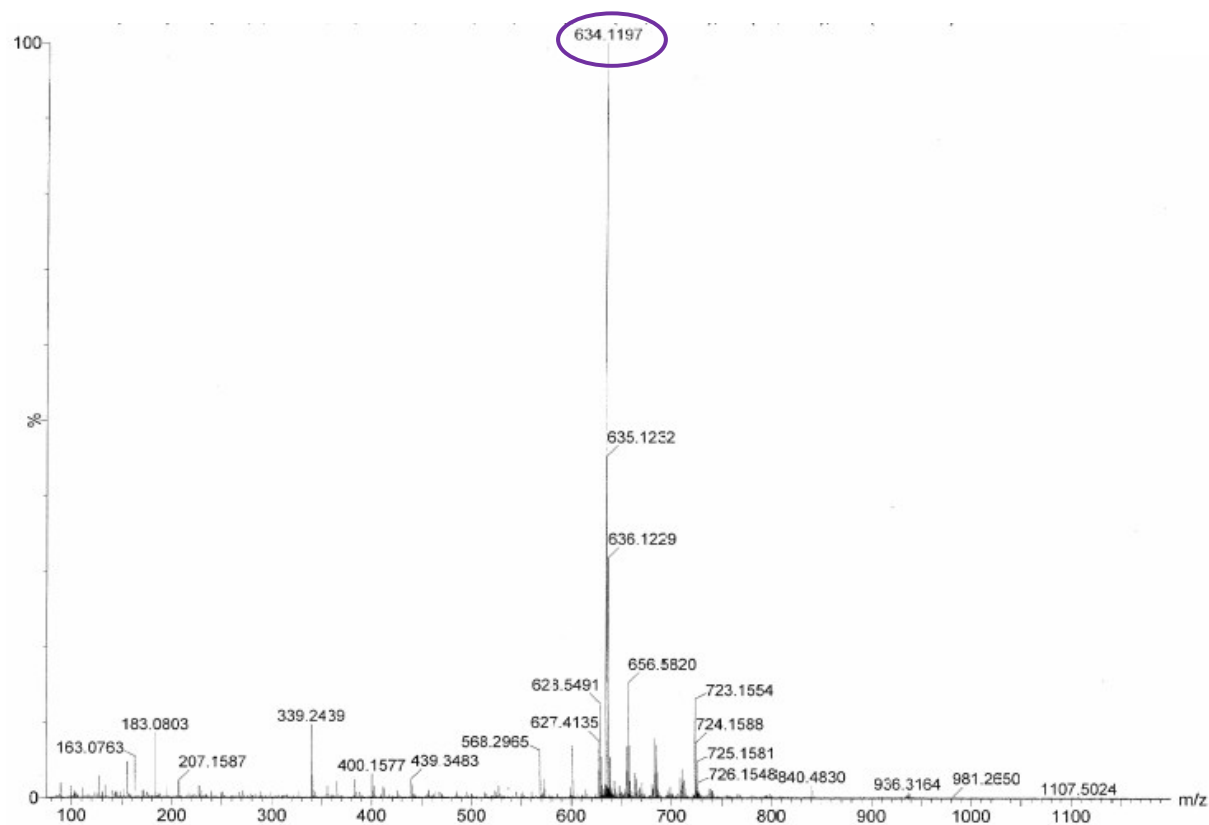
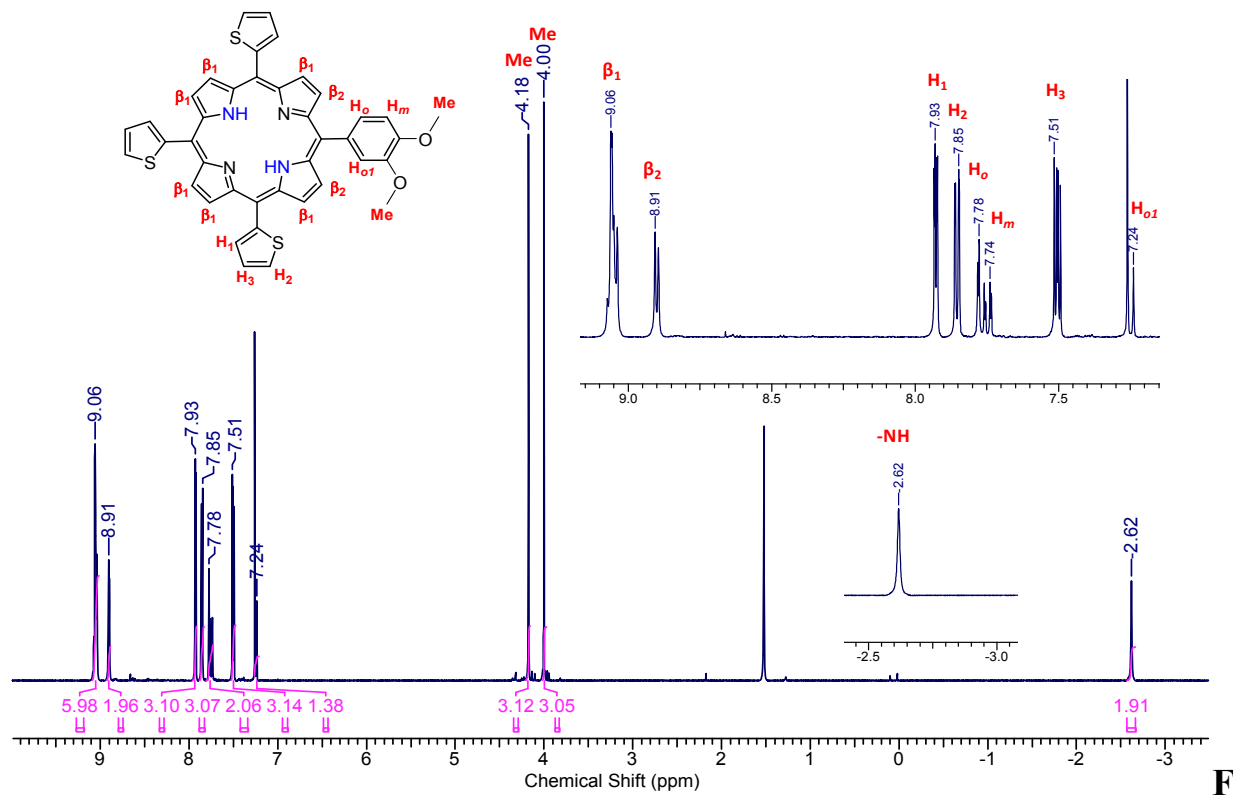


