

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.

Cindy Patinote ¹, Sandy Raevens ¹, Amélie Baumann ¹, Eloise Pellegrin ¹, Carine Deleuze-Masquéfa ¹, Pierre-Antoine Bonnet ^{1,*}.

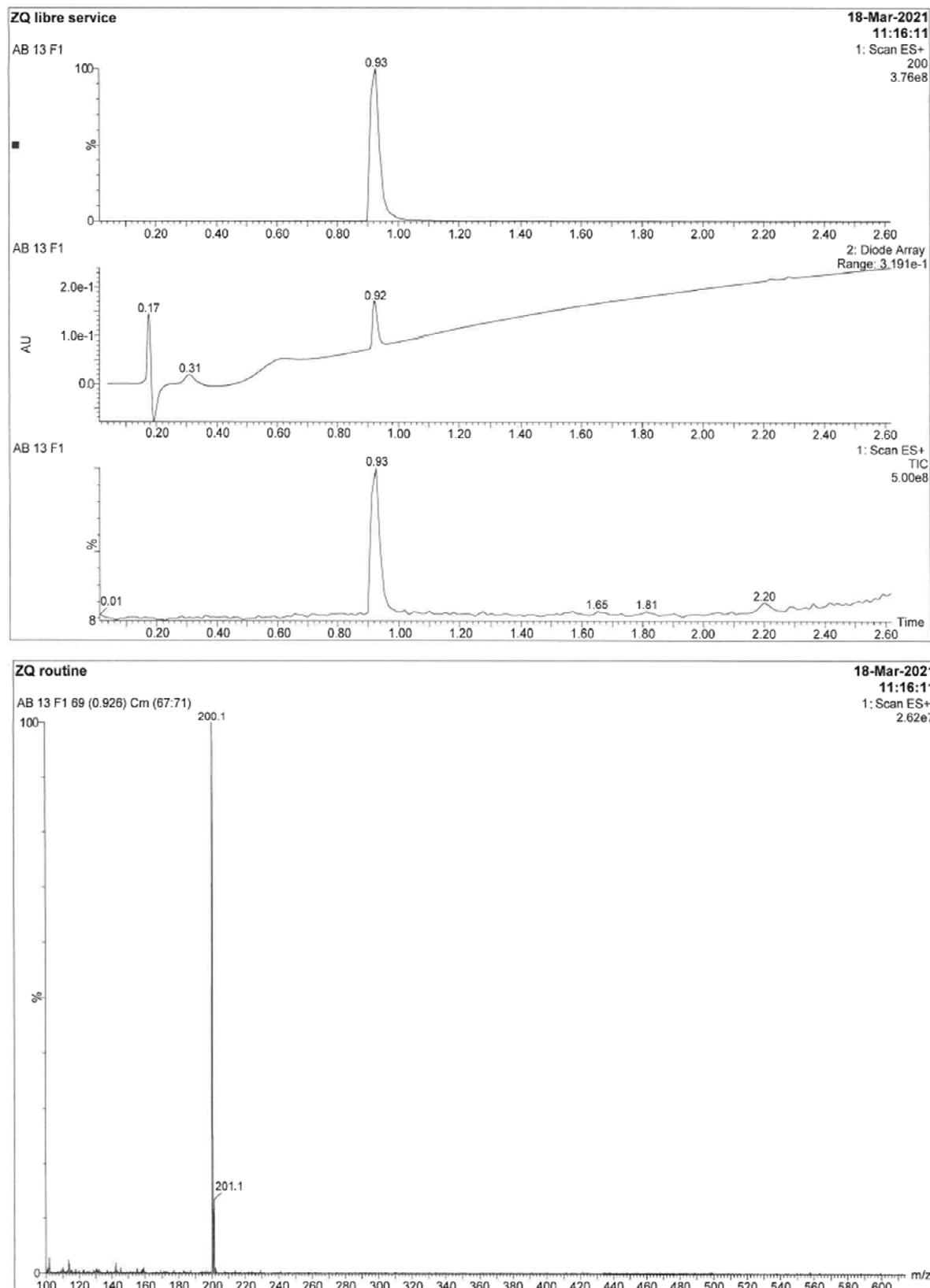
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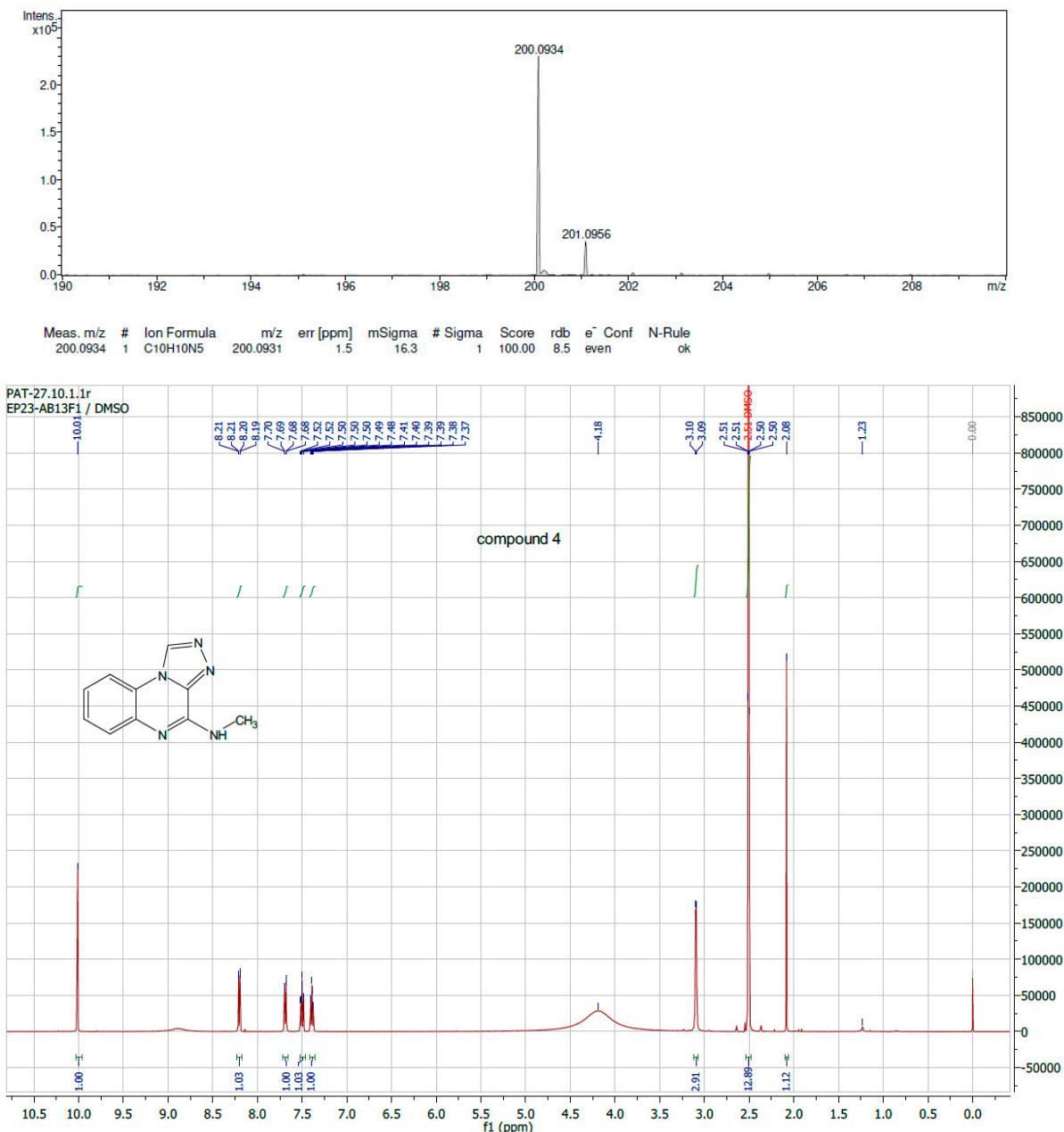
* Correspondence: pierre-antoine.bonnet@umontpellier.fr

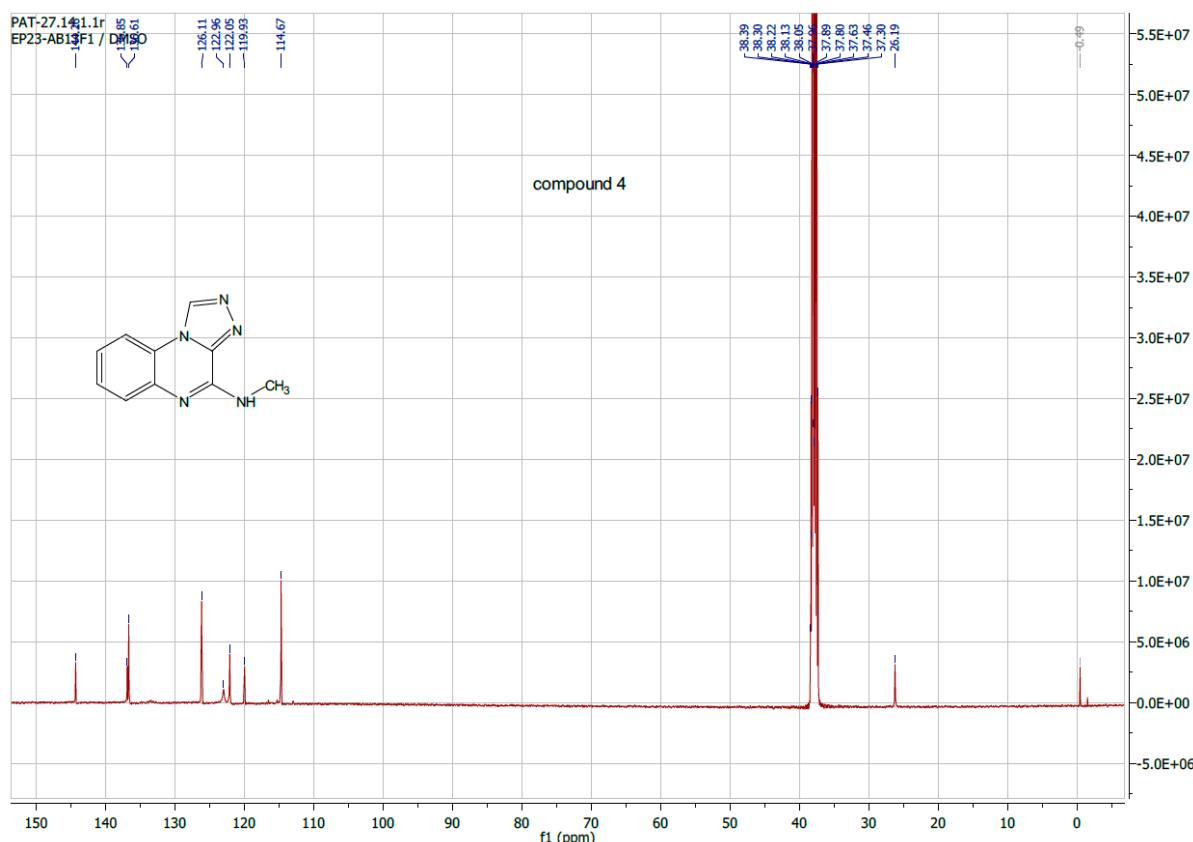
Compounds descriptions

S1.	N-methyl-[1,2,4]triazolo[4,3- <i>a</i>]quinoxalin-4-yl-amine (4).....	3
S2.	8-Bromo-[1,2,4]triazolo[4,3- <i>a</i>]quinoxalin-4-yl)-methyl-amine (7).....	5
S3.	[8-(3,4-Dimethoxy-phenyl)-[1,2,4]triazolo[4,3- <i>a</i>]quinoxalin-4-yl]-methyl-amine (8a).	8
S4.	[8-(3-Methoxy-phenyl)-[1,2,4]triazolo[4,3- <i>a</i>]quinoxalin-4-yl]-methyl-amine (8b).	10
S5.	Methyl-(8-phenyl-[1,2,4]triazolo[4,3- <i>a</i>]quinoxalin-4-yl)-amine (8c).....	13
S6.	Methyl-[8-(3,4,5-trimethoxy-phenyl)-[1,2,4]triazolo[4,3- <i>a</i>]quinoxalin-4-yl]-amine (8d).	15
S7.	2-chloro-3-(2-(3,4-dimethoxybenzylidene)hydrazinyl)quinoxaline (14a).	17
S8.	2-chloro-3-(2-(3-methoxybenzylidene)hydrazinyl)quinoxaline (14b).	19
S9.	2-(2-benzylidenehydrazinyl)-3-chloroquinoxaline (14c).	21
S10.	2-chloro-3-(2-(3,4,5-trimethoxybenzylidene)hydrazinyl)quinoxaline (14d).	23
S11.	2-chloro-3-(2-(pyridin-3-ylmethylene)hydrazinyl)quinoxaline (14e).	25
S12.	2-chloro-3-(2-(3-phenylpropylidene)hydrazinyl)quinoxaline (14f).	27
S13.	2-chloro-3-(2-pentylidenehydrazinyl)quinoxaline (14g).	29
S14.	2-chloro-3-(2-(3-methylbutylidene)hydrazinyl)quinoxaline (14h).	31
S15.	2-chloro-3-(2-ethylidenehydrazinyl)quinoxaline (14i).	33
S16.	4-chloro-1-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[4,3- <i>a</i>]quinoxaline (15a).	34
S17.	4-chloro-1-(3-methoxyphenyl)-[1,2,4]triazolo[4,3- <i>a</i>]quinoxaline (15b).	36
S18.	4-chloro-1-phenyl-[1,2,4]triazolo[4,3- <i>a</i>]quinoxaline (15c).	38
S19.	4-chloro-1-(3,4,5-trimethoxyphenyl)-[1,2,4]triazolo[4,3- <i>a</i>]quinoxaline (15d).	40

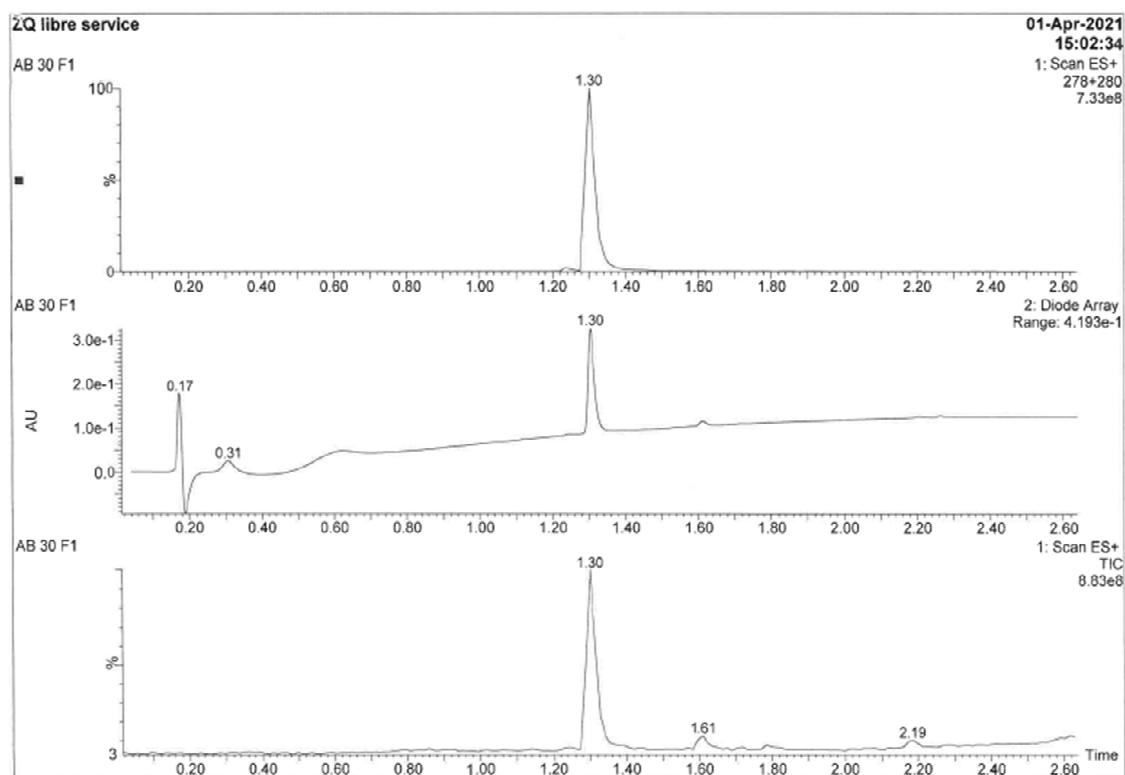
S20.	4-chloro-1-(pyridin-3-yl)-[1,2,4]triazolo[4,3-a]quinoxaline (15e).	42
S21.	4-chloro-1-phenethyl-[1,2,4]triazolo[4,3-a]quinoxaline (15f).	44
S22.	1-butyl-4-chloro-[1,2,4]triazolo[4,3-a]quinoxaline (15g).	46
S23.	4-chloro-1-isobutyl-[1,2,4]triazolo[4,3-a]quinoxaline (15h).	48
S24.	4-chloro-1-methyl-[1,2,4]triazolo[4,3-a]quinoxaline (15i).	50
S25.	1-(3,4-dimethoxyphenyl)-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16a).	52
S26.	1-(3-methoxyphenyl)-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16b).	56
S27.	N-methyl-1-phenyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16c).	59
S28.	N-methyl-1-(3,4,5-trimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16d).	62
S29.	N-methyl-1-(pyridin-3-yl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16e).	65
S30.	N-methyl-1-phenethyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16f).	68
S31.	1-butyl-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16g).	71
S32.	1-isobutyl-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16h).	74
S33.	N,1-dimethyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16i).	77
S34.	1-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16j).	80
S35.	4-(4-(methylamino)-[1,2,4]triazolo[4,3-a]quinoxalin-1-yl)benzene-1,2-diol (17a).	83

