Novel tetracyclic azaphenothiazines with the quinoline ring as new anticancer and antibacterial derivatives of chlorpromazine.

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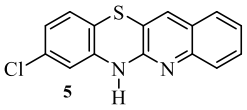
Content:

1. NMR spectra and HR MS of 6*H*-8-chloroquinobenzothiazine (**5**).



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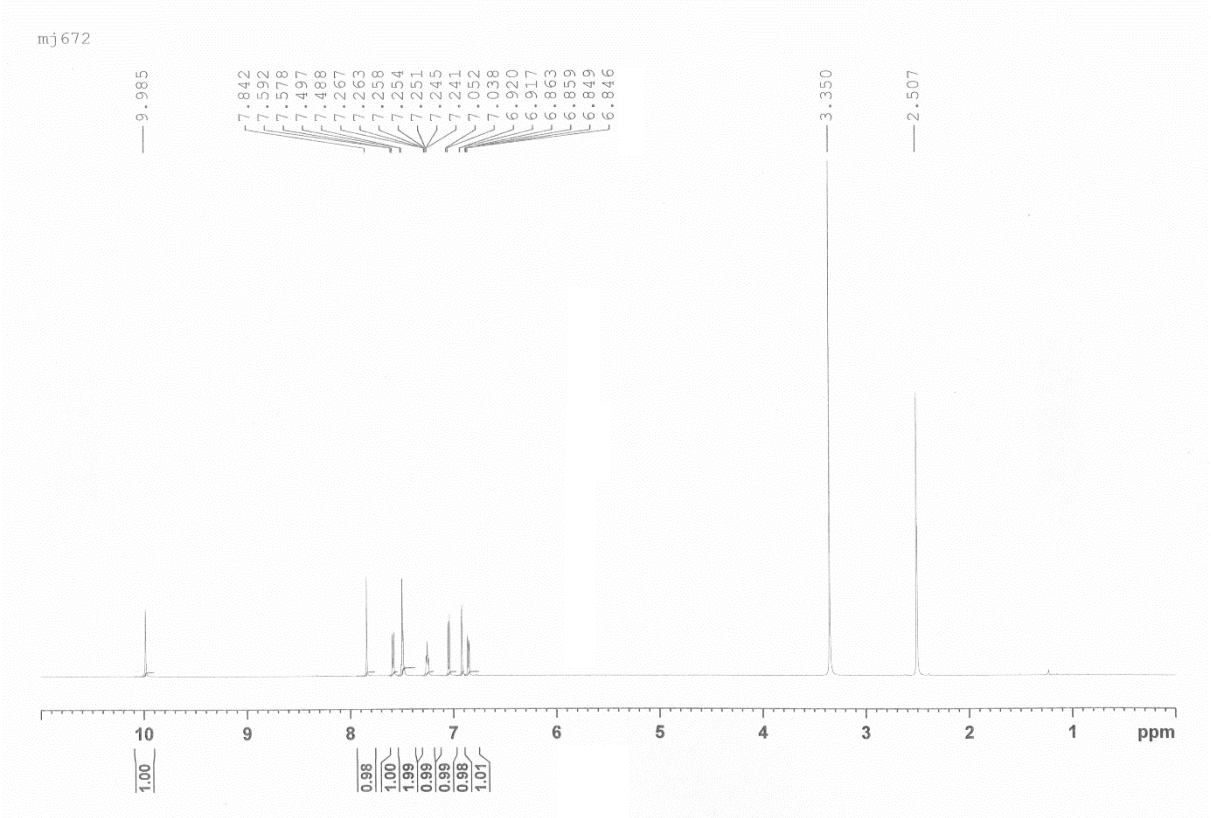

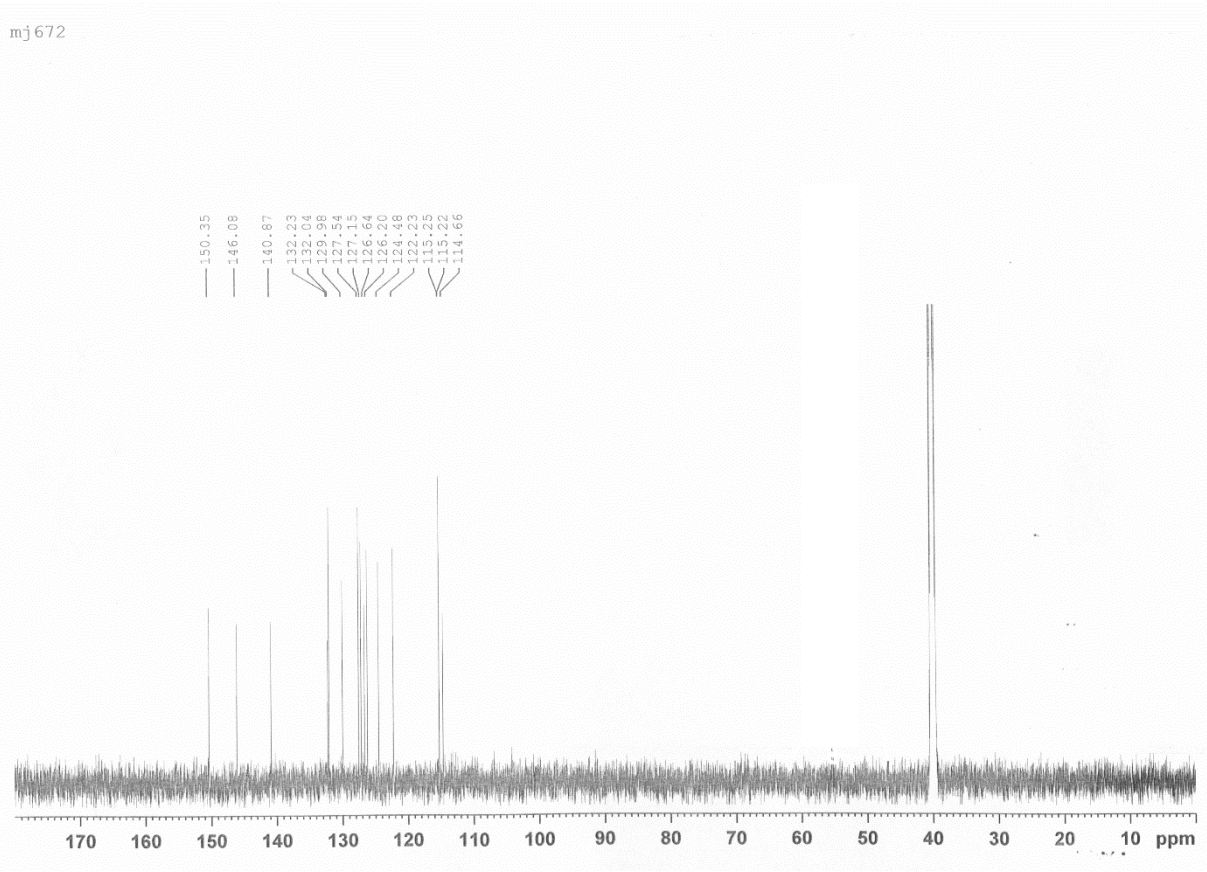

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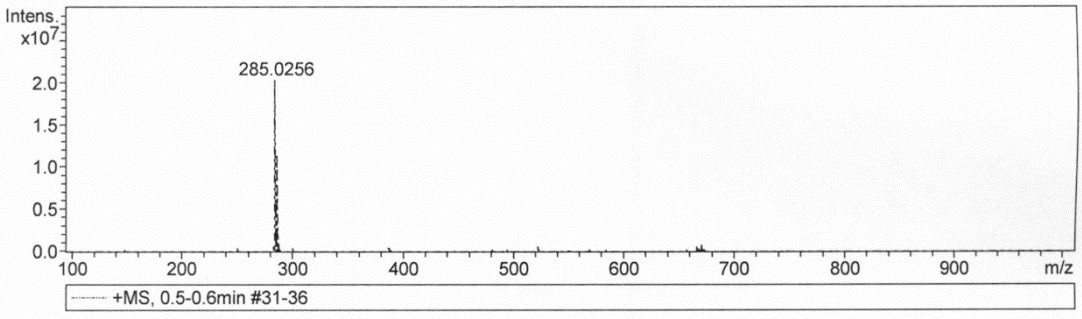

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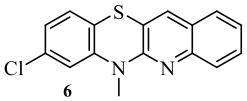
1	285.0256	17668	56320.7	20377480	100.0	0.0161
2	287.0218	37360	31654.5	11533646	56.6	0.0077

2. NMR spectra and HR MS of 8-chloro-6-methylquinobenzothiazine (**6**).



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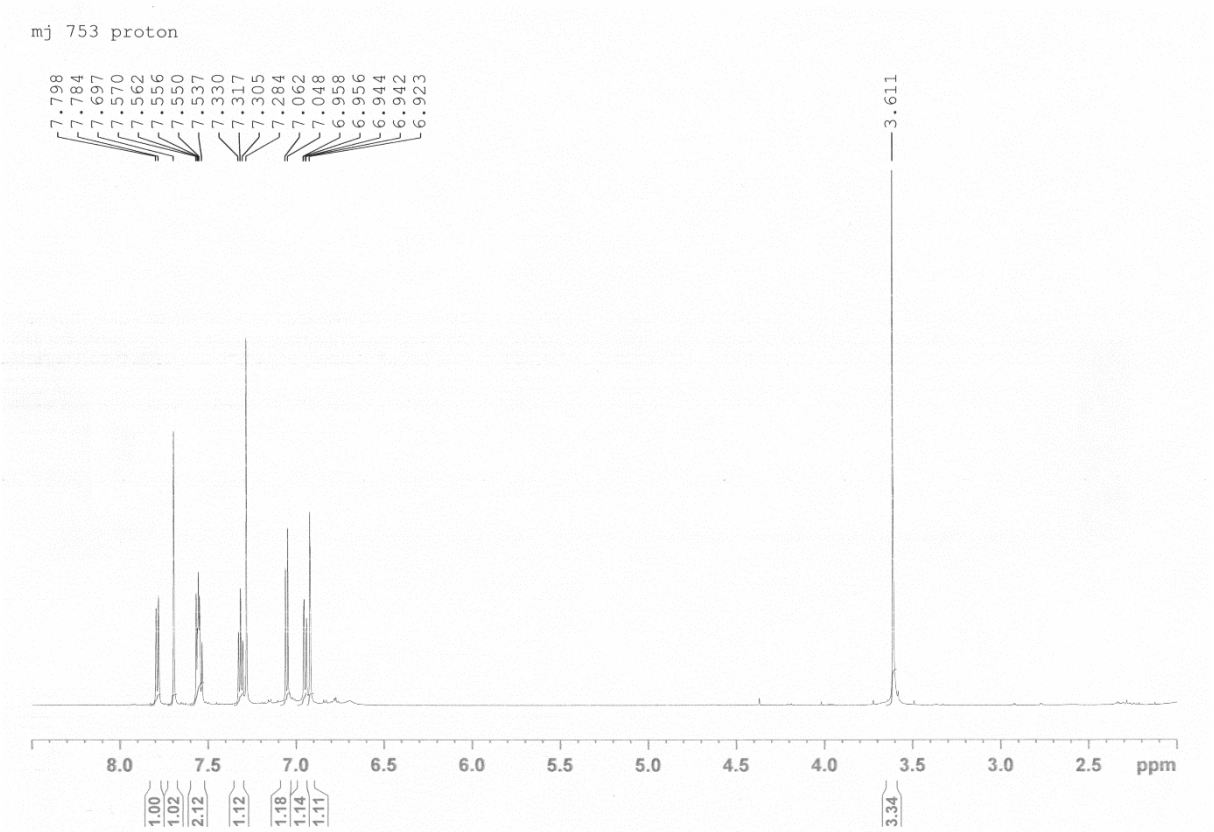
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6.942
6.923
3.611
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5.5
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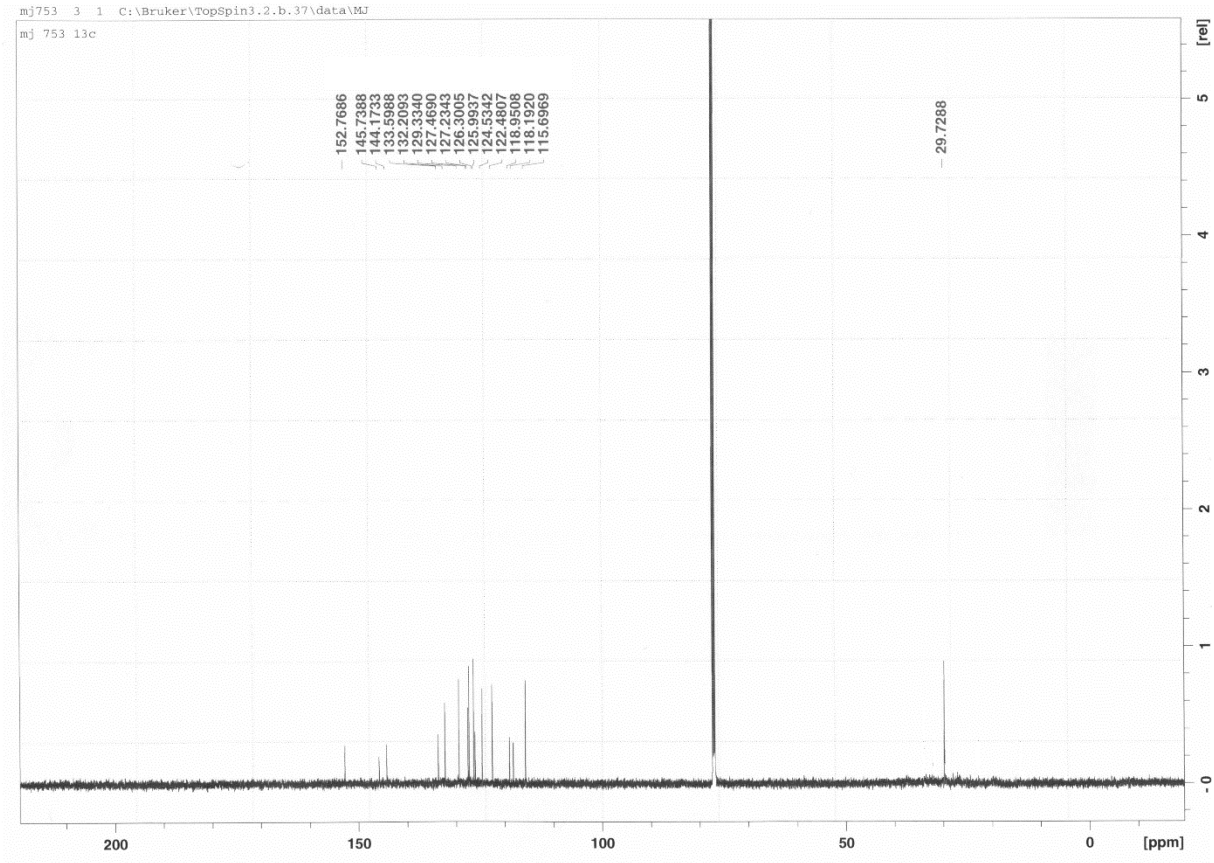
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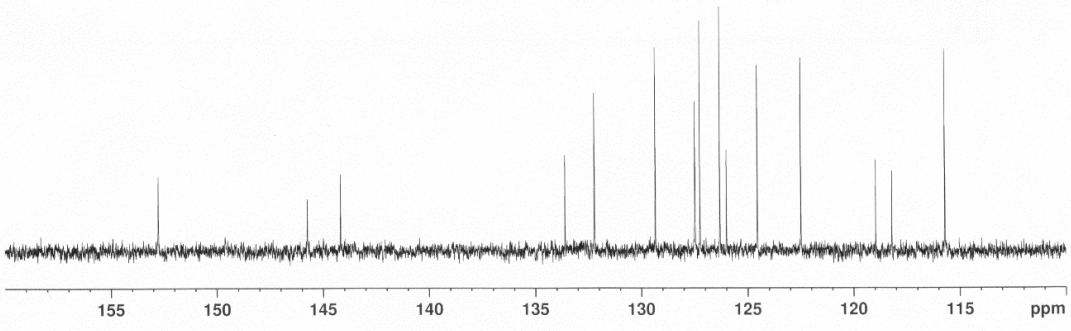

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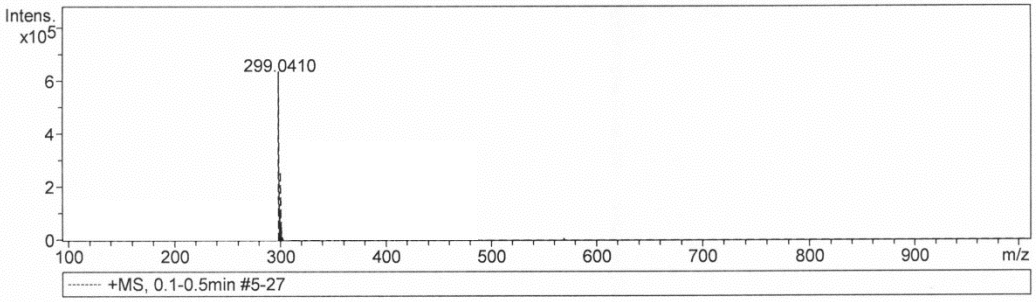

#	m/z	Res.	S/N	I	I %	FWHM
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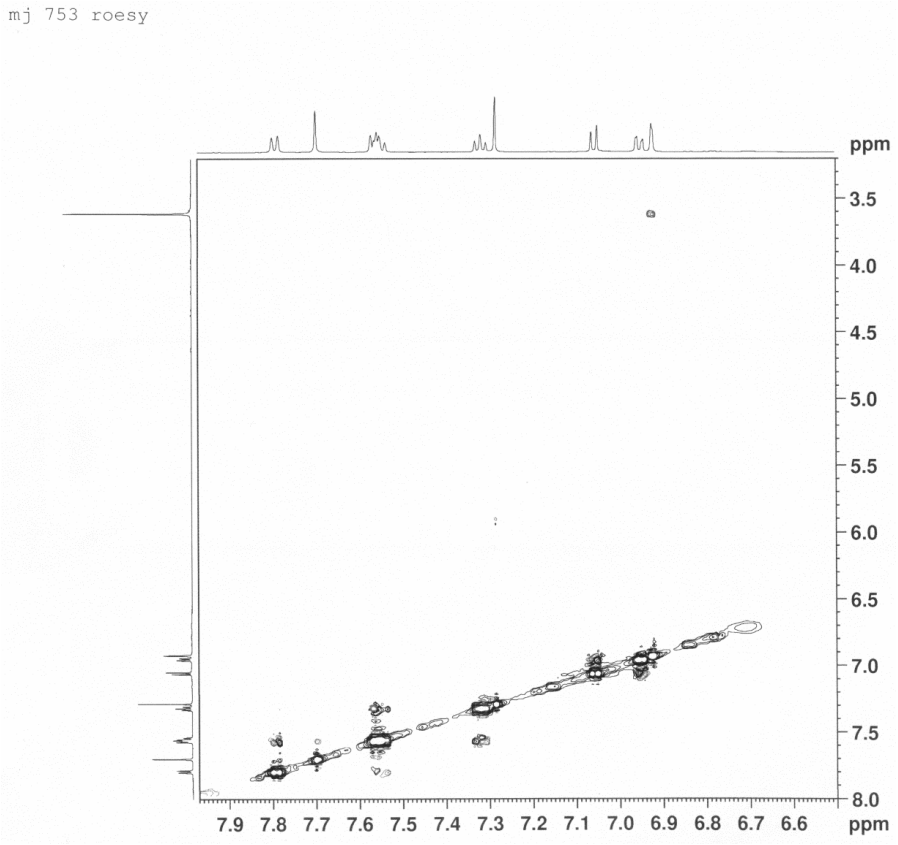
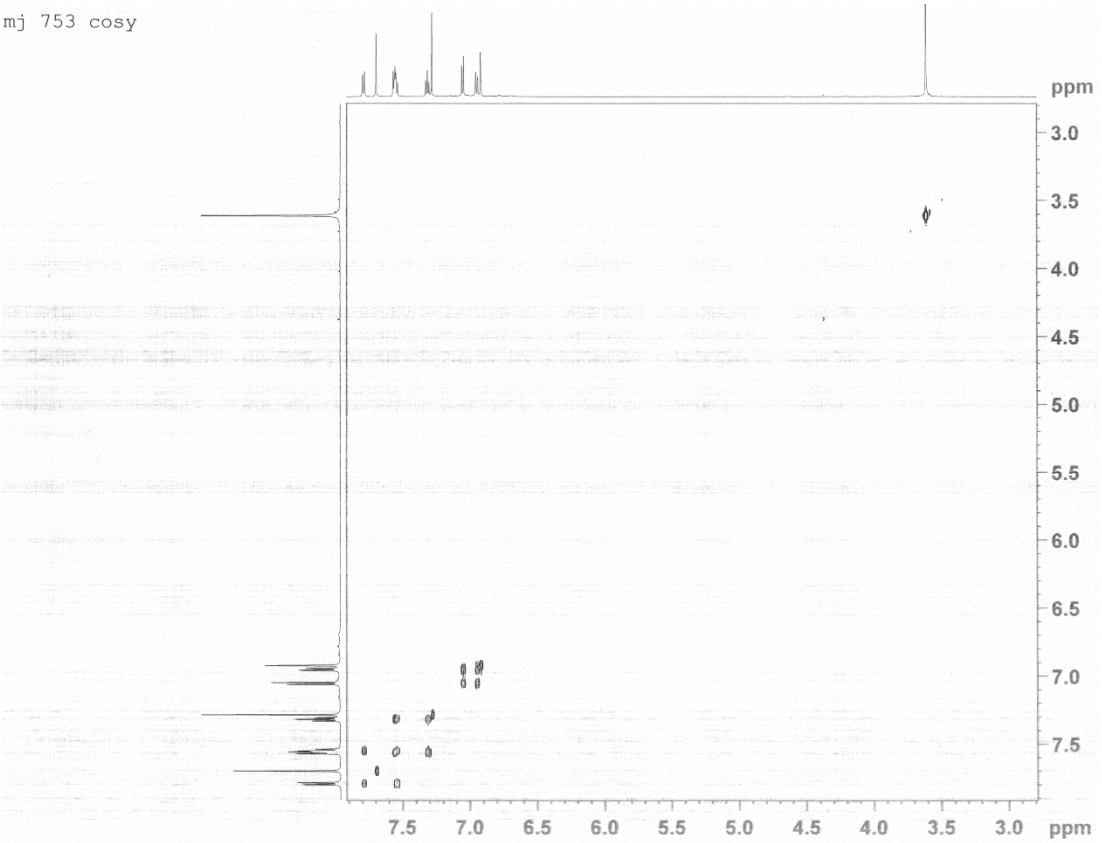
mj 753 roesy



mj 753 cosy



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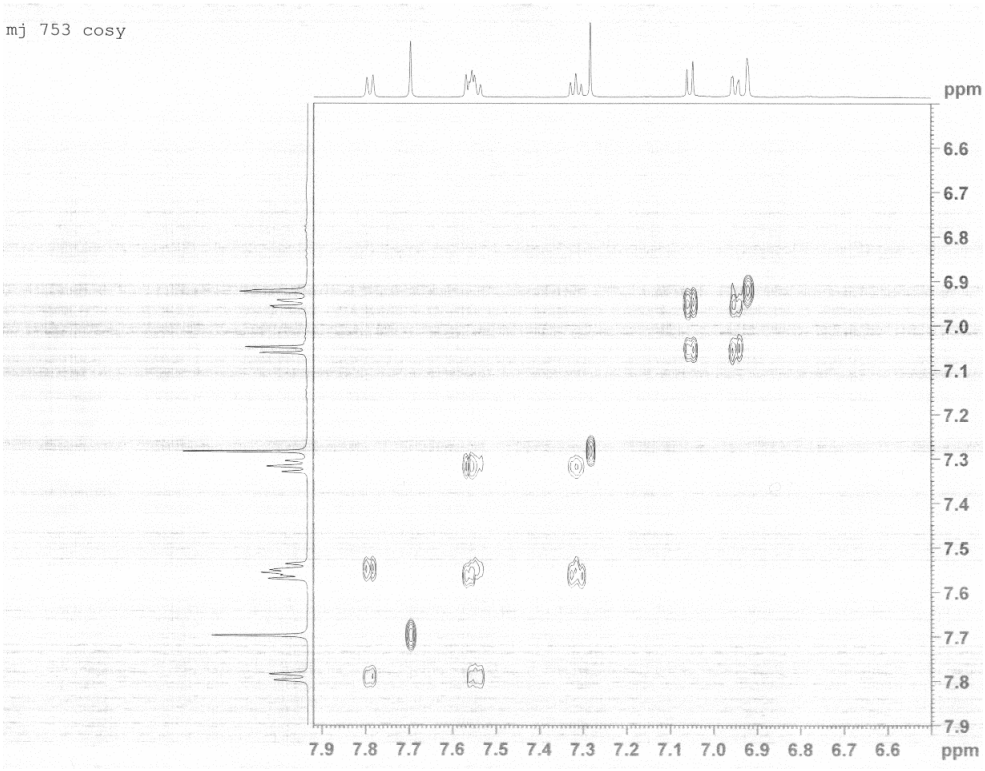