Fig. S5 ESI-TOF⁺ Mass spectrum of porphyrin **5**



ig. S6 ¹H-NMR (400MHz, CDCl₃) spectrum of porphyrin 4

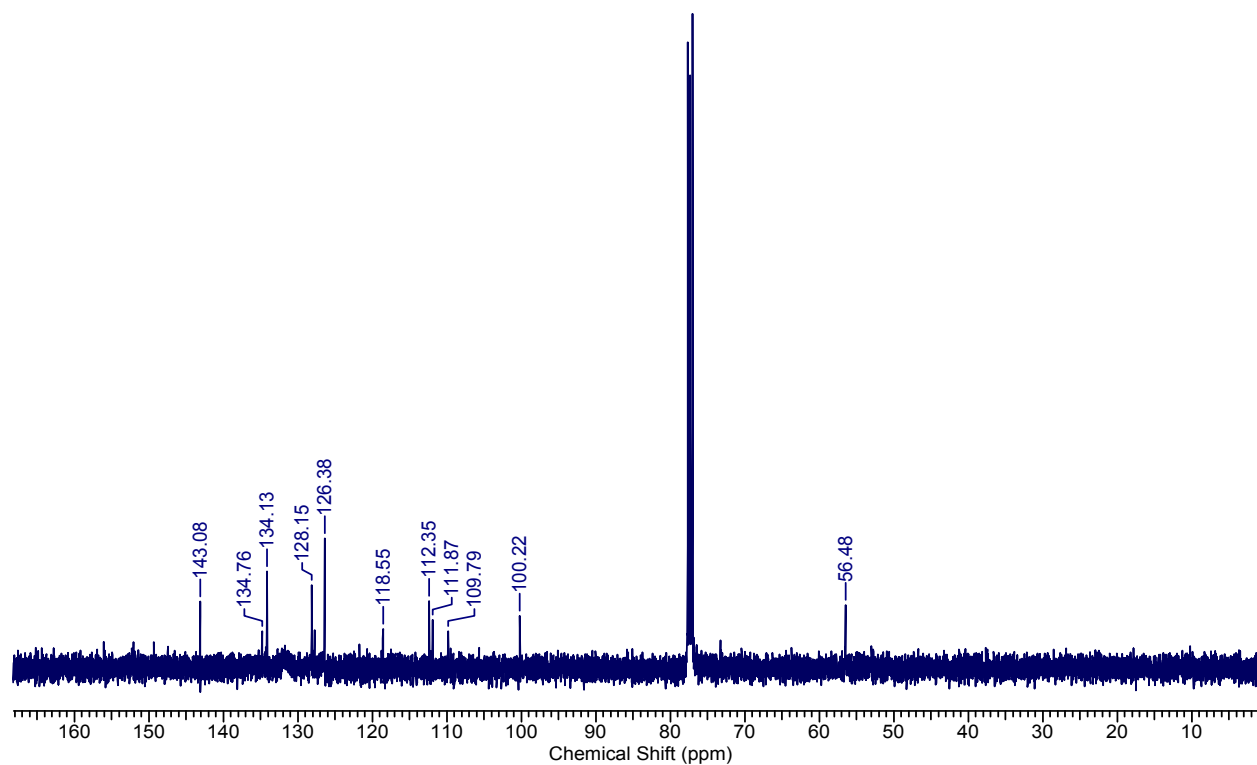


Fig. S7 ¹³C – NMR (400MHz, CDCl₃) spectrum of porphyrin 4

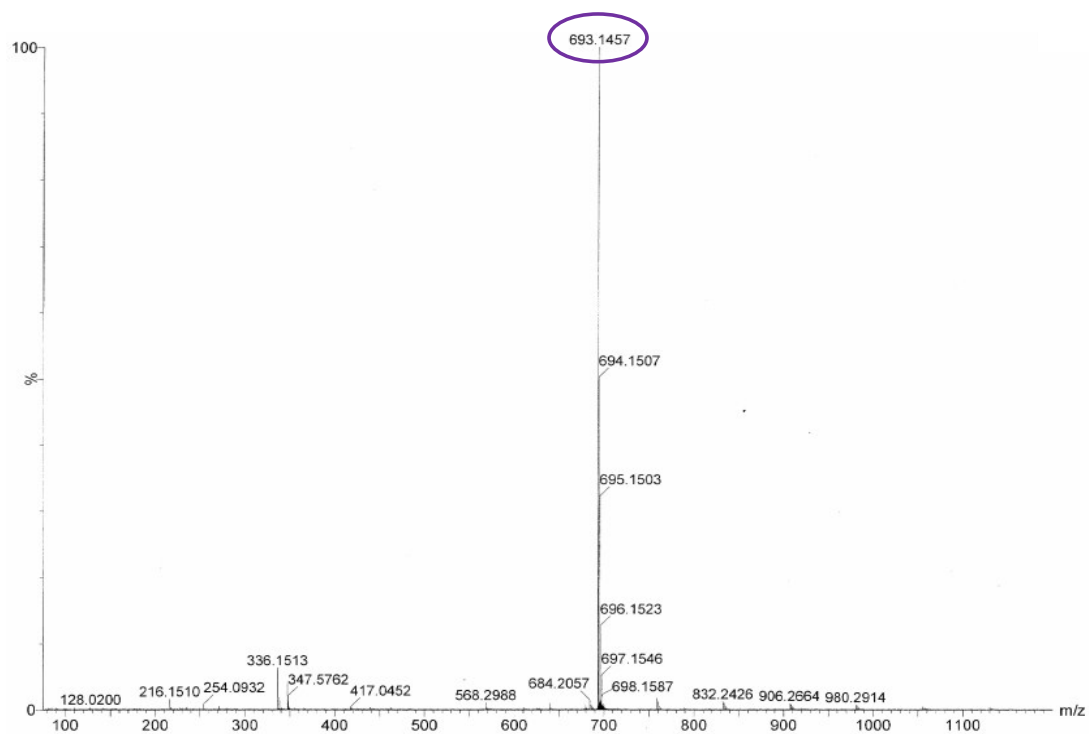


Fig. S8 ESI-TOF⁺ Mass spectrum of porphyrin **4**

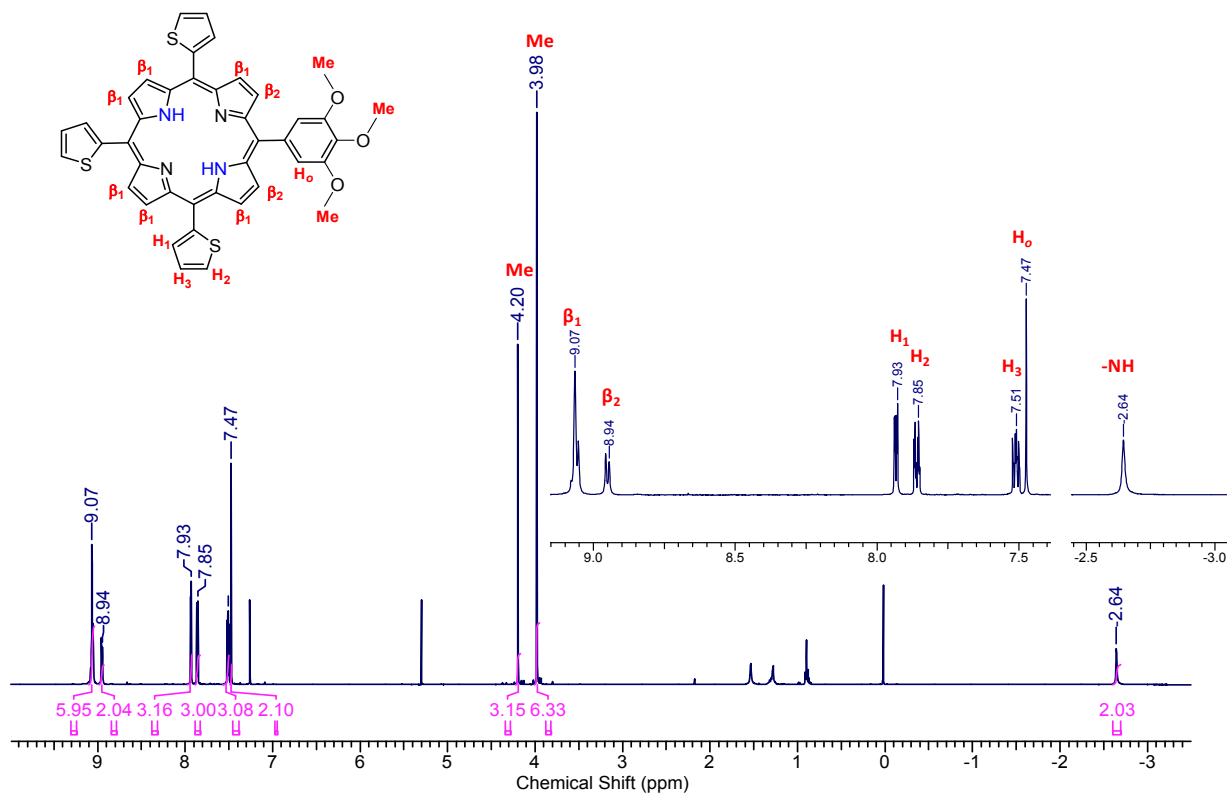
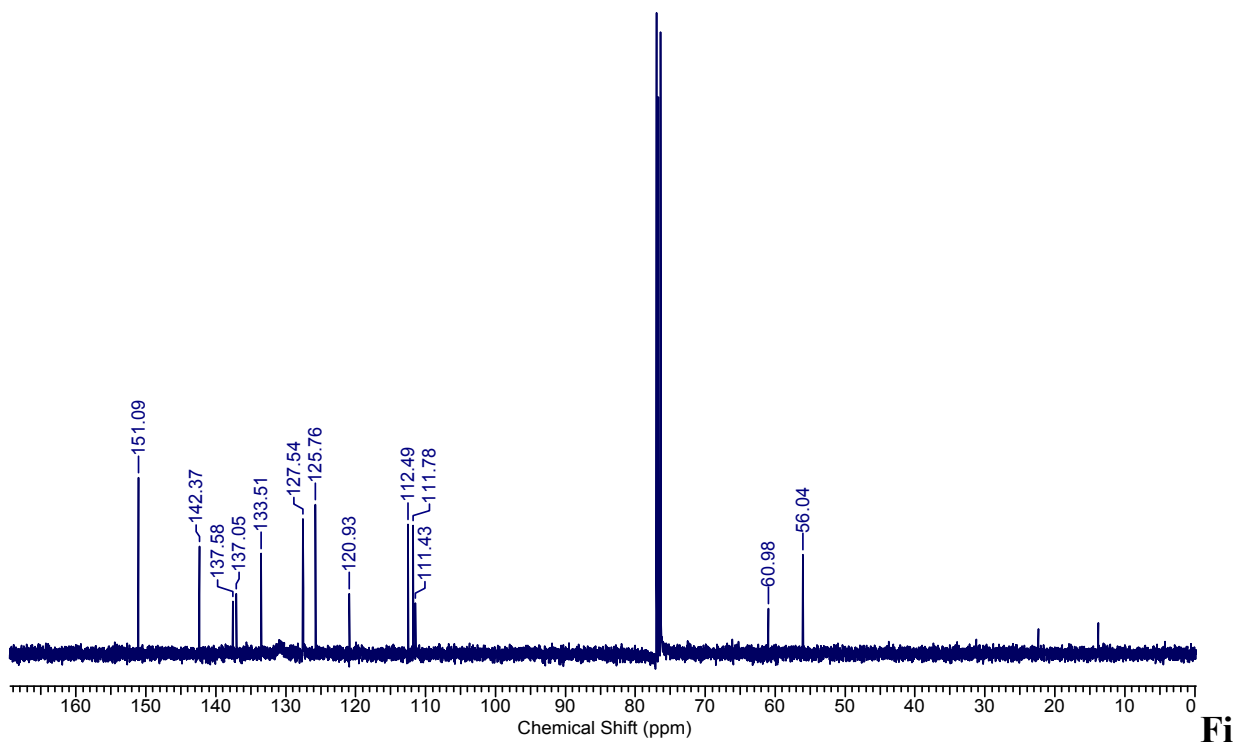


Fig. S9 ¹H-NMR (400MHz, CDCl₃) spectrum of porphyrin **3**



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g. S10 ^{13}C – NMR (400MHz, CDCl_3) spectrum of porphyrin **3**

