Supporting Information

Article

Synthesis, Stability, and Biological Evaluation of Novel Aminoderivatives Incorporating the Aza-acridine Scaffold

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Compound name	Linear range (mg L^{-1})	Equation of the calibration curve	R^2
16	5.0-15.0	y= (7.81 ± 0.17) x× 10^{-2}-(22.00±1.7) ×10^{-2}	0.998
17	5.0-12.5	y= (6.82 ± 0.12) x×10^{-2}-(3.9±1.0) ×10^{-2}	0.9990

Table S1- Linearity results of the investigated compounds

	Absorbance of compound 16						
Concentration	5 mg L^{-1}	6.25 mg L^{-1}	7.5 mg L^{-1}	8.75 mg L^{-1}	10 mg L^{-1}	12.5 mg L^{-1}	15 mg L^{-1}
Repilcate 1	0.179	0.274	0.356	0.45	0.580	0.742	0.963
Repilcate 2	0.189	0.273	0.357	0.434	0.590	0.742	0.963
Repilcate 3	0.188	0.272	0.357	0.441	0.590	0.743	0.963
Repilcate 4	0.178	0.272	0.357	0.45	0.580	0.743	0.963
Repilcate 5	0.170	0.273	0.357	0.45	0.580	0.743	0.963
Average	0.181	0.273	0.357	0.445	0.584	0.742	0.963
SD	0.01	0.00	0.00	0.01	0.01	0.00	0.00
%RSD	4.34	0.31	0.13	1.64	0.94	0.07	0.00

Table S2: Repeatability results for the compound 16

	Absorbance of compound 17					
Concentration	5 mg L^{-1}	6.25 mg L^{-1}	7.5 mg L^{-1}	8.75 mg L^{-1}	10 mg L^{-1}	12.5 mg L^{-1}
Repilcate 1	0.304	0.385	0.483	0.555	0.641	0.813
Repilcate 2	0.304	0.385	0.483	0.554	0.641	0.817
Repilcate 3	0.304	0.385	0.484	0.553	0.641	0.819
Repilcate 4	0.304	0.385	0.485	0.553	0.641	0.821
Repilcate 5	0.304	0.385	0.485	0.556	0.64	0.822
Average	0.304	0.385	0.484	0.554	0.641	0.818
SD	0.00	0.00	0.00	0.00	0.00	0.00
%RSD	0.00	0.00	0.21	0.24	0.07	0.44

Table S3: Repeatability results for the compound 17

Difference 1A-9A	19	24	16	58	52
ELF CPs	-6.1×10^{-9}	6.0×10^{-9}	-1.69×10^{-8}	1.1×10^{-2}	2.64×10^{-2}
LOL CPs	-4.8×10^{-9}	2.4×10^{-9}	-8.8×10^{-9}	5.97×10^{-3}	2.1×10^{-3}

Table S4: ELF LOL: ELF (Electron Localization Function) and LOL (Localized Orbital Locator) values of selected CPs of 1A and 9A along with their corresponding differences

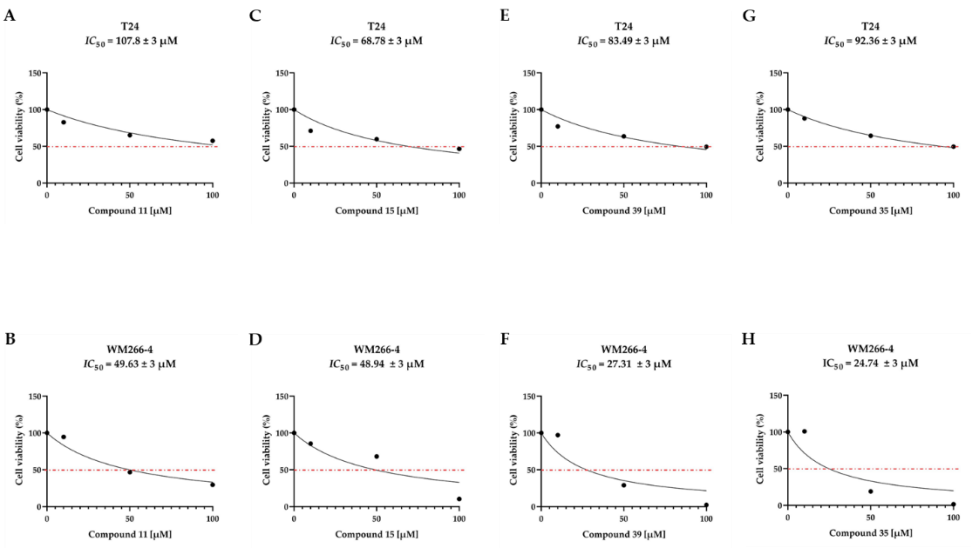


Figure S1: Determination of IC_{50} values using MTT assay.

Percentage of cell viability [%] is plotted on the Y-axis, while the concentration of the test compound [in µM] is shown on the X-axis. The IC_{50} value—defined as the concentration at which 50% inhibition of cell viability is observed—is determined as the point where the dose-response curve crosses the 50% viability level. Nonlinear regression (Inhibitor vs. normalized response) is used for curve fitting in GraphPad Prism 9.0.

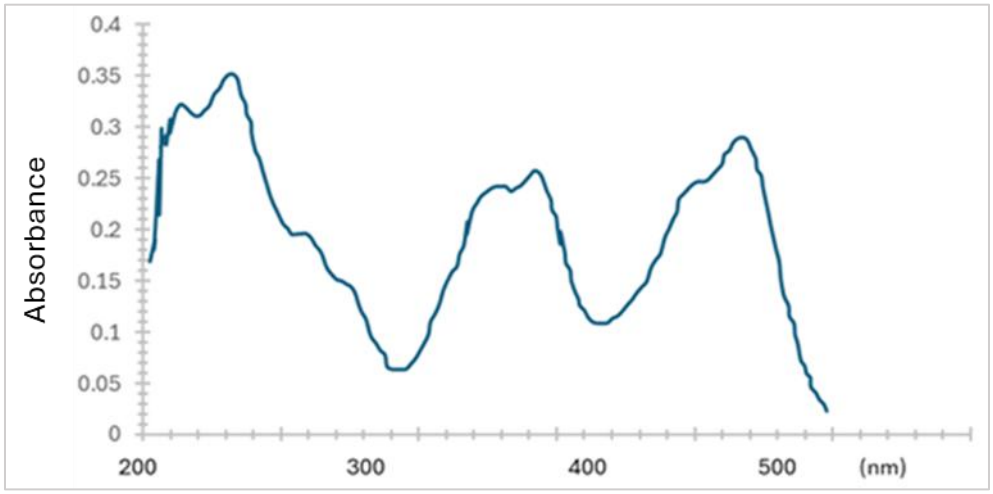


Figure S2: Absorbance spectrum of the compound 16

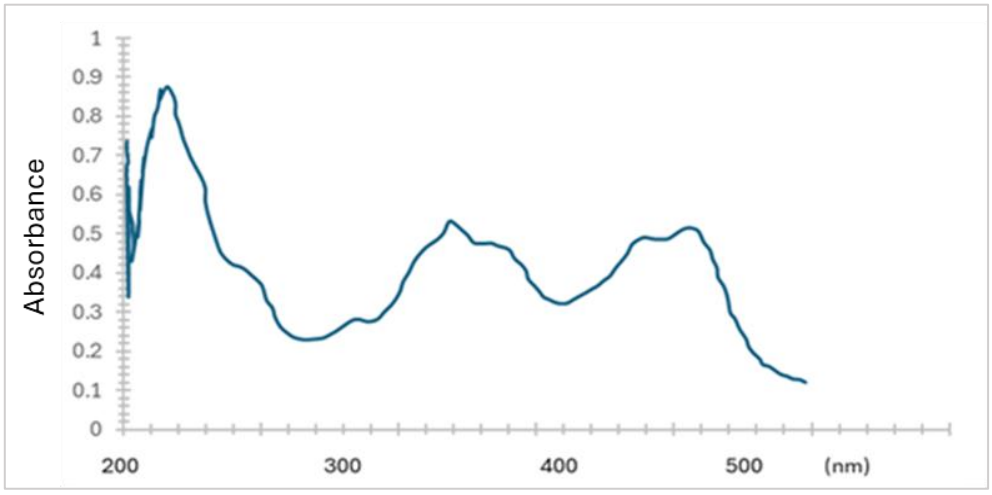
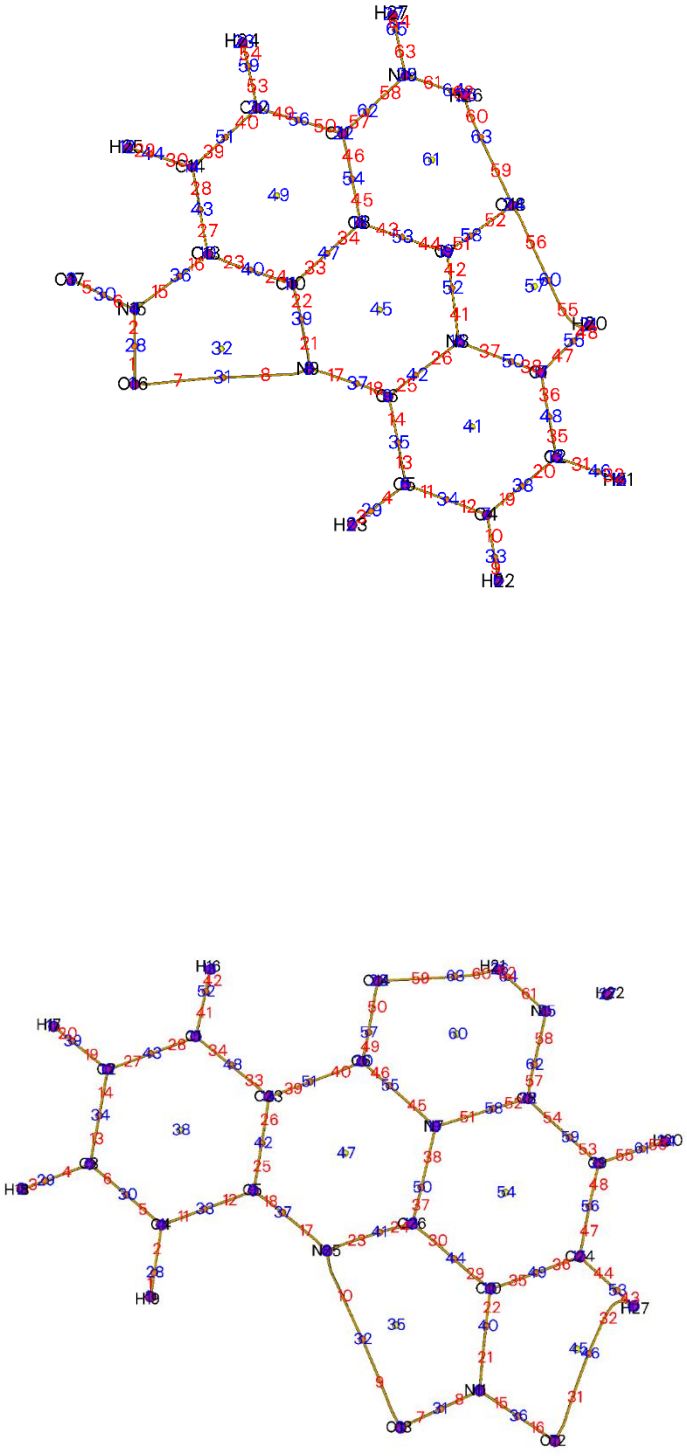


Figure S3: Absorbance spectrum of the compound 17

A



B

Figure S4: CPs numbering of the 1A (A) and 9A(B) molecules as shown in Fig S ELFLOL

