Supporting Information

Synthesis and Photophysical Investigation of Squaraine Rotaxanes by "Clicked Capping"

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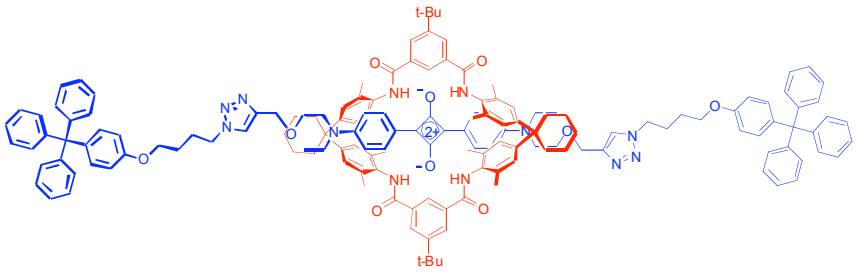
Contents

Synthesis:

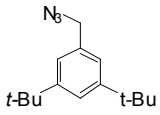
Compounds **M2**,[1] **M3**,[2] **D1**,[2] **D2**,[2] **S1**[3] and **S3**[4] were prepared from previously reported procedures.



Procedure to synthesize rotaxane M2⊃T1 and dye thread T1

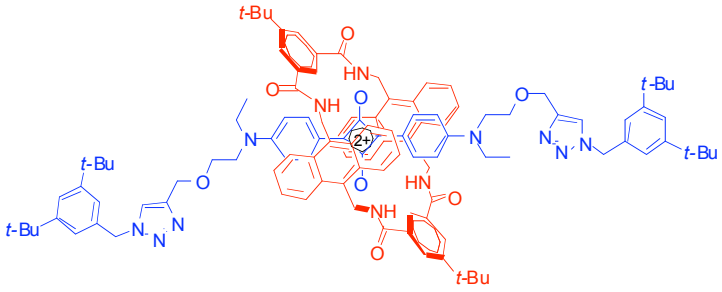
Macrocycle **M2** (23 mg, 0.023 mmol), squaraine dye **D1** (24 mg, 0.050 mmol), trityl azide **S3** (75 mg, 0.17 mmol), triethylamine (0.017 mL, 0.12 mmol), and *tris*(triphenylphosphine)-copper(I) bromide (8.0 mg, 0.0086 mmol) were mixed with dichloromethane (2 mL) at 50 °C for 2 days in a sealed tube. The solution was purified by column chromatography on silica gel with a gradient starting from pure chloroform to 3% methanol in chloroform. The first blue fraction collected was the desired product, **M2⊃T1** (21 mg, 0.009 mmol, yield of 40%). λ_{max} (abs, $CHCl_3$) = 645 nm, log ε = 5.23, λ_{max} (em, $CHCl_3$) = 656 nm; δ_H (600 MHz, $CDCl_3$) 9.15 (s, 2 H), 8.72 (s, 4 H), 8.42 (d, *J*=1.5 Hz, 4 H), 7.86 (d, *J*=9.4 Hz, 4 H), 7.54 (s, 2 H), 7.26 - 7.21 (m, 12 H), 7.21 - 7.15 (m, 18 H), 7.10 (d, *J*=9.1 Hz, 4 H), 6.76 (s, 8 H), 6.73 (d, *J*=9.1 Hz, 4 H), 6.64 (d, *J*=9.4 Hz, 4 H), 4.60 (s, 4 H), 4.40 (t, *J*=7.0 Hz, 4 H), 3.94 (t, *J*=5.9 Hz, 4 H), 3.75 (t, *J*=5.6 Hz, 4 H), 3.65 (t, *J*=5.6 Hz, 4 H), 3.56 (q, *J*=7.3 Hz, 4 H), 2.23 (br s, 8 H), 2.10 (dt, *J*=14.7, 7.6 Hz, 4 H), 2.04 (s, 24 H), 1.78 (dt, *J*=13.2, 6.5 Hz, 4 H), 1.55 (s, 18 H), 1.45 (s, 12 H), 1.23 (t, *J*=7.3 Hz, 6 H); δ_C (75 MHz, $CDCl_3$) 184.8, 184.2, 164.9, 156.6, 153.4, 153.3, 146.9, 144.1, 139.2, 134.4, 134.0, 132.2, 132.2, 131.0, 130.1, 129.0, 127.4, 125.8, 125.4, 125.3, 122.6 113.1, 112.3, 67.7, 66.7, 64.5, 64.3, 50.4, 50.0, 46.4, 44.9, 35.4, 34.4, 34.3, 31.3, 27.3, 26.2, 22.8, 18.8, 12.2; *m/z* (ESI) 1185.5 [$(M/2)^+$, 100%]

T1: The third colored fraction from the above column was pure "clicked" dye thread, **T1** (0.66 mg). λ_{max} (abs, $CHCl_3$) = 635 nm, log ε = 4.91, λ_{max} (em, $CHCl_3$) = 649; δ_H (600 MHz, $CDCl_3$) 8.29 (d, *J*=9.1 Hz, 4 H), 7.37 (s, 2 H), 7.19 - 7.14 (m, 12 H), 7.14 -7.09 (m, 18 H), 7.02 (d, *J*=8.8 Hz, 4 H), 6.68 (d, *J*=9.1 Hz, 4 H), 6.66 (d, *J*=8.8 Hz, 4 H), 4.56 (s, 4 H), 4.34 (t, *J*=7.0 Hz, 4 H), 3.87 (t, *J*=5.9 Hz, 4 H), 3.69 (t, *J*=5.3 Hz, 4 H), 3.59 (t, *J*=5.3 Hz, 4 H), 3.48 (q, *J*=6.8 Hz, 4 H), 2.01 (dt, *J*=14.7, 7.0 Hz, 4 H), 1.70 (dt, *J*=14.4, 6.5 Hz, 4 H), 1.15 (t, *J*=7.0 Hz, 6 H); δ_C (75 MHz, $CDCl_3$): 156.6, 155.3, 133.5, 147.0, 139.1, 133.3, 132.2, 131.1, 127.4, 125.8, 113.1, 112.5, 67.9, 66.7, 64.75, 50.2, 50.1, 46.3, 29.7, 27.3, 26.3, 12.3; *m/z* (FAB) 1352 [$(M-H)^+$ (2.5%)], 1351 (100).



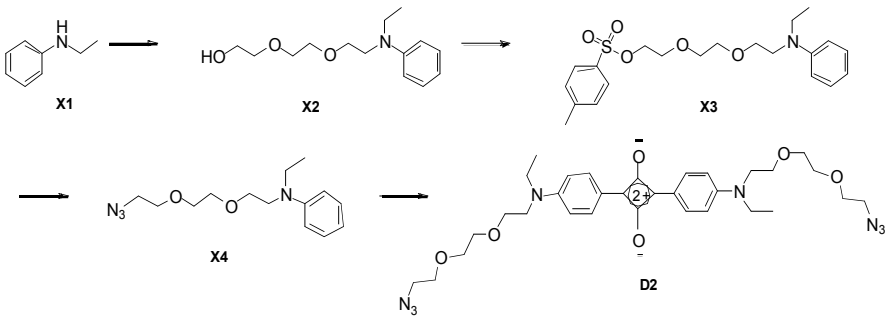
Procedure to prepare 3,5-di-(tert-butyl)benzyl azide S2

3,5-di-(*tert*-butyl)benzyl bromide (2.0 g, 7.0 mmol) was added in small portions to a solution of sodium azide in DMSO (0.5 M, 15.5 mL) at 25 °C, and the mixture was stirred for 3 h. Water (50 mL) was added to quench the reaction and the organic material was extracted with ether (3 x 35 mL), washed with water (2 x 50 mL) and brine (50 mL), dried (Na_2SO_4) and concentrated. The oily residue was purified by column chromatography using silica gel (0-2% ethyl acetate/hexane) to give 3,5-di-(*tert*-butyl)benzyl azide **S2** as a colorless oil (1.42 g, 0.006 mmol, yield of 82%); δ_H (500 MHz, $CDCl_3$) 7.40 (t, *J*=1.7, 1H), 7.14 (d, *J*=1.9, 2H), 4.34 (s, 2H), 1.34 (s, 18H); δ_C (125 MHz, $CDCl_3$) 151.4, 134.5, 122.4, 122.3, 55.5, 34.8, 31.4; *m/z* (FAB) 245 [(M^+), 10%], 203 [(M^+-N_3), 100%].



Procedure to synthesize rotaxane M3⊃T2

The squaraine dye **D1** (10 mg, 0.021 mmol) and the anthrylene macrocycle **M3** (22 mg, 0.026 mmol) were dissolved in chloroform (0.4 mL). 3,5-di-(*tert*-butyl)benzyl azide **S2** (13 mg, 0.053 mmol) dissolved in chloroform (0.1 mL), *tris*(triphenylphosphine)copper(I) bromide (4.0 mg, 0.0043 mmol) and diisopropylethylamine (3.0 mg, 0.027 mmol) were added and the reaction mixture was stirred at 50 °C for 21 hours. The solution was concentrated and the crude material was purified twice by column chromatography using silica gel (0-0.2% MeOH/$CHCl_3$) to give the squaraine rotaxane **M3⊃T1** as a dark green solid (35 mg, 0.019 mmol, yield of 90%); λ_{max} (abs, $CHCl_3$) = 661 nm, log ε = 5.24, λ_{max} (em, $CHCl_3$) = 704 nm; λ_{max} (abs, MeOH) = 666 nm, ε = 5.29; λ_{max} (em, MeOH) = 705 nm; δ_H (500 MHz, $CDCl_3$) 9.35 (s, 2H), 8.52 (s, 4H), 8.24 (t, *J*=6.0, 4H), 7.71 (m, 8H), 7.52 (br s, 2H), 7.40 (br s, 2H), 7.09 (d, *J*=1.5, 4H), 6.97 (d, *J*=9.0, 4H), 6.28 (m, 8H), 6.08 (d, *J*=9.0, 4H), 5.49 (s, 4H), 5.19 (d, *J*=6.0, 8H), 4.71 (s, 4H), 3.79 (t, *J*=5.5, 4H), 3.63 (t, *J*=5.5, 4H), 3.58 (q, *J*=7.0, 4H), 1.53 (s, 18H), 1.27 (s, 36H), 1.26 (t, *J*=7.0, 6H); δ_C (125 MHz, $CDCl_3$) 183.9, 179.6, 167.1, 153.1, 152.8, 151.9, 144.5, 133.6, 133.3, 132.9, 130.4, 128.9, 128.5, 125.7, 123.9, 122.8, 122.6, 122.5, 122.4, 117.1, 111.4, 67.9, 64.5, 54.8, 50.2, 46.3, 38.0, 35.3, 34.8, 31.4, 31.3, 12.5; *m/z* (FAB) 1819 [$(M)^+$, 56%], 1818 [$(M-H)^+$, 60%], 974 (100).



