Table 1. Optimized cartesian coordinates (Å) of the 16 molecules studied in their singlet ground state.

1p PORPHYRIN

C1	0.12116	−0.49995	−2.15925
C2	−2.13899	−0.63092	−1.9861
C3	−1.58707	−0.3779	−0.68668
N4	−0.22609	−0.3085	−0.84582
C5	−1.10145	−0.7049	−2.88038
C6	−2.50636	0.16055	2.99291
C7	−1.70994	0.01903	1.77794
C8	−1.62513	0.38996	3.99733
C9	−0.30067	0.3859	3.38397
N10	−0.38013	0.15899	2.0422
C11	4.80781	−0.0709	−1.54755
C12	4.01124	0.07671	−0.33353
C13	3.9265	−0.30031	−2.55201
C14	2.60162	−0.29015	−1.93938
N15	2.68106	−0.06086	−0.59798
C16	4.43893	0.7334	3.42924
C17	3.88717	0.47903	2.13015
N18	2.52636	0.40802	2.28982
C19	2.17923	0.60129	3.60308
C20	3.40185	0.80764	4.32384
C21	1.4204	−0.49214	−2.66188
H22	−3.35041	−0.31406	0.46733
C23	−2.26879	−0.2281	0.51899
H24	0.78289	0.76005	5.1745
C25	0.88032	0.59077	4.10591
H26	5.65098	0.41179	0.97759
C27	4.56929	0.32661	0.92521
H28	1.86561	0.23715	1.53771
H29	0.4349	−0.13738	−0.09394
H30	1.51801	−0.66235	−3.73031
H31	4.13025	−0.46189	−3.60363
H32	5.8876	−0.00485	−1.60027
H33	5.49601	0.84182	3.6318
H34	3.459	0.9877	5.38923
H35	−1.82847	0.54758	5.04965
H36	−3.58581	0.09051	3.04623
H37	−3.19623	−0.7393	−2.1891
H38	−1.15752	−0.88453	−3.94575

1c CHLORIN

C1	3.01276	0.92133	−0.02711
C2	4.31374	−0.93569	−0.01827
C3	2.93794	−1.3372	−0.00066
N4	2.19593	−0.1905	−0.00789
C5	4.3578	0.43623	−0.0344
C6	0.7572	−4.5529	0.09079
C7	1.12903	−3.07413	0.03362
C8	−0.77436	−4.5165	−0.03395
C9	−1.07285	−3.02046	0.00043
N10	0.04699	−2.27115	0.01258
C11	−0.48084	4.1286	−0.00387
C12	−0.91822	2.74331	0.00248
C13	0.87846	4.09543	−0.01831
C14	1.24799	2.69038	−0.01968
N15	0.14483	1.89288	−0.00585
C16	−4.13088	0.64013	0.01433
C17	−2.7647	1.06119	0.01288
N18	−2.00078	−0.0878	0.00673
C19	−2.79585	−1.19822	0.0057
C20	−4.15111	−0.73227	0.00933
C21	2.57571	2.23786	−0.03195
H22	3.21269	−3.42381	0.03514
C23	2.45013	−2.65014	0.024
H24	−3.17069	−3.2692	−0.01161
C25	−2.37177	−2.53315	−0.00054
H26	−3.00686	3.15024	0.01718
C27	−2.26612	2.35547	0.01206
H28	−0.98704	−0.08326	0.00845
H29	1.18349	−0.13983	−0.00178
H30	3.35334	2.9965	−0.04459
H31	1.56992	4.92979	−0.02706
H32	−1.13108	4.99553	0.00119
H33	−4.97754	1.314	0.01767
H34	−5.01706	−1.38077	0.00795
H35	−1.12505	−4.95173	−0.97774
H36	1.24331	−5.12434	−0.70634
H37	5.14897	−1.62375	−0.01786
H38	5.2356	1.06935	−0.04943
H39	−1.28705	−5.05314	0.77226
H40	1.08662	−4.99078	1.041

2p FOTOFRIN PORPHYRIN				**2c FOTOFRIN CHLORIN**			
C1	0.263	2.68638	0.24053	C1	0.27839	2.55647	0.29259
C2	2.53166	2.51107	0.10771	C2	2.54242	2.31916	0.3738
C3	1.94333	1.19385	0.05793	C3	1.9271	1.01555	0.33711
N4	0.58489	1.35879	0.1258	N4	0.57835	1.21078	0.27405
C5	1.50188	3.42423	0.22812	C5	1.52974	3.26195	0.34823
C6	2.80745	-2.54861	-0.15814	C6	2.78925	-2.79908	0.50684
C7	2.02648	-1.30365	-0.11424	C7	2.00884	-1.49224	0.31205
C8	1.89561	-3.55115	-0.32482	C8	1.86663	-3.79587	-0.23788
C9	0.58279	-2.89612	-0.36452	C9	0.53102	-3.05867	-0.13908
N10	0.69239	-1.54607	-0.22322	N10	0.69584	-1.73487	0.07929
C11	-4.46549	2.10843	0.25585	C11	-4.46004	2.06868	0.12806
C12	-3.66683	0.89301	0.05025	C12	-3.68909	0.82909	0.04471
C13	-3.56167	3.12121	0.40415	C13	-3.53489	3.07309	0.22952
C14	-2.23469	2.49714	0.28911	C14	-2.22581	2.41606	0.21225
N15	-2.33128	1.15399	0.09247	N15	-2.34835	1.06306	0.11067
C16	-4.18056	-2.88667	-0.54629	C16	-4.24543	-2.97113	-0.37304
C17	-3.5977	-1.58059	-0.34666	C17	-3.66212	-1.66482	-0.20084
N18	-2.23739	-1.75225	-0.3435	N18	-2.29543	-1.84815	-0.1596
C19	-1.90992	-3.071	-0.51753	C19	-1.97406	-3.16597	-0.30594
C20	-3.1467	-3.79774	-0.65514	C20	-3.21283	-3.8894	-0.44316
C21	-1.02537	3.20313	0.34284	C21	-0.99964	3.09692	0.27802
H22	3.68681	0.017	-0.00371	H22	3.65168	-0.17777	0.5213
C23	2.60274	-0.03087	-0.0167	C23	2.57618	-0.228	0.39702
H24	-0.54677	-4.66829	-0.65522	H24	-0.63147	-4.78236	-0.48177
C25	-0.61826	-3.59309	-0.52513	C25	-0.68202	-3.70992	-0.32044
H26	-5.32729	-0.40156	-0.23694	H26	-5.37046	-0.45487	-0.19565
C27	-4.24803	-0.36011	-0.17046	C27	-4.29162	-0.43006	-0.10618
H28	-1.56434	-0.99856	-0.24151	H28	-1.63592	-1.08172	-0.07727
H29	-0.09206	0.60279	0.09359	H29	-0.12057	0.47715	0.23919
C30	4.0002	2.79305	-0.03754	C30	4.02476	2.56548	0.3692
H31	4.59394	2.05019	0.50648	H31	4.54347	1.83356	0.99774
H32	4.25165	3.75716	0.41545	H32	4.25015	3.54081	0.8125
C33	4.44147	2.80339	-1.51199	C33	4.61771	2.51277	-1.0501
H34	3.87294	3.5471	-2.08486	H34	4.14378	3.25662	-1.70237
H35	4.22903	1.84122	-1.99395	H35	4.41635	1.54254	-1.52202
C36	5.91416	3.10638	-1.68008	C36	6.11267	2.74421	-1.072
O37	6.6972	3.35727	-0.79007	O37	6.82618	2.89548	-0.10432
O38	6.28073	3.07069	-2.98563	O38	6.59279	2.76263	-2.3406
H39	7.23494	3.27448	-3.00379	H39	7.55538	2.90289	-2.26346
C40	4.29267	-2.66326	0.03651	C40	4.28708	-2.81445	0.15401
H41	4.66528	-3.59352	-0.40536	H41	4.58472	-3.82558	-0.14599
H42	4.82374	-1.85934	-0.4865	H42	4.49131	-2.17685	-0.71274
C43	4.68232	-2.63063	1.52532	C43	5.17946	-2.3958	1.32969
H44	4.18498	-3.4386	2.0764	H44	5.07981	-3.10195	2.16502
H45	4.34085	-1.70277	2.00152	H45	4.88984	-1.42323	1.7466
C46	6.17361	-2.75457	1.74792	C46	6.64602	-2.31781	0.96332
O47	7.02038	-2.84978	0.88659	O47	7.12043	-2.50948	-0.13462
O48	6.47969	-2.74858	3.07065	O48	7.40613	-1.99286	2.03912
H49	7.45106	-2.82735	3.12183	H49	8.32624	-1.94848	1.71734
H50	-1.08256	4.27997	0.45997	H50	-1.03981	4.17997	0.32232
C51	-3.81646	4.57465	0.70619	C51	-3.76984	4.5505	0.40593
C52	1.59711	4.91881	0.31453	C52	1.65967	4.75622	0.36326
H53	1.16364	5.4054	-0.56881	H53	1.32552	5.20227	-0.58249
H54	2.63682	5.24843	0.39536	H54	2.69604	5.06602	0.52477

H55	1.06122	5.30395	1.19044
H56	-2.92632	5.15669	0.42185
C57	-4.07857	4.81058	2.20198
H58	-3.22667	4.4761	2.80407
H59	-4.96654	4.25737	2.52421
H60	-4.23788	5.87826	2.40809
O61	-4.92525	5.0223	-0.08626
H62	-5.10867	5.93897	0.17403
C63	-5.96511	2.1501	0.30159
H64	-6.40229	1.71518	-0.60628
H65	-6.32119	3.17729	0.3843
H66	-6.35383	1.57171	1.15101
C67	-5.65258	-3.20423	-0.53913
H68	-5.78596	-4.20269	-0.98254
C69	-6.23315	-3.23526	0.88388
H70	-7.30389	-3.47933	0.85844
H71	-6.10836	-2.26437	1.37304
H72	-5.73151	-3.99521	1.49275
O73	-6.33144	-2.23751	-1.35159
H74	-7.28059	-2.43048	-1.2936
C75	-3.22525	-5.28235	-0.86045
H76	-4.22527	-5.59383	-1.17425
H77	-2.98357	-5.83395	0.05766
H78	-2.52153	-5.6146	-1.63219
C79	2.13356	-5.02768	-0.43468
H80	1.69285	-5.57675	0.40826
H81	3.20261	-5.26151	-0.45444
H82	1.69187	-5.4399	-1.35079

H55	1.05492	5.20323	1.16148
H56	-2.85539	5.09299	0.11847
C57	-4.09408	4.91008	1.86464
H58	-3.2759	4.6122	2.52952
H59	-5.00517	4.39757	2.18954
H60	-4.24299	5.99314	1.97826
O61	-4.83293	4.95544	-0.46903
H62	-5.00732	5.89287	-0.28845
C63	-5.95864	2.15066	0.10345
H64	-6.36429	1.70551	-0.81396
H65	-6.29175	3.18802	0.14115
H66	-6.40351	1.60524	0.94641
C67	-5.71826	-3.2854	-0.38099
H68	-5.84901	-4.29194	-0.8067
C69	-6.31648	-3.28633	1.03486
H70	-7.38699	-3.53083	1.00177
H71	-6.1967	-2.30459	1.5033
H72	-5.82239	-4.03272	1.66635
O73	-6.38535	-2.33359	-1.22023
H74	-7.33563	-2.52255	-1.16757
C75	-3.29495	-5.3785	-0.61264
H76	-4.30124	-5.69841	-0.89693
H77	-3.0308	-5.91043	0.31105
H78	-2.60891	-5.72785	-1.39302
C79	2.23568	-4.03539	-1.71394
H80	1.47998	-4.66454	-2.19621
H81	3.20352	-4.53892	-1.81123
H82	2.28464	-3.09051	-2.2669
H83	2.69564	-3.04046	1.57907
H84	1.82866	-4.76272	0.2778

3p LEVULAN PORPHYRIN				**3c LEVULAN CHLORIN**			
C1	0.24789	2.90466	−0.17554	C1	0.29581	2.86742	−0.10067
C2	−2.03413	2.8587	−0.18559	C2	−1.97972	2.78513	−0.23417
C3	−1.52653	1.50931	−0.11566	C3	−1.44862	1.44349	−0.28245
N4	−0.15822	1.59673	−0.11193	N4	−0.09165	1.54786	−0.18368
C5	−0.94464	3.71182	−0.21098	C5	−0.90753	3.6544	−0.1127
C6	−2.61398	−2.17013	0.13731	C6	−2.53641	−2.29212	−0.66979
C7	−1.75355	−0.97907	0.05403	C7	−1.67149	−1.05101	−0.41551
C8	−1.76545	−3.23	0.27931	C8	−1.68096	−3.38124	0.02471
C9	−0.41065	−2.6617	0.26869	C9	−0.30045	−2.72923	−0.03093
N10	−0.43493	−1.30722	0.13071	N10	−0.37725	−1.38895	−0.18928
C11	4.9358	2.04787	−0.22238	C11	4.99533	2.07014	−0.07091
C12	4.07122	0.87711	−0.07046	C12	4.1549	0.88267	−0.00938
C13	4.09463	3.1221	−0.37051	C13	4.1346	3.13819	−0.1797
C14	2.72919	2.57129	−0.25607	C14	2.78453	2.56026	−0.13392
N15	2.75331	1.22184	−0.09373	N15	2.82946	1.2035	−0.05402
C16	4.35044	−2.95811	0.31459	C16	4.47021	−2.95922	0.2824
C17	3.83815	−1.60725	0.19707	C17	3.95977	−1.61256	0.14926
N18	2.47229	−1.6967	0.21457	N18	2.58972	−1.71334	0.07625
C19	2.07006	−3.00286	0.34184	C19	2.19007	−3.01819	0.16648
C20	3.25719	−3.81058	0.41569	C20	3.37653	−3.81923	0.30351
C21	1.56636	3.35109	−0.24225	C21	1.60668	3.32302	−0.08834
H22	−3.33239	0.43351	−0.06608	H22	−3.2333	0.36466	−0.54778
C23	−2.25514	0.32218	−0.05957	C23	−2.16413	0.24686	−0.43749
H24	0.60701	−4.50909	0.47908	H24	0.73299	−4.54265	0.24368
C25	0.74688	−3.43847	0.37624	C25	0.86319	−3.47028	0.1361
H26	5.64443	−0.53743	0.06144	H26	5.75005	−0.51004	0.13731
C27	4.5656	−0.42691	0.06826	C27	4.66949	−0.42128	0.09408
H28	1.84028	−0.90631	0.13158	H28	1.97365	−0.91283	−0.01575
H29	0.46684	0.79831	−0.06444	H29	0.55484	0.76694	−0.1927
C30	−3.48615	3.25803	−0.24984	C30	−3.43477	3.16791	−0.32027
H31	−4.07215	2.49296	−0.76807	H31	−3.97091	2.49948	−1.00126
H32	−3.56944	4.16858	−0.85287	H32	−3.50299	4.16852	−0.75967
C33	−4.1542	3.53618	1.11577	C33	−4.19289	3.19124	1.02786
H34	−5.03126	4.18252	0.96778	H34	−5.03401	3.8966	0.9646
H35	−3.48444	4.07144	1.79433	H35	−3.5577	3.54106	1.84673
C36	−4.67818	2.29202	1.80444	C36	−4.8115	1.86073	1.4066
O37	−5.07842	1.29006	1.24796	O37	−5.16932	0.99823	0.62977
O38	−4.70981	2.43523	3.14786	O38	−4.98436	1.74588	2.74141
H39	−5.09642	1.6118	3.50289	H39	−5.42791	0.88824	2.88873
C40	−4.11312	−2.17896	0.03292	C40	−4.02961	−2.23691	−0.30117
H41	−4.52028	−3.09967	0.46264	H41	−4.38603	−3.2488	−0.07865
H42	−4.54868	−1.35673	0.61305	H42	−4.18428	−1.65423	0.61254
C43	−4.59546	−2.0685	−1.42605	C43	−4.91621	−1.67072	−1.41595
H44	−4.13296	−2.85257	−2.04143	H44	−4.81265	−2.26591	−2.3347
H45	−4.29038	−1.11976	−1.88047	H45	−4.64218	−0.64871	−1.69411
C46	−6.09557	−2.21522	−1.5599	C46	−6.38204	−1.66479	−1.04263
O47	−6.84972	−2.65664	−0.72077	O47	−6.87476	−2.17397	−0.05991
O48	−6.52939	−1.80756	−2.78102	O48	−7.12741	−1.02076	−1.97694
H49	−7.49293	−1.96226	−2.78707	H49	−8.04945	−1.07065	−1.66226
H50	1.69945	4.42536	−0.28186	H50	1.73268	4.39796	−0.04049
C51	4.48864	4.51026	−0.60672	C51	4.50988	4.54334	−0.32888
H52	5.42116	4.81706	−0.13096	H52	5.42349	4.83937	0.18874
C53	−0.94944	5.21013	−0.26791	C53	−0.93692	5.1508	−0.01043
H54	−0.65337	5.65208	0.69217	H54	−0.73319	5.48987	1.01384

H55	-1.94219	5.59806	-0.51314
H56	-0.25136	5.58664	-1.02417
C57	6.43387	2.02814	-0.25261
H58	6.81537	1.48466	-1.12721
H59	6.85008	1.53862	0.63725
H60	6.84435	3.0407	-0.29694
H61	2.95468	5.18479	-1.92564
C62	3.8556	5.41827	-1.36635
H63	4.24727	6.42596	-1.47323
C64	3.2642	-5.29636	0.60729
H65	3.23516	-5.83578	-0.34909
H66	2.40125	-5.62832	1.19356
H67	4.17114	-5.61287	1.13127
C68	-2.09389	-4.68692	0.41464
H69	-1.64301	-5.12167	1.31611
H70	-1.72486	-5.2694	-0.44036
H71	-3.17417	-4.84876	0.47861
C72	5.77473	-3.27908	0.33779
H73	6.42407	-2.49926	0.73487
C74	6.35187	-4.41381	-0.08614
H75	7.42661	-4.55188	-0.01212
H76	5.78928	-5.22384	-0.53916

H55	-1.91119	5.5556	-0.29973
H56	-0.18261	5.61383	-0.65696
C57	6.49485	2.08439	-0.06233
H58	6.91253	1.59416	-0.95185
H59	6.89911	1.56047	0.81318
H60	6.88501	3.1062	-0.0443
H61	3.00163	5.26312	-1.65313
C62	3.88164	5.48135	-1.05558
H63	4.25731	6.49996	-1.096
C64	3.38747	-5.30661	0.48783
H65	3.49087	-5.8435	-0.46541
H66	2.46583	-5.65963	0.96105
H67	4.22728	-5.60955	1.12215
C68	-2.07113	-3.66816	1.4875
H69	-1.35791	-4.36505	1.93998
H70	-3.06875	-4.11406	1.55875
H71	-2.06326	-2.7492	2.08474
C72	5.89092	-3.26766	0.40884
H73	6.5077	-2.45989	0.80079
C74	6.50834	-4.41697	0.09304
H75	7.57791	-4.53009	0.24467
H76	5.98996	-5.26445	-0.34212
H77	-2.46425	-2.48807	-1.7526
H78	-1.70117	-4.32246	-0.53631