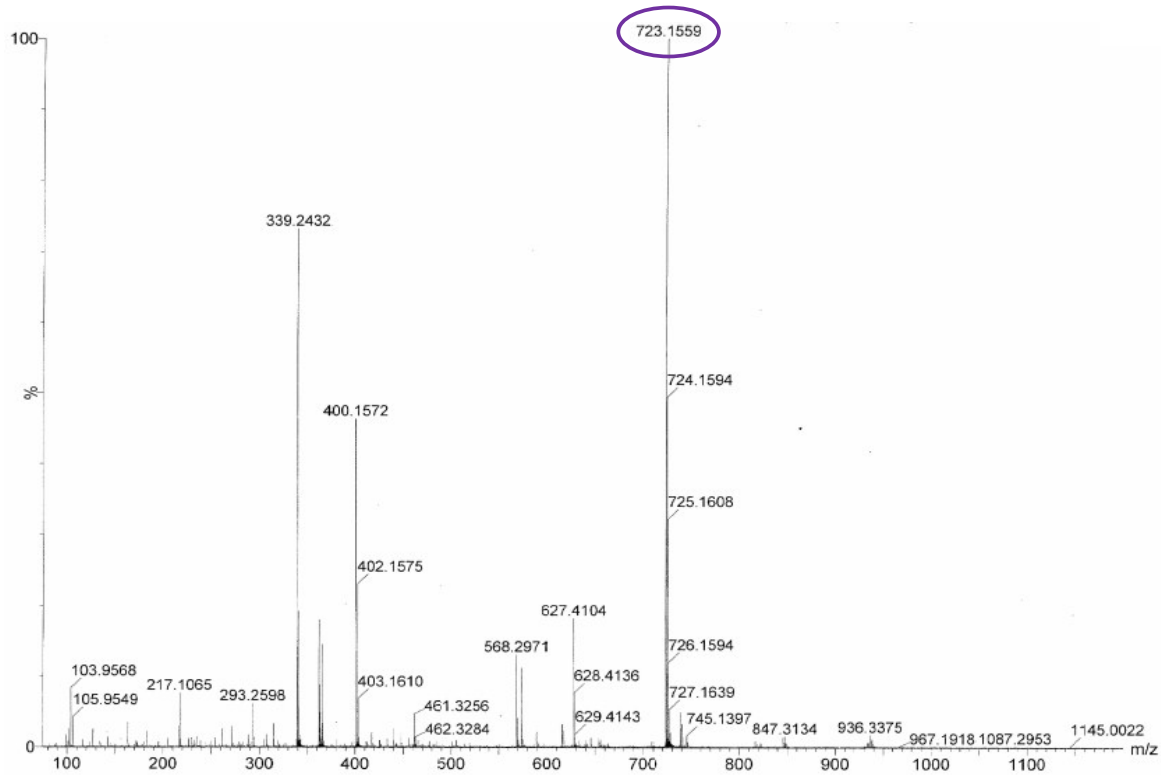


Fig. S11 ESI-TOF⁺ Mass spectrum of porphyrin **3**

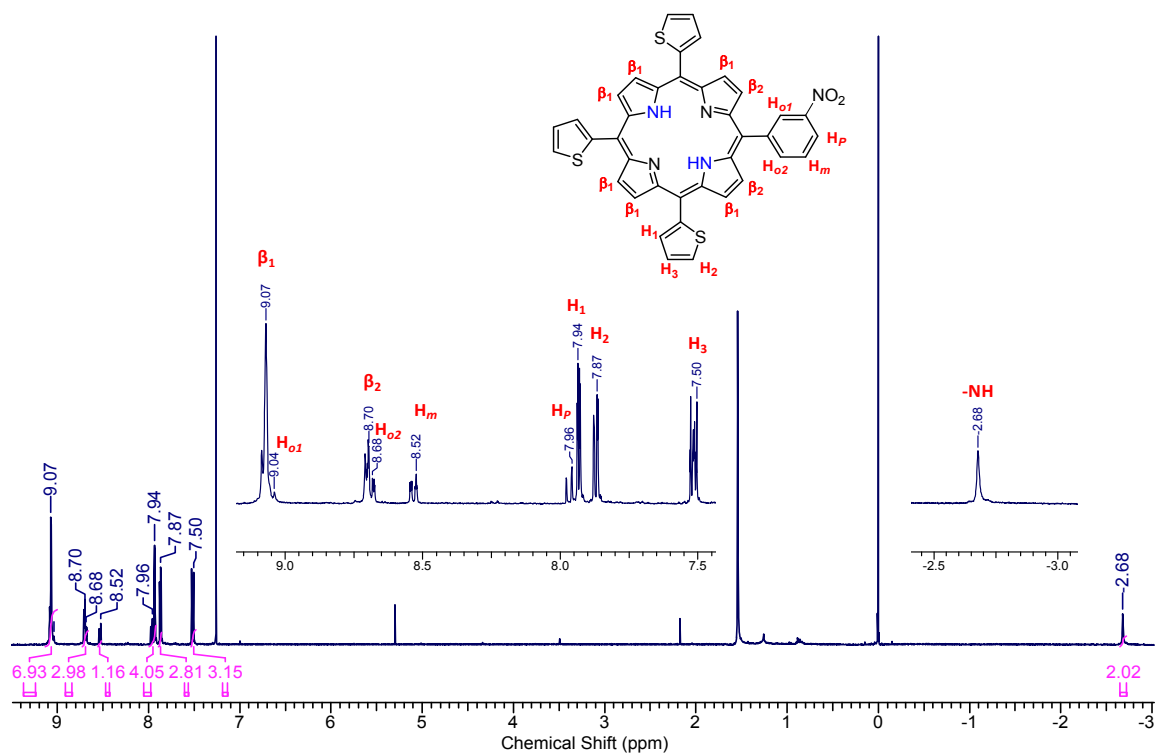
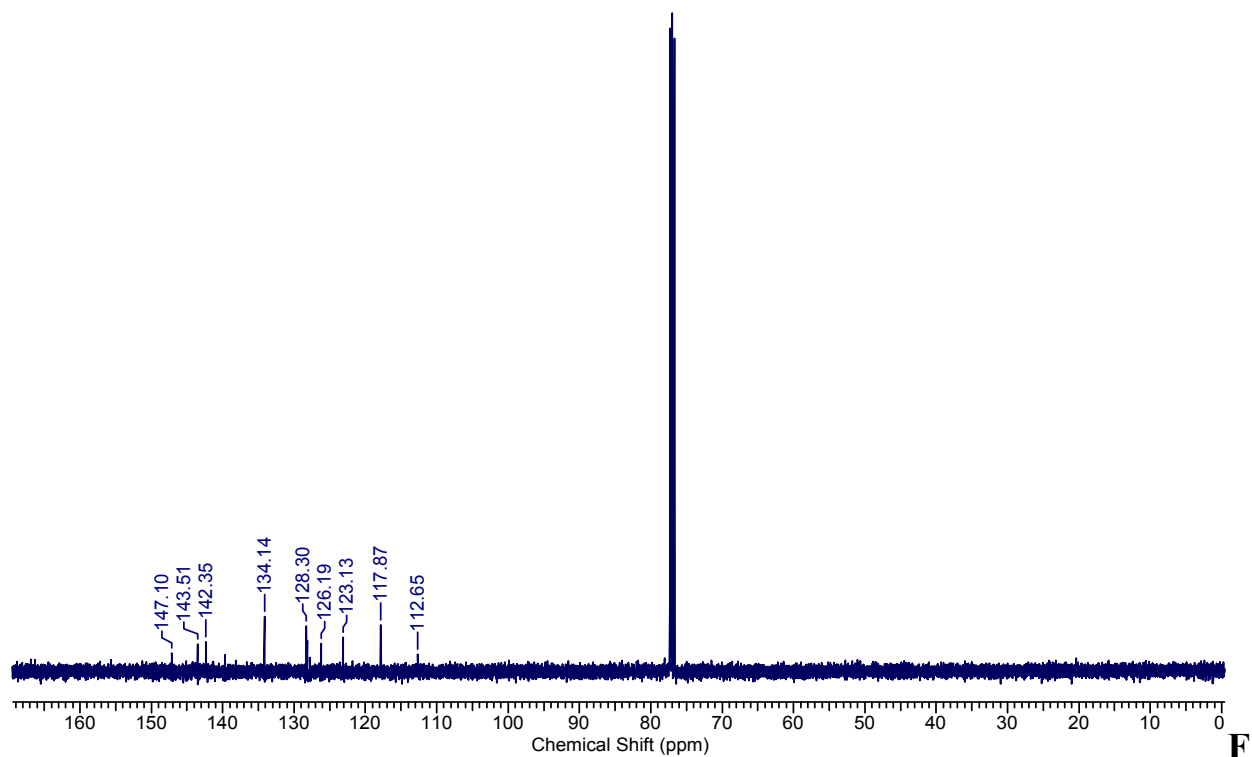


