

## Supporting Materials

Article

### **[1,2,4]triazolo[4,3-*a*]quinoxaline as novel scaffold in the Imiquinalines family : candidates with cytotoxic activities on melanoma cell lines.**

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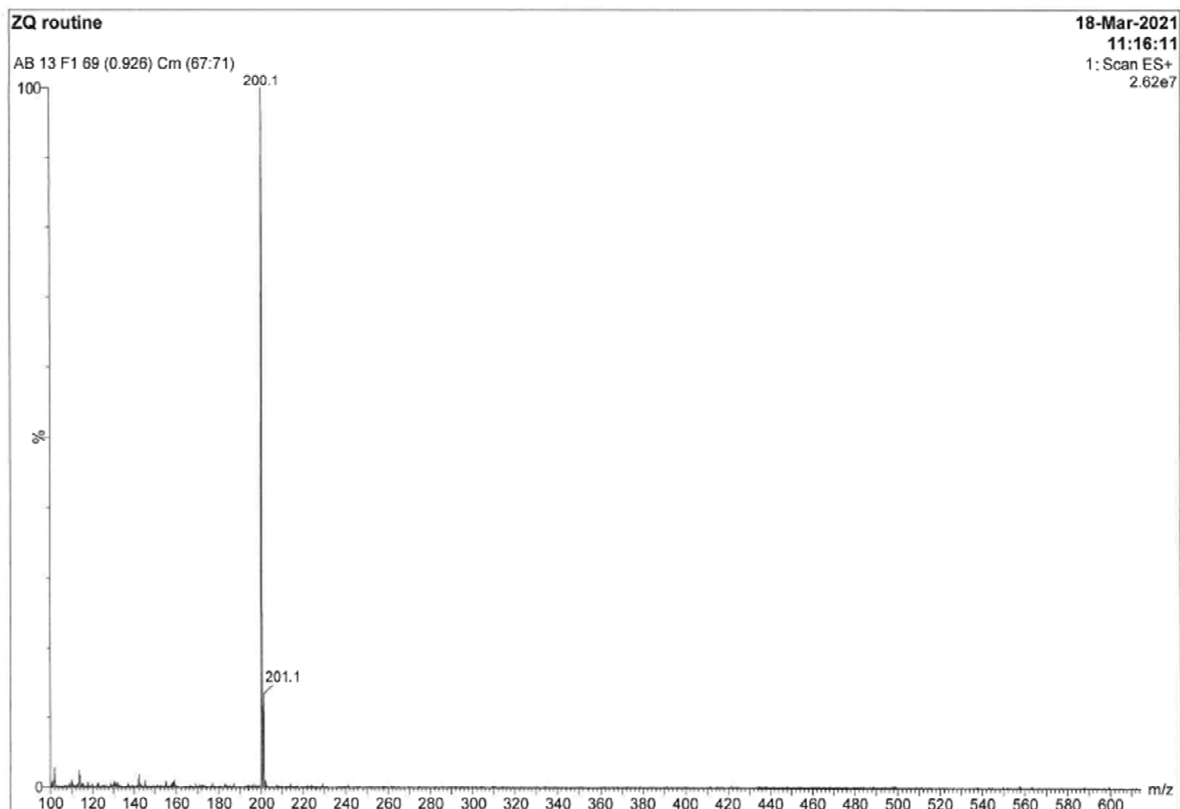
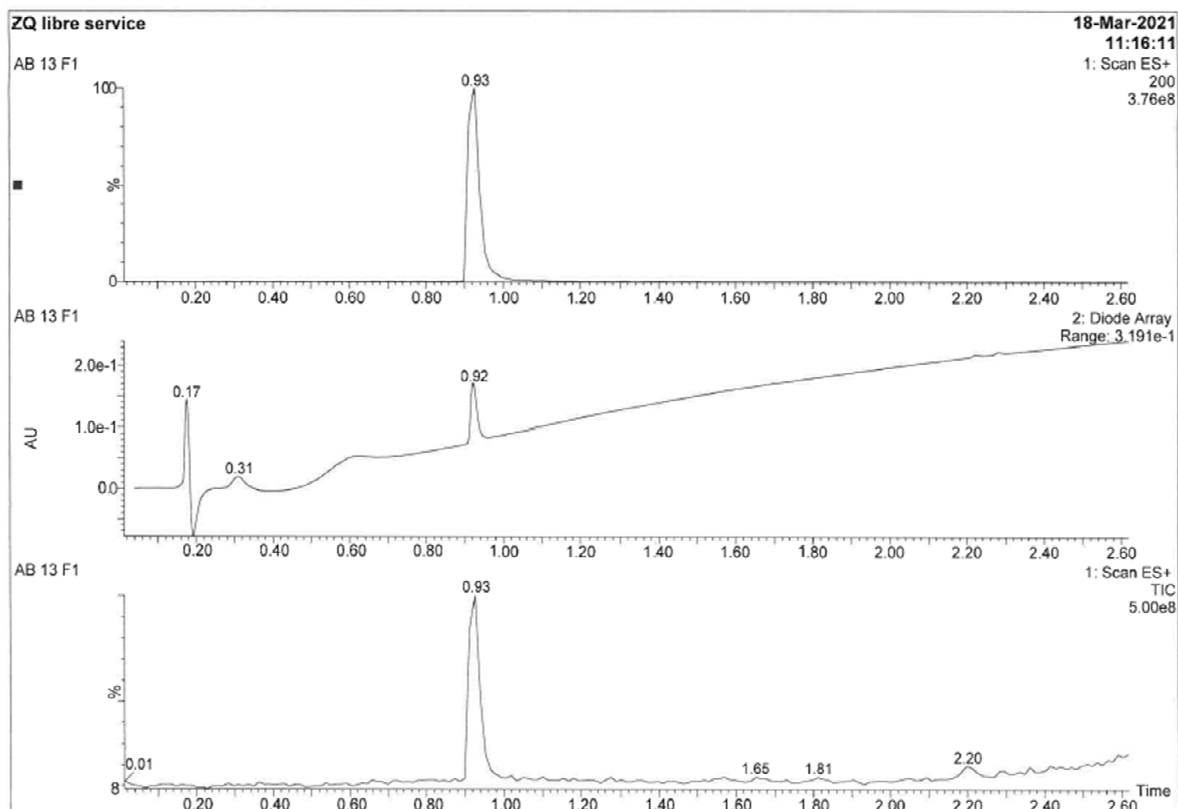


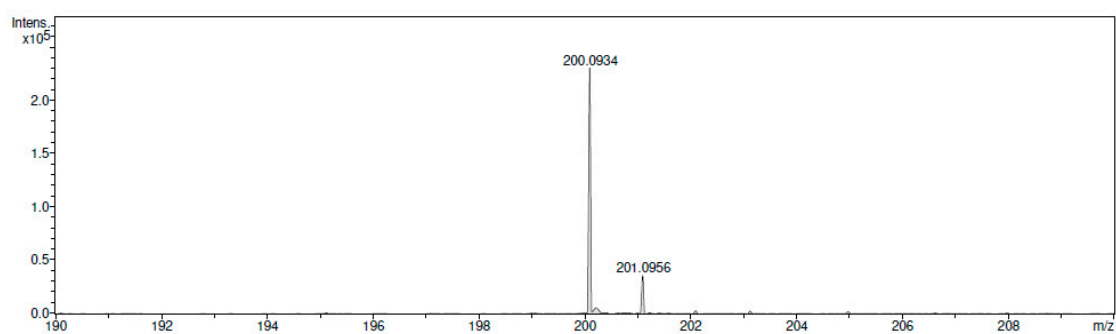
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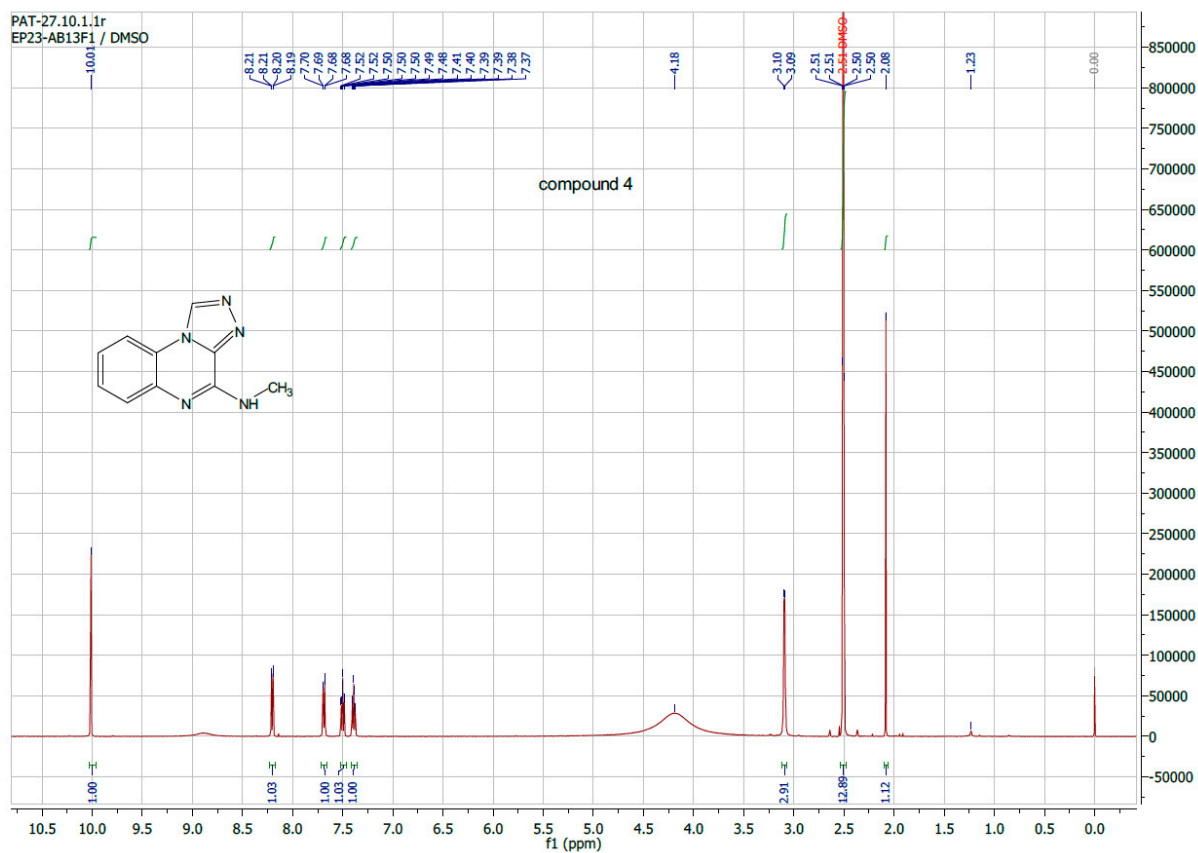


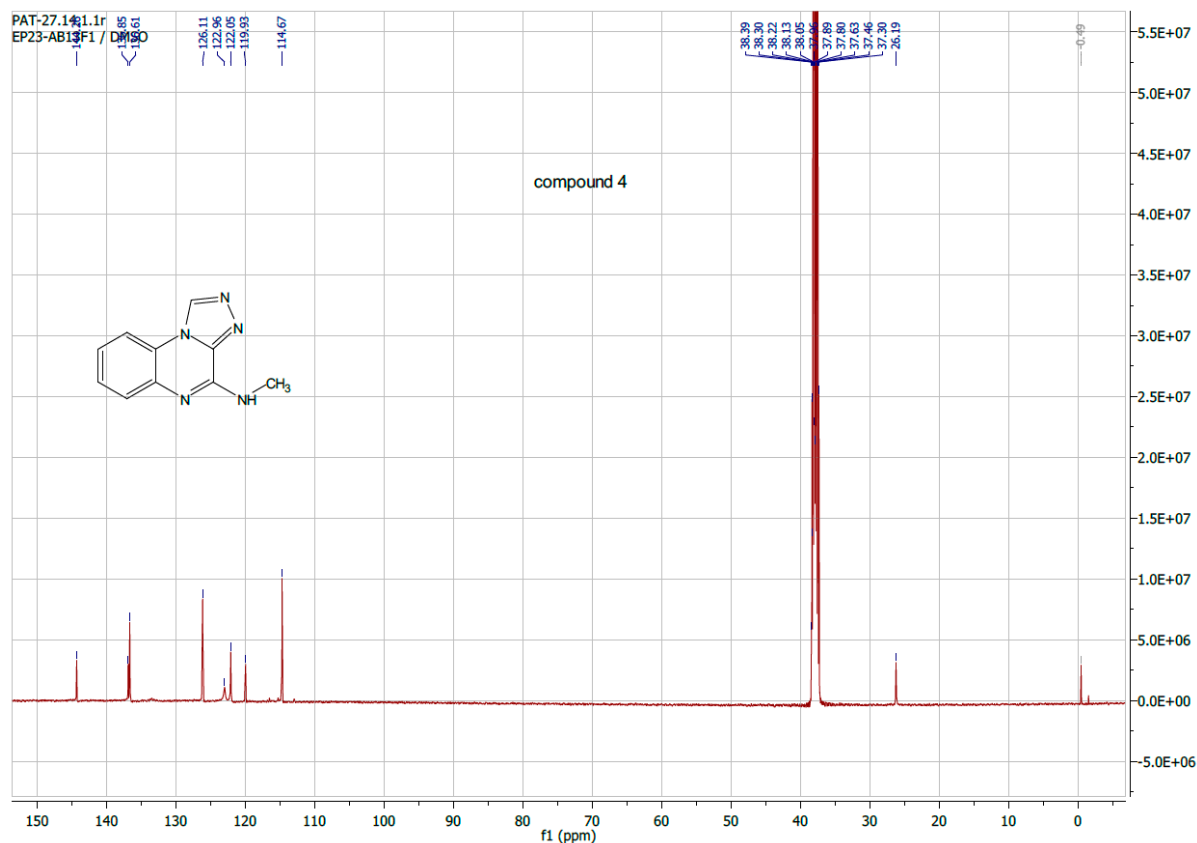
S1. *N*-methyl-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-yl-amine (4).



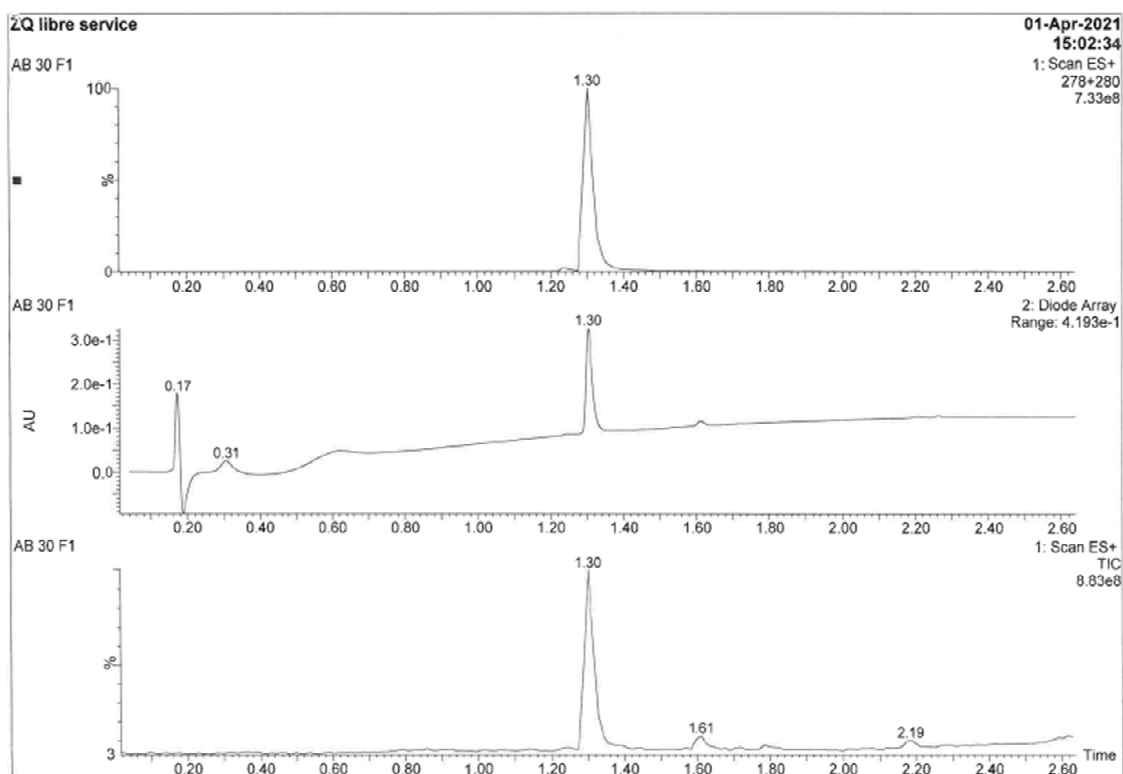


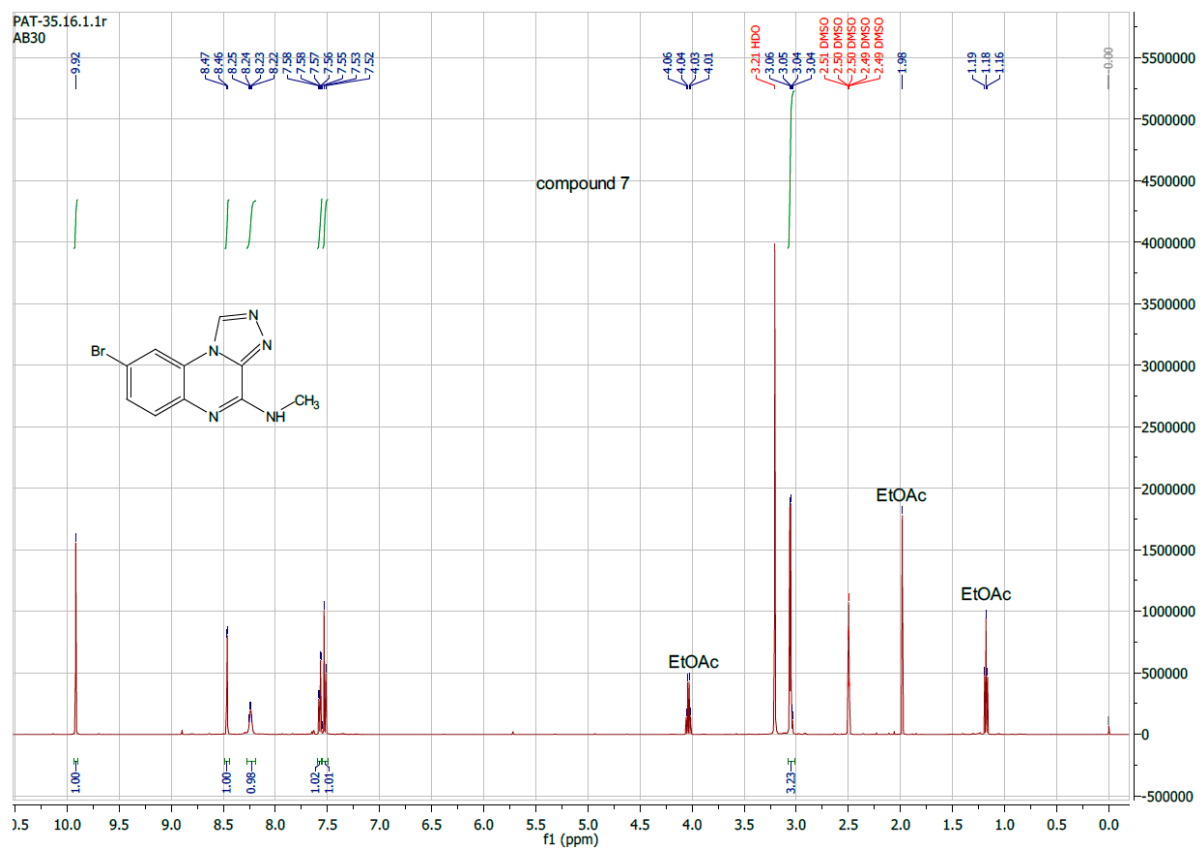
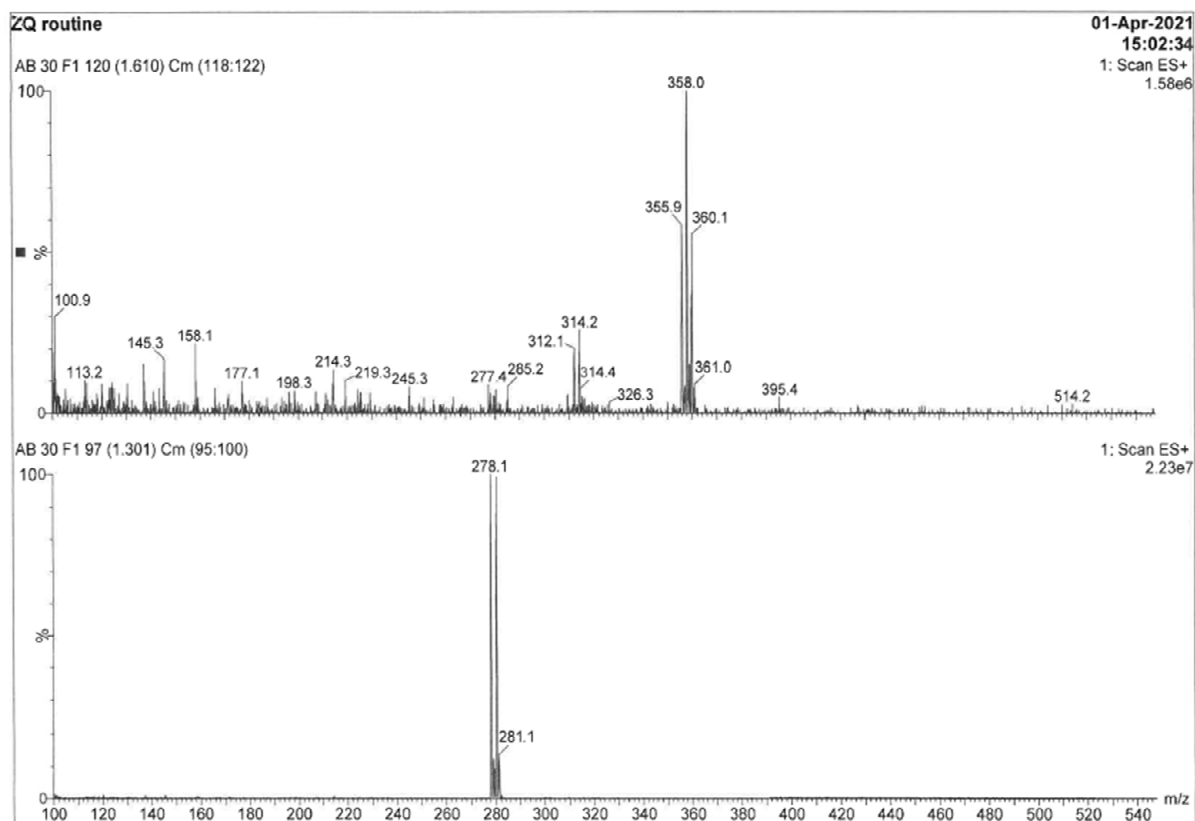
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
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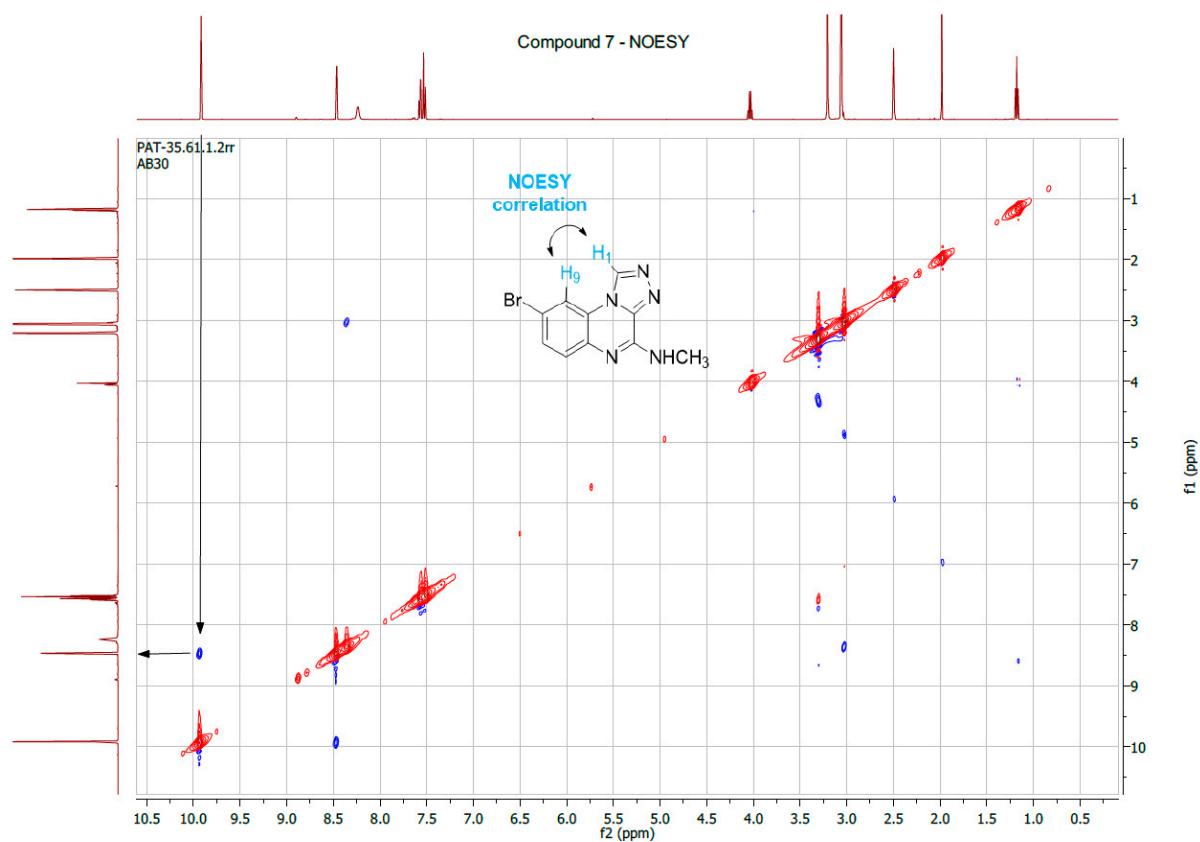
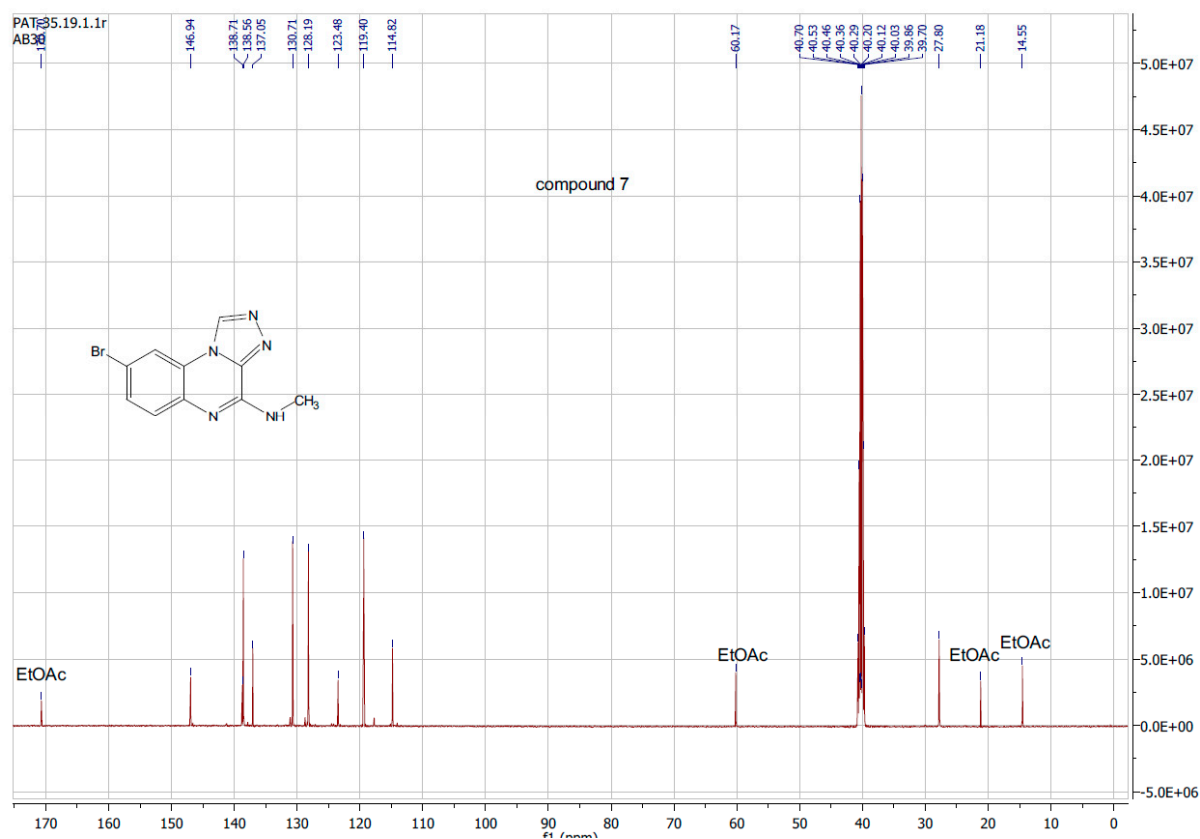


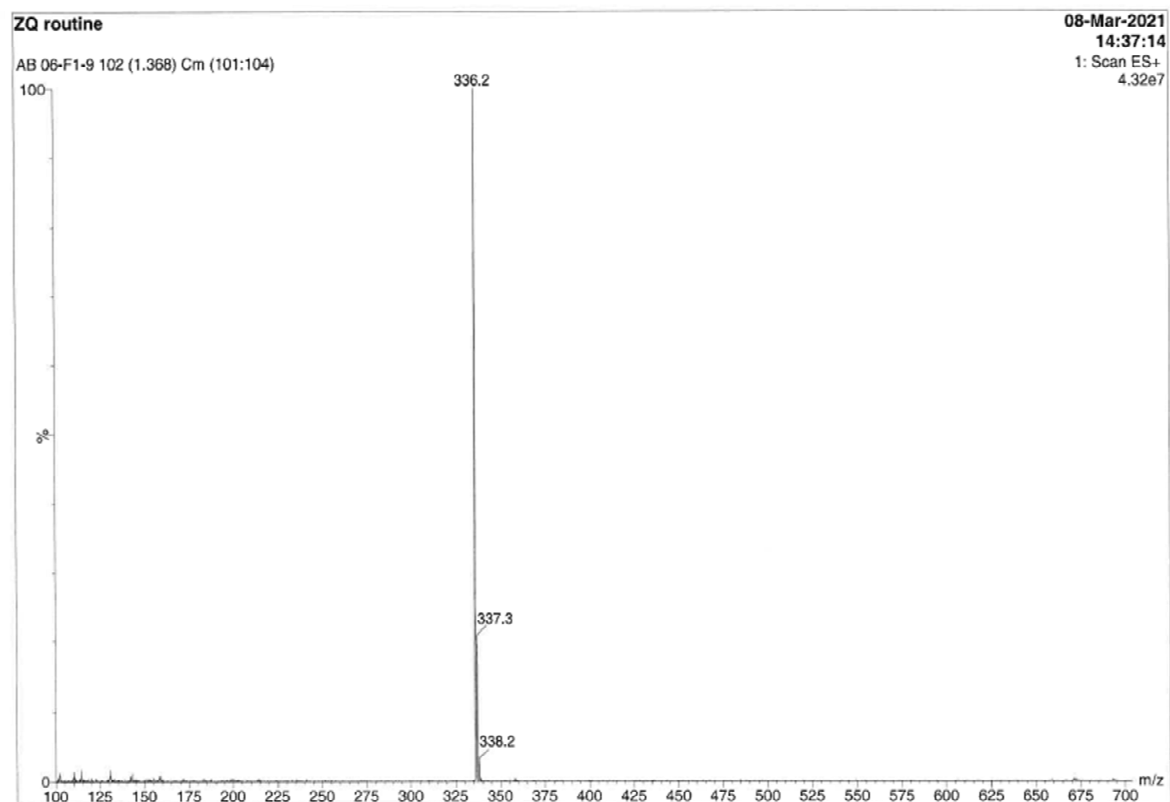
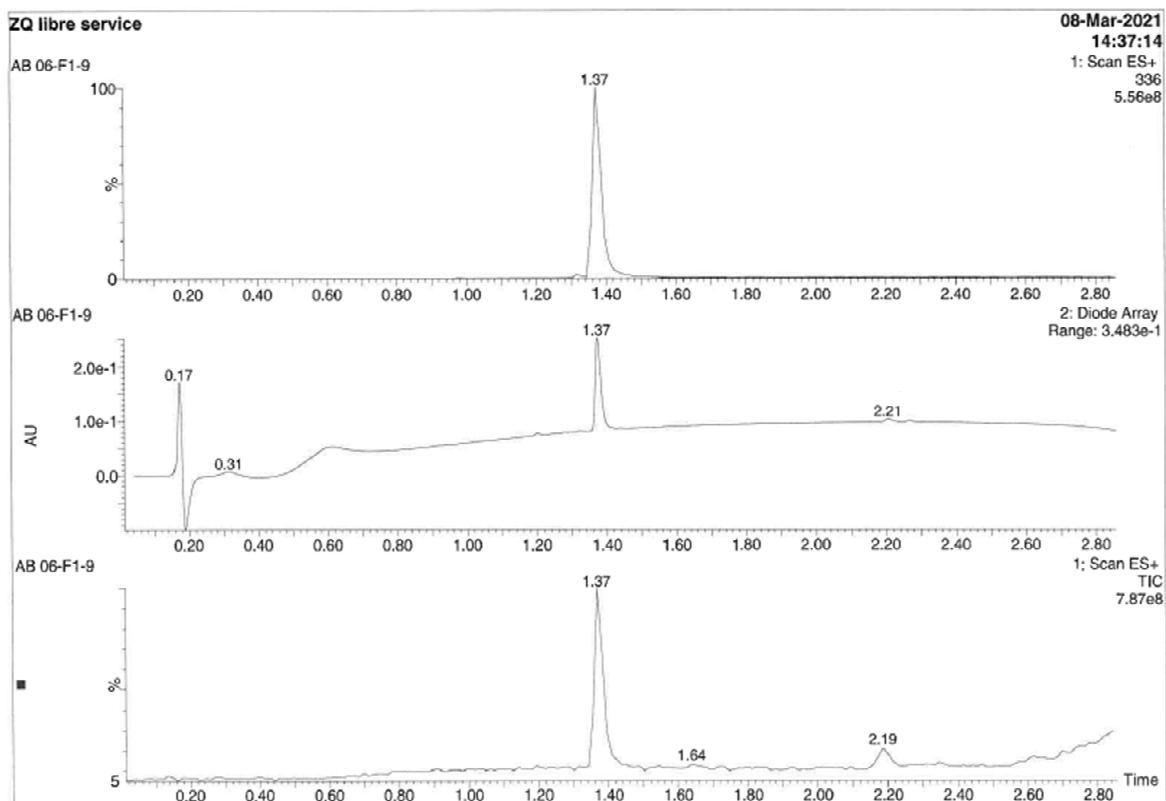


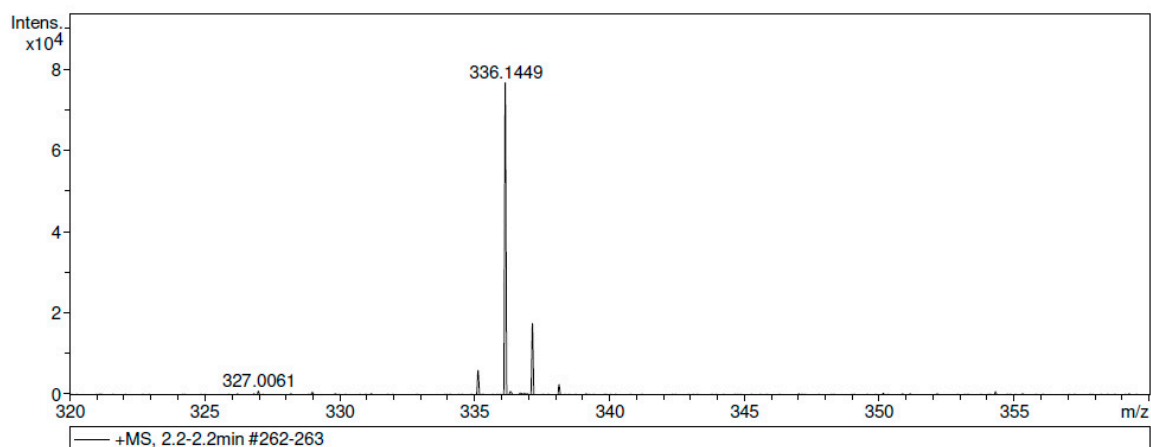
S2. 8-Bromo-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl)-methyl-amine (**7**).



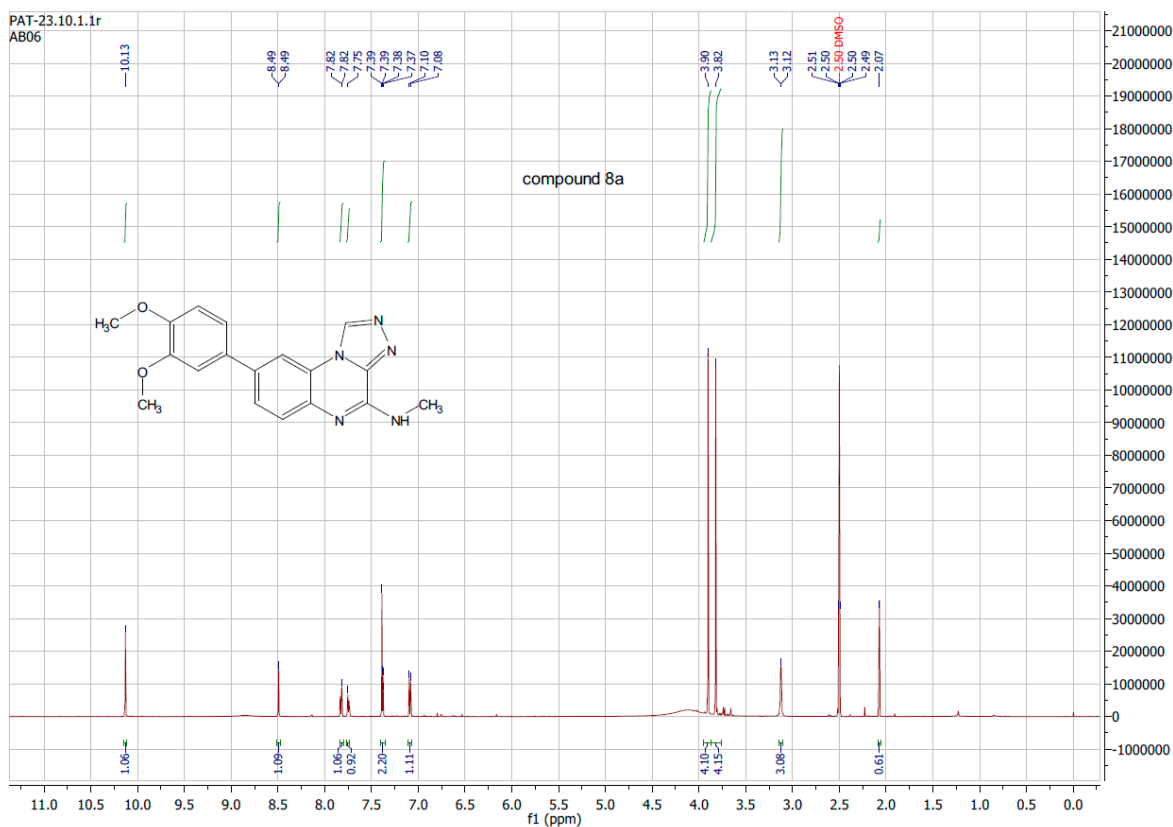


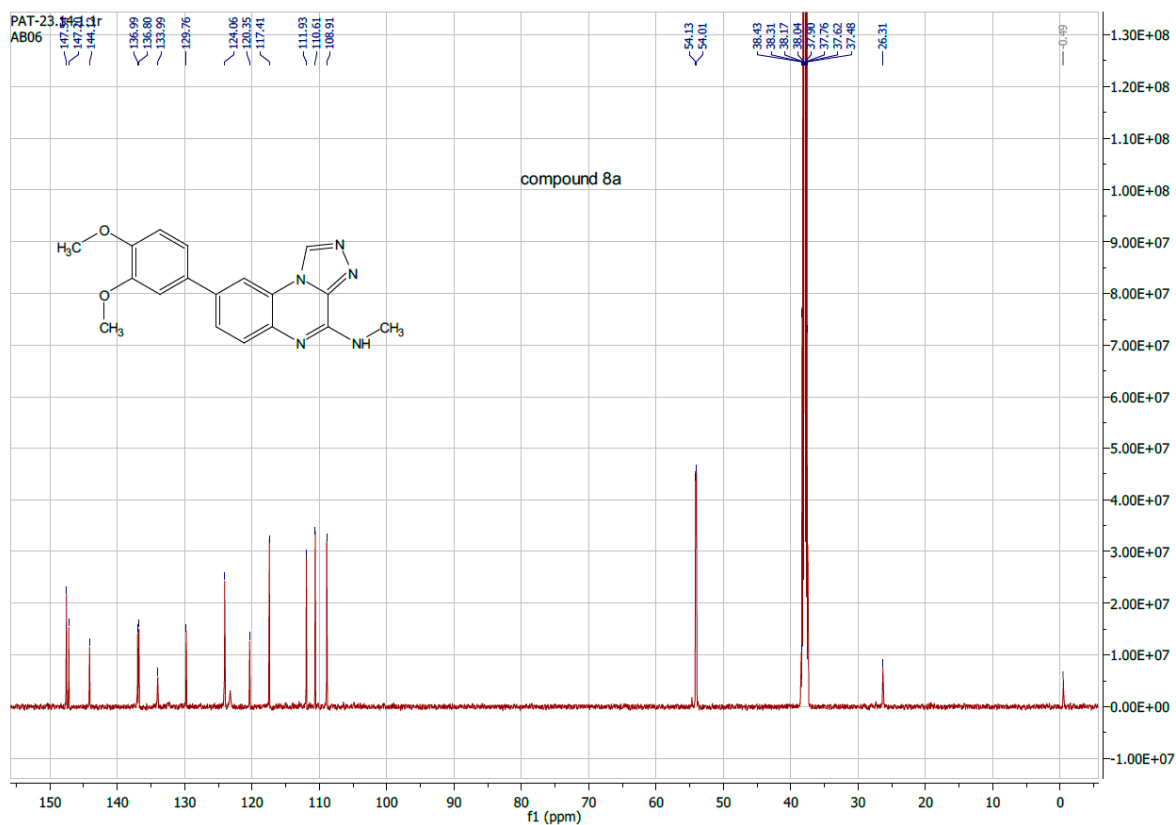


S3. [8-(3,4-Dimethoxy-phenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl]-methyl-amine (**8a**).

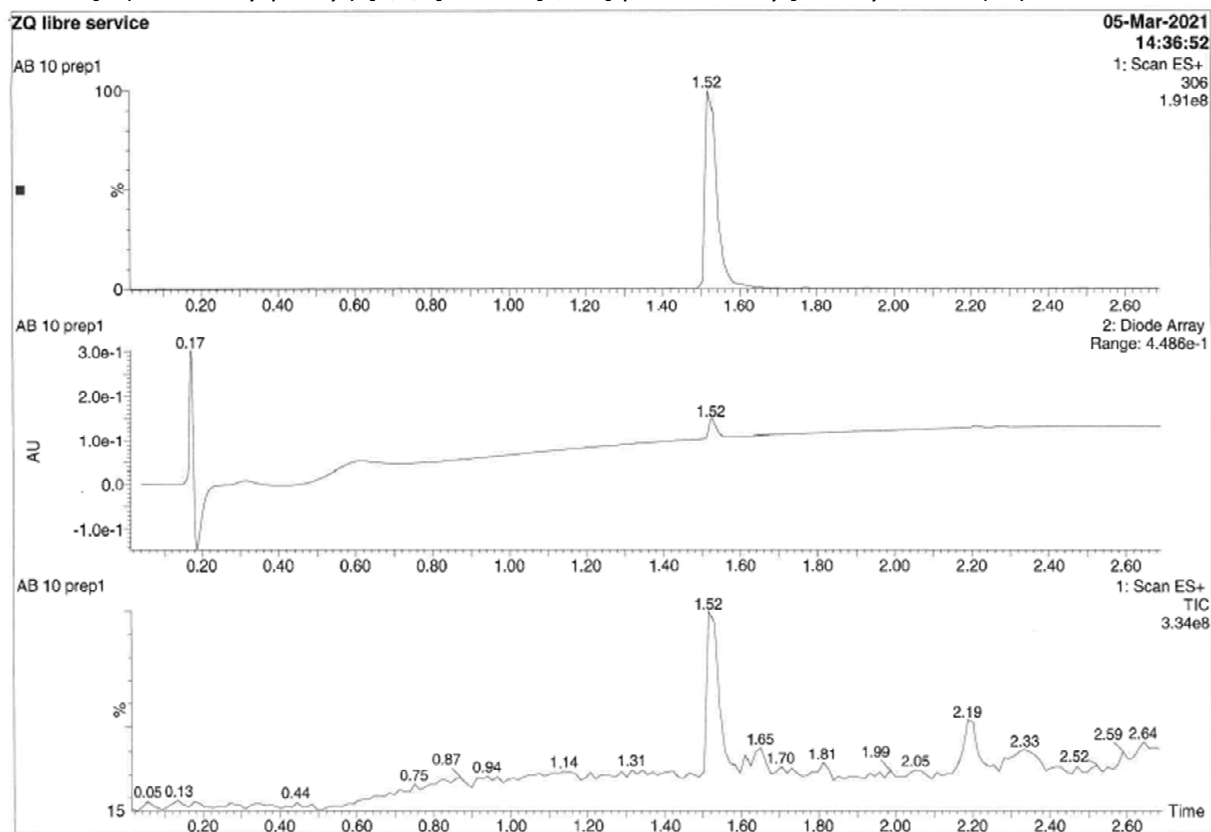


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
336.1449	1	C <sub>18</sub> H <sub>18</sub> N <sub>5</sub> O <sub>2</sub>	336.1455	-1.9	8.2	1	100.00	12.5	even		ok
	2	C <sub>17</sub> H <sub>22</sub> N <sub>5</sub> O <sub>6</sub>	336.1442	-2.1	20.6	2	74.52	7.5	even		ok

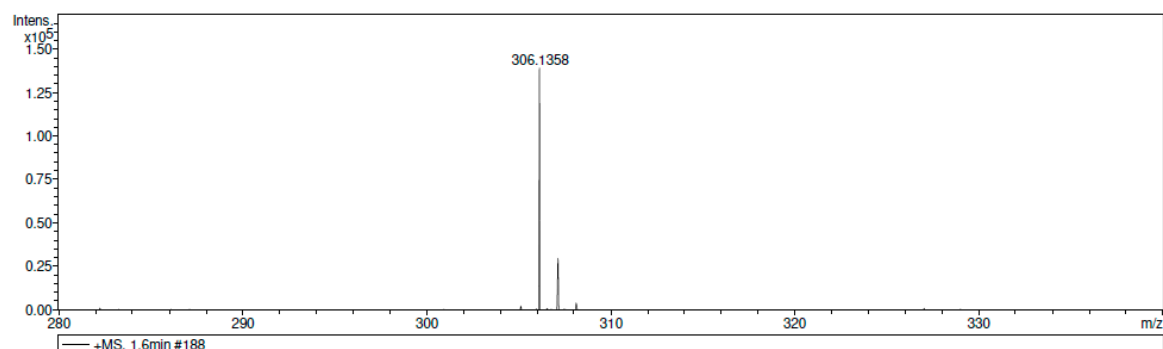
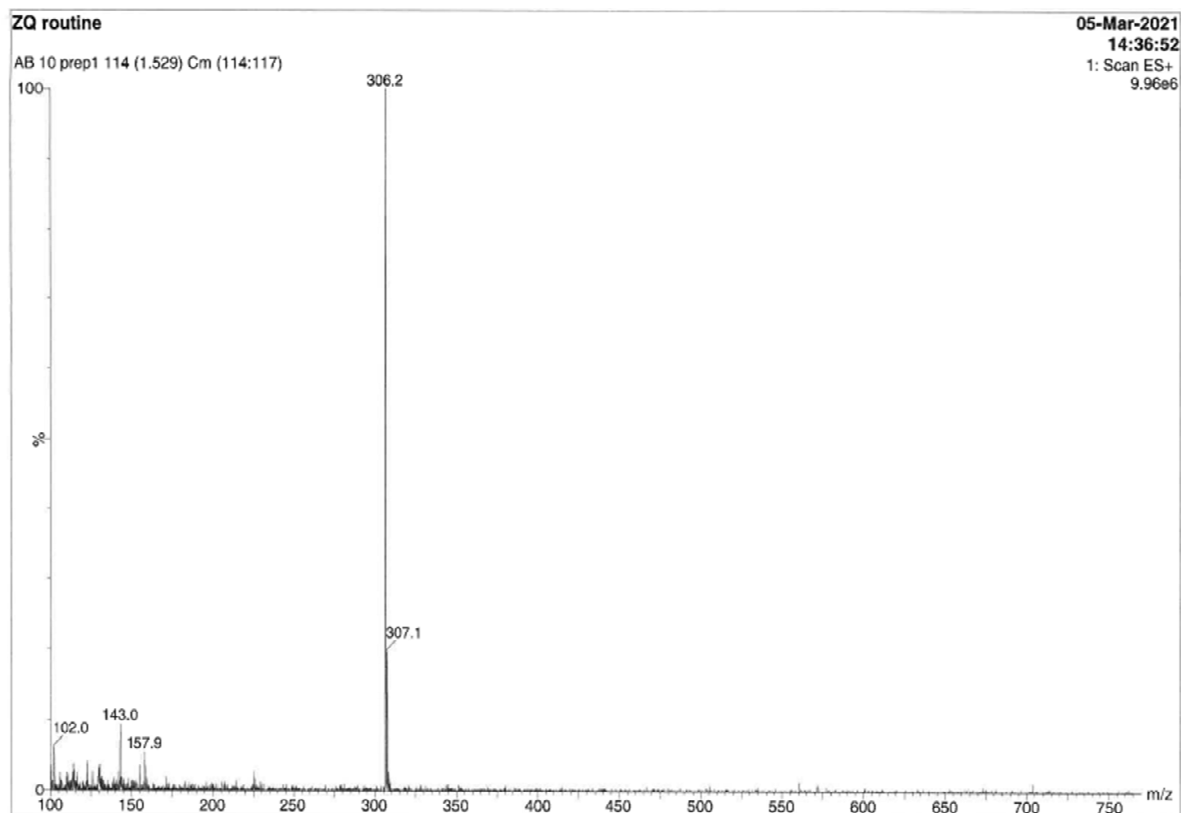




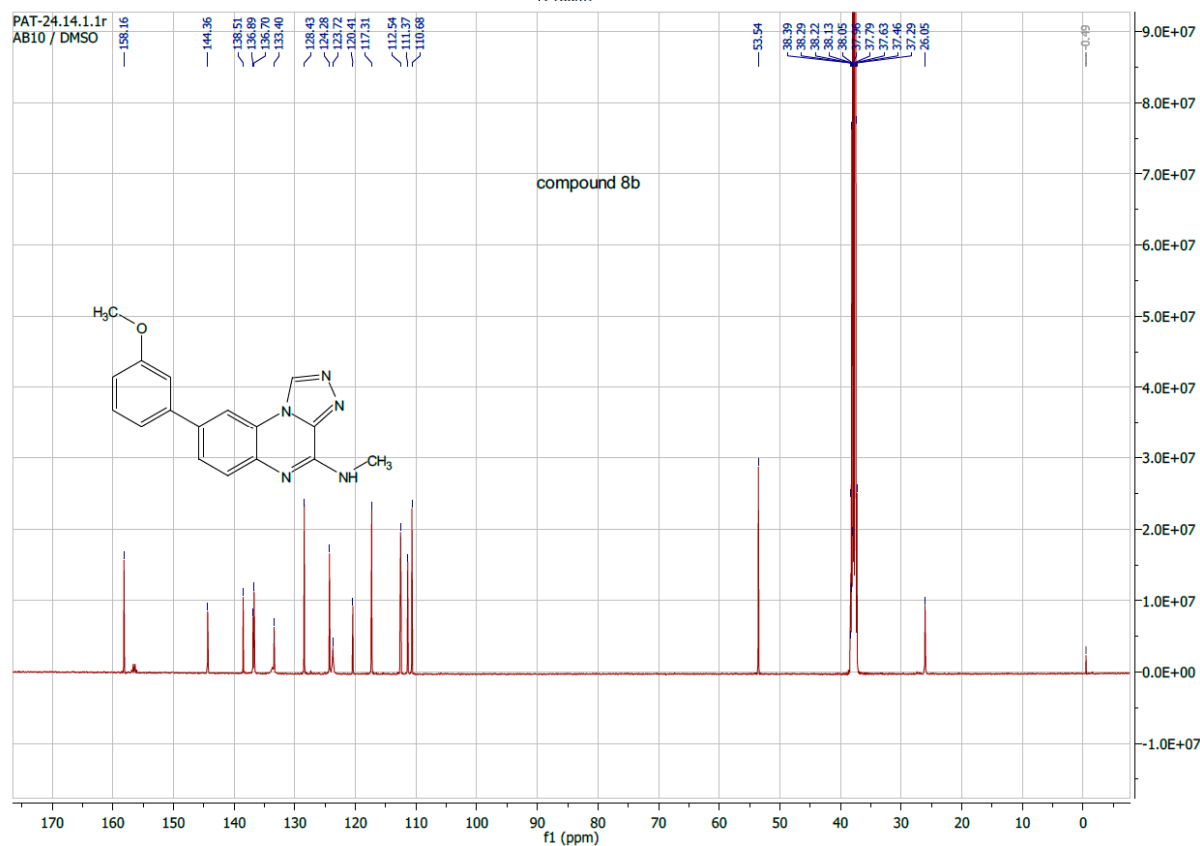
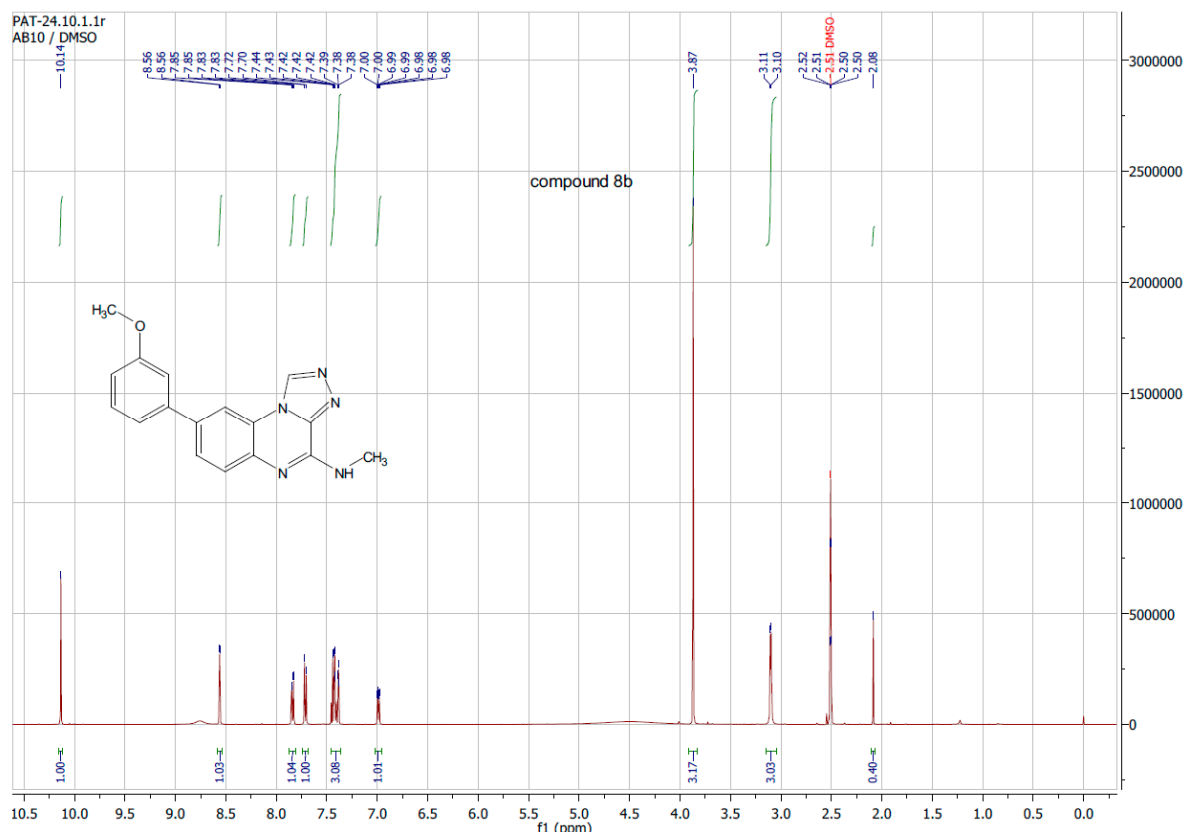
S4. [8-(3-Methoxy-phenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl]-methyl-amine (**8b**).