4p VISUDYNE PORPHYRIN				**4c VISUDYNE CHLORIN**			
C1	0.6118	-1.61568	0.41232	C1	2.31144	-1.40843	-1.10625
C2	-1.36554	-2.74348	0.27654	C2	0.36907	-2.50586	-1.54824
C3	-1.60648	-1.3321	0.10614	C3	0.15944	-1.08848	-1.69781
N4	-0.38451	-0.70485	0.1956	N4	1.35386	-0.47768	-1.42777
C5	-0.00969	-2.91844	0.46708	C5	1.68647	-2.70137	-1.1773
C6	-4.38561	1.25026	-0.49416	C6	-2.69063	1.40695	-2.59237
C7	-3.05669	0.67412	-0.26661	C7	-1.3176	0.89968	-2.15118
C8	-4.18853	2.59884	-0.61555	C8	-2.54062	2.94758	-2.42665
C9	-2.74821	2.80898	-0.44777	C9	-1.04824	3.08253	-2.12515
N10	-2.09125	1.63197	-0.24196	N10	-0.43634	1.89403	-1.94572
C11	2.94143	2.0526	0.10007	C11	4.62175	2.24505	-1.26632
C12	4.13131	0.07256	0.69408	C12	5.76757	0.302	-0.5189
C13	2.62321	-0.11218	0.44285	C13	4.28049	0.10269	-0.84561
N14	2.00502	1.06211	0.20283	N14	3.67905	1.26383	-1.15768
C15	1.21532	5.46344	-0.30369	C15	2.94793	5.66308	-1.77425
C16	1.43813	4.04819	-0.19233	C16	3.15068	4.25272	-1.64292
N17	0.20655	3.44653	-0.19736	N17	1.90648	3.6638	-1.67473
C18	-0.79588	4.37905	-0.32341	C18	0.92449	4.60332	-1.83524
C19	-0.15649	5.67616	-0.35623	C19	1.57726	5.89078	-1.8591
C20	1.97612	-1.34208	0.54655	C20	3.6419	-1.135	-0.80043
H21	-3.69024	-1.35342	-0.1624	H21	-1.86808	-1.13178	-2.23495
C22	-2.82513	-0.70074	-0.10522	C22	-1.04118	-0.45919	-2.03593
H23	-2.7967	4.92174	-0.65013	H23	-1.05219	5.18984	-2.23481
C24	-2.14472	4.0742	-0.47593	C24	-0.43025	4.32317	-2.04784
H25	3.53984	4.06518	-0.12368	H25	5.24537	4.24052	-1.52893
C26	2.67637	3.40888	-0.08408	C26	4.37168	3.59785	-1.4922
H27	0.03441	2.44742	-0.17007	H27	1.73266	2.66675	-1.65266
H28	-0.25817	0.29769	0.11594	H28	1.5229	0.51984	-1.4526
C29	-2.4507	-3.77799	0.20025	C29	-0.71051	-3.52354	-1.76114
H30	-3.3389	-3.40792	0.7229	H30	-1.61654	-3.19584	-1.24197
H31	-2.14786	-4.69436	0.71731	H31	-0.42856	-4.47915	-1.30991
C32	-2.84214	-4.12266	-1.26499	C32	-1.05987	-3.75352	-3.25656
H33	-2.11951	-4.81419	-1.70475	H33	-0.33396	-4.41846	-3.72722
H34	-2.84649	-3.20373	-1.85934	H34	-1.03554	-2.79543	-3.78369
C35	-4.22004	-4.74918	-1.35105	C35	-2.44093	-4.34929	-3.4156
O36	-4.46341	-5.91047	-1.59533	O36	-2.69151	-5.4567	-3.82619
O37	-5.17117	-3.82016	-1.09497	O37	-3.37867	-3.46199	-3.00895
C38	-5.68095	0.48752	-0.53191	C38	-3.91031	0.68258	-1.99073
H39	-6.41423	1.02397	-1.14543	H39	-4.82324	1.20228	-2.30662
H40	-5.55062	-0.48738	-1.01409	H40	-3.97756	-0.30973	-2.44663
C41	-6.27689	0.2667	0.87237	C41	-3.92889	0.48787	-0.47077
H42	-6.47536	1.21893	1.37526	H42	-4.06819	1.41963	0.08034
H43	-5.55657	-0.26285	1.51101	H43	-2.96731	0.08132	-0.13081
C44	-7.5523	-0.55214	0.84422	C44	-4.99919	-0.48569	-0.03282
O45	-7.90115	-1.28832	-0.05707	O45	-5.53525	-1.31899	-0.72799
O46	-8.2716	-0.37676	1.97368	O46	-5.29175	-0.33317	1.27087
H47	2.59887	-2.20853	0.72769	H47	4.25135	-1.99379	-0.55179
C48	0.73516	-4.20166	0.68329	C48	2.38789	-3.99494	-0.89588
H49	1.27192	-4.20132	1.64069	H49	2.71257	-4.05737	0.15056
H50	1.47961	-4.36914	-0.10471	H50	3.28404	-4.10827	-1.51753
H51	0.05735	-5.06001	0.68536	H51	1.73795	-4.85143	-1.09151
C52	-5.20318	3.67424	-0.86671	C52	-3.41007	3.64565	-1.37007
H53	-5.27865	4.37231	-0.02216	H53	-3.15401	3.33106	-0.3541
H54	-6.19976	3.25271	-1.03125	H54	-4.47528	3.45206	-1.53768

H55	-4.94953	4.27027	-1.75242
C56	-6.53468	-4.28452	-1.13246
H57	-6.77492	-4.66537	-2.12905
H58	-7.1429	-3.41429	-0.88843
H59	-6.68206	-5.08688	-0.40398
C60	2.30187	6.4961	-0.30943
H61	3.00339	6.33854	-1.13796
H62	2.88617	6.47309	0.61908
H63	1.89039	7.50333	-0.40921
C64	-0.82553	6.97594	-0.42322
H65	-0.30093	7.74442	-0.99076
H66	-2.53815	6.623	0.79374
C67	-1.98242	7.31262	0.16561
H68	-2.39494	8.3111	0.05293
C69	5.12523	-0.88244	-0.05193
H70	4.74889	-1.04176	-1.07201
C71	6.51037	-0.22988	-0.14018
H72	7.63846	1.53238	-0.28195
C73	6.6423	1.11991	-0.15183
C74	5.50027	2.00527	-0.11867
H75	5.62917	3.04211	-0.41889
C76	4.28895	1.49591	0.19251
C77	4.35856	0.09529	2.23464
H78	5.40195	0.32275	2.46758
H79	4.11087	-0.86793	2.68507
H80	3.72155	0.86372	2.68349
C81	7.74281	-1.0175	-0.38644
O82	8.87979	-0.59856	-0.2753
O83	7.46532	-2.27831	-0.80841
C84	5.2251	-2.25845	0.61137
O85	5.75698	-2.4872	1.67534
O86	4.62531	-3.21539	-0.1346
C87	8.61266	-3.10342	-1.05859
H88	9.19606	-3.23337	-0.14302
H89	9.24927	-2.65278	-1.82444
H90	8.2164	-4.05985	-1.40222
C91	4.73977	-4.54879	0.38959
H92	4.26315	-4.62326	1.37082
H93	5.79247	-4.82679	0.48653
H94	4.23599	-5.19184	-0.33299
C95	-9.48735	-1.13993	2.05784
H96	-10.15783	-0.88559	1.23257
H97	-9.93602	-0.87046	3.01442
H98	-9.27254	-2.21156	2.02283

H55	-3.26518	4.72998	-1.42167
C56	-4.74489	-3.91469	-3.0357
H57	-5.0786	-4.04591	-4.06919
H58	-5.31675	-3.13494	-2.5336
H59	-4.83873	-4.86843	-2.51026
C60	4.04624	6.68344	-1.77243
H61	4.7991	6.46618	-2.54016
H62	4.56729	6.71699	-0.80734
H63	3.65615	7.68541	-1.96521
C64	0.93362	7.19892	-1.95703
H65	1.50236	7.95661	-2.4957
H66	-0.85532	6.89236	-0.84176
C67	-0.2478	7.56519	-1.43841
H68	-0.63054	8.57224	-1.57768
C69	6.77844	-0.75903	-1.07802
H70	6.35576	-1.19689	-1.9913
C71	8.12621	-0.12928	-1.41536
H72	9.25614	1.57034	-1.87156
C73	8.27312	1.20576	-1.58707
C74	7.16254	2.12203	-1.54025
H75	7.29471	3.12592	-1.93537
C76	5.95677	1.67324	-1.13583
C77	5.90384	0.49342	1.02093
H78	6.93941	0.71388	1.29123
H79	5.59381	-0.40493	1.5615
H80	5.26854	1.32211	1.34679
C81	9.30218	-0.9722	-1.72063
O82	10.44045	-0.5708	-1.85915
O83	8.95881	-2.27775	-1.88105
C84	7.00043	-1.9078	-0.09446
O85	7.73495	-1.87397	0.86268
O86	6.26797	-2.99687	-0.40538
C87	10.04932	-3.16001	-2.17902
H88	10.78096	-3.1517	-1.36663
H89	10.54568	-2.85877	-3.10525
H90	9.60532	-4.15053	-2.28682
C91	6.45693	-4.12291	0.46516
H92	6.17827	-3.8696	1.49142
H93	7.50287	-4.43905	0.45095
H94	5.81123	-4.90894	0.07305
C95	-6.26722	-1.24068	1.80143
H96	-7.21788	-1.13438	1.27266
H97	-6.38067	-0.9698	2.85118
H98	-5.92267	-2.27387	1.70762
H99	-2.75961	3.4317	-3.38553
H100	-2.75757	1.21075	-3.67139

5p TETRASULFO PORPHYRIN			**5c TETRASULFO CHLORIN**		
C1	-0.69036	0.17391	C1	0.95362	2.94125	-0.01776
C2	1.57251	0.16044	-2.79922	C2	-0.93411	4.18871	0.08221
C3	1.01628	0.26436	-1.48313	C3	-1.30111	2.8034	0.07631
N4	-0.35034	0.27646	-1.63388	N4	-0.1354	2.09016	0.00997
C5	0.53989	0.0939	-3.69385	C5	0.43128	4.27075	0.02224
C6	1.94514	0.13441	2.23359	C6	-2.99992	0.95876	0.14657
C7	1.15125	0.19308	1.01141	C7	-2.89172	-1.23507	0.03457
C8	1.06452	0.02038	3.2526	N8	-2.16642	-0.09984	0.09207
C9	-0.26491	0.05379	2.65148	C9	4.25173	-0.45957	0.11819
N10	-0.18484	0.14948	1.29162	C10	2.88032	-0.93556	0.12147
C11	-5.38573	0.26433	-2.30759	C11	4.18492	0.89297	0.05311
C12	-4.59238	0.27602	-1.08283	C12	2.77311	1.2309	0.04175
C13	-4.5043	0.20247	-3.33088	N13	2.00153	0.10666	0.08266
C14	-3.17763	0.17109	-2.72654	C14	0.84952	-4.19207	0.07958
N15	-3.25694	0.21957	-1.36376	C15	1.23876	-2.8185	0.15372
C16	-5.00739	0.2816	2.73839	N16	0.07082	-2.07907	0.15202
C17	-4.46231	0.22691	1.41389	C17	-1.01885	-2.90247	0.06736
N18	-3.09973	0.10307	1.55601	C18	-0.51714	-4.2444	0.02651
C19	-2.75379	0.06755	2.88637	C19	2.29656	2.56067	-0.01827
C20	-3.97437	0.17636	3.62961	C20	-2.37834	-2.53094	0.00961
C21	-1.99139	0.1279	-3.48785	C21	2.53789	-2.30724	0.15673
C22	-1.45347	0.00154	3.41035	H22	0.05078	-1.06556	0.16391
C23	-5.17037	0.30052	0.20451	H23	-0.05563	1.07957	0.01124
H24	-2.4398	0.06427	0.78532	H24	1.53397	-5.02714	0.05041
H25	-1.01813	0.31524	-0.87001	H25	5.00951	1.58956	0.01456
H26	-6.05504	0.4041	2.96706	H26	5.14095	-1.07126	0.16141
H27	-4.72091	0.19045	-4.38881	H27	-1.13007	-5.13021	-0.04763
H28	-6.46345	0.28812	-2.36714	H28	-1.63251	5.0098	0.1378
H29	-4.03841	0.20077	4.70715	H29	1.03187	5.16874	0.02464
H30	1.28617	-0.0756	4.30453	C30	-3.34692	-3.67148	-0.1104
H31	3.02231	0.16981	2.29547	C31	-5.04354	-5.86383	-0.36589
H32	2.62827	0.10868	-3.01731	C32	-3.83723	-4.05129	-1.36748
H33	0.61299	-0.01966	-4.76427	C33	-3.73217	-4.40945	1.0178
C34	-1.33258	-0.14159	4.89509	C34	-4.57807	-5.50893	0.89901
C35	-1.0075	-0.49292	7.643	C35	-4.68298	-5.14794	-1.50521
C36	-0.74214	0.86247	5.67889	H36	-3.52737	-3.49551	-2.24823
C37	-1.78879	-1.3104	5.52639	H37	-3.34743	-4.12701	1.99384
C38	-1.63294	-1.4924	6.89768	H38	-4.85574	-6.09959	1.76577
C39	-0.57246	0.69237	7.05105	C39	3.30904	3.66277	-0.08633
H40	-0.41128	1.78224	5.20594	C40	5.23239	5.67277	-0.25133
H41	-2.25273	-2.09083	4.9305	C41	3.47412	4.39873	-1.26954
H42	-1.98565	-2.39603	7.38371	C42	4.12555	3.96184	1.0141
C43	-2.1015	-0.00338	-4.97429	C43	5.08831	4.9645	0.93956
C44	-2.23706	-0.30509	-7.74443	C44	4.43749	5.39893	-1.36313
C45	-1.64677	1.01454	-5.82721	H45	2.8569	4.16482	-2.13132
C46	-2.64626	-1.16718	-5.54187	H46	4.0052	3.39901	1.93422
C47	-2.72115	-1.32361	-6.923	H47	5.7315	5.18829	1.78402
C48	-1.70937	0.87039	-7.21169	C48	3.64927	-3.31019	0.15175
H49	-1.24737	1.92976	-5.40007	C49	5.70768	-5.18831	0.11599
H50	-3.0042	-1.95899	-4.89076	C50	4.46548	-3.45573	-0.98124
H51	-3.14768	-2.22038	-7.36007	C51	3.88485	-4.13207	1.26397
C52	-6.6614	0.38974	0.29835	C52	4.91351	-5.07103	1.25429
C53	-9.44586	0.52108	0.39268	C53	5.49115	-4.39449	-1.00977
C54	-7.33807	1.53843	-0.1425	H54	4.28115	-2.83378	-1.85138

C55	-7.41078	-0.68133	0.81075
C56	-8.80105	-0.62267	0.86311
C57	-8.72838	1.61105	-0.09947
H58	-6.76633	2.38079	-0.52057
H59	-6.89749	-1.57413	1.15554
H60	-9.25244	2.50104	-0.43202
C61	1.72689	0.26839	-0.27349
C62	3.21831	0.34609	-0.37802
C63	5.99653	0.54736	-0.52533
C64	3.82638	1.51426	-0.86506
C65	4.03366	-0.72907	0.00917
C66	5.42192	-0.63549	-0.0605
C67	5.21228	1.62217	-0.94352
H68	3.20428	2.3496	-1.17264
H69	3.57325	-1.64671	0.36321
H70	6.05357	-1.4691	0.22842
H71	-0.11763	1.46724	7.65919
H72	5.68172	2.52357	-1.32304
H73	-1.36699	1.6598	-7.87259
H74	-9.37992	-1.44967	1.2605
S75	-0.75097	-0.74121	9.39154
O76	-0.39636	0.52776	10.02805
O77	-1.82446	-1.57835	9.90766
S78	-11.22985	0.58501	0.41386
O79	-11.71289	-0.26183	1.49484
O80	-11.67913	1.9696	0.26396
S81	-2.29253	-0.51411	-9.5162
O82	-3.43402	-1.35309	-9.8511
O83	-2.06665	0.77304	-10.17483
S84	7.77445	0.69334	-0.58864
O85	8.38526	-0.63417	-0.51044
O86	8.12581	1.63476	-1.64195
O87	8.06417	1.42457	0.86289
H88	8.75996	0.8965	1.29949
O89	-11.56801	-0.17116	-1.01419
H90	-12.1917	0.41071	-1.48964
O91	-0.92185	-1.40445	-9.75043
H92	-0.42644	-0.95884	-10.46428
O93	0.63012	-1.64647	9.3535
H94	1.23798	-1.24282	10.00255

H55	3.2621	-4.02577	2.14648
H56	6.10593	-4.52477	-1.89429
C57	-2.61739	2.29955	0.14575
C58	-3.69765	3.33739	0.22749
C59	-5.63335	5.33258	0.3978
C60	-4.11992	4.02214	-0.92182
C61	-4.27184	3.67046	1.46159
C62	-5.23723	4.66896	1.5565
C63	-5.08532	5.02214	-0.84599
H64	-3.67317	3.77466	-1.8808
H65	-3.93776	3.15737	2.35922
H66	-5.66249	4.95093	2.51381
H67	-5.03853	-5.46477	-2.47998
H68	-5.39572	5.57059	-1.72936
H69	4.5883	5.94611	-2.28786
H70	5.09612	-5.71202	2.11024
S71	-6.05088	-7.32136	-0.54163
O72	-5.97301	-7.81279	-1.91276
O73	-5.81662	-8.22149	0.58189
S74	6.98966	-6.42322	0.07197
O75	6.76365	-7.41718	1.11619
O76	7.22593	-6.83954	-1.3057
S77	6.51337	6.90271	-0.38271
O78	7.50692	6.70734	0.66861
O79	6.92608	7.03241	-1.77516
S80	-6.8063	6.66653	0.52148
O81	-6.8535	7.15263	1.89563
O82	-6.6212	7.5975	-0.58679
O83	-8.17663	5.79376	0.22917
H84	-8.91642	6.42888	0.16625
O85	8.24499	-5.46071	0.54394
H86	9.03155	-6.03305	0.63541
O87	5.60643	8.22266	0.01875
H88	6.22128	8.97482	0.12268
O89	-7.52433	-6.60681	-0.33297
H90	-8.19902	-7.31053	-0.3975
C91	-4.46599	0.54455	0.20176
H92	-5.06643	1.06017	-0.55247
H93	-4.90303	0.80412	1.17216
C94	-4.39189	-0.96875	-0.00838
H95	-4.80943	-1.27147	-0.97488
H96	-4.93152	-1.5415	0.75121