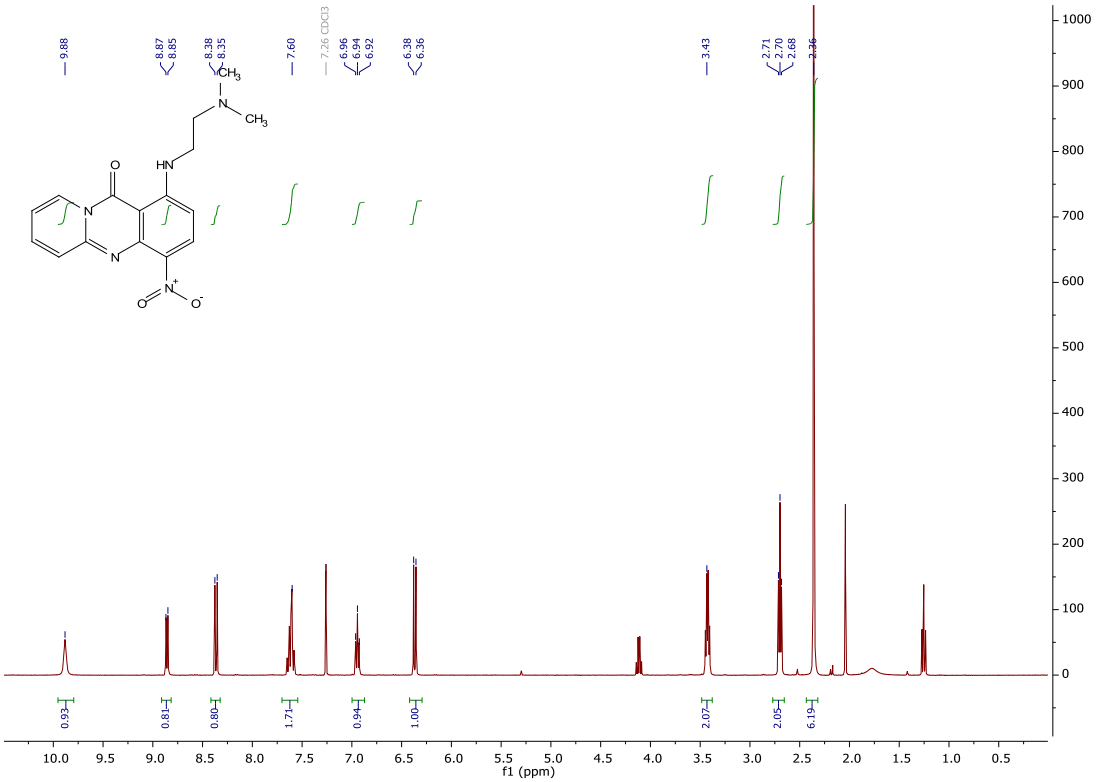


Figure S5: ^{1}H NMR spectrum of 11

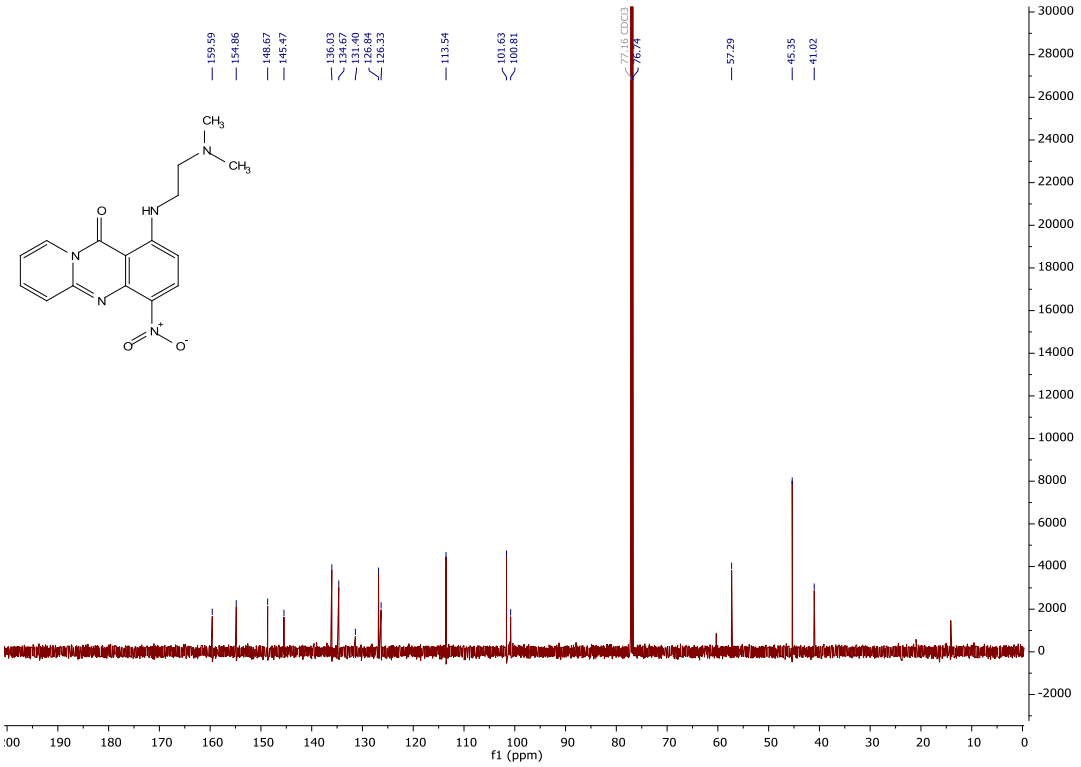


Figure S6: ^{13}C NMR spectrum of 11

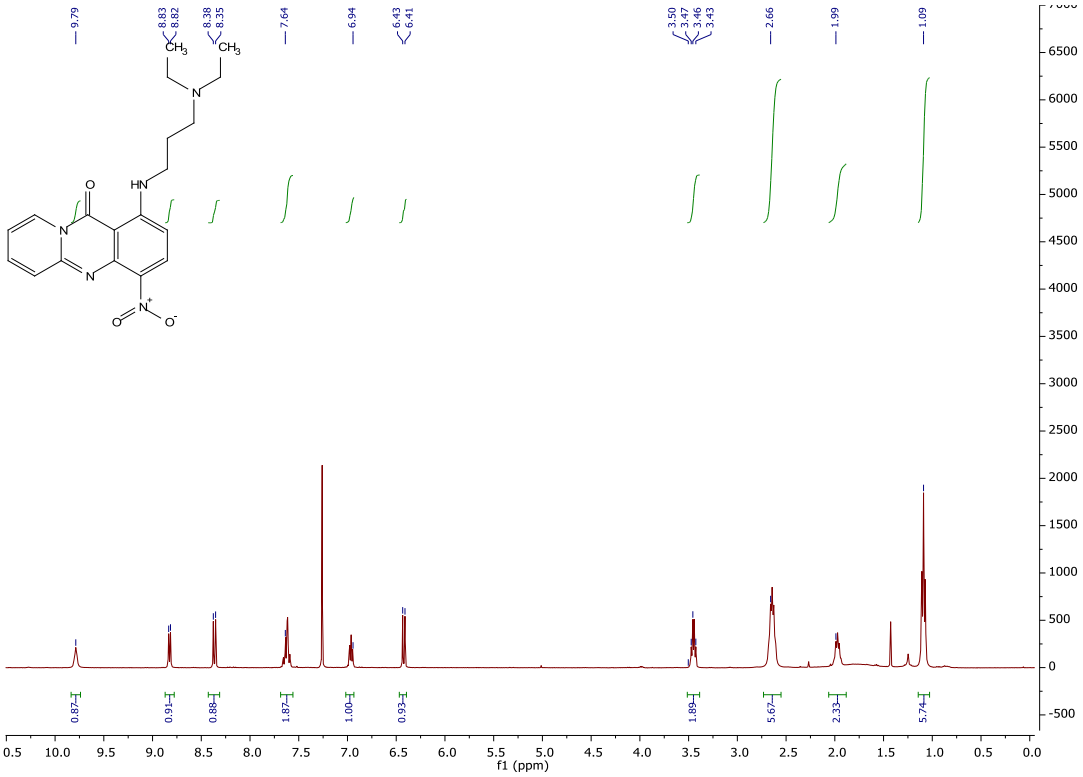


Figure S7: ^{1}H NMR spectrum of 12

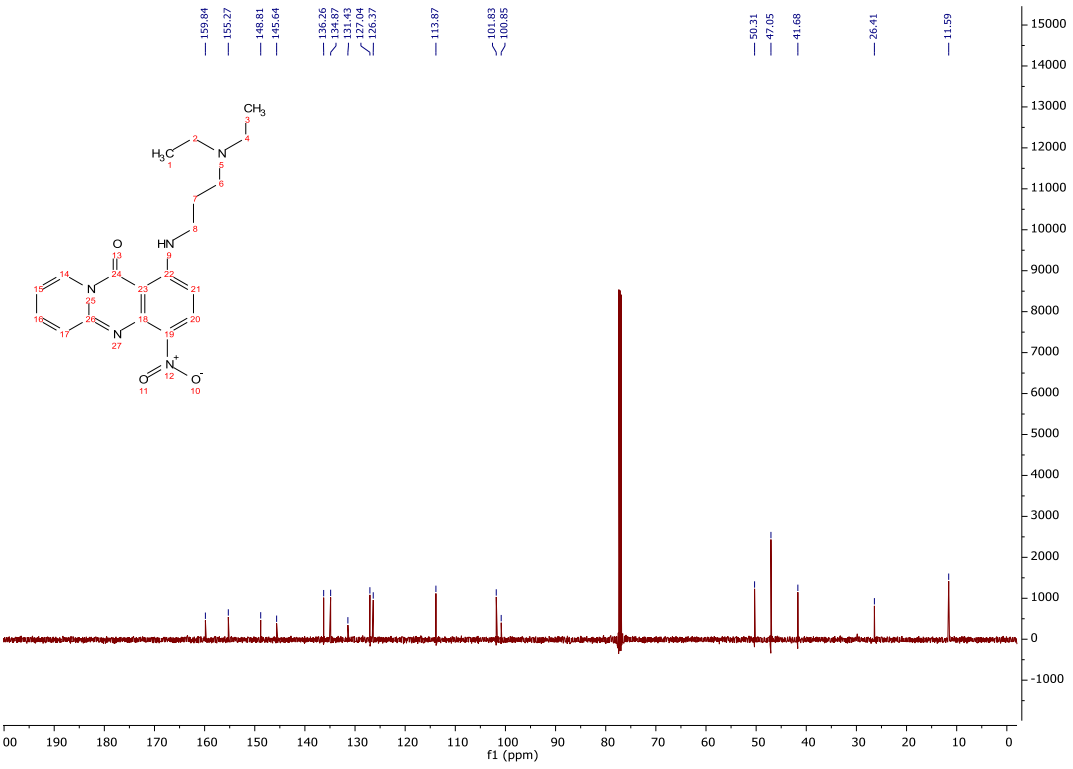


Figure S8: ^{13}C NMR spectrum of 12

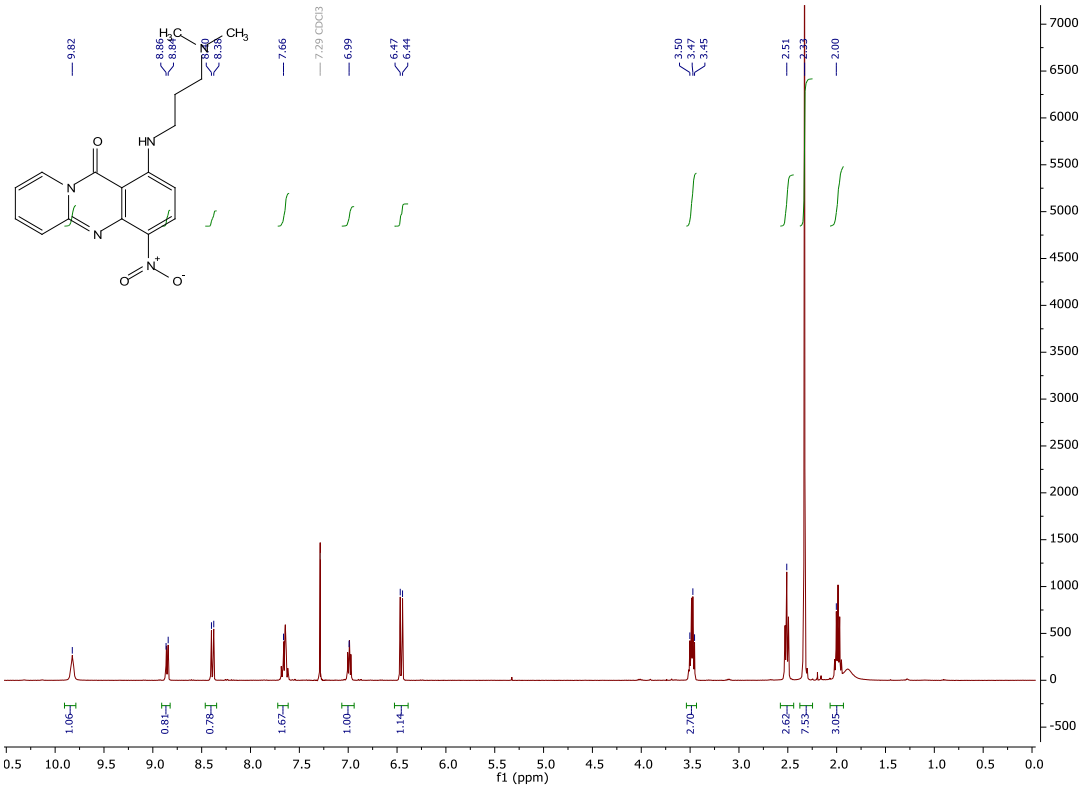


Figure S9: ^{1}H NMR spectrum of 13

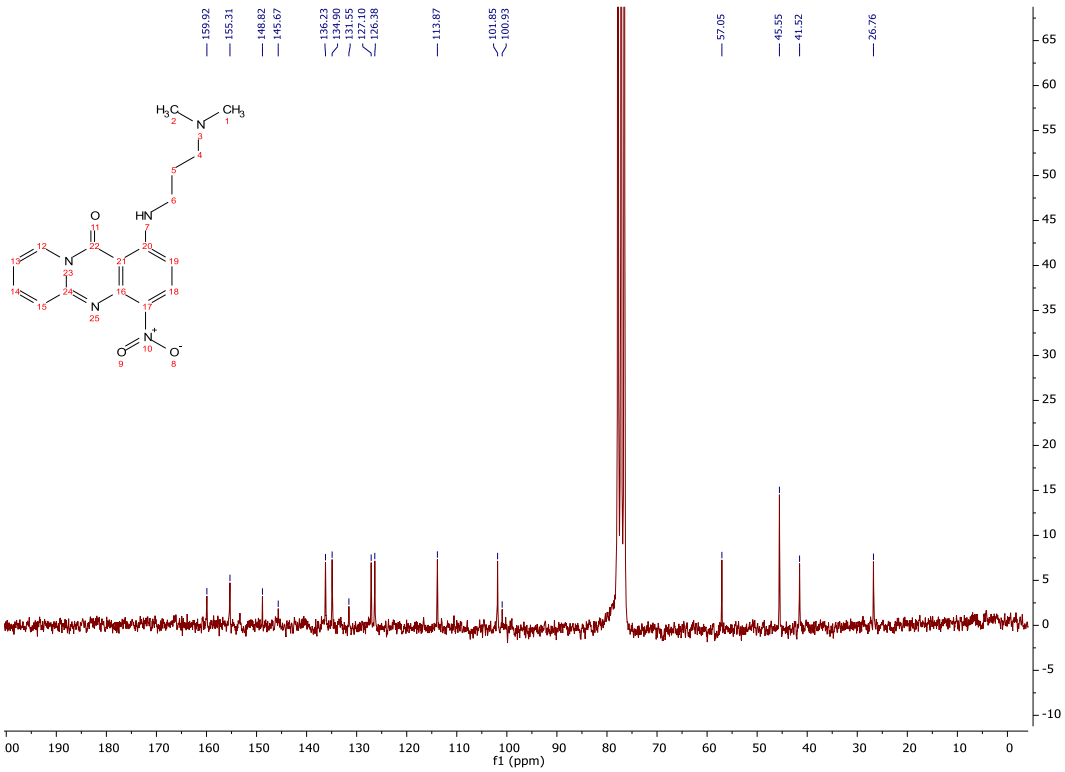


Figure S10: ^{13}C NMR spectrum of 13

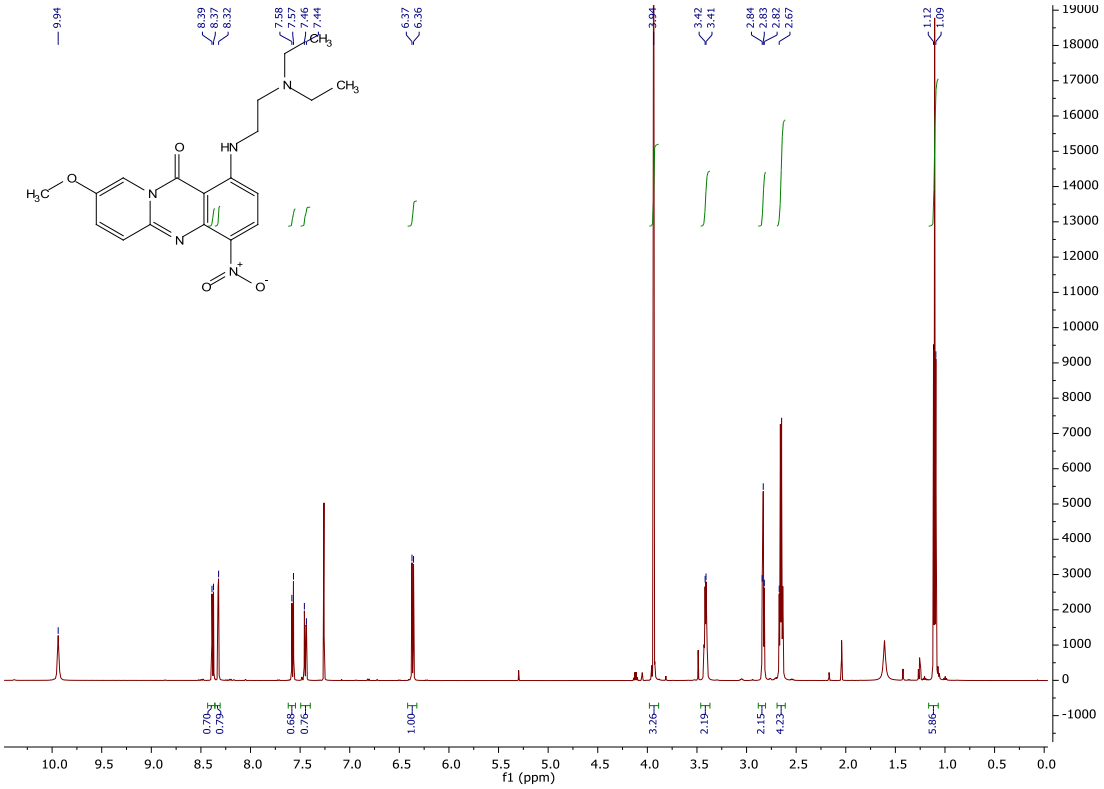