Procedure to synthesize D2

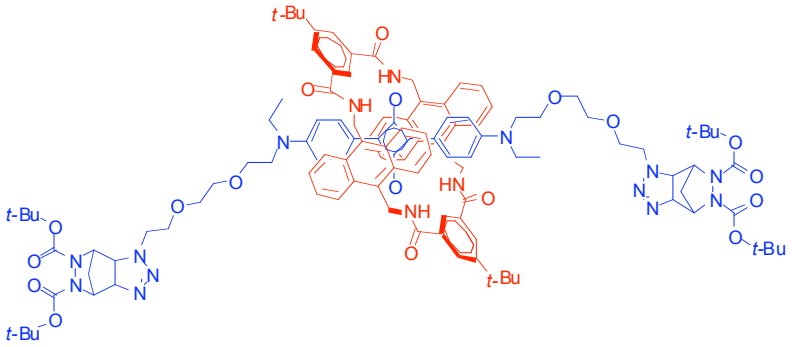
Commercially available N-ethylaniline (**X1**) (1.0 g, 8.2 mmol), 2-[2-(2-chloroethoxy)ethoxy]ethanol (1.3 mL, 9.0 mmol) and powdered $CaCO_3$ (8.0 g, 80 mmol) were mixed in of water (100 mL) and stirred at reflux for 3 days in the dark**.** The resulting light sensitive compound was chromatographed on silica (40% EtOAc / 60% Hex) to give **X2** (0.8707 g, 3.4 mmol, yield of 42%) as a transparent oil. δ_H (400 MHz, $CDCl_3$) 7.24 - 7.17 (m, 2 H), 6.72 - 6.62 (m, 3 H), 3.76 - 3.70 (m, *J*=4.8, 4.8 Hz, 2 H), 3.69 - 3.58 (m, 8 H), 3.51 (t, *J*=6.8 Hz, 2 H), 3.41 (q, *J*=7.1 Hz, 2 H), 2.28 (br s, 1 H), 1.15 (t, *J*=7.1 Hz, 3 H) δ_C (125 MHz, $CDCl_3$) 148.7, 129.4, 117.4, 113.0, 72.7, 71.6, 70.9, 70.6, 62.0, 42.9, 38.7, 15.1; *m/z* (FAB) 253 [$(M)^+$, 100%].

2-(2-(2-(ethyl(phenyl)amino)ethoxy)ethoxy)ethanol (**X2**) (0.87 g, 3.4 mmol) was dissolved in dry pyridine (10 mL) and cooled to 0 °C. *p*-Toluenesulfonyl chloride (0.78 g, 4.1 mmol) was added and the mixture was allowed to warm to room temperature and stir overnight. The reaction was poured into water (50 mL) and extracted with methylene chloride. The organic layer was washed with 10% HCl (100 mL) and dried with sodium sulfate. The solvent was reduced to give 2-(2-(2-(ethyl(phenyl)amino)ethoxy)ethoxy)ethyl 4-toluenesulfonate (**X3**) (1.3 g, 3.2 mmol, yield of 94%) as a light yellow oil and was used without further purification. δ_H (400 MHz, $CDCl_3$) 7.79 (d, *J*=8.3 Hz, 2 H), 7.34 (d, *J*=8.0 Hz, 2 H), 7.24 - 7.12 (m, 2 H), 6.72 - 6.60 (m, 3 H), 4.14 (t, *J*=4.7 Hz, 2 H), 3.68 (t, *J*=4.5 Hz, 2 H), 3.60 (m, 6 H), 3.48 (t, *J*=5.7 Hz, 2 H), 3.39

(q, *J*=6.8 Hz, 2 H), 2.44 (s, 3 H), 1.14 (t, *J*=6.8 Hz, 3 H); δ_C (125 MHz, $CDCl_3$) 170.7, 148.0, 145.1 130.1, 129.5, 128.3 115.9, 112.0, 71.1, 70.9, 69.5, 69.2, 69.0, 50.2, 45.6, 21.9, 12.4; *m/z* (FAB) 407 [$(M)^+$, 100%].

Conversion to azide (**X4**) was achieved by redissolving the oil in DMF (20 mL), adding sodium azide (5 mol equivalents) and heating to 100 °C for 24 hours. Addition of water (50 mL) and extraction with methylene chloride followed by drying ($MgSO_4$) provided N-(2-(2-(2-azidoethoxy)ethoxy)ethyl)-N-ethylaniline as a yellow oil quantitatively. δ_H (400 MHz, $CDCl_3$) 7.25- 7.19 (m, 2 H), 6.71 (d, *J*=8.8 Hz, 2 H), 6.69 - 6.63 (t, *J*=7.1, 7.1 Hz, 1 H), 3.70 - 3.63 (m, 8 H), 3.52 (t, *J*=6.5 Hz, 2 H), 3.46 - 3.37 (m, 4 H), 1.17 (t, *J*=7.1 Hz, 3 H); δ_C (125 MHz, $CDCl_3$) 148.0, 129.5, 115.8, 111.9, 70.9, 70.3, 69.1, 50.9, 50.1, 44.5, 12.3; *m/z* (FAB) 278 [$(M)^+$, 100%].

N-(2-(2-(2-azidoethoxy)ethoxy)ethyl)-N-ethylaniline (**X4)** (0.64 g, 2.3 mmol)**,** squaric acid (0.12 g, 1.1 mmol), benzene (30 mL) and n-butanol (40 mL) were added to a 250 mL round bottom flask fitted with a stir bar and Dean-Stark apparatus. The mixture was heated to 100 °C for 24 hours. Evaporation of solvent and chromatography on silica using a gradient starting from pure chloroform to 10% methanol in chloroform gave **D2** (0.26 g, 0.40 mmol, yield of 37%) as a green solid. λ_{max} (abs, $CHCl_3$) = 634 nm, λ_{max} (em, $CHCl_3$) = 650 nm; δ_H (400 MHz, $CDCl_3$) 8.35 (d, *J*=8.8 Hz, 4 H), 6.76 (d, *J*=8.8 Hz, 4 H), 3.78 - 3.51 (m, 22 H), 3.34 (t, *J*=4.5 Hz, 4 H), 1.23 (t, *J*=7.0 Hz, 6 H); δ_C (125 MHz, $CDCl_3$) 188.5, 183.5, 153.7, 133.5, 120.0, 112.6, 71.1, 70.9, 70.3, 69.0, 50.8, 50.6, 46.6, 12.5; HRMS *m/z* (FAB) found 634.3227, calcd for $C_{32}H_{44}N_8O_6$ 634.3238.



Procedure to synthesize M3⊃T3

Macrocycle **M3** (17 mg, 0.017 mmol), **D2** (12 mg, 0.017 mmol) and alkene stopper **S3** (10 mg, 0.034 mmol) were mixed in $CDCl_3$ (3 mL) which had been filtered through a plug of neutral alumina and magnesium sulfate. The mixture was heated to 50 °C in a capped vial for 3 days in the dark (yield <95% by NMR). The rotaxane can be purified by column chromatography ($CHCl_3$:MeOH 95:5) but this results in diminished yield. The purified sample was stored in deuterated chloroform that had been passed through neutral alumina and placed in the dark at -20 °C to slow the rate of decomposition. λ_{max} (abs, $CHCl_3$) = 662 nm, λ_{max} (em, $CHCl_3$) = 704 nm; δ_H (400 MHz, $CDCl_3$) 9.37 (s, 2 H), 8.53 (d, *J*=1.3 Hz, 4 H), 8.26 (t, *J*=3.8 Hz, 4 H), 7.74 (dd, *J*=6.8, 3.27 Hz, 8 H), 7.00 (d, *J*=9.6 Hz, 4 H), 6.67 (dd, *J*=6.8, 3.0 Hz, 8 H), 6.11 (d, *J*=8.6 Hz, 4 H), 5.23 (d, *J*=3.3 Hz, 8 H), 4.93 (br s, 2 H), 4.72 (br s, 2 H), 3.80 - 3.52 (m, 32 H), 1.54 (s, 22 H), 1.50 (br s, 18 H), 1.48 (s, 18 H), 1.31 (t, *J*=7.3 Hz, 6 H); δ_C (125 MHz, $CDCl_3$) 184.0, 179.5, 167.1, 152.9, 133.3, 133.0, 130.5, 129.0, 128.6, 125.7, 123.9, 122.7, 117.1, 111.4, 70.8, 70.4, 68.8, 50.4, 46.5, 38.0, 35.4, 31.4, 31.3, 29.7, 28.1, 12.6; *m/z* (ESI) 2072 [$(M)^+$, 50%), 2045 [$(M+H-N_2)^+$, 100%].

Labeled Spectra of Dye Compounds:

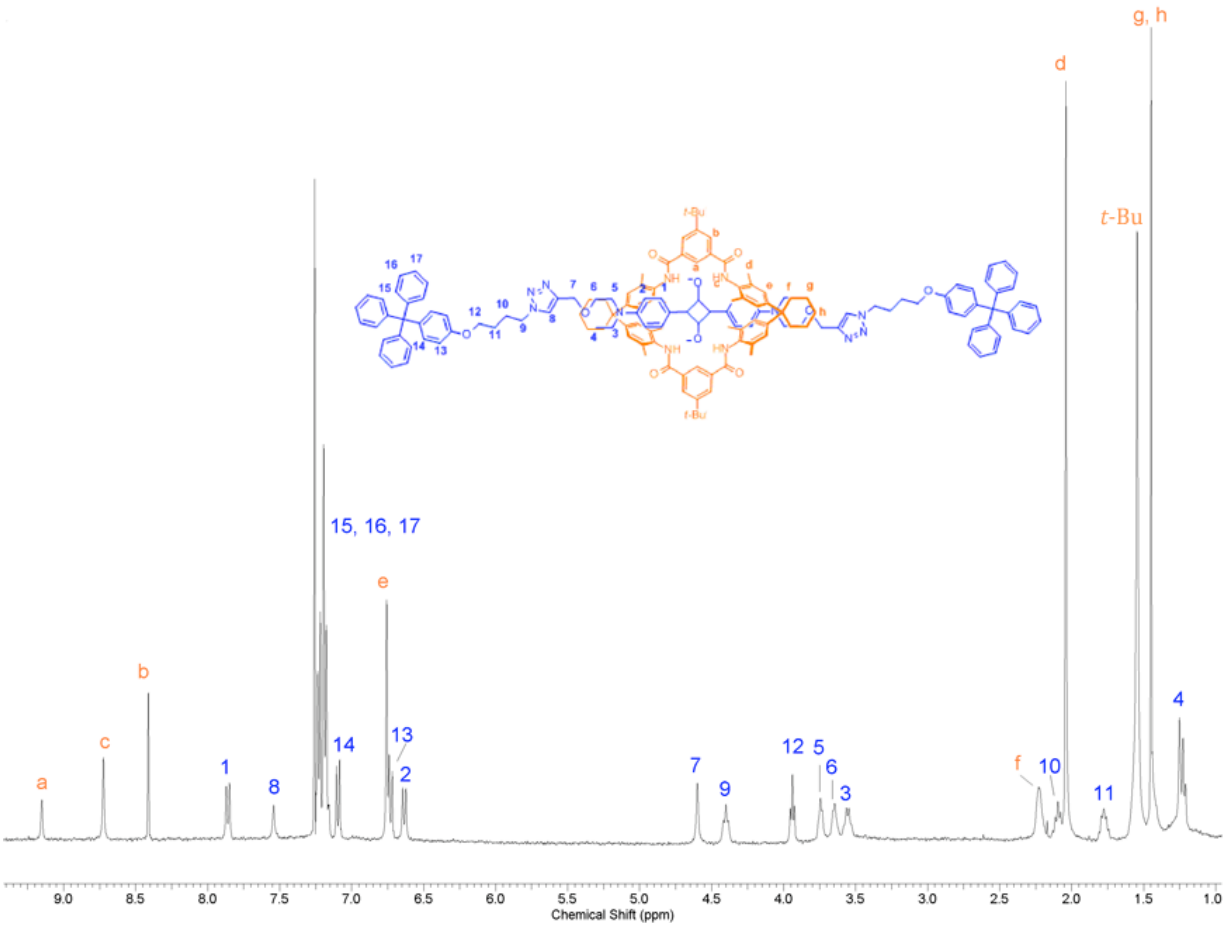


Figure S1: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of M2⊃T1 The assignment of 5 and 6 could be interchanged.

