Supporting Information

Directed Synthesis of [2]Catenanes Incorporating Naphthalenediimide and Crown Ethers by Associated Interactions of Templates

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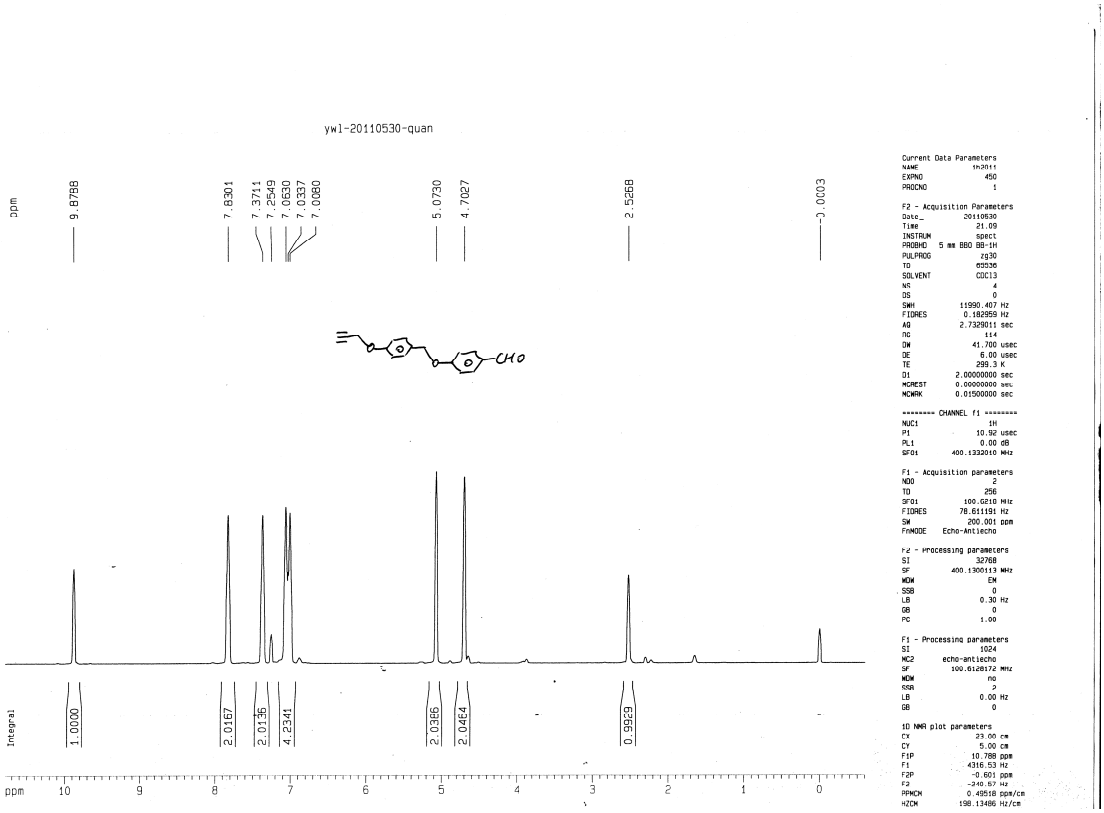
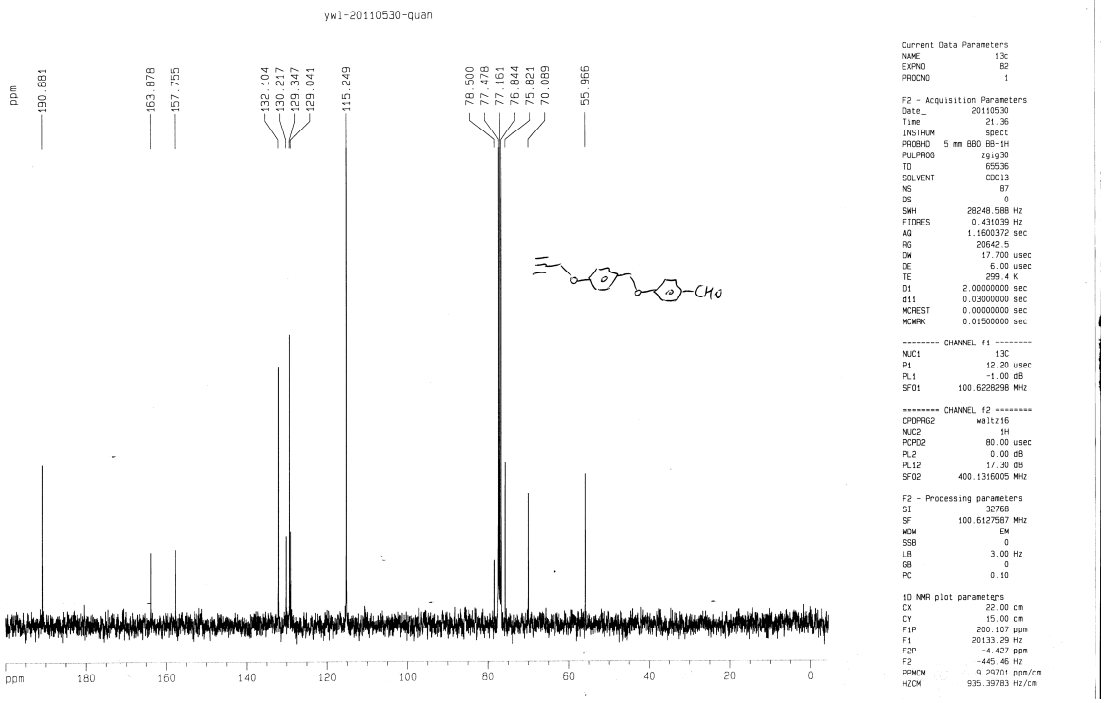
§1. NMR and MS spectra

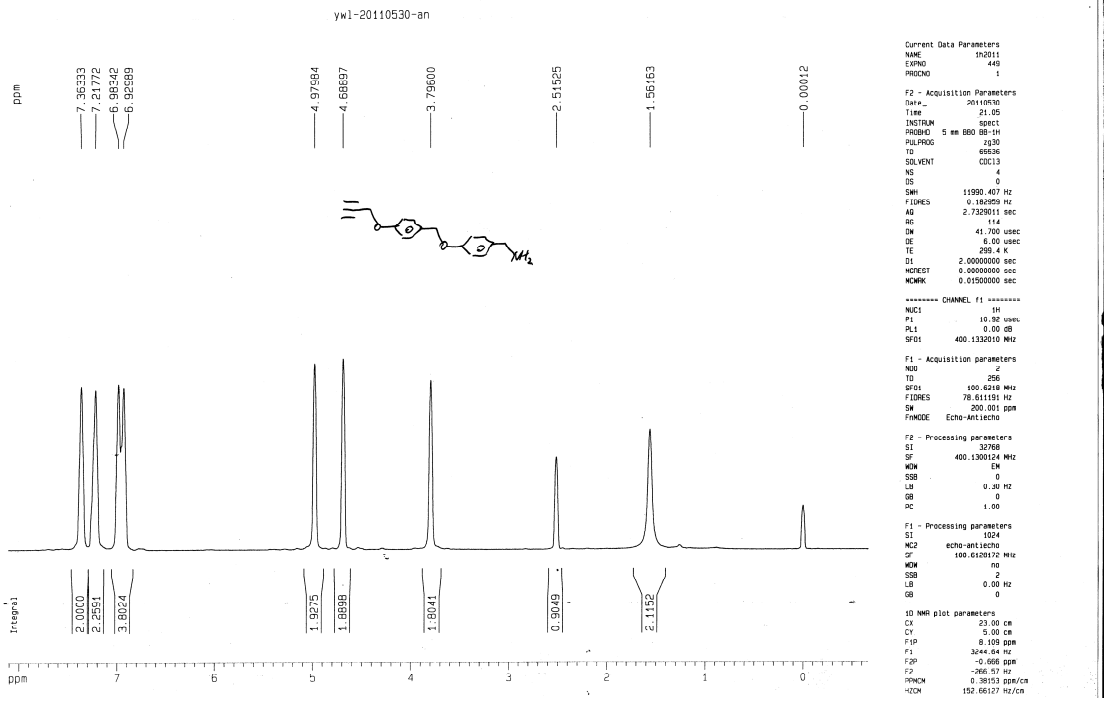
^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of **S-1**



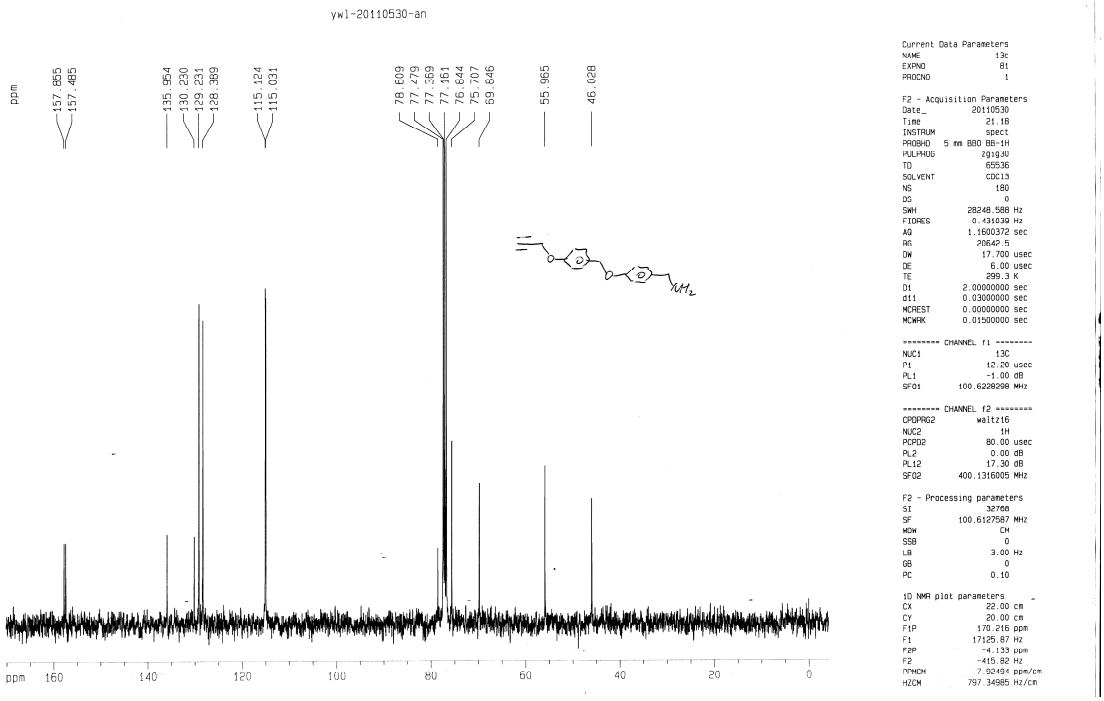
^{13}C NMR spectrum (400 MHz, 298 K, $CDCl_3$) of **S-1**



