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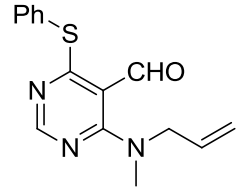
SUPPORTING INFORMATION

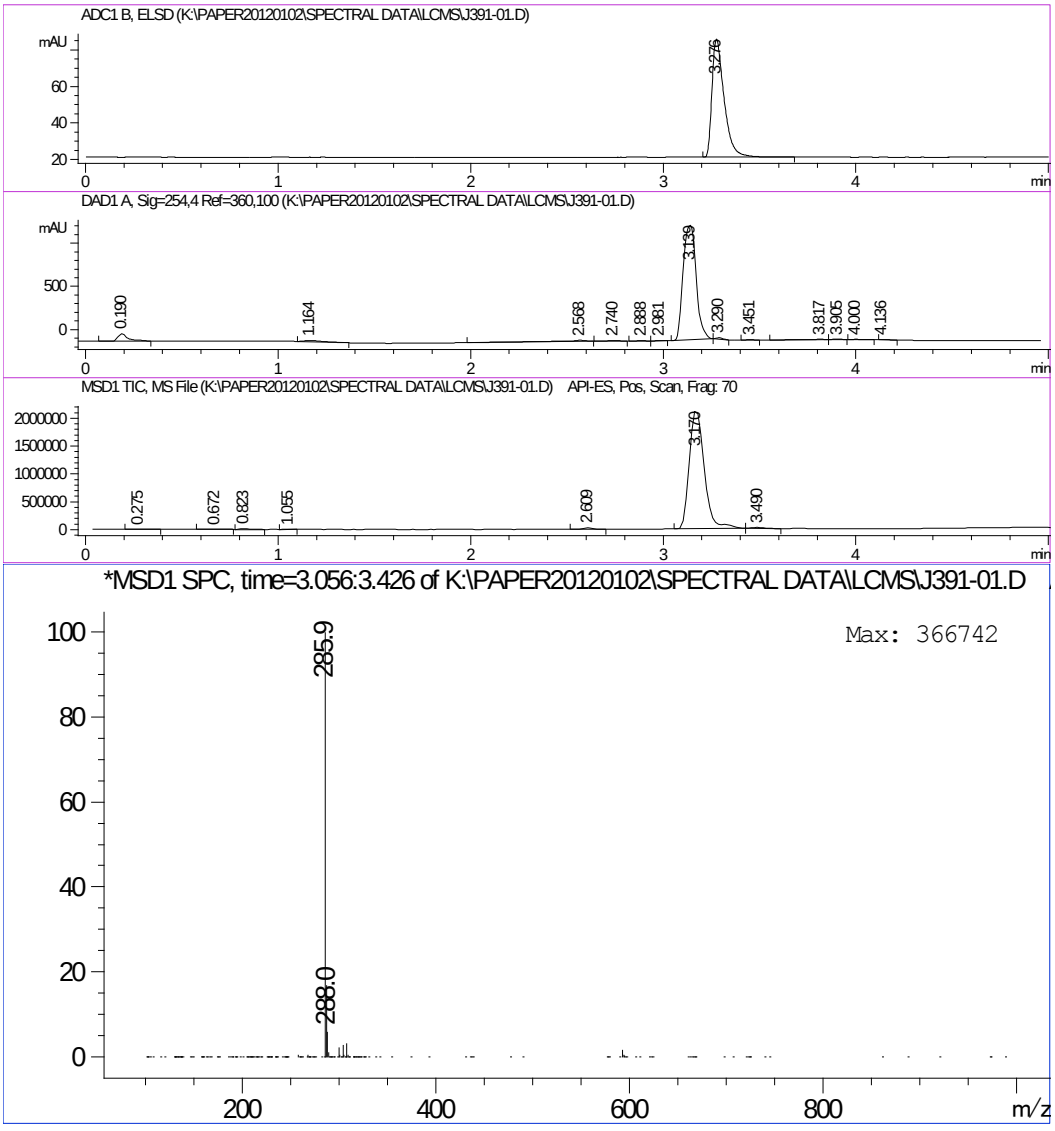
DOI: 10.1002/ejoc.201301318
Title: On-Demand Selection of the Reaction Path from Imino Diels–Alder to Ene-Type Cyclization: Synthesis of Epiminopyrimido[4,5-*b*]azepines
Author(s): Yuewei Zhang, Yue Zhu, Lianyou Zheng, Lian-Gang Zhuo, Fengzhi Yang, Qun Dang, Zhi-Xiang Yu,* Xu Bai*

1. LC-MS-ELSD Spectra and NMR Spectra for Compounds

LC-MS-ELSD spectra of Compound **1a**

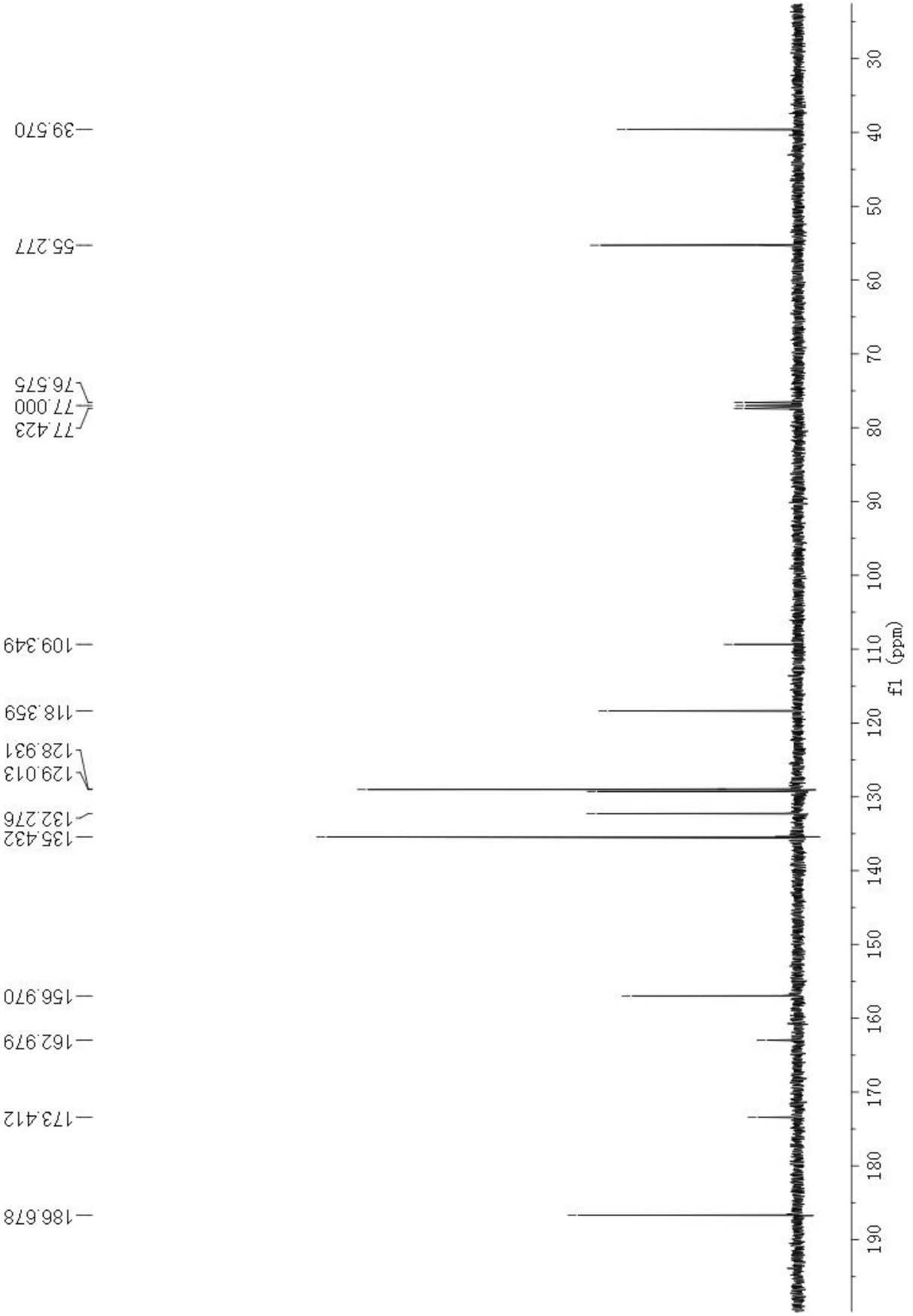


$C_{15}H_{15}N_3OS$
Exact Mass: 285.09
Mol. Wt.: 285.36

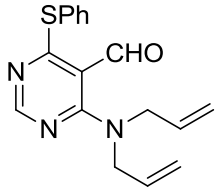


^{1}H NMR spectrum of Compound **1a**

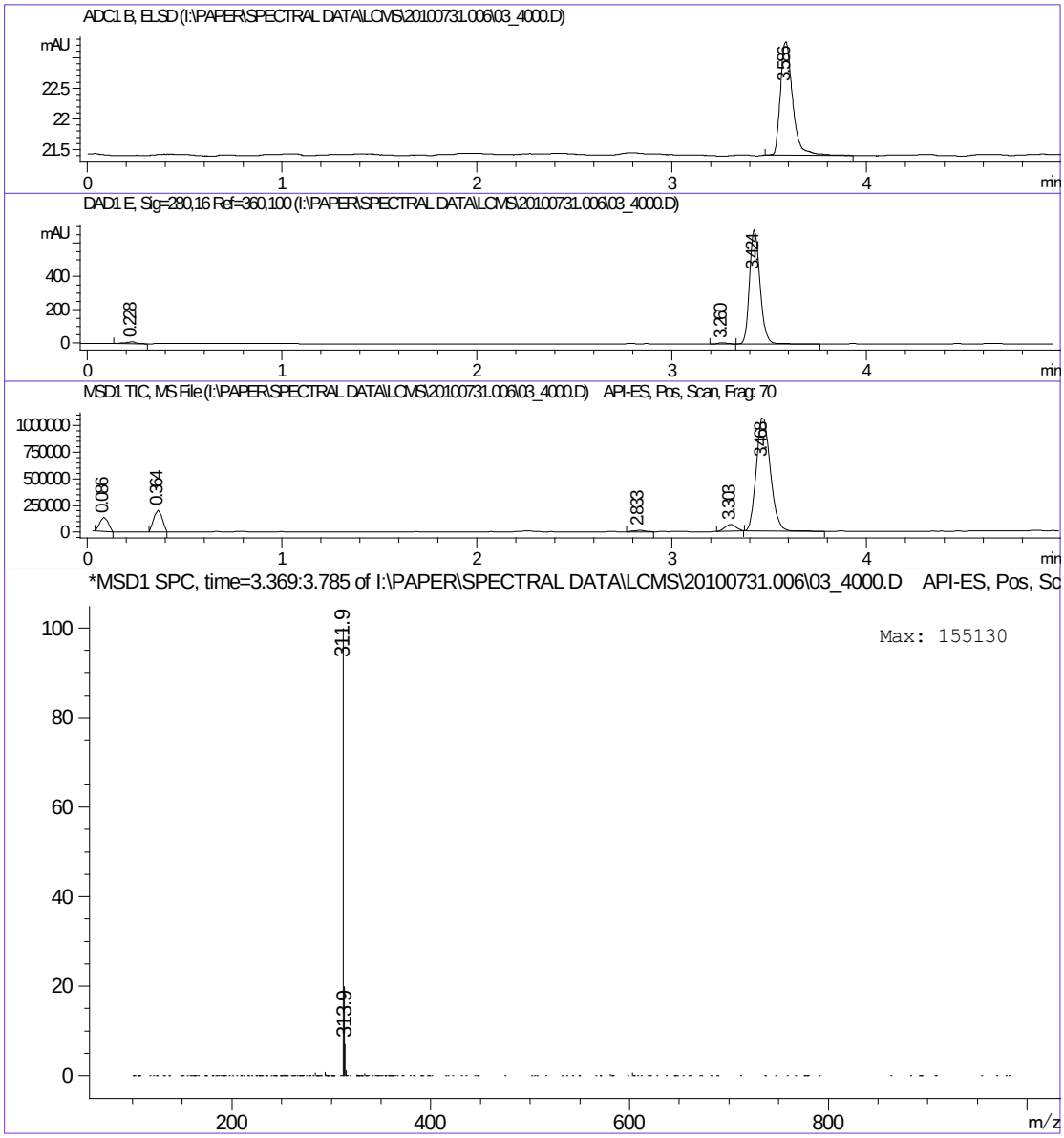
^{13}C NMR spectrum of Compound **1a**



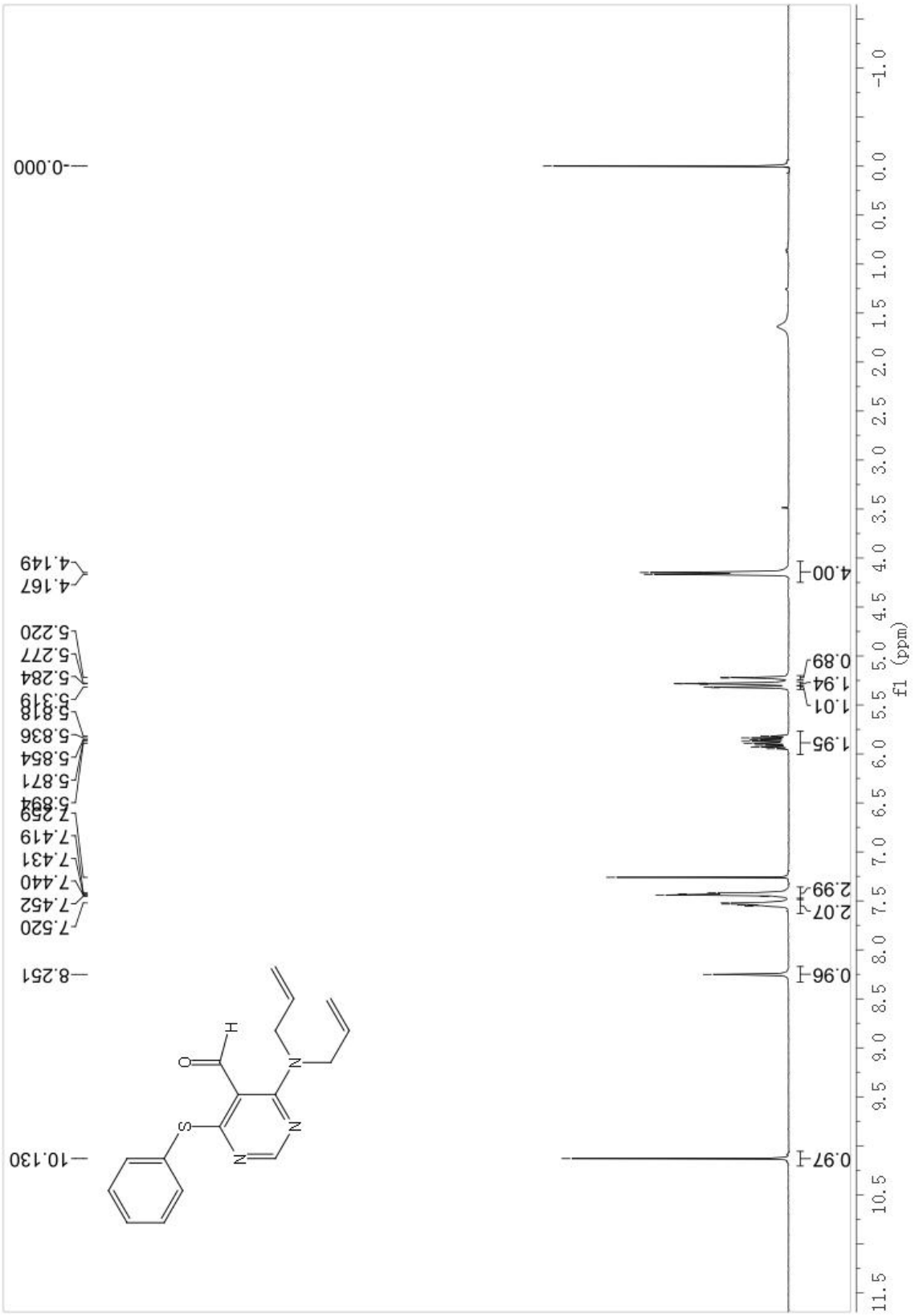
LC-MS-ELSD spectra of Compound **1b**



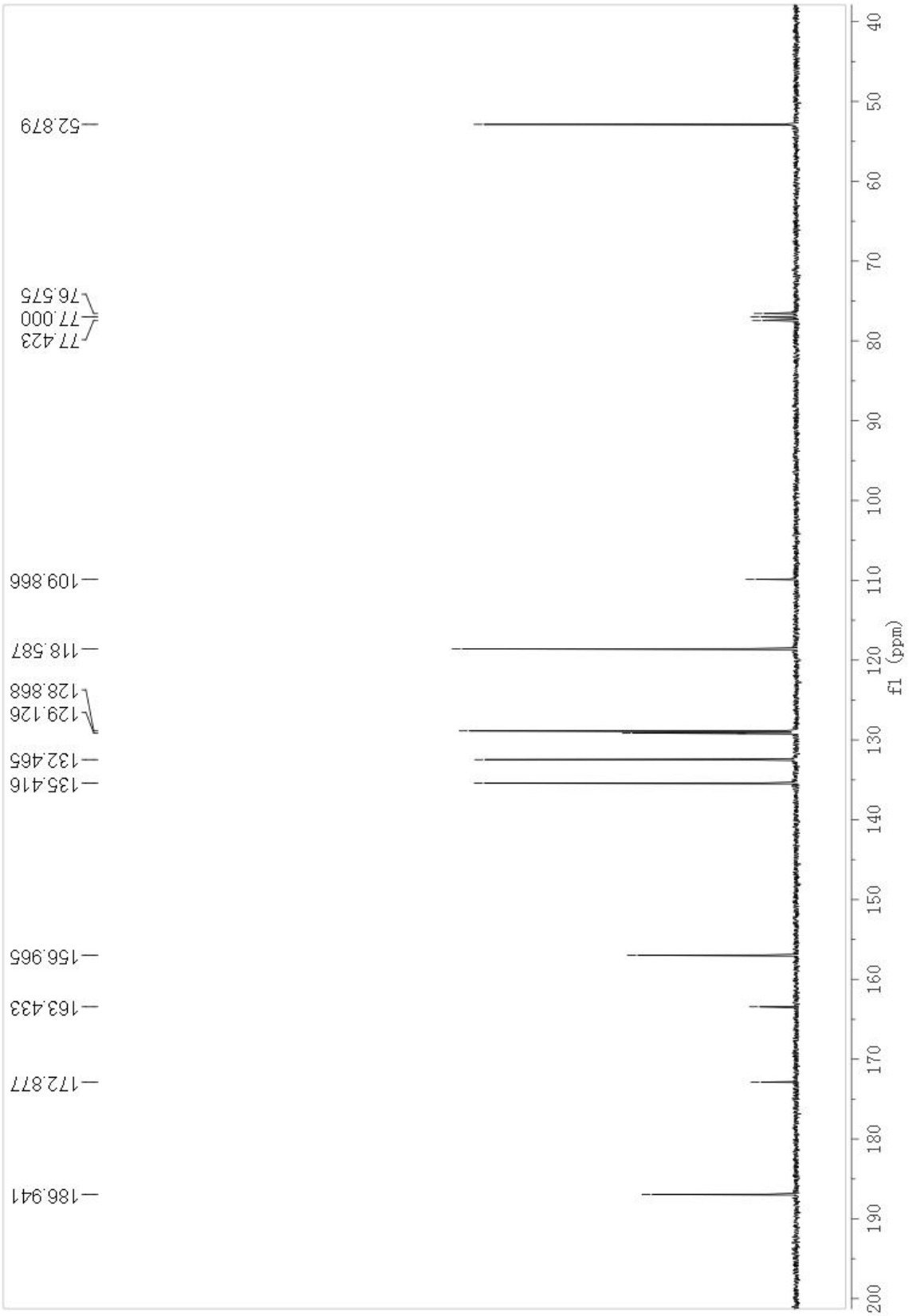
$C_{17}H_{17}N_3OS$
Exact Mass: 311.1
Mol. Wt.: 311.4