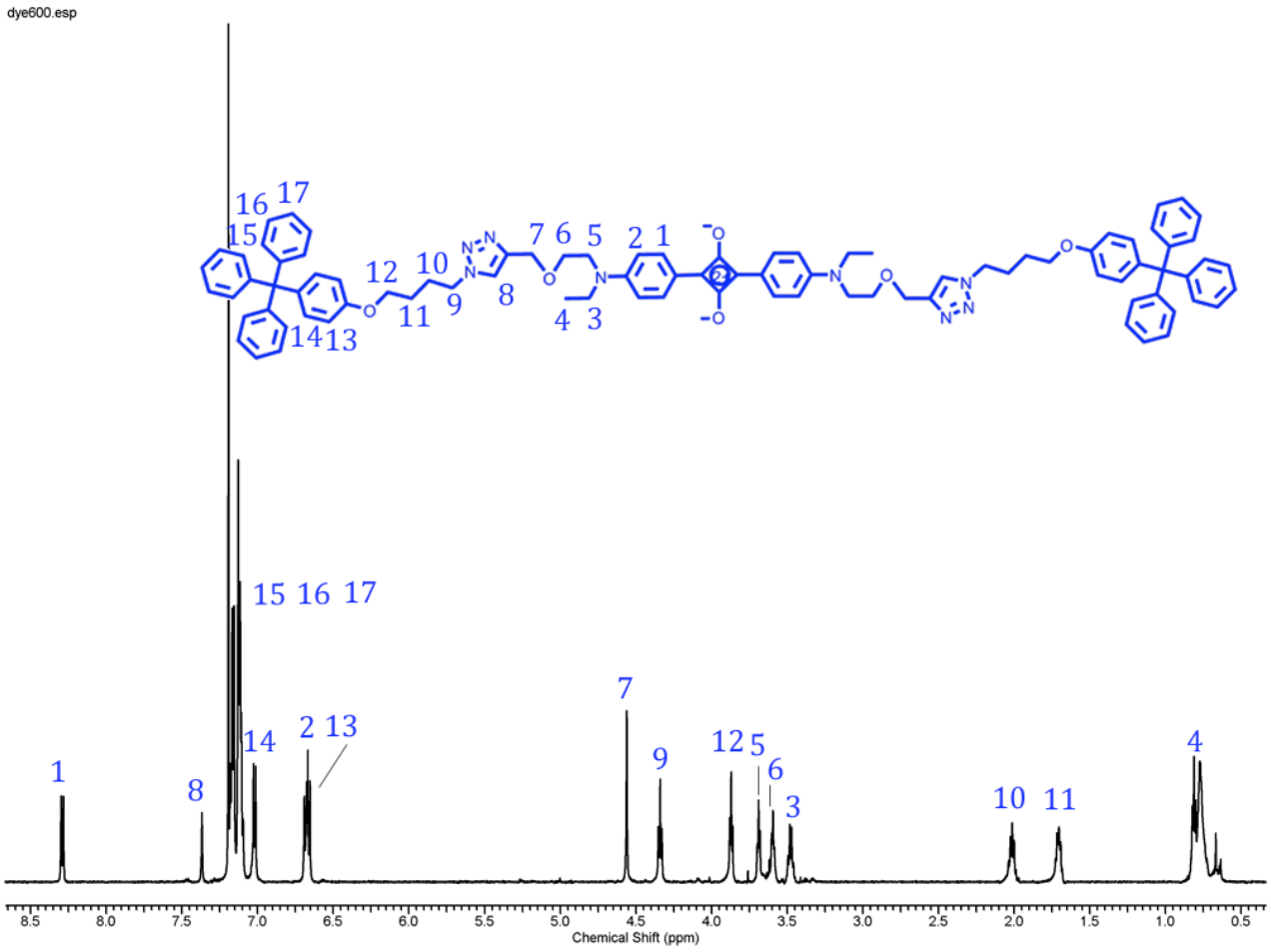


Figure S2: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of dilute T1 with water and solvent removed for clarity (ACDLabs 1D spectrum editor). The assignment of 5 and 6 could be interchanged.

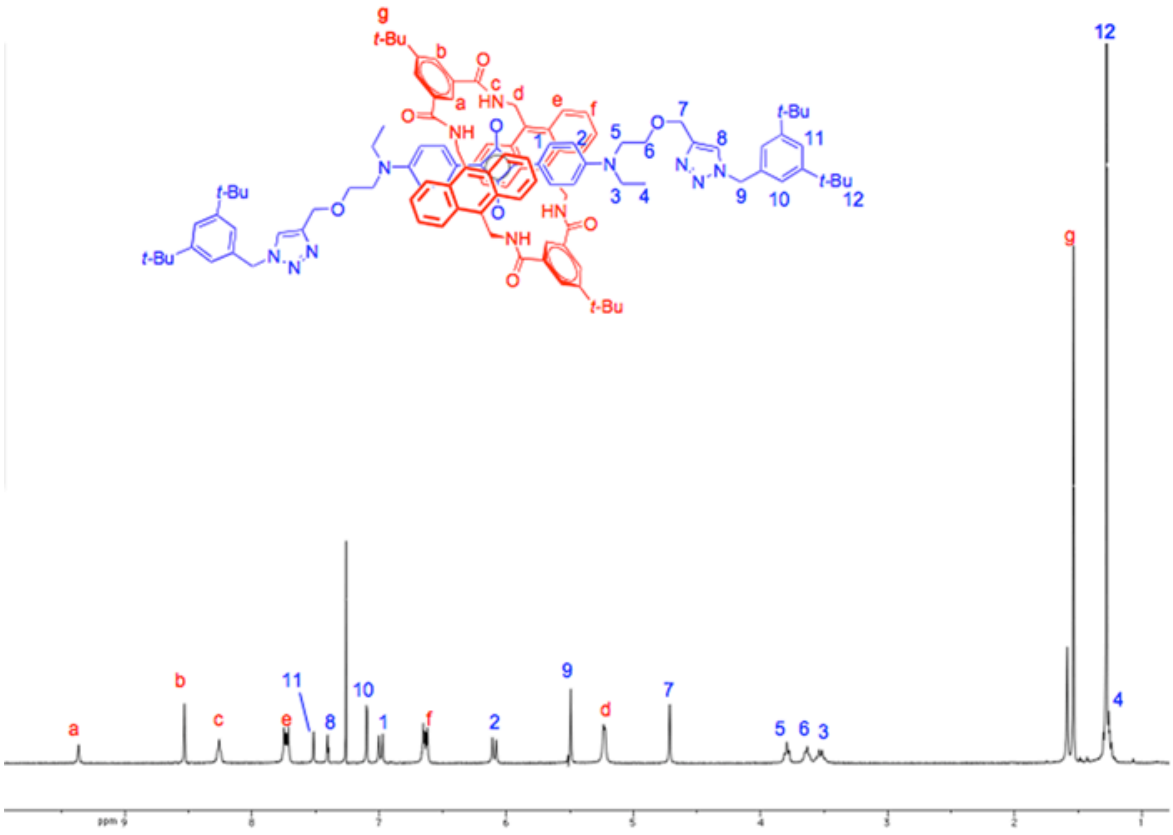


Figure S3: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of M3⊃T2 The assignment of 5 and 6 and 8 and 11 could be interchanged.

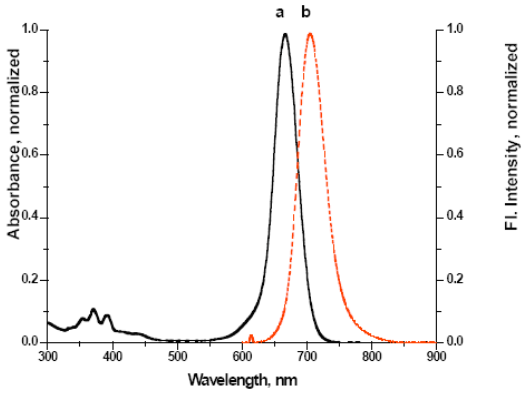


Figure S4 (a) Absorption spectrum of M3⊃T2 in methanol (6.0 μM), λ_{max} (abs) = 666 nm; (b) fluorescence emission spectrum of M3⊃T2 in methanol (6.0 μM), excited at 613 nm, λ_{max} (em) = 705 nm. Spectrum b was unchanged after sitting for 0.5 h.

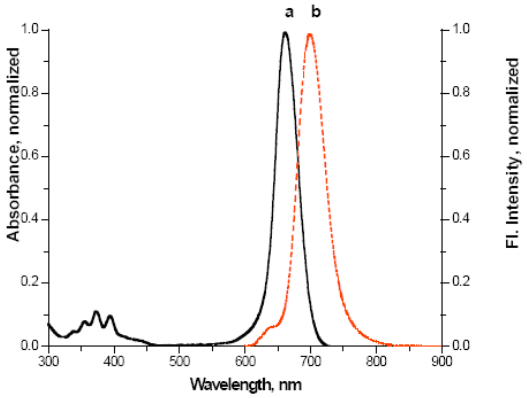


Figure S5 (a) Absorption spectrum of M3⊃T2 in chloroform (6.0 μM), λ_{max} (abs) = 661 nm; (b) fluorescence emission spectrum of M3⊃T2 in chloroform (6.0 μM), excited at 613 nm, λ_{max} (em) = 704 nm.