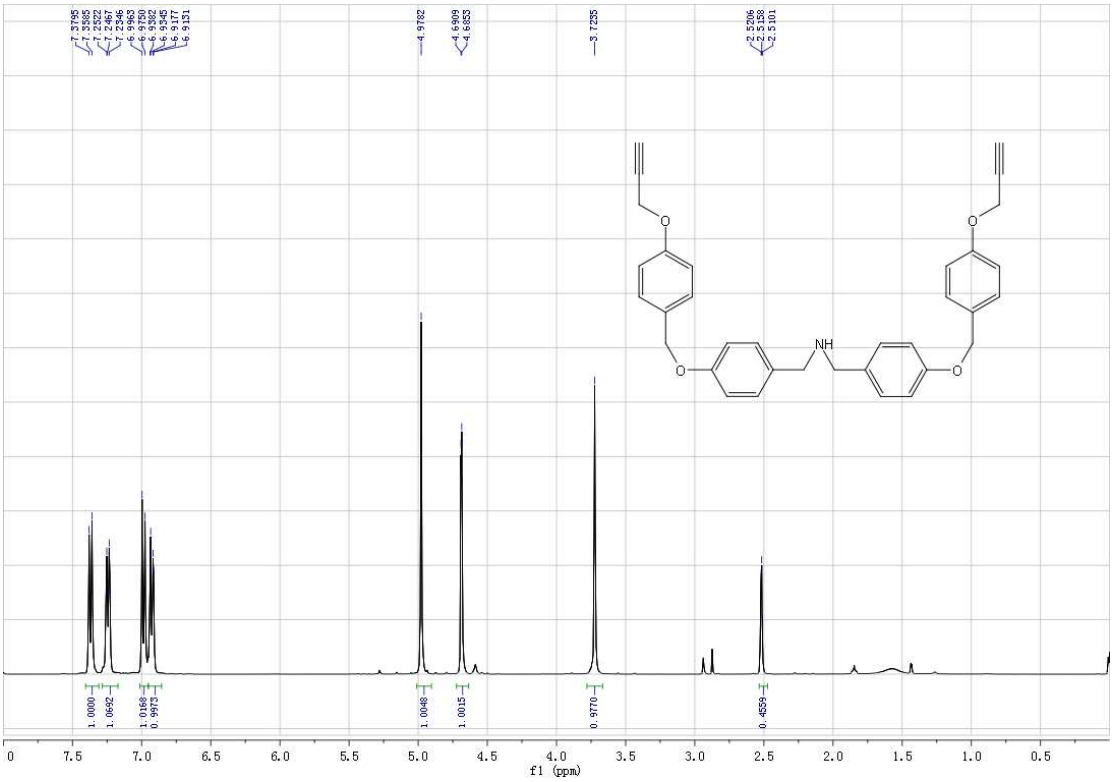
^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of **S-3**



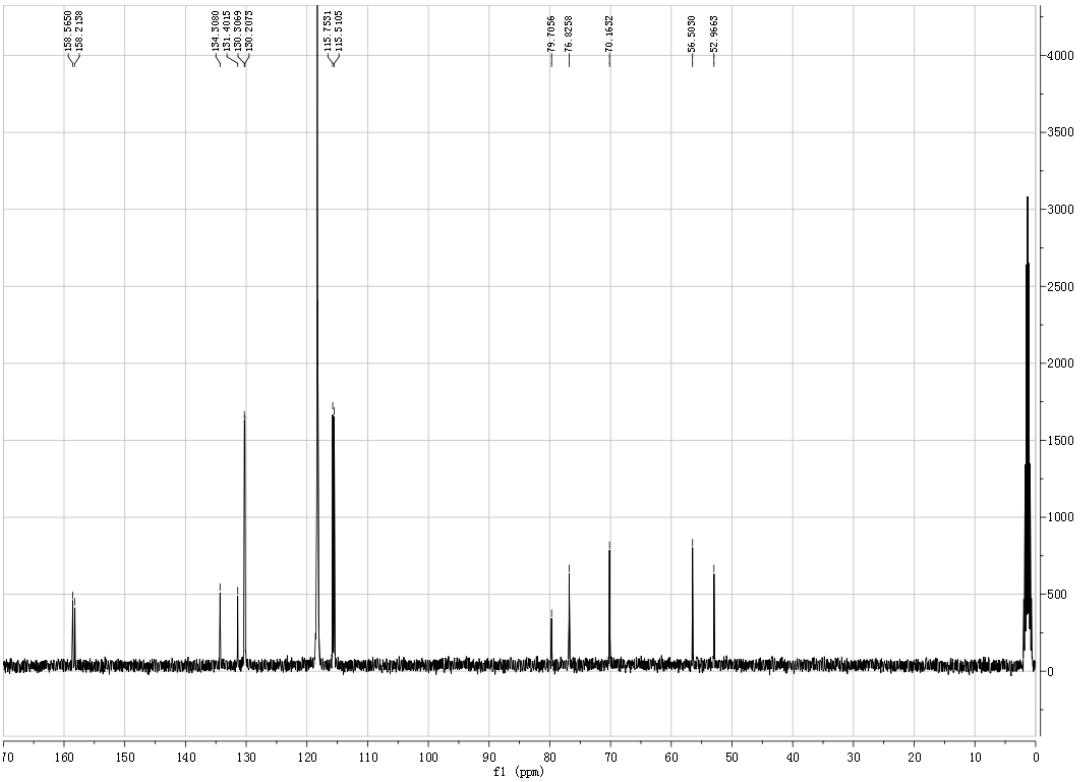
^{13}C NMR spectrum (400 MHz, 298 K, $CDCl_3$) of **S-3**



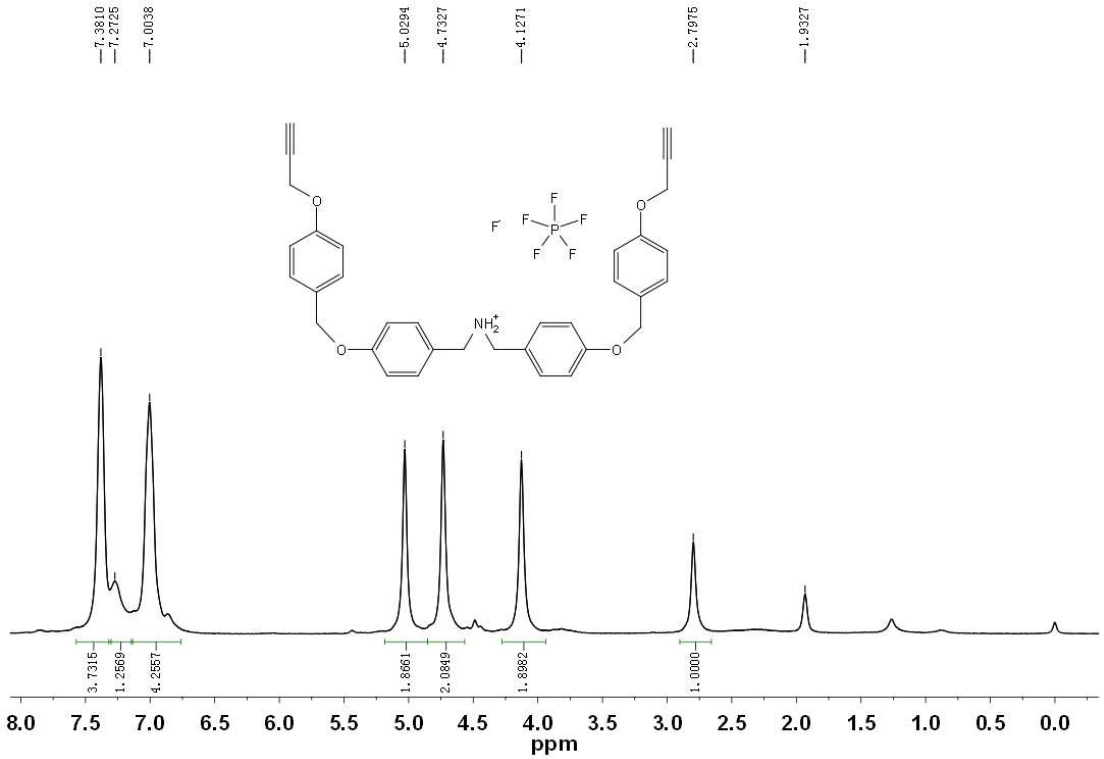
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **S-4**



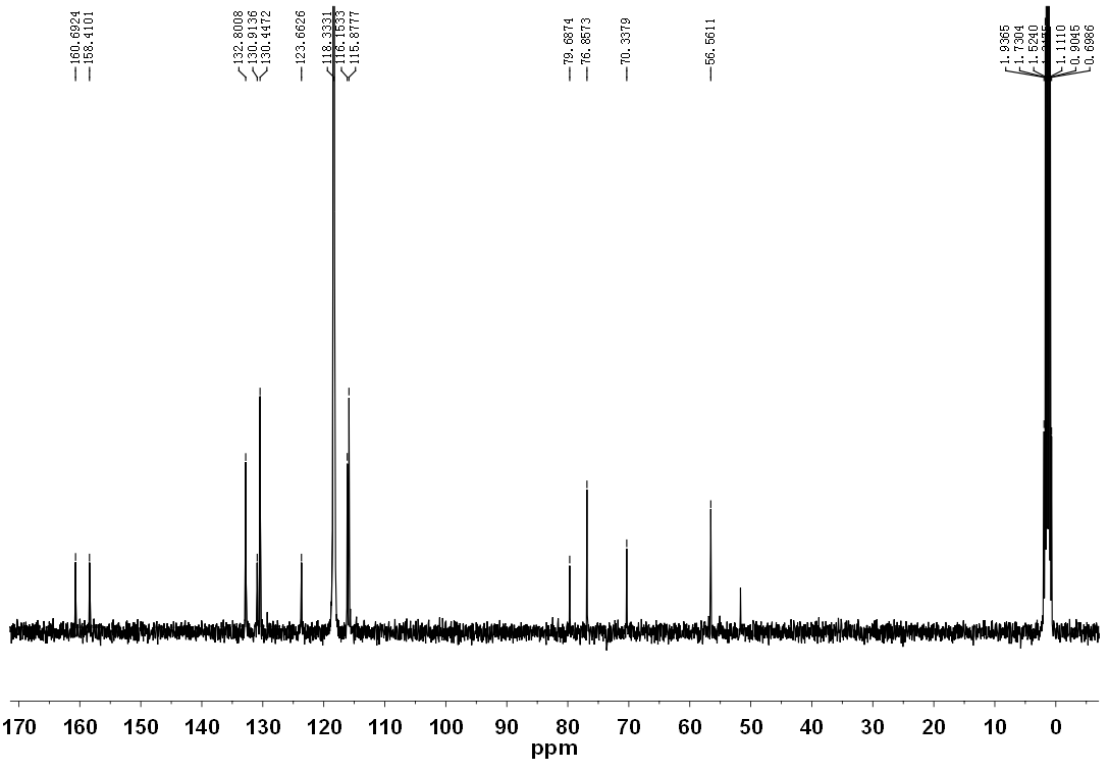
^{13}C NMR spectrum (400 MHz, 298 K, CD_3CN) of **S-4**



