Supporting Information

An Anthracene-Containing Bistable [2]Rotaxane Featuring Color and Fluorescence Changes

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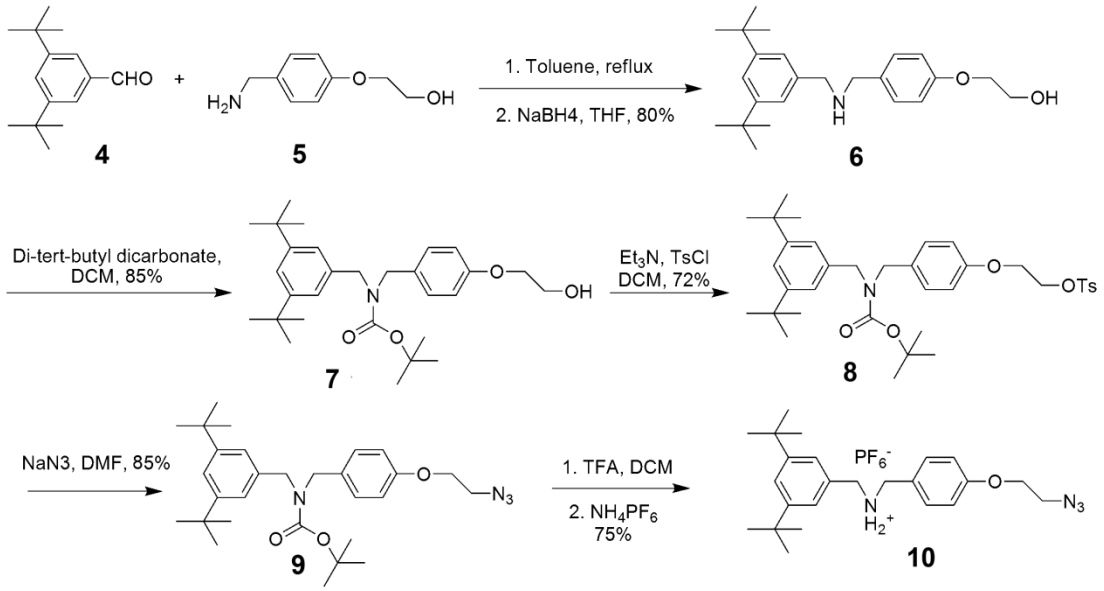
Experimental Section

General method: ^{1}H NMR and ^{13}C NMR spectra were measured on a Brüker AV-400 spectrometer. The electronic spray ionization (ESI) mass spectra were tested on a LCT Premier XE mass spectrometer. The UV-Vis absorption spectra and fluorescence spectra were obtained on a Varian Cary 100 spectrometer and a Varian Cary Eclipse (1-cm quartz cell used), respectively. The quantum yields of fluorescence were measured by using a Fluoromax-4 fluorescence spectrophotometer equipped with the quantum yield measuring accessory and report generator program.

Materials: Chemicals were used as received from Acros, Aldrich. All solvents were reagent grade, which were dried and distilled prior to use according to standard procedures. The molecular structures were confirmed via ^{1}H NMR, ^{13}C NMR and high-resolution ESI mass spectroscopy.



Scheme S1 Synthetic strategy to prepare compound **10**

Synthesis of the compound 6

A mixture of 3,5-Ditert-butylbenzaldehyde (0.65 g, 2.99 mmol) and compound **5** (0.5 g, 2.99 mmol) in dry toluene (70 mL) was refluxed overnight under argon atmosphere. The solvent was removed under vacuum, and the residue was dissolved in THF (50 mL). To the solution was added $NaBH_4$ (1.2 g, 30.0 mmol) in portion under ice bath. After the mixture was stirred for overnight,

the solution was poured into water, and the mixture was extracted by DCM (3 × 50 mL). The organic layer was dried over anhydrous sodium sulfate, and then concentrated to give the free amine compound. The residue was purified via column chromatography (SiO_2, CH_2Cl_2/MeOH = 20/1) to give a pale solid **6** (0.88g, 80%). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ = 7.32 (t, *J* = 1.6 Hz, 1H), 7.26 (d, *J* = 8.8 Hz, 2H), 7.16 (d, *J* = 1.6 Hz, 2H), 6.87 (d, *J* = 8.6 Hz, 2H), 4.06 (m, 2H), 3.93 (m, 2H), 3.77 (d, *J* = 6.4 Hz, 4H), 1.33 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 157.7, 150.8, 139.0, 132.6, 129.5, 122.4, 121.0, 114.4, 69.3, 61.2, 53.6, 52.5, 34.8, 31.5. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{36}NO_2$, 370.2746; found, 370.2744.

Synthesis of the compound 7

To the solution of amine **6** (1 g, 2.71 mmol) in dry DCM (50 mL) was added di-tert-butyldicarbonate (1.18 g, 5.42 mmol) and the mixture was stirred for 5 h at room temperature. The residue was washed with water, dried over Na_2SO_4 and evaporated in vacuo to give a crude product, which was purified by column chromatography (SiO_2, CH_2Cl_2/MeOH = 100/1) to give product **7** (1.08 g, 85 %) as a colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K):δ = 7.31 (t, *J* = 1.6 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 7.08 (m, 3H), 6.87 (d, *J* = 8.5 Hz, 2H), 4.35 (m, 4H), 4.07 (m, 2H), 3.96 (m, 2H), 1.50 (s, 9H), 1.31 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 156.0, 150.8, 121.1, 114.5, 79.8, 69.2, 61.4, 60.2, 34.7, 34.3, 31.4, 31.3, 28.51, 24.6, 22.3, 14.2, 13.9. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{29}H_{44}NO_4$, 470.3270; found, 470.3272.

Synthesis of the compound 8

To the solution of compound **7** (1.08 g, 2.30 mmol) in dry DCM (50 mL) was added 4-toluene sulfonyl chloride (0.88 g, 4.65 mmol) and triethylamine (0.65 ml, 4.65 mmol), then the mixture was stirred for 12 h at room temperature. The residue was washed with water, dried over Na_2SO_4 and evaporated in vacuo to give a crude product, which was purified by column chromatography (SiO_2, CH_2Cl_2) to give product **8** (1.01 g, 72 %) as a colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ = 7.82 (d, J = 8.3 Hz, 2H), 7.38-7.30 (m, 3H), 7.14 (d, J = 7.2 Hz, 1H), 7.04 (m, 3H), 6.73 (d, J = 8.6 Hz, 2H), 4.36 (m, 4H), 4.27 (m, 2H), 4.18-4.10 (m, 2H), 2.44 (s, 3H), 1.50 (s, 9H), 1.33 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 157.2, 156.0, 150.8, 145.0, 132.8, 129.9, 129.4, 128.8, 128.0, 121.9, 121.1, 114.5, 79.8, 68.2, 65.5, 34.8, 31.5, 29.7, 28.5, 21.7. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{36}H_{50}NO_6S$, 624.3359; found, 624.3355.

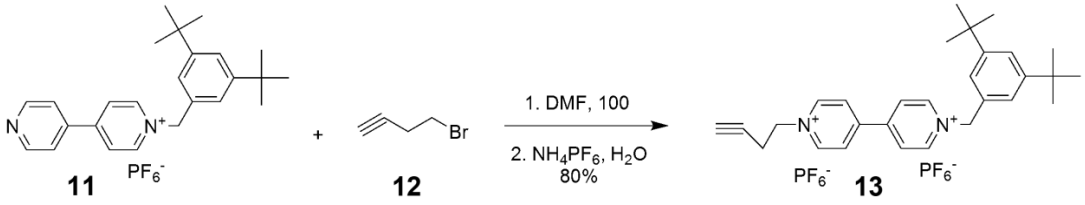
Synthesis of the compound 9

A mixture of compound **8** (1 g, 1.65 mmol) and sodium azide (0.54 g, 8.25 mmol) in dry DMF (50 mL) was stirred at 80 ^{o}C for 16 h under argon atmosphere. After the reaction mixture had been cooled to room temperature, the solution was evaporated under reduced pressure. The residue was purified via column chromatography (SiO_2, CH_2Cl_2) to give **9** (0.69 g, 85%) as a colorless oil. ^{1}H NMR (CDCl3, 400 MHz, 298 K): δ = 7.31 (t, *J* = 1.6 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 7.07 (m, 3H), 6.87 (d, *J* = 8.5 Hz, 2H), 4.4-4.27 (m, 4H), 4.18-4.12 (m, 2H), 3.59 (m, 2H), 1.50 (s, 9H), 1.31 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 156.4, 154.9, 149.7, 136.1, 129.9, 128.4, 127.8, 121.2, 120.8, 120.0, 113.5, 78.7, 65.9, 49.1, 33.7, 30.4, 27.4. HRMS (ESI) *m/z*: $[M+H]^+$ calcd for $C_{29}H_{43}N_4O_3$, 495.3335; found, 495.3339.

Synthesis of the compound 10

TFA (0.8 mL, 10.4 mmol) was added to a solution of product **9** (0.5 g, 1.01 mmol) in dichloromethane (10 mL) and the mixture was stirred for 10 h. A saturated aqueous solution of NH_4PF_6 (20 mL) was added to the reaction mixture for 4 h. The organic layer was separated and evaporated under reduced pressure to get the yellow solid, which was dissolved in MeOH (10 mL)

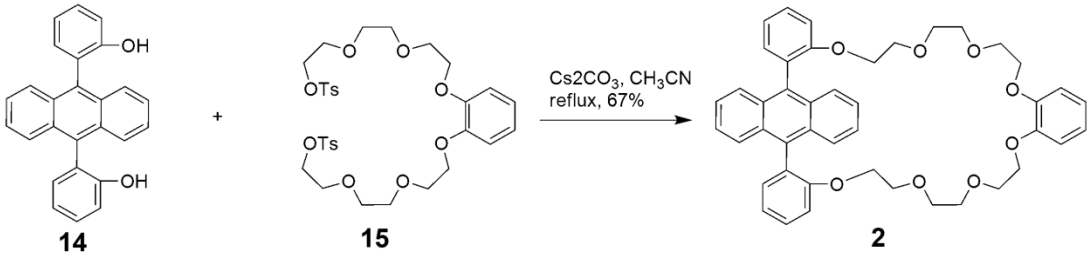
and added 20 mL saturated aqueous solution of NH_4PF_6. After stirring for 5 h, the mixture was diluted with CH_2Cl_2 (10 mL), the organic layer was separated and evaporated under reduced pressure to get the crude product, which was purified by column chromatography (SiO_2, CH_2Cl_2/MeOH = 50/1) to afford product **10** (0.41 g, 75 %) as a faint yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ = 7.45 (t, *J* = 1.6 Hz, 1H), 7.26 (m, 2H), 7.17 (d, *J* = 1.6 Hz, 2H), 6.92 (d, *J* = 8.7 Hz, 2H), 4.14-4.08 (m, 2H), 4.03 (s, 2H), 3.99 (s, 2H), 3.58 (t, *J* = 4.9 Hz, 2H), 1.32 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 159.1, 152.2, 131.2, 130.1, 123.7, 115.2, 66.7, 51.7, 50.5, 50.6, 34.9, 31.3, 29.7. HRMS (ESI) *m/z*: $[M\text{-}PF_6]^+$ calcd for $C_{24}H_{35}N_4O_2$, 395.2811; found, 395.2813.



