Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Benign Synthesis of Fused-thiazoles with Enone-based Natural Products and Drugs for Lead Discovery

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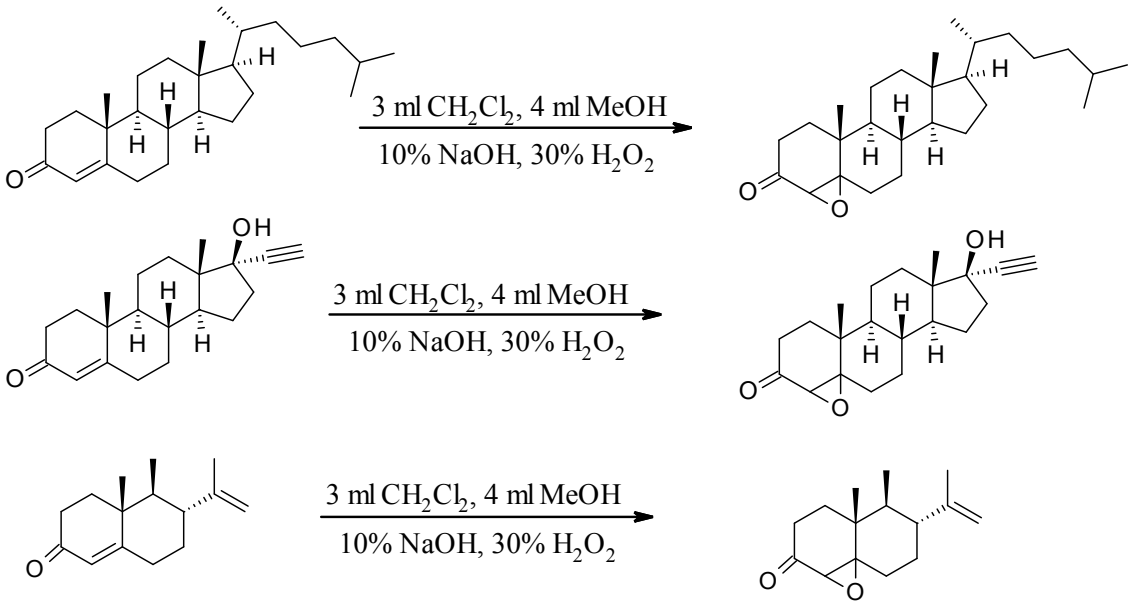
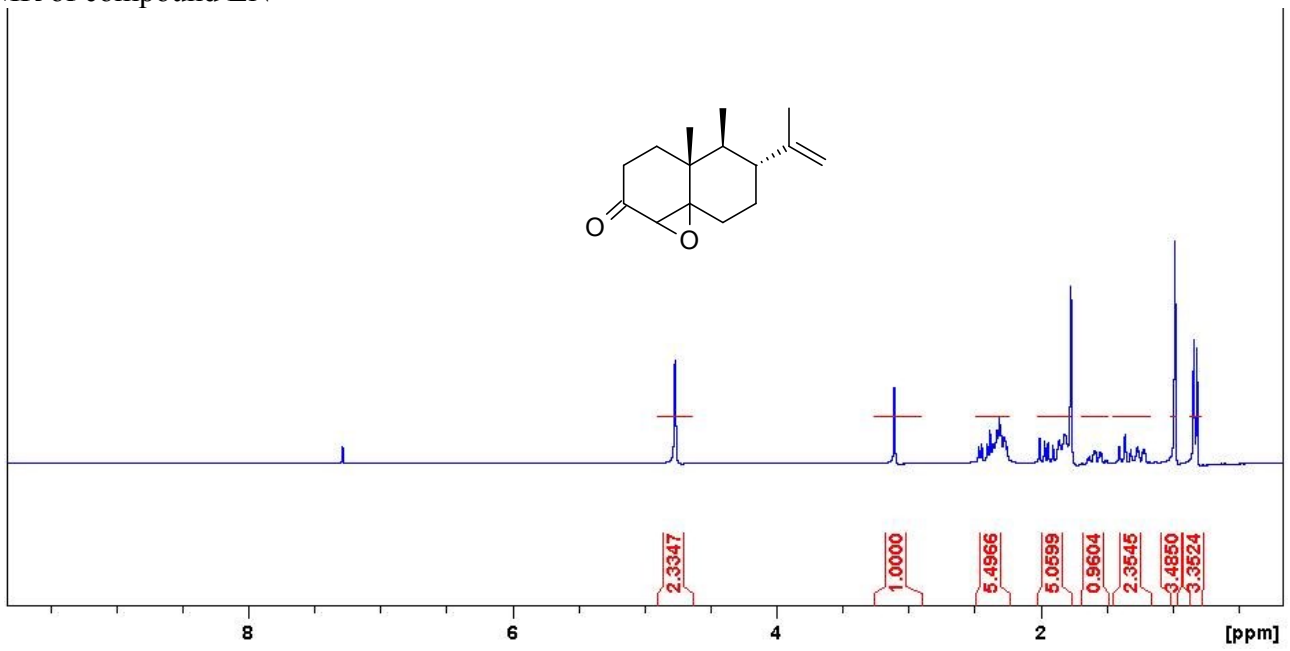


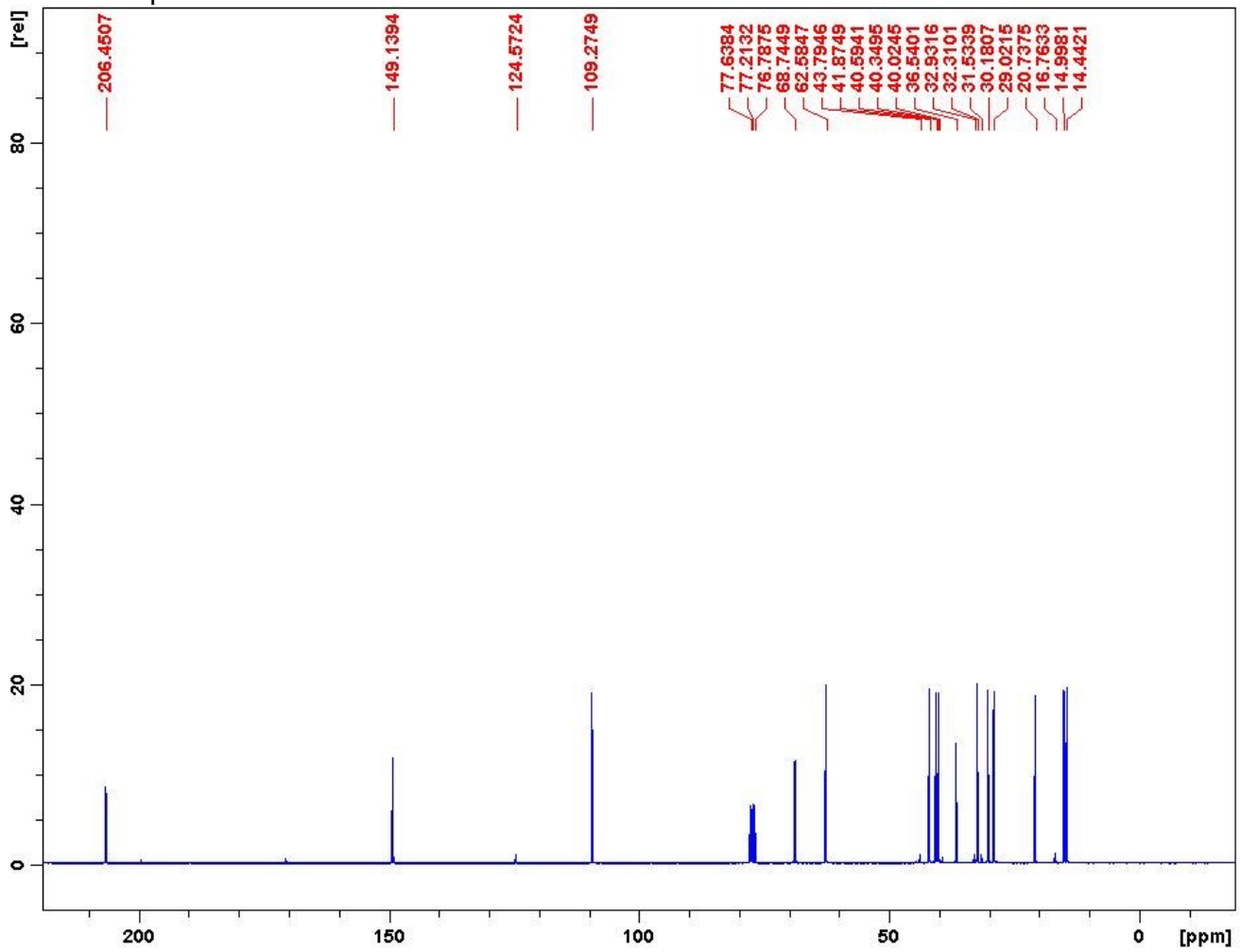
Scheme. The synthesis of epoxy-ketone

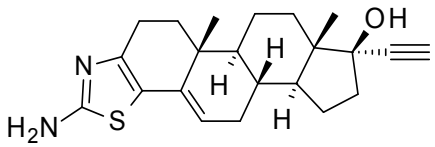
(1aS,4aS,8aR)-6-isopropenyl-4,4a-dimethyl-3,4,5,6,7,8-hexahydro-1aH-naphtho[1,8a-b] oxiren-2-one (EN)

^{1}H NMR of compound **EN**



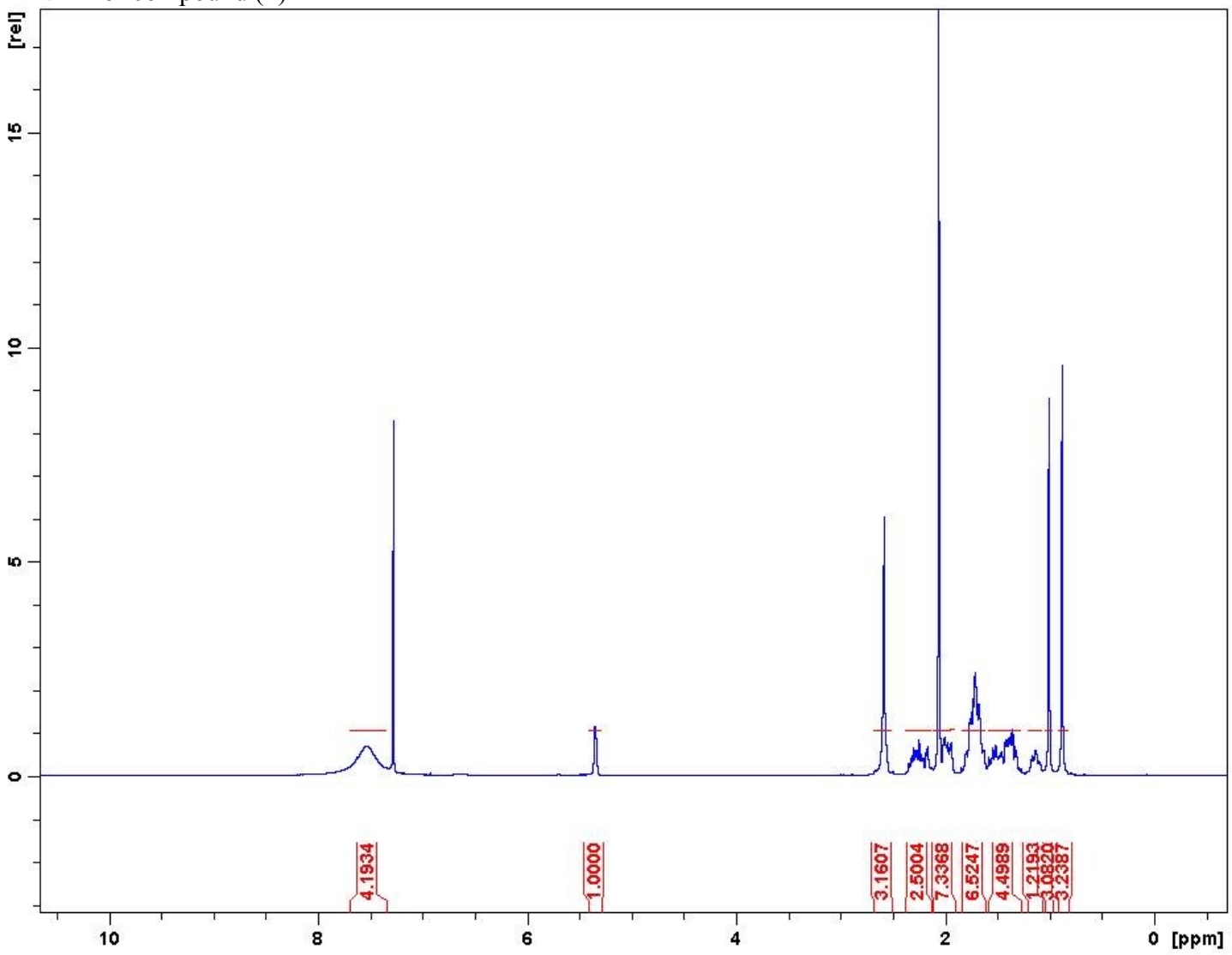
^{13}C NMR of compound **EN**



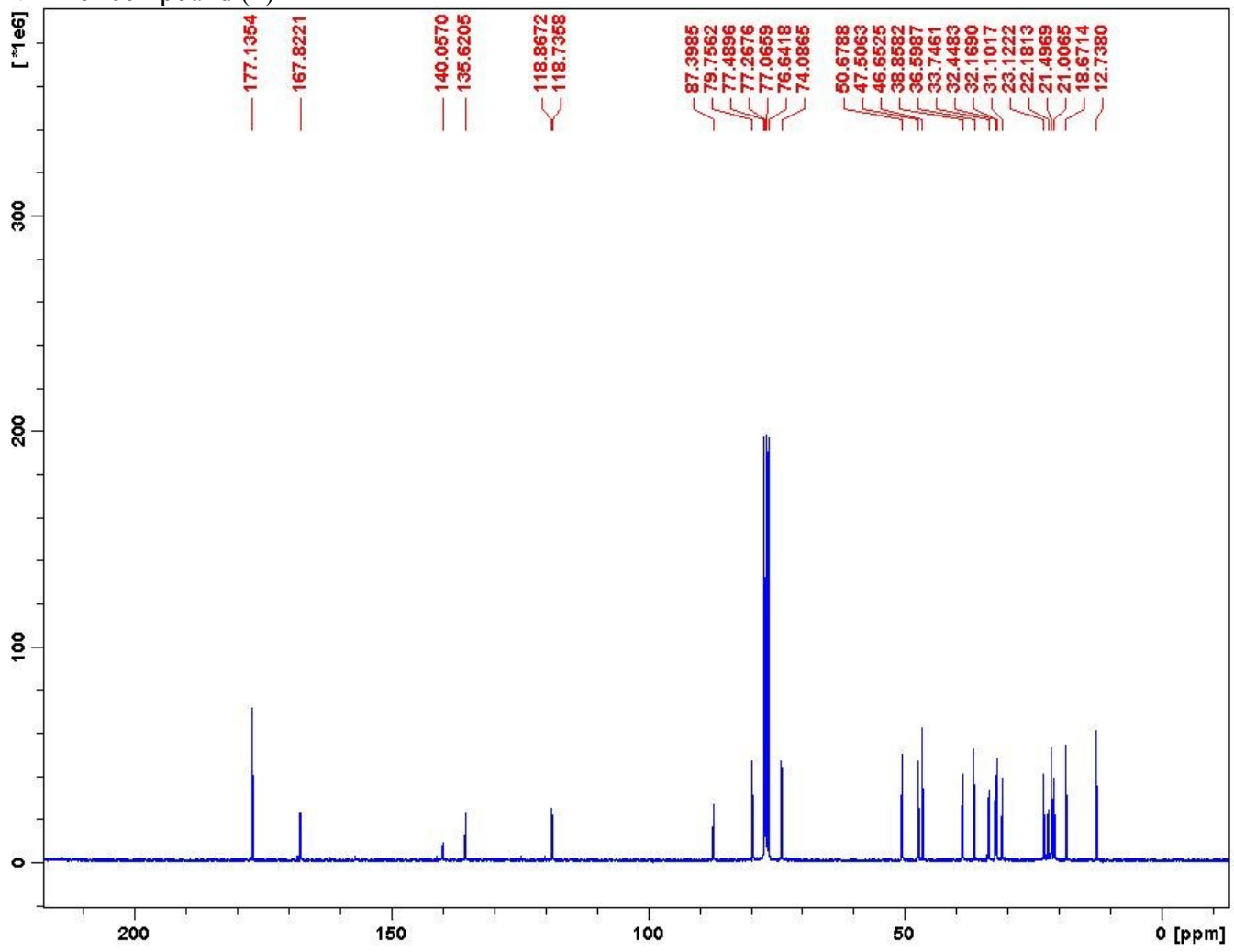


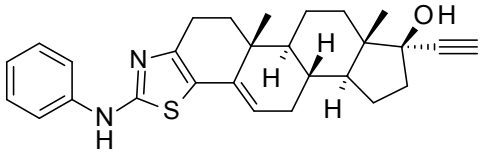
(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-7-amino-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (1).

^{1}H NMR of compound (**1**)



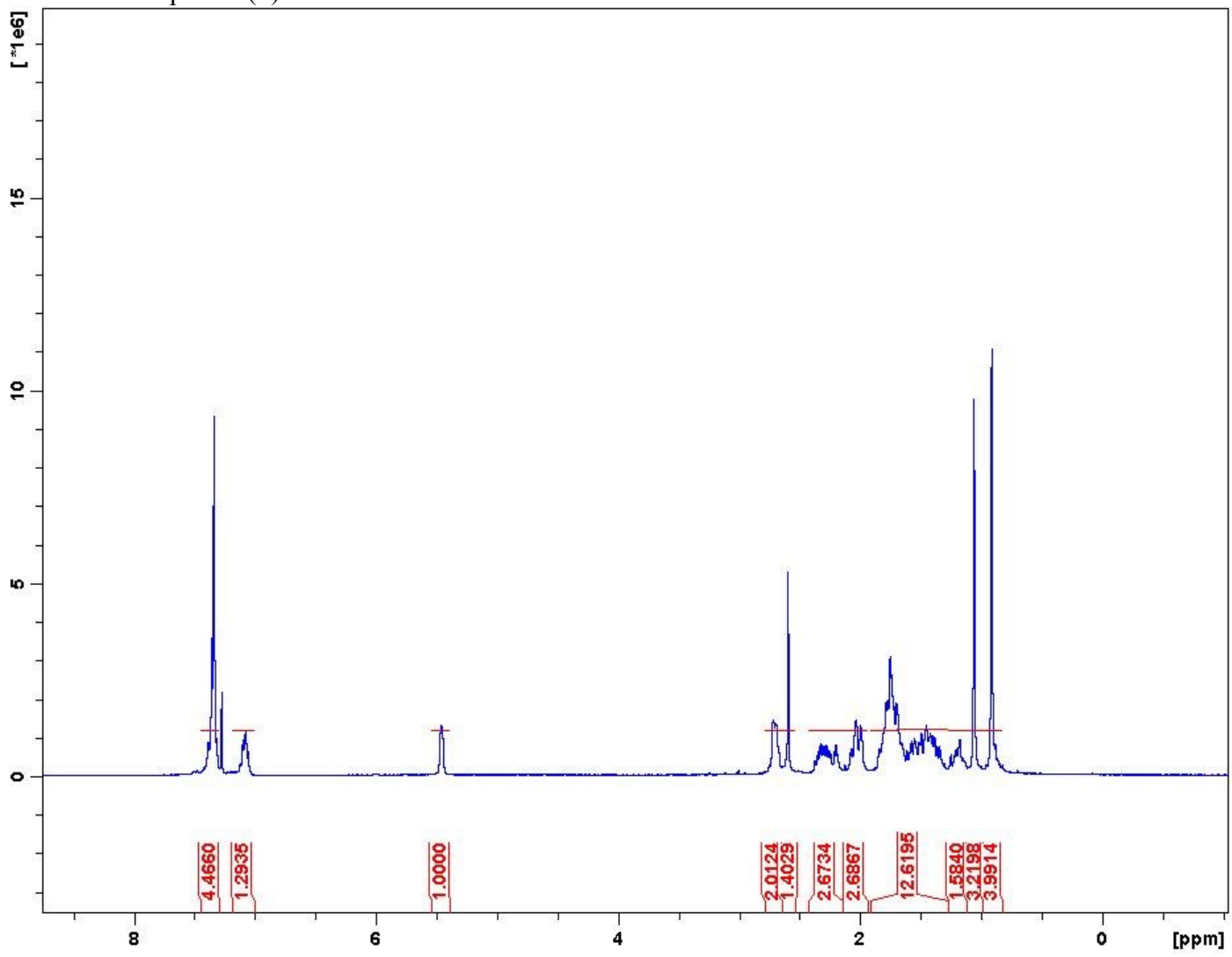
^{13}C NMR of compound (**1**)



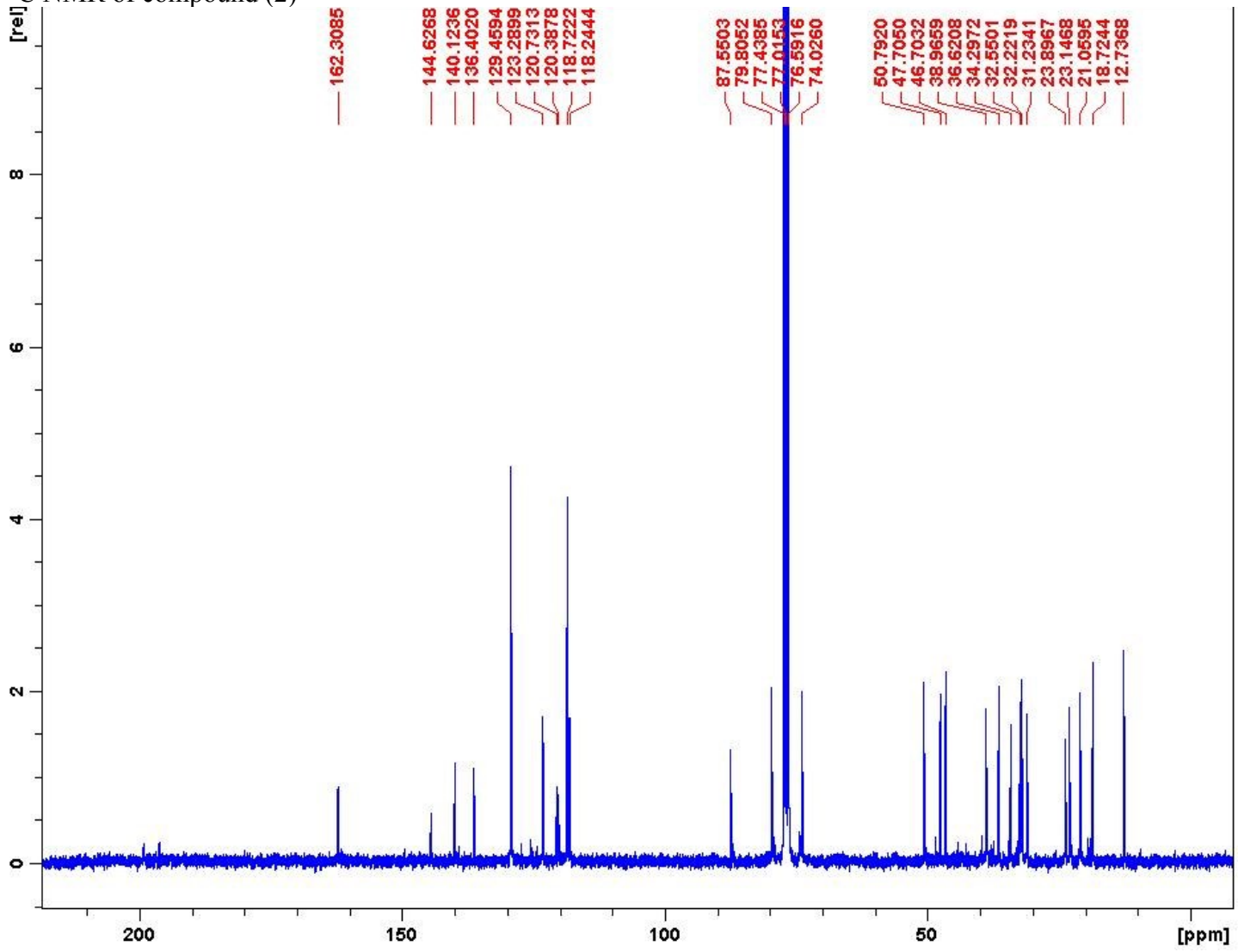


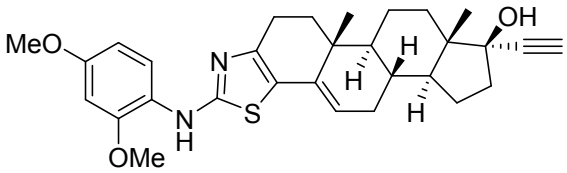
1-[(1R,13R,14R)-17-ethynyl-17-hydroxy-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-yl]guanidine (2).

^{1}H NMR of compound (**2**)



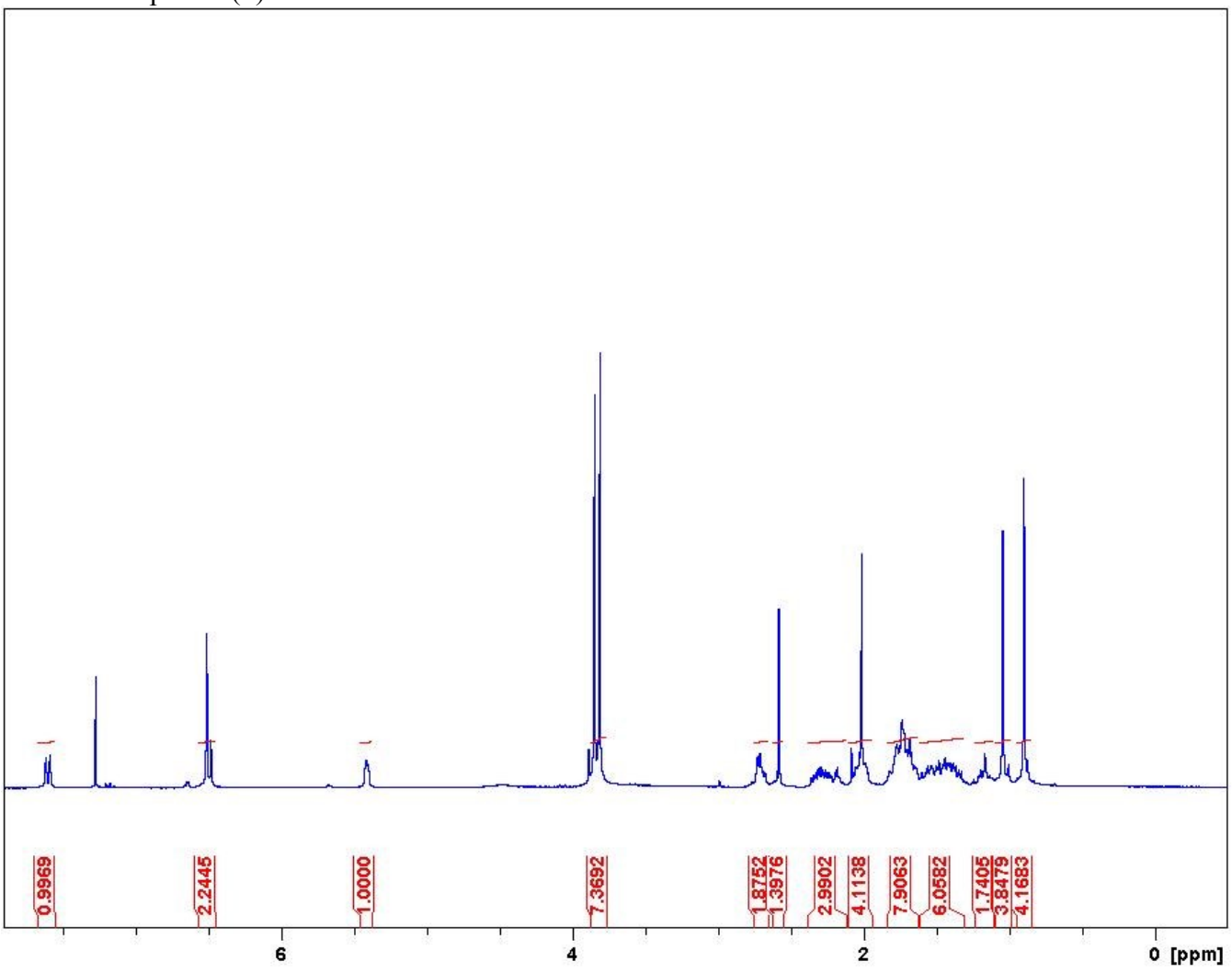
^{13}C NMR of compound (**2**)



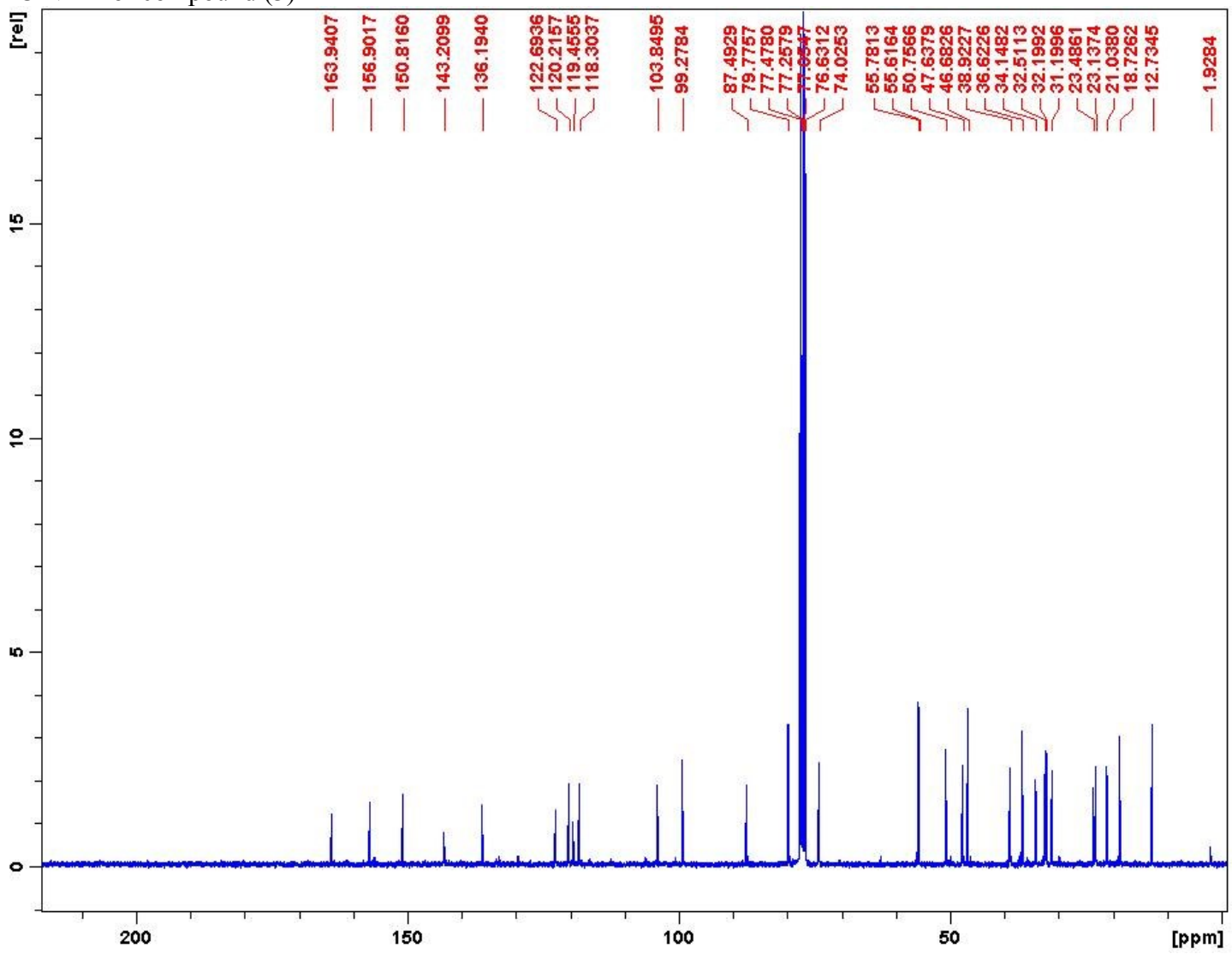


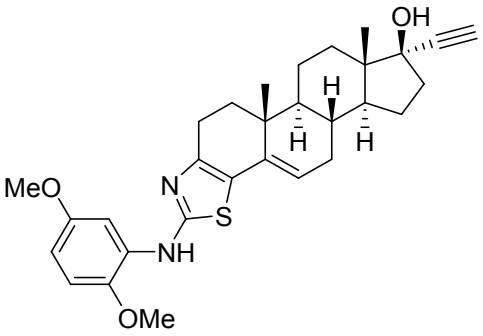
(1R,13R,14S)-7-(2,4-dimethoxyanilino)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (3).

^{1}H NMR of compound (**3**)



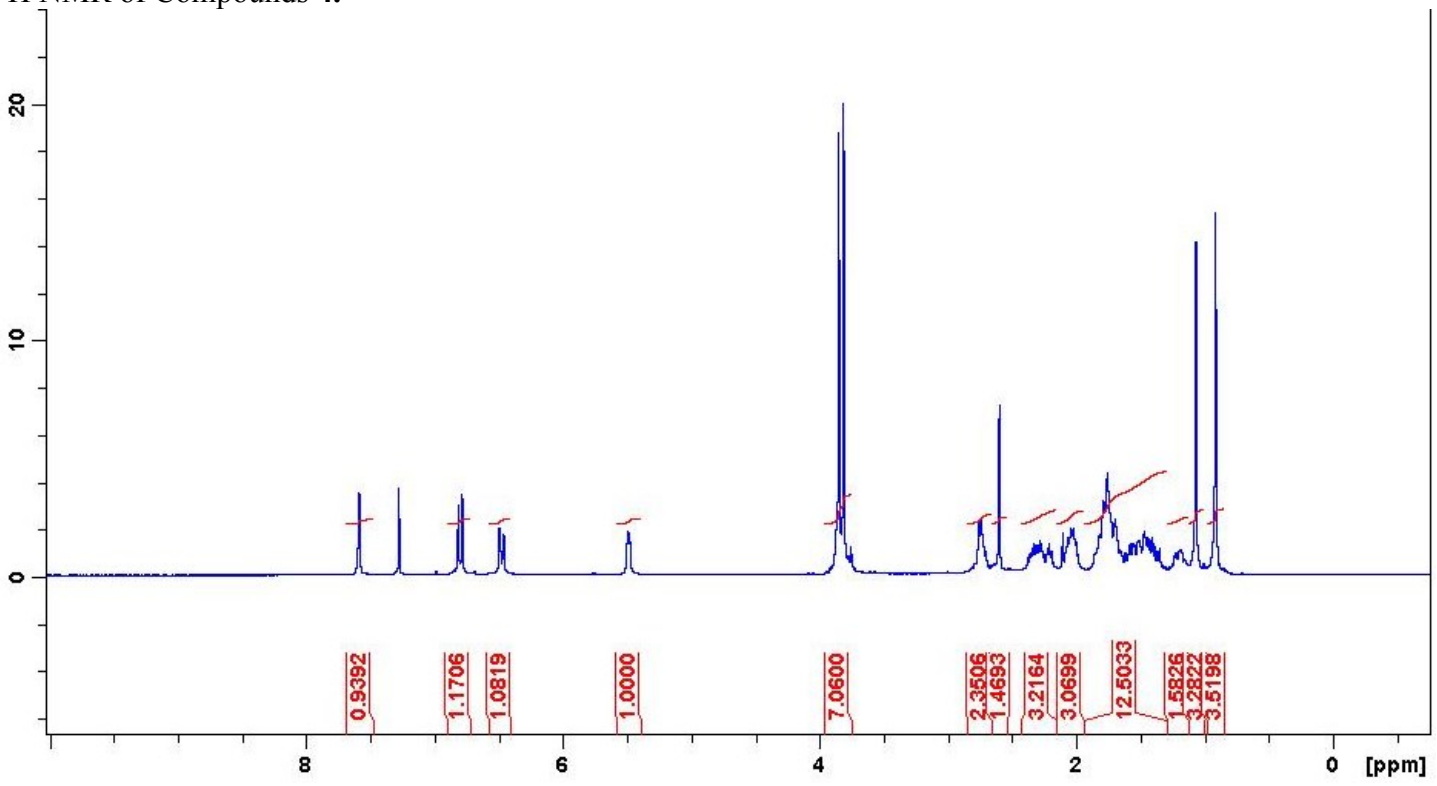
^{13}C NMR of compound (**3**)



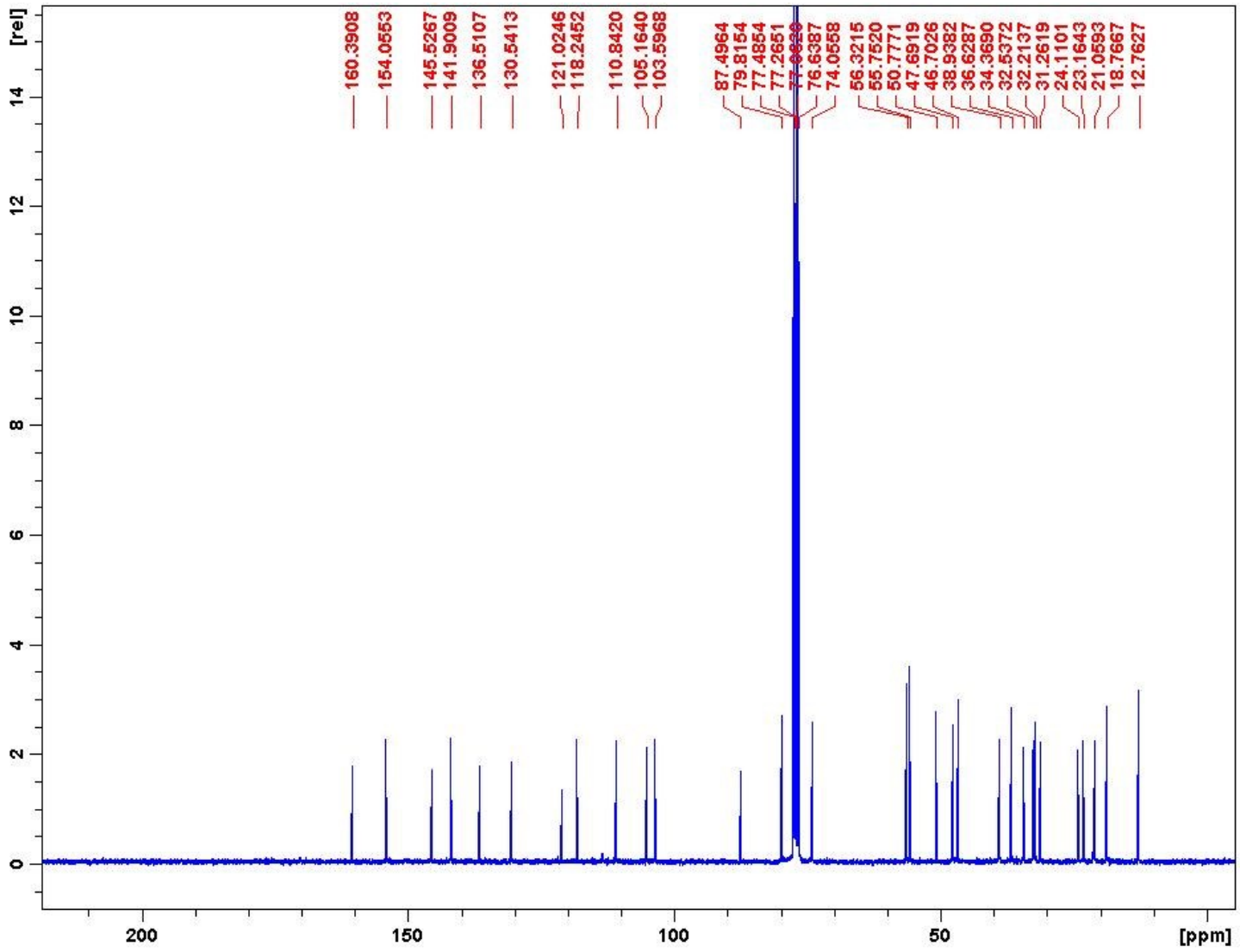


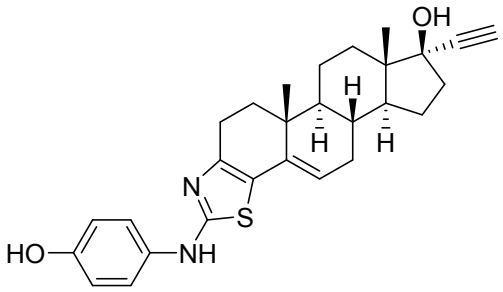
(1S,2R,13R,14S,17R,18S)-7-(2,5-dimethoxyanilino)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (4).

^{1}H NMR of Compounds **4.**



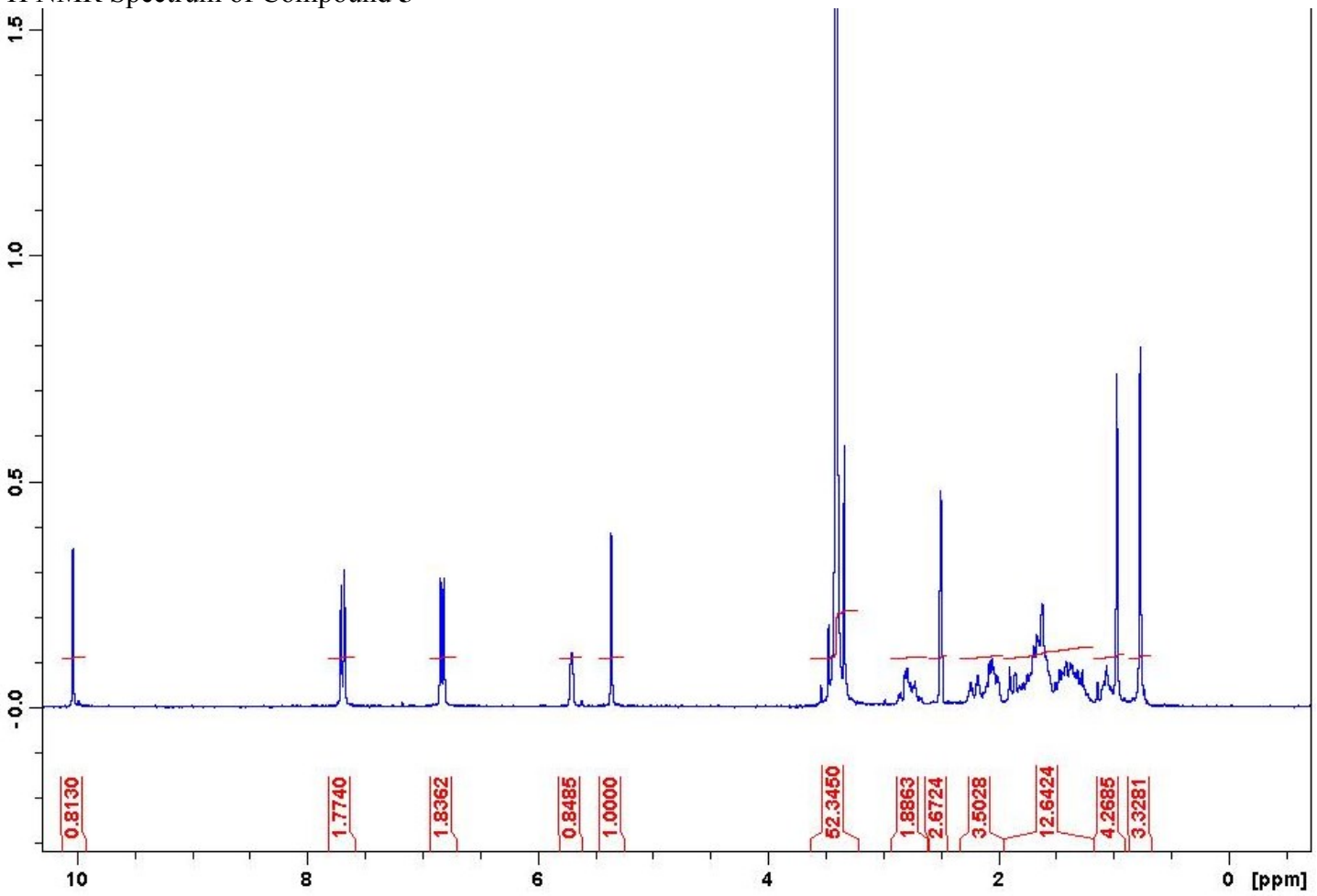
^{13}C NMR of Compounds 4.



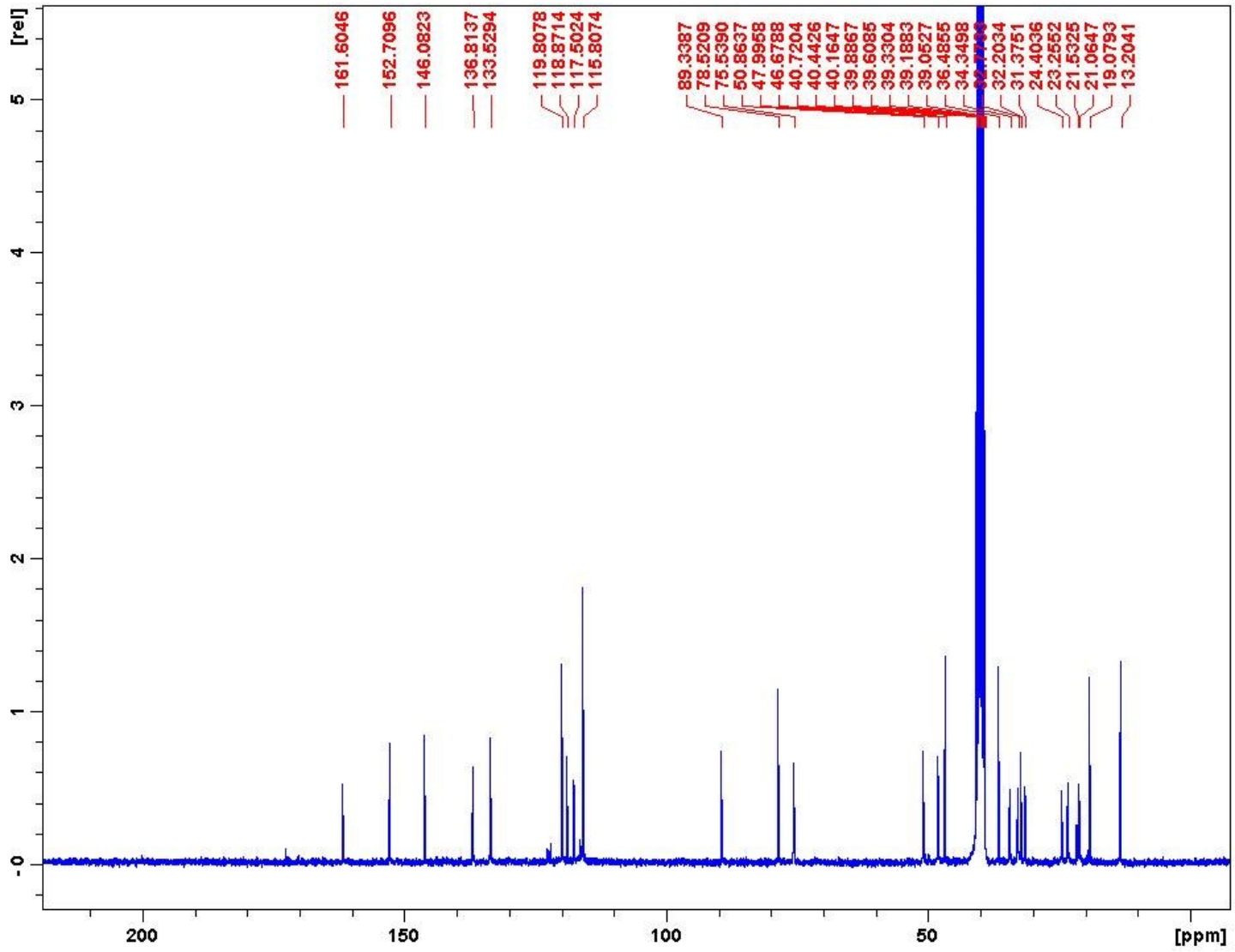


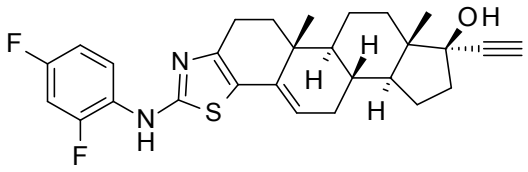
(1S,2R,13R,14S,17R,18S)-17-ethynyl-7-(4-hydroxyanilino)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (5).

^{1}H NMR Spectrum of Compound **5**



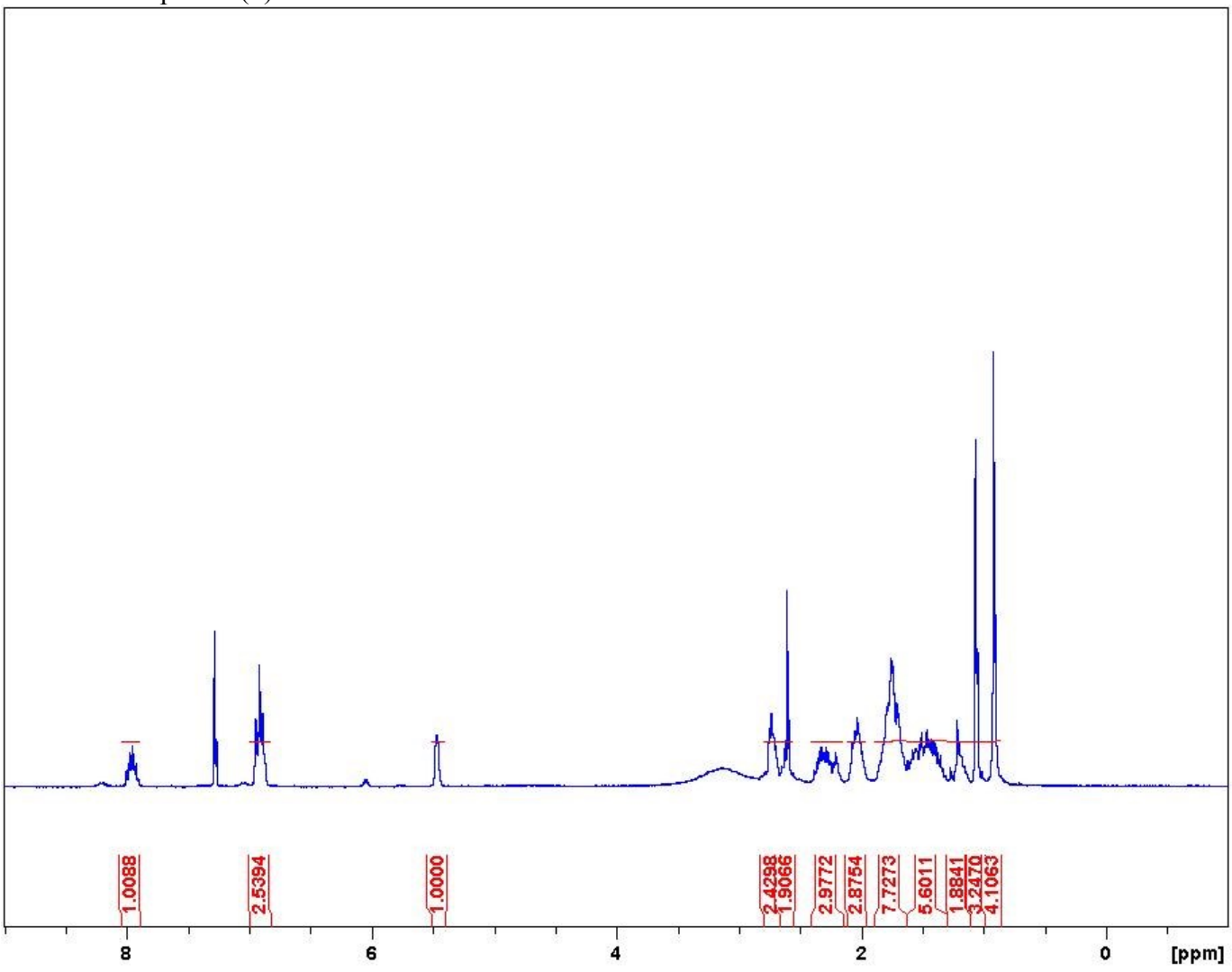
^{13}C NMR Spectrum of Compound **5**



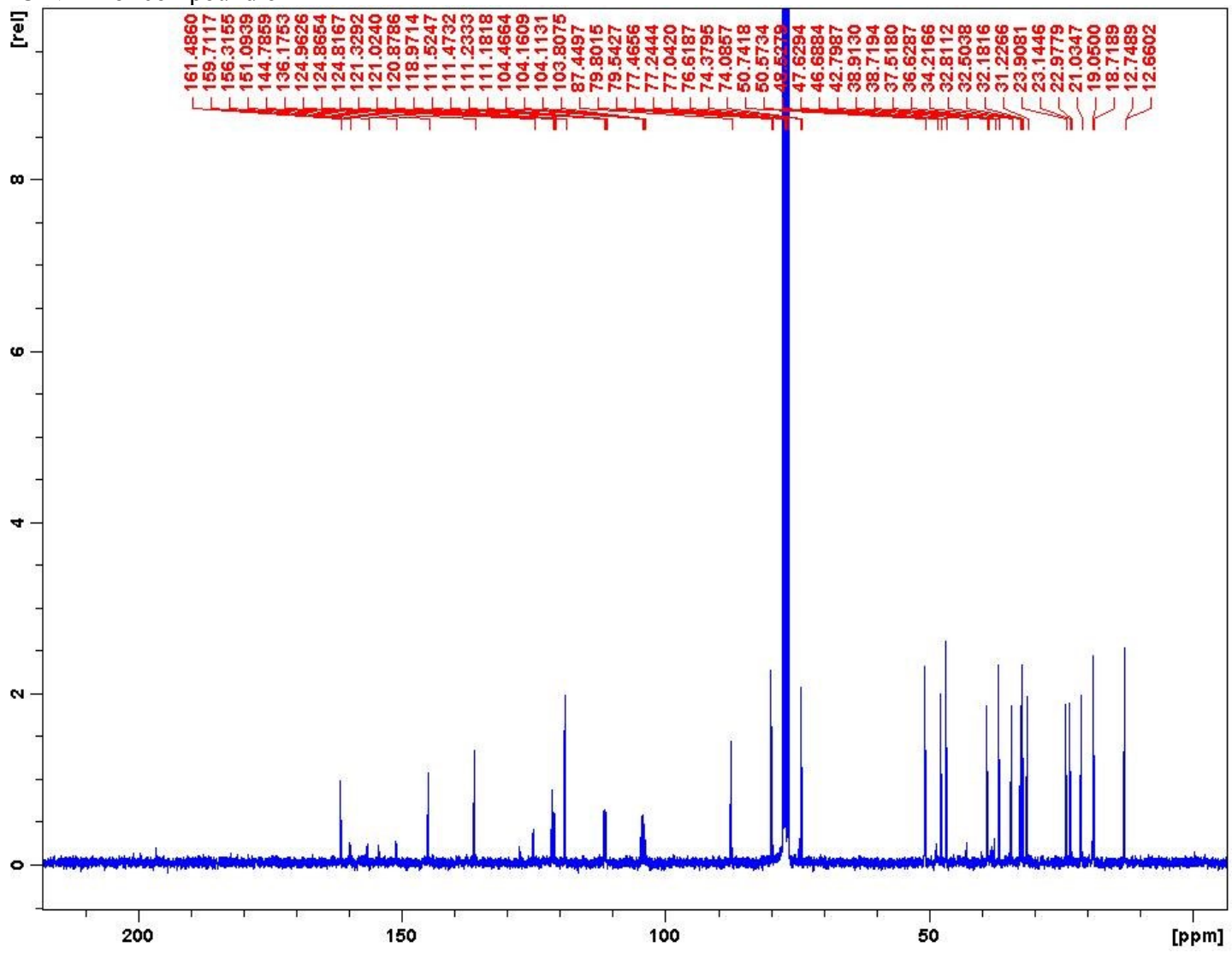


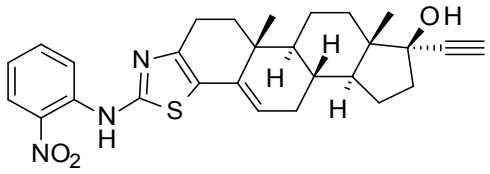
(1S,2R,13R,14S,17R,18S)-7-(2,4-difluoroanilino)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (6).