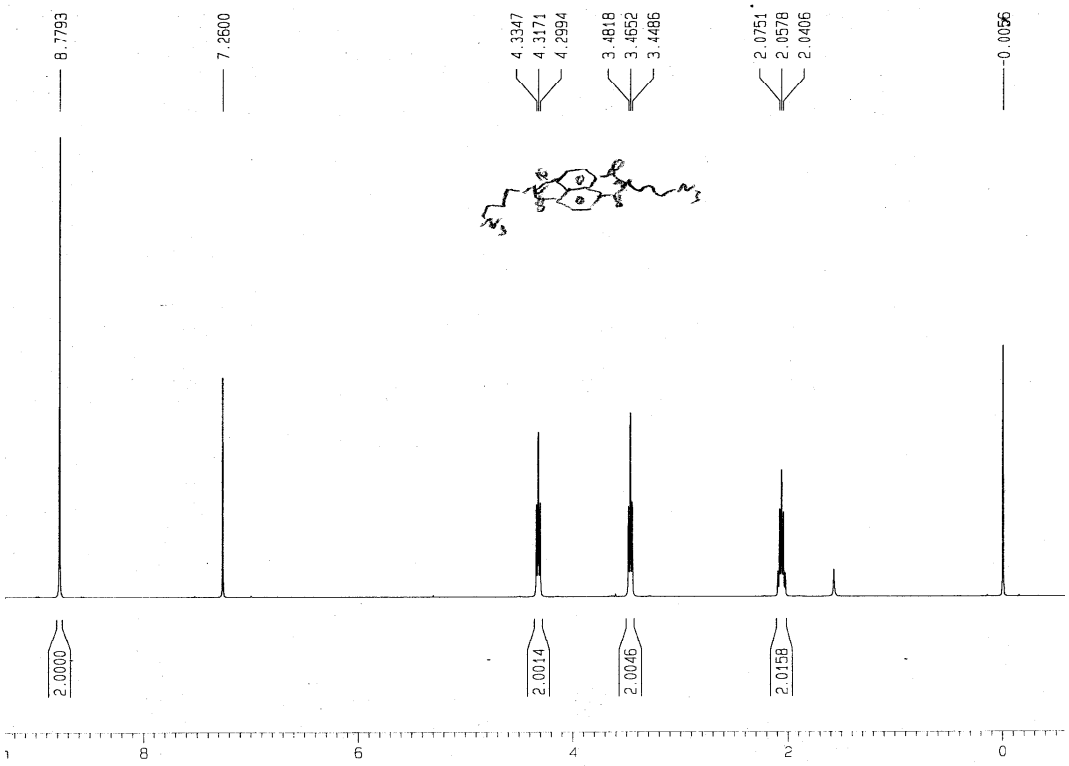
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **1**



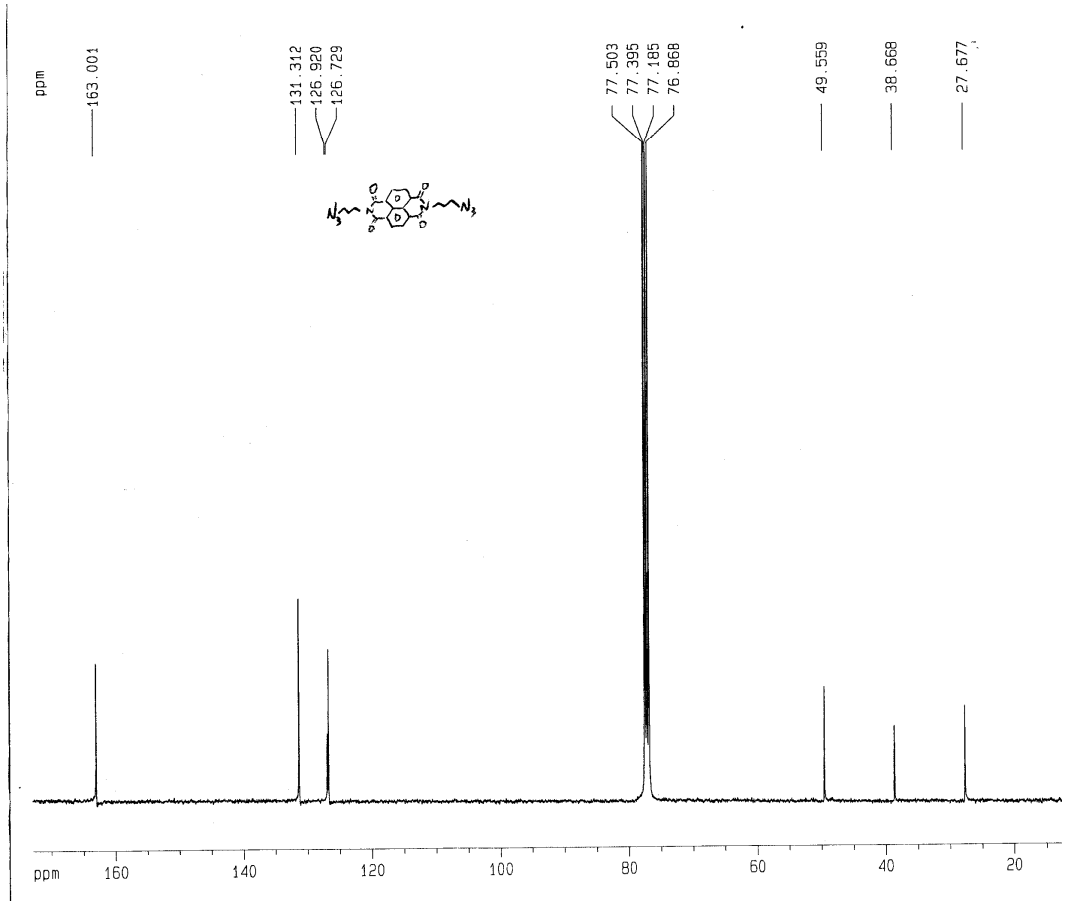
^{13}C NMR spectrum (100 MHz, 298 K, CD_3CN) of **1**



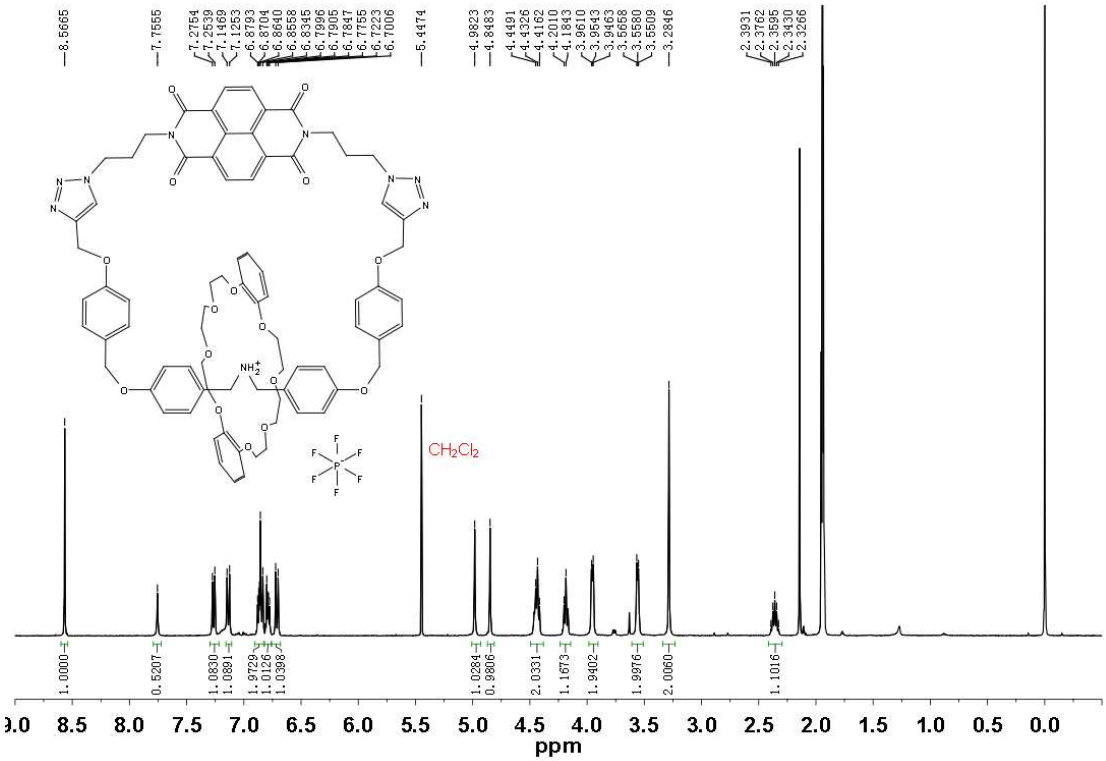
^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of **2**



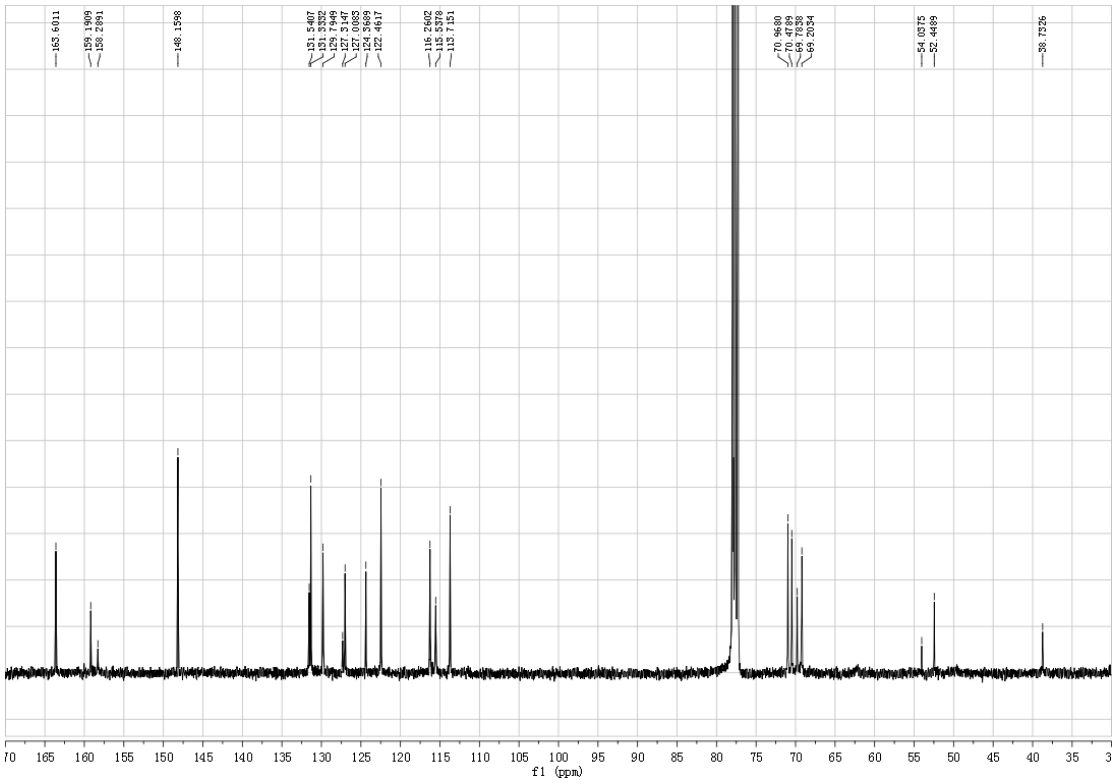
^{13}C NMR spectrum (400 MHz, 298 K, $CDCl_3$) of **2**



