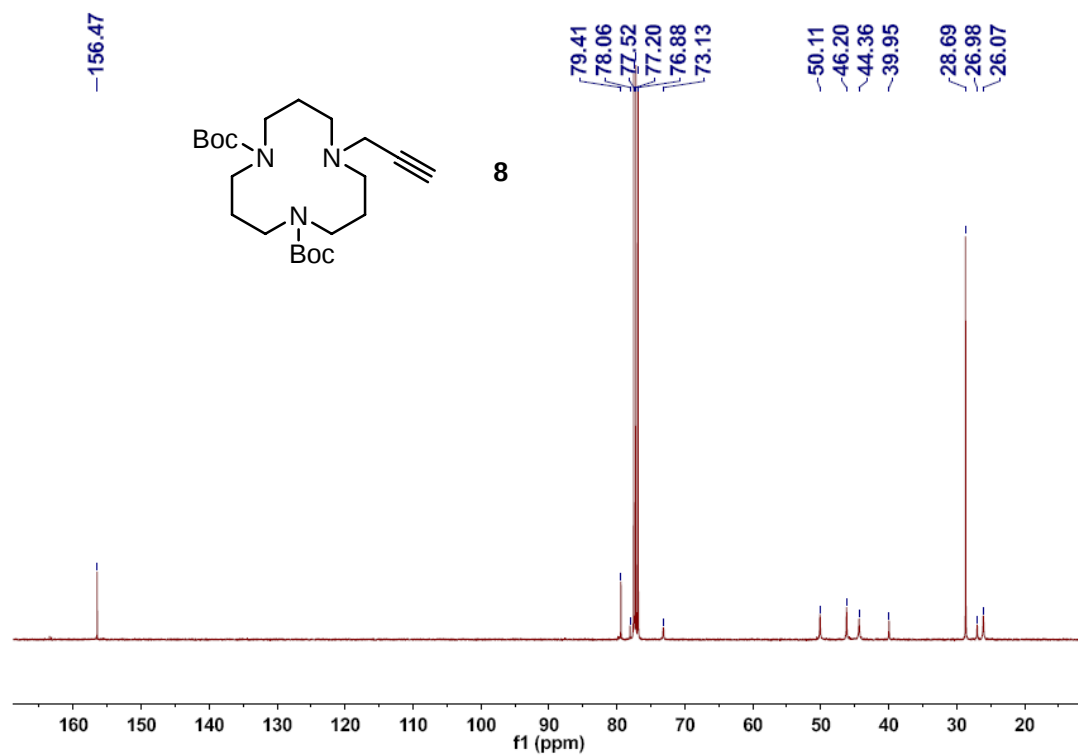
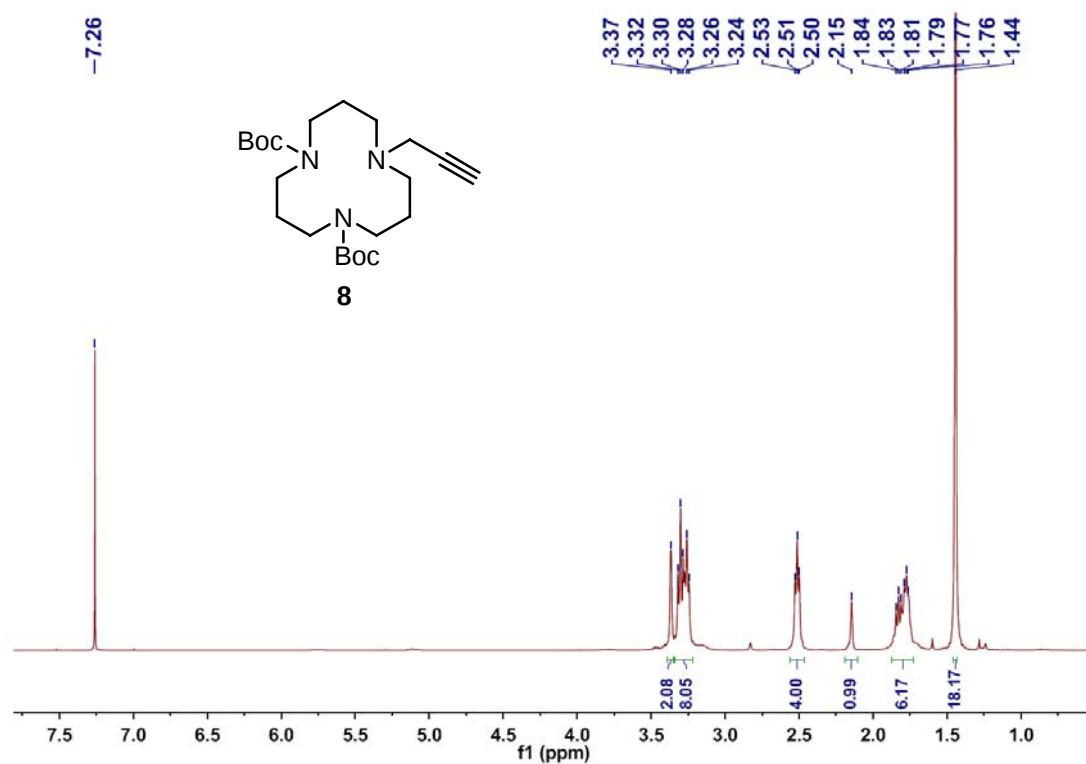
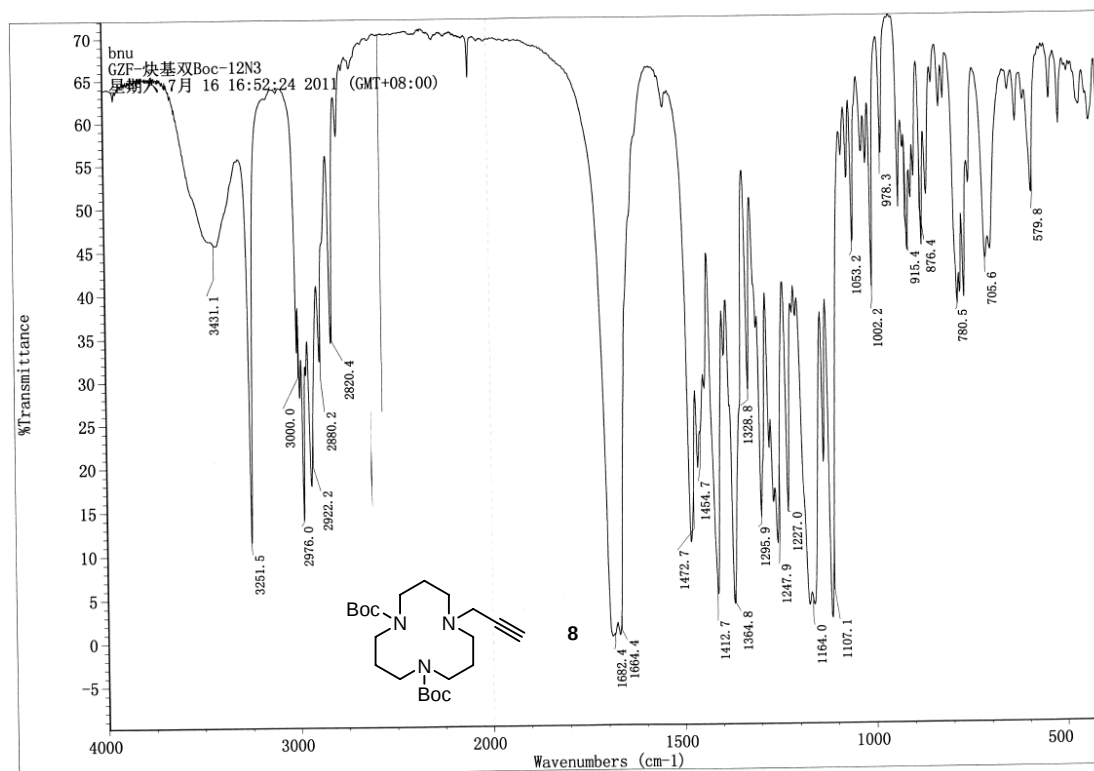






Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

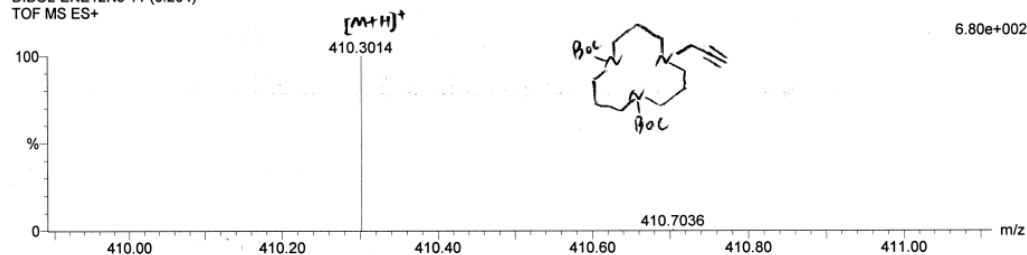
731 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-40 H: 0-70 N: 0-15 O: 0-10

DIBOL-ENE12N3 11 (0.204)

TOF MS ES+



Minimum:

Maximum:

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

410.3014

410.3019

-0.5

-1.2

4.5

n/a

C₂₂ H₄₀ N₃ O₄ ✓

410.3032

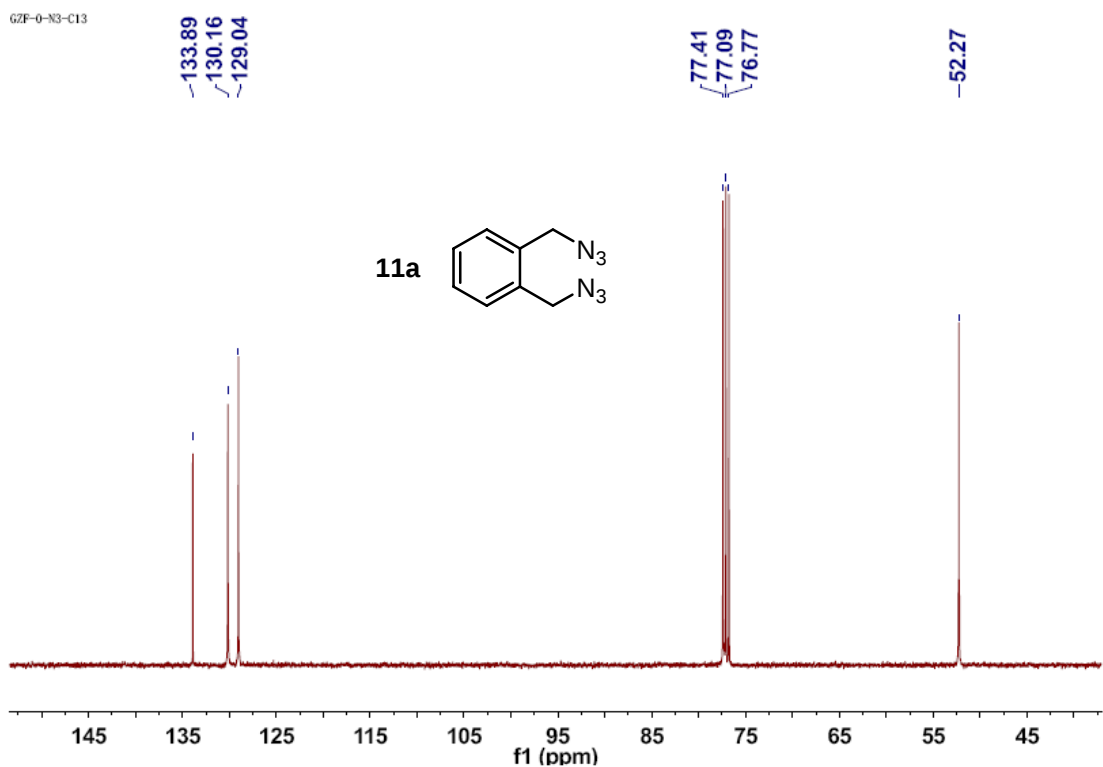
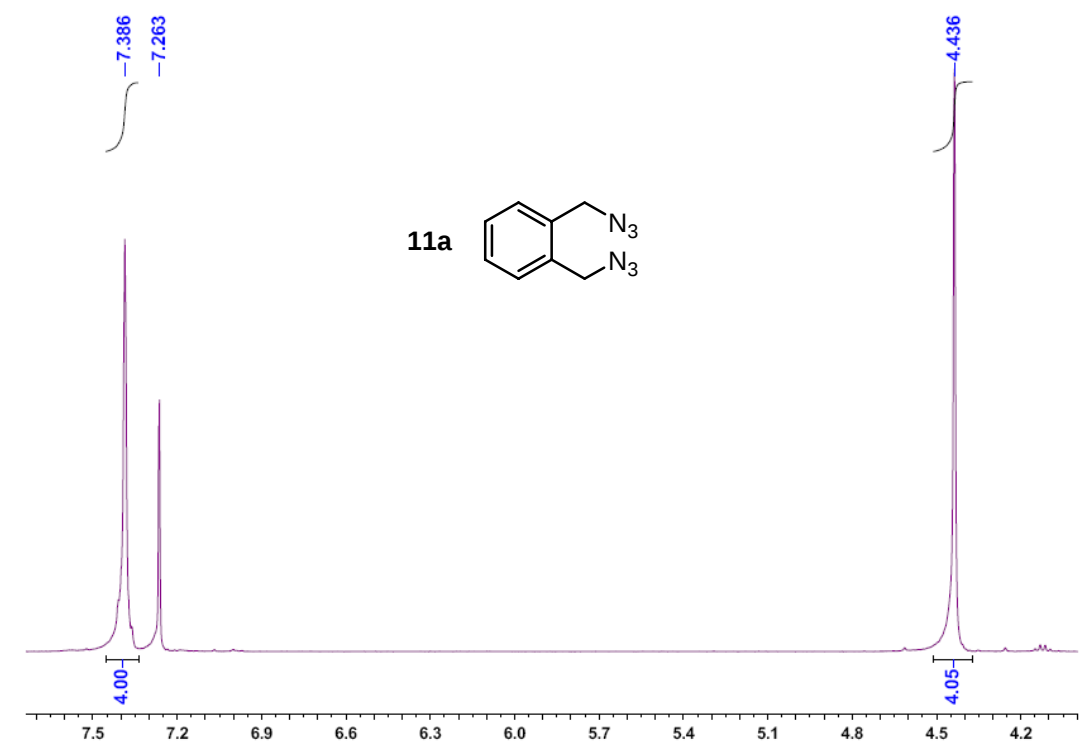
-1.8

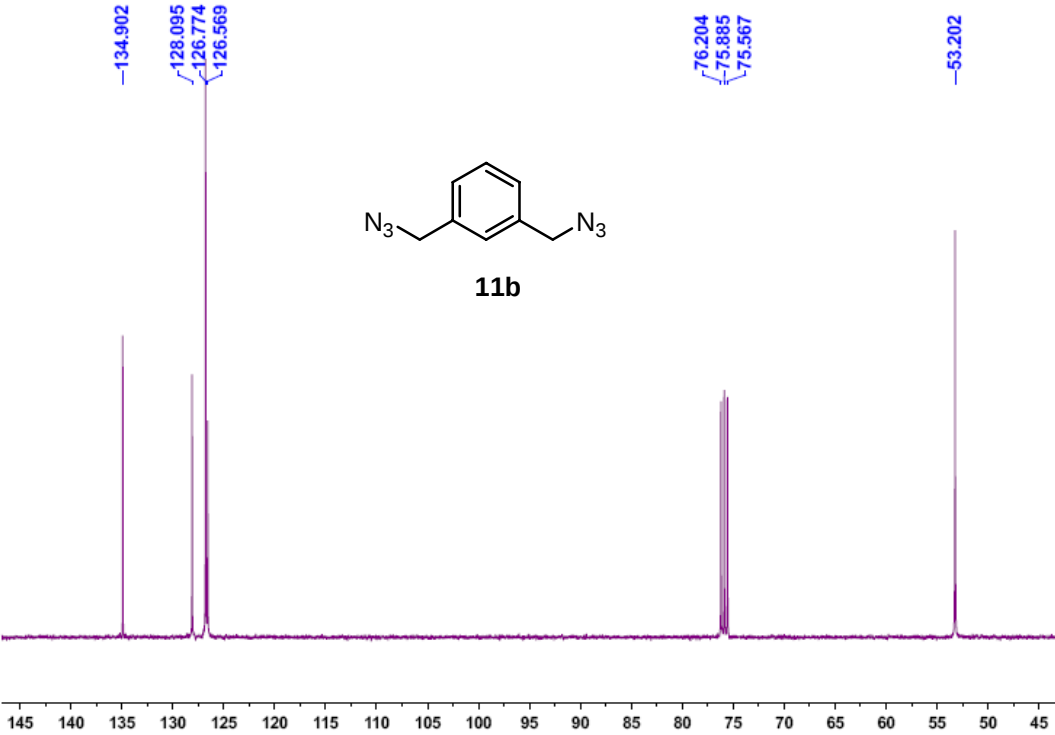
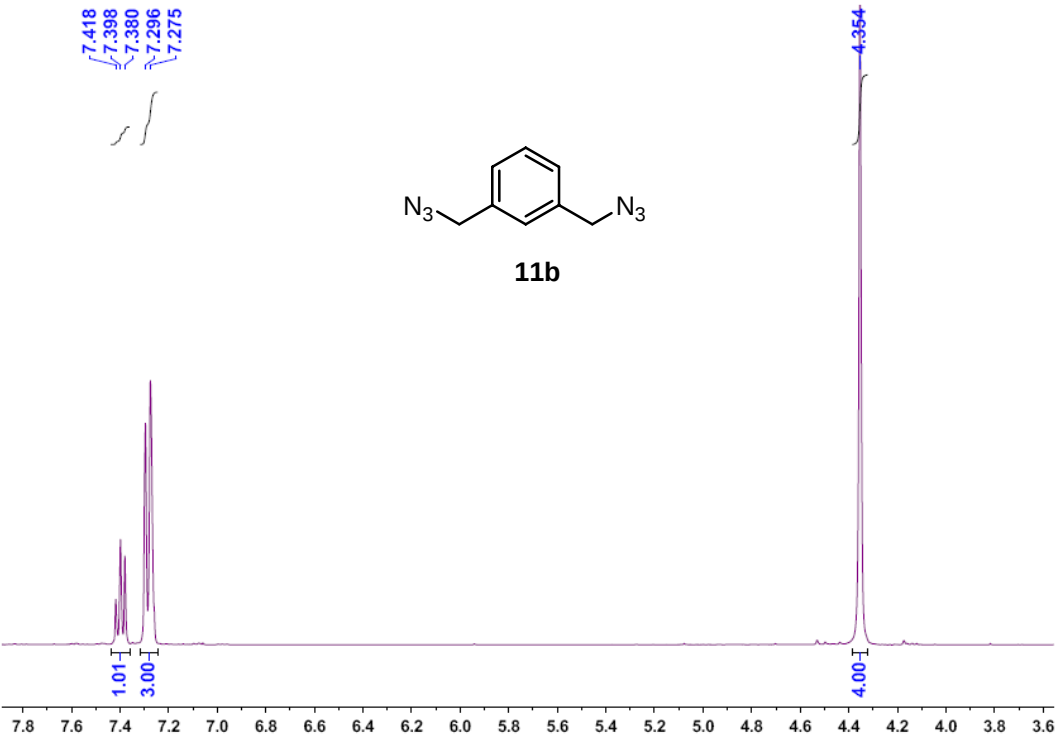
-4.4