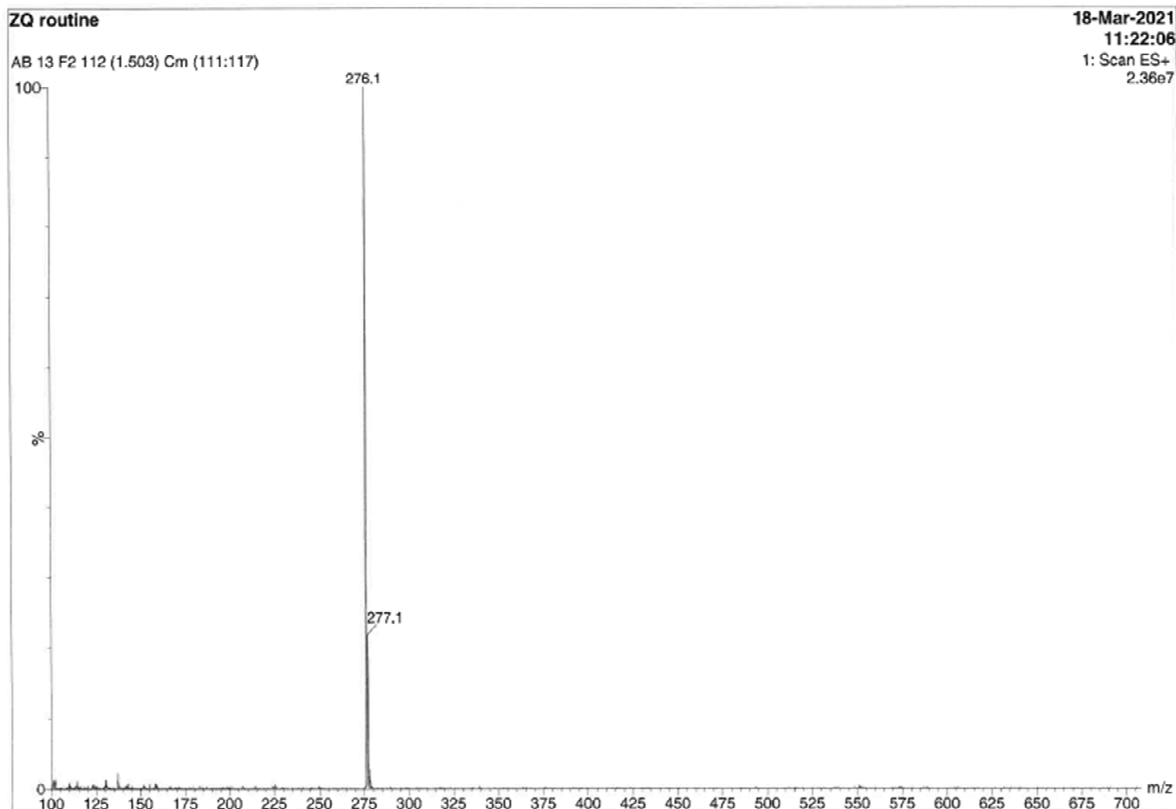
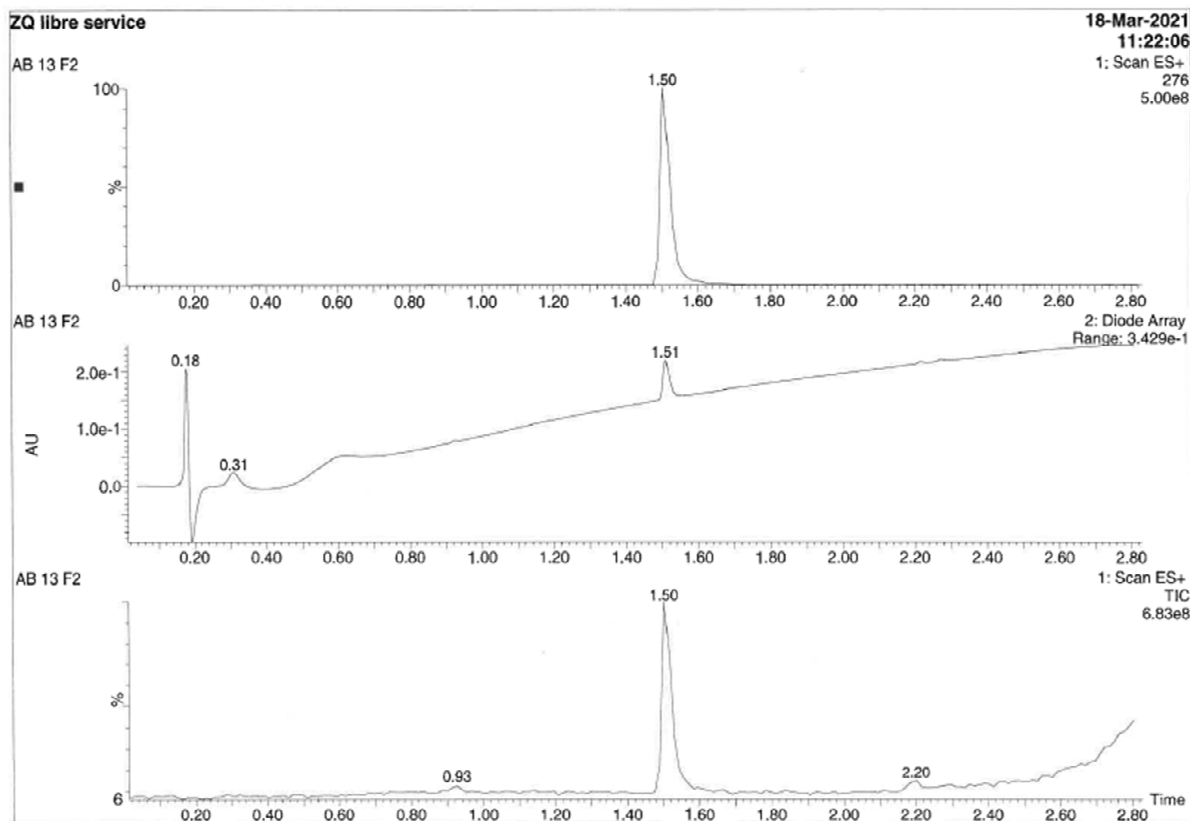


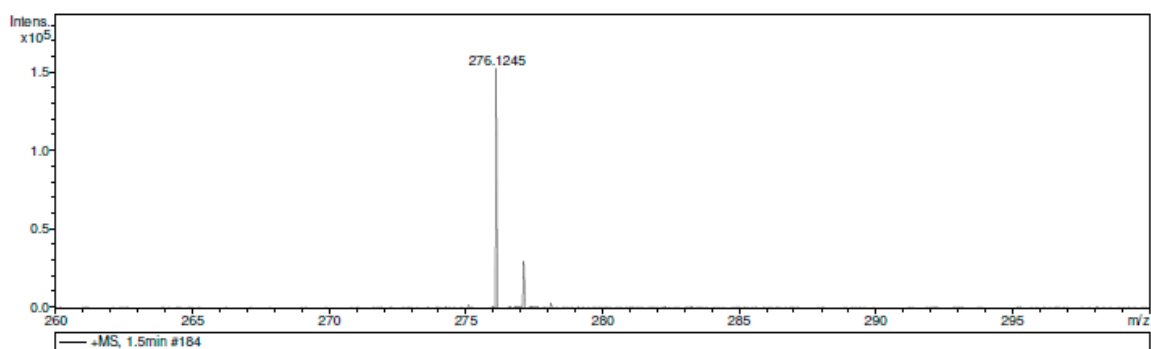
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
306.1358	1	C17H16N5O	306.1349	-2.7	7.6	1	100.00	12.5	even		ok



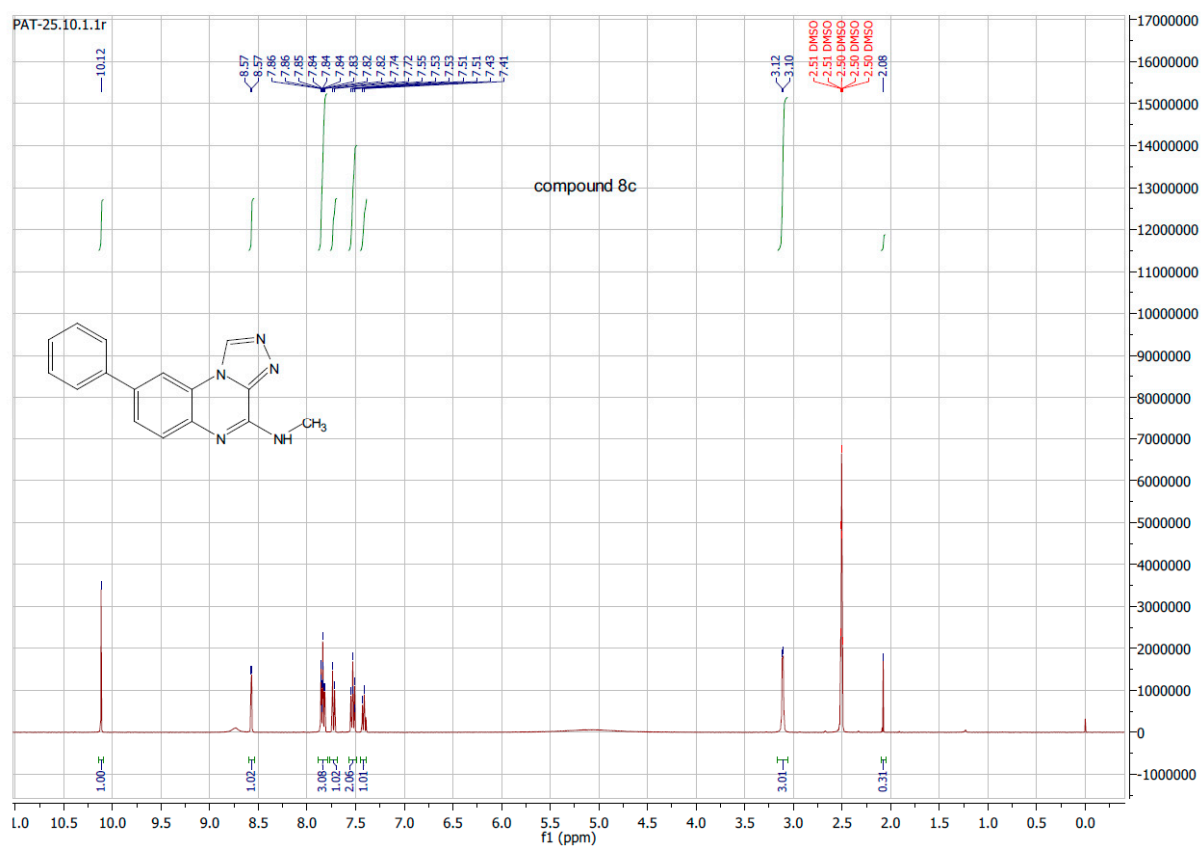


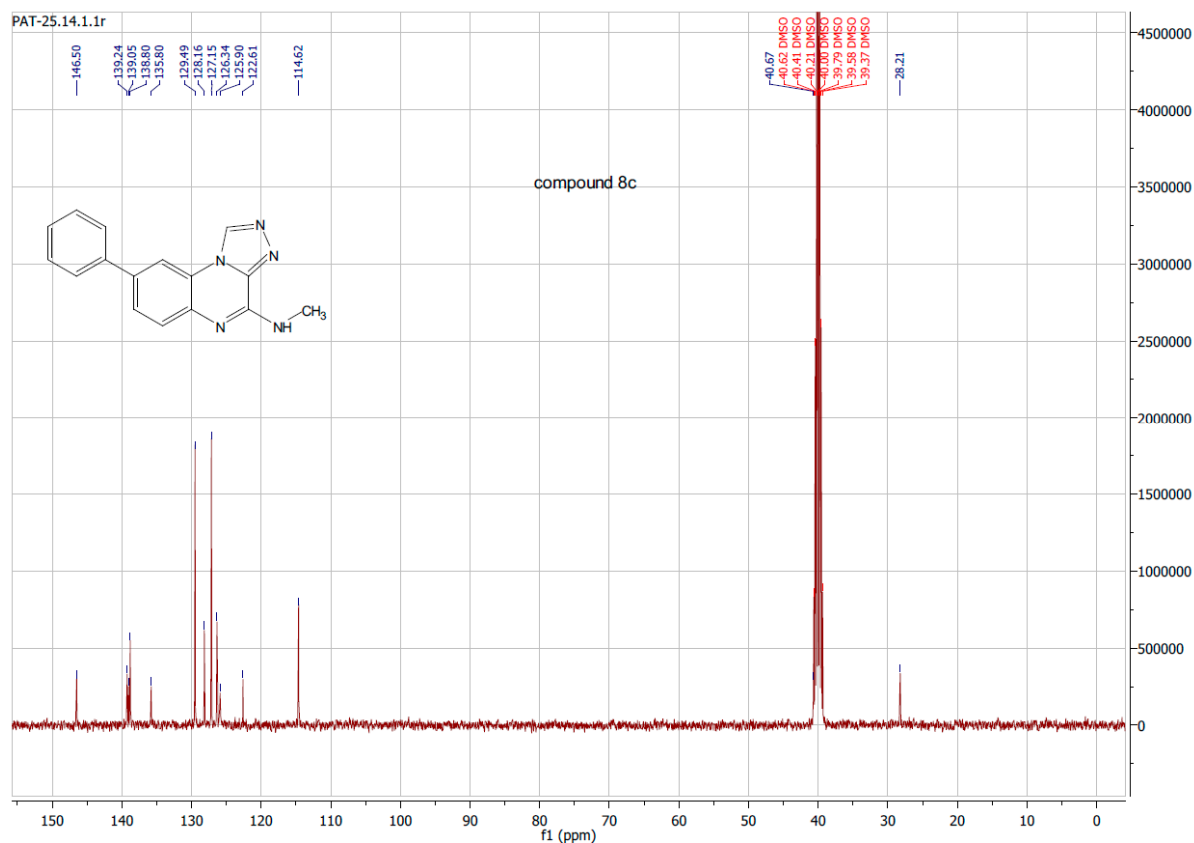
S5. Methyl-(8-phenyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl)-amine (**8c**).



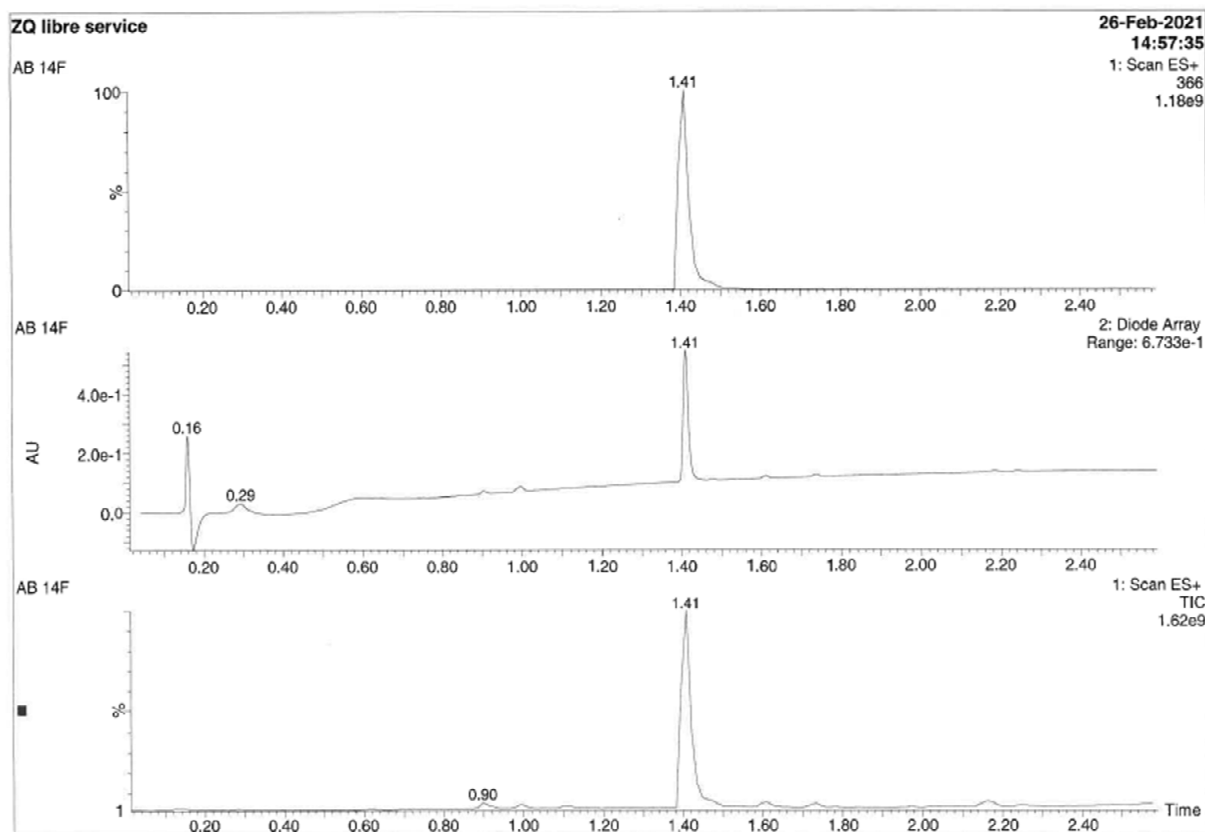


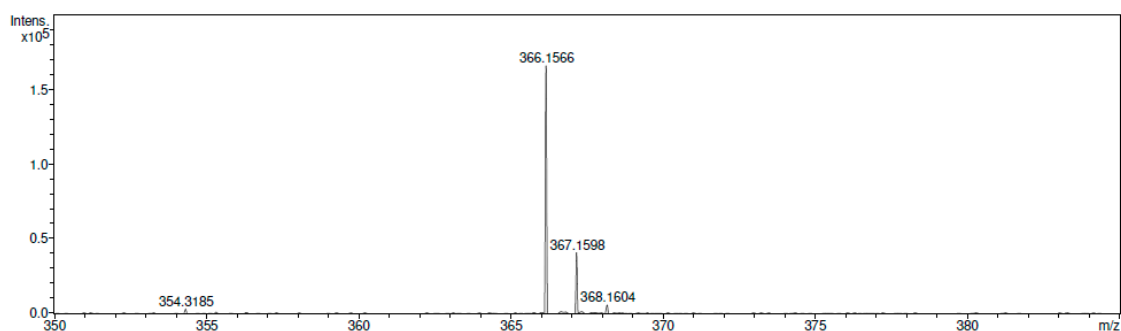
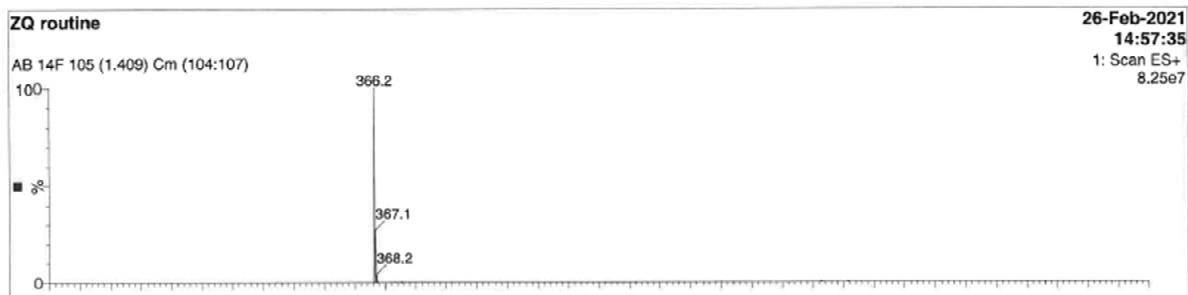
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
276.1245	1	C <sub>16</sub> H <sub>14</sub> N <sub>5</sub>	276.1244	-0.3	1.7	1	100.00	12.5	even	ok	



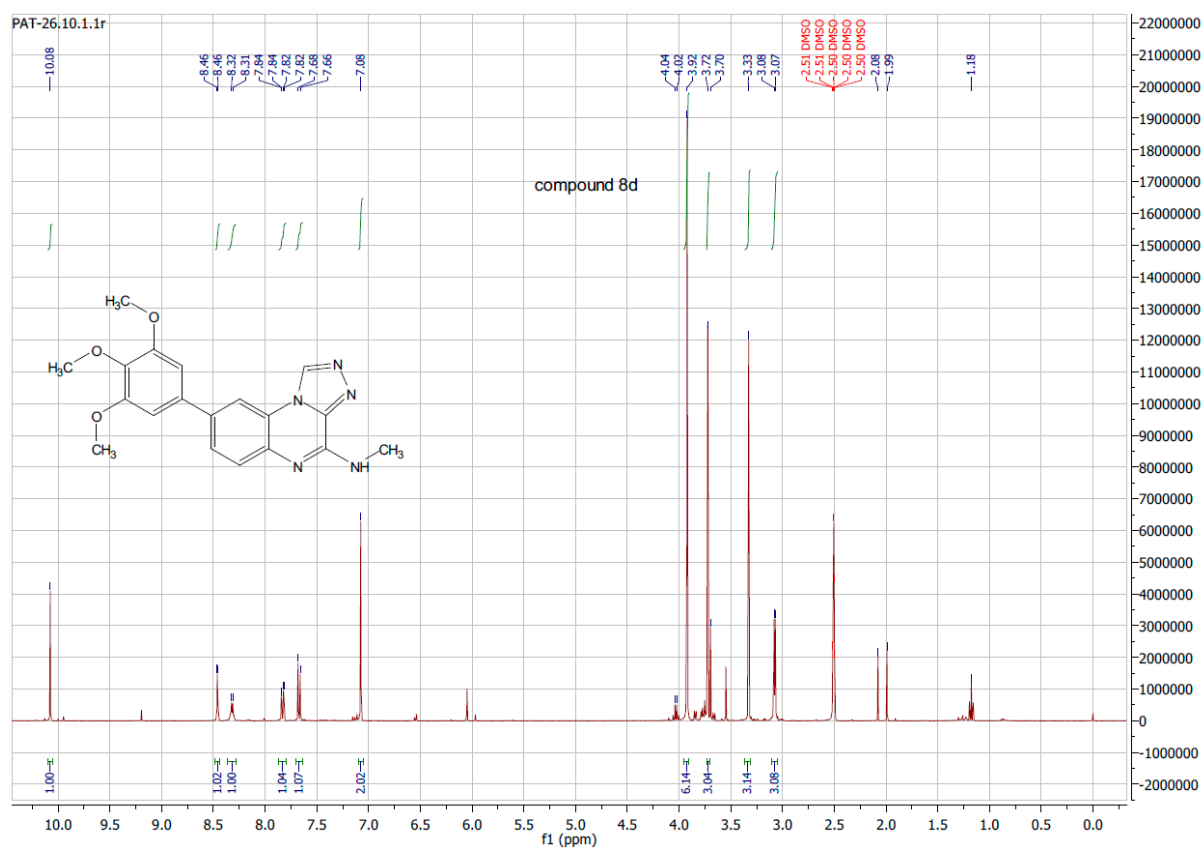


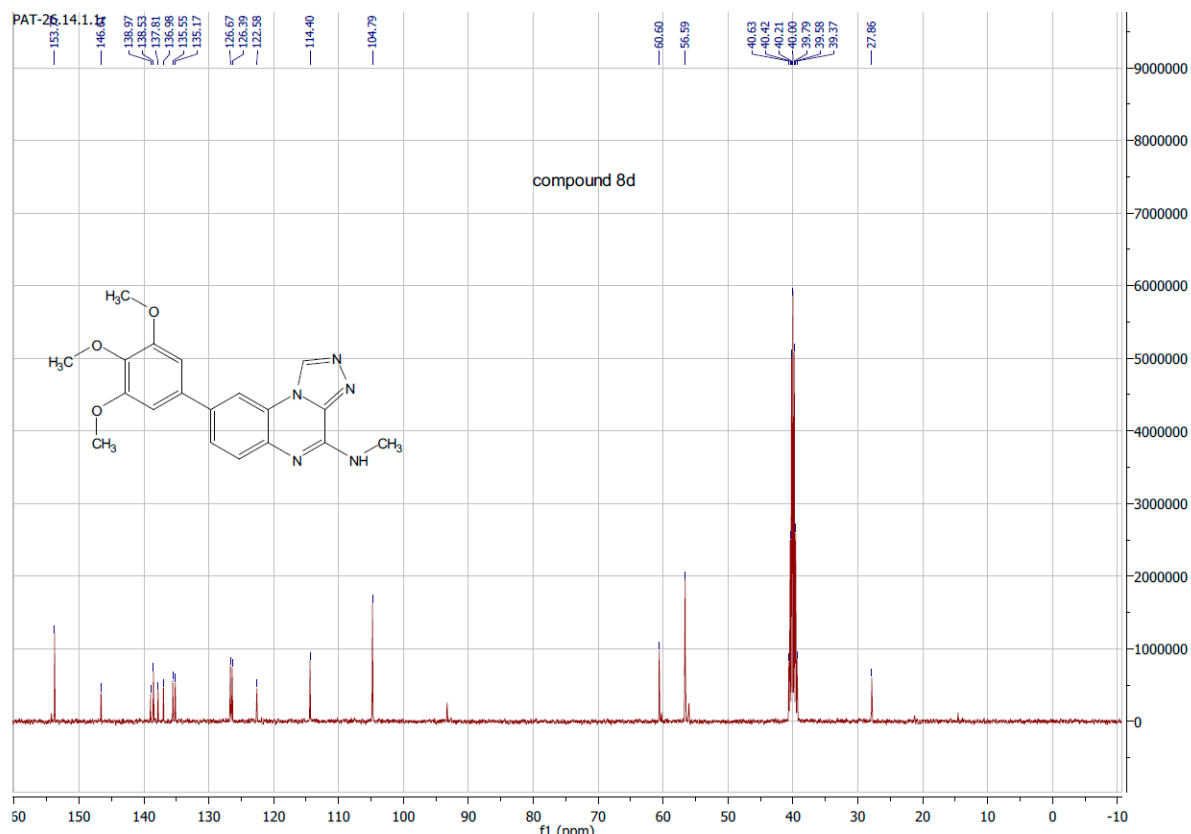
S6. Methyl-[8-(3,4,5-trimethoxy-phenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl]-amine (**8d**).



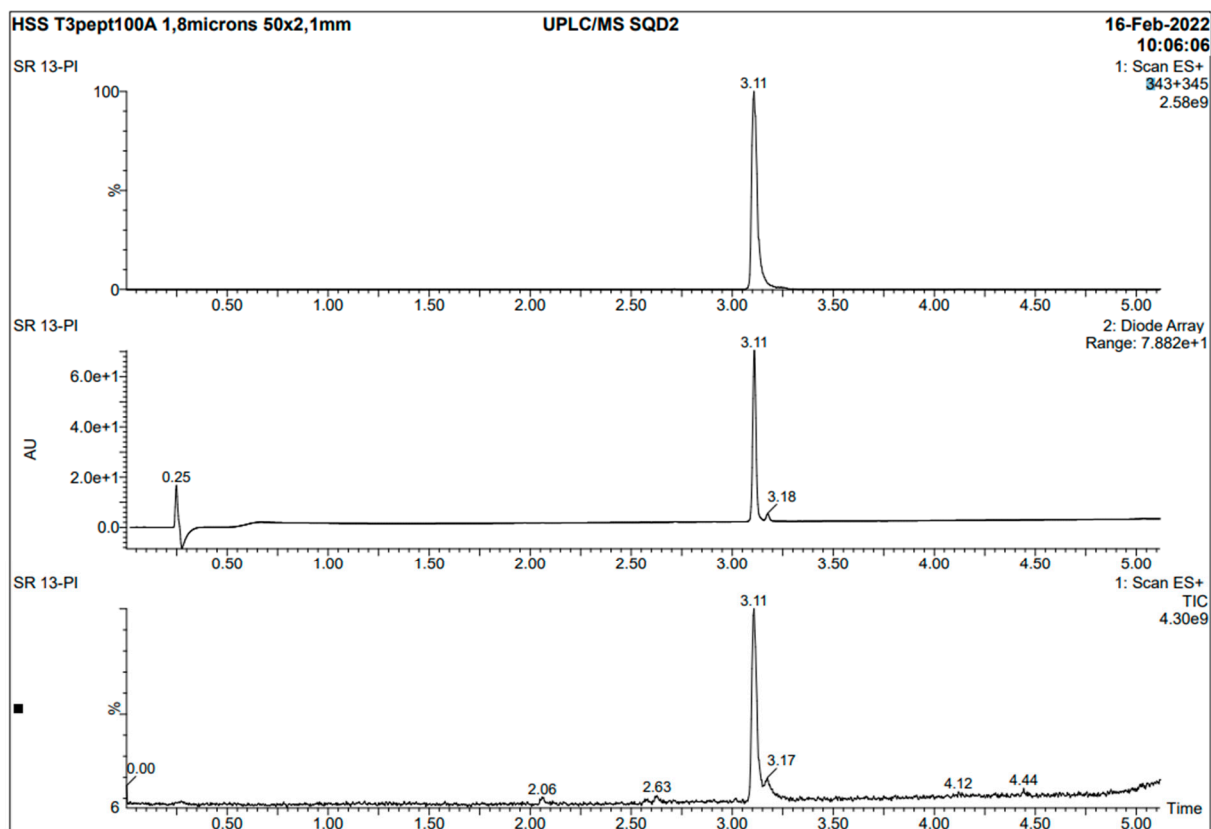


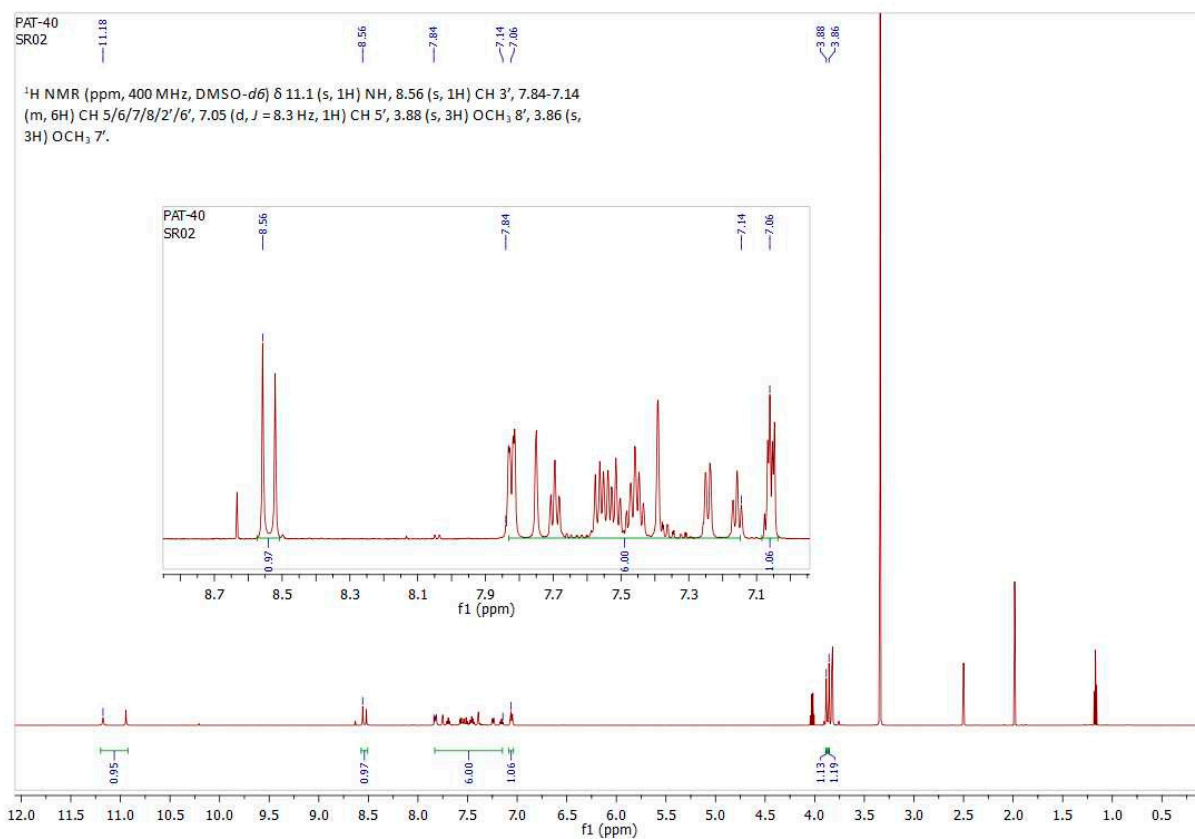
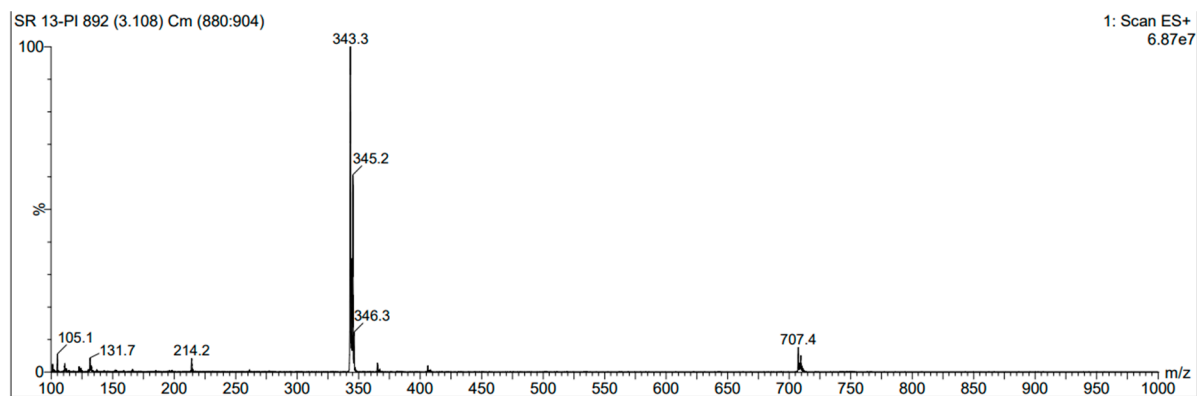
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
366.1566	1	C <sub>19</sub> H <sub>20</sub> N <sub>5</sub> O <sub>3</sub>	366.1561	-1.4	10.4	1	100.00	12.5	even		ok



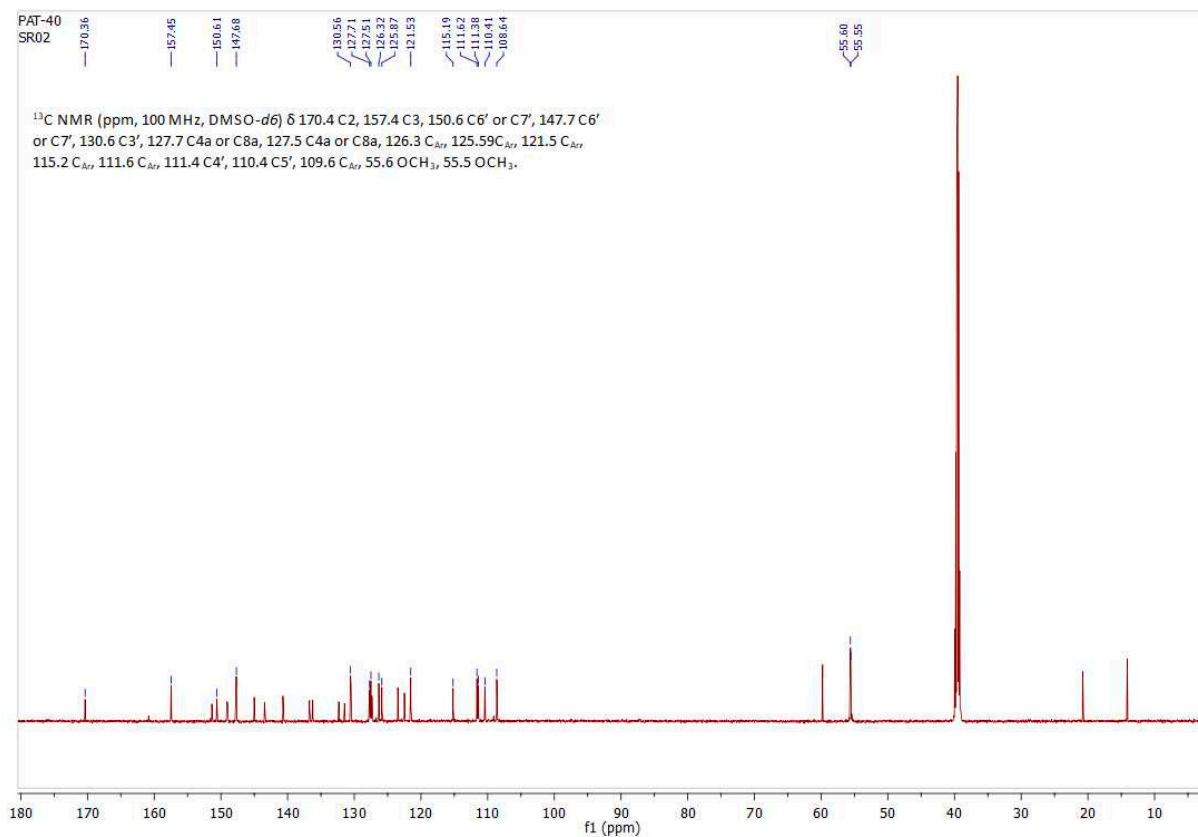


S7. 2-chloro-3-(2-(3,4-dimethoxybenzylidene)hydrazinyl)quinoxaline (**14a**).

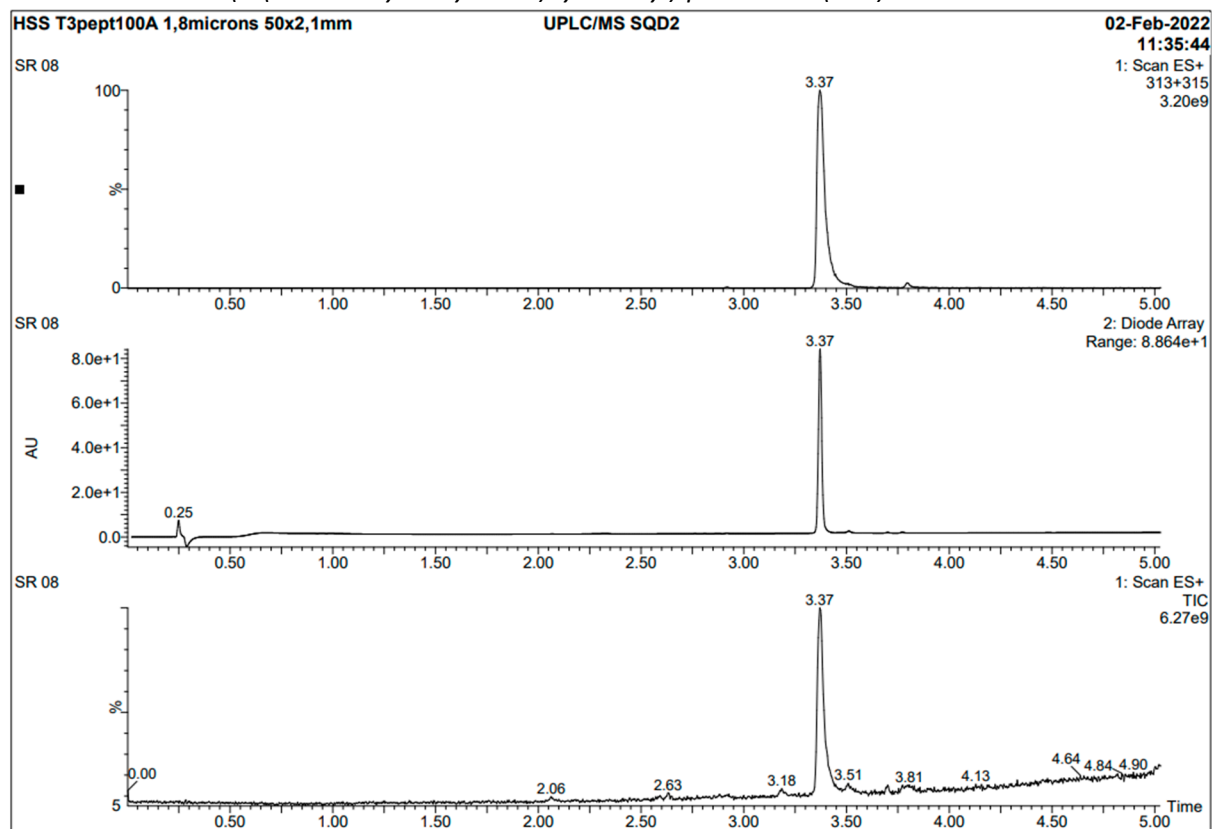


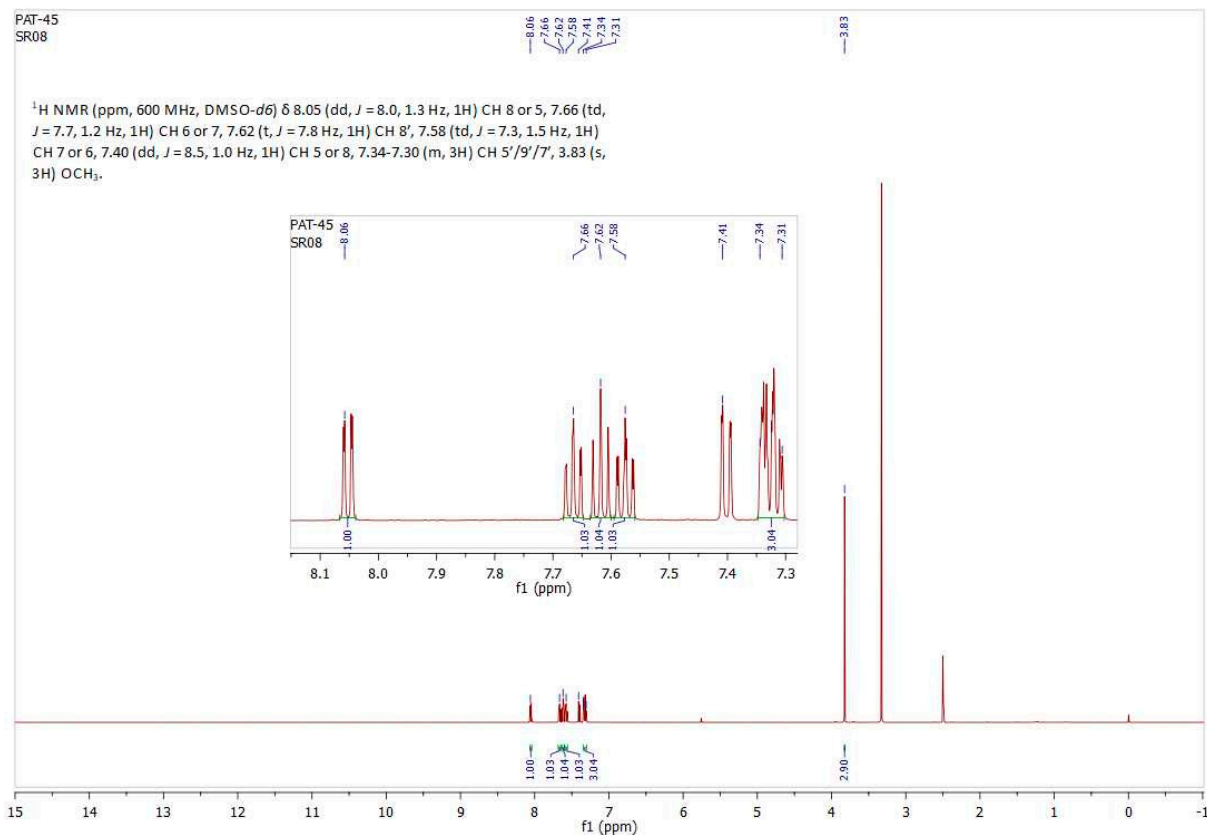
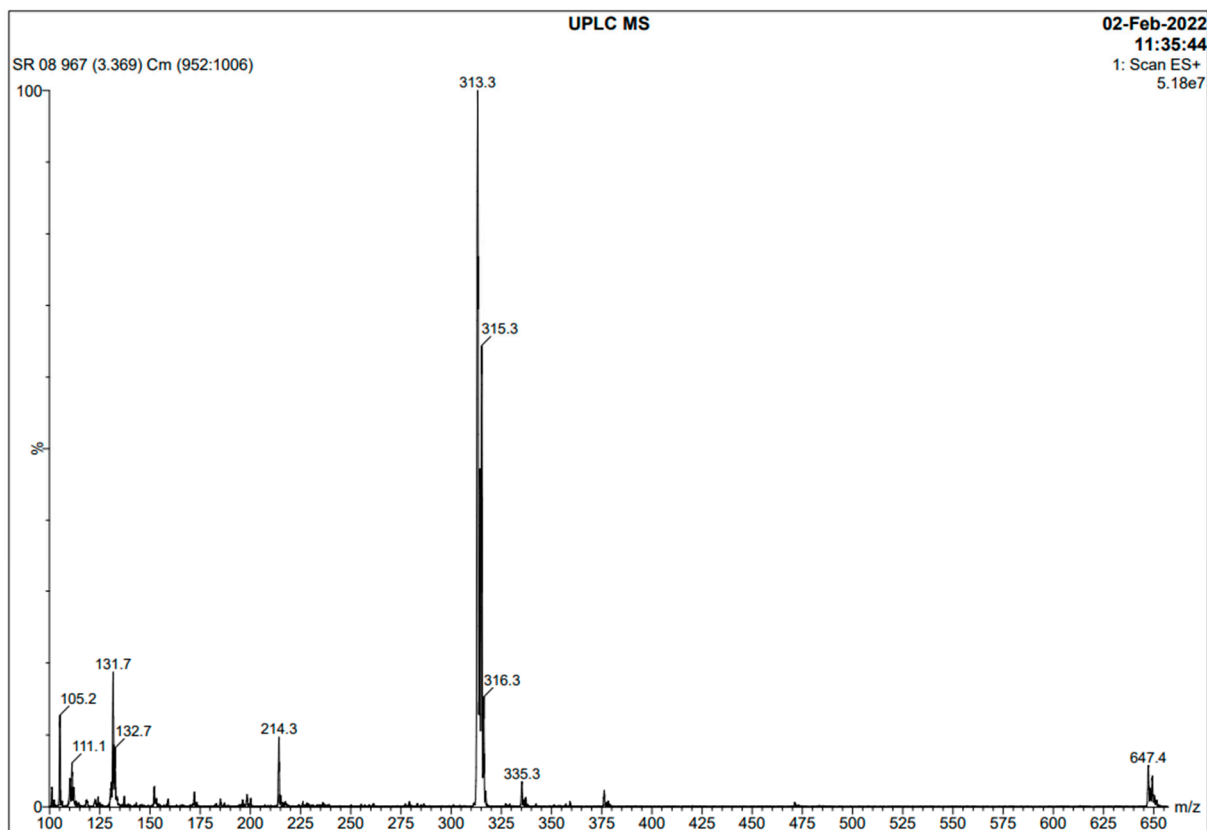


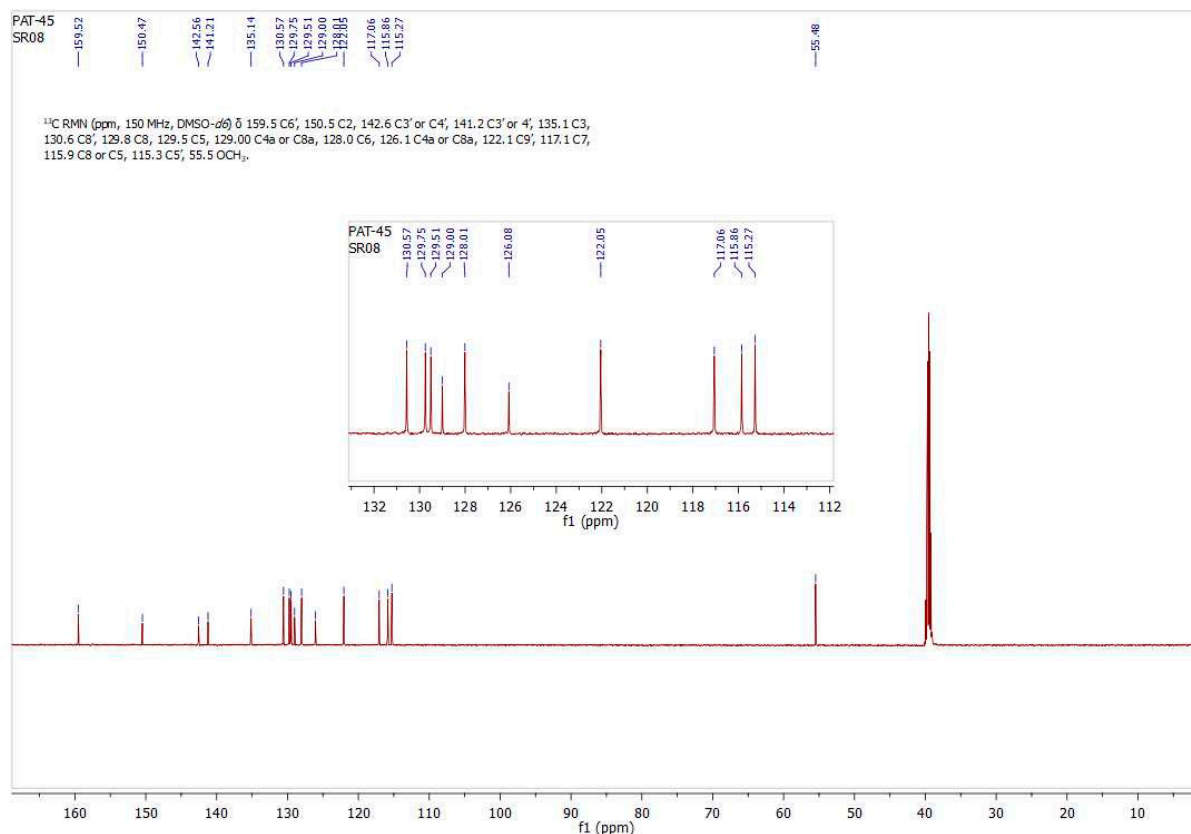




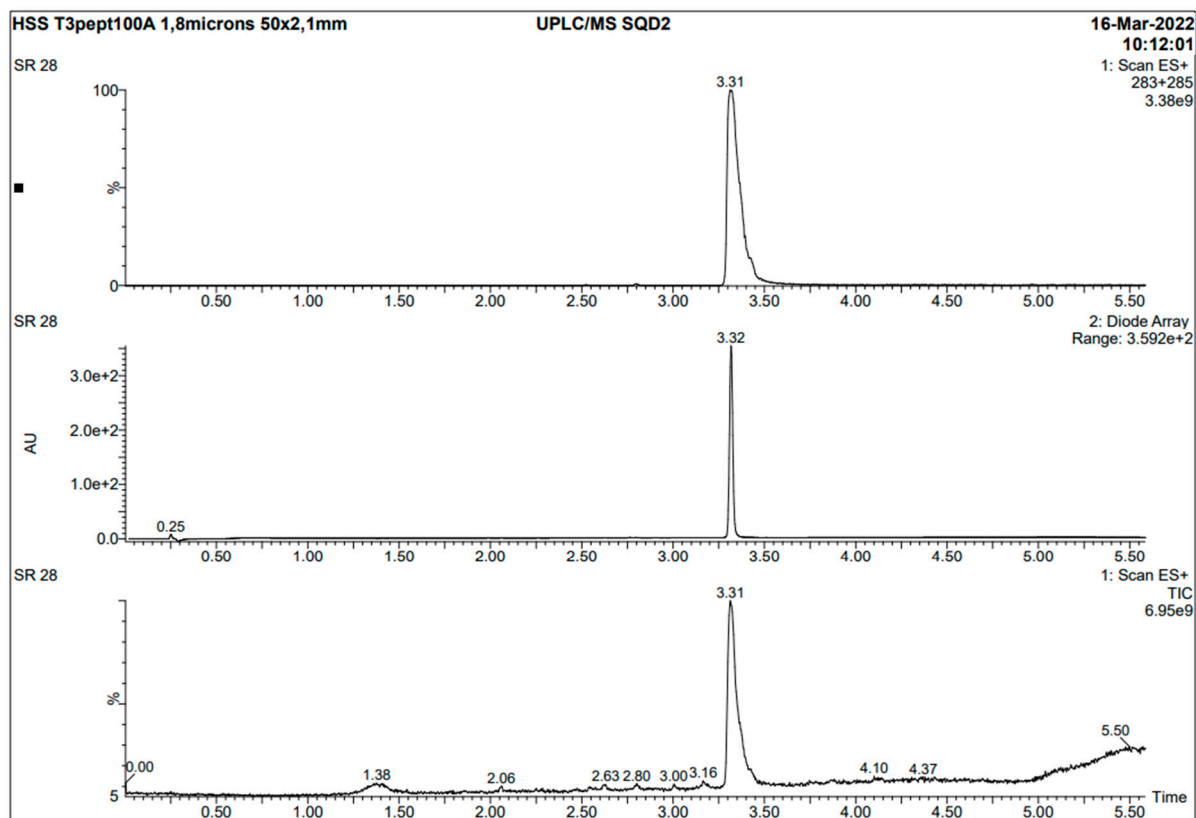
S8. 2-chloro-3-(2-(3-methoxybenzylidene)hydrazinyl)quinoxaline (**14b**).

