

Supporting information

**Cooperative Catalysis by Bovine Serum Albumin-Iodine Towards Cascade
Oxidative Coupling-C(sp²)-H Sulfenylation of Indoles/Hydroxyaryls with
Thiophenols on water**

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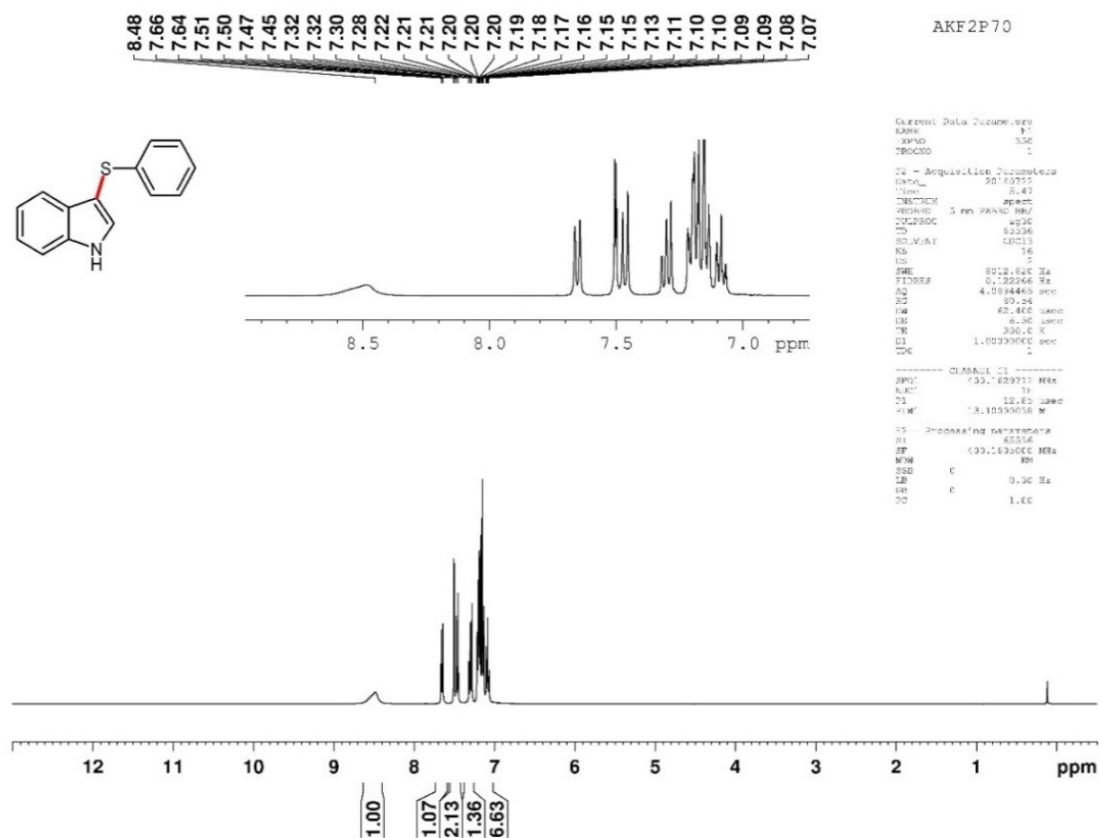
*E-mail: aksinha08@rediffmail.com, ak.sinha@cdri.res.in

CDRI communication no:

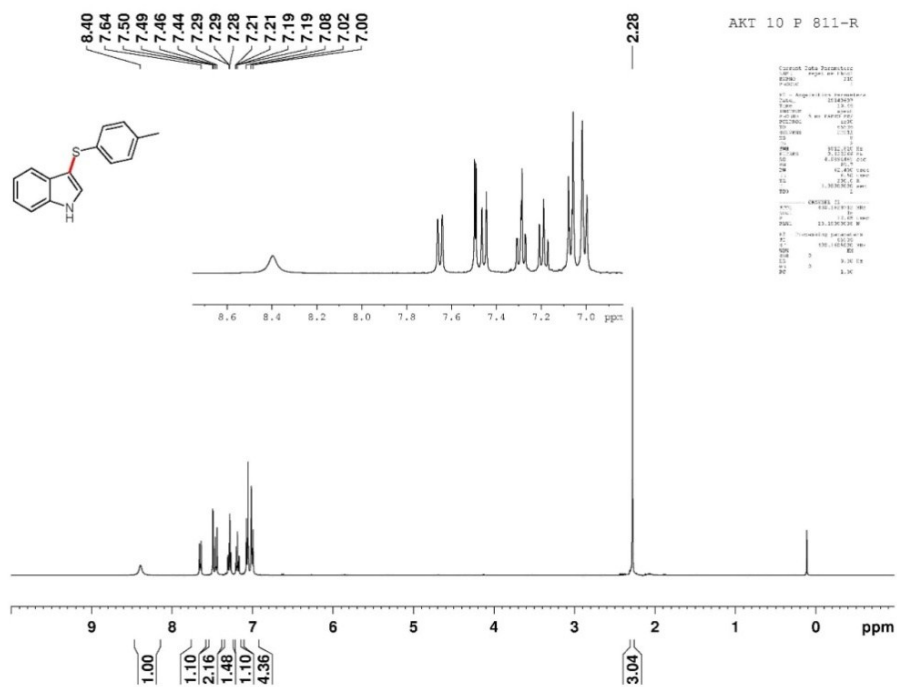
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[1] ¹ H, ¹³ C NMR and HRMS spectra of synthesized compounds	S2-S84
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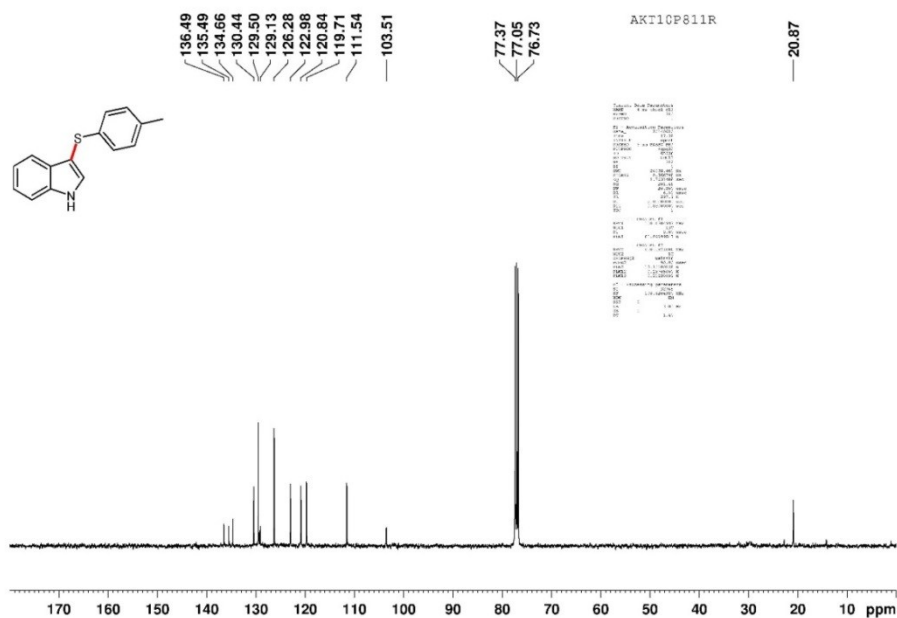
11. NMR spectras and HRMS of synthesised compounds:



¹H-NMR spectrum of 3-(phenylthio)-1H-indole (Table2, 3a).

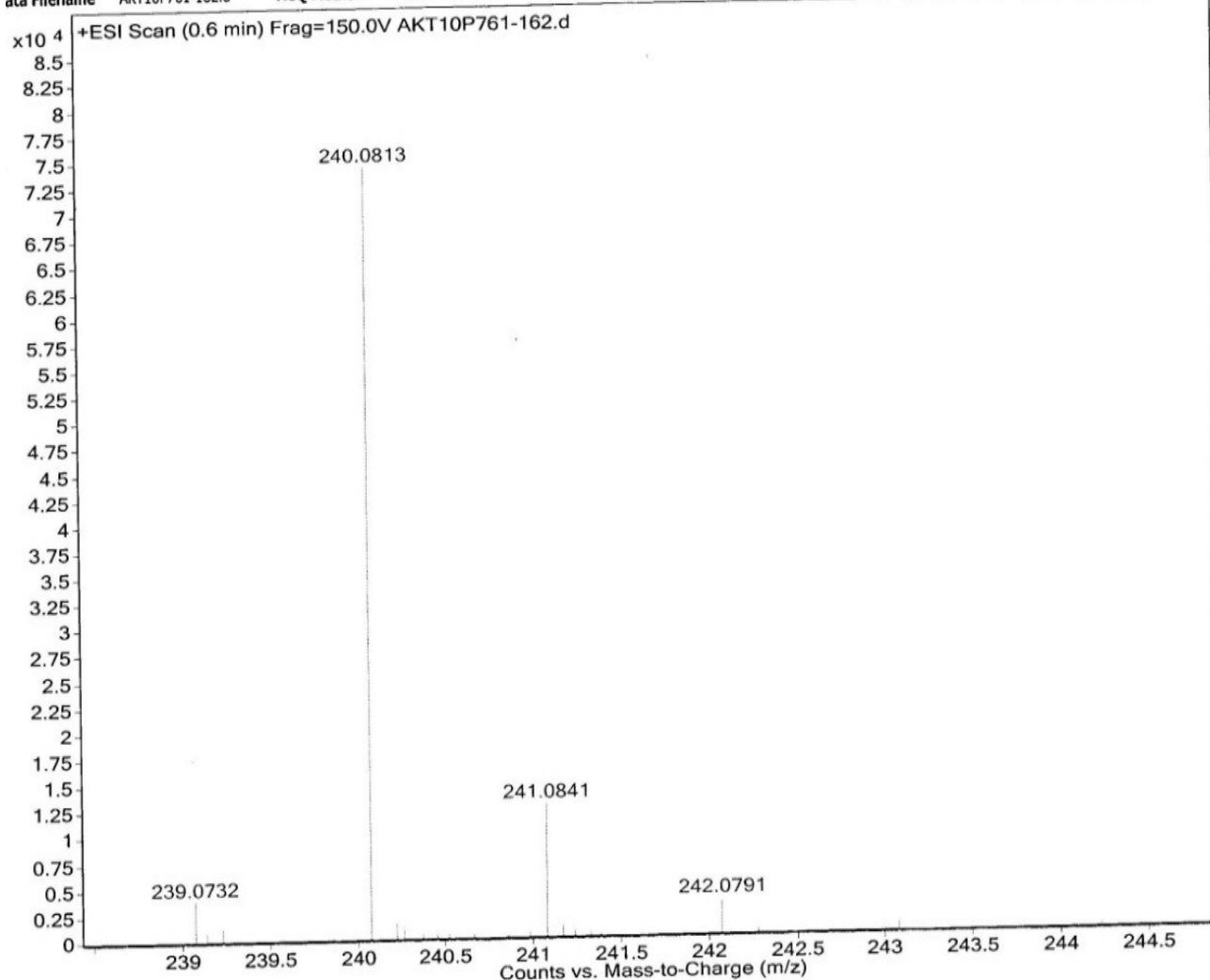


¹H-NMR spectrum of 3-(p-tolylthio)-1H-indole (Table2, 3b).

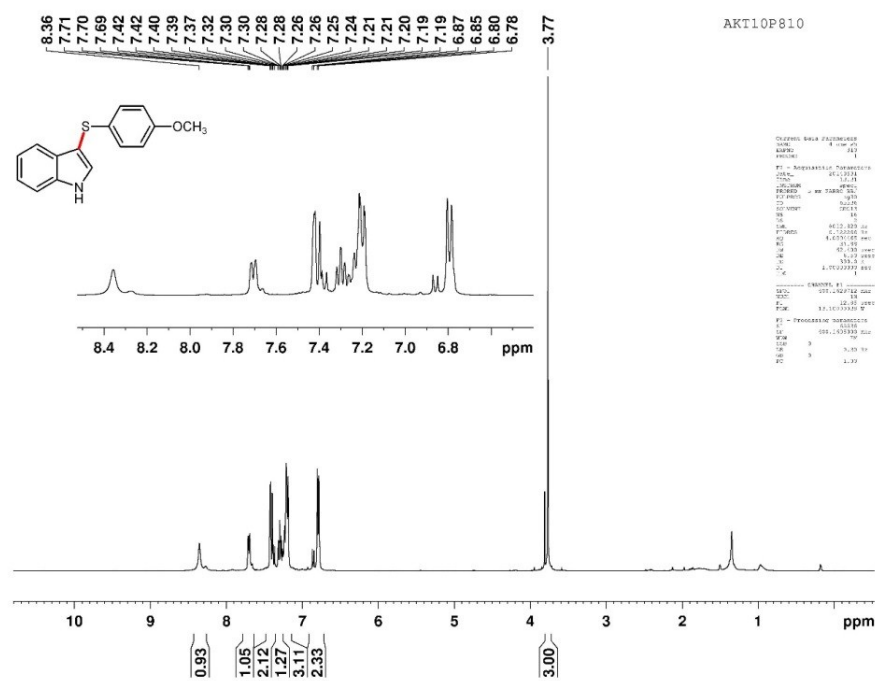


¹³C-NMR spectrum of 3-(p-tolylthio)-1H-indole (Table 2, 3b).

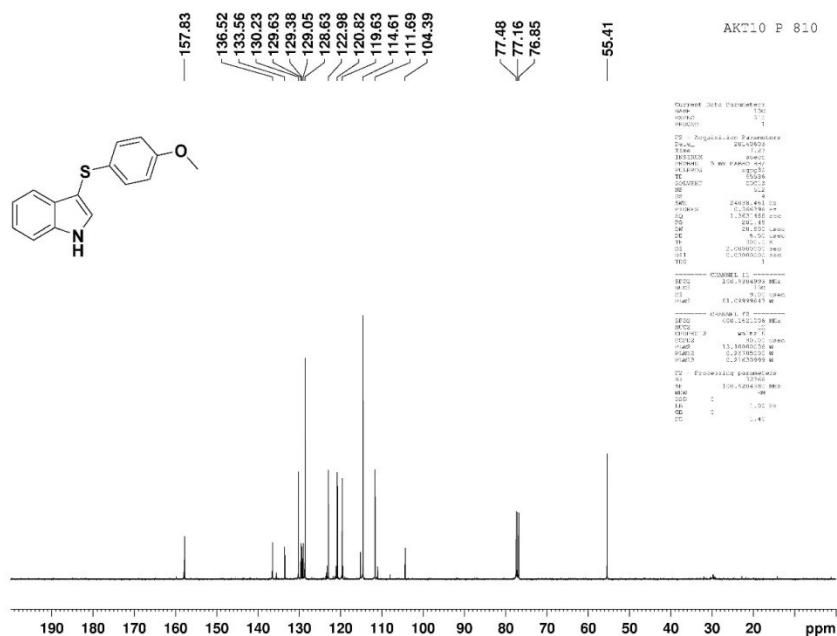
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HRMS spectrum of 3-(p-tolylthio)-1H-indole (Table 2, 3b).

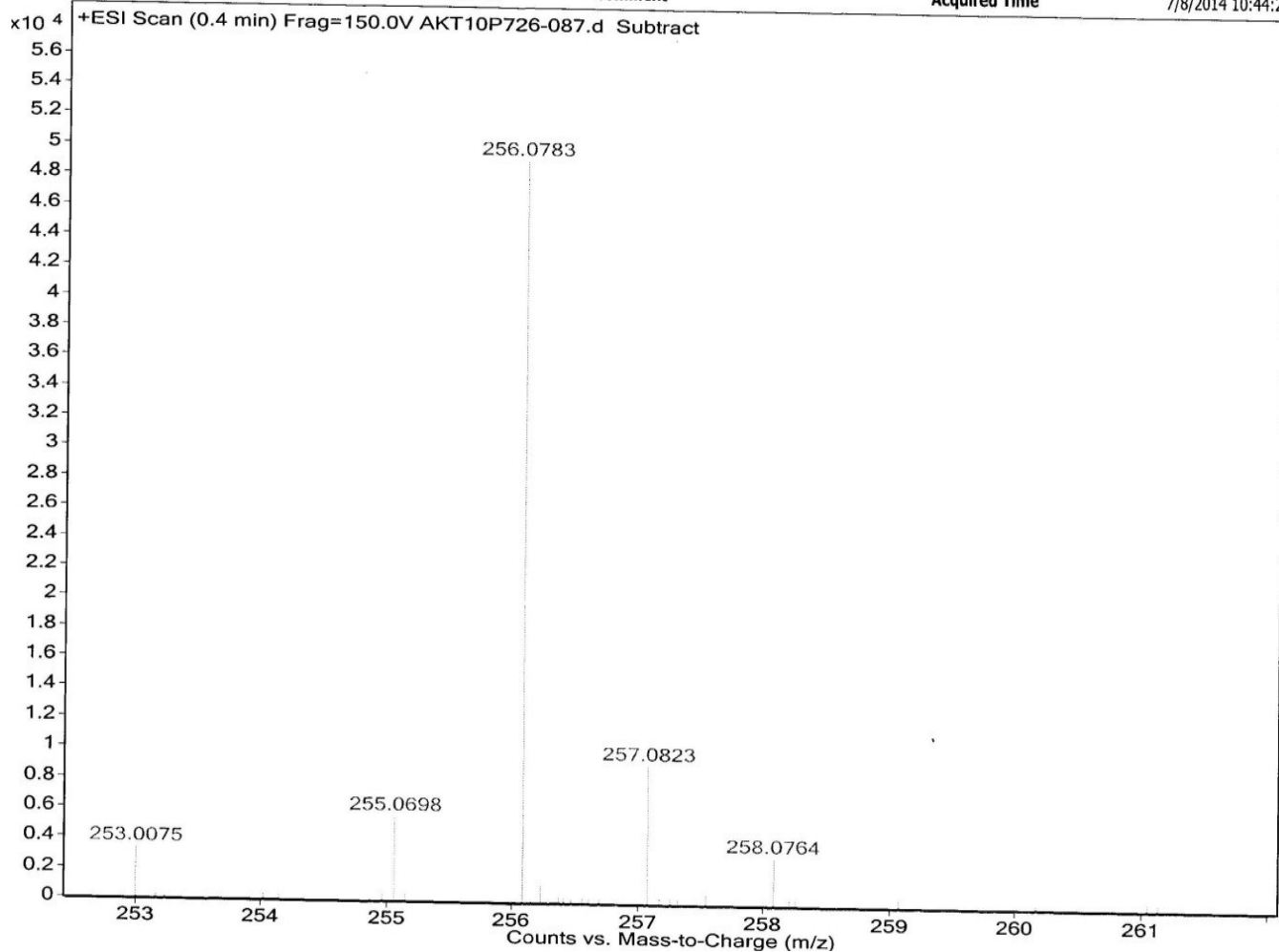


¹H-NMR spectrum of 3-((4-methoxyphenyl)thio)-1H-indole (Table 2, 3c)

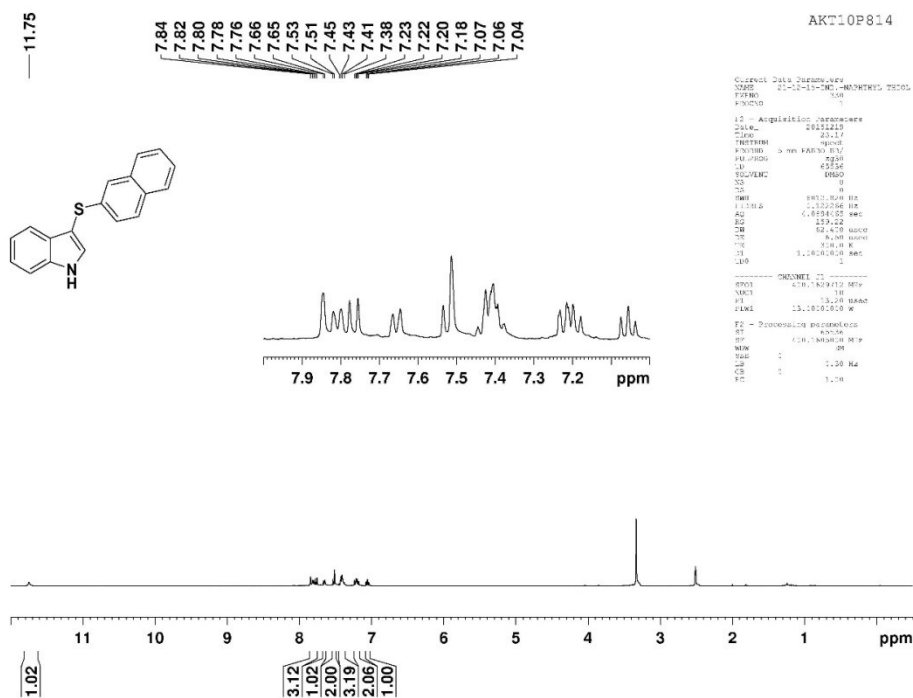


¹³C-NMR spectrum of 3-((4-methoxyphenyl)thio)-1H-indole (Table 2, 3c)

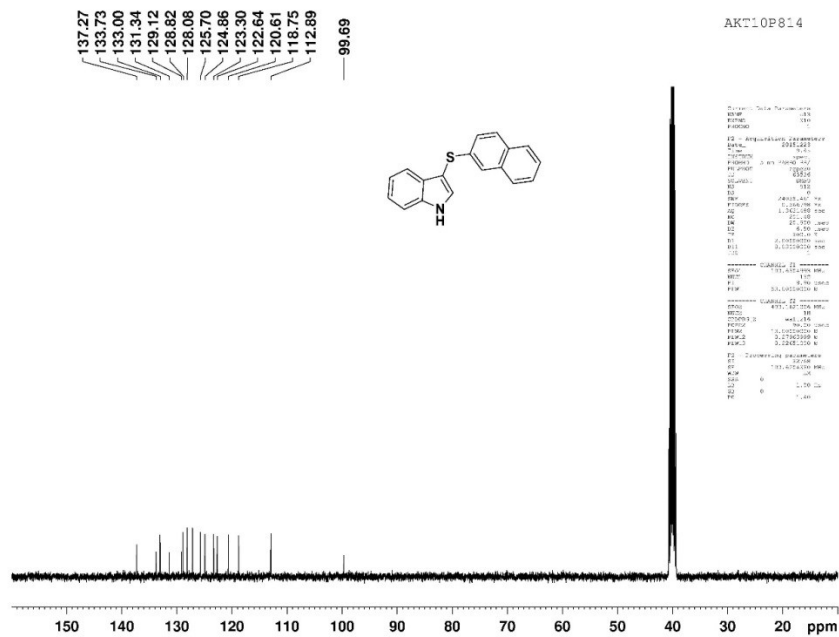
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HRMS spectrum of 3-((4-methoxyphenyl)thio)-1H-indole (Table 2, 3c)

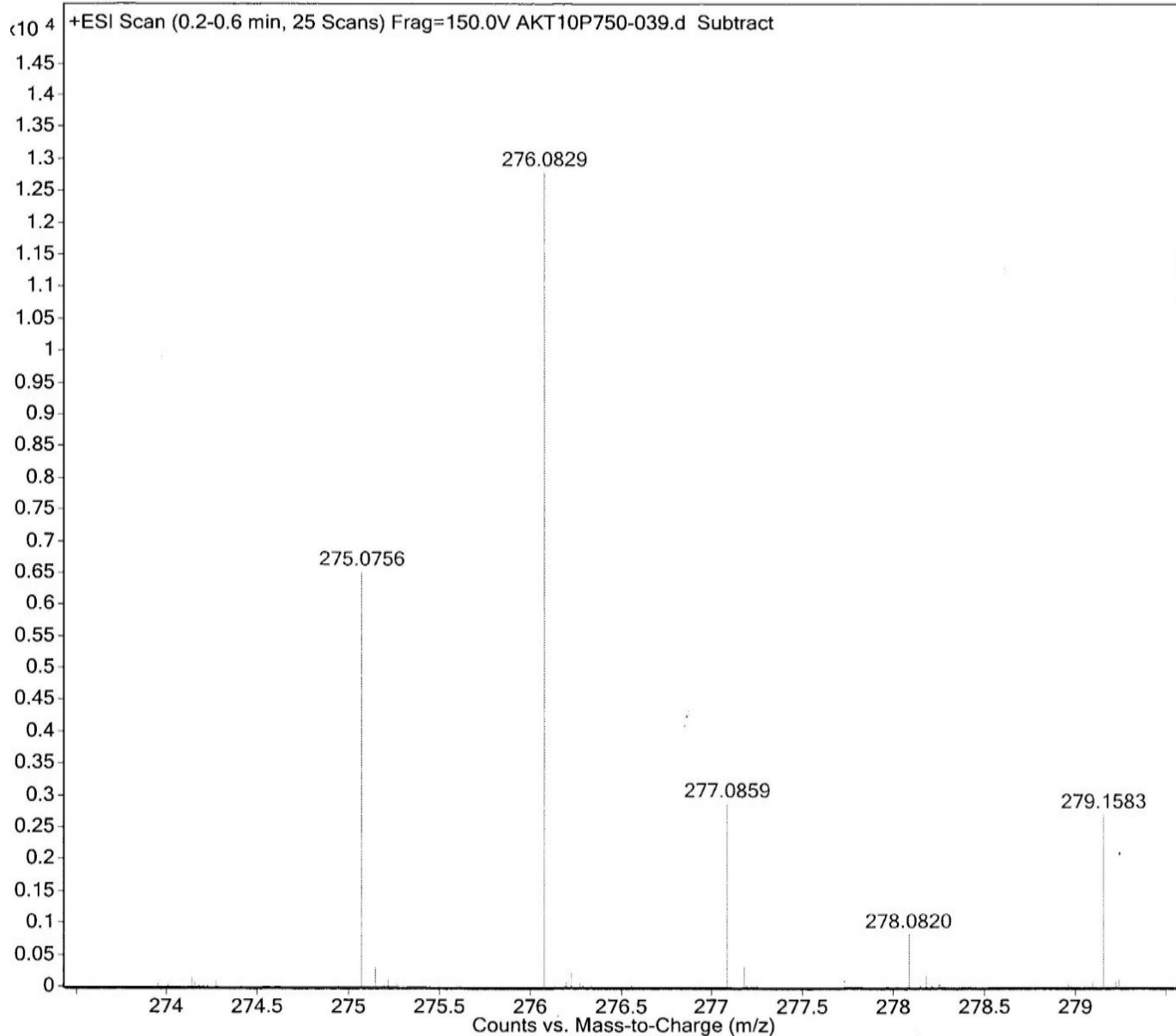


¹H-NMR spectrum of 3-(naphthalen-1-ylthio)-1H-indole (Table 2, 3d)

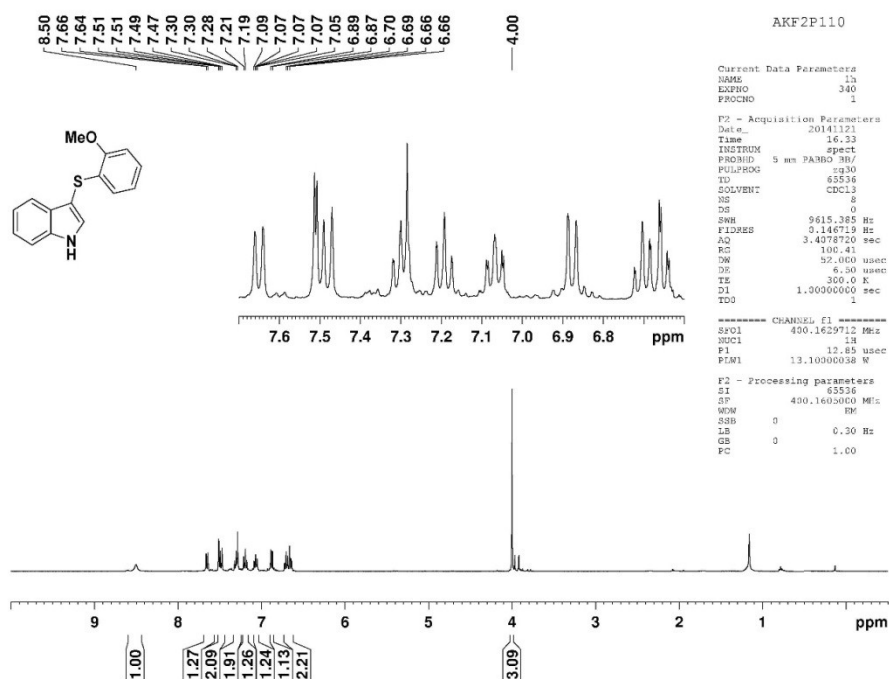


¹³C-NMR spectrum of 3-(naphthalen-1-ylthio)-1H-indole (Table 2, 3d)

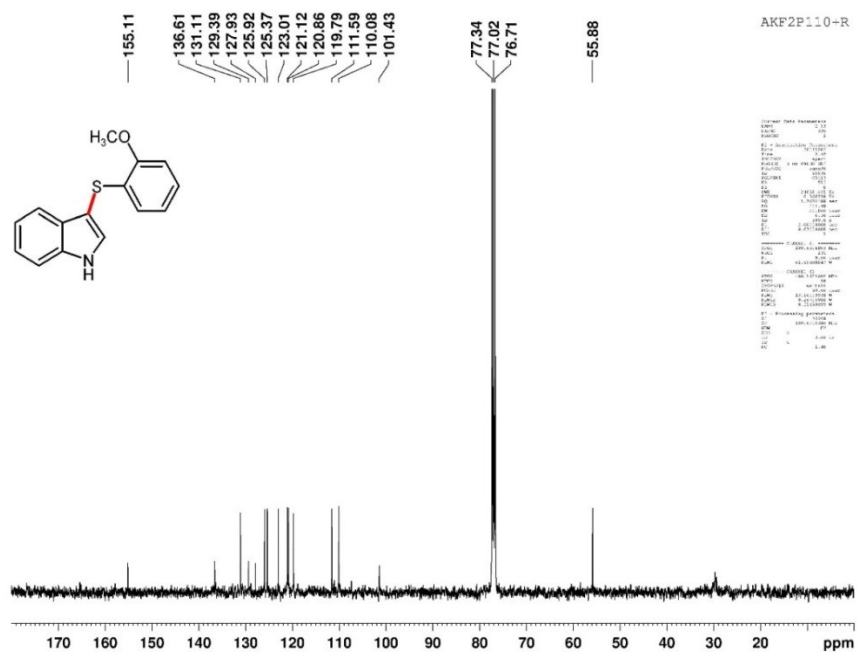
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HRMS spectrum of 3-(naphthalen-1-ylthio)-1H-indole (Table 2, 3d)



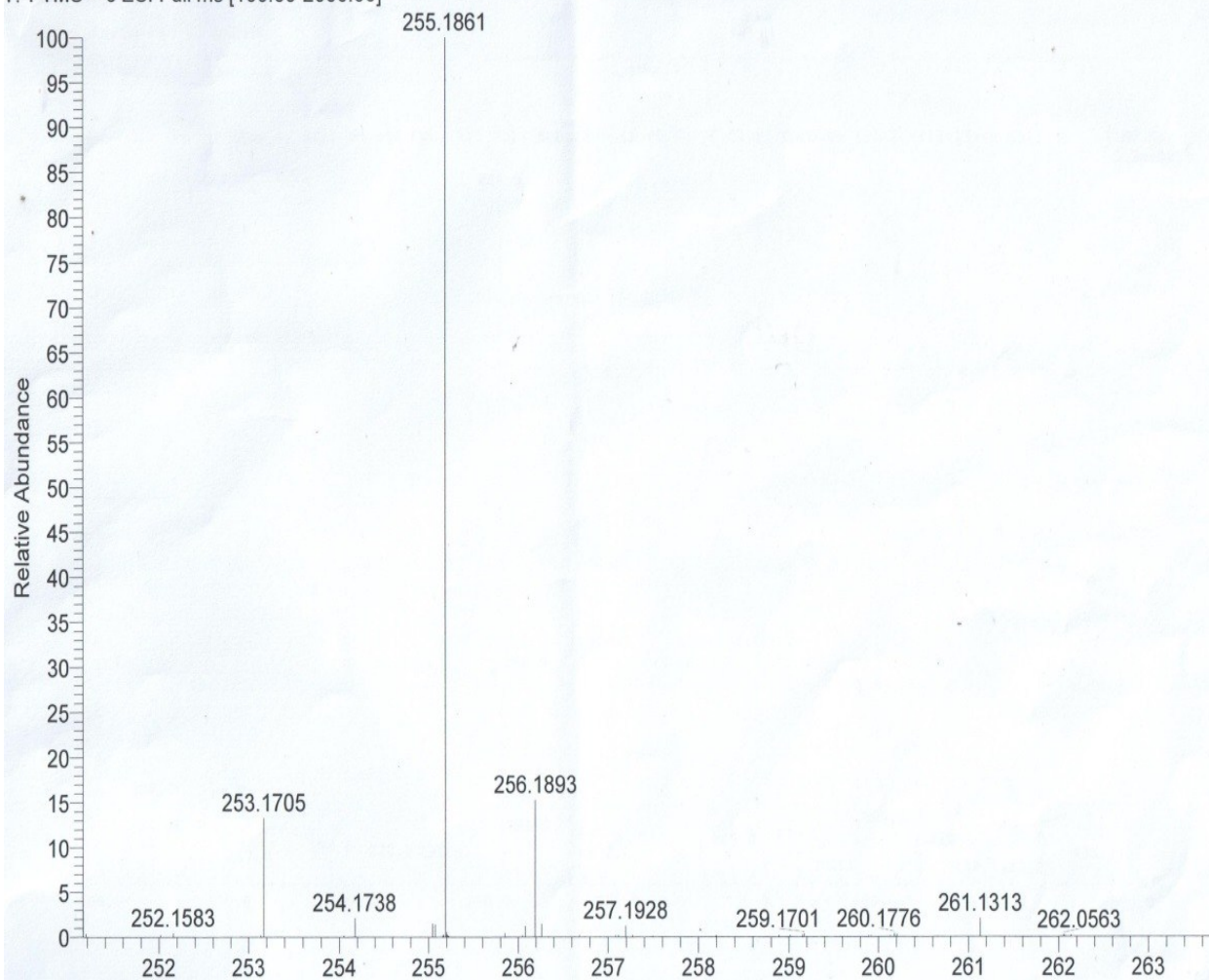
¹H-NMR spectrum of 3-((2-methoxyphenyl)thio)-1H-indole (Table 2, 3e)



¹³C-NMR spectrum of 3-((2-methoxyphenyl)thio)-1H-indole (Table 2, 3e)

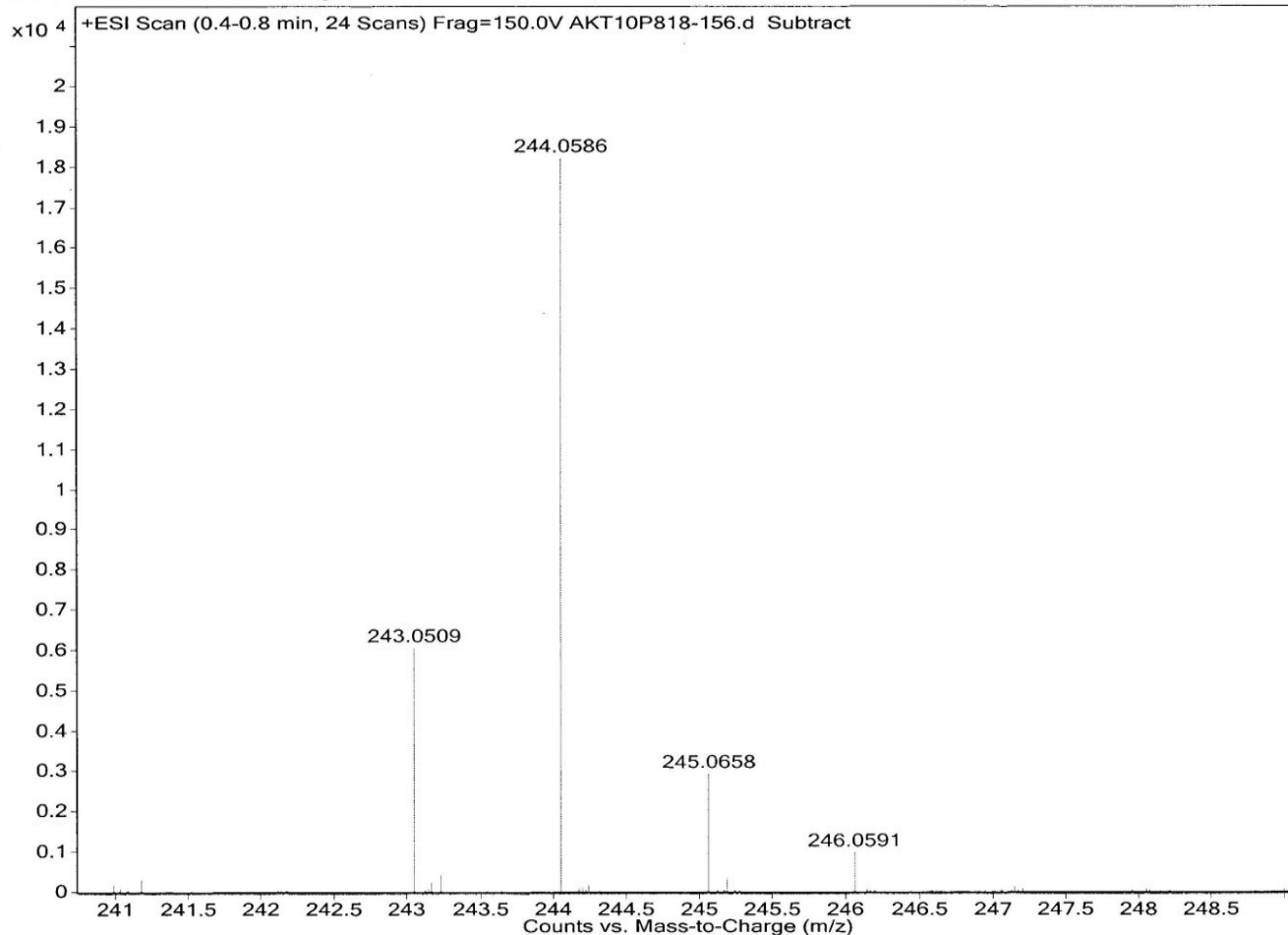
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T: FTMS + c ESI Full ms [100.00-2000.00]