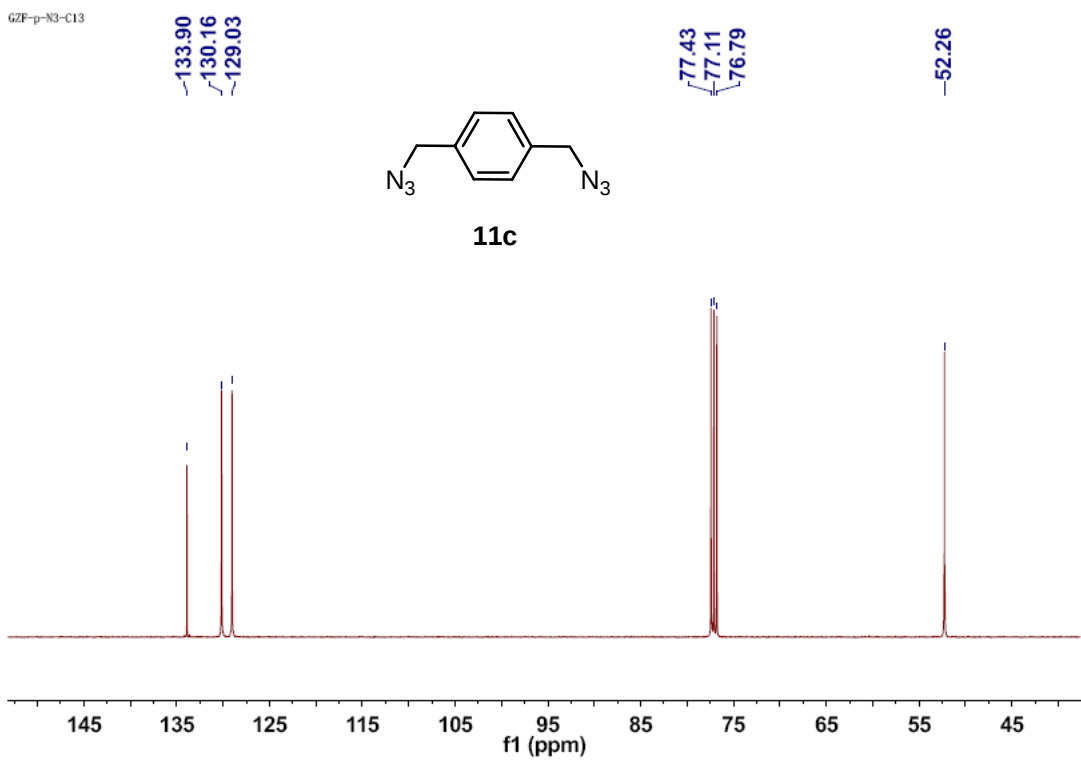
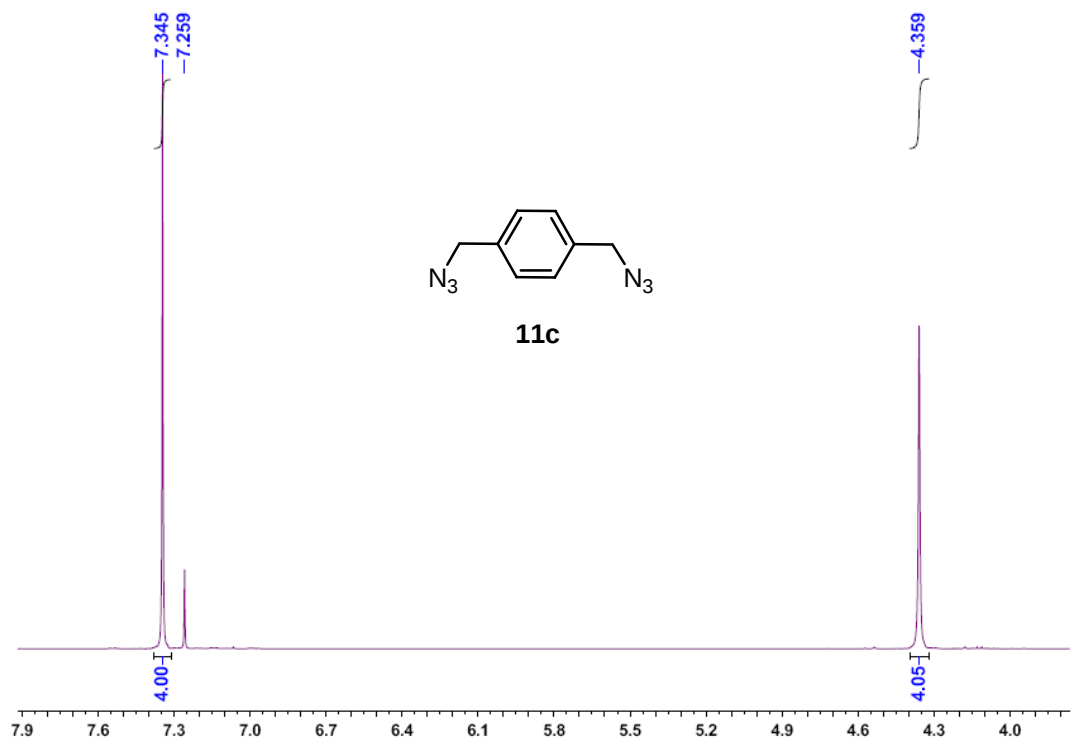
9.5

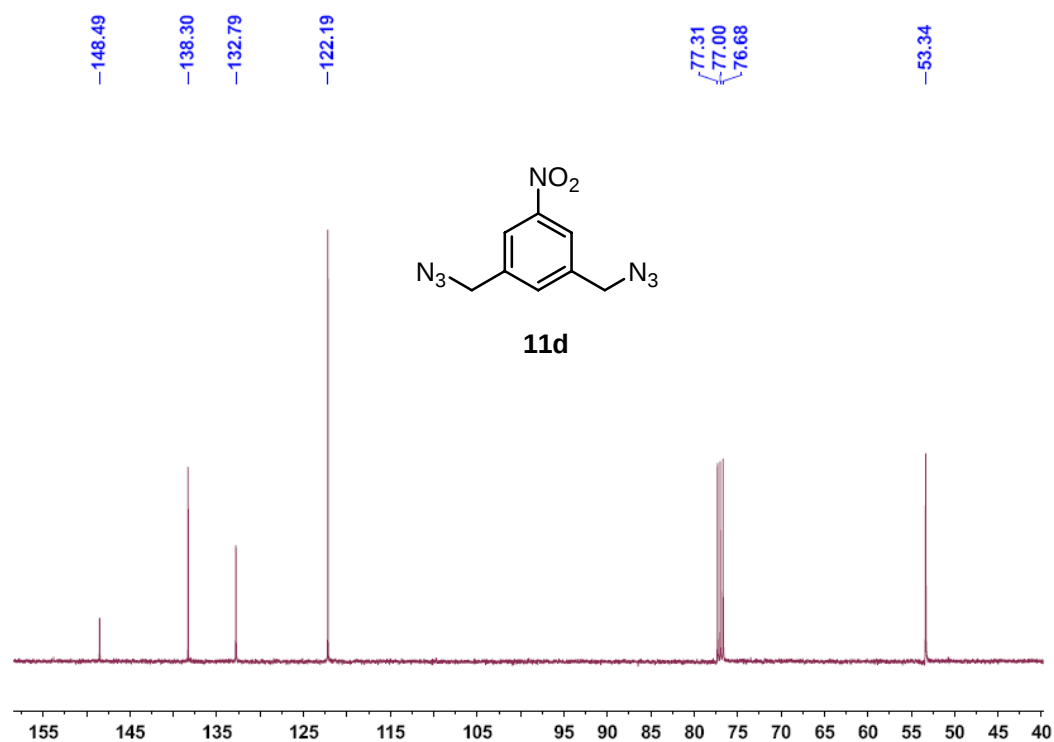
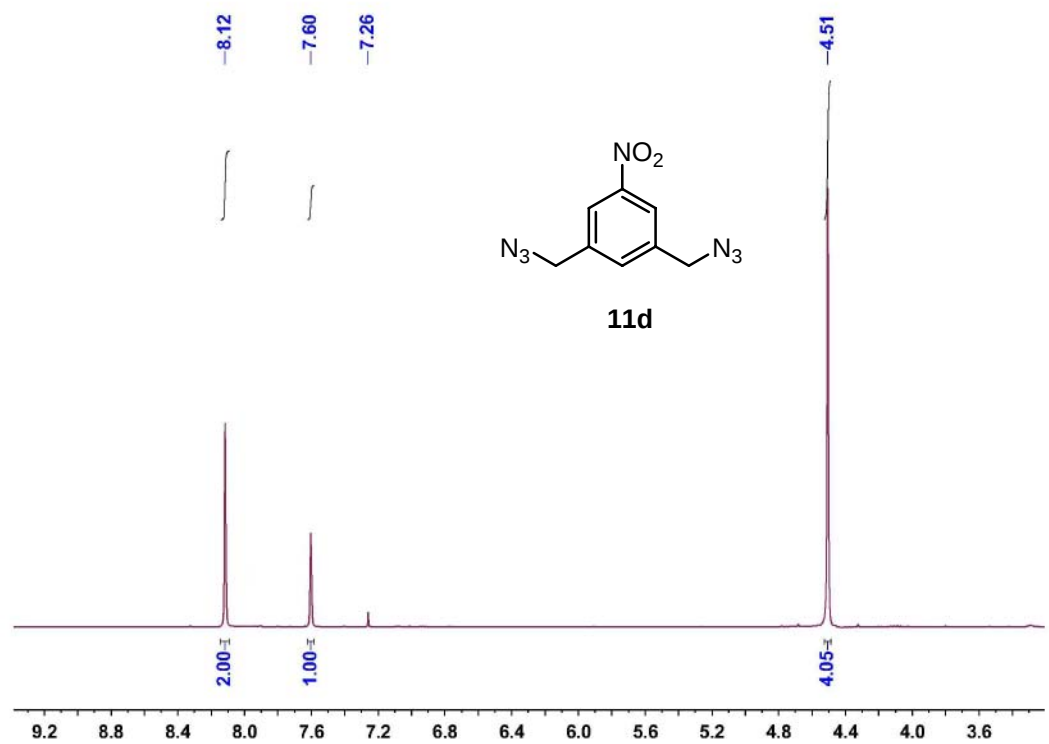
n/a

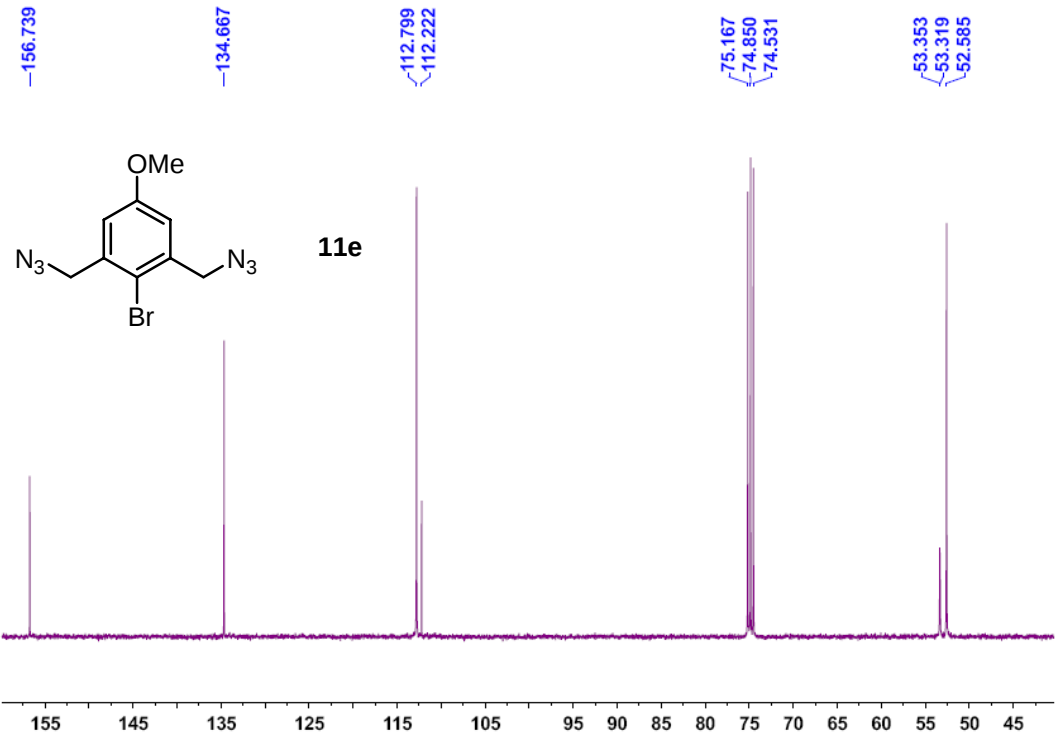
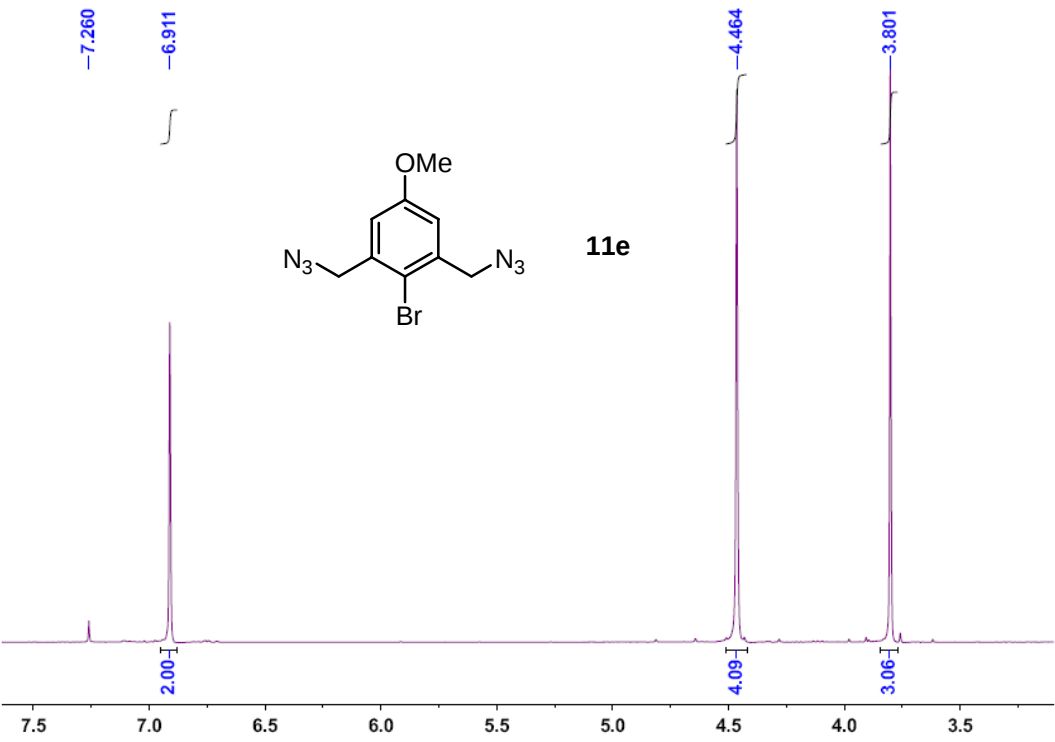
C₂₃ H₃₆ N₇

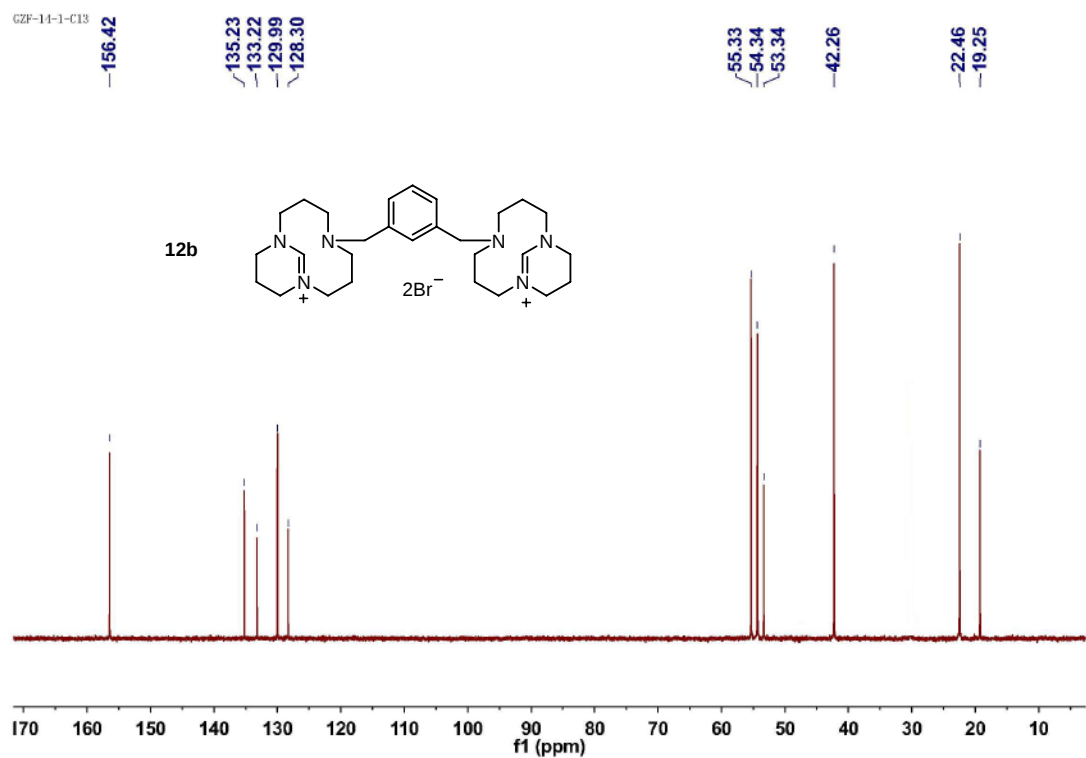
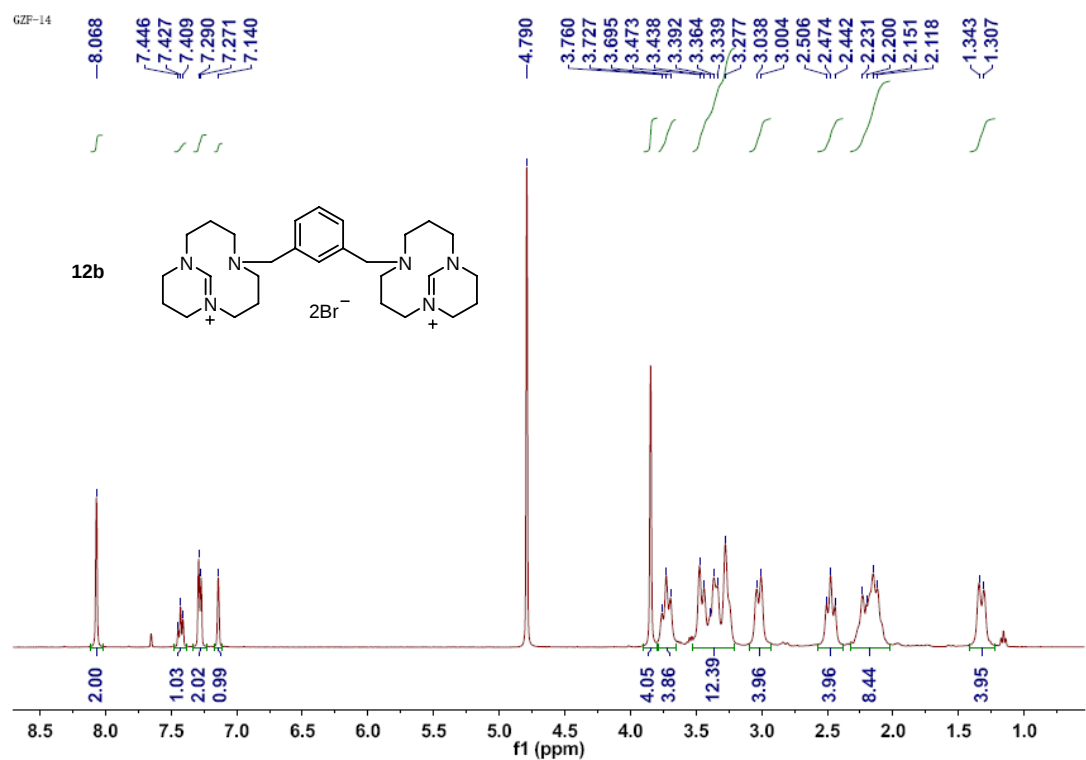