6p FOSCAN PORPHYRIN				**6c FOSCAN CHLORIN**			
C1	0.04933	-3.09801	0.14728	C1	0.39729	-3.07755	0.26183
C2	-2.13078	-3.72505	0.08079	C2	-1.68866	-3.94507	0.04854
C3	-2.05764	-2.30294	-0.08174	C3	-1.76464	-2.52585	-0.13535
N4	-0.72374	-1.97373	-0.03222	N4	-0.48929	-2.04832	-0.00343
C5	-0.85775	-4.20326	0.23995	C5	-0.38547	-4.27307	0.32215
C6	-3.04112	-0.00838	-0.14304	C6	-3.06108	-0.38955	-0.24479
C7	-2.28553	2.01081	0.12905	C7	-2.5468	1.70937	0.19198
N8	-1.891	0.70699	0.04478	N8	-2.03957	0.47409	-0.02762
C9	4.19201	-0.87667	-0.38962	C9	4.24862	-0.4065	-0.32
C10	3.03869	0.0066	-0.25927	C10	3.0024	0.33635	-0.27253
C11	3.73262	-2.13427	-0.19151	C11	3.93741	-1.6942	-0.02099
C12	2.29368	-2.01626	0.01899	C12	2.49724	-1.73474	0.16113
N13	1.89665	-0.71157	-0.03778	N13	1.9491	-0.494	0.00057
C14	2.13736	3.71875	0.04304	C14	1.6415	3.91859	-0.21266
C15	2.05664	2.29878	-0.13412	C15	1.75374	2.49552	-0.29731
N16	0.72632	1.96862	-0.03038	N16	0.48065	1.99402	-0.0962
C17	-0.0381	3.09063	0.19384	C17	-0.41153	3.00727	0.13012
C18	0.873	4.19452	0.26361	C18	0.33671	4.22851	0.07165
C19	1.45191	-3.13852	0.18595	C19	1.7843	-2.94252	0.37186
C20	-1.43831	3.13083	0.28314	C20	-1.80431	2.88332	0.33309
C21	3.13193	1.41275	-0.31395	C21	2.92152	1.74005	-0.44056
H22	0.35818	1.02344	-0.06582	H22	0.27081	1.00392	-0.04886
H23	-0.35829	-1.02742	-0.06768	H23	-0.20921	-1.07654	-0.06965
H24	3.05642	4.28489	0.02819	H24	2.46884	4.60286	-0.32681
H25	4.29217	-3.05812	-0.22265	H25	4.6047	-2.54233	0.0284
H26	5.20325	-0.56644	-0.60713	H26	5.22148	0.00227	-0.54992
H27	0.58296	5.21582	0.45621	H27	-0.08689	5.21024	0.21811
H28	-3.05025	-4.29068	0.10211	H28	-2.53766	-4.61105	0.0081
H29	-0.55913	-5.22667	0.40676	H29	0.01172	-5.25353	0.53622
C30	-2.07397	4.46175	0.53589	C30	-2.53695	4.13725	0.71242
C31	-3.30717	6.93593	1.04611	C31	-3.89276	6.47118	1.4921
C32	-2.81562	4.65692	1.70704	C32	-2.90486	4.33015	2.04769
C33	-1.95403	5.5193	-0.38214	C33	-2.8536	5.12361	-0.23464
C34	-2.57022	6.74179	-0.12219	C34	-3.52566	6.27975	0.16002
C35	-3.42782	5.88676	1.96182	C35	-3.58015	5.48997	2.43734
H36	-2.92113	3.85876	2.43469	H36	-2.65791	3.5891	2.80203
H37	-1.39921	5.37137	-1.30289	H37	-2.56988	4.98021	-1.27328
H38	-2.48411	7.55385	-0.83955	H38	-3.76839	7.043	-0.5749
H39	-3.78764	7.89267	1.24434	H39	-4.41823	7.37575	1.79428
C40	2.09328	-4.47291	0.4055	C40	2.5784	-4.16654	0.70454
C41	3.33081	-6.9586	0.87587	C41	4.11664	-6.42444	1.38892
C42	2.84877	-4.68745	1.56828	C42	3.30419	-4.20113	1.90496
C43	1.96463	-5.51756	-0.5208	C43	2.63332	-5.27514	-0.15131
C44	2.5845	-6.74572	-0.27956	C44	3.40043	-6.38969	0.19617
C45	3.46089	-5.92077	1.80351	C45	4.06554	-5.32096	2.24596
H46	2.94984	-3.8836	2.29496	H46	3.26852	-3.34441	2.57513
H47	1.39969	-5.35878	-1.43364	H47	2.09467	-5.25254	-1.09358
H48	2.48902	-7.54774	-1.00697	H48	3.44649	-7.24161	-0.47739
H49	3.8165	-7.90874	1.07518	H49	4.71741	-7.28389	1.6699
C50	4.47052	2.04161	-0.55173	C50	4.17663	2.49675	-0.75349
C51	6.95919	3.25815	-1.0303	C51	6.52345	3.90827	-1.38378
C52	5.51016	1.92666	0.38658	C52	5.22219	2.59132	0.18025
C53	4.68959	2.7717	-1.72576	C53	4.31559	3.11978	-1.99882
C54	5.92749	3.37398	-1.96602	C54	5.48487	3.81828	-2.31407

C55	6.74008	2.53434	0.14212	C55	6.38172	3.2941	-0.13964
H56	5.344	1.37564	1.3064	H56	5.11697	2.11821	1.15154
H57	3.90655	2.87135	-2.47073	H57	3.52699	3.05584	-2.74187
H58	7.5395	2.45022	0.87373	H58	7.18698	3.36889	0.58668
H59	7.92215	3.73087	-1.21677	H59	7.4328	4.45521	-1.628
C60	-3.13903	-1.41383	-0.20508	C60	-2.94545	-1.77601	-0.34246
C61	-4.4896	-2.03472	-0.38753	C61	-4.17781	-2.57744	-0.65458
C62	-7.00942	-3.229	-0.77835	C62	-6.4433	-4.11292	-1.30915
C63	-4.76532	-2.75622	-1.55896	C63	-4.43445	-2.93947	-1.98376
C64	-5.48926	-1.91911	0.58887	C64	-5.06516	-2.99333	0.3458
C65	-6.73498	-2.51729	0.38618	C65	-6.18815	-3.75448	0.01159
C66	-6.01665	-3.34539	-1.75541	C66	-5.55885	-3.70247	-2.31058
H67	-3.99772	-2.84473	-2.32578	H67	-3.74276	-2.62833	-2.76536
H68	-5.28347	-1.37285	1.50408	H68	-4.86753	-2.72823	1.38066
H69	-7.50333	-2.42972	1.14993	H69	-6.87156	-4.07784	0.79259
H70	-7.97446	-3.69609	-0.9483	H70	-7.30959	-4.70751	-1.58173
O71	-6.32672	-4.04766	-2.88822	O71	-5.84058	-4.08011	-3.59499
H72	-5.55971	-4.04186	-3.48199	H72	-5.14453	-3.7436	-4.18097
O73	-4.13249	6.00213	3.12914	O73	-3.90256	5.60946	3.76204
H74	-4.50366	6.89624	3.18603	H74	-4.34828	6.45927	3.90228
O75	6.06692	4.06458	-3.13931	O75	5.55387	4.39161	-3.55498
H76	6.96702	4.42209	-3.18949	H76	6.41447	4.82779	-3.65206
O77	4.19951	-6.17118	2.92797	O77	4.78302	-5.39333	3.40893
H78	4.20732	-5.37565	3.48294	H78	4.66548	-4.56666	3.90259
C79	-4.19776	0.87651	-0.22697	C79	-4.40393	0.3267	-0.34313
H80	-5.21614	0.5684	-0.41159	H80	-5.20318	-0.19659	0.18378
C81	-3.73066	2.13178	-0.0336	H81	-4.71204	0.39707	-1.3955
H82	-4.2906	3.05561	-0.03487	C82	-4.07163	1.70483	0.24022
				H83	-4.4187	1.79577	1.27774
				H84	-4.50919	2.54049	-0.31194

7p MACE PORPHYRIN				**7c MACE CHLORIN**			
C1	3.31633	-1.55569	0.18814	C1	4.05527	-1.75325	-0.22807
C2	2.2637	-3.20583	-0.96418	C2	2.84171	-3.62827	-0.6442
C3	1.49804	-1.98193	-1.10452	C3	1.93396	-2.57421	-0.25147
N4	2.21118	-1.02534	-0.42401	N4	2.71154	-1.46501	-0.07707
C5	3.34751	-2.94918	-0.13443	C5	4.14803	-3.128	-0.58431
C6	-0.41112	-0.48498	-1.69486	C6	-0.26502	-1.4773	0.19034
C7	-0.52611	1.69351	-1.69412	C7	-0.89794	0.61874	0.40567
N8	0.28729	0.65566	-1.39474	N8	0.15436	-0.18399	0.14946
C9	5.50225	2.32013	1.94644	C9	5.88053	2.62297	0.36655
C10	4.3629	2.58743	1.06375	C10	4.42795	2.571	0.19451
C11	5.58322	0.96083	2.04684	C11	6.30807	1.32395	0.33776
C12	4.48531	0.43706	1.21797	C12	5.10008	0.51525	0.14214
N13	3.75946	1.44101	0.66283	N13	3.97839	1.29581	0.0882
C14	2.34476	5.40495	-0.61179	C14	1.31691	4.85805	-0.00297
C15	2.87349	4.13273	-0.16315	C15	2.23058	3.73105	0.00458
N16	1.99687	3.16461	-0.57459	N16	1.45464	2.5933	0.04552
C17	0.90411	3.72394	-1.1756	C17	0.13148	2.90896	0.16396
C18	1.11773	5.1494	-1.2042	C18	0.03407	4.34751	0.12533
C19	4.27703	-0.91729	0.97756	C19	5.11923	-0.86588	-0.04065
C20	0.20207	-1.76091	-1.64149	C20	0.5383	-2.60869	0.03845
H21	-1.00229	3.71939	-2.0034	H21	-1.89152	2.46723	0.52999
C22	-0.2243	3.06041	-1.63641	C22	-0.92093	2.01209	0.3559
H23	4.53782	4.71788	0.99955	H23	4.0992	4.68224	0.17475
C24	3.96951	3.86621	0.64754	C24	3.6102	3.71744	0.11355
H25	2.15577	2.18163	-0.3585	H25	1.86457	1.66316	0.07768
H26	1.88405	-0.06047	-0.39602	H26	2.33873	-0.56527	0.20868
H27	4.98872	-1.59466	1.43644	H27	6.10025	-1.32735	-0.05719
C28	4.4249	-3.89381	0.30375	C28	5.41535	-3.86289	-0.89877
H29	5.41569	-3.53664	-0.00042	H29	6.25492	-3.17685	-1.03416
H30	4.26989	-4.89051	-0.10777	H30	5.30894	-4.46475	-1.80567
H31	4.43501	-3.9904	1.39634	H31	5.66806	-4.56641	-0.09734
C32	6.36887	3.36484	2.58041	C32	6.69112	3.87276	0.54178
H33	5.77418	4.09561	3.14301	H33	6.31634	4.48794	1.36992
H34	6.94135	3.92788	1.83135	H34	6.67213	4.50186	-0.3585
H35	7.08855	2.92051	3.27415	H35	7.73976	3.64156	0.75283
C36	0.16993	6.13524	-1.81554	C36	-1.25698	5.10695	0.18036
H37	0.50742	7.16162	-1.65556	H37	-1.08514	6.18586	0.20914
H38	-0.83607	6.04393	-1.38847	H38	-1.84416	4.83928	1.06786
H39	0.07699	5.98609	-2.89843	H39	-1.88193	4.90145	-0.69896
C40	6.58733	0.14181	2.80712	C40	7.71393	0.80303	0.46602
H41	6.93719	0.71288	3.6752	H41	8.3025	1.49706	1.07902
H42	6.10406	-0.75351	3.21757	H42	7.71041	-0.14601	1.01777
C43	7.80579	-0.28037	1.96434	C43	8.43037	0.60207	-0.88356
H44	8.50402	-0.8802	2.55988	H44	9.44508	0.21446	-0.733
C45	2.99051	6.70829	-0.47809	C45	1.67983	6.2687	-0.12202
H46	2.31673	7.55924	-0.37948	H46	1.01568	6.96869	0.3842
H47	4.69257	7.96312	-0.39435	H47	2.89576	7.84348	-0.84054
C48	4.30914	6.95239	-0.4999	C48	2.71285	6.77322	-0.81348
H49	5.04222	6.16623	-0.65163	H49	3.38725	6.14836	-1.39052
C50	-3.00035	-0.98599	-2.44252	C50	-2.45655	-1.96028	-0.99868
H51	-2.80031	-1.70459	-3.24378	H51	-1.82829	-2.67872	-1.53758
H52	-3.78105	-0.33417	-2.83917	H52	-2.50497	-1.07039	-1.64043
C53	-3.59864	-1.74745	-1.24399	C53	-3.86082	-2.59157	-0.85377
H54	-2.81228	-2.18602	-0.62135	H54	-3.78992	-3.52372	-0.2847

H55	7.50082	-0.87438	1.09564
C56	-1.83298	1.23166	-2.1561
C57	-1.79212	-0.13273	-2.1391
H58	-4.20544	-2.58742	-1.60721
O59	-4.5444	0.33579	-0.44065
C60	-4.47634	-0.87813	-0.35011
H61	-5.11602	-2.58964	0.60453
N62	-5.19385	-1.58165	0.58233
C63	-6.10974	-0.95204	1.51789
H64	-6.03281	0.11969	1.33923
C65	-5.7531	-1.30609	2.96281
H66	-4.70481	-1.06399	3.16326
H67	-5.86892	-2.38333	3.12886
C68	-7.52544	-1.42387	1.18447
O69	-7.99799	-2.47293	1.5611
O70	-8.16332	-0.57637	0.35965
H71	-9.03652	-0.97275	0.17654
C72	-6.62838	-0.58692	3.96073
O73	-7.54953	0.14903	3.69035
O74	-6.2595	-0.86474	5.23069
H75	-6.87401	-0.37244	5.8075
C76	-0.50017	-2.9788	-2.20094
H77	-1.41823	-2.69443	-2.70511
H78	0.10986	-3.45036	-2.97004
C79	-0.8974	-4.0353	-1.18541
O80	-1.21306	-3.85071	-0.03361
O81	-0.90391	-5.26779	-1.75062
H82	-1.1524	-5.89194	-1.04254
H83	8.34349	0.5975	1.58969
C84	-2.96957	2.13649	-2.5232
H85	-2.62848	2.98014	-3.13415
H86	-3.45971	2.53651	-1.62857
H87	-3.73943	1.61487	-3.09354
C88	2.13477	-4.52613	-1.62063
O89	2.21451	-5.59618	-1.06045
O90	2.022	-4.44451	-2.97432
H91	1.9405	-5.3668	-3.28421

H55	7.8869	-0.10456	-1.5207
C56	-2.14253	-0.15364	0.82291
C57	-1.78934	-1.57612	0.34854
H58	-2.06701	-2.30852	1.1099
H59	-4.24571	-2.84136	-1.85136
O60	-5.06998	-1.81099	1.09102
C61	-4.8548	-1.70768	-0.11008
H62	-5.28134	-0.72124	-1.8804
N63	-5.46963	-0.75412	-0.88677
C64	-6.35721	0.26103	-0.3331
H65	-6.23824	0.22261	0.74997
C66	-7.81753	0.00539	-0.72616
H67	-8.11613	-1.00074	-0.41489
H68	-7.93107	0.05623	-1.81593
C69	-5.8771	1.61077	-0.86648
O70	-6.12084	2.01928	-1.98143
O71	-5.07428	2.2569	0.00138
H72	-4.79437	3.07968	-0.44409
C73	-8.74808	1.02416	-0.1085
O74	-8.39565	2.02501	0.47821
O75	-10.04579	0.6964	-0.29121
H76	-10.57049	1.40949	0.12022
C77	-0.07968	-3.94708	0.3969
H78	-1.07823	-4.0814	-0.03357
H79	0.49102	-4.78988	0.02101
C80	-0.23023	-4.14583	1.9029
O81	-0.17087	-3.29995	2.76581
O82	-0.47717	-5.45156	2.18294
H83	-0.58768	-5.5025	3.15131
H84	8.50444	1.54829	-1.43081
H85	-3.02752	0.24729	0.31821
C86	-2.36642	-0.0753	2.34488
H87	-2.4904	0.96331	2.67085
H88	-1.51453	-0.5068	2.88218
H89	-3.26813	-0.63458	2.61334
C90	2.57323	-4.93316	-1.26536
O91	3.33498	-5.88346	-1.26203
O92	1.39803	-4.98551	-1.96028
H93	1.37078	-5.88522	-2.33781

8p CLORINP6 PORPHYRIN				8c CLORINP6 CHLORIN			
C1	0.94672	-2.61053	0.01317	C1	1.30305	-2.76758	0.1074
C2	-1.01505	-3.45602	-0.74998	C2	-0.76533	-3.6648	-0.1106
C3	-1.15715	-2.0219	-0.5853	C3	-0.90407	-2.25824	0.16315
N4	0.06864	-1.57175	-0.1742	N4	0.36008	-1.76176	0.23465
C5	0.25568	-3.8178	-0.3372	C5	0.59091	-3.98349	-0.10719
C6	-2.27934	0.21589	-0.51637	C6	-2.15335	-0.07975	0.28752
C7	-1.46454	2.22958	-0.41848	C7	-1.48497	2.01283	0.30464
N8	-1.11199	0.91788	-0.47037	N8	-1.07275	0.72855	0.22381
C9	4.99171	-0.27117	0.98723	C9	5.29463	-0.15317	0.28996
C10	3.87665	0.56492	0.53793	C10	4.05604	0.60804	0.16658
C11	4.50297	-1.54485	1.04104	C11	4.92034	-1.46806	0.34309
C12	3.09951	-1.44661	0.61682	C12	3.45929	-1.46499	0.25033
N13	2.74675	-0.16636	0.34593	N13	2.96605	-0.19635	0.16919
C14	2.91606	4.19664	-0.29865	C14	2.75074	4.21884	-0.19677
C15	2.92637	2.76463	-0.09543	C15	2.87337	2.78012	-0.09278
N16	1.63311	2.33118	-0.21531	N16	1.59576	2.27775	0.01494
C17	0.78408	3.38675	-0.39435	C17	0.68247	3.28669	0.05909
C18	1.59019	4.57736	-0.45122	C18	1.4068	4.5277	-0.06796
C19	2.2697	-2.55471	0.44045	C19	2.68662	-2.62353	0.18694
C20	-2.29849	-1.19448	-0.6767	C20	-2.09012	-1.48293	0.3487
H21	-1.08853	4.29951	-0.5077	H21	-1.24096	4.09459	0.27873
C22	-0.60642	3.33009	-0.44973	C22	-0.69981	3.15563	0.2136
H23	4.93308	2.4167	0.45867	H23	4.95553	2.53942	-0.00186
C24	3.97408	1.93939	0.29828	C24	4.01236	2.00744	0.01605
H25	1.3831	1.35096	-0.09882	H25	1.41713	1.28122	0.10657
H26	0.24805	-0.57955	-0.03138	H26	0.56571	-0.78028	0.39068
H27	2.72197	-3.52383	0.61991	H27	3.23666	-3.55808	0.18272
C28	0.8733	-5.18176	-0.32147	C28	1.20298	-5.32885	-0.34513
H29	1.75155	-5.22735	-0.97644	H29	2.27563	-5.25844	-0.53932
H30	0.15605	-5.93779	-0.63781	H30	0.72976	-5.82791	-1.19503
H31	1.2093	-5.44281	0.68945	H31	1.04695	-5.98558	0.51764
C32	6.37085	0.21954	1.30532	C32	6.67503	0.42841	0.33894
H33	6.35384	1.02102	2.05465	H33	6.77207	1.18361	1.12911
H34	6.8742	0.62262	0.41663	H34	6.94658	0.91724	-0.60609
H35	6.998	-0.5859	1.69717	H35	7.42347	-0.34561	0.53033
C36	1.05538	5.95954	-0.67214	C36	0.77136	5.8845	-0.09259
H37	1.8397	6.71186	-0.55861	H37	1.52488	6.67262	-0.16772
H38	0.25863	6.19959	0.04145	H38	0.18295	6.07033	0.81455
H39	0.63531	6.07421	-1.6791	H39	0.09236	5.99753	-0.94677
C40	5.22687	-2.80569	1.42017	C40	5.80414	-2.67902	0.45006
H41	6.02374	-2.56486	2.13291	H41	6.70414	-2.42185	1.02179
H42	4.54672	-3.48009	1.95503	H42	5.29966	-3.45909	1.03344
C43	5.8412	-3.5513	0.22003	C43	6.22657	-3.25846	-0.91372
H44	6.3505	-4.46525	0.54729	H44	6.84543	-4.1542	-0.78382
C45	4.08132	5.07584	-0.33896	C45	3.84631	5.16186	-0.41467
H46	3.91915	6.09024	0.02501	H46	3.74711	6.12996	0.07647
H47	6.10674	5.49183	-0.79051	H47	5.68873	5.71584	-1.29748
C48	5.3002	4.76445	-0.804	C48	4.92368	4.95317	-1.18491
H49	5.52608	3.79452	-1.23642	H49	5.06312	4.03442	-1.74652
C50	-4.91159	0.82979	-0.19559	C50	-4.17779	0.56945	-1.11077
H51	-5.30322	0.23592	-1.01989	H51	-3.95518	-0.41473	-1.52556
H52	-5.4576	1.77554	-0.20348	H52	-3.77639	1.31391	-1.8078
C53	-5.24549	0.11332	1.12561	C53	-5.70199	0.68105	-1.04254
H54	-4.68079	-0.81055	1.2639	H54	-6.10443	-0.05494	-0.34254

