SUPPLEMENTARY MATERIAL

Design and Synthesis of New Derivatives of Alkaloid Lupinine: Structural Characterization, Acetylcholinesterase Inhibition Evaluation, and Molecular Modeling Study

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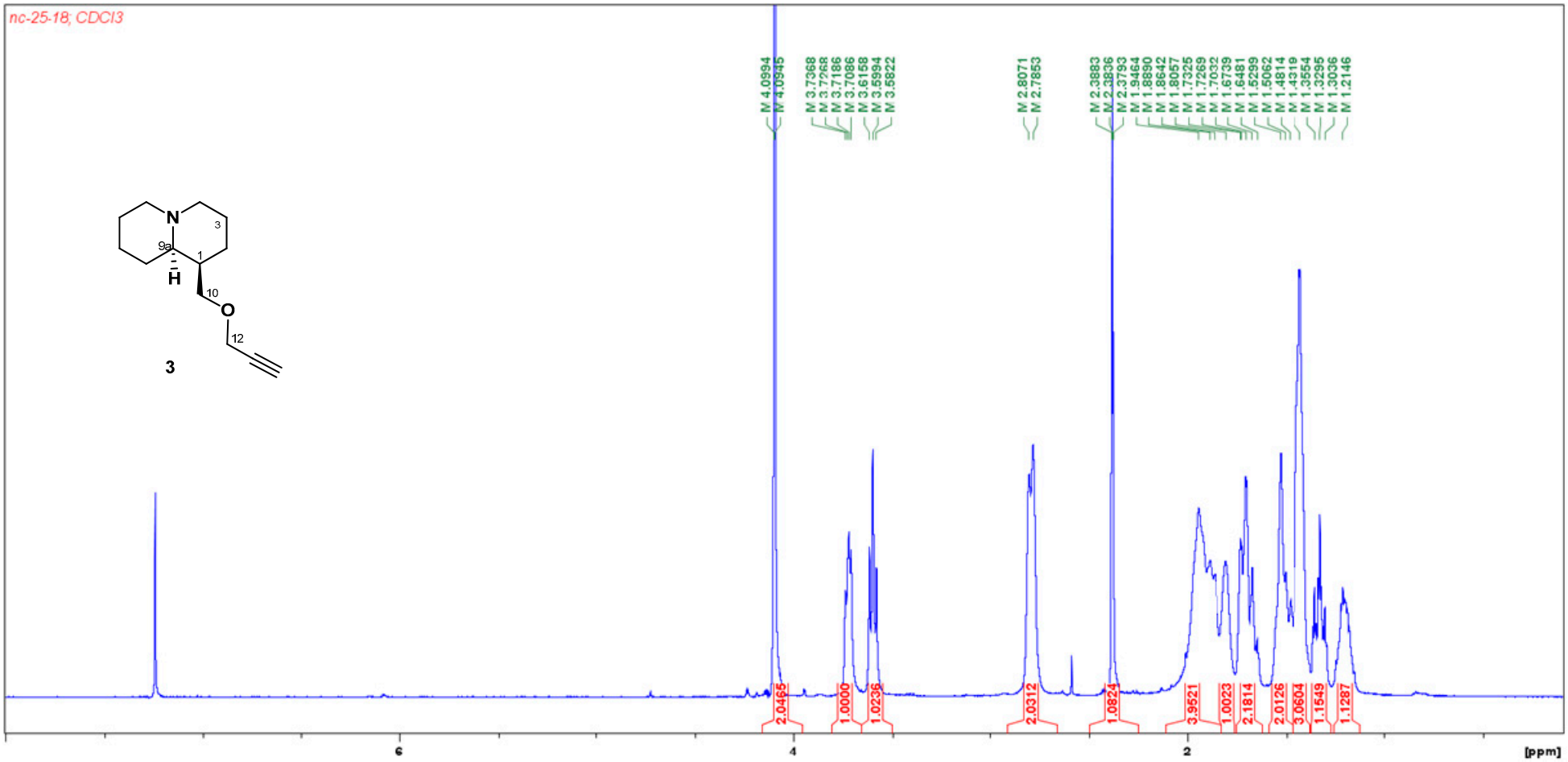


Figure S1. ^{1}H NMR spectrum of (1*R*,9a*R*)-1-((prop-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**3**) ($CDCl_3$, 500 MHz).

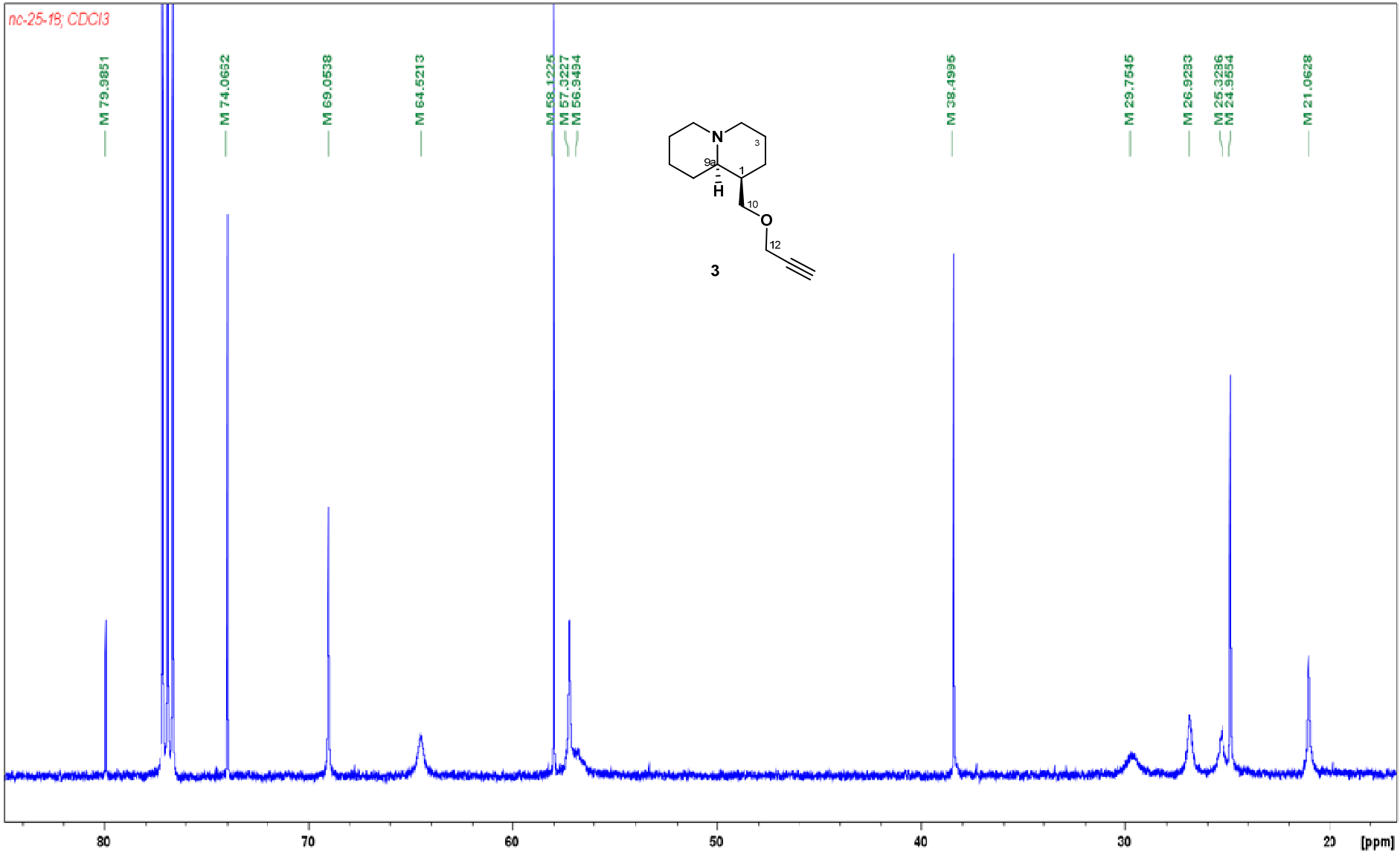
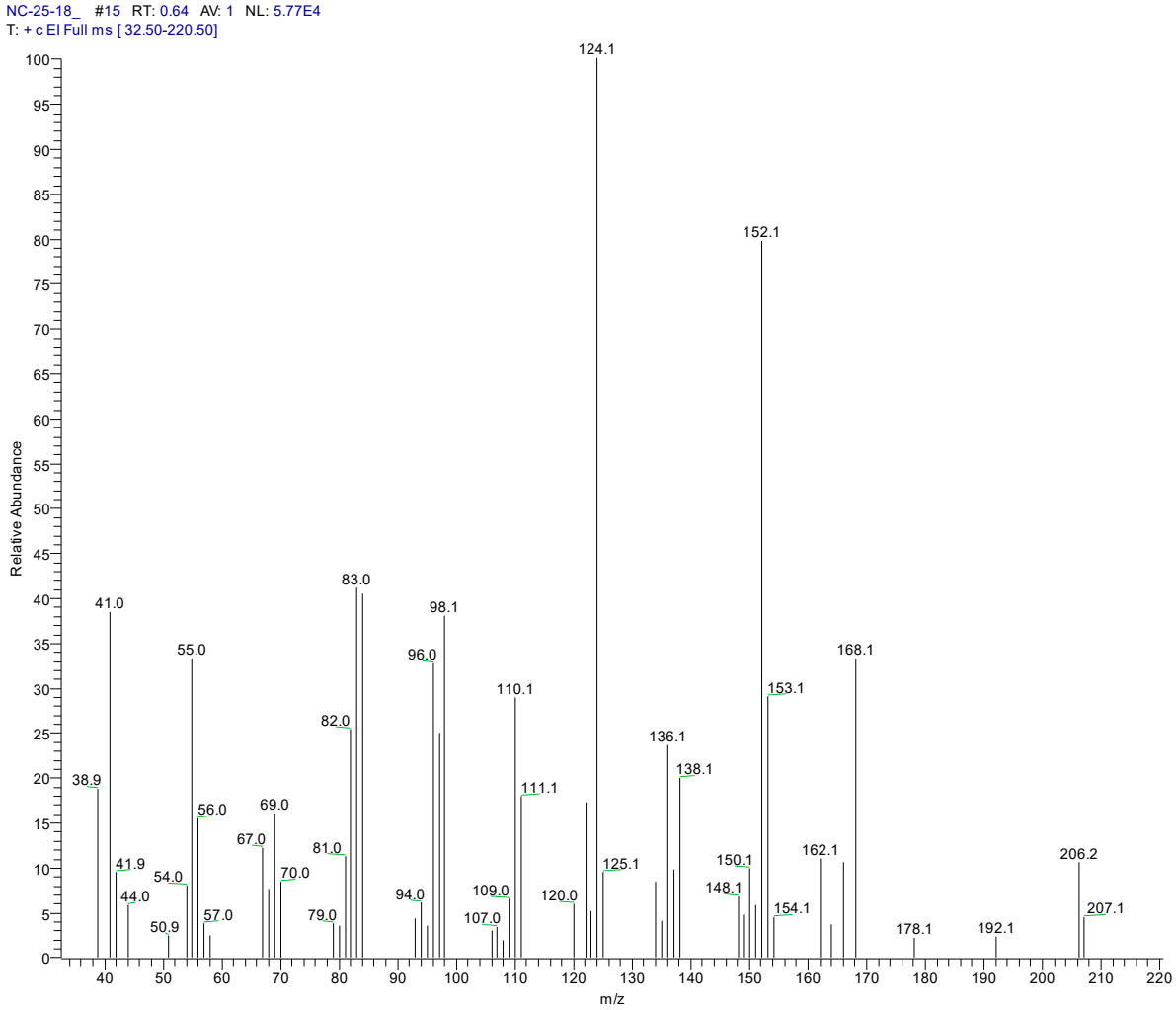
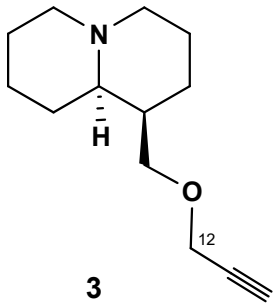


Figure S2. ^{13}C NMR spectrum of (1*R*,9a*R*)-1-((prop-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**3**) ($CDCl_3$, 125 MHz).

Figure S3. HR-MS spectrum of (1*R*,9a*R*)-1-((prop-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**3**)





3

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Tprobe=180˚C
Calculated: m/z= 206.1539
(C13 H20 O1 N1)$^{+\cdot}$
Found: m/z= 206.1538

1	**C13 H20 O1 N1**	
RDB	**(ppm)**	
4.5	**-0.684**	
Isotope	**min**	**max**
12 C	**10**	**16**
1 H	**15**	**30**
16 O	**0**	**3**
14 N	**0**	**3**

m/z	Intensity	Relative
38.9	10768.0	18.65
41.0	22124.0	38.32
41.9	5437.0	9.42
44.0	3358.0	5.82
54.0	4558.0	7.89
54.9	3465.0	6.00
55.0	19191.0	33.24

m/z	Intensity	Relative
56.0	8876.0	15.37
67.0	7037.0	12.19
68.0	4318.0	7.48
69.0	5784.0	10.02
69.0	9249.0	16.02
70.0	4824.0	8.36
81.0	5944.0	10.30
81.0	6450.0	11.17
82.0	14607.0	25.30
83.0	23750.0	41.14
84.1	23323.0	40.40
94.0	3491.0	6.05
96.0	18872.0	32.69
97.0	14367.0	24.88
98.0	9356.0	16.21
98.1	21910.0	37.95
109.0	3731.0	6.46
110.1	16633.0	28.81
111.1	10315.0	17.87
120.0	3385.0	5.86
122.1	9915.0	17.17
123.1	2958.0	5.12
124.1	57735.0	100.00
125.1	5464.0	9.46
134.1	4824.0	8.36
136.1	13647.0	23.64
137.1	5597.0	9.69
138.1	11488.0	19.90
148.1	3918.0	6.79
149.1	2692.0	4.66
150.1	5650.0	9.79
151.1	3305.0	5.72
152.1	45980.0	79.64
153.1	16766.0	29.04
162.1	6317.0	10.94
166.1	6077.0	10.53
168.1	19191.0	33.24
206.2	6077.0	10.53
207.1	2585.0	4.48

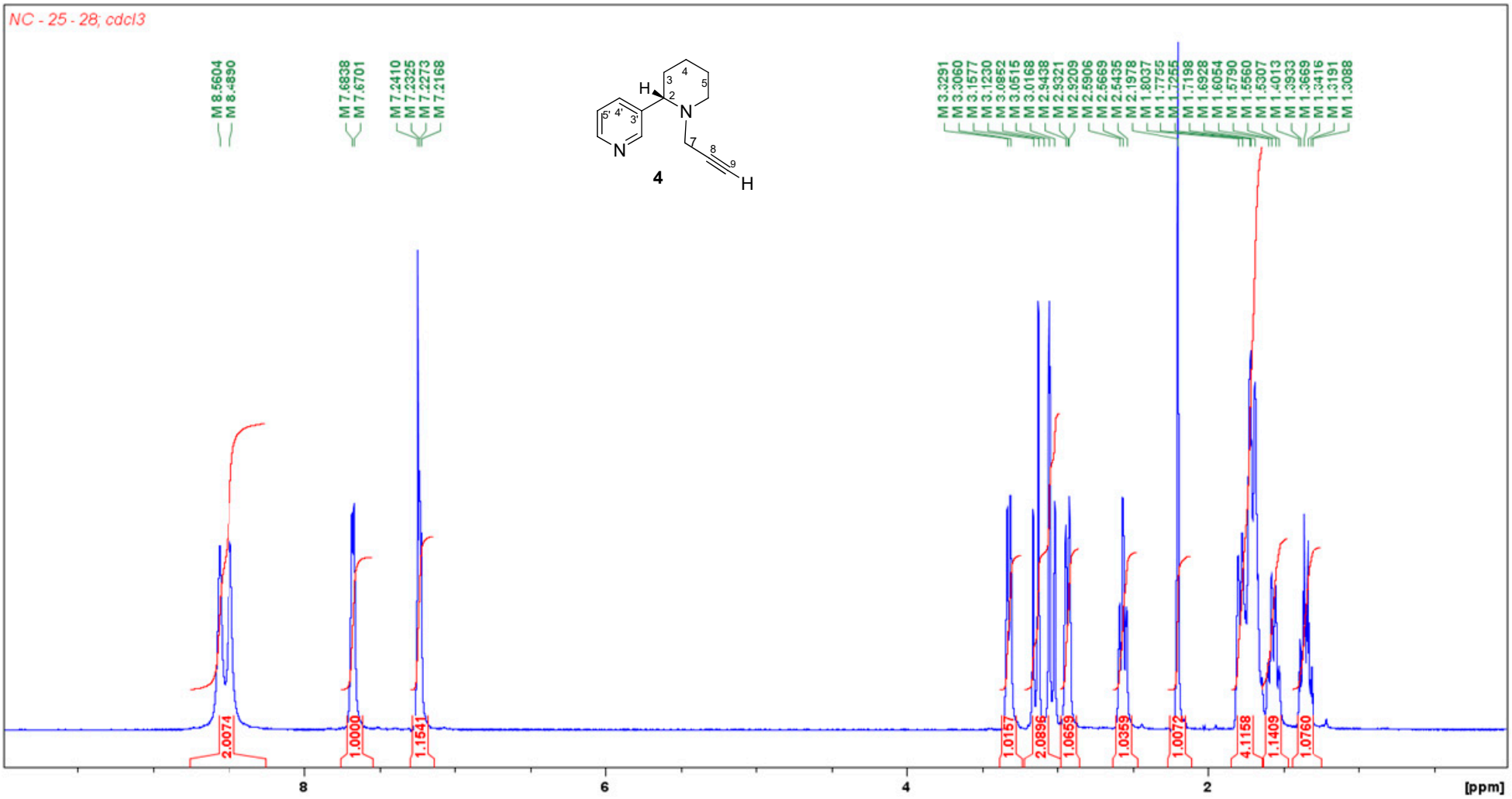


Figure S4. ^{1}H NMR spectrum of (*S*)-N-(prop-2-ynyl)anabasine (**4**) ($CDCl_3$, 400 MHz).

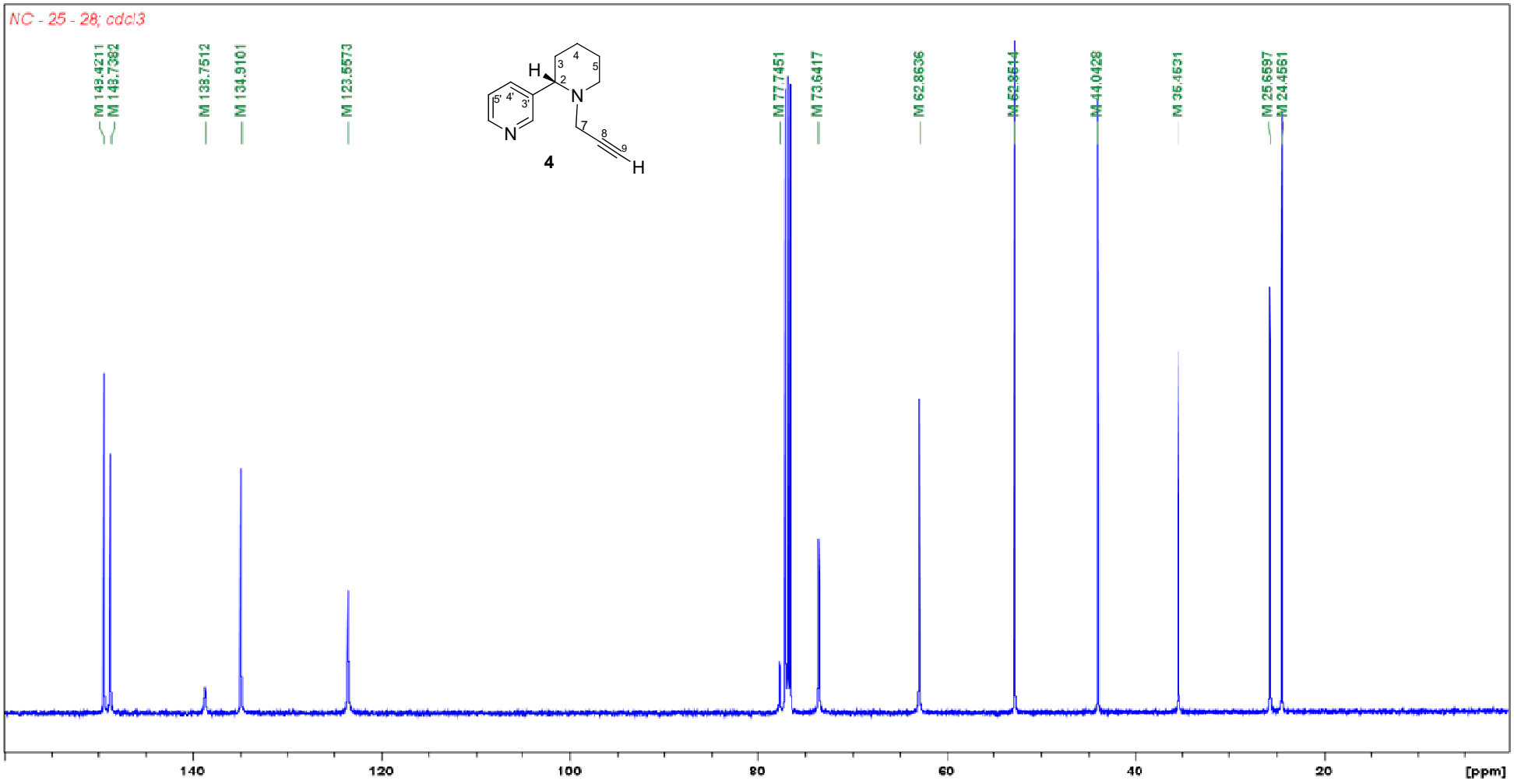
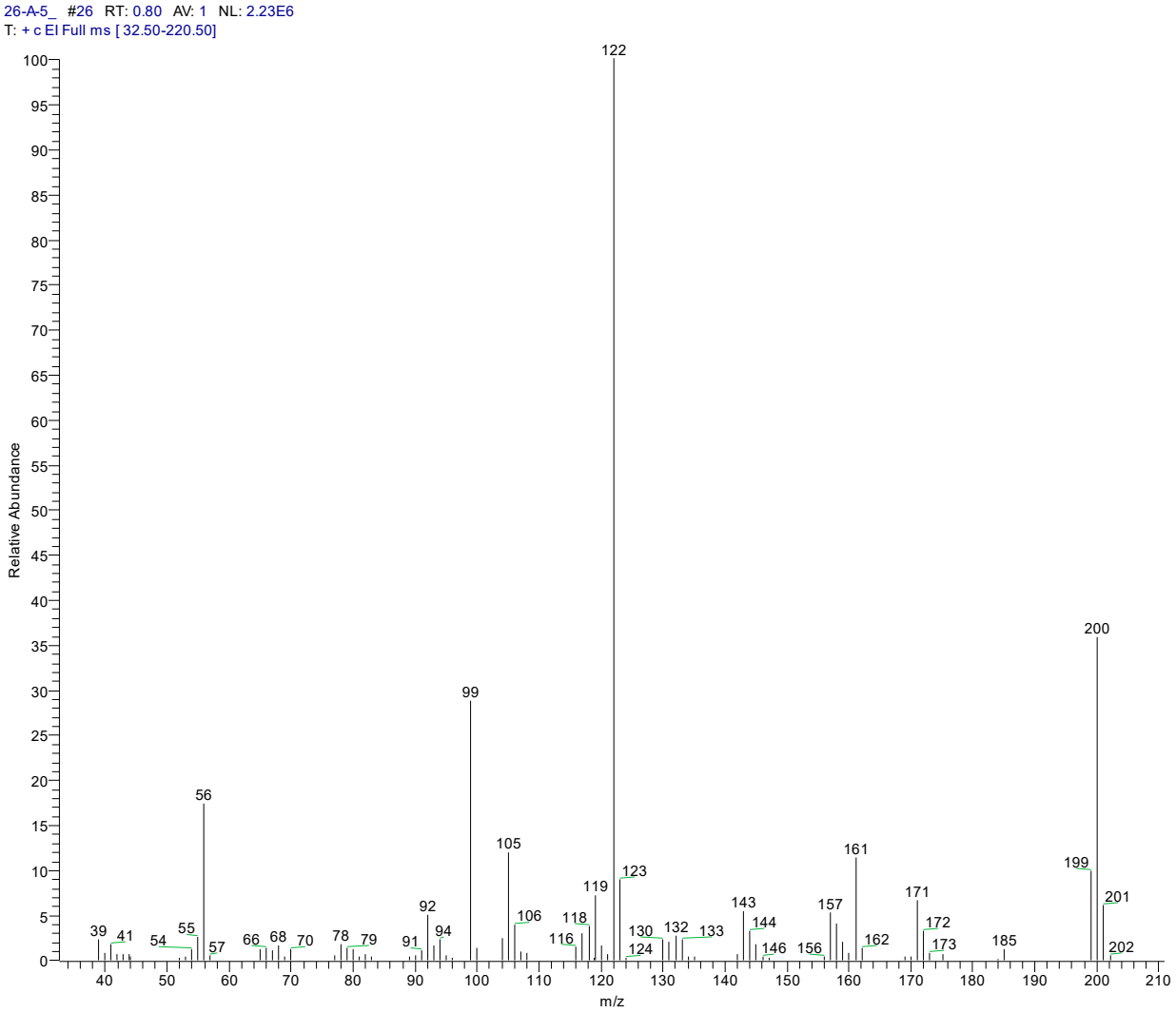
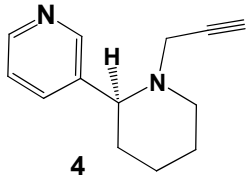


Figure S5. ^{13}C NMR spectrum of (*S*)-N-(prop-2-ynyl)anabasine (**4**) ($CDCl_3$, 101 MHz).