Scheme S2 Synthetic strategy to prepare compound **13**

Synthesis of the compound 13

The pyridinium salt **11** (0.3 g, 0.53 mmol) was added to a CH_3CN solution (10 mL) of 4-bromo-1-butyne **12** (0.15 g, 1.1 mmol); this mixture was then stirred at 100 °C for 24 h. Saturated aqueous NH_4PF_6 (20 mL) was added to the solution; the organic solvent was evaporated and the residue was extracted with CH_2Cl_2 (2 × 20 mL). The organic phases were combined, dried (Na_2SO_4), and concentrated to afford a crude product, which was purified by column chromatography (SiO_2, CH_2Cl_2/MeOH = 25/1) to give compound **13** as a light-yellow solid (0.29 g, 80 %). ^{1}H NMR (CD_3SOCD_3, 400 MHz, 298 K): δ = 9.59 (d, *J* = 6.2 Hz, 2H), 9.39 (d, *J* = 6.0 Hz, 2H), 8.79 (t, *J* = 6.3 Hz, 4H), 7.55 (s, 2H), 7.47 (s, 1H), 5.87 (s, 2H), 4.84 (t, *J* = 6.2 Hz, 1H), 3.11 (s, 1H), 3.04 (s, 2H), 1.29 (s, 18H). ^{13}C NMR (100 MHz, CD_3SOCD_3, 298 K) δ = 151.5, 149.1, 148.8, 145.9, 145.4, 133.3, 128.0, 127.2, 126.4, 125.4, 123.3, 123.1, 79.0, 75.3, 64.1, 58.7, 34.7, 31.1, 20.3. HRMS (ESI) *m/z*: $[M\text{-}PF_6]^+$ calcd for $C_{29}H_{36}N_2PF_6$, 557.2520; found, 557.2518.

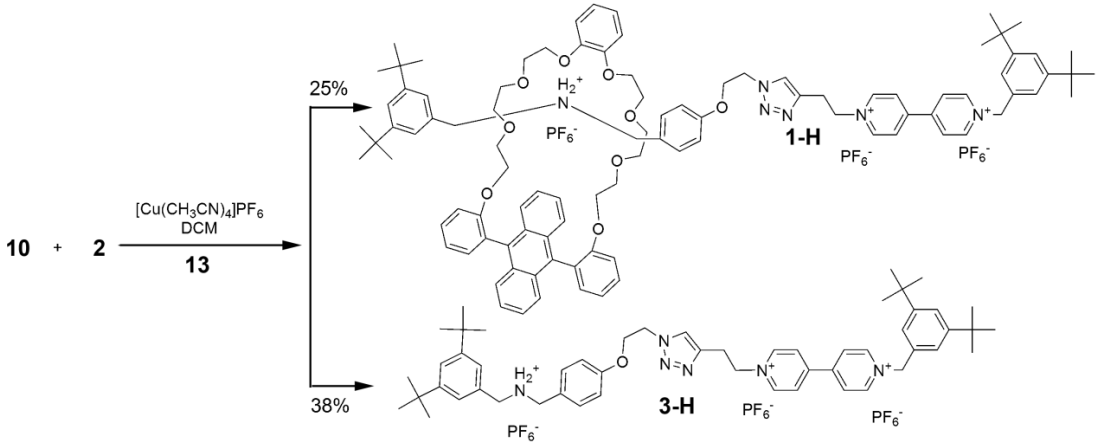


Scheme S3 Synthetic strategy to prepare compound **2**

Synthesis of the compound 2

A solution of diphenol **14** (1.2 g, 3.31 mmol), compound **15** (2.2 g, 3.31 mmol), and Cs_2CO_3 (3.9 g, 12 mmol) in CH_3CN (100 mL) was heated to reflux under N_2 for 24 h. Then the organic solvent was evaporated and the residue was extracted with CH_2Cl_2 (3 × 50 mL), and the combined organic layer was washed with brine (3 × 50 mL), dried over Na_2SO_4 and evaporated in vacuo to obtain oily liquid, which was purified by column chromatography (SiO_2, CH_2Cl_2/MeOH = 30/1) to give product **2** (1.56 g, 67 %) as a blue solid. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ = 7.64 (dd, *J* = 6.7, 3.2 Hz, 4H), 7.52 (t, *J* = 7.8 Hz, 2H), 7.33-7.28 (m, 6H), 7.22-7.12 (m, 4H), 6.88-6.78 (m, 4H),

4.01 (t, *J* = 4.6 Hz, 8H), 3.69-3.65 (m, 4H), 3.37 (t, *J* = 5.1 Hz, 4H), 3.25-3.20 (m, 4H), 3.06-3.02 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 157.3, 148.8, 133.7, 133.0, 130.0, 129.3, 127.9, 126.9, 124.7, 121.2, 121.1, 113.7, 112.7, 70.8, 70.3, 69.4, 68.9, 68.8, 68.7. HRMS (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{44}H_{44}O_8Na$, 723.2934; found, 723.2933.



Scheme S4 Synthetic strategy to prepare compound **1**-H and **3**-H

Synthesis of the compound 3-H and 1-H

A mixture of azide **10** (0.16 g, 0.29 mmol) and crown ether **2** (0.21 g, 0.29 mmol) was stirred in dry CH_2Cl_2 (5 mL) at room temperature for 1 h. After alkyne **13** (0.25 g, 0.35 mmol) and $Cu(CH_3CN)_4PF_6$ (0.024 g, 0.058 mmol) were added to the solution, the mixture was stirred for two days. After removal of the solvent, the residue was first purified via column chromatography (SiO_2, CH_2Cl_2/MeOH = 100/1) to give compound **1-H** (0.14 g, 25 %) as a light orange powder, ^{1}H NMR (CD_3COCD_3, 400 MHz, 298 K): δ = 9.29 (d, *J* = 6.1 Hz, 2H), 9.07 (d, *J* = 6.0 Hz, 2H), 8.43 (m, 5.8 Hz, 4H), 7.81 (s, 1H), 7.68-7.57 (m, 7H), 7.55 (d, *J* = 1.4 Hz, 2H), 7.51 (m, 2.9 Hz, 3H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.37 (m, 2H), 7.32 (d, *J* = 1.4 Hz, 2H), 7.26-7.15 (m, 8H), 6.71 (m, 6H), 5.96 (s, 2H), 5.05 (t, *J* = 6.4 Hz, 2H), 4.74 (t, *J* = 5.0 Hz, 2H), 4.29 (t, *J* = 5.0 Hz, 2H), 4.05 (m, 12H), 3.66-3.31 (m, 18H), 1.32 (s, 18H), 1.25 (s, 18H). ^{13}C NMR (100 MHz, CD_3COCD_3, 298 K) δ = 158.86, 157.06, 152.42, 151.47, 149.84, 147.37, 145.37, 134.19, 133.25, 132.39, 131.55, 130.08, 129.74, 127.70, 127.28, 127.00, 126.96, 126.71, 125.28, 125.16, 124.14, 123.81, 123.76, 123.38, 121.55, 121.32, 114.47, 114.11, 113.75, 112.80, 70.15, 69.35, 69.08, 68.16, 67.76, 66.34, 65.41, 60.74, 49.32, 34.76, 34.62, 33.57, 31.73, 30.73, 26.73, 22.42, 13.45. HRMS (ESI) *m/z*: $[M-2PF_6]^{2+}$ calcd for $C_{97}H_{115}N_6O_9PF_6$, 826.9201; found, 826.9189; $[M-3PF_6]^{3+}$ calcd for $C_{97}H_{115}N_6O_9$, 502.9586; found, 502.9527. Then purified via column chromatography (SiO_2, CH_2Cl_2/MeOH = 20/1) to give compound **3-H** (0.13 g, 38 %) as a light orange solid. ^{1}H NMR (CD_3SOCD_3, 400 MHz, 298 K): δ = 9.57 (d, *J* = 6.9 Hz, 2H), 9.37 (d, *J* = 6.9 Hz, 2H), 9.04 (s, 2H), 8.75 (m, 4H), 8.07 (s, 2H), 7.54 (d, *J* = 1.6 Hz, 2H), 7.45-7.39 (m, 4H), 7.29 (d, *J* = 1.6 Hz, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 5.86 (s, 2H), 5.00 (t, *J* = 7.1 Hz, 2H), 4.74 (t, *J* = 4.9 Hz, 2H), 4.40 (t, *J* = 4.9 Hz, 2H), 4.17-4.08 (m, 4H), 3.44 (t, *J* = 7.2 Hz, 2H), 1.29 (s, 36H). ^{13}C NMR (100 MHz, CD_3SOCD_3, 298 K) δ = 158.2, 151.5, 150.8, 148.8, 145.9, 145.4, 141.7, 133.3, 131.6, 131.1, 127.1, 126.3, 124.1, 123.7, 123.6, 123.6, 123.2, 123.1, 122.5, 114.6, 50.3, 49.7, 48.9, 34.7, 34.5, 31.1, 31.1, 26.5. HRMS (ESI) *m/z*: $[M-PF_6]^+$ calcd for $C_{53}H_{71}N_6P_2F_{12}$, 1097.4973; found, 1097.4977.

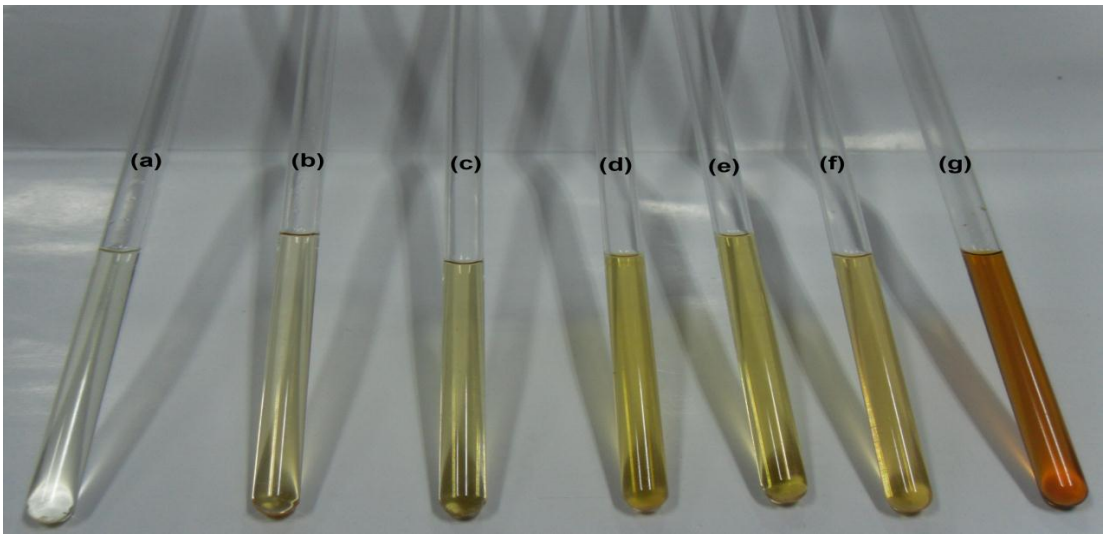


Fig. S1 Photograph of (a) [2]rotaxane **1**-H in CD_3COCD_3, (b) [2]rotaxane **1**-H in CD_3SOCD_3, (c) the mixture obtained after addition of 2 equiv Bu_3N to sample a, (d) the mixture obtained after addition of 3.5 equiv TBAF to sample a, (e) the mixture obtained after addition of 3.5 equiv TBACl to sample a, (f) the mixture obtained after addition of 3.5 equiv TBABr to sample a, and (g) the mixture obtained after addition of 2 equiv TBAI to sample a.