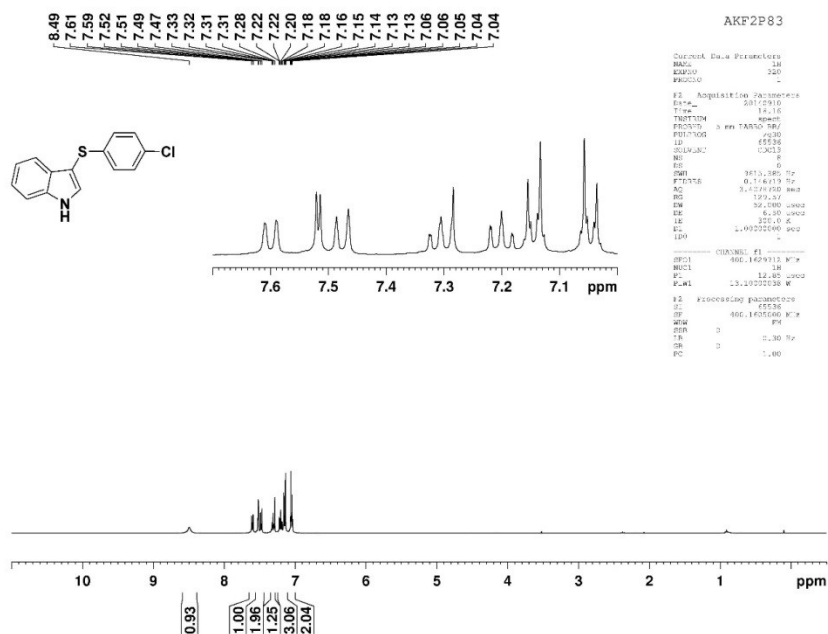


HRMS spectrum of 3-((2-methoxyphenyl)thio)-1H-indole (Table 2, 3e)

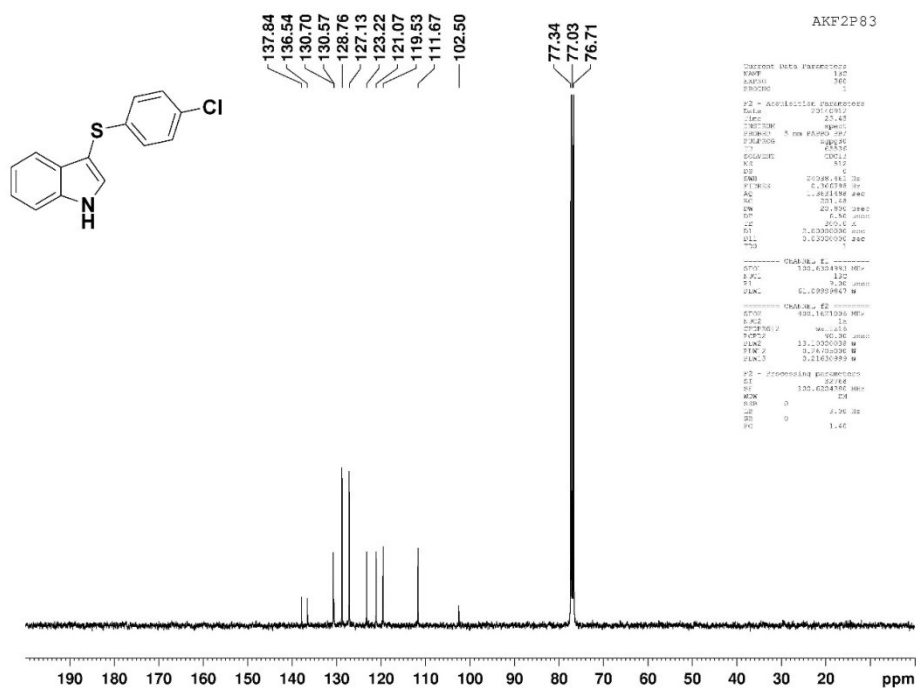
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HRMS spectrum of 3-((4-fluorophenyl)thio)-1H-indole (Table 2, 3f)

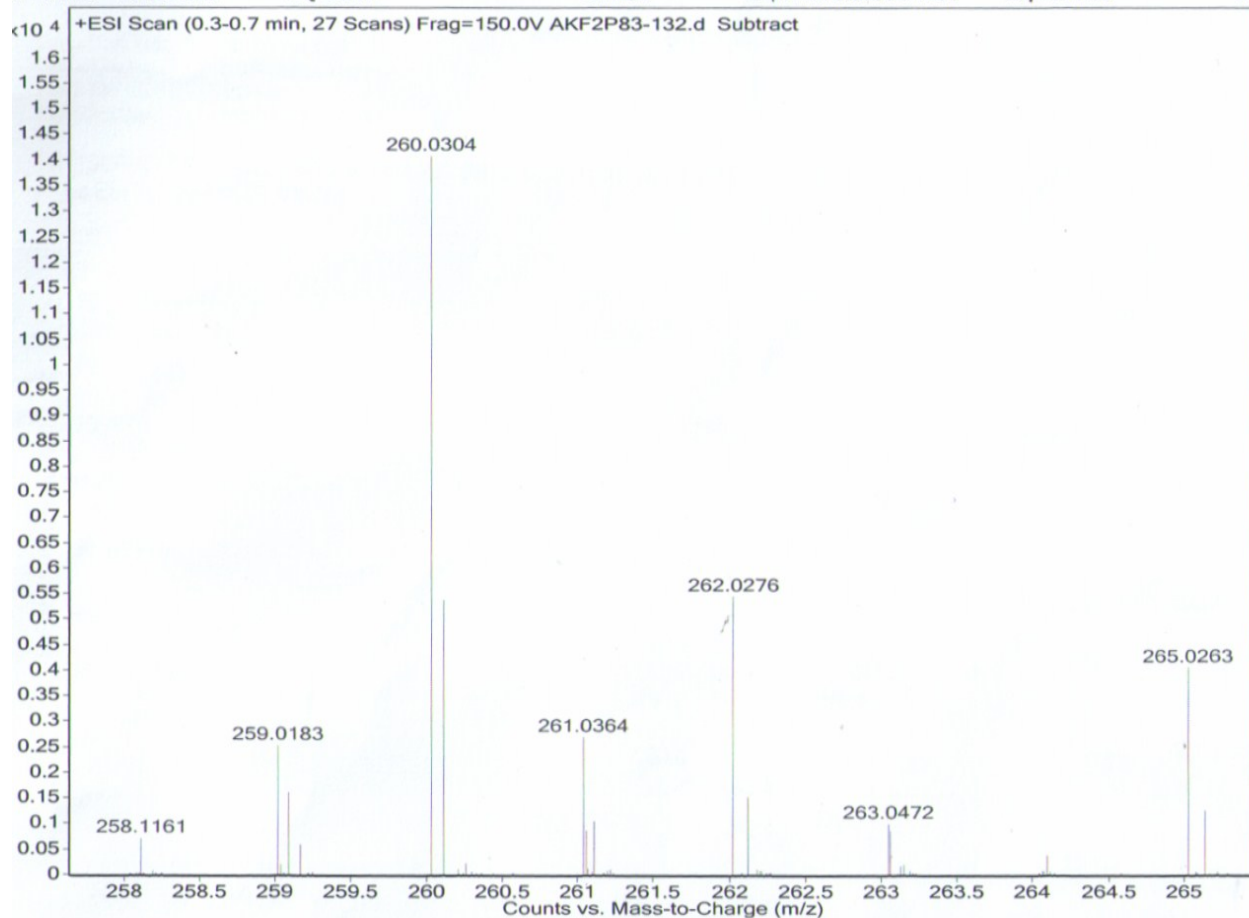


¹H-NMR spectrum of 3-((4-chlorophenyl)thio)-1H-indole (Table 2, 3g)

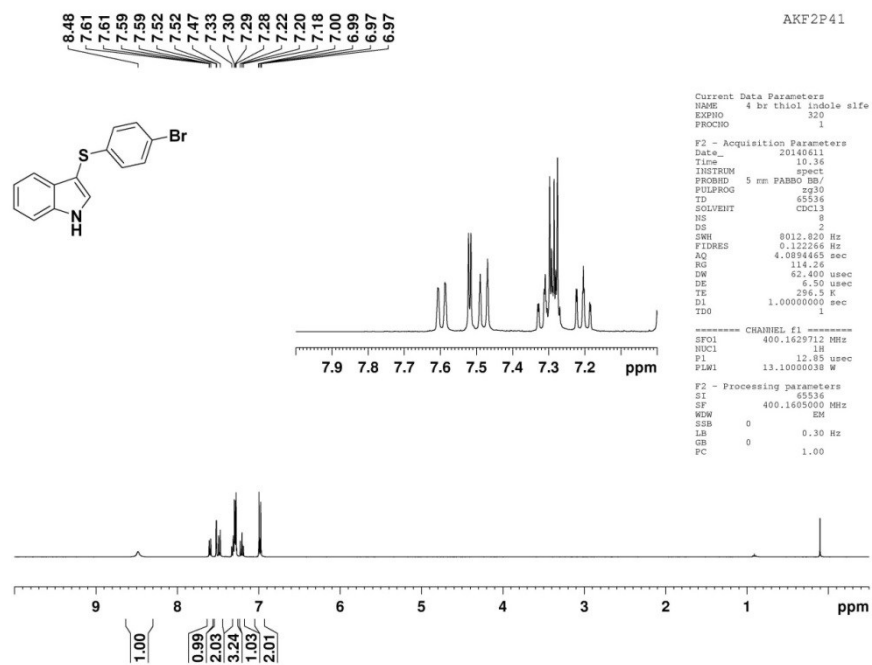


¹³C-NMR spectrum of 3-((4-chlorophenyl)thio)-1H-indole (Table 2, 3g)

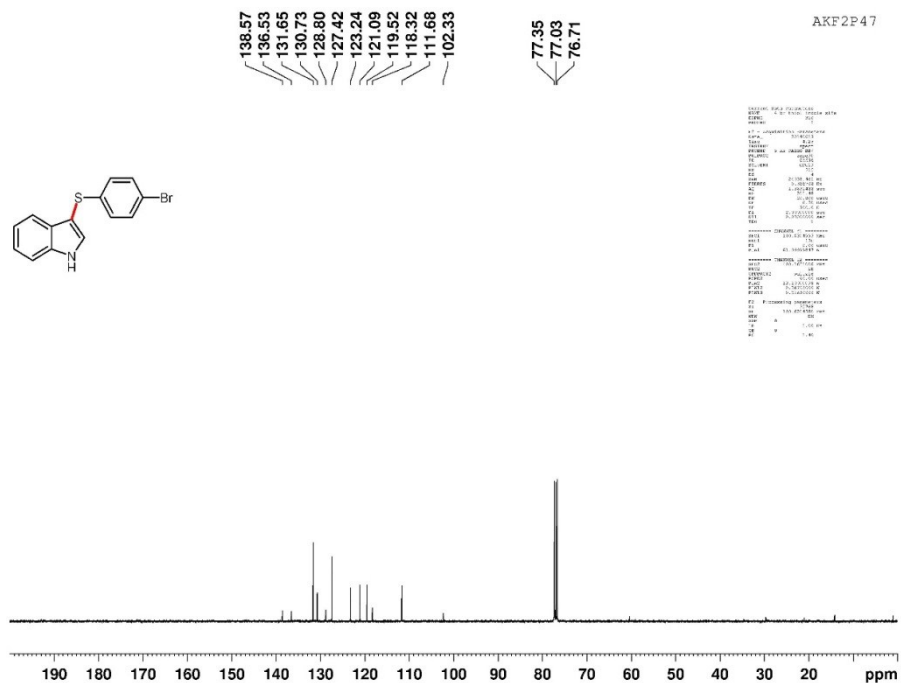
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HRMS spectrum of 3-((4-chlorophenyl)thio)-1H-indole (Table 2, 3g)

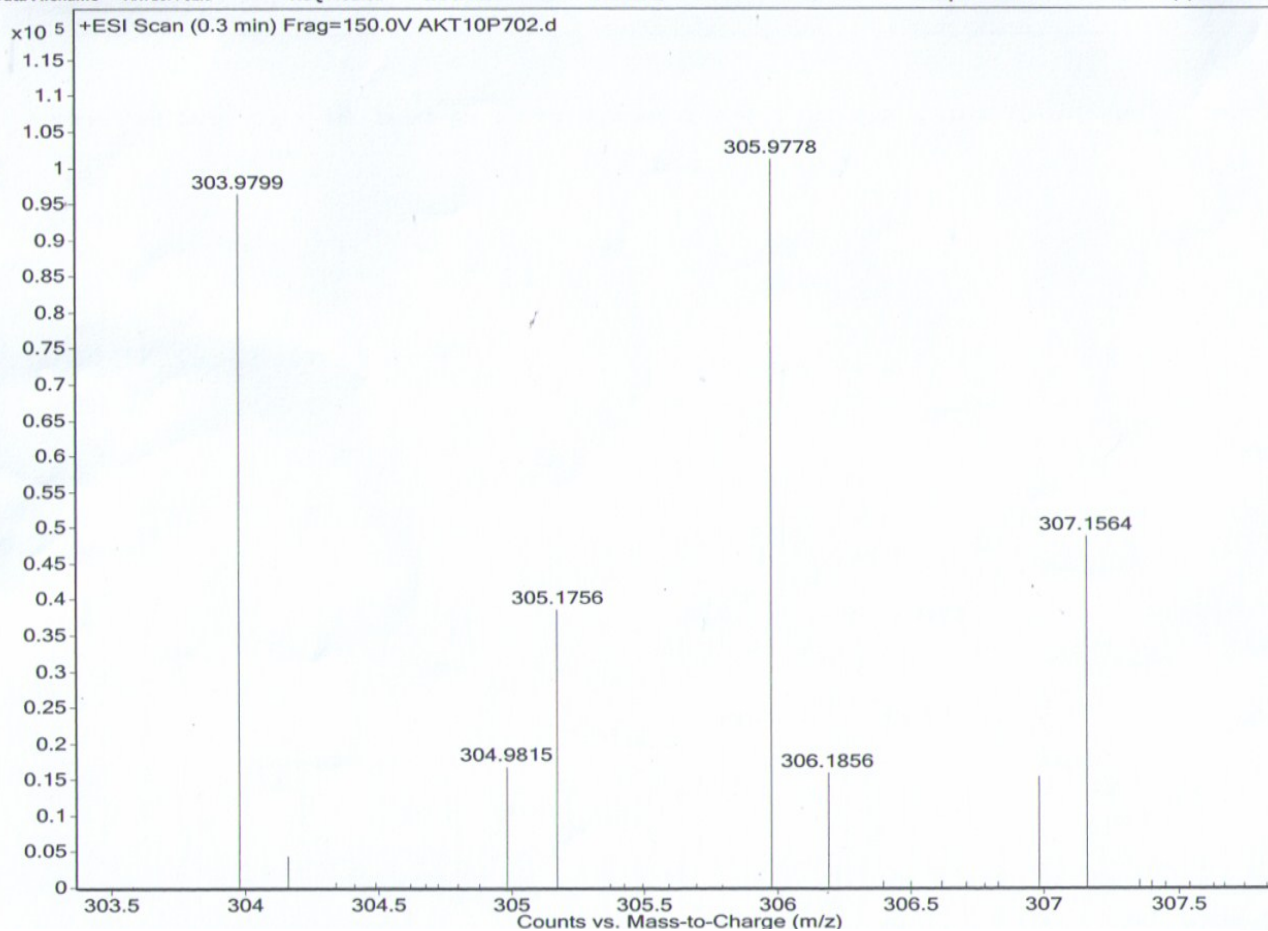


¹H-NMR spectrum of 3-((4-bromophenyl)thio)-1H-indole (Table 2, 3h)

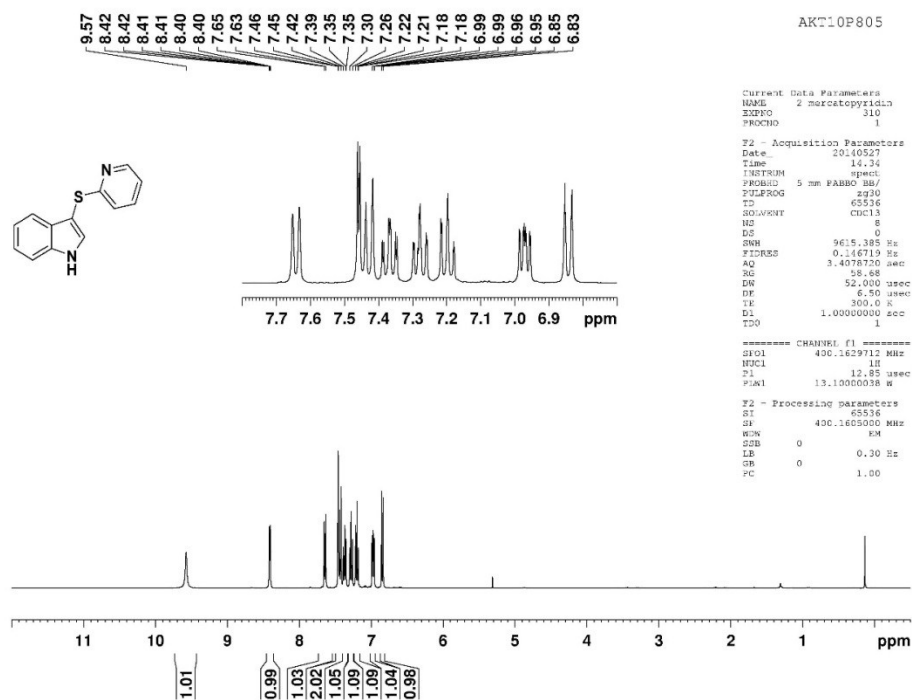


¹³C-NMR spectrum of 3-((4-bromophenyl)thio)-1H-indole (Table 2, 3h)

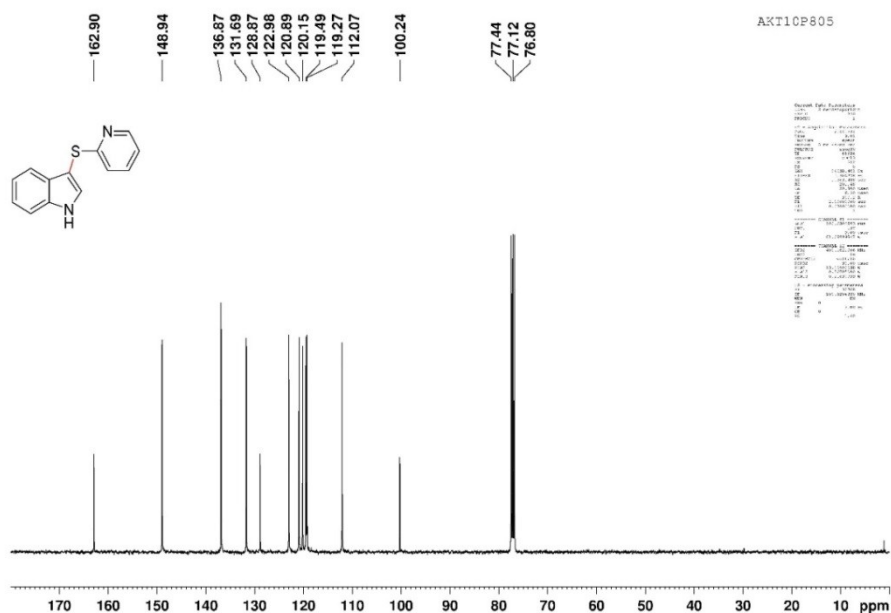
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HRMS spectrum of 3-((4-bromophenyl)thio)-1H-indole (Table 2, 3h)

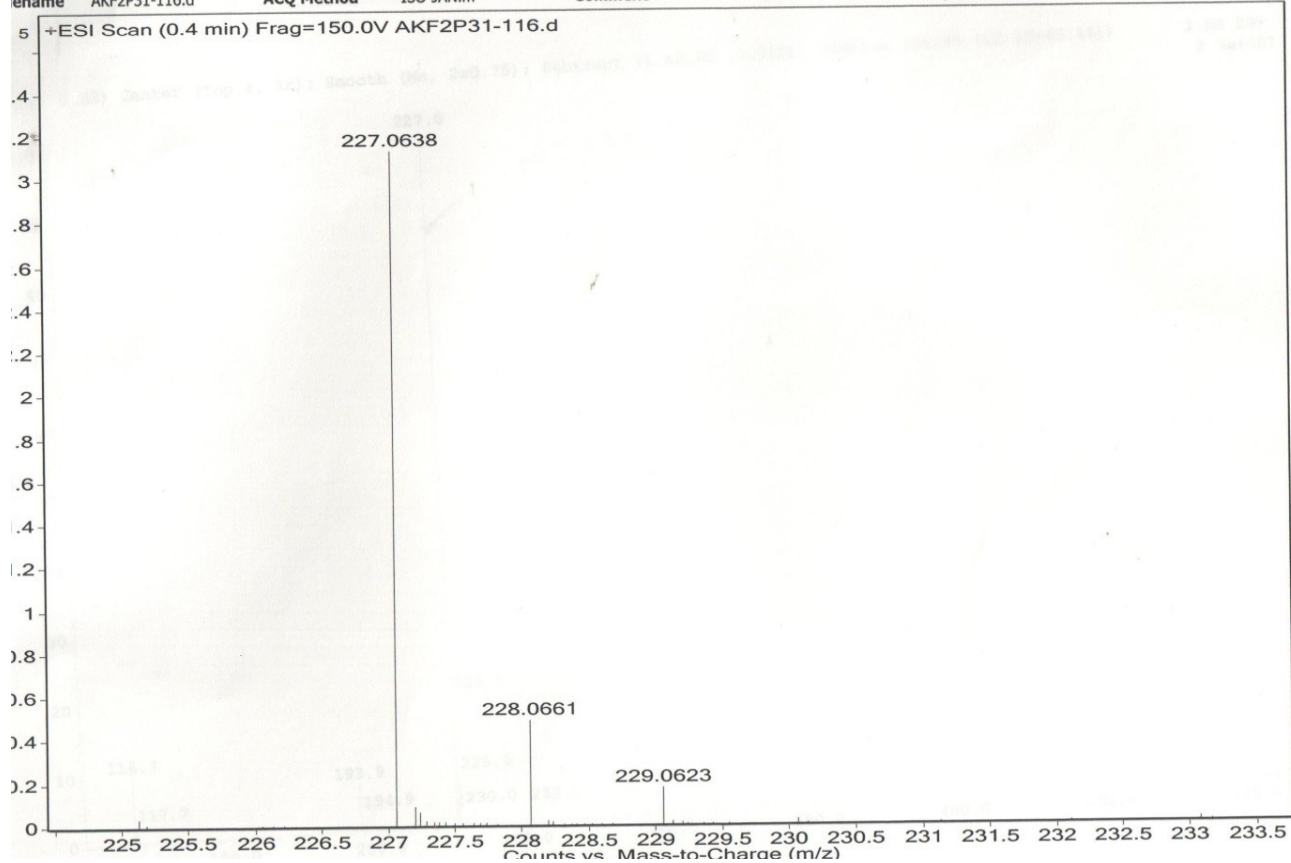


¹H-NMR spectrum of 3-(pyridin-2-ylthio)-1H-indole (Table 2, 5a).

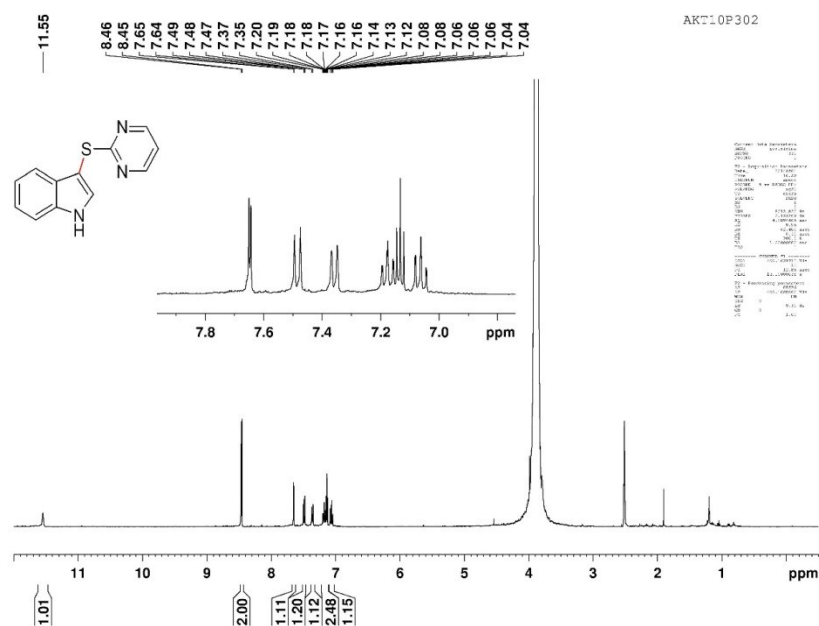


¹³C-NMR spectrum of 3-(pyridin-2-ylthio)-1H-indole (Table 2, 5a).

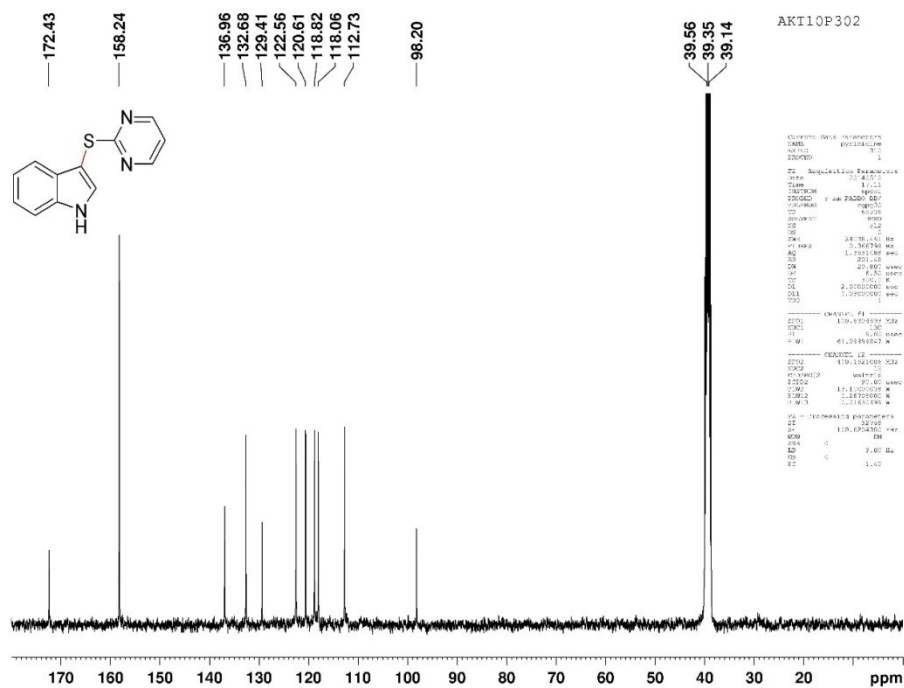
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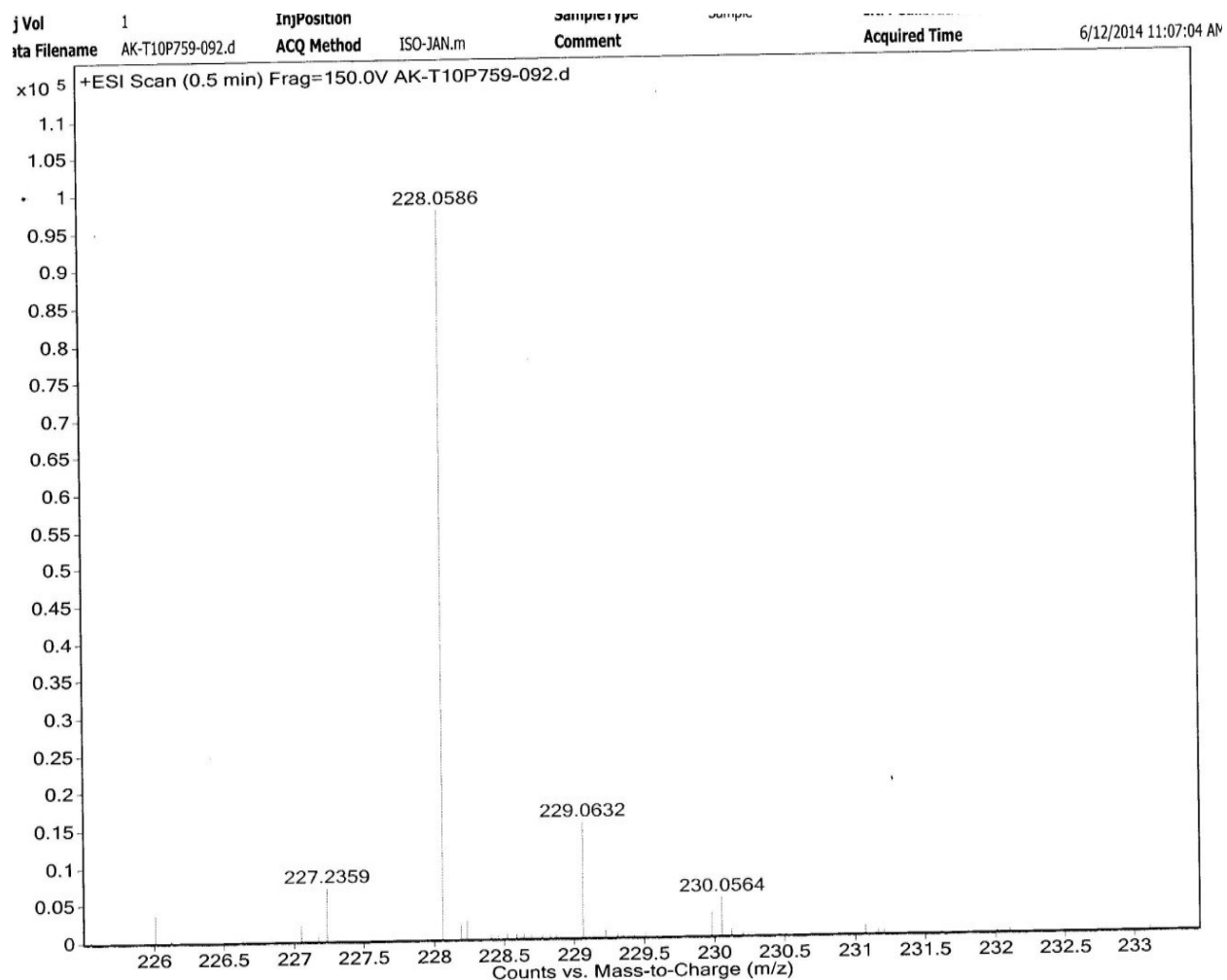
HRMS spectrum of 3-(pyridin-2-ylthio)-1H-indole (Table 2, 5a).