Figure S6. HR-MS spectrum of (*S*)-N-(prop-2-ynyl)anabasine (**4**)





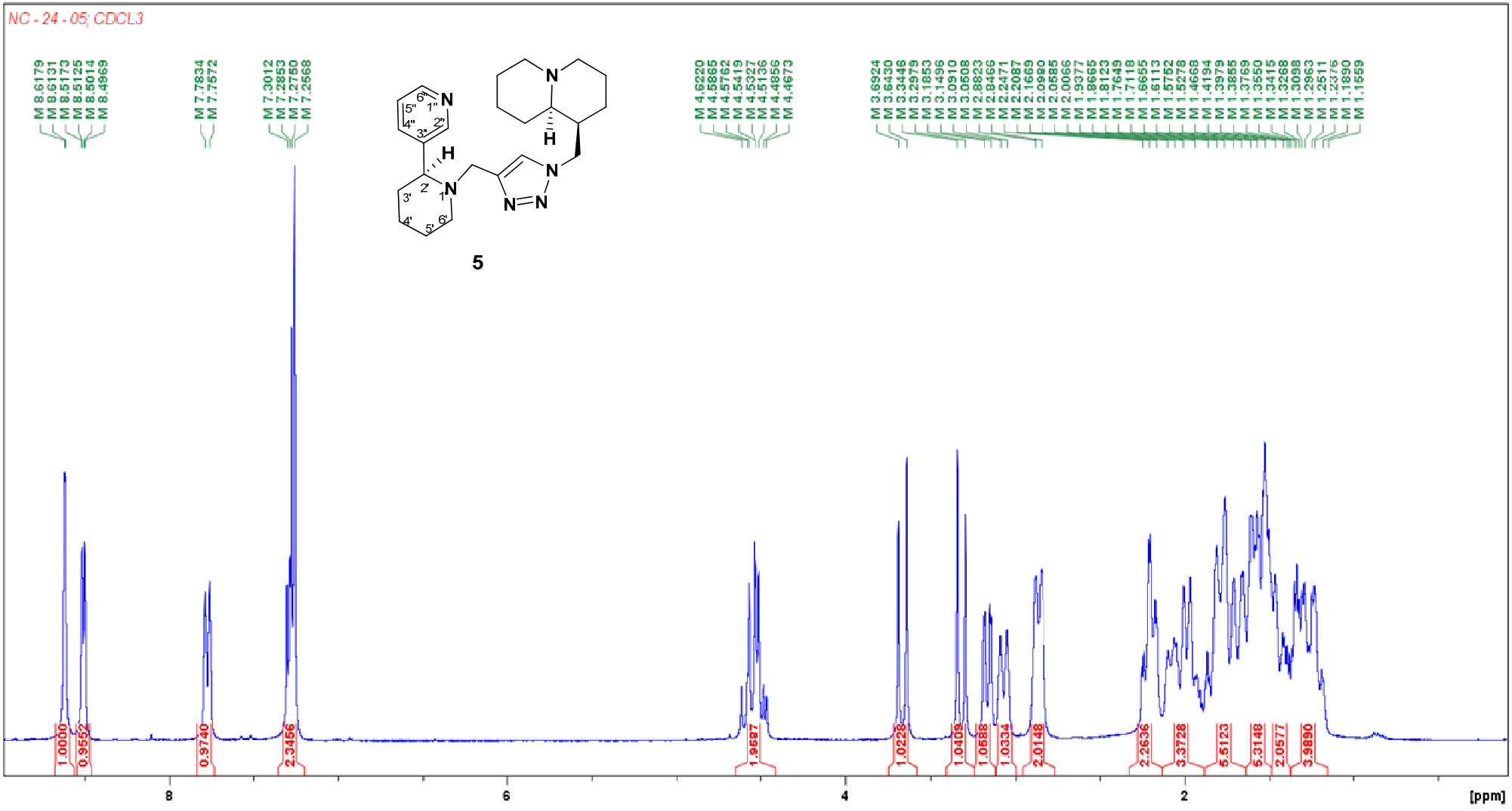
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$(C13\ H16\ N2)^{+\cdot}$
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Isotope	**min**	**max**
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1 H	10	25
14 N	0	4

m/z	Intensity	Relative
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55	54813.0	2.46
55	50717.0	2.27
56	385667.0	17.27
65	25877.0	1.16
66	30077.0	1.35
68	36248.0	1.62
70	26240.0	1.18
78	37545.0	1.68
79	29766.0	1.33
80	25514.0	1.14
92	110301.0	4.94
93	34018.0	1.52
94	50405.0	2.26
99	642468.0	28.78
100	29662.0	1.33
104	53361.0	2.39
105	264112.0	11.83
106	84995.0	3.81
116	30440.0	1.36
117	65600.0	2.94
118	84528.0	3.79
119	159929.0	7.16
120	34122.0	1.53
122	2232588.0	100.00
123	200016.0	8.96
130	50561.0	2.26
131	45271.0	2.03
132	58703.0	2.63
133	49472.0	2.22
143	119843.0	5.37
144	72238.0	3.24
145	36404.0	1.63
157	116472.0	5.22
158	88573.0	3.97
159	42990.0	1.93
161	253585.0	11.36
162	28158.0	1.26
171	148573.0	6.65
172	71045.0	3.18
185	26914.0	1.21
199	221381.0	9.92
200	800064.0	35.84
201	134726.0	6.03



5

Figure S7. ^{1}H NMR spectrum of (1*S*,9a*R*)-1-((4-(((*S*)-2-(pyridin-3-yl)piperidin-1-yl)methyl)-1H-1,2,3-triazol-1-yl)methyl)octahydro-1*H*-quinolizine (**5**) ($CDCl_3$, 400 MHz).

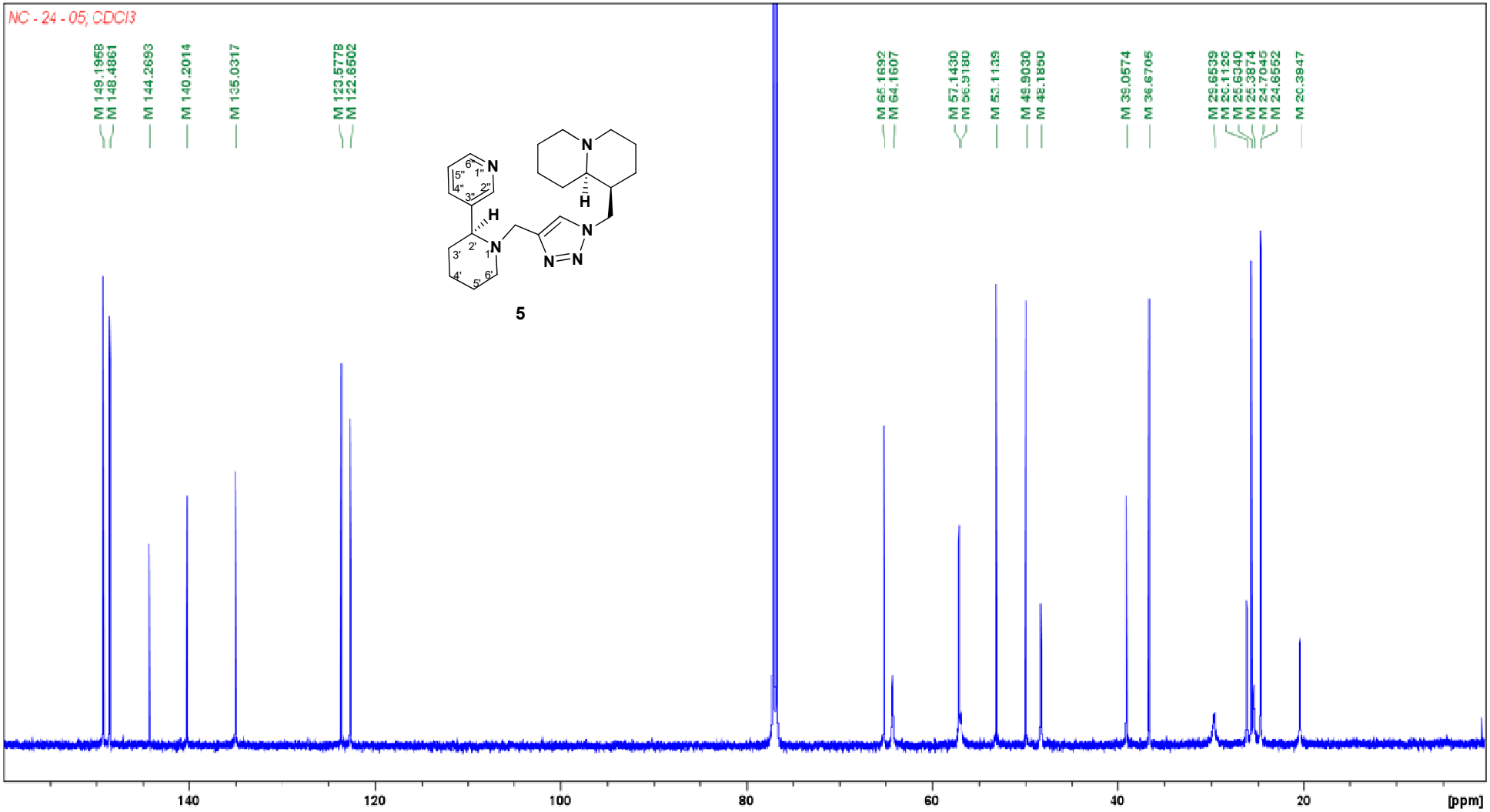
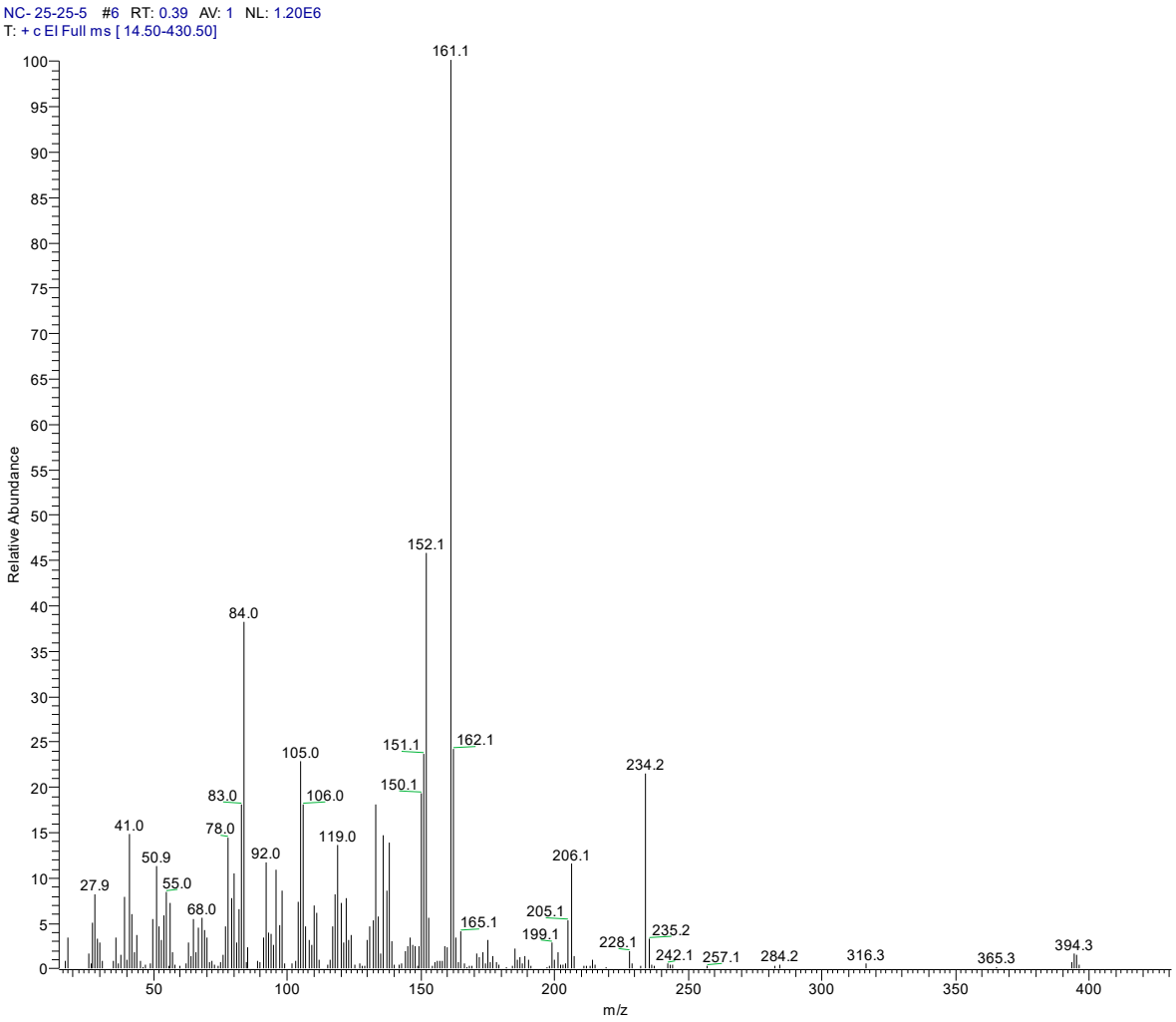
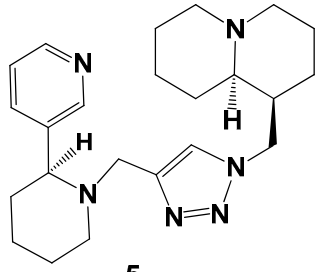


Figure S8. ^{13}C NMR spectrum of of (1*S*,9a*R*)-1-((4-(((*S*)-2-(pyridin-3-yl)piperidin-1-yl)methyl)-1H-1,2,3-triazol-1-yl)methyl)octahydro-1*H*-quinolizine (**5**) ($CDCl_3$), 125 MHz).

Figure S9. HR-MS spectrum of (1*S*,9a*R*)-1-((4-(((*S*)-2-(pyridin-3-yl)piperidin-1-yl)methyl)-1H-1,2,3-triazol-1-yl)methyl)octahydro-1*H*-quinolizine (**5**)





5

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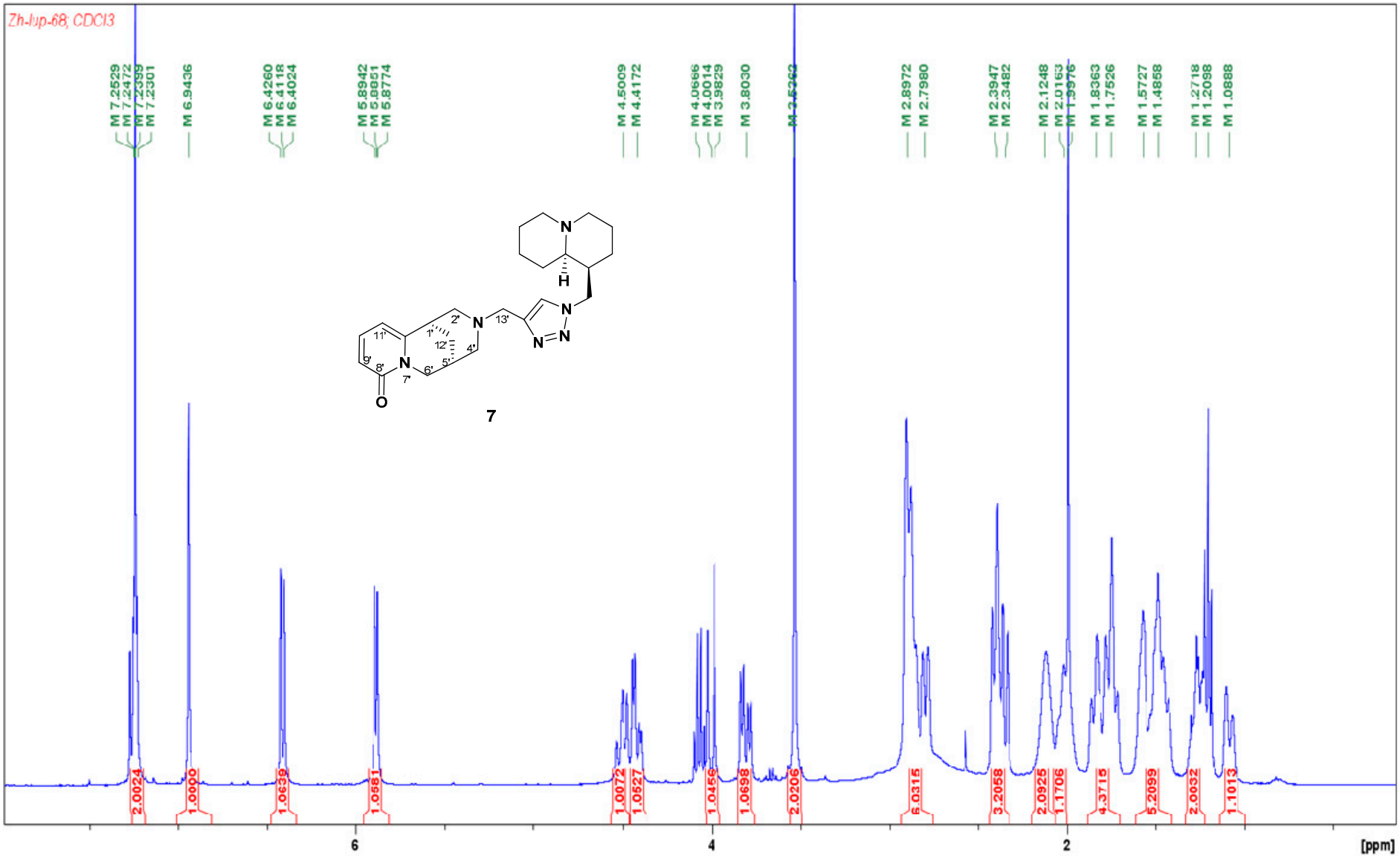
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Isotope	min	max
12 C	20	26
1 H	25	40
14 N	0	8

m/z	Intensity	Relative
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50.9	134194.0	11.20
78.0	171025.0	14.27
80.0	124430.0	10.38
83.0	215921.0	18.02
84.0	457521.0	38.17
92.0	139786.0	11.66
96.0	129837.0	10.83

m/z	Intensity	Relative
105.0	272992.0	22.78
106.0	215056.0	17.94
119.0	161972.0	13.51
133.0	215736.0	18.00
136.1	175011.0	14.60
137.1	102368.0	8.54
138.1	164475.0	13.72
150.1	230228.0	19.21
151.1	283034.0	23.61
152.1	547900.0	45.71
161.1	1198540.0	100.00
162.1	289708.0	24.17
171.0	19188.0	1.60
172.0	13842.0	1.15
173.1	20764.0	1.73
175.1	36368.0	3.03
177.1	15696.0	1.31
185.1	25429.0	2.12
186.1	11339.0	0.95
187.1	14306.0	1.19
189.1	15603.0	1.30
199.1	33648.0	2.81
200.1	11154.0	0.93
201.1	20022.0	1.67
205.1	62477.0	5.21
206.1	138180.0	11.53
207.2	16160.0	1.35
228.1	21660.0	1.81
234.2	257233.0	21.46
235.2	38005.0	3.17
257.1	1977.0	0.16
284.2	3862.0	0.32
316.3	5098.0	0.43
393.3	7106.0	0.59
394.3	19404.0	1.62
395.3	16747.0	1.40
396.3	4758.0	0.40



7

Figure S10. ^{1}H NMR spectrum of (1*R*,5*S*)-3-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl-1,2,3,4,5,6-hexahydro-8*H*-1,5-methanopyrido[1,2-*a*][1,5]diazocine-8 one (**7**) ($CDCl_3$, 400 MHz).

