Electronic Supplementary Material (ESI) for RSC Advances.

Structure and dynamics processes in free-base chlorins controlled by chemical modifications of macroring and aryl groups in meso-positions†

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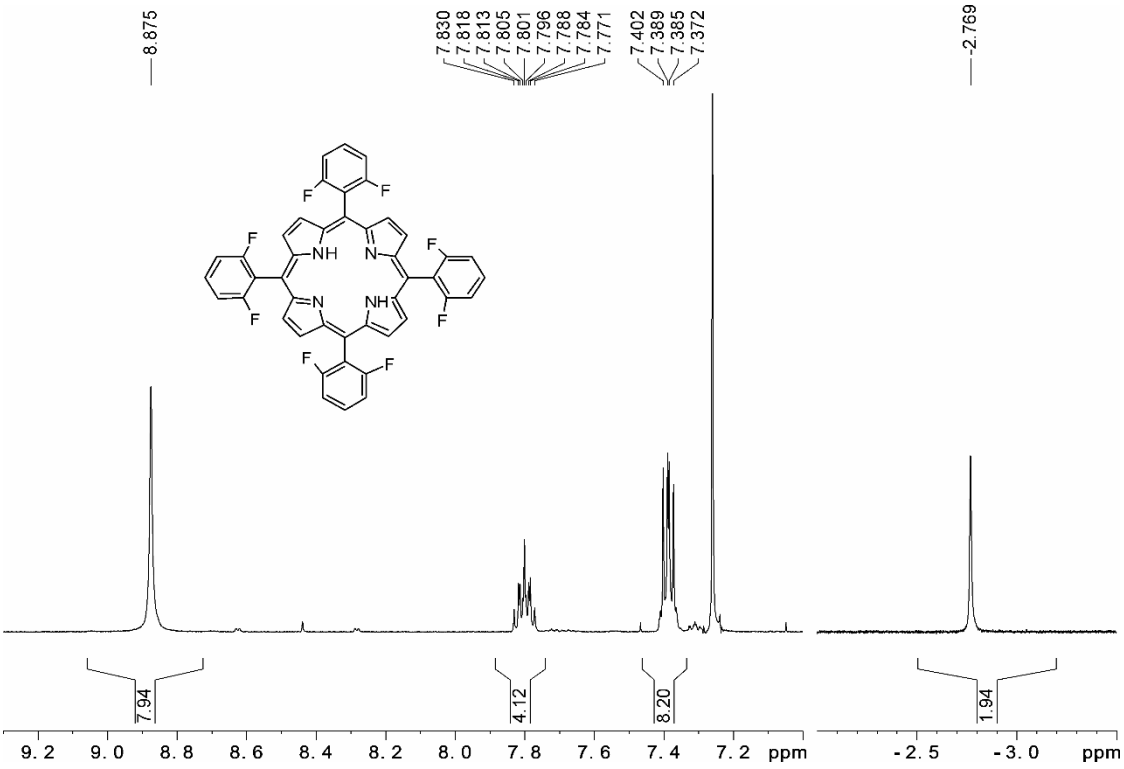


Figure S1 ^{1}H-NMR spectrum in $CDCl_3$ of compound **5** recorded in $CDCl_3$ at 500 MHz.

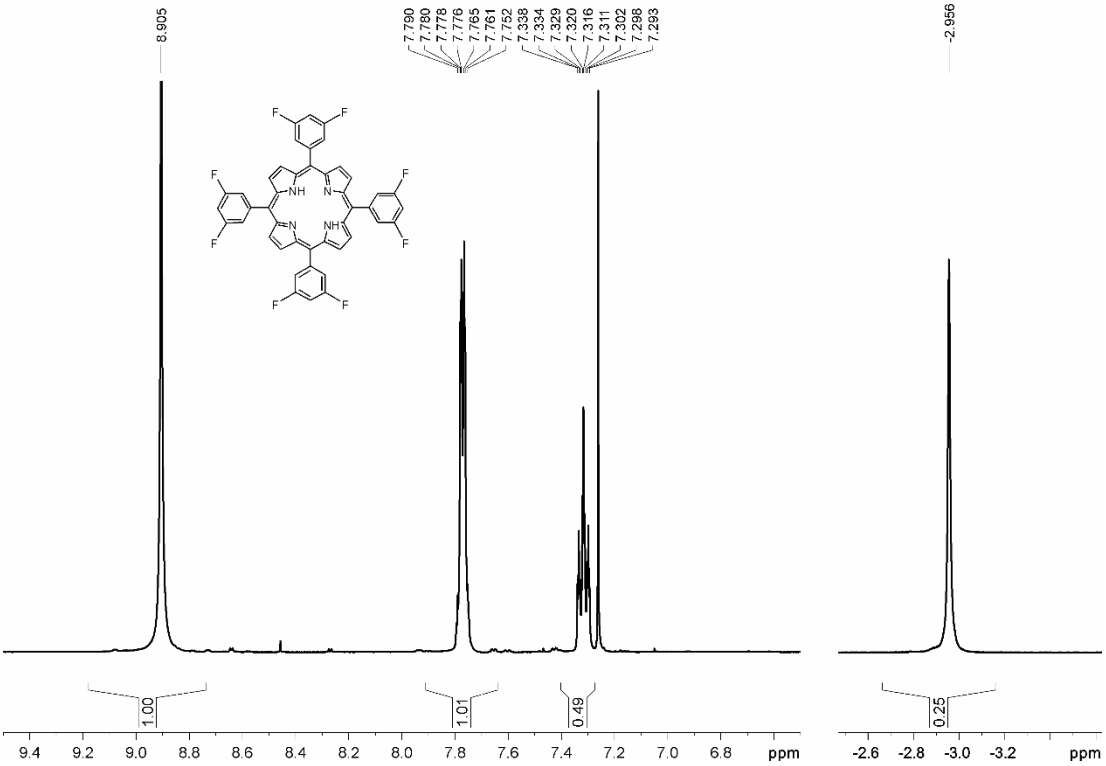


Figure S2 ^{1}H-NMR spectrum in $CDCl_3$ of compound **6** recorded in $CDCl_3$ at 500 MHz

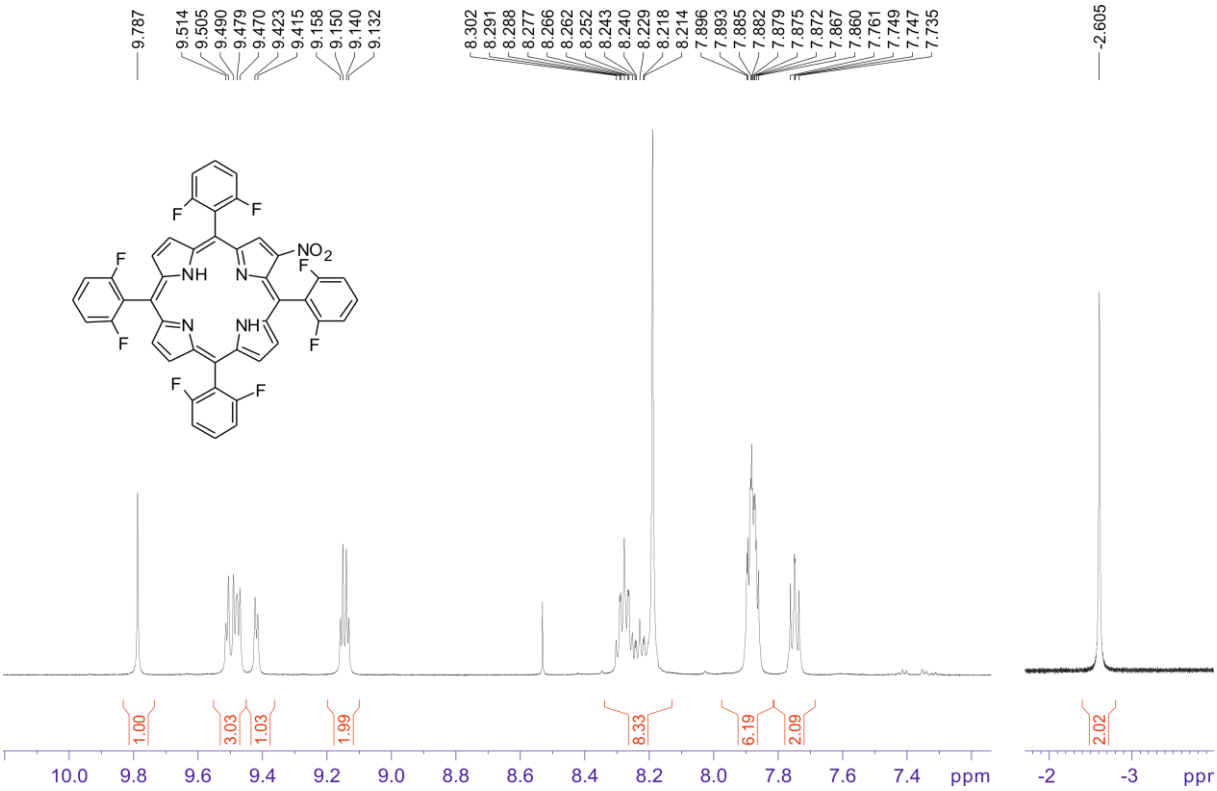


Figure S 3 ^{1}H NMR spectrum in DMF-d_7 of compound **17** recorded in DMF-d_7 at 600MHz

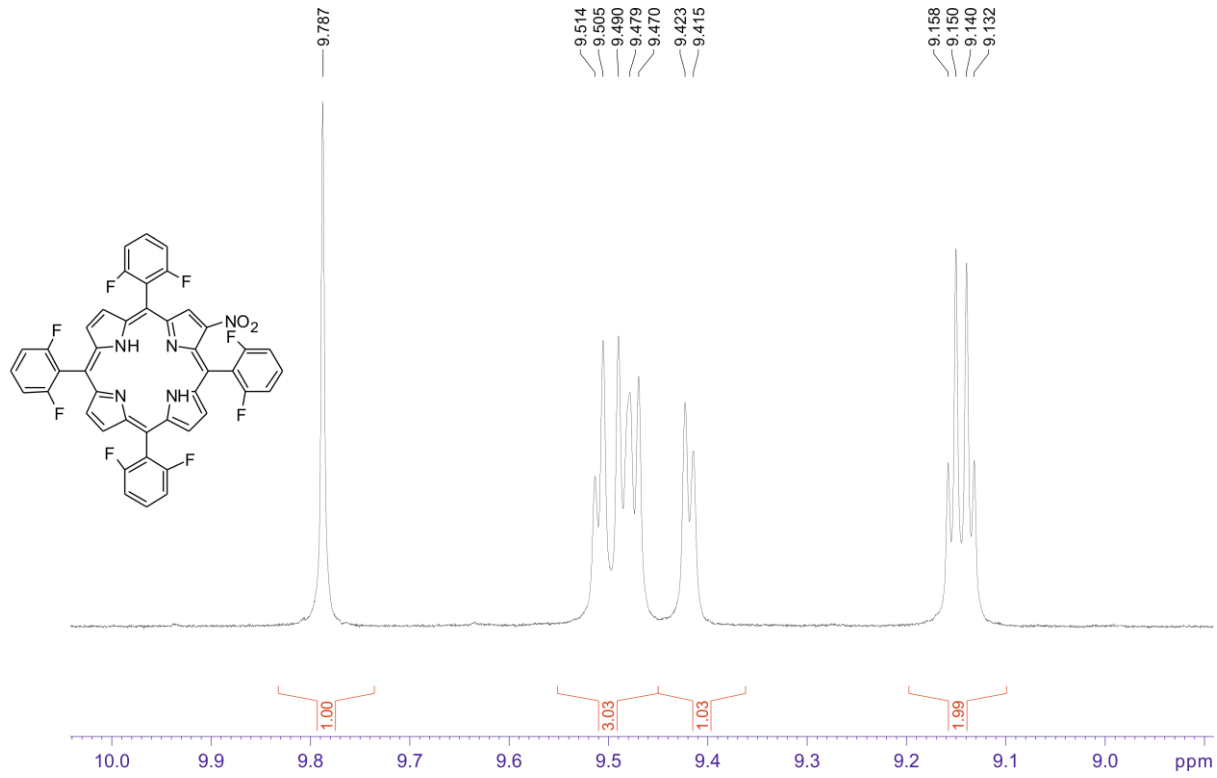


Figure S 4 ^{1}H NMR spectrum in DMF-d_7 of compound **17** (expansion of 9.00-10.00 ppm region) recorded in DMF-d_7 at 600 MHz

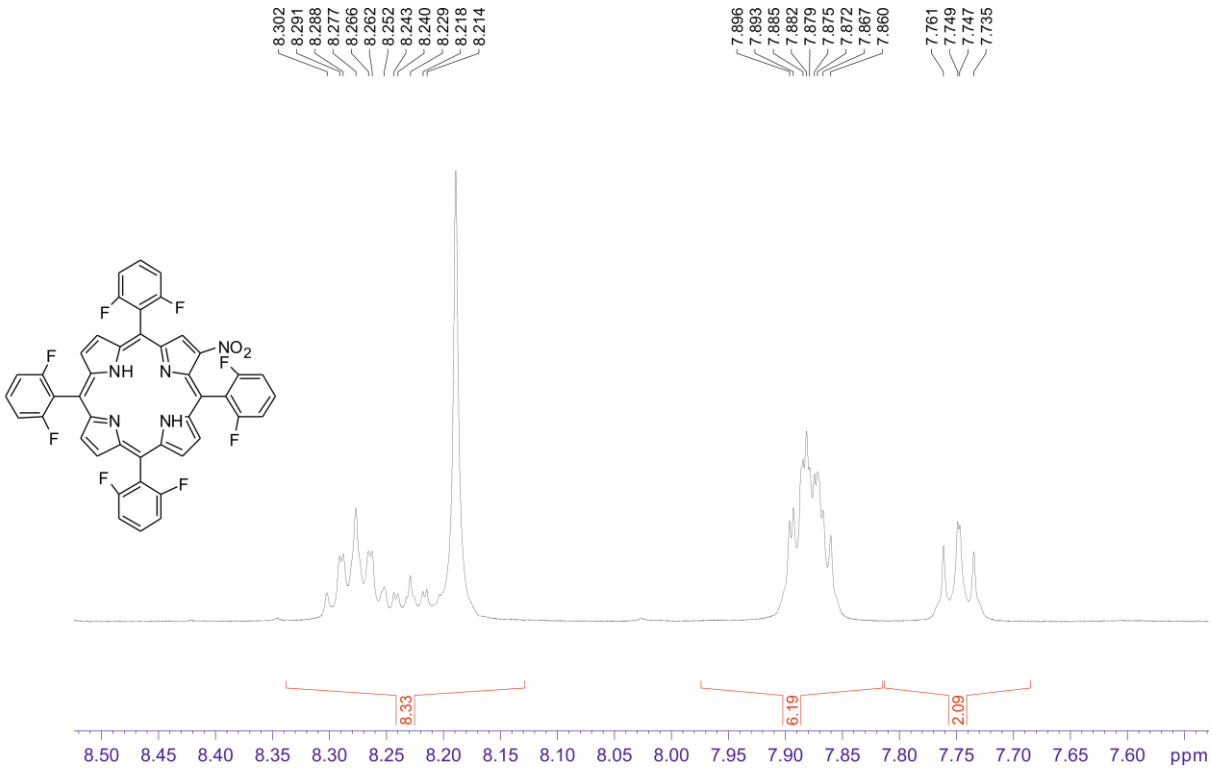


Figure S 5 ^{1}H NMR spectrum in DMF-d_7 of compound **17** (expansion of 7.60-8.50 ppm region) recorded in DMF-d_7 at 600MHz.

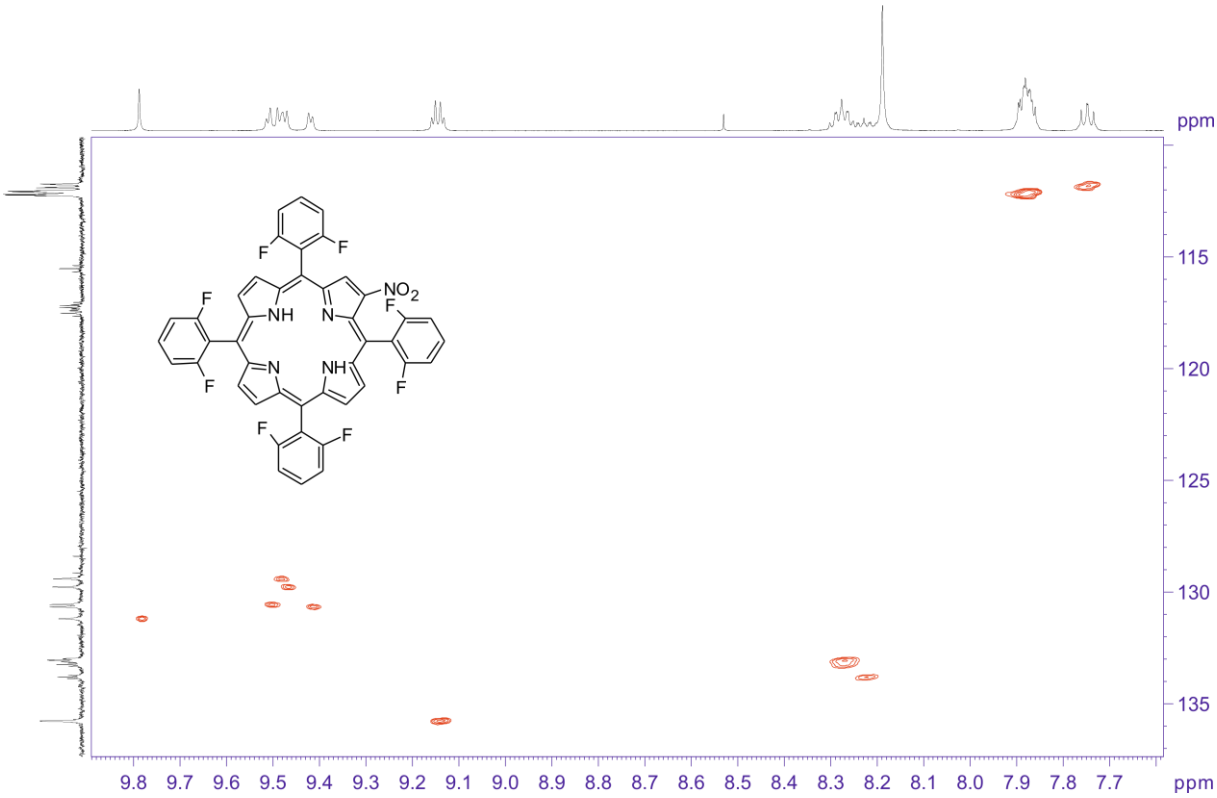


Figure S 6 ^{1}H-^{13}C HSQC NMR spectrum in DMF-d_7 of compound **17** recorded in d_7-DMF. The spectrum obtained at 600 MHz spectrometer.

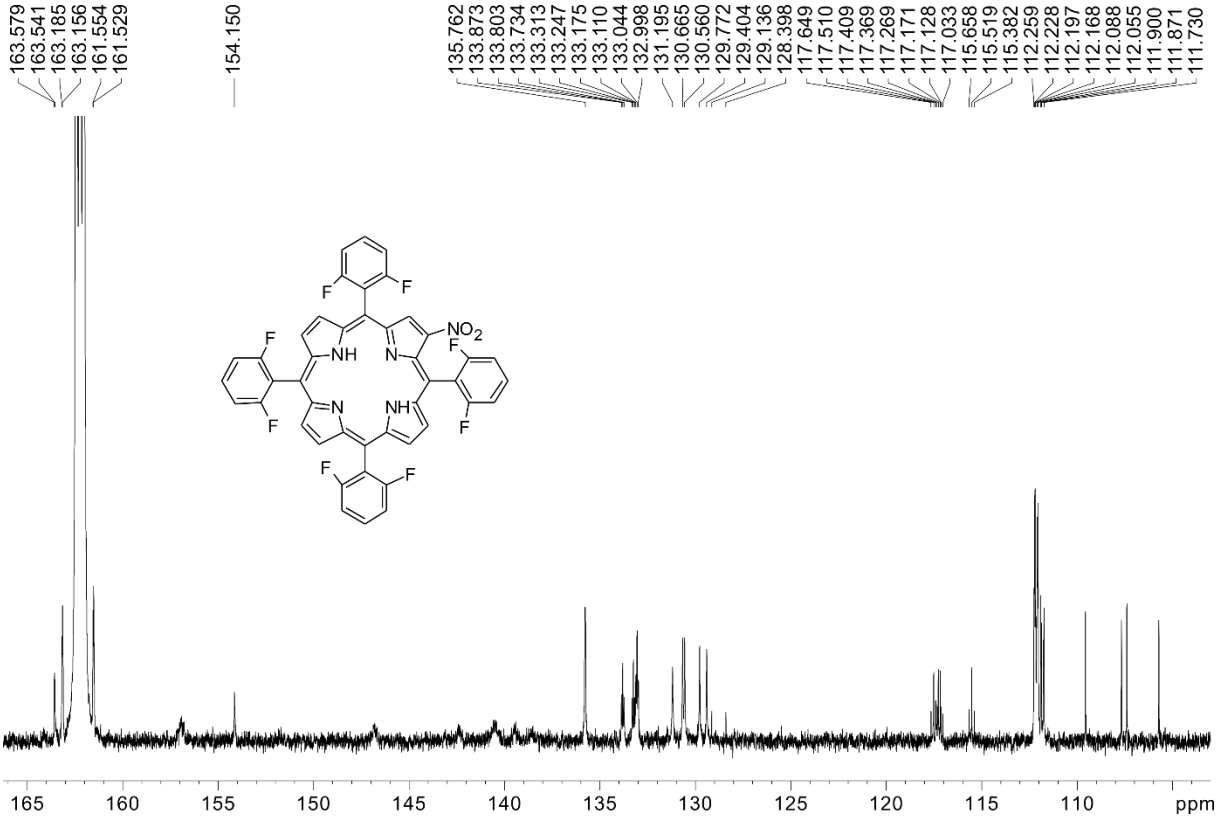


Figure S 7 ^{13}C NMR spectrum in DMF-d_7 of compound **17** at 600 MHz spectrometer.

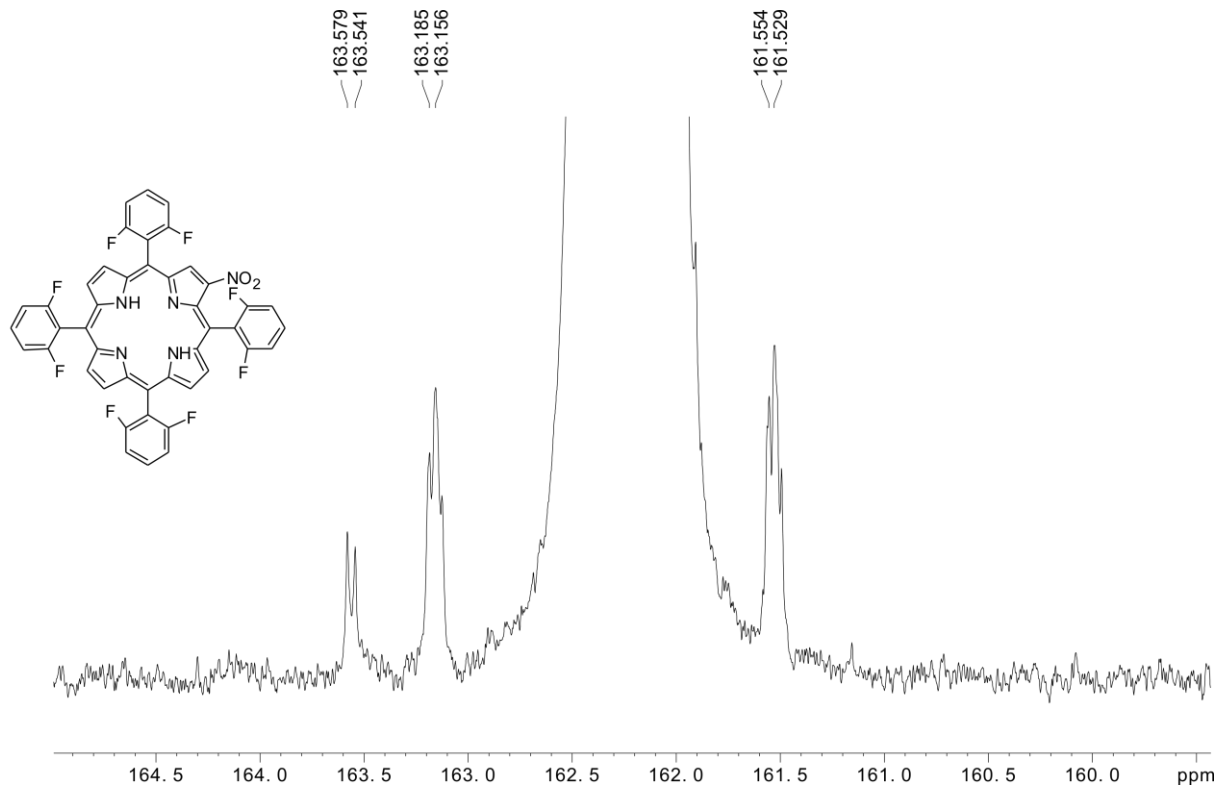


Figure S 8 ^{13}C NMR spectrum in DMF-d_7 of compound **17** (expansion of 159.5-165 ppm region) at 600 MHz spectrometer.

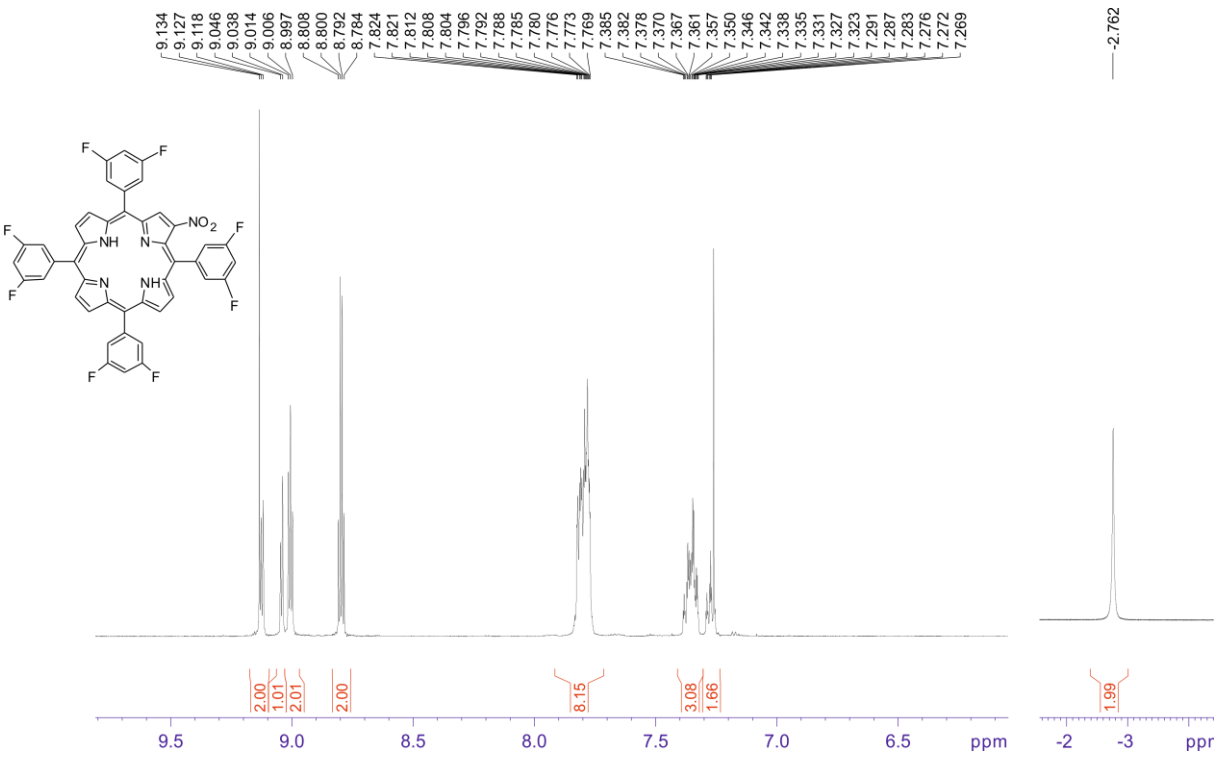


Figure S 9 ^{1}H NMR spectrum in $CDCl_3$ of compound **18** at 600 MHz.

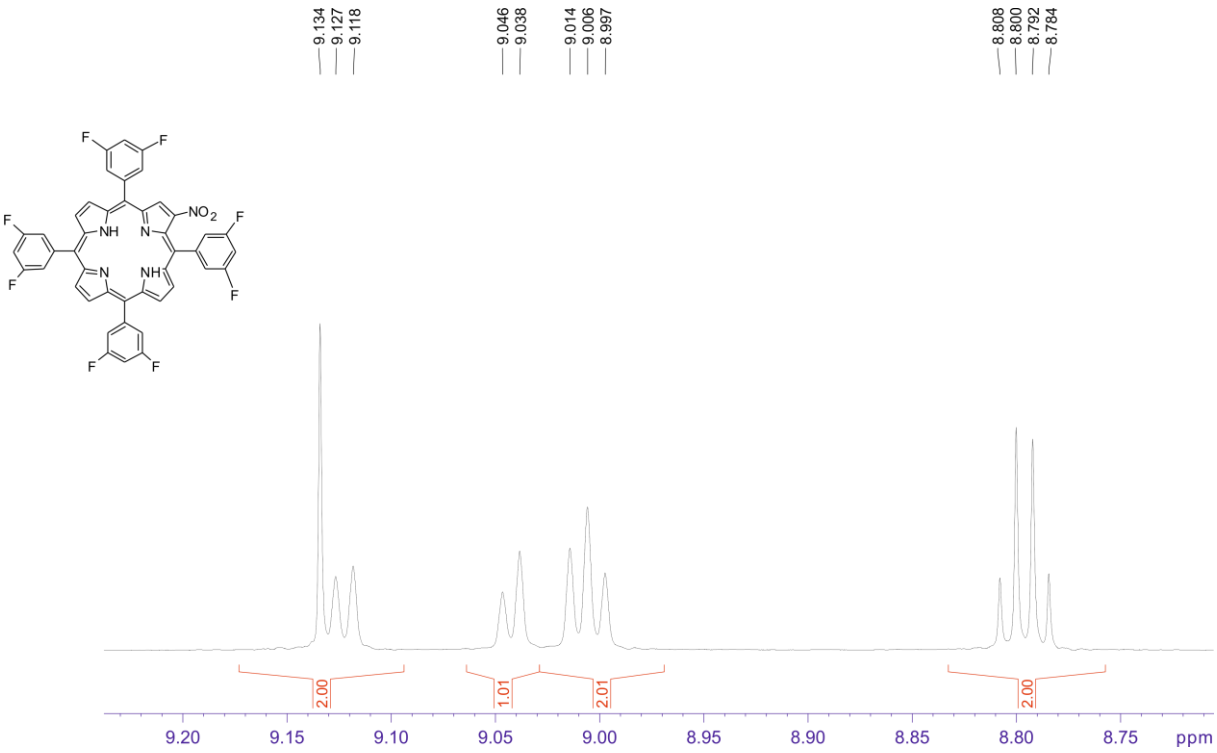
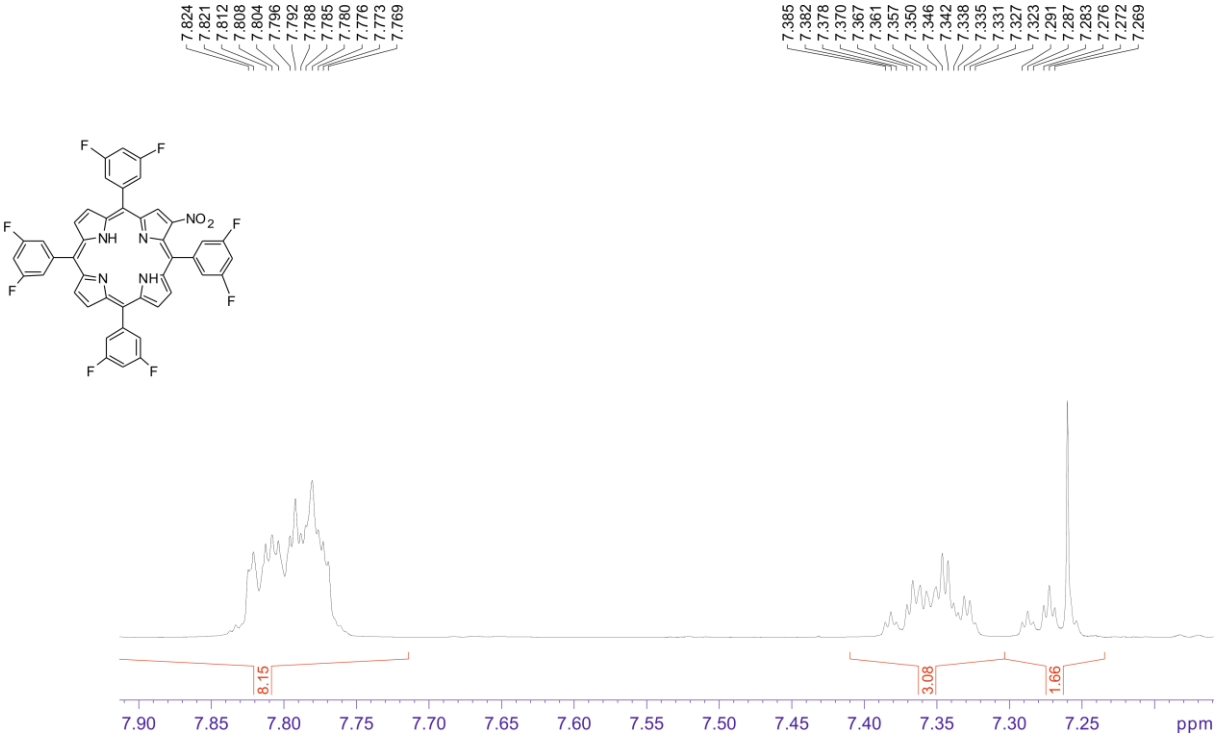


Figure S 10 ^{1}H NMR spectrum in $CDCl_3$ of compound **18 (**expansion of 8.75 – 9.20 ppm region) at 600 MHz.



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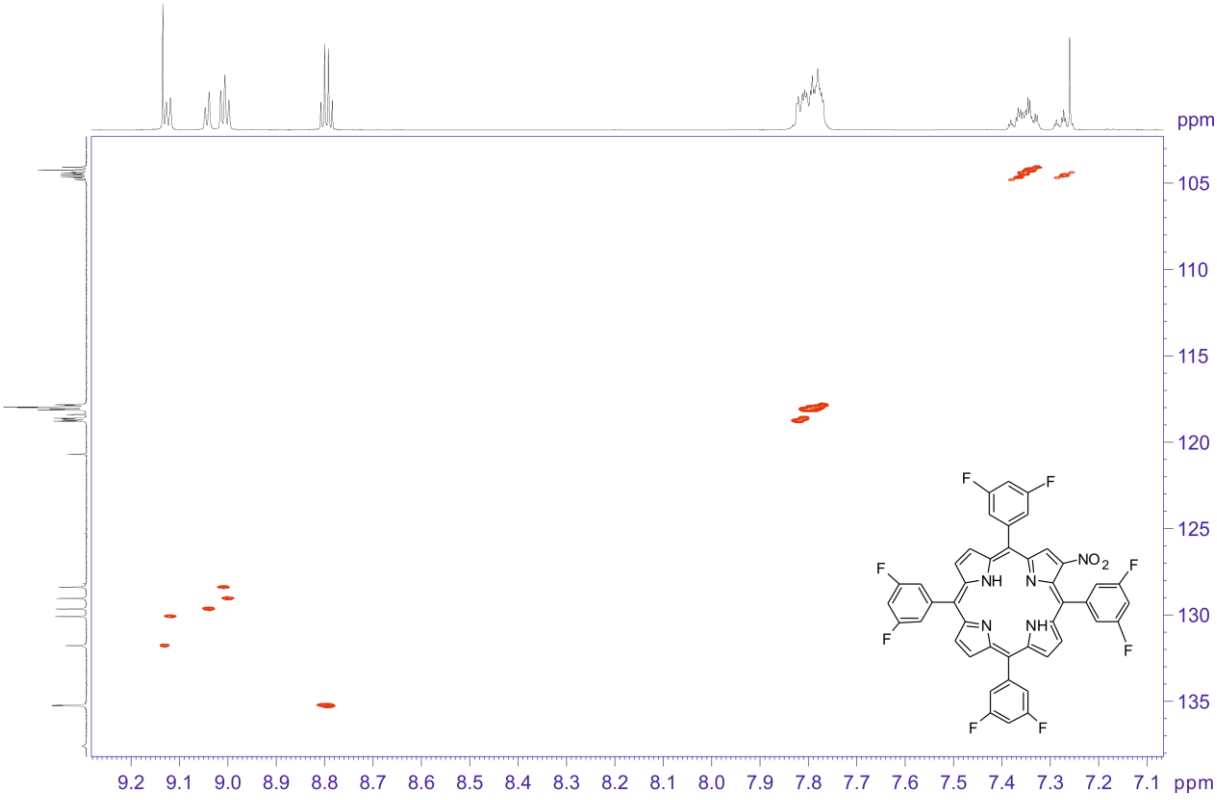


Figure S 12 ^{1}H-^{13}C HSQC spectrum in $CDCl_3$ of compound **18.** The spectrum obtained at 600 MHz spectrometer.