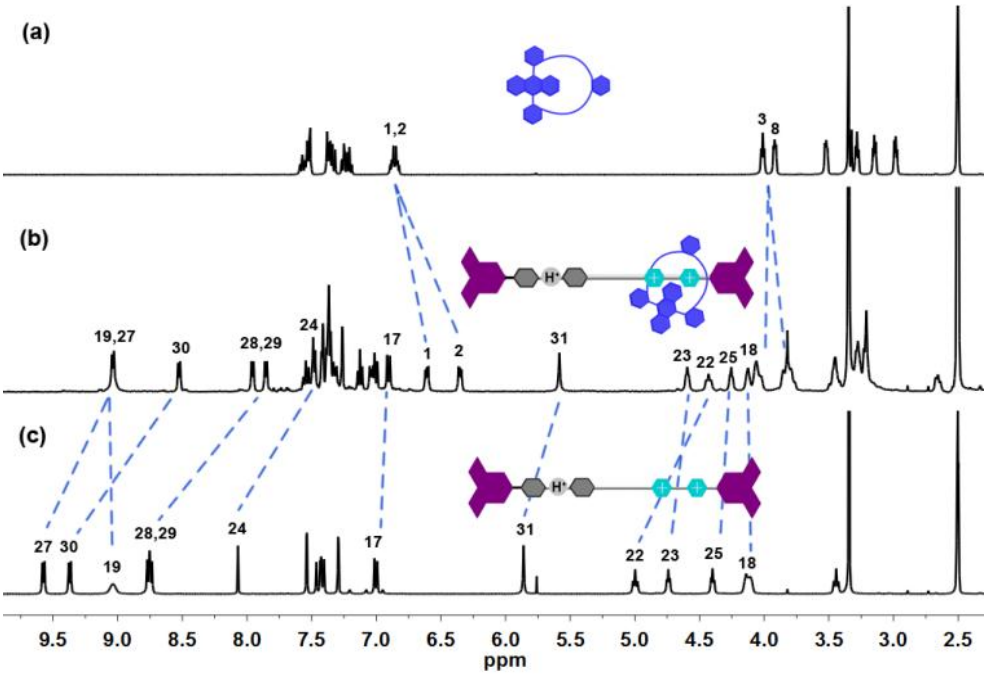


Fig. S2 Partial ^{1}H NMR spectra (400 MHz, DMSO-d_6, 298 K) of (a) macrocycle 2, (b) [2]rotaxane **1-H**, (c) thread component **3-H**.

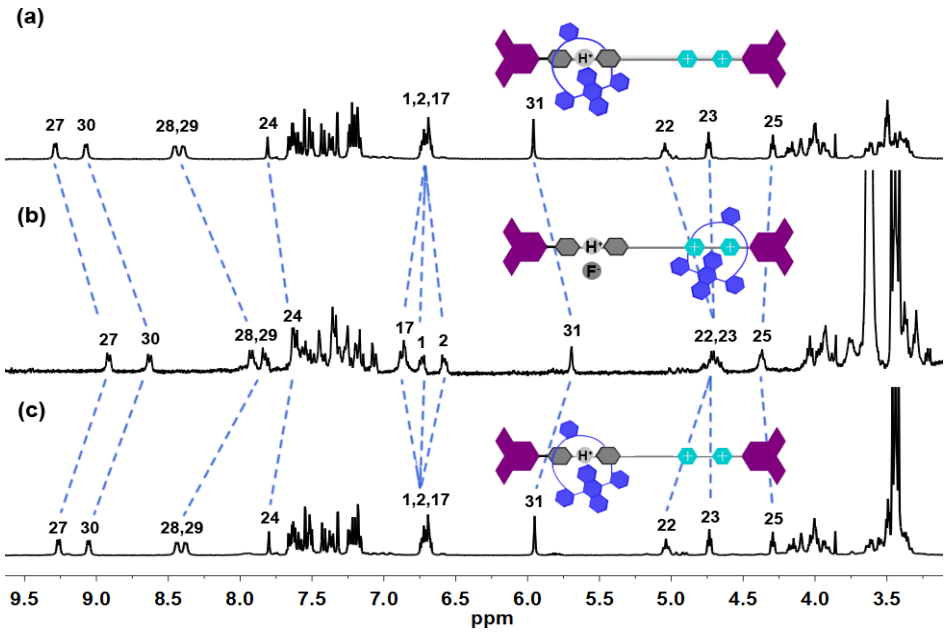


Fig. S3 Partial ^{1}H NMR spectra (400 MHz, CD_3COCD_3, 298 K) of (a) [2]rotaxane **1-H**, (b) the solution obtained after adding 3.5 equiv of TBAF to the solution of a, and (c) the solution obtained after adding 4 equiv of $Ca(PF_6)_2$ to the solution of b.

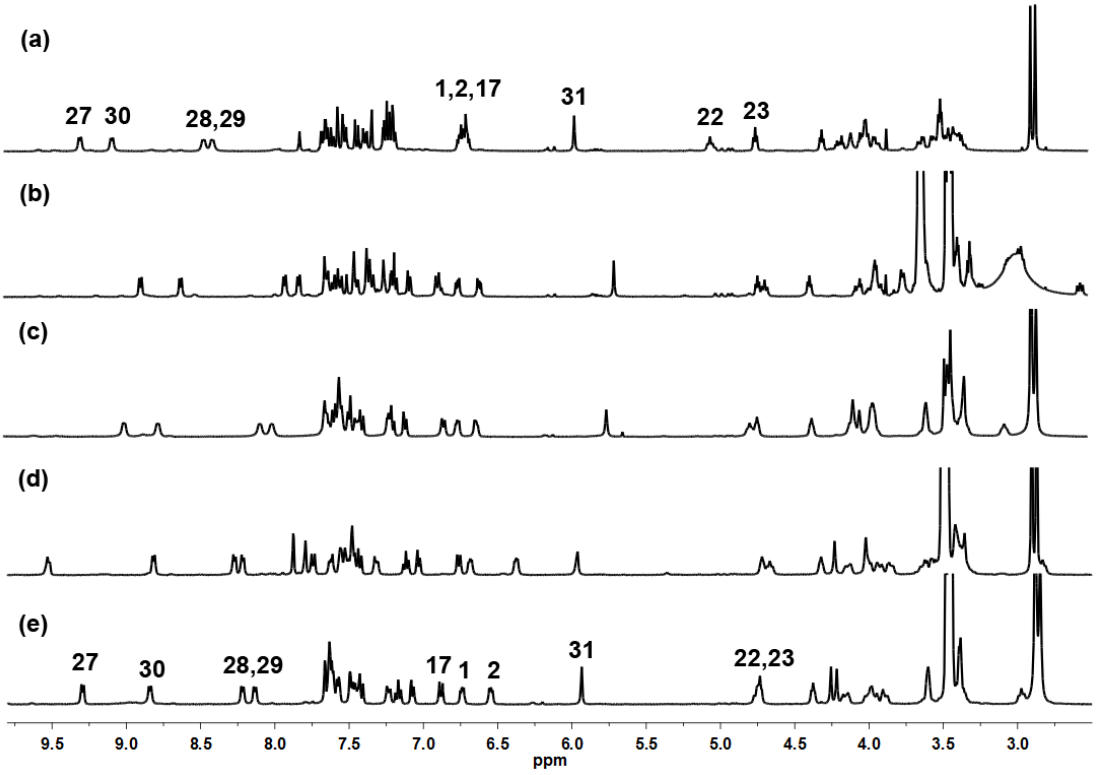


Fig. S4 Partial ^{1}HNMR spectra (CD_3COCD3, 400 MHz, 298 K) of (a) [2]rotaxane **1-H**, (b) the mixture obtained after addition of 3.5 equiv TBAF to sample a, (c) the mixture obtained after addition of 3.5 equiv TBACl to sample a, (d) the mixture obtained after addition of 3.5 equiv TBABr to sample a, and (e) the mixture obtained after addition of 3.5 equiv TBAI to sample a.

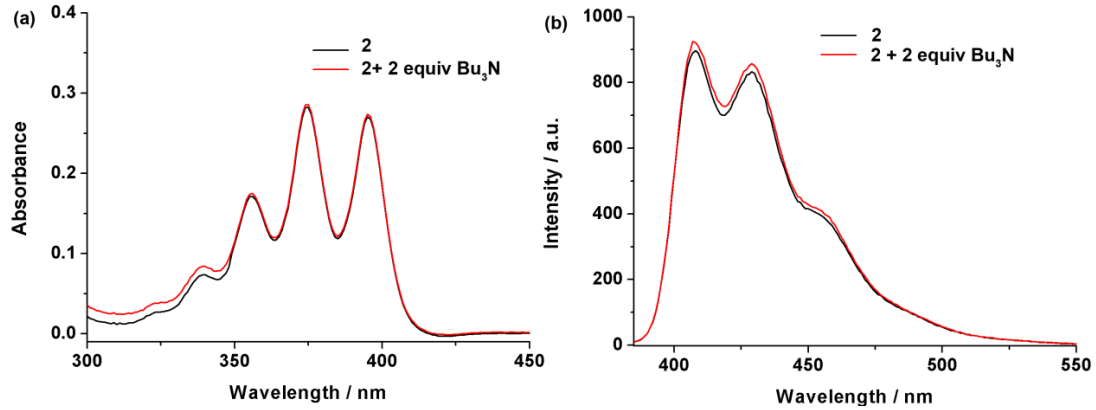


Fig. S5 (a) Absorption and (b) fluorescence spectral changes of **2** in CH_2Cl_2 (2×10^{-5} M) upon addition of 2 equiv of Bu_3N. Excitation wavelength was 375 nm.