H55	5.07326	-3.83187	-0.50937
C56	-2.91872	2.38708	-0.35001
C57	-3.44549	1.12899	-0.38449
H58	-6.30508	-0.17575	1.11743
H59	6.57177	-2.92071	-0.29844
C60	-3.65334	3.69067	-0.23661
H61	-3.95389	4.07283	-1.22175
H62	-3.03869	4.46047	0.23881
H63	-4.55067	3.58158	0.37586
C64	-1.93409	-4.40629	-1.40488
O65	-2.08741	-5.56979	-1.10675
O66	-2.55033	-3.85466	-2.47939
H67	-3.11849	-4.55066	-2.85787
C68	-5.05725	0.98718	2.34459
O69	-5.14902	2.19279	2.37842
O70	-4.80186	0.25111	3.45271
H71	-4.72901	0.88834	4.18858
C72	-3.6017	-1.86665	-0.95417
O73	-4.3914	-1.56997	-1.8171
O74	-3.85269	-2.88293	-0.09154
H75	-4.69359	-3.28002	-0.37995

H55	5.35246	-3.53277	-1.51549
C56	-2.97496	2.13536	0.56714
C57	-3.4651	0.70894	0.2631
H58	-4.14462	0.3464	1.03693
H59	-6.12961	0.42385	-2.02114
H60	6.80374	-2.52519	-1.48826
H61	-3.43233	2.86273	-0.10695
C62	-3.25121	2.57509	2.01551
H63	-2.80827	3.55459	2.2248
H64	-2.83563	1.85817	2.73364
H65	-4.3301	2.64893	2.1899
C66	-1.79356	-4.63013	-0.51707
O67	-1.71021	-5.83414	-0.39188
O68	-2.84746	-4.04974	-1.1531
H69	-3.45177	-4.77933	-1.38324
C70	-6.25061	2.04583	-0.70435
O71	-5.68101	3.10689	-0.82965
O72	-7.53052	1.96973	-0.26195
H73	-7.8166	2.8909	-0.11307
C74	-3.32206	-2.19889	0.76892
O75	-4.47443	-1.91156	0.51854
O76	-3.04511	-3.22964	1.61574
H77	-3.90957	-3.62664	1.826

Table 2. Optimized cartesian coordinates (Å) of the 16 molecules studied in its first triplet excited state.

1p PORPHYRIN

C1	0.10576	−0.50531	−2.17208
C2	−2.15026	−0.63268	−1.97321
C3	−1.59637	−0.38333	−0.7036
N4	−0.23713	−0.31187	−0.85549
C5	−1.09555	−0.70882	−2.88668
C6	−2.53088	0.16577	3.00377
C7	−1.7463	0.01849	1.78187
C8	−1.64698	0.39373	4.00176
C9	−0.31596	0.38592	3.38655
N10	−0.39011	0.15986	2.05489
C11	4.83152	−0.06663	−1.55976
C12	4.04688	0.07984	−0.3378
C13	3.94769	−0.29475	−2.55774
C14	2.61667	−0.28793	−1.94248
N15	2.69077	−0.06218	−0.61077
C16	4.45103	0.72956	3.41752
C17	3.89708	0.48058	2.14786
N18	2.53785	0.40914	2.29978
C19	2.19503	0.6023	3.61642
C20	3.39636	0.80553	4.33105
C21	1.43151	−0.49268	−2.66793
H22	−3.366	−0.31228	0.48095
C23	−2.28436	−0.22568	0.54135
H24	0.76715	0.75943	5.18005
C25	0.86922	0.59007	4.11211
H26	5.66656	0.4106	0.9631
C27	4.58496	0.32364	0.90276
H28	1.87836	0.23795	1.54748
H29	0.42229	−0.14028	−0.10319
H30	1.5335	−0.66187	−3.73591
H31	4.14769	−0.45471	−3.61038
H32	5.91075	0.00042	−1.61953
H33	5.50765	0.8385	3.62218
H34	3.45969	0.98574	5.39544
H35	−1.84697	0.55421	5.05433
H36	−3.61013	0.09936	3.06355
H37	−3.20687	−0.74171	−2.17787
H38	−1.15884	−0.88929	−3.95103

1c CHLORIN

C1	0.01451	−0.00952	−0.00218
C2	2.28543	−0.01363	−0.00899
C3	1.82949	1.34209	−0.00415
N4	0.45511	1.29279	0.00029
C5	1.17832	−0.83742	−0.00718
C6	3.17461	4.97959	−0.02613
C7	2.18238	3.82462	0.00238
C8	2.2675	6.20741	0.10988
C9	0.87147	5.60049	0.06057
N10	0.88754	4.24117	0.02573
C11	−4.62782	1.01484	−0.01941
C12	−3.73454	2.19132	−0.0098
C13	−3.82895	−0.06769	−0.01648
C14	−2.44128	0.43898	−0.00679
N15	−2.42208	1.80621	−0.00274
C16	−3.88039	6.0261	0.02207
C17	−3.43581	4.66882	0.01065
N18	−2.06143	4.70167	0.02382
C19	−1.60528	5.99898	0.04393
C20	−2.76422	6.83741	0.04295
C21	−1.33756	−0.40522	−0.00429
H22	3.69286	2.34273	−0.0212
C23	2.61957	2.50694	−0.00756
H24	−0.09794	7.48138	0.08958
C25	−0.25866	6.40776	0.06472
H26	−5.29115	3.635	−0.01371
C27	−4.21495	3.49487	−0.00612
H28	−1.47868	3.87083	0.01804
H29	−0.16391	2.09693	0.00449
H30	−1.52237	−1.47469	−0.00727
H31	−4.10789	−1.11458	−0.02089
H32	−5.71039	1.05707	−0.02639
H33	−4.91889	6.32852	0.01619
H34	−2.7323	7.91839	0.05669
H35	2.41777	6.73556	1.0598
H36	3.91302	4.89021	0.77845
H37	3.32715	−0.30529	−0.01341
H38	1.15758	−1.91858	−0.01013
H39	2.40903	6.94601	−0.68699
H40	3.73423	4.97527	−0.96989

2p FOTOFRIN PORPHYRIN				**2c FOTOFRIN CHLORIN**			
C1	0.03398	0.187	-2.60732	C1	0.26388	2.58556	0.21534
C2	-2.23089	0.06927	-2.37048	C2	2.53412	2.35853	0.22804
C3	-1.62345	0.07721	-1.08943	C3	1.93223	1.06918	0.27188
N4	-0.27014	0.15111	-1.26677	N4	0.58029	1.24144	0.2466
C5	-1.19975	0.13586	-3.32072	C5	1.50261	3.30178	0.1953
C6	-2.44926	-0.01746	2.69616	C6	2.78396	-2.75674	0.58304
C7	-1.70577	0.07144	1.43171	C7	2.03915	-1.44017	0.36716
C8	-1.52865	0.14552	3.68529	C8	1.89643	-3.72044	-0.24502
C9	-0.22529	0.31746	3.00908	C9	0.55854	-2.98961	-0.15742
N10	-0.3416	0.26589	1.67493	N10	0.68134	-1.69855	0.1319
C11	4.79741	0.55032	-2.09241	C11	-4.50216	2.04779	0.24451
C12	4.02799	0.5435	-0.84025	C12	-3.73	0.79728	0.11161
C13	3.87994	0.44865	-3.09306	C13	-3.58156	3.04522	0.30273
C14	2.55612	0.36638	-2.4329	C14	-2.2501	2.38766	0.2257
N15	2.65885	0.41533	-1.09736	N15	-2.3582	1.05396	0.13229
C16	4.54475	0.78557	2.9642	C16	-4.22416	-2.97407	-0.45892
C17	3.95173	0.67744	1.67996	C17	-3.65058	-1.69065	-0.22323
N18	2.60077	0.57605	1.85596	N18	-2.29535	-1.84521	-0.18916
C19	2.28419	0.60926	3.19452	C19	-1.95138	-3.16461	-0.3927
C20	3.50836	0.74819	3.91127	C20	-3.17332	-3.88906	-0.57155
C21	1.33138	0.26351	-3.14029	C21	-1.03011	3.10705	0.23163
H22	-3.34971	-0.11879	0.14167	H22	3.67056	-0.13671	0.53837
C23	-2.27152	0.00334	0.18648	C23	2.59783	-0.20082	0.3942
H24	0.91318	0.533	4.79974	H24	-0.56429	-4.74055	-0.60399
C25	0.98655	0.49755	3.71878	C25	-0.65056	-3.67771	-0.40316
H26	5.67137	0.80562	0.44278	H26	-5.39295	-0.474	-0.12232
C27	4.59788	0.66847	0.39711	C27	-4.31371	-0.43003	-0.05581
H28	1.92546	0.50401	1.10141	H28	-1.64665	-1.07397	-0.06378
H29	0.41343	0.18824	-0.51762	H29	-0.10489	0.49449	0.26667
C30	-3.71216	0.06183	-2.62814	C30	4.01493	2.6141	0.1779
H31	-4.2316	-0.57616	-1.90382	H31	4.55184	1.93034	0.8452
H32	-3.92762	-0.37813	-3.60742	H32	4.24229	3.6182	0.55097
C33	-4.3206	1.47478	-2.57321	C33	4.58835	2.46829	-1.24277
H34	-3.83699	2.13757	-3.3022	H34	4.11032	3.17253	-1.9349
H35	-4.14417	1.94238	-1.59637	H35	4.37419	1.47158	-1.64991
C36	-5.8093	1.48719	-2.84263	C36	6.08454	2.6842	-1.3007
O37	-6.4929	0.52637	-3.1212	O37	6.81415	2.89271	-0.35585
O38	-6.32175	2.73953	-2.73768	O38	6.54824	2.61209	-2.57428
H39	-7.27613	2.65683	-2.92365	H39	7.51285	2.74832	-2.51755
C40	-3.91537	-0.31527	2.83106	C40	4.29849	-2.79756	0.32926
H41	-4.29662	0.06522	3.78424	H41	4.59795	-3.81929	0.06803
H42	-4.49425	0.20148	2.05724	H42	4.56566	-2.17957	-0.53449
C43	-4.20376	-1.82504	2.74737	C43	5.11805	-2.3677	1.55226
H44	-3.65111	-2.37023	3.52297	H44	4.92205	-3.03214	2.40487
H45	-3.85298	-2.24194	1.79518	H45	4.84422	-1.36571	1.90439
C46	-5.67277	-2.1542	2.89748	C46	6.60969	-2.37808	1.29656
O47	-6.56954	-1.35905	3.07418	O47	7.15414	-2.66624	0.25355
O48	-5.89117	-3.49109	2.81319	O48	7.30304	-2.01738	2.40547
H49	-6.85362	-3.61385	2.91765	H49	8.24572	-2.04038	2.1546
H50	1.3843	0.25916	-4.22306	H50	-1.09238	4.18878	0.24721
C51	4.08371	0.36837	-4.58294	C51	-3.76906	4.52857	0.48081
C52	-1.32823	0.16356	-4.81479	C52	1.62002	4.7954	0.14699
H53	-1.05076	1.14054	-5.23408	H53	1.23525	5.20643	-0.79624
H54	-2.35467	-0.04645	-5.13036	H54	2.66085	5.11802	0.24394

H55	-0.68221	-0.58482	-5.29068
H56	3.20195	0.80739	-5.07665
C57	4.22662	-1.08532	-5.06169
H58	3.34669	-1.6771	-4.78751
H59	5.10837	-1.54599	-4.60473
H60	4.33407	-1.12884	-6.15446
O61	5.23499	1.14107	-4.9418
H62	5.36982	1.02344	-5.89539
C63	6.29336	0.64367	-2.15955
H64	6.65026	1.57397	-1.69978
H65	6.63873	0.62486	-3.19251
H66	6.76279	-0.18384	-1.61181
C67	6.01763	0.84941	3.26833
H68	6.13547	1.23615	4.29246
C69	6.69152	-0.53047	3.20242
H70	7.76026	-0.45417	3.44604
H71	6.59316	-0.95916	2.19985
H72	6.23451	-1.22218	3.91856
O73	6.63661	1.7638	2.35083
H74	7.59018	1.74809	2.53032
C75	3.62066	0.8123	5.40623
H76	4.53557	1.32634	5.71856
H77	3.63893	-0.18674	5.86494
H78	2.77778	1.35462	5.84896
C79	-1.7288	0.14485	5.17005
H80	-1.19352	-0.68516	5.65162
H81	-2.78663	0.05173	5.43441
H82	-1.35513	1.07086	5.62742

H55	1.05346	5.27122	0.95768
H56	-2.96004	5.04654	-0.05954
C57	-3.69371	4.93417	1.96197
H58	-2.73753	4.63326	2.40329
H59	-4.50087	4.45219	2.523
H60	-3.78918	6.0231	2.07411
O61	-5.02056	4.92096	-0.09329
H62	-5.13216	5.86701	0.0898
C63	-5.99984	2.1026	0.30968
H64	-6.44878	1.68158	-0.59904
H65	-6.34809	3.12931	0.4146
H66	-6.37599	1.51041	1.15467
C67	-5.69509	-3.29028	-0.50965
H68	-5.81432	-4.28048	-0.97582
C69	-6.33335	-3.34453	0.8874
H70	-7.40287	-3.58625	0.81724
H71	-6.22799	-2.38203	1.39806
H72	-5.85644	-4.11486	1.50322
O73	-6.34346	-2.30781	-1.33066
H74	-7.29511	-2.49648	-1.30601
C75	-3.24683	-5.36731	-0.81387
H76	-4.24438	-5.67323	-1.14179
H77	-3.00959	-5.94427	0.09051
H78	-2.53835	-5.68017	-1.59004
C79	2.32891	-3.8873	-1.71404
H80	1.59626	-4.48818	-2.26347
H81	3.29918	-4.38987	-1.78874
H82	2.40663	-2.91553	-2.21443
H83	2.61165	-3.0295	1.63786
H84	1.83636	-4.71205	0.22024

3p LEVULAN PORPHYRIN				**3c LEVULAN CHLORIN**			
C1	-1.5378	3.24727	-4.52555	C1	0.38183	2.91226	-0.03605
C2	-2.81881	1.494	-3.85285	C2	-1.90282	2.87972	-0.07615
C3	-1.58323	1.47217	-3.14049	C3	-1.40447	1.54861	-0.21683
N4	-0.84407	2.54447	-3.57969	N4	-0.04465	1.60618	-0.17454
C5	-2.78832	2.60908	-4.70857	C5	-0.79471	3.72459	0.03731
C6	0.40944	-0.45839	-0.43409	C6	-2.55739	-2.19222	-0.56343
C7	0.07193	0.56115	-1.45378	C7	-1.6912	-0.94177	-0.38394
C8	1.6303	-0.10991	0.05534	C8	-1.67399	-3.2562	0.14042
C9	2.0283	1.10523	-0.66958	C9	-0.29745	-2.61153	0.00823
N10	1.04295	1.47923	-1.58704	N10	-0.34831	-1.30155	-0.21175
C11	1.84125	6.52632	-5.34691	C11	5.09913	2.05436	-0.0984
C12	2.13511	5.54766	-4.2891	C12	4.25461	0.85545	-0.03533
C13	0.63807	6.1585	-5.88323	C13	4.24667	3.11806	-0.18049
C14	0.19297	4.98905	-5.10398	C14	2.87418	2.54165	-0.11355
N15	1.15568	4.63916	-4.15702	N15	2.90508	1.20014	-0.0549
C16	4.97225	4.71627	-1.7768	C16	4.49172	-2.97468	0.26957
C17	3.7486	4.70046	-2.52885	C17	4.00364	-1.63786	0.12411
N18	3.02252	3.61896	-2.09993	N18	2.64525	-1.69151	0.06131
C19	3.70351	2.94543	-1.11775	C19	2.2068	-2.99832	0.17123
C20	4.92543	3.60749	-0.89177	C20	3.36409	-3.82028	0.30455
C21	-1.03256	4.38807	-5.22568	C21	1.7097	3.33588	-0.03243
H22	-1.85966	-0.22149	-1.91056	H22	-3.21873	0.48174	-0.55078
C23	-1.14838	0.55302	-2.16729	C23	-2.15854	0.33601	-0.39428
H24	3.87144	1.3513	0.28621	H24	0.69365	-4.46209	0.29524
C25	3.20841	1.76758	-0.46457	C25	0.86432	-3.39874	0.16525
H26	4.02222	6.38647	-3.77479	H26	5.83097	-0.53155	0.06545
C27	3.33415	5.5849	-3.5348	C27	4.75299	-0.42143	0.04757
H28	2.11208	3.35194	-2.46013	H28	2.05666	-0.86867	-0.02854
H29	0.08405	2.7815	-3.24365	H29	0.56817	0.80026	-0.23048
C30	-3.93718	0.49217	-3.74859	C30	-3.35178	3.29763	-0.07331
H31	-3.55702	-0.48001	-3.41954	H31	-3.84284	2.99818	-1.00646
H32	-4.36312	0.33426	-4.74687	H32	-3.38941	4.38969	-0.054
C33	-5.09076	0.90462	-2.80885	C33	-4.21121	2.75145	1.09642
H34	-5.97941	0.29436	-3.02612	H34	-4.87714	3.53915	1.47516
H35	-5.38328	1.94783	-2.95943	H35	-3.60057	2.43386	1.94644
C36	-4.77695	0.6777	-1.34418	C36	-5.11498	1.60603	0.6768
O37	-4.05156	-0.18914	-0.9014	O37	-5.49755	1.41969	-0.46678
O38	-5.44969	1.53584	-0.54428	O38	-5.46089	0.81455	1.70173
H39	-5.21905	1.2928	0.37295	H39	-6.01069	0.07597	1.33696
C40	-0.44225	-1.64493	-0.08519	C40	-4.02866	-2.12686	-0.11111
H41	-0.14924	-2.05603	0.88568	H41	-4.3431	-3.12472	0.21775
H42	-1.49332	-1.34835	0.01828	H42	-4.12773	-1.47416	0.76087
C43	-0.33955	-2.76211	-1.14071	C43	-5.00437	-1.67551	-1.20961
H44	0.70871	-3.05961	-1.28021	H44	-4.97757	-2.35571	-2.06764
H45	-0.68096	-2.42166	-2.12427	H45	-4.75494	-0.67746	-1.58951
C46	-1.11606	-4.00262	-0.75689	C46	-6.42755	-1.58004	-0.71321
O47	-1.55111	-4.2623	0.34336	O47	-6.78224	-1.29993	0.42166
O48	-1.26247	-4.84431	-1.81258	O48	-7.32644	-1.83866	-1.67948
H49	-1.74652	-5.61973	-1.47104	H49	-8.20806	-1.69714	-1.28384
H50	-1.716	4.82486	-5.94455	H50	1.86113	4.40398	0.05433
C51	-0.04199	6.79449	-7.01074	C51	4.62983	4.52048	-0.32558
H52	0.08548	7.87499	-7.08527	H52	5.58396	4.78819	0.12968
C53	-3.87287	3.05495	-5.64599	C53	-0.7708	5.21459	0.20364
H54	-4.58214	3.74023	-5.16134	H54	-0.36791	5.50632	1.18244