Fig. S12 ¹H-NMR (400MHz, CDCl₃) spectrum of porphyrin **2**



ig. S13 ^{13}C – NMR (400MHz, CDCl_3) spectrum of porphyrin **2**

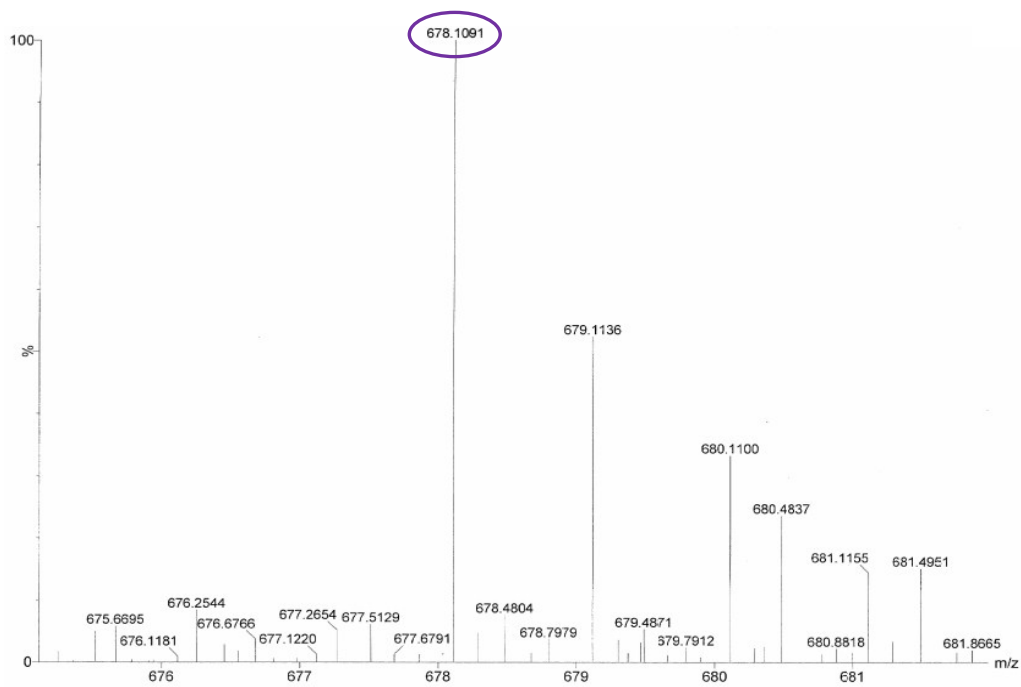


Fig. S14 ESI-TOF⁺ Mass spectrum of porphyrin **2**

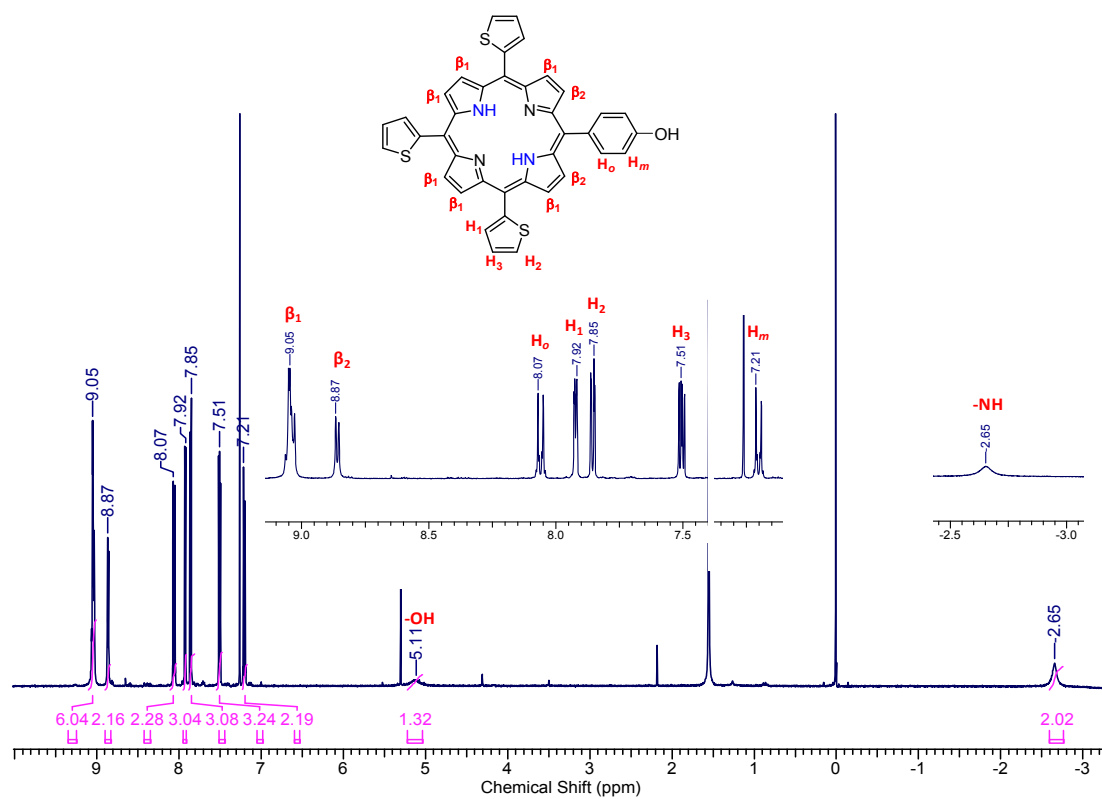


Fig. S15 ^1H -NMR (400MHz, CDCl_3) spectrum of porphyrin **1**

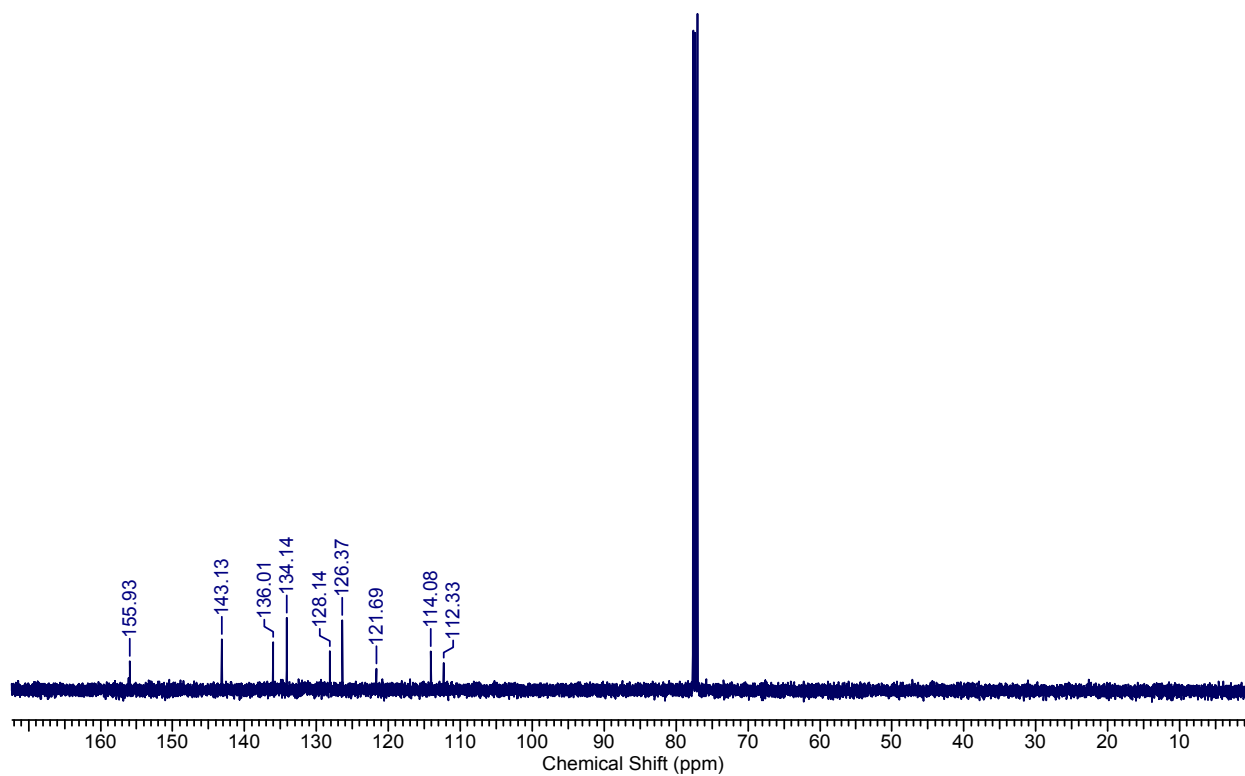


Fig. S16 ^{13}C – NMR (400MHz, CDCl_3) spectrum of porphyrin **1**

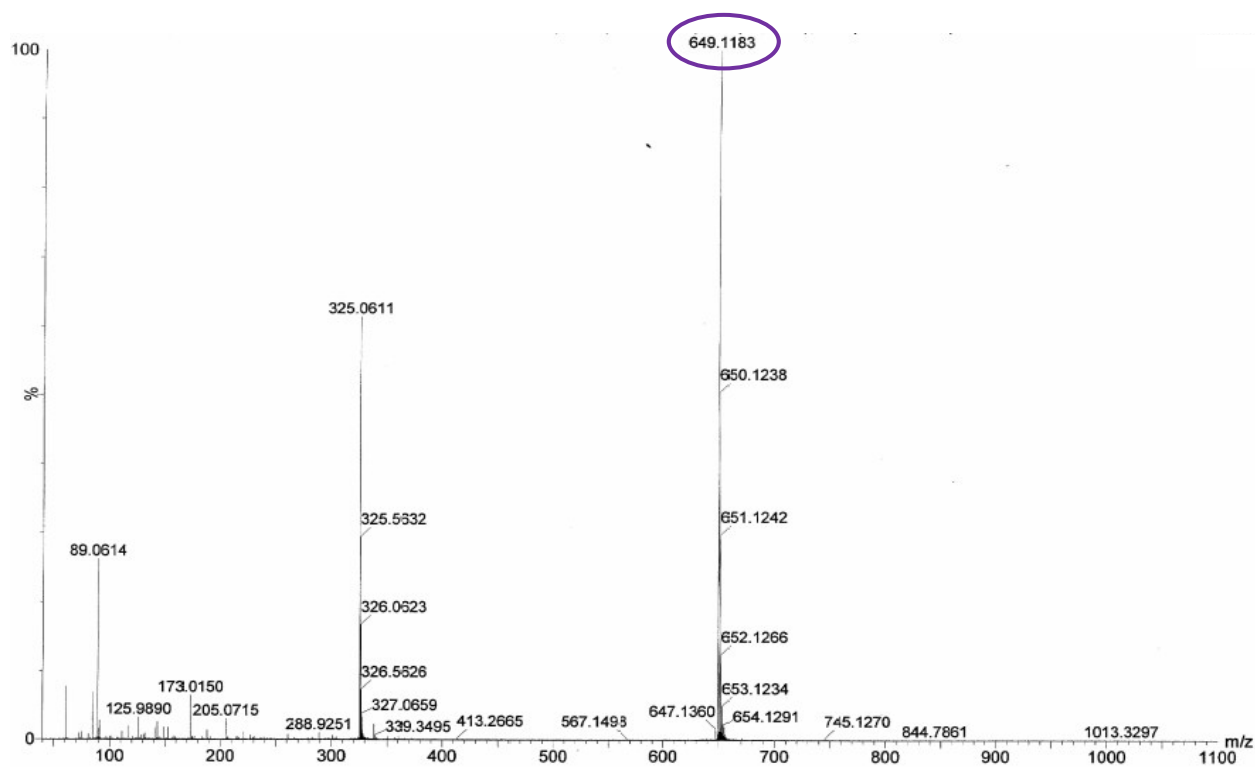


Fig. S17 ESI-TOF⁺ Mass spectrum of porphyrin **1**

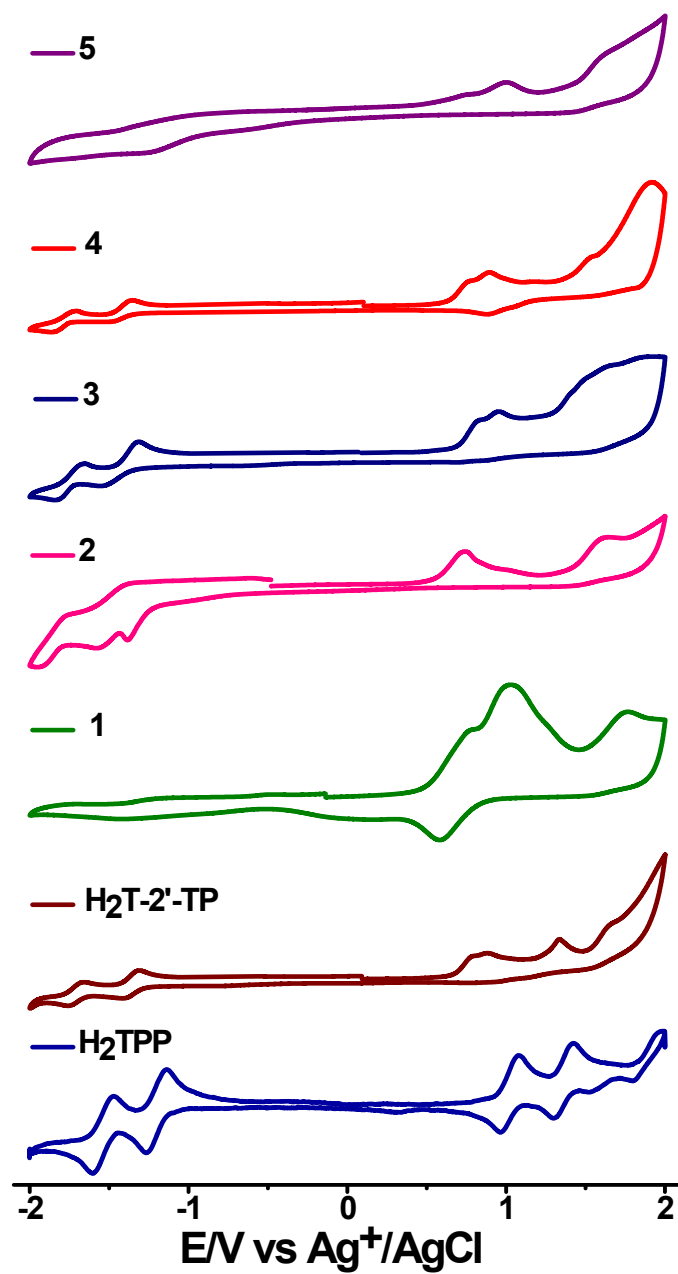
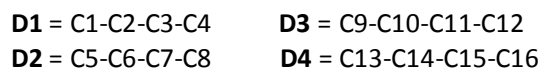
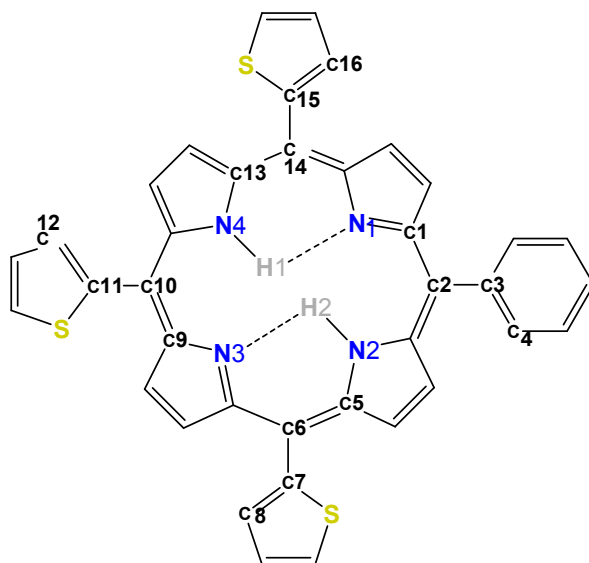


Fig. S18 Cyclic voltammograms of porphyrin **1-5** (1 mM) in CH₂Cl₂ containing 0.1 M TBAPF₆ using Ag/AgCl as a reference electrode with a scan rate of 0.10 V/s at 298 K.

Table S2. Scheme of atom numbering and pertinent bond lengths (Å) and dihedral angles (°) of porphyrins **1-5** obtained from the B3LYP/6-31G(d,p) optimized geometries.



Porphyrins	State	D1	D2	D3	D4	N4-H1	N2-H2	N1-H1	N3-H2
1	S ₀	62.9	63.9	64.6	65	1.013	1.014	2.320	2.317
	S ₁	54.0	52.6	52.7	53.4	1.012	1.012	2.345	2.340
2	S ₀	64.7	64.8	63.7	64	1.013	1.014	2.314	2.312
	S ₁	58.6	52.7	52.6	52.4	1.012	1.013	2.315	2.310
3	S ₀	65.9	65.5	65.2	64.4	1.013	1.013	2.312	2.311
	S ₁	56.2	53.6	52.8	53.0	1.012	1.012	2.333	2.329
4	S ₀	64.0	65.5	64.5	64.0	1.014	1.013	2.321	2.320
	S ₁	55.6	54.0	53.1	53.3	1.012	1.012	2.338	2.333
5	S ₀	64.0	66.2	65.6	64.5	1.013	1.014	2.311	2.311
	S ₁	57.0	53.3	52.7	52.9	1.012	1.012	2.327	2.320

Table S3. Comparison of calculated and experimental absorption maxima (λ_{max}) of Porphyrin **1** at various density functionals in combination with 6-311G(d,p) basis set.

Functionals	λ_{max} (in nm)
B3LYP	416.0
CAM-B3LYP	376.8
M06-2X	380.9
M06	404.6
M05-2X	376.4
M05	401.1
PBE	458.9
PBE0	399.7
ω-B97X-D	375.5
Experimental	423

Table S4. Comparison of calculated and experimental absorption maxima (λ_{max}) of Porphyrin **1** at B3LYP functional in combination with various basis sets.