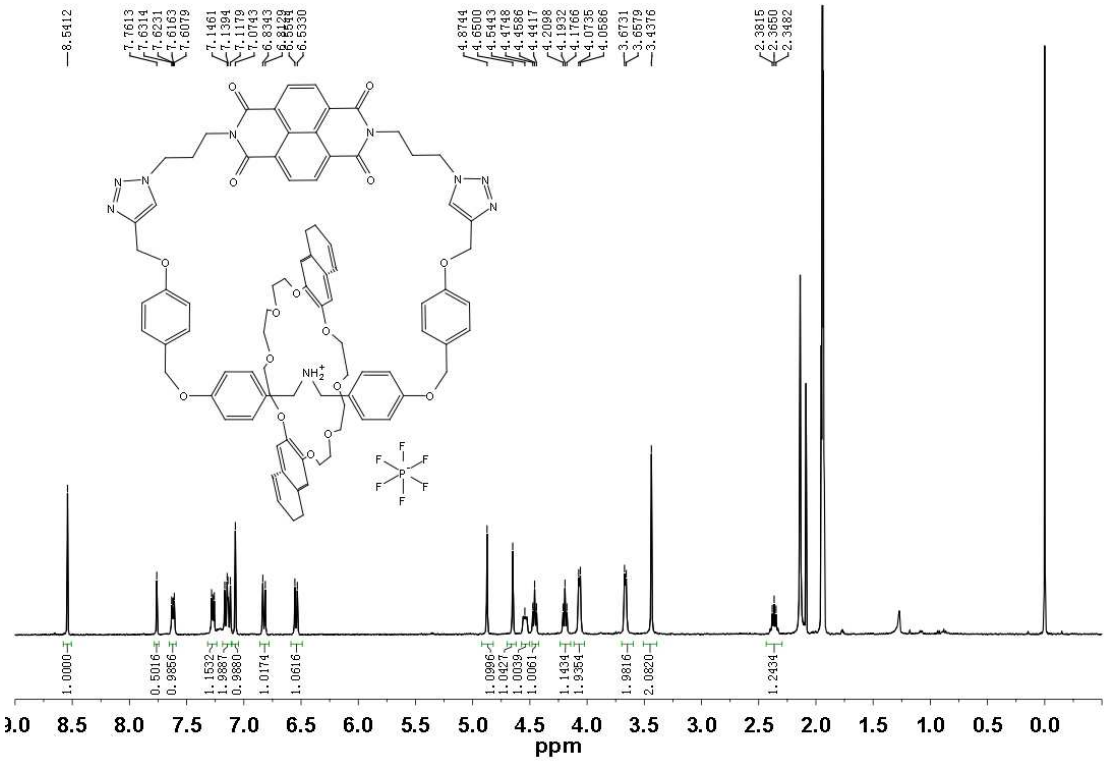
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **4B**



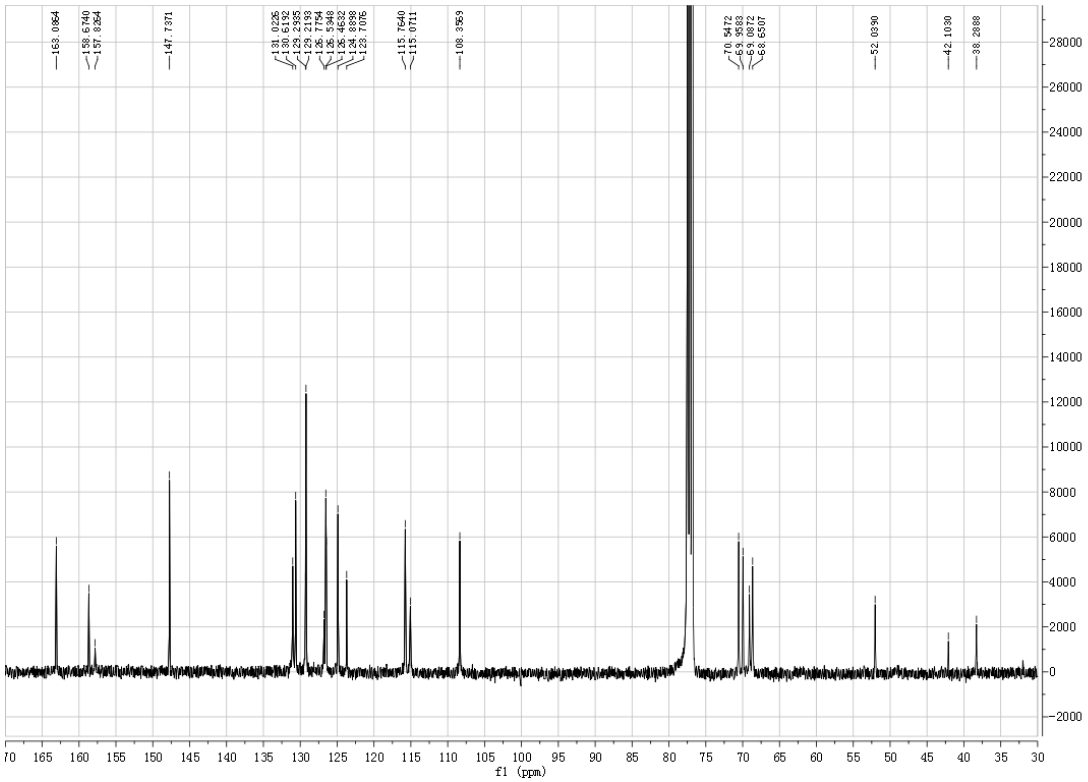
^{13}C NMR spectrum (400 MHz, 298 K, CD_3CN) of **4B**



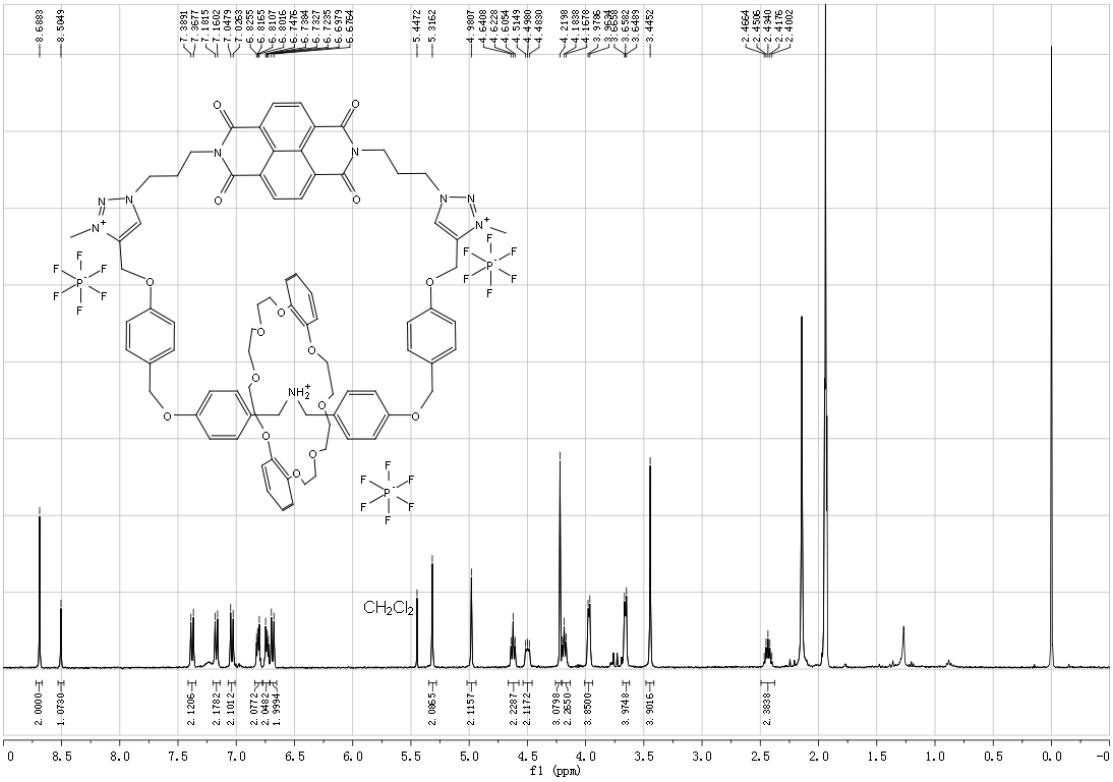
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **4A**



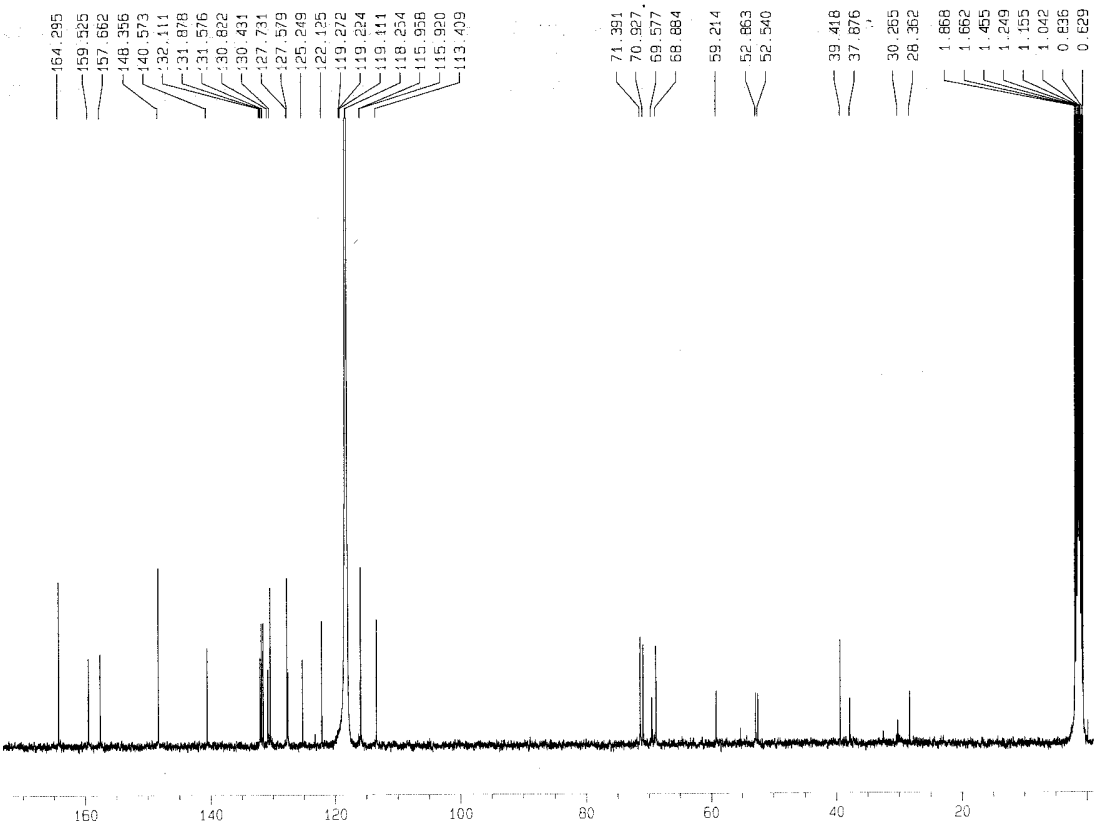
^{13}C NMR spectrum (400 MHz, 298 K, CD_3CN) of **4A**



