



Molecular Docking, Computational, and Antithrombotic Studies of Novel 1,3,4-Oxadiazole Derivatives

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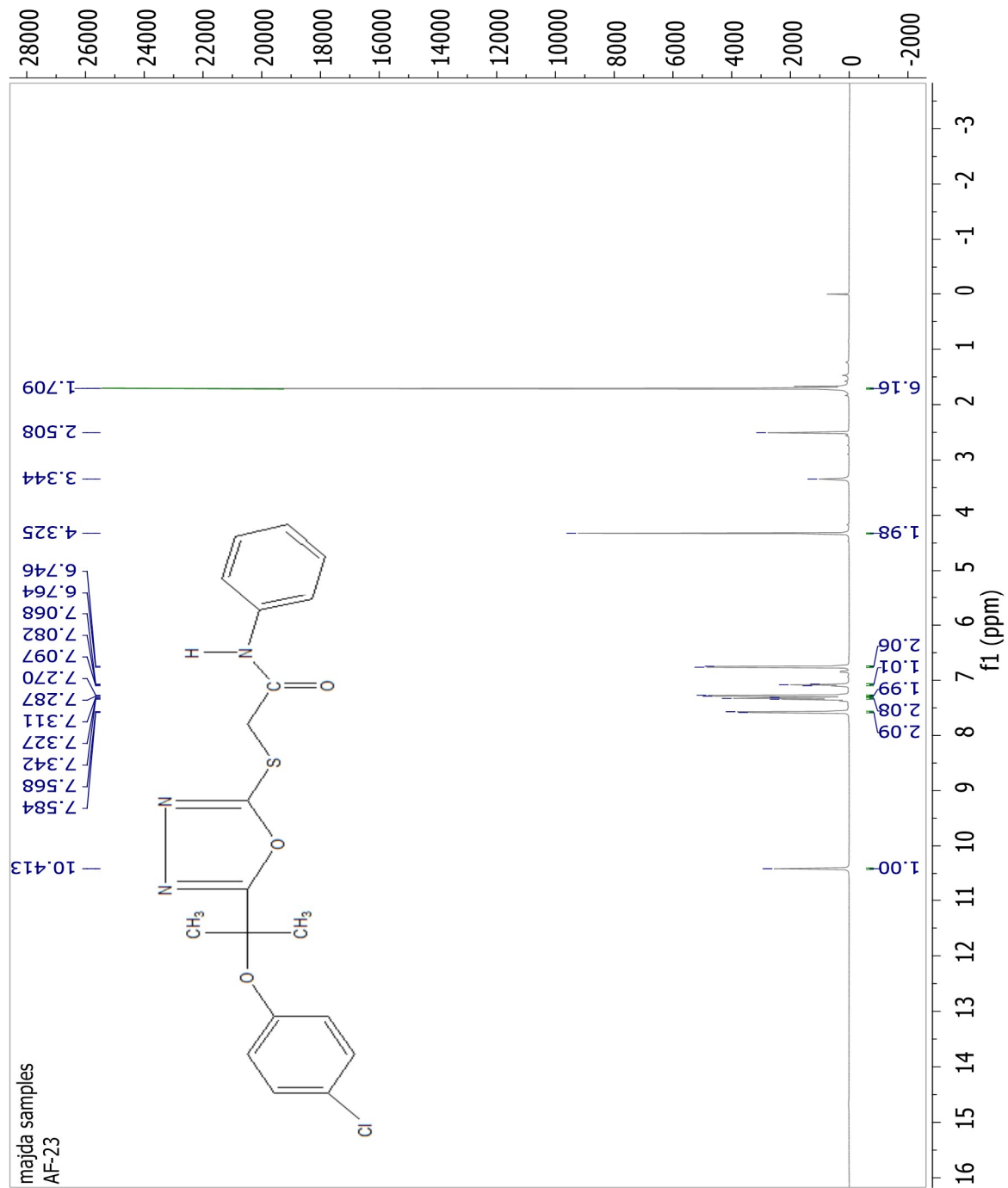
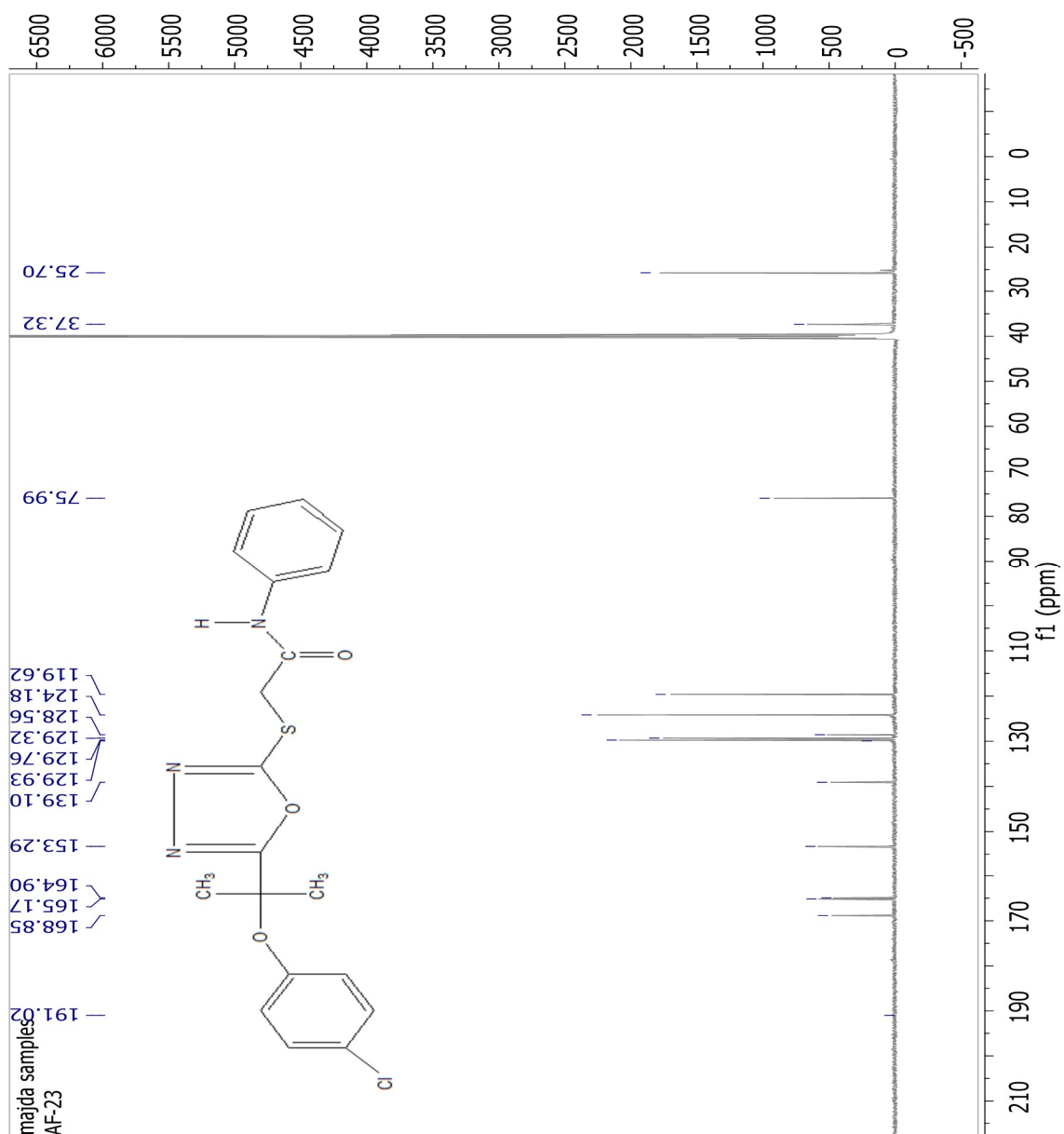


Figure S1. ¹H-NMR spectrum of compound 3a.

Figure S2. ¹³C-NMR spectrum of compound 3a.

Mass Lab (104)
6/19/2017 1:14:38 PM

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 Inlet: Direct Probe
 Ionization mode: EI+

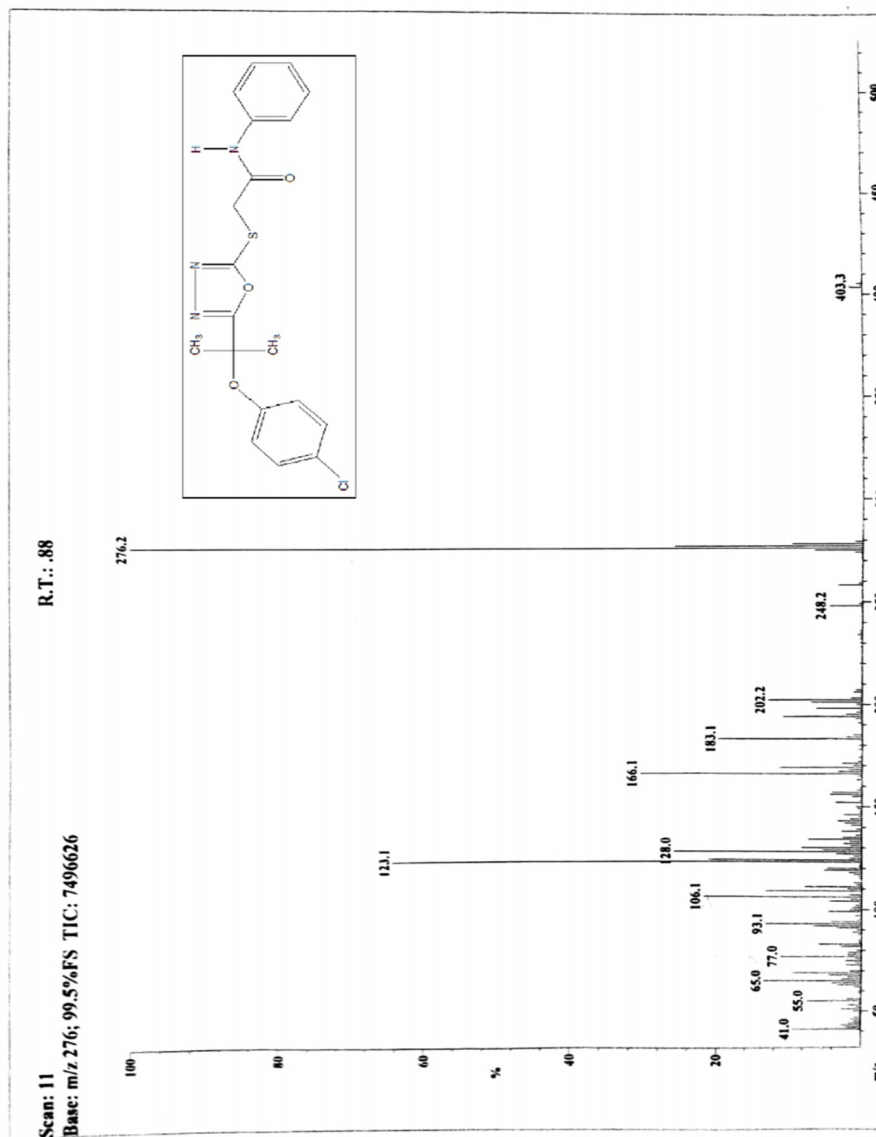


Figure S3. EI-MS of compound 3a.