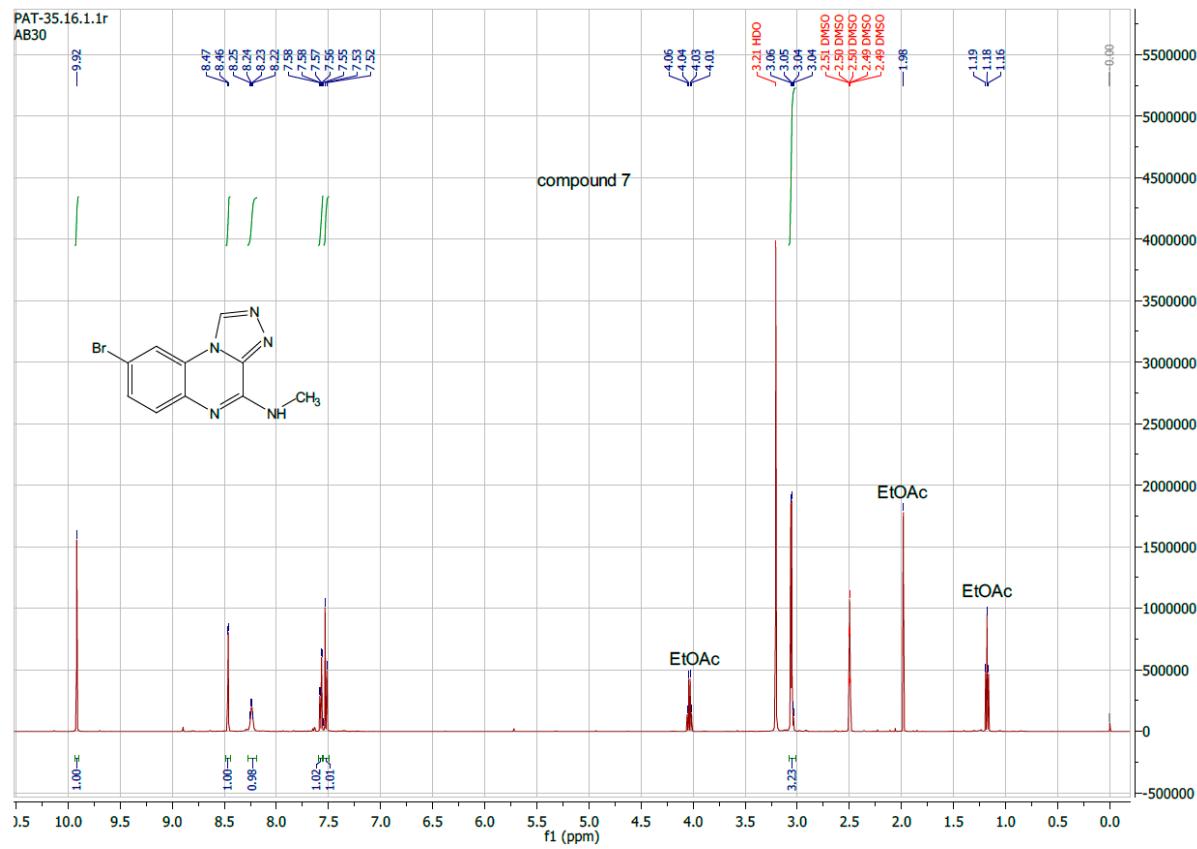
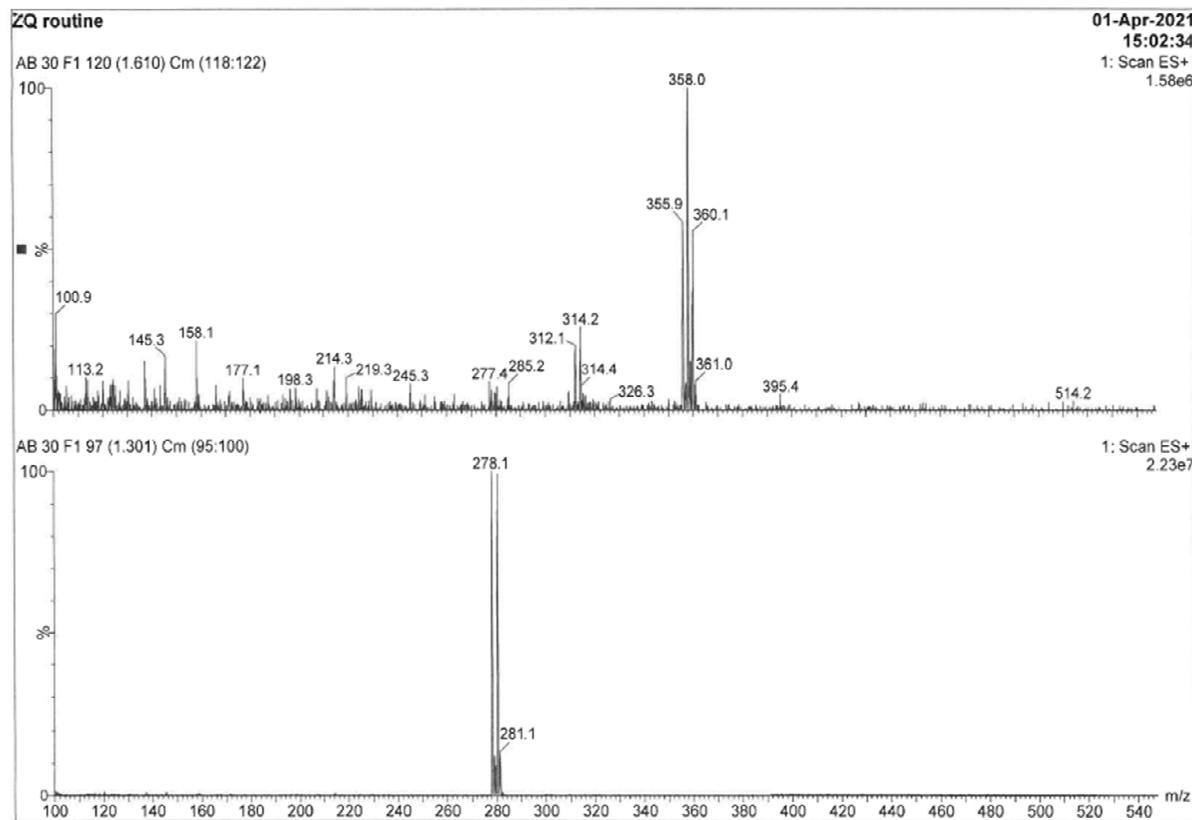
S1. *N*-methyl-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-yl-amine (**4**).

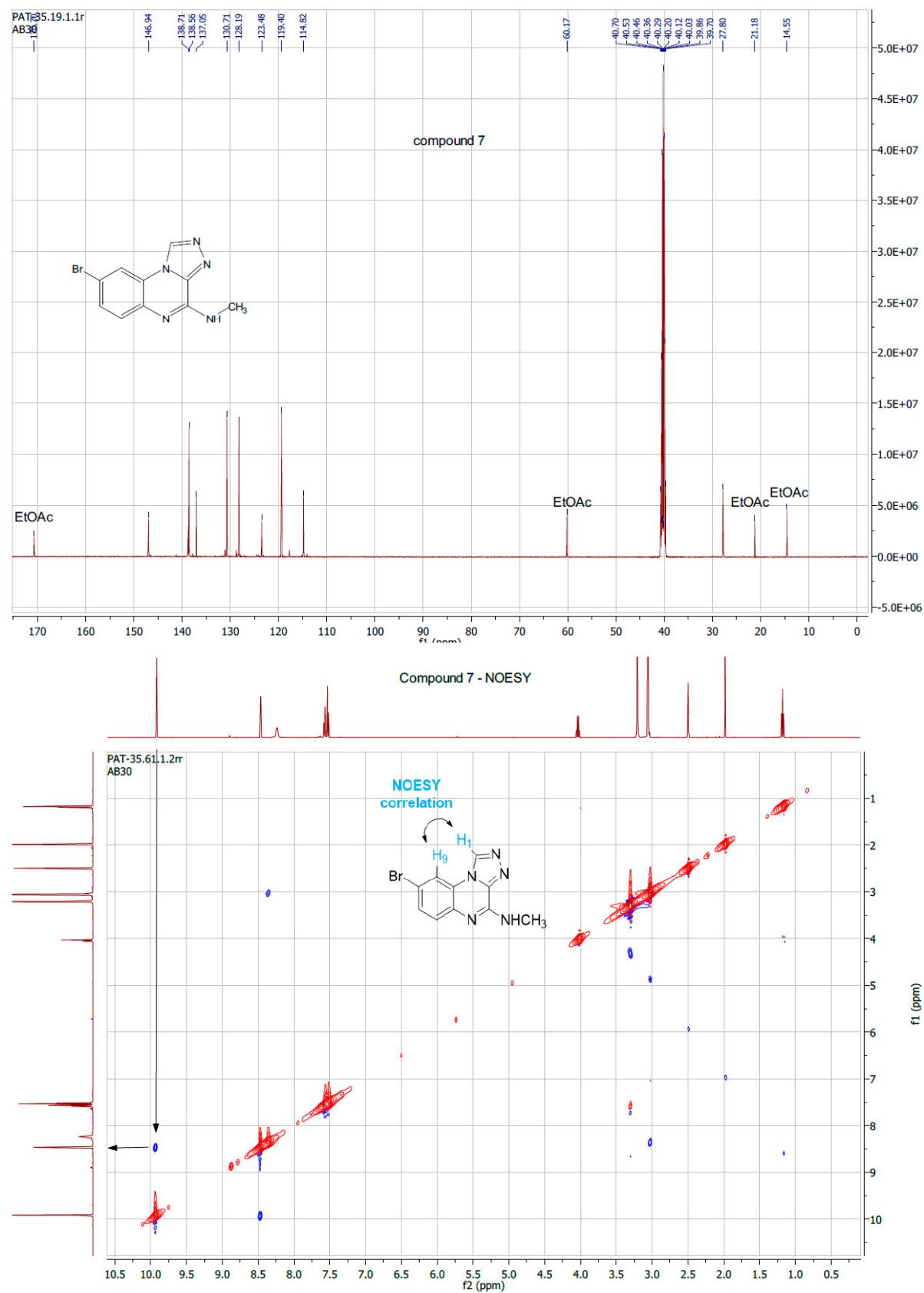




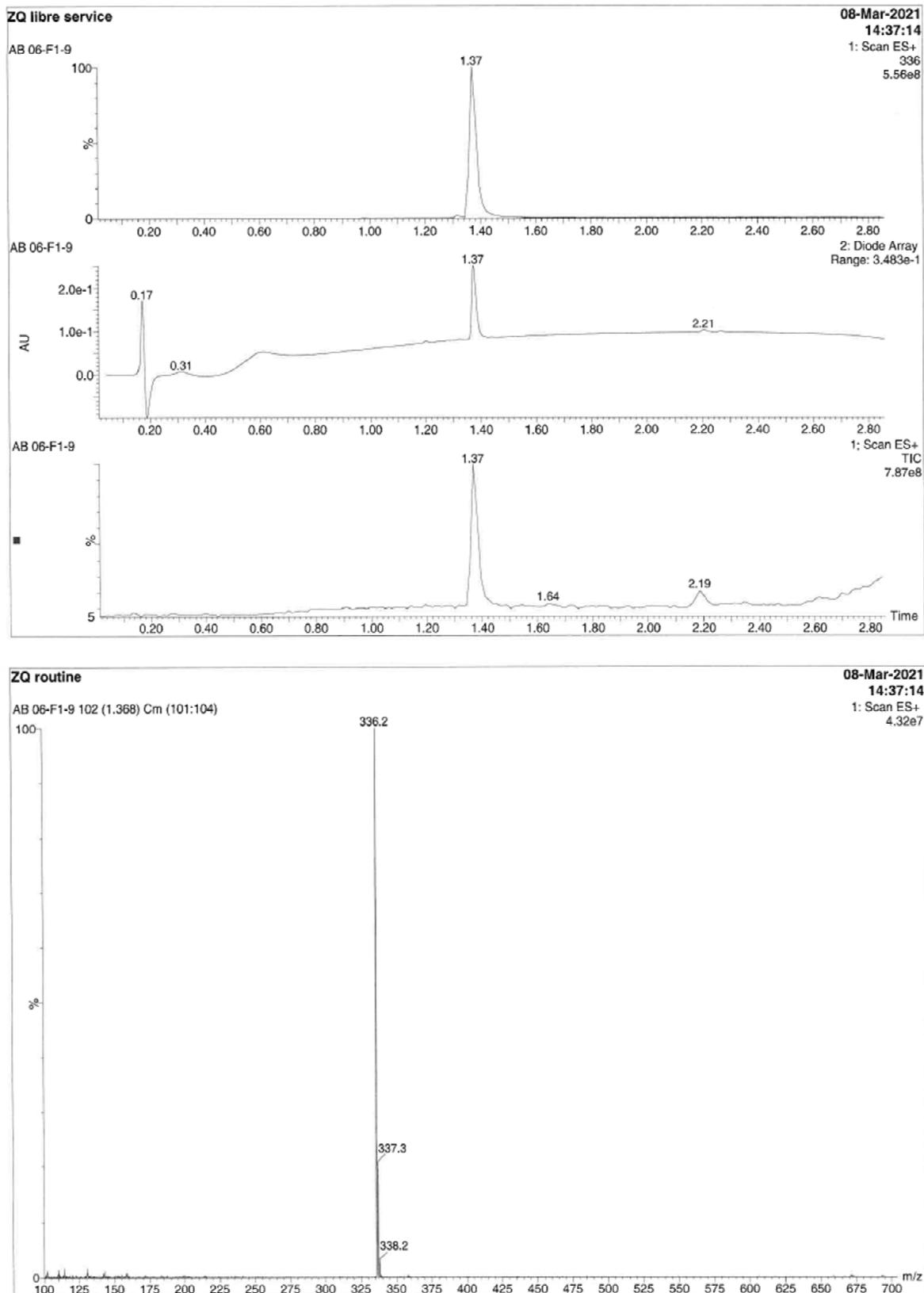
S2. 8-Bromo-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl)-methyl-amine (7).