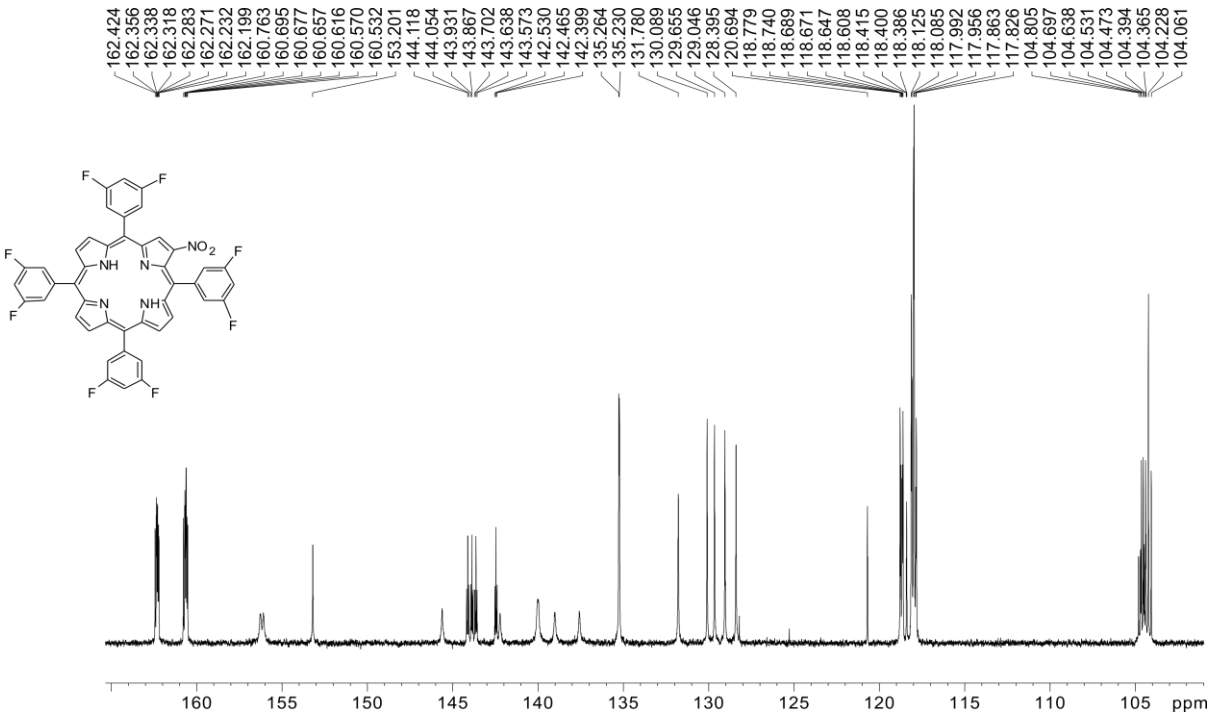


Figure S 13 ^{13}C NMR spectrum in $CDCl_3$ of compound **18** at 600 MHz spectrometer.

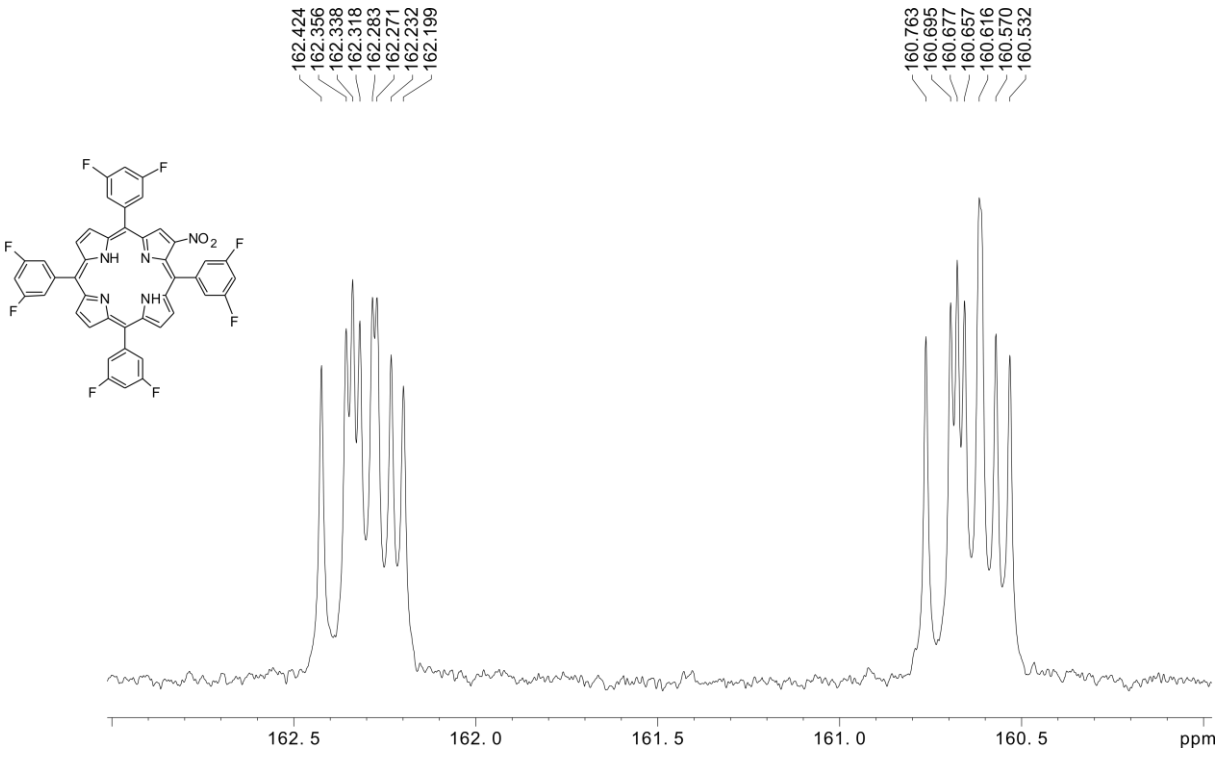


Figure S 14 ^{13}C NMR spectrum in $CDCl_3$ of compound **18 (**expansion of 160 - 163 ppm region) at 600 MHz spectrometer.

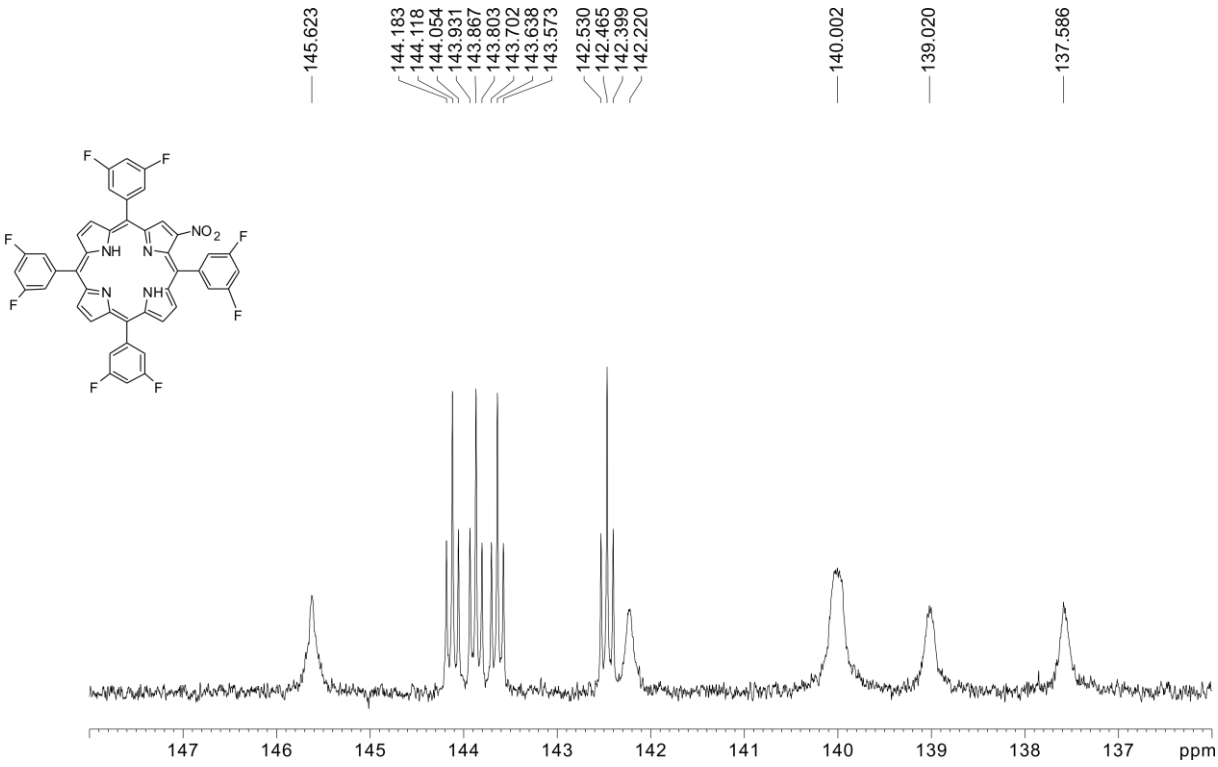


Figure S 15 ^{13}C NMR spectrum in $CDCl_3$ of compound **18 (**expansion of 136 - 147 ppm region) at 600 MHz spectrometer.

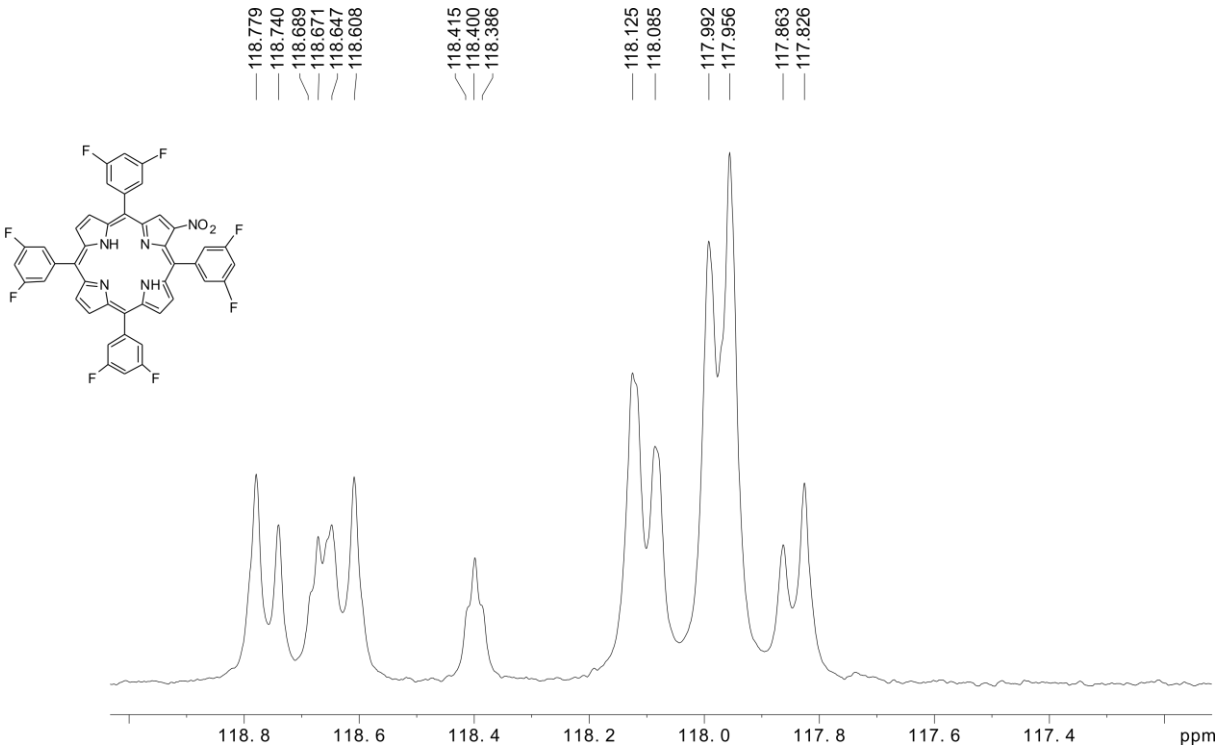
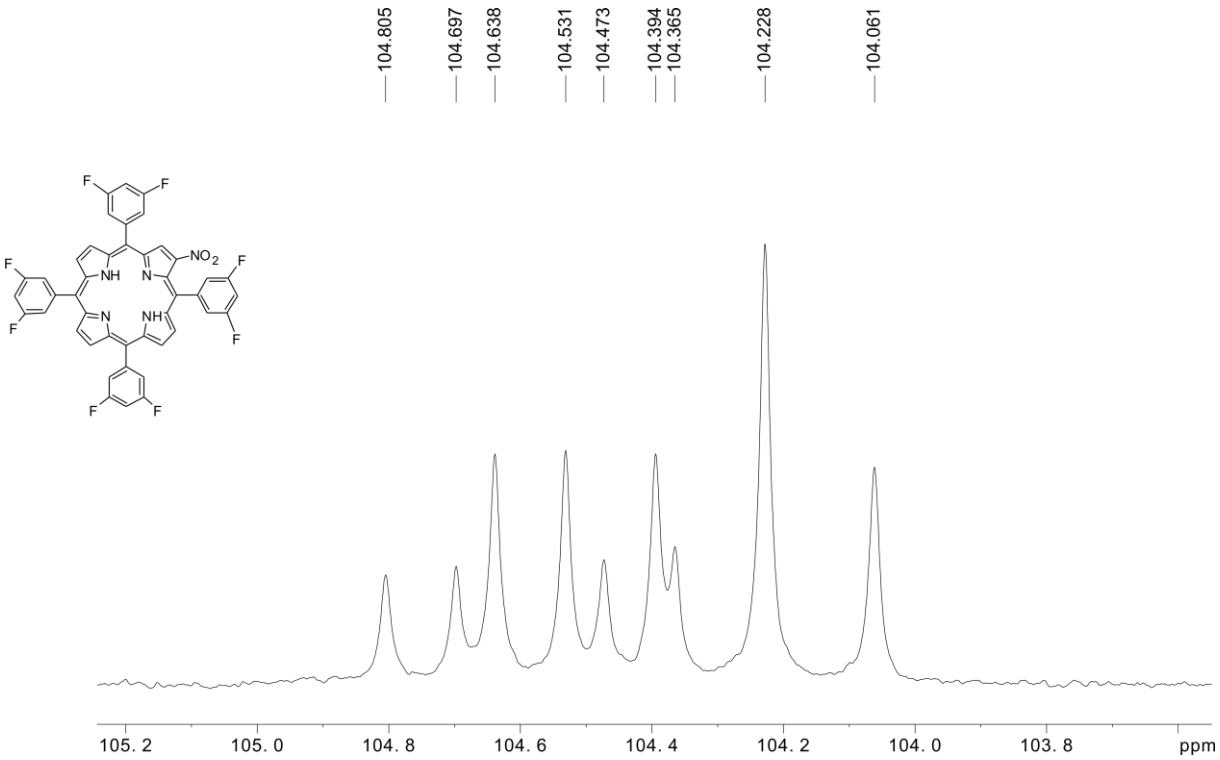


Figure S 16 ^{13}C NMR spectrum in $CDCl_3$ of compound **18 (**expansion of 117 - 119 ppm region) at 600 MHz spectrometer.



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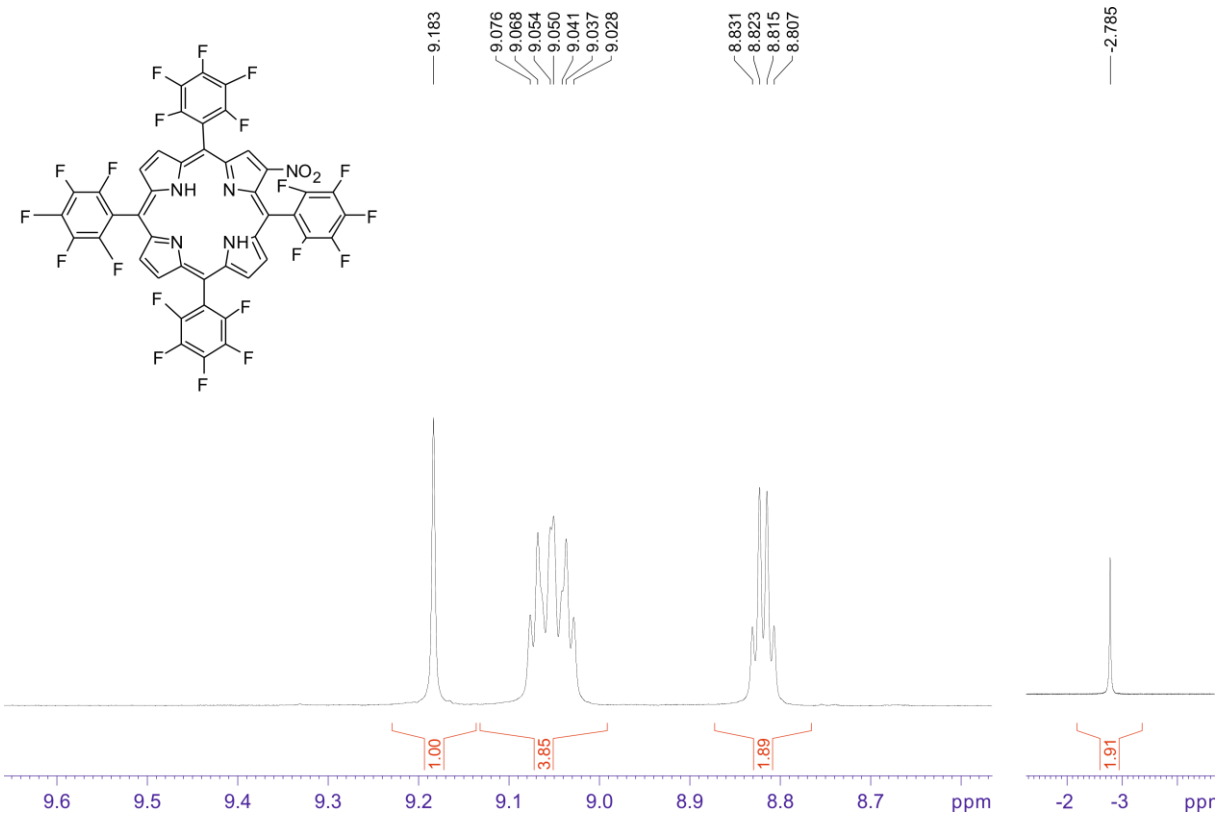


Figure S 18 ^{1}H NMR spectrum in $CDCl_3$ of compound **19** at 600 MHz.

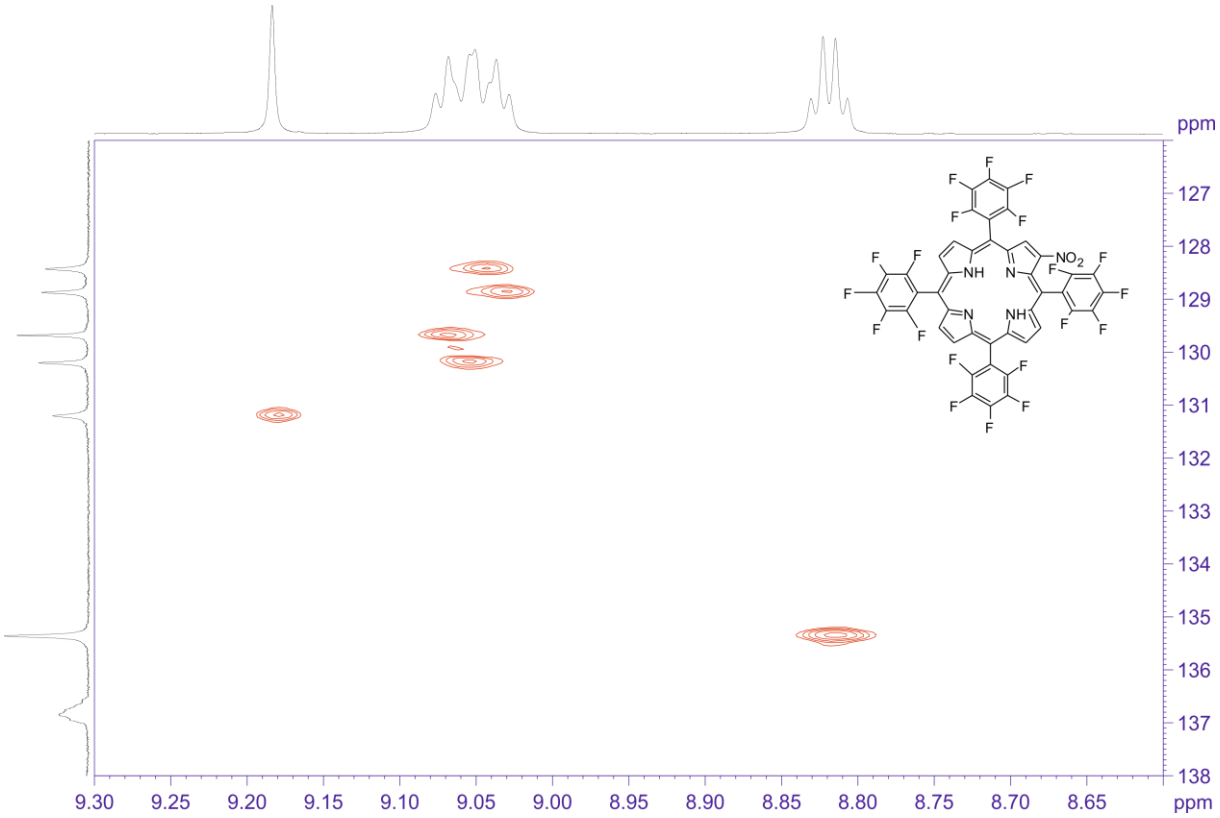


Figure S 19 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **19.** The spectrum obtained at 600 MHz spectrometer.

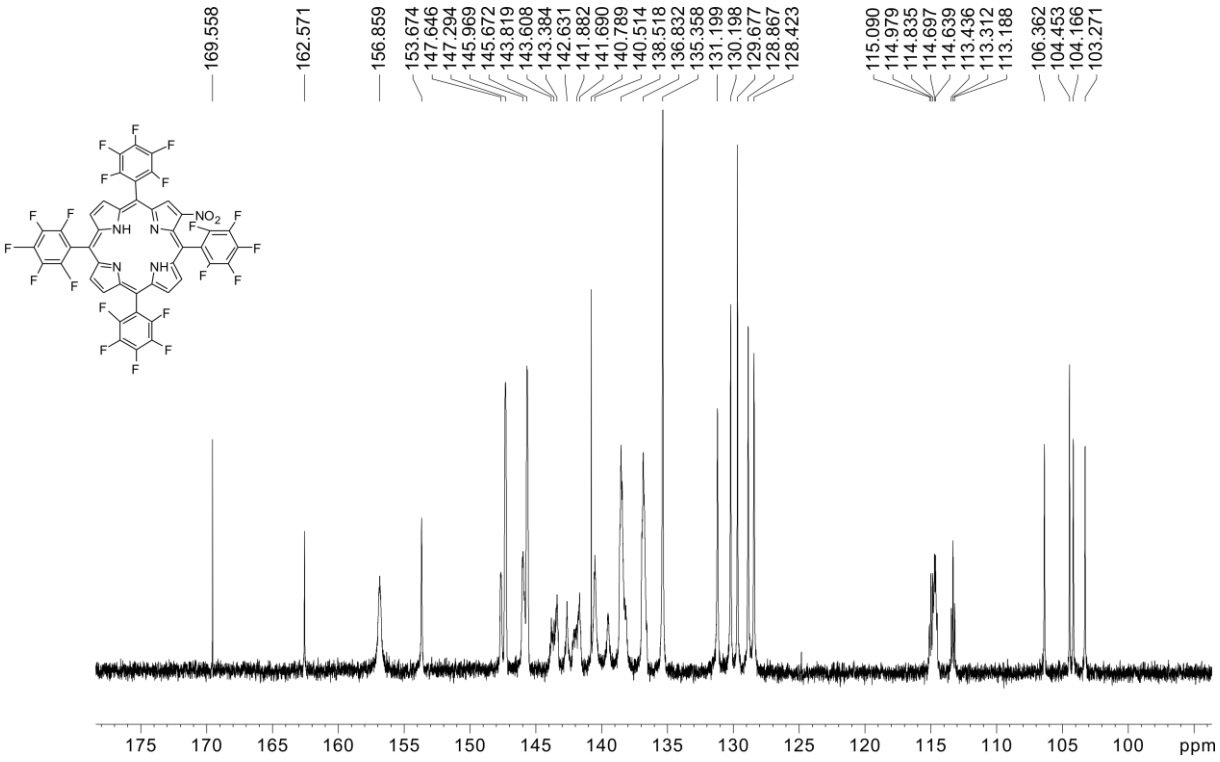


Figure S 20 ^{13}C NMR spectrum in $CDCl_3$ of compound **19** at 600 MHz spectrometer.

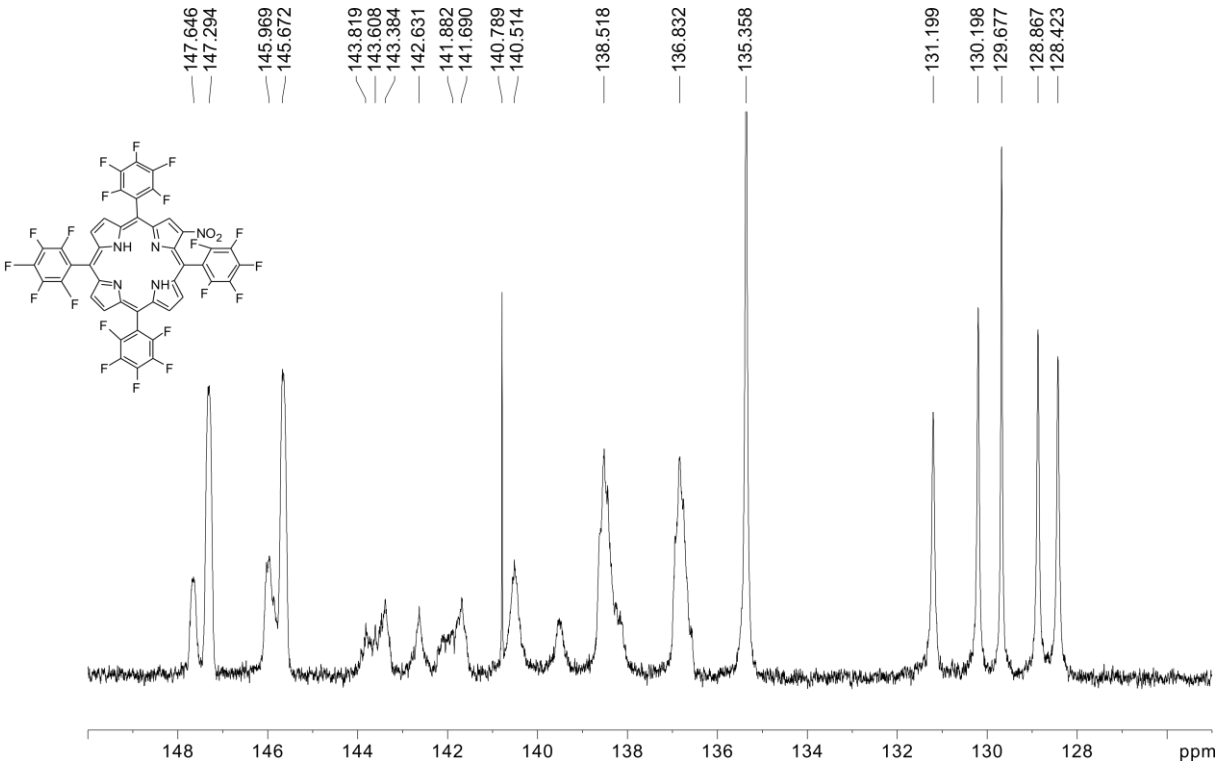
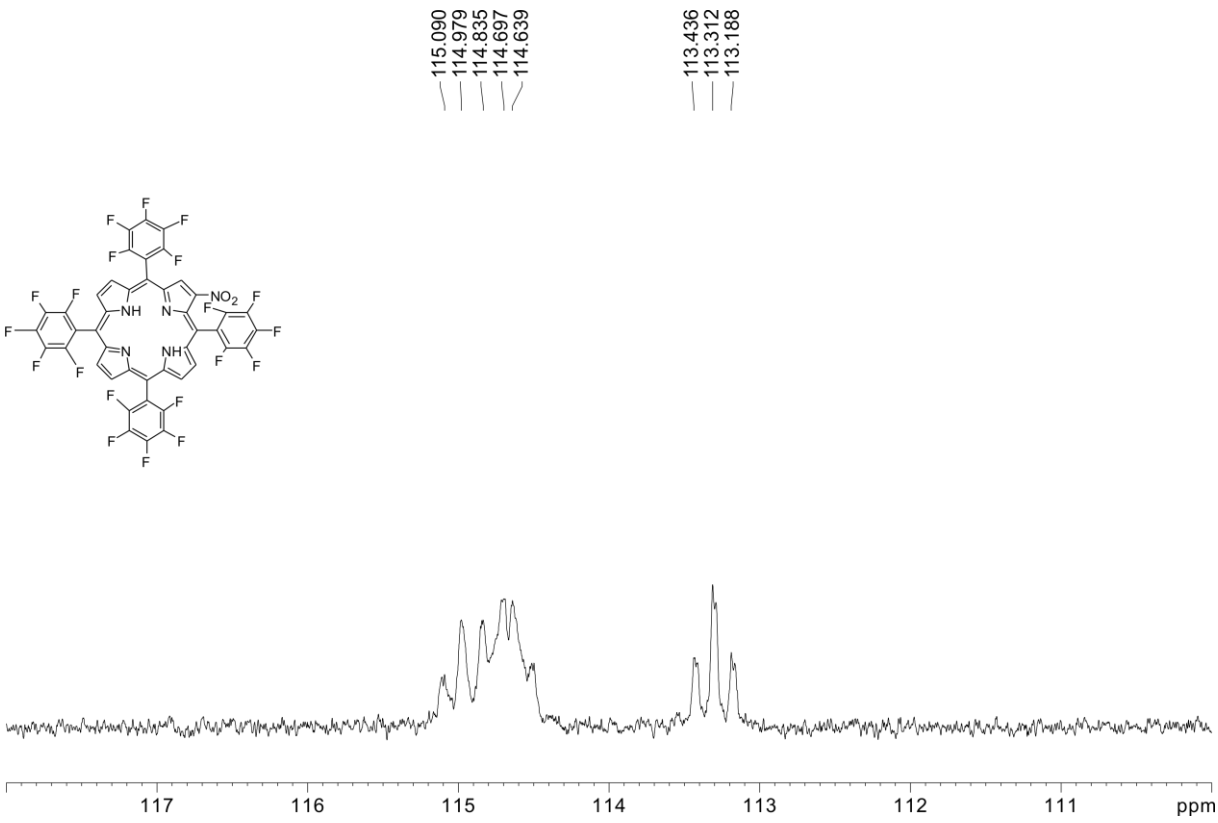


Figure S 21 ^{13}C NMR spectrum in $CDCl_3$ of compound **19 (**expansion of 127 - 149 ppm region) at 600 MHz spectrometer.



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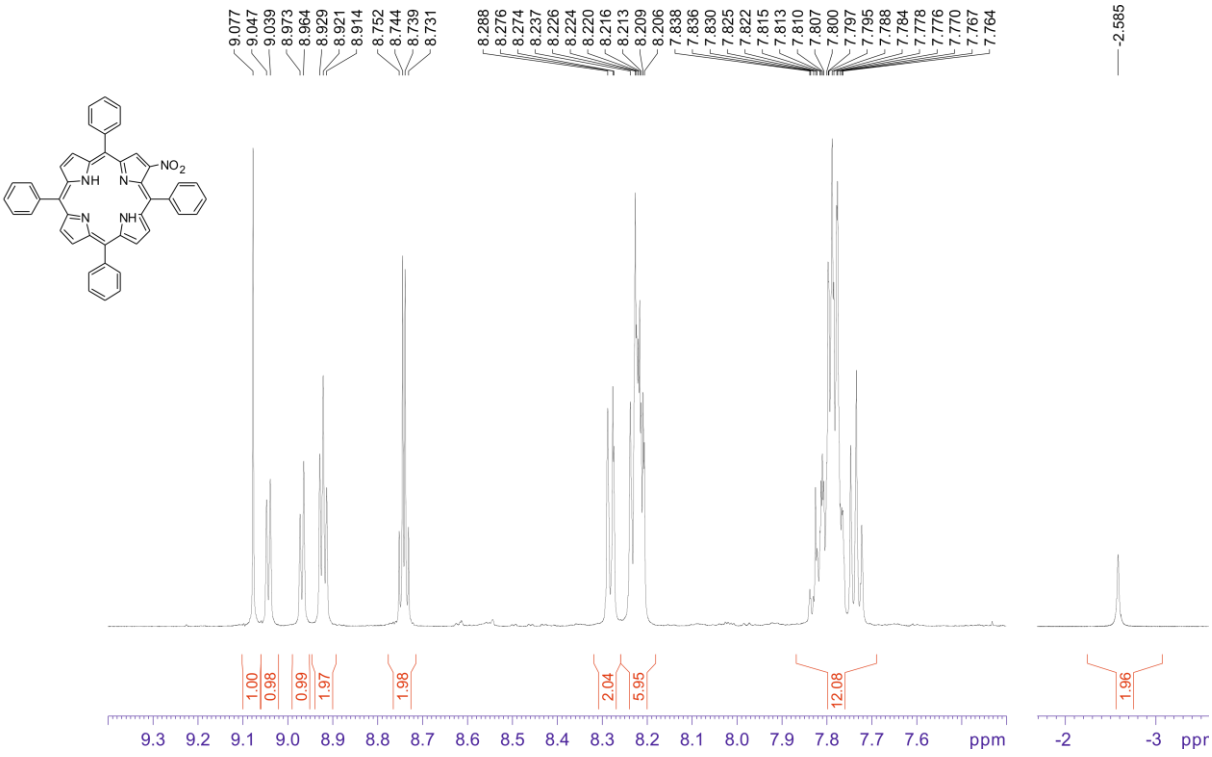


Figure S 23 ^{1}H NMR spectrum in $CDCl_3$ of compound **20** at 600 MHz.