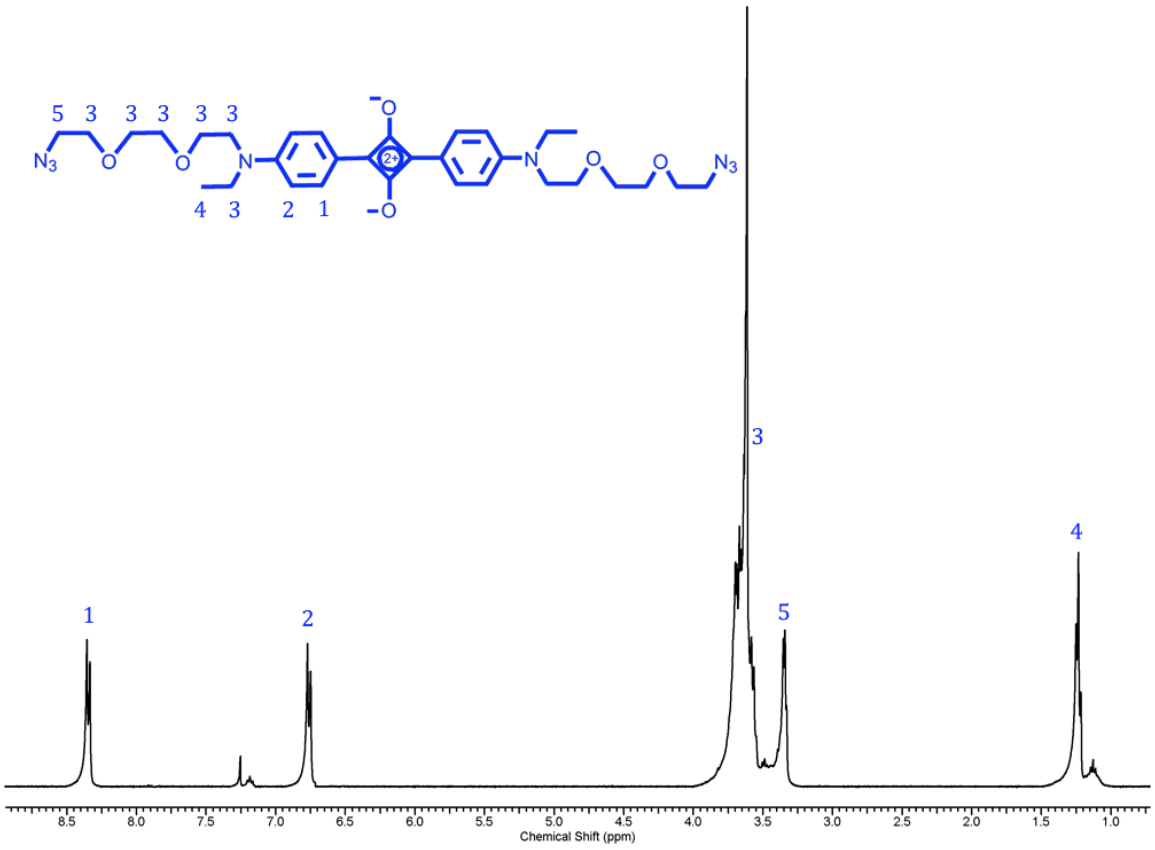


Figure S6: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of D2.

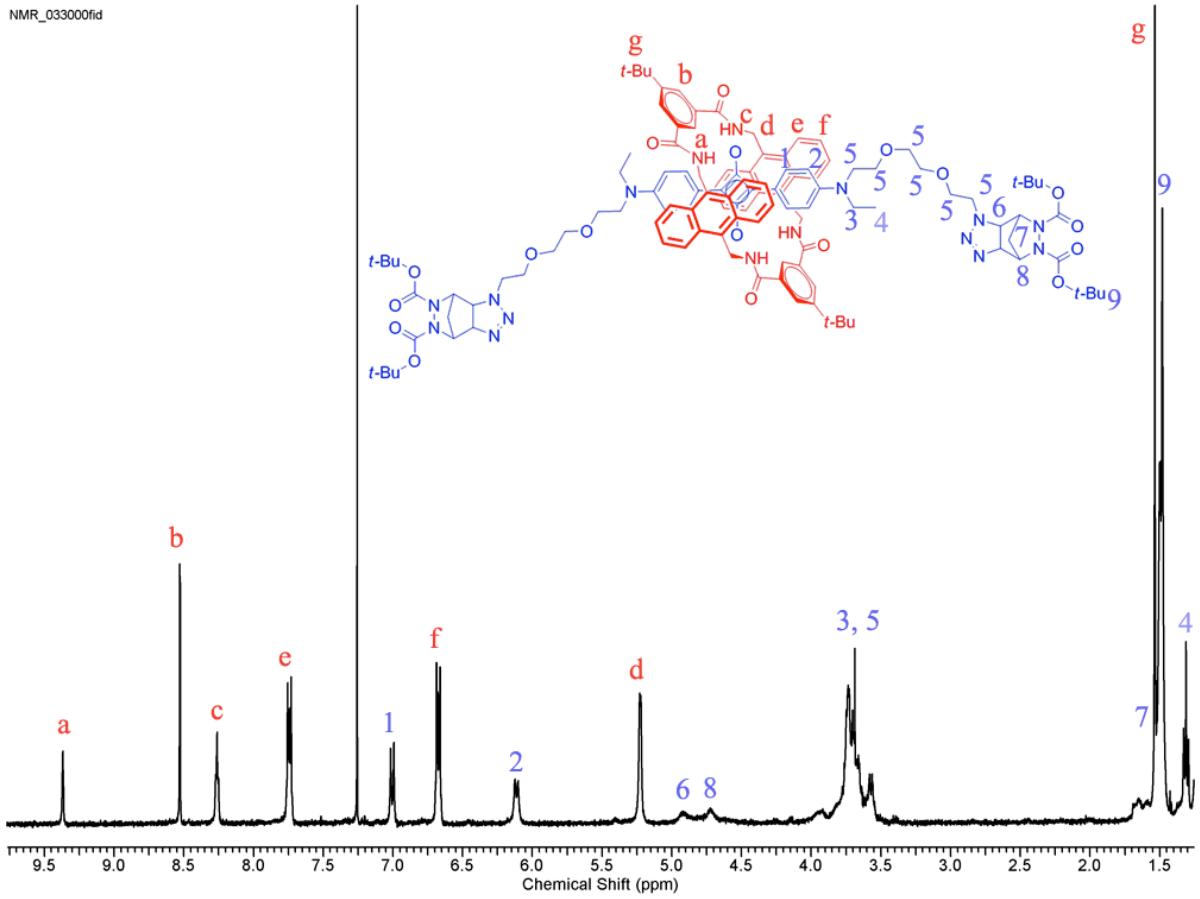


Figure S7: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of rotaxane M3⊃T3.

Analytical Methods:

Quantum Yield Determination

Measurements of all reported quantum yields followed a previously described procedure.[5] The quantum yield was determined by the relative method using Equation S1 below:

$$\Phi_u = \frac{A_s F_u n_u^2}{A_u F_s n_s^2} \Phi_s \qquad \text{Equation S1}$$

Each experiment was performed in spectroscopic grade chloroform at 22 °C. Fluorescence quantum yields were determined using 4,4-[bis-(*N*,*N*-dimethylamino)phenyl]squaraine dye as the standard (Φ_f) 0.70 in $CHCl_3$.

NMR titrations

NMR titrations to determine **D1** binding constant with **M2** were performed according to a previously published procedure.[6] A solution of **M2** in CD_2Cl_2 (3.0 mM) was prepared in an NMR tube and an initial measurement was made of the chemical shift corresponding to **M2** proton *c* (see structure in the article). Aliquots of **D1** (30 mM) were titrated into the NMR tube and spectra were taken after equilibrium was achieved; the chemical shift of proton *c* was recorded for each consecutive addition. Titration was performed at 25 °C until movement became saturated. The resulting titration curve was fitted to a 1:1 binding model using non-linear least squares method in Origin software.

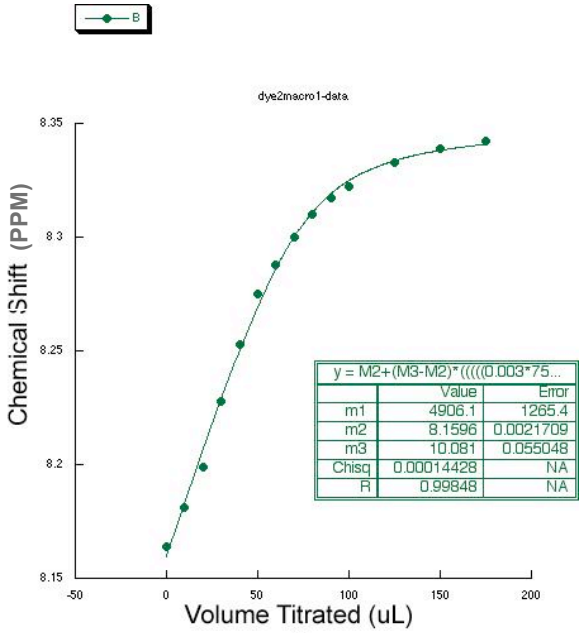


Figure S8: Chemical shift of M2 proton *c* after addition of a 30 mM solution of D1.

Ancillary Spectra

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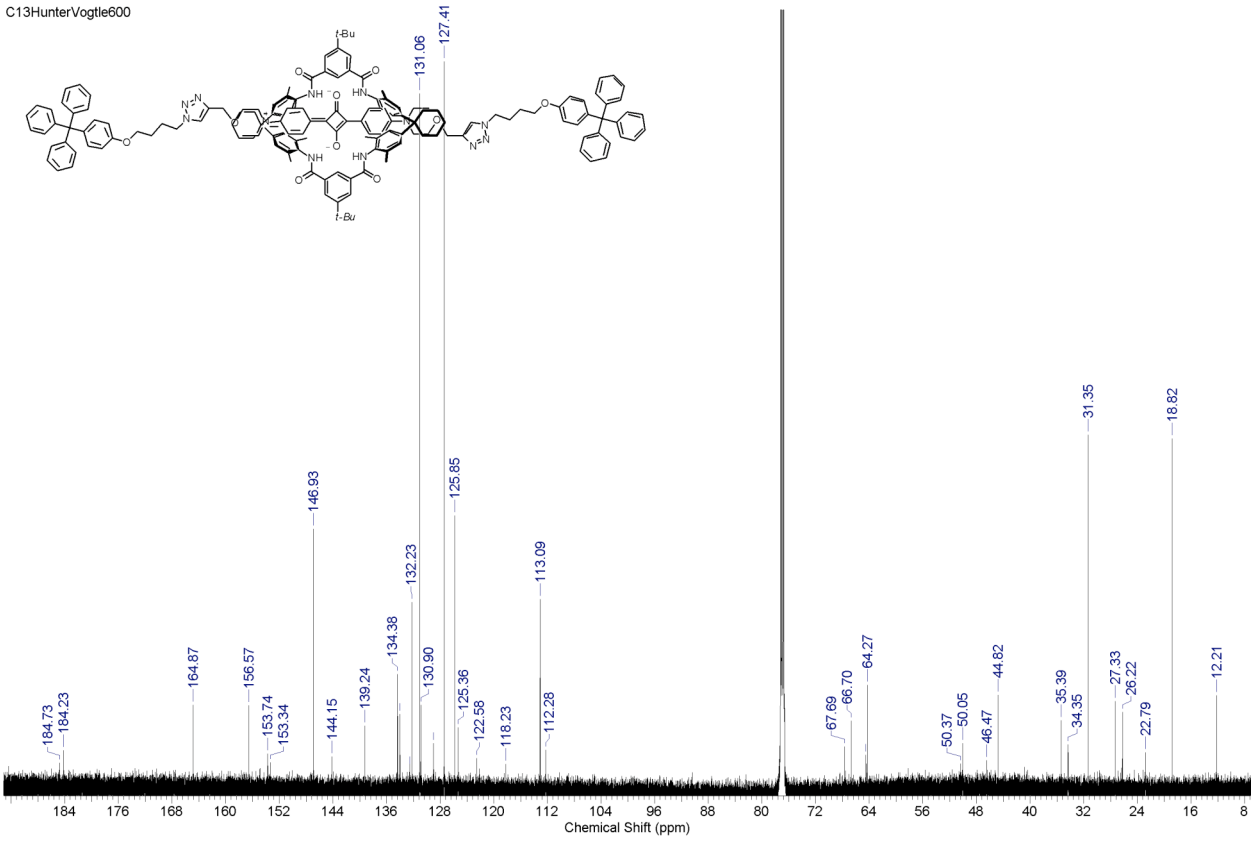