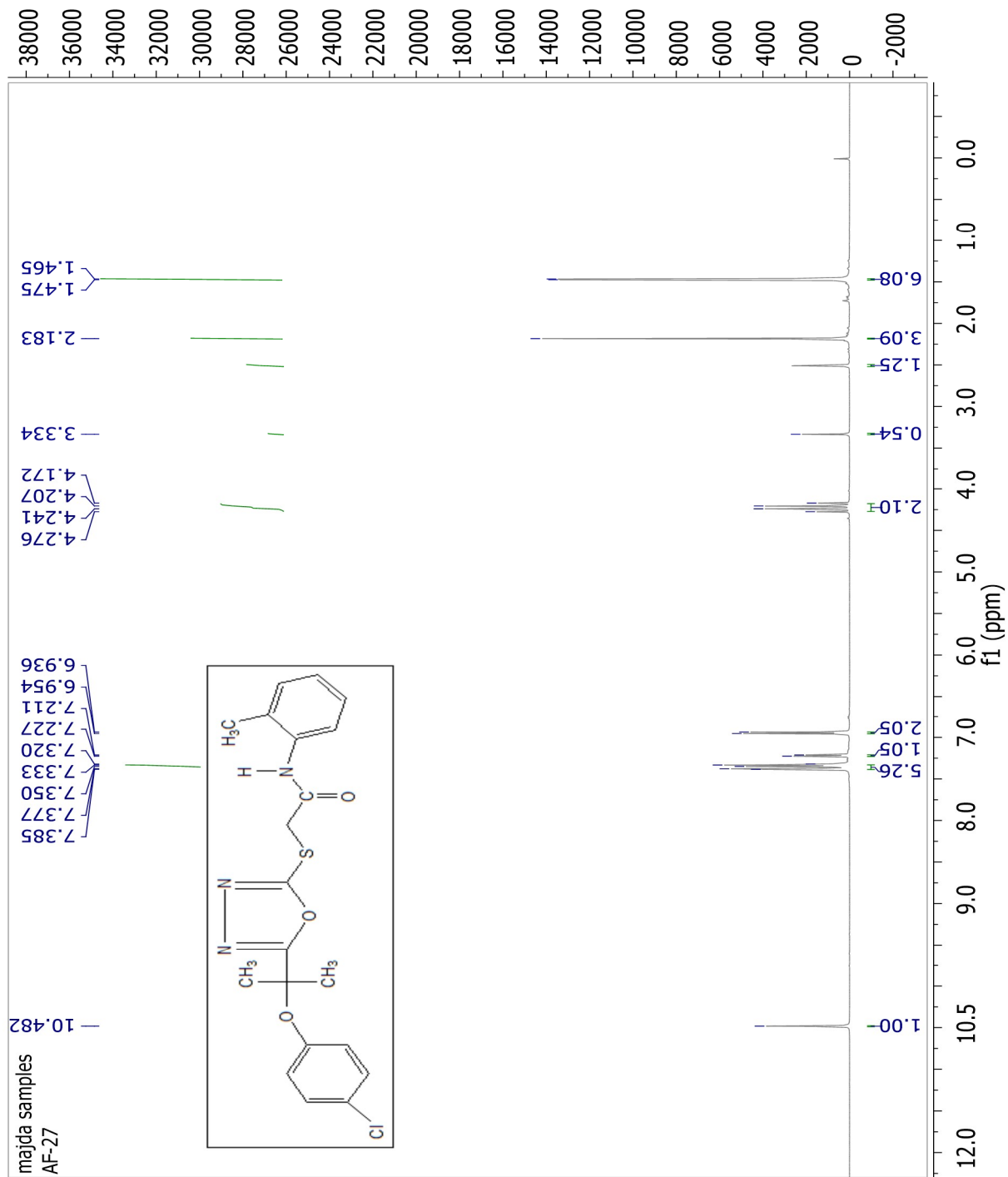
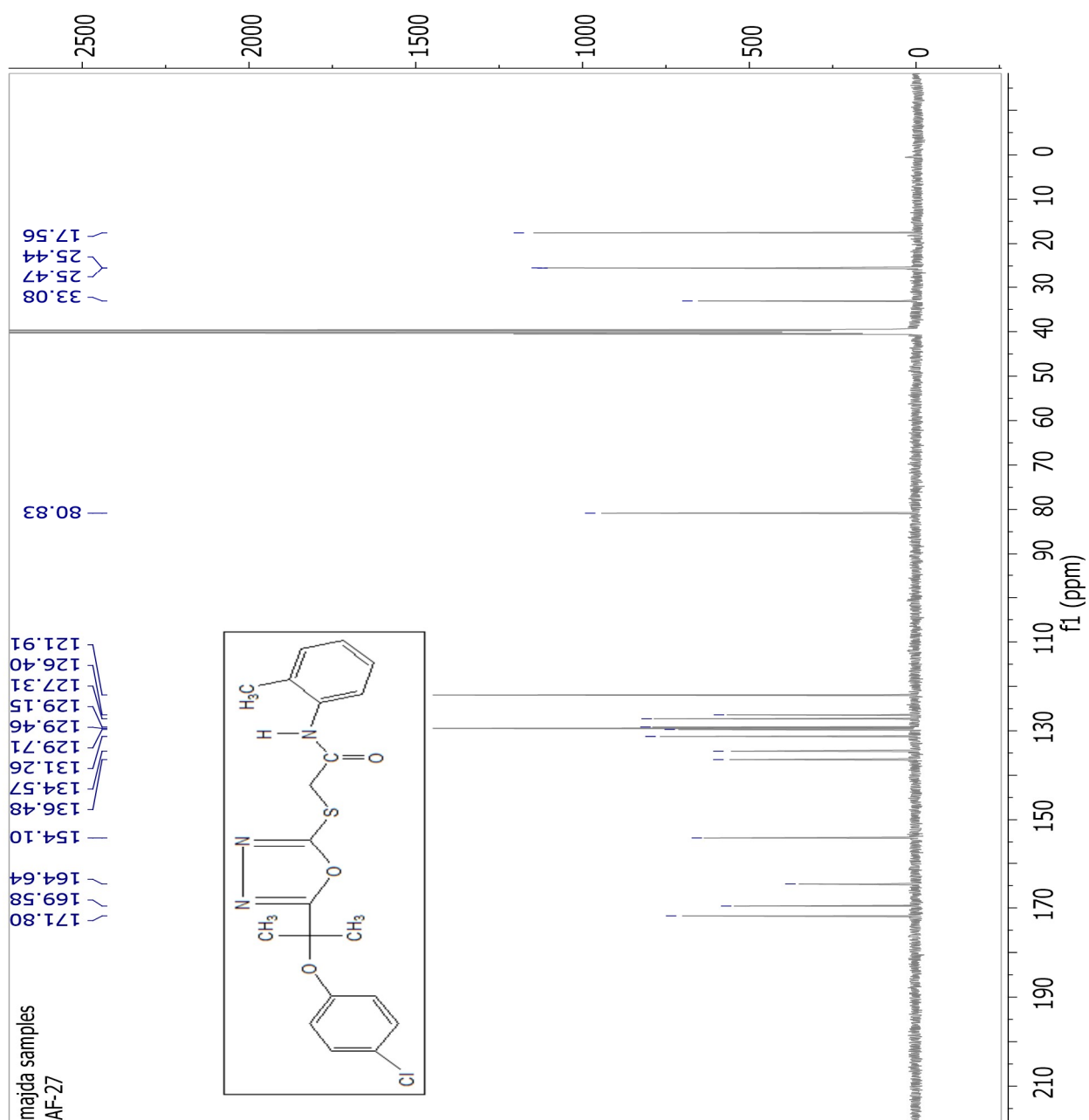


Figure S4. ¹H-NMR spectrum of compound 3b.

Figure S5. ^{13}C -NMR spectrum of compound 3b.

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Instrument: JEOL 600 MSRoute
Inlet: Direct Probe
Ionization mode: EI+

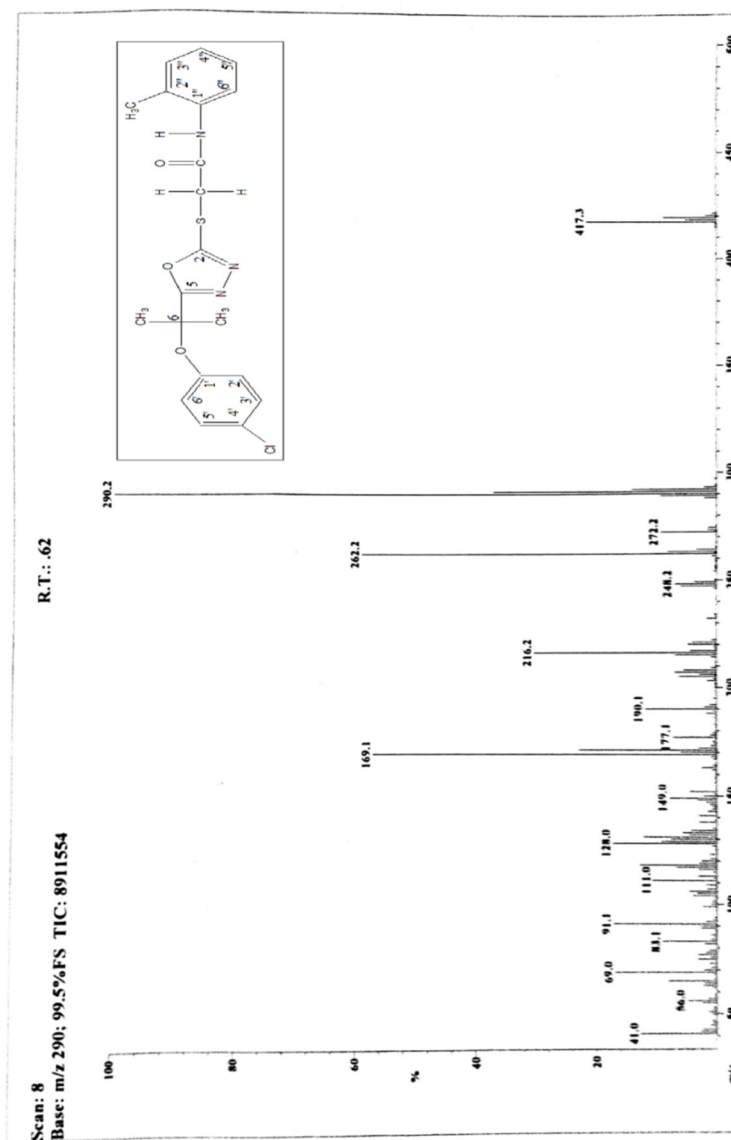


Figure S6. EI-MS of compound 3b.

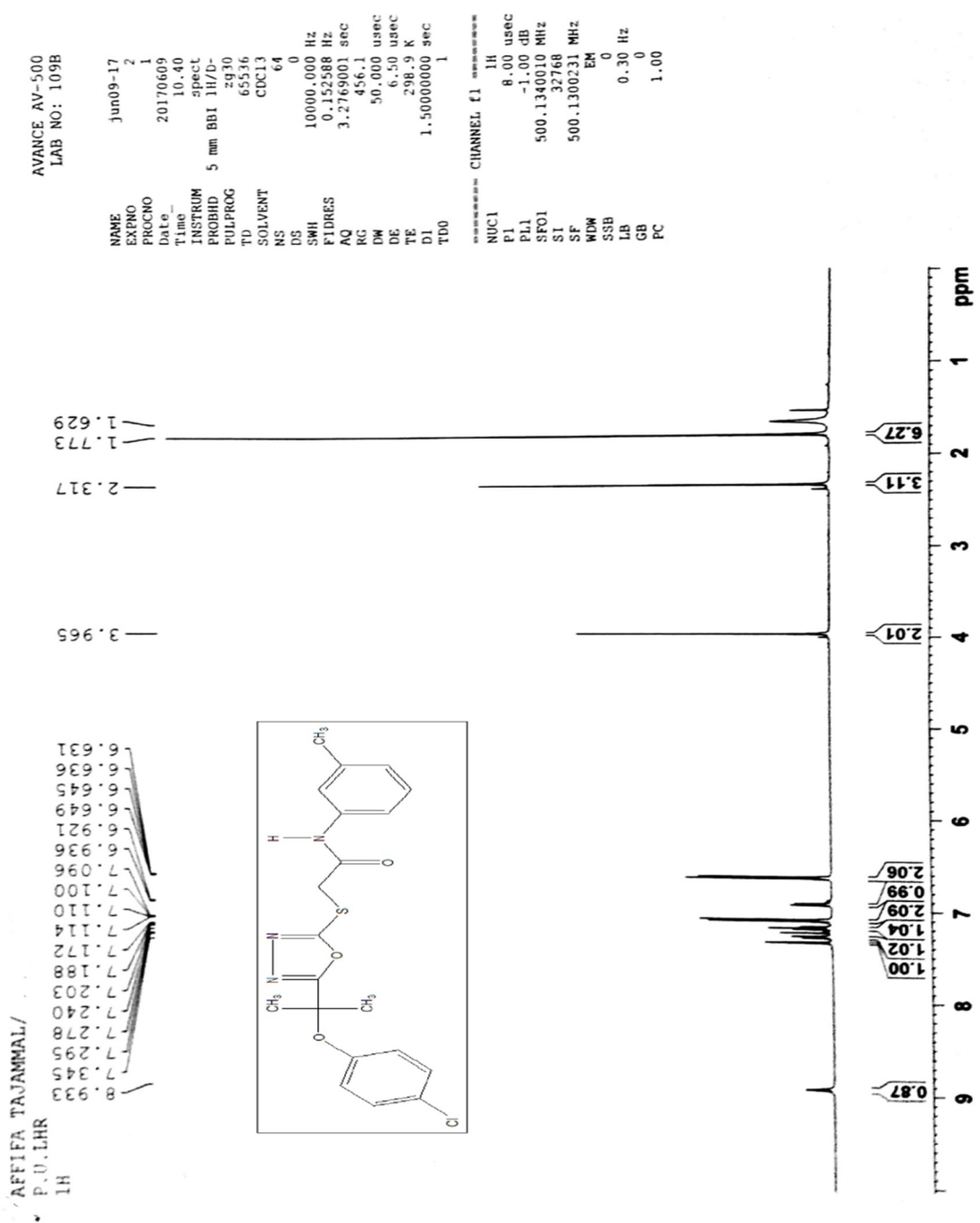


Figure S7. ¹H-NMR spectrum of compound 3c.