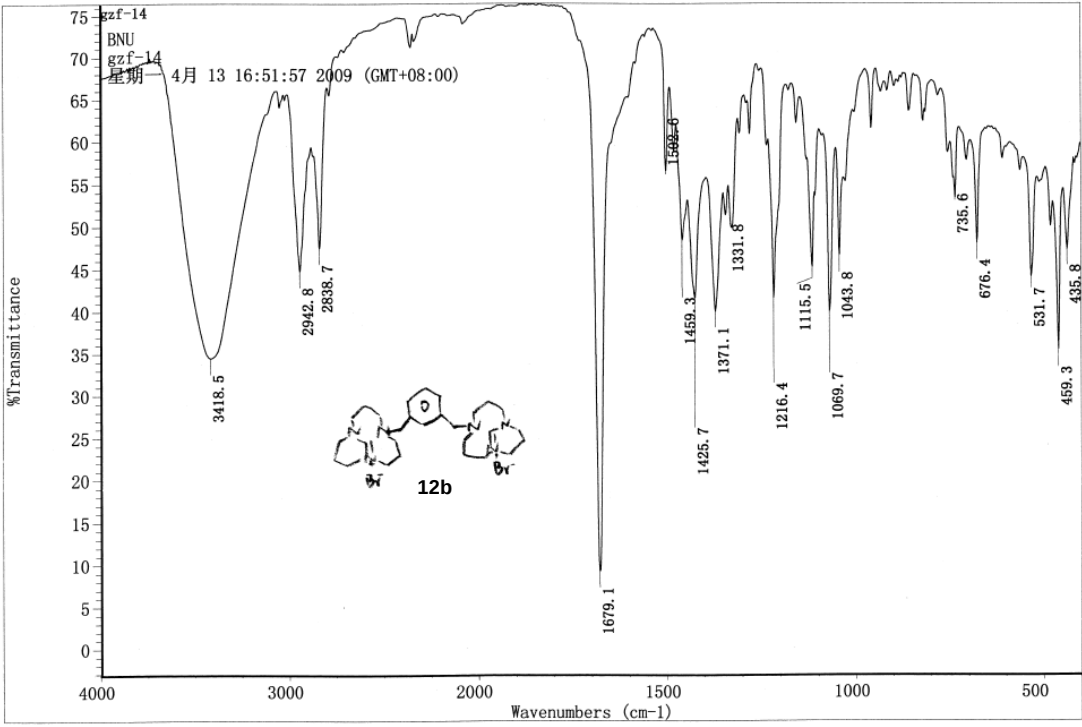
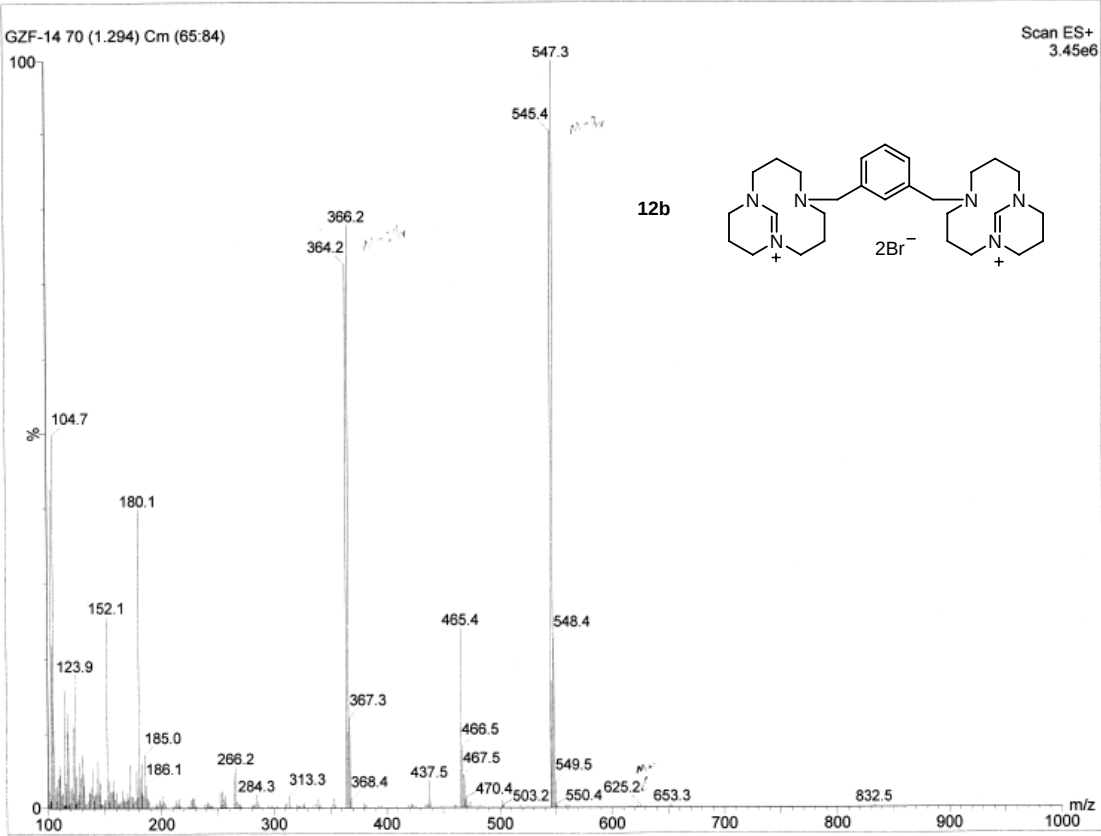


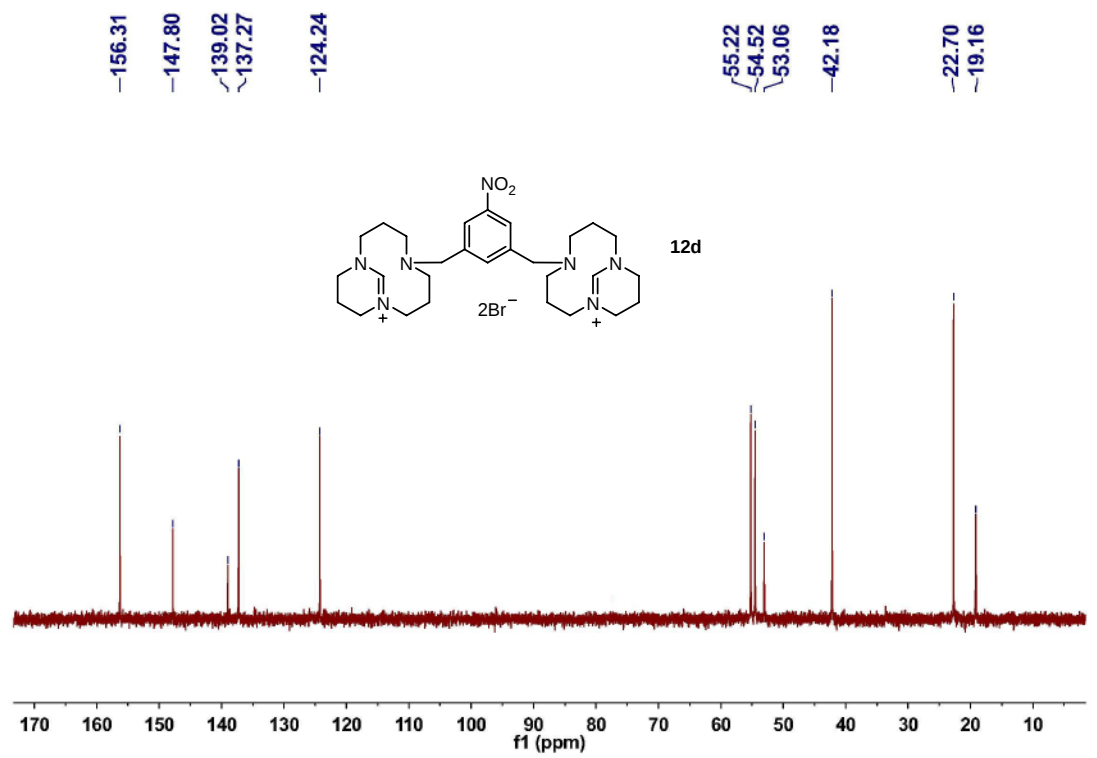
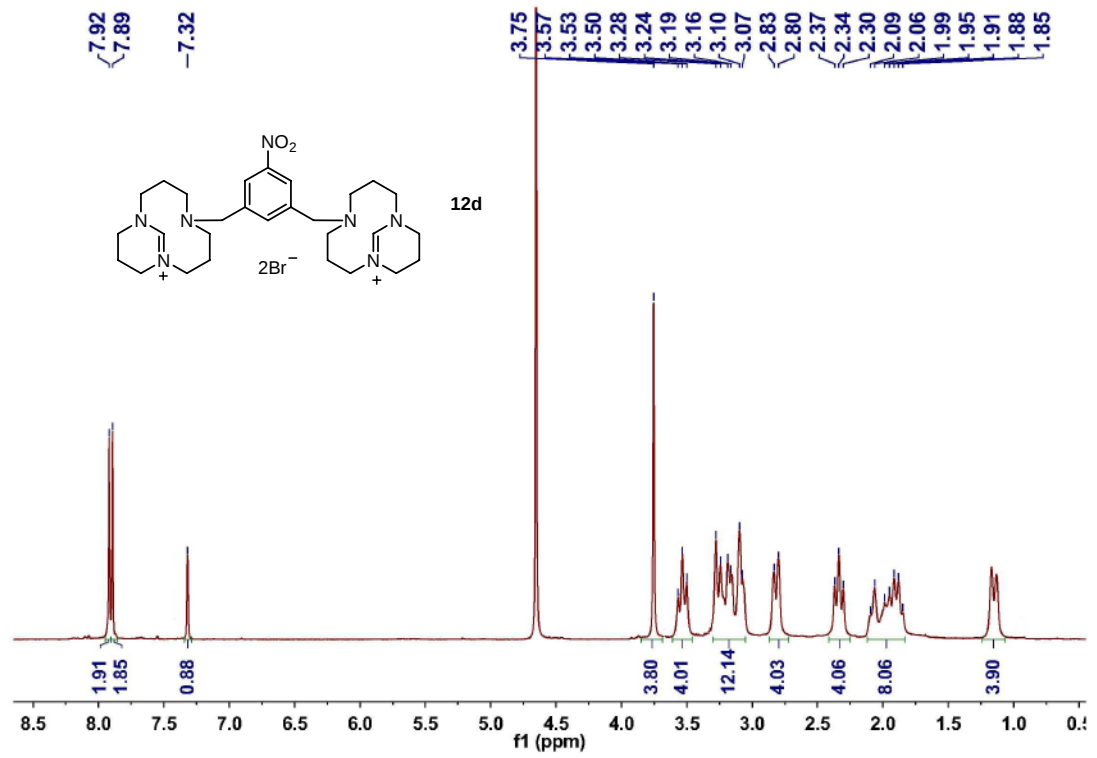


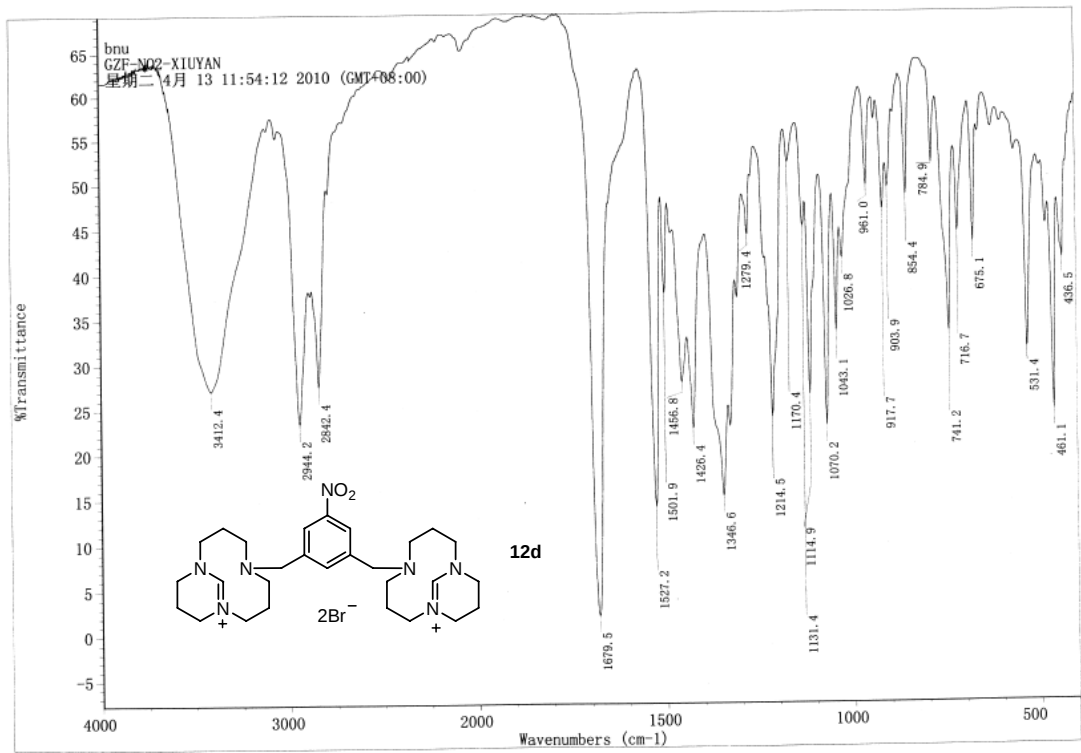
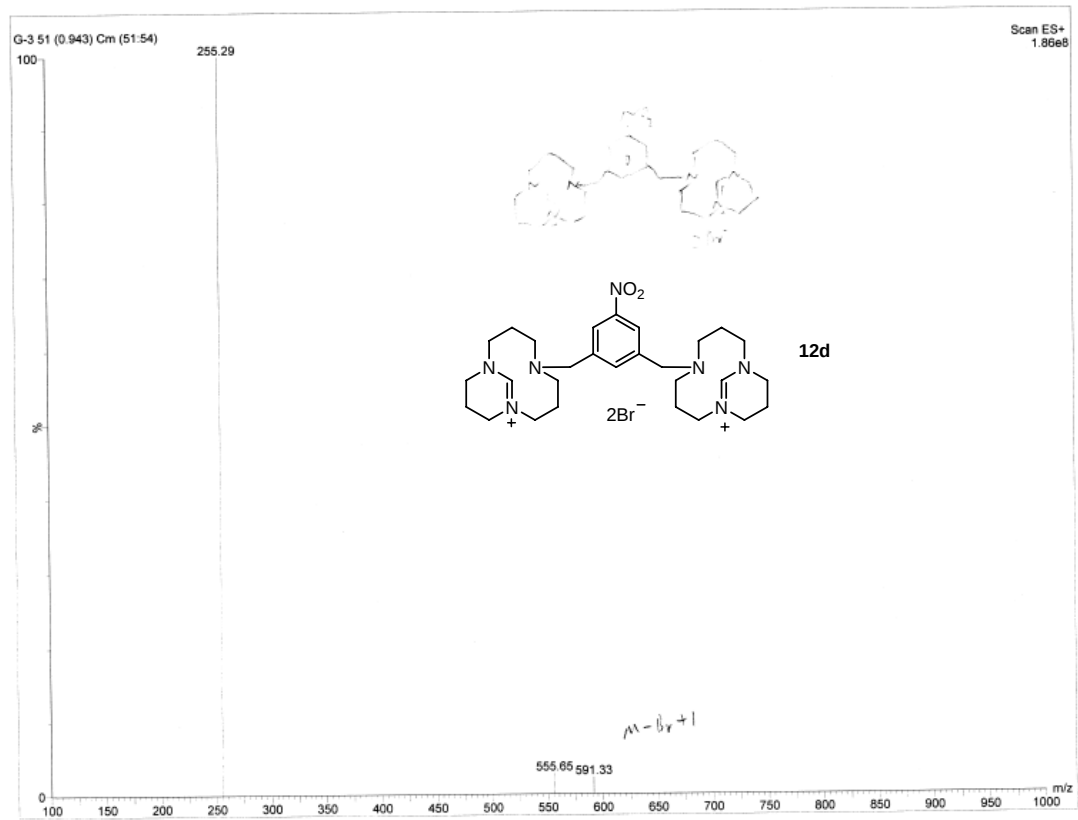


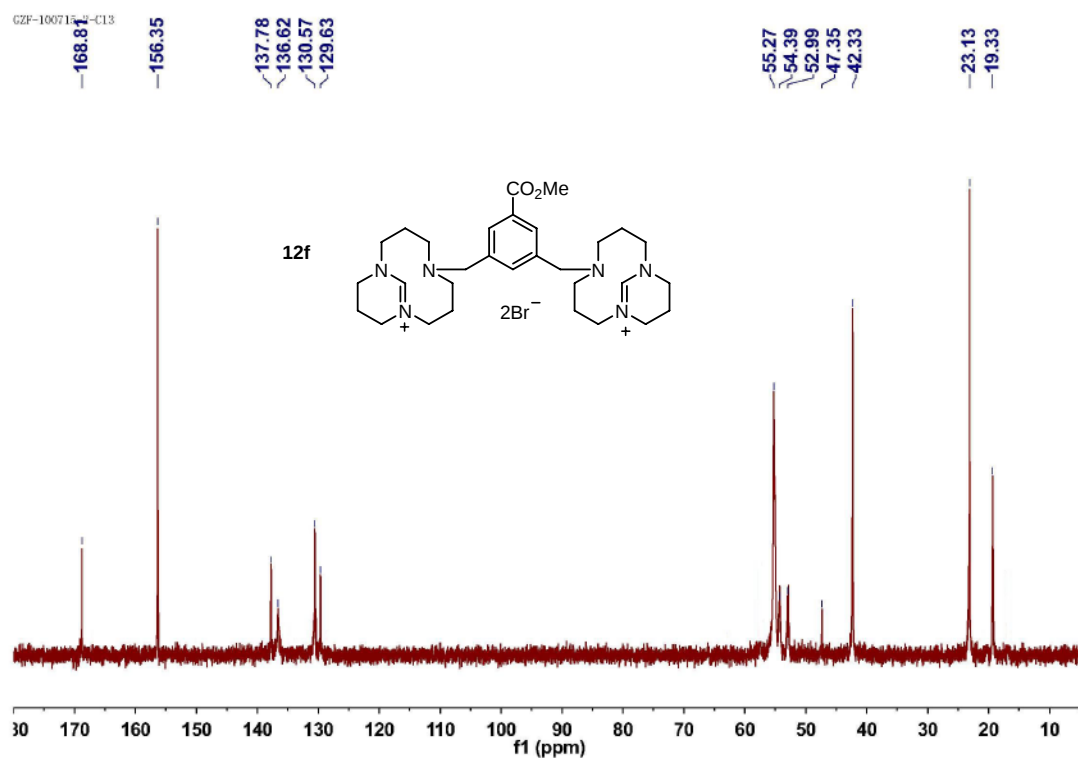
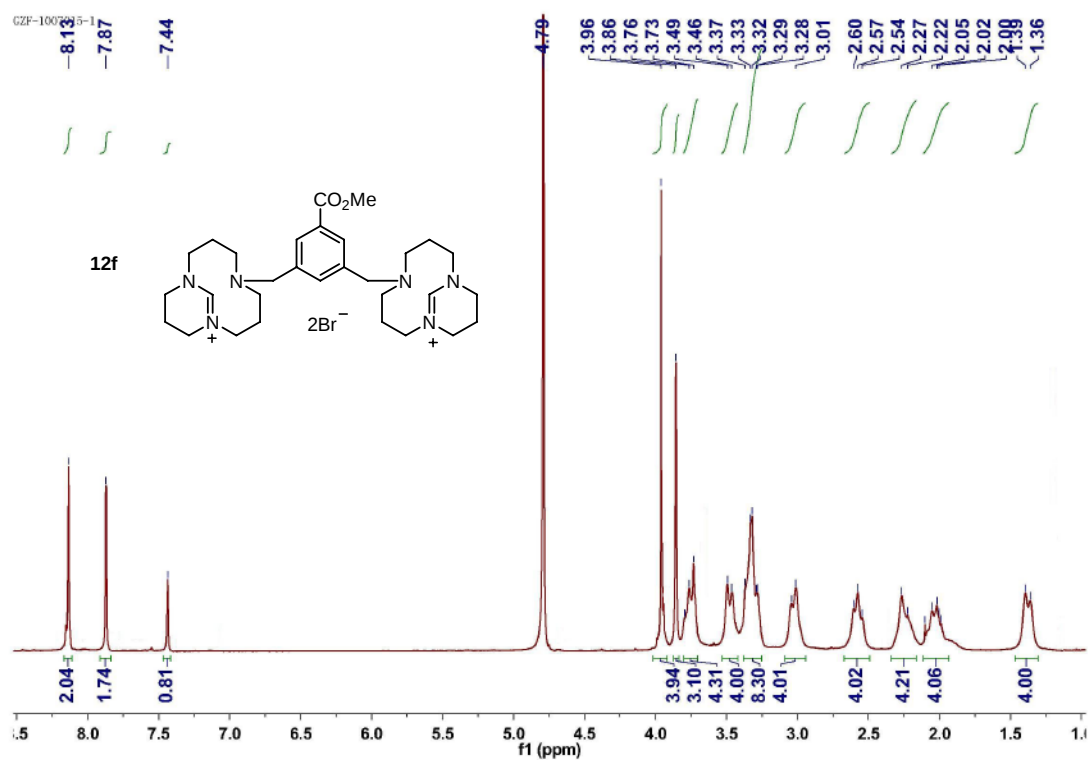