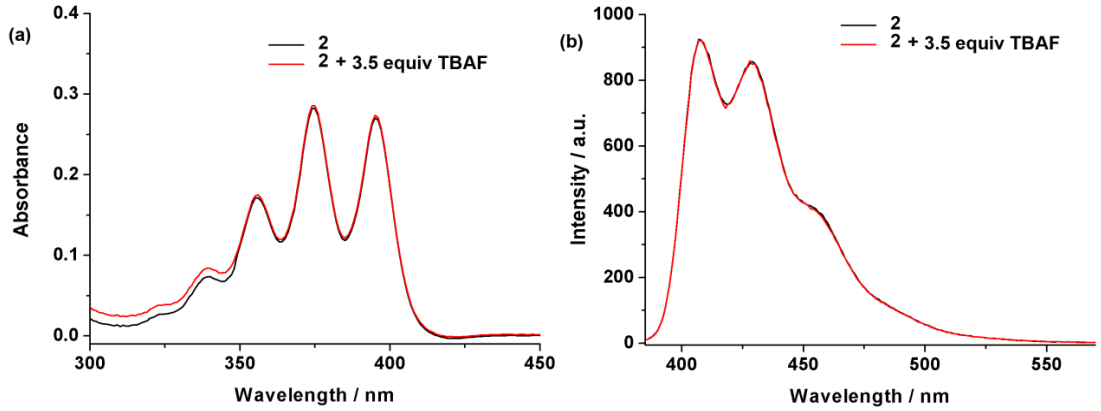


Fig. S6 (a) Absorption and (b) fluorescence spectral changes of **2** in CH_2Cl_2 (2×10^{-5} M) upon addition of 3.5 equiv of TBAF. Excitation wavelength was 375 nm.

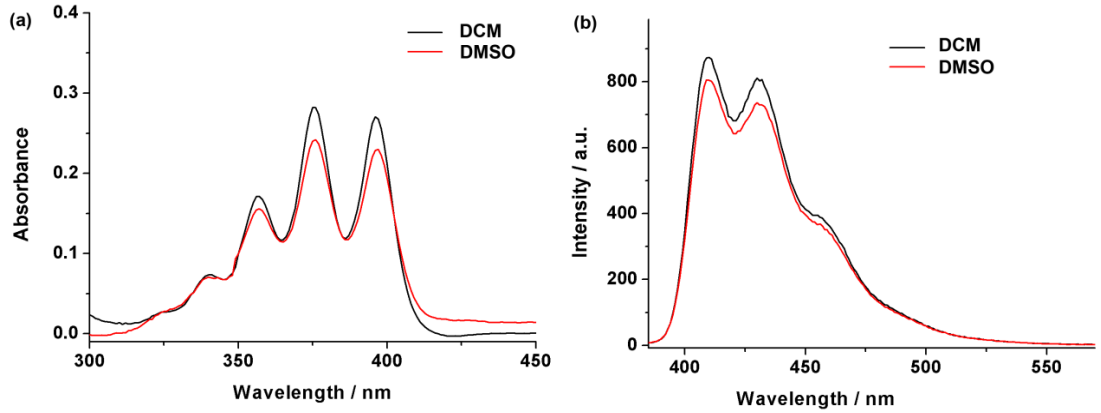


Fig. S7 (a) Absorption and (b) fluorescence spectra of macrocycle **2** (2×10^{-5} M) in DCM and DMSO. Excitation wavelength was 375 nm.

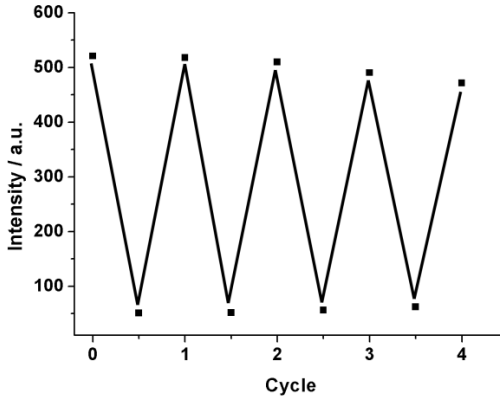


Fig. S8 Fluorescence intensity of **1-H** in CH_2Cl_2 (2×10^{-5} M) at 410 nm upon addition of alternate external stimuli (Bu_3N and TFA) for four cycles. The excitation wavelength was 375 nm.

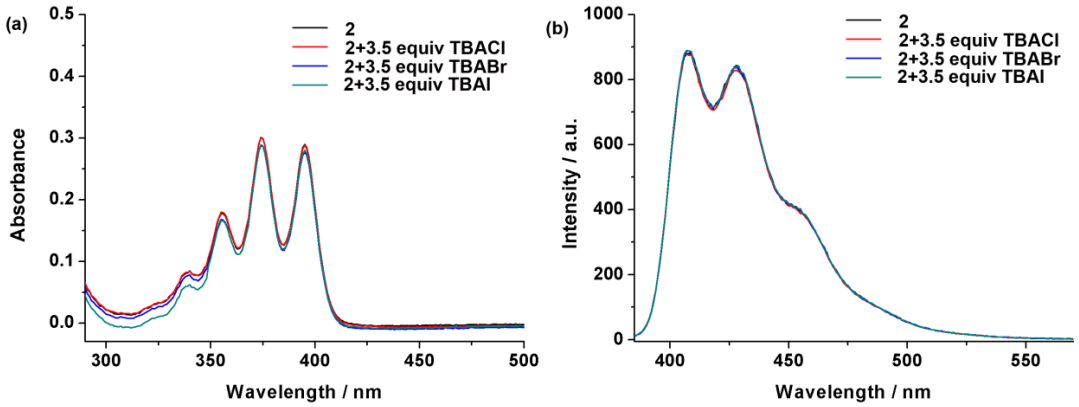


Fig. S9 (a) Absorption and (b) fluorescence spectral changes of **2** in CH_2Cl_2 (2×10^{-5} M) upon addition of 3.5 equiv of TBACl, TBABr, and TBAI. Excitation wavelength was 375 nm.

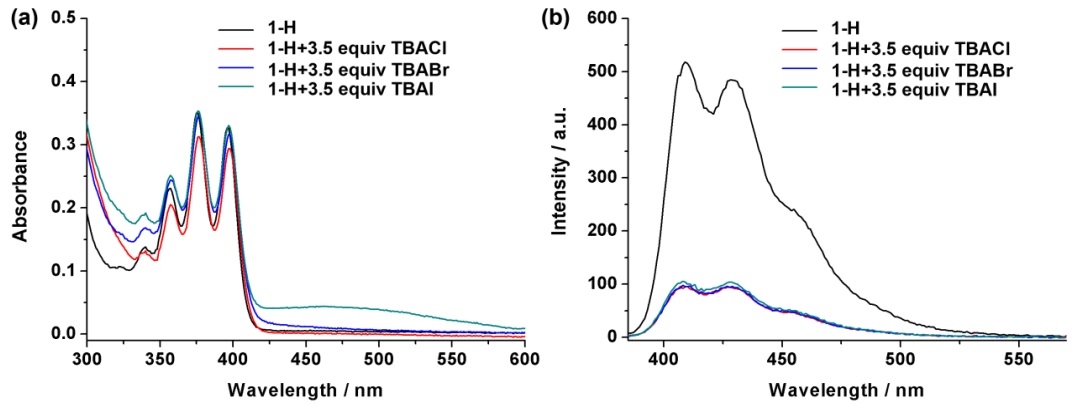
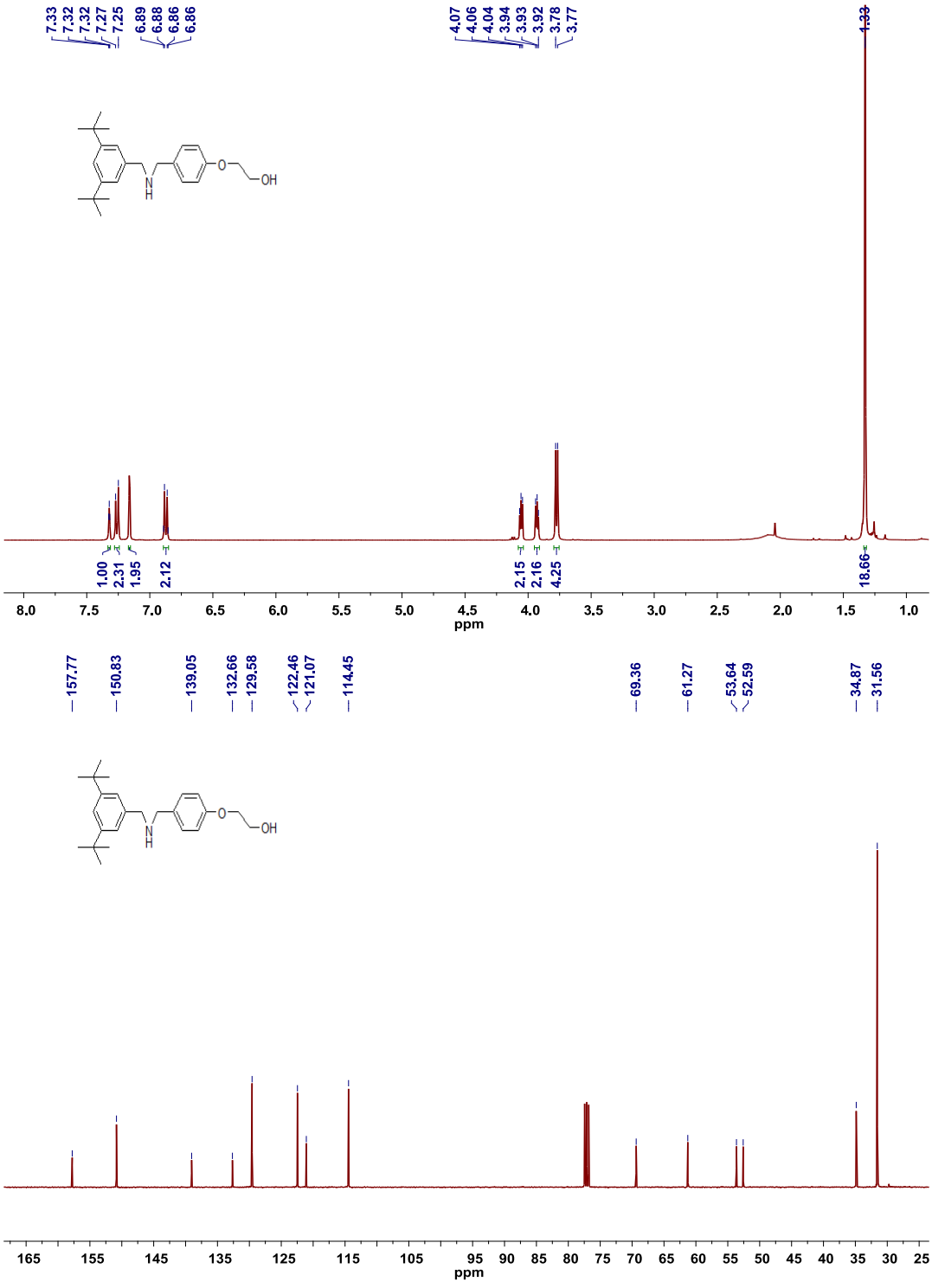


Fig. S10 (a) Absorption and (b) fluorescence spectral changes of **1**-H in CH_2Cl_2 (2×10^{-5} M) upon addition of 3.5 equiv of TBACl, TBABr, and TBAI. Excitation wavelength was 375 nm.