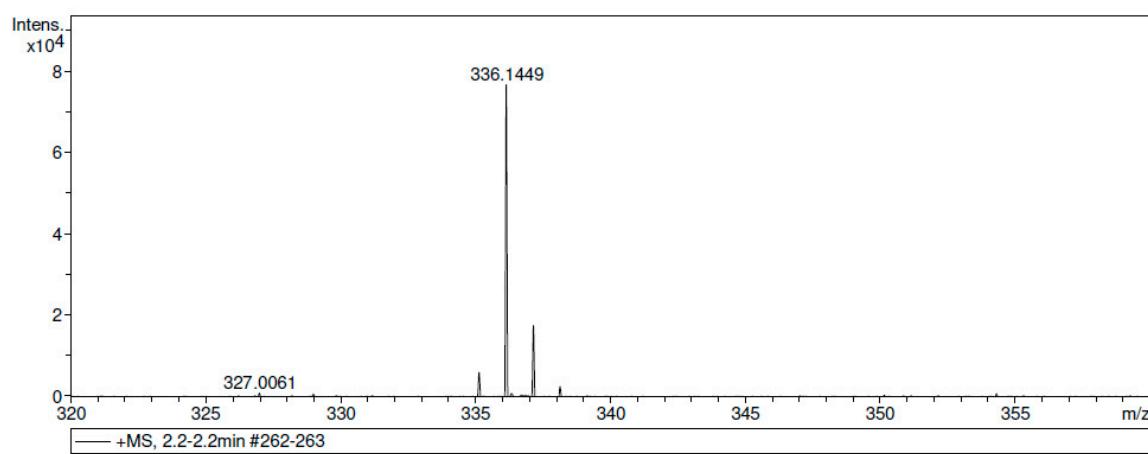




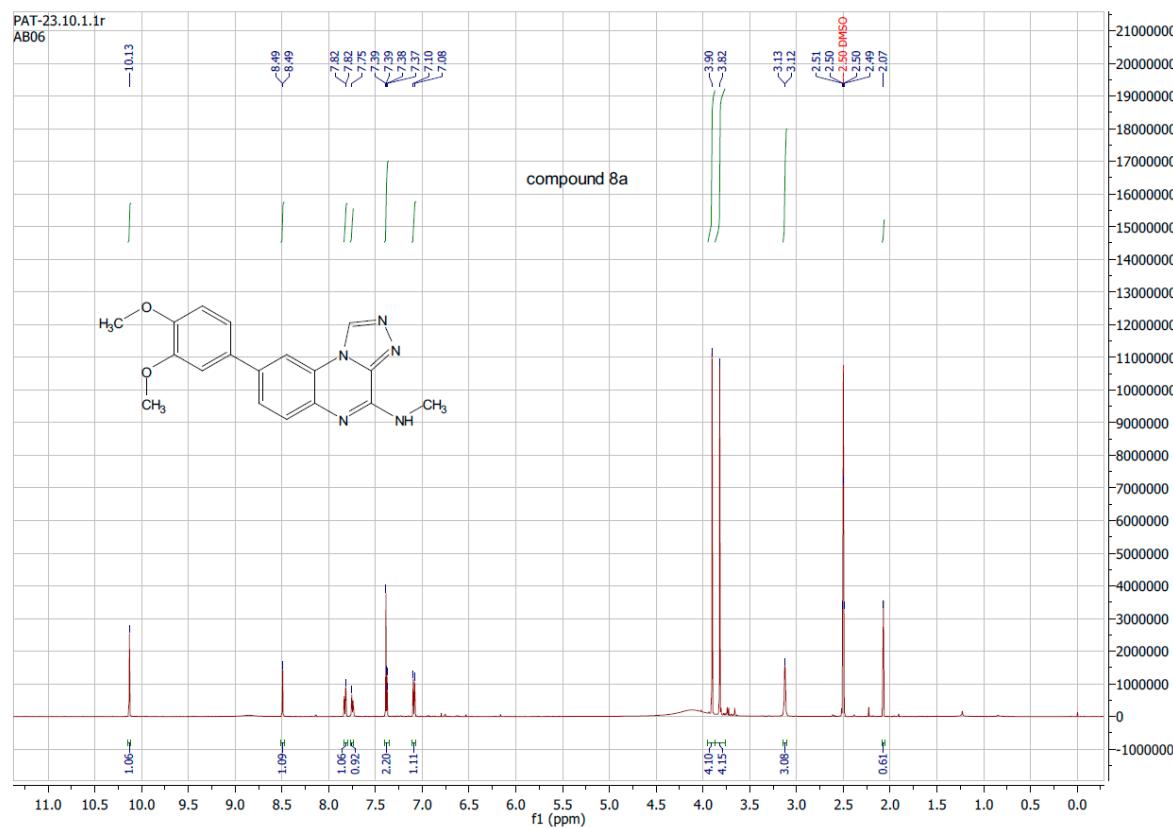


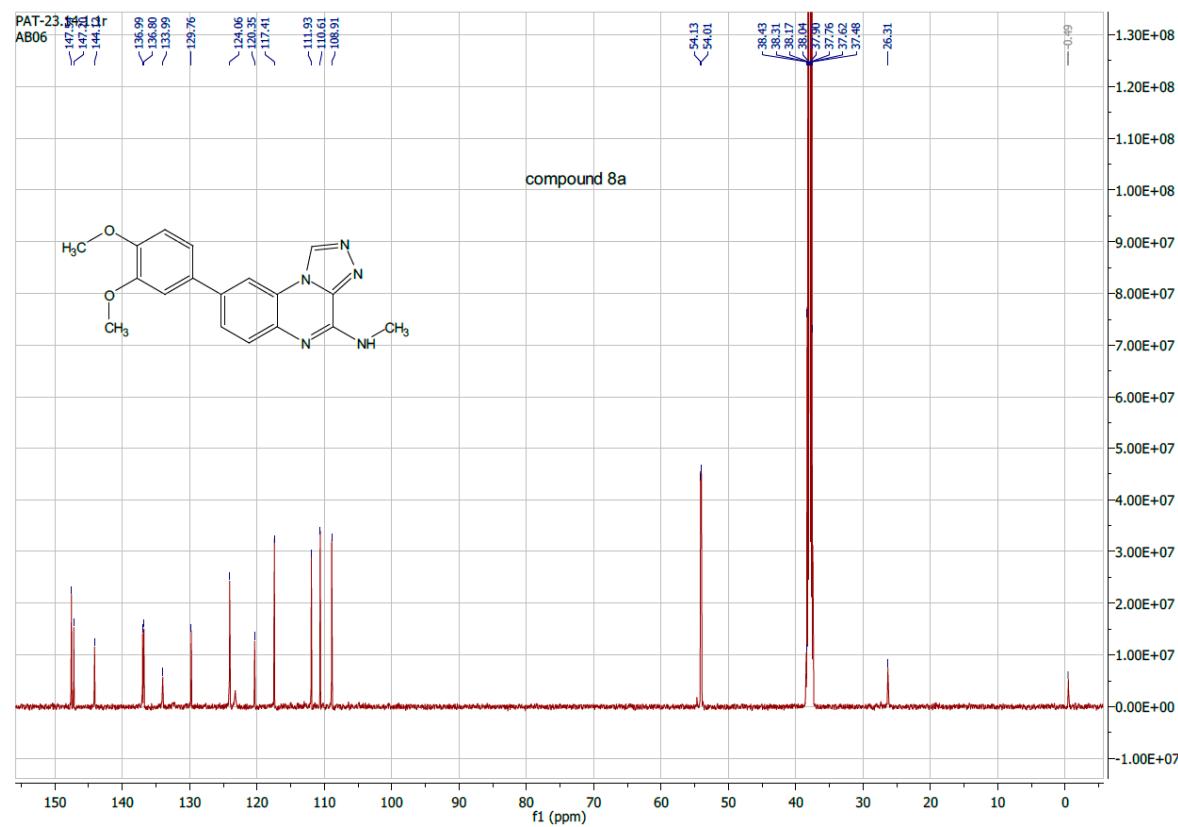
S3. [8-(3,4-Dimethoxy-phenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl]-methyl-amine (**8a**).



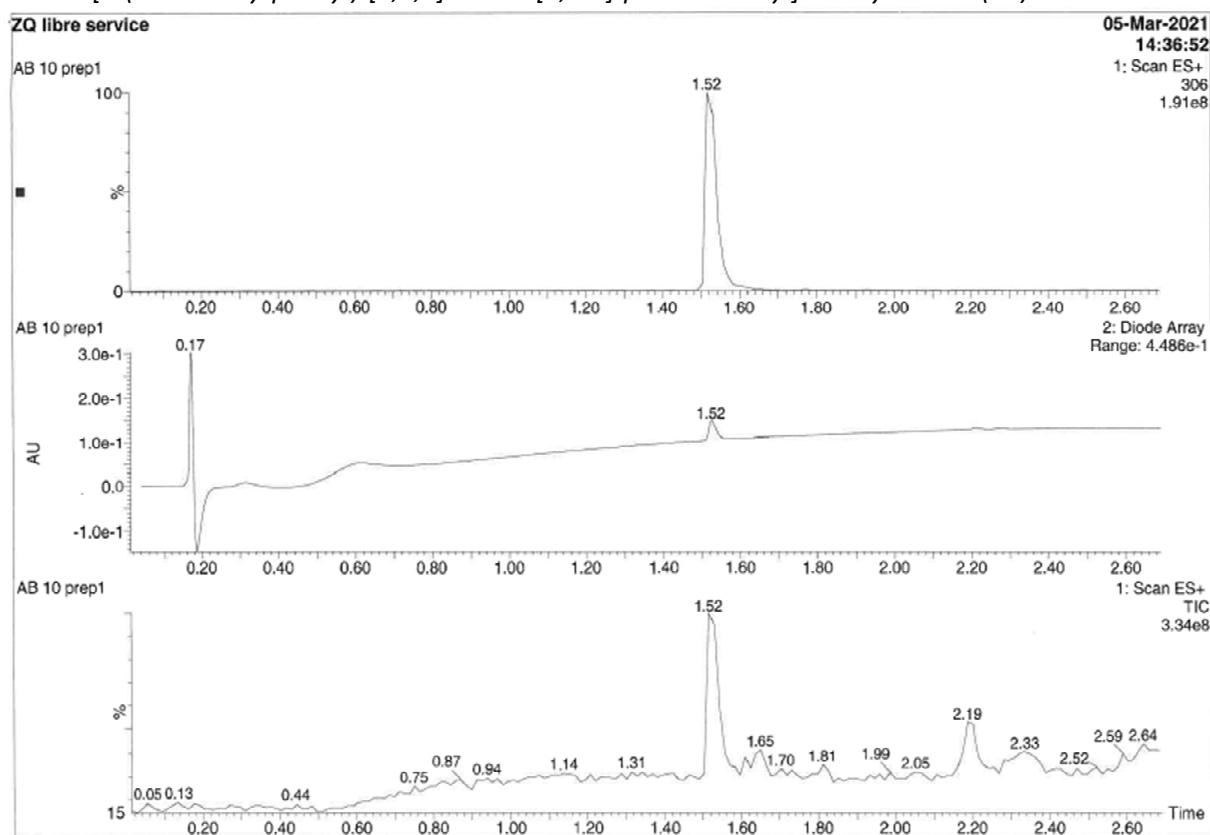


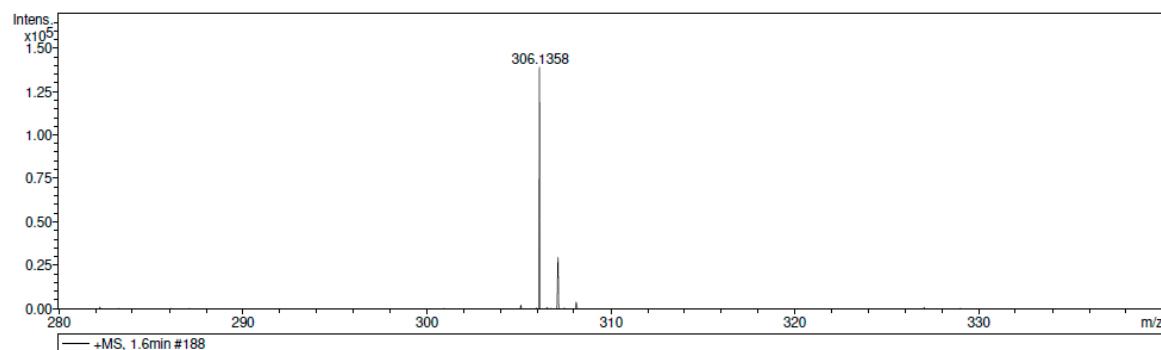
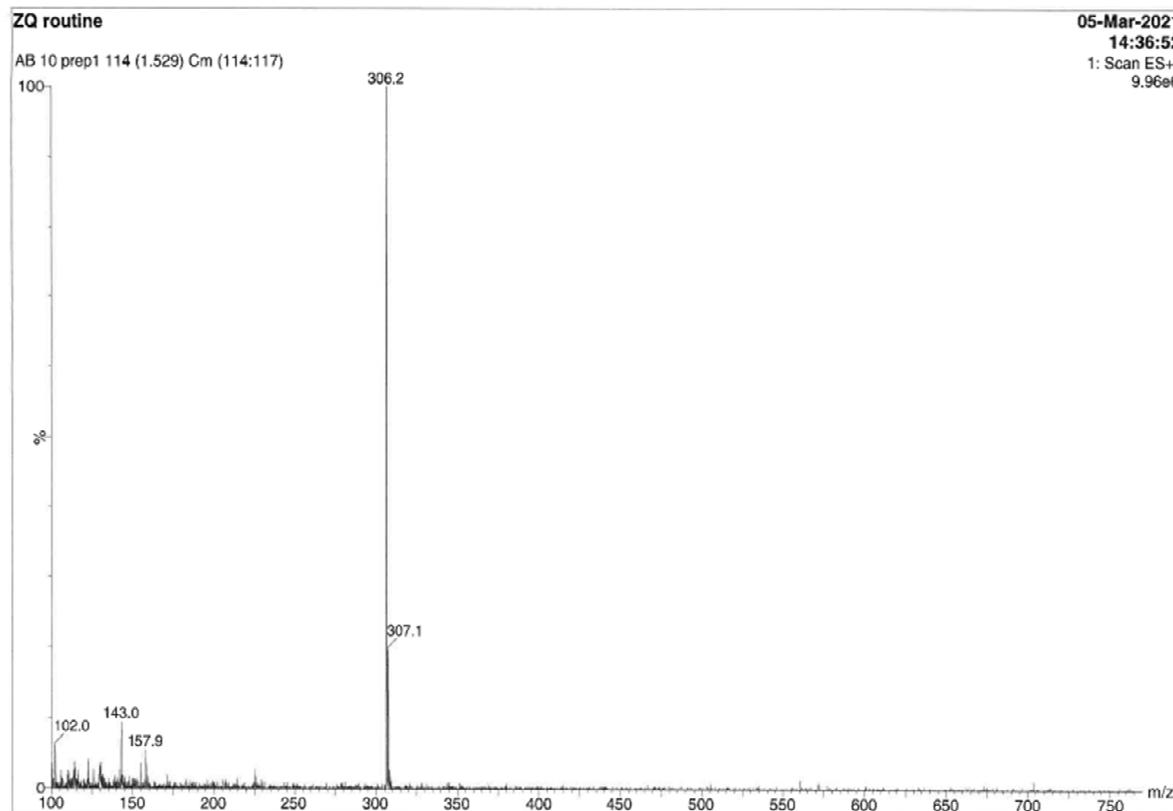
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
336.1449	1	C ₁₈ H ₁₈ N ₅ O ₂	336.1455	-1.9	8.2	1	100.00	12.5	even	ok
	2	C ₁₇ H ₂₂ N ₆	336.1442	-2.1	20.6	2	74.52	7.5	even	ok