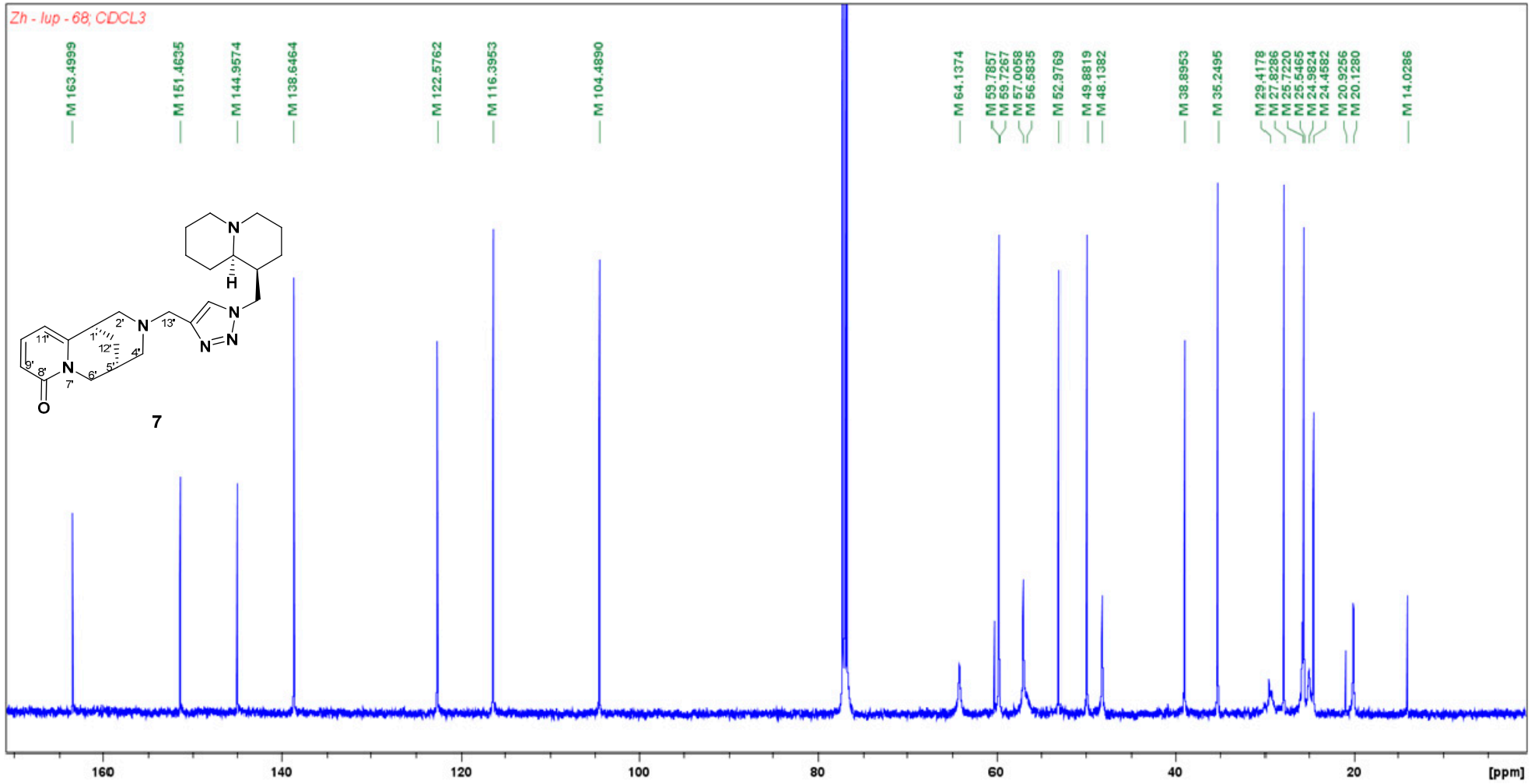
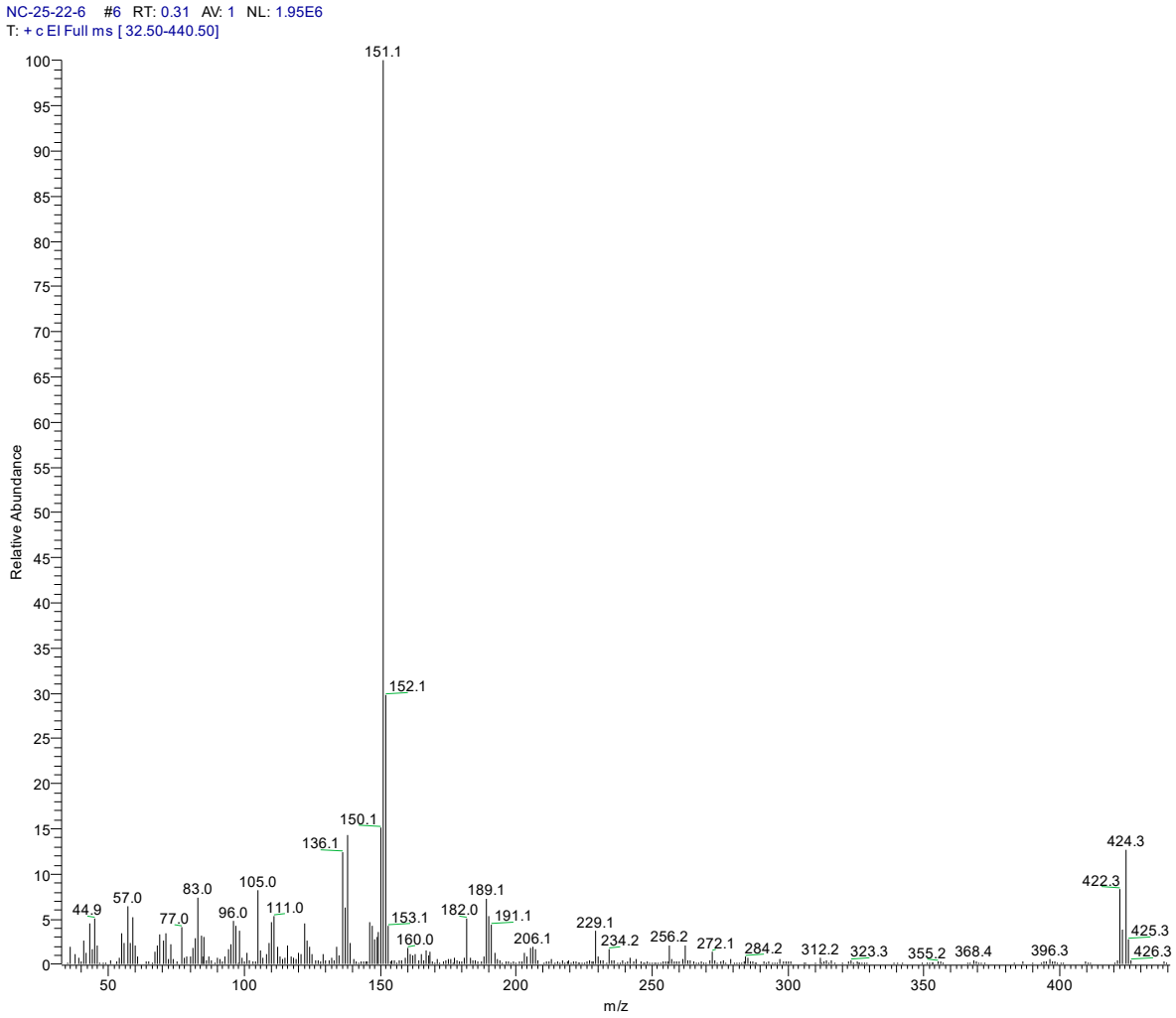
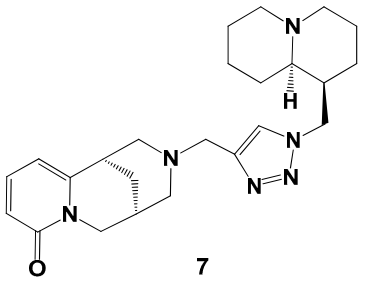


Figure S11. ^{13}C NMR spectrum of (1*R*,5*S*)-3-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl-1,2,3,4,5,6-hexahydro-8*H*-1,5-methanopyrido[1,2-*a*][1,5]diazocine-8 one (**7**) ($CDCl_3$, 125 MHz).

Figure S12. HR-MS spectrum of(1*R*,5*S*)-3-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl-1,2,3,4,5,6-hexahydro-8*H*-1,5-methanopyrido[1,2-*a*][1,5]diazocine-8 one (**7**).





7

Tsource=100˚C
Tprobe=280˚C

Calculated: m/z= 422.2789
(C24 H34 O1 N6) $^{+\cdot}$
Found: m/z= 422.2790

1 C24 H34 O1 N6

RDB	(ppm)
11.0	0.328

Isotope	min	max
12 C	18	28
1 H	30	45
16 O	0	3
14 N	0	8

m/z	Intensity	Relative
42.9	86021.0	4.42
44.9	95422.0	4.90
57.0	124176.0	6.37
59.0	99589.0	5.11

m/z	Intensity	Relative
83.0	142668.0	7.32
96.0	92598.0	4.75
97.0	80580.0	4.14
105.0	158543.0	8.14
110.0	88603.0	4.55
111.0	102963.0	5.29
122.0	84781.0	4.35
136.1	239502.0	12.29
137.1	119837.0	6.15
138.1	277037.0	14.22
146.0	87811.0	4.51
147.0	80959.0	4.16
150.1	292120.0	15.00
151.1	1948081.0	100.00
152.1	577113.0	29.62
153.1	80545.0	4.13
160.0	34057.0	1.75
167.0	26756.0	1.37
168.1	24897.0	1.28
182.0	97453.0	5.00
189.1	137813.0	7.07
190.1	102412.0	5.26
191.1	83094.0	4.27
192.1	23278.0	1.19
205.1	33230.0	1.71
206.1	36846.0	1.89
207.1	30303.0	1.56
229.1	71041.0	3.65
234.2	30097.0	1.54
256.2	39635.0	2.03
262.1	37122.0	1.91
272.1	25448.0	1.31
422.3	160437.0	8.24
423.3	73555.0	3.78
424.3	244461.0	12.55
425.3	52824.0	2.71

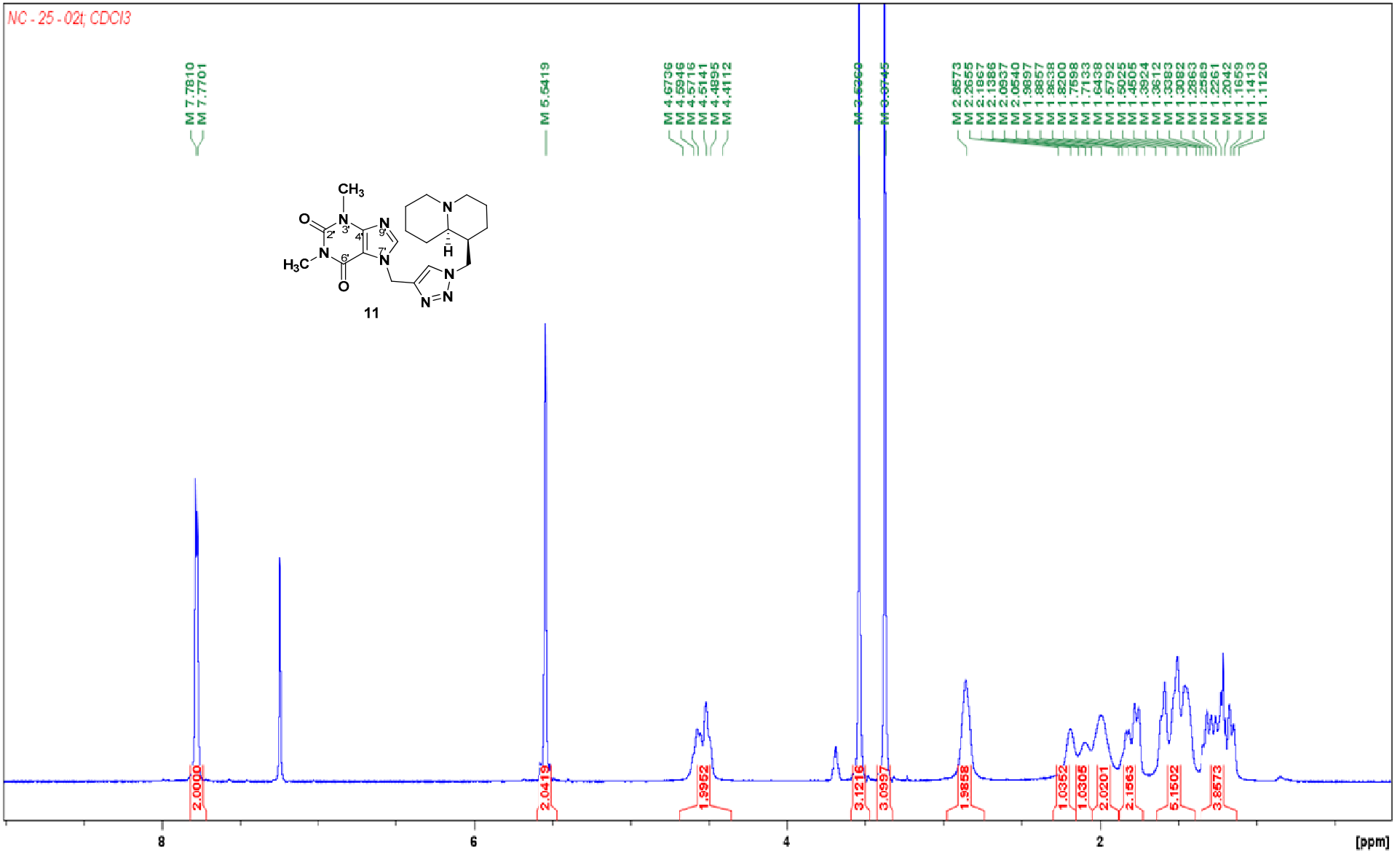


Figure S13. ^{1}H NMR spectrum of 1,3-dimethyl-7-((1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl) methyl)-1*H*-purine-2,6(3*H*,7*H*)-dione (**11**) ($CDCl_3$, 500 MHz).

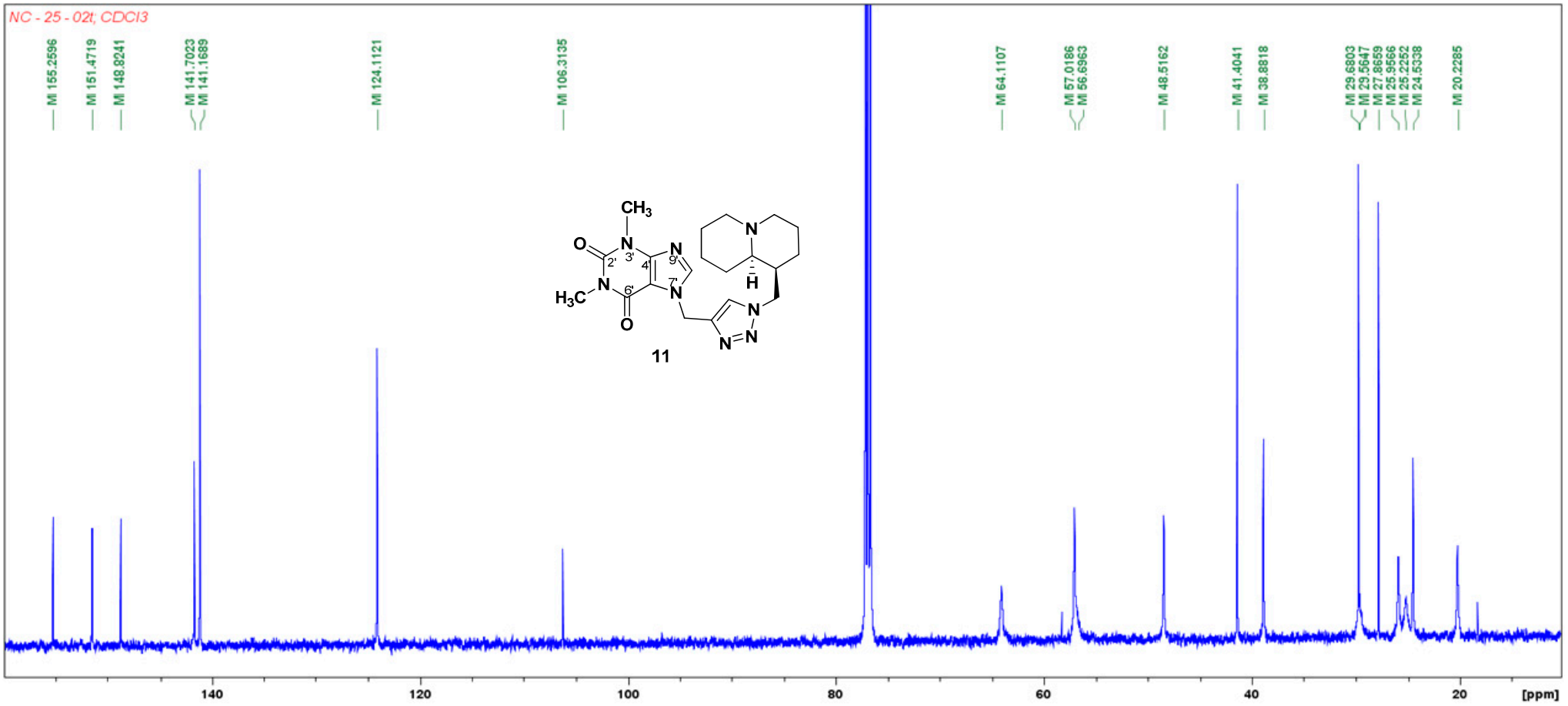
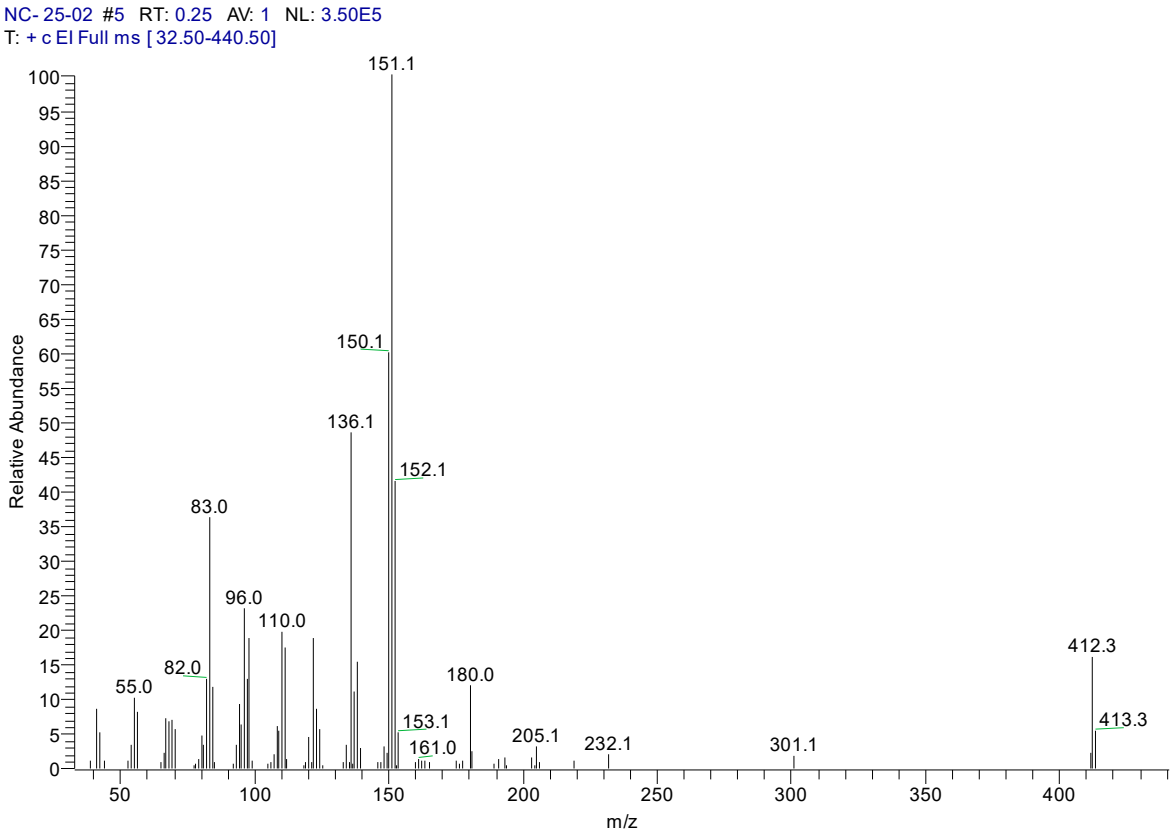
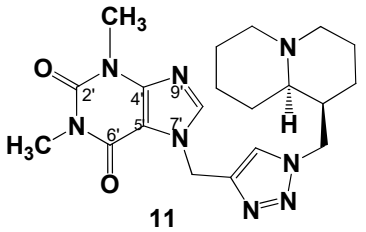


Figure S14. ^{13}C NMR spectrum of 1,3-dimethyl-7-((1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl) methyl)-1*H*-purine-2,6(3*H*,7*H*)-dione (**11** ($CDCl_3$, 125 MHz).

Figure S15. HR-MS spectrum of 1,3-dimethyl-7-((1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl) methyl)-1*H*-purine-2,6(3*H*,7*H*)-dione (**11**)





11

Tsource=110˚C
Tprobe=300˚C

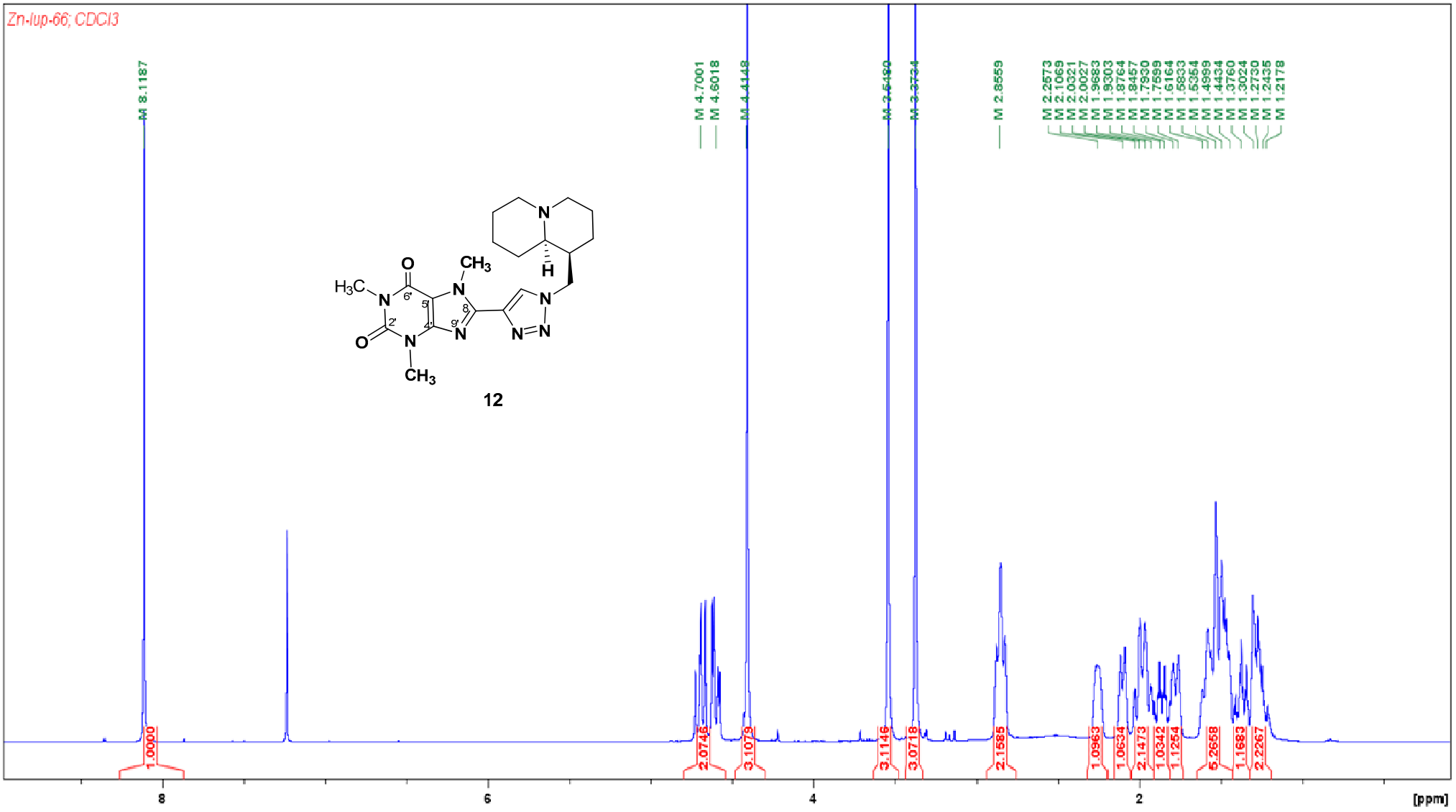
Calculated: m/z= 412.2330
$(C20\ H28\ O2\ N8)^{+\cdot}$
Found: m/z= 412.2334

1	C20 H28 O2 N8	
RDB		(ppm)
11.0		1.033

Isotope	min	max
12 C	15	25
1 H	20	35
16 O	0	4
14 N	0	10

m/z	Intensity	Relative
40.9	30044.0	8.59
55.0	35580.0	10.17
56.0	27960.0	7.99
82.0	44818.0	12.81

m/z	Intensity	Relative
83.0	126524.0	36.17
84.0	40775.0	11.66
94.0	32470.0	9.28
96.0	80865.0	23.12
97.0	45129.0	12.90
98.0	65190.0	18.64
110.0	68798.0	19.67
111.1	60929.0	17.42
122.0	65221.0	18.64
123.1	29391.0	8.40
136.1	169351.0	48.41
137.1	38629.0	11.04
138.1	53682.0	15.35
150.1	210095.0	60.06
151.1	349807.0	100.00
152.1	144936.0	41.43
163.1	3390.0	0.97
165.1	2736.0	0.78
175.0	3856.0	1.10
175.1	3918.0	1.12
176.1	1803.0	0.52
177.1	3483.0	1.00
180.0	41614.0	11.90
181.0	8273.0	2.37
189.0	1803.0	0.52
191.1	4261.0	1.22
193.0	4914.0	1.40
194.0	1586.0	0.45
203.1	5100.0	1.46
205.1	10885.0	3.11
206.1	2892.0	0.83
219.1	3856.0	1.10
232.1	6593.0	1.88
301.1	6002.0	1.72
411.3	7868.0	2.25
412.3	56108.0	16.04
413.3	18754.0	5.36



12

Figure S16. ^{1}H NMR spectrum of 1,3,7-trimethyl-8-(1-((((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)-1*H*-purine-2,6(3H,7*H*)-dione (**12**) ($CDCl_3$, 400 MHz).