H55	-4.45343	2.20329	-6.01808	H55	-1.77023	5.64965	0.11937
H56	-3.46846	3.57649	-6.51919	H56	-0.14188	5.69404	-0.5568
C57	2.74178	7.6524	-5.75107	C57	6.59659	2.05197	-0.11377
H58	3.71049	7.28403	-6.11498	H58	6.98853	1.57035	-1.01898
H59	2.95205	8.32425	-4.90808	H59	7.00405	1.50369	0.74476
H60	2.29996	8.25064	-6.55246	H60	7.00237	3.06701	-0.08371
H61	-0.88097	5.1067	-8.00581	H61	3.04472	5.30074	-1.52226
C62	-0.75606	6.18479	-7.96959	C62	3.97273	5.48461	-0.9901
H63	-1.21217	6.75564	-8.77343	H63	4.37352	6.4928	-1.04502
C64	5.95213	3.22248	0.13007	C64	3.34976	-5.30511	0.49491
H65	6.84501	2.77741	-0.32878	H65	3.58528	-5.845	-0.43296
H66	5.55909	2.49603	0.84668	H66	2.37425	-5.66127	0.8394
H67	6.28581	4.09784	0.69955	H67	4.09595	-5.60652	1.23853
C68	2.45036	-0.78891	1.11071	C68	-2.00098	-3.49066	1.62907
H69	2.70599	-0.10077	1.9268	H69	-1.25467	-4.15163	2.08267
H70	3.39662	-1.17129	0.70535	H70	-2.98263	-3.95845	1.75811
H71	1.91488	-1.63551	1.55042	H71	-1.99461	-2.54774	2.18717
C72	6.00128	5.72449	-1.93937	C72	5.90275	-3.30786	0.39544
H73	5.69927	6.60074	-2.51206	H73	6.54778	-2.47332	0.66776
C74	7.26843	5.71306	-1.48274	C74	6.49828	-4.50064	0.22172
H75	7.92909	6.55208	-1.67938	H75	7.56949	-4.60635	0.36601
H76	7.69429	4.88626	-0.92656	H76	5.96375	-5.39356	-0.08167
				H77	-2.53602	-2.43898	-1.63744
				H78	-1.71186	-4.21928	-0.38324

4p VISUDYNE PORPHYRIN				4c VISUDYNE CHLORIN			
C1	0.50949	-1.05317	-3.11905	C1	2.33708	-1.38095	-1.03163
C2	-1.7665	-0.9075	-3.00423	C2	0.38153	-2.48681	-1.39206
C3	-1.19425	-0.56339	-1.71999	C3	0.17352	-1.083	-1.579
N4	0.17028	-0.66608	-1.84769	N4	1.36803	-0.45858	-1.35082
C5	-0.73291	-1.21475	-3.85787	C5	1.71519	-2.67427	-1.05055
C6	-2.16147	0.53356	1.82975	C6	-2.64231	1.43451	-2.52487
C7	-1.34406	0.14508	0.67601	C7	-1.2925	0.88878	-2.0737
C8	-1.27505	0.81902	2.83021	C8	-2.4904	2.95219	-2.24582
C9	0.05841	0.58104	2.26455	C9	-0.9834	3.07028	-2.04347
N10	-0.00868	0.18072	0.97094	N10	-0.36861	1.89154	-1.89603
C11	4.45457	-0.56814	-1.2956	C11	4.65961	2.28158	-1.33209
C12	4.371	-1.25111	-3.53872	C12	5.8019	0.3331	-0.59412
C13	3.00198	-1.00742	-2.89704	C13	4.30318	0.1469	-0.87266
N14	3.09077	-0.65932	-1.61481	N14	3.69132	1.30553	-1.18525
C15	4.81983	0.41162	2.43234	C15	2.99211	5.70216	-1.74975
C16	4.24642	0.09102	1.13484	C16	3.1996	4.29295	-1.6528
N17	2.87467	0.14165	1.28981	N17	1.96108	3.69348	-1.67928
C18	2.53526	0.4917	2.57044	C18	0.96816	4.62958	-1.81121
C19	3.78651	0.62664	3.31586	C19	1.61635	5.92859	-1.81308
C20	1.79398	-1.22565	-3.60415	C20	3.68164	-1.09623	-0.77189
H21	-2.96286	-0.16503	-0.66097	H21	-1.87396	-1.12791	-2.12075
C22	-1.88223	-0.19914	-0.56993	C22	-1.04654	-0.4541	-1.93209
H23	1.14592	1.06781	4.03512	H23	-1.03015	5.1854	-2.17104
C24	1.24623	0.72772	3.01281	C24	-0.38315	4.33604	-1.99869
H25	6.0271	-0.17601	0.08714	H25	5.31075	4.2684	-1.59256
C26	4.94691	-0.20849	-0.00658	C26	4.43463	3.63175	-1.53975
H27	2.19037	0.00808	0.55316	H27	1.80044	2.69257	-1.66275
H28	0.83318	-0.48165	-1.10316	H28	1.53068	0.53953	-1.41548
C29	-3.24038	-0.85044	-3.28241	C29	-0.70123	-3.50948	-1.56216
H30	-3.78667	-1.27832	-2.43487	H30	-1.6134	-3.1571	-1.06808
H31	-3.49223	-1.46313	-4.15399	H31	-0.42661	-4.44529	-1.06545
C32	-3.73888	0.6044	-3.51647	C32	-1.03262	-3.80305	-3.05096
H33	-3.51568	0.92863	-4.53561	H33	-0.27811	-4.4583	-3.48972
H34	-3.22504	1.27594	-2.82093	H34	-1.03773	-2.86278	-3.60968
C35	-5.23158	0.73803	-3.28651	C35	-2.38904	-4.45478	-3.19631
O36	-6.07258	0.91822	-4.13937	O36	-2.59313	-5.60508	-3.50287
O37	-5.51332	0.61148	-1.96818	O37	-3.36407	-3.56275	-2.90569
C38	-3.66325	0.53754	1.88614	C38	-3.90898	0.69038	-2.05816
H39	-4.00822	1.26979	2.62548	H39	-4.78658	1.25766	-2.39406
H40	-4.0965	0.85405	0.93135	H40	-3.96478	-0.26528	-2.58937
C41	-4.23222	-0.84709	2.25552	C41	-4.03833	0.39019	-0.55913
H42	-3.84334	-1.19091	3.21941	H42	-4.13822	1.28806	0.05033
H43	-3.91057	-1.59607	1.51873	H43	-3.13463	-0.12136	-0.20389
C44	-5.74694	-0.86664	2.29905	C44	-5.20935	-0.52107	-0.26133
O45	-6.48236	-0.08729	1.72687	O45	-5.66163	-1.36569	-1.00386
O46	-6.20044	-1.88644	3.05896	O46	-5.69607	-0.28918	0.97602
H47	1.87784	-1.55455	-4.63238	H47	4.30132	-1.94606	-0.52525
C48	-0.80325	-1.6276	-5.29574	C48	2.42227	-3.95971	-0.75438
H49	-0.28284	-2.57758	-5.4662	H49	2.73572	-4.01781	0.2964
H50	-0.33336	-0.88307	-5.95136	H50	3.32667	-4.07016	-1.3651
H51	-1.83829	-1.75071	-5.62571	H51	1.78	-4.82138	-0.95391
C52	-1.55254	1.27417	4.23098	C52	-3.25824	3.54021	-1.04944
H53	-1.224	0.53528	4.97452	H53	-2.92833	3.10659	-0.10059
H54	-2.62123	1.44696	4.3919	H54	-4.3369	3.38004	-1.15239

H55	-1.03002	2.21144	4.46109
C56	-6.90573	0.70678	-1.60716
H57	-7.29818	1.68979	-1.88175
H58	-6.93488	0.56012	-0.52821
H59	-7.48482	-0.06176	-2.12673
C60	6.29081	0.43876	2.71138
H61	6.80988	1.13979	2.04682
H62	6.74469	-0.54841	2.55764
H63	6.49821	0.73701	3.74162
C64	3.92351	0.92484	4.74205
H65	4.80516	1.50434	5.01388
H66	2.23882	-0.09849	5.55132
C67	3.10843	0.526	5.72936
H68	3.31223	0.79665	6.76131
C69	4.76606	-0.35045	-4.77133
H70	4.58716	0.68937	-4.46681
C71	6.26526	-0.50479	-5.02645
H72	8.19139	-0.61291	-4.1262
C73	7.12537	-0.63418	-3.92419
C74	6.65662	-0.71238	-2.61638
H75	7.35533	-0.64063	-1.78663
C76	5.26587	-0.84941	-2.3944
C77	4.52452	-2.76921	-3.83529
H78	5.54134	-2.98466	-4.17623
H79	3.82978	-3.0918	-4.6118
H80	4.33498	-3.34151	-2.92162
C81	6.90733	-0.37065	-6.33776
O82	8.09593	-0.56127	-6.55329
O83	6.04985	0.02072	-7.32081
C84	3.88146	-0.59356	-5.99283
O85	3.67597	-1.6615	-6.53096
O86	3.28523	0.55462	-6.37672
C87	6.63173	0.12336	-8.6263
H88	7.0275	-0.84377	-8.94902
H89	7.44358	0.85588	-8.63017
H90	5.82296	0.44413	-9.28458
C91	2.47119	0.45756	-7.55373
H92	1.64902	-0.24776	-7.40179
H93	3.07212	0.12034	-8.40289
H94	2.08628	1.4629	-7.72863
C95	-7.63076	-2.013	3.13719
H96	-8.07278	-1.10666	3.55956
H97	-7.81313	-2.86884	3.7879
H98	-8.05654	-2.18665	2.14513

H55	-3.0906	4.62056	-0.99145
C56	-4.71526	-4.05845	-2.94112
H57	-5.00367	-4.29238	-3.97034
H58	-5.32642	-3.25436	-2.53366
H59	-4.80353	-4.96424	-2.33567
C60	4.09465	6.71811	-1.72903
H61	4.81663	6.54604	-2.53758
H62	4.65447	6.68708	-0.78541
H63	3.70807	7.73372	-1.84297
C64	0.97817	7.23571	-1.86333
H65	1.59284	8.02776	-2.29129
H66	-0.90652	6.88711	-0.92121
C67	-0.24157	7.58428	-1.41948
H68	-0.59529	8.6067	-1.51548
C69	6.78622	-0.74234	-1.17949
H70	6.35007	-1.15403	-2.09694
C71	8.14117	-0.12581	-1.52163
H72	9.27584	1.56262	-2.01389
C73	8.29255	1.2059	-1.72122
C74	7.18305	2.12375	-1.68558
H75	7.30518	3.11479	-2.11603
C76	5.98497	1.69357	-1.23499
C77	5.98641	0.52959	0.93984
H78	7.03314	0.73196	1.17954
H79	5.67635	-0.36041	1.49325
H80	5.37435	1.37071	1.27745
C81	9.32137	-0.977	-1.79971
O82	10.45932	-0.57513	-1.93574
O83	8.98085	-2.2835	-1.93808
C84	6.99976	-1.91316	-0.21885
O85	7.70582	-1.88773	0.75997
O86	6.30087	-3.00701	-0.57956
C87	10.07481	-3.17557	-2.19539
H88	10.77876	-3.16566	-1.35873
H89	10.60232	-2.88416	-3.10727
H90	9.62745	-4.16385	-2.3096
C91	6.47869	-4.15001	0.27133
H92	6.15919	-3.92476	1.29229
H93	7.52968	-4.44927	0.2872
H94	5.86009	-4.93691	-0.16081
C95	-6.78411	-1.13543	1.38412
H96	-7.632	-1.02665	0.70248
H97	-7.05337	-0.80247	2.38713
H98	-6.47247	-2.18342	1.39878
H99	-2.78804	3.52682	-3.13049
H100	-2.64579	1.33057	-3.61978

5p TETRASULPHO PORPHYRIN			**5c TETRASULPHO CHLORIN**		
C1	-0.68113	0.2094	C1	0.94631	2.95289	-0.01526
C2	1.5762	0.25979	C2	-0.93286	4.18746	0.19478
C3	1.01623	0.43163	C3	-1.30283	2.82335	0.07361
N4	-0.35038	0.40973	N4	-0.12907	2.10654	-0.05461
C5	0.52974	0.10985	C5	0.45101	4.26356	0.13749
C6	2.00381	0.31163	C6	-2.98637	0.93093	0.05064
C7	1.20418	0.36634	C7	-2.88749	-1.27233	-0.10413
C8	1.1426	0.09869	N8	-2.14868	-0.09321	-0.0183
C9	-0.19841	0.09138	C9	4.28222	-0.4387	-0.02874
N10	-0.14302	0.24567	C10	2.89764	-0.92153	0.01579
C11	-5.4032	0.2858	C11	4.2192	0.90504	-0.09389
C12	-4.60543	0.33802	C12	2.80249	1.25787	-0.05179
C13	-4.53334	0.16089	N13	2.0239	0.10315	0.00372
C14	-3.19537	0.14487	C14	0.88254	-4.19697	0.04109
N15	-3.25645	0.25049	C15	1.26357	-2.83297	0.0992
C16	-4.9495	0.39036	N16	0.09128	-2.09531	0.08833
C17	-4.42652	0.29835	C17	-0.98842	-2.92768	0.01378
N18	-3.07117	0.09489	C18	-0.50092	-4.25221	-0.00788
C19	-2.71522	0.04856	C19	2.33524	2.55621	-0.06811
C20	-3.89493	0.22419	C20	-2.38063	-2.5378	-0.07604
C21	-2.01293	0.08505	C21	2.56948	-2.30541	0.08239
C22	-1.3819	-0.05766	H22	0.06145	-1.08224	0.09828
C23	-5.15314	0.40046	H23	-0.05643	1.09677	-0.11867
H24	-2.42452	0.02938	H24	1.56583	-5.03176	0.01035
H25	-1.02282	0.47045	H25	5.0446	1.59771	-0.16255
H26	-5.98301	0.57616	H26	5.17064	-1.05228	-0.01201
H27	-4.76228	0.10265	H27	-1.11097	-5.14042	-0.07357
H28	-6.48103	0.31791	H28	-1.62046	5.0091	0.32729
H29	-3.9471	0.26355	H29	1.05654	5.15391	0.21759
H30	1.38278	-0.03482	C30	-3.34184	-3.68543	-0.16253
H31	3.07693	0.40854	C31	-5.08693	-5.8451	-0.32106
H32	2.63253	0.21149	C32	-3.84939	-4.09986	-1.40066
H33	0.61675	-0.07603	C33	-3.72003	-4.38122	0.99453
C34	-1.2819	-0.34128	C34	-4.59265	-5.46266	0.92428
C35	-1.05782	-0.98273	C35	-4.72122	-5.1817	-1.48937
C36	-0.62855	0.52714	H36	-3.5419	-3.57908	-2.30323
C37	-1.85615	-1.52005	H37	-3.31733	-4.0733	1.95536
C38	-1.7464	-1.84763	H38	-4.87499	-6.0158	1.81389
C39	-0.51106	0.21161	C39	3.32756	3.67118	-0.13308
H40	-0.22079	1.46333	C40	5.23528	5.69404	-0.31618
H41	-2.37929	-2.19127	C41	3.38288	4.5026	-1.263
H42	-2.18828	-2.75904	C42	4.23886	3.89126	0.91193
C43	-2.12399	-0.16913	C43	5.19668	4.89797	0.8255
C44	-2.23437	-0.74588	C44	4.33954	5.50608	-1.36736
C45	-1.59597	0.72748	H45	2.68756	4.3382	-2.08011
C46	-2.7345	-1.34934	H46	4.19619	3.26315	1.79569
C47	-2.79536	-1.642	H47	5.91493	5.05705	1.62296
C48	-1.64821	0.44656	C48	3.68127	-3.29869	0.10571
H49	-1.14635	1.65598	C49	5.73012	-5.19048	0.13382
H50	-3.14662	-2.05124	C50	4.55402	-3.42766	-0.98696
H51	-3.26626	-2.55443	C51	3.85909	-4.14711	1.2108
C52	-6.62995	0.57872	C52	4.8792	-5.09294	1.23266
C53	-9.39887	0.88905	C53	5.57498	-4.37166	-0.98246
C54	-7.24432	1.73029	H54	4.41396	-2.79465	-1.85748

C55	-7.43234	-0.40002	0.92479
C56	-8.81494	-0.25293	0.98569
C57	-8.62653	1.89182	-0.14806
H58	-6.6296	2.50478	-0.65427
H59	-6.96836	-1.29085	1.33684
H60	-9.10198	2.78503	-0.53955
C61	1.74208	0.4876	-0.2756
C62	3.223	0.63299	-0.40289
C63	5.98728	0.97087	-0.53758
C64	3.77275	1.81261	-0.93126
C65	4.08892	-0.39146	0.01298
C66	5.47083	-0.22914	-0.0506
C67	5.15188	1.99078	-0.99538
H68	3.11157	2.60301	-1.27379
H69	3.67256	-1.32172	0.3874
H70	6.14121	-1.02236	0.26363
H71	-0.01603	0.88683	7.79543
H72	5.57838	2.90539	-1.39345
H73	-1.24925	1.14373	-8.00186
H74	-9.43536	-1.01058	1.45244
S75	-0.88042	-1.41867	9.29437
O76	-0.42062	-0.25452	10.05206
O77	-2.04608	-2.18937	9.69982
S78	-11.17639	1.06287	0.47303
O79	-11.68703	0.35324	1.63615
O80	-11.53969	2.45201	0.19164
S81	-2.25553	-1.14163	-9.43777
O82	-3.45988	-1.90559	-9.726
O83	-1.88336	0.04227	-10.21306
S84	7.75632	1.21434	-0.56506
O85	8.43254	-0.0777	-0.44332
O86	8.07868	2.15465	-1.62766
O87	7.9821	1.99304	0.87257
H88	8.62703	1.4582	1.37433
O89	-11.59991	0.1916	-0.86273
H90	-12.1017	0.79976	-1.43834
O91	-0.97974	-2.1839	-9.53711
H92	-0.35321	-1.78933	-10.17333
O93	0.39751	-2.46112	9.22208
H94	1.08018	-2.09669	9.81715

H55	3.19062	-4.05698	2.06166
H56	6.23174	-4.48997	-1.83784
C57	-2.61898	2.3035	0.10721
C58	-3.70923	3.3211	0.21082
C59	-5.67957	5.27794	0.42399
C60	-4.00464	4.15939	-0.87555
C61	-4.42364	3.48757	1.40623
C62	-5.40518	4.46705	1.52246
C63	-4.9884	5.13858	-0.77757
H64	-3.44947	4.04423	-1.80186
H65	-4.18292	2.86514	2.26344
H66	-5.93575	4.62156	2.45603
H67	-5.09946	-5.52265	-2.44731
H68	-5.206	5.79966	-1.60993
H69	4.40957	6.12244	-2.2574
H70	5.01052	-5.75499	2.0821
S71	-6.14386	-7.27334	-0.43251
O72	-6.10711	-7.80756	-1.78844
O73	-5.92258	-8.14642	0.71521
S74	6.99466	-6.44267	0.11876
O75	6.64508	-7.51448	1.04468
O76	7.37126	-6.74659	-1.25682
S77	6.51213	6.9247	-0.4775
O78	7.6225	6.6103	0.41456
O79	6.75201	7.20076	-1.88911
S80	-6.87244	6.58985	0.59444
O81	-7.04754	6.9068	2.00616
O82	-6.59547	7.64499	-0.37464
O83	-8.20242	5.76455	0.07216
H84	-8.91777	6.41822	-0.0524
O85	8.20605	-5.55265	0.80154
H86	8.97612	-6.14442	0.90776
O87	5.68474	8.2001	0.16504
H88	6.29955	8.9588	0.19631
O89	-7.58948	-6.50579	-0.2133
H90	-8.27666	-7.19729	-0.14954
C91	-4.45313	0.51979	0.05115
H92	-5.03341	1.07513	-0.69067
H93	-4.91177	0.7359	1.02208
C94	-4.37675	-0.98121	-0.22449
H95	-4.73473	-1.22206	-1.23169
H96	-4.97437	-1.58067	0.4669