^{1}H NMR, ^{13}C NMR and Mass Spectra

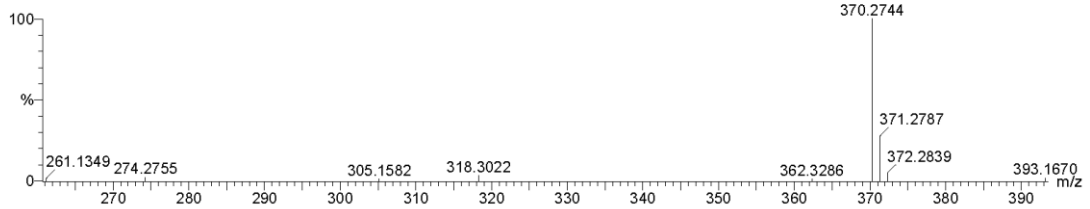
Compound **6**



Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

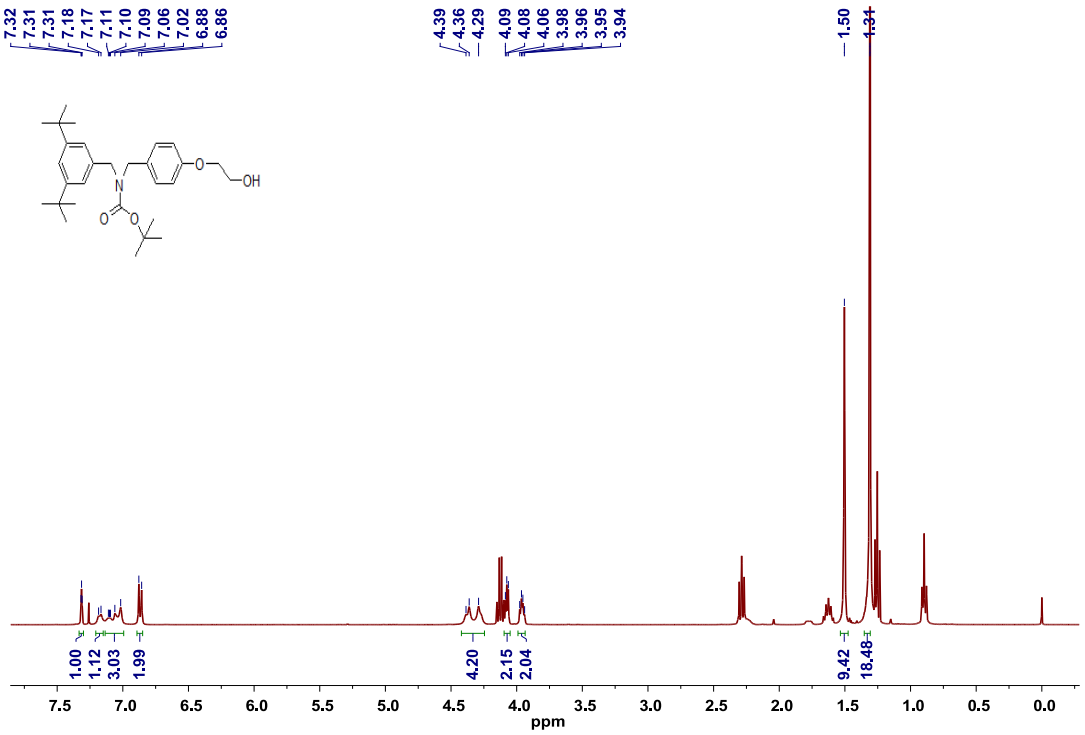
Monoisotopic Mass, Even Electron Ions
579 formula(e) evaluated with 38 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-65 H: 0-120 N: 0-10 O: 0-14

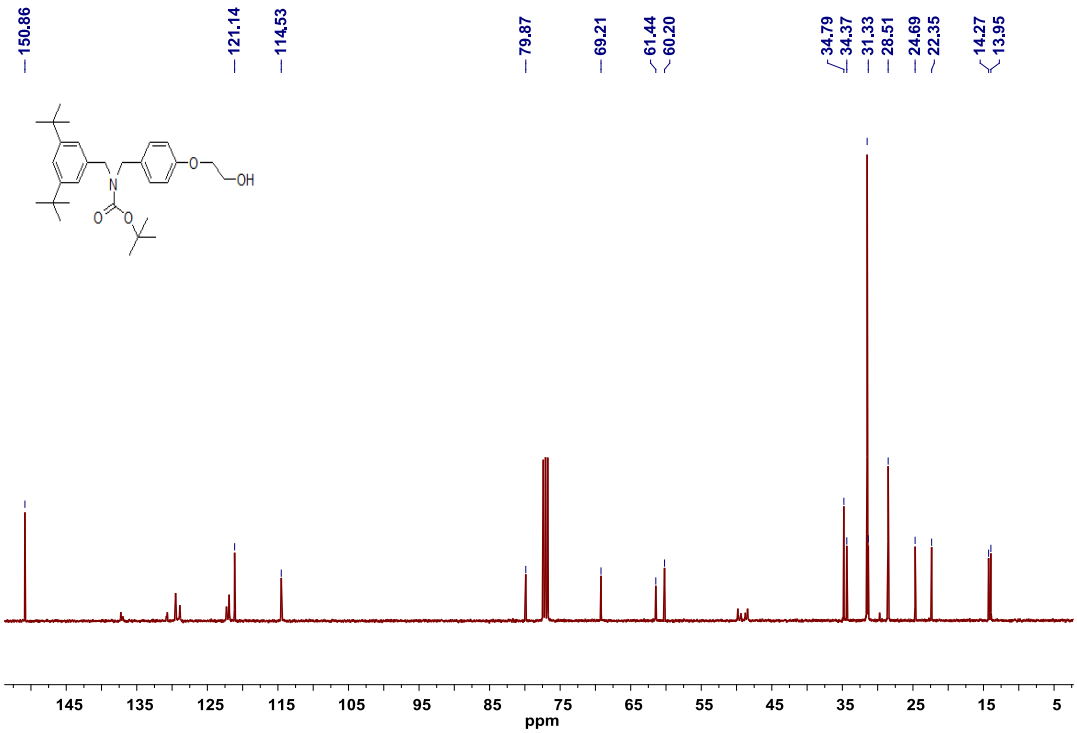
H-TIAN ECUST institute of Fine Chem 02-Dec-2012 21:45:24
TH-ZW-9 36 (1.181) Cm (31:40) 1: TOF MS ES+ 6.00e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
370.2744	370.2746	-0.2	-0.5	7.5	7.3	0.0	C24 H36 N O2

Compound 7

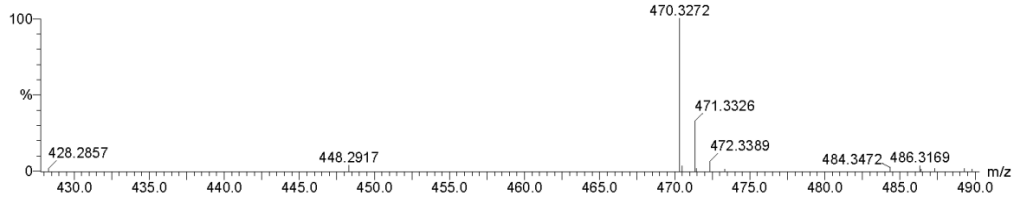




Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

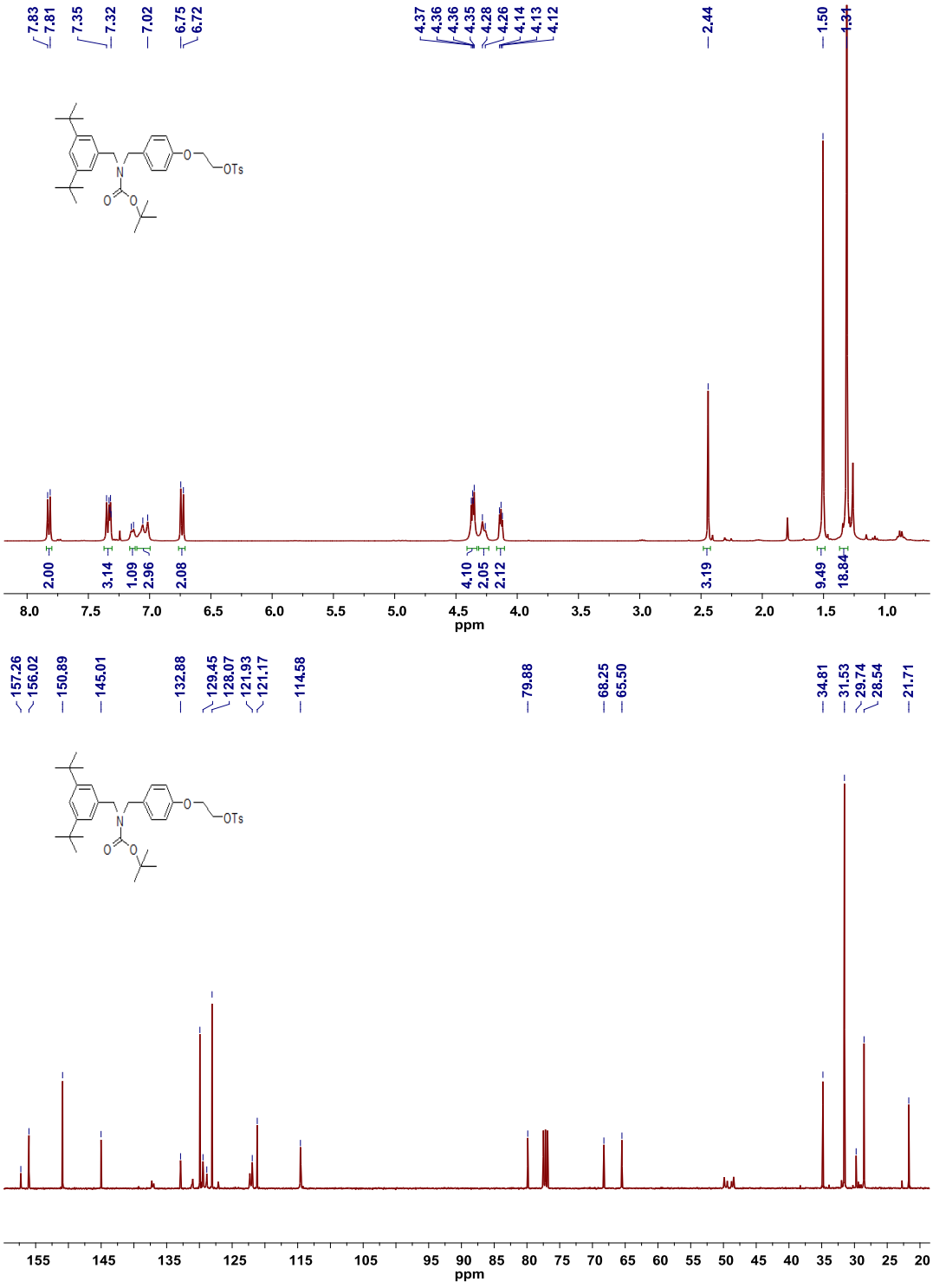
Monoisotopic Mass, Even Electron Ions
132 formula(e) evaluated with 15 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-35 H: 0-47 N: 0-5 O: 0-5

H-TIAN ECUST institute of Fine Chem 01-Dec-2012 11:25:48
TH-ZW-10 48 (1.553) Cm (46:48) 1: TOF MS ES+ 6.60e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
470.3272	470.3270	0.2	0.4	8.5	29.7	0.0	C29 H44 N O4