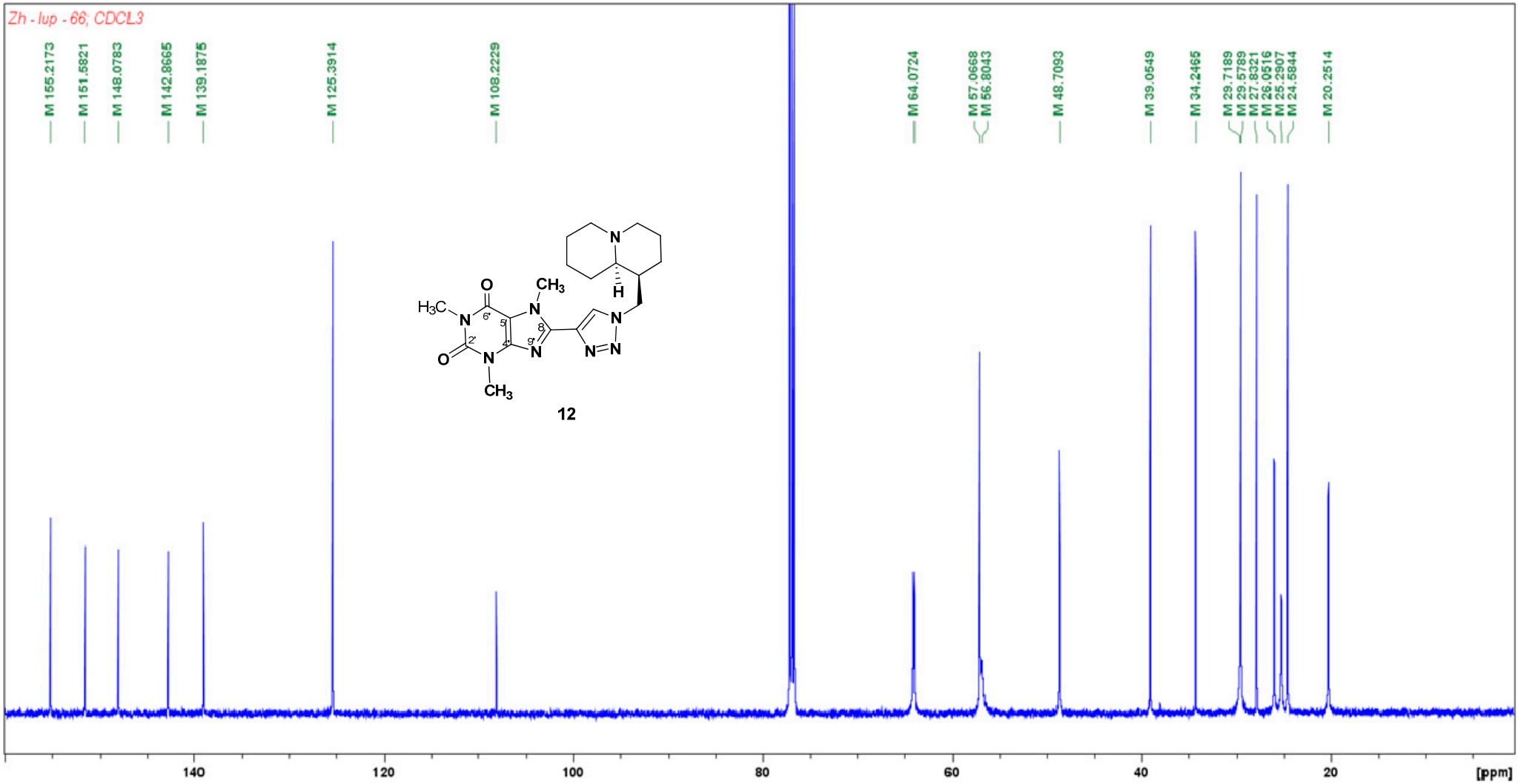
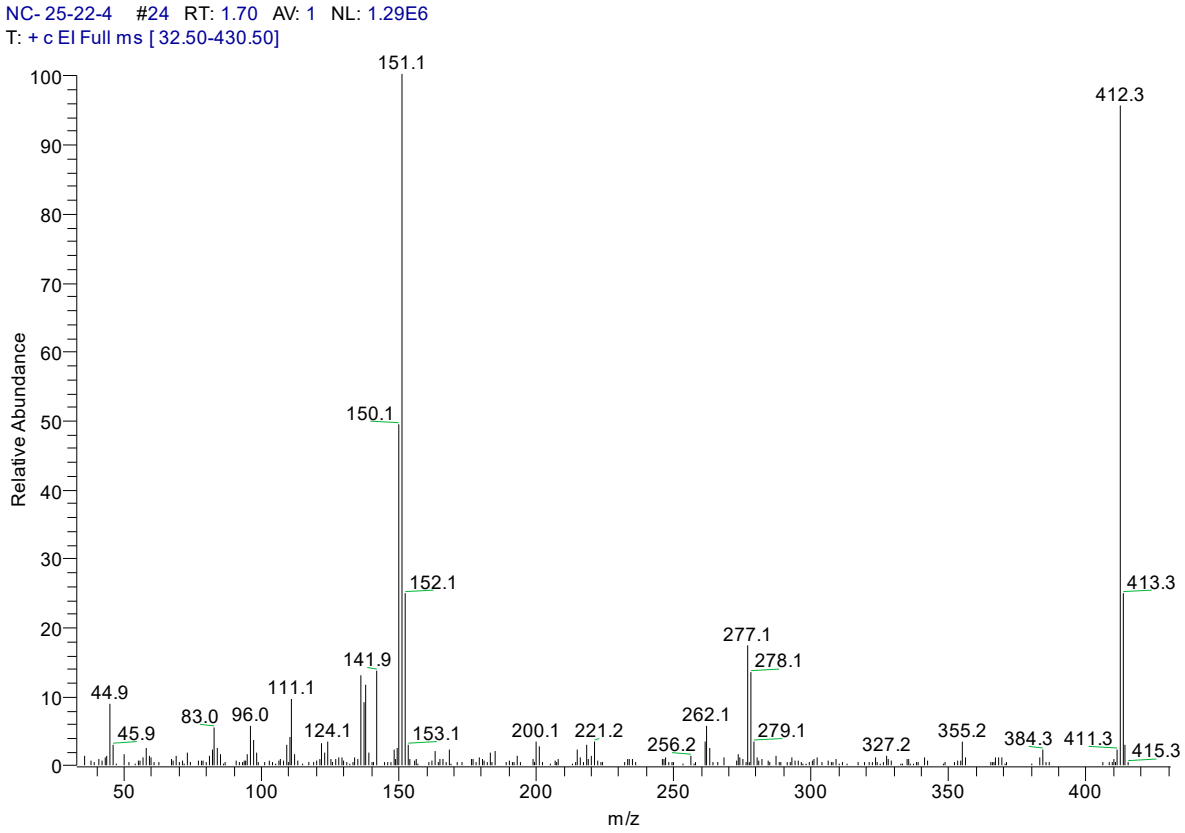
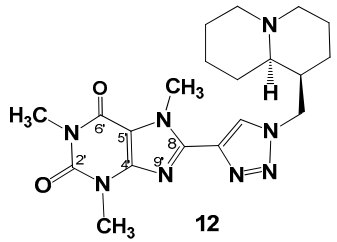


Figure S17. ^{13}C NMR spectrum of 1,3,7-trimethyl-8-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)-1*H*-purine-2,6(3H,7*H*)-dione (**12**) ($CDCl_3$, 125 MHz).

Figure S18. HR-MS spectrum of 1,3,7-trimethyl-8-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)-1*H*-purine-2,6-dione (**12**)





Tsource=100˚C
Tprobe=270˚C
Calculated: m/z= 412.2330
(C20 H28 O2 N8) $^{+\cdot}$
Found: m/z= 412.2329

1	**C20 H28 O2 N8**	
RDB	**(ppm)**	
11.0	**-0.179**	

Isotope	**min**	**max**
12 C	**15**	**25**
1 H	**22**	**35**
16 O	**0**	**4**
14 N	**0**	**10**

m/z	**Intensity**	**Relative**
44.9	**114280.0**	**8.83**
45.9	**37482.0**	**2.89**
58.0	**31328.0**	**2.42**
83.0	**68417.0**	**5.28**
84.0	**31917.0**	**2.47**
96.0	**72837.0**	**5.63**
97.0	**46092.0**	**3.56**
109.0	**35583.0**	**2.75**
110.0	**53261.0**	**4.11**

m/z	**Intensity**	**Relative**
111.1	**121711.0**	**9.40**
122.0	**39250.0**	**3.03**
124.1	**44193.0**	**3.41**
136.1	**168589.0**	**13.02**
137.1	**117750.0**	**9.09**
138.1	**149439.0**	**11.54**
141.9	**176085.0**	**13.60**
150.1	**639396.0**	**49.38**
151.1	**1294799.0**	**100.00**
152.1	**320811.0**	**24.78**
153.1	**36434.0**	**2.81**
200.1	**43113.0**	**3.33**
201.0	**33619.0**	**2.60**
218.1	**37220.0**	**2.87**
221.2	**41967.0**	**3.24**
261.1	**43244.0**	**3.34**
262.1	**72084.0**	**5.57**
263.1	**31262.0**	**2.41**
277.1	**224535.0**	**17.34**
278.1	**173598.0**	**13.41**
279.1	**43964.0**	**3.40**
287.1	**15254.0**	**1.18**
302.2	**13912.0**	**1.07**
327.2	**17415.0**	**1.34**
341.2	**13879.0**	**1.07**
355.1	**12963.0**	**1.00**
355.2	**41509.0**	**3.21**
356.3	**13061.0**	**1.01**
367.2	**14076.0**	**1.09**
368.2	**13356.0**	**1.03**
383.3	**14371.0**	**1.11**
384.3	**27432.0**	**2.12**
411.3	**29200.0**	**2.26**
412.3	**1236890.0**	**95.53**
413.3	**321531.0**	**24.83**
414.3	**38399.0**	**2.97**

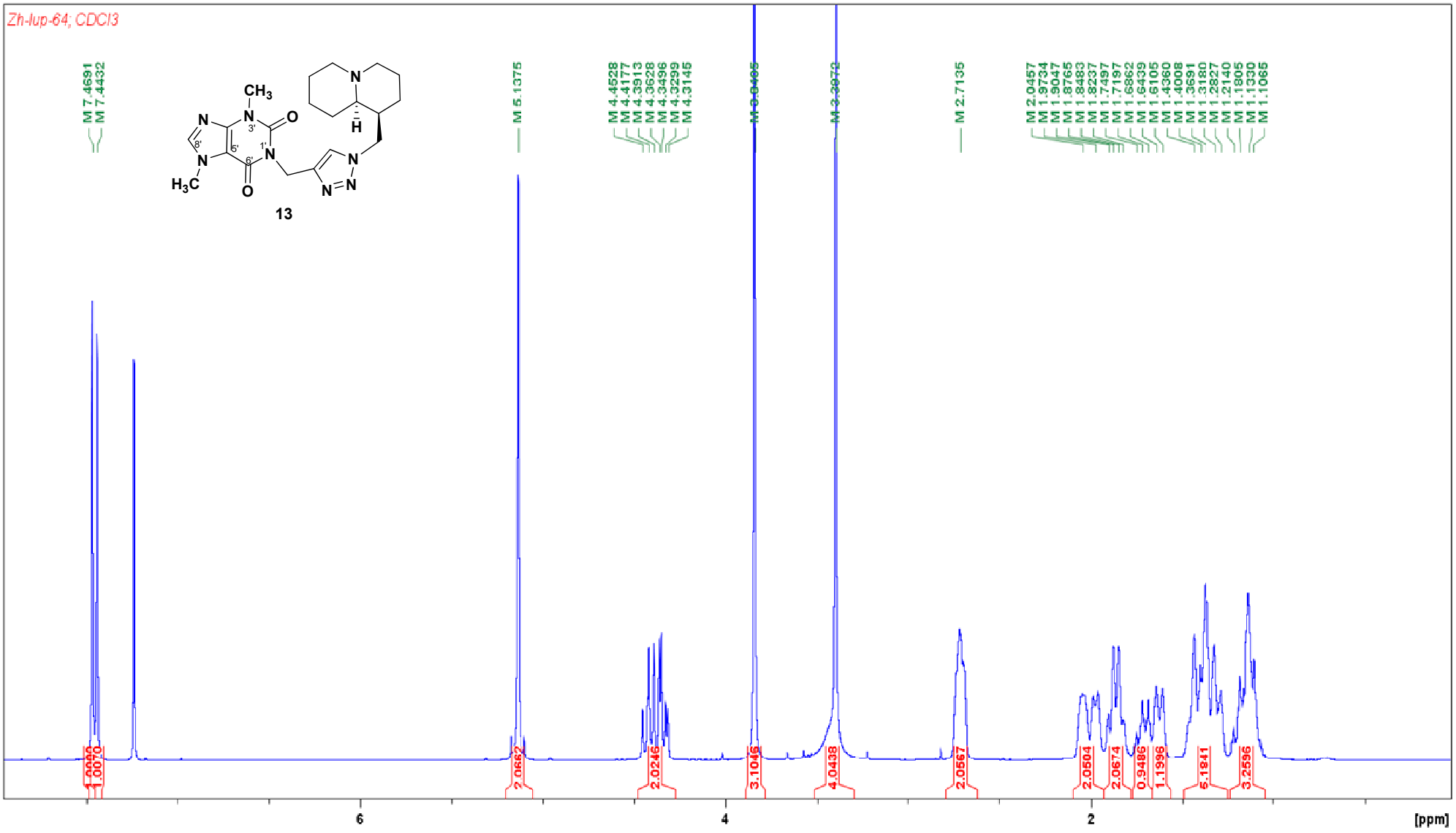


Figure S19. ^{1}H NMR spectrum of 3,7-dimethyl-1-((1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-purine-2,6(3*H*,7*H*)-dione (**13**) ($CDCl_3$, 400 MHz).

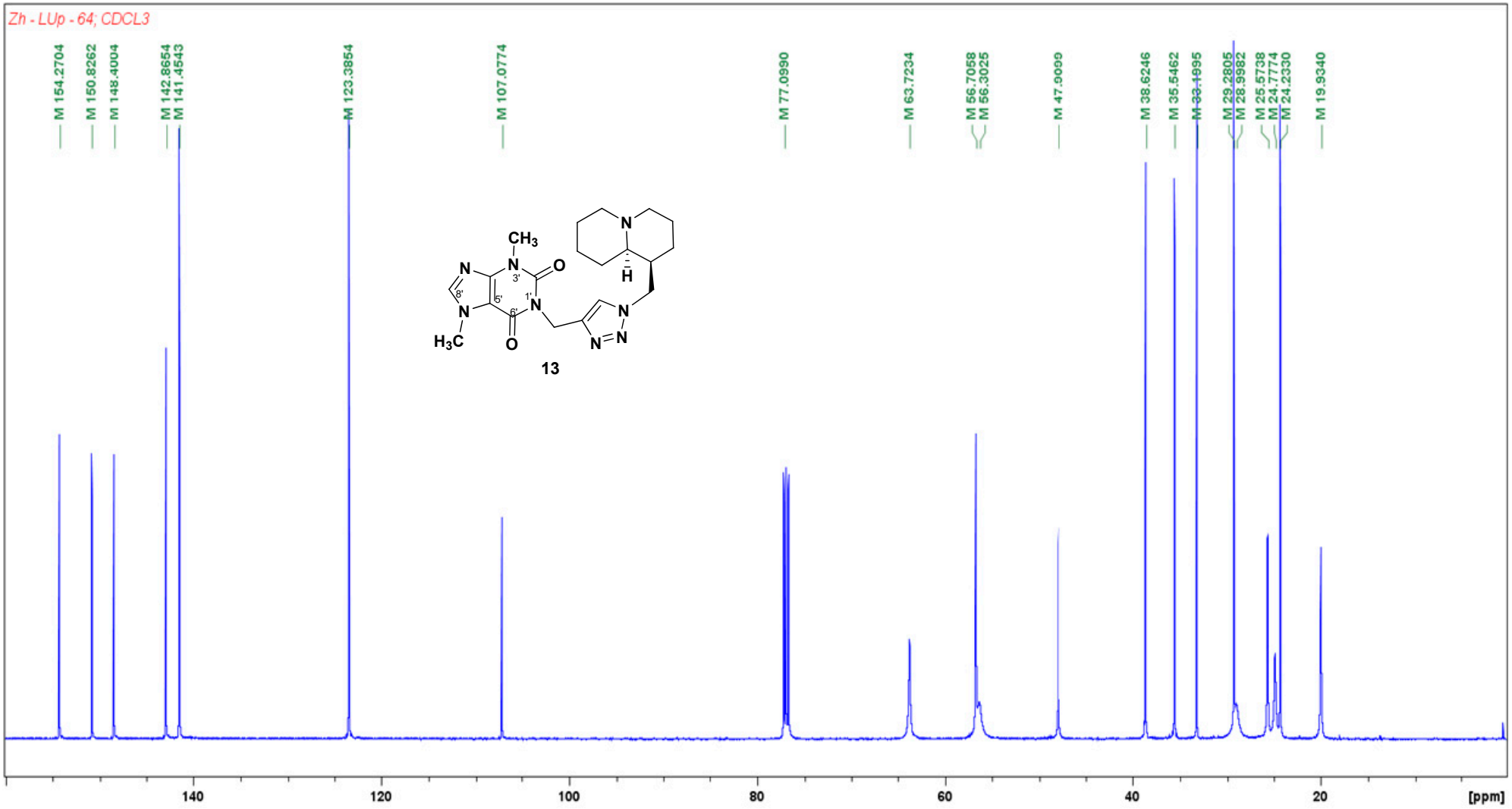
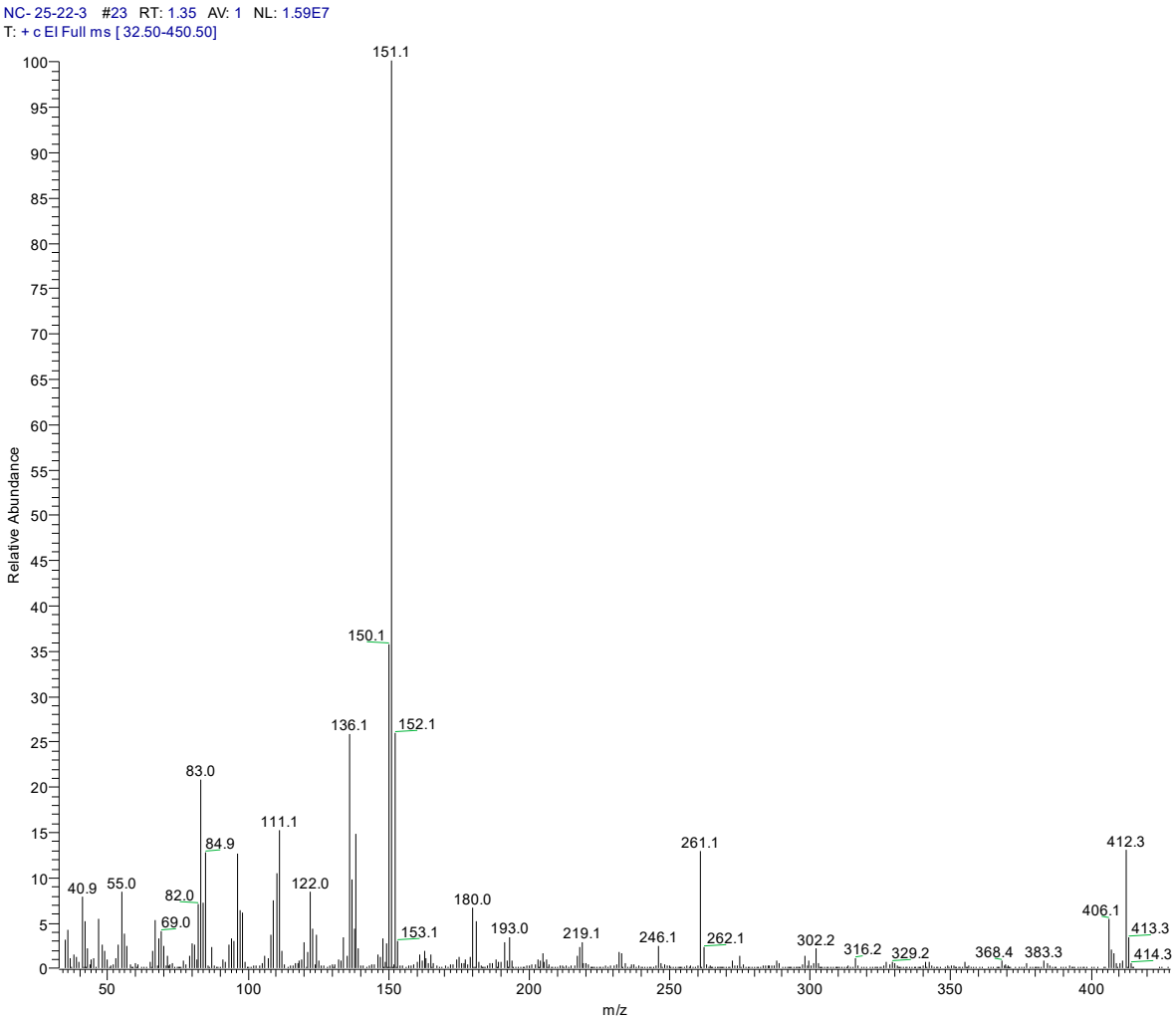
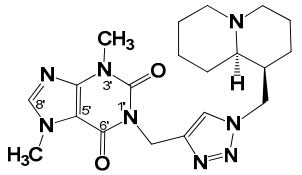


Figure S20. ^{13}C NMR spectrum of 3,7-dimethyl-1-((1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-purine-2,6(3*H*,7*H*)-dione (**13**) ($CDCl_3$, 125 MHz).

Figure S21. HR-MS spectrum of 3,7-dimethyl-1-((1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-purine-2,6(3*H*,7*H*)-dione (**13**) .