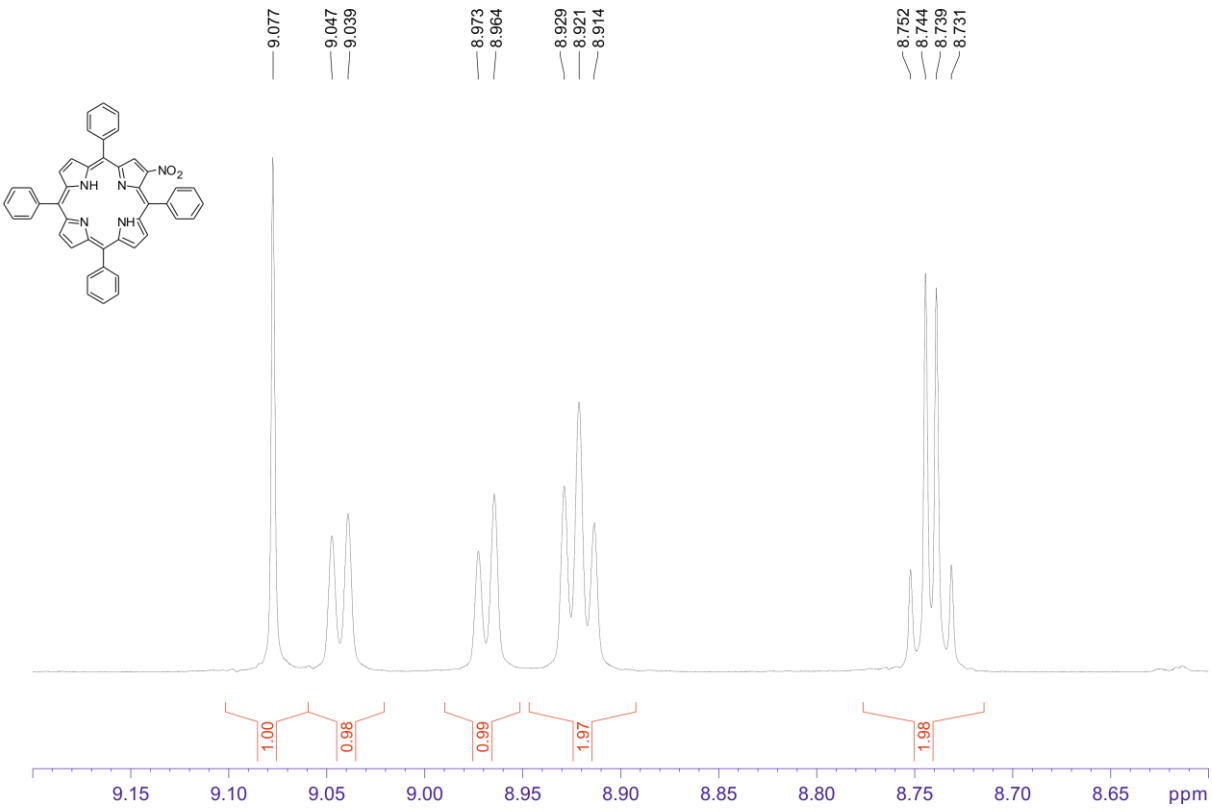


Figure S 24 ^{1}H NMR spectrum in $CDCl_3$ of compound **20 (**expansion of 8.60 – 9.20 ppm region) at 600 MHz.

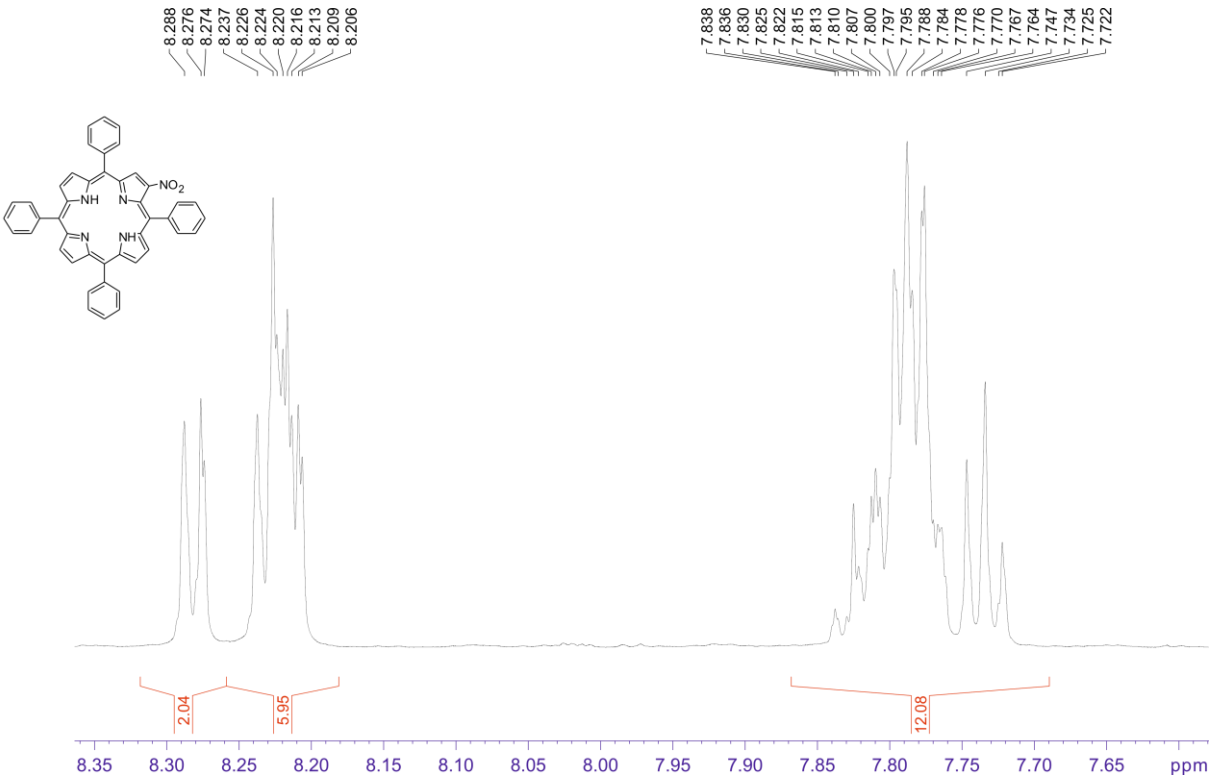


Figure S 25 ^{1}H NMR spectrum in $CDCl_3$ of compound **20 (**expansion of 7.60-8.35 ppm region) at 600 MHz.

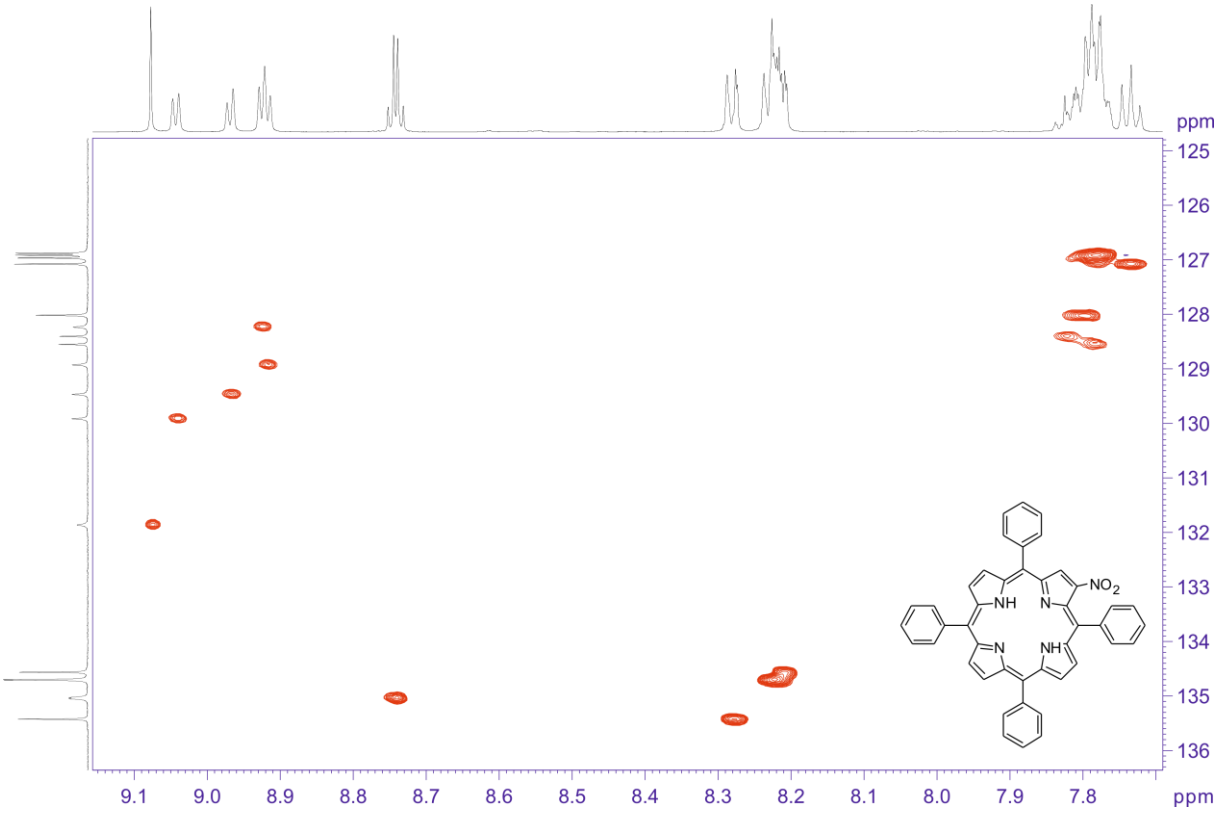


Figure S 26 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **20.** The spectrum obtained at 600 MHz spectrometer.

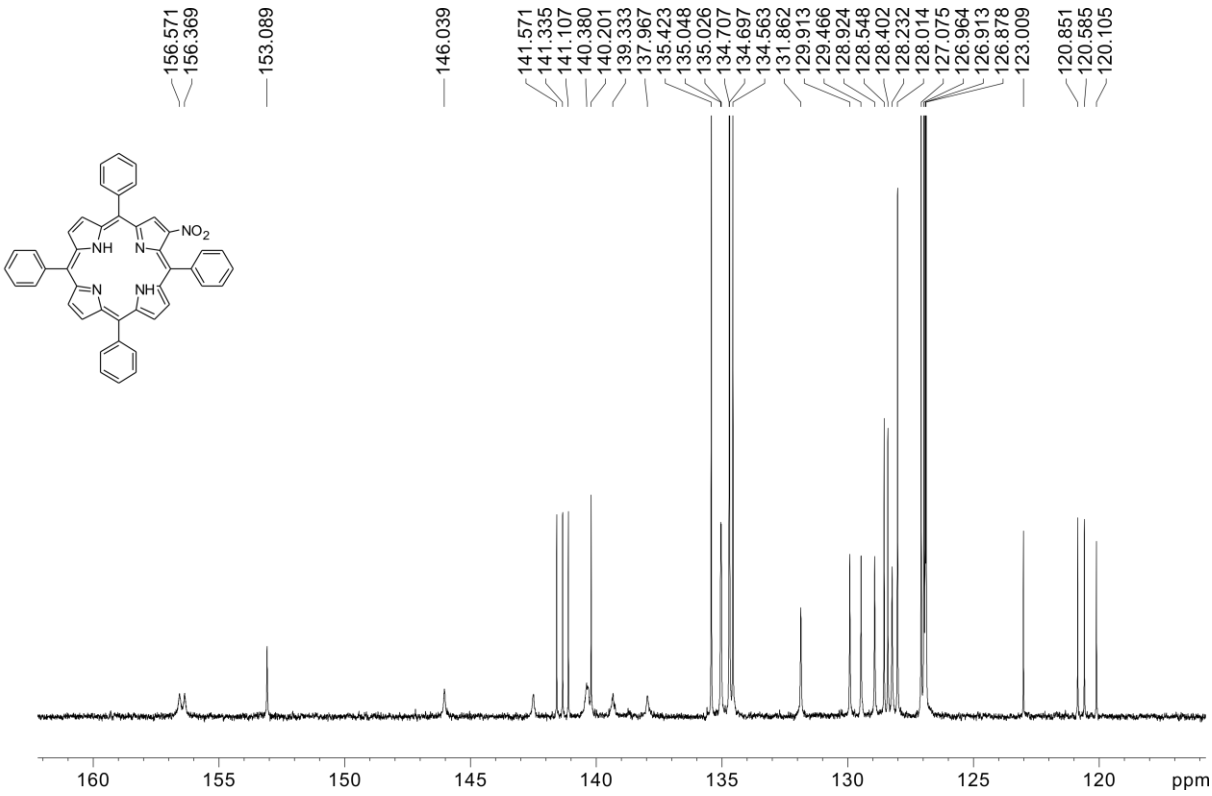


Figure S 27 ^{13}C NMR spectrum in $CDCl_3$ of compound **20** at 600 MHz spectrometer.

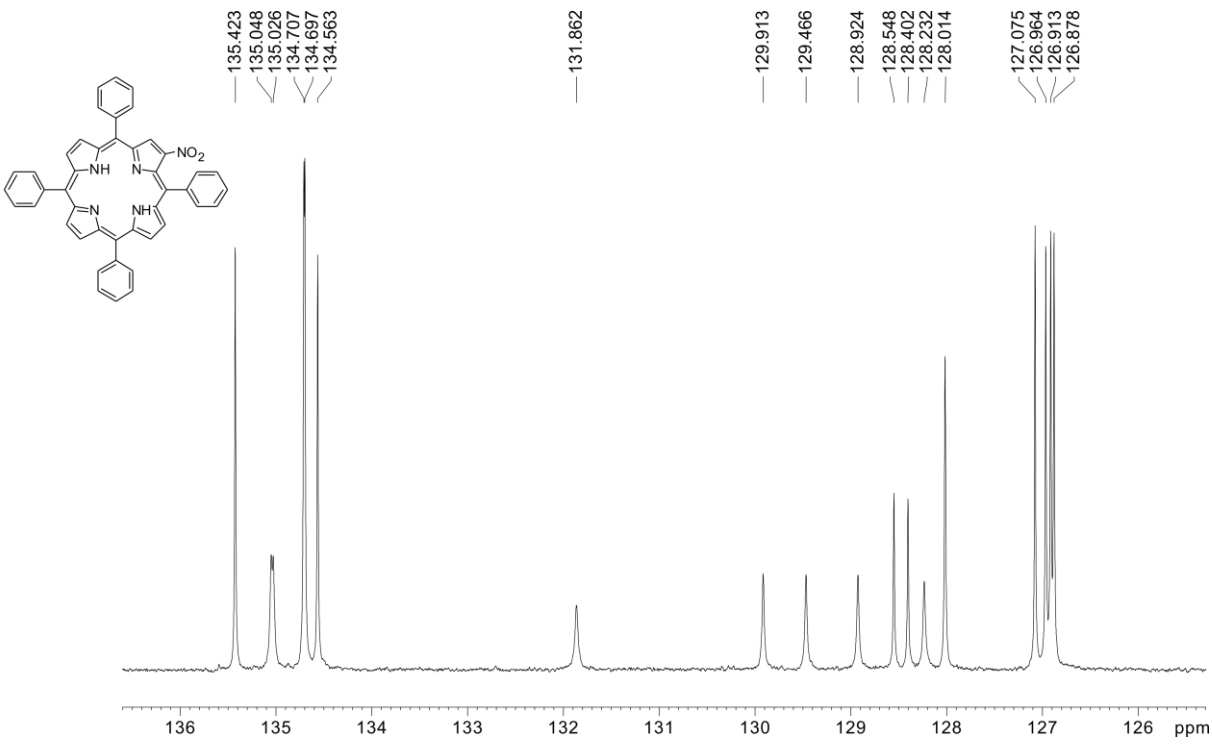


Figure S 28 ^{13}C NMR spectrum in $CDCl_3$ of compound **18 (**expansion of 126 - 136 ppm region) at 600 MHz spectrometer.

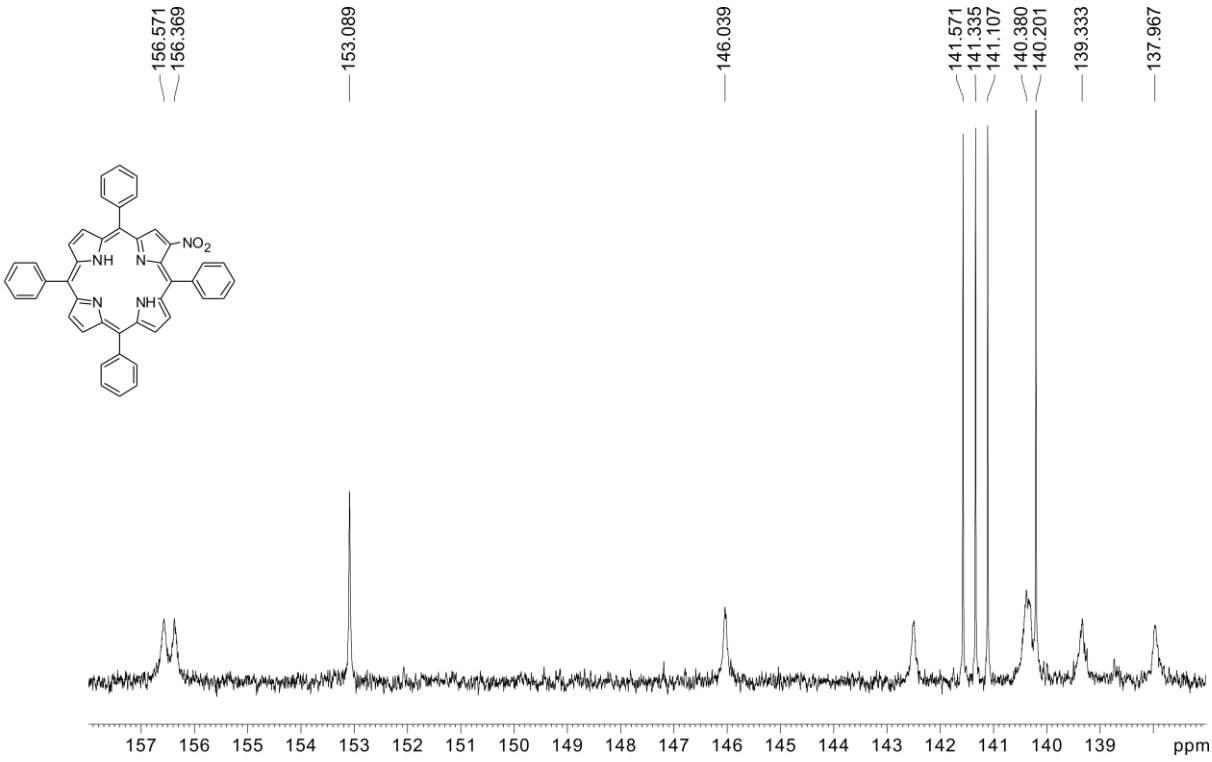


Figure S 29 ^{13}C NMR spectrum in $CDCl_3$ of compound **18 (**expansion of 138-157 ppm region) at 600 MHz spectrometer.

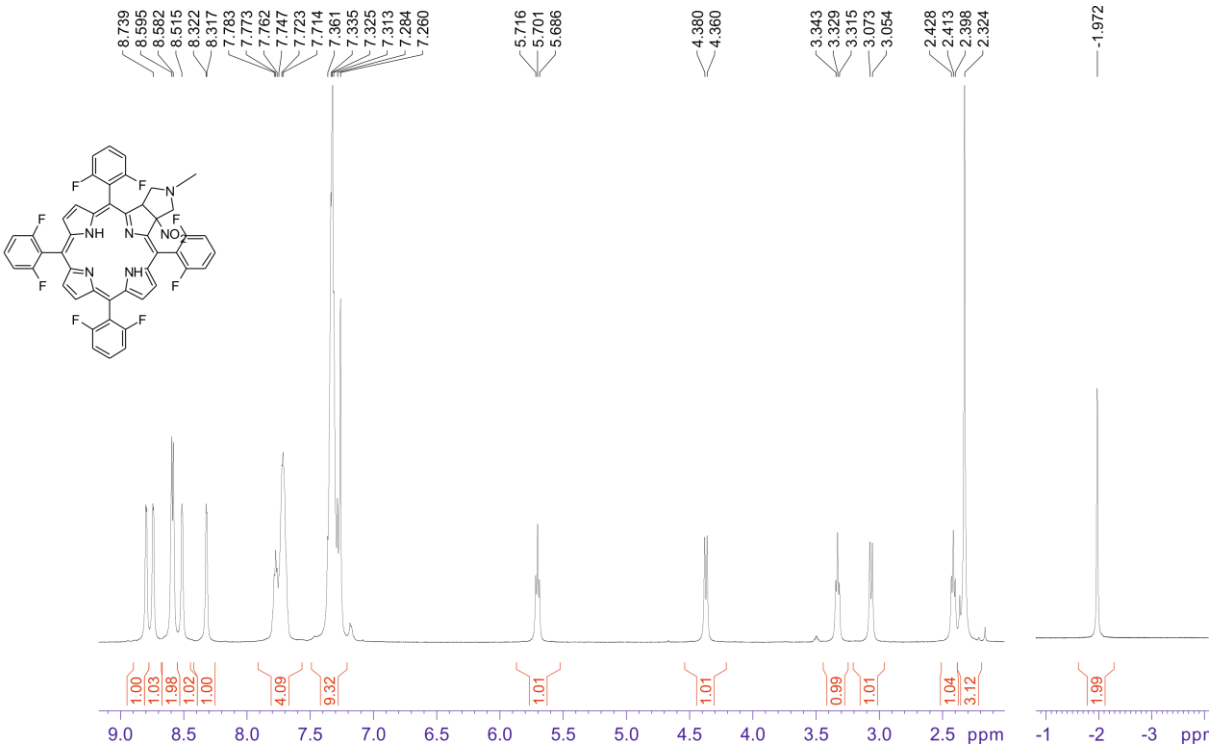


Figure S 30 ^{1}H NMR spectrum in $CDCl_3$ of compound **1** at 600 MHz.

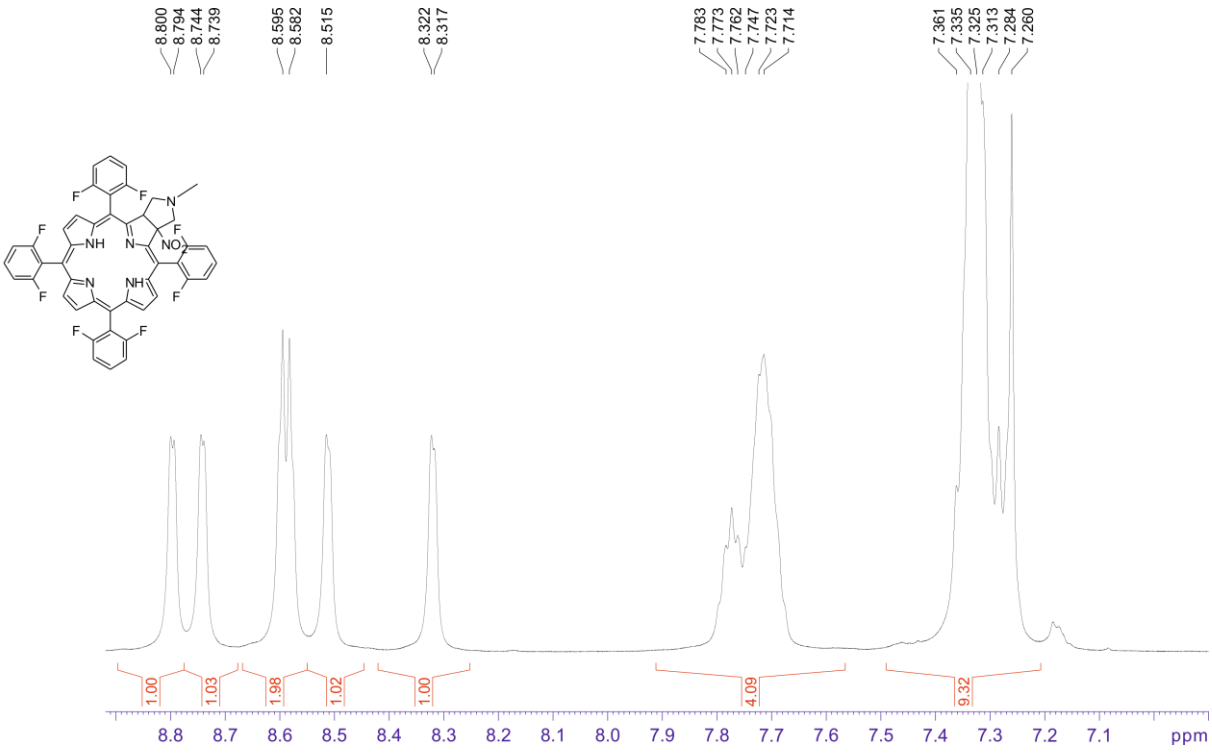
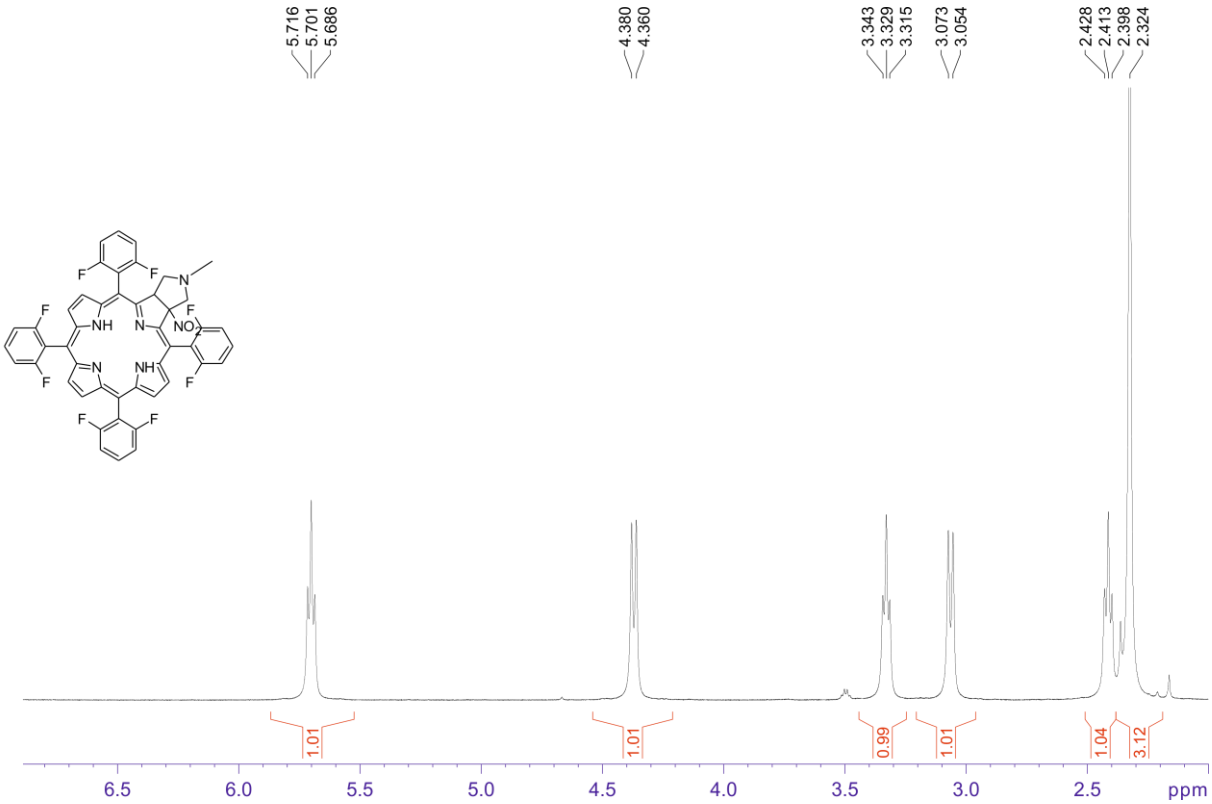


Figure S 31 ^{1}H NMR spectrum in $CDCl_3$ of compound **1** (expansion of 7.1-8.9 ppm region) at 600 MHz.



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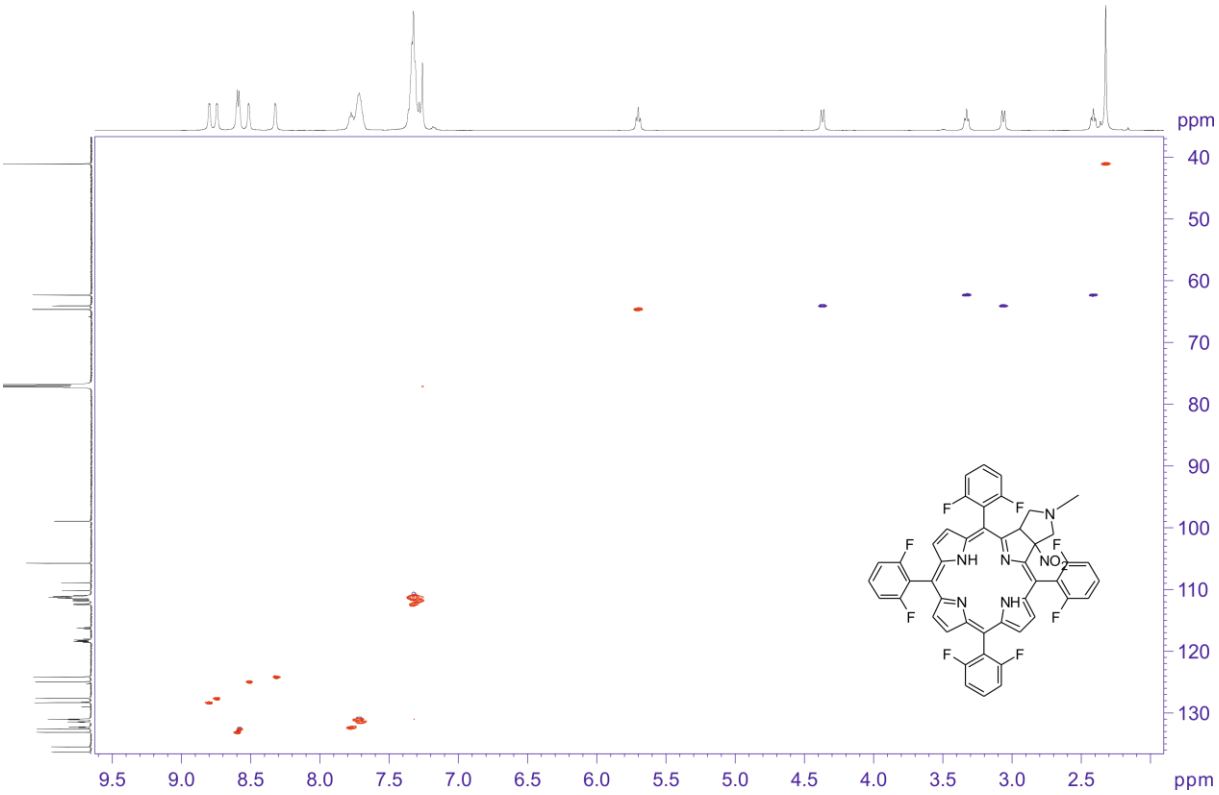

Figure S 33 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **1.** The spectrum obtained at 600 MHz spectrometer.

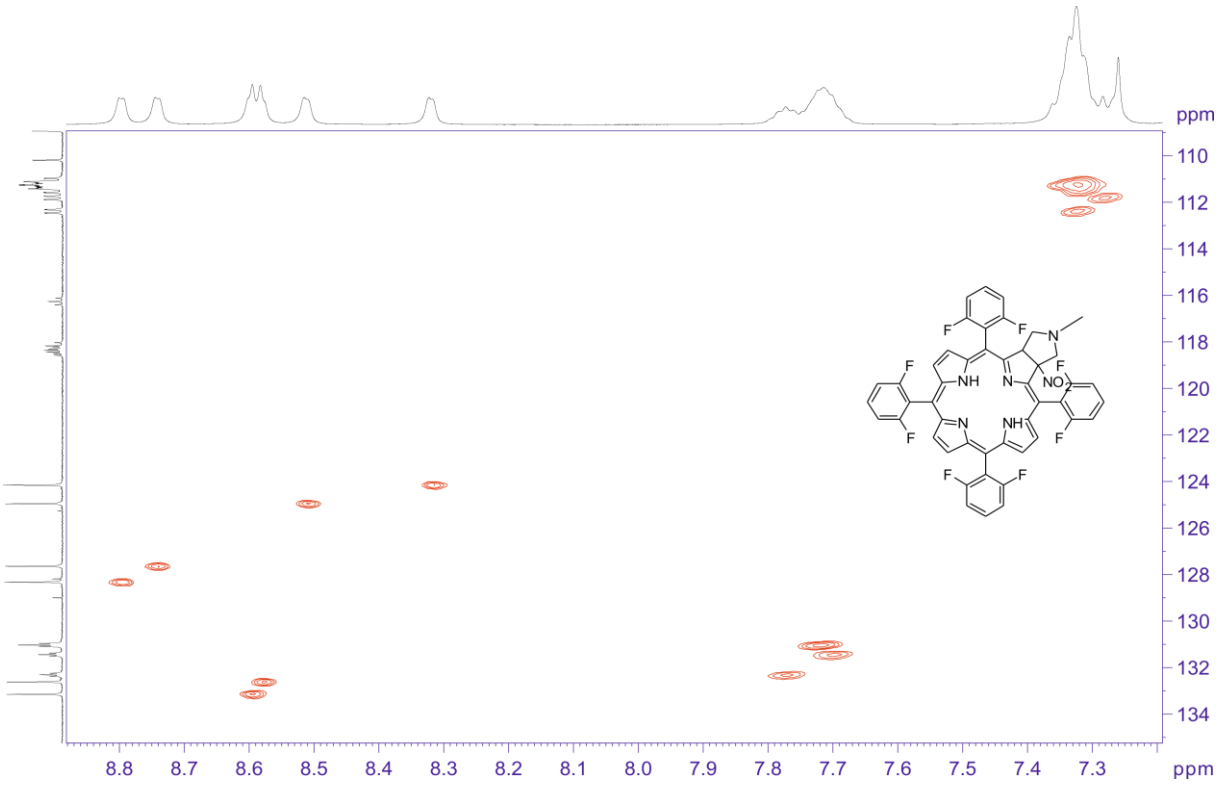

Figure S 34 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **1.** The spectrum obtained at 600 MHz spectrometer.

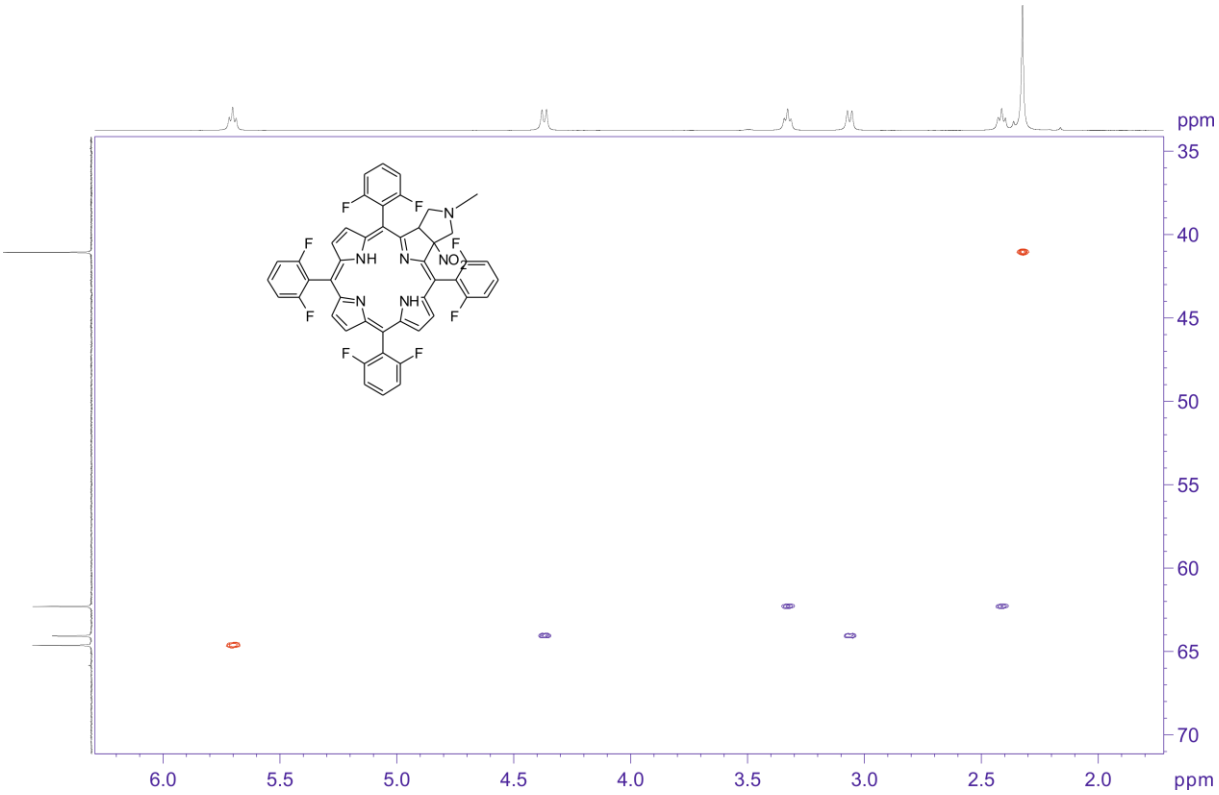

Figure S 35 ^{1}H-^{13}C NMR spectrum in $CDCl_3$ of compound **1.** The spectrum obtained at 600 MHz spectrometer.

