Synthesis of Triphyrin(2.1.1)-Triphyrin(2.1.1) Homo Dimers and Bis-Re(I) Triphyrin Dimer Complex

Gurpreet Kaur and Mangalampalli Ravikanth*

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076,

India, E-mail: ravikanth@chem.iitb.ac.in

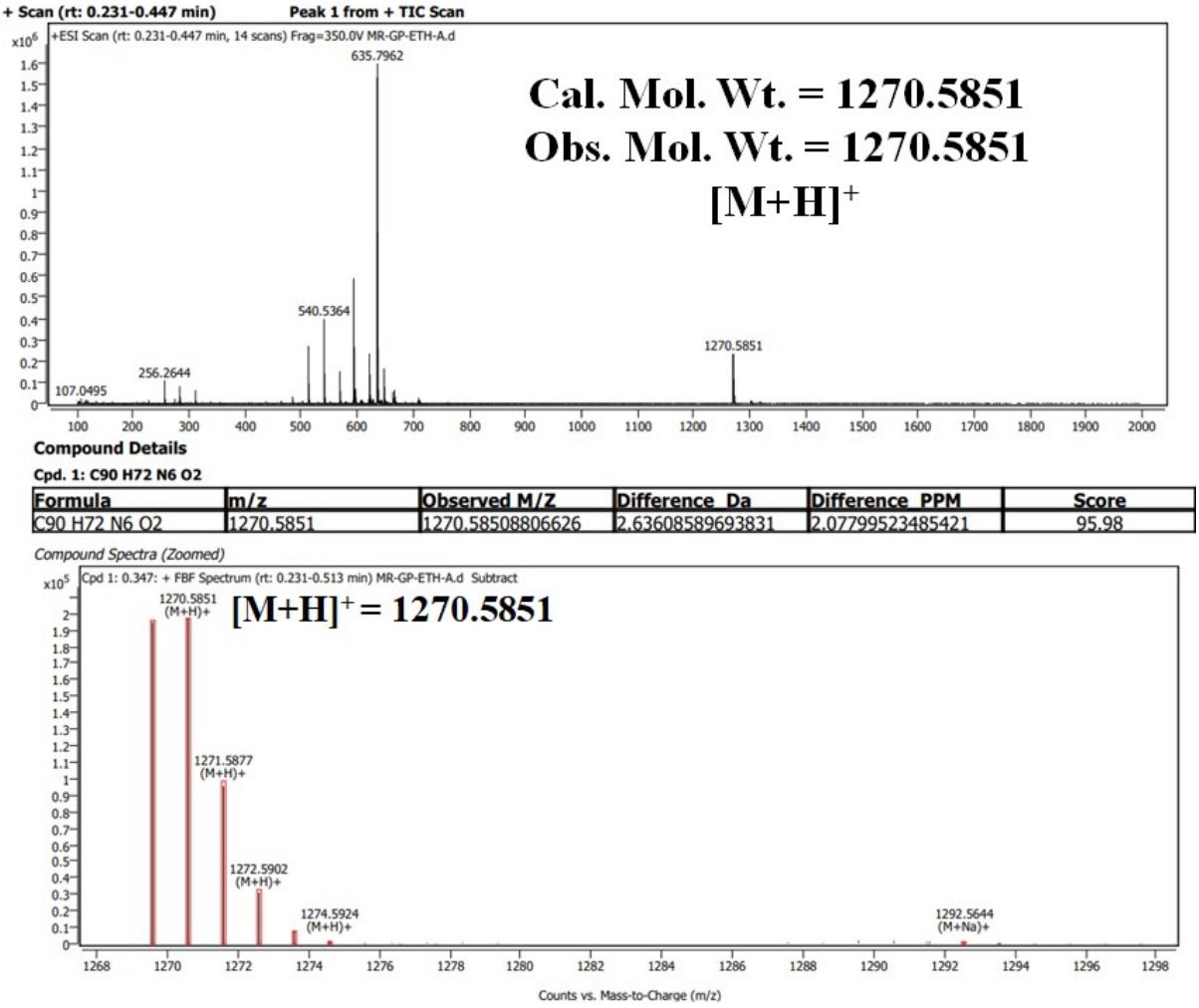


Figure S1. HR mass spectrum of the compound **3**.

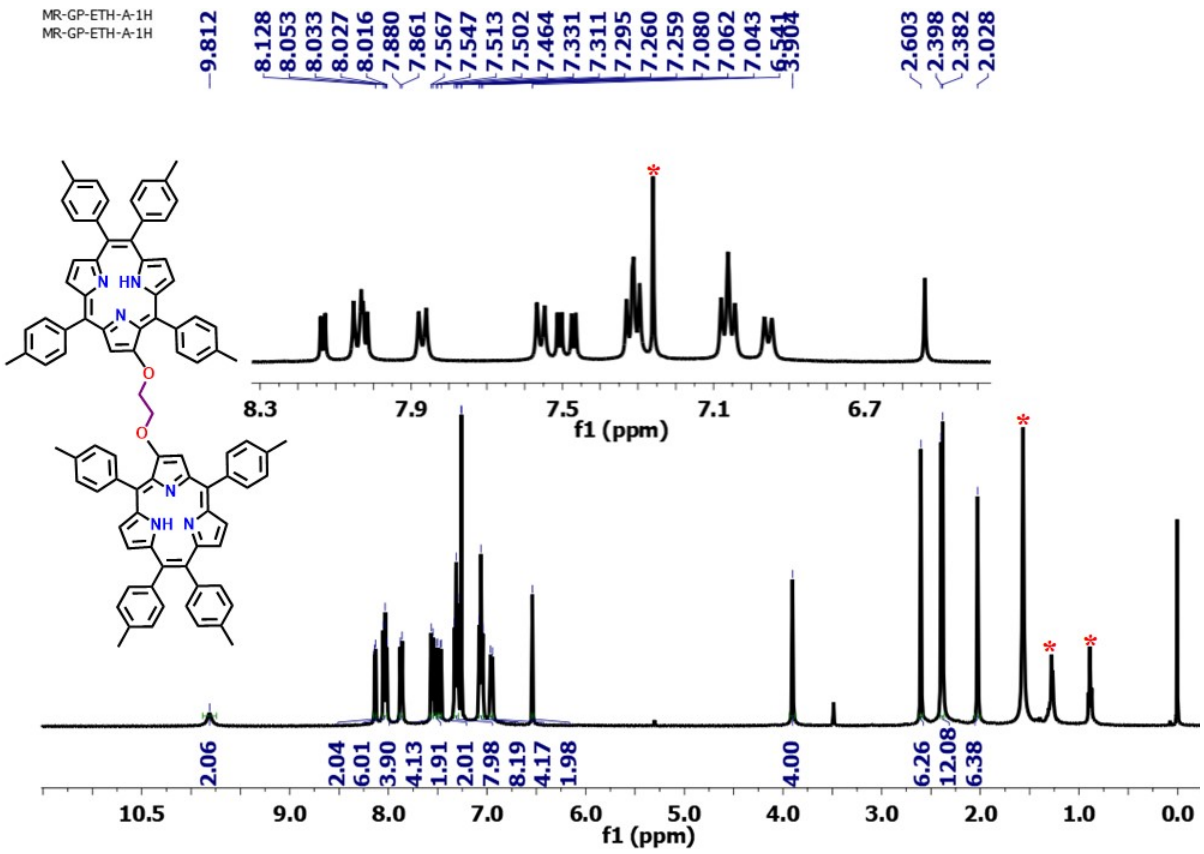


Figure S2. ^{1}H NMR spectrum of the compound **3** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

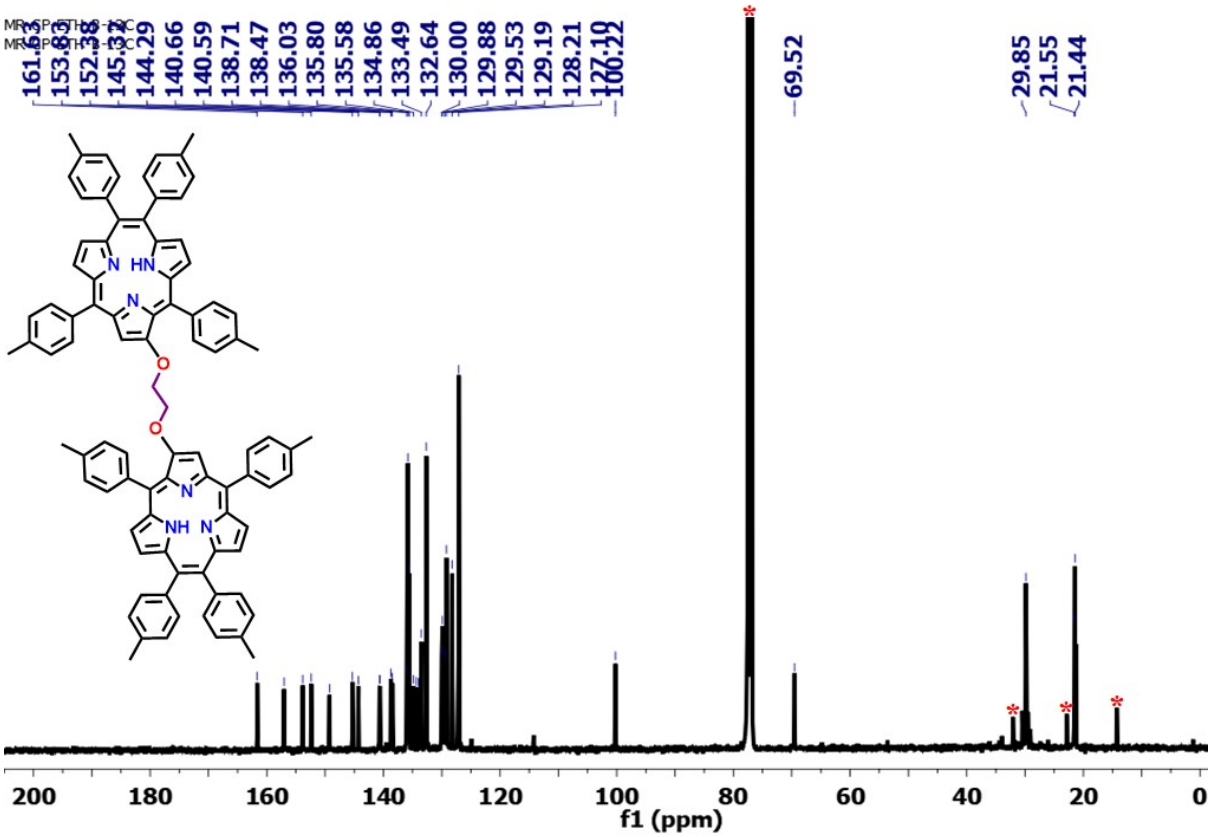


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

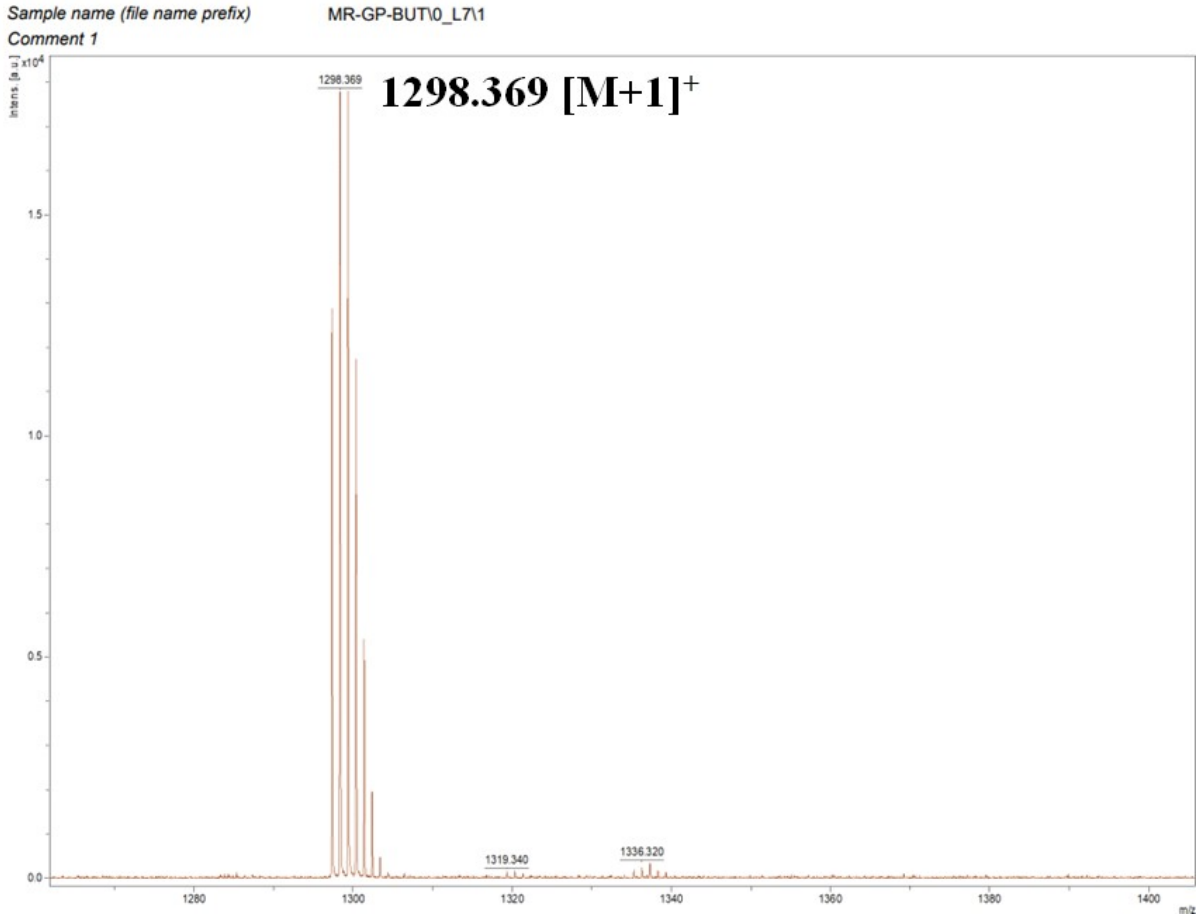


Figure S4. MALDI-TOF mass spectrum of the compound **4**.

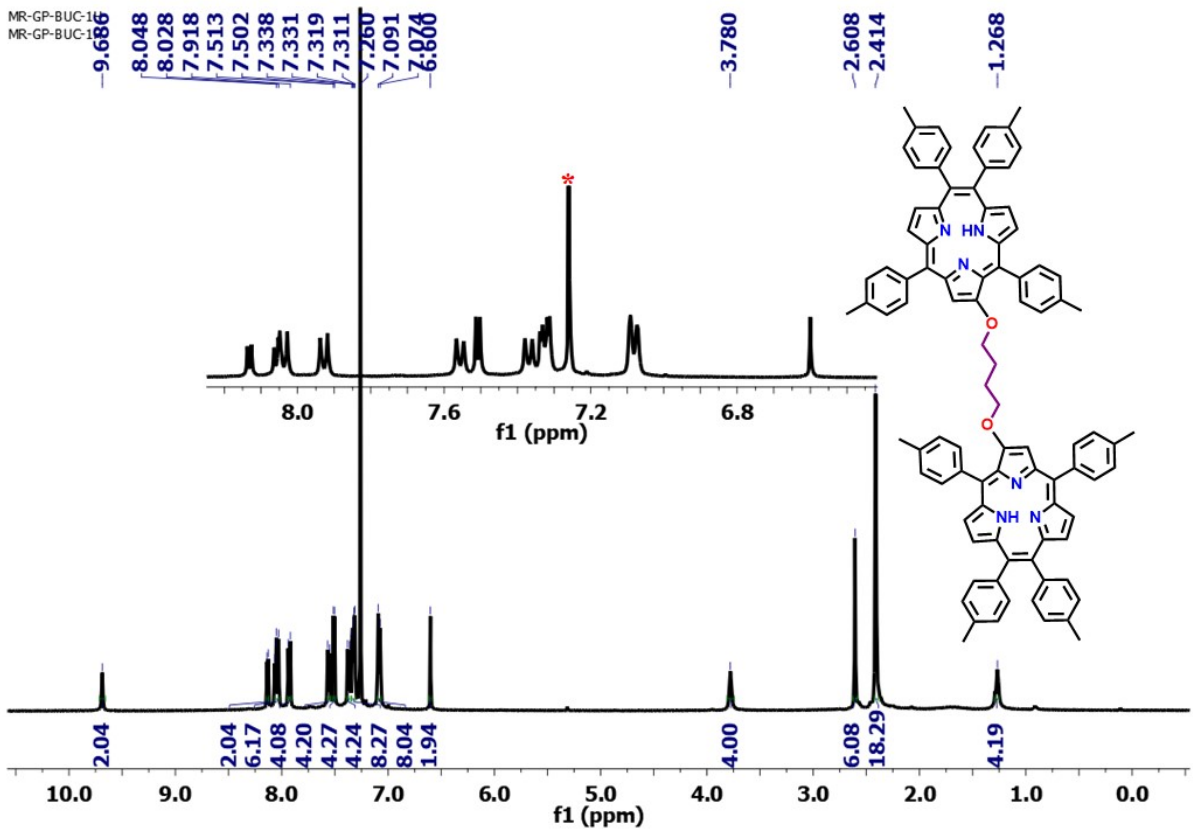


Figure S5. ^{1}H NMR spectrum of the compound **4** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometers. Note: Peaks marked with asterisk (*) are due to residual solvents.

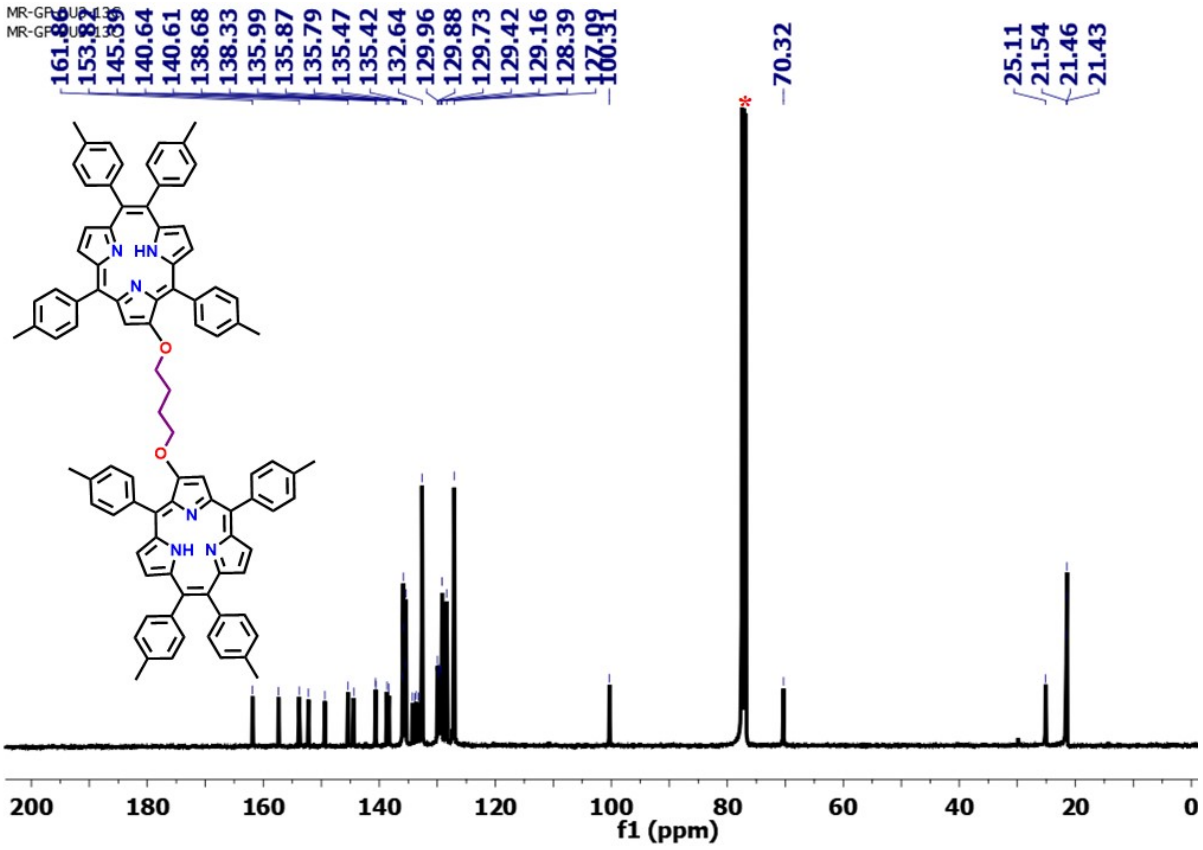


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

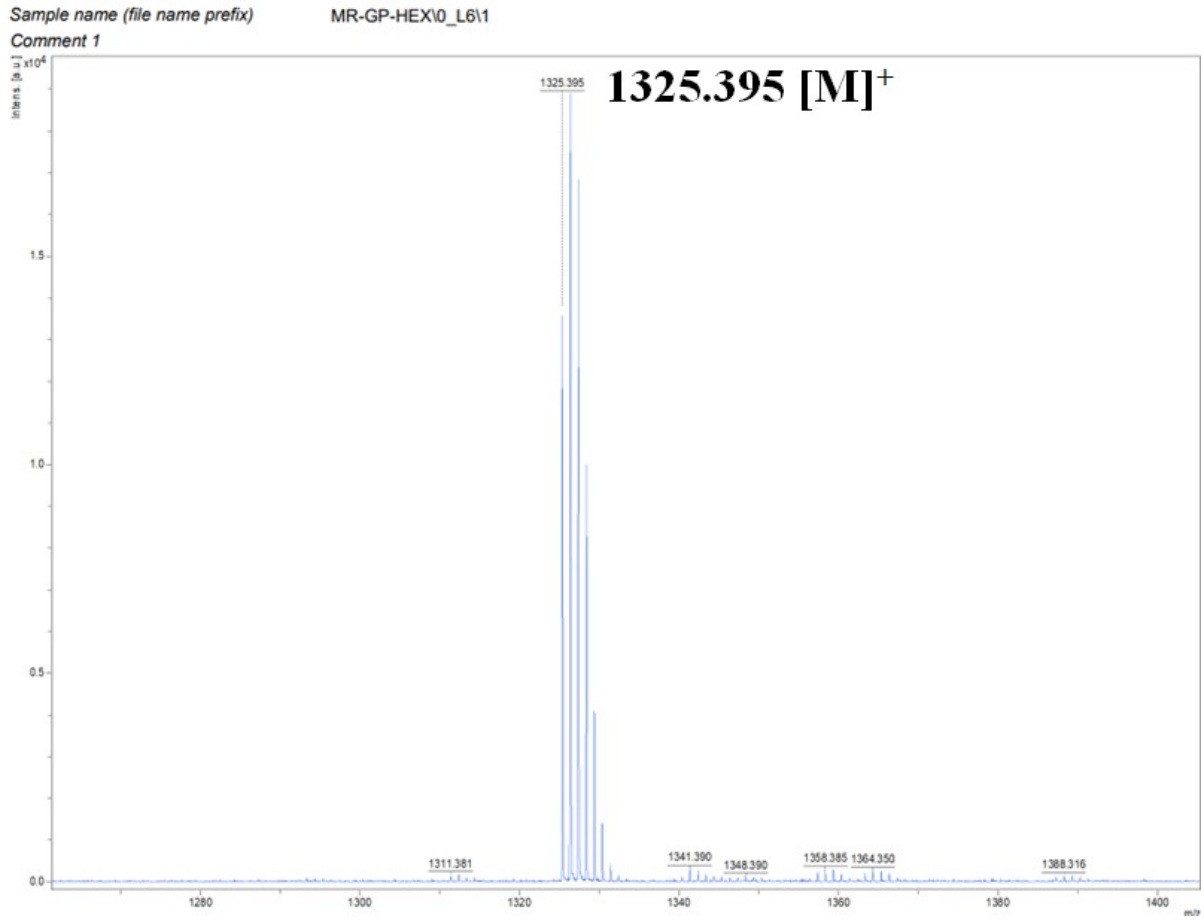


Figure S7. MALDI-TOF mass spectrum of the compound **5**.