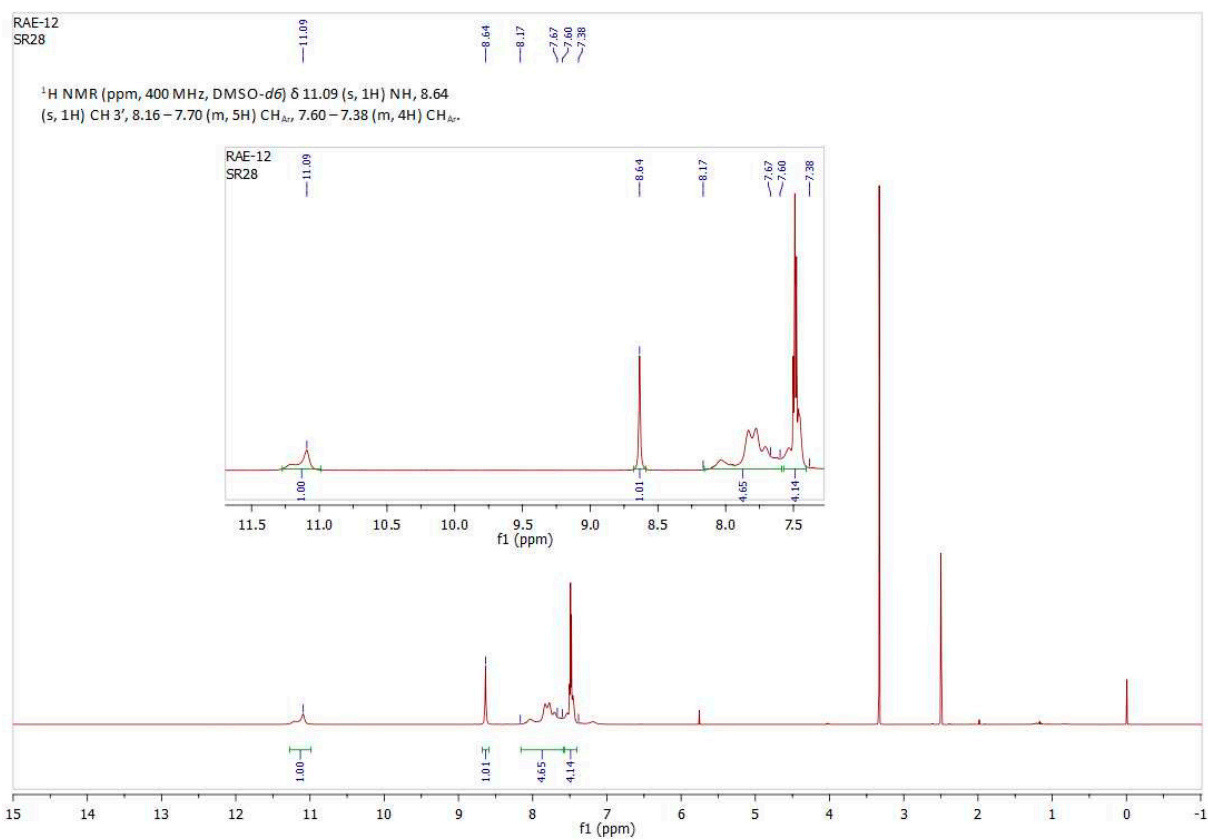
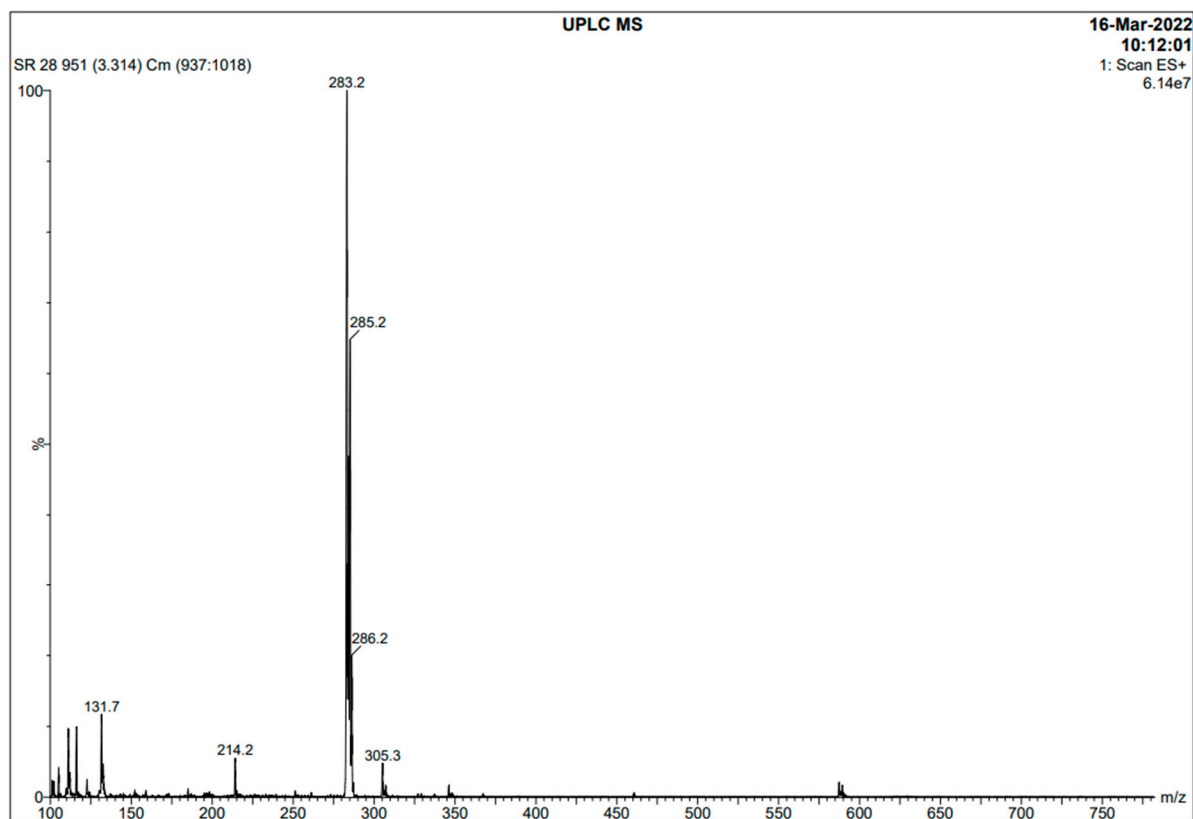


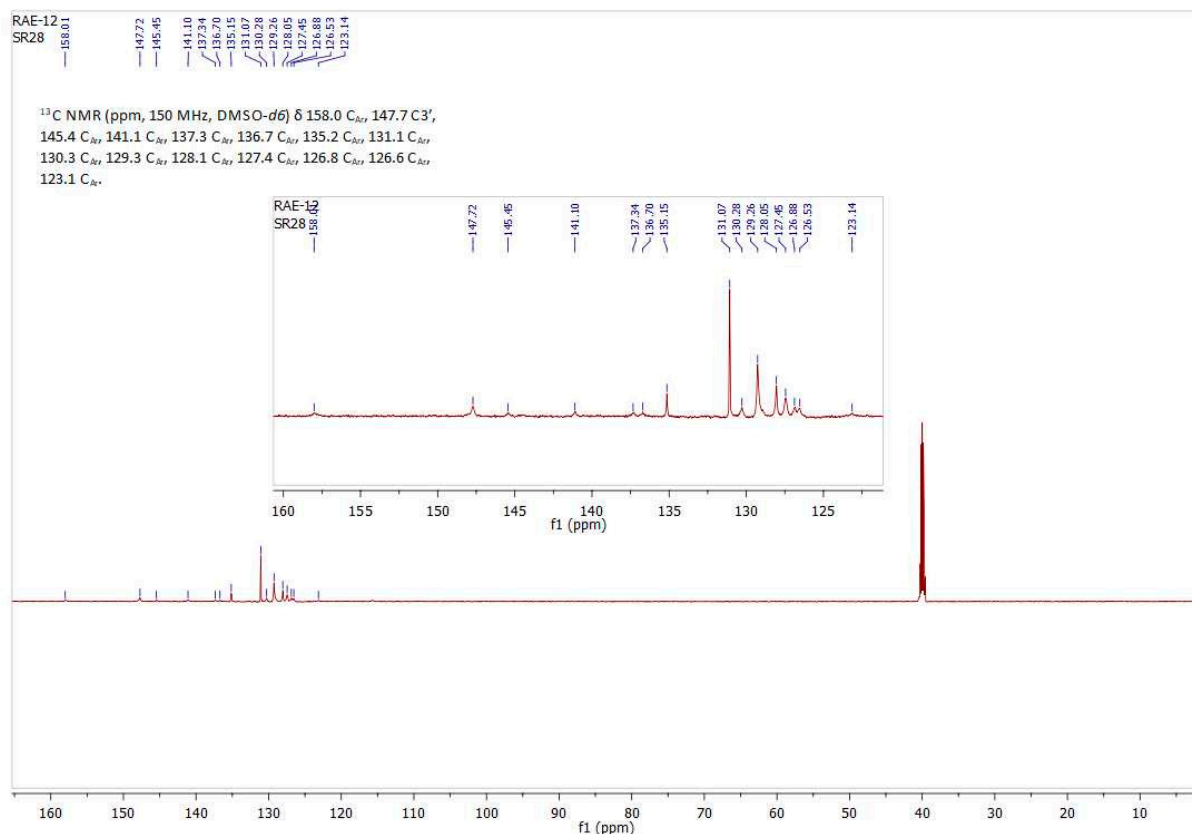




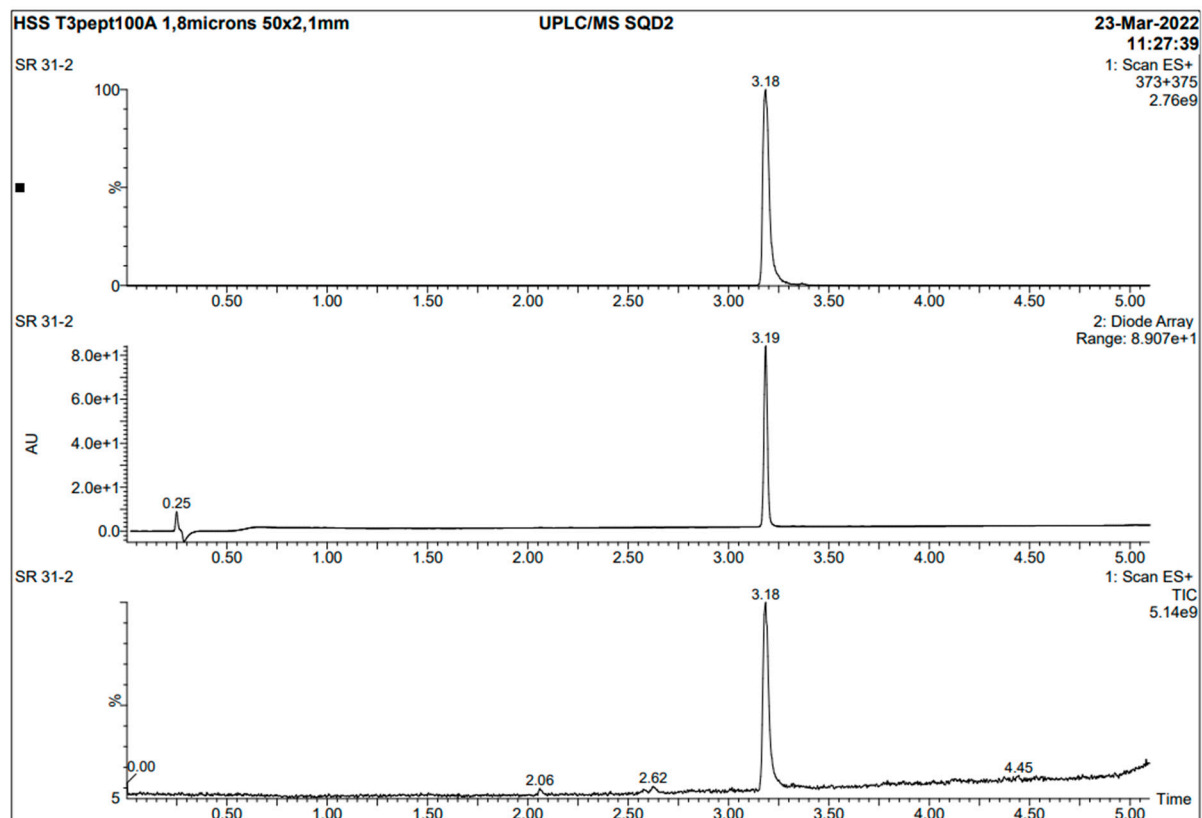
S9. 2-(2-benzylidenehydrazinyl)-3-chloroquinoxaline (**14c**).

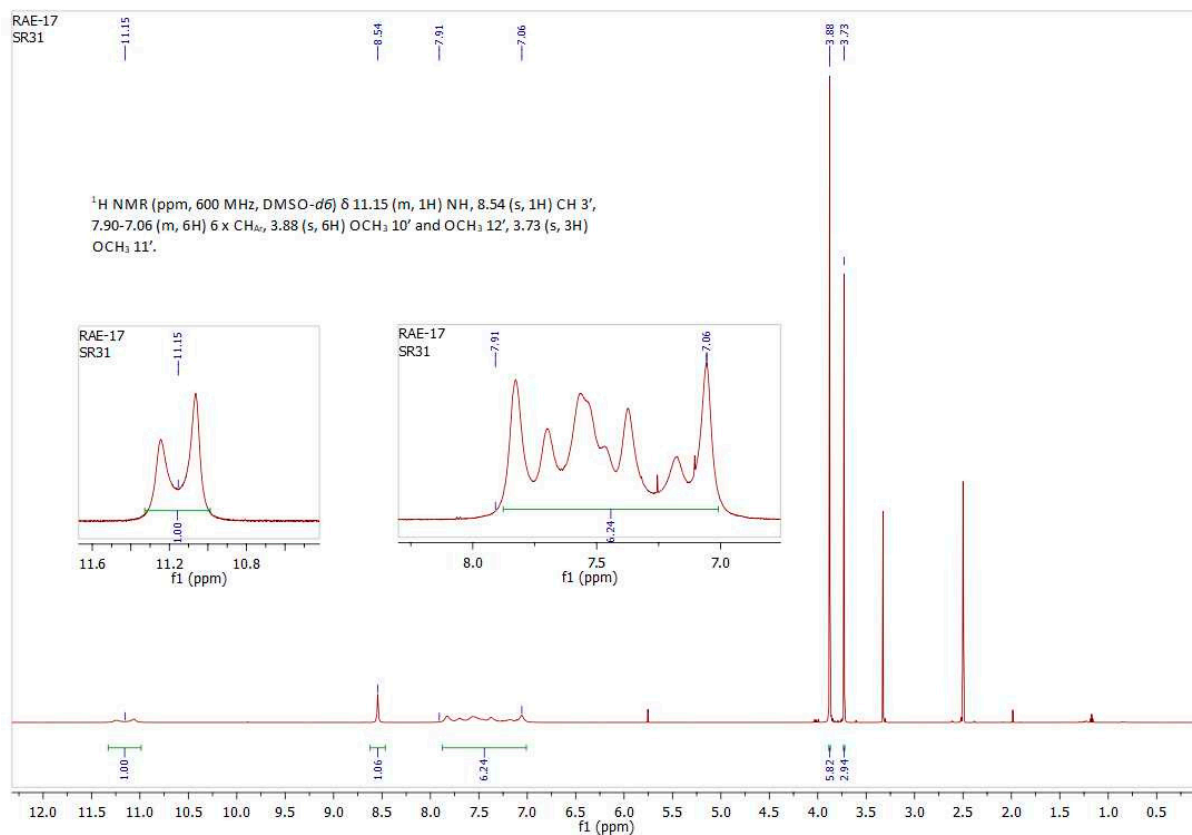
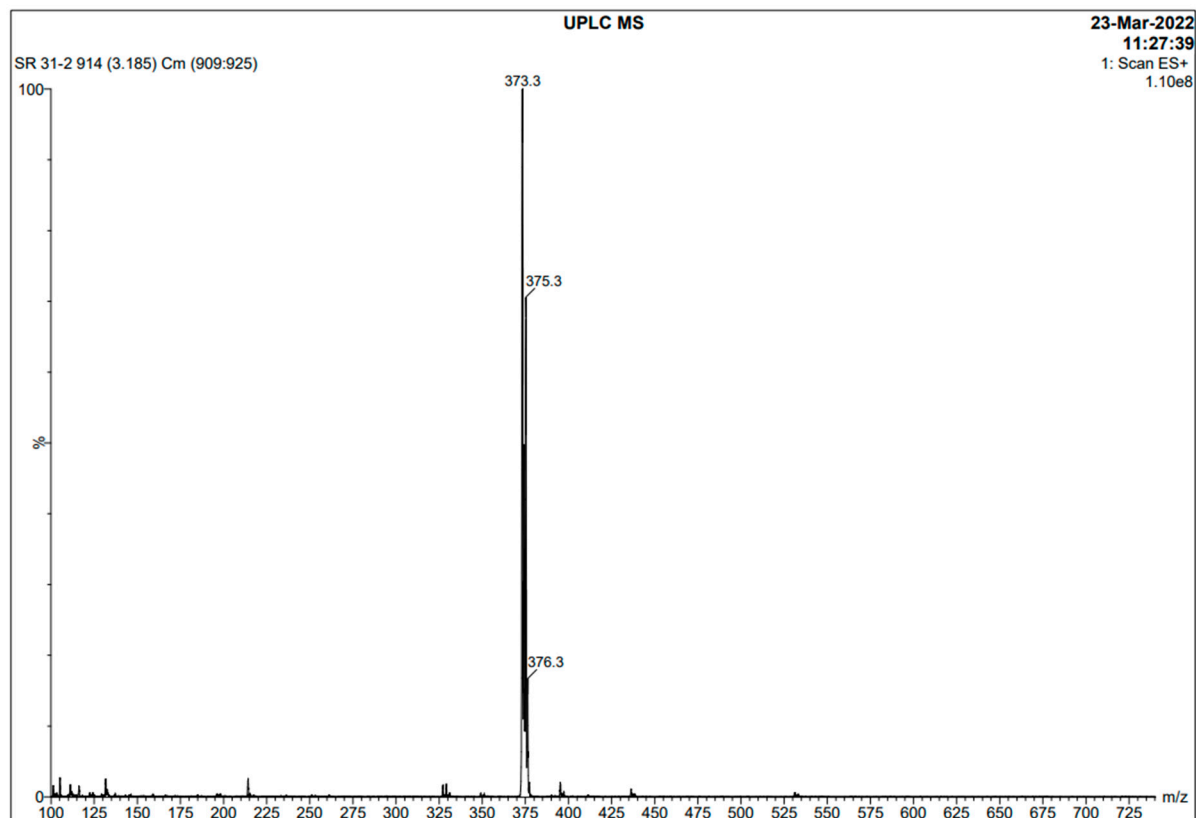


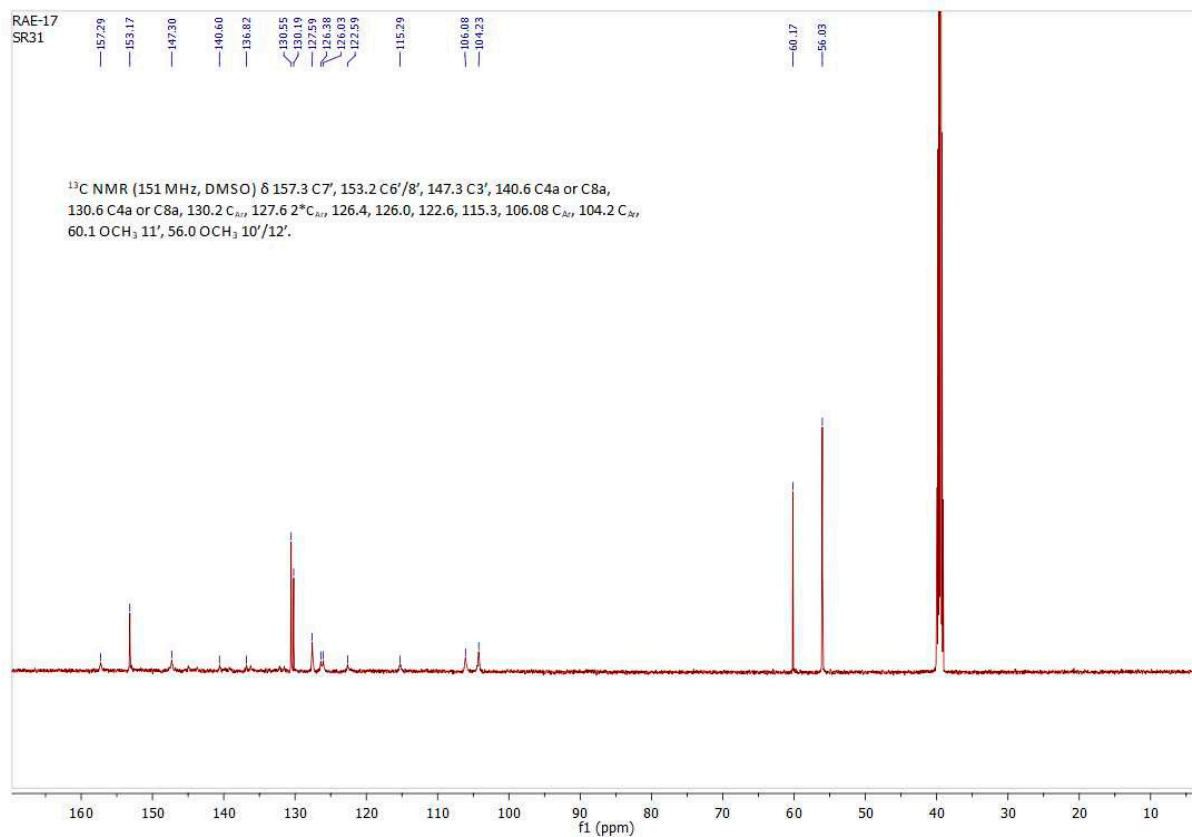




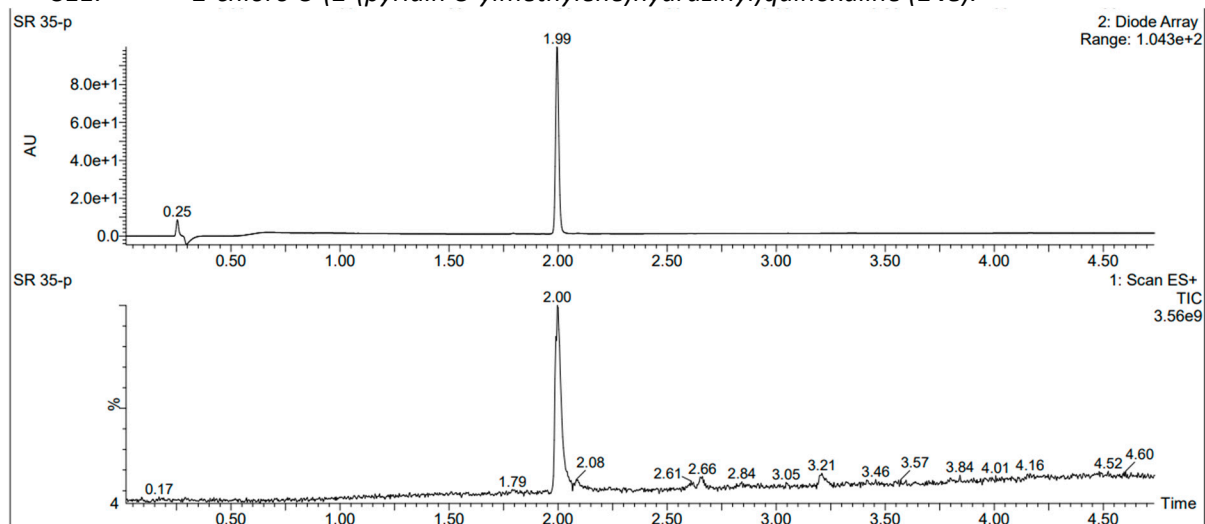
S10. 2-chloro-3-(2-(3,4,5-trimethoxybenzylidene)hydrazinyl)quinoxaline (**14d**).

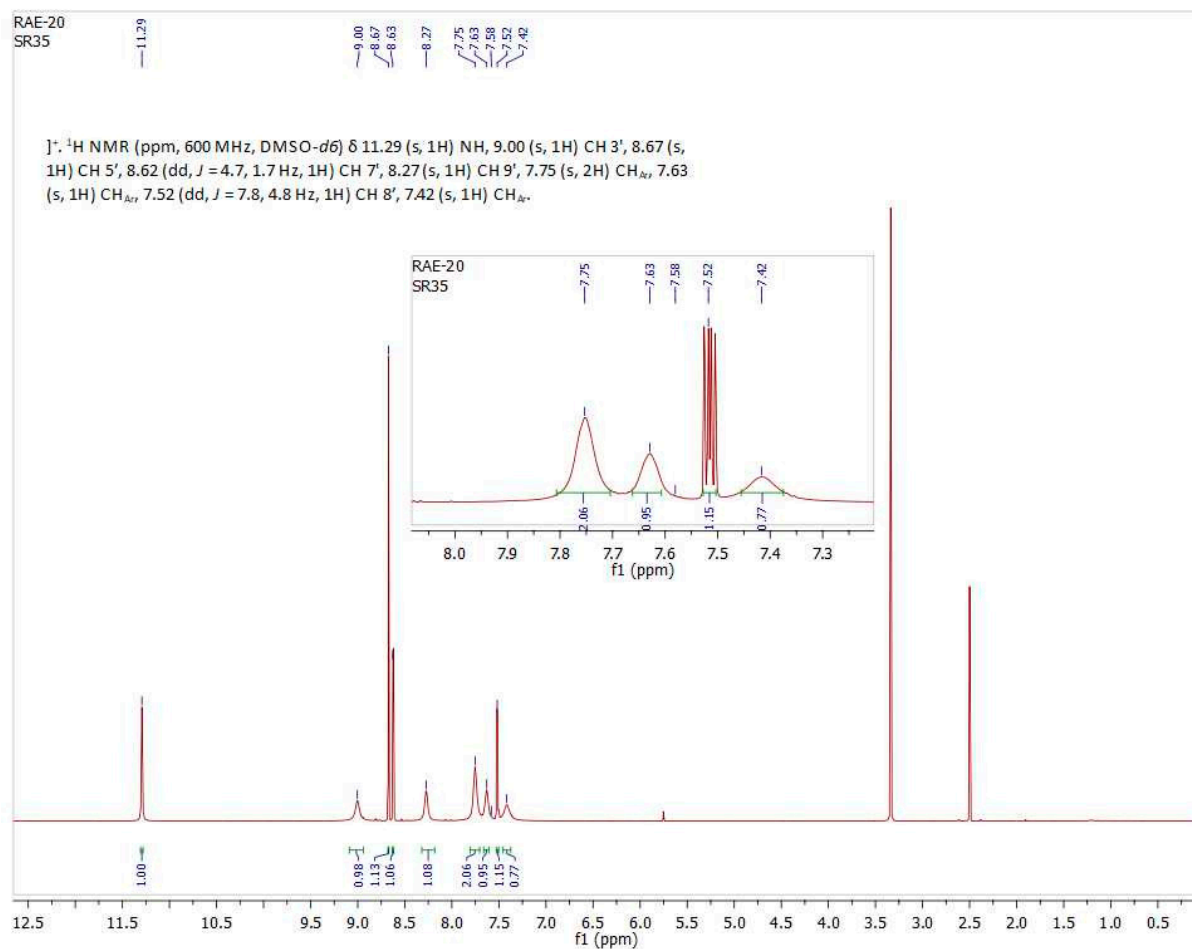
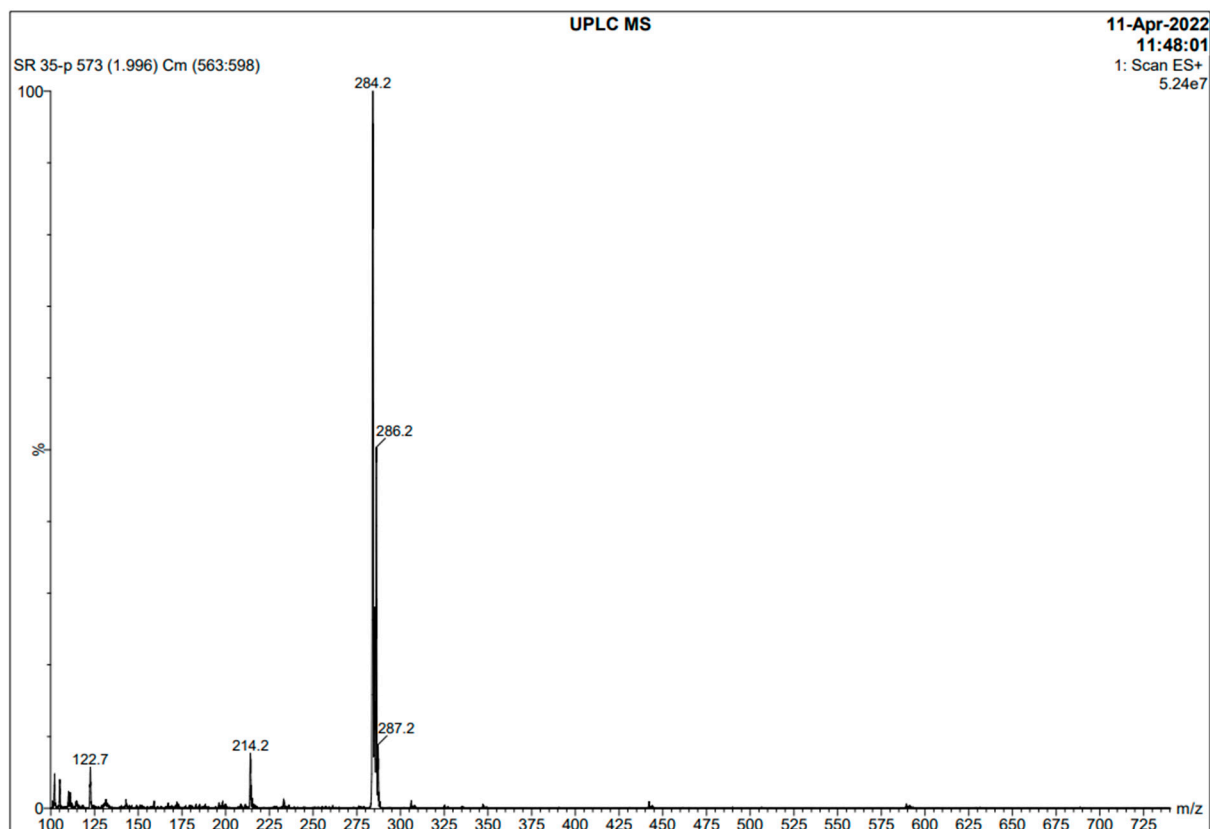




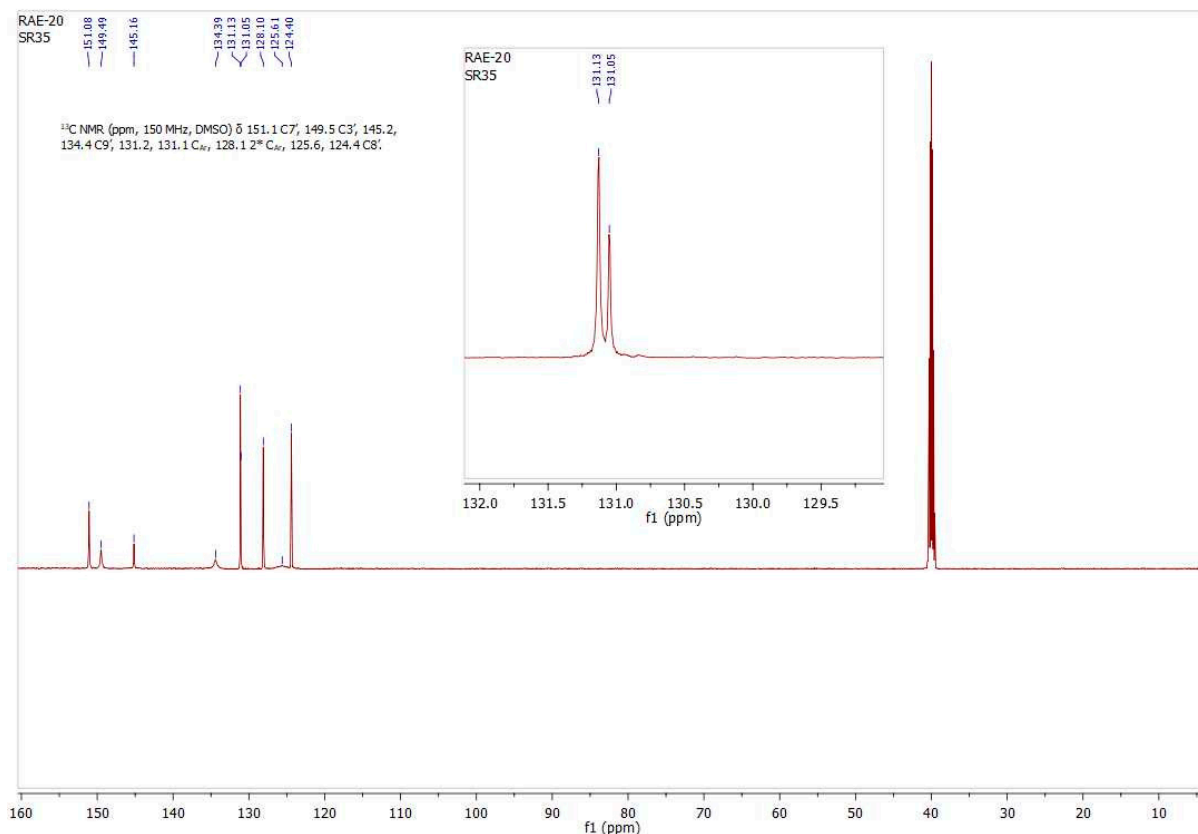


S11. 2-chloro-3-(2-(pyridin-3-ylmethylene)hydrazinyl)quinoxaline (**14e**).

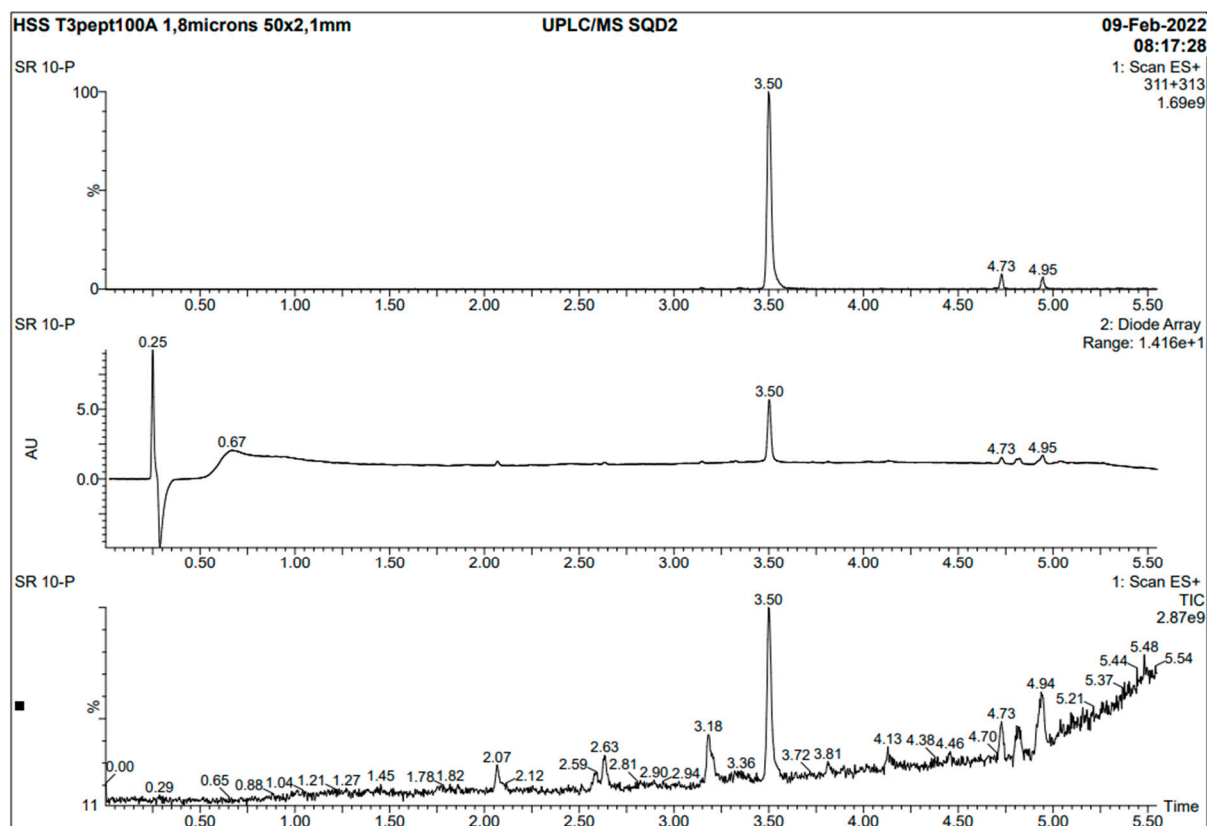


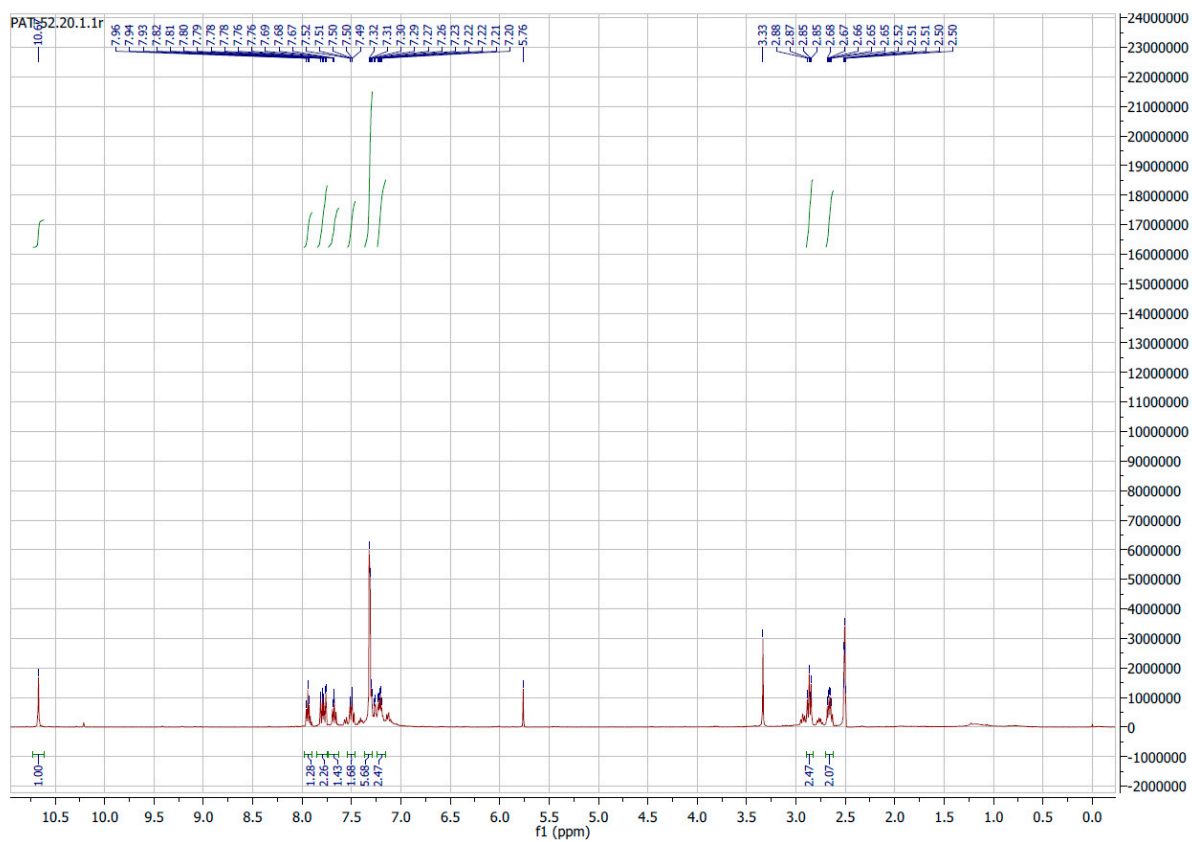
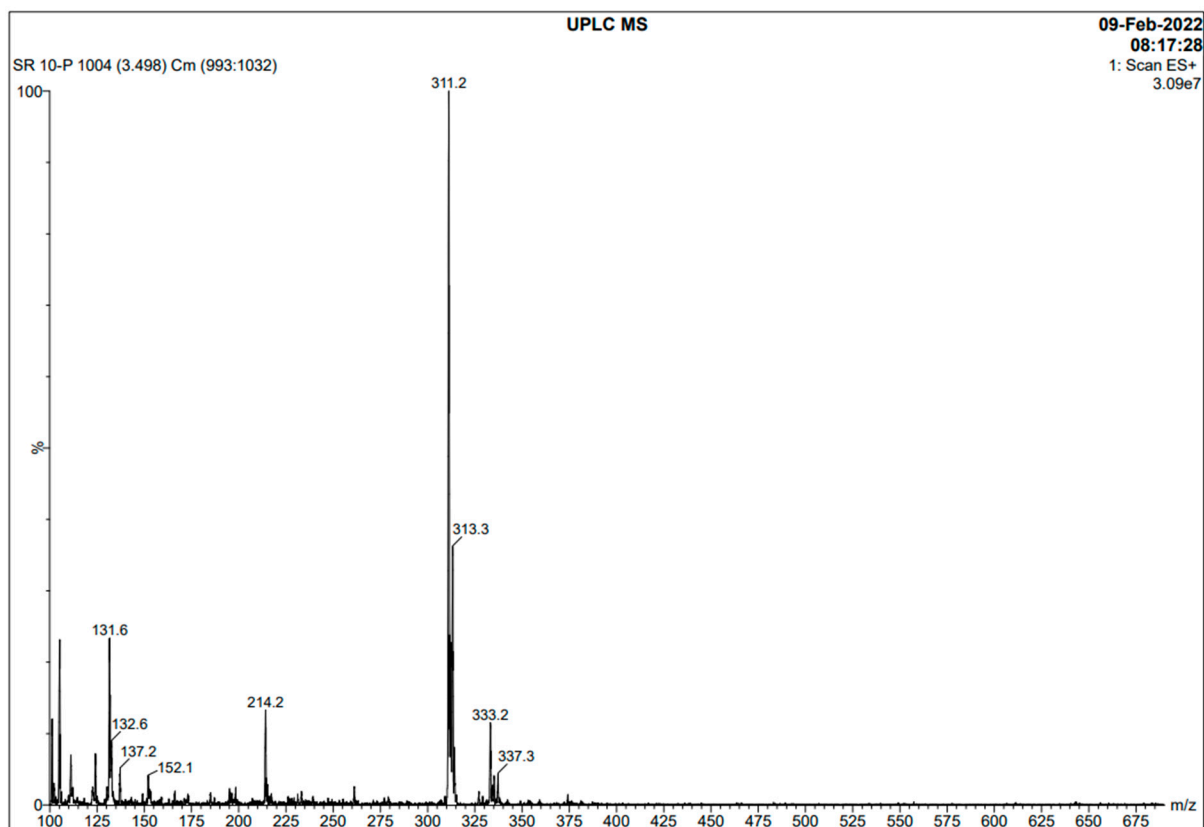


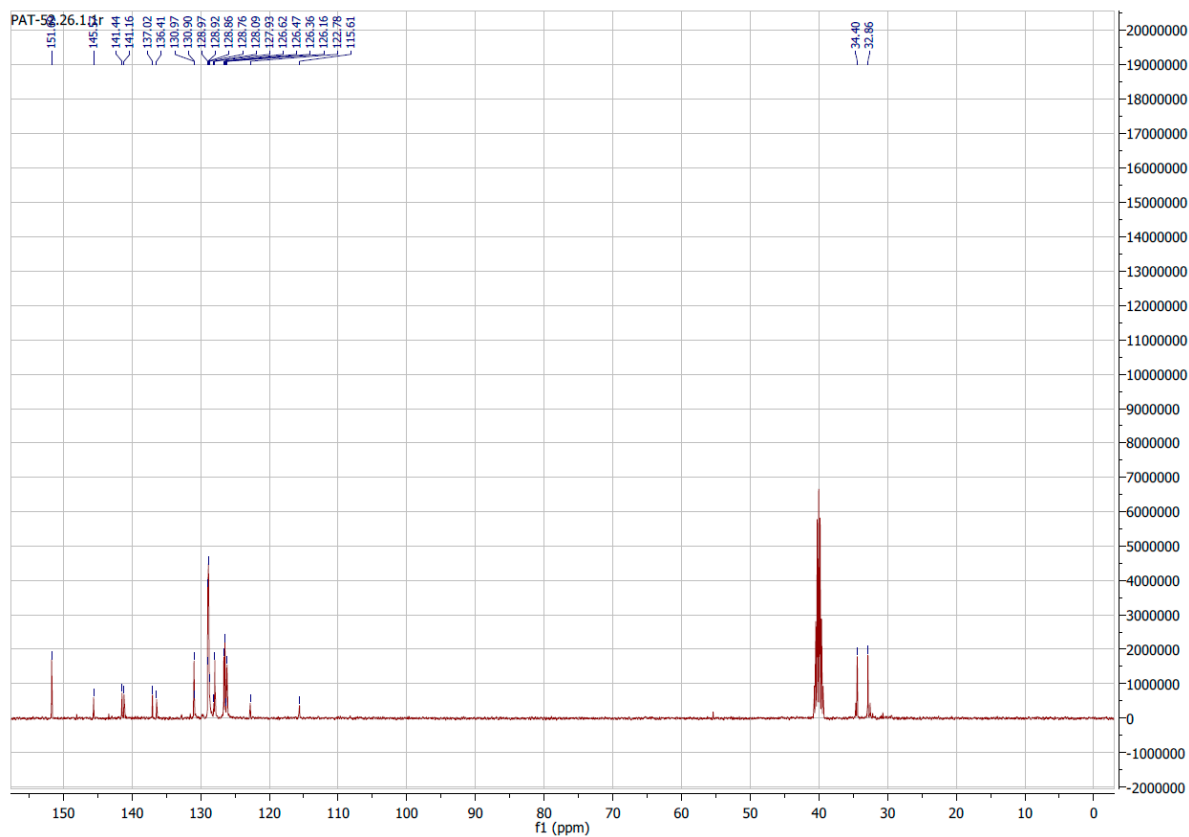




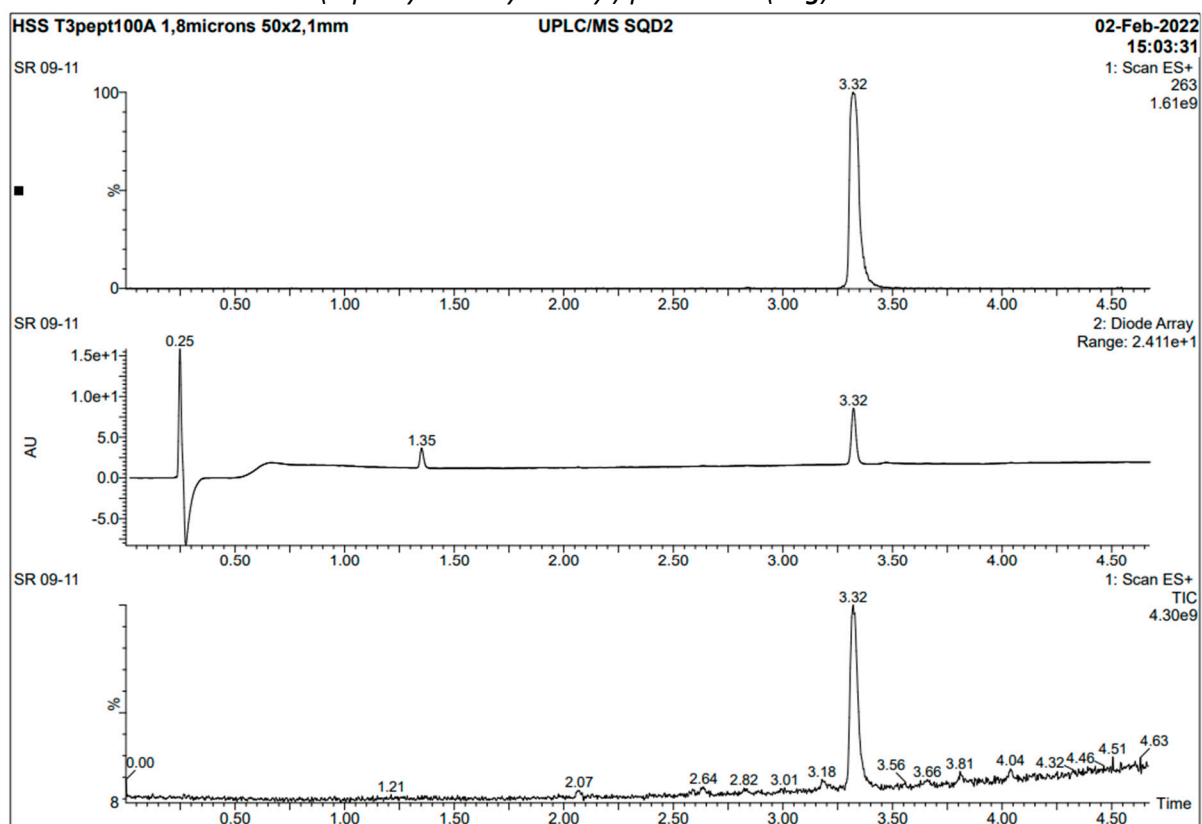
S12. 2-chloro-3-(2-(3-phenylpropylidene)hydrazinyl)quinoxaline (**14f**).

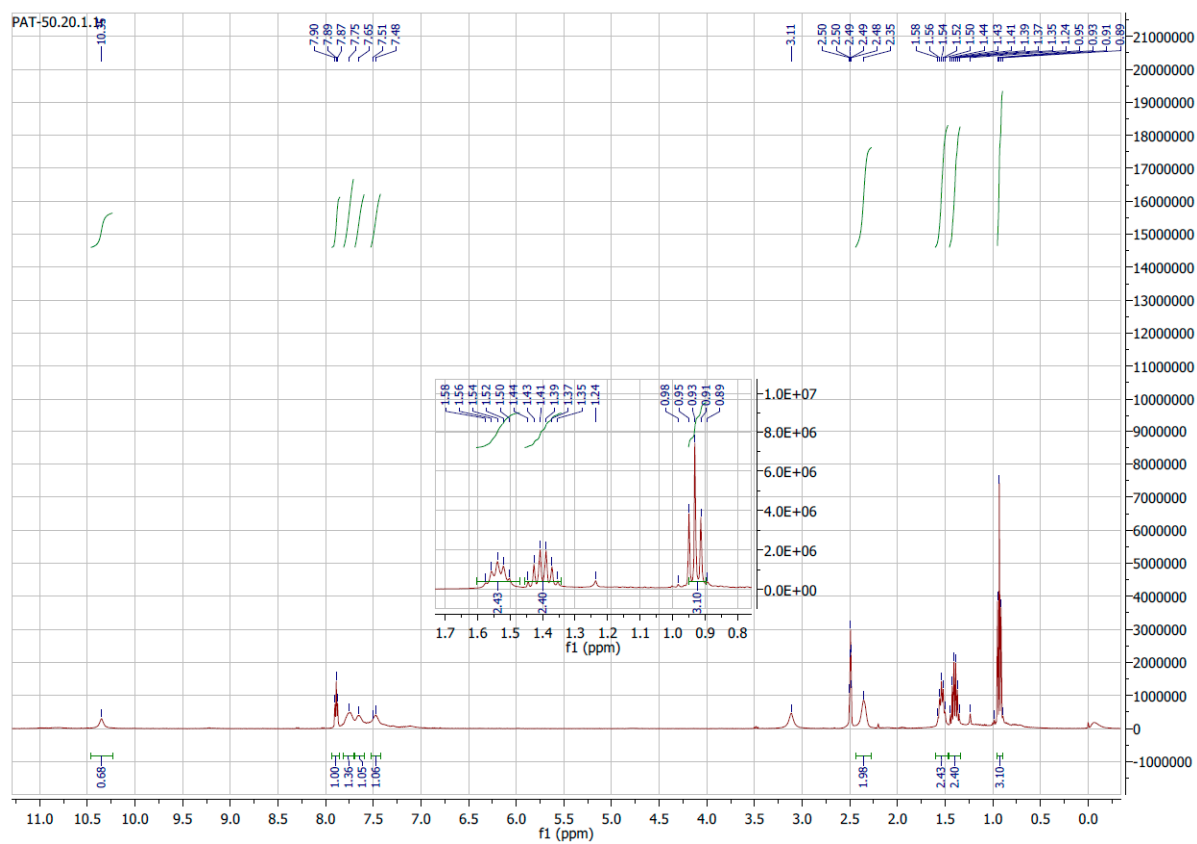
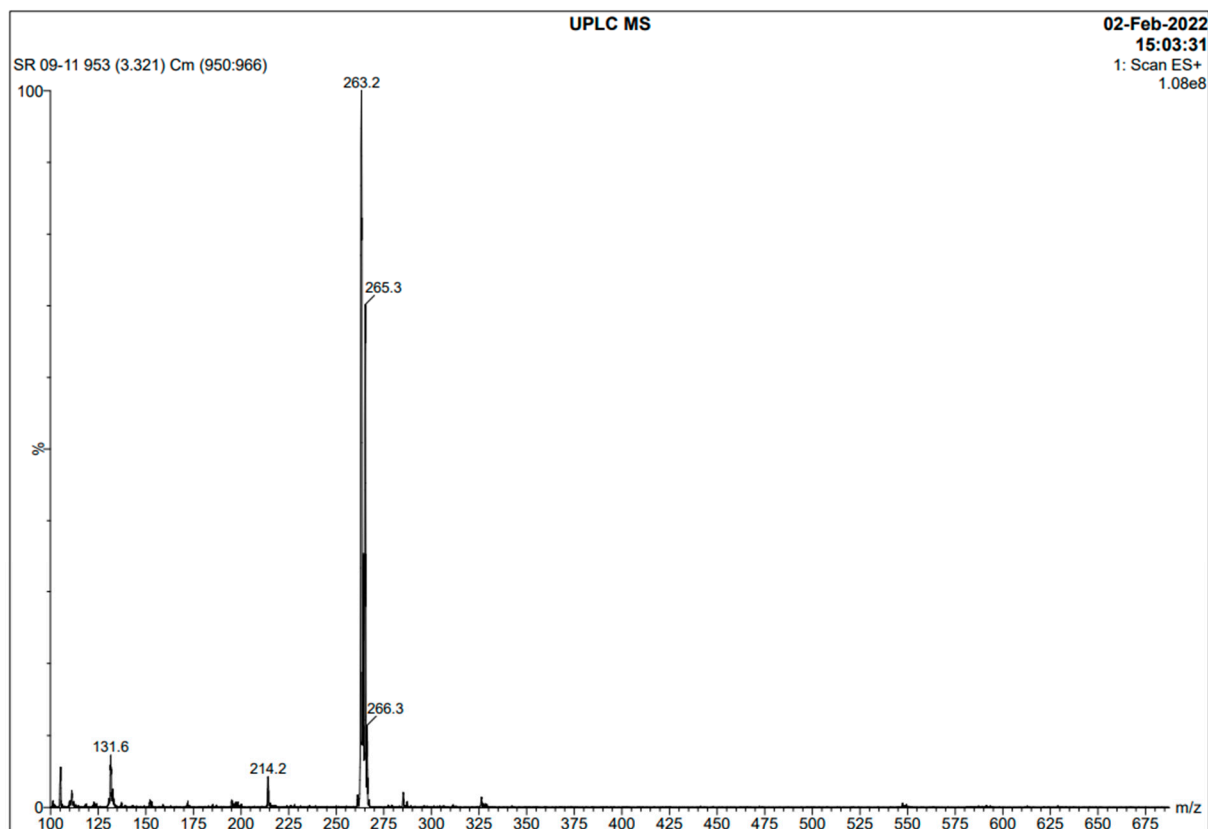


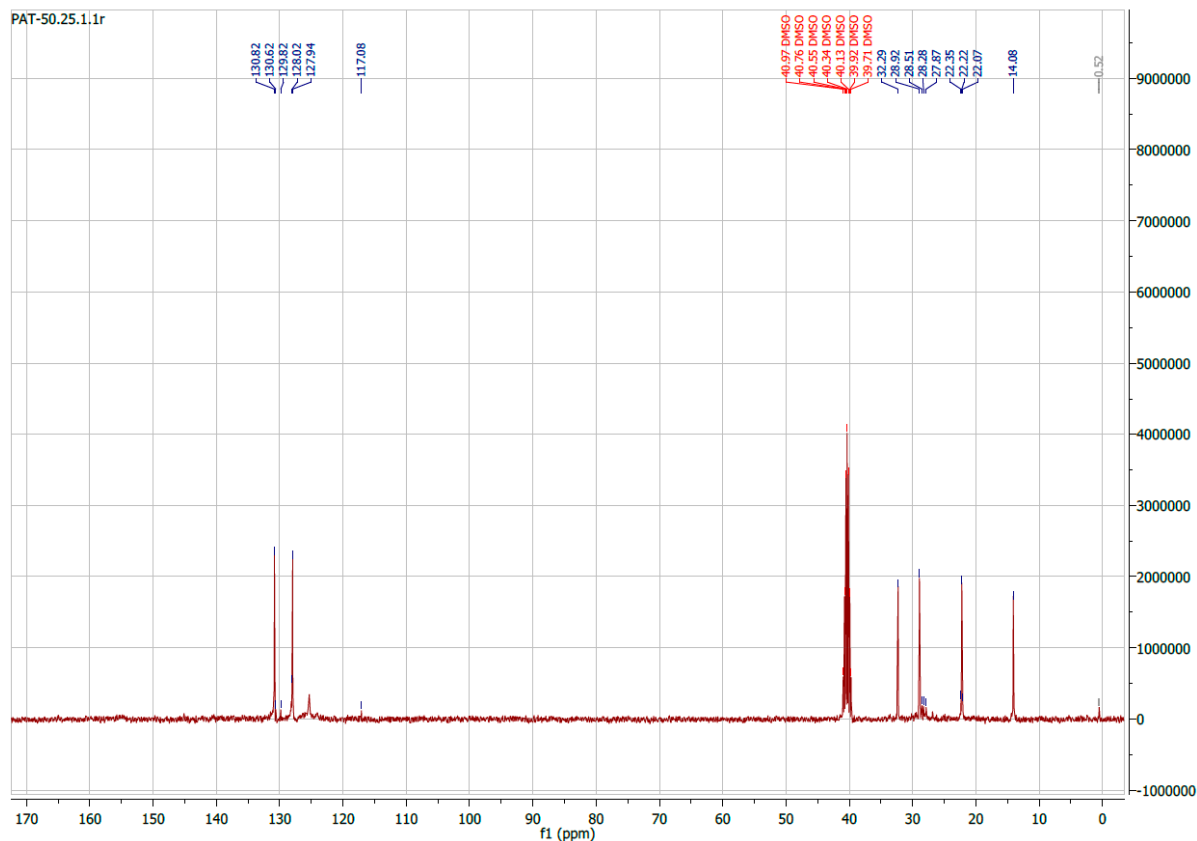




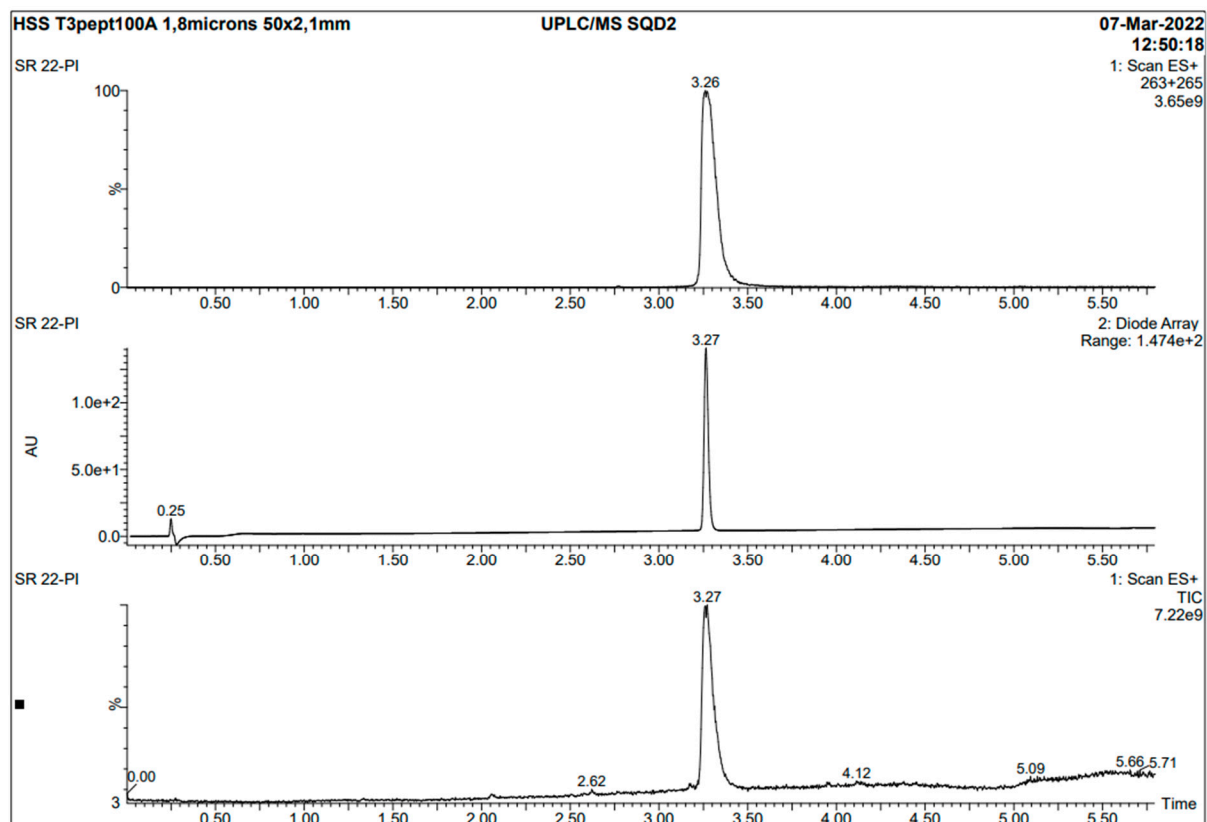
S13. 2-chloro-3-(2-pentylidenehydrazinyl)quinoxaline (14g).