Basis sets	λ_{max} (in nm)
6-31G(d)	418.7
6-31G(d,p)	419.2
6-311G(d)	416.1
6-311G(d,p)	416.0
6-31+G(d)	413.4
6-31+G(d,p)	413.7
6-311+G(d)	411.7
6-311+G(d,p)	411.3
6-31++G(d)	413.6
6-31++G(d,p)	413.9
6-311++G(d)	411.8
6-311++G(d,p)	411.5
Experimental	423

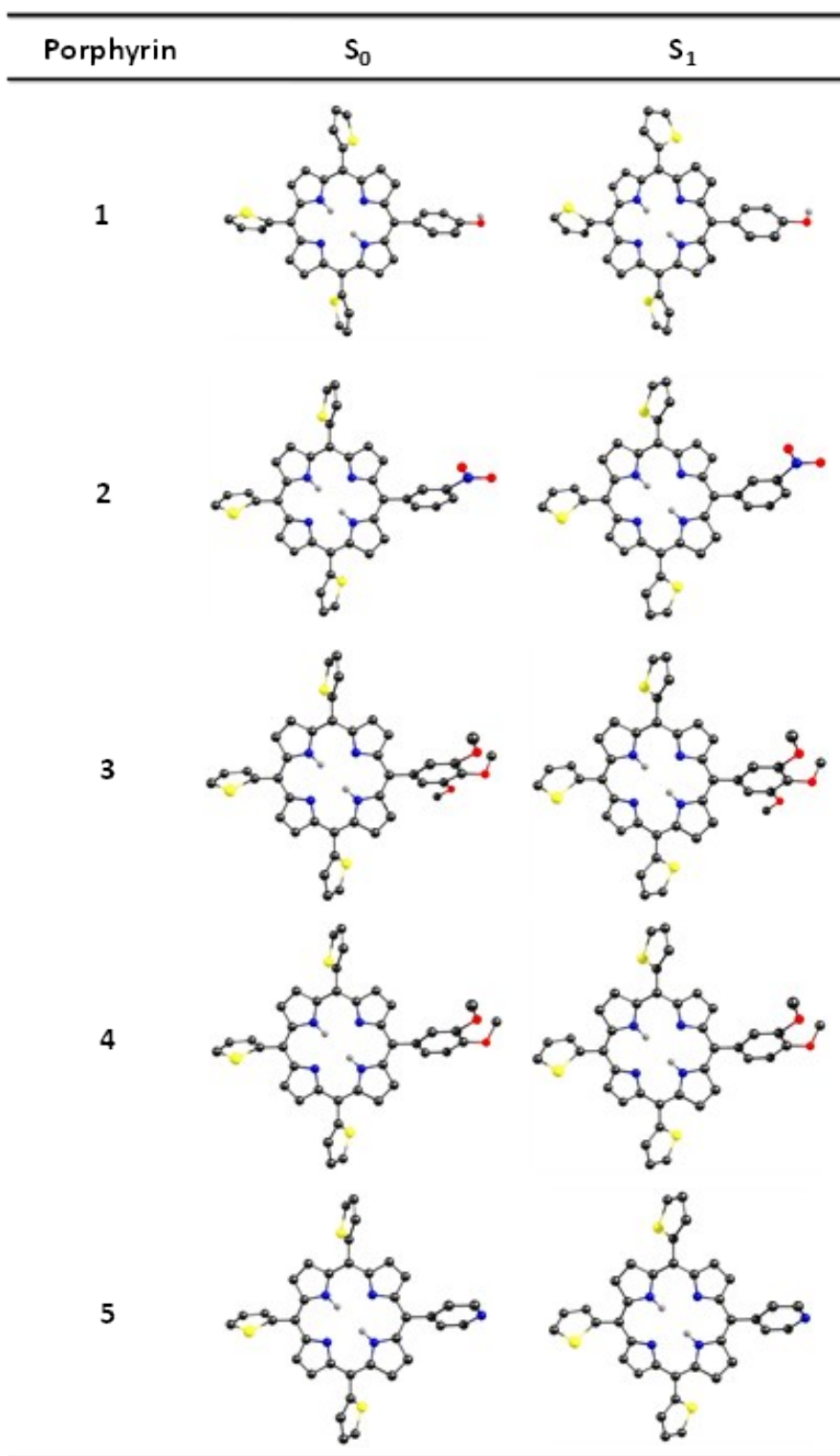


Figure. S19 TD-B3LYP/6-31G(d,p) optimized ground and excited-state geometries of porphyrins **1-5**. All hydrogen atoms attached to the carbons are hidden for better view.

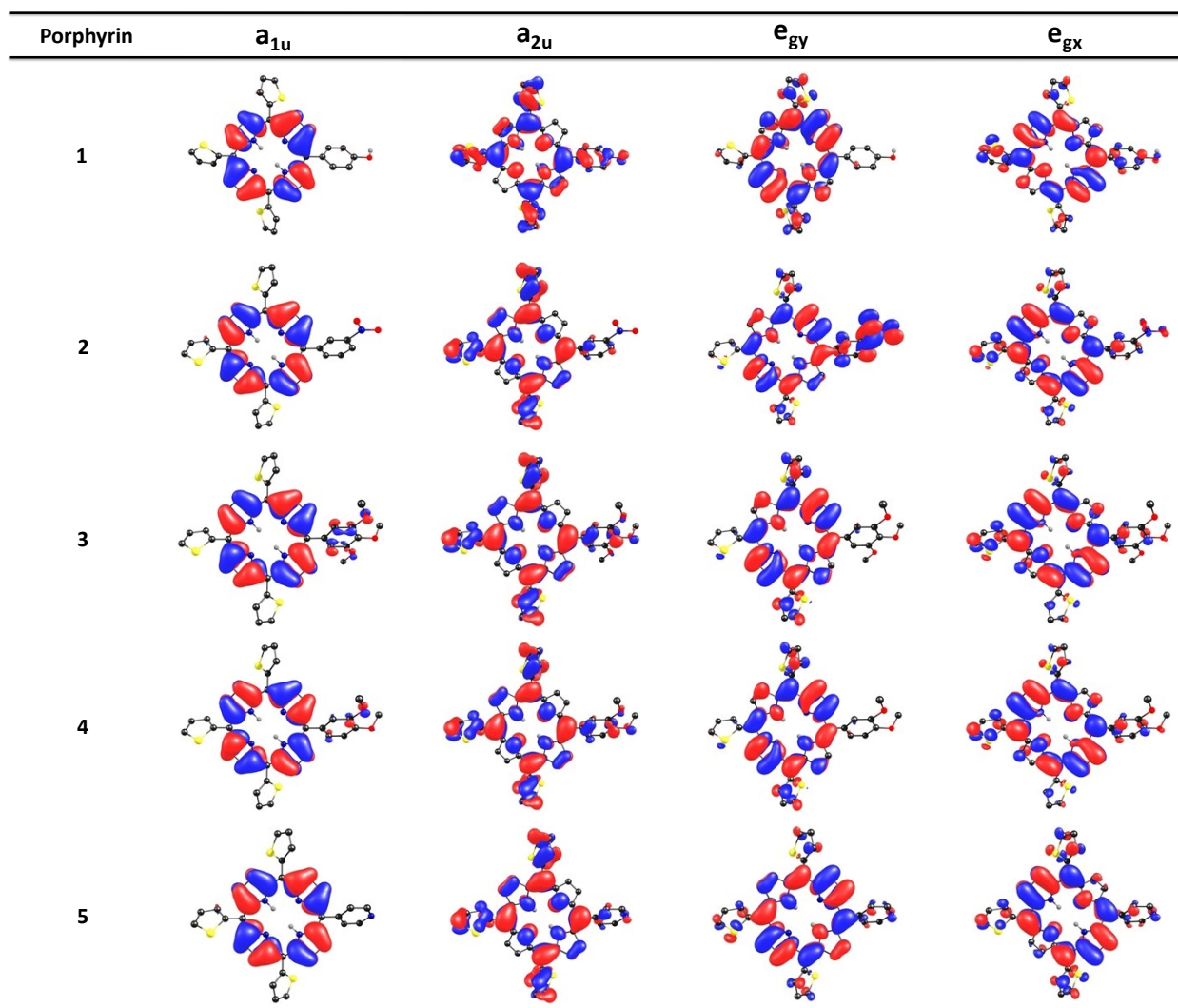


Figure S20. Frontier molecular orbitals of porphyrins **1-5** in S_1 state.

Cartesian coordinates of B3LYP/6-31G(d,p) optimized ground-state geometries

Porphyrin 1

7	-1.336590000	1.331715000	-0.045965000
7	-1.164633000	-1.598648000	-0.081786000
1	-0.502988000	-0.831076000	-0.117126000
6	-1.251646000	2.691349000	-0.124922000
6	-2.564807000	3.286894000	-0.346267000
1	-2.766439000	4.338199000	-0.485793000
6	-3.446616000	2.259915000	-0.378974000
1	-4.511878000	2.306297000	-0.547959000
6	-2.667651000	1.043169000	-0.173497000
6	-3.248982000	-0.243058000	-0.121379000
6	-2.532688000	-1.450714000	-0.038328000

6	-3.078529000	-2.767698000	0.108968000
1	-4.131357000	-2.986560000	0.194839000
6	-2.039930000	-3.660230000	0.139020000
1	-2.097255000	-4.731616000	0.249933000
6	-0.817115000	-2.924746000	0.011440000
6	0.489519000	-3.451255000	-0.023547000
7	1.758541000	-1.324491000	-0.007412000
7	1.588431000	1.604855000	-0.033731000
1	0.929534000	0.836778000	-0.097436000
6	1.675404000	-2.686617000	-0.082883000
6	2.997428000	-3.283072000	-0.249420000
1	3.204063000	-4.335491000	-0.372250000
6	3.879335000	-2.256966000	-0.254471000
1	4.950878000	-2.301477000	-0.376012000
6	3.091641000	-1.039011000	-0.086532000
6	3.670222000	0.249540000	-0.012231000
6	2.952630000	1.458386000	0.054223000
6	3.493877000	2.774080000	0.230350000
1	4.542832000	2.992234000	0.355034000
6	2.455148000	3.665569000	0.233959000
1	2.509215000	4.735725000	0.357203000
6	1.236255000	2.931824000	0.057680000
6	-0.066024000	3.457509000	-0.020827000
6	5.150147000	0.340451000	0.011799000
6	6.015604000	-0.130595000	0.969171000
16	6.055139000	1.062653000	-1.310433000
6	7.390891000	0.089699000	0.660645000
1	5.666705000	-0.614489000	1.874144000
6	7.569146000	0.723111000	-0.538130000
1	8.209066000	-0.206697000	1.307020000
1	8.496464000	1.014515000	-1.011755000
6	0.594819000	-4.930572000	-0.001055000
6	0.163224000	-5.832004000	-0.944134000
16	1.283664000	-5.782846000	1.371603000
6	0.389392000	-7.193922000	-0.584476000
1	-0.291384000	-5.519167000	-1.877210000
6	0.985664000	-7.324984000	0.639289000
1	0.124728000	-8.036120000	-1.213561000
1	1.273190000	-8.232913000	1.151319000
6	-0.173107000	4.936213000	0.001318000
6	0.309171000	5.840442000	-0.914457000
16	-0.935364000	5.784801000	1.337100000
6	0.064172000	7.201229000	-0.563558000
1	0.813653000	5.529855000	-1.822266000
6	-0.597443000	7.328865000	0.626551000
1	0.362796000	8.045155000	-1.174852000
1	-0.911577000	8.235398000	1.125250000
6	-4.740217000	-0.350095000	-0.147698000
6	-5.405627000	-1.002396000	-1.200581000
6	-5.521429000	0.195416000	0.881848000
6	-6.792095000	-1.107741000	-1.229553000

1	-4.823555000	-1.422630000	-2.015059000
6	-6.911287000	0.094288000	0.866509000
1	-5.032378000	0.697733000	1.710516000
6	-7.552450000	-0.558664000	-0.191246000
1	-7.496230000	0.518104000	1.680168000
1	-7.302082000	-1.603728000	-2.048558000
8	-8.909417000	-0.691094000	-0.265929000
1	-9.312192000	-0.268675000	0.504168000