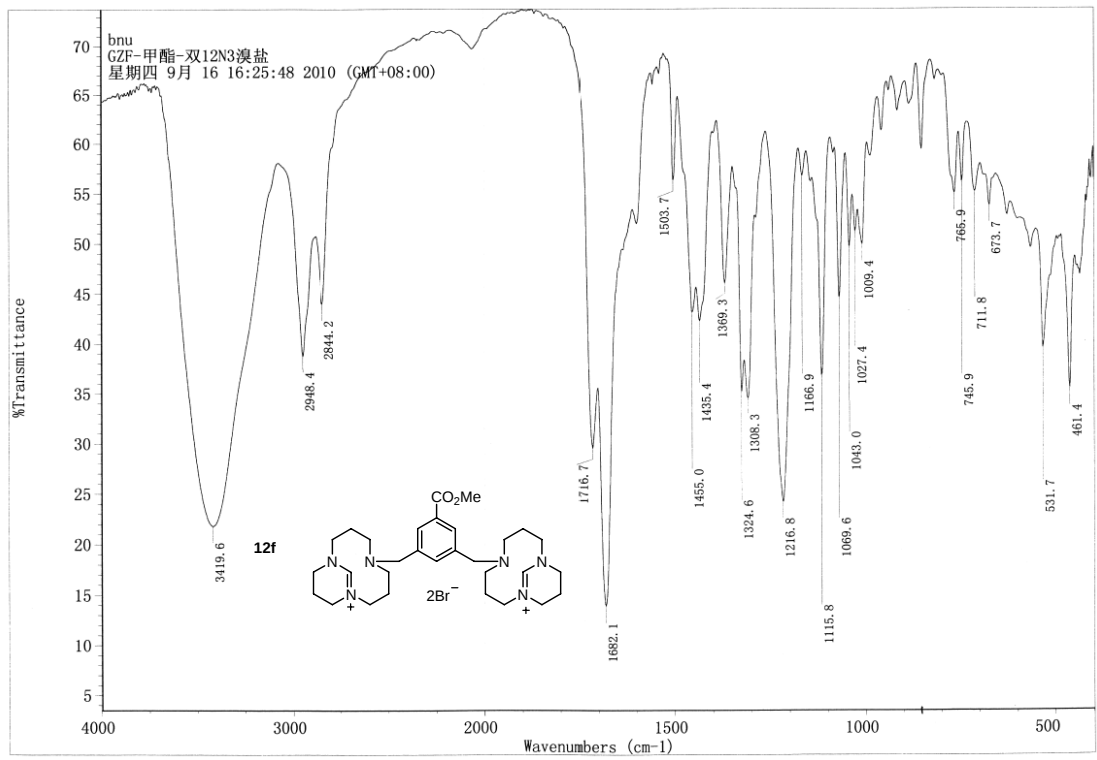
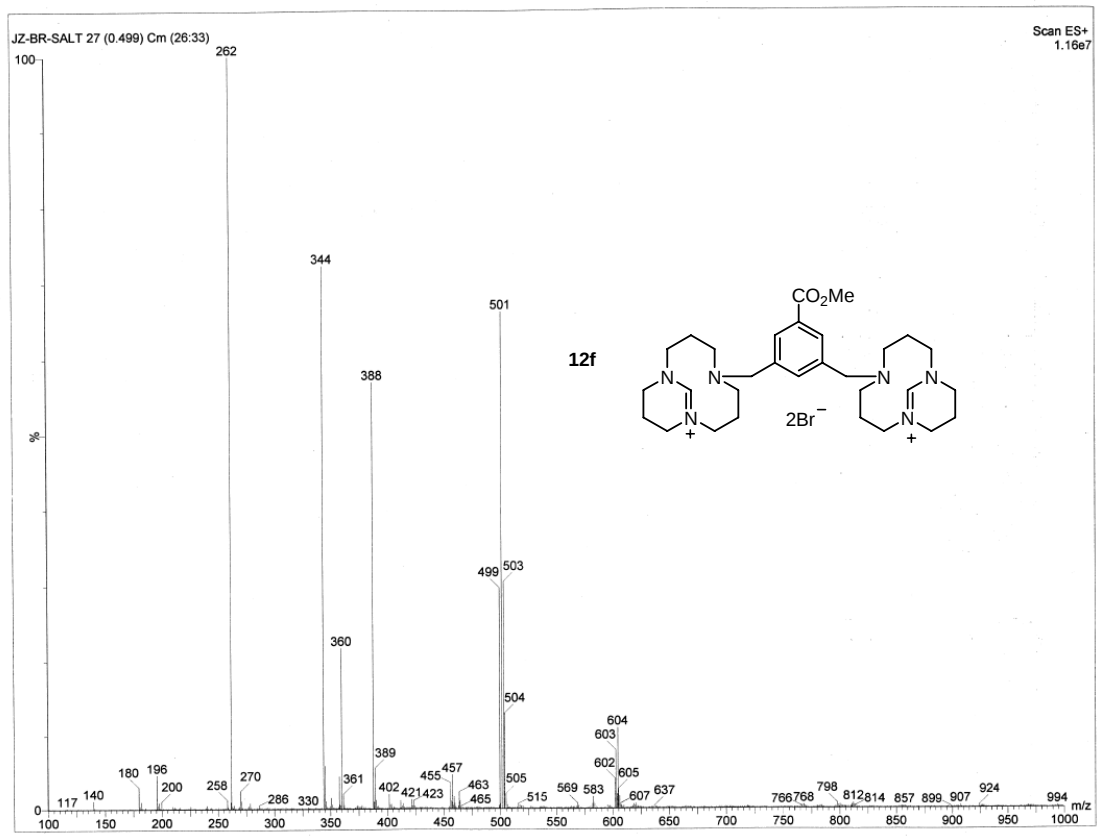


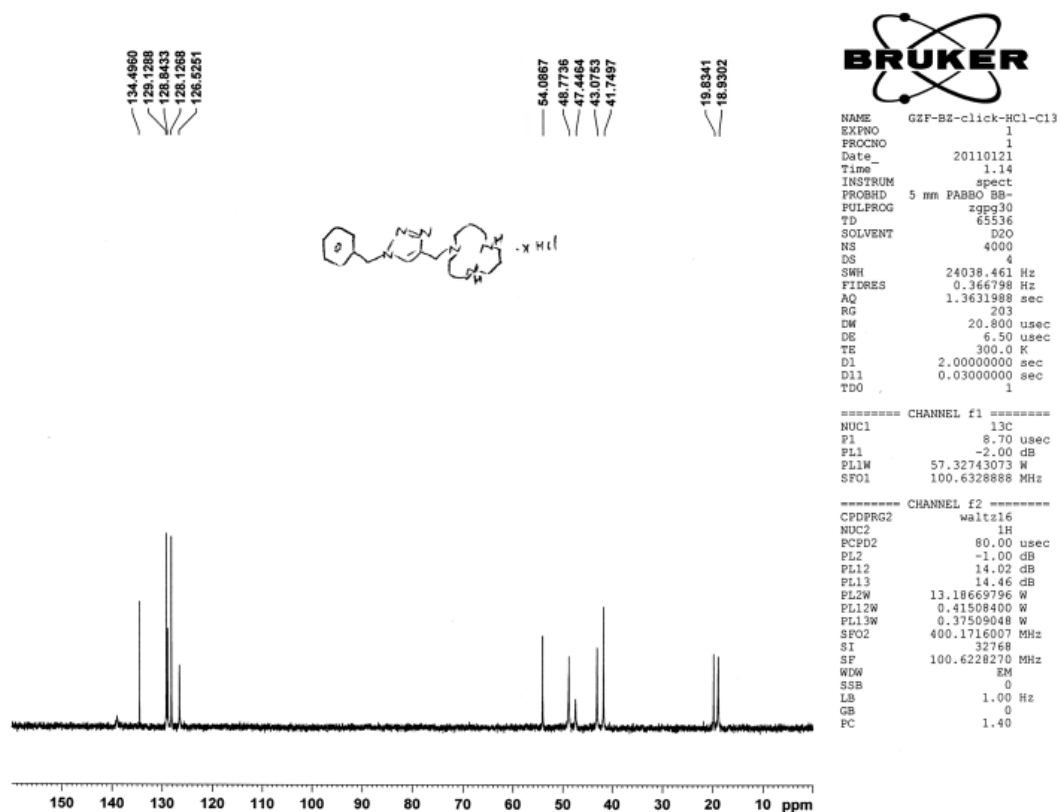
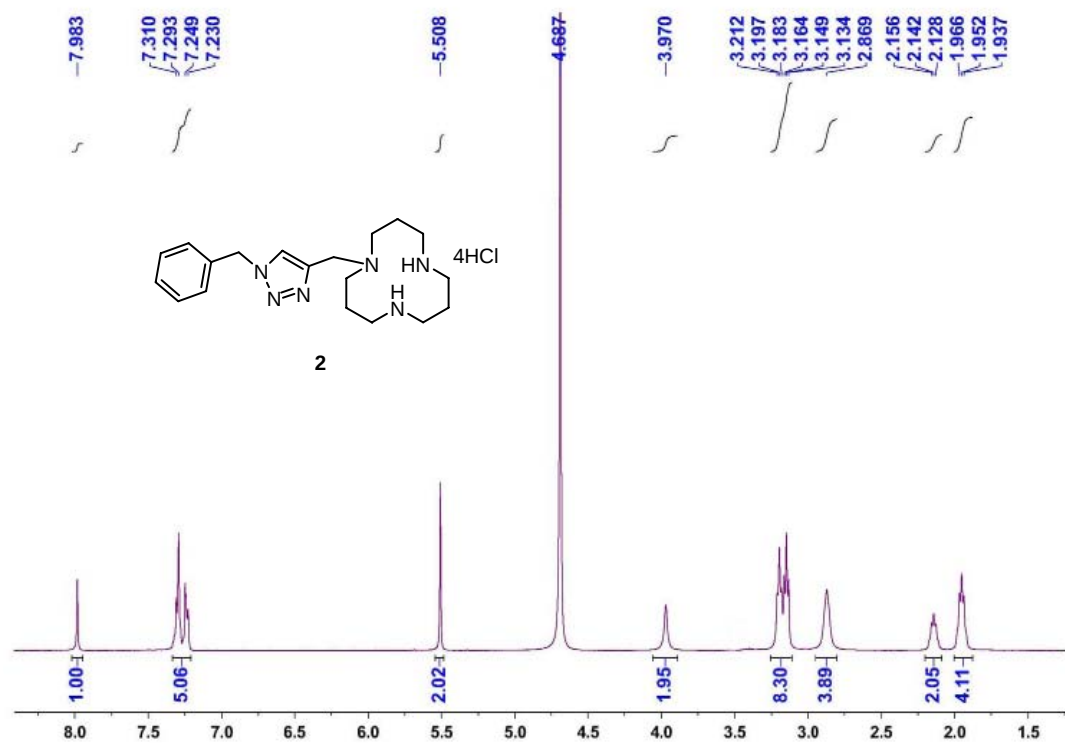












Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

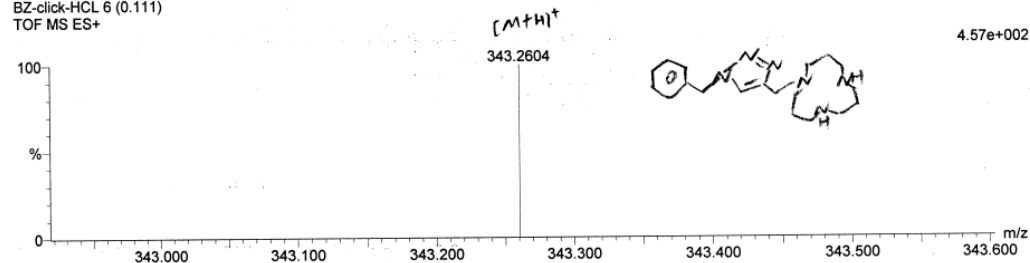
596 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-40 H: 0-70 N: 0-15 O: 0-10

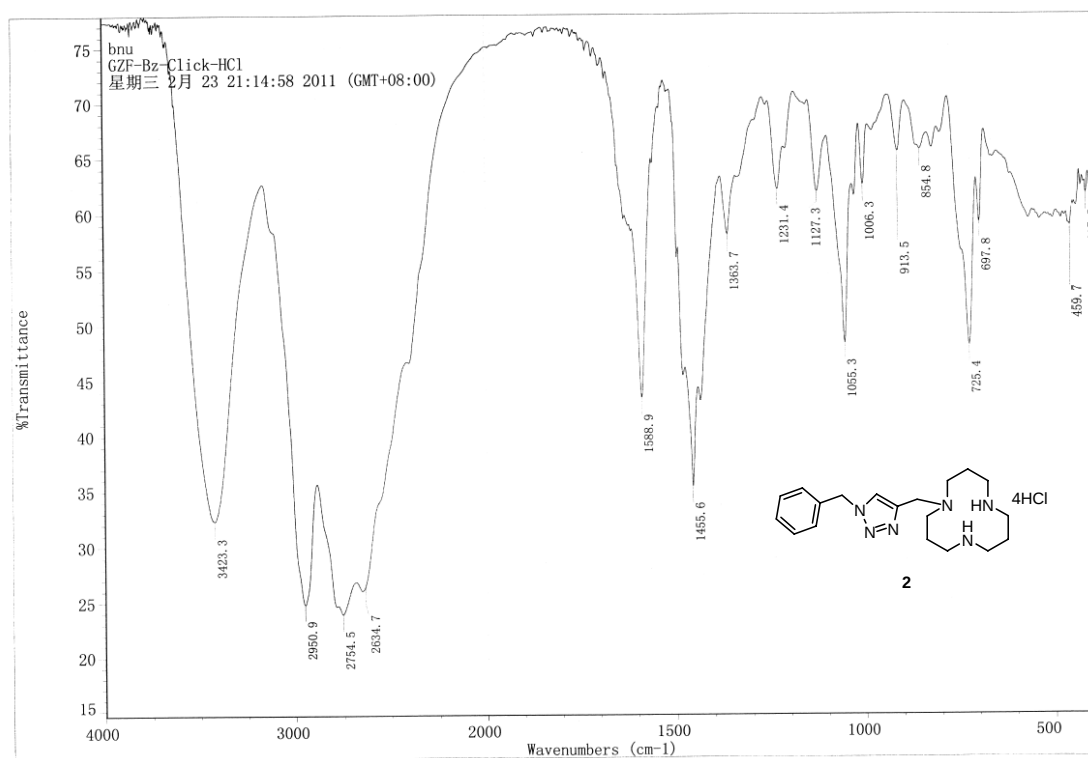
BZ-click-HCL 6 (0.111)

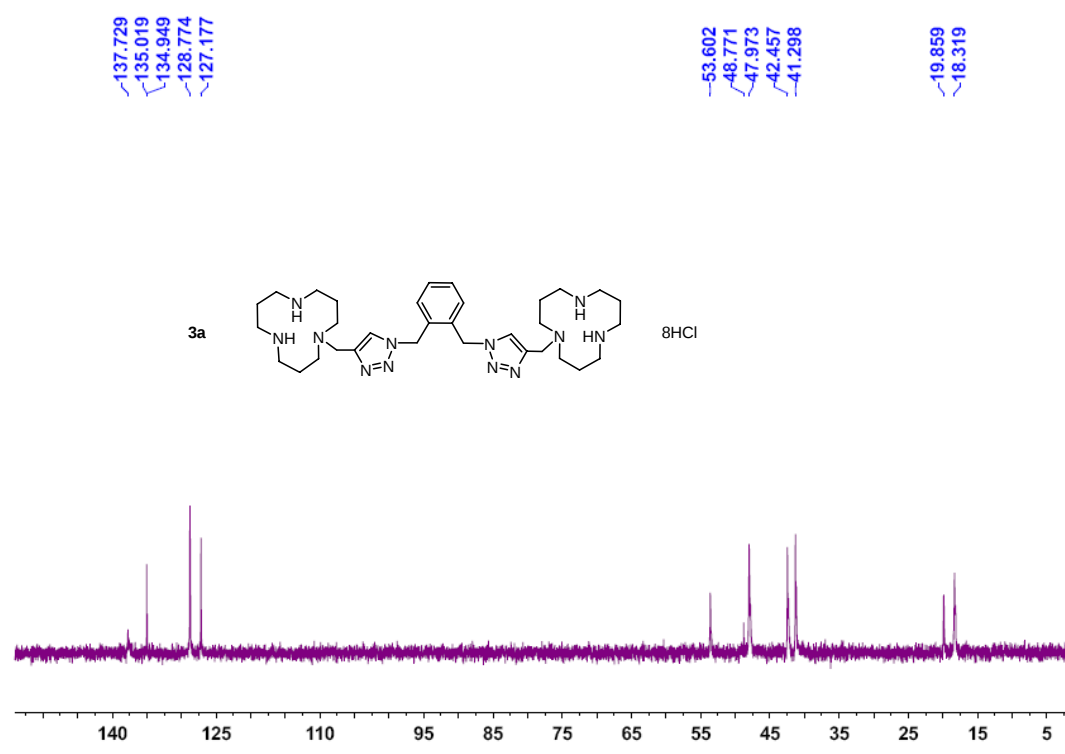
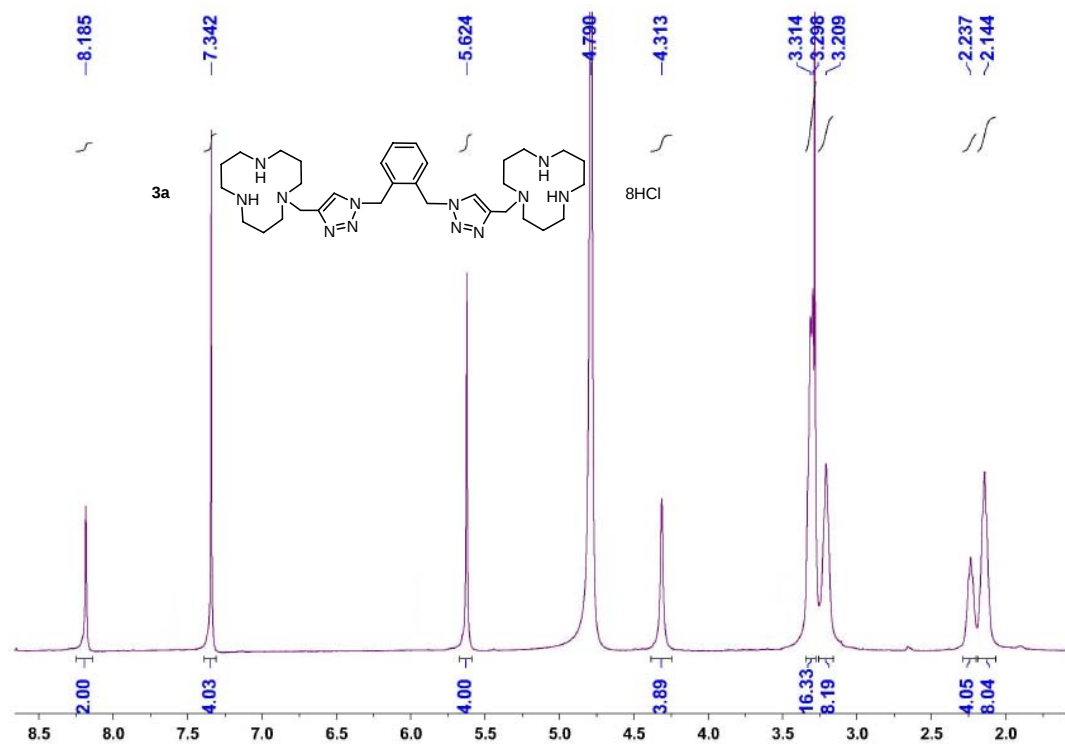
TOF MS ES+



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.2604	343.2610	-0.6	-1.7	7.5	n/a	C19 H31 N6
	343.2597	0.7	2.0	2.5	n/a	C18 H35 N2 O4





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

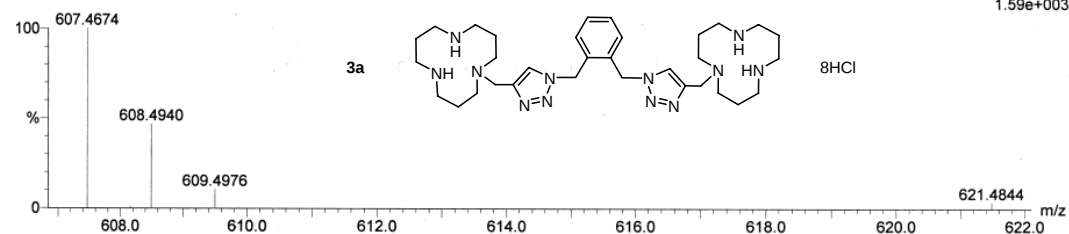
901 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)

Elements Used:

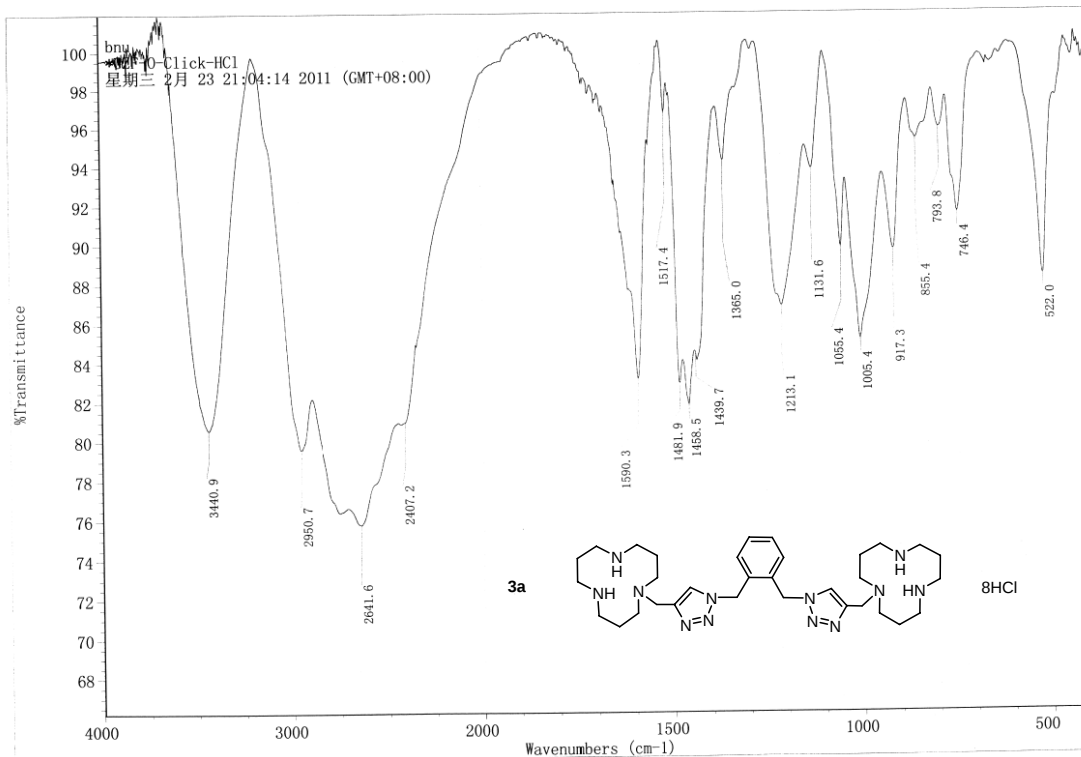
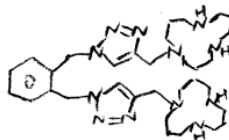
C: 0-40 H: 0-70 N: 0-15 O: 0-10