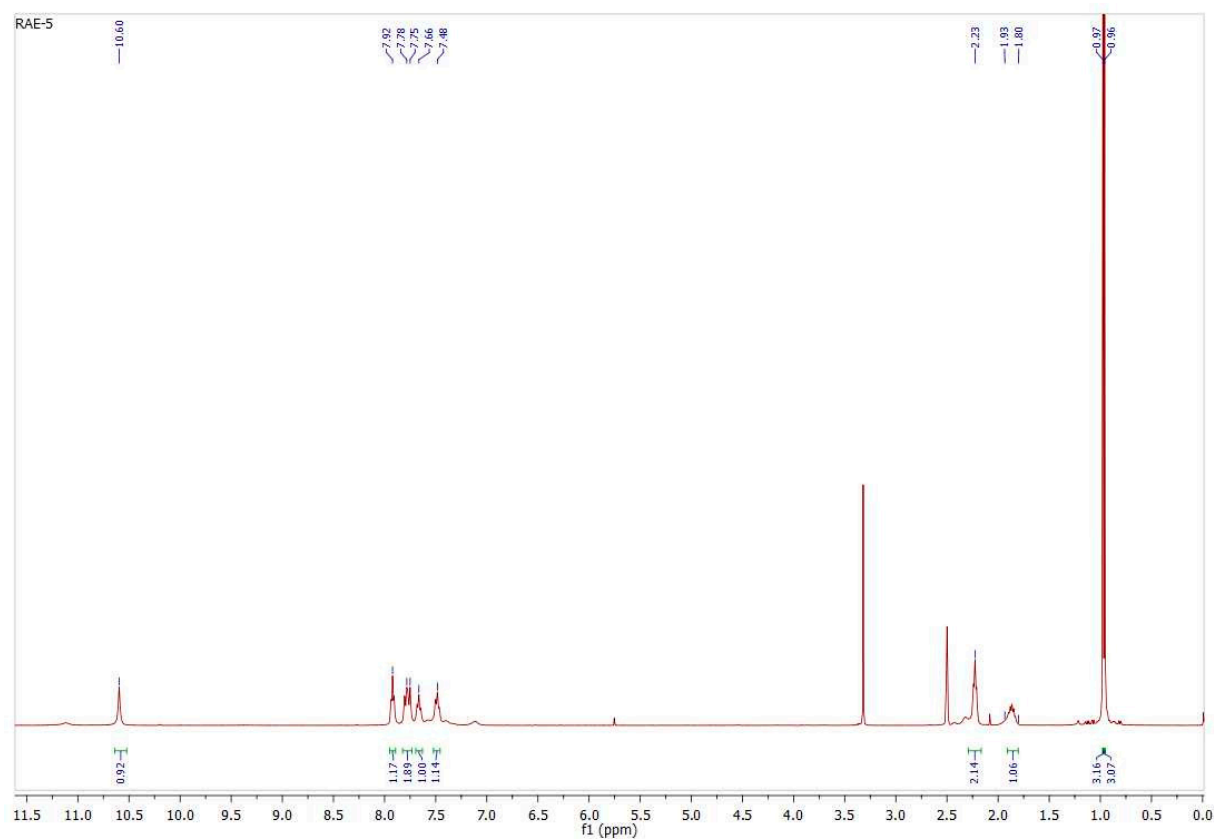
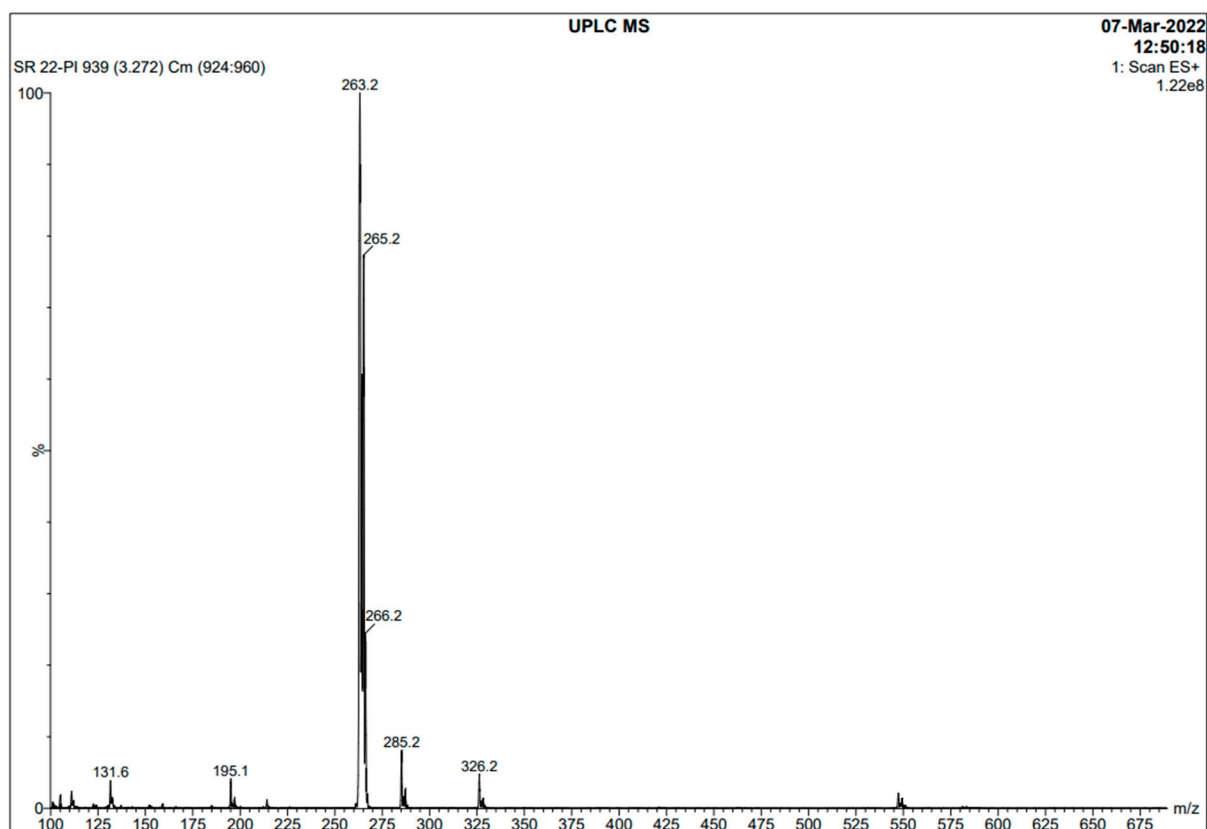


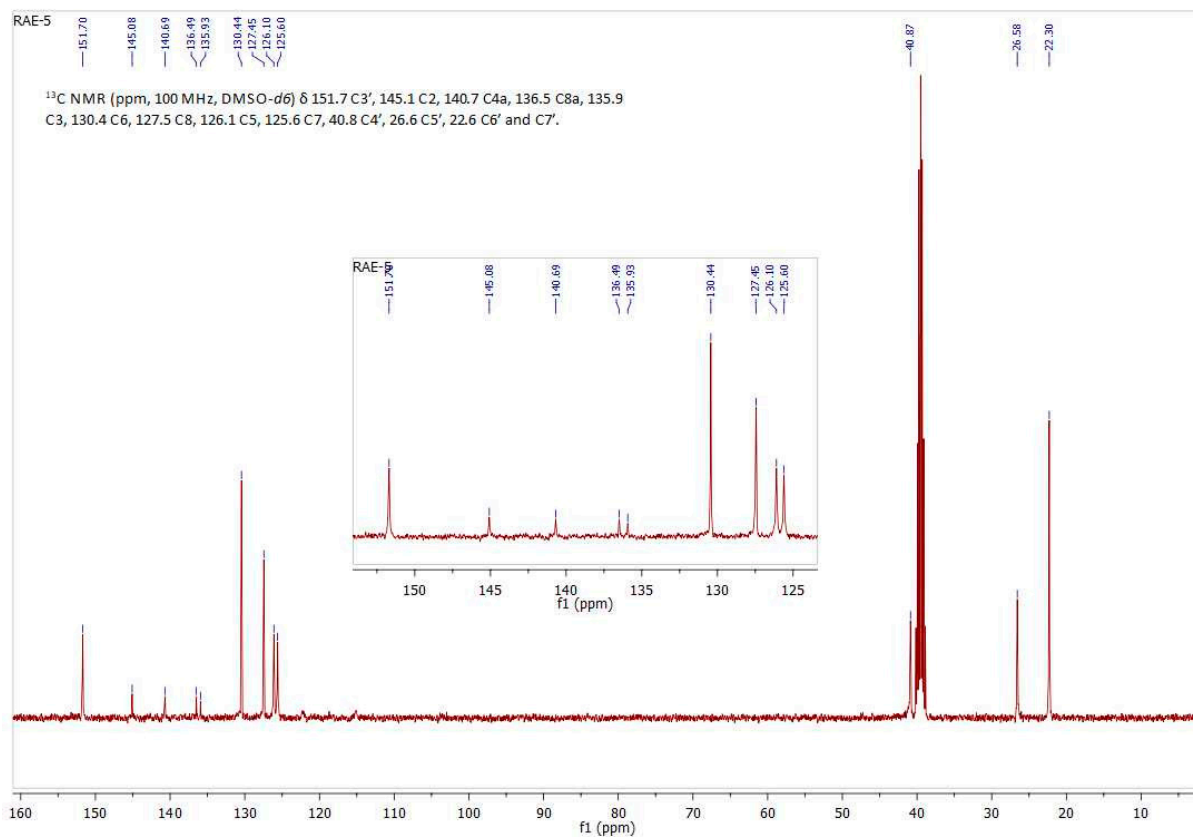




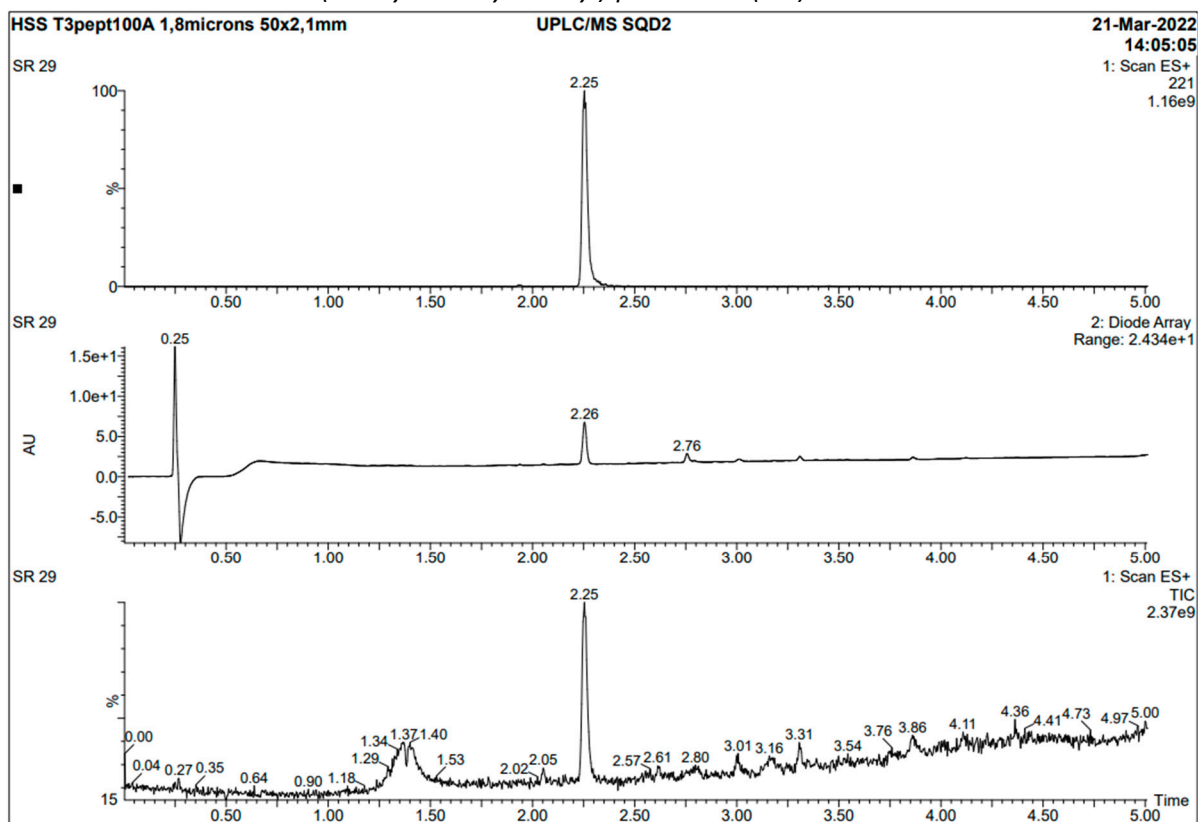
S14. 2-chloro-3-(2-(3-methylbutylidene)hydrazinyl)quinoxaline (**14h**).

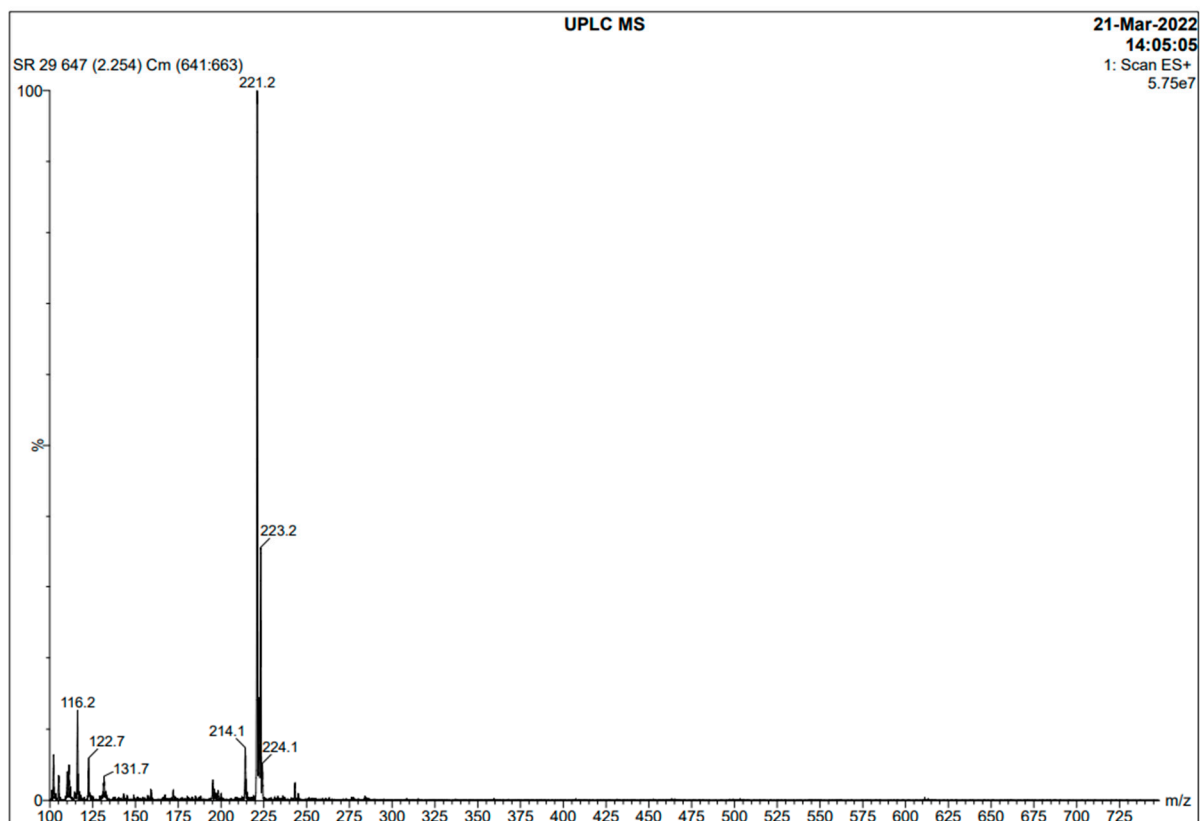




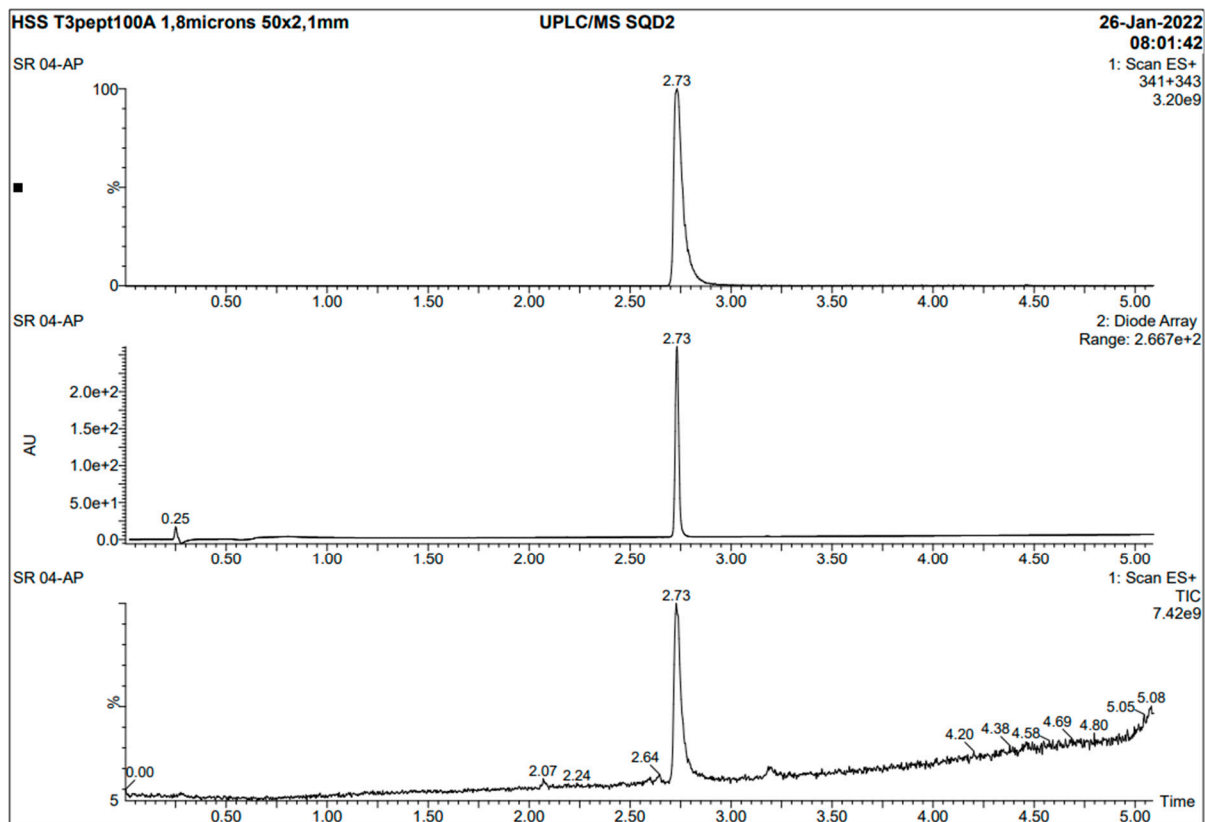


S15. 2-chloro-3-(2-ethylidenehydrazinyl)quinoxaline (**14i**).

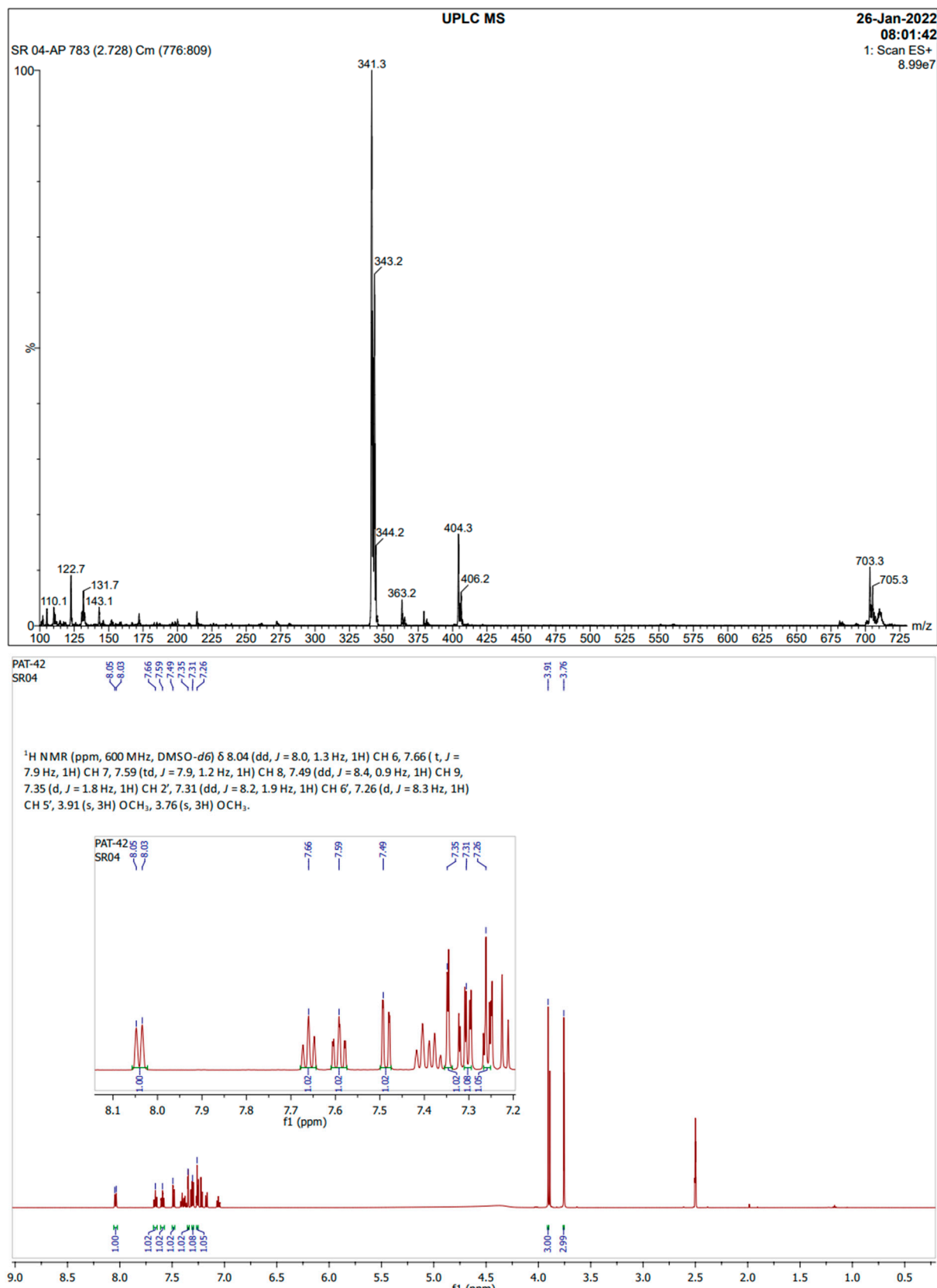


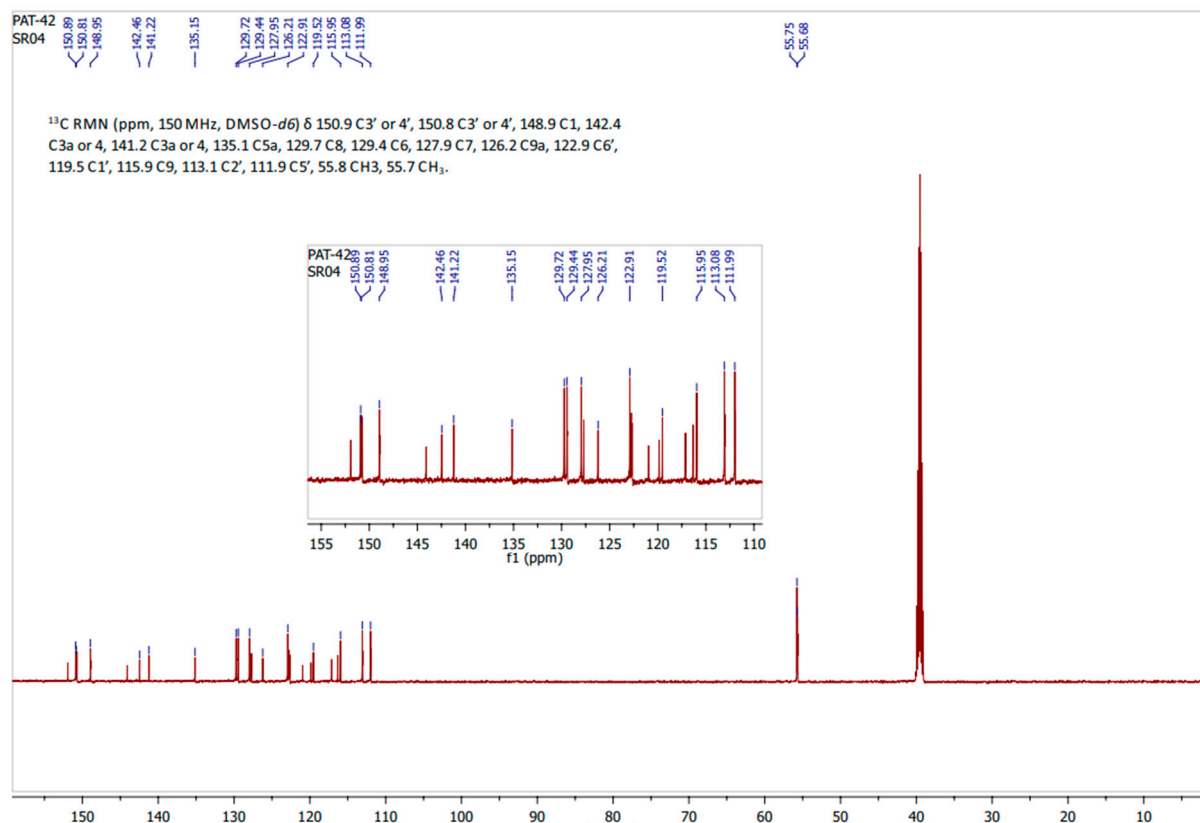


S16. 4-chloro-1-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxaline (**15a**).

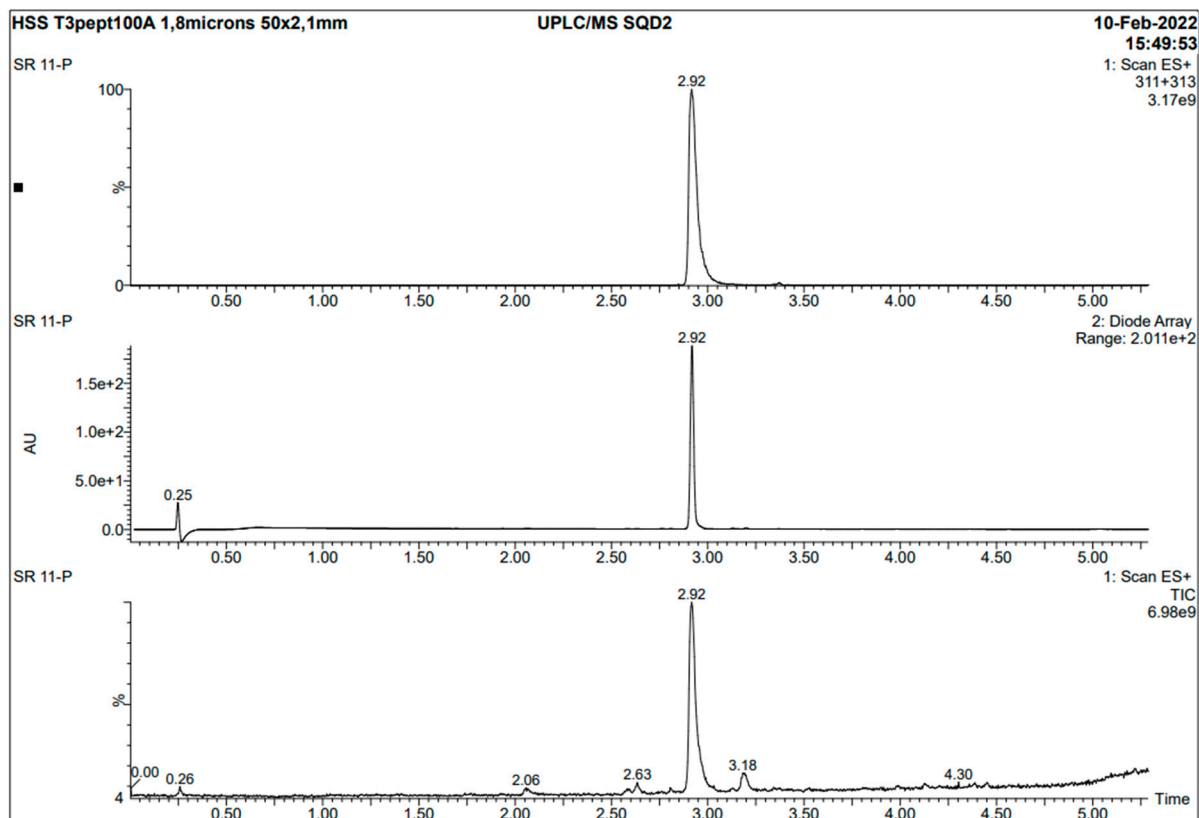


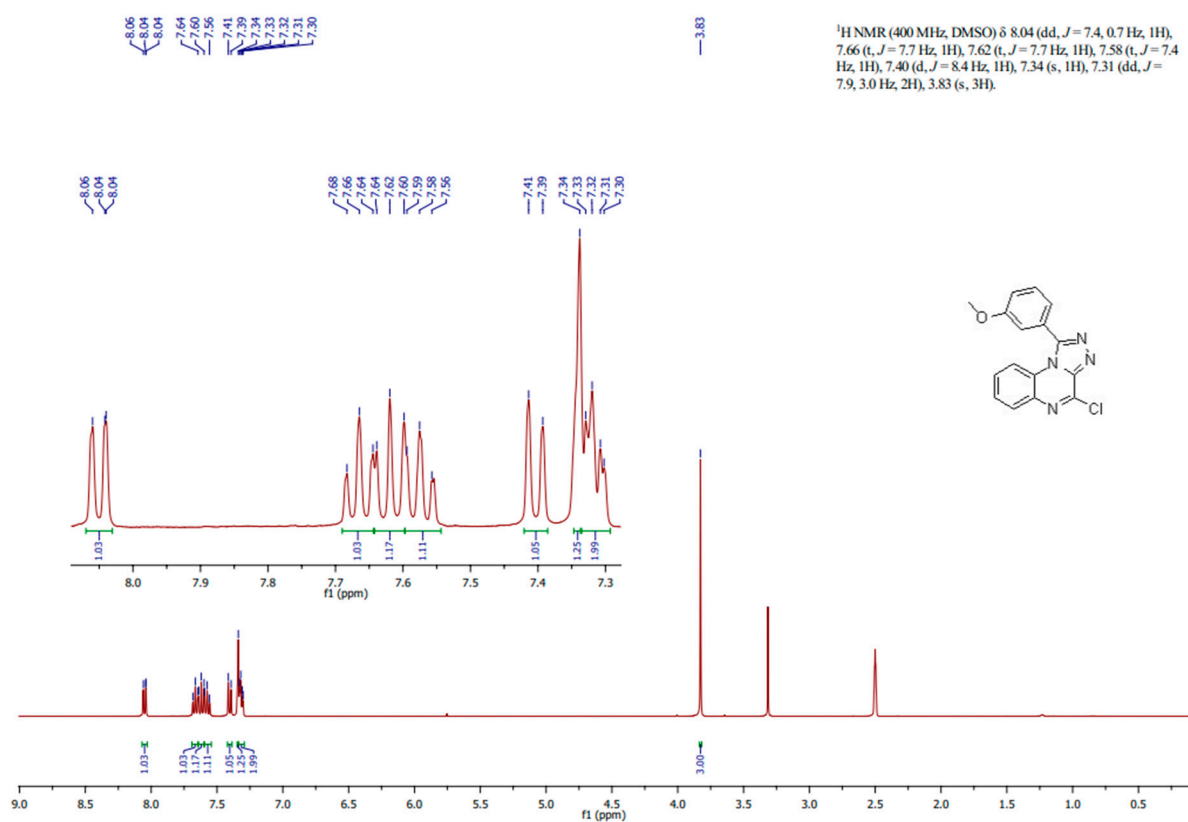
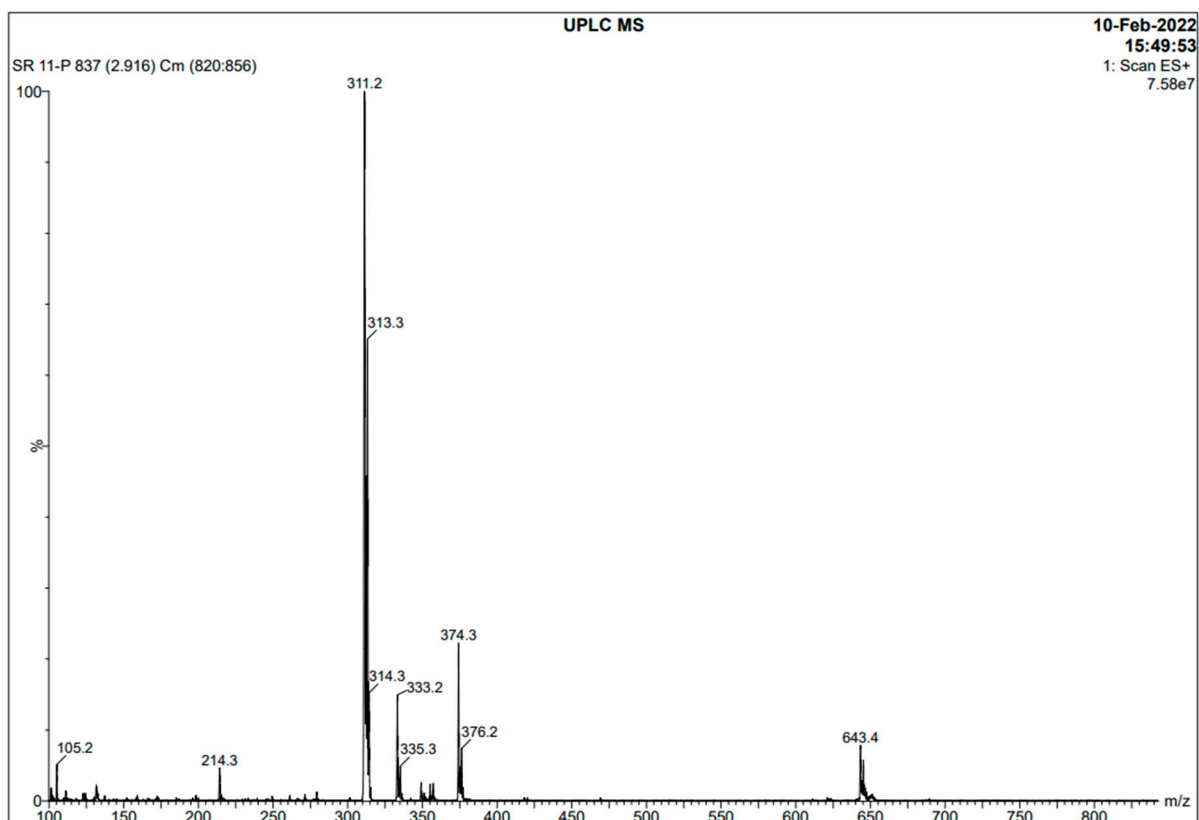


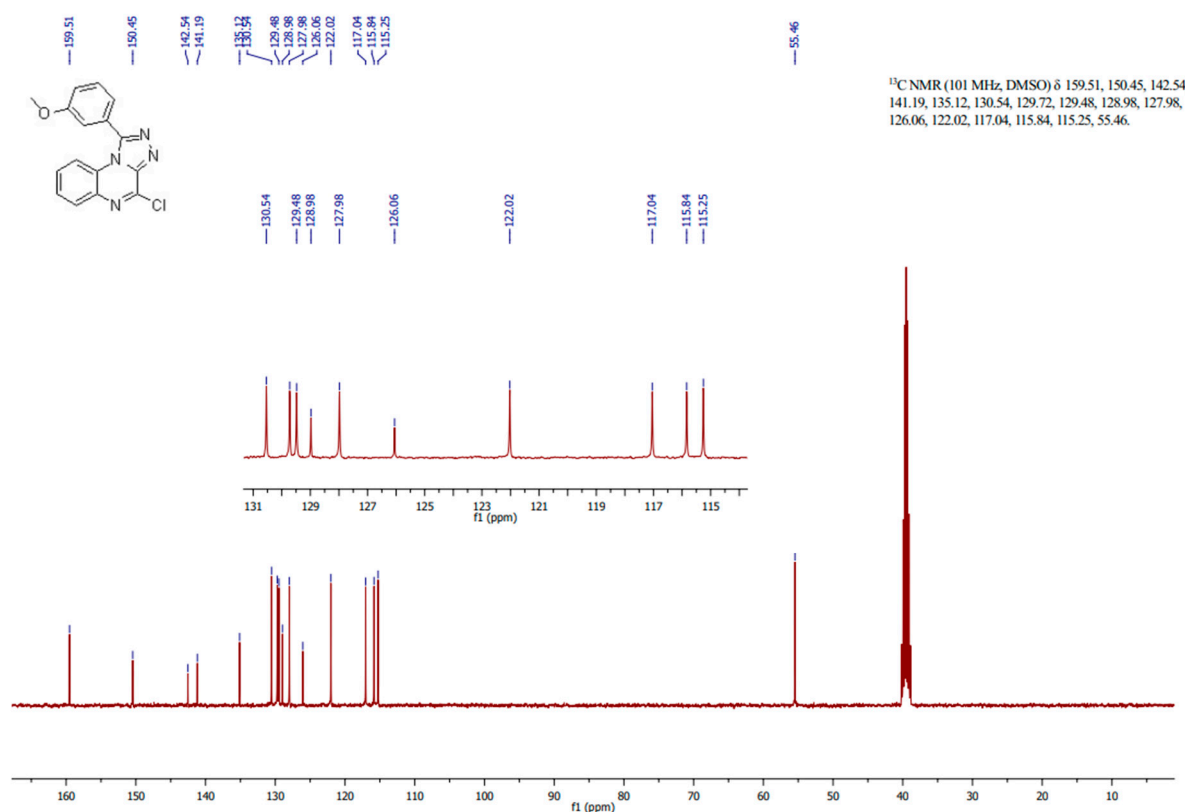




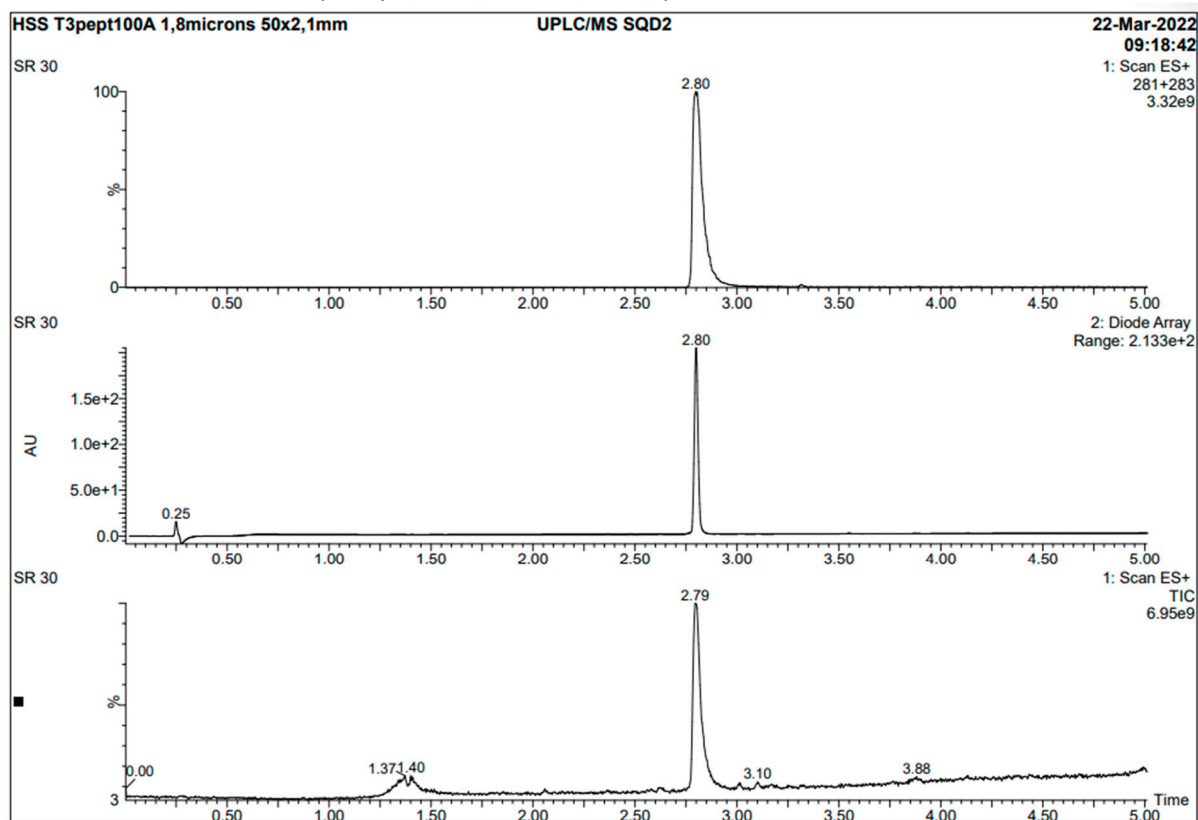
S17. 4-chloro-1-(3-methoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxaline (**15b**).

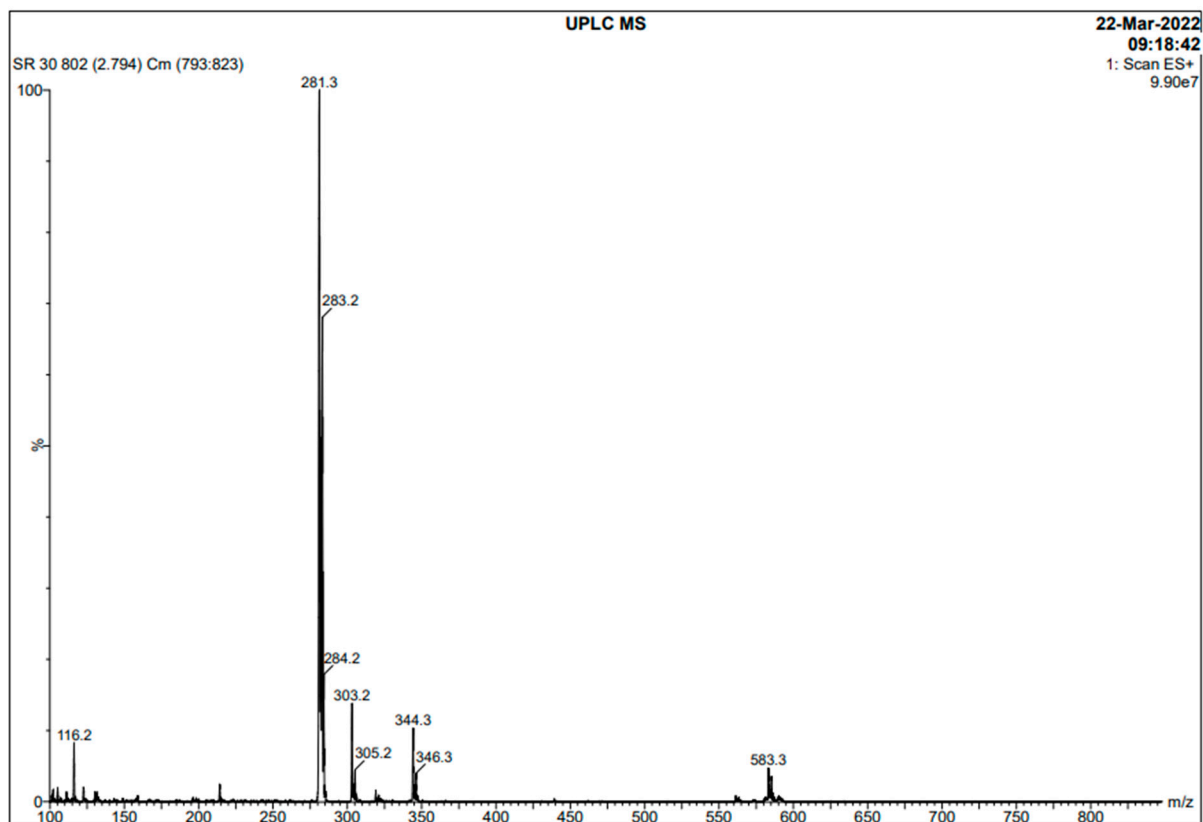




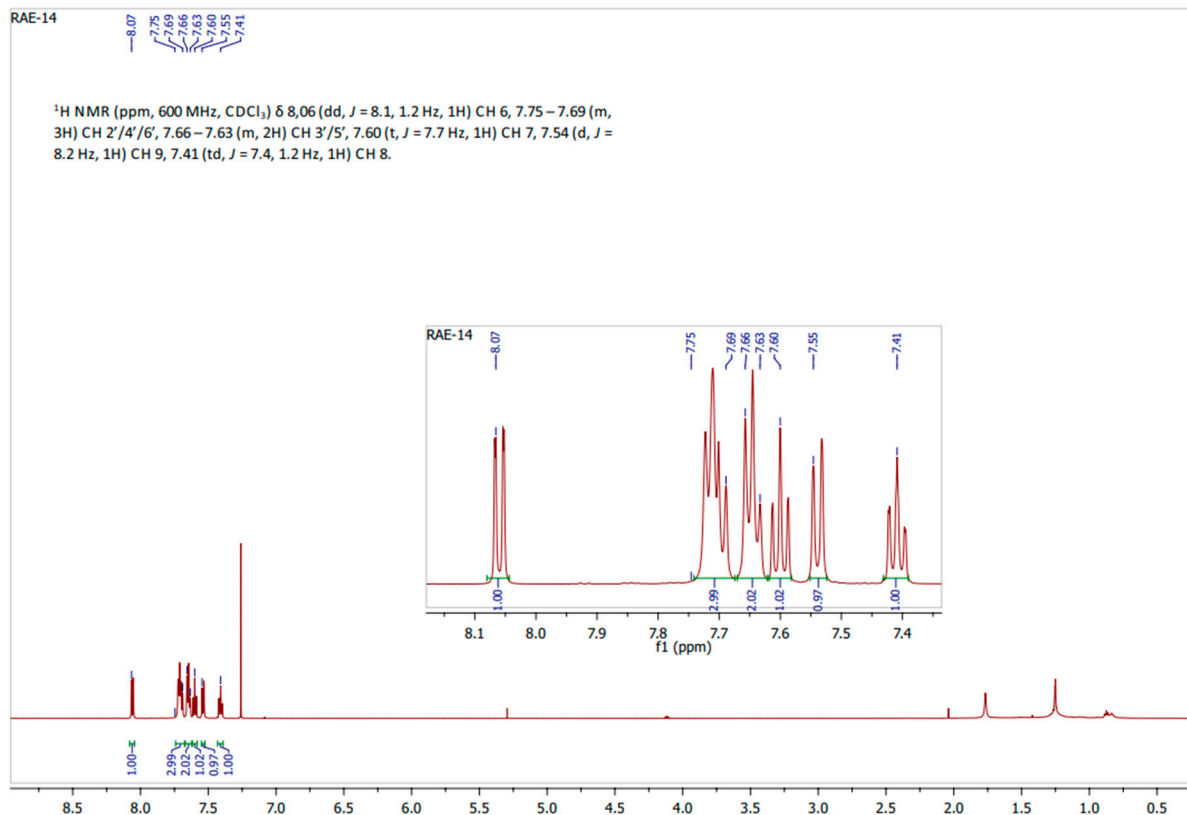


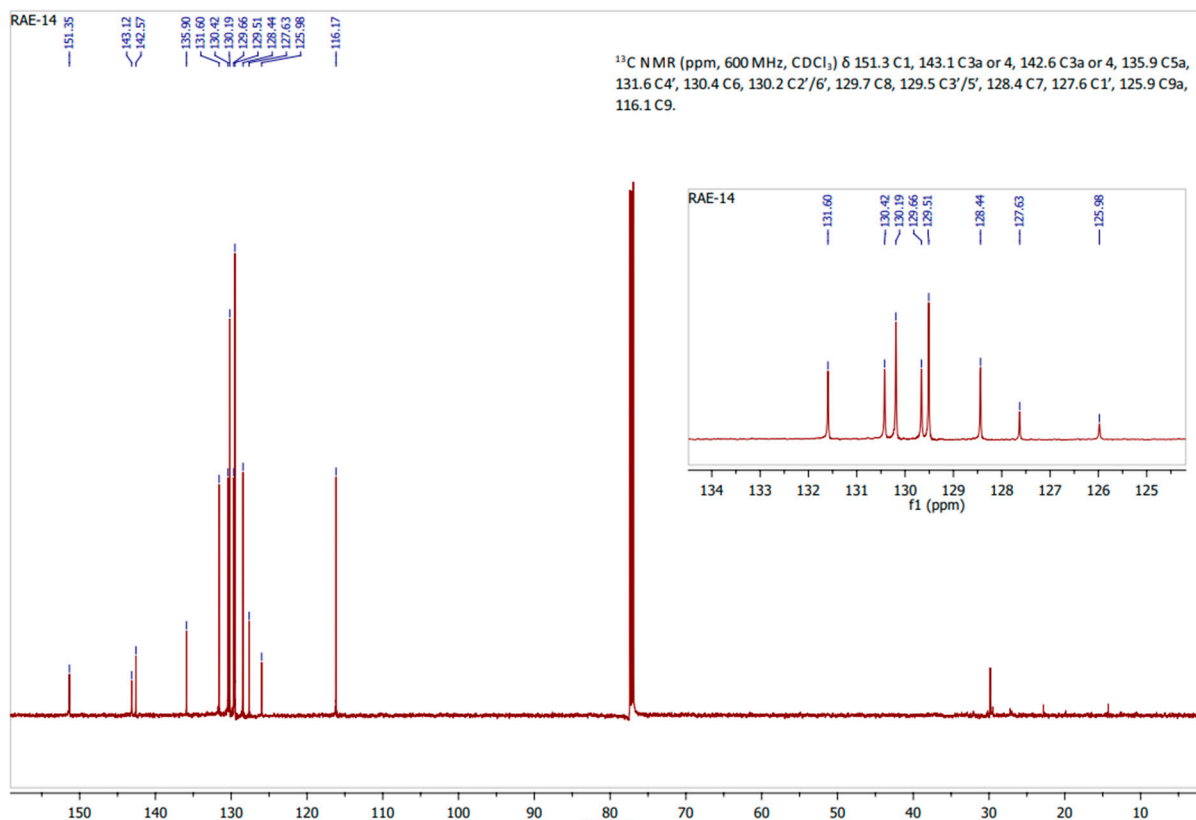
S18. 4-chloro-1-phenyl-[1,2,4]triazolo[4,3-a]quinoxaline (15c).