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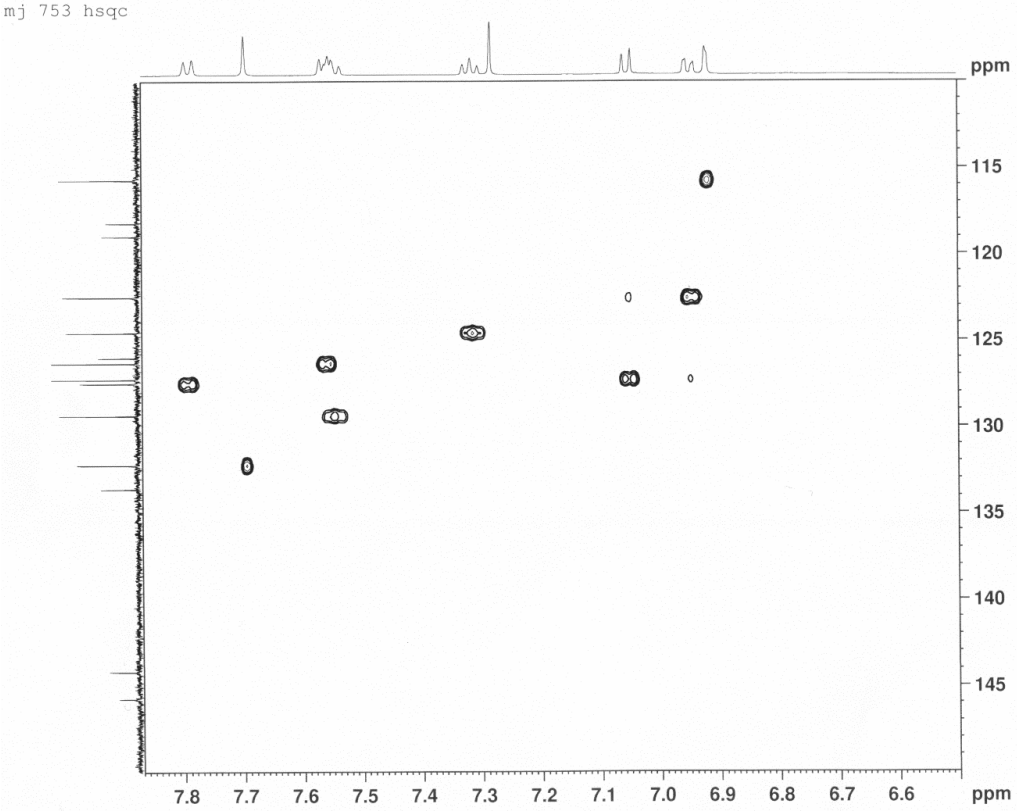
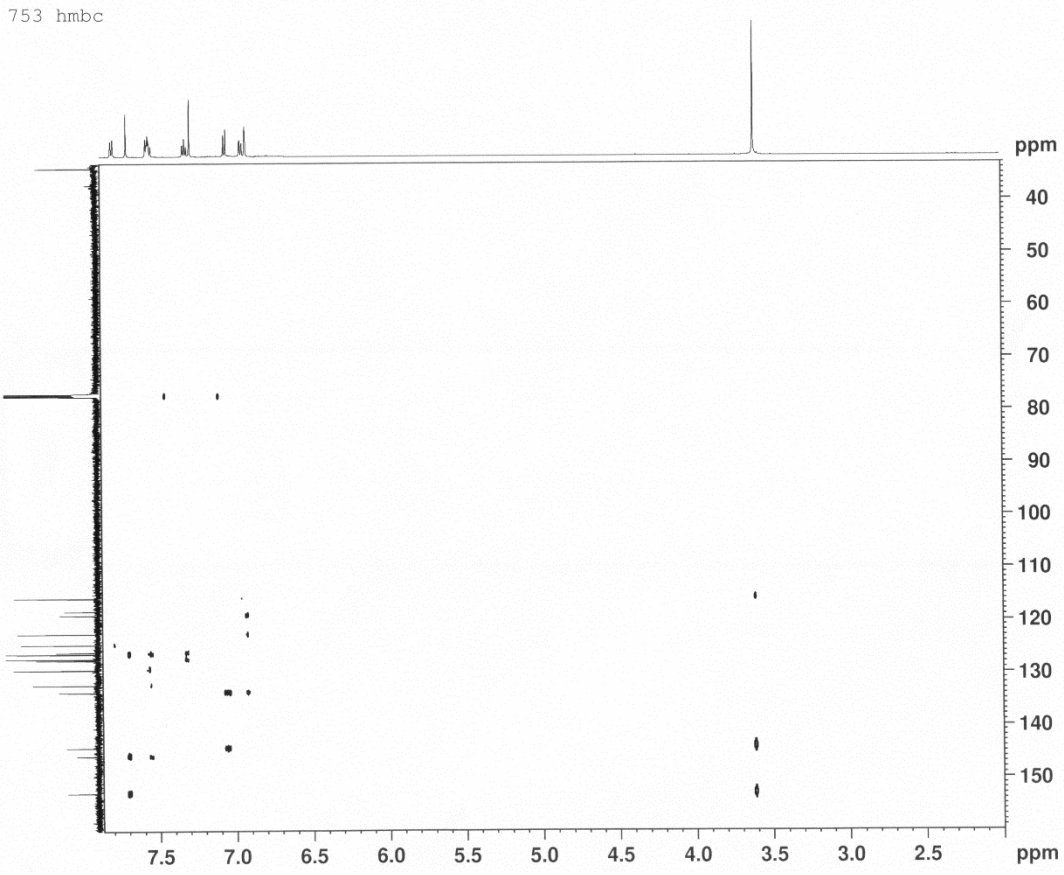


753 hmbc



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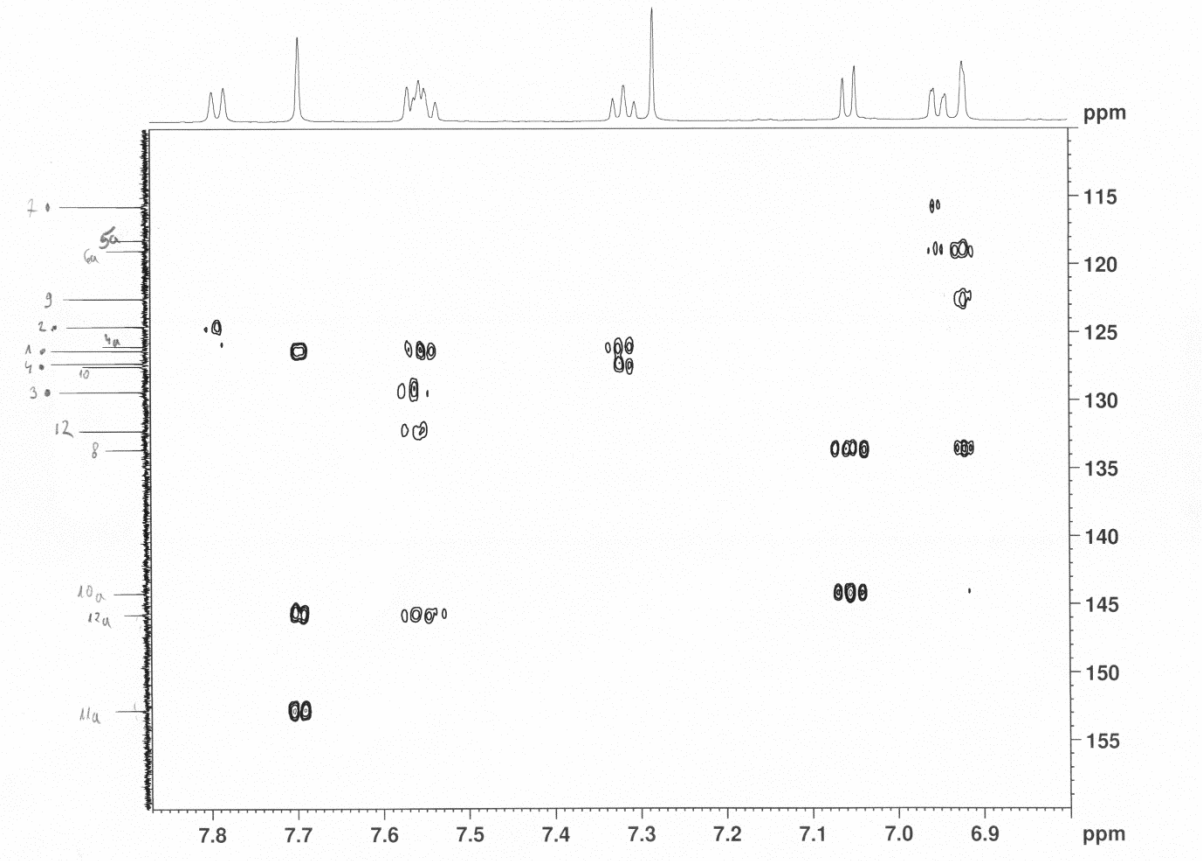
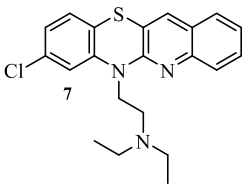


3. NMR spectra and HR MS of 6-(2-diethylaminoethyl)-8-chloroquinobenzothiazine (**7**)



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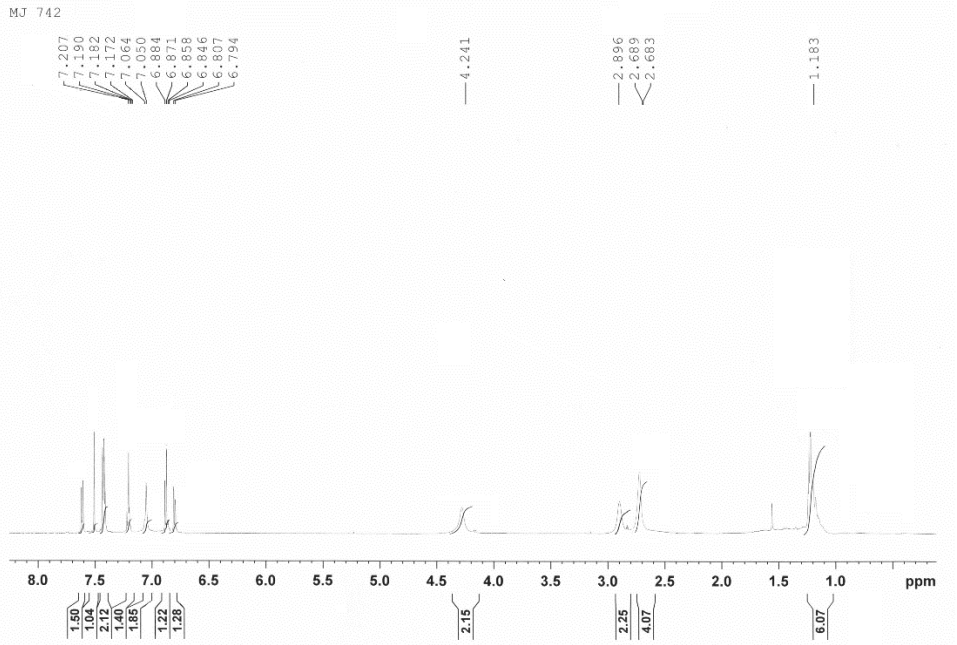

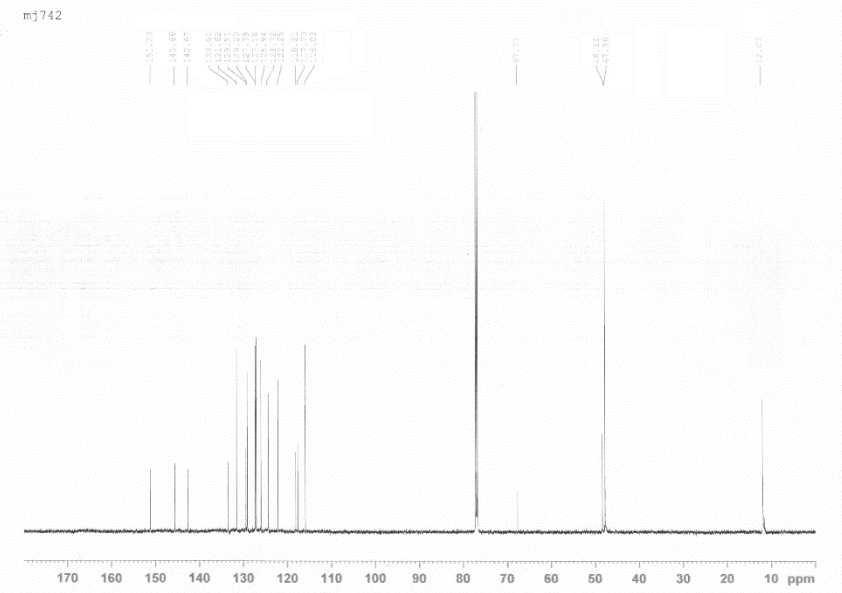

Acquisition Parameter

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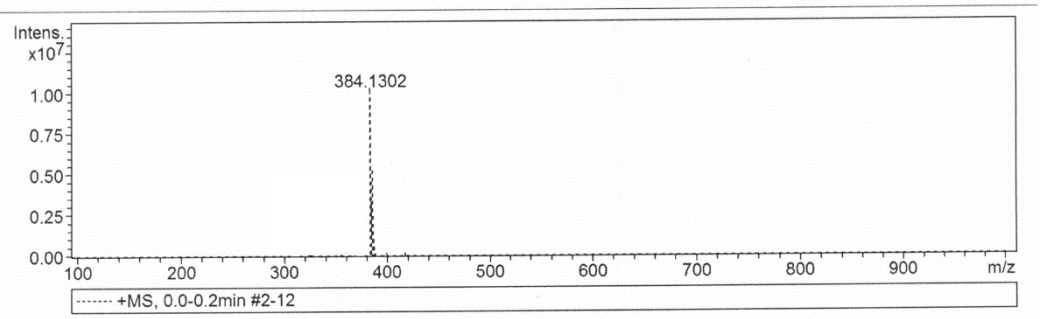
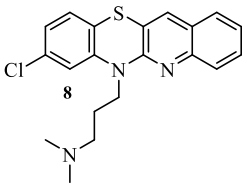
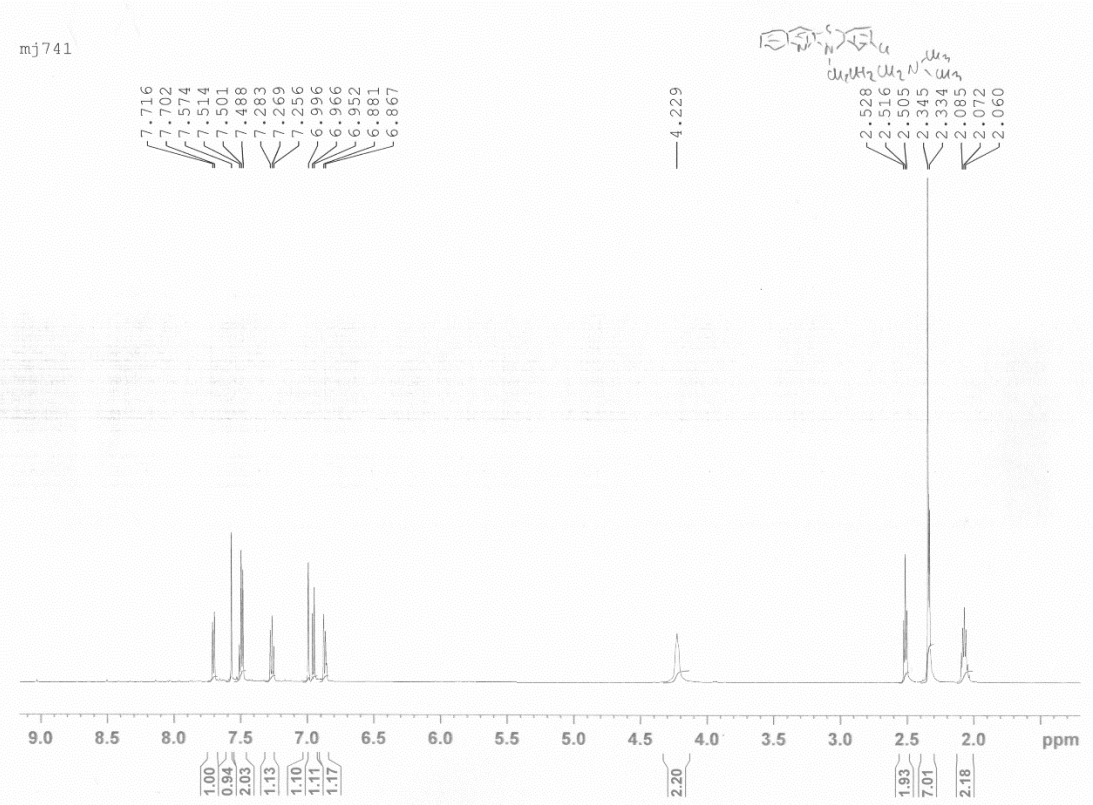
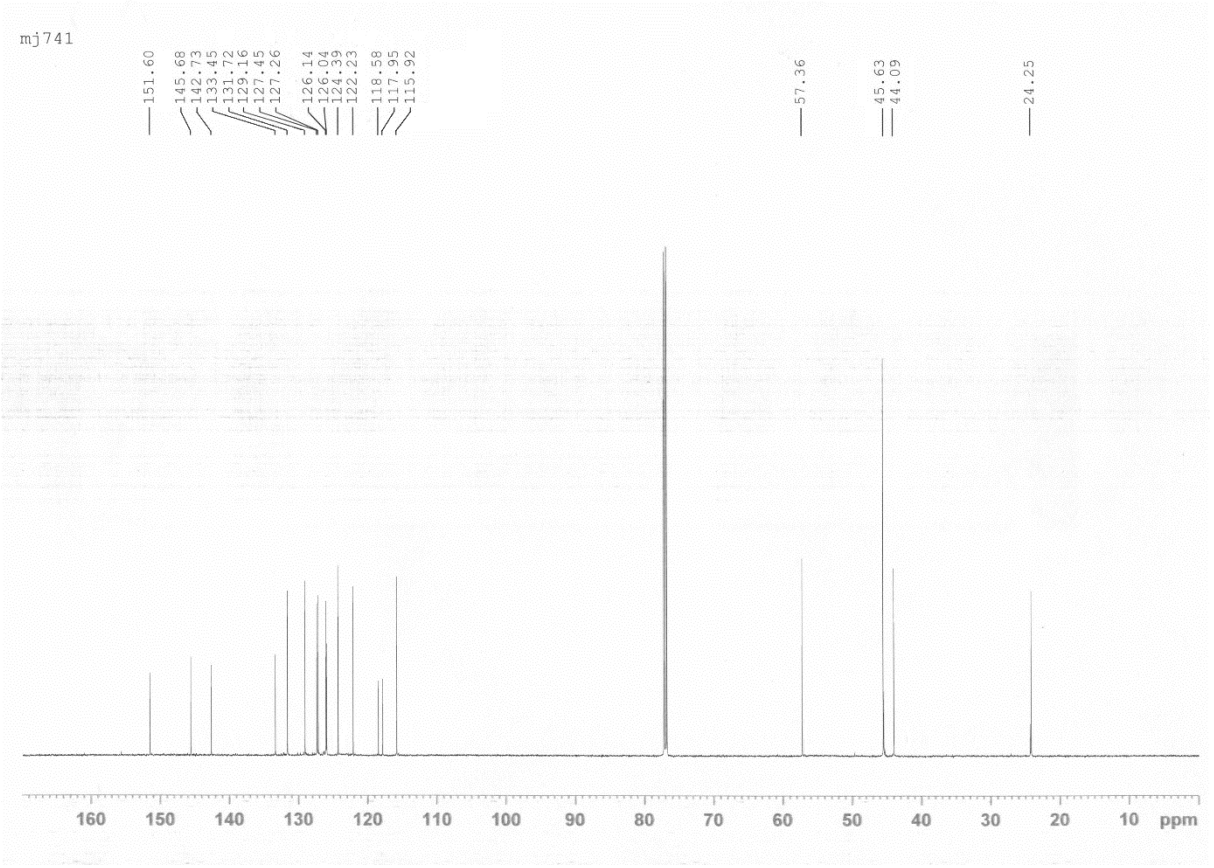


#	m/z	Res.	S/N	I	I %	FWHM
1	384.1302	10222	54428.6	10071745	100.0	0.0376
2	386.1272	13564	29049.0	5380588	53.4	0.0285

4. NMR spectra and HR MS of 6-(3-dimethylaminopropyl)-8-chloroquinobenzothiazine (**8**).







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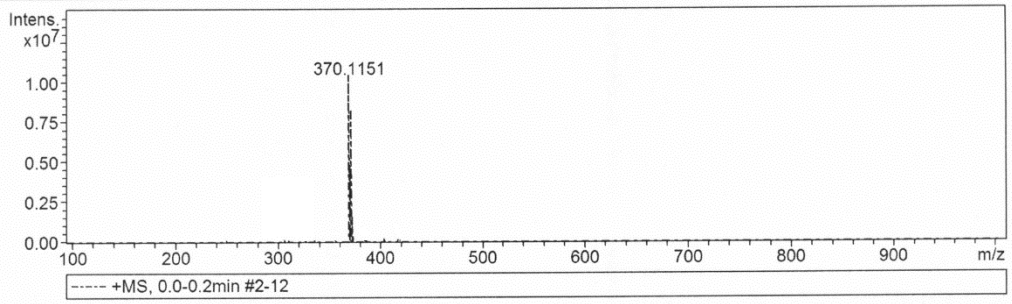
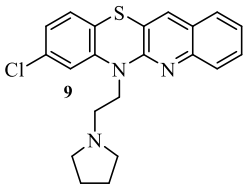


#	m/z	Res.	S/N	I	I %	FWHM
1	370.1151	8103	56136.2	10188798	100.0	0.0457
2	372.1123	13546	43737.8	7961009	78.1	0.0275

5. NMR spectra and HR MS of 6-(1-Pyrrolidylethyl)-8-chloroquinobenzothiazine (**9**).



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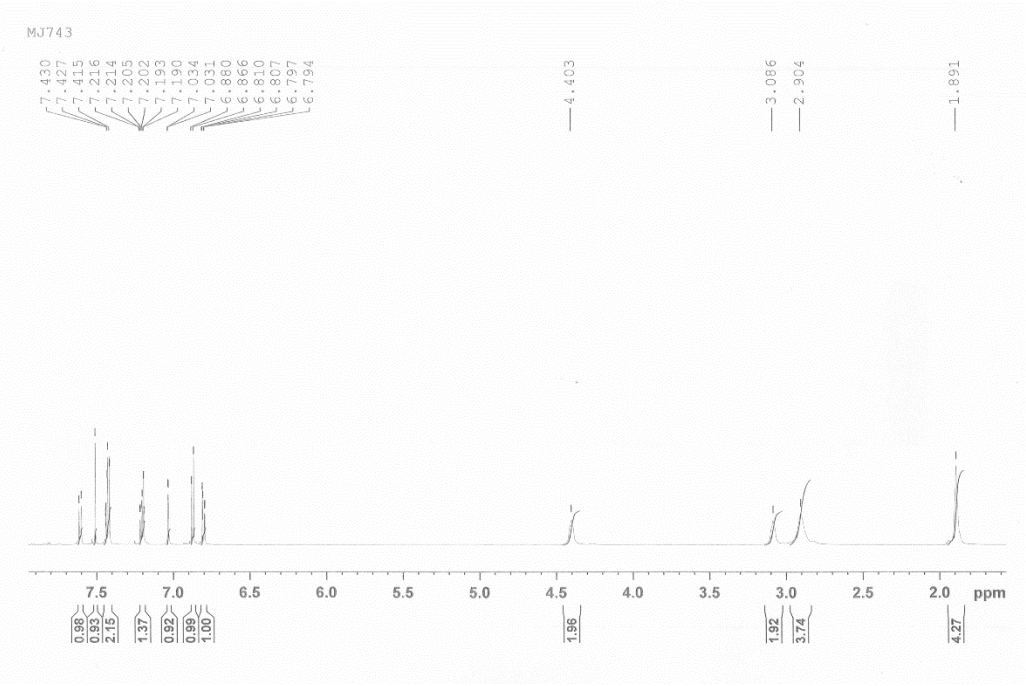

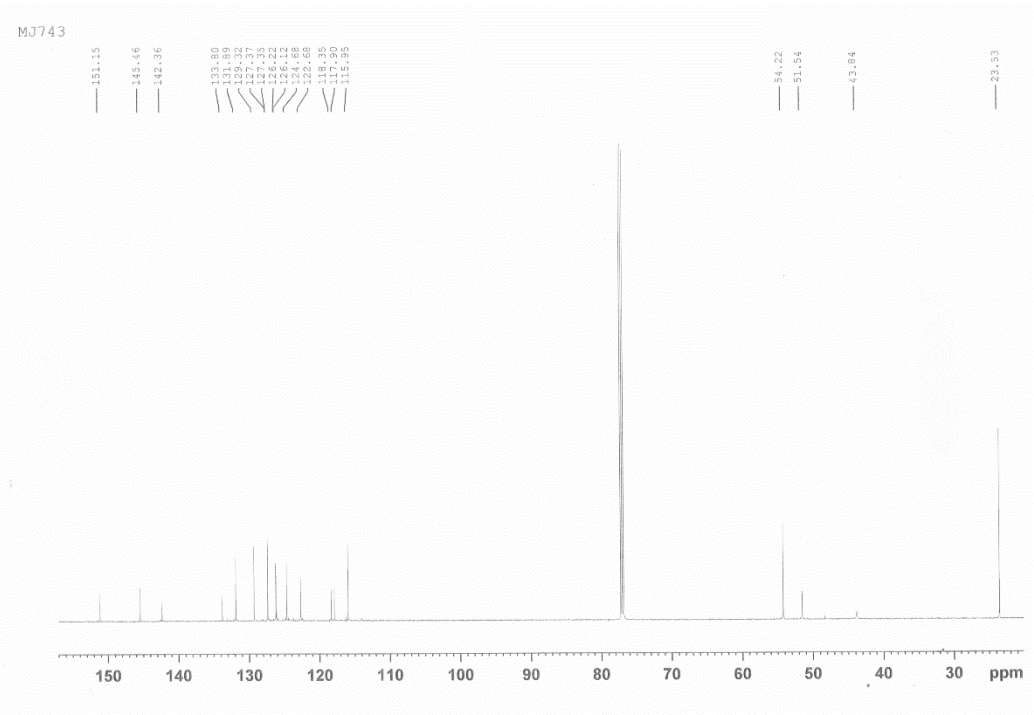

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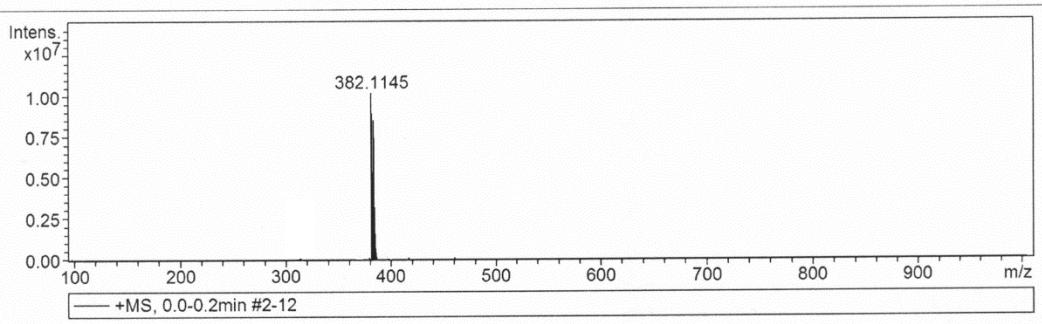
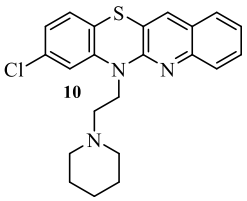