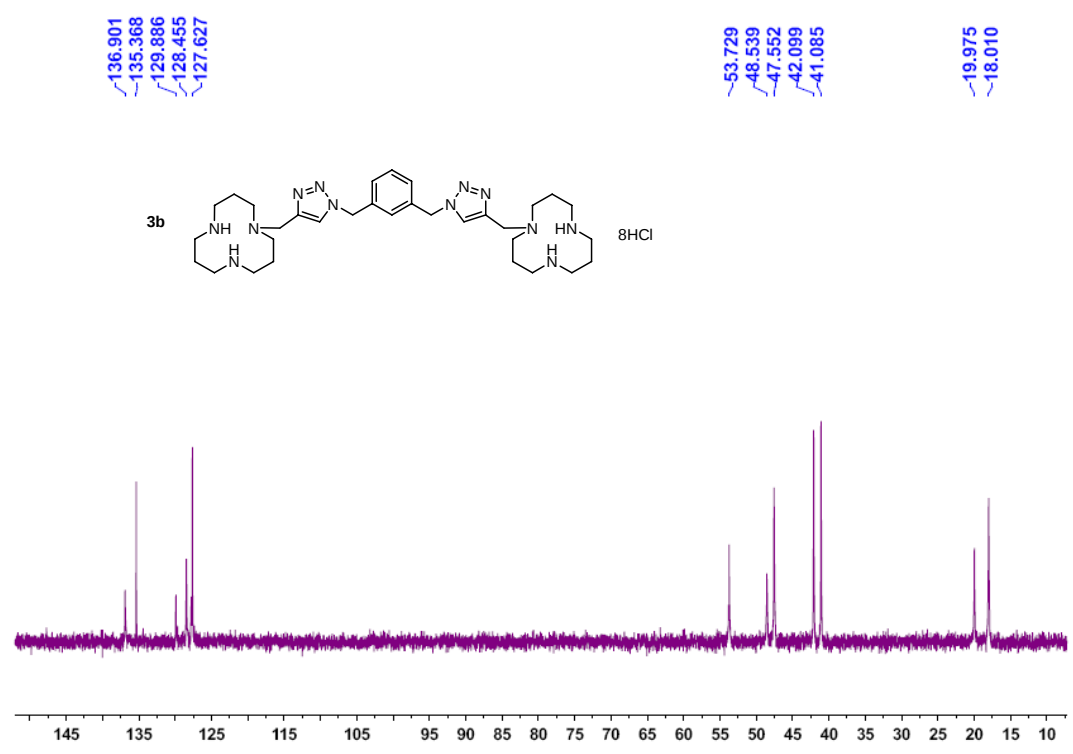
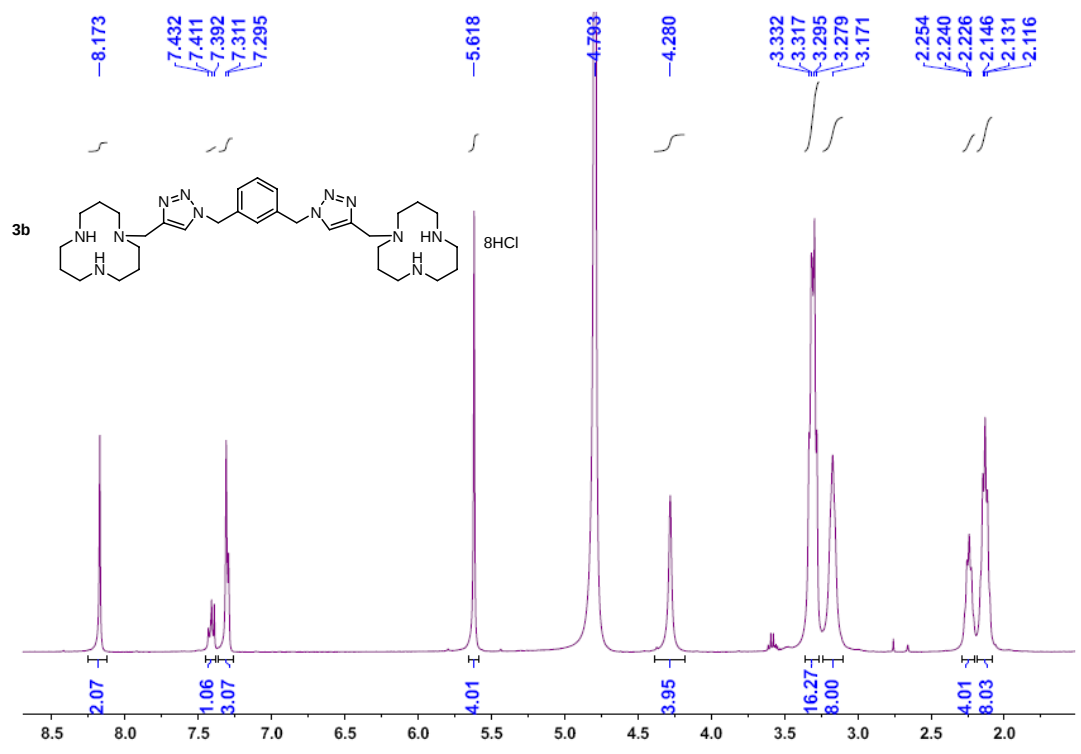
O-click-HCL 3 (0.055)

TOF MS ES+



Minimum:				-1.5		
Maximum:	10.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
607.4674	607.4673	0.1	0.2	11.5	11.0	C32 H55 N12 ✓
	607.4686	-1.2	-2.0	5.5	8.0	C35 H63 N2 O6
	607.4659	1.5	2.5	6.5	16.0	C31 H59 N8 O4
	607.4691	-1.7	-2.8	-1.5	66.8	C20 H59 N14 O7
	607.4700	-2.6	-4.3	10.5	4.9	C36 H59 N6 O2
	607.4646	2.8	4.6	1.5	22.6	C30 H63 N4 O8





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

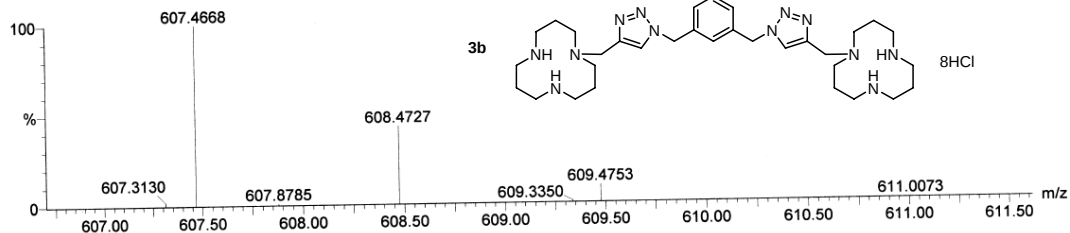
1041 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

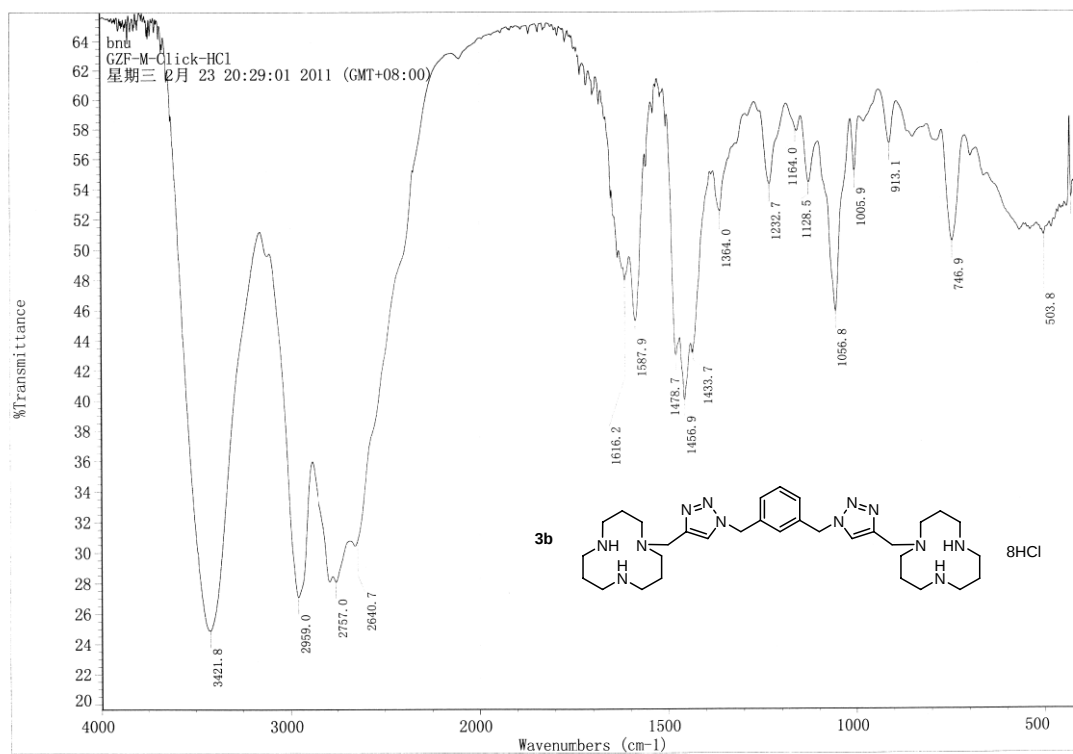
C: 0-35 H: 0-60 N: 0-15 54Fe: 0-1 56Fe: 0-1 57Fe: 0-1 58Fe: 0-1

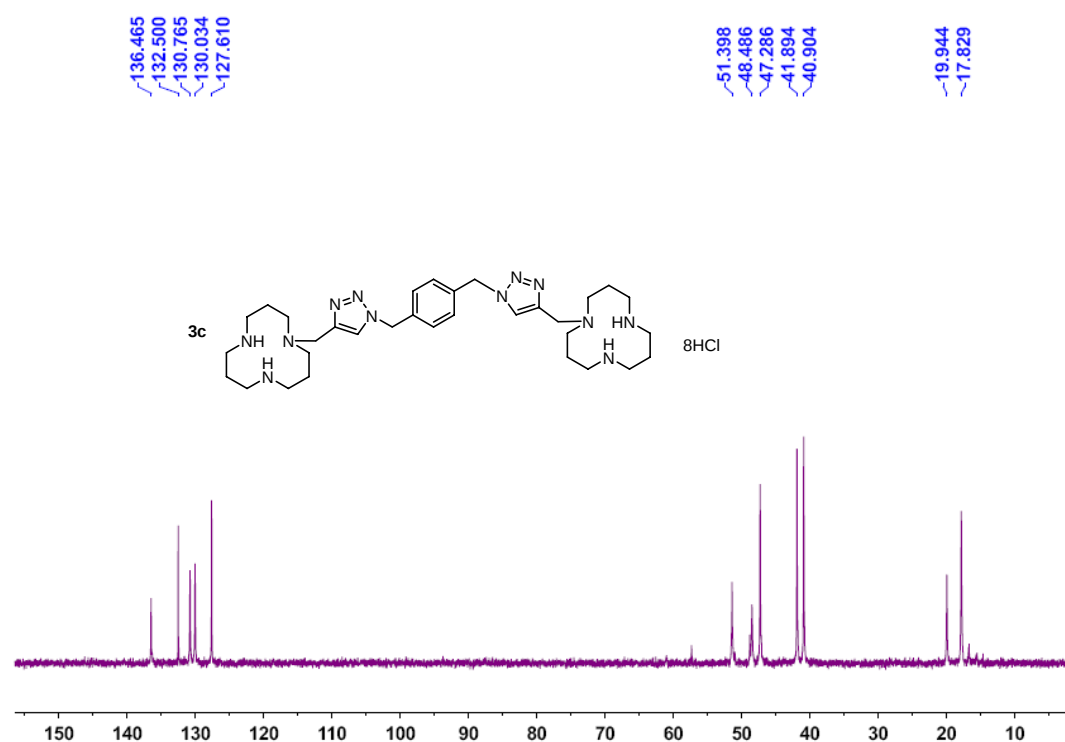
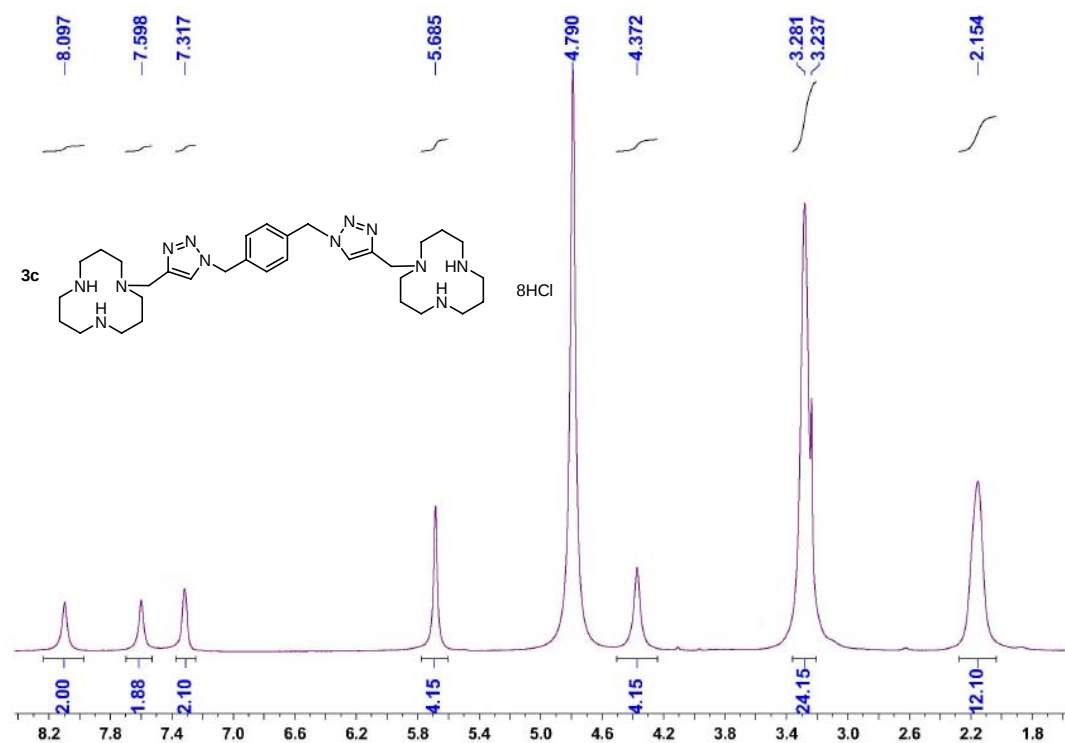
YANH-1 36 (0.666)

TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
607.4668	607.4673	-0.5	-0.8	11.5	12.8	C32 H55 N12





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

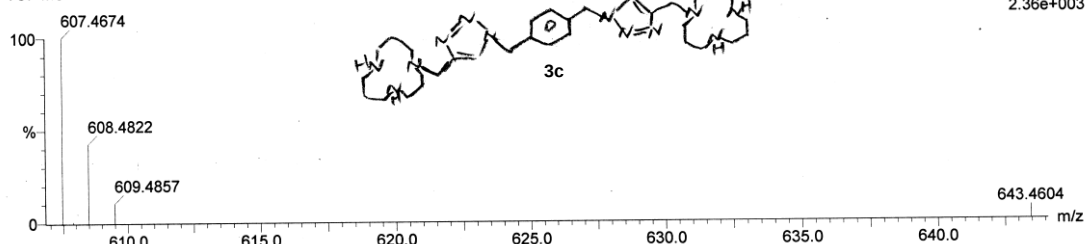
901 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)

Elements Used:

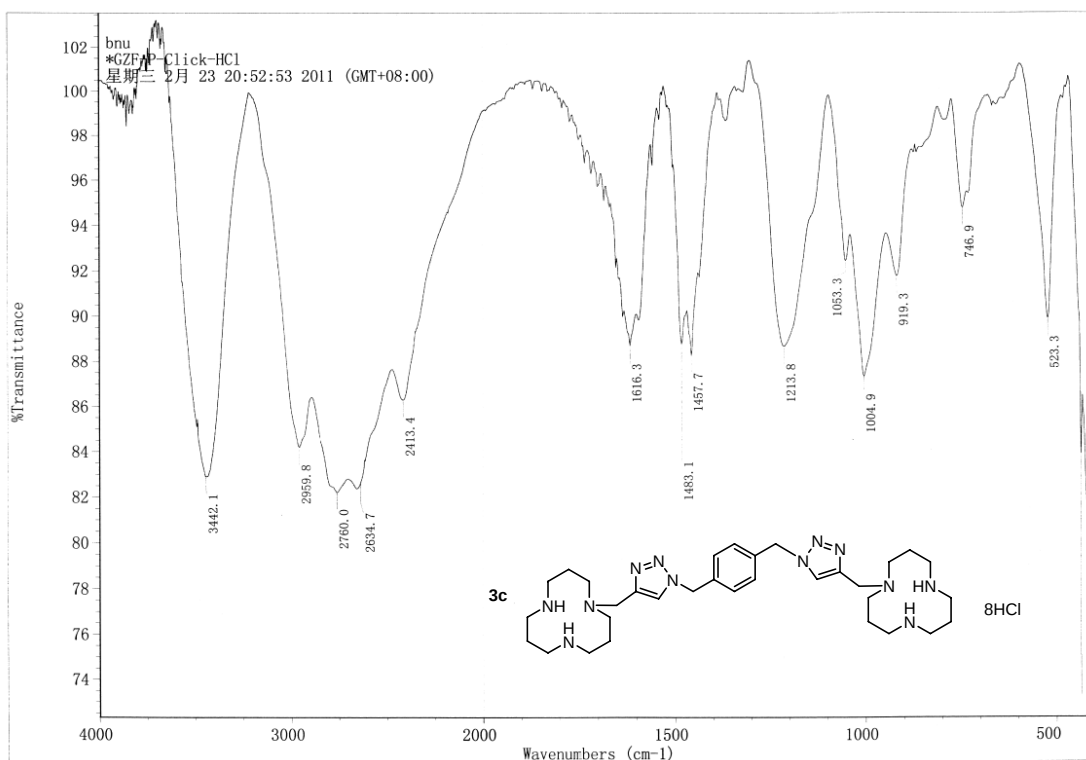
C: 0-40 H: 0-70 N: 0-15 O: 0-10

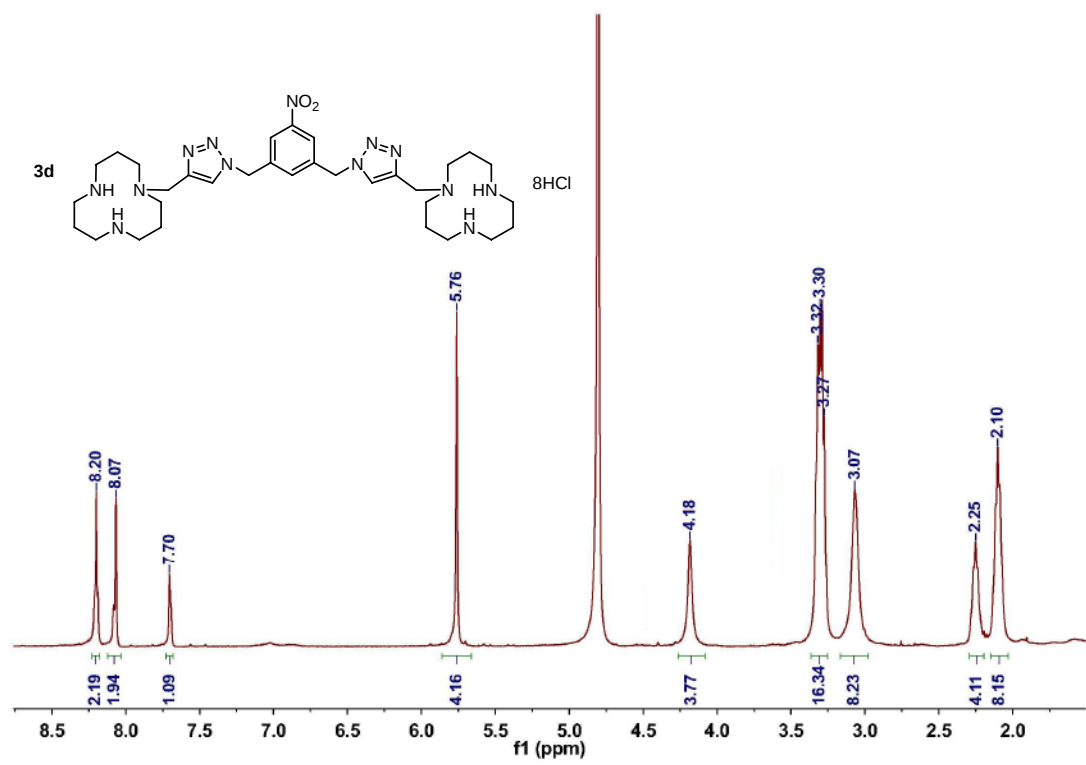
P-click-HCL 9 (0.167)