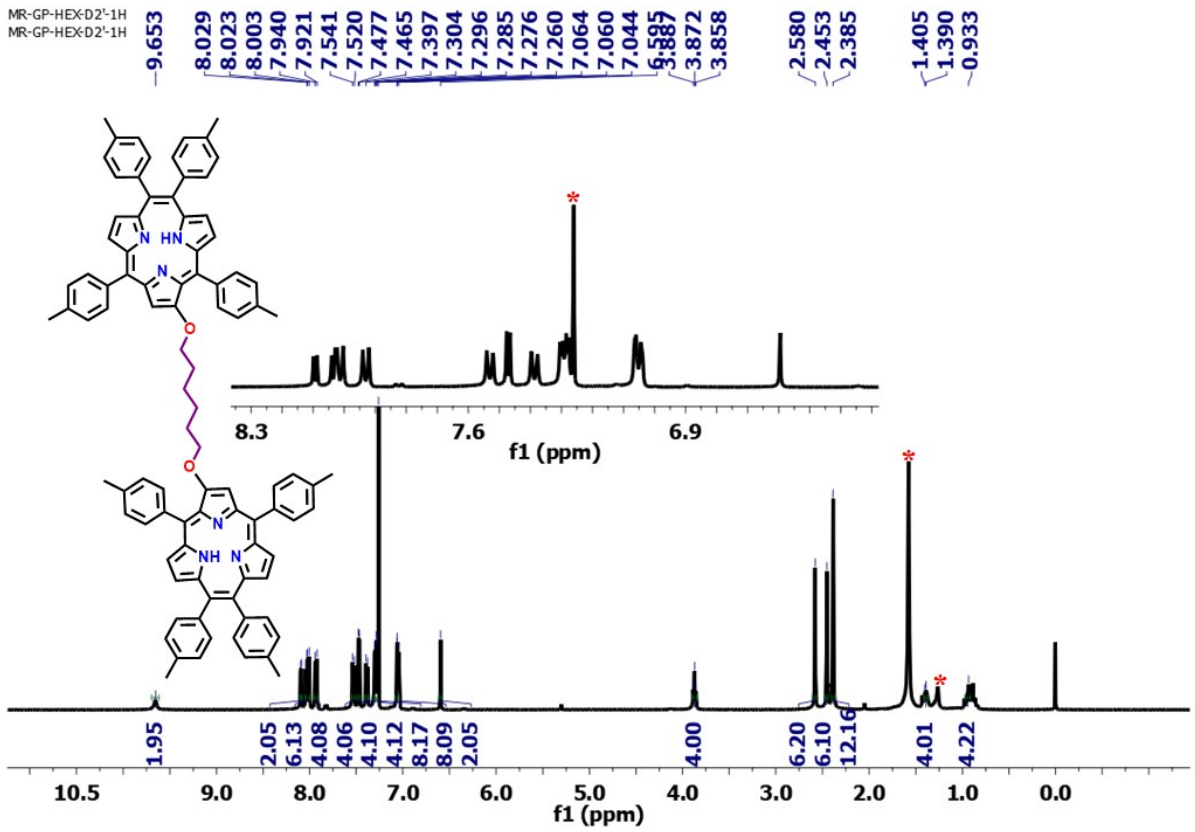


Figure S8. ^{1}H NMR spectrum of the compound **5** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

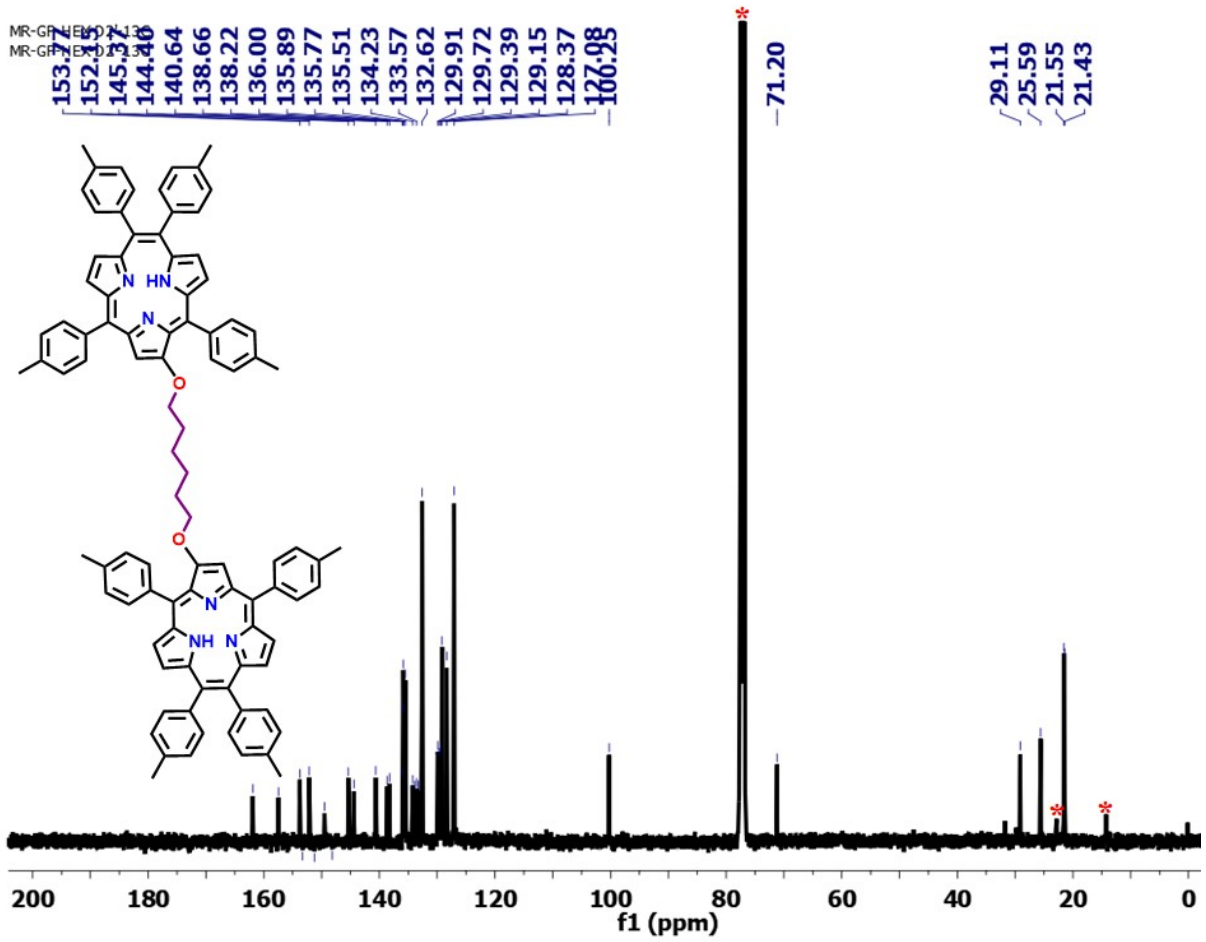


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

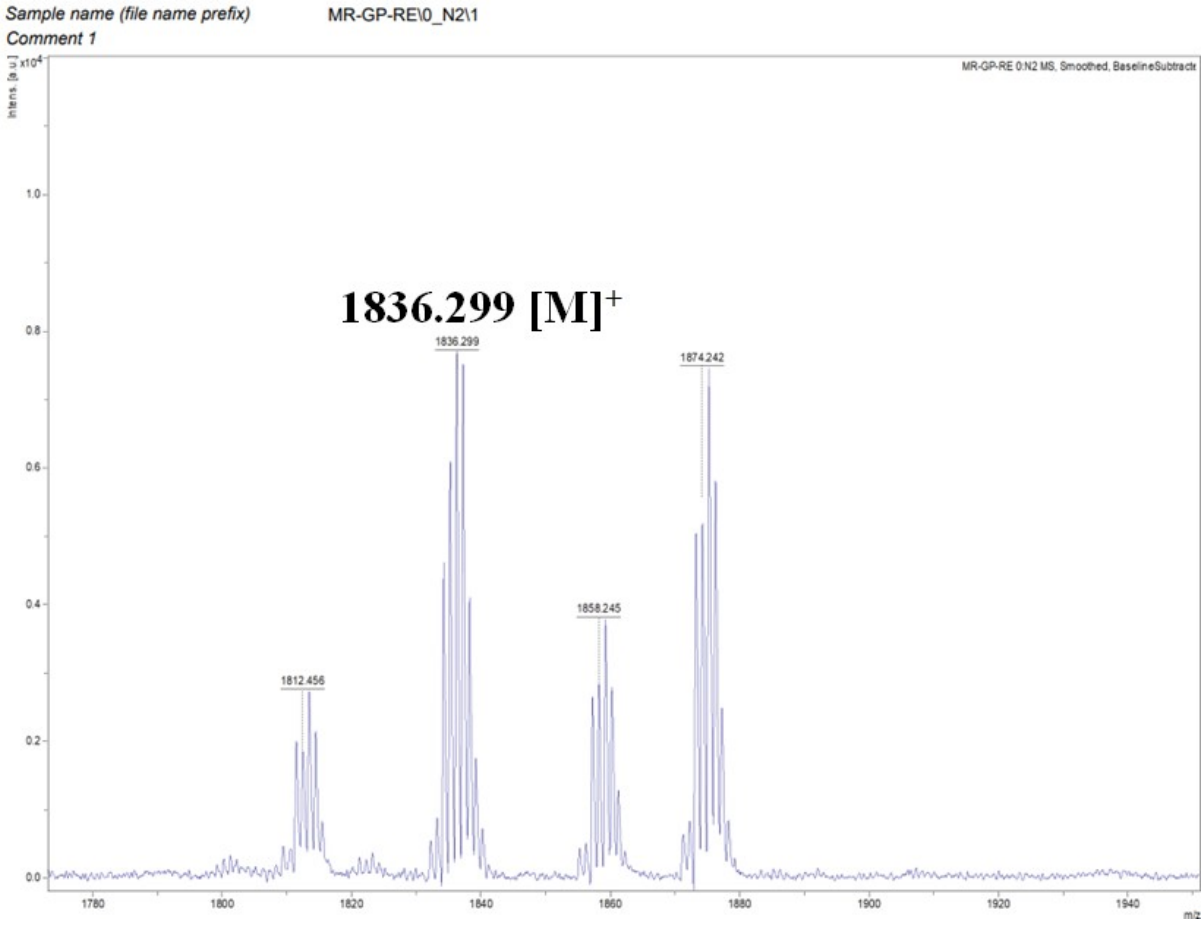


Figure S10. MALDI-TOF mass spectrum of the compound **4-Re**.

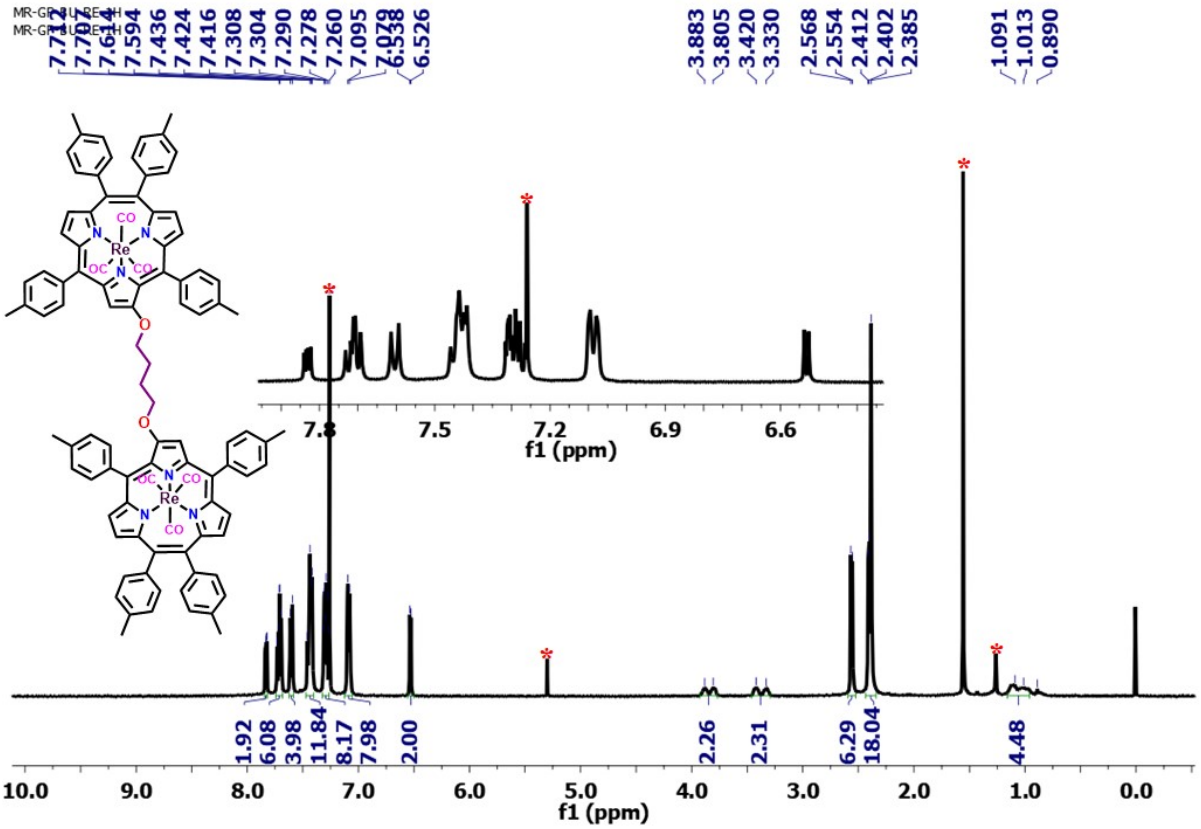


Figure S11. ^{1}H NMR spectrum of the compound **4-Re** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

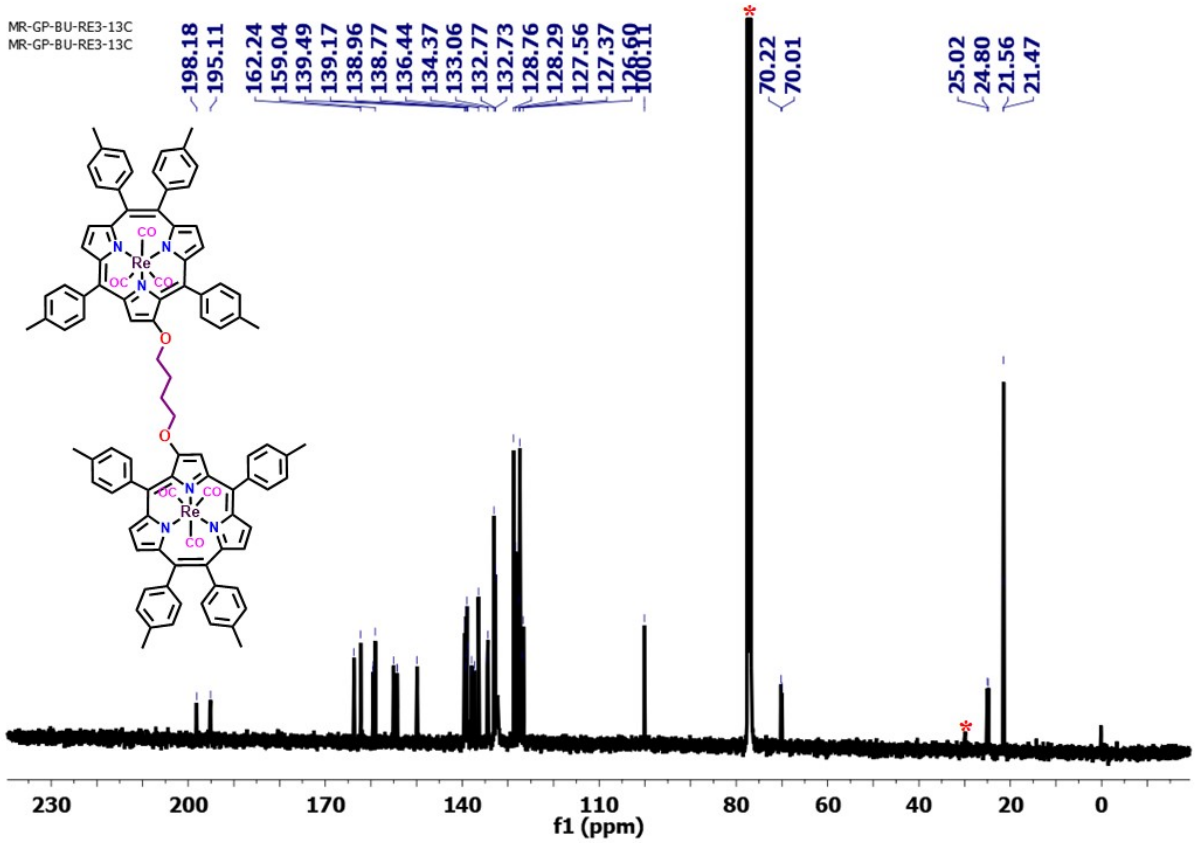
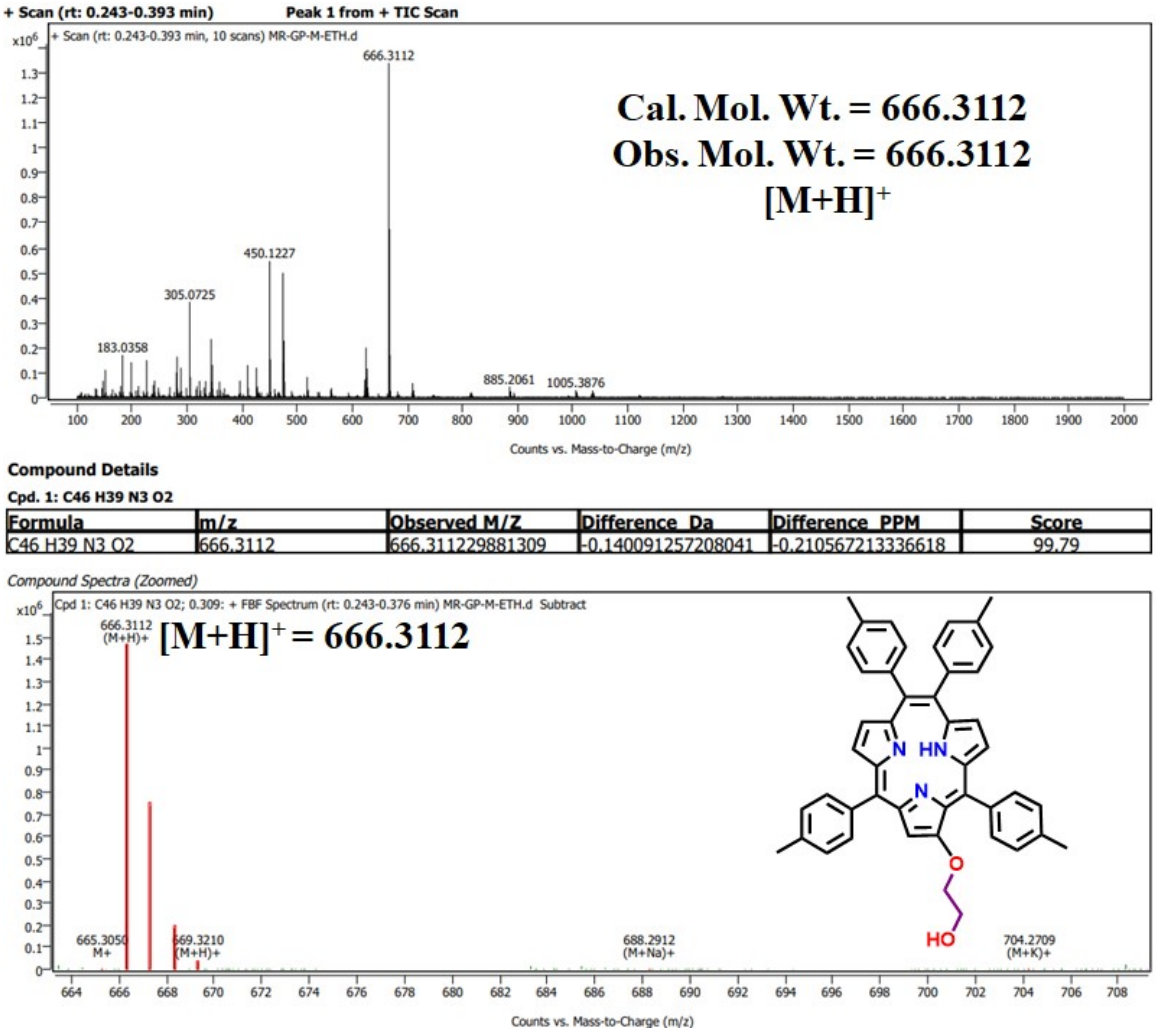


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4-Re** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound Details

Cpd. 1: C46 H39 N3 O2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C46 H39 N3 O2	666.3112	666.311229881309	-0.140091257208041	-0.210567213336618	99.79

Figure S13. HR mass spectrum of the compound **2-O(CH_2)$_2$-OH**.