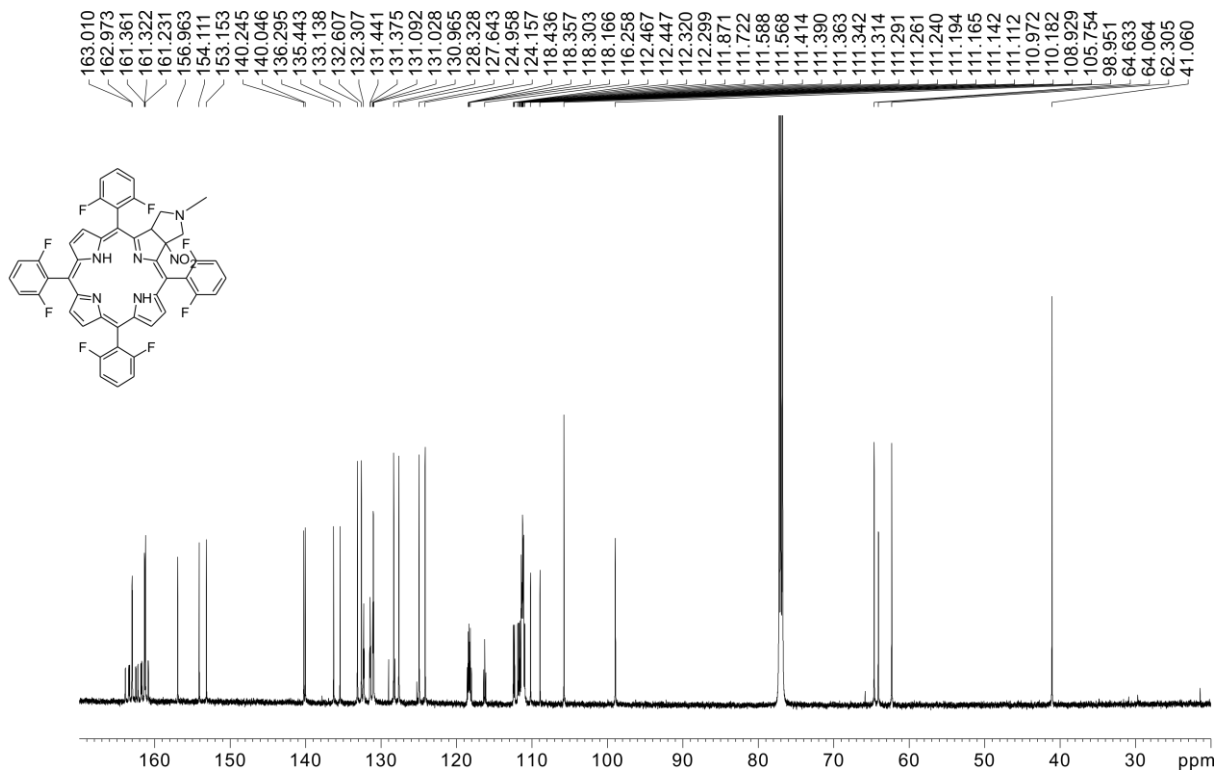

Figure S 36 ^{13}C NMR spectrum in $CDCl_3$ of compound **1** at 600 MHz spectrometer.

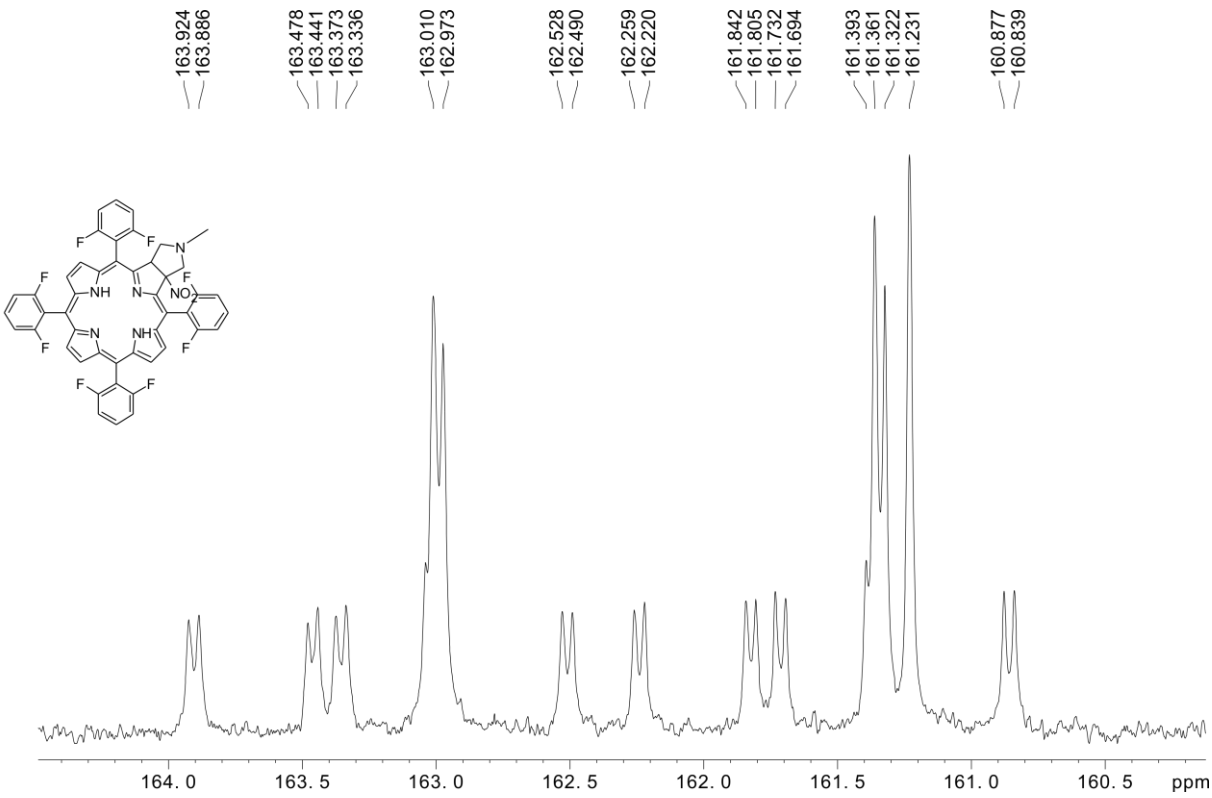

Figure S 37 ^{13}C NMR spectrum in $CDCl_3$ of compound **1** (expansion of 160-164 ppm region) at 600 MHz spectrometer.

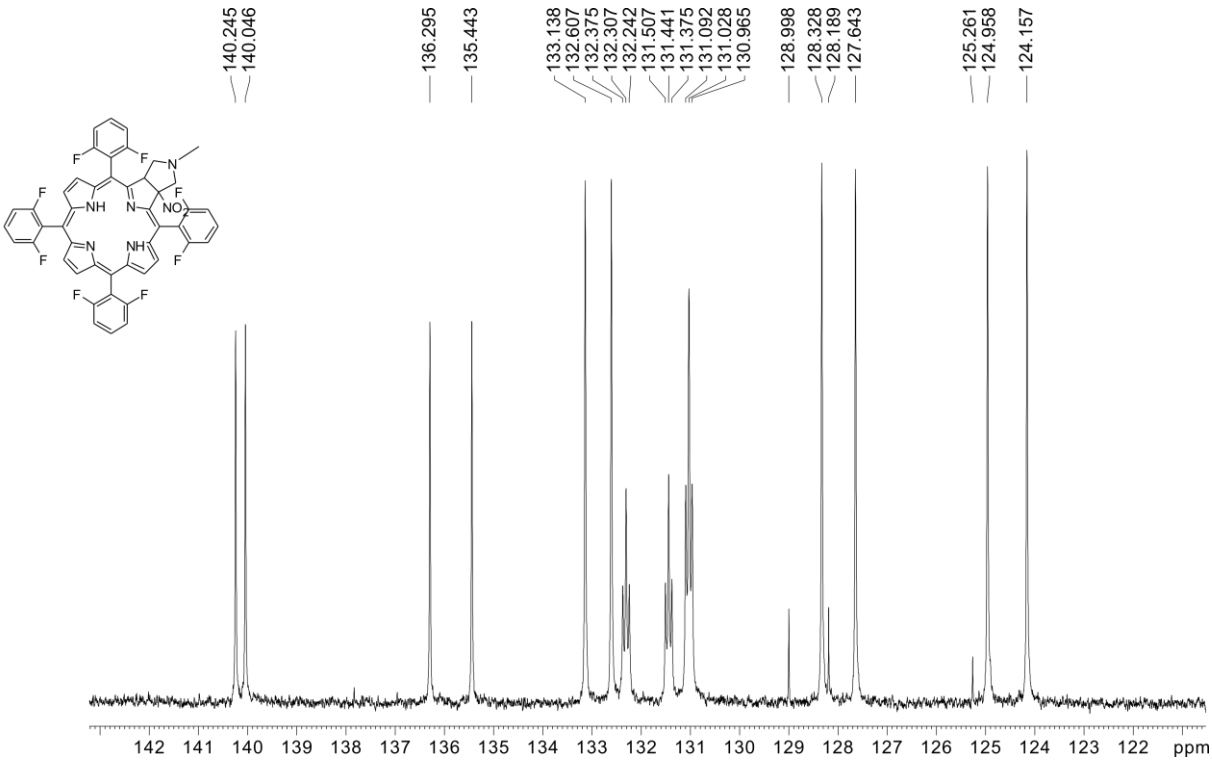

Figure S 38 ^{13}C NMR spectrum in $CDCl_3$ of compound **1** (expansion of 121-143 ppm region) at 600 MHz spectrometer.

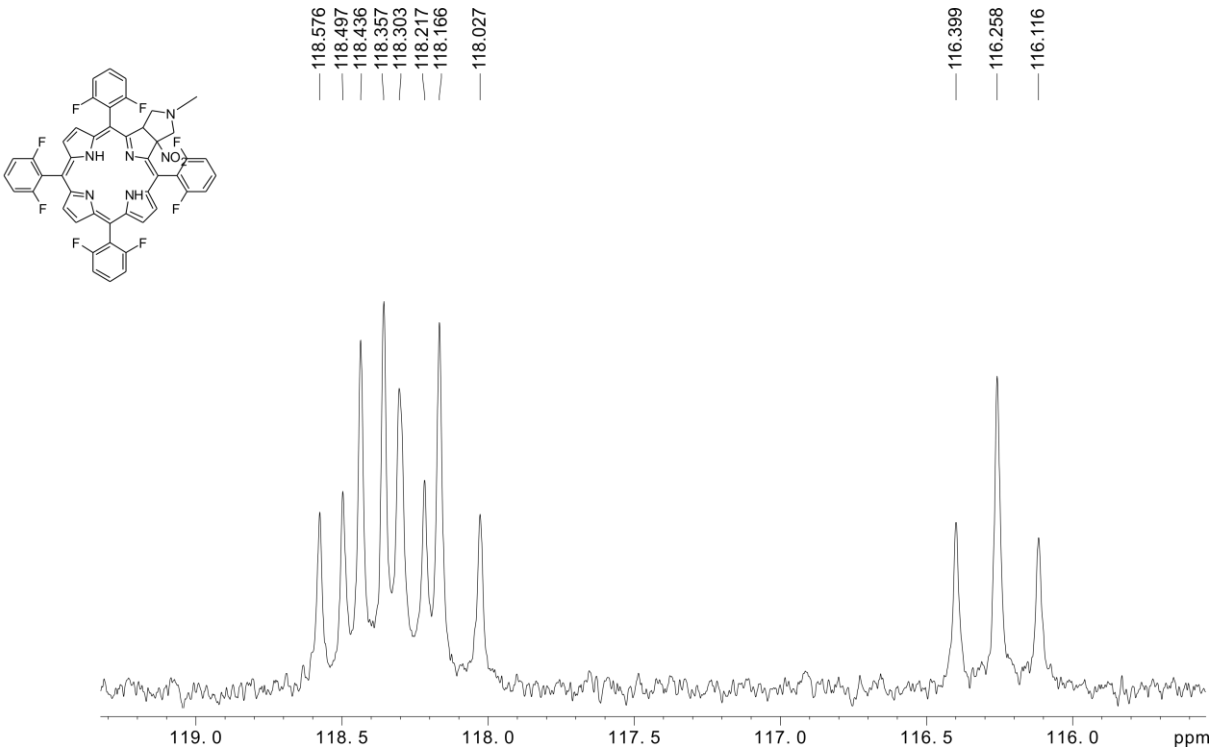

Figure S 39 ^{13}C NMR spectrum in $CDCl_3$ of compound **1** (expansion of 115-119 ppm region) at 600 MHz spectrometer.

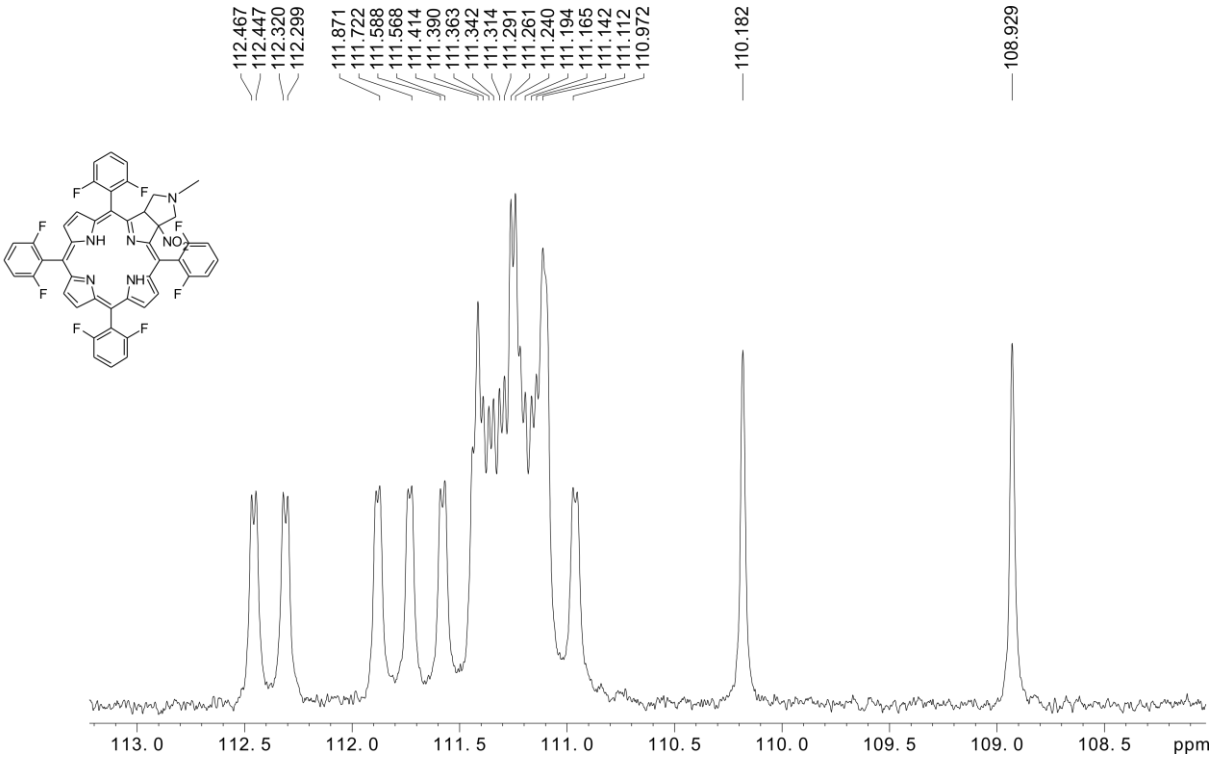

Figure S 40 ^{13}C NMR spectrum in $CDCl_3$ of compound **1** (expansion of 108-113 ppm region) at 600 MHz spectrometer.

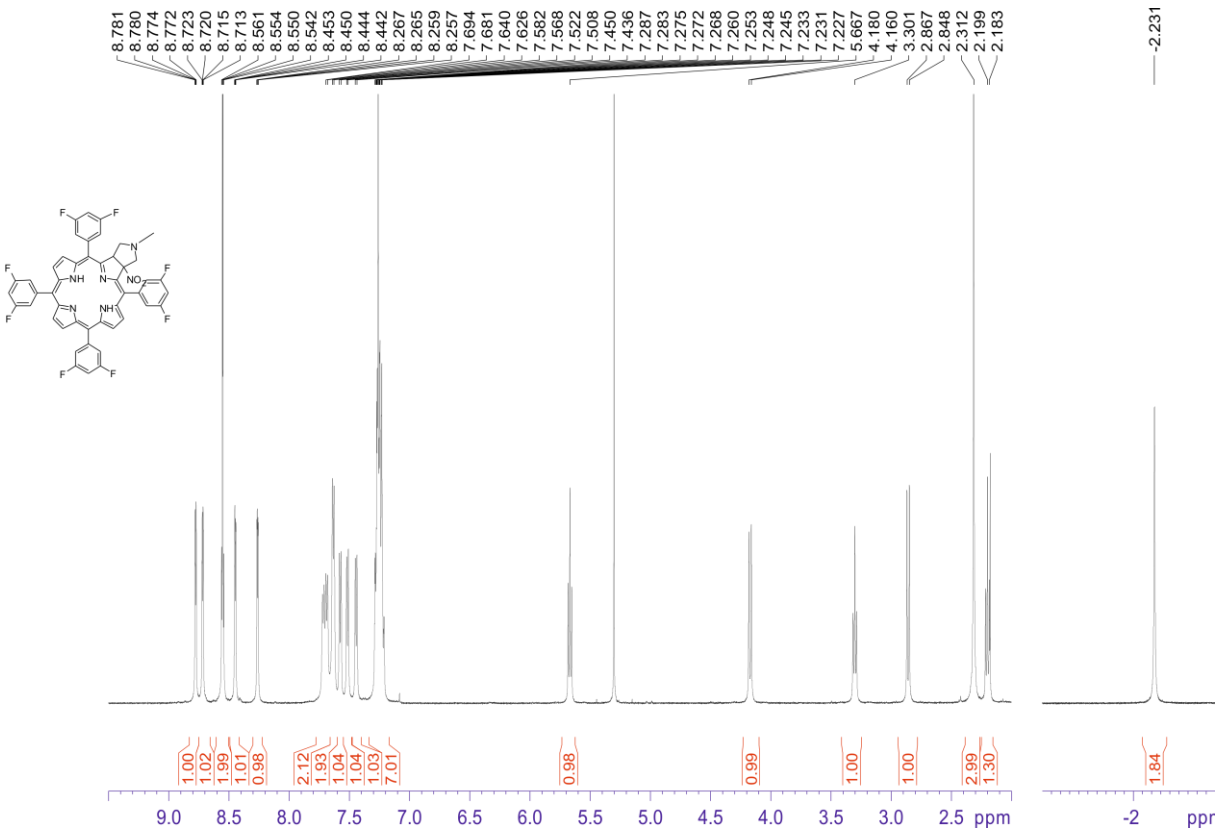

Figure S 41 ^{1}H NMR spectrum in $CDCl_3$ of compound **2** at 600 MHz.

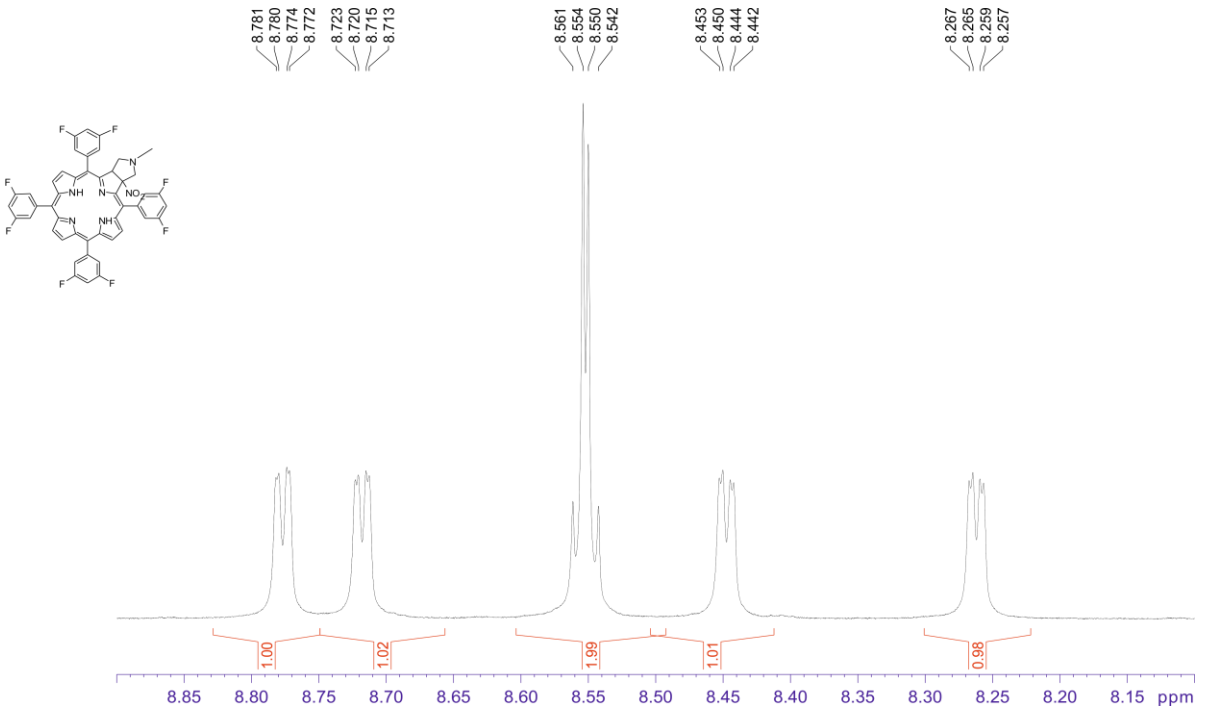

Figure S 42 ^{1}H NMR spectrum in $CDCl_3$ of compound **2** (expansion of 8.15-8.86 ppm region) at 600 MHz.

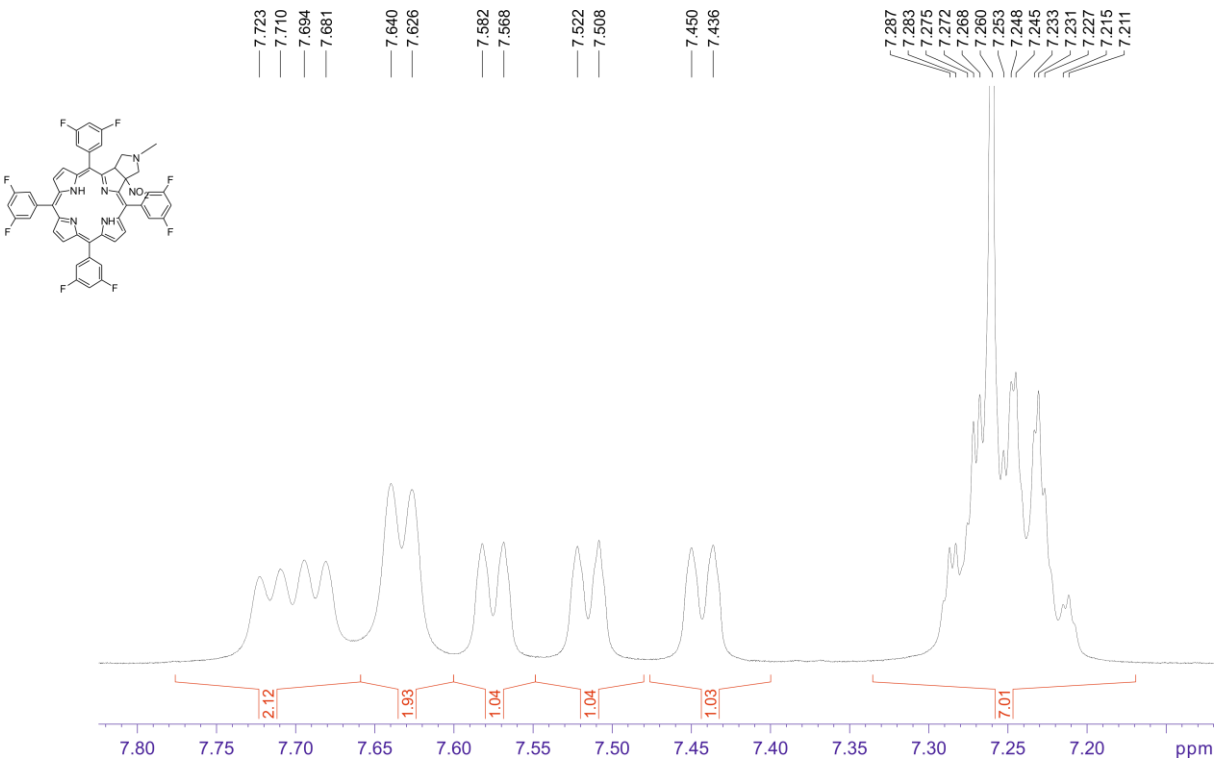

Figure S 43 ^{1}H NMR spectrum in $CDCl_3$ of compound **2** (expansion of 7.15-7.80 ppm region) at 600 MHz.

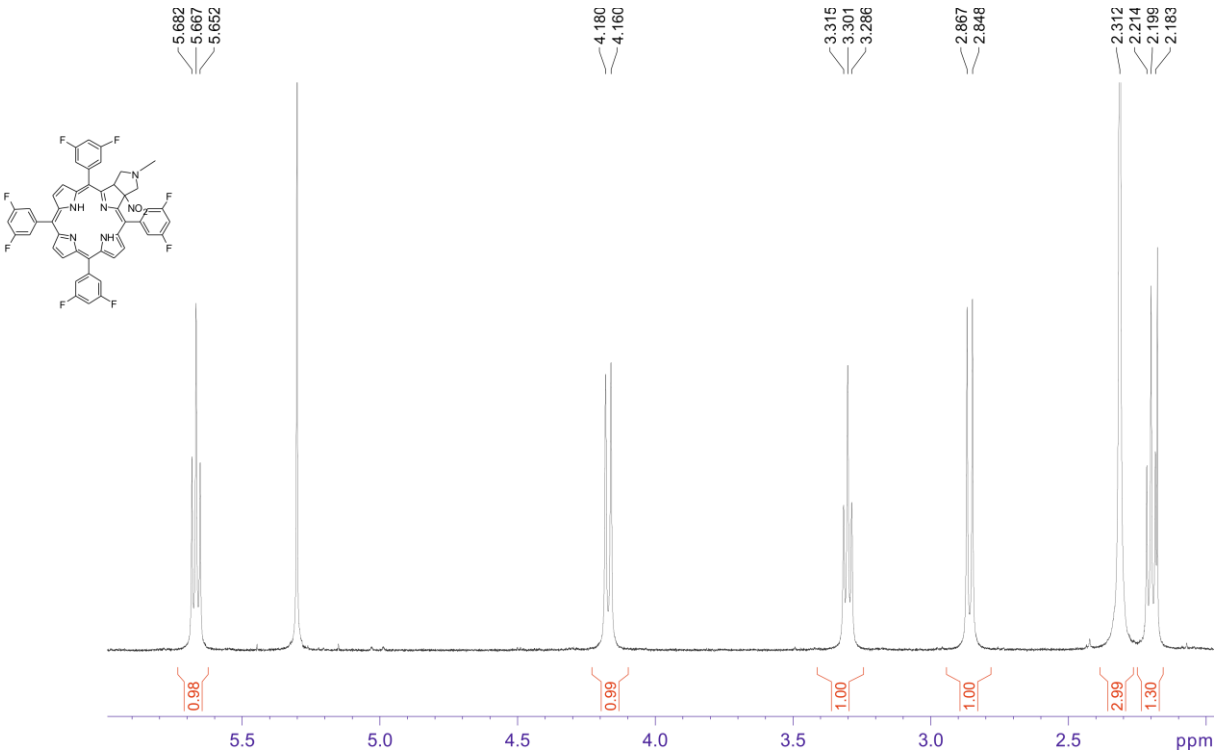

Figure S 44 ^{1}H NMR spectrum in $CDCl_3$ of compound **2** (expansion of 2.0-6.0 ppm region) at 600 MHz.

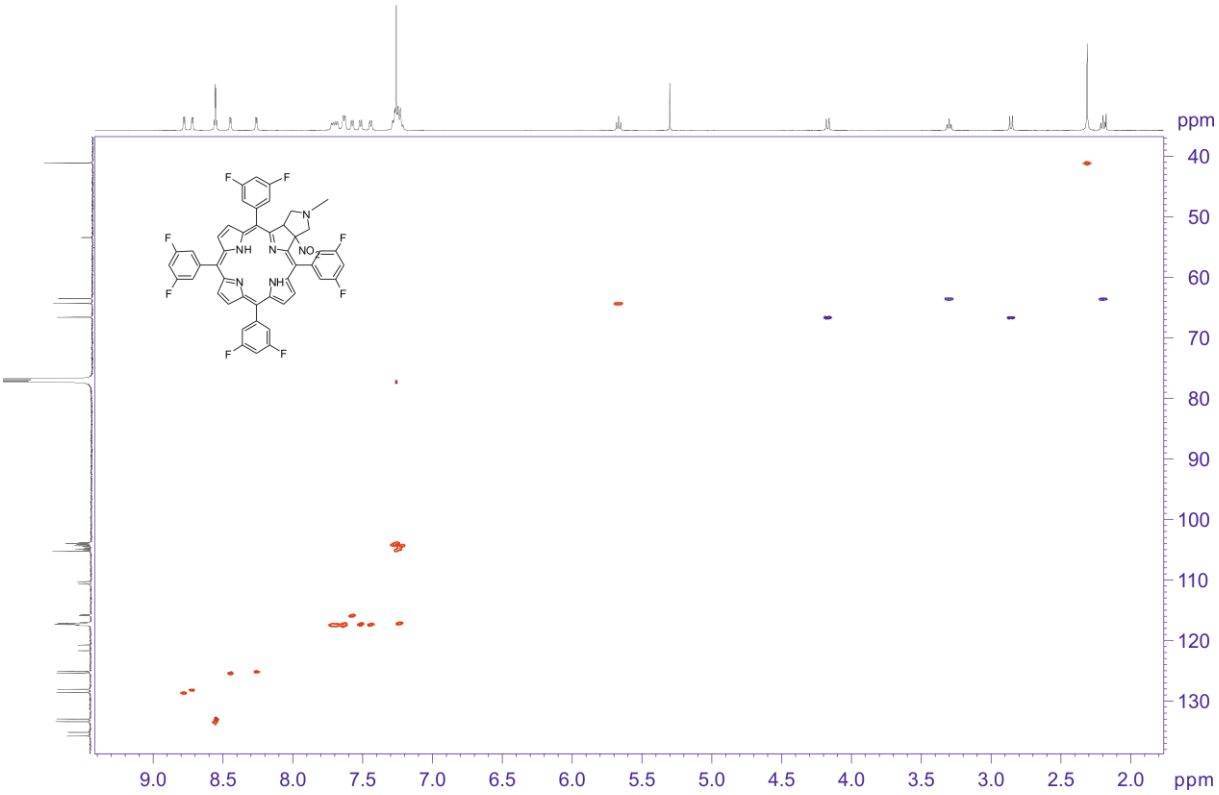

Figure S 45 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **2.** The spectrum obtained at 600 MHz spectrometer.

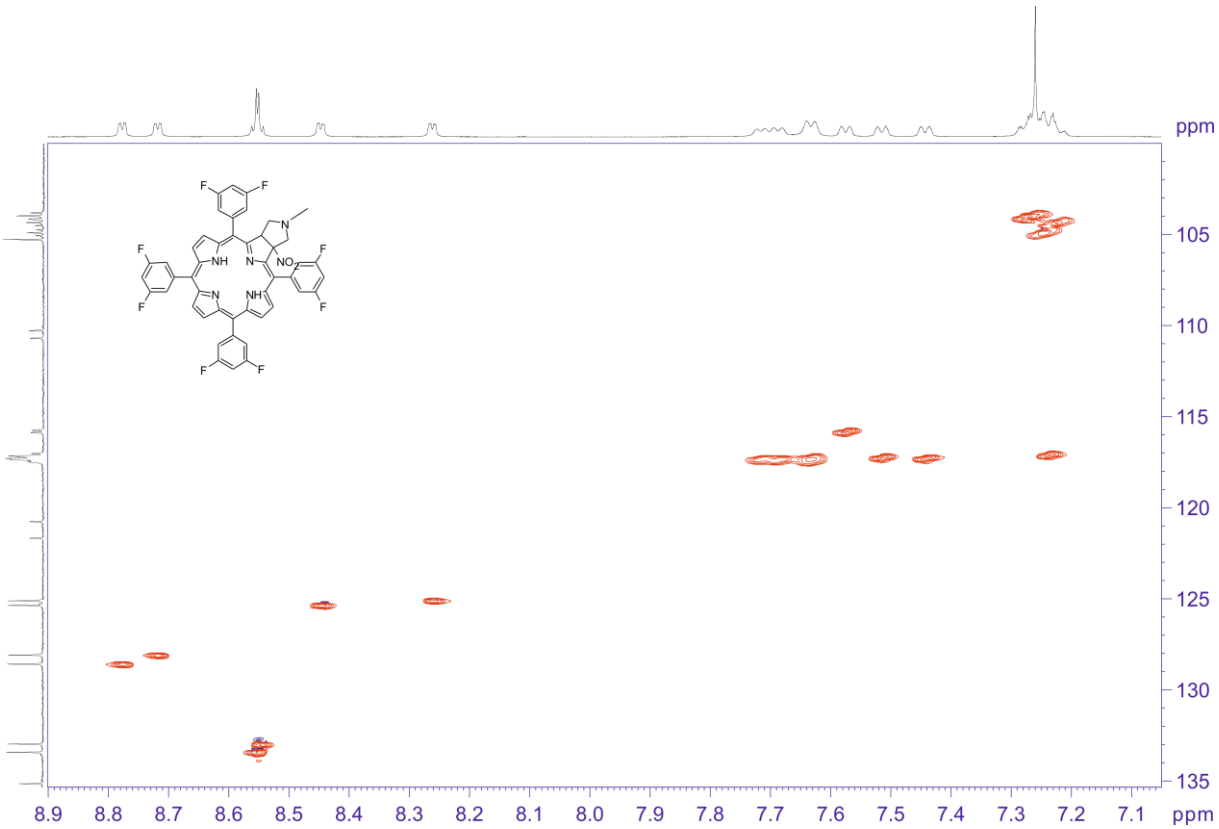

Figure S 46 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **2.** The spectrum obtained at 600 MHz spectrometer.

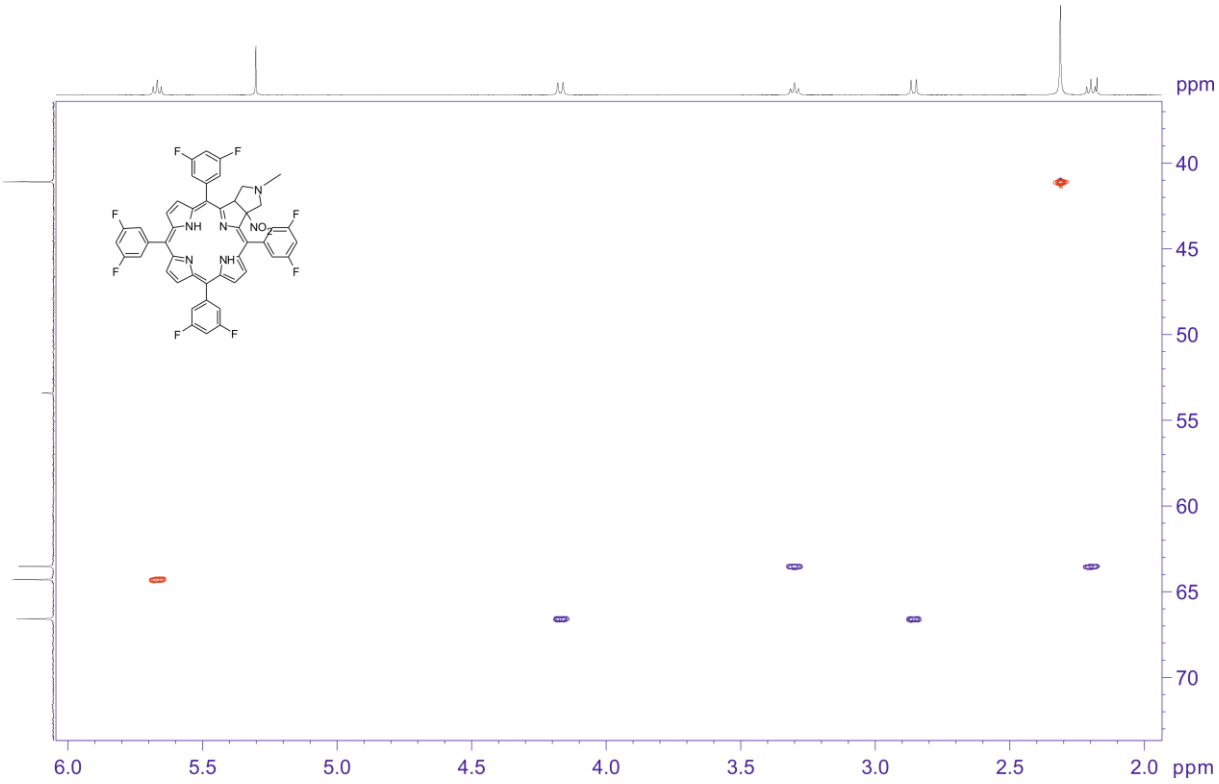

Figure S 47 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **2.** The spectrum obtained at 600 MHz spectrometer.