AFFIA /42P/CH:DEPT:U.O.PUNJAB/BB/

AVANCE 400
LAB NO 117

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PROCNO   1
Date_    20170609
Time_    12.53
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PULPROG  zgpg
TD        32768
SOLVENT  DMSO
NS        18432
DS        2
SWH       24154.590 Hz
FIDRES   0.737140 Hz
AQ        0.6783476 sec
RG        18390.4
EW        20.700 usec
DE        6.50 usec
TE        300.0 K
D1        1.50000000 sec
D11       0.03000000 sec
TDO       18
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NUC1      13C
P1        8.55 usec
PL1       7.00 dB
SFO1      100.6243395 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2     80.00 usec
PZ2       0.00 dB
PL2       19.00 dB
PL13      20.00 dB
SFO2      400.1324008 MHz
SI        16384
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WDM       EM
SSB       0
LB        1.00 Hz
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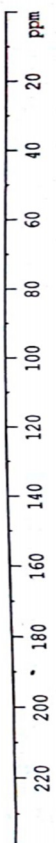
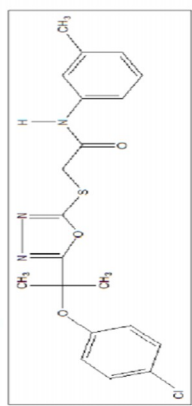


Figure S8. ¹³C-NMR spectrum of compound 3c.

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 Inlet: Direct Probe
 Ionization mode: EI+

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 Base: m/z 290; 99.5%FS TIC: 10286106

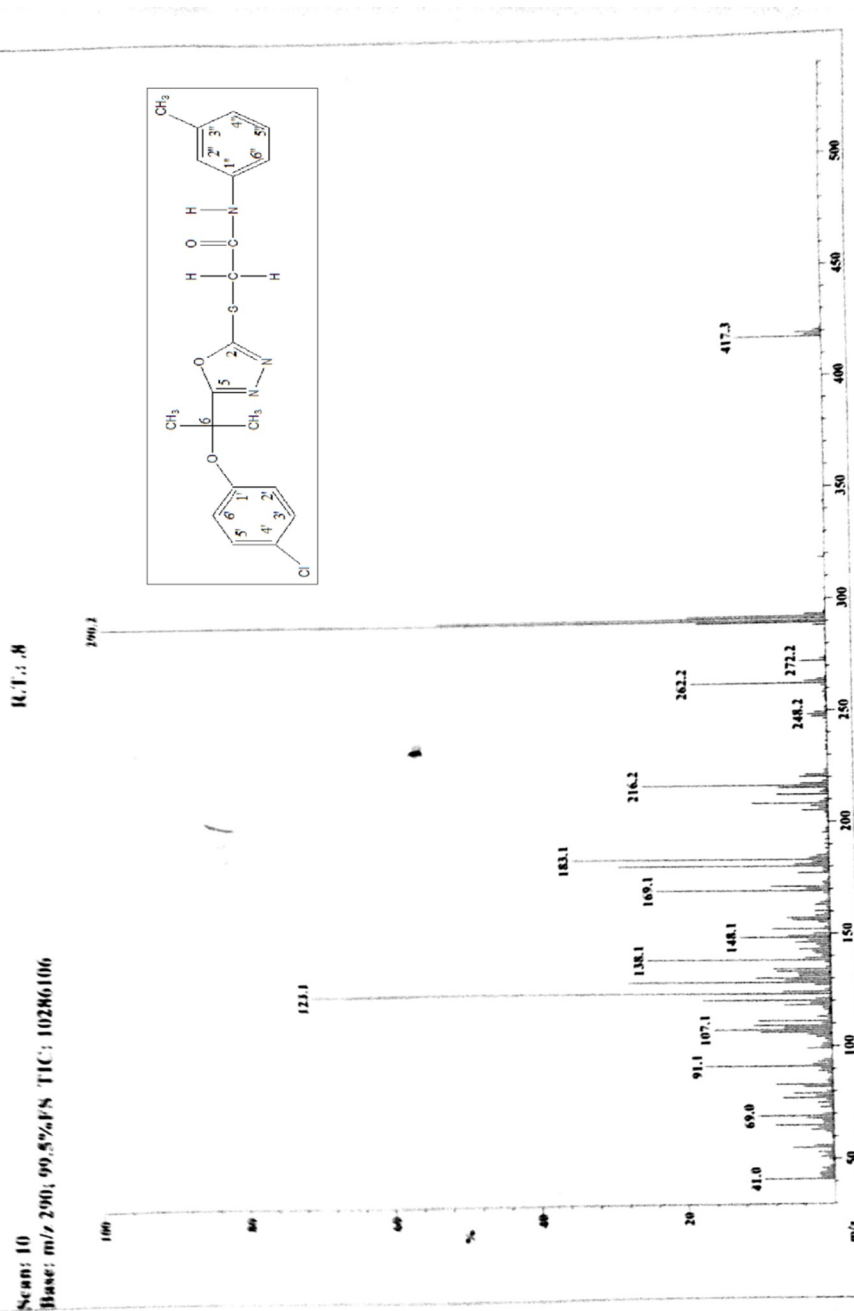


Figure S9. EI-MS of compound 3c.

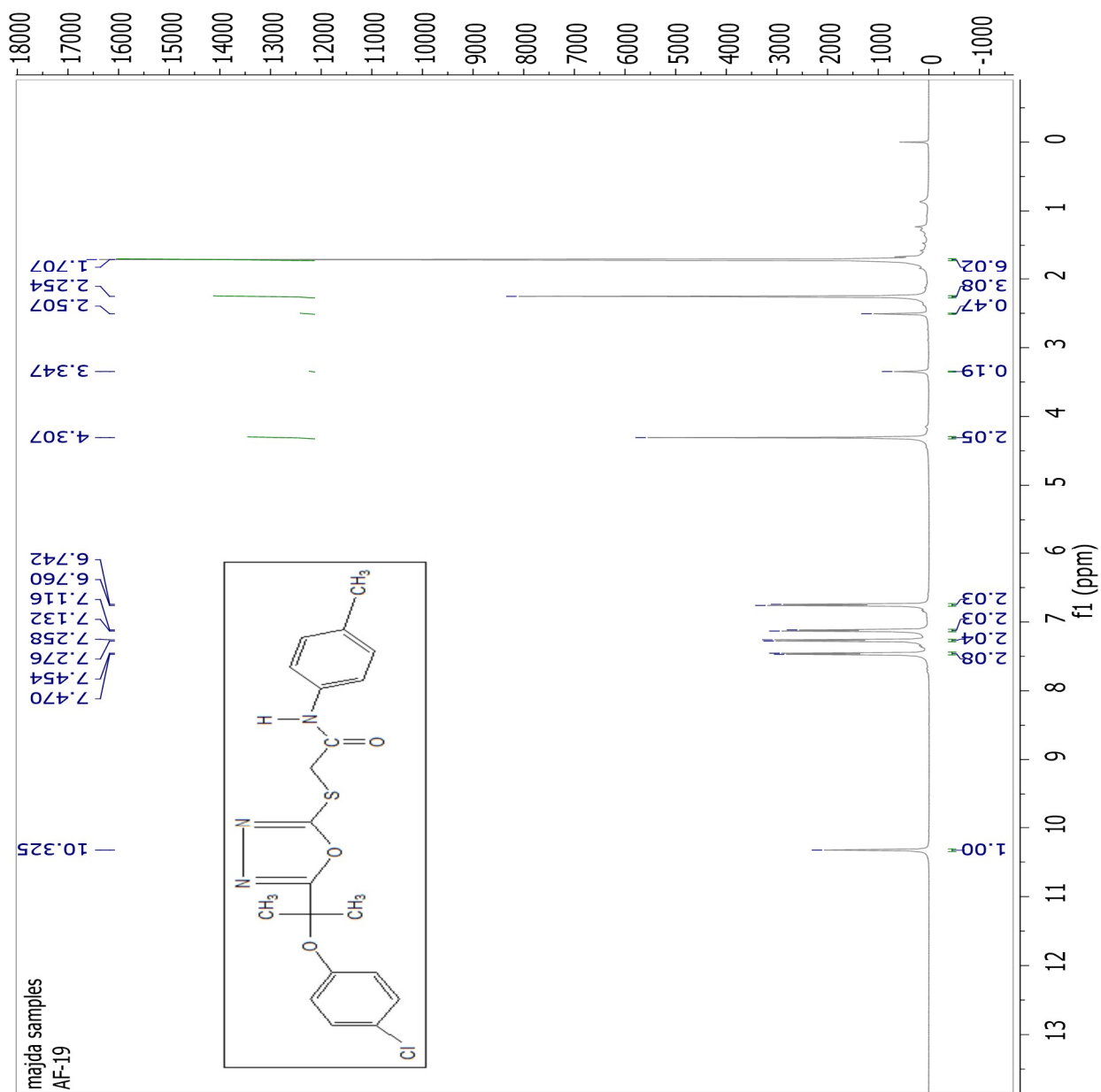


Figure S10. ¹H-NMR spectrum of compound 3d.

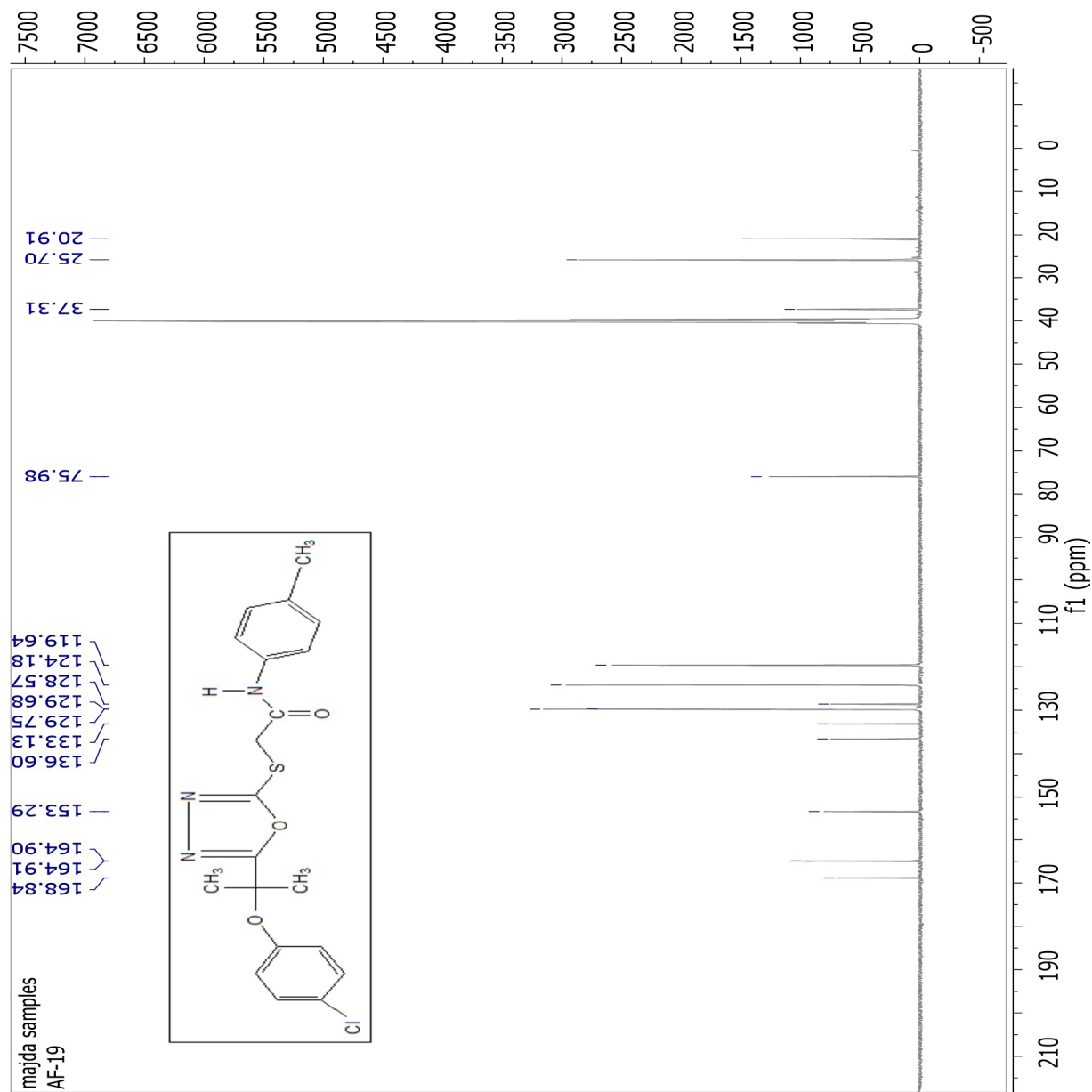


Figure S11. ¹³C-NMR spectrums of compound 3d.