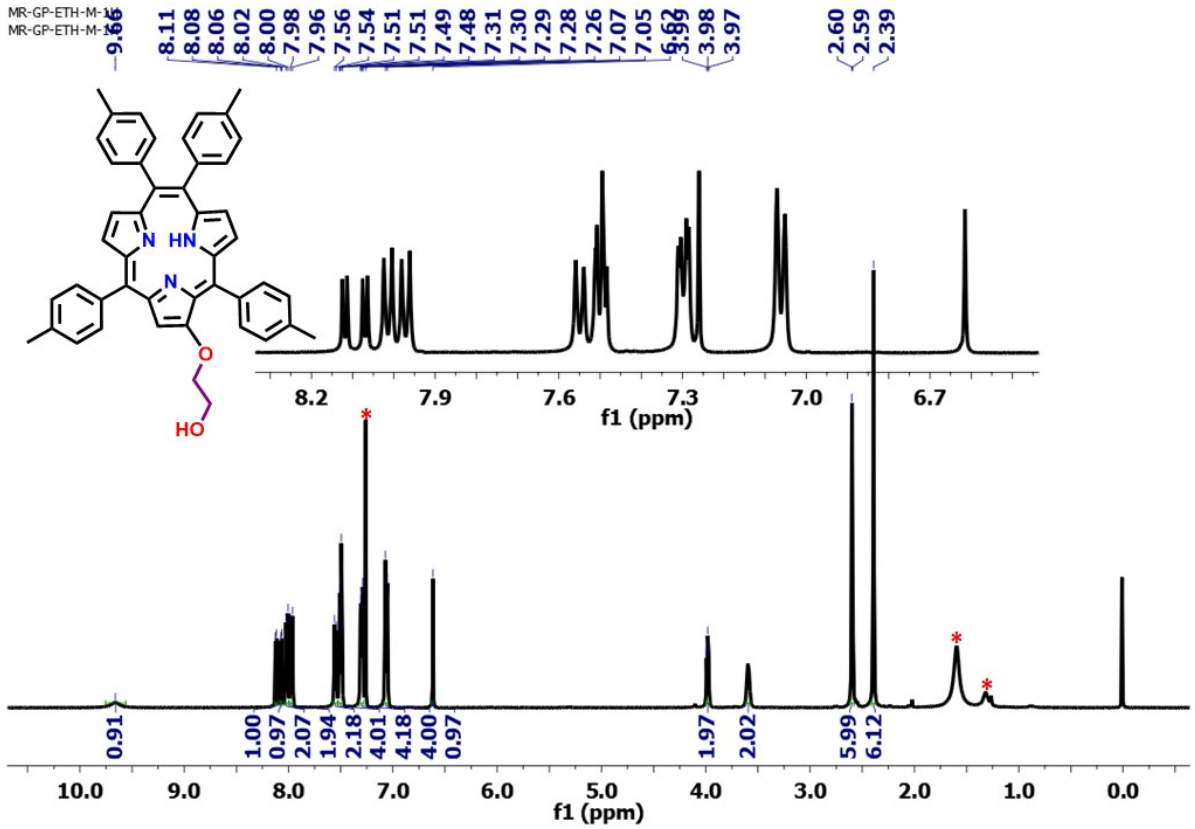


Figure S14. ^{1}H NMR spectrum of the compound **2-O(CH$_2$)$_2$-OH** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

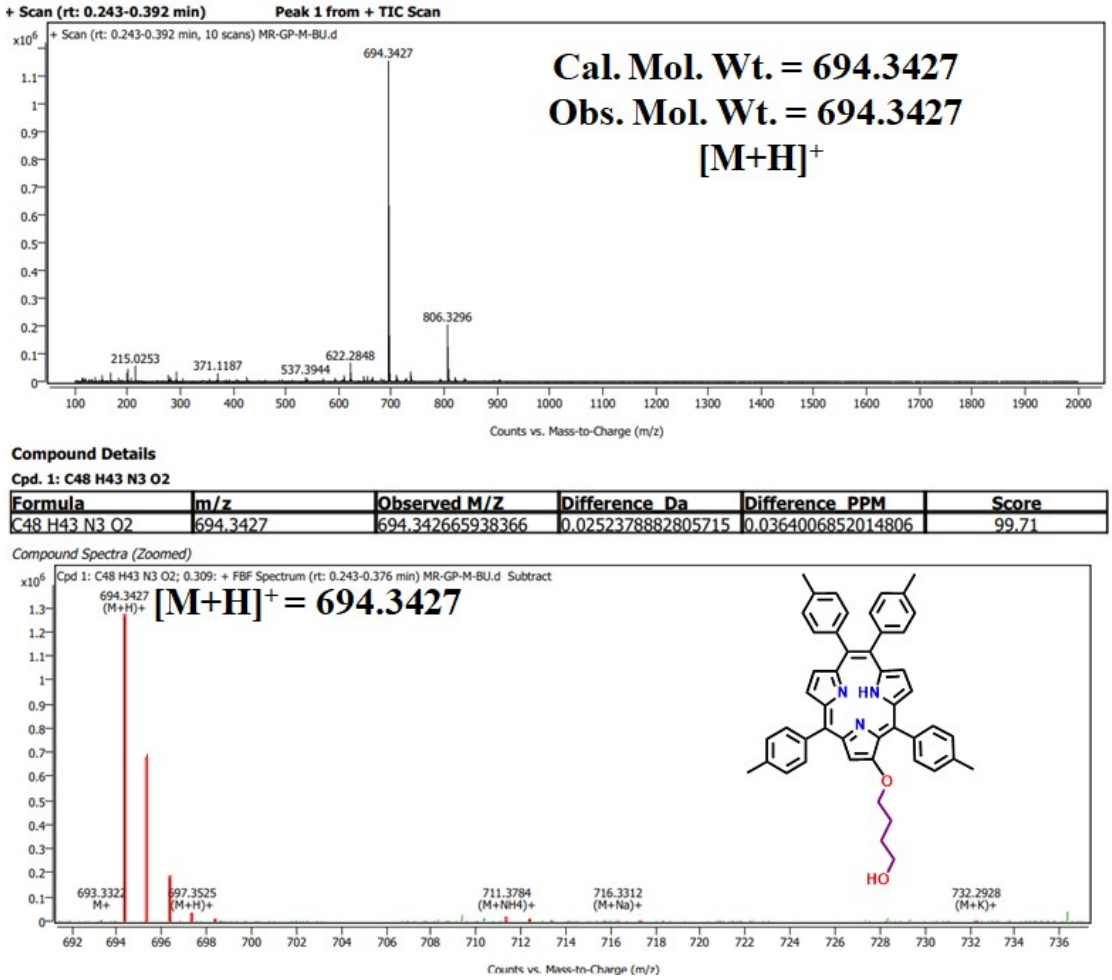


Figure S15. HR mass spectrum of the compound **2-O(CH_2)$_4$-OH**.

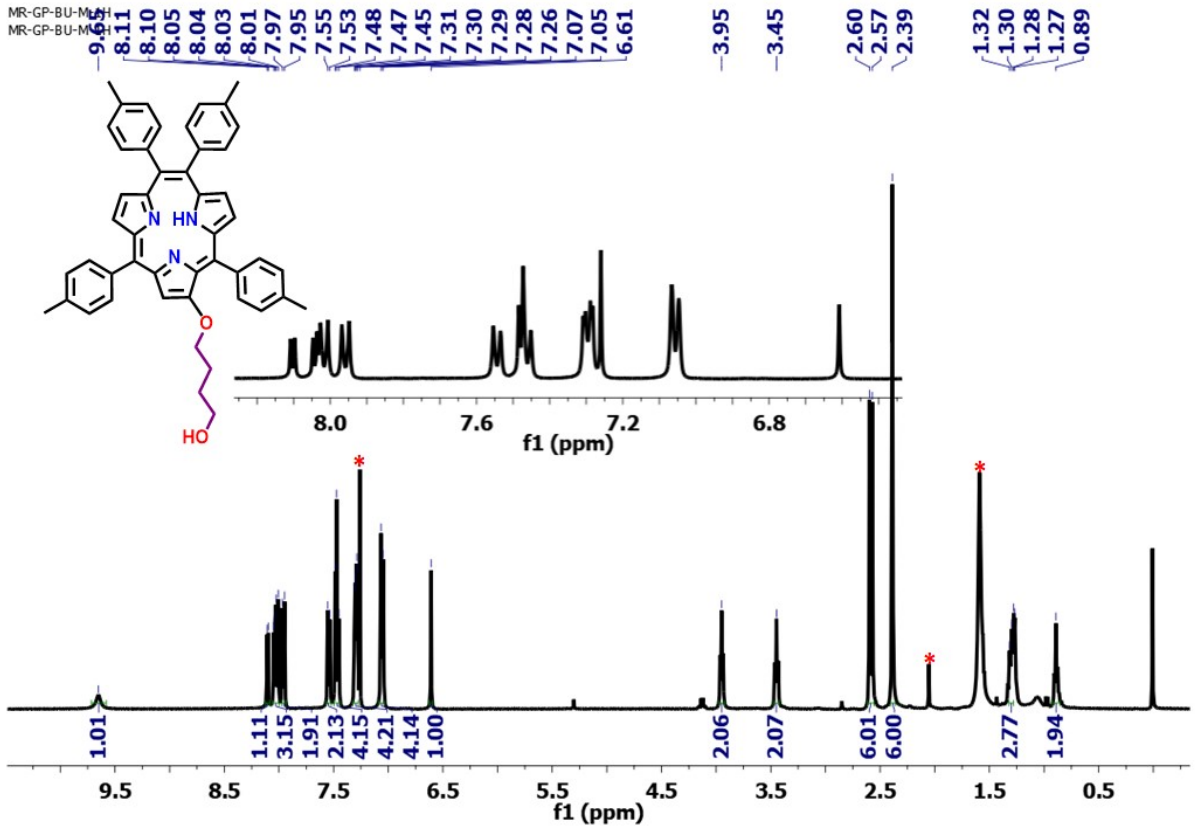


Figure S16. ^{1}H NMR spectrum of the compound **2-O(CH$_2$)$_4$-OH** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

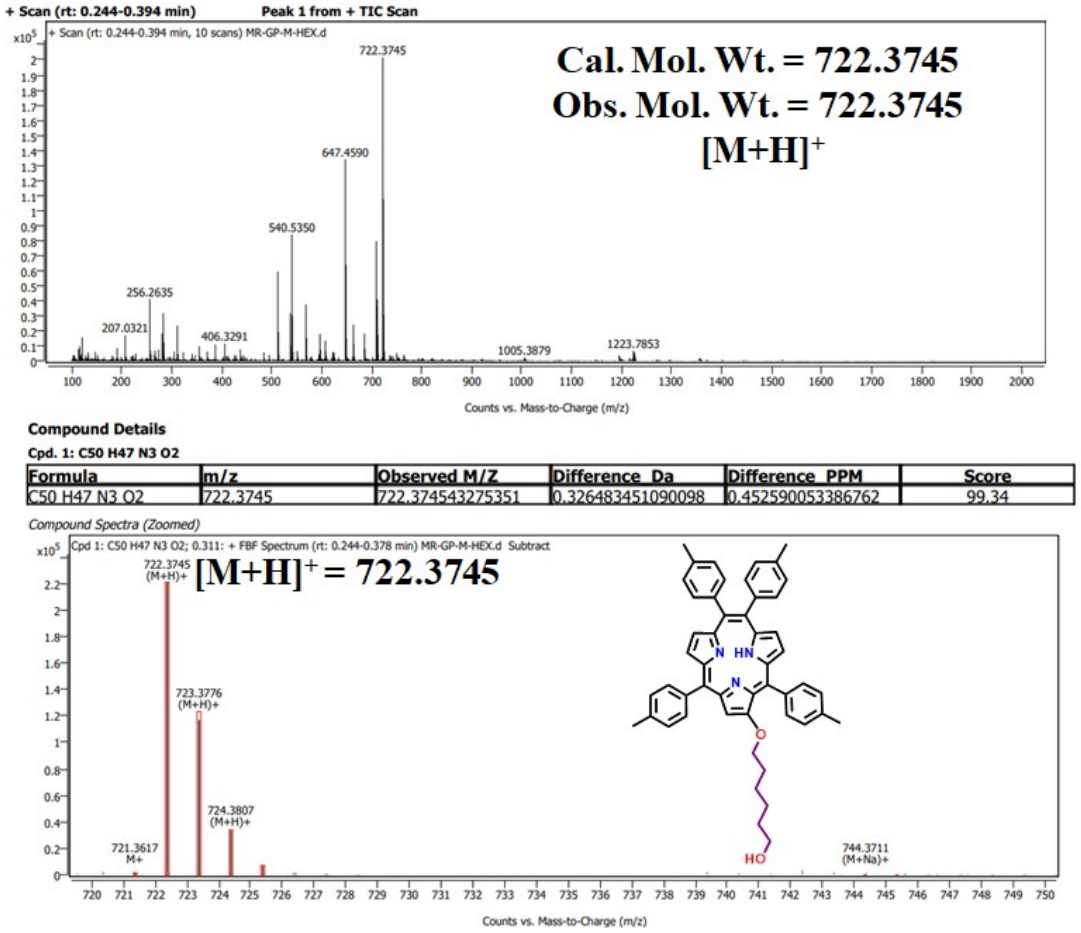


Figure S17. HR mass spectrum of the compound **2-O(CH_2)$_6$-OH**.

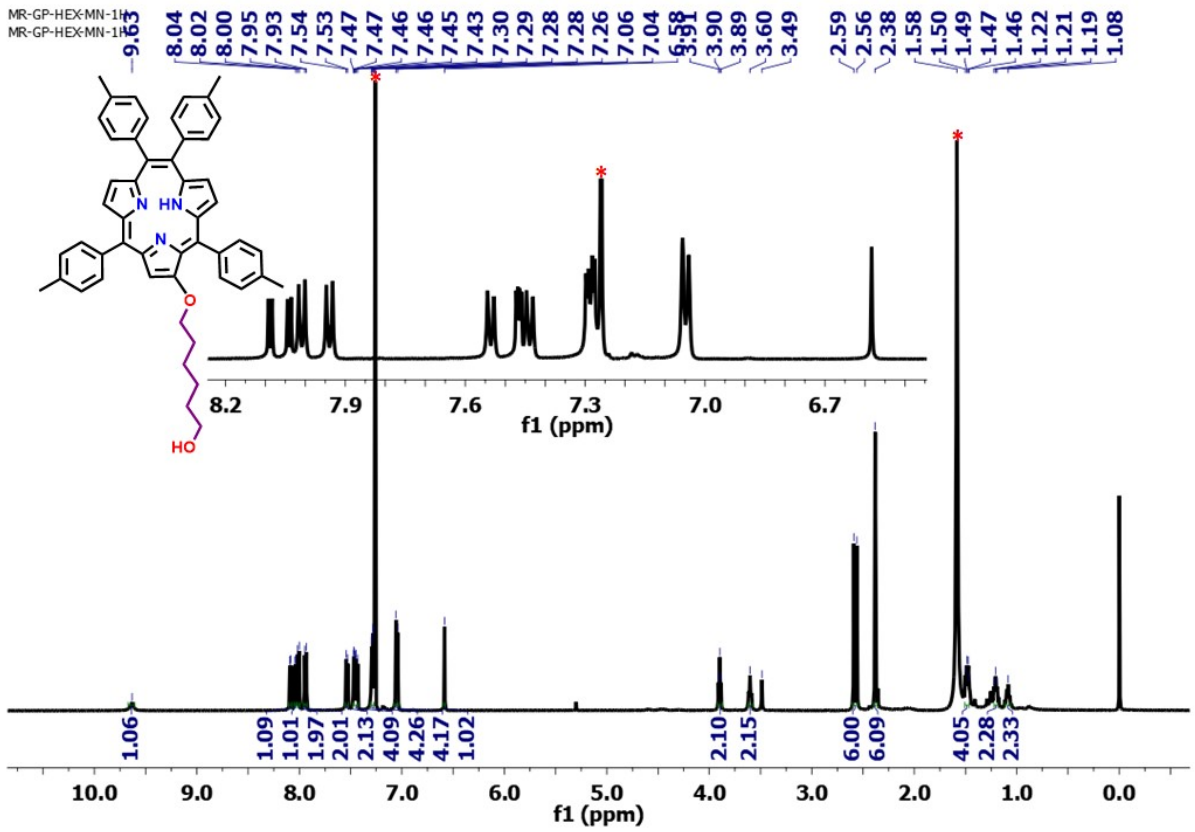


Figure S18. ^{1}H NMR spectrum of the compound **2-O(CH$_2$)$_6$-OH** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

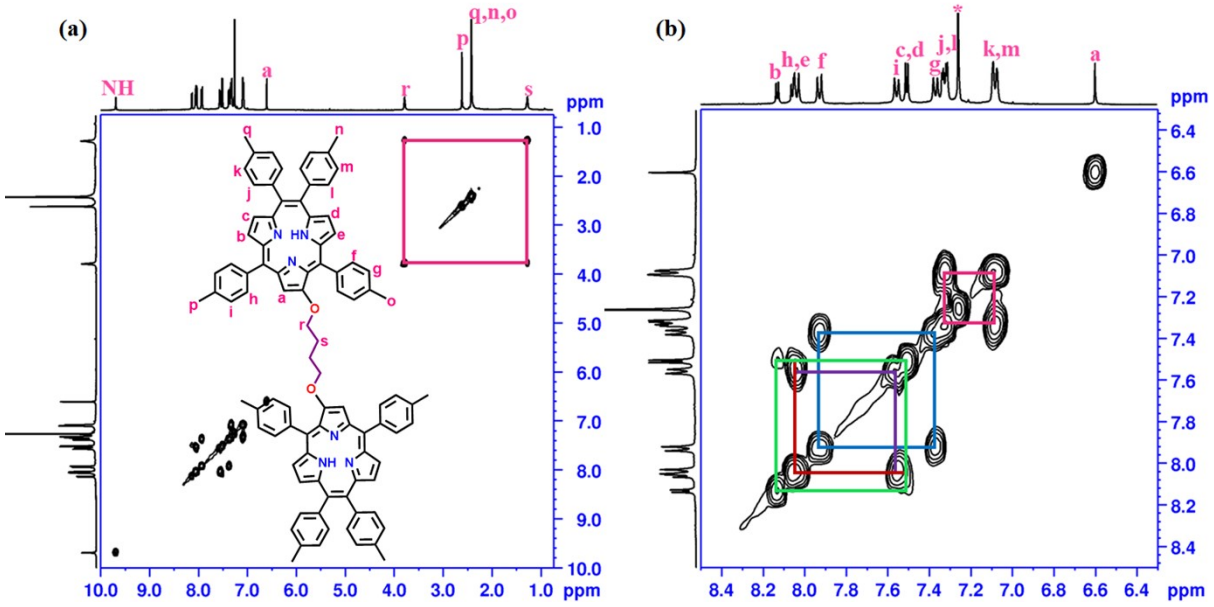


Figure S19. (a) ^{1}H-^{1}H COSY spectra of (a) **4** in full range, (b) **4** in selected region recorded in $CDCl_3$ at room temperature (25 °C).

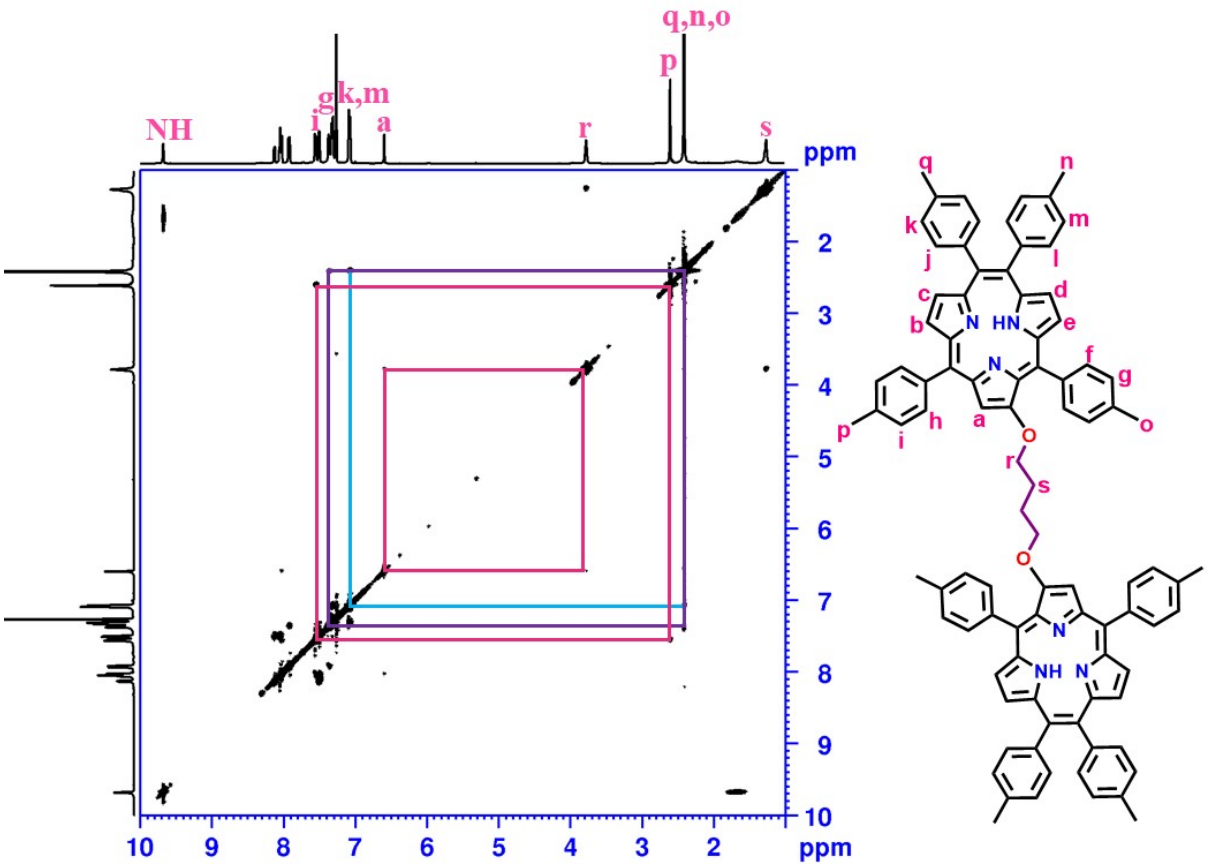


Figure S20. ^{1}H-^{1}H NOESY spectrum (full range) of compound **4** recorded in $CDCl_3$ at room temperature (25 °C).