Figure S11: ^{1}H NMR spectrum of 14

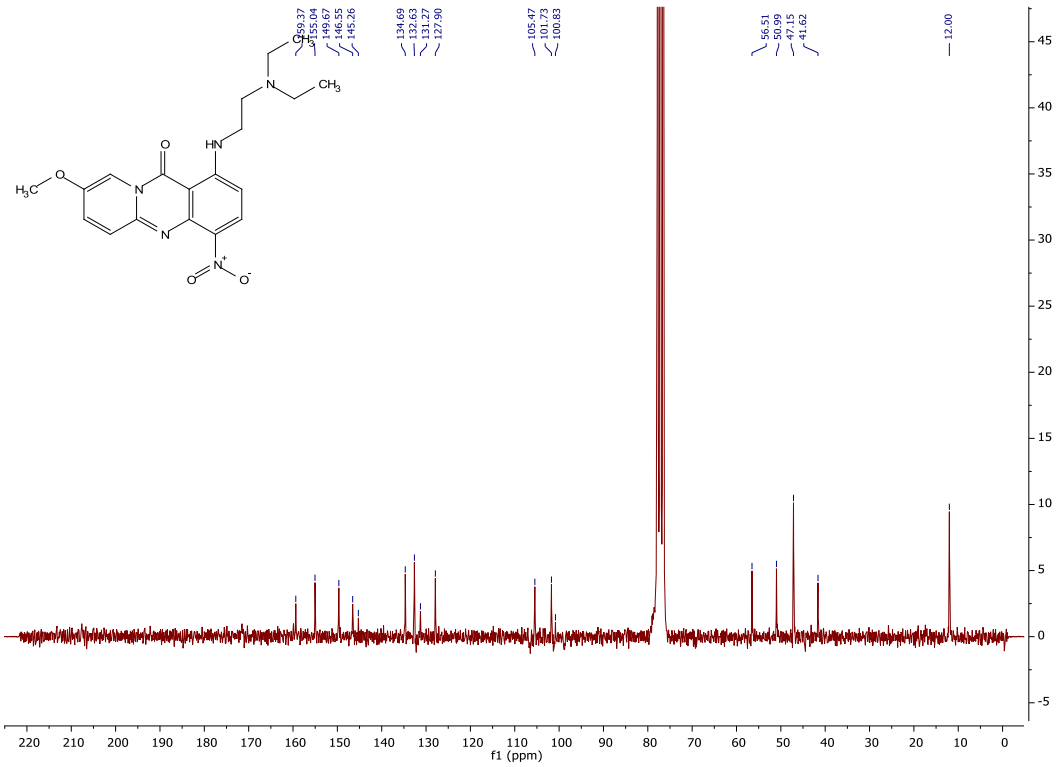


Figure S12: ^{13}C NMR spectrum of 14

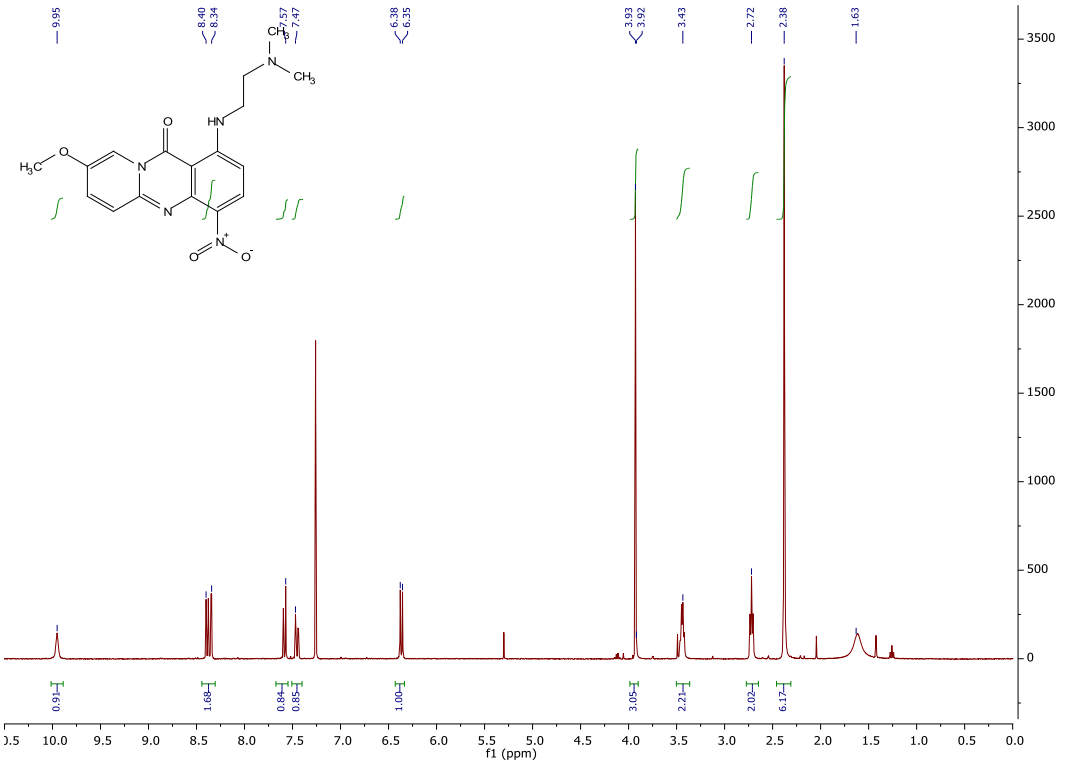


Figure S13: ^{1}H NMR spectrum of 15

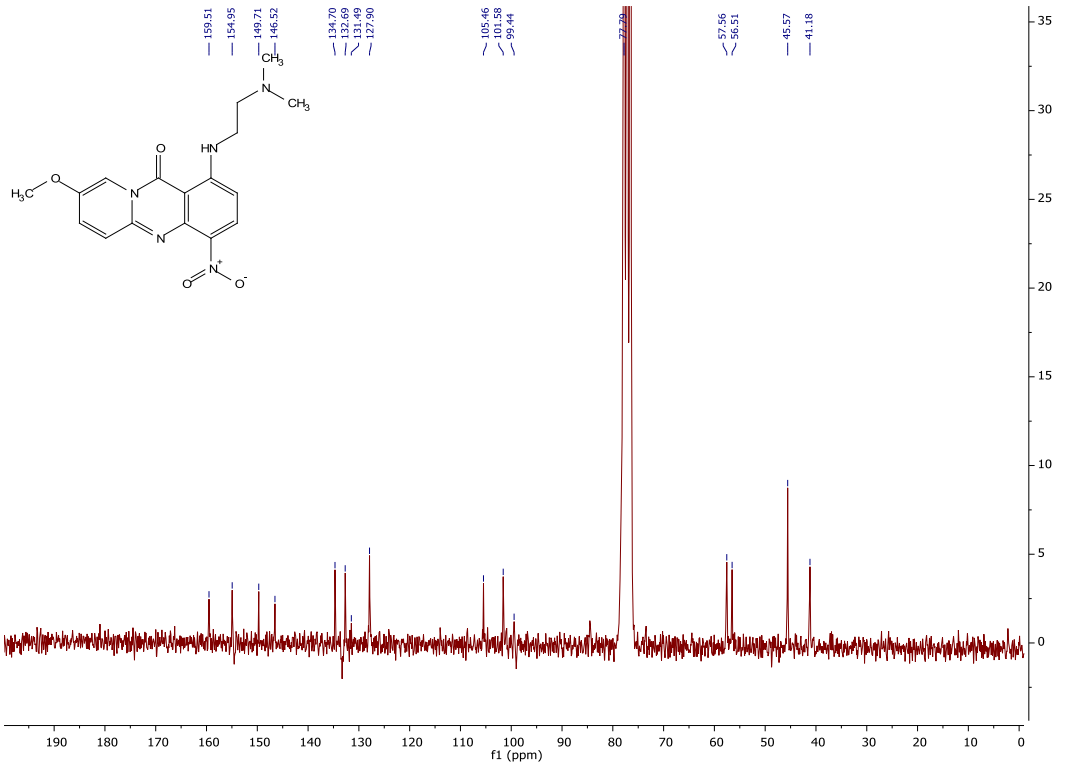


Figure S14: ^{13}C NMR spectrum of 15

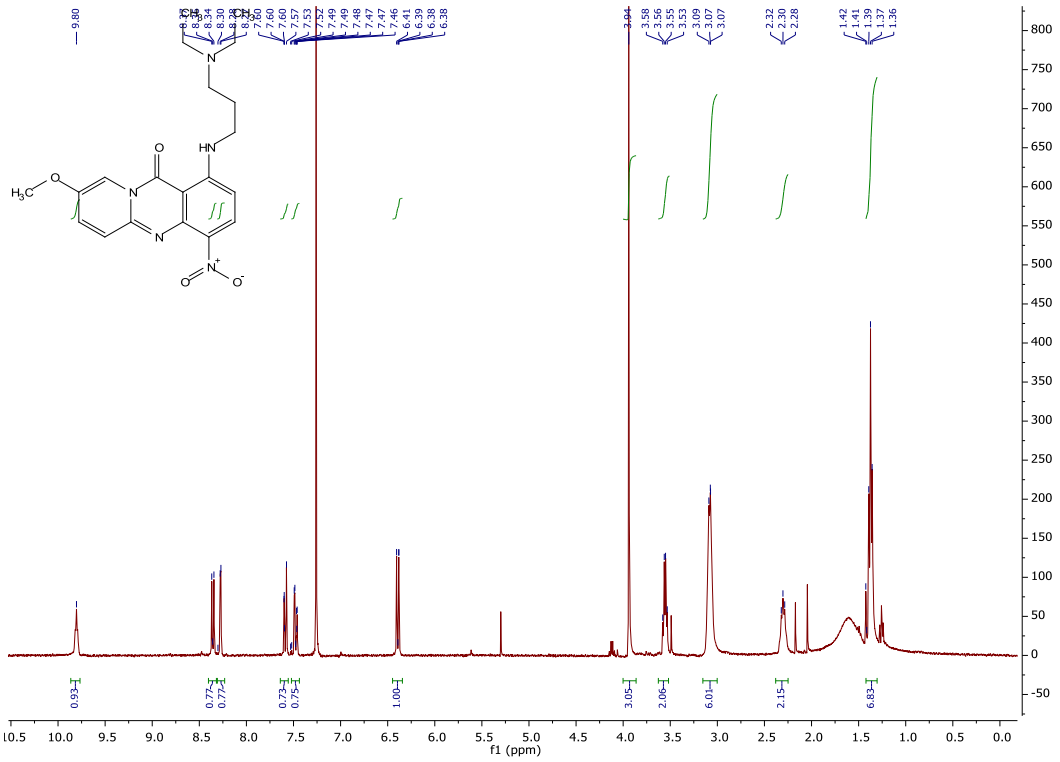


Figure S15: ^{1}H NMR spectrum of 16

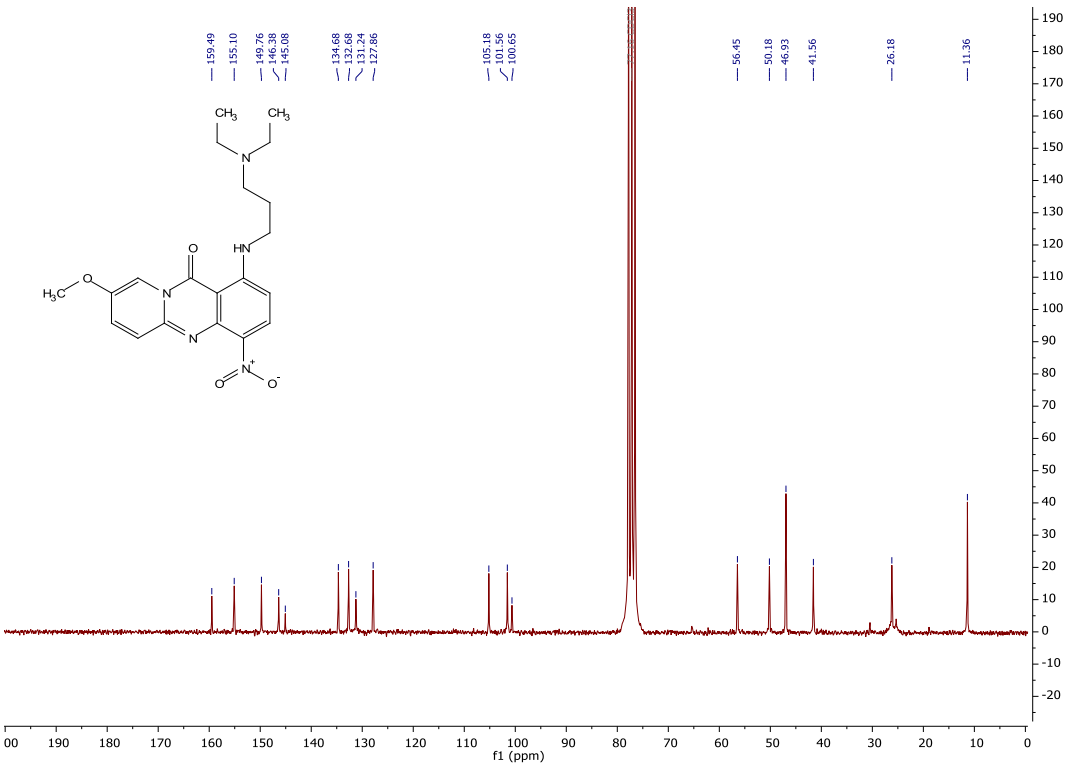


Figure S16: ^{13}C NMR spectrum of 16

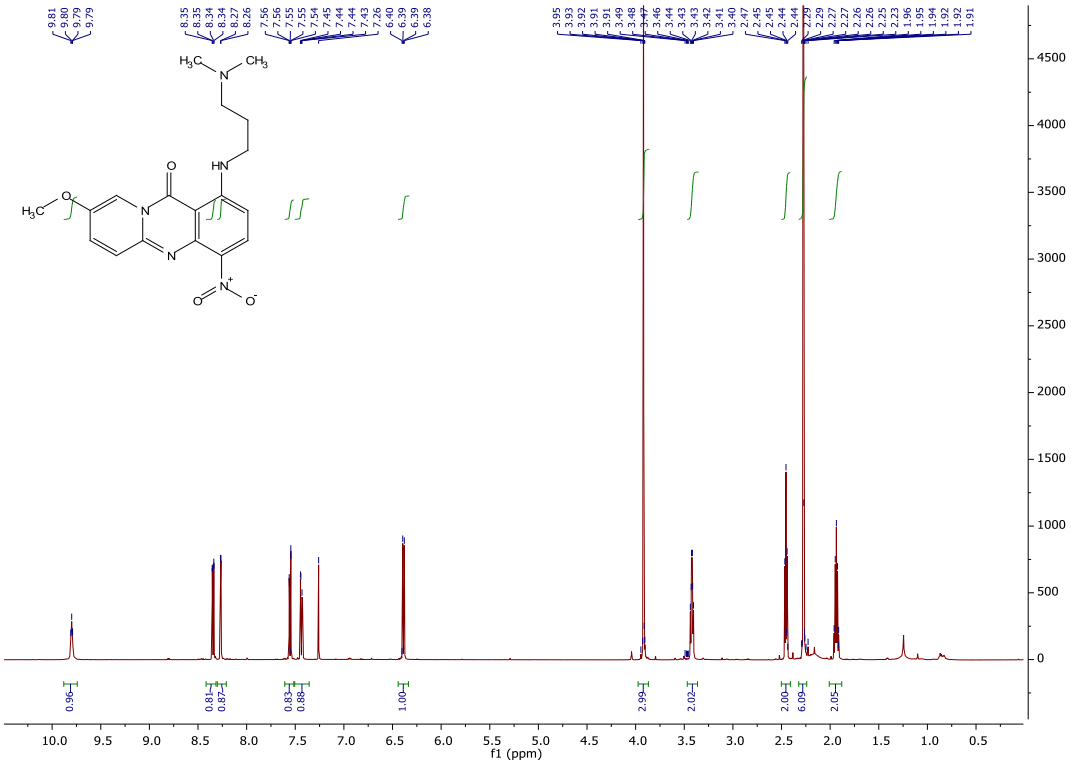