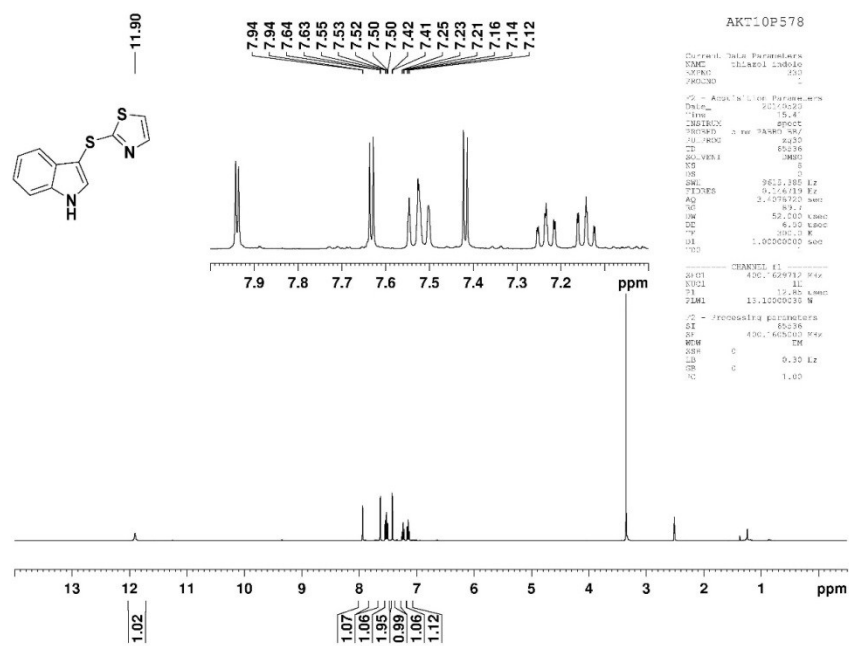
¹H-NMR spectrum of 3-(pyrimidin-2-ylthio)-1H-indole (Table 2, 5b)



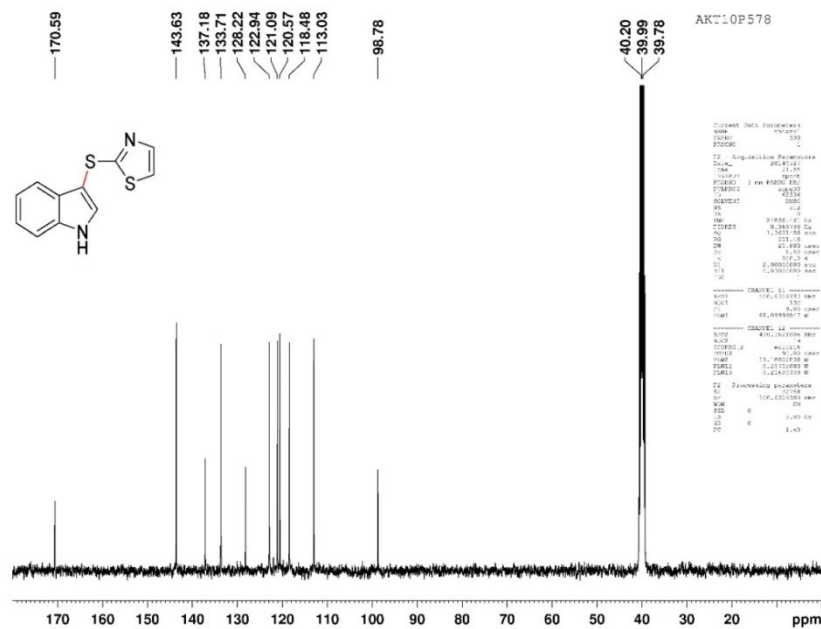
¹³C-NMR spectrum of 3-(pyrimidin-2-ylthio)-1H-indole (Table 2, 5b)



HRMS spectrum of 3-(pyrimidin-2-ylthio)-1H-indole (Table 2, 5b)

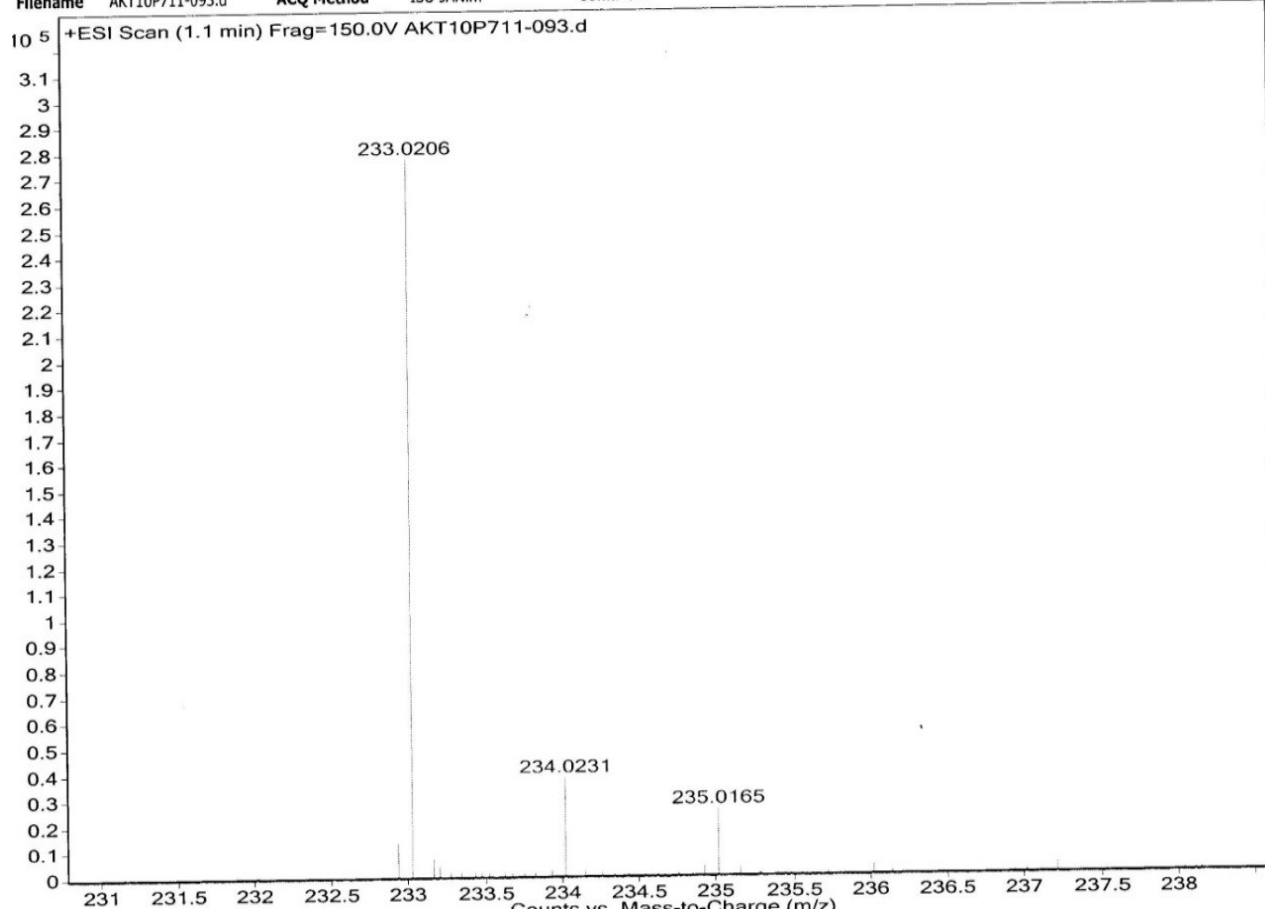


¹H-NMR spectrum of 2-((1H-indol-3-yl)thio)thiazole (Table 2, 5c)

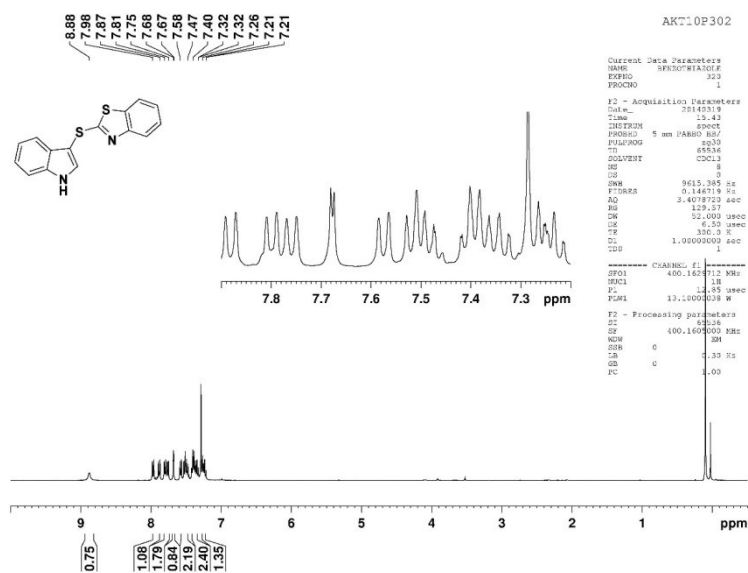


¹³C-NMR spectrum of 2-((1H-indol-3-yl)thio)thiazole (Table 2, 5c)

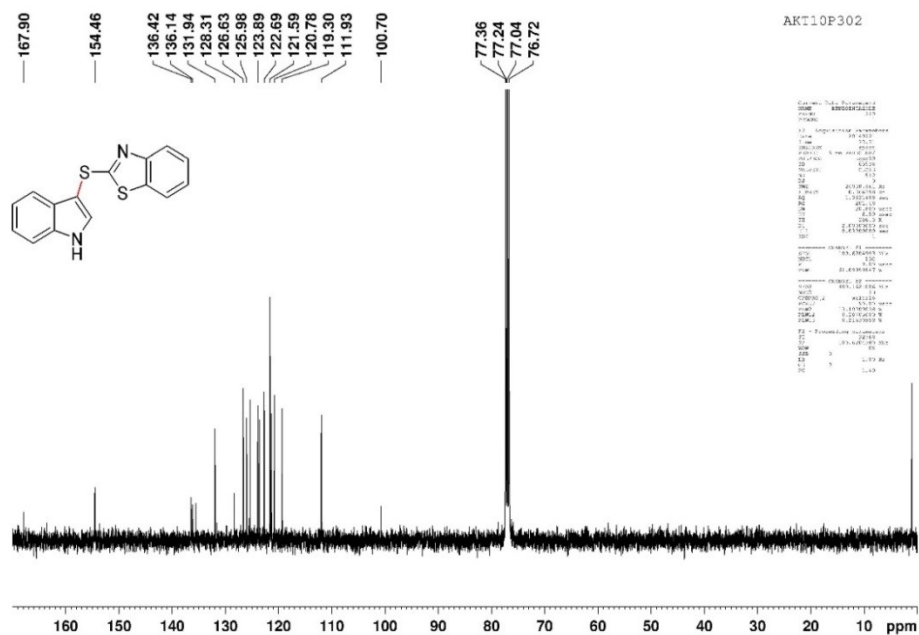
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HRMS spectrum of 2-((1H-indol-3-yl)thio)thiazole(Table 2, 5c)

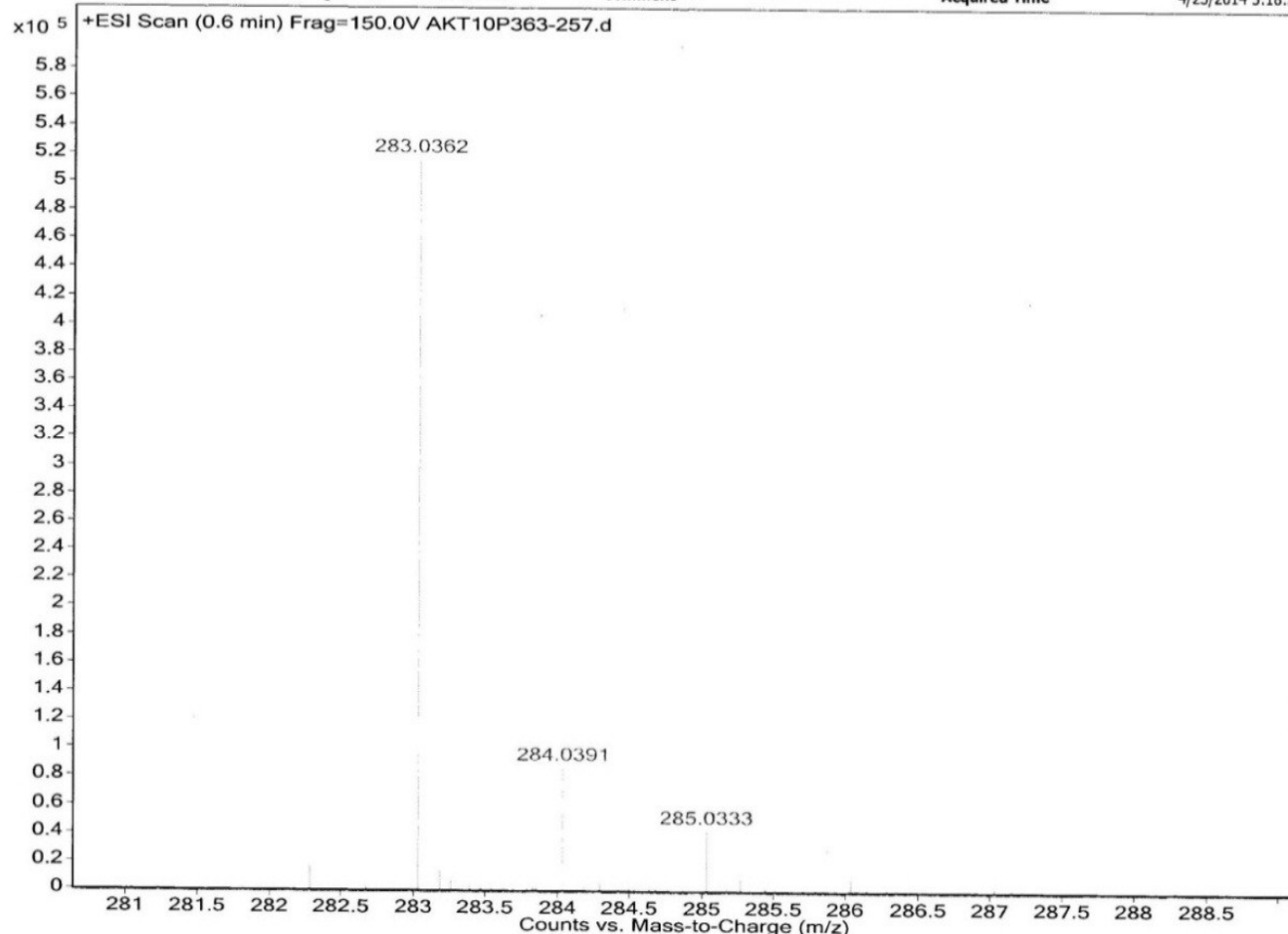


¹H-NMR spectrum of 2-((1H-indol-3-yl)thio)benzo[d]thiazole (Table 2, 5d)

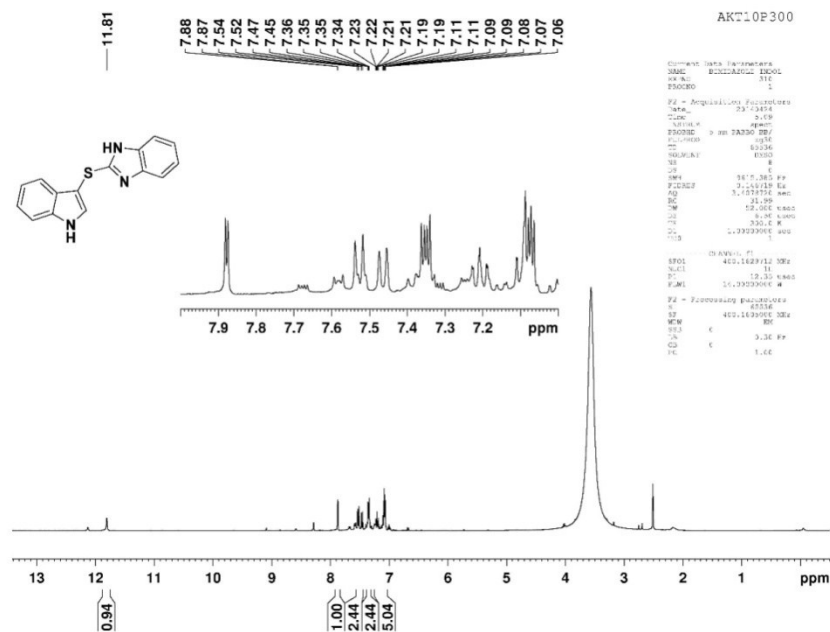


¹³C-NMR spectrum of 2-((1H-indol-3-yl)thio)benzo[d]thiazole (Table 2, 5d)

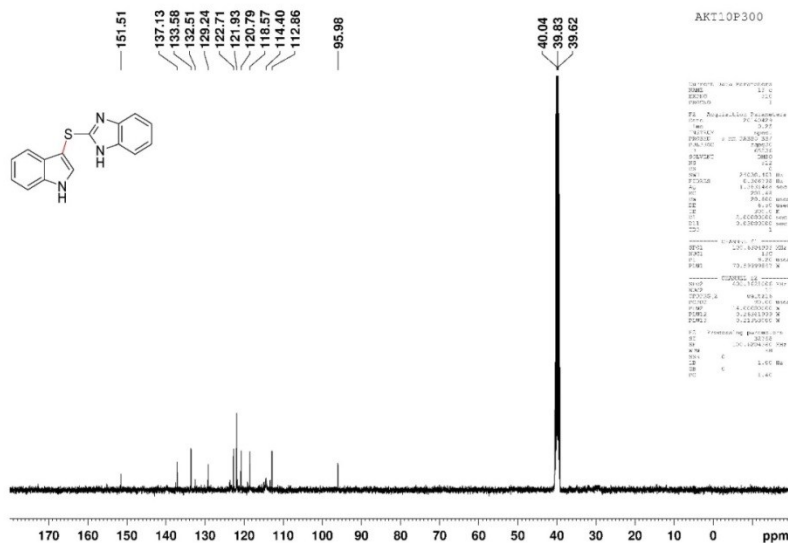
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HRMS spectrum of 2-((1H-indol-3-yl)thio)benzo[d]thiazole(Table 2, 5d)

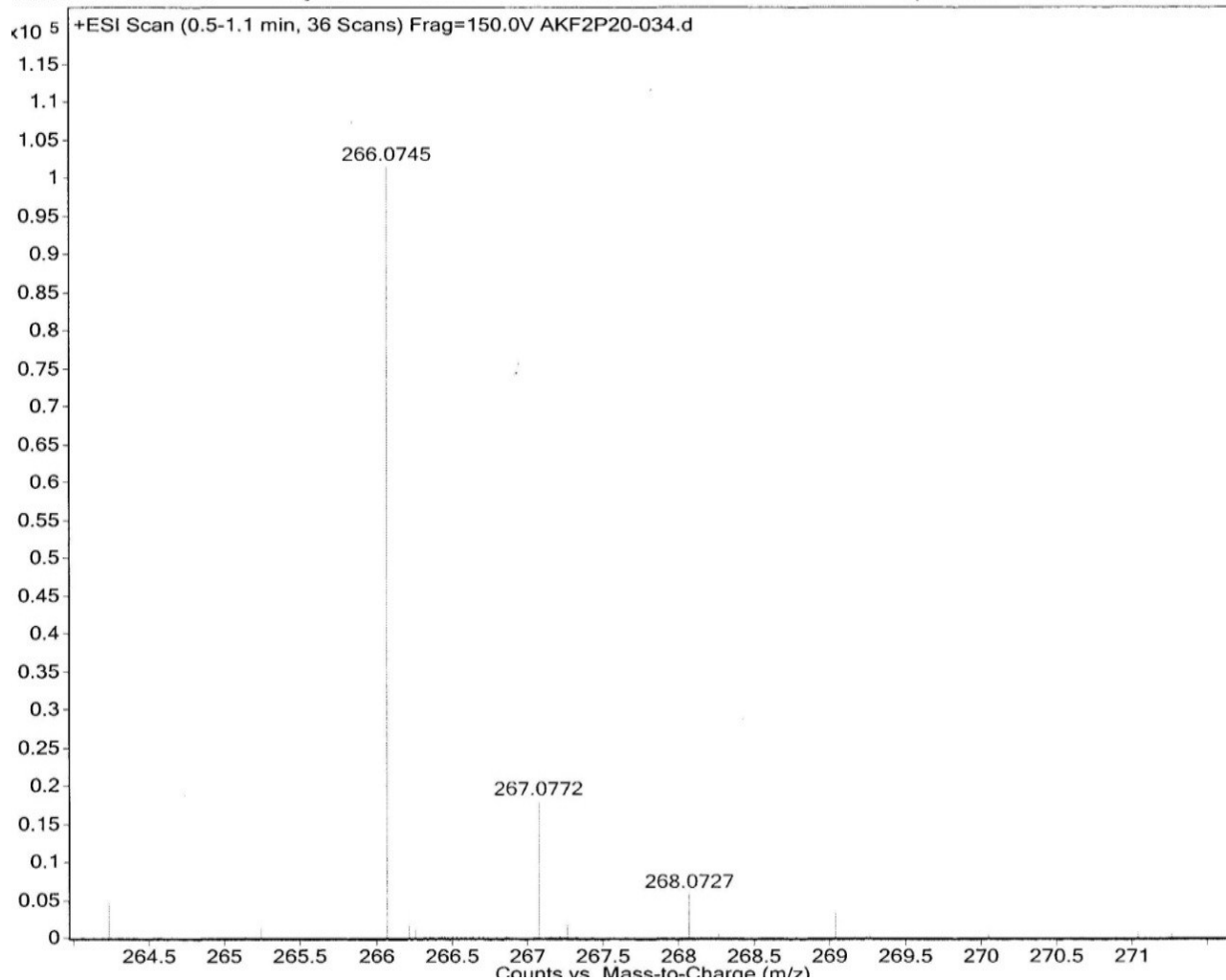


¹H-NMR spectrum of 2-((1H-indol-3-yl)thio)-1H-benzo[d]imidazole (Table 2, 5e)

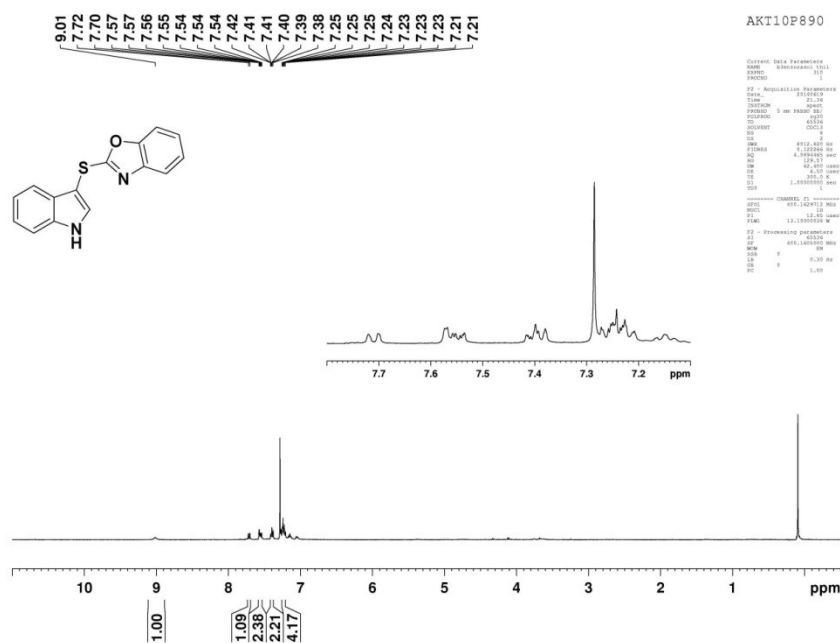


¹³C-NMR spectrum of 2-((1H-indol-3-yl)thio)-1H-benzo[d]imidazole (Table 2, 5e)

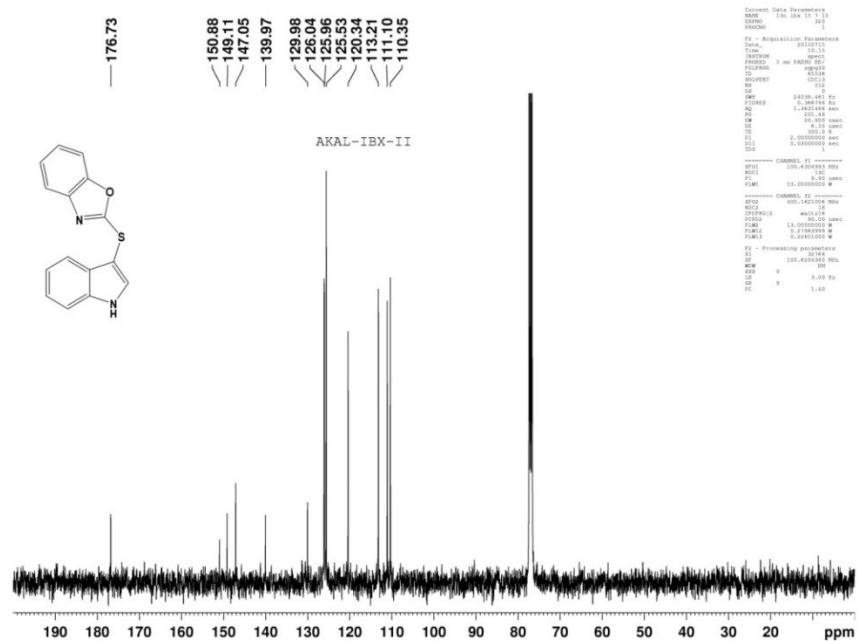
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HRMS spectrum of 2-((1H-indol-3-yl)thio)-1H-benzo[d]imidazole (Table 2, 5e)

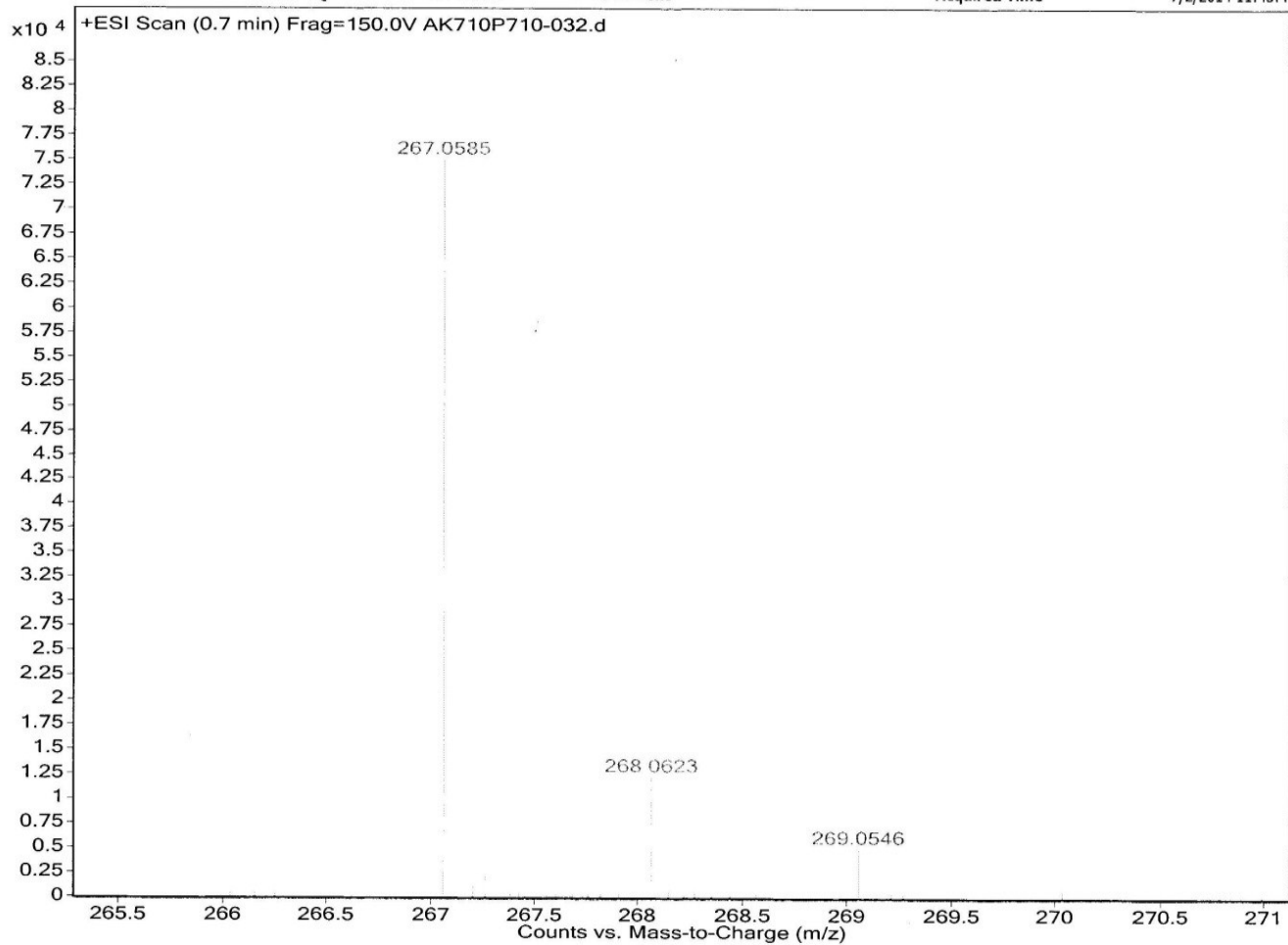


¹H-NMR spectrum of 2-((1H-indol-3-yl)thio)benzo[d]oxazole (Table 2, 5f).

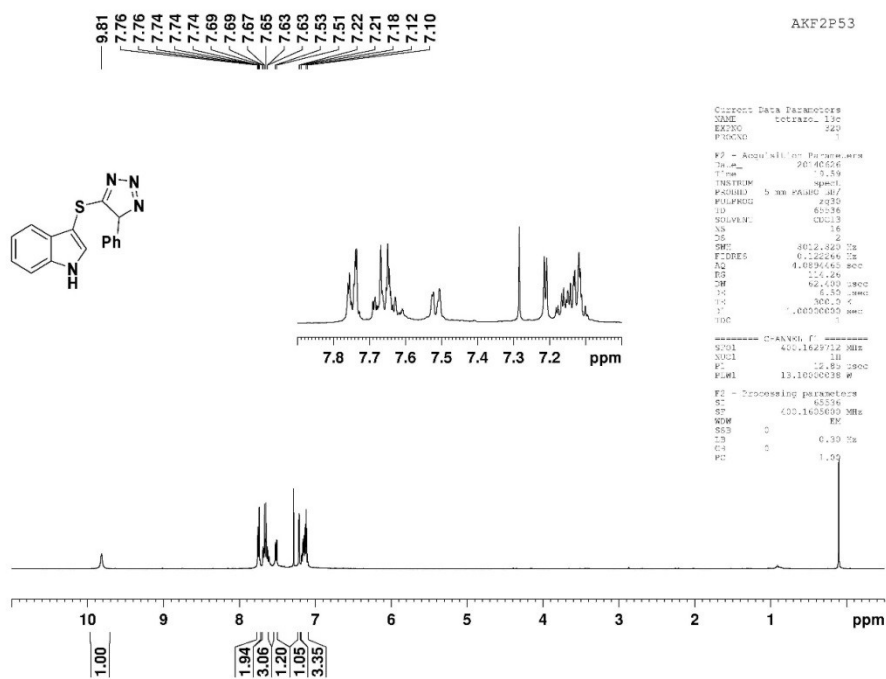


¹³C-NMR spectrum of 2-((1H-indol-3-yl)thio)benzo[d]oxazole (Table 2, 5f).

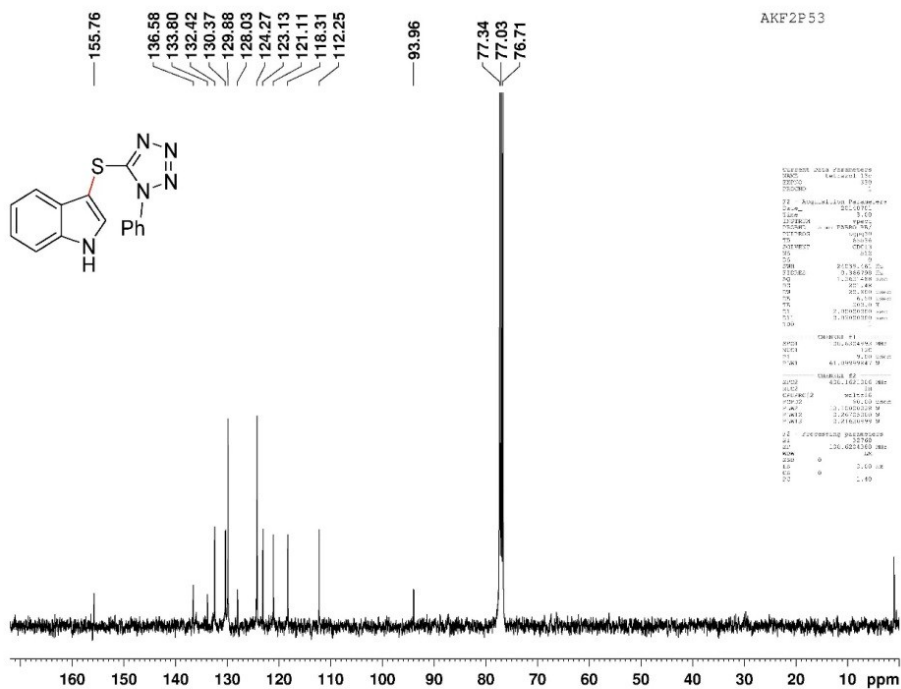
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HRMS spectrum of 2-((1H-indol-3-yl)thio)benzo[d]oxazole(Table 2, 5f).

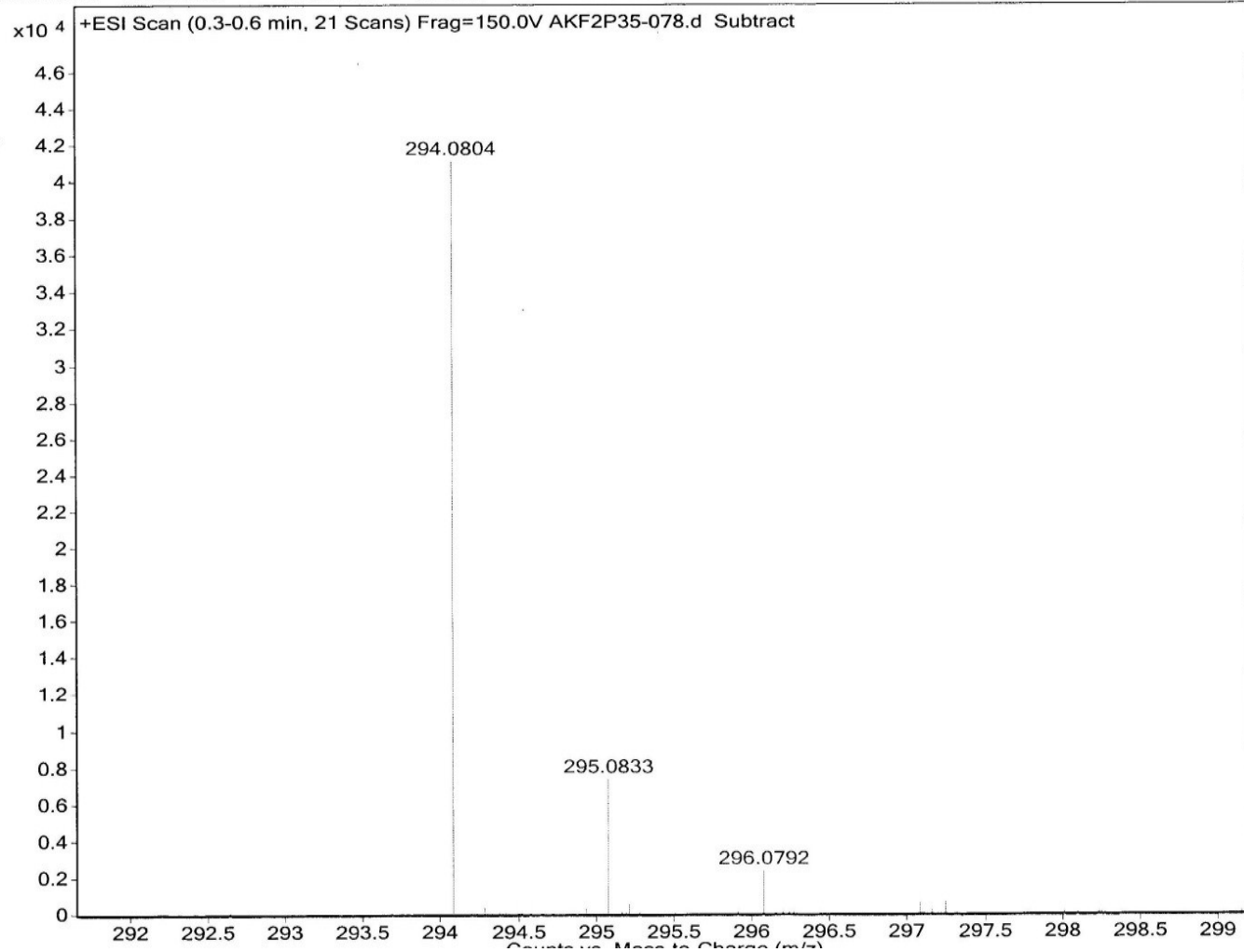


¹H-NMR spectrum of 3-((1-phenyl-1H-tetrazol-5-yl)thio)-1H-indole (Table 2, 5g)

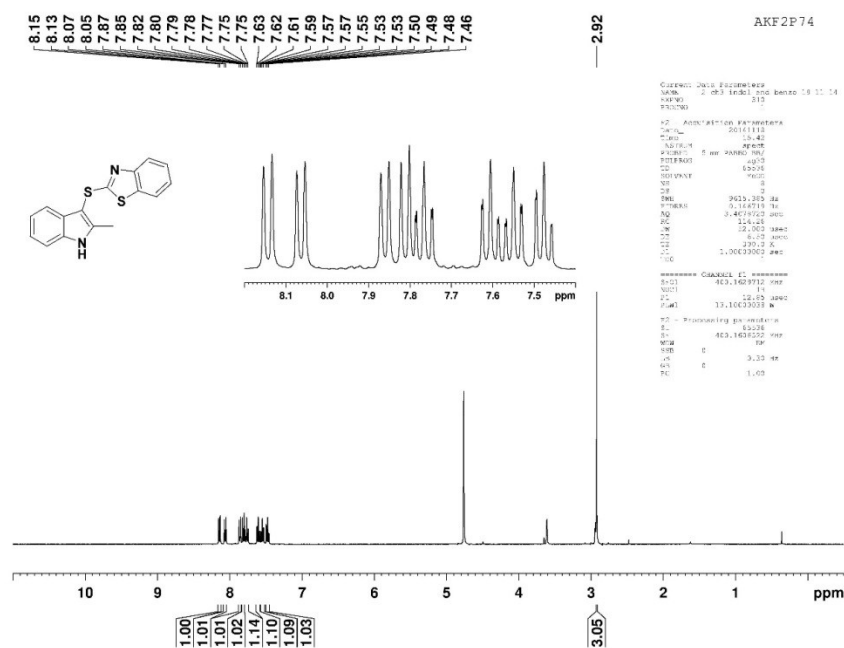


¹³C-NMR spectrum of 3-((1-phenyl-1H-tetrazol-5-yl)thio)-1H-indole (Table 2, 5g)

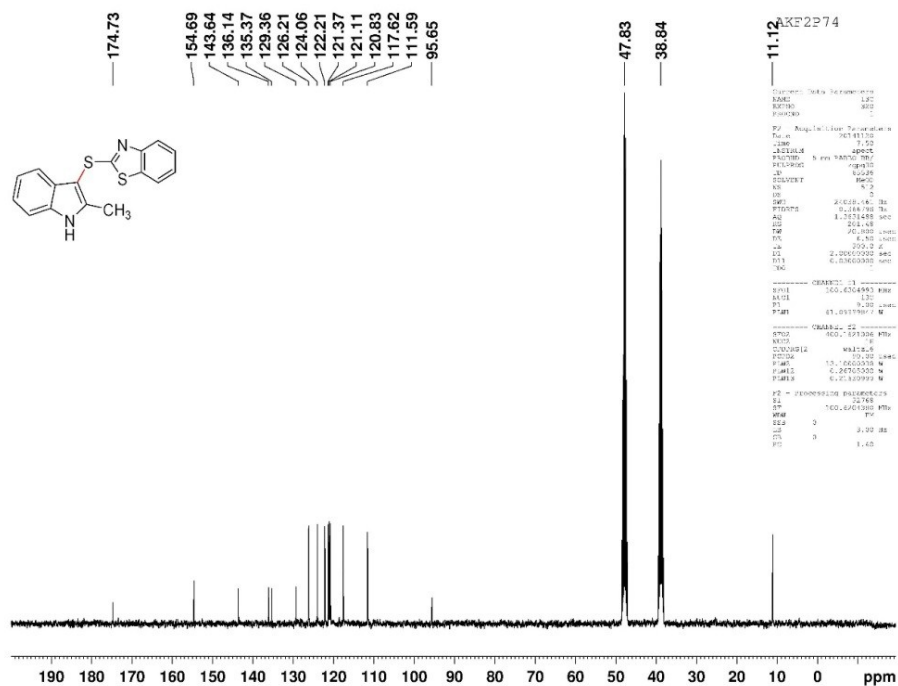
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HRMS spectrum of 3-((1-phenyl-1H-tetrazol-5-yl)thio)-1H-indole(Table 2, 5g)

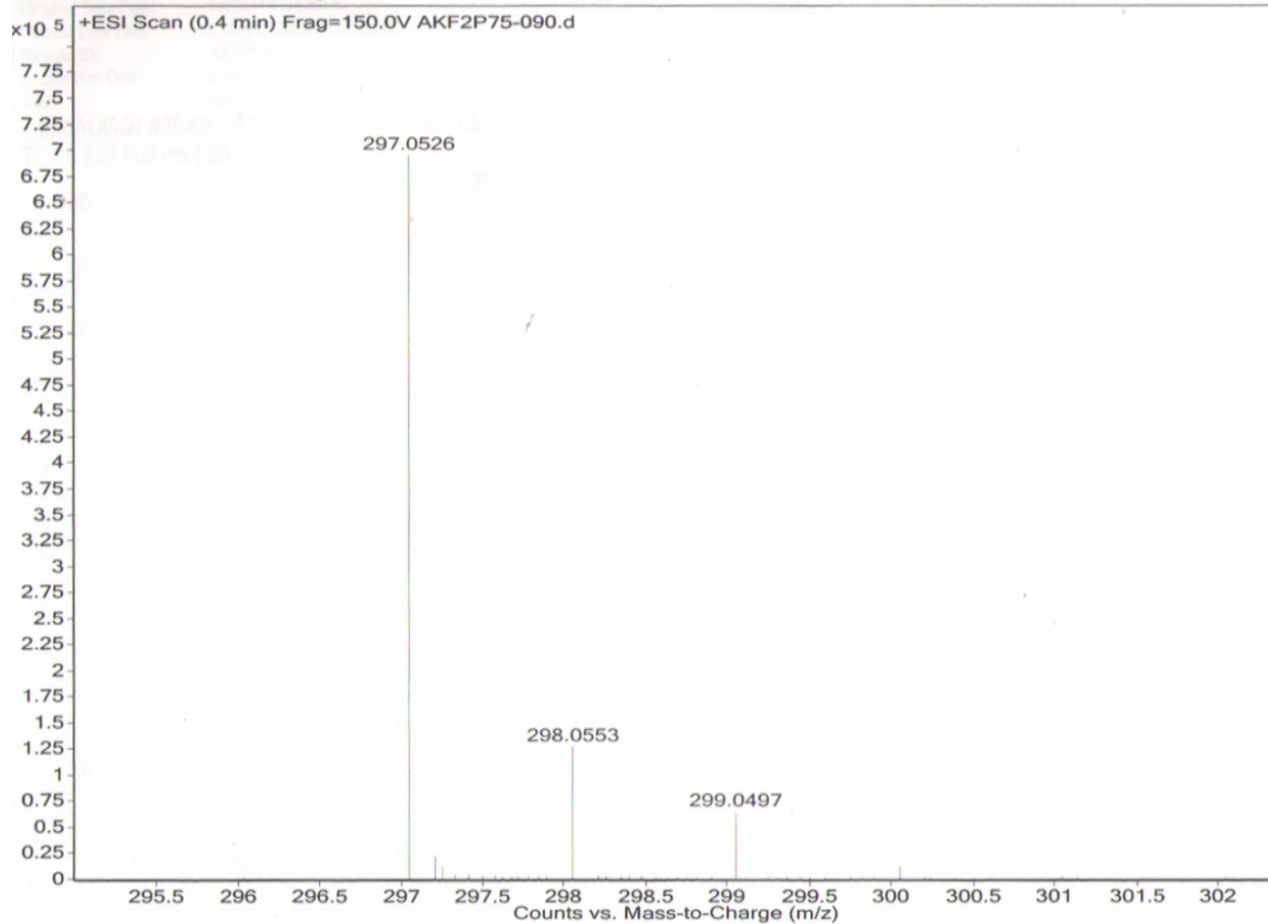


¹H-NMR spectrum of 2-((2-methyl-1H-indol-3-yl)thio)benzo[d]thiazole (Table 2, 5h)



¹³C-NMR spectrum of 2-((2-methyl-1H-indol-3-yl)thio)benzo[d]thiazole (Table 2, 5h)

Sample Name	Dr. A. K. SINHA	Position	Vial 20	Instrument Name	Instrument 1	User Name	
Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
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HRMS spectrum of 2-((2-methyl-1H-indol-3-yl)thio)benzo[d]thiazole (Table 2, 5h)



AKF2P71

Chemical structure of AKF2P71 (1-phenyl-5-nitro-1H-indole-3-thiol) is shown above the spectrum.