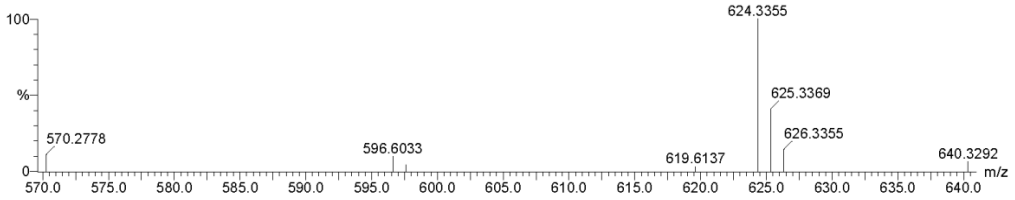
Compound 8



Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

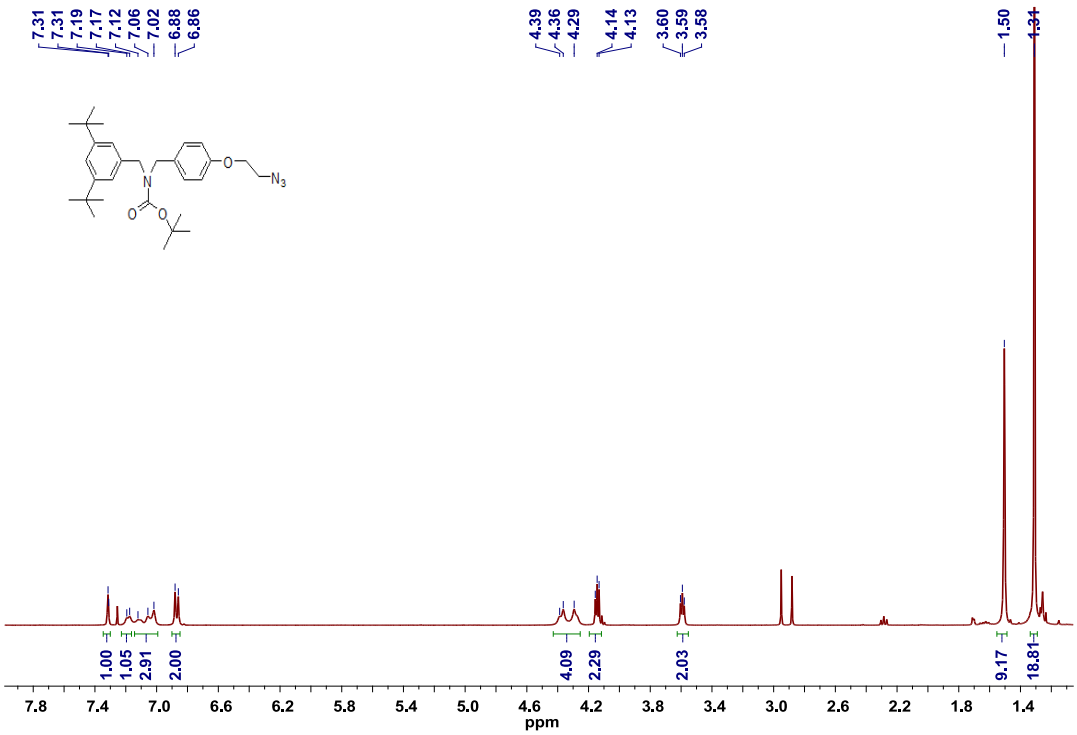
Monoisotopic Mass, Even Electron Ions
1259 formula(e) evaluated with 75 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-44 H: 0-80 N: 0-4 O: 0-6 S: 0-5

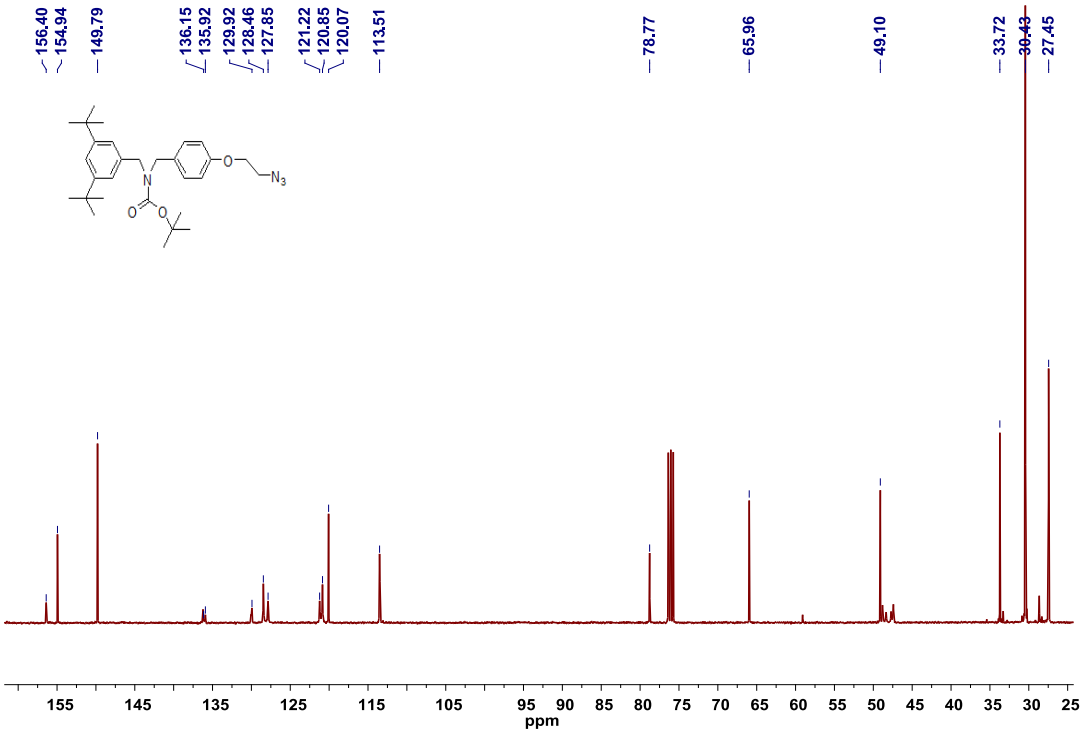
H-TIAN ECUST institute of Fine Chem 02-Dec-2012 11:54:52
TH-ZW-11 35 (1.159) Cm (34:35) 1: TOF MS ES+ 1.03e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
624.3355	624.3359	-0.4	-0.6	12.5	7.9	0.0	C36 H50 N O6 S

Compound 9

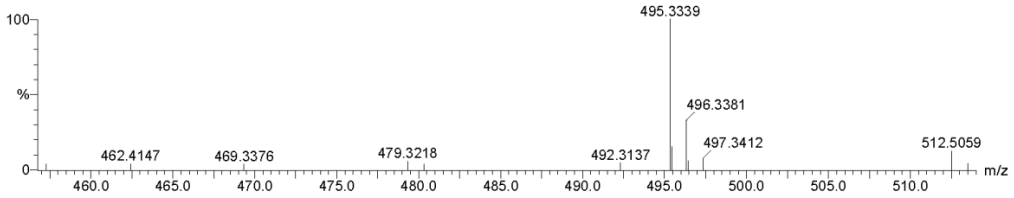




Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

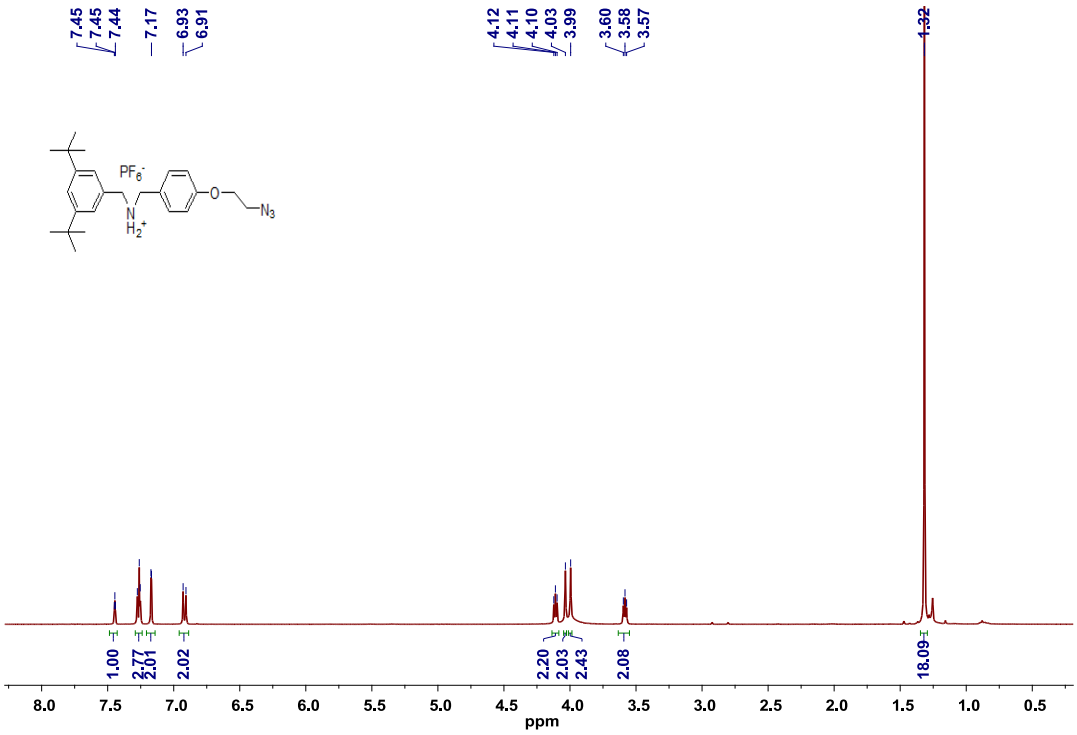
Monoisotopic Mass, Odd and Even Electron Ions
158 formula(e) evaluated with 27 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-40 H: 0-80 N: 0-4 O: 0-4