Figure S17: ^{1}H NMR spectrum of 17

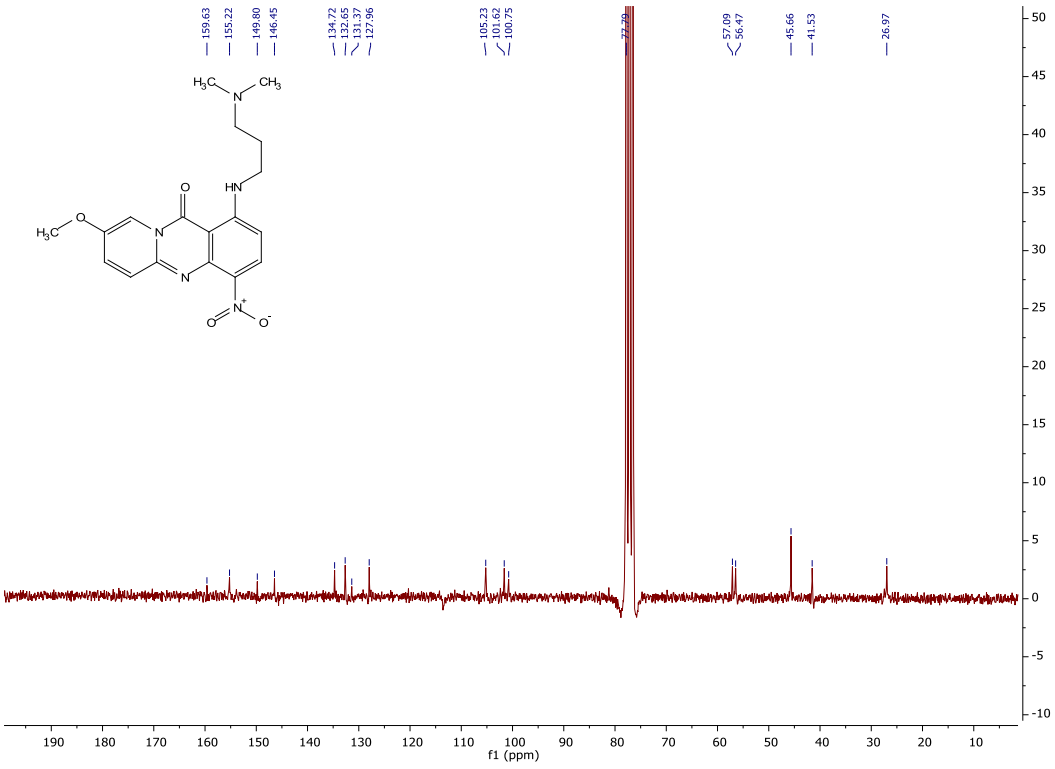


Figure S18: ^{13}C NMR spectrum of 17

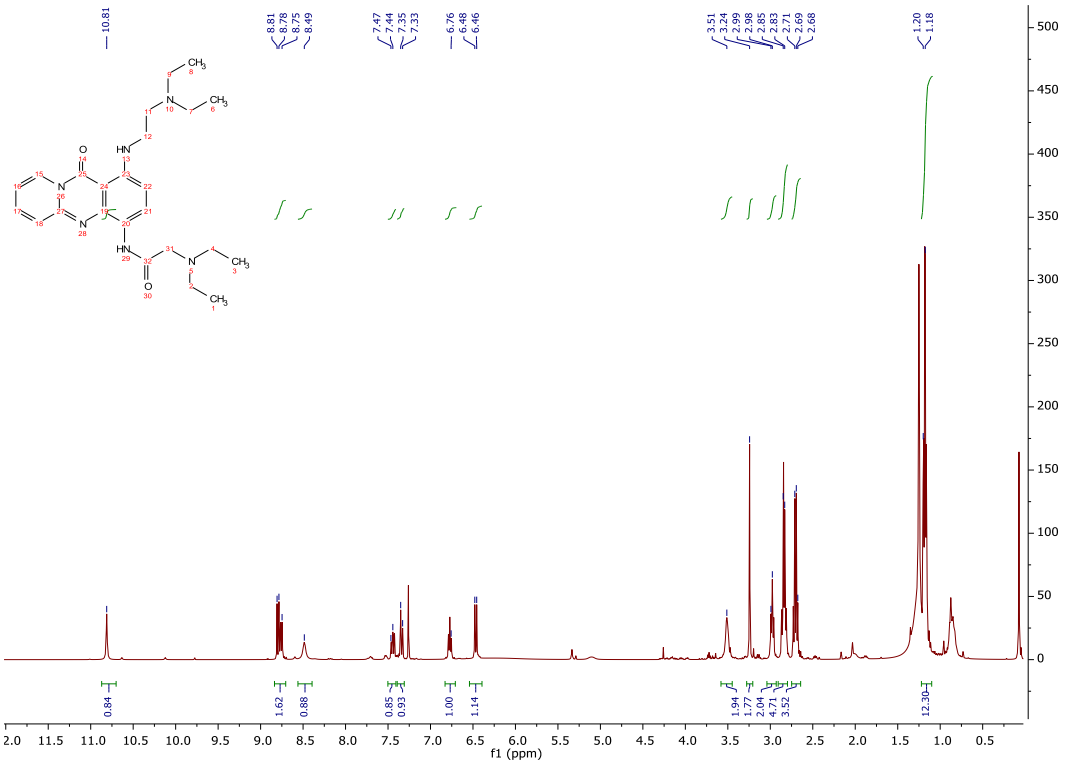


Figure S19: ^{1}H NMR spectrum of 34

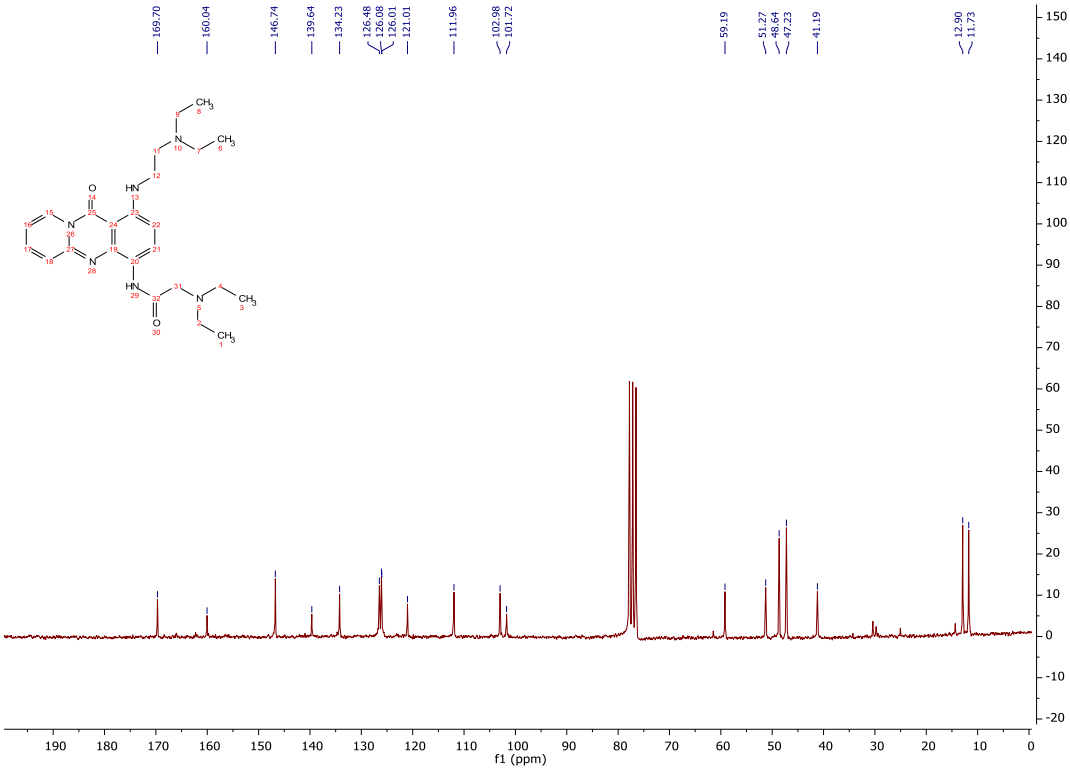


Figure S20: ^{13}C NMR spectrum of 34

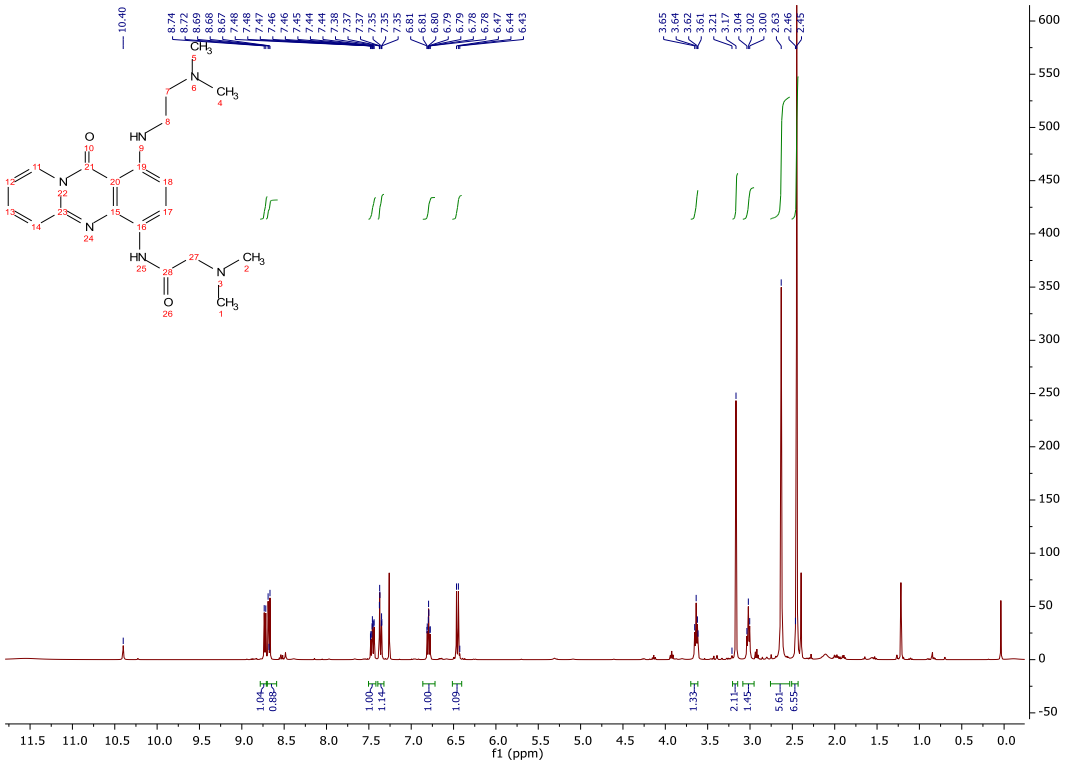


Figure S21: ^{1}H NMR spectrum of 35

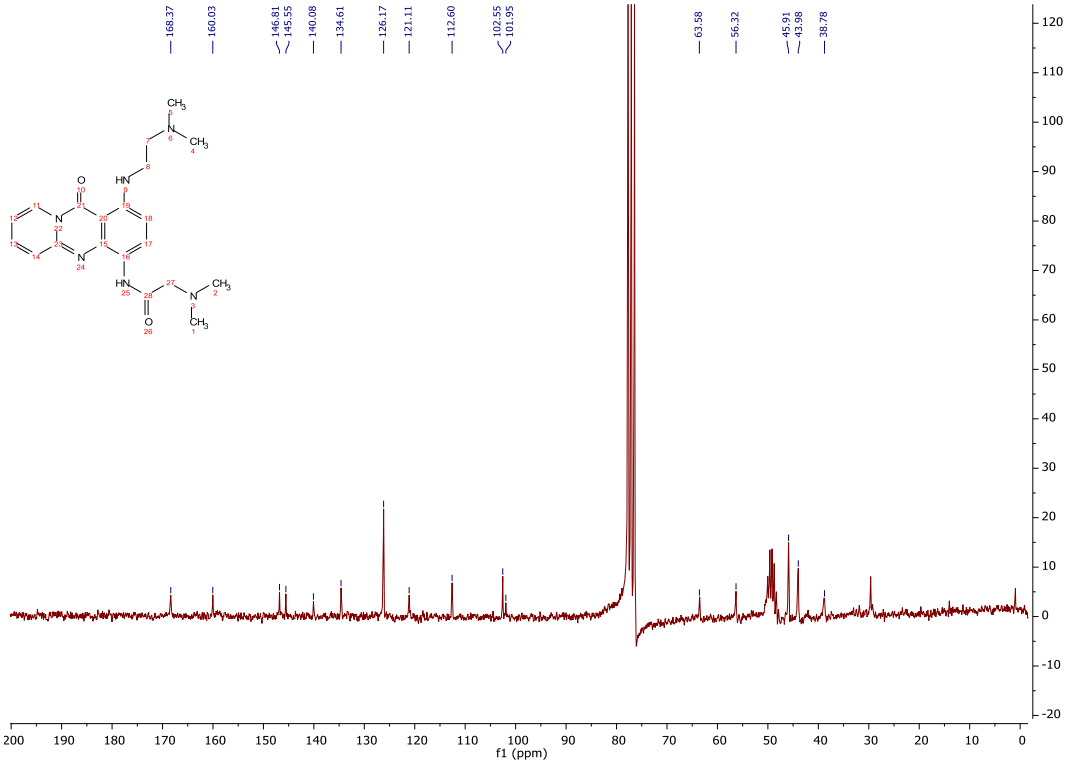


Figure S22: ^{13}C NMR spectrum of 35

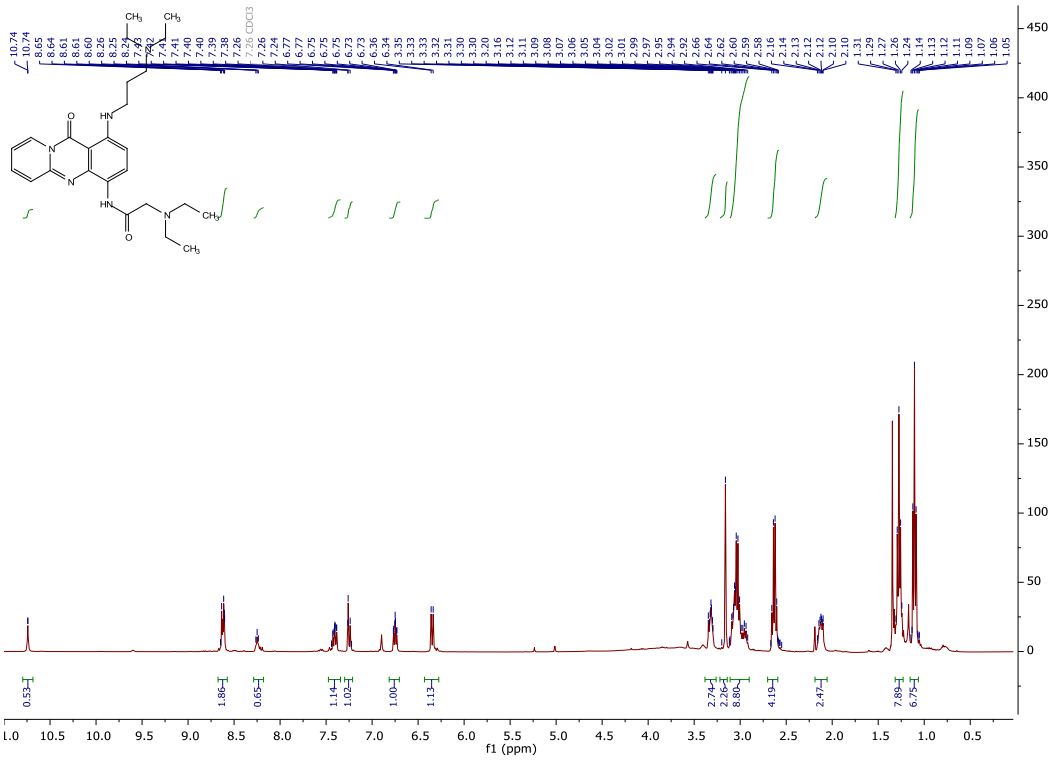


Figure S23: ^{1}H NMR spectrum of 36