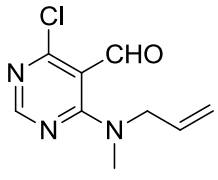
^{1}H NMR spectrum of Compound **1b**



^{13}C NMR spectrum of Compound **1b**



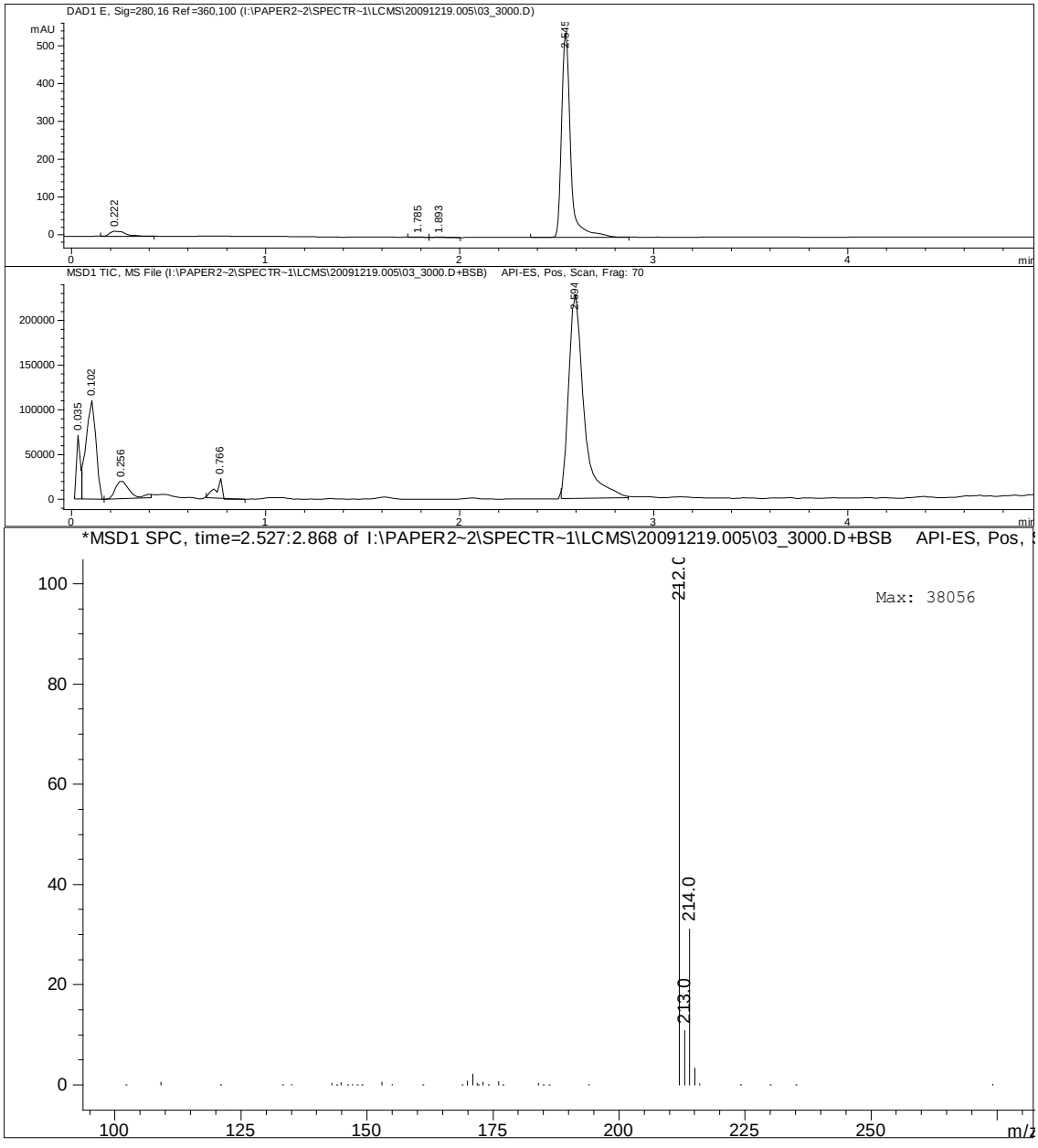
LC-MS-ELSD spectra of Compound **1c**



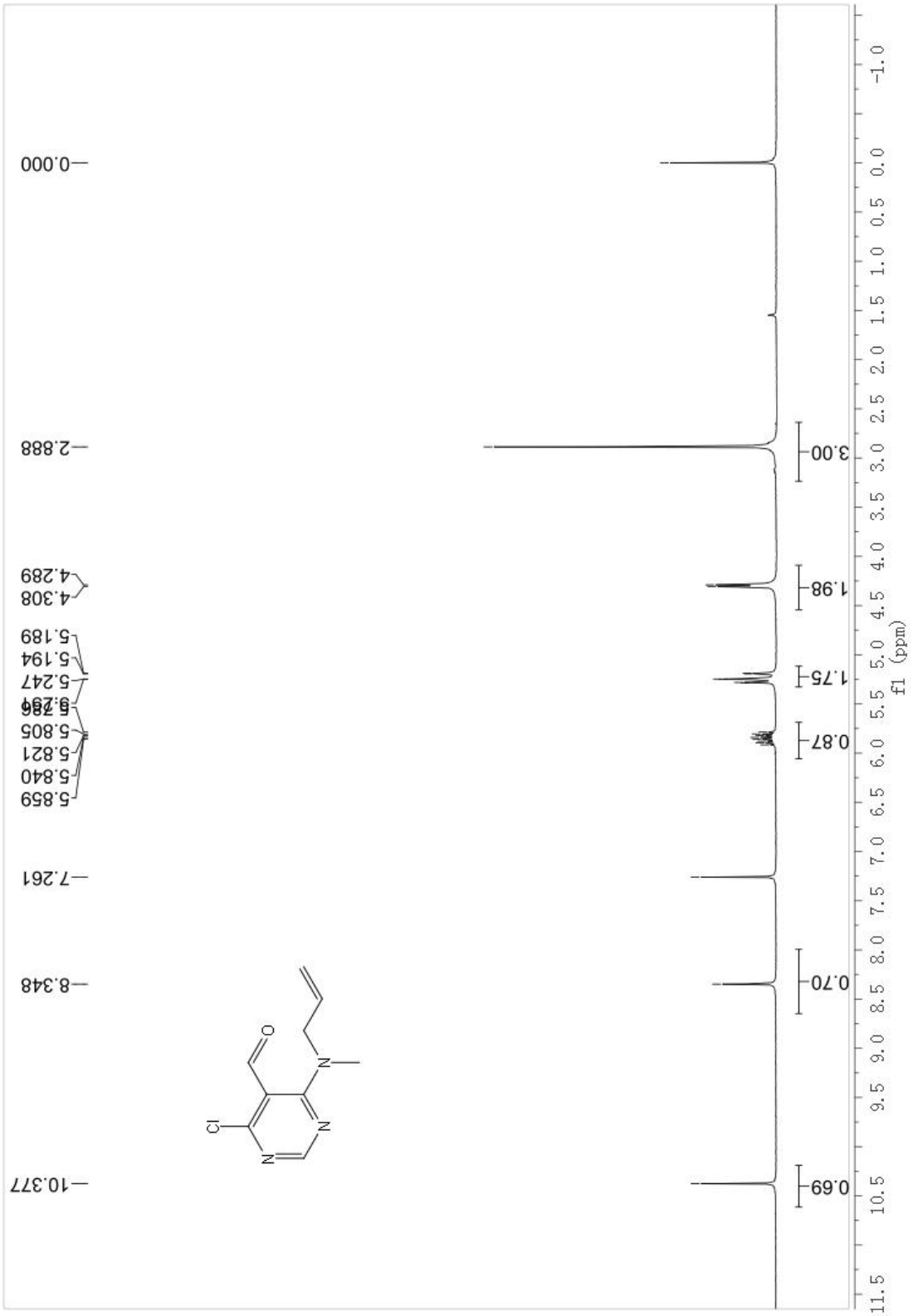
$C_9H_{10}ClN_3O$

Exact Mass: 211.1

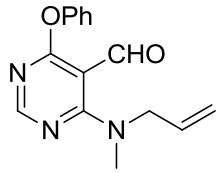
Mol. Wt.: 211.6



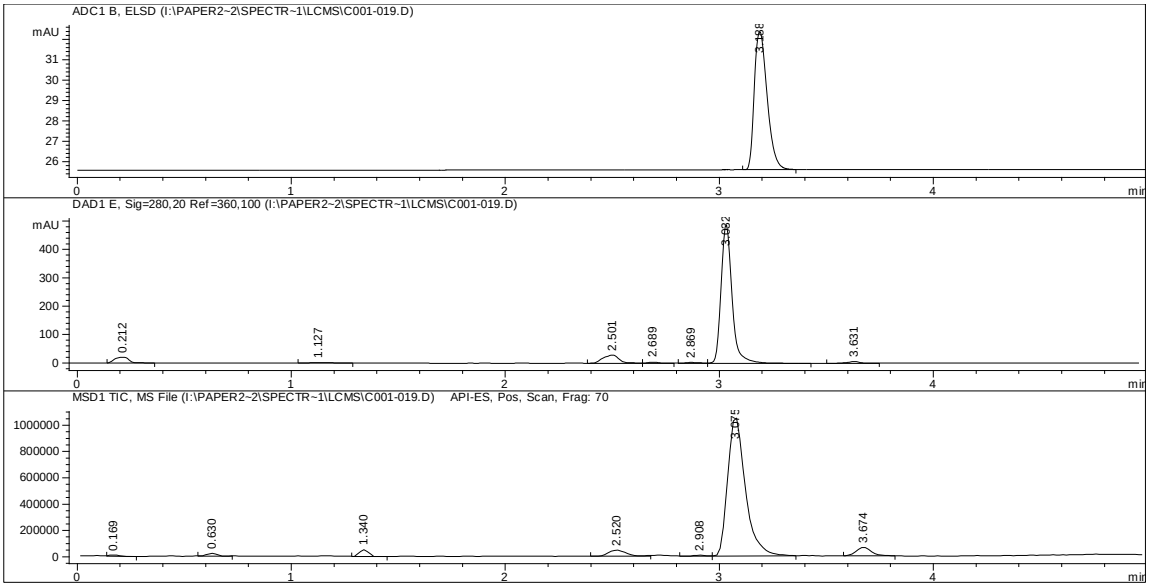
^{1}H NMR spectrum of Compound **1c**

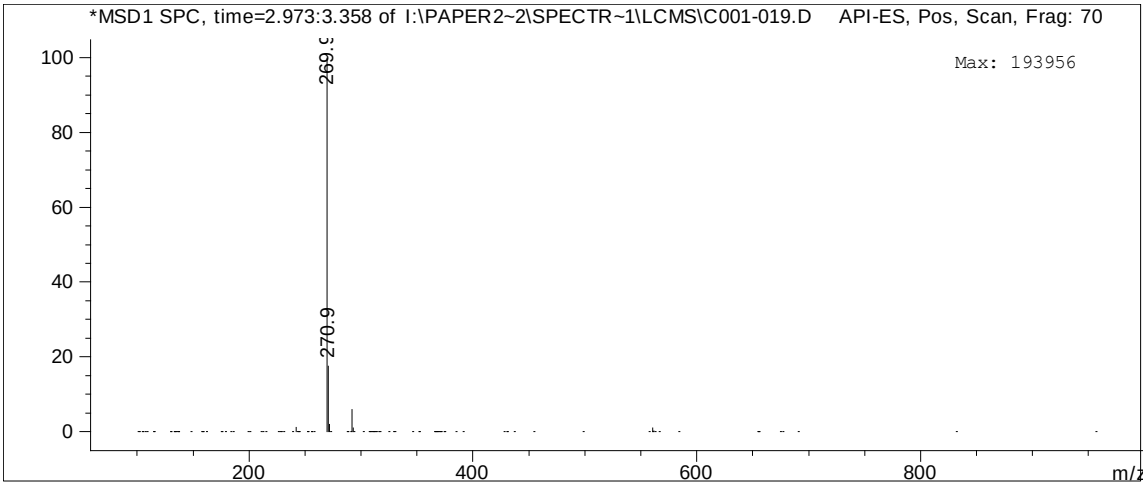


LC-MS-ELSD spectra of Compound **1d**

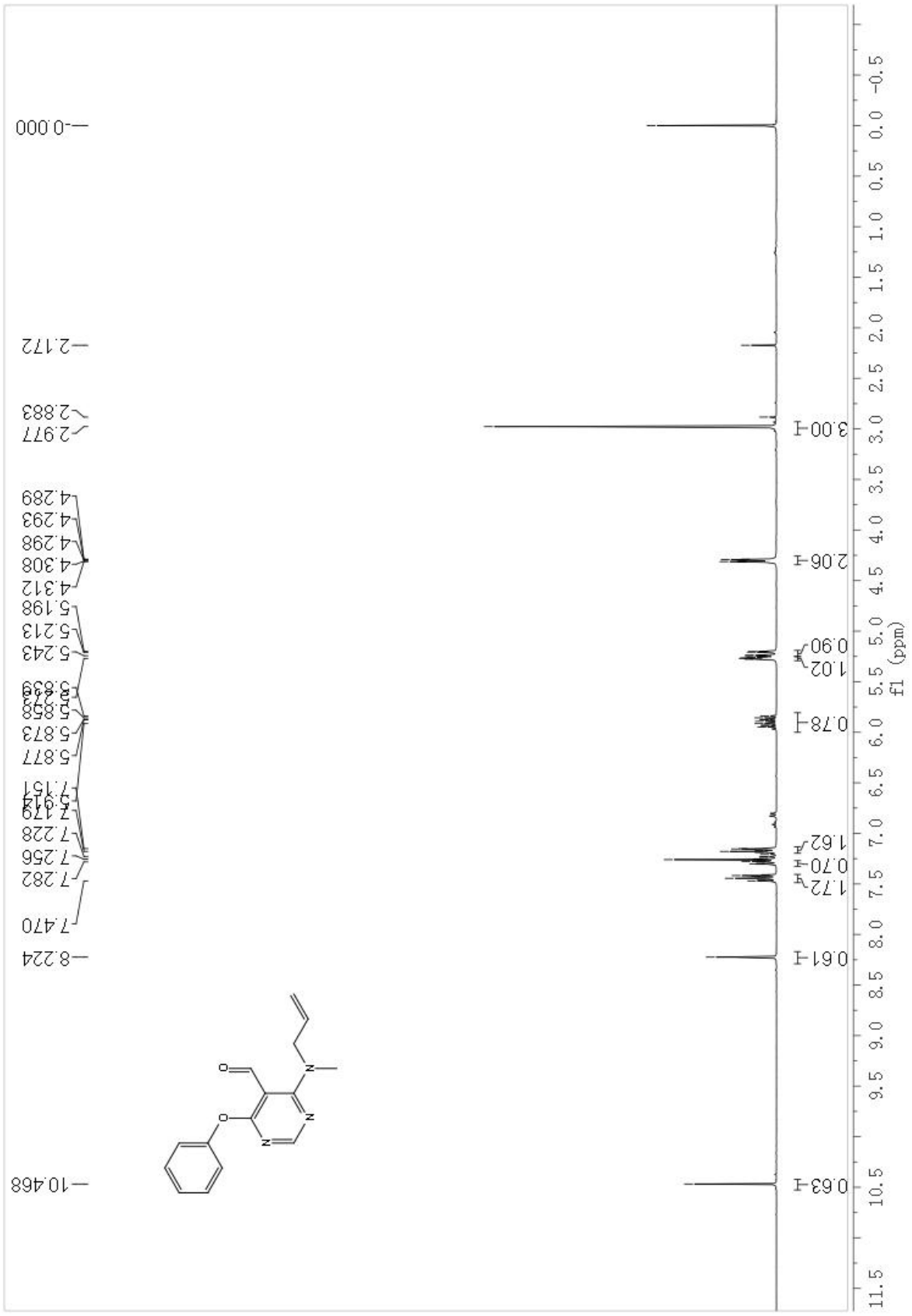


$C_{15}H_{15}N_3O_2$
Exact Mass: 269.1
Mol. Wt.: 269.3

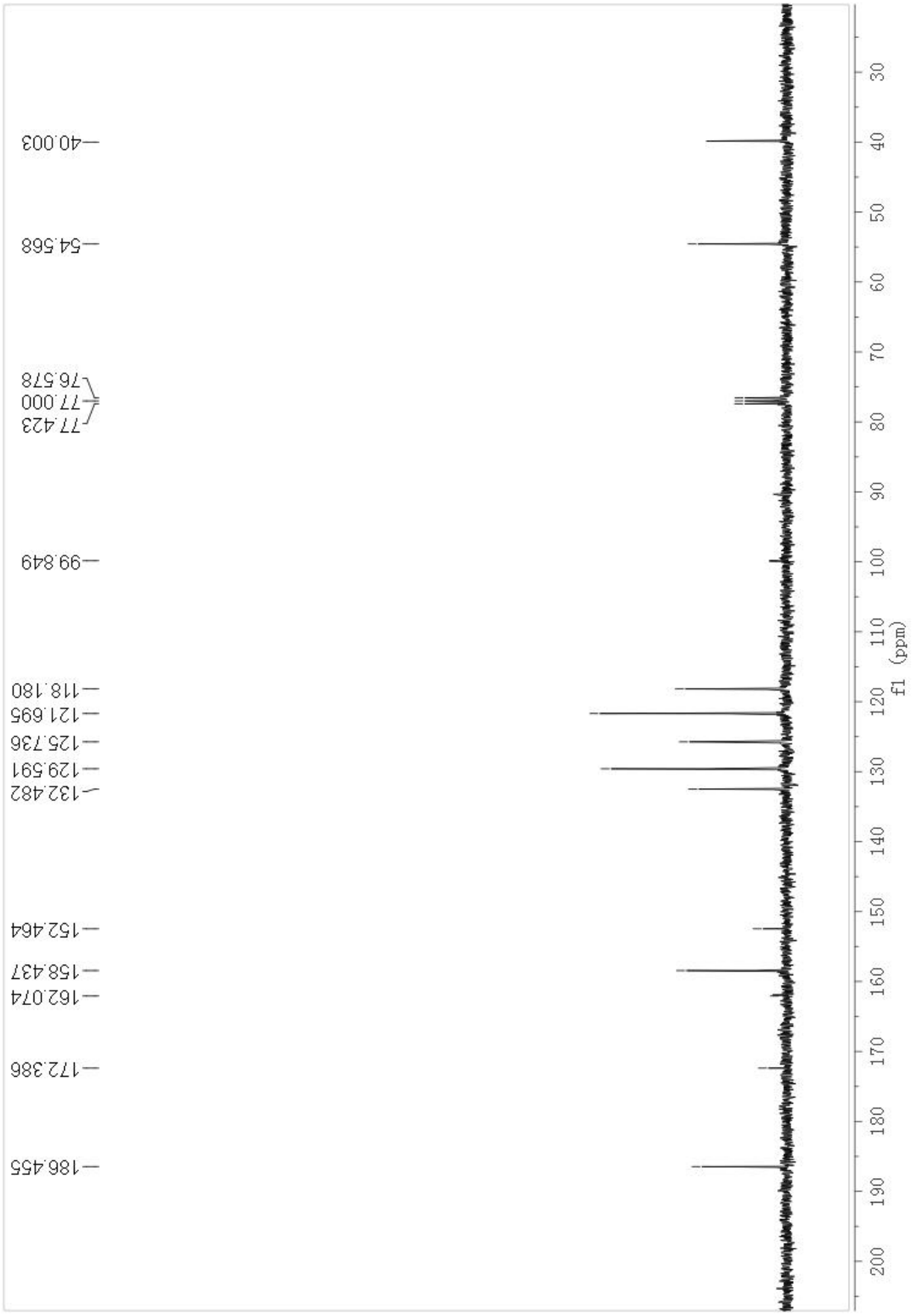




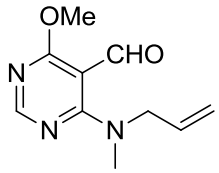
^{1}H NMR spectrum of Compound **1d**



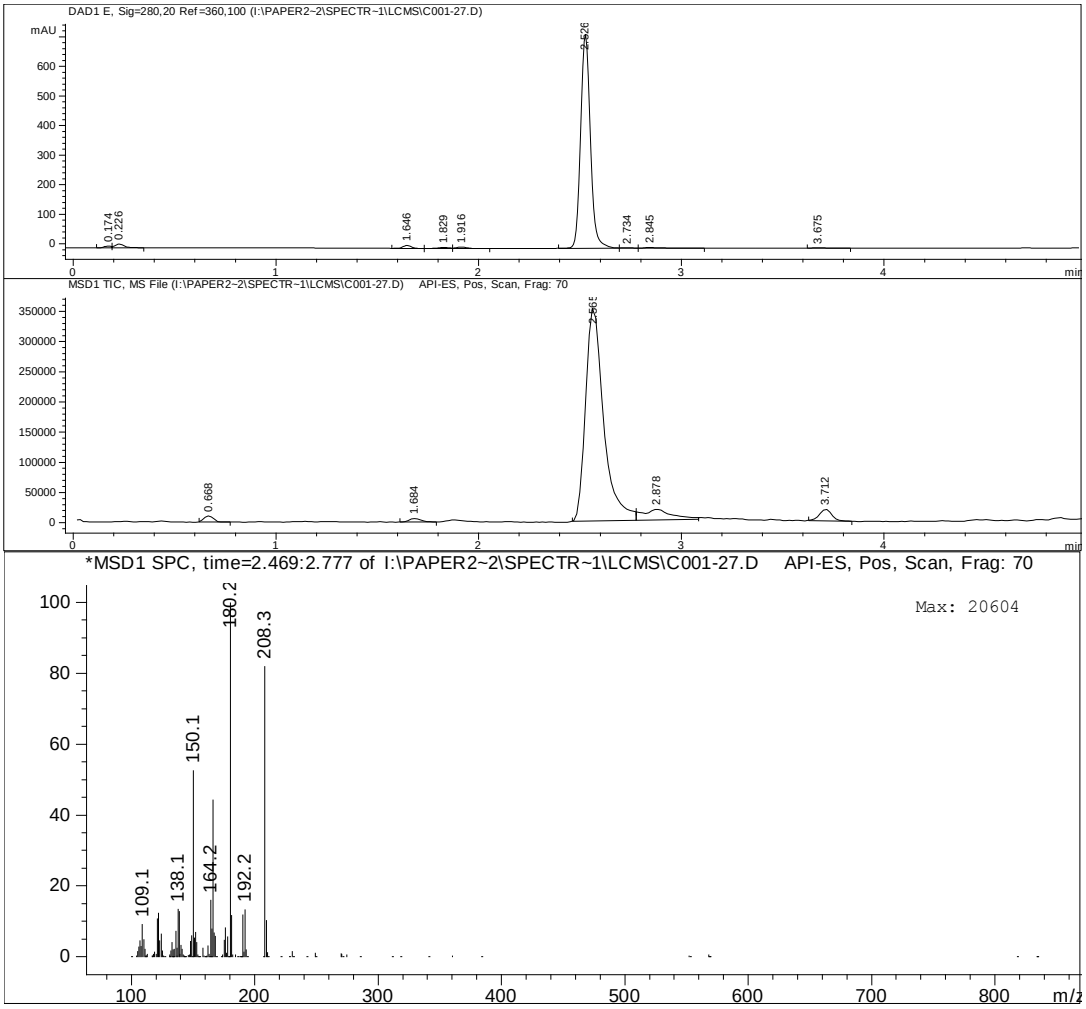
^{13}C NMR spectrum of Compound **1d**



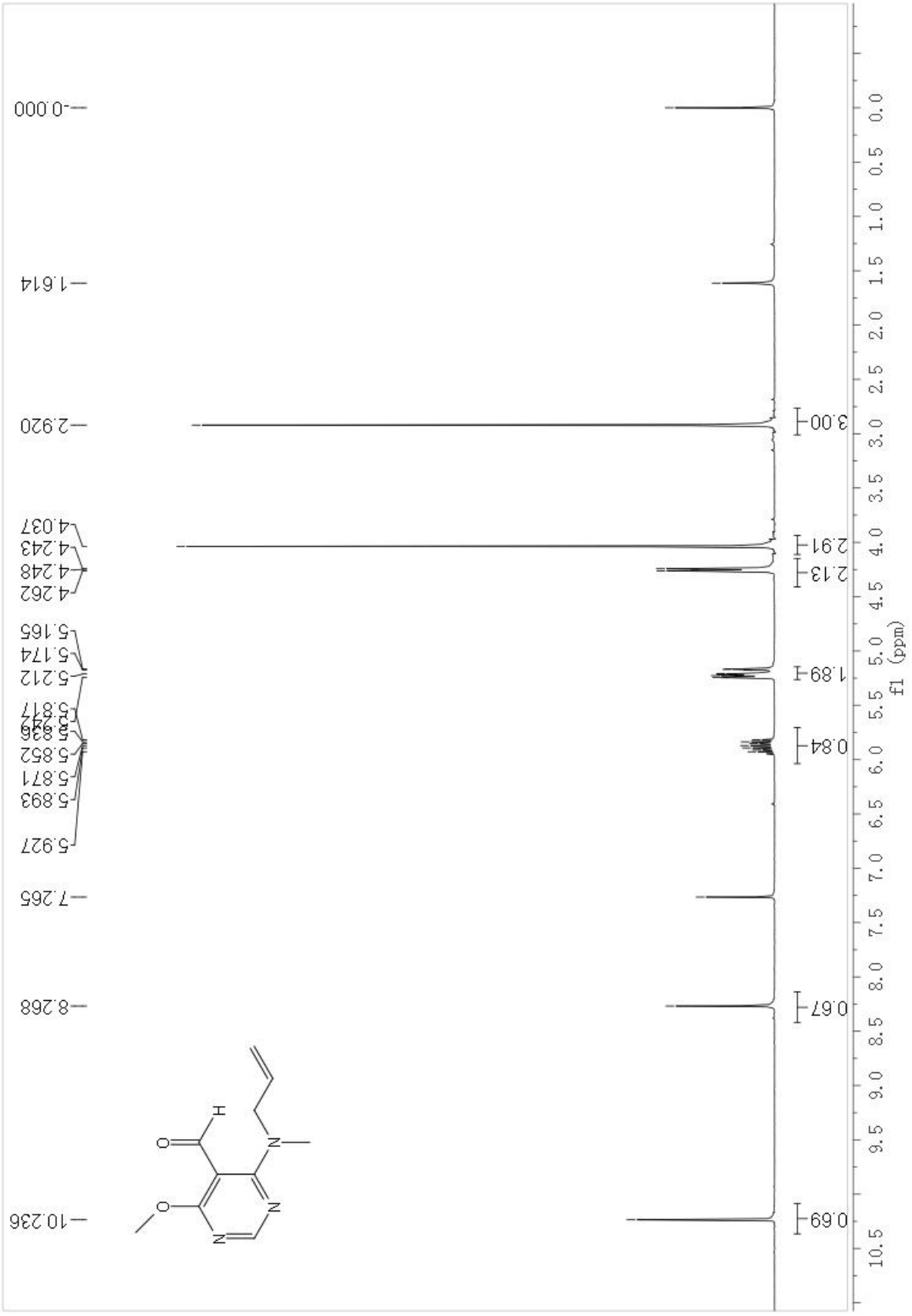
LC-MS-ELSD spectra of Compound **1e**



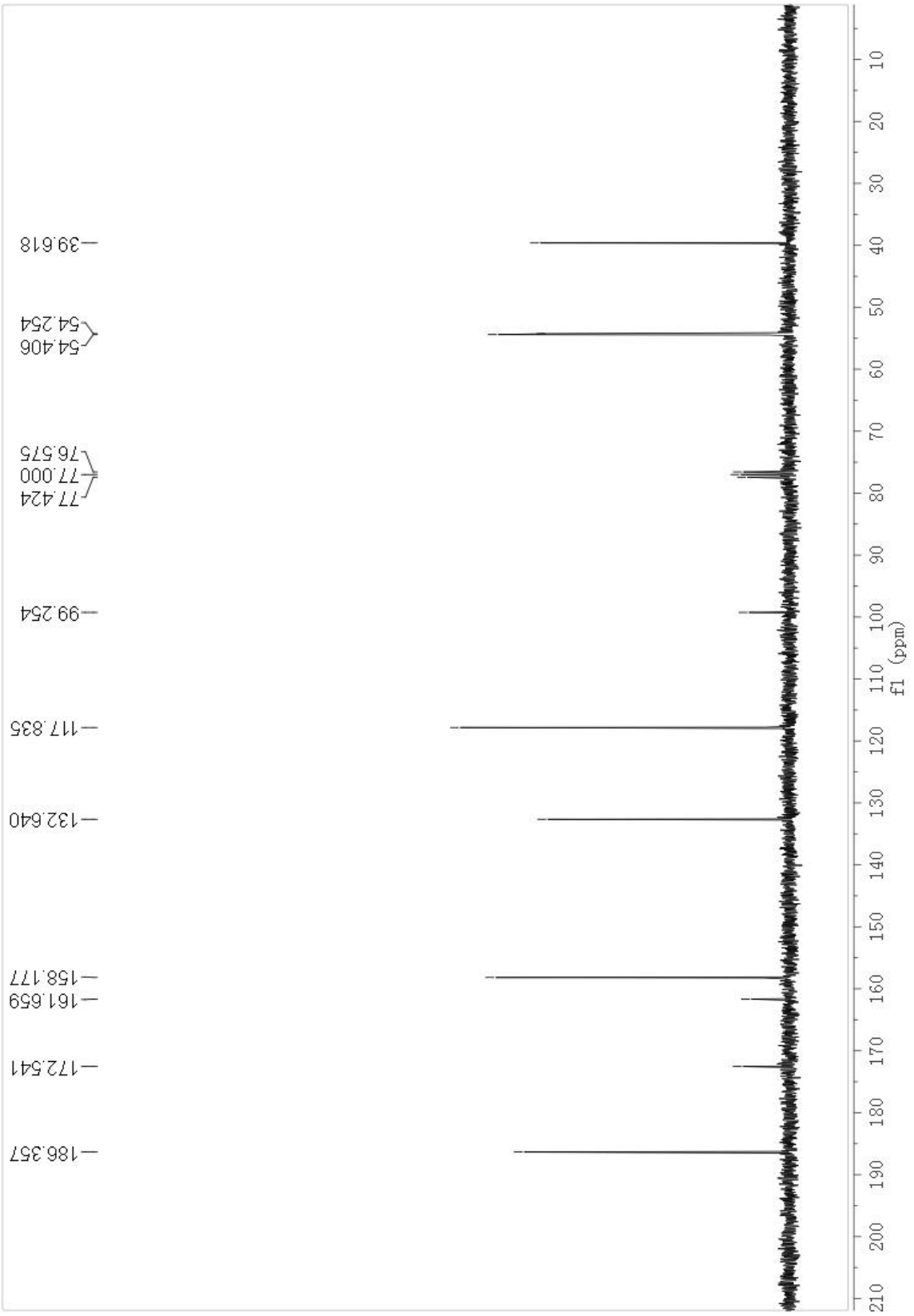
$C_{10}H_{13}N_3O_2$
Exact Mass: 207.1
Mol. Wt.: 207.2