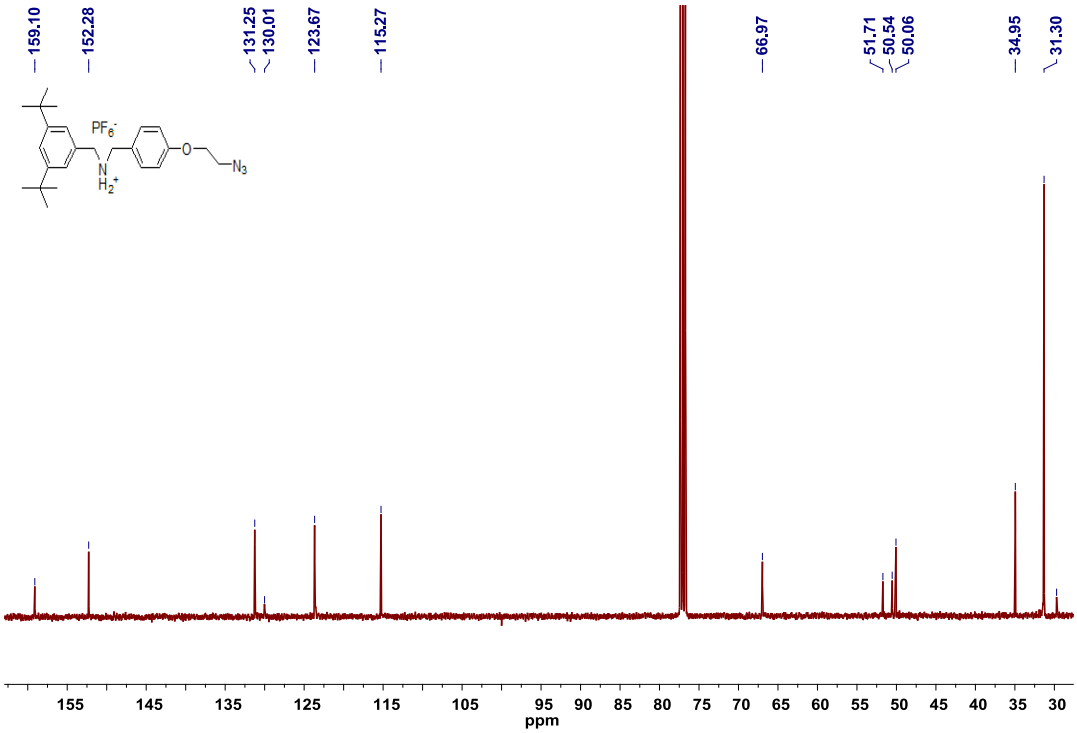
H-TIAN ECUST institute of Fine Chem 02-Dec-2012 12:58:05
TH-ZW-12 14 (0.520) Cm (8:14) 1: TOF MS ES+ 2.19e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
495.3339	495.3335	0.4	0.8	10.5	29.1	0.0	C29 H43 N4 O3

Compound 10

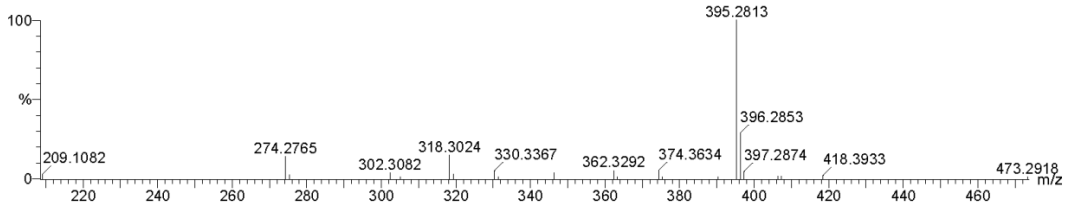




Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

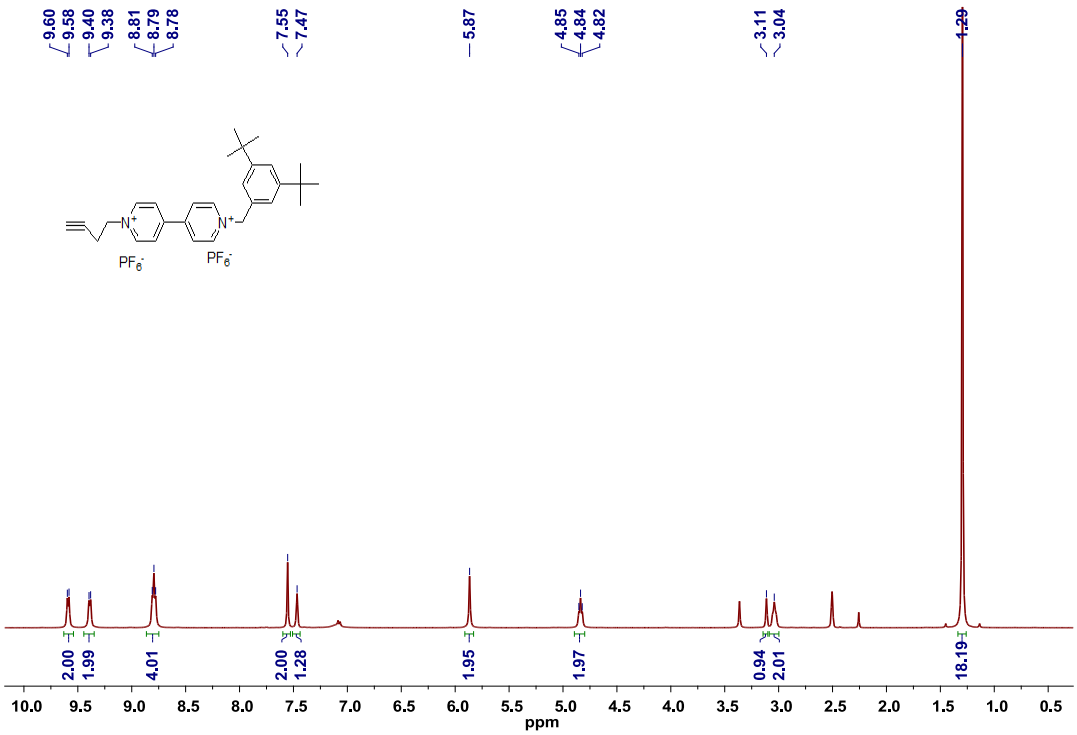
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-24 H: 0-80 N: 0-4 O: 0-1

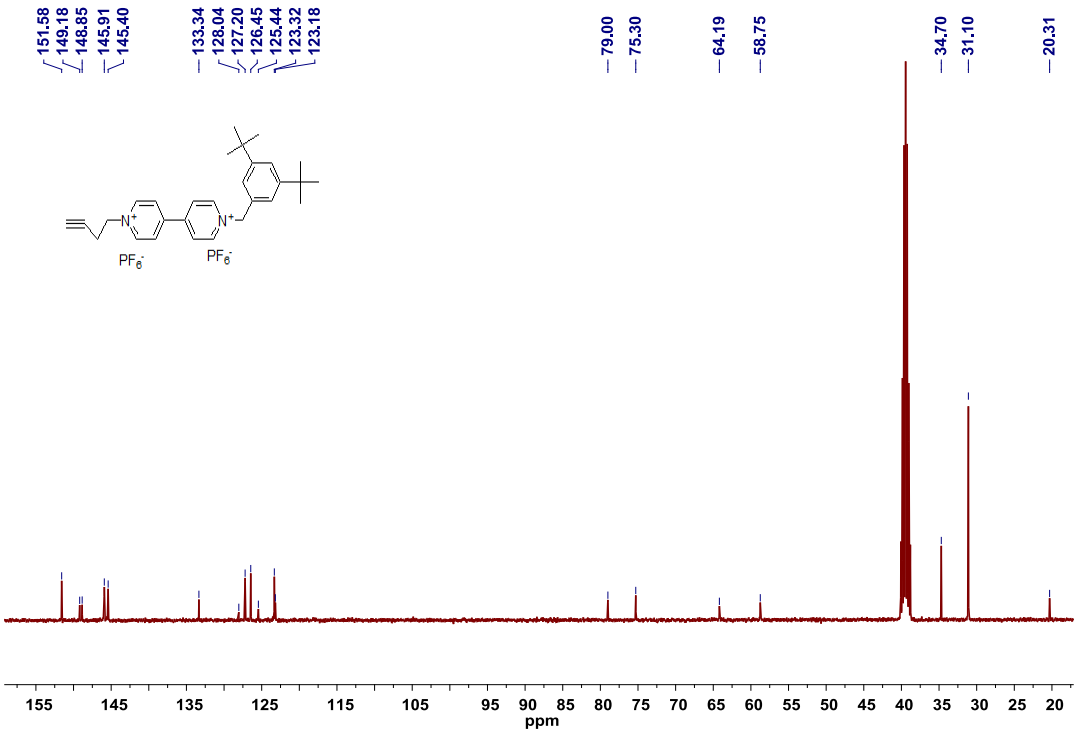
H-TIAN ECUST institute of Fine Chem 02-Dec-2012 12:44:45
TH-ZW-13 6 (0.275) Cm (6:10) 1: TOF MS ES+ 4.30e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
395.2813	395.2811	0.2	0.5	9.5	7.1	0.0	C24 H35 N4 O

Compound 13

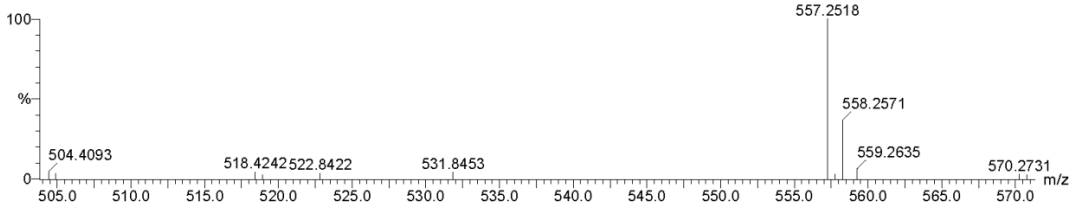




Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

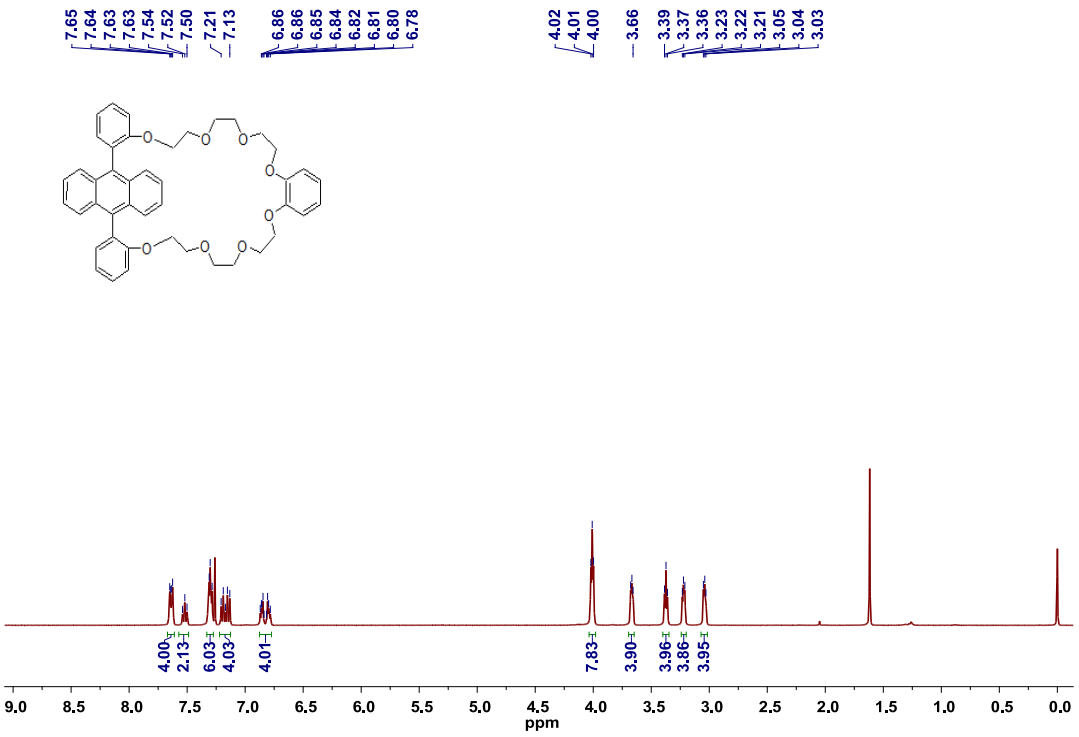
Monoisotopic Mass, Even Electron Ions
287 formula(e) evaluated with 23 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-29 H: 0-80 N: 0-6 F: 0-6 P: 0-2