13

Tsource=110˚C
Tprobe=270˚C
Calculated: m/z=412.2330
(C20 H28 O2 N8) $^{+\cdot}$
Found: m/z= 412.2326
1 C20 H28 O2 N8

RDB	(ppm)
11.0	-0.907

Isotope	min	max
12 C	16	25
1 H	20	35
16 O	0	4
14 N	0	10

m/z	Intensity	Relative
40.9	1238564.0	7.81
55.0	1329211.0	8.38
82.0	1118255.0	7.05
82.9	2995528.0	18.88
83.0	3291690.0	20.74
84.0	1136298.0	7.16

m/z	Intensity	Relative
84.9	2020297.0	12.73
96.0	1996506.0	12.58
97.0	1005015.0	6.33
98.0	951162.0	5.99
109.0	1169741.0	7.37
110.0	1639205.0	10.33
111.1	2405170.0	15.16
122.0	1328381.0	8.37
136.1	4085842.0	25.75
137.1	1544778.0	9.74
138.1	2334165.0	14.71
150.1	5667045.0	35.71
151.1	15868160.0	100.00
152.1	4108373.0	25.89
161.1	218487.0	1.38
163.0	294902.0	1.86
180.0	1044760.0	6.58
181.0	810719.0	5.11
191.1	437834.0	2.76
193.0	534014.0	3.37
205.0	244737.0	1.54
218.1	353120.0	2.23
219.1	440877.0	2.78
232.1	267299.0	1.68
233.1	255157.0	1.61
246.1	370948.0	2.34
261.1	2042675.0	12.87
262.1	357423.0	2.25
302.2	344236.0	2.17
406.1	861314.0	5.43
407.1	316941.0	2.00
408.1	245321.0	1.55
412.3	2058228.0	12.97
413.3	538287.0	3.39

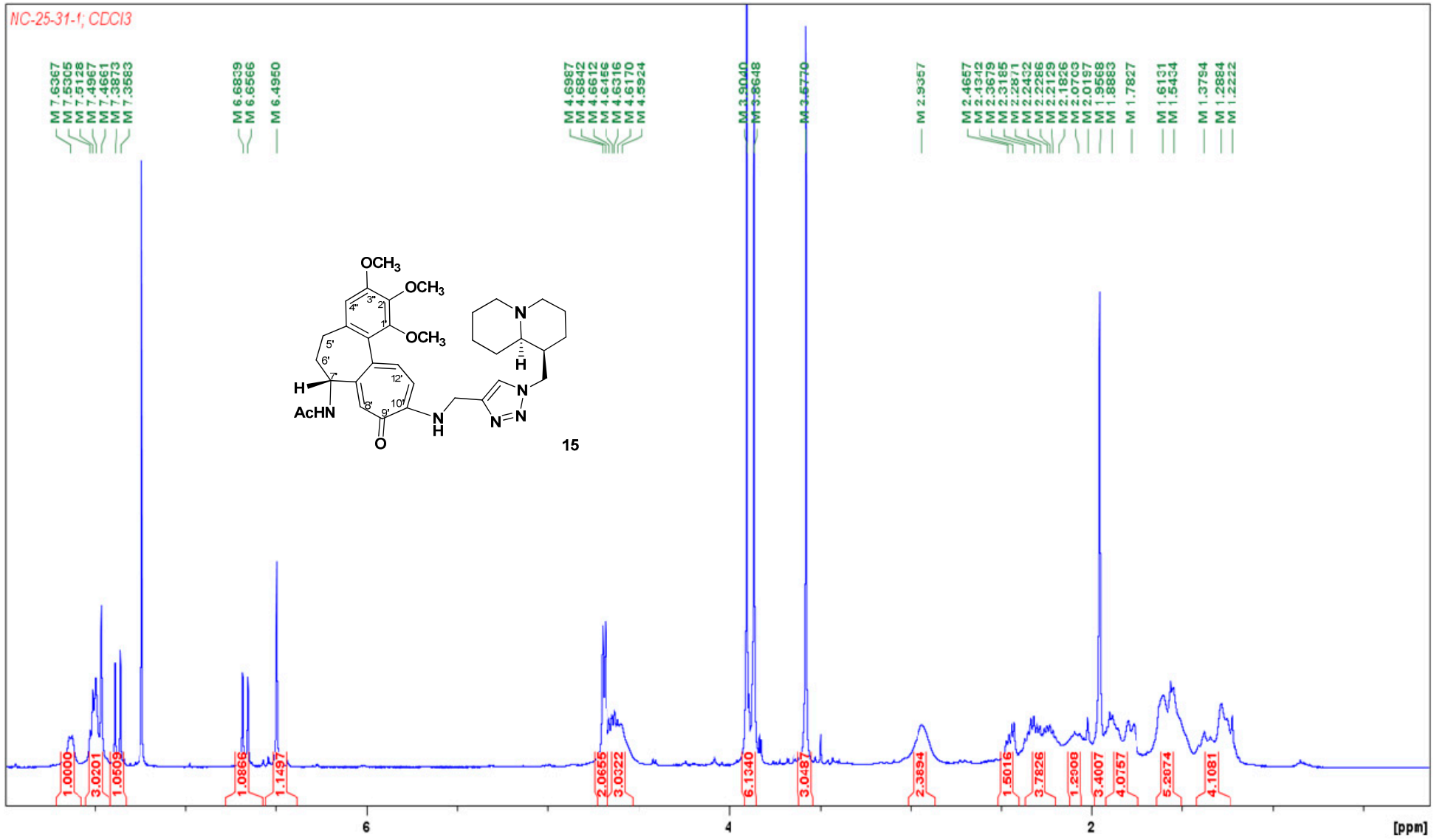


Figure S22. ^{1}H NMR spectrum of 1*R*,5*S*)-10-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methylamino-N-[(7*S*)-acetylamino-1,2,3,-trimethoxy-6,7-dihydro-5*H*-benzo[*a*]heptalen-9-one (**15**) ($CDCl_3$, 400 MHz).

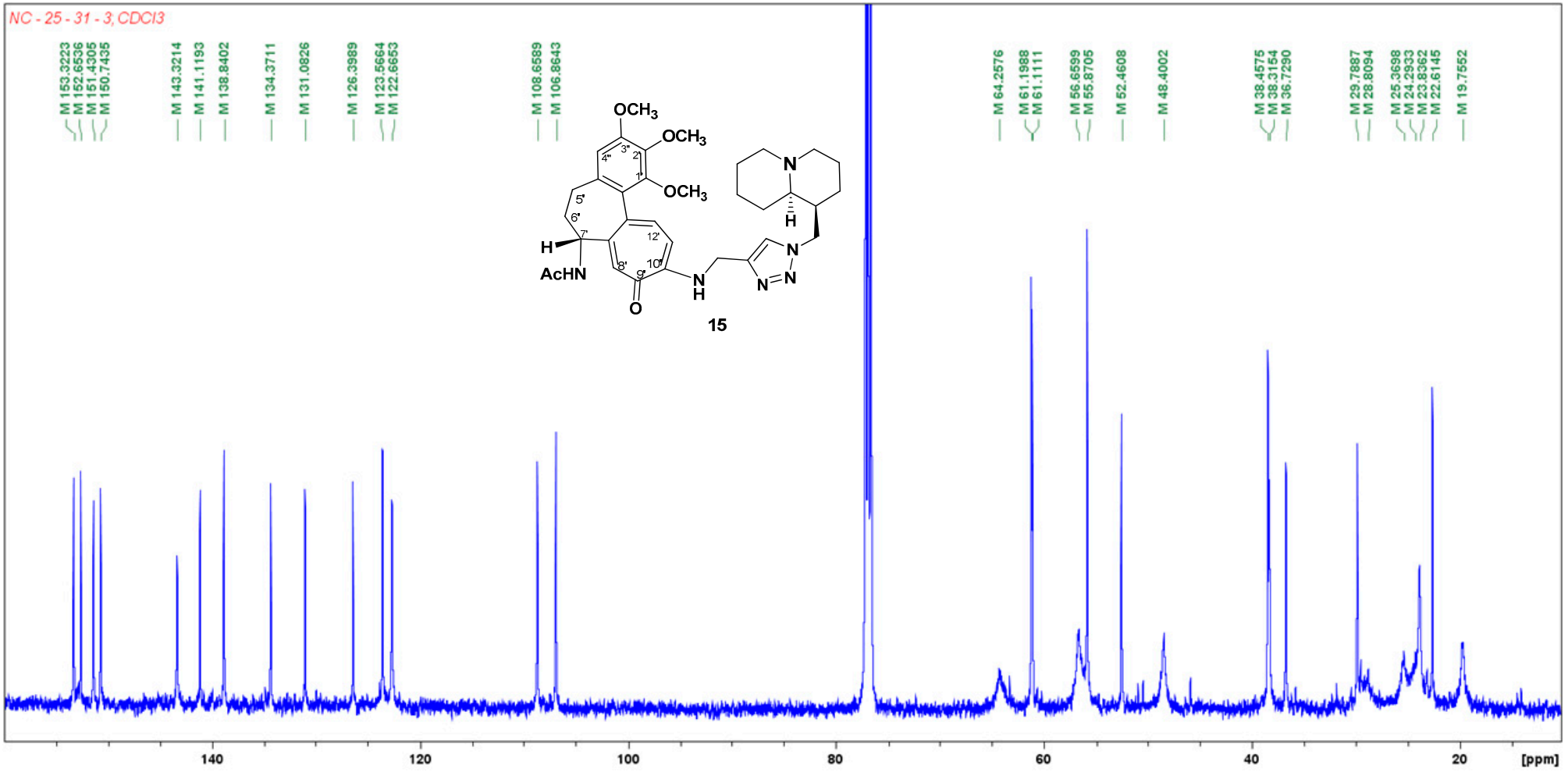
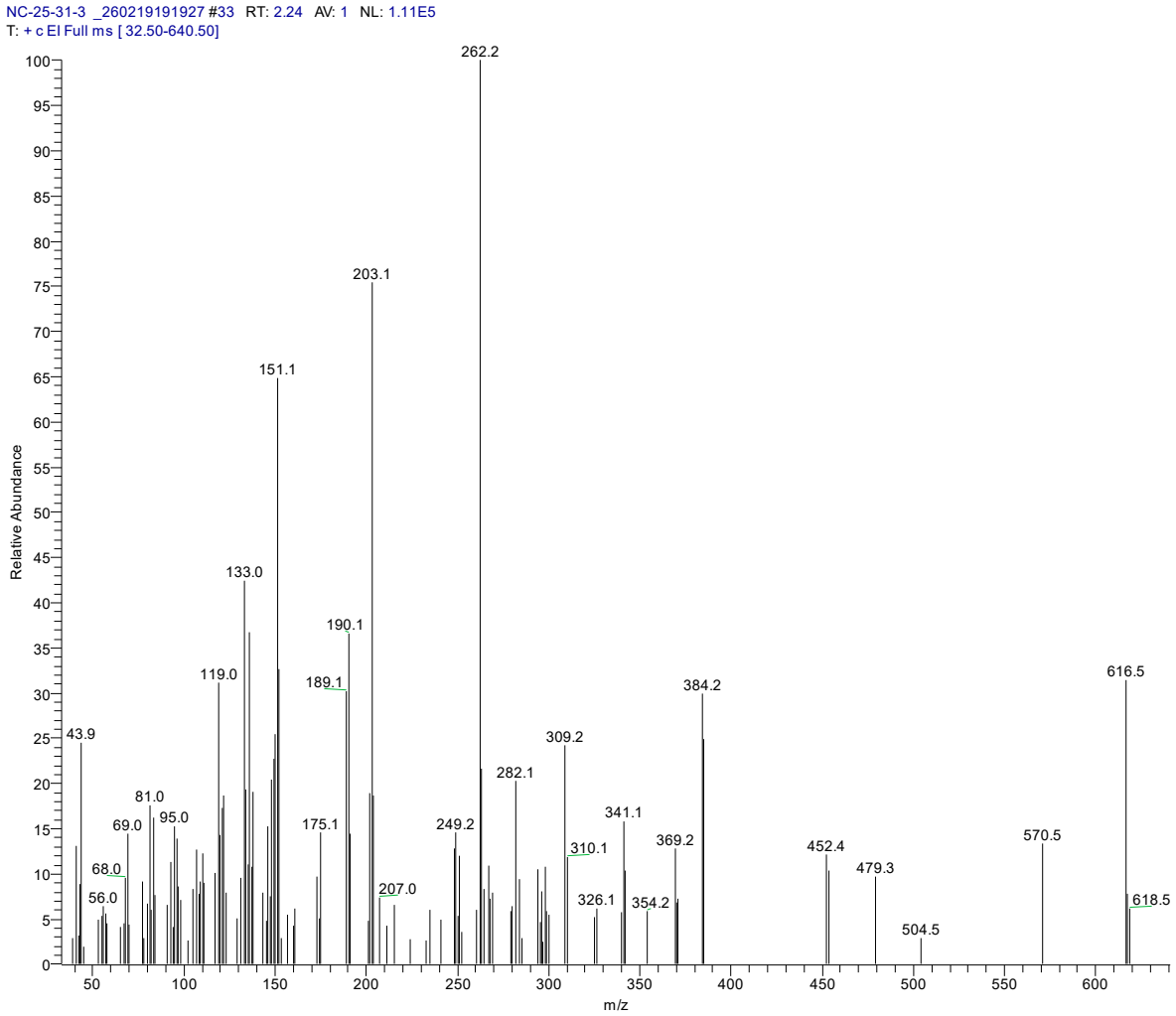
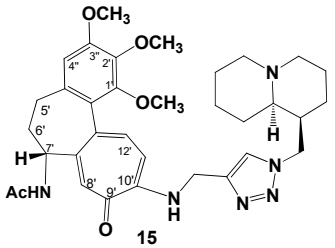


Figure S23. ^{13}C NMR spectrum of of 1*R*,5*S*)-10-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methylamino-N-[(7*S*)-acetylamino-1,2,3,-trimethoxy-6,7-dihydro-5*H*-benzo[*a*]heptalen-9-one (**15**) ($CDCl_3$, 125 MHz).

Figure S24. HR-MS spectrum of of 1*R*,5*S*)-10-(1-(((1*S*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methylamino-N-[(7*S*)-acetylamino-1,2,3,-trimethoxy-6,7-dihydro-5*H*-benzo[*a*]heptalen-9-one (**15**).





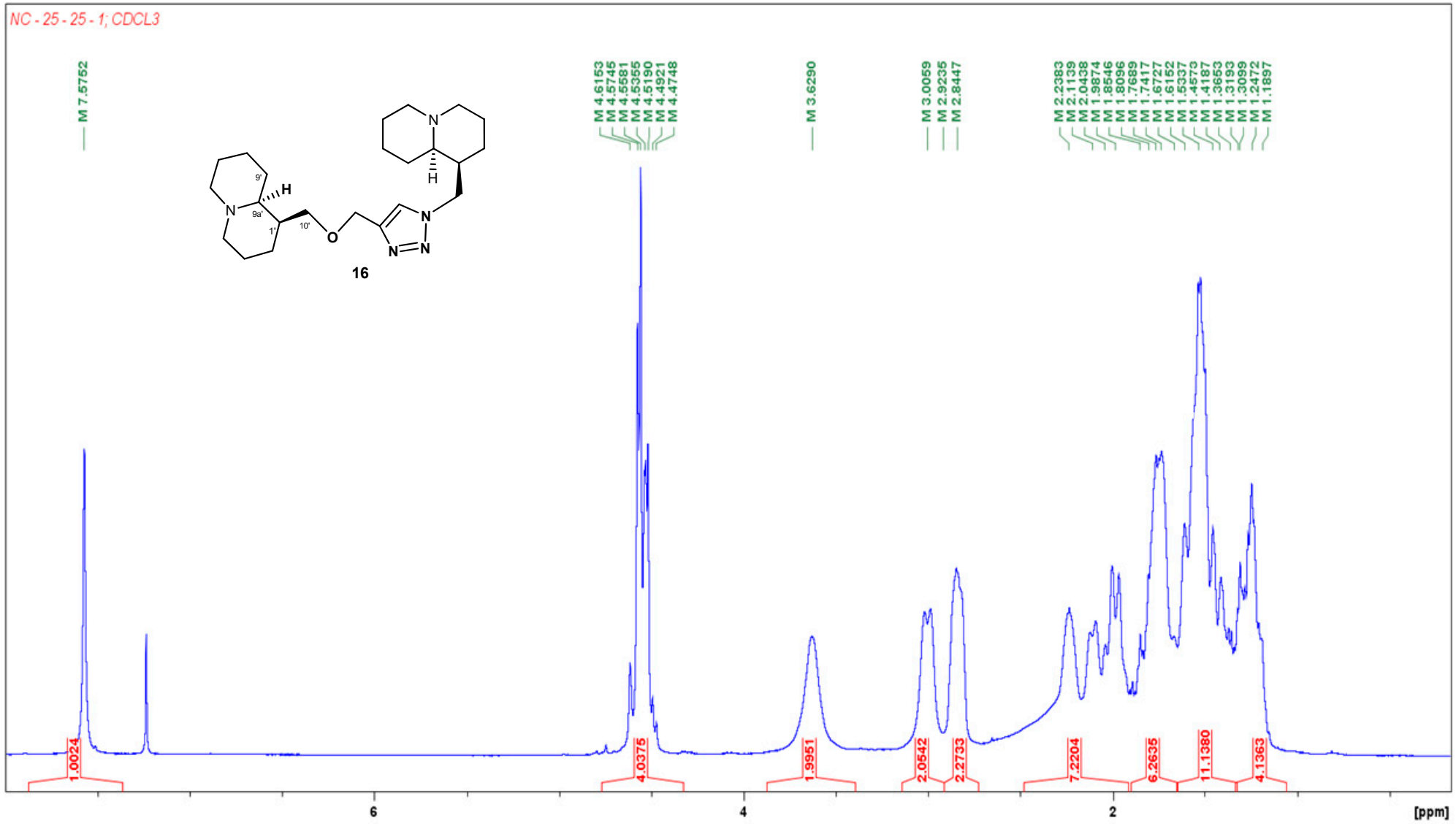
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Tprobe=340˚C
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(C24 H34 O1 N6) $^{+\cdot}$
Found: m/z= 616.3367

1	C24 H34 O1 N6
RDB	(ppm)
11.0	-0.114

Isotope	min	max
12 C	30	40
1 H	35	55
16 O	0	7
14 N	0	8

m/z	Intensity	Relative
43.9	27171.0	24.40
81.0	19445.0	17.46
119.0	34545.0	31.02
122.0	20630.0	18.53

m/z	Intensity	Relative
133.0	47100.0	42.29
134.0	21377.0	19.20
136.1	40822.0	36.66
138.1	21157.0	19.00
148.1	22606.0	20.30
149.1	25239.0	22.66
150.1	28268.0	25.38
151.1	72164.0	64.80
152.1	36301.0	32.60
189.1	33492.0	30.07
190.1	40647.0	36.50
202.1	21026.0	18.88
203.1	83972.0	75.40
204.1	20674.0	18.56
262.2	111363.0	100.00
263.2	23923.0	21.48
282.1	22474.0	20.18
284.1	10359.0	9.30
294.1	11500.0	10.33
296.1	8823.0	7.92
298.1	11895.0	10.68
309.2	26820.0	24.08
310.1	13080.0	11.75
341.1	17470.0	15.69
342.1	11412.0	10.25
369.2	14178.0	12.73
370.1	7506.0	6.74
371.2	7901.0	7.09
384.2	33272.0	29.88
385.2	27654.0	24.83
452.4	13388.0	12.02
453.3	11456.0	10.29
479.3	10622.0	9.54
504.5	3116.0	2.80
570.5	14705.0	13.20
616.5	34853.0	31.30
617.6	8559.0	7.69
618.5	6803.0	6.11



16

Figure S25. ^{1}H NMR spectrum of (1*S*,9a*R*)-1-((4-((((1*S*,9a*S*)-octahydro-1*H*-quinolizin-1-yl)methoxy)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)octahydro-1*H*-quinolizine (**16**) ($CDCl_3$, 300 MHz).

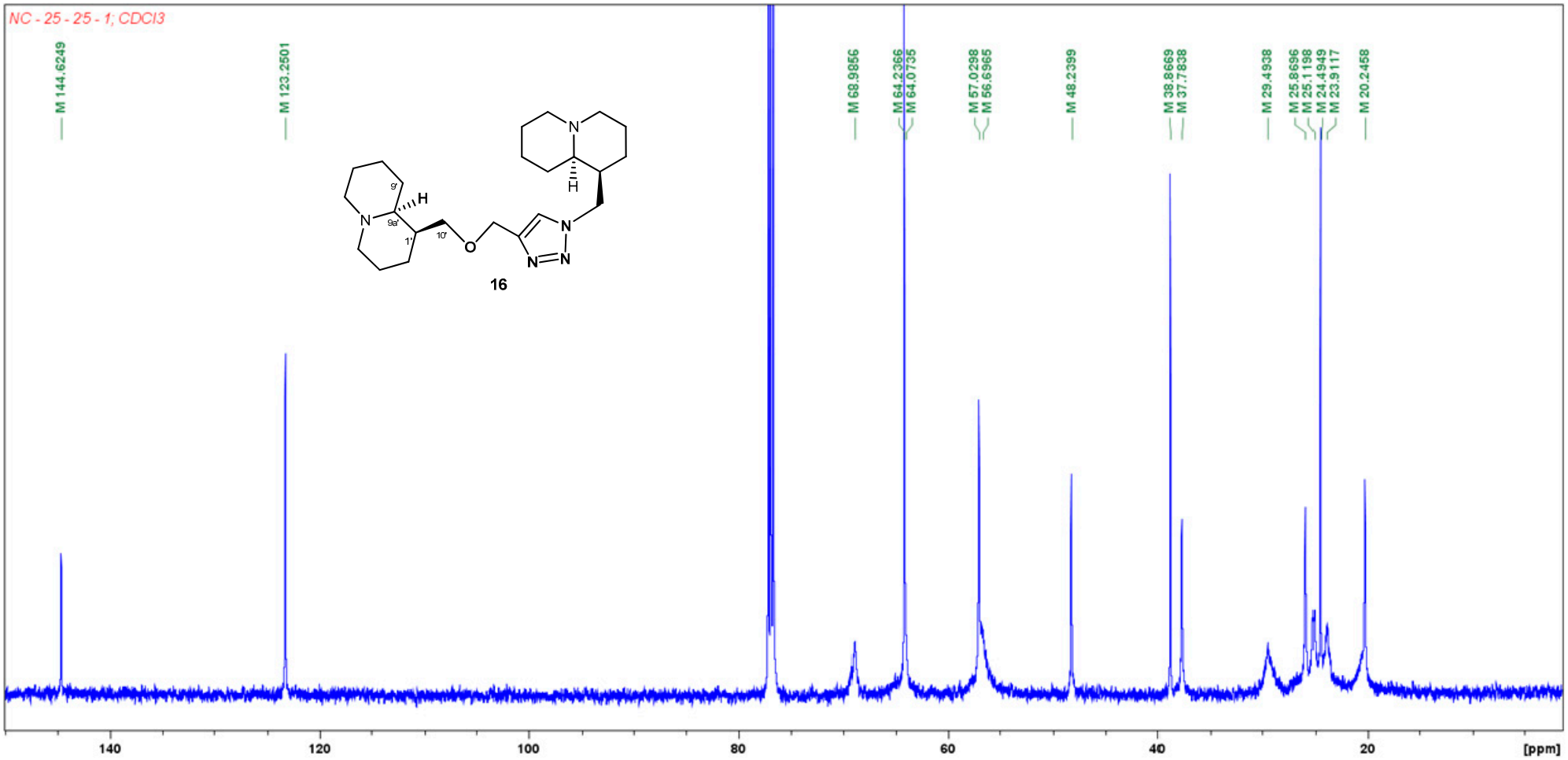
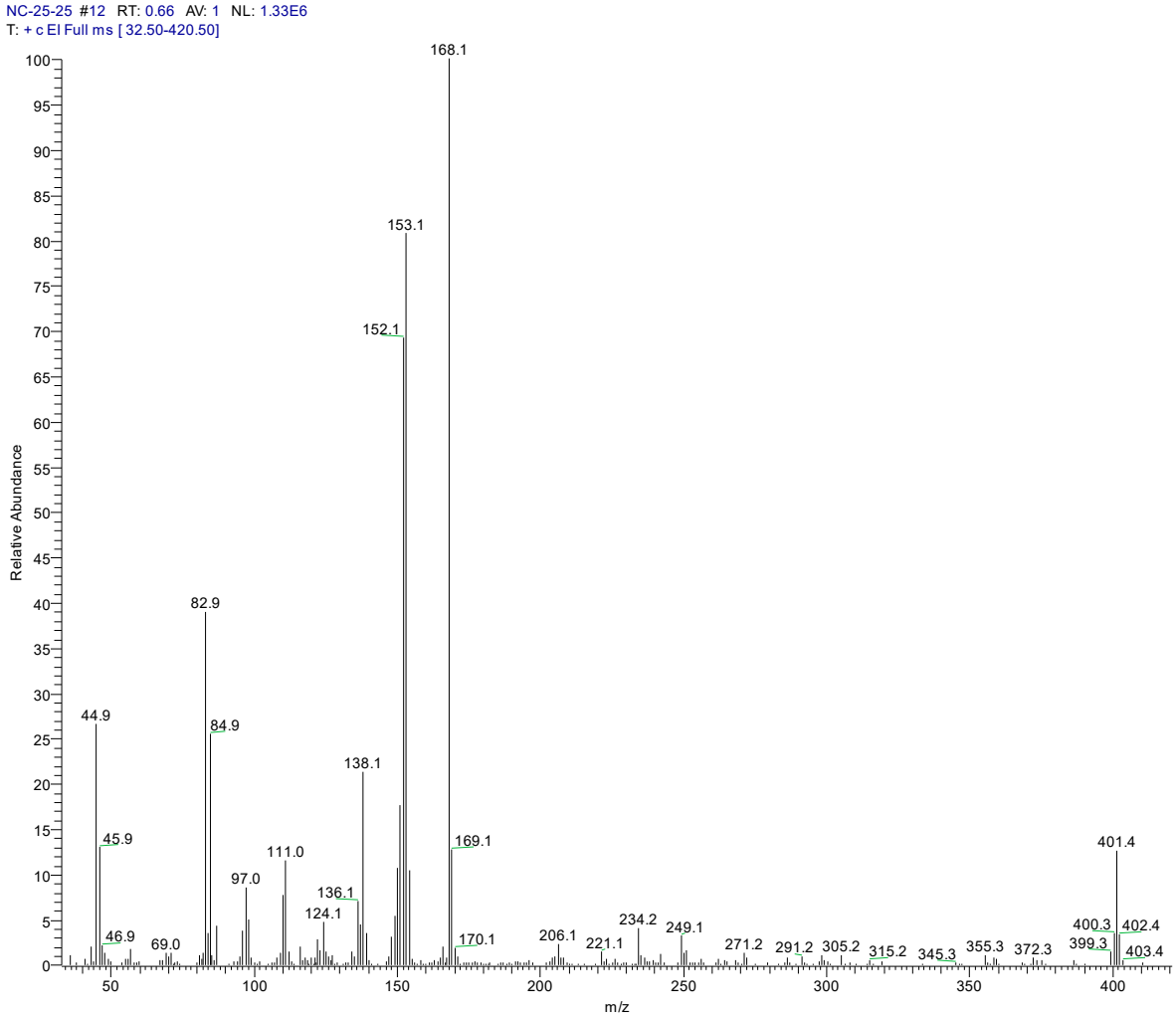
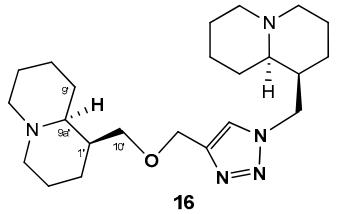


Figure S26. ^{13}C NMR spectrum of (1*S*,9a*R*)-1-((4-((((1*S*,9a*S*)-octahydro-1*H*-quinolizin-1-yl)methoxy)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)octahydro-1*H*-quinolizine (**16**) ($CDCl_3$, 125 MHz).