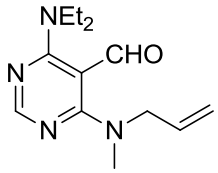
^{1}H NMR spectrum of Compound **1e**



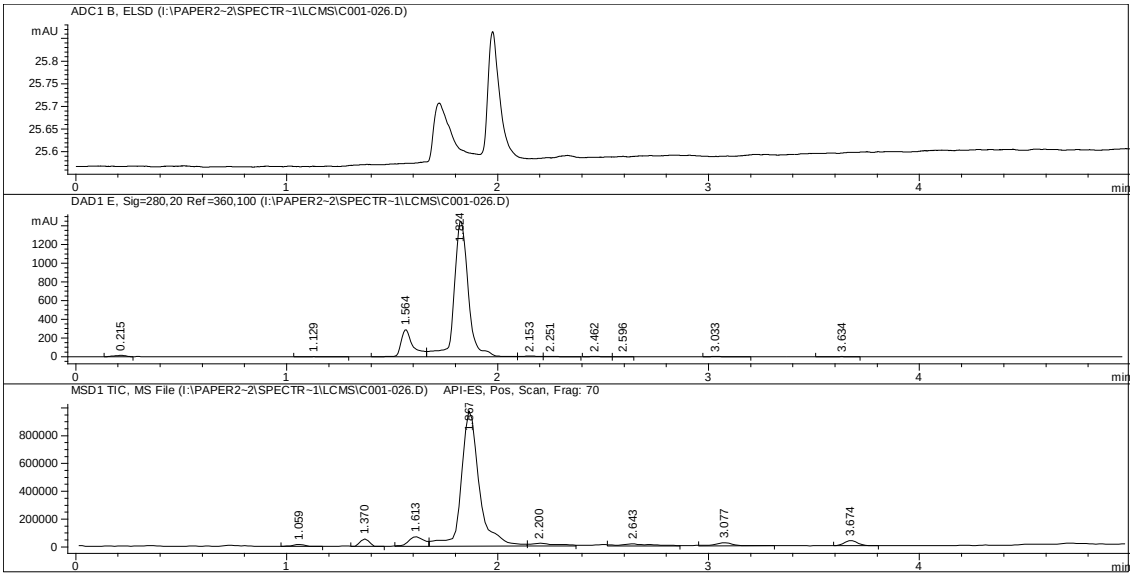
^{13}C NMR spectrum of Compound **1e**

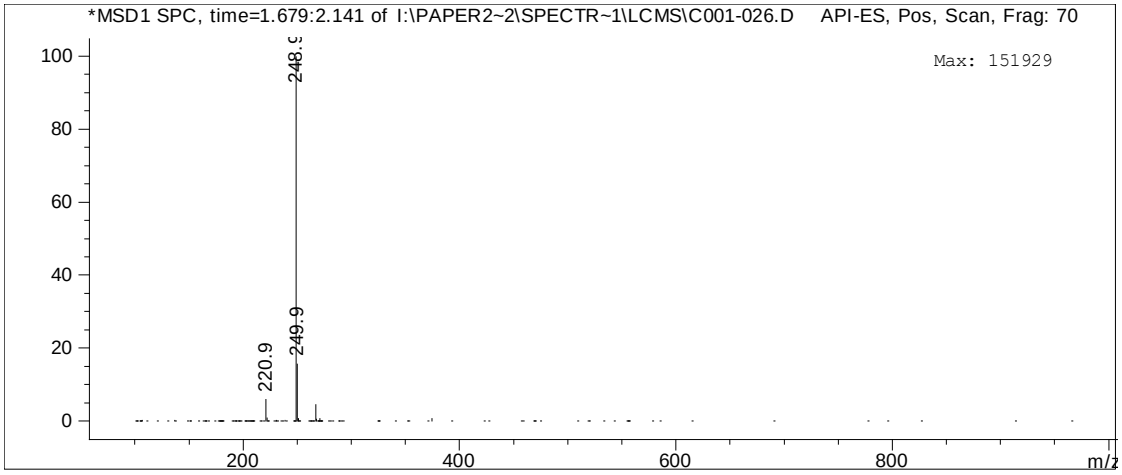


LC-MS-ELSD spectra of Compound **1f**

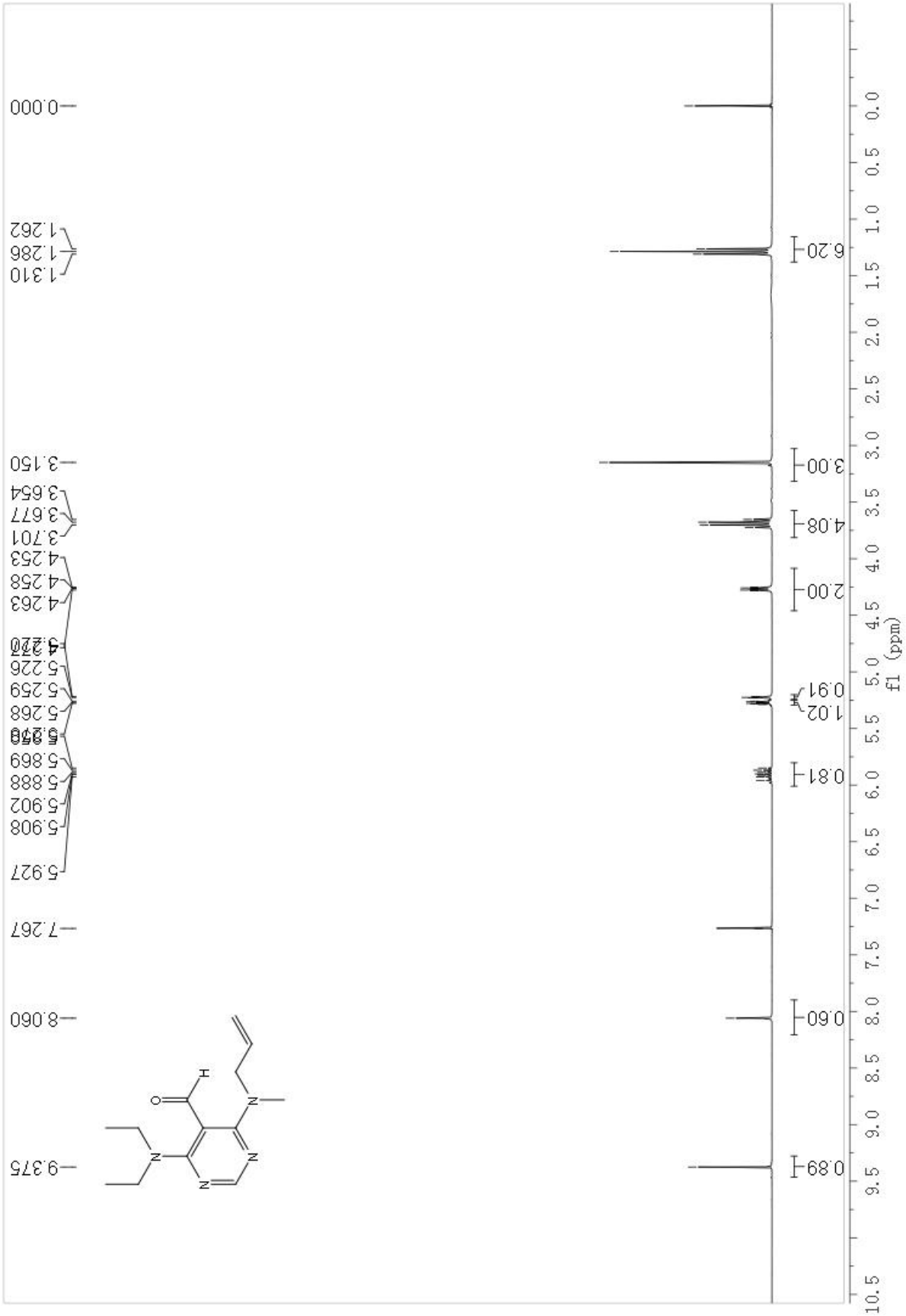


$C_{13}H_{20}N_4O$
Exact Mass: 248.2
Mol. Wt.: 248.3

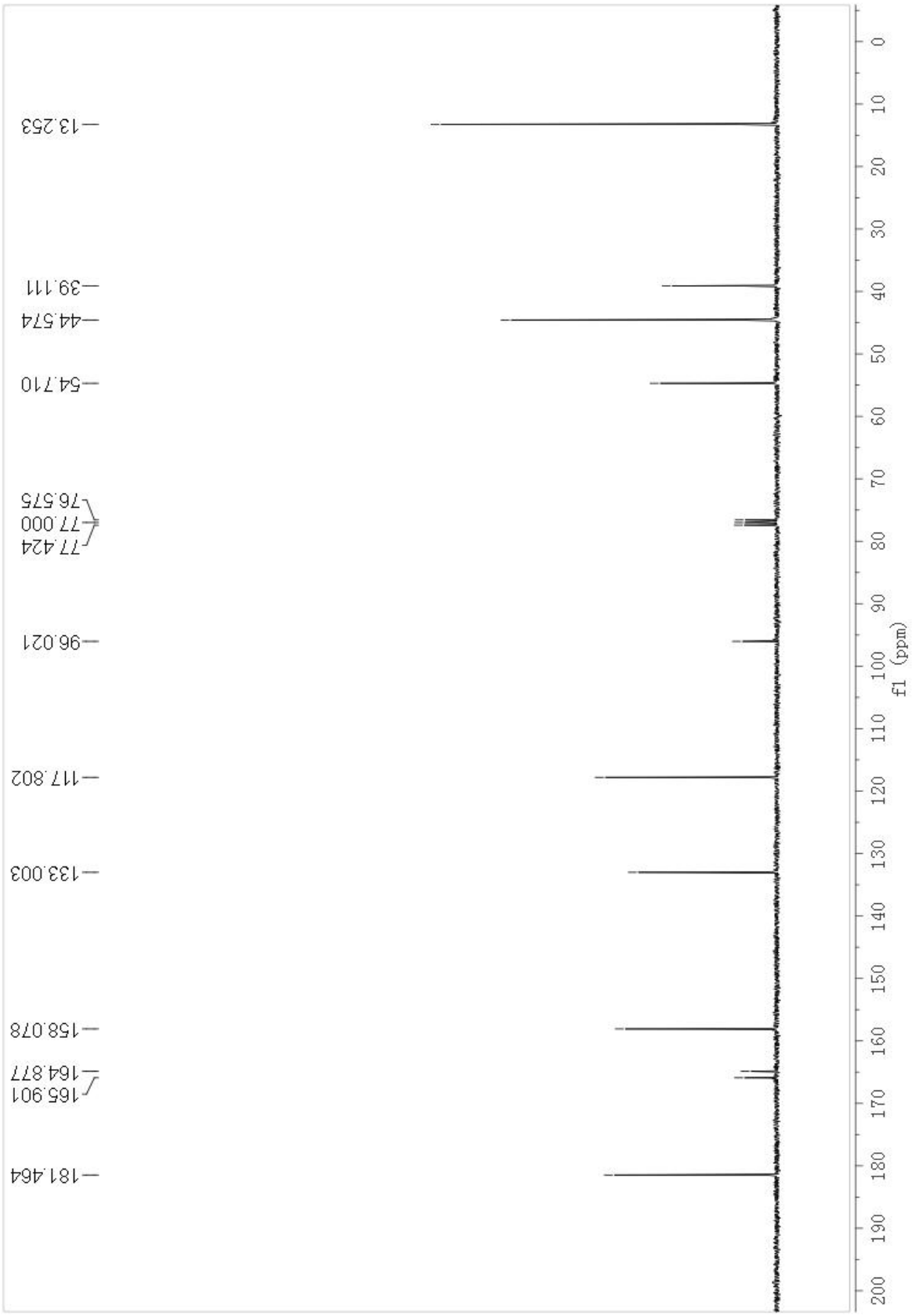




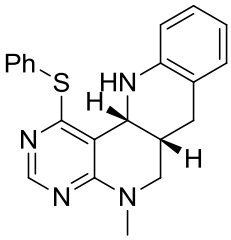
^{1}H NMR spectrum of Compound **1f**



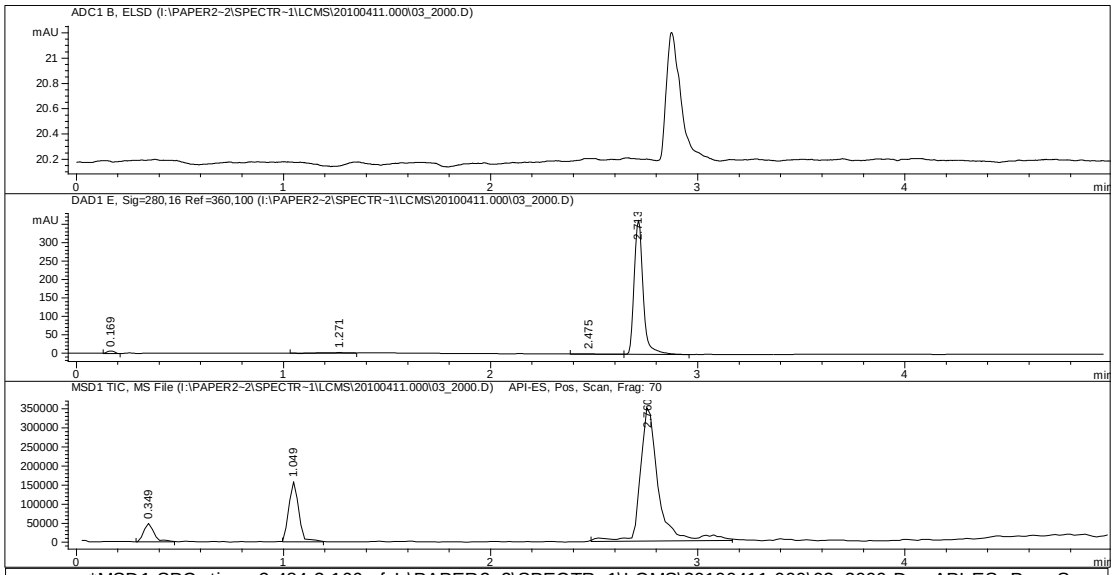
^{13}C NMR spectrum of Compound **1f**

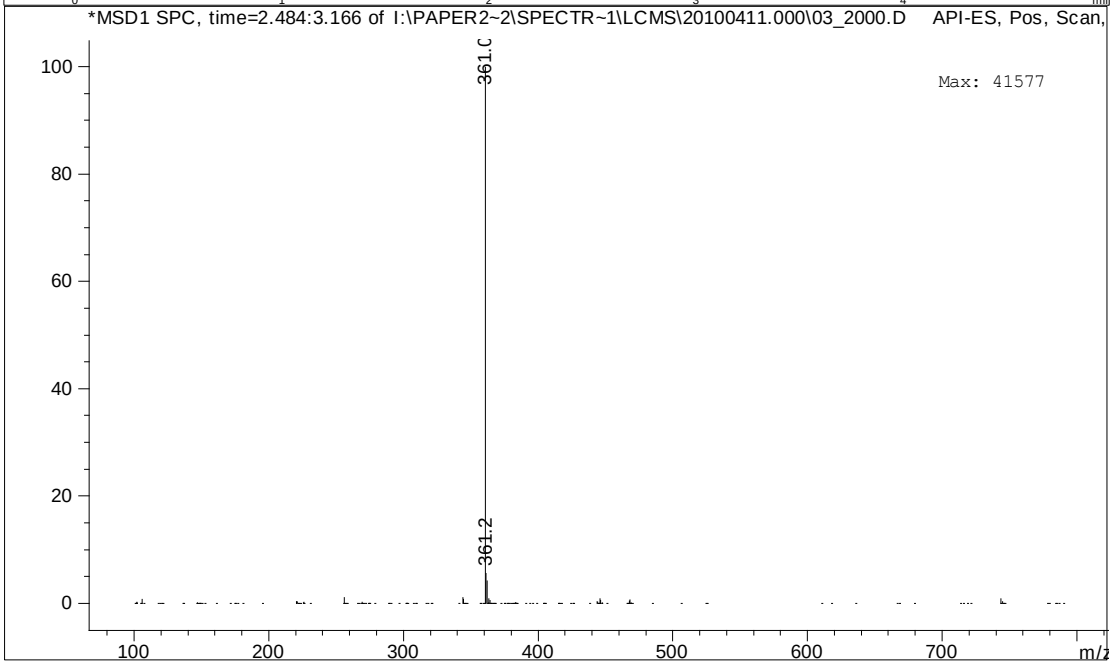


LC-MS-ELSD spectra of Compound **2a**

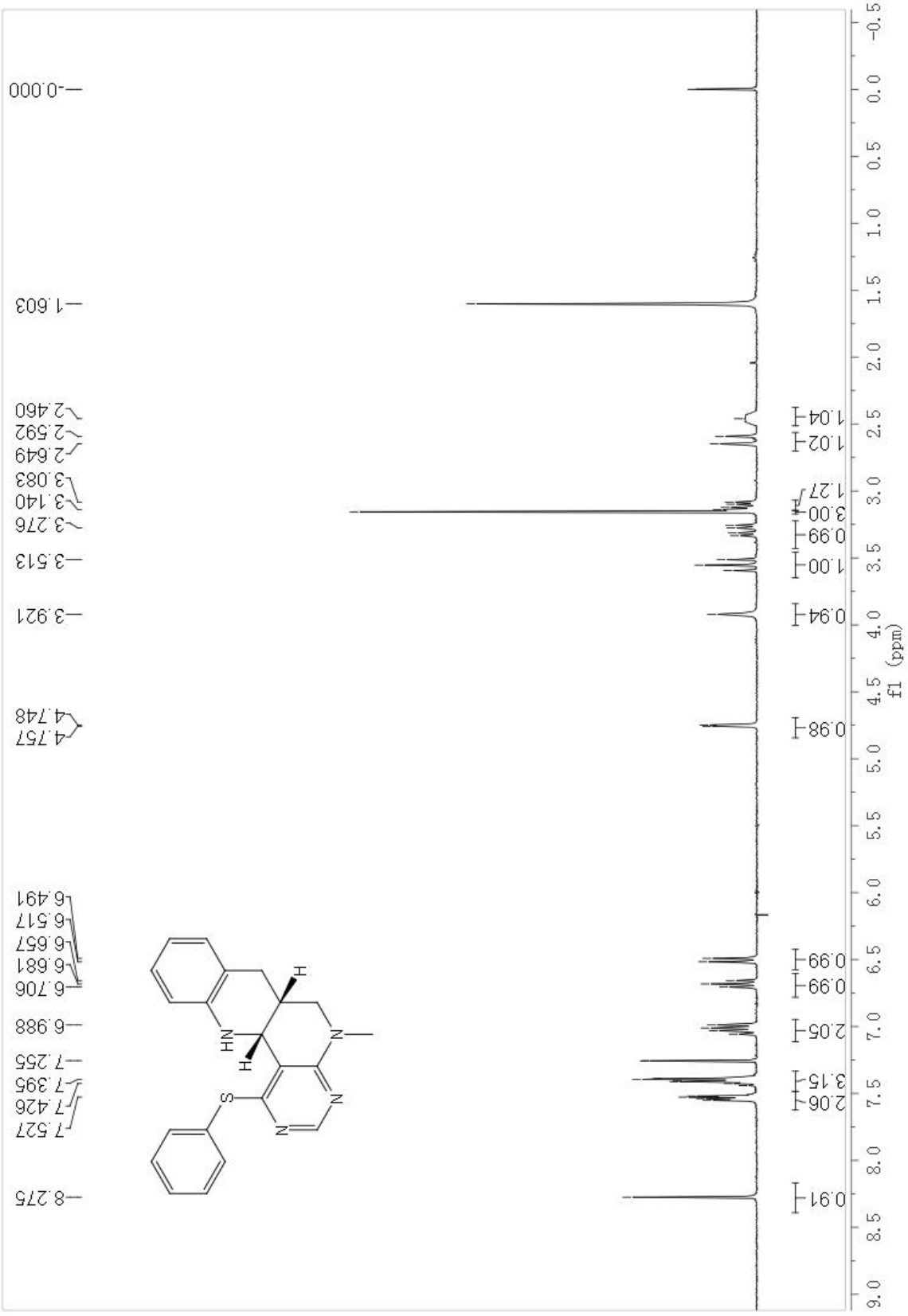


$C_{21}H_{20}N_4S$
Exact Mass: 360.14
Mol. Wt: 360.48

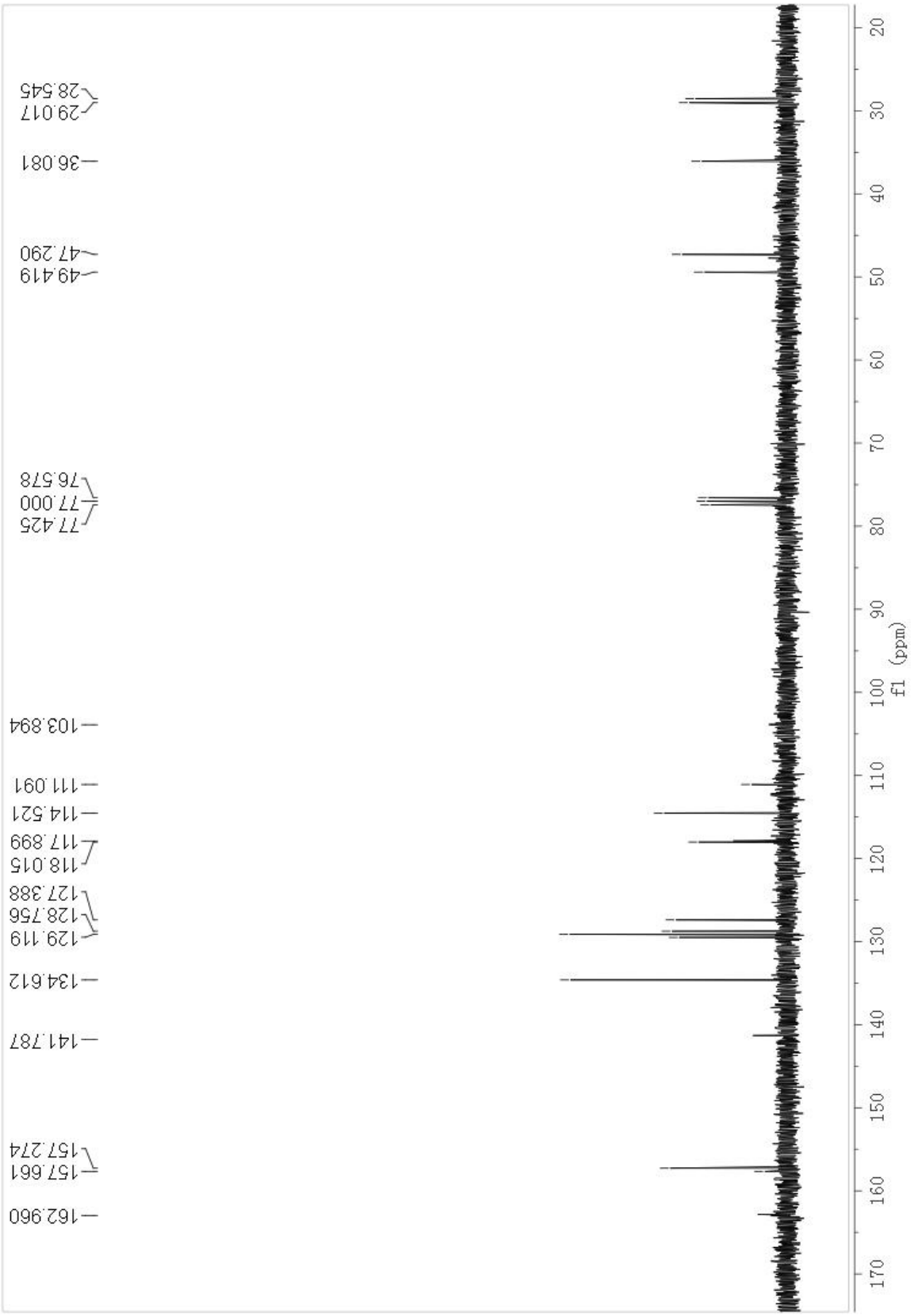




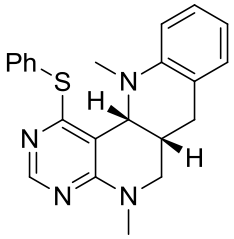
^{1}H NMR spectrum of Compound **2a**



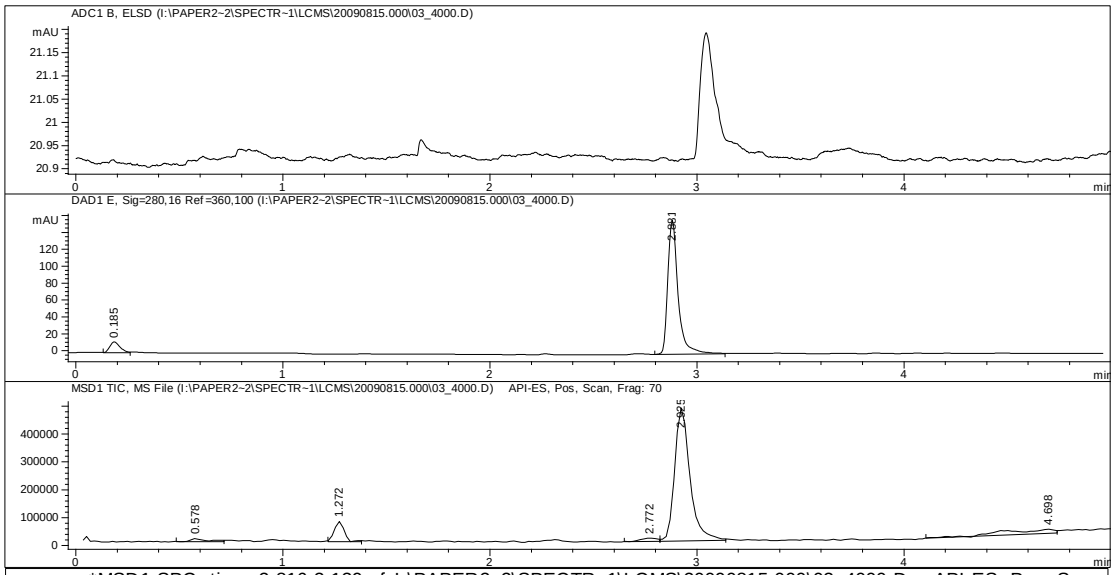
^{13}C NMR spectrum of Compound **2a**

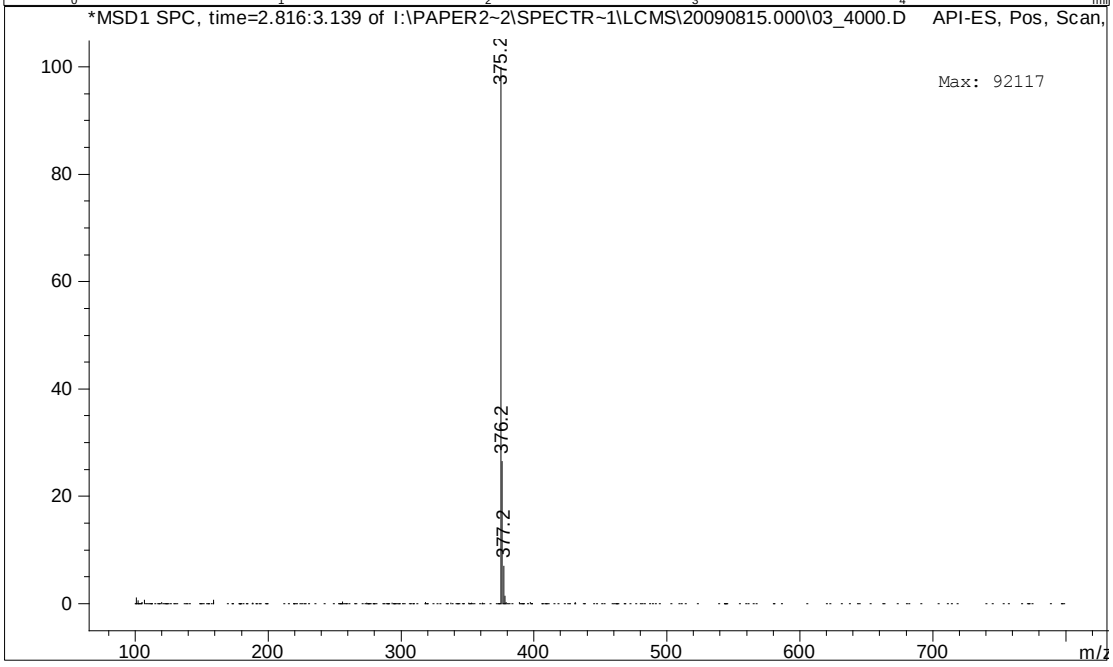


LC-MS-ELSD spectra of Compound **2b**

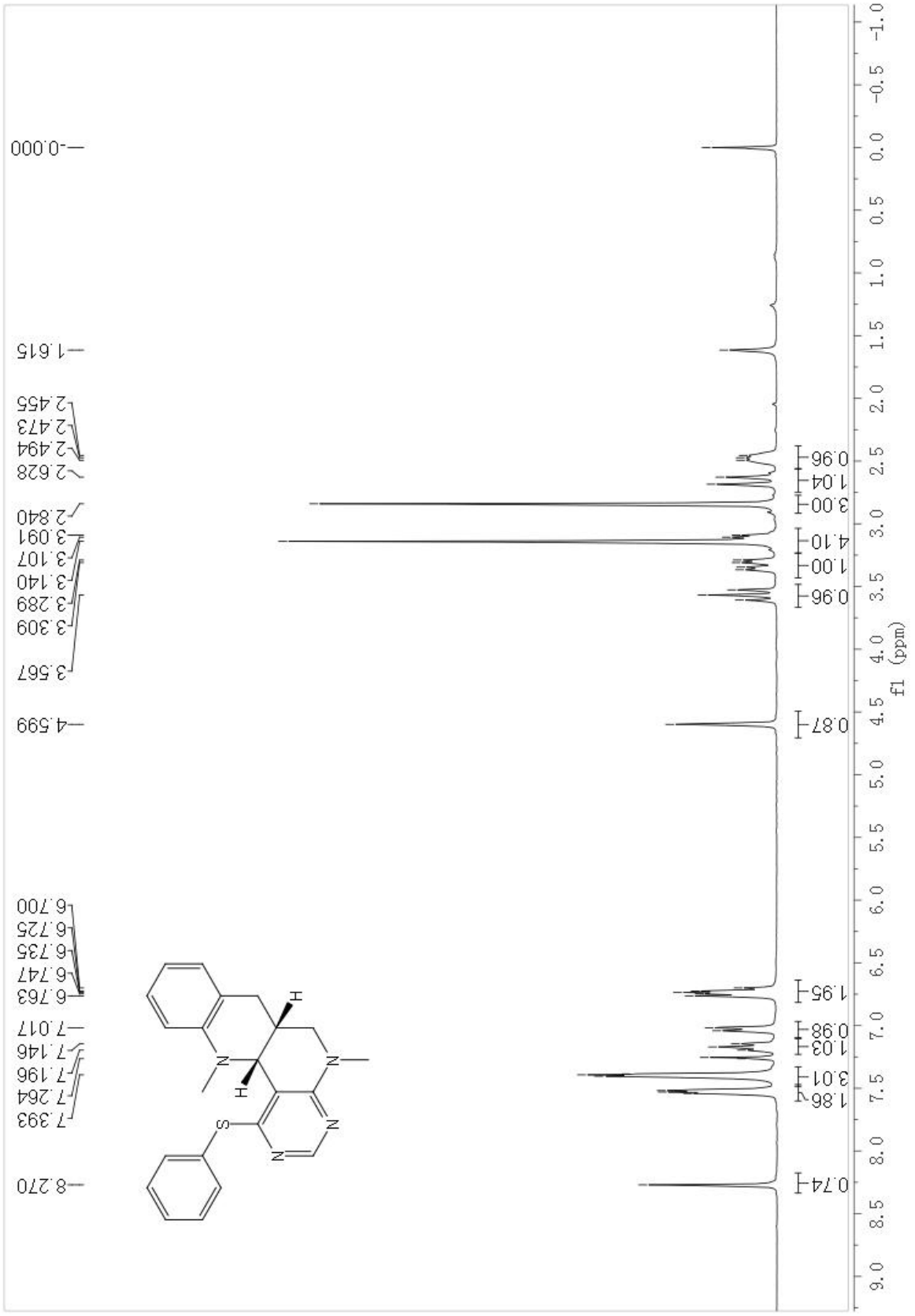


$C_{22}H_{22}N_4S$
Exact Mass: 374.16
Mol. Wt: 374.50

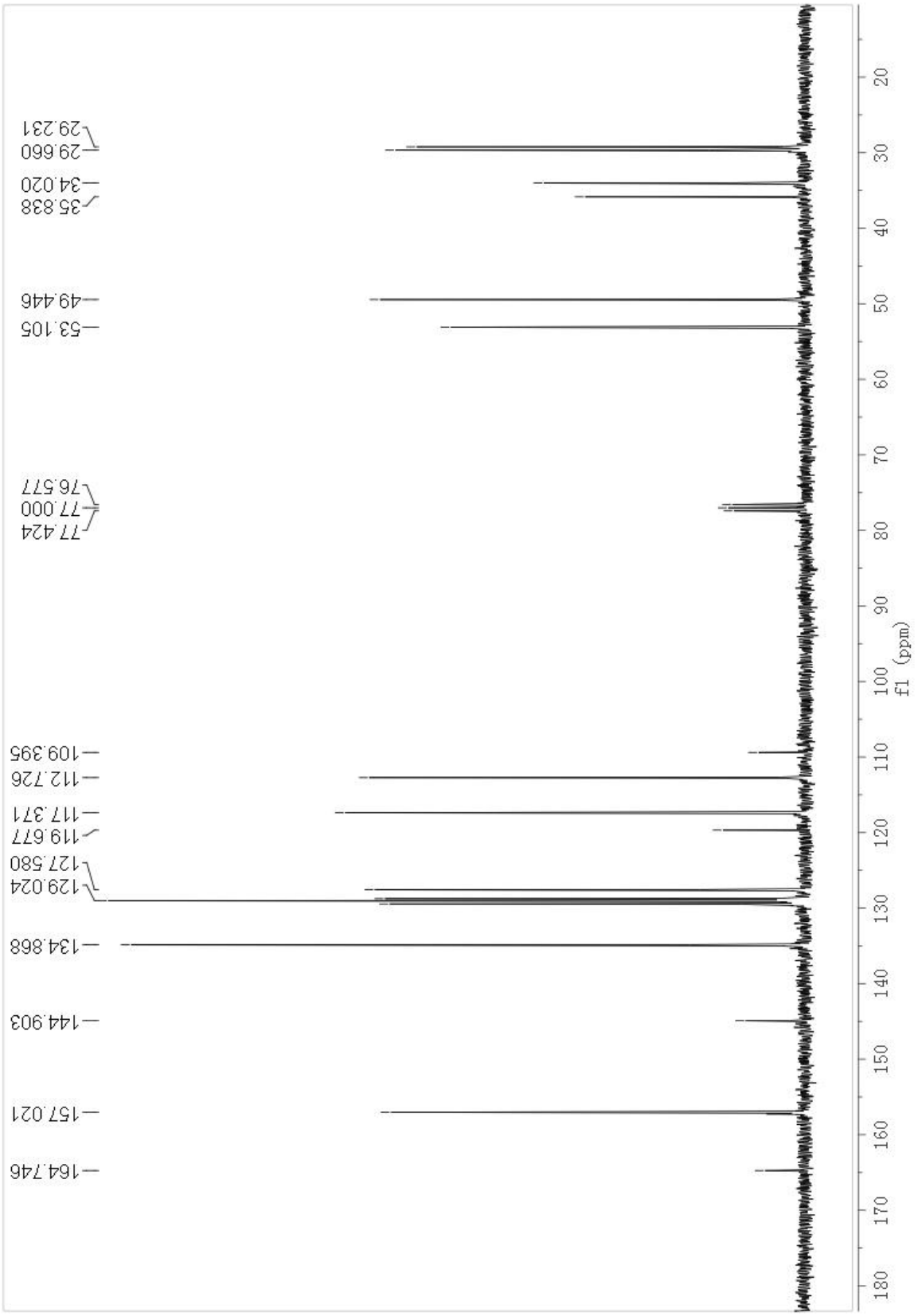




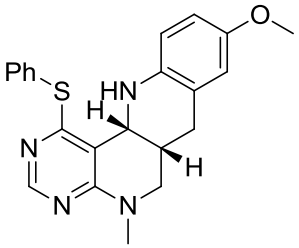
^{1}H NMR spectrum of Compound **2b**



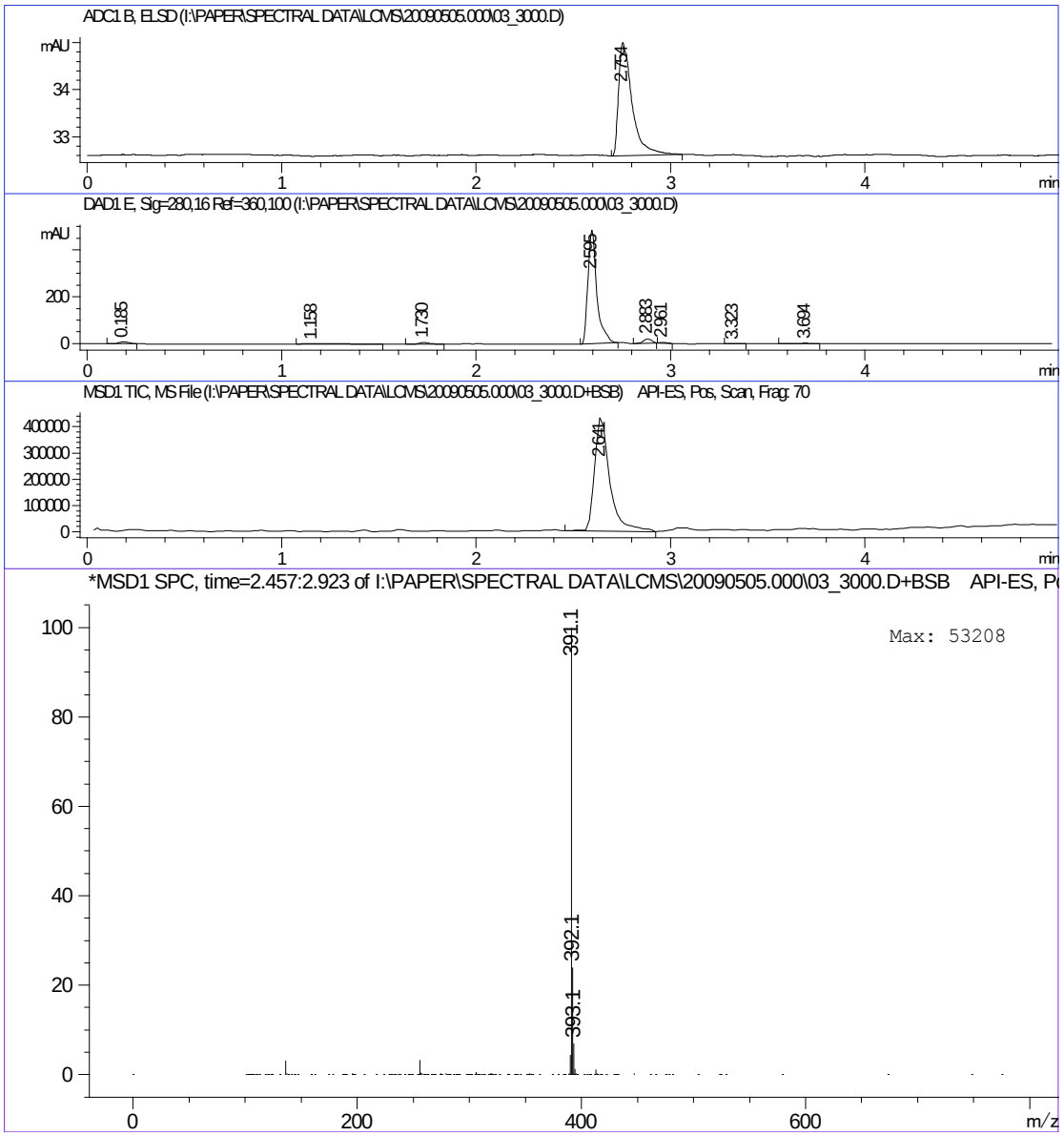
^{13}C NMR spectrum of Compound **2b**



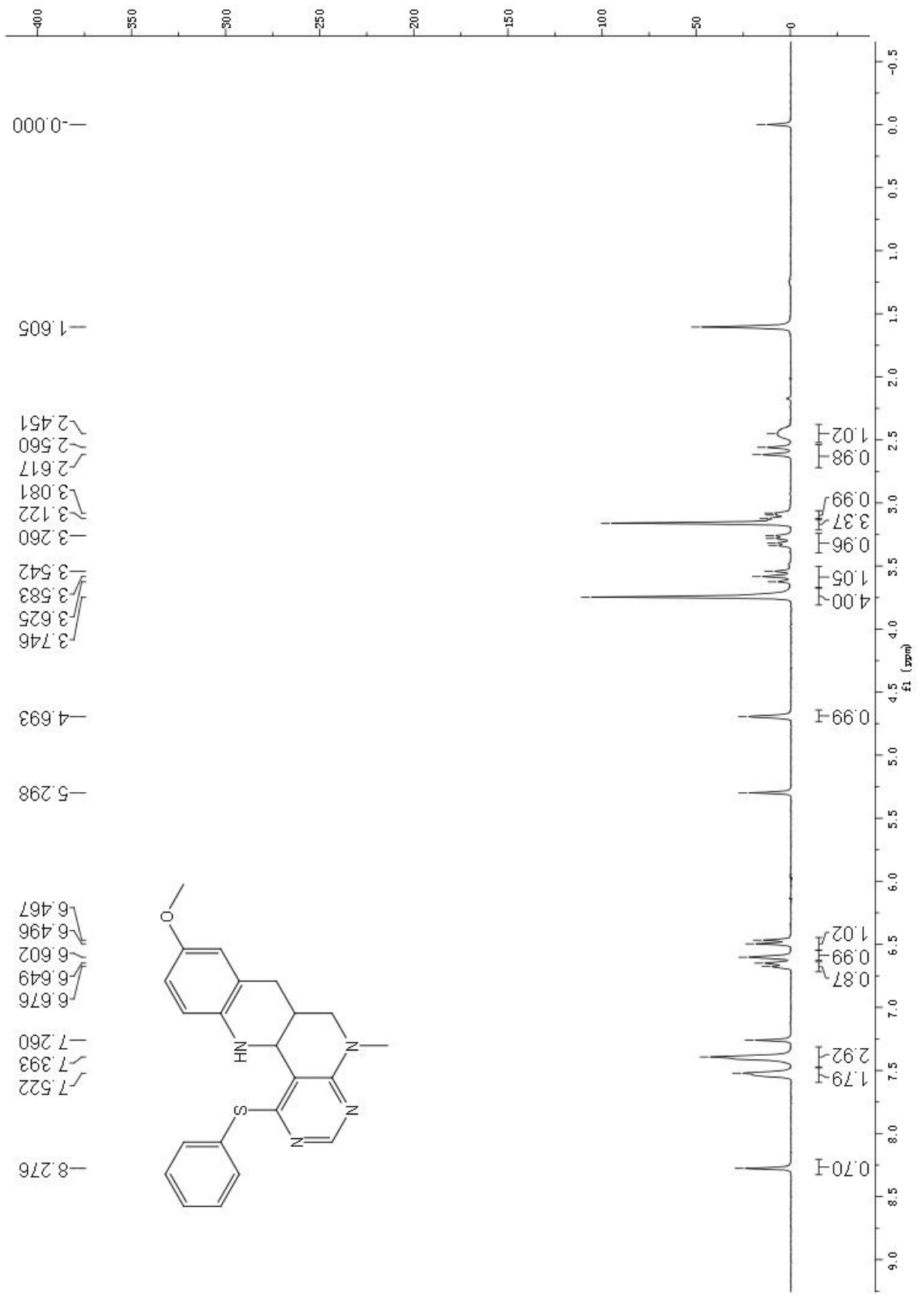
LC-MS-ELSD spectra of Compound **2e**



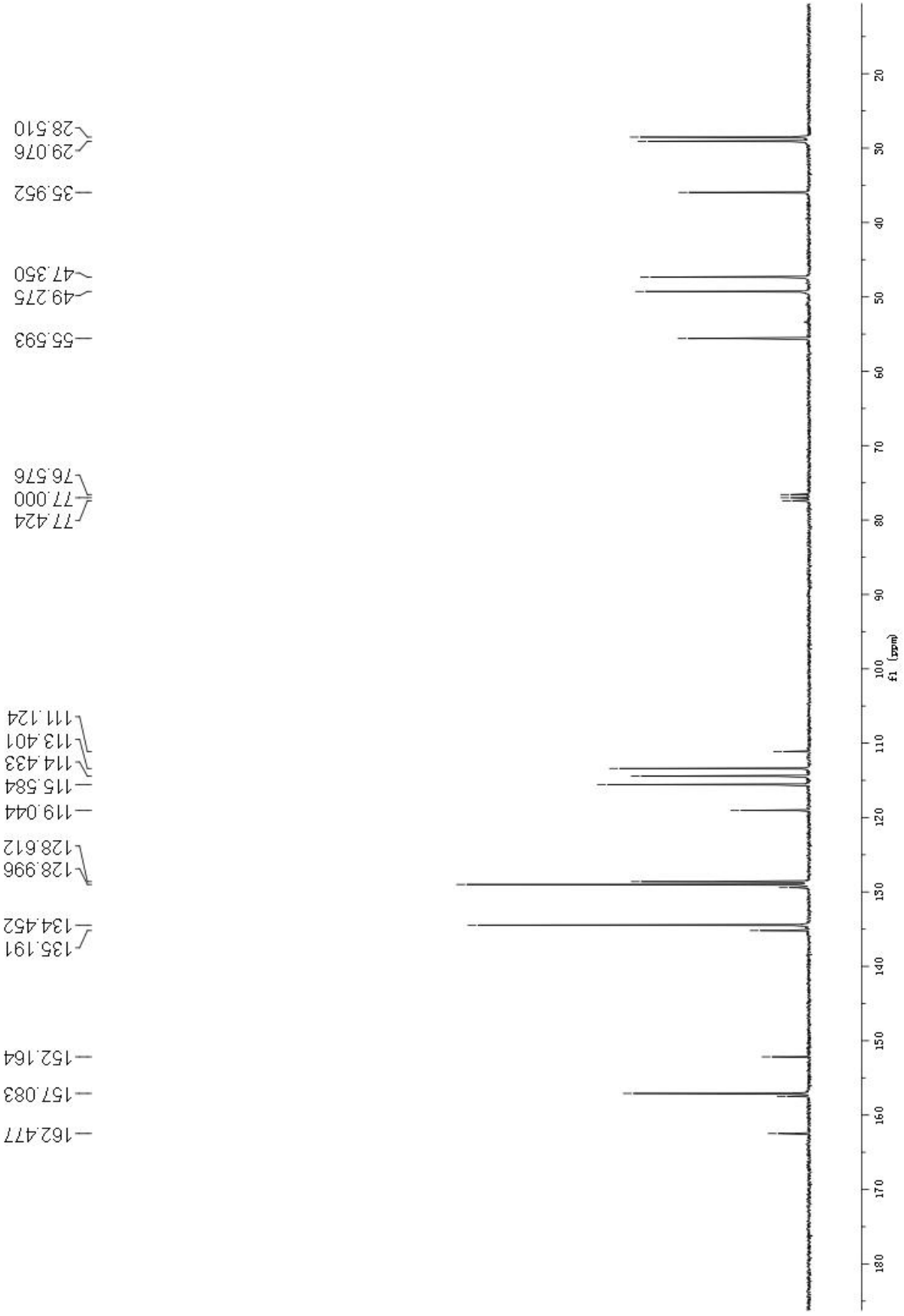
$C_{22}H_{22}N_4OS$
Exact Mass: 390.15
Mol. Wt.: 390.5