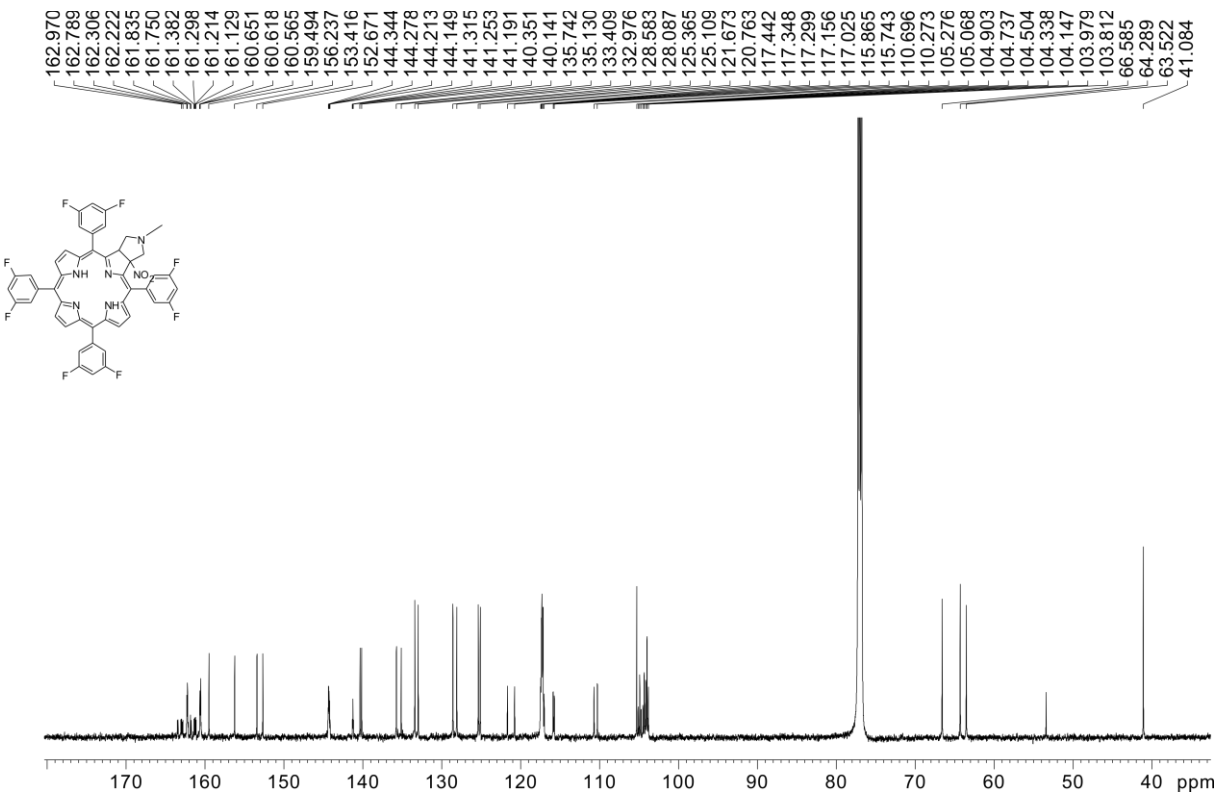

Figure S 48 ^{13}C NMR spectrum in $CDCl_3$ of compound **2** at 600 MHz spectrometer.

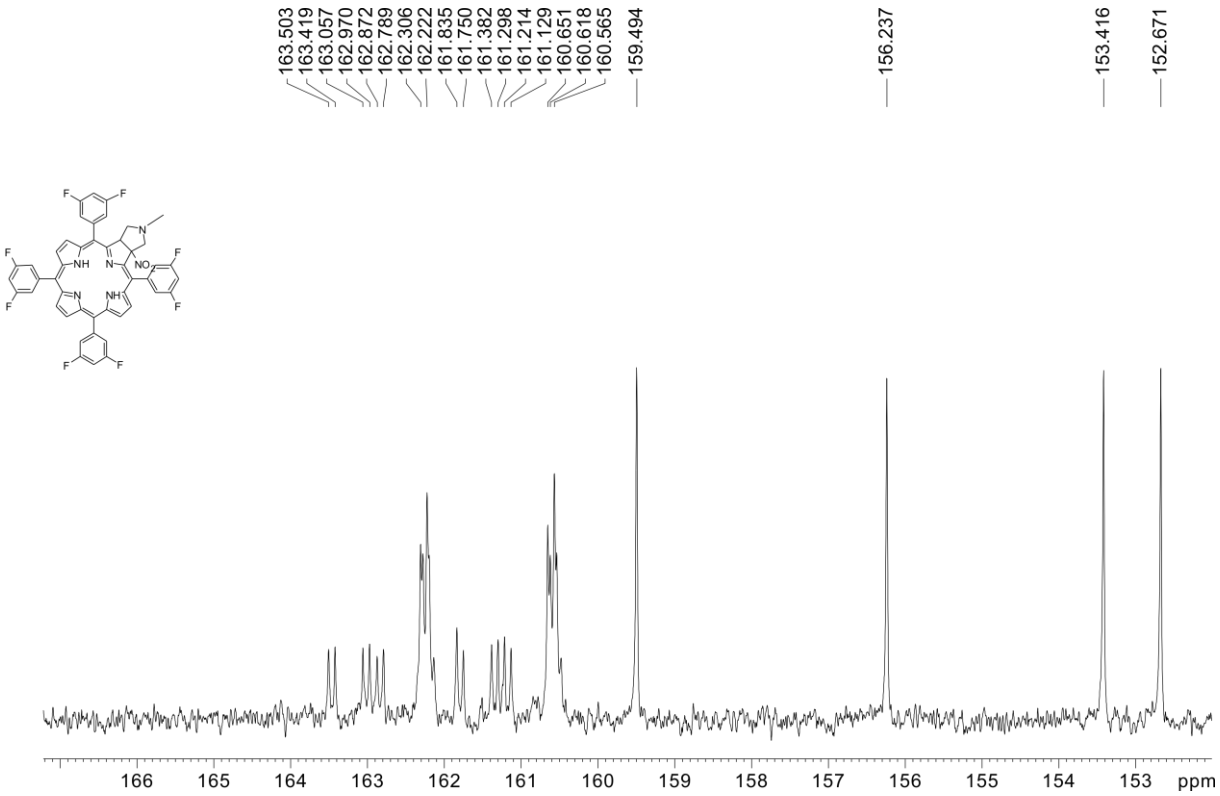

Figure S 49 ^{13}C NMR spectrum in $CDCl_3$ of compound **2** (expansion of 152-166 ppm region) at 600 MHz spectrometer.

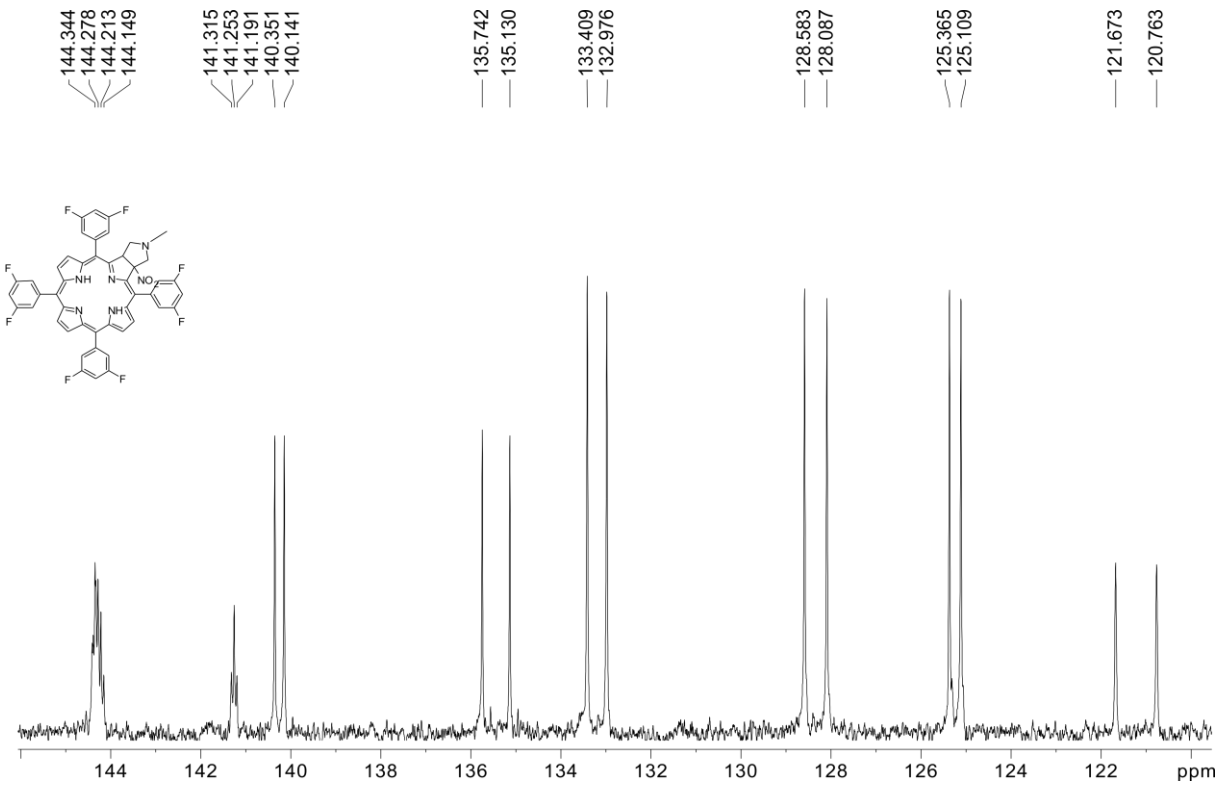

Figure S 50 ^{13}C NMR spectrum in $CDCl_3$ of compound **2** (expansion of 120-146 ppm region) at 600 MHz spectrometer.

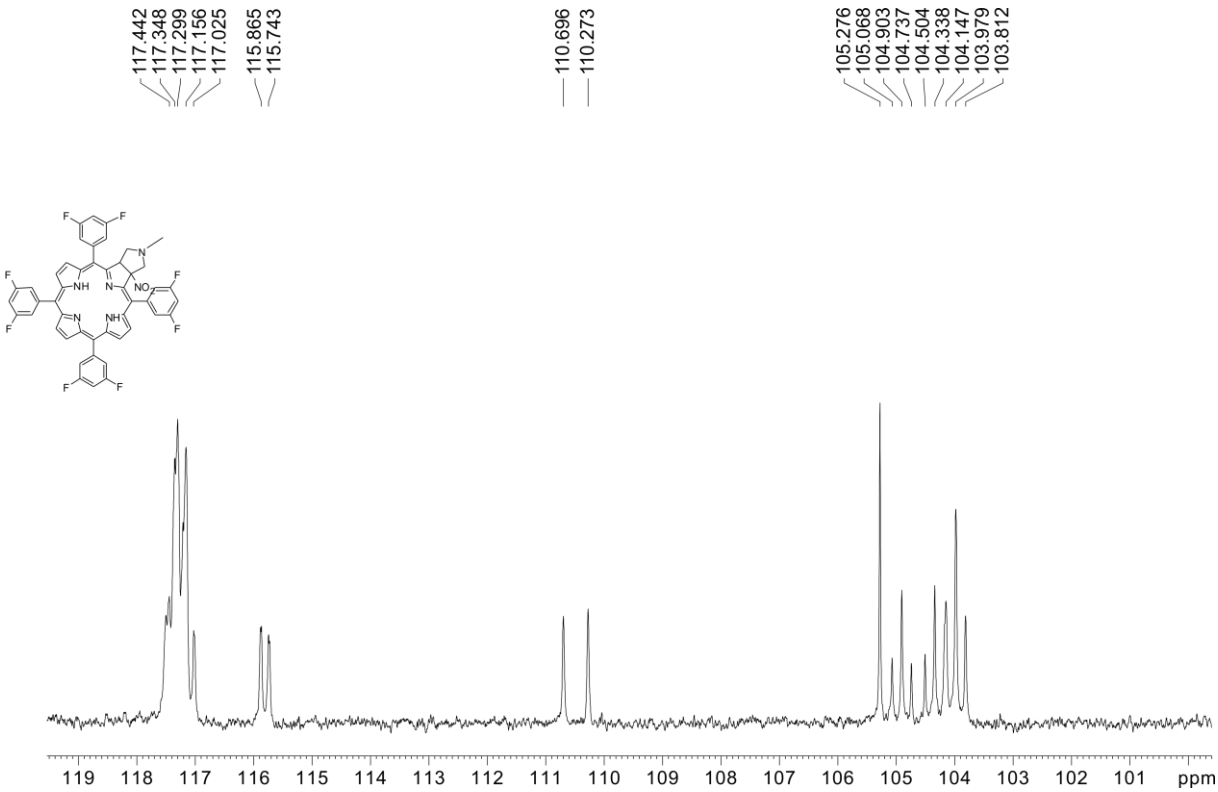

Figure S 51 ^{13}C NMR spectrum in $CDCl_3$ of compound **2** (expansion of 100-119 ppm region) at 600 MHz spectrometer.

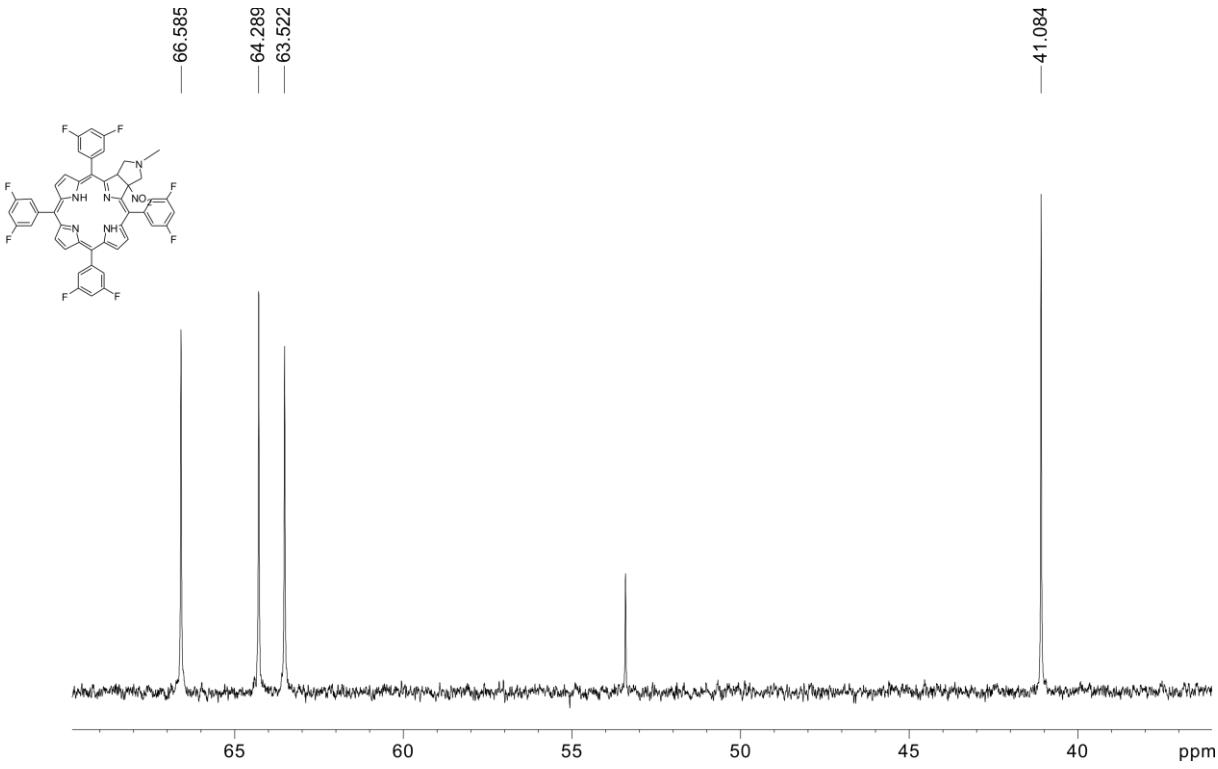

Figure S 52 ^{13}C NMR spectrum in $CDCl_3$ of compound **2** (expansion of 35-70 ppm region) at 600 MHz spectrometer.

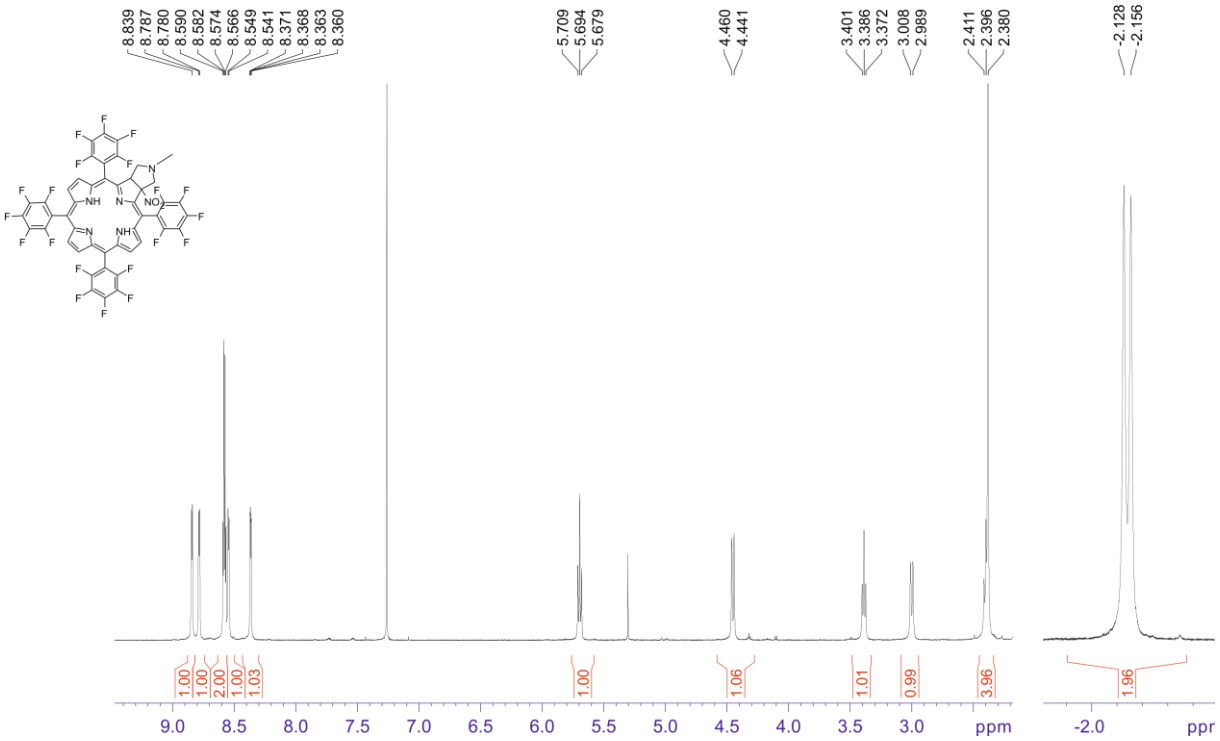

Figure S 53 ^{1}H NMR spectrum in $CDCl_3$ of compound **3** at 600 MHz.

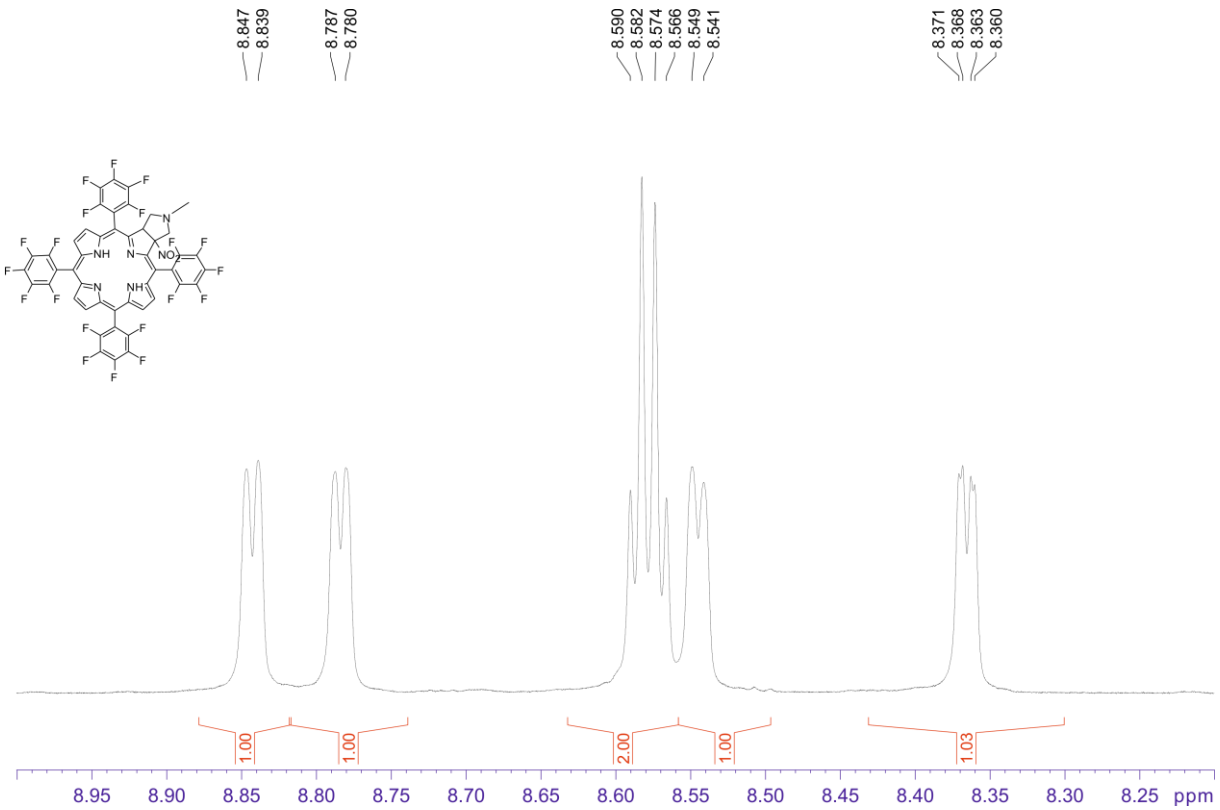

Figure S 54 ^{1}H NMR spectrum in $CDCl_3$ of compound **3** (expansion of 8.10-9.00 ppm region) at 600 MHz.

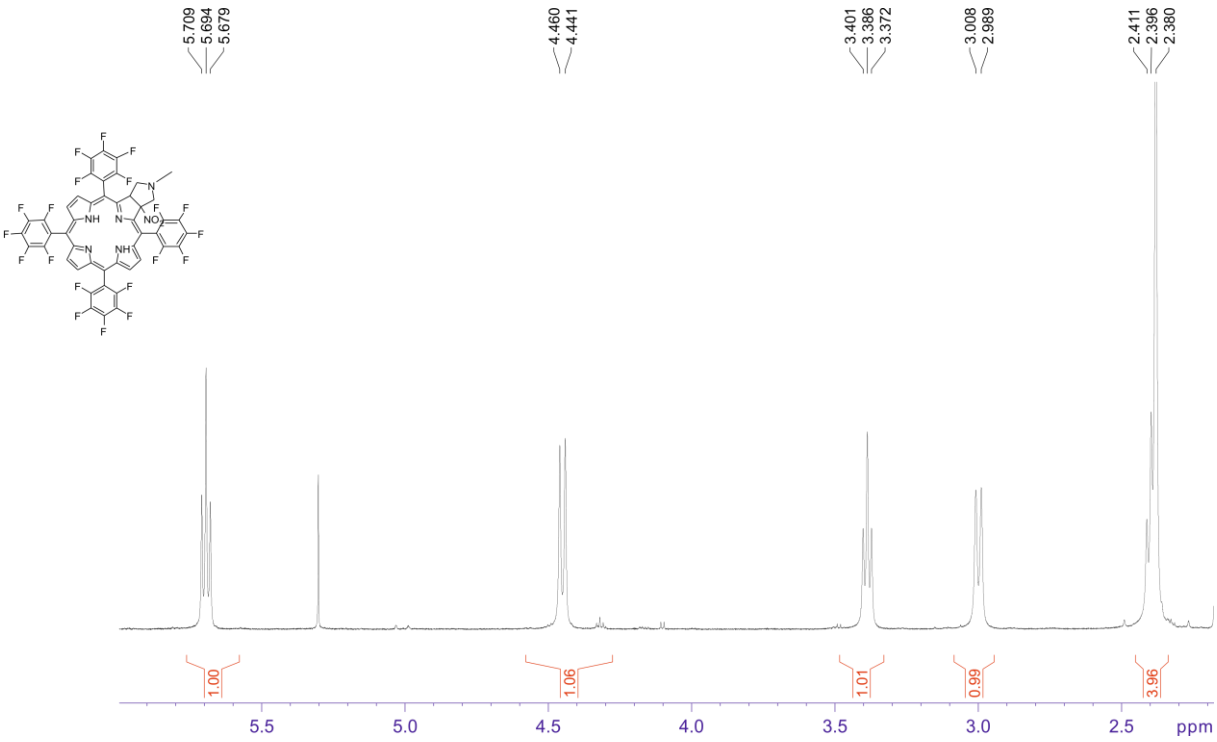

Figure S 55 ^{1}H NMR spectrum in $CDCl_3$ of compound **3** (expansion of 2.0-6.0 ppm region) at 600 MHz.

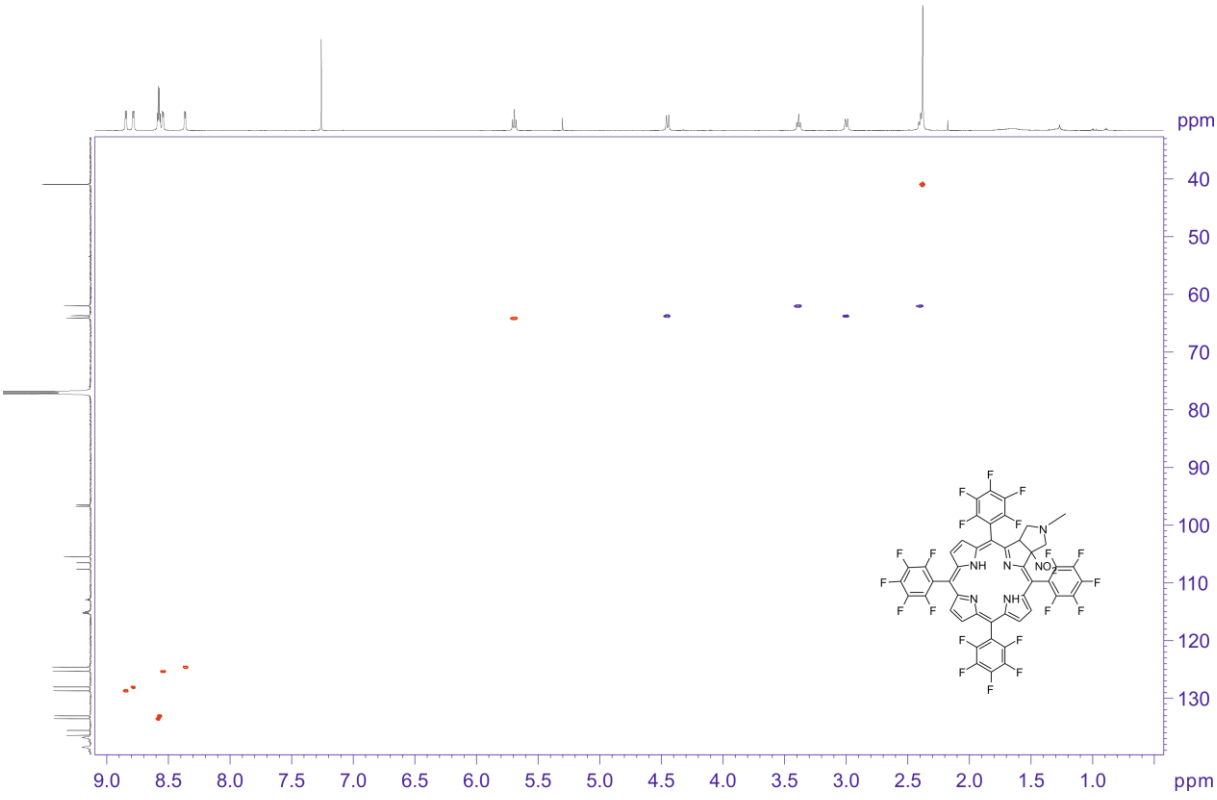

Figure S 56 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **3.** The spectrum obtained at 600 MHz spectrometer.

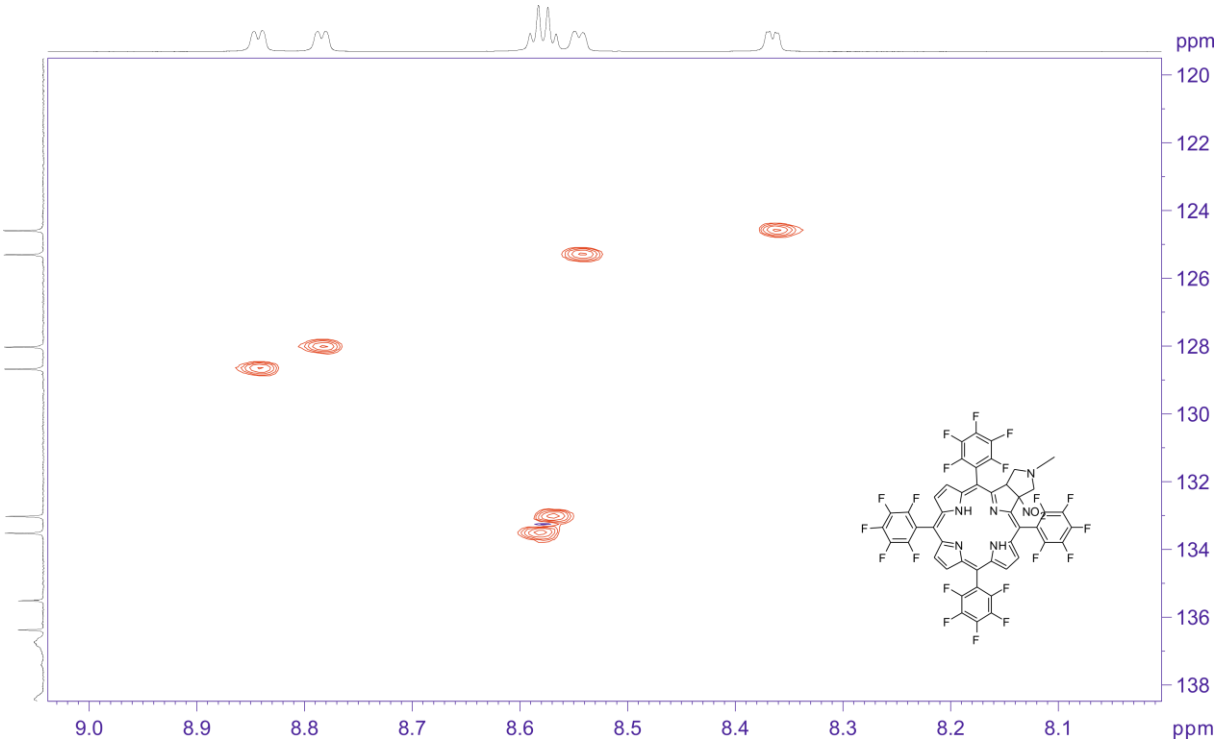

Figure S 57 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **3.** The spectrum obtained at 600 MHz spectrometer.

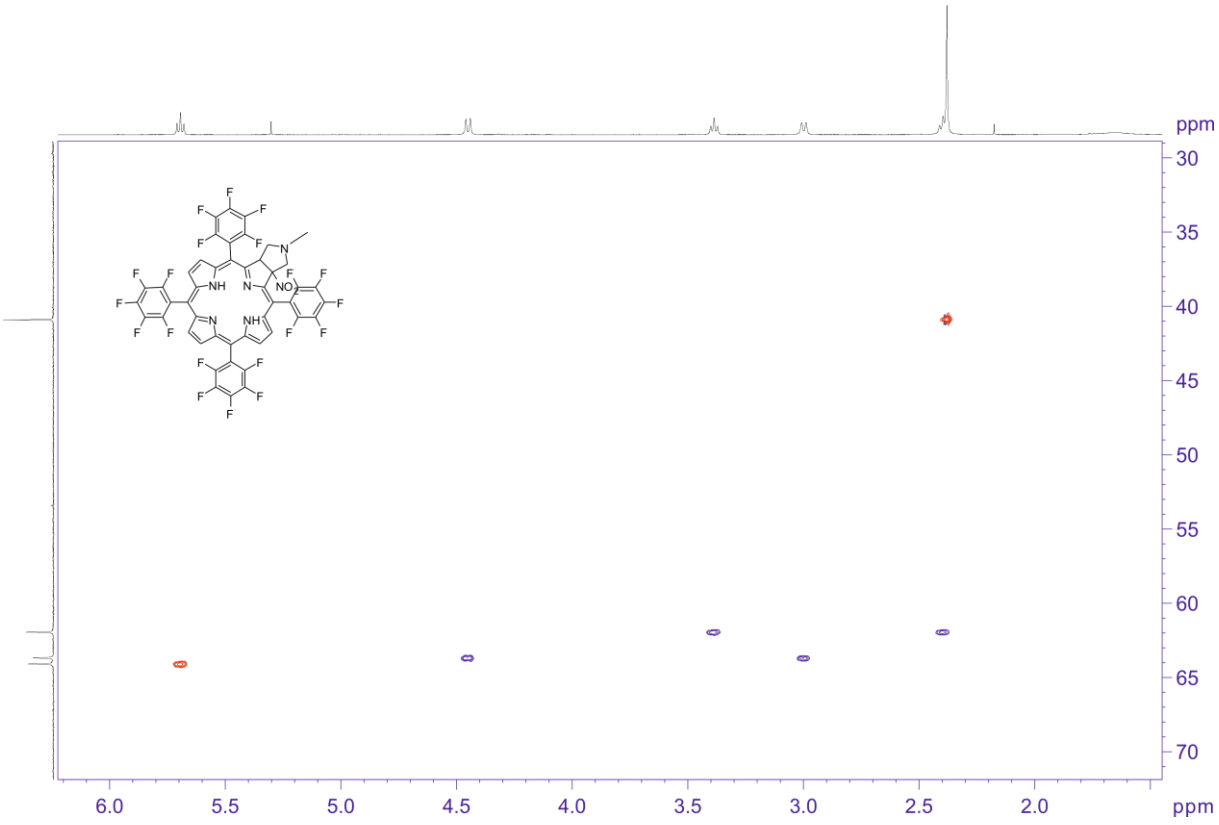

Figure S 58 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **3.** The spectrum obtained at 600 MHz spectrometer.

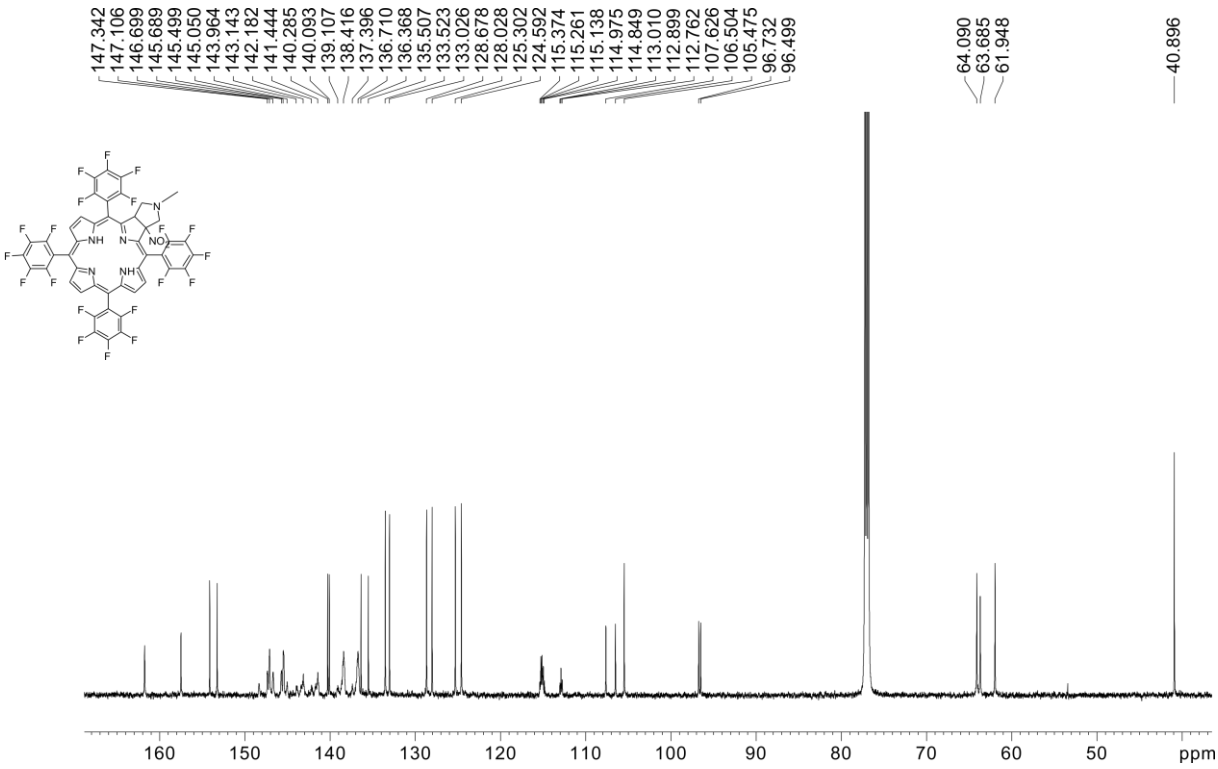

Figure S 59 ^{13}C NMR spectrum in $CDCl_3$ of compound **3** at 600 MHz spectrometer.