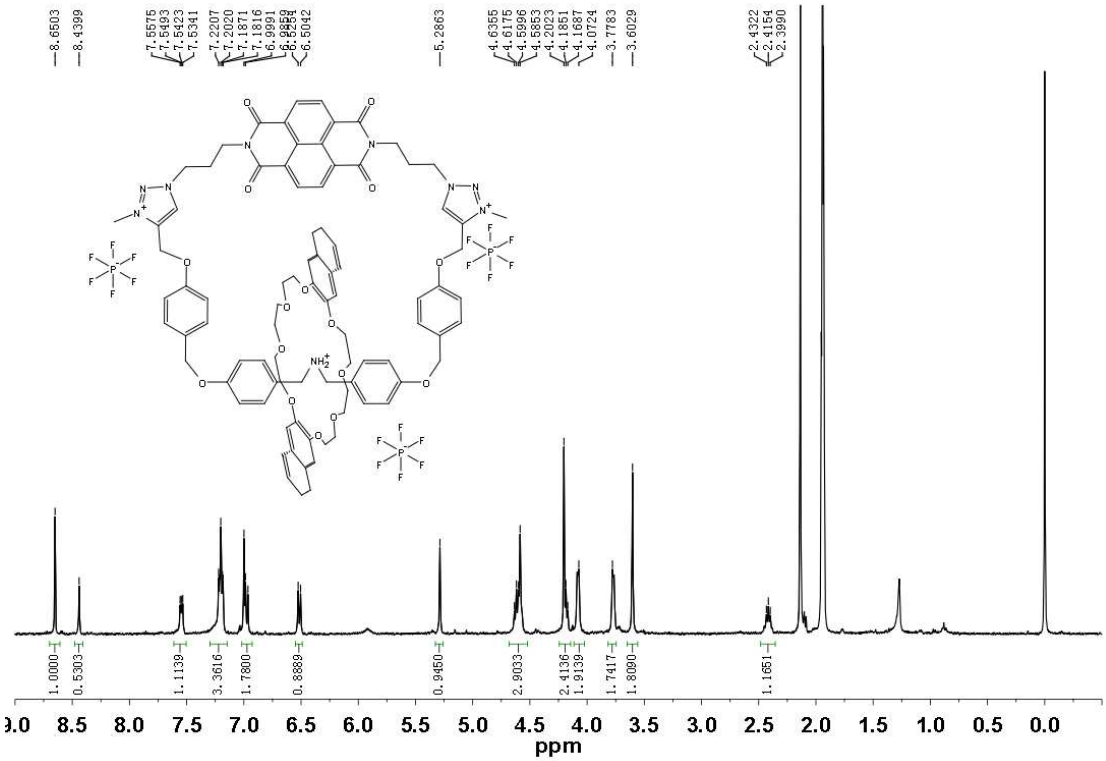
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **5B**



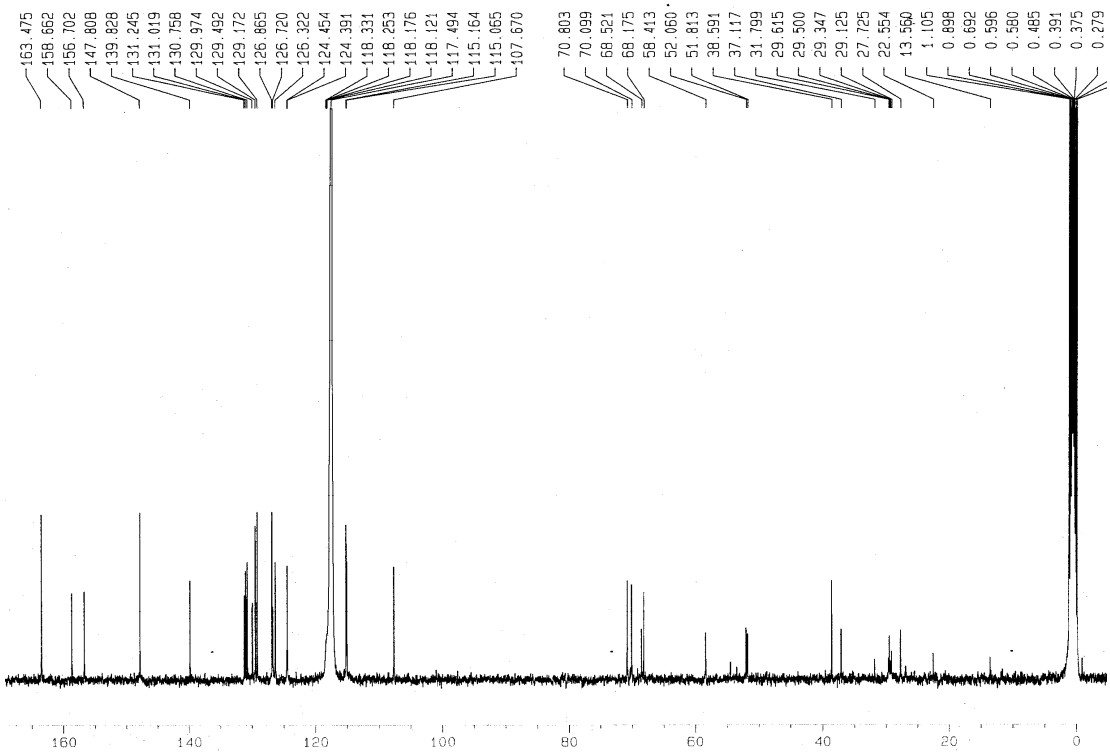
^{13}C NMR spectrum (400 MHz, 298 K, CD_3CN) of **5B**



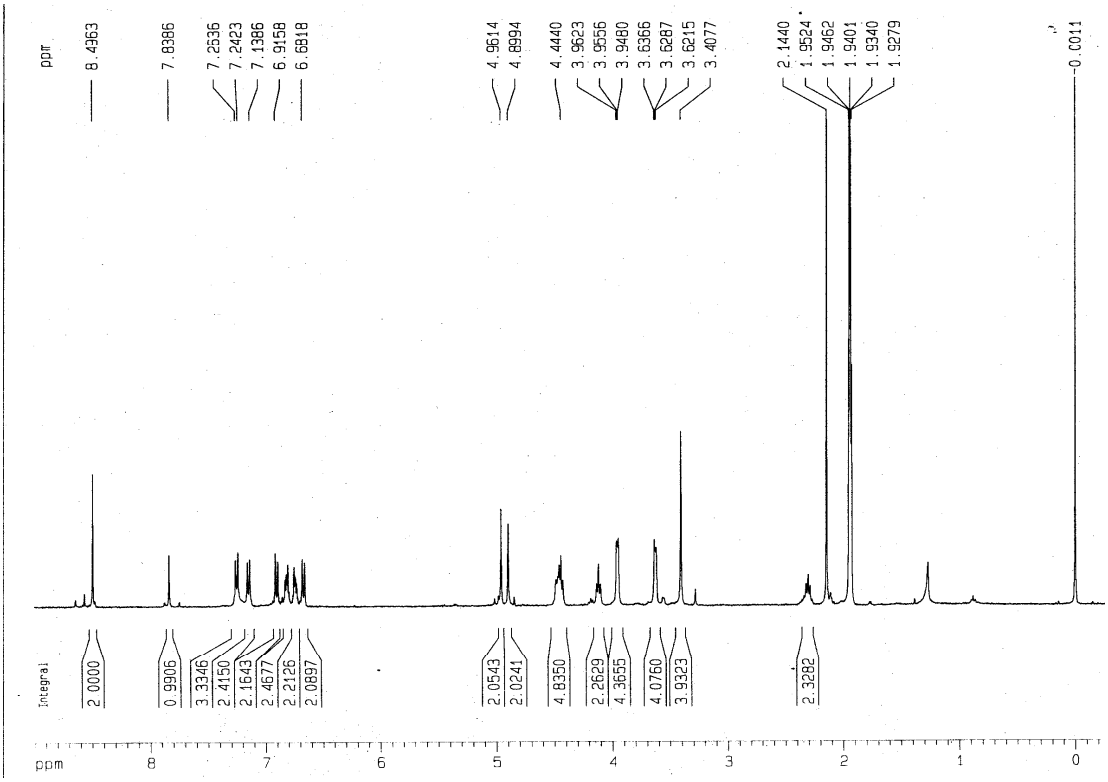
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **5A**



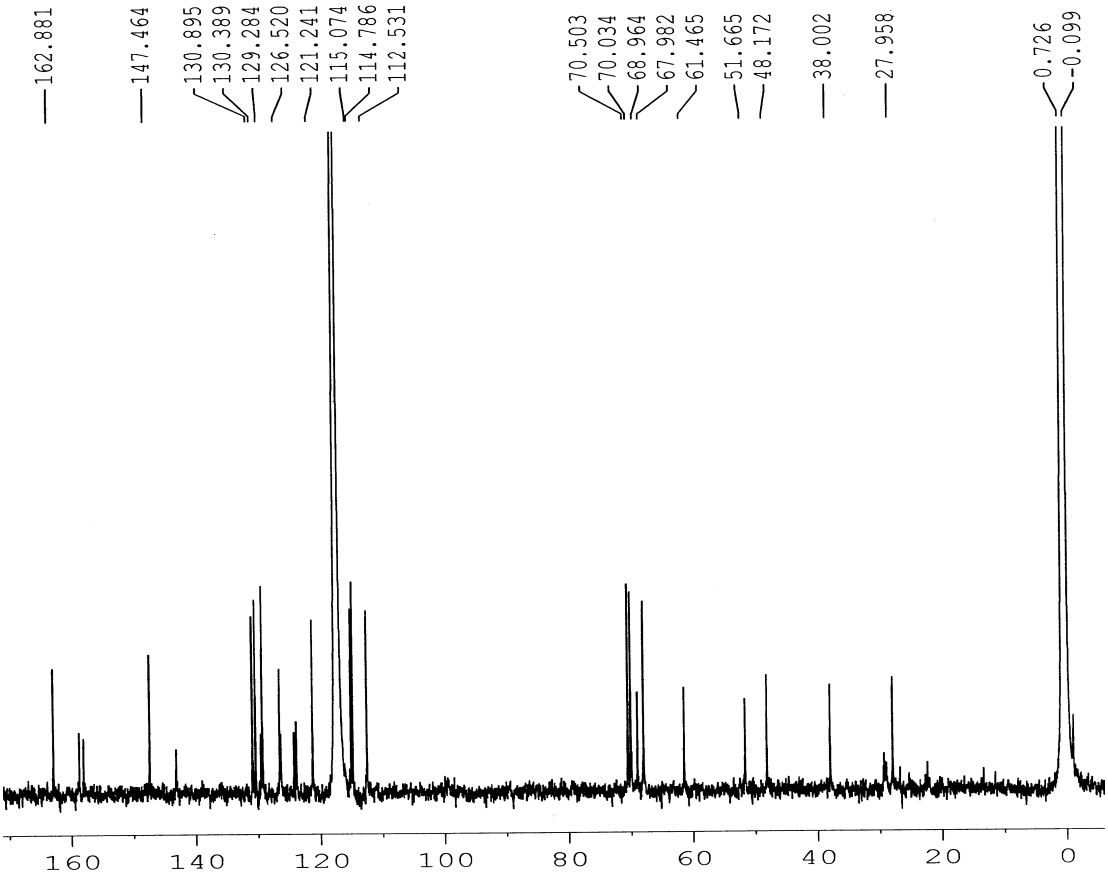
^{13}C NMR spectrum (400 MHz, 298 K, CD_3CN) of **5A**