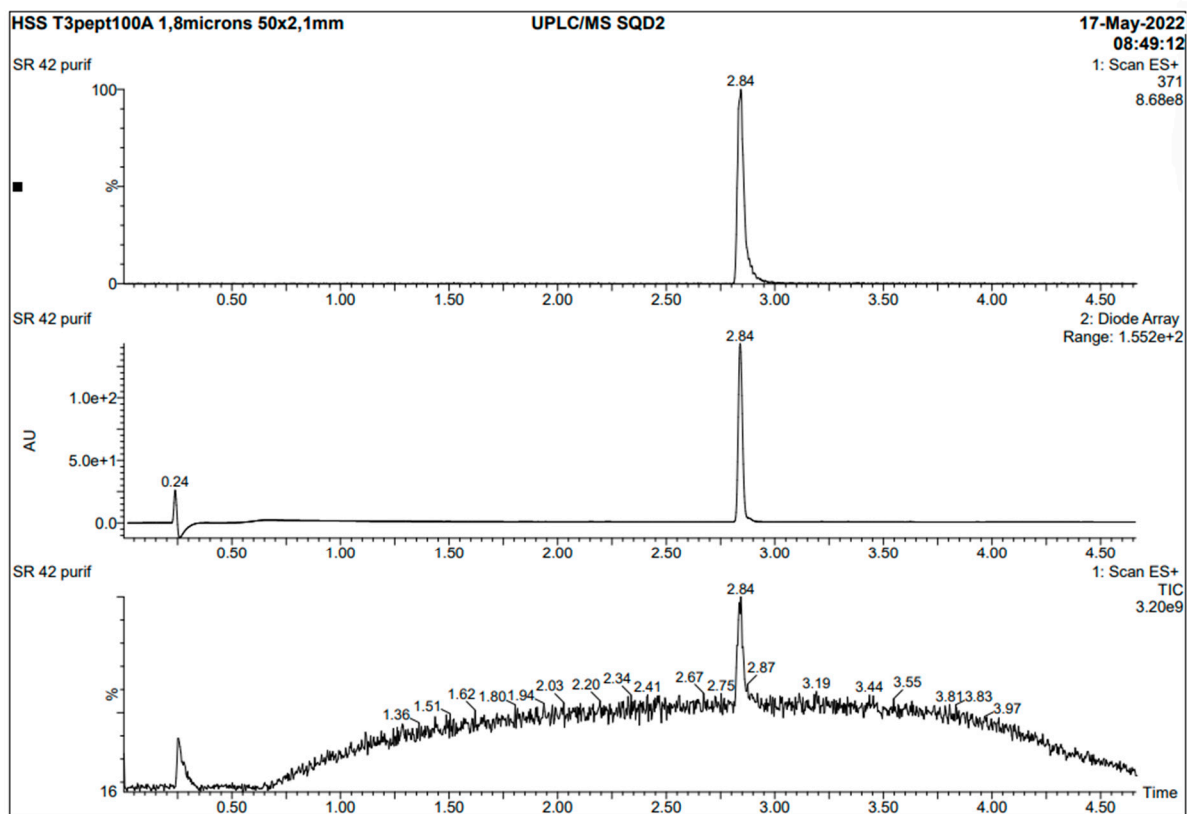


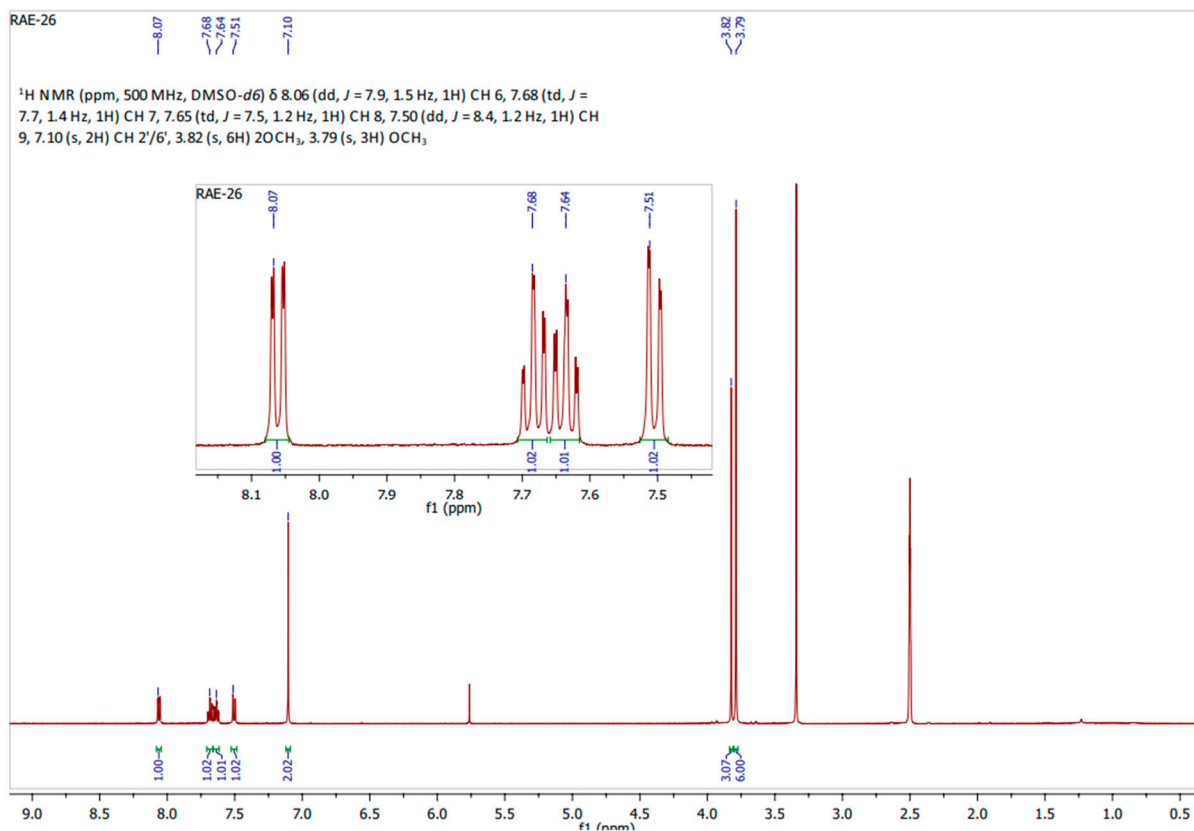
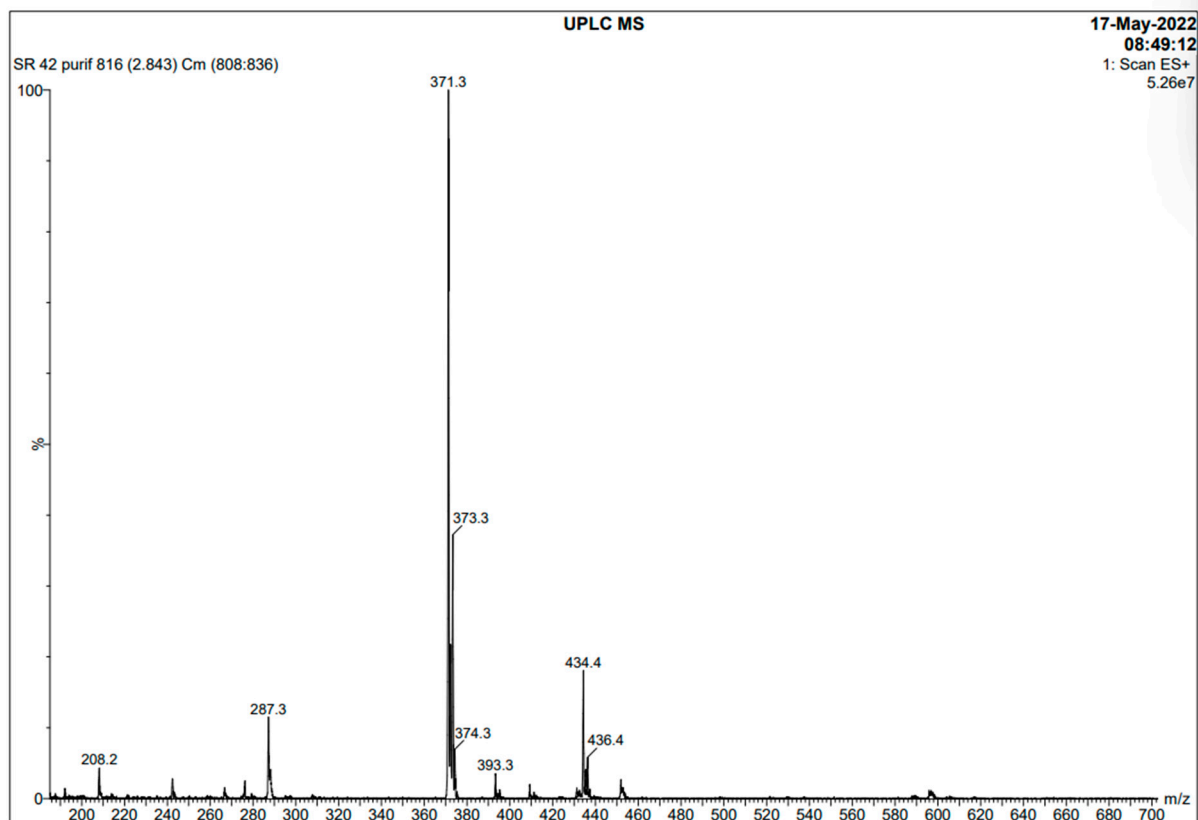
RAE-14

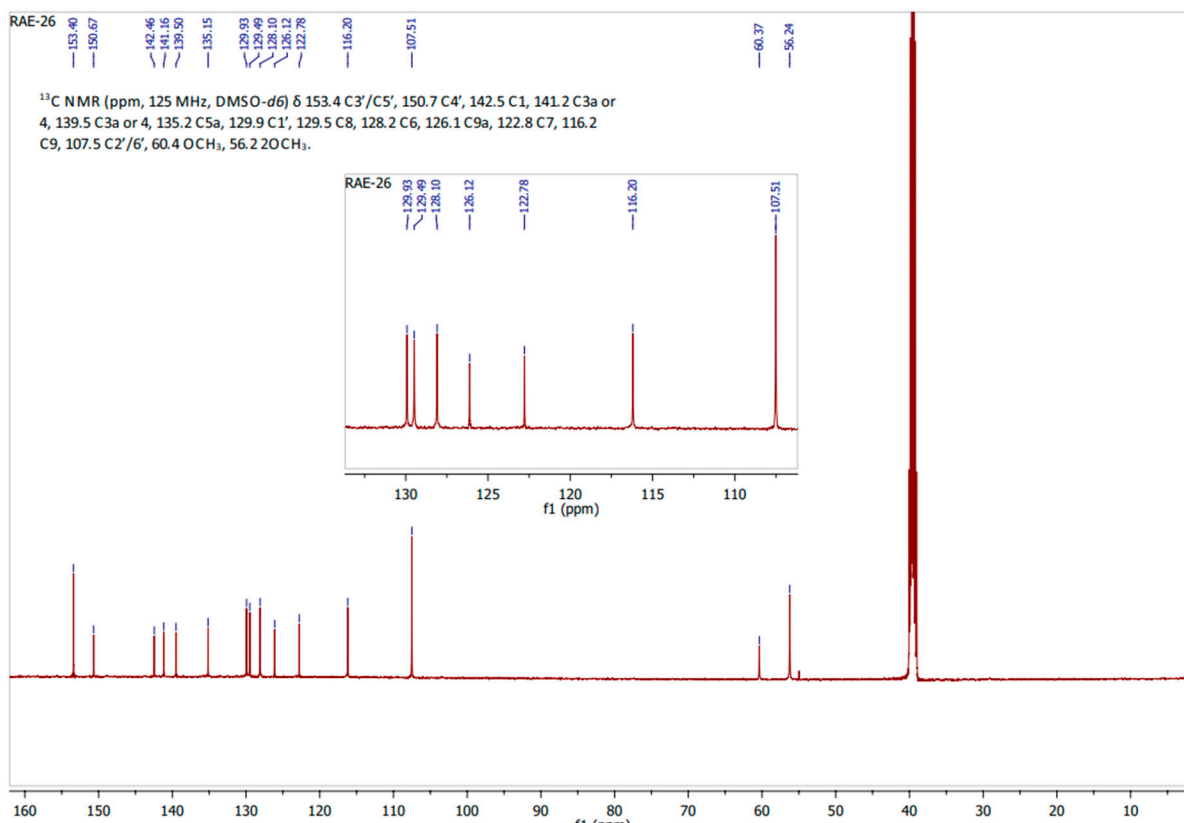




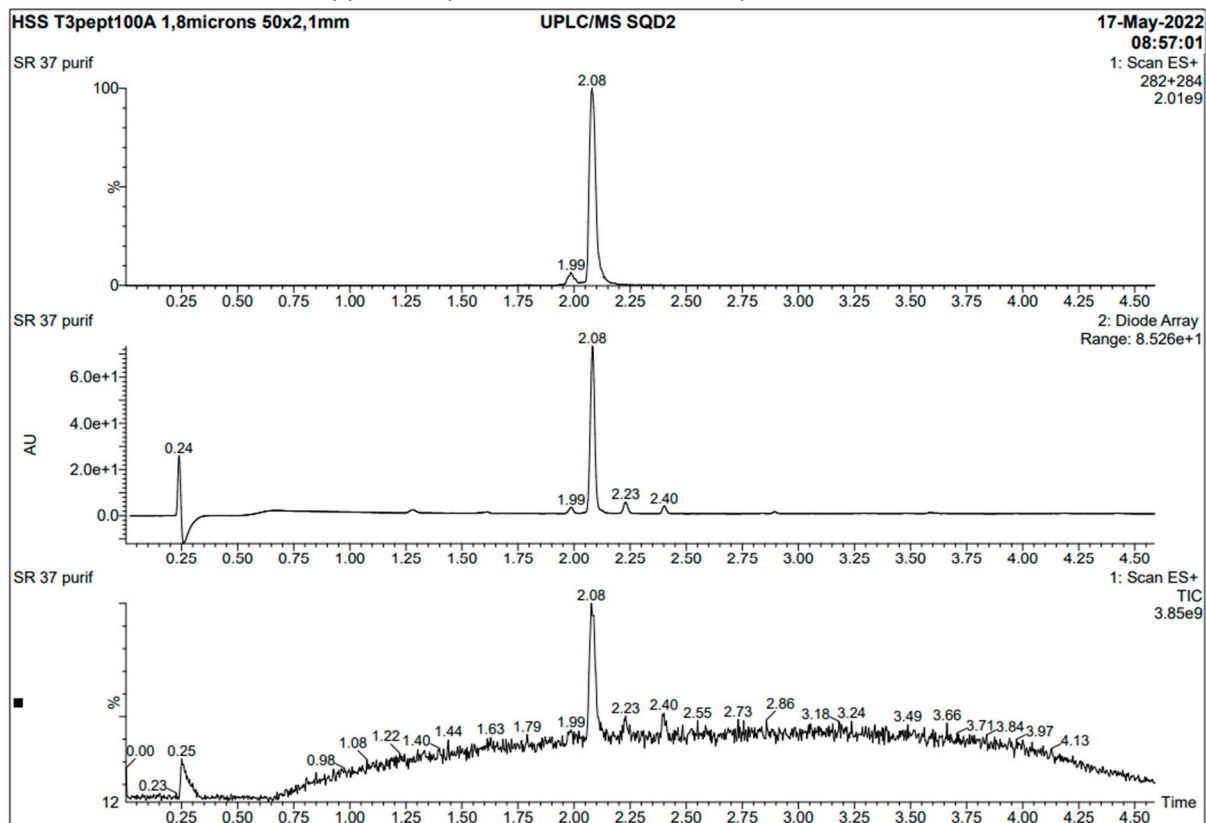
S19. 4-chloro-1-(3,4,5-trimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxaline (**15d**).



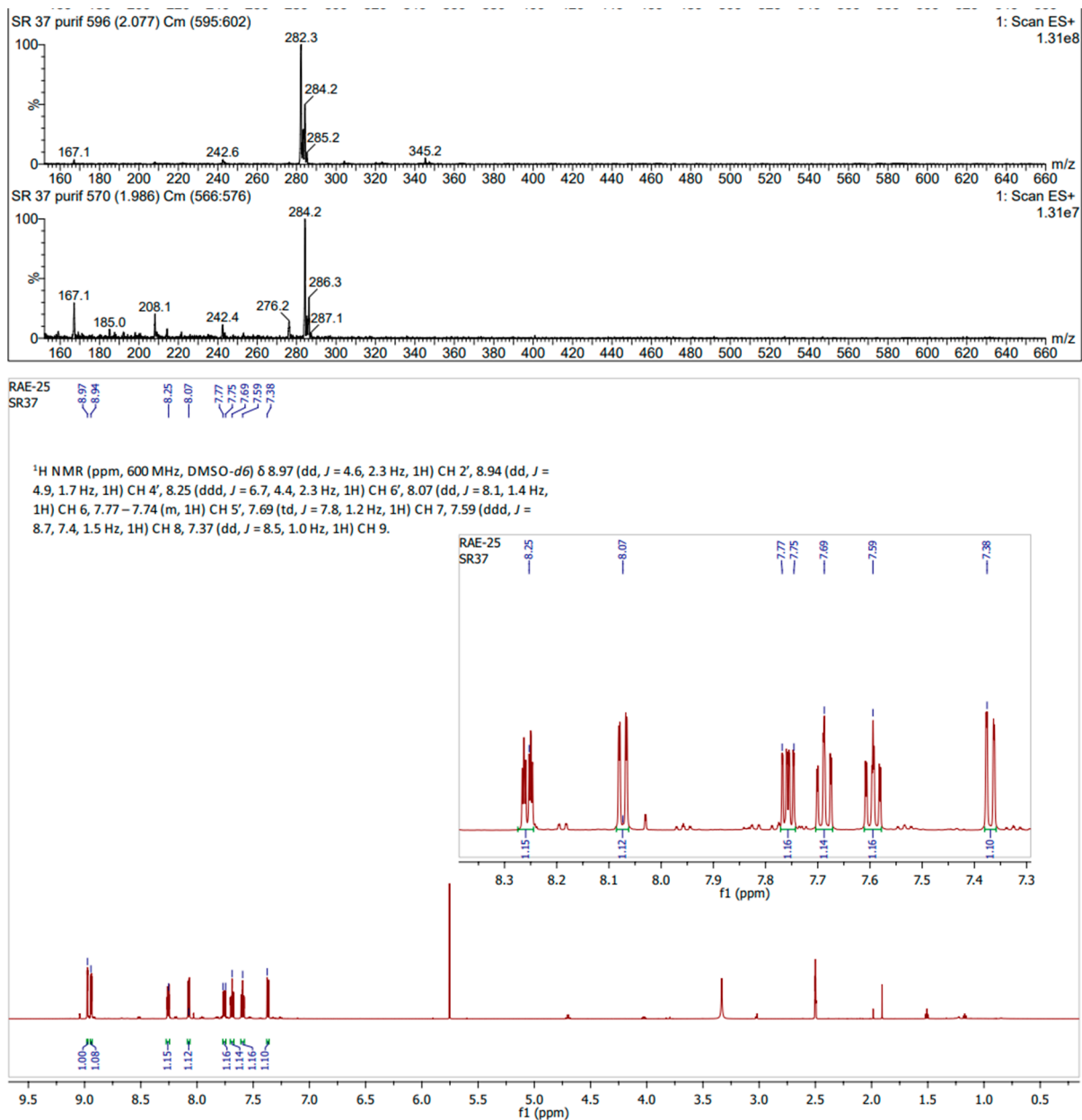


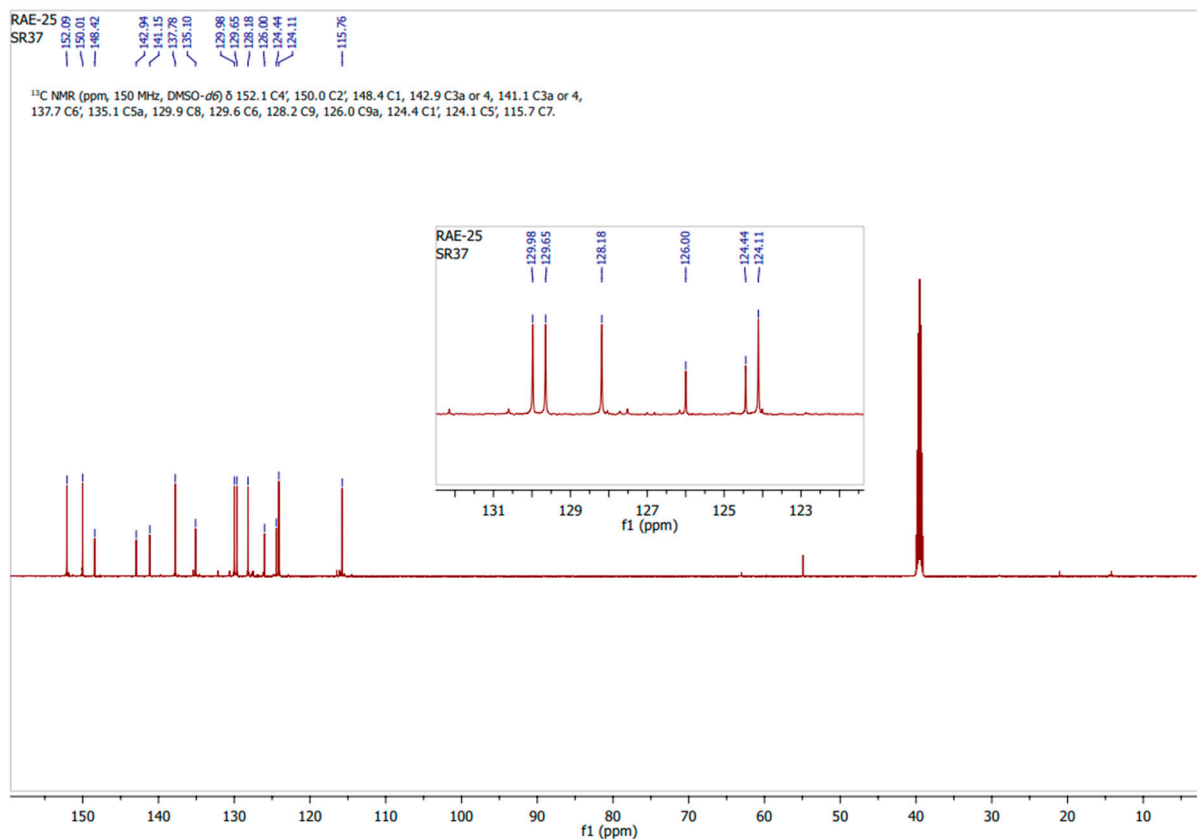


S20. 4-chloro-1-(pyridin-3-yl)-[1,2,4]triazolo[4,3-a]quinoxaline (15e).

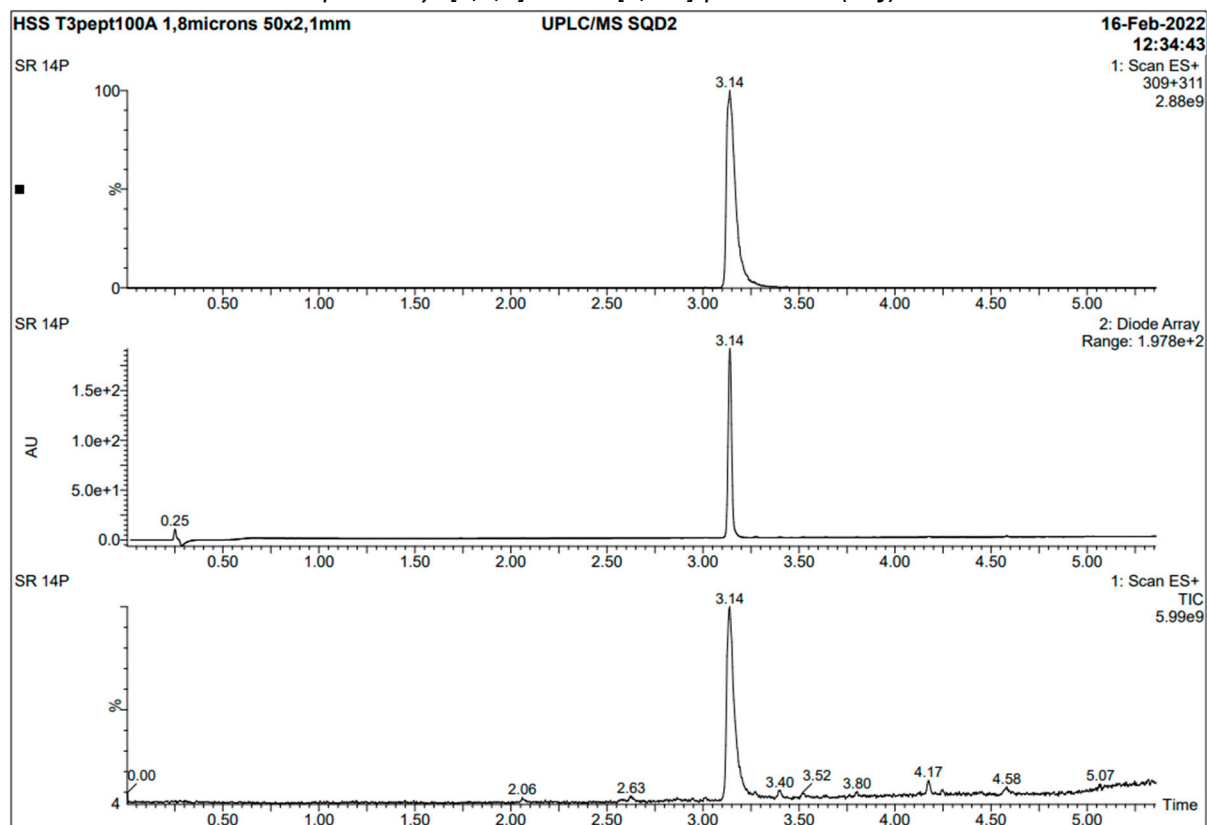


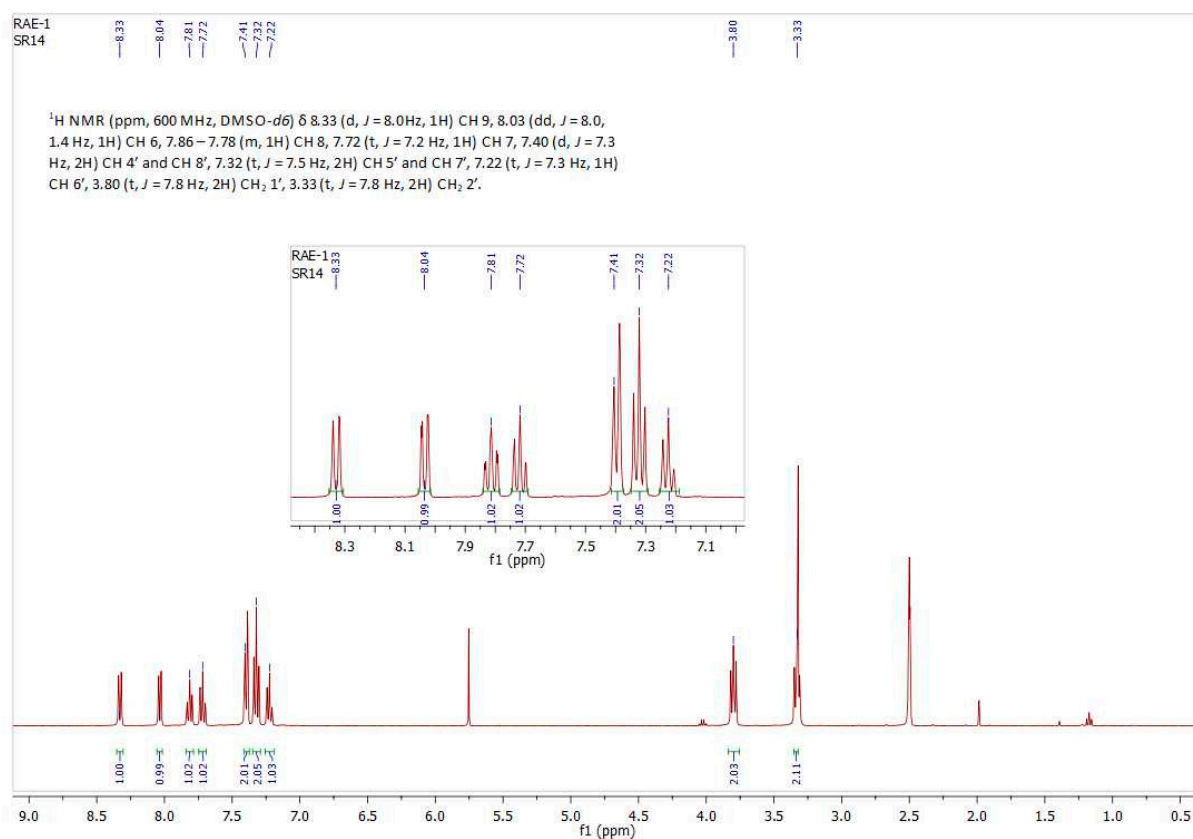
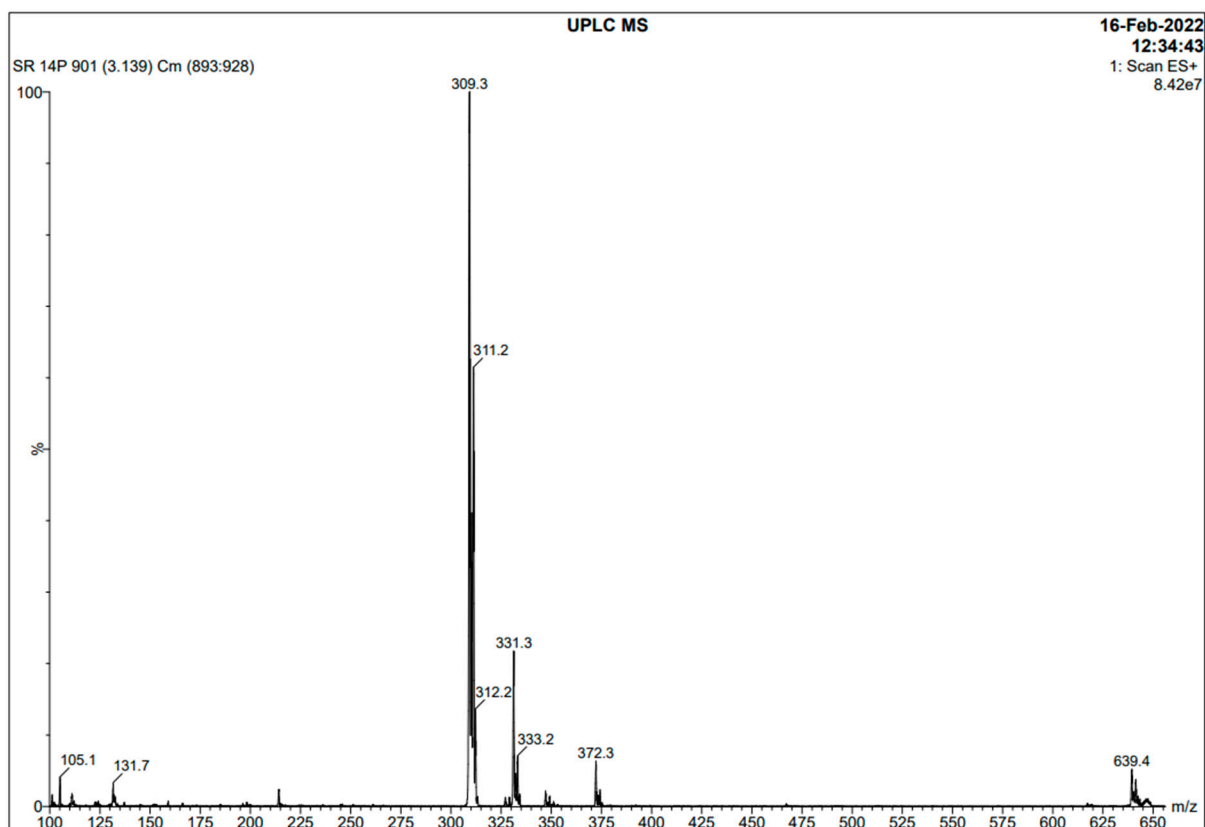


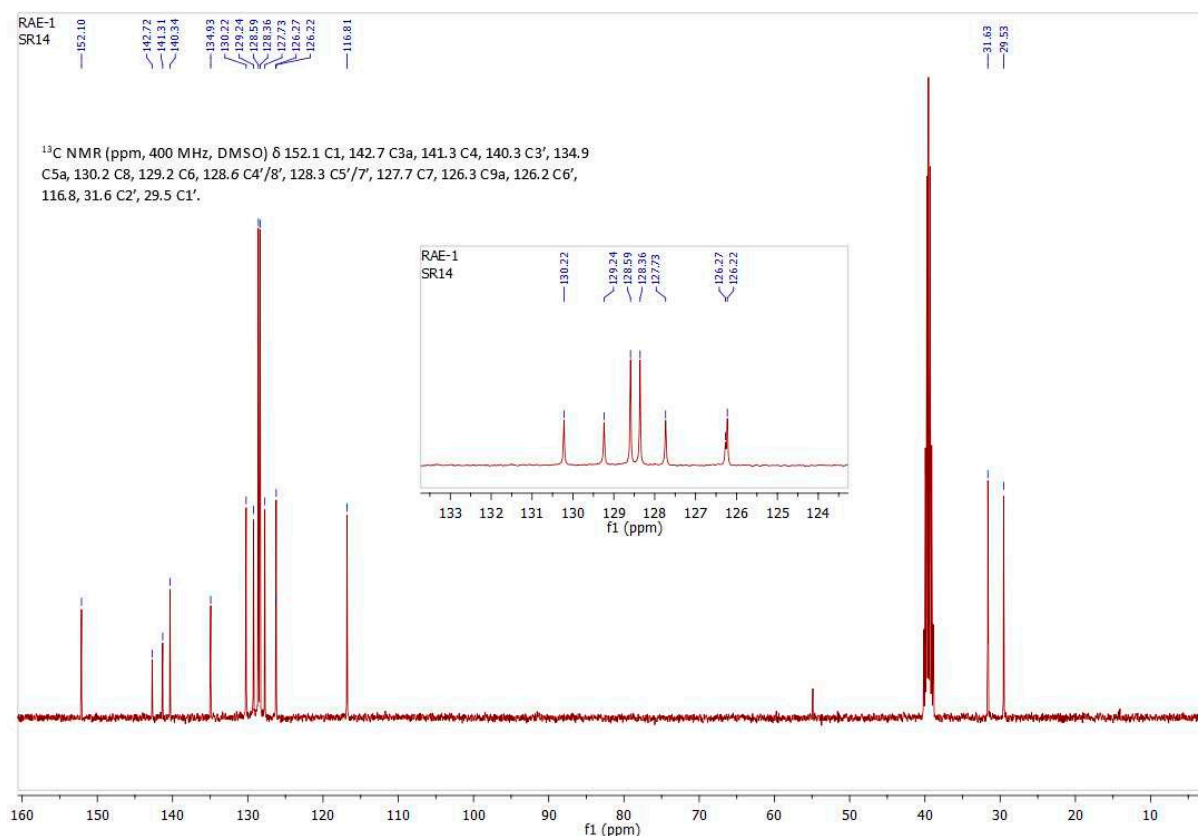




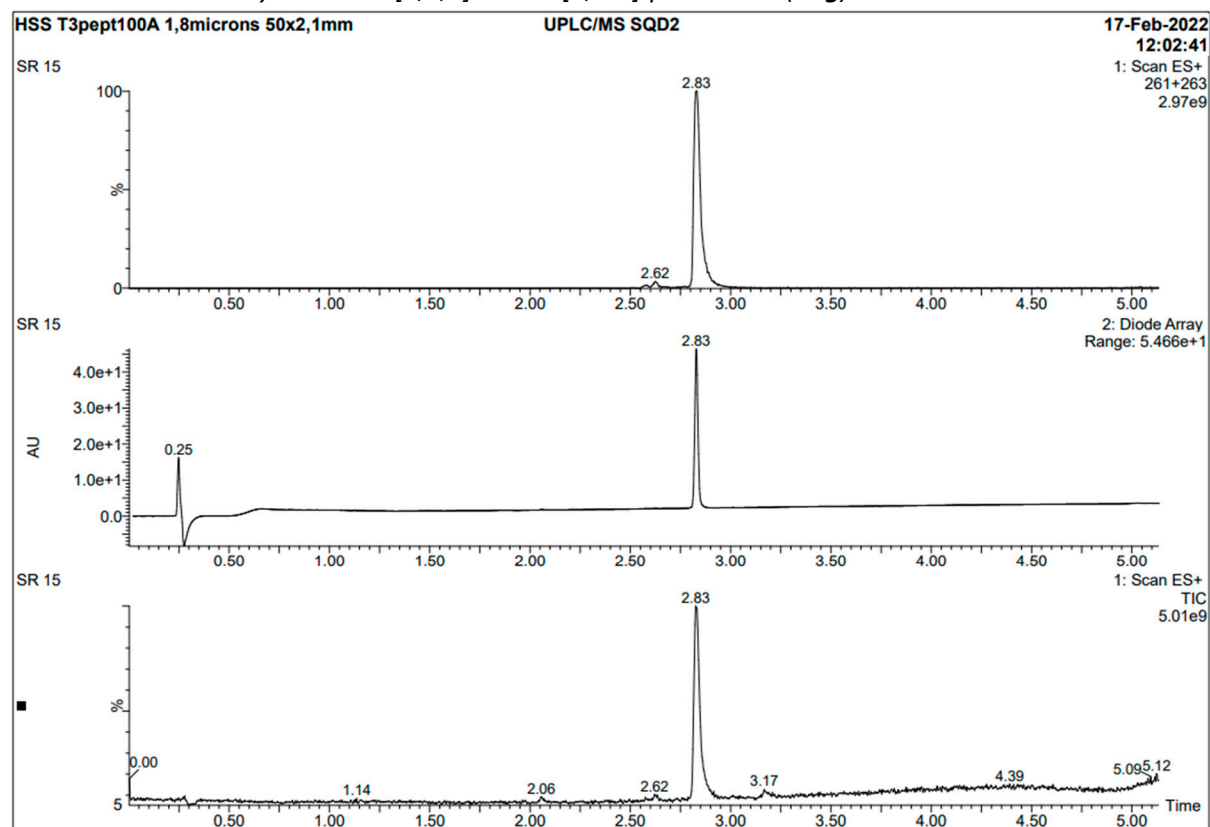
S21. 4-chloro-1-phenethyl-[1,2,4]triazolo[4,3-a]quinoxaline (**15f**).

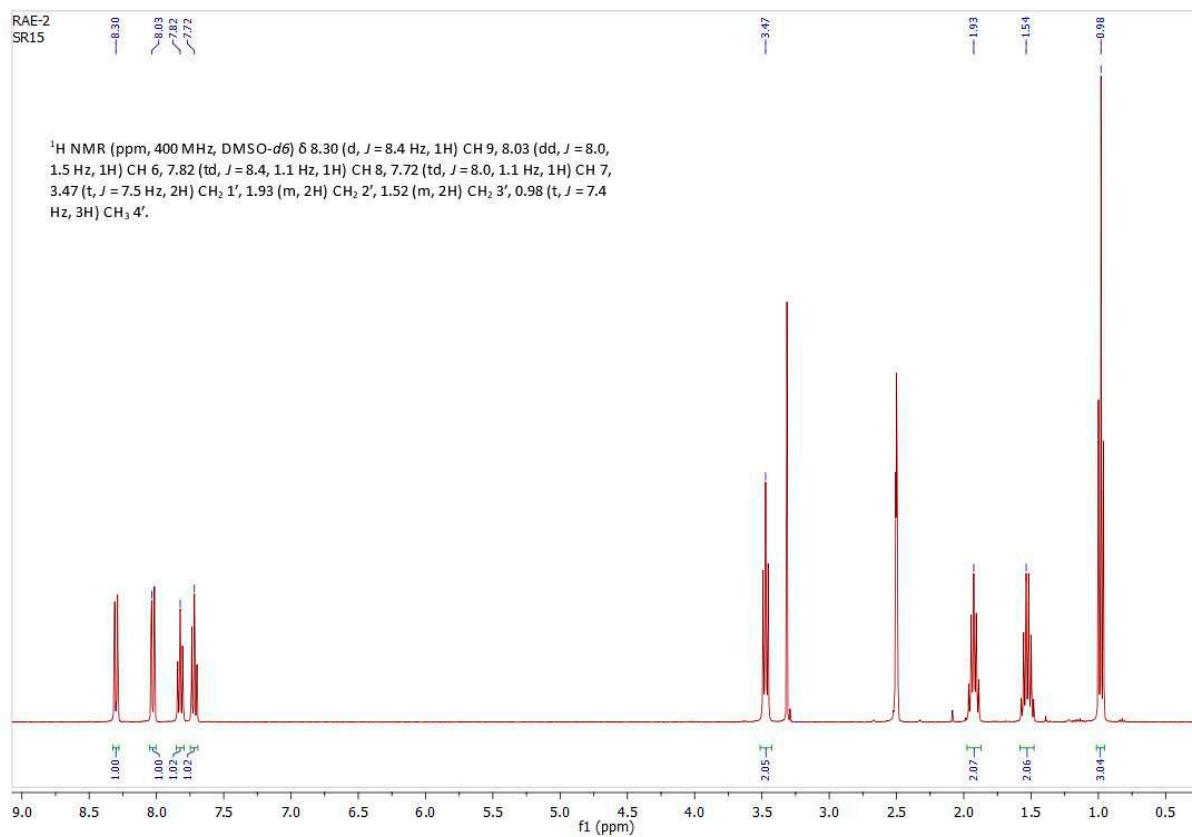
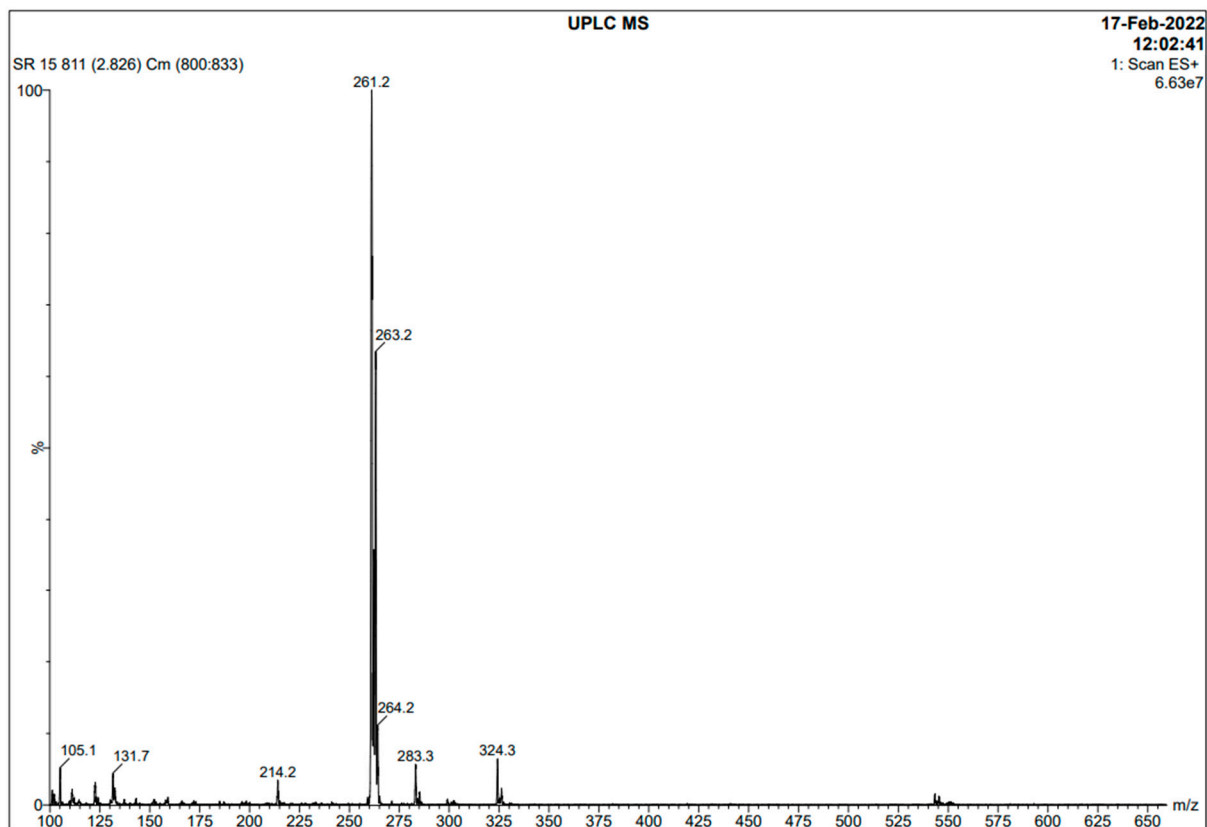


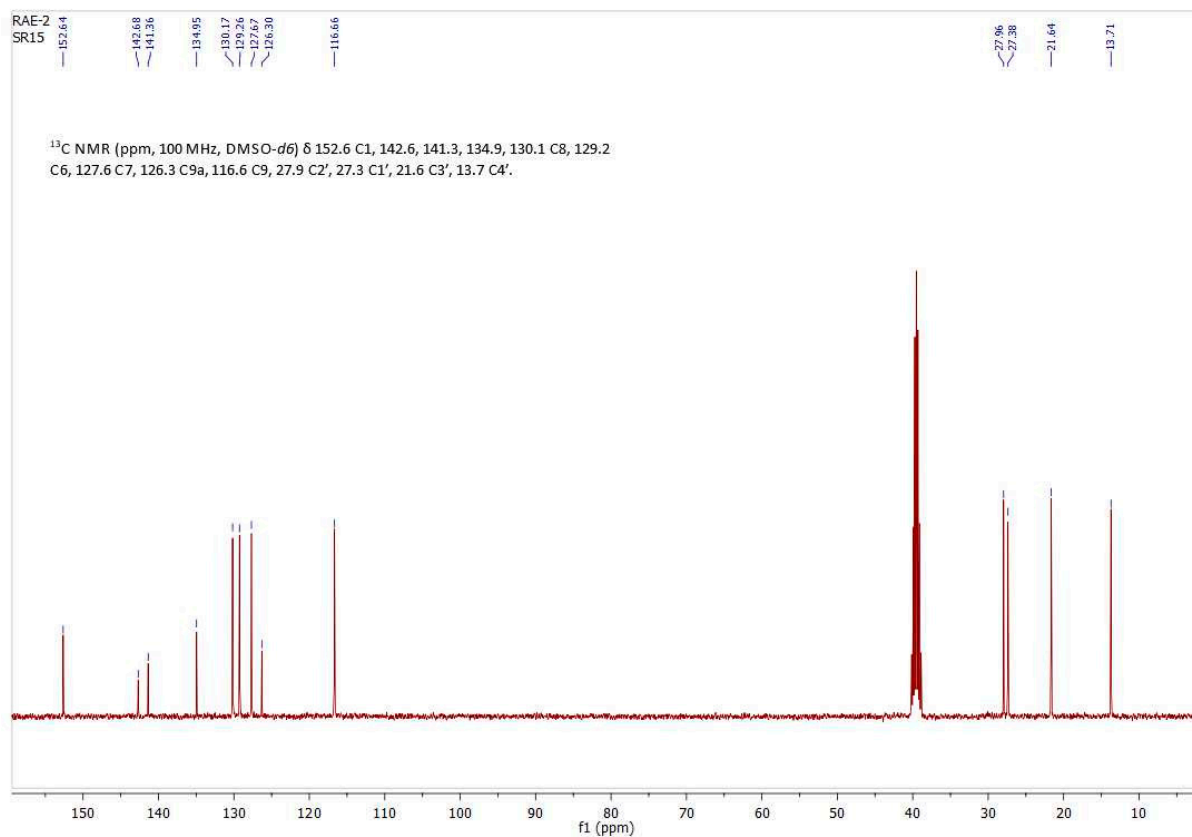




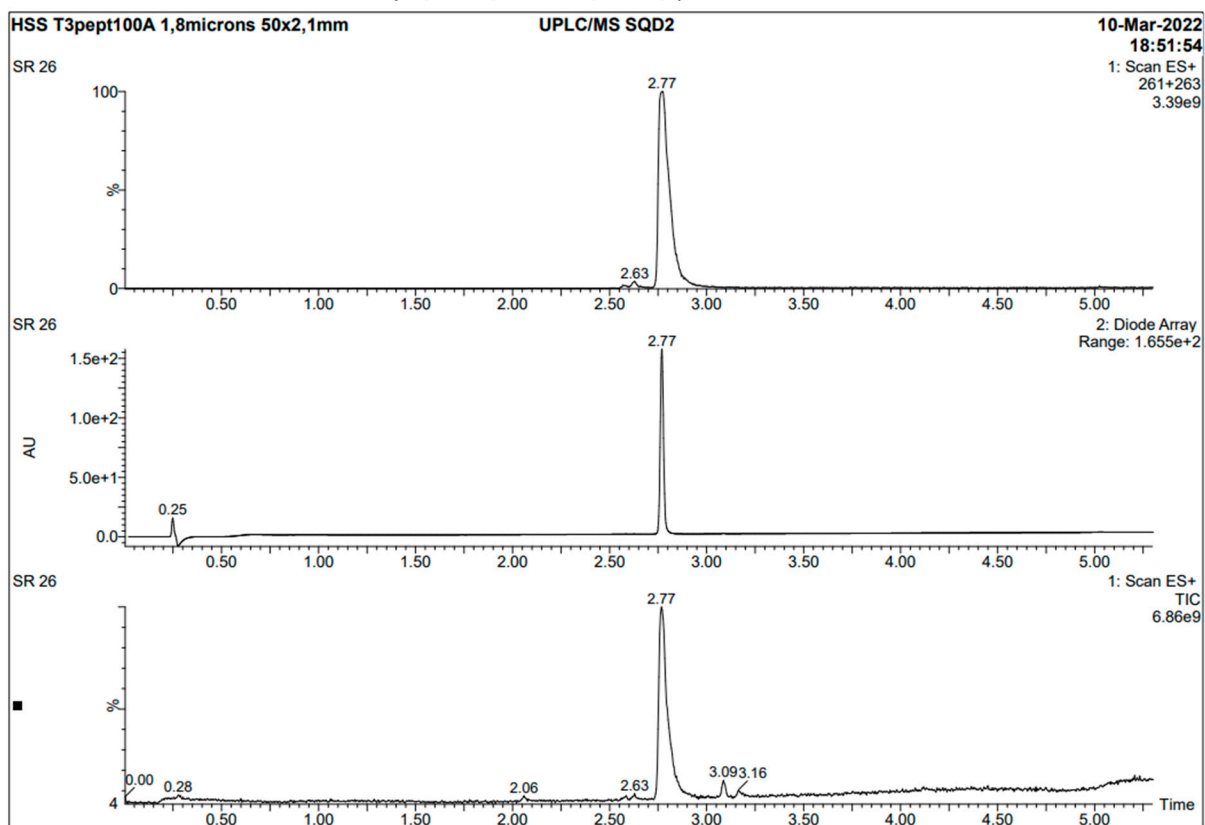
S22. 1-butyl-4-chloro-[1,2,4]triazolo[4,3-a]quinoxaline (15g).

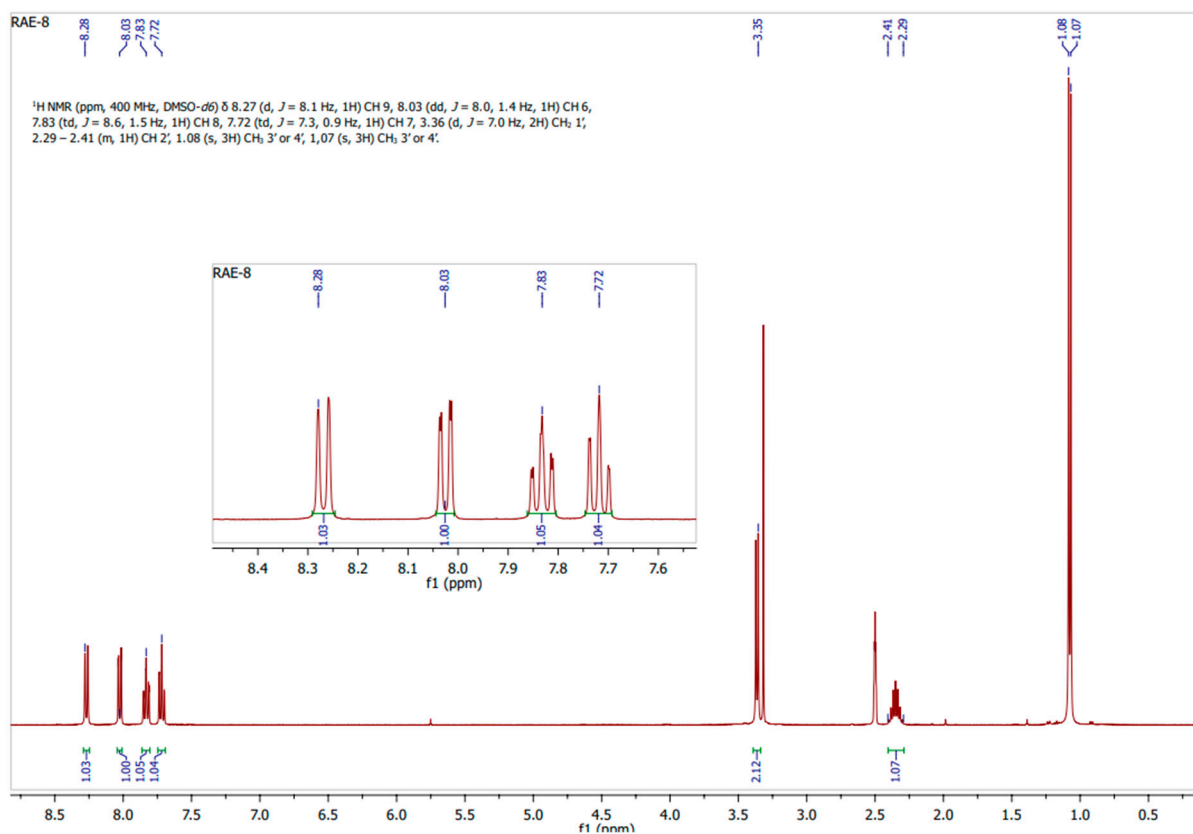
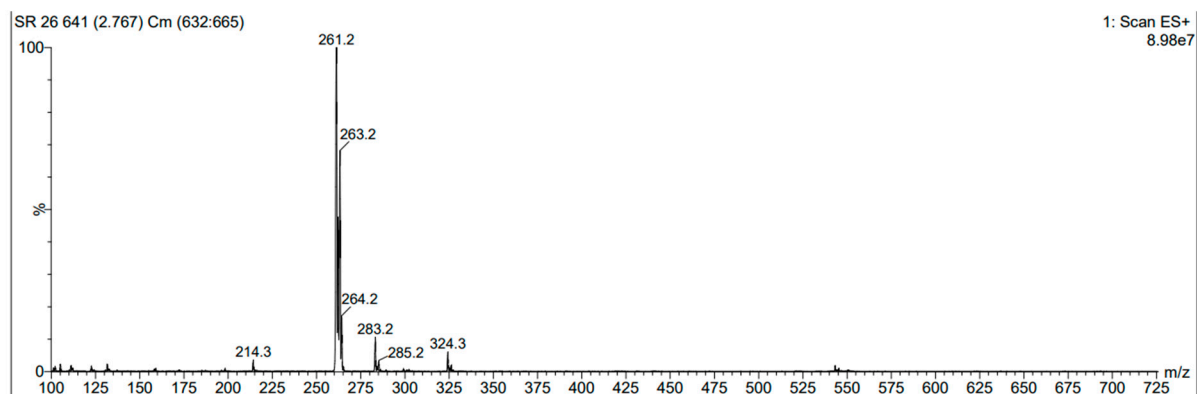


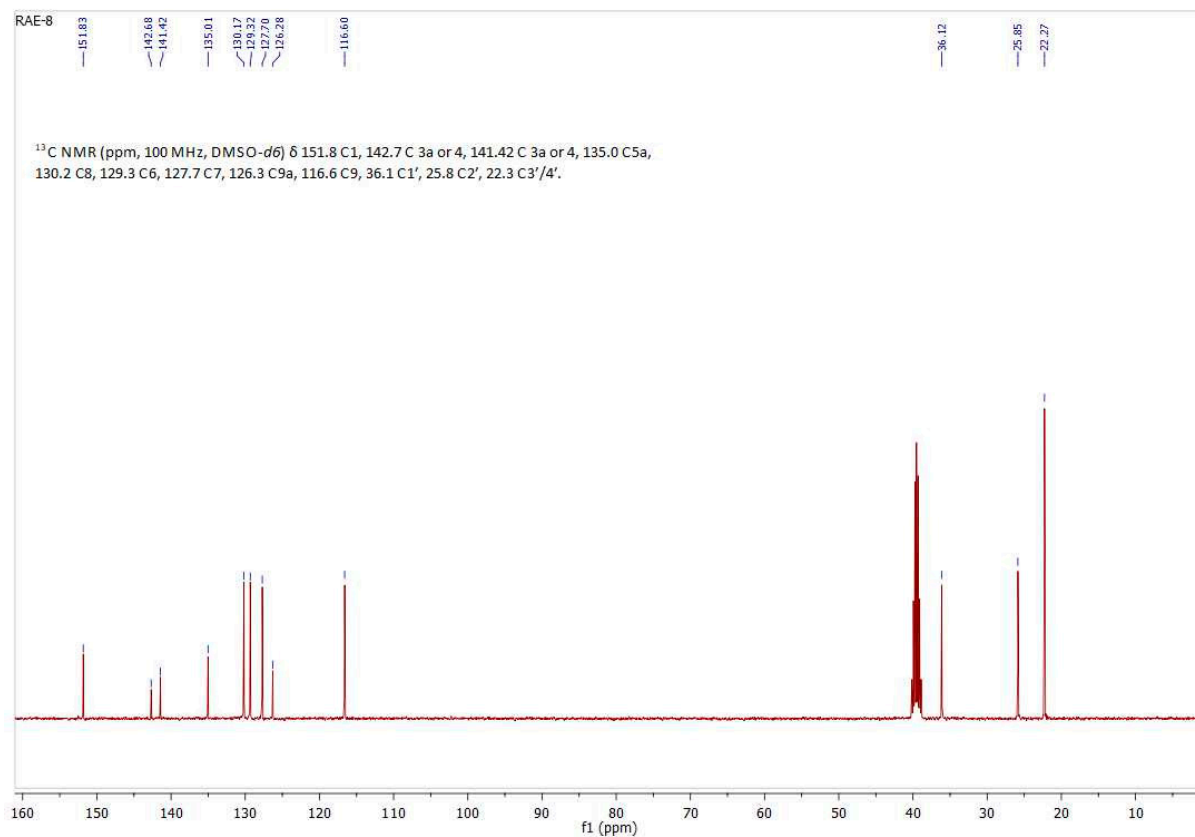




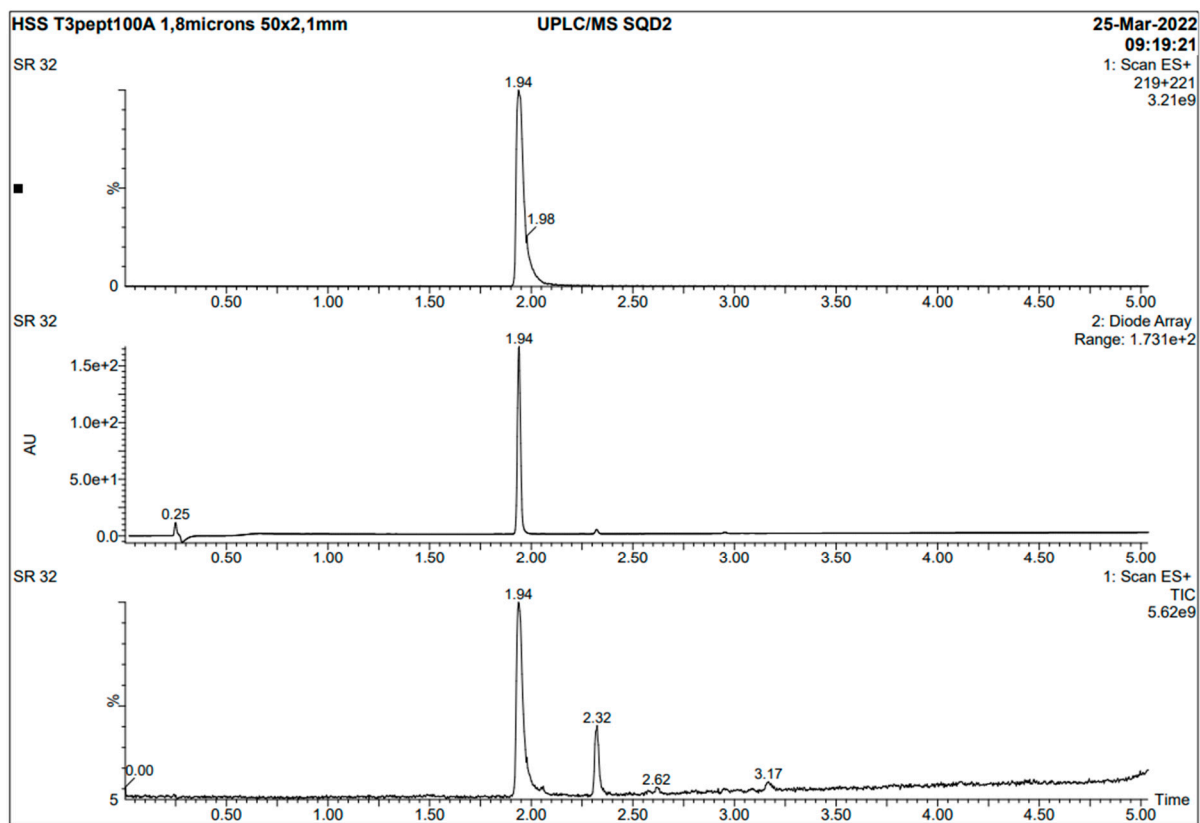
S23. 4-chloro-1-isobutyl-[1,2,4]triazolo[4,3-*a*]quinoxaline (**15h**).