Figure S27. HR-MS spectrum of (1*S*,9a*R*)-1-((4-((((1*S*,9a*S*)-octahydro-1*H*-quinolizin-1-yl)methoxy)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)octahydro-1*H*-quinolizine (**16**)





16

Tsource=100˚C
Tprobe=260˚C
Calculated: m/z= 401.3149
$(C_{23}H_{39}O_1N_5)^{+\cdot}$
Found: m/z= 401.3150

1	C23 H39 O1 N5	
RDB		(ppm)
7.0		0.217
Isotope	min	max
12 C	18	28
1 H	30	50
16 O	0	3
14 N	0	7

m/z	Intensity	Relative
44.9	352499.0	26.51
45.9	171802.0	12.92
82.9	517834.0	38.94
83.0	71644.0	5.39
84.9	338226.0	25.43
97.0	112534.0	8.46
98.0	66699.0	5.02
110.0	101402.0	7.62
111.0	153363.0	11.53

m/z	Intensity	Relative
124.1	62533.0	4.70
136.1	92633.0	6.97
138.1	282316.0	21.23
149.1	71644.0	5.39
150.1	140956.0	10.60
151.1	233683.0	17.57
152.1	921516.0	69.29
153.1	1075097.0	80.84
154.1	138748.0	10.43
168.1	1329894.0	100.00
169.1	169159.0	12.72
205.1	11660.0	0.88
206.1	29447.0	2.21
208.1	10541.0	0.79
221.1	18564.0	1.40
234.2	53422.0	4.02
235.2	12842.0	0.97
242.2	15765.0	1.19
249.1	41730.0	3.14
250.2	16791.0	1.26
251.2	20647.0	1.55
271.2	17351.0	1.30
291.2	11132.0	0.84
298.2	13619.0	1.02
305.2	13930.0	1.05
355.3	13744.0	1.03
358.3	9421.0	0.71
359.3	7307.0	0.55
372.3	10790.0	0.81
373.3	7058.0	0.53
375.3	6747.0	0.51
399.3	19030.0	1.43
400.3	45803.0	3.44
401.4	167231.0	12.57
402.4	43595.0	3.28

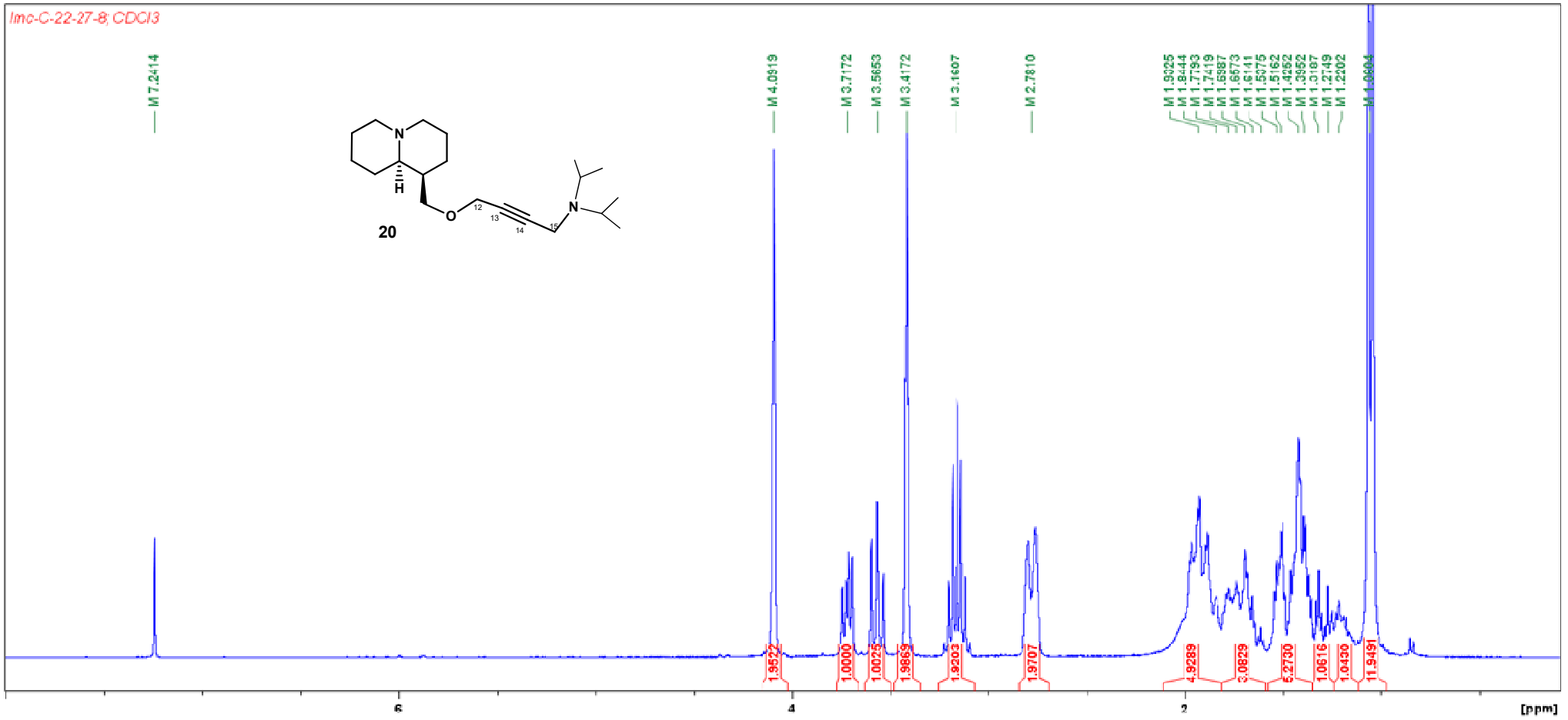


Figure S28. ^{1}H NMR spectrum of N,N-diisopropyl-4-(((1*R*,9a*R*)-octahydro-1H-quinolizin-1-yl)methoxy)but-2-yn-1-amine (**20**) ($CDCl_3$, 300 MHz).

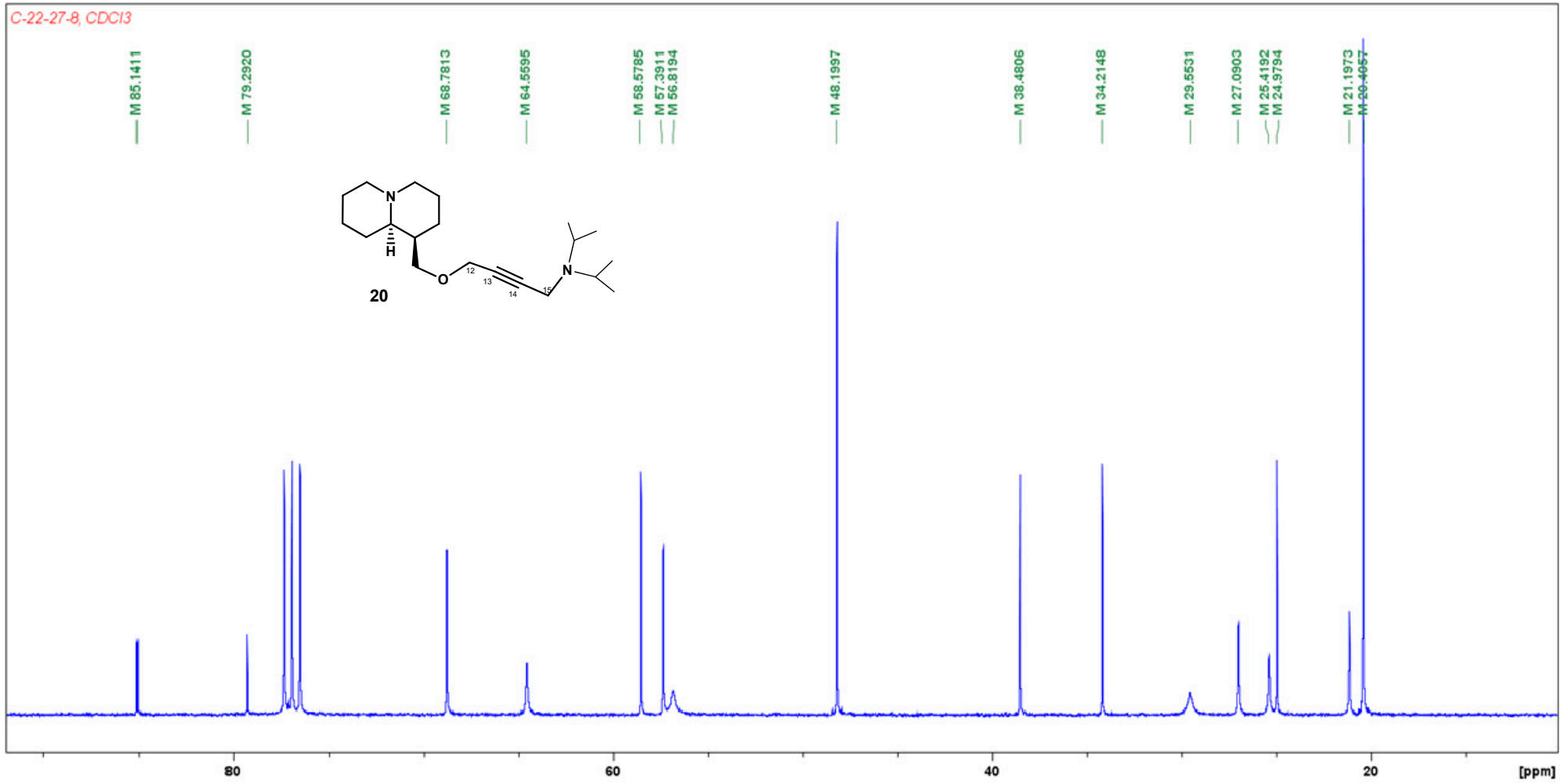
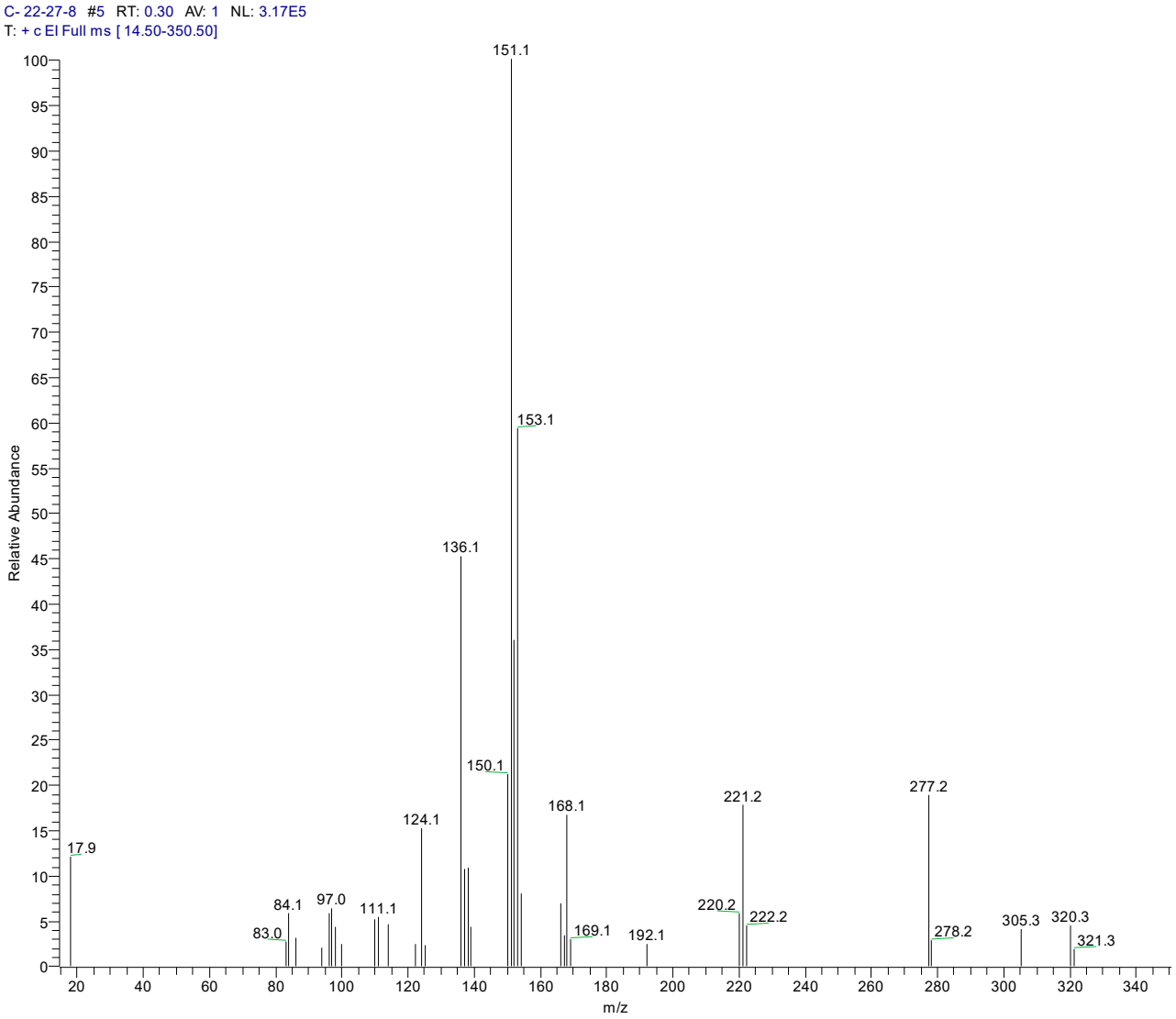
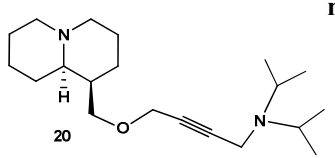


Figure S29. ^{13}C NMR spectrum of N,N-diisopropyl-4-(((1*R*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methoxy)but-2-yn-1-amine (**20**) ($CDCl_3$, 125 MHz).

Figure S30. HR-MS spectrum of N,N-diisopropyl-4-(((1*R*,9a*R*)-octahydro-1H-quinolizin-1-yl)methoxy)but-2-yn-1-amine (**20**)





Tsource=80˚C
Tprobe=220˚C

Calculated
m/z= 320.2822
$(C_{20}H_{36}O_1N_2)^{+\cdot}$

Found

m/z= 320.2819

Элементный состав
1 C20 H36 O1 N2

RDB	Ошибка (ppm)
4.0	-0.985

Интервал значений чисел атомов элементов:

Isotope	min	max
12 C	17	25
1 H	25	45
16 O	0	3
14 N	0	4

m/z	Intensity	Relative
17.9	38192.0	12.06
83.0	8338.0	2.63
84.1	18427.0	5.82
86.1	9643.0	3.04
96.0	18427.0	5.82
97.0	19892.0	6.28
98.1	13431.0	4.24
100.1	7320.0	2.31
110.1	16104.0	5.08
111.1	16963.0	5.36
114.1	14322.0	4.52
122.0	7447.0	2.35
124.1	47804.0	15.09
136.1	142936.0	45.13
137.1	33641.0	10.62
138.1	34118.0	10.77
139.1	13526.0	4.27
150.1	67028.0	21.16
151.1	316712.0	100.00
152.1	113718.0	35.91
153.1	187971.0	59.35
154.1	25239.0	7.97
166.1	21833.0	6.89
167.1	10598.0	3.35
168.1	52833.0	16.68
169.1	9070.0	2.86
192.1	7670.0	2.42
220.2	18364.0	5.80
221.2	56143.0	17.73
222.2	14131.0	4.46
277.2	59612.0	18.82
278.2	9007.0	2.84
305.3	12699.0	4.01
320.3	14163.0	4.47
321.3	5665.0	1.79

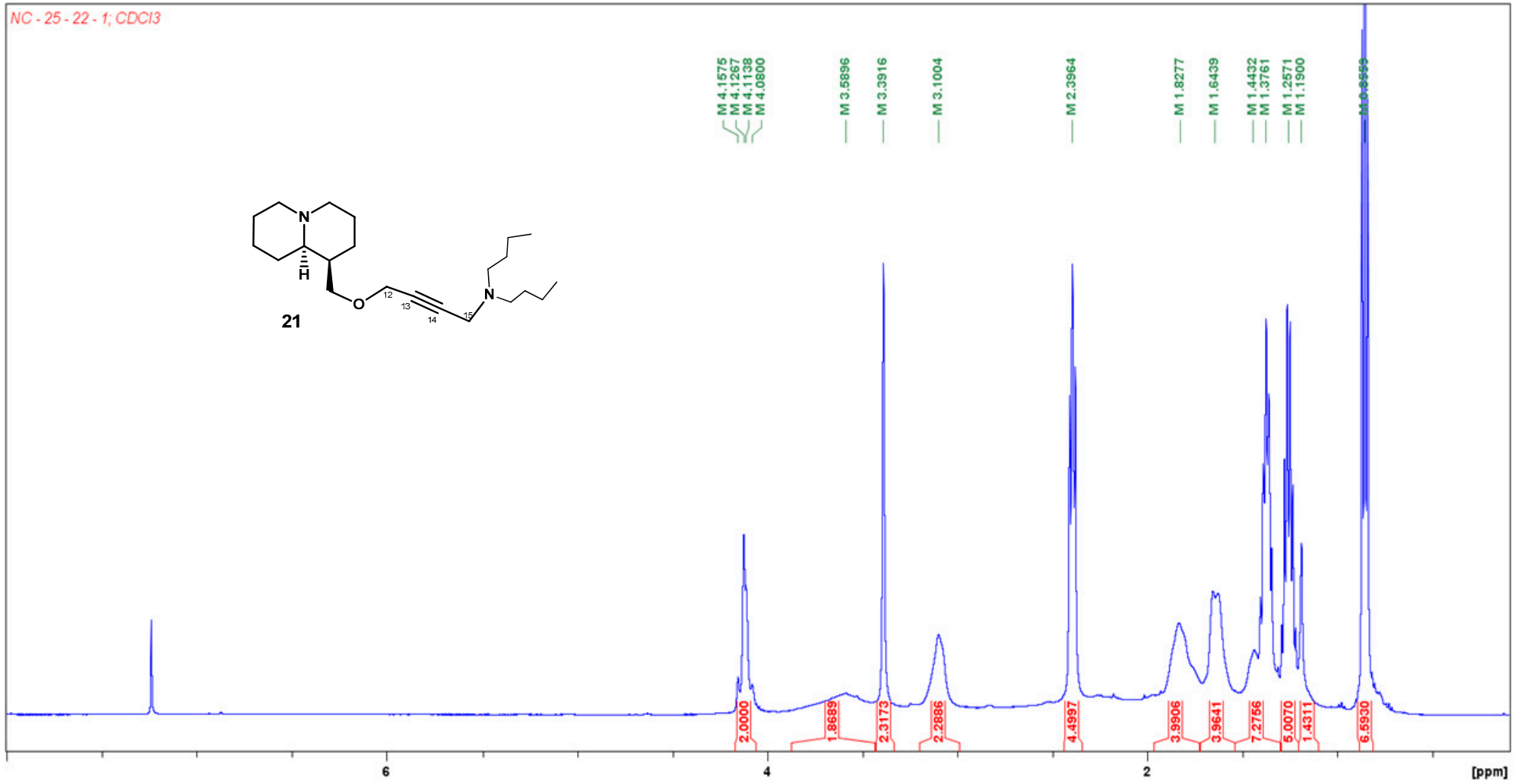


Figure S31. ^{1}H NMR spectrum of N,N-dibutyl-4-(((1*R*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methoxy)but-2-yn-1-amine (**21**) ($CDCl_3$, 500 MHz).