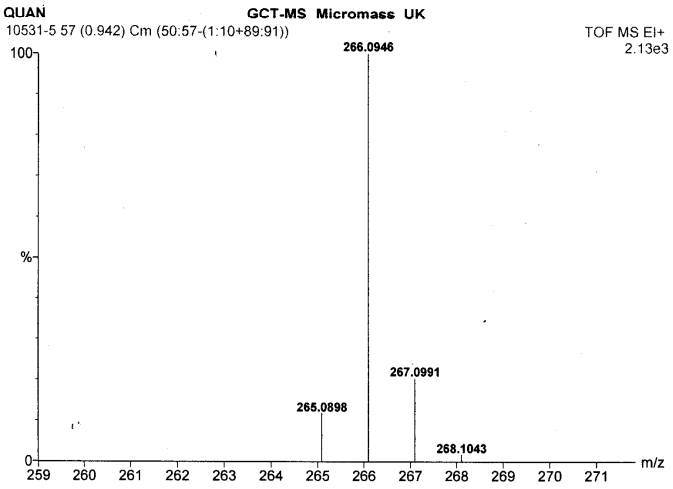
^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of **7**



^{13}C NMR spectrum (600 MHz, 298 K, CD_3CN) of **7**



GCT-MS of compound **S-1**



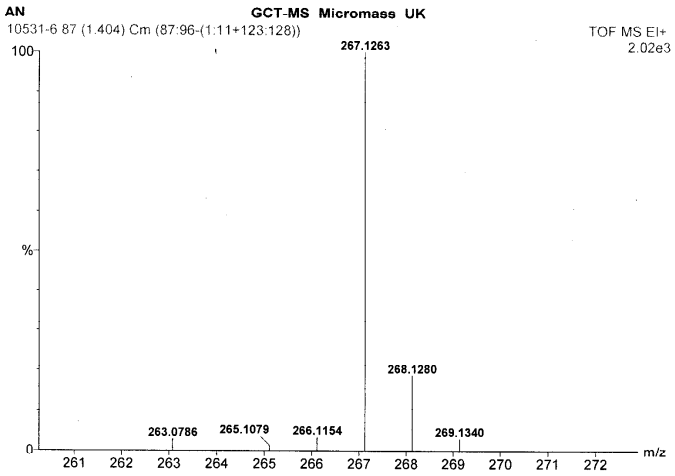
Elemental Composition Report

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:	80.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
266.0946	100.00	266.0943	0.3	1.1	11.0	1	C17 H14 O3

GCT-MS of compound **S-3**



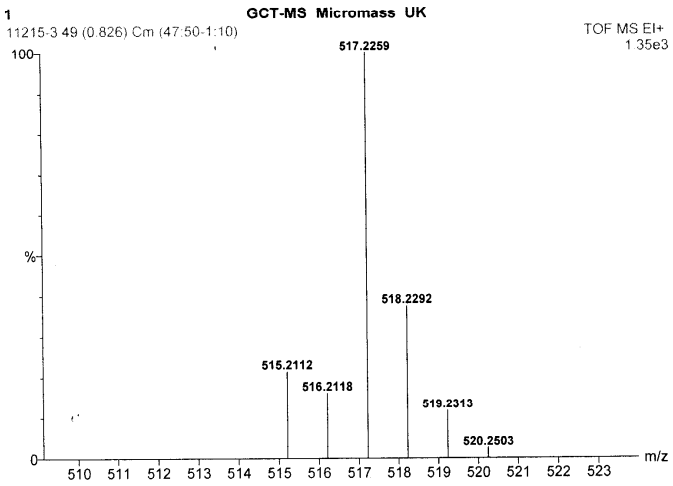
Elemental Composition Report

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:	80.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
267.1263	100.00	267.1259	0.4	1.4	10.0	1	C17 H17 N O2

GCT-MS of compound **1**

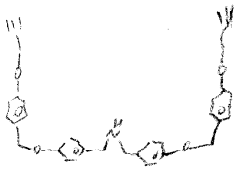


Elemental Composition Report

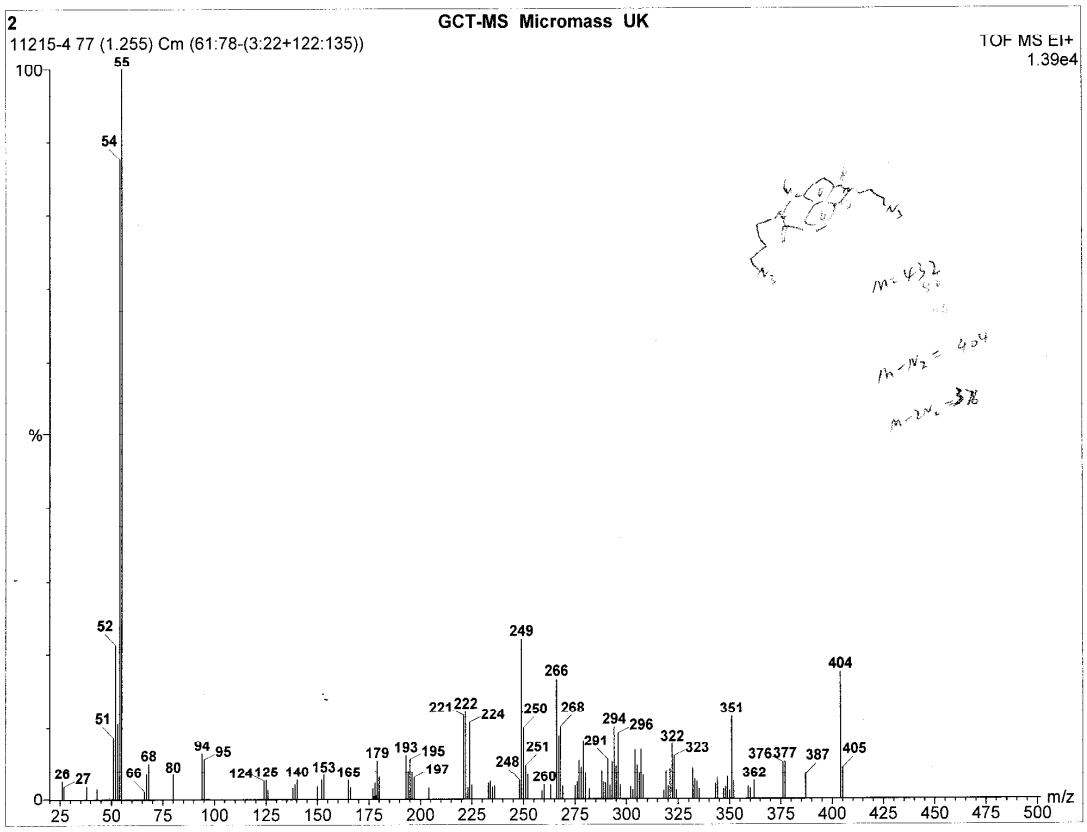
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

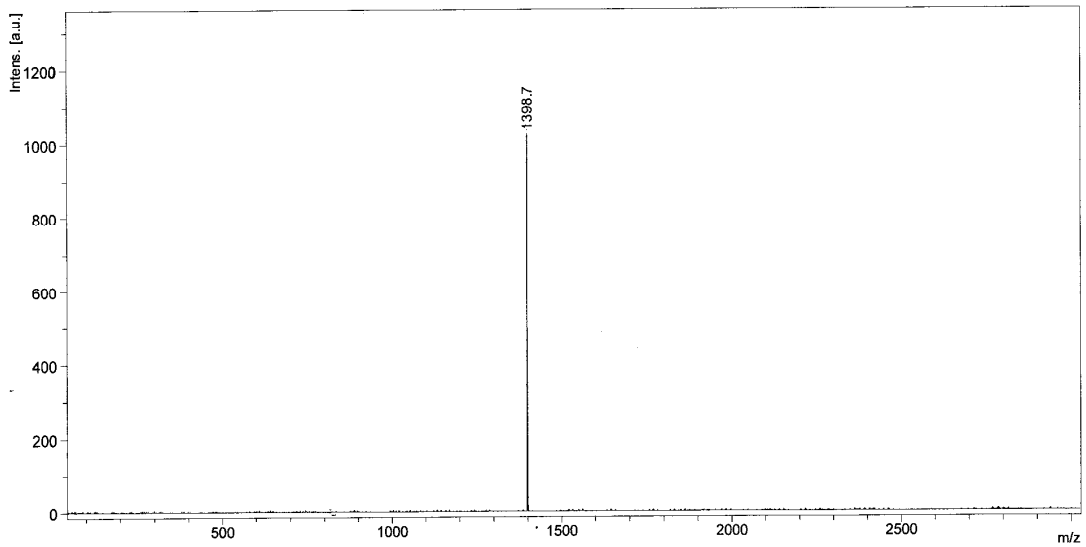
Minimum:	80.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
517.2259	100.00	517.2253	0.6	1.1	20.0	1	C34 H31 N O4