#	m/z	Res.	S/N	I	I %	FWHM
1	382.1145	7782	81007.5	10188798	100.0	0.0491
2	384.1118	13403	67270.0	8484336	83.3	0.0287

6. NMR spectra and HR MS of 6-(1-Piperidylethyl)-8-chloroquinobenzothiazine (**10**).



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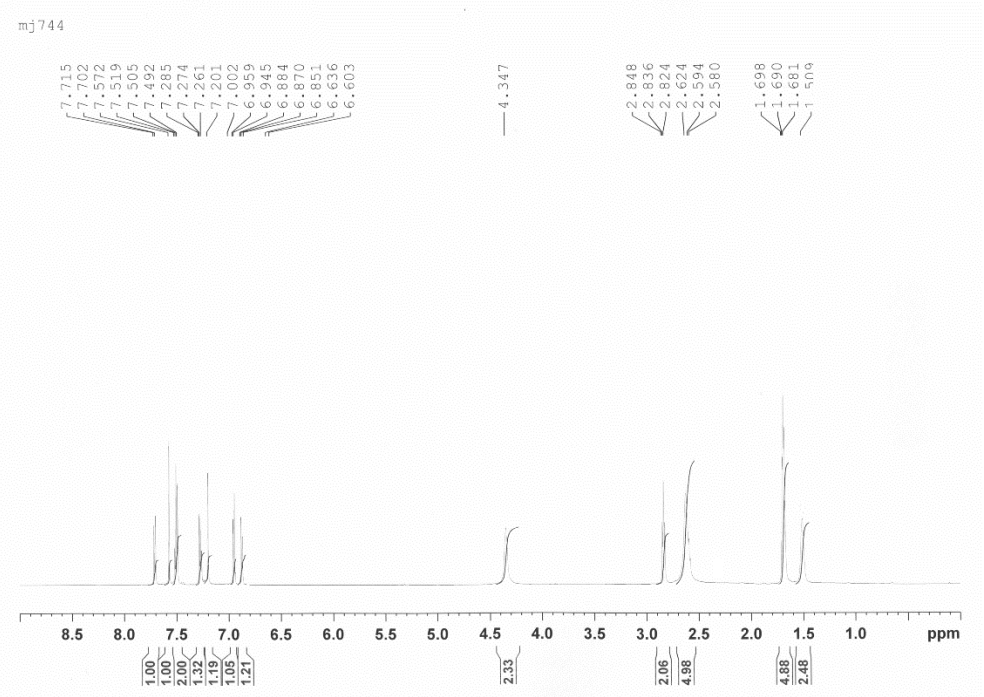

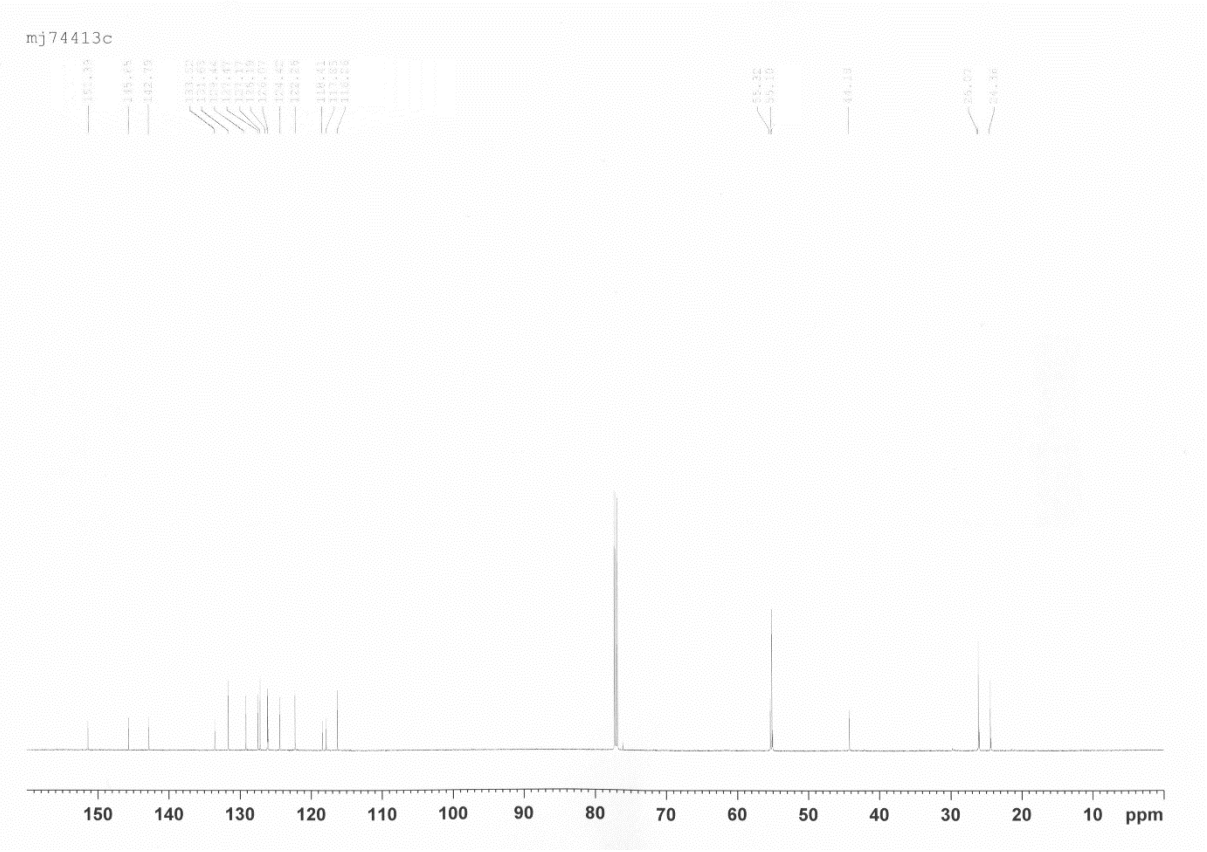

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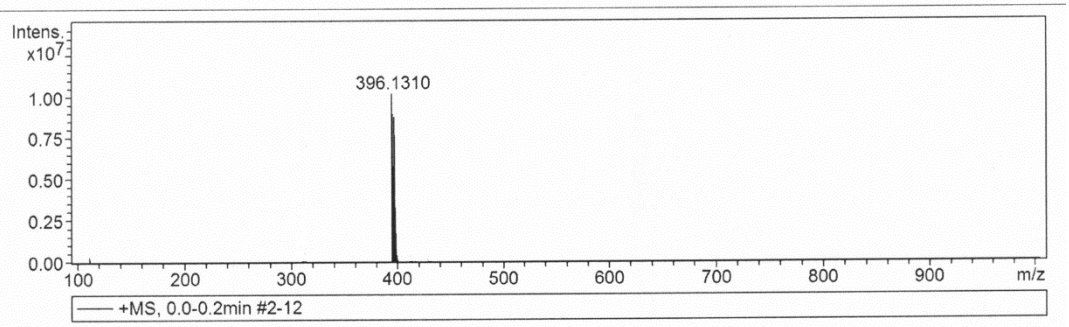
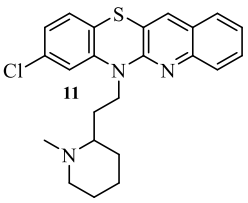


#	m/z	Res.	S/N	I	I %	FWHM
1	396.1310	7738	94773.6	10188798	100.0	0.0512
2	398.1282	13593	81523.1	8789789	86.3	0.0293

7. NMR spectra and HR MS of 6-(1-Methyl-2-piperidylethyl)-8-chloroquinobenzothiazine (**11**).



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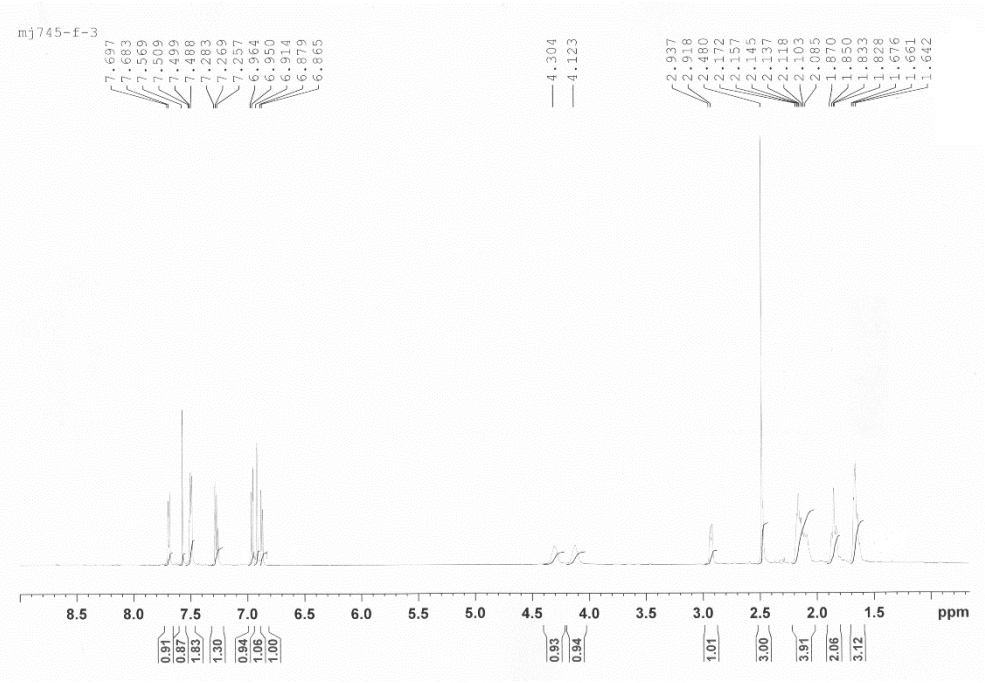

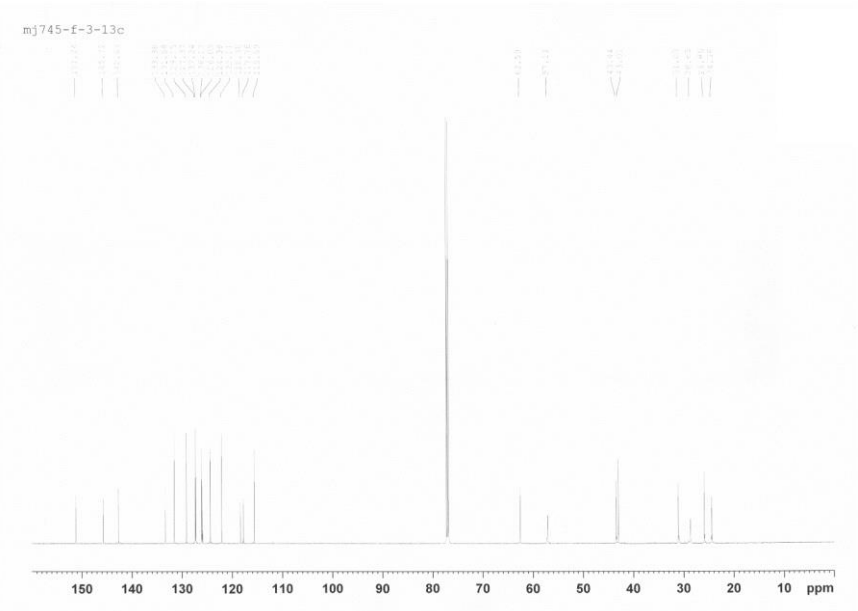

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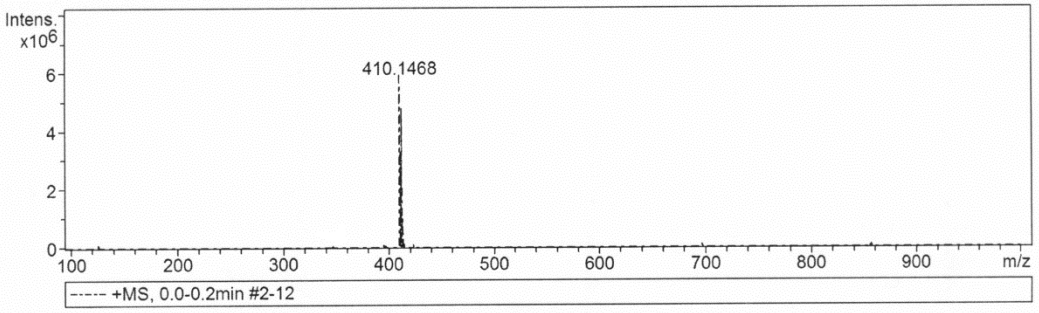
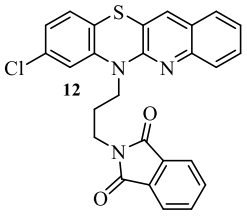


#	m/z	Res.	S/N	I	I %	FWHM
1	410.1468	8116	88496.9	5767489	100.0	0.0505
2	412.1442	13609	70653.7	4628476	80.3	0.0303

8. NMR spectra and HR MS of 8-Chloro-6-phthalimidopropylquinobenzothiazine (**12**).



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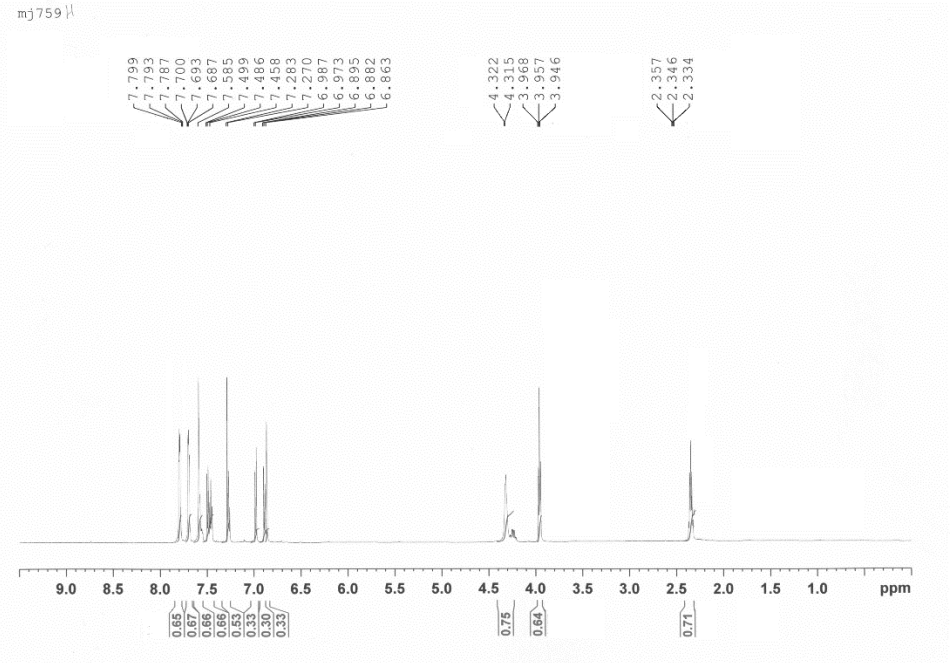

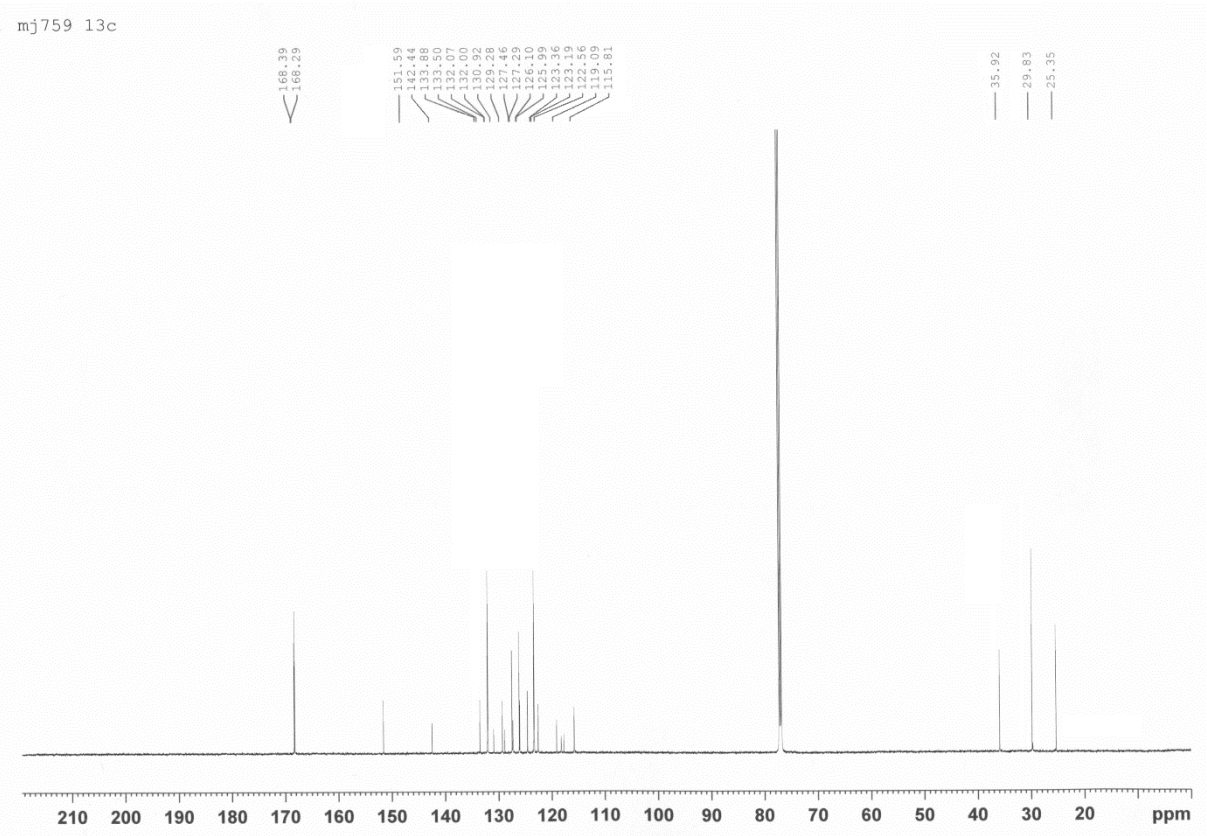

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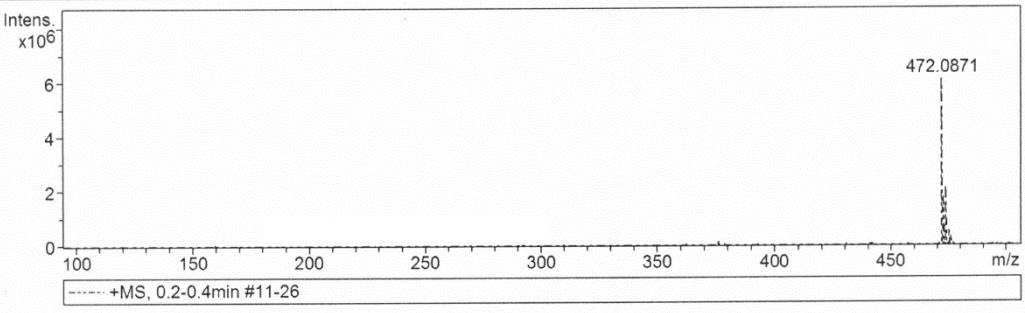
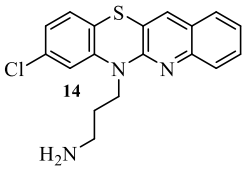
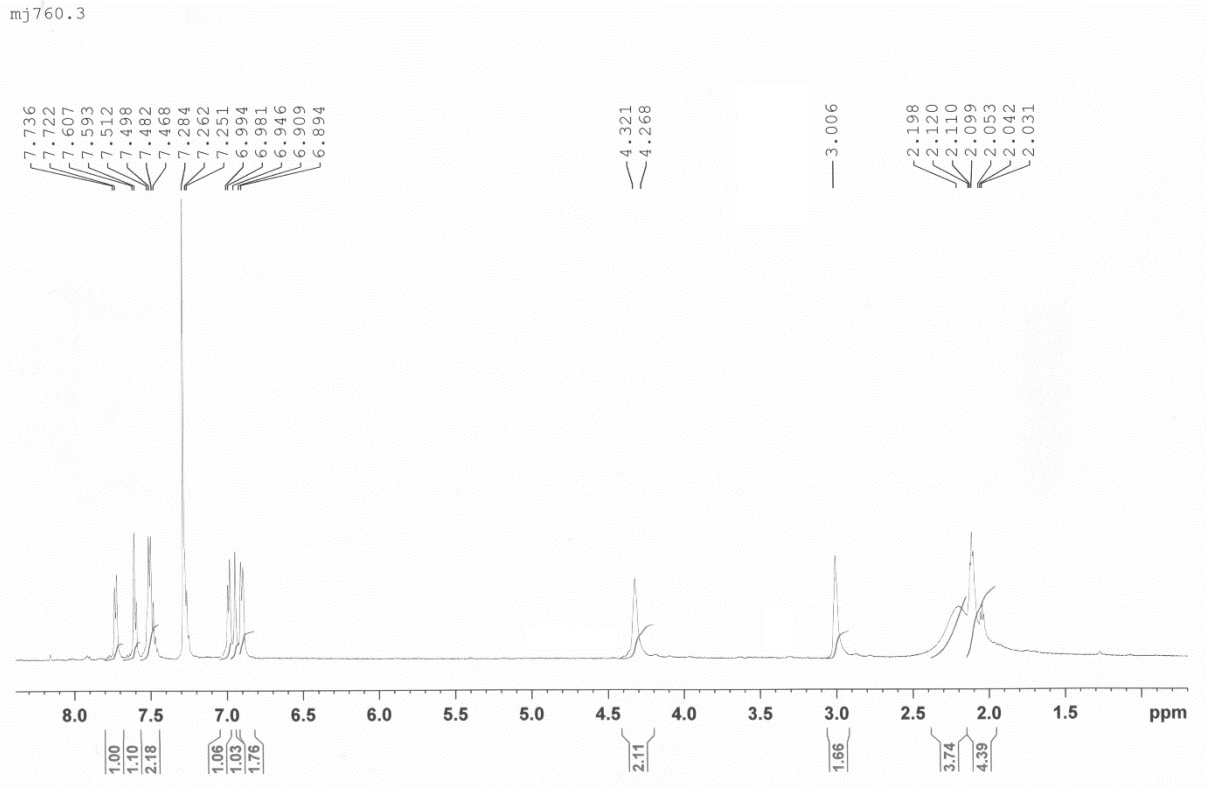
		Set Corona	0 nA	Set APCI Heater	0 °C



#	m/z	Res.	S/N	I	I %	FWHM
1	472.0871	37225	12528.0	6128841	100.0	0.0127
2	474.0836	26588	4409.6	2159305	35.2	0.0178

9. NMR spectra and HR MS of 6-Aminopropyl-8-chloroquinobenzothiazine (**14**).





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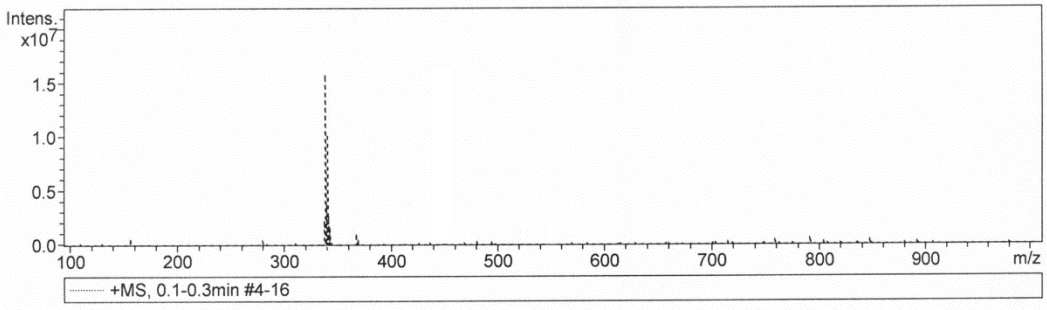
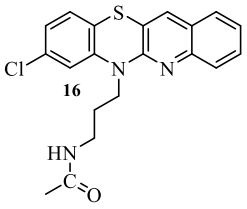


#	m/z	Res.	S/N	I	I %	FWHM
1	342.0844	23653	278.3	110821	100.0	0.0145

10. NMR spectra and HR MS of 6-Acetylaminopropyl-8-chloroquinobenzothiazine (**16**).



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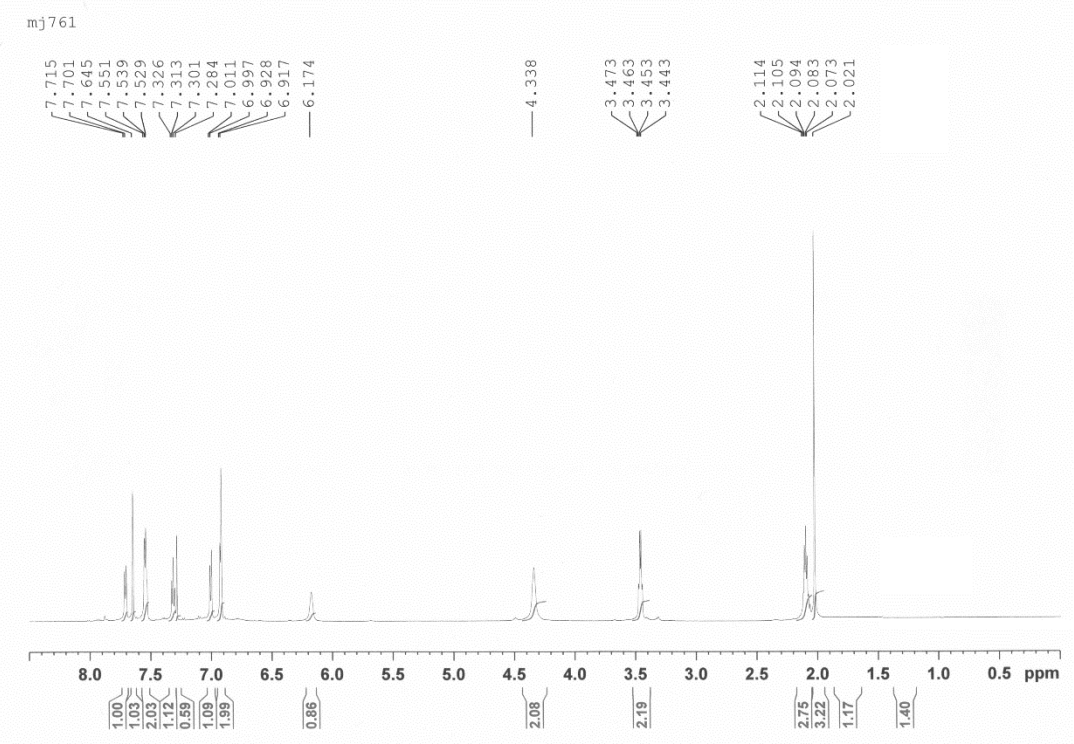
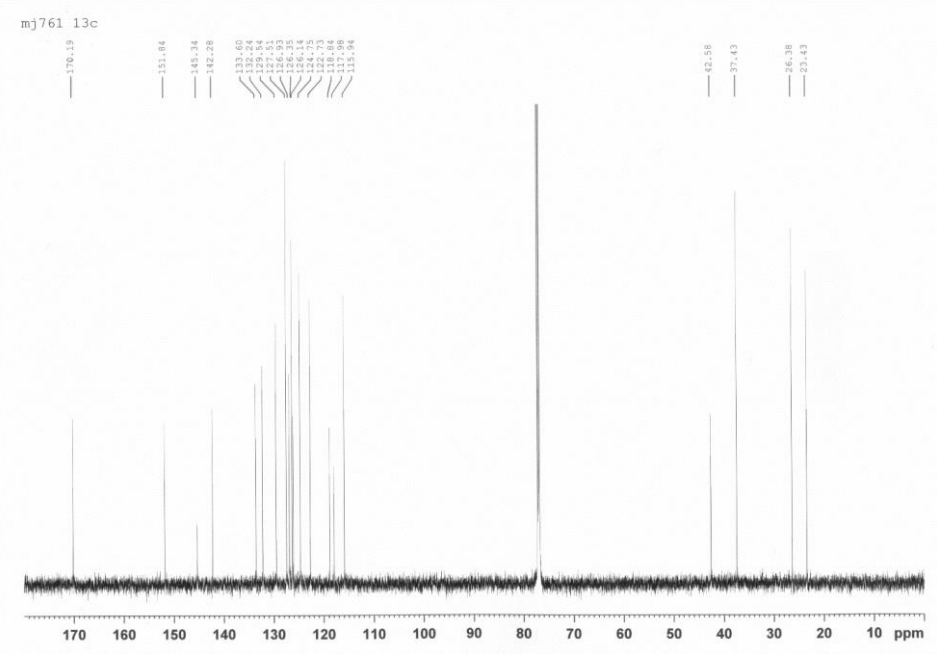
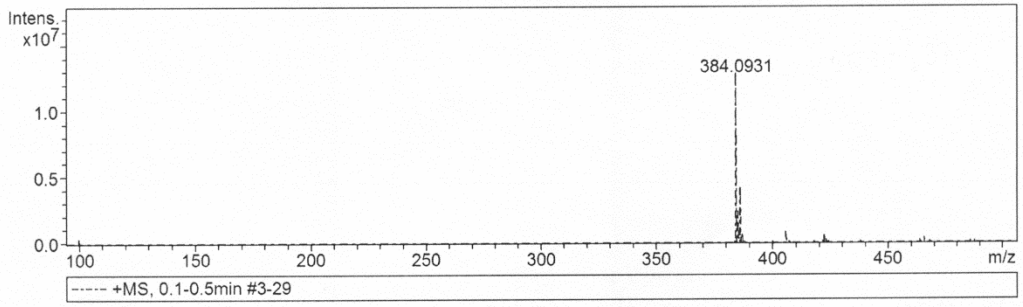