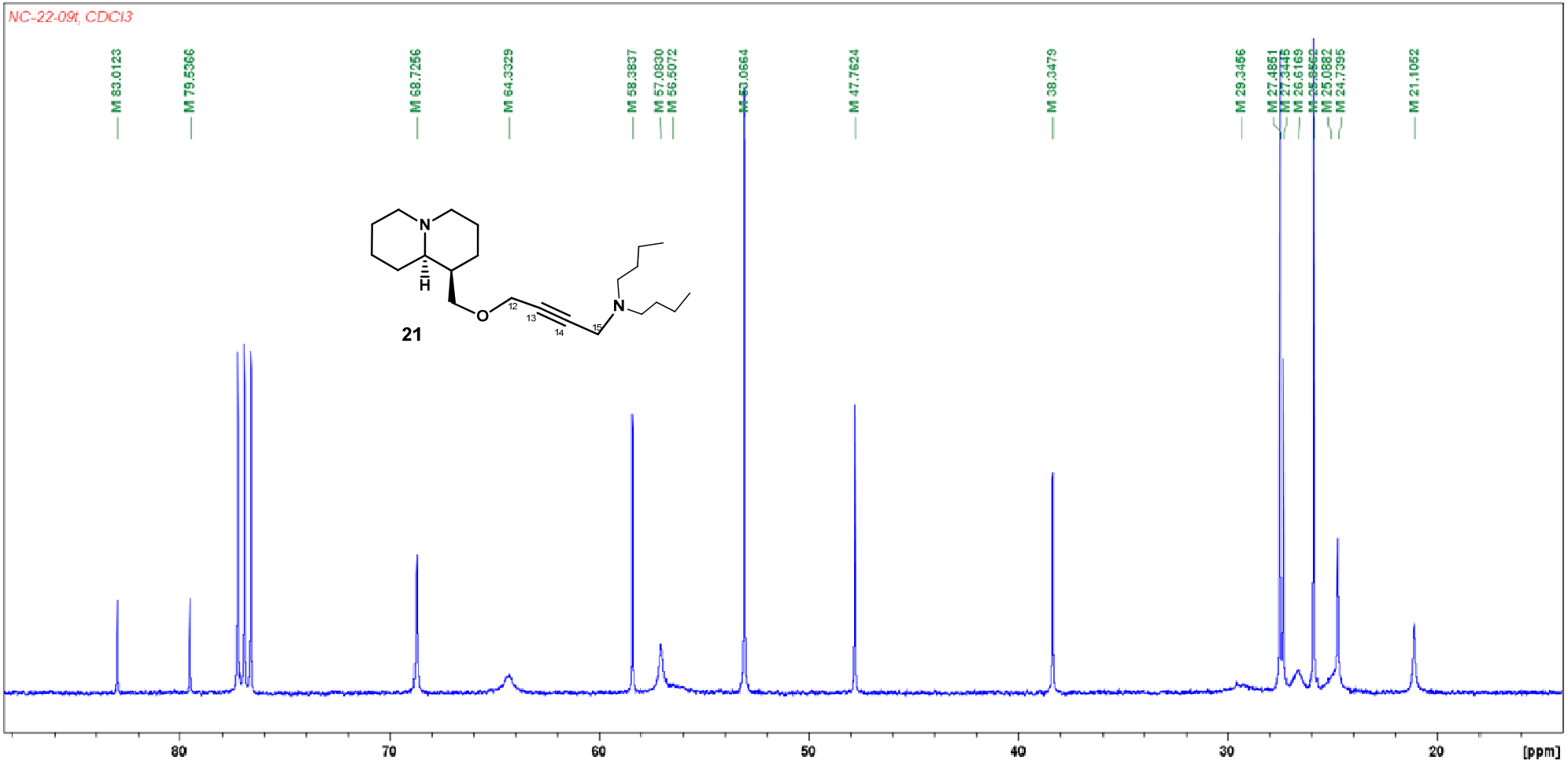
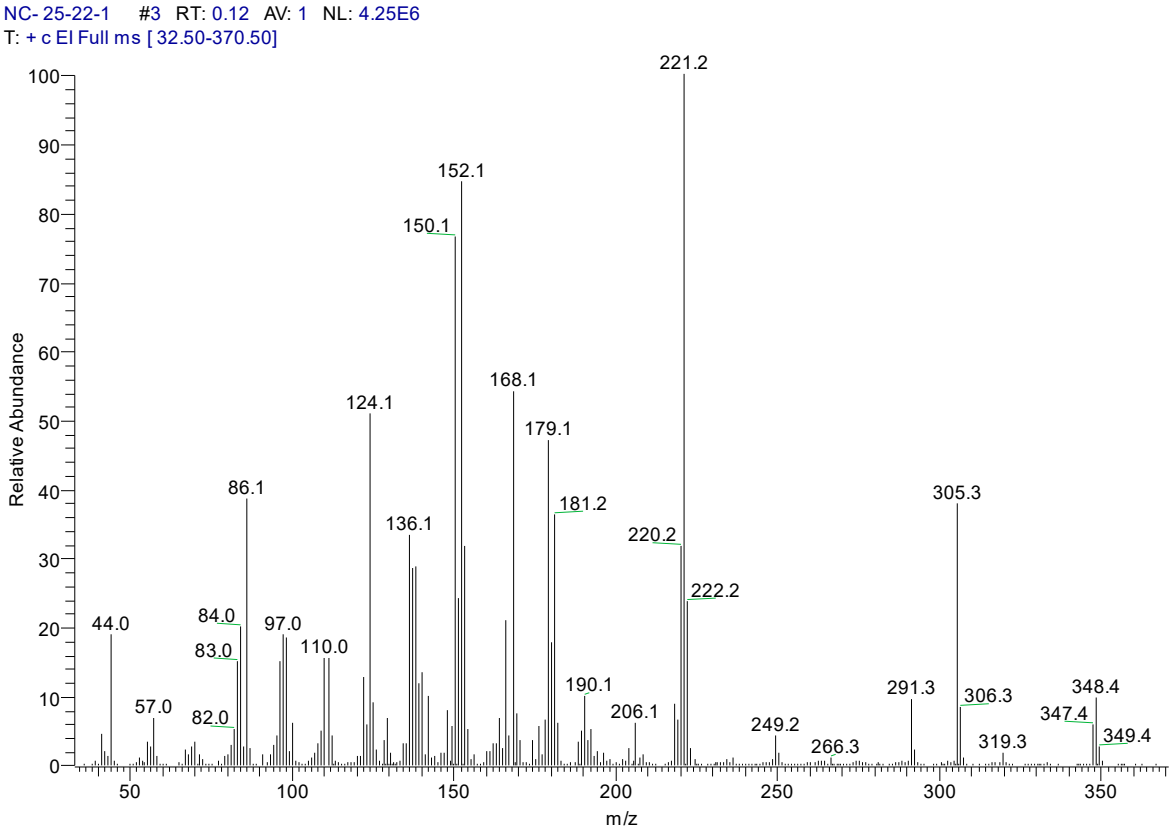
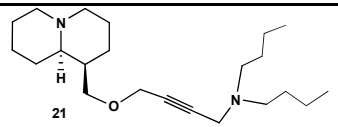


Figure S32. ^{13}C NMR spectrum of N,N-dibutyl-4-(((1*R*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methoxy)but-2-yn-1-amine (**21**) ($CDCl_3$, 125 MHz).

Figure S33. HR-MS spectrum of N,N-dibutyl-4-(((1*R*,9a*R*)-octahydro-1*H*-quinolizin-1-yl)methoxy)but-2-yn-1-amine (**21**).





Tsource=100°C

Calculated: m/z= 347.3057
$(C22\ H39\ O1\ N2)^{+\cdot}$
Found: m/z= 347.3055

1	C22 H39 O1 N2
RDB	(ppm)
4.5	-0.549

Isotope	min	max
12 C	16	26
1 H	30	45
16 O	0	3
14 N	0	4

m/z	Intensity	Relative
44.0	805284.0	18.97
83.0	633873.0	14.93
84.0	853752.0	20.11
86.1	1635752.0	38.53
96.0	640941.0	15.10
97.0	801857.0	18.89
98.0	780959.0	18.39
110.0	654741.0	15.42
111.1	652813.0	15.38
124.1	2157421.0	50.81
136.1	1414220.0	33.31
137.1	1211109.0	28.53
138.1	1214628.0	28.61

m/z	Intensity	Relative
150.1	3248708.0	76.52
151.1	1023572.0	24.11
152.1	3593428.0	84.64
153.1	1343997.0	31.66
166.1	886798.0	20.89
168.1	2296827.0	54.10
179.1	1997546.0	47.05
180.1	751034.0	17.69
181.2	1542305.0	36.33
220.2	1349230.0	31.78
221.2	4245661.0	100.00
222.2	1006590.0	23.71
234.2	29496.0	0.69
236.2	40022.0	0.94
248.2	33933.0	0.80
249.2	181417.0	4.27
250.2	68968.0	1.62
262.2	21969.0	0.52
263.2	22306.0	0.53
264.2	21694.0	0.51
266.3	39012.0	0.92
274.3	24233.0	0.57
275.3	21021.0	0.50
288.3	28119.0	0.66
290.3	20286.0	0.48
291.3	405273.0	9.55
292.3	87816.0	2.07
302.3	21571.0	0.51
304.3	19674.0	0.46
305.3	1607510.0	37.86
306.3	355184.0	8.37
307.3	40359.0	0.95
319.3	77199.0	1.82
347.4	244724.0	5.76
348.4	412831.0	9.72
349.4	111959.0	2.64
350.4	20684.0	0.49

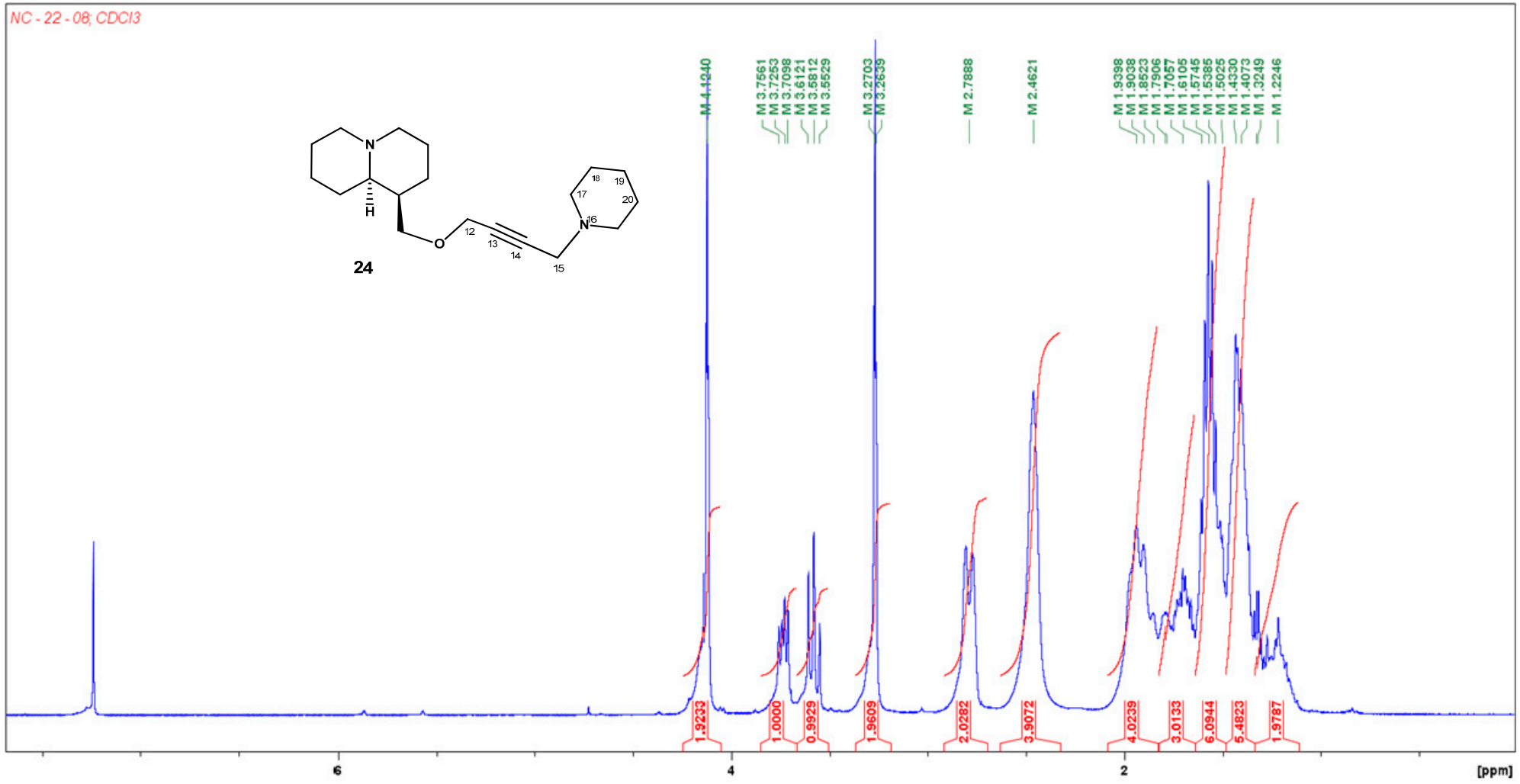


Figure S34. ^{1}H NMR spectrum of (1*R*,9a*R*)-1-((4-(piperidin-1-yl)but-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**24**) ($CDCl_3$, 300MHz).

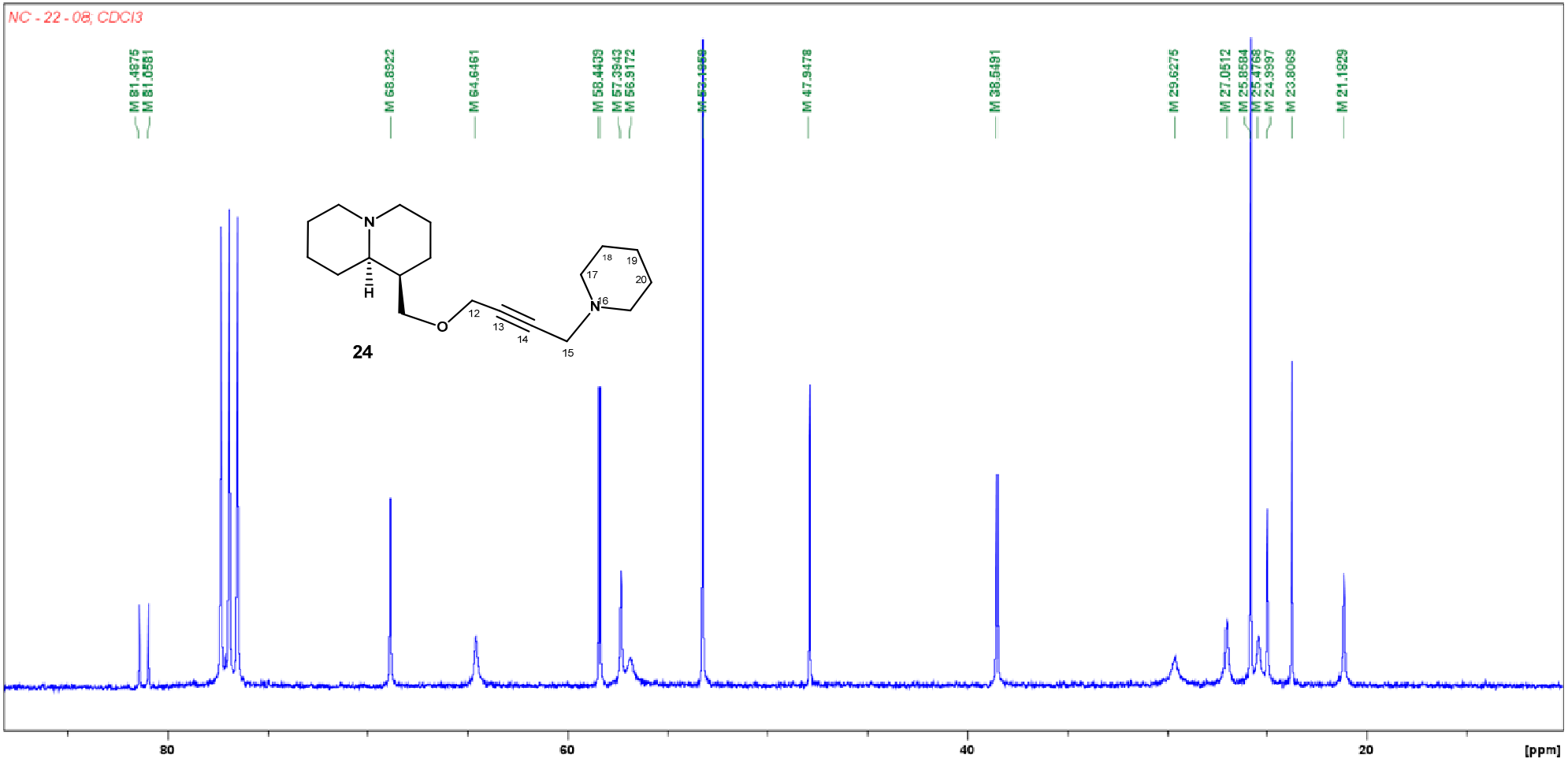
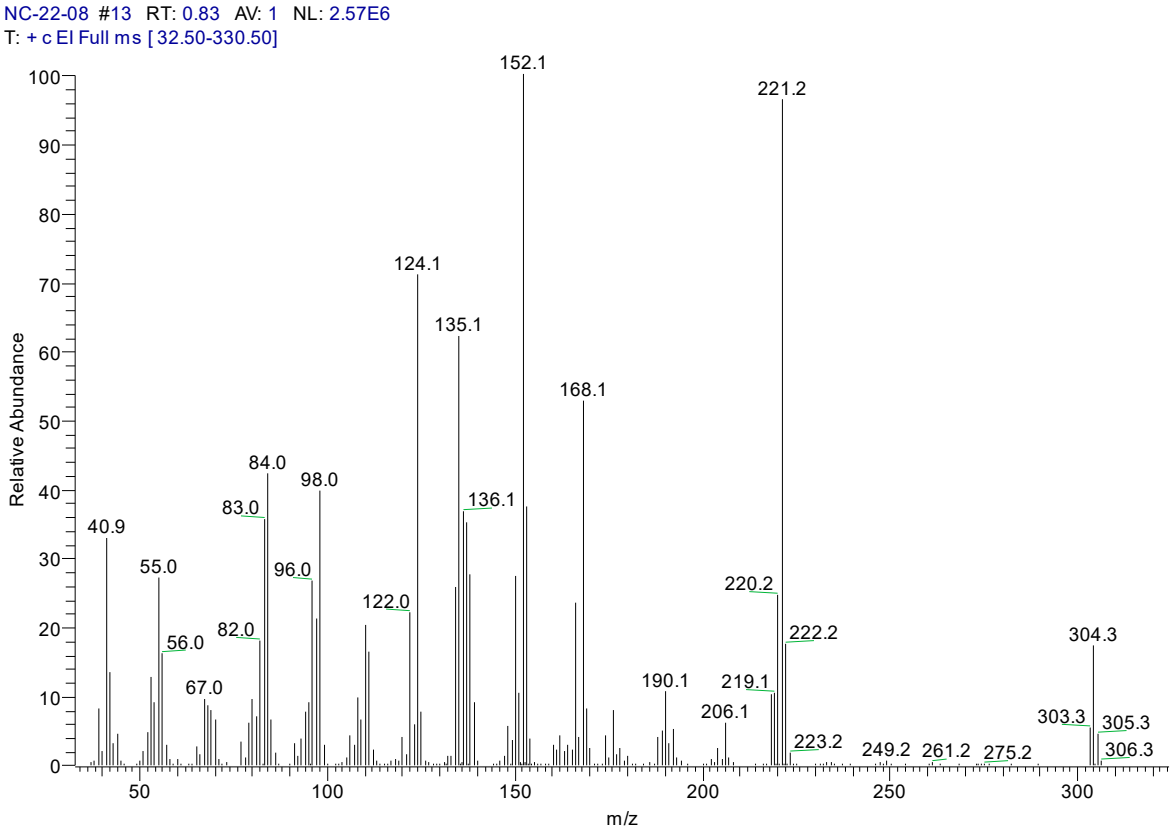
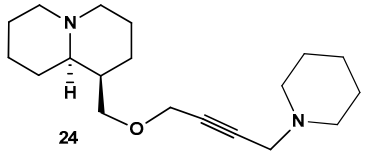


Figure S35. ^{13}C NMR spectrum of (1*R*,9a*R*)-1-((4-(piperidin-1-yl)but-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**24**) ($CDCl_3$, 100 MHz).

Figure S36. HR-MS spectrum of (1*R*,9a*R*)-1-((4-(piperidin-1-yl)but-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**24**).





24

Tsource=80˚C
Tprobe=230˚C
Calculated:
m/z= 304.2509

Found:
Измеренное значение
m/z= 304.2507
1 C19 H32 O1 N2

RDB	Ошибка (ppm
5	-0.708

Isotope	min	max
12 C	15	22
1 H	25	40
16 O	0	3
14 N	0	4

m/z	Intensity	Relative
38.9	205598.0	8.01
40.9	844549.0	32.92
41.9	342832.0	13.36
53.0	323582.0	12.61
54.0	234123.0	9.13
55.0	695861.0	27.12
56.0	412678.0	16.09
67.0	245103.0	9.55
68.0	219176.0	8.54
69.0	201156.0	7.84
80.0	244768.0	9.54
82.0	462827.0	18.04
83.0	913194.0	35.59
84.0	1083646.0	42.24
94.0	197747.0	7.71
96.0	681501.0	26.56
97.0	545553.0	21.26

m/z	Intensity	Relative
98.0	1015951.0	39.60
108.0	250886.0	9.78
110.0	519626.0	20.25
111.0	421730.0	16.44
122.0	566059.0	22.06
124.1	1825411.0	71.15
134.0	658424.0	25.66
135.1	1593075.0	62.10
136.1	940210.0	36.65
137.1	899811.0	35.07
138.1	707595.0	27.58
139.1	230547.0	8.99
150.1	699940.0	27.28
151.1	264297.0	10.30
152.1	2565527.0	100.00
153.1	958873.0	37.38
166.1	599027.0	23.35
168.1	1352246.0	52.71
169.1	208532.0	8.13
174.1	111111.0	4.33
176.1	200513.0	7.82
188.1	100689.0	3.92
189.1	125806.0	4.90
190.1	273265.0	10.65
191.1	77752.0	3.03
192.1	133992.0	5.22
204.1	59173.0	2.31
206.1	152795.0	5.96
207.1	27016.0	1.05
218.1	259072.0	10.10
219.1	265330.0	10.34
220.2	632692.0	24.66
221.2	2476850.0	96.54
221.3	11259.0	0.44
222.2	449836.0	17.53
223.2	43416.0	1.69
303.3	136032.0	5.30
304.3	445617.0	17.37
305.3	111725.0	4.35
306.3	13466.0	0.52

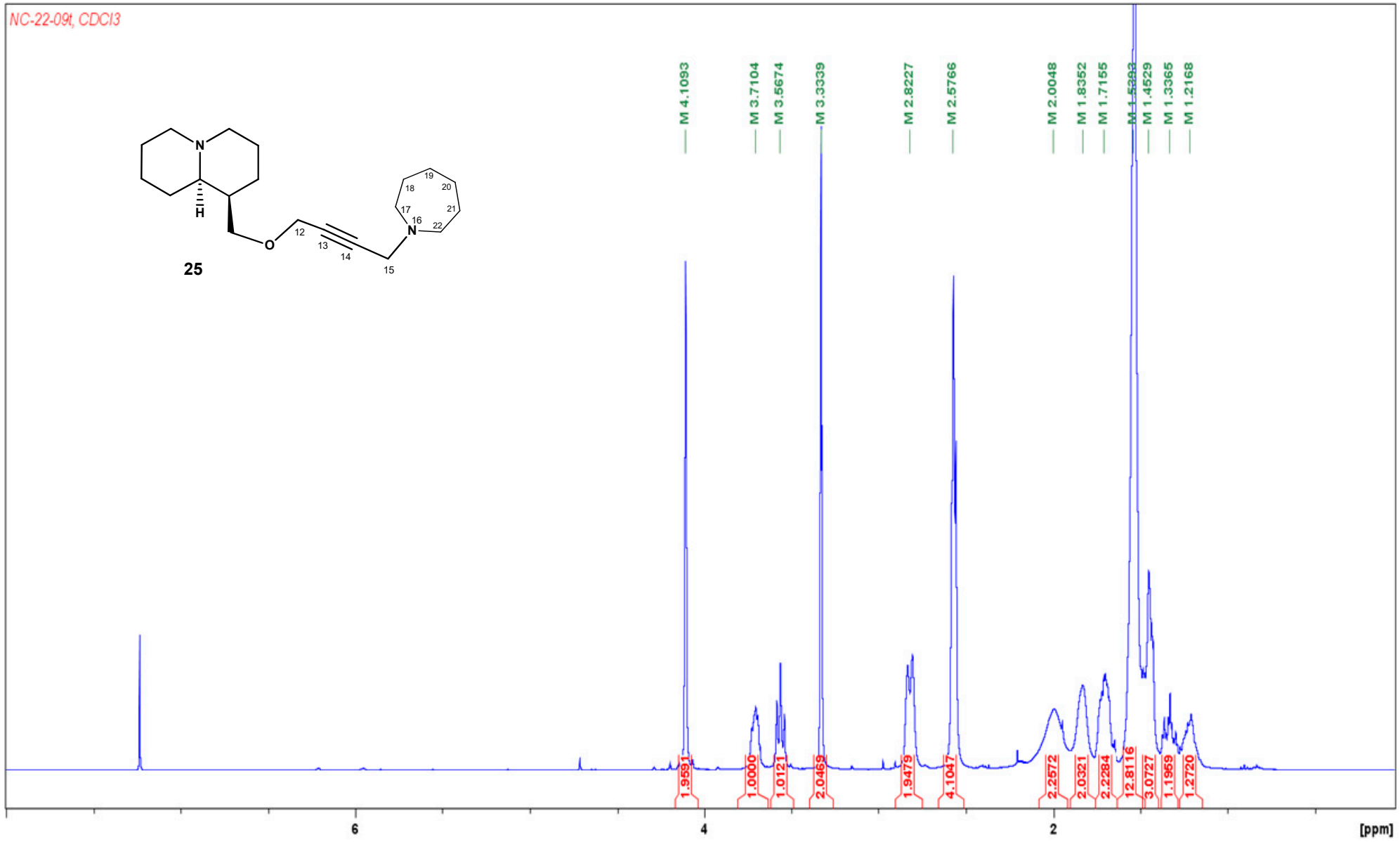


Figure S37. ^{1}H NMR spectrum of (1*R*,9a*R*)-1-((4-(azepan-1-yl)but-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**25**) ($CDCl_3$, 300 MHz).