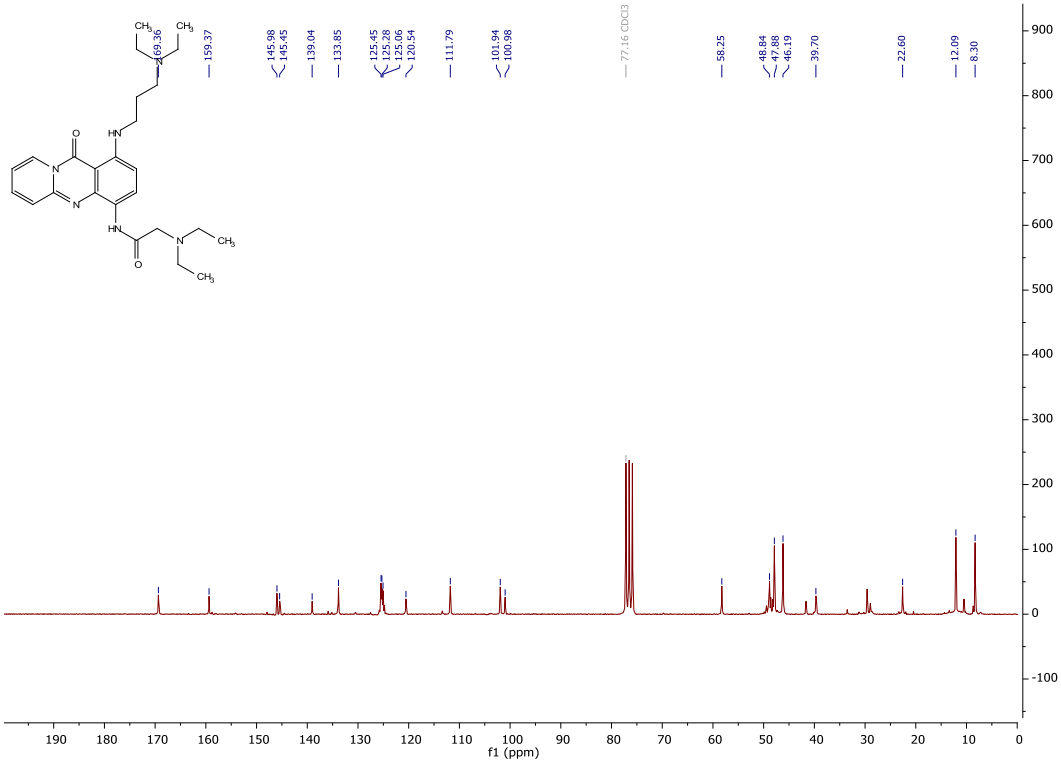


Figure S24: ^{13}C NMR spectrum of 36

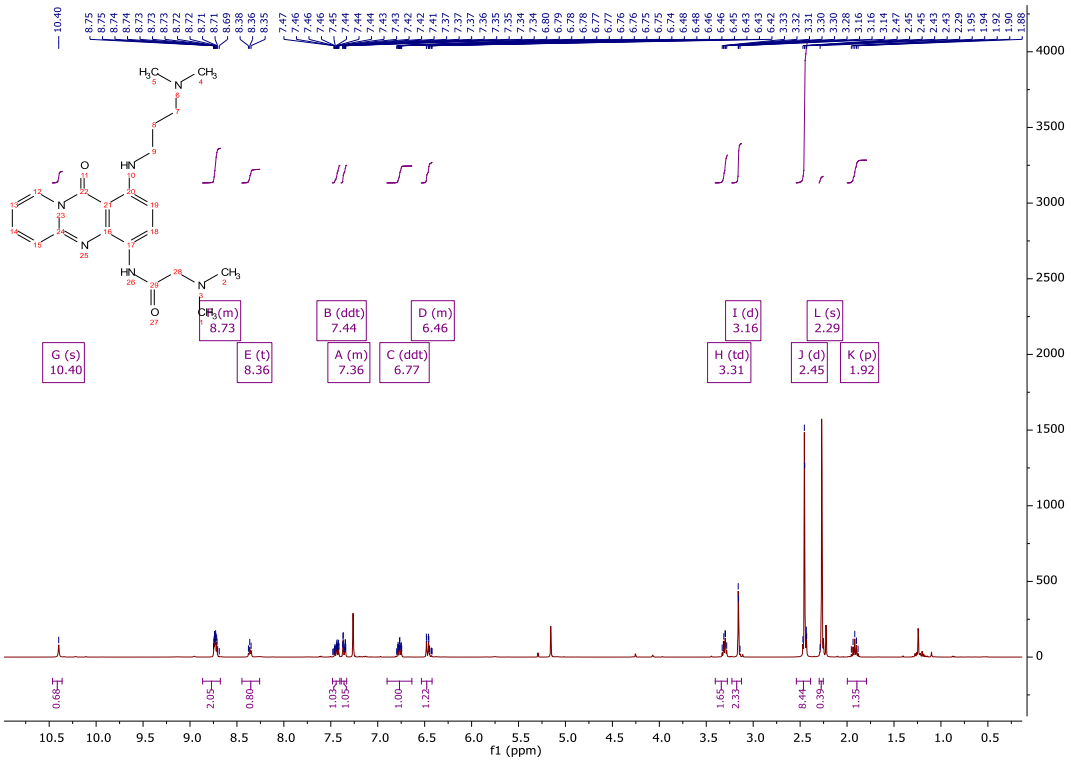


Figure S25: ^{1}H NMR spectrum of 37

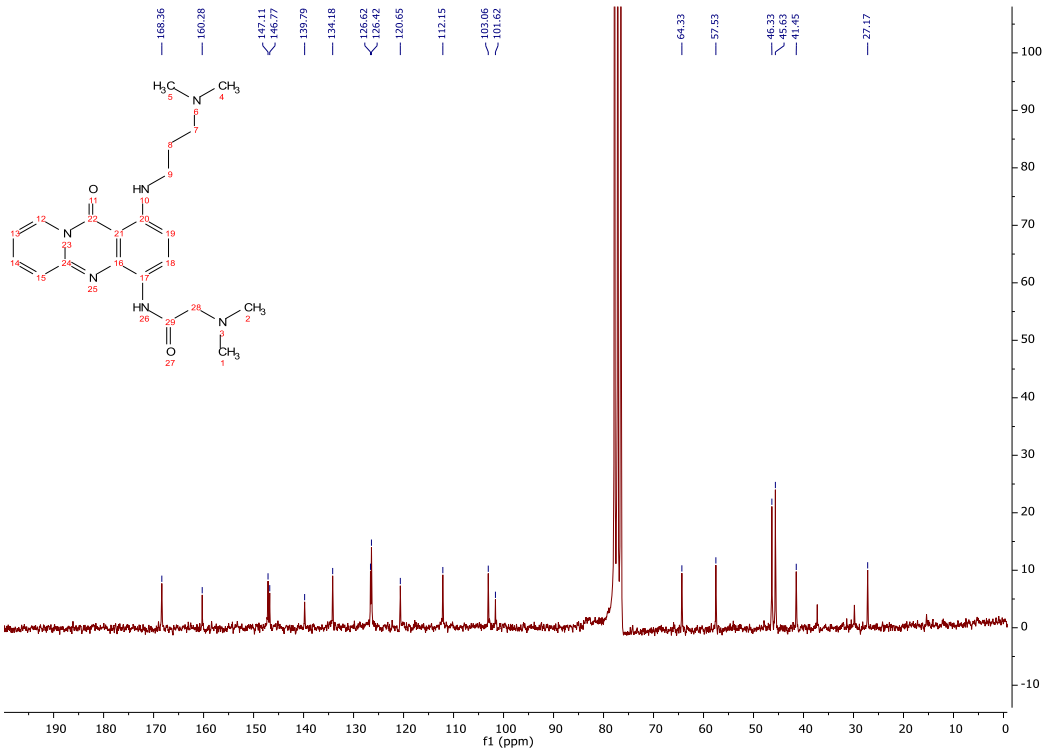


Figure S26: ^{13}C NMR spectrum of 37

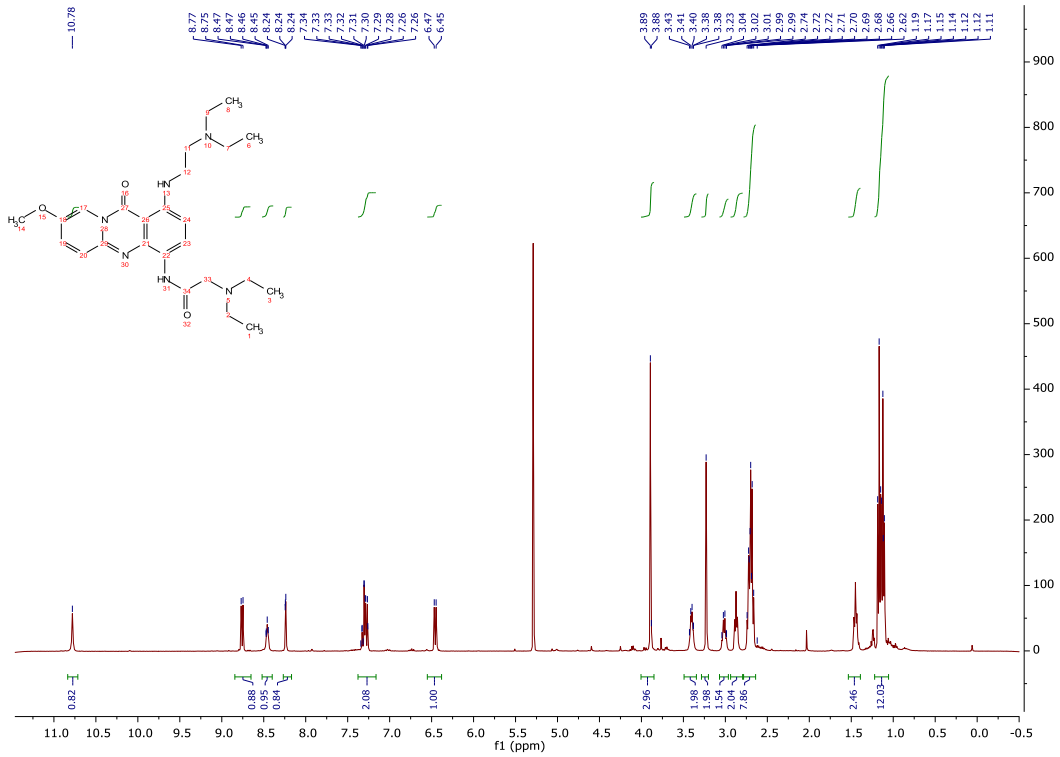


Figure S27: ^{1}H NMR spectrum of 38

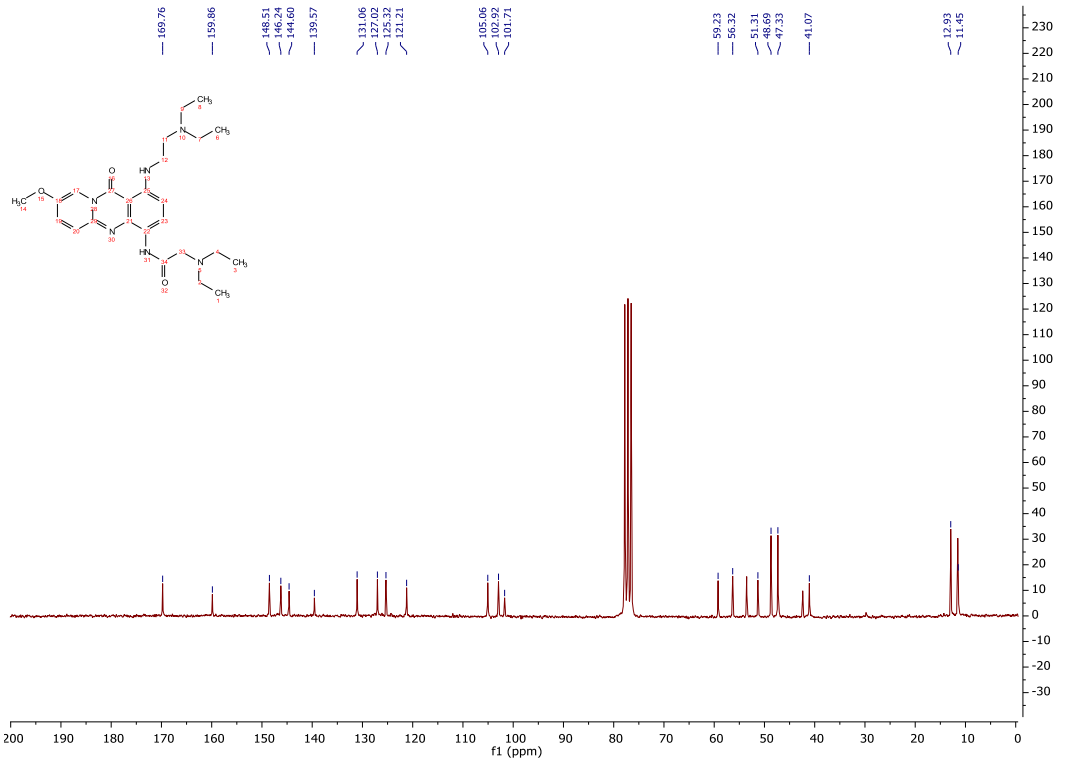


Figure S28: ^{13}C NMR spectrum of 38

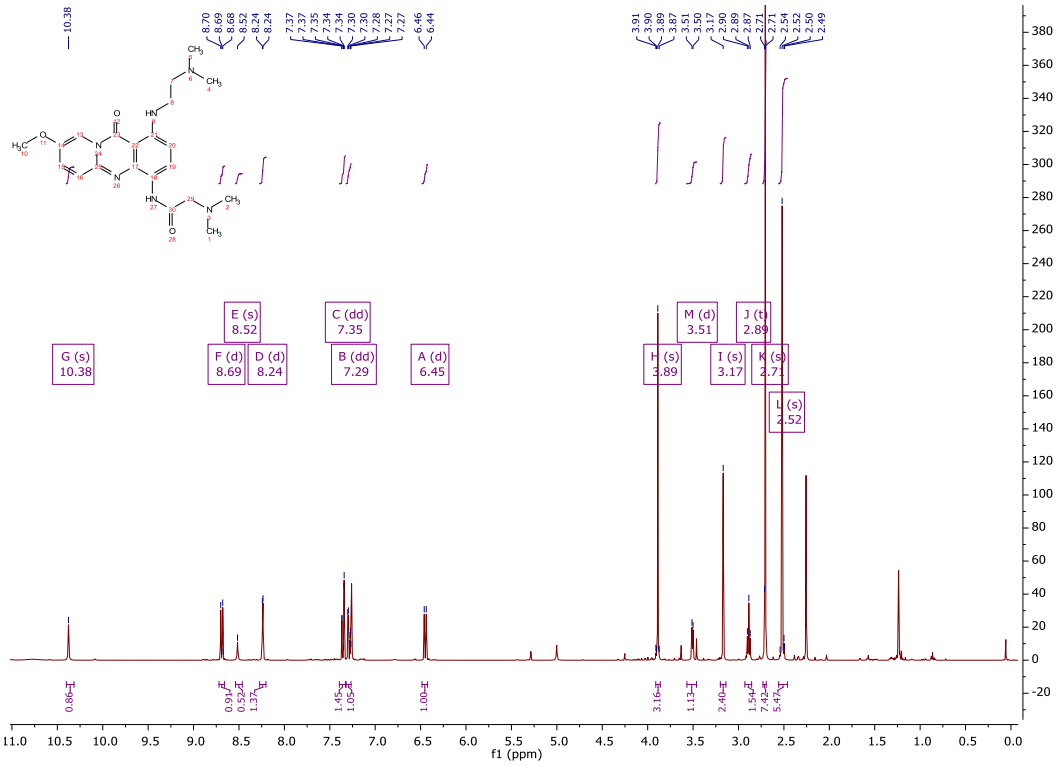


Figure S29: ^{1}H NMR spectrum of 39