Mass Lab (104)
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File: 10P Date Run: 06-19-2017 (Time Run: 13:58:24)
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 Inlet: Direct Probe

Ionization mode: EI+

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R.T.: .98

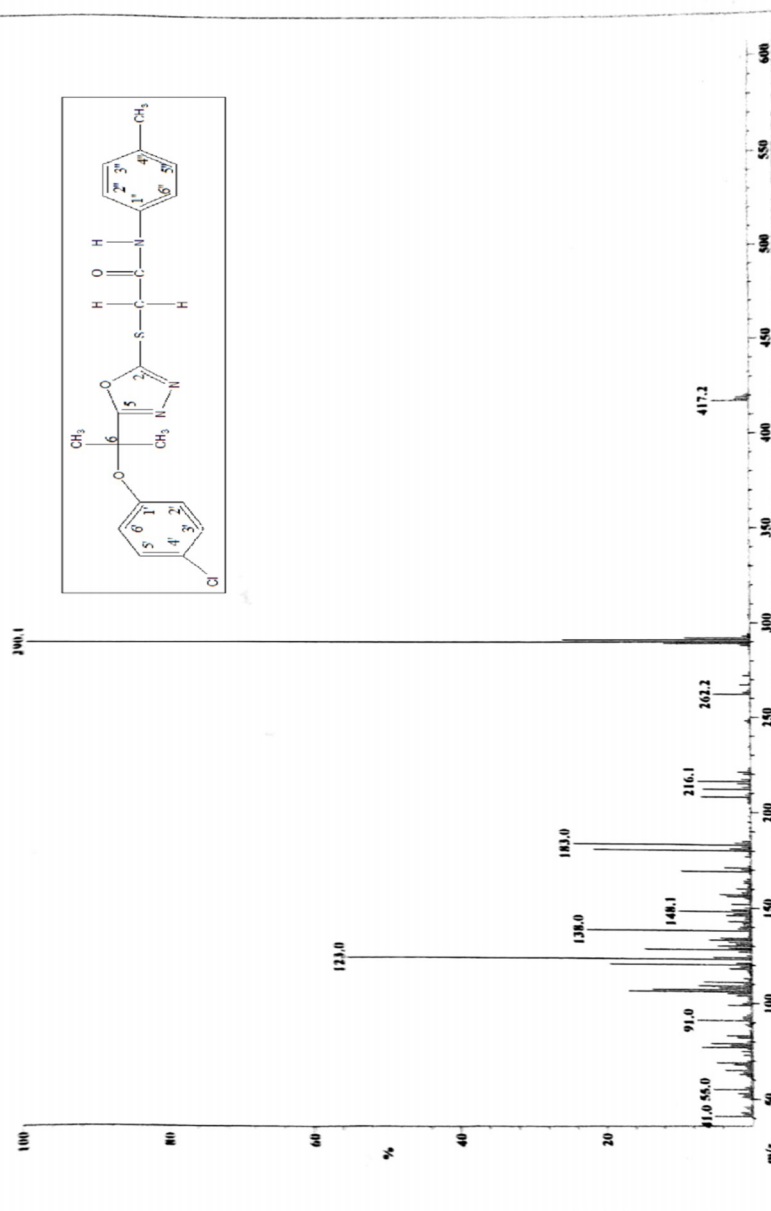


Figure S12. EI-MS of compound 3d.

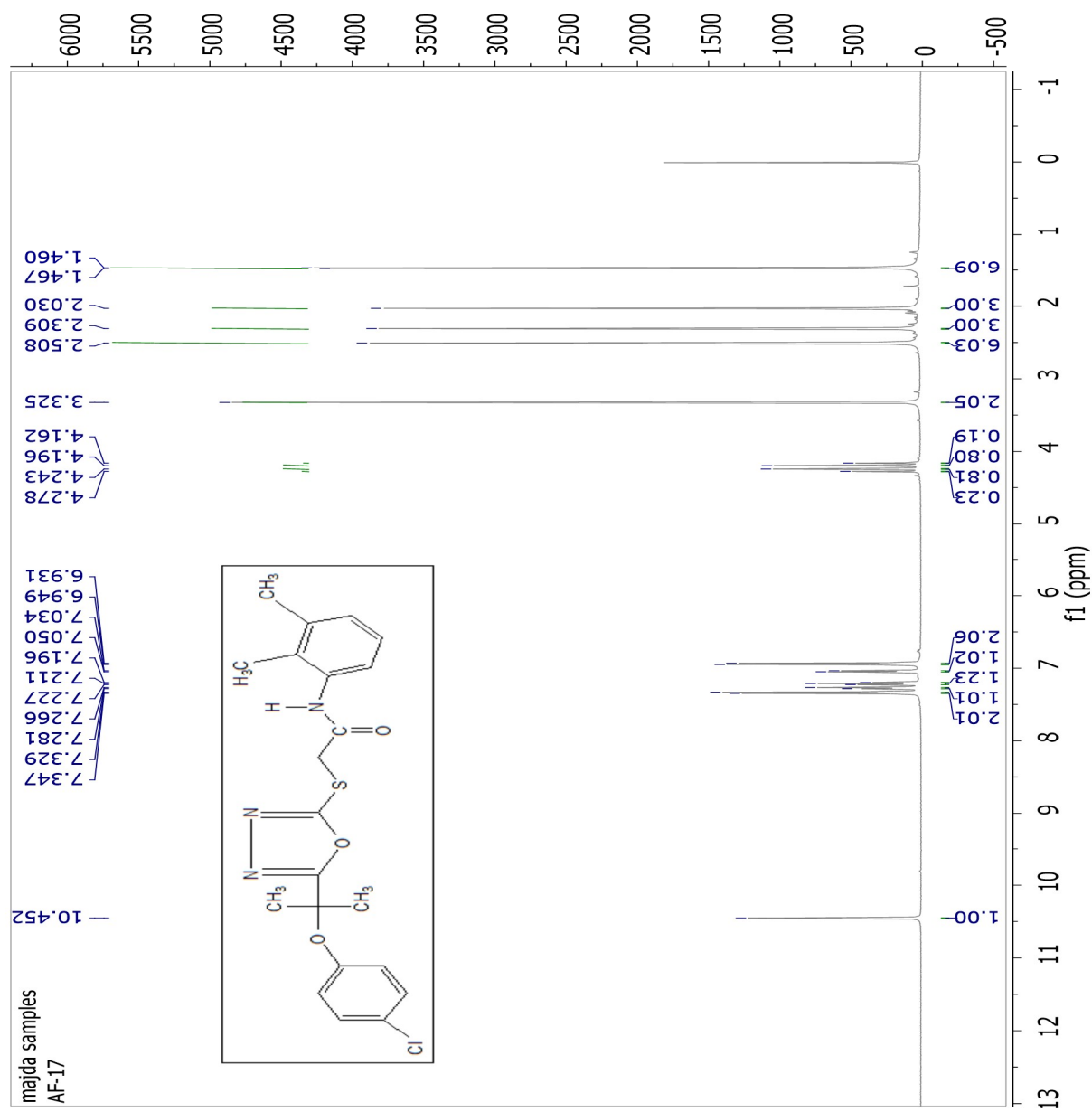


Figure S13. ¹H-NMR spectrum of compound 3e.

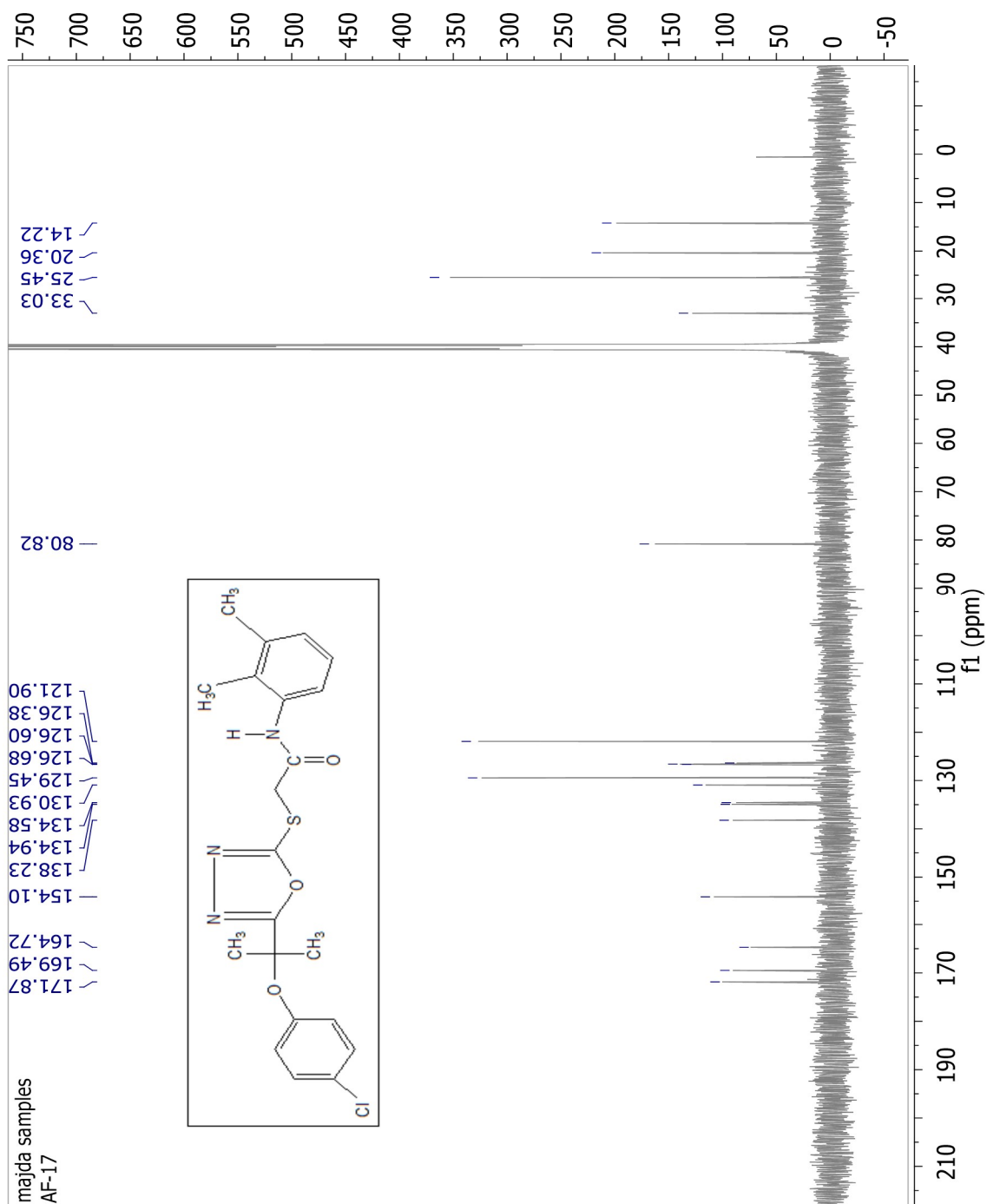


Figure S14. ¹³C-NMR spectrum of compound 3e.