TOF MS ES+



Minimum:				-1.5					
Maximum:		10.0	5.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula			
607.4674	607.4673	0.1	0.2	11.5	7.3	C32	H55	N12	✓
	607.4686	-1.2	-2.0	5.5	2.7	C35	H63	N2	O6
	607.4659	1.5	2.5	6.5	10.5	C31	H59	N8	O4
	607.4691	-1.7	-2.8	-1.5	71.3	C20	H59	N14	O7
	607.4700	-2.6	-4.3	10.5	2.0	C36	H59	N6	O2
	607.4646	2.8	4.6	1.5	16.2	C30	H63	N4	O8

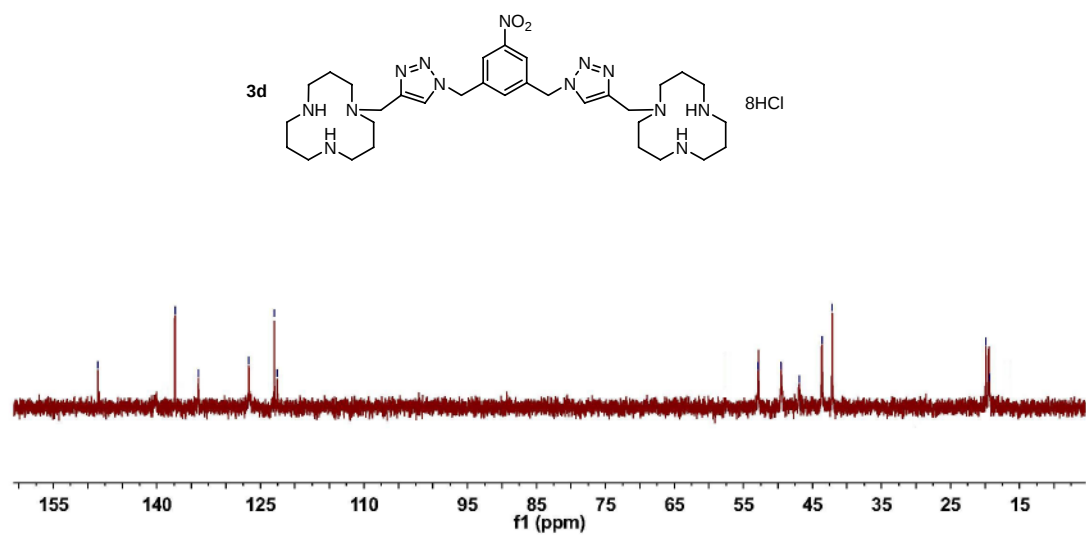




148.55
137.37
133.97
126.66
122.97
122.55

52.86
49.56
46.90
43.62
42.13

19.88
19.36



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

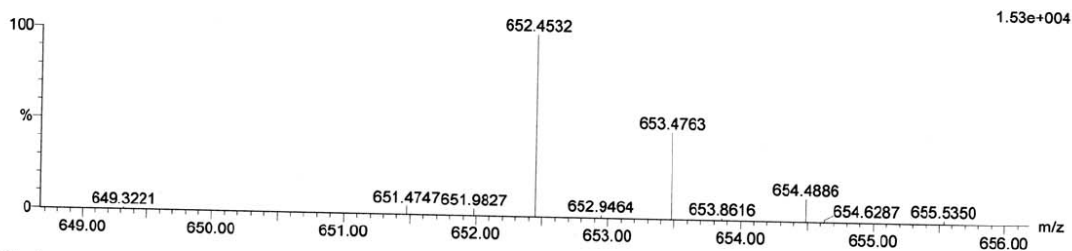
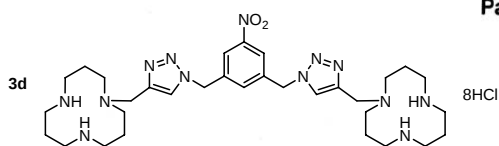
597 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-35 H: 0-60 N: 0-15 O: 0-3 Br: 0-2

yanh-3 24 (0.444)

TOF MS ES+



Minimum:

Maximum:

5.0

5.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

652.4532

652.4523

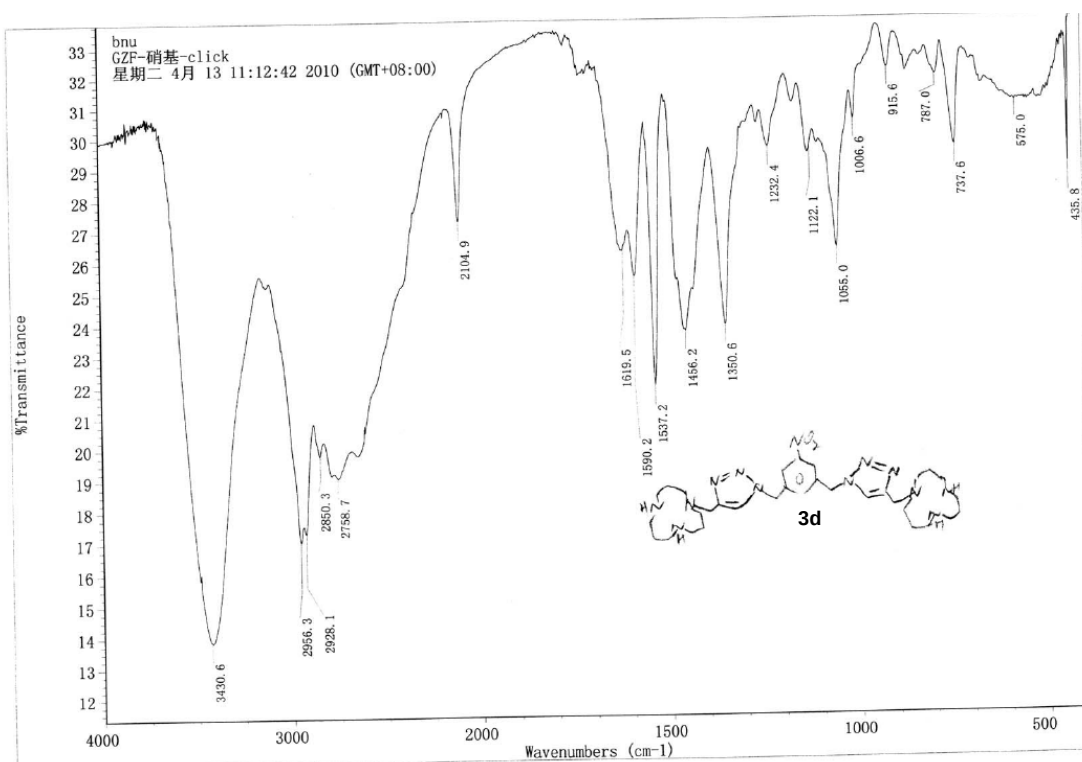
0.9

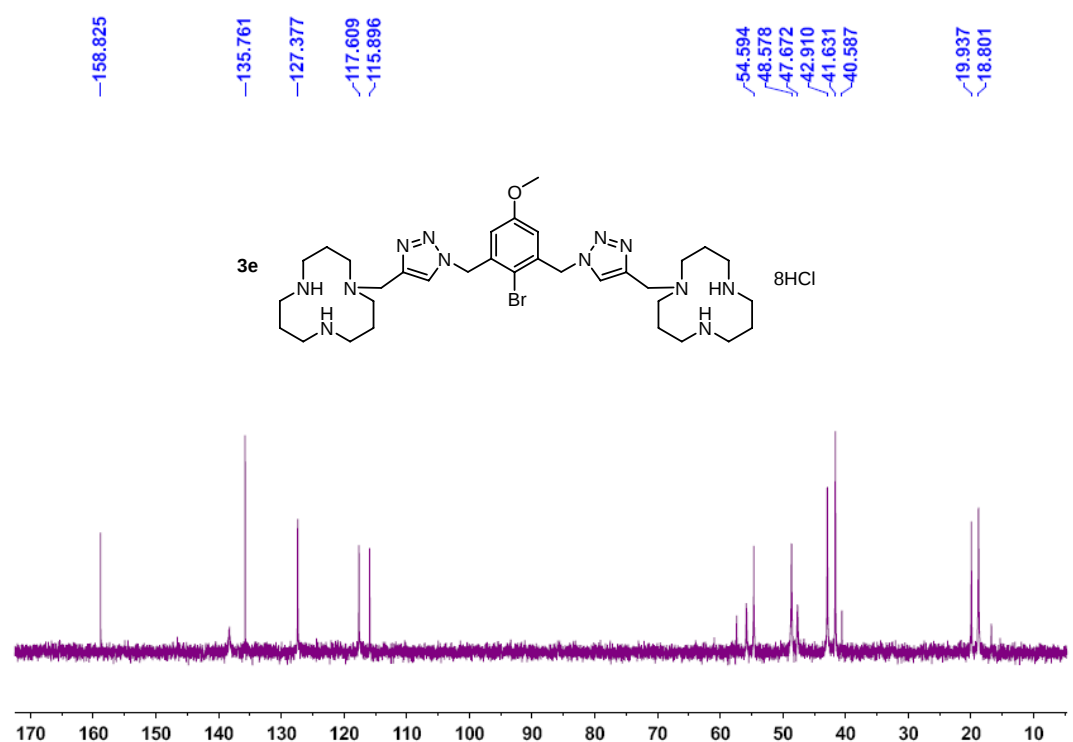
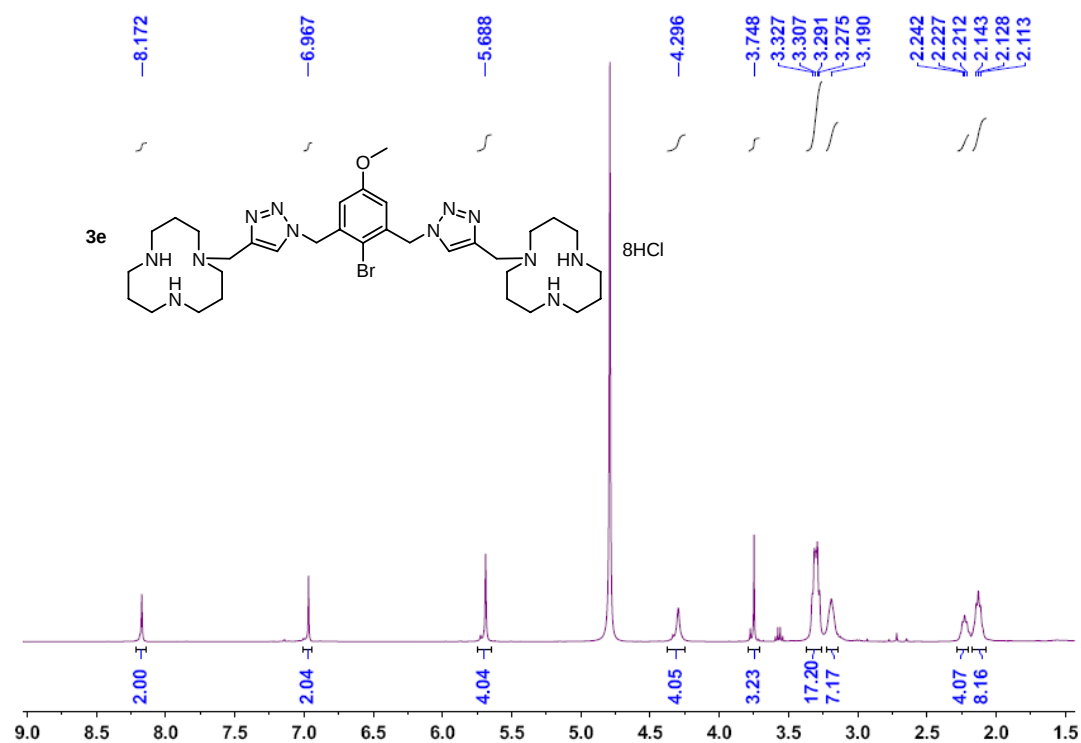
1.4

12.5

135.9

C32 H54 N13 O2





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

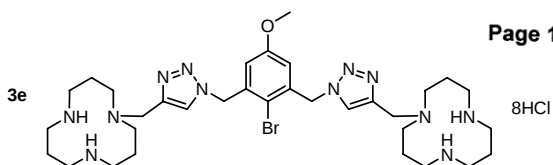
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

393 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

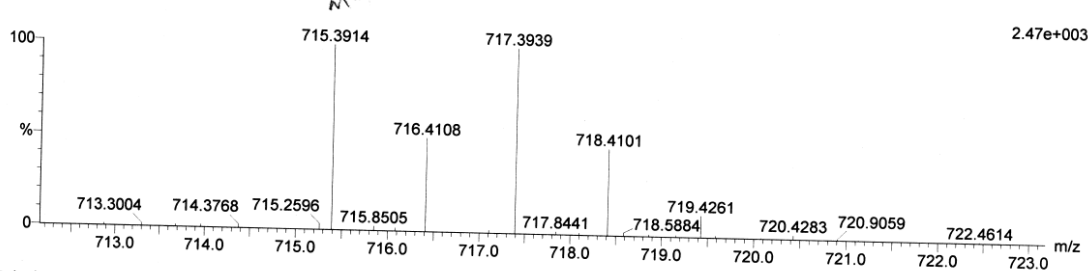
Elements Used:

C: 0-35 H: 0-60 N: 0-15 O: 0-3 Br: 0-2

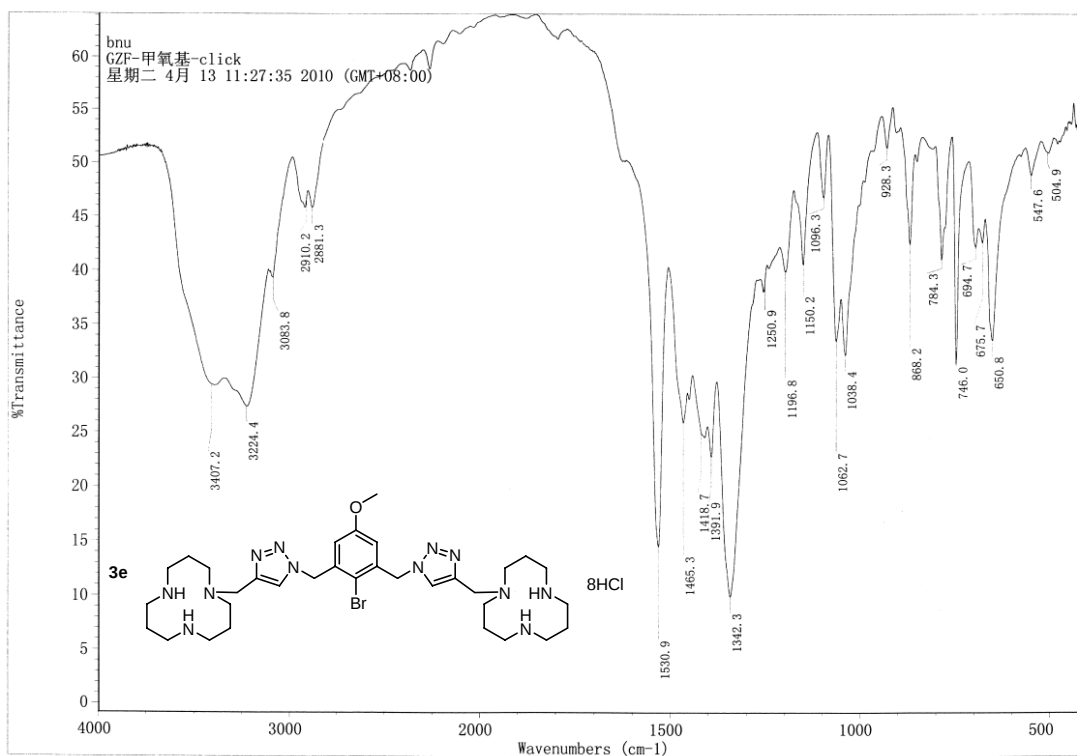


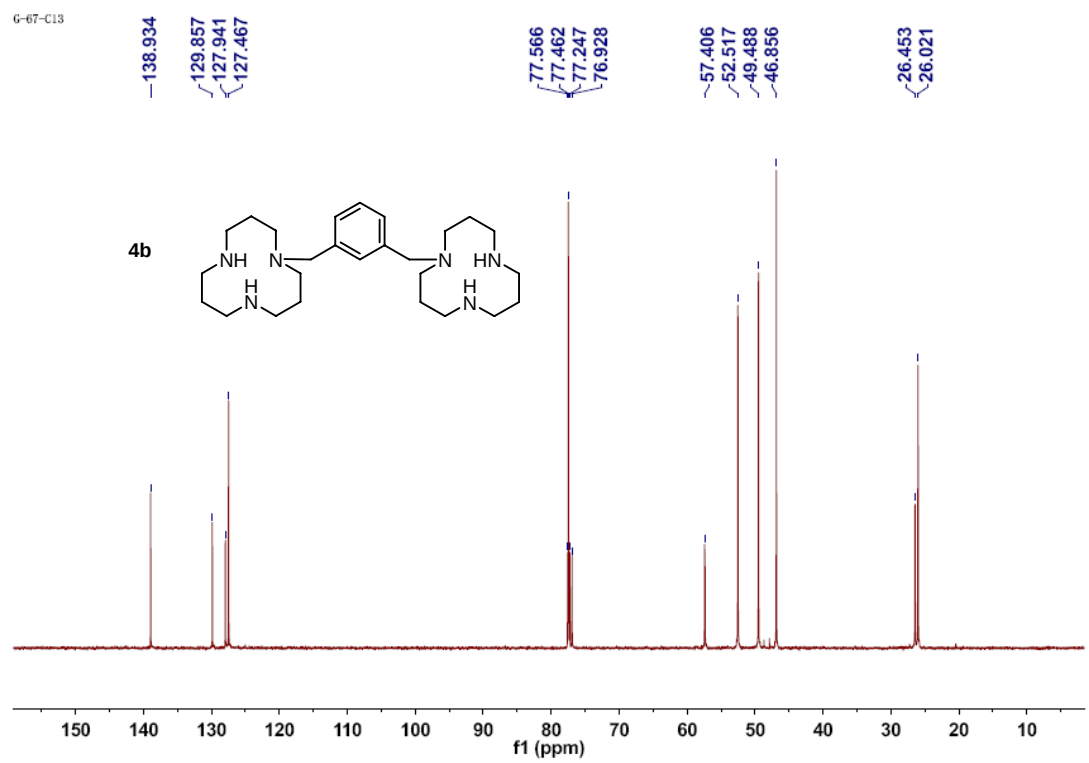
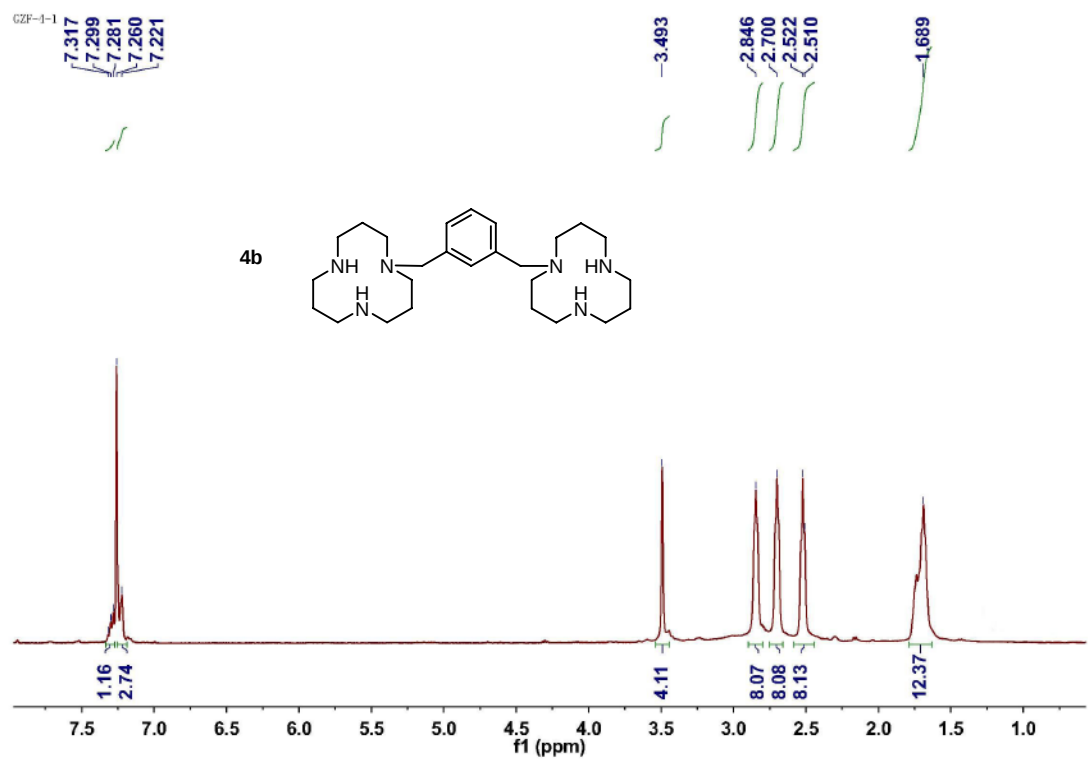
yanh-2 64 (1.409)