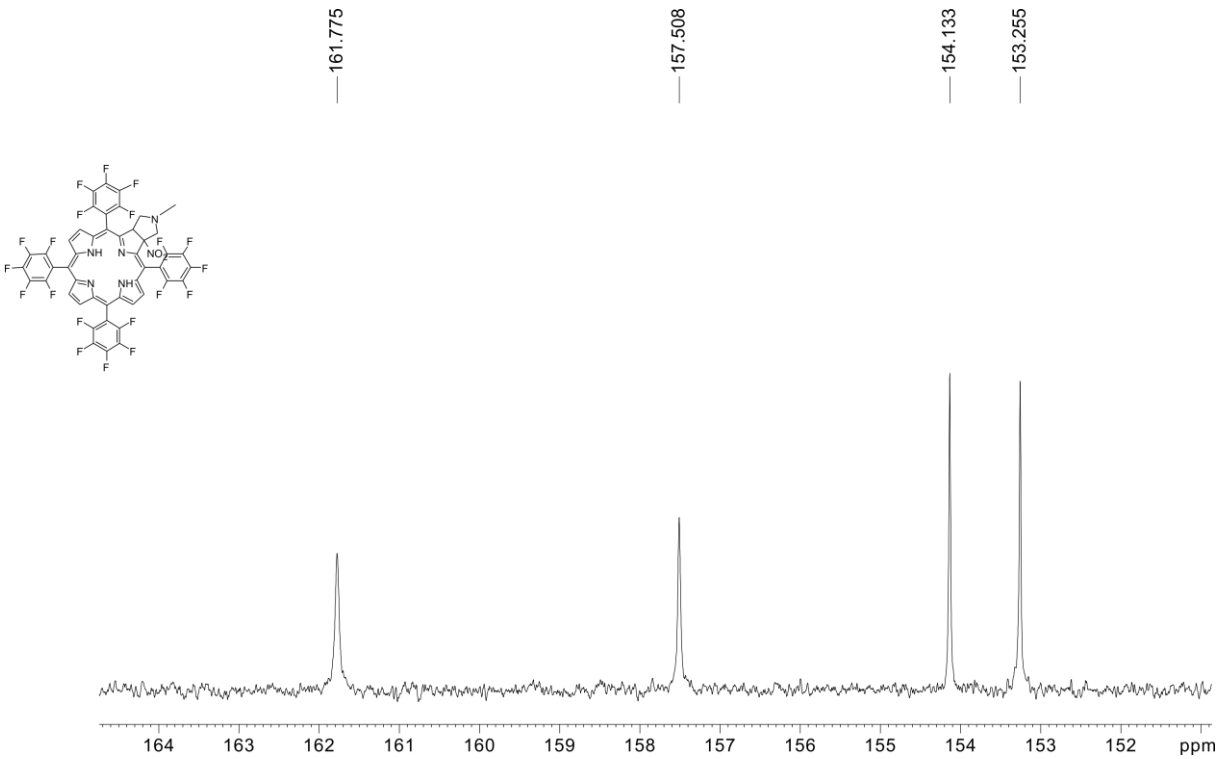

Figure S 60 ^{13}C NMR spectrum in $CDCl_3$ of compound **3** (expansion of 151-165 ppm region) at 600 MHz spectrometer.

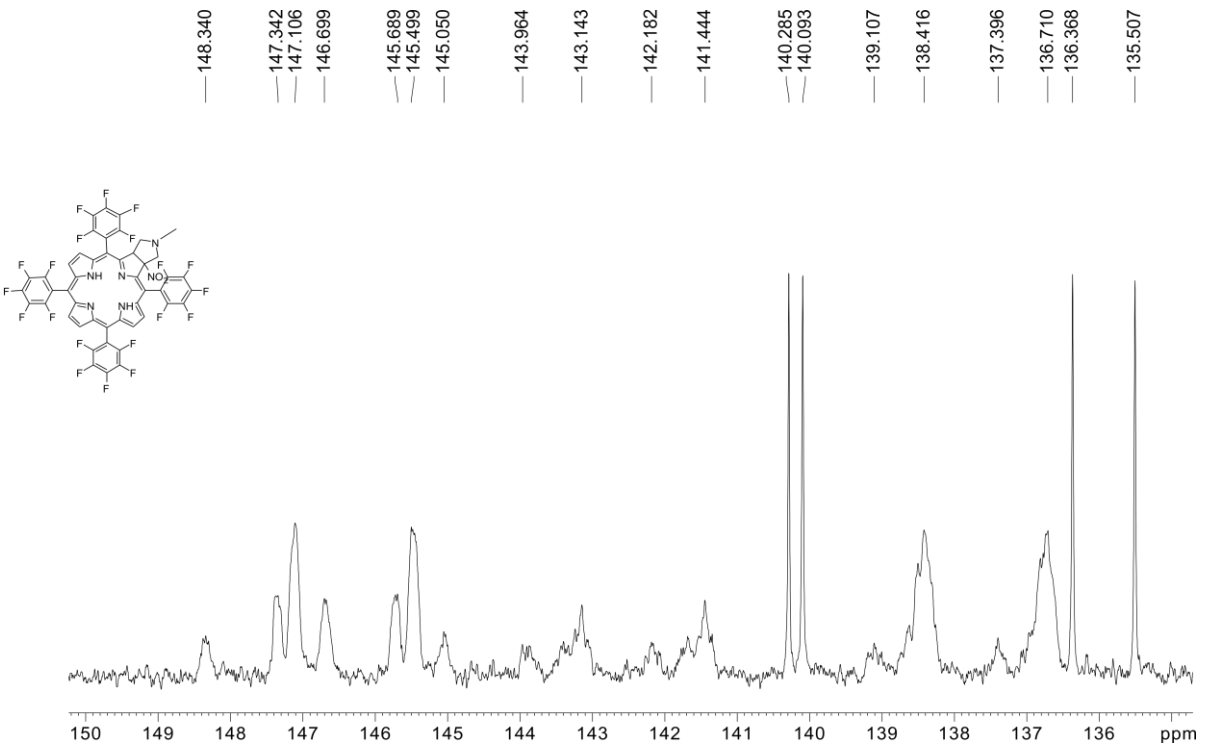

Figure S 61 ^{13}C NMR spectrum in $CDCl_3$ of compound **3** (expansion of 135-150 ppm region) at 600 MHz spectrometer.

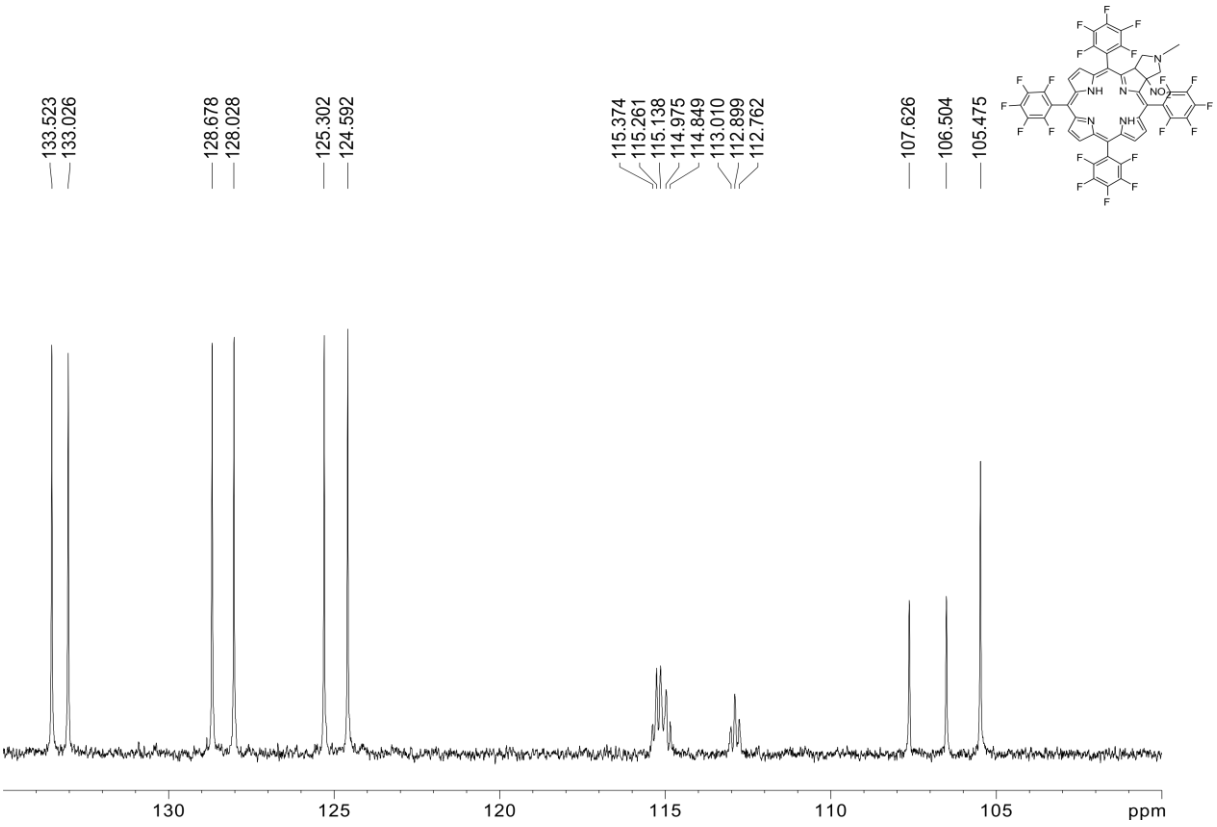

Figure S 62 ^{13}C NMR spectrum in $CDCl_3$ of compound **3** (expansion of 100-135 ppm region) at 600 MHz spectrometer.

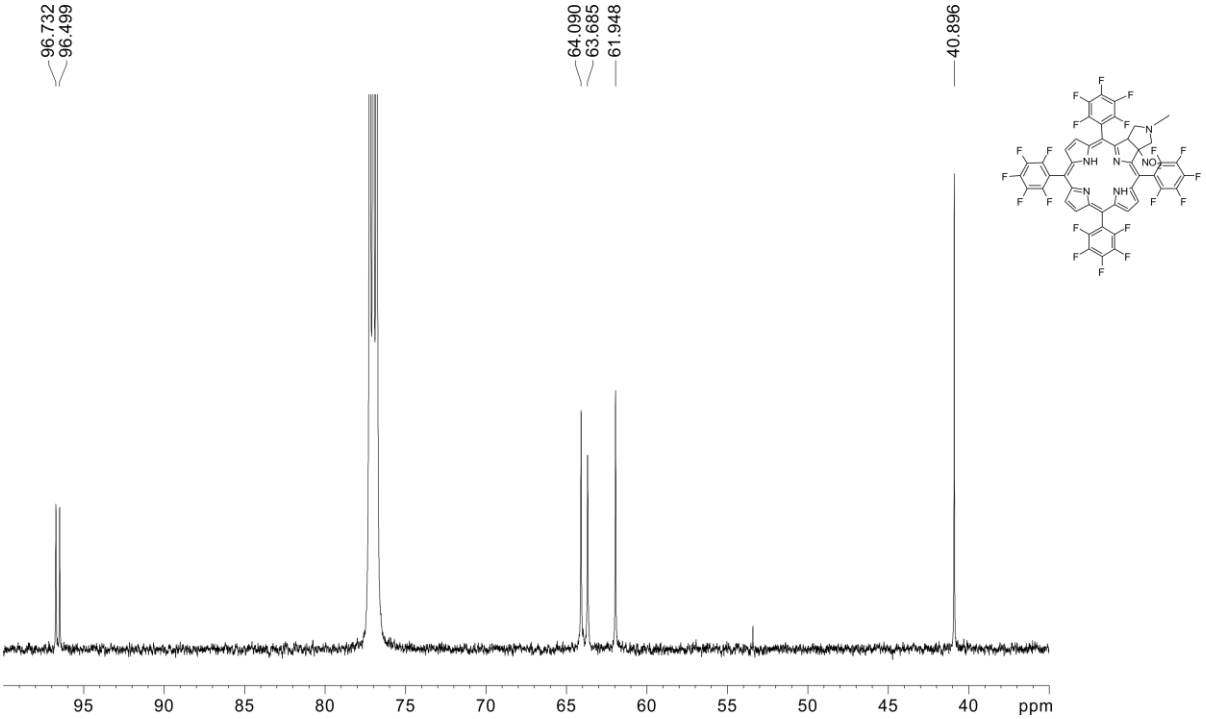

Figure S 63 ^{13}C NMR spectrum in $CDCl_3$ of compound **3** (expansion of 35-100 ppm region) at 600 MHz spectrometer.

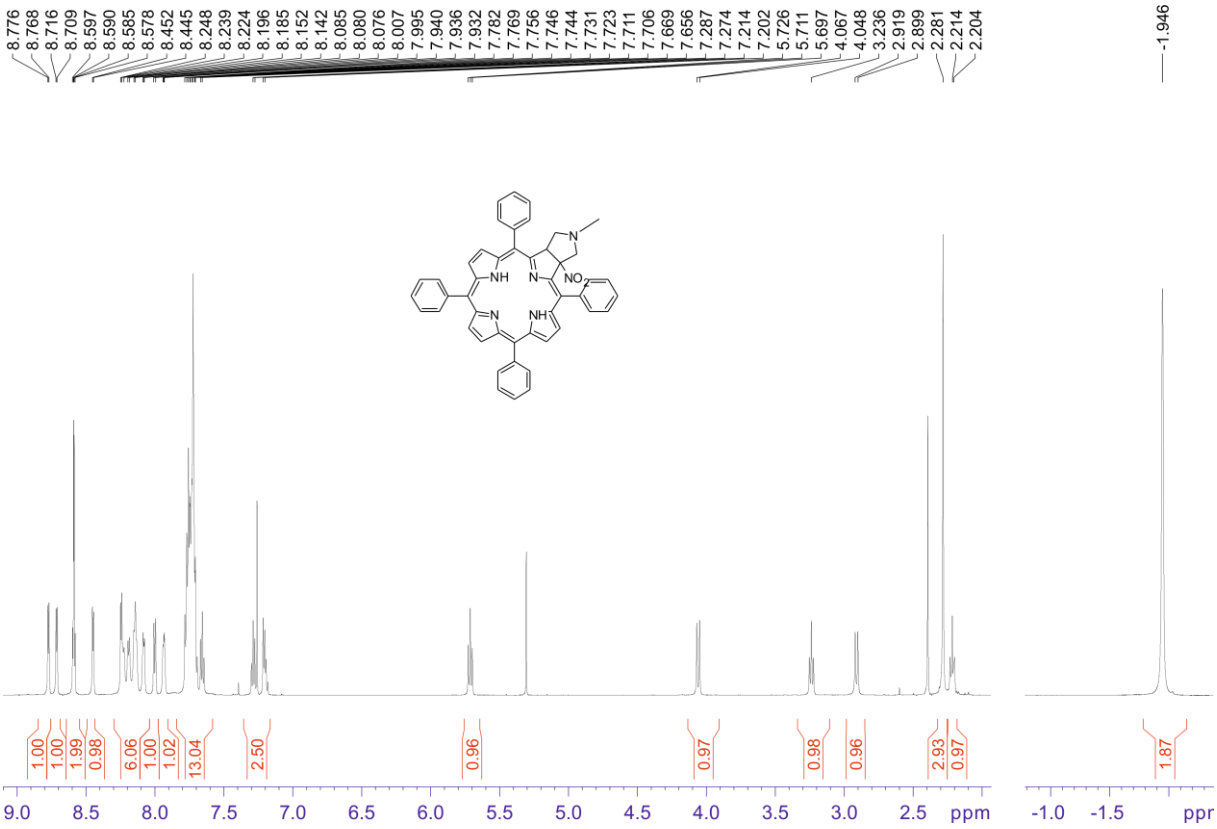

Figure S 64 ^{1}H NMR spectrum in $CDCl_3$ of compound **4** at 600 MHz.

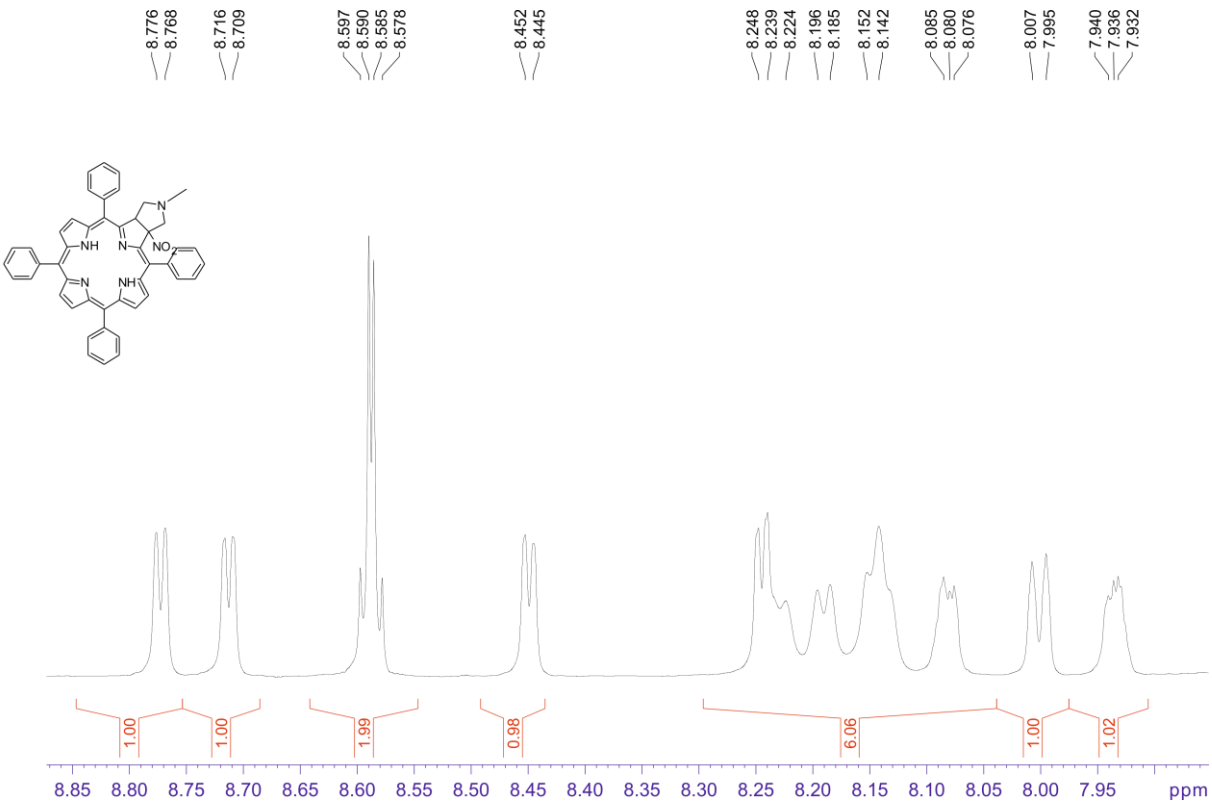

Figure S 65 ^{1}H NMR spectrum in $CDCl_3$ of compound **4** (expansion of 7.90-8.85 ppm region) at 600 MHz.

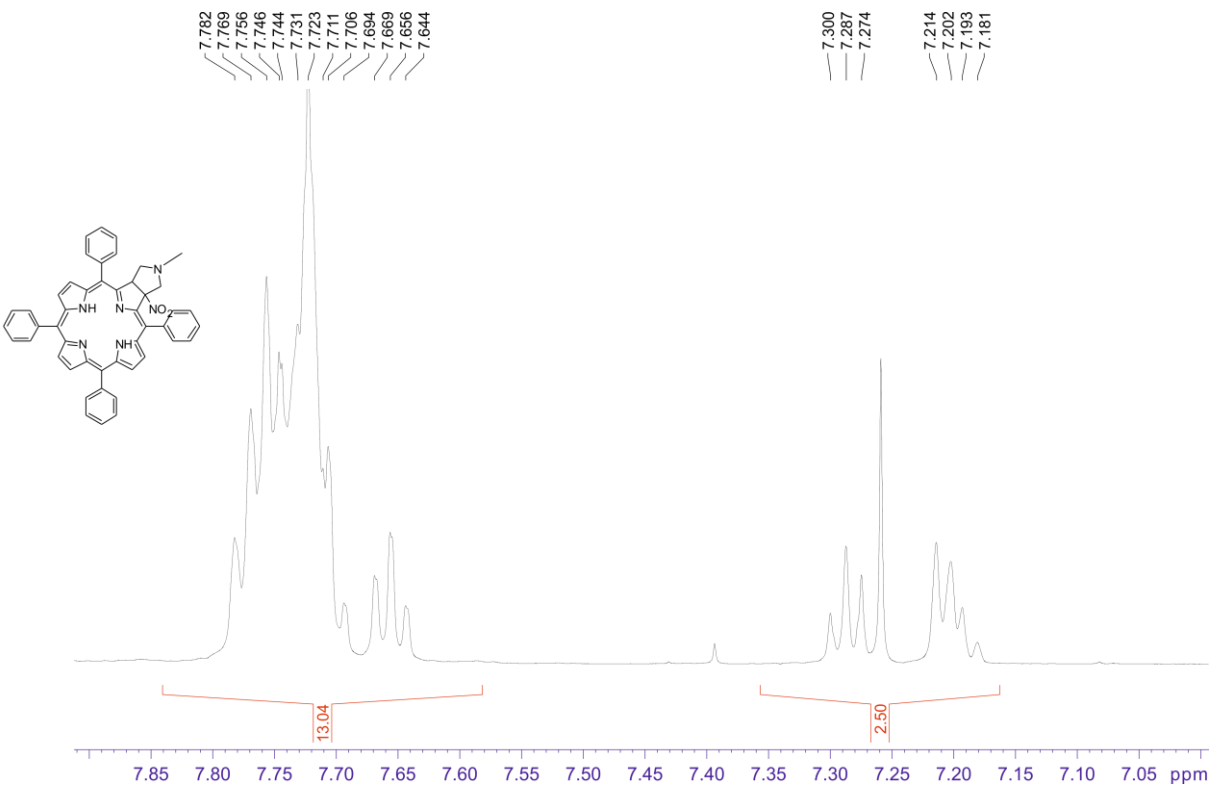

Figure S 66 ^{1}H NMR spectrum in $CDCl_3$ of compound **4** (expansion of 7.0-7.9 ppm region) at 600 MHz.

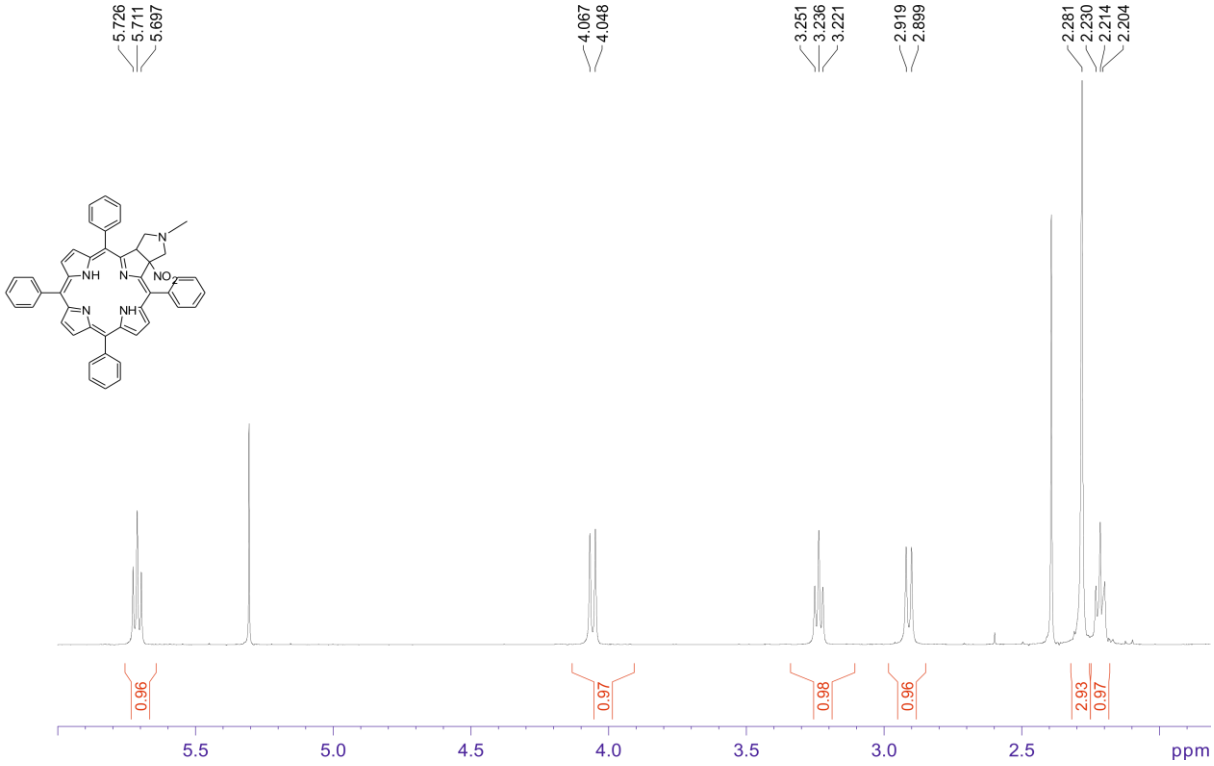

Figure S 67 ^{1}H NMR spectrum in $CDCl_3$ of compound **4** (expansion of 2.0-6.0 ppm region) at 600 MHz.

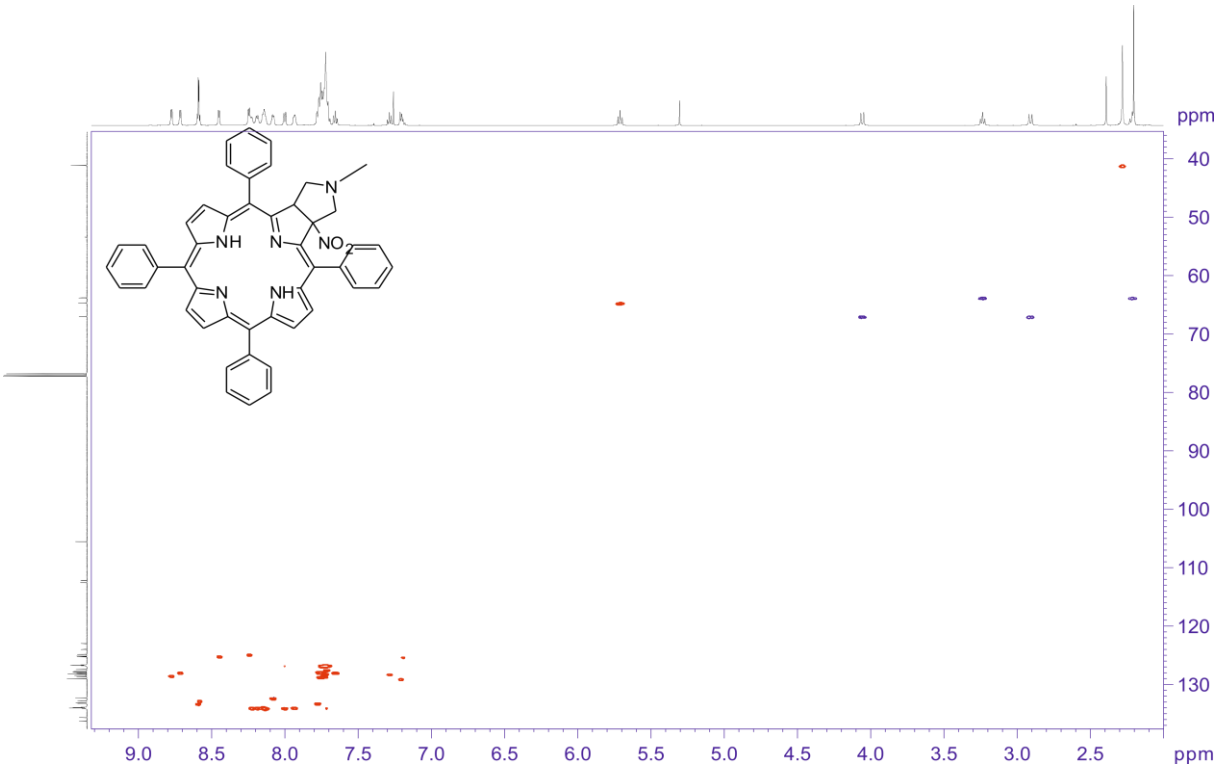

Figure S 68 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **4.** The spectrum obtained at 600 MHz spectrometer.

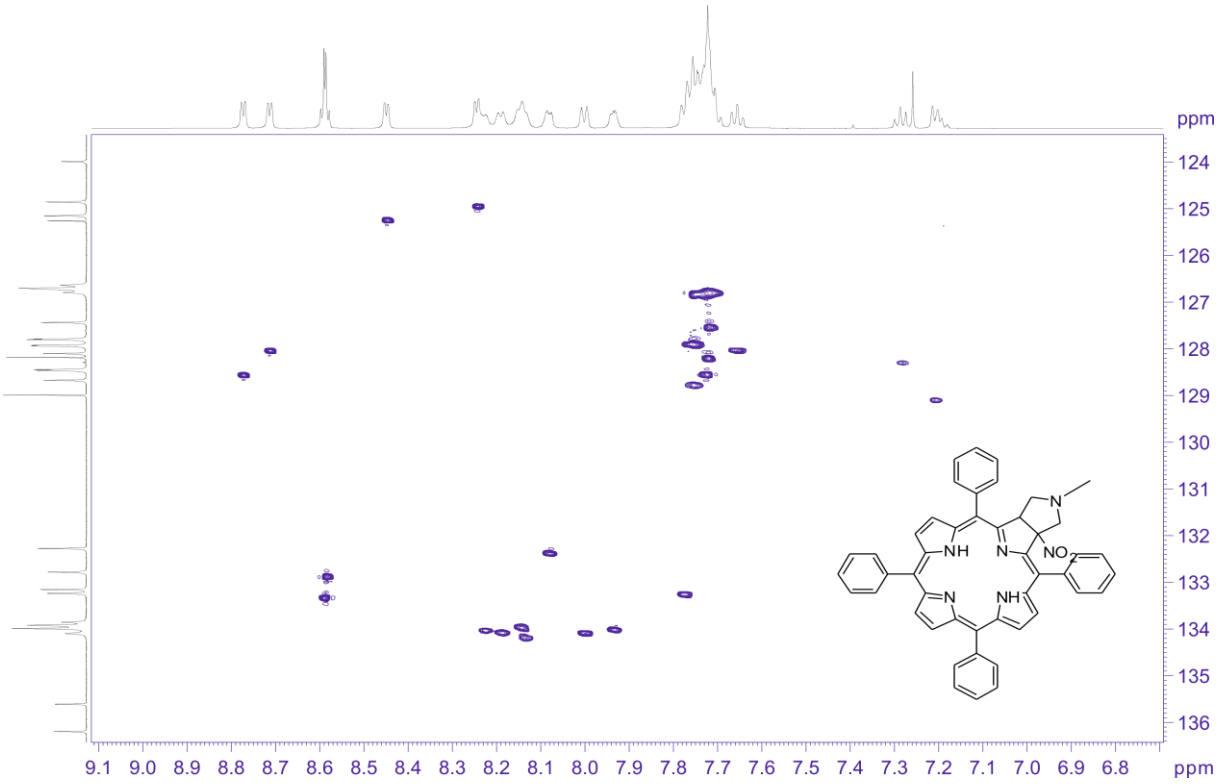

Figure S 69 ^{1}H-^{13}C HSQC NMR spectrum in $CDCl_3$ of compound **4.** The spectrum obtained at 600 MHz spectrometer.

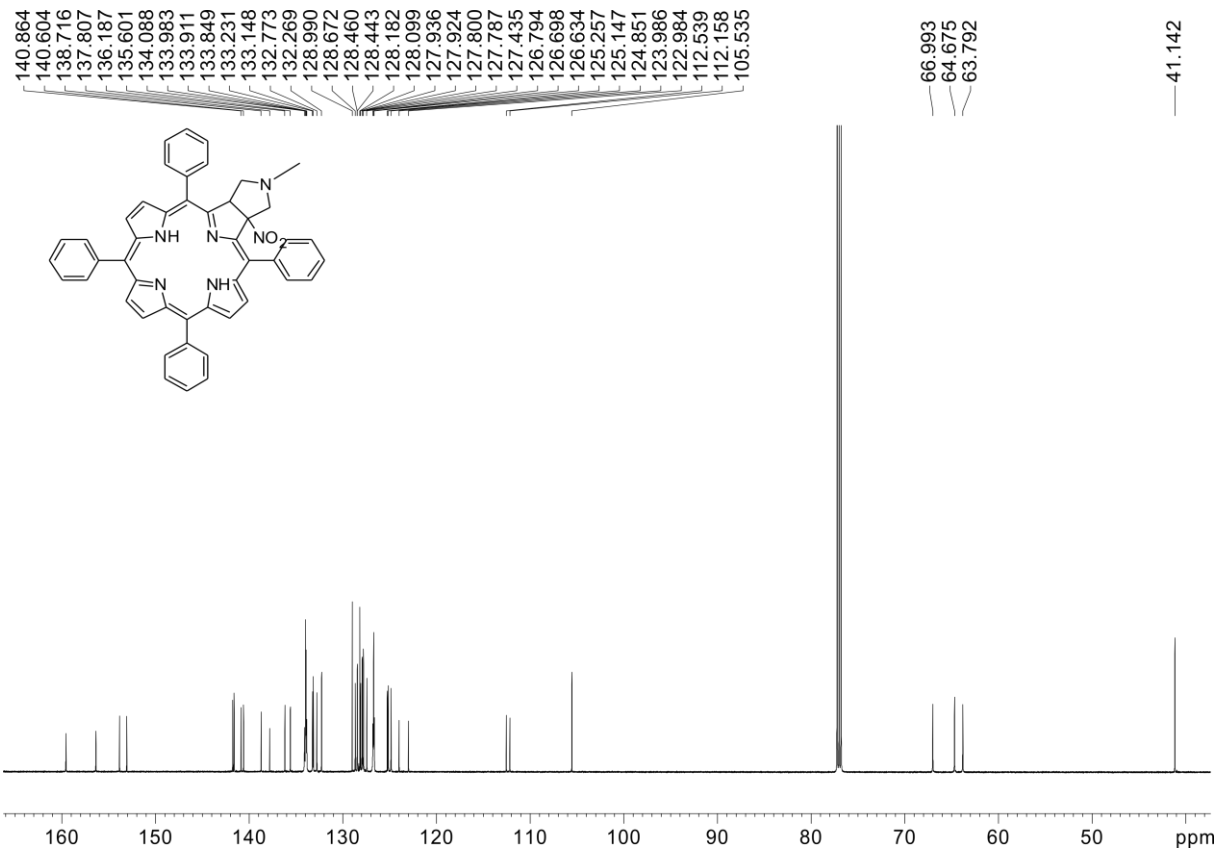

Figure S 70 ^{13}C NMR spectrum in $CDCl_3$ of compound **4** at 600 MHz spectrometer.