¹³C NMR spectrum (CDCl₃) showing peaks at 142.45, 139.80, 138.21, 134.38, 128.87, 126.19, 125.34, 118.28, 116.68, 112.06, 105.39, 77.39, 77.08, and 76.76 ppm.

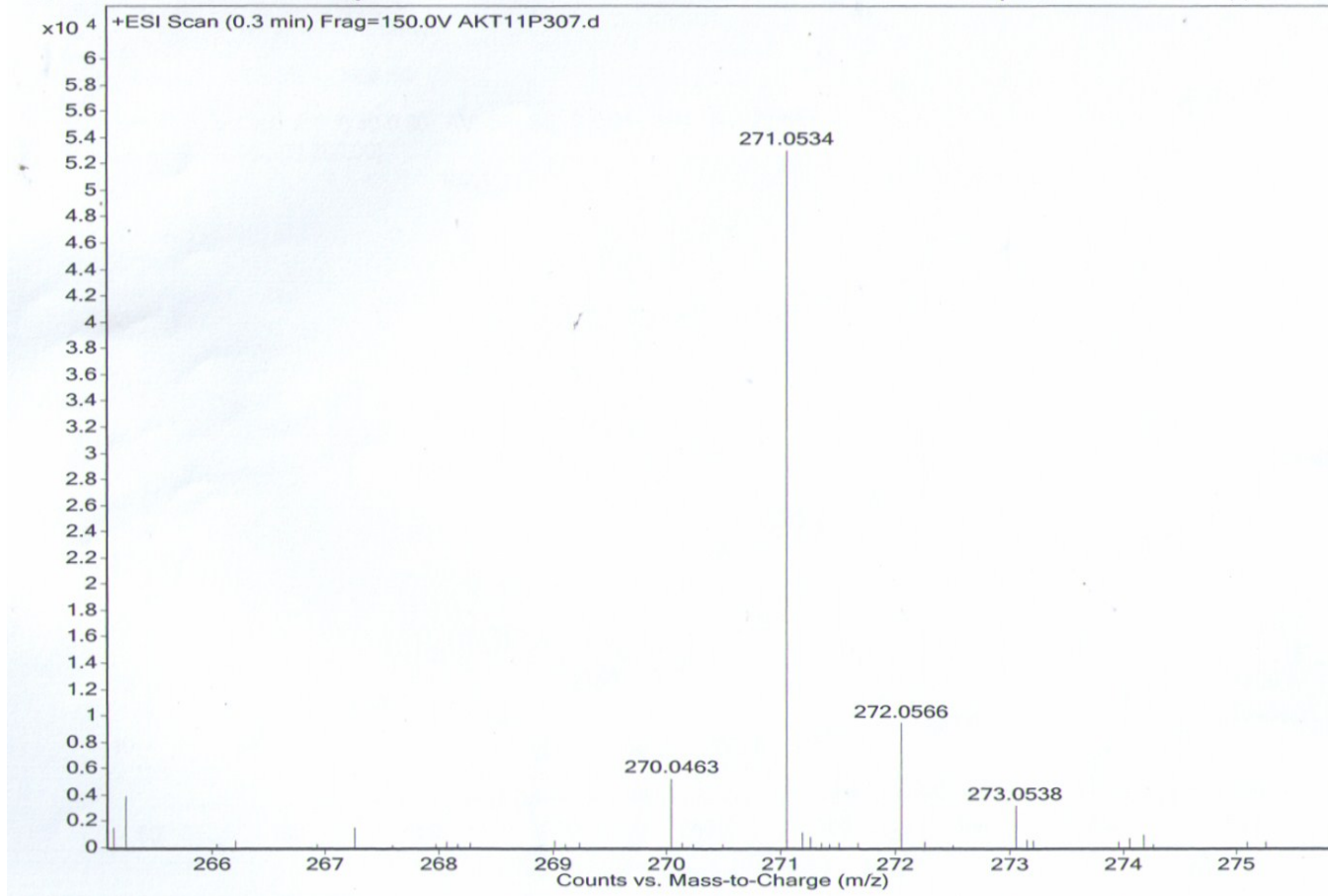
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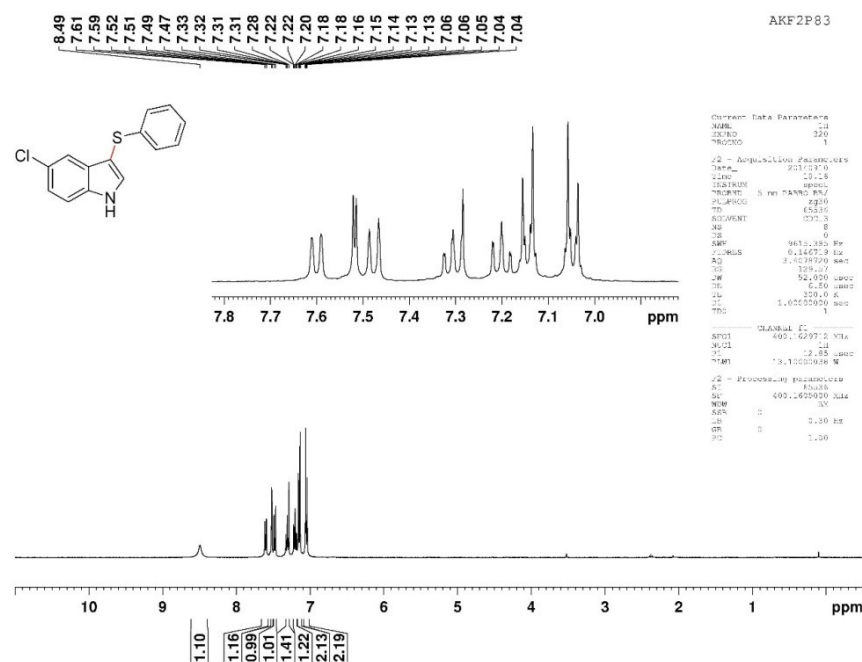
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- PROBHT5: 1.5 mm QNP 1H/13
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- PROBHT57: 1.5 mm QNP 1H/13
- PROBHT58: 1.5 mm QNP 1H/13
- PROBHT59: 1.5 mm QNP 1H/13
- PROBHT60: 1.5 mm QNP 1H/13
- PROBHT61: 1.5 mm QNP 1H/13
- PROBHT62: 1.5 mm QNP 1H/13
- PROBHT63: 1.5 mm QNP 1H/13
- PROBHT64: 1.5 mm QNP 1H/13
- PROBHT65: 1.5 mm QNP 1H/13
- PROBHT66: 1.5 mm QNP 1H/13
- PROBHT67: 1.5 mm QNP 1H/13
- PROBHT68: 1.5 mm QNP 1H/13
- PROBHT69: 1.5 mm QNP 1H/13
- PROBHT70: 1.5 mm QNP 1H/13
- PROBHT71: 1.5 mm QNP 1H/13
- PROBHT72: 1.5 mm QNP 1H/13
- PROBHT73: 1.5 mm QNP 1H/13
- PROBHT74: 1.5 mm QNP 1H/13
- PROBHT75: 1.5 mm QNP 1H/13
- PROBHT76: 1.5 mm QNP 1H/13
- PROBHT77: 1.5 mm QNP 1H/13
- PROBHT78: 1.5 mm QNP 1H/13
- PROBHT79: 1.5 mm QNP 1H/13
- PROBHT80: 1.5 mm QNP 1H/13
- PROBHT81: 1.5 mm QNP 1H/13
- PROBHT82: 1.5 mm QNP 1H/13
- PROBHT83: 1.5 mm QNP 1H/13
- PROBHT84: 1.5 mm QNP 1H/13
- PROBHT85: 1.5 mm QNP 1H/13
- PROBHT86: 1.5 mm QNP 1H/13
- PROBHT87: 1.5 mm QNP 1H/13
- PROBHT88: 1.5 mm QNP 1H/13
- PROBHT89: 1.5 mm QNP 1H/13
- PROBHT90: 1.5 mm QNP 1H/13
- PROBHT91: 1.5 mm QNP 1H/13
- PROBHT92: 1.5 mm QNP 1H/13
- PROBHT93: 1.5 mm QNP 1H/13
- PROBHT94: 1.5 mm QNP 1H/13
- PROBHT95: 1.5 mm QNP 1H/13
- PROBHT96: 1.5 mm QNP 1H/13
- PROBHT97: 1.5 mm QNP 1H/13
- PROBHT98: 1.5 mm QNP 1H/13
- PROBHT99: 1.5 mm QNP 1H/13
- PROBHT100: 1.5 mm QNP 1H/13
- PROBHT101: 1.5 mm QNP 1H/13
- PROBHT102: 1.5 mm QNP 1H/13
- PROBHT103: 1.5 mm QNP 1H/13
- PROBHT104: 1.5 mm QNP 1H/13
- PROBHT105: 1.5 mm QNP 1H/13
- PROBHT106: 1.5 mm QNP 1H/13
- PROBHT107: 1.5 mm QNP 1H/13
- PROBHT108: 1.5 mm QNP 1H/13
- PROBHT109: 1.5 mm QNP 1H/13
- PROBHT110: 1.5 mm QNP 1H/13
- PROBHT111: 1.5 mm QNP 1H/13
- PROBHT112: 1.5 mm QNP 1H/13
- PROBHT113: 1.5 mm QNP 1H/13
- PROBHT114: 1.5 mm QNP 1H/13
- PROBHT115: 1.5 mm QNP 1H/13
- PROBHT116: 1.5 mm QNP 1H/13
- PROBHT117: 1.5 mm QNP 1H/13
- PROBHT118: 1.5 mm QNP 1H/13
- PROBHT119: 1.5 mm QNP 1H/13
- PROBHT120: 1.5 mm QNP 1H/13
- PROBHT121: 1.5 mm QNP 1H/13
- PROBHT122: 1.5 mm QNP 1H/13
- PROBHT123: 1.5 mm QNP 1H/13
- PROBHT124: 1.5 mm QNP 1H/13
- PROBHT125: 1.5 mm QNP 1H/13
- PROBHT126: 1.5 mm QNP 1H/13
- PROBHT127: 1.5 mm QNP 1H/13
- PROBHT128: 1.5 mm QNP 1H/13
- PROBHT129: 1.5 mm QNP 1H/13
- PROBHT130: 1.5 mm QNP 1H/13
- PROBHT131: 1.5 mm QNP 1H/13
- PROBHT132: 1.5 mm QNP 1H/13
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- PROBHT134: 1.5 mm QNP 1H/13
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- PROBHT136: 1.5 mm QNP 1H/13
- PROBHT137: 1.5 mm QNP 1H/13
- PROBHT138: 1.5 mm QNP 1H/13
- PROBHT139: 1.5 mm QNP 1H/13
- PROBHT140: 1.5 mm QNP 1H/13
- PROBHT141: 1.5 mm QNP 1H/13
- PROBHT142: 1.5 mm QNP 1H/13
- PROBHT143: 1.5 mm QNP 1H/13
- PROBHT144: 1.5 mm QNP 1H/13
- PROBHT145: 1.5 mm QNP 1H/13
- PROBHT146: 1.5 mm QNP 1H/13
- PROBHT147: 1.5 mm QNP 1H/13
- PROBHT148: 1.5 mm QNP 1H/13
- PROBHT149: 1.5 mm QNP 1H/13
- PROBHT150: 1.5 mm QNP 1H/13
- PROBHT151: 1.5 mm QNP 1H/13
- PROBHT152: 1.5 mm QNP 1H/13
- PROBHT153: 1.5 mm

S34

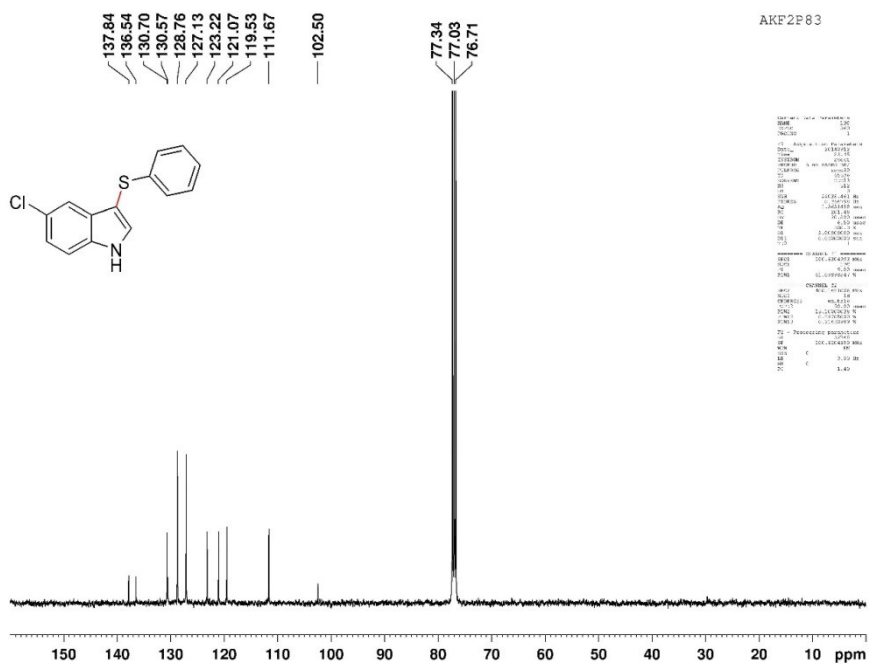
Sample Name	Dr. A. K. SINHA	Position	Vial 76	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKT11P307.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	10/1/2014 10:32:35



HRMS spectrum of 5-nitro-3-(phenylthio)-1H-indole (Table 2, 6a).

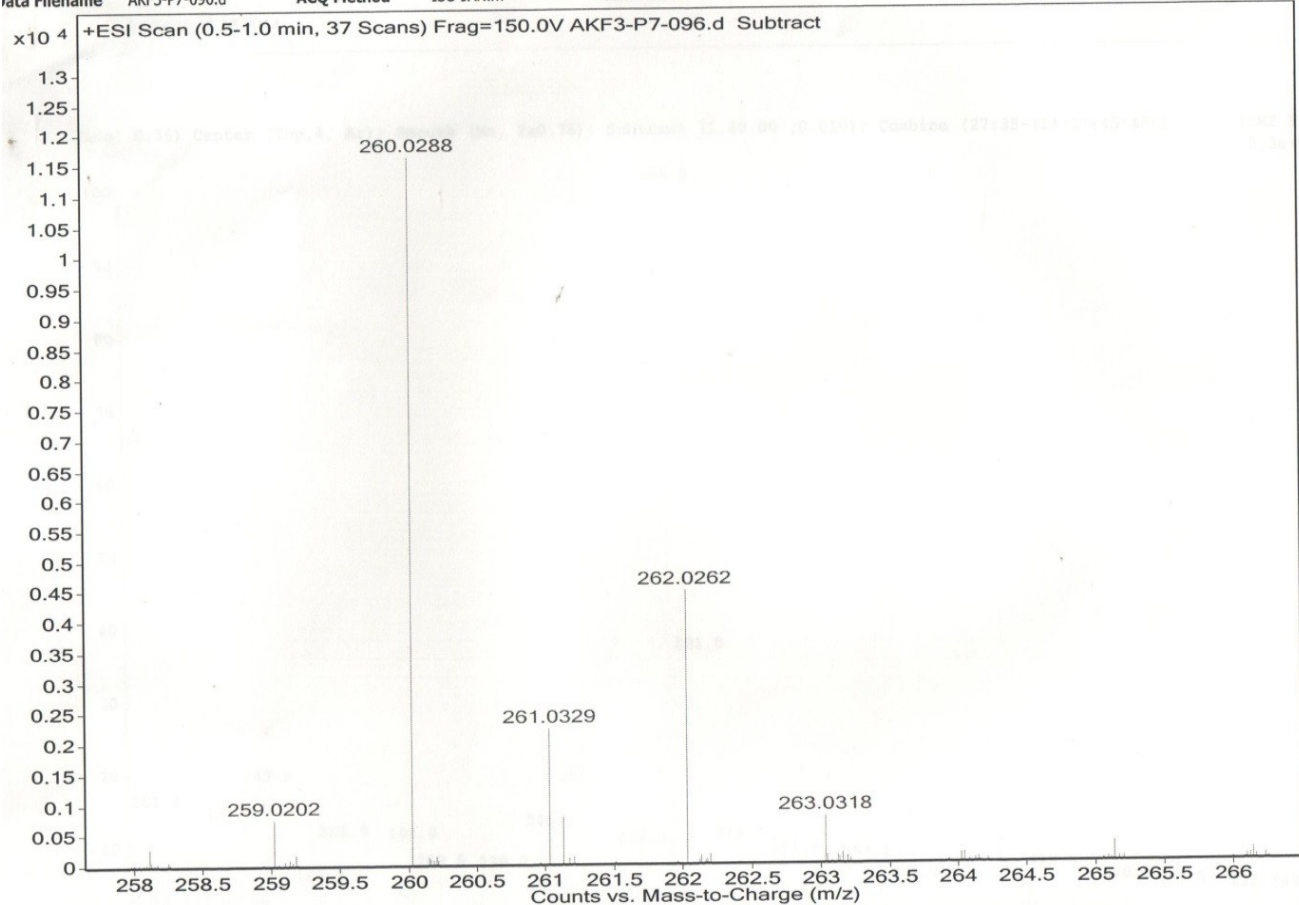


¹H-NMR spectrum of 5-chloro-3-(phenylthio)-1H-indole (Table 2, 6b).

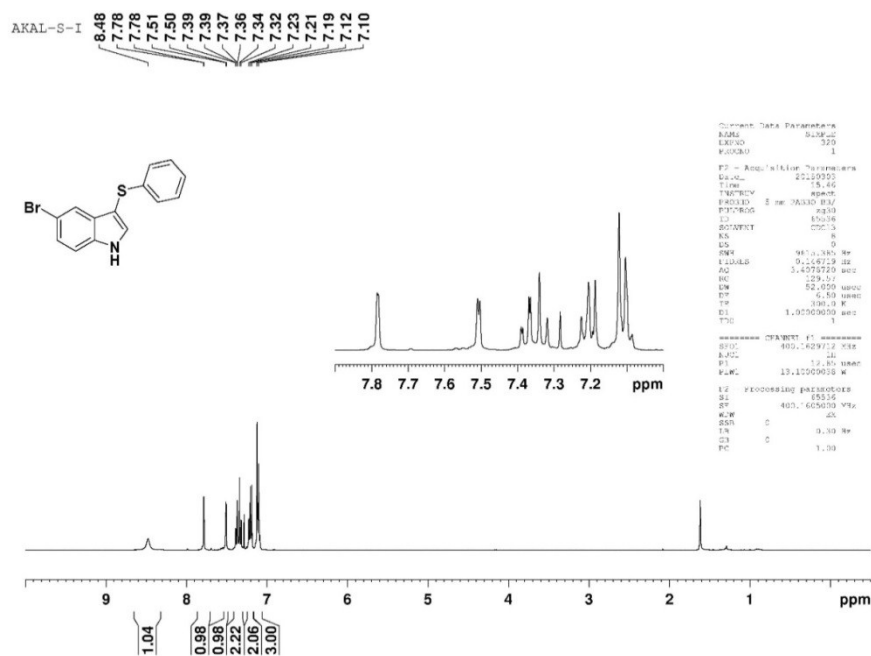


¹³C-NMR spectrum of 5-chloro-3-(phenylthio)-1H-indole (Table 2, 6b).

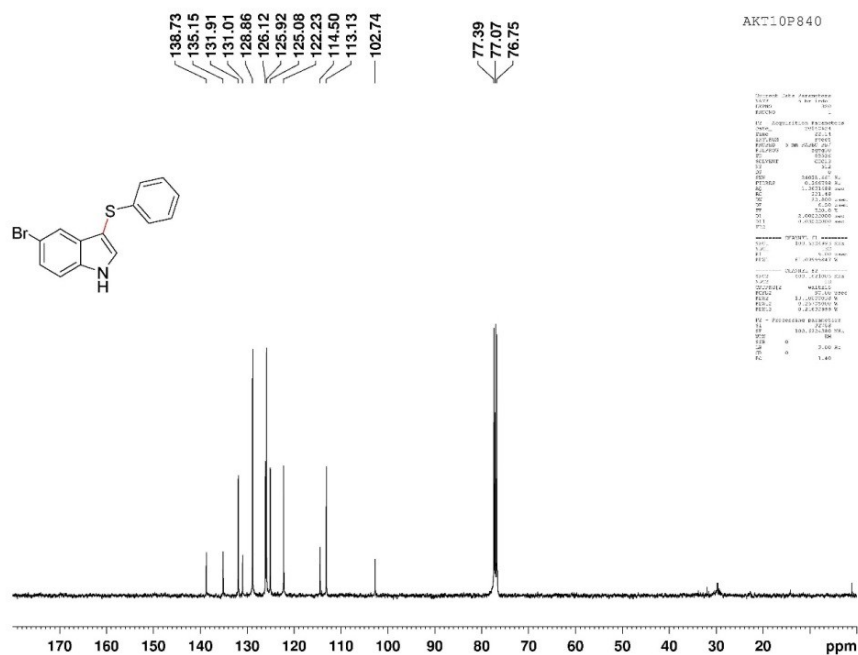
Sample Name	Dr. Sinha	Position	Vial 20	Assignment Name	Assignment	IRM Calibration Status	Some Ions Missed
nj Vol	1	InjPosition	ISO-JAN.m	SampleType	Sample	Acquired Time	7/9/2014 10:09:54 A
ata Filename	AKF3-P7-096.d	ACQ Method		Comment			



HRMS spectrum of 5-chloro-3-(phenylthio)-1H-indole (Table 2, 6b).

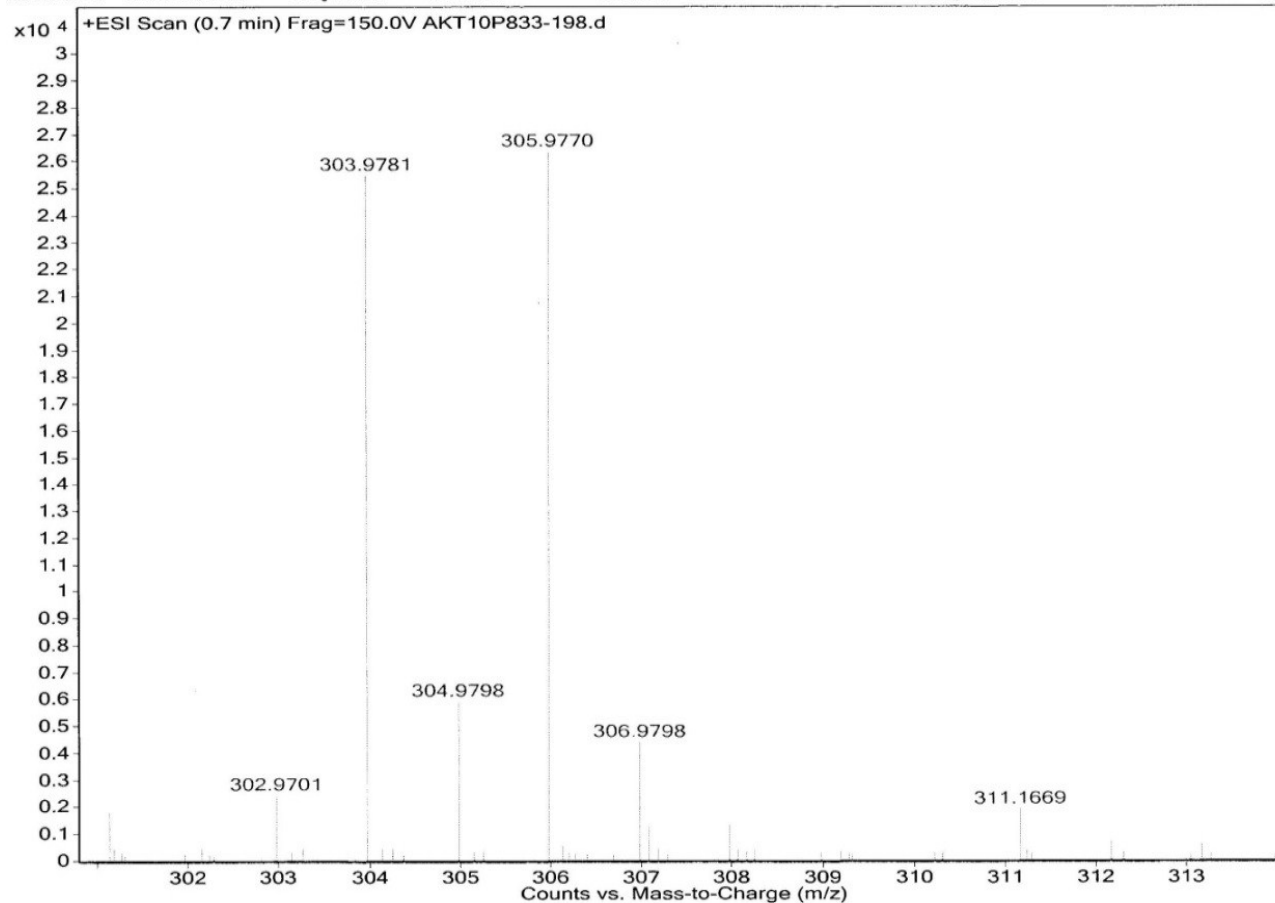


¹H-NMR spectrum of 5-bromo-3-(phenylthio)-1H-indole (Table 2,6c).

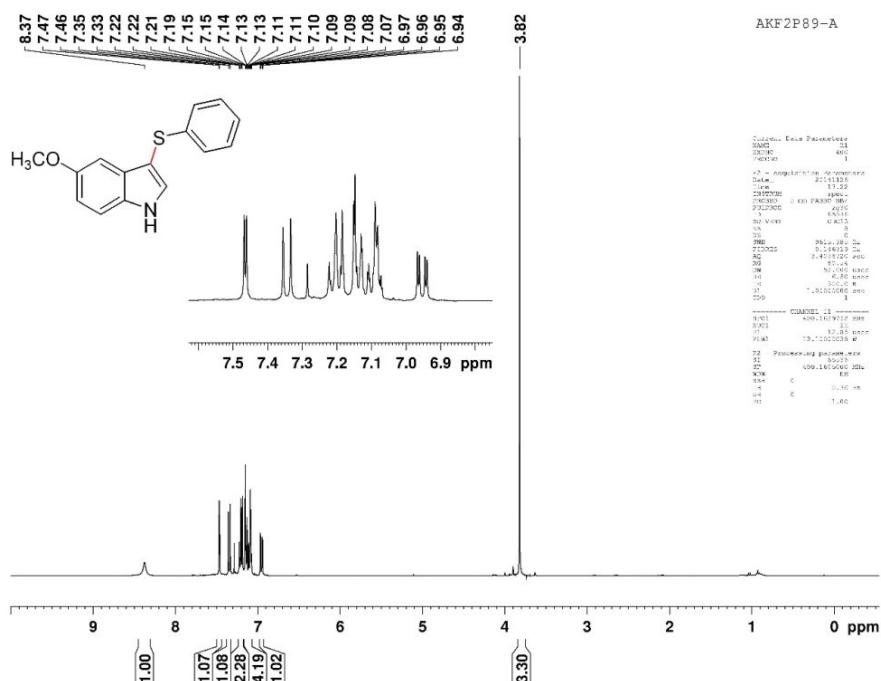


¹³C-NMR spectrum of 5-bromo-3-(phenylthio)-1H-indole (Table 2, 6c).

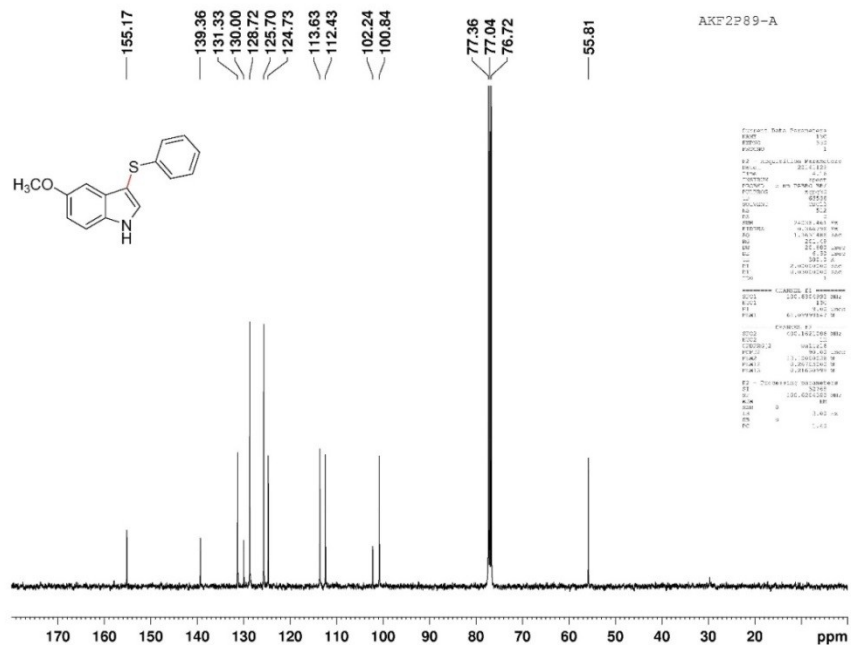
Sample Name	Dr. Sinha	Position	Vial 19	Instrument Name	Instrument 1	User Name	
Injection Volume	1	Injection Position		Sample Type	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKT10P833-198.d	Acquisition Method	ISO-JAN.m	Comment		Acquired Time	6/30/2014 10:58:24



HRMS spectrum of 5-bromo-3-(phenylthio)-1H-indole (Table 2, 6c).

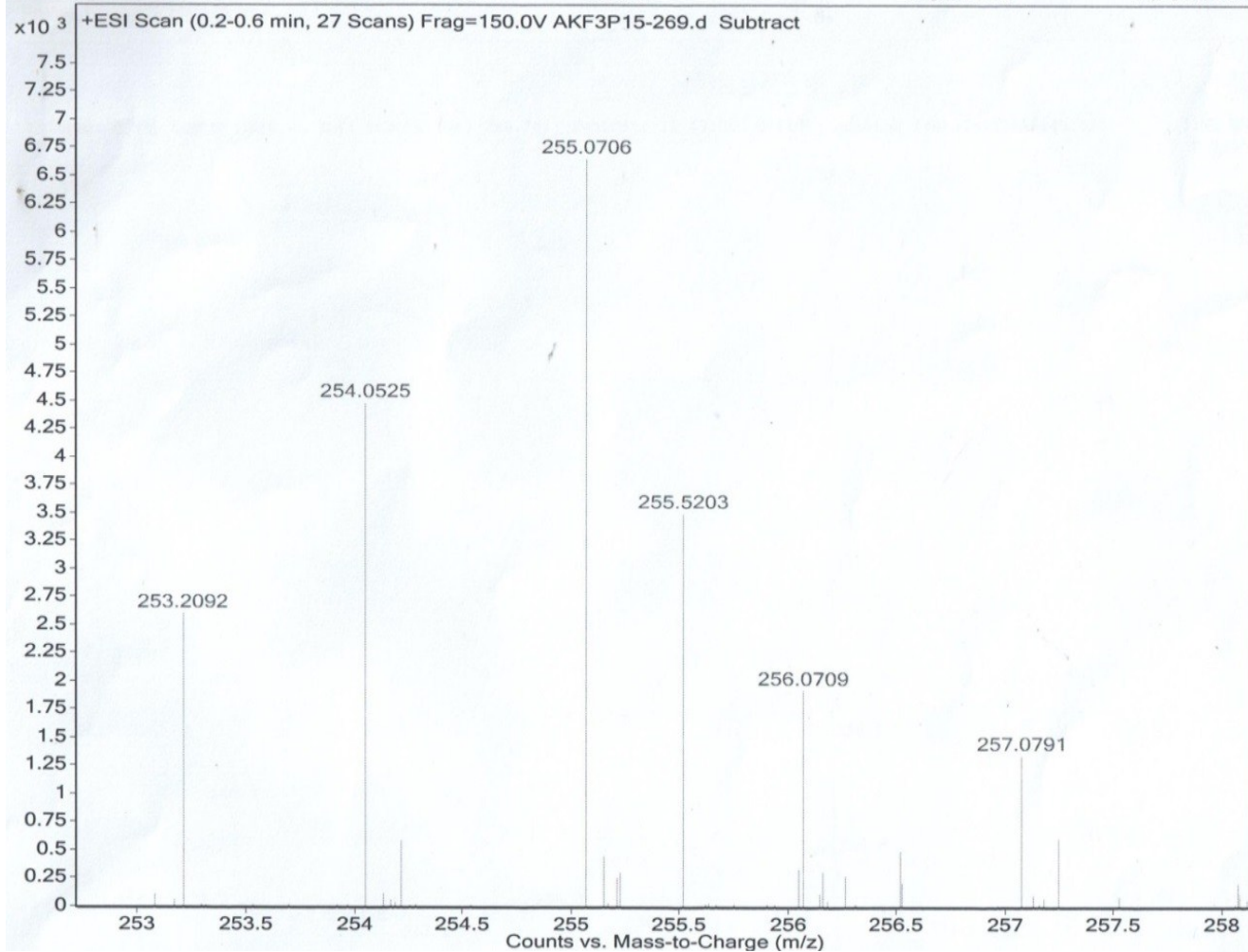


¹H-NMR spectrum of 5-methoxy-3-(phenylthio)-1H-indole (Table 2, 6d).