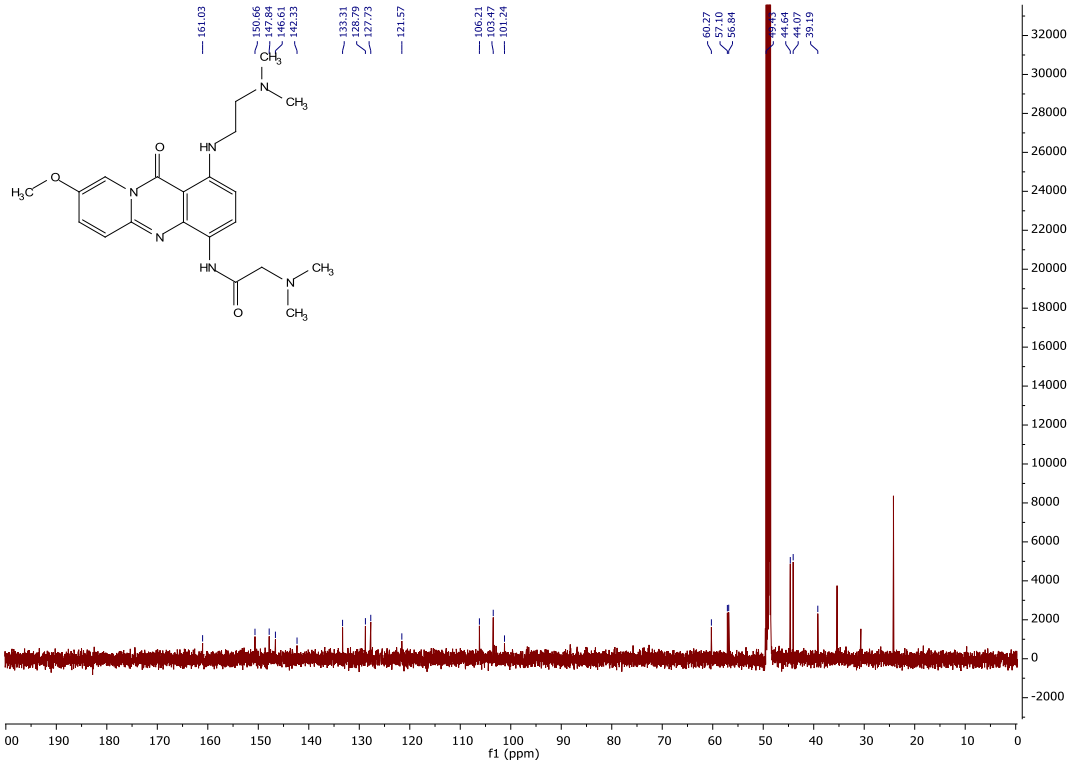


Figure S30: ^{13}C NMR spectrum of 39

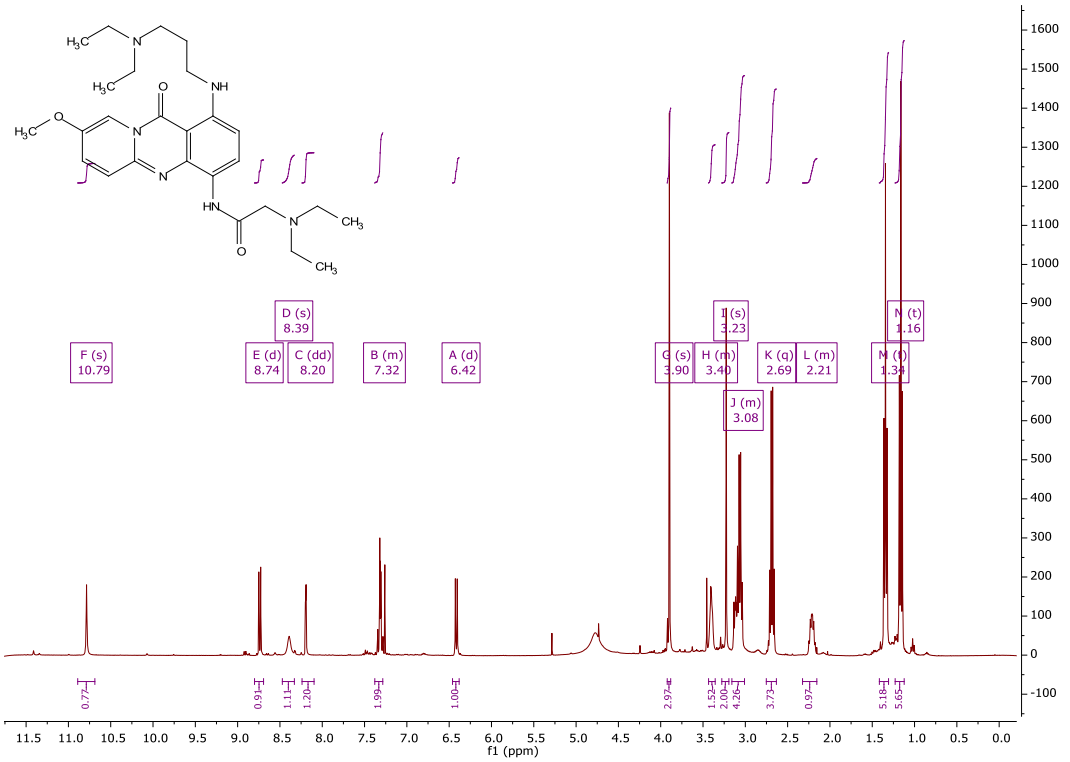


Figure S31: ^{1}H NMR spectrum of 40

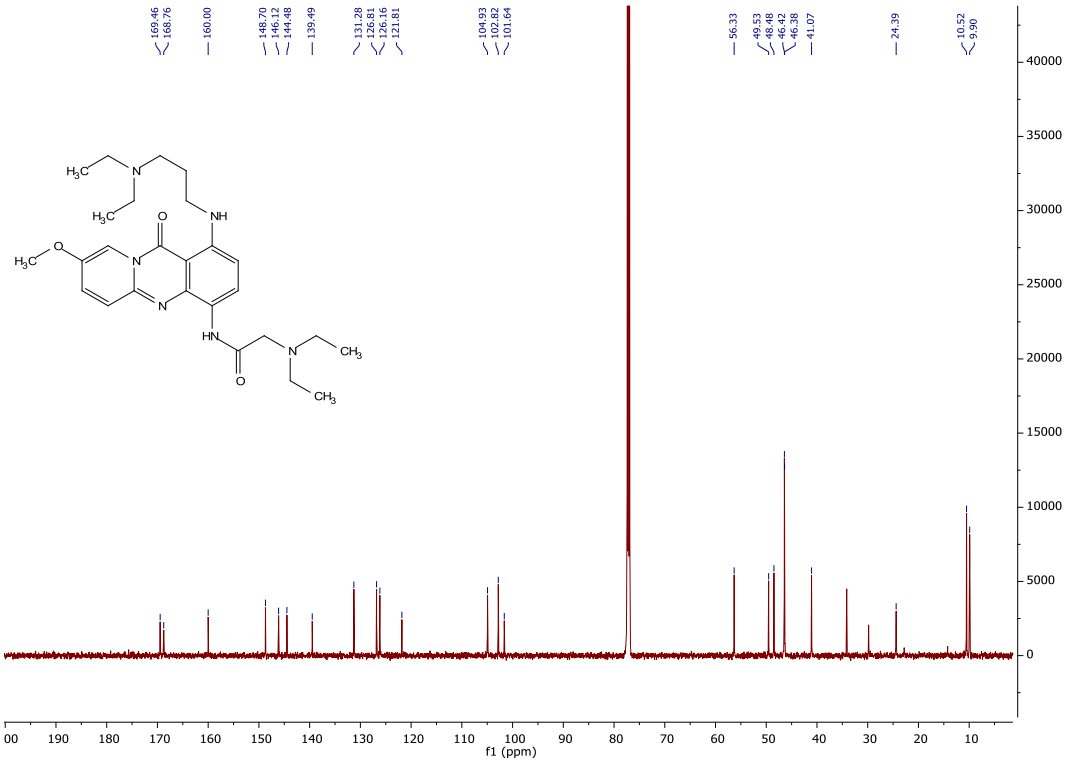


Figure S32: ^{13}C NMR spectrum of 40

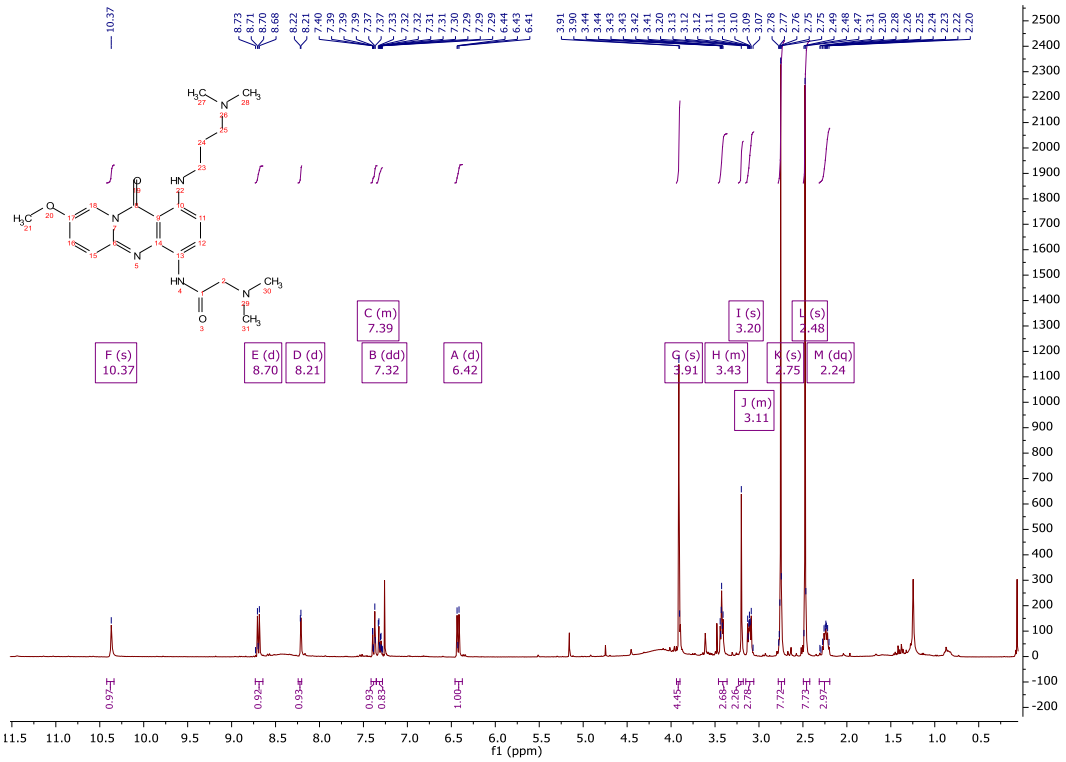


Figure S33: ^{1}H NMR spectrum of 41

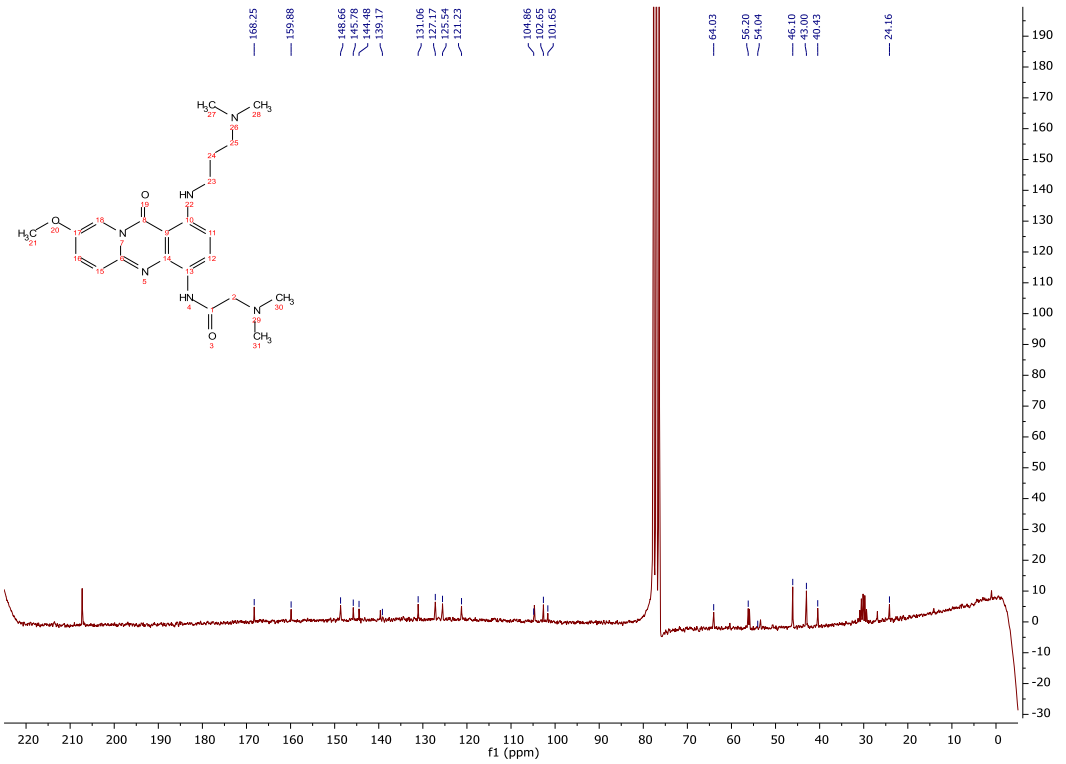


Figure S34: ^{13C} NMR spectrum of 41

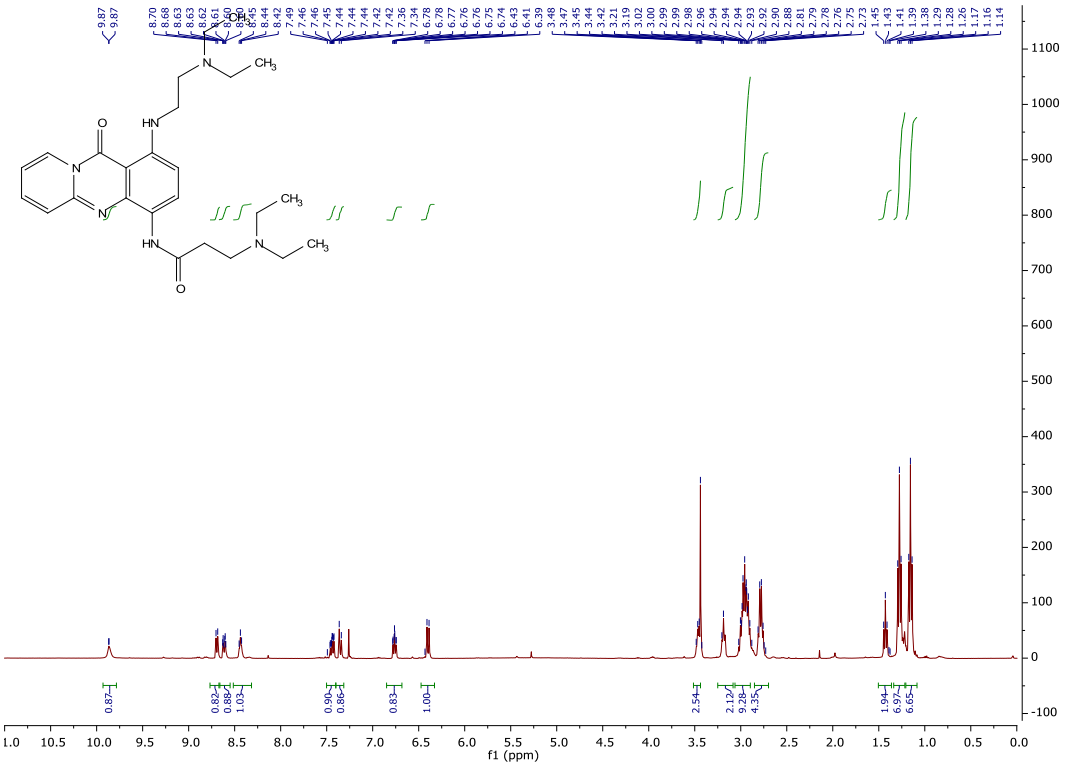


Figure S35: ^{1}H NMR spectrum of 50

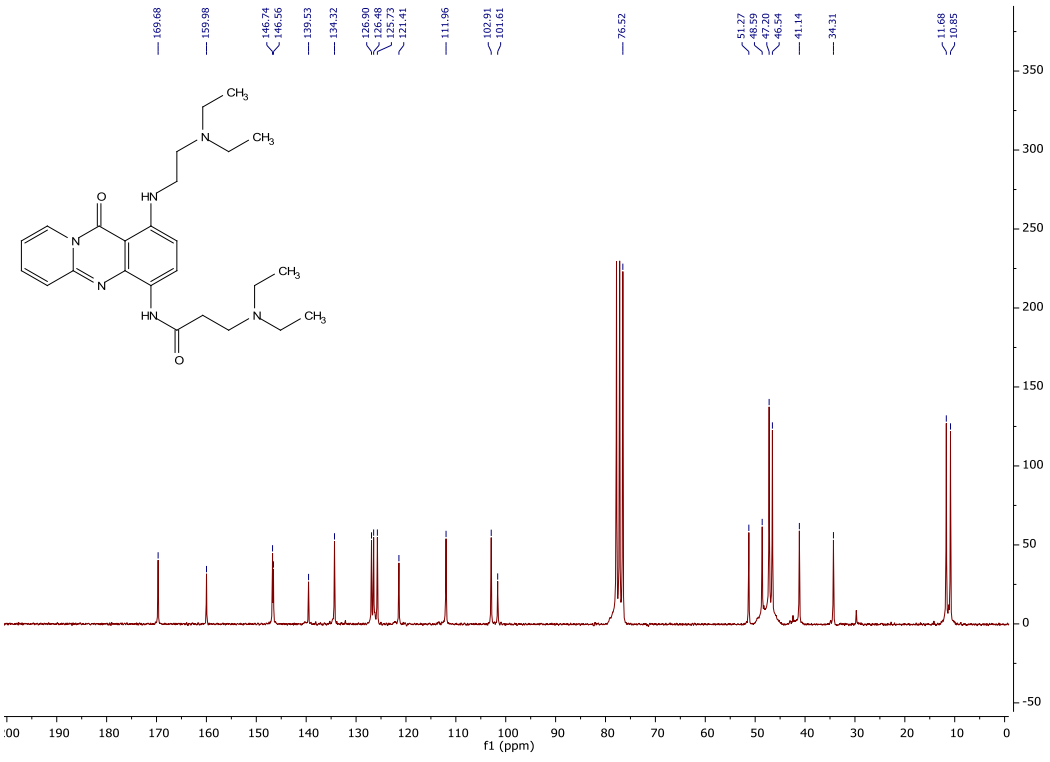