Porphyrin 2

7	1.157818000	1.188479000	-0.211732000
7	0.709101000	-1.717842000	-0.189533000
1	0.121835000	-0.891429000	-0.211521000
6	1.200930000	2.548403000	-0.323039000
6	2.561661000	3.011209000	-0.575629000
1	2.858834000	4.036461000	-0.734862000
6	3.342452000	1.905801000	-0.586540000
1	4.406646000	1.853177000	-0.761412000
6	2.452935000	0.772666000	-0.347515000
6	2.904199000	-0.562800000	-0.285221000
6	2.084358000	-1.699678000	-0.177687000
6	2.507650000	-3.062259000	-0.039938000
1	3.535390000	-3.383671000	0.027764000
6	1.390535000	-3.853277000	0.011120000
1	1.353925000	-4.924989000	0.126966000
6	0.239979000	-3.006237000	-0.090733000
6	-1.110329000	-3.406330000	-0.090238000
7	-2.162174000	-1.167570000	0.021013000
7	-1.717997000	1.736426000	-0.052600000
1	-1.138968000	0.909111000	-0.143551000
6	-2.218704000	-2.529159000	-0.085372000
6	-3.600381000	-2.989933000	-0.183177000
1	-3.914604000	-4.014329000	-0.312408000
6	-4.375505000	-1.883733000	-0.104219000
1	-5.451666000	-1.823102000	-0.162435000
6	-3.462862000	-0.752808000	0.034853000
6	-3.908788000	0.584283000	0.152930000
6	-3.078731000	1.720820000	0.145315000
6	-3.481324000	3.085392000	0.323248000
1	-4.493727000	3.401070000	0.519891000
6	-2.369107000	3.875359000	0.213858000
1	-2.317158000	4.948409000	0.310597000
6	-1.240301000	3.025709000	-0.029809000
6	0.097582000	3.425756000	-0.200065000
6	-5.362741000	0.840555000	0.289649000
6	-6.196003000	1.515347000	-0.570185000
16	-6.256213000	0.325354000	1.710957000
6	-7.541928000	1.612760000	-0.107914000
1	-5.849459000	1.916332000	-1.515836000
6	-7.726214000	1.018240000	1.109949000

1	-8.336590000	2.098940000	-0.662087000
1	-8.637102000	0.941091000	1.687430000
6	-1.382977000	-4.863454000	-0.078027000
6	-2.008027000	-5.602412000	0.897267000
16	-0.962133000	-5.896458000	-1.435998000
6	-2.142956000	-6.984979000	0.573504000
1	-2.350591000	-5.160744000	1.825912000
6	-1.625689000	-7.293568000	-0.654224000
1	-2.600760000	-7.716240000	1.229705000
1	-1.591626000	-8.256245000	-1.145386000
6	0.366911000	4.883459000	-0.234602000
6	1.092374000	5.636835000	0.656331000
16	-0.205337000	5.896654000	-1.551258000
6	1.185812000	7.015244000	0.301059000
1	1.536621000	5.209302000	1.547831000
6	0.535598000	7.305745000	-0.866362000
1	1.710567000	7.756280000	0.893005000
1	0.444237000	8.261563000	-1.363551000
6	4.379844000	-0.810154000	-0.341282000
6	5.217328000	-0.349771000	0.683144000
6	4.957328000	-1.505587000	-1.417370000
6	6.586366000	-0.591512000	0.606253000
1	4.817979000	0.185207000	1.535194000
6	6.332958000	-1.737441000	-1.473898000
1	4.317254000	-1.857167000	-2.220343000
6	7.166687000	-1.280096000	-0.456623000
1	6.756984000	-2.271295000	-2.318319000
1	8.236918000	-1.441128000	-0.469686000
7	7.453754000	-0.104122000	1.693881000
8	6.921749000	0.502047000	2.622882000
8	8.660119000	-0.332468000	1.606845000

Porphyrin 3

7	0.454073000	1.414316000	-0.005438000
7	0.406495000	-1.524694000	0.056741000
1	-0.286384000	-0.789260000	-0.027632000
6	0.319504000	2.764733000	-0.149517000
6	1.619490000	3.406661000	-0.316854000
1	1.784352000	4.460816000	-0.480425000
6	2.542249000	2.418592000	-0.246878000
1	3.614298000	2.501950000	-0.343026000
6	1.801238000	1.178026000	-0.041982000
6	2.429394000	-0.079628000	0.082182000
6	1.763090000	-1.315326000	0.160549000
6	2.358973000	-2.603261000	0.359864000
1	3.415550000	-2.771656000	0.497691000
6	1.360356000	-3.540859000	0.356411000
1	1.462597000	-4.605516000	0.496320000
6	0.113874000	-2.863240000	0.157641000
6	-1.166357000	-3.447236000	0.083285000

7	-2.520764000	-1.374598000	0.058848000
7	-2.473282000	1.561471000	-0.064601000
1	-1.779762000	0.821910000	-0.079992000
6	-2.382473000	-2.733479000	-0.005344000
6	-3.678977000	-3.383816000	-0.170906000
1	-3.841275000	-4.445031000	-0.282325000
6	-4.601792000	-2.394172000	-0.178207000
1	-5.670270000	-2.484678000	-0.302913000
6	-3.863596000	-1.144224000	-0.023814000
6	-4.495147000	0.120643000	0.015182000
6	-3.830699000	1.360789000	0.026892000
6	-4.430062000	2.660038000	0.120027000
1	-5.489355000	2.835760000	0.222010000
6	-3.431514000	3.594697000	0.068899000
1	-3.535786000	4.666782000	0.127077000
6	-2.180249000	2.905421000	-0.053221000
6	-0.900658000	3.482664000	-0.134414000
6	-5.977284000	0.175355000	0.036947000
6	-6.828095000	0.681472000	-0.915953000
16	-6.896813000	-0.392102000	1.421525000
6	-8.206220000	0.608033000	-0.554016000
1	-6.469090000	1.082145000	-1.857114000
6	-8.399154000	0.052790000	0.680793000
1	-9.015892000	0.948330000	-1.189402000
1	-9.332131000	-0.126760000	1.197014000
6	-1.234727000	-4.927955000	0.115514000
6	-1.806429000	-5.733242000	1.070586000
16	-0.596001000	-5.911726000	-1.193316000
6	-1.728789000	-7.125861000	0.771059000
1	-2.261352000	-5.330326000	1.968123000
6	-1.102975000	-7.376884000	-0.418635000
1	-2.117921000	-7.904382000	1.417228000
1	-0.905554000	-8.332465000	-0.884506000
6	-0.831347000	4.963080000	-0.193791000
6	-0.298605000	5.828575000	0.730427000
16	-1.415755000	5.859964000	-1.587291000
6	-0.363493000	7.199292000	0.340059000
1	0.119394000	5.484250000	1.669379000
6	-0.940555000	7.372719000	-0.887534000
1	-0.000873000	8.018349000	0.950592000
1	-1.118689000	8.296302000	-1.420820000
6	3.926481000	-0.123439000	0.134198000
6	4.604660000	0.440101000	1.222894000
6	4.648167000	-0.728236000	-0.903618000
6	6.003557000	0.395905000	1.276853000
1	4.032576000	0.901035000	2.017507000
6	6.046954000	-0.771821000	-0.851781000
1	4.111379000	-1.144264000	-1.746320000
6	6.732235000	-0.222635000	0.245923000
8	8.095447000	-0.334253000	0.337384000
6	8.821411000	0.729668000	-0.280419000

1	9.879933000	0.507807000	-0.129192000
1	8.612514000	0.779237000	-1.355524000
1	8.584418000	1.693395000	0.186183000
8	6.839401000	-1.320450000	-1.816253000
8	6.754560000	0.918685000	2.287114000
6	6.078283000	1.535100000	3.372422000
1	5.486013000	2.398980000	3.044747000
1	5.421257000	0.828082000	3.894075000
1	6.857952000	1.872256000	4.056829000
6	6.209578000	-1.929802000	-2.933100000
1	5.558425000	-2.758334000	-2.627744000
1	5.621349000	-1.207561000	-3.513415000
1	7.016737000	-2.318118000	-3.555702000

Porphyrin 4

7	0.860569000	1.252012000	-0.149631000
7	0.536129000	-1.666219000	-0.143542000
1	-0.082750000	-0.864130000	-0.184448000
6	0.846470000	2.611298000	-0.270816000
6	2.189631000	3.130899000	-0.505296000
1	2.443814000	4.167122000	-0.669388000
6	3.017482000	2.059613000	-0.497005000
1	4.085125000	2.044977000	-0.656736000
6	2.175123000	0.890787000	-0.263450000
6	2.687545000	-0.422747000	-0.186691000
6	1.909777000	-1.590941000	-0.096227000
6	2.385343000	-2.934075000	0.055850000
1	3.425025000	-3.207340000	0.145223000
6	1.300961000	-3.770685000	0.079402000
1	1.305380000	-4.842986000	0.195787000
6	0.118866000	-2.972150000	-0.052713000
6	-1.213960000	-3.428980000	-0.079174000
7	-2.364384000	-1.238284000	0.014684000
7	-2.042705000	1.677745000	-0.048288000
1	-1.429404000	0.873508000	-0.120791000
6	-2.359023000	-2.601269000	-0.093208000
6	-3.717852000	-3.121467000	-0.213553000
1	-3.985099000	-4.158480000	-0.348027000
6	-4.541741000	-2.050133000	-0.146882000
1	-5.618581000	-2.036324000	-0.221714000
6	-3.681712000	-0.880532000	0.006301000
6	-4.186905000	0.436229000	0.113421000
6	-3.405821000	1.606715000	0.118491000
6	-3.868724000	2.954505000	0.275954000
1	-4.898065000	3.228810000	0.445236000
6	-2.788079000	3.789510000	0.184200000
1	-2.783376000	4.864717000	0.271062000
6	-1.619236000	2.986419000	-0.027101000
6	-0.296772000	3.440647000	-0.174203000
6	-5.653298000	0.630164000	0.218802000

6	-6.498632000	1.255985000	-0.665584000
16	-6.551746000	0.092734000	1.629043000
6	-7.856905000	1.298302000	-0.231255000
1	-6.150984000	1.660894000	-1.609169000
6	-8.039437000	0.710435000	0.990020000
1	-8.661112000	1.741290000	-0.807538000
1	-8.957842000	0.598261000	1.549591000
6	-1.423432000	-4.896659000	-0.074279000
6	-2.033922000	-5.665413000	0.887118000
16	-0.931432000	-5.906616000	-1.425737000
6	-2.101844000	-7.051728000	0.558132000
1	-2.413603000	-5.241571000	1.809630000
6	-1.547646000	-7.333880000	-0.659860000
1	-2.539639000	-7.804229000	1.203992000
1	-1.461172000	-8.292941000	-1.151683000
6	-0.089875000	4.908758000	-0.216142000
6	0.573318000	5.702527000	0.687841000
16	-0.664591000	5.883231000	-1.560639000
6	0.616627000	7.080572000	0.320994000
1	1.008136000	5.303017000	1.596823000
6	-0.009566000	7.330904000	-0.868699000
1	1.088899000	7.850111000	0.920906000
1	-0.128583000	8.277226000	-1.378074000
6	4.173107000	-0.606672000	-0.203195000
6	4.955086000	-0.095340000	0.848684000
6	4.808042000	-1.287027000	-1.247581000
6	6.341641000	-0.257351000	0.861684000
1	4.456425000	0.414059000	1.663780000
6	6.196276000	-1.436830000	-1.246464000
1	4.220510000	-1.680866000	-2.070202000
6	6.973620000	-0.930360000	-0.209648000
8	8.325796000	-1.164048000	-0.221589000
6	9.163804000	-0.011655000	-0.347877000
1	10.187793000	-0.387310000	-0.395541000
1	8.937705000	0.536055000	-1.271878000
1	9.059116000	0.658531000	0.509759000
8	7.161558000	0.180443000	1.862717000
6	6.570731000	0.828231000	2.980279000
1	6.052568000	1.750312000	2.688335000
1	5.864643000	0.169383000	3.500442000
1	7.393809000	1.075050000	3.652125000
1	6.705031000	-1.954328000	-2.053370000