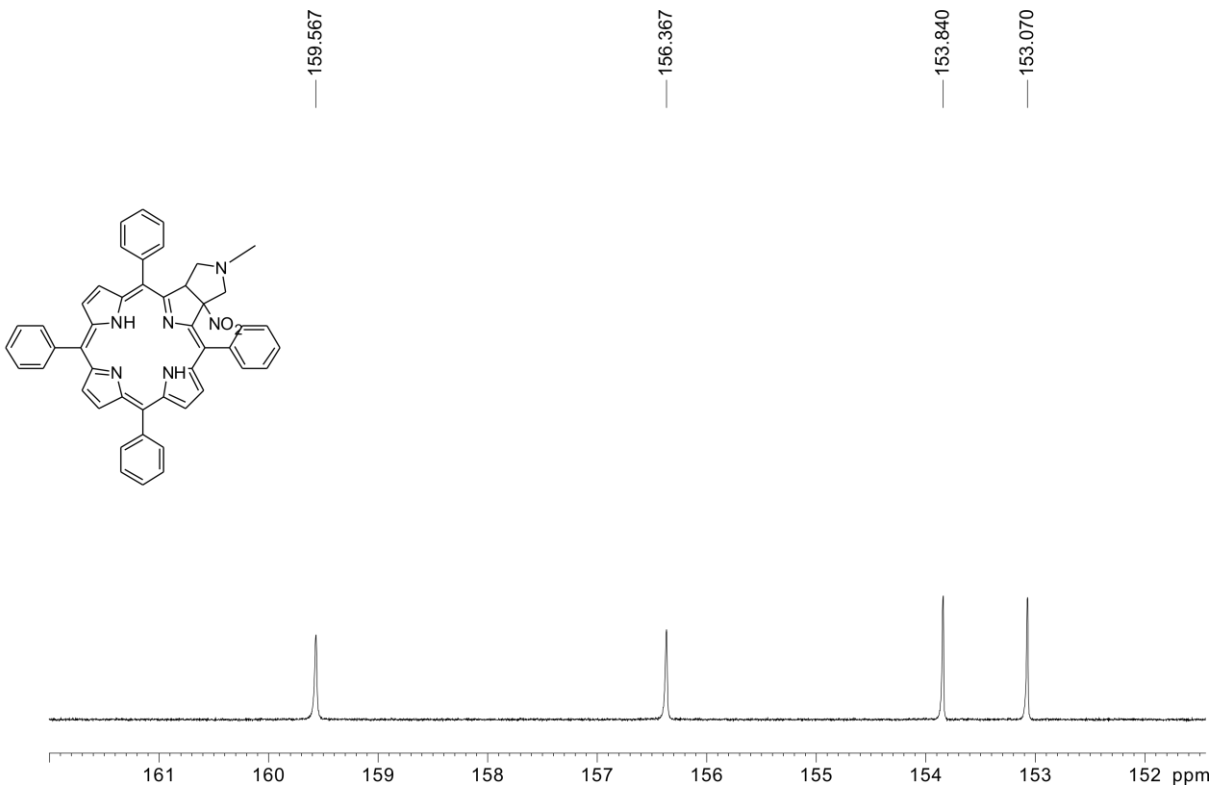

Figure S 71 ^{13}C NMR spectrum in $CDCl_3$ of compound **4** (expansion of 152-162 ppm region) at 600 MHz spectrometer.

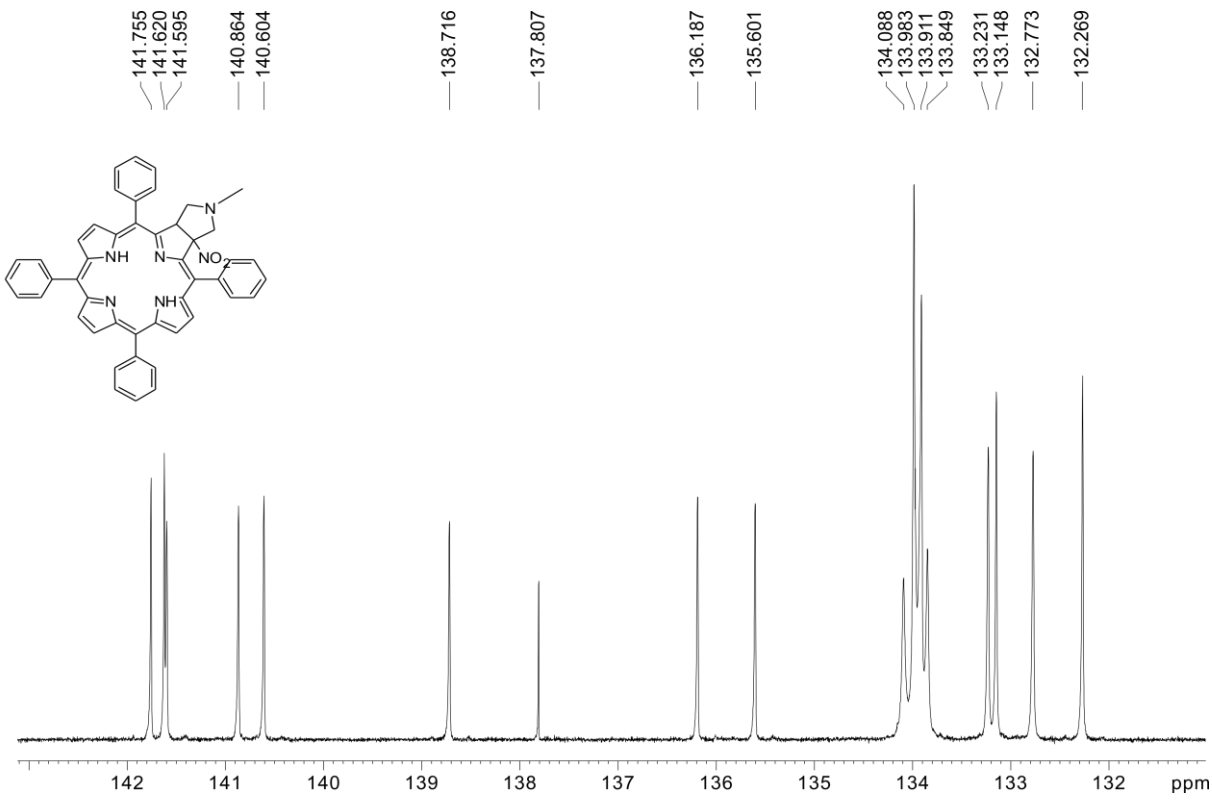

Figure S 72 ^{13}C NMR spectrum in $CDCl_3$ of compound **4** (expansion of 131-143 ppm region) at 600 MHz spectrometer.

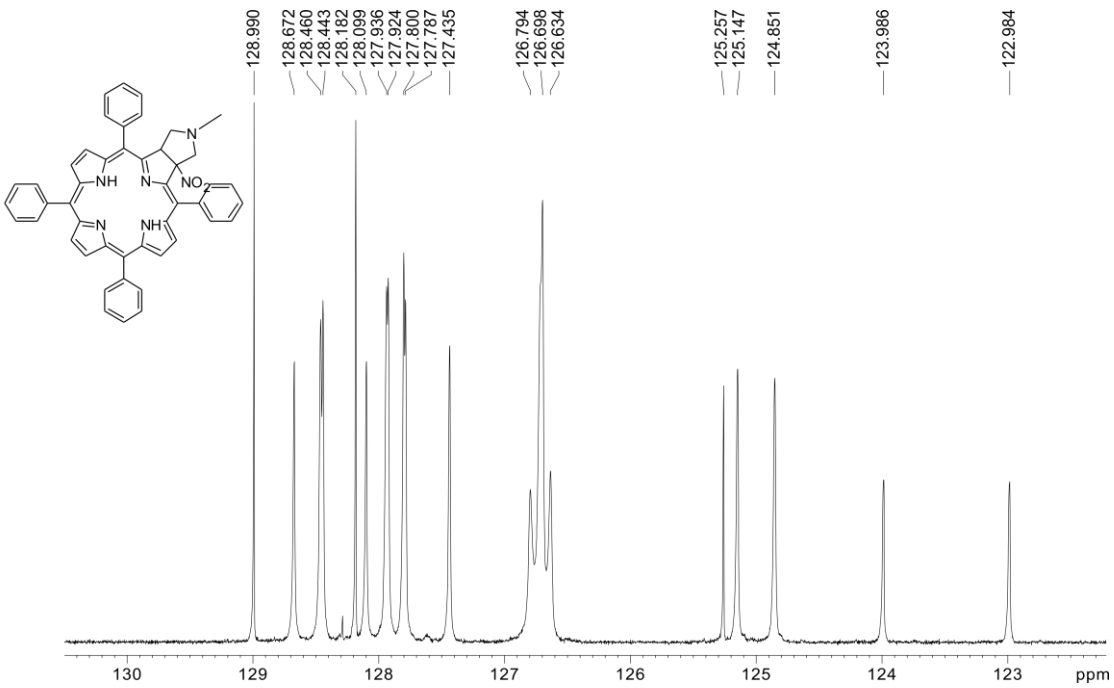

Figure S 73 ^{13}C NMR spectrum in $CDCl_3$ of compound **4** (expansion of 121-130 ppm region) at 600 MHz spectrometer.

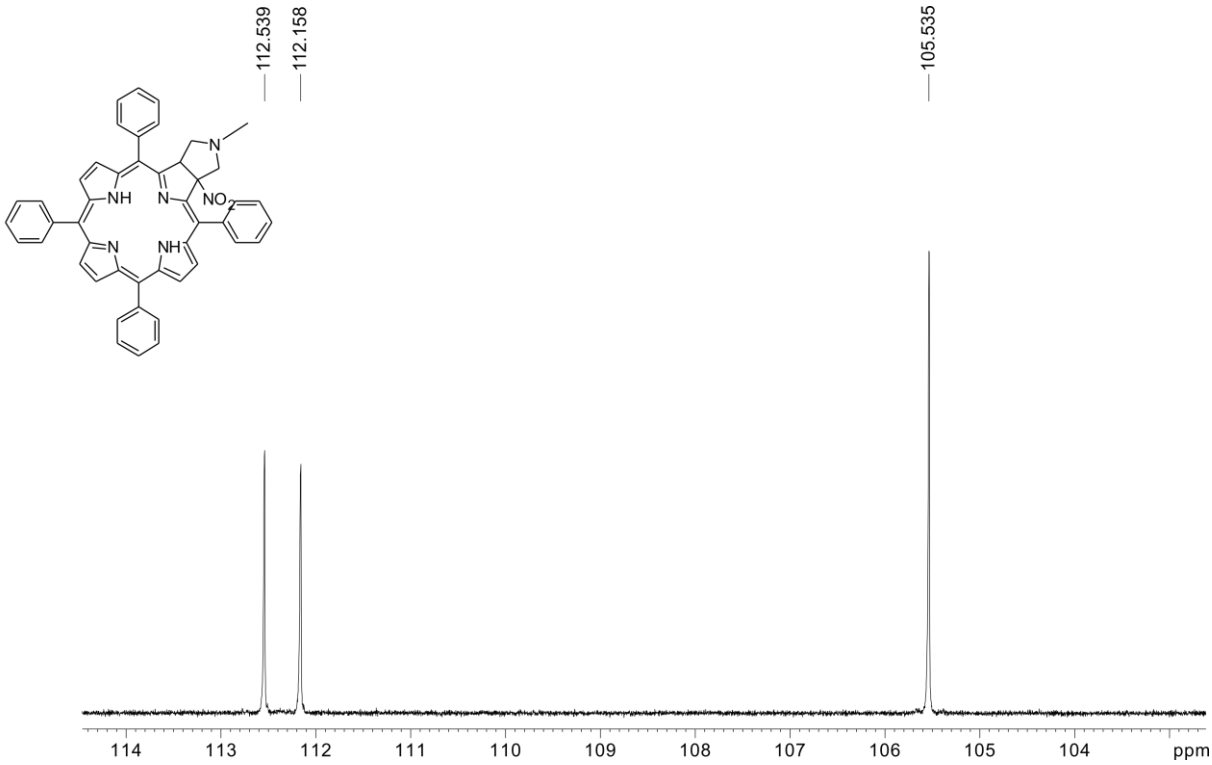

Figure S 74 ^{13}C NMR spectrum in $CDCl_3$ of compound **4** (expansion of 103-114 ppm region) at 600 MHz spectrometer.

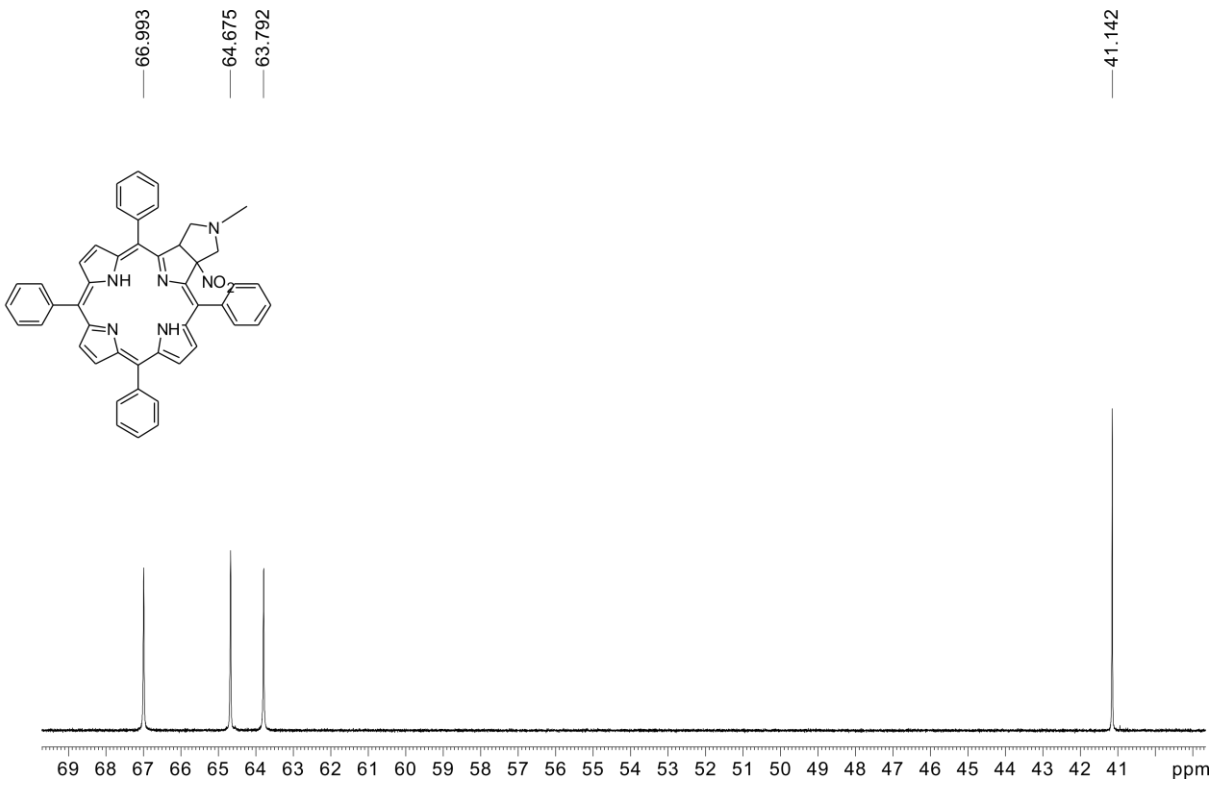

Figure S 75 ^{13}C NMR spectrum in $CDCl_3$ of compound **4** (expansion of 40-69 ppm region) at 600 MHz spectrometer.

Assignments of chlorin 2

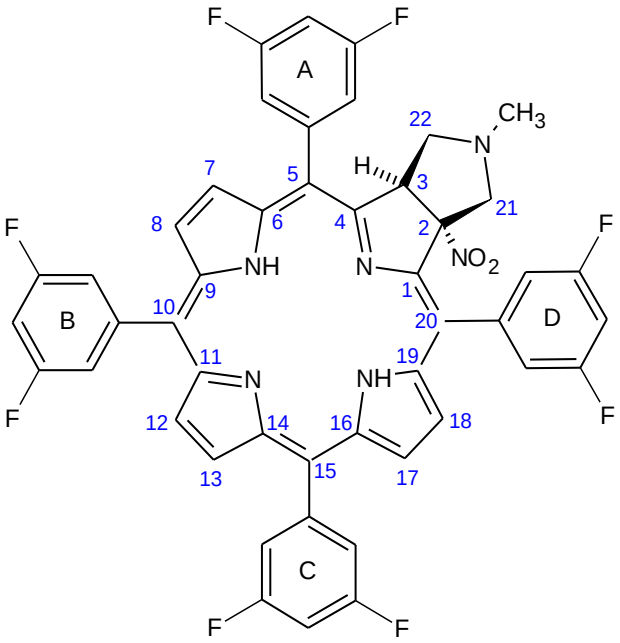

Figure S 76 Structure of chlorin **2** with labeling and numeration of atoms

In this case it impossible to use ^{19}F-^{1}H correlation based on dipolar coupling. Instead of that we have decided to use ^{19}F decoupled ^{1}H-^{1}H ROESY experiment. In such case after finding H_3, H_{21}, $H_{21'}$ and H_{22}, $H_{22'}$ it was possible to assign protons in β-pyrrolic positions. Proton in *o*-H_{Aup} position was assigned by looking for correlation with H_{22} and $H_{22'}$ protons in ^{1}H-^{1}H ROESY spectrum. Having in mind *o*-H_{Aup} correlation it was possible to assign H_7 proton in β-pyrrolic positions. In the analogues way we assign H_{18} using correlation with o-H_{Dup}. After this we found correlation between H_{18} and *o*-H_{Dup}. H_8 and H_{17} were assigned using ^{1}H-^{1}H COSY and theirs correlation with previous assigned H_7 and H_{18}. It were impossible to stereospecific assign of up and down *o*-proton in B and C position. Both of up/down protons were assigned by looking for correlation with H_8 or H_{17} for C and B rings respectively in ^{1}H-^{1}H ROESY spectrum. H_{12} and H_{13} signals were find by looking for correlation with *o*-protons of C or B ring. ^{19}F signals were assigned based on ^{19}F-^{1}H HETCOR (scalar based) correlation. In addition using this experiment protons in *para* position of phenyl rings were assigned. In this case we did not observe unexpected correlation on the ^{19}F-^{1}H HETCOR experiment. It is well understandable, when we considered the closest distance (more than 4A) between ^{19}F in *meta* position of phenyl ring and β-pyrrolic protons.

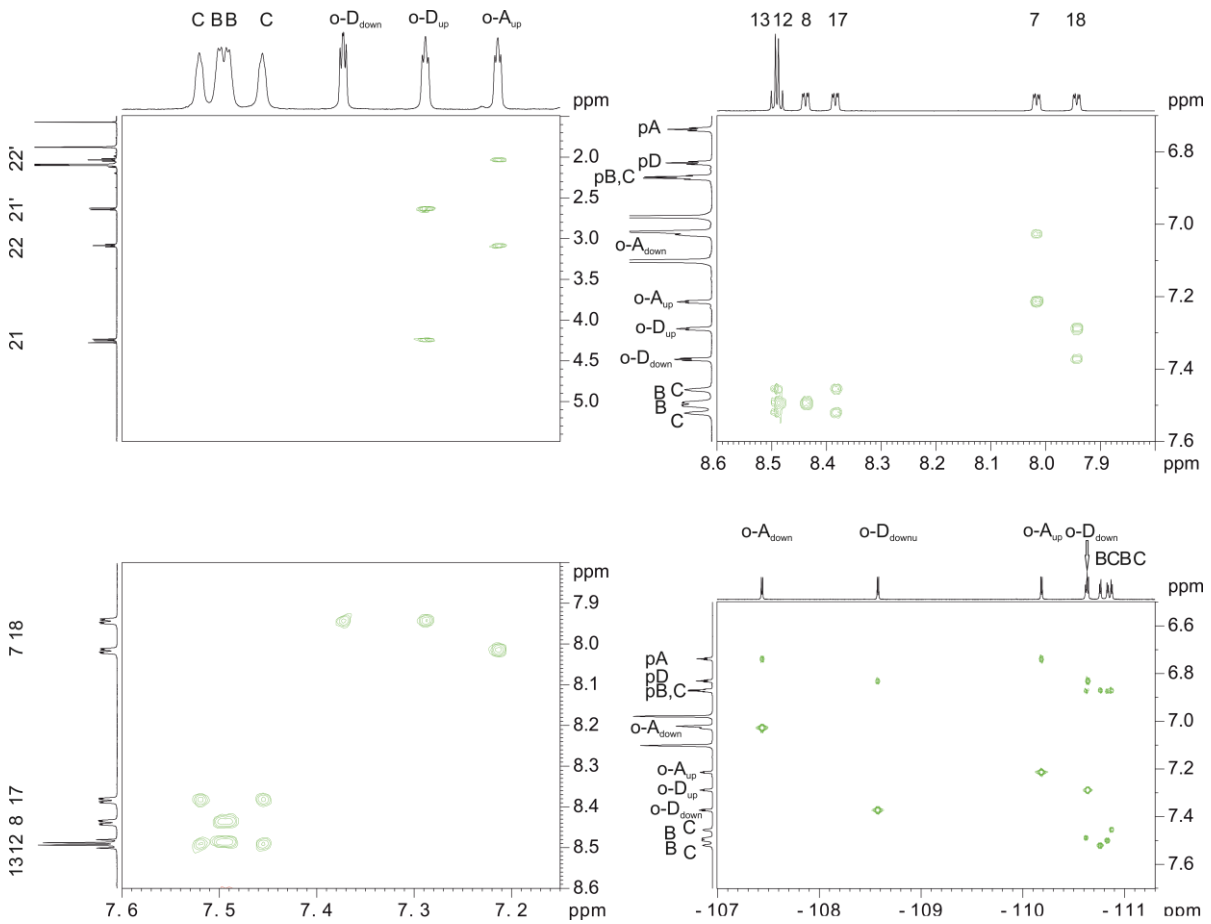

Figure S 77 a, b, c) ^{19}F decoupled ^{1}H-^{1}H ROESY (dipolar based) b) ^{1}H-^{19}F HETCOR (scalar based) for chlorin **2.** The spectra obtained at 600 MHz spectrometer.

Assignments of chlorin 3

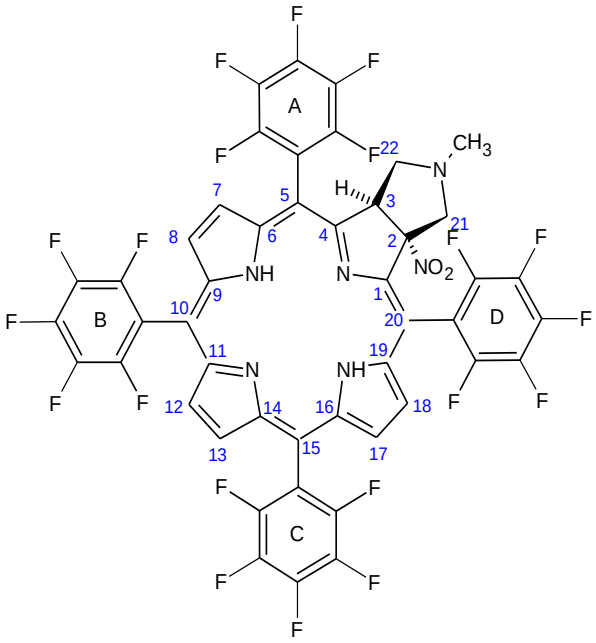

Figure S 78 Structure of chlorin **3** with labeling and numeration of atoms

Because *ortho*, *meta*, *para* fluorine atoms in the *meso*-perfluorinated phenyl ring are well resolved (-136 to -138 ppm, -156 to -162 ppm and -148 to 151 ppm for *o*-, *m*-, *p*- respectively) it is easy to find them. Having in mind characteristic ^{19}F chemical shifts it is easy to assign this compound in similar manner like chlorin **1** by finding correlation between protons in β-position and *o*-fluorine atoms of perfluorinated phenyl ring. *m*- and *p*- fluorine atoms were assigned using ^{19}F-^{19}F COSY correlation.

HRMS analysis

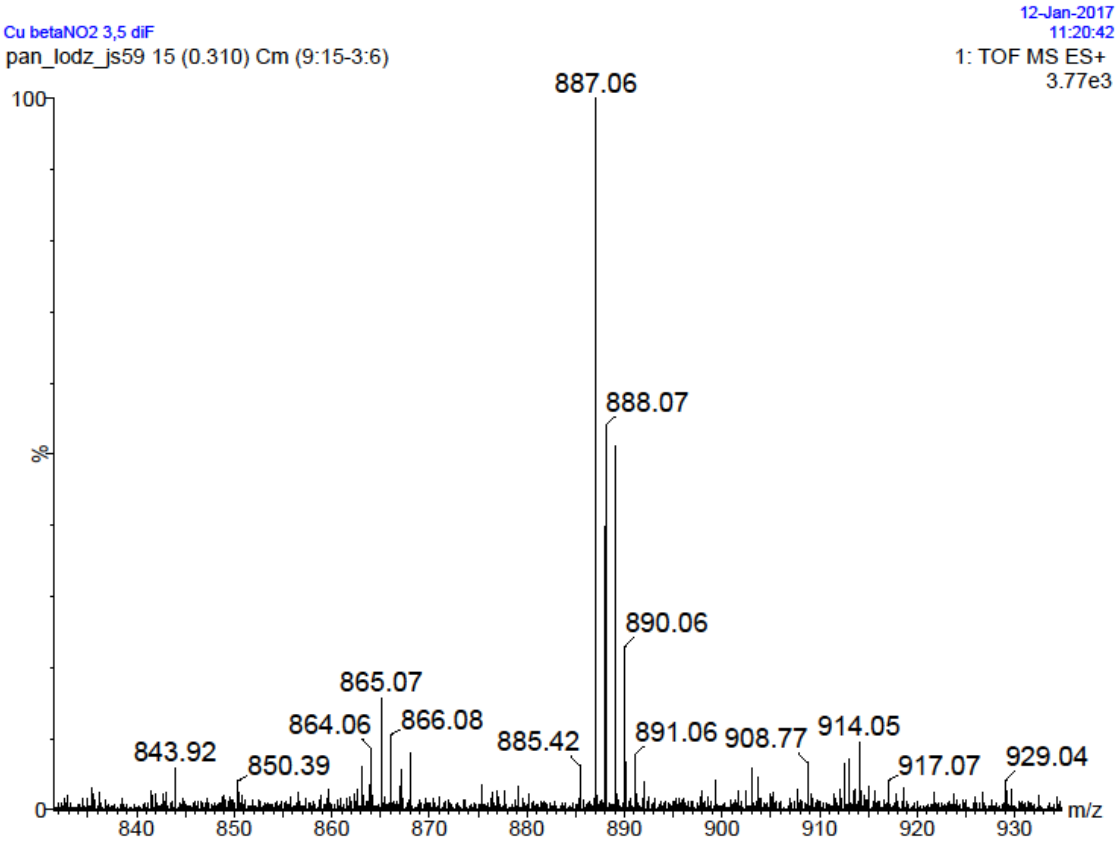

Figure S 79 HRMS spectrum of compound **14**

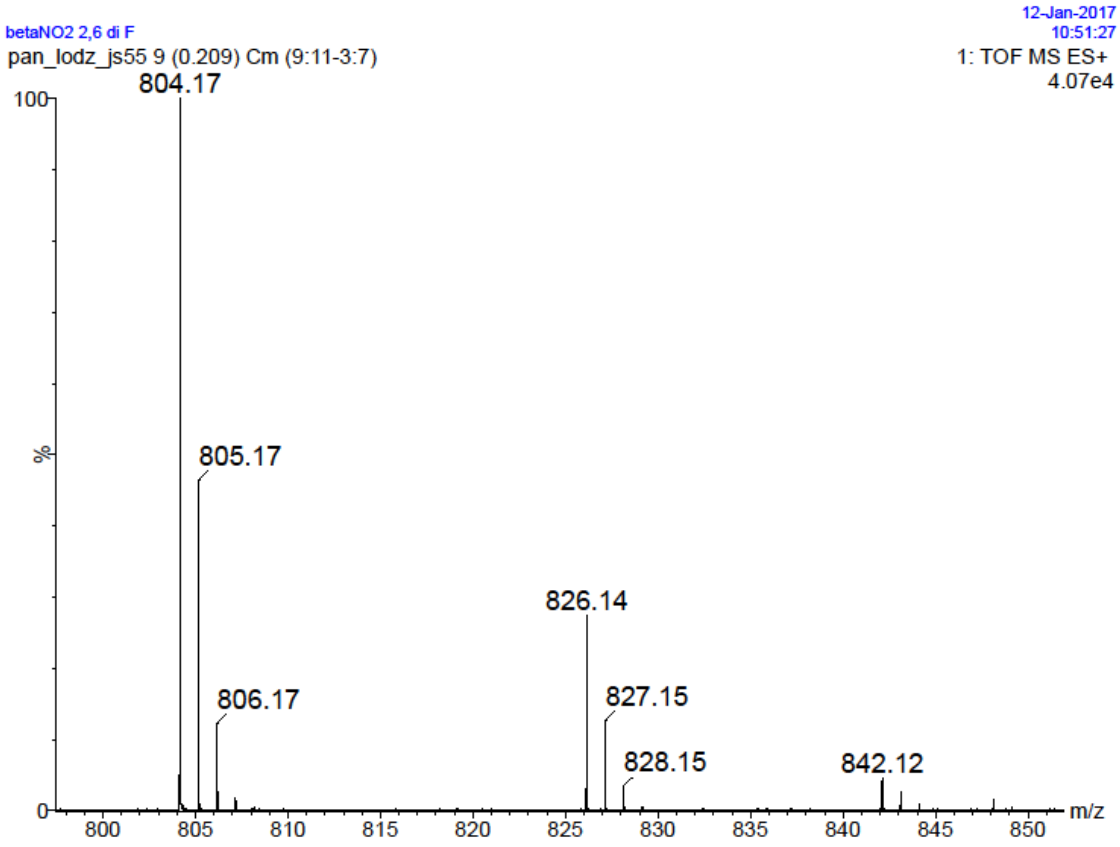

Figure S 80 HRMS spectrum of compound **17**

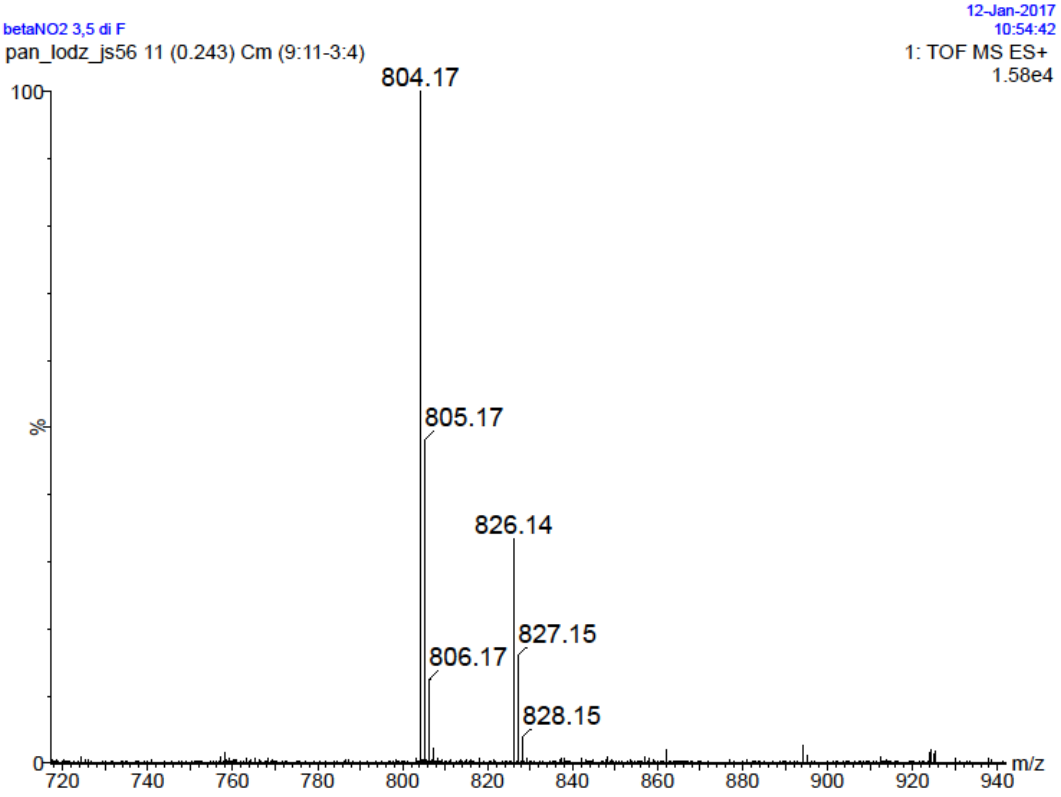

Figure S 81 HRMS spectrum of compound **18**

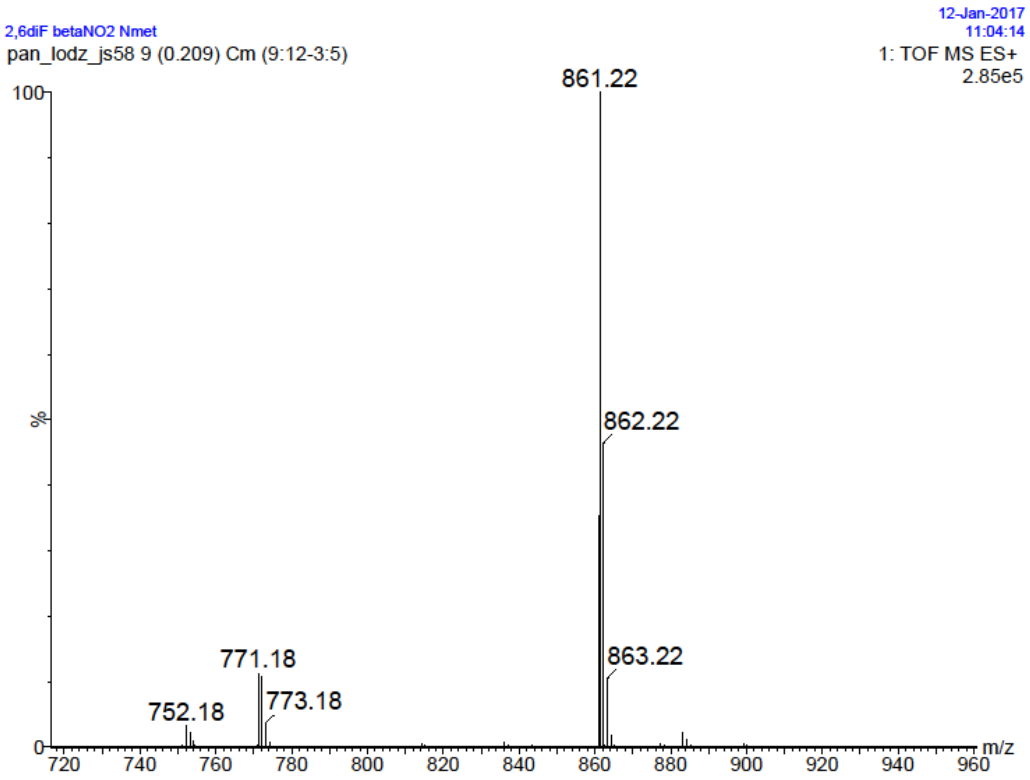

Figure S 82 HRMS spectrum of compound **1**

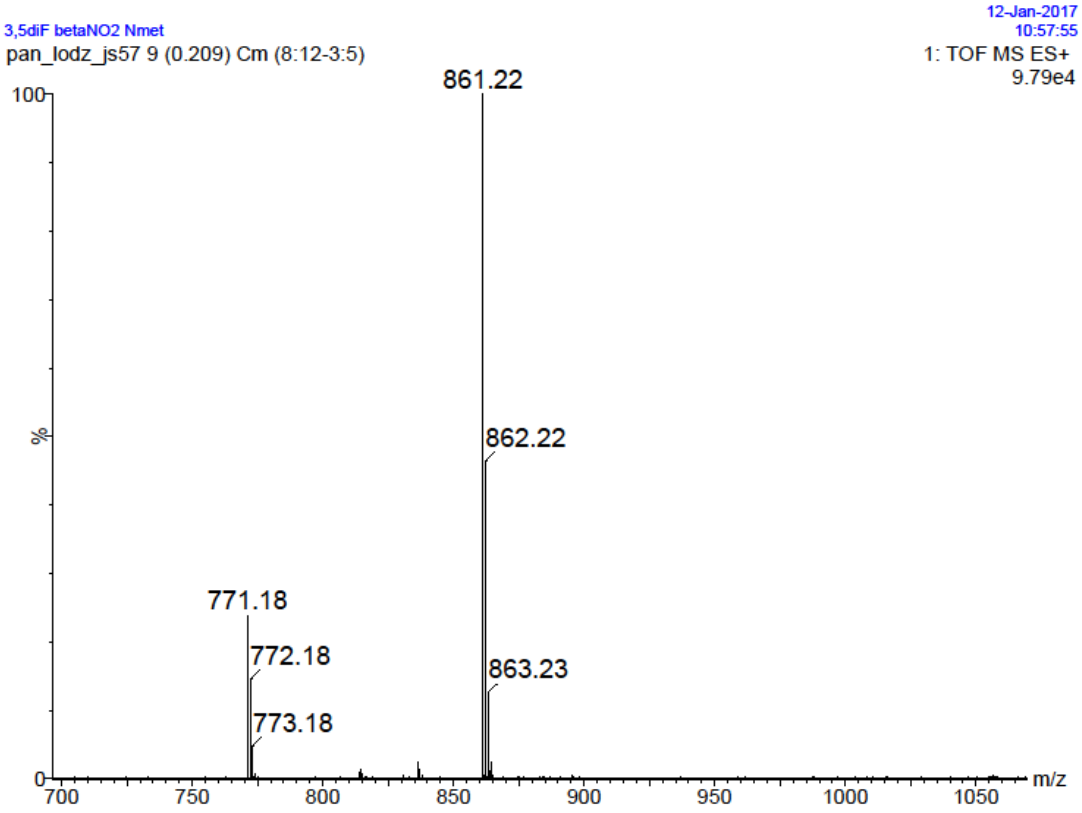

Figure S 83 HRMS spectrum of compound **2**

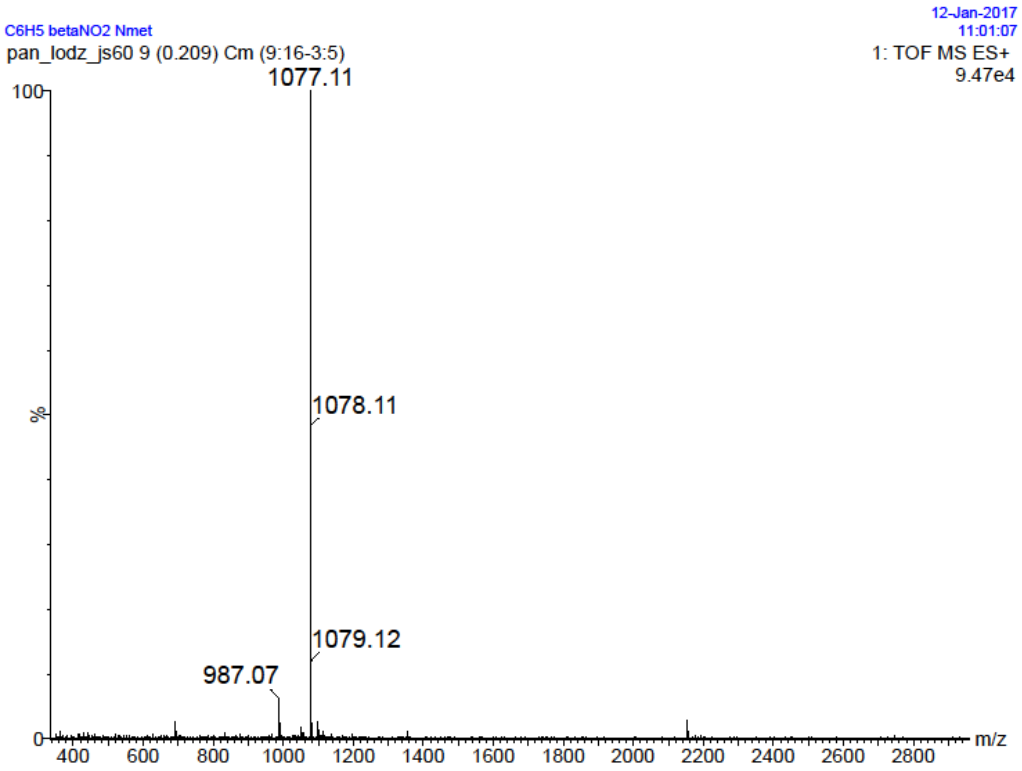

Figure S 84 HRMS spectrum of compound **3**

Absorption spectroscopy

Table S1 Molar absorbance coefficient from experimental data:

Chlorin	Soret band [nm]	Molar absorbance coefficient [$dm^3 \cdot mol^{-1} \cdot cm^{-1}$]
1	408	141 040
2	409	180 726
3	408	120 968
4	411	163 822

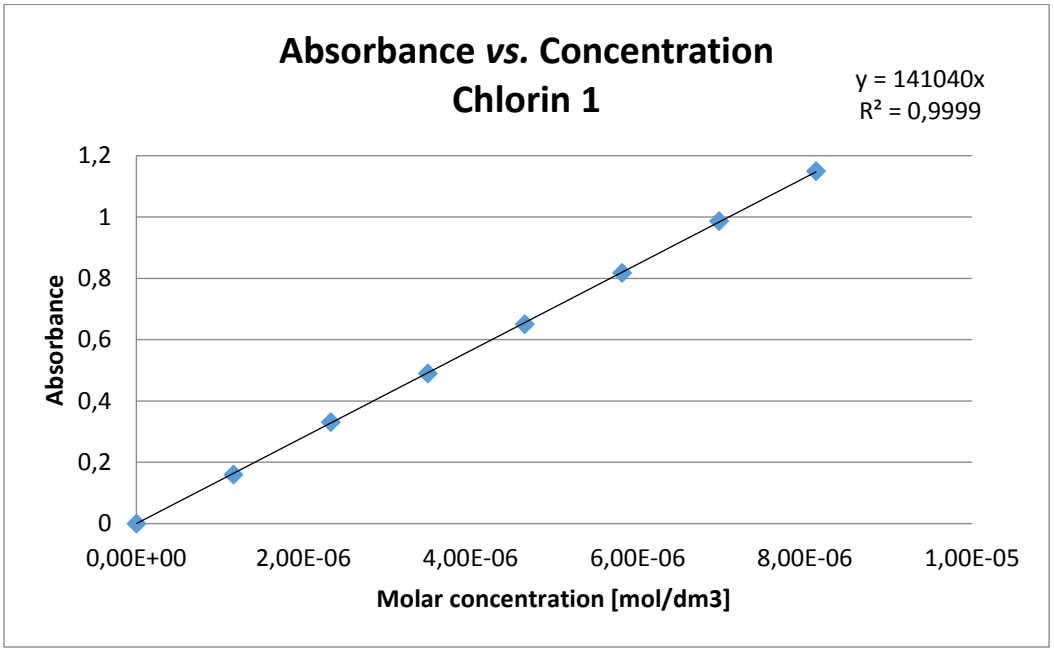

Figure S 85 Absorbance *vs.* concentration calibration curve for chlorin **1**

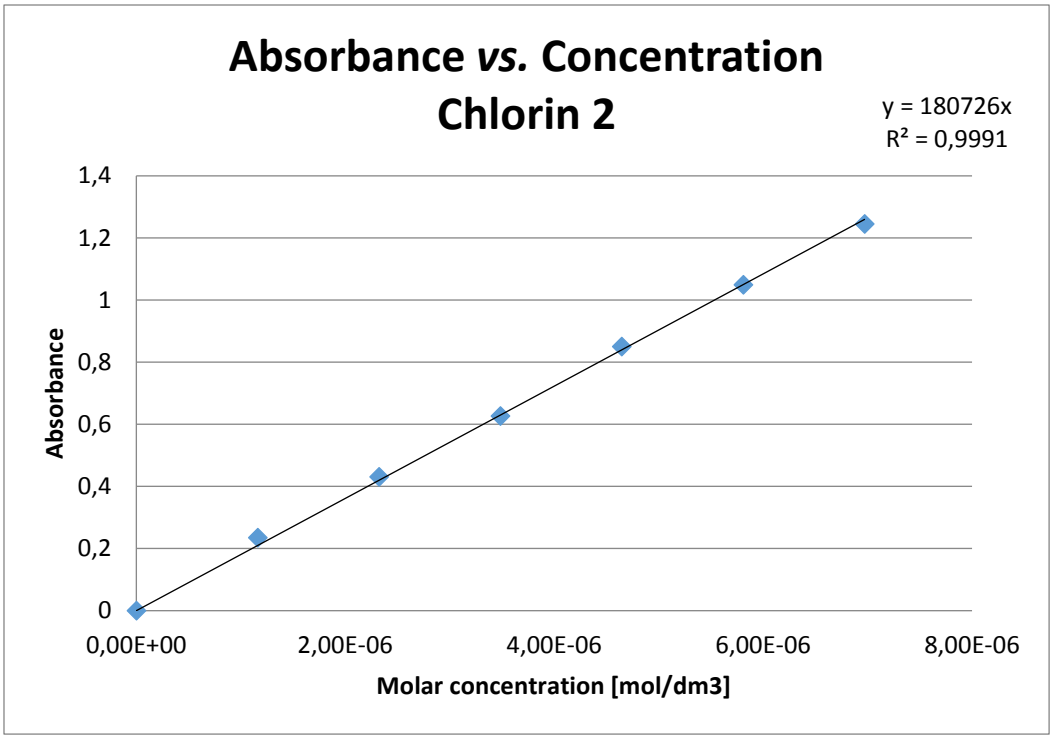

Figure S 86 Absorbance *vs.* concentration calibration curve for chlorin **2**

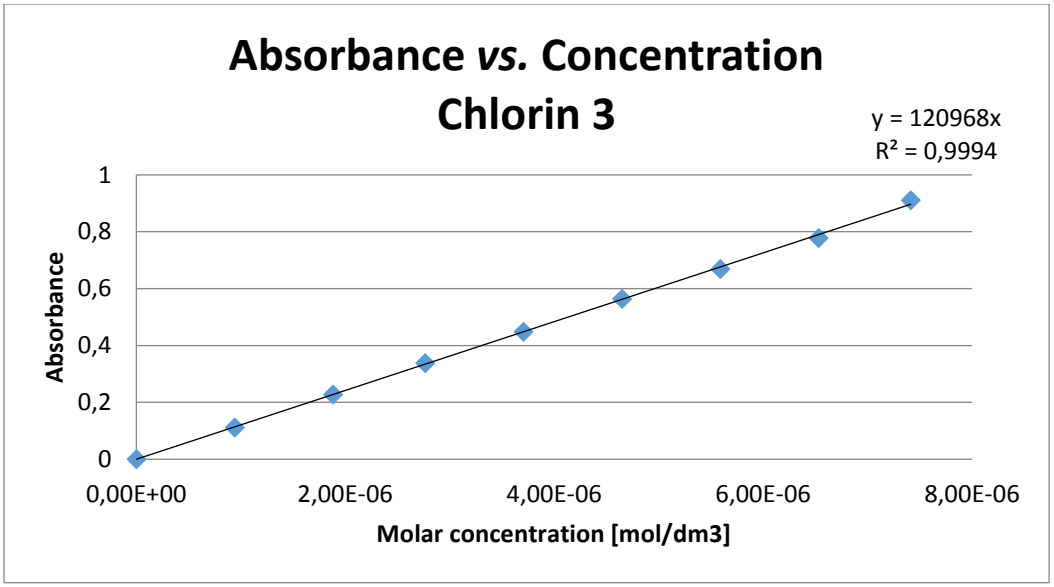

Figure S 87 Absorbance *vs.* concentration calibration curve for chlorin **3**

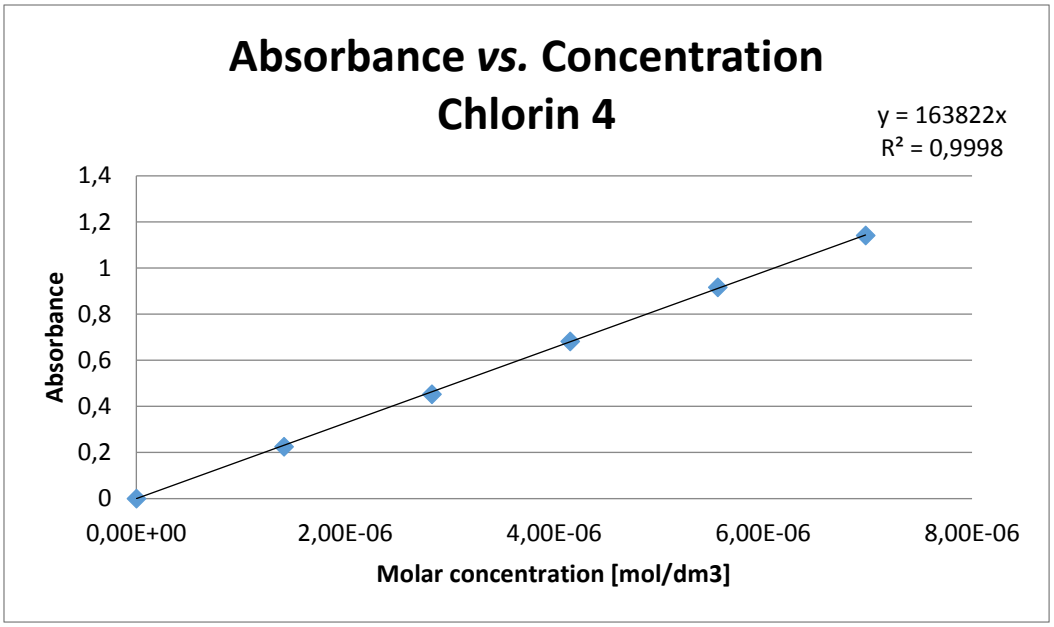

Figure S 88 Absorbance *vs.* concentration calibration curve for chlorin **4**

Calculations:

a) Chlorin 1

C	0.07805000	-2.96792200	-0.08074500
N	-0.94746000	-2.06478800	-0.03818700
C	-2.16775900	-2.71150900	-0.07047300
C	-3.66259000	-0.71780700	0.03268700
C	0.81744500	2.70176600	-0.04997800
C	2.38896700	0.74811400	-0.09151000
C	-3.42103200	-2.10527000	-0.03016700
N	-2.70315000	0.24916200	0.03584400
C	-0.52511900	-4.26743000	-0.15032100
N	-0.39413900	2.06836300	-0.00236900
N	1.47491900	-0.24830300	-0.04438600
C	2.08523300	-1.45015800	-0.03509900
C	2.10279500	2.11482000	-0.09434100
C	-3.37849700	1.43208000	0.09587300
C	-4.99200100	-0.13351500	0.10007800
C	-1.42307000	2.98929800	0.04442600
C	3.82413600	0.19506200	-0.10354200
C	-1.88332200	-4.11027200	-0.14405300
C	3.59882400	-1.33006300	-0.00224700
C	-2.78880700	2.71031600	0.09935800
C	0.54384100	4.10781800	-0.03557200
C	-0.81190800	4.27983500	0.02364700
C	-4.81445000	1.20917600	0.14184200
C	1.46138300	-2.70066100	-0.06049400
C	3.22180000	3.11564500	-0.14591600
C	3.71076200	3.62682200	-1.35123300
C	3.77883100	3.67851000	1.00485300
C	4.69979000	4.59504500	-1.42966800
C	4.76856500	4.64800400	0.98667400
C	5.23014300	5.10101200	-0.24718100
C	-3.70380900	3.89528600	0.16173000
C	-4.26187900	4.46857900	-0.98227600
C	-4.05998600	4.49798300	1.36931500
C	-5.11637000	5.56051400	-0.95161700
C	-4.90945300	5.59059300	1.45814700
C	-5.43735800	6.11918700	0.28290600
C	-4.60649100	-3.02008800	-0.05668100
C	-5.26245100	-3.35421500	-1.24295300
C	-5.13397600	-3.59317500	1.10182800
C	-6.36493600	-4.19379500	-1.29740600
C	-6.23340100	-4.43850200	1.10537100
C	-6.84765100	-4.73522200	-0.10867800
C	2.33778600	-3.91829400	-0.09289700
C	2.91365400	-4.39270200	-1.27435200
C	2.61103200	-4.67904300	1.04617900
C	3.70843600	-5.52739500	-1.34074800

C	3.39452400	-5.82306400	1.03861000
C	3.94522500	-6.24272000	-0.16989200
C	4.73490100	0.54503700	1.07995900
N	5.37382500	-0.72728500	1.40923600
C	4.30851400	-1.71976500	1.31343700
N	4.50353800	0.49245900	-1.46708200
O	5.57455000	1.07440900	-1.48171500
O	3.90575900	0.09460300	-2.45255300
C	6.09124800	-0.72374200	2.67211000
F	-4.79693300	-2.83345800	-2.39764500
F	-4.54318200	-3.30699300	2.28174000
F	-3.95221200	3.93158400	-2.18103800
F	-3.55076500	3.98863300	2.51138400
F	3.18530300	3.15642000	-2.49891000
F	2.68231900	-3.70814800	-2.41346400
F	2.08458900	-4.27580000	2.22430400
H	-0.85658100	-1.05827800	0.00224800
H	0.01940000	-5.19562000	-0.20172200
H	-0.53438900	1.06723400	-0.01095500
H	-5.92450300	-0.67598200	0.11461800
H	-2.62915900	-4.88733700	-0.18802000
H	4.05515300	-1.84987000	-0.84323500
H	1.29292500	4.88103800	-0.06655400
H	-1.34780600	5.21468900	0.04909000
H	-5.57431500	1.97306400	0.19602600
H	5.03859200	4.92944400	-2.40139600
H	5.15532400	5.03288900	1.92137100
H	6.00601000	5.85599600	-0.28585300
H	-5.51211200	5.95264300	-1.87954400
H	-5.14321300	6.00546200	2.43005900
H	-6.10315100	6.97245700	0.32937700
H	-6.82306600	-4.40902100	-2.25406100
H	-6.58925100	-4.84495200	2.04324000
H	-7.70826900	-5.39283500	-0.12850400
H	4.12144600	-5.83230700	-2.29355900
H	3.56188700	-6.36061400	1.96303200
H	4.56198400	-7.13277000	-0.19925700
H	4.10782400	0.91222900	1.90919900
H	3.60372700	-1.65780700	2.16312600
H	4.72155700	-2.72910600	1.28705100
H	6.55687100	-1.69890600	2.83355700
H	6.88418800	0.02726000	2.64275700
H	5.43644400	-0.50464200	3.53524700
F	3.31951000	3.26059700	2.20817300
H	5.47220500	1.30573800	0.83057800

b) Chlorin 2

C	0.08239400	-2.97054900	-0.11526600
N	-0.94178400	-2.06671700	-0.02300200
C	-2.16562500	-2.70897100	-0.07084800
C	-3.65469600	-0.71210300	0.08536400
C	0.82997100	2.69795800	-0.06471400
C	2.39465600	0.74026100	-0.03186900
C	-3.42025500	-2.10228400	0.00387700
N	-2.69530500	0.25649900	0.03813700
C	-0.52542900	-4.26286700	-0.24228200
N	-0.38494200	2.07050100	0.01292300
N	1.47904800	-0.25610700	-0.01200600
C	2.08974300	-1.45925600	-0.00760400
C	2.11403800	2.10750500	-0.07383100
C	-3.36718400	1.44132000	0.12724000
C	-4.97663400	-0.12625400	0.23445900
C	-1.41212900	2.99652300	0.01993200
C	3.82855500	0.18972400	0.01319900
C	-1.88381900	-4.10314500	-0.21481400
C	3.60059400	-1.33703100	0.09576200
C	-2.77993000	2.72335700	0.09312000
C	0.56008400	4.10388000	-0.11791000
C	-0.79545400	4.28277100	-0.06698700
C	-4.79718000	1.21712400	0.26070700
C	1.46828400	-2.70956100	-0.08457700
C	3.24531400	3.09928300	-0.15505600
C	3.75256500	3.48411800	-1.40046100
C	3.75021400	3.69173100	1.00864600
C	4.76307200	4.43260500	-1.45028000
C	4.76130700	4.63333200	0.89899900
C	5.29505600	5.02870700	-0.31738100
C	-3.69558100	3.91148500	0.12929400
C	-4.43869300	4.25859400	-1.00454900
C	-3.81179400	4.67713600	1.29468200
C	-5.27637300	5.36144000	-0.94447700
C	-4.66899800	5.76694500	1.29766900
C	-5.41862300	6.14106400	0.19331200
C	-4.60901700	-3.01570700	-0.00905800
C	-5.42969900	-3.08496200	-1.14068300
C	-4.90515500	-3.80313700	1.10954000
C	-6.52156400	-3.93876100	-1.12516800
C	-6.01315600	-4.63549700	1.06939600
C	-6.84627700	-4.73087400	-0.03431200
C	2.34723800	-3.92885900	-0.16010300
C	2.97805300	-4.26728200	-1.36293200
C	2.52505900	-4.74461000	0.96344300
C	3.77422700	-5.40191200	-1.40882200
C	3.33191500	-5.86747300	0.85970800
C	3.97613600	-6.22808800	-0.31337800

C	4.68929400	0.53155700	1.23846200
N	5.29435700	-0.74398800	1.60479100
C	4.23396300	-1.73075600	1.44863500
N	4.56551700	0.48408100	-1.31511800
O	5.71005800	0.89203400	-1.28167500
O	3.93146900	0.24499400	-2.33377200
C	5.95318300	-0.74686000	2.89893200
F	-4.78335300	6.50014100	2.42790600
F	-5.98805400	5.69746500	-2.04339200
F	-6.29860700	-5.38925000	2.15501300
F	-7.30782900	-4.00799000	-2.22248500
F	3.50309200	-6.64709200	1.95137900
F	4.37782000	-5.72555300	-2.57280400
F	5.24805600	5.19779600	2.02822900
F	5.25054300	4.79966300	-2.65368300
H	-0.84594700	-1.06181400	0.03872900
H	0.01590700	-5.18783200	-0.34817100
H	-0.52969100	1.07007500	0.03028900
H	-5.90531200	-0.66757300	0.31948700
H	-2.63079800	-4.87531800	-0.29651200
H	4.10861700	-1.85917700	-0.71280300
H	-1.32807200	5.21894600	-0.09334200
H	-5.55176800	1.97954300	0.37013400
H	5.44551300	1.28480100	1.02737600
H	3.48015000	-1.66426400	2.25667500
H	4.63867000	-2.74335300	1.44544500
H	6.40169000	-1.72594300	3.08168700
H	6.75322900	-0.00321400	2.90670200
H	5.26049400	-0.52142000	3.73064500
H	4.02467300	0.91115900	2.03537600
H	1.31217400	4.87116400	-0.18969100
H	-3.25589200	4.42844400	2.18928200
H	-4.36591400	3.68742800	-1.92082800
H	-6.08015100	6.99632300	0.21773000
H	3.36075400	3.43701900	1.98563500
H	3.37767600	3.05223900	-2.31935200
H	6.08556700	5.76416600	-0.38006700
H	2.04633100	-4.51432100	1.90653000
H	4.60170300	-7.10835500	-0.37259200
H	2.84827000	-3.66714100	-2.25474100
H	-4.29492400	-3.76378100	2.00241400
H	-5.22339400	-2.49187600	-2.02198400
H	-7.70490700	-5.38839900	-0.04413000

c) Chlorin 3

C	0.13718500	-2.98320000	-0.07239400
N	-0.86220300	-2.05201700	-0.02650000
C	-2.09923200	-2.66475700	-0.06375100

C	-3.54001000	-0.62877300	0.03468900
C	1.03268200	2.66328300	-0.03981800
C	2.55356100	0.66530700	-0.02598900
C	-3.33390400	-2.02176600	-0.02283200
N	-2.55426500	0.31076300	0.03140300
C	-0.50148300	-4.26520900	-0.15228400
N	-0.19610000	2.06450200	0.00095800
N	1.61103300	-0.30435900	-0.00147000
C	2.18856800	-1.52221800	0.01308200
C	2.30077700	2.03899500	-0.05426800
C	-3.19768600	1.51139900	0.07877800
C	-4.85355700	-0.00824300	0.09615000
C	-1.19831500	3.01461400	0.02362800
C	3.97278600	0.07301300	0.01119400
C	-1.85425300	-4.07075700	-0.14514800
C	3.70343500	-1.44572800	0.08265900
C	-2.57088400	2.77158000	0.06998800
C	0.79897700	4.07684300	-0.04737900
C	-0.55129400	4.28768200	-0.00706100
C	-4.63959200	1.32879000	0.12502600
C	1.52686100	-2.75277100	-0.03837100
C	3.44824300	3.00738800	-0.11433300
C	3.92772400	3.48921000	-1.33400900
C	4.02563600	3.53890000	1.03932600
C	4.95162200	4.42571900	-1.41032600
C	5.05302300	4.47260800	0.99255300
C	5.51950400	4.91461200	-0.24015400
C	-3.45459600	3.98196200	0.10909100
C	-3.99416700	4.52872400	-1.05513000
C	-3.77937700	4.60686700	1.31284600
C	-4.82276000	5.64488200	-1.03029900
C	-4.60504500	5.72416300	1.36483000
C	-5.12847300	6.24378100	0.18645700
C	-4.54502200	-2.90373100	-0.04336200
C	-5.20942700	-3.20123200	-1.23322200
C	-5.06187400	-3.45896300	1.12717300
C	-6.33844500	-4.01199300	-1.26470300
C	-6.18892600	-4.27288400	1.12271100
C	-6.82883300	-4.54933800	-0.08001300
C	2.36927800	-3.99448900	-0.08429400
C	2.92993400	-4.45001100	-1.27896900
C	2.60333100	-4.76836800	1.05308100
C	3.69185700	-5.61133300	-1.34536900
C	3.35837000	-5.93479600	1.01494000
C	3.90542200	-6.35674000	-0.19146700
C	4.84165200	0.38117600	1.23778900
N	5.44724200	-0.90792300	1.55704000
C	4.36800900	-1.87713900	1.40987100
N	4.71432900	0.37757100	-1.31770600
O	5.77181700	0.98208500	-1.28014300

O	4.16831800	-0.02613300	-2.33015400
C	6.13424500	-0.94643000	2.83783700
F	-4.76050700	-2.70166800	-2.39110300
F	-4.47048900	-3.20924600	2.30248200
F	-3.71696800	3.97655000	-2.24257700
F	-3.29269600	4.12935900	2.46549200
F	3.58058400	3.15788500	2.24754500
F	3.39312500	3.04927200	-2.47744000
F	2.73637300	-3.76091300	-2.40954400
F	2.09462200	-4.39027200	2.23460100
F	-4.89901500	6.29907000	2.53402800
F	-5.92129400	7.31437600	0.22324000
F	-5.32385000	6.14531700	-2.16244400
F	-6.65984300	-4.78891100	2.26104300
F	-7.90959600	-5.32889900	-0.09739400
F	-6.95138000	-4.28012100	-2.42049200
F	3.56472000	-6.64850100	2.12539800
F	4.63164700	-7.47258400	-0.24149700
F	4.21260700	-6.01804000	-2.50491900
F	5.58850900	4.95211100	2.11947300
F	6.50396200	5.81015900	-0.29781100
F	5.39154700	4.85719000	-2.59301200
H	-0.74315800	-1.04863800	0.01875600
H	0.01365100	-5.20956600	-0.20914300
H	-0.36518400	1.06779400	0.00223000
H	-5.80224300	-0.52147600	0.11526800
H	-2.61889000	-4.82887600	-0.19484300
H	4.16536100	-1.96227800	-0.75730500
H	-1.05760200	5.23910900	-0.00010500
H	-5.38090100	2.11104500	0.17167600
H	5.60119900	1.13382700	1.03447400
H	3.64067800	-1.82168400	2.24080000
H	4.76592200	-2.89238700	1.37340800
H	6.57725800	-1.93357700	2.98720300
H	6.94178400	-0.21113800	2.84381000
H	5.46250400	-0.73391800	3.68853900
H	4.18922000	0.74073500	2.05119900
H	1.56740400	4.83070400	-0.07780700

d) Chlorin 4

C	-0.01030400	-2.96339300	-0.12697300
N	-1.04586200	-2.07199300	-0.03345800
C	-2.26282800	-2.72848700	-0.07893400
C	-3.77273500	-0.75030400	0.08718400
C	0.67141300	2.71519200	-0.08856500
C	2.25569400	0.77682200	-0.08338500
C	-3.52603600	-2.13899700	0.00109400
N	-2.82564100	0.23060100	0.03241100

C	-0.60313300	-4.26262300	-0.25133100
N	-0.53578900	2.07302100	-0.00105800
N	1.35224200	-0.23084100	-0.04835300
C	1.97588700	-1.42760500	-0.04063200
C	1.96389600	2.14204000	-0.11114600
C	-3.50981300	1.40807800	0.13247900
C	-5.09915000	-0.18002000	0.25251300
C	-1.57546100	2.98583500	0.01007800
C	3.69620700	0.24199300	-0.06602000
C	-1.96396100	-4.11885300	-0.22332000
C	3.48598500	-1.28550400	0.04883200
C	-2.94072300	2.69912000	0.09504500
C	0.38295700	4.11703900	-0.14467600
C	-0.97508800	4.27885600	-0.08611700
C	-4.93505600	1.16597100	0.28168400
C	1.37345600	-2.68792200	-0.10251100
C	3.08450700	3.14619800	-0.18085800
C	3.54510700	3.78033900	0.98050000
C	3.63774800	3.51875000	-1.41108500
C	4.54796200	4.74534200	0.91651200
C	4.64225900	4.48312400	-1.47680500
C	5.10152700	5.09727400	-0.31399200
C	-3.86886800	3.87618900	0.14127900
C	-4.65223400	4.20889400	-0.97065000
C	-3.96904800	4.66389100	1.29428700
C	-5.51284400	5.30437900	-0.93144800
C	-4.83383800	5.75641900	1.33608400
C	-5.60703300	6.08063800	0.22262800
C	-4.70401800	-3.06518100	-0.01068400
C	-5.54416800	-3.13387100	-1.12902400
C	-4.98811700	-3.87773500	1.09385300
C	-6.63918100	-3.99563000	-1.14358300
C	-6.08669700	-4.73570100	1.08211800
C	-6.91463600	-4.79808100	-0.03734400
C	2.26821100	-3.89604700	-0.16891000
C	2.91303000	-4.24128900	-1.36318500
C	2.45861000	-4.71176300	0.95322500
C	3.73522300	-5.36499800	-1.43077800
C	3.27879900	-5.83730300	0.88746900
C	3.92177700	-6.16566600	-0.30489300
C	4.58663000	0.61637600	1.12765500
N	5.19673000	-0.65034900	1.52145000
C	4.13511200	-1.64253700	1.40333000
N	4.39697600	0.51074900	-1.41895200
O	5.55787500	0.87353300	-1.42442400
O	3.72585800	0.28870700	-2.41784700
C	5.86539100	-0.61678300	2.80881300
H	-0.96228800	-1.06576900	0.02490200
H	-0.04814300	-5.17948200	-0.35782100
H	-0.66711100	1.07075900	0.01742100

H	-6.01887900	-0.73492500	0.34751700
H	-2.70372600	-4.89798400	-0.30504900
H	3.99559300	-1.82044400	-0.75020500
H	1.12664200	4.89153600	-0.22672600
H	-1.52214500	5.20661500	-0.11506300
H	-5.69522200	1.92088800	0.40400800
H	3.10708200	3.51980000	1.93781400
H	3.28106300	3.04780500	-2.31992500
H	4.89352400	5.22442800	1.82597800
H	5.06584000	4.75067300	-2.43810400
H	5.88360000	5.84642400	-0.36532600
H	-4.58008700	3.60742100	-1.86979600
H	-3.37184600	4.41180400	2.16347100
H	-6.10818900	5.55162800	-1.80339900
H	-4.90443300	6.35206800	2.23947600
H	-6.27813300	6.93161000	0.25397200
H	-5.33212900	-2.51158900	-1.99107500
H	-4.34957200	-3.82686900	1.96869500
H	-7.27596200	-4.04069200	-2.02013200
H	-6.29646700	-5.35248100	1.94900900
H	-7.76838400	-5.46629400	-0.04752300
H	2.76270600	-3.62763500	-2.24494800
H	1.95921100	-4.46031400	1.88263100
H	4.22537200	-5.61676300	-2.36464800
H	3.41540400	-6.45609600	1.76753400
H	4.56087300	-7.03986100	-0.35737000
H	5.33915700	1.36146400	0.87737500
H	3.94189900	1.02216200	1.92714500
H	3.39030700	-1.55481100	2.21778400
H	4.53915100	-2.65528800	1.42093300
H	6.31642900	-1.59010800	3.01599900
H	6.66470500	0.12785900	2.79013100
H	5.17918900	-0.36857500	3.64032700

NBO analysis

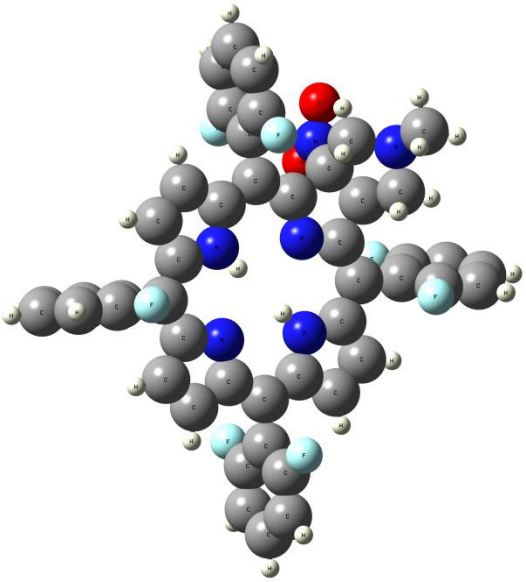

Figure S 89 Chlorin **1**

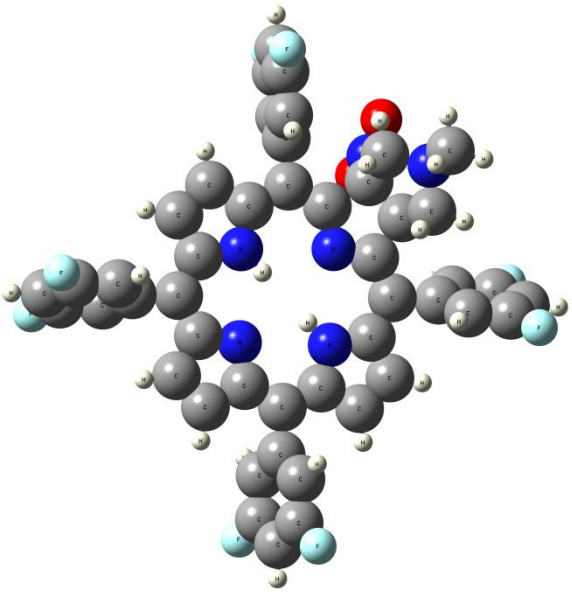

Figure S 90 Chlorin **2**

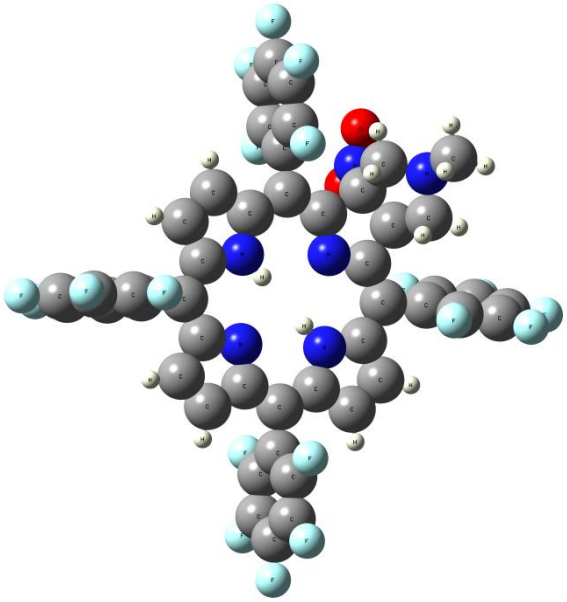

Figure S 91 Chlorin **3**

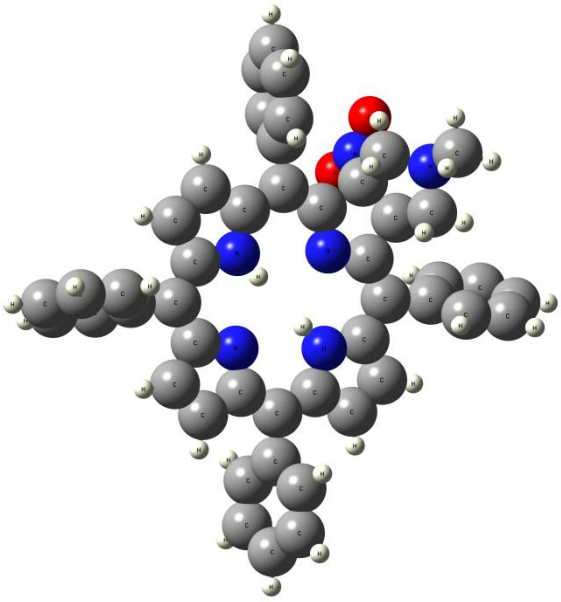

Figure S 92 Chlorin **4**