^{1}H NMR of compound (**6**)



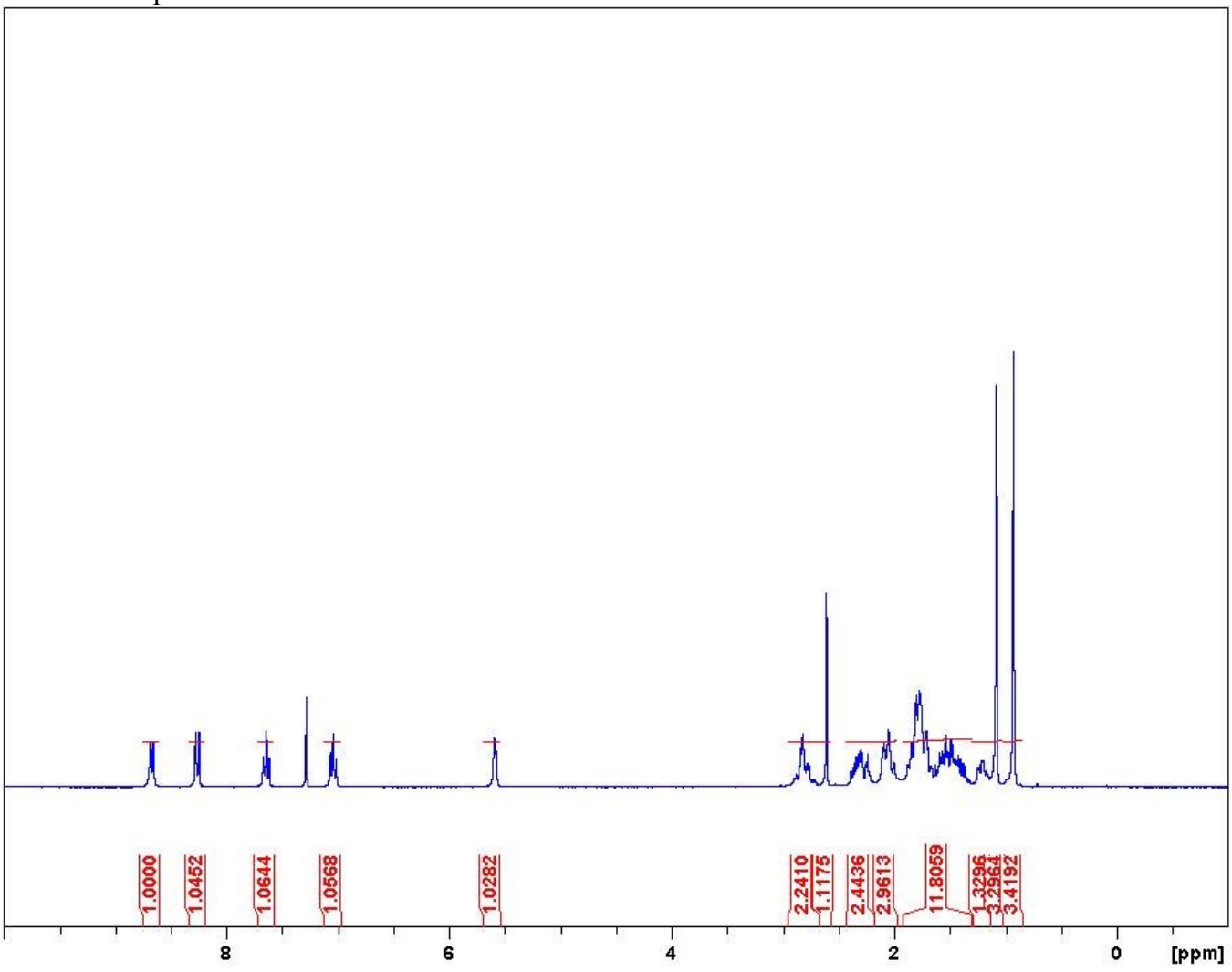
^{13}C NMR of compound **6**



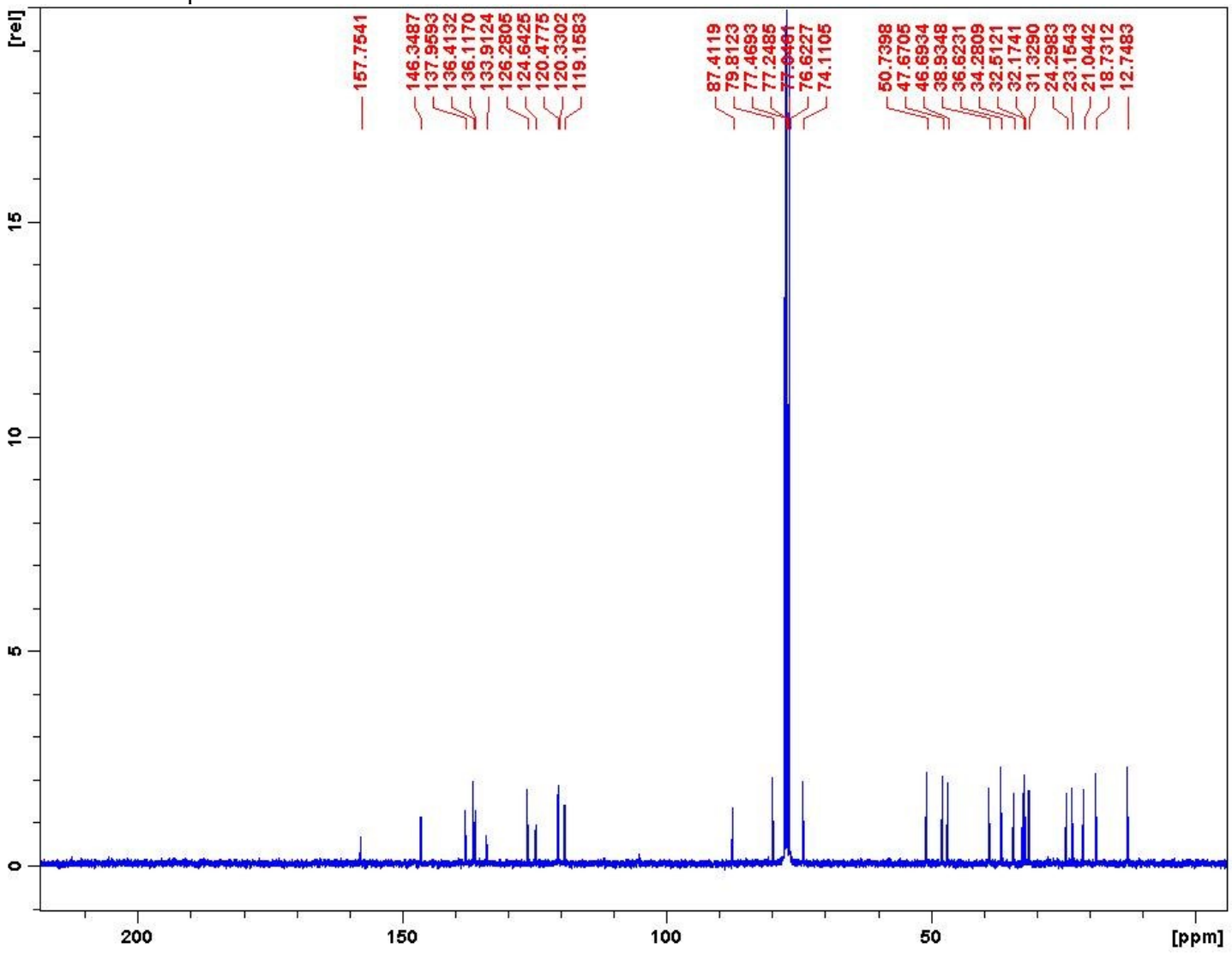


(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-ethynyl-2,18-dimethyl-7-(2-nitroanilino)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (7).

^{1}H NMR of compound **7**

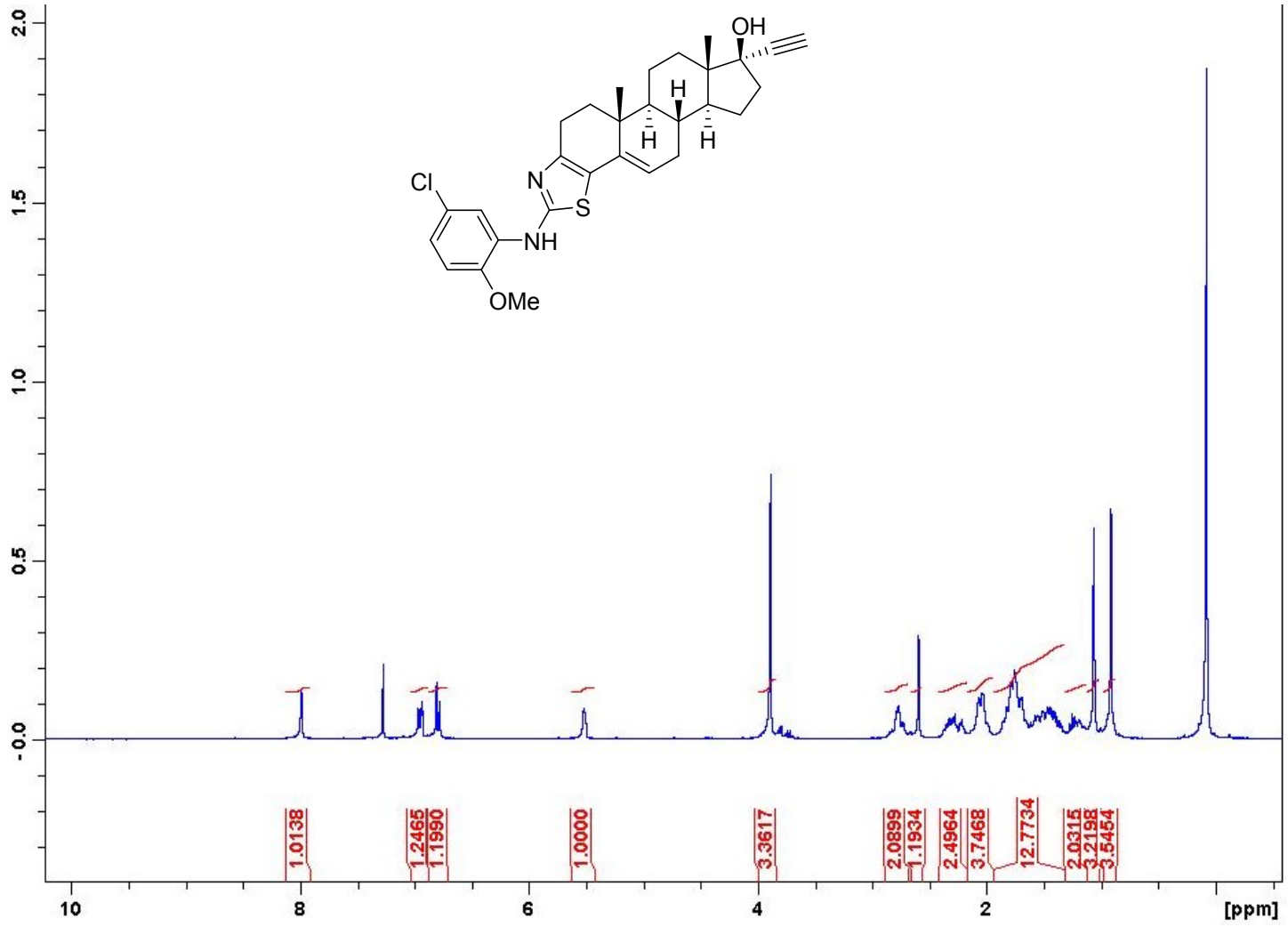


^{13}C NMR of compound **7**

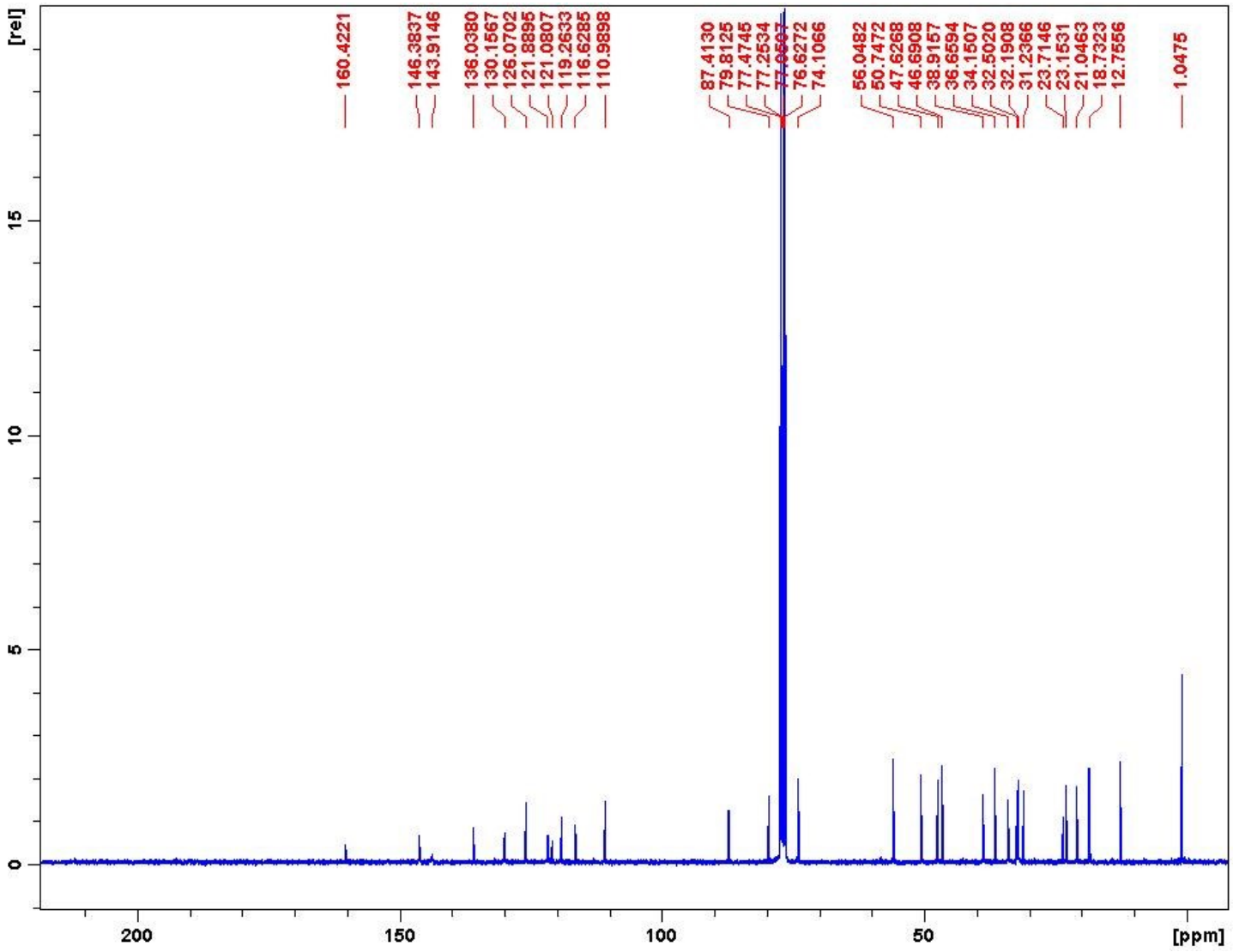


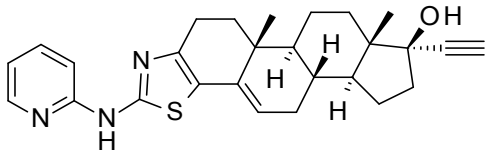
(1S,2R,13R,14S,17R,18S)-7-(5-chloro-2-methoxy-anilino)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (8)

^{1}H NMR of compound (**8**)



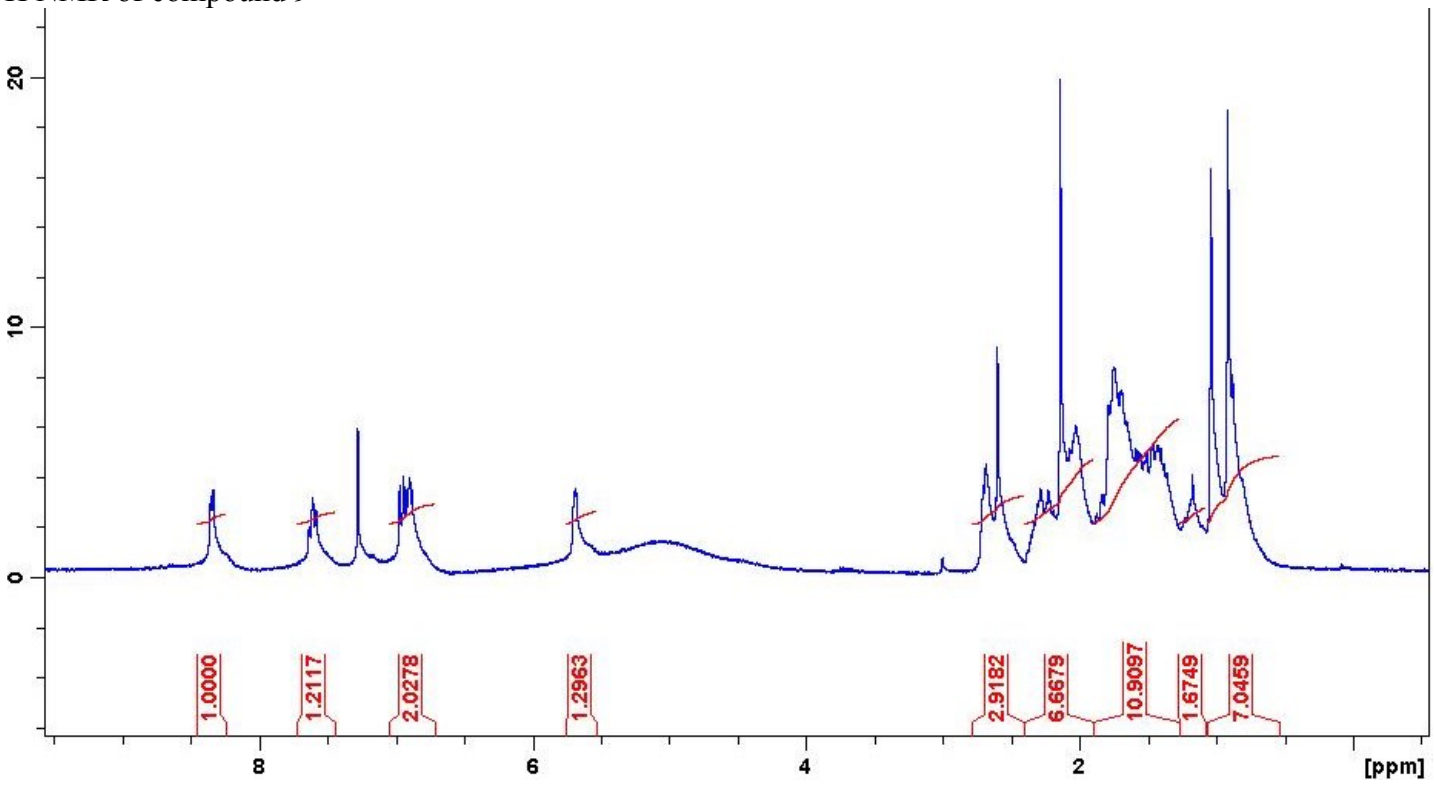
^{13}C NMR of compound (**8**)



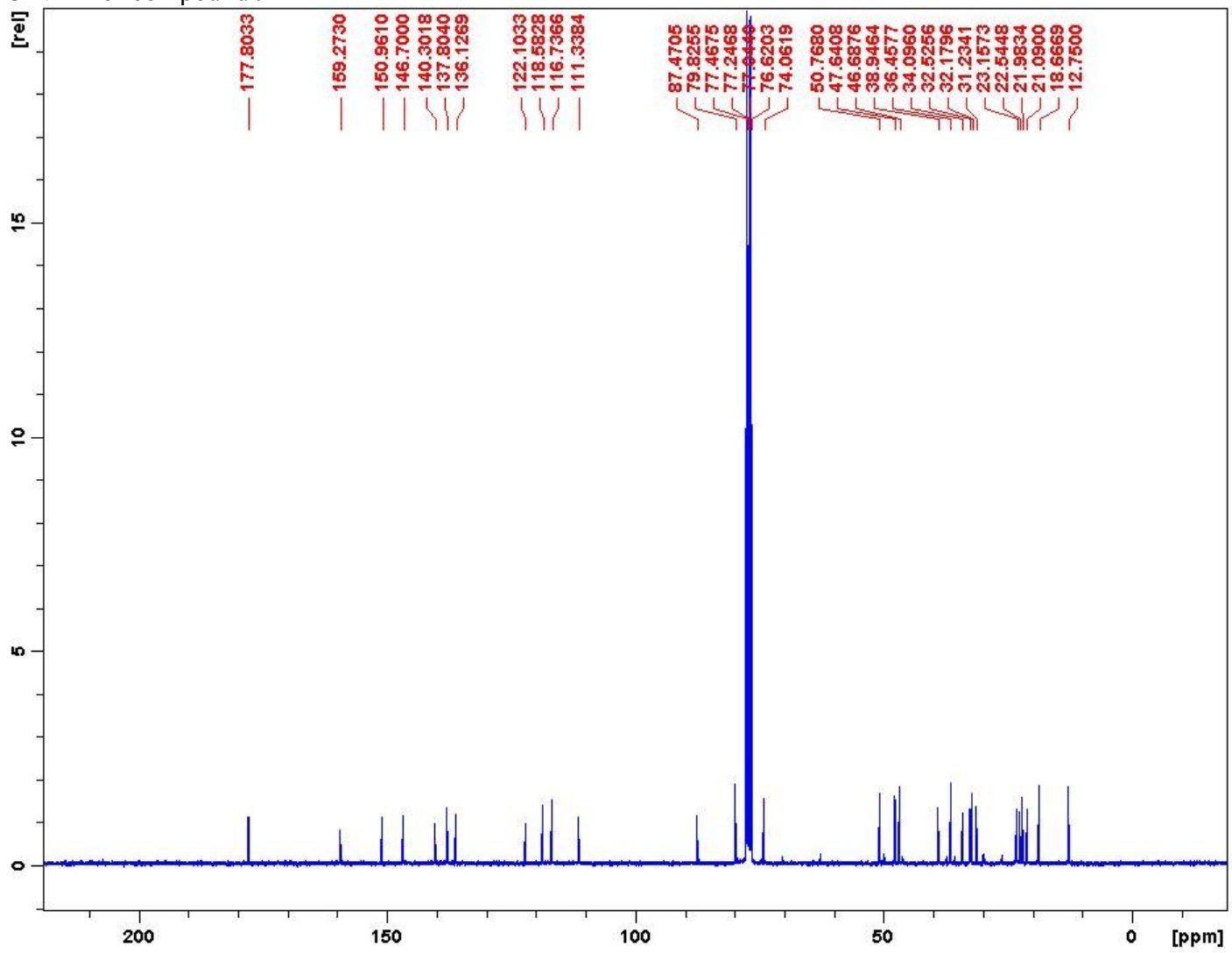


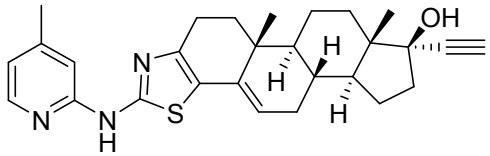
(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-(2-pyridylamino)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (9).

^{1}H NMR of compound **9**



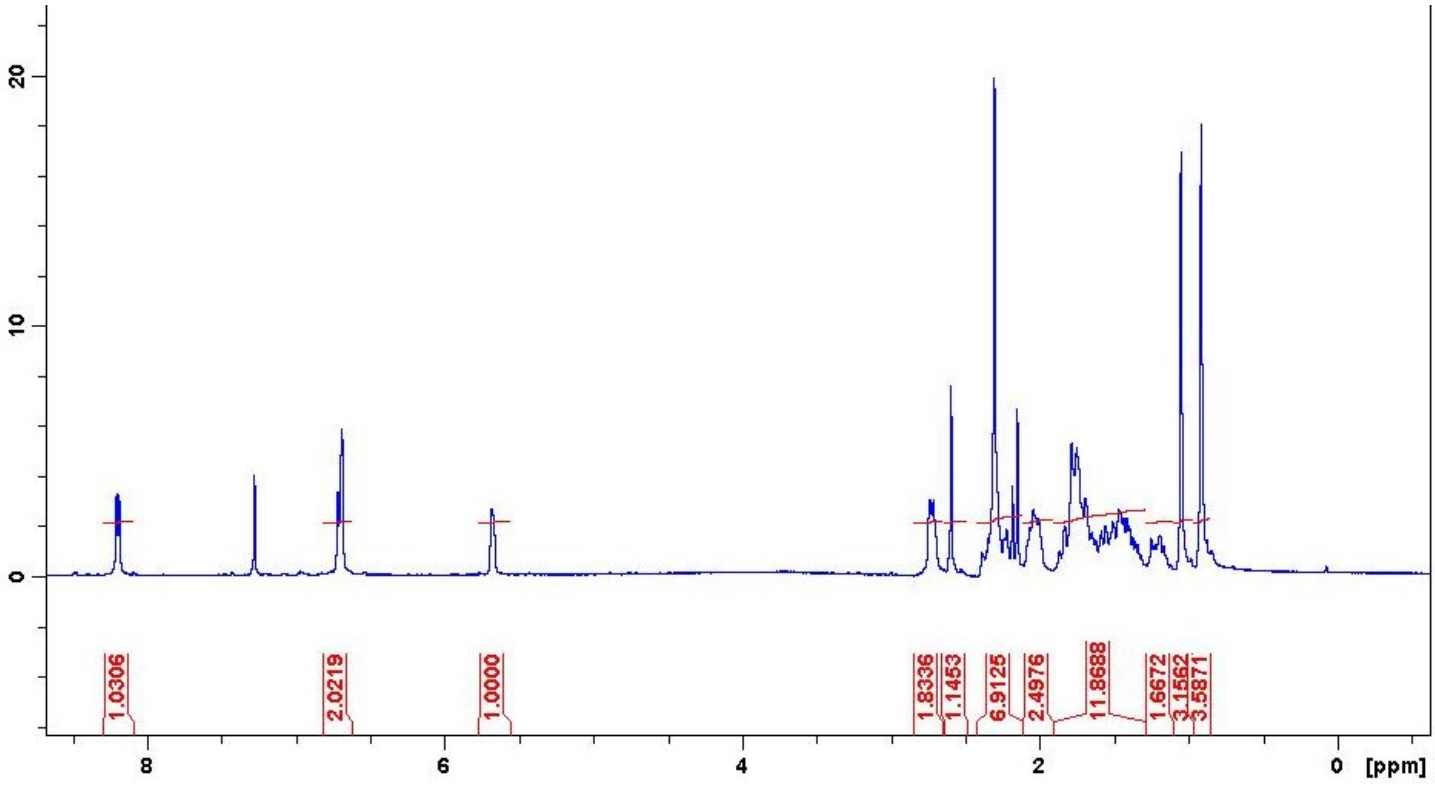
^{13}C NMR of compound **9**



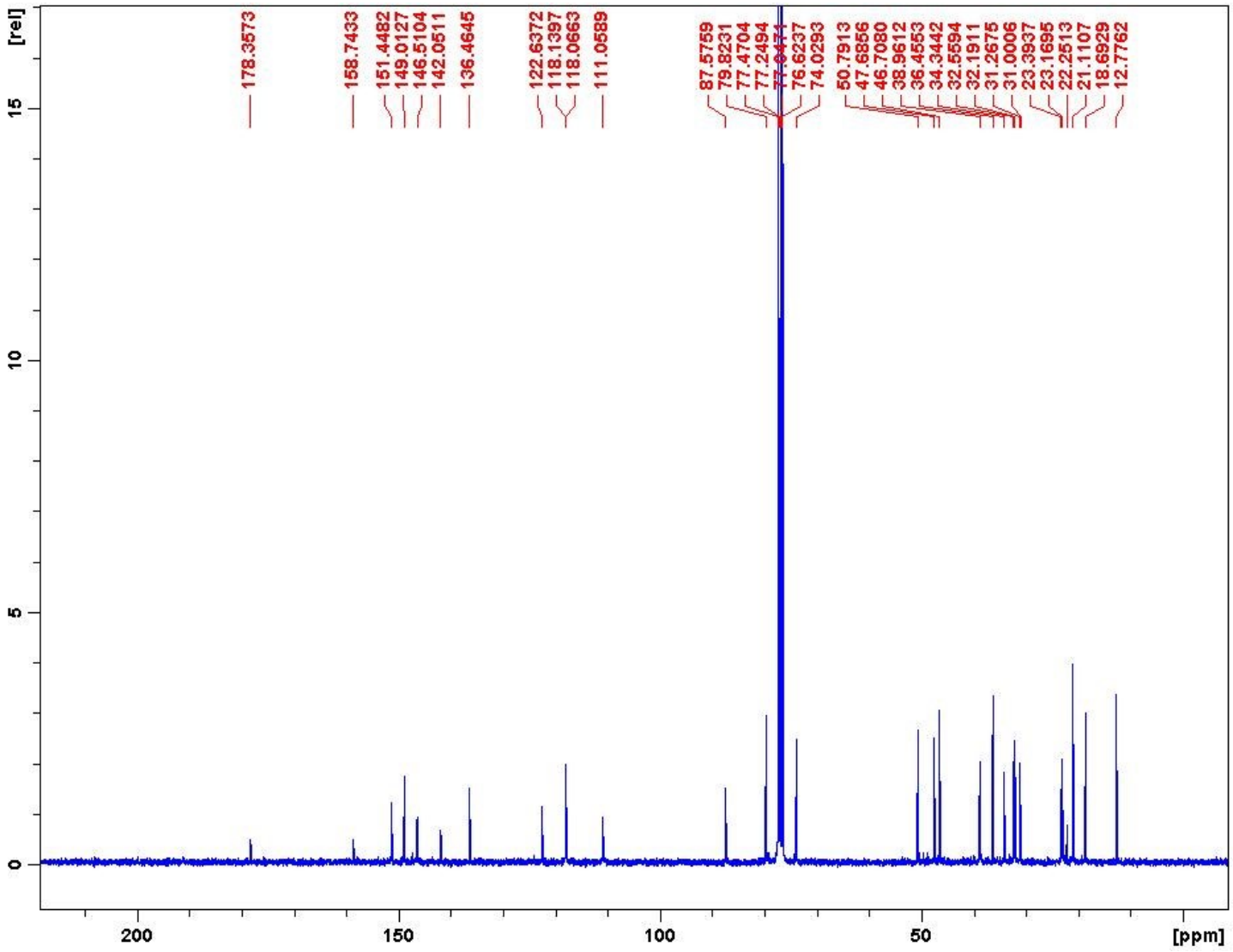


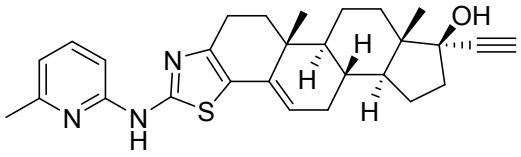
(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-ethynyl-2,18-dimethyl-7-[(4-methyl-2-pyridyl)amino]-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (10):

^{1}H NMR of compound (**10**)



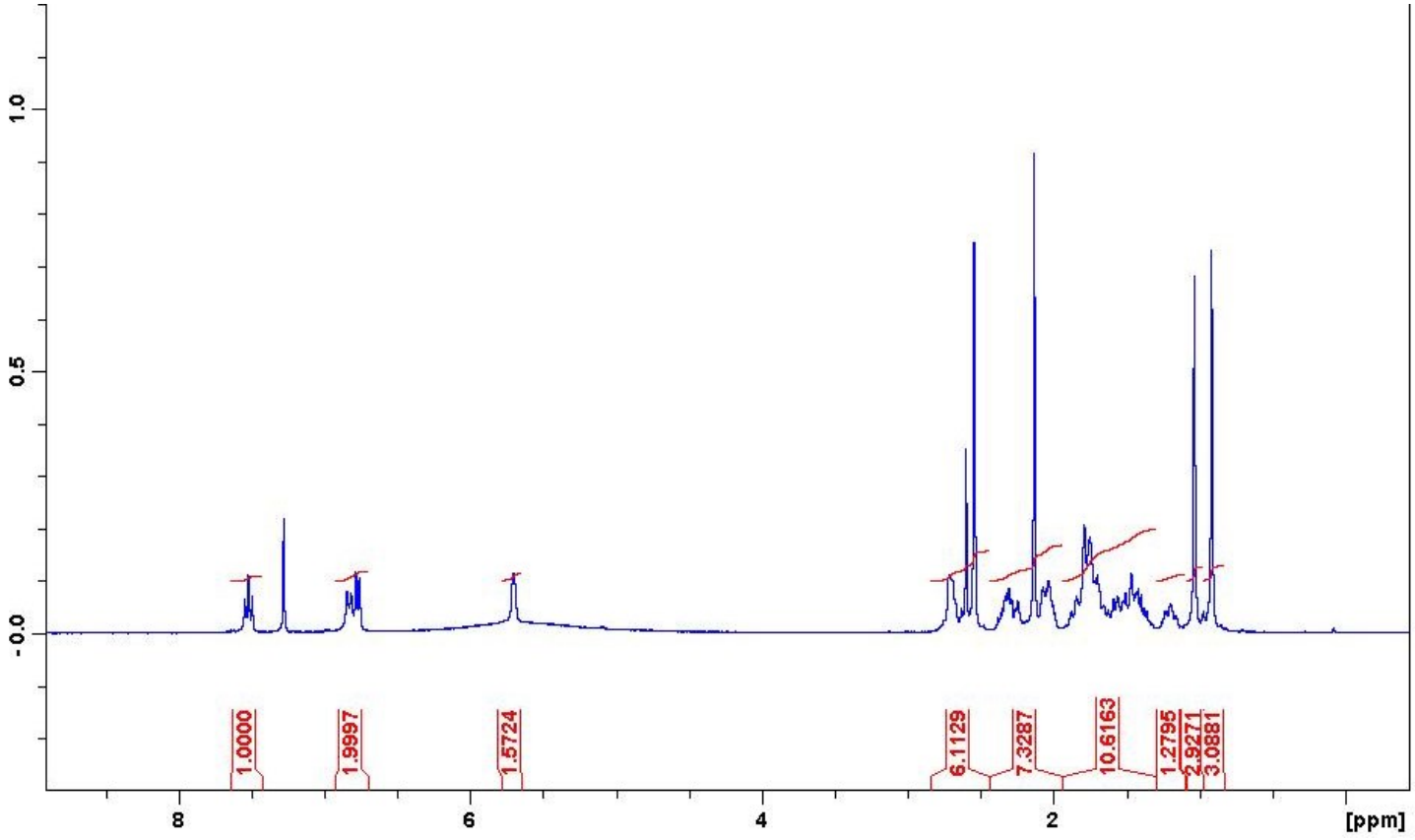
^{13}C NMR of compound (**10**)



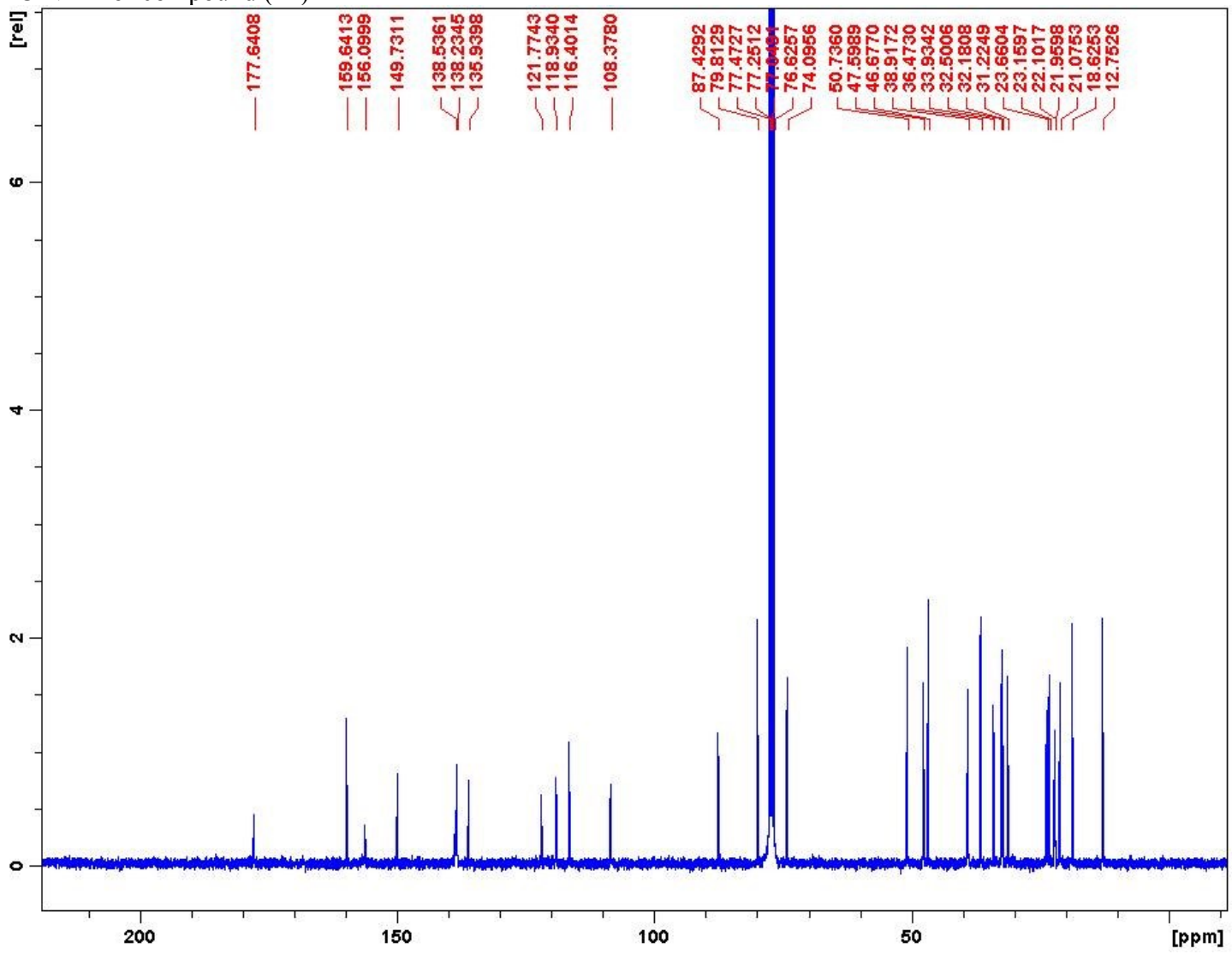


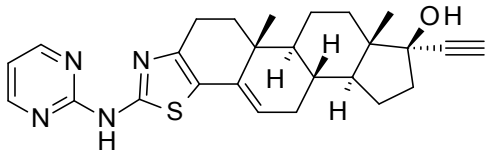
(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-[(6-methyl-2-pyridyl)amino]-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (11).

^{1}H NMR of compound **11**



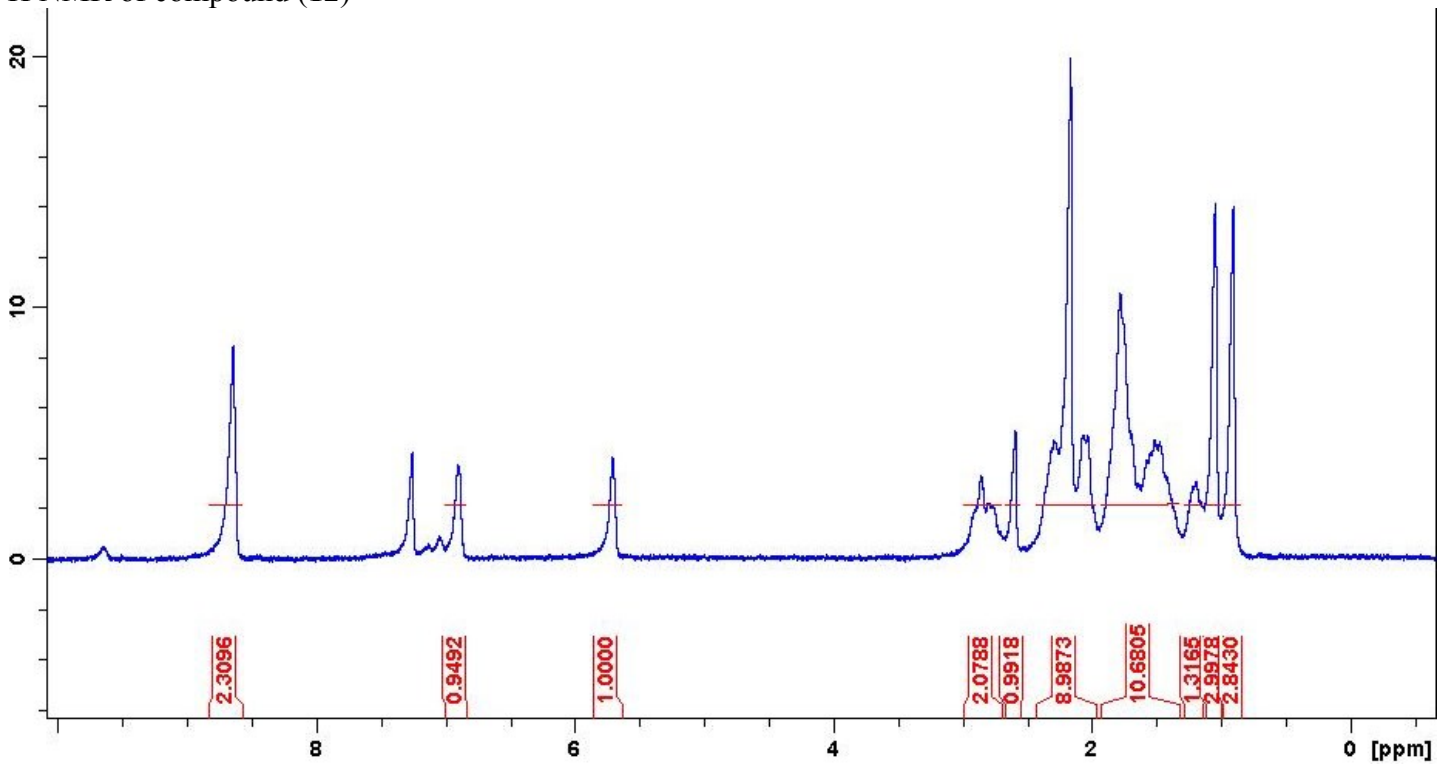
^{13}C NMR of compound (**11**)



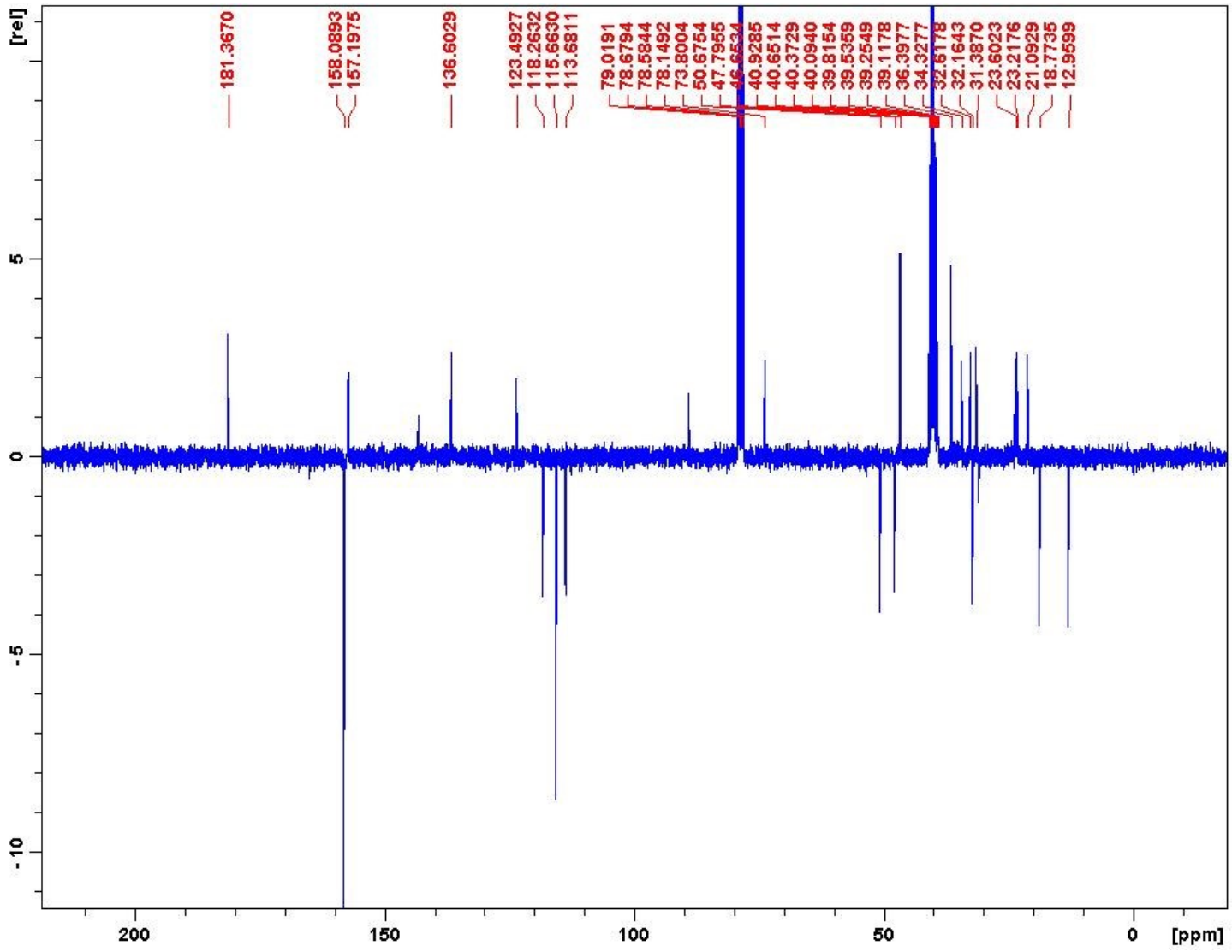


(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-(pyrimidin-2-ylamino)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (12).

^{1}H NMR of compound (**12**)



APT NMR spectrum of compound **12**


[rel]
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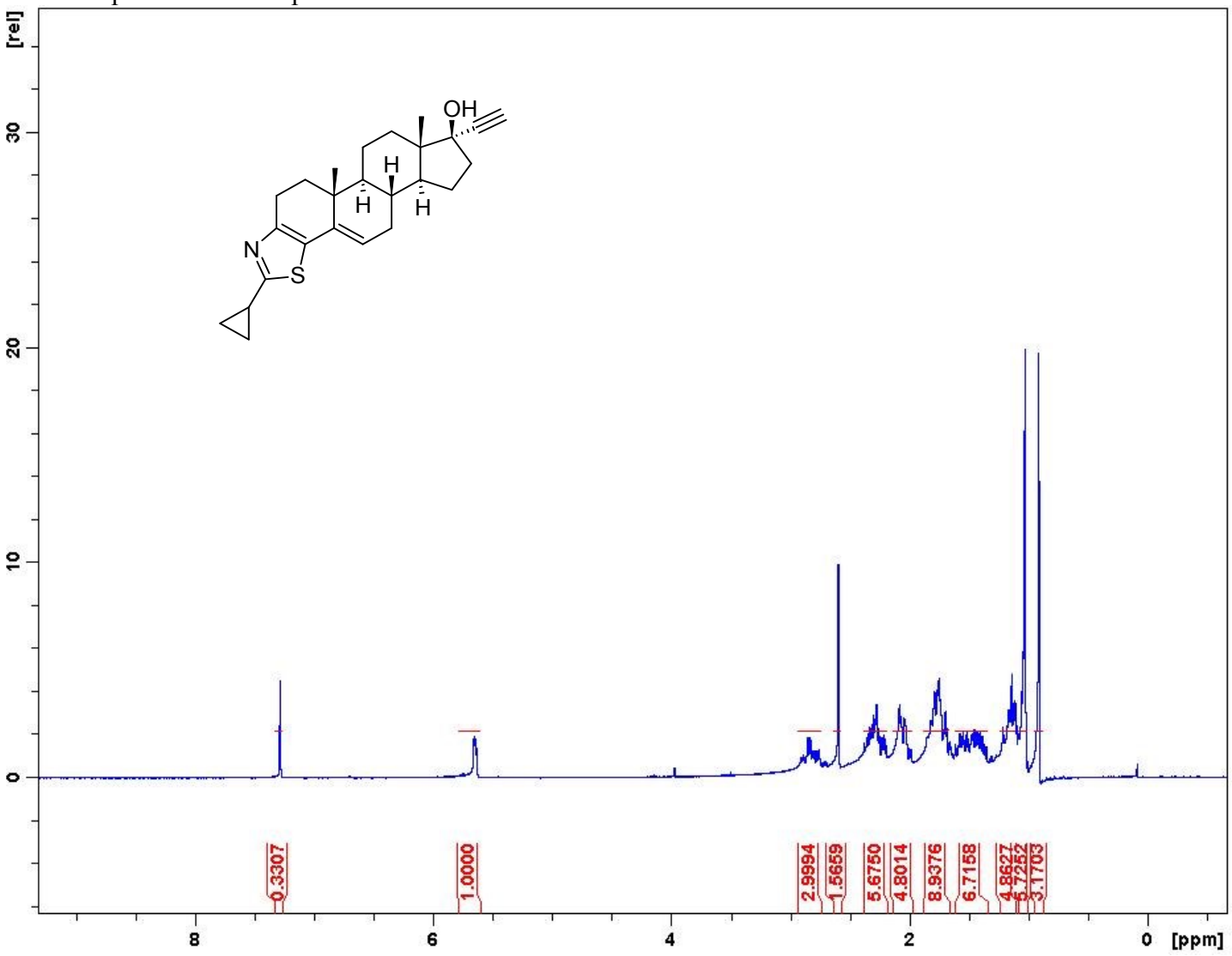
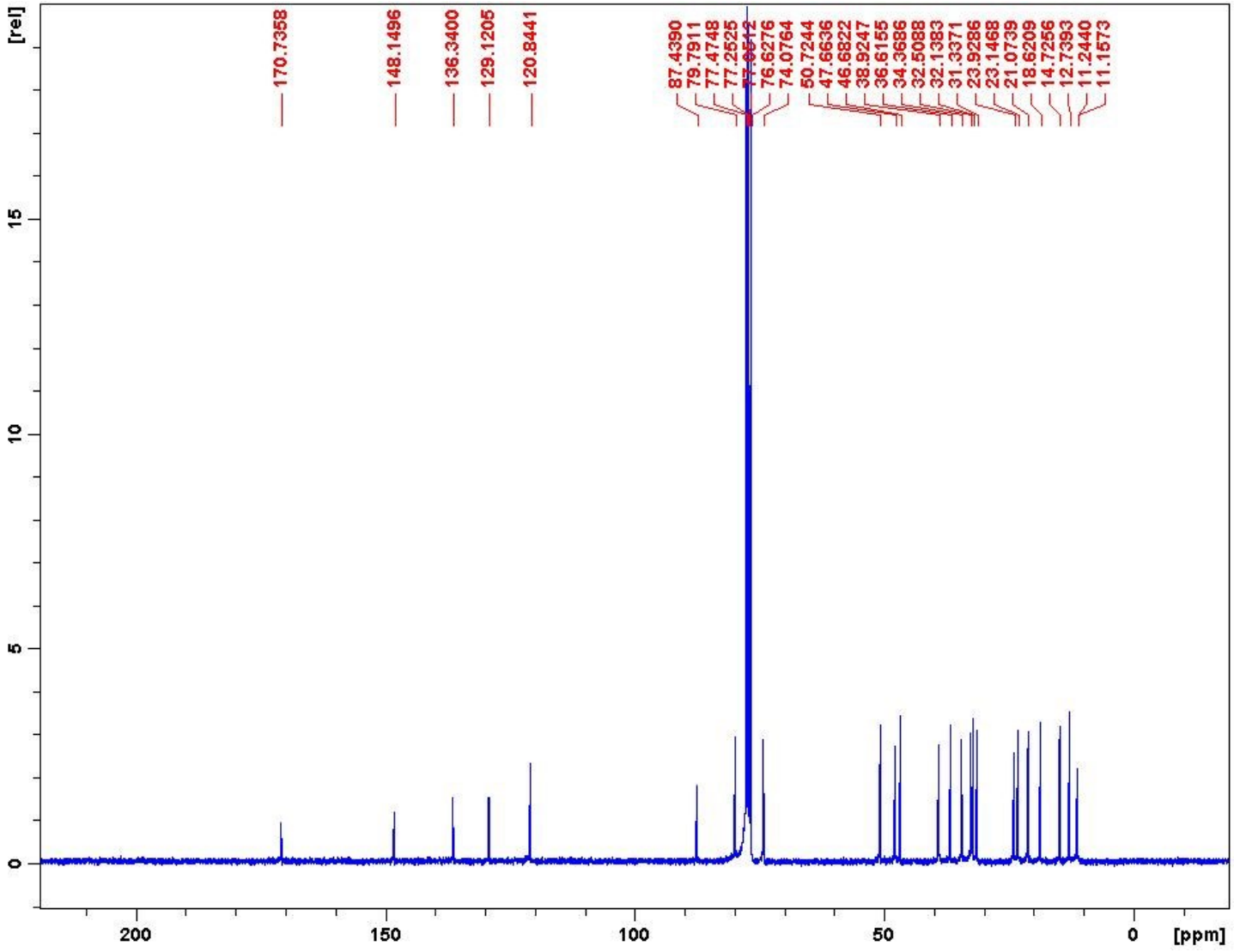
158.0893
157.1975
136.6029
123.4927
118.2632
115.6630
113.6811
79.0191
78.6794
78.5844
78.1492
73.8004
50.6754
47.7955
40.9285
40.6514
40.3729
40.0940
39.8154
39.5359
39.2549
39.1178
36.3977
34.3277
32.6178
32.1643
31.3870
23.6023
23.2176
21.0929
18.7735
12.9599
5
0
-5
-10
200
150
100
50
0
[ppm]

(1S,2R,13R,14S,17R,18S)-7-cyclopropyl-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (13).

^{1}H NMR spectrum of Compound **13**

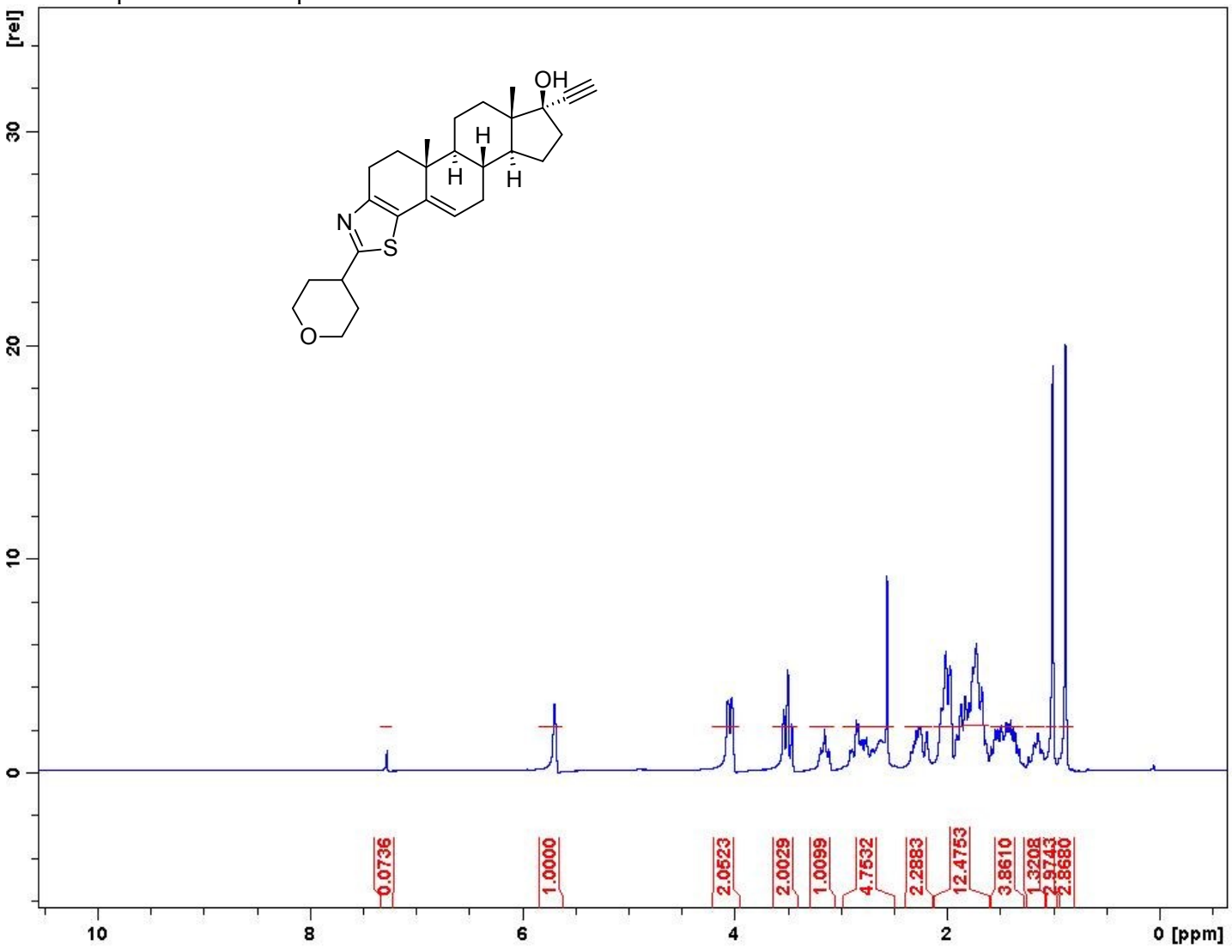


^{13}C NMR Spectrum of Compound **13**

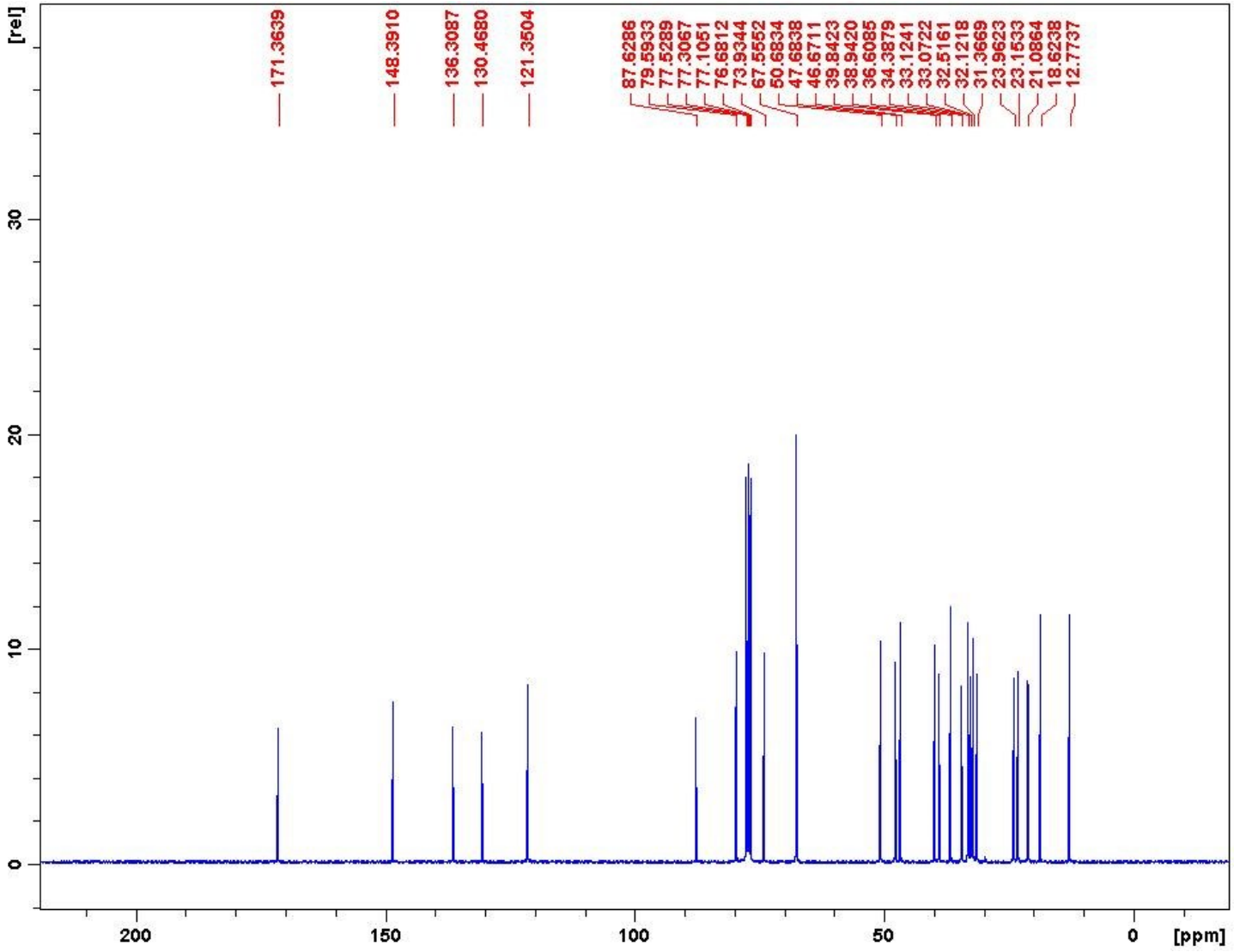


(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-tetrahydropyran-4-yl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (14).