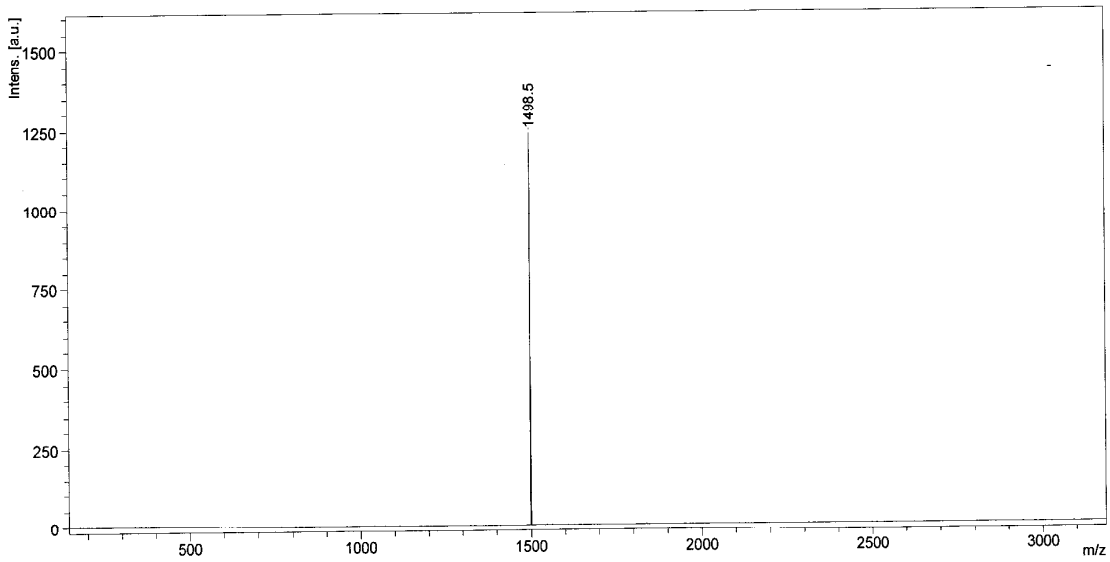
MS of compound **2**



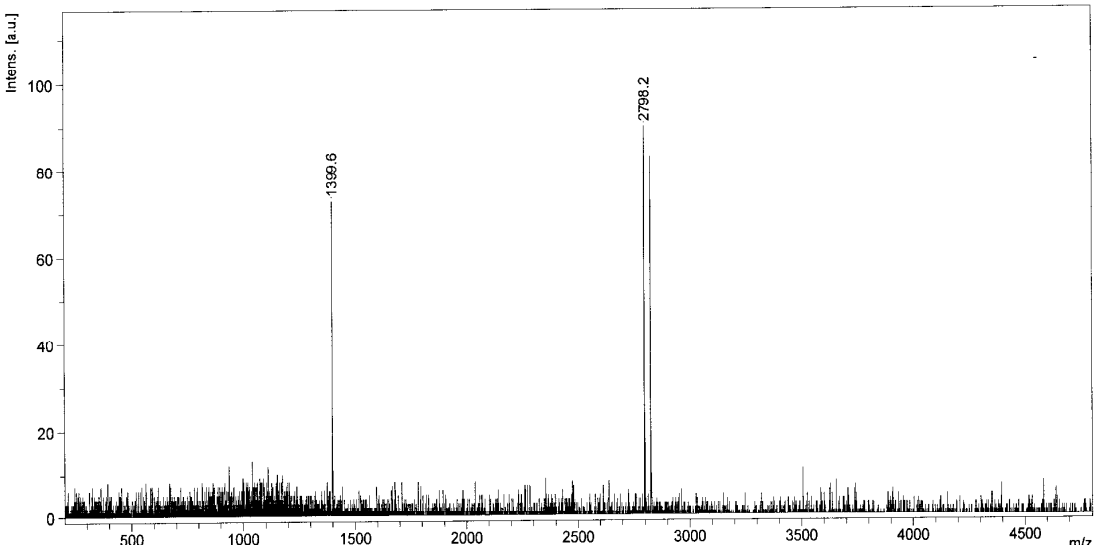
MALDI-TOF of **4B**



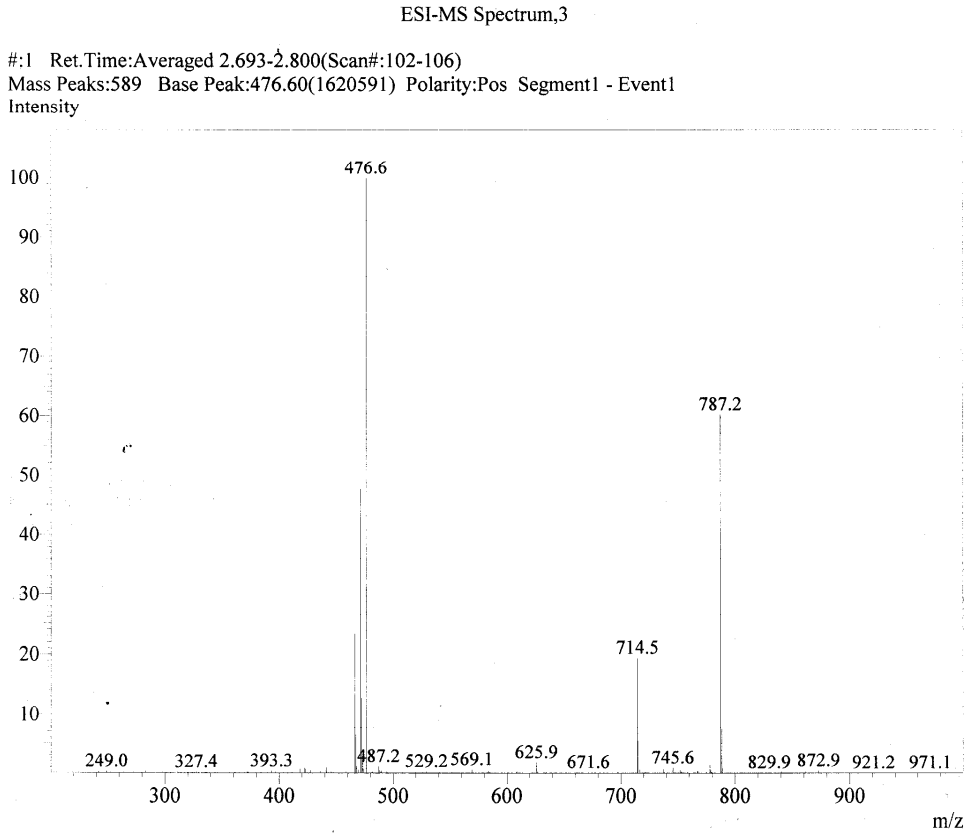
MALDI-TOF of **4A**



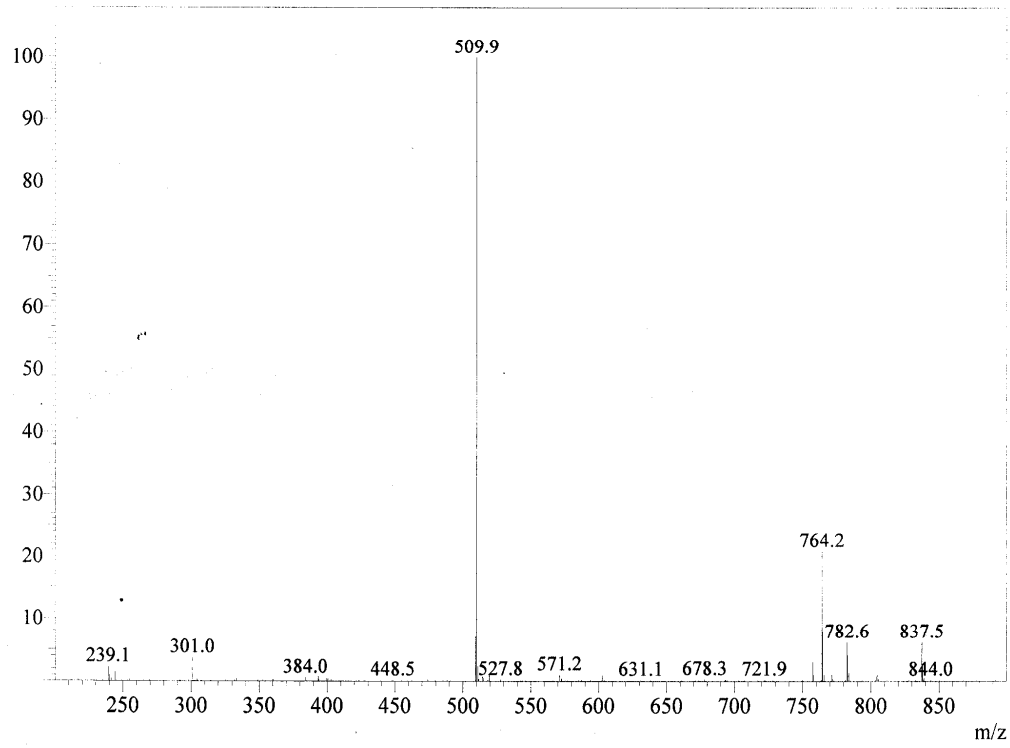
MALDI-TOF of **7**



ESI-MS of **5B**

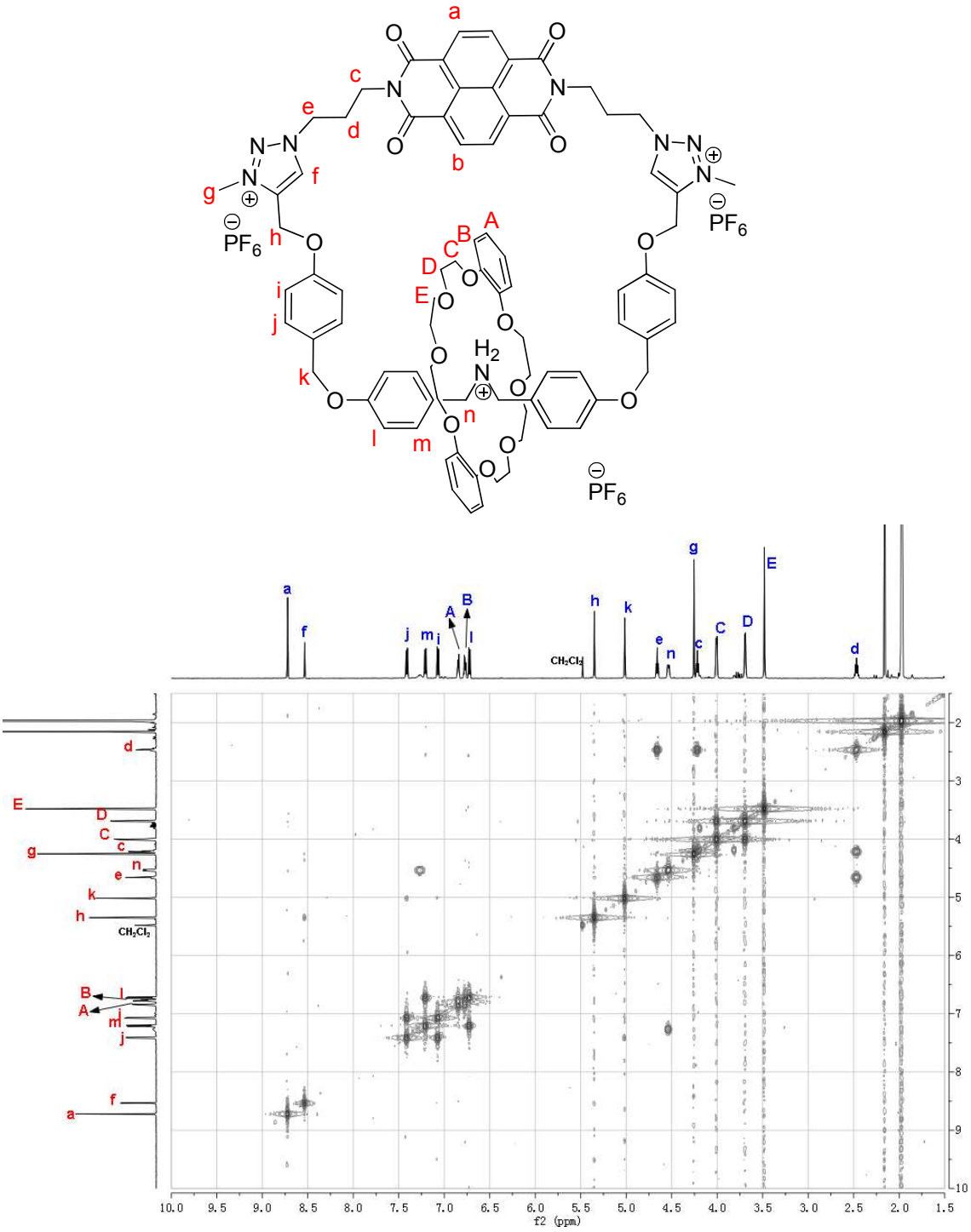


ESI-MS of **5A**

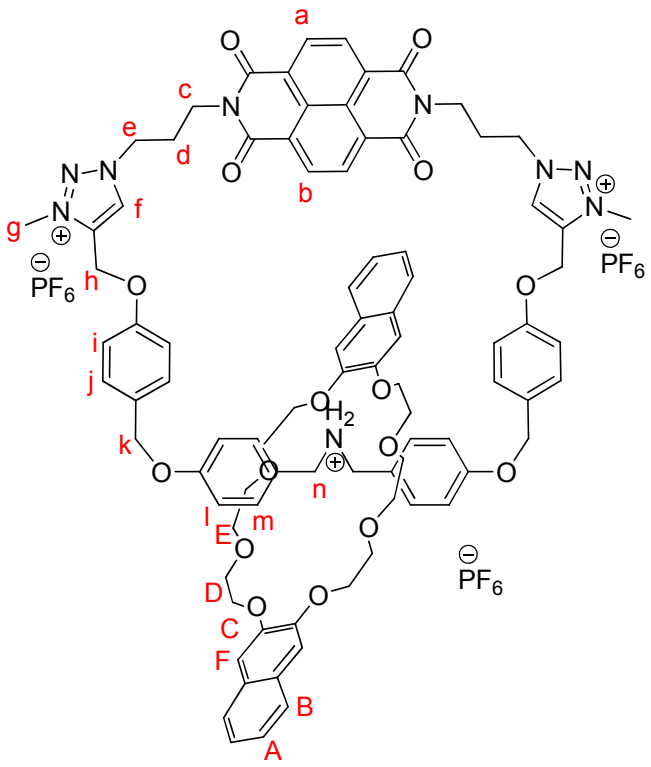


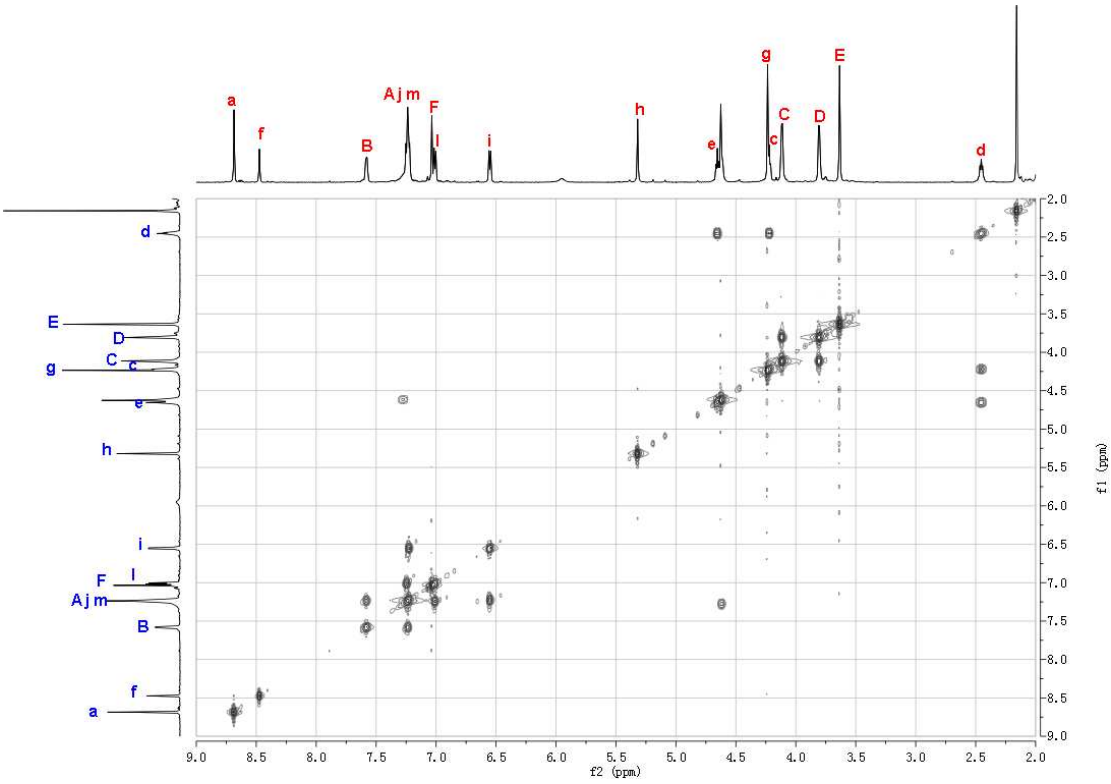
§2. COSY-NMR spectra

COSY-NMR spectra of **5B**



COSY-NMR spectra of **5A**





§3. ^{1}H NMR spectra of compound 5B