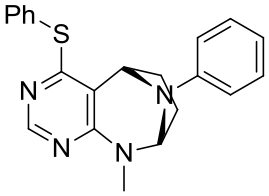
^{1}H NMR spectrum of Compound **2e**



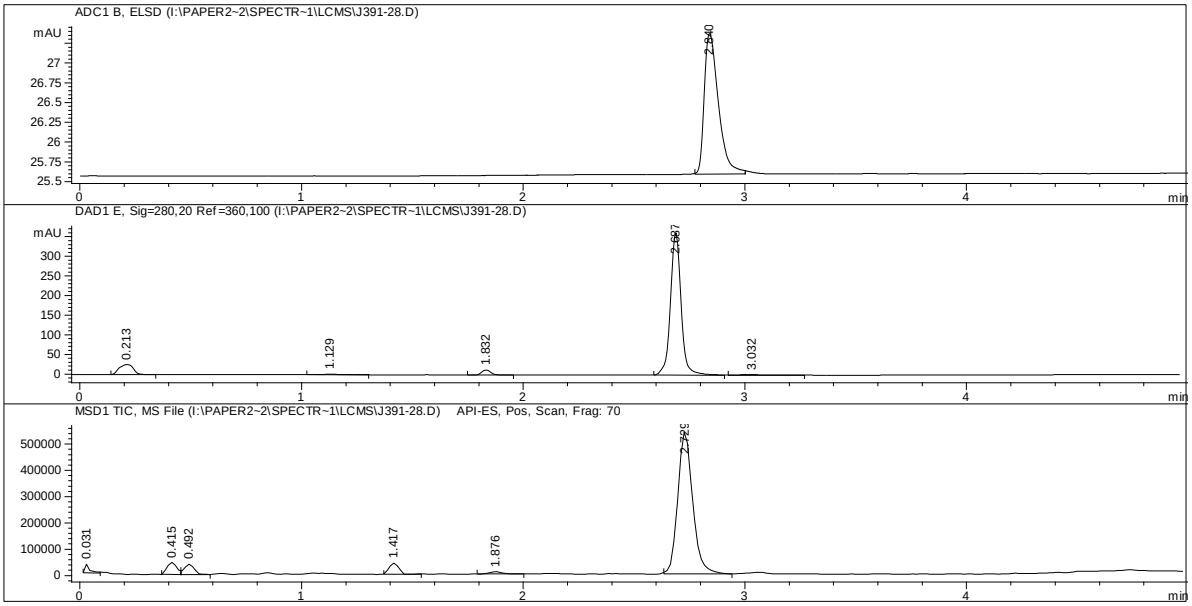
^{13}C NMR spectrum of Compound **2e**

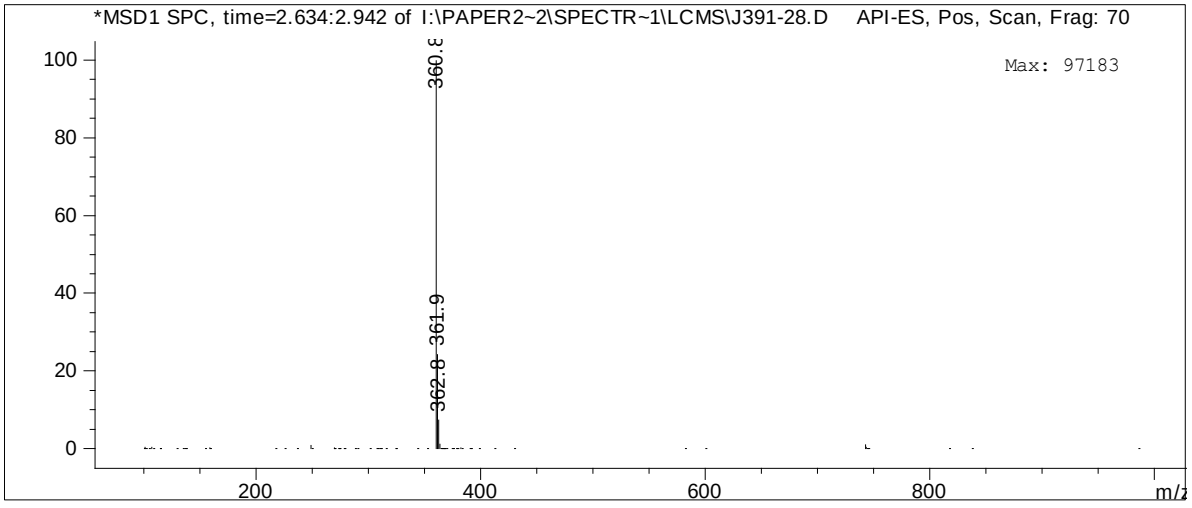


LC-MS-ELSD spectra of Compound **3a**

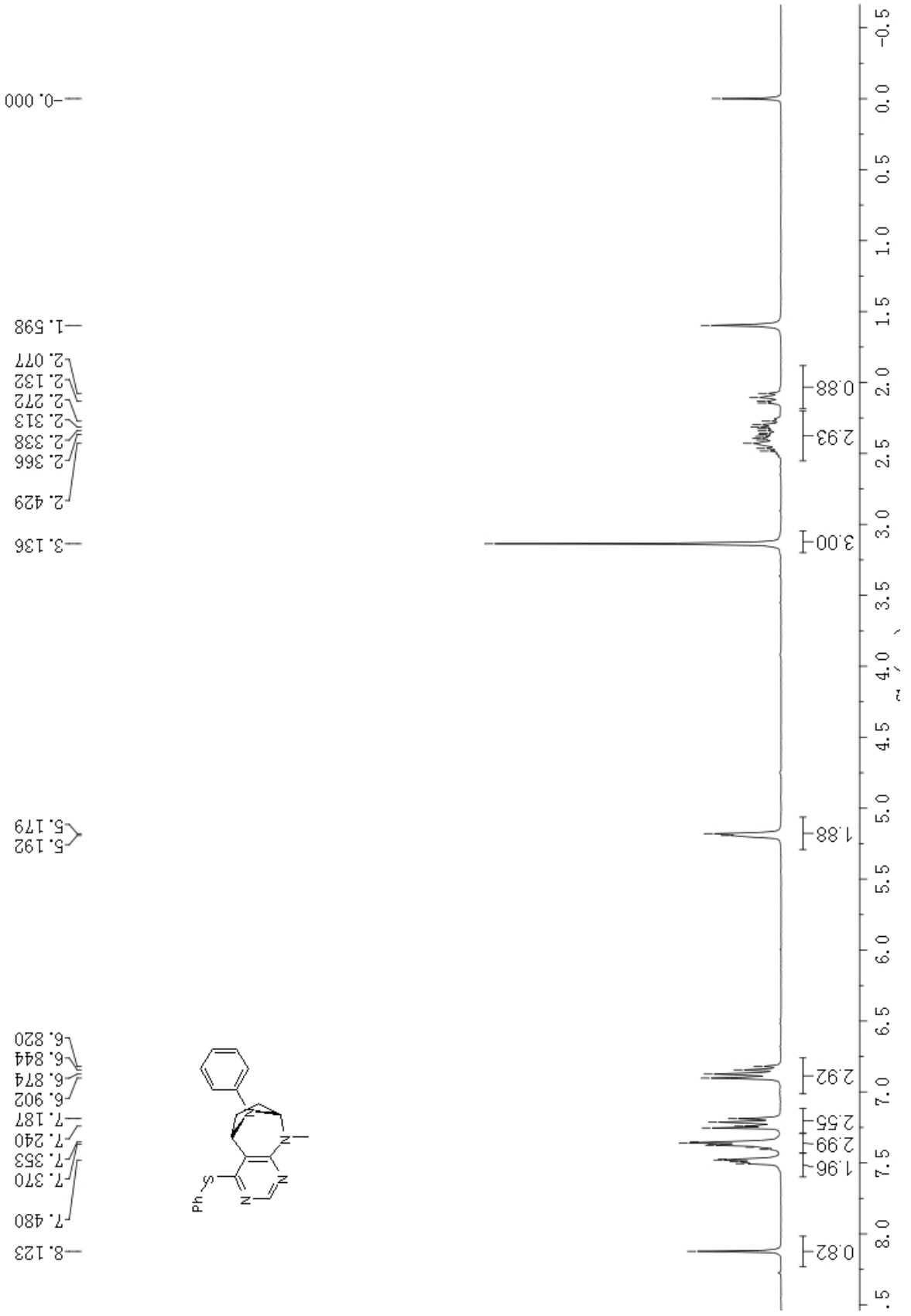


$C_{21}H_{20}N_4S$
Exact Mass: 360.1
Mol. Wt: 360.5

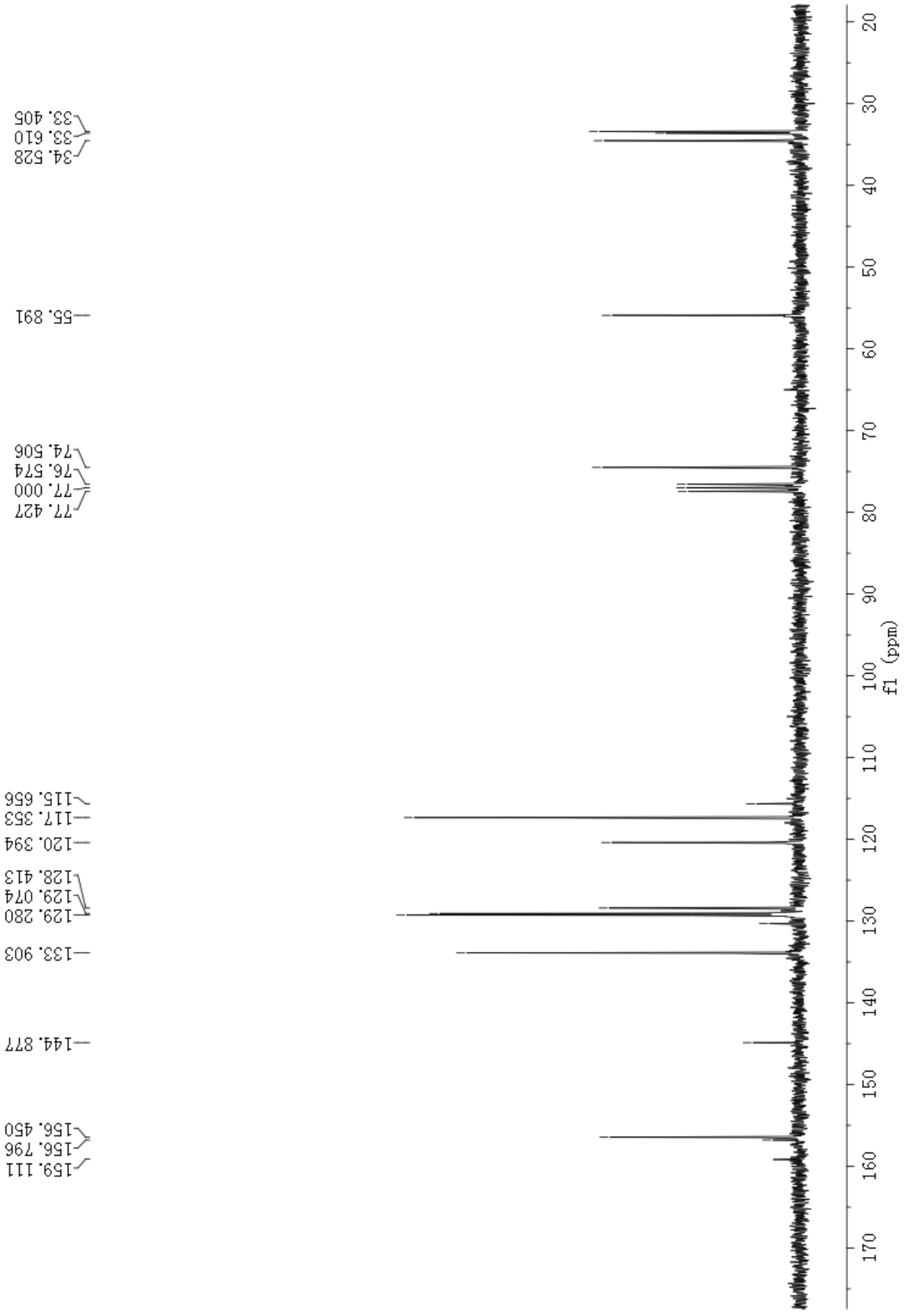




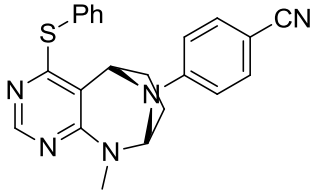
^{1}H NMR spectrum of Compound **3a**



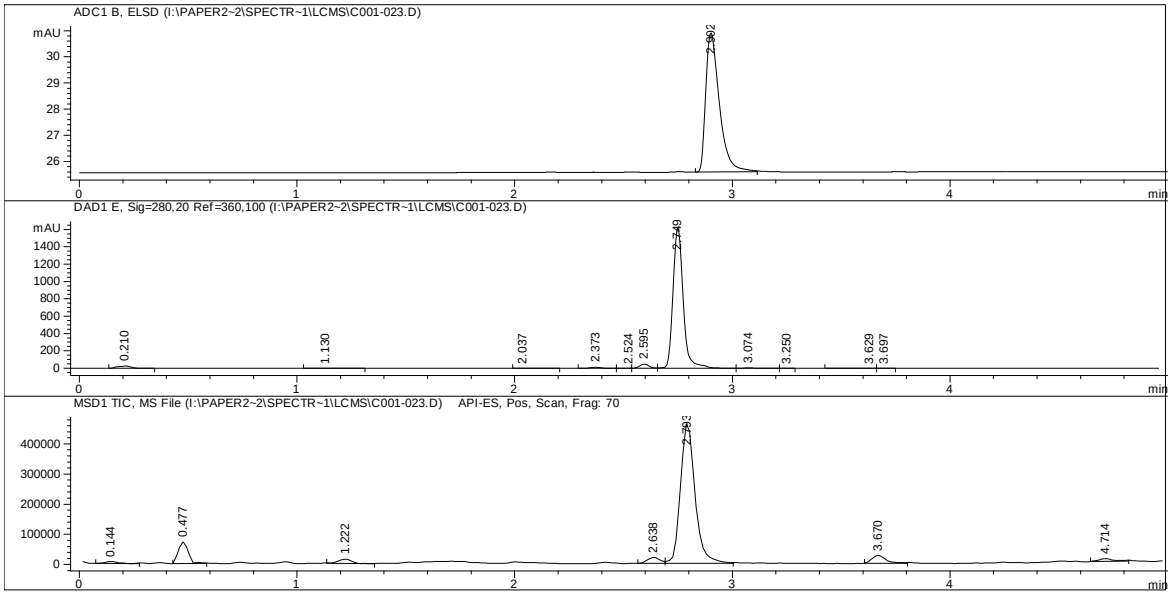
^{13}C NMR spectrum of Compound **3a**

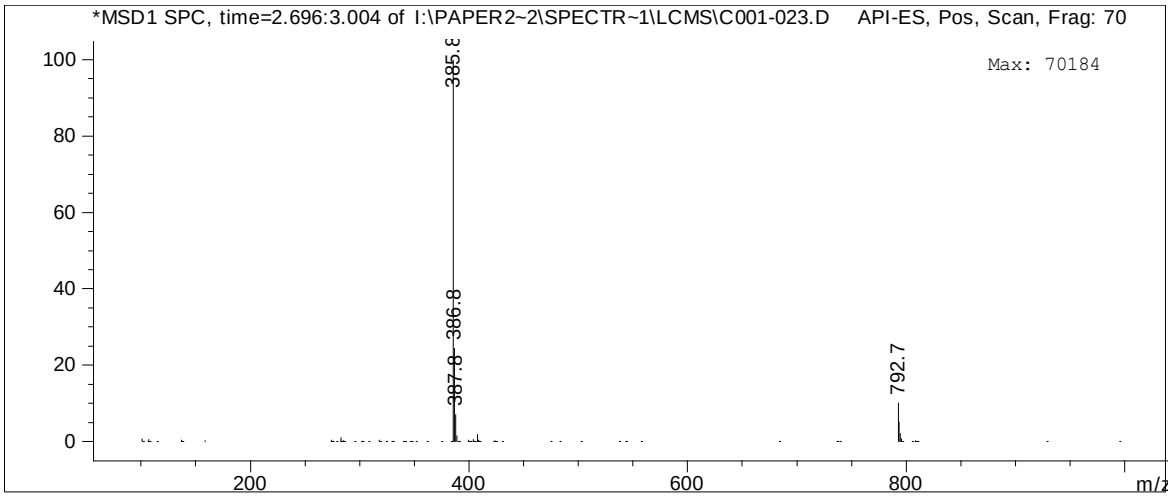


LC-MS-ELSD spectra of Compound **3b**

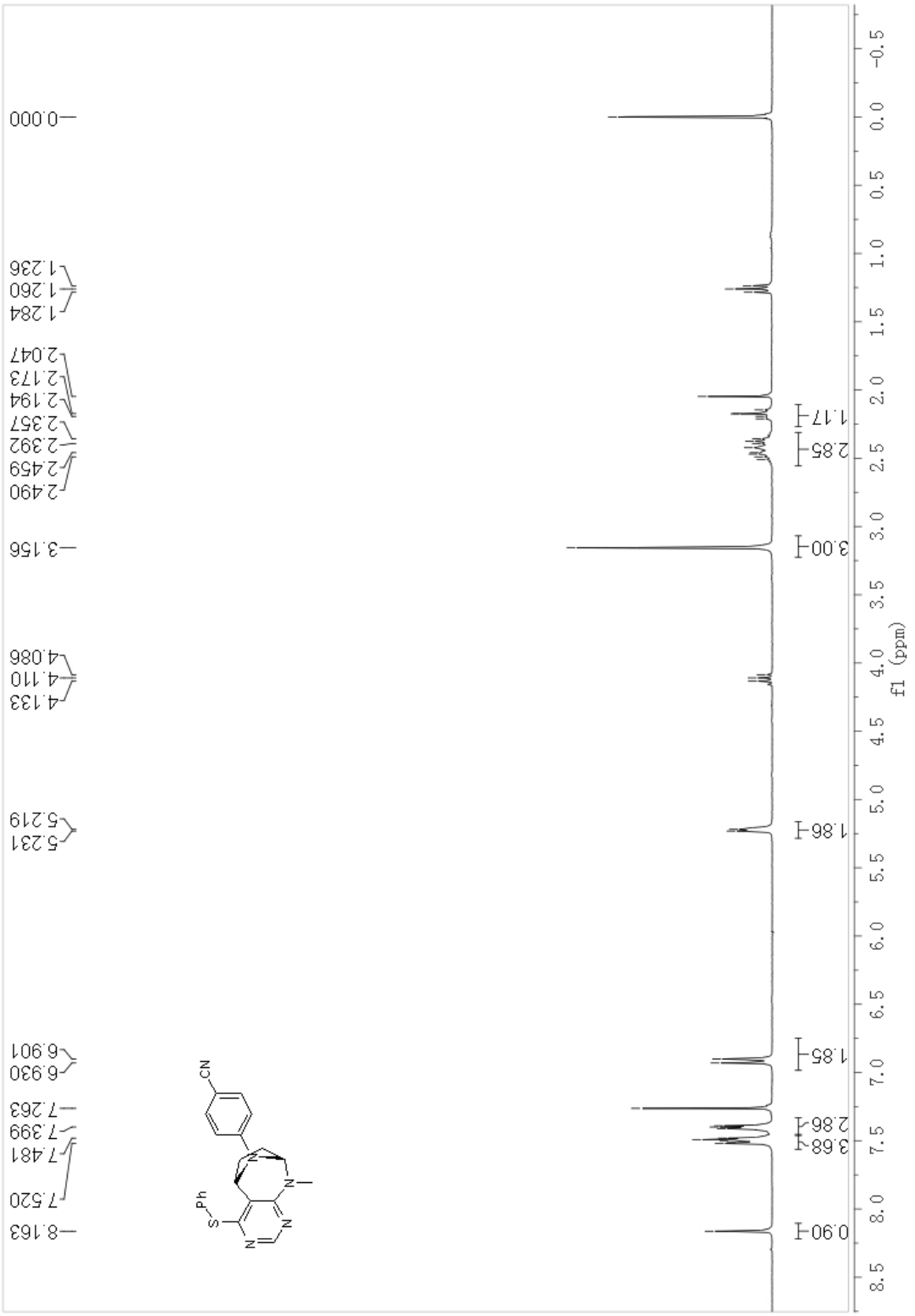


$C_{22}H_{19}N_5S$
Exact Mass: 385.14
Mol. Wt.: 385.48

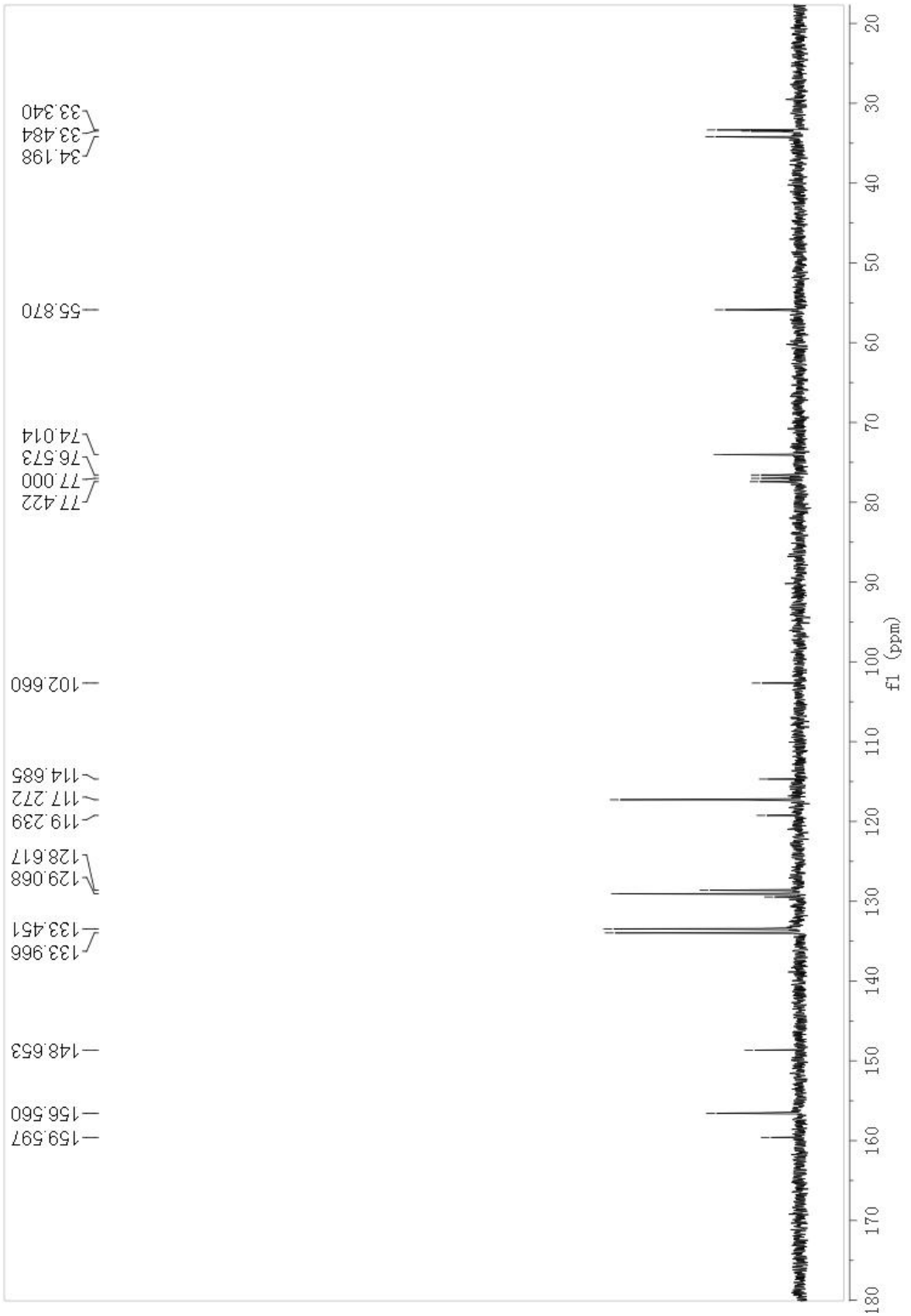




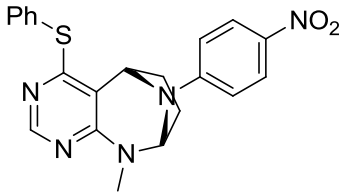
^{1}H NMR spectrum of Compound **3b**



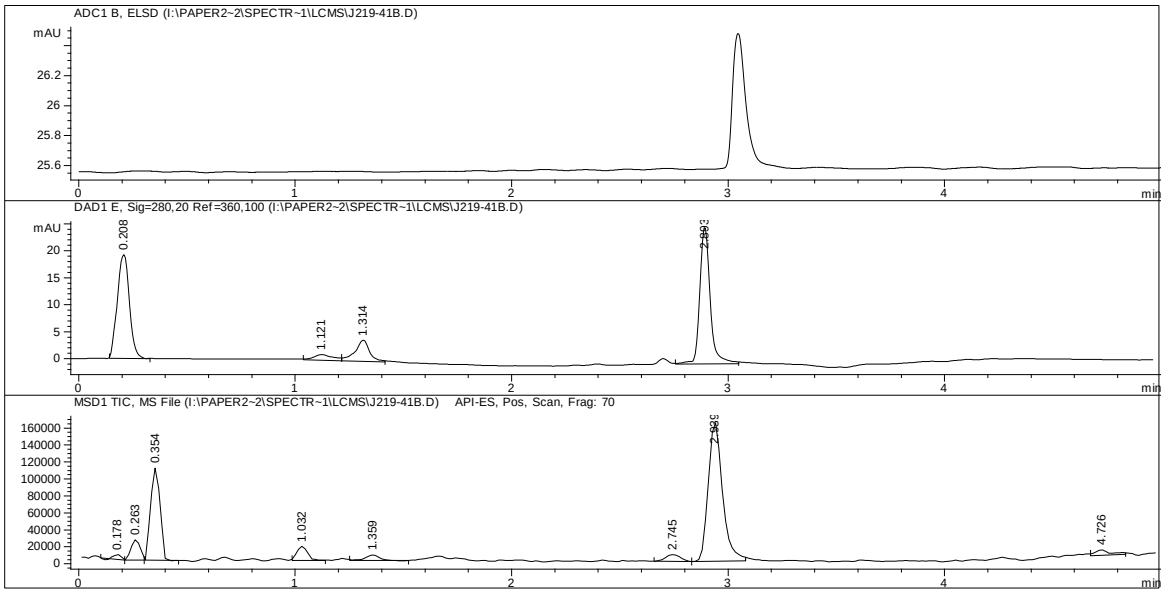
^{13}C NMR spectrum of Compound **3b**

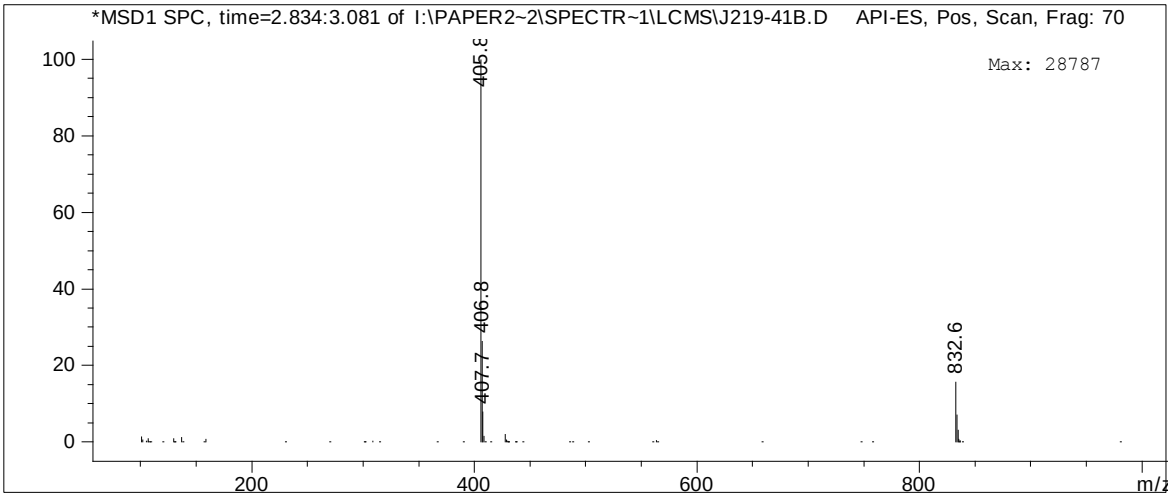


LC-MS-ELSD spectra of Compound **3c**

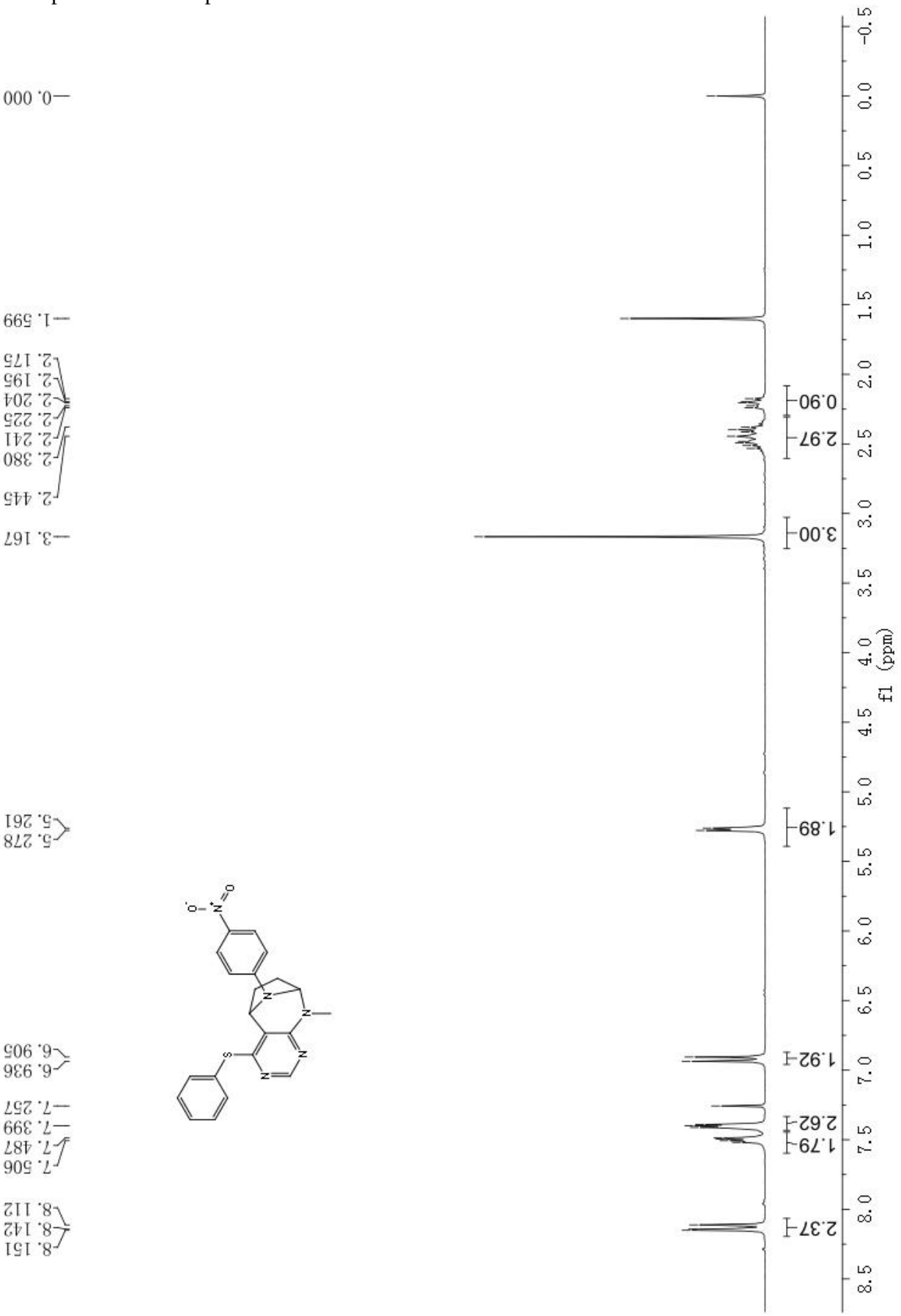


$C_{21}H_{19}N_5O_2S$
Exact Mass: 405.13
Mol. Wt.: 405.47

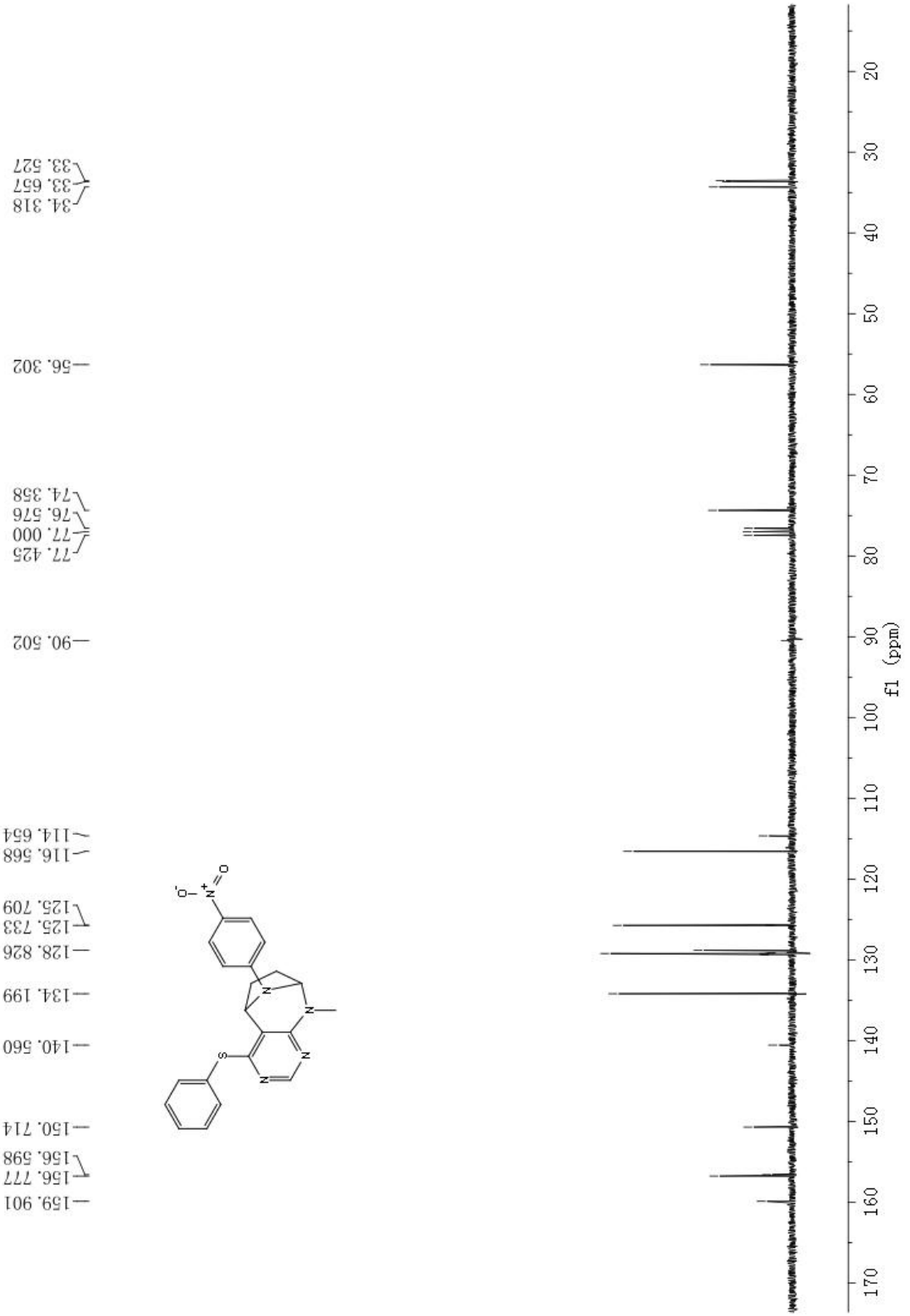




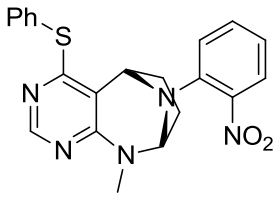
^{1}H NMR spectrum of Compound **3c**



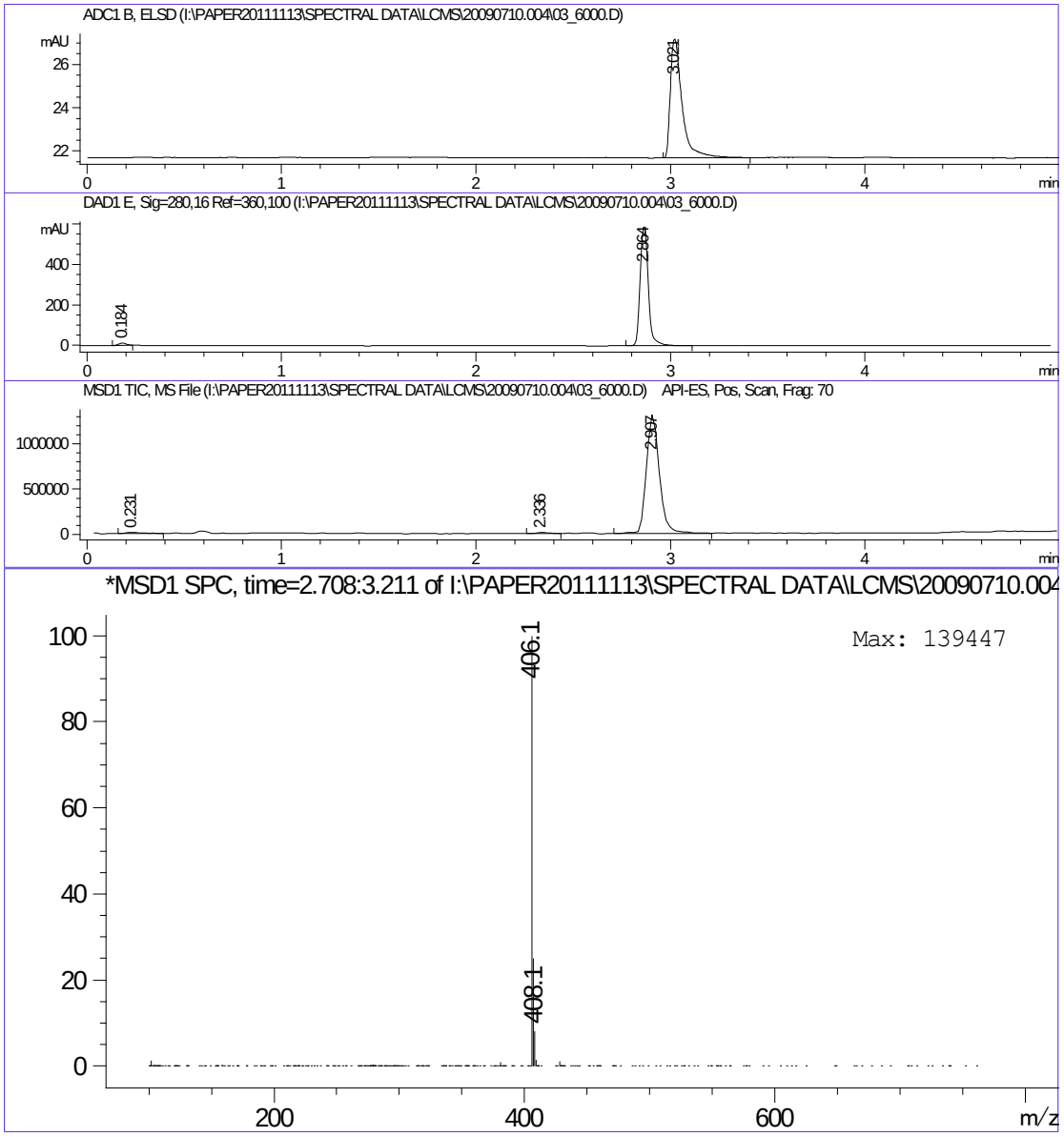
^{13}C NMR spectrum of Compound **3c**



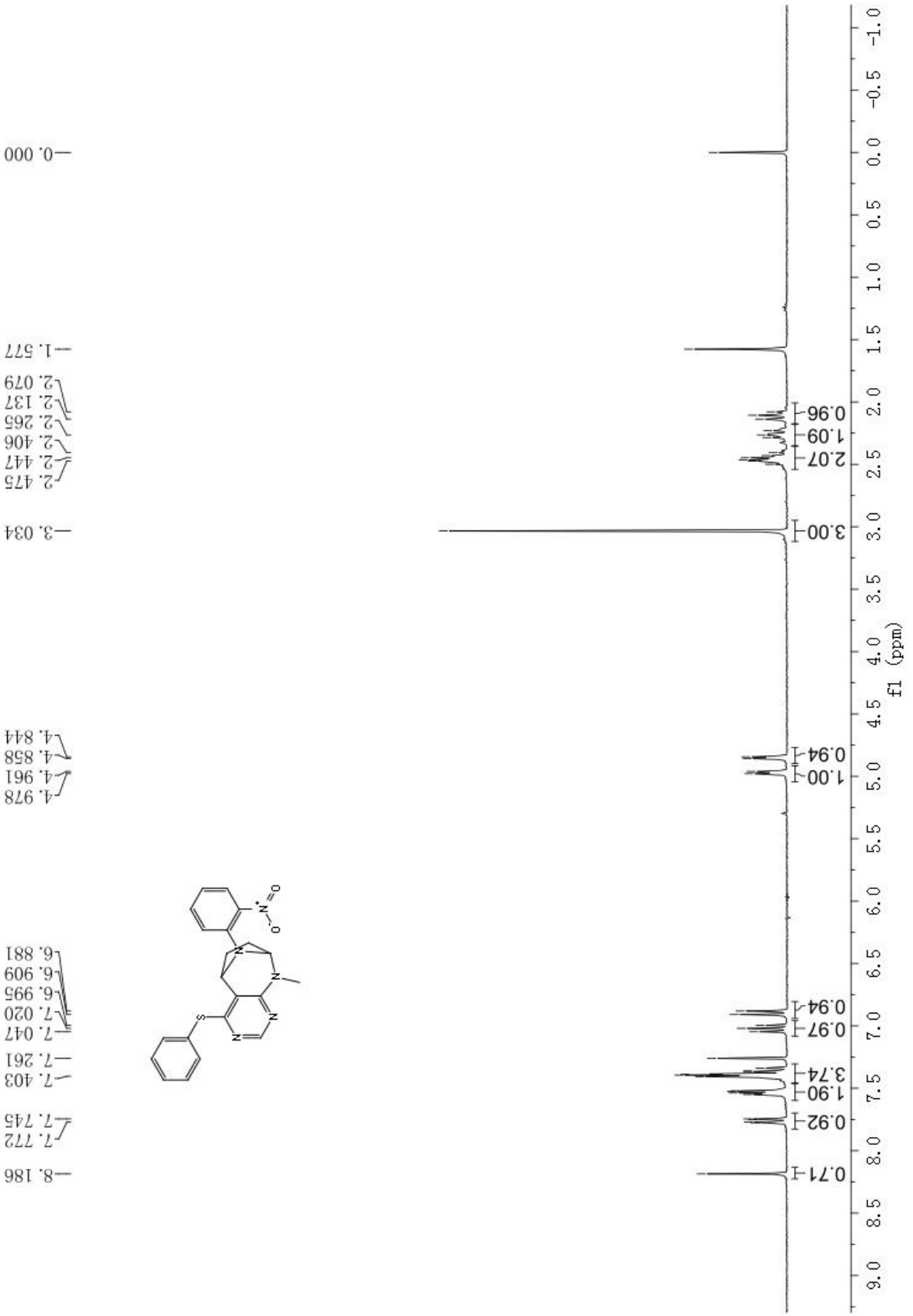
LC-MS-ELSD spectra of Compound **3d**



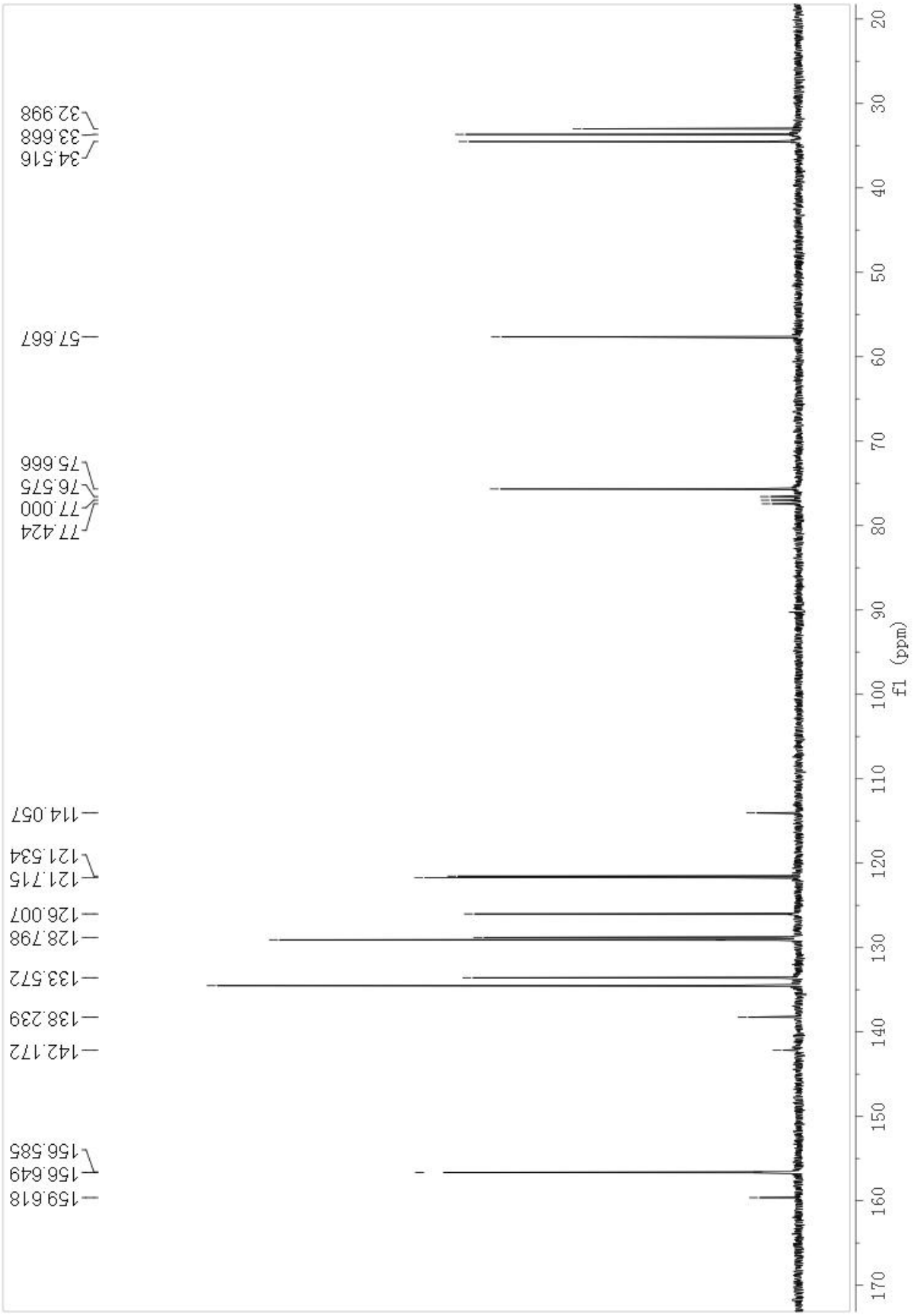
$C_{21}H_{19}N_5O_2S$
Exact Mass: 405.13
Mol. Wt: 405.47