6p FOSCAN PORPHYRIN				**6c FOSCAN CHLORIN**			
C1	0.00274	-3.1135	0.20511	C1	0.44594	-0.89621	-2.89597
C2	-2.19682	-3.66432	0.20654	C2	-1.78826	-1.08466	-2.53697
C3	-2.07974	-2.29611	-0.10356	C3	-1.20171	-0.49004	-1.40036
N4	-0.74033	-1.99352	-0.09924	N4	0.136	-0.38375	-1.64593
C5	-0.9159	-4.16745	0.41652	C5	-0.77474	-1.36058	-3.44778
C6	-3.07033	0.01389	-0.25962	C6	-1.31141	0.08757	1.04151
C7	-2.29166	2.02017	0.10855	C7	0.21029	-0.15378	2.63239
N8	-1.90686	0.72991	0.02613	N8	0.05759	-0.05248	1.31781
C9	4.14625	-0.93461	-0.6296	C9	4.84013	0.8348	-2.66556
C10	3.03141	-0.02419	-0.4024	C10	4.19711	0.68987	-1.36172
C11	3.68572	-2.17984	-0.37429	C11	4.04207	0.21106	-3.5596
C12	2.26819	-2.03729	-0.0373	C12	2.86636	-0.25639	-2.81777
N13	1.88107	-0.74628	-0.07995	N13	2.96528	0.04662	-1.50881
C14	2.18126	3.64746	0.15875	C14	4.86934	0.7271	2.37586
C15	2.0525	2.28109	-0.15614	C15	4.1837	0.78904	1.14514
N16	0.71534	1.97481	-0.0895	N16	2.88365	0.44135	1.38803
C17	-0.01466	3.09071	0.25547	C17	2.70429	0.13997	2.72412
C18	0.91121	4.14559	0.43152	C18	3.96801	0.30348	3.34603
C19	1.42662	-3.15608	0.24313	C19	1.73839	-0.85627	-3.46384
C20	-1.43579	3.1349	0.35576	C20	1.46137	-0.19992	3.31732
C21	3.1258	1.35745	-0.43323	C21	4.75801	1.07106	-0.15699
H22	0.32019	1.04414	-0.17158	H22	2.17716	0.30083	0.67482
H23	-0.34689	-1.06276	-0.18914	H23	0.8432	-0.06257	-0.99446
H24	3.11481	4.18785	0.20022	H24	5.91808	0.94548	2.50886
H25	4.2245	-3.11401	-0.44477	H25	4.19049	0.11108	-4.6254
H26	5.13924	-0.64961	-0.94386	H26	5.77705	1.33739	-2.85388
H27	0.65813	5.15163	0.72613	H27	4.17038	0.13577	4.39252
H28	-3.12939	-4.20141	0.2927	H28	-2.84157	-1.29677	-2.64723
H29	-0.65104	-5.17547	0.69391	H29	-0.87752	-1.83526	-4.41128
C30	-2.06129	4.43418	0.71768	C30	1.46146	-0.57979	4.75875
C31	-3.24812	6.87504	1.46562	C31	1.47656	-1.3685	7.45727
C32	-2.90141	4.50594	1.83832	C32	1.06077	-1.8711	5.12427
C33	-1.8289	5.60318	-0.03158	C33	1.8669	0.31848	5.76154
C34	-2.42261	6.80532	0.34326	C34	1.87011	-0.08027	7.09622
C35	-3.4856	5.71755	2.21265	C35	1.07082	-2.26491	6.46403
H36	-3.09175	3.62554	2.44281	H36	0.76404	-2.59417	4.37046
H37	-1.20079	5.55759	-0.91475	H37	2.16856	1.32499	5.48951
H38	-2.2463	7.70136	-0.24618	H38	2.18058	0.61875	7.86839
H39	-3.70559	7.81857	1.7586	H39	1.48514	-1.67676	8.50115
C40	2.07829	-4.44515	0.58953	C40	1.93498	-1.42286	-4.82372
C41	3.34812	-6.85612	1.31849	C41	2.37315	-2.54601	-7.37457
C42	2.98095	-4.48715	1.66706	C42	2.93167	-2.39447	-5.02256
C43	1.82609	-5.63017	-0.12087	C43	1.16389	-1.01855	-5.92586
C44	2.46248	-6.8169	0.24518	C44	1.38989	-1.57905	-7.18377
C45	3.6053	-5.68069	2.03121	C45	3.14668	-2.95237	-6.28319
H46	3.17794	-3.57872	2.23286	H46	3.53012	-2.72487	-4.17593
H47	1.15197	-5.61184	-0.97055	H47	0.40893	-0.24948	-5.79825
H48	2.26824	-7.72575	-0.31852	H48	0.79409	-1.25114	-8.03172
H49	3.84453	-7.77432	1.61647	H49	2.55661	-2.99096	-8.34745
C50	4.44814	1.98746	-0.72511	C50	6.07622	1.77108	-0.13448
C51	6.92276	3.17962	-1.31289	C51	8.52649	3.14995	-0.08237
C52	5.56441	1.75096	0.09607	C52	7.23718	1.18211	-0.66437
C53	4.58085	2.83574	-1.83156	C53	6.16203	3.04749	0.43783
C54	5.81345	3.41971	-2.13009	C54	7.37592	3.73617	0.45536

C55	6.78717	2.34936	-0.201
H56	5.46243	1.11497	0.96867
H57	3.73538	3.03724	-2.48042
H58	7.64616	2.17103	0.44059
H59	7.88122	3.64164	-1.54408
C60	-3.16517	-1.36688	-0.31907
C61	-4.49371	-1.99266	-0.58458
C62	-6.98318	-3.17895	-1.14707
C63	-4.65054	-2.83051	-1.70066
C64	-5.59449	-1.76742	0.25518
C65	-6.82439	-2.36349	-0.03108
C66	-5.88742	-3.40998	-1.98557
H67	-3.80138	-3.01475	-2.3557
H68	-5.47829	-1.14297	1.13432
H69	-7.67086	-2.19035	0.62832
H70	-7.93529	-3.64374	-1.38331
O71	-6.08881	-4.21385	-3.07403
H72	-5.25779	-4.28903	-3.56857
O73	-4.27893	5.70974	3.32749
H74	-4.60526	6.6088	3.4879
O75	5.87368	4.21931	-3.23834
H76	6.77964	4.54967	-3.34037
O77	4.47657	-5.76167	3.08308
H78	4.55799	-4.88597	3.49216
C79	-4.19401	0.92898	-0.42122
H80	-5.20013	0.65052	-0.69623
C81	-3.72279	2.16847	-0.16059
H82	-4.26504	3.1029	-0.18398

C55	8.4474	1.87264	-0.63488
H56	7.18737	0.18181	-1.08249
H57	5.28394	3.52642	0.85918
H58	9.34298	1.41056	-1.04226
H59	9.47331	3.6871	-0.06416
C60	-1.88736	-0.08359	-0.18136
C61	-3.36789	0.11648	-0.32678
C62	-6.13123	0.54772	-0.63696
C63	-3.84894	1.34332	-0.80356
C64	-4.28295	-0.89649	-0.0133
C65	-5.65363	-0.67279	-0.16883
C66	-5.22073	1.55936	-0.95633
H67	-3.14284	2.13252	-1.05756
H68	-3.91871	-1.85415	0.34819
H69	-6.35913	-1.46254	0.07625
H70	-7.19313	0.73449	-0.76316
O71	-5.73077	2.74458	-1.41305
H72	-4.99626	3.34671	-1.61021
O73	0.67892	-3.54598	6.73972
H74	0.75419	-3.70048	7.69398
O75	7.37723	4.98674	1.01185
H76	8.27012	5.35911	0.946
O77	4.10043	-3.90776	-6.50912
H78	4.55506	-4.10069	-5.67421
C79	-2.06964	0.40265	2.32133
H80	-3.06991	-0.03126	2.34945
H81	-2.18226	1.49079	2.43217
C82	-1.11541	-0.14925	3.38952
H83	-1.39358	-1.17027	3.68166
H84	-1.07223	0.44401	4.30657

7p MACE-e6 PORPHYRIN			
C1	3.30205	-1.64936	0.21739
C2	2.37445	-3.28597	-1.04661
C3	1.6089	-2.07346	-1.23123
N4	2.24131	-1.11995	-0.46217
C5	3.3829	-3.02235	-0.10605
C6	-0.33201	-0.56042	-1.77849
C7	-0.62483	1.59972	-1.7187
N8	0.31619	0.57973	-1.54966
C9	5.35408	2.31475	1.95704
C10	4.26411	2.53095	0.98733
C11	5.43534	0.96699	2.13499
C12	4.40165	0.38322	1.26544
N13	3.69654	1.38617	0.60362
C14	2.22502	5.33632	-0.72661
C15	2.78212	4.07298	-0.30061
N16	1.90515	3.09395	-0.6988
C17	0.78909	3.65156	-1.25578
C18	0.96818	5.06009	-1.28286
C19	4.21133	-0.95696	1.07849
C20	0.3661	-1.83831	-1.86293
H21	-1.21207	3.58903	-1.91191
C22	-0.37831	2.94497	-1.65144
H23	4.43797	4.67498	0.86796
C24	3.87926	3.81808	0.51488
H25	2.06554	2.11144	-0.48881
H26	1.93343	-0.15108	-0.45403
H27	4.87436	-1.61673	1.6288
C28	4.4106	-3.97358	0.43015
H29	5.41347	-3.53256	0.41605
H30	4.43169	-4.89998	-0.14449
H31	4.18644	-4.24979	1.46892
C32	6.16298	3.40368	2.59005
H33	5.52236	4.13548	3.09975
H34	6.74884	3.96012	1.84591
H35	6.86472	3.00585	3.32885
C36	-0.02219	6.04006	-1.84083
H37	0.3012	7.07092	-1.67614
H38	-1.00858	5.92751	-1.37362
H39	-0.1592	5.91119	-2.92183
C40	6.39652	0.20083	2.99816
H41	6.66539	0.81047	3.86871
H42	5.904	-0.69209	3.40191
C43	7.68396	-0.21622	2.26246
H44	8.3463	-0.78366	2.92645
C45	2.84057	6.64672	-0.59882
H46	2.14753	7.48377	-0.51618
H47	4.50974	7.94735	-0.49616
C48	4.15516	6.92647	-0.60419
H49	4.91039	6.16	-0.74735
C50	-2.93243	-1.29442	-2.02833
H51	-2.74668	-2.1401	-2.69245
H52	-3.81389	-0.79498	-2.44337
C53	-3.30363	-1.89539	-0.64635
H54	-2.39226	-2.22163	-0.14034

7c MACE-e6 CHLORIN			
C1	0.45419	-0.83034	-3.43676
C2	-1.60901	-0.4704	-4.32986
C3	-1.66673	-0.18532	-2.93318
N4	-0.41045	-0.36816	-2.45148
C5	-0.29603	-0.91463	-4.63163
C6	-2.73267	0.74507	-0.86459
C7	-1.86899	1.59252	0.98011
N8	-1.55753	1.14061	-0.23529
C9	4.57164	-0.69542	-0.9527
C10	3.47088	0.0772	-0.36266
C11	4.06878	-1.26436	-2.08139
C12	2.65085	-0.83308	-2.15984
N13	2.30405	-0.06646	-1.11454
C14	2.60709	2.45237	2.53555
C15	2.5435	1.62799	1.37069
N16	1.23374	1.52042	1.01023
C17	0.42426	2.17283	1.91773
C18	1.27858	2.76539	2.88957
C19	1.80935	-1.14649	-3.24802
C20	-2.81611	0.11097	-2.07723
H21	-1.44673	2.58749	2.79869
C22	-0.97935	2.1523	1.91946
H23	4.56057	0.94244	1.22157
C24	3.59154	0.88201	0.74082
H25	0.9315	1.00639	0.18599
H26	-0.15076	-0.19634	-1.48714
H27	2.27777	-1.66235	-4.07746
C28	0.23088	-1.32387	-5.97102
H29	1.31992	-1.37624	-5.97466
H30	-0.08745	-0.62641	-6.74544
H31	-0.15794	-2.3016	-6.26844
C32	5.95353	-0.79337	-0.37952
H33	5.93337	-1.13957	0.66112
H34	6.463	0.17939	-0.38265
H35	6.57651	-1.48954	-0.94866
C36	0.80931	3.59177	4.05104
H37	1.64185	3.86933	4.70256
H38	0.07543	3.04882	4.66451
H39	0.33116	4.52528	3.72218
C40	4.76736	-2.15612	-3.0687
H41	5.59349	-2.67659	-2.56865
H42	4.07728	-2.94229	-3.40398
C43	5.32568	-1.40693	-4.2934
H44	5.80931	-2.10416	-4.98754
C45	3.80925	2.87737	3.24767
H46	3.68656	3.02257	4.32163
H47	5.85104	3.4357	3.34855
C48	5.01943	3.13159	2.71922
H49	5.21531	3.0717	1.6525
C50	-4.7017	2.35366	-0.64472
H51	-4.63691	2.32441	-1.73792
H52	-4.1836	3.27447	-0.34117
C53	-6.20335	2.43522	-0.27868
H54	-6.73171	1.58654	-0.72634

H55	7.45762	-0.84014	1.39086
C56	-1.9357	1.03838	-2.01167
C57	-1.78601	-0.31828	-2.00878
H58	-3.90215	-2.79823	-0.81043
O59	-3.59795	0.15756	0.59556
C60	-4.03594	-0.93607	0.27473
H61	-5.5427	-2.33193	0.49153
N62	-5.24056	-1.4	0.73976
C63	-6.04125	-0.67075	1.70799
H64	-5.61449	0.32971	1.7623
C65	-6.01577	-1.35881	3.07627
H66	-4.98227	-1.4845	3.41265
H67	-6.45147	-2.36174	3.00154
C68	-7.4655	-0.59958	1.16492
O69	-8.26473	-1.50549	1.24406
O70	-7.71212	0.55363	0.52108
H71	-8.628	0.49379	0.1886
C72	-6.78933	-0.59398	4.12138
O73	-7.44915	0.39916	3.92049
O74	-6.66579	-1.1601	5.34218
H75	-7.20222	-0.61766	5.95094
C76	-0.21584	-2.92798	-2.72452
H77	-1.0181	-2.53233	-3.3481
H78	0.53138	-3.29241	-3.42984
C79	-0.76777	-4.13444	-1.98407
O80	-1.10369	-4.17987	-0.82587
O81	-0.85832	-5.21303	-2.79895
H82	-1.2134	-5.93418	-2.24656
H83	8.2308	0.66311	1.90481
C84	-3.18887	1.84356	-2.16727
H85	-3.03576	2.70251	-2.83182
H86	-3.53047	2.21971	-1.19662
H87	-4.0046	1.25028	-2.58878
C88	2.28661	-4.60361	-1.69486
O89	2.35542	-5.67238	-1.12443
O90	2.21884	-4.54589	-3.05257
H91	2.14048	-5.47063	-3.35082

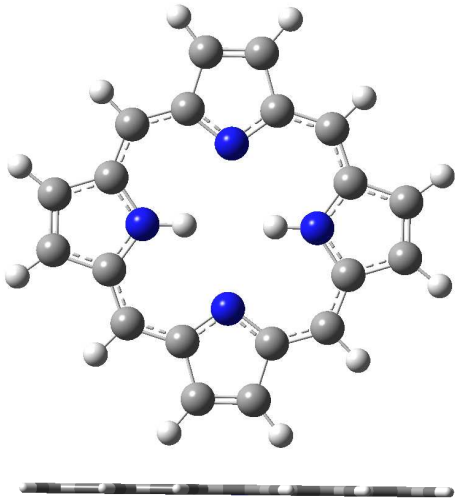
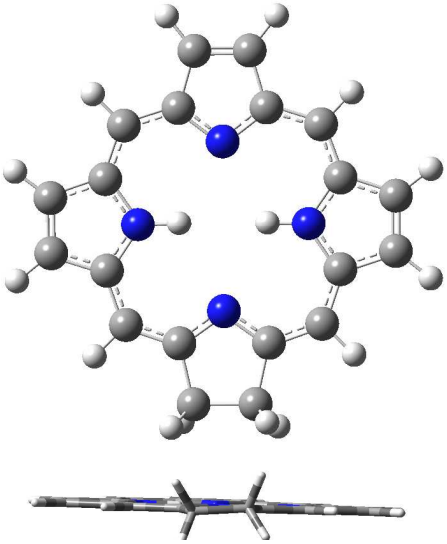
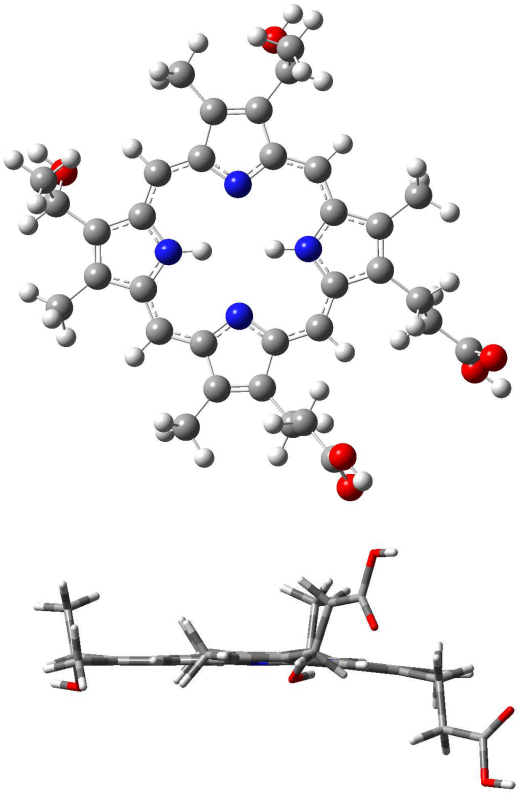
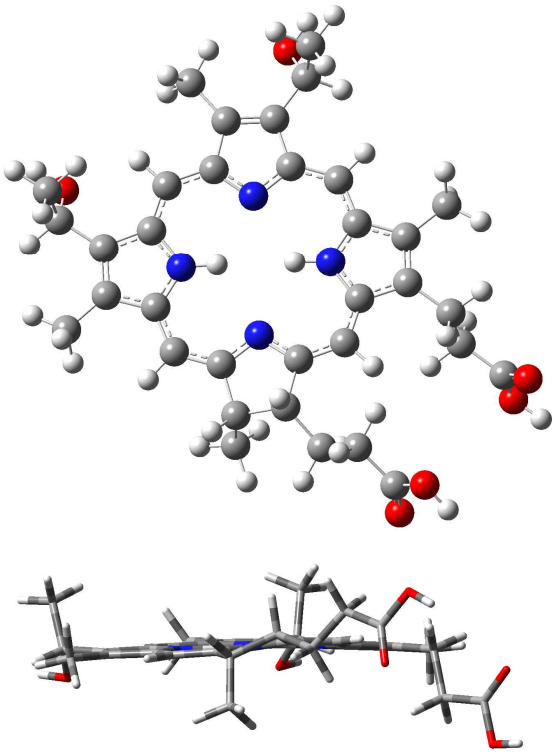
H55	4.53373	-0.87796	-4.83479
C56	-3.33832	1.41939	1.34474
C57	-3.96498	1.12826	-0.03516
H58	-4.66376	0.28966	0.03664
H59	-6.62716	3.35439	-0.70663
O60	-6.76595	1.31644	1.79171
C61	-6.49566	2.36636	1.21794
H62	-6.20483	4.41515	1.36404
N63	-6.41114	3.57003	1.88247
C64	-6.57495	3.68622	3.32738
H65	-6.57324	2.67265	3.72328
C66	-7.87731	4.40698	3.68703
H67	-8.72732	3.89237	3.22834
H68	-7.86287	5.42911	3.29309
C69	-5.36551	4.46137	3.84808
O70	-5.22936	5.65567	3.72269
O71	-4.42096	3.66229	4.37071
H72	-3.68516	4.24499	4.64153
C73	-8.08095	4.48888	5.18359
O74	-7.25555	4.18913	6.01707
O75	-9.30905	4.95408	5.49885
H76	-9.34871	4.99354	6.47409
C77	-4.14588	-0.50223	-2.47021
H78	-4.9874	0.17429	-2.29086
H79	-4.20398	-0.73319	-3.52798
C80	-4.45601	-1.78696	-1.70575
O81	-3.92267	-2.18697	-0.6945
O82	-5.47307	-2.45758	-2.30735
H83	-5.63661	-3.2473	-1.75661
H84	6.06887	-0.6619	-3.98798
H85	-3.73126	2.3379	1.79772
C86	-3.53258	0.25848	2.34255
H87	-2.9855	0.44164	3.27514
H88	-3.1751	-0.68486	1.9104
H89	-4.595	0.15209	2.57727
C90	-2.58562	-0.18383	-5.38105
O91	-2.58334	-0.66751	-6.49435
O92	-3.51206	0.76476	-5.04762
H93	-4.07053	0.86025	-5.84188