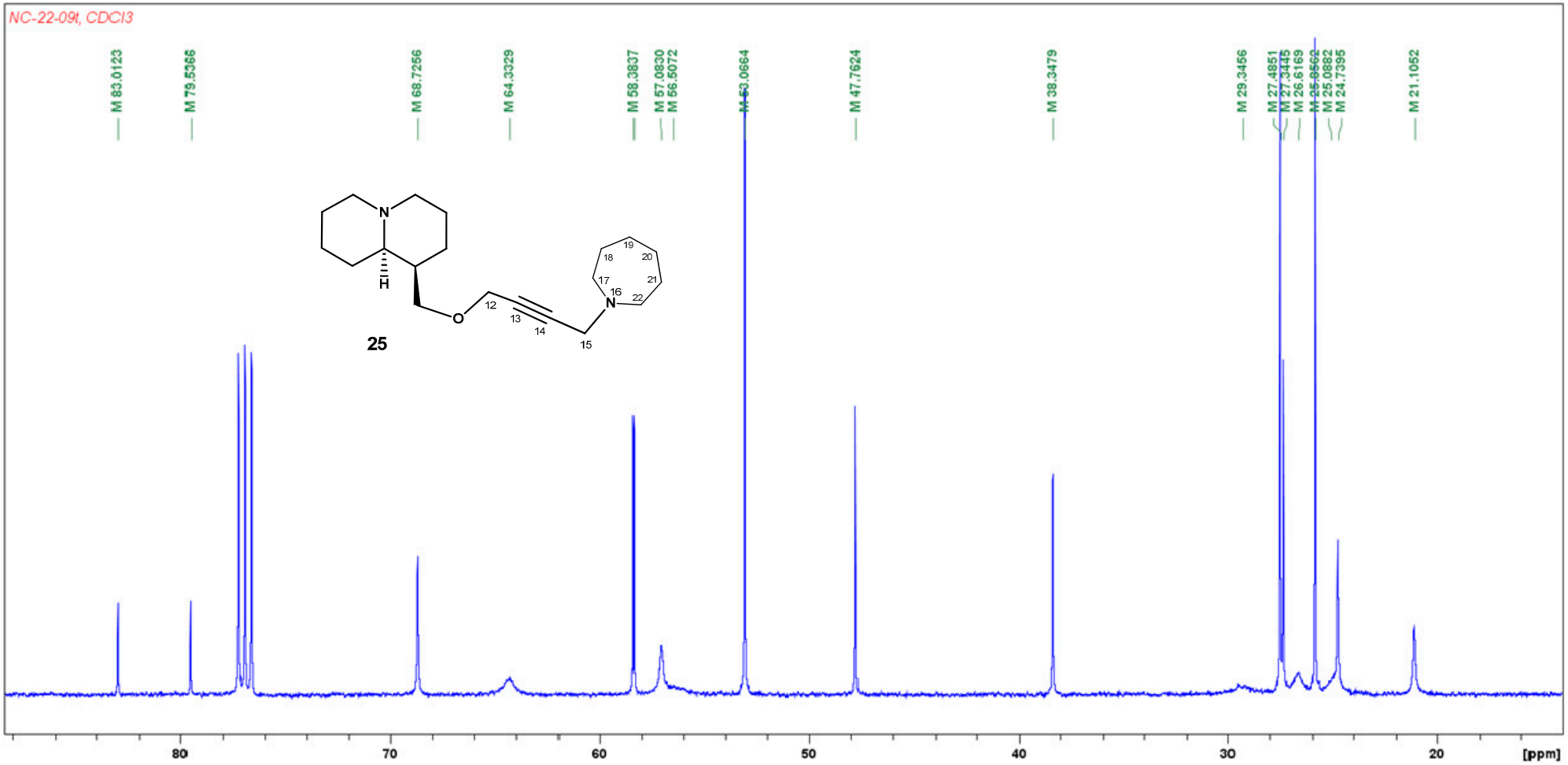
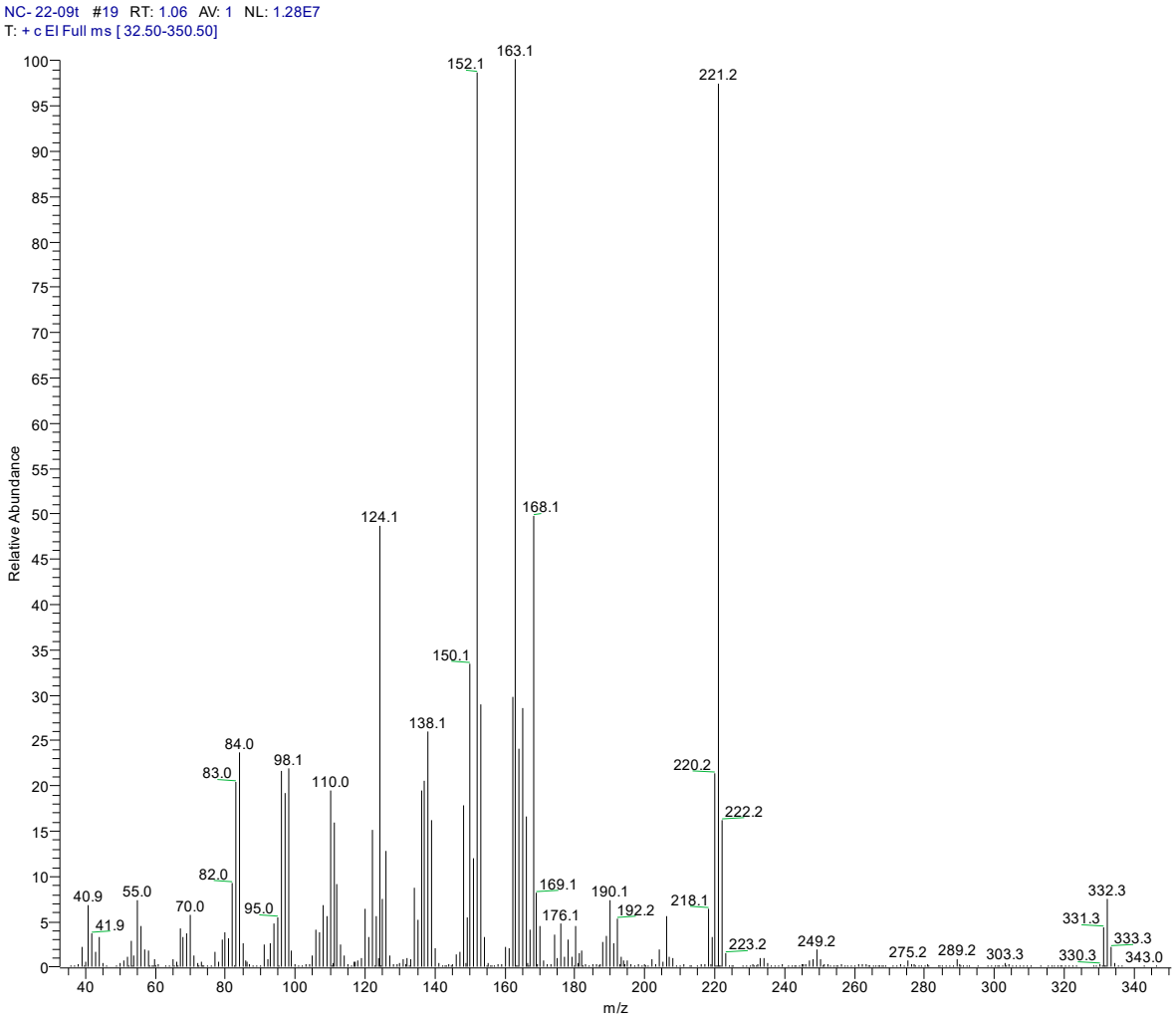
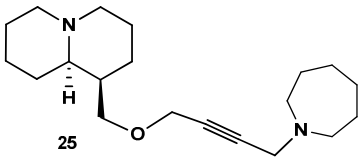


Figure S38. ^{13}C NMR spectrum of (1*R*,9a*R*)-1-((4-(azepan-1-yl)but-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**25**) ($CDCl_3$, 100 MHz).

Figure S39. HR-MS spectrum of (1*R*,9a*R*)-1-((4-(azepan-1-yl)but-2-ynyloxy)methyl)octahydro-1*H*-quinolizine (**25**).





25

Tsource=90˚C
Tprobe=220˚C

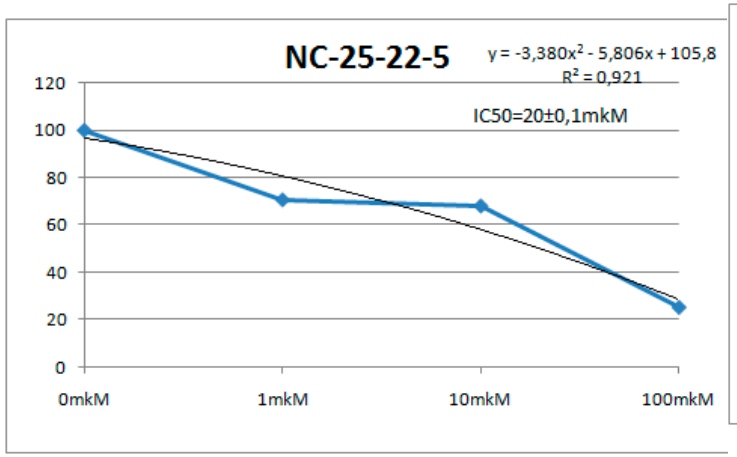
Calculated: m/z= 332.2822
(C21 H36 O1 N2)$^{+\cdot}$
Found: m/z= 332.2816

1	C21 H36 O1 N2	
	RDB	(ppm)
	5.0	-1.853

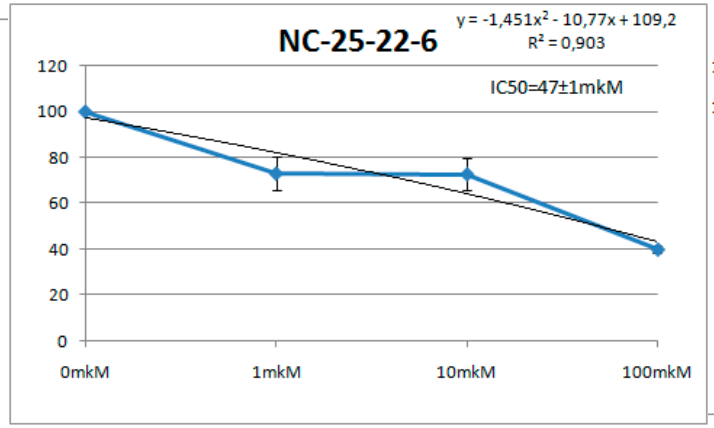
Isotope	min	max
12 C	16	25
1 H	25	45
16 O	0	3
14 N	0	4

m/z	Intensity	Relative
83.0	2602643.0	20.33
84.0	3021274.0	23.60
96.0	2758544.0	21.54
97.0	2441780.0	19.07
98.1	2786065.0	21.76
110.0	2480155.0	19.37
111.1	2019661.0	15.77
122.1	1915158.0	14.96
124.1	6217055.0	48.55
126.1	1631652.0	12.74
136.1	2471007.0	19.30
137.1	2617605.0	20.44

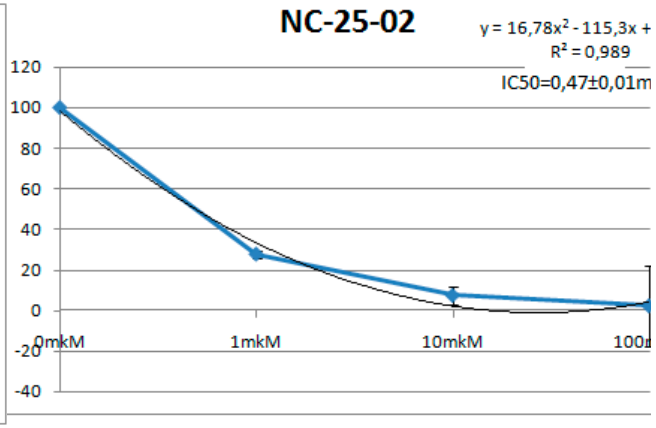
m/z	Intensity	Relative
138.1	3308966.0	25.84
139.1	2062454.0	16.11
148.1	2273552.0	17.76
150.1	4263289.0	33.29
151.1	1518932.0	11.86
152.1	12630528.0	98.64
153.1	3700308.0	28.90
162.1	3808145.0	29.74
163.1	12804608.0	100.00
164.1	3064455.0	23.93
165.1	3645576.0	28.47
166.1	2120752.0	16.56
168.1	6351637.0	49.60
174.1	435065.0	3.40
180.1	570035.0	4.45
182.1	210633.0	1.64
188.1	343509.0	2.68
189.1	427313.0	3.34
190.1	924166.0	7.22
191.1	329322.0	2.57
192.2	668801.0	5.22
206.1	706865.0	5.52
218.1	814702.0	6.36
219.2	417002.0	3.26
220.2	2722495.0	21.26
221.2	12460800.0	97.31
222.2	2054391.0	16.04
223.2	181019.0	1.41
249.2	228386.0	1.78
331.3	550654.0	4.30
332.3	946260.0	7.39
333.3	270637.0	2.11



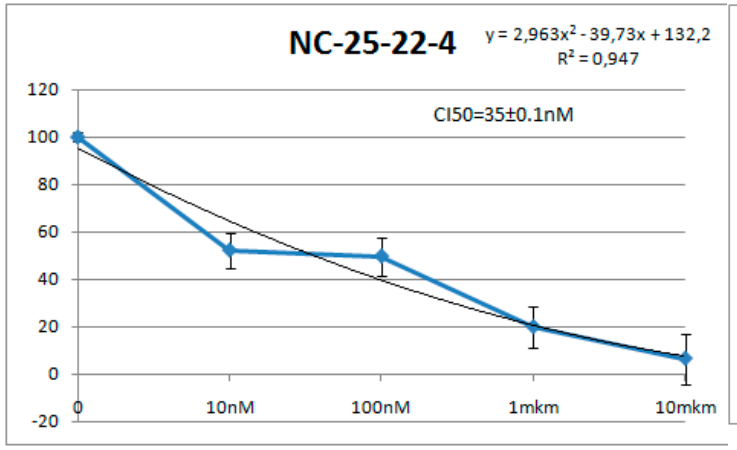
Compound **5**: IC_{50} = 20.1±0.1 μM



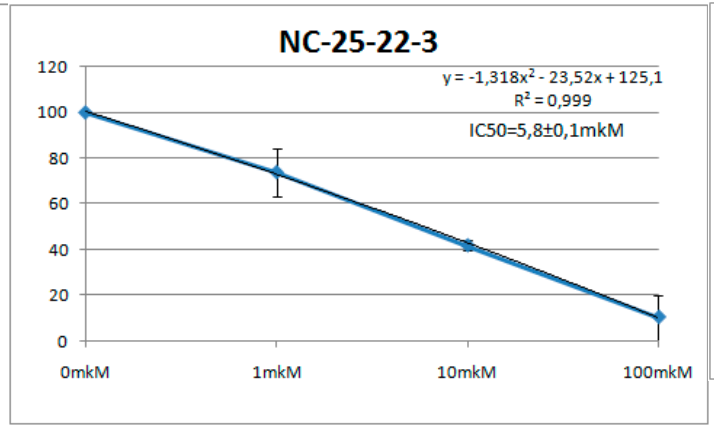
Compound **7**: IC_{50} = 47.0±1.1 μM



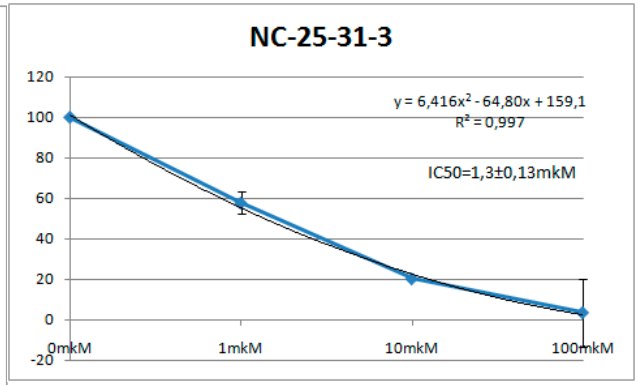
Compound **11**: IC_{50} = 0.47±0.01 μM



Compound **12**: IC_{50} = 0.035±0.0001 μM

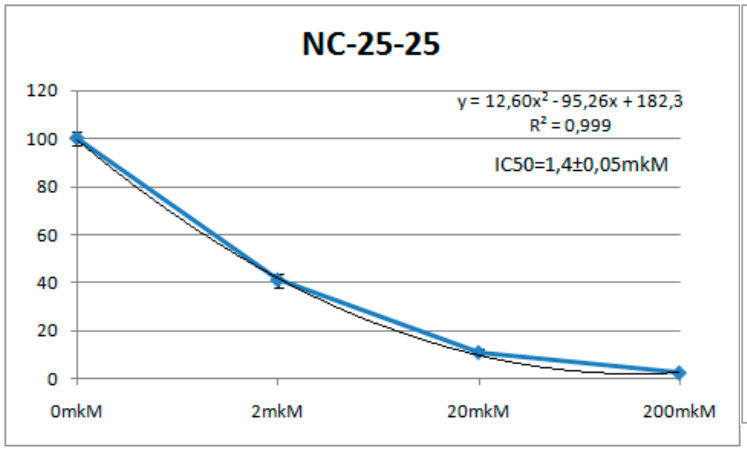


Compound **13**: IC_{50} = 5.8±0.1 μM

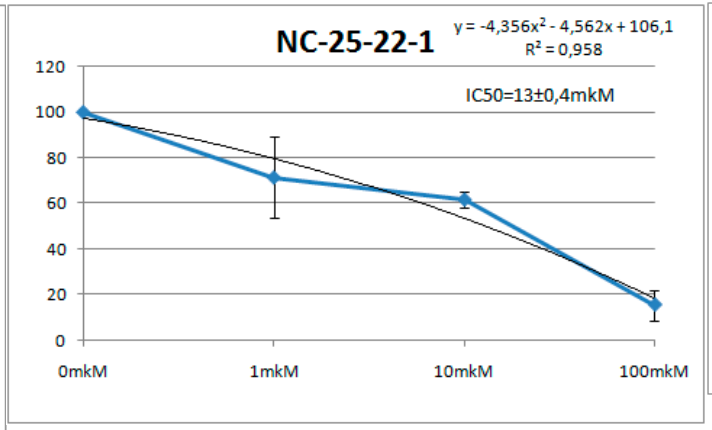


Compound **15**: IC_{50} = 1.3±0.13 μM

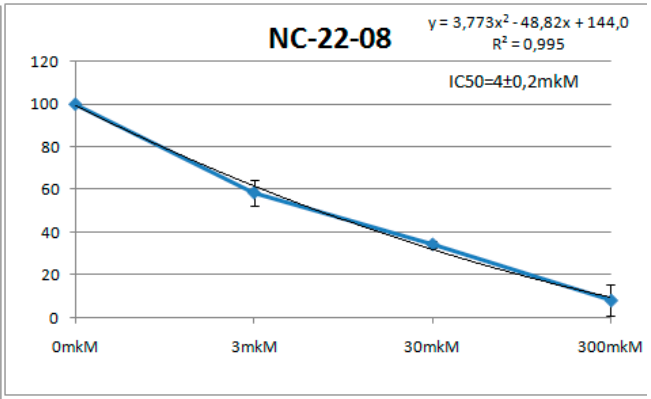
Figure S40A–F: The curves for AChE inhibition by compounds **5**, **7**, **11**, **12**, **13**, **15.**



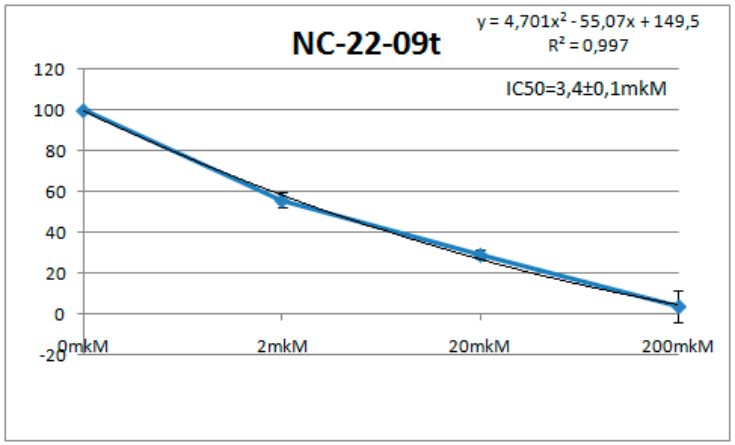
Compound **16**: IC_{50} = 1.4±0.05 μM



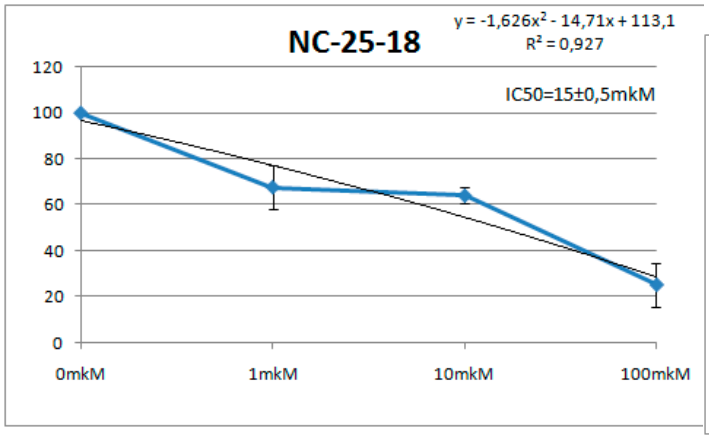
Compound **21**: IC_{50} = 13±0.4 μM



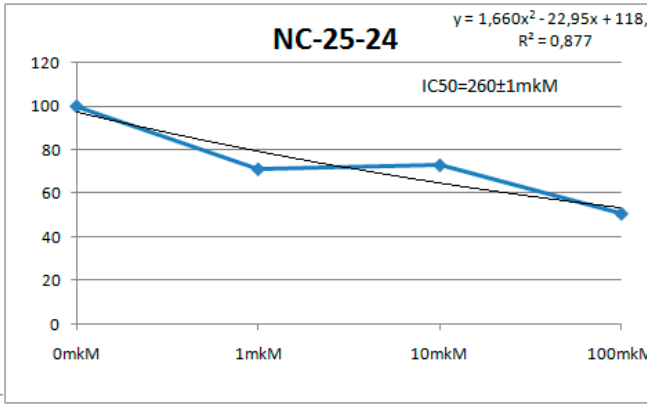
Compound **24**: IC_{50} = 4.0±0.2 μM



Compound **25**: IC_{50} = 3.4±0.1 μM



Compound **3**: IC_{50} = 15.0±0.5 μM



Compound **4**: IC_{50} = 260.0±1.1 μM

Figure S40G–L: The curves for AChE inhibition by compounds **16**, **21**, **24**, **25**, **3**, **4.**