^{1}H NMR Spectrum of Compound **14**.

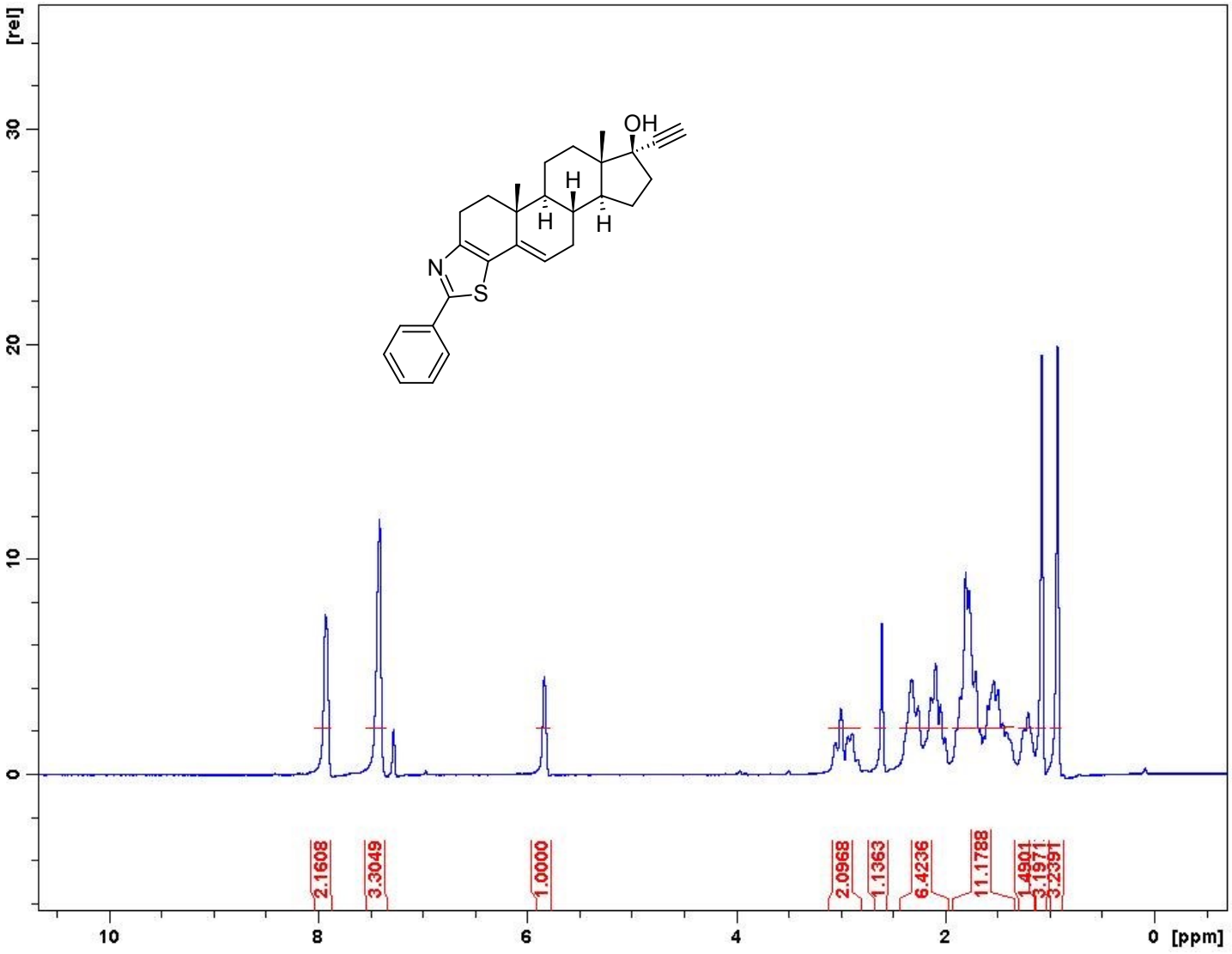


^{13}C NMR spectrum of Compound **14**.

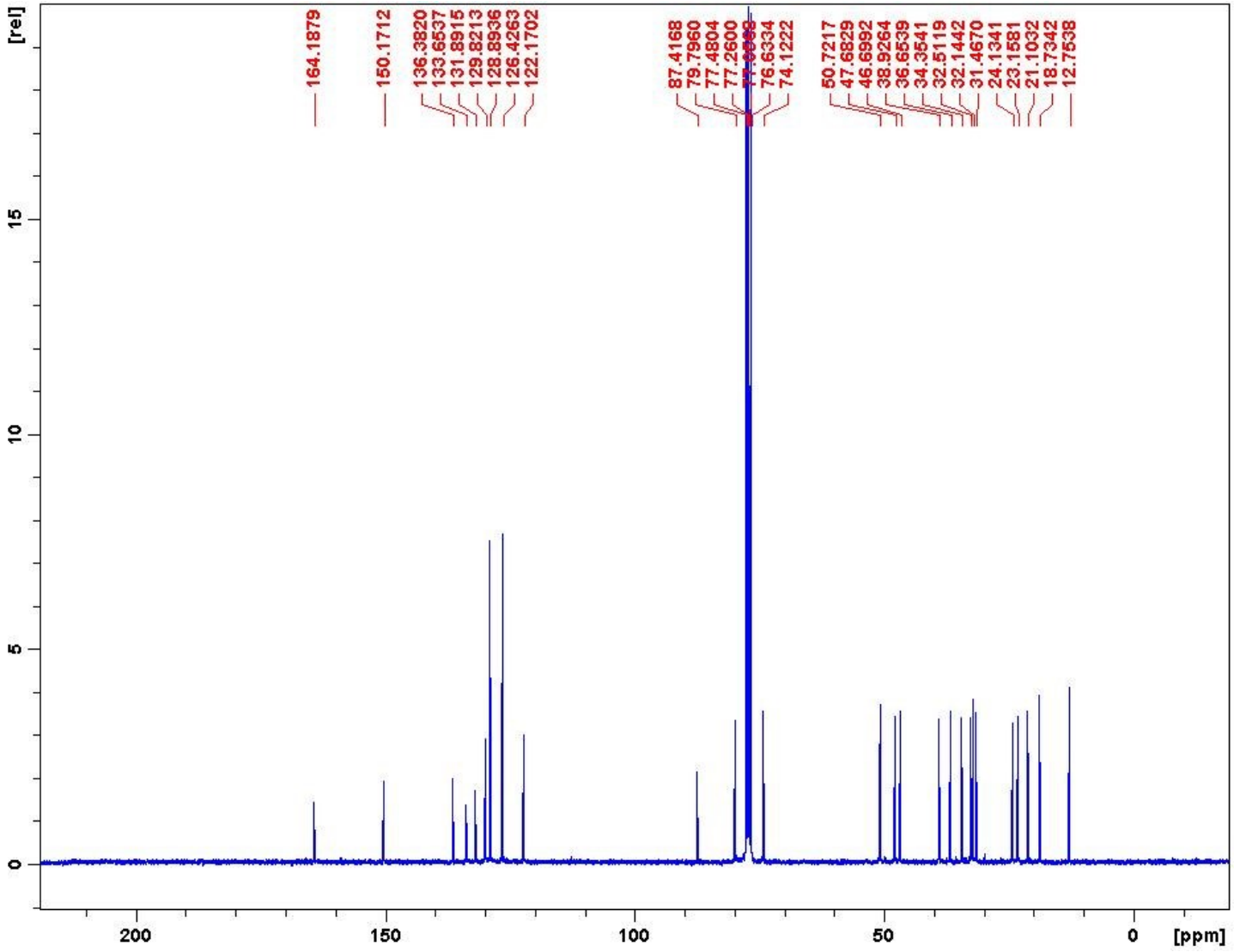


(1*S*,2*R*,13*R*,14*S*,17*R*,18*S*)-17-ethynyl-2,18-dimethyl-7-phenyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (15).

^{1}H NMR Spectrum of Compound **15**.

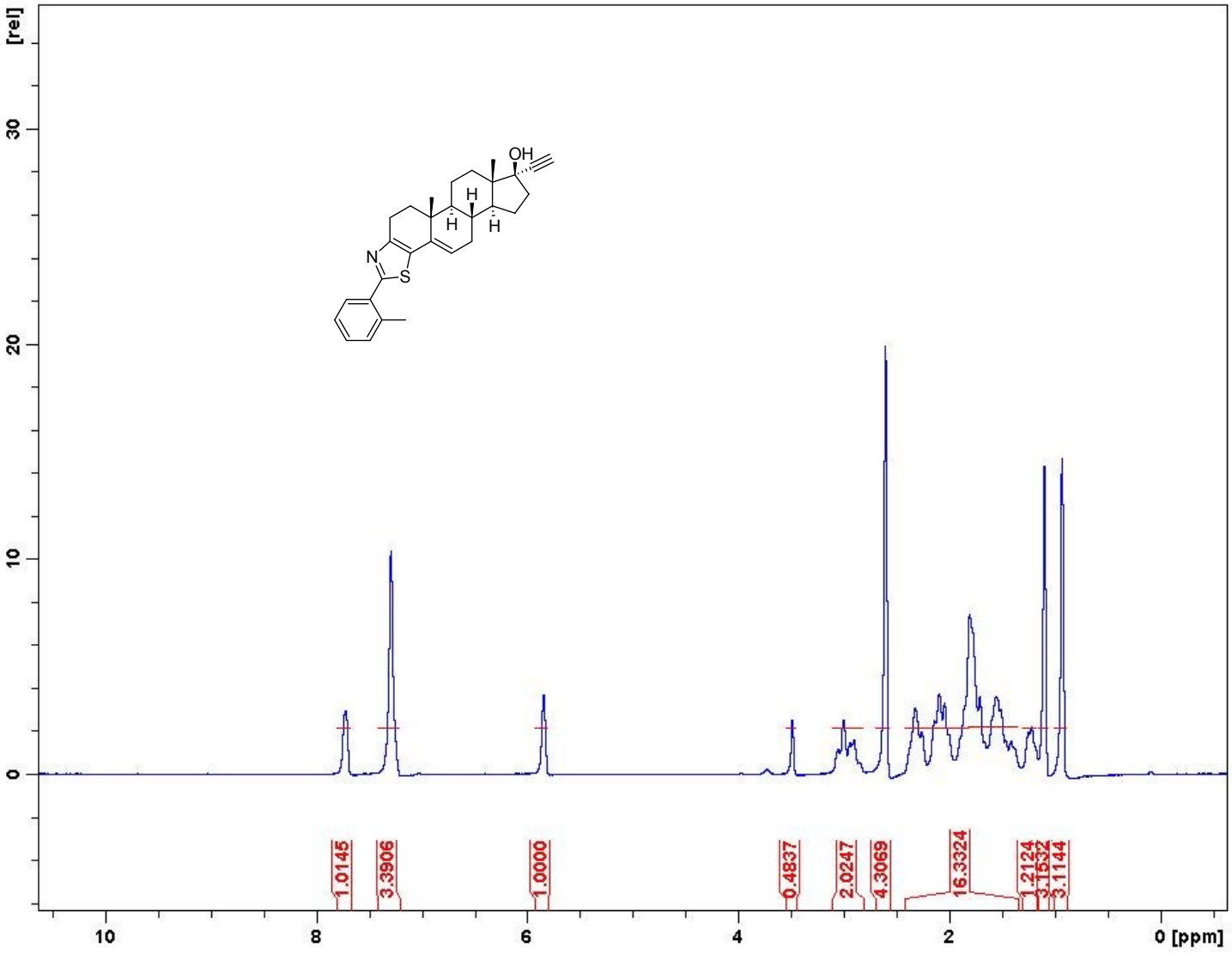


^{13}C NMR Spectrum of Compound **15**.

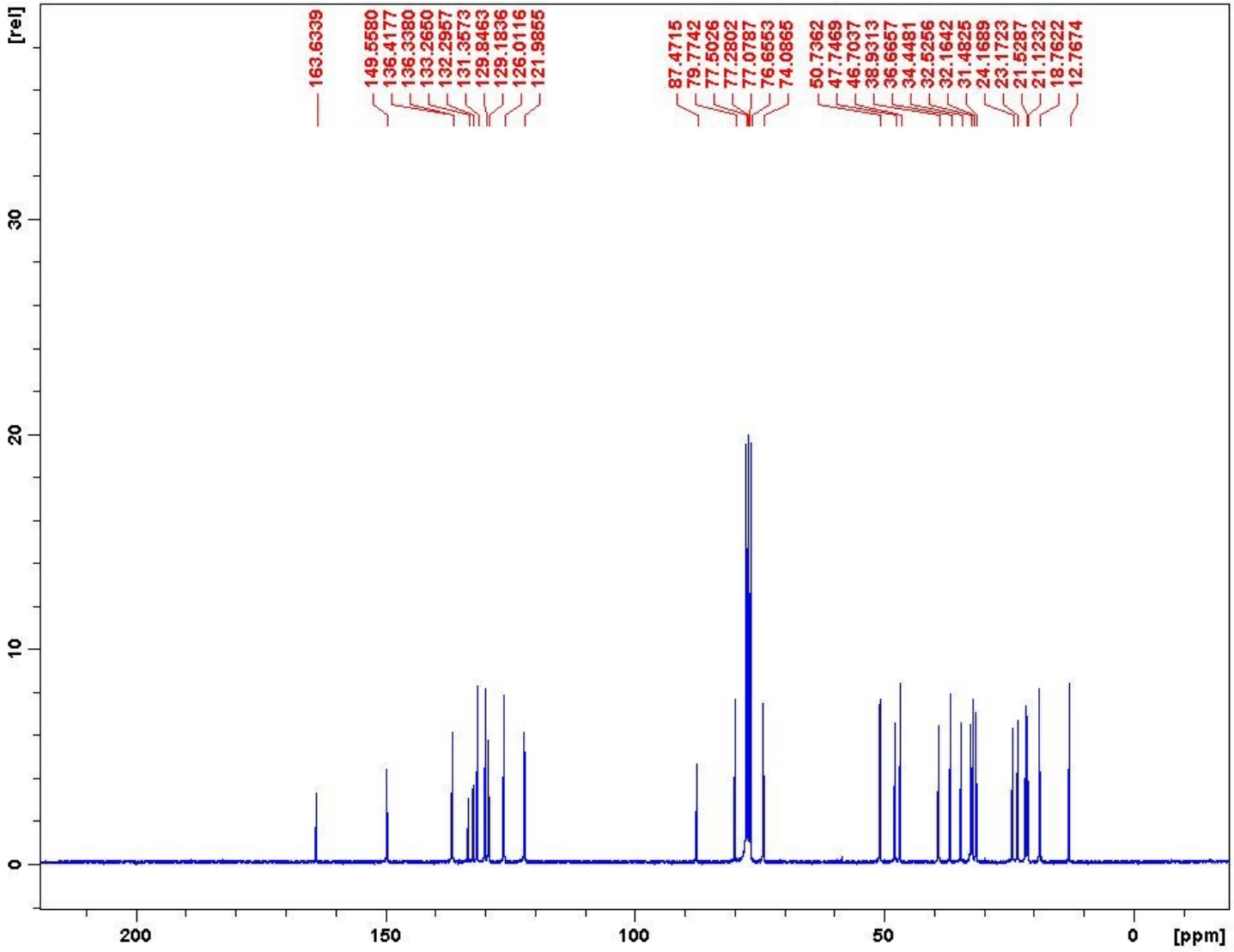


(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-(o-tolyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (16).

^{1}H NMR Spectrum of Compound **16**.

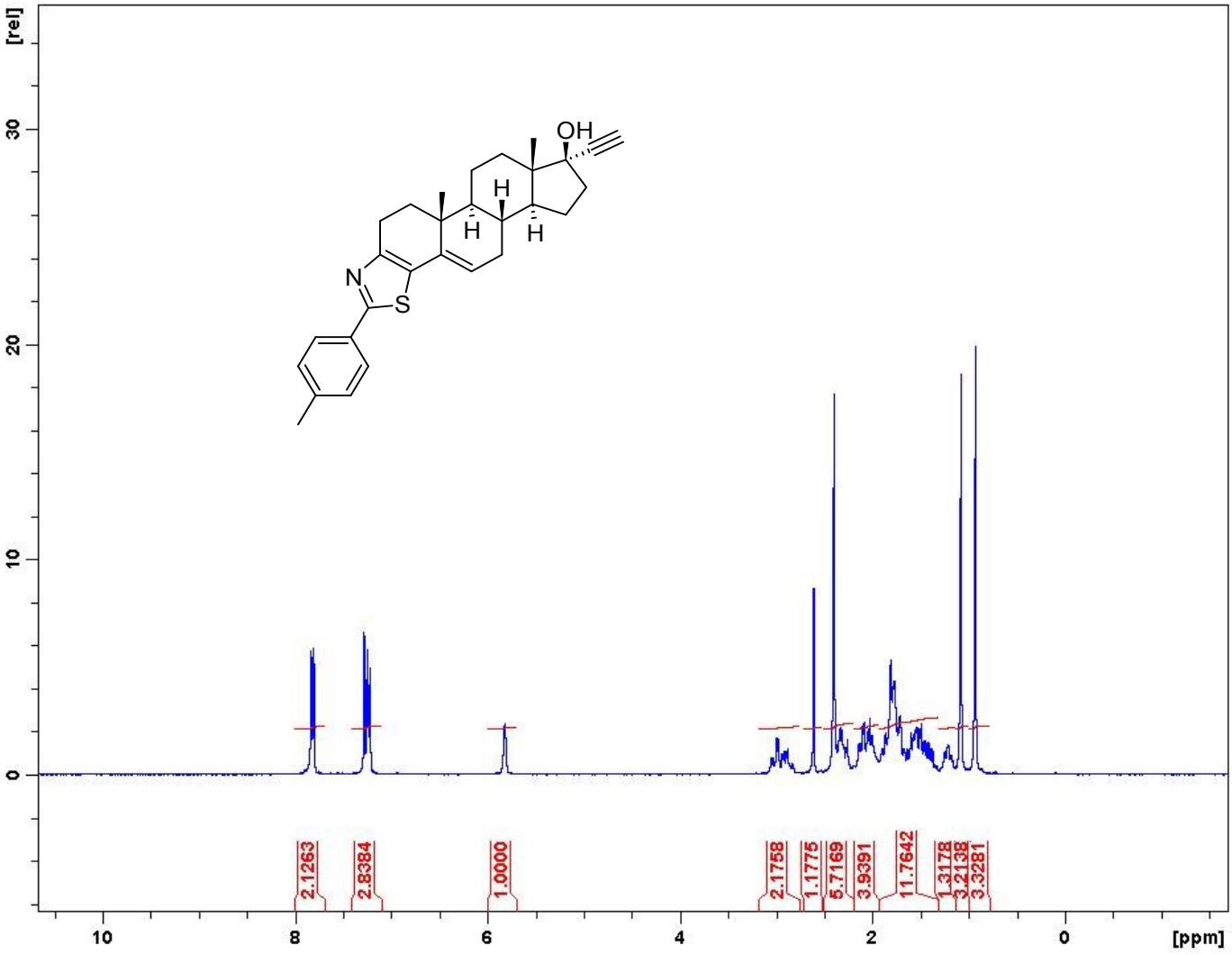


^{13}C NMR Spectrum of Compound **16**.

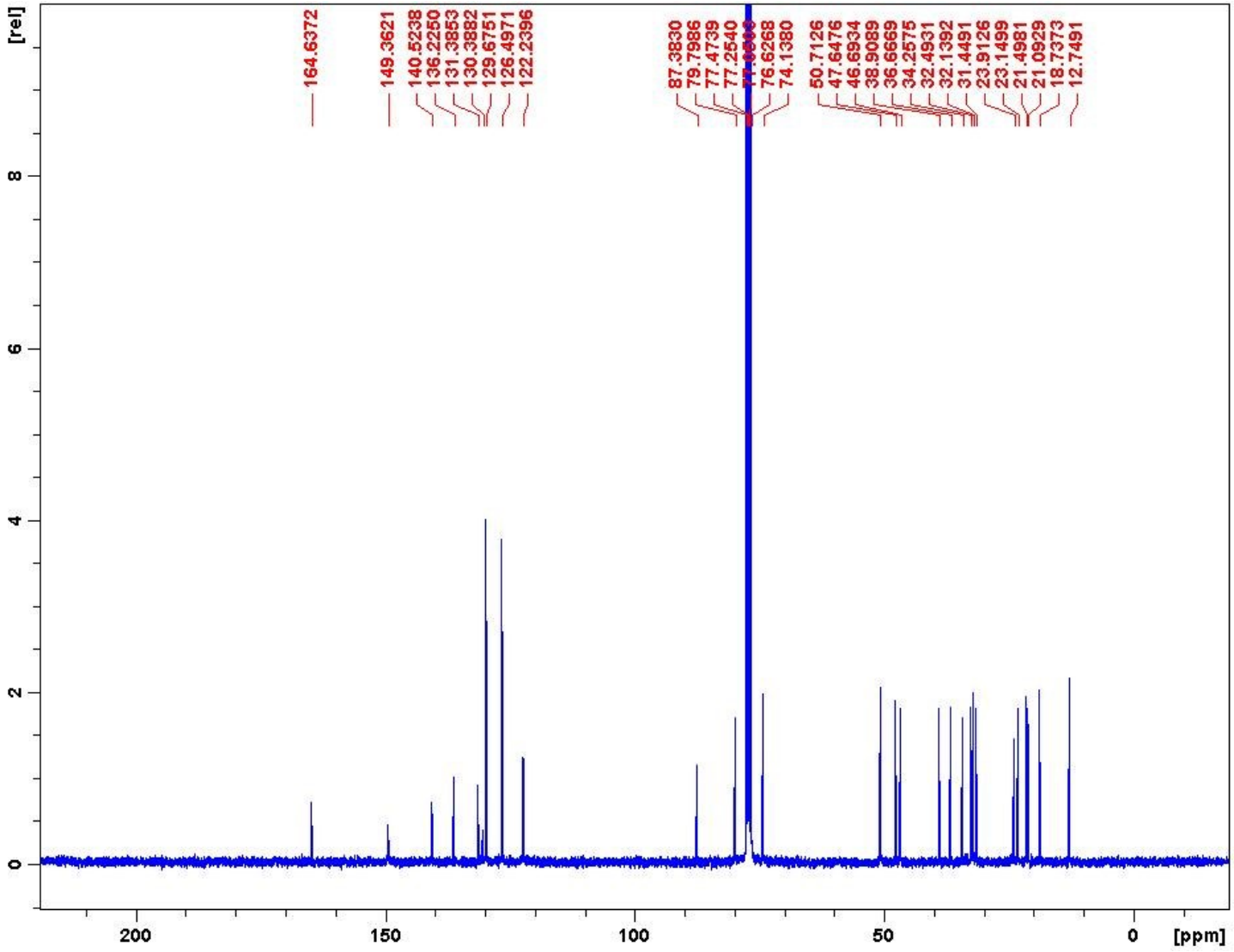


(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-(p-tolyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (17).

^{1}H NMR spectrum of compound **17**

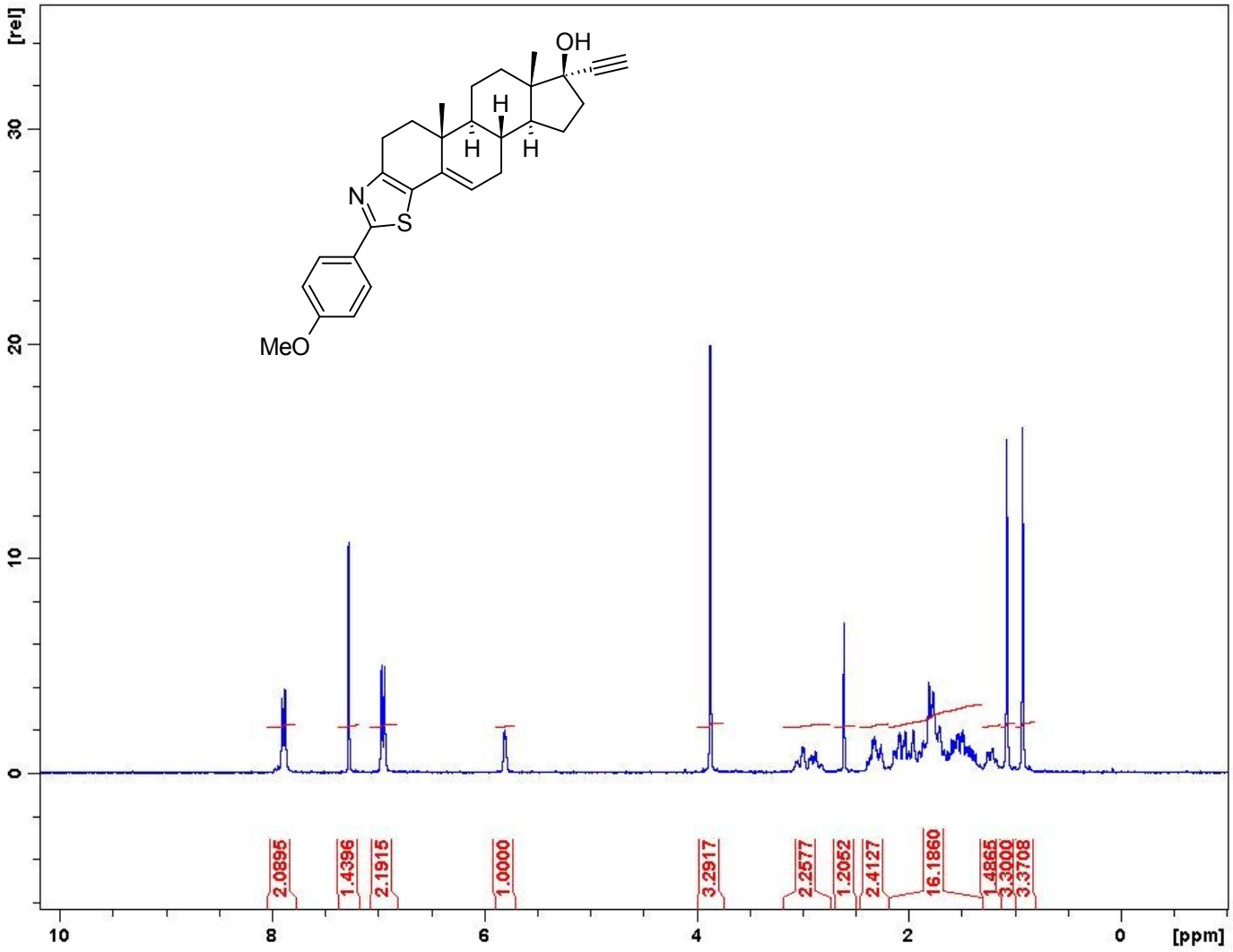


^{13}C NMR spectrum of compound **17**

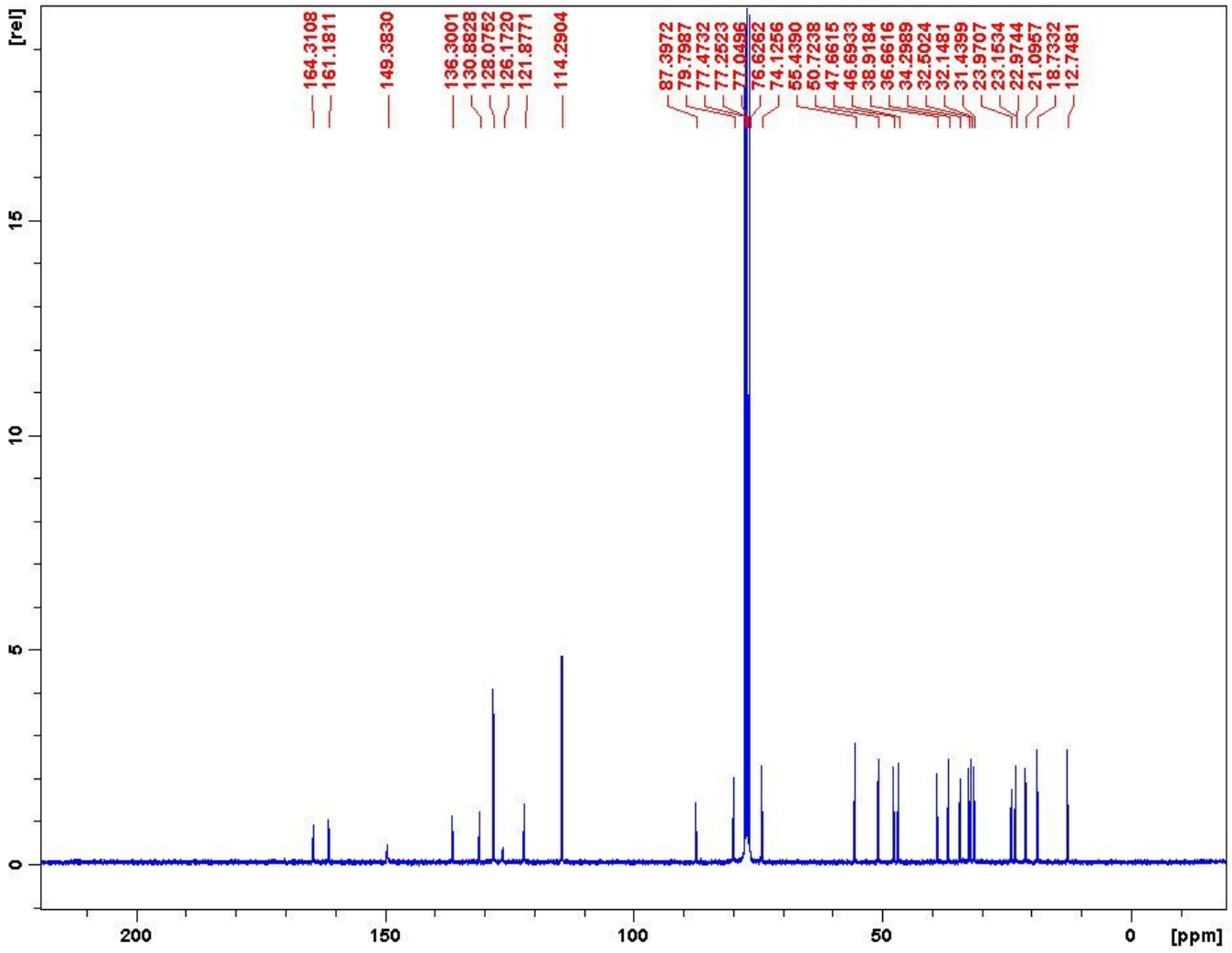


(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-(4-methoxyphenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (18).

^{1}H NMR Spectrum of Compound **18**.

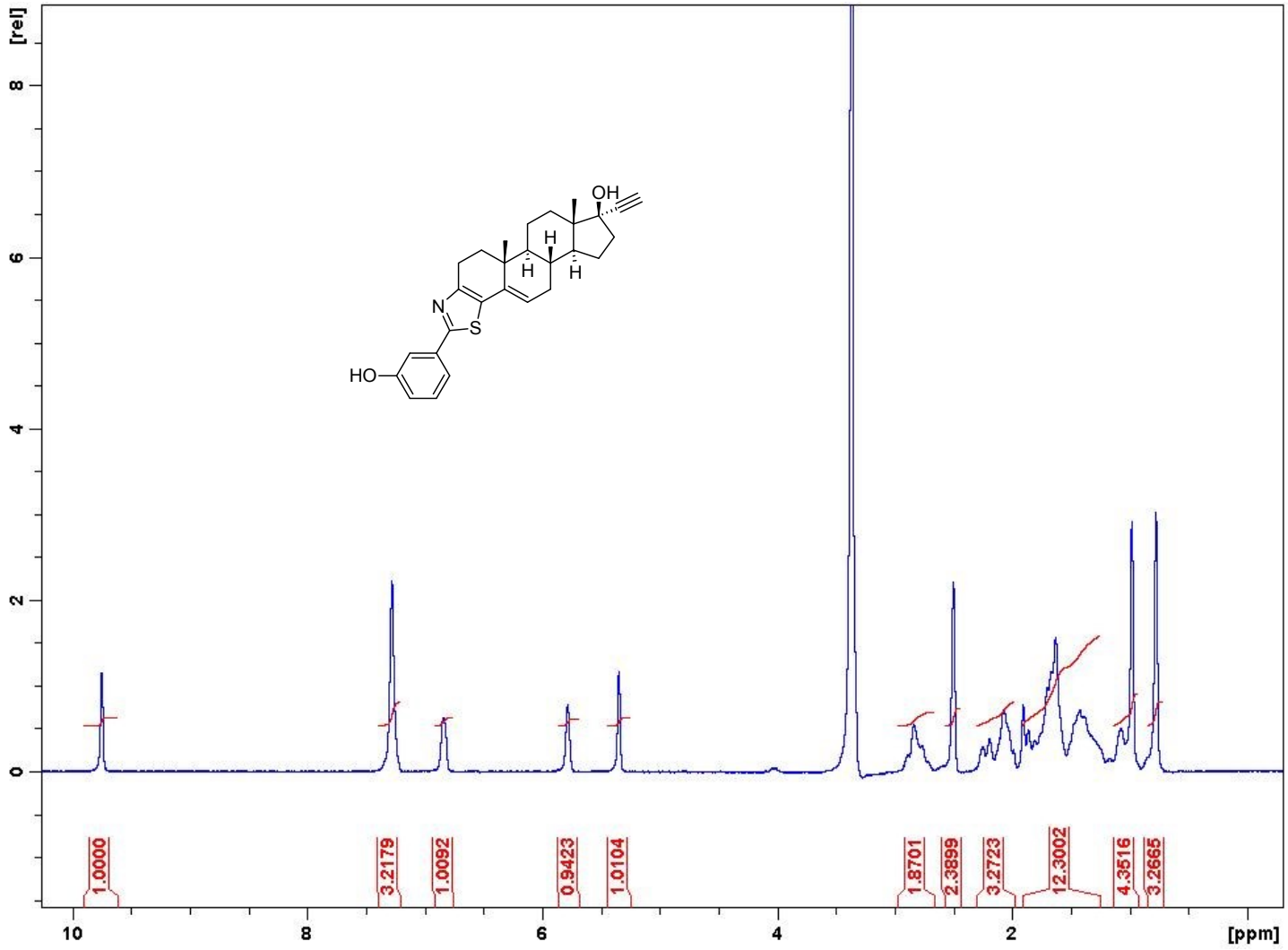


^{13}C NMR Spectrum of Compound **18**.

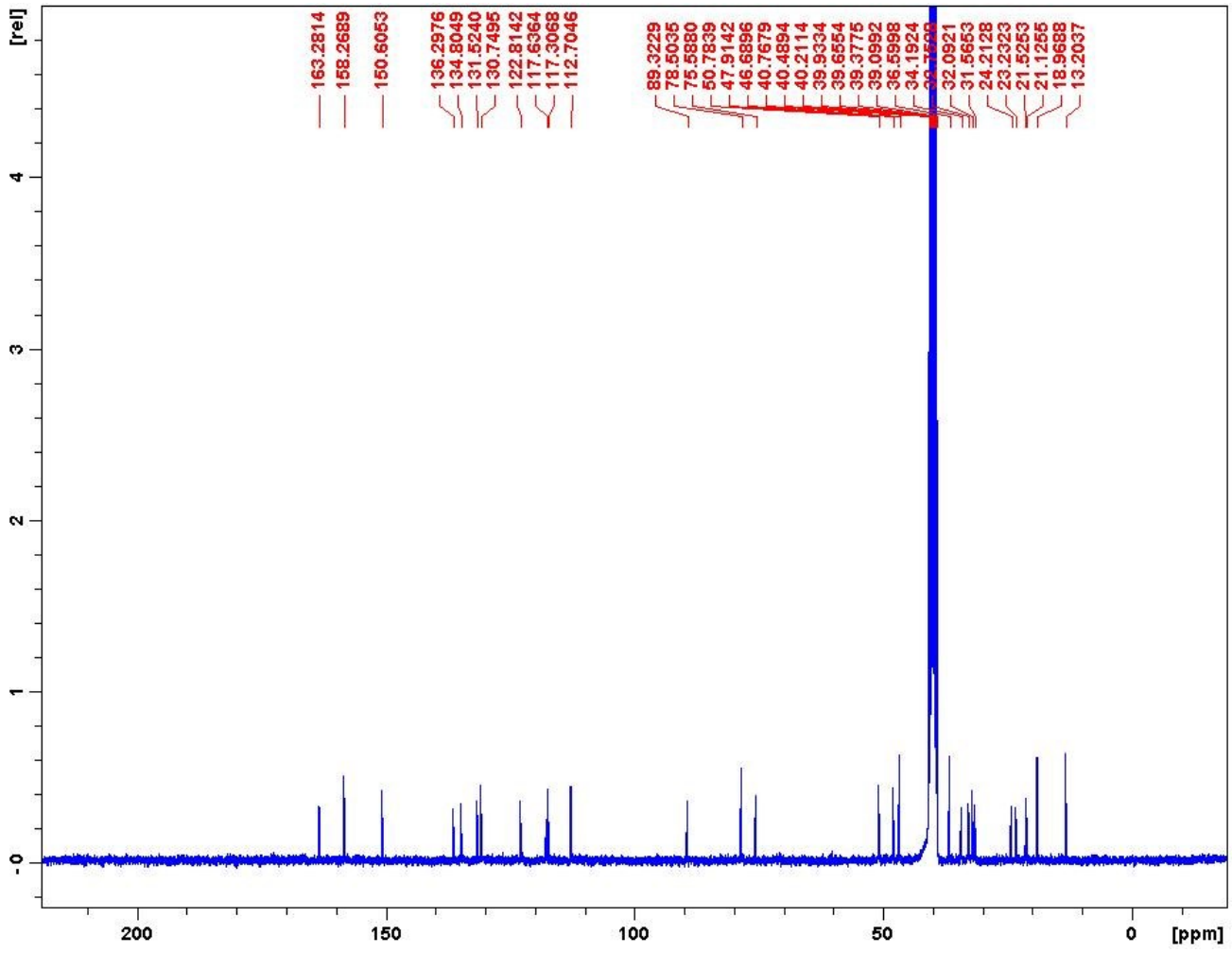


(1S,2R,13R,14S,17R,18S)-17-ethynyl-7-(3-hydroxyphenyl)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (19).

^{1}H NMR Spectrum of Compound **19**.

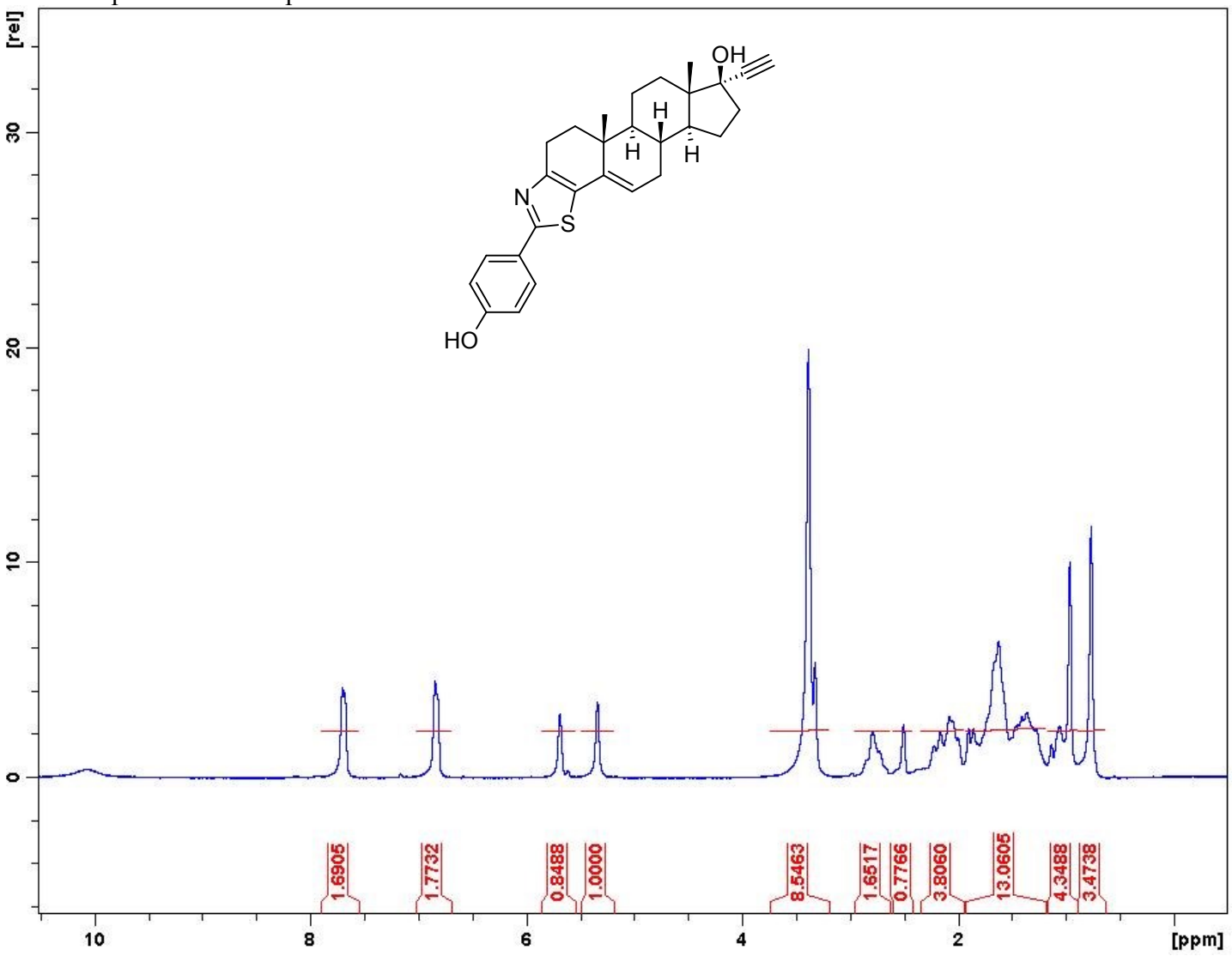


^{13}C NMR Spectrum of Compound **19**.

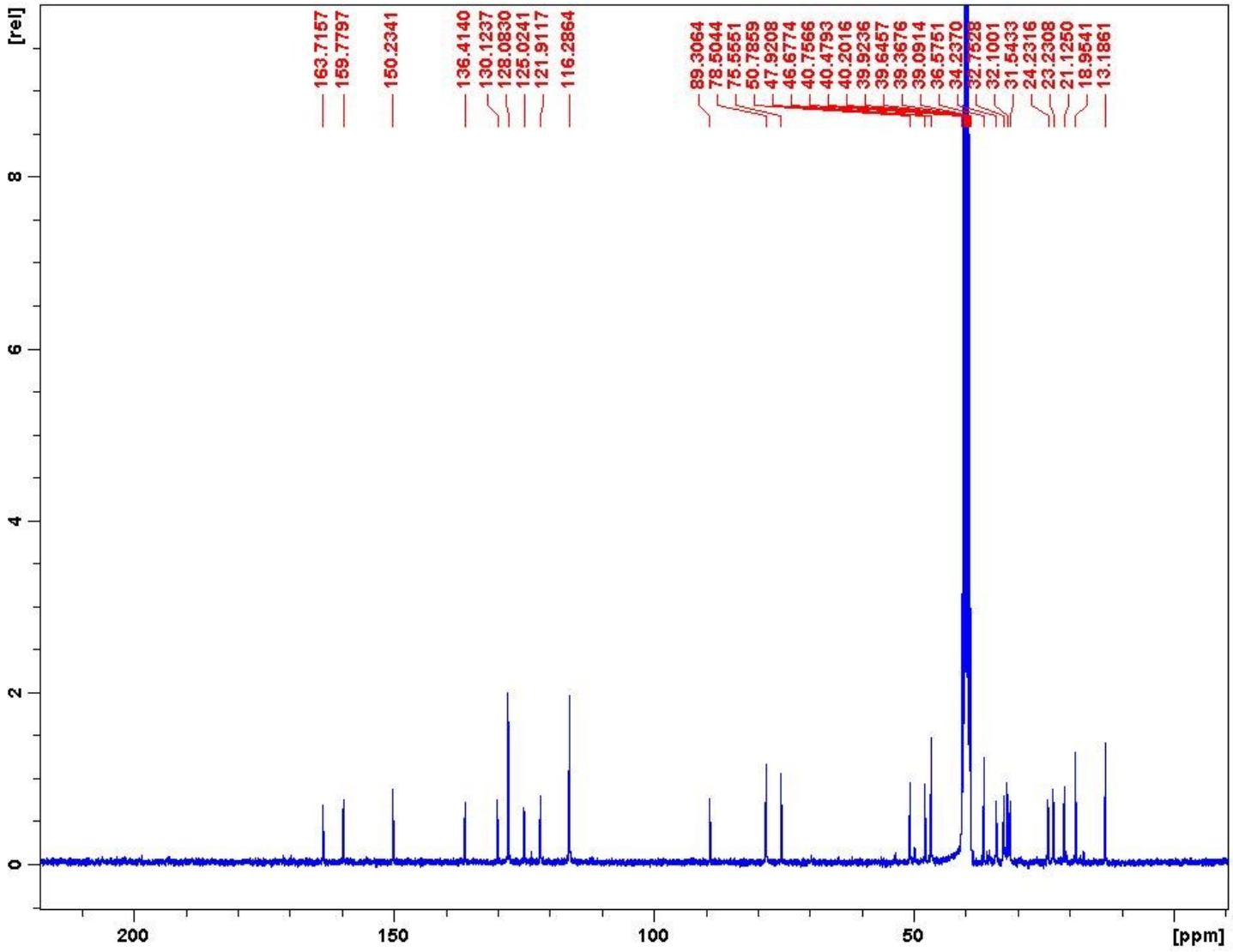


(1S,2R,13R,14S,17R,18S)-17-ethynyl-7-(4-hydroxyphenyl)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (**20**).

^{1}H NMR spectrum of compound **20**

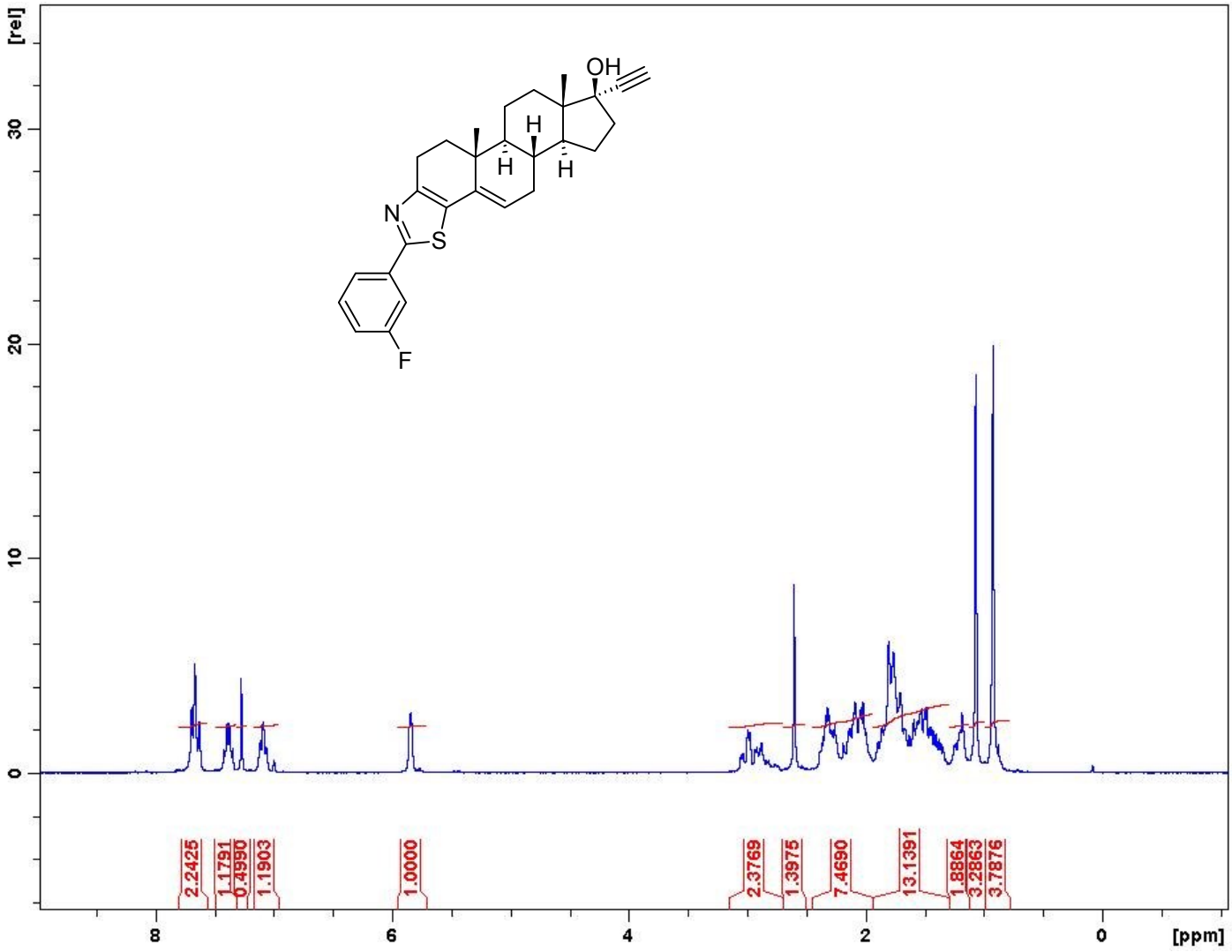


^{13}C NMR spectrum of compound **20**

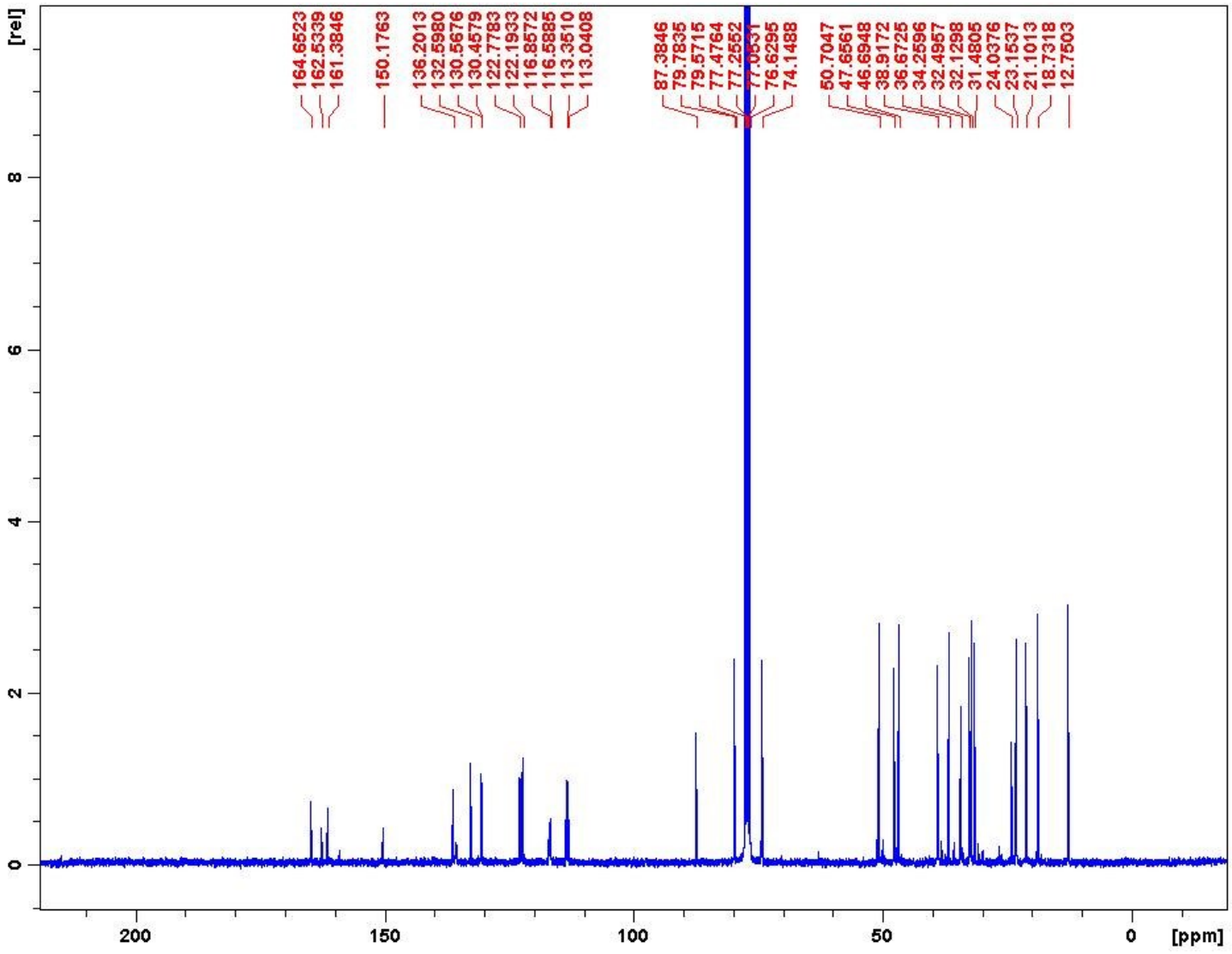


(1S,2R,13R,14S,17R,18S)-17-ethynyl-7-(3-fluorophenyl)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (21).

^{1}H NMR spectrum of compound **21**.

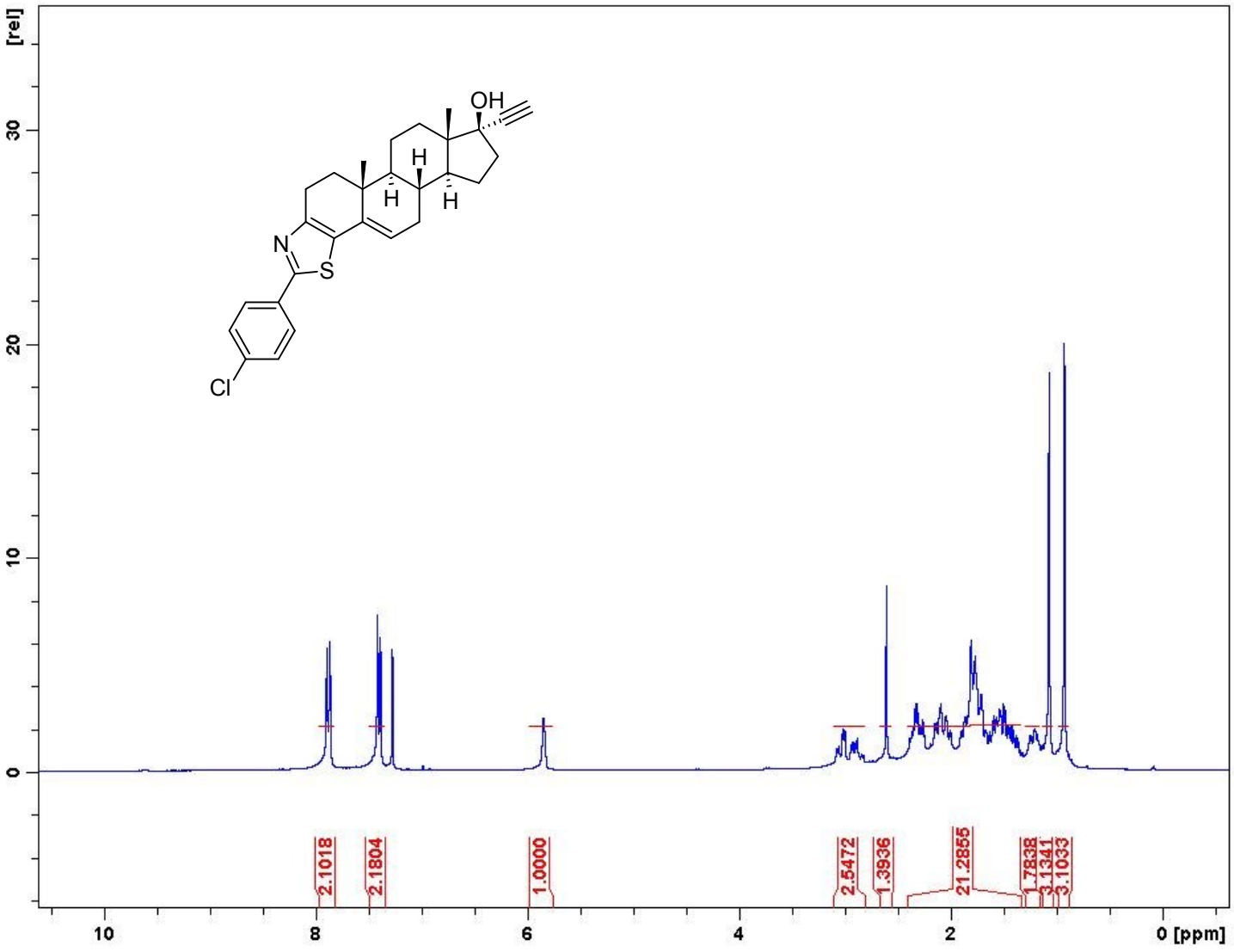


^{13}C NMR Spectrum of Compound **21**.