Figure S36: ^{13}C NMR spectrum of 50

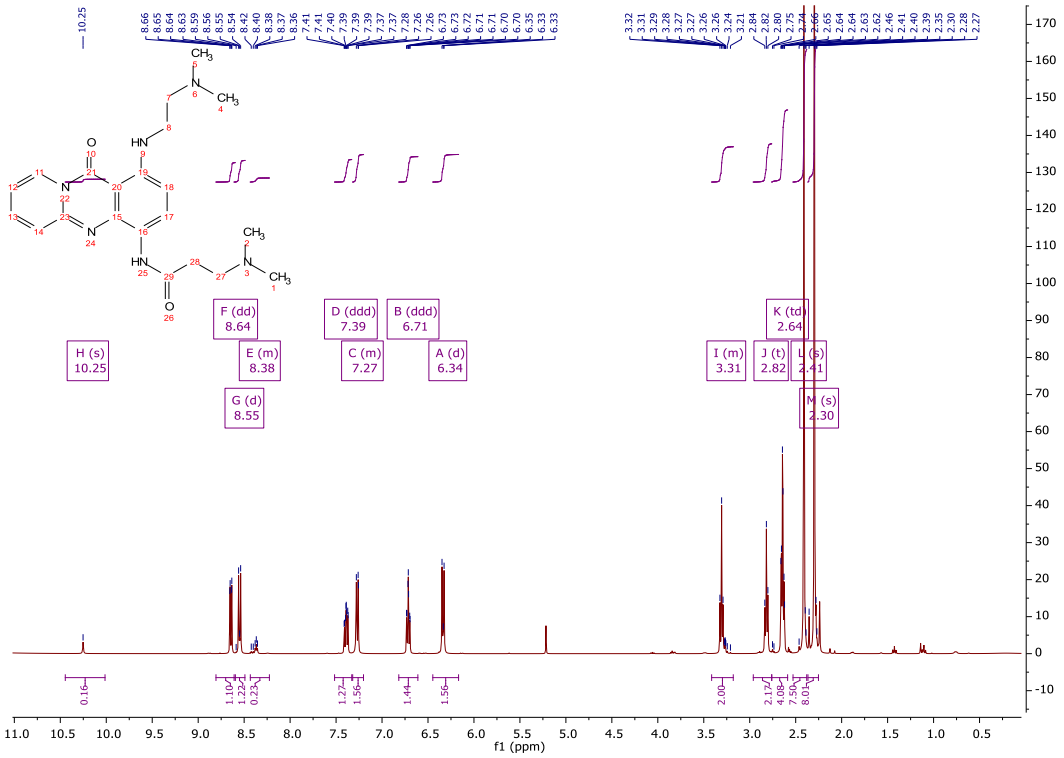


Figure S37: ^{1}H NMR spectrum of 51

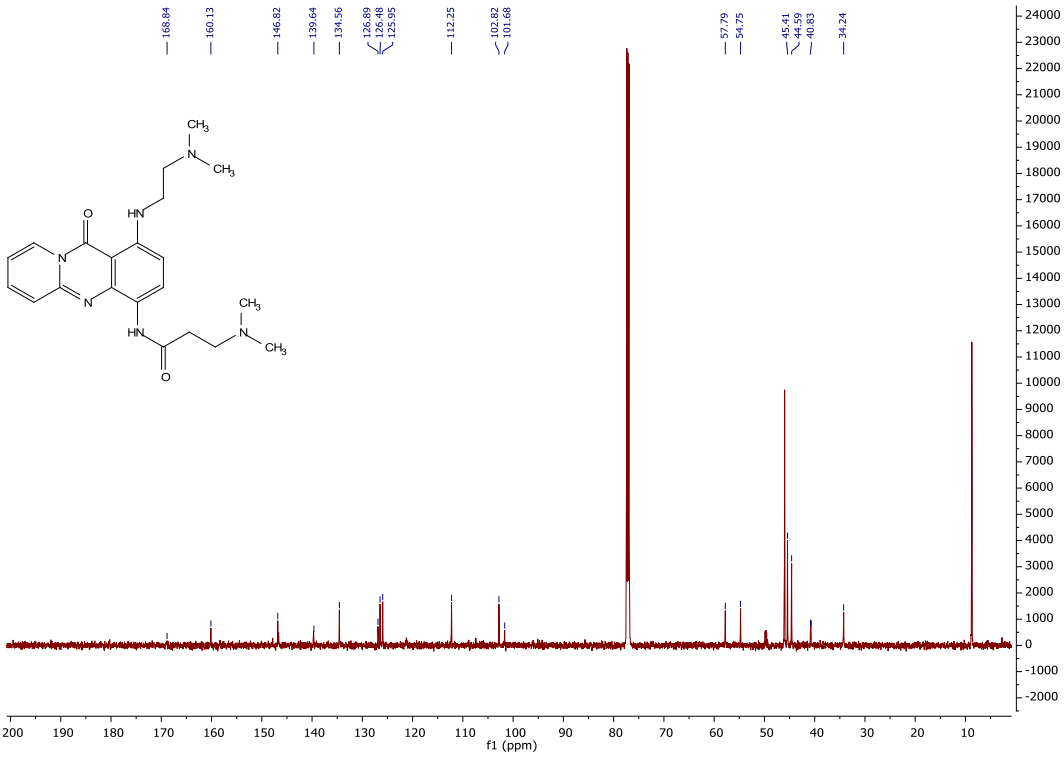


Figure S38: ^{13}C NMR spectrum of 51

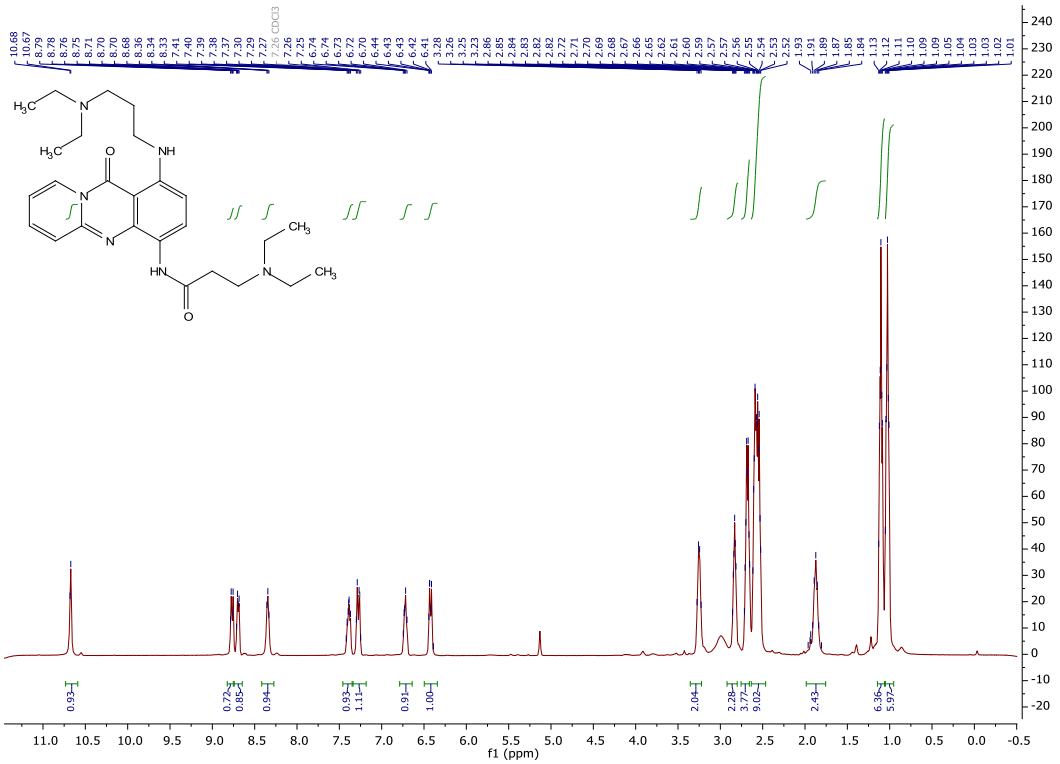


Figure S39: ^{1}H NMR spectrum of 52

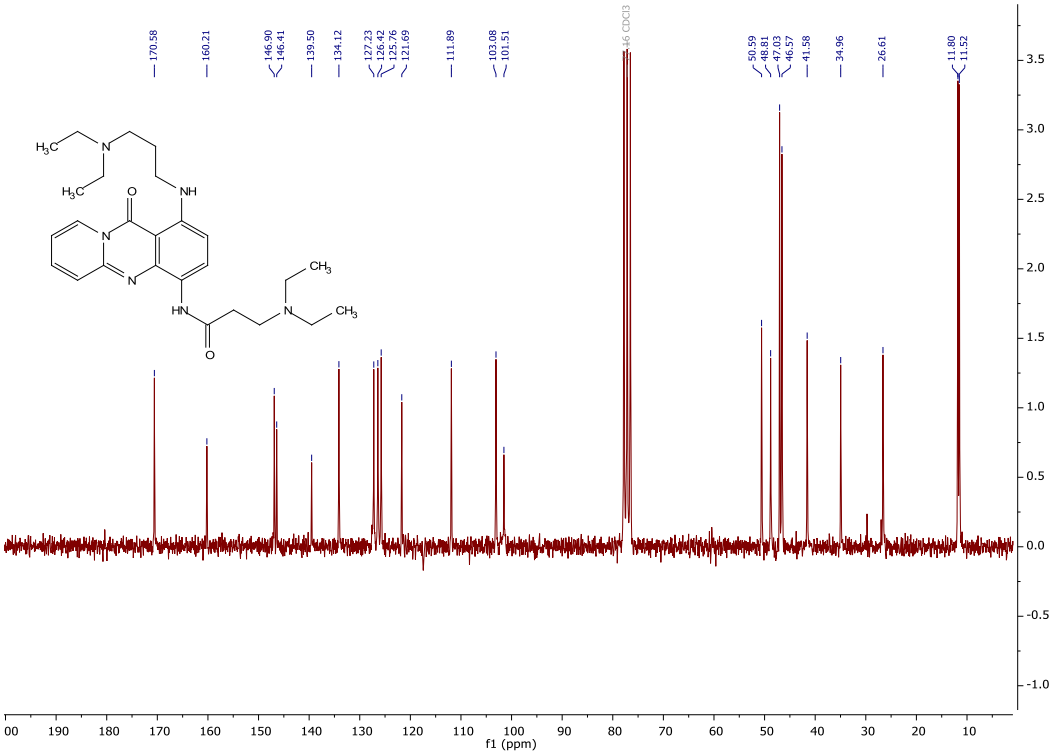


Figure S40: ^{13}C NMR spectrum of 52

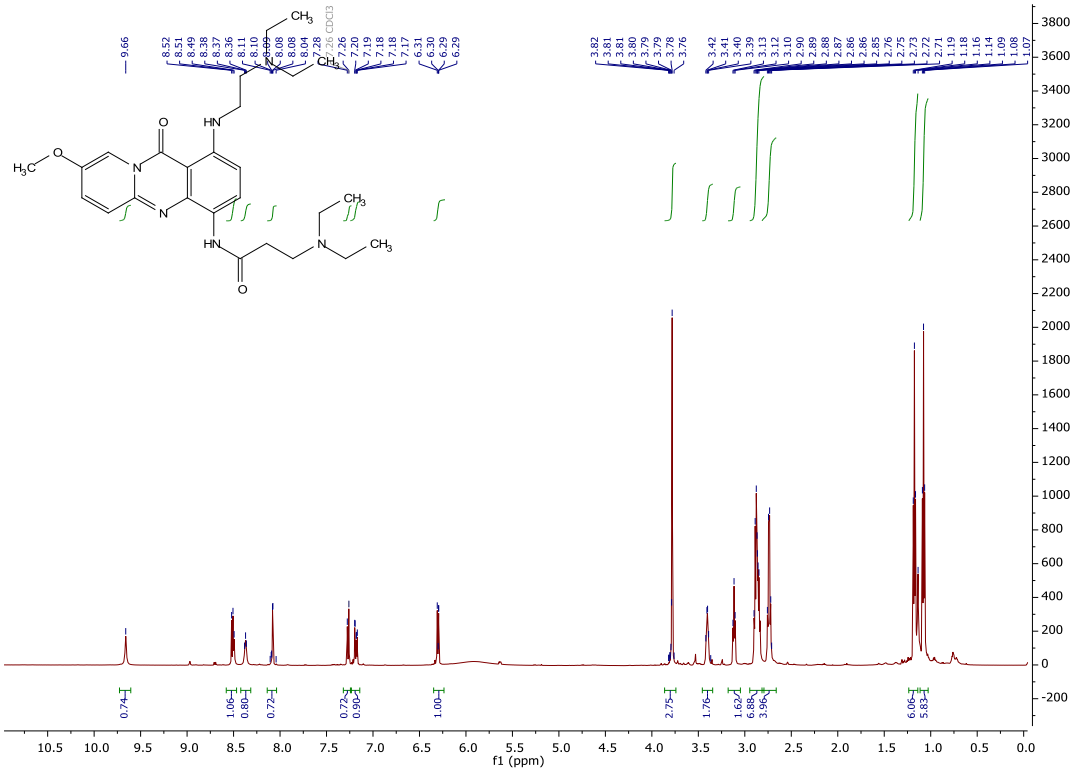


Figure S41: ^{1}H NMR spectrum of 54

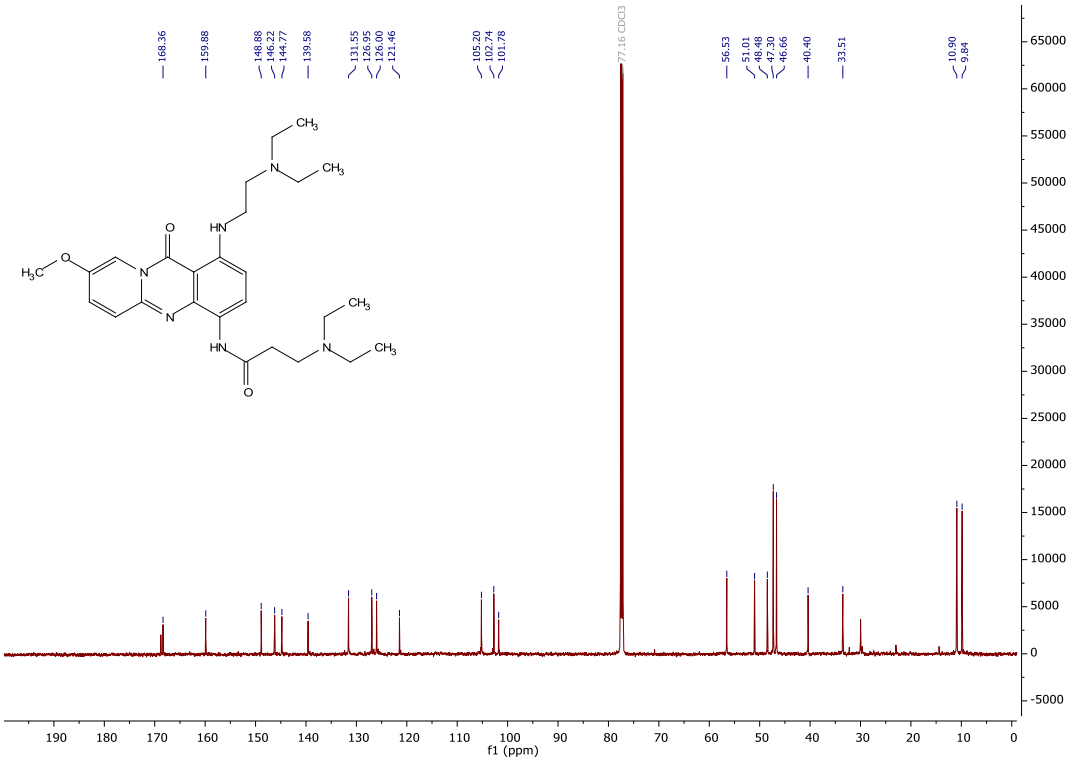