File: 2P Date Run: 06-20-2017 (Time Run: 09:13:10)
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 Instrument: JEOL 600 MSRoute
 Inlet: Direct Probe Ionization mode: EI+

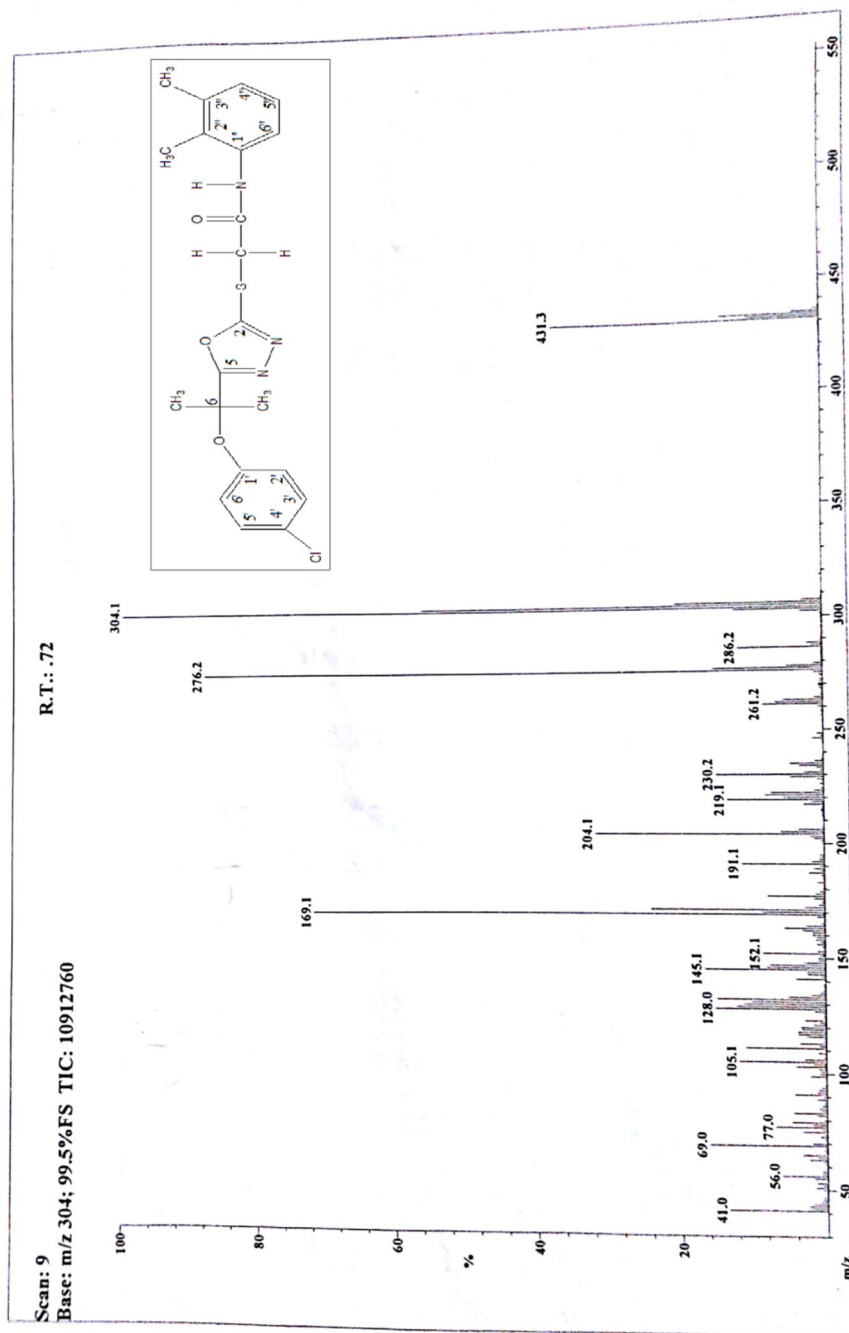


Figure S15. EI-MS of compound 3e.

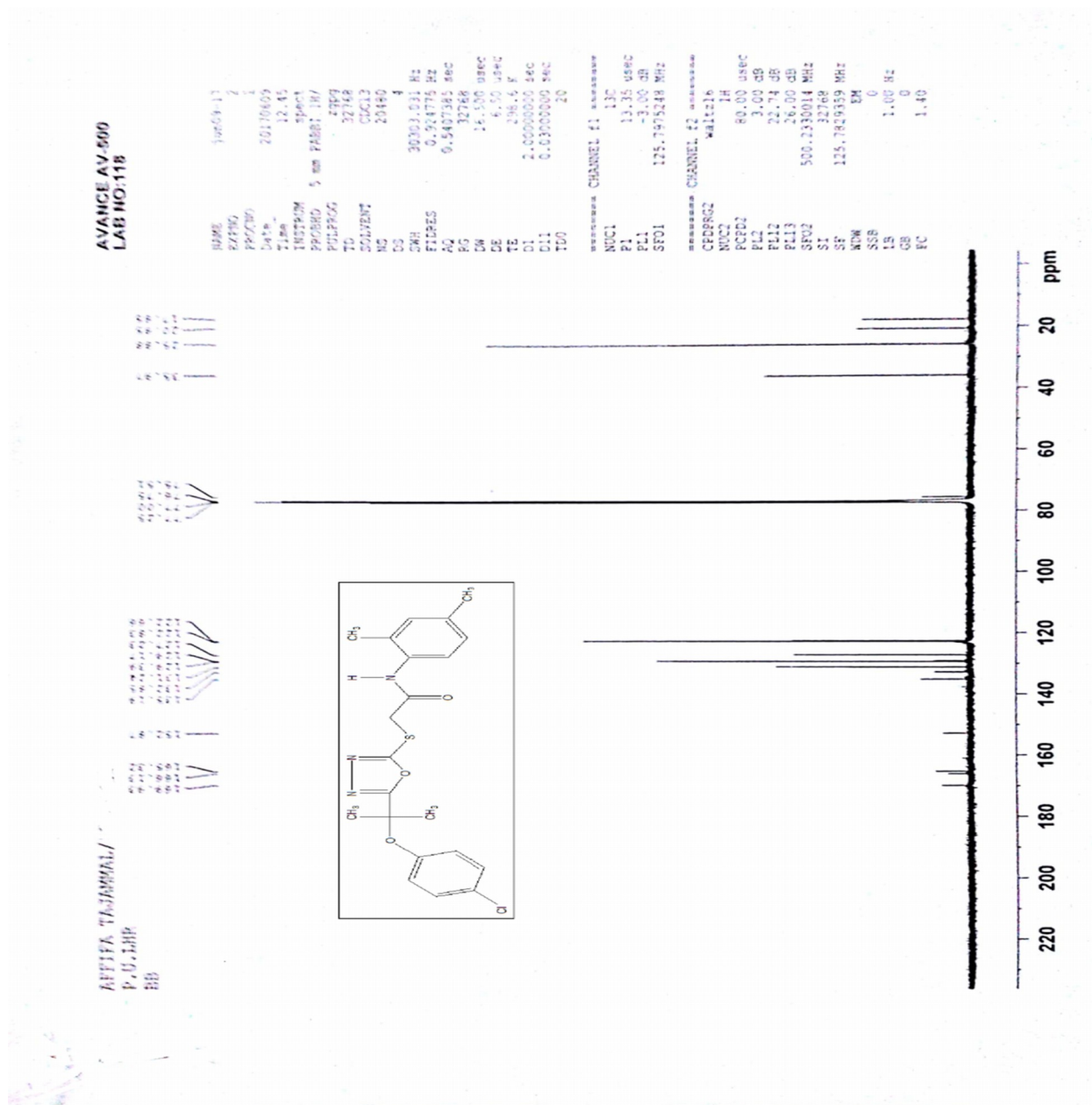


Figure S17. ¹³C-NMR spectrum of compound 3f.

Mass Lab (104)
6/19/2017 1:44:50 PM Page 1

File: IP
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Instrument: JEOL 600 MSRoute
Inlet: Direct Probe
Ionization mode: EI+

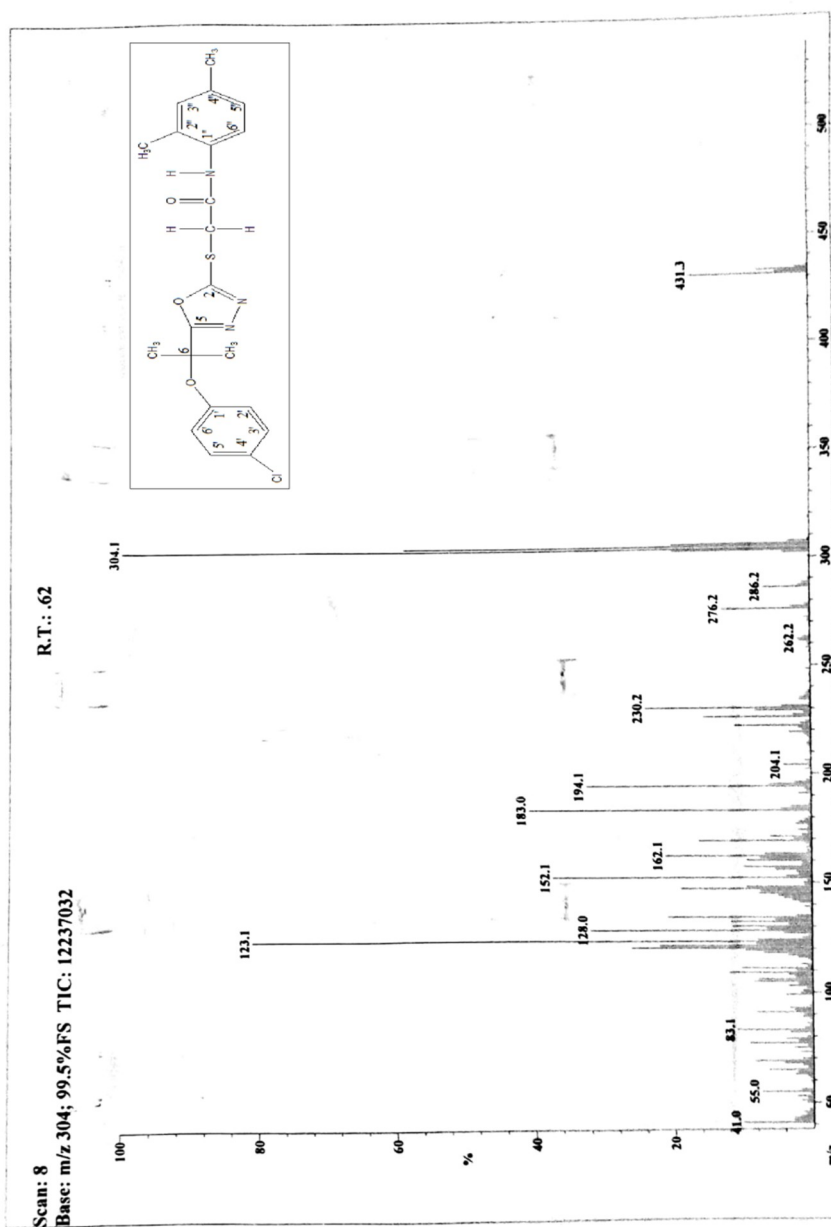


Figure S18. EI-MS of compound 3f.

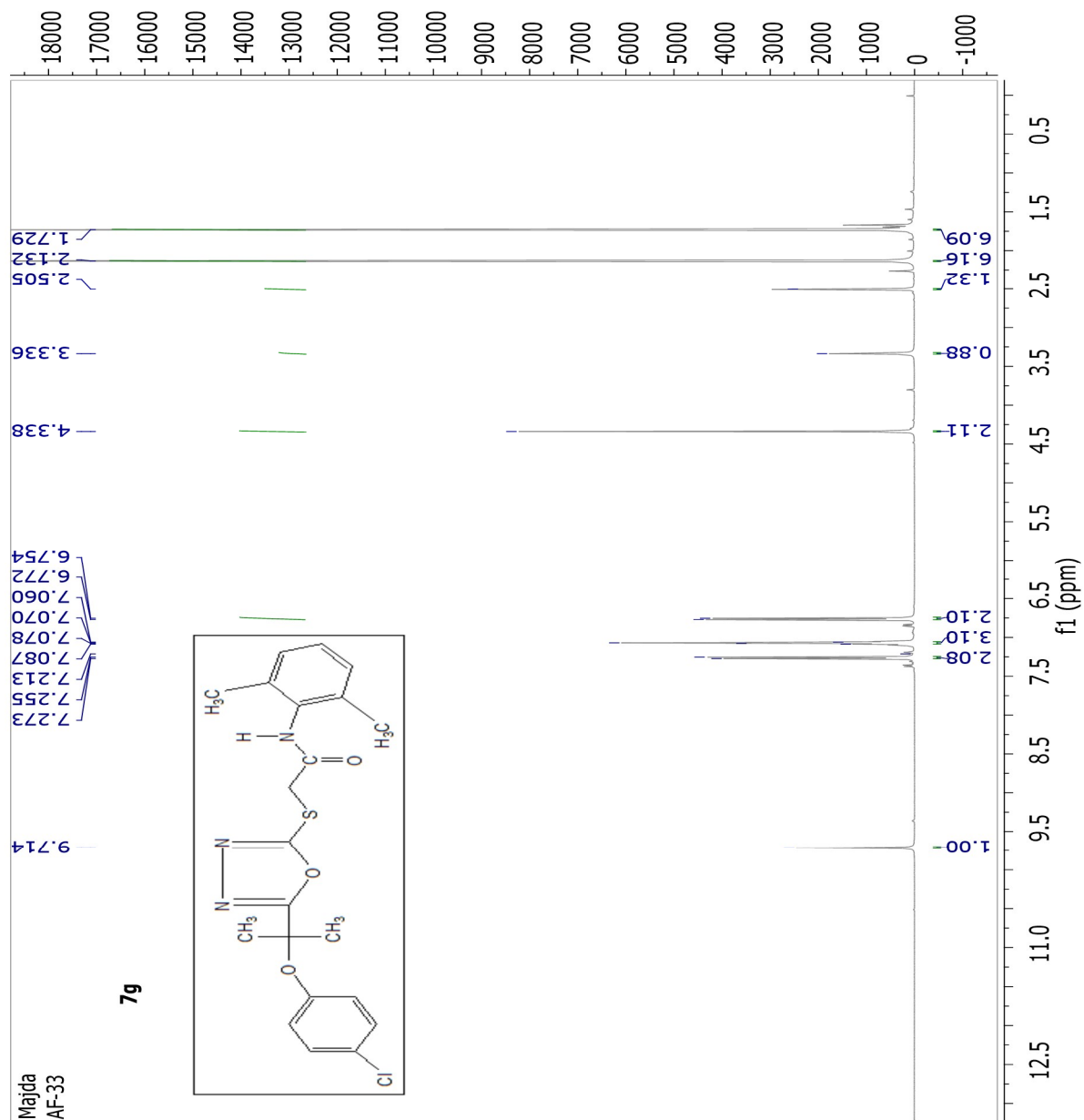


Figure S19. ¹H-NMR spectrum of compound 3g.