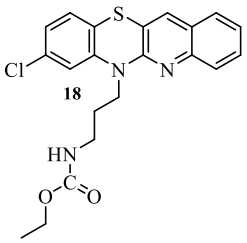
Acquisition Parameter

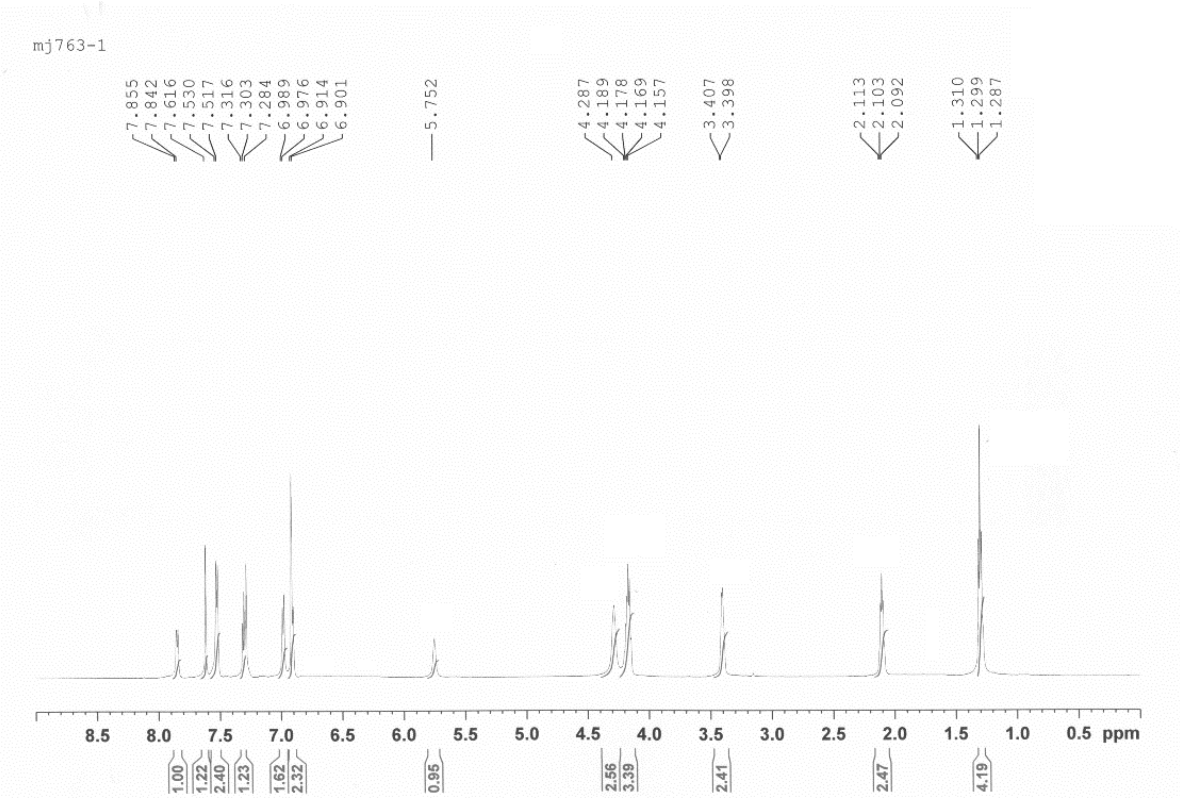
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

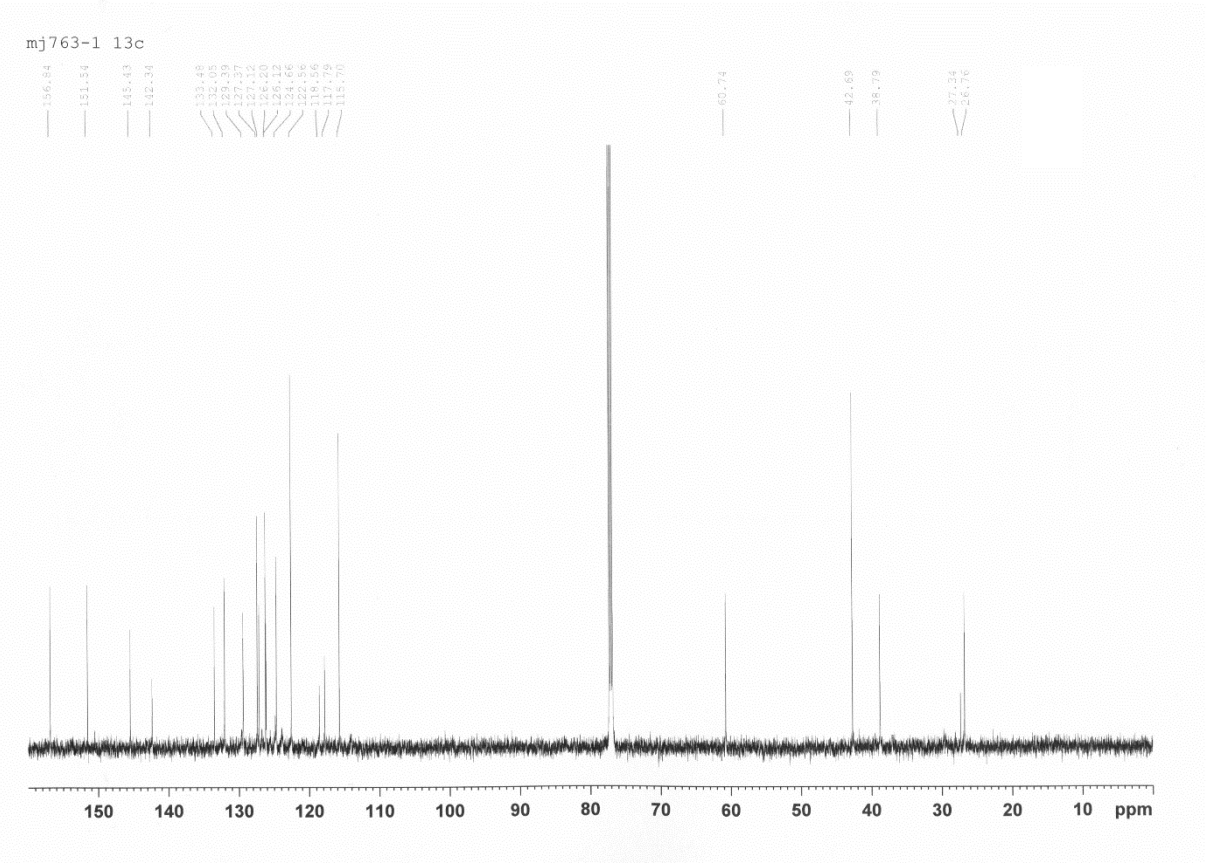


#	m/z	Res.	S/N	I	I %	FWHM
1	384.0931	38530	80379.1	12531551	100.0	0.0100
2	386.0898	32092	27159.5	4284578	34.2	0.0120

11. NMR spectra and HR MS of 6-Ethoxycarbonylaminopropyl-8-chloroquinobenzothiazine (**18**).

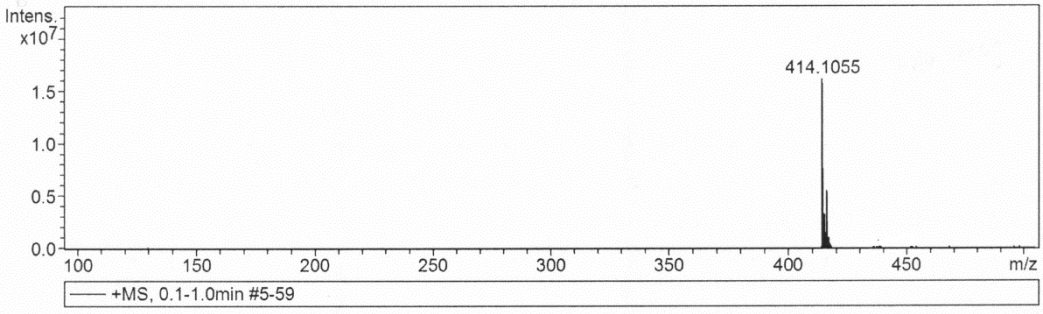






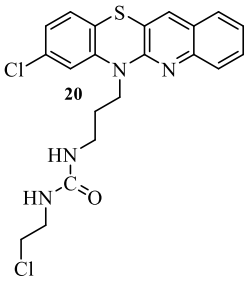
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

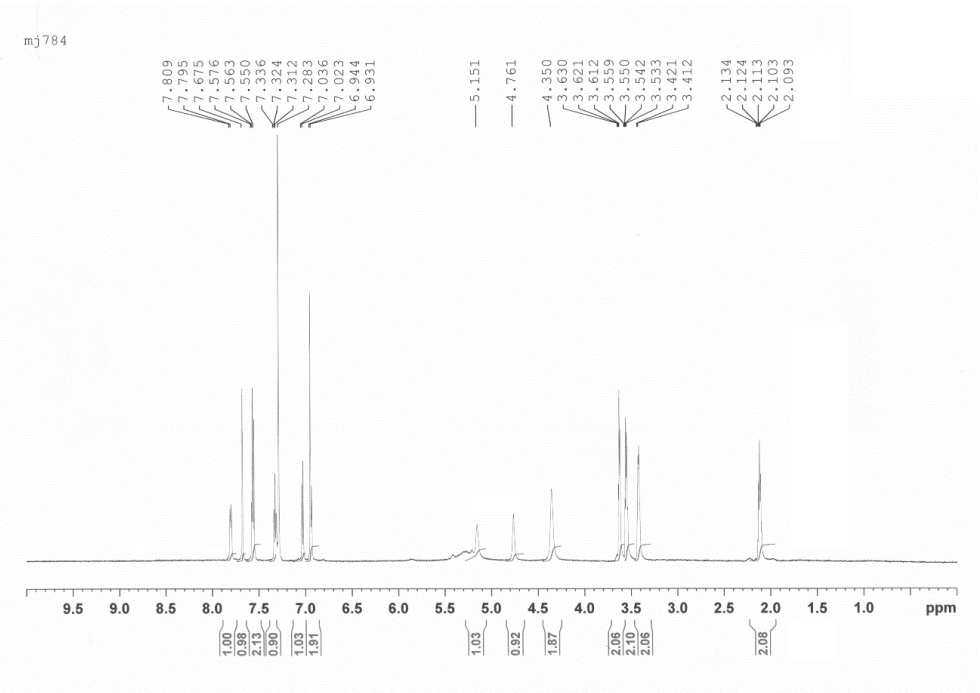


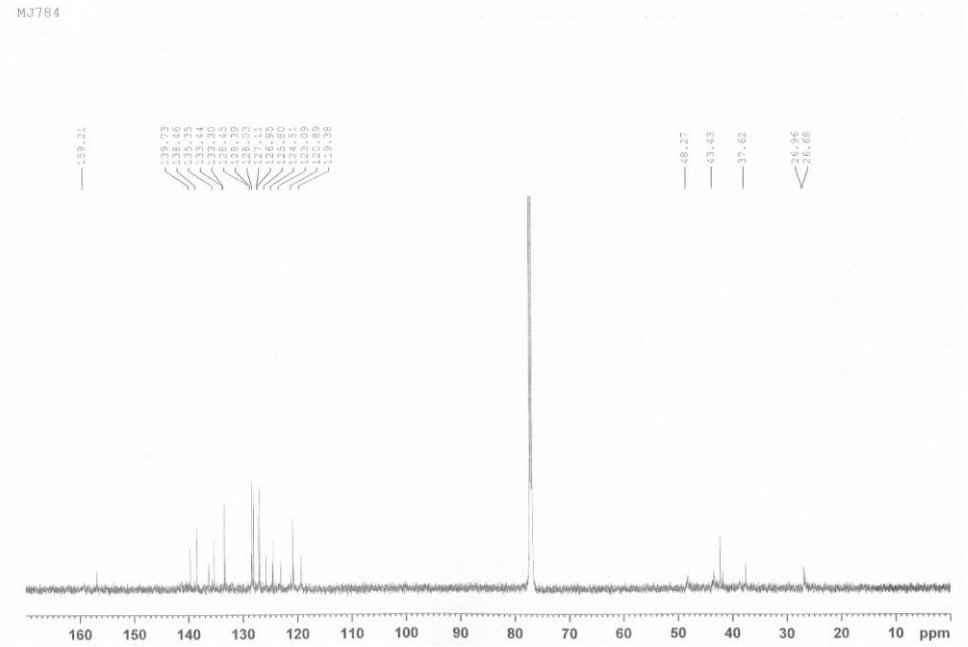
#	m/z	Res.	S/N	I	I %	FWHM
1	414.1055	34600	96812.6	16221700	100.0	0.0120
2	416.1021	33931	32773.3	5547655	34.2	0.0123

12. NMR spectra and HR MS of 6-Chloroethylureidopropyl-8-chloroquinobenzothiazine (**20**).



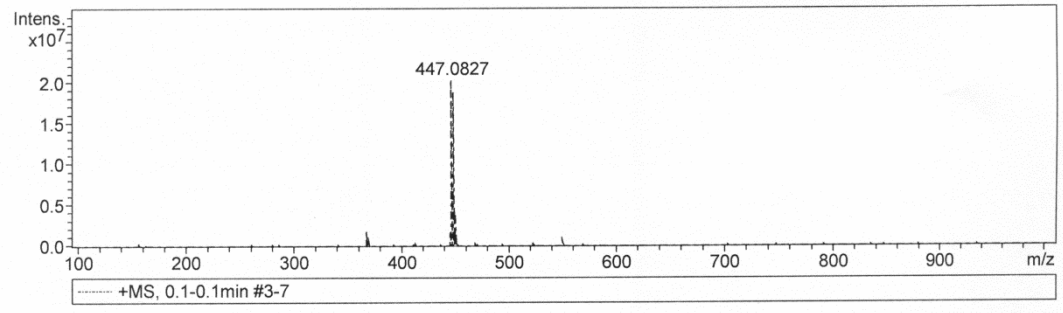
20





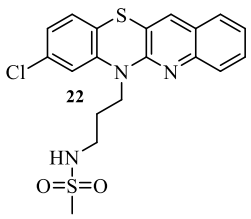
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

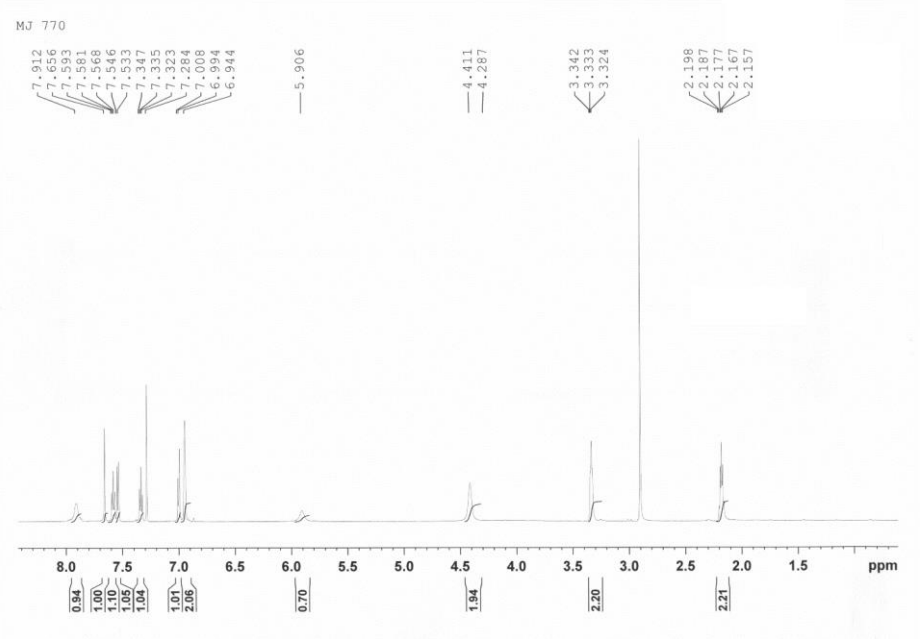


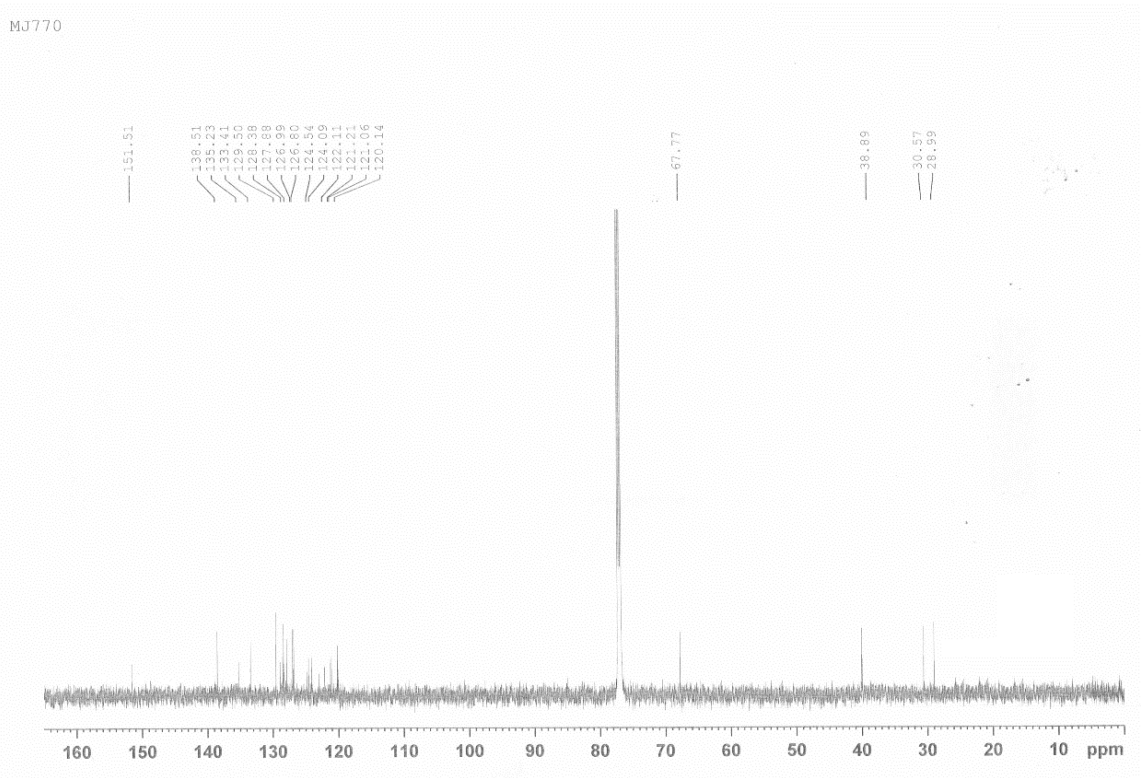
#	m/z	Res.	S/N	I	I %	FWHM
1	447.0827	22029	37433.2	20371780	100.0	0.0203
2	449.0793	39034	33448.2	18212446	89.4	0.0115

13. NMR spectra and HR MS of 8-Chloro-6-methanesulfonylaminopropylquinobenzothiazine (**22**).



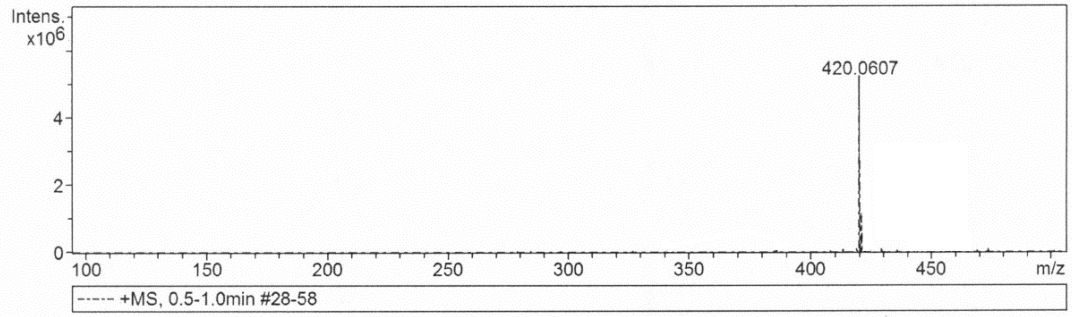
22





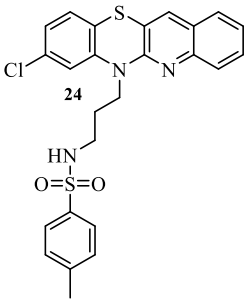
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

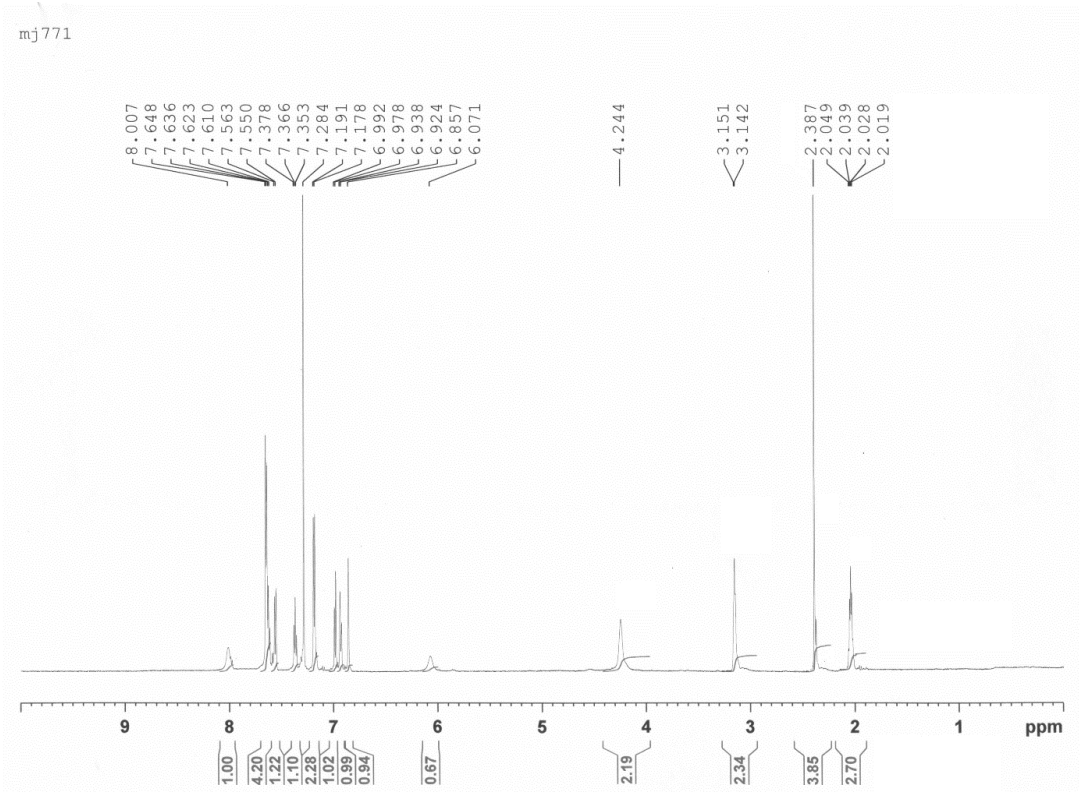


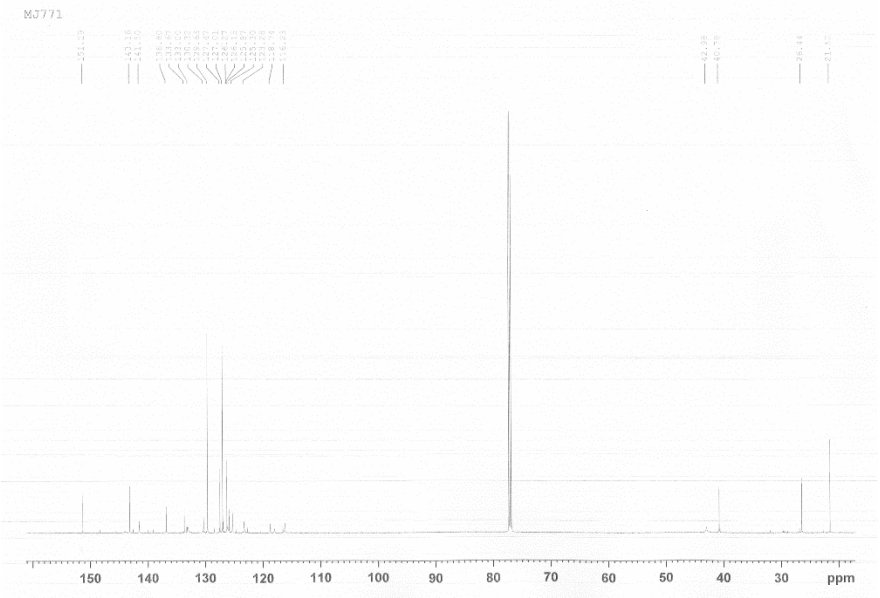
#	m/z	Res.	S/N	I	I %	FWHM
1	420.0607	34065	20988.5	5131382	100.0	0.0123
2	422.0575	26272	7957.4	1969690	38.4	0.0161

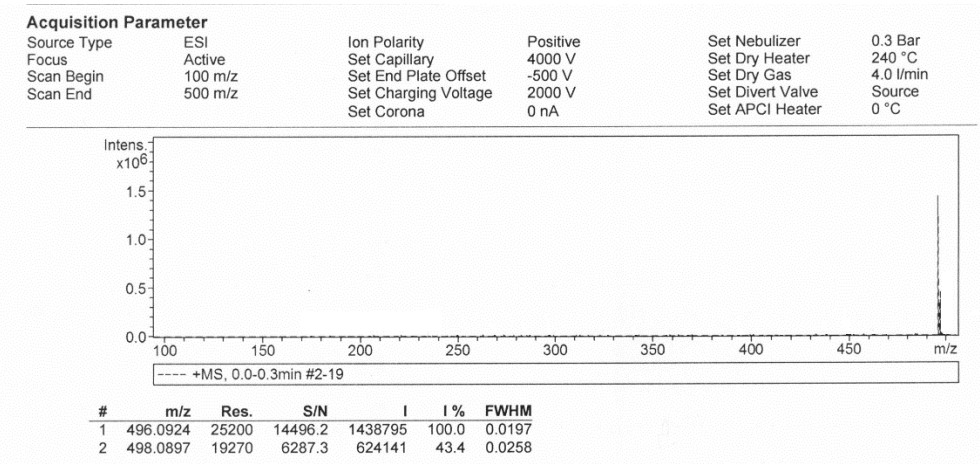
14. NMR spectra and HR MS of 8-Chloro-6-p-toluenesulfonylaminopropylquinobenzothiazine (**24**).