Porphyrin 5

7	1.782387000	-1.022932000	-0.068646000
7	1.057127000	1.827232000	-0.041099000
1	0.554403000	0.948871000	0.022917000
6	1.964969000	-2.372311000	0.029381000
6	3.381268000	-2.702587000	0.150895000
1	3.788032000	-3.694914000	0.272736000

6	4.050801000	-1.527542000	0.098916000
1	5.116327000	-1.370376000	0.174851000
6	3.038900000	-0.484882000	-0.047851000
6	3.353992000	0.888190000	-0.132283000
6	2.423173000	1.941412000	-0.156893000
6	2.702959000	3.339021000	-0.310681000
1	3.688337000	3.756580000	-0.447096000
6	1.514804000	4.018895000	-0.270390000
1	1.367091000	5.082625000	-0.370726000
6	0.461200000	3.064747000	-0.092214000
6	-0.917601000	3.334069000	0.007305000
7	-1.756038000	1.004604000	-0.022261000
7	-1.030171000	-1.843755000	0.015682000
1	-0.525948000	-0.964577000	0.046869000
6	-1.935003000	2.355771000	0.080578000
6	-3.344590000	2.684181000	0.272590000
1	-3.745863000	3.675887000	0.415167000
6	-4.013504000	1.508164000	0.257176000
1	-5.072286000	1.345313000	0.390837000
6	-3.008271000	0.467532000	0.062925000
6	-3.330782000	-0.907511000	-0.004864000
6	-2.398437000	-1.959959000	-0.056065000
6	-2.683920000	-3.359757000	-0.179028000
1	-3.675963000	-3.772430000	-0.273503000
6	-1.496070000	-4.039428000	-0.165613000
1	-1.350521000	-5.104732000	-0.252794000
6	-0.435928000	-3.082643000	-0.038341000
6	0.943759000	-3.351276000	0.007727000
6	-4.760394000	-1.303362000	-0.015382000
6	-5.458135000	-2.010067000	0.934217000
16	-5.803343000	-0.940200000	-1.380642000
6	-6.819814000	-2.252973000	0.584443000
1	-5.004829000	-2.332529000	1.864662000
6	-7.151395000	-1.736441000	-0.637621000
1	-7.520271000	-2.783790000	1.218945000
1	-8.106465000	-1.770544000	-1.143451000
6	-1.327715000	4.758975000	0.021393000
6	-2.080535000	5.435999000	-0.907368000
16	-0.923268000	5.825310000	1.358210000
6	-2.327008000	6.798701000	-0.565046000
1	-2.437657000	4.964769000	-1.815818000
6	-1.765858000	7.153432000	0.630498000
1	-2.893266000	7.483624000	-1.185688000
1	-1.792769000	8.114228000	1.125772000
6	1.353226000	-4.777005000	0.017748000
6	2.039844000	-5.472484000	-0.947555000
16	1.036857000	-5.818225000	1.397025000
6	2.306009000	-6.830005000	-0.598513000
1	2.335592000	-5.018753000	-1.886497000
6	1.825804000	-7.161861000	0.638066000
1	2.827958000	-7.527500000	-1.243539000

1	1.884177000	-8.113904000	1.147336000
6	4.797528000	1.274830000	-0.202019000
6	5.602262000	0.900525000	-1.287294000
6	5.408212000	2.028055000	0.810505000
6	6.942138000	1.286523000	-1.307731000
1	5.185325000	0.322926000	-2.105752000
6	6.757564000	2.361007000	0.693366000
1	4.841125000	2.339658000	1.681686000
1	7.243777000	2.940644000	1.476147000
1	7.575568000	1.005186000	-2.147203000
7	7.528617000	2.005701000	-0.342135000

Cartesian coordinates of B3LYP/6-31G(d,p) optimized excited-state geometries

Porphyrin 1

7	-1.401584000	1.280958000	-0.067859000
7	-1.101139000	-1.662711000	-0.092261000
1	-0.471900000	-0.876898000	-0.202743000
6	-1.359947000	2.637397000	-0.248224000
6	-2.652123000	3.146997000	-0.659699000
1	-2.877862000	4.167889000	-0.926570000
6	-3.495358000	2.076004000	-0.685758000
1	-4.536466000	2.063683000	-0.970918000
6	-2.707758000	0.926359000	-0.291379000
6	-3.240129000	-0.386207000	-0.128067000
6	-2.470834000	-1.553697000	0.044644000
6	-2.947391000	-2.863235000	0.378444000
1	-3.977485000	-3.105268000	0.588221000
6	-1.874197000	-3.715877000	0.414917000
1	-1.883748000	-4.765742000	0.660452000
6	-0.693934000	-2.965291000	0.099809000
6	0.625007000	-3.452536000	-0.027693000
7	1.825621000	-1.279672000	-0.014529000
7	1.526463000	1.665033000	-0.060952000
1	0.904876000	0.880969000	-0.216825000
6	1.784676000	-2.636306000	-0.201699000
6	3.085236000	-3.146599000	-0.584603000
1	3.315094000	-4.167119000	-0.849424000
6	3.930509000	-2.077512000	-0.590268000
1	4.976728000	-2.065764000	-0.853912000
6	3.136722000	-0.928235000	-0.208048000
6	3.664152000	0.387425000	-0.022228000
6	2.887260000	1.555934000	0.137257000
6	3.344787000	2.857737000	0.520712000
1	4.360121000	3.097866000	0.792274000
6	2.269037000	3.708376000	0.523083000
1	2.265157000	4.752299000	0.792708000
6	1.107276000	2.963932000	0.138432000

6	-0.206153000	3.452972000	-0.033416000
6	5.126440000	0.525787000	0.010467000
6	6.034570000	-0.209307000	0.745452000
16	5.989097000	1.671443000	-1.016065000
6	7.390809000	0.144707000	0.509221000
1	5.721492000	-0.970438000	1.449902000
6	7.524665000	1.141863000	-0.420779000
1	8.231407000	-0.317788000	1.013657000
1	8.433929000	1.598965000	-0.786252000
6	0.786533000	-4.912241000	0.013347000
6	0.102525000	-5.871797000	-0.706137000
16	1.912124000	-5.695591000	1.121044000
6	0.472585000	-7.207346000	-0.386819000
1	-0.626584000	-5.611638000	-1.464275000
6	1.434557000	-7.270891000	0.585896000
1	0.049357000	-8.082066000	-0.867165000
1	1.897337000	-8.150251000	1.012472000
6	-0.366293000	4.912011000	0.012839000
6	0.354235000	5.874638000	-0.666370000
16	-1.537699000	5.691567000	1.075128000
6	-0.024072000	7.208929000	-0.352653000
1	1.116306000	5.617404000	-1.392378000
6	-1.028806000	7.268835000	0.576195000
1	0.424467000	8.085624000	-0.805609000
1	-1.506427000	8.146773000	0.989132000
6	-4.717190000	-0.545298000	-0.133773000
6	-5.358491000	-1.449343000	-1.003792000
6	-5.528214000	0.206973000	0.735209000
6	-6.739878000	-1.600063000	-1.009114000
1	-4.759143000	-2.025905000	-1.700944000
6	-6.911527000	0.057902000	0.746152000
1	-5.062485000	0.905169000	1.422704000
6	-7.524867000	-0.846721000	-0.128668000
1	-7.515614000	0.639521000	1.439405000
1	-7.228554000	-2.286749000	-1.692108000
8	-8.875174000	-1.034647000	-0.169972000
1	-9.296999000	-0.454984000	0.478147000

Porphyrin 2

7	1.229282000	1.119612000	-0.229175000
7	0.604078000	-1.790094000	-0.181298000
1	0.052512000	-0.944956000	-0.269462000
6	1.345969000	2.469059000	-0.425494000
6	2.684777000	2.818914000	-0.859957000
1	3.024619000	3.805333000	-1.134428000
6	3.395658000	1.657667000	-0.881952000
1	4.425225000	1.521488000	-1.176927000
6	2.481459000	0.612110000	-0.465918000
6	2.859921000	-0.747417000	-0.295401000

6	1.979821000	-1.827305000	-0.095529000
6	2.329507000	-3.182891000	0.210099000
1	3.335641000	-3.535670000	0.374670000
6	1.174379000	-3.918816000	0.280401000
1	1.088188000	-4.966592000	0.518739000
6	0.070595000	-3.045202000	0.014548000
6	-1.299443000	-3.384061000	-0.063356000
7	-2.235144000	-1.086888000	0.021231000
7	-1.612745000	1.823043000	-0.089498000
1	-1.081410000	0.979007000	-0.264717000
6	-2.363995000	-2.438551000	-0.174886000
6	-3.734992000	-2.789351000	-0.484798000
1	-4.095213000	-3.774289000	-0.738191000
6	-4.447983000	-1.630214000	-0.432709000
1	-5.497797000	-1.494956000	-0.641882000
6	-3.503131000	-0.584755000	-0.092545000
6	-3.867292000	0.781640000	0.114919000
6	-2.960556000	1.861139000	0.200752000
6	-3.254901000	3.211854000	0.575886000
1	-4.220943000	3.558454000	0.906012000
6	-2.101074000	3.946380000	0.478515000
1	-1.974925000	4.989440000	0.720058000
6	-1.050949000	3.074921000	0.044446000
6	0.298230000	3.414909000	-0.200682000
6	-5.290017000	1.121118000	0.246233000
6	-5.999775000	2.105381000	-0.413935000
16	-6.342937000	0.304792000	1.399663000
6	-7.360295000	2.202431000	-0.013922000
1	-5.551551000	2.718587000	-1.186590000
6	-7.689480000	1.299242000	0.962173000
1	-8.065943000	2.906492000	-0.439487000
1	-8.646698000	1.154869000	1.444174000
6	-1.663399000	-4.806304000	-0.027452000
6	-2.619564000	-5.416842000	0.759466000
16	-0.942979000	-5.996430000	-1.110773000
6	-2.763456000	-6.809657000	0.516800000
1	-3.184439000	-4.870723000	1.505281000
6	-1.928587000	-7.265093000	-0.469540000
1	-3.453732000	-7.447821000	1.056238000
1	-1.831635000	-8.271421000	-0.853182000
6	0.657110000	4.838542000	-0.216732000
6	1.692129000	5.464157000	0.449451000
16	-0.195043000	6.012475000	-1.219418000
6	1.793907000	6.855692000	0.179821000
1	2.344112000	4.930990000	1.130848000
6	0.846137000	7.294940000	-0.707089000
1	2.536427000	7.504241000	0.630093000
1	0.697315000	8.296698000	-1.086059000
6	4.315522000	-1.064703000	-0.329133000
6	5.188661000	-0.460635000	0.587128000
6	4.846875000	-1.967817000	-1.268638000

6	6.543997000	-0.777402000	0.552679000
1	4.825363000	0.235619000	1.331731000
6	6.211315000	-2.266112000	-1.288766000
1	4.182533000	-2.426185000	-1.993869000
6	7.077928000	-1.673928000	-0.375242000
1	6.600607000	-2.959524000	-2.027614000
1	8.139701000	-1.883050000	-0.364953000
7	7.440797000	-0.148306000	1.529451000
8	6.948088000	0.637811000	2.342421000
8	8.638594000	-0.440211000	1.476973000