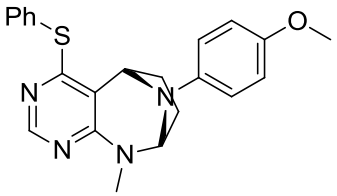
^{1}H NMR spectrum of Compound **3d**



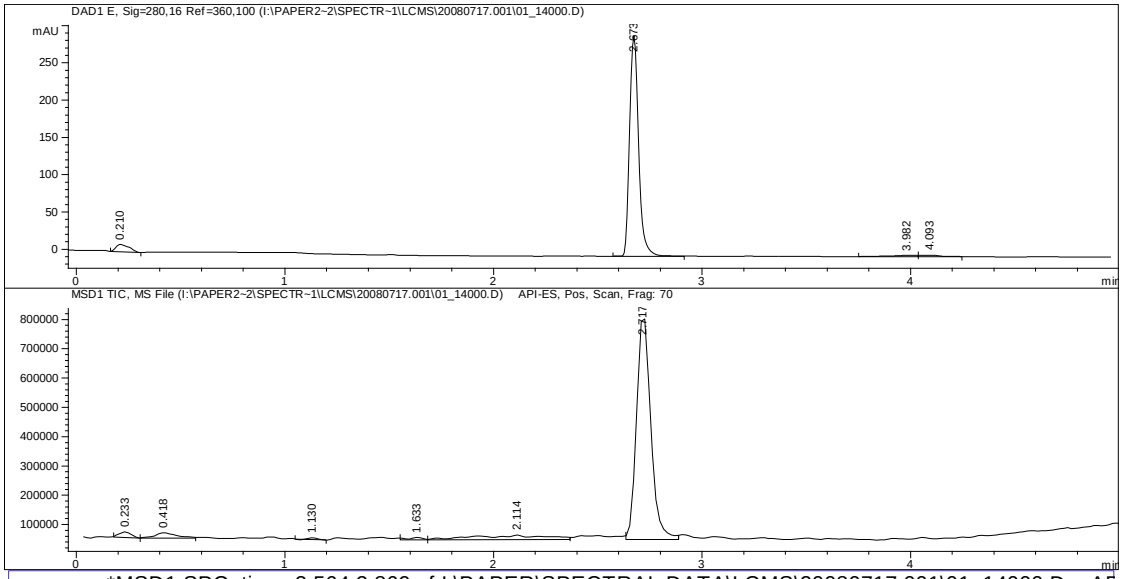
^{13}C NMR spectrum of Compound **3d**

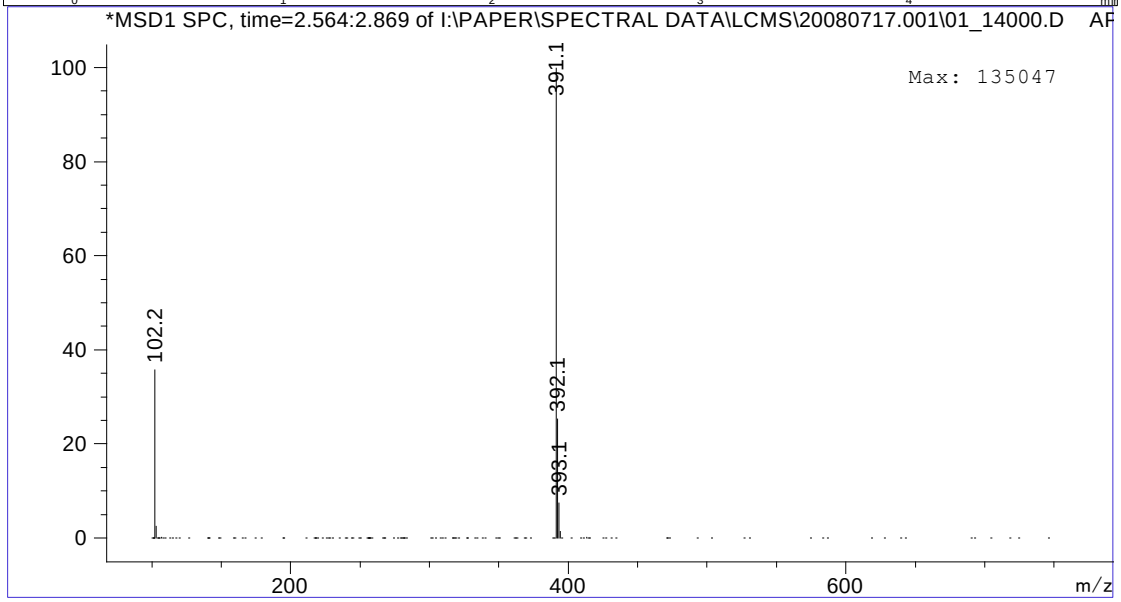


LC-MS-ELSD spectra of Compound **3e**

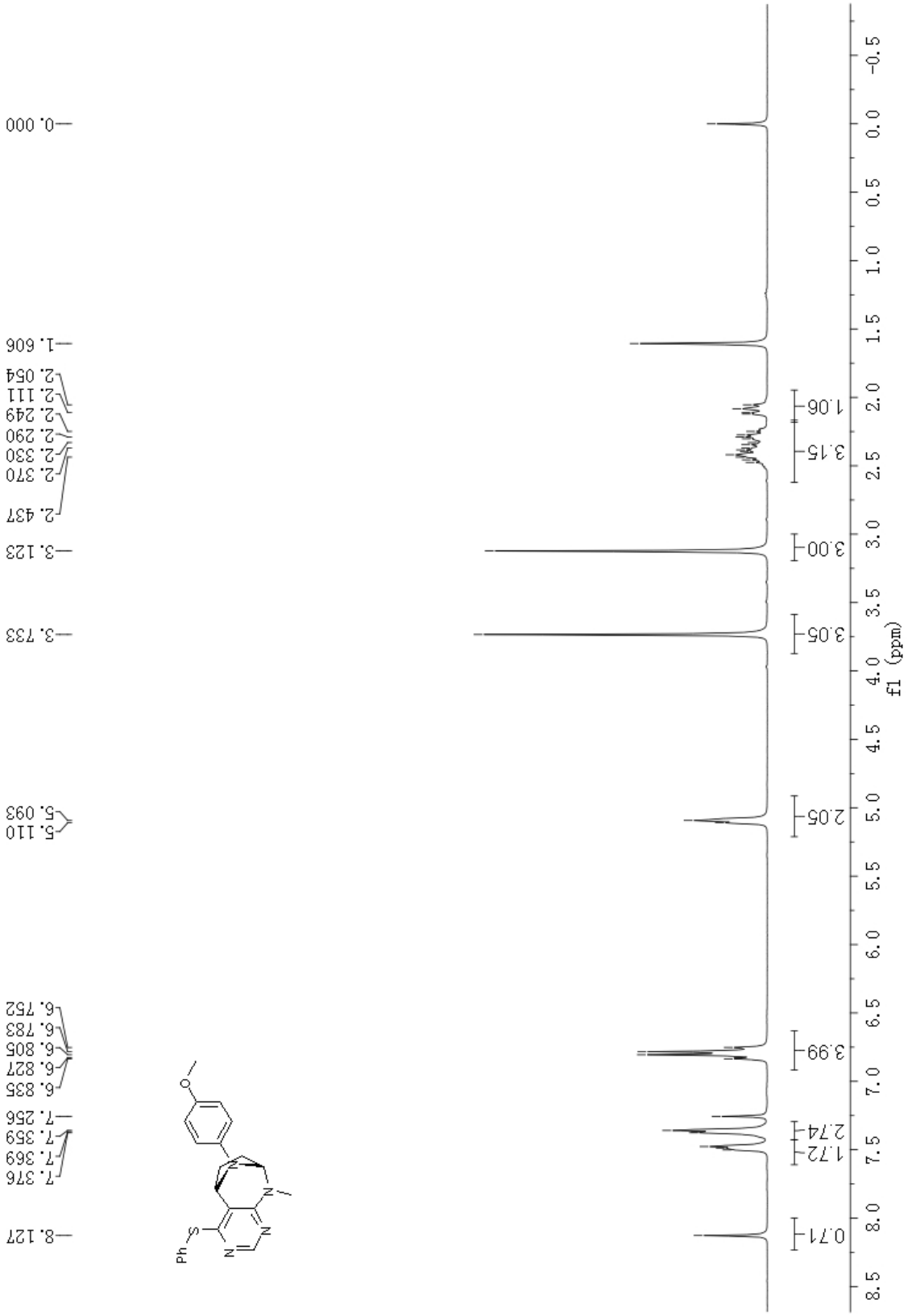


$C_{22}H_{22}N_4OS$
Exact Mass: 390.15
Mol. Wt.: 390.5

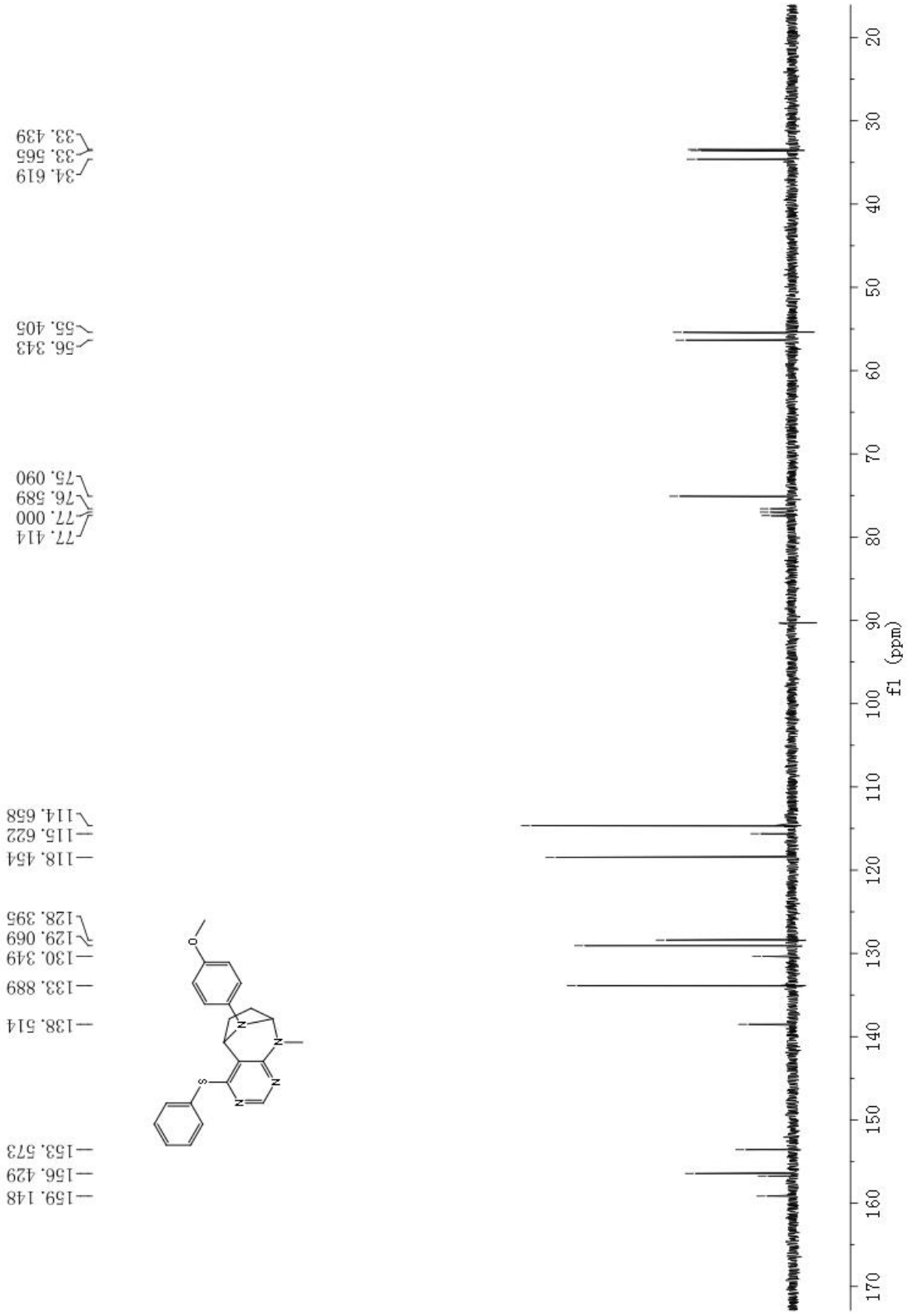




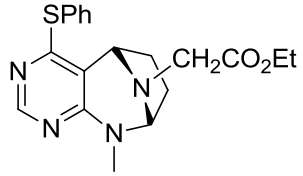
^{1}H NMR spectrum of Compound **3e**



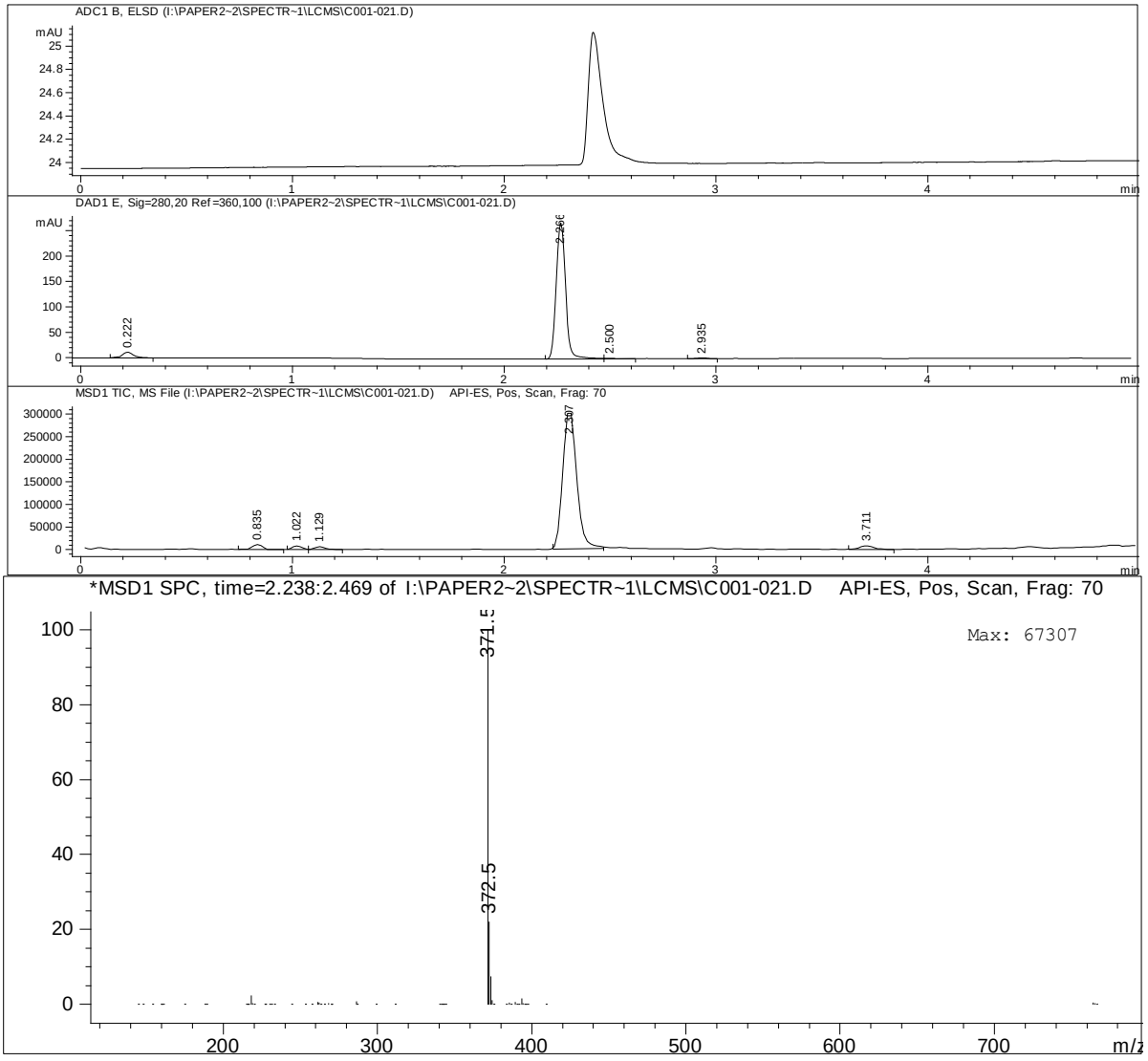
^{13}C NMR spectrum of Compound **3e**



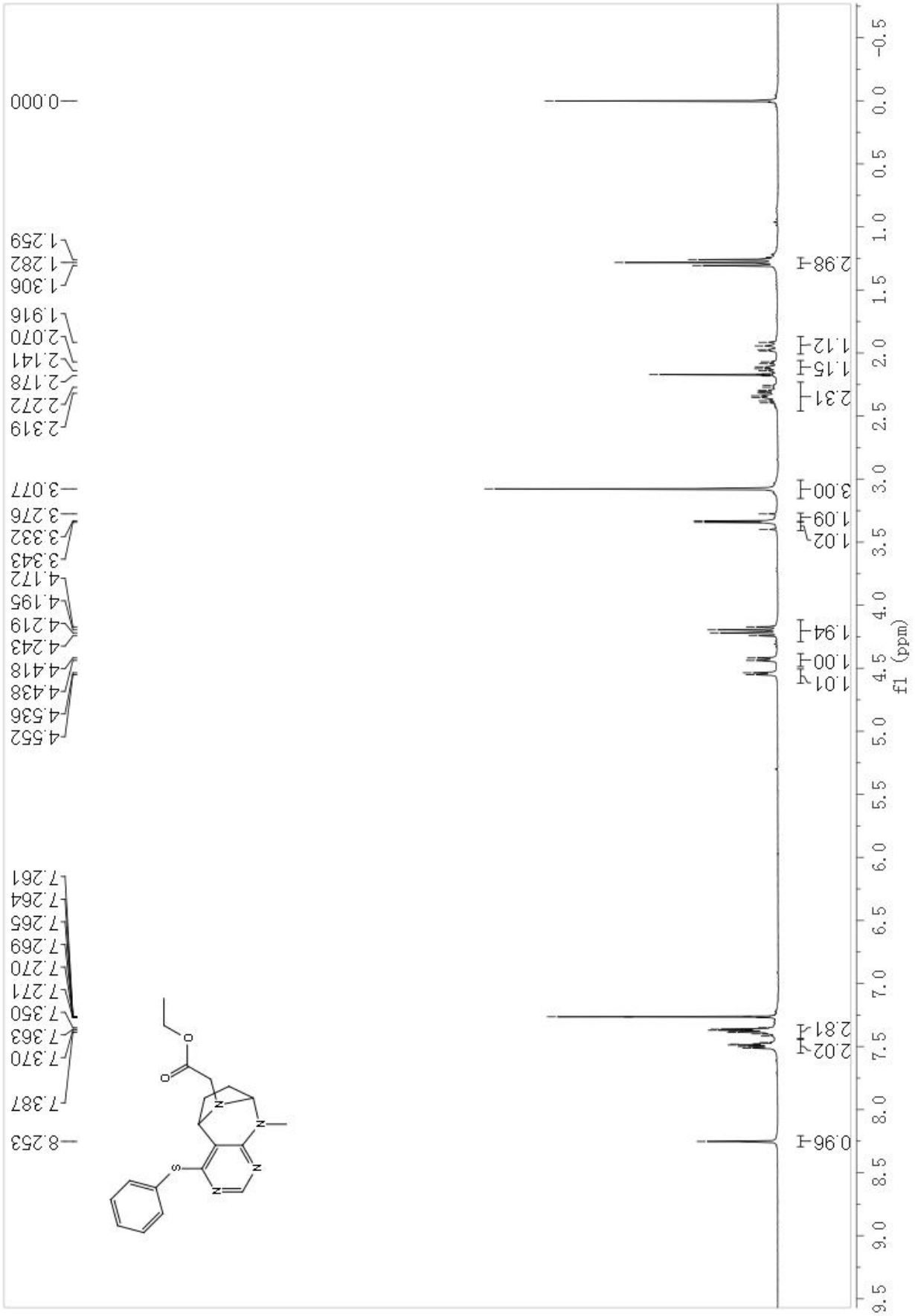
LC-MS-ELSD spectra of Compound **3f**



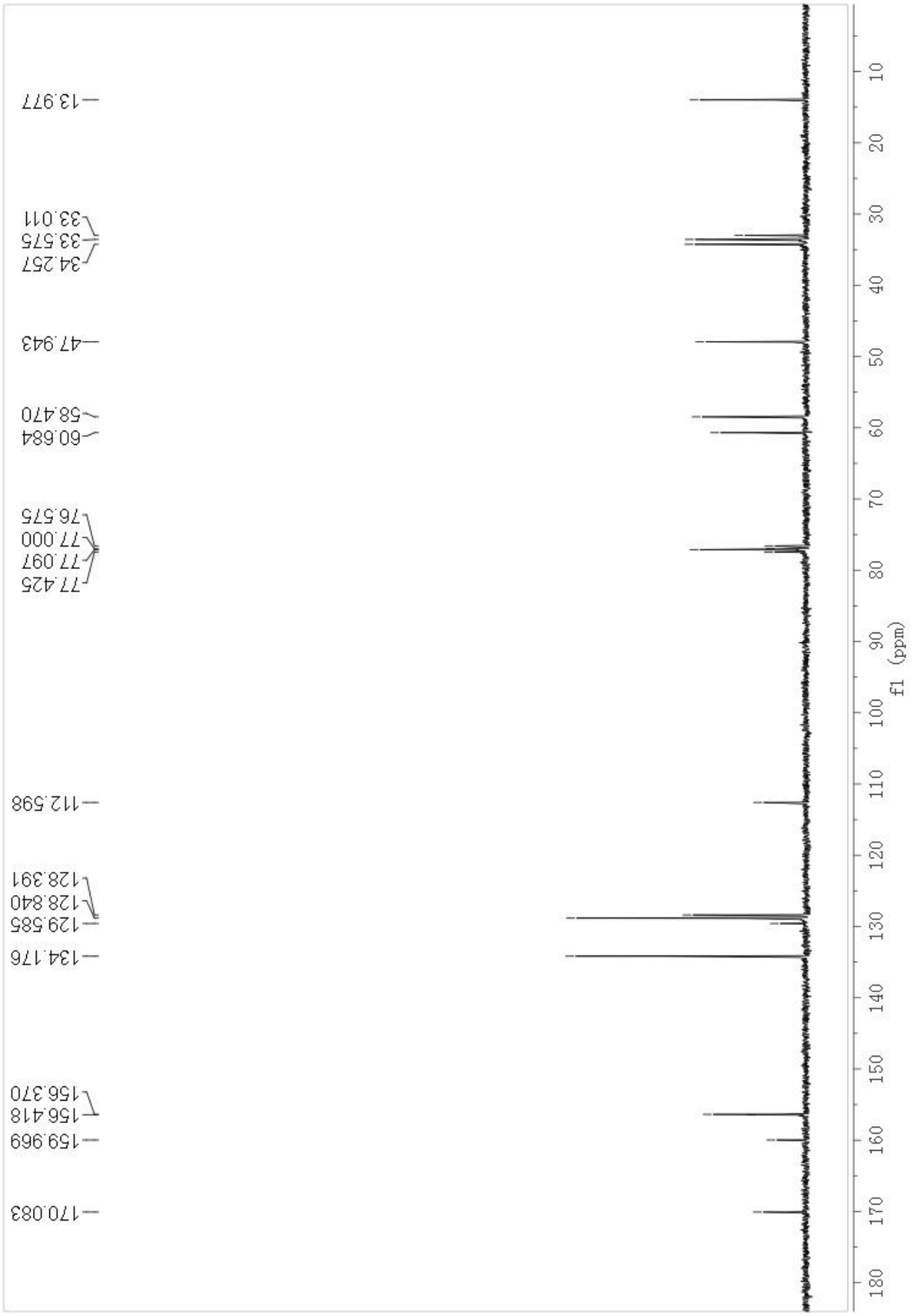
$C_{19}H_{22}N_4O_2S$
Exact Mass: 370.1
Mol. Wt.: 370.5



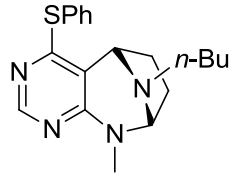
^{1}H NMR spectrum of Compound **3f**



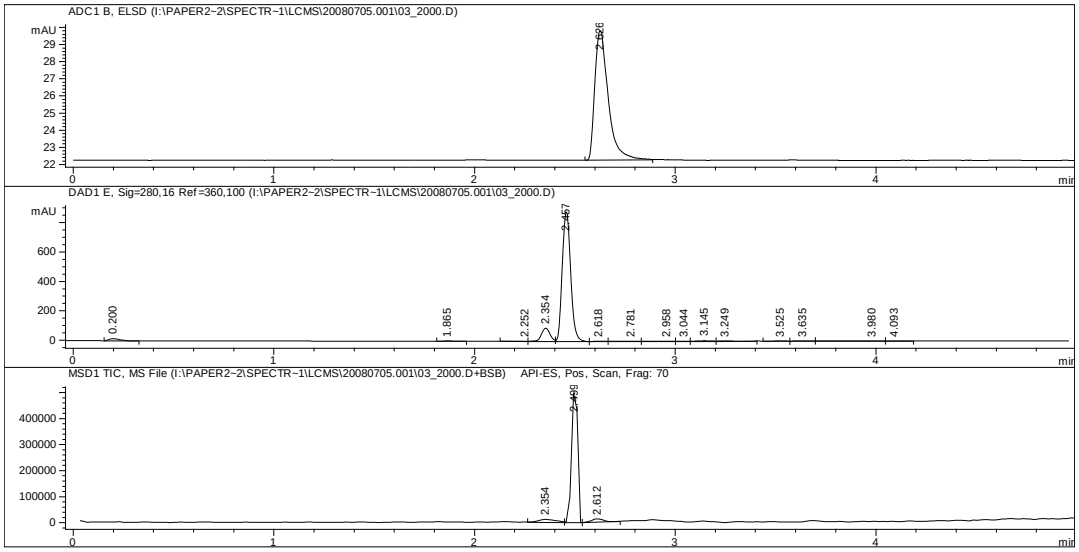
^{13}C NMR spectrum of Compound **3f**

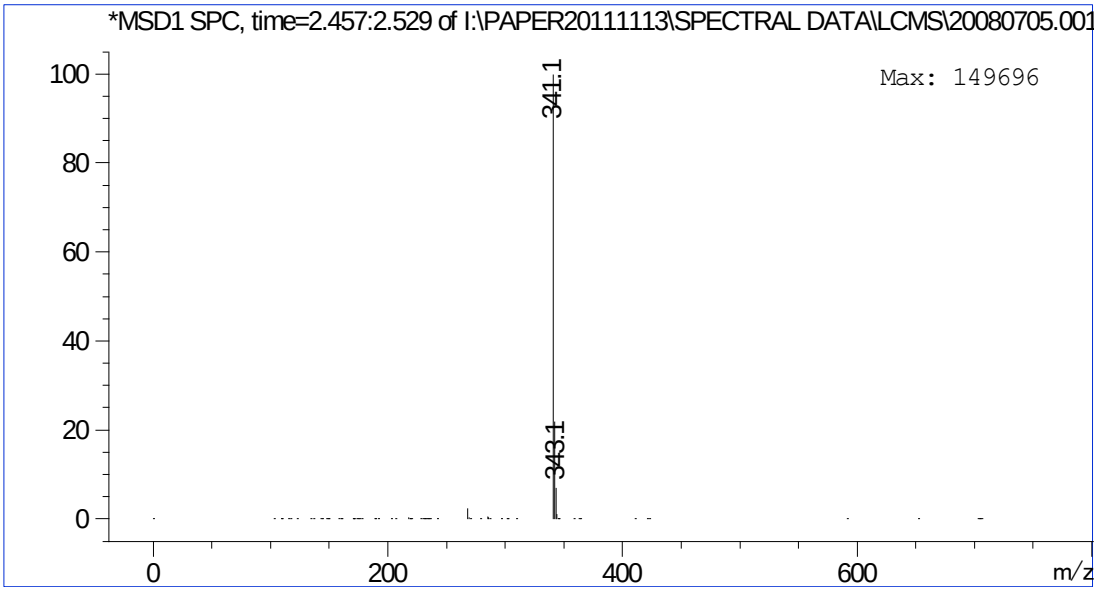


LC-MS-ELSD spectra of Compound **3g**

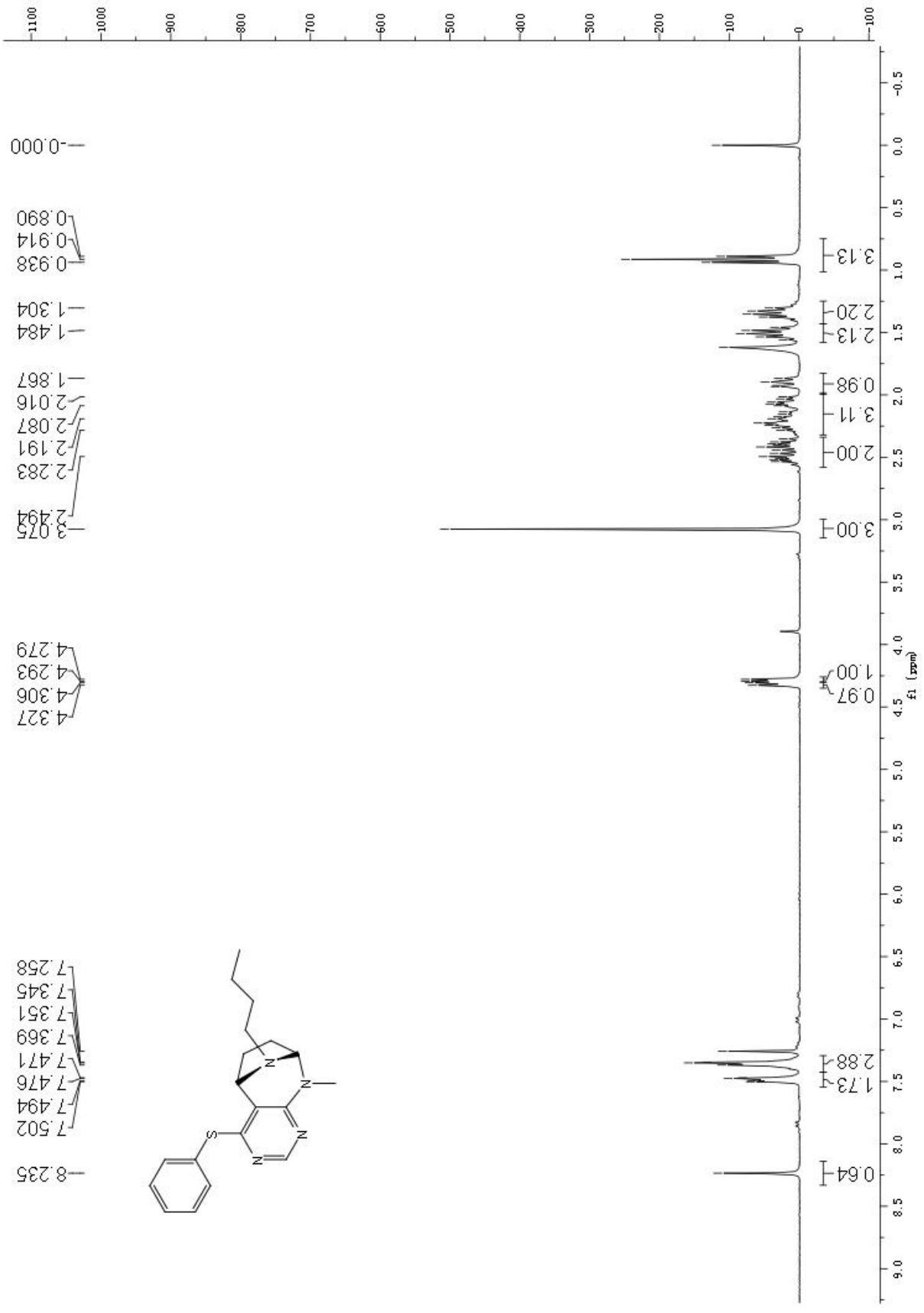


$C_{19}H_{24}N_4S$
Exact Mass: 340.17
Mol. Wt.: 340.49

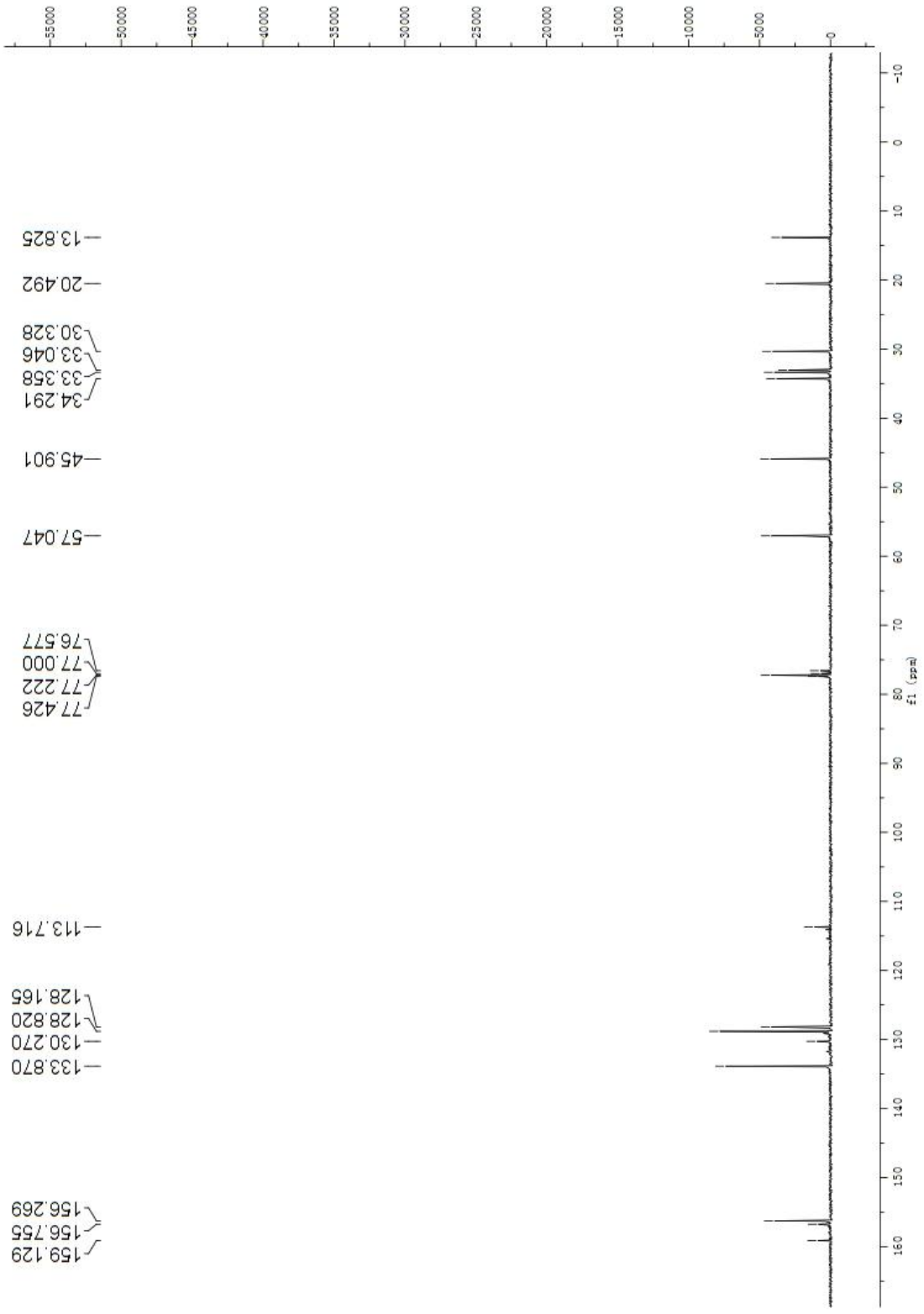




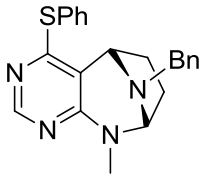
^{1}H NMR spectrum of Compound **3g**



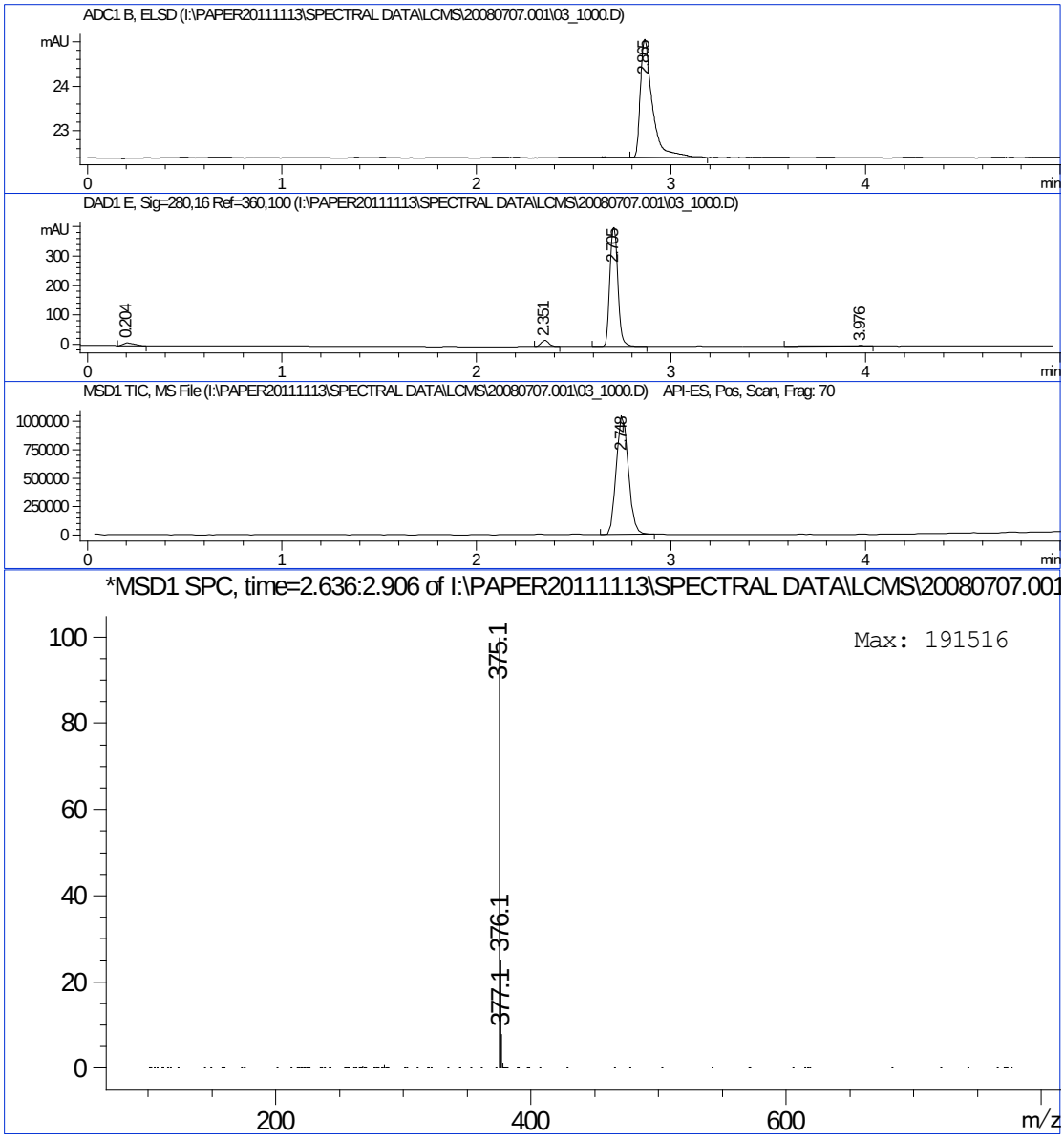
^{13}C NMR spectrum of Compound **3g**



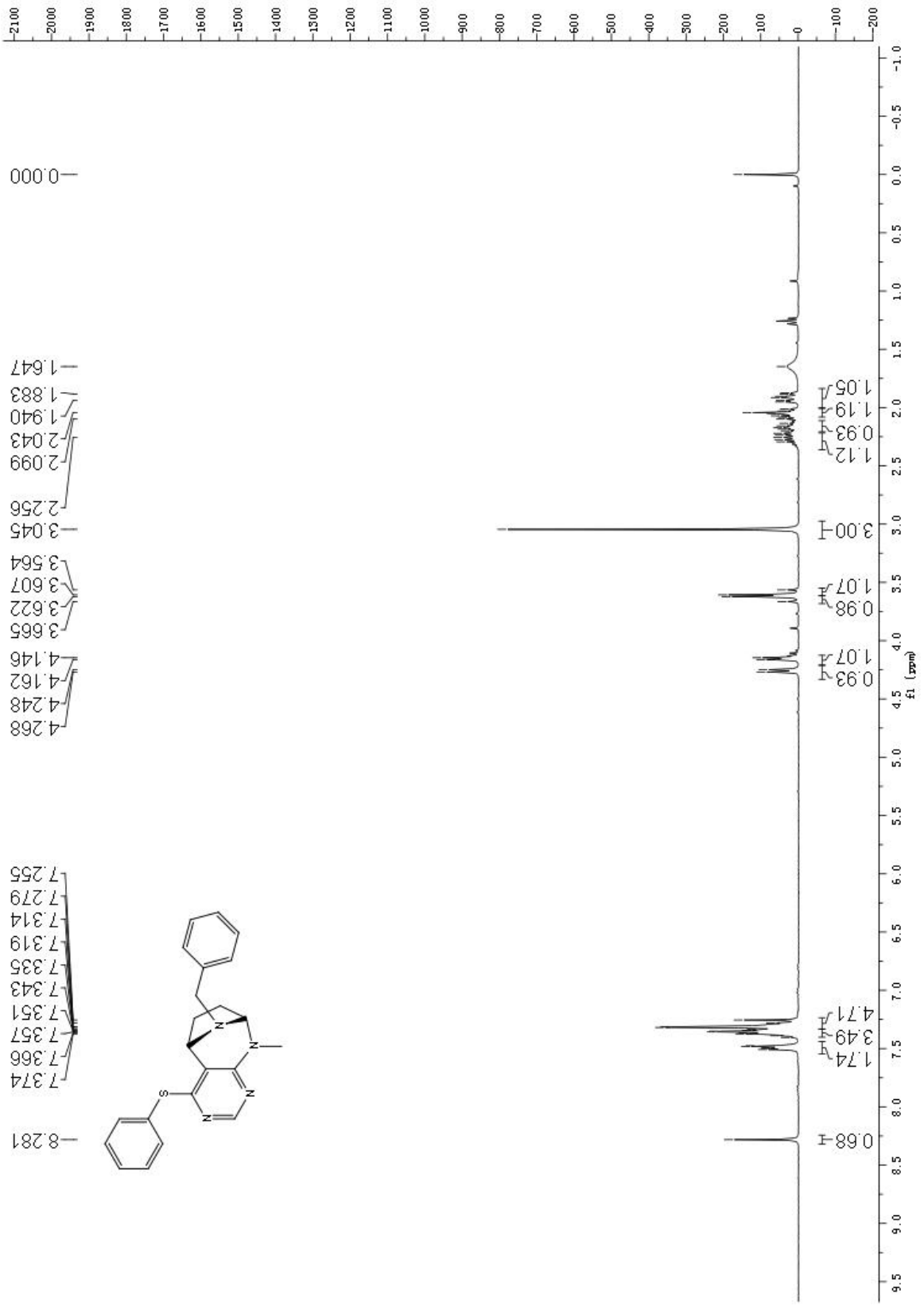
LC-MS-ELSD spectra of Compound **3h**



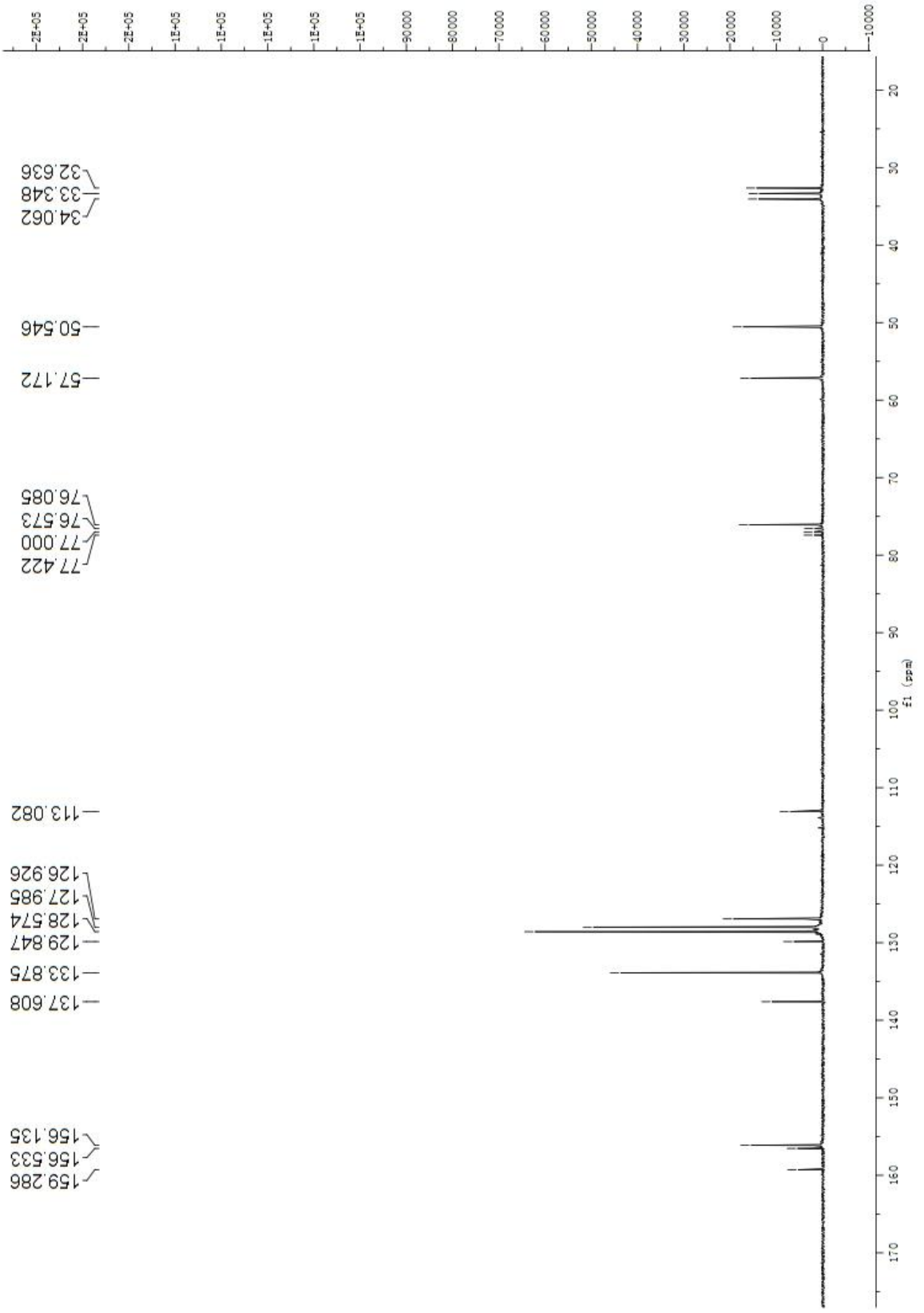
$C_{22}H_{22}N_4S$
Exact Mass: 374.16
Mol. Wt.: 374.50