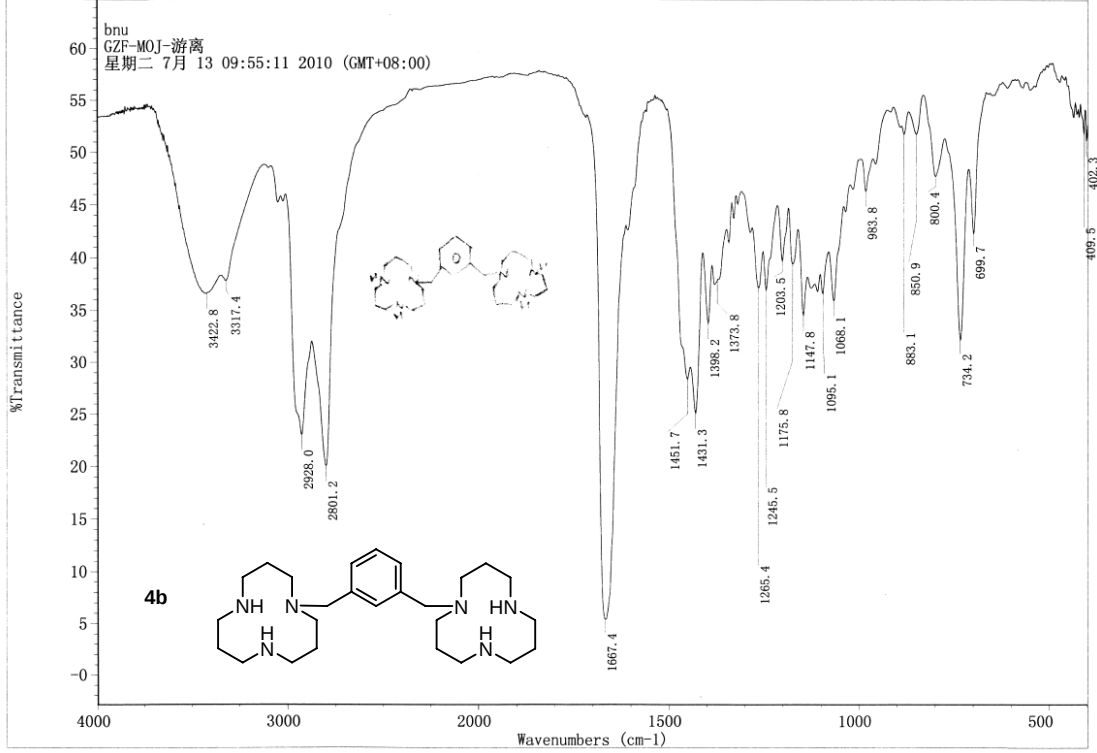
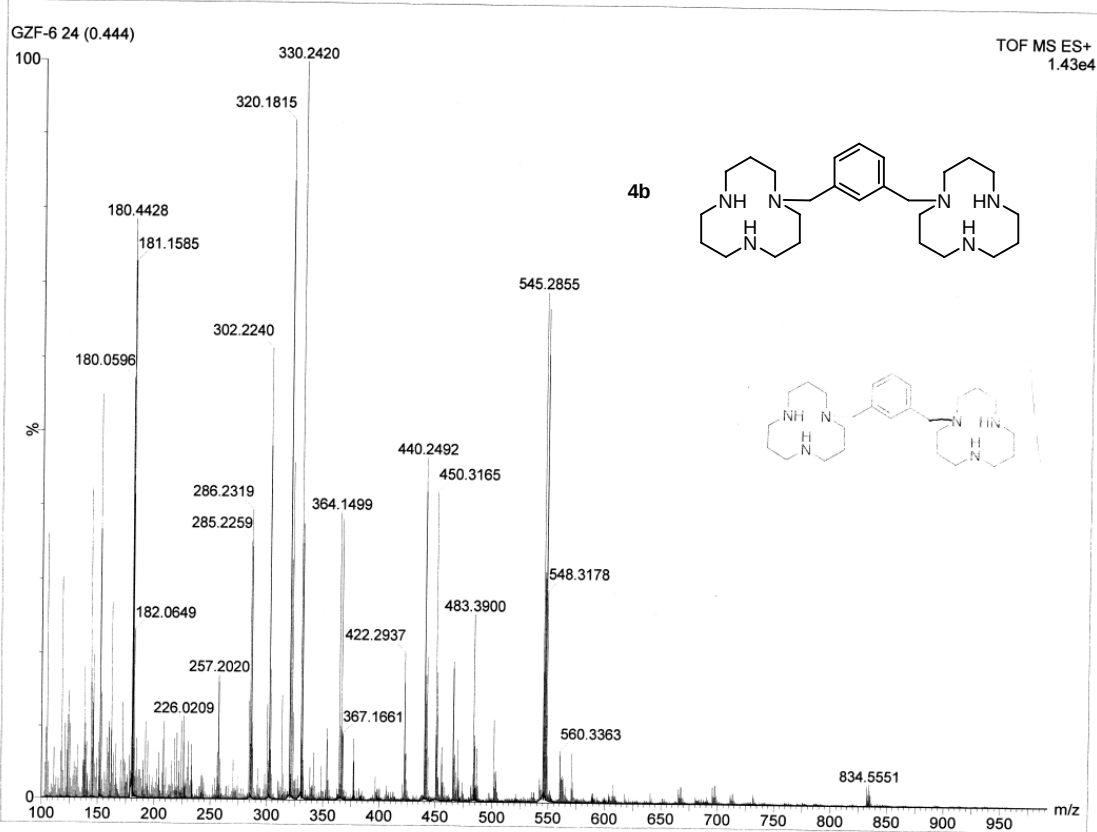
1: TOF MS ES+

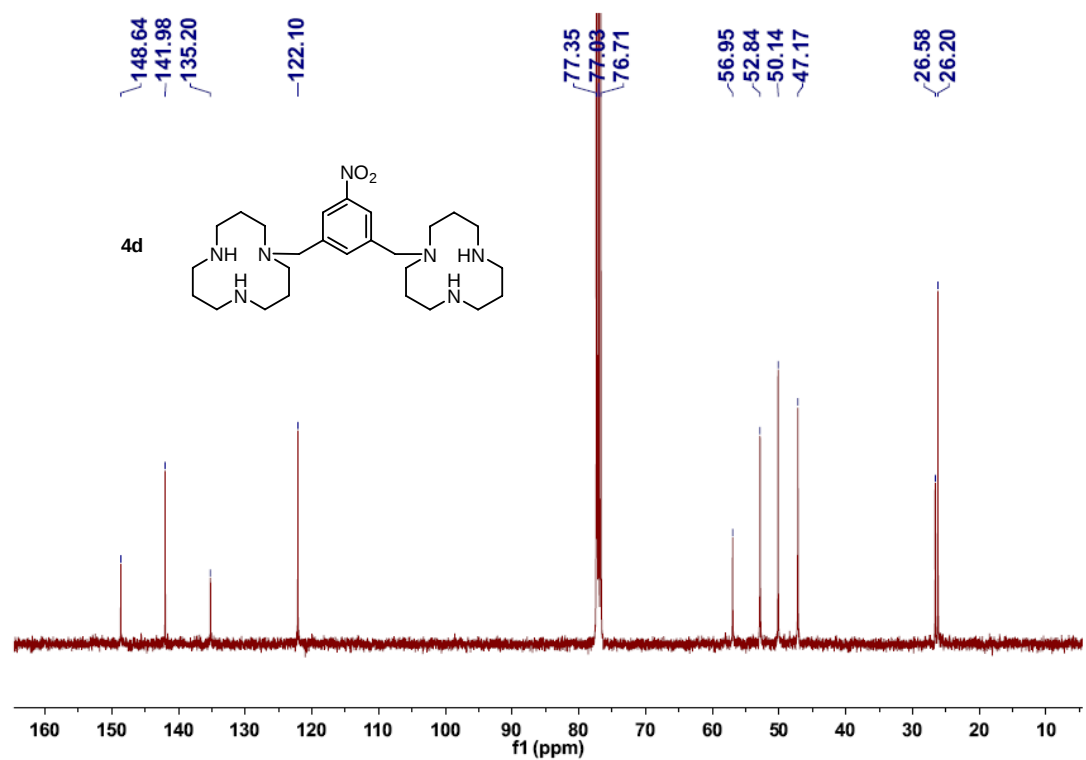
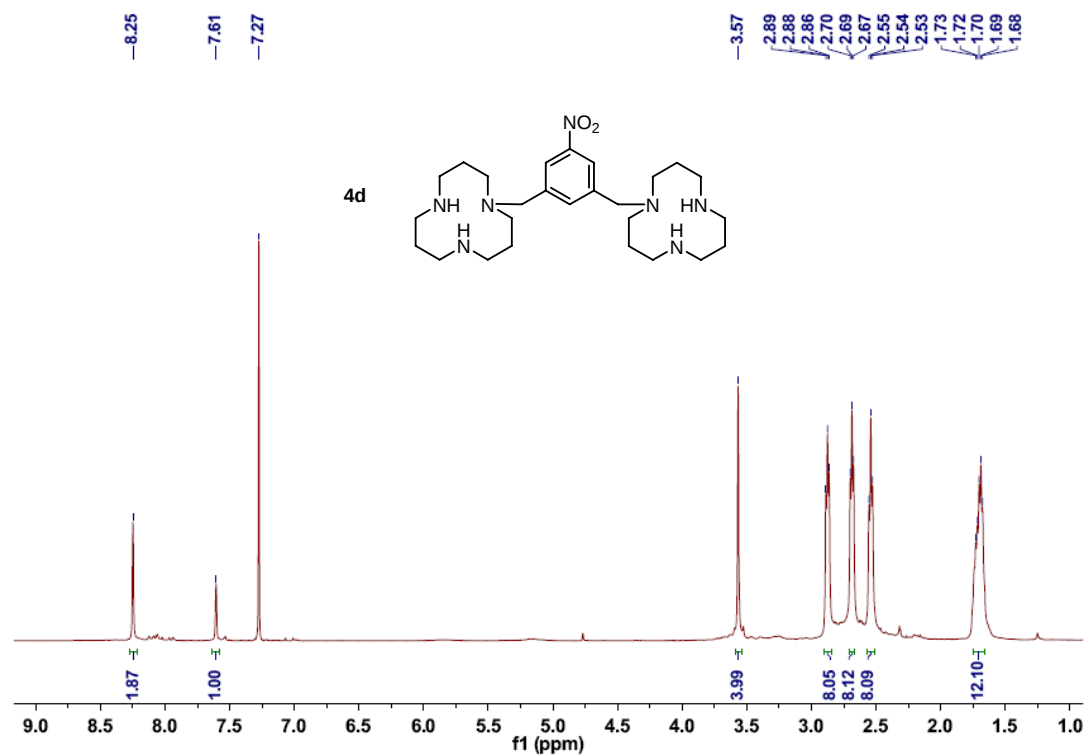


Minimum:						
Maximum:		5.0	5.0	-1.5	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
715.3914	715.3883	3.1	4.3	11.5	25.2	C33 H56 N12 O Br









Elemental Composition Report

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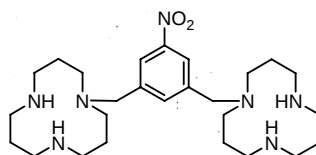
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

4d



Monoisotopic Mass, Even Electron Ions

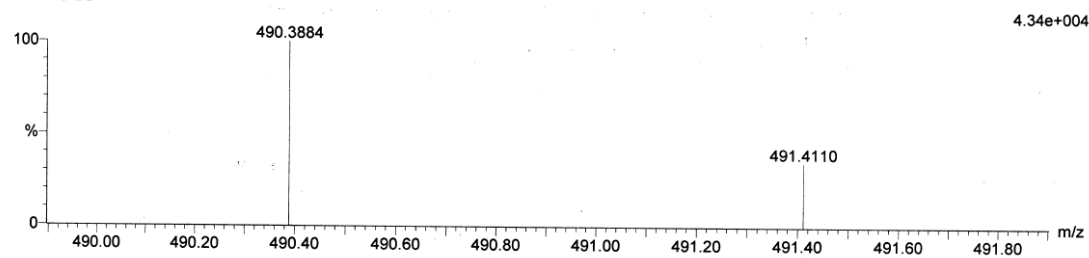
286 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

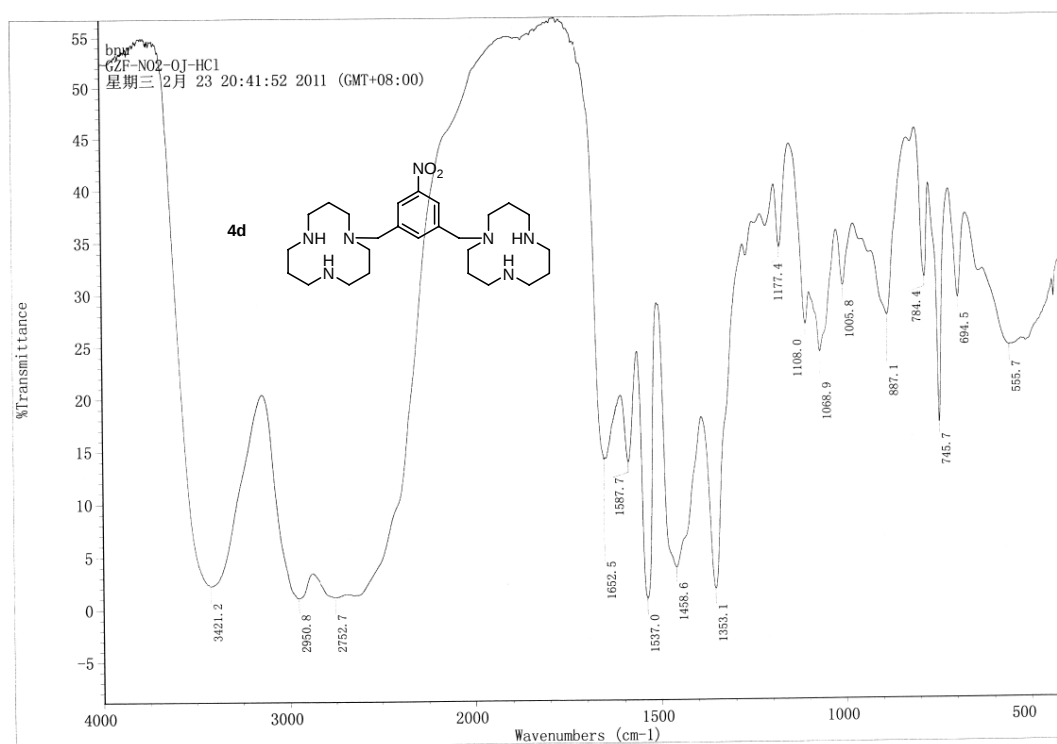
C: 0-40 H: 0-50 N: 0-10 O: 0-5

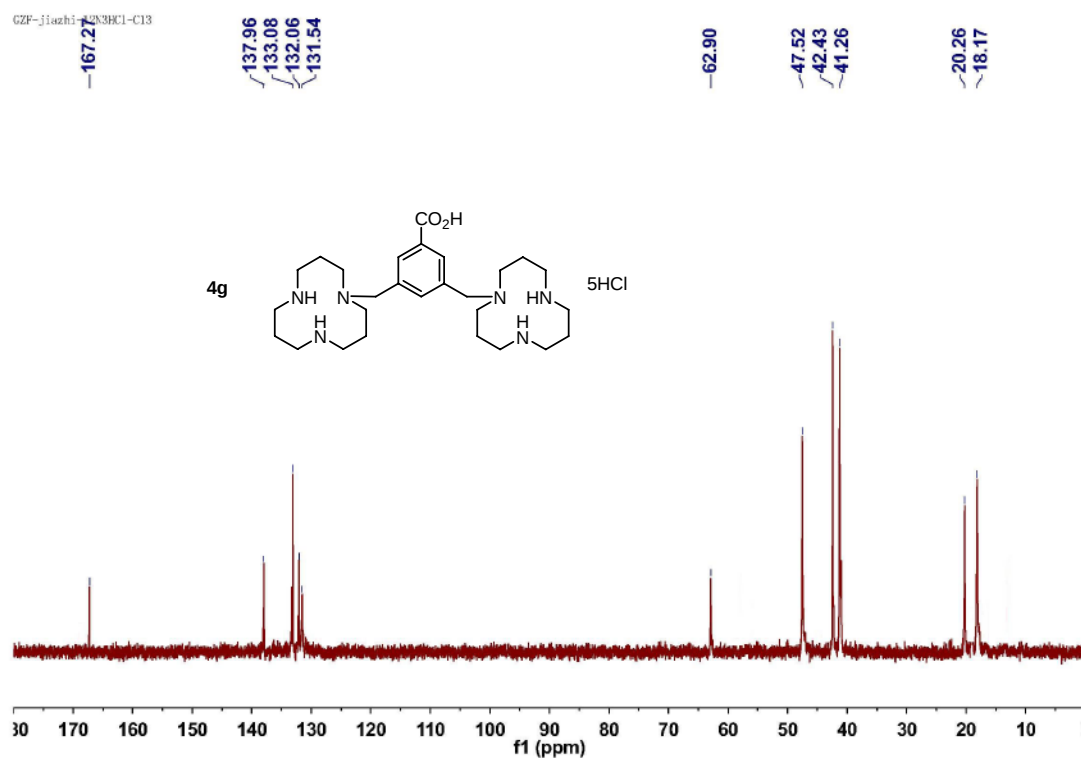
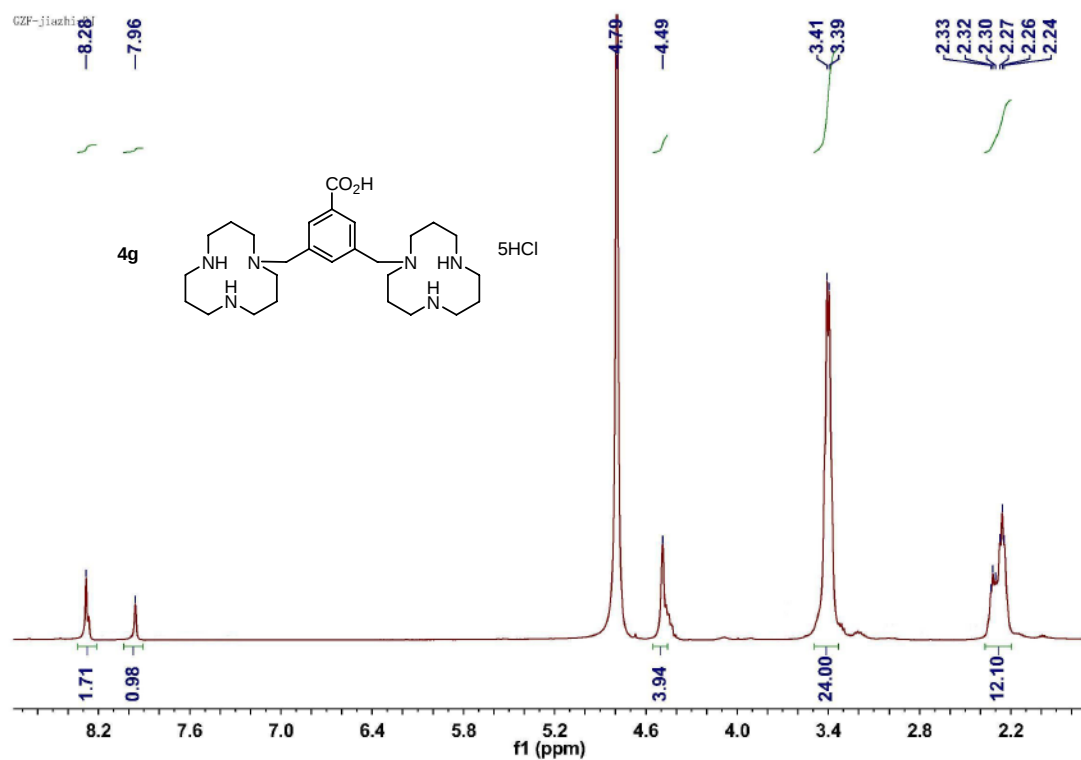
GZF-4 71 (1.314)