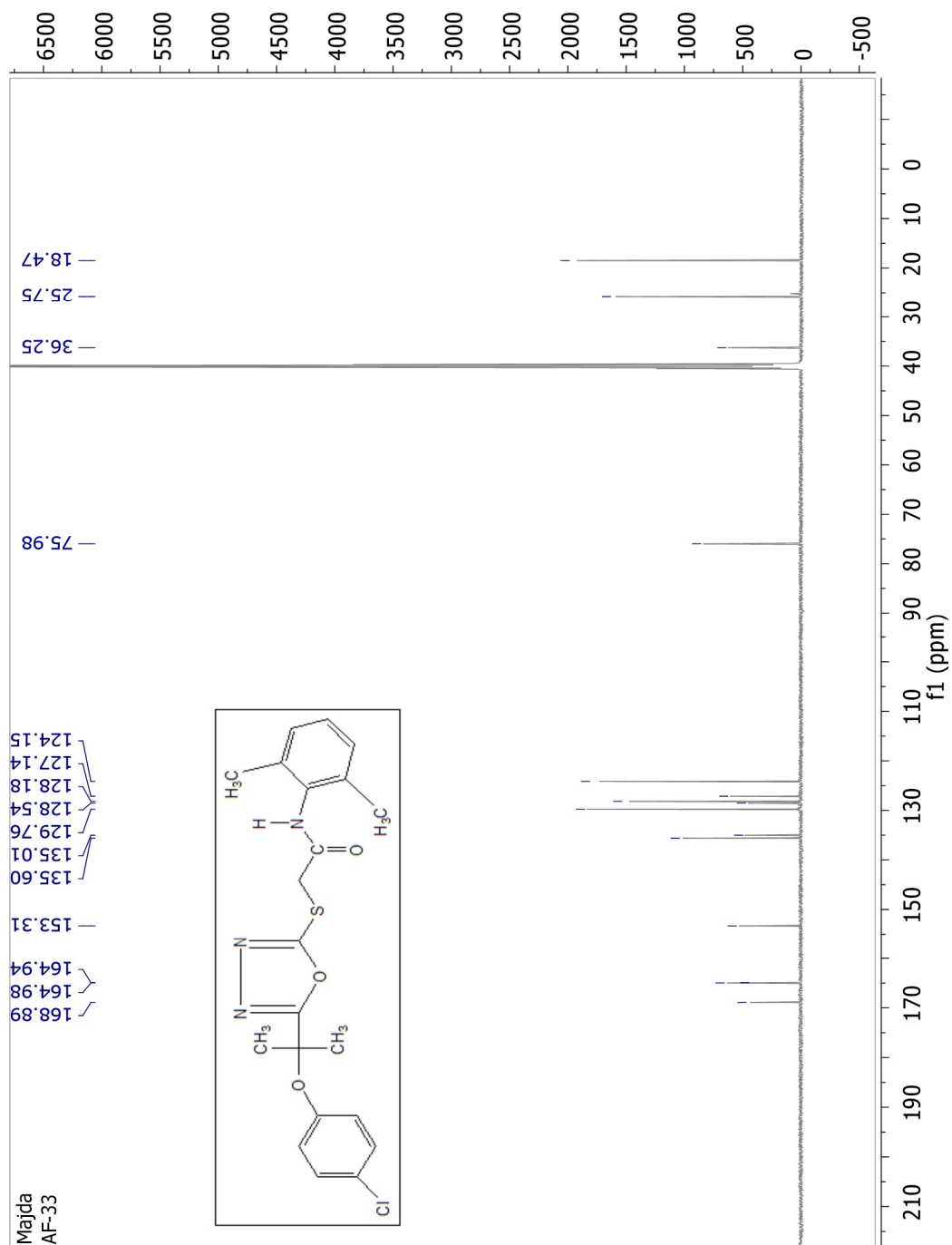


Figure S20. ¹³C-NMR spectrum of compound 3g.

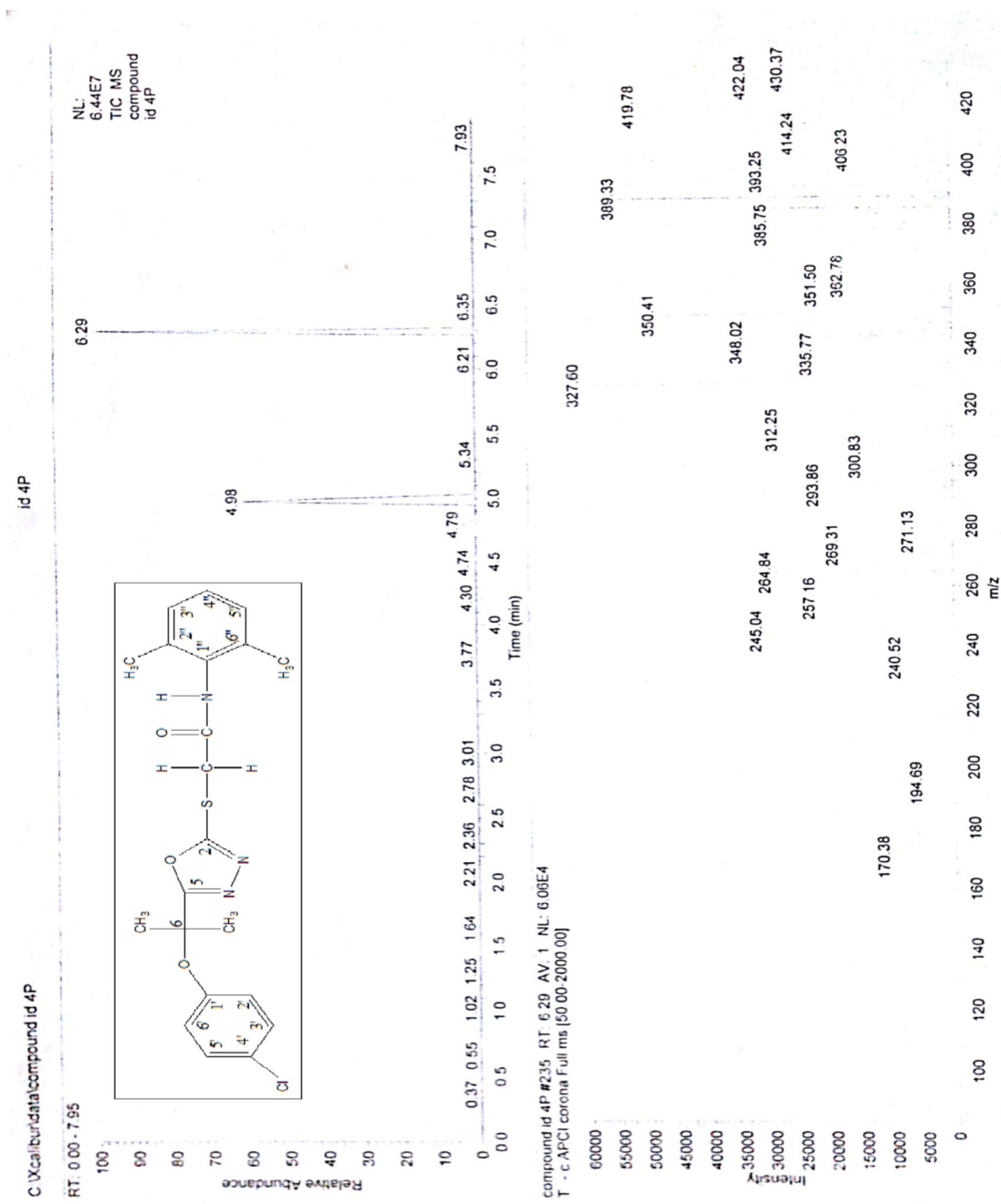


Figure S21. EI-MS of compound 3g.

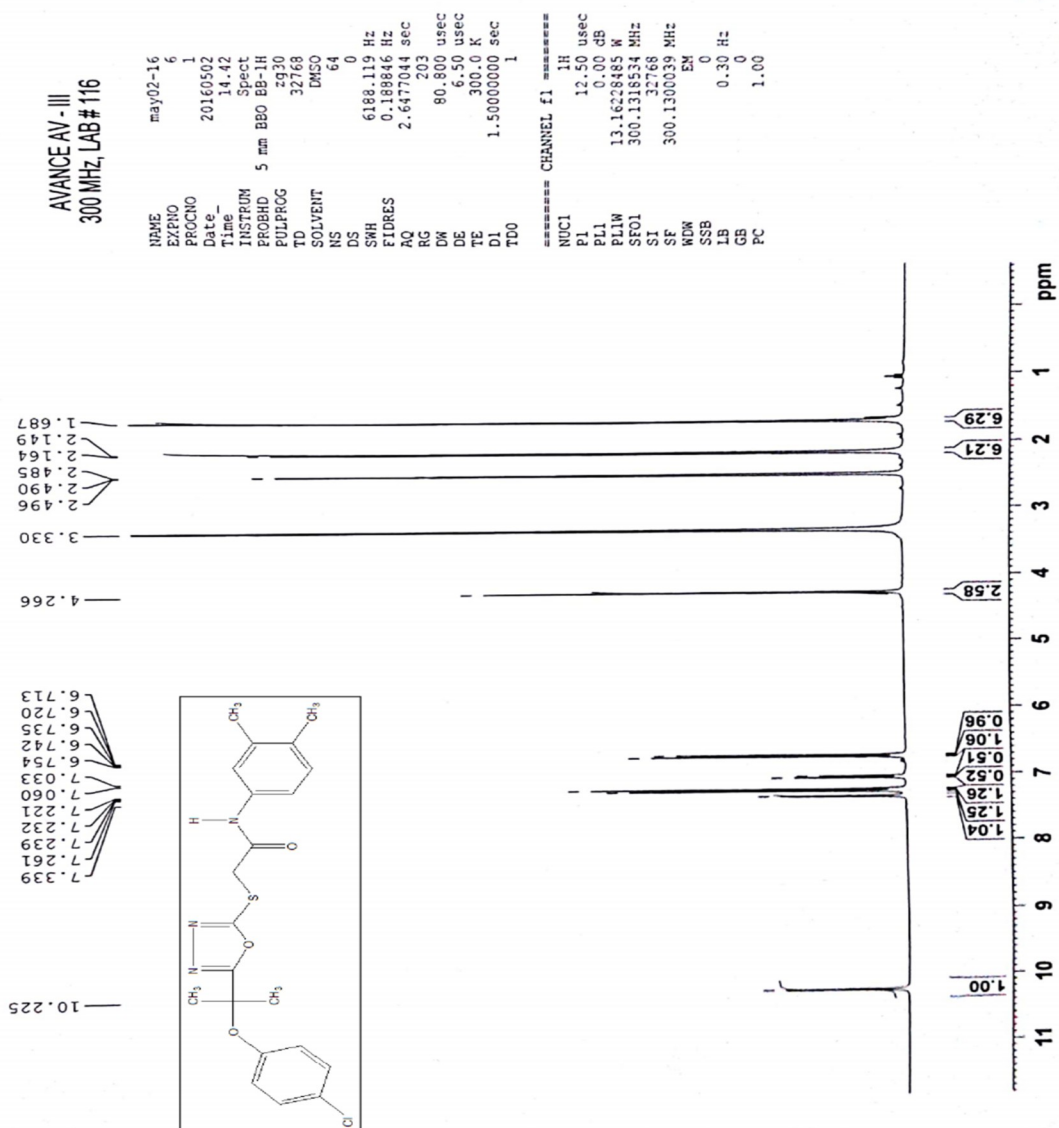


Figure S22. ¹H-NMR spectrum of compound 3h.