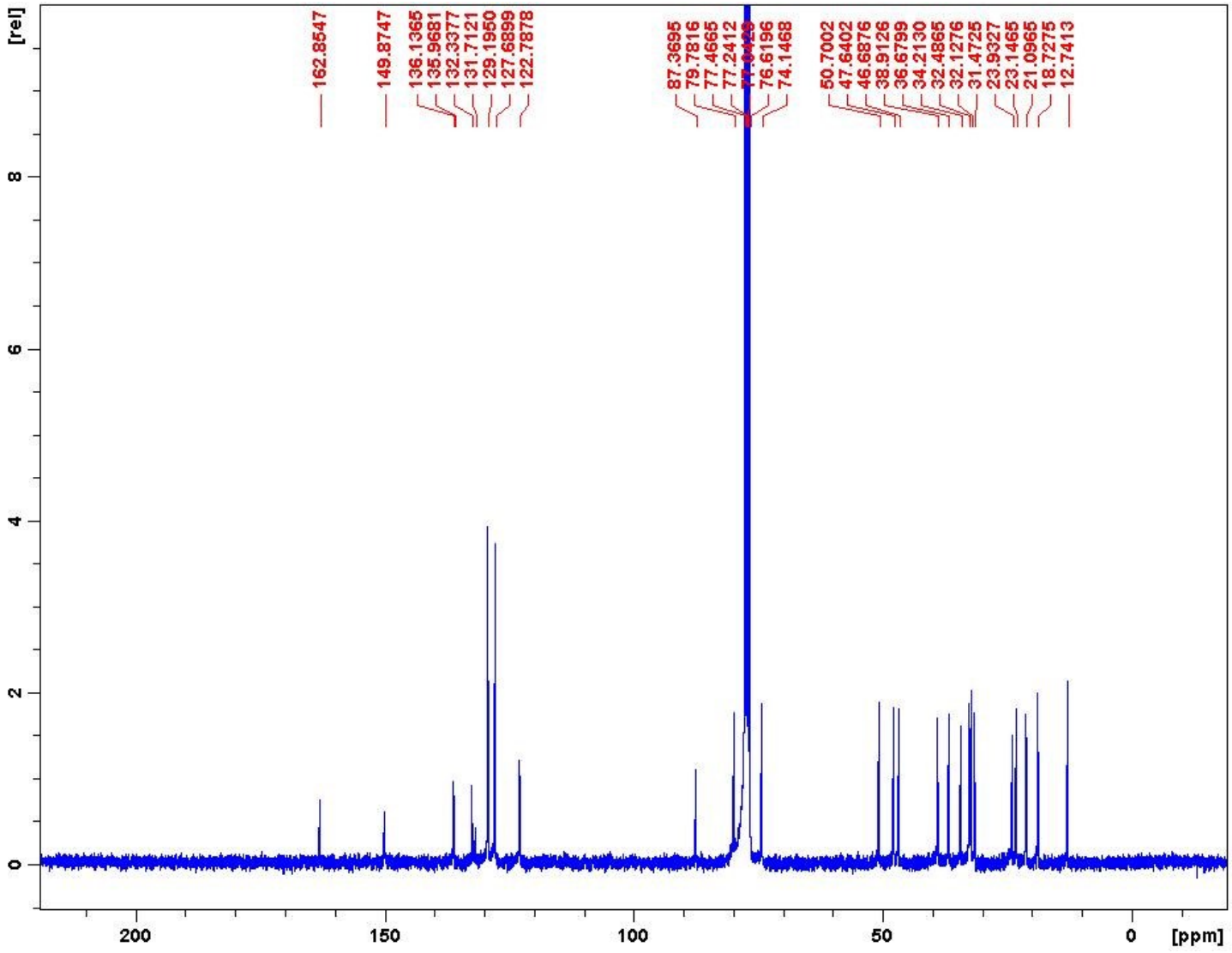


(1S,2R,13R,14S,17R,18S)-17-ethynyl-7-(4-chlorophenyl)-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (22).

^{1}H NMR Spectrum of Compound **22**

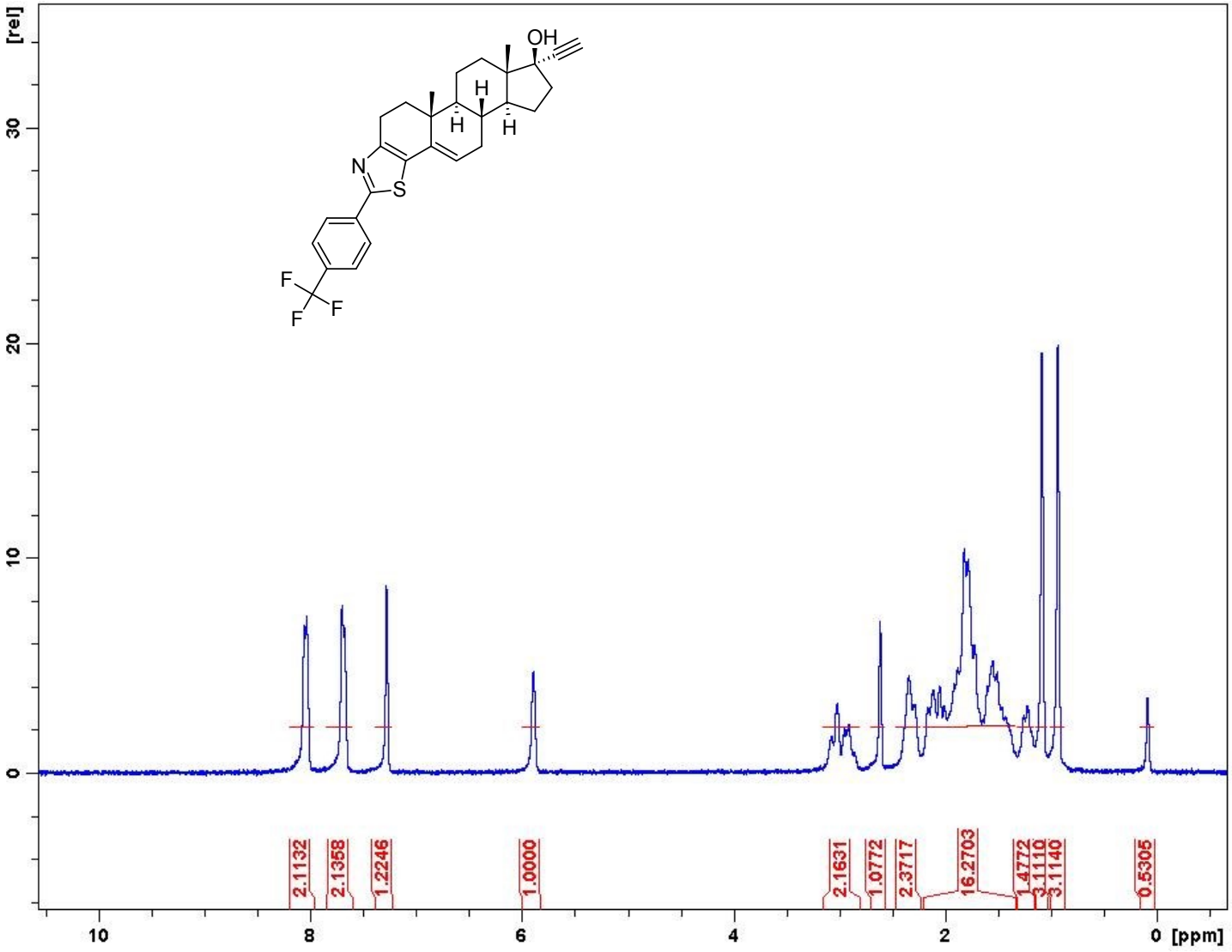


^{13}C NMR spectrum of compound **22**.

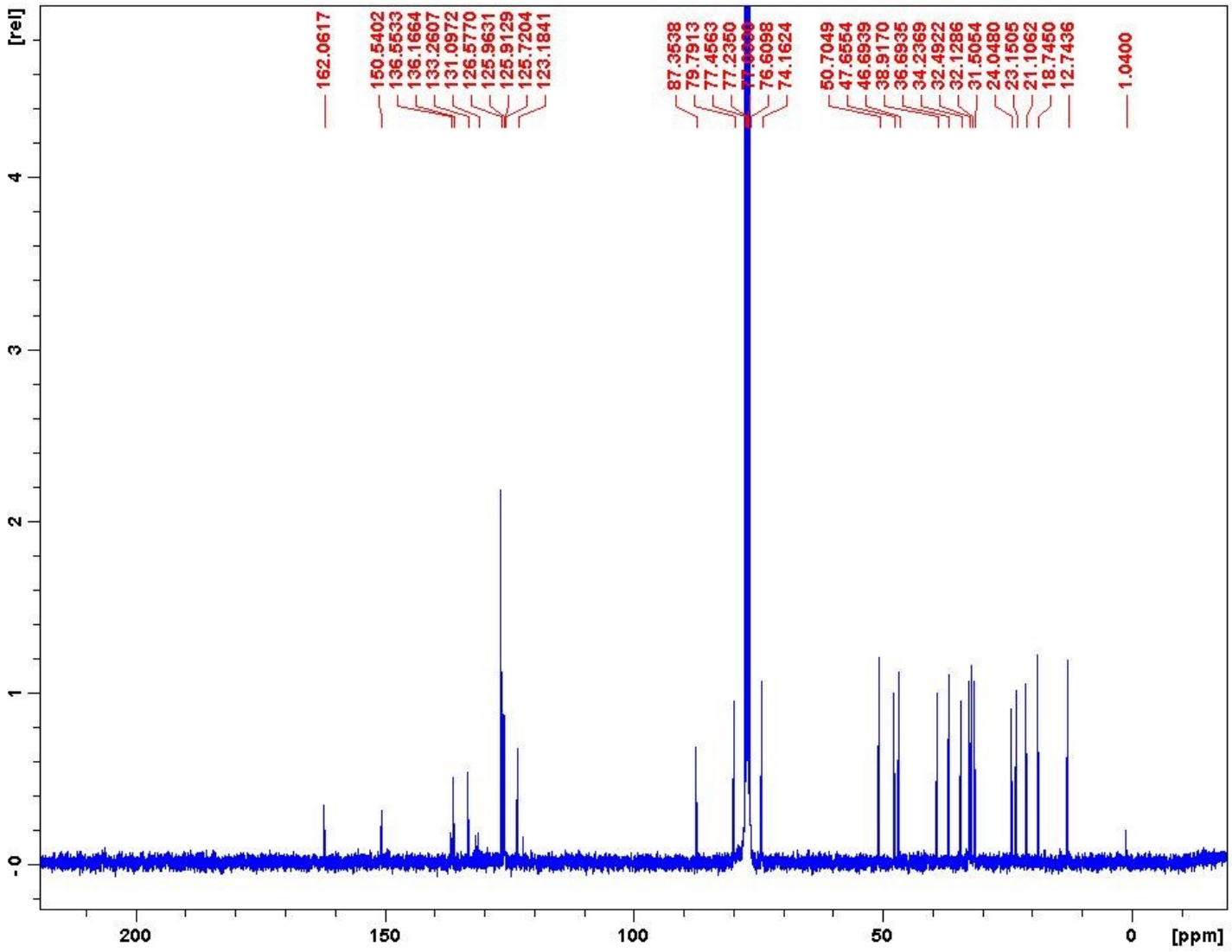


(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-[4-(trifluoromethyl)phenyl]-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (23).

^{1}H NMR Spectrum of Compound **23**.

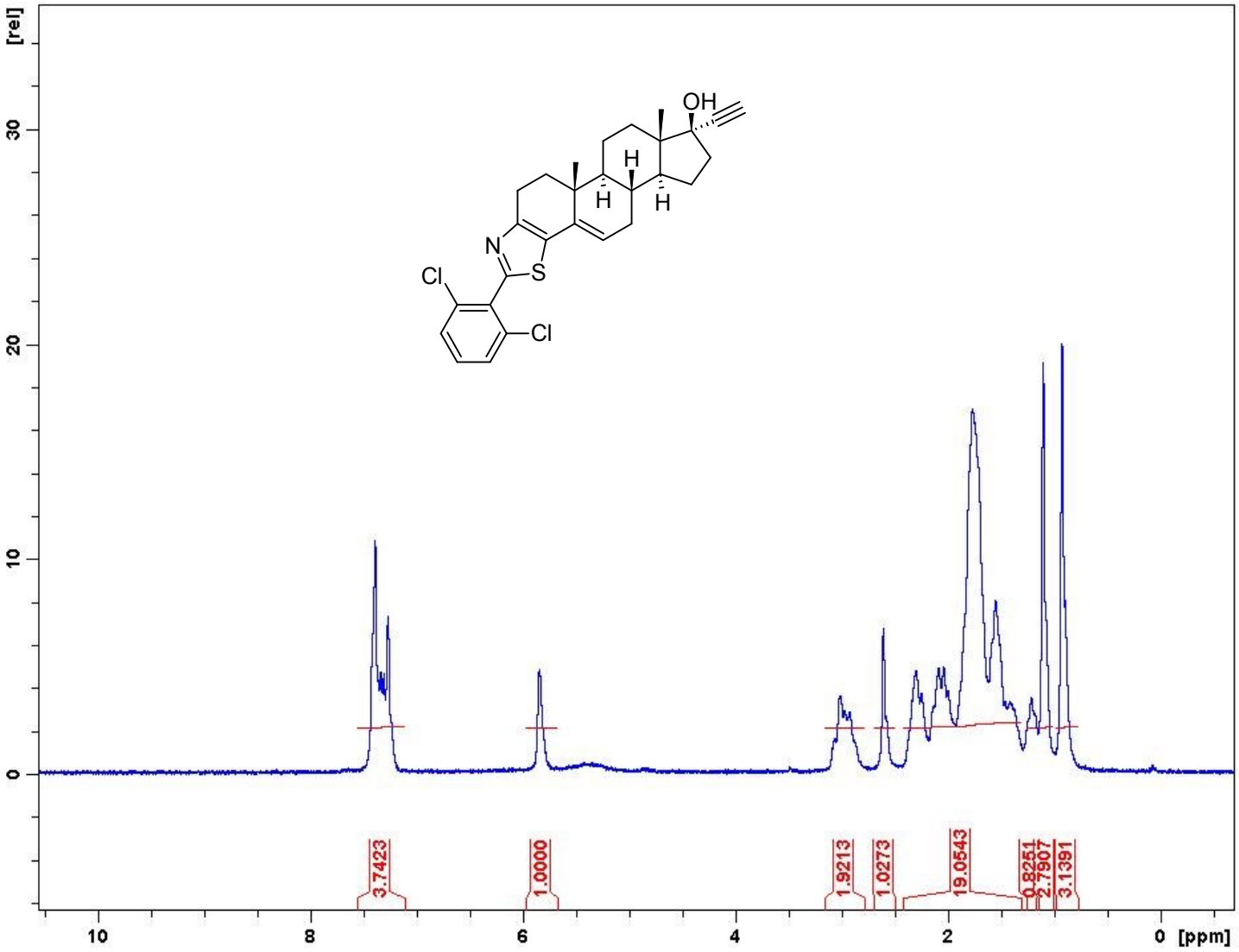


^{13}C NMR spectrum of compound **23**.

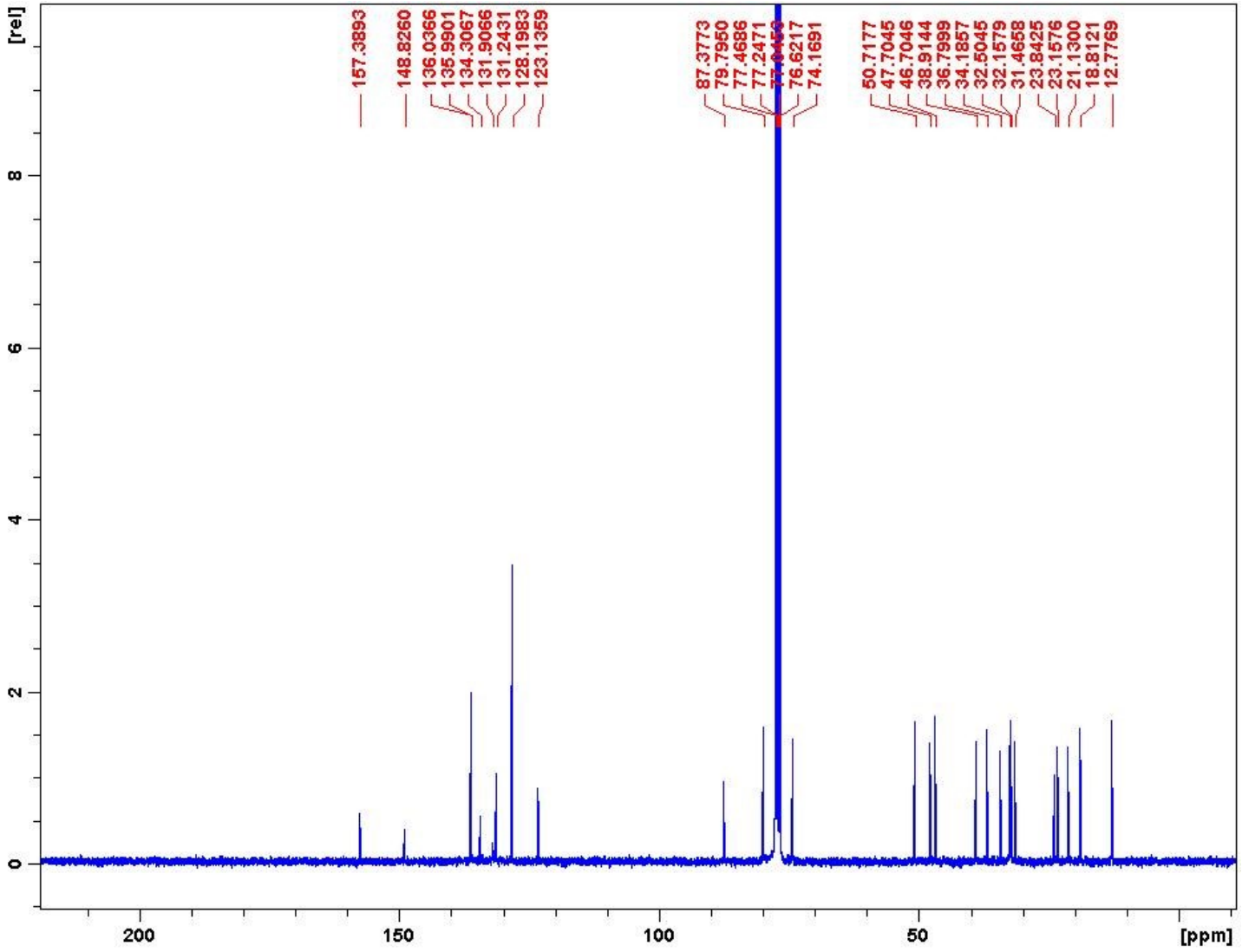


(1S,2R,13R,14S,17R,18S)-7-(2,6-dichlorophenyl)-17-ethynyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (24).

^{1}H NMR Spectrum of Compound **24**.

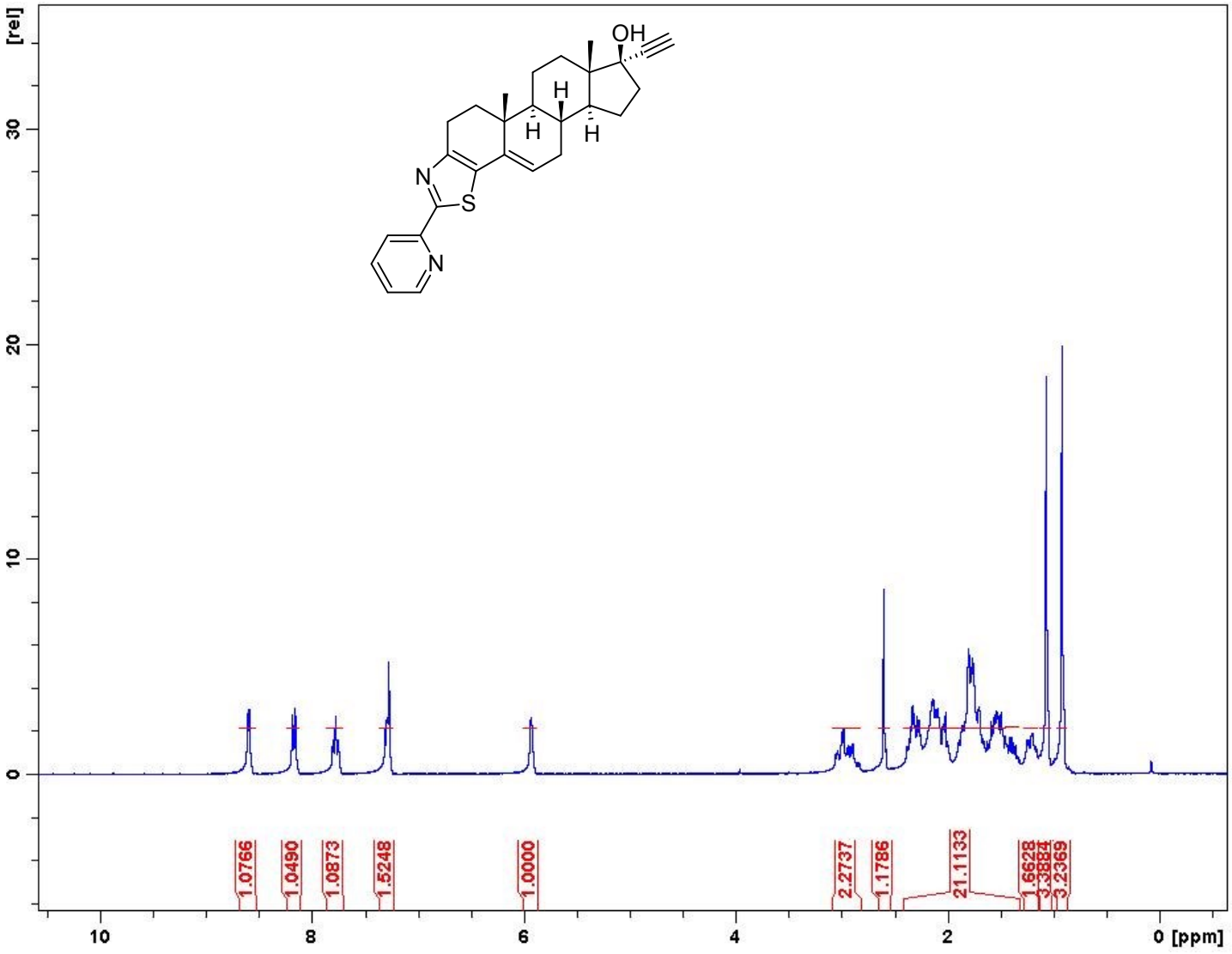


^{13}C NMR Spectrum of Compound **24**.

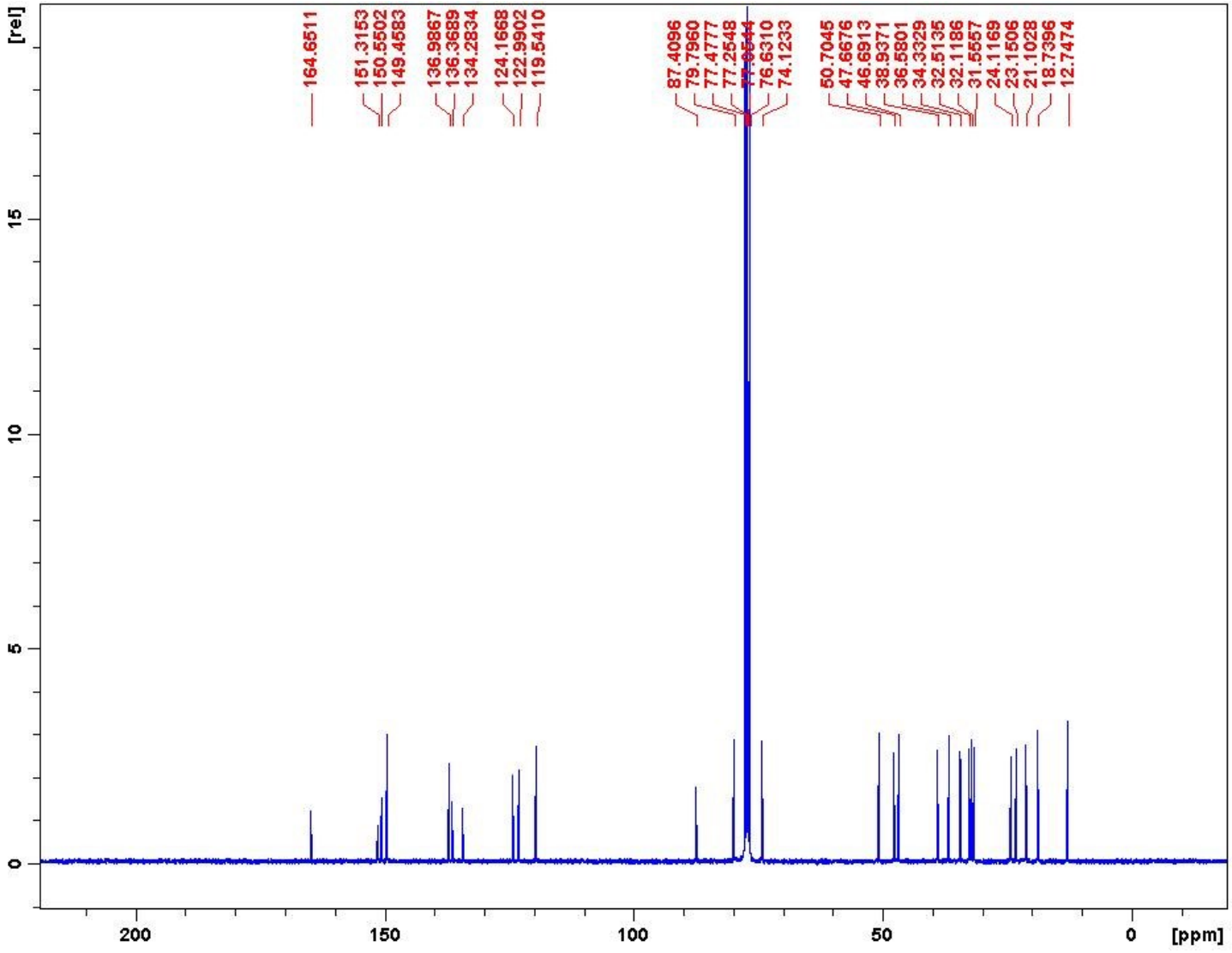


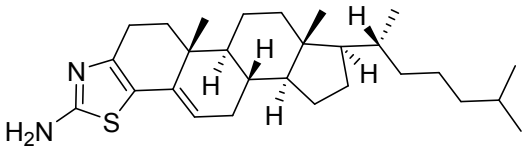
(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-(2-pyridyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-ol (25).

^{1}H NMR spectrum of compound **25**



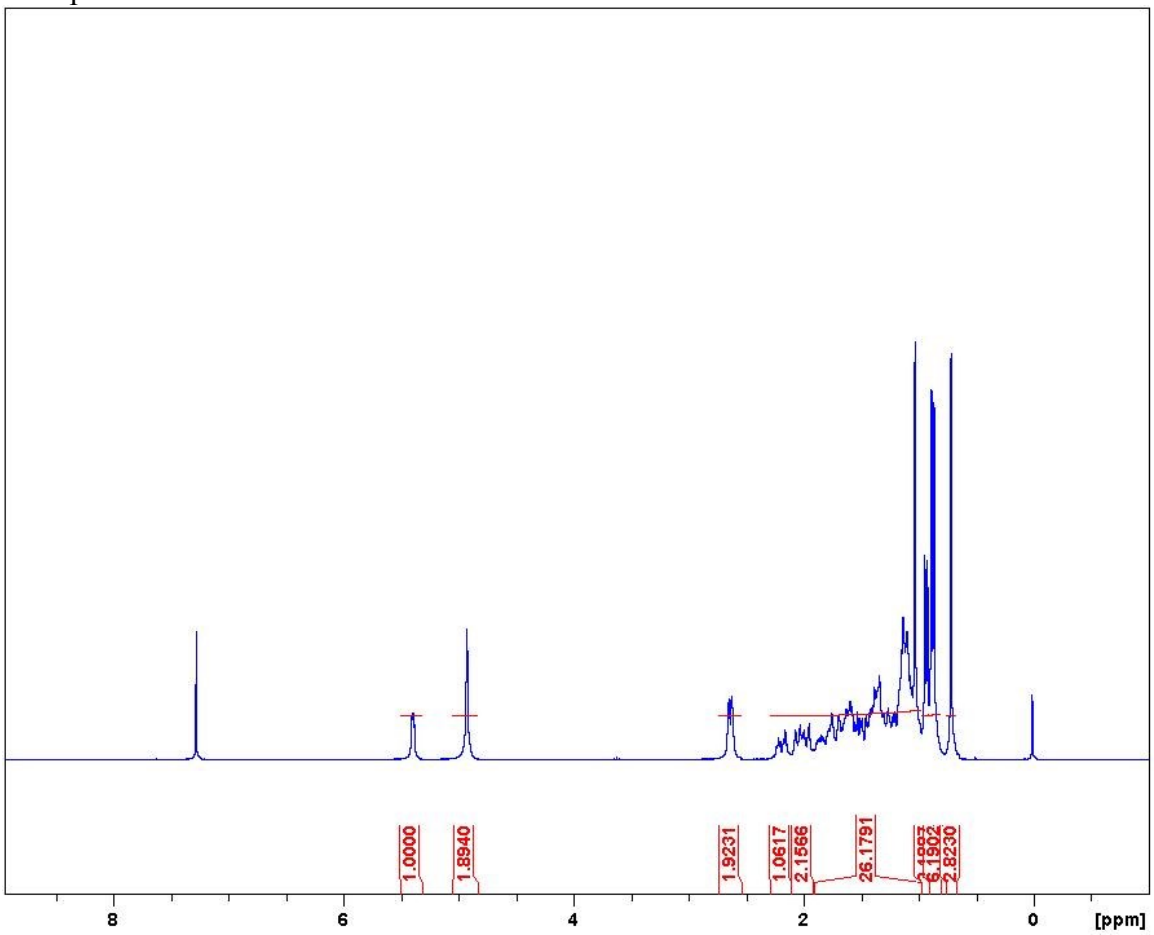
^{1}H NMR spectrum of compound **25**



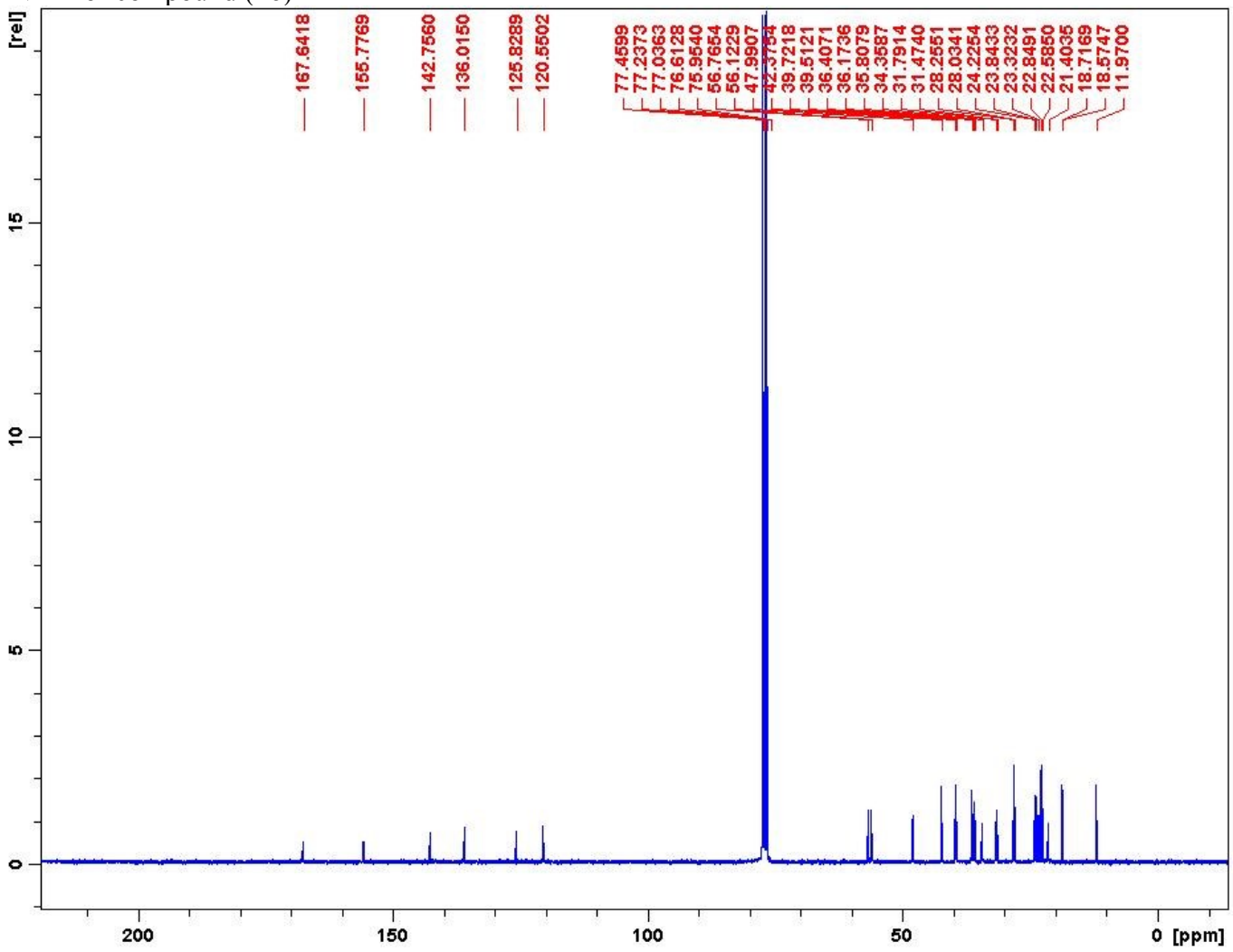


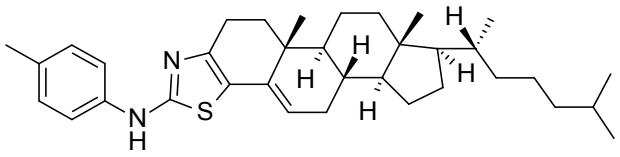
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (26)

^{1}H NMR of compound **26**



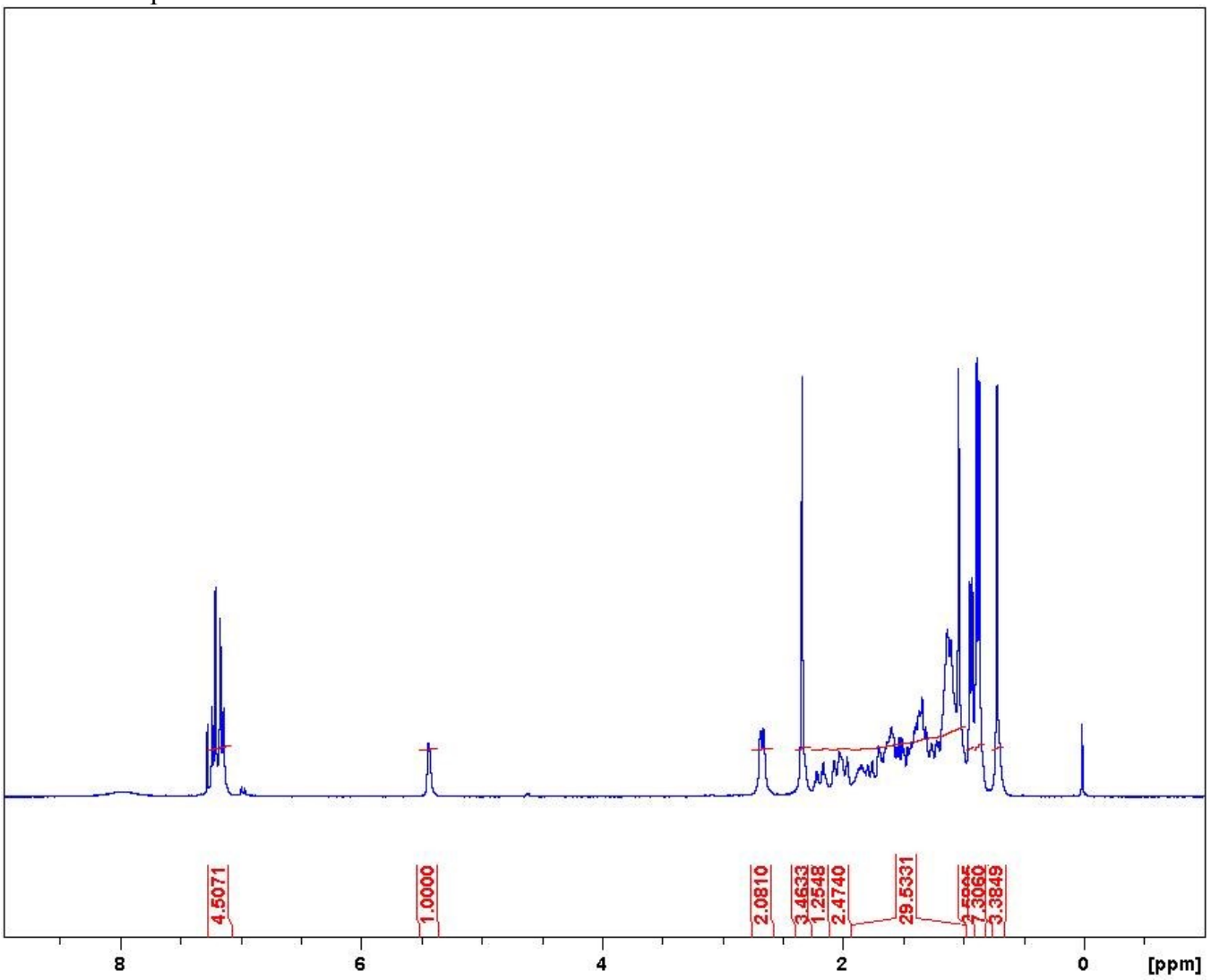
^{13}C NMR of compound (**26**)



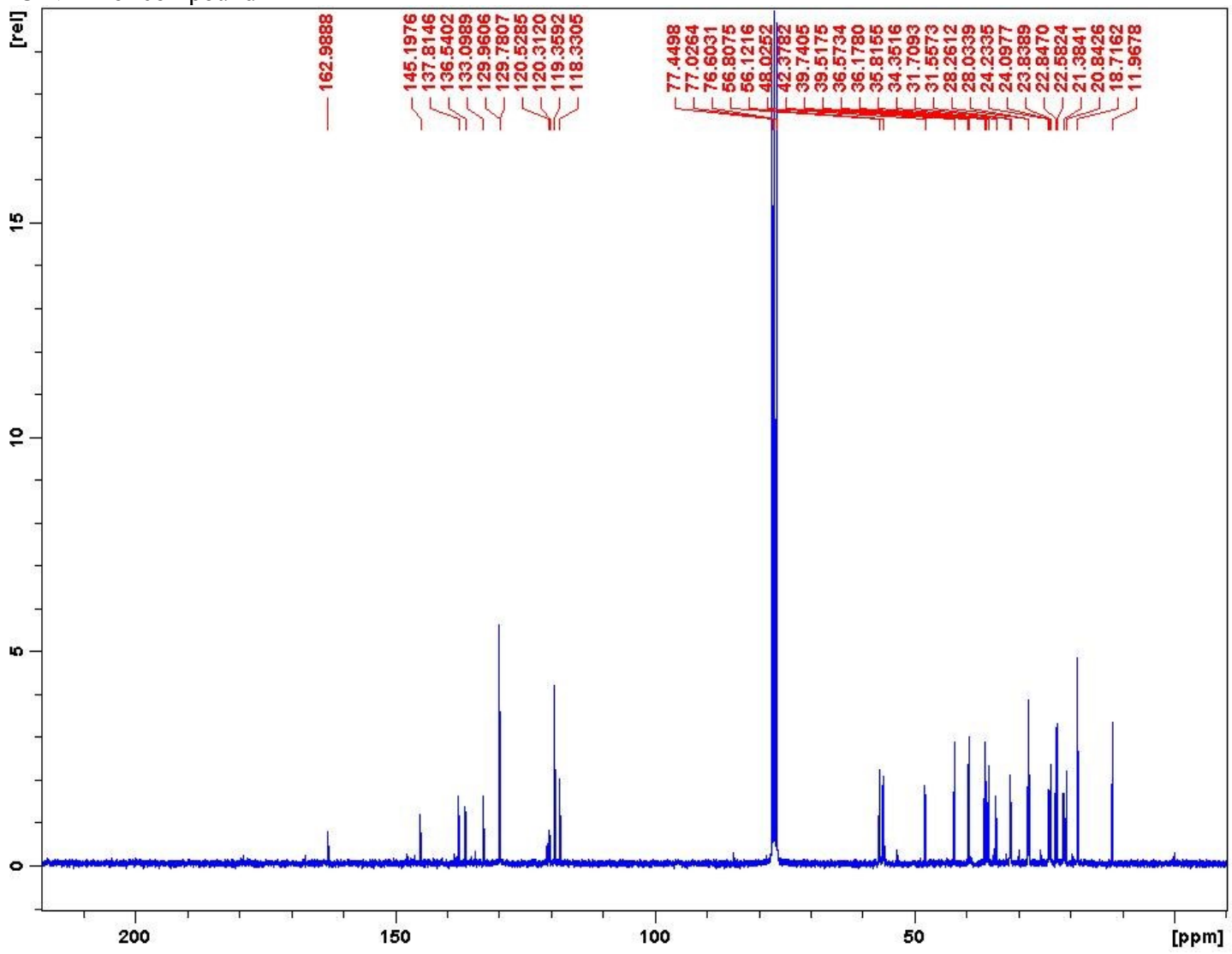


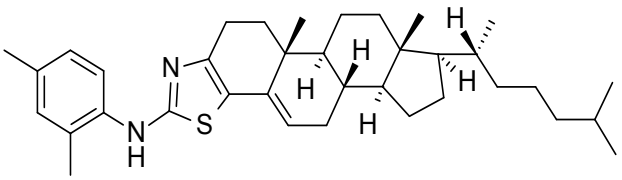
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(p-tolyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (27).

^{1}H NMR of compound **27**



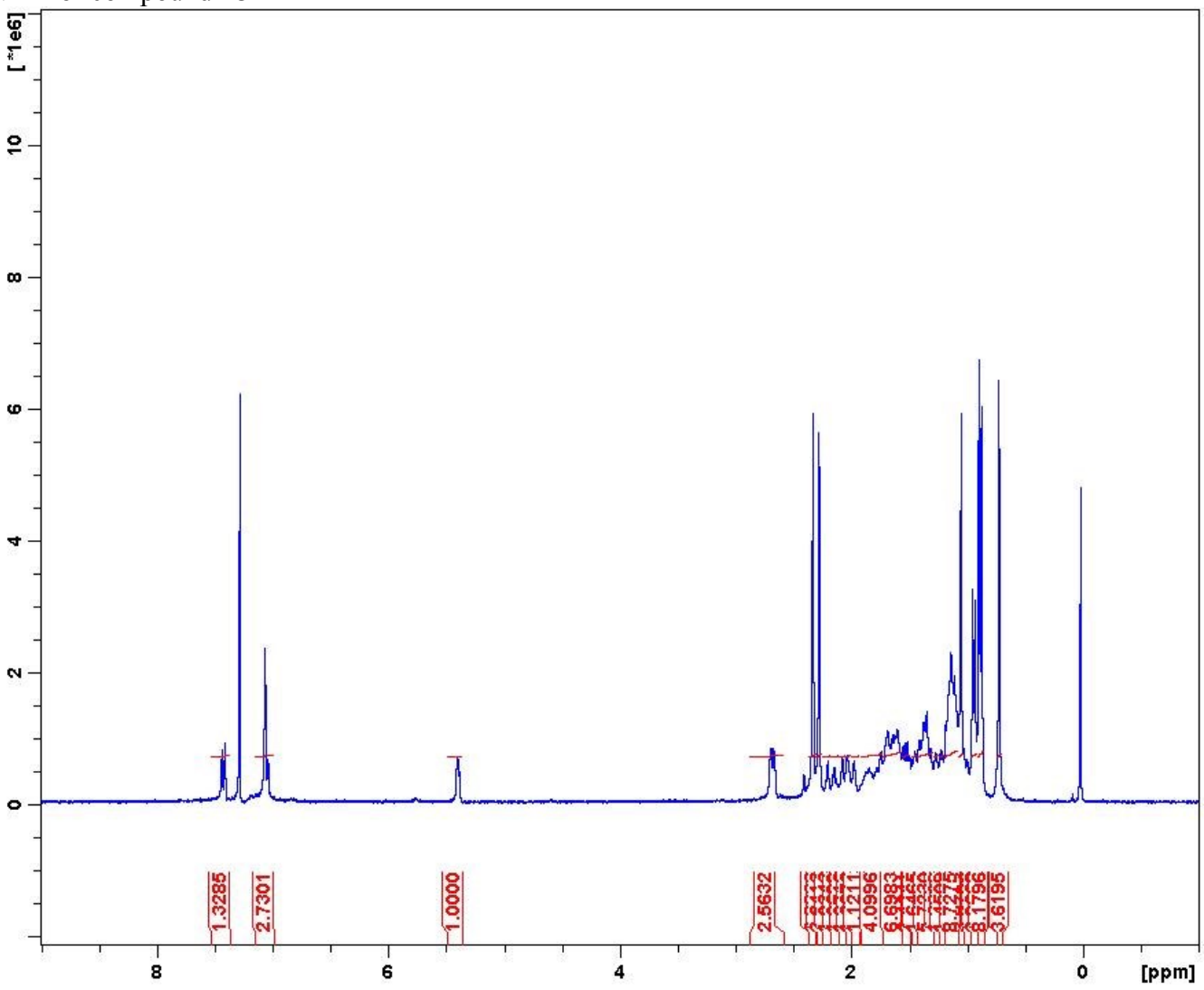
^{13}C NMR of compound **27**



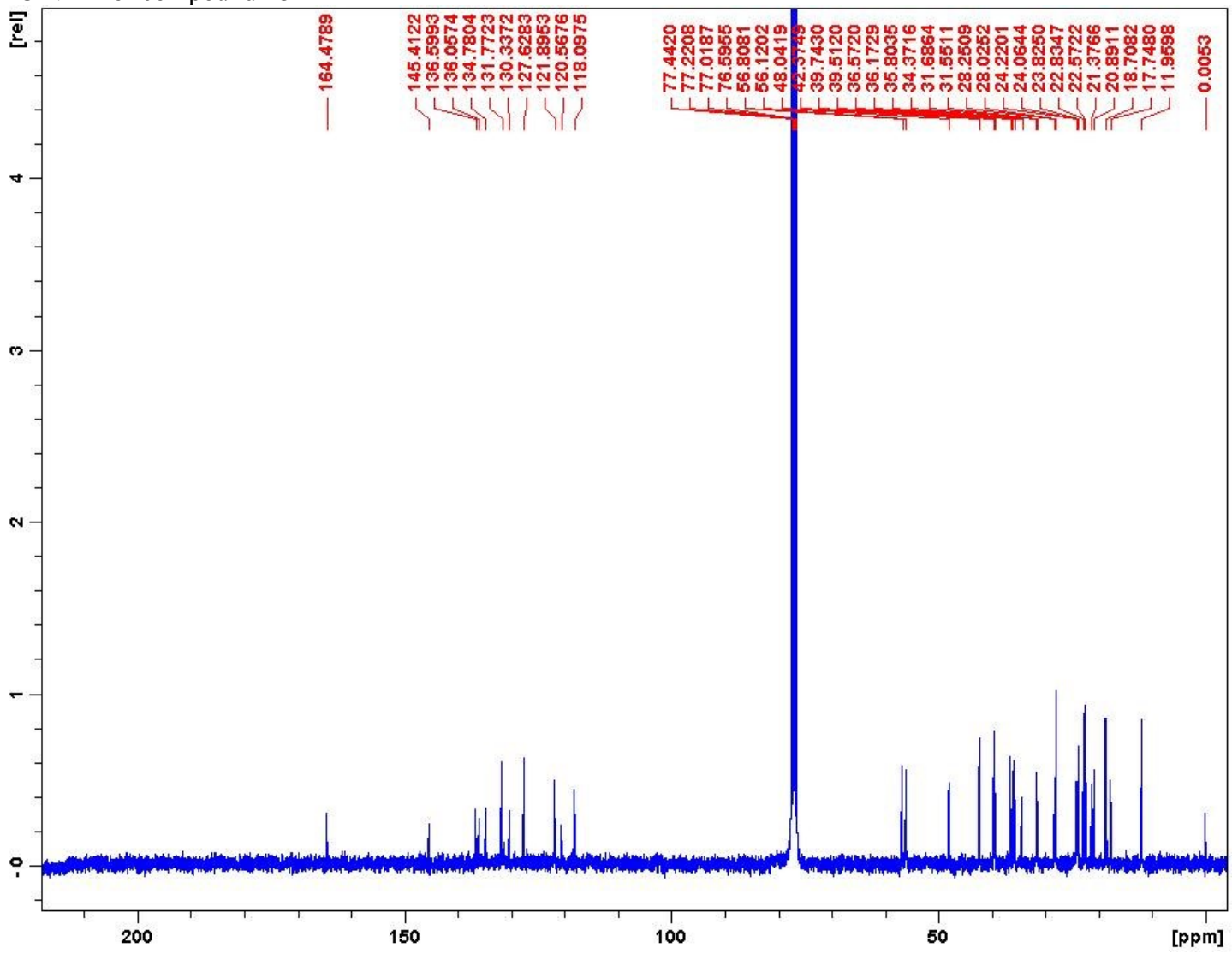


(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2,4-dimethylphenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (28).

^{1}H NMR of compound **28**

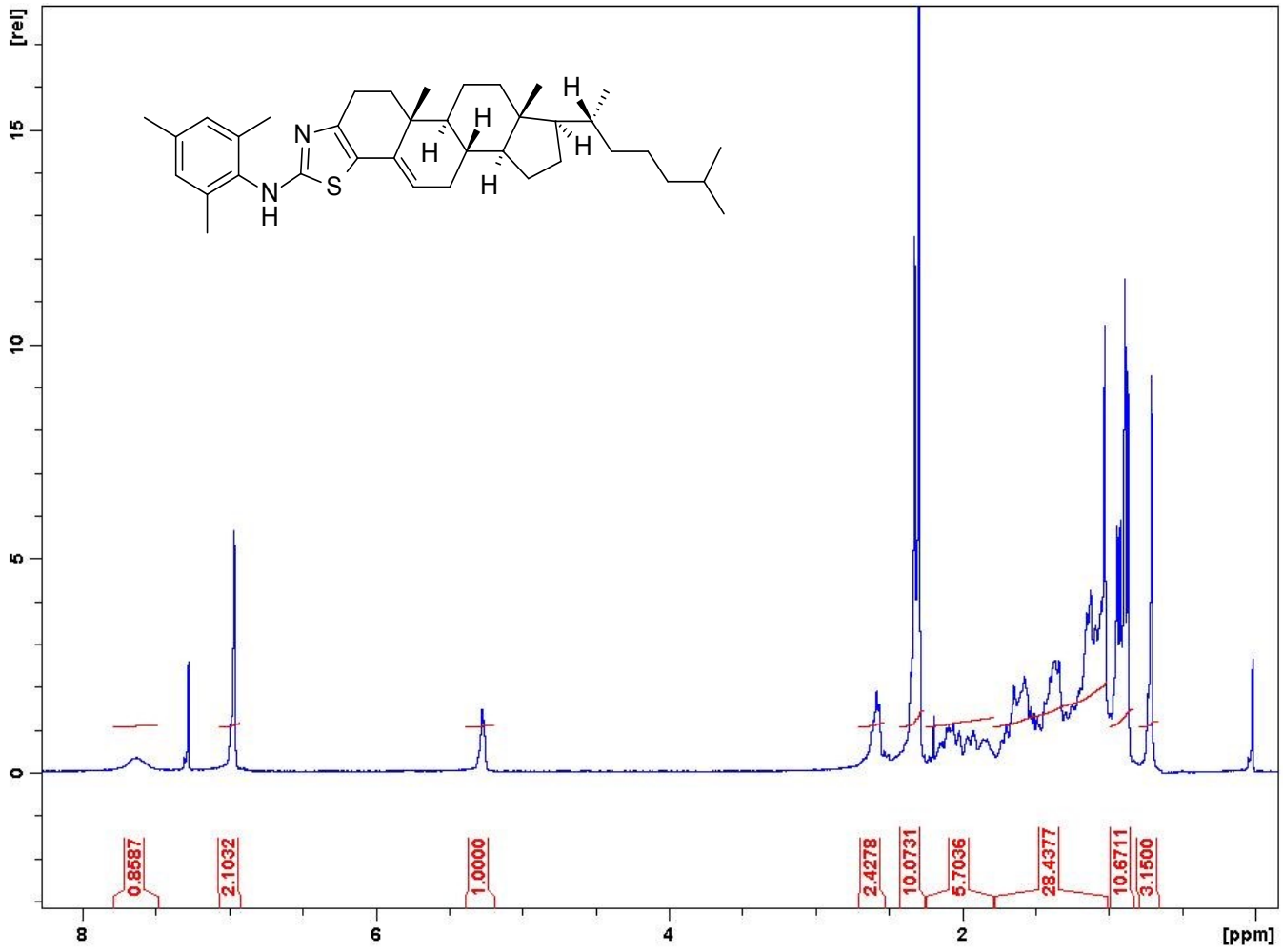


^{13}C NMR of compound **28**

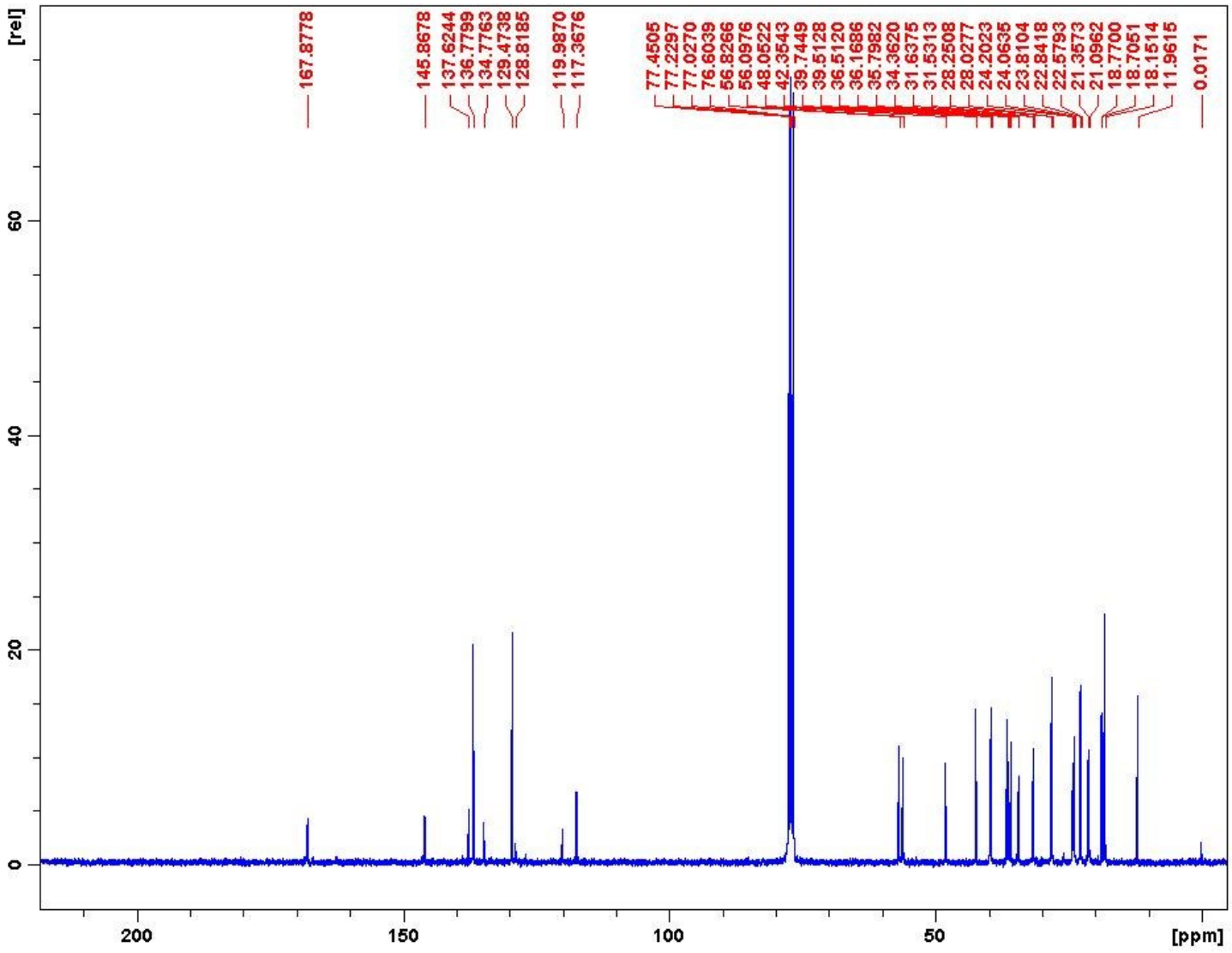


(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2,4,6-trimethylphenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (29).