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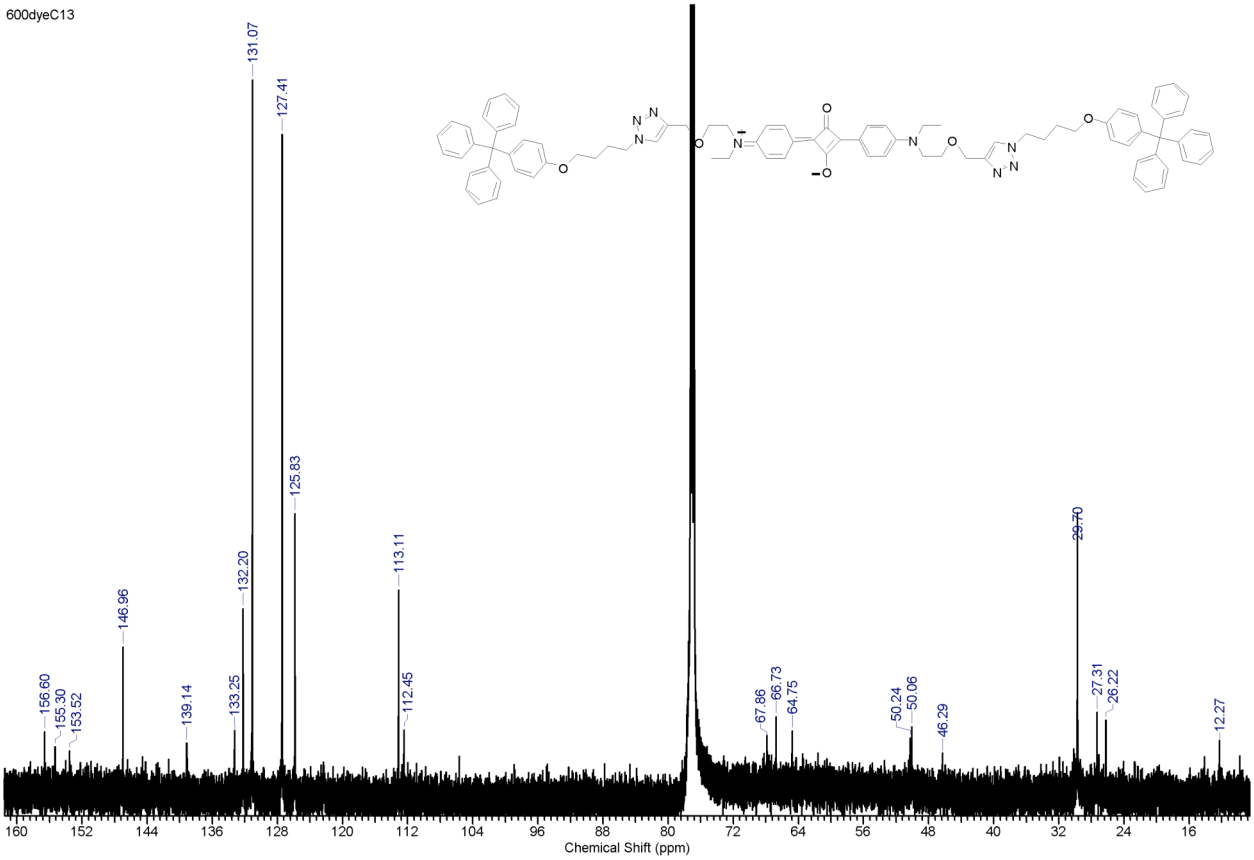

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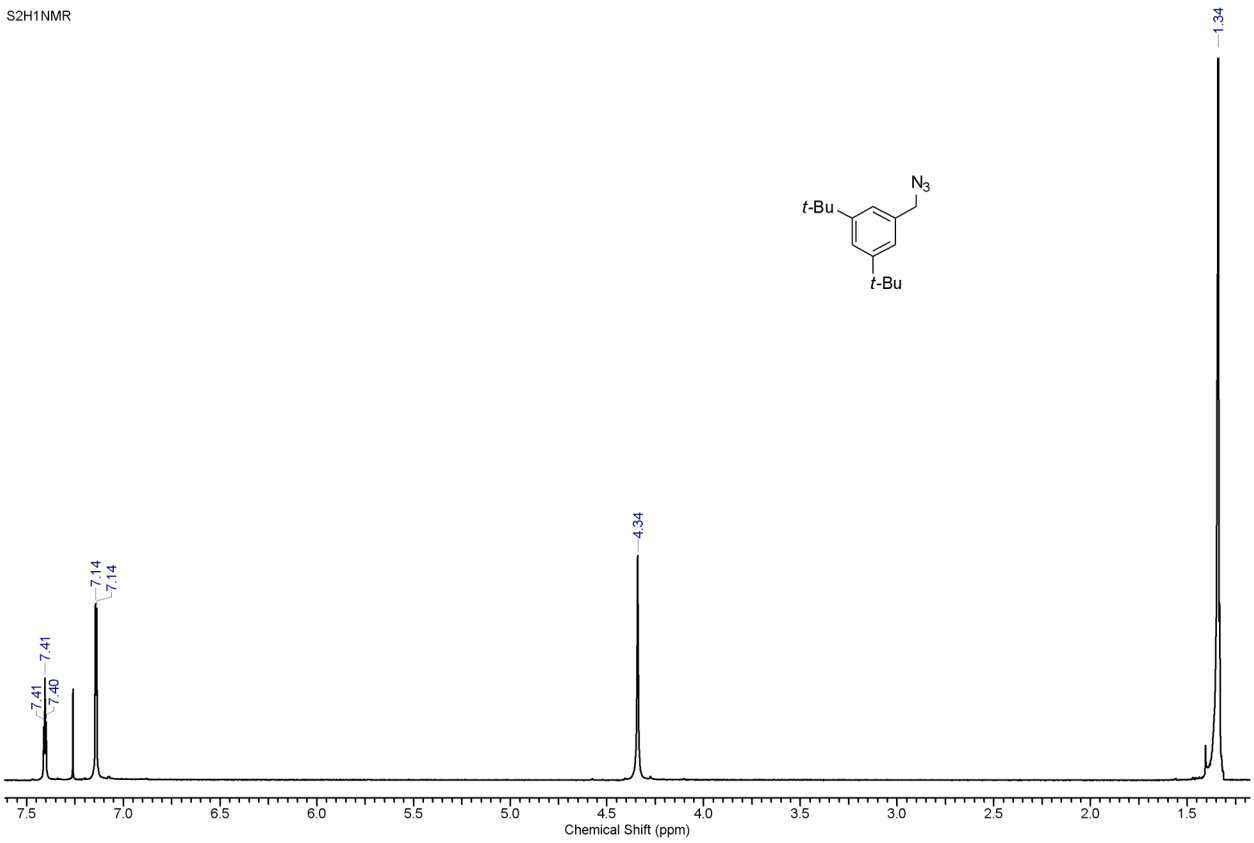
S2H1NMR



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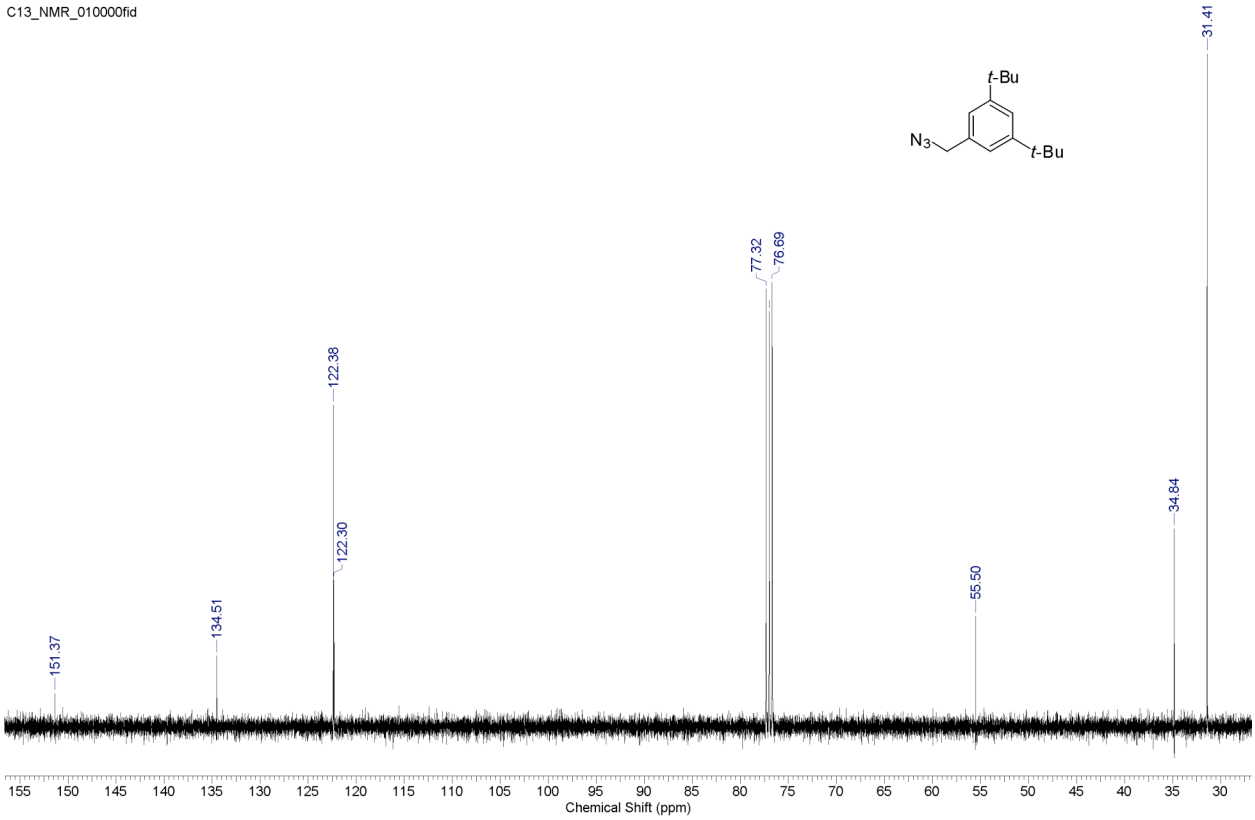
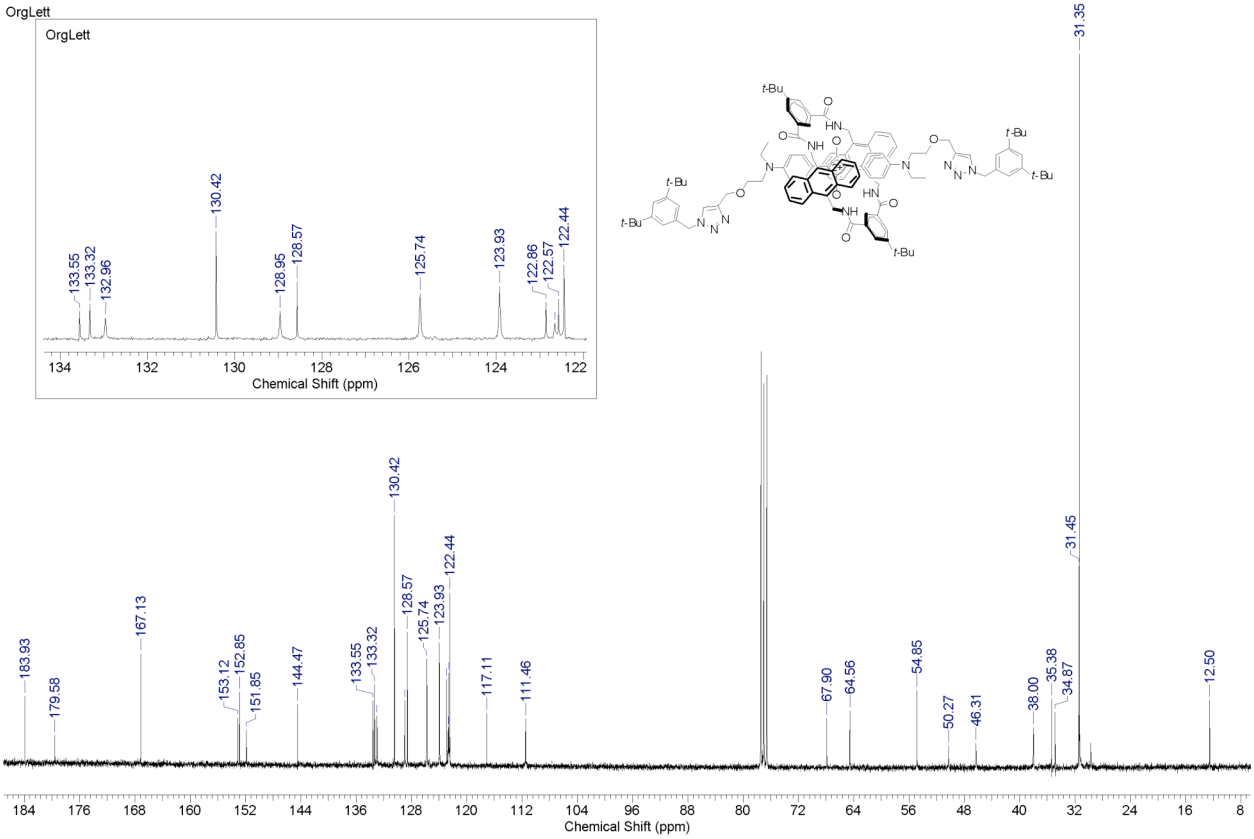
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	137	***Origin***	spect
Original Points Count	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	9195.20	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10055.4824	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	23.000		