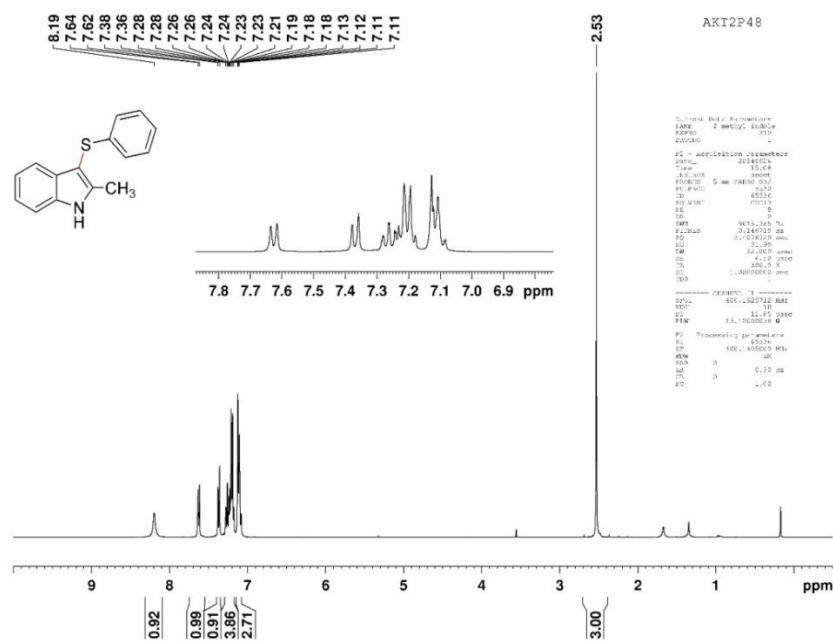


¹³C-NMR spectrum of 5-methoxy-3-(phenylthio)-1H-indole (Table 2, 6d).

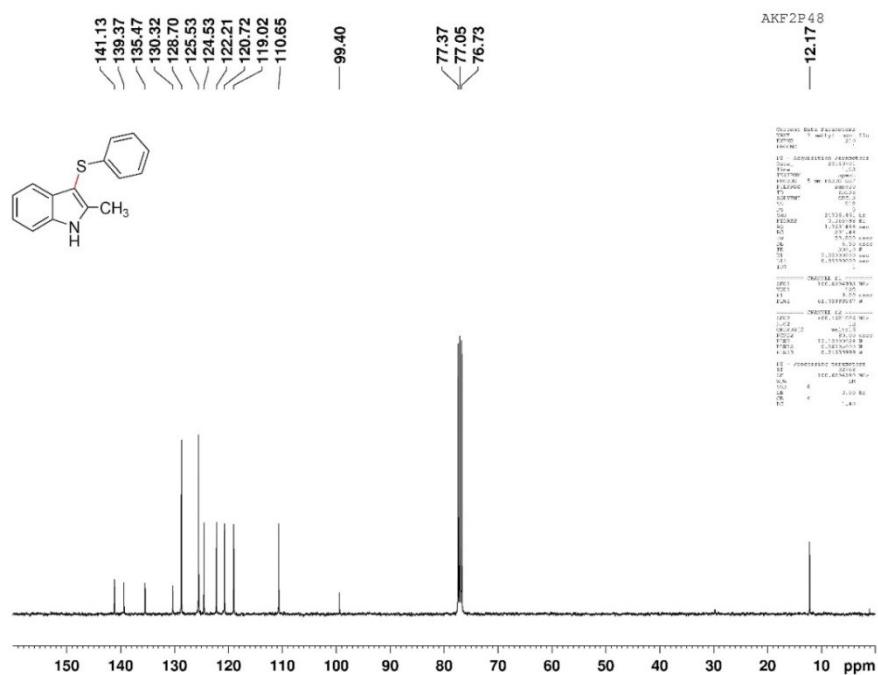
Sample Name	Dr. SINHA	Position	Vial 17	Instrument Name	Instrument 1	User Name	
Injection Vol	5	Injection Position		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	AKF3P15-269.d	Acquisition Method	ISO-OCT.m	Comment		Acquired Time	10/30/2014 3:12:31



HRMS spectrum of 5-methoxy-3-(phenylthio)-1H-indole (Table 2, 6d).

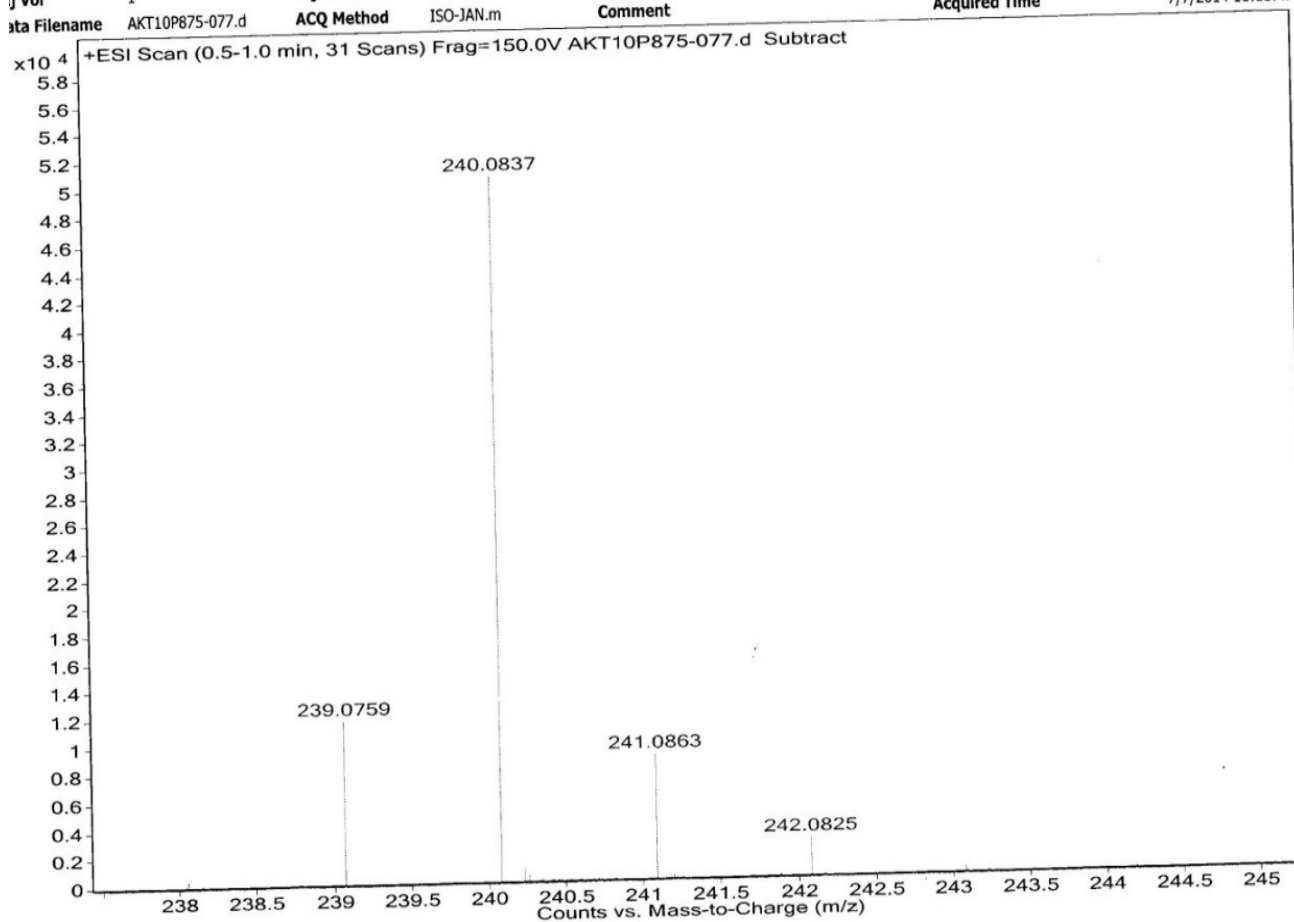


¹H-NMR spectrum of 2-methyl-3-(phenylthio)-1H-indole (Table 2, 6e).

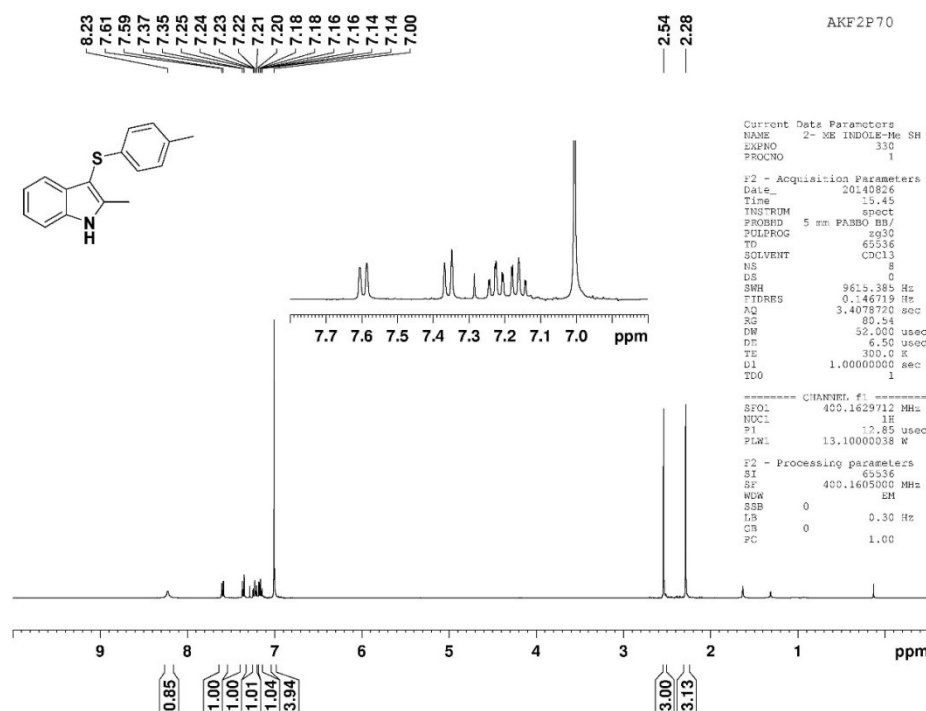


¹³C-NMR spectrum of 2-methyl-3-(p-tolylthio)-1H-indole (Table 2, 6e)

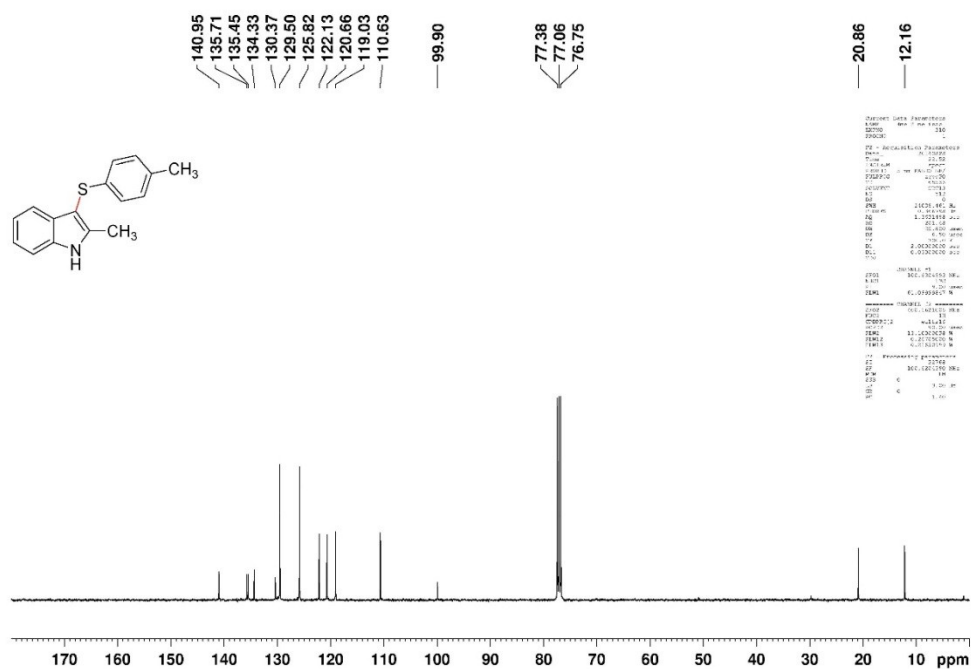
Sample Name	Dr. SINHA	Position	Vial 34	Instrument Name	Instrument 1	User Name	
Injection Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Sample Filename	AKT10P875-077.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	7/7/2014 11:18:47 A



HRMS spectrum of 2-methyl-3-(p-tolylthio)-1H-indole (Table 2, 6e)

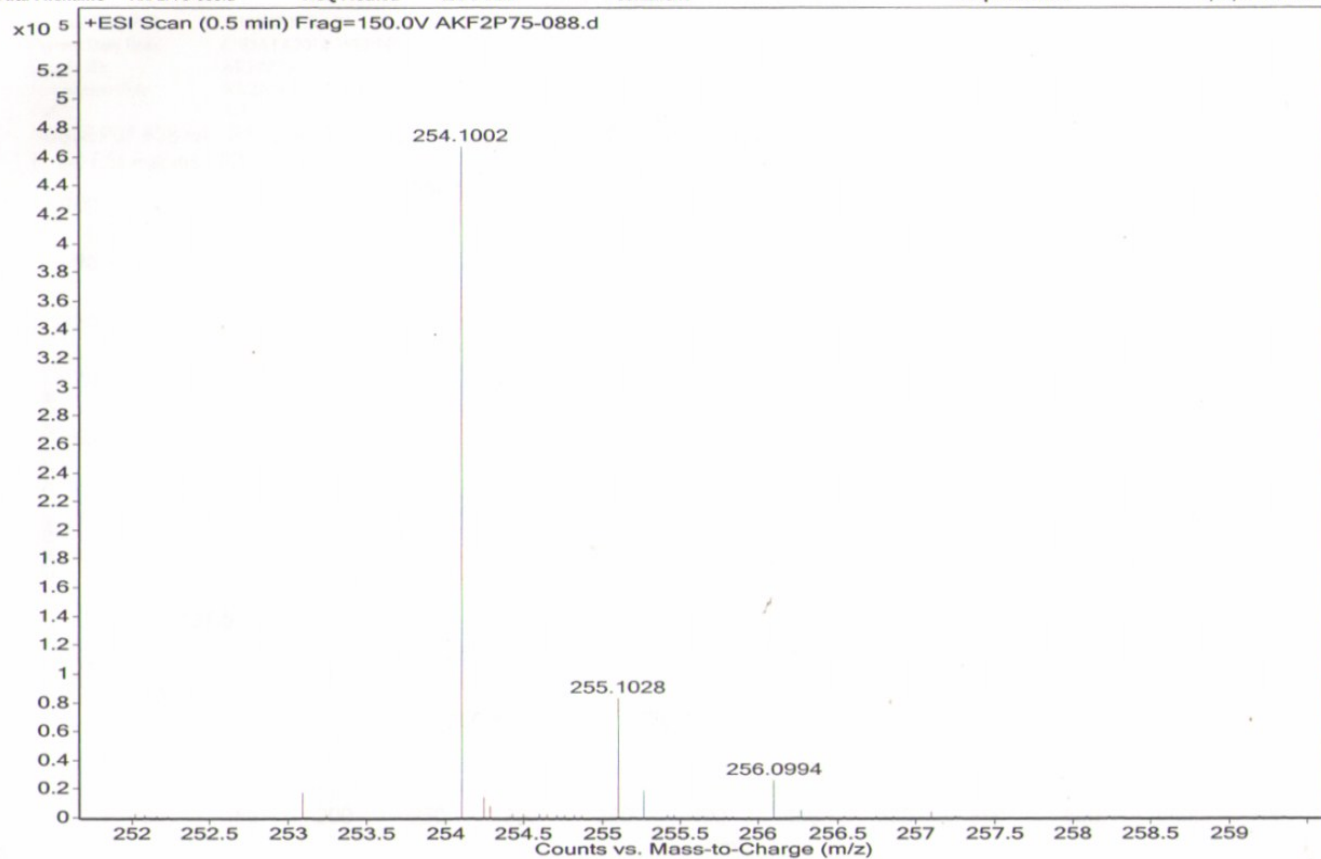


¹H-NMR spectrum of 2-methyl-3-(p-tolylthio)-1H-indole (Table 2, 6f)

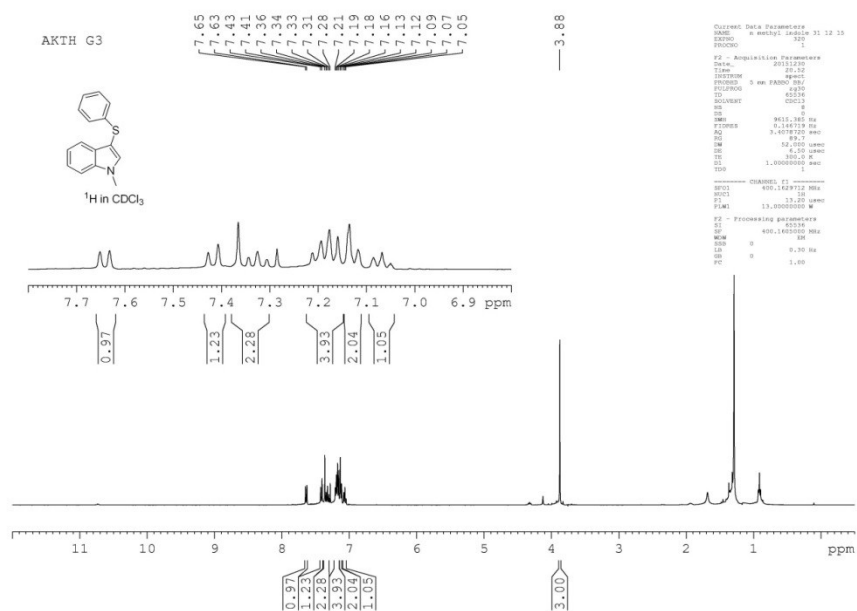


¹³C-NMR spectrum of 2-methyl-3-(p-tolylthio)-1H-indole (Table 2, 6f)

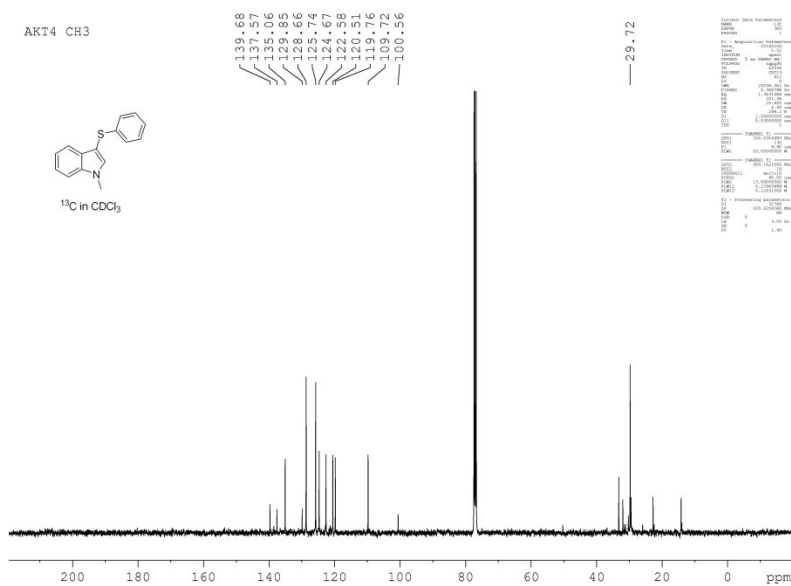
Sample Name	Dr. A. K. SINHA	Position	Vial 18	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKF2P75-088.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	9/11/2014 10:52:45



HRMS spectrum of 2-methyl-3-(p-tolylthio)-1H-indole (Table 2, 6f)

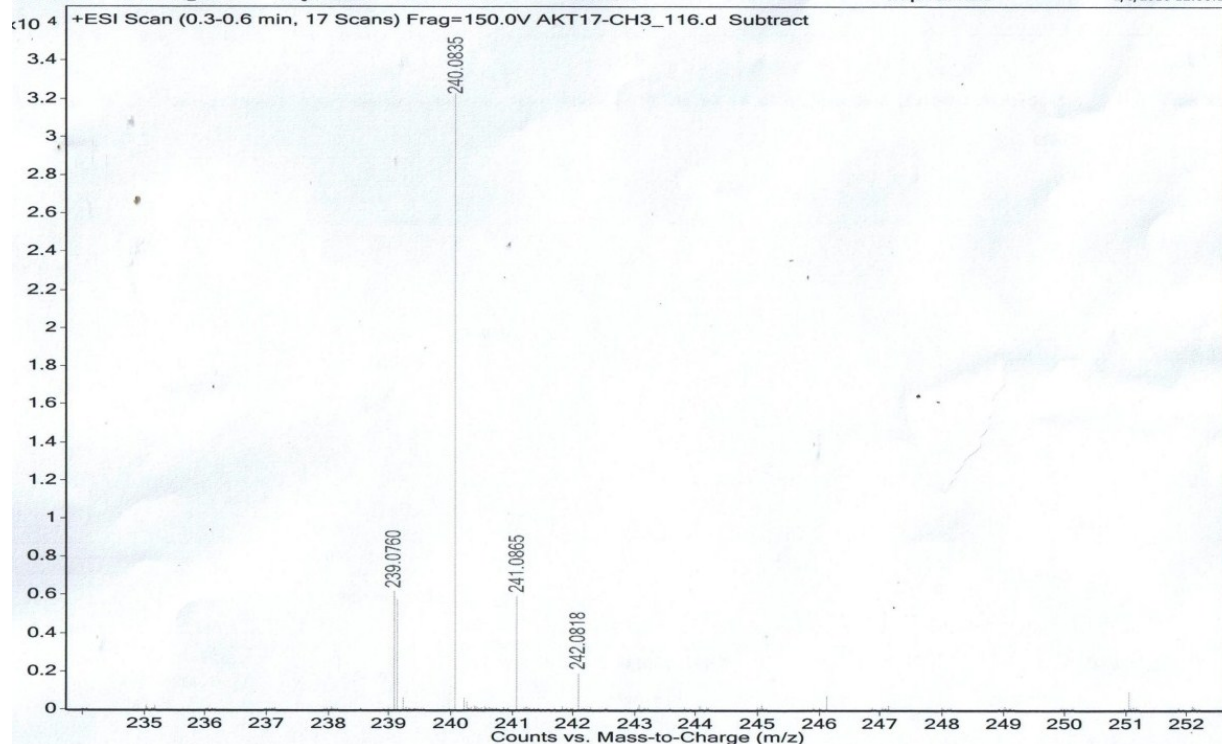


¹H-NMR spectrum of 1-methyl-3-(phenylthio)indoline (Table 2, 6g)

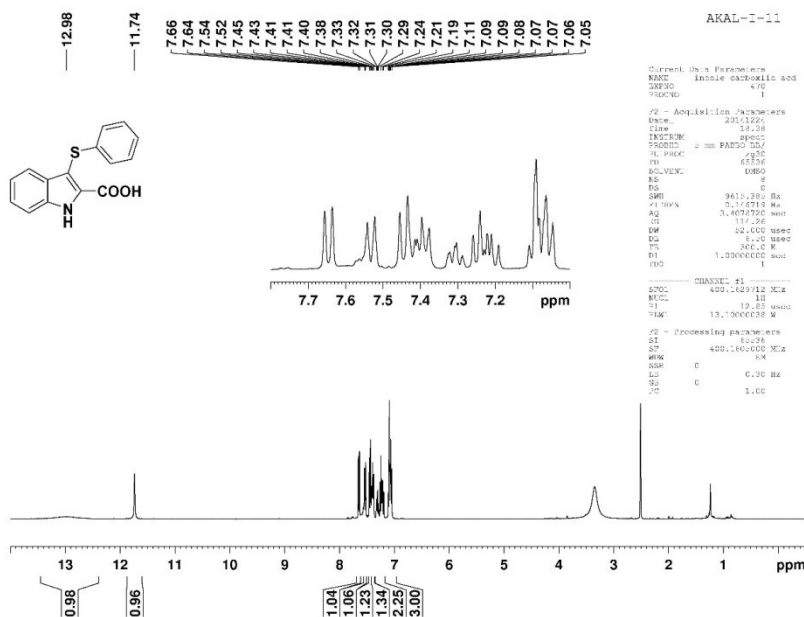


¹³C-NMR spectrum of 1-methyl-3-(phenylthio)indoline (Table 2, 6g)

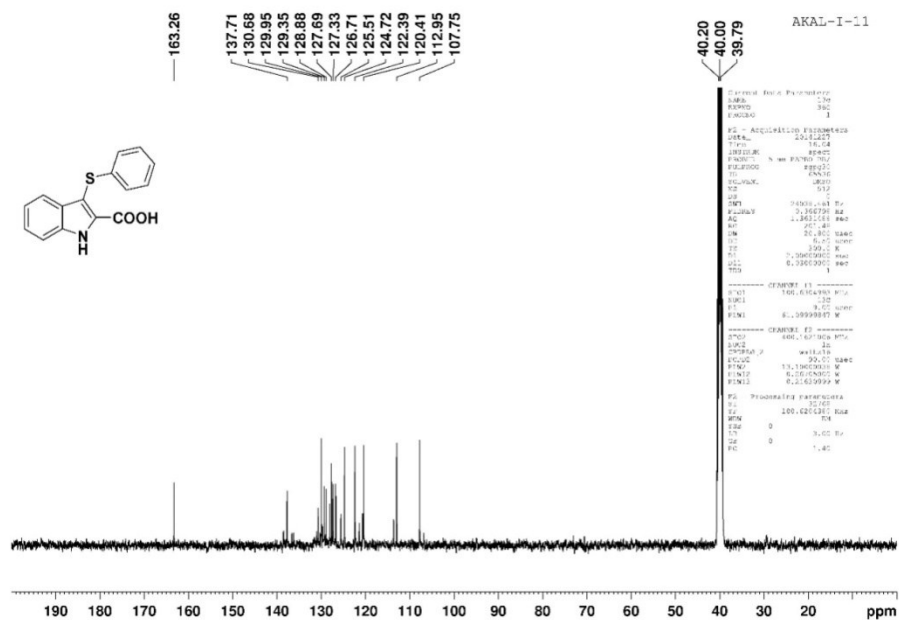
Sample Name	Dr. SINHA/SAIMA	Position	Vial 17	Instrument Name	Instrument 1	User Name	
Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
File Name	AKT17-CH3_116.d	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	1/8/2016 12:08:19 PM



HRMS spectrum of 1-methyl-3-(phenylthio)indoline (Table 2, 6g).

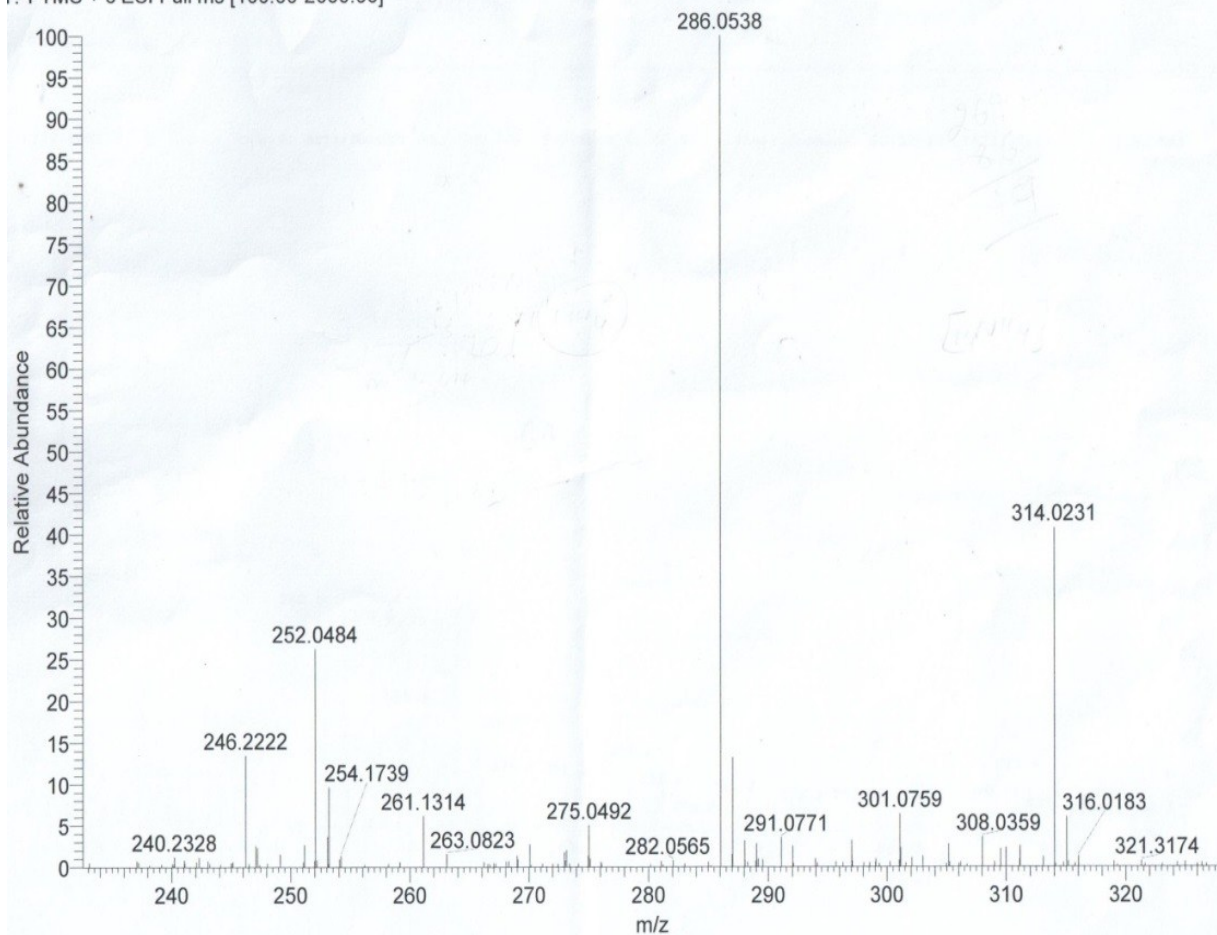


¹H-NMR spectrum of 3-(phenylthio)-1H-indole-2-carboxylic acid (Table 3, 7a).

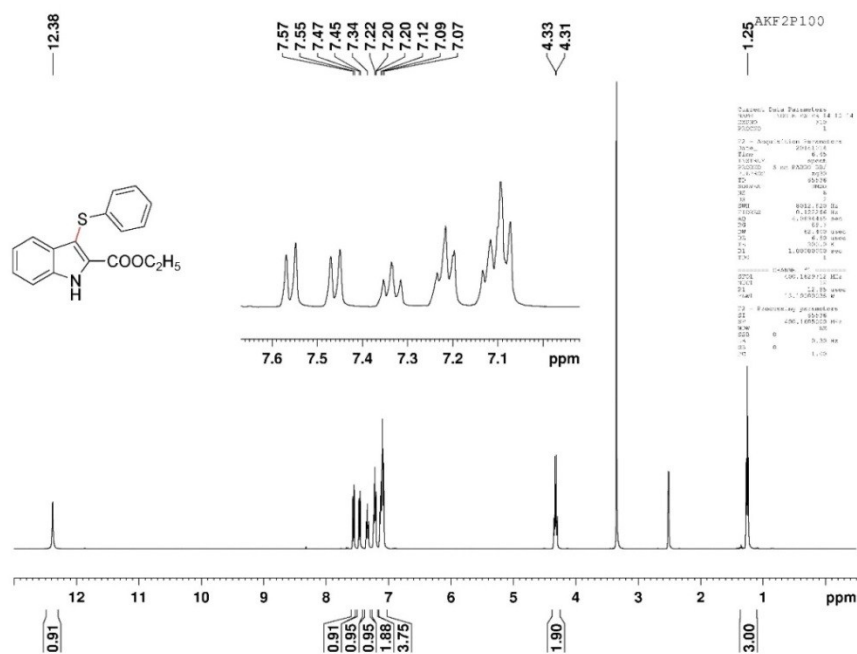


¹³C-NMR spectrum of 3-(phenylthio)-1H-indole-2-carboxylic acid (Table 3, 7a).

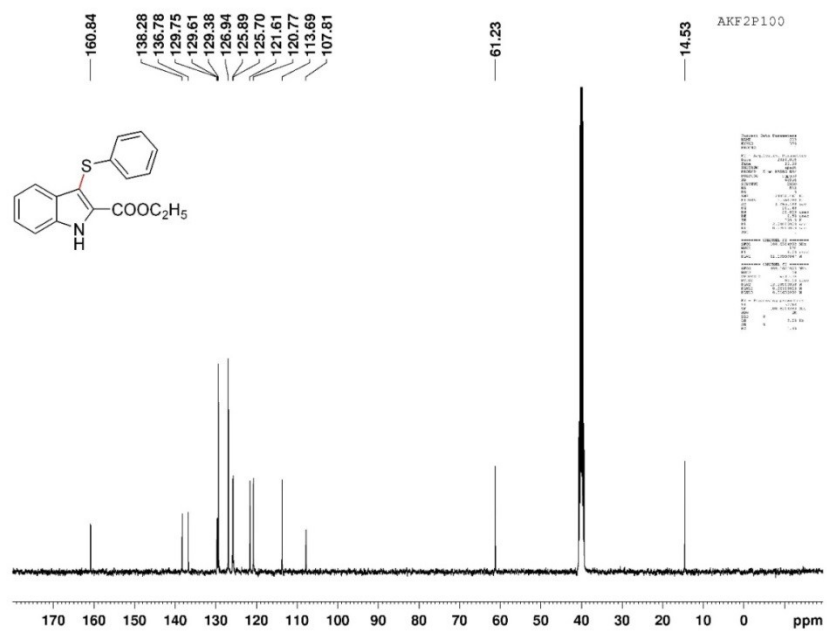
AKT10P860_150112120902 #24 RT: 0.22 AV: 1 SB: 6 0.03-0.08 NL: 2.79E5
F: FTMS + c ESI Full ms [100.00-2000.00]



HRMS spectrum of 3-(phenylthio)-1H-indole-2-carboxylic acid (Table 3, 7a).