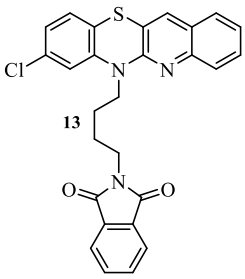
24

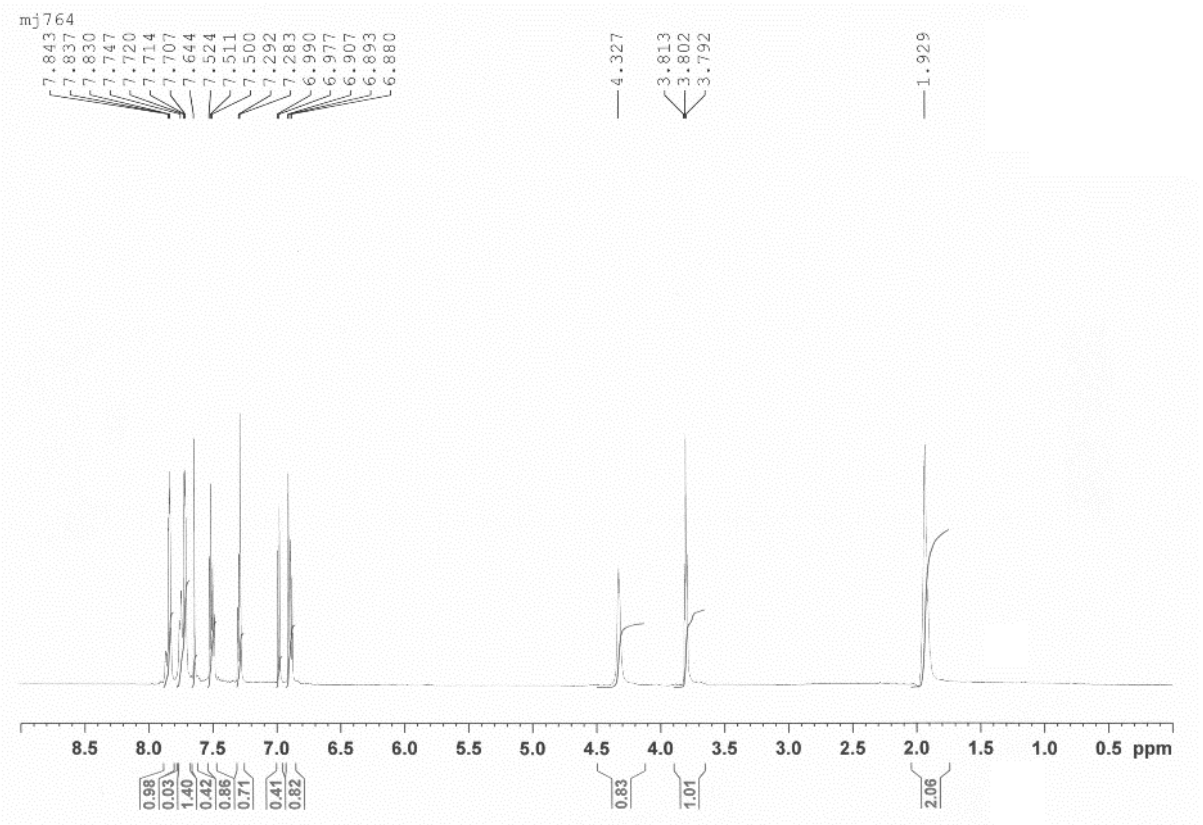




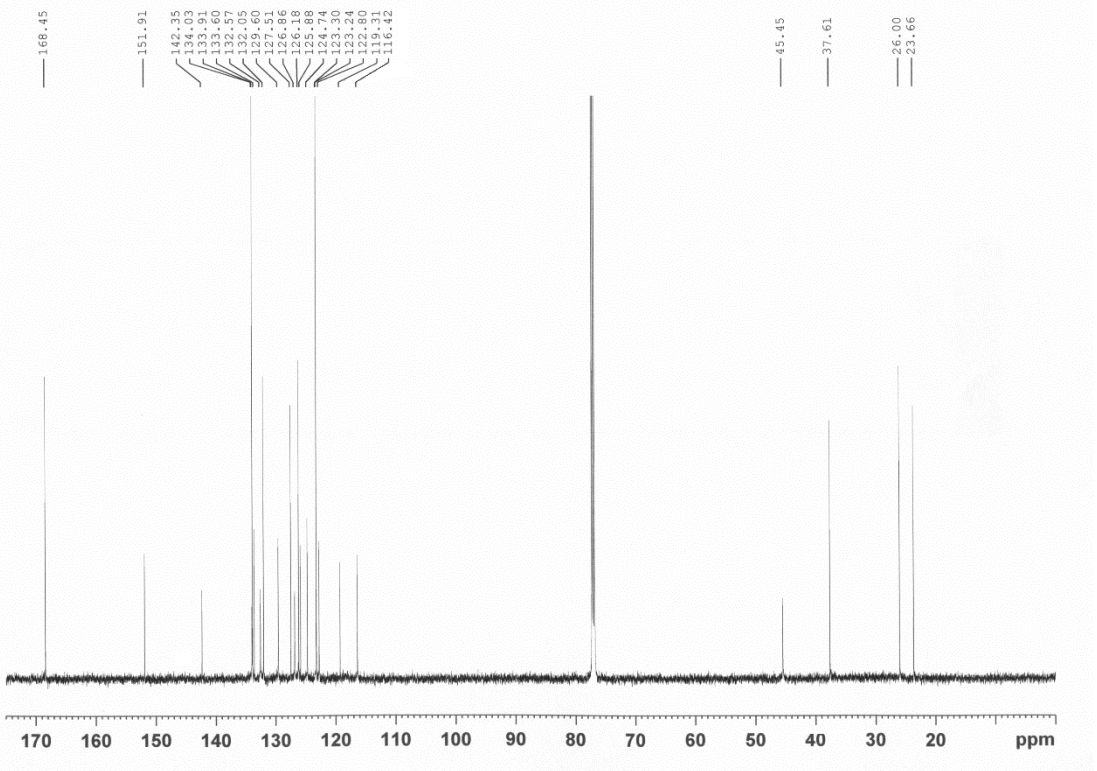


15. NMR spectra and HR MS of 8-Chloro-6-phthalimidobutylquinobenzothiazine (**13**).



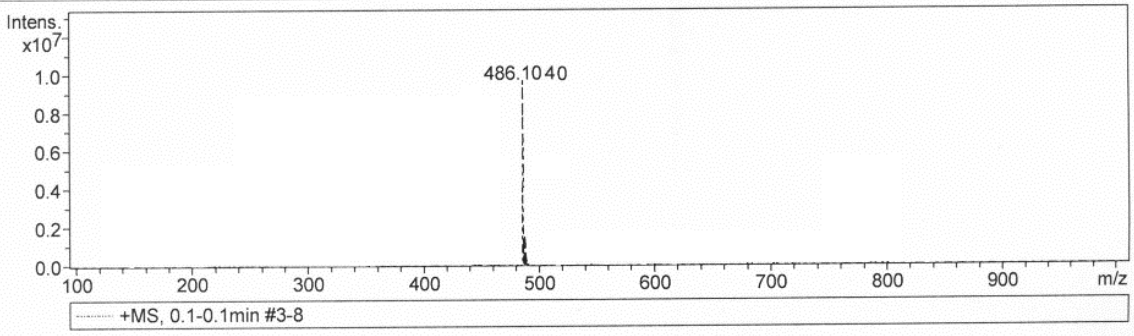


mj764 13c



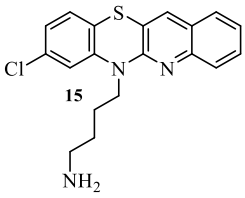
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

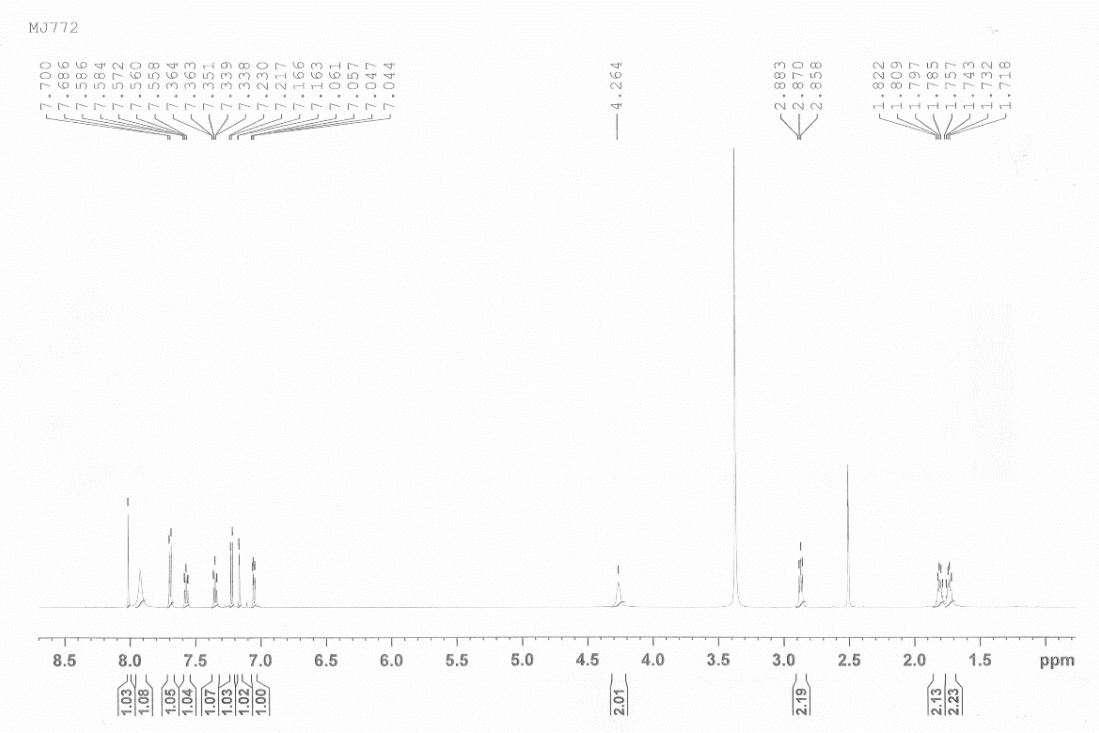


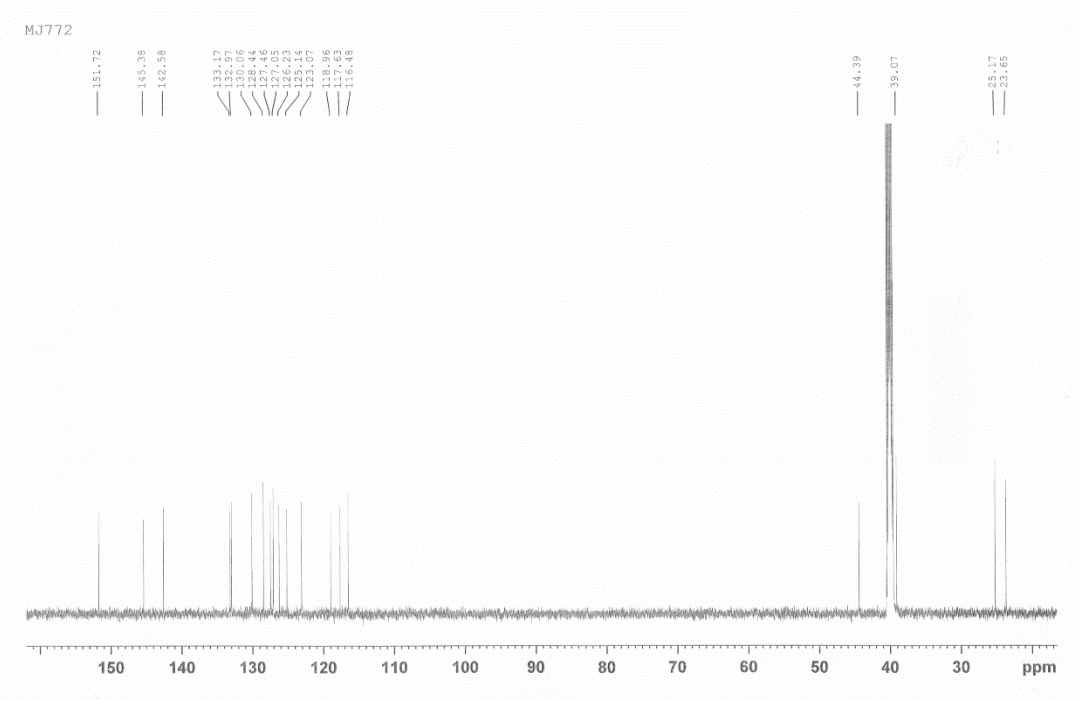
#	m/z	Res.	S/N	I	I %	FWHM
1	486.1040	41233	6045.6	4573534	100.0	0.0118

16. NMR spectra and HR MS of 6-Aminobutyl-8-chloroquinobenzothiazine (**15**).



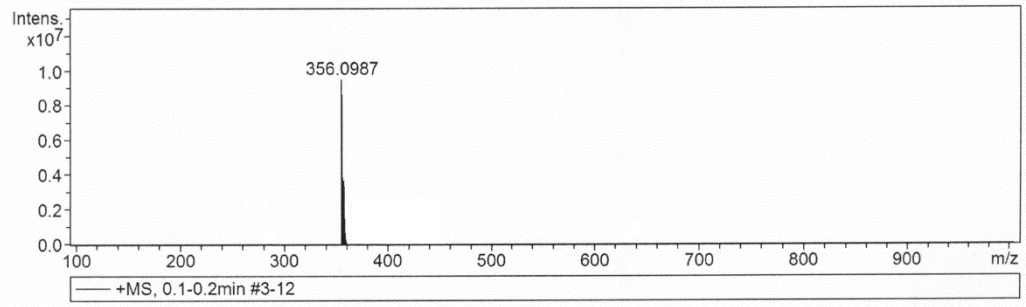
15





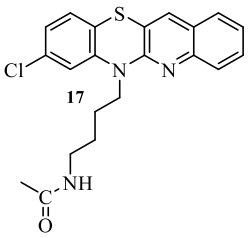
Acquisition Parameter

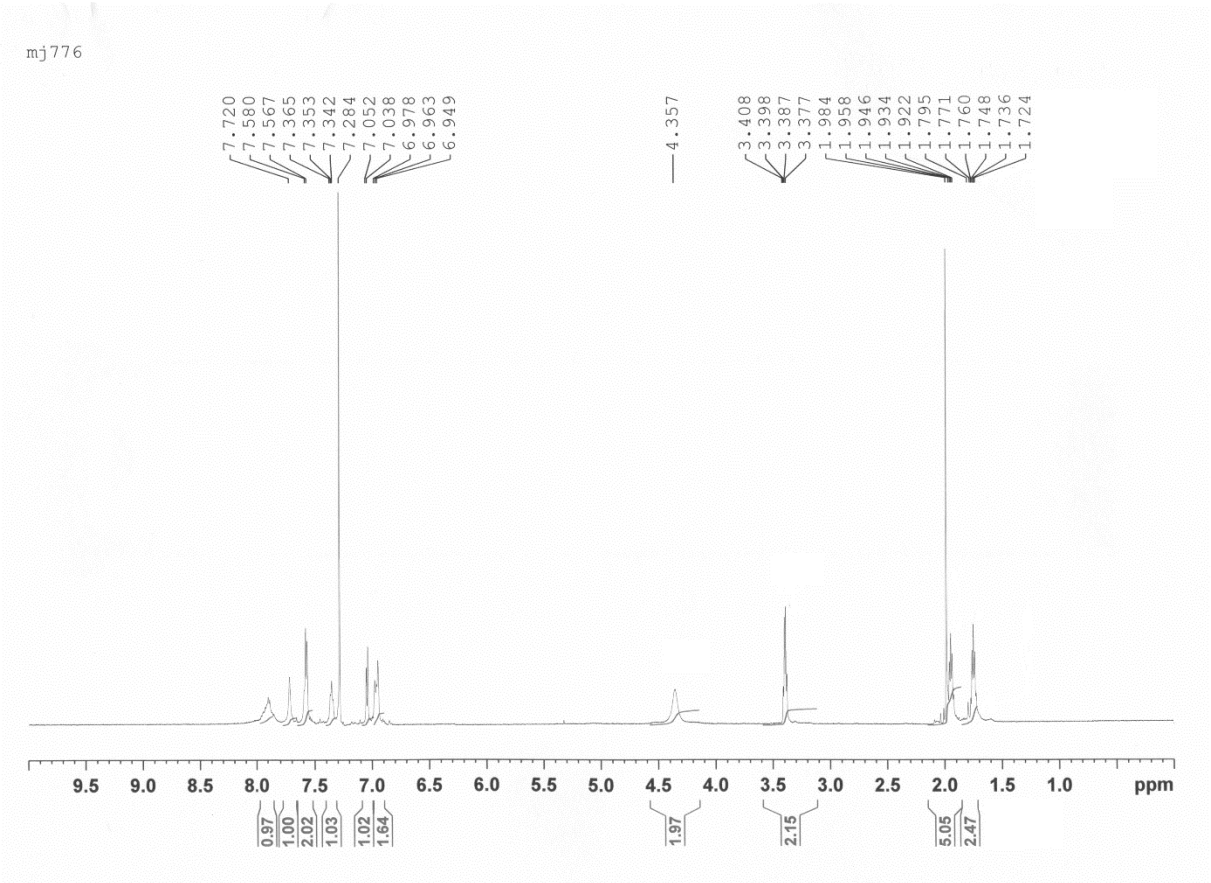
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

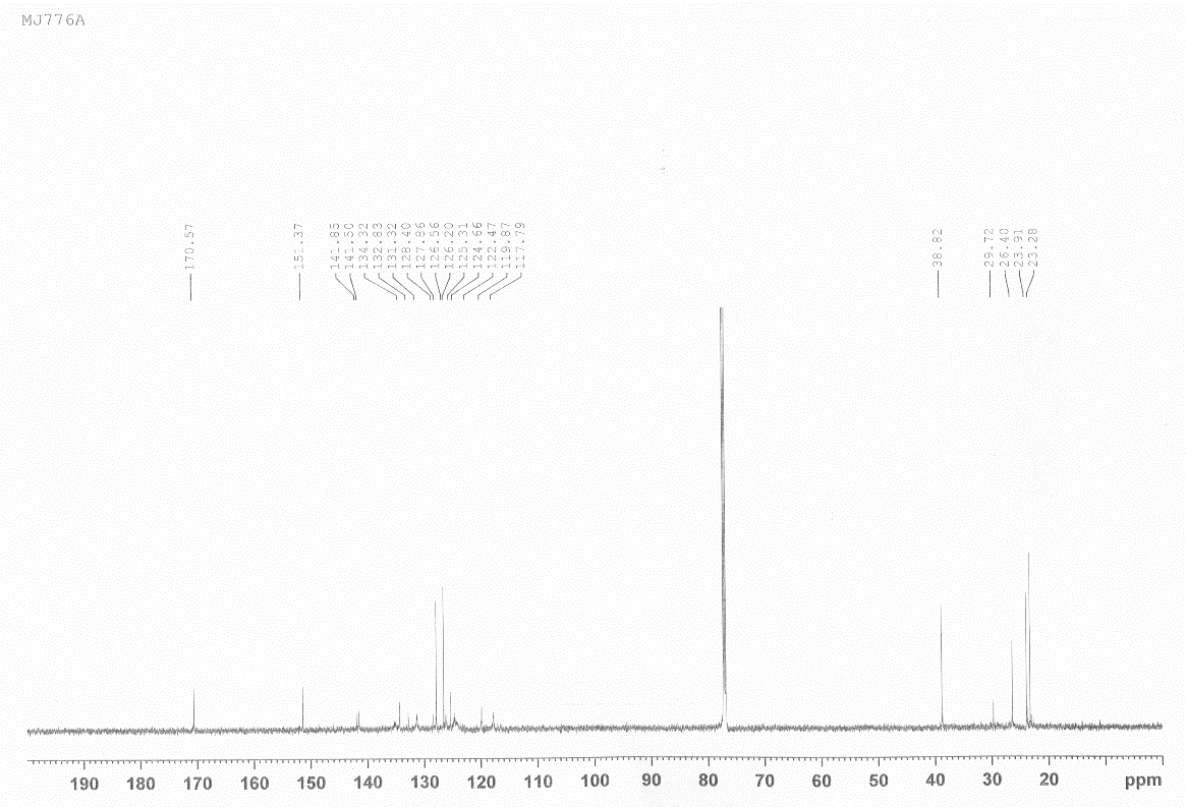


#	m/z	Res.	S/N	I	I %	FWHM
1	356.0987	12588	110224.2	9527740	100.0	0.0283
2	358.0954	13358	42185.6	3668580	38.5	0.0268

17. NMR spectra and HR MS of 6-Acetylaminobutyl-8-chloroquinobenzothiazine (**17**).

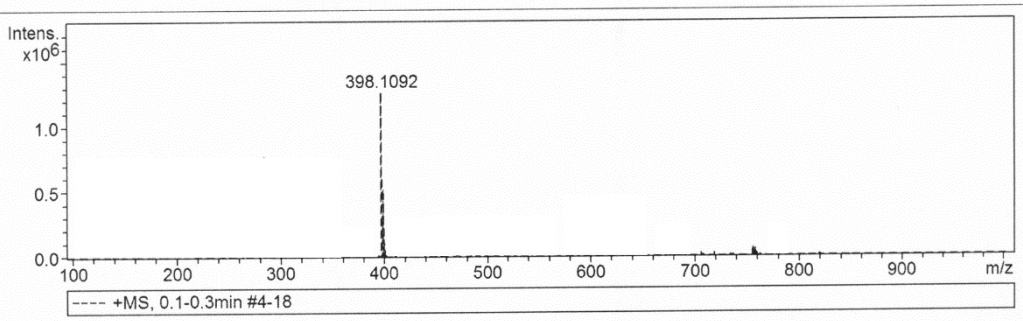






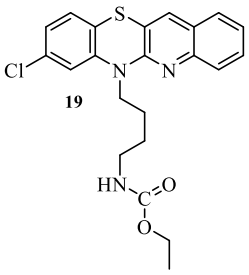
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