^{1}H NMR of compound **29**



^{13}C NMR of Compound **29**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40
60
200
150
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128.8185
119.9870
117.3676
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77.0270
76.6039
56.8266
56.0976
48.0522
42.3543
39.7449
39.5128
36.5120
36.1686
35.7982
34.3620
31.6375
31.5313
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28.0277
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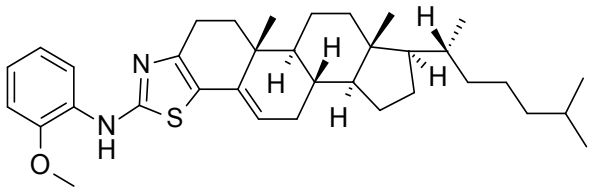
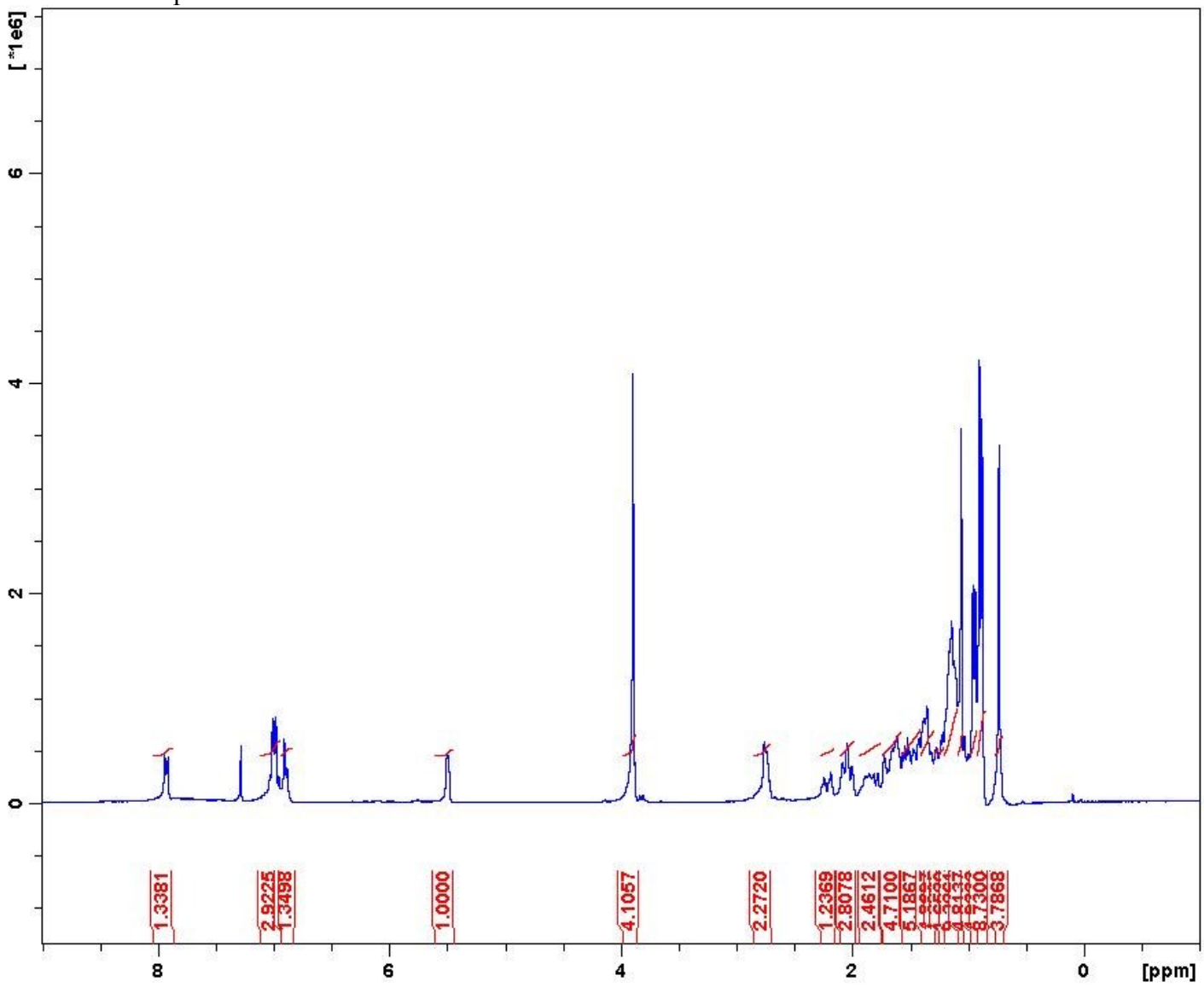
18.1514
11.9615
0.0171

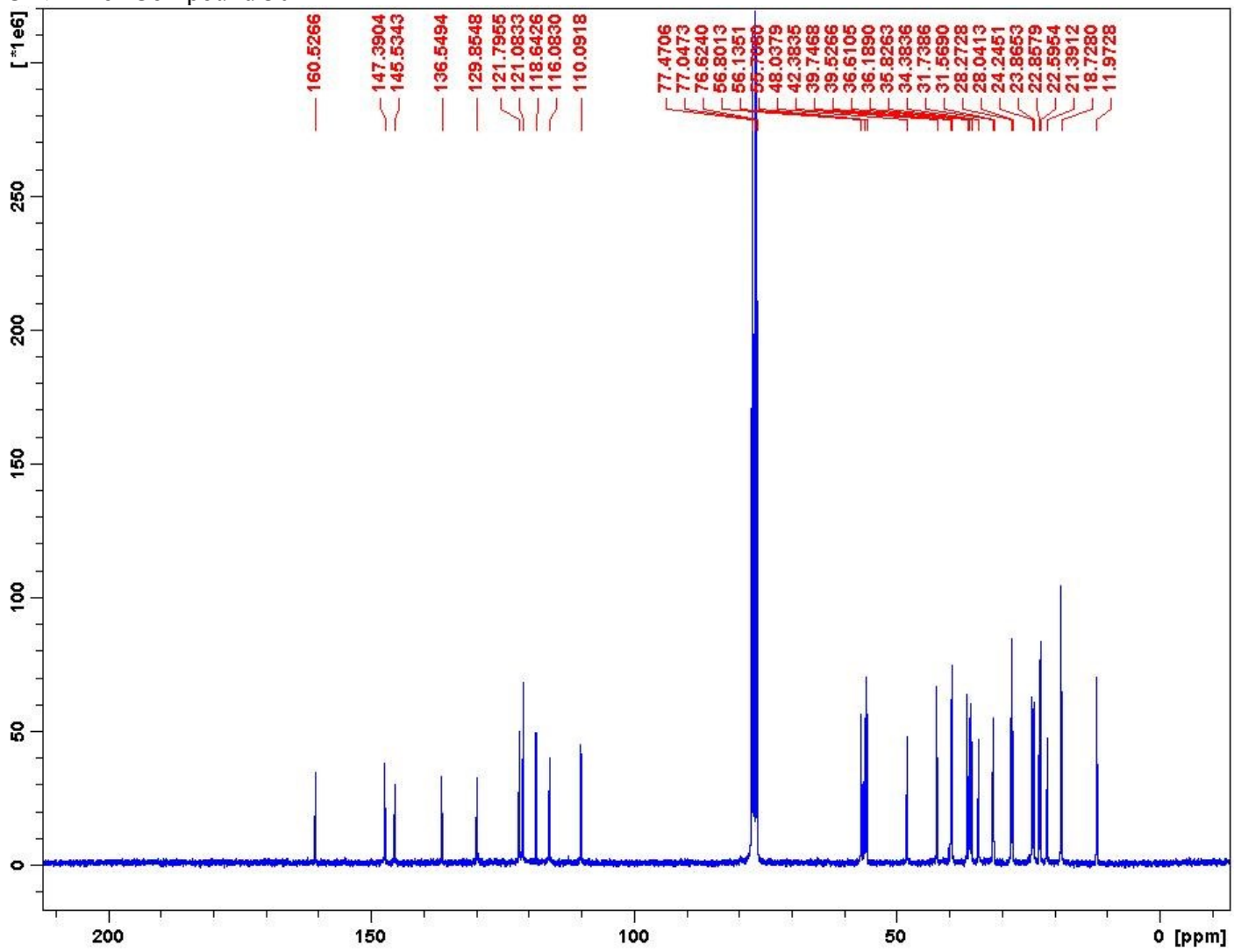


(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2-methoxyphenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (30).

^{1}H NMR of Compound **30**

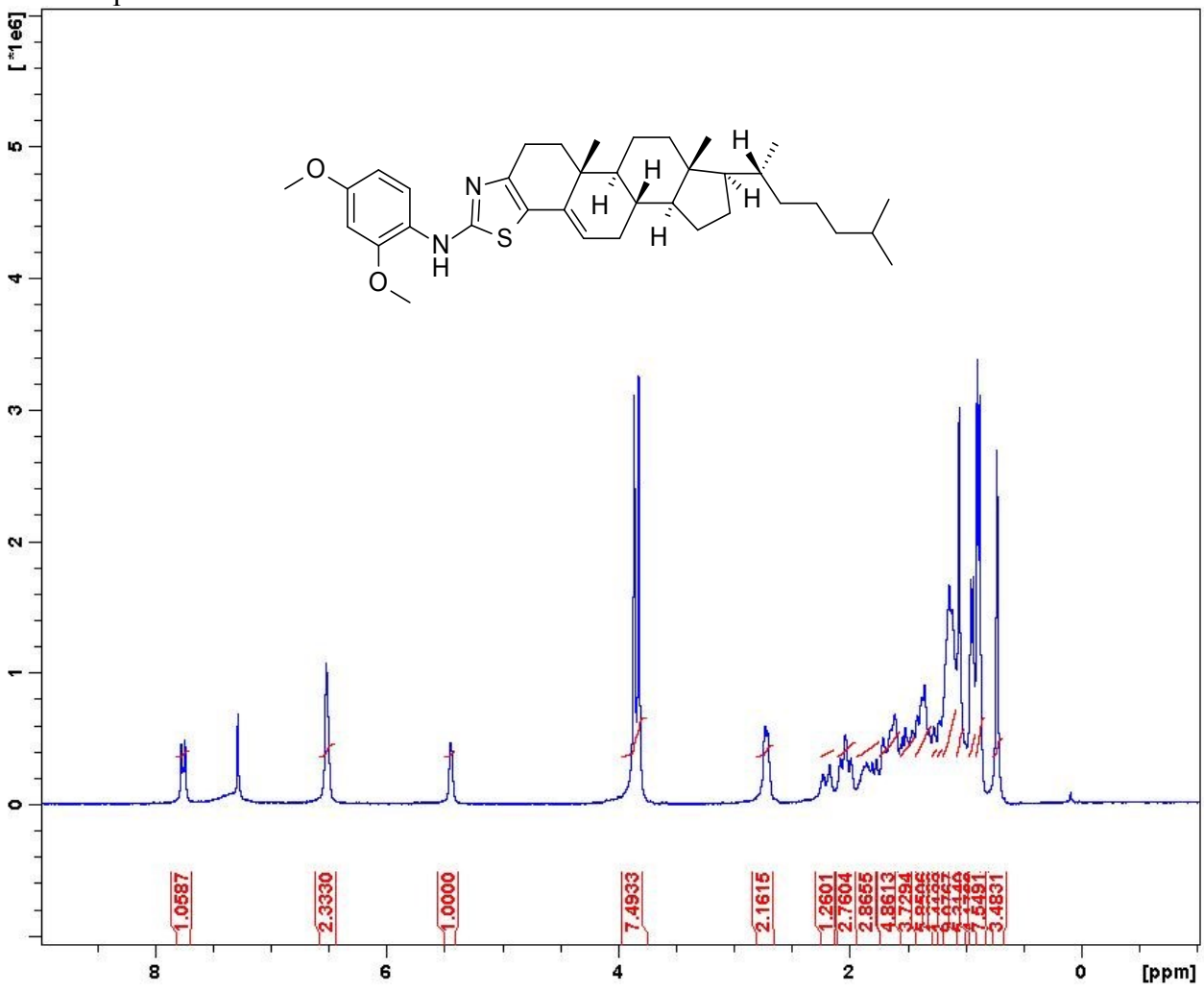


^{13}C NMR of Compound **30**

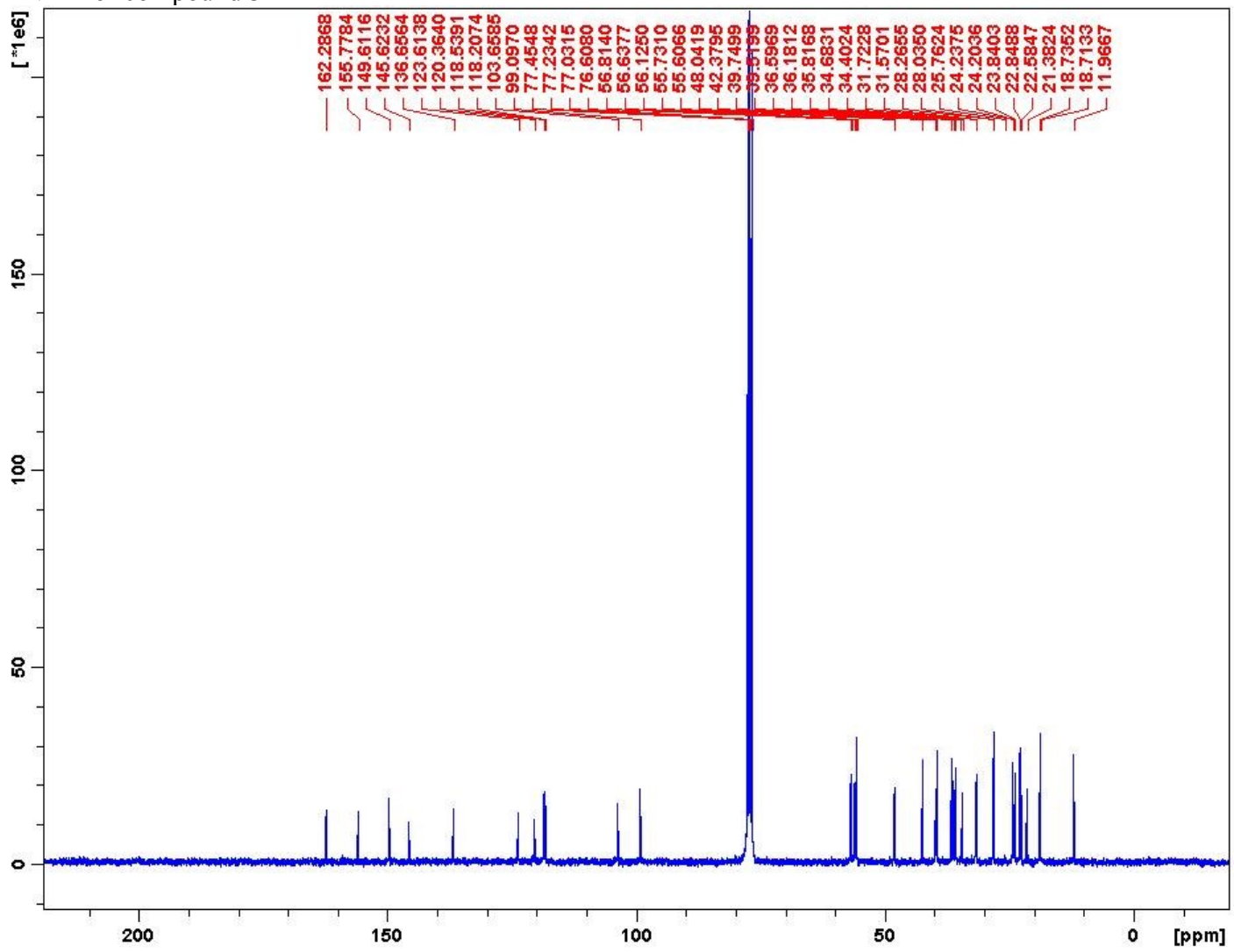


(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2,4-dimethoxyphenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (31).

^{1}H NMR of compound **31**

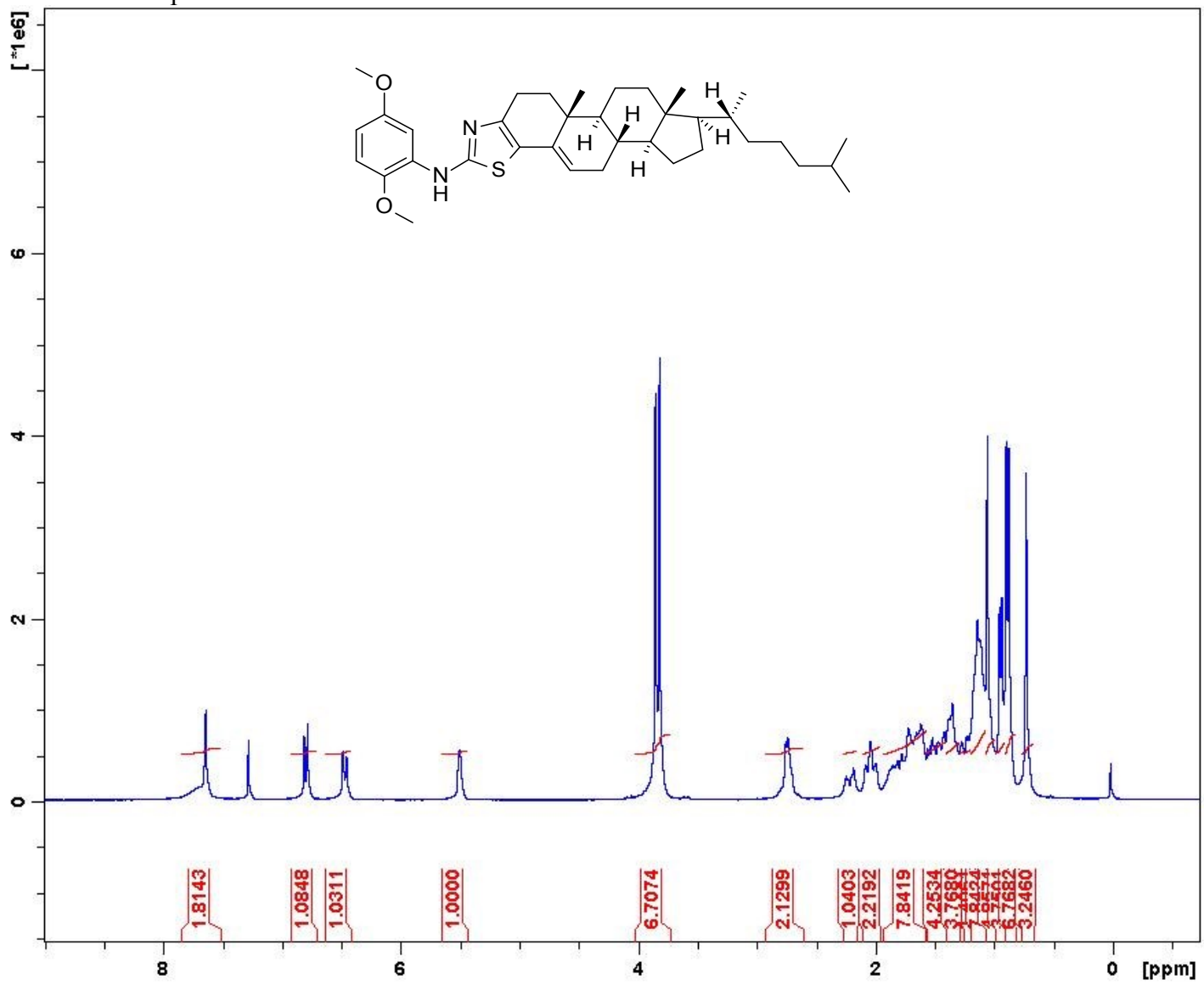


^{1}H NMR of compound **31**

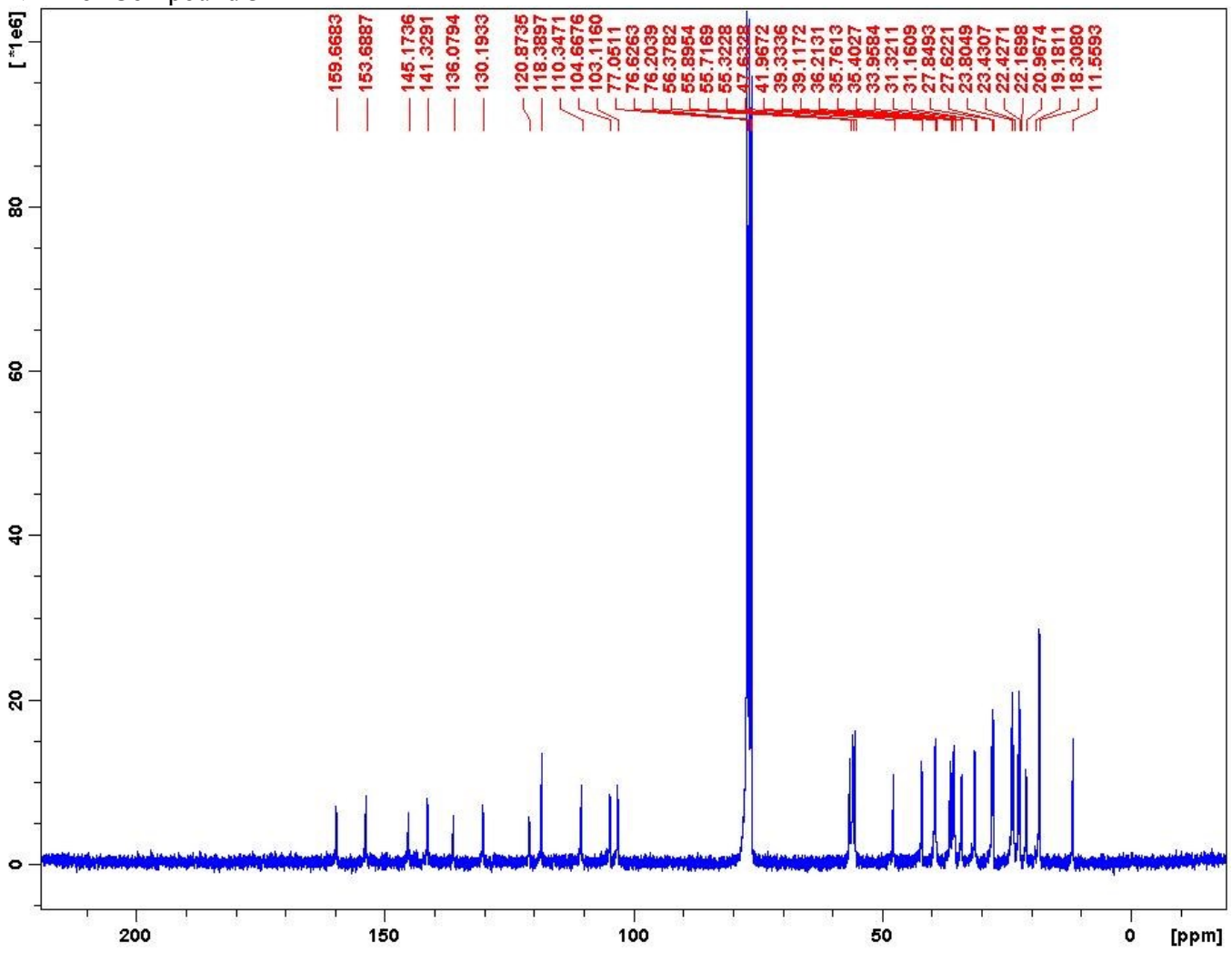


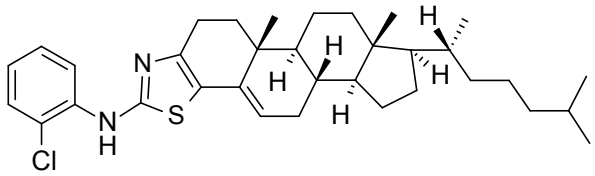
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2,5-dimethoxyphenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (32).

^{1}H NMR of compound **32**



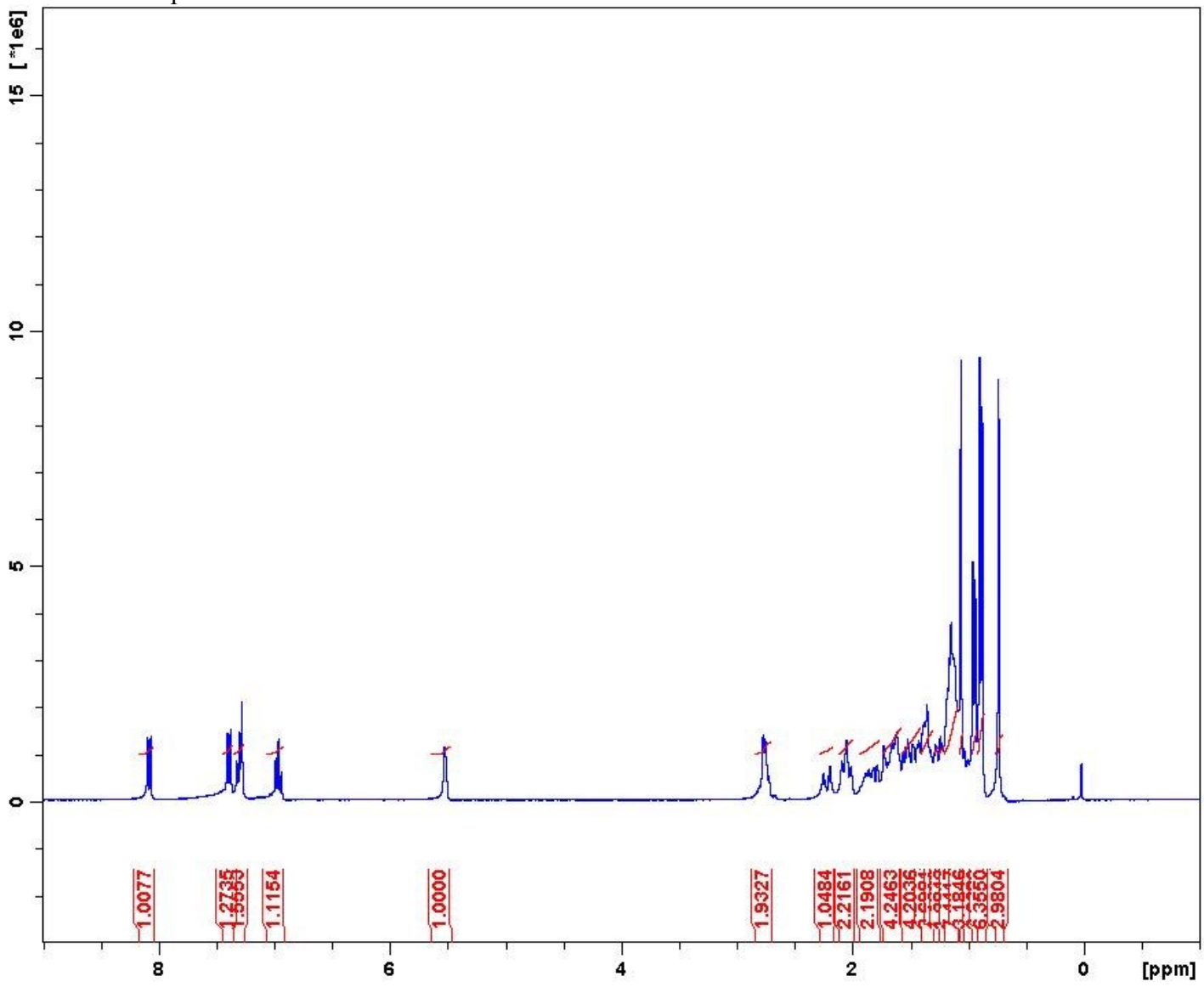
^{13}C NMR of Compound **32**



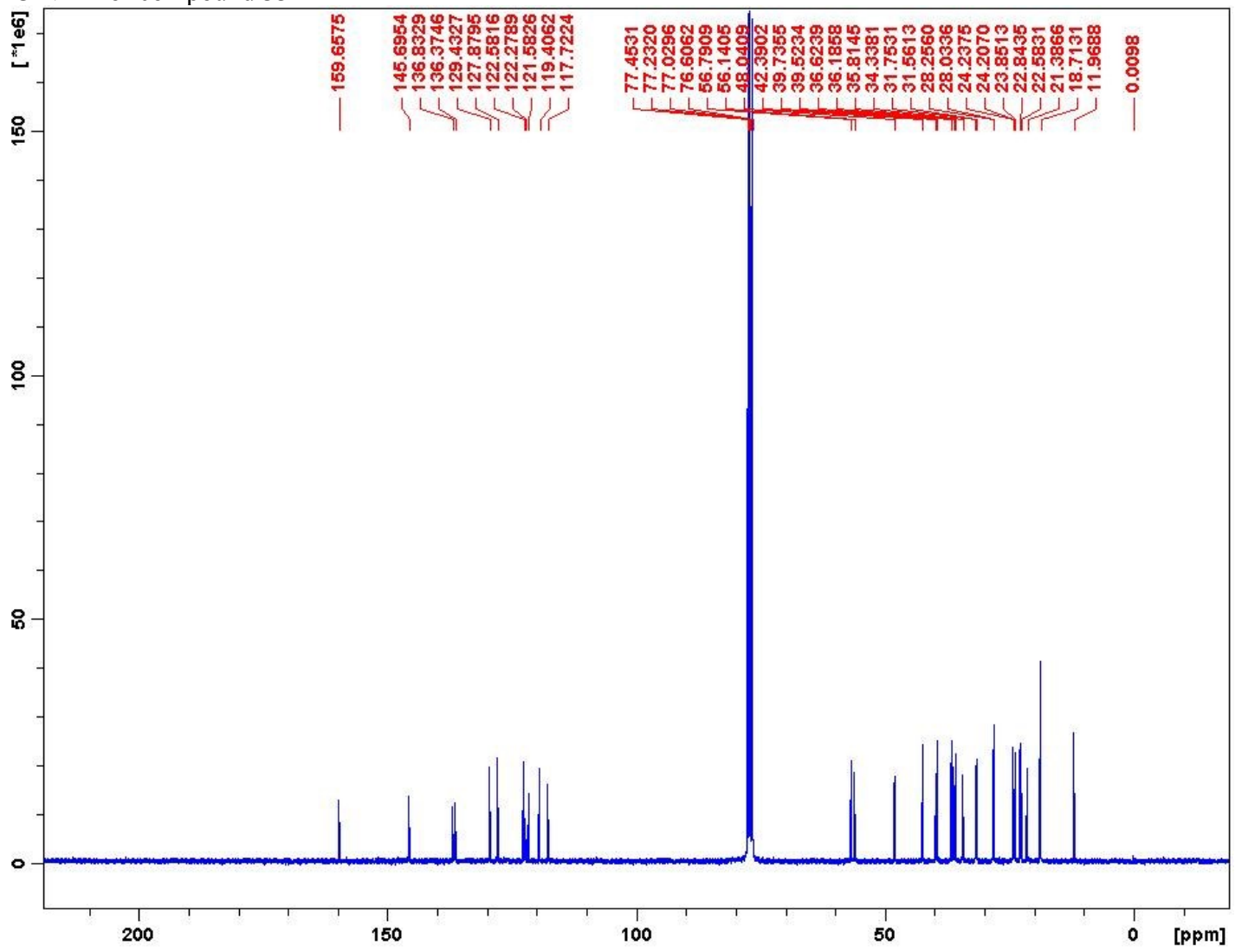


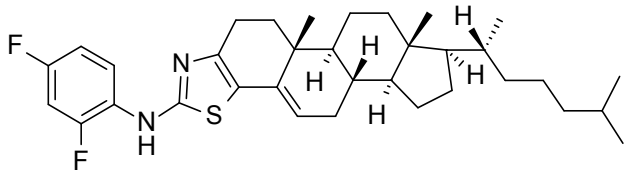
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2-chlorophenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (33)

^{1}H NMR of compound **33**



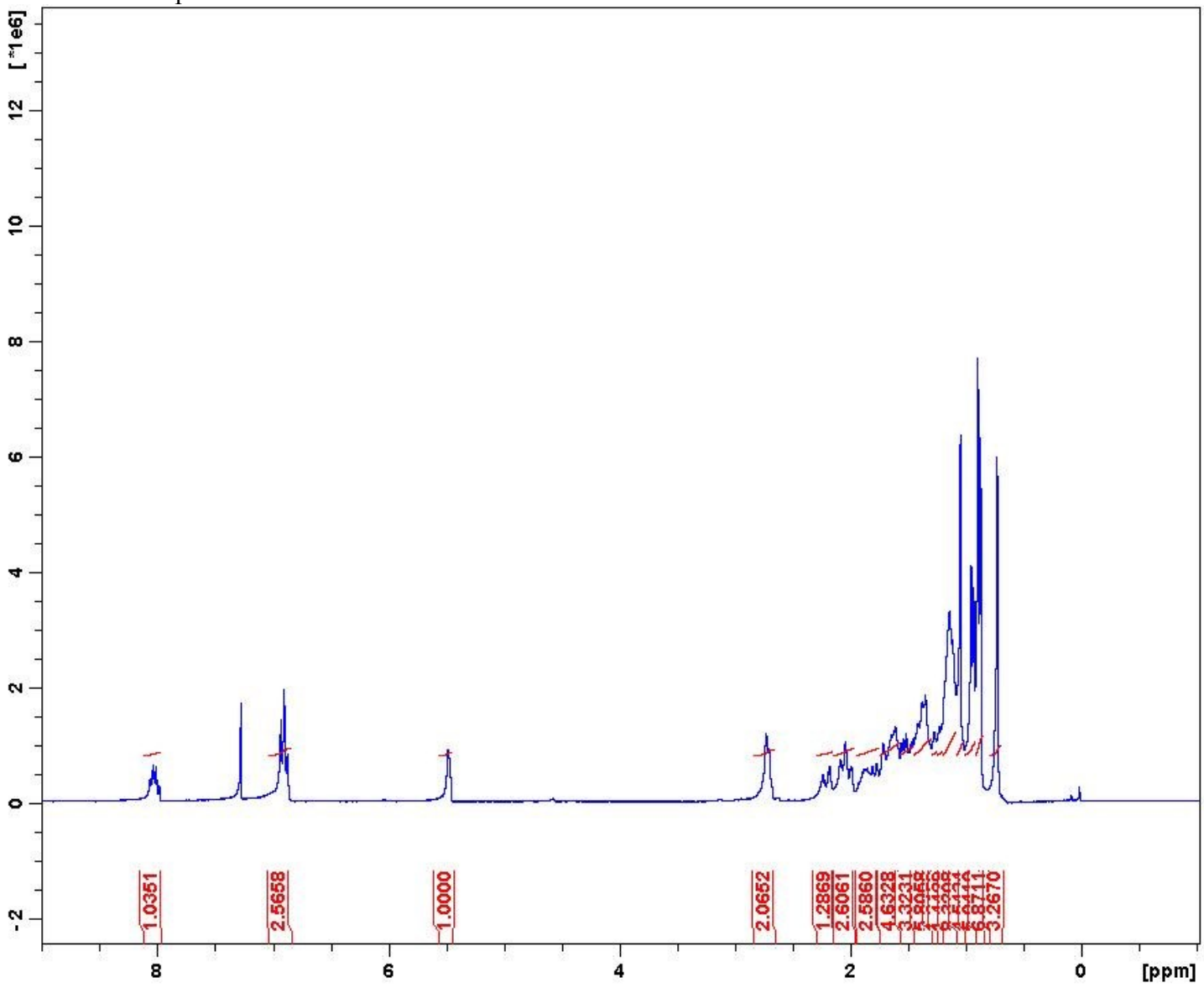
^{13}C NMR of compound **33**



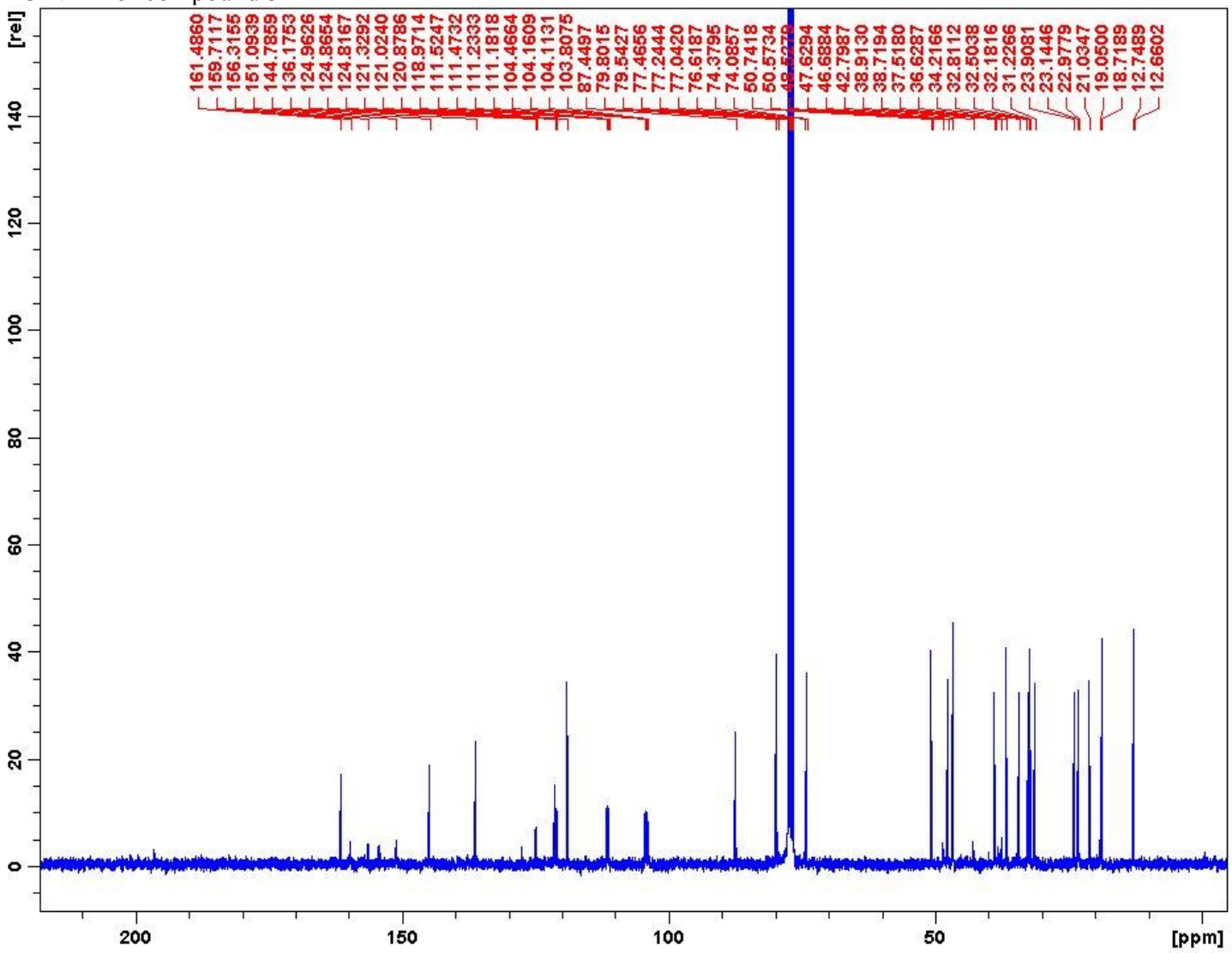


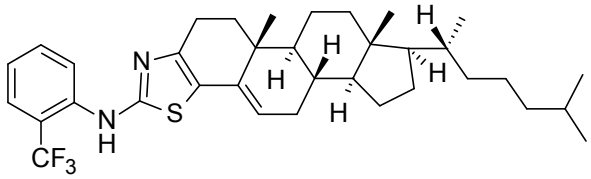
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2,4-difluorophenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (34).

^{1}H NMR of compound **34**



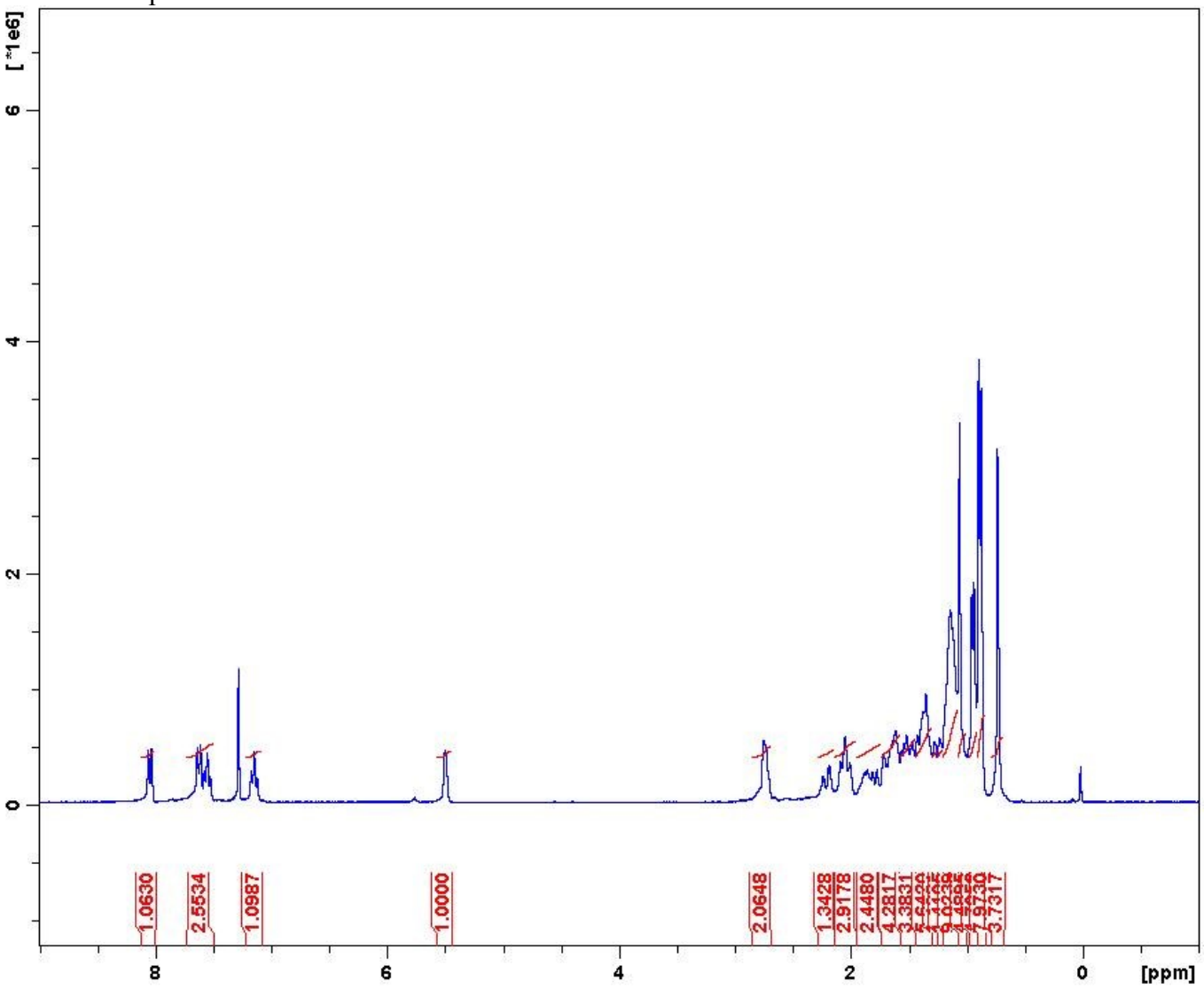
^{13}C NMR of compound **34**



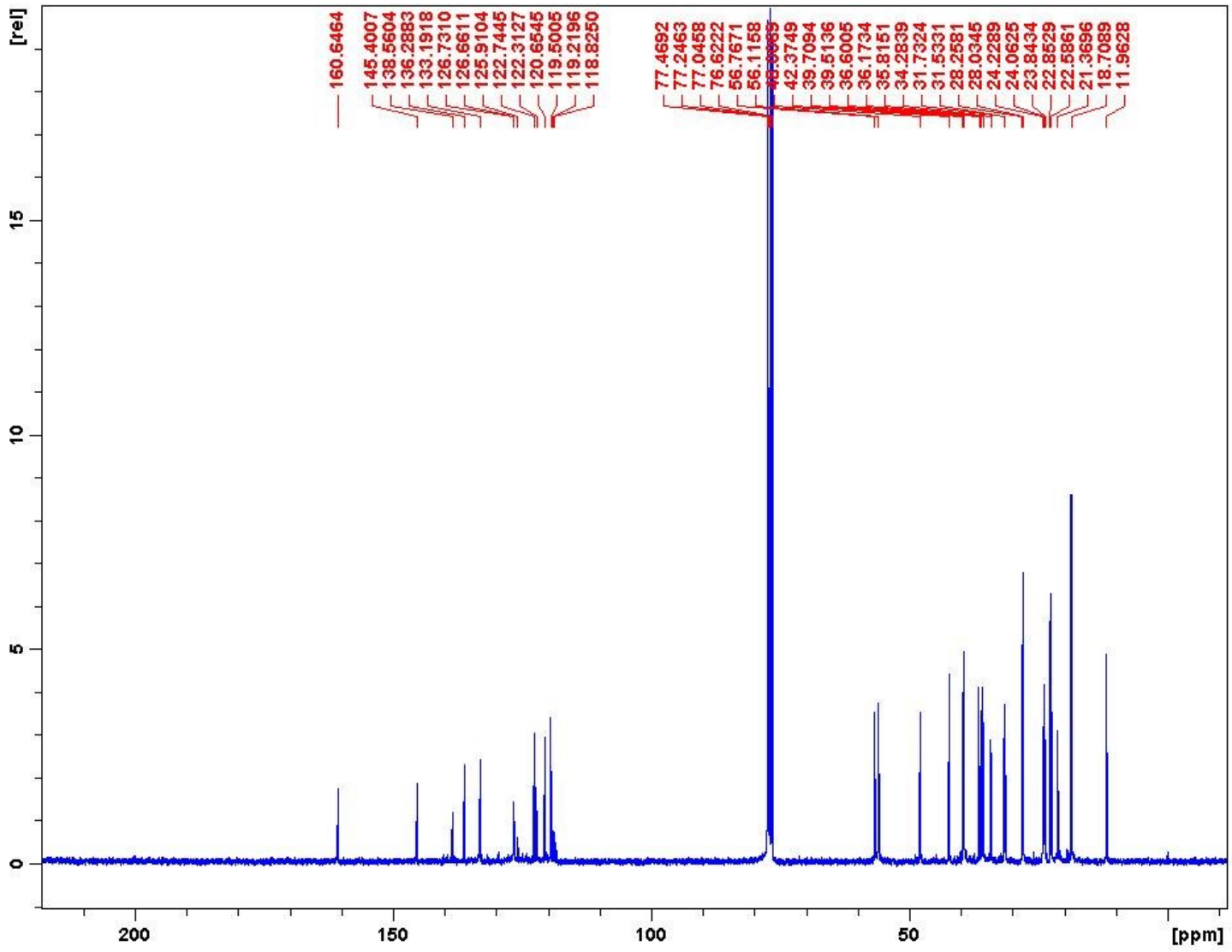


(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-[2-(trifluoromethyl)phenyl]-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (35).

^{1}H NMR of compound **35**



^{13}C NMR of compound **35**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133.1918
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126.6611
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122.7445
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120.6545
119.5005
119.2196
118.8250
77.4692
77.2463
77.0458
76.6222
56.7671
56.1158
42.3749
39.7094
39.5136
36.6005
36.1734
35.8151
34.2839
31.7324
31.5331
28.2581
28.0345
24.2289
24.0625
23.8434
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11.9628
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5
10
15
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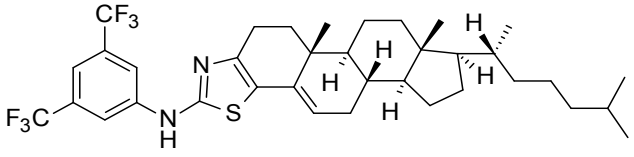
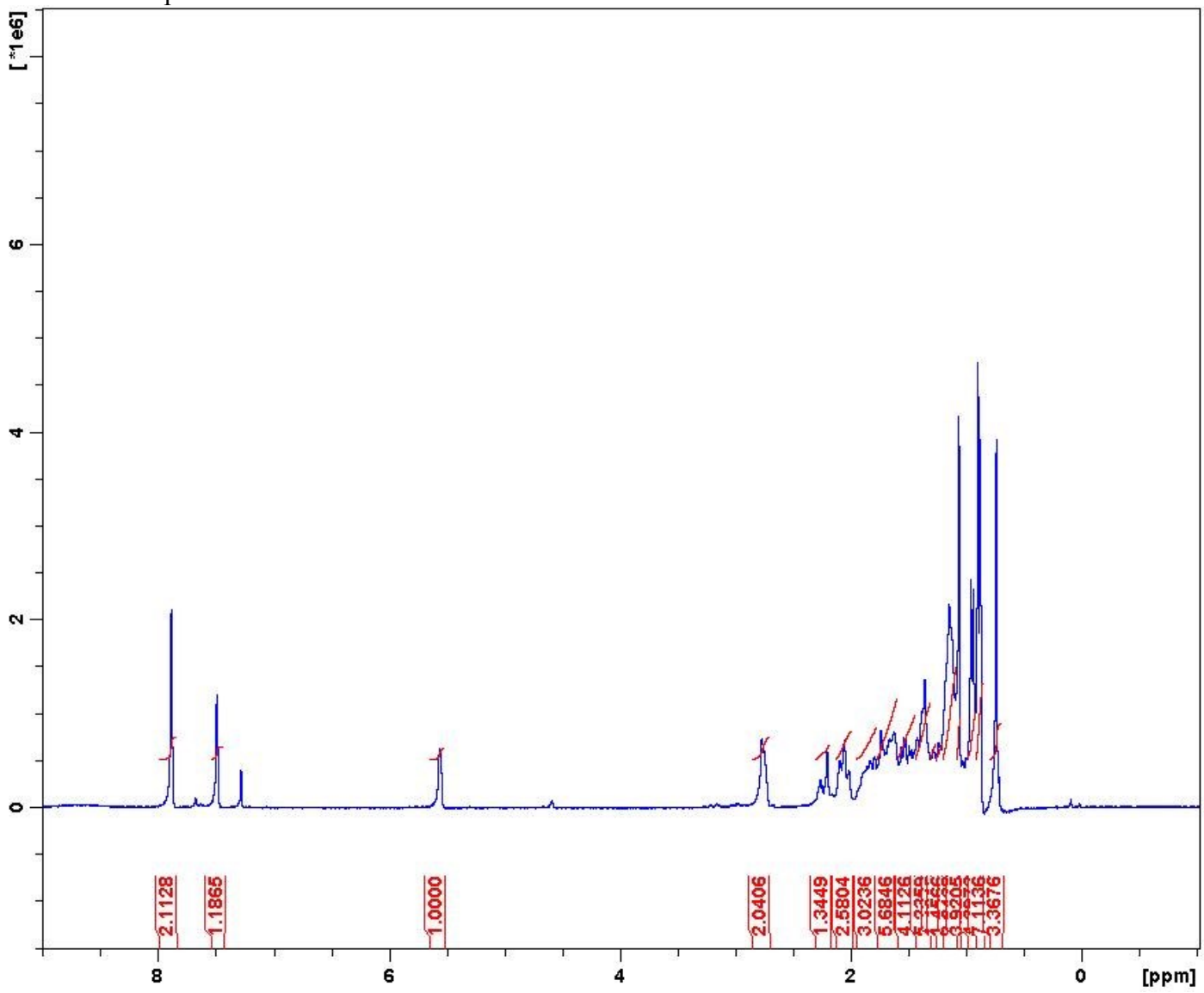
150
100
50
[ppm]

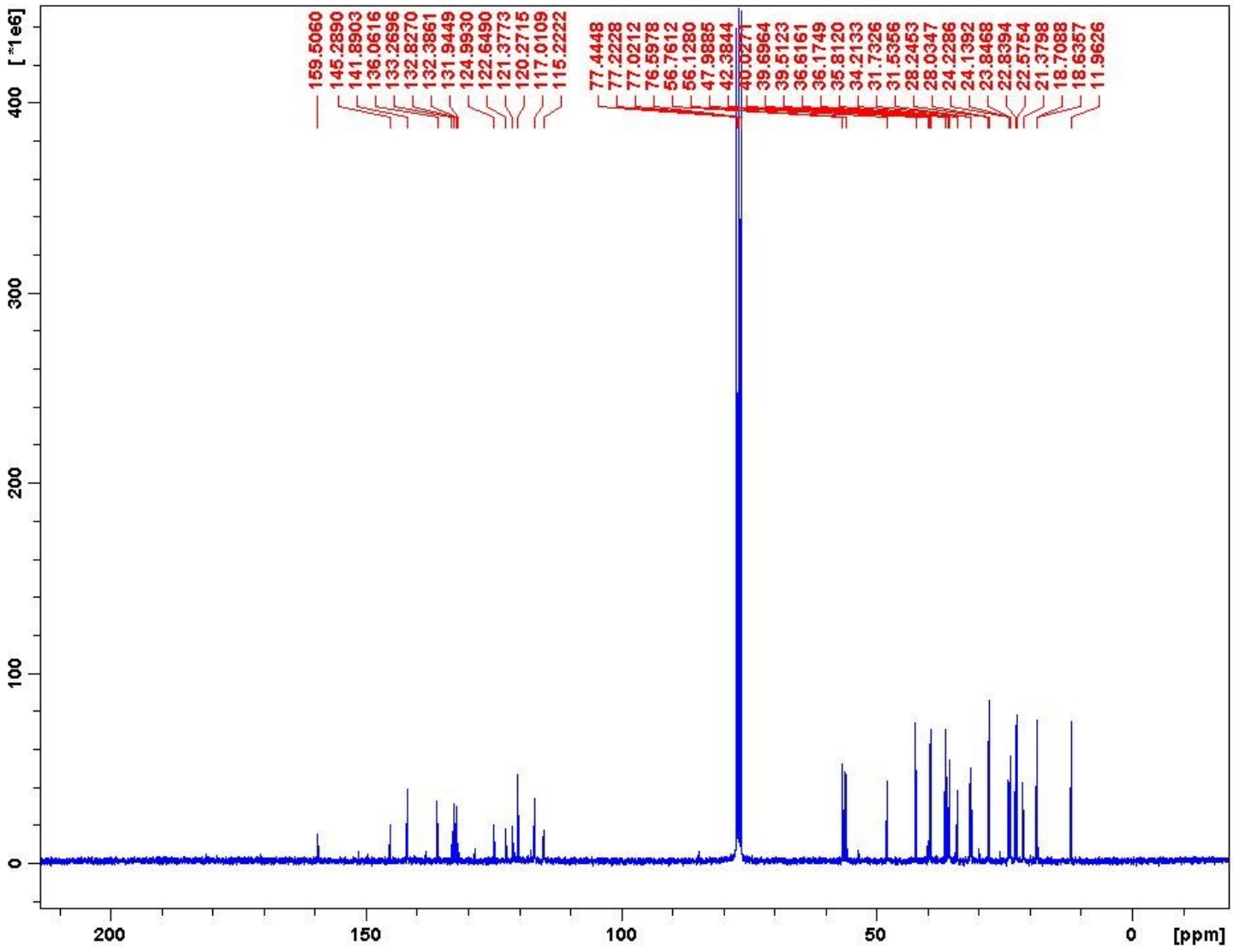

CF3
F3C
N
H
S
N
H
H
H
H
H

(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-[3,5-bis(trifluoromethyl)phenyl]-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (36).

^{1}H NMR of compound **36**



^{13}C NMR of compound **36**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120.2715
117.0109
115.2222
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77.2228
77.0212
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56.1280
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42.3844
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36.6161
36.1749
35.8120
34.2133
31.7326
31.5356
28.2453
28.0347
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24.1392
23.8468
22.8394
22.5754
21.3798
18.7088
18.6357
11.9626
[*1e6]
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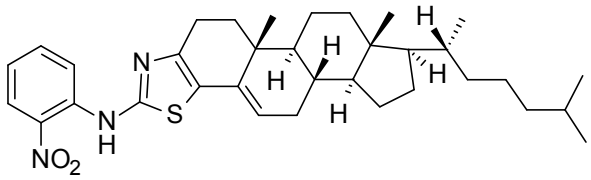
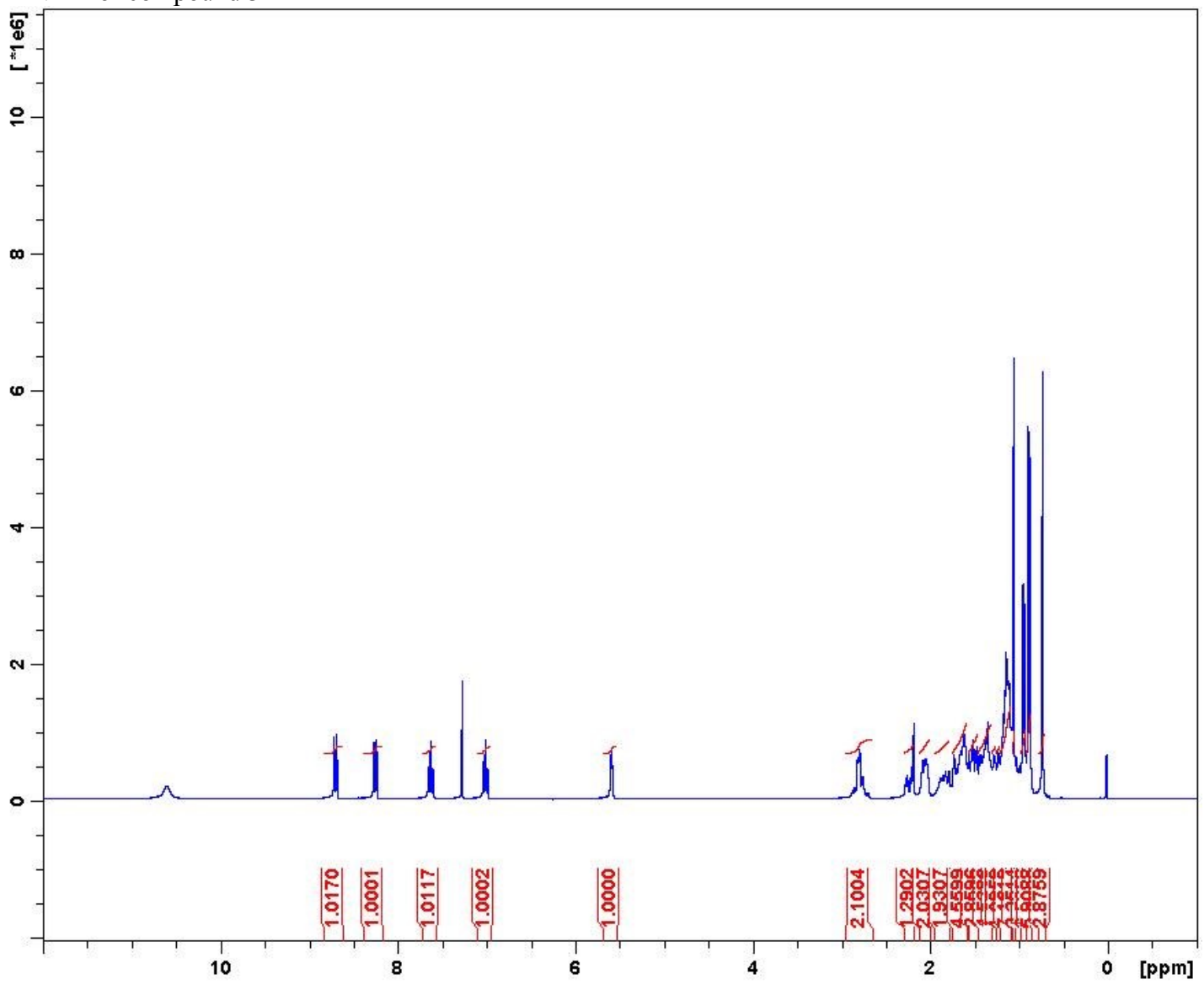
300
200
100
0
200
150
100
50
0
[ppm]

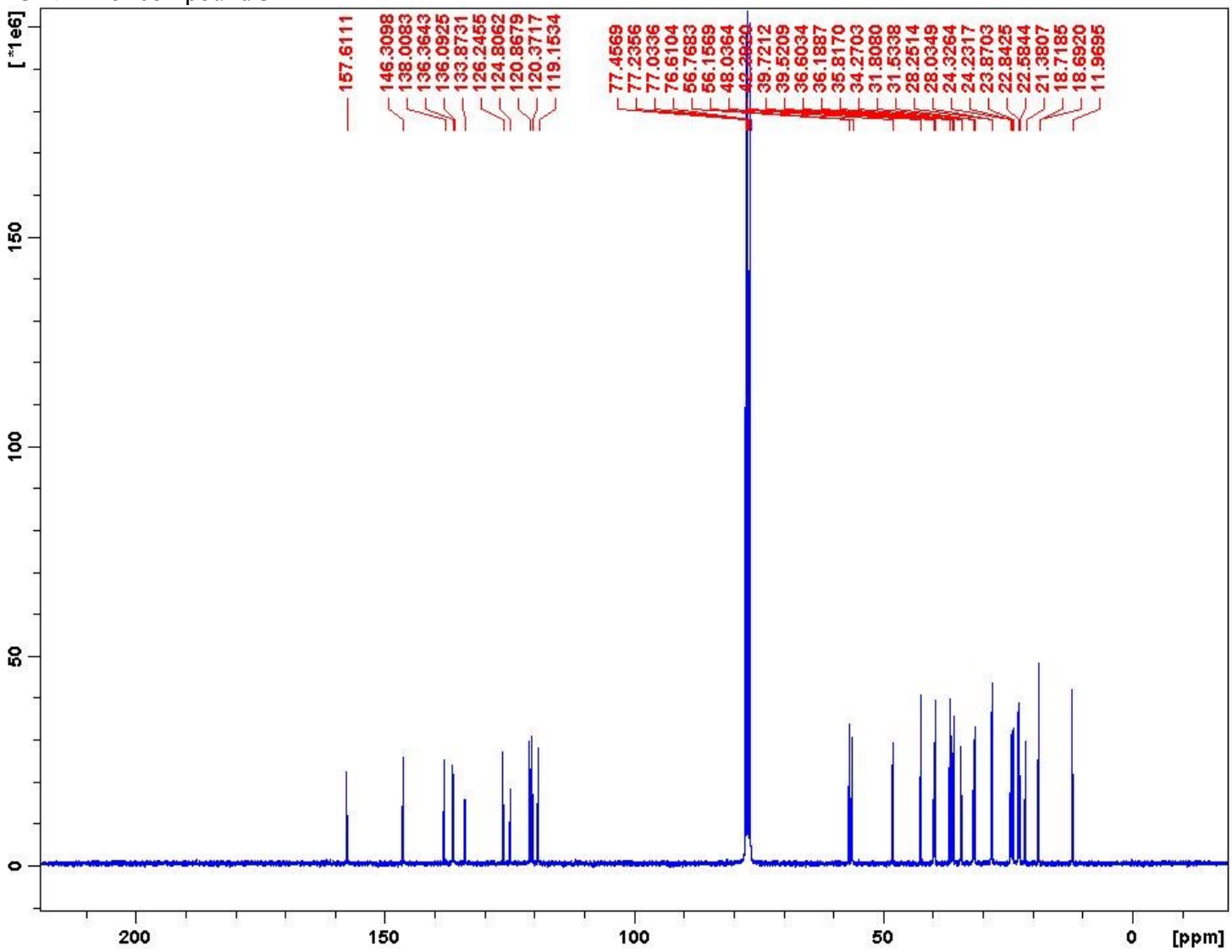


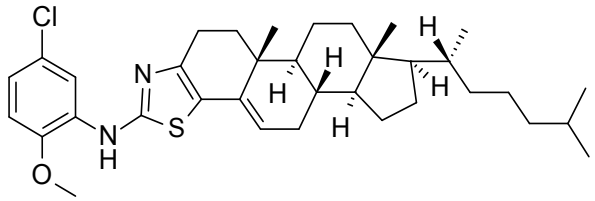
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2-nitrophenyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (37).