Affifa/Dr,Riffat
 Ins:O.Ch:U.O. Punjab/
 DEPT135

AVANCE AV - III
 300 MHz, LAB # 116

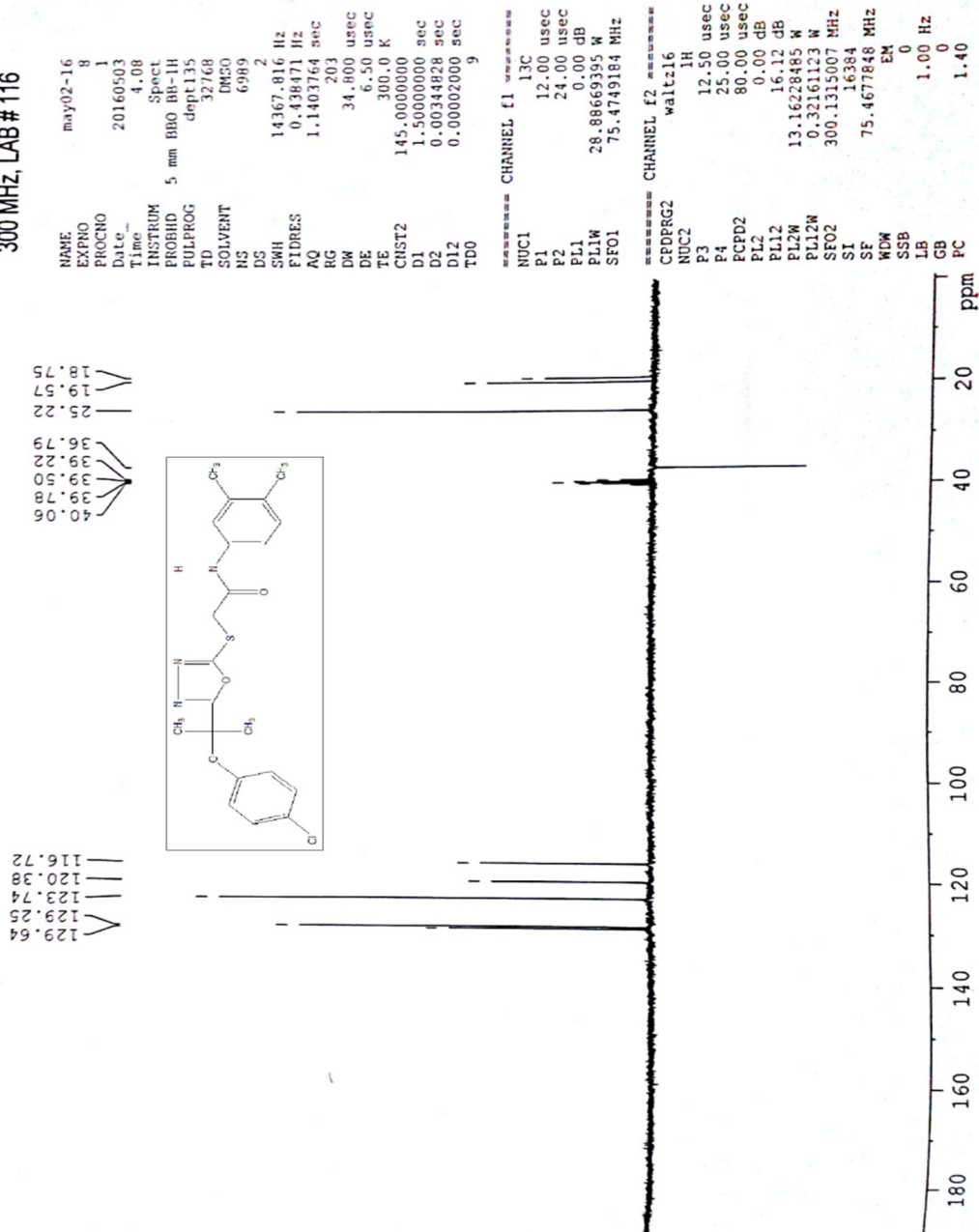


Figure S23. ¹³C-NMR spectrum of compound 3h.

Mass Lab (104)
6/20/2017 10:10:39 AM

Page 1

File: SP
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Inlet: Direct Probe

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Ionization mode: EI+

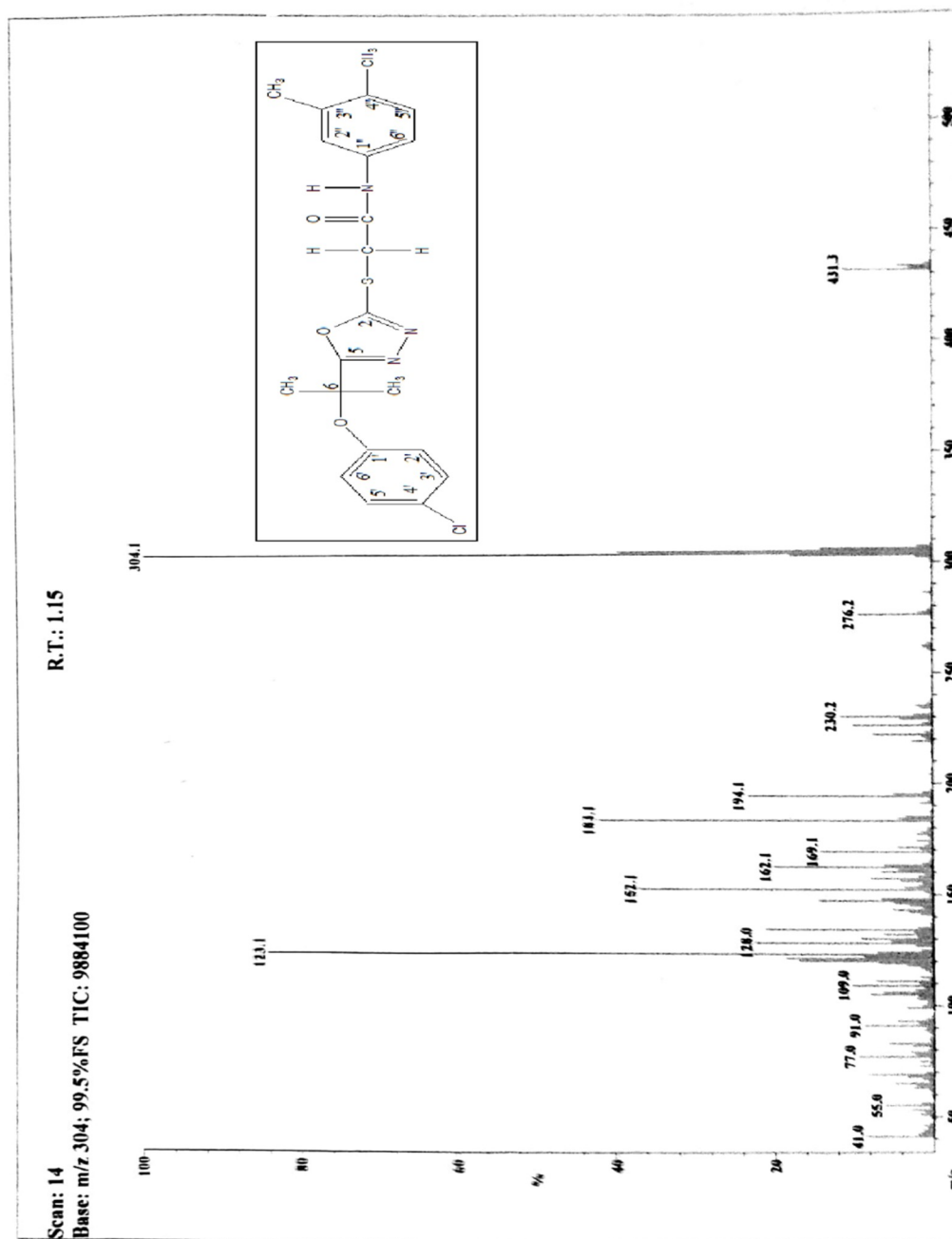


Figure S24. EI-MS of compound 3h.

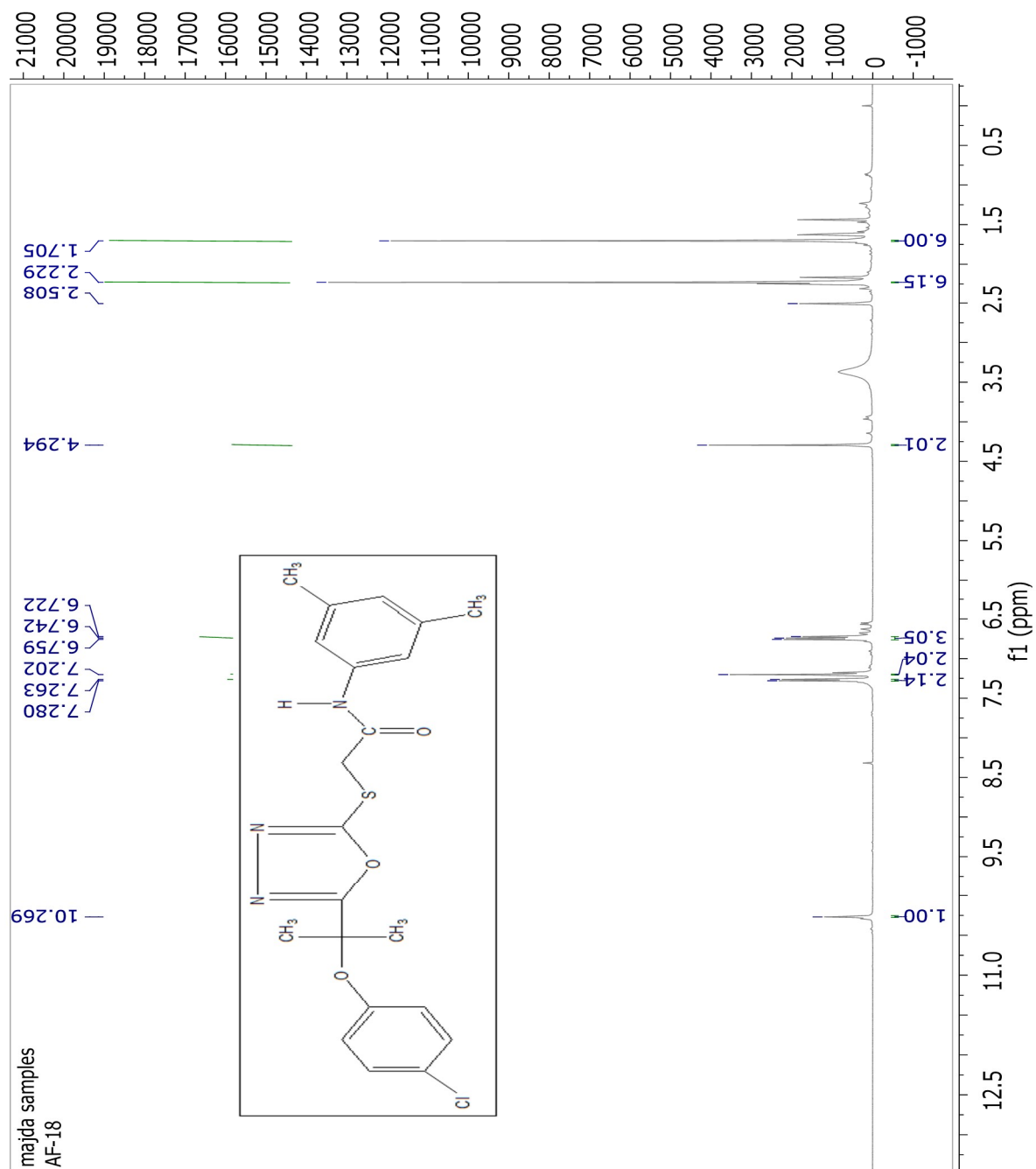


Figure S25. ¹H-NMR spectrum of compound 3i.