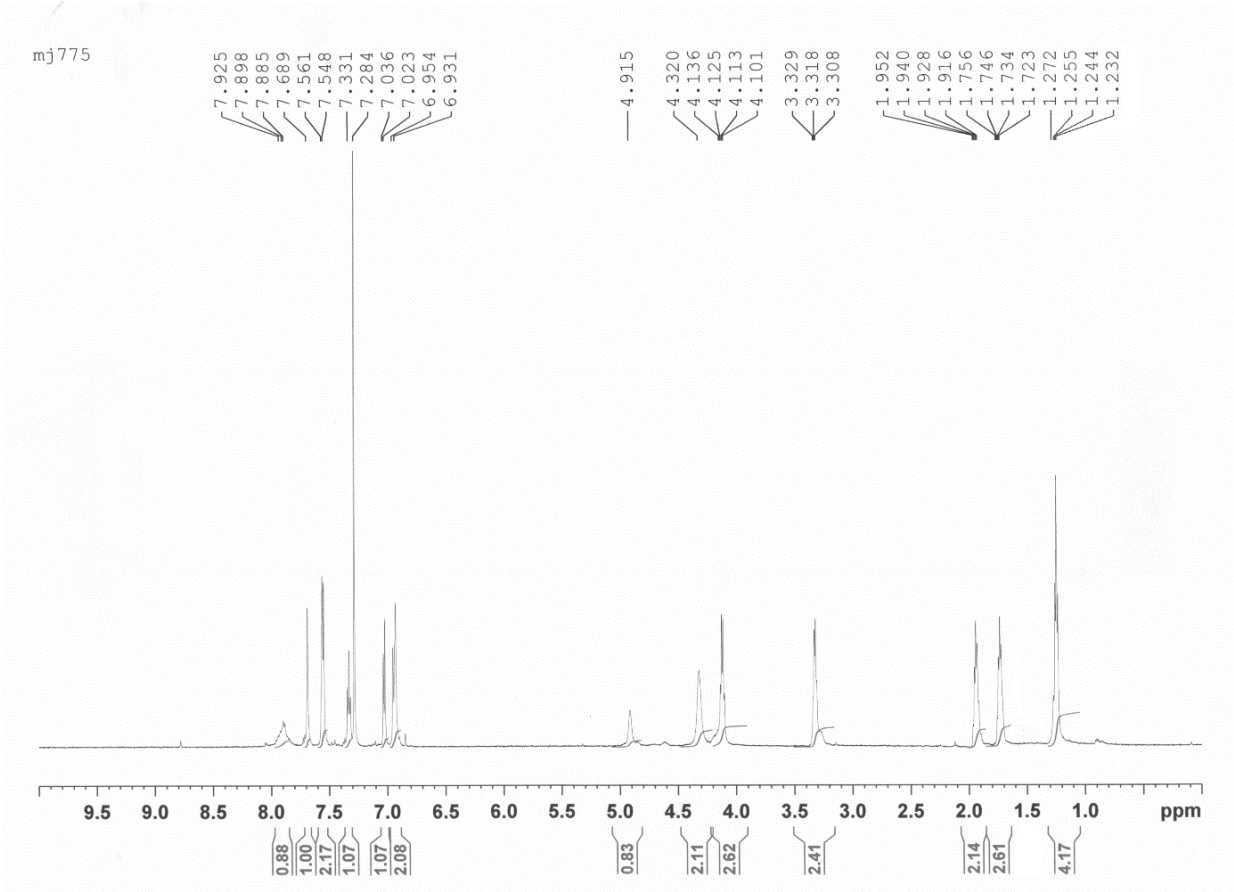


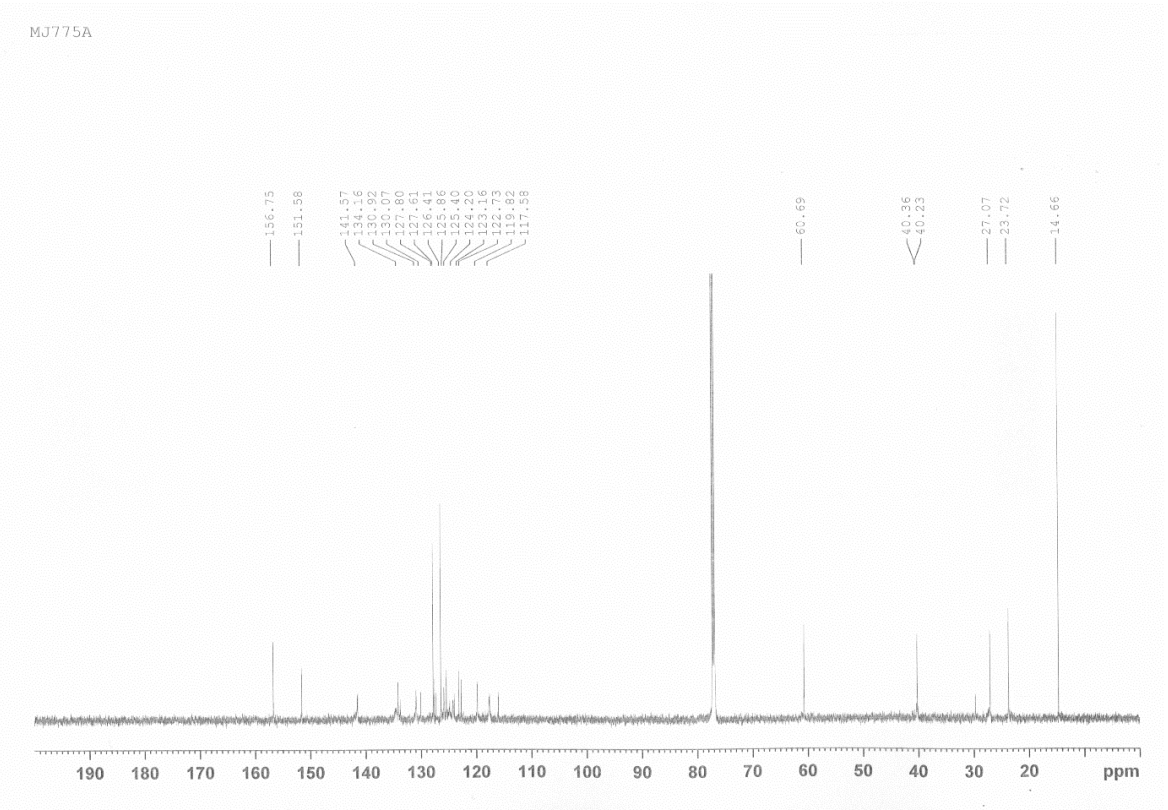
#	m/z	Res.	S/N	I	I %	FWHM
1	398.1092	13619	9225.4	1268062	100.0	0.0292
2	400.1063	13496	3545.4	490455	38.7	0.0296

18. NMR spectra and HR MS of 8-Chloro-6-ethoxycarbonylaminobutylquinobenzothiazine (**19**).



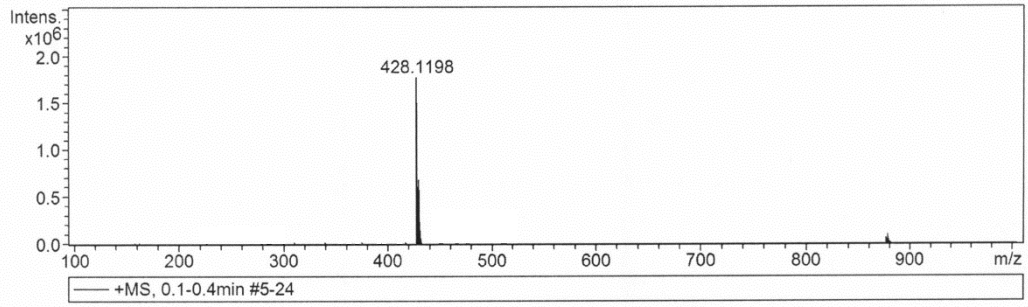
19





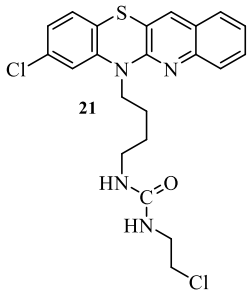
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

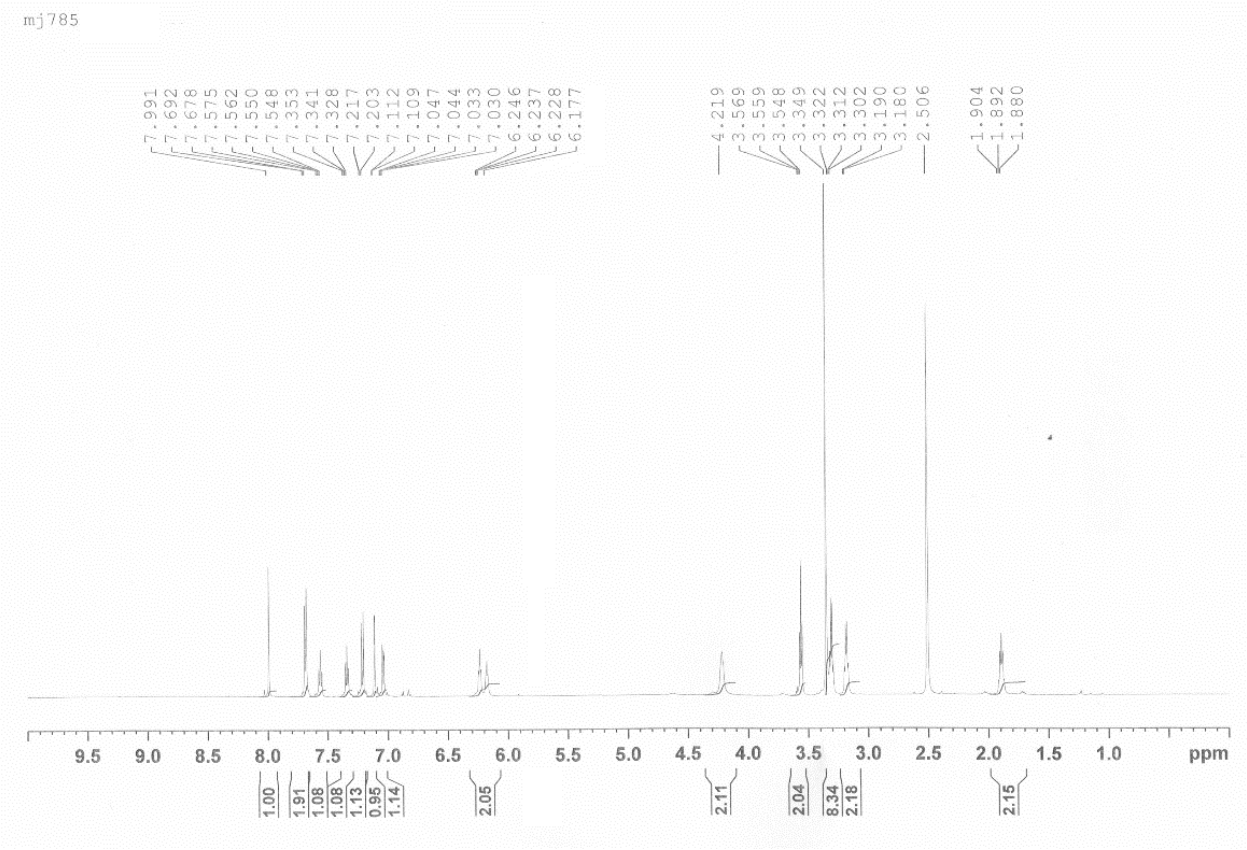


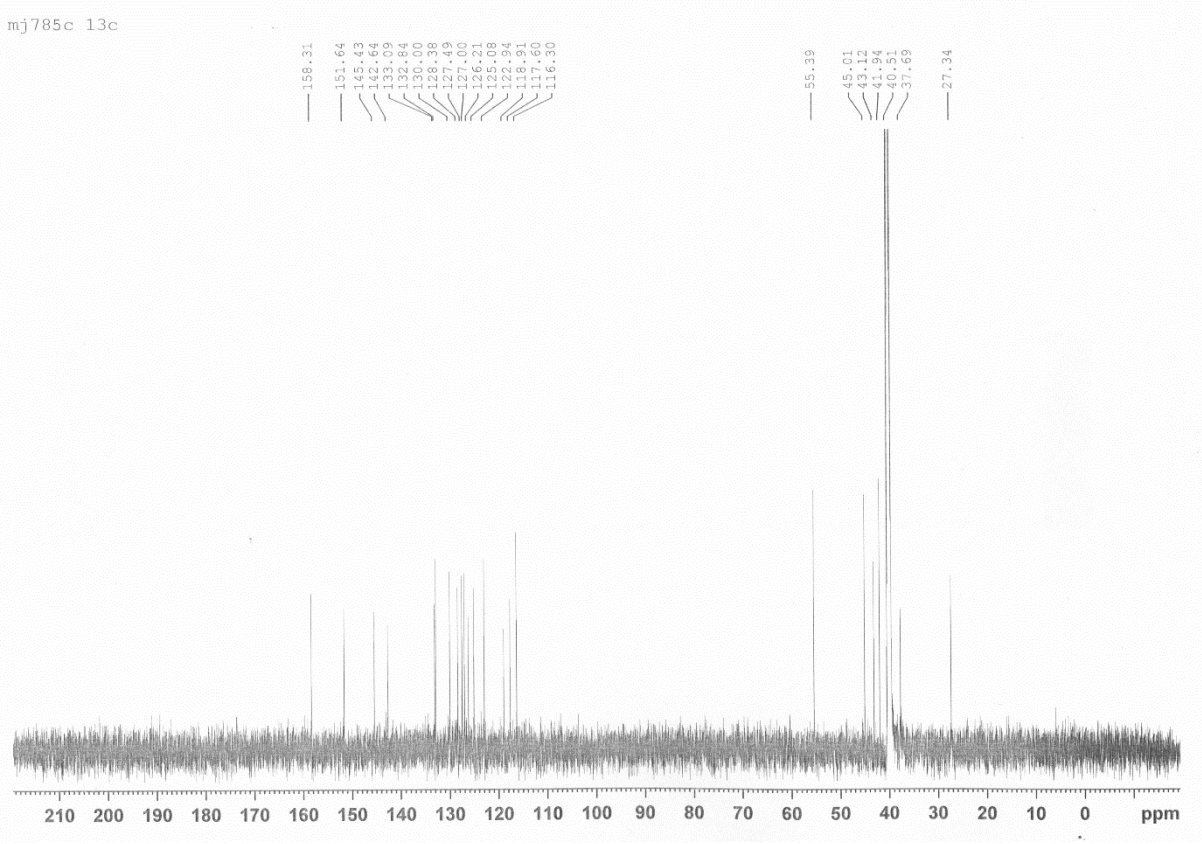
#	m/z	Res.	S/N	I	I %	FWHM
1	428.1198	13986	21640.4	1773247	100.0	0.0306
2	430.1171	13745	8352.5	686719	38.7	0.0313

19. NMR spectra and HR MS of 6-Chloroethylureidobutyl-8-chloroquinobenzothiazine (**21**).



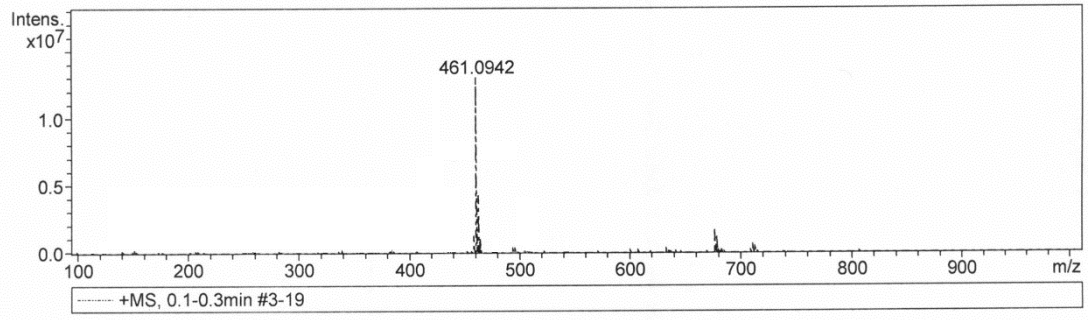
21





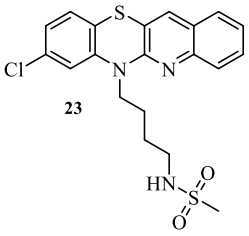
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

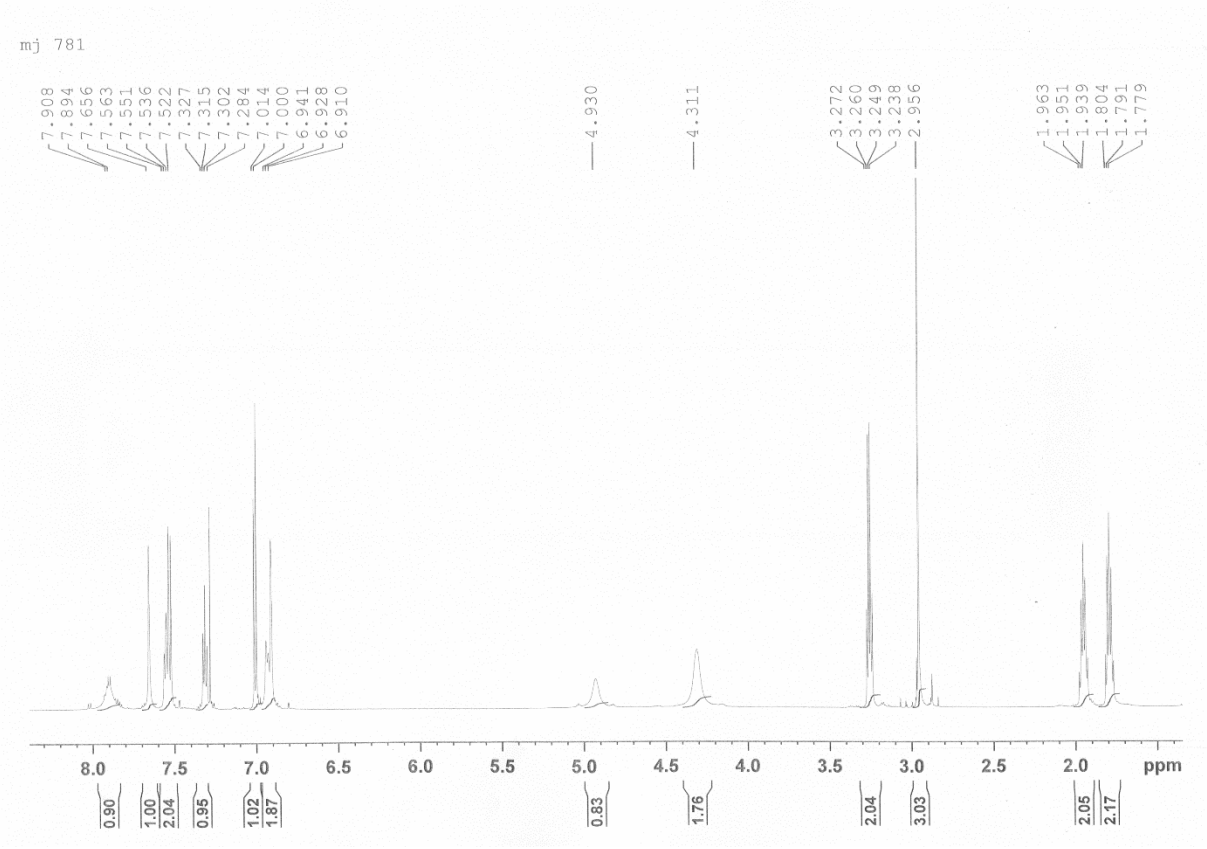


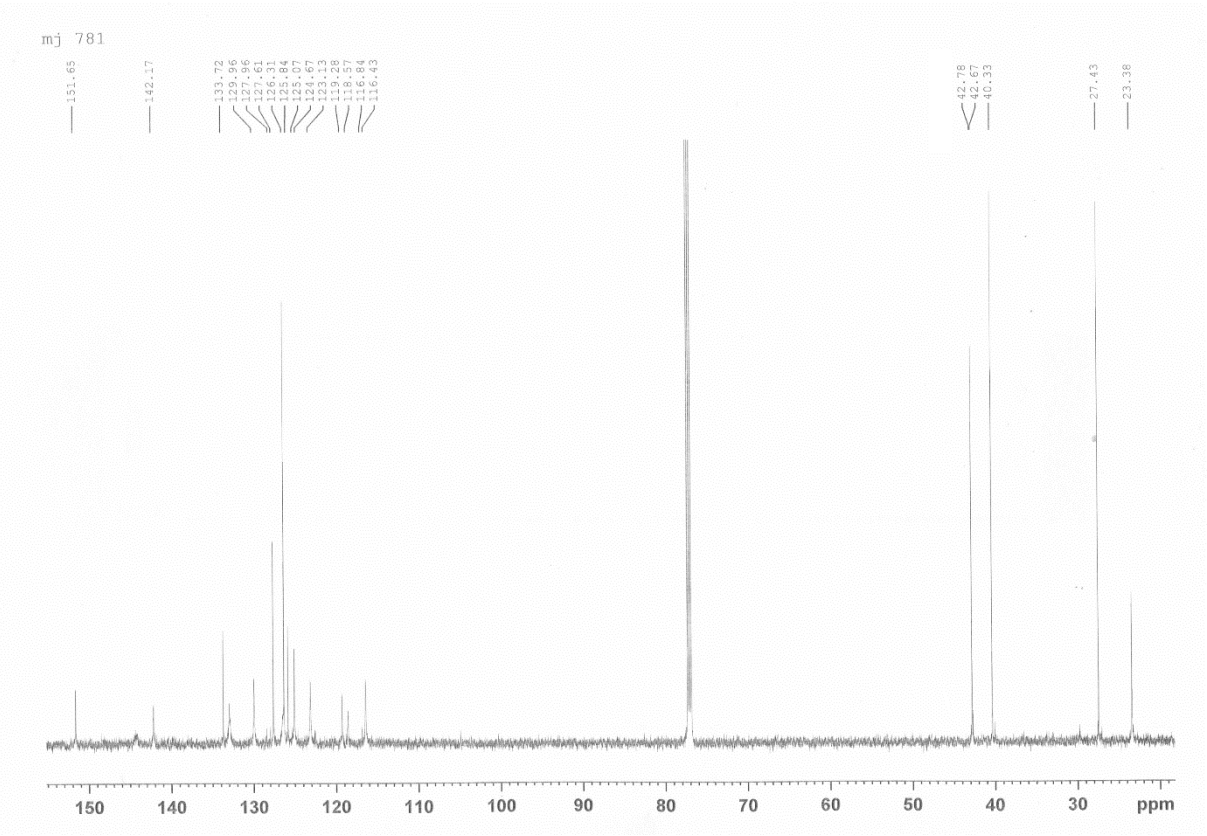
#	m/z	Res.	S/N	I	I %	FWHM
1	461.0942	43730	5526.7	6555349	100.0	0.0105
2	463.0719	41548	3633.5	4332482	66.1	0.0111

20. NMR spectra and HR MS of 8-Chloro-6-methanesulfonylaminobutylquinobenzothiazine (**23**).



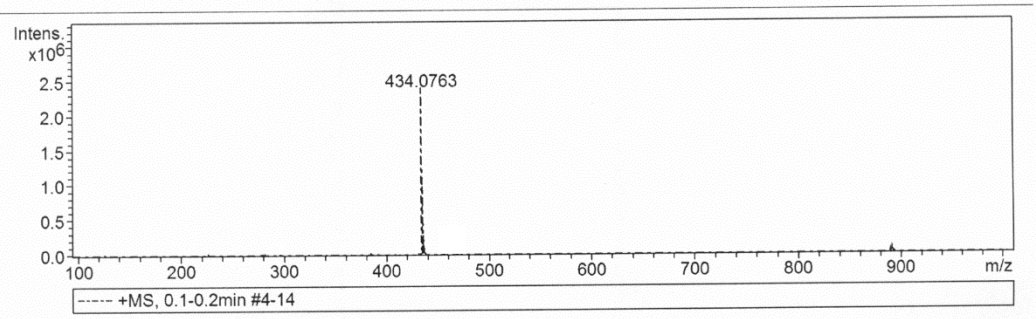
23





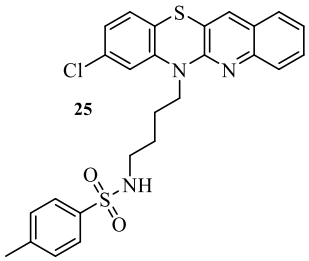
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

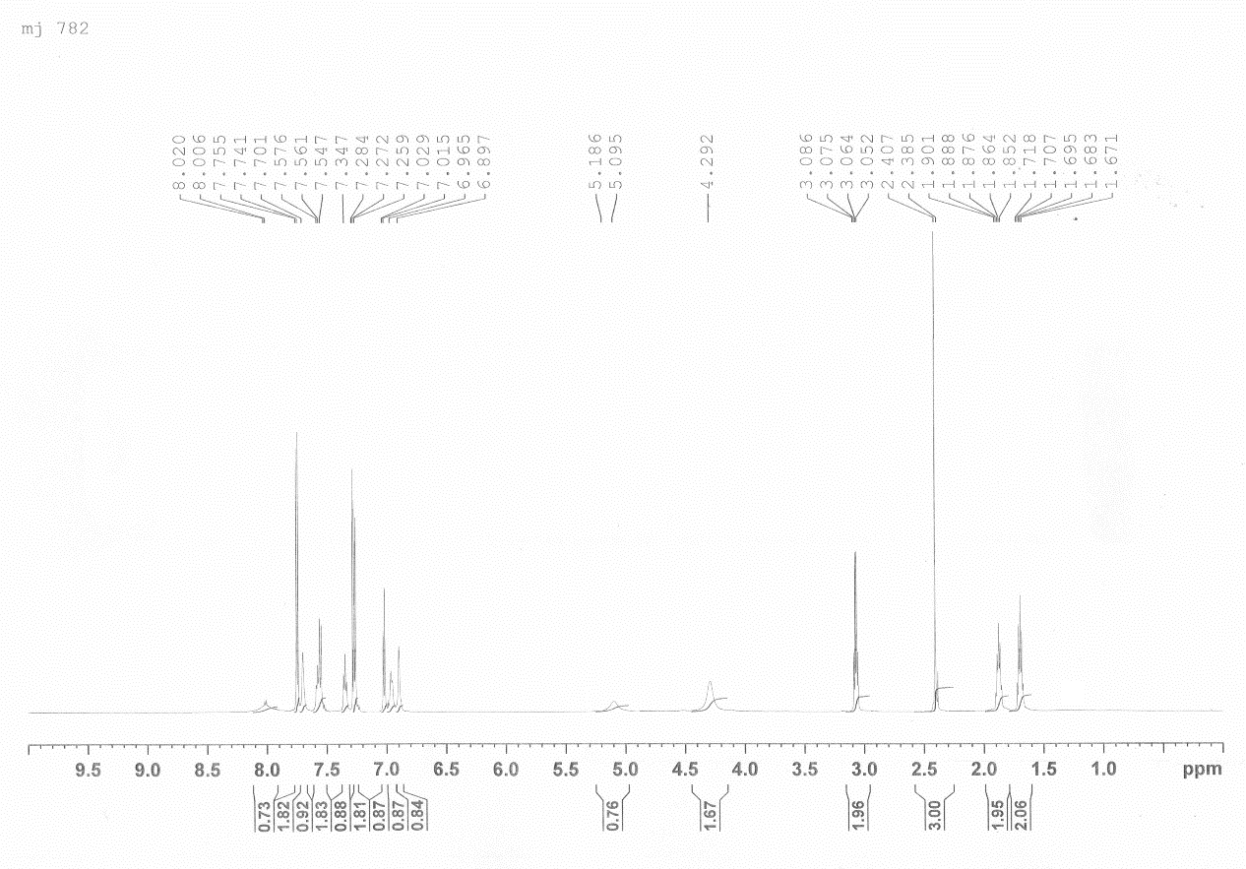


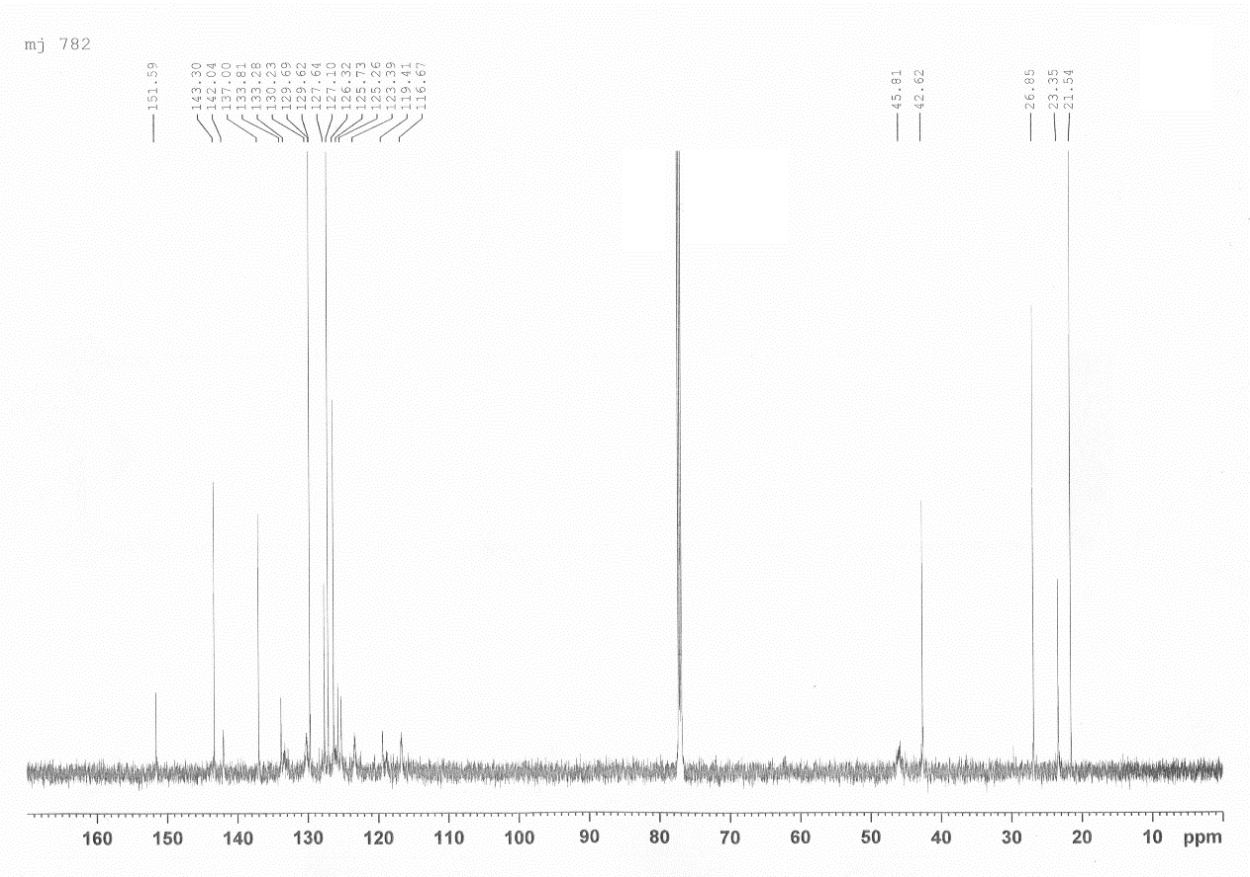
#	m/z	Res.	S/N	I	I %	FWHM
1	434.0763	13896	36384.3	2348999	100.0	0.0312
2	436.0732	13652	15313.9	993562	42.3	0.0319