^{1}H NMR of compound **37**



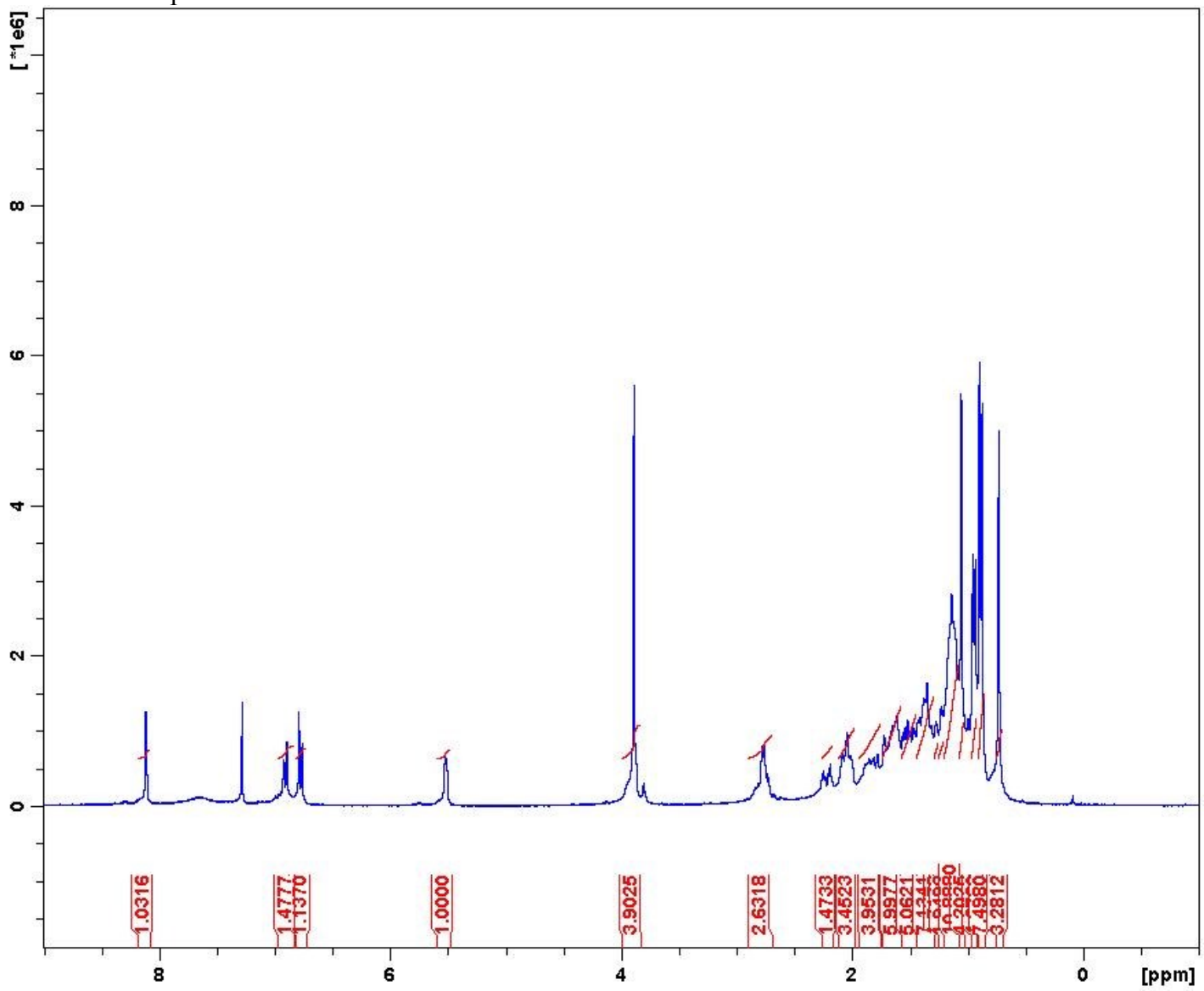
^{13}C NMR of compound **37**



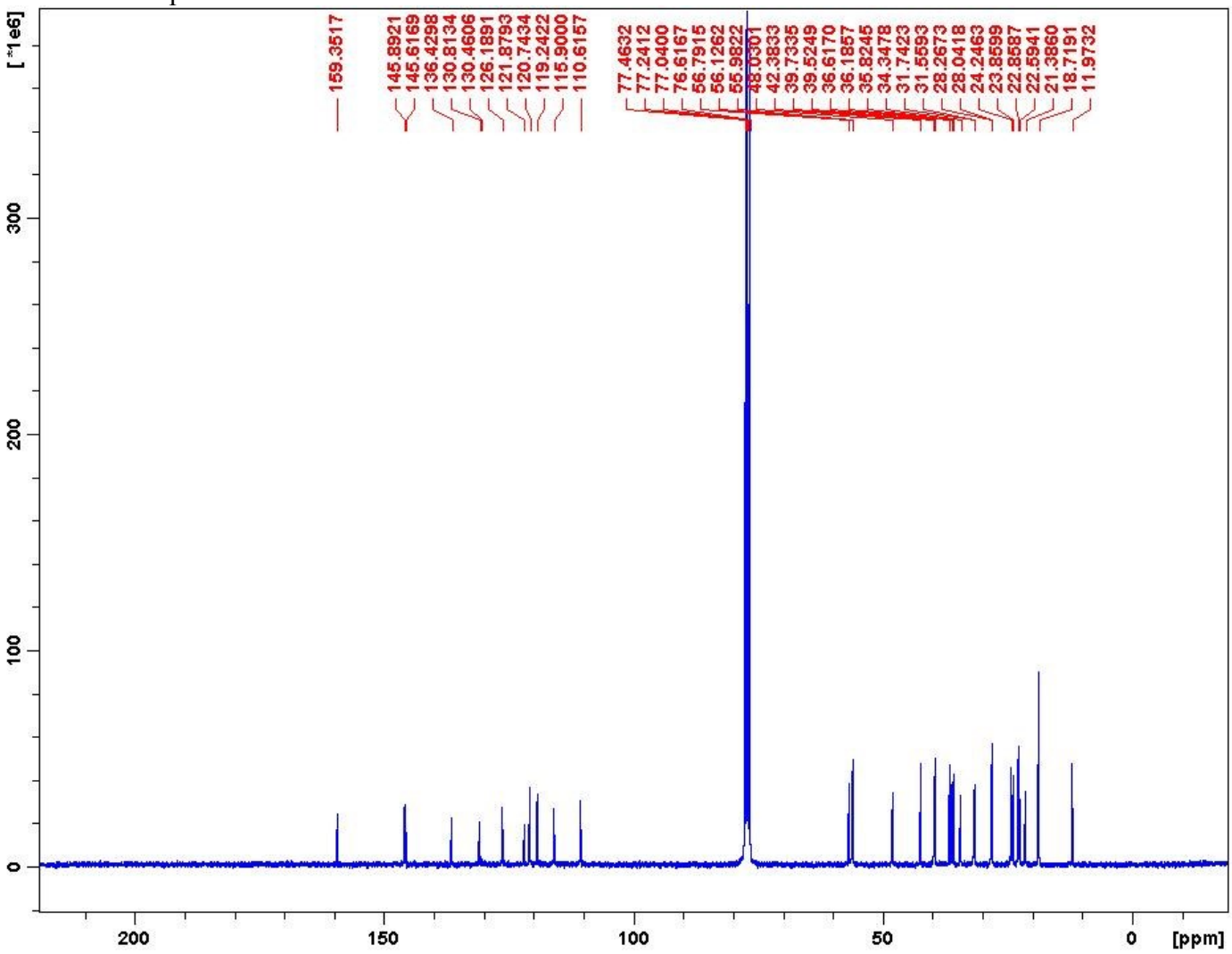


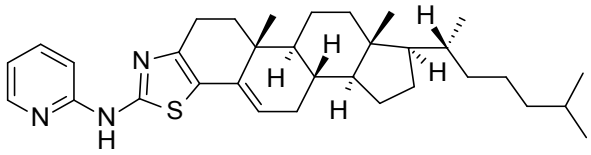
(1S,2R,13S,14S,17R,18R)-N-(5-chloro-2-methoxy-phenyl)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (38).

^{1}H NMR of compound **38**



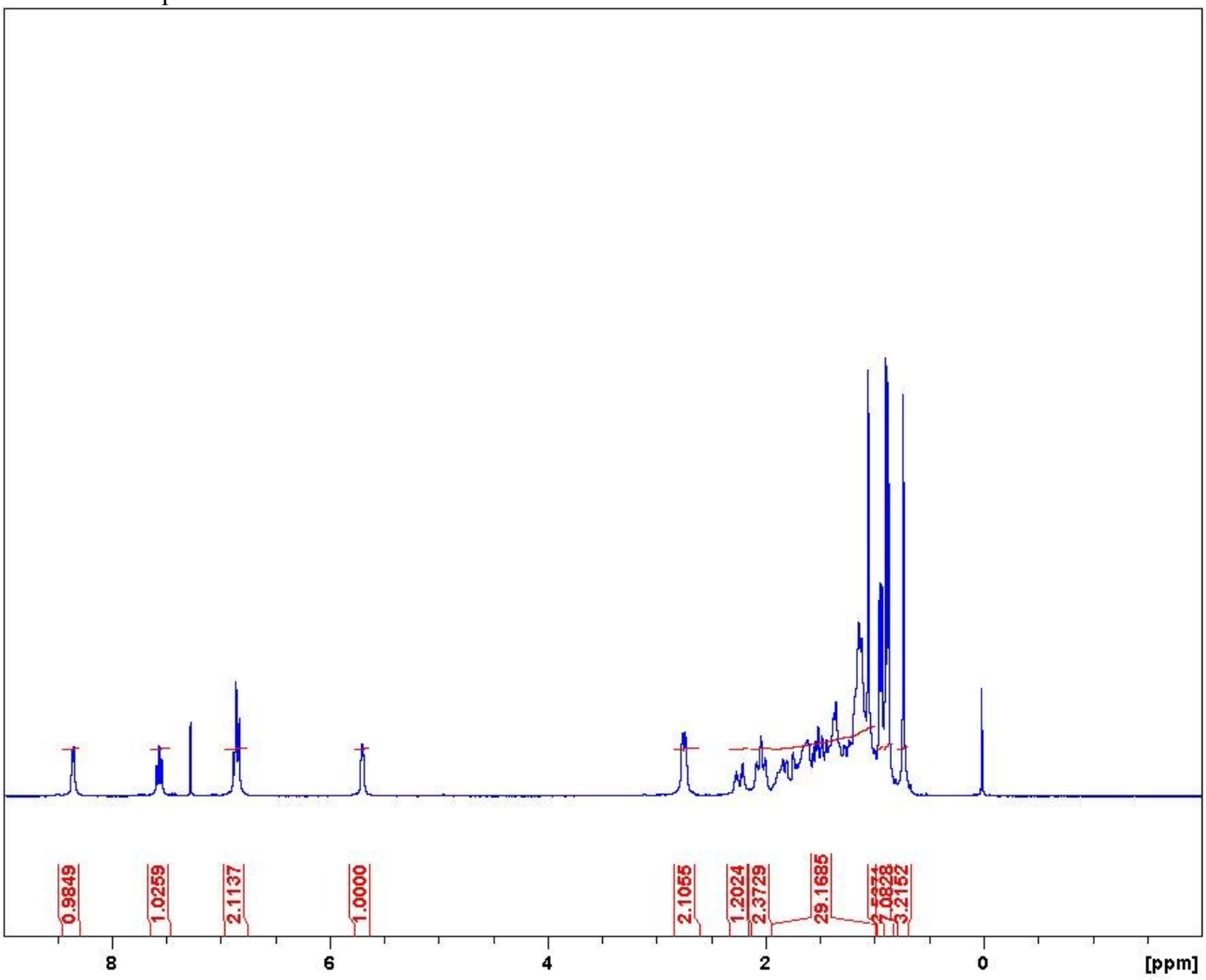
^{13}C NMR of compound **38**



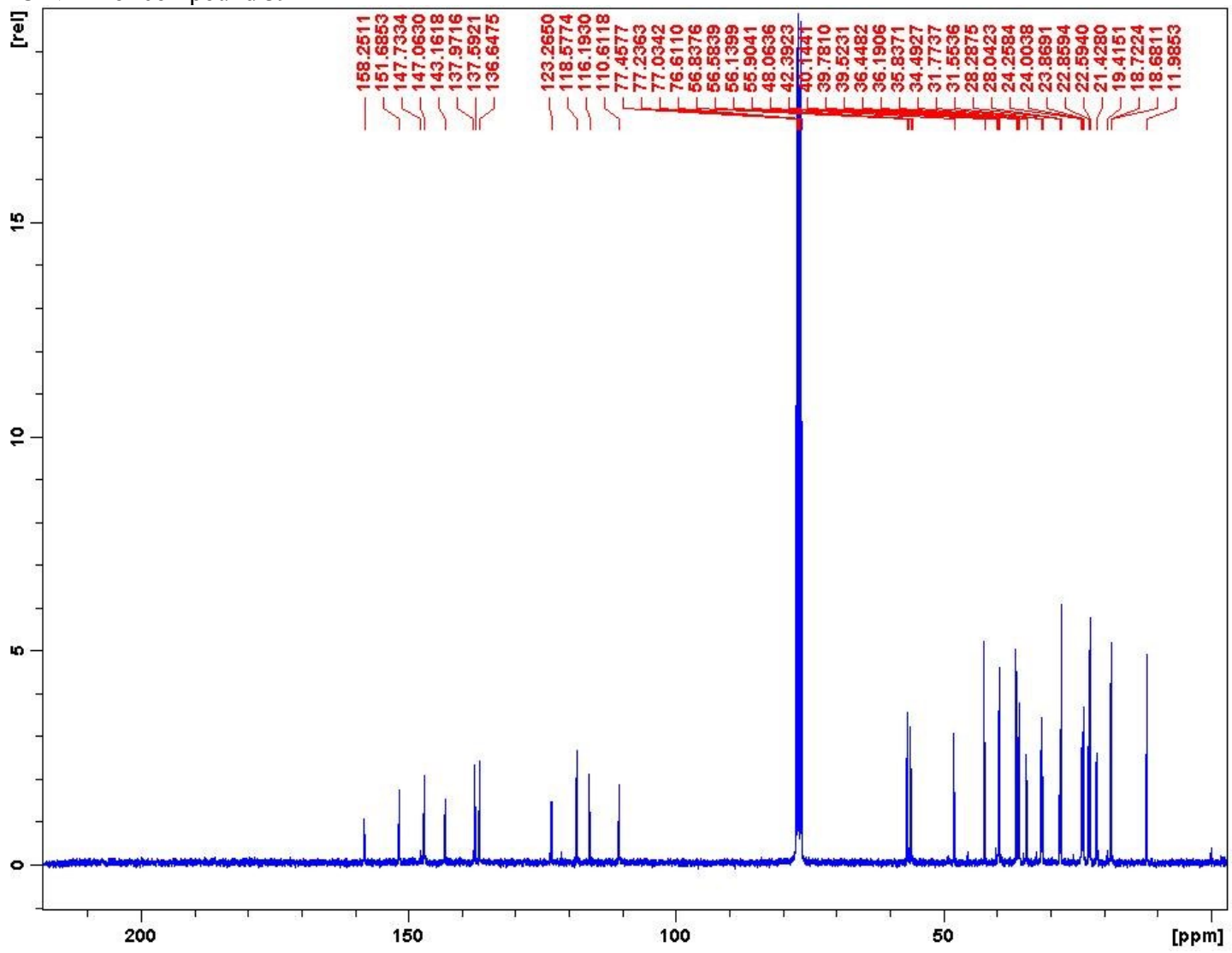


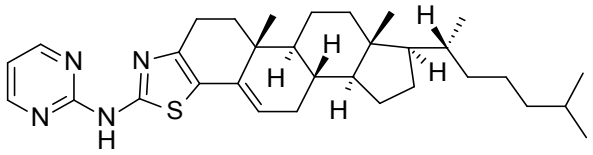
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-(2-pyridyl)-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (39).

^{1}H NMR of compound **39**



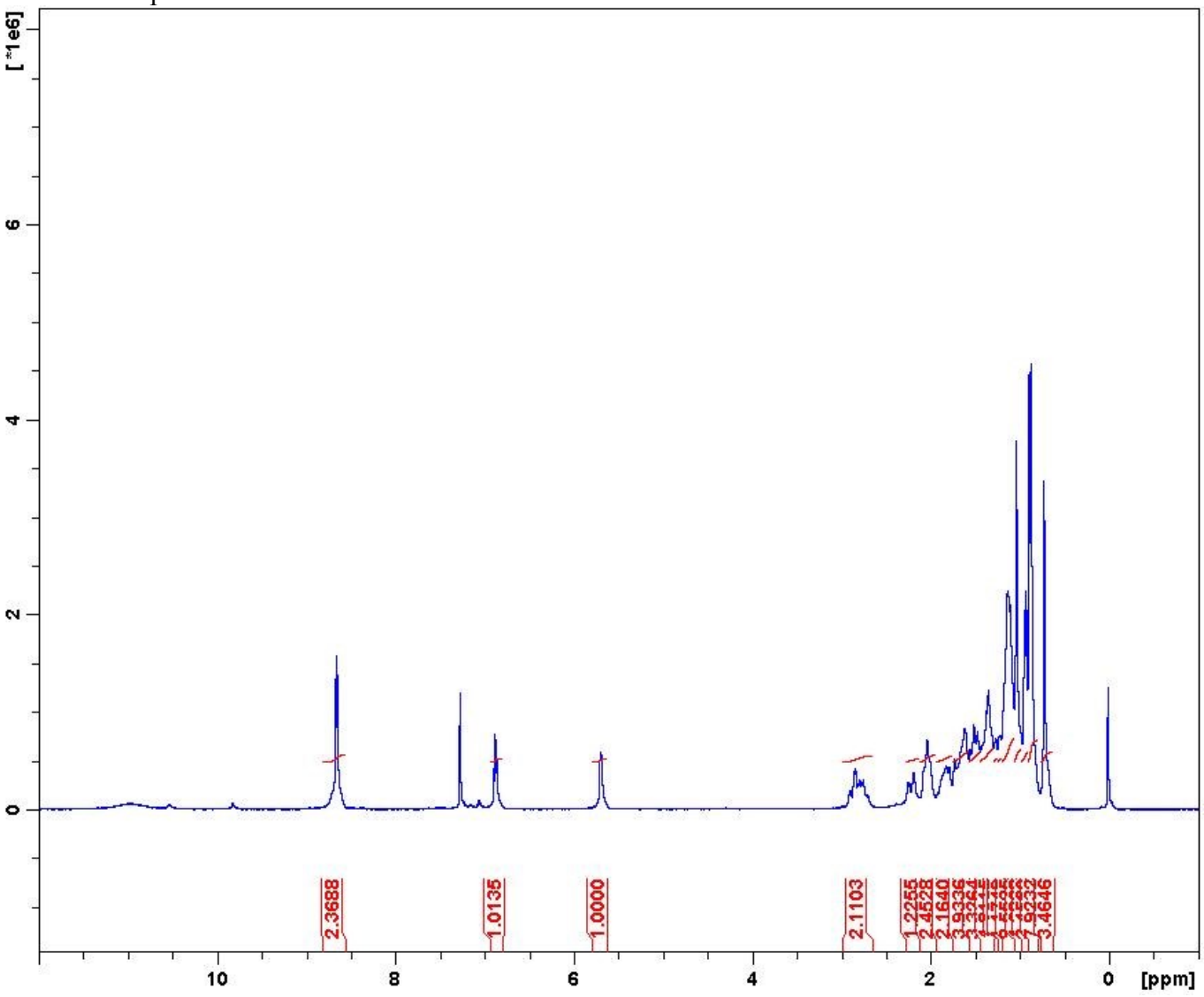
^{13}C NMR of compound **39**



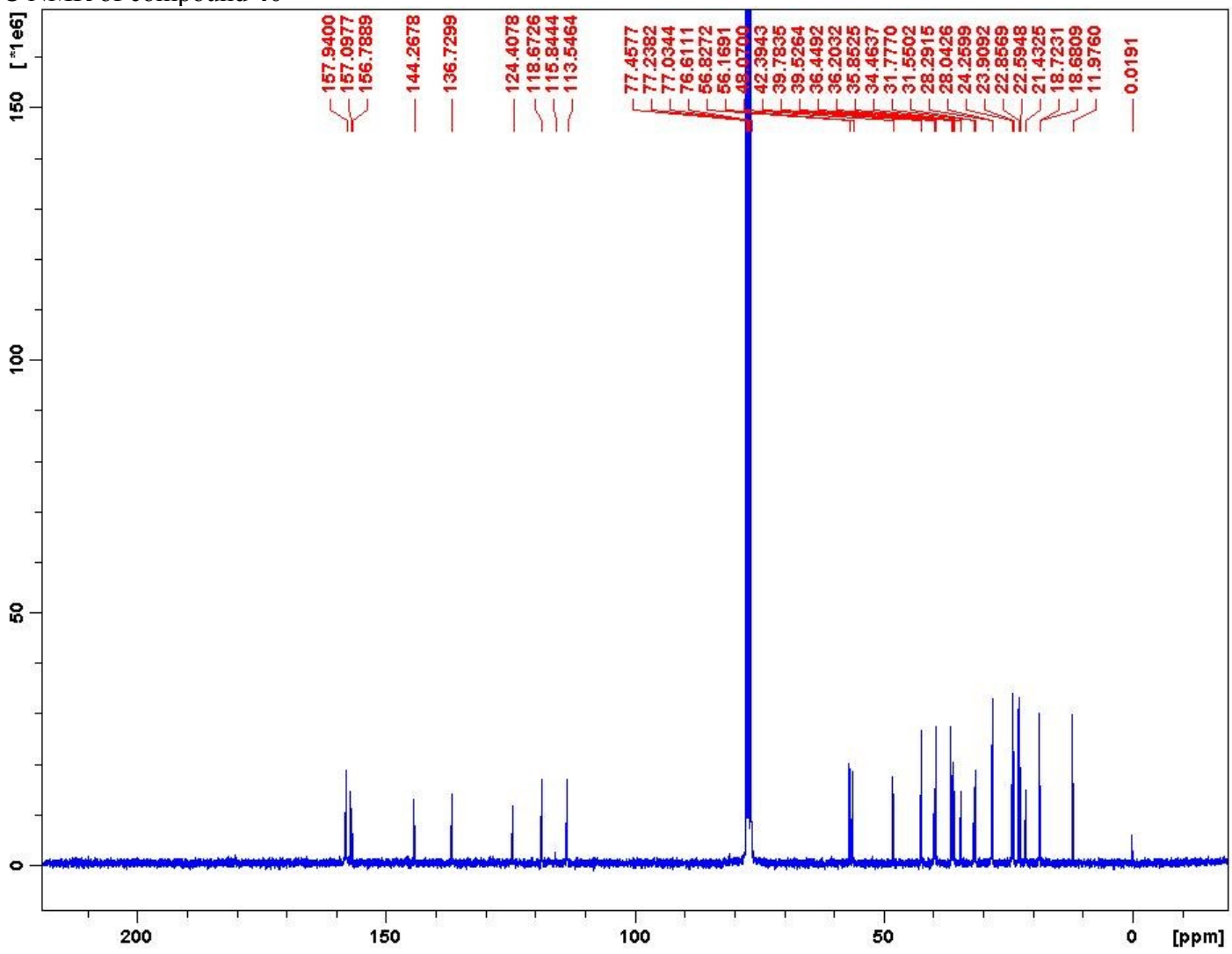


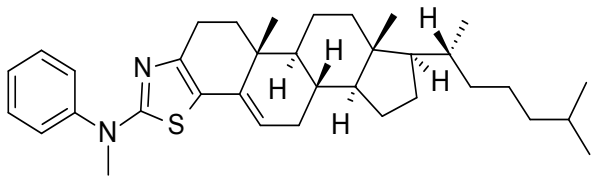
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-N-pyrimidin-2-yl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (40).

^{1}H NMR of compound **40**



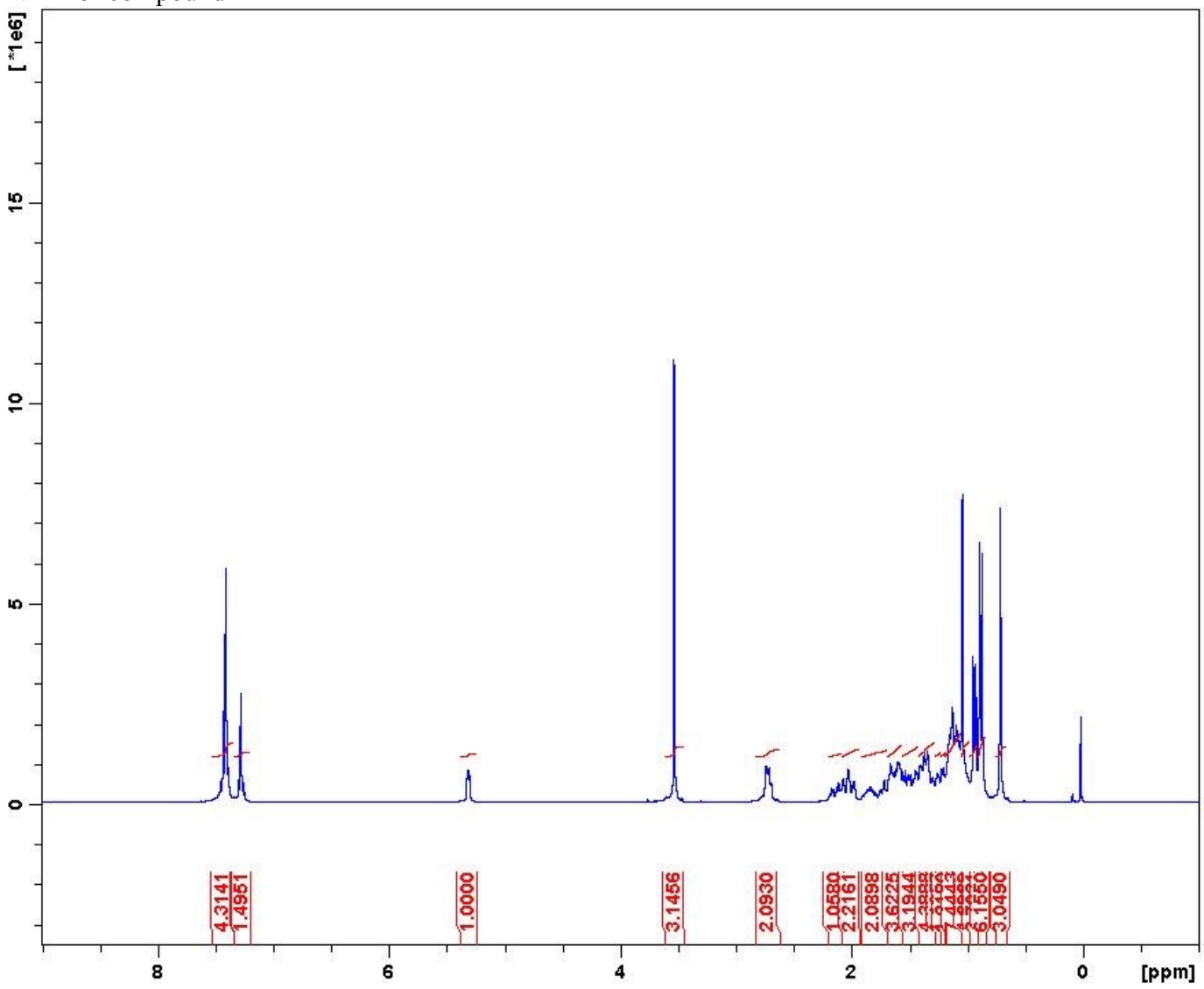
^{13}C NMR of compound **40**



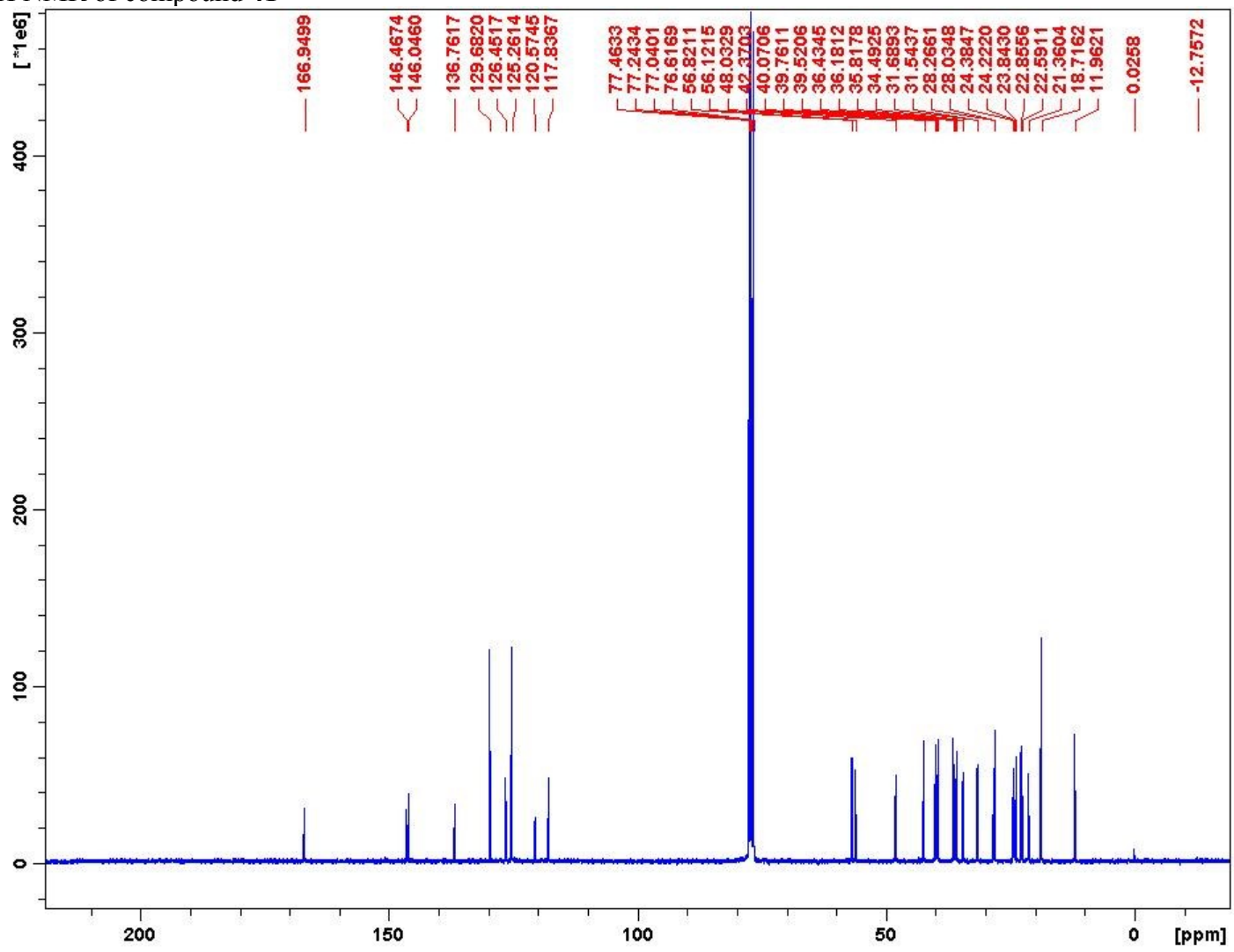


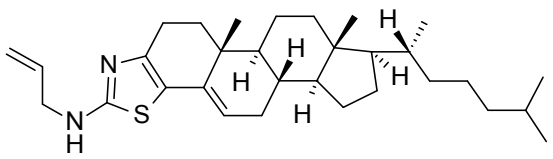
(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-N,2,18-trimethyl-N-phenyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (41).

^{1}H NMR of compound **41**



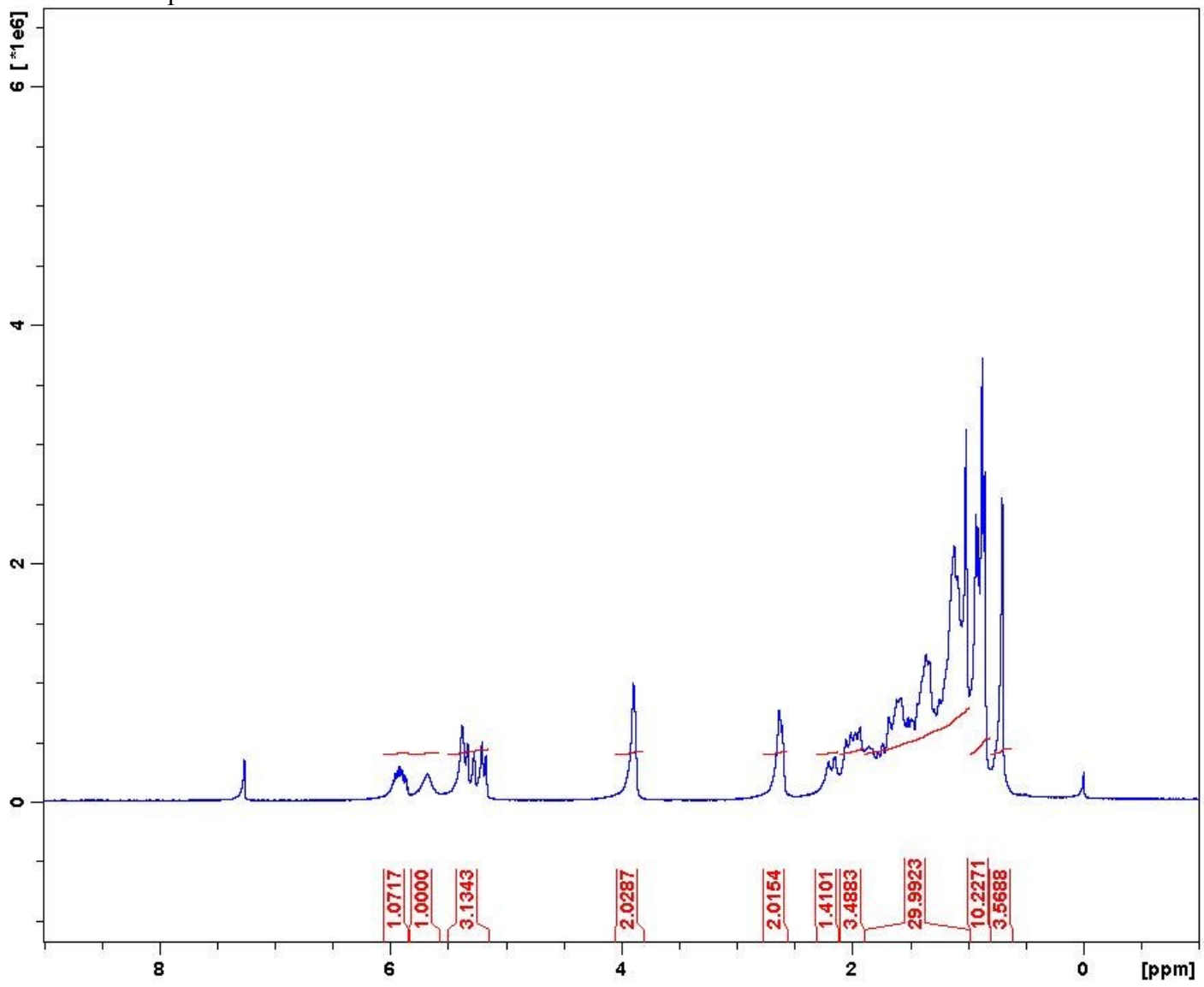
^{1}H NMR of compound **41**



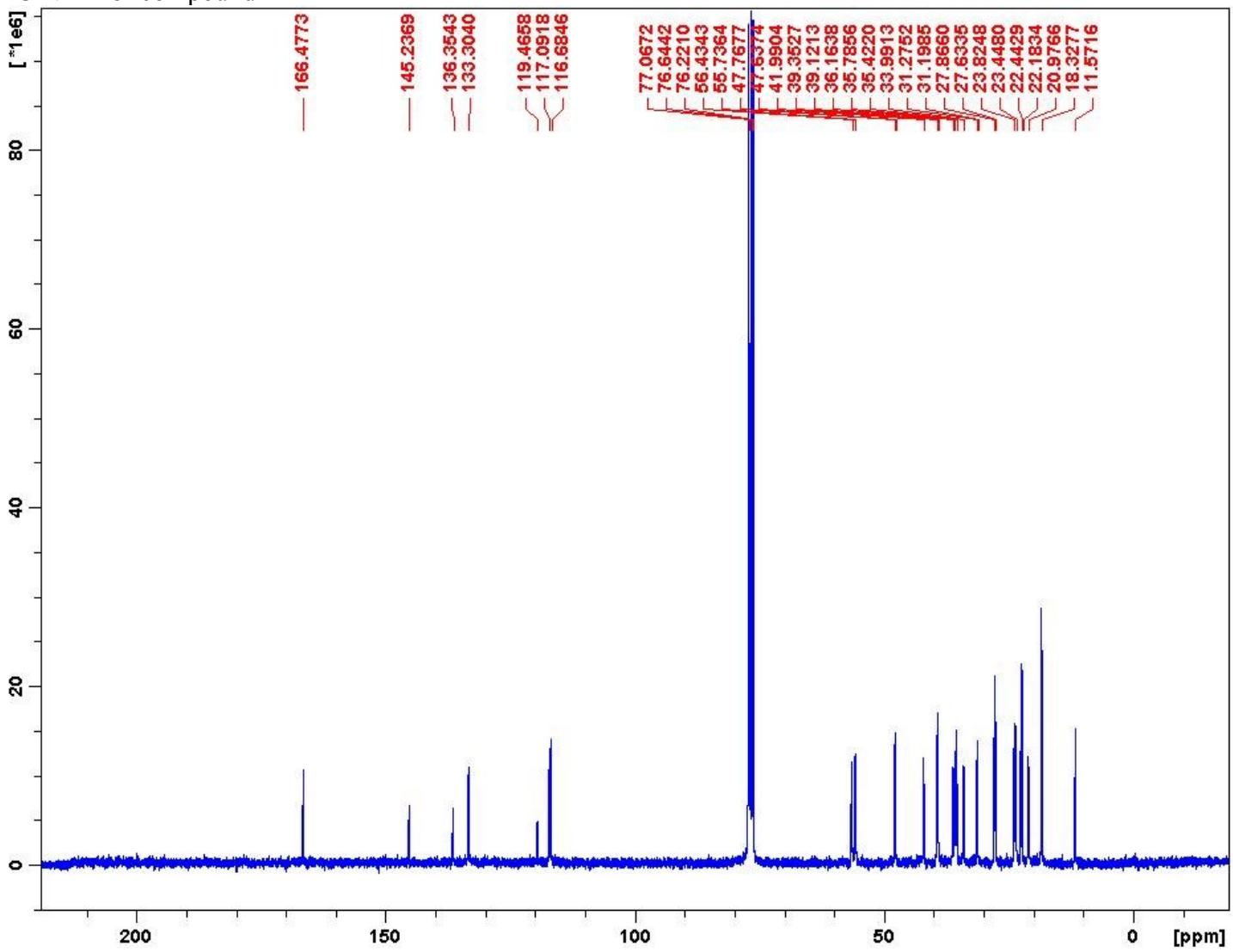


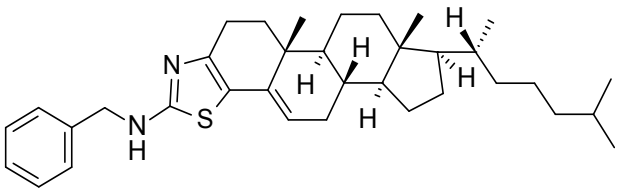
(1S,2R,13S,14S,17R,18R)-N-allyl-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (42).

^{1}H NMR of compound **42**



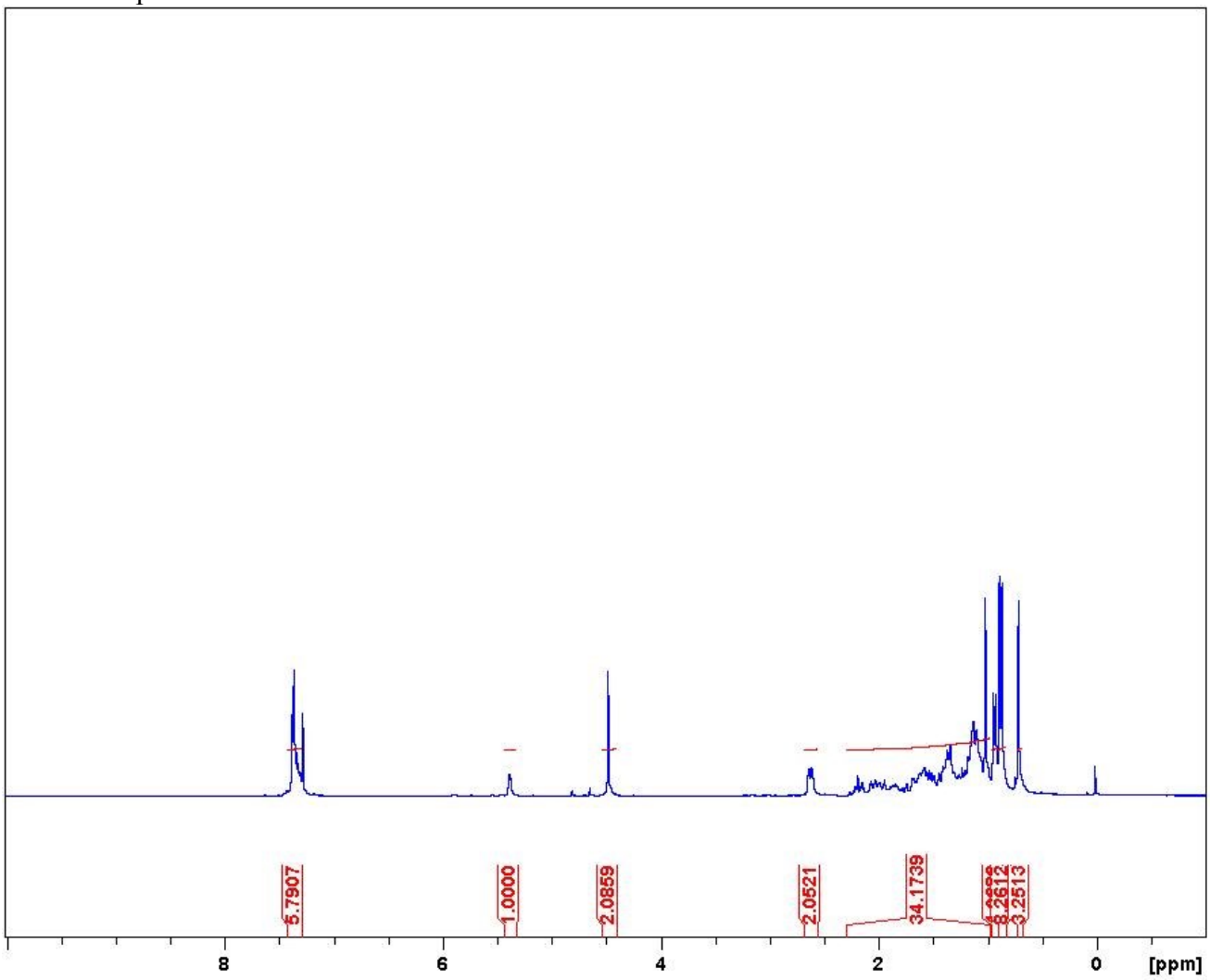
^{13}C NMR of compound **42**



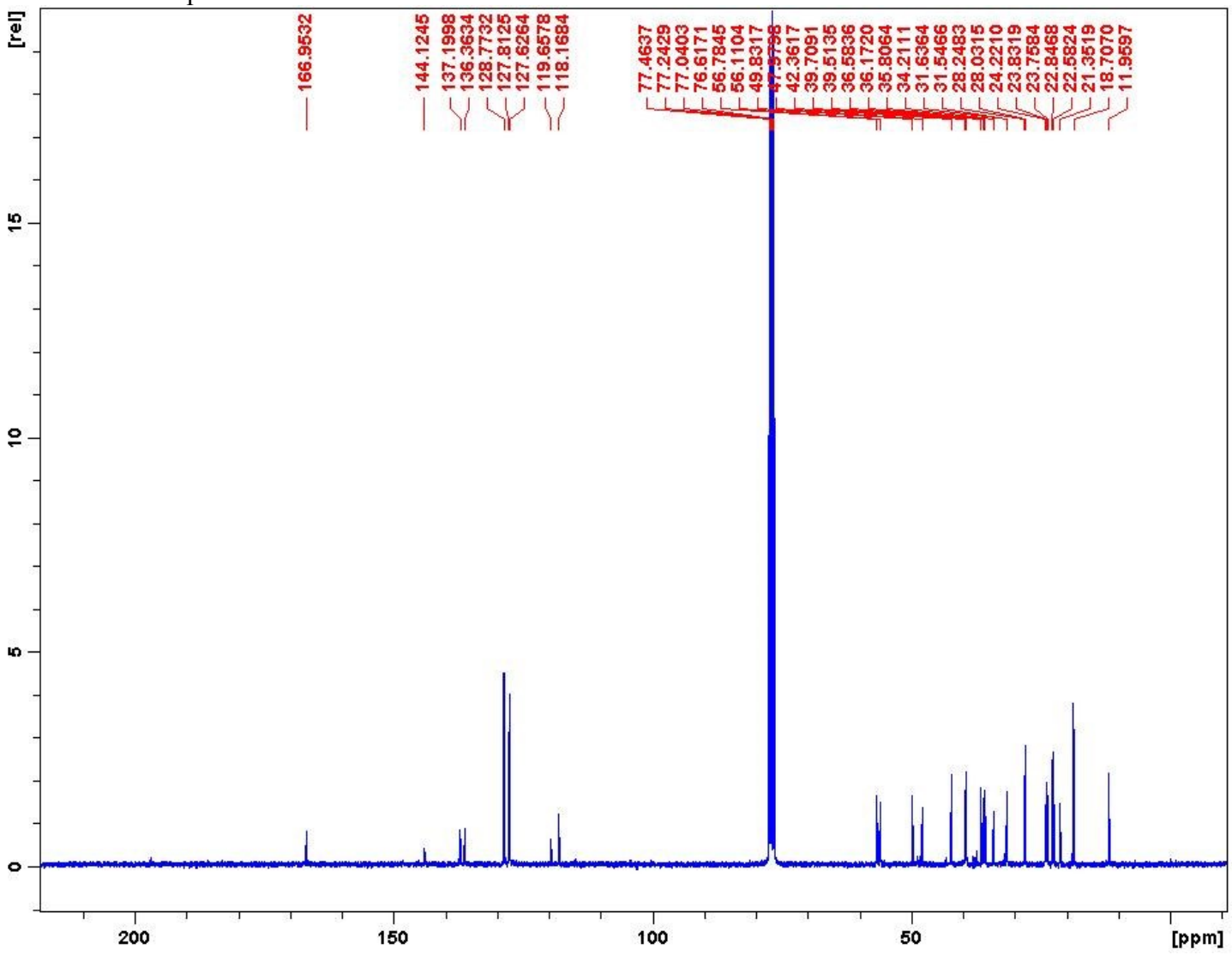


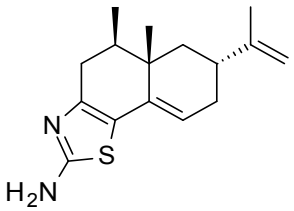
(1S,2R,13S,14S,17R,18R)-N-benzyl-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-amine (43).

^{1}H NMR of compound **43**



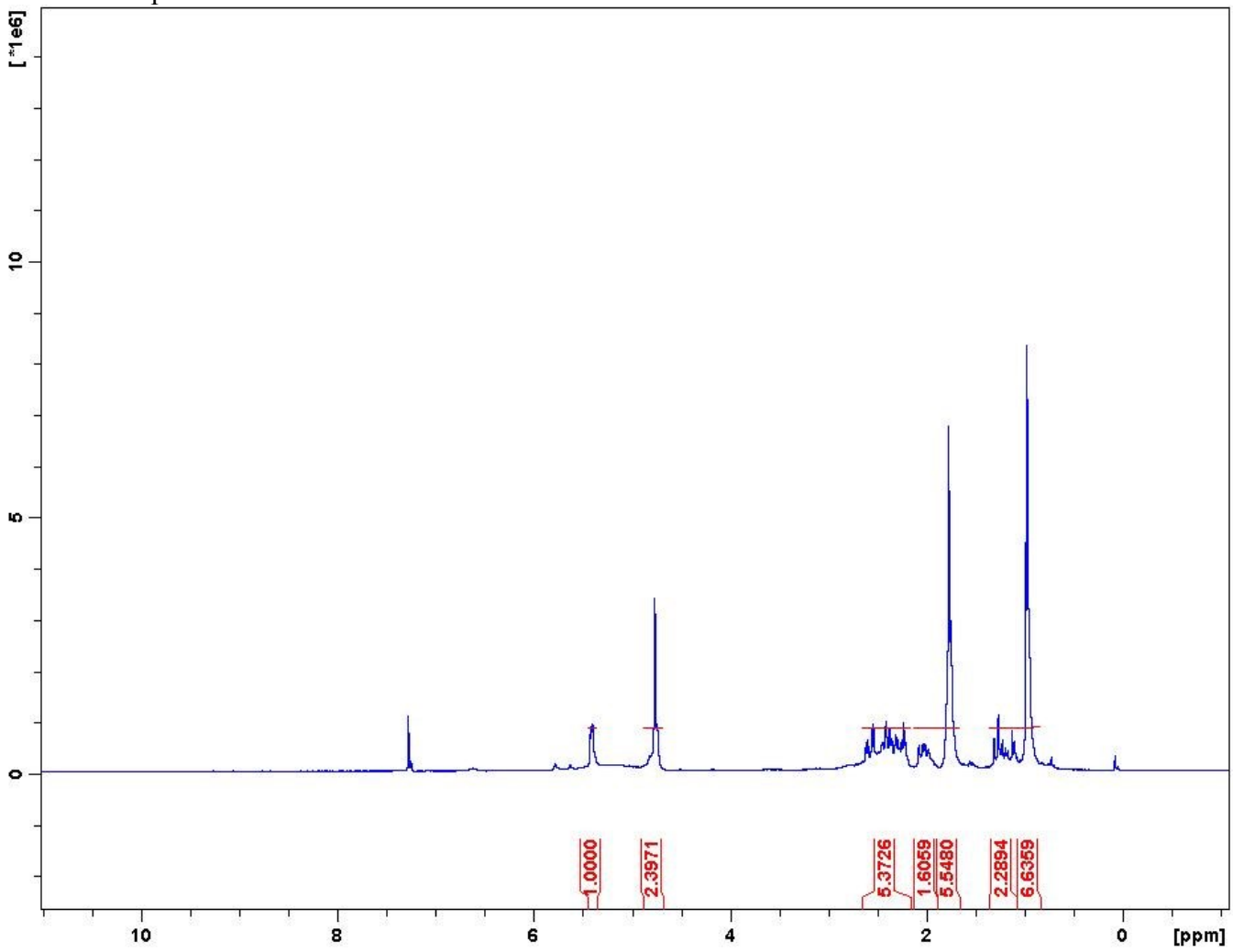
^{13}C NMR of compound **43**



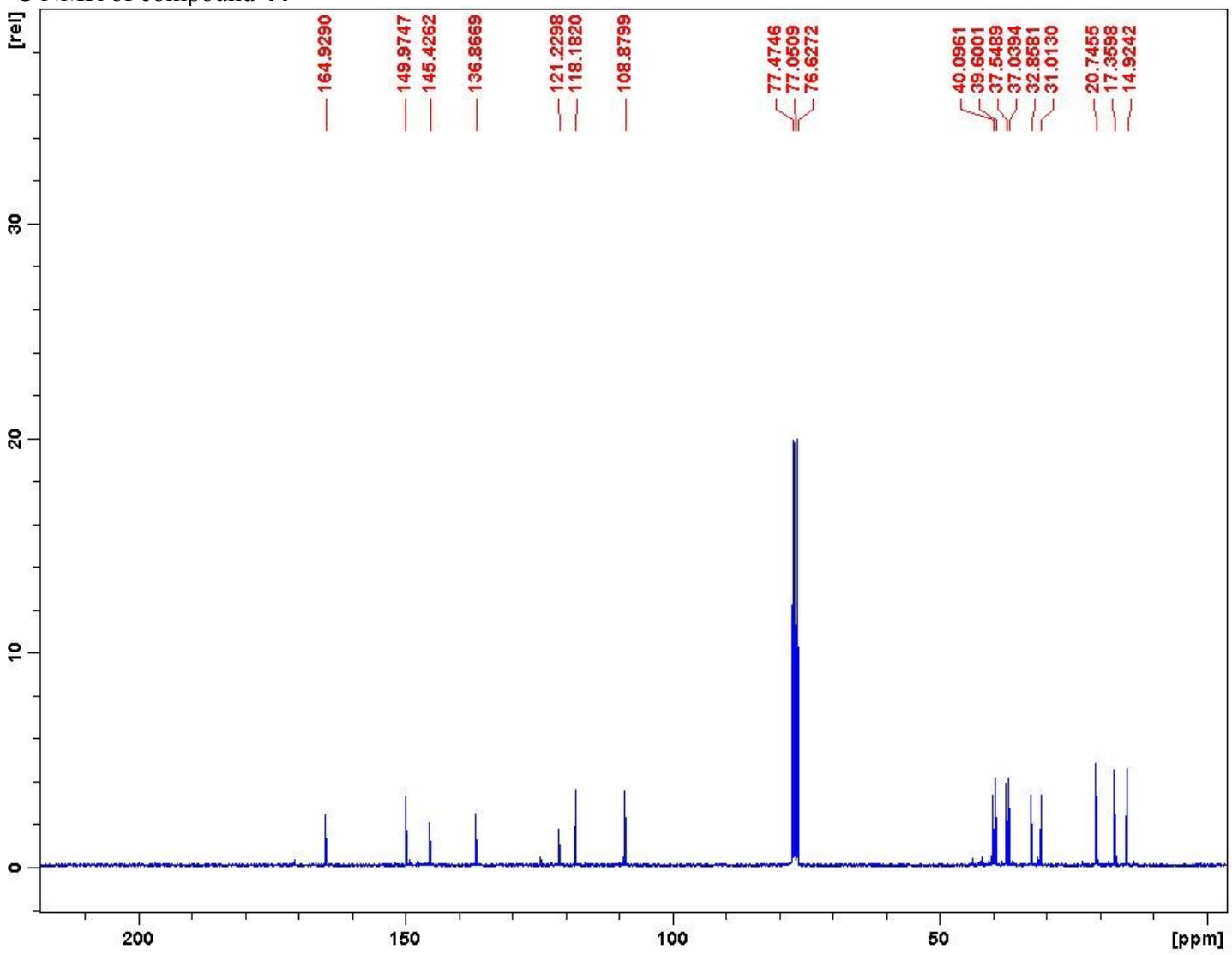


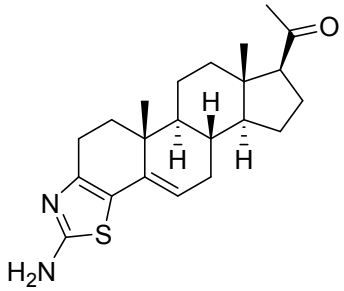
(5R,5aS,7R)-7-isopropenyl-5,5a-dimethyl-5,6,7,8,9,9a-hexahydro-4*H*-benzo[g][1,3]benzothiazol-2-amine (44).