C13_NMR_010000fid

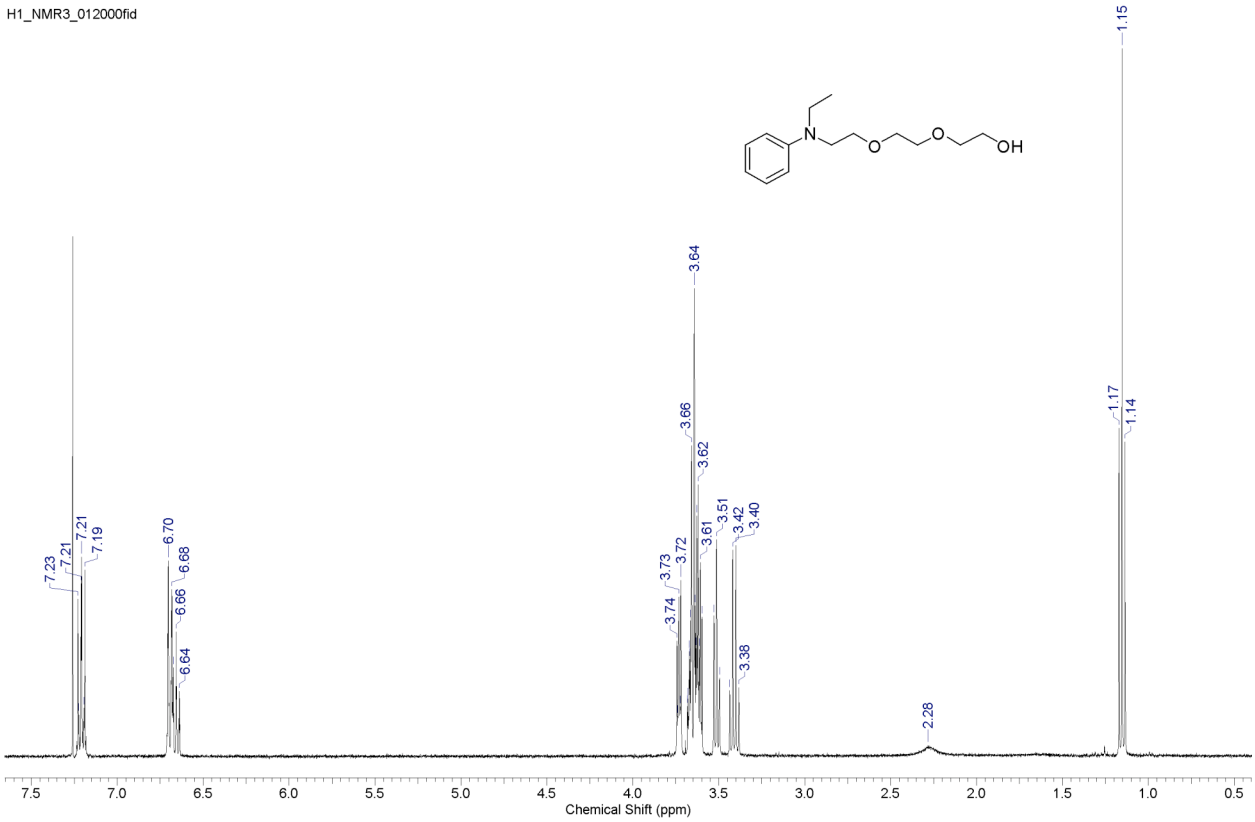


Acquisition Time (sec)	0.9572	***Comment***	Imported from VNMR.			***Date***	May 30 2008
Date Stamp	May 30 2008	***File Name***	C:\Documents and Settings\Jeremiah Gassensmith\My Documents\OrgLett\OrgLett				
Frequency (MHz)	75.43	***Nucleus***	13C	***Number of Transients***	18500	***Original Points Count***	16384
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	60.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	7538.6616	***Sweep Width (Hz)***	17115.96	***Temperature (degree C)***	29.000		



Acquisition Time (sec)	3.9715	***Comment***	aniline alcohol ?			***Date***	28 May 2008 14:43:12
Date Stamp	28 May 2008 14:43:12			***File Name***	\\afs\auto2\Private\NMR\H1_NMR3\H1_NMR3_012000fid		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	4.00	***SW(cyclical) (Hz)***	8250.83	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2449.1282	***Sweep Width (Hz)***	8250.57	***Temperature (degree C)***	22.700		

H1_NMR3_012000fid



Acquisition Time (sec)	1.3631	***Comment***	PEG aniline alcohol			***Date***	12 Nov 2007 23:23:44
Date Stamp	12 Nov 2007 23:23:44			***File Name***	\\afs\auto2\Private\NMR\C13_NMR\C13_NMR_007000fid		
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	149	***Origin***	spect
Original Points Count	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	9195.20	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
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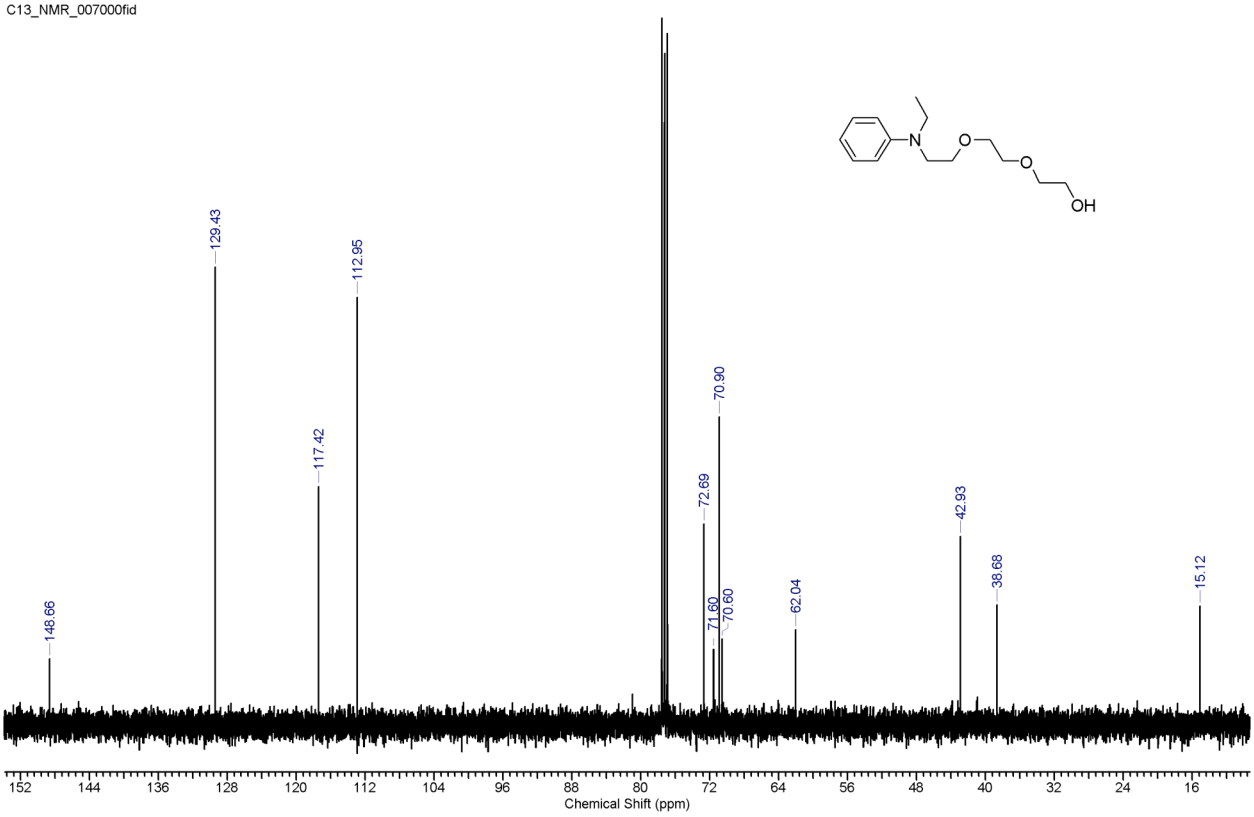
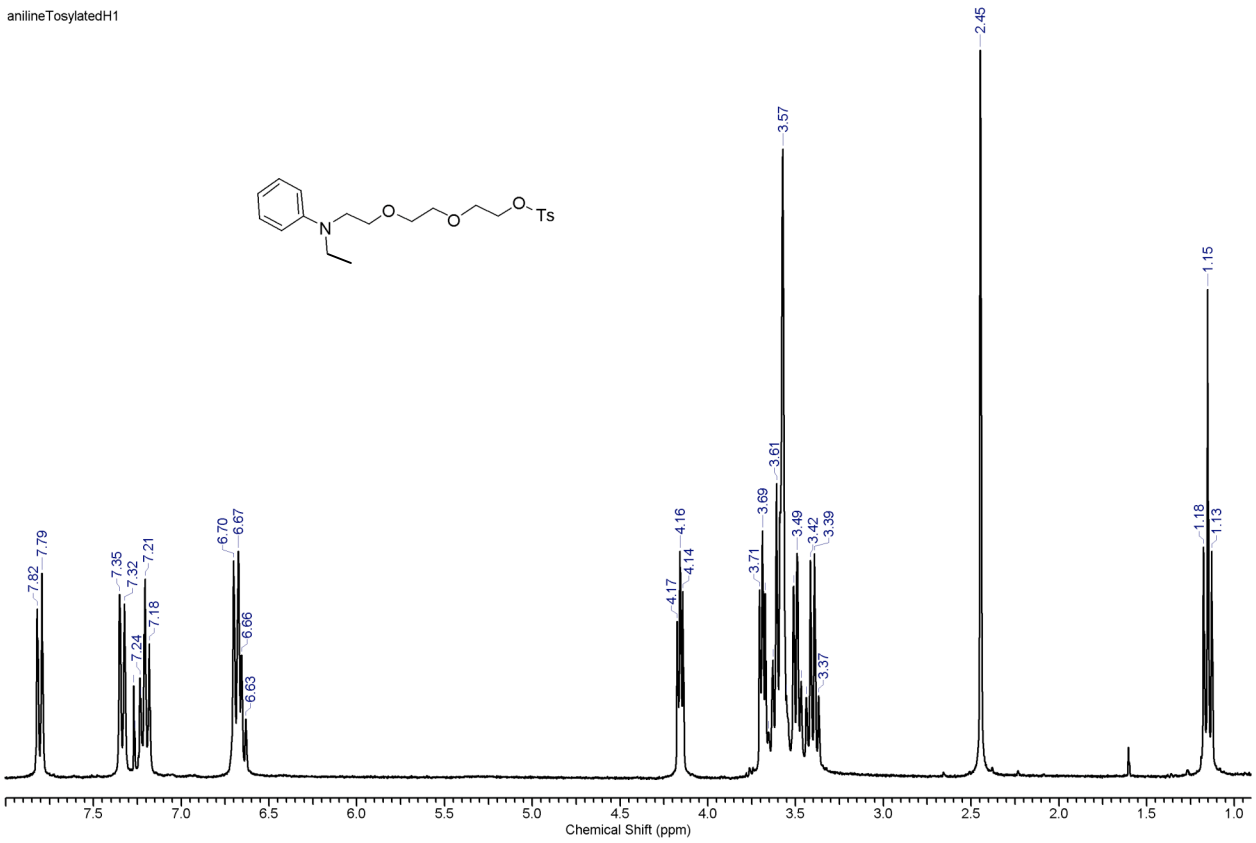
C13_NMR_007000fid