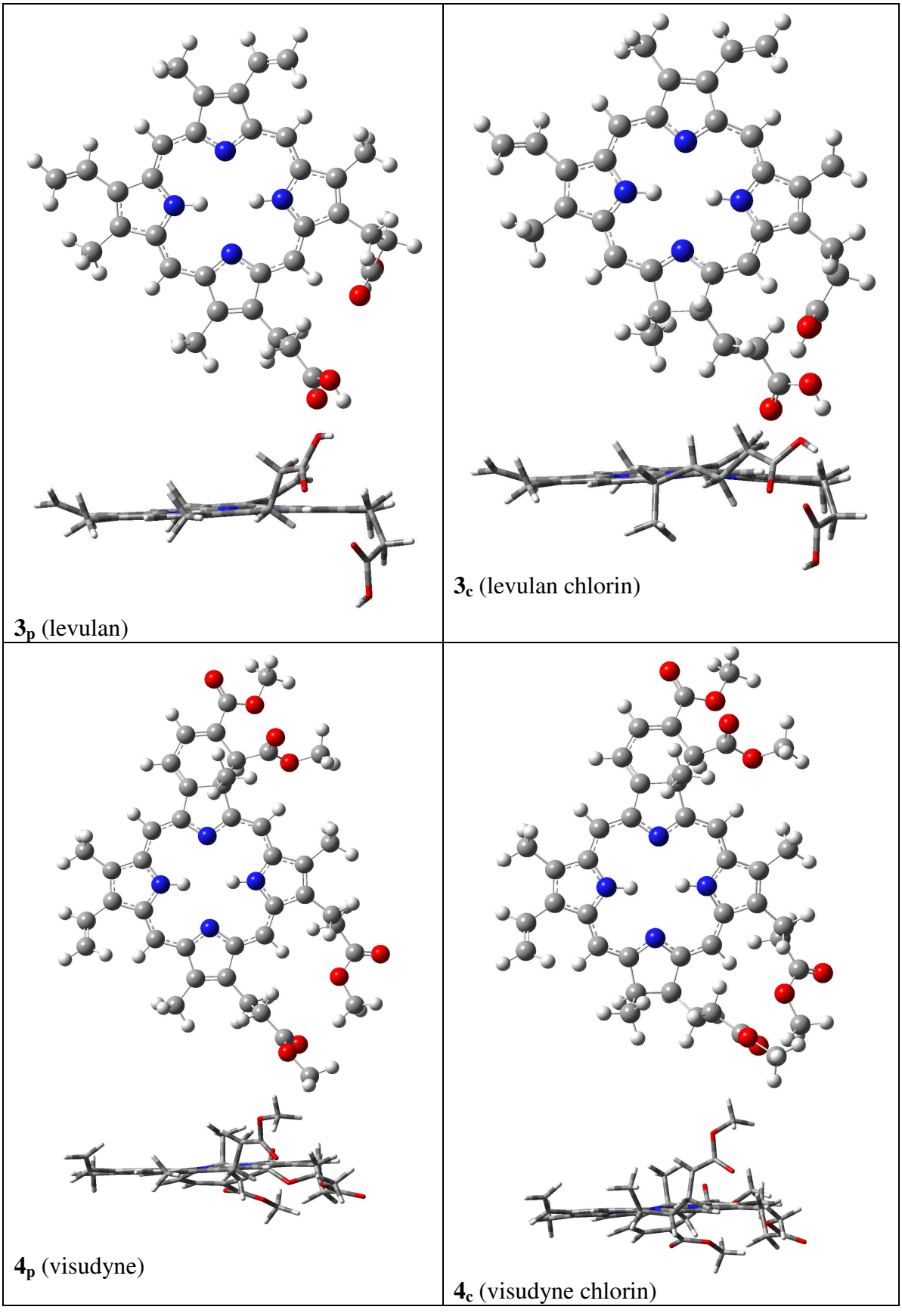
8p P6 PORPHYRIN				**8c P6 CHLORIN**			
C1	0.87018	-2.61623	0.08994	C1	1.33191	-2.79826	0.00983
C2	-1.01669	-3.40503	-0.87754	C2	-0.78337	-3.54759	-0.33824
C3	-1.18923	-1.99924	-0.61158	C3	-0.85401	-2.22366	0.18078
N4	0.00071	-1.57413	-0.06612	N4	0.42186	-1.79817	0.3407
C5	0.24137	-3.78799	-0.39101	C5	0.57361	-3.92457	-0.40208
C6	-2.28749	0.27965	-0.49231	C6	-2.14812	-0.0761	0.35105
C7	-1.50078	2.30657	-0.35677	C7	-1.49789	2.00941	0.07653
N8	-1.14374	0.95959	-0.49653	N8	-1.06784	0.7398	0.09952
C9	4.91682	-0.27939	1.07482	C9	5.31438	-0.1819	0.50917
C10	3.81714	0.53329	0.51841	C10	4.0758	0.59408	0.34086
C11	4.41541	-1.53464	1.23182	C11	4.95024	-1.48973	0.44752
C12	3.02556	-1.47325	0.75455	C12	3.47695	-1.49367	0.26929
N13	2.6982	-0.17585	0.36148	N13	2.97204	-0.2485	0.2417
C14	2.92896	4.1613	-0.49202	C14	2.79453	4.1749	-0.2258
C15	2.91951	2.73938	-0.23986	C15	2.87808	2.75769	-0.04325
N16	1.60945	2.33131	-0.29348	N16	1.6095	2.26164	-0.0386
C17	0.78157	3.40554	-0.46103	C17	0.69053	3.28377	-0.16514
C18	1.58941	4.56635	-0.588	C18	1.42984	4.49968	-0.27788
C19	2.20005	-2.55219	0.61796	C19	2.72359	-2.67315	0.09568
C20	-2.32077	-1.16017	-0.72421	C20	-2.04407	-1.44612	0.54276
H21	-1.09925	4.35217	-0.39838	H21	-1.24546	4.09056	-0.17203
C22	-0.63837	3.36964	-0.41426	C22	-0.7014	3.15297	-0.11429
H23	4.92755	2.36352	0.30435	H23	4.97037	2.50231	0.28163
C24	3.95512	1.90661	0.1747	C24	4.03773	1.95827	0.20151
H25	1.3363	1.36295	-0.14544	H25	1.40413	1.26894	0.0395
H26	0.18912	-0.59413	0.12413	H26	0.68794	-0.8588	0.61083
H27	2.61297	-3.51889	0.88772	H27	3.28375	-3.59418	-0.01739
C28	0.88073	-5.14276	-0.43683	C28	1.12505	-5.2362	-0.86514
H29	1.79281	-5.13565	-1.04641	H29	2.21474	-5.20721	-0.94983
H30	0.19184	-5.88113	-0.84514	H30	0.70911	-5.51481	-1.83837
H31	1.16688	-5.47501	0.56917	H31	0.84884	-6.04323	-0.17719
C32	6.28657	0.23698	1.38735	C32	6.67962	0.41097	0.68054
H33	6.24612	1.101	2.06355	H33	6.71119	1.11387	1.52273
H34	6.8112	0.56815	0.48093	H34	6.99446	0.96677	-0.21268
H35	6.90624	-0.52845	1.86313	H35	7.42974	-0.36338	0.86496
C36	1.06907	5.95553	-0.81406	C36	0.81962	5.86003	-0.4357
H37	1.86911	6.69686	-0.74703	H37	1.58681	6.63721	-0.48293
H38	0.3085	6.22781	-0.07213	H38	0.15162	6.10381	0.40065
H39	0.60927	6.06274	-1.80441	H39	0.22489	5.93378	-1.35516
C40	5.11816	-2.75878	1.74587	C40	5.82274	-2.71108	0.51752
H41	5.88171	-2.45712	2.47227	H41	6.72904	-2.47994	1.09036
H42	4.41161	-3.38743	2.30127	H42	5.30771	-3.50189	1.07864
C43	5.78559	-3.59724	0.63906	C43	6.23141	-3.25261	-0.86712
H44	6.28065	-4.47831	1.06328	H44	6.84919	-4.1525	-0.76645
C45	4.09331	5.02172	-0.6198	C45	3.90614	5.11822	-0.3278
H46	3.92869	6.06921	-0.36738	H46	3.7076	6.11434	0.06803
H47	6.12056	5.40559	-1.09637	H47	5.8673	5.6777	-0.88911
C48	5.3205	4.67315	-1.04282	C48	5.11177	4.89762	-0.87478
H49	5.55772	3.66862	-1.37796	H49	5.37686	3.95582	-1.34577
C50	-4.89104	0.81263	0.02812	C50	-4.36056	0.29165	-0.83829
H51	-5.32136	0.27276	-0.81592	H51	-4.16025	-0.75344	-1.08351
H52	-5.46247	1.73752	0.13401	H52	-4.08245	0.88693	-1.71637
C53	-5.11043	-0.02096	1.30275	C53	-5.86688	0.40569	-0.58183
H54	-4.5042	-0.92952	1.32705	H54	-6.13469	-0.12822	0.3363

H55	5.05073	-3.9405	-0.09729
C56	-2.94101	2.4345	-0.18548
C57	-3.45226	1.16875	-0.23719
H58	-6.15468	-0.35945	1.33839
H59	6.538	-3.0081	0.10352
C60	-3.6858	3.71797	0.03372
H61	-4.07945	4.12287	-0.90842
H62	-3.04652	4.4867	0.47874
H63	-4.52463	3.56688	0.717
C64	-1.86129	-4.29686	-1.68378
O65	-1.9821	-5.49383	-1.53288
O66	-2.45195	-3.65055	-2.72356
H67	-2.96717	-4.32621	-3.2011
C68	-4.87657	0.75925	2.5759
O69	-4.93627	1.96112	2.69757
O70	-4.62059	-0.06134	3.62312
H71	-4.52079	0.5187	4.40186
C72	-3.60939	-1.76392	-1.13152
O73	-4.35834	-1.32414	-1.97451
O74	-3.92659	-2.87793	-0.42496
H75	-4.75285	-3.21376	-0.81408

H55	5.35393	-3.50824	-1.47129
C56	-2.98585	2.16571	0.34548
C57	-3.46562	0.69992	0.36914
H58	-4.0122	0.47142	1.28739
H59	-6.42108	-0.09992	-1.38551
H60	6.80651	-2.50386	-1.42278
H61	-3.46444	2.72014	-0.46771
C62	-3.26359	2.91976	1.65974
H63	-2.84171	3.93075	1.6416
H64	-2.83325	2.39093	2.51855
H65	-4.34356	3.01204	1.81558
C66	-1.87295	-4.38203	-0.8471
O67	-1.79629	-5.57655	-1.07699
O68	-3.01358	-3.68835	-1.13035
H69	-3.64217	-4.35641	-1.46104
C70	-6.42082	1.81056	-0.51285
O71	-5.84513	2.84042	-0.80101
O72	-7.71402	1.80898	-0.10201
H73	-8.00124	2.74155	-0.11442
C74	-3.159	-2.16226	1.19119
O75	-4.31939	-1.79239	1.31039
O76	-2.75689	-3.32479	1.78238
H77	-3.56561	-3.69009	2.18553

Figure 1. Drawings of the optimized geometries of the 16 studied molecules.

Porphyrins	Chlorins
 **1_P** (porphyrin)	 **1_c** (chlorin)
 **2_p** (photofrin)	 **2_c** (photofrin chlorin)

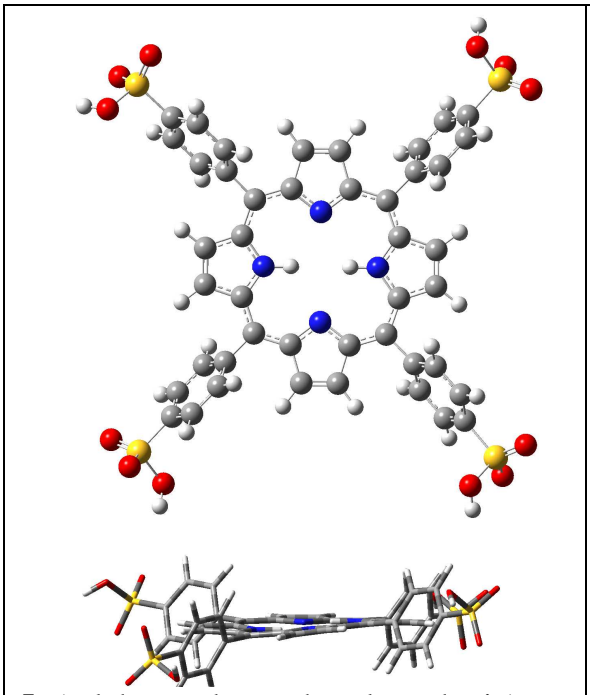


3_p (levulan)

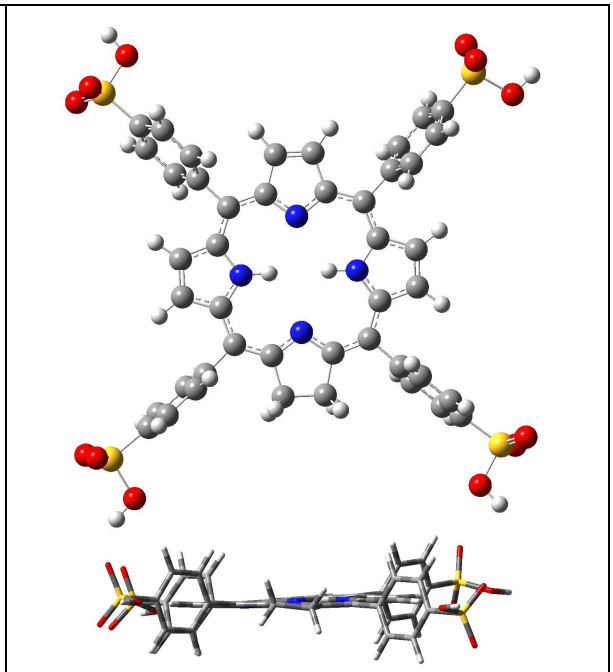
3_c (levulan chlorin)

4_p (visudyne)

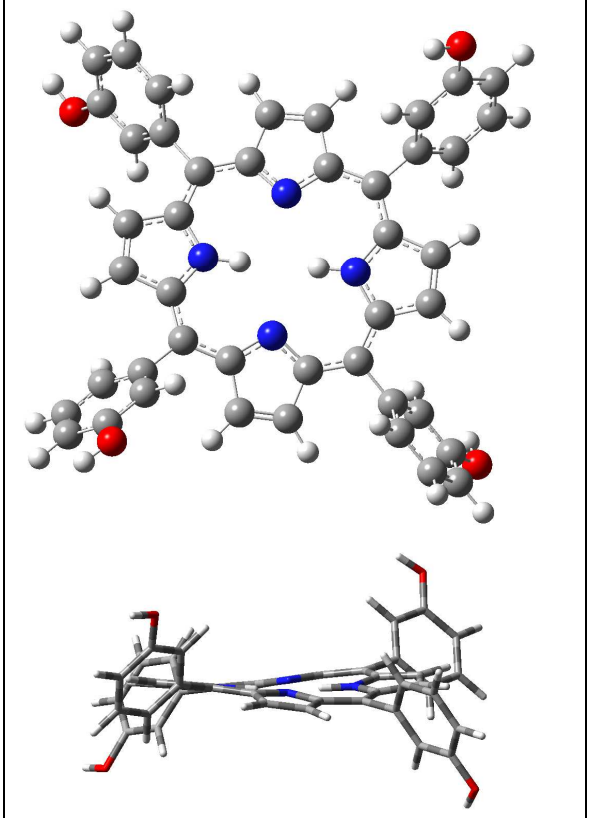
4_c (visudyne chlorin)



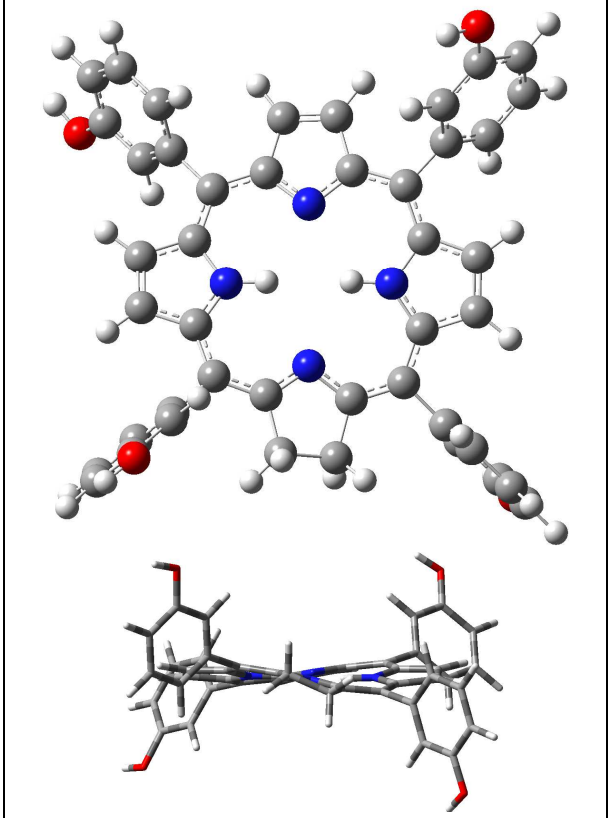
5$_p$ (sulphonated-tetraphenyl porphyrin)