^{1}H NMR of compound **44**



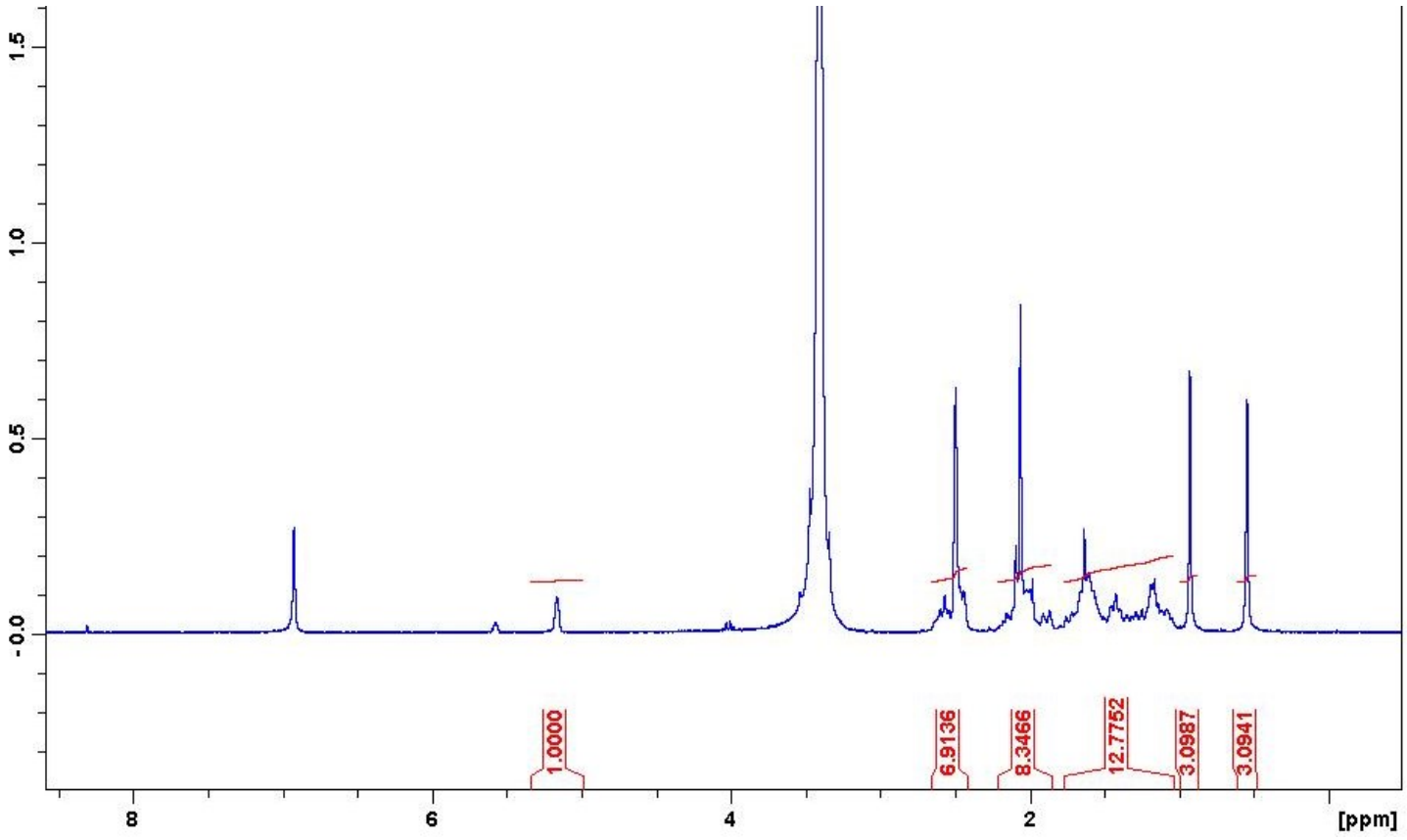
^{13}C NMR of compound **44**



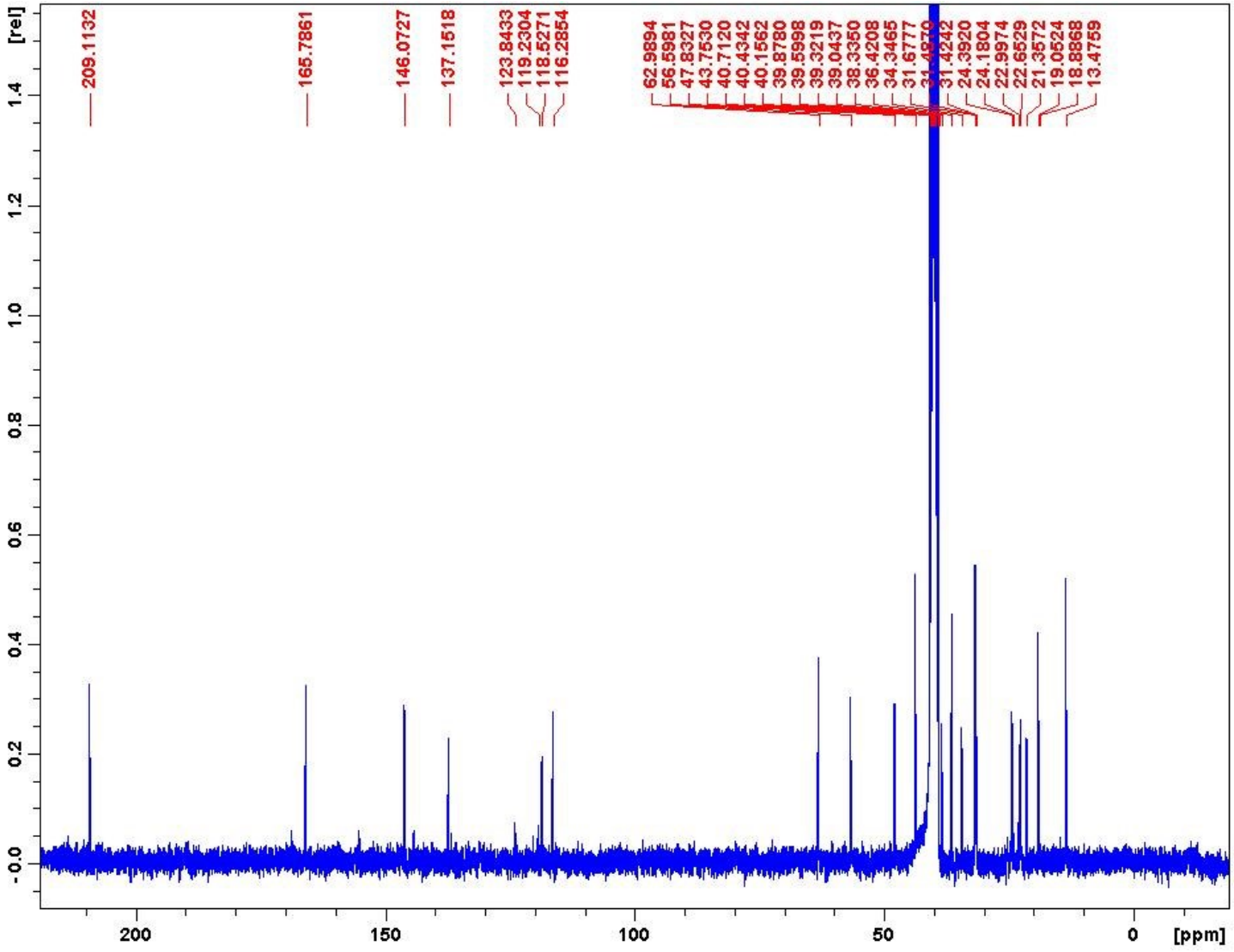


1-[(1S,2R,13S,14S,17S,18S)-7-amino-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-17-yl]ethanone (45).

^{1}H NMR Spectrum of Compound **45**.

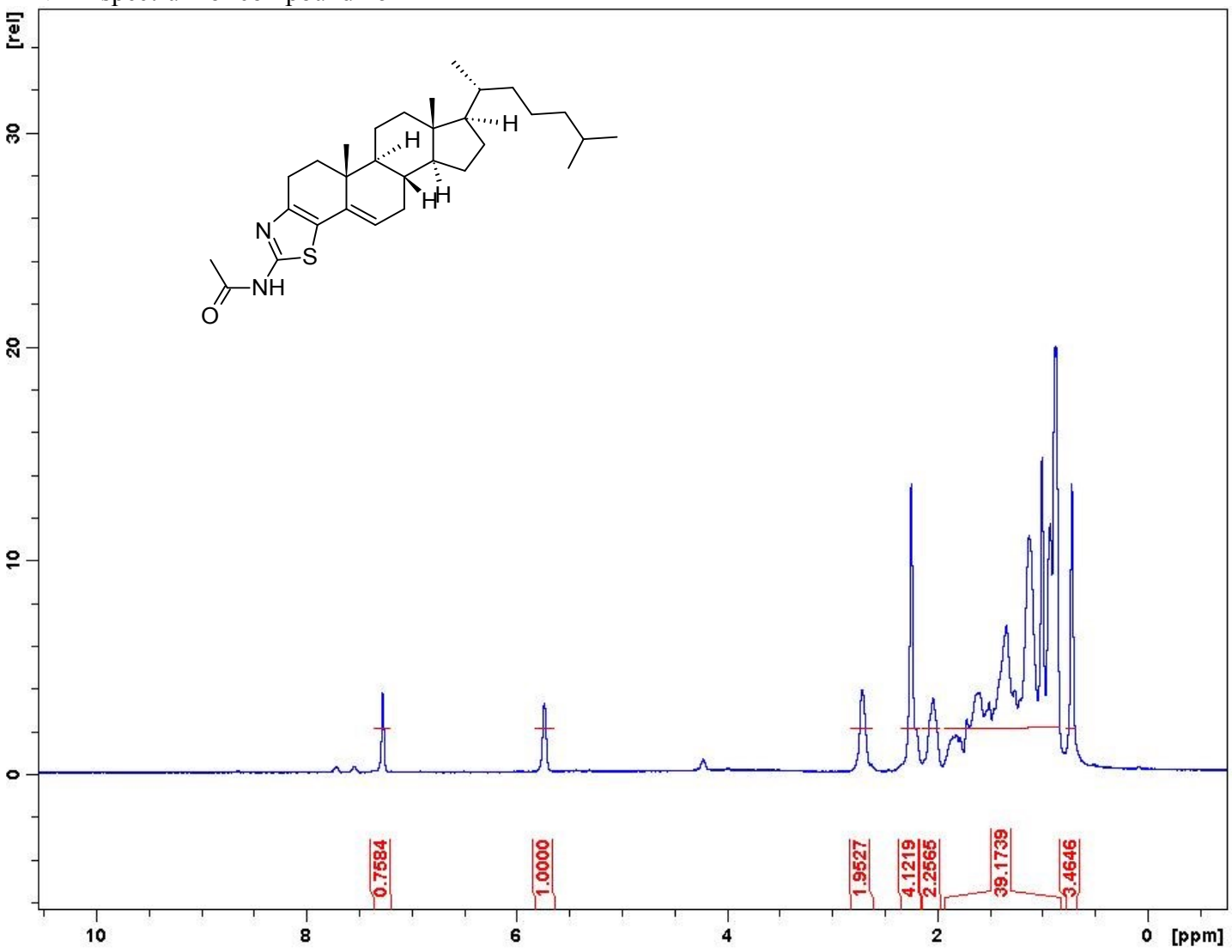


^{13}C NMR spectrum of compound **45**.

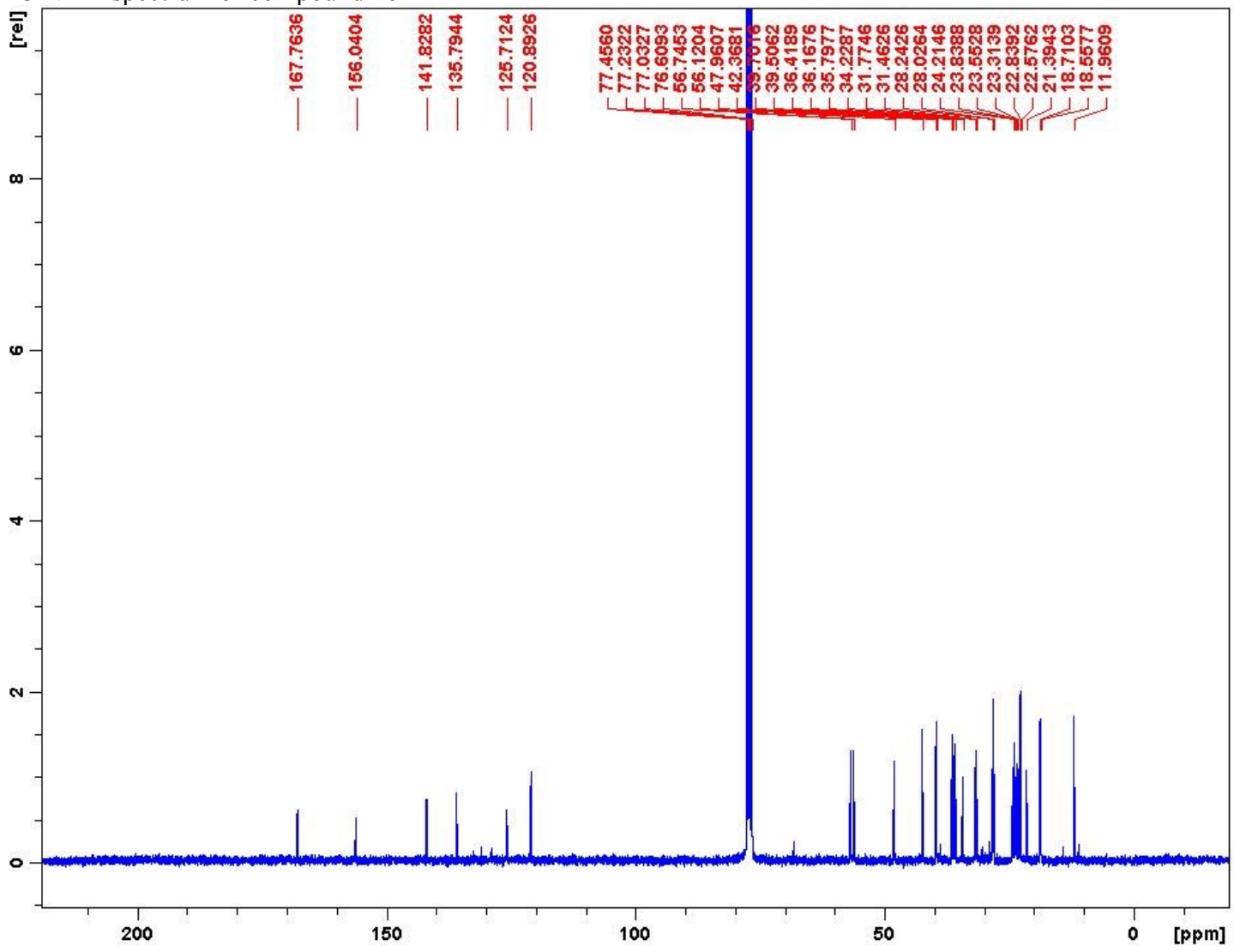


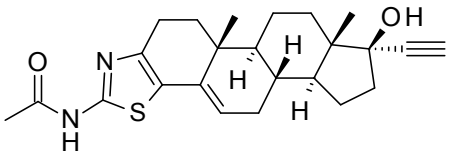
N-[(1S,2R,13S,14S,17R,18R)-17-[(1R)-1,5-dimethylhexyl]-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-yl]acetamide (46).

^{1}H NMR spectrum of compound **46**



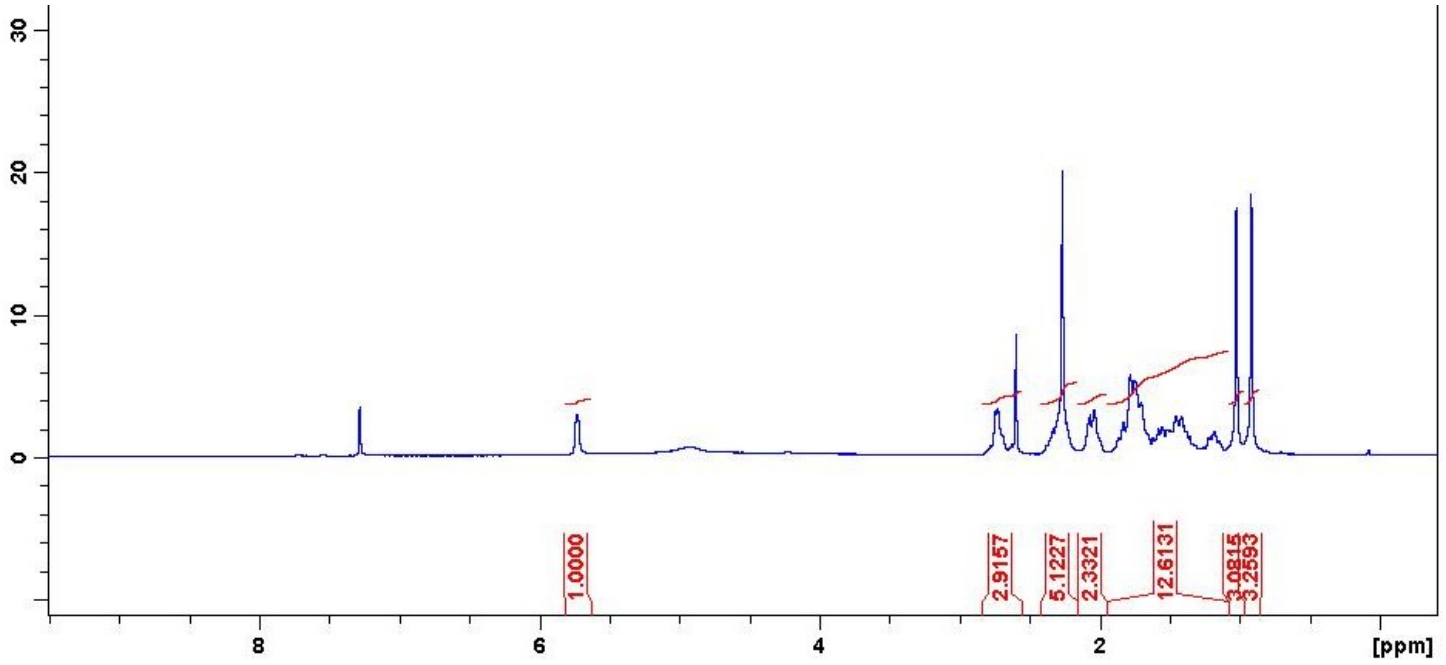
^{13}C NMR spectrum of compound **46**



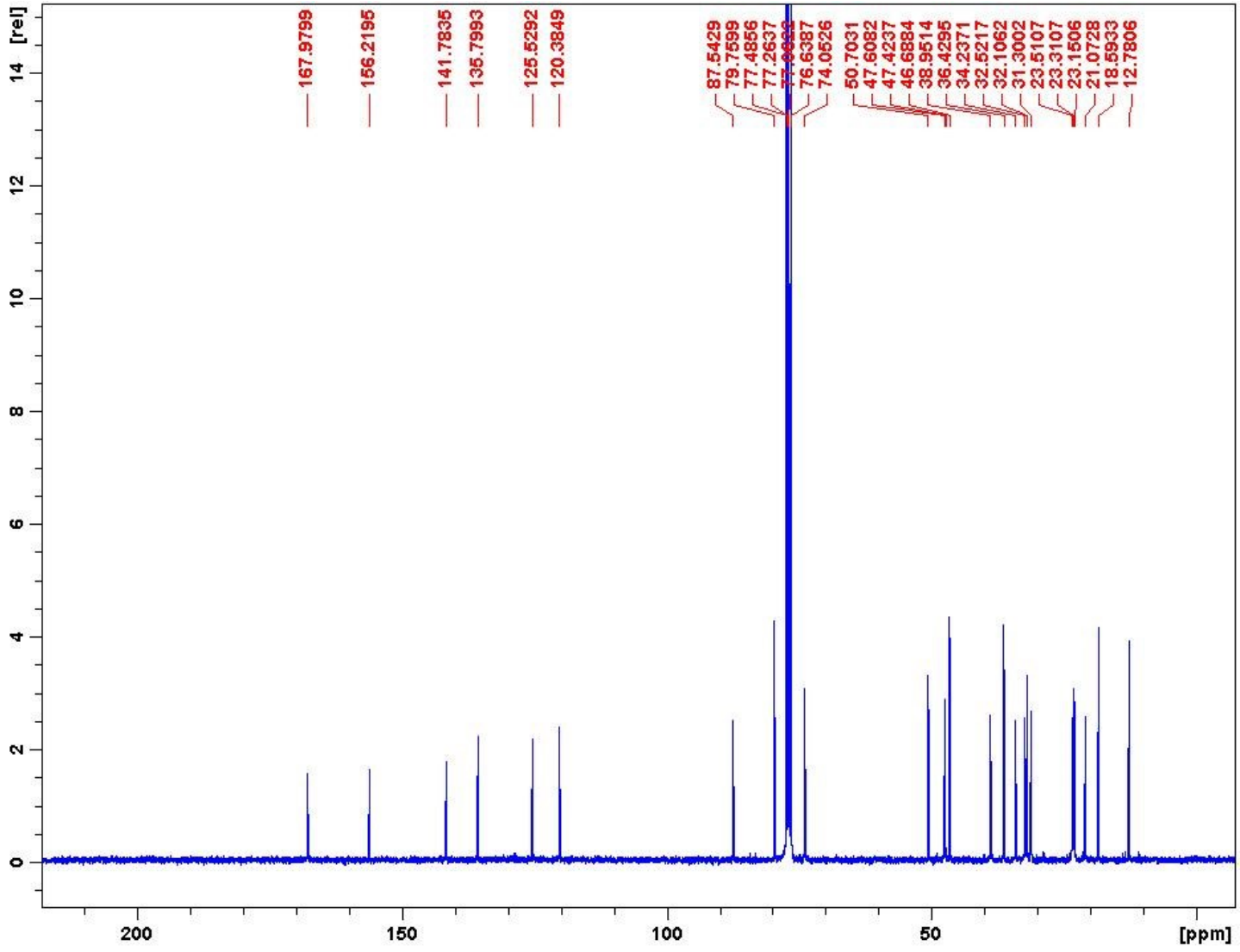


N-[(1S,2R,13R,14S,17R,18S)-17-ethynyl-17-hydroxy-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-yl]acetamide (47).

^{1}H NMR spectrum of compound **47**.

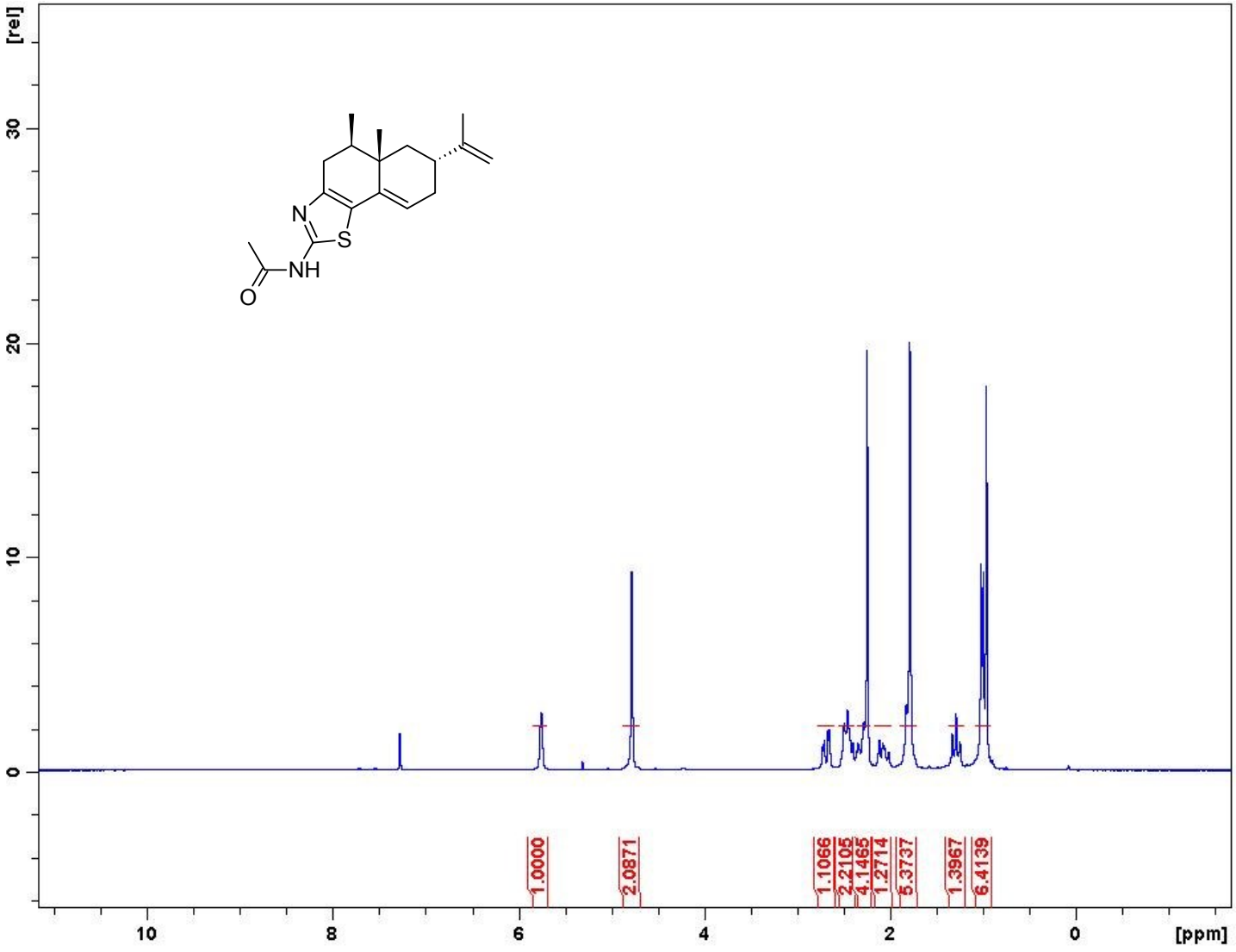


^{13}C NMR spectrum of compound **47**.

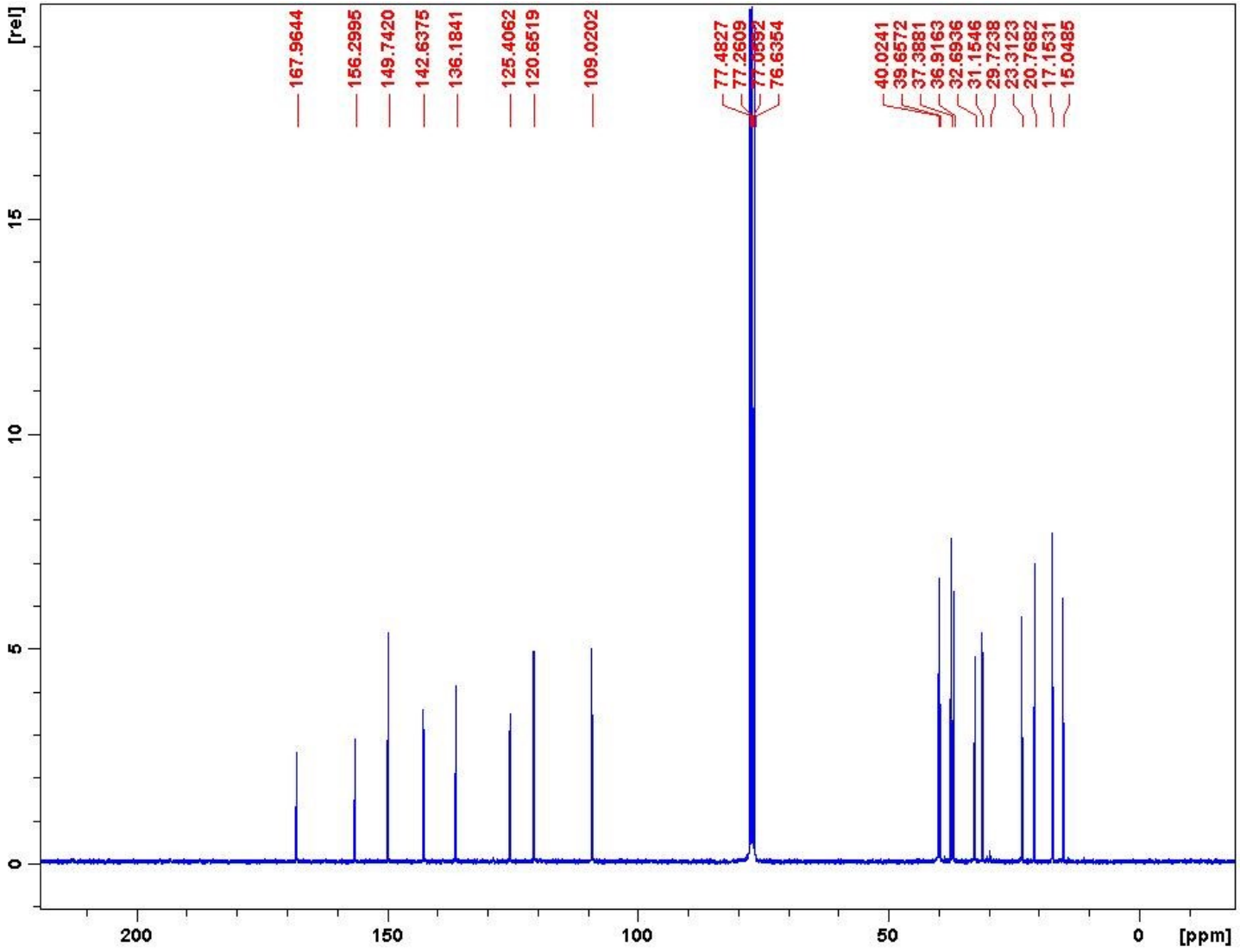


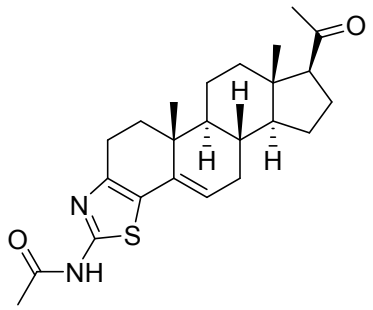
N-[(5R,5aS,7R)-7-isopropenyl-5,5a-dimethyl-5,6,7,8,9,9a-hexahydro-4*H*-benzo[g][1,3]benzothiazol-2-yl]acetamide (48).

^{1}H NMR spectrum of compound **48**.



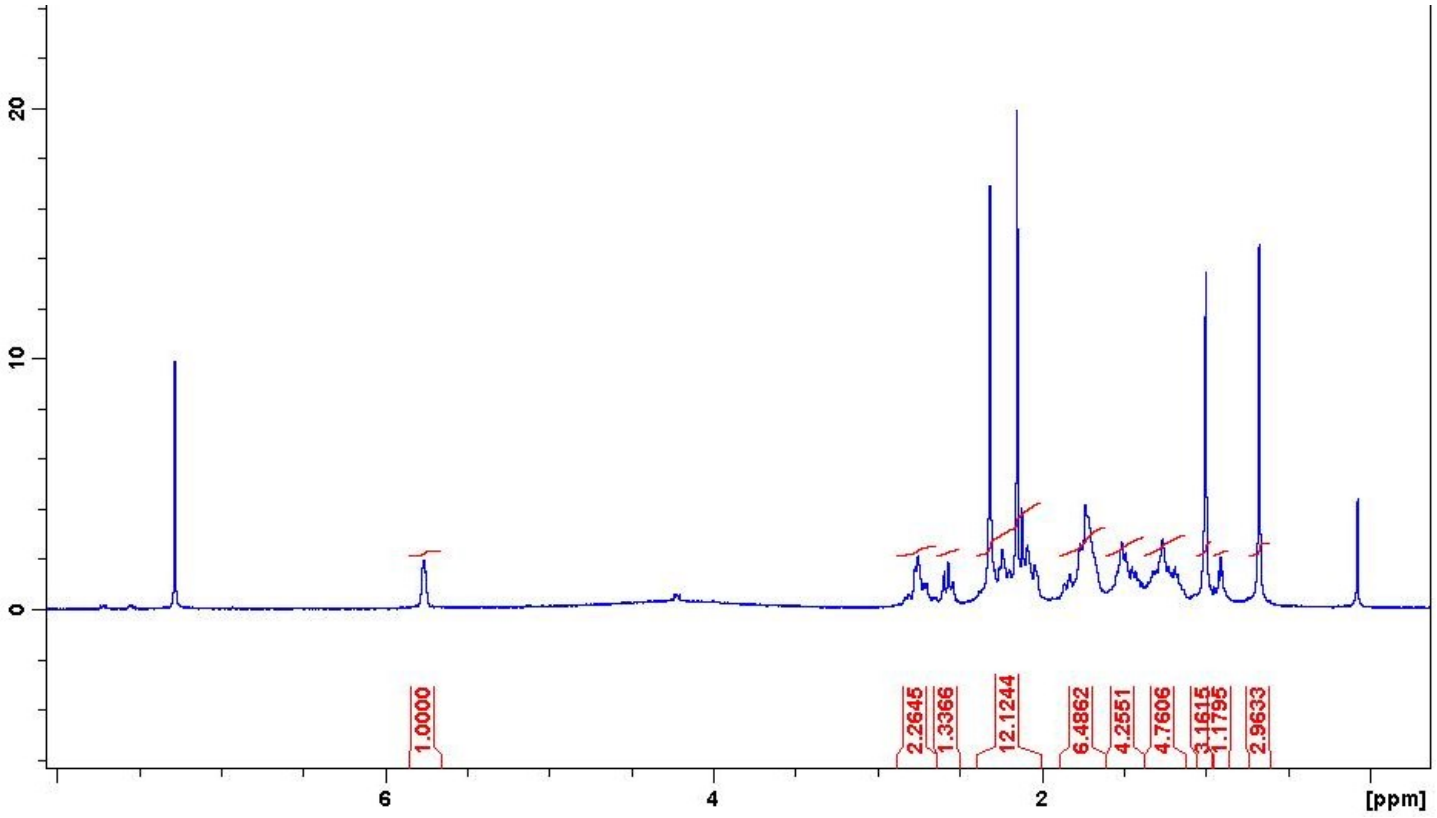
^{13}C NMR Spectrum of Compound **48**.



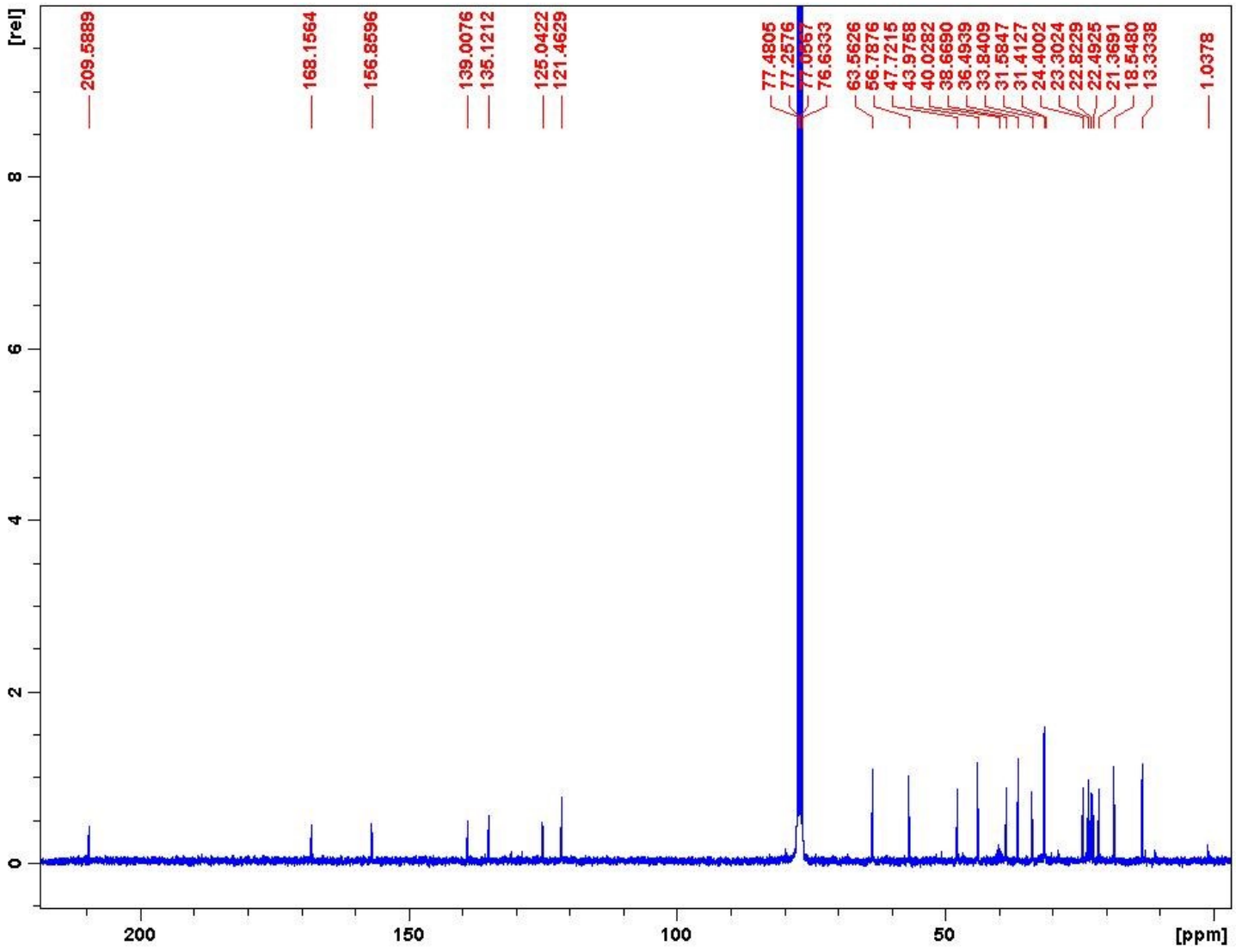


N-[(1S,2R,13S,14S,17S,18S)-17-acetyl-2,18-dimethyl-8-thia-6-azapentacyclo[11.7.0.02,10.05,9.014,18]icosa-5(9),6,10-trien-7-yl]acetamide (49).

^{1}H NMR spectrum of compound 49.



^{13}C NMR spectrum of compound **49**.



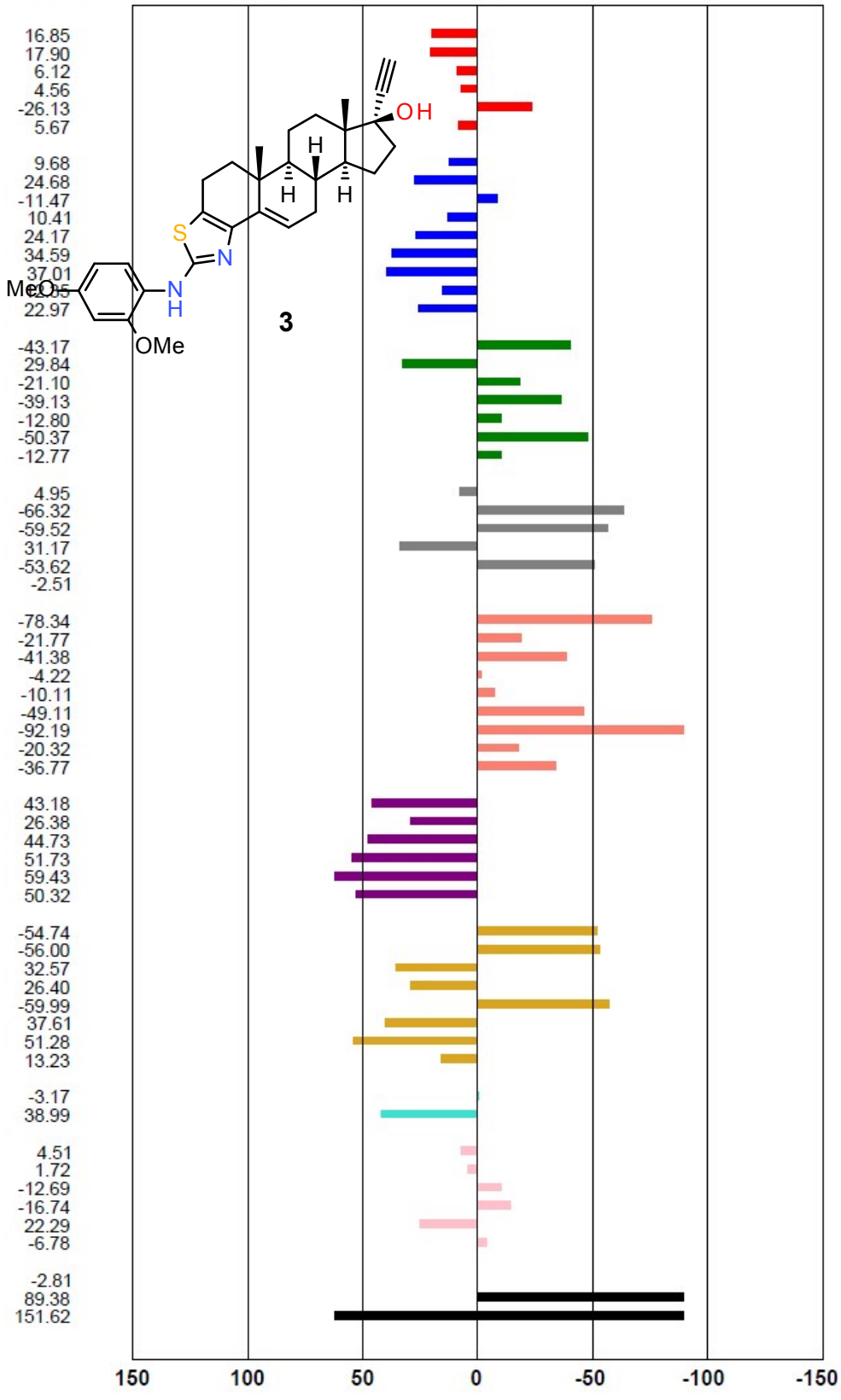
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-818583 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Sep 16, 2019
Experiment ID: 1909OS65		**Report Date:** Dec 07, 2019

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	16.85
HL-60(TB)	17.90
K-562	6.12
MOLT-4	4.56
RPMI-8226	-26.13
SR	5.67
Non-Small Cell Lung Cancer	
A549/ATCC	9.68
EKVX	24.68
HOP-62	-11.47
HOP-92	10.41
NCI-H226	24.17
NCI-H23	34.59
NCI-H322M	37.01
NCI-H460	22.85
NCI-H522	22.97
Colon Cancer	
COLO 205	-43.17
HCC-2998	29.84
HCT-116	-21.10
HCT-15	-39.13
HT29	-12.80
KM12	-50.37
SW-620	-12.77
CNS Cancer	
SF-268	4.95
SF-295	-66.32
SF-539	-59.52
SNB-19	31.17
SNB-75	-53.62
U251	-2.51
Melanoma	
LOX IMVI	-78.34
MALME-3M	-21.77
M14	-41.38
MDA-MB-435	-4.22
SK-MEL-2	-10.11
SK-MEL-28	-49.11
SK-MEL-5	-92.19
UACC-257	-20.32
UACC-62	-36.77
Ovarian Cancer	
IGROV1	43.18
OVCAR-3	26.38
OVCAR-4	44.73
OVCAR-5	51.73
OVCAR-8	59.43
NCI/ADR-RES	50.32
Renal Cancer	
786-0	-54.74
A498	-56.00
ACHN	32.57
CAKI-1	26.40
RXF 393	-59.99
SN12C	37.61
TK-10	51.28
UO-31	13.23
Prostate Cancer	
PC-3	-3.17
DU-145	38.99
Breast Cancer	
MCF7	4.51
MDA-MB-231/ATCC	1.72
HS 578T	-12.69
BT-549	-16.74
T-47D	22.29
MDA-MB-468	-6.78
Mean	-2.81
Delta	89.38
Range	151.62

Mean Growth Percent - Growth Percent



GI50, TGI, and LC50 values of compound **3** against NCI-60 cancer cell lines

NSC : D - 818583 / 1	Experiment ID : 1911NS88	Test Type : 08	Units : Molar
Report Date : December 07, 2019	Test Date : November 04, 2019	QNS :	MC :
COMI : L-2,4xOMe	Stain Reagent : SRB Dual-Pass Related	SSPL : 0ZRW	

			Log10 Concentration											
	Time		Mean Optical Densities					Percent Growth						
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.560	2.742	2.665	2.711	1.271	0.606	0.287	96	99	33	2	-49	5.44E-7	1.10E-5	> 1.00E-4
HL-60(TB)	0.917	3.353	3.317	3.330	2.436	0.748	0.656	99	99	62	-18	-28	1.42E-6	5.91E-6	> 1.00E-4
K-562	0.194	2.070	1.948	2.072	0.767	0.226	0.169	94	100	31	2	-13	5.25E-7	1.30E-5	> 1.00E-4
MOLT-4	0.642	2.767	2.771	2.805	1.146	0.568	0.434	100	102	24	-12	-32	4.60E-7	4.69E-6	> 1.00E-4
RPMI-8226	0.911	2.606	2.561	2.411	0.827	0.626	0.510	97	89	-9	-31	-44	2.48E-7	8.04E-7	> 1.00E-4
SR	0.388	2.420	2.260	2.204	1.090	0.398	0.354	92	89	35	.	-9	5.23E-7	1.12E-5	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.458	2.743	2.481	2.622	2.293	0.678	0.434	89	95	80	10	-5	2.68E-6	4.39E-5	> 1.00E-4
EKVX	0.823	2.198	2.096	2.185	1.872	1.022	0.465	93	99	76	14	-44	2.66E-6	1.78E-5	> 1.00E-4
HOP-62	0.655	1.957	1.827	1.922	1.625	0.581	0.299	90	97	74	-11	-54	1.93E-6	7.37E-6	7.92E-5
HOP-92	1.228	1.955	1.838	1.913	1.815	1.046	0.522	84	94	81	-15	-57	2.10E-6	7.00E-6	6.67E-5
NCI-H226	1.361	2.463	2.416	2.474	2.375	1.038	0.683	96	101	92	-24	-50	2.30E-6	6.23E-6	> 1.00E-4
NCI-H23	0.582	1.852	1.772	1.868	1.515	0.632	0.312	94	101	73	4	-46	2.18E-6	1.20E-5	> 1.00E-4
NCI-H322M	0.918	2.303	2.204	2.275	1.955	1.164	0.632	93	98	75	18	-31	2.72E-6	2.31E-5	> 1.00E-4
NCI-H460	0.404	3.290	3.254	3.309	2.889	0.428	0.106	99	101	86	1	-74	2.65E-6	1.03E-5	4.80E-5
NCI-H522	1.037	2.794	2.559	2.645	2.650	0.741	0.564	87	92	92	-29	-46	2.22E-6	5.79E-6	> 1.00E-4
Colon Cancer															
COLO 205	0.437	1.743	1.616	1.856	1.710	0.236	0.194	90	109	97	-46	-56	2.14E-6	4.78E-6	2.58E-5
HCC-2998	0.648	1.921	1.744	1.743	1.808	0.449	0.125	86	86	91	-31	-81	2.17E-6	5.59E-6	2.43E-5
HCT-116	0.285	2.511	2.501	2.499	1.659	0.053	0.035	100	99	62	-81	-88	1.21E-6	2.70E-6	6.03E-6
HCT-15	0.234	1.792	1.670	1.726	1.187	0.148	0.181	92	96	61	-37	-23	1.30E-6	4.20E-6	> 1.00E-4
HT29	0.226	1.797	1.676	1.797	1.136	0.195	0.167	92	100	58	-14	-26	1.29E-6	6.40E-6	> 1.00E-4
KM12	0.874	3.360	3.328	3.336	3.034	0.616	0.208	99	99	87	-30	-76	2.07E-6	5.57E-6	2.74E-5
SW-620	0.358	2.865	2.695	2.800	2.236	0.155	0.157	93	97	75	-57	-56	1.55E-6	3.71E-6	8.89E-6
CNS Cancer															
SF-268	1.102	2.847	2.701	2.833	2.341	0.934	0.582	92	99	71	-15	-47	1.75E-6	6.65E-6	> 1.00E-4
SF-295	1.271	3.249	3.199	3.263	0.926	0.430	0.505	97	101	-27	-66	-60	2.49E-7	6.13E-7	3.84E-6
SF-539	0.781	2.599	2.424	2.350	1.198	0.184	0.177	90	86	23	-76	-77	3.74E-7	1.70E-6	5.42E-6
SNB-19	0.769	2.523	2.410	2.493	1.918	0.804	0.295	94	98	65	2	-62	1.75E-6	1.07E-5	6.56E-5
U251	0.446	2.226	2.059	2.082	1.241	0.320	0.175	91	92	45	-28	-61	7.70E-7	4.09E-6	4.63E-5
Melanoma															
LOX IMVI	0.616	2.953	2.819	2.920	2.398	0.091	0.265	94	99	76	-85	-57	1.45E-6	2.97E-6	6.05E-6
MALME-3M	0.634	1.274	1.189	1.262	0.885	0.336	0.192	87	98	39	-47	-70	6.55E-7	2.85E-6	1.35E-5
M14	0.419	1.821	1.732	1.738	1.351	0.190	0.060	94	94	66	-55	-86	1.37E-6	3.53E-6	9.13E-6
MDA-MB-435	0.508	2.592	2.449	2.536	2.191	0.280	0.260	93	97	81	-45	-49	1.76E-6	4.39E-6	> 1.00E-4
SK-MEL-2	1.085	3.002	2.933	2.912	2.166	0.937	0.545	96	95	56	-14	-50	1.23E-6	6.39E-6	> 1.00E-4
SK-MEL-28	0.703	1.960	1.935	1.864	1.240	0.307	0.132	98	92	43	-56	-81	7.12E-7	2.70E-6	8.63E-6
SK-MEL-5	1.246	3.215	3.190	3.188	3.090	0.138	0.152	99	99	94	-89	-88	1.73E-6	3.26E-6	6.12E-6
UACC-257	0.795	2.254	2.121	2.185	1.807	0.557	0.384	91	95	69	-30	-52	1.57E-6	4.99E-6	8.30E-5
UACC-62	0.953	2.840	2.777	2.847	2.405	0.642	0.401	97	100	77	-33	-58	1.76E-6	5.04E-6	4.86E-5
Ovarian Cancer															
IGROV1	0.474	2.141	2.062	2.156	1.760	0.411	0.323	95	101	77	-13	-32	1.99E-6	7.11E-6	> 1.00E-4
OVCAR-3	0.561	1.947	1.901	1.928	1.619	0.241	0.137	97	99	76	-57	-76	1.58E-6	3.74E-6	8.86E-6
OVCAR-4	1.073	2.104	2.110	2.028	2.139	1.289	1.112	101	93	103	21	4	4.44E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.576	1.646	1.620	1.605	1.428	0.640	0.212	98	96	80	6	-63	2.53E-6	1.22E-5	6.43E-5
OVCAR-8	0.563	2.820	2.669	2.761	2.588	0.815	0.621	93	97	90	11	3	3.20E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.593	2.062	2.064	2.082	1.734	0.647	0.521	100	101	78	4	-12	2.36E-6	1.70E-5	> 1.00E-4
SK-OV-3	0.832	1.861	1.786	1.868	1.578	0.723	0.530	93	101	73	-13	-36	1.83E-6	7.02E-6	> 1.00E-4
Renal Cancer															
786-0	0.741	2.648	2.564	2.613	1.305	0.433	0.255	96	98	30	-42	-66	5.04E-7	2.60E-6	2.24E-5
A498	1.676	2.319	2.056	2.060	1.717	0.622	0.282	59	60	6	-63	-83	1.52E-7	1.23E-6	6.51E-6
ACHN	0.544	2.407	2.338	2.398	1.898	0.550	0.308	96	99	73	.	-43	2.06E-6	1.02E-5	> 1.00E-4
CAKI-1	1.234	3.098	2.924	3.003	2.380	0.994	0.886	91	95	61	-19	-28	1.39E-6	5.74E-6	> 1.00E-4
RXF 393	0.955	1.768	1.800	1.828	0.673	0.330	0.453	104	107	-30	-65	-53	2.62E-7	6.08E-7	3.72E-6
SN12C	0.566	2.246	2.131	2.241	2.058	0.820	0.350	93	100	89	15	-38	3.36E-6	1.92E-5	> 1.00E-4
TK-10	1.066	2.020	1.805	1.865	2.055	1.189	0.495	77	84	104	13	-54	3.90E-6	1.56E-5	8.84E-5
UO-31	1.009	2.324	2.138	2.181	1.819	0.758	0.321	86	89	62	-25	-68	1.36E-6	5.16E-6	3.80E-5
Prostate Cancer															
PC-3	0.532	1.646	1.573	1.615	1.048	0.521	0.422	93	97	46	-2	-21	8.45E-7	9.02E-6	> 1.00E-4
DU-145	0.477	2.067	2.015	2.093	1.704	0.523	0.086	97	102	77	3	-82	2.32E-6	1.08E-5	4.20E-5
Breast Cancer															
MCF7	0.406	2.047	1.949	1.888	1.220	0.132	0.179	94	90	50	-68	-56	9.78E-7	2.65E-6	7.08E-6
MDA-MB-231/ATCC	0.812	2.180	2.112	2.224	1.605	0.636	0.577	95	103	58	-22	-29	1.26E-6	5.34E-6	> 1.00E-4
HS 578T	1.691	2.855	2.708	2.809	1.937	1.090	0.941	87	96	21	-36	-44	4.11E-7	2.36E-6	> 1.00E-4
BT-549	1.314	2.509	2.406	2.415	1.799	1.061	0.569	91	92	41	-19	-57	6.56E-7	4.76E-6	6.62E-5
T-47D	0.831	1.883	1.784	1.826	1.722	0.866	0.719	91	95	85	3	-14	2.67E-6	1.57E-5	> 1.00E-4
MDA-MB-468	0.946	1.545	1.493	1.580	1.477	0.412	0.461	91	106	89	-57	-51	1.84E-6	4.08E-6	9.02E-6

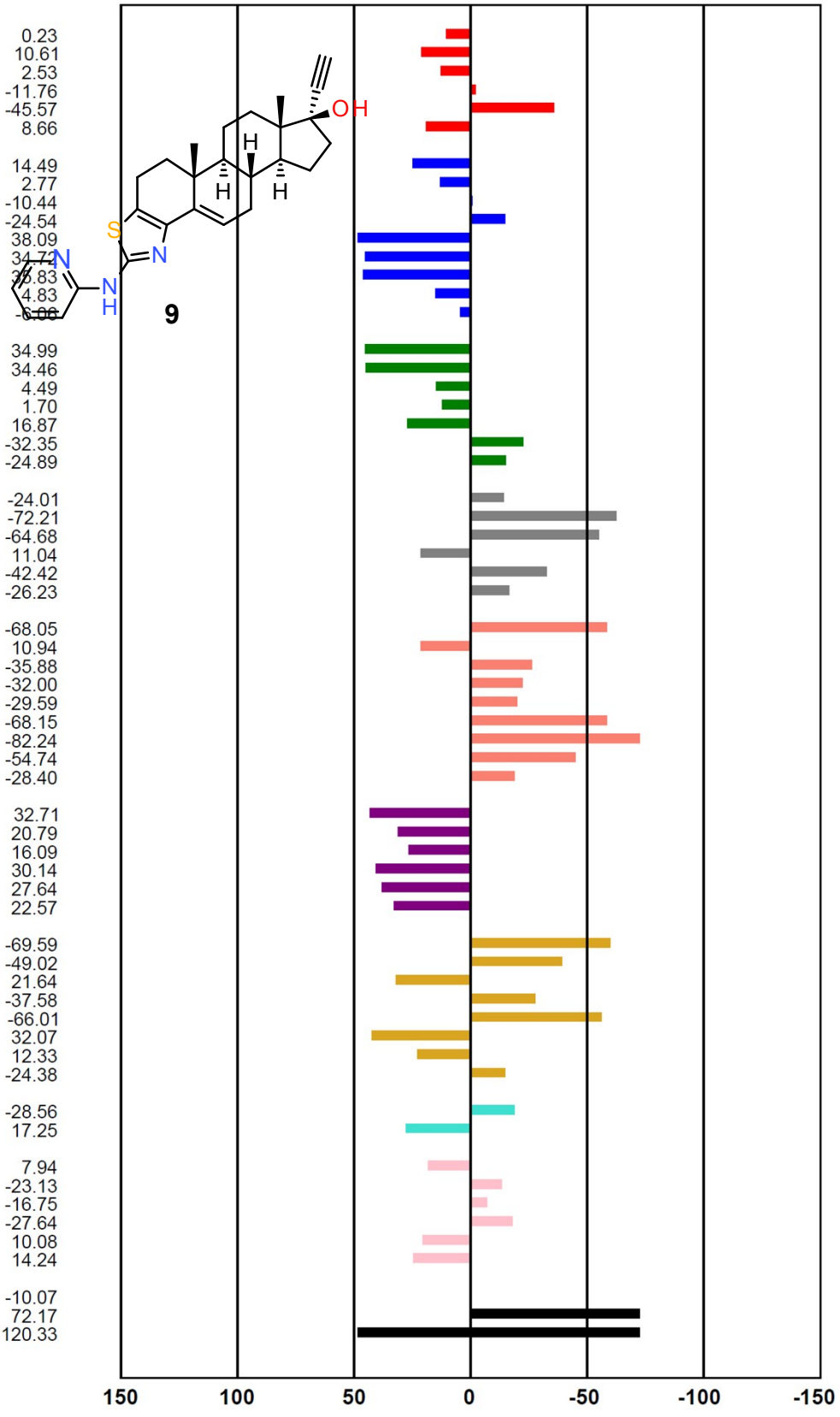
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-818584 / 1 | **Conc:** 1.00E-5 Molar | **Test Date:** Sep 16, 2019