Acquisition Time (sec)	3.6205	***Comment***	STANDARD 1H OBSERVE			***Date***	May 29 2008
Date Stamp	May 29 2008	***File Name***	\\afs\auto2\Private\NMR\anilineTosylatedH1			***Frequency (MHz)***	299.95
Nucleus	1H	***Number of Transients***	16	***Original Points Count***	16384	***Points Count***	16384
Pulse Sequence	s2pul	***Receiver Gain***	51.00	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	1974.1495	***Sweep Width (Hz)***	4525.40	***Temperature (degree C)***	29.000		

anilineTosylatedH1



Acquisition Time (sec)	0.9572	***Comment***	new experiment			***Date***	May 29 2008
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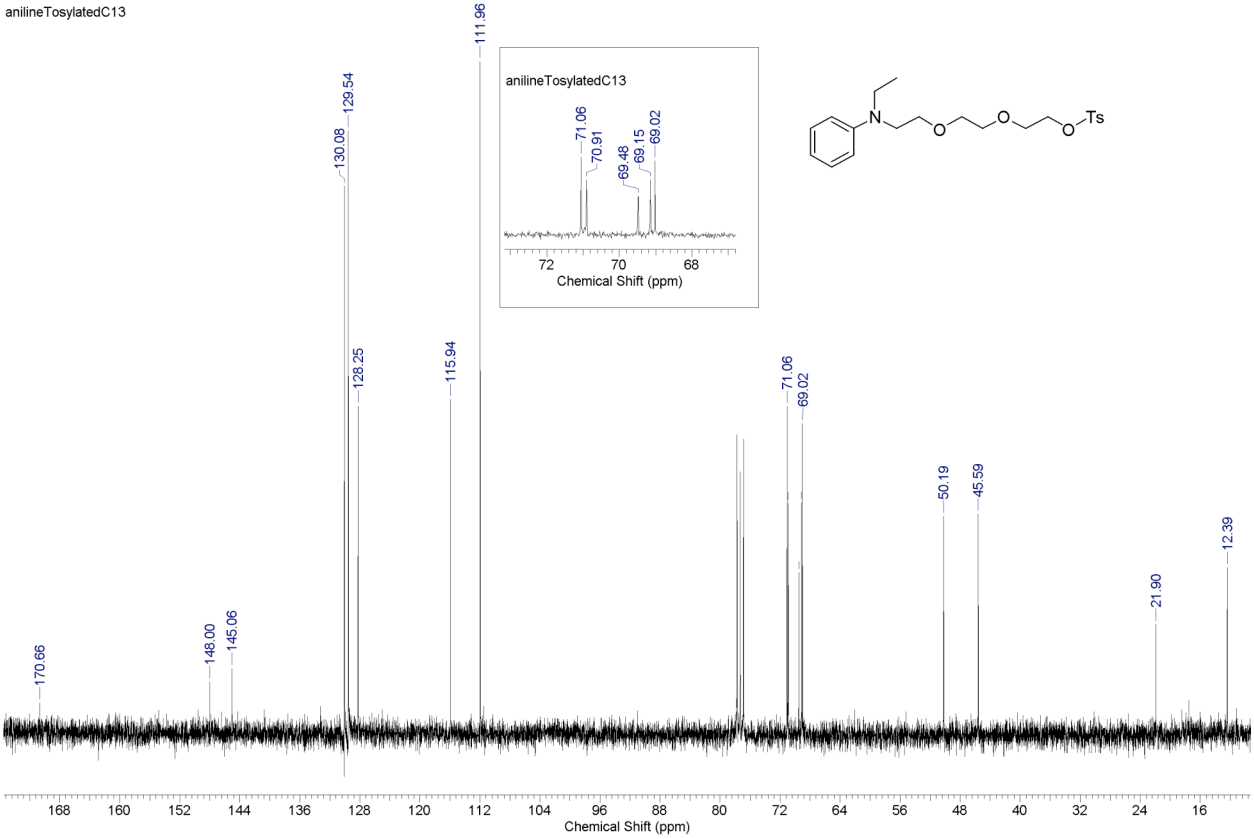
Nucleus	13C	***Number of Transients***	1000	***Original Points Count***	16384	***Points Count***	16384
Pulse Sequence	s2pul	***Receiver Gain***	60.00	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	7559.6538	***Sweep Width (Hz)***	17115.96	***Temperature (degree C)***	29.000		



Acquisition Time (sec)	3.9715	***Comment***	aniline azide ?			***Date***	30 May 2008 23:30:08
Date Stamp	30 May 2008 23:30:08			***File Name***	\\afs\auto2\Private\NMR\H1_NMR3\H1_NMR3_013000fid		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	4.00	***SW(cyclical) (Hz)***	8250.83	***Solvent***	CHLOROFORM-d		
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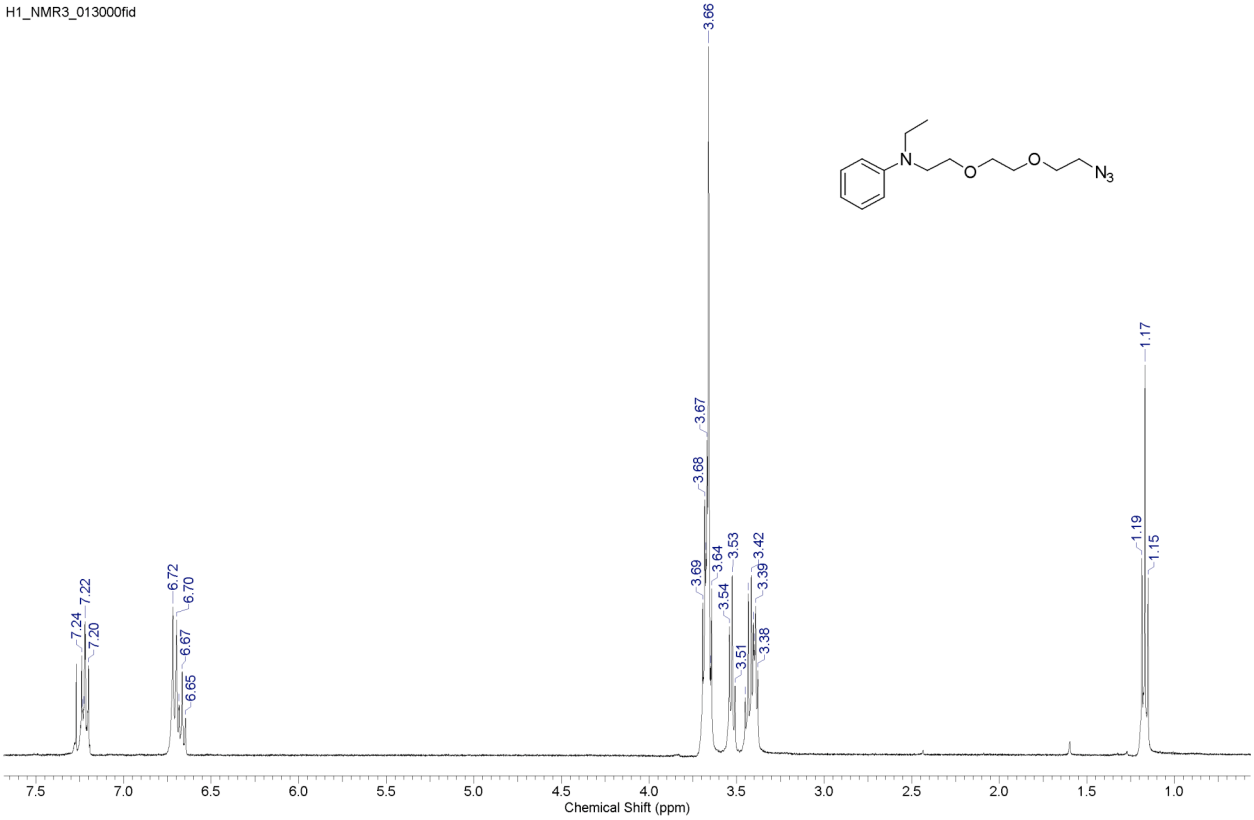
H1_NMR3_013000fid