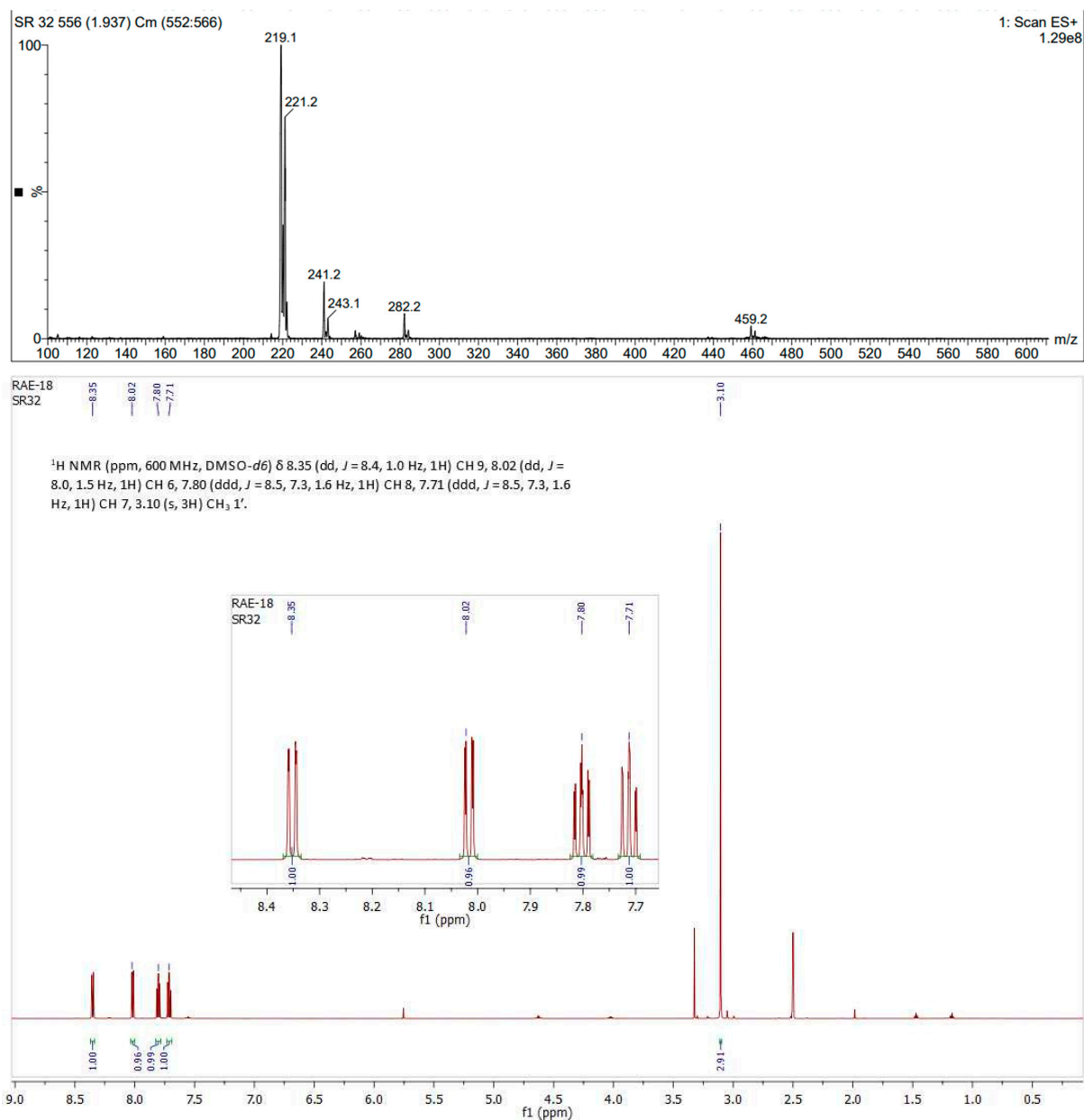


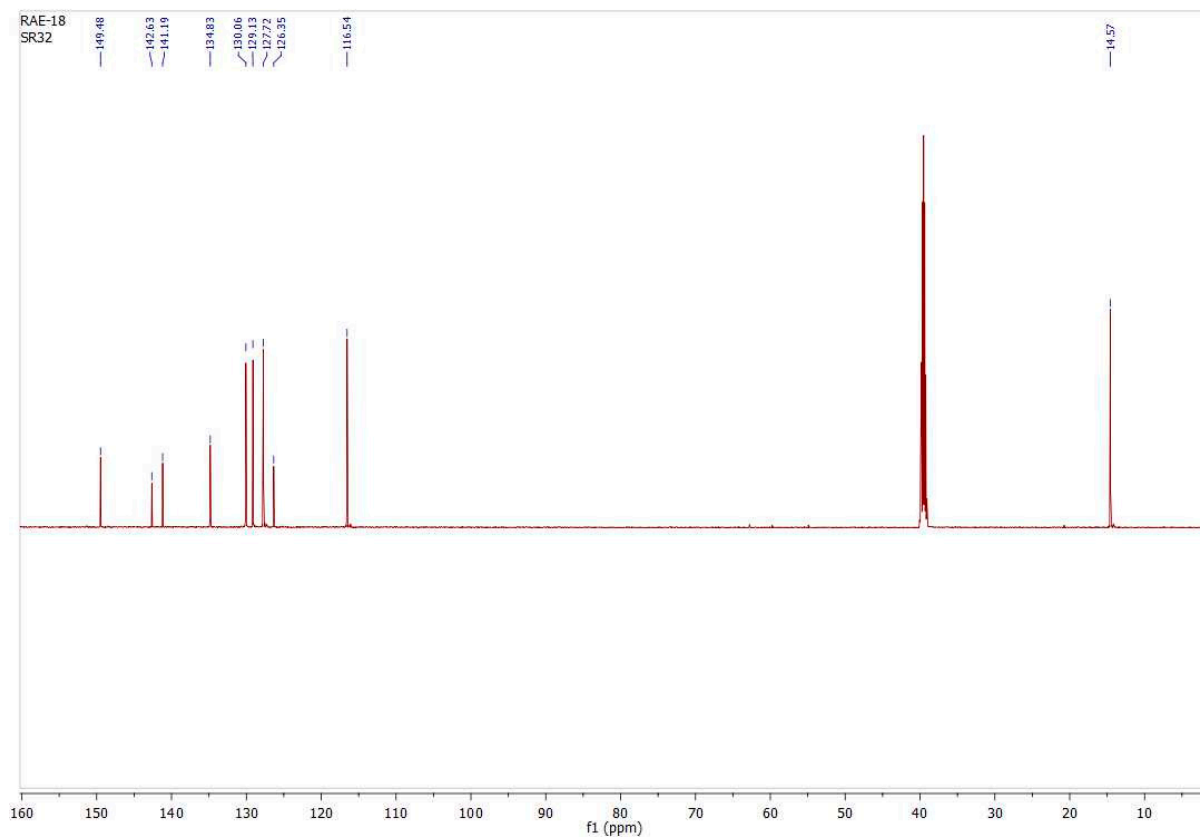


S24. 4-chloro-1-methyl-[1,2,4]triazolo[4,3-a]quinoxaline (**15i**).

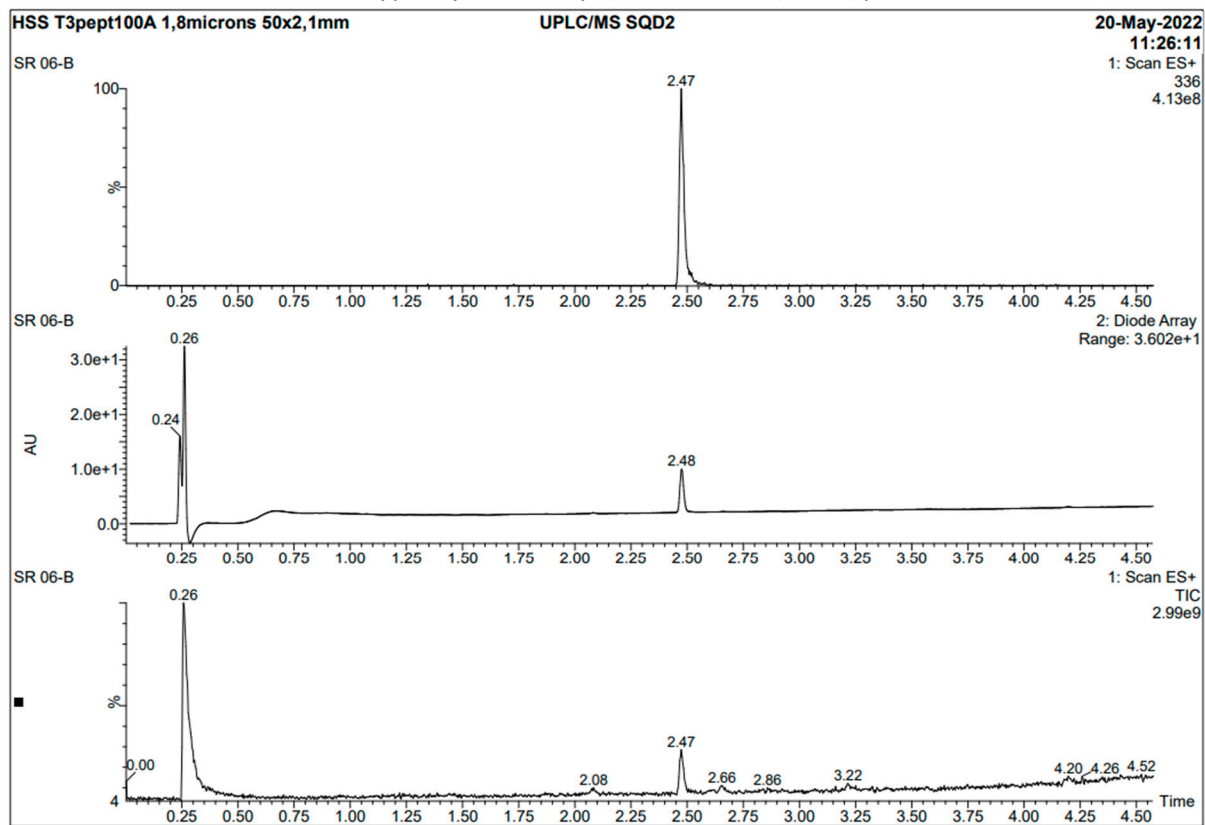


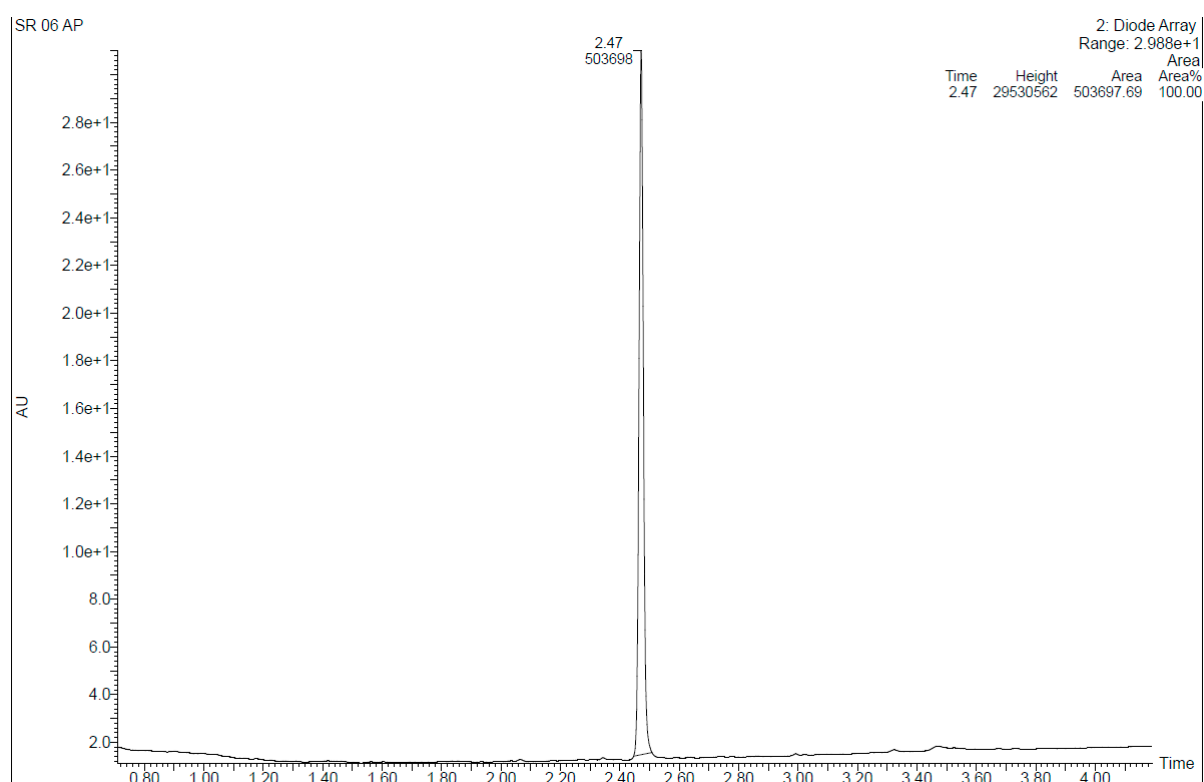
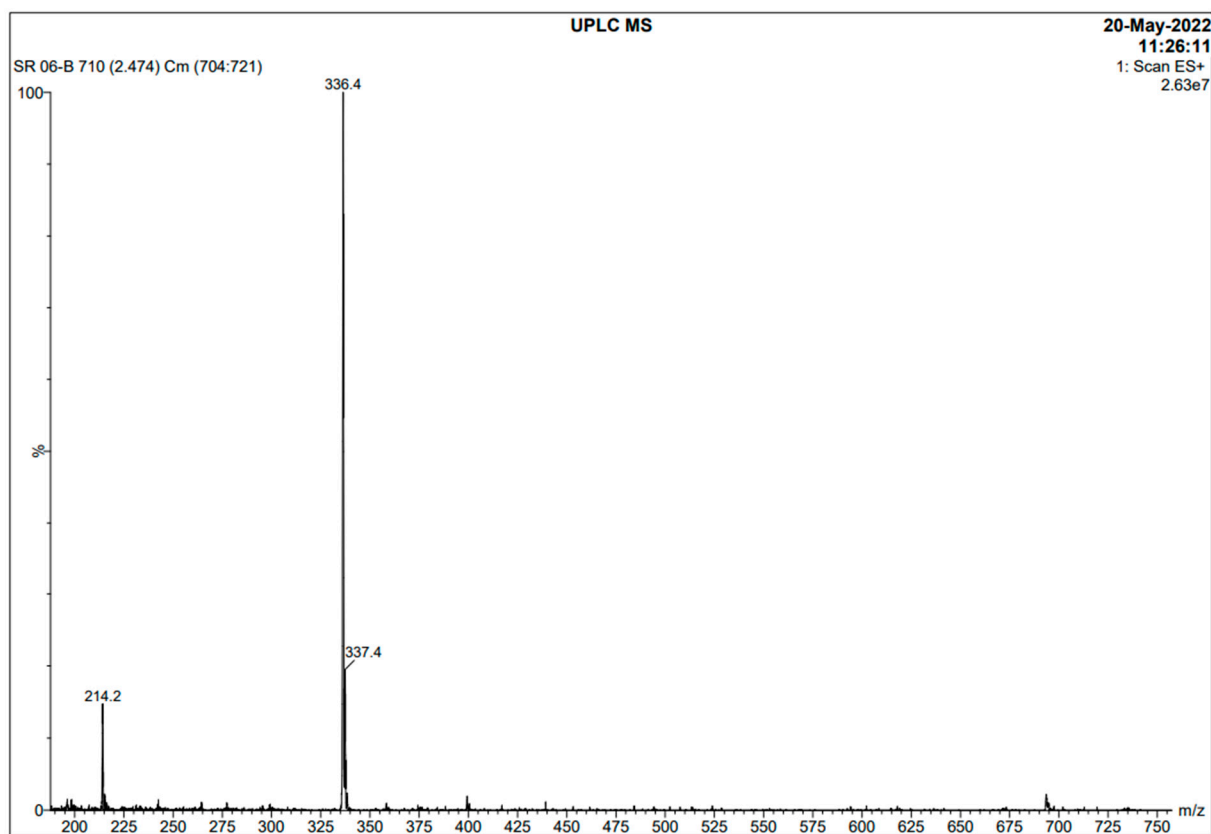






S25. 1-(3,4-dimethoxyphenyl)-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16a**).

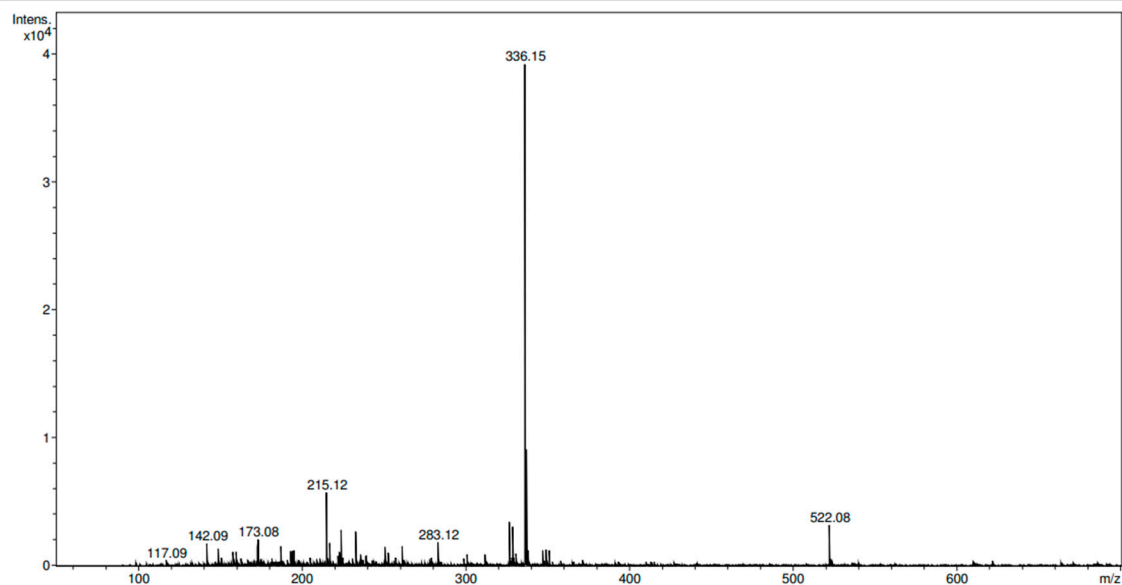






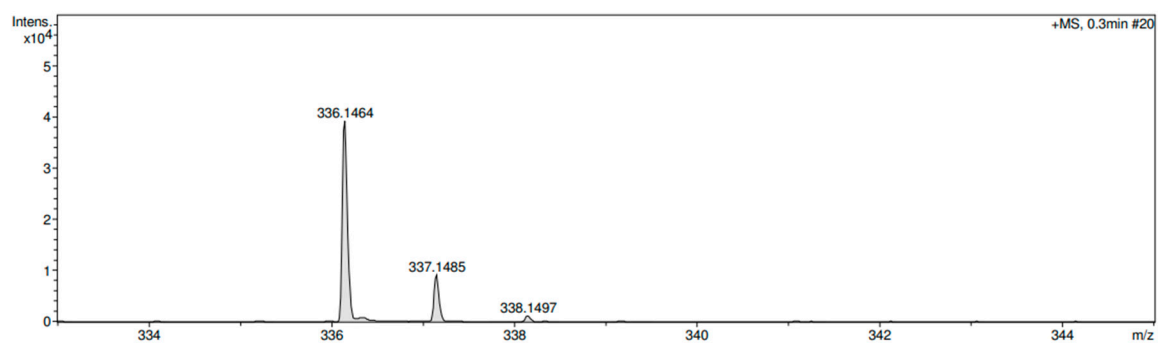
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

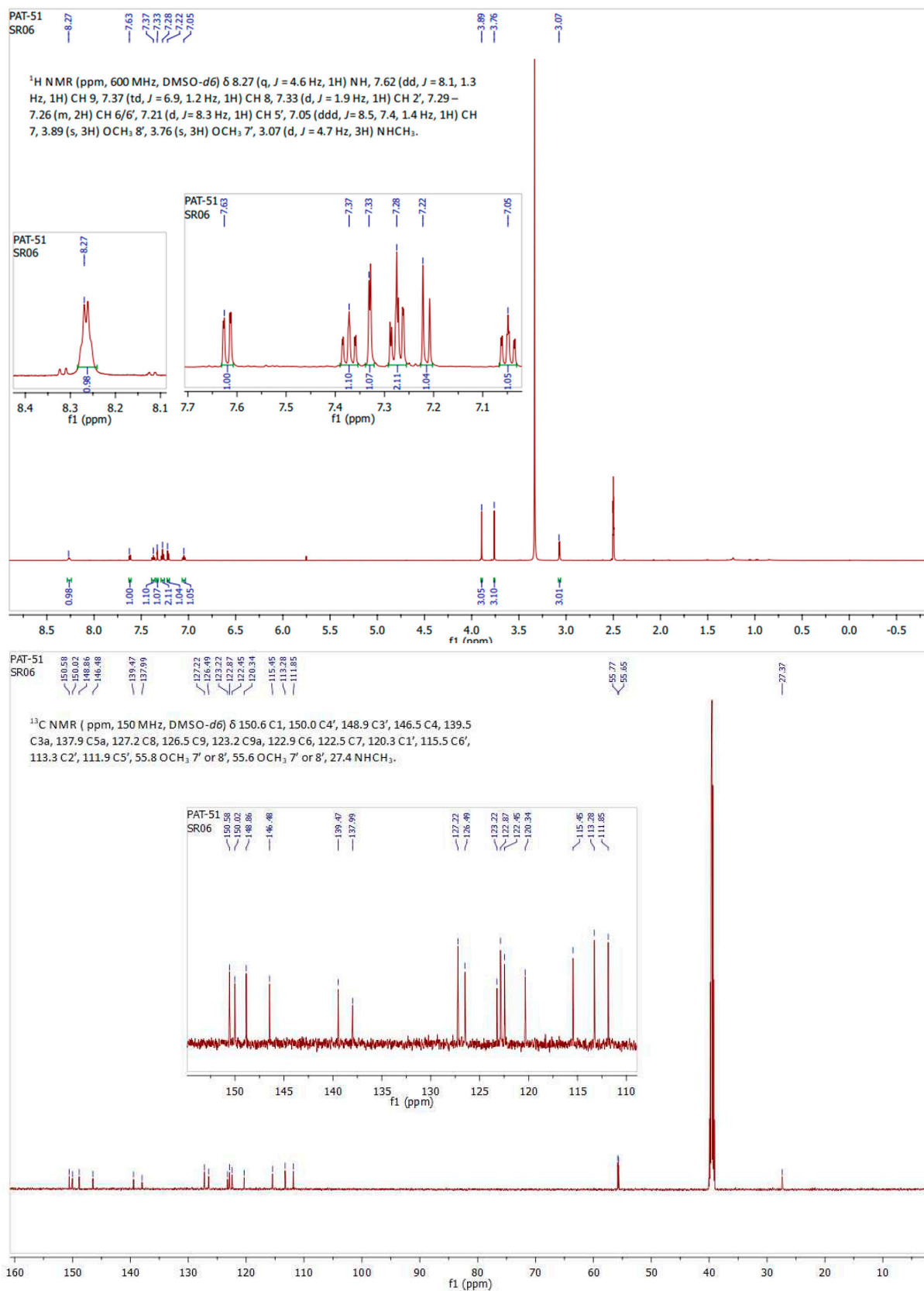


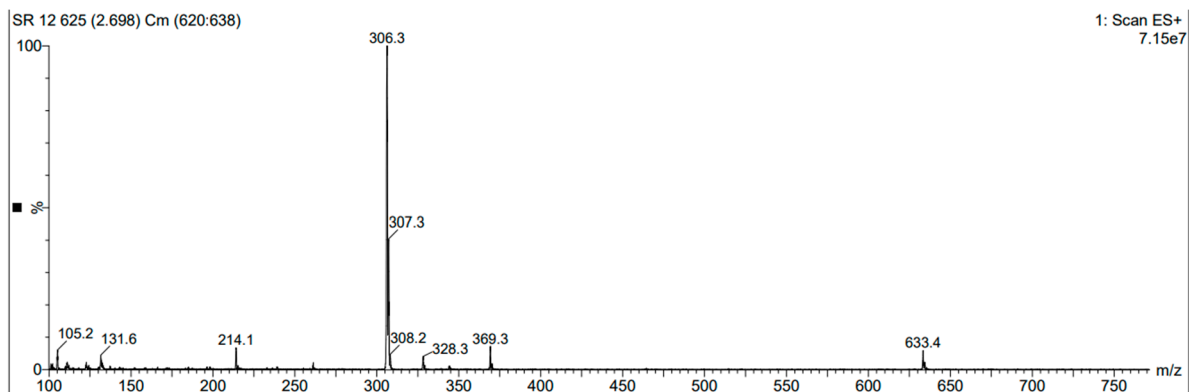
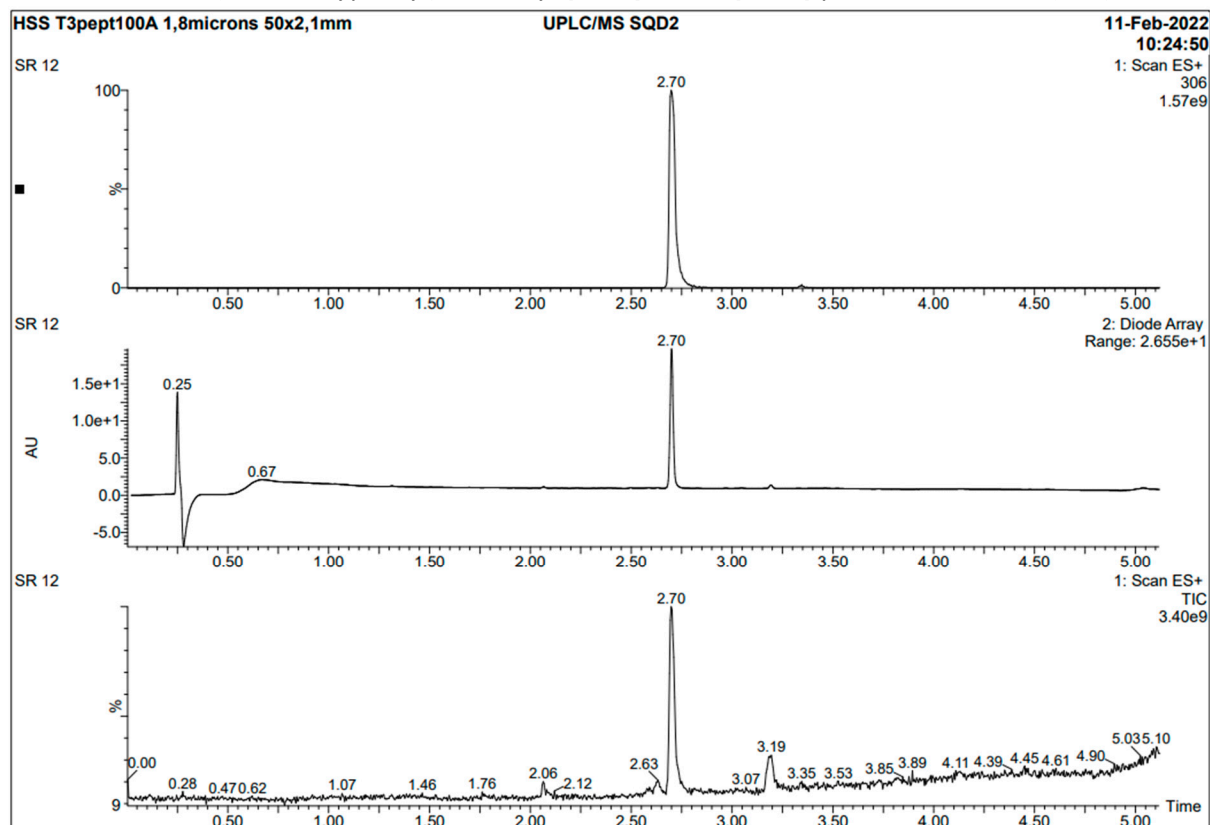
## Acquisition Parameter

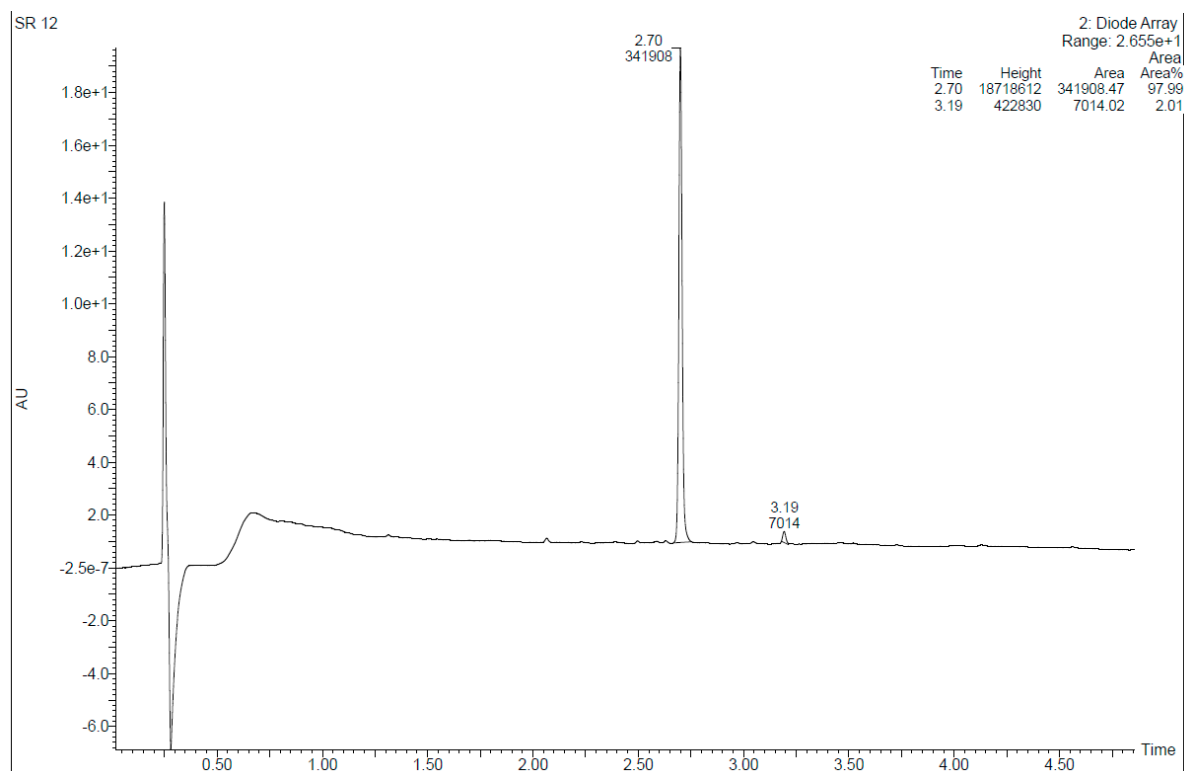
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
336.1464	1	C18H18N5O2	336.1455	-2.6	9.8	1	100.00	12.5	even		ok

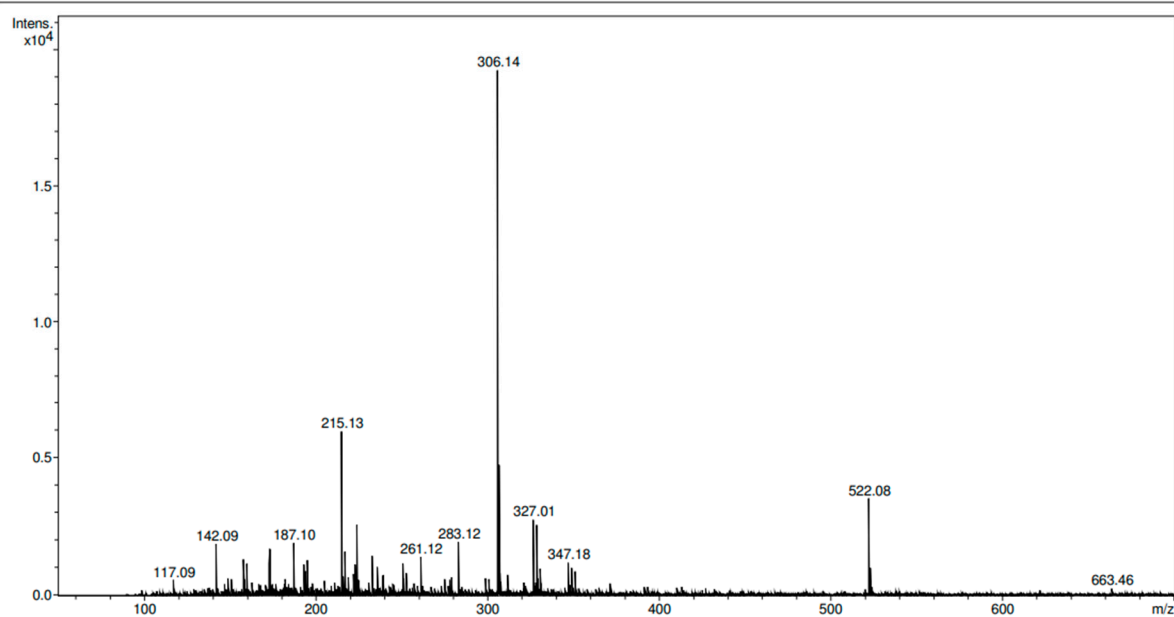


S26. 1-(3-methoxyphenyl)-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16b**).



#### Acquisition Parameter

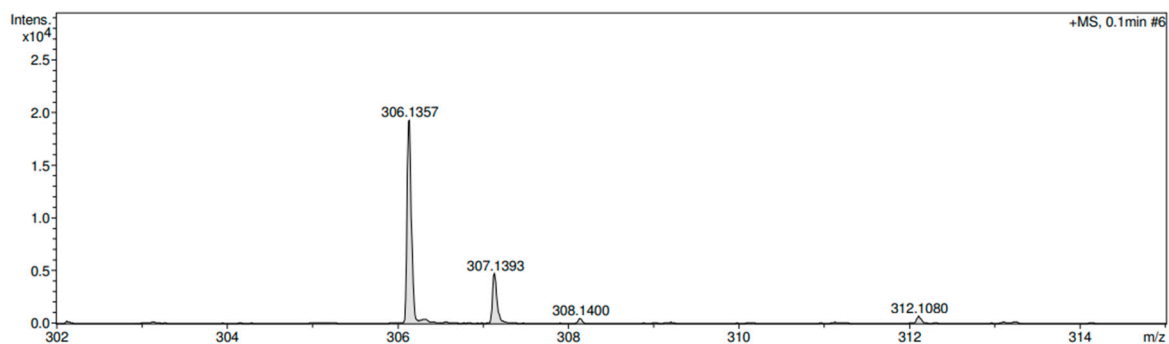
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



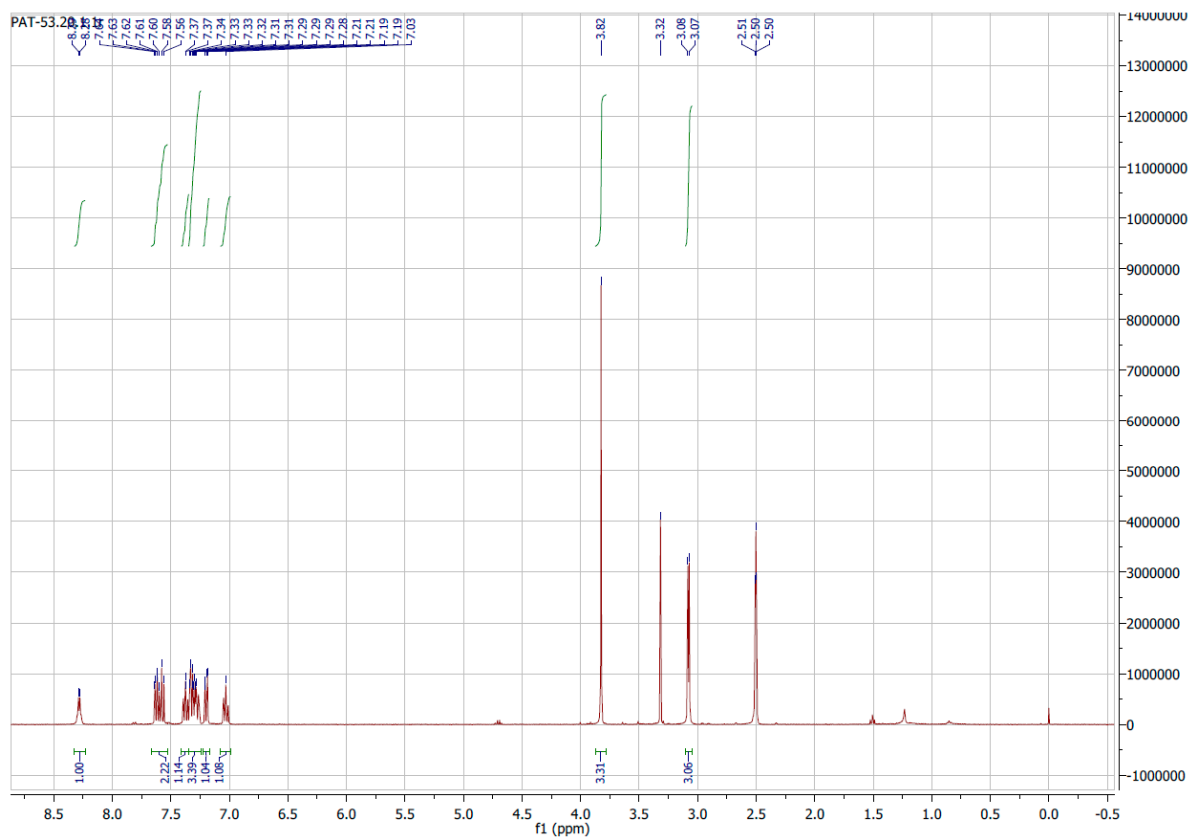


## Acquisition Parameter

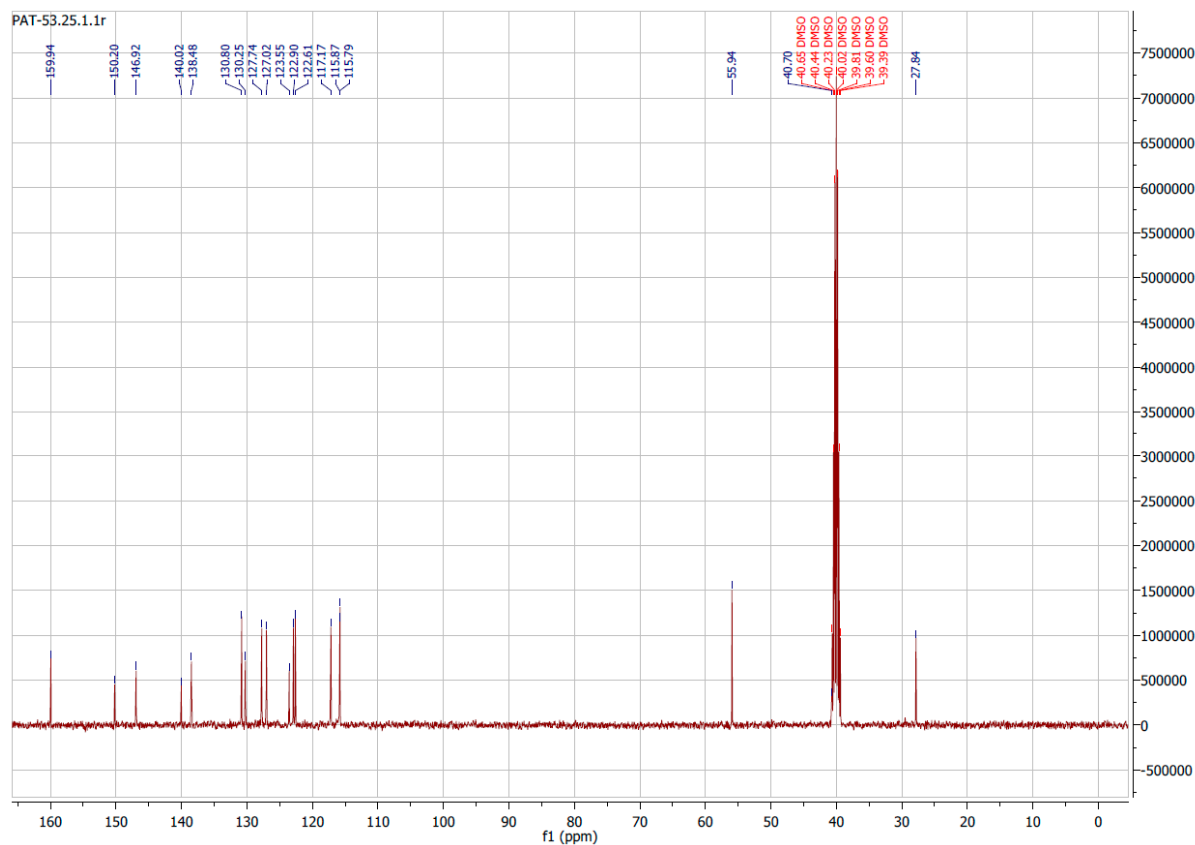
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



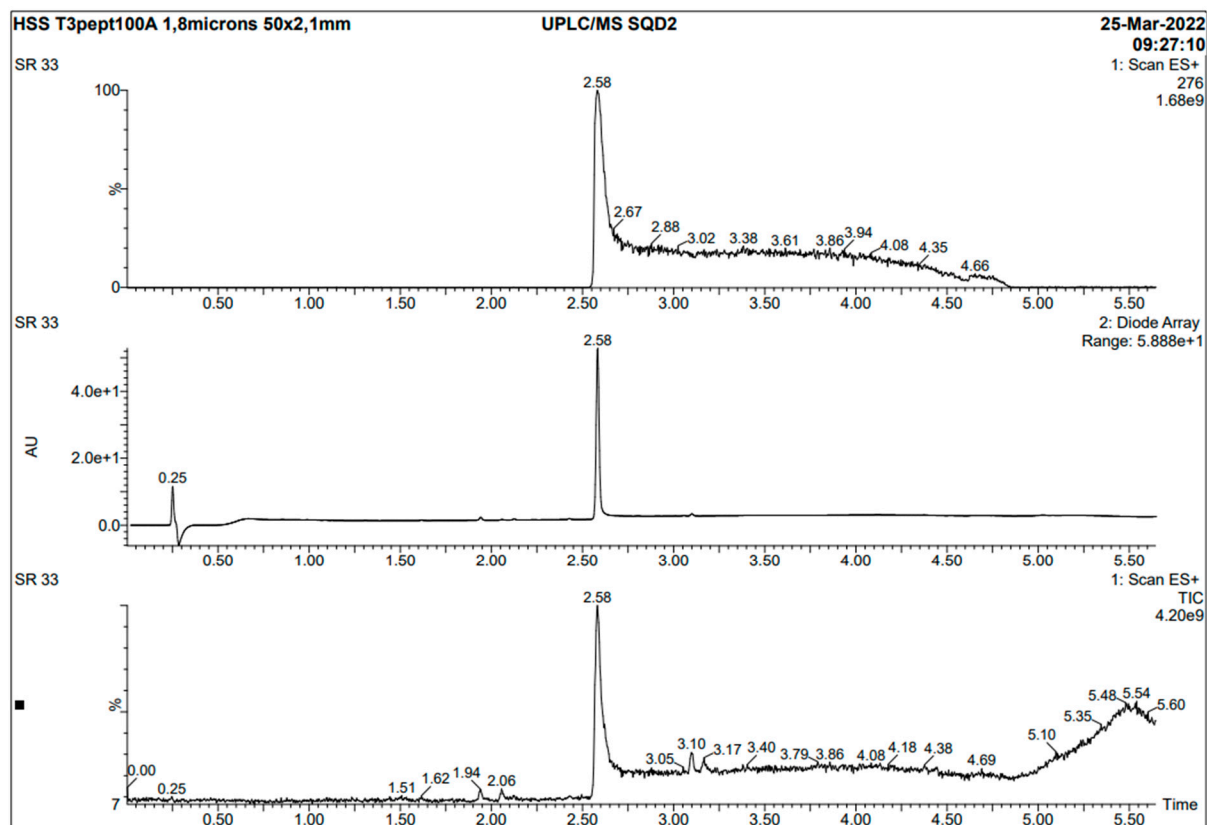
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
306.1357	1	C17H16NSO	306.1349	-2.4	24.3	1	100.00	12.5	even	ok
	2	C16H20NO5	306.1336	-6.7	37.7	2	30.36	7.5	even	ok

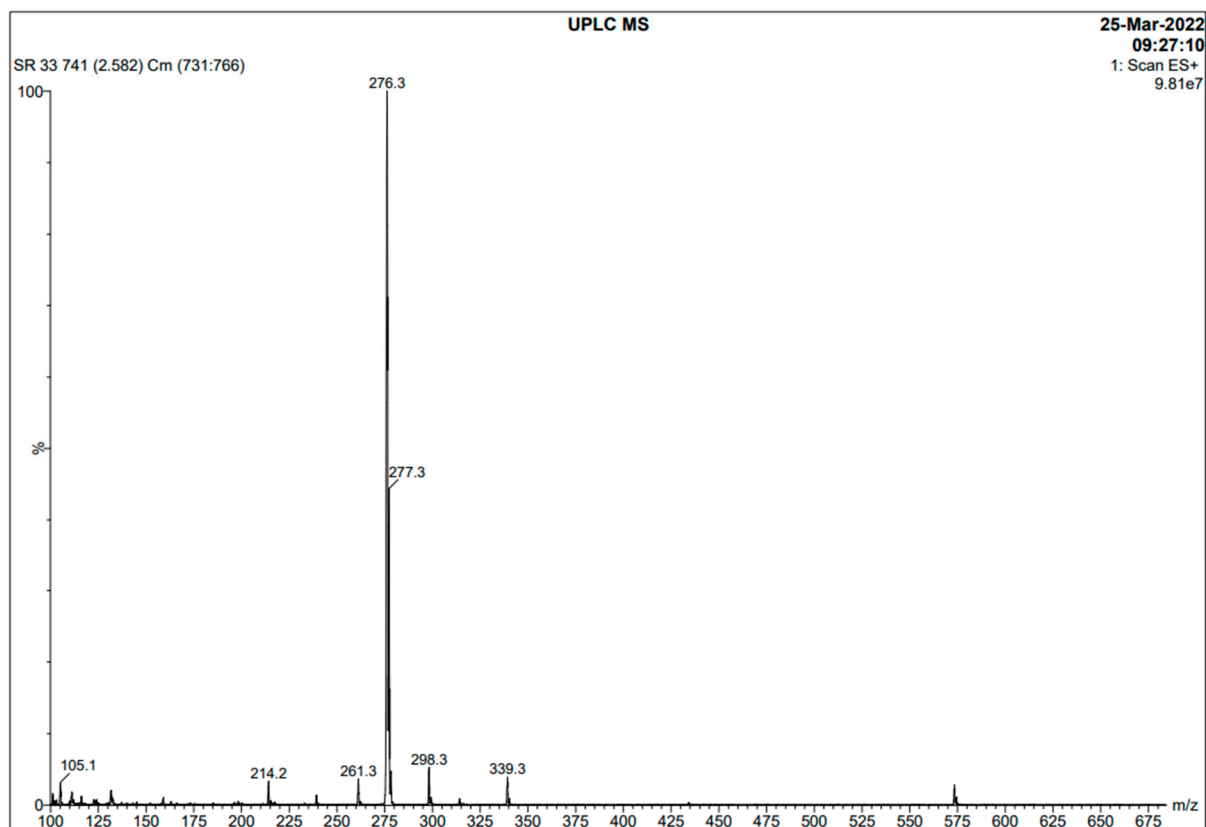






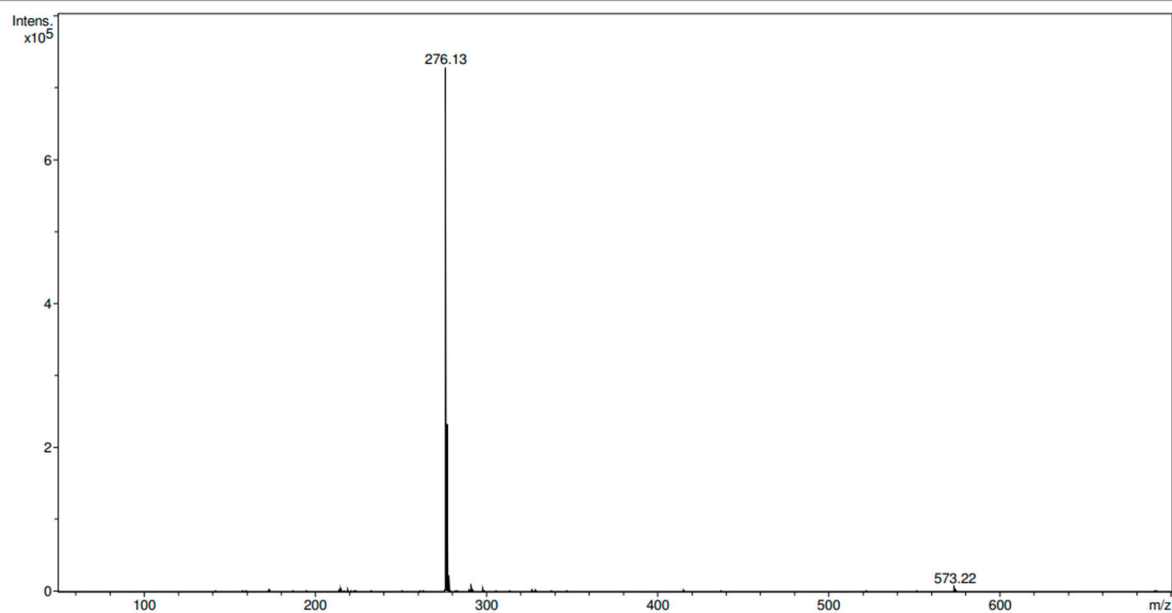
S27. *N*-methyl-1-phenyl-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-amine (**16c**).