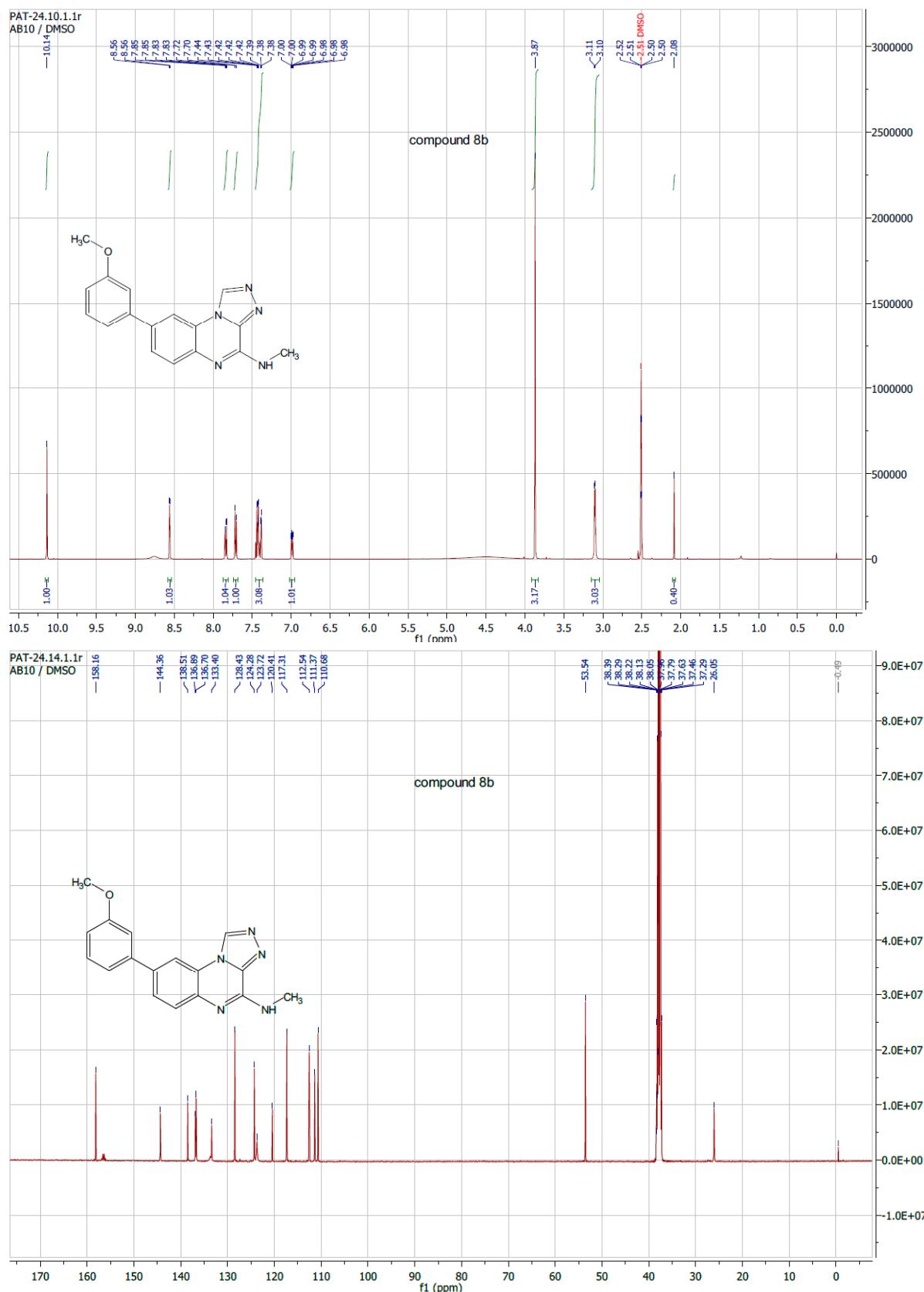


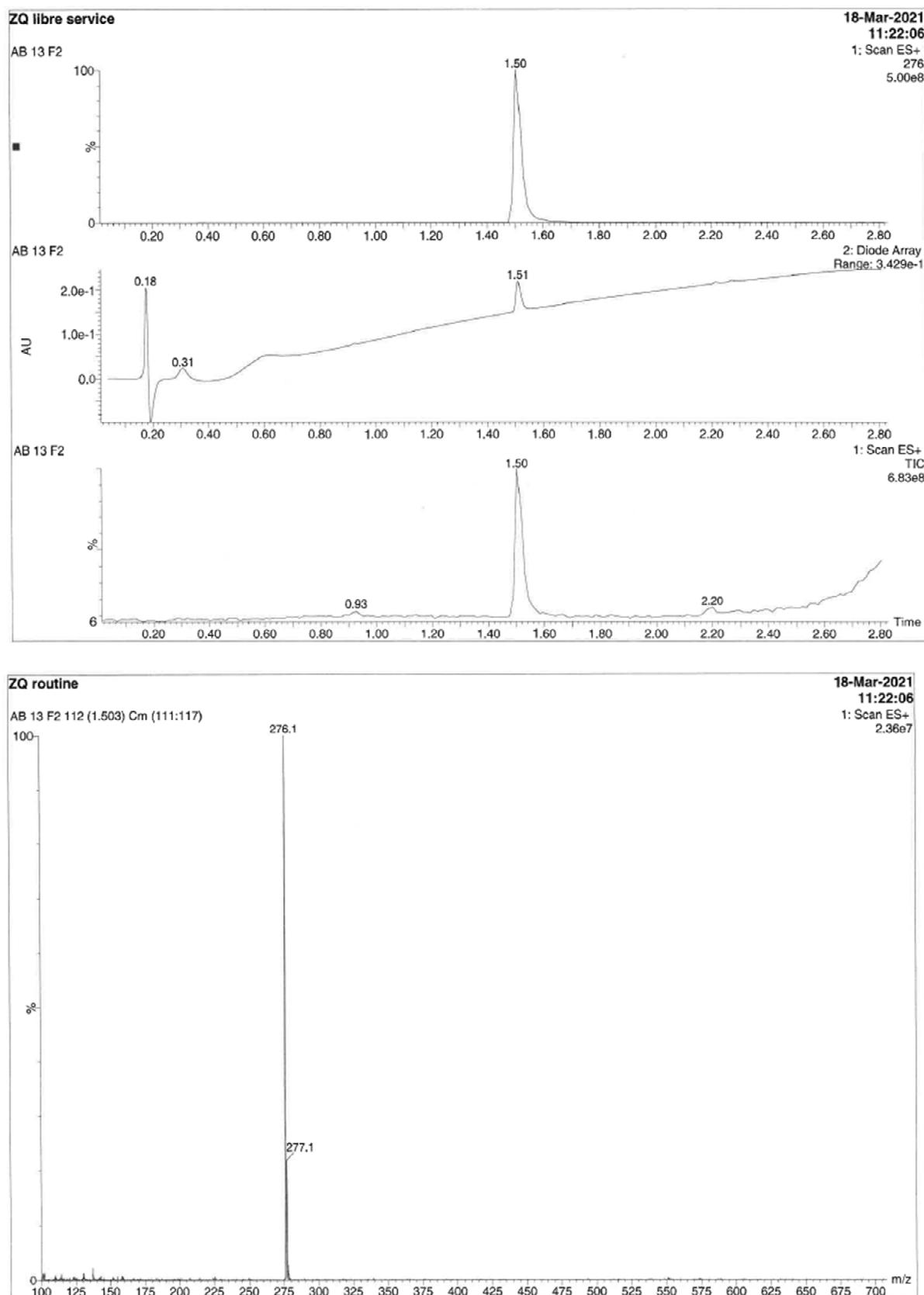
S4. [8-(3-Methoxy-phenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl]-methyl-amine (**8b**).

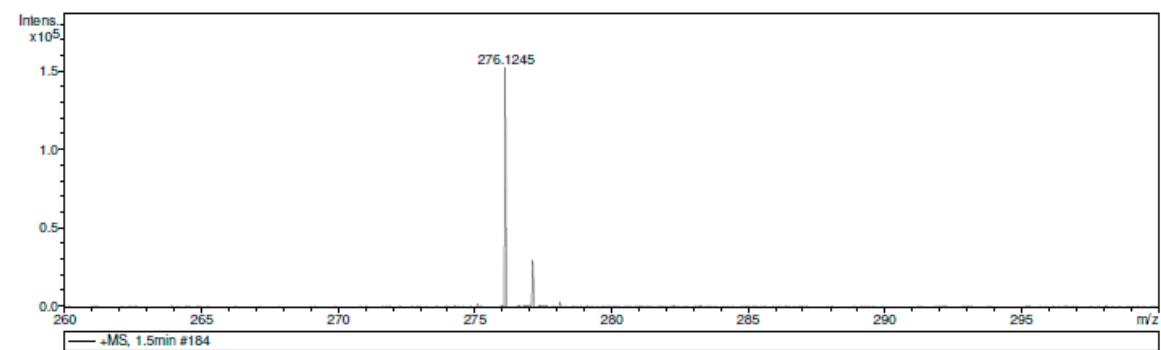




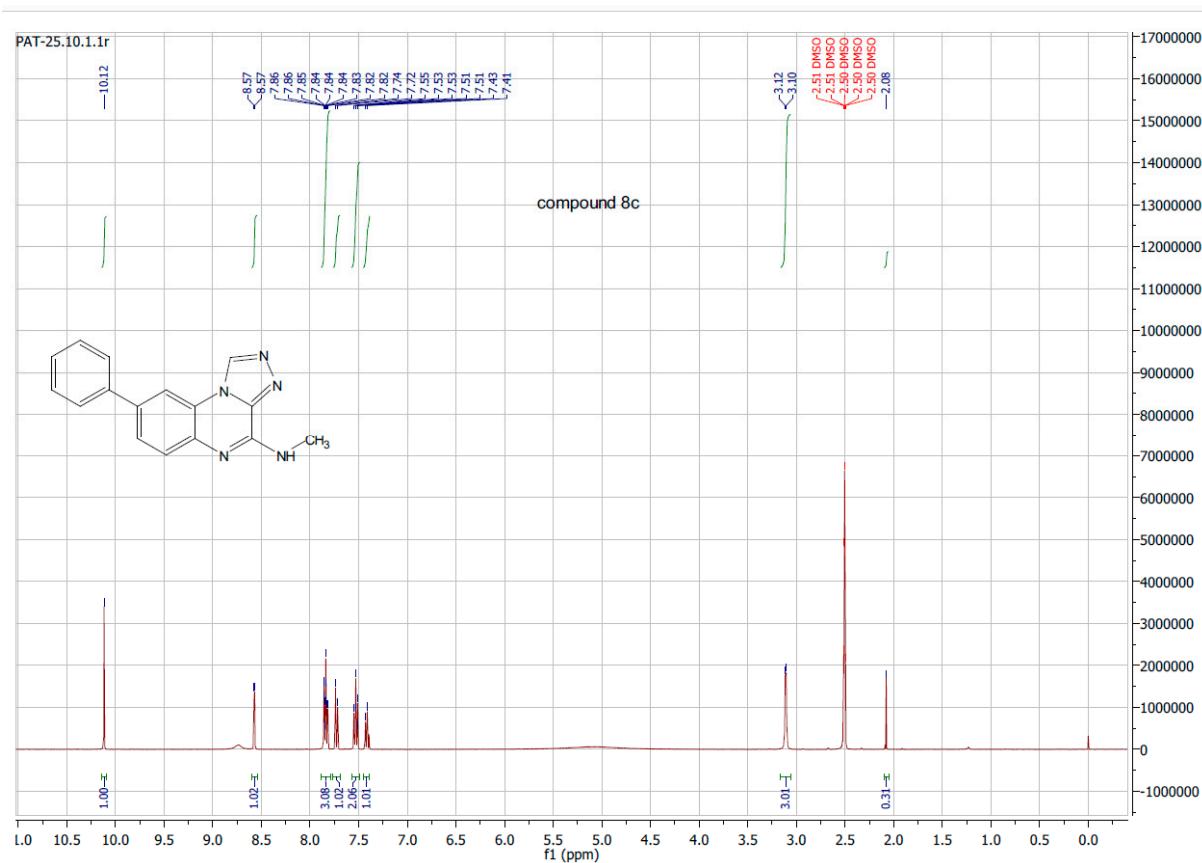
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
306.1358	1	C ₁₇ H ₁₆ N ₅ O	306.1349	-2.7	7.6	1	100.00	12.5	even	ok

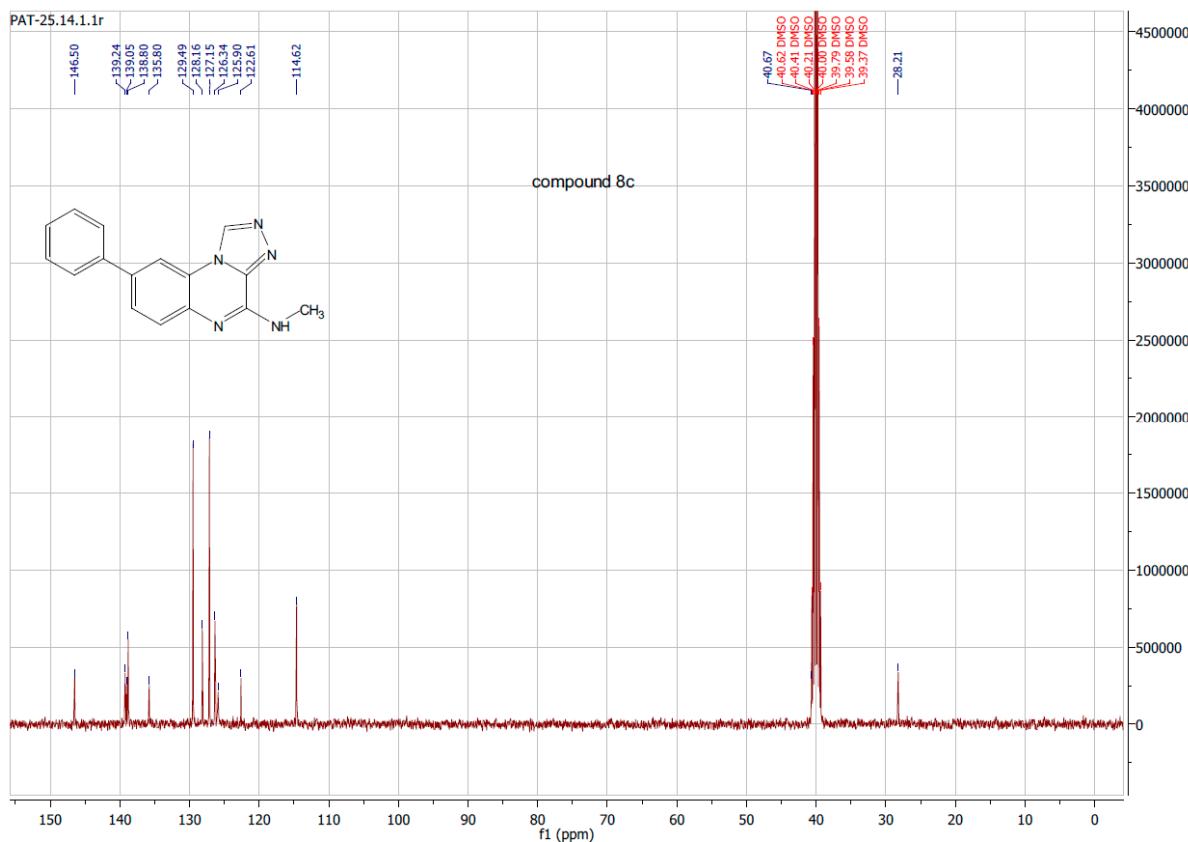


S5. Methyl-(8-phenyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl)-amine (**8c**).