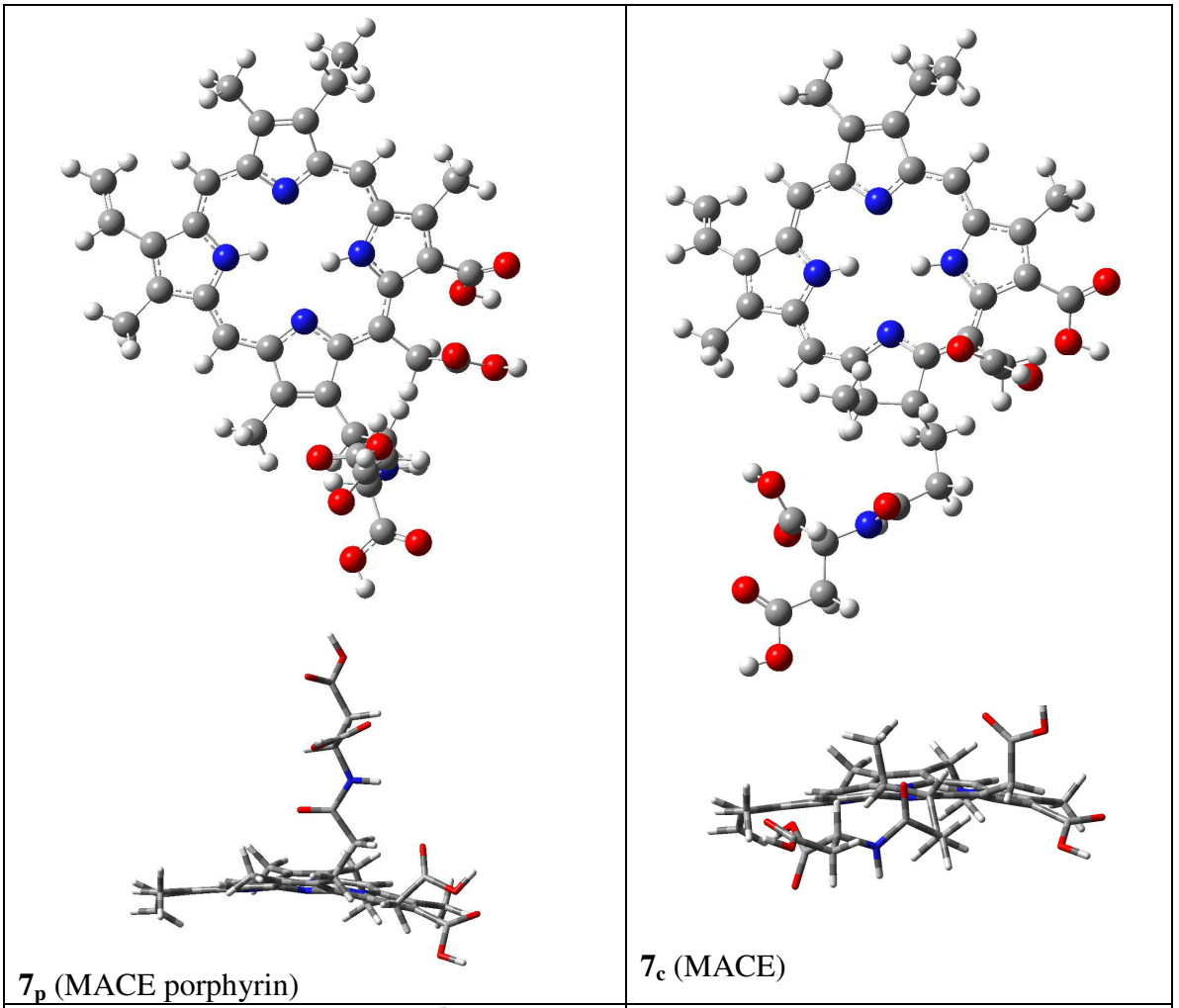
5$_c$ (sulphonated-tetraphenyl chlorin)



6$_p$ (phoscan porphyrin)

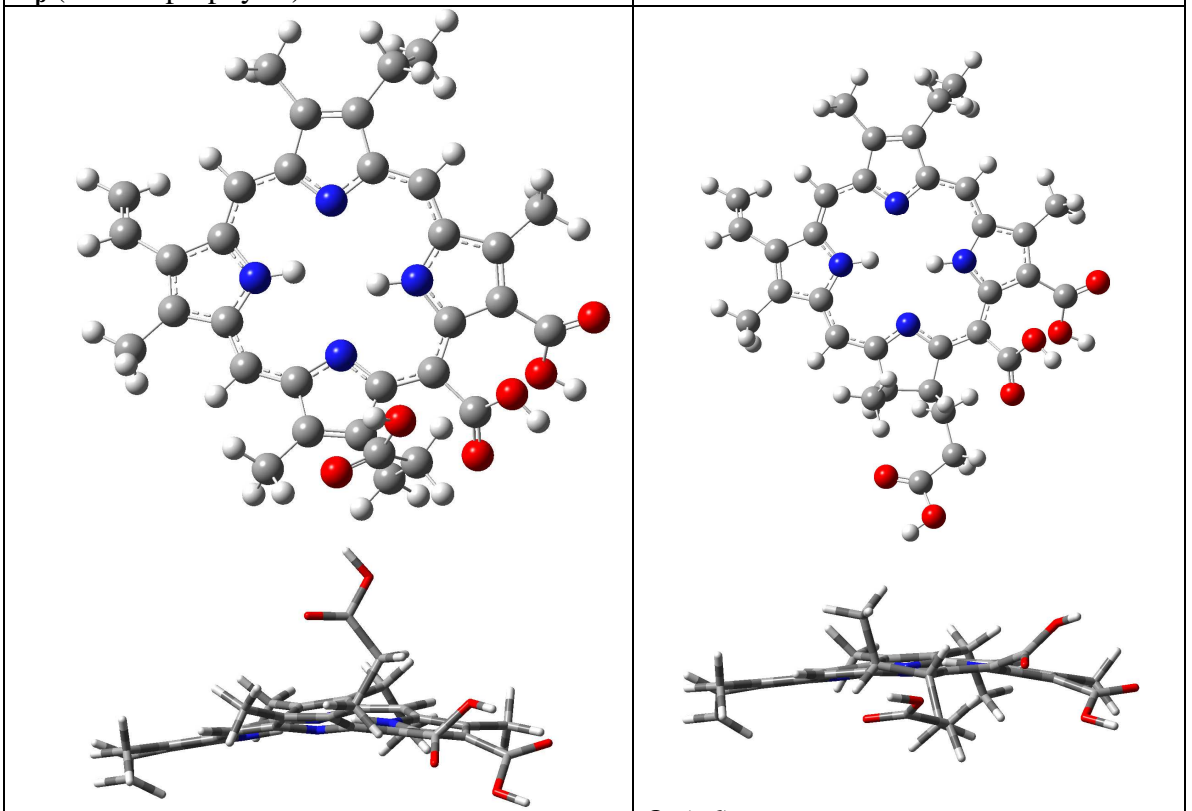


6$_c$ (phoscan)



7_p (MACE porphyrin)

7_c (MACE)



8_p (p6 porphyrin)

8_c (p6)

Table 3. Interatomic distances (Å) calculated at B3LYP/6-31G(d) level for the ground state and the first triplet excited state of porphyrin and chlorin derivatives. Italic numbers correspond to chlorins.

Interatomic distances	rC5···C15	rC10···C20	rN21-N23	rN22-N24
$1_P/1_C$ Singlet:	6.88/*6.88*	6.87/*6.87*	4.05/*4.17*	4.23/*4.20*
$1_P/1_C$ Triplet:	6.90/*6.90*	6.89/*6.91*	4.08/*4.11*	4.26/*4.24*
$2_P/2_C$ Singlet:	6.86/*6.84*	6.86/*6.89*	4.07/*4.13*	4.23/*4.22*
$2_P/2_C$ Triplet:	6.87/*6.82*	6.91/*6.93*	4.09/*4.10*	4.26/*4.24*
$3_P/3_C$ Singlet:	6.87/*6.84*	6.86/*6.89*	4.08/*4.13*	4.23/*4.21*
$3_P/3_C$ Triplet:	6.89/*6.79*	6.88/*6.97*	4.08/*4.11*	4.28/*4.26*
$4_P/4_C$ Singlet:	6.88/*6.92*	6.87/*6.79*	4.16/*4.24*	4.21/*4.19*
$4_P/4_C$ Triplet:	6.92/*6.89*	6.85/*6.85*	4.12/*4.16*	4.22/*4.21*
$5_P/5_C$ Singlet:	6.92/*6.91*	6.91/*6.91*	4.06/*4.17*	4.21/*4.18*
$5_P/5_C$ Triplet:	6.91/*6.95*	6.94/*6.93*	4.11/*4.18*	4.23/*4.21*
$6_P/6_C$ Singlet:	6.90/*6.84*	6.88/*6.84*	4.05/*4.10*	4.20/*4.16*
$6_P/6_C$ Triplet:	6.91/*6.82*	6.86/*6.75*	4.07/*4.06*	4.23/*4.18*
$7_P/7_C$ Singlet:	6.55/*6.70*	7.15/*7.04*	4.12/*4.10*	4.20/*4.25*
$7_P/7_C$ Triplet:	6.61/*6.74*	7.07/*7.04*	4.09/*4.14*	4.23/*4.27*
$8_P/8_C$ Singlet:	6.61/*6.70*	7.08/*7.04*	4.09/*4.14*	4.21/*4.23*
$8_P/8_C$ Triplet:	6.65/*6.76*	7.04/*6.98*	4.10/*4.16*	4.23/*4.25*

Table 4. Electronic absorption spectra calculated at the TD-DFT level with different exchange correlation functionals in the solution phase using the explicit modelling of the solvent (methanol) and the polarizable continuum model (CPCM). The oscillator strengths (f)[a] of the transitions are included for each transition.

Porphyrin **1p**		Exchange Correlation Functional								
		Explicit Solvent Model		Continuum Solvent Model						
State	Exp[b]	BLYP[c]	BHANDHLYP	BLYP[c]	BPW91	PBE0	B3LYP	PBE1	BHANDH	BHANDHLYP
1	2.02 613	2.08 596 f=0.0001	2.30 538 f=0.0042	2.19 566 f=0.0026	2.20 562 f=0.0029	2.20 561 f=0.0029	2.30 538 f=0.0003	2.33 530 f=0.0002	2.33 530 f=0.0016	2.29 540 f=0.0028
2	2.21 561	2.09 591 f=0.0009	2.45 505 f=0.0039	2.31 534 f=0.0005	2.32 533 f=0.0006	2.33 532 f=0.0007	2.43 508 f=0.0002	2.48 499 f=0.0003	2.49 496 f=0.0044	2.44 507 f=0.0060
3	3.17 391	2.17 569 f=0.0011	3.66 338 f=0.8855	2.99 414 f=0.0000	3.02 409 f=0.0076	3.02 409 f=0.0016	3.27 378 f=0.9506	3.34 371 f=1.0464	3.51 352 f=1.4101	3.49 354 f=1.3910
4		2.22 557 f=0.0006	3.72 333 f=1.0794	3.00 412 f=0.2390	3.02 409 f=0.3095	3.03 409 f=0.3176	3.35 369 f=1.2629	3.40 363 f=1.3301	3.55 348 f=1.5416	3.54 350 f=1.5431
5		2.26 547 f=0.0007	4.05 306 f=0.0025	3.06 404 f=0.0000	3.08 401 f=0.1984	3.08 401 f=0.2001	3.48 355 f=0.0000	3.60 344 f=0.0000	4.06 304 f=0.0000	4.05 306 f=0.0000
6		2.31 534 f=0.0001	4.34 285 f=0.4503	3.07 403 f=0.1053	3.09 400 f=0.0000	3.09 400 f=0.0000	3.68 336 f=0.0000	3.83 323 f=0.0000	4.29 288 f=0.3643	4.28 289 f=0.3883
7		2.96 418 f=0.0065	4.46 278 f=0.0015	3.34 370 f=1.1005	3.31 374 f=1.0749	3.31 374 f=1.0754	3.74 330 f=0.5765	3.85 321 f=0.5257	4.48 276 f=0.0000	4.47 277 f=0.0000
8		3.01 411 f=0.0074	4.58 270 f=0.1047	3.41 362 f=0.0001	3.39 365 f=0.9405	3.39 365 f=0.9396	3.76 329 f=0.2036	3.91 316 f=0.1621	4.57 270 f=0.0972	4.58 271 f=0.1029
9		3.02 409 f=0.996	4.83 256 f=0.0013	3.42 362 f=0.9490	3.43 360 f=0.0000	3.42 361 f=0.0000	4.13 299 f=0.0000	4.30 287 f=0.0000	4.90 253 f=0.0000	4.88 254 f=0.0000
10		3.05 405.80 f=0.0325	4.91 252.69 f=0.0002	3.43 360 f=0.0039	3.44 359 f=0.0002	3.43 360 f=0.0002	4.18 296 f=0.0000	4.32 286 f=0.0000	4.92 252 f=0.0000	4.91 252 f=0.0000

Chlorin **1c**		Exchange Correlation Functional								
	Exp[d]	Explicit Solvent Molecules		Continuum Solvent Model						
State		BLYP[c]	BHANDHLYP	BLYP[c]	BPW91	PBE0	B3LYP	PBE1	BHANDH	BHANDHLYP
1	1.98 626	2.20 564 f=0.0042	2.26 549 f=0.1044	2.21 559 f=0.0742	2.21 562 f=0.0873	2.21 561 f=0.0884	2.27 547 f=0.1249	2.29 542 f=0.1340	2.25 550 f=0.1637	2.22 558 f=0.1621
2	2.29 541	2.21 560 f=0.0432	2.60 476 f=0.0006	2.32 533 f=0.0050	2.32 534 f=0.0053	2.32 533 f=0.0053	2.48 500 f=0.0054	2.53 490 f=0.0055	2.63 471 f=0.0017	2.60 478 f=0.0010
3	3.18 390	2.29 541 f=0.0039	3.74 331 f=1.0669	2.97 417 f=0.0129	3.00 412 f=0.0304	3.00 412 f=0.0315	3.34 372 f=0.9221	3.41 363 f=0.9705	3.57 347 f=1.5305	3.56 348 f=1.5299
4		2.46 504 f=0.0004	3.83 324 f=0.8589	3.08 402 f=0.5626	3.07 403 f=0.6436	3.08 403 f=0.6457	3.38 367 f=1.1607	3.43 361 f=1.2790	3.68 337 f=1.2379	3.68 337 f=1.2421
5		2.64 470 f=0.0010	4.30 288 f=0.1118	3.32 373 f=1.0752	3.27 378 f=1.1374	3.27 379 f=1.1402	3.60 344 f=0.2430	3.74 331 f=0.1601	4.35 285 f=0.0824	4.34 286 f=0.0865
6		2.87 432 f=0.0149	4.54 273 f=0.2290	3.41 363 f=0.0006	3.43 361 f=0.0003	3.43 361 f=0.0003	3.97 312 f=0.2307	4.09 303 f=0.2382	4.58 271 f=0.2045	4.57 272 f=0.2178
7		2.93 422.54 f=0.0040	4.73 261.87 f=0.0112	3.49 354.38 f=0.1161	3.51 353 f=0.0297	3.51 353 f=0.0121	4.10 303 f=0.0098	4.22 294 f=0.0040	4.77 260 f=0.0050	4.79 259 f=0.0041
8		3.14 394.64 f=0.3213	4.85 255.70 f=0.0613	3.55 349.13 f=0.0144	3.52 352 f=0.0407	3.52 352 f=0.0481	4.17 297 f=0.0005	4.31 287 f=0.0007	4.87 255 f=0.0469	4.88 254 f=0.0447
9		3.39 366.02 f=0.5987	5.03 246.36 f=0.0133	3.58 345.94 f=0.0803	3.58 346 f=0.1087	3.58 346 f=0.1159	4.19 296 f=0.0441	4.32 287 f=0.0473	4.90 253 f=0.0000	4.90 253 f=0.0001
10		3.41 363.63 f=0.0428	5.07 244.35 f=0.0236	3.64 340.29 f=0.0939	3.64 340 f=0.0703	3.64 340 f=0.0677	4.24 293 f=0.0024	4.36 284 f=0.0021	5.04 246 f=0.0634	5.03 247 f=0.0530

[a] One-electron excitations, with coefficients larger than 0,1 in a given electronic transition, are included.[b] [63] measured in ethanol. These are the three low-lying experimental bands. Only the Q band is assigned to the first calculated one. [c] basis set 6-31G(d). [d] [60] measured in benzene. These are the three low-lying experimental bands. Only the Q band is assigned to the first calculated one.

Table 5. Excitation energies (eV) and oscillator strengths (*f*) calculated at the TD-DFT level in the gas phase. In parenthesis are included the values in *nm.* Experimental data are also included.

		Gas Phase			
Molecule	$E_{exp.}$	BLYP	*f*	Transition[a]	
$\mathbf{1_p}$	1.98 (627) [b]	2.17 (571)	0.0009	H-1→L	0.43
		(8.8%)		H→L+1	0.53
$\mathbf{1_c}$	1.98 (626)[c]	2.22 (558)	0.047	H→L	0.52
		(12.1%)		H-1→L+1	0.42
$\mathbf{2_p}$	1.97 (630)	2.12 (585)	0.0004	H→L	0.23
		(7.1%)		H→L+1	0.47
				H-1→L	-0.40
				H-1→L+1	0.19
$\mathbf{2_c}$		2.15 (576)	0.0870	H→L	0.53
				H-1→L+1	-0.39
$\mathbf{3_p}$	1.95 (635)	2.07 (600)	0.0020	H→L	-0.15
		(5.5%)		H→L+1	0.50
				H-1→L	-0.43
				H-1→L+1	-0.10
$\mathbf{3_c}$		2.07 (599)	0.0920	H→L	0.53
				H-1→L+1	-0.39
$\mathbf{4_p}$	1.80 (690)	1.88 (659)	0.0440	H→L	0.41
		(4.5%)		H→L+1	-0.28
				H-1→L	-0.34
				H-1→L+1	-0.32
$\mathbf{4_c}$		1.83 (678)	0.152	H→L	0.55
				H-1→L+1	-0.27
				H-1→L+2	-0.14
$\mathbf{5_p}$	2.10 (590)	2.02 (615)	0.0300	H→L+1	0.54
		(-4.2%)		H-1→L	0.40
$\mathbf{5_c}$		2.10 (590)	0.0430	H→L	0.52
				H-1→L+1	0.42
$\mathbf{6_p}$		2.01 (618)	0.0270	H→L	-0.28
				H→L+1	0.47
				H-1→L	-0.35
				H-1→L+1	-0.21
$\mathbf{6_c}$	1.90 (652)	2.10 (590)	0.0420	H→L	0.38
		(9.5%)		H→L+1	0.30
				H-1→L	-0.36
				H-1→L+1	0.30
$\mathbf{7_p}$		2.02 (615)	0.005	H→L	-0.25
				H→L+1	0.44
				H-1→L	-0.43
				H-1→L+1	-0.15
7c	1.90 (654)	2.04 (607)	0.112	H→L	0.54
		(7.2%)		H-1→L+1	-0.38
$\mathbf{8_p}$		2.01 (616)	0.011	H-1→L	0.38
				H-1→L+1	0.23
				H→L	0.34
				H→L+1	-0.38
$\mathbf{8_c}$	1.88 (660)	2.04 (608)	0.132	H→L	0.55
		(7.9%)		H-1→L+1	-0.34

[a] One-electron excitations, with coefficients larger than 0,1 in a given electronic transition, are included. [b] [63]. [c] [60].