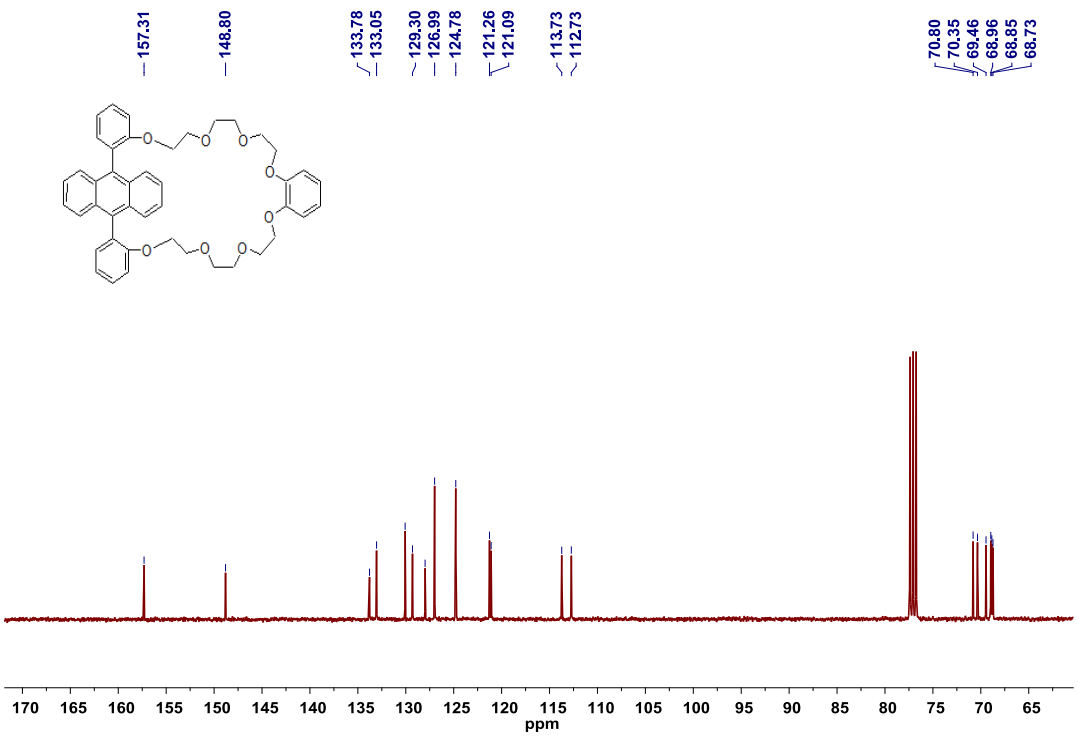
H-TIAN ECUST institute of Fine Chem 02-Dec-2012 12:23:14
TH-ZW-1 22 (0.766) Cm (20:26) 1: TOF MS ES+ 2.33e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
557.2518	557.2520	-0.2	-0.4	10.5	17.5	0.0	C29 H36 N2 F6 P

Compound 2

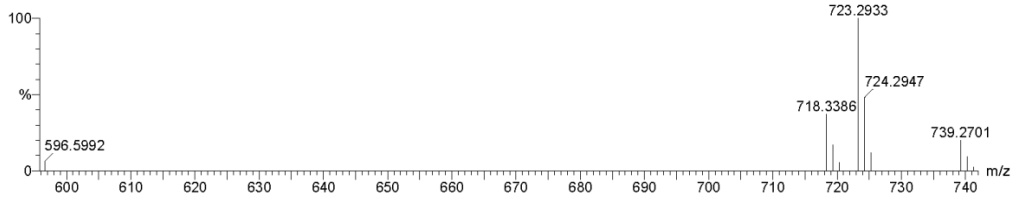




Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

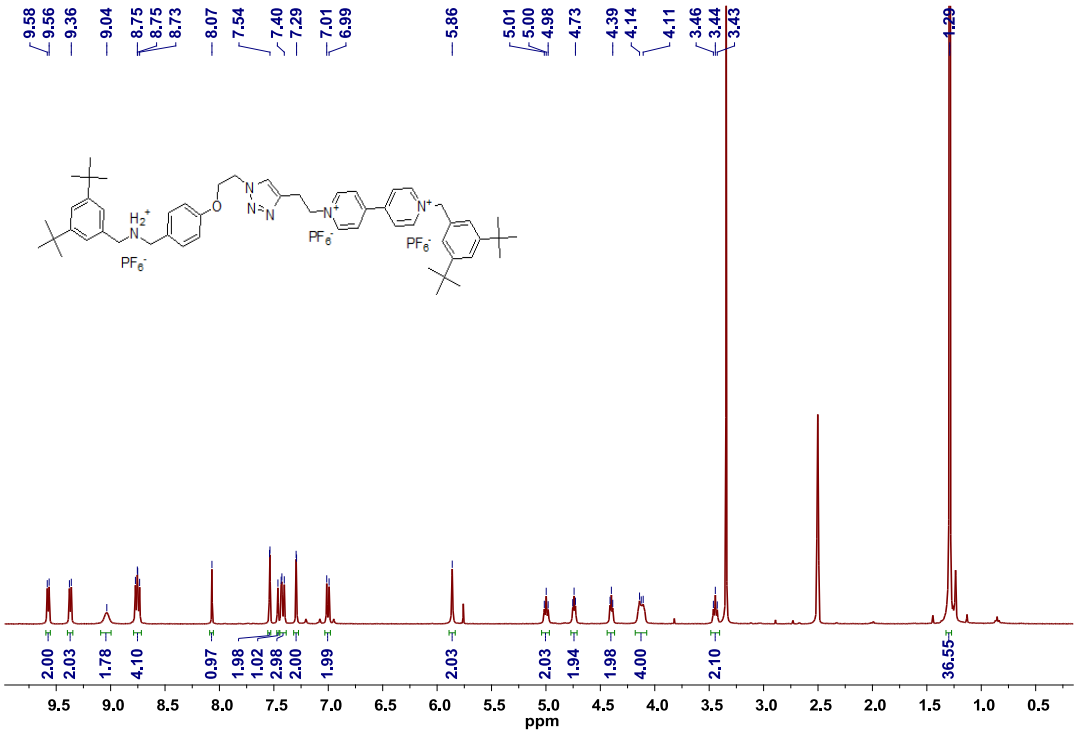
Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-44 H: 0-80 O: 0-8 Na: 0-1

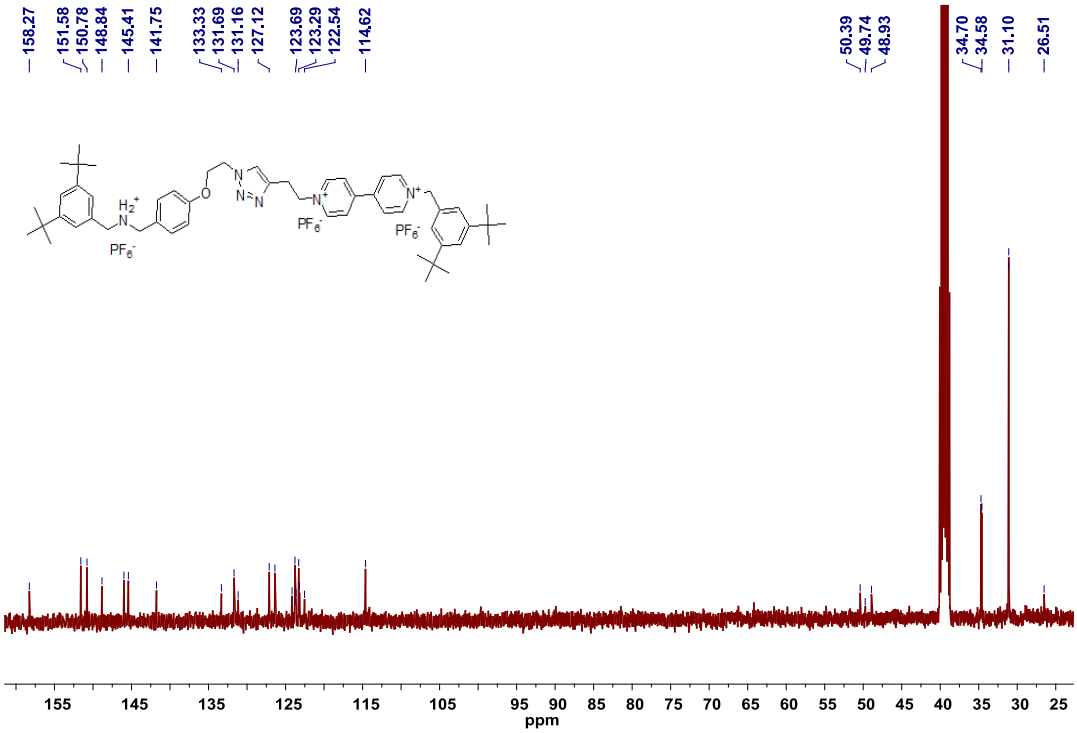
H-TIAN ECUST institute of Fine Chem 02-Dec-2012 12:28:15
TH-ZW-15 44 (1.428) Cm (38:45) 1: TOF MS ES+ 2.44e+003



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
723.2933	723.2934	-0.1	-0.1	22.5	8.8	0.0	C44 H44 O8 Na

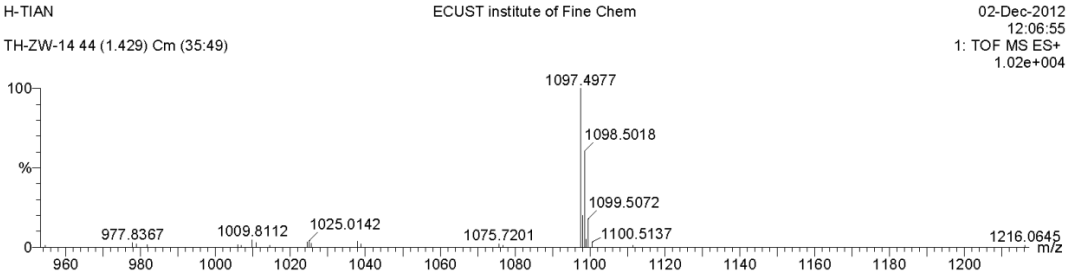
Compound **3-H**





Single Mass Analysis
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
1920 formula(e) evaluated with 51 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-53 H: 0-80 N: 0-6 O: 0-6 F: 0-12 P: 0-2



Minimum:				-1.5			
Maximum:		50.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1097.4977	1097.4973	0.4	0.4	16.5	25.5	0.0	C53 H71 N6 O F12 P2

Compound **1-H**