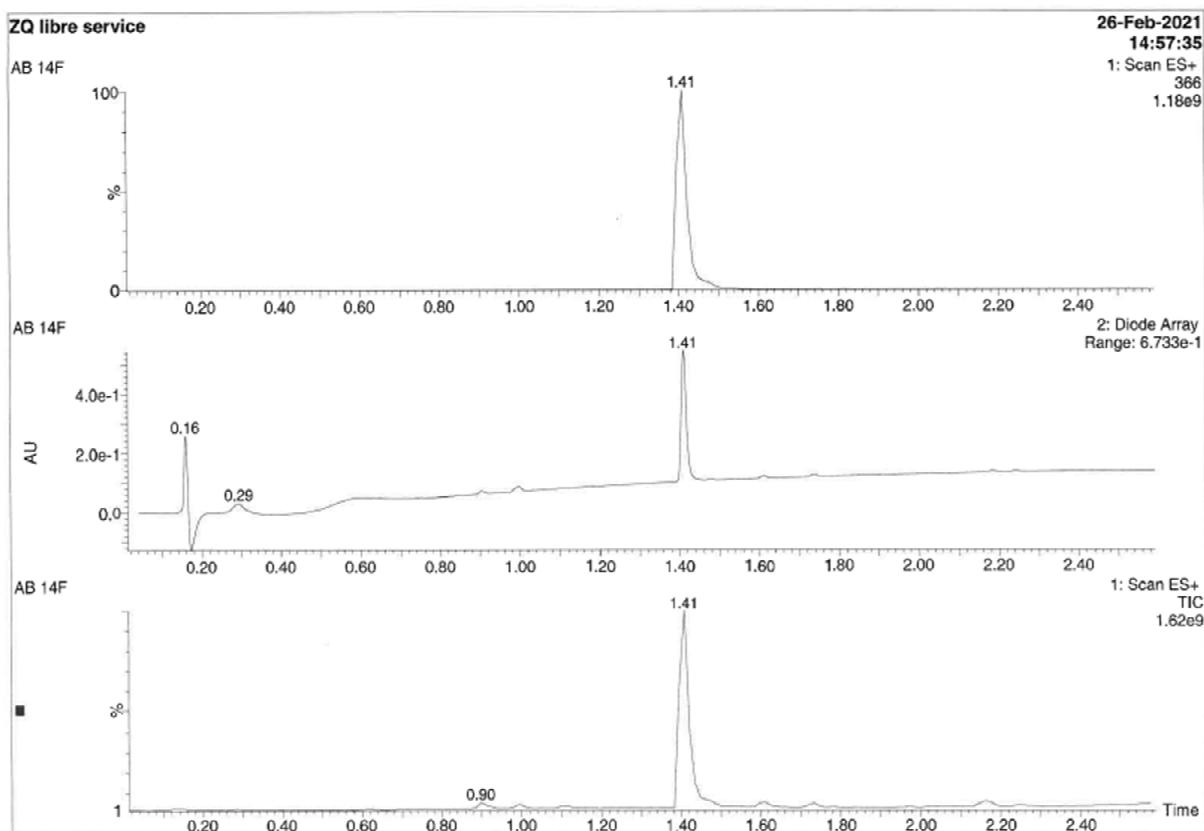


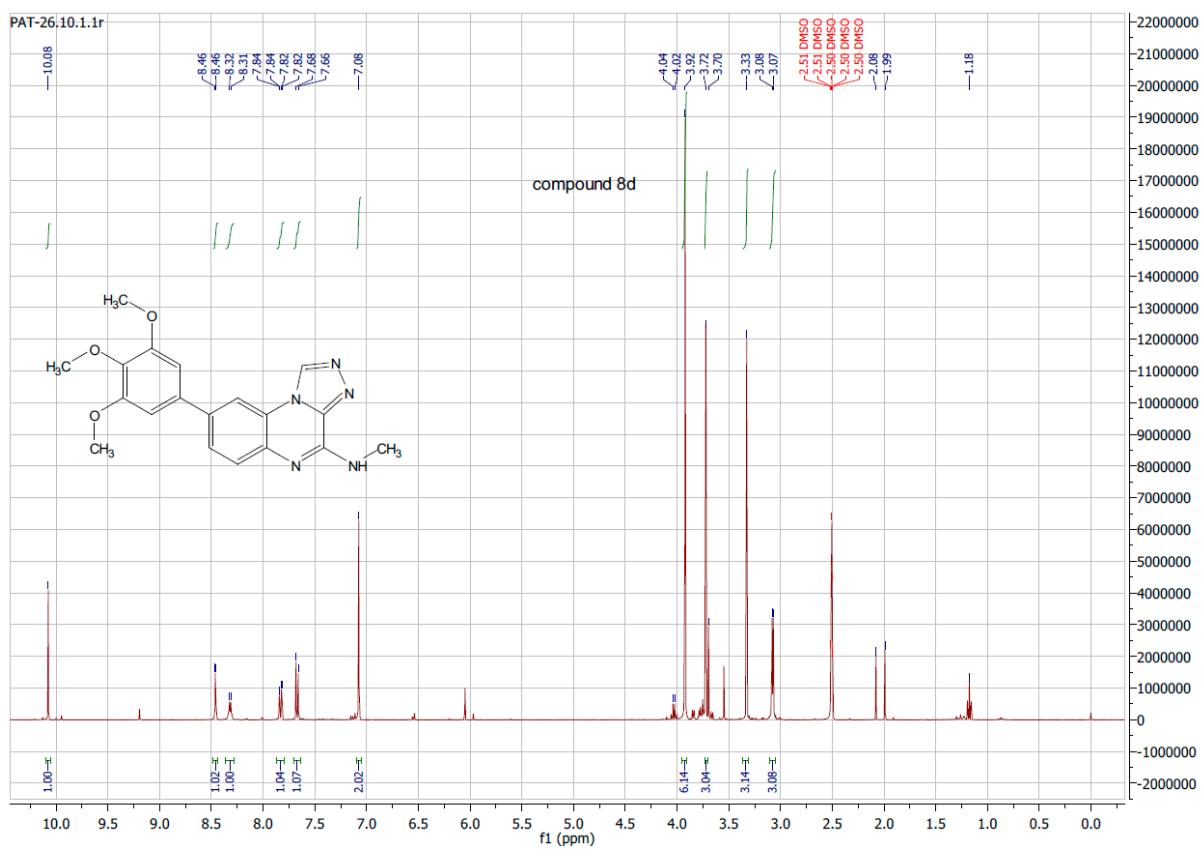
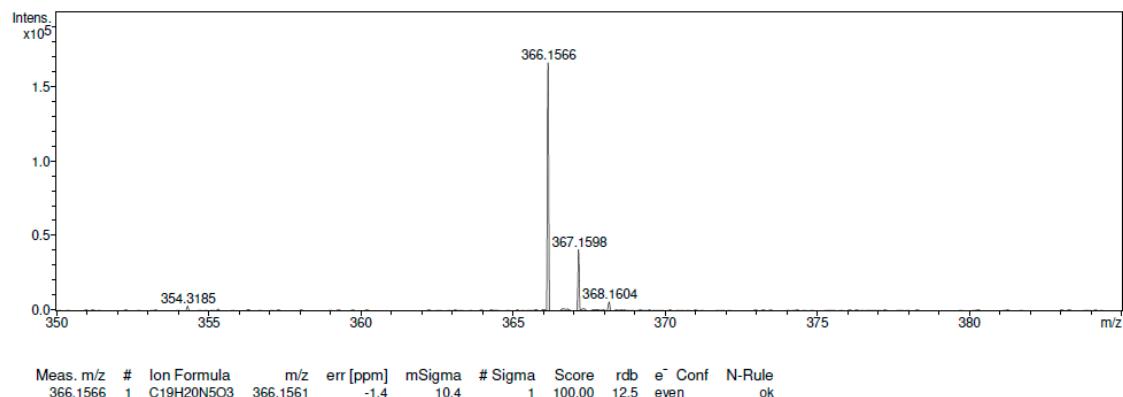
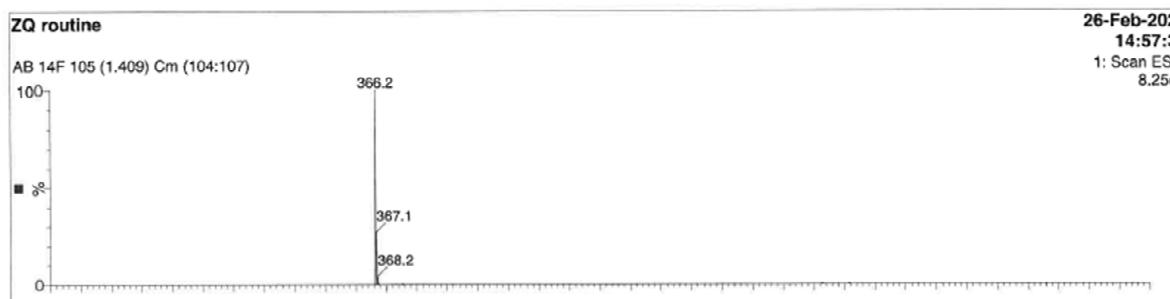
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
276.1245	1	C ₁₆ H ₁₄ N ₅	276.1244	-0.3	1.7	1	100.00	12.5	even	ok

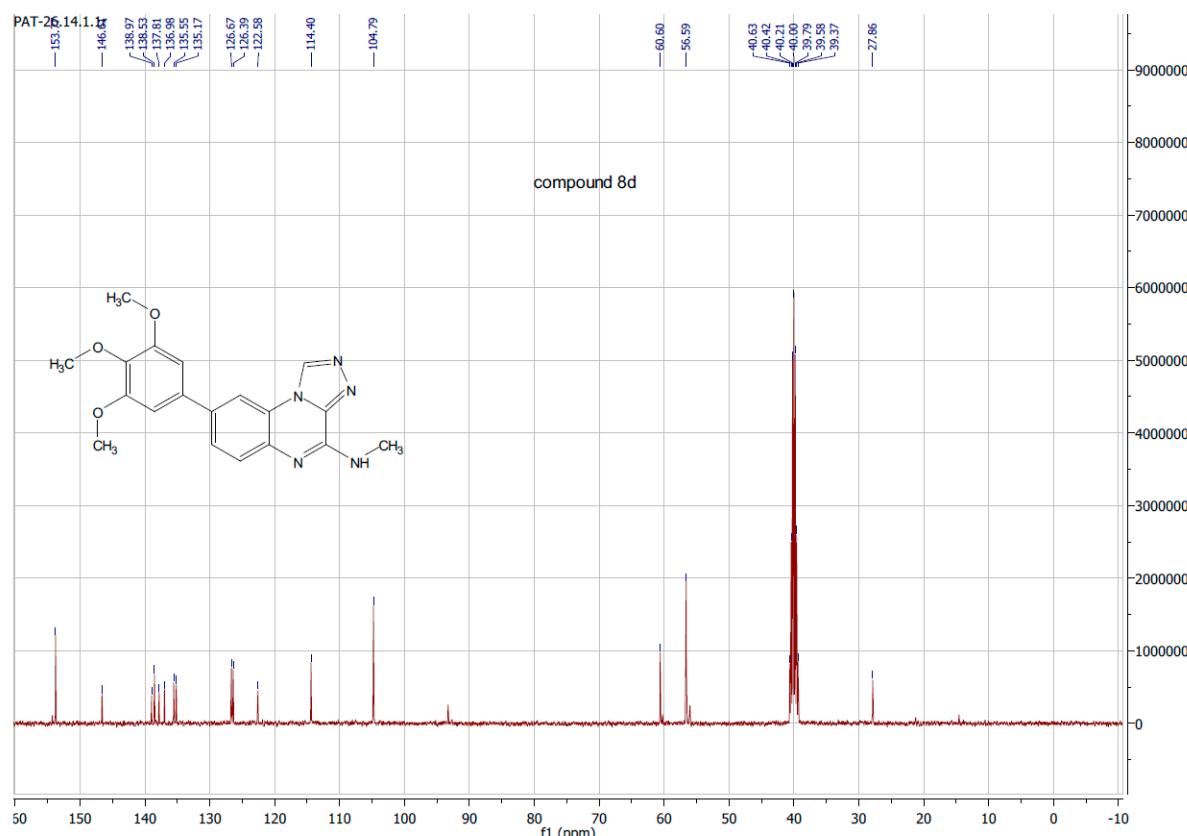




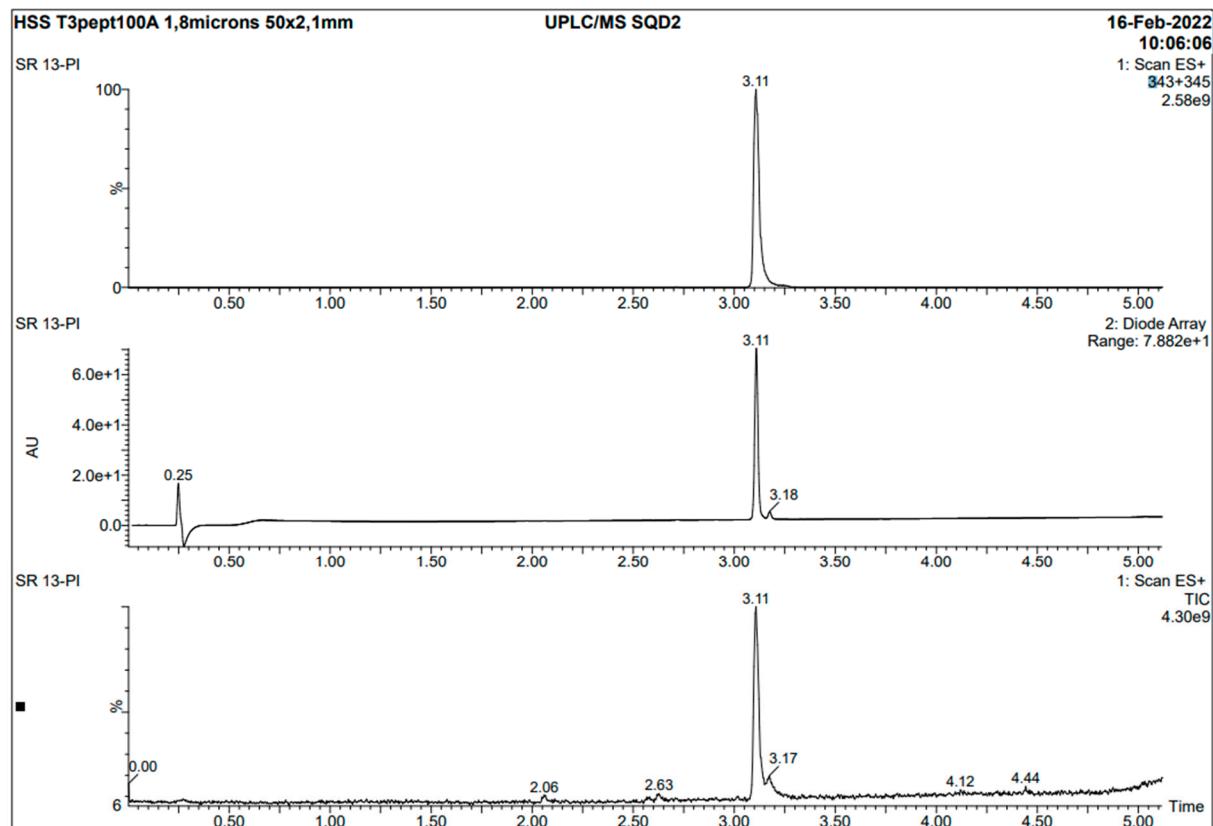
S6. Methyl-[8-(3,4,5-trimethoxy-phenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-yl]-amine (8d).

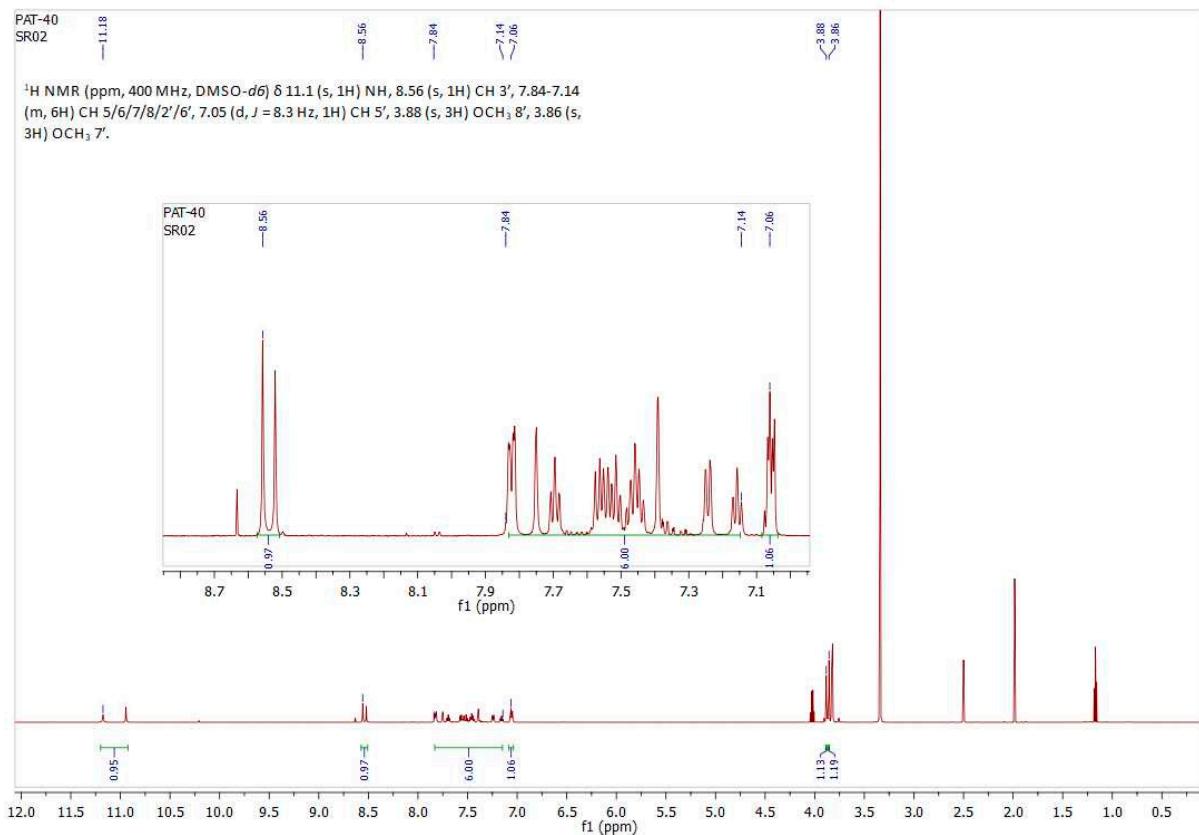
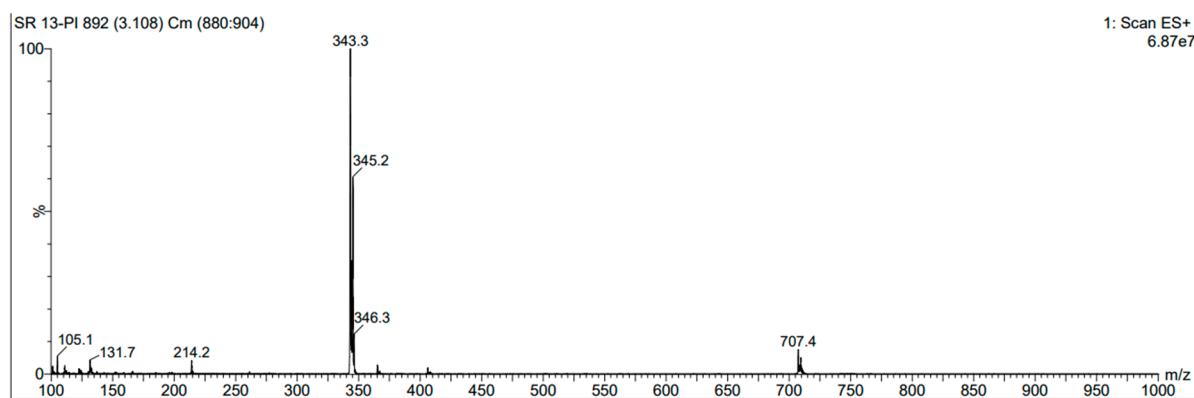