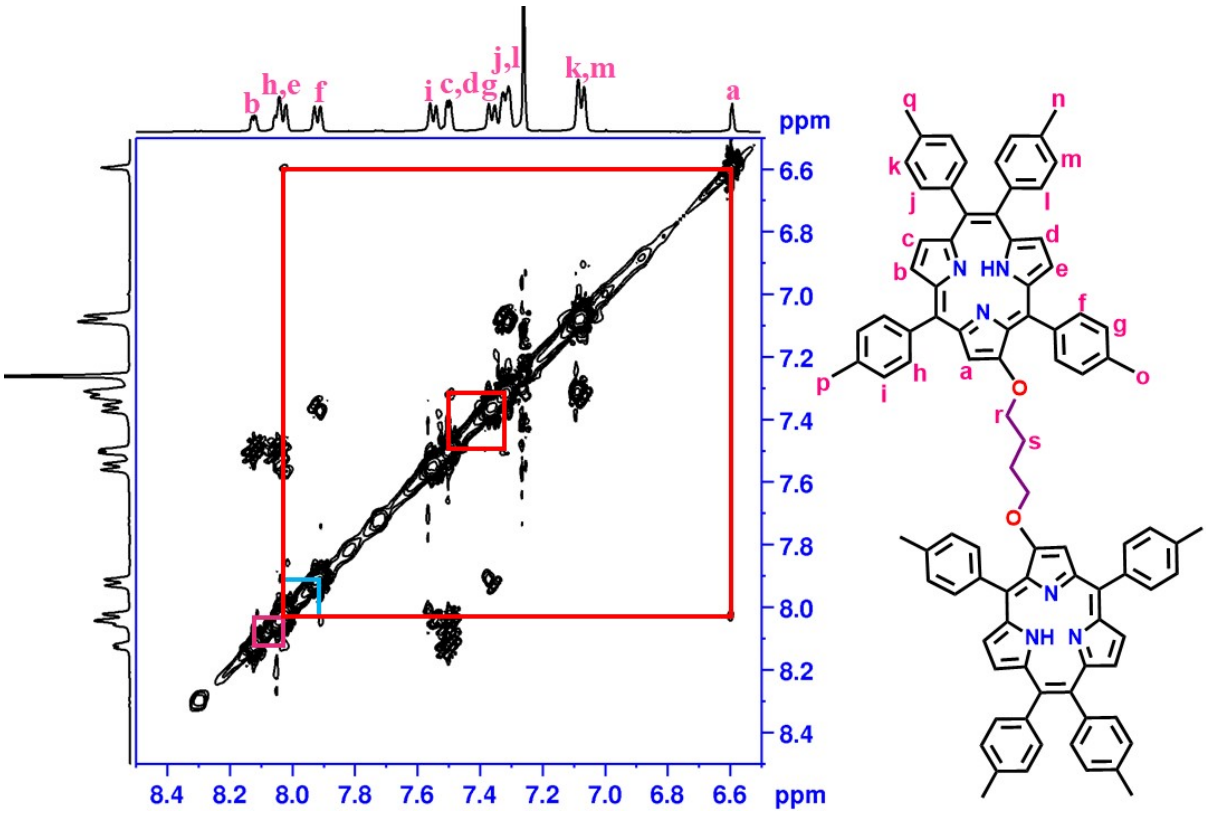


Figure S21. ^{1}H-^{1}H NOESY spectrum (selected region) of compound **4** recorded in $CDCl_3$ at room temperature (25 °C).

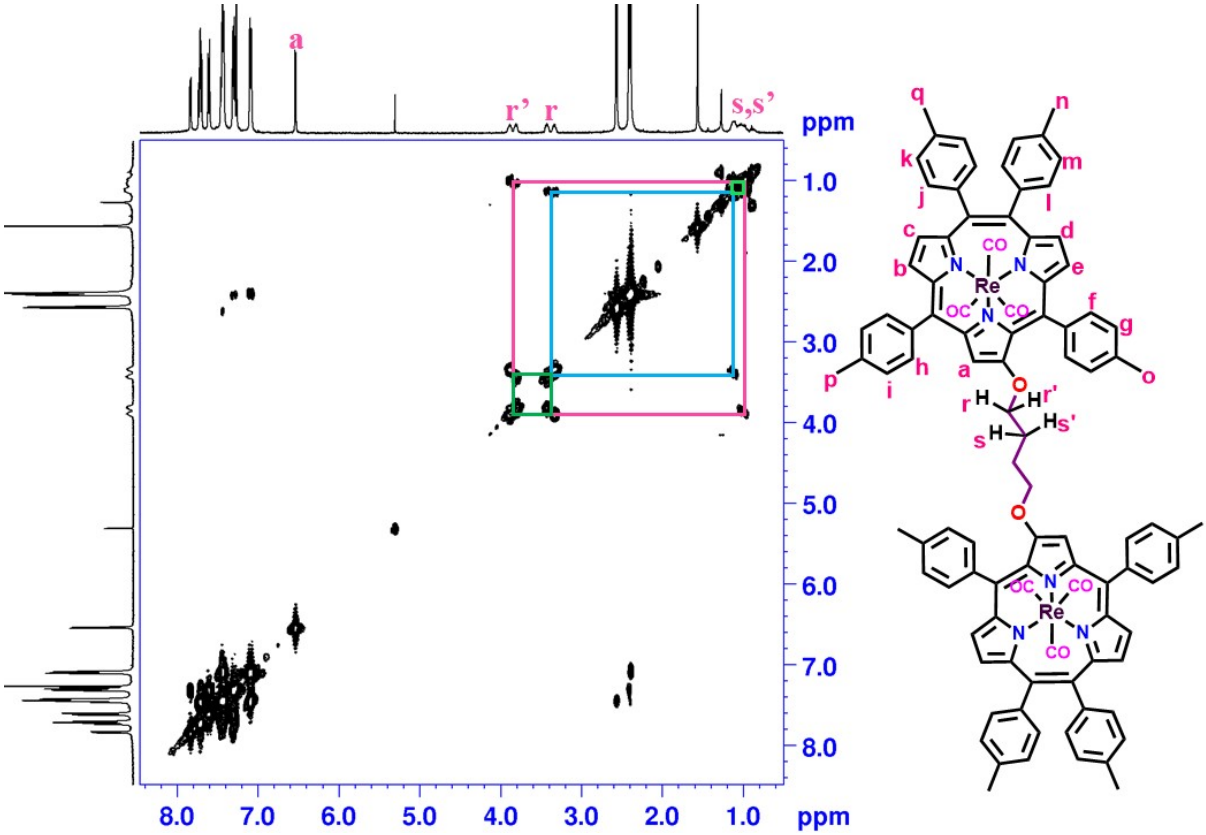


Figure S22. ^{1}H-^{1}H COSY spectrum (full range) of compound **4-Re** recorded in $CDCl_3$ at room temperature (25 °C).

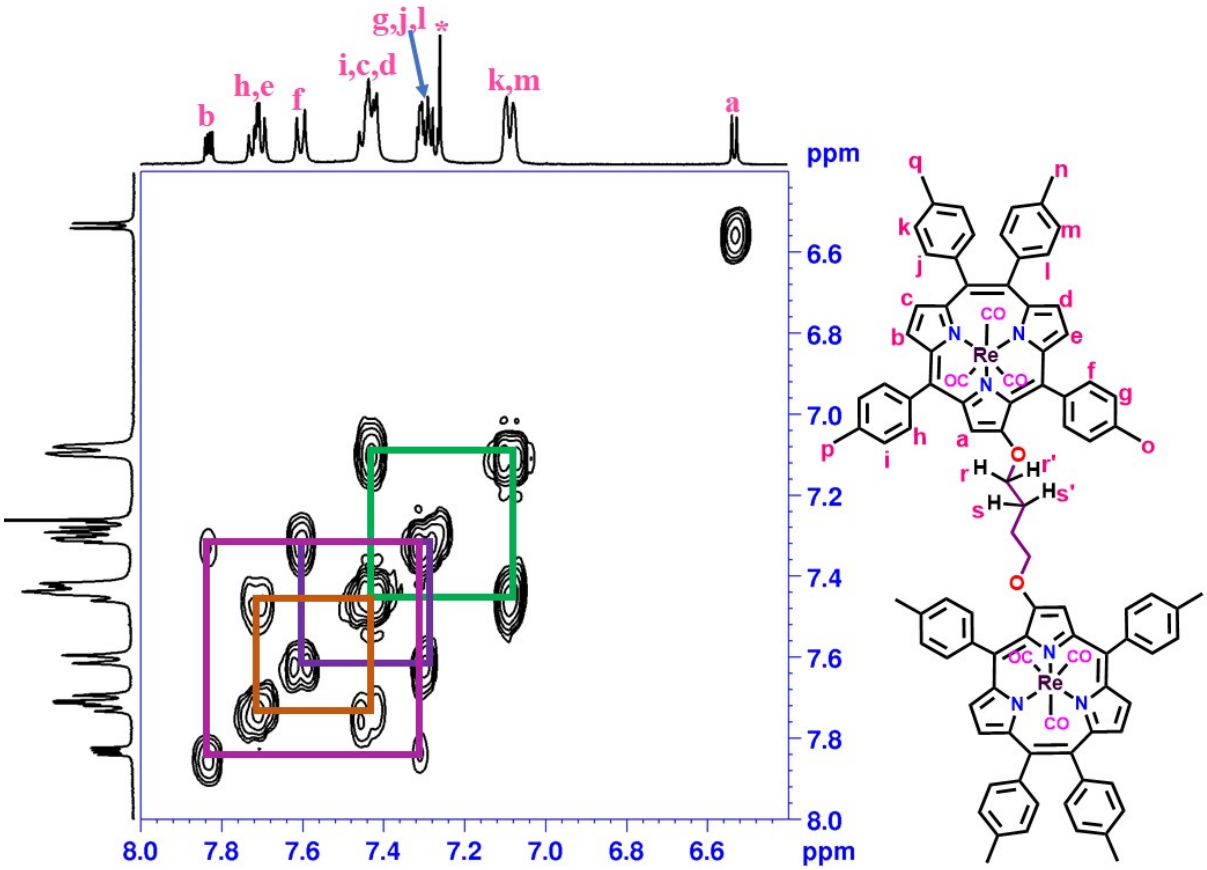


Figure S23. ^{1}H-^{1}H COSY spectrum (selected region) of compound **4-Re** recorded in $CDCl_3$ at room temperature (25 °C).

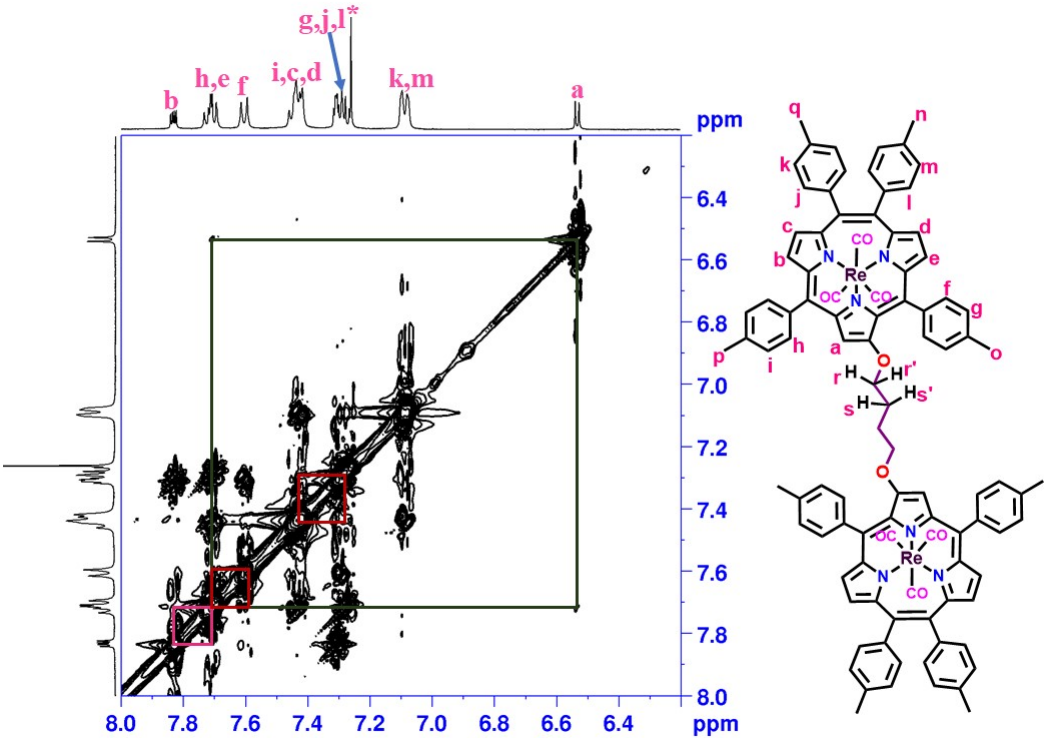


Figure S24. ^{1}H-^{1}H NOESY spectrum (selected region) of compound **4-Re** recorded in $CDCl_3$ at room temperature (25 °C).

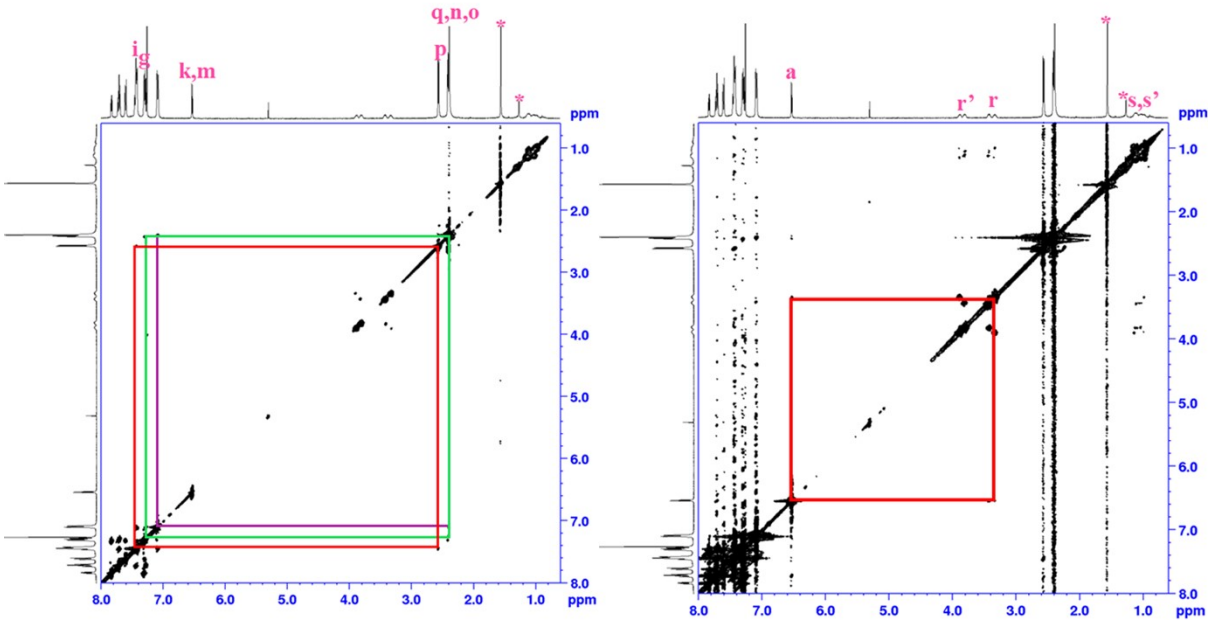


Figure S25. ^{1}H-^{1}H NOESY spectra (full range) of compound **4-Re** recorded in $CDCl_3$ at room temperature (25 °C).

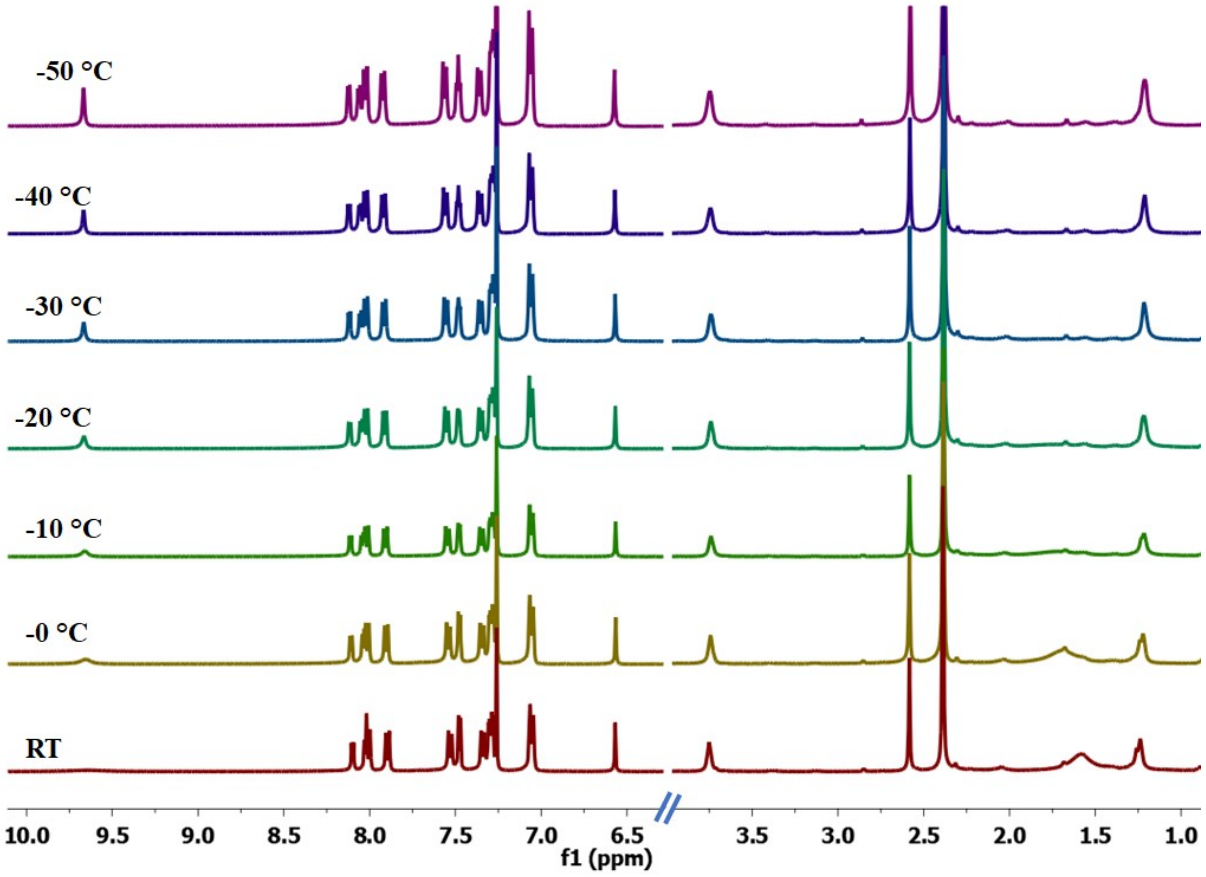


Figure S26. ^{1}H-NMR spectra of compound **4** recorded in $CDCl_3$ at variable low temperature.

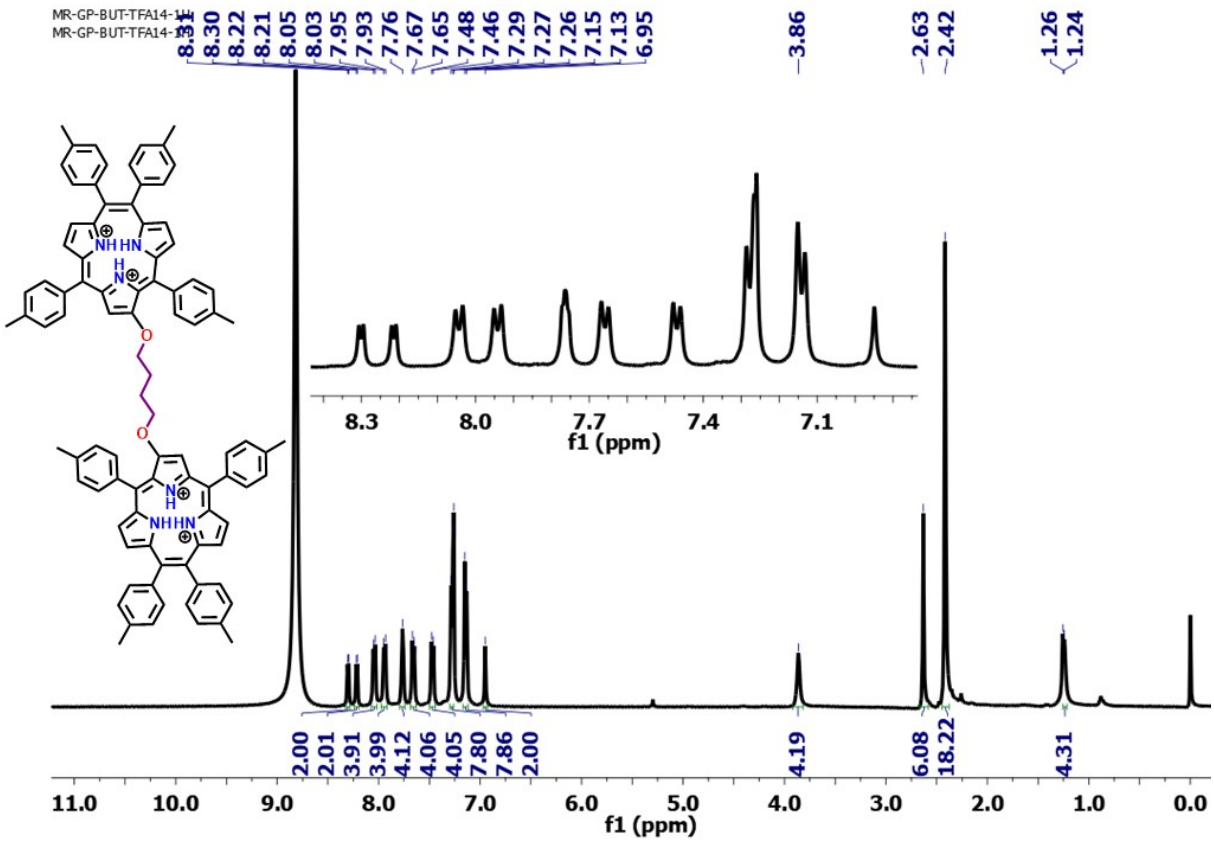


Figure S27. ^{1}H-NMR spectrum of **4.4H**$^{+}$ recorded in $CDCl_3$ at room temperature (25 °C).