Figure S42: ^{13}C NMR spectrum of 54

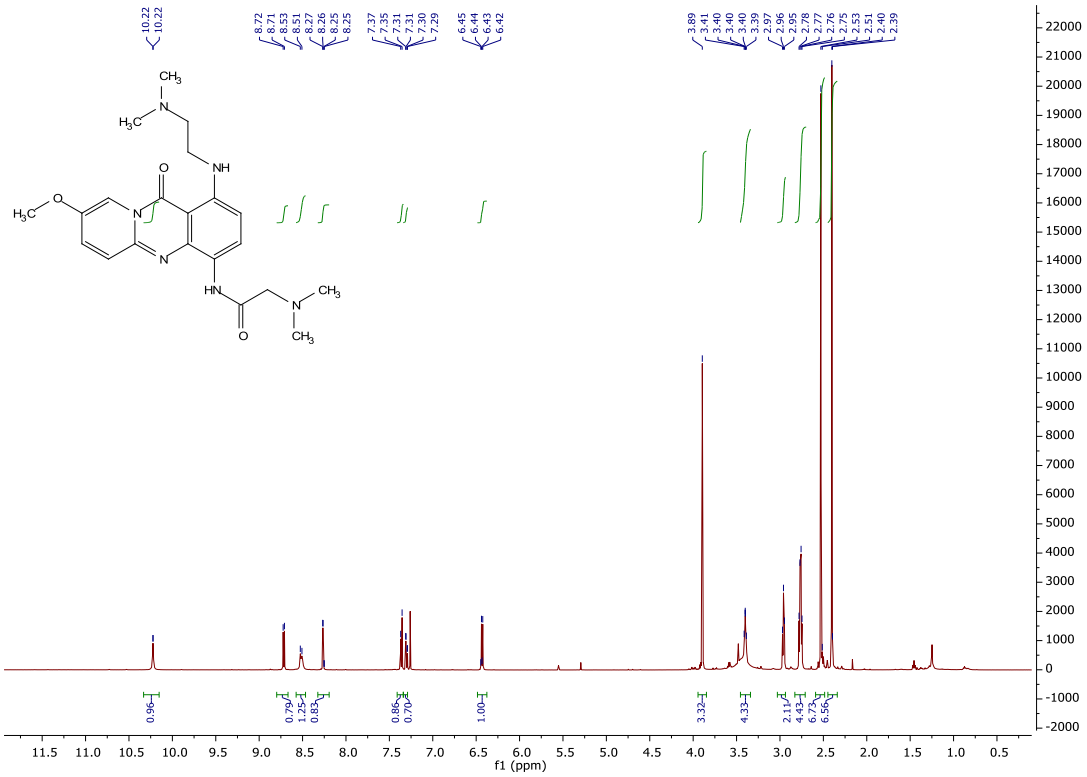


Figure S43: ^{1}H NMR spectrum of 55

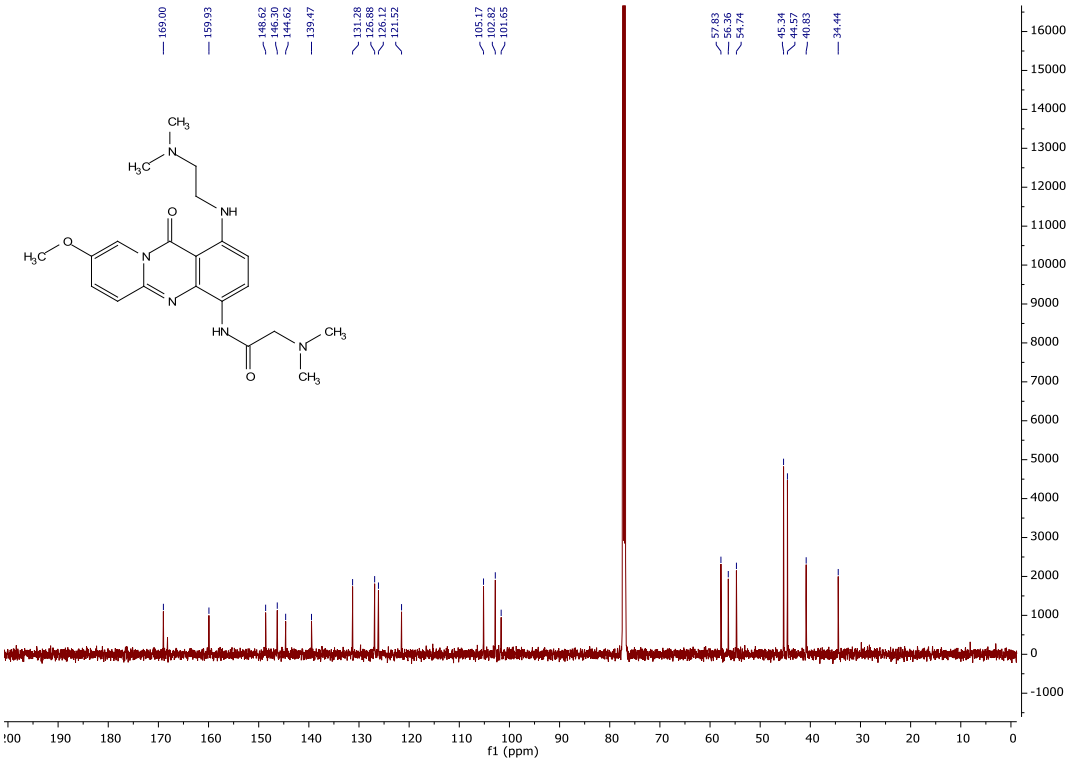


Figure S44: ^{13}C NMR spectrum of 55

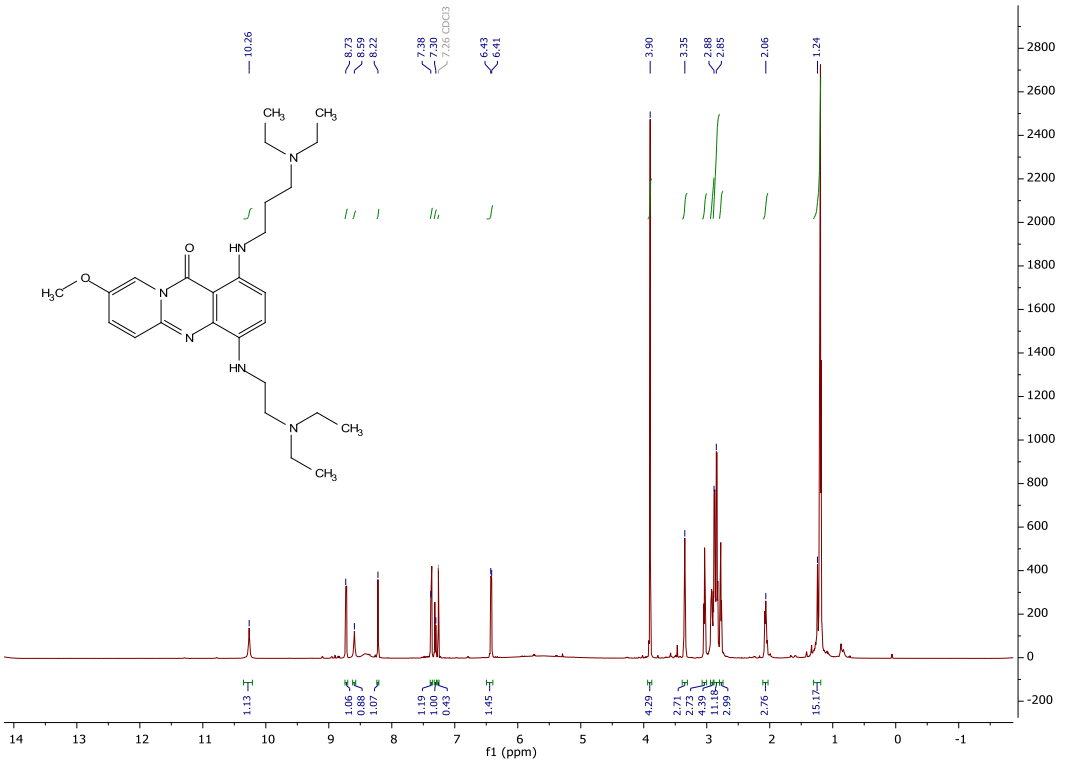


Figure S45: ^{1}H NMR spectrum of 56

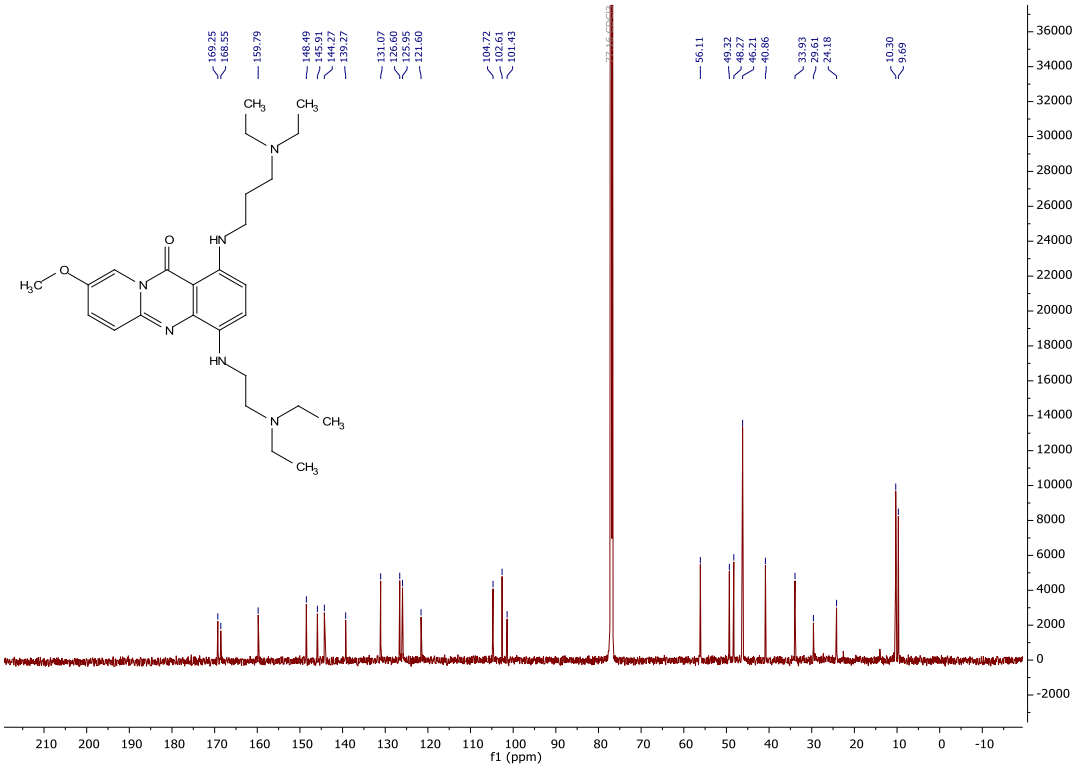


Figure S46: ^{13}C NMR spectrum of 56

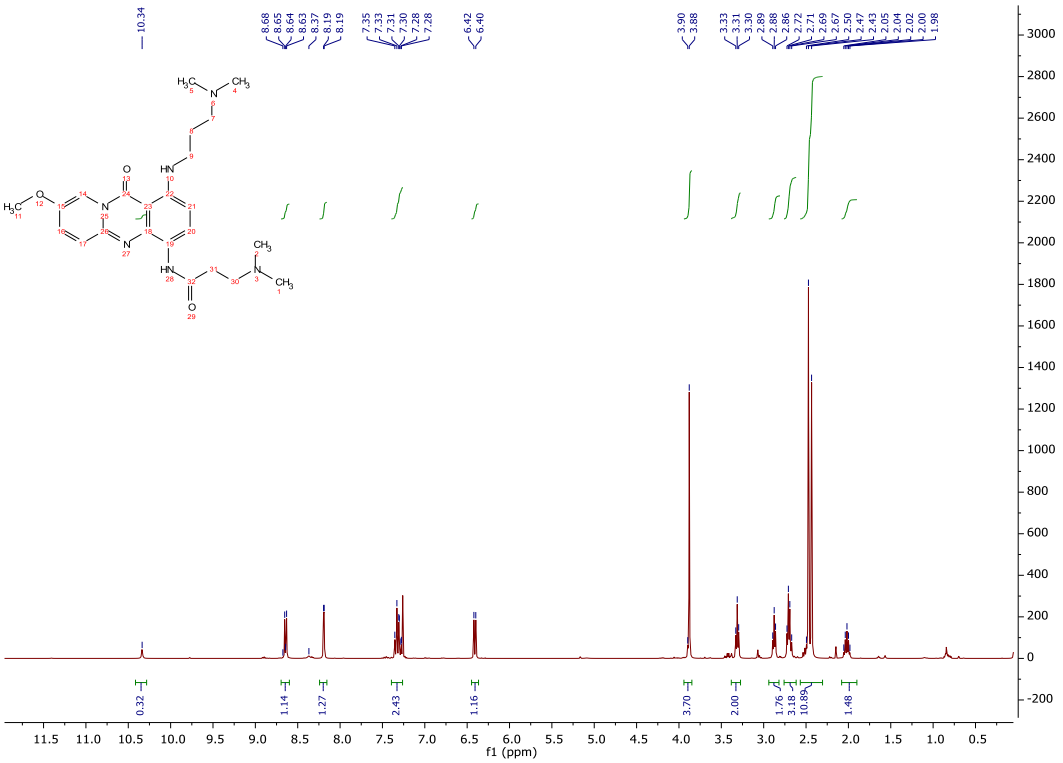


Figure S47: ^{1}H NMR spectrum of 57

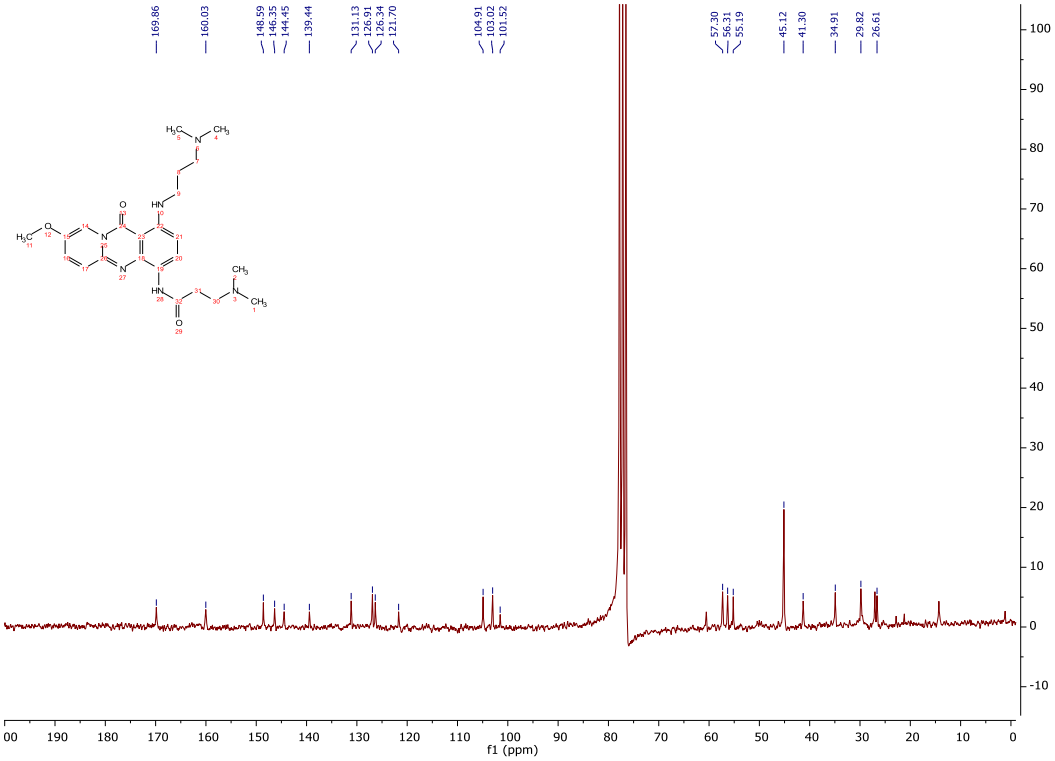


Figure S48: 13C NMR spectrum of 57