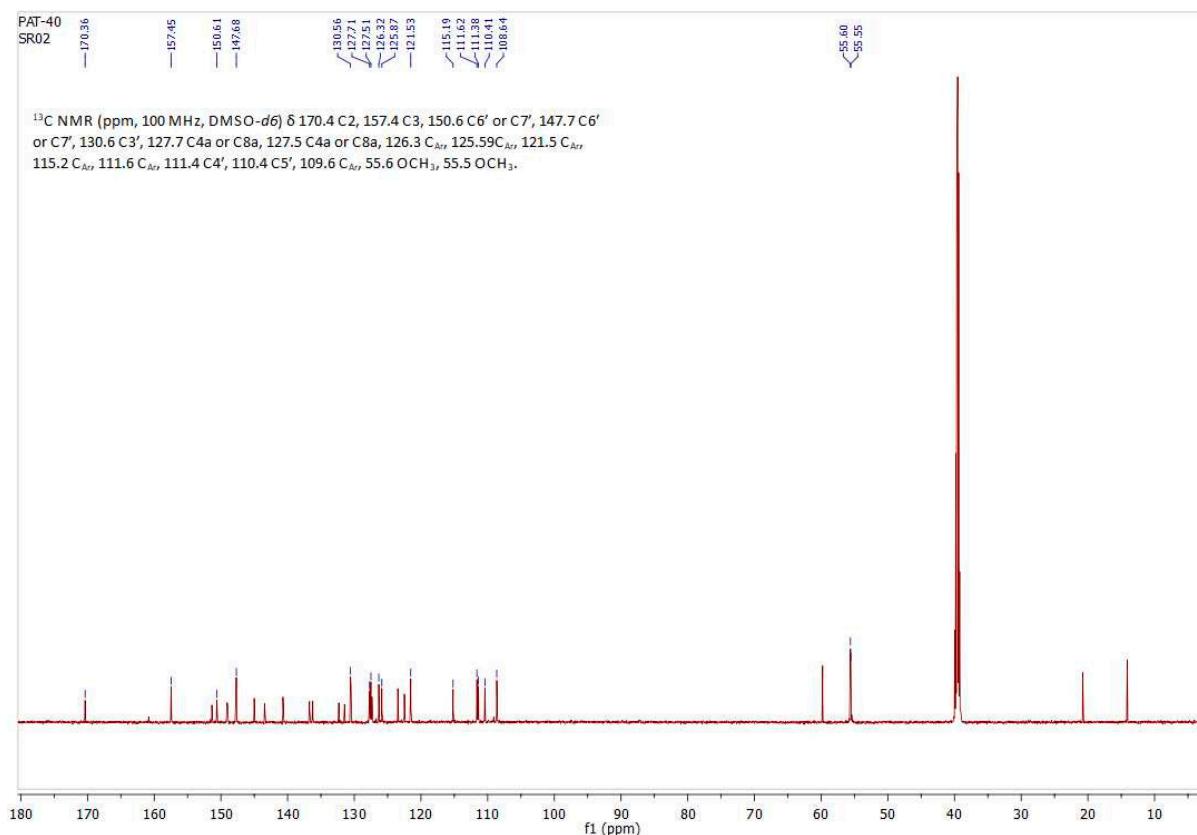




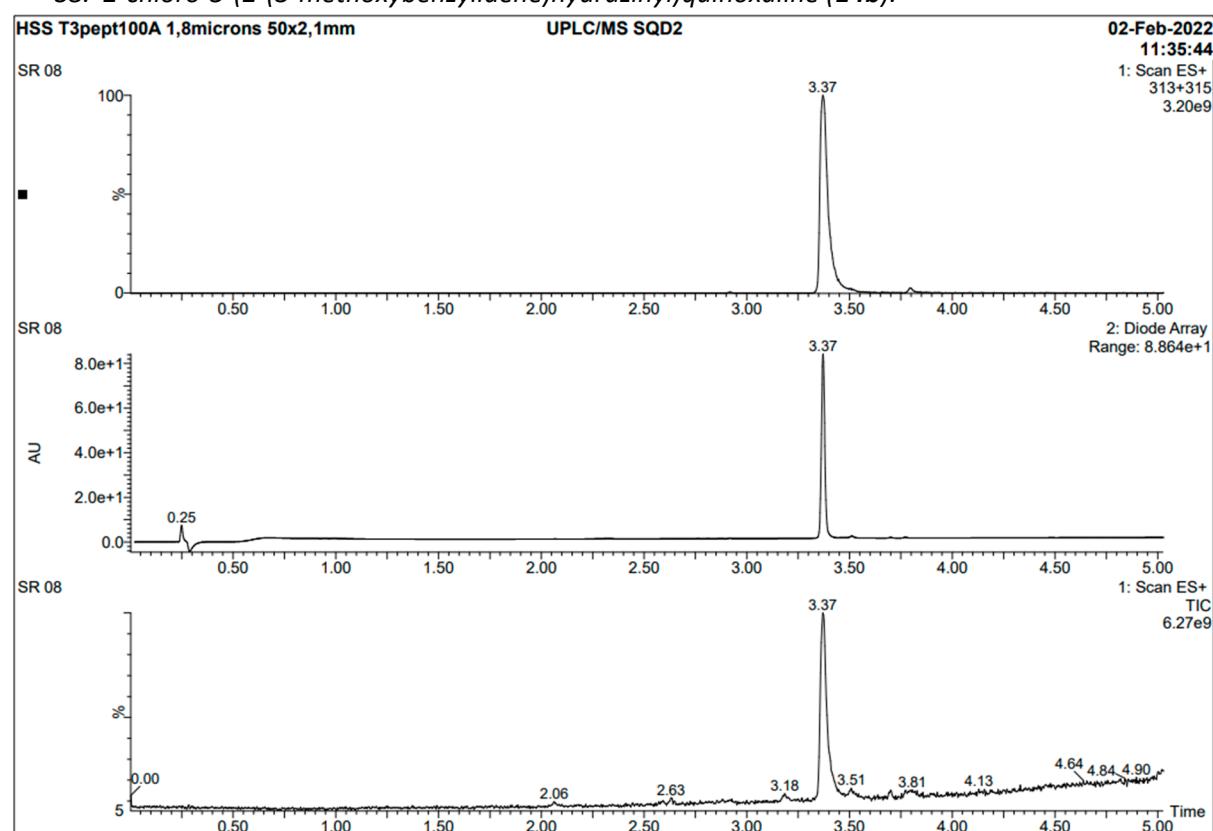
S7. 2-chloro-3-(2-(3,4-dimethoxybenzylidene)hydrazinyl)quinoxaline (**14a**).

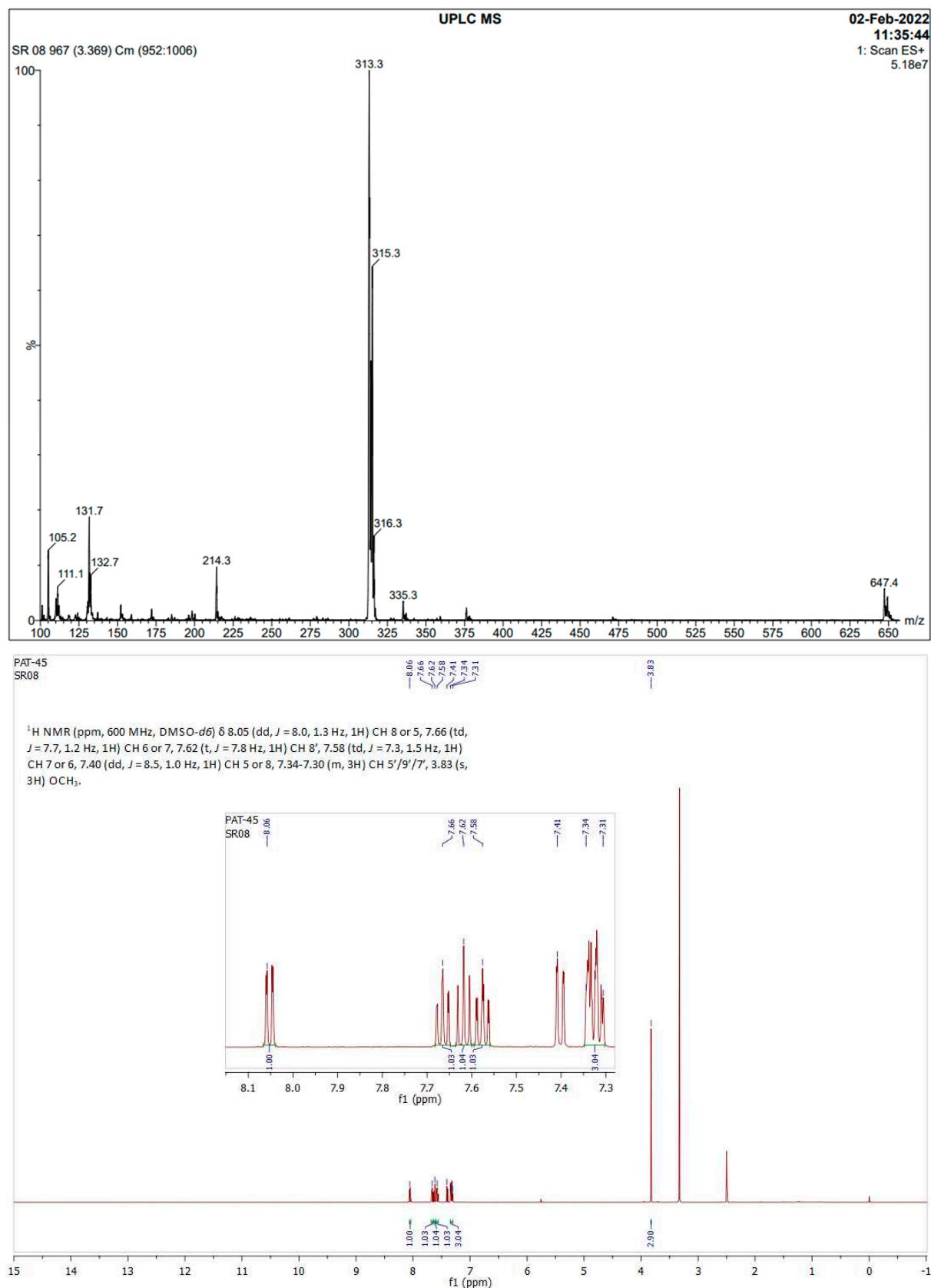


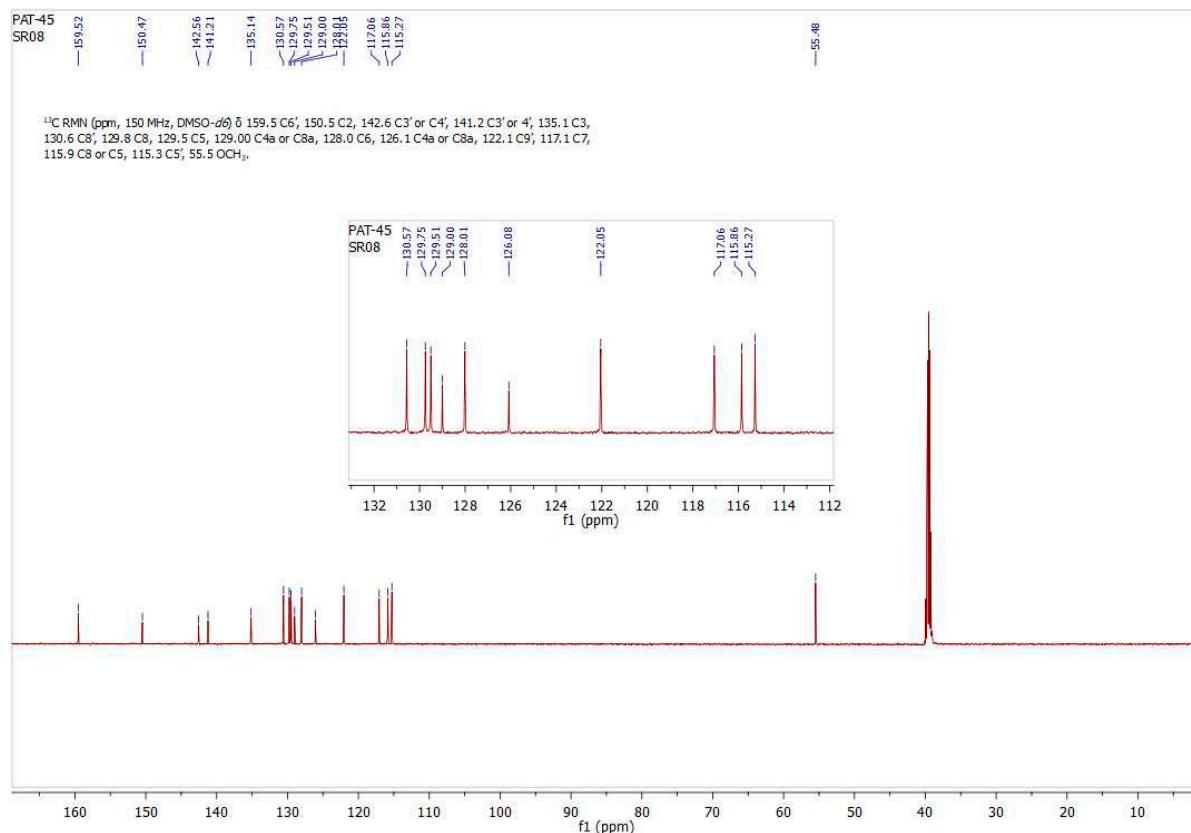




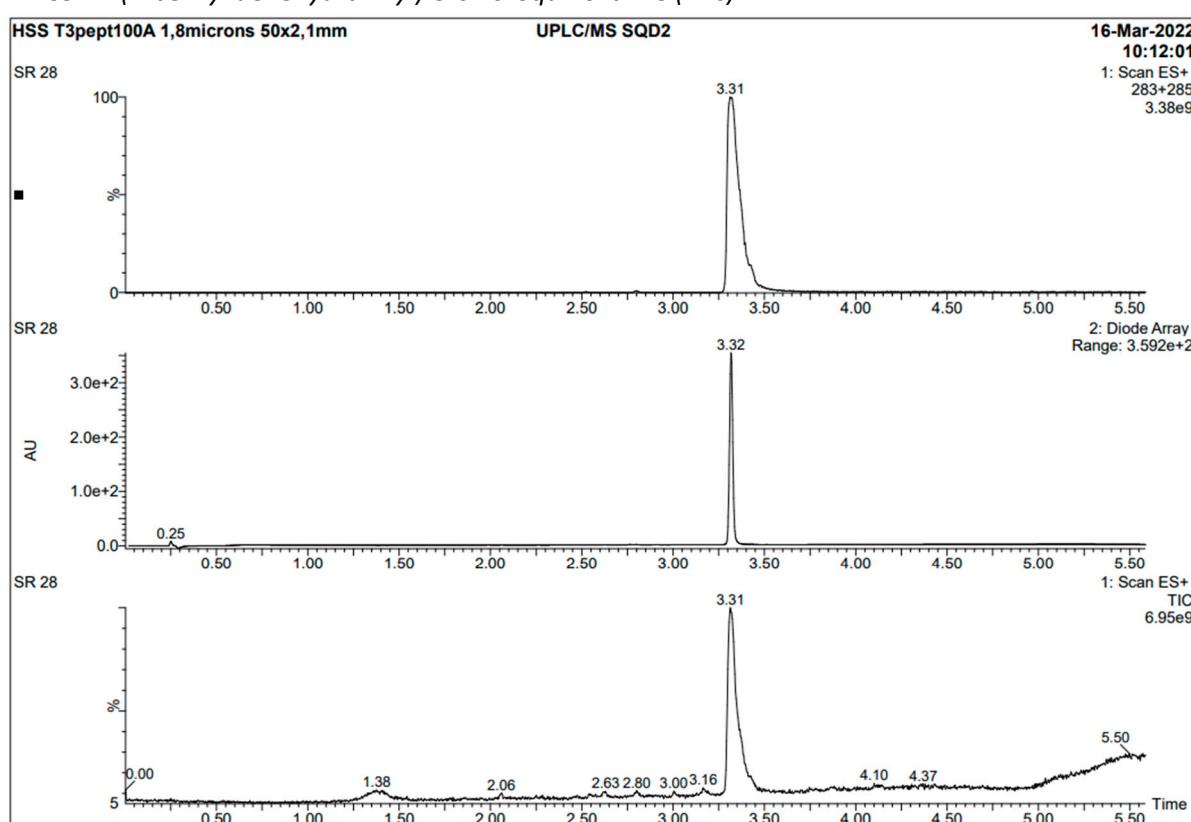
S8. 2-chloro-3-(2-(3-methoxybenzylidene)hydrazinyl)quinoxaline (**14b**).