Experiment ID: 1909OS65 | **Report Date:** Dec 07, 2019

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	0.23
HL-60(TB)	10.61
K-562	2.53
MOLT-4	-11.76
RPMI-8226	-45.57
SR	8.66
Non-Small Cell Lung Cancer	
A549/ATCC	14.49
EKVX	2.77
HOP-62	-10.44
HOP-92	-24.54
NCI-H226	38.09
NCI-H23	34.74
NCI-H322M	38.83
NCI-H460	4.83
NCI-H522	-6.06
Colon Cancer	
COLO 205	34.99
HCC-2998	34.46
HCT-116	4.49
HCT-15	1.70
HT29	16.87
KM12	-32.35
SW-620	-24.89
CNS Cancer	
SF-268	-24.01
SF-295	-72.21
SF-539	-64.68
SNB-19	11.04
SNB-75	-42.42
U251	-26.23
Melanoma	
LOX IMVI	-68.05
MALME-3M	10.94
M14	-35.88
MDA-MB-435	-32.00
SK-MEL-2	-29.59
SK-MEL-28	-68.15
SK-MEL-5	-82.24
UACC-257	-54.74
UACC-62	-28.40
Ovarian Cancer	
IGROV1	32.71
OVCAR-3	20.79
OVCAR-4	16.09
OVCAR-5	30.14
OVCAR-8	27.64
NCI/ADR-RES	22.57
Renal Cancer	
786-0	-69.59
A498	-49.02
ACHN	21.64
CAKI-1	-37.58
RXF 393	-66.01
SN12C	32.07
TK-10	12.33
UO-31	-24.38
Prostate Cancer	
PC-3	-28.56
DU-145	17.25
Breast Cancer	
MCF7	7.94
MDA-MB-231/ATCC	-23.13
HS 578T	-16.75
BT-549	-27.64
T-47D	10.08
MDA-MB-468	14.24
Mean	-10.07
Delta	72.17
Range	120.33



GI50, TGI, and LC50 values of compound **9** against NCI-60 cancer cell lines

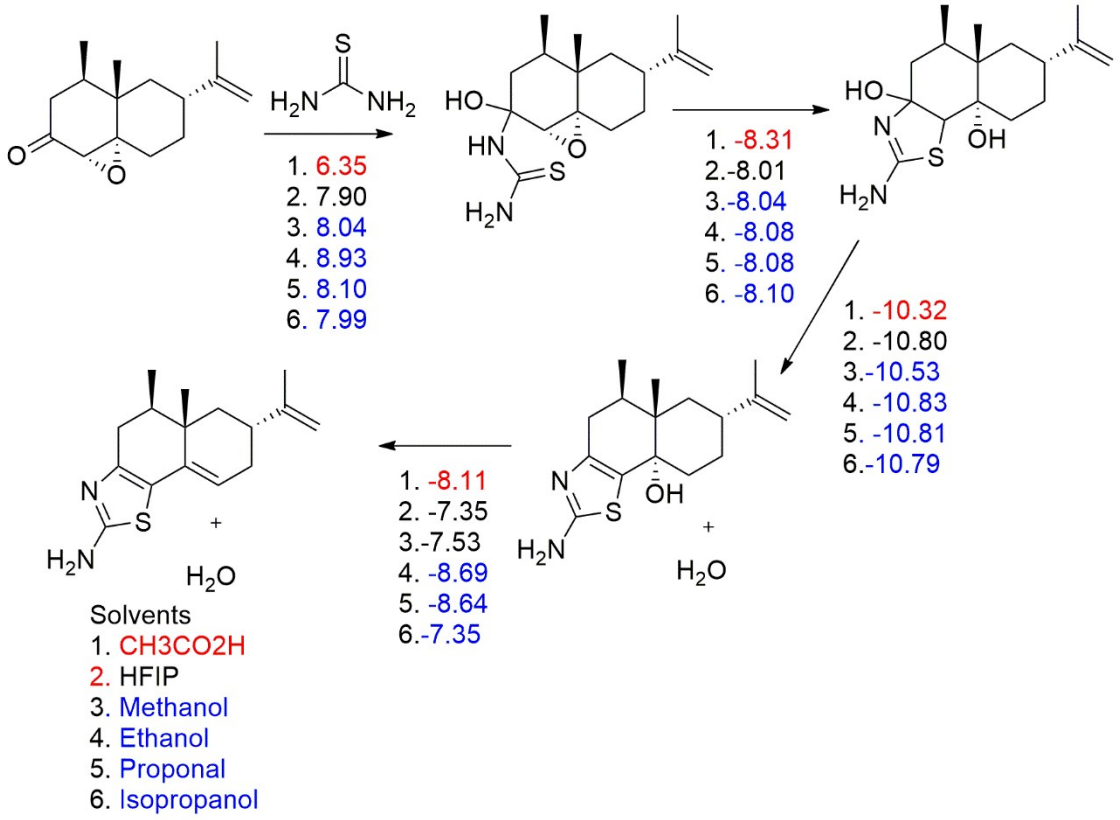
NSC : D - 818584 / 1	Experiment ID : 1911NS88	Test Type : 08	Units : Molar
Report Date : December 07, 2019	Test Date : November 04, 2019	QNS :	MC :
COMI : L-2Py	Stain Reagent : SRB Dual-Pass Related	SSPL : 0ZRW	

			Log10 Concentration											
	Time		Mean Optical Densities					Percent Growth						
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.560	2.631	2.470	2.512	1.170	0.460	0.384	92	94	29	-18	-32	4.82E-7	4.18E-6	> 1.00E-4
HL-60(TB)	0.917	3.281	3.225	3.264	1.321	0.537	0.635	98	99	17	-41	-31	3.98E-7	1.96E-6	> 1.00E-4
K-562	0.194	1.904	1.739	1.750	0.457	0.133	0.171	90	91	15	-31	-12	3.48E-7	2.13E-6	> 1.00E-4
MOLT-4	0.642	2.668	2.579	2.489	0.935	0.333	0.303	96	91	14	-48	-53	3.44E-7	1.70E-6	2.42E-5
RPMI-8226	0.911	2.553	2.460	2.144	0.718	0.504	0.687	94	75	-21	-45	-25	1.82E-7	6.02E-7	> 1.00E-4
SR	0.388	2.124	1.934	1.984	0.992	0.259	0.233	89	92	35	-33	-40	5.42E-7	3.24E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.458	2.551	2.350	2.394	1.902	0.522	0.160	90	92	69	3	-65	1.94E-6	1.11E-5	6.01E-5
EKVX	0.823	2.272	2.158	2.183	1.781	0.801	0.211	92	94	66	-3	-74	1.72E-6	9.14E-6	4.57E-5
HOP-62	0.655	1.891	1.735	1.770	1.338	0.247	0.225	87	90	55	-62	-66	1.11E-6	2.95E-6	7.85E-6
HOP-92	1.228	1.896	1.739	1.857	1.778	0.675	0.153	76	94	82	-45	-88	1.80E-6	4.43E-6	1.31E-5
NCI-H226	1.361	2.537	2.353	2.483	2.205	0.689	0.640	84	95	72	-49	-53	1.51E-6	3.91E-6	1.46E-5
NCI-H23	0.582	1.848	1.778	1.765	1.451	0.496	0.269	94	93	69	-15	-54	1.67E-6	6.64E-6	8.00E-5
NCI-H322M	0.918	2.254	2.200	2.285	1.953	0.964	0.135	96	102	77	3	-85	2.35E-6	1.09E-5	4.00E-5
NCI-H460	0.404	3.217	3.194	3.203	2.124	0.105	0.157	99	99	61	-74	-61	1.21E-6	2.83E-6	6.64E-6
NCI-H522	1.037	2.611	2.384	2.406	2.440	0.459	0.422	86	87	89	-56	-59	1.86E-6	4.12E-6	9.12E-6
Colon Cancer															
COLO 205	0.437	1.627	1.542	1.593	1.473	0.192	0.151	93	97	87	-56	-65	1.81E-6	4.05E-6	9.05E-6
HCC-2998	0.648	1.913	1.770	1.778	1.715	0.425	0.165	89	89	84	-34	-75	1.95E-6	5.13E-6	2.44E-5
HCT-116	0.285	2.515	2.428	2.517	1.540	0.078	0.039	96	100	56	-73	-86	1.12E-6	2.73E-6	6.66E-6
HCT-15	0.234	1.768	1.608	1.720	1.222	0.063	0.104	90	97	64	-73	-56	1.27E-6	2.94E-6	6.77E-6
HT29	0.226	1.571	1.526	1.614	1.253	0.109	0.074	97	103	76	-52	-67	1.60E-6	3.94E-6	9.69E-6
KM12	0.874	3.317	3.283	3.292	2.759	0.517	0.161	99	99	77	-41	-82	1.70E-6	4.50E-6	1.67E-5
SW-620	0.358	2.702	2.574	2.631	1.831	0.098	0.147	95	97	63	-73	-59	1.24E-6	2.91E-6	6.79E-6
CNS Cancer															
SF-268	1.102	2.816	2.687	2.817	2.362	0.944	0.429	92	100	74	-14	-61	1.85E-6	6.87E-6	5.79E-5
SF-295	1.271	3.307	3.190	3.273	0.707	0.367	0.226	94	98	-44	-71	-82	2.18E-7	4.89E-7	1.62E-6
SF-539	0.781	2.445	2.257	1.979	0.698	0.042	0.039	89	72	-11	-95	-95	1.85E-7	7.44E-7	2.94E-6
SNB-19	0.769	2.477	2.391	2.488	1.816	0.610	0.082	95	101	61	-21	-89	1.37E-6	5.59E-6	2.67E-5
U251	0.446	2.047	1.934	1.785	1.051	0.102	0.046	93	84	38	-77	-90	5.41E-7	2.13E-6	5.80E-6
Melanoma															
LOX IMVI	0.616	2.996	2.872	2.941	2.235	0.022	0.199	95	98	68	-97	-68	1.29E-6	2.59E-6	5.22E-6
MALME-3M	0.634	1.228	1.129	1.226	0.871	0.195	0.092	83	100	40	-69	-85	6.77E-7	2.32E-6	6.66E-6
M14	0.419	1.826	1.683	1.734	1.210	0.190	0.069	90	93	56	-55	-84	1.14E-6	3.21E-6	9.06E-6
MDA-MB-435	0.508	2.389	2.298	2.300	1.839	0.314	0.105	95	95	71	-38	-79	1.55E-6	4.45E-6	1.93E-5
SK-MEL-2	1.085	2.715	2.585	2.586	1.707	0.653	0.283	92	92	38	-40	-74	6.03E-7	3.08E-6	1.98E-5
SK-MEL-28	0.703	1.865	1.858	1.746	0.708	0.181	0.084	99	90	.	-74	-88	2.79E-7	1.01E-6	4.73E-6
SK-MEL-5	1.246	3.243	3.207	3.255	3.006	0.028	0.078	98	101	88	-98	-94	1.60E-6	2.98E-6	5.53E-6
UACC-257	0.795	2.018	1.911	2.046	1.329	0.288	0.078	91	102	44	-64	-90	7.78E-7	2.55E-6	7.43E-6
UACC-62	0.953	2.807	2.716	2.772	2.031	0.214	0.113	95	98	58	-78	-88	1.15E-6	2.68E-6	6.26E-6
Ovarian Cancer															
IGROV1	0.474	2.091	2.023	2.131	1.704	0.518	0.131	96	102	76	3	-72	2.27E-6	1.09E-5	5.03E-5
OVCAR-3	0.561	1.864	1.793	1.796	1.495	0.185	0.181	94	95	72	-67	-68	1.43E-6	3.29E-6	7.54E-6
OVCAR-4	1.073	1.939	1.972	1.948	1.908	1.046	0.530	104	101	96	-3	-51	2.94E-6	9.42E-6	9.71E-5
OVCAR-5	0.576	1.582	1.541	1.562	1.332	0.341	0.103	96	98	75	-41	-82	1.65E-6	4.44E-6	1.66E-5
OVCAR-8	0.563	2.599	2.420	2.452	1.968	0.519	0.329	91	93	69	-8	-42	1.77E-6	7.89E-6	> 1.00E-4
NCI/ADR-RES	0.593	2.030	2.014	1.989	1.621	0.477	0.477	99	97	72	-20	-20	1.72E-6	6.10E-6	> 1.00E-4
SK-OV-3	0.832	1.752	1.672	1.757	1.383	0.642	0.191	91	100	60	-23	-77	1.32E-6	5.29E-6	3.16E-5
Renal Cancer															
786-0	0.741	2.724	2.614	2.727	1.042	0.360	0.129	94	100	15	-51	-83	3.89E-7	1.69E-6	9.50E-6
A498	1.676	2.298	2.042	2.181	1.714	0.416	0.167	59	81	6	-75	-90	2.60E-7	1.19E-6	4.89E-6
ACHN	0.544	2.341	2.314	2.246	1.581	0.562	0.024	98	95	58	1	-96	1.37E-6	1.02E-5	3.37E-5
CAKI-1	1.234	3.071	2.957	2.940	2.393	0.428	0.327	94	93	63	-65	-74	1.26E-6	3.10E-6	7.59E-6
RXF 393	0.955	1.834	1.812	1.843	0.482	0.422	0.263	98	101	-50	-56	-73	2.18E-7	4.69E-7	1.17E-6
SN12C	0.566	2.159	2.145	2.154	1.981	0.169	0.095	99	100	89	-70	-83	1.75E-6	3.62E-6	7.46E-6
TK-10	1.066	1.887	1.730	1.821	1.870	0.632	0.125	81	92	98	-41	-88	2.22E-6	5.08E-6	1.57E-5
UO-31	1.009	2.358	2.086	2.139	1.849	0.149	0.099	80	84	62	-85	-90	1.21E-6	2.64E-6	5.77E-6
Prostate Cancer															
PC-3	0.532	1.594	1.469	1.412	0.906	0.408	0.216	88	83	35	-23	-59	4.89E-7	3.99E-6	5.48E-5
DU-145	0.477	1.986	1.944	1.926	1.635	0.463	0.051	97	96	77	-3	-89	2.16E-6	9.16E-6	3.50E-5
Breast Cancer															
MCF7	0.406	2.138	1.929	1.989	1.262	0.256	0.191	88	91	49	-37	-53	9.68E-7	3.73E-6	6.44E-5
MDA-MB-231/ATCC	0.812	2.178	2.111	2.173	1.497	0.394	0.168	95	100	50	-51	-79	1.00E-6	3.11E-6	9.67E-6
HS 578T	1.691	2.803	2.655	2.708	1.969	1.001	0.932	87	91	25	-41	-45	4.21E-7	2.40E-6	> 1.00E-4
BT-549	1.314	2.494	2.413	2.452	1.800	0.652	0.158	93	96	41	-50	-88	6.92E-7	2.82E-6	9.90E-6
T-47D	0.831	1.740	1.600	1.696	1.512	0.652	0.459	85	95	75	-22	-45	1.81E-6	5.98E-6	> 1.00E-4
MDA-MB-468	0.946	1.562	1.456	1.613	1.382	0.675	0.442	83	108	71	-29	-53	1.62E-6	5.15E-6	7.33E-5

All the Quantum Chemical calculations were done using Gaussian 09 Software.

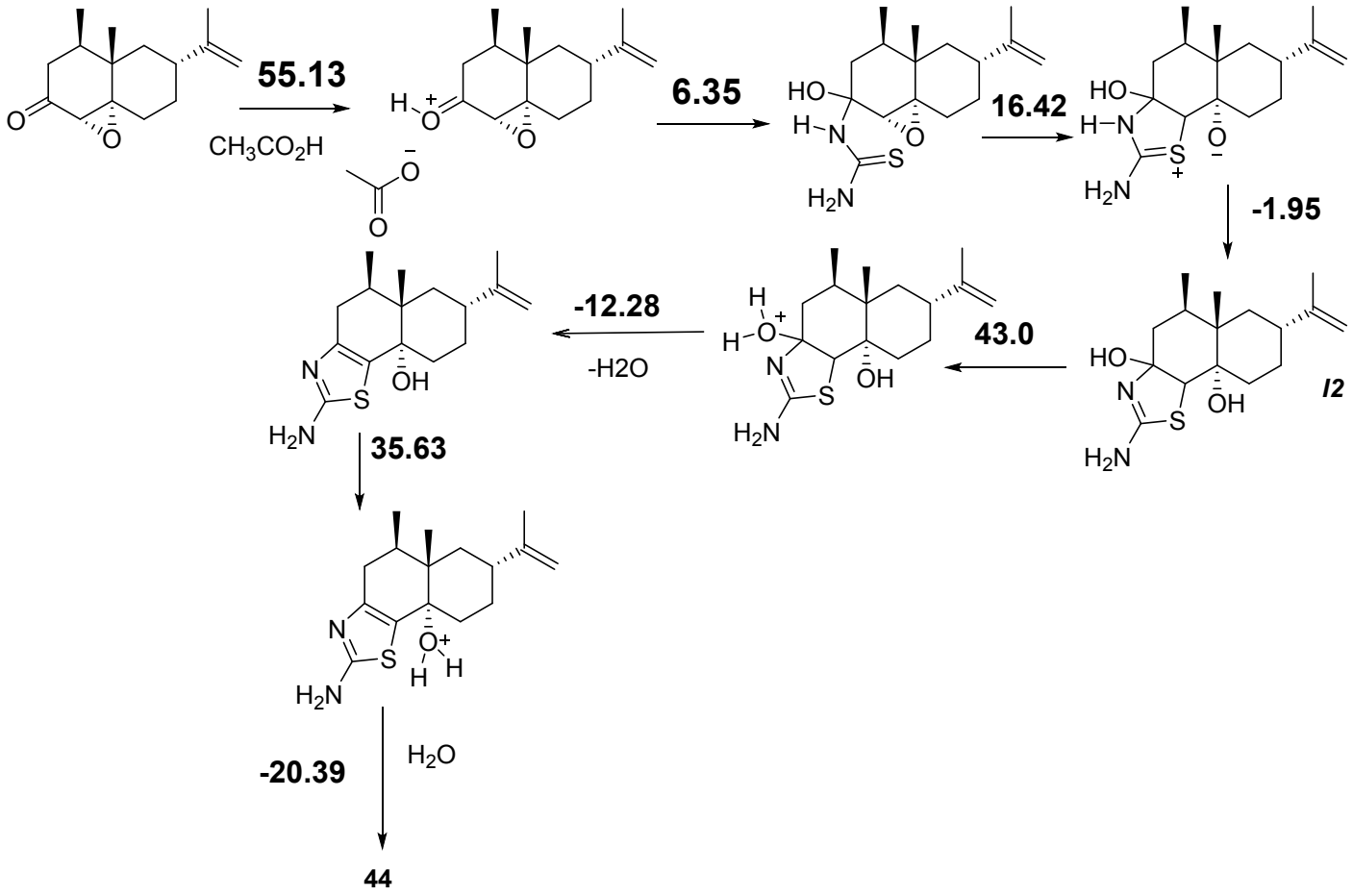
ΔG was Calculated using M06-2X/6-31+G(d,p) + PCP [different solvents]

The calculation shown in red color (Acetic Acid) is more feasible than other solvents. All the energies shown in this scheme is with respect to reactants.



Protonation Mechanism

ΔG was calculated using M06-2X/6-31+G(d,p) + PCP (Solvent =AcOH)



Optimized geometry of Reactants, Intermediates and Products using M06-2X/6-31+G(d,p) + PCM (Solvent= AcOH).

Reactant (EN)

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,-3.9338819484,-3.1445708734,-2.0947763282

C,0,-2.5012805684,-2.9085342614,-2.6294272259

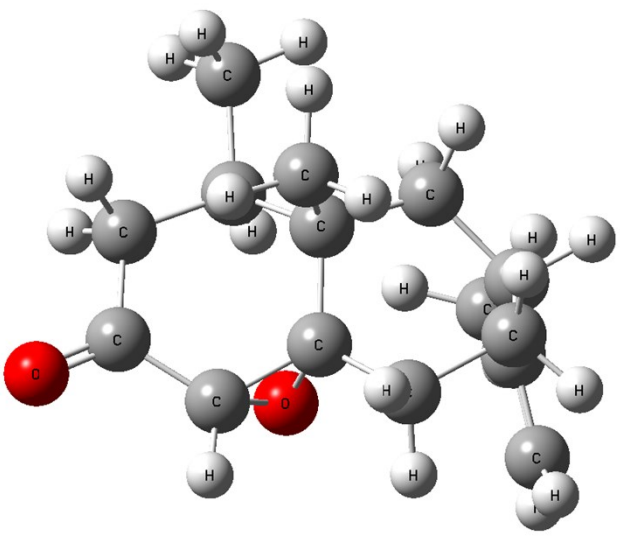
C,0,-2.3920578468,-1.4545223725,-3.0969739678

C,0,-2.5659678415,-0.4745366084,-1.9206901916

C,0,-3.3756611454,-1.0732231486,-0.7820965933

C,0,-4.5088730763,-2.0249922349,-1.1690971178

H,0,-1.4430435384,-1.2679573577,-3.6077792342



H,0,-2.4018712784,-3.5634317033,-3.5078678637

H,0,-4.5958404027,-3.2437739008,-2.9628807461

H,0,-3.9739445762,-4.1063455552,-1.5773166464

H,0,-1.6000393321,-0.1812583795,-1.5001098079

H,0,-3.0594656799,0.4413483914,-2.2634524086

H,0,-3.1763200697,-1.2858651316,-3.8437012483

C,0,-3.4621618433,-0.2919272687,0.4749040123

H,0,-2.9249934784,0.6512010952,0.5636876511

C,0,-4.69677865,-0.4002616616,1.3070841307

C,0,-5.1055619444,-2.6688849546,0.1106387715

H,0,-4.2952309006,-3.2571804098,0.5558999884

C,0,-5.5580512355,-1.633001685,1.1512387556

H,0,-5.645222385,-2.1025152264,2.138059454

H,0,-6.5622943993,-1.2572509799,0.9132726948

C,0,-6.2750229057,-3.6150401505,-0.1755127114

H,0,-7.1482645633,-3.0679894905,-0.5455656454

H,0,-6.0183328885,-4.382044075,-0.9113917364

H,0,-6.5738995736,-4.1247645264,0.7456841185

C,0,-5.5644840955,-1.1986159877,-1.9243648031

H,0,-5.1352337132,-0.7349449813,-2.8173434196

H,0,-6.3901186242,-1.8353296204,-2.253542746

H,0,-5.9757504117,-0.3972886852,-1.3000630045

O,0,-5.0250689771,0.5223913089,2.0316520886

O,0,-2.6429509388,-1.4568010665,0.3775430497

C,0,-1.3832046013,-3.3437649069,-1.6859170961

C,0,-0.2215459767,-2.6911012562,-1.5817255886

H,0,-0.0178051391,-1.7654427372,-2.1093546154

C,0,-1.6052806568,-4.6223275232,-0.9176004626

H,0,-0.6760210073,-4.9673936855,-0.4592345825

H,0,-2.3421155717,-4.476853837,-0.1189541467

H,0,-1.9882984595,-5.416646064,-1.569353232

H,0,0.5719945844,-3.0713265485,-0.9445455152

Thermochemistry Data

Zero-point correction= 0.345289 (Hartree/Particle)

Thermal correction to Energy= 0.361452

Thermal correction to Enthalpy= 0.362396

Thermal correction to Gibbs Free Energy= 0.303129

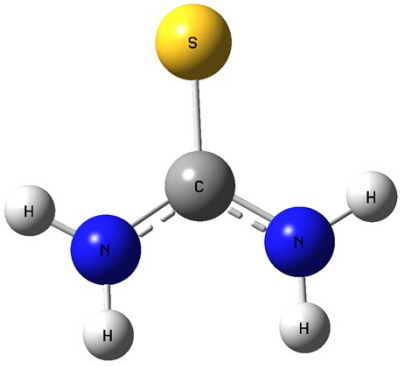
Sum of electronic and zero-point Energies= -734.626758

Sum of electronic and thermal Energies= -734.610595

Sum of electronic and thermal Enthalpies= -734.609651

Sum of electronic and thermal Free Energies= -734.668918

$NH_2C(=S)NH_2$



Charge = 0 Multiplicity = 1

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N,0,-0.091282287,-2.0873637978,-0.0845652395

H,0,-0.9138643197,-2.6729377646,-0.0658022098

H,0,0.3213431555,-1.810555574,0.7919910733

C,0,0.5298623789,-1.7444251579,-1.2248828943

N,0,-0.0440094365,-2.1543858233,-2.3678419282

H,0,-0.9272503853,-2.6435358941,-2.390375387

H,0,0.3865775976,-1.8999427231,-3.2425344643

S,0,1.9660878151,-0.8395563547,-1.2217083643

Thermochemistry Data

Zero-point correction= 0.061464 (Hartree/Particle)

Thermal correction to Energy= 0.066400

Thermal correction to Enthalpy= 0.067345

Thermal correction to Gibbs Free Energy= 0.034565

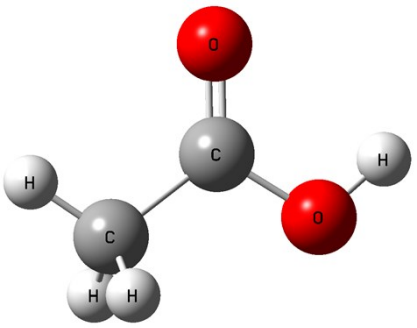
Sum of electronic and zero-point Energies= -548.083649

Sum of electronic and thermal Energies= -548.078712

Sum of electronic and thermal Enthalpies= -548.077767

Sum of electronic and thermal Free Energies= -548.110547

CH_3COOH



Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,-3.4415414205,-0.0613688708,0.0048850861

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H,0,-2.7841503603,0.1004774913,-0.8525940776

H,0,-4.4251101616,0.3606975277,-0.1900857398

C,0,-2.8466844945,0.5866818534,1.2200219028

O,0,-3.368329984,1.449093181,1.8908239499

O,0,-1.6265809876,0.0982599855,1.5059019694

H,0,-1.2945985089,0.5530306114,2.2968020198t

Thermochemistry Data

Zero-point correction= 0.062385 (Hartree/Particle)

Thermal correction to Energy= 0.066877

Thermal correction to Enthalpy= 0.067821

Thermal correction to Gibbs Free Energy= 0.035485

Sum of electronic and zero-point Energies= -228.945701

Sum of electronic and thermal Energies= -228.941210

Sum of electronic and thermal Enthalpies= -228.940265

Sum of electronic and thermal Free Energies= -228.972602

Hydrogen bonded complex CH_3COOH with R_1 (C=O)[EH1]

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

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C,0,1.496972485,-2.089886413,1.1905980871

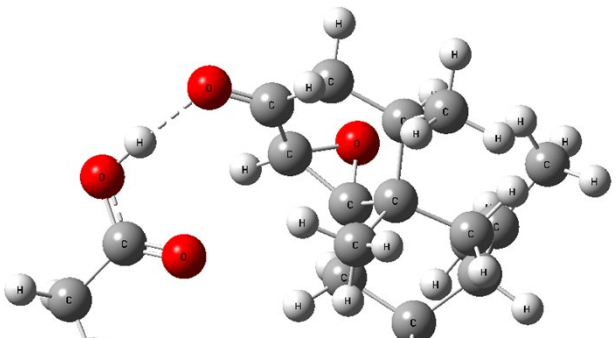
C,0,0.2641769472,-1.7369206707,0.3362937783

C,0,0.2935148994,-0.3011497117,-0.1555903173

C,0,0.9118729434,0.7396356179,0.778914679

H,0,1.73882033,-3.1514096397,1.0862739358

H,0,3.5353137317,-1.4733276658,1.4833035007



H,0,2.4249910965,0.3526787644,2.2855986579

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H,0,-0.6570544773,-1.8801644089,0.9108833921

H,0,1.2725966406,-1.9325976298,2.2517969497

C,0,-0.7724031469,0.0998967746,-1.1036629671

H,0,-1.4902872949,-0.6439769679,-1.4435375571

C,0,-1.2675465799,1.4966368388,-1.0196260064

C,0,1.0210278833,2.0985421302,0.0370833292

H,0,1.7159619681,1.9327286937,-0.7929668535

C,0,-0.318732669,2.5711518211,-0.5581998416

H,0,-0.1347403472,3.2362597797,-1.4111057691

H,0,-0.8863967108,3.1664341131,0.1677550237

C,0,1.5861193701,3.2224420697,0.9095228223

H,0,0.8956800964,3.4843943165,1.7175204534

H,0,2.5470842494,2.9549360957,1.3571920685

H,0,1.7398581375,4.1214296974,0.3043820872

C,0,-0.0019409148,0.8501204406,2.0115760219

H,0,-0.1126156458,-0.1186908843,2.5077591207

H,0,0.4194356117,1.5472425581,2.741057058

H,0,-1.0072804583,1.1890507621,1.7390438204

O,0,-2.4456090971,1.7494198472,-1.246159925

O,0,0.5702199322,-0.0981853612,-1.5397595134

C,0,3.2113284952,-1.4039156586,-0.5885512128

C,0,2.9629971021,-2.5044934315,-1.3059173192

H,0,2.3120330259,-3.300303683,-0.9592581108

C,0,4.1215275868,-0.334334756,-1.1381034012

H,0,4.6145500599,-0.675466455,-2.0509435791

H,0,3.5594095482,0.5753320541,-1.3785943705

H,0,4.8918440222,-0.0544531135,-0.4095866486

H,0,3.4093046873,-2.6369551025,-2.2876820435

C,0,-4.9250748532,-1.9301526326,0.6026821177

H,0,-5.0008592129,-2.6540324878,-0.2123511585

H,0,-5.9150120094,-1.4916427059,0.7490359296

H,0,-4.5954009922,-2.4244704199,1.514412183

C,0,-3.9503871388,-0.8505996176,0.2260324156

O,0,-2.9436505351,-0.575200517,0.8511922833

O,0,-4.3009145699,-0.2121400341,-0.8919233882

H,0,-3.6382863581,0.497941618,-1.0842545311

Thermochemistry Data

Zero-point correction= 0.409261 (Hartree/Particle)

Thermal correction to Energy= 0.431558

Thermal correction to Enthalpy= 0.432502

Thermal correction to Gibbs Free Energy= 0.356960

Sum of electronic and zero-point Energies= -963.584621

Sum of electronic and thermal Energies= -963.562325

Sum of electronic and thermal Enthalpies= -963.561380

Sum of electronic and thermal Free Energies= -963.636923

Hydrogen bonded complex CH_3COOH with R_1 (epoxy group) (EH2)

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,-1.9844894162,-1.762455885,0.2246665408

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C,0,-0.5464080339,-2.3109027659,-1.740640618

C,0,-0.0391867219,-0.8633898391,-1.8794413028

C,0,-0.5079967804,0.0245808548,-0.7401916967

C,0,-1.8981022865,-0.2528528212,-0.1700050899

H,0,0.1681901178,-3.0059471351,-2.190149499

H,0,-1.2078353548,-3.6881720168,-0.2298868573

H,0,-2.9143776743,-2.1707905283,-0.1874911794

H,0,-2.0720965345,-1.8537758078,1.3102657253

H,0,1.0545069844,-0.8238611044,-1.8909826388

H,0,-0.3824232328,-0.4293533858,-2.824652394

H,0,-1.4816222598,-2.4346292043,-2.2980404647

C,0,0.0765898654,1.3831474366,-0.6484548982

H,0,0.8440051693,1.6956041026,-1.3543448746

C,0,-0.7510175918,2.4893723322,-0.0771432009

C,0,-2.1311517321,0.6237498396,1.0903672033

H,0,-1.3980972862,0.2859541977,1.8313427279

C,0,-1.8905631434,2.1219873866,0.8453268752

H,0,-1.72493455,2.6361270818,1.7991823456

H,0,-2.7809736321,2.5917975666,0.4068399053

C,0,-3.5257884659,0.4464281949,1.6973072938

H,0,-4.3009591695,0.8564153361,1.042155005

H,0,-3.7637893919,-0.6033457161,1.8898795226

H,0,-3.5861765136,0.9812995165,2.6500841301

C,0,-2.9190910424,0.0708977122,-1.2746045391

H,0,-2.744418504,-0.5393262487,-2.1657203491

H,0,-3.9349571655,-0.1408489369,-0.9305849686

H,0,-2.8708272661,1.1231729114,-1.577218961

O,0,-0.5508394469,3.6370603845,-0.4270193378

O,0,0.4722752898,0.3464295947,0.2552063029

C,0,0.4191875431,-2.6574064405,0.6076764722

C,0,1.6578391918,-2.777799021,0.1184343738

H,0,1.8710461223,-2.8154146878,-0.9450280677

C,0,0.197763649,-2.5965356439,2.0977546431

H,0,1.118332351,-2.8303661119,2.6368375668

H,0,-0.1266278943,-1.5943317221,2.401890199

H,0,-0.5806991555,-3.3001732611,2.4152365391

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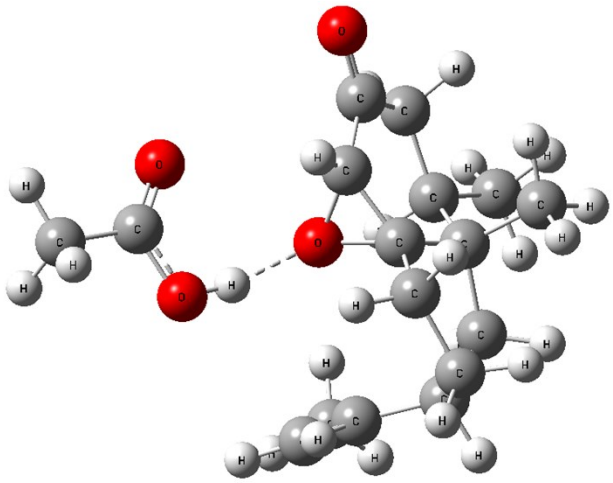

H,0,5.4347118565,0.9318413687,-0.9712320581

H,0,5.6139327503,0.7636636678,0.7760713387

H,0,5.449686905,2.3934723269,0.059113543

C,0,3.6419143922,1.2647066451,0.1365707517

O,0,2.9033170684,2.2137395577,0.3076967165

O,0,3.1973309378,0.0061406946,0.0556669137

H,0,2.2169566612,0.0001134125,0.1687585784

Thermochemistry Data

Zero-point correction= 0.409034 (Hartree/Particle)

Thermal correction to Energy= 0.431401

Thermal correction to Enthalpy= 0.432345

Thermal correction to Gibbs Free Energy= 0.355990

Sum of electronic and zero-point Energies= -963.583745

Sum of electronic and thermal Energies= -963.561378

Sum of electronic and thermal Enthalpies= -963.560434

Sum of electronic and thermal Free Energies= -963.636789

Intermediate HA

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,-3.8148972206,-3.4166424828,-1.9038666675

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C,0,-2.4700058001,-1.8622245022,-3.3419015483

C,0,-2.8416084264,-0.6278736816,-2.4922097136

C,0,-3.6118200093,-1.0129952117,-1.241142929

C,0,-4.599122769,-2.1617690587,-1.4098199685

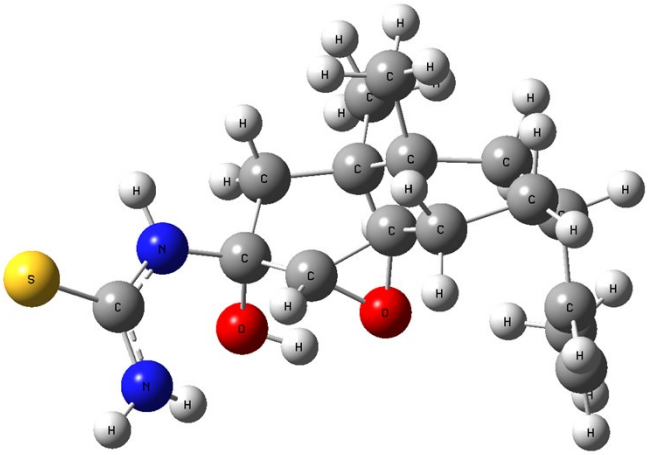
H,0,-1.5263358554,-1.6877978026,-3.8651930758

H,0,-2.1870507549,-3.9820576347,-3.1542049091

H,0,-4.4080023526,-3.9017242919,-2.6877377363

H,0,-3.7396762052,-4.1448147257,-1.0917988248

H,0,-1.9455775195,-0.0925425128,-2.1649310687



H,0,-3.4404586998,0.0734905407,-3.0833615296

H,0,-3.2177071343,-2.0223338032,-4.1256619746

C,0,-3.772549352,-0.0227009051,-0.1607854365

H,0,-3.3517956236,0.9743698594,-0.2958512069

C,0,-4.8708148637,-0.1379193944,0.903581057

C,0,-5.2936390464,-2.4639194475,-0.0556991819

H,0,-4.5101008552,-2.8298500562,0.6231543594

C,0,-5.910245894,-1.2016571229,0.5520158231

H,0,-6.4473006193,-1.4441670933,1.4752257361

H,0,-6.6407444299,-0.7856616251,-0.151605961

C,0,-6.3614097517,-3.5564321992,-0.1548877752

H,0,-7.2560255731,-3.193988422,-0.6712551034

H,0,-5.9947372924,-4.4375271009,-0.6894875483

H,0,-6.6655061552,-3.8733457635,0.8467193889

C,0,-5.6293433459,-1.7357355885,-2.4749864302

H,0,-5.1552730028,-1.5890828027,-3.4474466629

H,0,-6.3881880361,-2.5124147584,-2.6019068363

H,0,-6.1316072561,-0.7990987105,-2.2140772289

O,0,-4.2464346632,-0.4558830279,2.1433544733

O,0,-2.8057151953,-1.064239053,-0.0481560918

C,0,-1.2671374783,-3.1350042676,-1.4695726445

C,0,-0.1683203385,-2.3867219824,-1.610045467

H,0,-0.0407228671,-1.6711777453,-2.4154924018

C,0,-1.3829632174,-4.0931462909,-0.311464791

H,0,-0.4368985808,-4.1646470693,0.2295070654

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H,0,-1.6684533011,-5.097214024,-0.6467101937

H,0,0.6483076077,-2.4653946365,-0.8978150944

N,0,-5.5569502654,1.1322002365,1.073772337

H,0,-6.5049114444,1.198908728,0.7299811971

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N,0,-3.7879093948,2.2760360754,2.0077965214

H,0,-3.4155310802,3.1418544404,2.36638779

H,0,-3.3941477544,1.3974696387,2.3247601421

S,0,-5.9040487947,3.7510164053,1.3391484807

H,0,-3.5509618626,-1.1040398633,1.9488545227

Thermochemistry Data

Zero-point correction= 0.412784 (Hartree/Particle)

Thermal correction to Energy= 0.433385

Thermal correction to Enthalpy= 0.434329

Thermal correction to Gibbs Free Energy= 0.365449

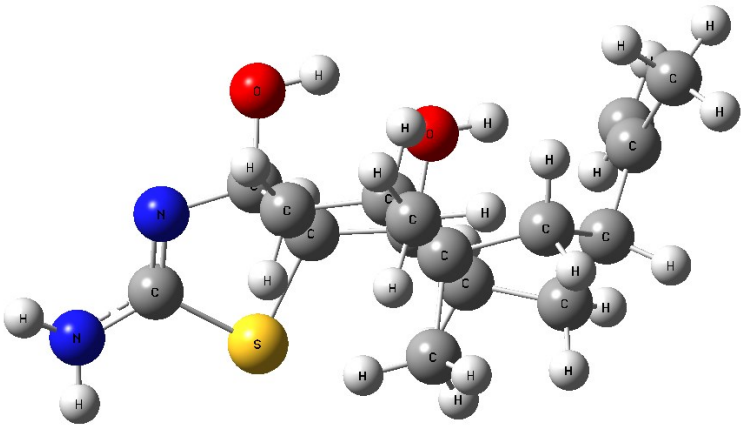
Sum of electronic and zero-point Energies= -1282.722003

Sum of electronic and thermal Energies= -1282.701402

Sum of electronic and thermal Enthalpies= -1282.700458

Sum of electronic and thermal Free Energies= -1282.769338

Intermediate TZ



Charge = 0 Multiplicity = 1

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C,0,-2.2188869359,-1.5662105686,-1.2999671417

C,0,-0.8892863204,-1.7993775954,-0.5535369014

C,0,-0.2925285788,-0.5303523754,0.0799259819

C,0,-0.5791061911,0.7301459127,-0.78265147

H,0,-2.8371459962,-2.4677253643,-1.2567792975

H,0,-3.8185366144,-0.1802339598,-1.5325680956

H,0,-2.359416461,1.4964907336,-1.7348564235

H,0,-2.407111126,1.580240385,0.0083835768

H,0,-0.9988482871,-2.5378335525,0.2495150427

H,0,-0.1674762893,-2.2277155529,-1.2568921255

H,0,-2.0105169733,-1.4018984464,-2.3607665819

C,0,1.1848273635,-0.7466155706,0.4706302286

C,0,1.8750722688,0.5225080842,1.0385230605

C,0,0.0611312549,1.9631230512,-0.0812964763

H,0,-0.4441257198,2.0647411239,0.8880176548

C,0,1.5547305823,1.7597892418,0.1890943297

H,0,1.9609720298,2.6254118116,0.7240188229

H,0,2.101879172,1.6862336158,-0.7586125363

C,0,-0.147094797,3.2689141744,-0.8526457585

H,0,0.4069613954,3.2643535946,-1.7974564617

H,0,-1.2022629926,3.4507540736,-1.0777176527

H,0,0.2176799278,4.1139779193,-0.2608215092

C,0,-0.0295612238,0.5936719067,-2.2180936073

H,0,-0.2698989806,-0.3714477049,-2.6696239283

H,0,-0.4681429889,1.3675078852,-2.8549021281

H,0,1.0551662374,0.7018493882,-2.2600616027

O,0,1.4802517878,0.7242540738,2.3810722447

O,0,-0.8822903275,-0.2979919169,1.3778840164

C,0,-3.7544957789,-0.5642166652,0.5080854567

C,0,-3.7803759755,-1.7294330329,1.1704523525

H,0,-3.2383521879,-2.6083445739,0.8359910285

C,0,-4.5390418087,0.6195931632,1.0210795301

H,0,-5.2833848067,0.3062655956,1.7560262524

H,0,-3.88434335,1.3550472321,1.500477482

H,0,-5.0500116738,1.132288835,0.1989536004

H,0,-4.3693294569,-1.837297972,2.0769209335

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C,0,3.6530674912,-0.5378940897,0.1301670168

N,0,4.937273479,-0.8890737734,-0.1550982691

H,0,5.1320479226,-1.3978411693,-1.0035941974

H,0,5.6563029941,-0.2521263951,0.1588537466

S,0,2.349694346,-1.3502827274,-0.8028292101

H,0,0.5276139614,0.5454270456,2.4336691114

H,0,-1.7663441084,-0.6902930048,1.4374459021

H,0,1.1823632064,-1.5041923454,1.2625578856

Thermochemistry Data

Zero-point correction= 0.411810 (Hartree/Particle)

Thermal correction to Energy= 0.432475

Thermal correction to Enthalpy= 0.433419

Thermal correction to Gibbs Free Energy= 0.365464

Sum of electronic and zero-point Energies= -1282.736234

Sum of electronic and thermal Energies= -1282.715569

Sum of electronic and thermal Enthalpies= -1282.714625

Sum of electronic and thermal Free Energies= -1282.782580

Intermediate HT

Charge = 0 Multiplicity = 1

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C,0,-2.9714686727,-0.3398765838,-0.7563995791

C,0,-2.1618707925,-1.5154383411,-1.3376668529

C,0,-0.7215301857,-1.6857080163,-0.8039371835

C,0,-0.1512753087,-0.4411494242,-0.098599918

C,0,-0.6125893618,0.8603908326,-0.8235431101

H,0,-2.7260526599,-2.4411124087,-1.191326931

H,0,-3.7765260684,-0.1396905432,-1.4754739842

H,0,-2.5163699612,1.7152939876,-1.3603743943

H,0,-2.3164566974,1.4288083575,0.3537709061

H,0,-0.6566745102,-2.5159010585,-0.0897307171

H,0,-0.0656246463,-1.9455471409,-1.6409329157

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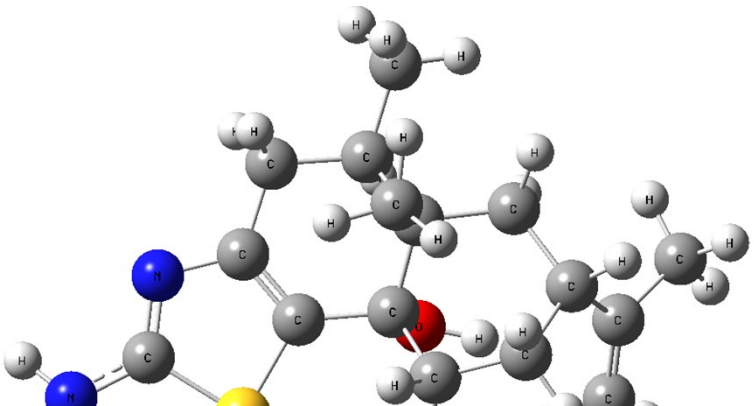

C,0,1.3487900953,-0.4602896237,-0.0407315591

C,0,2.1568865033,0.6255087682,-0.1303942218

C,0,0.1022726373,2.0645497006,-0.1444109208

H,0,-0.0789549089,1.9467311854,0.9319725847

C,0,1.6215725883,2.0042740951,-0.3632871137

H,0,2.1220431067,2.7052523648,0.3146789889

H,0,1.875713984,2.3278300086,-1.3834569992

C,0,-0.4296350889,3.4367520306,-0.5614698003

H,0,-0.3065153247,3.6152248525,-1.6350957581

H,0,-1.4874564614,3.5599144701,-0.3147932764

H,0,0.1244892793,4.2212757454,-0.0359073514

C,0,-0.2603732211,0.8166148517,-2.3217717522

H,0,-0.8751727408,0.1013930464,-2.8693118823

H,0,-0.4370085979,1.7959601389,-2.7762729045

H,0,0.7874953792,0.549973598,-2.4859437326

O,0,-0.5773239801,-0.4149228314,1.2729106285

C,0,-3.699317476,-0.6574790277,0.5430813756

C,0,-3.4877906764,-1.7615496576,1.27215461

H,0,-2.7730201579,-2.5270655692,0.9823233947

C,0,-4.7480081108,0.346994471,0.9507916752

H,0,-5.2135462879,0.075594002,1.9004969994

H,0,-4.333375652,1.3552779539,1.0465915501

H,0,-5.5292477753,0.3966413637,0.1831977379

H,0,-4.0438041597,-1.938896617,2.1882597474

N,0,3.5167223604,0.395280469,0.0028835147

C,0,3.7431715021,-0.8678862125,0.2112429098

N,0,4.9992613661,-1.412188436,0.3172792332

H,0,5.086998665,-2.2639747677,0.8537937019

H,0,5.7190941164,-0.7298158859,0.5198600632

S,0,2.3174188285,-1.8873078852,0.2539992914

H,0,-1.5149037726,-0.6514601593,1.3350924442

Thermochemistry Data

Zero-point correction= 0.383783 (Hartree/Particle)

Thermal correction to Energy= 0.403288

Thermal correction to Enthalpy= 0.404232

Thermal correction to Gibbs Free Energy= 0.338398

Sum of electronic and zero-point Energies= -1206.355967

Sum of electronic and thermal Energies= -1206.336463

Sum of electronic and thermal Enthalpies= -1206.335519

Sum of electronic and thermal Free Energies= -1206.401352

Product (44)

Charge = 0 Multiplicity = 1

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C,0,2.3664645743,-0.9830329315,2.0164137947

C,0,0.9252750849,-1.2893159984,1.5521265467

C,0,0.5377510345,-0.4708824491,0.3105141189

C,0,0.9984282689,1.0041511399,0.4334209907

H,0,2.8536925723,-1.890511312,2.3860988378

H,0,4.1800027968,-0.0495618404,1.3647604249

H,0,2.8879378491,1.8006292867,1.1389772092

H,0,2.9380738409,1.2712806339,-0.5249226041

H,0,0.814667608,-2.353706694,1.3131556478

H,0,0.2187641217,-1.0800934587,2.3639194126

H,0,2.3423115258,-0.292447034,2.865957845

C,0,-0.9253482737,-0.5282372117,-0.0116620647

C,0,-1.6553683502,0.4780726893,-0.5536855257

C,0,0.4825971118,1.7801816321,-0.8119422103

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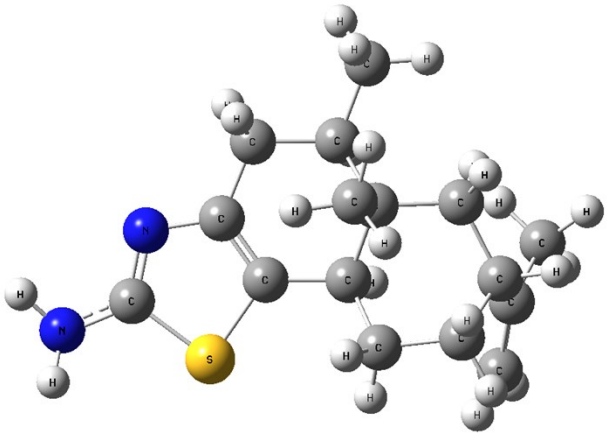

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H,0,0.6753192598,3.8383551093,-0.1093844694

H,0,2.1154679504,3.2385540417,-0.9467691444

H,0,0.6665792371,3.6611027124,-1.8638708094

C,0,0.4377124017,1.6407693175,1.7174802387

H,0,0.8648138387,1.1837797773,2.6131920149

H,0,0.6826084101,2.7067200761,1.7547029081

H,0,-0.6501518519,1.5366303216,1.7781383936

C,0,3.5902933962,-1.2663331673,-0.2251340479

C,0,3.3827645471,-2.587838074,-0.1995189749

H,0,2.8666159379,-3.085476765,0.614516918

C,0,4.3078371153,-0.6368704525,-1.3954573285

H,0,4.7934782946,-1.3981077883,-2.0098356898

H,0,3.6136950707,-0.0816456349,-2.0364537589

H,0,5.0684437142,0.0753400979,-1.0549767447

H,0,3.7283934449,-3.2187156066,-1.0139036871

N,0,-3.0019464032,0.2214722855,-0.7728695425

C,0,-3.2970079701,-0.9892756159,-0.4092249237

N,0,-4.5360500431,-1.5642383985,-0.5747327981

H,0,-4.7899189449,-2.2916092321,0.0797215735

H,0,-5.2733230207,-0.8867874712,-0.7250995039

S,0,-1.955916031,-1.9223331982,0.2323652906

H,0,1.0834190369,-0.8997220922,-0.5429700799

Thermochemistry Data

Zero-point correction= 0.379031 (Hartree/Particle)

Thermal correction to Energy= 0.397472

Thermal correction to Enthalpy= 0.398416

Thermal correction to Gibbs Free Energy= 0.334257

Sum of electronic and zero-point Energies= -1131.159273

Sum of electronic and thermal Energies= -1131.140832

Sum of electronic and thermal Enthalpies= -1131.139888

Sum of electronic and thermal Free Energies= -1131.204047

H_2O

Charge = 0 Multiplicity = 1

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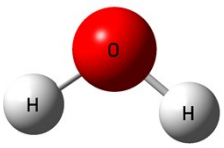

O,0,-0.70503387,-0.7575507791,0.

H,0,0.2576884437,-0.7236584422,0.

H,0,-0.9944488631,0.1612647113,0.

Zero-point correction= 0.021537 (Hartree/Particle)

Thermal correction to Energy= 0.024373

Thermal correction to Enthalpy= 0.025317

Thermal correction to Gibbs Free Energy= 0.003893

Sum of electronic and zero-point Energies= -76.380031

Sum of electronic and thermal Energies= -76.377196

Sum of electronic and thermal Enthalpies= -76.376251

Sum of electronic and thermal Free Energies= -76.397676

Intermediate IT

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

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C,0,1.7605299197,-1.9394609454,0.3347153714

C,0,0.8860685906,-0.8287740553,-0.2722542863

C,0,1.1368747462,0.552141267,0.3951660281

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H,0,4.575170685,0.1033869556,0.5695829146

H,0,2.9398390187,1.5406398339,1.0581964243

H,0,2.7222615615,1.5901144114,-0.6713037632

H,0,1.8507833715,-2.7206369329,-0.42912953

H,0,1.2321916147,-2.4001135063,1.1737565638

H,0,3.0809392884,-1.1838017629,1.8760560111

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C,0,-1.4624523832,-0.1589264147,-0.9190877798

C,0,0.2738944011,1.6226541202,-0.3319868584

H,0,0.651203824,1.6696288831,-1.3593385469

C,0,-1.2137668832,1.2378565257,-0.4165360885

H,0,-1.7622419132,1.9354992308,-1.0548094338

H,0,-1.6701774911,1.2909111023,0.5830011819

C,0,0.3948141336,3.0174999176,0.2858532636

H,0,-0.0410693654,3.0481646518,1.2898471496

H,0,1.4371501293,3.3412335627,0.3564782323

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H,0,1.1860327835,-0.3661898441,2.3980454044

H,0,1.218047044,1.3951789714,2.3980383969

H,0,-0.2863760565,0.5450717175,2.0791667044

O,0,-2.3439217858,-0.42846282,-1.7173890913

O,0,1.1405724543,-0.6804073391,-1.6773143379

C,0,4.1212777041,-0.5080634066,-1.3644725641

C,0,4.231791711,-1.7383601175,-1.8847307488

H,0,3.9558388916,-2.6345194718,-1.3386825696

C,0,4.52984214,0.6982688682,-2.1753944056

H,0,5.1335408843,0.4037496752,-3.0360186515

H,0,3.6540167728,1.2397236929,-2.5494278262

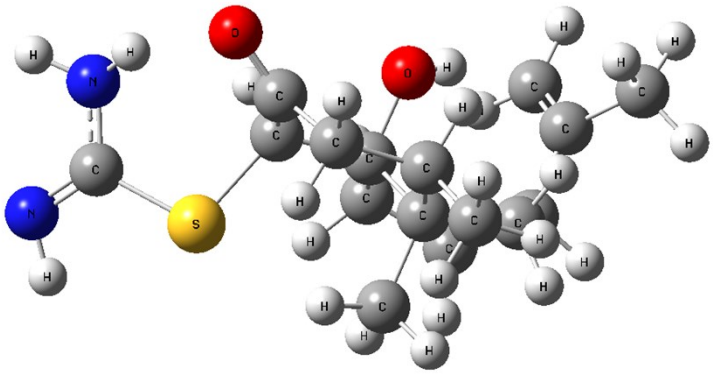
H,0,5.1070321805,1.401604829,-1.5652529547

H,0,4.6252239148,-1.8818056666,-2.8870591416

N,0,-2.9245395269,-3.9058291771,1.6773524148

H,0,-2.4646737478,-3.782750779,2.576941607

C,0,-2.501929809,-3.0721491477,0.806556451



N,0,-2.8653871249,-3.1411244048,-0.5048723397

H,0,-2.8817490113,-2.3010252086,-1.0745478313

H,0,-3.5821027834,-3.8279895937,-0.7019730275

S,0,-1.3733132181,-1.7470573736,1.2845764244

H,0,2.036354128,-0.9833808311,-1.8896584465

H,0,-0.6515232447,-2.1398852575,-0.9581306908

Thermochemistry Data

Zero-point correction= 0.410202 (Hartree/Particle)

Thermal correction to Energy= 0.431788

Thermal correction to Enthalpy= 0.432732

Thermal correction to Gibbs Free Energy= 0.361598

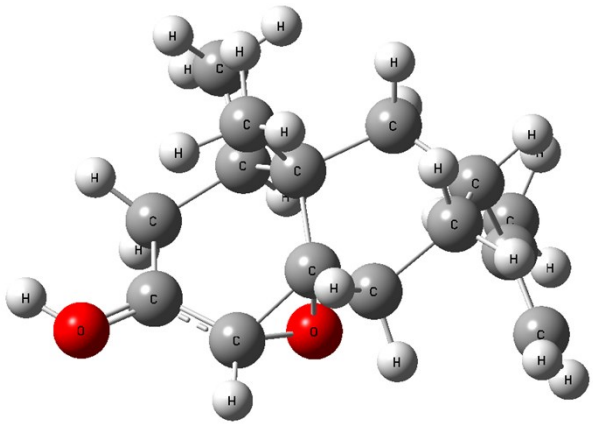
Sum of electronic and zero-point Energies= -1282.722789

Sum of electronic and thermal Energies= -1282.701203

Sum of electronic and thermal Enthalpies= -1282.700259

Sum of electronic and thermal Free Energies= -1282.771393

Cation (EI)



Charge = 1 Multiplicity = 1

Redundant internal coordinates found in file.

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C,0,1.9939878963,-0.6369888119,1.6468330864

C,0,0.8327900314,-1.5559675432,1.2087467481

C,0,-0.1399930963,-0.8196280625,0.3087107923

C,0,-0.4156864433,0.6511877874,0.6065370689

H,0,2.9003039083,-1.2321625173,1.7840796024

H,0,3.0276657804,1.139668979,1.0337666009

H,0,0.9784303783,2.0056089567,1.5644114016

H,0,1.0136183445,2.1114352201,-0.1800413149

H,0,1.1916381899,-2.4228629354,0.6483549592

H,0,0.2963037383,-1.9320520057,2.085108415

H,0,1.7663953143,-0.1938275378,2.6221453851

C,0,-1.2357437454,-1.6943557261,-0.3123627653

H,0,-1.2450203087,-2.762365328,-0.1174655738

C,0,-2.489167064,-1.0052450104,-0.4182196819

C,0,-1.2902560088,1.2451174315,-0.5251685863

H,0,-0.6926923084,1.193056201,-1.4389947558

C,0,-2.5826464728,0.4249362553,-0.7718414323

H,0,-2.837395671,0.4593534257,-1.842074955

H,0,-3.4410280057,0.8523782394,-0.2382091179

C,0,-1.6887808408,2.7030045901,-0.2932771989

H,0,-2.3580989076,2.8042044155,0.5661429698

H,0,-0.8134159976,3.3331822914,-0.1201824231

H,0,-2.2108249289,3.0920575802,-1.171848223

C,0,-1.1132995119,0.7397205793,1.9732626985

H,0,-0.5112096453,0.2682303871,2.7546657194

H,0,-1.2572100391,1.7841084487,2.2588604012

H,0,-2.0948670504,0.2494762485,1.9725316554

O,0,-3.5190085617,-1.7005856878,-0.0984642525

O,0,-0.1509067072,-1.1667537674,-1.0517001153

C,0,2.6752091441,0.0531585788,-0.7310885768

C,0,3.1927787026,-1.1559139112,-0.9694072565

H,0,3.2677752521,-1.9272037827,-0.2102310886

C,0,2.6063492487,1.0805251563,-1.8332438978

H,0,3.1726621915,0.7511913649,-2.706456593

H,0,1.5712710143,1.2532728859,-2.151411926

H,0,3.0064385772,2.0461146443,-1.5027560675

H,0,3.5699937781,-1.4102840934,-1.955744437

H,0,-4.3557186556,-1.1985945616,-0.0924009111

Thermochemistry Data

Zero-point correction= 0.358365 (Hartree/Particle)

Thermal correction to Energy= 0.374666

Thermal correction to Enthalpy= 0.375610

Thermal correction to Gibbs Free Energy= 0.316034

Sum of electronic and zero-point Energies= -735.006590

Sum of electronic and thermal Energies= -734.990289

Sum of electronic and thermal Enthalpies= -734.989345

Sum of electronic and thermal Free Energies= -735.048921