21. NMR spectra and HR MS of 8-Chloro-6-p-toluenesulfonylaminobutylquinobenzothiazine (**25**).



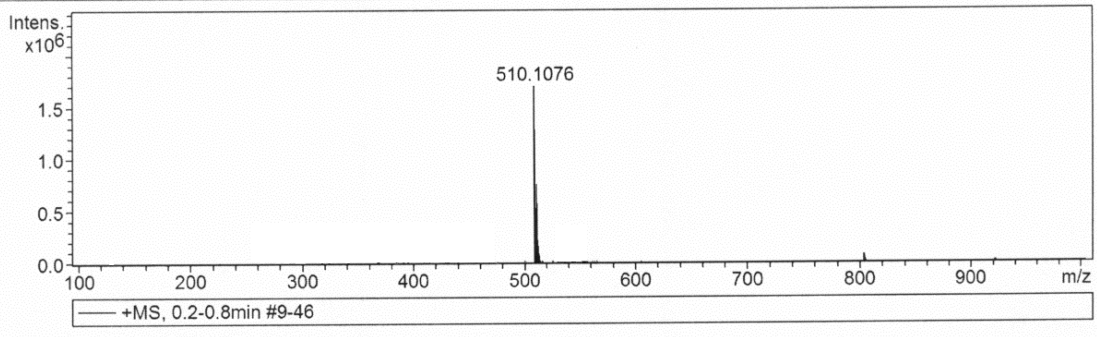
25





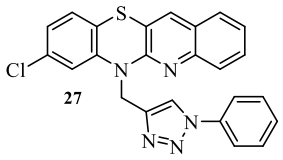
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

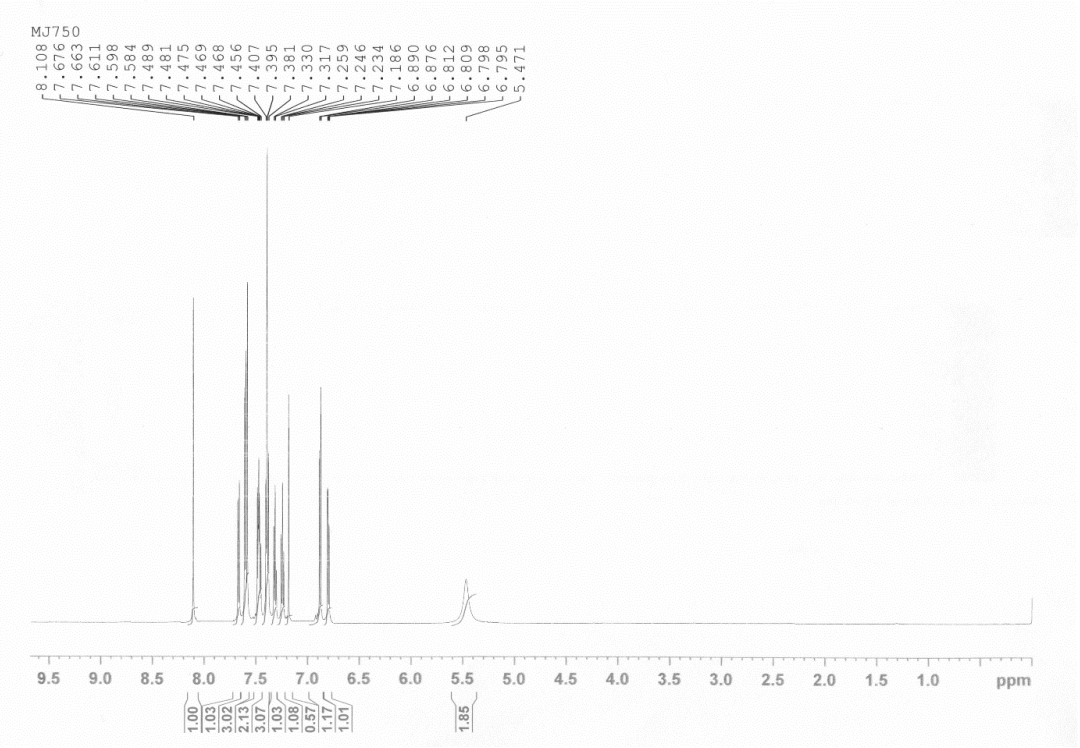


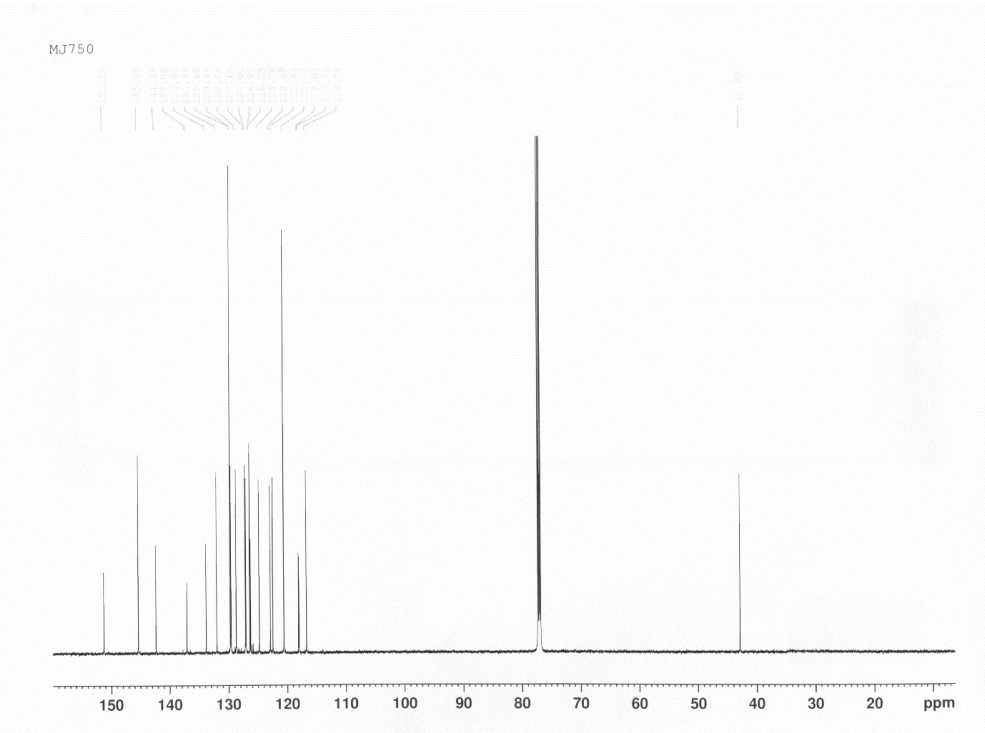
#	m/z	Res.	S/N	I	I %	FWHM
1	510.1076	13939	14844.9	1708201	100.0	0.0366
2	512.1048	13680	6597.7	761488	44.6	0.0374

22. NMR spectra and HR MS of 8-chloro-6-[(1-phenyl-1H-1,2,3-triazol-4-yl)methyl]-quinobenzo[1,4]thiazine (**27**).



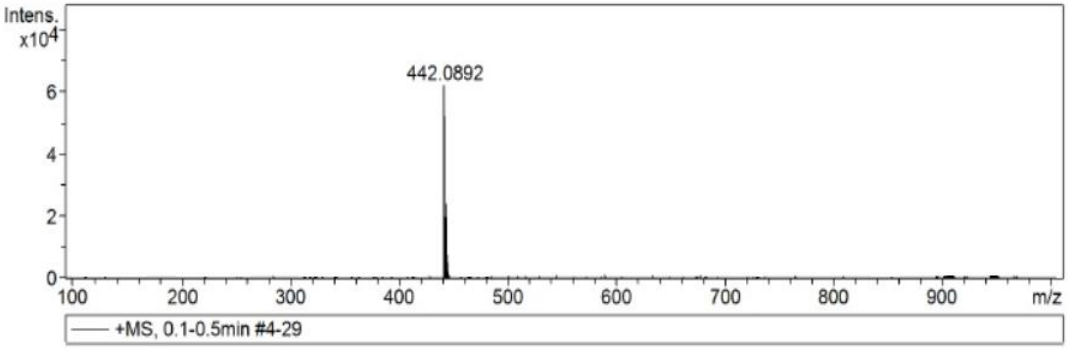
27





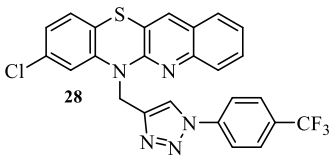
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

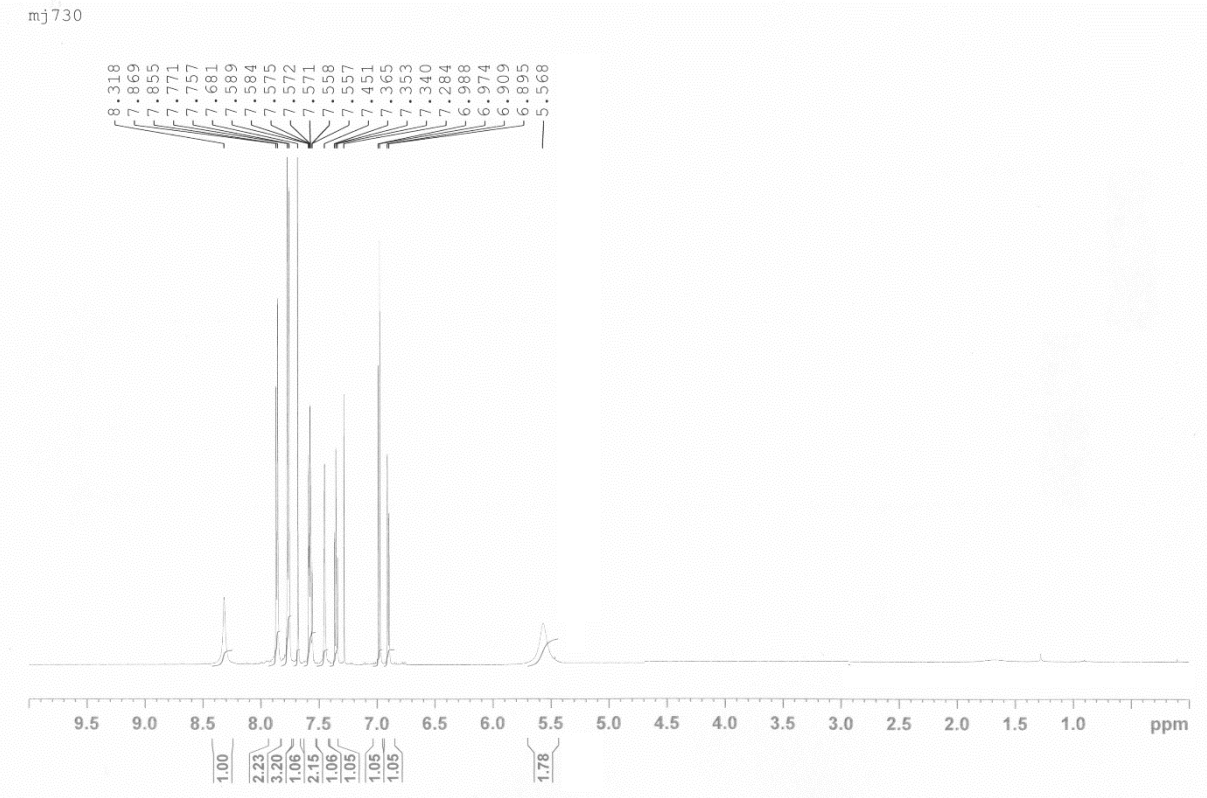


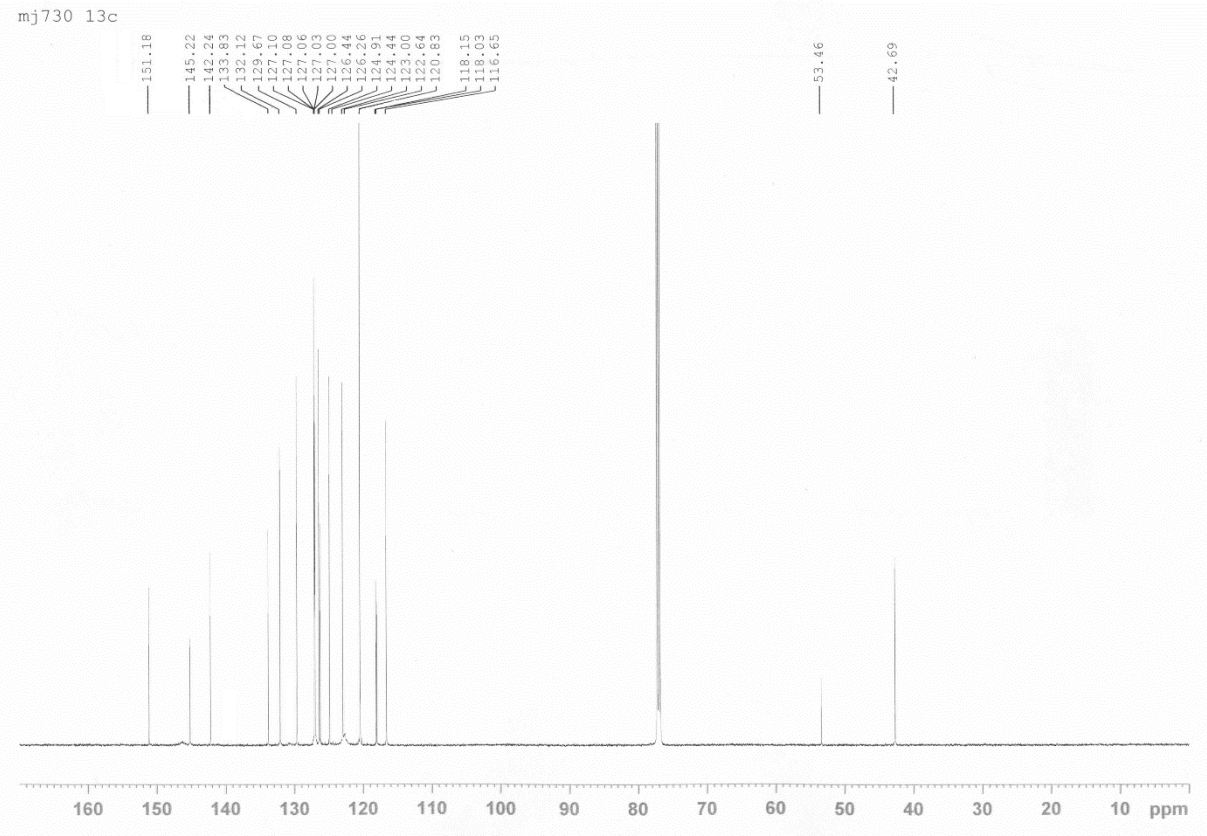
#	m/z	Res.	S/N	I	I %	FWHM
1	442.0892	22688	4657.9	61769	100.0	0.0195
2	444.0868	21031	1818.3	24166	39.1	0.0211

23. NMR spectra and HR MS of 8-chloro-6-[(1-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)methyl]-quinobenzo[1,4]thiazine (**28**).



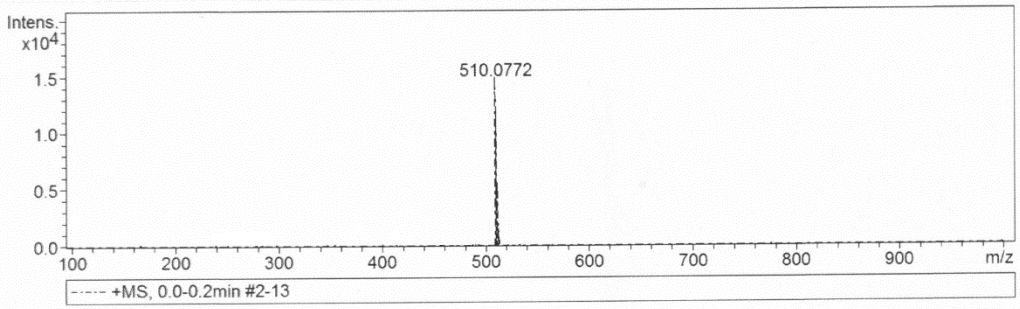
28





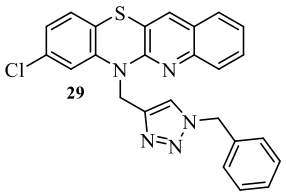
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

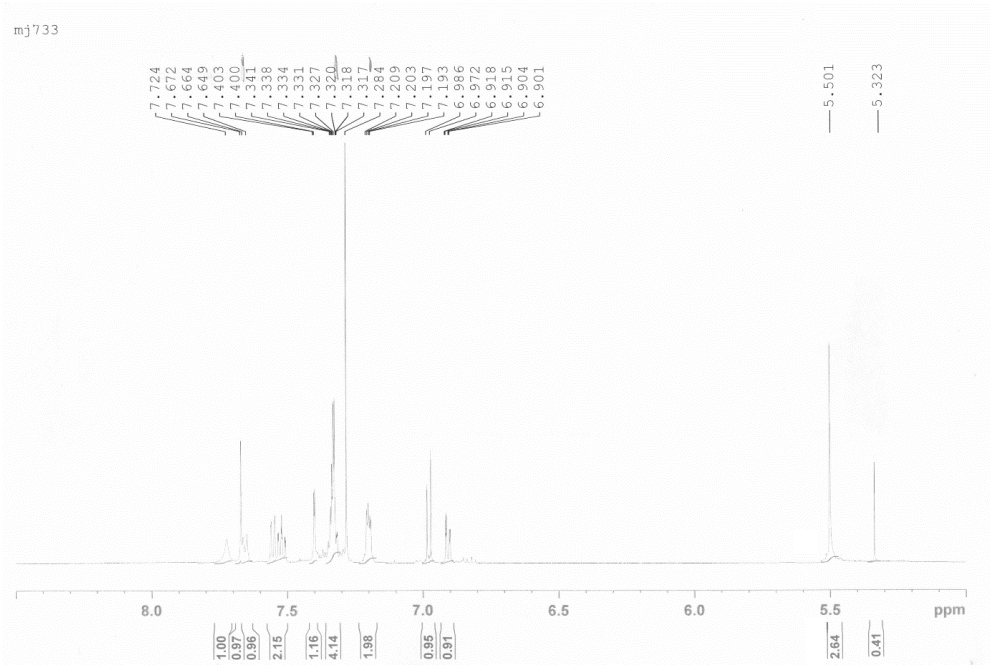


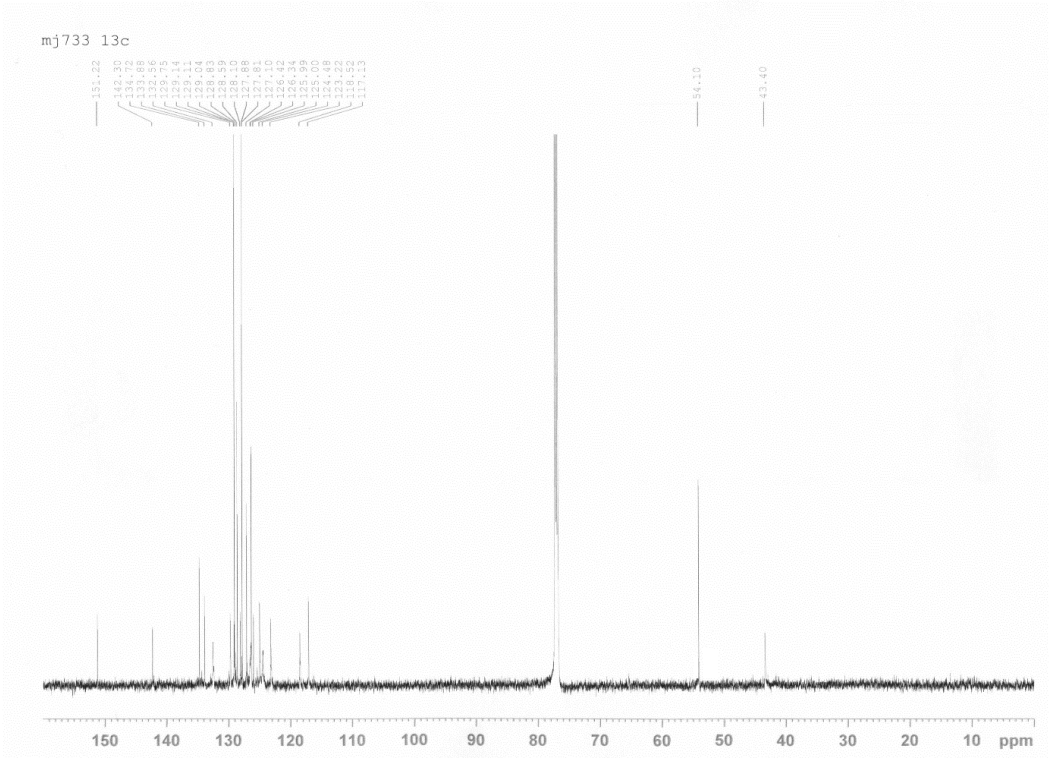
#	m/z	Res.	S/N	I	I %	FWHM
1	510.0772	22849	1149.1	14607	100.0	0.0223

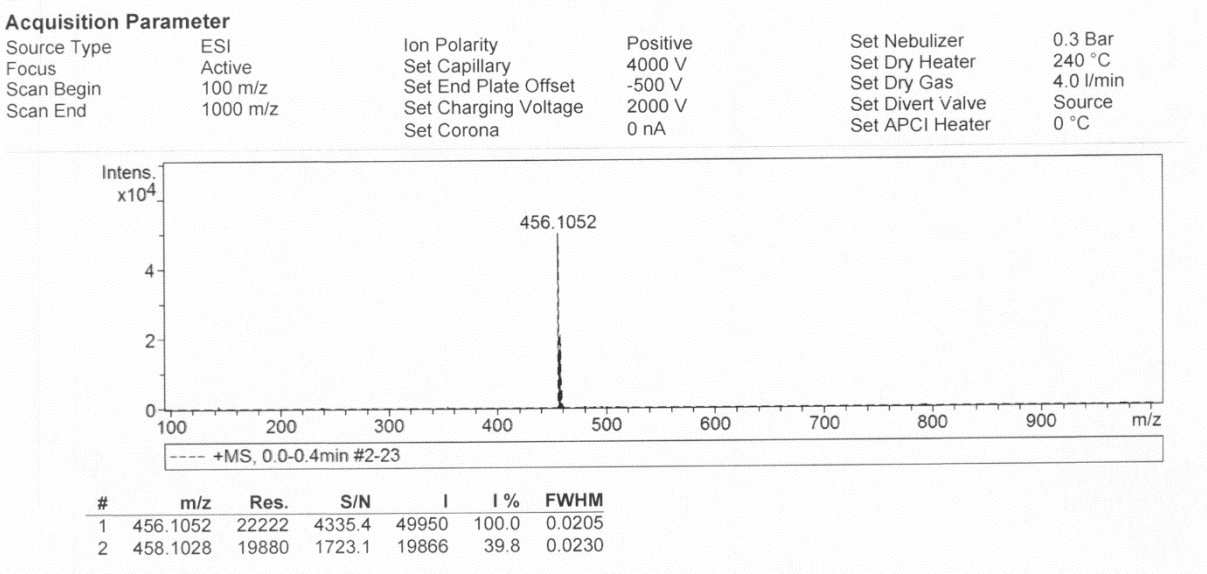
24. NMR spectra and HR MS of 8-chloro-6-[(1-Benzyl-1H-1,2,3-triazol-4-yl)-methyl]-quinobenzo[1,4]thiazine (**29**).