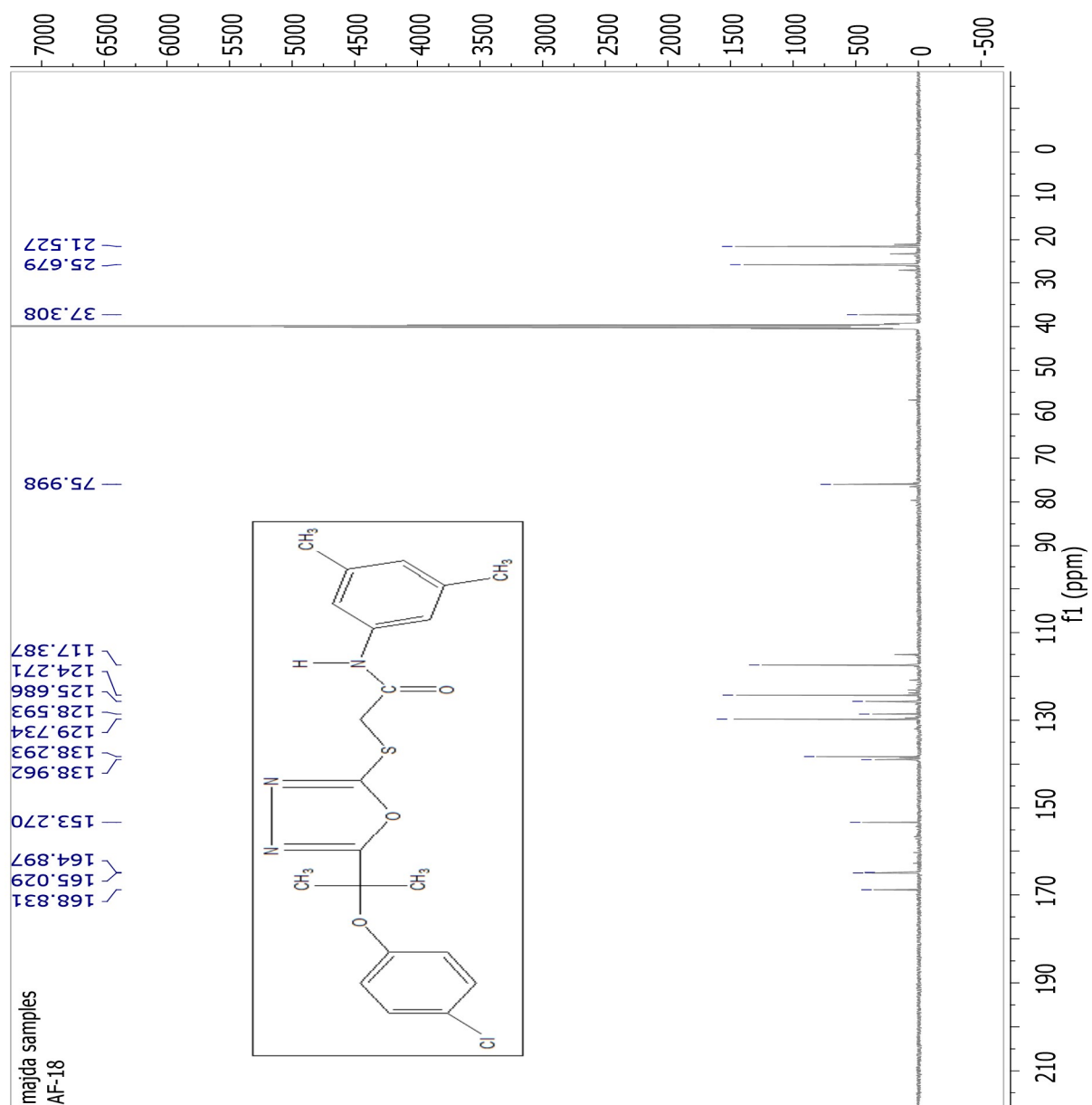


Figure S26. ^{13}C -NMR spectrum of compound 3i.

Mass Lab (104)
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File: 61P Date Run: 06-20-2017 (Time Run: 10:36:17)
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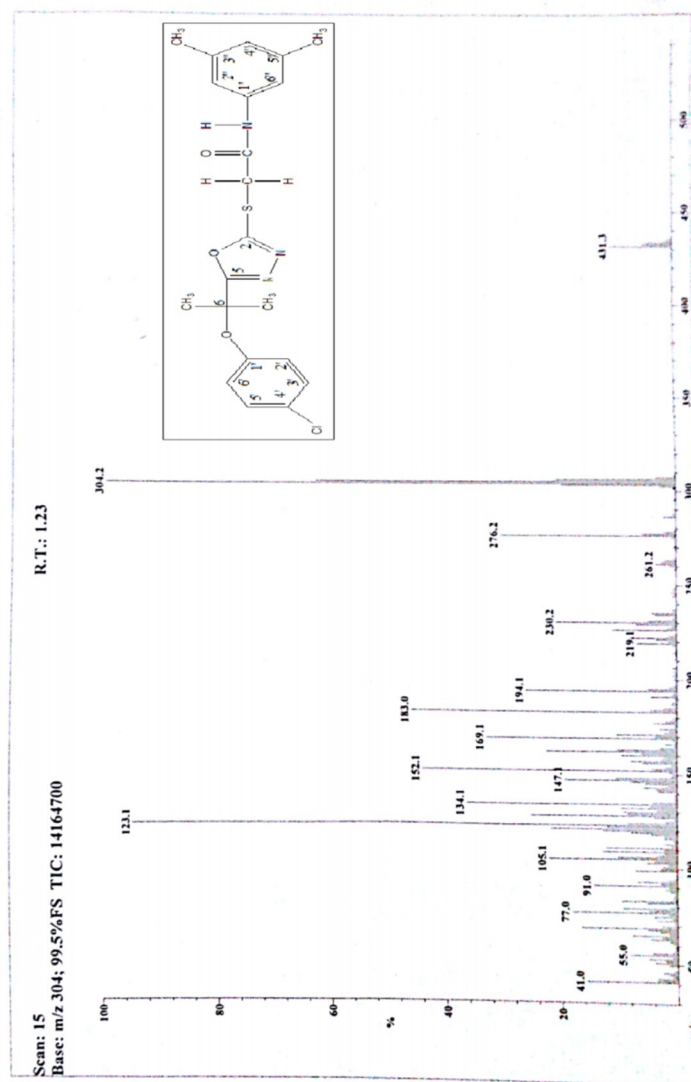


Figure S27. EI-MS of compound 3i.

Table S1. Docking results for the highest ranked biologically active ligand F-Xa.

Compd. No.	Score	<i>In-vivo</i> anticoagulant activity at 7 th h (Sec)	ACE Kcal/mole	Amino acids showing hydrogen bond contacts	Distance (Å)	Amino acids showing van der Waals contacts lie within 4 Å	Amino acids showing hydrophobic contacts lie within 4 Å	Amino acids showing arene-cation contacts
1	3562	74	-197.87	Glu ⁴⁹	3.22	Ser ⁴⁸ , Leu ⁴⁷ , Met ²⁴² , Ala ²⁴ , Cys ¹²² , Pro ⁴³ , Tyr ⁴²	Pro ¹²⁰ , Phe ¹¹⁴ , Cys ⁴⁴ , Arg ²⁵ , Leu ¹²³	Arg ²⁵
3a	6270	342	-352.28	Arg ²⁵	2.94	Tyr ⁴² , Met ²⁴² , Phe ¹¹⁴ , Cys ¹²² , Leu ⁴⁷ , Ser ⁴⁸ , Pro ¹²⁰ , Gly ²⁶ , Gly ⁴⁰ , Thr ³⁹	Ala ²⁴ , Pro ⁴³	-
3b	5312	108	-370.05	-	-	Leu ⁴⁷ , SER ⁴⁸ , Pro ¹²⁰ , Tyr ⁴² , Phe ¹¹⁴ , Pro ⁴¹ , Gly ⁴⁰ , Pro ¹²⁴ , Glu ¹²⁴	Cys ⁴⁴ , Pro ⁴³ , Gly ²⁶ , Pro ¹²⁴ , Met ²⁴² , Phe ¹¹ , Ala ²⁴ , Leu ¹²³	Arg ²⁵
3c	5324	95	-253.57	Arg ²⁵	2.83	Arg ¹²⁵ , Glu ¹²⁴ , Pro ¹²⁴ , Ala ²⁴ , Cys ¹²² , Phe ¹¹⁴ , Glu ⁴⁹ , Ser ⁴⁸ , Leu ⁴⁷ , Met ²⁴² , Asp ²³⁹	Leu ¹²³ , Arg ²⁵ , Pro ¹²⁰ , Leu ²³⁵ , Lys ²³⁶	-
3d	5646	132	-287.52	Arg ²⁵ , Leu ¹²³	3.19, 3.25	-	Cys ⁴⁴ , Pro ¹²⁰ , Arg ²⁵ , Leu ²³⁵ , Lys ²³⁶	-
3e	5658	167	-189.68	Arg ²⁵ , Leu ¹²³ , Pro ¹²⁴	2.98, 3.03, 3.17	Arg ¹²⁵ , Glu ¹²⁴ , Phe ¹¹⁴ , Glu ⁴⁴ , Ser ⁴⁸	Lys ²³⁶ , Ala ²⁴ , Arg ²⁵ , Leu ¹²³ , Cys ⁴⁴	-
3f	5626	84	-340.54	Arg ²⁵ , Arg ²⁵	2.99, 2.74	Ala ²⁴ , Gly ²⁶ , Phe ¹¹⁴ , Gly ⁴⁰ , Pro ⁴³ , Tyr ⁴² , Leu ⁴⁷ , Met ²⁴² , Glu ¹²⁴	Phe ¹¹ , Leu ¹²³ , Leu ²³⁵ , Cys ⁴⁴ , Pro ⁴¹ , Pro ¹²⁰	-
3g	5442	92	-262.48	-	-	Asp ²³⁹ , Pro ¹²⁴ , Glu ¹²⁴ , Trp ¹²⁷ , Cys ¹²²	Ala ²⁴ , Phe ¹¹ , Cys ⁴⁴ , Arg ²⁵ , Lys ²³⁶ , Arg ¹²⁵ , Leu ²³⁵	-
3h	5612	130	-311.48	-	-	Thr ³⁹ , Gly ⁴⁰ , Pro ⁴¹ , Gly ²⁶ , Pro ¹²⁰ , Cys ⁴⁴ , Leu ⁴⁷ , Asp ²³⁹ , Ala ²⁴ , Phe ¹¹ , Glu ¹²⁴	Pro ⁴³ , Leu ¹²³ , Phe ¹¹⁴	Arg ²⁵

3i	5662	214	-312.12	-	-	Pro ⁴¹ , Tyr ⁴² , Pro ¹²⁰ , Leu ⁴⁷ , Cys ⁴⁴ , Met ²⁴² , Ala ²⁴ , Asp ²³⁹ , Gly ²⁶ , Pro ⁴³ , Thr ³⁹ , Gly ⁴⁰	Arg ²⁵	Arg ²⁵
RPR200095	5192	110	-197.81	-	-	Leu ⁴⁷ , Ser ⁴⁸ , Cys ²³ , Tyr ⁵¹ , Cys ¹²² , Gly ²⁶ , Ala ²⁴ , Phe ¹¹ , Pro ¹²⁴ , Leu ²³⁵ , Asp ²³⁹ , Leu ²³⁵	Lys ²⁴³ , Arg ²⁵ , Met ²⁴²	-

No. = Specific code assigned to ligand; ACE= Atomic contact energy calculated by *Patch Dock* (kcal/mol); Distance = hydrogen bond length calculated from docked pose by using *Ligand interaction* tool of *Patch Dock*.

Table S2. DFT computed molecular properties (all in eV, except dipole moment which is in the units of Debye) for oxadiazoles derivatives obtained at B3LYP/6-31G** level of theory.

Sr. No.	Compound name	E _{HOMO}	E _{LUMO}	E _{gap}	Ionisation potential (I)	Electron affinity (A)	Chemical hardness (η)	Chemical softness (S)	Chemical potential (μ)	Electronegativity (χ)	Electrophilicity (ω)	Dipole moment (D)
1	1	-6.60	-0.58	6.02	6.60	0.58	3.01	0.17	-3.59	3.59	2.14	3.66
2	3a	-6.25	-0.64	5.61	6.25	0.64	2.80	0.18	-3.44	3.44	2.12	1.84
3	3b	-6.14	-0.64	5.51	6.14	0.64	2.75	0.18	-3.39	3.39	2.09	1.83
4	3c	-6.15	-0.60	5.54	6.15	0.60	2.77	0.18	-3.37	3.37	2.06	2.20
5	3d	-6.05	-0.57	5.48	6.05	0.57	2.74	0.18	-3.31	3.31	1.99	2.39
6	3e	-6.07	-0.58	5.49	6.07	0.58	2.75	0.18	-3.32	3.32	2.01	2.19
7	3f	-5.95	-0.57	5.39	5.95	0.57	2.69	0.19	-3.26	3.26	1.97	2.36
8	3g	-6.41	-0.54	5.87	6.41	0.54	2.94	0.17	-3.47	3.47	2.05	2.14
9	3h	-5.97	-0.53	5.43	5.97	0.53	2.72	0.18	-3.25	3.25	1.94	2.67
10	3i	-6.08	-0.54	5.54	6.08	0.54	2.77	0.18	-3.31	3.31	1.98	2.37



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