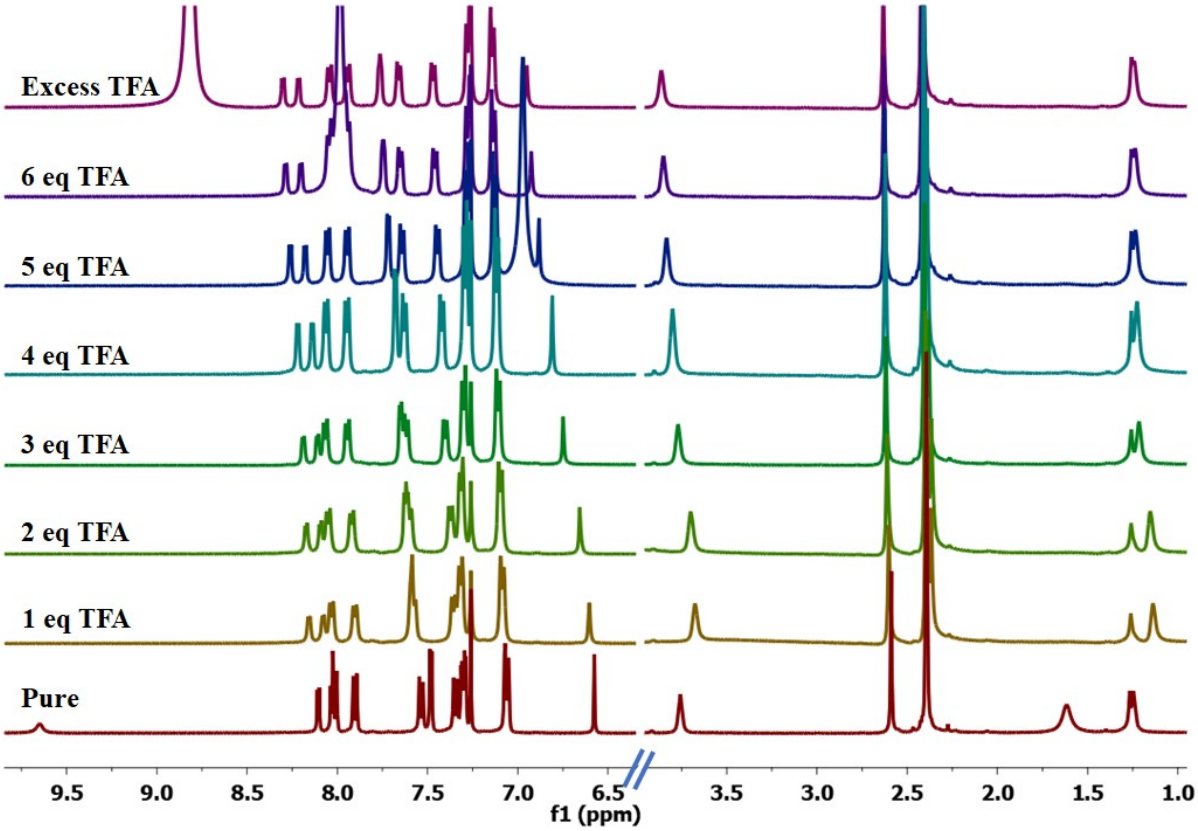


Figure S28. ^{1}H NMR titration experiment of the compound **4** with dilute solution of TFA recorded in $CDCl_3$ at room temperature (25 °C).

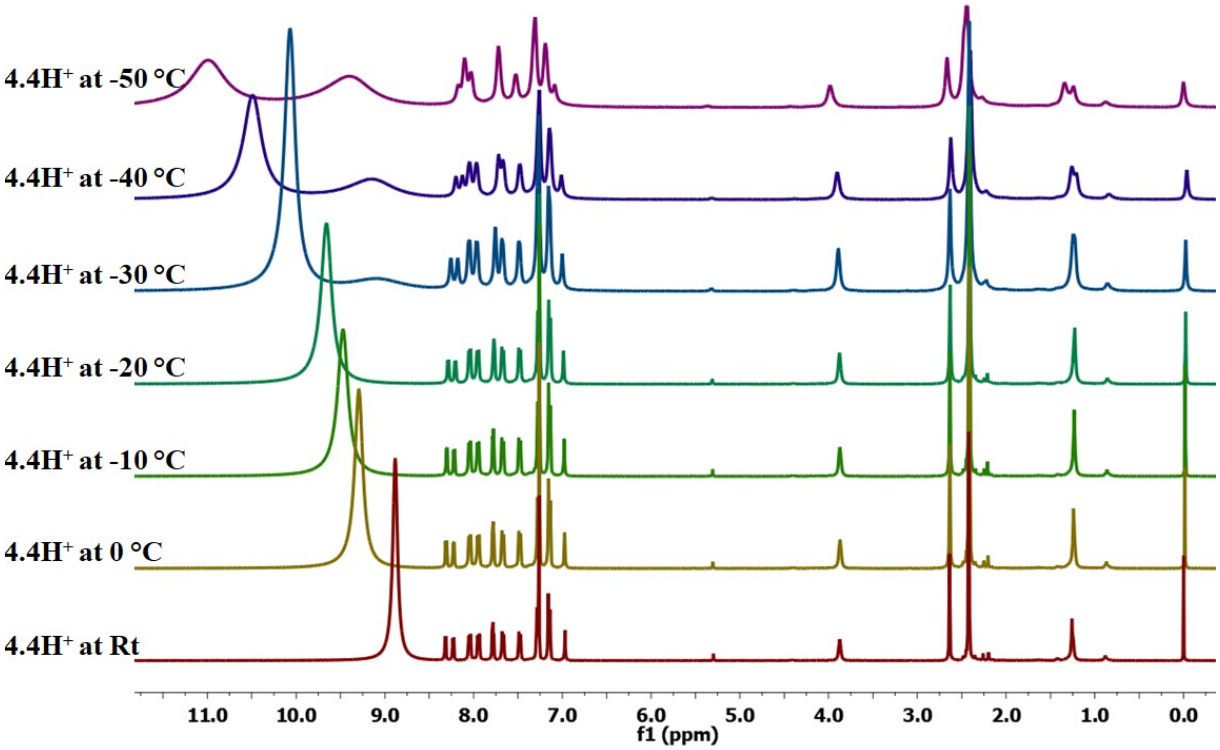


Figure S29. ^{1}H-NMR spectrum of **4.4H**$^{+}$ recorded in $CDCl_3$ at variable low temperature.

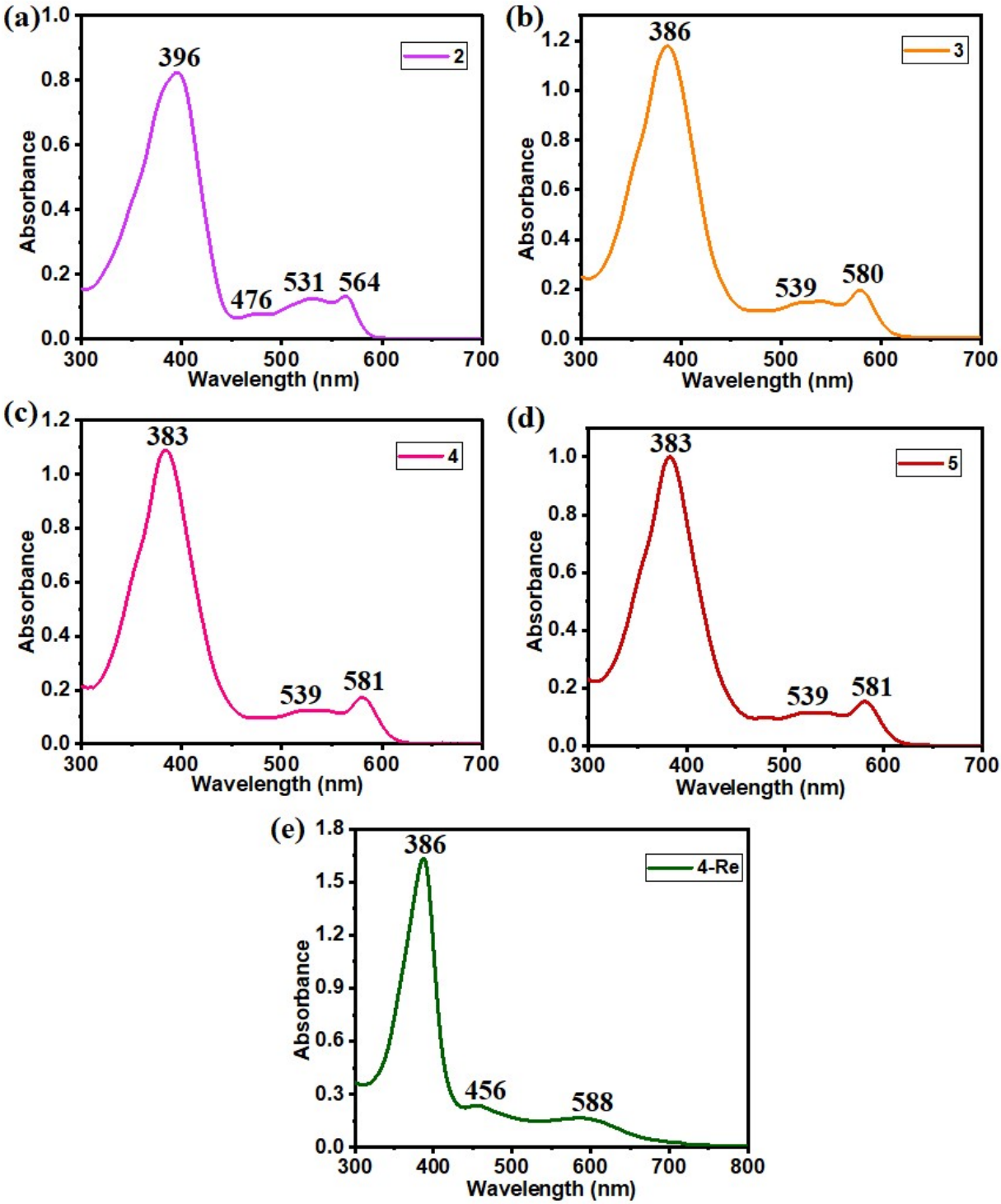
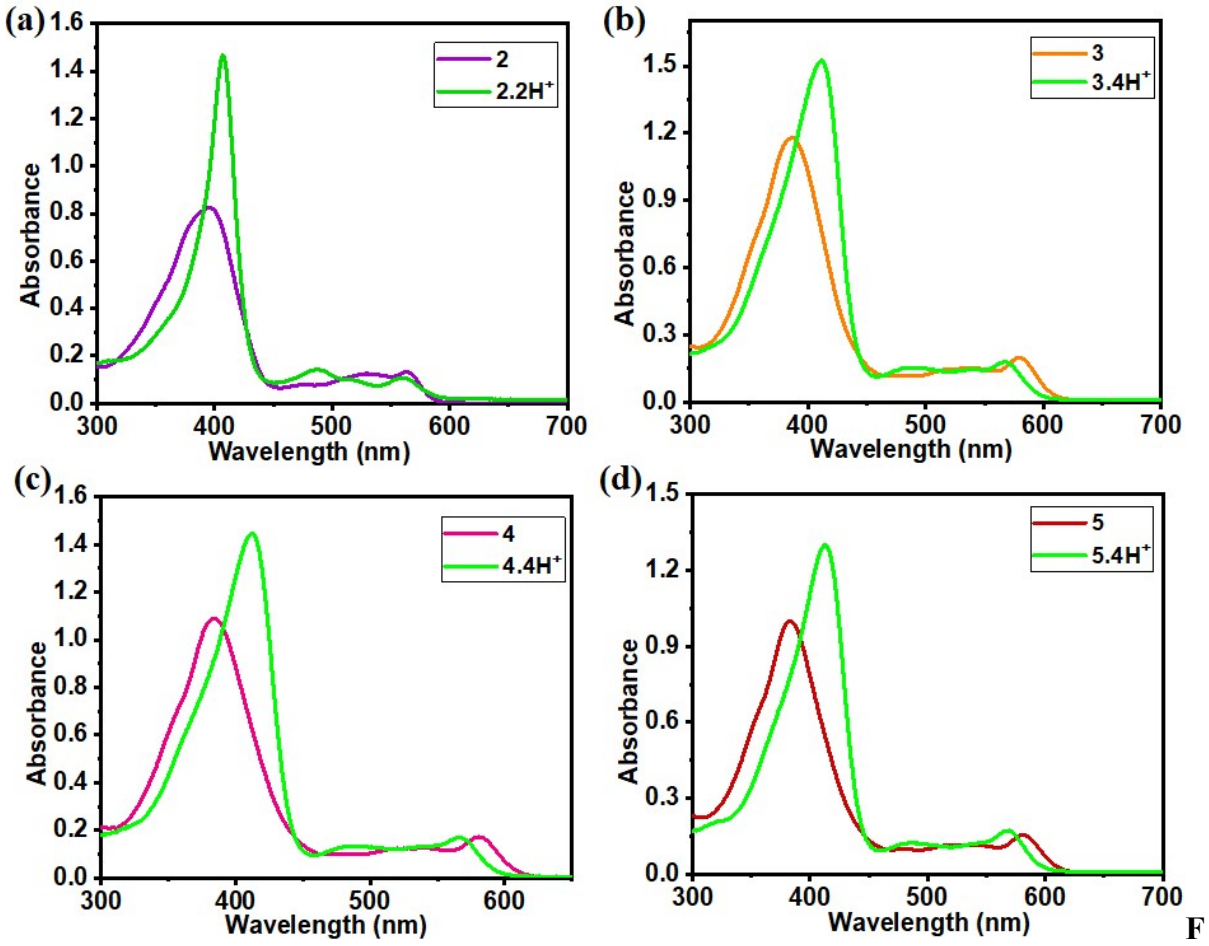


Figure S30. Absorption spectra of compounds **2-5** and **4-Re** (1×10^{-5} M) recorded in $CHCl_3$.



igure S31. Comparison of the absorption spectra of compounds **2-5** and **2.2H$^+$, 3.4H$^+$-5.4H$^+$** respectively in chloroform.

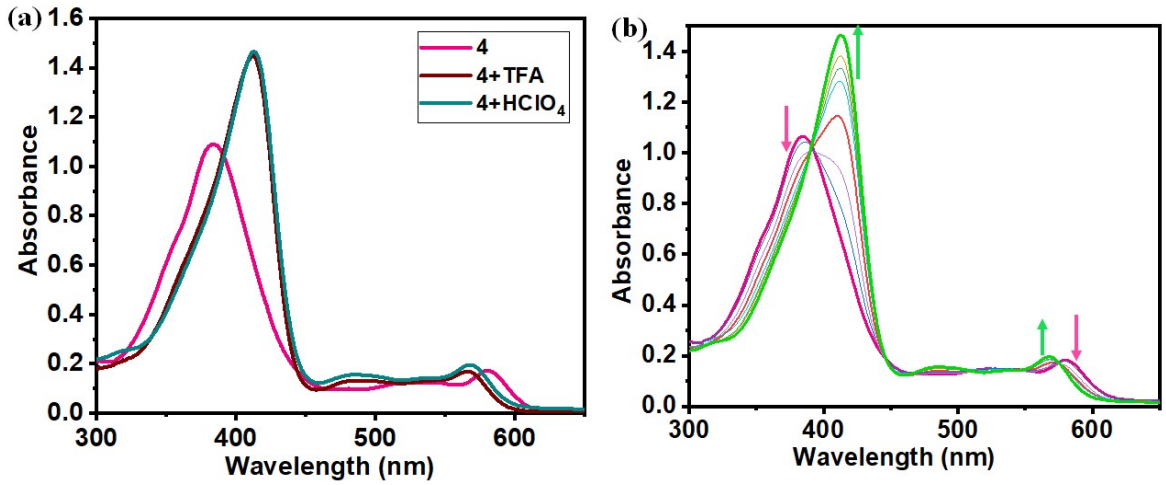


Figure S32. (a) Comparison of absorption spectra of compound **4** and in the presence of an excess of two different acids in $CHCl_3$; (b) Systematic protonation studies of compound **4** (1×10^{-5} M) by addition of increasing amounts of $HClO_4$ in $CHCl_3$ at room temperature.

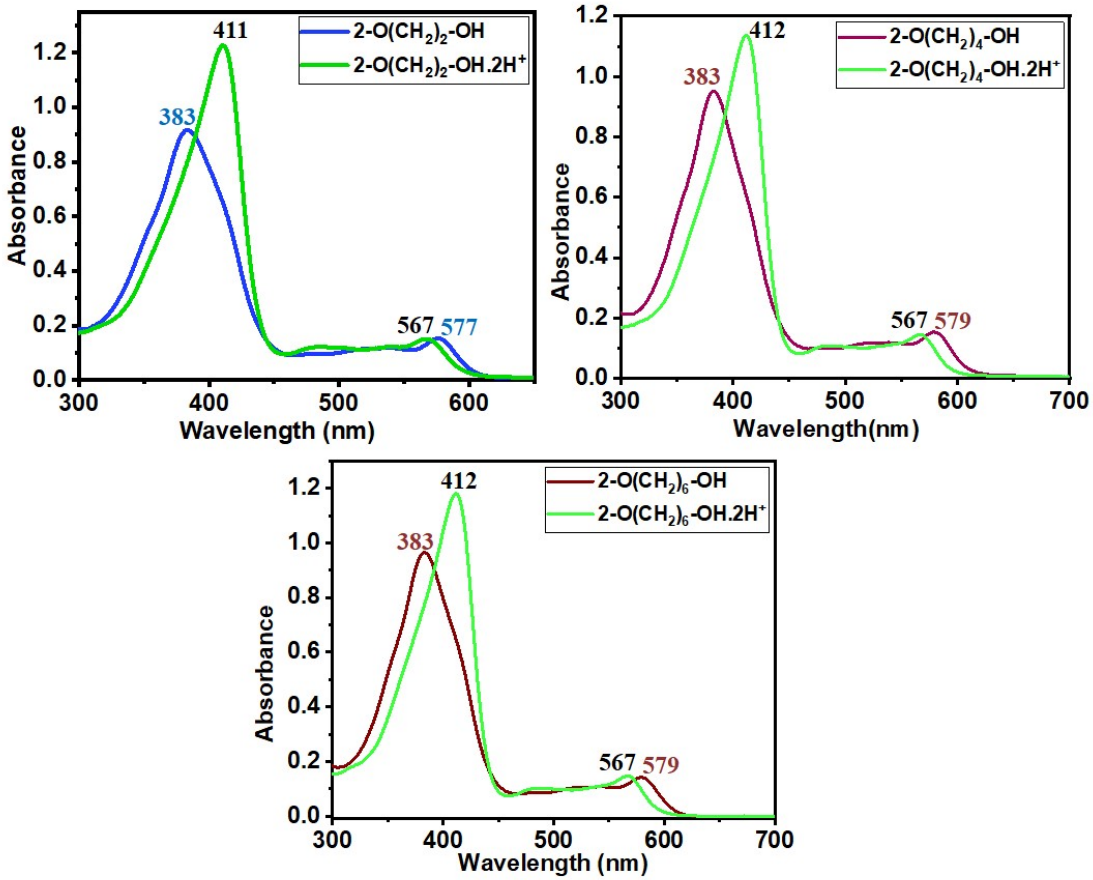


Figure S33. Comparison of the absorption spectra of compounds **2-O$(CH_2)_n$-OH** and their protonated derivatives respectively in chloroform.