Acquisition Parameter

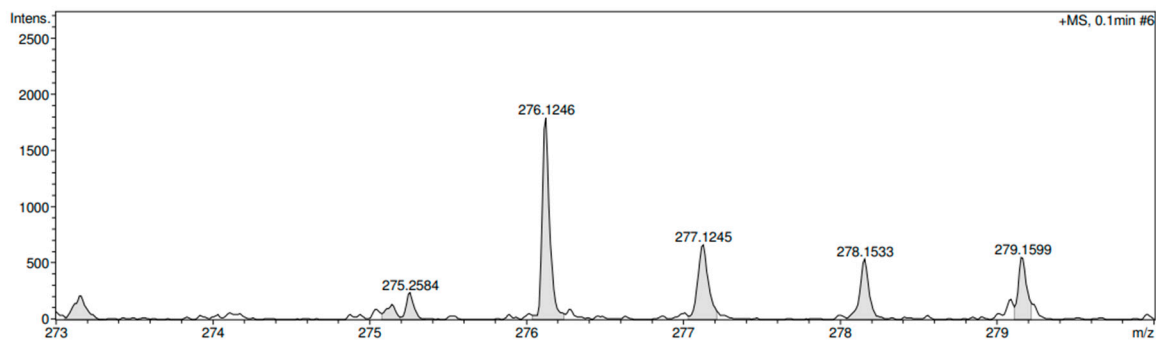
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



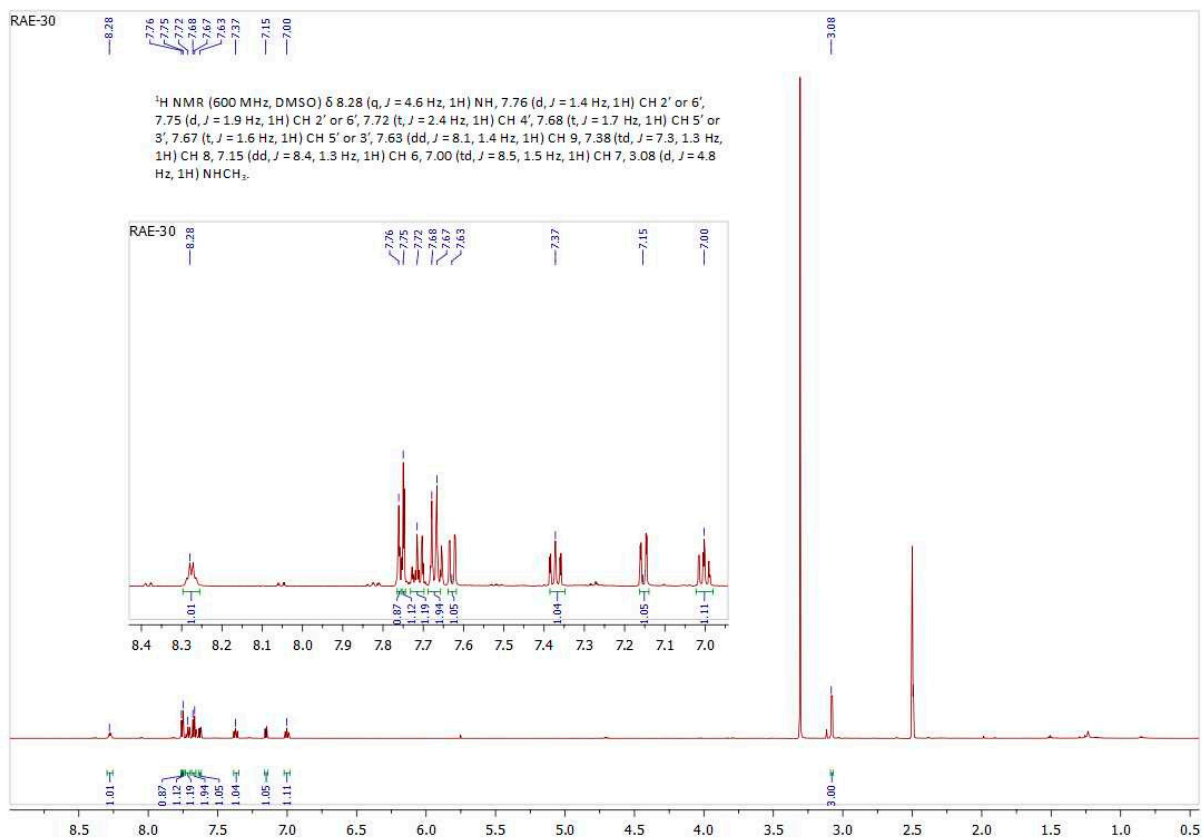


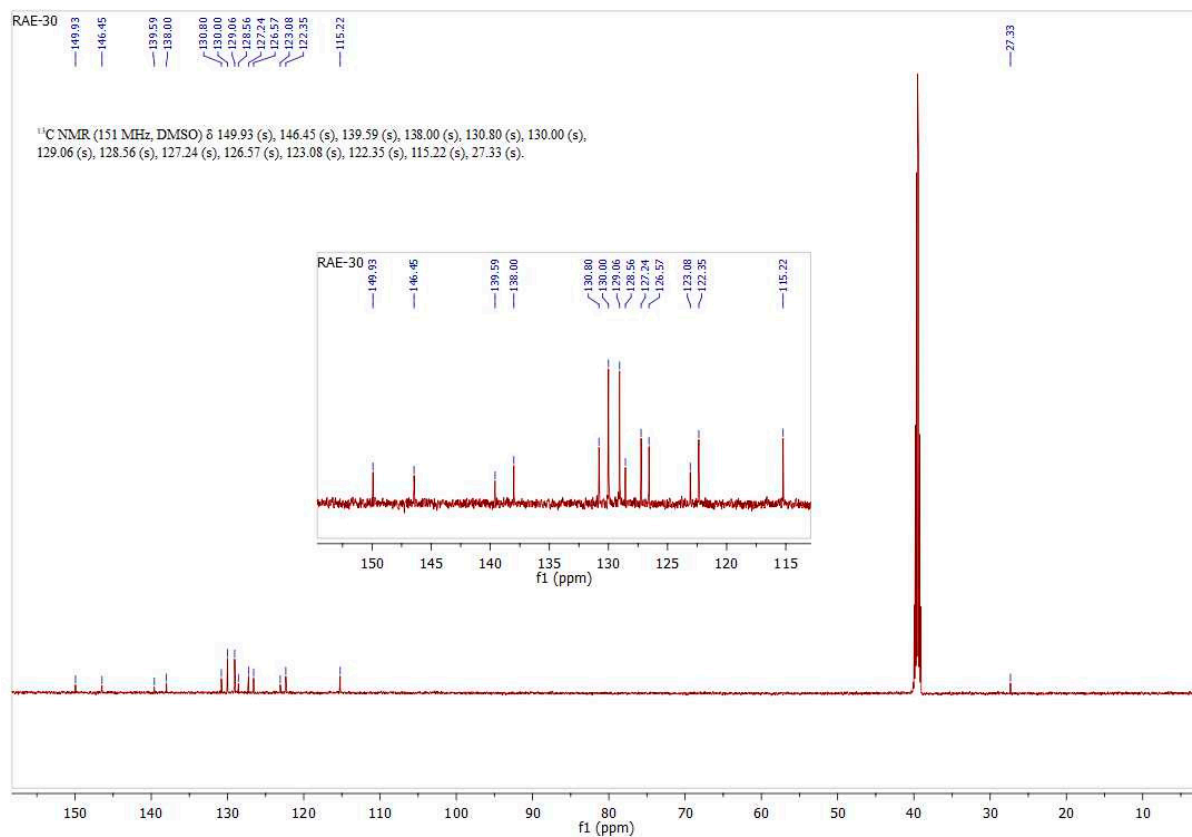
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

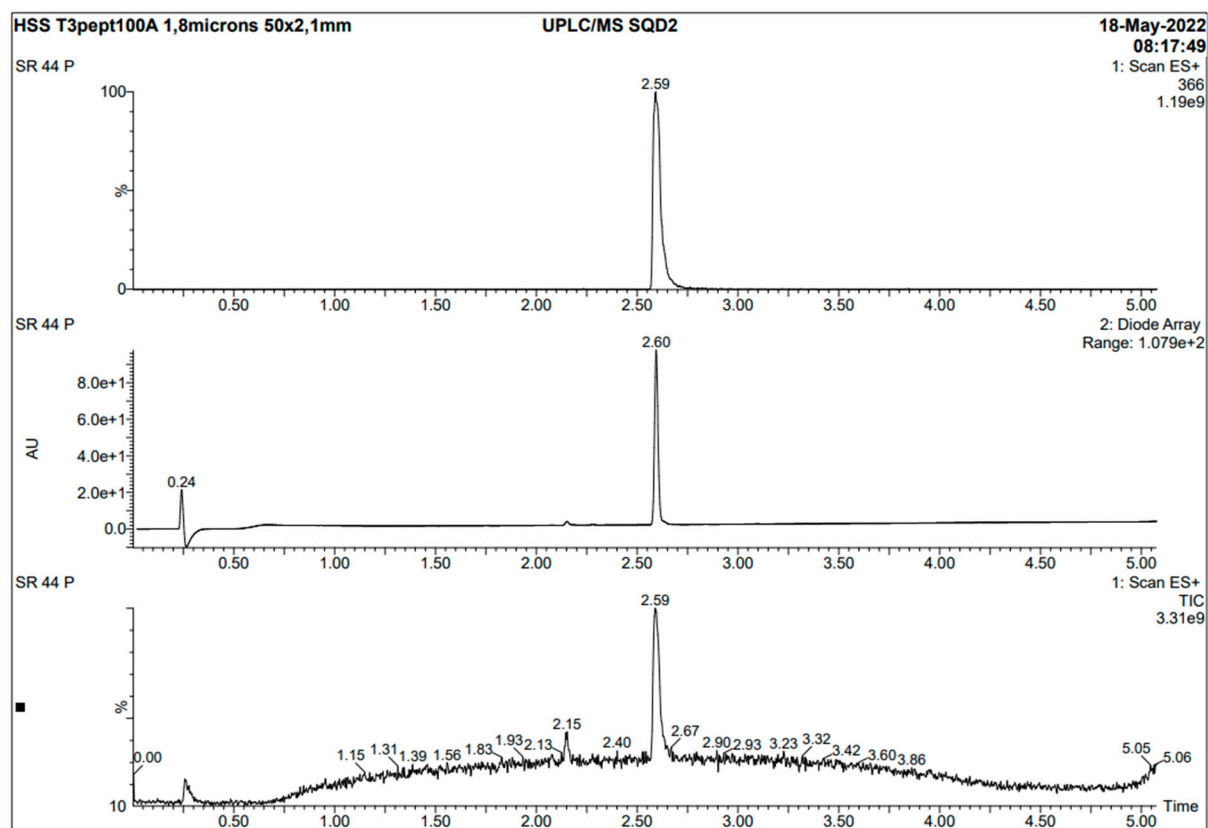


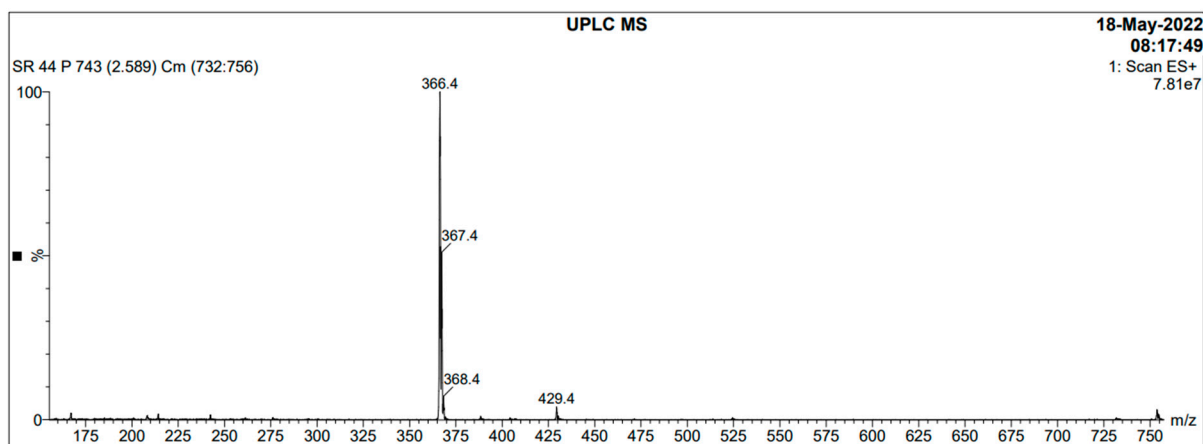
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
276.1246	1	C16H14N5	276.1244	-0.7	193.1	1	100.00	12.5	even	ok
	2	C15H18NO4	276.1230	-5.6	198.9	2	29.82	7.5	even	ok





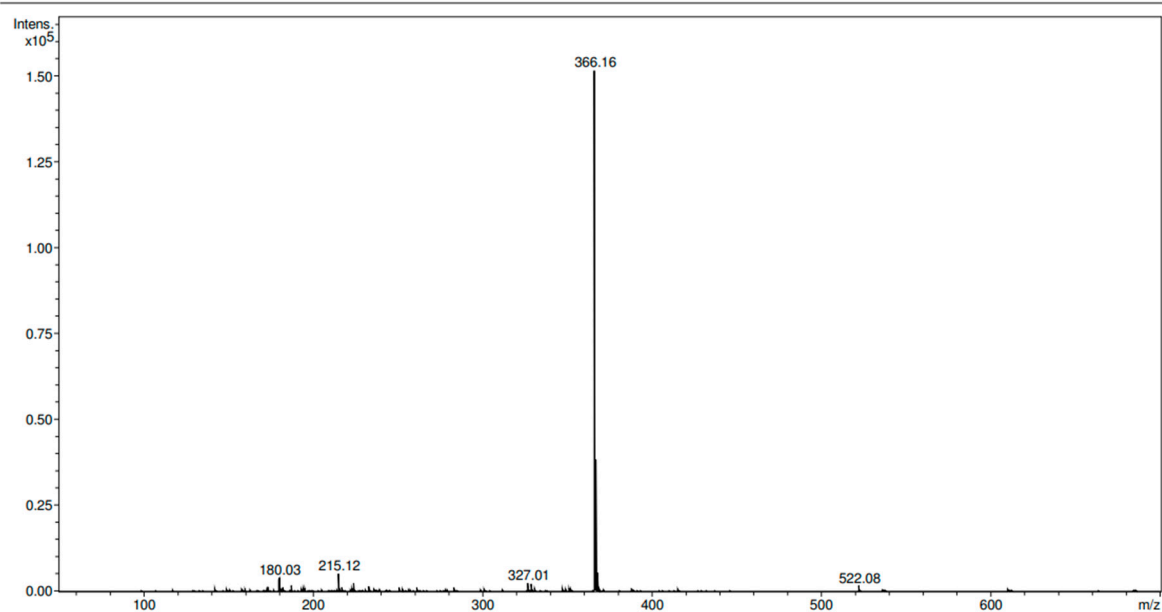
S28. *N*-methyl-1-(3,4,5-trimethoxyphenyl)-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-amine (**16d**).





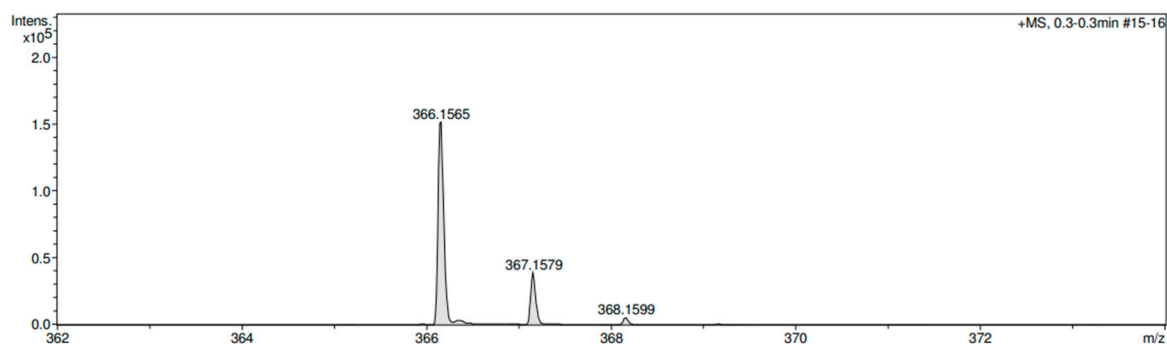
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

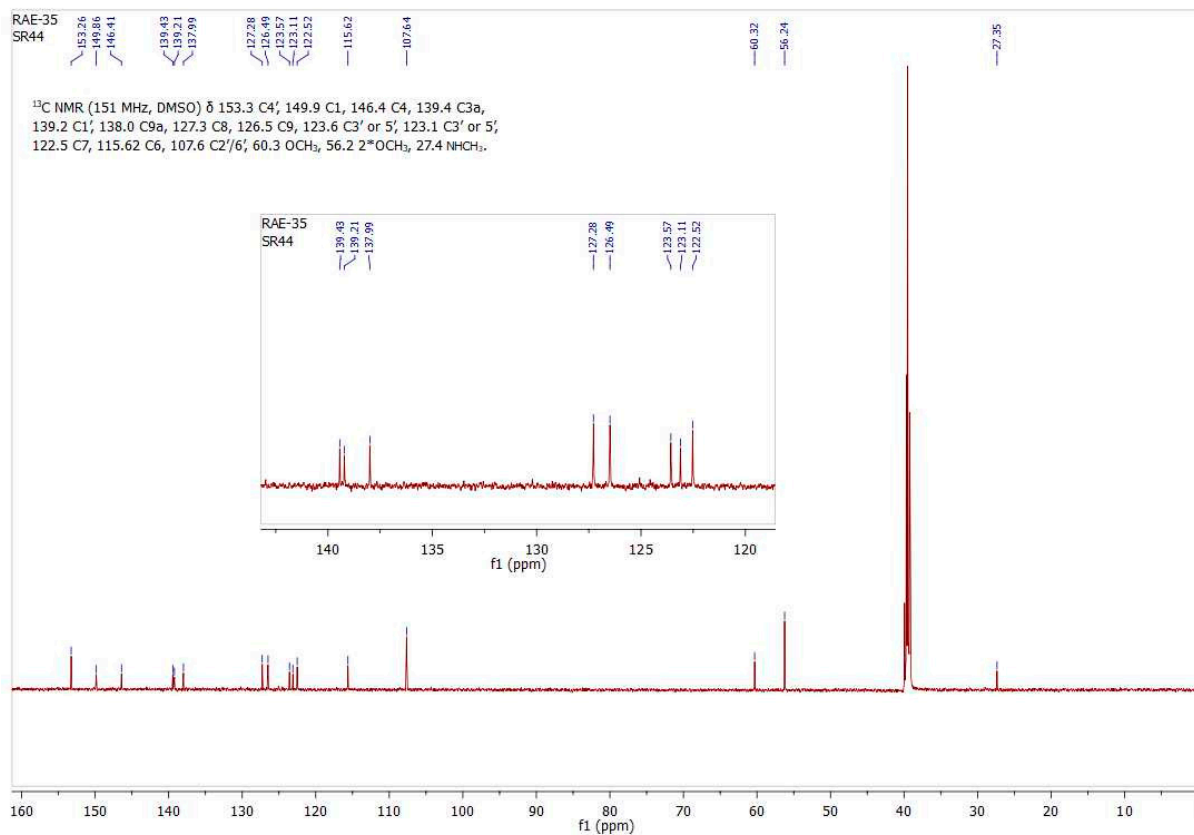
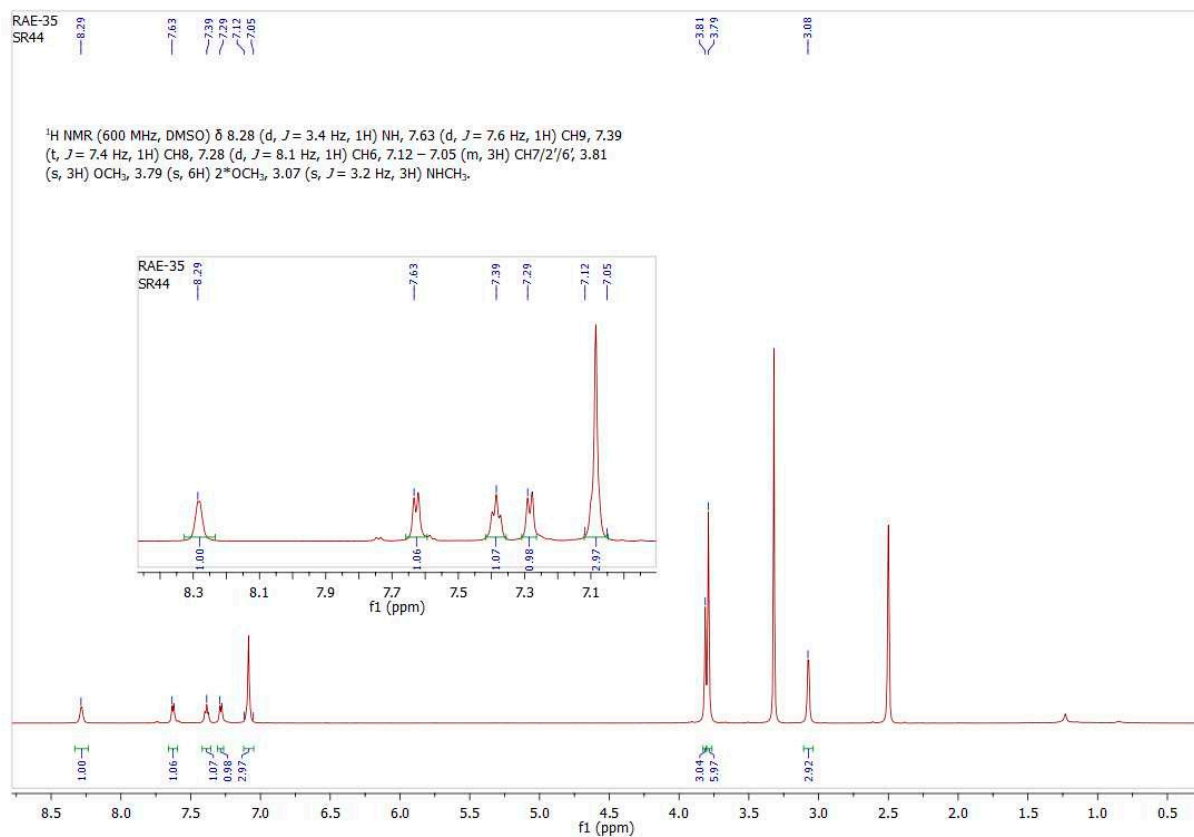


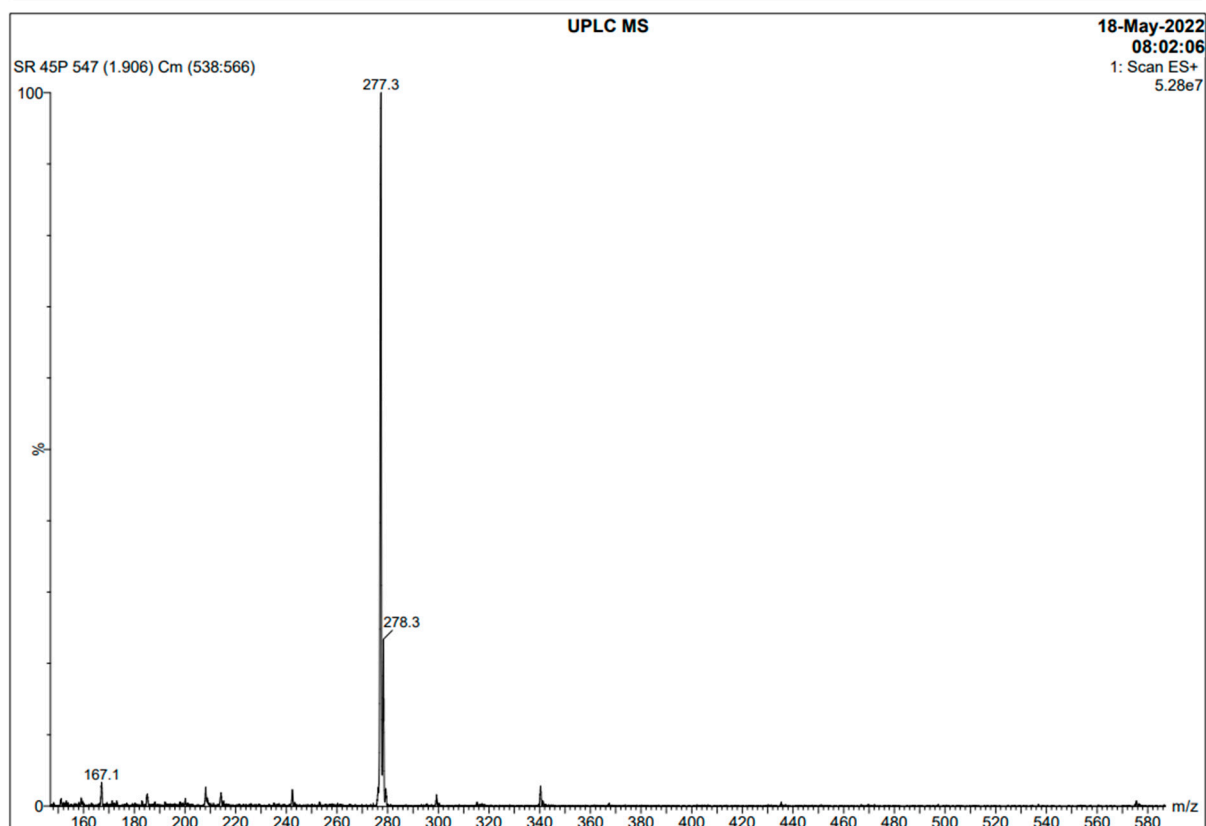
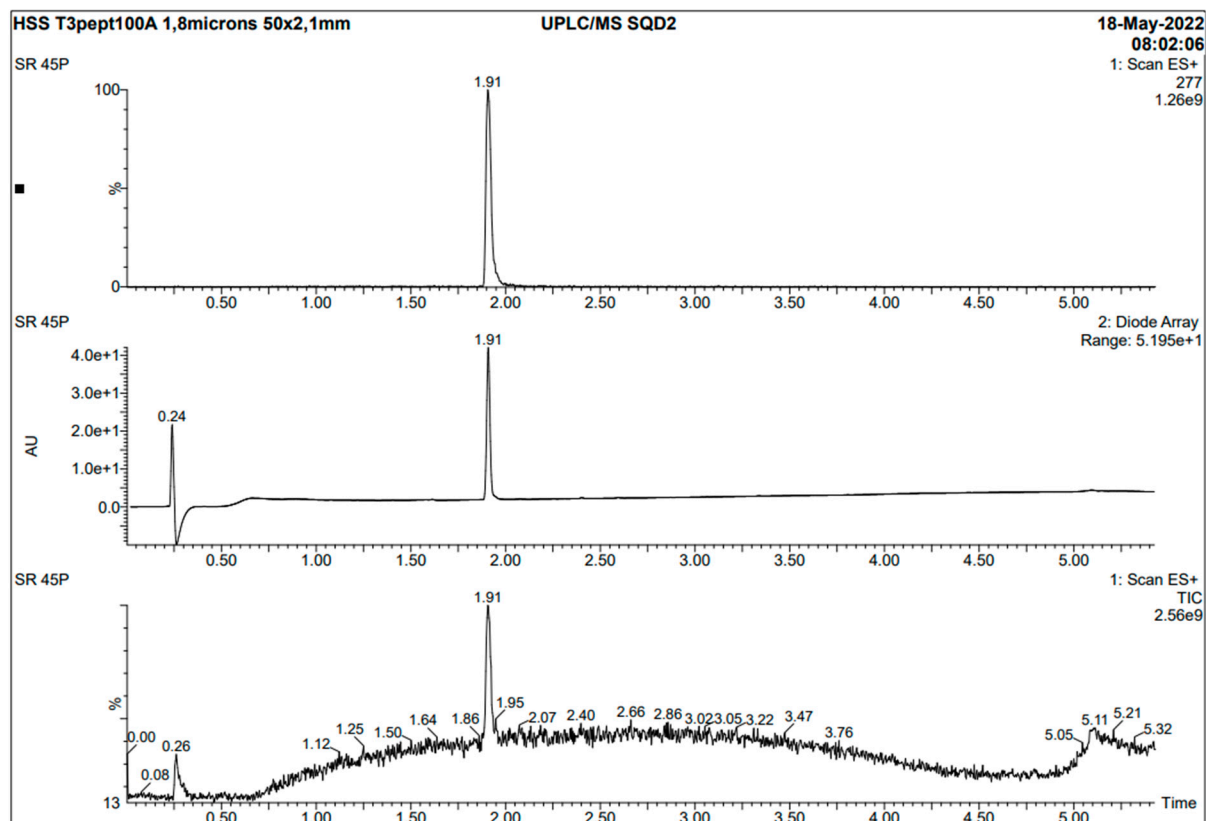
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
366.1565	1	C <sub>19</sub> H <sub>20</sub> N <sub>5</sub> O <sub>3</sub>	366.1561	1.1	15.8	1	100.00	12.5	even	ok

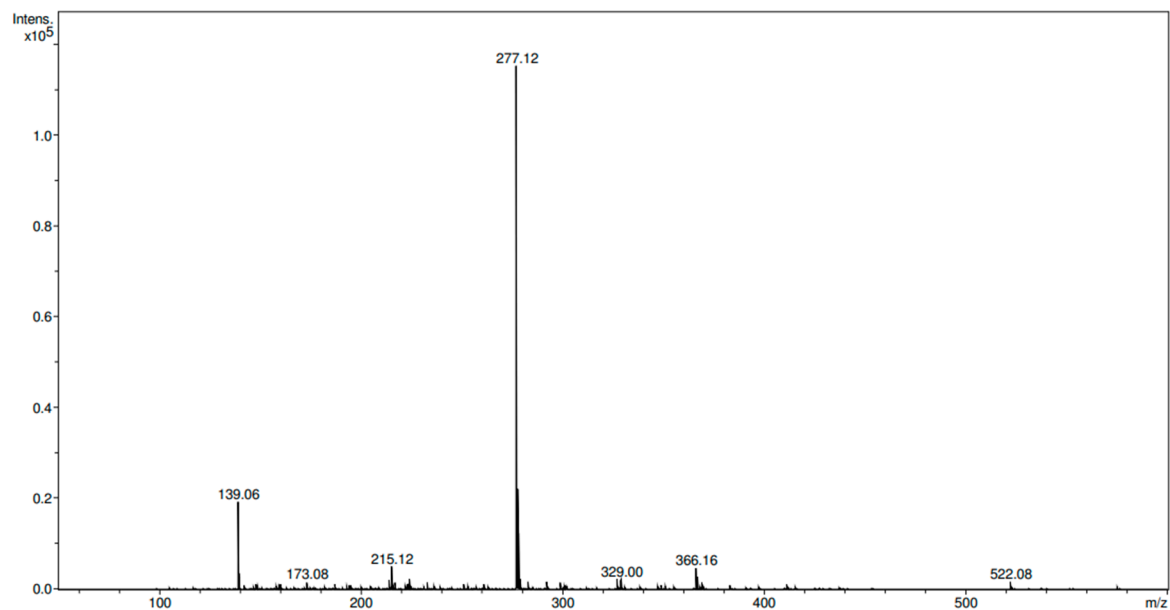


S29. *N*-methyl-1-(pyridin-3-yl)-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-amine (**16e**).



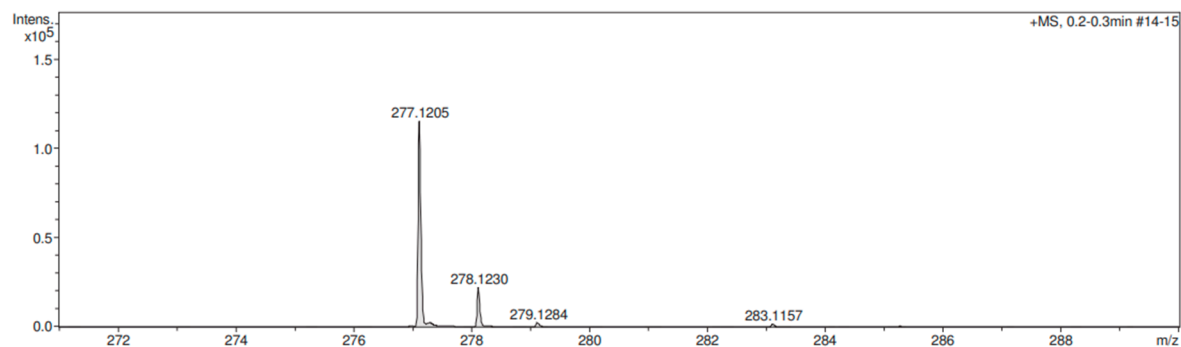
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



## Acquisition Parameter

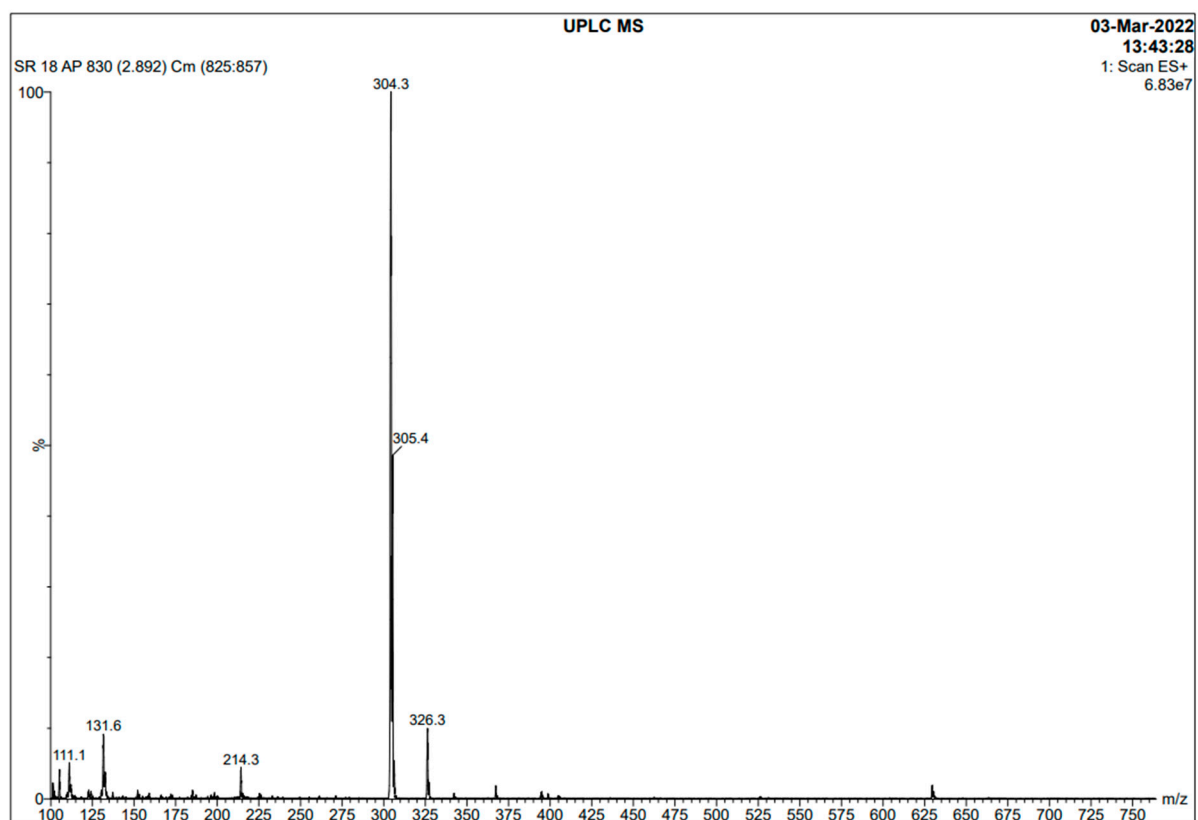
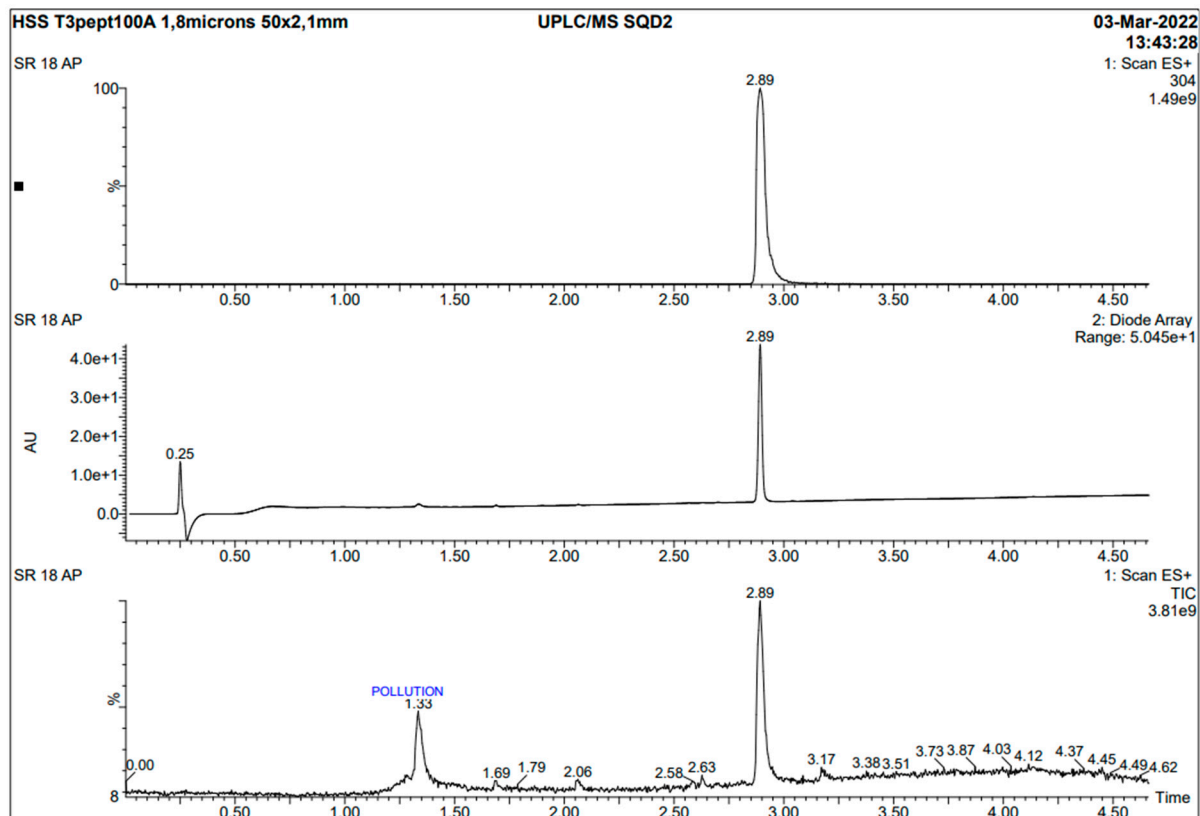
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
277.1205	1	C <sub>15</sub> H <sub>13</sub> N <sub>6</sub>	277.1196	3.0	4.1	1	100.00	12.5	even	ok



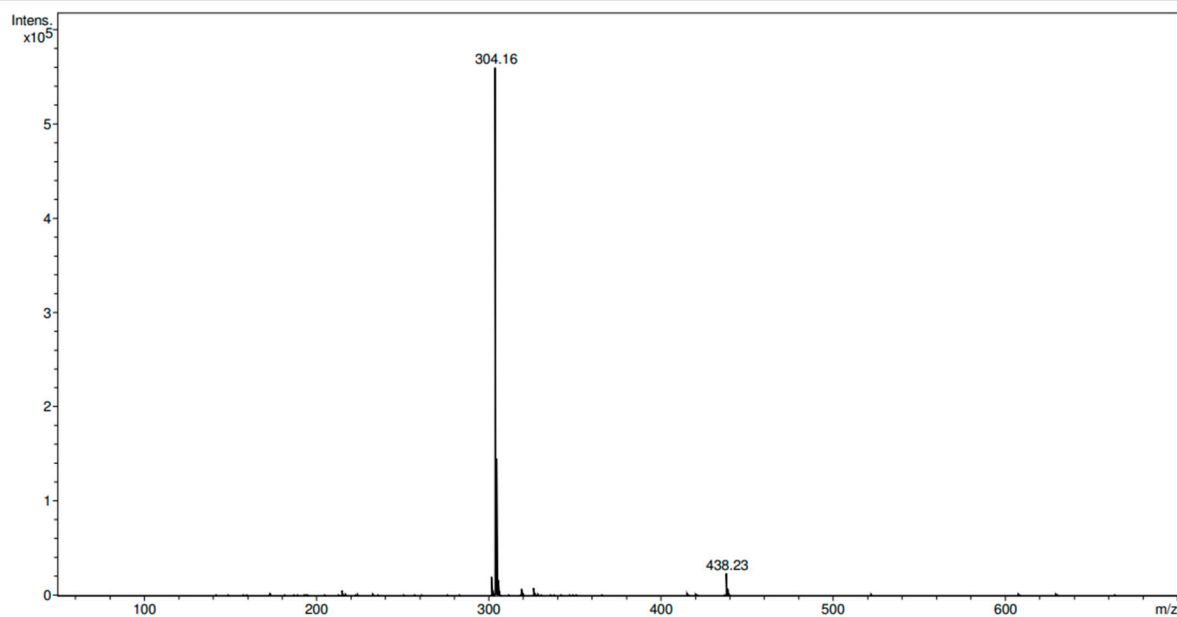


S30. *N*-methyl-1-phenethyl-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-amine (**16f**).



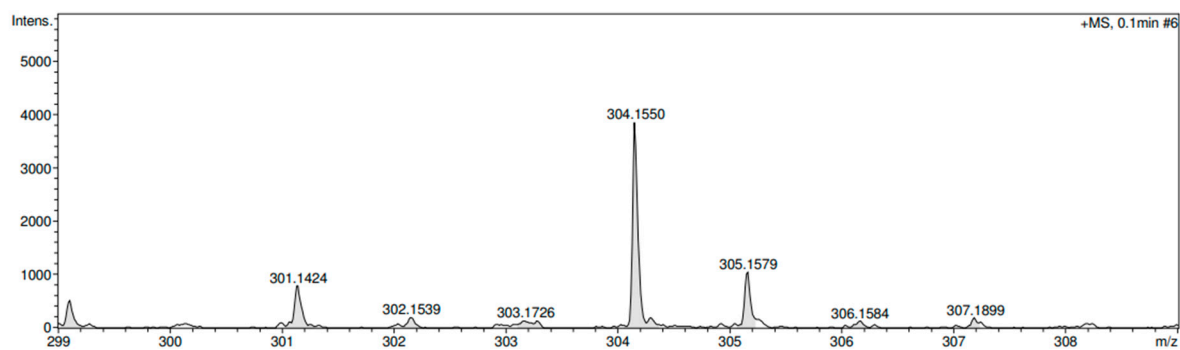
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

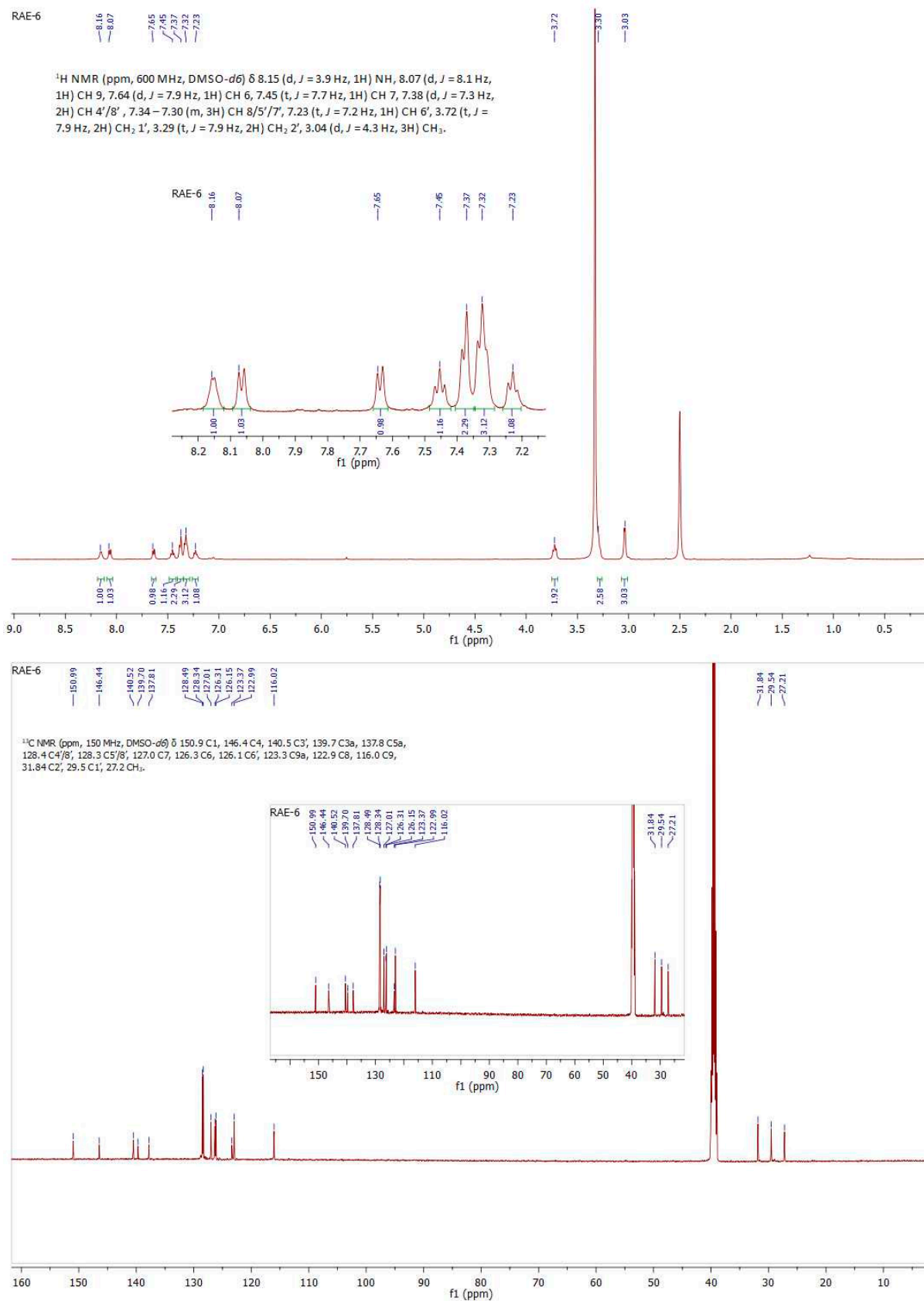


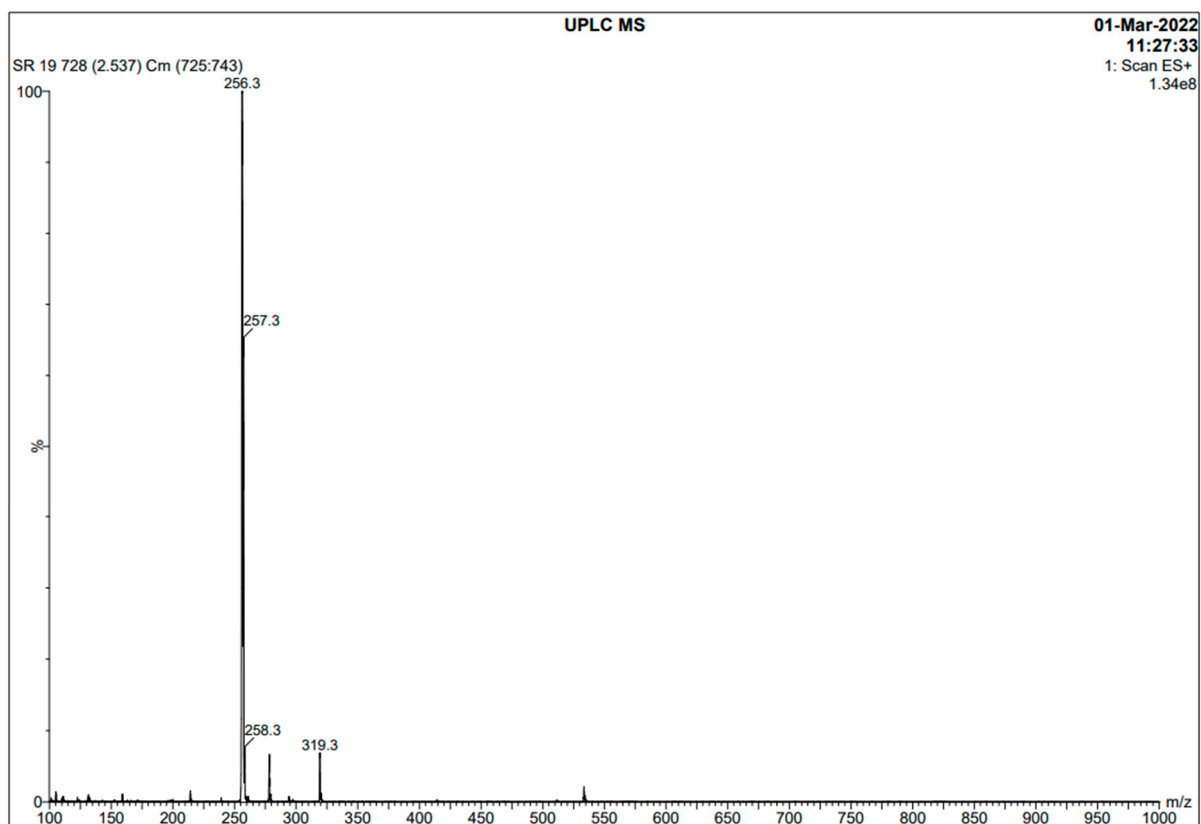
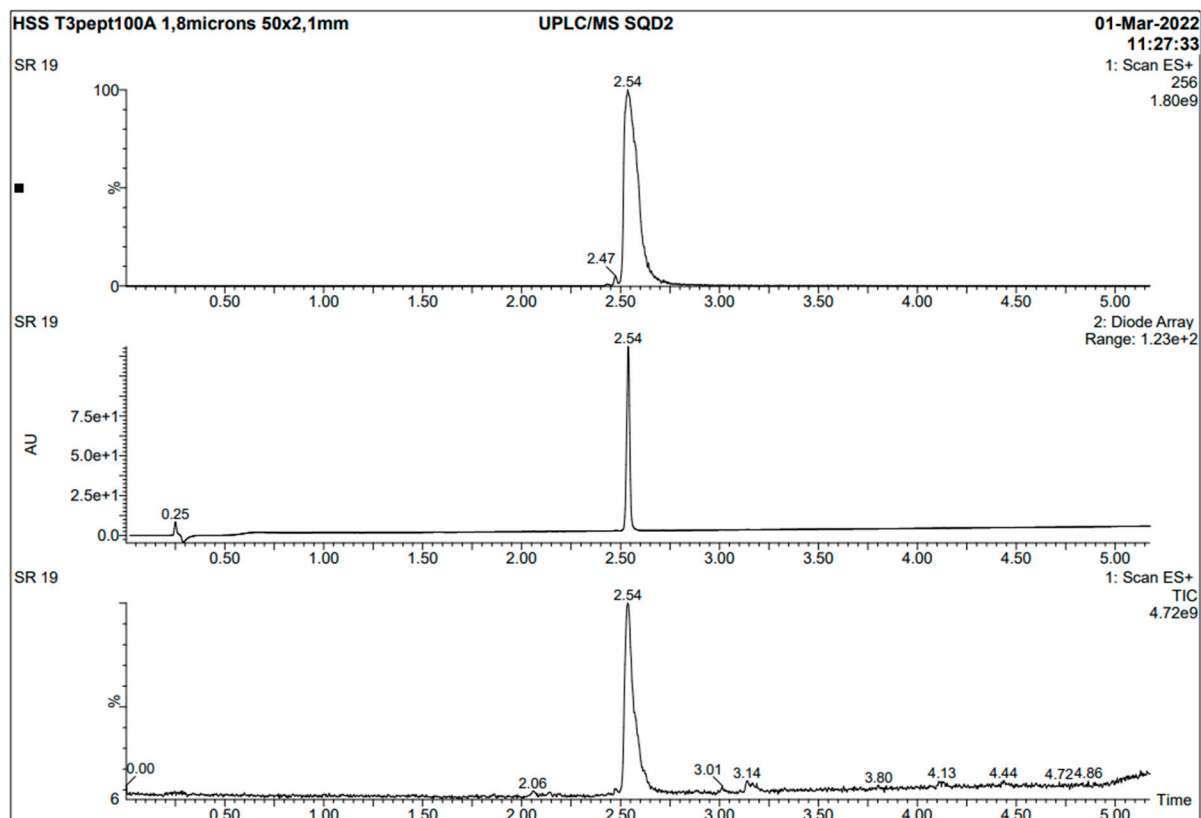
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
304.1550	1	C <sub>18</sub> H <sub>18</sub> N <sub>5</sub>	304.1557	2.1	32.5	1	100.00	12.5	even	ok

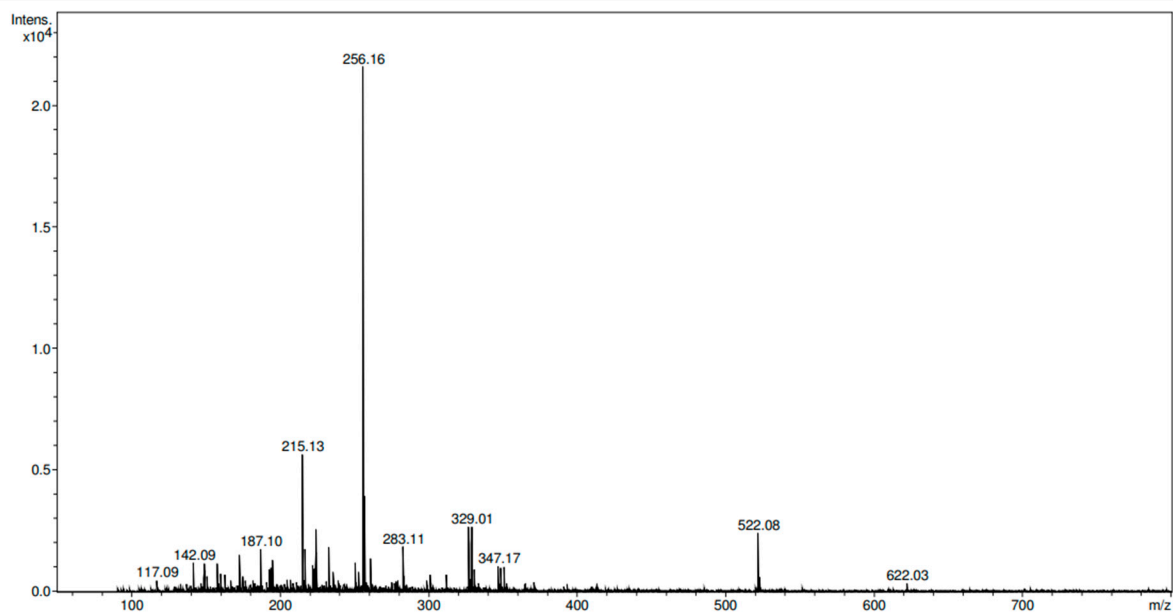


S31. 1-butyl-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16g**).