TOF MS ES+



Minimum:				-1.5			
Maximum:	10.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
490.3884	490.3869	1.5	3.1	6.5	n/a	C ₂₆ H ₄₈ N ₇ O ₂	



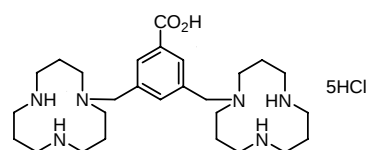


Single Mass Analysis

4g

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

2696 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

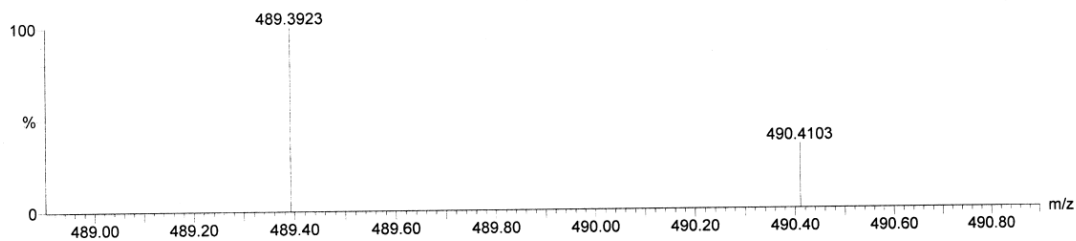
Elements Used:

C: 0-50 H: 0-100 N: 0-10 O: 0-5 Na: 0-1 S: 0-3

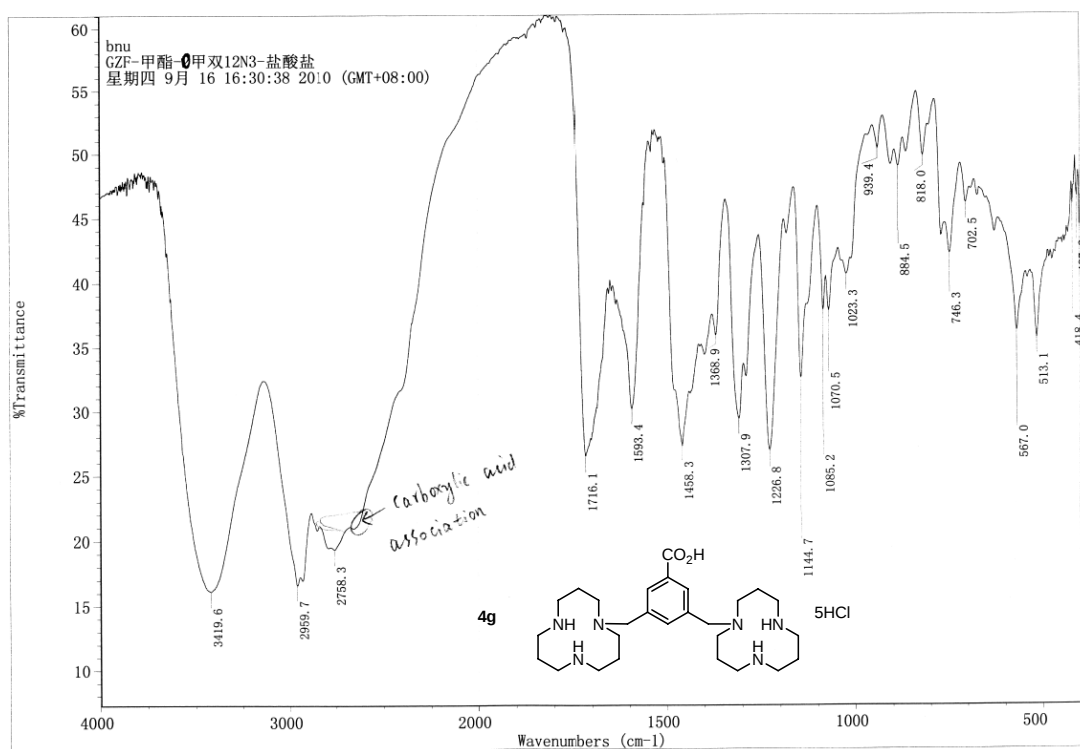
GZF-JZ-3 4 (0.074)

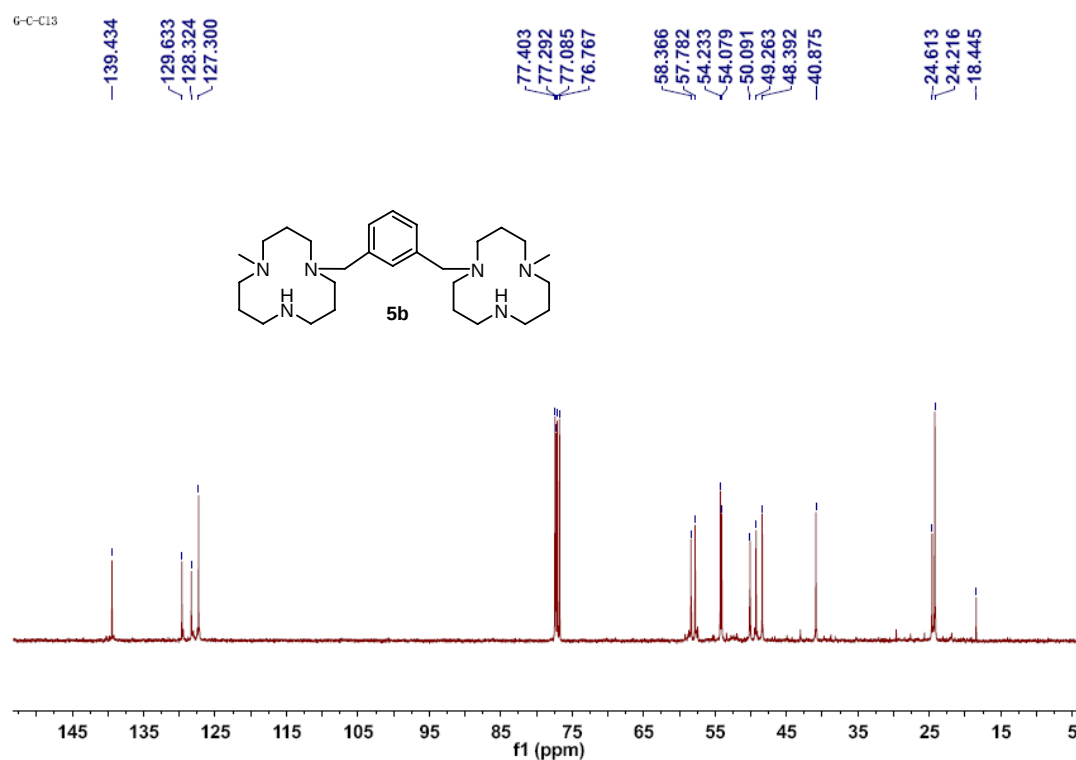
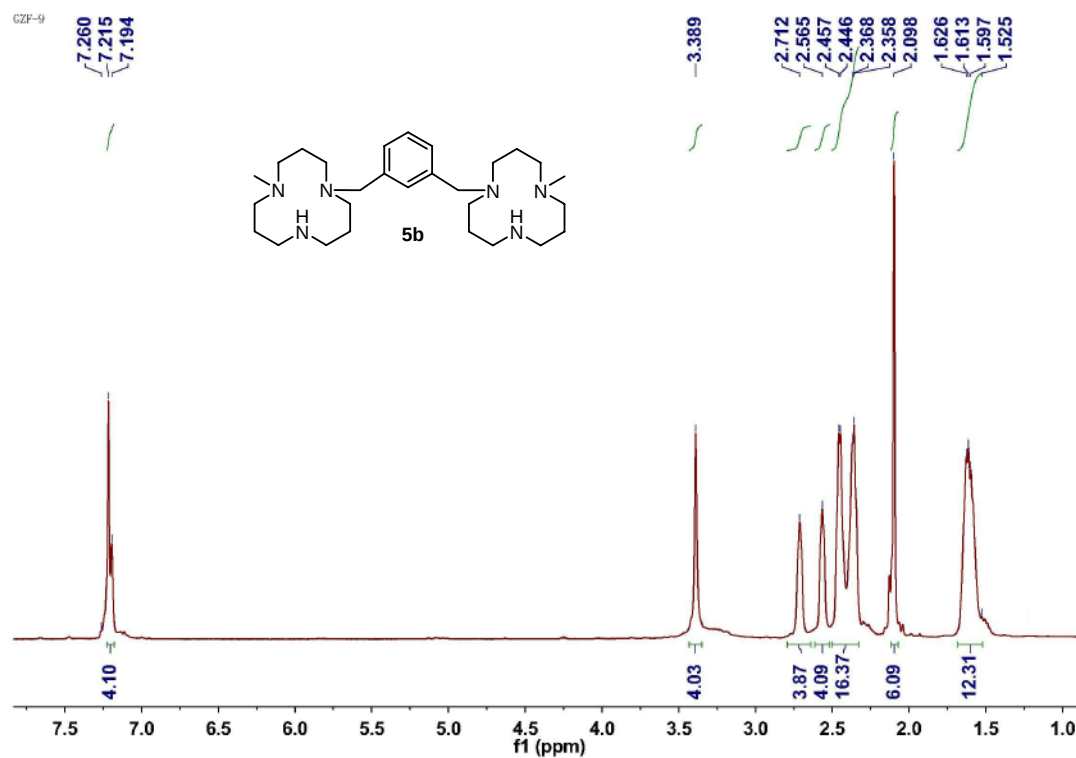
TOF MS ES+

8.43e+002



Minimum:				-1.5									
Maximum:				10.0	3.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula							
489.3923	489.3920	0.3	0.6	2.5	n/a	C29	H54	O4	Na				
	489.3927	-0.4	-0.8	-1.5	n/a	C22	H54	N6	O2	Na	S		
	489.3917	0.6	1.2	6.5	n/a	C27	H49	N6	O2	✓			
	489.3933	-1.0	-2.0	7.5	n/a	C30	H50	N4	Na				
	489.3912	1.1	2.2	0.5	n/a	C27	H57	N2	O	S2			



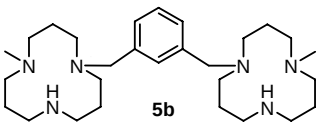


Elemental Composition Report

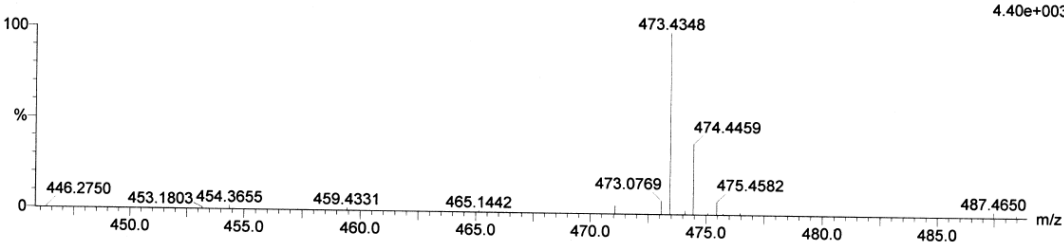
Page 1

Single Mass Analysis

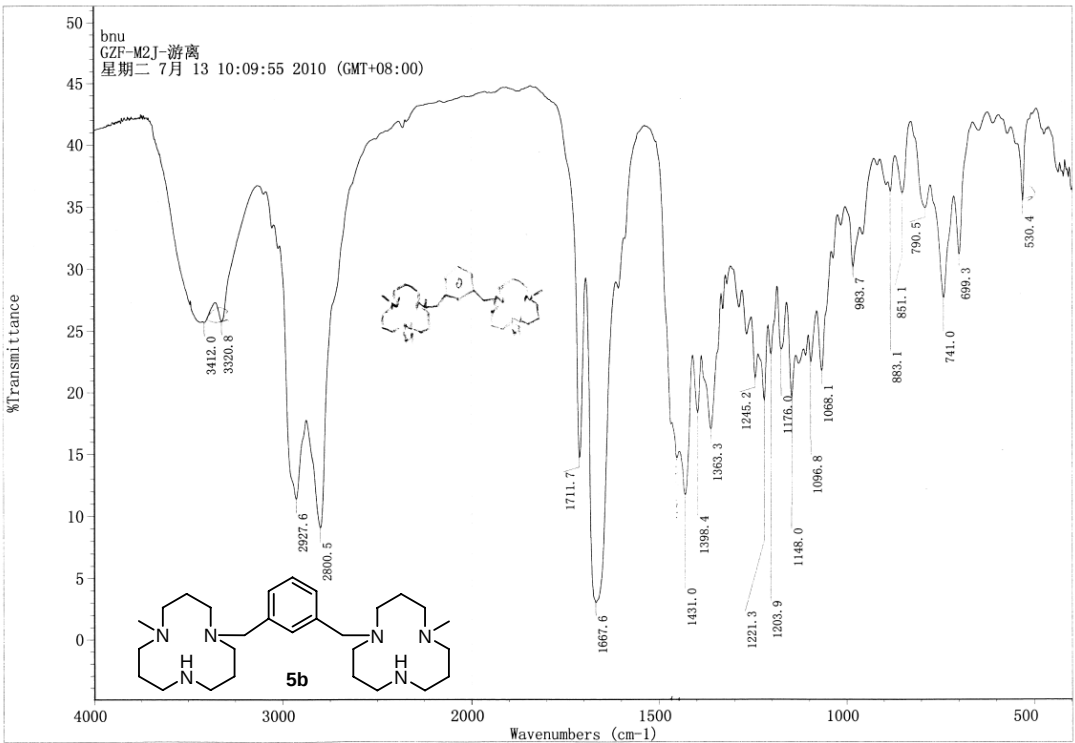
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

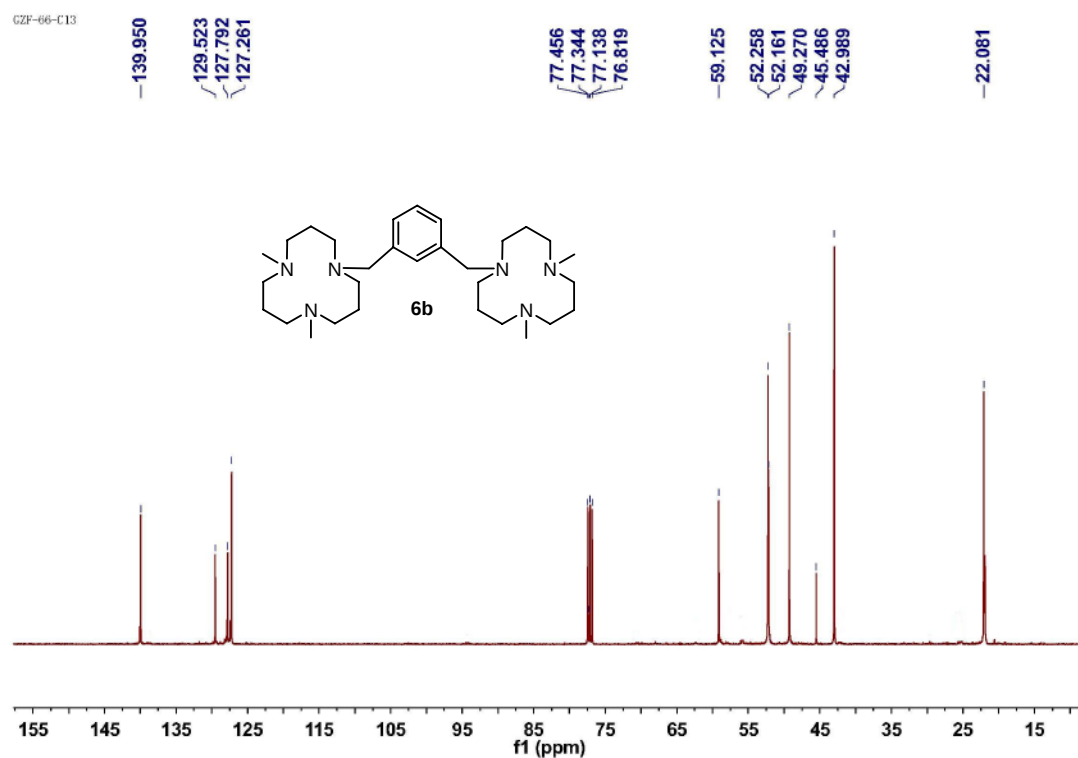
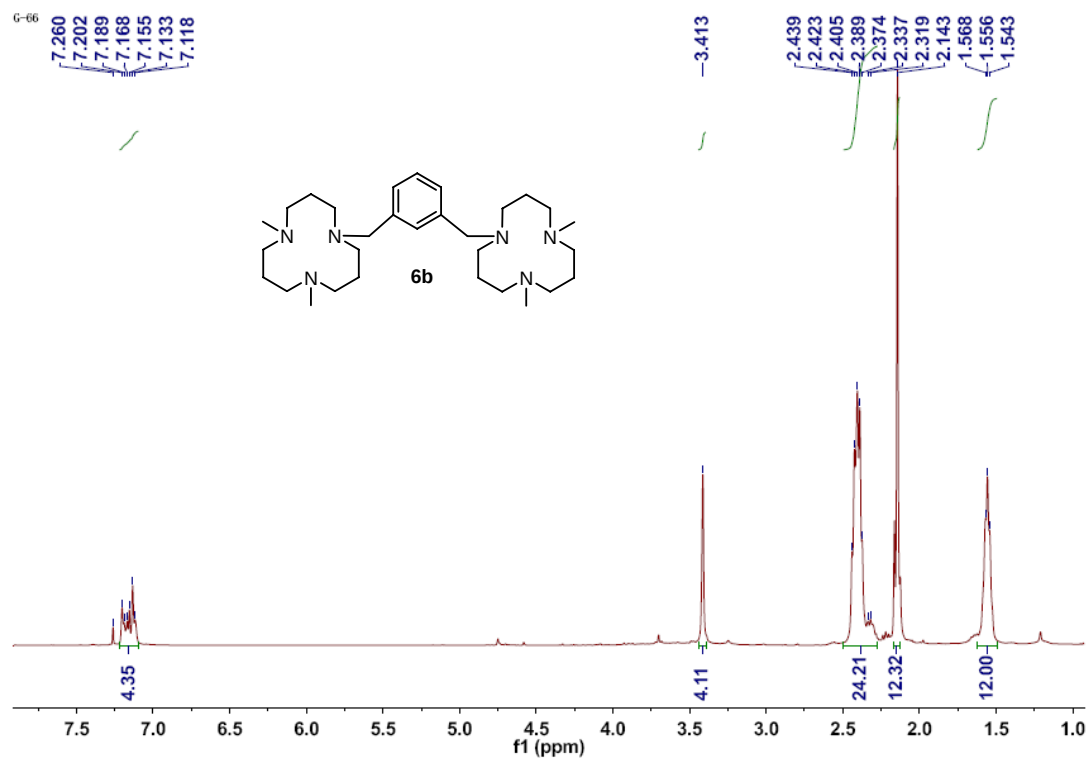


Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-35 H: 0-60 N: 0-10
GZF-5 32 (0.705)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:	5.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
473.4348	473.4332	1.6	3.4	5.5	15.2	C28 H53 N6





Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

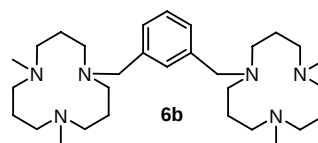
36 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

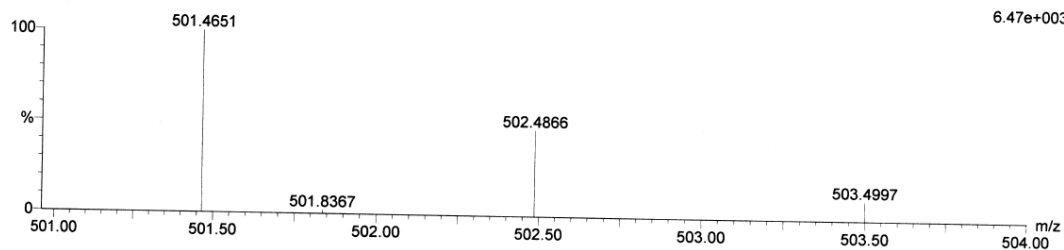
C: 0-35 H: 0-60 N: 0-10

GZF-7 16 (0.296)

TOF MS ES+



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Minimum:

Maximum:

5.0

5.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

501.4651

501.4645

0.6

1.2

5.5

123.2

C30 H57 N6