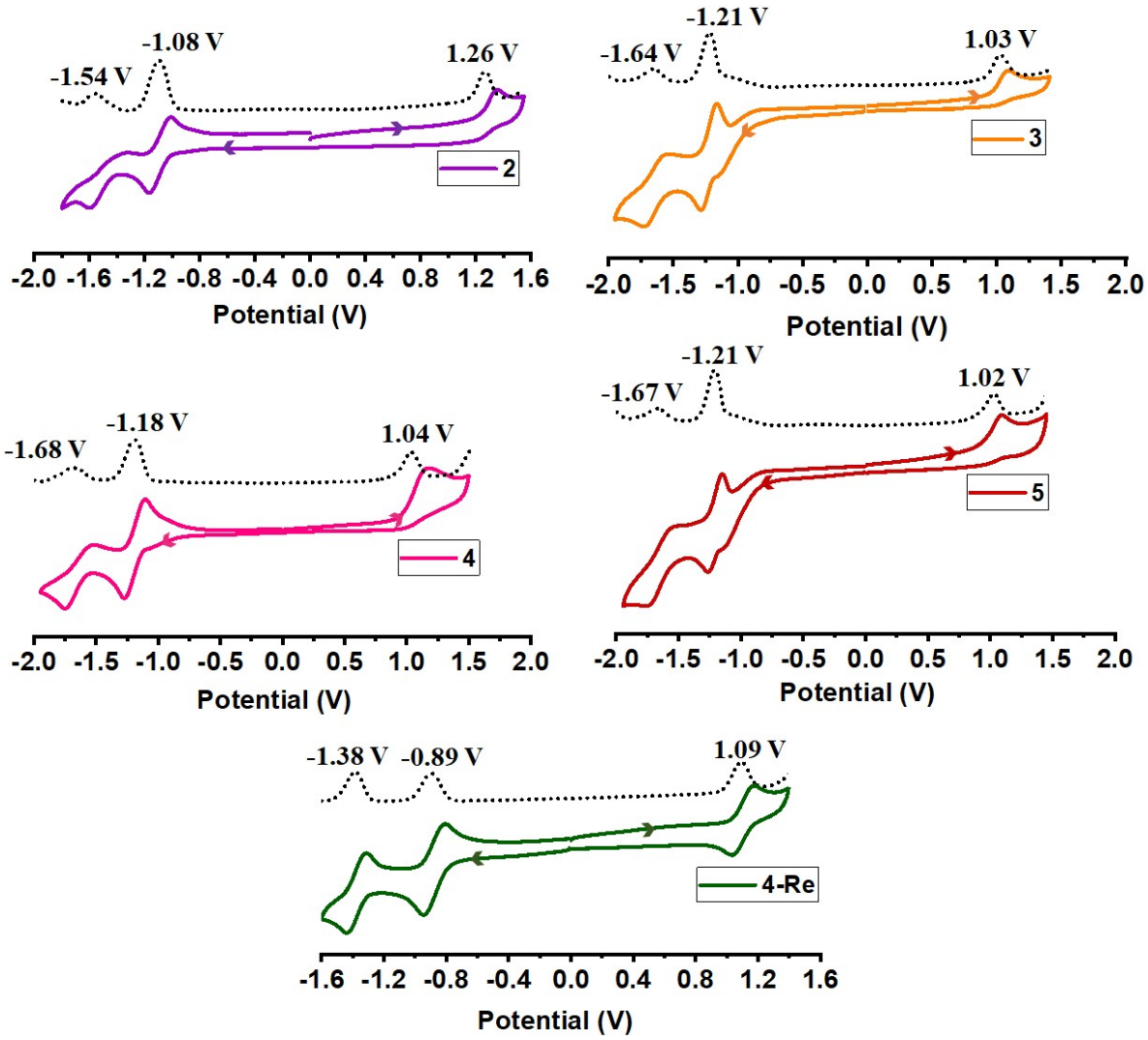


Figure S34. Comparison of cyclic voltammograms (coloured solid line) with their differential pulse voltammogram (dotted black line) of compounds **2-5** and **4-Re** recorded in dry CH_2Cl_2 with 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at a scan rate of 50 mV s^{-1}. A saturated calomel electrode (SCE) was employed as the reference electrode, glassy carbon as the working electrode, and platinum wire as the auxiliary electrode. (Note that polarographic convention has been followed for plotting CV starting at 0 V). All the potentials were calibrated by using ferrocene as an external standard, taking $E_{1/2}$ (Fc/Fc^+) = 0.42 V *versus* SCE.

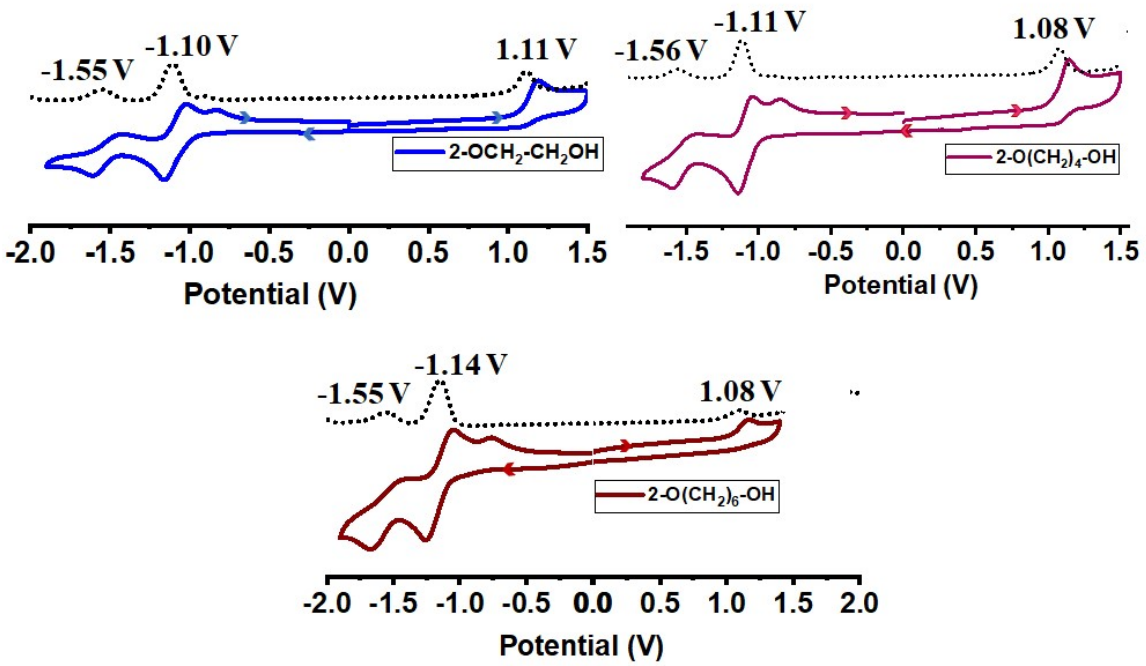


Figure S35. Comparison of cyclic voltammograms (coloured solid line) with their differential pulse voltammogram (dotted black line) of compounds **2-O(CH$_2$)$_n$-OH** recorded in dry CH_2Cl_2 with 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at a scan rate of 50 mV s^{-1}. A saturated calomel electrode (SCE) was employed as the reference electrode, glassy carbon as the working electrode, and platinum wire as the auxiliary electrode. (Note that polarographic convention has been followed for plotting CV starting at 0 V). All the potentials were calibrated by using ferrocene as an external standard, taking $E_{1/2}$ (Fc/Fc^+) = 0.42 V *versus* SCE.

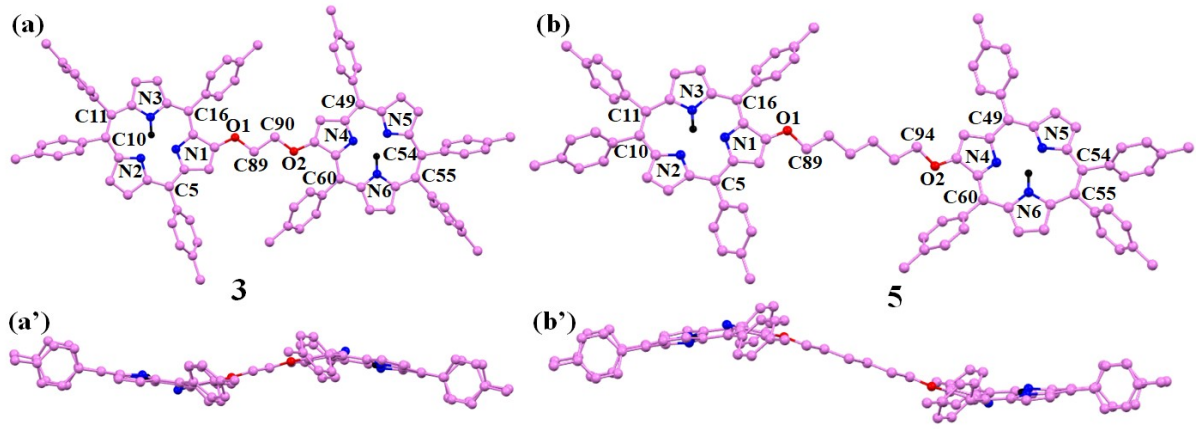


Figure S36. Ground state optimized structures with top view and side view of compounds **3** (a and a') and **5** (b and b') at B3LYP/6-31G (d, p) level of theory. Hydrogen atoms except inner NH were omitted for clarity.

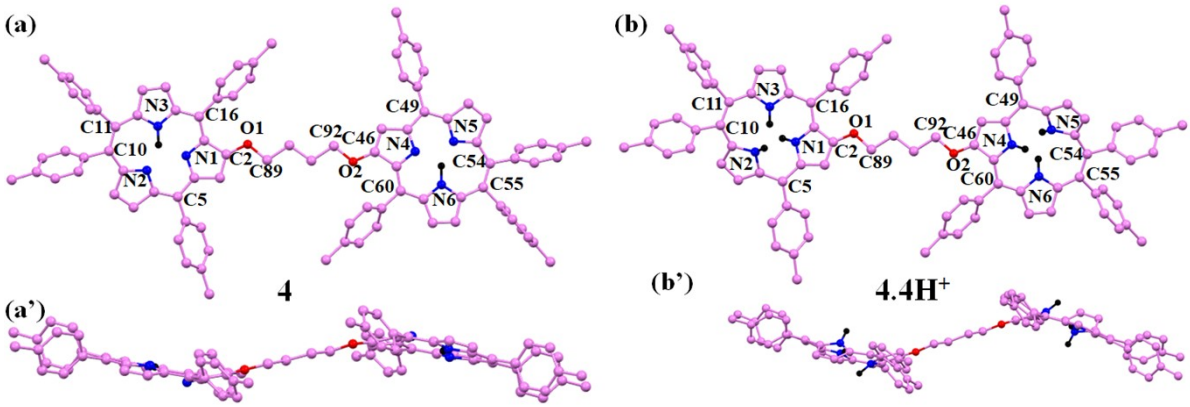


Figure S37. Ground state optimized structures with top view and side view of compounds **4** (a and a') and **4.4H**$^{+}$ (b and b') at B3LYP/6-31G (d, p) level of theory. Hydrogen atoms except inner NH were omitted for clarity.

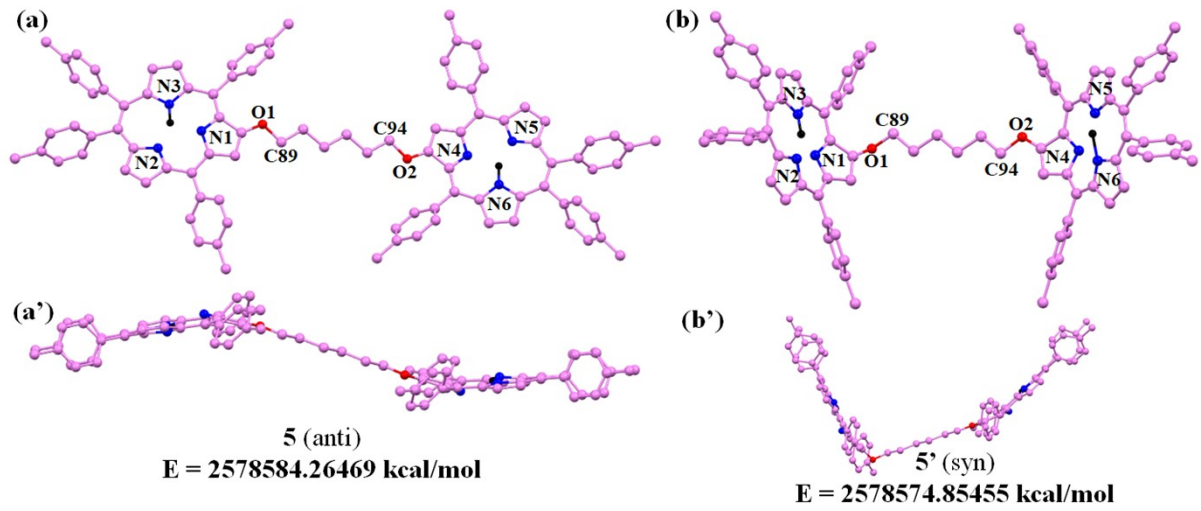


Figure S38. Ground state optimized structures with top view and side view of compounds **5** (a and a') in *anti*-conformation and **5'** (b and b') in *syn*-conformation at B3LYP/6-31G (d, p) level of theory. Hydrogen atoms except inner NH were omitted for clarity.

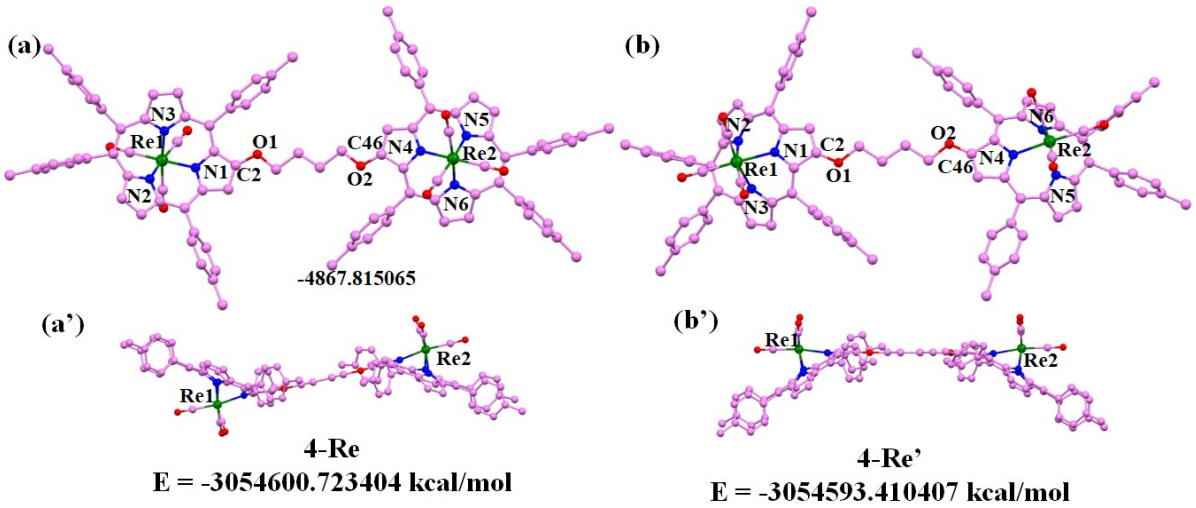


Figure S39. Ground state optimized structures with top view and side view of compounds **4-Re** (a and a') and **4-Re'** (b and b') at B3LYP/6-31G (d, p) and LANL2DZ level of theory. Hydrogen atoms except inner NH were omitted for clarity.

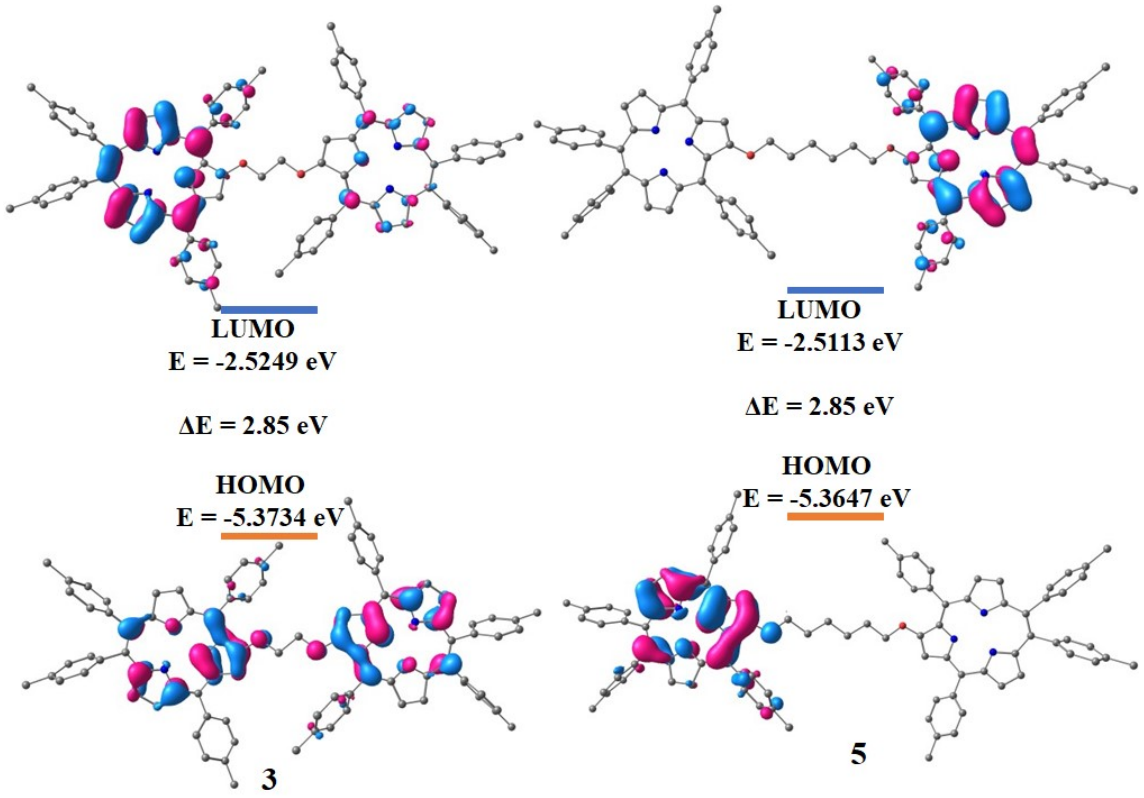


Figure S40. Energy-level diagram (selected FMOs) of compounds **3** and **5** calculated by the B3LYP/6-31g(d, p) method.

Table S1. S_0 optimized geometry of the compound **3** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3951.966766

Atom	X	Y	Z	Atom	X	Y	Z
N	-7.35269	-1.39906	-0.25128	C	12.7218	1.740834	-1.68302
N	-5.05869	-0.54866	-1.12564	H	12.98628	2.2049	-2.63018
N	-6.87924	1.121851	-0.45474	C	9.301613	-1.0552	0.034772
H	-6.76685	0.066701	-0.41822	C	3.169998	1.736069	0.670092
C	-7.90772	-3.59404	-0.63166	H	2.509193	2.544309	0.39594
H	-7.79956	-4.64462	-0.86196	C	4.135342	-0.30282	1.07737
C	-8.69087	-1.50018	-0.2521	C	11.40471	1.337931	-1.46246
C	-3.11469	-1.63344	-0.53921	H	10.6568	1.495173	-2.23443
H	-2.44487	-2.4313	-0.25686	C	3.420912	-3.76451	0.072487
C	-6.81935	-2.6312	-0.50076	H	4.131106	-3.75944	-0.74806

C	-4.54201	-1.74957	-0.82681	C	4.498194	-1.67168	0.981656
C	-11.0336	-0.83348	0.072114	C	8.721599	1.456327	0.153962
C	-9.33895	0.993586	-0.10667	C	9.144748	2.845444	0.342649
C	-8.09892	1.694273	-0.31466	H	10.16362	3.20366	0.358715
C	-4.11364	0.390725	-0.93917	C	2.450568	-4.76143	0.141735
C	-9.06956	-2.89471	-0.49031	H	2.425691	-5.53433	-0.62262
H	-10.0771	-3.27726	-0.56153	C	9.59725	0.323486	-0.02338
C	-7.89655	3.117878	-0.43441	C	1.562138	-3.76552	2.137117
H	-8.67086	3.865944	-0.3666	H	0.846521	-3.76425	2.955635
C	-5.89771	2.056358	-0.67237	C	8.008093	3.576963	0.521169
C	-2.84443	-0.28966	-0.60868	H	7.936478	4.634716	0.732097
C	-10.5009	1.930208	0.112039	C	6.891575	2.639655	0.461539
C	-4.87794	-4.23028	-0.59687	C	11.92591	-3.16847	-1.75311
C	-5.4267	-2.85946	-0.65906	H	12.2782	-3.32026	-2.77068
C	-4.5154	1.74768	-0.8302	C	13.70726	1.560087	-0.70579
C	-9.60212	-0.39316	-0.09065	C	4.996005	4.289306	0.606074
C	-11.982	-0.64577	-0.94323	C	12.01573	0.544653	0.721004
H	-11.6893	-0.14197	-1.85881	H	11.74908	0.07997	1.664875
C	-2.52673	2.917128	-1.80867	C	5.513239	2.906709	0.67464
H	-2.5014	2.160305	-2.58611	C	13.3279	0.956224	0.500626
C	-12.6479	3.737702	0.545055	H	14.07123	0.805598	1.279936
C	-6.55795	3.334045	-0.66306	C	1.502349	-4.78169	1.172789
H	-6.07339	4.28558	-0.82442	C	12.02545	-3.67626	0.588349
C	-3.5375	3.846491	0.168825	H	12.45843	-4.2252	1.421144
H	-4.28036	3.802091	0.958672	C	5.433779	5.194846	-0.37837
C	-12.7544	-1.94457	1.386095	H	6.155924	4.864705	-1.11776
H	-13.045	-2.44915	2.304388	C	11.0029	-2.75874	0.8314
C	-3.522	2.846965	-0.81836	H	10.64819	-2.60435	1.846588
C	-1.5958	3.950107	-1.81528	C	4.021938	4.738067	1.517967
H	-0.84712	3.988678	-2.60285	H	3.674186	4.063638	2.293887
C	-11.0519	2.104055	1.388956	C	3.96499	6.93808	0.476915
H	-10.6515	1.535515	2.222811	C	3.520091	6.034704	1.452554
C	-12.0947	3.564918	-0.72901	H	2.776921	6.355575	2.178575
H	-12.4974	4.127414	-1.56795	C	4.927037	6.490085	-0.4381
C	-2.59609	4.873864	0.161829	H	5.276639	7.162958	-1.21728
H	-2.62628	5.629681	0.942777	O	-1.69467	0.379452	-0.37372
C	-13.7028	-1.75478	0.374866	O	1.701807	-0.24817	0.591156
C	-13.2902	-1.09871	-0.79305	C	13.5926	-4.91268	-0.97642
H	-14.0042	-0.94014	-1.59781	H	14.15833	-5.14271	-0.06904
C	-5.33407	-5.16696	0.349586	H	13.17492	-5.85615	-1.34975
H	-6.09541	-4.87026	1.063418	H	14.29794	-4.55216	-1.73206
C	-11.4406	-1.50005	1.235582	C	15.12688	2.024653	-0.92988
H	-10.721	-1.66644	2.032169	H	15.35654	2.109195	-1.99602
C	-11.0374	2.680424	-0.94284	H	15.2995	3.010386	-0.47962
H	-10.6261	2.564527	-1.94169	H	15.84944	1.33529	-0.48179
C	-1.60829	4.946466	-0.82783	C	3.44449	8.35435	0.43086
C	-4.79739	-6.4501	0.405442	H	4.043223	9.016178	1.069386
H	-5.16253	-7.14756	1.155364	H	3.481923	8.762276	-0.58353