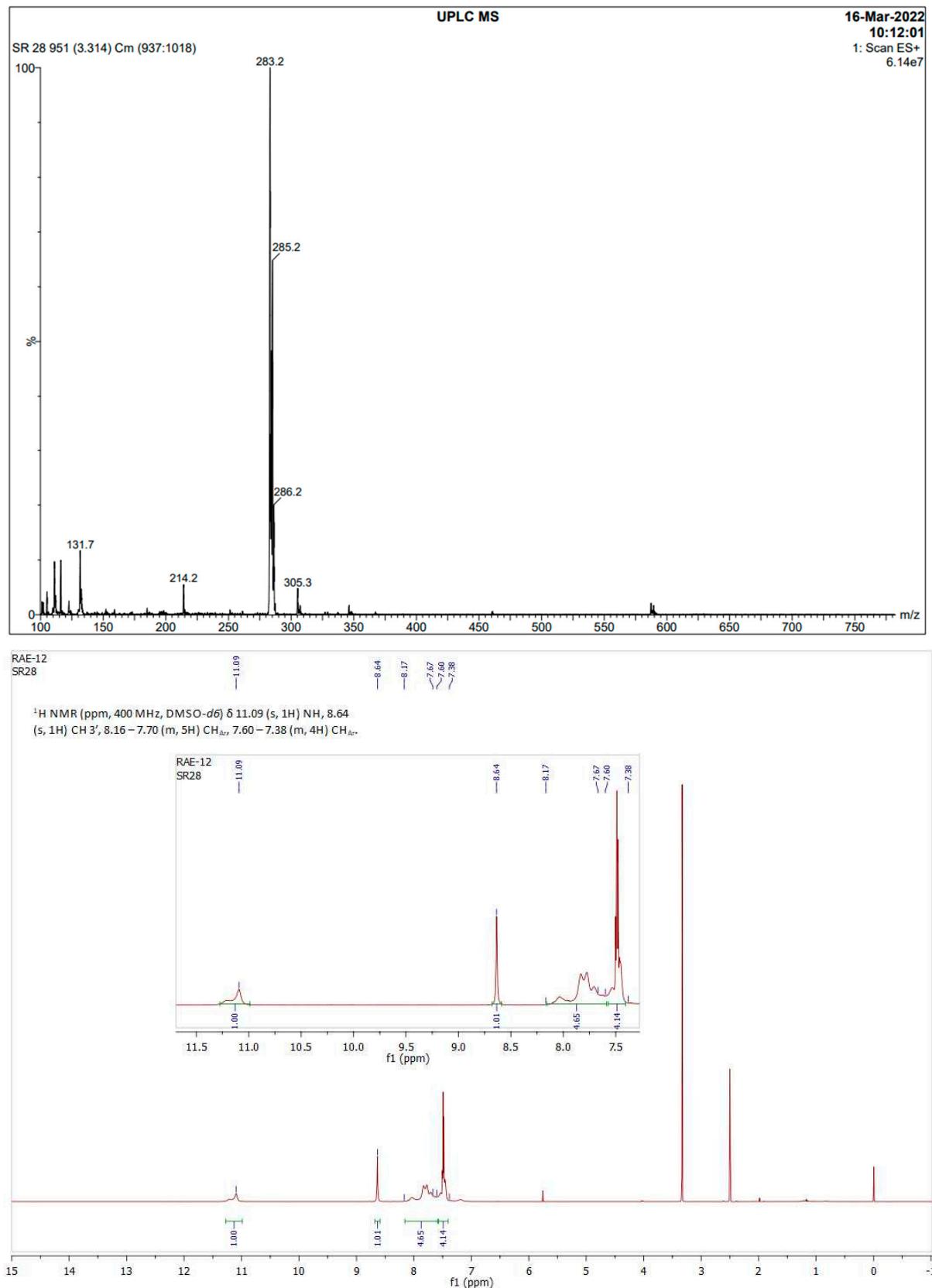


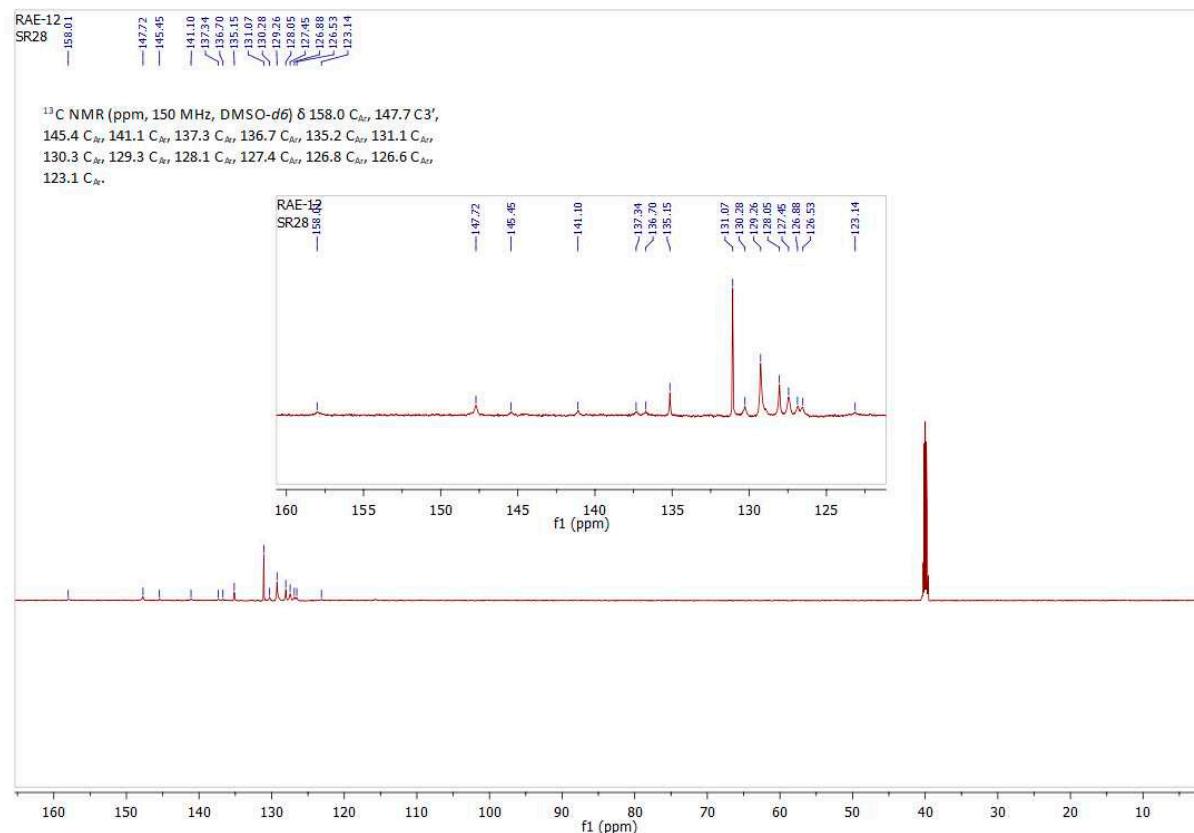




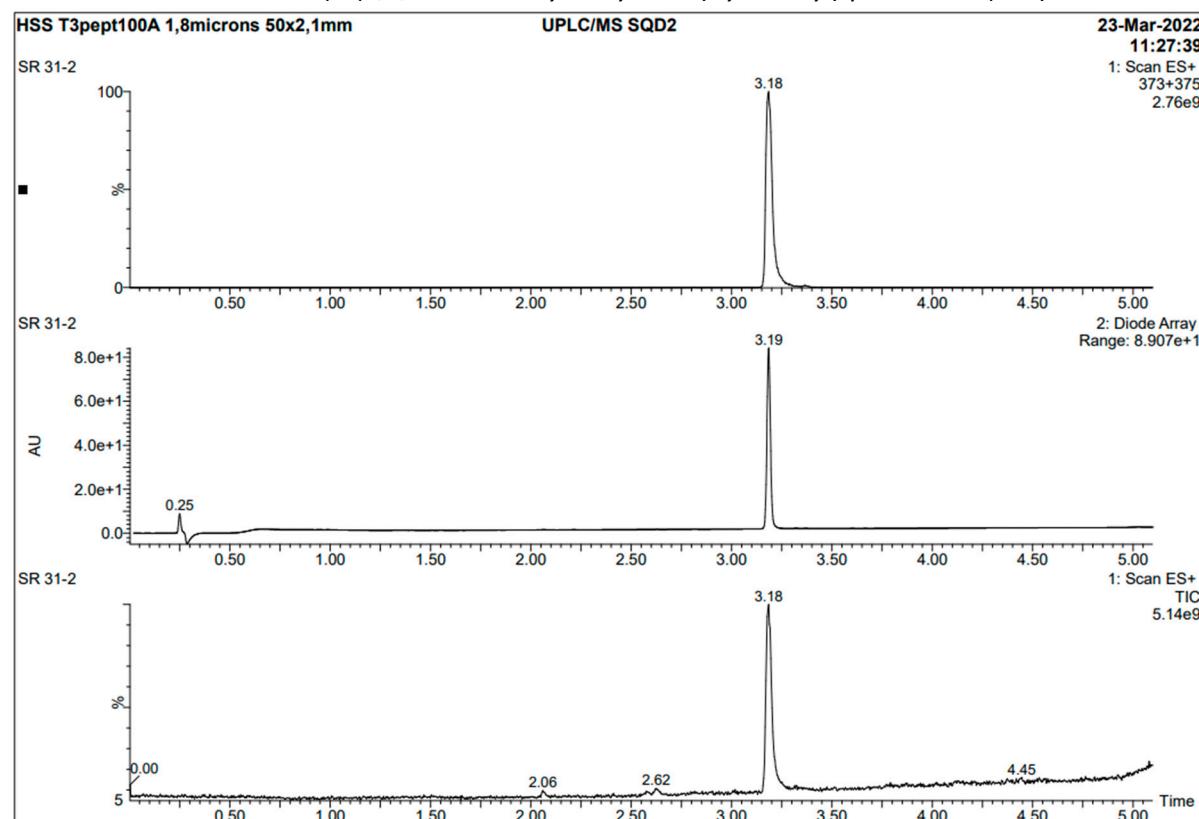
S9. 2-(2-benzylidenehydrazinyl)-3-chloroquinoxaline (**14c**).

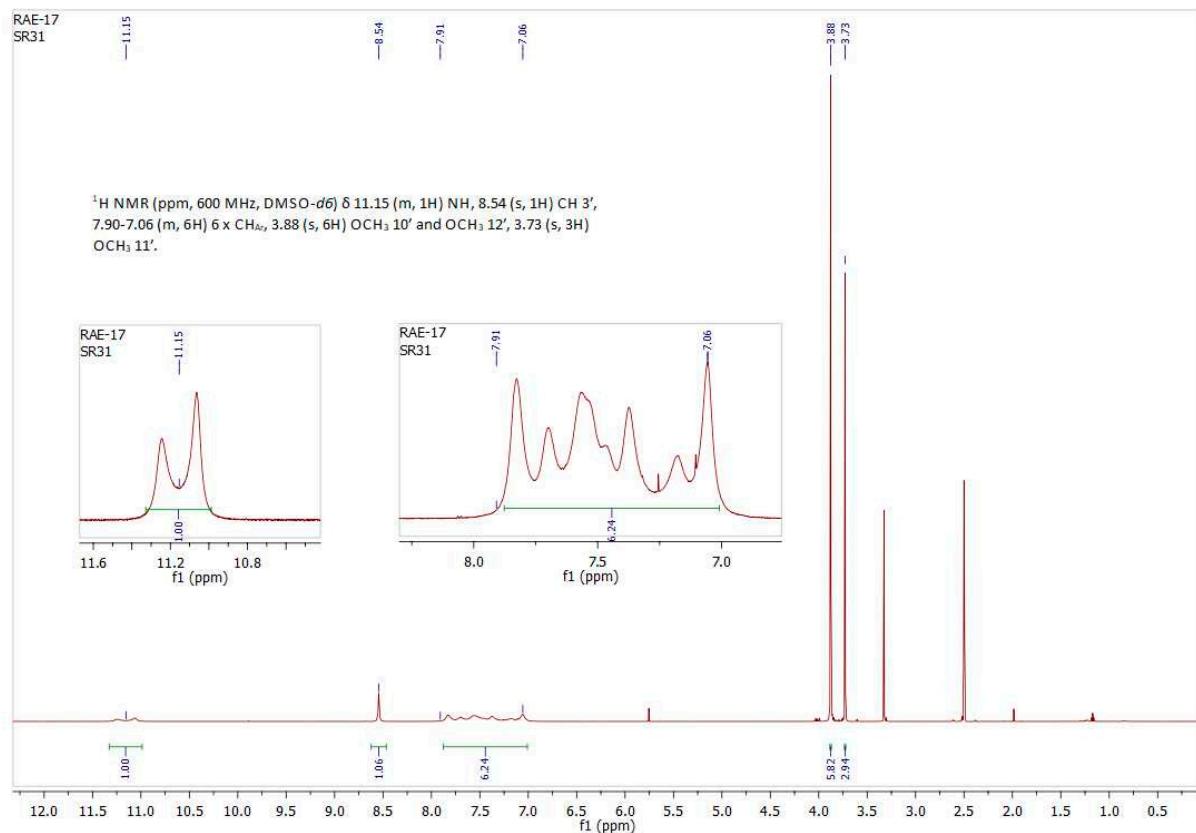
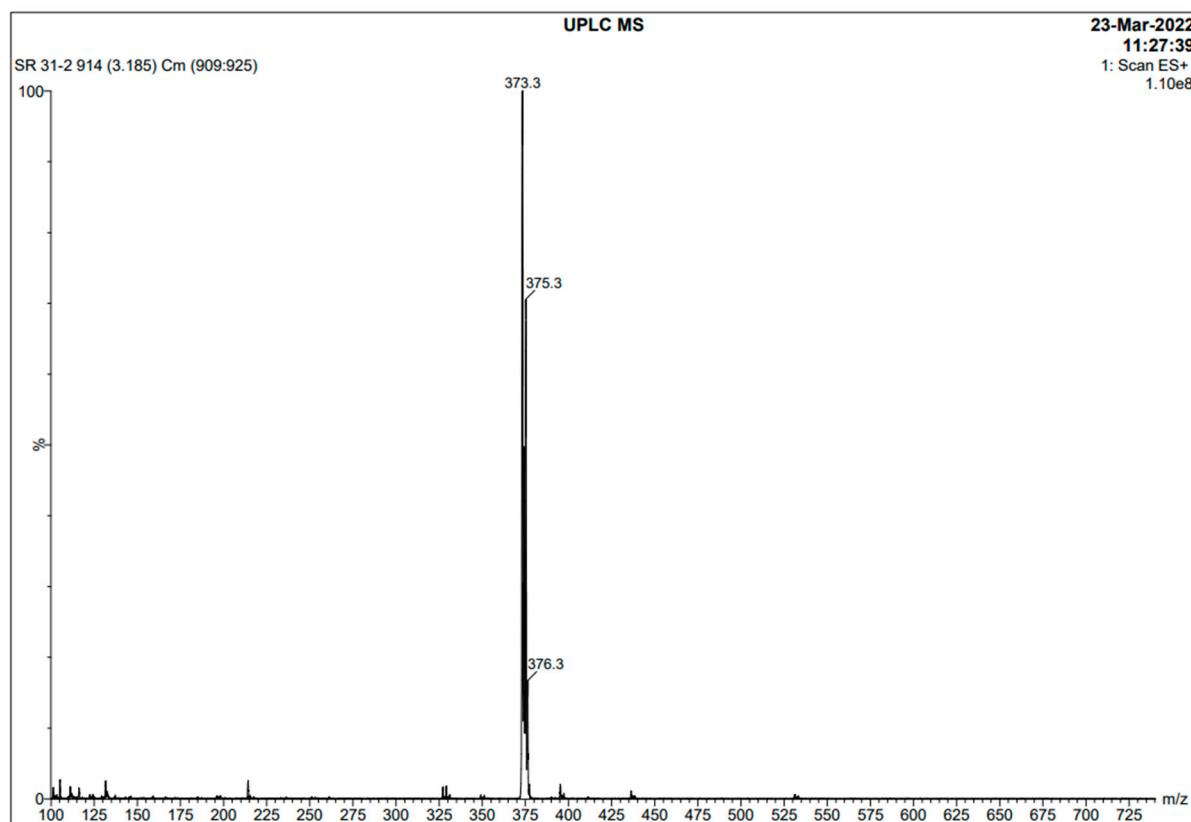