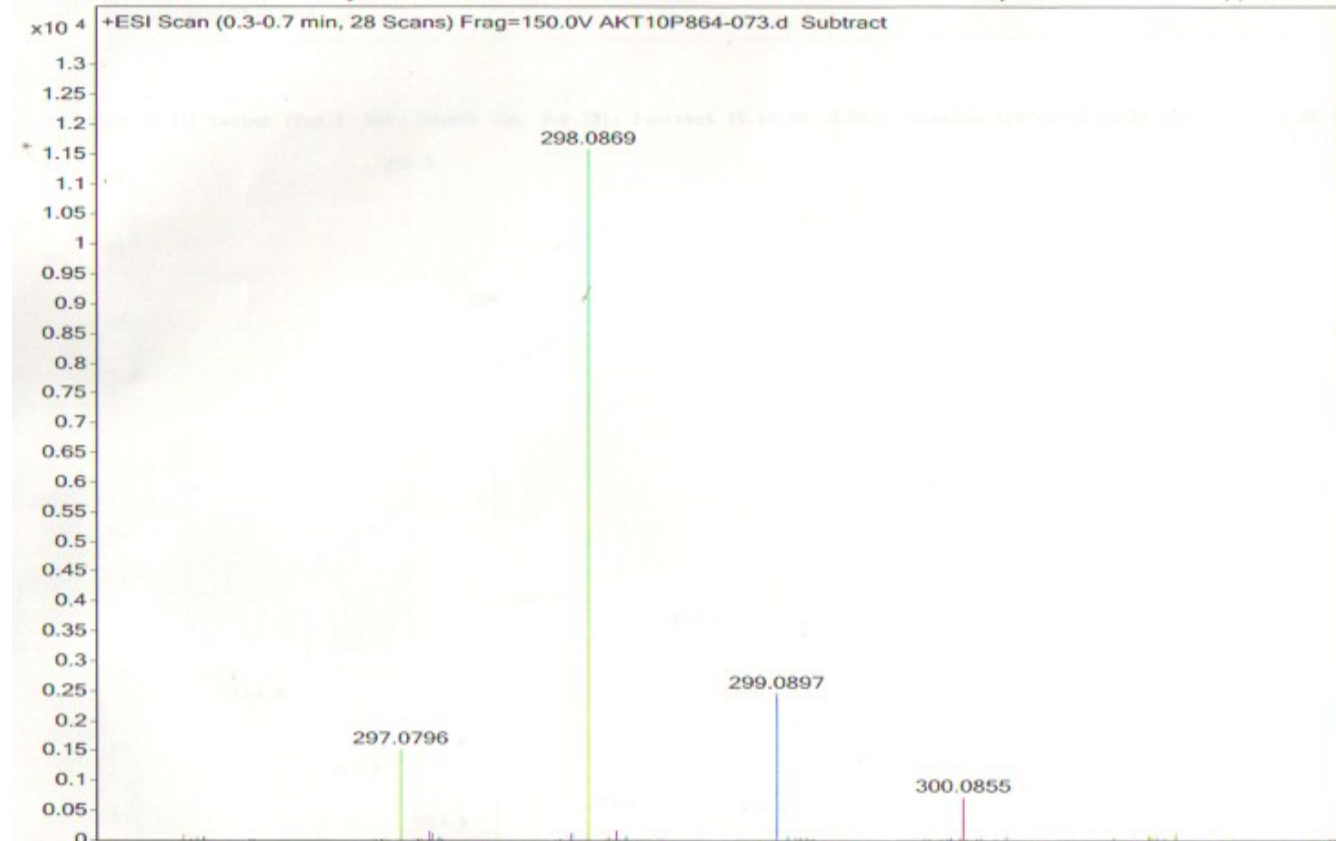


¹H-NMR spectrum of ethyl 3-(phenylthio)-1H-indole-2-carboxylate (Table 3, 7b)

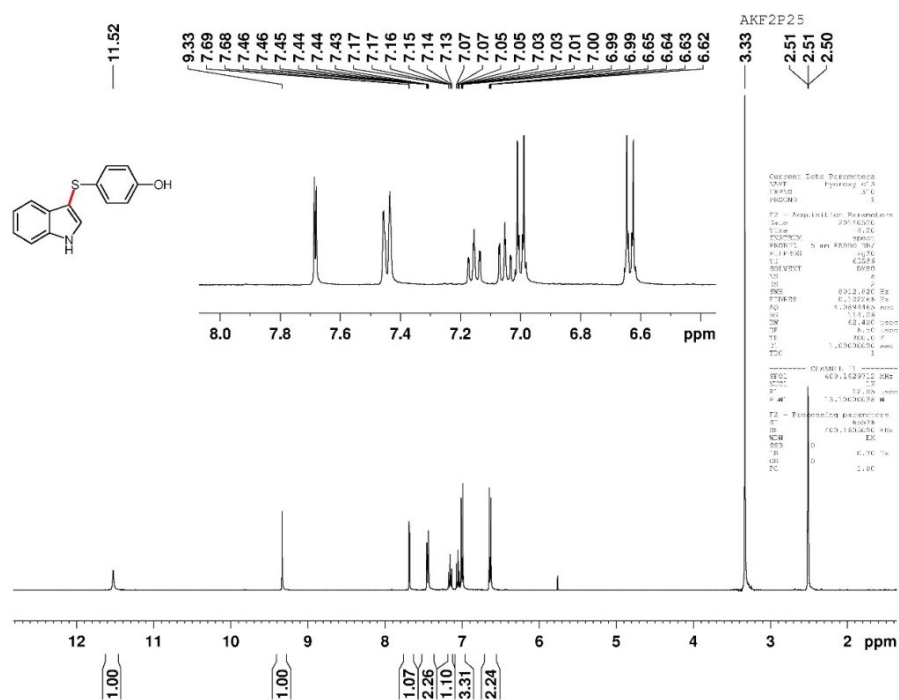


¹³C-NMR spectrum of ethyl 3-(phenylthio)-1H-indole-2-carboxylate (Table 3, 7b)

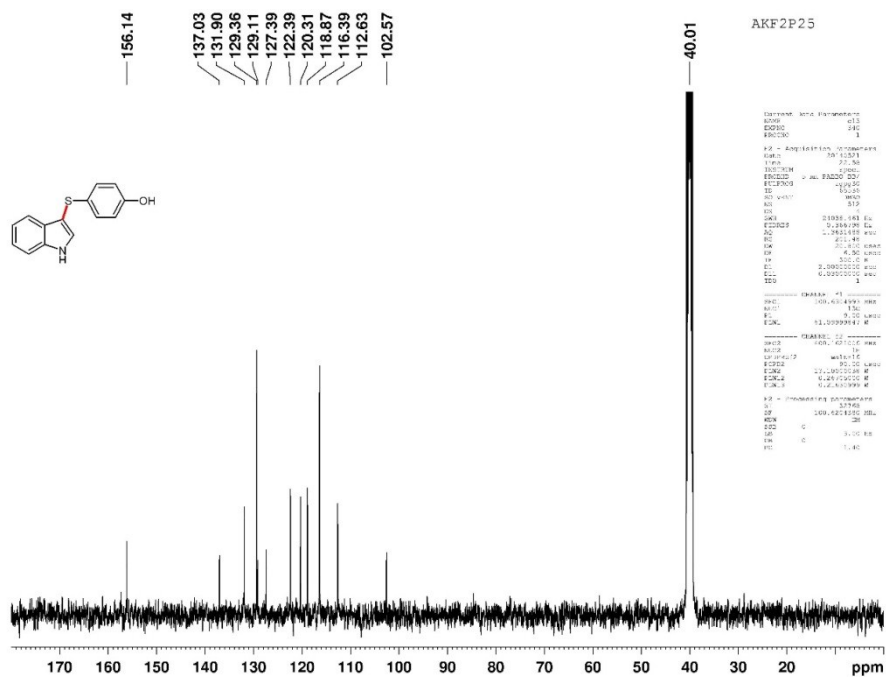
Sample Name	Dr. SINHA	Position	Vial 41	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKT10P864-073.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	8/6/2014 4:28:45 PM



HRMS spectrum of ethyl 3-(phenylthio)-1H-indole-2-carboxylate (Table 3, 7b)

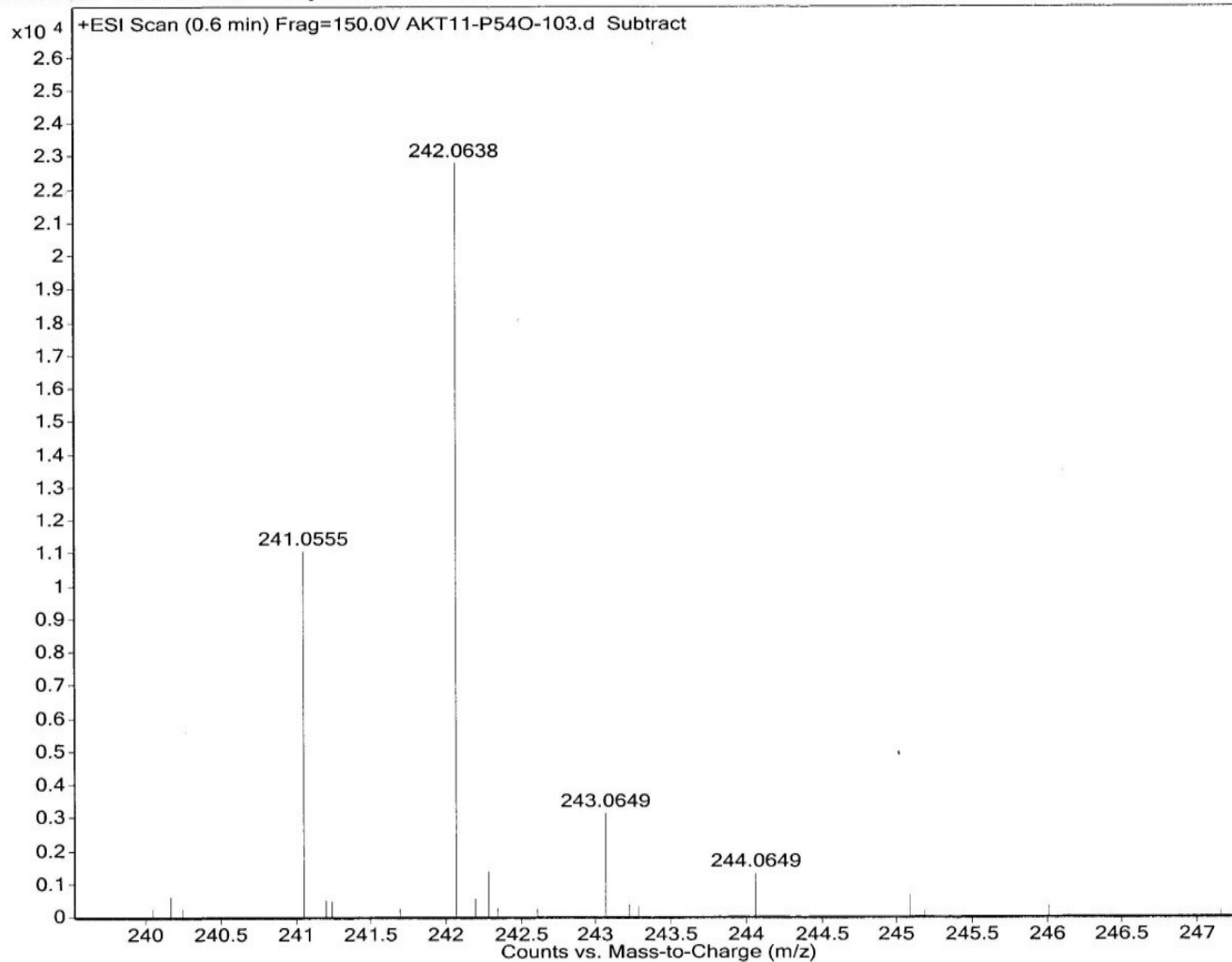


¹H-NMR spectrum of 4-((1H-indol-3-yl)thio)phenol (Table 3, 7c)

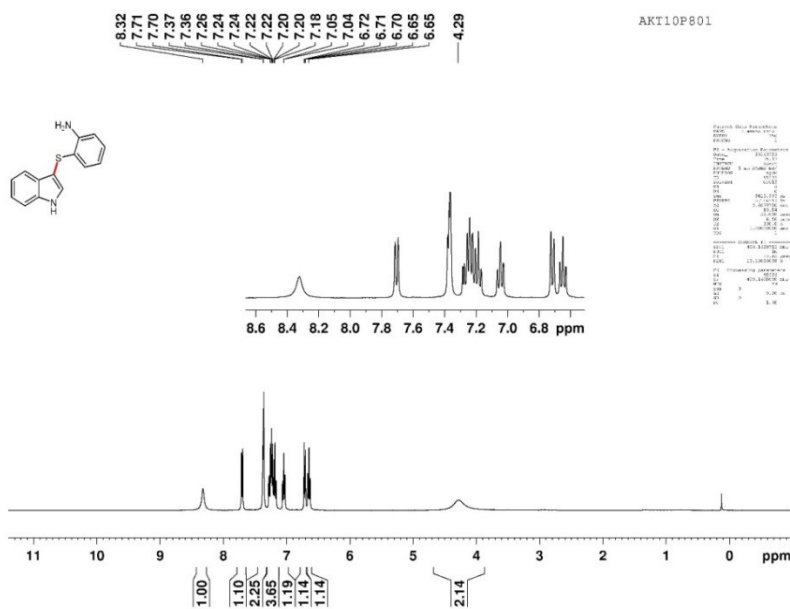


¹³C-NMR spectrum of 4-((1H-indol-3-yl)thio)phenol (Table 3, 7c)

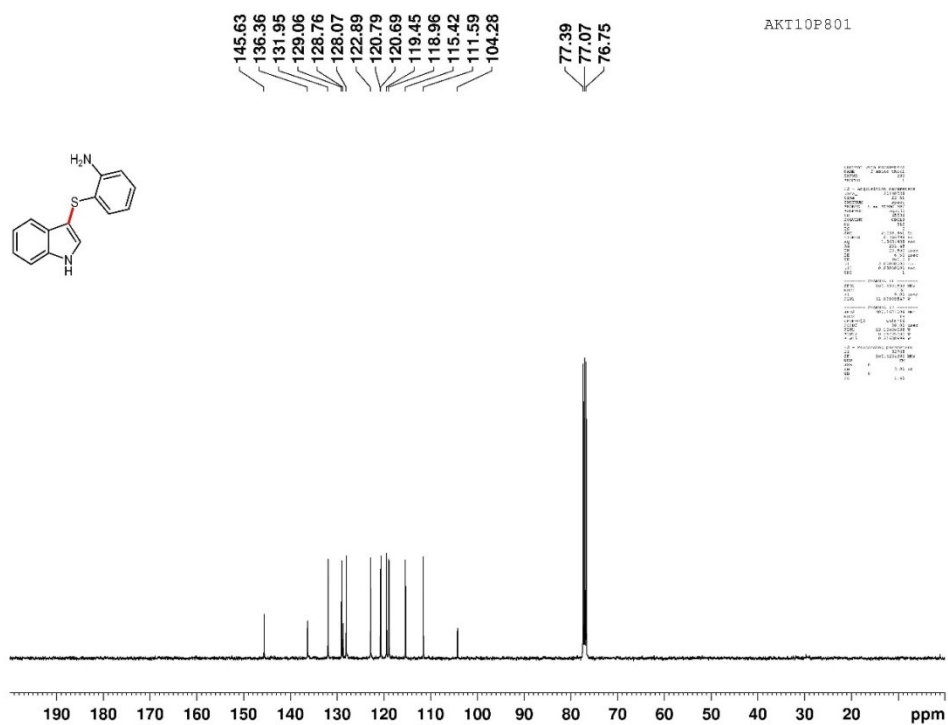
Sample Name	Dr. A.N. SINHA	Position	Vidit 12	Instrument Name	MSU-010000-1	User Name	
Inj Vol	1	Inj Position		Sample Type	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKT11-P540-103.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	6/13/2014 10:42:04 A



HRMS spectrum of 4-((1H-indol-3-yl)thio)phenol (Table 3, 7c)

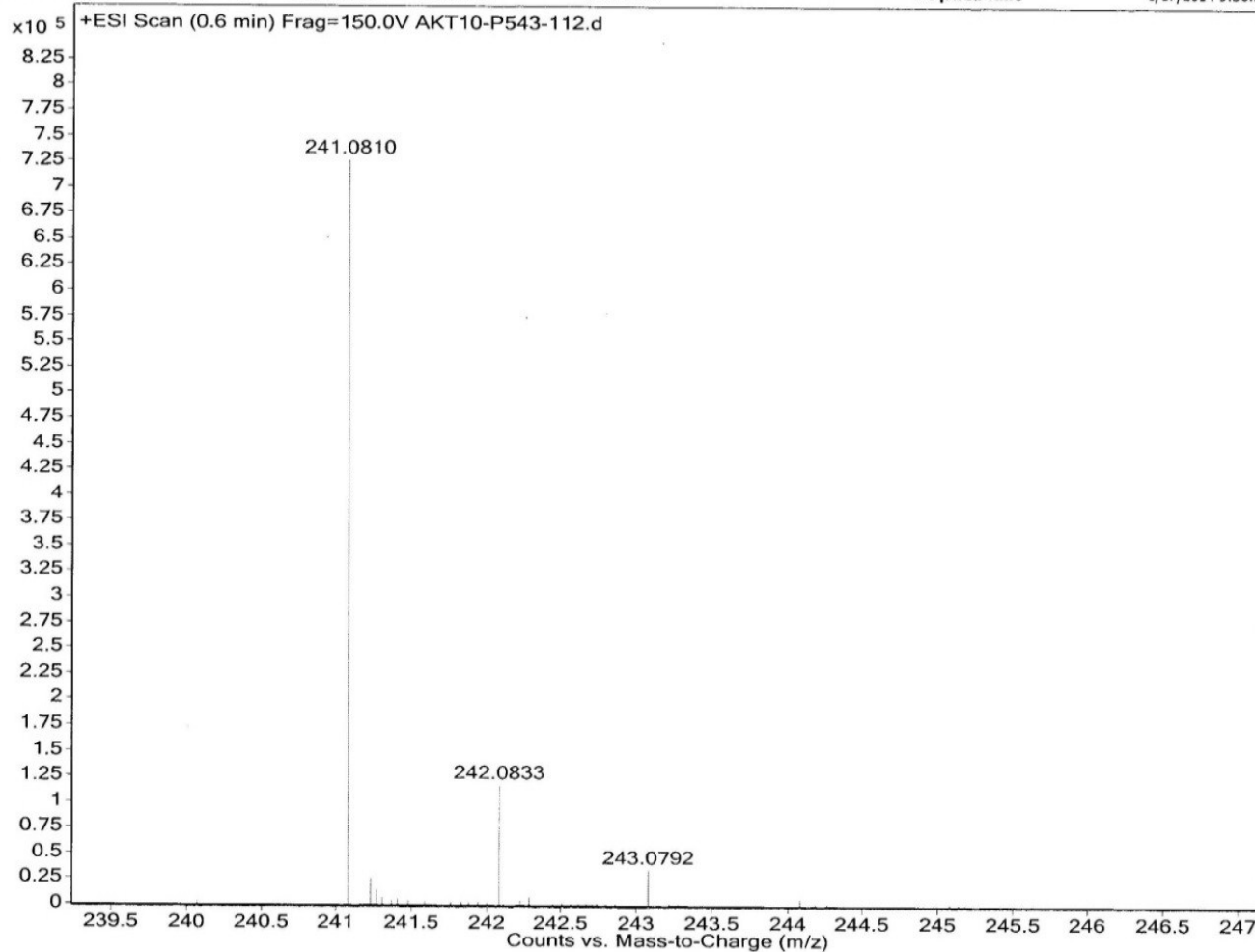


¹H-NMR spectrum of 2-((1H-indol-3-yl)thio)aniline (Table 3, 7d).

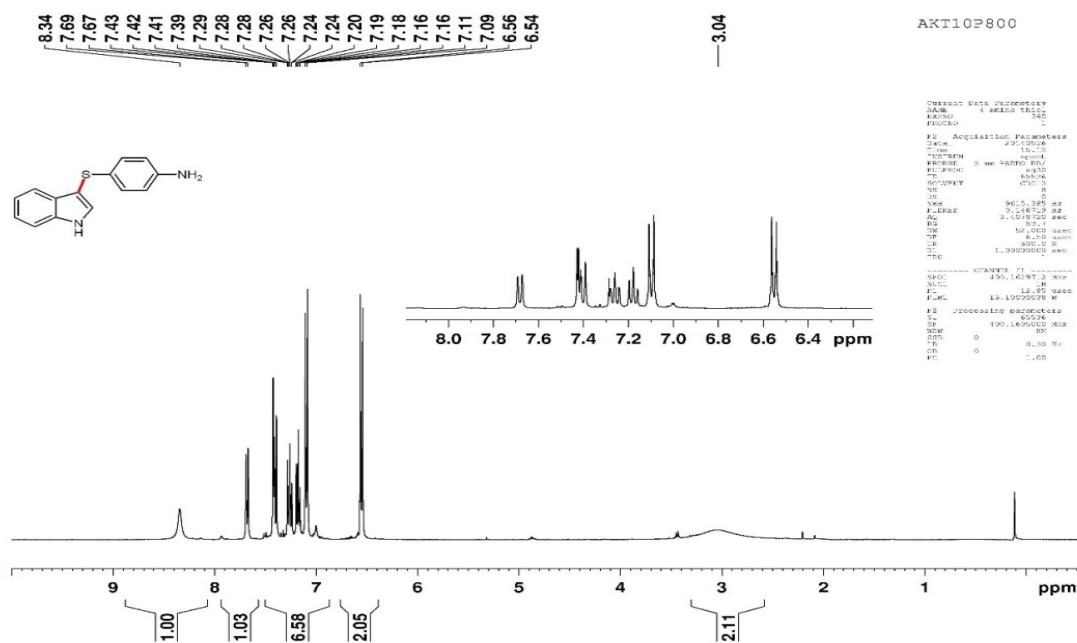


¹³C-NMR spectrum of 2-((1H-indol-3-yl)thio)aniline (Table 3, 7d).

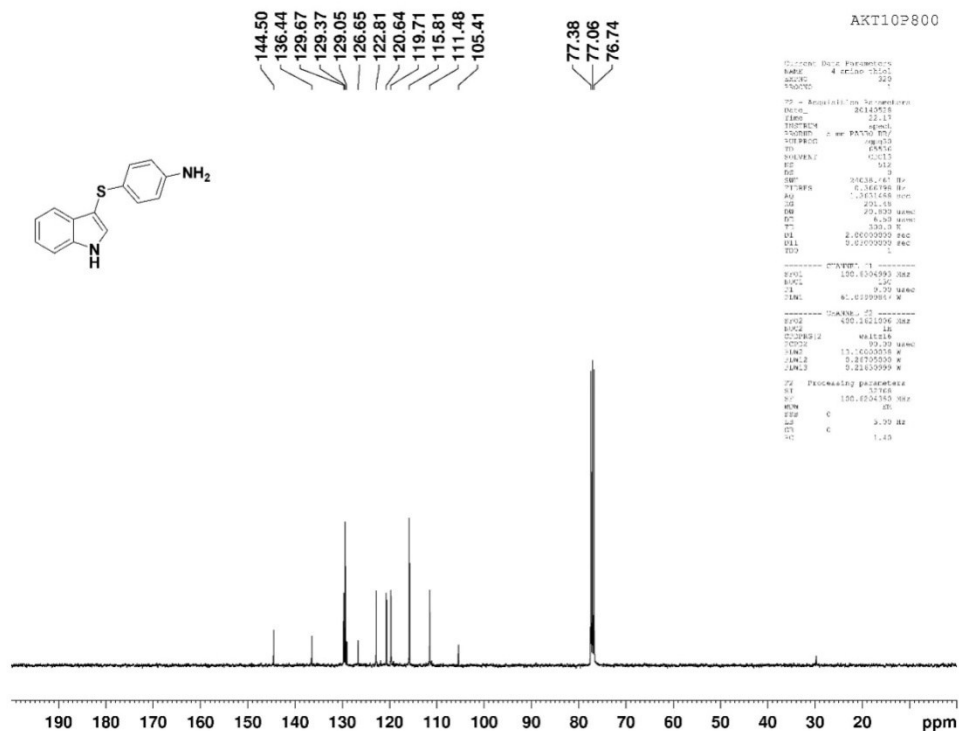
Sample Name	Dr. N. RASTOGI	Position	Vial 19	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKT10-P543-112.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	6/17/2014 9:56:29 A



HRMS spectrum of 2-((1H-indol-3-yl)thio)aniline (Table 3, 7d)

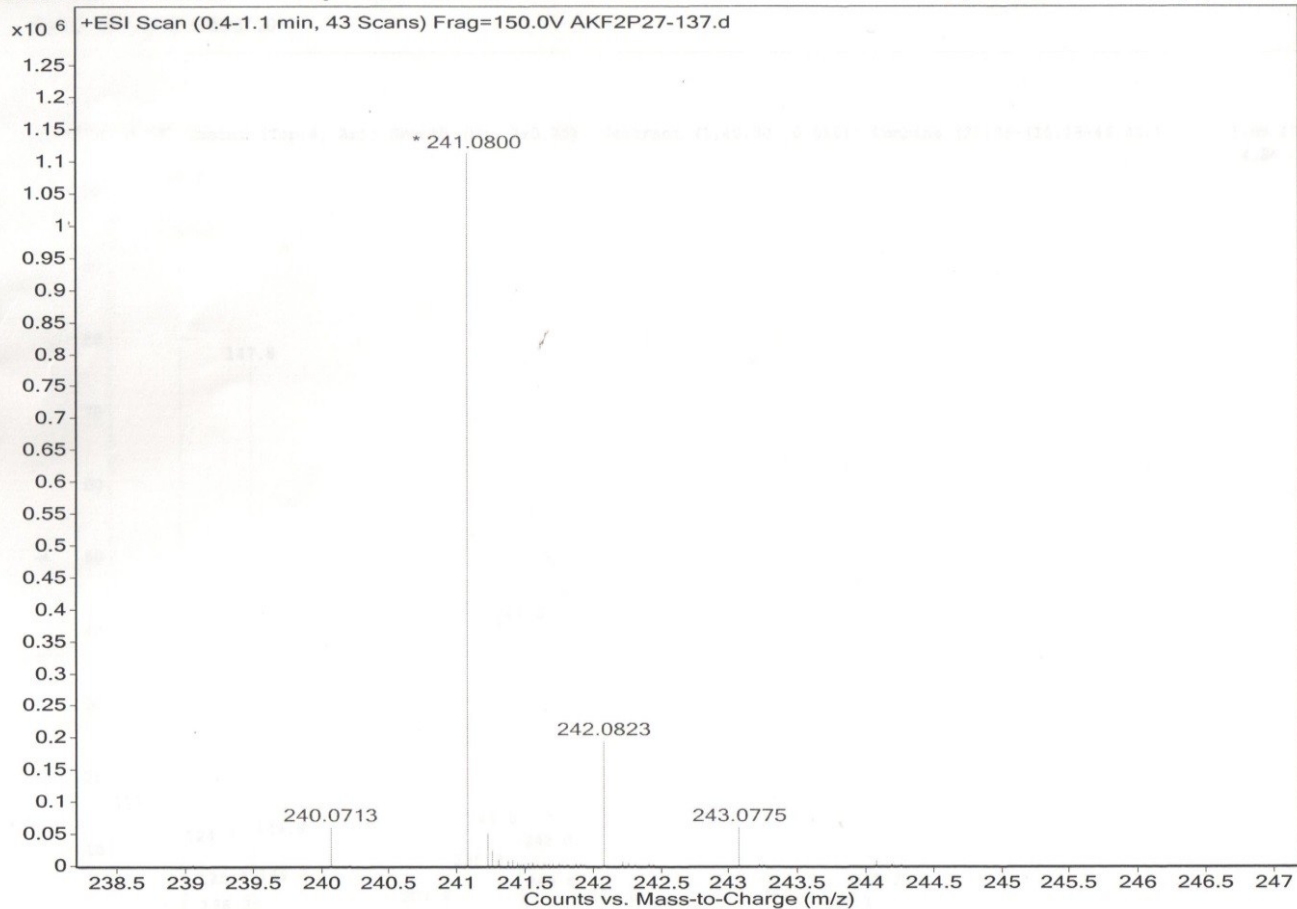


¹H-NMR spectrum of 4-((1H-indol-3-yl)thio)aniline (Table 3, 7e)

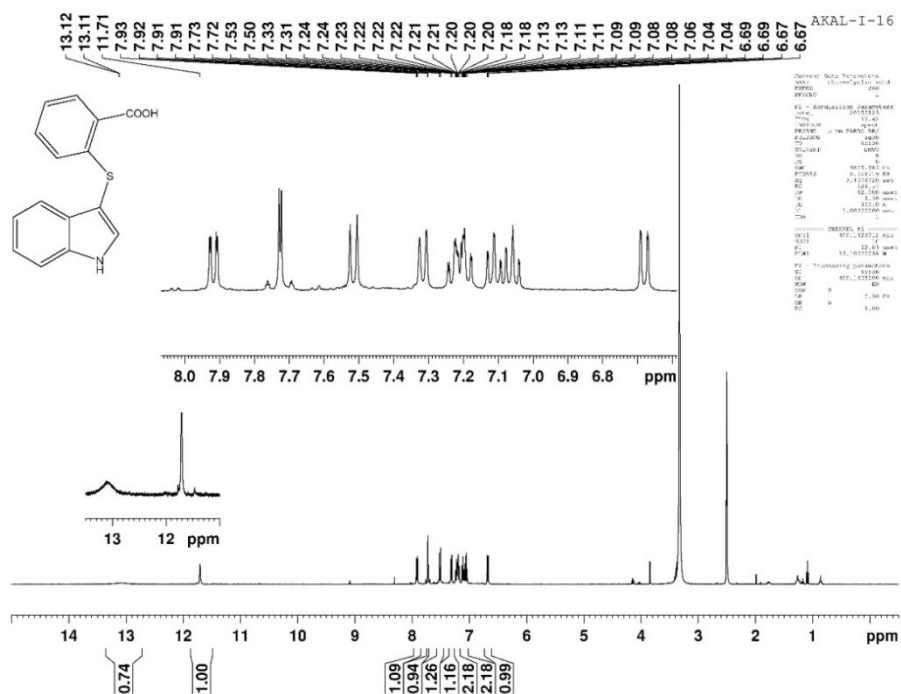


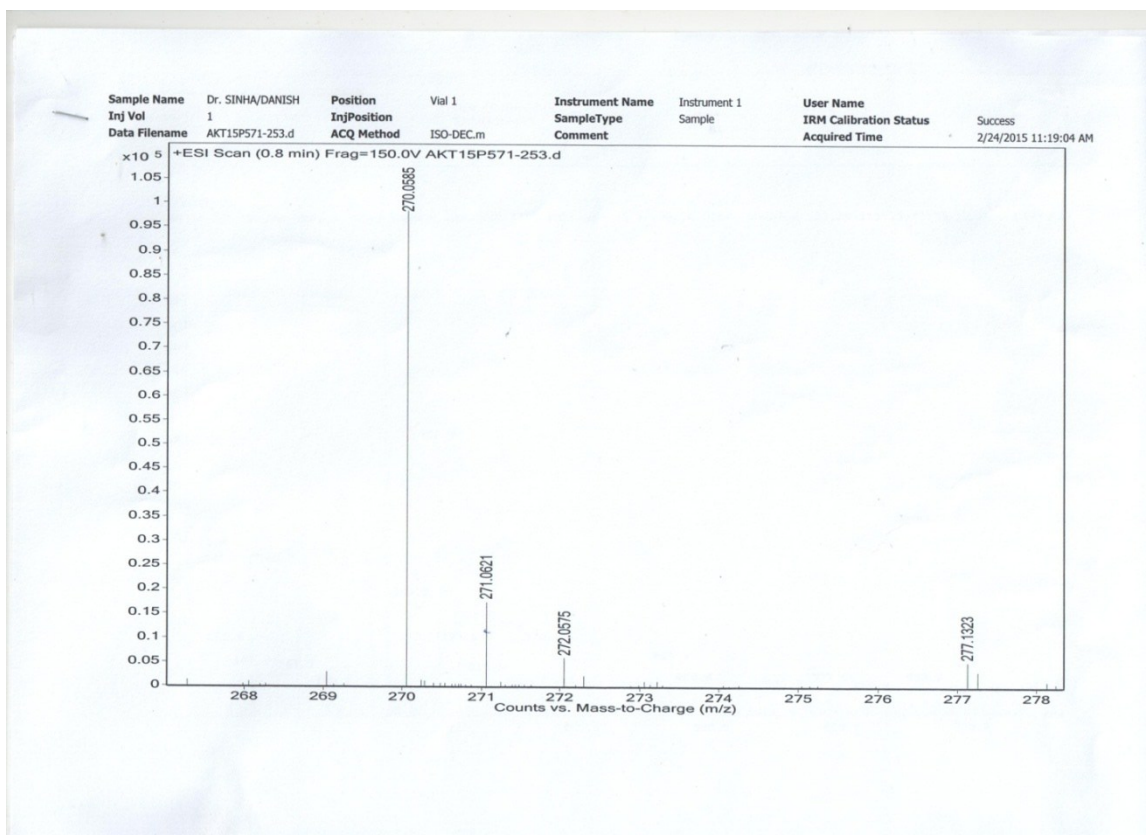
¹³C-NMR spectrum of 4-((1H-indol-3-yl)thio)aniline (Table 3, 7e)

Sample Name	Dr. A.K. SINHA	Position	Vial 20	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKF2P27-137.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	6/20/2014 11:46:20



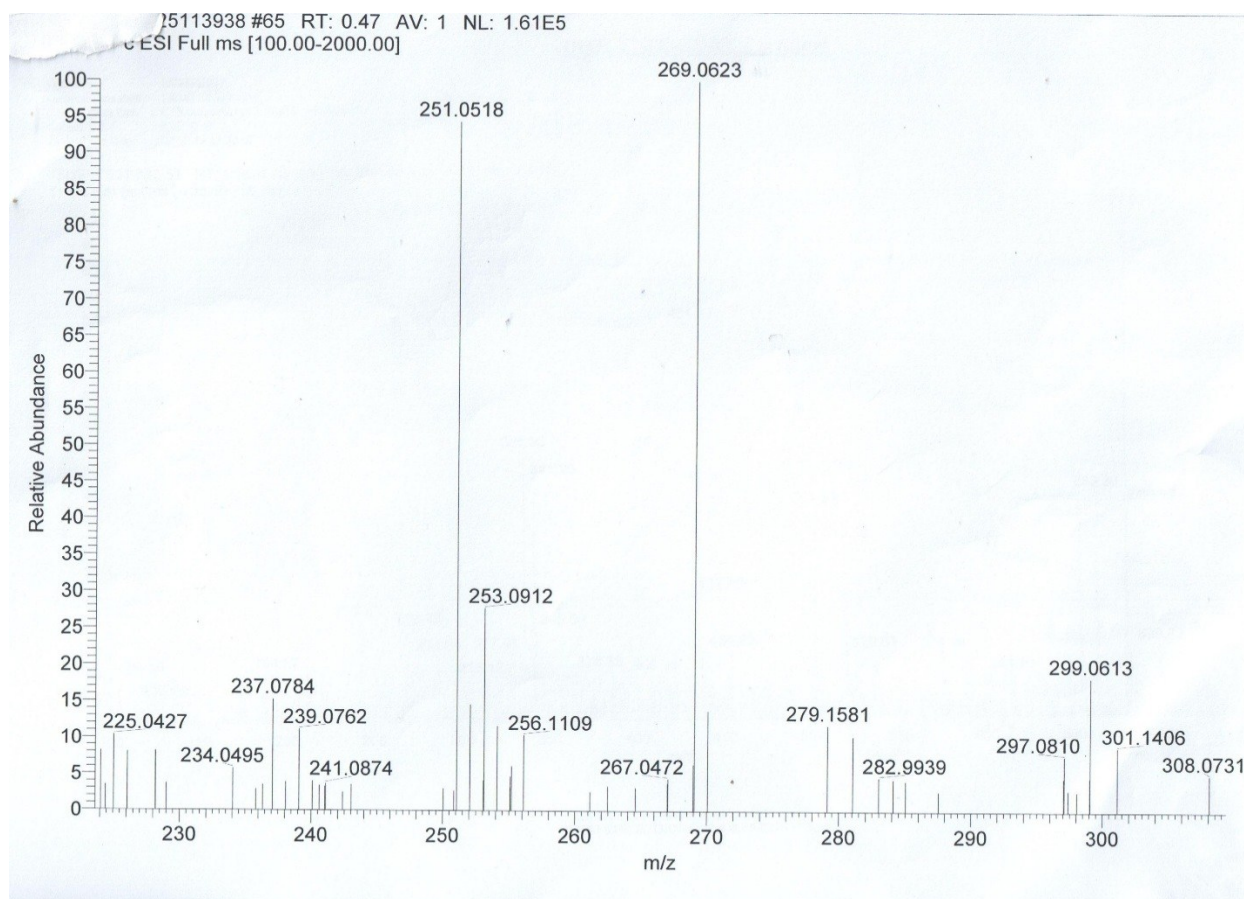
HRMS spectrum of 4-((1H-indol-3-yl)thio)aniline (Table 3, 7e)



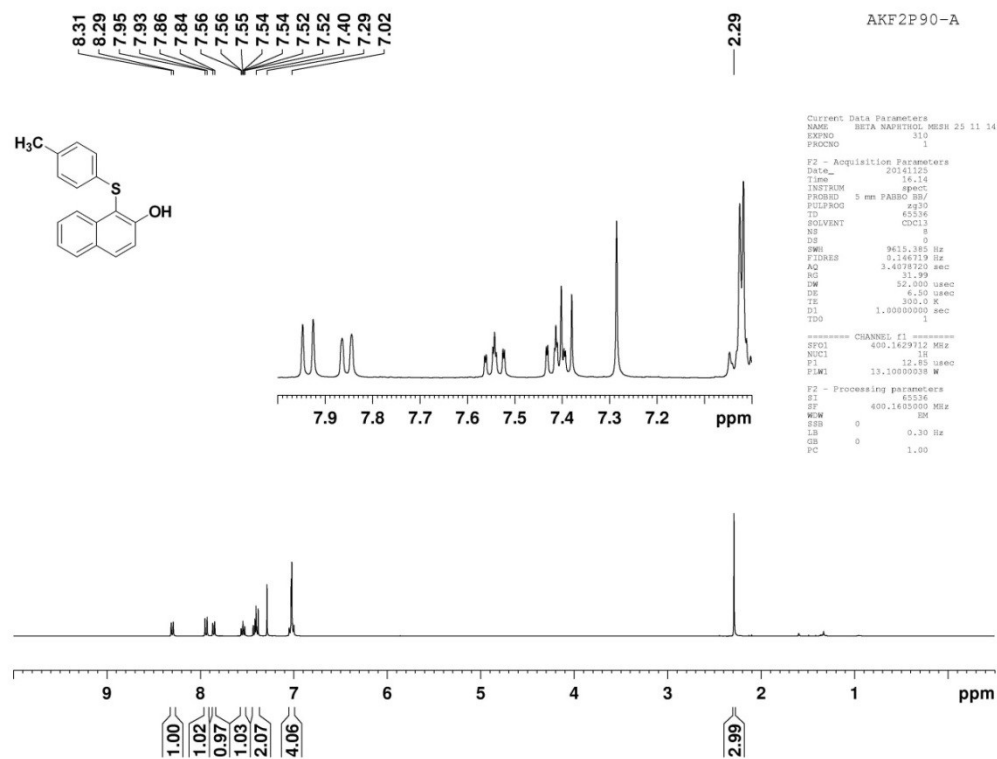


HRMS spectrum of 3-(phenylthio)-1H-indole-2-carboxylic acid (Table 3, 7f).