Porphyrin 3

7	0.467771000	1.437497000	-0.037179000
7	0.407381000	-1.527683000	0.049583000
1	-0.282705000	-0.803440000	-0.107293000
6	0.327999000	2.778531000	-0.280755000
6	1.597780000	3.375302000	-0.644922000
1	1.753880000	4.402212000	-0.937394000
6	2.523443000	2.377880000	-0.576279000
1	3.577852000	2.437873000	-0.799381000
6	1.807946000	1.182198000	-0.177152000
6	2.433615000	-0.077328000	0.053230000
6	1.757215000	-1.299360000	0.231093000
6	2.329853000	-2.555690000	0.615418000
1	3.368280000	-2.702277000	0.867339000
6	1.332470000	-3.496363000	0.631943000
1	1.425482000	-4.534804000	0.906312000
6	0.105839000	-2.856201000	0.256888000
6	-1.163510000	-3.455207000	0.102577000
7	-2.532393000	-1.384970000	0.057821000
7	-2.473044000	1.578671000	-0.100078000
1	-1.782979000	0.844989000	-0.204915000
6	-2.382222000	-2.738019000	-0.106313000
6	-3.635474000	-3.356123000	-0.487901000
1	-3.779687000	-4.397309000	-0.731790000
6	-4.563552000	-2.358504000	-0.511781000
1	-5.604287000	-2.435909000	-0.786104000
6	-3.865009000	-1.143152000	-0.146992000
6	-4.497698000	0.130380000	-0.003961000
6	-3.821673000	1.365423000	0.100948000
6	-4.391554000	2.644264000	0.403010000
1	-5.427110000	2.808676000	0.654221000
6	-3.393476000	3.583262000	0.350703000
1	-3.484689000	4.637751000	0.555864000

6	-2.168713000	2.918206000	0.019652000
6	-0.896259000	3.505298000	-0.155510000
6	-5.964904000	0.189743000	0.030953000
6	-6.808073000	1.001391000	-0.702259000
16	-6.912079000	-0.791831000	1.147067000
6	-8.184951000	0.839236000	-0.386626000
1	-6.438178000	1.673802000	-1.467090000
6	-8.395564000	-0.089824000	0.597579000
1	-8.984586000	1.382312000	-0.877114000
1	-9.335905000	-0.409803000	1.025128000
6	-1.247459000	-4.920974000	0.161608000
6	-2.112610000	-5.693244000	0.909649000
16	-0.246801000	-5.966721000	-0.846517000
6	-1.969520000	-7.091957000	0.698620000
1	-2.817746000	-5.254706000	1.605406000
6	-1.003805000	-7.393370000	-0.224932000
1	-2.554929000	-7.842893000	1.216698000
1	-0.688685000	-8.368119000	-0.571073000
6	-0.819641000	4.972316000	-0.202716000
6	0.014413000	5.807012000	0.512567000
16	-1.796165000	5.929165000	-1.316651000
6	-0.133149000	7.184674000	0.193064000
1	0.699191000	5.429169000	1.262174000
6	-1.071236000	7.406018000	-0.780307000
1	0.428830000	7.978499000	0.671694000
1	-1.382507000	8.348884000	-1.208522000
6	3.921386000	-0.117687000	0.108529000
6	4.613038000	0.695090000	1.021084000
6	4.641351000	-0.963912000	-0.750468000
6	6.008666000	0.650133000	1.084654000
1	4.048444000	1.337164000	1.683800000
6	6.039435000	-0.996549000	-0.701175000
1	4.100383000	-1.564774000	-1.469251000
6	6.733326000	-0.200461000	0.228147000
8	8.094590000	-0.303186000	0.325956000
6	8.827207000	0.741202000	-0.319345000
1	9.883792000	0.513481000	-0.164590000
1	8.616250000	0.762486000	-1.395430000
1	8.597901000	1.717401000	0.121620000
8	6.822951000	-1.759776000	-1.513366000
8	6.766896000	1.385779000	1.947473000
6	6.098478000	2.243085000	2.861546000
1	5.513740000	3.013341000	2.343205000
1	5.436190000	1.680408000	3.530891000

1	6.882767000	2.720940000	3.450091000
6	6.183072000	-2.605368000	-2.457111000
1	5.532425000	-3.340566000	-1.967230000
1	5.592070000	-2.031816000	-3.182470000
1	6.984855000	-3.128024000	-2.980467000

Porphyrin 4

7	0.906080000	1.229216000	-0.142822000
7	0.489590000	-1.708042000	-0.120443000
1	-0.110983000	-0.899944000	-0.228498000
6	0.920734000	2.582317000	-0.358152000
6	2.239163000	3.029691000	-0.760671000
1	2.507695000	4.036239000	-1.041963000
6	3.039277000	1.926790000	-0.744408000
1	4.083914000	1.865002000	-1.009475000
6	2.199006000	0.817317000	-0.339620000
6	2.675541000	-0.514317000	-0.160776000
6	1.863220000	-1.651169000	0.010531000
6	2.292512000	-2.980133000	0.331801000
1	3.314101000	-3.261647000	0.532936000
6	1.189032000	-3.793308000	0.361850000
1	1.165758000	-4.844817000	0.598671000
6	0.035969000	-2.996484000	0.060261000
6	-1.302574000	-3.432250000	-0.052225000
7	-2.410325000	-1.211936000	0.018237000
7	-1.997606000	1.724498000	-0.079334000
1	-1.409612000	0.913890000	-0.229882000
6	-2.433412000	-2.568098000	-0.182900000
6	-3.769206000	-3.019994000	-0.514824000
1	-4.050451000	-4.028976000	-0.773817000
6	-4.569316000	-1.917900000	-0.470340000
1	-5.623552000	-1.862404000	-0.693672000
6	-3.711799000	-0.805730000	-0.115447000
6	-4.177641000	0.530814000	0.081874000
6	-3.352489000	1.672412000	0.177497000
6	-3.748873000	3.004248000	0.524445000
1	-4.745020000	3.287724000	0.824102000
6	-2.646973000	3.816329000	0.441307000
1	-2.600305000	4.869816000	0.665839000
6	-1.527261000	3.014488000	0.046817000
6	-0.201363000	3.447603000	-0.173510000
6	-5.623936000	0.766394000	0.185270000
6	-6.393038000	1.688885000	-0.496204000
16	-6.633773000	-0.115763000	1.329059000
6	-7.764171000	1.688728000	-0.119642000
1	-5.977755000	2.326606000	-1.267367000
6	-8.043020000	0.772381000	0.859446000
1	-8.512264000	2.334820000	-0.564425000
1	-8.995585000	0.560680000	1.325517000

6	-1.560192000	-4.878913000	-0.031954000
6	-2.475513000	-5.569118000	0.736318000
16	-0.741938000	-5.998925000	-1.121373000
6	-2.512466000	-6.966327000	0.475944000
1	-3.088778000	-5.075695000	1.480730000
6	-1.635271000	-7.346642000	-0.505105000
1	-3.158881000	-7.660543000	1.000566000
1	-1.457378000	-8.338747000	-0.896706000
6	0.048045000	4.895887000	-0.205950000
6	0.999795000	5.614782000	0.487612000
16	-0.845677000	5.978447000	-1.273253000
6	1.006672000	7.004888000	0.188264000
1	1.660269000	5.147349000	1.207985000
6	0.068464000	7.350500000	-0.748055000
1	1.675717000	7.719065000	0.654536000
1	-0.142560000	8.329939000	-1.154770000
6	4.147431000	-0.732407000	-0.159130000
6	4.964617000	-0.023835000	0.744735000
6	4.753566000	-1.635522000	-1.044261000
6	6.345569000	-0.213532000	0.773666000
1	4.493295000	0.657770000	1.441187000
6	6.137482000	-1.808945000	-1.035603000
1	4.144320000	-2.176907000	-1.759621000
6	6.945840000	-1.110907000	-0.142641000
8	8.290478000	-1.374061000	-0.132607000
6	9.159765000	-0.284836000	-0.459482000
1	10.169575000	-0.699401000	-0.467280000
1	8.926150000	0.113766000	-1.454953000
1	9.096815000	0.516853000	0.280478000
8	7.190403000	0.399492000	1.654678000
6	6.630334000	1.274309000	2.624175000
1	6.129849000	2.131326000	2.156427000
1	5.916144000	0.751085000	3.271554000
1	7.468296000	1.629699000	3.225149000
1	6.621096000	-2.492667000	-1.725685000

Porphyrin 5

7	-0.553465000	2.007390000	0.032811000
7	2.036473000	0.551798000	0.030273000
1	1.067248000	0.286114000	-0.095943000
6	-1.806619000	2.527320000	-0.151716000
6	-1.741677000	3.941091000	-0.468139000
1	-2.579995000	4.575270000	-0.711354000
6	-0.423923000	4.282730000	-0.427572000
1	0.012307000	5.249570000	-0.629045000
6	0.301747000	3.072342000	-0.095719000
6	1.711488000	3.018528000	0.091731000
6	2.478926000	1.845513000	0.214499000

6	3.873359000	1.753373000	0.535166000
1	4.507039000	2.593884000	0.771027000
6	4.232281000	0.430316000	0.514947000
1	5.204060000	0.020227000	0.737572000
6	3.074682000	-0.343219000	0.175891000
6	2.997545000	-1.742008000	-0.005517000
7	0.525502000	-1.967495000	0.014996000
7	-2.066335000	-0.511578000	-0.044704000
1	-1.098916000	-0.245364000	-0.180606000
6	1.783829000	-2.472504000	-0.192755000
6	1.724484000	-3.860473000	-0.603139000
1	2.566063000	-4.474971000	-0.882870000
6	0.406420000	-4.204419000	-0.601813000
1	-0.025877000	-5.151040000	-0.886936000
6	-0.323685000	-3.021386000	-0.191787000
6	-1.740998000	-2.981511000	-0.010843000
6	-2.507407000	-1.805214000	0.141565000
6	-3.894300000	-1.712729000	0.488841000
1	-4.518974000	-2.554047000	0.742532000
6	-4.253236000	-0.389375000	0.477185000
1	-5.219067000	0.021739000	0.723145000
6	-3.100123000	0.385070000	0.127747000
6	-3.022263000	1.788051000	-0.013077000
6	-2.485365000	-4.247234000	0.015507000
6	-3.620873000	-4.588931000	-0.692815000
16	-2.037591000	-5.571242000	1.089402000
6	-4.121487000	-5.884951000	-0.391298000
1	-4.060063000	-3.927715000	-1.430310000
6	-3.374772000	-6.532231000	0.557284000
1	-4.992889000	-6.320846000	-0.866155000
1	-3.526779000	-7.521102000	0.967714000
6	4.250375000	-2.509446000	-0.004411000
6	4.543419000	-3.653380000	0.710389000
16	5.612247000	-2.100420000	-1.047146000
6	5.835307000	-4.184283000	0.446588000
1	3.845712000	-4.082277000	1.419571000
6	6.527908000	-3.456079000	-0.484564000
1	6.235570000	-5.066517000	0.932684000
1	7.523119000	-3.633439000	-0.868433000
6	-4.279495000	2.548332000	-0.005513000
6	-4.599383000	3.662130000	0.744262000
16	-5.616884000	2.161667000	-1.087666000
6	-5.891873000	4.188576000	0.474019000
1	-3.921580000	4.071765000	1.483453000

6	-6.558236000	3.486777000	-0.495839000
1	-6.311259000	5.048705000	0.983096000
1	-7.547529000	3.668036000	-0.892955000
6	2.448105000	4.311015000	0.164855000
6	2.117330000	5.289071000	1.116683000
6	3.502164000	4.615102000	-0.711261000
6	2.838007000	6.481158000	1.149970000
1	1.316470000	5.112823000	1.826757000
6	4.154580000	5.841969000	-0.596429000
1	3.795533000	3.910149000	-1.481974000
1	2.595535000	7.241042000	1.890837000
1	4.967280000	6.089736000	-1.277160000
7	3.844282000	6.773259000	0.314388000