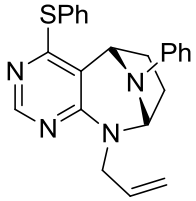
^{1}H NMR spectrum of Compound **3h**



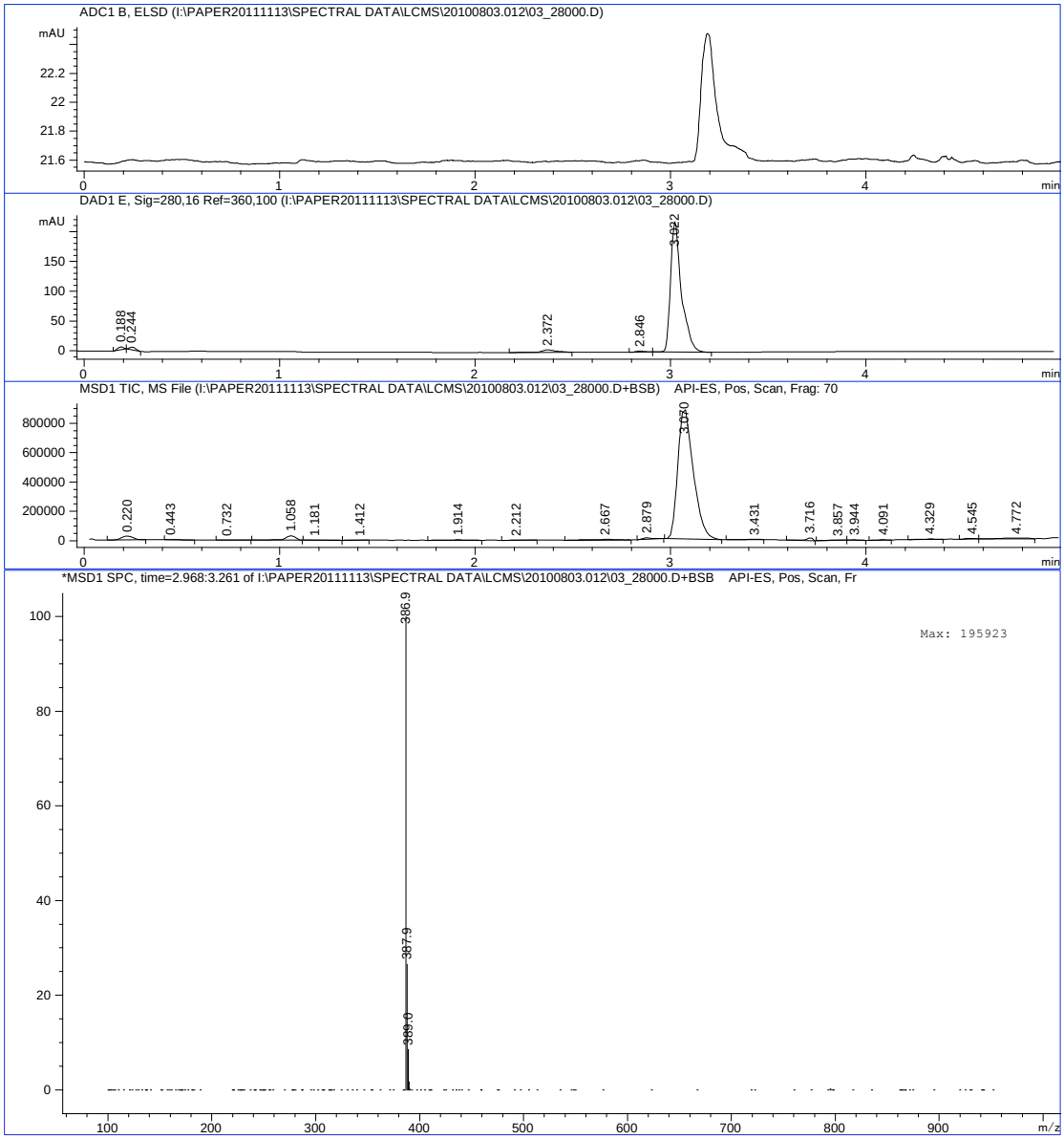
^{13}C NMR spectrum of Compound **3h**



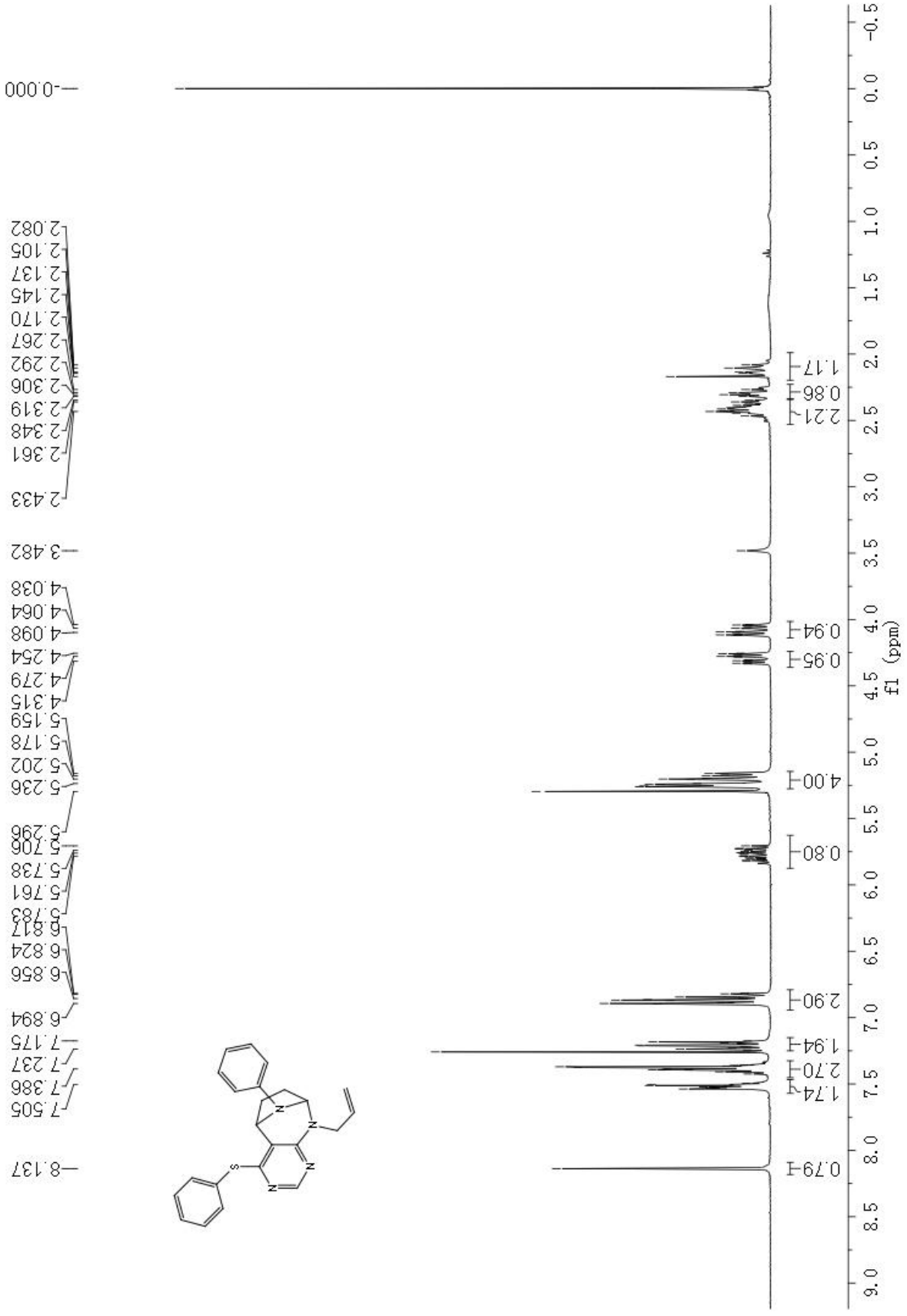
LC-MS-ELSD spectra of Compound **3i**



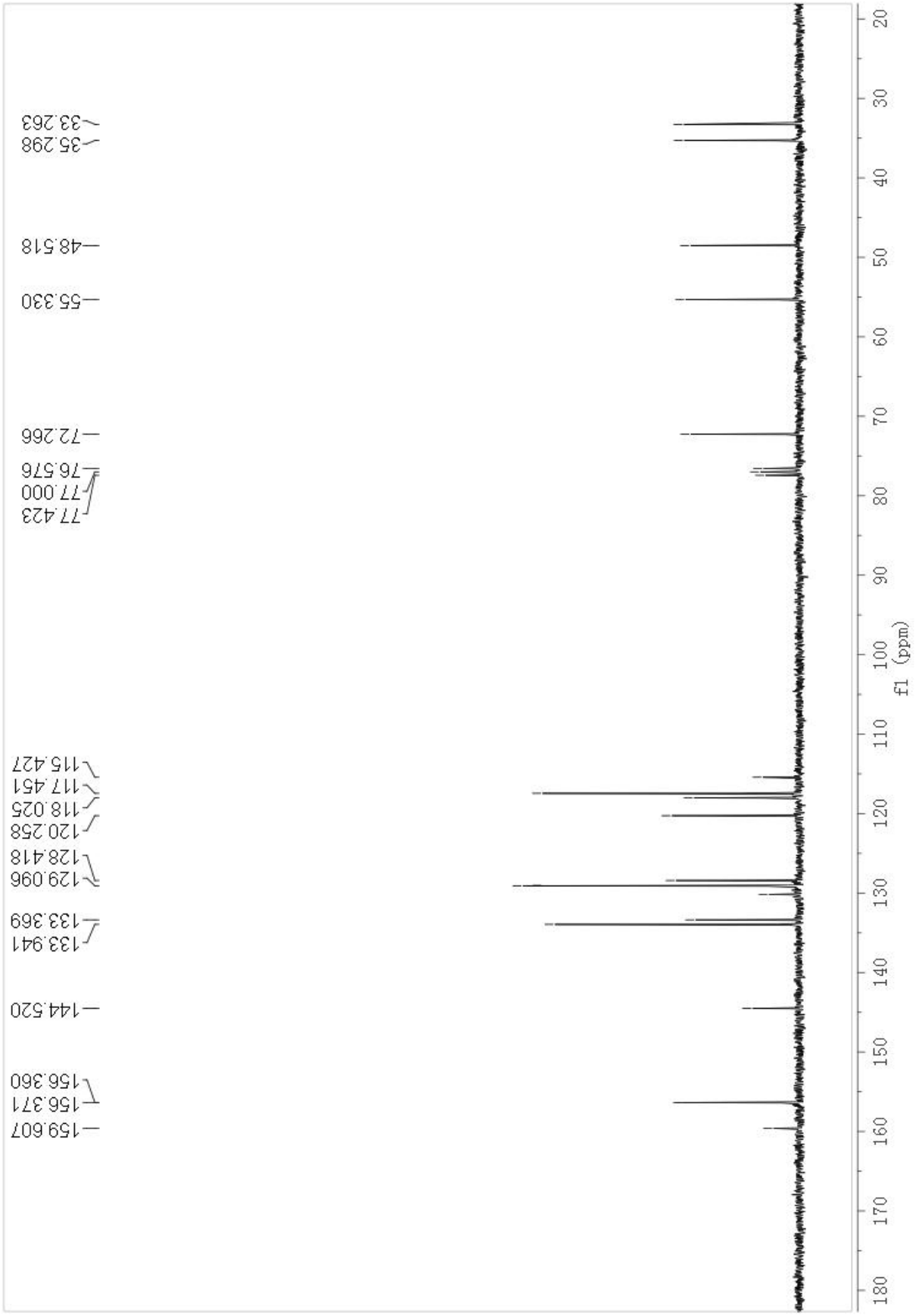
$C_{23}H_{22}N_4S$
Exact Mass: 386.2
Mol.Wt: 386.5