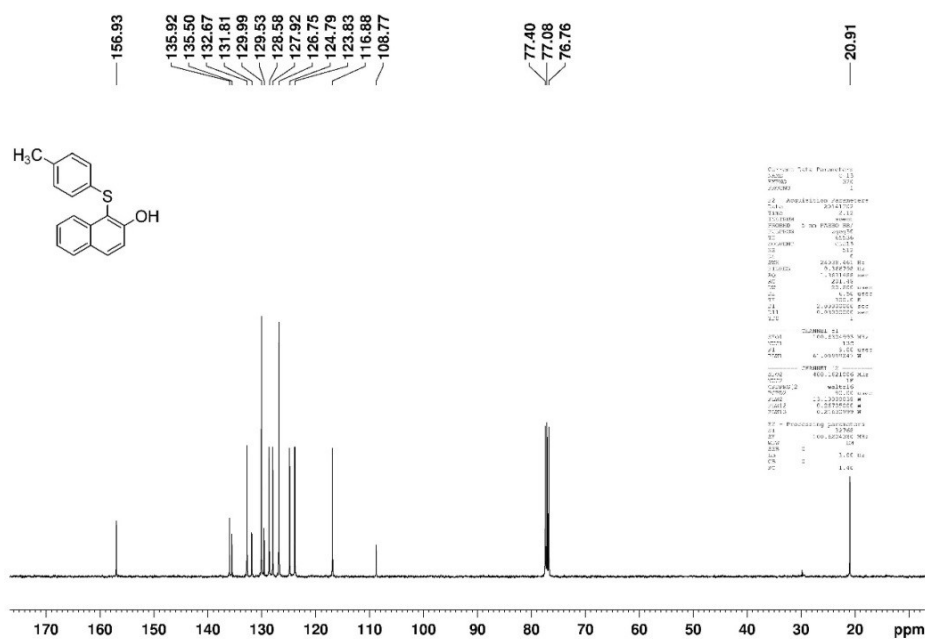




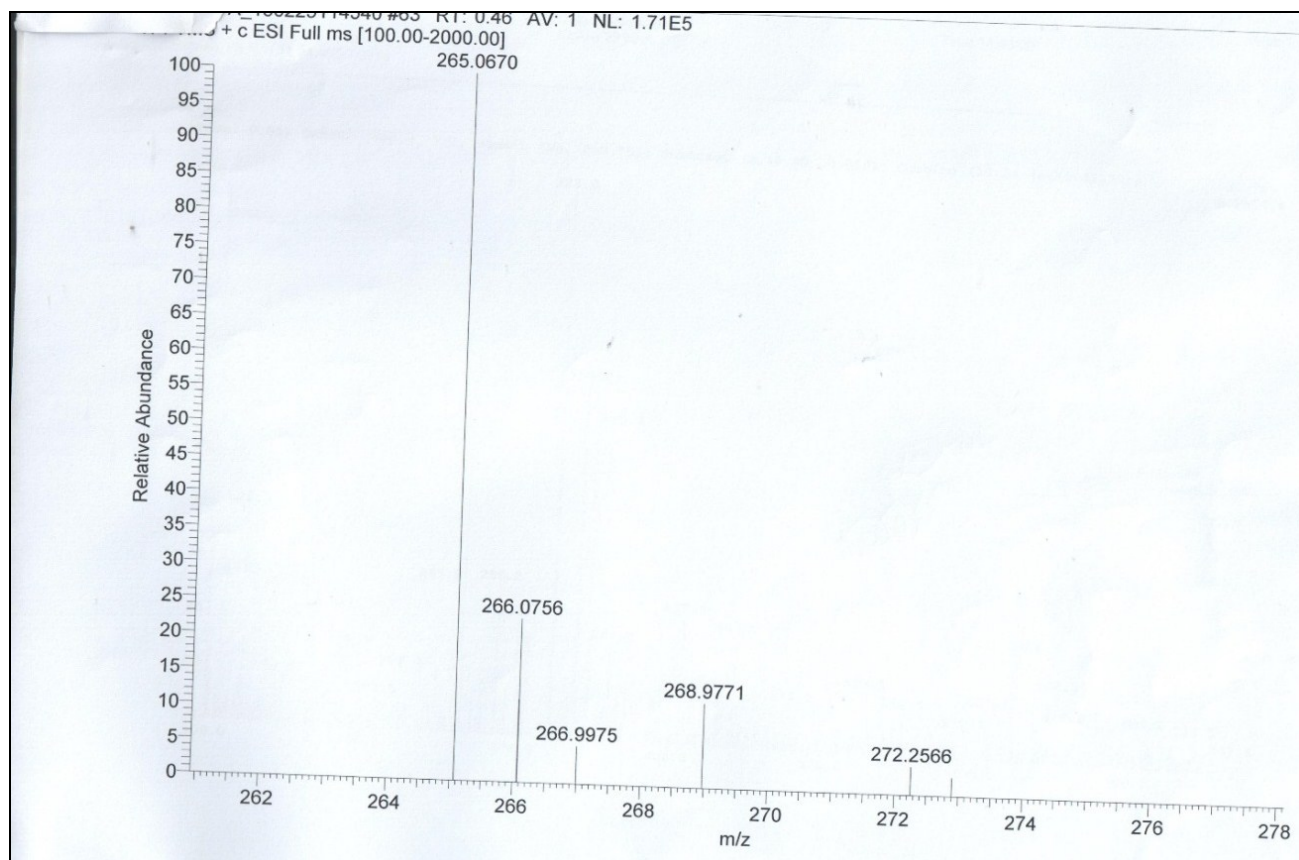
HRMS spectrum of 1-(phenylthio)naphthalen-2-ol (Table 4, 10a)



¹H-NMR spectrum of 1-(p-tolylthio)naphthalen-2-ol (Table 4,10b)

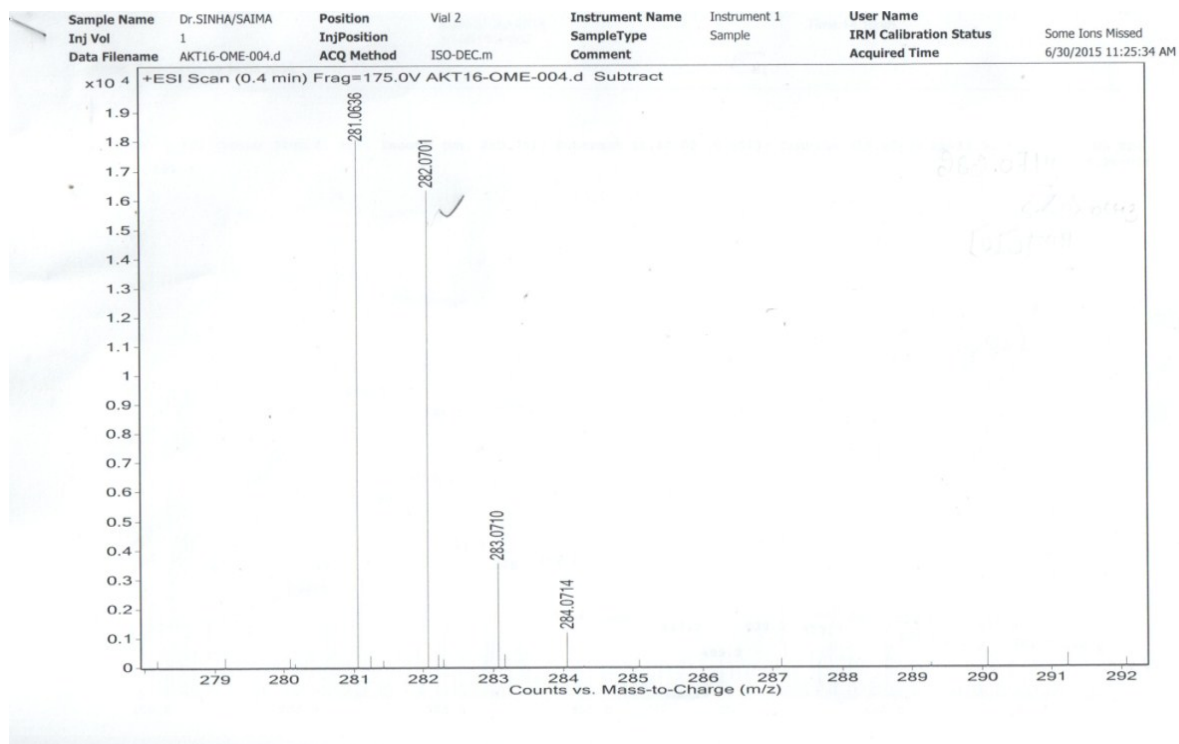


¹³C-NMR spectrum of 1-(p-tolylthio)naphthalen-2-ol (Table 4, 10b)

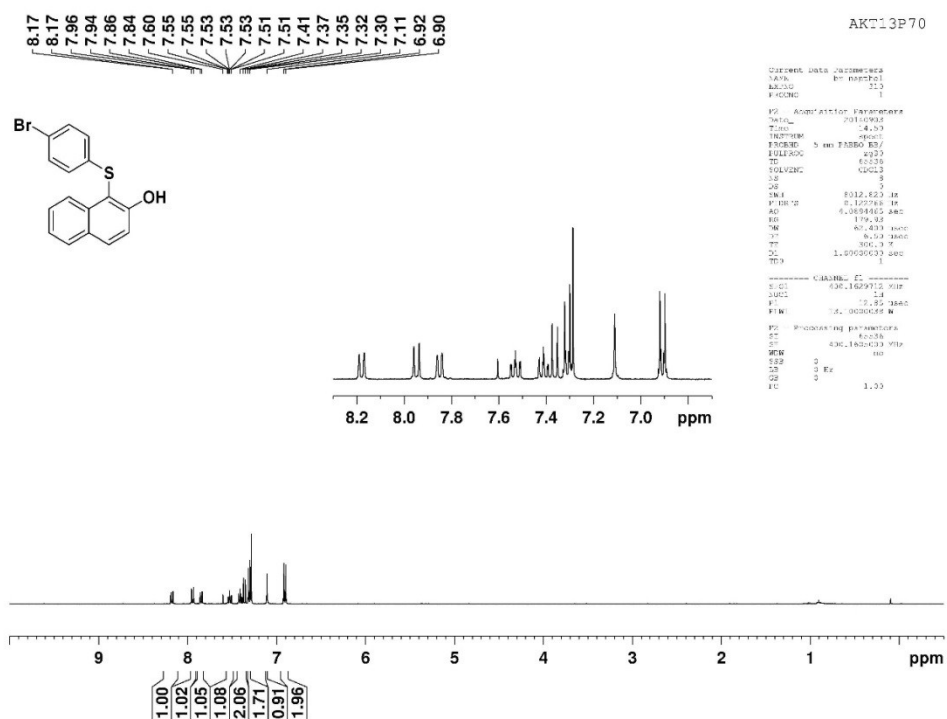


HRMS spectrum of 1-(p-tolylthio)naphthalen-2-ol (Table 4, 10b)

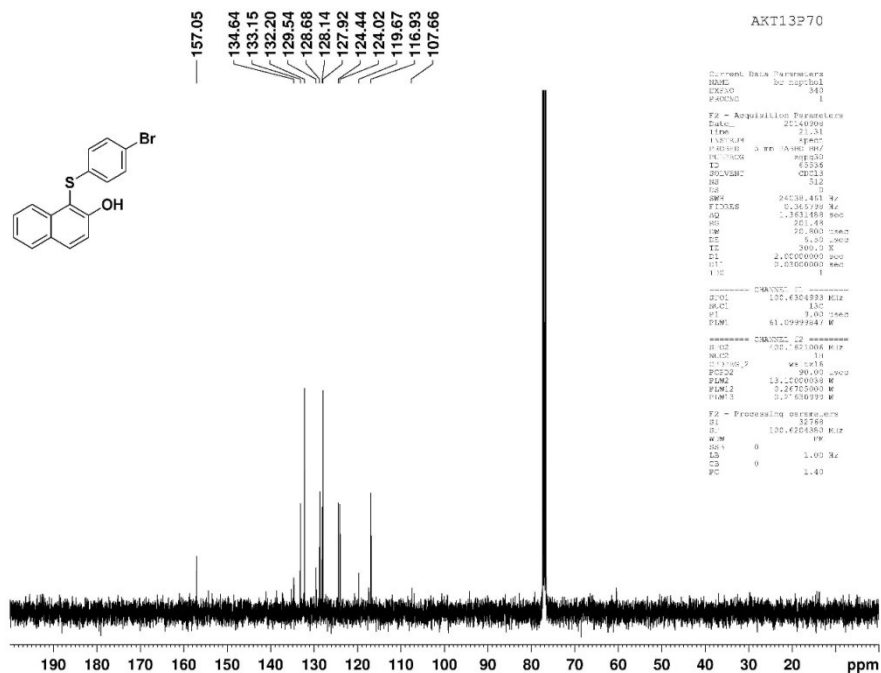




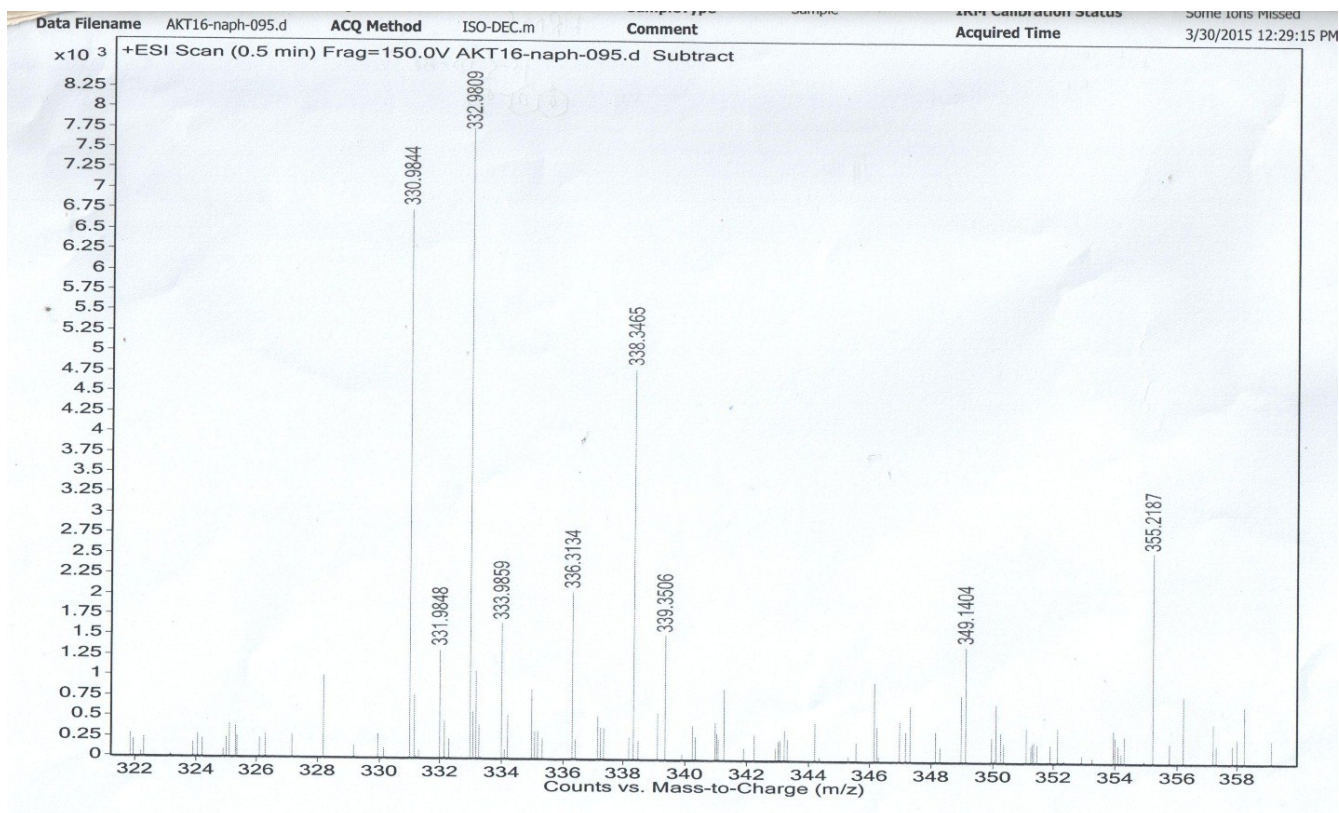
HRMS spectrum of 1-((4-methoxyphenyl)thio)naphthalen-2-ol (Table 4, 10c)



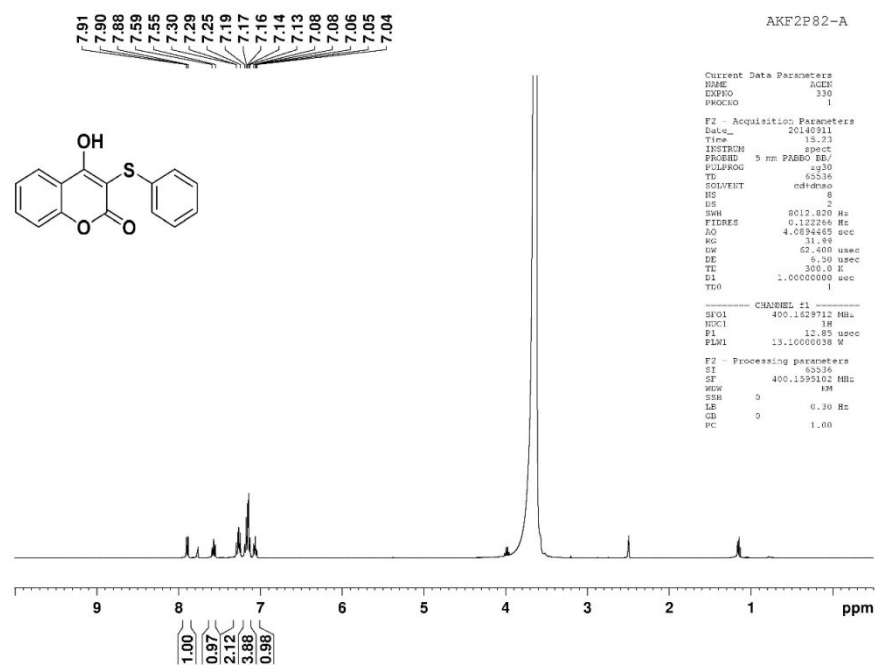
¹H-NMR spectrum of 1-((4-bromophenyl)thio)naphthalen-2-ol) (Table 4, 10d)



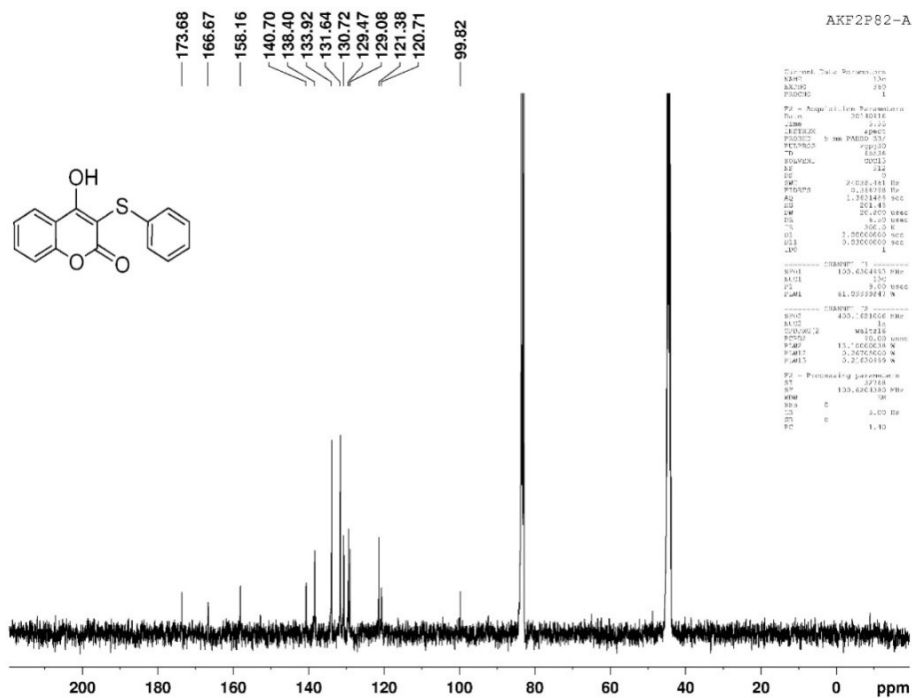
¹³C-NMR spectrum of 1-((4-bromophenyl)thio)naphthalen-2-ol) (Table 4, 10d)



HRMS spectrum of 1-((4-bromophenyl)thio)naphthalen-2-ol) (Table 4, 10d)

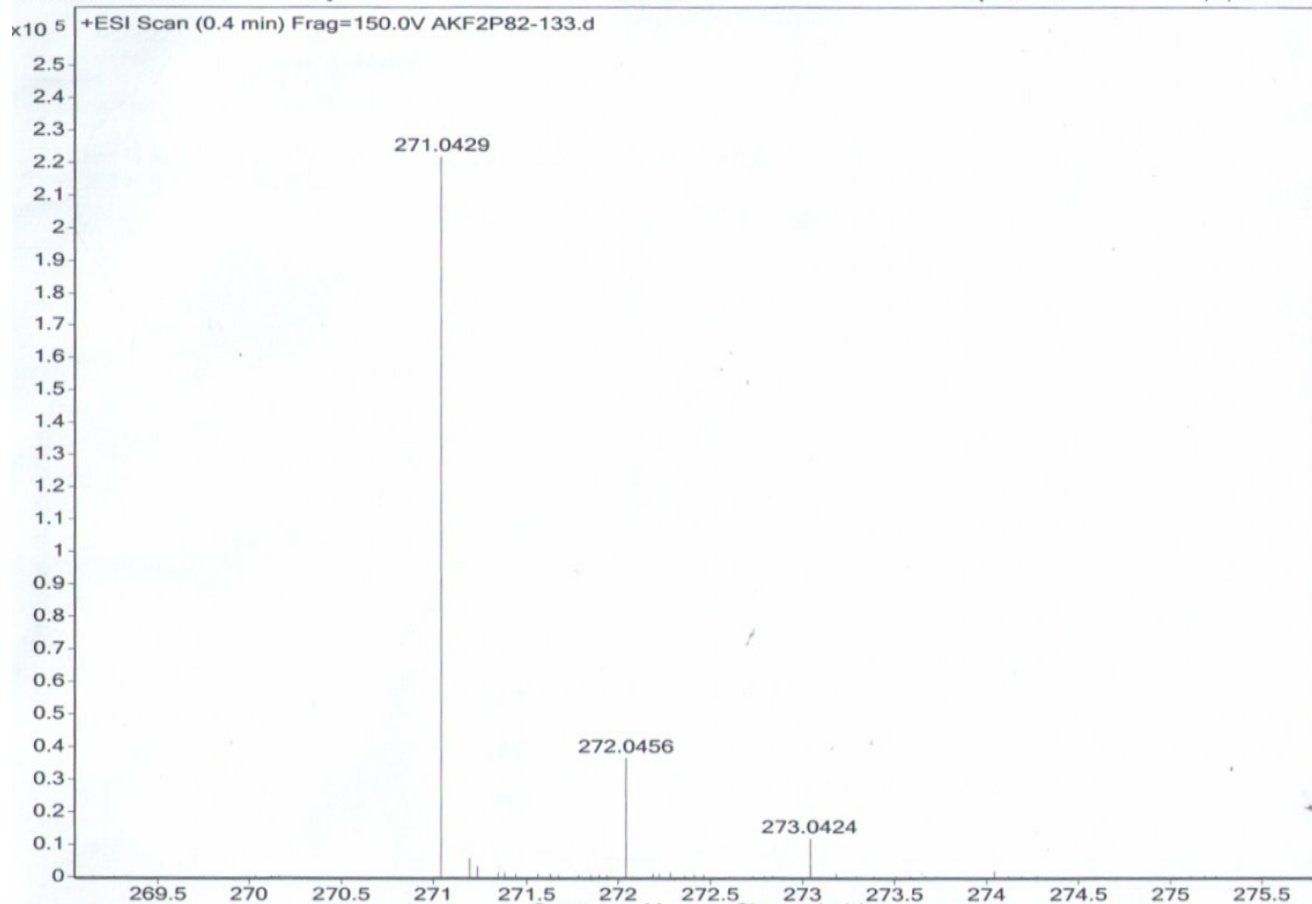


¹H-NMR spectrum of 4-hydroxy-3-(phenylthio)-2H-chromen-2-one (Table 4, 11a)

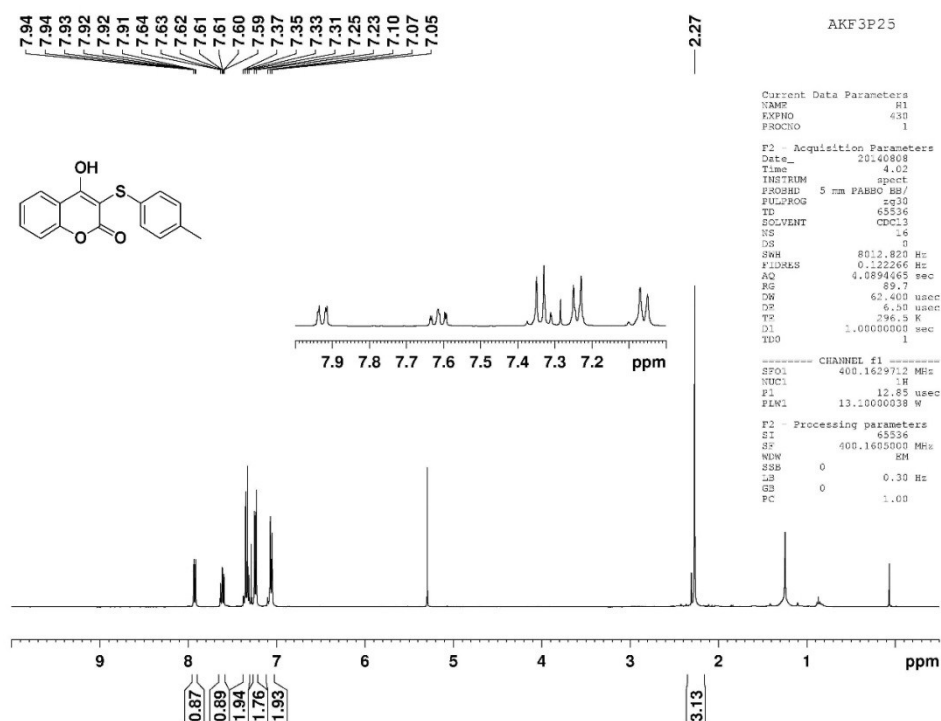


¹³C-NMR spectrum of 4-hydroxy-3-(phenylthio)-2H-chromen-2-one (Table 4, 11a)

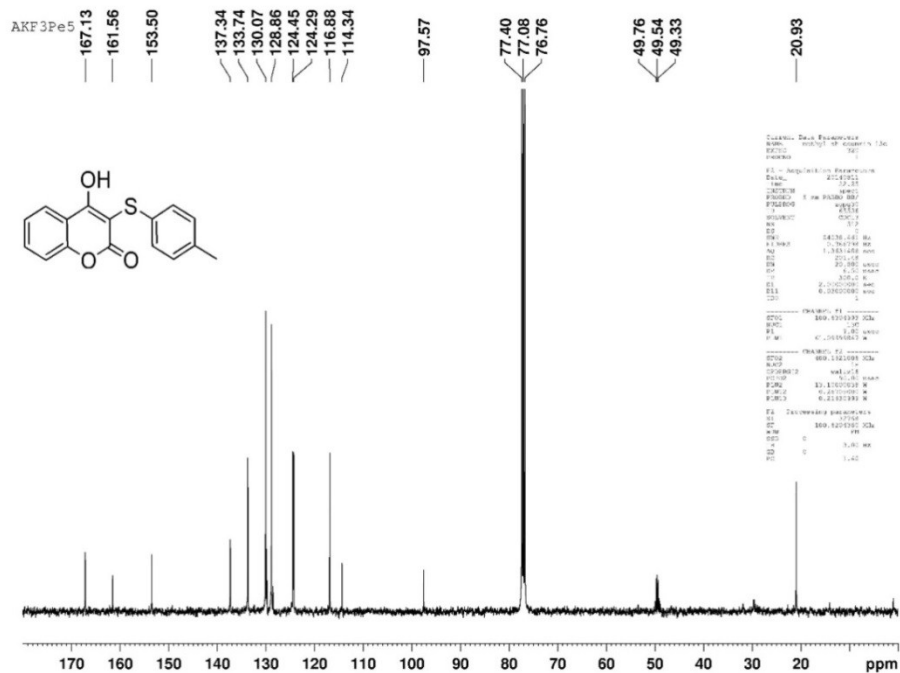
Sample Name	Dr. SINHA	Position	Vial 24	Instrument Name	Instrument 1	User Name	
Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
File Name	AKF2P82-133.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	9/15/2014 2:00:06



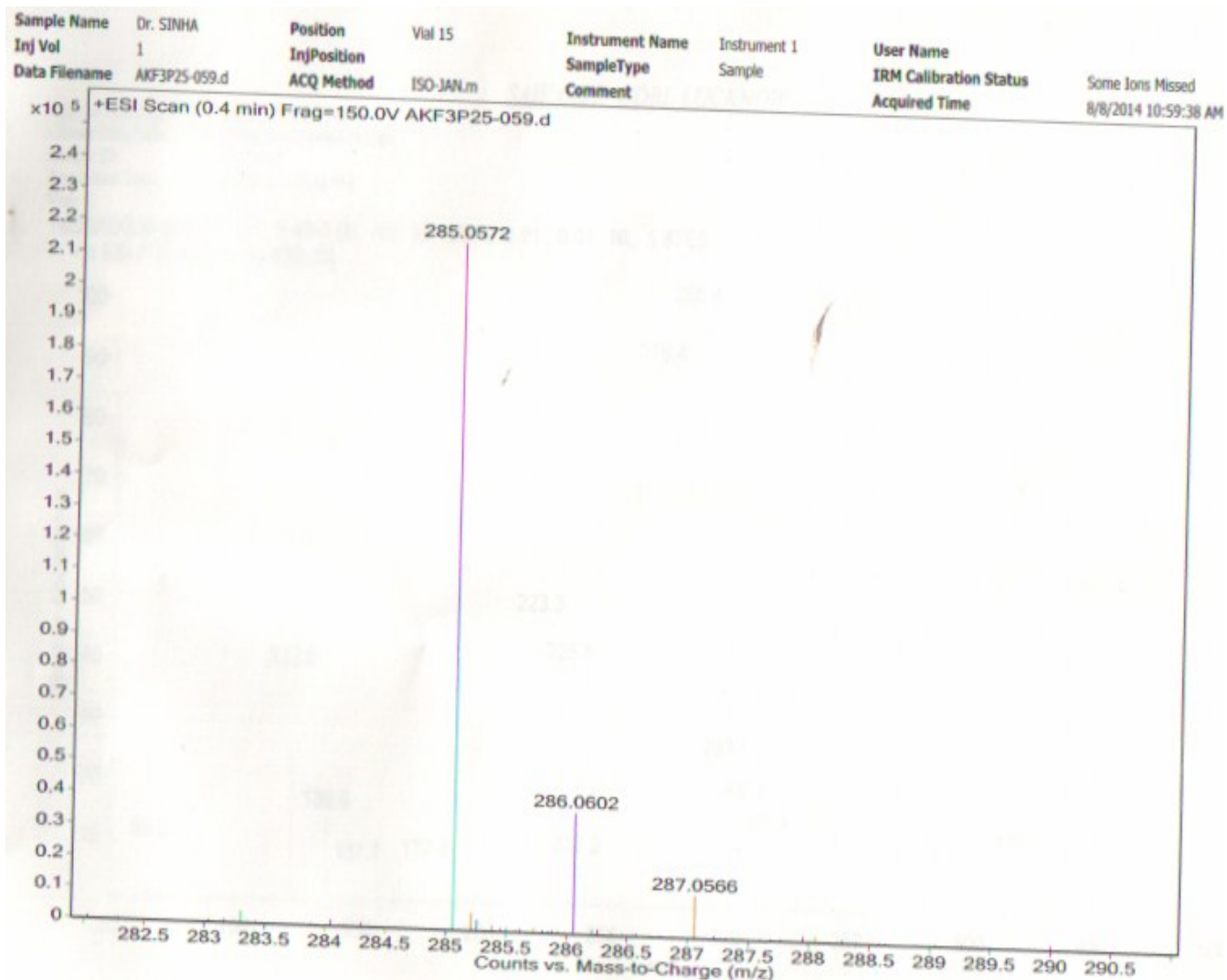
HRMS spectrum of 4-hydroxy-3-(phenylthio)-2H-chromen-2-one (Table 4, 11a)



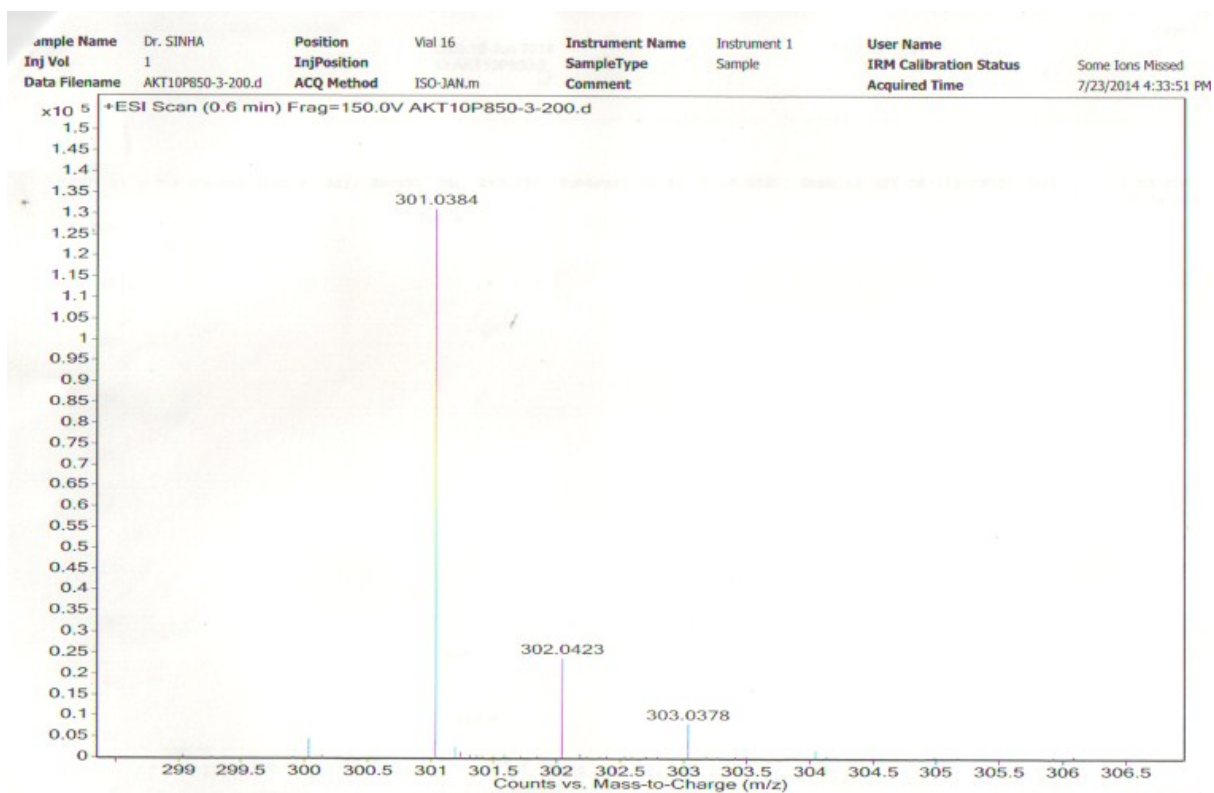
¹H-NMR spectrum of 4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (Table 4, 11b)



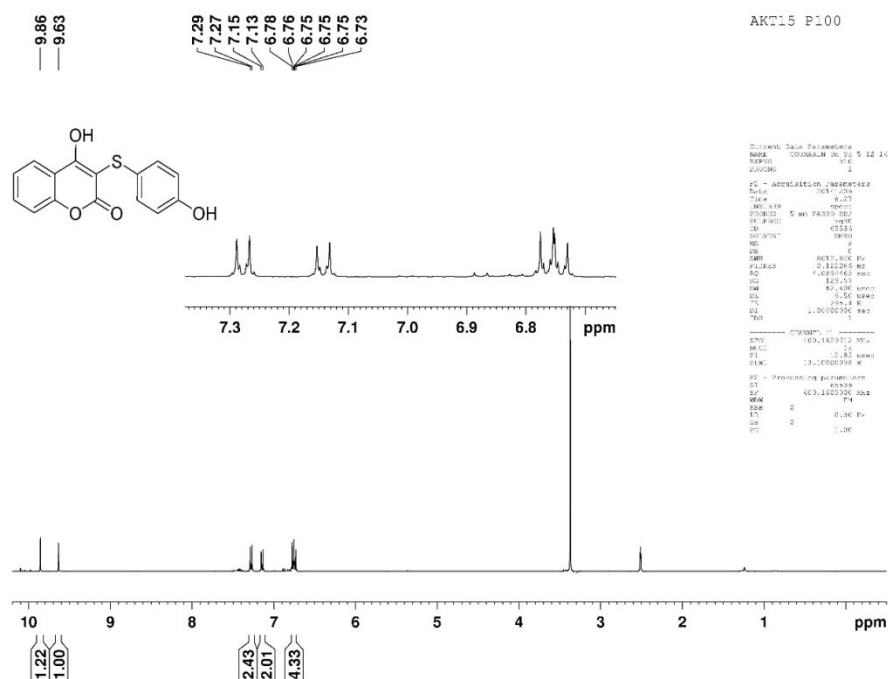
¹³C-NMR spectrum of 4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (Table 4, 11b)