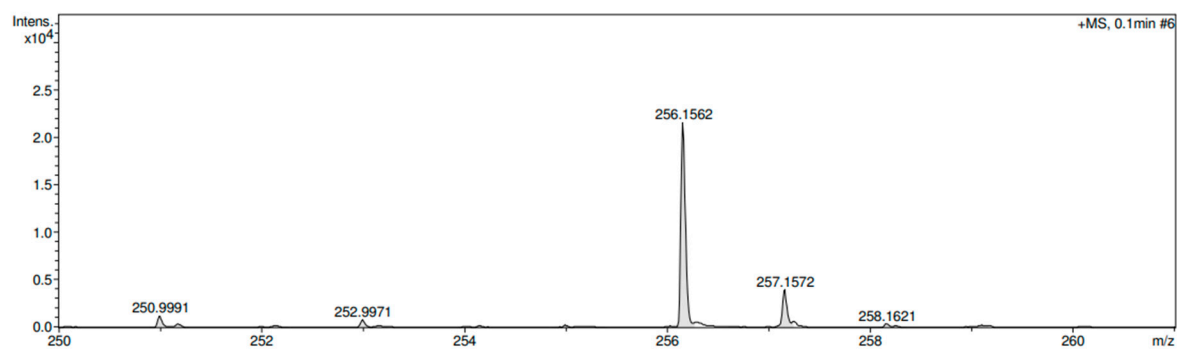
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

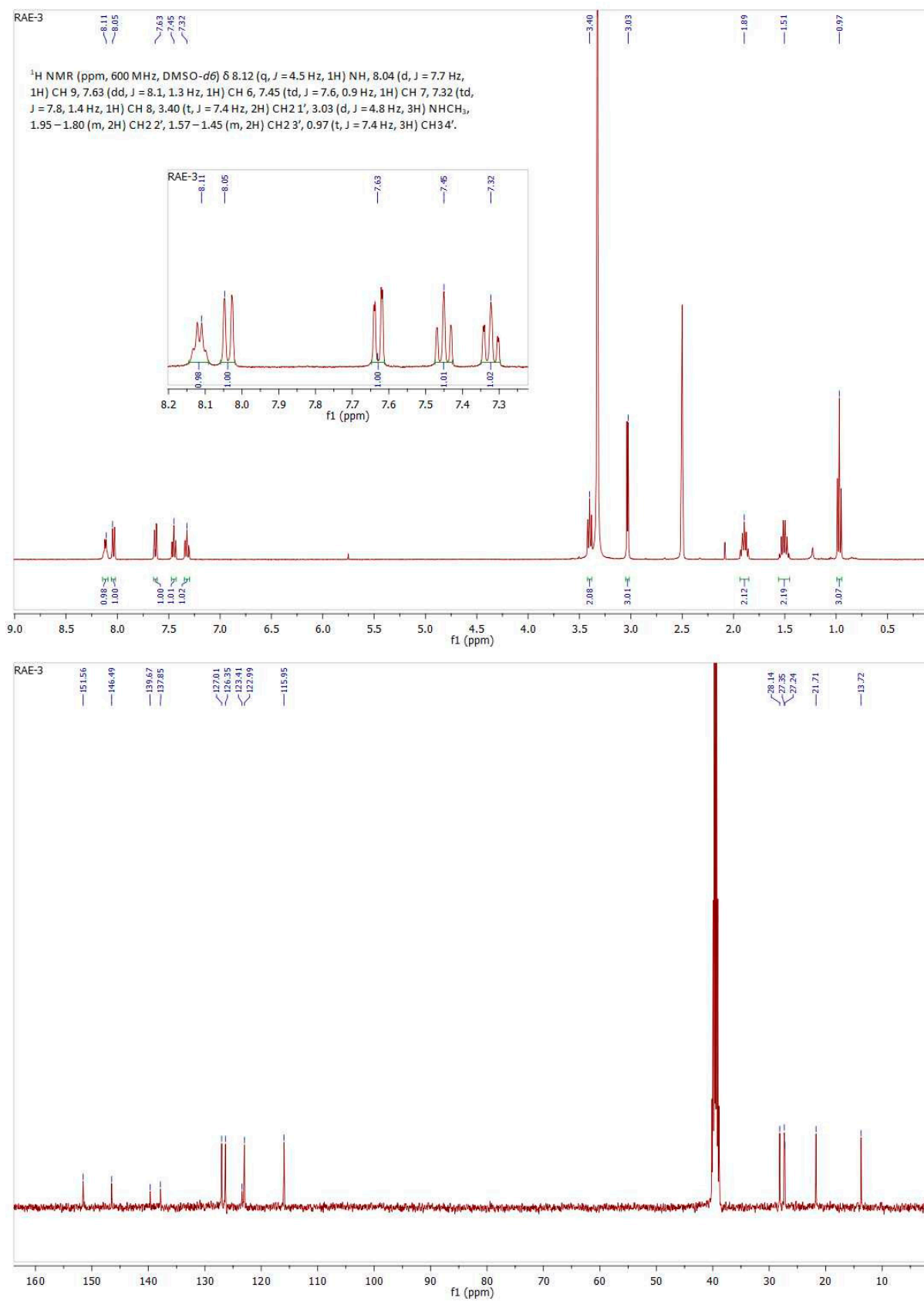


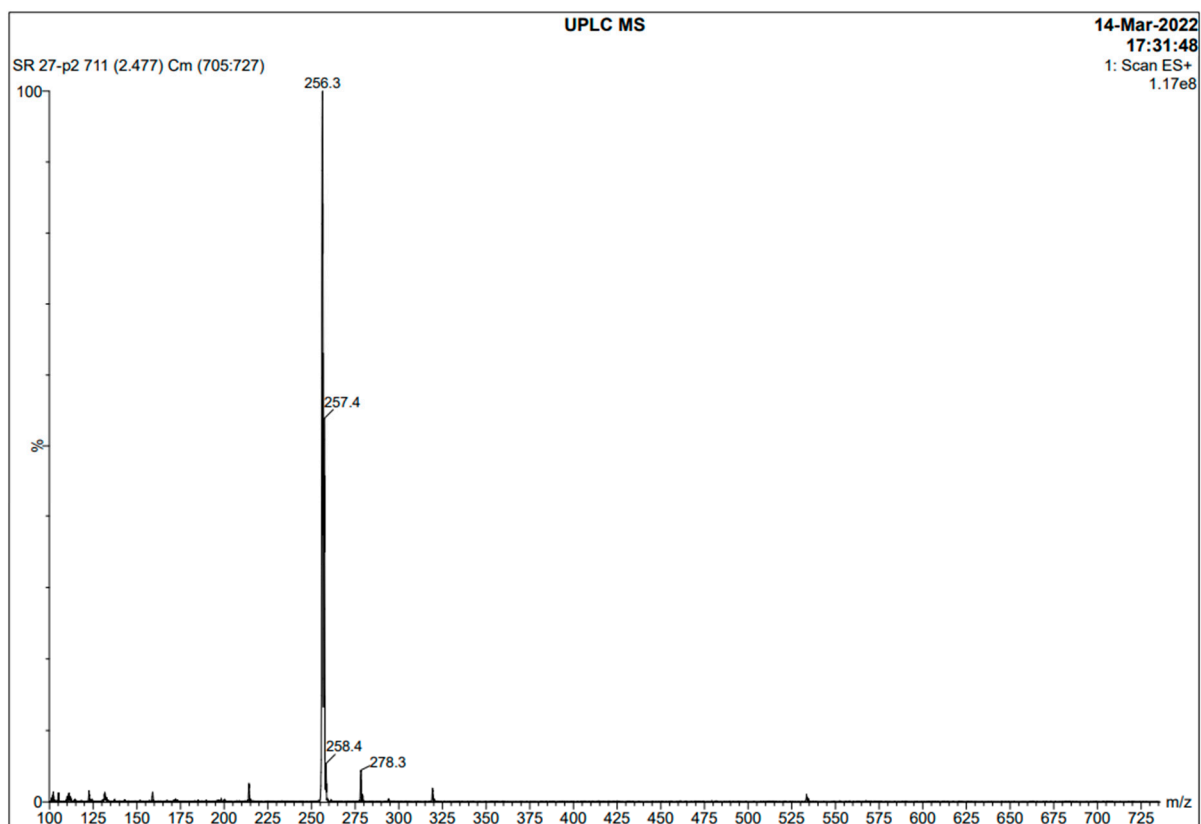
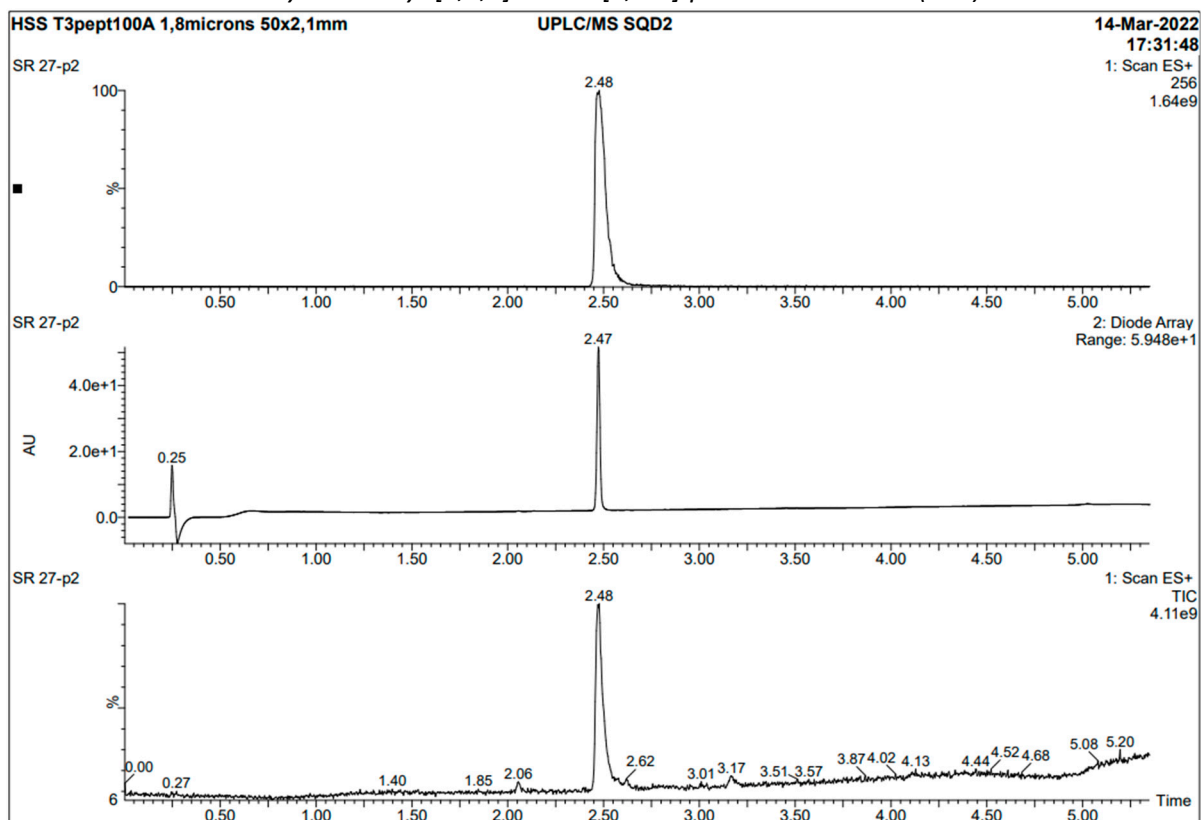
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
256.1562	1	C <sub>14</sub> H <sub>18</sub> N <sub>5</sub>	256.1557	2.1	6.6	1	100.00	8.5	even		ok



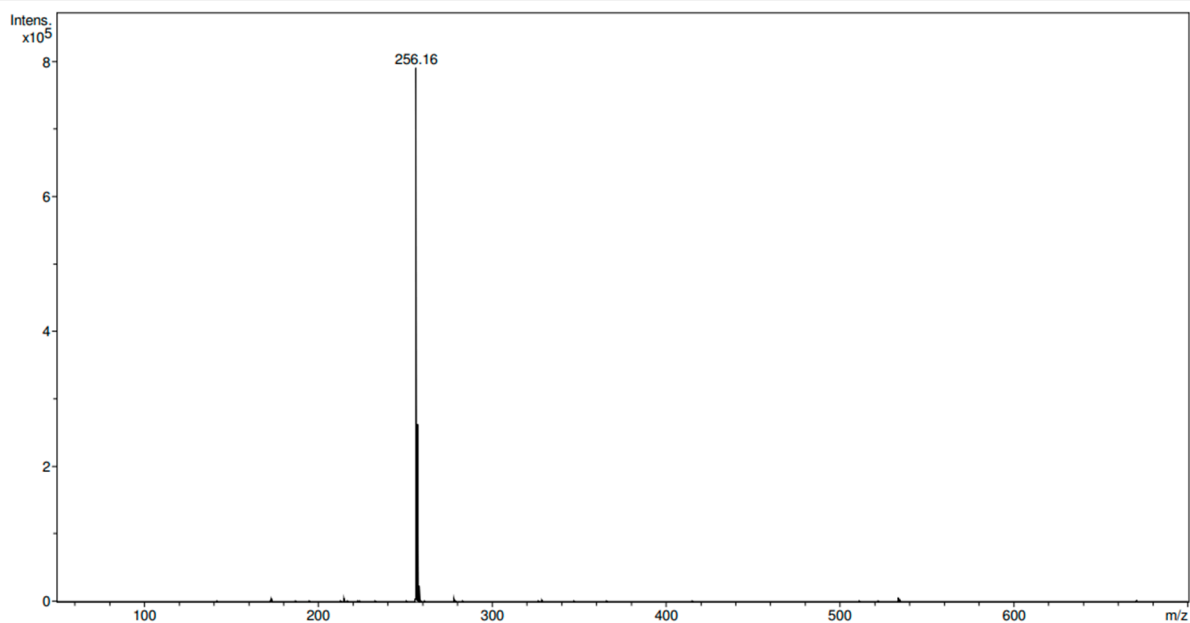
S32. 1-isobutyl-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16h**).





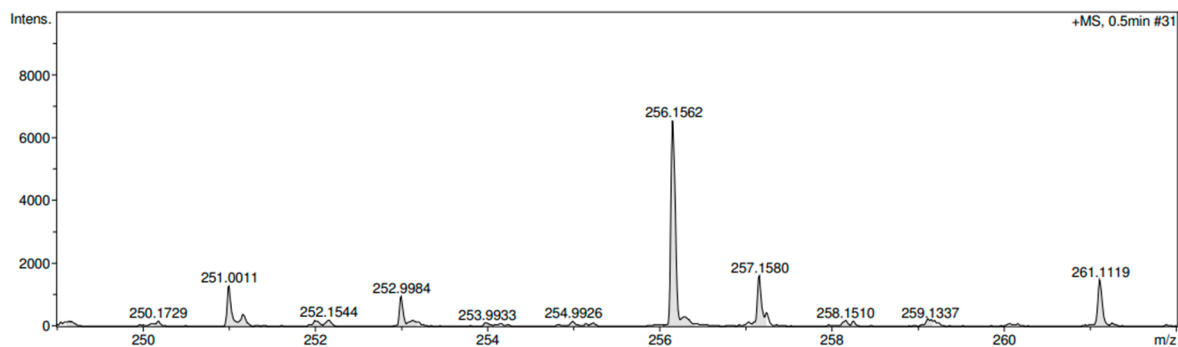
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

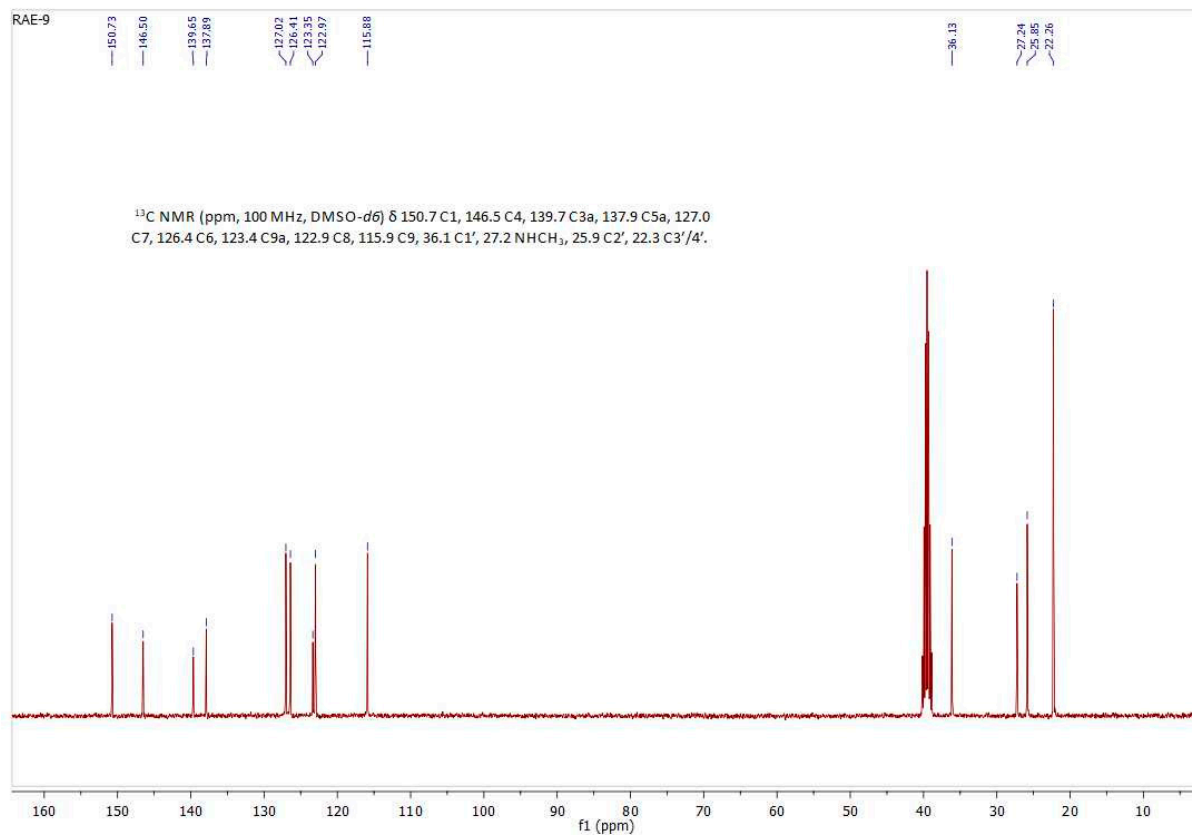
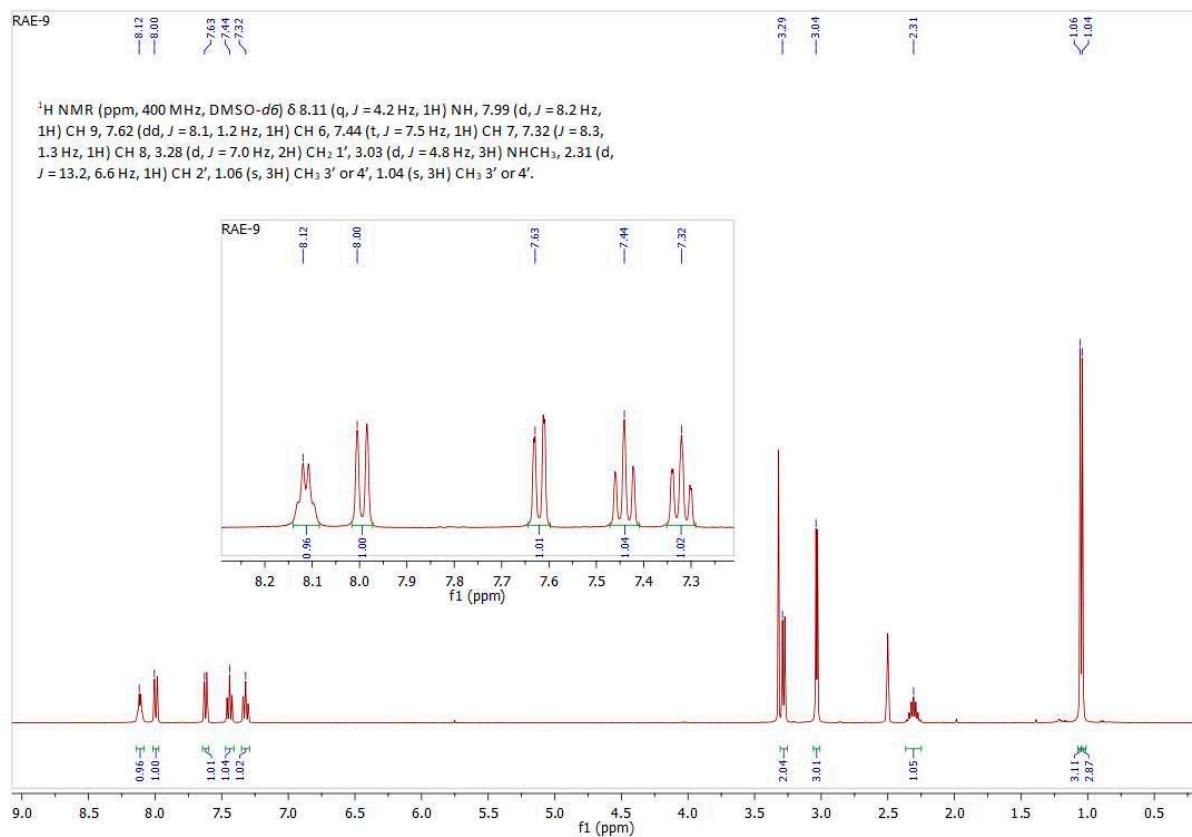


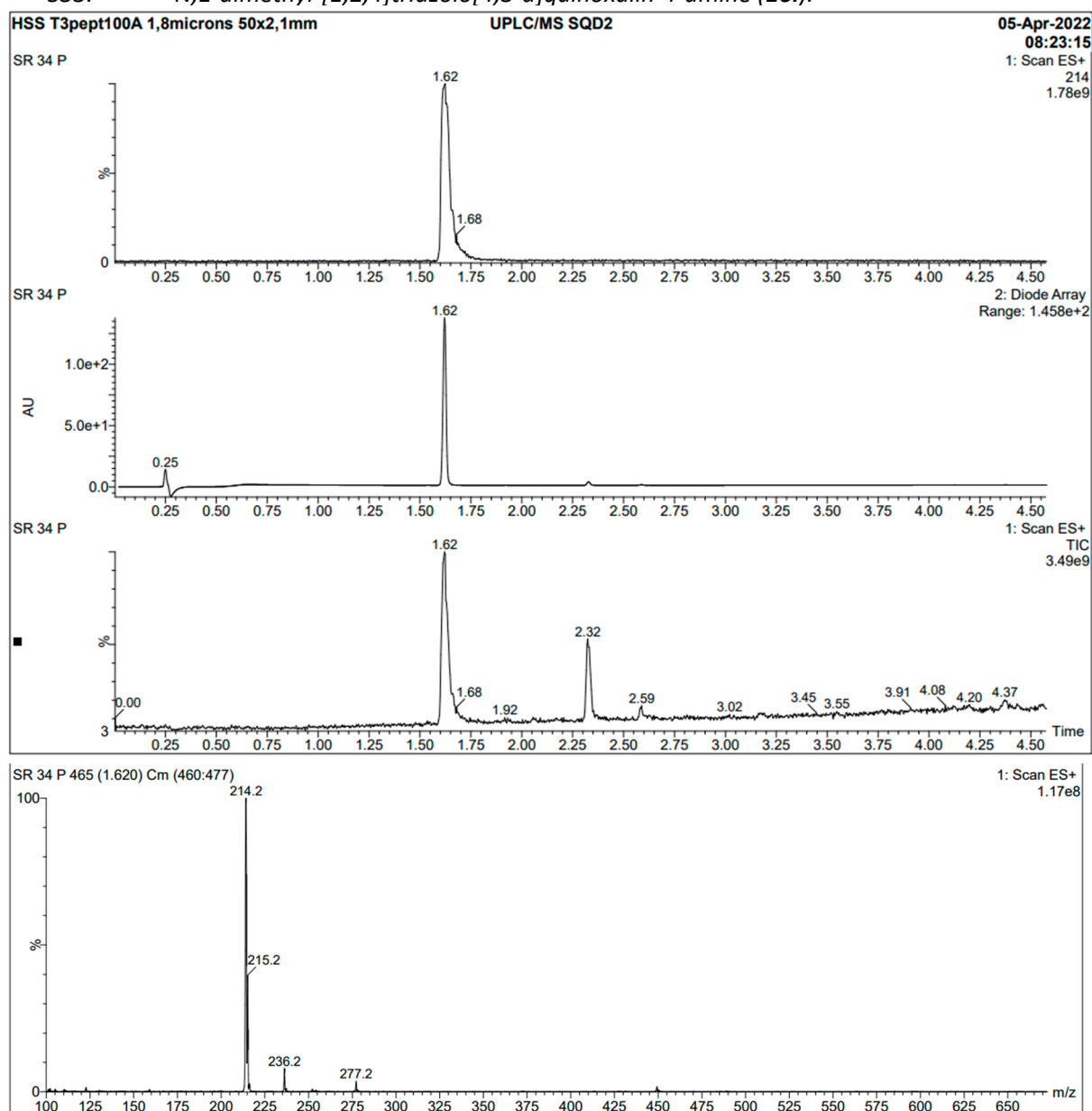
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
256.1562	1	C <sub>14</sub> H <sub>18</sub> N <sub>5</sub>	256.1557	2.0	43.7	1	100.00	8.5	even		ok
	2	C <sub>13</sub> H <sub>22</sub> NO <sub>4</sub>	256.1543	-7.2	56.7	2	29.86	3.5	even		ok

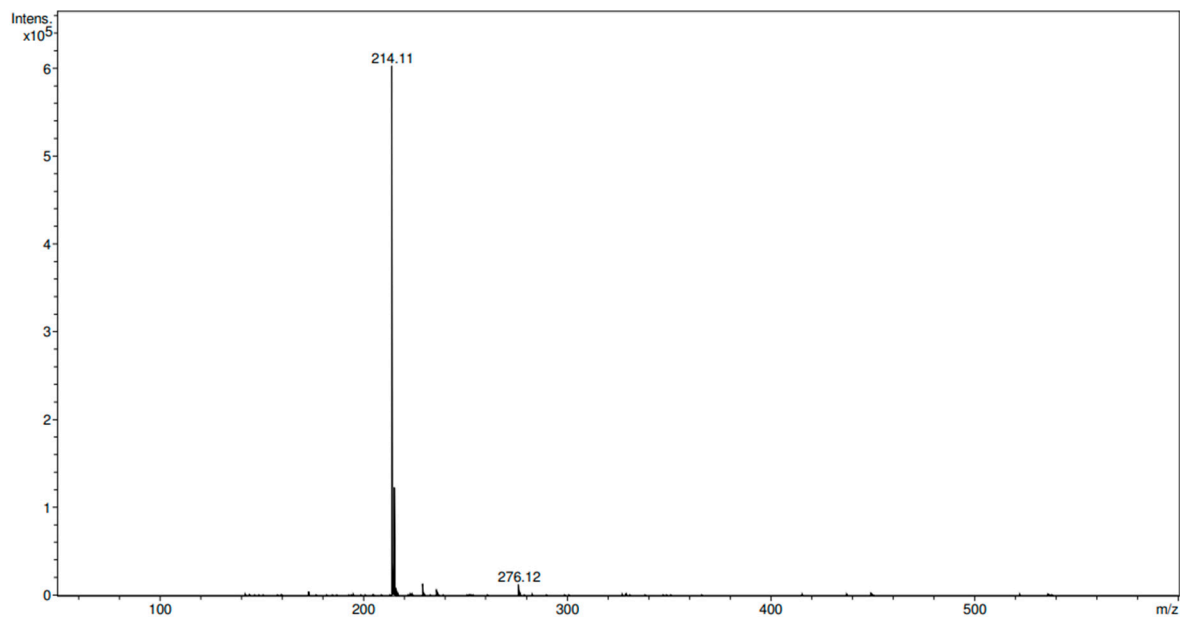


S33. *N*,1-dimethyl-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-amine (**16i**).



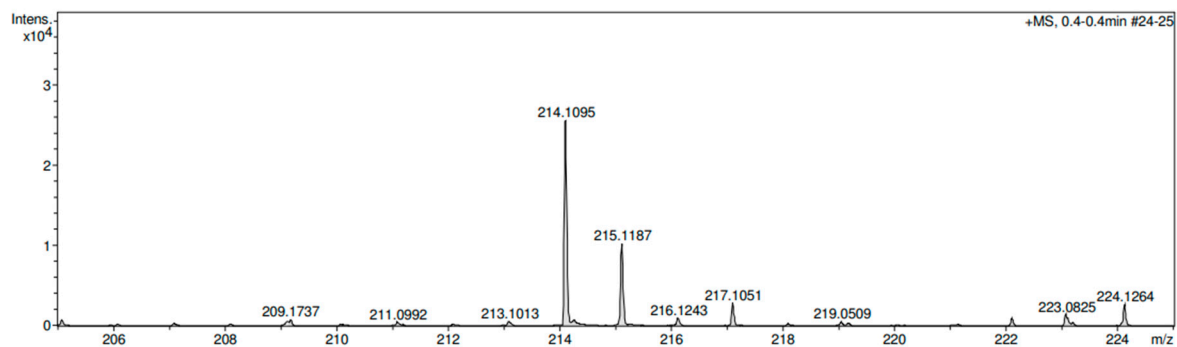
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

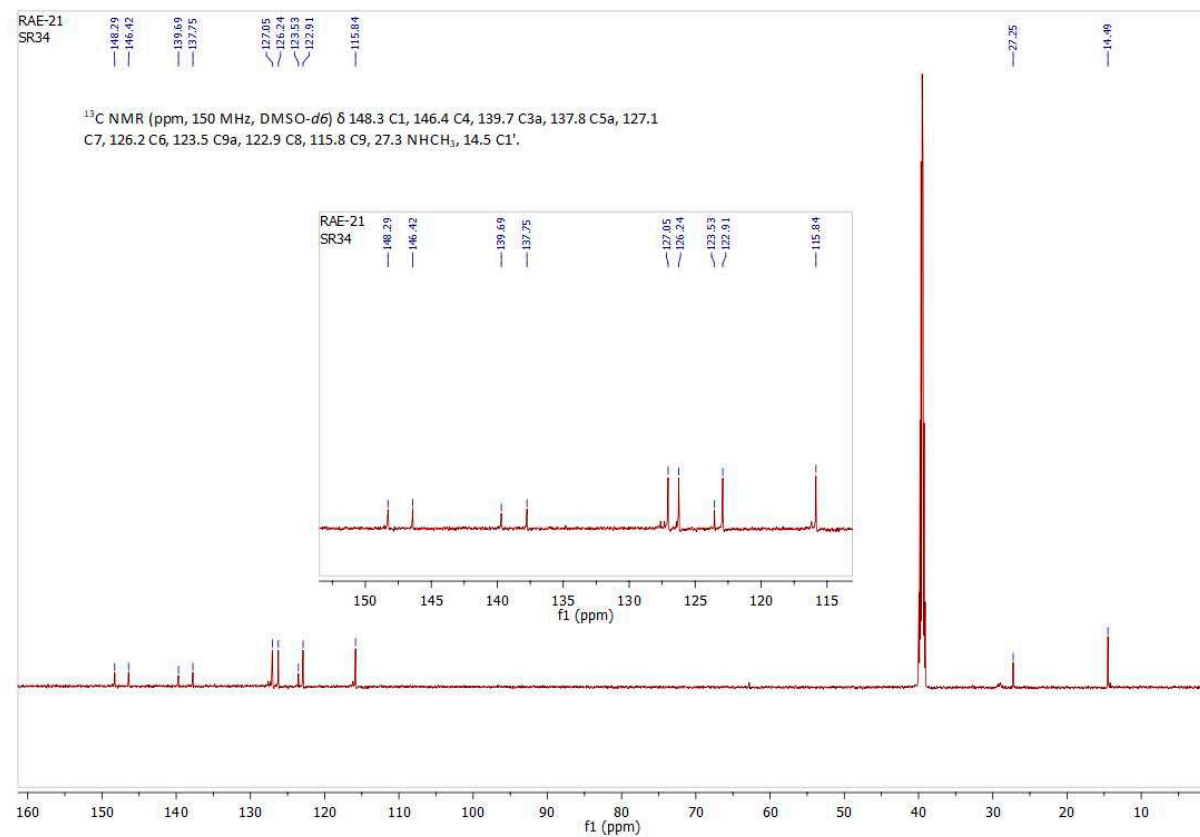
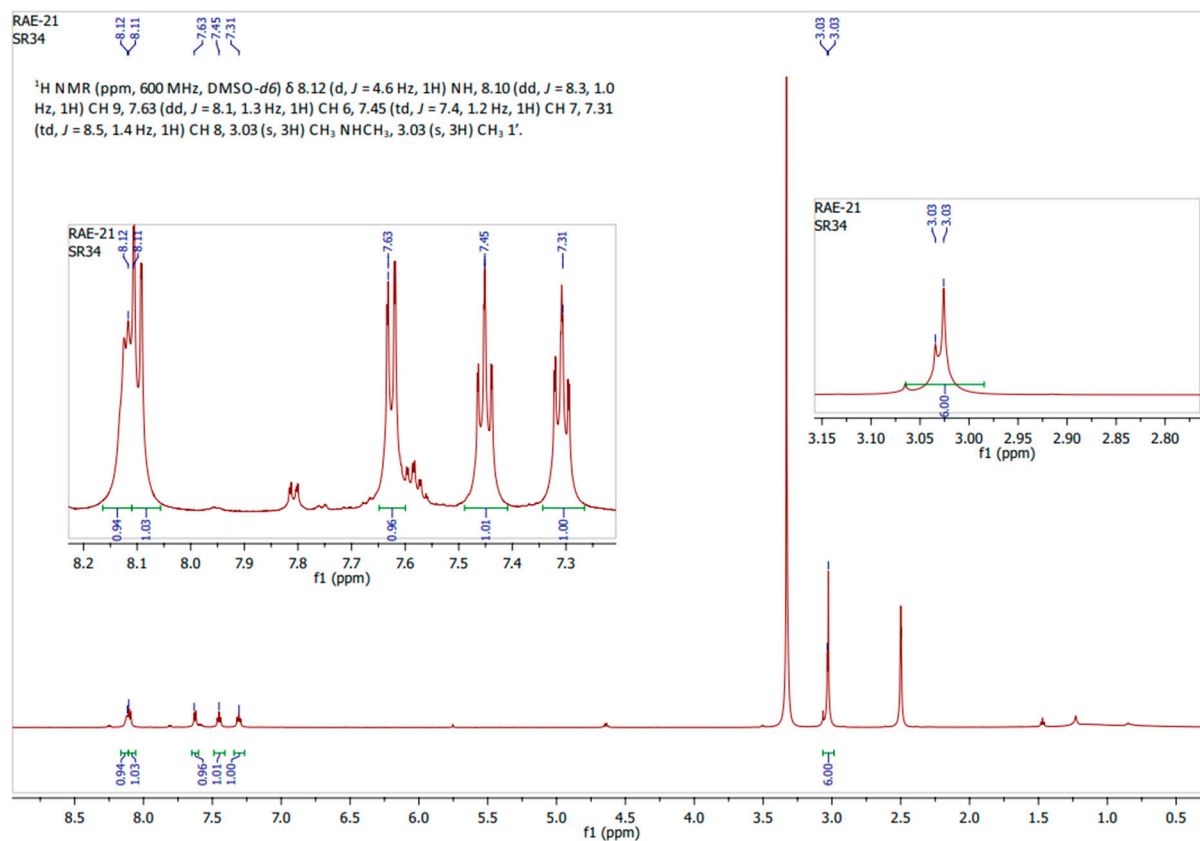


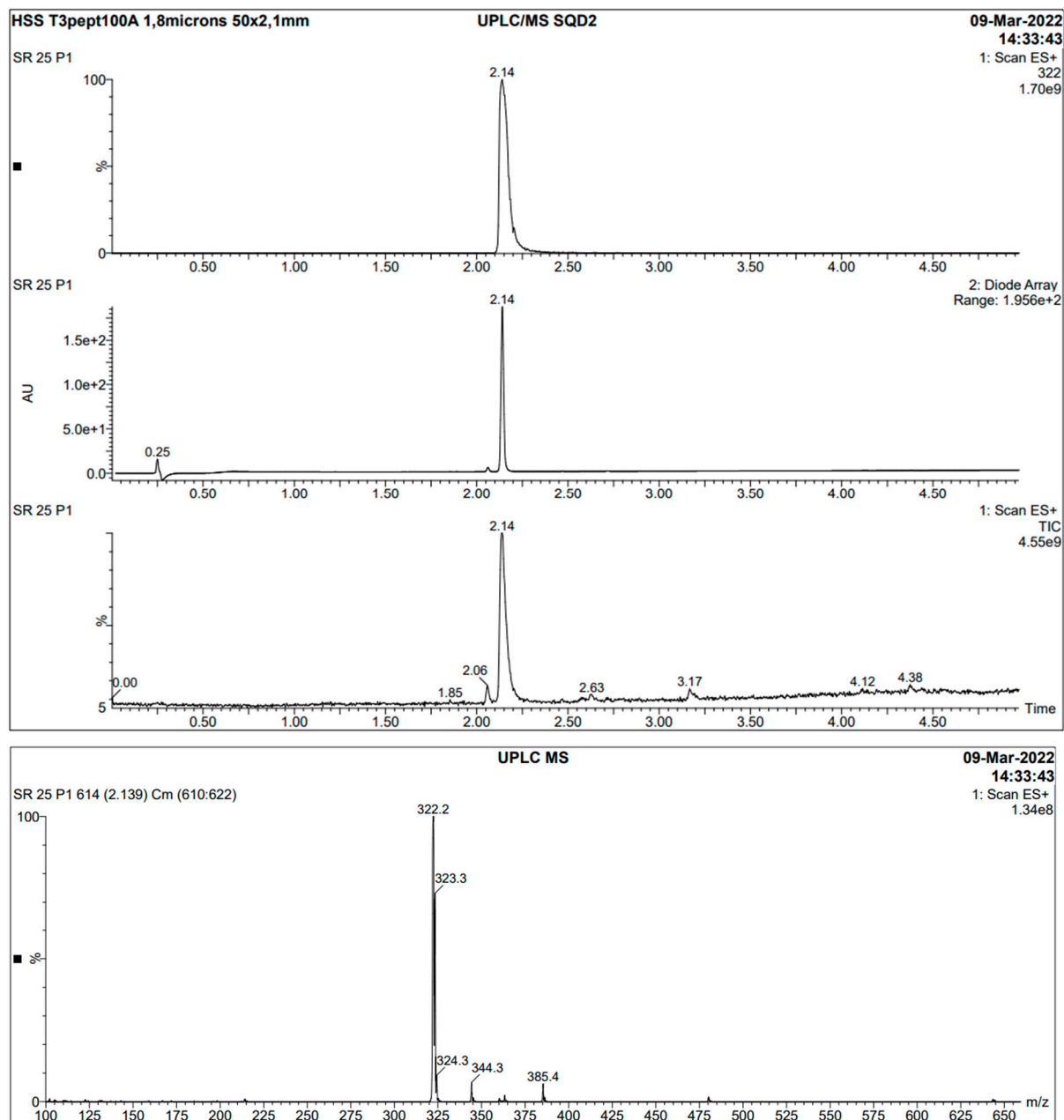
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
214.1095	1	C11H12N5	214.1087	3.8	153.8	1	100.00	8.5	even		ok

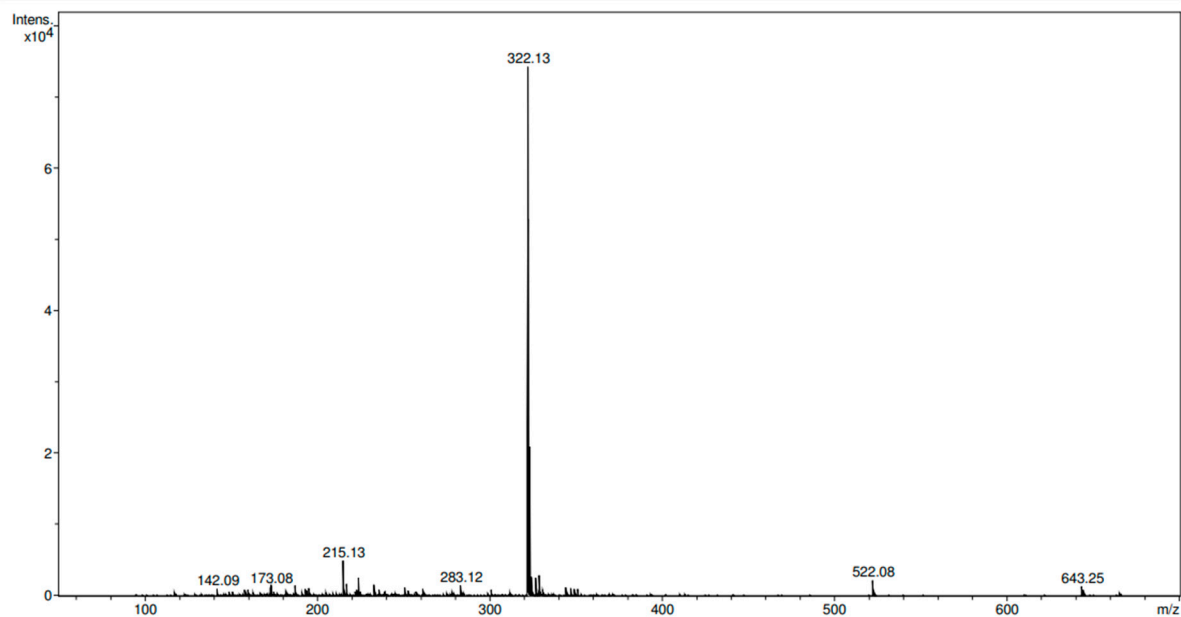


S34. 1-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16j**).



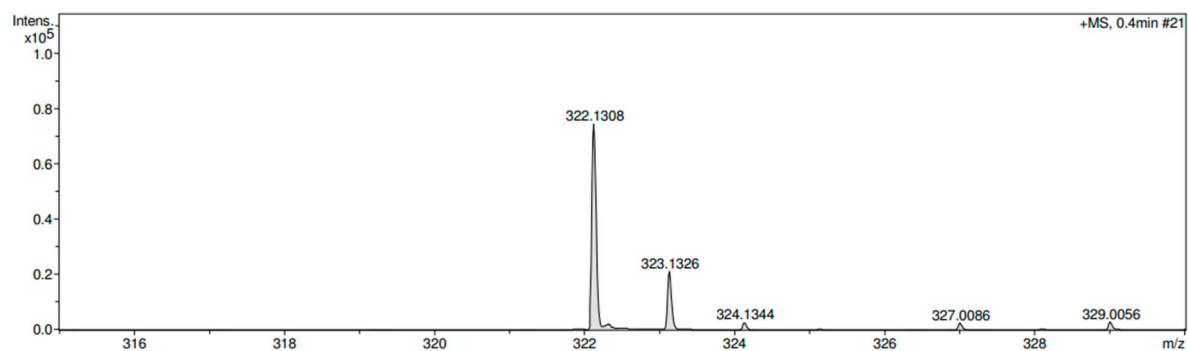
## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

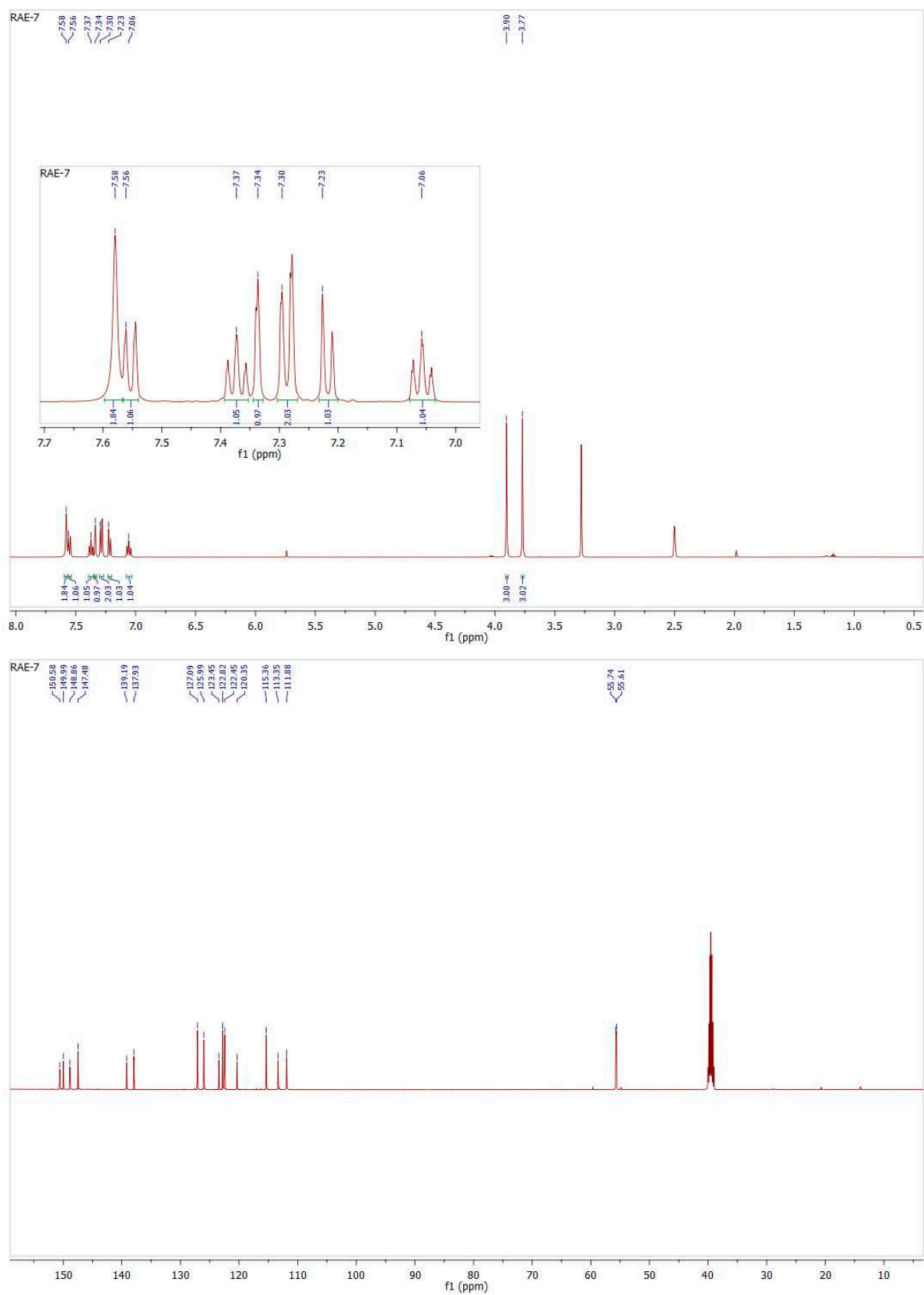


## Acquisition Parameter

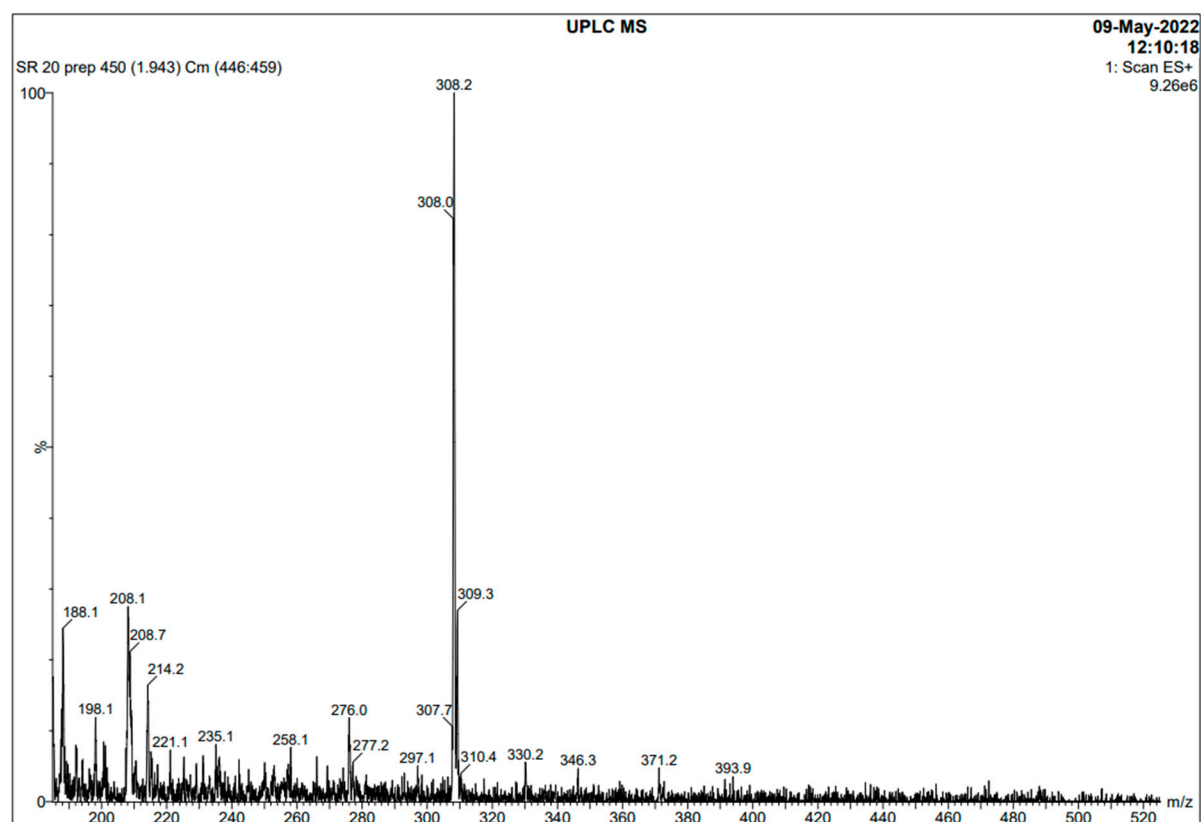
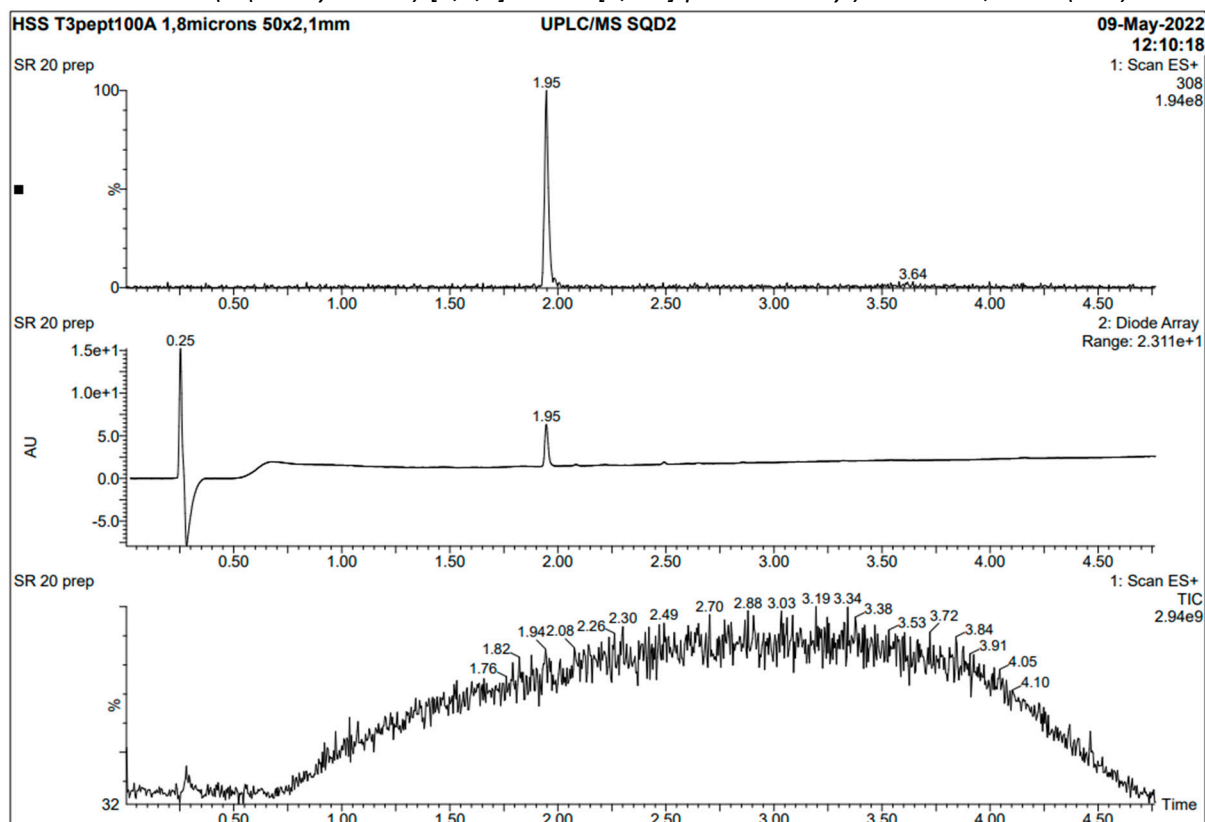
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

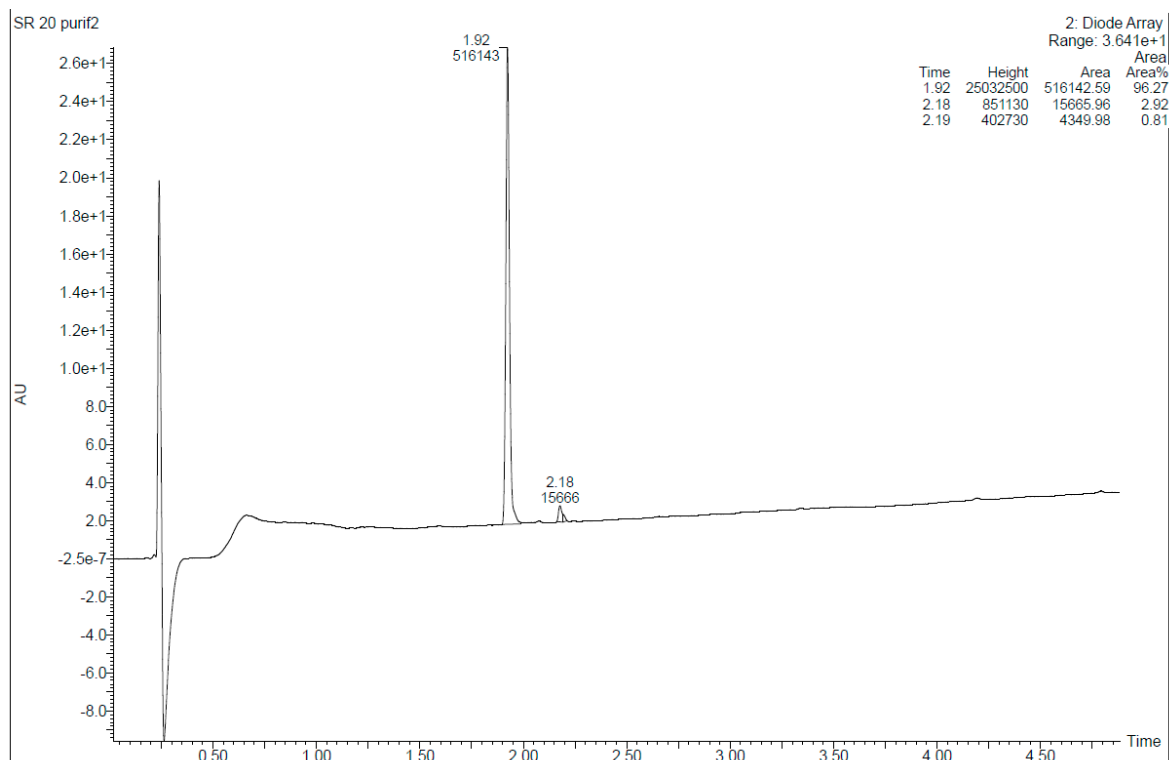


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
322.1308	1	C <sub>17</sub> H <sub>16</sub> N <sub>5</sub> O <sub>2</sub>	322.1299	-3.0	45.8	2	100.00	12.5	even		ok
	2	C <sub>16</sub> H <sub>20</sub> NO <sub>6</sub>	322.1285	7.2	59.0	3	26.15	7.5	even		ok



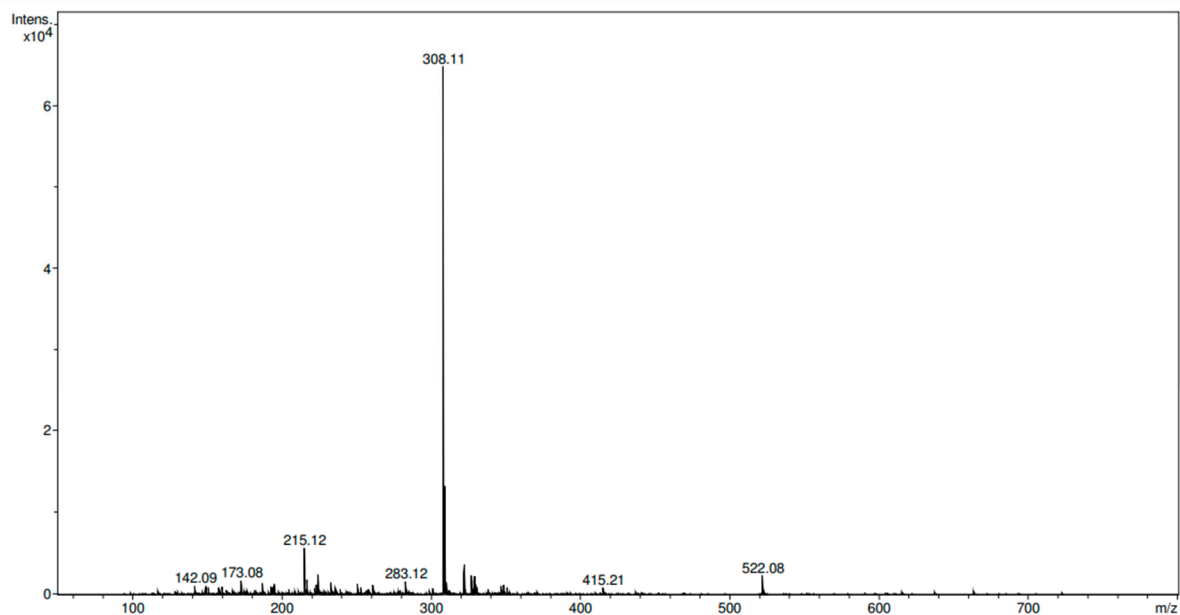


S35. 4-(4-(methylamino)-[1,2,4]triazolo[4,3-a]quinoxalin-1-yl)benzene-1,2-diol (**17a**).



#### Acquisition Parameter

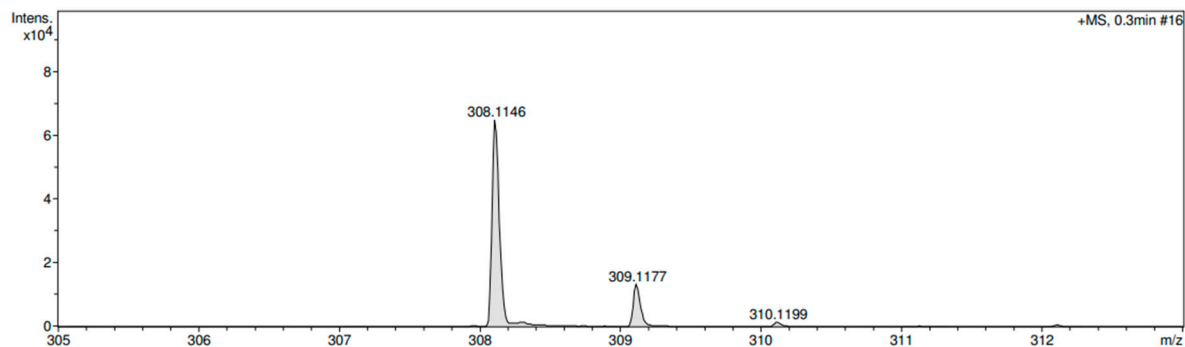
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z





## Acquisition Parameter

Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
308.1146	1	C16H14N5O2	308.1142	1.3	6.6	1	100.00	12.5	even	ok