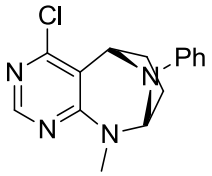
^{1}H NMR spectrum of Compound **3i**



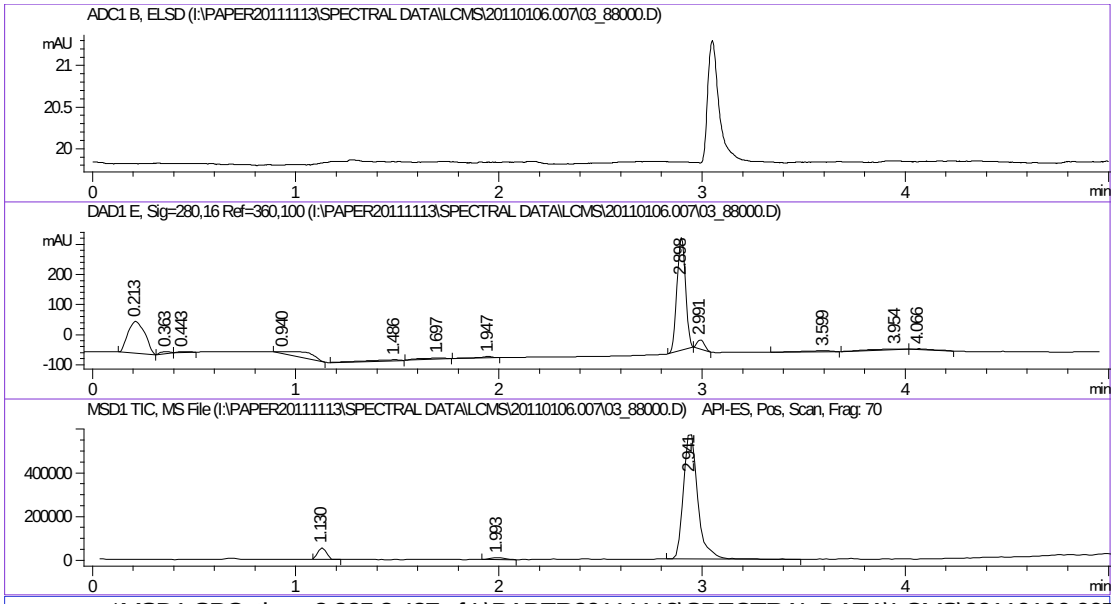
^{13}C NMR spectrum of Compound **3i**

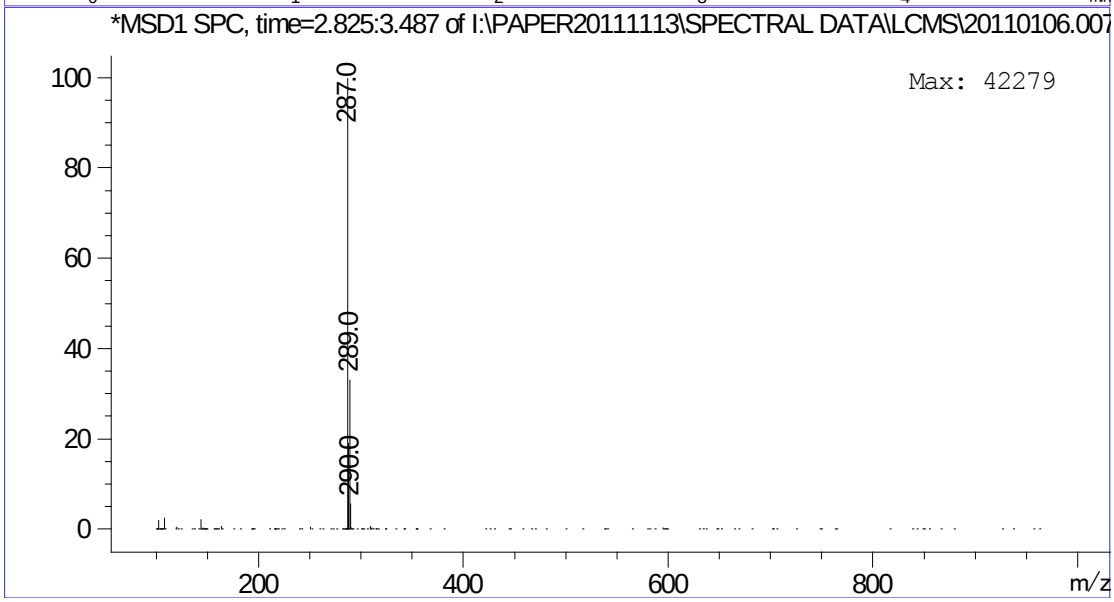


LC-MS-ELSD spectra of Compound **3j**

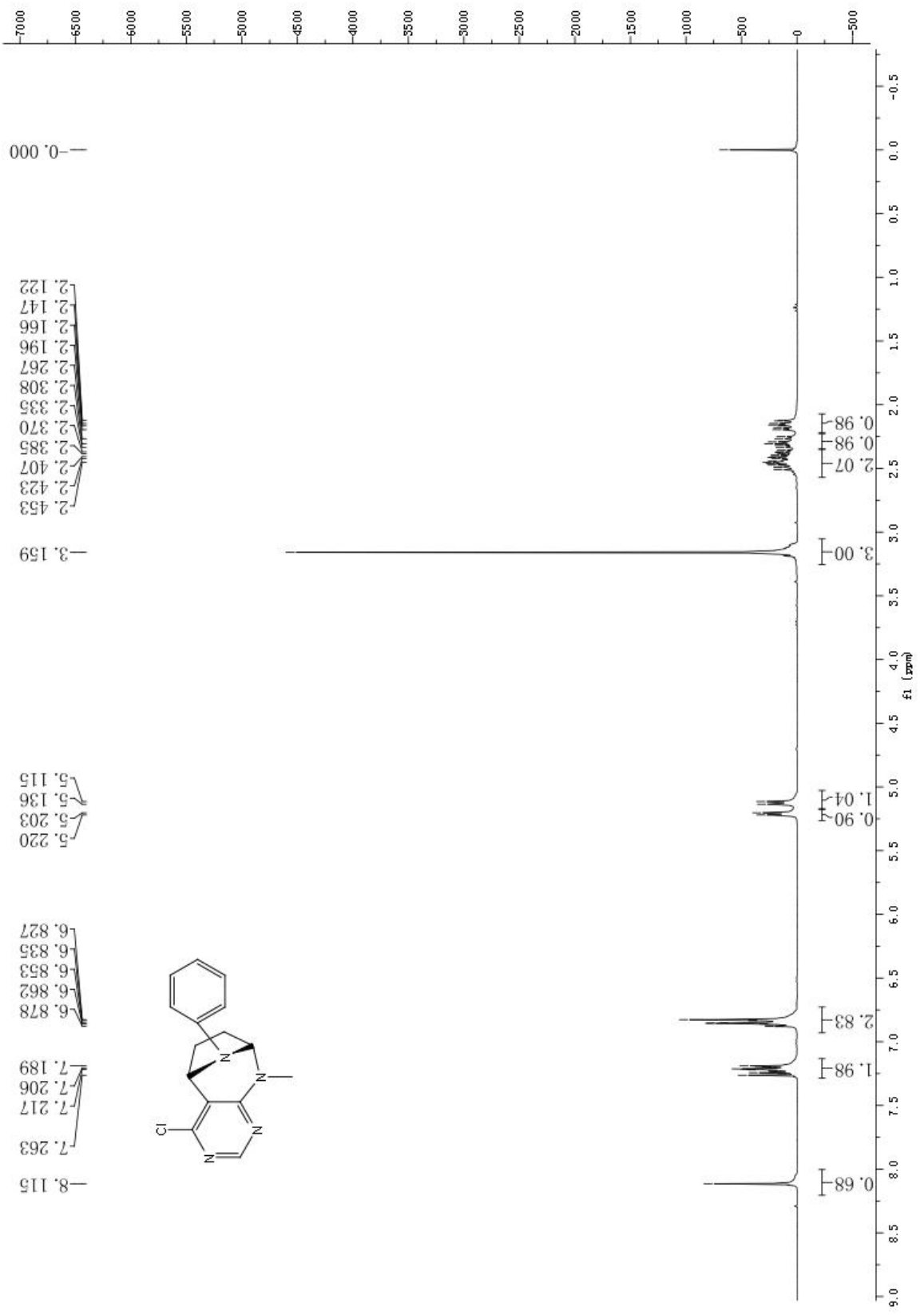


$C_{15}H_{15}ClN_4$
Exact Mass: 286.1
Mol. Wt: 286.8

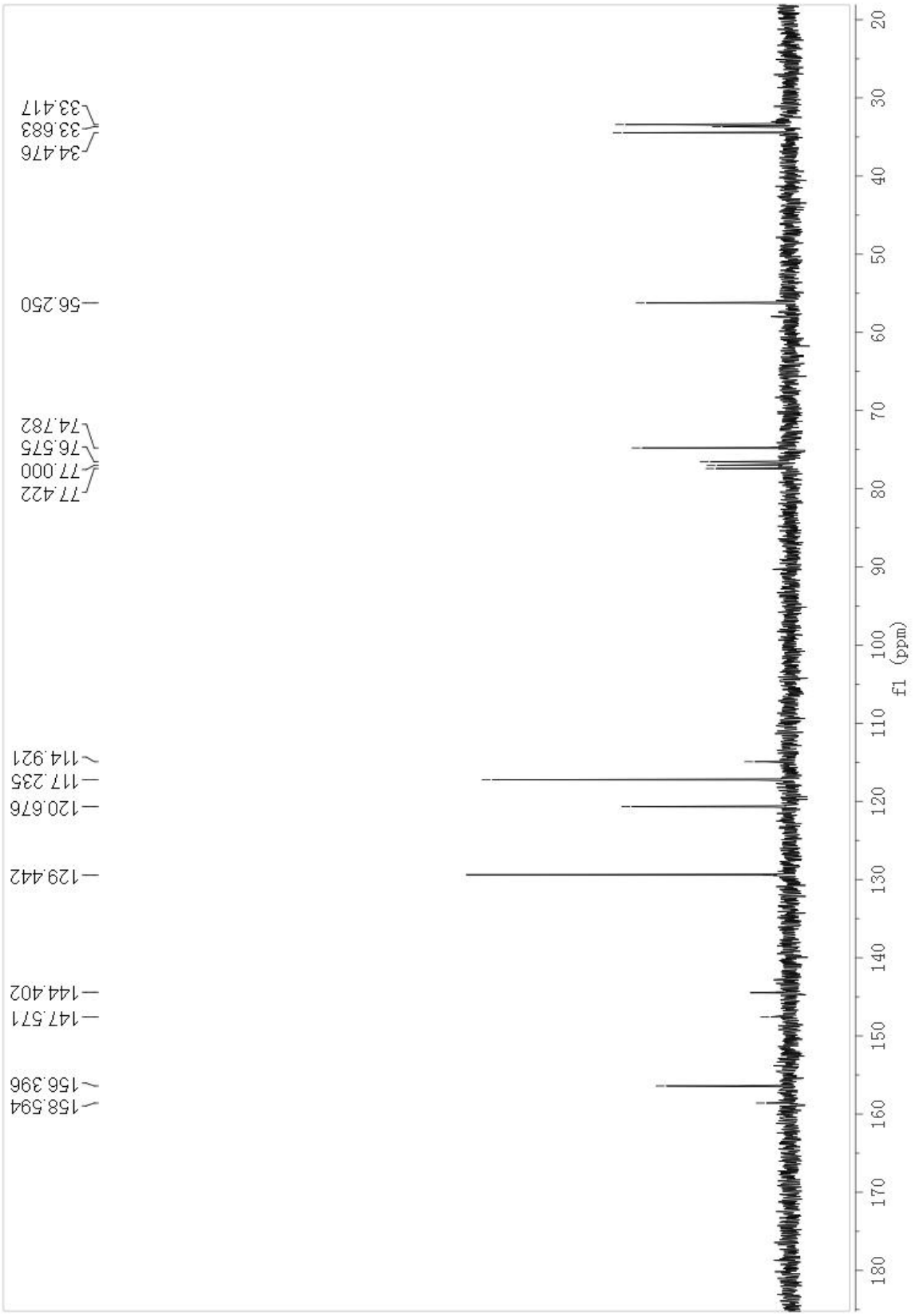




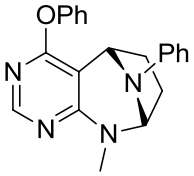
^{1}H NMR spectrum of Compound **3j**



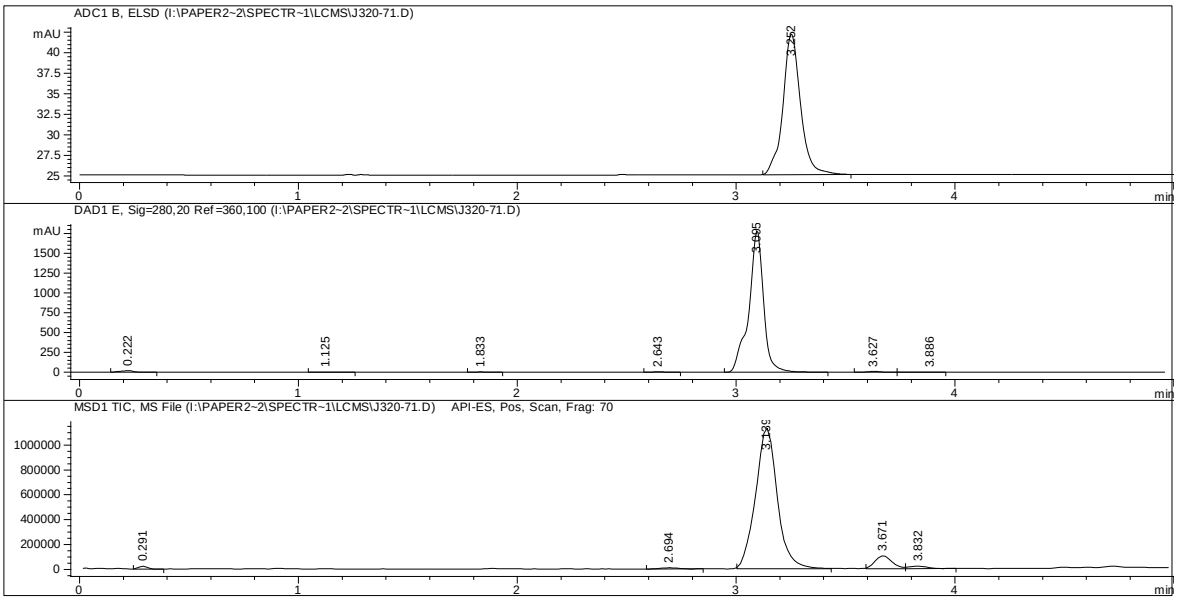
^{13}C NMR spectrum of Compound **3j**

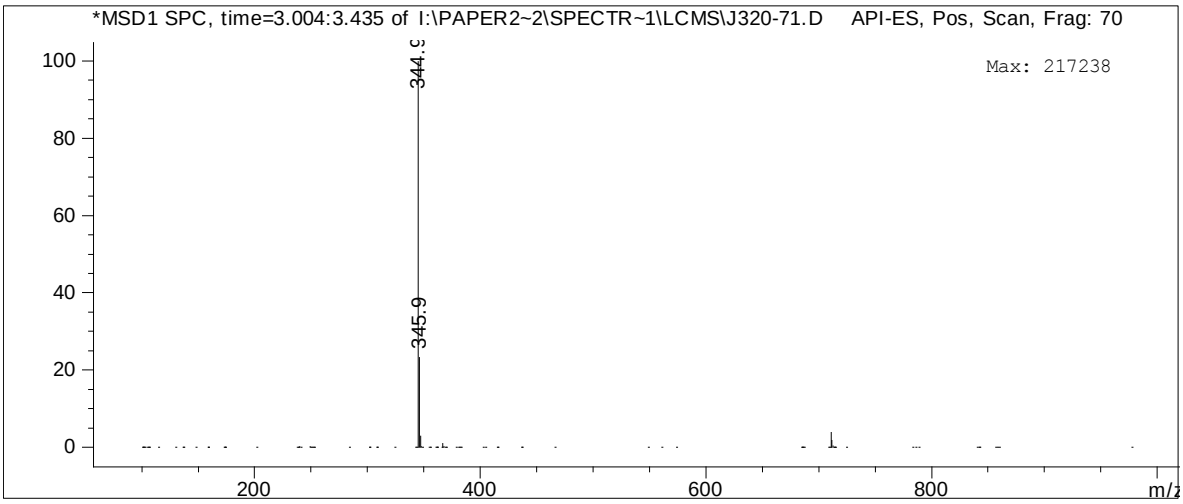


LC-MS-ELSD spectra of Compound **3k**

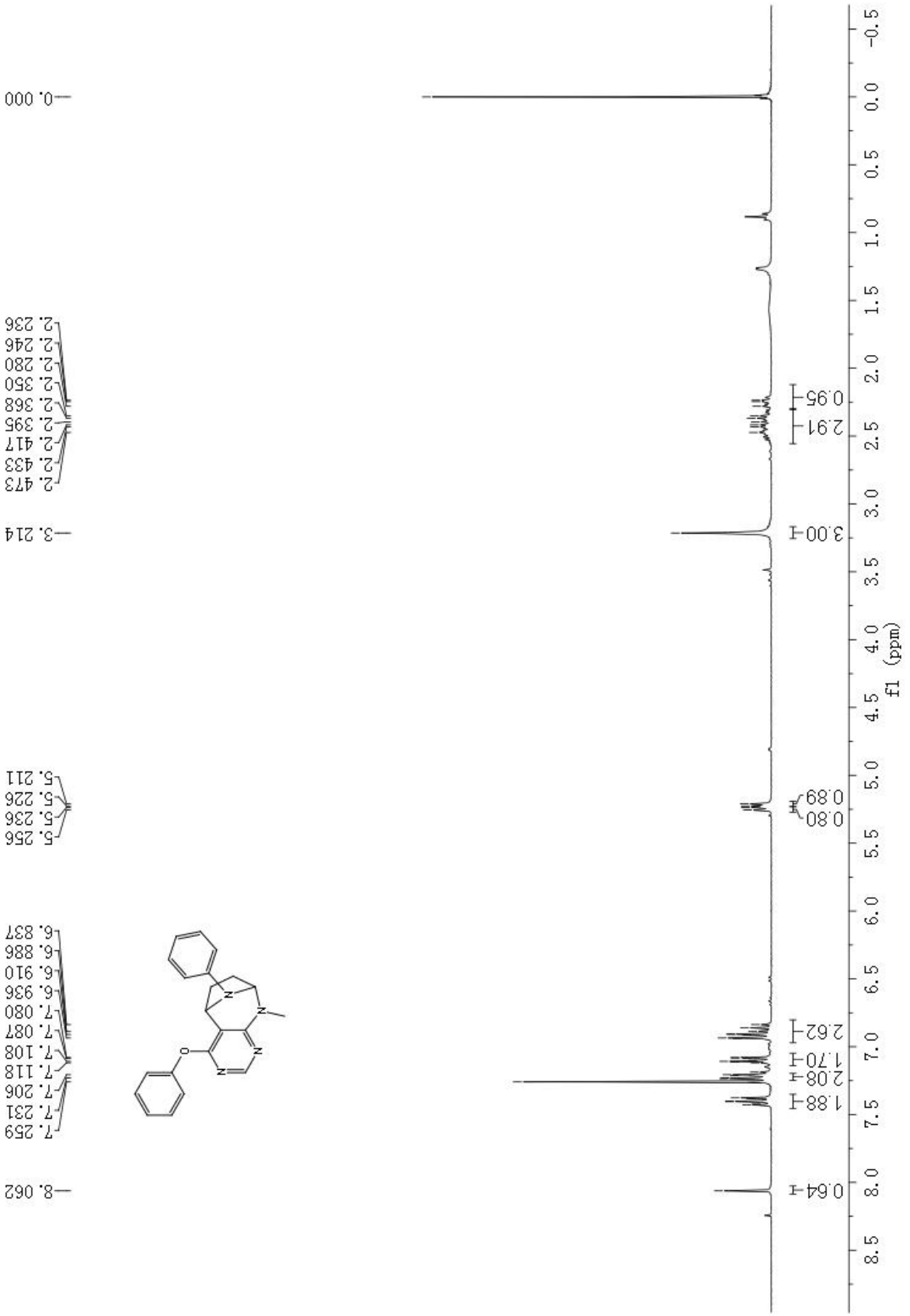


$C_{21}H_{20}N_4O$
Exact Mass: 344.2
Mol. Wt: 344.4

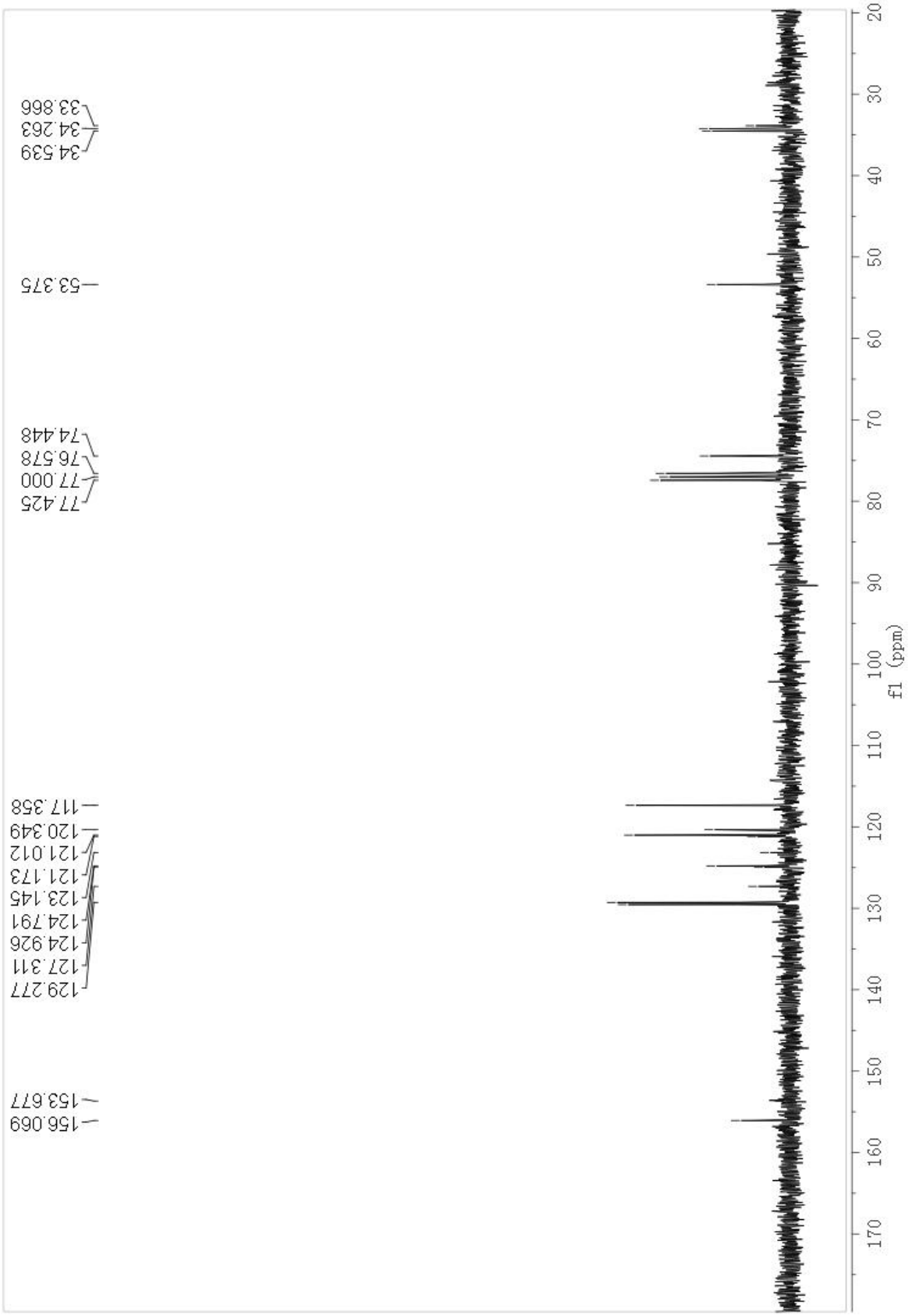




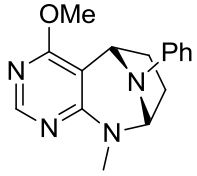
^{1}H NMR spectrum of Compound **3k**



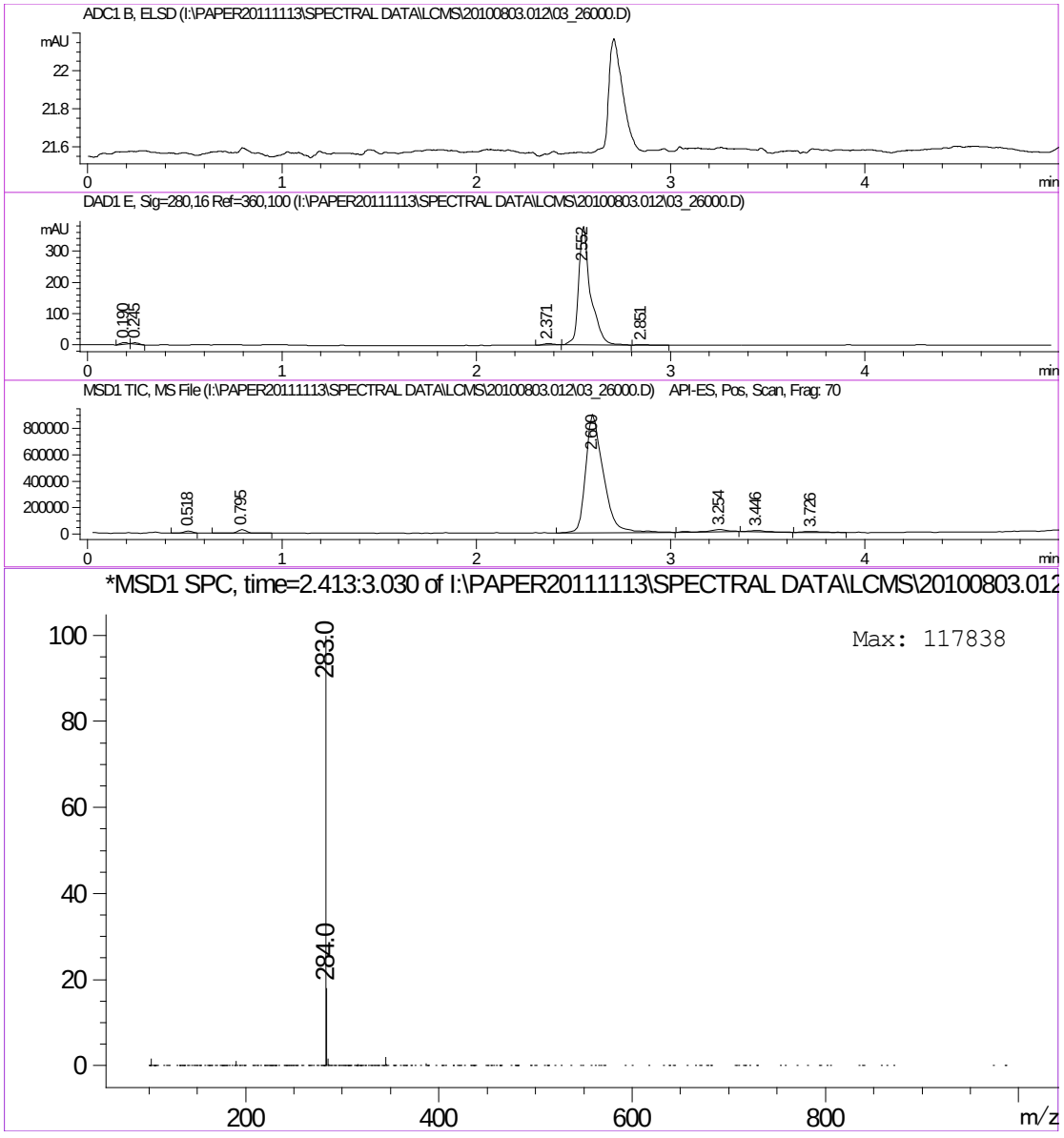
^{13}C NMR spectrum of Compound **3k**



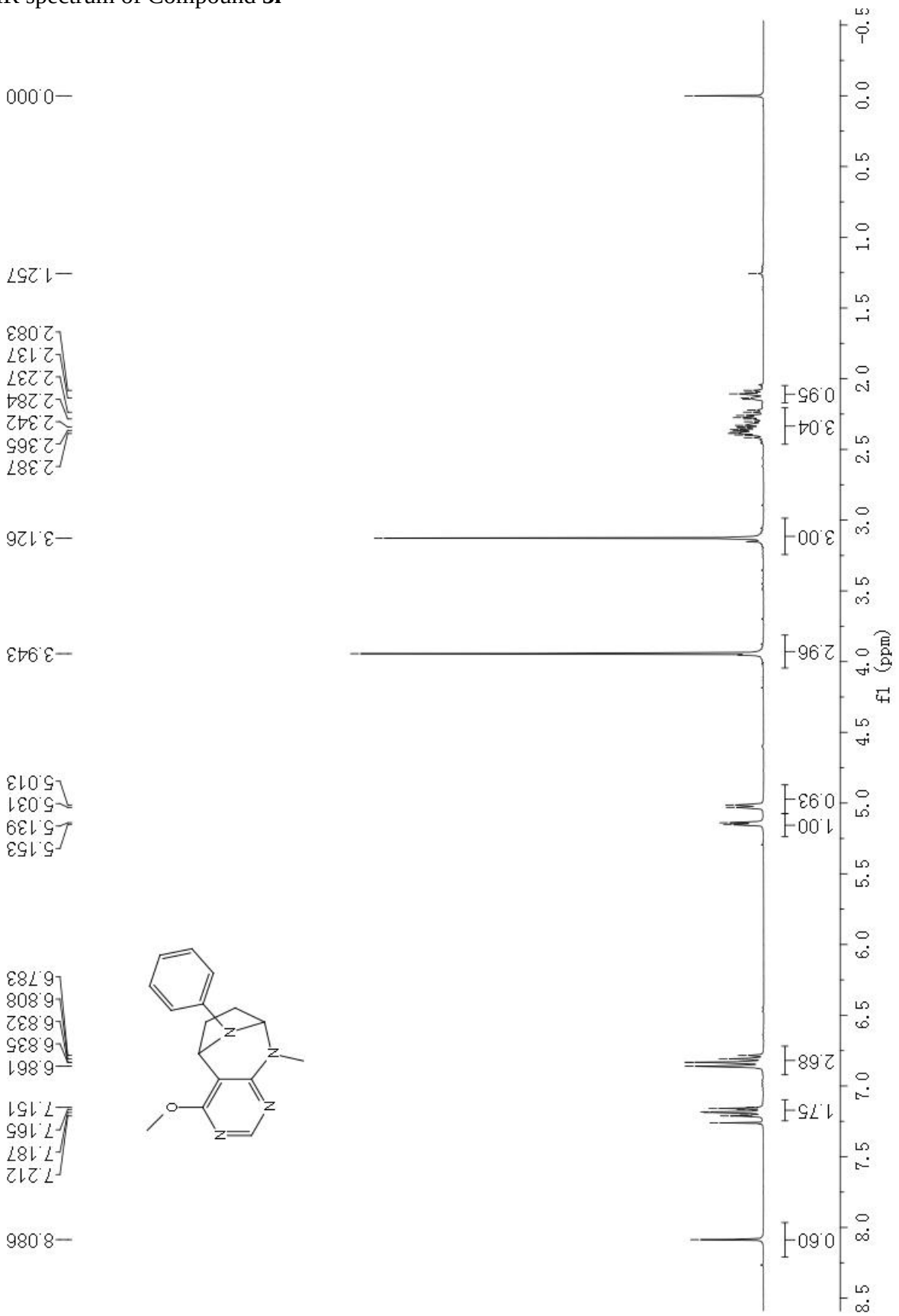
LC-MS-ELSD spectra of Compound **3l**



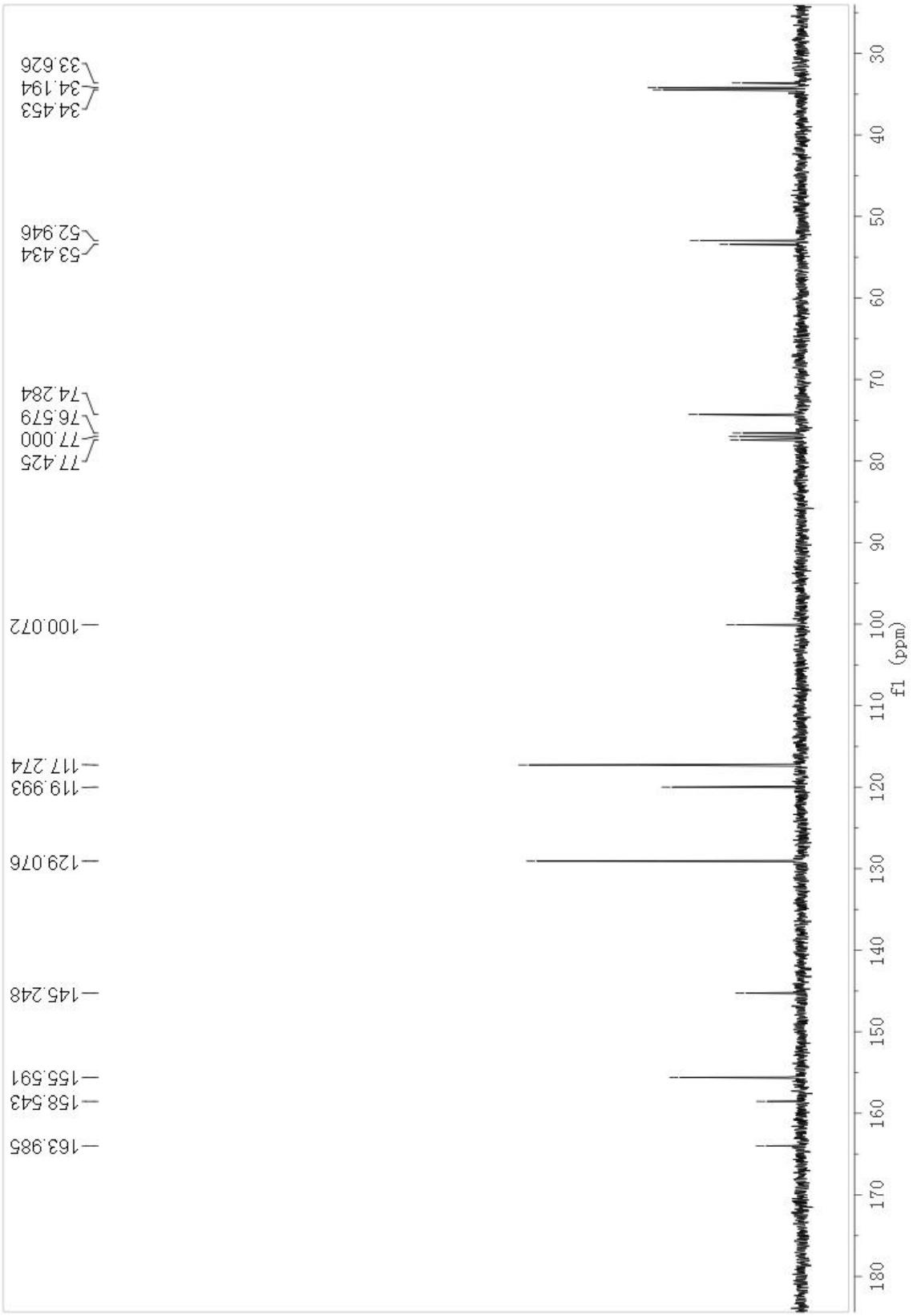
$C_{16}H_{18}N_4O$
Exact Mass: 282.1
Mol. Wt: 282.3



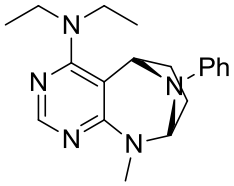
^{1}H NMR spectrum of Compound **3l**



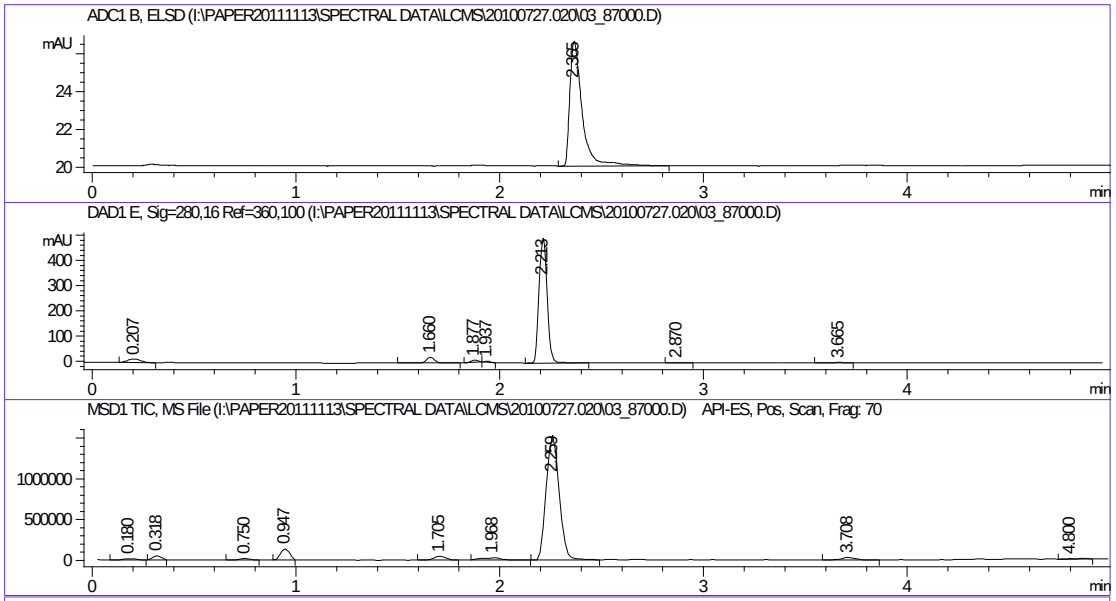
^{13}C NMR spectrum of Compound **3l**

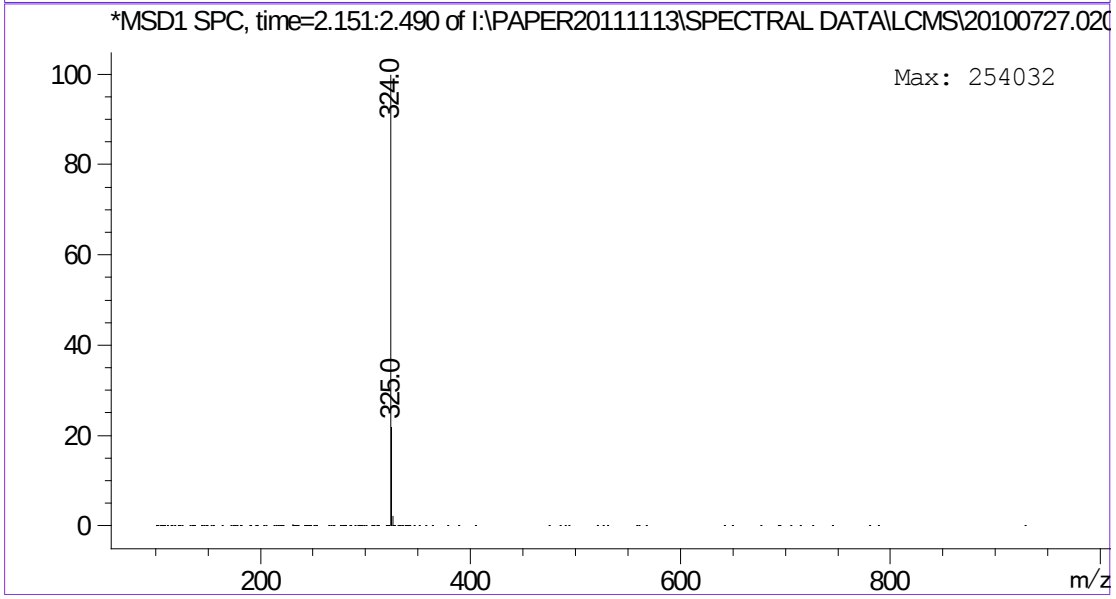


LC-MS-ELSD spectra of Compound **3m**

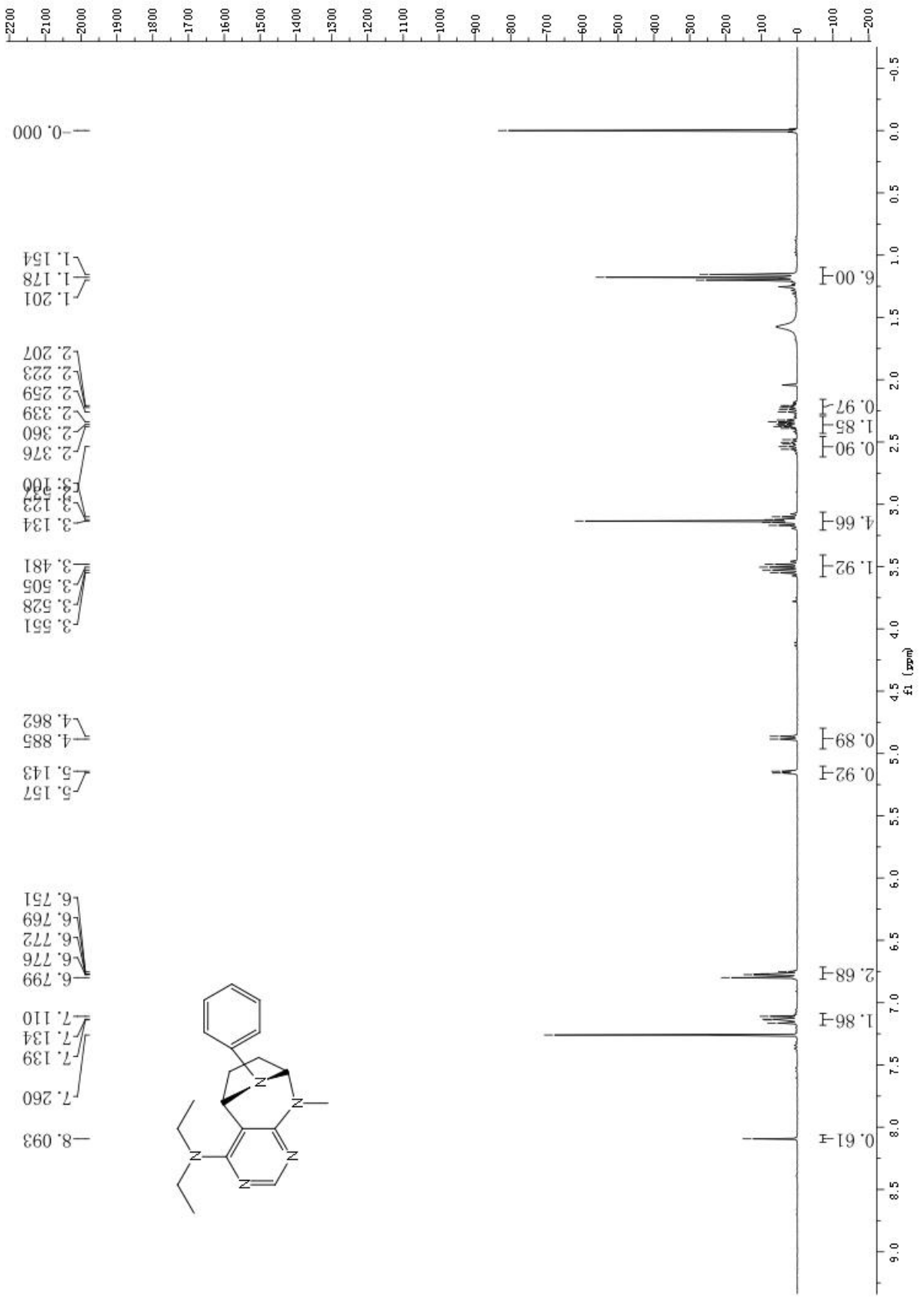


$C_{19}H_{25}N_5$
Exact Mass: 323.2
Mol. Wt: 323.4

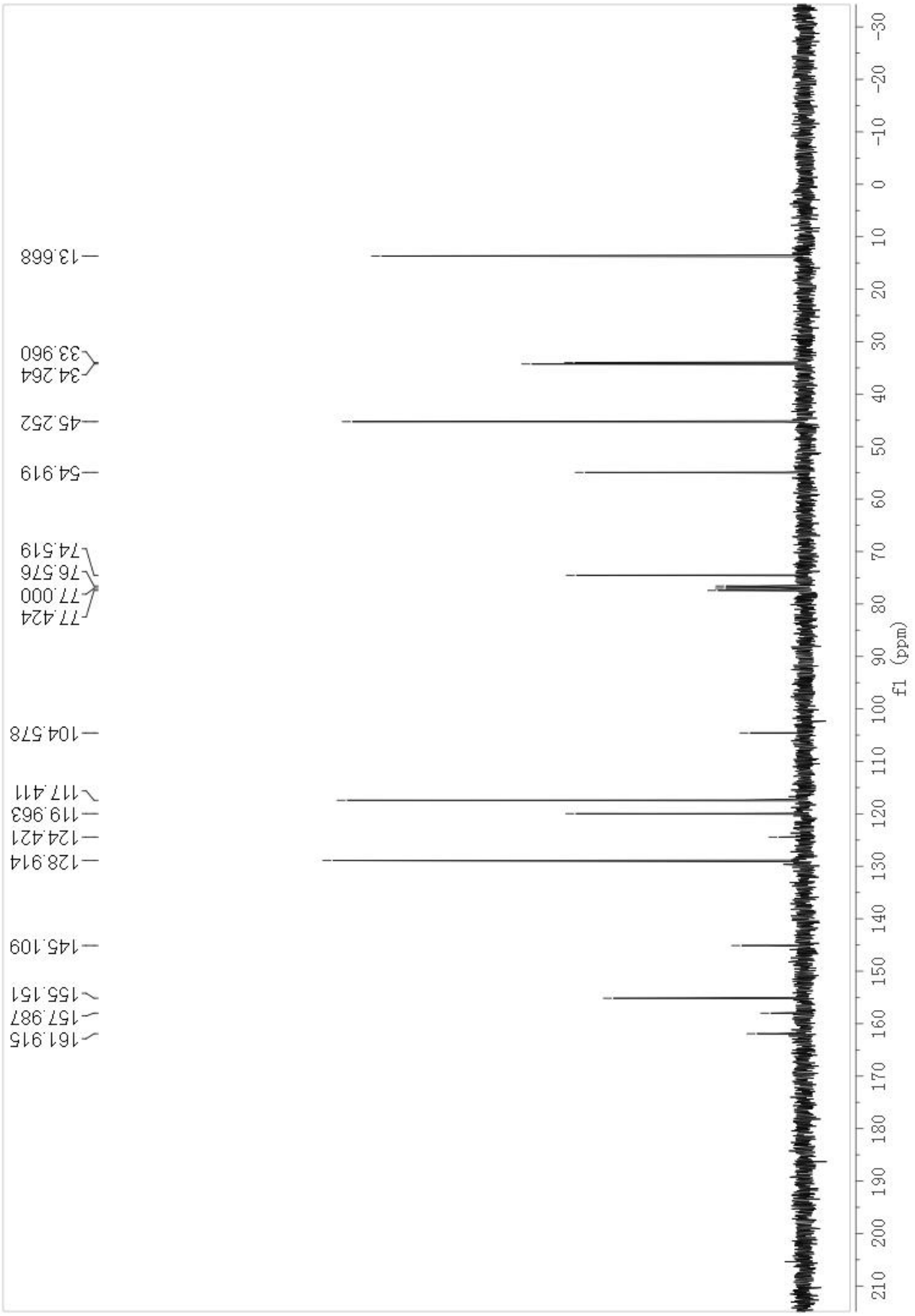




^{1}H NMR spectrum of Compound **3m**

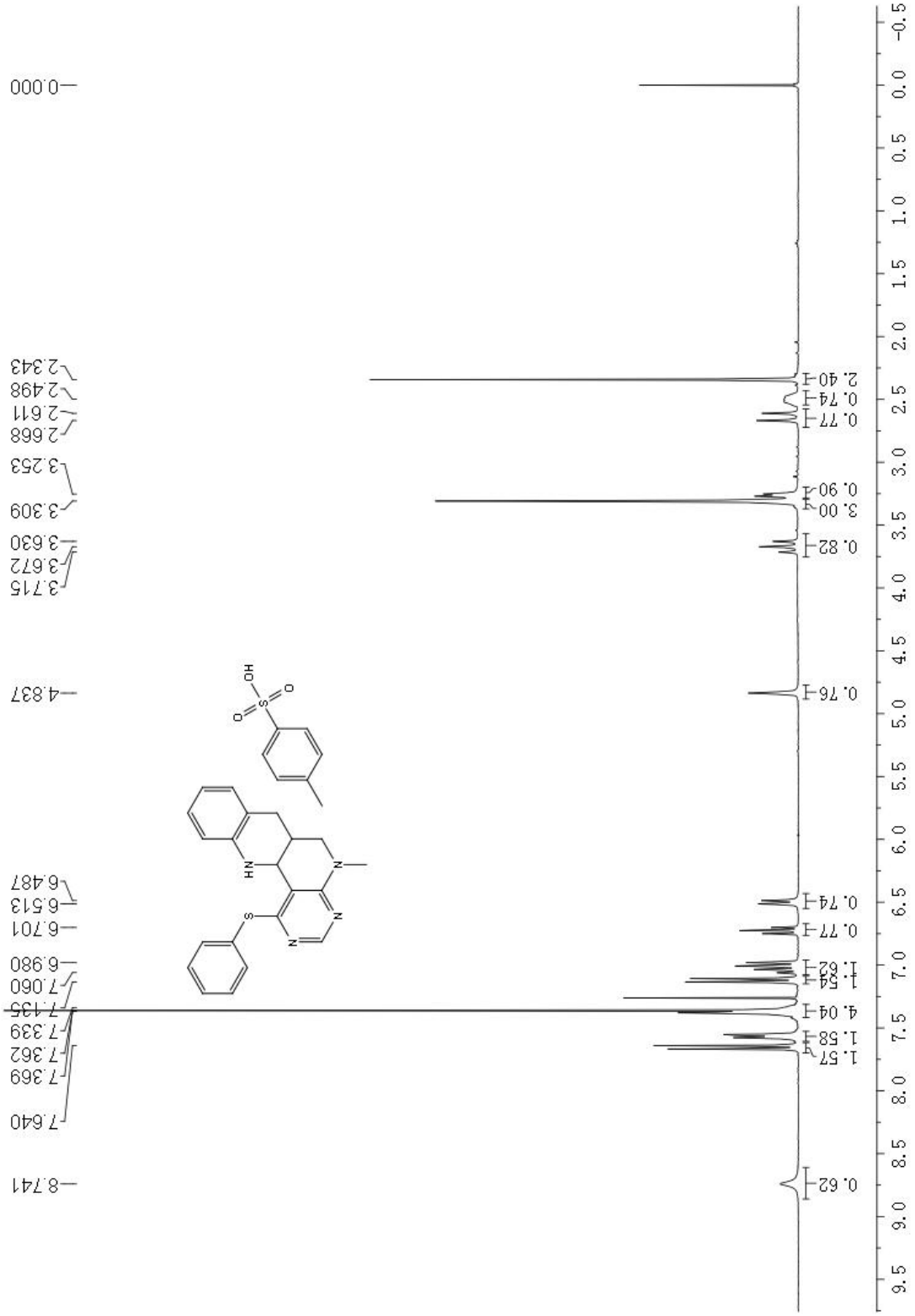


^{13}C NMR spectrum of Compound **3m**



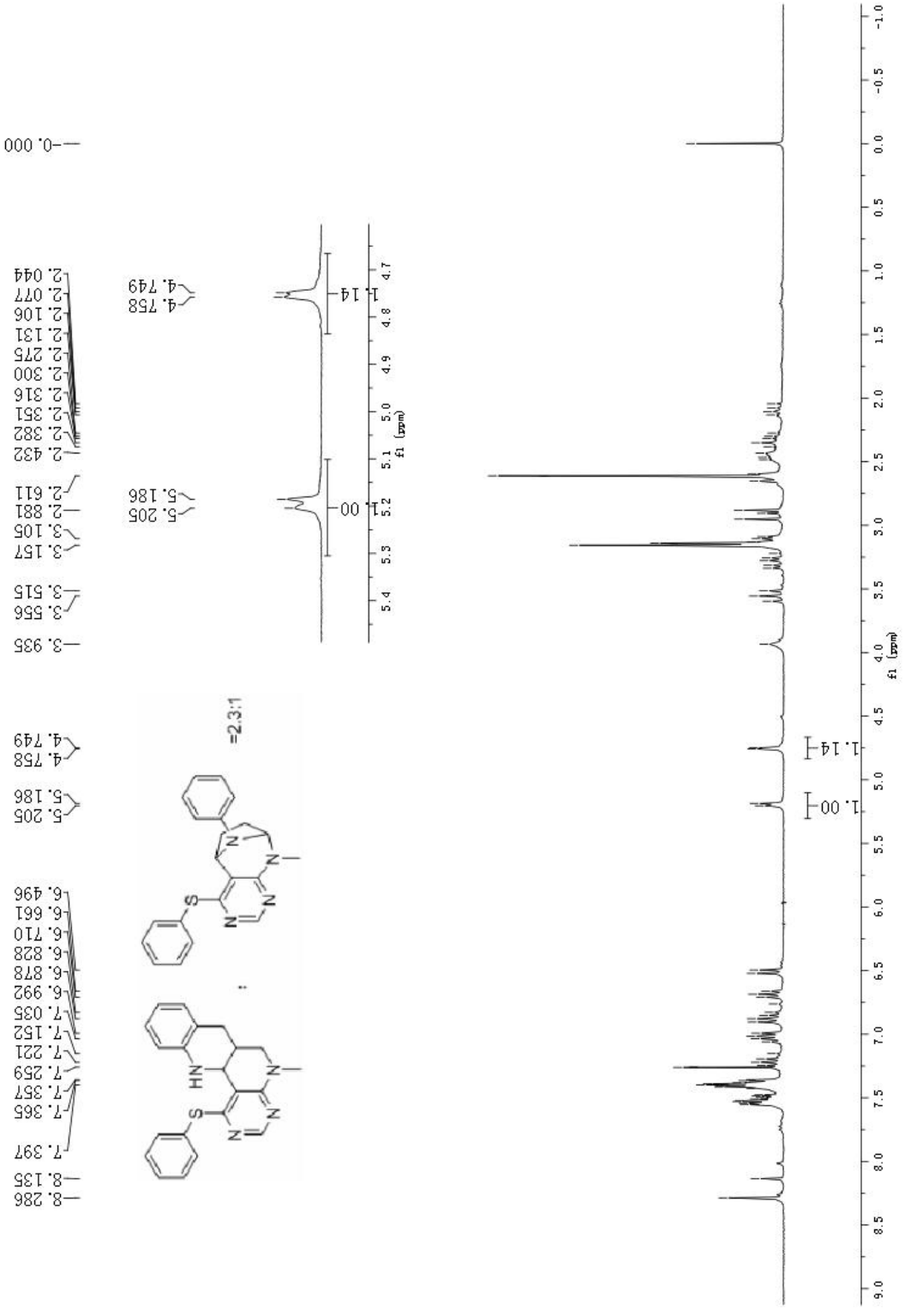
^{1}H NMR spectrum of mixture of **2a** and **3a**

Entry 5, Table 1



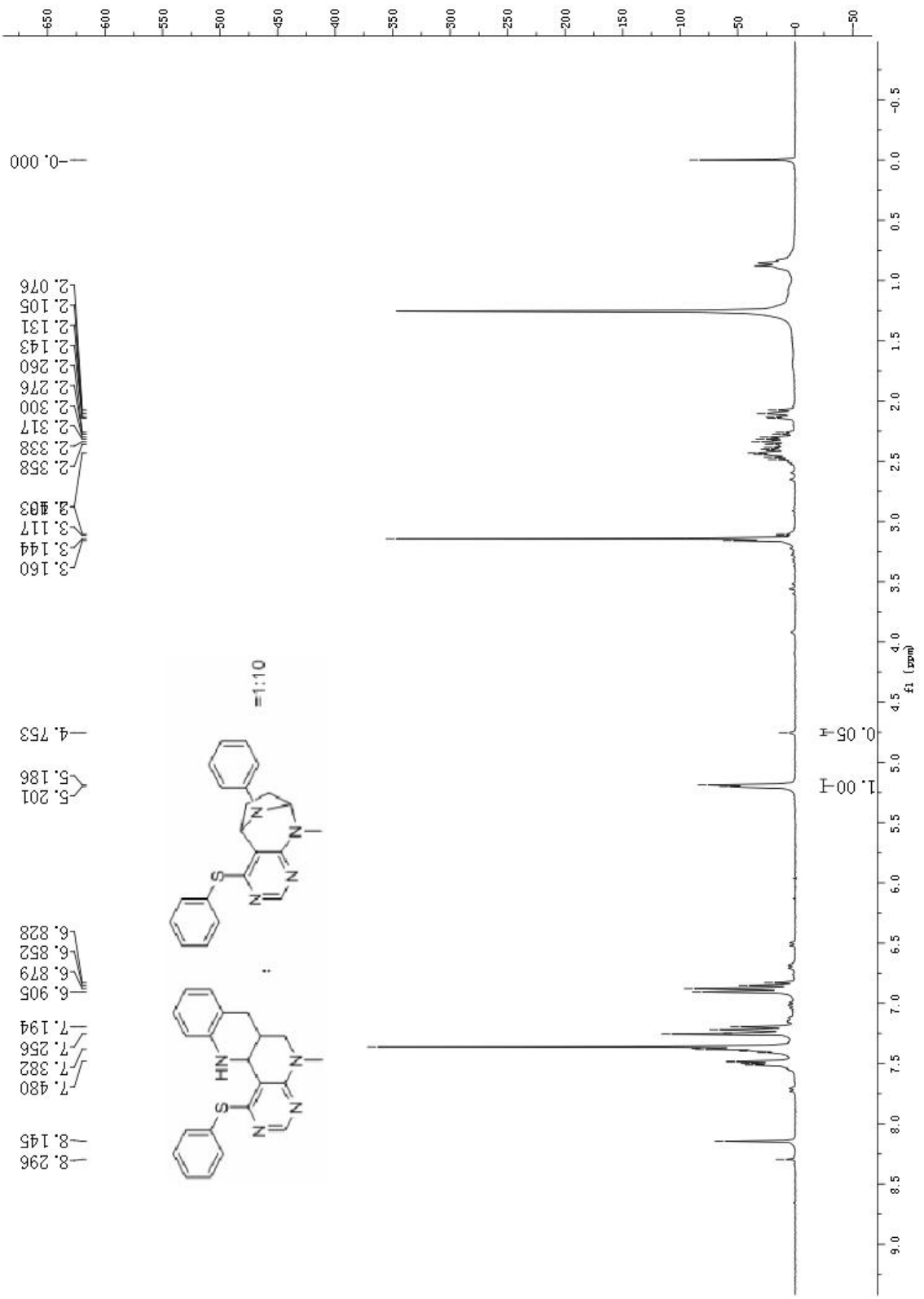
^{1}H NMR spectrum of mixture of **2a** and **3a**

Entry 8, Table 1



^{1}H NMR spectrum of mixture of **2a** and **3a**

Entry 10, Table 1



2. Additional computational results and discussion

2.1. Potential energy surface between In2 and TS2

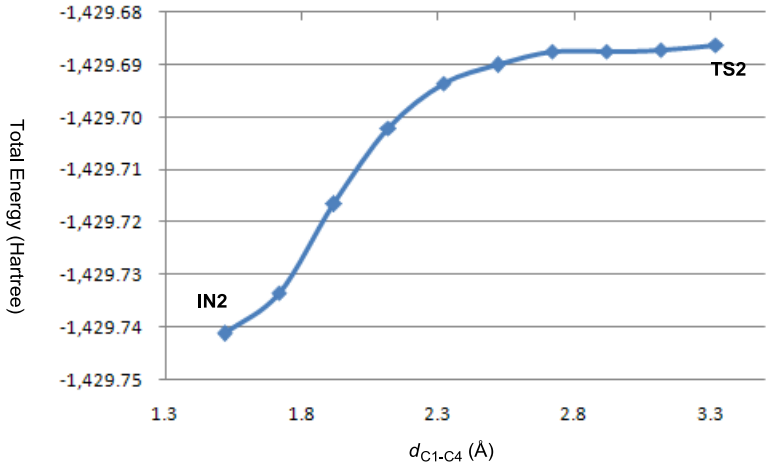


Figure S1. Energy diagram for the formation of the C1-C4 bond after **TS2** at B3LYP/6-311+(d,p) level in the gas phase. Potential energy surfaces were scanned at 0.2 Å intervals for the formation of the C-C bond. The formation of **IN2** after **TS2** is found to be a downhill process, with no intervening intermediates or transition states.

2.2. FMO analysis

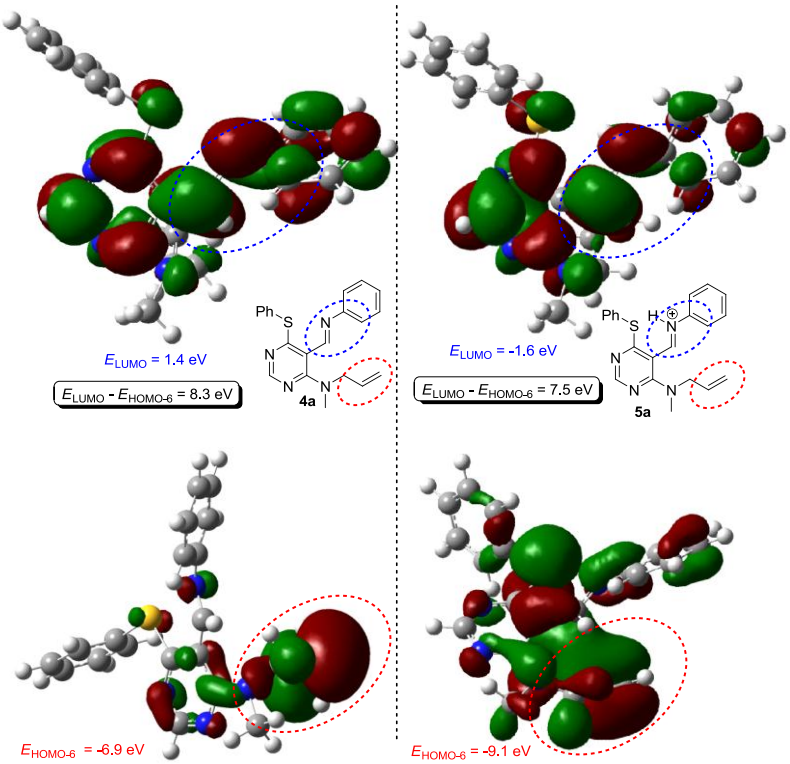
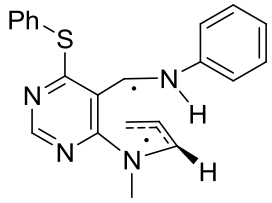


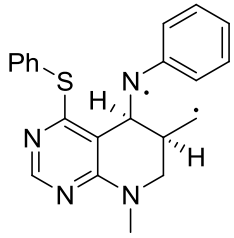
Figure S2. FMOs of **4a** and **5a** (calculated by HF/6-31G(d) based on the B3LYP/6-311+G(d,p) geometries).

2.3. Additional analysis of diradical pathways from 4a and 5a



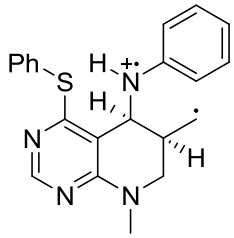
IN3'

IN3′ can be found only in this triplet state and is higher than **TS2** by 11.0 kcal/mol. When we searched its singlet diradical, it directly collapsed to **IN2**. This suggest that no involvement of such a diradical species with a siglet diradical character exists for the ene-type reaction shown in Figure 1.



***cis*-IN1'**

A possible diradical species of ***cis*-IN1′** in the D-A reaction could not be located in its singlet diradical state. Its triplet diradical state is higher than ***endo*-TS1** by 10.6 kcal/mol. Therefore, diradical pathway of the D-A reaction can be ruled out.



***cis*-HIN1'**

A possible diradical cation species of ***cis*-HIN1′** in the D-A reaction could not be located in its singlet diradical state. Its triplet diradical state is higher than ***endo*-TS1** by 15.9 kcal/mol. Therefore, diradical pathway of the D-A reaction can be ruled out.