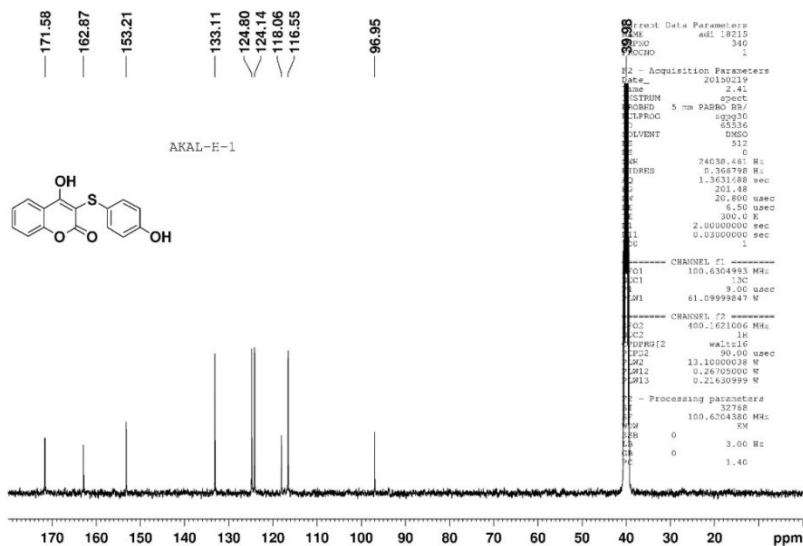
HRMS spectrum of 4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (Table 4, 11b)



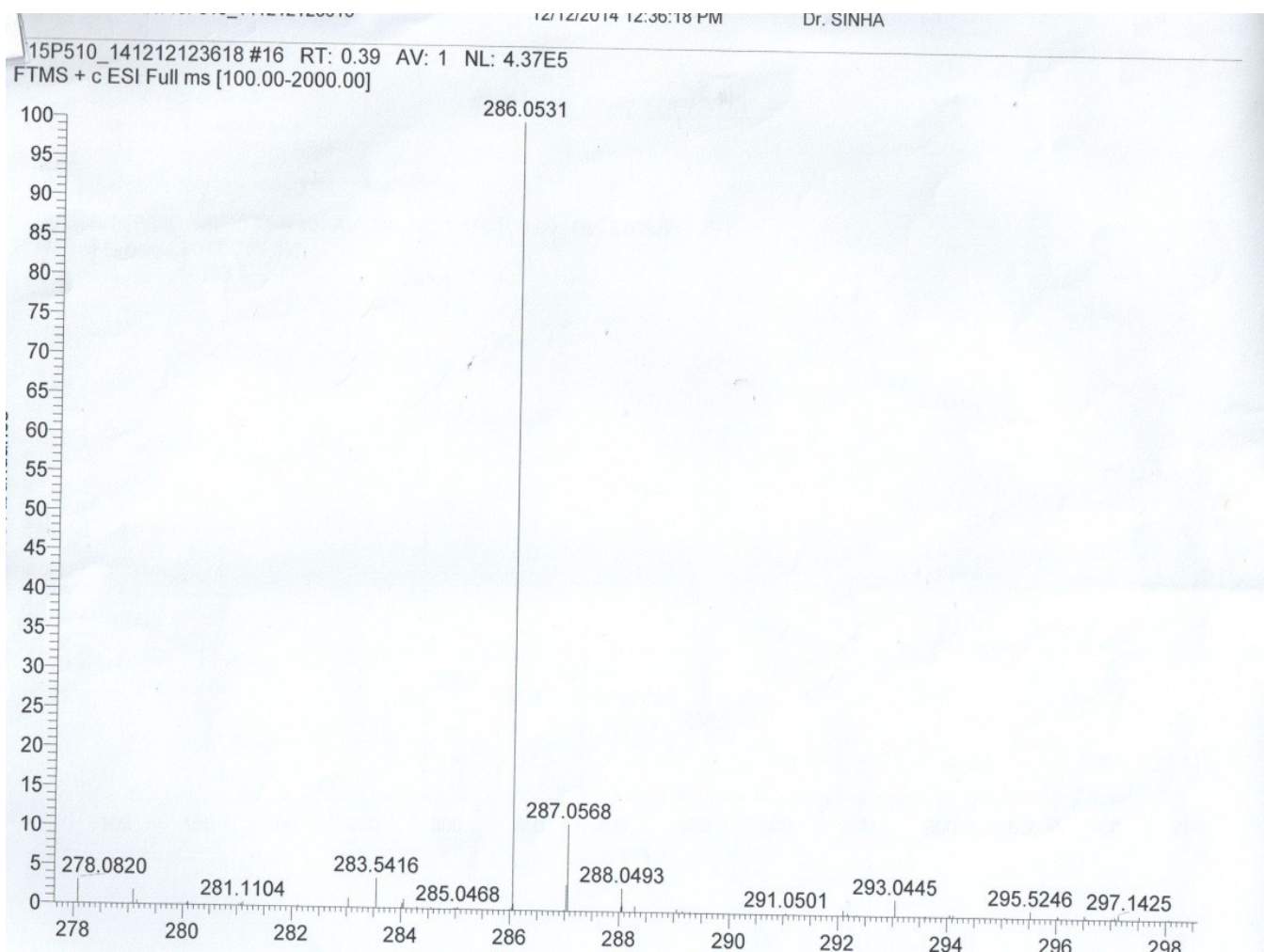
**HRMS spectrum of 4-hydroxy-3-((4-methoxyphenyl)thio)-2H-chromen-2-one
(Table 4, 11c)**



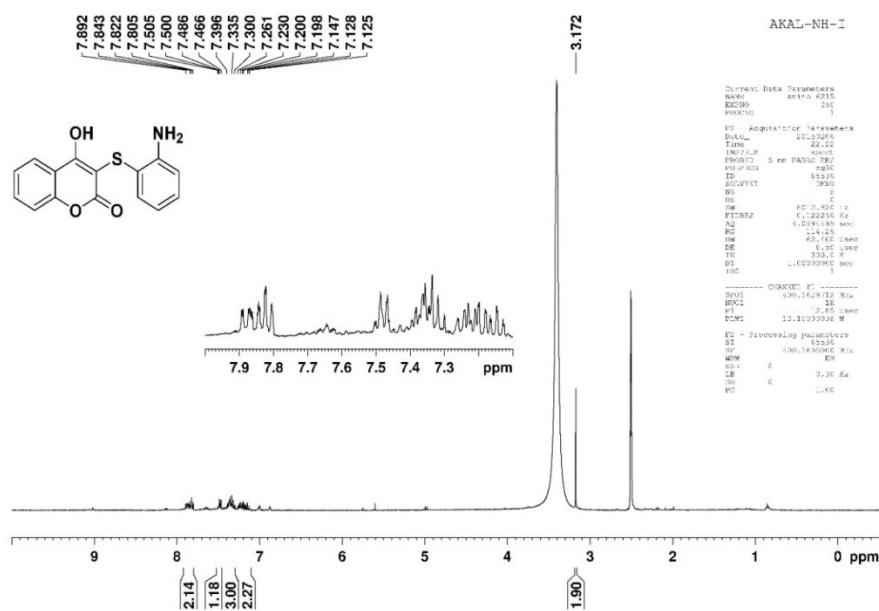
¹H-NMR spectrum of 4-hydroxy-3-((4-hydroxyphenyl)thio)-2H-chromen-2-one (Table 4, 11d)



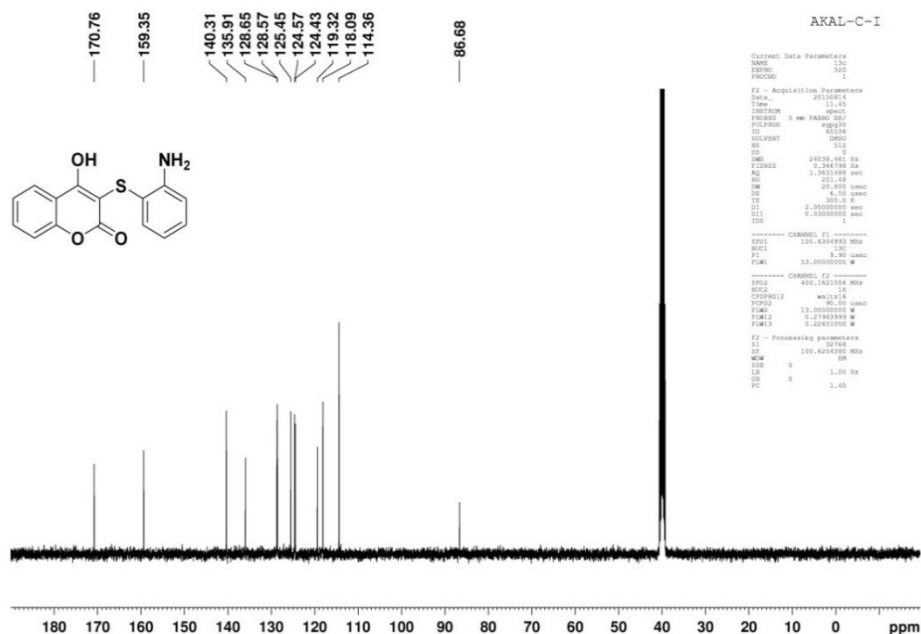
¹³C-NMR spectrum of 4-hydroxy-3-((4-hydroxyphenyl)thio)-2H-chromen-2-one (Table 4, 11d)



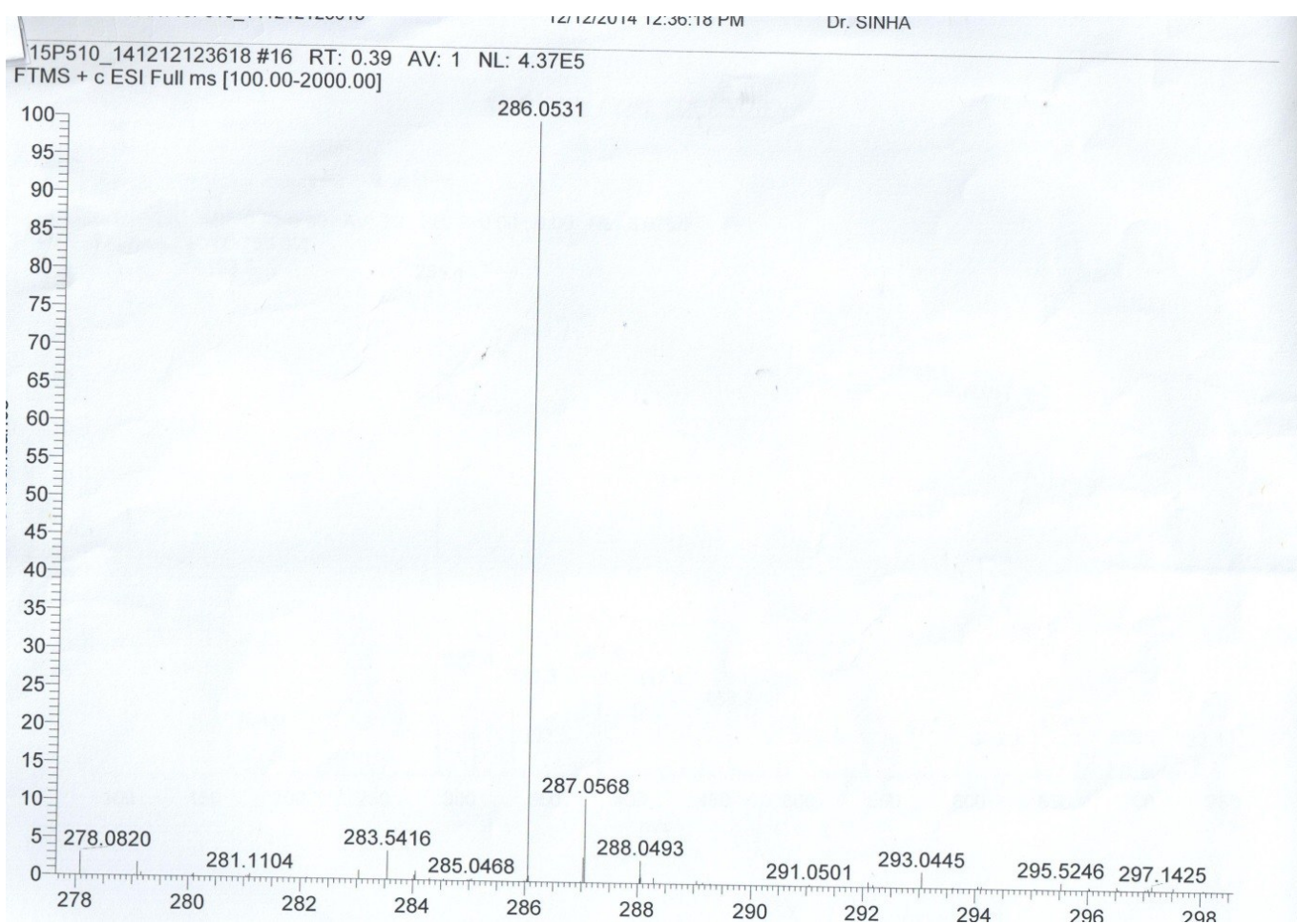
HRMS spectrum of 4-hydroxy-3-((4-hydroxyphenyl)thio)-2H-chromen-2-one (Table 4, 11d)



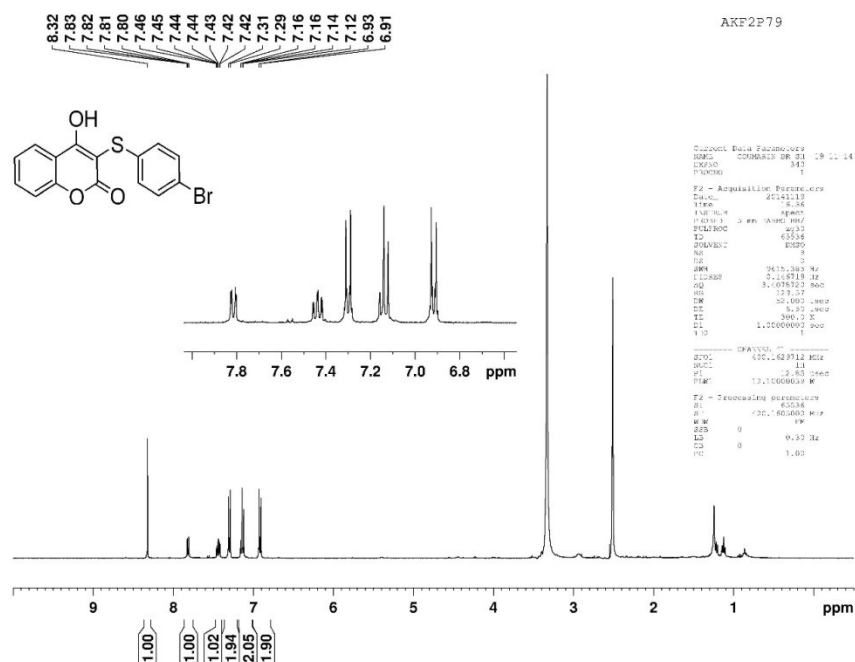
¹H-NMR spectrum of 3-((2-aminophenyl)thio)-4-hydroxy-2H-chromen-2-one (Table 4, 11e)



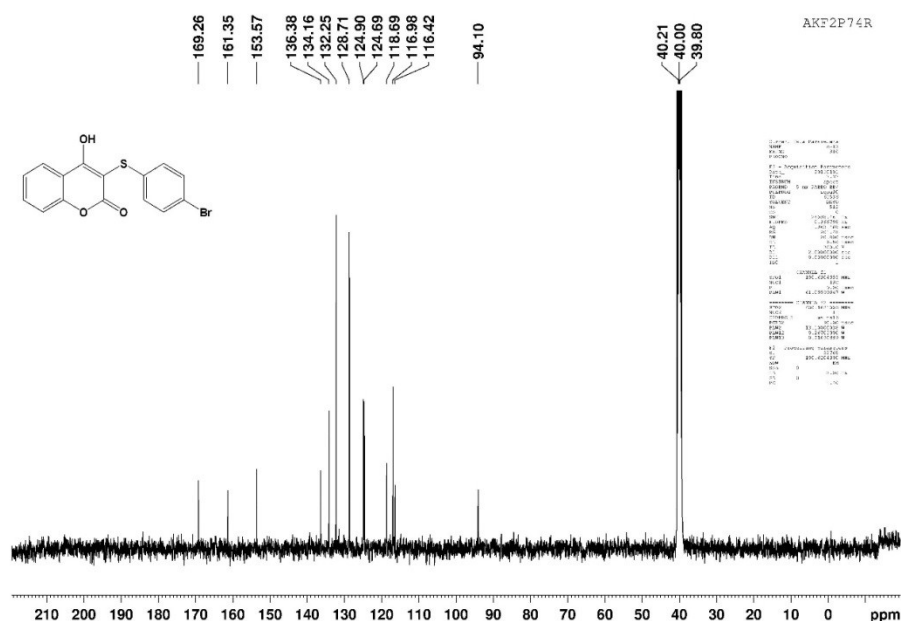
¹³C-NMR spectrum of 3-((2-aminophenyl)thio)-4-hydroxy-2H-chromen-2-one (Table 4, 11e)



HRMS spectrum of 3-((2-aminophenyl)thio)-4-hydroxy-2H-chromen-2-one (Table 4, 11e)

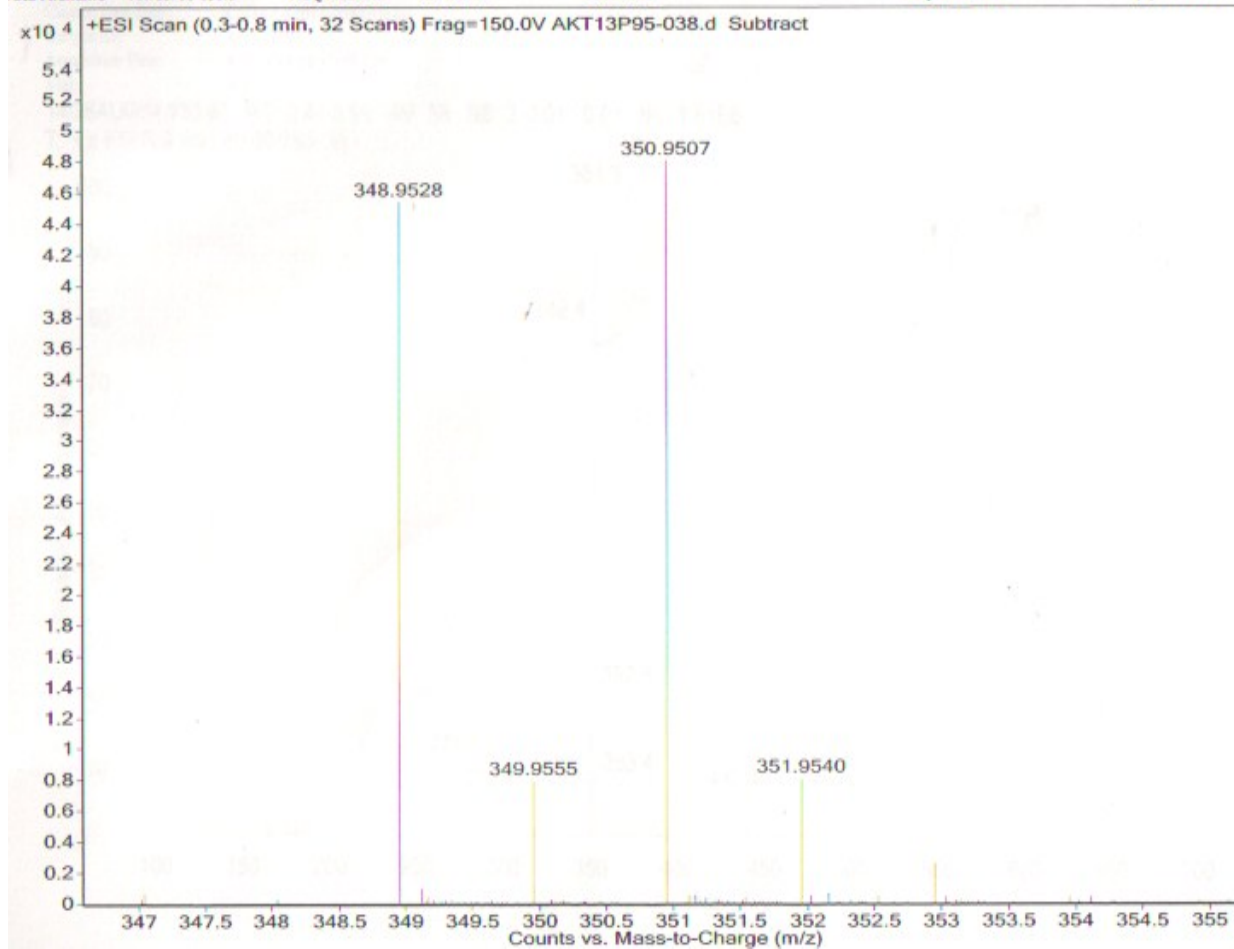


¹H-NMR spectrum of 3-((4-bromophenyl)thio)-4-hydroxy-2H-chromen-2-one (Table 4, 11f)

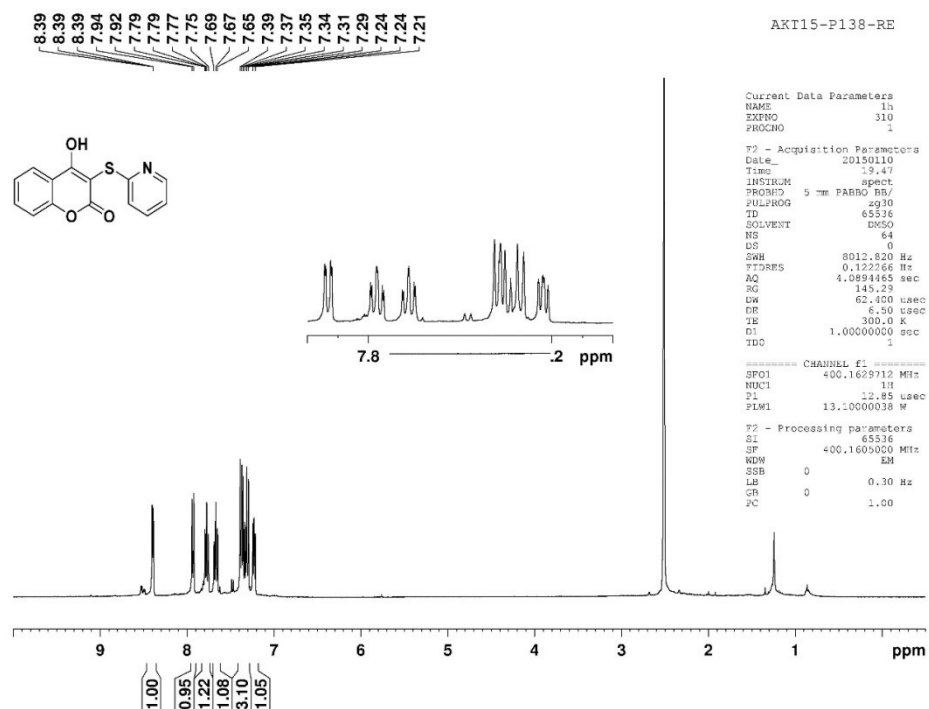


¹³C-NMR spectrum of 3-((4-bromophenyl)thio)-4-hydroxy-2H-chromen-2-one (Table 4, 11f)

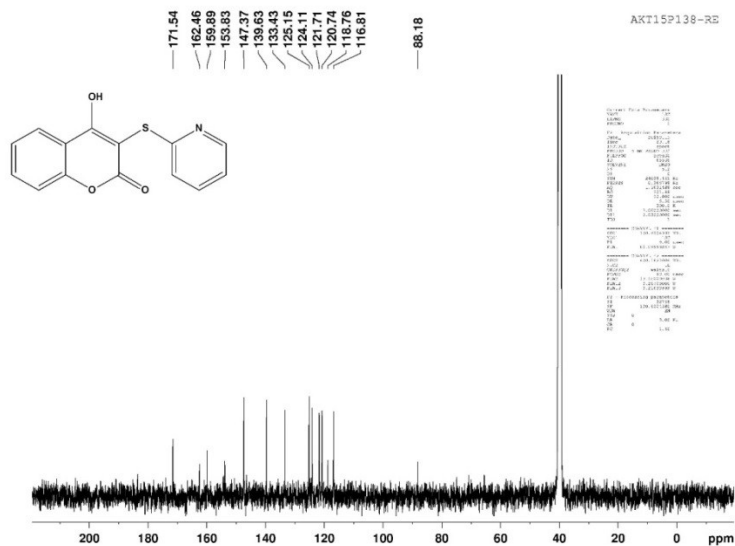
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Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	AKT13P95-038.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	9/8/2014 12:11:52



HRMS spectrum of 3-((4-bromophenyl)thio)-4-hydroxy-2H-chromen-2-one (Table 4, 11f)

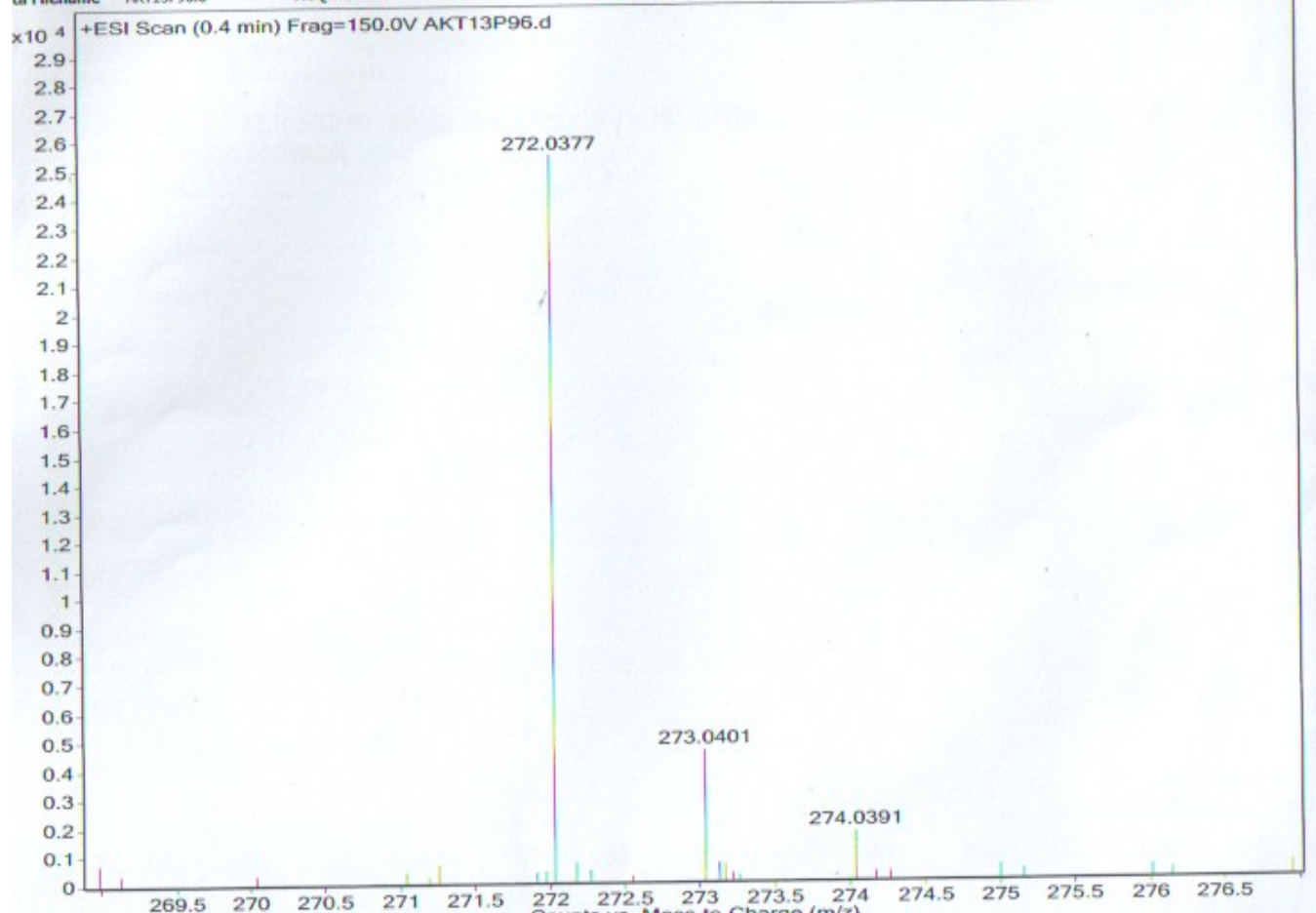


¹H-NMR spectrum of 4-hydroxy-3-(pyridin-2-ylthio)-2H-chromen-2-one (Table 4, 11g)

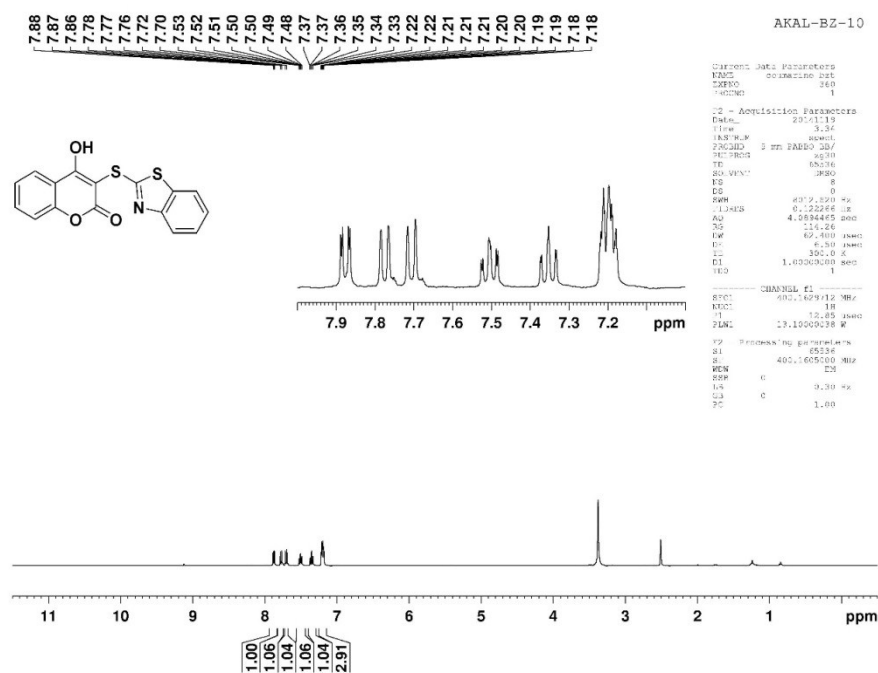


¹³C-NMR spectrum of 4-hydroxy-3-(pyridin-2-ylthio)-2H-chromen-2-one (Table 4, 11g)

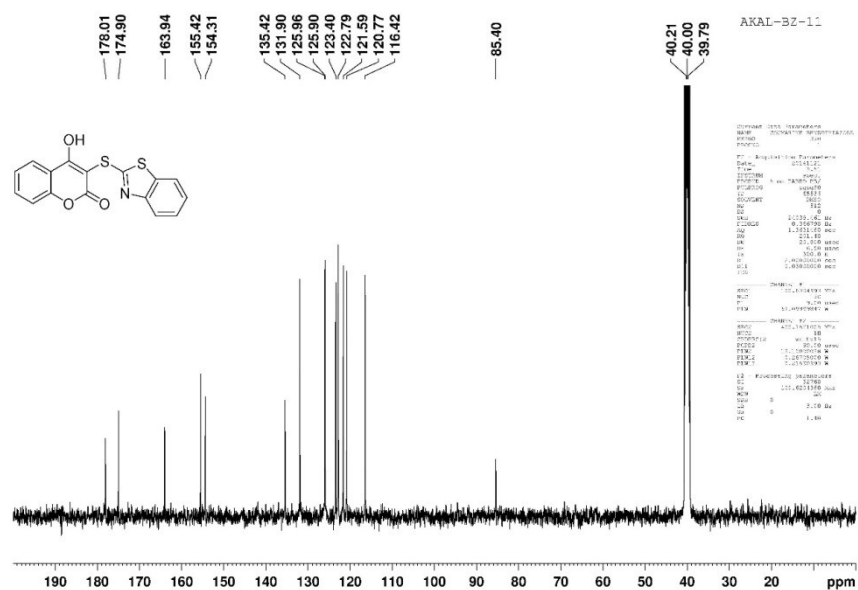
Sample Name	Dr. A. K. SINHA	Position	Vial 86	Instrument Name	Instrument 1	User Name	
Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
File Name	AKT13P96.d	ACQ Method	ISO-JAN.m	Comment		Acquired Time	10/1/2014 10:58:28 AM



HRMS spectrum of 4-hydroxy-3-(pyridin-2-ylthio)-2H-chromen-2-one (Table 4, 11g)

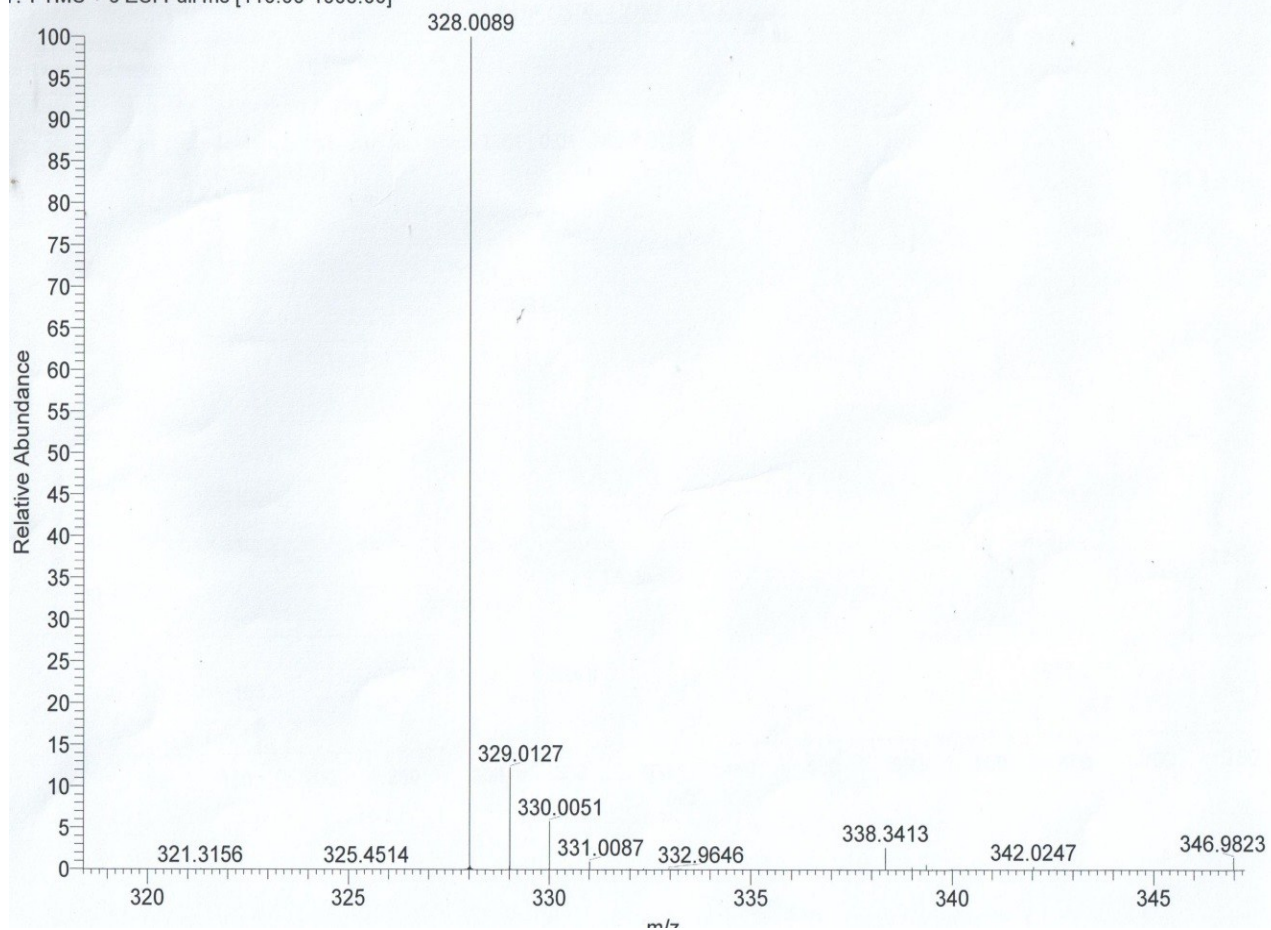


¹H-NMR spectrum of 3-(benzo[d]thiazol-2-ylthio)-4-hydroxy-2H-chromen-2-one (Table 4, 11h)



¹³C-NMR spectrum of 3-(benzo[d]thiazol-2-ylthio)-4-hydroxy-2H-chromen-2-one (Table 4, 11h)

AKT15P100_141113115412 #18 RT: 0.42 AV: 1 NL: 2.36E6
F: FTMS + c ESI Full ms [110.00-1000.00]



**HRMS spectrum of 3-(benzo[d]thiazol-2-ylthio)-4-hydroxy-2H-chromen-2-one
(Table 4, 11h)**