C	-3.85505	-4.63558	-1.47472	H	2.410474	8.414032	0.783562
H	-3.49201	-3.93675	-2.22145	C	0.433231	-5.84649	1.227571
C	-12.1065	2.989636	1.598912	H	-0.44967	-5.55612	0.643758
H	-12.5163	3.101967	2.599915	H	0.793399	-6.796	0.819698
C	-3.32326	-5.92066	-1.41343	H	0.097741	-6.0235	2.253652
H	-2.54217	-6.20788	-2.11322	C	-3.23244	-8.25881	-0.43539
C	-3.78586	-6.85492	-0.47604	H	-3.26939	-8.67504	0.575769
N	5.108846	0.616538	1.209295	H	-3.81009	-8.92995	-1.08354
N	7.382654	1.389163	0.216319	H	-2.19432	-8.29134	-0.77908
N	6.857269	-1.11405	0.491471	C	-0.57264	6.045217	-0.82017
H	6.769872	-0.05697	0.437295	H	-0.92501	6.921826	-0.26873
C	6.492135	-3.31274	0.762958	H	0.359408	5.712369	-0.34583
H	5.992193	-4.24814	0.966315	H	-0.31944	6.362898	-1.83644
C	7.824406	-3.13509	0.472357	C	-13.7734	4.716365	0.783468
H	8.577047	-3.90335	0.388146	H	-13.3951	5.673268	1.164702
C	2.871549	0.400913	0.776933	H	-14.3221	4.927359	-0.13897
C	5.864103	-2.01901	0.772081	H	-14.4864	4.335237	1.521362
C	2.523103	-2.762	2.068623	C	-15.1177	-2.26263	0.521345
H	2.552983	-1.98863	2.82949	H	-15.2579	-3.21045	-0.01339
C	8.055372	-1.7199	0.311909	H	-15.373	-2.43864	1.570222
C	4.609531	1.823163	0.903093	H	-15.8428	-1.55221	0.11147
C	10.42919	-2.02557	-0.21545	C	0.5897	0.547664	0.194691
C	3.476571	-2.74334	1.036579	C	-0.57746	-0.40951	0.022057
C	10.906	-2.25042	-1.51417	H	0.804057	1.068641	-0.74698
H	10.47462	-1.69654	-2.34243	H	0.361536	1.300585	0.959849
C	12.50492	-3.89982	-0.70732	H	-0.3455	-1.15997	-0.74424
C	11.03062	0.722786	-0.26018	H	-0.78909	-0.93378	0.962561

Table S2. S_0 optimized geometry of the compound **4** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -4030.601435

Atom	X	Y	Z	Atom	X	Y	Z
N	-8.59871	-1.40112	-0.35013	C	4.477481	1.84273	0.738911
N	-6.34378	-0.48352	-1.26361	H	3.825901	2.648125	0.436003
N	-8.14187	1.130333	-0.41549	C	5.413799	-0.18621	1.249148
H	-8.0242	0.075767	-0.44769	C	12.58207	1.064583	-1.74264
C	-9.16298	-3.56872	-0.85461	H	11.79833	1.165194	-2.48805
H	-9.06145	-4.60099	-1.15878	C	4.597033	-3.70679	0.563355
C	-9.93556	-1.50919	-0.30451	H	5.261193	-3.77833	-0.29195
C	-4.37562	-1.59279	-0.82178	C	5.744766	-1.56619	1.244234
H	-3.69569	-2.40522	-0.61551	C	9.991044	1.388494	-0.00119

C	-8.07277	-2.61084	-0.70371	C	10.45188	2.777135	0.059697
C	-5.81233	-1.69798	-1.06159	H	11.47718	3.111142	-0.00307
C	-12.2654	-0.87795	0.155369	C	3.621961	-4.68159	0.764487
C	-10.5848	0.966166	0.025751	H	3.548547	-5.51297	0.067684
C	-9.35702	1.685669	-0.19077	C	10.83367	0.224683	-0.13051
C	-5.39428	0.447157	-1.05684	C	2.839871	-3.50521	2.70532
C	-10.3199	-2.88682	-0.61955	H	2.159451	-3.41897	3.5491
H	-11.3285	-3.26923	-0.67528	C	9.34145	3.547219	0.240537
C	-9.16554	3.114796	-0.23501	H	9.302913	4.619119	0.374393
H	-9.93873	3.852978	-0.09017	C	8.203954	2.63577	0.306806
C	-7.17419	2.082041	-0.61962	C	13.02609	-3.45183	-1.64647
C	-4.10926	-0.24536	-0.81756	H	13.33365	-3.69867	-2.6599
C	-11.7391	1.879586	0.355112	C	14.92259	1.312309	-1.12332
C	-6.13725	-4.19108	-0.99354	C	6.358505	4.341054	0.430556
C	-6.6876	-2.82093	-0.93417	C	13.29058	0.466022	0.473243
C	-5.79772	1.792477	-0.85219	H	13.06502	0.096574	1.468519
C	-10.8429	-0.4201	-0.03546	C	6.844148	2.951808	0.565074
C	-13.2531	-0.63346	-0.80897	C	14.59567	0.830515	0.151646
H	-12.998	-0.0717	-1.70184	H	15.37496	0.739648	0.904661
C	-3.86111	3.029159	-1.85005	C	2.730456	-4.60466	1.841452
H	-3.85281	2.303775	-2.65713	C	13.21491	-3.75434	0.724886
C	-13.8699	3.641823	1.001475	H	13.67367	-4.23638	1.584873
C	-7.839	3.352574	-0.50834	C	6.761996	5.166409	-0.63523
H	-7.36654	4.315292	-0.63507	H	7.429364	4.76633	-1.39142
C	-4.79945	3.851085	0.20897	C	12.21823	-2.79933	0.926671
H	-5.50161	3.754173	1.030646	H	11.90874	-2.54952	1.937674
C	-13.93	-2.07928	1.462452	C	5.453435	4.878217	1.365393
H	-14.1829	-2.64165	2.358134	H	5.132975	4.265569	2.202013
C	-4.81458	2.900235	-0.82504	C	5.398184	7.00768	0.187533
C	-2.94685	4.076511	-1.84851	C	4.987033	6.183685	1.244481
H	-2.22788	4.158178	-2.66022	H	4.295908	6.573503	1.987943
C	-12.2344	1.964346	1.663575	C	6.289429	6.470836	-0.75086
H	-11.796	1.343441	2.438861	H	6.610256	7.080331	-1.59213
C	-13.3729	3.557445	-0.30414	O	-2.9551	0.414633	-0.58565
H	-13.8136	4.172652	-1.08496	O	2.964536	-0.10762	0.848036
C	-3.87454	4.893401	0.209434	C	14.69508	-5.1542	-0.7857
H	-3.87717	5.607872	1.028927	H	15.31967	-5.28625	0.102507
C	-14.9176	-1.83336	0.501828	H	14.24571	-6.12822	-1.01691
C	-14.5529	-1.10326	-0.6375	H	15.34956	-4.89462	-1.62378
H	-15.2979	-0.89926	-1.40293	C	16.33619	1.726321	-1.45777
C	-6.54988	-5.19308	-0.09534	H	16.49785	1.760589	-2.53897
H	-7.27481	-4.94791	0.673748	H	16.56366	2.723633	-1.06082
C	-12.6249	-1.61807	1.289793	H	17.06846	1.035011	-1.02831
H	-11.8747	-1.82941	2.046422	C	4.915102	8.433647	0.077866
C	-12.3238	2.694845	-0.62295	H	5.561219	9.114689	0.646147
H	-11.9567	2.648026	-1.64438	H	4.91511	8.777977	-0.96048
C	-2.93685	5.031261	-0.82084	H	3.900991	8.545798	0.473289
C	-6.01528	-6.47669	-0.15835	C	1.69912	-5.6809	2.081094

H	-6.34412	-7.22648	0.557148	H	1.455677	-6.21527	1.158273
C	-5.15983	-4.53153	-1.94736	H	2.062727	-6.42392	2.802119
H	-4.83118	-3.77977	-2.65778	H	0.771946	-5.26504	2.487517
C	-13.281	2.827806	1.978332	C	-4.49903	-8.21914	-1.20257
H	-13.6468	2.870651	3.00152	H	-4.47163	-8.69984	-0.22001
C	-4.63141	-5.81777	-2.00568	H	-5.11876	-8.84846	-1.85383
H	-3.8839	-6.0537	-2.75923	H	-3.48533	-8.22692	-1.61398
C	-5.0507	-6.81664	-1.11649	C	-1.9587	6.181091	-0.8397
N	6.412305	0.7155	1.275807	H	-1.83266	6.615676	0.156018
N	8.656083	1.35891	0.132057	H	-0.97432	5.865065	-1.19951
N	8.091199	-1.10365	0.613475	H	-2.30245	6.98274	-1.50545
H	8.023183	-0.05164	0.483609	C	-14.9867	4.595512	1.354647
C	7.695859	-3.26468	1.076151	H	-14.5966	5.514734	1.809518
H	7.187155	-4.16933	1.374461	H	-15.5589	4.887287	0.469318
C	9.018044	-3.14083	0.71871	H	-15.6811	4.1503	2.074315
H	9.751813	-3.92994	0.666329	C	-16.3229	-2.36068	0.670055
C	4.152406	0.524897	0.948272	H	-16.4665	-3.29544	0.11355
C	7.093771	-1.96052	1.006493	H	-16.5494	-2.56836	1.719842
C	3.804995	-2.52451	2.505004	H	-17.0657	-1.6477	0.298439
H	3.873298	-1.68426	3.188472	C	1.850977	0.687858	0.436631
C	9.269035	-1.74878	0.435473	C	0.640582	-0.22719	0.324062
C	5.926843	1.909941	0.906855	H	2.077484	1.165251	-0.52726
C	11.61324	-2.14951	-0.15717	H	1.679444	1.486197	1.173203
C	4.710481	-2.6095	1.433308	C	-0.62845	0.539071	-0.06673
C	12.03214	-2.496	-1.44879	H	0.86145	-1.00593	-0.41594
H	11.57646	-2.00728	-2.30453	H	0.498251	-0.73814	1.283745
C	13.63615	-4.10009	-0.56435	C	-1.82135	-0.38762	-0.24864
C	12.26007	0.57092	-0.47147	H	-0.87677	1.283676	0.698805
C	13.89227	1.419921	-2.06399	H	-0.47065	1.090393	-1.00168
H	14.1155	1.789303	-3.06204	H	-1.63553	-1.11526	-1.05157
C	10.51486	-1.13724	0.053996	H	-2.03301	-0.95168	0.671004

Table S3. S_0 optimized geometry of the compound **5** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -4109.234714

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
N	9.911595	1.360146	-0.24321	C	-13.6526	-1.38414	-1.88589
N	7.630481	0.652095	-1.2678	H	-12.8121	-1.53856	-2.55652
N	9.327066	-1.1273	-0.54849	C	-5.96014	3.822343	0.456935
H	9.26423	-0.06938	-0.48325	H	-6.57669	3.805531	-0.43599
C	10.5956	3.532128	-0.53602	C	-7.09324	1.712117	1.252092
H	10.55278	4.591999	-0.74404	C	-11.1865	-1.46274	0.040143
C	11.25139	1.392851	-0.17029	C	-11.6186	-2.85198	0.205643
C	5.713015	1.816011	-0.74713	H	-12.6311	-3.21818	0.118803
H	5.071292	2.639917	-0.47455	C	-5.0207	4.836833	0.629523

C	9.454986	2.623447	-0.48941	H	-4.92738	5.610766	-0.12836
C	7.157135	1.868702	-0.95998	C	-12.0464	-0.34043	-0.24777
C	13.53744	0.598869	0.258965	C	-4.32108	3.843476	2.699867
C	11.76741	-1.13302	-0.06634	H	-3.6864	3.844269	3.582774
C	10.50855	-1.76399	-0.36409	C	-10.5032	-3.57106	0.518291
C	6.632224	-0.24305	-1.15872	H	-10.448	-4.62449	0.754192
C	11.71158	2.771315	-0.34996	C	-9.39258	-2.62601	0.561355
H	12.73939	3.103373	-0.35655	C	-14.2138	3.121335	-2.2329
C	10.24613	-3.17061	-0.54786	H	-14.4568	3.26836	-3.28269
H	10.97907	-3.95788	-0.46557	C	-16.0261	-1.63953	-1.41396
C	8.31662	-2.00389	-0.85597	C	-7.51627	-4.25896	0.938665
C	5.380021	0.488913	-0.86809	C	-14.5361	-0.59454	0.203891
C	12.868	-2.13284	0.188089	H	-14.3924	-0.12921	1.173835
C	7.609336	4.324418	-0.65811	C	-8.04272	-2.87827	0.920071
C	8.086664	2.927184	-0.71753	C	-15.8048	-1.03035	-0.17144
C	6.961991	-1.62109	-1.07952	H	-16.6381	-0.89832	0.514709
C	12.09665	0.237288	0.006613	C	-4.18938	4.872053	1.755599
C	14.52637	0.404131	-0.71526	C	-14.5672	3.632012	0.083344
H	14.25641	-0.04633	-1.66507	H	-15.0915	4.178367	0.863627
C	4.993705	-2.64826	-2.23551	C	-7.83981	-5.18848	-0.06699
H	5.047189	-1.84971	-2.96849	H	-8.47493	-4.87764	-0.88986
C	14.89304	-4.0597	0.688574	C	-13.5663	2.725678	0.436506
C	8.914043	-3.31202	-0.85878	H	-13.3194	2.57775	1.484093
H	8.395316	-4.23223	-1.08297	C	-6.65105	-4.68201	1.965396
C	5.827488	-3.71517	-0.24511	H	-6.39312	-3.98679	2.757873
H	6.51023	-3.73678	0.598169	C	-6.47663	-6.90552	0.991316
C	15.24112	1.563496	1.704102	C	-6.14558	-5.9782	1.989022
H	15.50881	2.013513	2.657136	H	-5.48641	-6.27907	2.799771
C	5.922379	-2.67154	-1.18053	C	-7.32815	-6.48298	-0.03805
C	4.025047	-3.63803	-2.35756	H	-7.58549	-7.17568	-0.83562
H	3.326382	-3.60078	-3.18997	O	4.194623	-0.13306	-0.70406
C	13.32506	-2.37842	1.490201	O	-4.25943	0.304046	1.123801
H	12.89782	-1.82024	2.317717	C	-15.9779	4.841784	-1.64405
C	14.43349	-3.81534	-0.61049	H	-16.5563	5.166678	-0.77466
H	14.86256	-4.36839	-1.4426	H	-15.5422	5.73742	-2.10364
C	4.848478	-4.69921	-0.36798	H	-16.6759	4.41534	-2.37244
H	4.789839	-5.48818	0.377739	C	-17.4105	-2.07682	-1.83004
C	16.2302	1.365965	0.733836	H	-17.371	-2.86016	-2.59266
C	15.84642	0.781122	-0.48051	H	-17.9822	-2.461	-0.97939
H	16.59247	0.618252	-1.25476	H	-17.9817	-1.23989	-2.25128
C	8.05584	5.217339	0.333564	C	-5.95104	-8.31987	1.038266
H	8.751387	4.865584	1.088376	H	-6.6113	-8.96763	1.62881
C	13.91638	1.19521	1.46916	H	-5.88124	-8.75494	0.036935
H	13.16588	1.365169	2.235901	H	-4.95938	-8.36417	1.498675
C	13.43591	-2.87177	-0.85783	C	-3.19789	5.991972	1.960865
H	13.09655	-2.70139	-1.87569	H	-2.92221	6.462246	1.012544
C	3.93456	-4.68485	-1.42849	H	-3.61435	6.776578	2.605197
C	7.591085	6.528895	0.379576	H	-2.28207	5.633801	2.441409

H	7.945595	7.19197	1.164937	C	6.189204	8.438127	-0.52528
C	6.670304	4.802466	-1.59164	H	6.232599	8.852119	0.486378
H	6.31662	4.137002	-2.37266	H	6.812006	9.076433	-1.16479
C	14.32004	-3.32224	1.733421	H	5.159678	8.527227	-0.88514
H	14.65736	-3.4897	2.753616	C	2.898466	-5.77208	-1.58305
C	6.211914	6.115283	-1.54061	H	2.690104	-6.26596	-0.62957
H	5.493633	6.45813	-2.28148	H	1.955984	-5.37531	-1.97337
C	6.665273	7.005969	-0.5576	H	3.237547	-6.54531	-2.28395
N	-7.70538	-0.57647	1.453136	C	15.95396	-5.09937	0.962335
N	-9.86266	-1.38343	0.243706	H	15.51178	-6.03096	1.33723
N	-9.3868	1.127516	0.533476	H	16.51564	-5.34584	0.05677
H	-9.28644	0.070622	0.501226	H	16.66667	-4.75494	1.718642
C	-9.07236	3.331184	0.824782	C	17.65885	1.793771	0.973354
H	-8.60524	4.273337	1.070438	H	17.85946	2.778228	0.531986
C	-10.3671	3.137861	0.403411	H	17.88142	1.864808	2.041979
H	-11.1148	3.897891	0.238495	H	18.3681	1.090157	0.526124
C	-5.43605	-0.34907	1.221665	C	-3.11773	-0.49347	0.798451
C	-8.43552	2.044277	0.905679	C	-1.91019	0.425031	0.687387
C	-5.25042	2.823684	2.529248	H	-3.30221	-1.02218	-0.14771
H	-5.33724	2.039787	3.274719	H	-2.96788	-1.25237	1.580202
C	-10.567	1.719869	0.230636	C	-0.63202	-0.34014	0.324185
C	-7.17166	-1.78343	1.213921	H	-2.1207	1.190374	-0.06927
C	-12.8769	1.997751	-0.54136	H	-1.77927	0.953384	1.639522
C	-6.09678	2.796709	1.407232	C	0.600719	0.563881	0.198926
C	-13.2156	2.215153	-1.88437	H	-0.43701	-1.11253	1.081189
H	-12.6919	1.665127	-2.66028	H	-0.78242	-0.87497	-0.62398
C	-14.9088	3.847788	-1.25603	H	0.403299	1.34205	-0.55146
C	-13.4371	-0.75759	-0.65087	H	0.761832	1.090687	1.149744
C	-14.926	-1.81091	-2.26199	C	1.867339	-0.21059	-0.18412
H	-15.0649	-2.28973	-3.22835	C	3.088561	0.686788	-0.31688
C	-11.7717	1.040901	-0.169	H	1.715322	-0.73358	-1.13608
C	-5.71834	-1.68876	1.111173	H	2.079554	-0.9826	0.565281
H	-5.03335	-2.49802	0.909509	H	2.928528	1.465655	-1.07666
C	-6.72908	0.348174	1.397126	H	3.32135	1.189758	0.632661

Table S4. S_0 optimized geometry of the compound **4.4H**$^+$ at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -4031.929924

Atom	X	Y	Z	Atom	X	Y	Z
N	-8.56845	-1.54279	-0.1891	C	5.30431	-0.12402	1.453405
N	-6.28036	-0.65124	-1.53253	C	12.45559	1.464856	-1.17193
N	-8.05055	1.199429	-0.70771	H	11.64607	1.973687	-1.68456
H	-7.92187	0.202492	-0.64102	C	4.423745	-3.67777	1.132661
C	-9.1836	-3.05549	-1.72405	H	5.057187	-3.87119	0.273733
H	-9.1376	-3.83005	-2.47626	C	5.614531	-1.49163	1.544011
C	-9.9137	-1.29993	-0.46176	C	9.95378	1.221253	0.304083
C	-4.40405	-1.70431	-0.87761	C	10.37089	2.267888	1.132453
H	-3.75264	-2.46367	-0.47542	H	11.33747	2.329081	1.610717
C	-8.11063	-2.61998	-0.95633	C	3.451809	-4.60299	1.488741
C	-5.783	-1.8923	-1.17281	H	3.355607	-5.52078	0.915817
C	-12.1405	-0.63856	0.242306	C	10.74896	0.034556	-0.02788
C	-10.4223	1.180624	0.120483	C	2.720351	-3.16465	3.277589
C	-9.19463	1.842197	-0.30356	H	2.074138	-2.96949	4.128665
C	-5.31947	0.349423	-1.42807	C	9.286885	3.150708	1.324495
C	-10.2977	-2.24506	-1.41811	H	9.268187	4.017512	1.969609
H	-11.2647	-2.2798	-1.89829	C	8.199456	2.658374	0.613726
C	-8.90483	3.227669	-0.38879	C	12.72673	-3.21041	-2.24153
H	-9.57246	4.031999	-0.12848	H	13.06728	-3.14327	-3.27016
C	-7.04475	2.090914	-1.0273	C	14.84365	1.186723	-0.78245
C	-4.10222	-0.3533	-1.05376	C	6.43583	4.465613	0.458889
C	-11.4414	2.081125	0.713299	C	13.24492	-0.24359	0.367988
C	-6.28271	-4.36777	-1.03219	H	13.04987	-1.01783	1.099273
C	-6.68273	-2.98135	-1.03146	C	6.785415	3.076865	0.637729
C	-5.67813	1.704146	-1.32956	C	14.54806	0.154401	0.131174
C	-10.7503	-0.19683	0.023229	H	15.35967	-0.32748	0.667486
C	-13.2608	0.034237	-0.31829	C	2.594853	-4.37754	2.579733
H	-13.105	0.904629	-0.94315	C	12.71562	-4.3252	-0.09895
C	-3.77673	2.69702	-2.58881	H	13.08345	-5.10914	0.556669
H	-3.85575	1.879069	-3.29792	C	7.295897	5.342221	-0.25617
C	-13.3415	3.809429	1.931146	H	8.20648	4.952525	-0.69792
C	-7.60855	3.377152	-0.87444	C	11.81014	-3.39914	0.390468
H	-7.11359	4.31073	-1.09062	H	11.49656	-3.45613	1.427606
C	-4.54649	3.835942	-0.59656	C	5.247419	5.016553	1.007262
H	-5.17636	3.876643	0.28561	H	4.599271	4.395419	1.615756
C	-13.6783	-2.27134	1.201568	C	5.793563	7.219565	0.121722
H	-13.8447	-3.15544	1.809488	C	4.942392	6.356263	0.839485
C	-4.65959	2.750262	-1.49039	H	4.041342	6.759088	1.292354
C	-2.85175	3.709257	-2.80457	C	6.974262	6.676461	-0.42447
H	-2.20965	3.665924	-3.67969	H	7.642908	7.319708	-0.98882
C	-11.9385	1.823514	2.014508	O	-2.95962	0.290914	-0.82206
H	-11.5715	0.96396	2.565011	O	2.948838	-0.06154	0.831958
C	-12.8689	4.049277	0.620794	C	14.13132	-5.30344	-1.95614
H	-13.2603	4.894944	0.062841	H	14.92816	-5.51441	-1.23615
C	-3.60206	4.831224	-0.80938	H	13.60261	-6.2501	-2.12702
H	-3.52499	5.651001	-0.10098	H	14.58479	-5.00134	-2.90212
C	-14.7897	-1.59528	0.648382	C	16.25584	1.623344	-1.03104