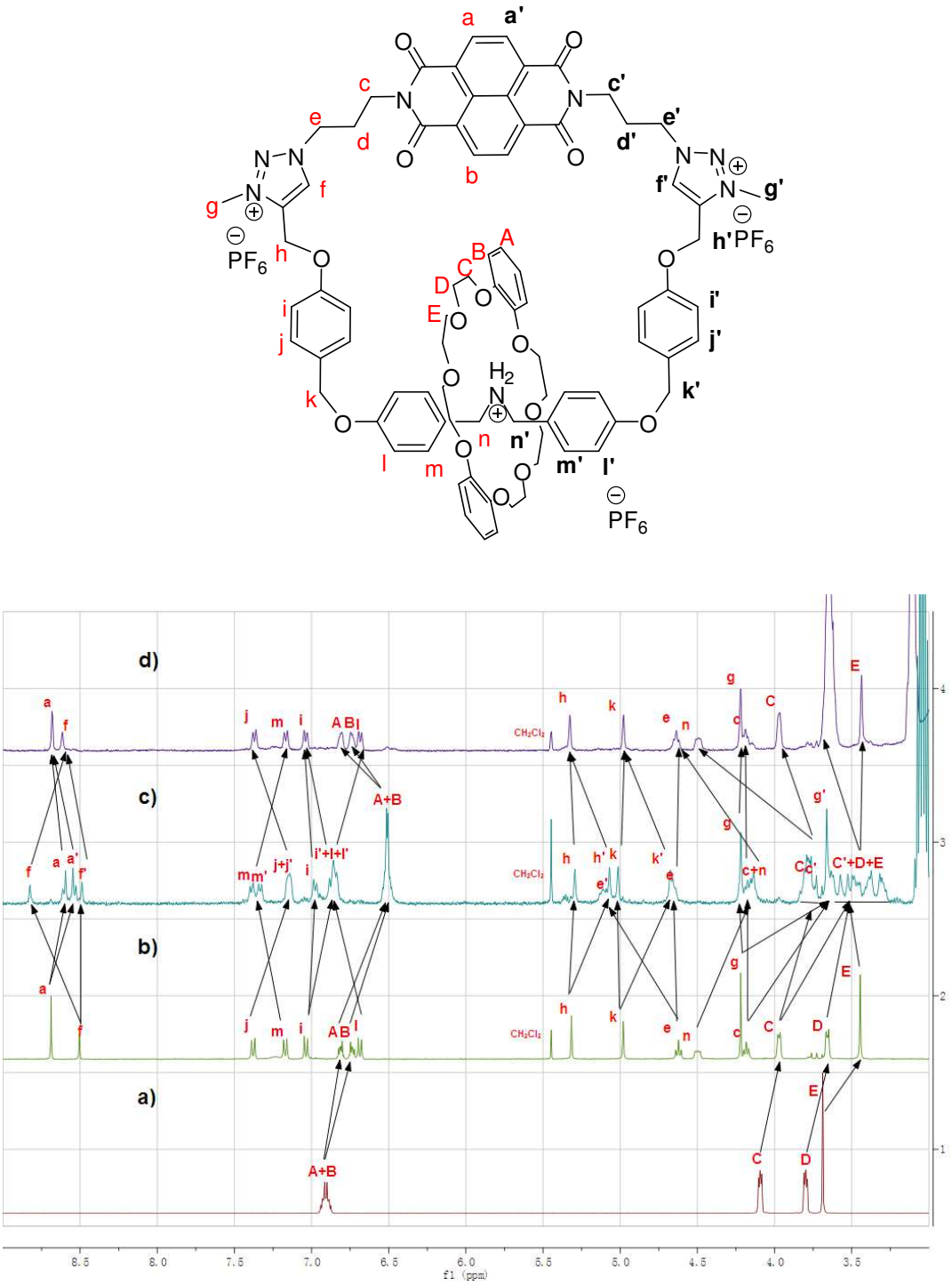


Figure S1. ^{1}H NMR spectra (400 MHz, CD_3CN, 298 K) of a) DB24C8, b) [2]catenane **5B**, c)deprotonation of [2]catenane **5B**, and d) reprotonation of [2]catenane **5B**.

§4. Absorption spectra of [2]catenane 4B and 5B

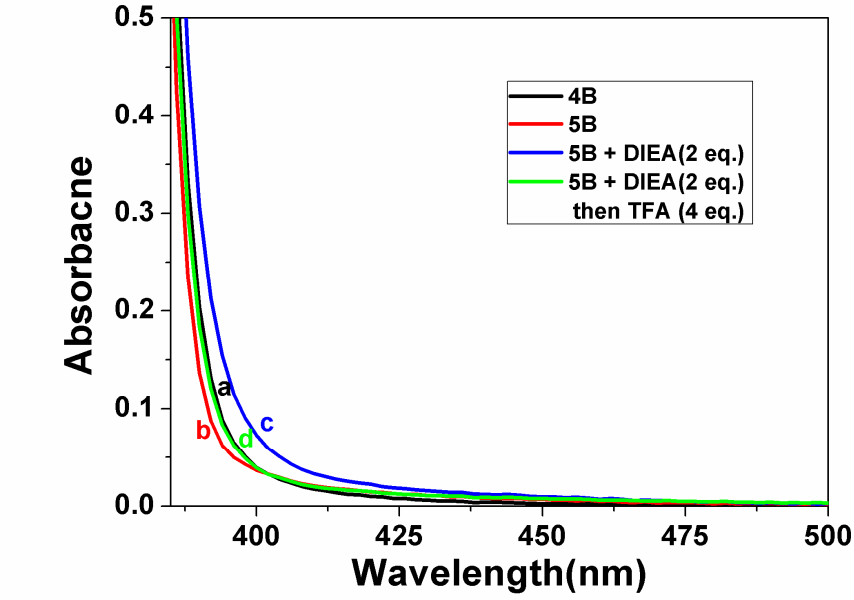


Figure S2. Absorption spectra of (a) [2]catenane **4B** (1×10^{-4} M), (b) [2]catenane **5B** (1×10^{-4} M), (c) **5B** (1×10^{-4} M) + DIEA (2 eq.), (d) **5B** (1×10^{-4} M) + DIEA (2 eq.) then TFA (4 eq.) in CH_3CN.