2.4. Computed Energies of All Stationary Points

Thermal enthalpy corrections (*H*, in Hartree)
Thermal free energy corrections (*G*, in Hartree)
Thermal correction to Gibbs free energy (*TCGFE*, in Hartree)
Total free energy in solution (E_{sol}, in Hartree)
Thermal corrected Gibbs free energy in toluene solution (G_{sol}, in Hartree)
Single-point energy (SP, in Hartree)

	H	*G*	G_{sol}	*TCGFE*	$E_{sol(B3LYP)}$
4a	-1429.328535	-1429.409938	-1429.433293	0.308856	-1429.742149
***exo*-TS1**	-1429.279792	-1429.354964	-1429.380934	0.313949	-1429.694883
***endo*-TS1**	-1429.281491	-1429.358423	-1429.389333	0.312377	-1429.701710
***cis*-IN1**	-1429.330572	-1429.405682	-1429.436853	0.317885	-1429.754738
***trans*-INN1**	-1429.332500	-1429.408104	-1429.440521	0.317304	-1429.757825
TS2	-1429.297237	-1429.376340	-1429.394808	0.305822	-1429.700630
IN2	-1429.351580	-1429.427038	-1429.451528	0.316404	-1429.767932
5a	-1429.708116	-1429.789950	-1429.847581	0.322449	-1430.170030
***exo*-HTS1**	-1429.668793	-1429.744807	-1429.814257	0.327318	-1430.141575
***endo*-HTS1**	-1429.672586	-1429.749609	-1429.822044	0.326289	-1430.148333
***cis*-HIN1**	-1429.720485	-1429.795083	-1429.868294	0.332624	-1430.200918
***trans*-HIN1**	-1429.719064	-1429.794273	-1429.869589	0.331717	-1430.201306
HTS3	-1429.668718	-1429.749384	-1429.815519	0.318104	-1430.133623

	SP			SP
4a	-1429.718794		**5a**	-1430.112399
IN3′ (triplet)	-1429.664655		**cis-HIN1′** (triplet)	-1430.050466
cis-IN1′ (triplet)	-1429.651940			

2. 5. Coordinates of All Stationary Points

4a

C	2.31763000	3.55862500	1.58987900
C	1.41282900	-0.01625500	-0.38387300
C	3.08362400	-2.25788000	-1.23025300
C	2.05692400	3.08432600	2.80542900
C	0.29104300	0.91157200	-0.35796500
C	-1.05546400	0.51620100	-0.16697100
C	-1.76339000	2.54955000	-0.88149300
S	-1.45516900	-1.13241800	0.38492400
N	1.39647100	-1.15513500	0.19957200
C	2.45155800	-2.06323700	0.00845000
C	2.84862000	-2.84368100	1.10449400
C	3.88757600	-3.75865200	0.97716000
C	4.52560900	-3.93506700	-0.25183500
C	4.11270300	-3.18807900	-1.35406900
N	-0.54987800	3.07527200	-1.01194800
N	1.75001200	2.84680000	-0.74239800
C	2.66774700	2.68609200	0.40963300
C	1.87622500	4.13395200	-1.43188500
N	-2.07449900	1.34388200	-0.41859700
C	0.48392900	2.28317200	-0.69054500
H	-2.59852100	3.18639600	-1.16113400
H	2.27507500	0.31504600	-0.97503700
H	2.33352200	-2.70917800	2.04829700
H	4.19357600	-4.34561000	1.83606700
H	5.32533500	-4.65970100	-0.35288300
H	4.58532600	-3.33789700	-2.31867000
H	2.74342600	-1.70662800	-2.09956300
H	3.67125500	2.92815700	0.04453300
H	2.68973700	1.64625000	0.72864600
H	2.93835600	4.31908800	-1.60683700
H	1.36019000	4.08821200	-2.38899200
H	1.45243100	4.97042900	-0.86638100
H	2.28683400	4.63126900	1.41594600
H	1.81791300	3.74270300	3.63310000
H	2.07495800	2.01937500	3.01745800
C	-3.25113200	-1.12495200	0.23305500
C	-4.03941200	-0.81784800	1.34302900
C	-3.85246200	-1.52580600	-0.96137600
C	-5.42773900	-0.89654200	1.25199700
H	-3.56675600	-0.51364200	2.26914400
C	-5.24086100	-1.60107200	-1.04878300
H	-3.23528500	-1.77439600	-1.81648700
C	-6.02991100	-1.28566800	0.05659700
H	-6.03779000	-0.65339000	2.11483200
H	-5.70524500	-1.90889600	-1.97903200
H	-7.11024900	-1.34714600	-0.01223400

***exo*-TS1**

C	2.60995100	1.15703100	0.91626400
C	1.29734900	0.31759900	-0.37796700
C	3.65573100	-1.08840900	-0.65417400
C	3.79394100	0.39605200	0.92209300
C	0.08372200	1.11787800	-0.15173200
C	-1.22306200	0.62112700	0.01091800
C	-2.04179400	2.74022500	0.02273700
S	-1.55970800	-1.13947400	0.07587700
N	1.28281800	-0.98783300	-0.09347400
C	2.41680800	-1.68610400	-0.23476000
C	2.44426600	-3.03654400	0.23811400
C	3.61092100	-3.75087400	0.26088500
C	4.82859200	-3.16858000	-0.19354400
C	4.84261500	-1.88403300	-0.66570700
N	-0.86126500	3.34092800	-0.05894500
N	1.44307600	3.13939500	-0.18123300
C	2.68433100	2.55633100	0.35406700
C	1.50499700	4.59188200	-0.32122800
N	-2.28190400	1.43627100	0.09557800

C	0.21303400	2.53162000	-0.11675500
H	-2.91236700	3.39061900	0.05006200
H	1.90063500	0.68614200	-1.21540300
H	1.50950700	-3.46044200	0.58536000
H	3.61394100	-4.77182100	0.62631400
H	5.73821200	-3.75868500	-0.18775500
H	5.76085300	-1.45357300	-1.05176000
H	3.62057000	-0.25595600	-1.34679000
H	3.03260700	3.22689000	1.15277300
H	3.45081100	2.59028200	-0.43121300
H	2.47967100	4.85574000	-0.73942800
H	0.71937200	4.93539300	-0.98883900
H	1.38271700	5.10420300	0.64130800
H	1.94520800	1.02310800	1.76250700
H	3.95588500	-0.33043000	1.70694900
H	4.69770000	0.82011200	0.49888700
C	-3.36153100	-1.14568200	0.02382200
C	-4.08940000	-1.23381300	1.21159700
C	-4.02791500	-1.17033100	-1.20309000
C	-5.47916700	-1.33099600	1.17196100
H	-3.56787000	-1.21945500	2.16109400
C	-5.41740500	-1.26464600	-1.23927500
H	-3.45882400	-1.11209900	-2.12325300
C	-6.14505900	-1.34411000	-0.05245200
H	-6.04054400	-1.39508900	2.09756500
H	-5.93101200	-1.27883900	-2.19429400
H	-7.22637300	-1.41958100	-0.08225500

***endo*-TS1**

C	2.28119400	0.95497500	1.41013100
C	1.06132900	-0.03183900	0.21109900
C	3.07663800	-1.85195800	0.68016800
C	3.33377900	0.11172400	1.80004700
C	-0.02461100	0.95484400	-0.02939000
C	-1.36332800	0.56807700	-0.12758500
C	-1.99345400	2.68284700	-0.57388000
S	-1.75471100	-1.17579000	0.06083800
N	1.83773900	-0.37544600	-0.83215000
C	2.83317800	-1.24930900	-0.59797000
C	3.79729900	-1.46171500	-1.63357900
C	4.90867500	-2.23196100	-1.41664100
C	5.12811000	-2.84652600	-0.15372400
C	4.21913500	-2.67972600	0.86002800
N	-0.77694400	3.19585200	-0.47503900
N	1.46318000	2.88744300	0.03641000
C	2.61632700	2.12576000	0.50717000
C	1.74306500	4.27993500	-0.29653700
N	-2.36019000	1.41513900	-0.39377600
C	0.22674600	2.34413900	-0.16775500
H	-2.78912900	3.37928300	-0.82597000
H	0.79139200	-0.78895100	0.95339500
H	3.61367500	-0.98151200	-2.58772000
H	5.62997100	-2.37925500	-2.21292700
H	6.00395000	-3.46831200	-0.00571400
H	4.36233400	-3.18265300	1.81059100
H	2.25068000	-1.98769000	1.36507100
H	3.24340700	2.83186700	1.06248000
H	3.21102100	1.76118100	-0.34086200
H	2.55533300	4.33210500	-1.03053200
H	0.85088500	4.73852600	-0.71053400
H	2.04768400	4.83432600	0.59803600
H	1.52898900	1.15719900	2.16889400
H	3.29672400	-0.38208300	2.76200000
H	4.32290900	0.23600900	1.37707200
C	-3.54998800	-1.17561100	0.07100800
C	-4.24247500	-1.05093100	1.27667300
C	-4.24817000	-1.37605100	-1.12084900
C	-5.63418700	-1.11567700	1.28619900
H	-3.69357500	-0.90102300	2.19835200
C	-5.63979600	-1.44123400	-1.10548300

H	-3.70325000	-1.47366400	-2.05162800
C	-6.33384500	-1.31039200	0.09626800
H	-6.17055000	-1.01500200	2.22311300
H	-6.18049300	-1.59296700	-2.03292000
H	-7.41682900	-1.36186500	0.10589800

***cis*-HIN1**

N	-1.90111300	1.44159300	-0.77553700
C	-1.32330400	2.41324700	-1.48355100
N	-0.08920000	2.87545100	-1.34569500
C	0.69214500	2.26452000	-0.43940200
C	0.23902100	1.12227300	0.27195400
C	-1.11769600	0.81426200	0.09553200
N	1.93787100	2.78043600	-0.20961900
C	2.56812800	2.40656700	1.05167800
C	2.61365900	0.88518600	1.21129600
C	1.17058800	0.32582900	1.17620800
C	3.52595400	0.23743200	0.16052900
C	3.54371900	-1.28999700	0.34132400
C	2.14892600	-1.84000100	0.31347400
N	1.15671500	-1.10600500	0.75107900
C	4.52143400	-2.03930500	-0.51145600
C	4.22786800	-3.23887500	-1.04115500
C	2.91757400	-3.81409900	-0.83882900
C	1.91698200	-3.15936600	-0.18849600
S	-1.85984000	-0.46668200	1.12213900
C	2.31809200	4.06736000	-0.79800000
C	-3.50126900	-0.68369300	0.43215000
C	-3.70495800	-1.54230700	-0.64904900
C	-4.99493700	-1.73190500	-1.13672000
C	-6.07156400	-1.07468800	-0.54197500
C	-5.86097100	-0.22505400	0.54215100
C	-4.57330000	-0.02552200	1.03514600
H	-1.94009200	2.89169400	-2.23833500
H	2.03615800	2.85850600	1.90225400
H	3.58475800	2.80268900	1.05978900
H	3.03191000	0.66884400	2.19995200
H	0.77037600	0.32183500	2.19573700
H	4.54088500	0.62566200	0.27440000
H	3.19510100	0.48703500	-0.85088400
H	3.88700500	-1.48841800	1.37599700
H	0.21620500	-1.51041400	0.73864500
H	5.50635900	-1.59942400	-0.62409600
H	4.95999600	-3.79138700	-1.61632000
H	2.71842500	-4.79893900	-1.24749800
H	0.92756100	-3.59401000	-0.10345800
H	1.94432400	4.12538300	-1.81637000
H	3.40658000	4.13942400	-0.80392000
H	1.90591600	4.90995300	-0.23074500
H	-2.86667400	-2.05192900	-1.10795900
H	-5.15914300	-2.39405200	-1.97870400
H	-7.07469800	-1.22742000	-0.92243900
H	-6.69718600	0.28469800	1.00580000
H	-4.40277800	0.63566400	1.87549200

***trans*-IN1**

N	2.29433000	1.31212000	-0.69329600
C	2.09064200	2.61477700	-0.84617400
N	0.96086700	3.28341400	-0.65202400
C	-0.11347300	2.55785900	-0.28816900
C	-0.04506400	1.14632000	-0.15472500
C	1.22322800	0.58861100	-0.34124000
N	-1.27860200	3.24852900	-0.04600300
C	-2.37641500	2.56889200	0.62879300
C	-2.55926900	1.16586000	0.06638900
C	-1.26684700	0.34180800	0.23508300
C	-3.75158100	0.40541300	0.66905100
C	-3.45887100	-1.12796900	0.77076300
C	-2.46939200	-1.56070300	-0.30489300
N	-1.40259000	-0.88179500	-0.54475800

C	-4.70732100	-1.95563700	0.84502200
C	-4.89143500	-3.04200600	0.07957600
C	-3.88238200	-3.46696800	-0.88136700
C	-2.73950200	-2.77274900	-1.06356100
S	1.48098600	-1.17317400	-0.08488300
C	-1.26745200	4.70432000	0.02359500
C	3.26402700	-1.23153300	0.15687800
C	4.08986600	-1.62076500	-0.89871500
C	5.46406100	-1.74219500	-0.69955300
C	6.01663200	-1.47507600	0.55163500
C	5.19078500	-1.09142900	1.60774600
C	3.81626000	-0.97486100	1.41397400
H	2.95093800	3.20368800	-1.15410400
H	-3.28435300	3.15824100	0.47178900
H	-2.20457300	2.52589200	1.71765300
H	-2.70982100	1.26611100	-1.01350200
H	-1.16852800	0.07087100	1.30354200
H	-4.64222000	0.56388400	0.05643900
H	-3.98293000	0.77890500	1.67242500
H	-2.92207600	-1.26641000	1.72490300
H	-5.46482300	-1.64772300	1.56012300
H	-5.80243500	-3.62421000	0.16524100
H	-4.07267700	-4.35973700	-1.46733300
H	-1.99327200	-3.06986800	-1.79093800
H	-2.26617500	5.07480800	-0.21851800
H	-0.99175300	5.06497600	1.02445200
H	-0.54946700	5.09925500	-0.68951400
H	3.65642800	-1.81716400	-1.87167700
H	6.10222200	-2.04080100	-1.52383800
H	7.08608700	-1.56790600	0.70464600
H	5.61570500	-0.88641700	2.58420200
H	3.17094300	-0.68329600	2.23404200

TS2

H	2.74894100	0.90207300	-0.03802800
N	2.34384200	-0.16574500	-0.34745200
C	2.59332600	2.29050100	0.49691100
C	0.39355200	2.08821100	-0.61200800
C	0.10379000	0.72166000	-0.23912600
C	-1.29935200	0.43447600	-0.14766800
C	1.05832100	-0.30269200	-0.05546400
S	-1.81588400	-1.08292900	0.65665400
C	-1.79463200	2.37118700	-1.20540600
C	3.24647100	-1.24458400	-0.26247500
C	2.88572600	-2.53559600	-0.67517000
C	3.81664500	-3.56937200	-0.62824500
C	5.11644600	-3.33542800	-0.18274300
C	5.48052400	-2.04901500	0.21461800
C	4.55749700	-1.00968000	0.17686300
N	1.58847200	2.70740500	-0.41658500
N	-0.57413500	2.84412200	-1.19820700
C	1.86190900	3.95549900	-1.14990600
C	2.33299200	2.01417400	1.89598500
C	1.17900600	1.80508200	2.56005100
H	-2.55407100	2.96699600	-1.70340900
H	0.71653700	-1.26643800	0.31045800
H	1.88995500	-2.72128900	-1.05950800
H	3.52479000	-4.56142200	-0.95438300
H	5.83788300	-4.14327700	-0.15077000
H	6.48857100	-1.85300000	0.56251400
H	4.84110100	-0.01522400	0.50019000
N	-2.22920700	1.23188400	-0.62081200
H	3.52085800	2.82189800	0.31053100
H	1.29874300	3.98013100	-2.07791000
H	2.93206700	3.99371400	-1.35728100
H	1.58543500	4.82287600	-0.54502400
H	3.25717700	1.89640900	2.46066500
H	1.19777400	1.58148700	3.61977500
H	0.20416800	1.90028500	2.10283600
C	-3.58118200	-1.11373300	0.33381300

C	-4.46288600	-0.53820400	1.24972300
C	-4.07015600	-1.77595400	-0.79340600
C	-5.83619100	-0.61667200	1.02909000
H	-4.07436600	-0.02922800	2.12310700
C	-5.44455600	-1.85041200	-1.00891900
H	-3.37885200	-2.22491300	-1.49612700
C	-6.32787800	-1.27093600	-0.09929700
H	-6.52069600	-0.16591600	1.73875100
H	-5.82382400	-2.36180500	-1.88643600
H	-7.39710600	-1.33124500	-0.26834500

IN2

H	3.29144100	-0.04644700	-0.96671600
N	2.43008700	0.45712900	-1.12163300
C	3.14051600	-2.55292200	-0.39825200
C	1.22404100	-1.61558000	0.86685500
C	0.56890200	-0.92220400	-0.17450300
C	-0.80259200	-0.71203300	0.04123300
C	1.28788500	-0.40197600	-1.41242600
S	-1.80072800	-0.02752900	-1.29190000
C	-0.65893100	-1.51619000	2.14254300
C	2.35461400	1.69043100	-0.48056500
C	1.16541900	2.43221800	-0.38789100
C	1.16671800	3.68984400	0.21292400
C	2.33397600	4.23923700	0.73683400
C	3.51751300	3.50370200	0.65094800
C	3.53065000	2.24952300	0.05562600
N	2.53160500	-2.08650400	0.77568600
N	0.61704700	-1.85877800	2.04187900
C	3.18196200	-2.50042200	2.03056800
C	2.83988500	-2.38292100	-1.69631100
C	1.75358500	-1.55457900	-2.31975500
H	-1.13657200	-1.69364300	3.10207600
H	0.57514900	0.19044100	-1.98946600
H	0.23901400	2.03851400	-0.78554100
H	0.23579900	4.24413900	0.26927700
H	2.32416200	5.21716000	1.20293000
H	4.43995500	3.90919000	1.05270900
H	4.45998600	1.69125700	-0.00804400
N	-1.42448200	-1.00405100	1.18375200
H	4.01249600	-3.15493200	-0.17206300
H	2.96411300	-1.77825800	2.81311600
H	4.25818100	-2.53241200	1.86202100
H	2.83304700	-3.48130700	2.36553700
H	3.51108800	-2.88817100	-2.38238100
H	2.12356100	-1.13542600	-3.26156200
H	0.88160000	-2.16675400	-2.57418700
C	-3.41894700	0.13120700	-0.53244200
C	-4.38071700	-0.85415700	-0.75886100
C	-3.73724400	1.26552300	0.21642800
C	-5.66046900	-0.70710800	-0.22683700
H	-4.12583200	-1.73010700	-1.34271700
C	-5.01610900	1.40437500	0.74964700
H	-2.98702700	2.02825900	0.38418500
C	-5.97847900	0.41962000	0.52879300
H	-6.40616300	-1.47437300	-0.40186700
H	-5.26093300	2.28315900	1.33547200
H	-6.97429000	0.53207400	0.94248900

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C	2.06096500	2.24190700	1.97743600
C	1.33266300	0.22415800	-0.22714600
C	3.44530100	-1.65796900	-1.19910100
C	2.70273500	1.29649400	2.65895600
C	0.22940200	1.09874900	-0.20002500
C	-1.15921200	0.72354500	-0.08677400
C	-1.75498000	2.61761300	-1.16931200
S	-1.59477400	-0.76689600	0.76872200
N	1.36417700	-1.07647200	-0.01252600
C	2.48474400	-1.93518600	-0.22415500

C	2.58097800	-3.08209000	0.56726400
C	3.66056300	-3.94232600	0.39679100
C	4.63859300	-3.66041700	-0.55600700
C	4.52664200	-2.52100000	-1.35186900
N	-0.56572500	3.18004100	-1.13305400
N	1.58430600	3.17002700	-0.32901700
C	2.59205300	2.87019300	0.71921800
C	1.78584100	4.47199200	-0.99329000
N	-2.12649500	1.47116400	-0.57018100
C	0.43376100	2.49588100	-0.53748800
H	-2.53575000	3.15228500	-1.70175800
H	2.28160900	0.64556400	-0.53163100
H	0.50710500	-1.52825200	0.30646000
H	1.82581500	-3.29233700	1.31681400
H	3.73814100	-4.83072700	1.01152000
H	5.47751900	-4.33265200	-0.68786400
H	5.27063500	-2.31322100	-2.11133500
H	3.33902000	-0.80540400	-1.85948000
H	3.00574900	3.84708600	0.98689100
H	3.42877700	2.29458100	0.30910600
H	2.85056000	4.58431300	-1.20289700
H	1.22097000	4.50980400	-1.91875400
H	1.45772200	5.29146900	-0.34797500
H	1.14533300	2.67301400	2.37498400
H	2.33466500	0.94449400	3.61518600
H	3.63042300	0.85838500	2.30265500
C	-3.31495000	-1.04562700	0.33995800
C	-4.30839200	-0.58390300	1.20325700
C	-3.63322200	-1.77413200	-0.80718200
C	-5.64261700	-0.84751800	0.90230500
H	-4.04491900	-0.02604500	2.09304700
C	-4.97086600	-2.02852600	-1.09788400
H	-2.85128300	-2.13690200	-1.46294300
C	-5.97285700	-1.56611200	-0.24537000
H	-6.42169900	-0.49123300	1.56556800
H	-5.22848800	-2.59136100	-1.98718100
H	-7.01222300	-1.77020600	-0.47402000

***exo*-HTS1**

C	2.54336600	1.18516900	0.89786800
C	1.33335300	0.40379800	-0.35354600
C	3.67226300	-1.18969200	-0.74812800
C	3.73843500	0.44524900	0.96573600
C	0.08510500	1.17263500	-0.21062500
C	-1.24237100	0.67491000	-0.19056900
C	-2.06449800	2.78765200	-0.10802300
S	-1.60080600	-1.08172100	-0.32744600
N	1.34267200	-0.95512800	-0.13591100
C	2.47696800	-1.71900500	-0.20119800
C	2.48264900	-3.00840900	0.38109000
C	3.64701500	-3.74041600	0.40319800
C	4.84079200	-3.22450000	-0.15162500
C	4.84692100	-1.97671300	-0.73135000
N	-0.88707700	3.38531600	-0.08909000
N	1.40383700	3.22987900	-0.02301100
C	2.66599500	2.58416500	0.31899400
C	1.46247100	4.69795900	-0.04055100
N	-2.29842500	1.47491900	-0.13259900
C	0.20160000	2.59429400	-0.10825600
H	-2.93867400	3.43172500	-0.09605400
H	1.92455100	0.70077200	-1.21633900
H	0.55999300	-1.35306700	0.37836800
H	1.56973700	-3.40552500	0.81110400
H	3.64889000	-4.72601400	0.85312200
H	5.74146700	-3.82573200	-0.13834500
H	5.74625200	-1.59066700	-1.19589900
H	3.63547400	-0.33494100	-1.41073700
H	3.16391500	3.22025000	1.05836800
H	3.32633100	2.55339000	-0.55915700
H	2.41960500	4.99864700	-0.47041600

H	0.65162500	5.09257500	-0.64448500
H	1.37613300	5.10953500	0.96996800
H	1.90174500	1.09401900	1.77102500
H	3.88414100	-0.30538700	1.73065000
H	4.63720800	0.80824100	0.48248200
C	-3.37303400	-1.17440900	-0.07143100
C	-4.21546500	-1.19503500	-1.18326100
C	-3.88504900	-1.30277600	1.22051900
C	-5.58849100	-1.33360900	-0.99472600
H	-3.80375400	-1.10122900	-2.18035400
C	-5.25948500	-1.43843600	1.39764200
H	-3.22036700	-1.29466000	2.07554800
C	-6.10961900	-1.45324600	0.29247700
H	-6.24888700	-1.34868300	-1.85365800
H	-5.66466500	-1.53586500	2.39795400
H	-7.17838900	-1.56225300	0.43484400

***endo*-HTS1**

C	2.15197300	0.99792900	1.44237500
C	1.03434000	0.03290000	0.26845900
C	3.01047800	-2.03757300	0.61098800
C	3.18802500	0.16945500	1.88650200
C	-0.02887500	0.99409900	-0.07423600
C	-1.37300500	0.57719900	-0.19611100
C	-1.99687600	2.68935500	-0.69851700
S	-1.73973200	-1.15472500	0.01343100
N	1.84028900	-0.41651600	-0.76148700
C	2.90294900	-1.27396100	-0.57413700
C	3.92318200	-1.34684200	-1.54860100
C	5.01522900	-2.15990300	-1.33544700
C	5.12876200	-2.91937000	-0.15312600
C	4.13158500	-2.86476200	0.80051200
N	-0.79087200	3.21755100	-0.56428900
N	1.42345200	2.94897900	0.05962400
C	2.54802700	2.18723100	0.57393900
C	1.66440300	4.38369400	-0.13130800
N	-2.35228200	1.41555900	-0.50972500
C	0.20895600	2.38784500	-0.20900300
H	-2.79154700	3.36952500	-0.99014100
H	0.71016800	-0.76000300	0.93628000
H	1.83362600	0.12688300	-1.61624000
H	3.84161300	-0.76011800	-2.45750800
H	5.79577700	-2.21320800	-2.08488900
H	5.98925400	-3.56064500	-0.00740500
H	4.19306700	-3.47447400	1.69372500
H	2.16536000	-2.14144100	1.27709700
H	3.15223500	2.87224700	1.17435200
H	3.19914500	1.83210000	-0.23944500
H	2.56549300	4.52546000	-0.73414300
H	0.81273800	4.82478200	-0.63835600
H	1.80104300	4.87841400	0.83492800
H	1.38610000	1.20110100	2.18931400
H	3.08204600	-0.41197400	2.79328300
H	4.18358200	0.22452900	1.46343000
C	-3.53353700	-1.19650200	0.06525500
C	-4.24368800	-1.47010300	-1.10405400
C	-4.19548700	-1.02539700	1.28203800
C	-5.63285400	-1.55975100	-1.05318300
H	-3.71828100	-1.60731300	-2.04090300
C	-5.58458500	-1.11478600	1.32161400
H	-3.63310600	-0.82551800	2.18580300
C	-6.30219500	-1.38094900	0.15621700
H	-6.19008700	-1.76923700	-1.95861500
H	-6.10453700	-0.98049600	2.26285900
H	-7.38293400	-1.45289300	0.19174400

***cis*-HIN1**

N	-1.90111300	1.44159300	-0.77553700
C	-1.32330400	2.41324700	-1.48355100
N	-0.08920000	2.87545100	-1.34569500

C	0.69214500	2.26452000	-0.43940200
C	0.23902100	1.12227300	0.27195400
C	-1.11769600	0.81426200	0.09553200
N	1.93787100	2.78043600	-0.20961900
C	2.56812800	2.40656700	1.05167800
C	2.61365900	0.88518600	1.21129600
C	1.17058800	0.32582900	1.17620800
C	3.52595400	0.23743200	0.16052900
C	3.54371900	-1.28999700	0.34132400
C	2.14892600	-1.84000100	0.31347400
N	1.15671500	-1.10600500	0.75107900
C	4.52143400	-2.03930500	-0.51145600
C	4.22786800	-3.23887500	-1.04115500
C	2.91757400	-3.81409900	-0.83882900
C	1.91698200	-3.15936600	-0.18849600
S	-1.85984000	-0.46668200	1.12213900
C	2.31809200	4.06736000	-0.79800000
C	-3.50126900	-0.68369300	0.43215000
C	-3.70495800	-1.54230700	-0.64904900
C	-4.99493700	-1.73190500	-1.13672000
C	-6.07156400	-1.07468800	-0.54197500
C	-5.86097100	-0.22505400	0.54215100
C	-4.57330000	-0.02552200	1.03514600
H	-1.94009200	2.89169400	-2.23833500
H	2.03615800	2.85850600	1.90225400
H	3.58475800	2.80268900	1.05978900
H	3.03191000	0.66884400	2.19995200
H	0.77037600	0.32183500	2.19573700
H	4.54088500	0.62566200	0.27440000
H	3.19510100	0.48703500	-0.85088400
H	3.88700500	-1.48841800	1.37599700
H	0.21620500	-1.51041400	0.73864500
H	5.50635900	-1.59942400	-0.62409600
H	4.95999600	-3.79138700	-1.61632000
H	2.71842500	-4.79893900	-1.24749800
H	0.92756100	-3.59401000	-0.10345800
H	1.94432400	4.12538300	-1.81637000
H	3.40658000	4.13942400	-0.80392000
H	1.90591600	4.90995300	-0.23074500
H	-2.86667400	-2.05192900	-1.10795900
H	-5.15914300	-2.39405200	-1.97870400
H	-7.07469800	-1.22742000	-0.92243900
H	-6.69718600	0.28469800	1.00580000
H	-4.40277800	0.63566400	1.87549200

***trans*-HIN1**

N	2.28146200	1.50237500	-0.29912600
C	2.00579300	2.76312600	-0.63280200
N	0.82419300	3.35910500	-0.60074000
C	-0.23342400	2.61050500	-0.24028800
C	-0.08140200	1.22140300	0.04158100
C	1.24018200	0.75224700	0.04792600
N	-1.44458000	3.23784900	-0.15513100
C	-2.56707800	2.54088600	0.45390400
C	-2.59886300	1.09247800	-0.02219400
C	-1.29270600	0.38858300	0.39087600
C	-3.82696800	0.30440600	0.45641000
C	-3.51522200	-1.22518600	0.63823600
C	-2.38053000	-1.69642700	-0.22608100
N	-1.32054700	-0.92325200	-0.28762000
C	-4.73022900	-2.09048600	0.59226200
C	-4.76005500	-3.24565800	-0.09740000
C	-3.60145400	-3.67575300	-0.84163700
C	-2.45326600	-2.94383400	-0.90847000
S	1.58075800	-0.93812200	0.57319300
C	-1.55126400	4.69280200	-0.28184000
C	3.34158700	-1.12621500	0.28689700
C	3.80915800	-1.53724900	-0.96213600
C	5.17523300	-1.72866400	-1.15101600

C	6.06368900	-1.51851700	-0.09704300
C	5.58839300	-1.11626700	1.14968500
C	4.22356900	-0.91920600	1.34787200
H	2.84744000	3.37231600	-0.94877900
H	-2.51674800	2.58573300	1.55355800
H	-3.48643000	3.04867500	0.15420800
H	-2.59639700	1.11402100	-1.11683000
H	-1.31199100	0.18548600	1.47388500
H	-4.18893100	0.68322600	1.41583800
H	-4.63948200	0.41809000	-0.26267000
H	-3.11521500	-1.32528700	1.66439600
H	-0.47304400	-1.24881400	-0.74968900
H	-5.58973800	-1.75696200	1.16365000
H	-5.64676600	-3.86692000	-0.10488700
H	-3.65357800	-4.61767100	-1.37684400
H	-1.60543200	-3.28246700	-1.49258300
H	-1.45181800	5.18654400	0.69171200
H	-2.52609600	4.93849500	-0.70696400
H	-0.76586000	5.05755700	-0.93653100
H	3.11630200	-1.69962900	-1.77858700
H	5.54442300	-2.04312000	-2.12012600
H	7.12604400	-1.67094700	-0.24736200
H	6.27803800	-0.95430900	1.96963600
H	3.84859200	-0.60445900	2.31375900

HTS3

H	2.46635800	1.08434600	0.08315100
C	2.74510100	2.51974700	0.29264200
C	1.49279000	0.27990900	0.16392800
C	0.33500900	1.15912600	-0.17465700
C	-1.00715600	0.68975400	-0.21482600
C	0.49726400	2.51634100	-0.50523900
S	-1.35758300	-0.98952400	0.24967400
C	-1.71074000	2.73831800	-0.91558400
C	2.41614100	-1.98045900	-0.33719700
C	3.08379600	-2.15449200	0.88152000
C	3.81009300	-3.32012300	1.10492100
C	3.88051400	-4.31369800	0.12956100
C	3.21634100	-4.13579500	-1.08388100
C	2.48855200	-2.97712200	-1.32074400
N	1.78851400	3.07612100	-0.51298100
N	-0.50626400	3.29844000	-0.90345400
C	2.18250700	3.91775300	-1.65981500
C	2.65782900	2.54391700	1.76000400
C	1.73771800	3.21106700	2.46446400
H	-2.53827600	3.36471500	-1.23273000
H	1.60146700	0.07649700	1.23242700
H	3.04529500	-1.40081300	1.65800000
H	4.32391600	-3.45086700	2.04974300
H	4.44760700	-5.21771400	0.31343600
H	3.26343200	-4.90149100	-1.84868000
H	1.96913600	-2.84452100	-2.26443500
N	-2.00994600	1.48852200	-0.56351300
H	3.75710900	2.58077300	-0.10850100
H	2.48094300	3.30344900	-2.51508100
H	3.00248500	4.56807400	-1.36185700
H	1.32306000	4.52604200	-1.93378600
H	3.45254500	2.00664100	2.26974800
H	1.76936300	3.21667400	3.54711000
H	0.95581600	3.79401700	1.99126800
N	1.65944700	-0.83066700	-0.62685800
H	1.28166500	-0.78253000	-1.56431600
C	-3.15265300	-1.04368200	0.23936400
C	-3.85603400	-0.73443900	1.40453700
C	-3.82119000	-1.47119900	-0.90838900
C	-5.24475100	-0.83913600	1.41129300
H	-3.32580000	-0.41846000	2.29453800
C	-5.21022600	-1.57282400	-0.89112100
H	-3.26436500	-1.72085200	-1.80313000
C	-5.92085400	-1.25579000	0.26544400

H	-5.79655700	-0.59976400	2.31266100
H	-5.73514600	-1.90261200	-1.77988500
H	-7.00128000	-1.33918000	0.27581300

IN3′

H	2.70416000	0.69270200	0.11518700
N	2.36015500	-0.25040300	-0.03125000
C	2.53339400	2.66373600	0.39599100
C	0.35759500	1.96842200	-0.55199300
C	0.06915300	0.60936400	-0.26206000
C	-1.34978500	0.33935800	-0.17485300
C	1.01058600	-0.41640200	-0.11731600
S	-1.88692600	-1.31434000	0.27568400
C	-1.85103300	2.48061000	-0.74770100
C	3.32628600	-1.25944300	-0.04197500
C	3.03554900	-2.58811000	-0.38889300
C	4.04561900	-3.54599700	-0.37294700
C	5.35262400	-3.20751100	-0.02835900
C	5.64433100	-1.88333300	0.30429000
C	4.64621400	-0.91892800	0.30048700
N	1.71555200	2.38586000	-0.69027100
N	-0.57834300	2.87311200	-0.81180500
C	2.02354700	3.09781500	-1.93906900
C	2.26238300	2.63377700	1.76919300
C	1.09300600	2.41857500	2.46755900
H	-2.61477200	3.21753000	-0.97014500
H	0.65983300	-1.43456100	-0.05266100
H	2.03673000	-2.87587700	-0.68978000
H	3.80468800	-4.56783500	-0.64408700
H	6.13182500	-3.95998600	-0.02288800
H	6.65554700	-1.59997100	0.57381300
H	4.87848300	0.10590600	0.57224500
N	-2.26996100	1.24773900	-0.41720100
H	3.53273900	2.95594100	0.09348000
H	1.56885100	2.57054200	-2.77775300
H	3.10660900	3.10829200	-2.07718400
H	1.64888600	4.12497900	-1.92126600
H	3.15046800	2.82845400	2.36627900
H	1.10606400	2.44343100	3.54959500
H	0.13830100	2.24366400	1.99395600
C	-3.67371400	-1.18291100	0.18396100
C	-4.39617000	-0.71391800	1.28262700
C	-4.34073400	-1.62242400	-0.96035300
C	-5.78706200	-0.67300400	1.22801800
H	-3.87119500	-0.38129400	2.16950600
C	-5.73317400	-1.58321200	-1.00729800
H	-3.77246200	-1.98653800	-1.80755900
C	-6.45668200	-1.10741600	0.08460200
H	-6.34717900	-0.30347500	2.07957300
H	-6.25036200	-1.92353400	-1.89729800
H	-7.53978600	-1.07737700	0.04625800

***cis*-IN1′**

N	-1.33458000	-2.49009100	-1.26148200
C	-2.61187300	-2.68420700	-0.92584500
N	-3.40320000	-1.83606300	-0.28708600
C	-2.89084500	-0.64879800	0.08303100
C	-1.52756800	-0.31965700	-0.22401500
C	-0.83179100	-1.30984700	-0.90191400
N	-3.69684200	0.22265000	0.73762300
C	-3.16847900	1.47310400	1.27445900
C	-2.07220900	2.07389400	0.37480200
C	-0.94451600	0.99499300	0.25345300
C	-2.60017700	2.52244400	-0.94966500
C	1.68294300	2.25735700	1.11710400
C	1.19619500	2.25803900	-0.20453000
C	2.76368200	3.06118500	1.45221600
C	3.38269100	3.86258200	0.49028300

C	2.91135300	3.85459000	-0.82603800
C	1.83243900	3.06028800	-1.17542400
S	0.87764500	-1.04161600	-1.43955800
C	-5.06051700	-0.13530800	1.13575000
C	1.84696300	-2.00434900	-0.32075700
C	3.21102400	-2.11422400	-0.64909000
C	4.05651700	-2.84351200	0.17488800
C	3.55565400	-3.46574600	1.32037900
C	2.20038500	-3.35482600	1.64176000
C	1.34088100	-2.62483300	0.83137600
H	-3.04689500	-3.63752100	-1.20917200
H	-2.77784200	1.31755800	2.29001400
H	-3.99587600	2.18011600	1.35382400
H	-1.64103200	2.92781400	0.90336600
H	-0.52482000	0.84908500	1.25055800
H	-3.23839000	1.87594400	-1.54023400
H	-2.43742000	3.53395500	-1.29774200
H	1.23535000	1.62971500	1.87635800
H	3.13124100	3.05848900	2.47126500
H	4.22644400	4.48470400	0.76213900
H	3.38685600	4.47272500	-1.57783000
H	1.46679300	3.05629800	-2.19721000
H	-5.10887000	-0.32178900	2.21383400
H	-5.36863300	-1.03129700	0.60676700
H	-5.73430300	0.68796000	0.88903100
H	3.59546000	-1.64323500	-1.54663200
H	5.10508100	-2.93518900	-0.08111300
H	4.21707500	-4.04041500	1.95742800
H	1.81121100	-3.84621200	2.52554400
H	0.29001400	-2.55750700	1.07850900
N	0.13518600	1.45829000	-0.61285100
H	-0.17421900	1.64214300	-1.56254000

***cis*-HIN1′**

N	-1.97033900	1.62222900	-0.55551100
C	-1.72591200	2.92579500	-0.52029700
N	-0.57167200	3.52127000	-0.25179500
C	0.48134800	2.71759100	-0.01108700
C	0.36632500	1.30102500	-0.06751400
C	-0.92173000	0.82182400	-0.32173100
N	1.66883000	3.33042400	0.29819800
C	2.77780000	2.52834500	0.79078300
C	2.88551900	1.20998000	0.02099800
C	1.56356700	0.40698900	0.23188800
C	3.22340700	1.43078900	-1.41788400
C	2.79248600	-2.12858100	1.06321600
C	2.16505000	-1.89931500	-0.20108400
N	1.56588000	-0.76479400	-0.61544500
C	3.37748800	-3.34943900	1.34883400
C	3.36367700	-4.38816200	0.40885400
C	2.74884200	-4.19330800	-0.83466600
C	2.16093300	-2.98002600	-1.13597600
S	-1.25387300	-0.94803200	-0.32673200
C	1.71952300	4.76173800	0.56461200
C	-3.02441800	-0.97183200	-0.00013000
C	-3.92191600	-1.11909000	-1.05868600
C	-5.28887000	-1.21165500	-0.80321400
C	-5.76211900	-1.15866600	0.50672300
C	-4.86455300	-1.01740100	1.56436000
C	-3.49692900	-0.92955700	1.31344500
H	-2.56934600	3.58040200	-0.72489700
H	2.67390800	2.33242800	1.86985200
H	3.69749400	3.10392900	0.65563600
H	3.68927200	0.62444500	0.49586900
H	1.51805300	0.13799400	1.29820000
H	3.81035900	2.29366900	-1.70861000
H	2.95778500	0.70070700	-2.16869200
H	2.80961400	-1.34809100	1.81301500
H	3.84901100	-3.50528500	2.31305400
H	3.82381300	-5.34030600	0.64649400

H	2.73210400	-4.99771700	-1.56137600
H	1.67471400	-2.80639100	-2.08829000
H	1.51301100	4.98793500	1.61996100
H	0.98022500	5.27334200	-0.04495900
H	2.71768800	5.13089500	0.31798800
H	-3.54905500	-1.14962000	-2.07500500
H	-5.98353400	-1.32070000	-1.62867900
H	-6.82612200	-1.22945800	0.70327900
H	-5.22776300	-0.97918800	2.58544200
H	-2.79524800	-0.82664400	2.13263600