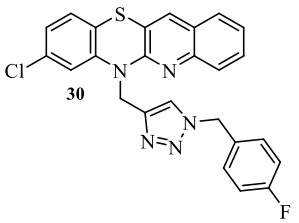
29

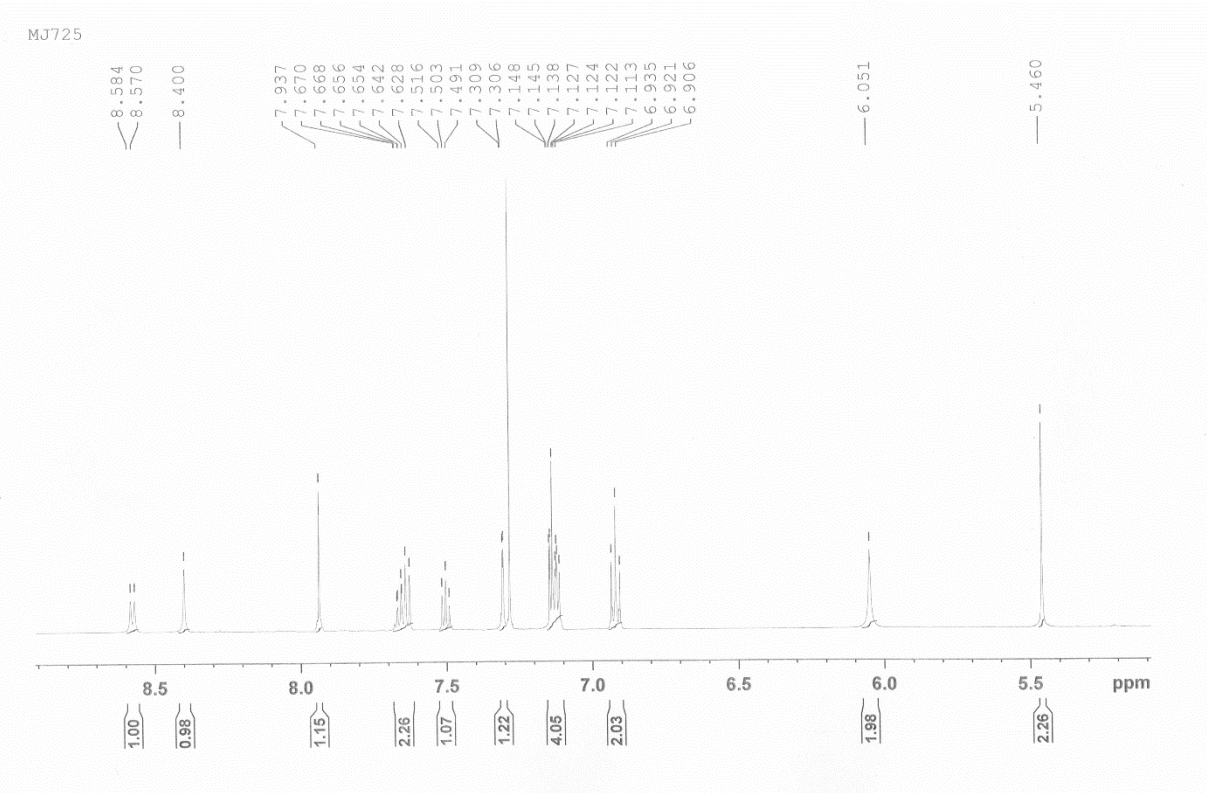


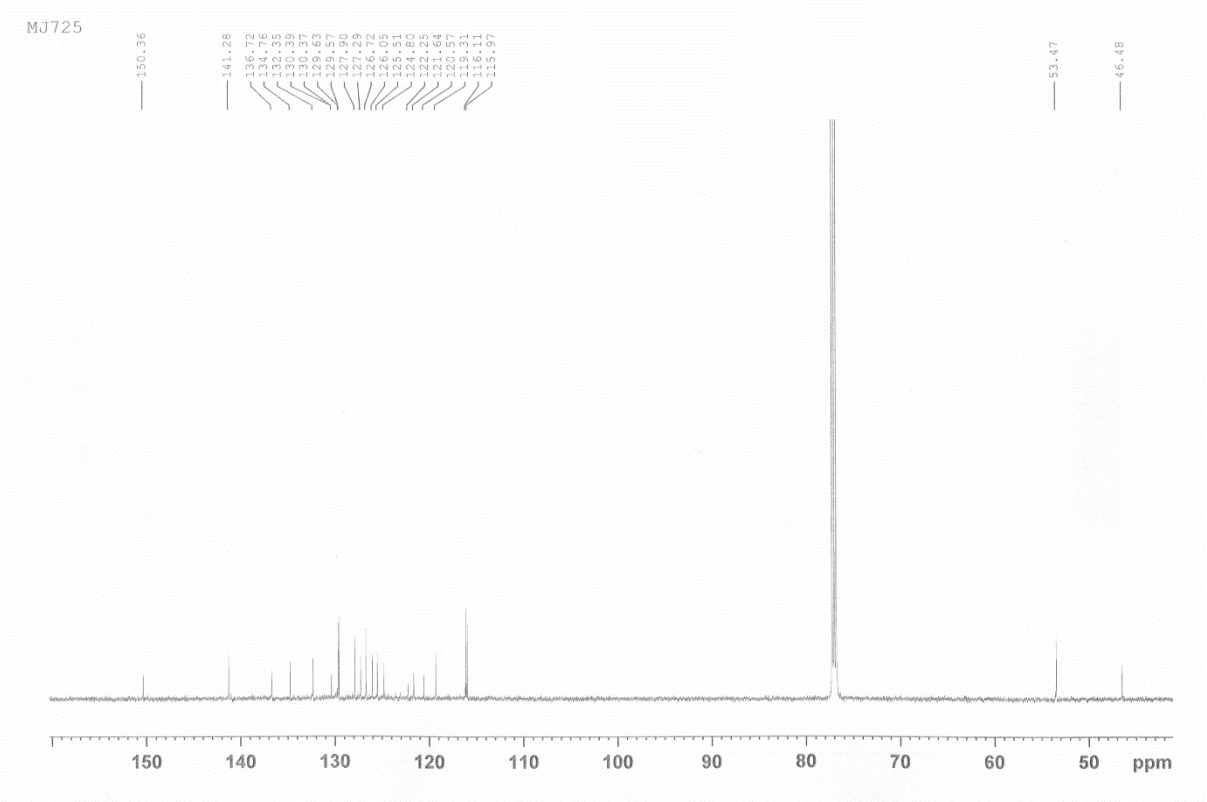




25. NMR spectra and HR MS of 8-chloro-6-[(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]-quinobenzo[1,4]thiazine (**30**).

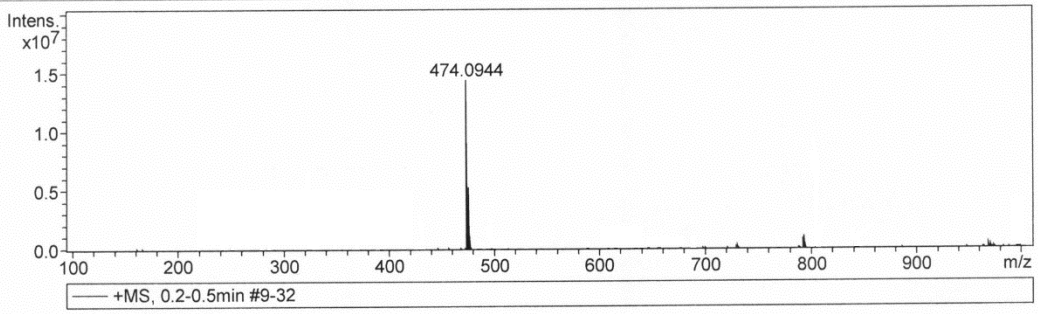






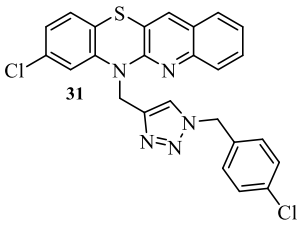
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

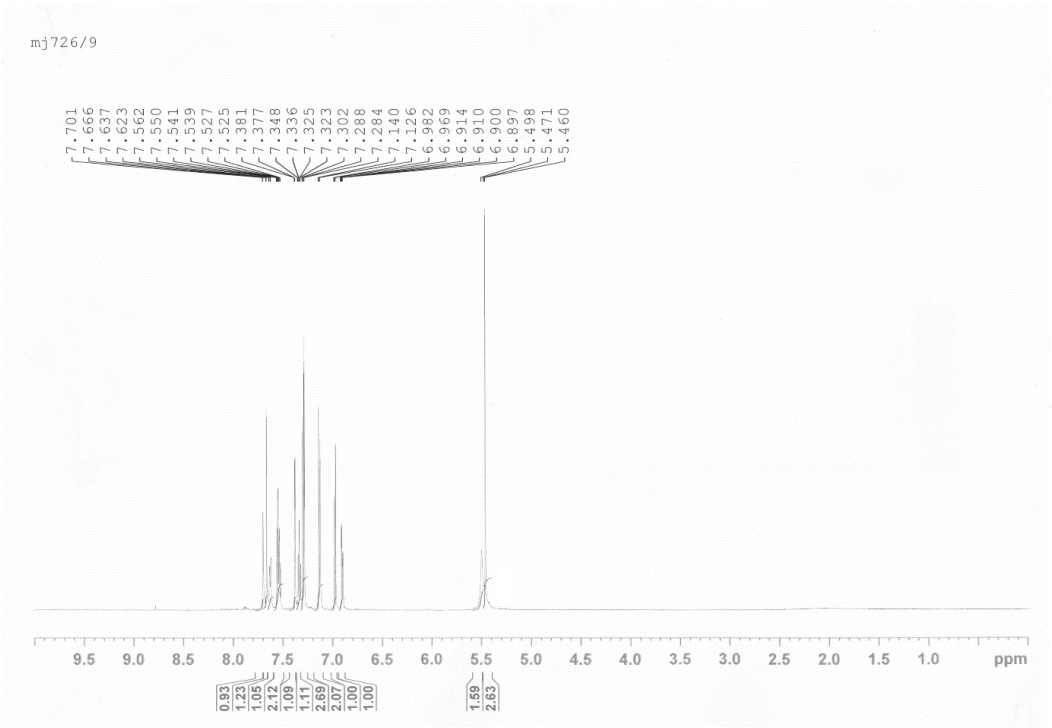


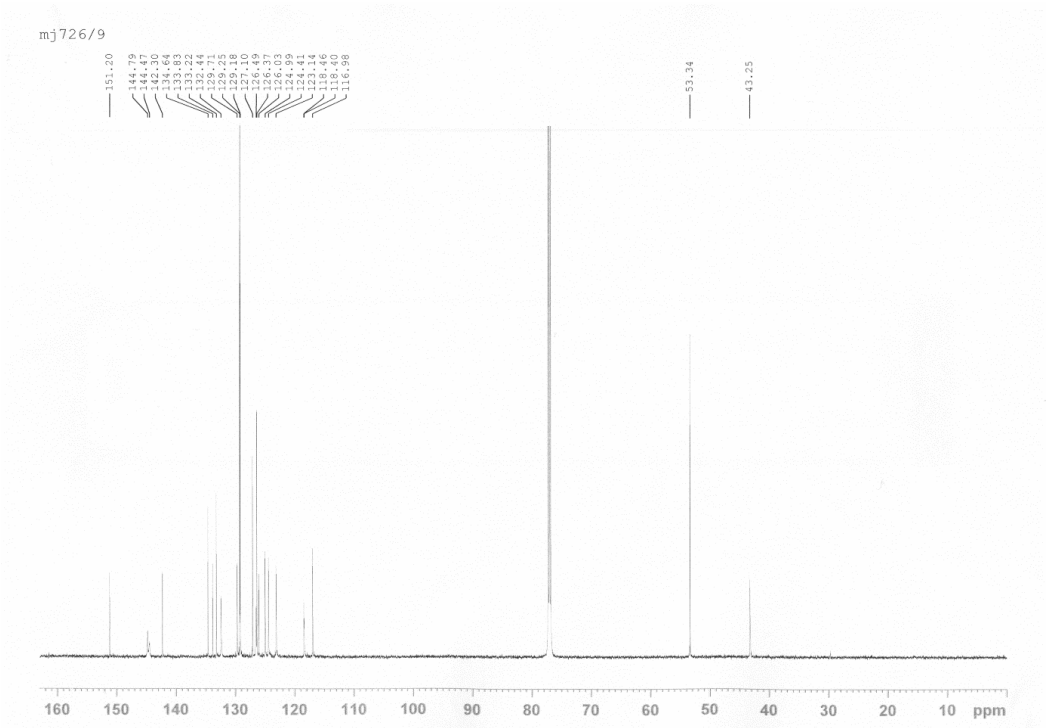
#	m/z	Res.	S/N	I	I %	FWHM
1	474.0944	48156	15401.2	14340540	100.0	0.0098
2	476.0916	46723	5583.8	5264247	36.7	0.0102

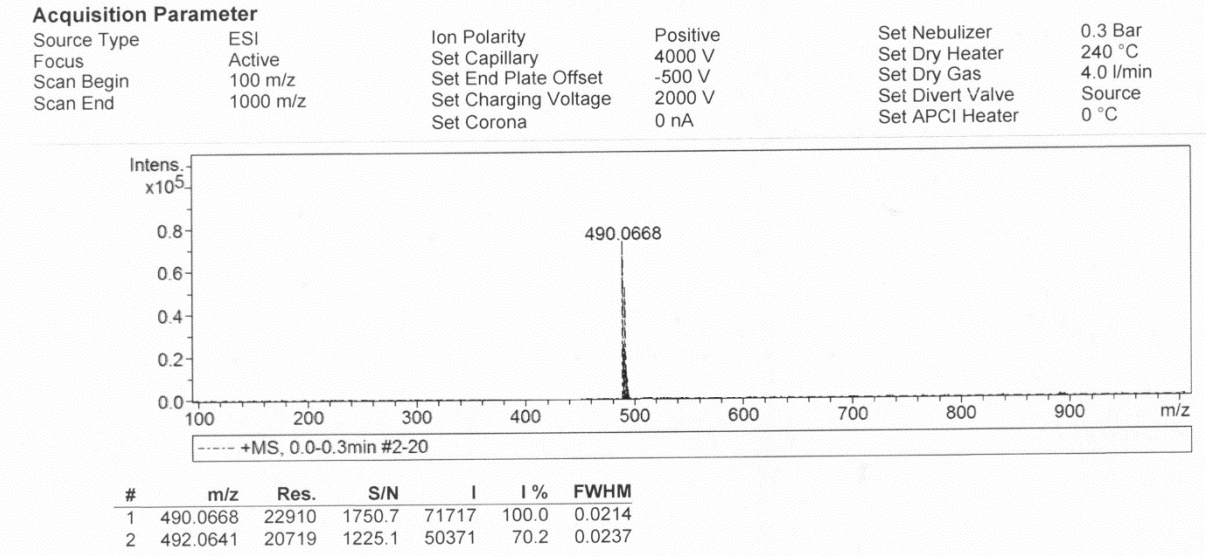
26. NMR spectra and HR MS of 8-chloro-6-[(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]-quinobenzo[1,4]thiazine (**31**).



31

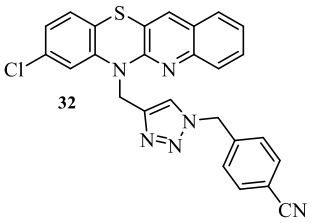




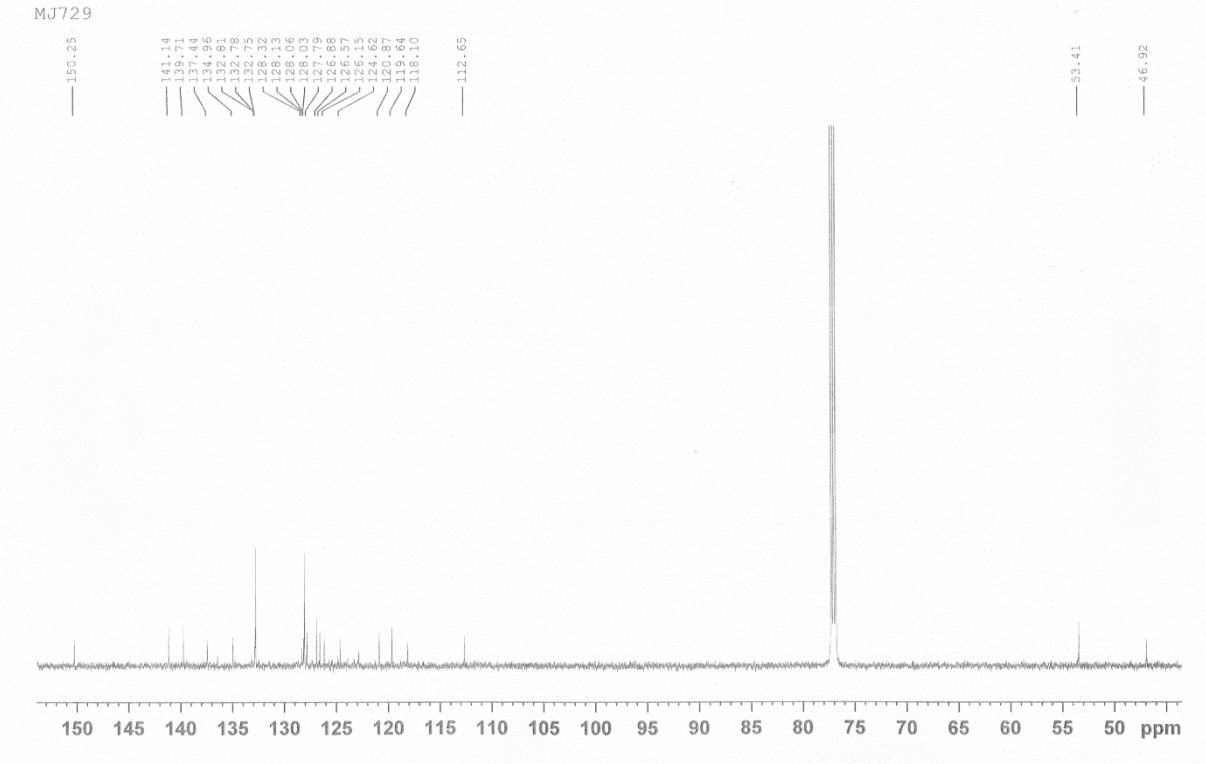


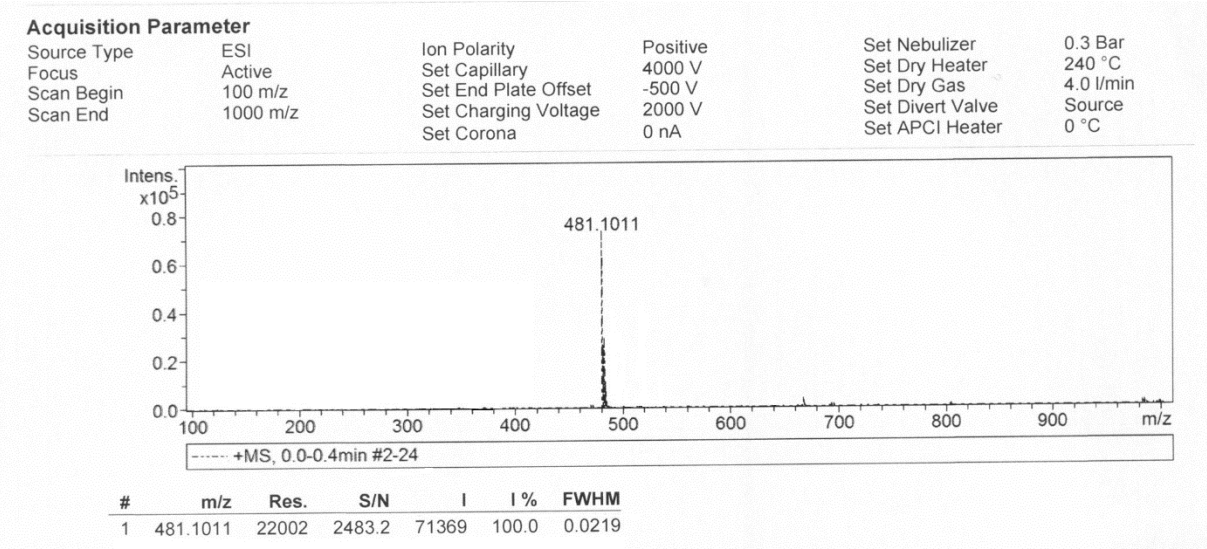
#	m/z	Res.	S/N	I	I %	FWHM
1	490.0668	22910	1750.7	71717	100.0	0.0214
2	492.0641	20719	1225.1	50371	70.2	0.0237

27. NMR spectra and HR MS of 8-chloro-6-[(1-(4-cyanobenzyl)-1H-1,2,3-triazol-4-yl)methyl]-quinobenzo[1,4]thiazine (**32**).

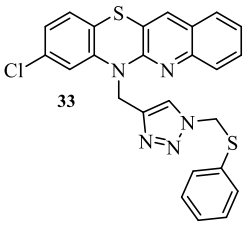


32

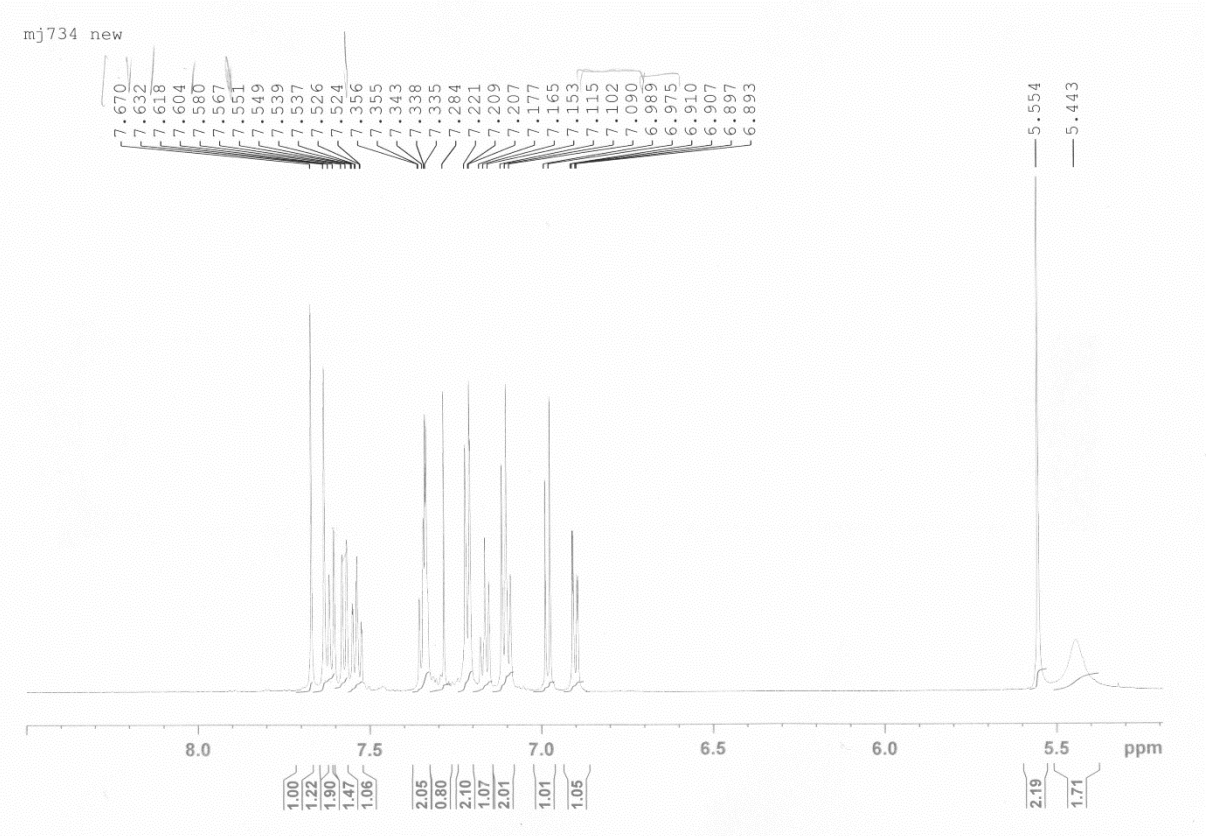


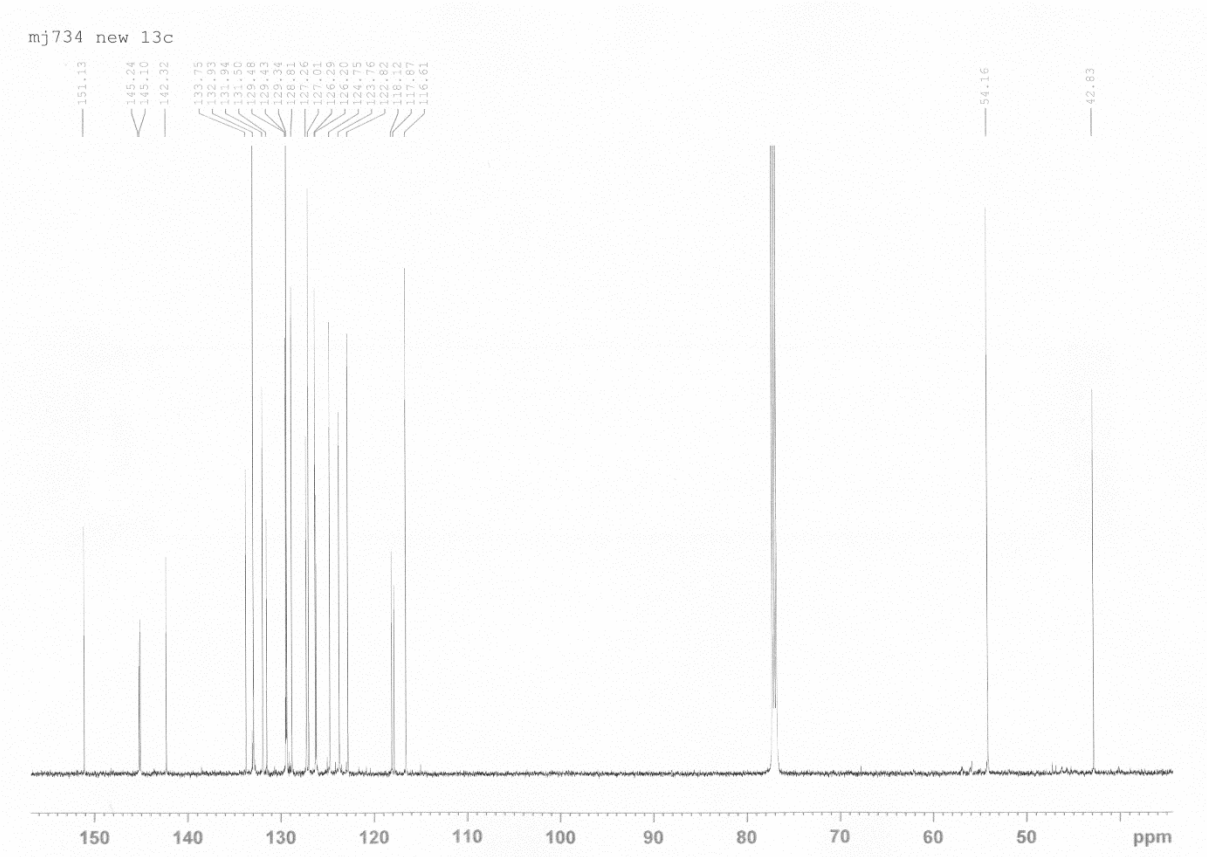


28. NMR spectra and HR MS of 8-chloro-6-[(1-phenylthiomethyl-1H-1,2,3-triazolo-4-ylo)methyl]-quinobenzo[1,4]thiazine (**33**).



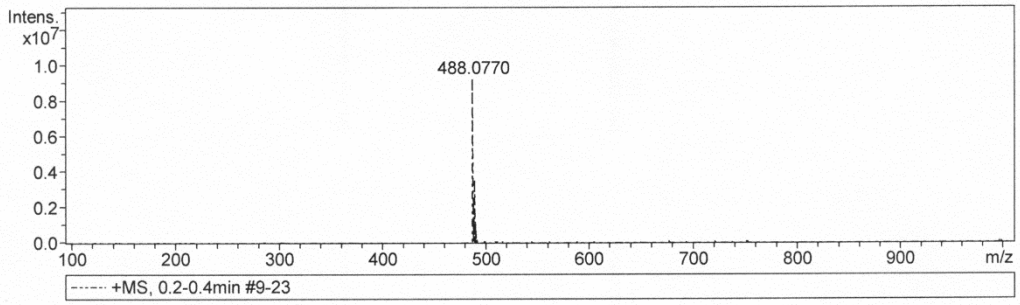
33





Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	240 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	m/z	Res.	S/N	I	I %	FWHM
1	488.0770	48345	16381.6	9268264	100.0	0.0101
2	490.0740	43308	6352.0	3594898	38.8	0.0113