Acquisition Time (sec)	1.3631	***Comment***	Aniline Azide	***Date***	30 May 2008 23:47:12		
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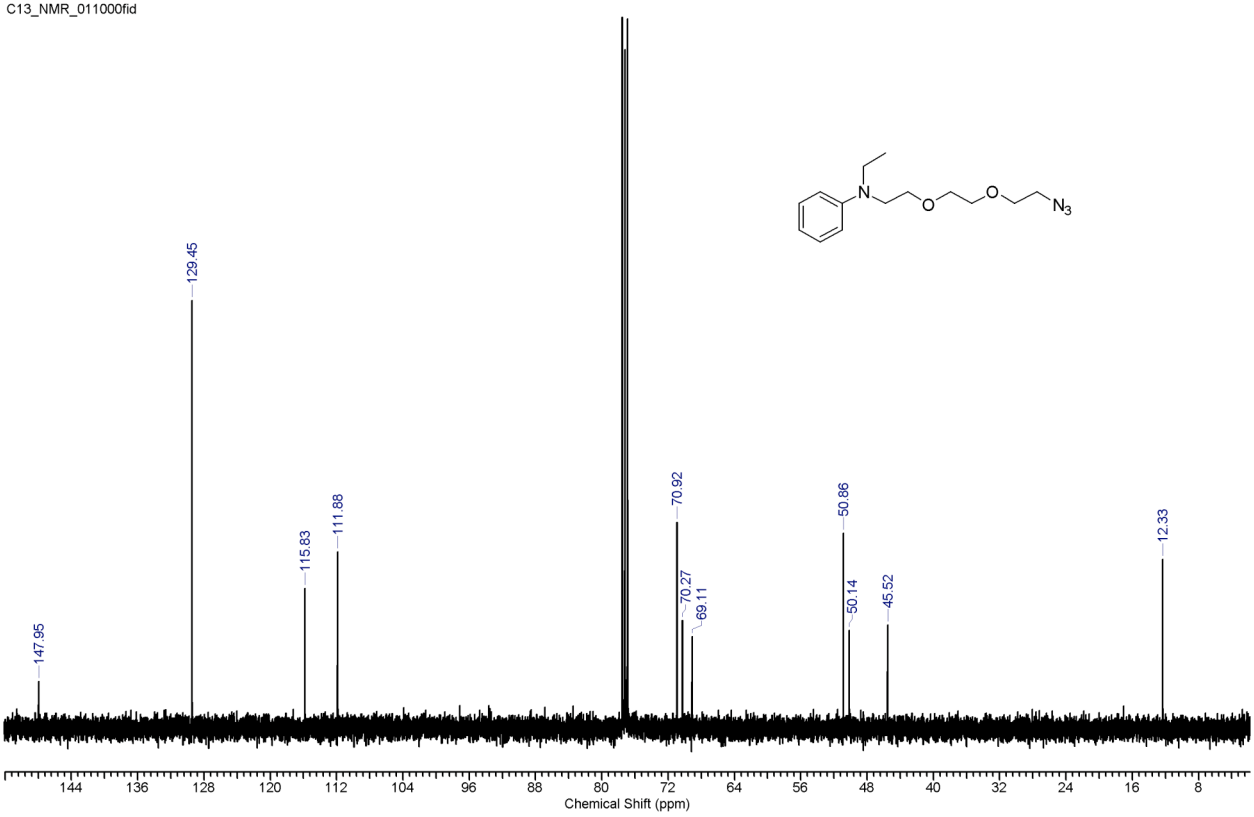
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	313	***Origin***	spect
Original Points Count	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	9195.20	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10075.3691	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	23.100		

C13_NMR_011000fid



Acquisition Time (sec)	1.3631	***Comment***	bisazide squaraine dye			***Date***	06 May 2008 17:59:28
Date Stamp	06 May 2008 17:59:28			***File Name***	\\afs\auto2\Private\NMR\C13_NMR\C13_NMR_009000fid		
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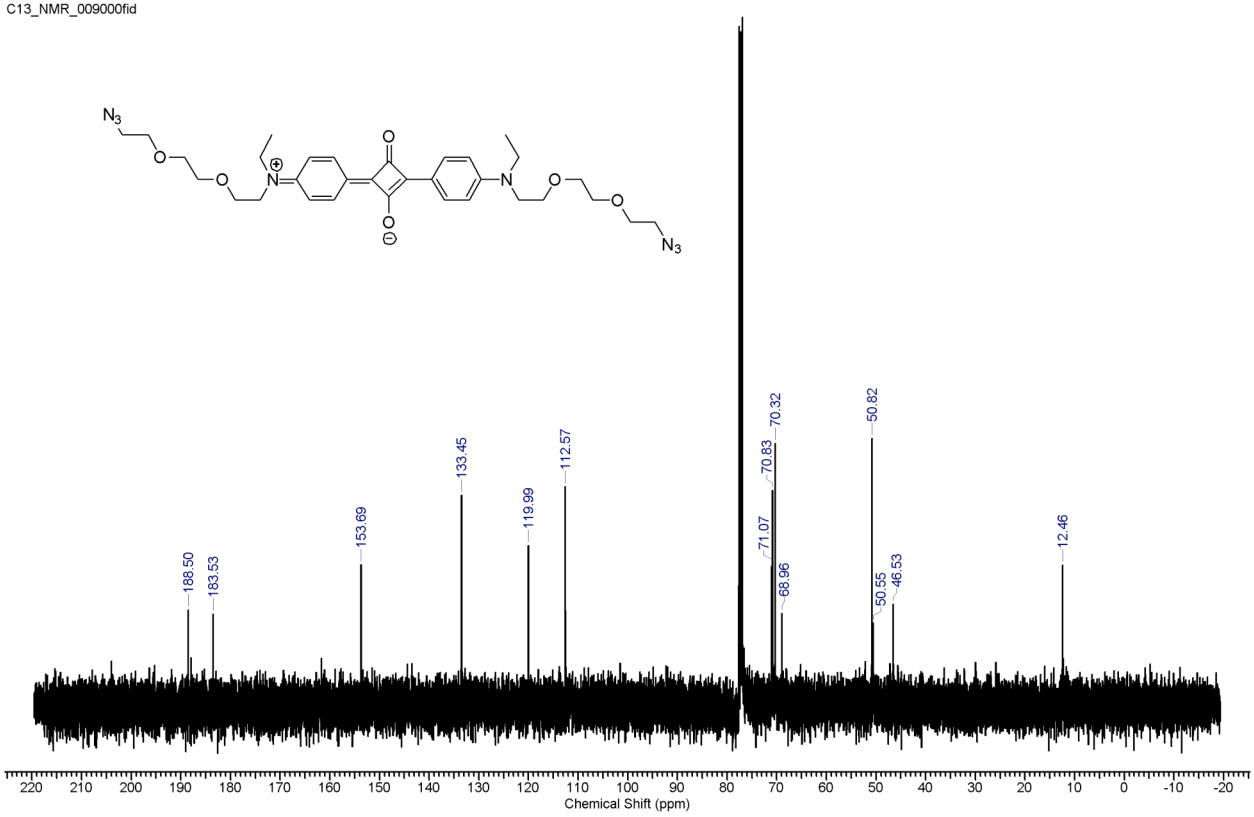
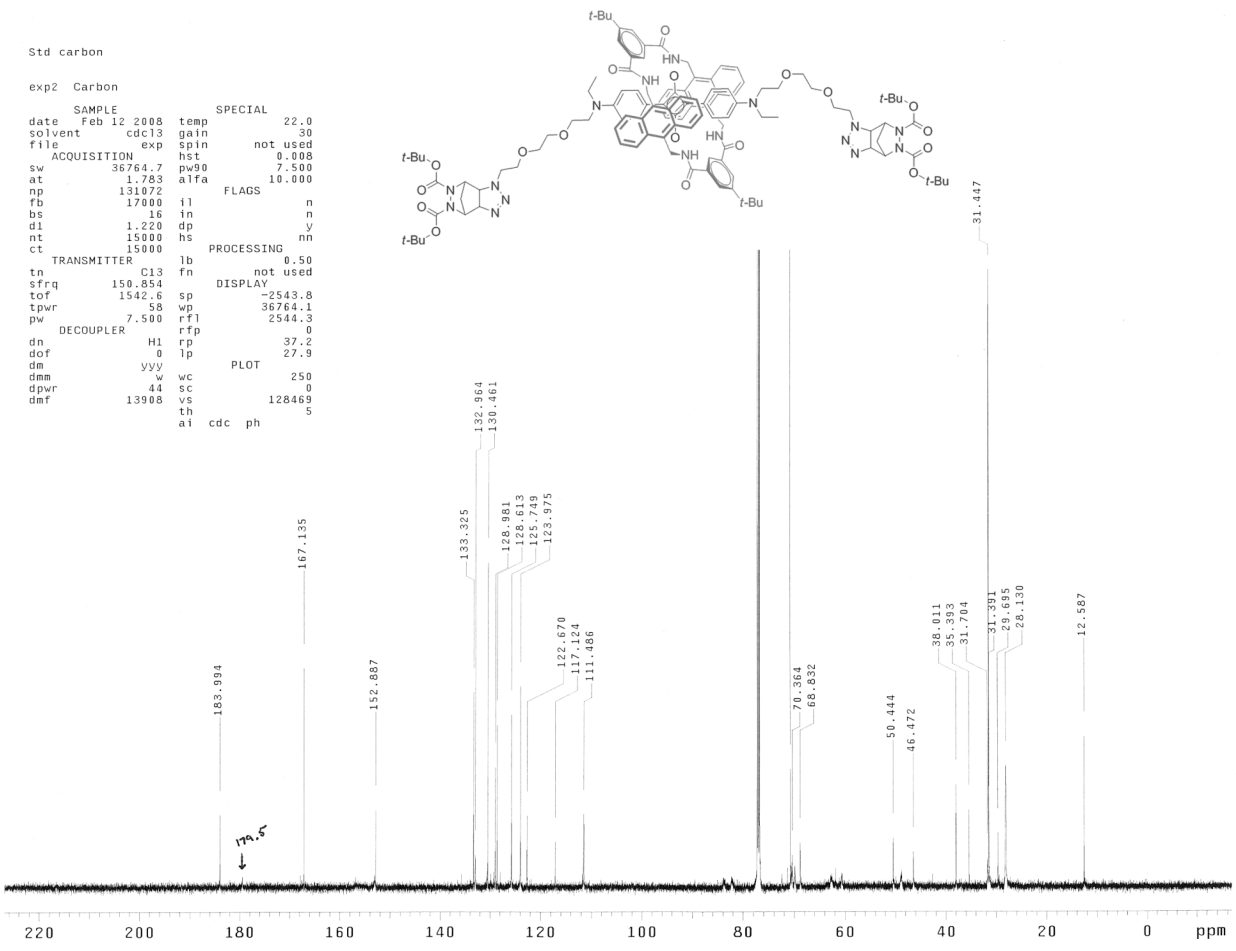
Original Points Count	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	9195.20	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10075.3691
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.400				

C13_NMR_009000fid

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ppm

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