C	-14.5447	-0.44187	-0.12521	H	16.41144	1.900546	-2.0775
H	-15.3806	0.073865	-0.58772	H	16.48689	2.512979	-0.42941
C	-7.11349	-5.3615	-0.44793	H	16.97585	0.8491	-0.75787
H	-8.04044	-5.06659	0.03151	C	5.478524	8.68025	-0.02847
C	-12.3883	-1.82789	0.97913	H	6.085263	9.274625	0.666593
H	-11.5539	-2.36679	1.41552	H	5.711687	9.036666	-1.03623
C	-11.9281	3.222085	0.031009	H	4.42915	8.894529	0.185109
H	-11.6089	3.41736	-0.98745	C	1.596545	-5.41987	3.00728
C	-2.75047	4.801589	-1.92695	H	1.240809	-6.00954	2.157997
C	-6.74307	-6.69401	-0.45302	H	2.055801	-6.12041	3.715648
H	-7.39046	-7.43004	0.014208	H	0.735121	-4.97258	3.510331
C	-5.0702	-4.7983	-1.63444	C	-5.1707	-8.57188	-1.0975
H	-4.44133	-4.07885	-2.14726	H	-5.49673	-9.09683	-0.19551
C	-12.8512	2.680481	2.610732	H	-5.66216	-9.0619	-1.94812
H	-13.1944	2.476161	3.620233	H	-4.09419	-8.7142	-1.21789
C	-4.71581	-6.13585	-1.63991	C	-1.78378	5.924555	-2.19331
H	-3.79657	-6.44293	-2.12996	H	-1.44517	6.393558	-1.26559
C	-5.53963	-7.11688	-1.05213	H	-0.90982	5.581142	-2.75325
N	6.300738	0.845856	1.430211	H	-2.26389	6.707156	-2.79368
N	8.61834	1.475258	-0.00558	C	-14.3293	4.741676	2.569576
N	8.0004	-1.15838	0.86029	H	-13.8401	5.683963	2.848015
H	7.902933	-0.17871	0.646267	H	-15.1366	5.000088	1.876972
C	7.492658	-3.27192	1.349155	H	-14.7675	4.315071	3.473866
H	6.970407	-4.14671	1.702845	C	-16.1818	-2.11476	0.846046
C	8.792723	-3.23606	0.851629	H	-16.4177	-2.8612	0.075156
H	9.434814	-4.09054	0.718031	H	-16.2937	-2.60996	1.814108
C	4.11265	0.567964	0.988501	H	-16.9273	-1.32042	0.764329
C	6.967923	-1.96136	1.305659	C	1.841343	0.678599	0.269564
C	3.674548	-2.22346	2.916782	C	0.627683	-0.2449	0.256075
H	3.773591	-1.30843	3.491961	H	2.106992	1.005932	-0.7434
C	9.124498	-1.88834	0.561994	H	1.659663	1.566182	0.888425
C	5.84735	2.048928	0.916753	C	-0.63072	0.466514	-0.27252
C	11.3559	-2.33399	-0.42416	H	0.862298	-1.11926	-0.36219
C	4.562449	-2.46981	1.848866	H	0.459872	-0.61081	1.275463
C	11.85016	-2.25524	-1.74964	C	-1.83301	-0.46995	-0.32863
H	11.50811	-1.45679	-2.3992	H	-0.883	1.320667	0.366372
C	13.18366	-4.26468	-1.43135	H	-0.45358	0.86224	-1.27928
C	12.15619	0.391522	-0.29008	H	-1.64785	-1.31094	-1.00817
C	13.76349	1.82672	-1.43314	H	-2.08035	-0.86849	0.663313
H	13.96927	2.617498	-2.14822	H	8.173338	1.131764	-0.84872
C	10.37218	-1.33152	0.053179	H	7.070279	0.825349	2.087089
C	4.46104	1.875122	0.646807	H	-7.04834	-0.57696	-2.18757
H	3.834885	2.601832	0.154197	H	-8.13118	-1.29343	0.690354

Table S5. S_0 optimized geometry of the compound **4-Re** at B3LYP/6-31g (d,p) and LANL2DZ level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -4867.815065

Atom	X	Y	Z	Atom	X	Y	Z
N	-8.70635	-1.40527	-0.02794	C	9.792483	1.480916	-0.51687
N	-6.41528	-0.72175	-1.18696	C	9.943631	2.810345	-1.08619
N	-8.0698	1.209226	-0.46626	H	10.75697	3.129794	-1.71991
C	-8.89231	-3.33802	1.185923	C	3.244022	-4.27087	-0.78993
H	-8.67858	-4.32306	1.572555	H	2.952334	-4.68341	-1.75286
C	-9.77284	-1.28136	0.790145	C	10.6702	0.363455	-0.7642
C	-4.48897	-1.8353	-0.66797	C	2.981828	-4.13867	1.593487
H	-3.83682	-2.63397	-0.35205	H	2.49142	-4.45579	2.510737
C	-8.07973	-2.60806	0.233206	C	8.846461	3.536887	-0.71855
C	-5.92657	-1.9195	-0.77879	H	8.614943	4.554883	-0.99361
C	-11.949	-0.41007	1.533701	C	8.002711	2.660542	0.068692
C	-10.2585	1.244136	0.732335	C	12.77436	-3.15238	-2.81252
C	-9.01593	1.82162	0.279777	H	13.00761	-3.32319	-3.86084
C	-5.41611	0.202229	-1.16553	C	14.66612	1.63198	-1.90333
C	-9.92827	-2.51916	1.536741	C	6.002996	4.18597	0.243354
H	-10.6996	-2.7151	2.266267	C	13.07036	0.885629	-0.21999
C	-8.54552	3.152263	0.618322	H	12.85009	0.632776	0.812846
H	-9.08712	3.872595	1.213018	C	6.657031	2.864535	0.449888
C	-6.9615	2.025419	-0.53943	C	14.35195	1.298563	-0.57843
C	-4.16621	-0.51834	-0.91387	H	15.12169	1.365066	0.186976
C	-11.2863	2.290902	1.085252	C	2.592977	-4.70565	0.371587
C	-6.15574	-4.23363	0.11212	C	13.1383	-3.62298	-0.48747
C	-6.77403	-2.91838	-0.21091	H	13.66096	-4.16212	0.299061
C	-5.68779	1.58441	-0.98279	C	5.938451	4.811055	-1.01216
C	-10.5881	-0.1035	0.957534	H	6.365997	4.315869	-1.87841
C	-13.0173	-0.6933	0.67152	C	12.15312	-2.69914	-0.14206
H	-12.8622	-0.65039	-0.40251	H	11.91969	-2.52083	0.903505
C	-3.96214	2.789968	-2.32455	C	5.391067	4.826129	1.334174
H	-4.32561	2.255167	-3.19711	H	5.427422	4.356704	2.312785
C	-13.1702	4.327648	1.668219	C	4.710605	6.693385	-0.07293
C	-7.28424	3.280494	0.10442	C	4.763216	6.059678	1.17612
H	-6.62184	4.127743	0.199077	H	4.307733	6.53921	2.039117
C	-4.0802	3.260171	0.035564	C	5.302014	6.041935	-1.16339
H	-4.51222	3.074251	1.01421	H	5.256514	6.5	-2.14845
C	-13.4336	-0.79696	3.41831	O	-2.97727	0.106697	-0.85809
H	-13.5851	-0.83254	4.494638	O	2.962204	-0.35562	0.488237
C	-4.56629	2.561552	-1.07896	C	14.50474	-4.90126	-2.19731
C	-2.91918	3.704024	-2.45099	H	15.32125	-4.92404	-1.46886

H	-2.47426	3.872269	-3.4288	H	14.07273	-5.90956	-2.22987
C	-11.426	2.78779	2.386722	H	14.9355	-4.69961	-3.18255
H	-10.8048	2.388345	3.183238	C	16.05328	2.100413	-2.27579
C	-13.0288	3.823372	0.368377	H	16.19219	2.11801	-3.3605
H	-13.6546	4.216572	-0.4294	H	16.24512	3.113593	-1.90164
C	-3.02875	4.166261	-0.097	H	16.82337	1.449749	-1.84778
H	-2.66222	4.689652	0.782965	C	4.055695	8.044592	-0.23279
C	-14.5061	-1.07531	2.562065	H	4.764263	8.854087	-0.01698
C	-14.2749	-1.01282	1.181544	H	3.690955	8.195665	-1.25309
H	-15.0906	-1.21958	0.492646	H	3.210749	8.16439	0.452217
C	-6.02723	-4.70832	1.427418	C	1.524277	-5.77149	0.314654
H	-6.37388	-4.09522	2.253407	H	1.055487	-5.8174	-0.6728
C	-12.1747	-0.46824	2.914603	H	1.944278	-6.76369	0.522458
H	-11.3598	-0.25431	3.600656	H	0.738948	-5.59309	1.056052
C	-12.0977	2.828212	0.075844	C	-4.32793	-8.0945	0.924999
H	-12.0073	2.450635	-0.93842	H	-3.86367	-8.12783	1.915192
C	-2.43418	4.410701	-1.34178	H	-5.08832	-8.88503	0.895816
C	-5.42883	-5.94049	1.684838	H	-3.56624	-8.3512	0.182631
H	-5.33193	-6.28055	2.713057	C	-1.32356	5.423584	-1.49006
C	-5.64518	-5.0251	-0.93031	H	-0.75293	5.532574	-0.5628
H	-5.73127	-4.67338	-1.95414	H	-0.628	5.142187	-2.28668
C	-12.3524	3.791768	2.670528	H	-1.72289	6.413559	-1.7443
H	-12.4431	4.161334	3.68922	C	-14.1572	5.430628	1.970382
C	-5.05458	-6.2588	-0.66516	H	-13.7549	6.412296	1.690042
H	-4.67795	-6.85691	-1.49132	H	-15.0908	5.295259	1.414939
C	-4.94003	-6.74276	0.645038	H	-14.4006	5.469578	3.036166
N	6.335293	0.553351	1.125956	C	-15.8628	-1.45564	3.106793
N	8.664632	1.458329	0.224818	H	-15.9891	-2.5454	3.134074
N	8.120995	-1.21232	0.307486	H	-16.0033	-1.08564	4.126745
C	7.465185	-3.21276	-0.58796	H	-16.67	-1.05328	2.486698
H	6.84645	-4.05988	-0.843	C	1.828017	0.43275	0.11613
C	8.750503	-2.97239	-0.98988	C	0.630256	-0.5007	0.018079
H	9.360809	-3.58361	-1.63795	H	2.027636	0.931108	-0.84318
C	4.118578	0.301438	0.683857	H	1.659355	1.212146	0.87246
C	7.046825	-2.0683	0.192785	C	-0.6422	0.241975	-0.40633
C	3.98635	-3.17646	1.655144	H	0.867605	-1.29927	-0.69487
H	4.275334	-2.75214	2.612211	H	0.486381	-0.98269	0.992623
C	9.139937	-1.68562	-0.44324	C	-1.85443	-0.6771	-0.44446
C	5.819936	1.772816	0.830937	H	-0.8558	1.066693	0.284304
C	11.47354	-1.97506	-1.13205	H	-0.51249	0.69009	-1.39863
C	4.64826	-2.75753	0.490873	H	-1.70505	-1.5051	-1.1519
C	11.797	-2.21703	-2.47304	H	-2.05512	-1.11085	0.545338
H	11.27899	-1.67211	-3.25658	Re	-8.40058	-0.37017	-1.90648
C	13.46326	-3.87139	-1.82752	Re	8.281407	0.191136	1.942466
C	12.05816	0.781833	-1.18519	C	-10.2507	0.018913	-2.30093
C	13.65078	1.531124	-2.86118	C	-8.50029	-1.96047	-2.99928
H	13.86669	1.779106	-3.89772	C	-7.85147	0.66333	-3.44246
C	10.38464	-1.01289	-0.72815	C	10.11611	-0.17111	2.425148

C	4.397136	1.649379	0.614564	C	8.226519	1.637279	3.223161
H	3.731152	2.455148	0.349768	C	7.683819	-1.04669	3.298052
C	5.382196	-0.39771	0.927843	O	-11.37	0.260053	-2.52907
C	12.36637	1.111823	-2.5103	O	-8.5273	-2.93884	-3.63014
H	11.59723	1.038923	-3.2745	O	-7.47413	1.294532	-4.34555
C	4.258402	-3.31545	-0.73477	O	11.22603	-0.39755	2.707094
H	4.735918	-2.98189	-1.6511	O	7.281807	-1.80278	4.087515
C	5.727819	-1.73459	0.596237	O	8.158583	2.529423	3.968387

Table S6. S_0 optimized geometry of the compound **4-Re'** at B3LYP/6-31g (d,p) and LANL2DZ level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -4867.803411

Atom	X	Y	Z	Atom	X	Y	Z
N	-8.6498	-1.33038	-0.00046	C	9.570906	1.39564	1.009498
N	-6.53121	-0.3205	-1.24428	C	9.612478	2.76959	1.484096
N	-7.99188	1.30524	0.237443	H	10.23471	3.12855	2.290475
C	-8.71215	-3.52755	0.642198	C	3.048656	-4.27912	-1.68587
H	-8.47299	-4.57854	0.702851	H	2.751798	-4.71736	-2.63572
C	-9.57732	-1.45319	0.971914	C	10.32002	0.305659	1.587471
C	-4.58758	-1.5145	-1.36805	C	2.784798	-4.06789	0.691789
H	-3.92251	-2.36295	-1.39513	H	2.272582	-4.3307	1.614351
C	-8.02864	-2.55058	-0.18216	C	8.664445	3.466419	0.790296
C	-6.02735	-1.57961	-1.27158	H	8.366149	4.49533	0.930339
C	-11.5917	-0.85551	2.244472	C	8.030255	2.529074	-0.11544
C	-9.97719	0.976846	1.713214	C	12.85244	-3.4386	2.37707
C	-8.79519	1.670754	1.261689	H	13.66364	-3.89221	1.81253
C	-5.50977	0.570163	-1.12052	C	14.02136	1.747422	3.342171
C	-9.65765	-2.8516	1.360517	C	6.289905	4.115734	-0.9198
H	-10.3157	-3.25109	2.117621	C	11.72744	0.973663	3.606378
C	-8.23505	2.855624	1.885242	H	10.88718	0.752436	4.257513
H	-8.65733	3.374182	2.732923	C	6.80465	2.722744	-0.79364
C	-6.88034	2.120463	0.228786	C	12.91633	1.455646	4.152635
C	-4.26157	-0.17823	-1.28345	H	12.98765	1.603478	5.227664
C	-10.9068	1.867497	2.500646	C	2.377206	-4.65375	-0.51334
C	-6.19419	-4.05325	-1.04093	C	11.65495	-3.13134	4.433237
C	-6.81288	-2.70791	-0.88593	H	11.52209	-3.34027	5.492228
C	-5.70393	1.839489	-0.51365	C	6.983478	5.02916	-1.73054

C	-10.3192	-0.38024	1.587053	H	7.870168	4.698031	-2.26291
C	-12.763	-0.96517	1.48215	C	10.7773	-2.25604	3.792888
H	-12.7507	-0.6637	0.438846	H	9.971388	-1.79454	4.357261
C	-4.17228	3.399277	-1.71783	C	5.139342	4.561758	-0.25147
H	-4.68365	3.126391	-2.63621	H	4.603138	3.882215	0.403774
C	-12.6187	3.629133	3.915515	C	5.378449	6.786461	-1.21502
C	-7.06092	3.137285	1.242198	C	4.694931	5.874962	-0.3995
H	-6.36464	3.930431	1.46977	H	3.804783	6.199491	0.134235
C	-3.90649	3.183181	0.667146	C	6.528468	6.33785	-1.87817
H	-4.18542	2.722076	1.60975	H	7.07552	7.02135	-2.52285
C	-12.8149	-1.72521	4.155472	O	-3.05743	0.418972	-1.25005
H	-12.8236	-2.01923	5.202459	O	3.00034	-0.36293	-1.2054
C	-4.58058	2.818971	-0.50681	C	13.64066	-4.70852	4.424615
C	-3.1375	4.329985	-1.74583	H	13.69788	-4.51594	5.500172
H	-2.84711	4.774878	-2.69458	H	13.30265	-5.74468	4.296324
C	-10.8002	2.010336	3.890101	H	14.65363	-4.64663	4.015062
H	-10.052	1.438559	4.431969	C	15.30022	2.291424	3.934203
C	-12.7232	3.478782	2.526971	H	16.17212	1.994064	3.343802
H	-13.4758	4.044339	1.982862	H	15.28851	3.388401	3.965724
C	-2.86358	4.108535	0.629748	H	15.44904	1.939156	4.959464
H	-2.3498	4.370126	1.55179	C	4.909716	8.215509	-1.35283
C	-13.99	-1.83019	3.400798	H	5.421117	8.870563	-0.63628
C	-13.9424	-1.43718	2.056869	H	5.114901	8.608503	-2.35321
H	-14.841	-1.50277	1.448073	H	3.835494	8.305387	-1.16634
C	-5.88887	-4.87817	0.053132	C	1.267258	-5.67764	-0.54842
H	-6.09371	-4.52851	1.060148	H	0.665351	-5.58559	-1.45803
C	-11.6341	-1.24468	3.589176	H	1.67016	-6.69812	-0.53065
H	-10.7368	-1.17152	4.197046	H	0.599833	-5.57625	0.312529
C	-11.8779	2.619029	1.825871	C	-4.37333	-7.95833	-1.62905
H	-11.9784	2.517103	0.749299	H	-3.85535	-8.30704	-0.73091
C	-2.46506	4.704025	-0.57357	H	-5.14262	-8.70195	-1.87202
C	-5.29417	-6.12456	-0.13815	H	-3.65634	-7.95513	-2.456
H	-5.05878	-6.74003	0.726706	C	-1.36287	5.736238	-0.60815
C	-5.86422	-4.51134	-2.3279	H	-0.71335	5.659189	0.268851
H	-6.08923	-3.88626	-3.18696	H	-0.74119	5.629486	-1.50292
C	-11.6425	2.878739	4.583829	H	-1.77406	6.753399	-0.62177
H	-11.542	2.970936	5.66283	C	-13.5116	4.589075	4.666171
C	-5.2764	-5.76075	-2.51104	H	-13.0505	5.581851	4.745327
H	-5.04195	-6.09572	-3.51852	H	-14.4738	4.718181	4.161657
C	-4.98436	-6.59313	-1.42149	H	-13.7073	4.240887	5.685063
N	6.474797	0.353043	-1.13195	C	-15.262	-2.37382	4.008029
N	8.664228	1.311007	0.014645	H	-15.3676	-3.44876	3.813875
N	7.945536	-1.31724	0.270717	H	-15.2786	-2.23591	5.093269
C	7.014014	-3.16334	1.248723	H	-16.1463	-1.88241	3.590548
H	6.312034	-3.95264	1.472678	C	1.859303	0.498605	-1.2528
C	8.209645	-2.9177	1.86688	C	0.618085	-0.38168	-1.23722
H	8.646659	-3.47003	2.684875	H	1.899321	1.111078	-2.16446
C	4.208119	0.226538	-1.21346	H	1.878405	1.177682	-0.38839

C	6.822689	-2.11819	0.26797	C	-0.67381	0.444036	-1.2519
C	3.834752	-3.1506	0.730042	H	0.656059	-1.051	-2.10504
H	4.122255	-2.69774	1.674195	H	0.656603	-1.02045	-0.34677
C	8.769665	-1.72235	1.263489	C	-1.91301	-0.43916	-1.26674
C	5.982374	1.617413	-1.16379	H	-0.72319	1.098047	-0.37308
C	10.92576	-1.96199	2.431482	H	-0.70214	1.09798	-2.13174
C	4.506448	-2.78482	-0.44474	H	-1.93954	-1.06816	-2.1676
C	11.9756	-2.5695	1.729304	H	-1.94095	-1.10286	-0.39086
H	12.10785	-2.35172	0.673711	Re	-8.588	0.203008	-1.5273
C	12.70724	-3.73949	3.737665	Re	8.517245	-0.20583	-1.50218
C	11.6036	0.773215	2.225332	C	-10.4643	0.661808	-1.51538
C	13.89372	1.542581	1.962435	C	-8.89057	-1.00319	-3.00544
H	14.73697	1.754515	1.309454	C	-8.2401	1.648007	-2.76036
C	9.971912	-1.0514	1.697432	C	8.093201	-1.62942	-2.74071
C	4.544816	1.561131	-1.30067	C	8.80396	1.0175	-2.96746
H	3.881986	2.407454	-1.3773	C	10.38276	-0.6978	-1.55574
C	5.446885	-0.53109	-1.02891	O	-11.5983	0.938357	-1.497
C	12.70276	1.074583	1.408643	O	-9.03366	-1.75685	-3.88143
H	12.62799	0.919384	0.336301	O	-7.98195	2.523011	-3.48417
C	4.090813	-3.35641	-1.65711	O	7.789491	-2.48674	-3.46775
H	4.601946	-3.08349	-2.57564	O	11.51426	-0.98471	-1.57153
C	5.636177	-1.81225	-0.44835	O	8.947347	1.792429	-3.82521