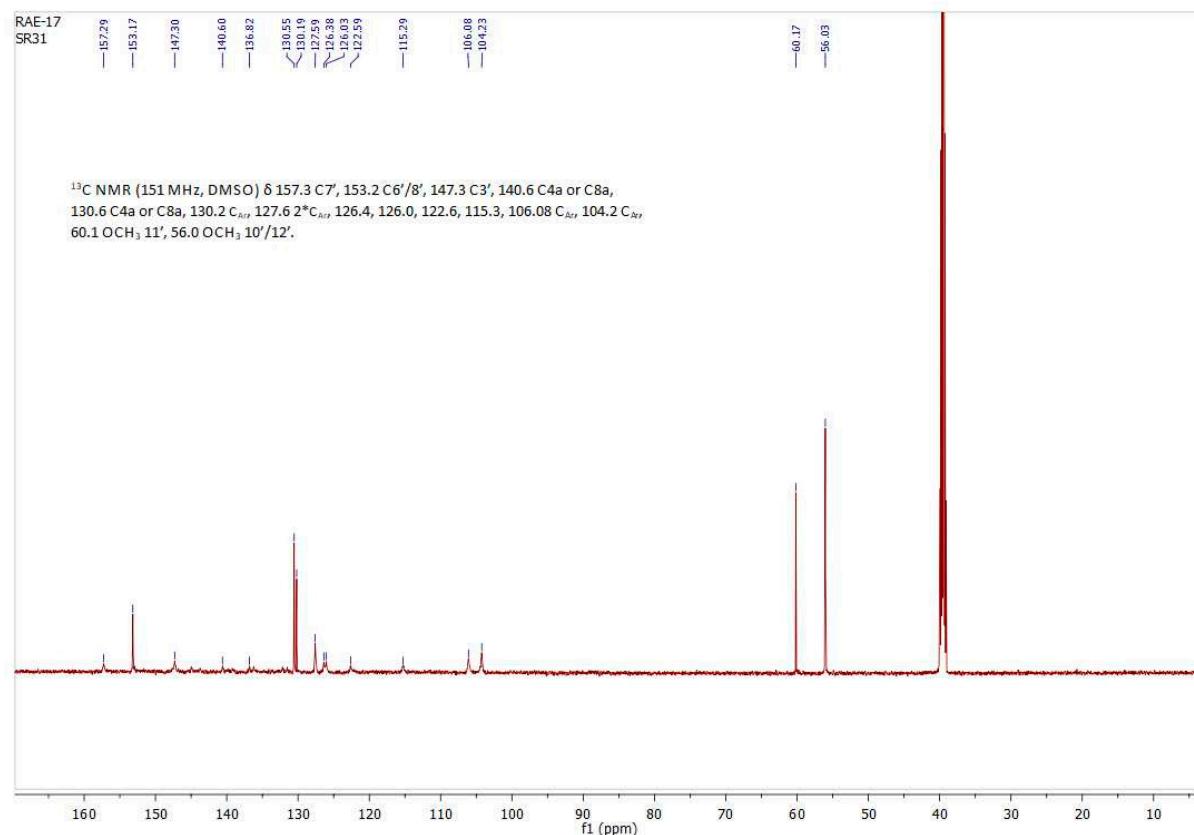




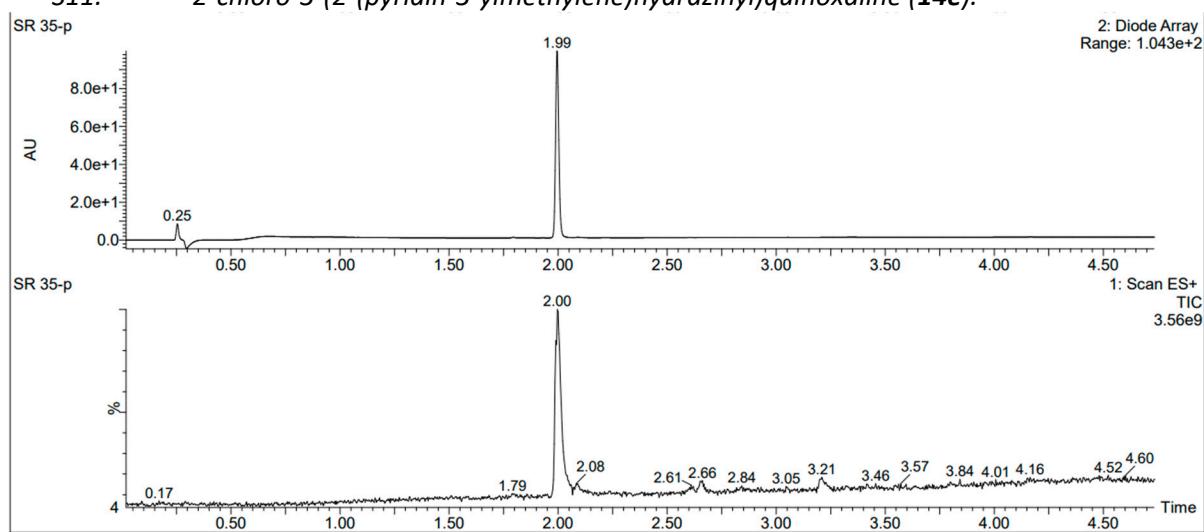
S10. 2-chloro-3-(2-(3,4,5-trimethoxybenzylidene)hydrazinyl)quinoxaline (**14d**).

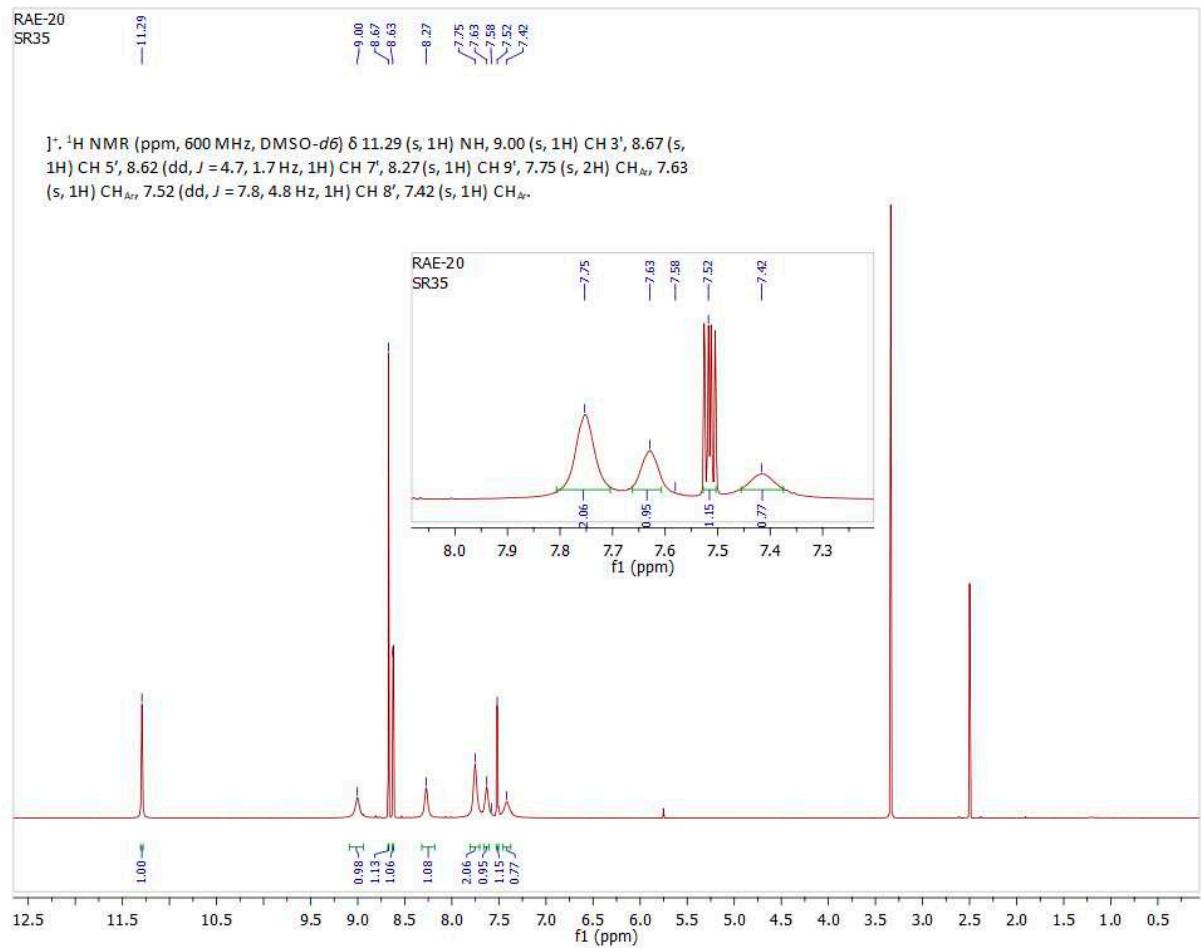
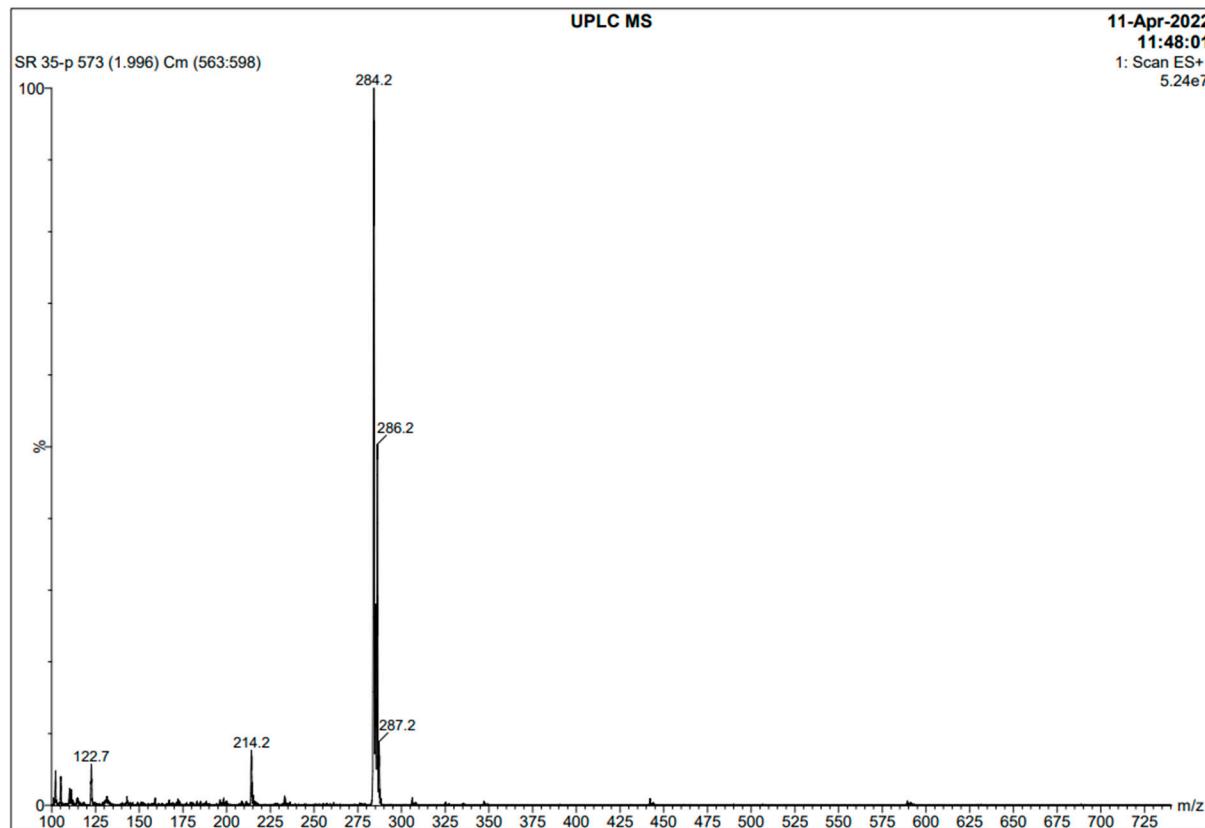


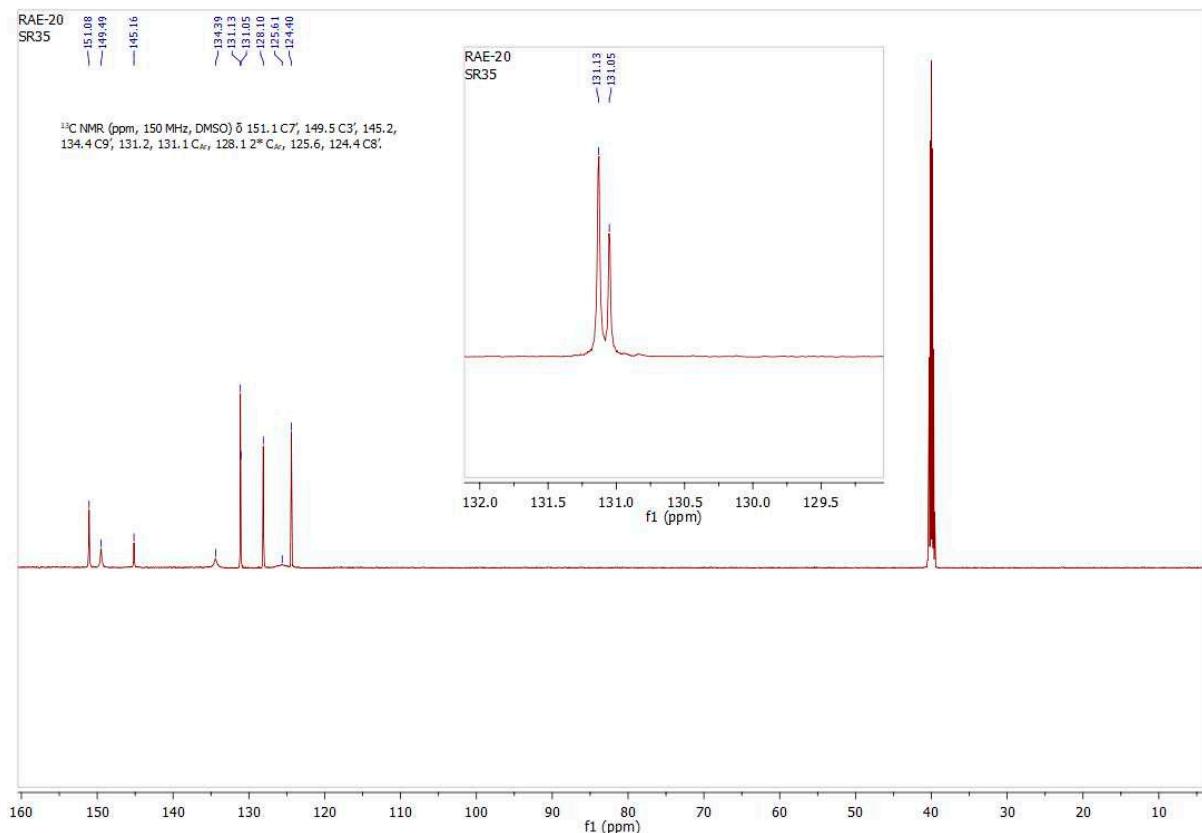




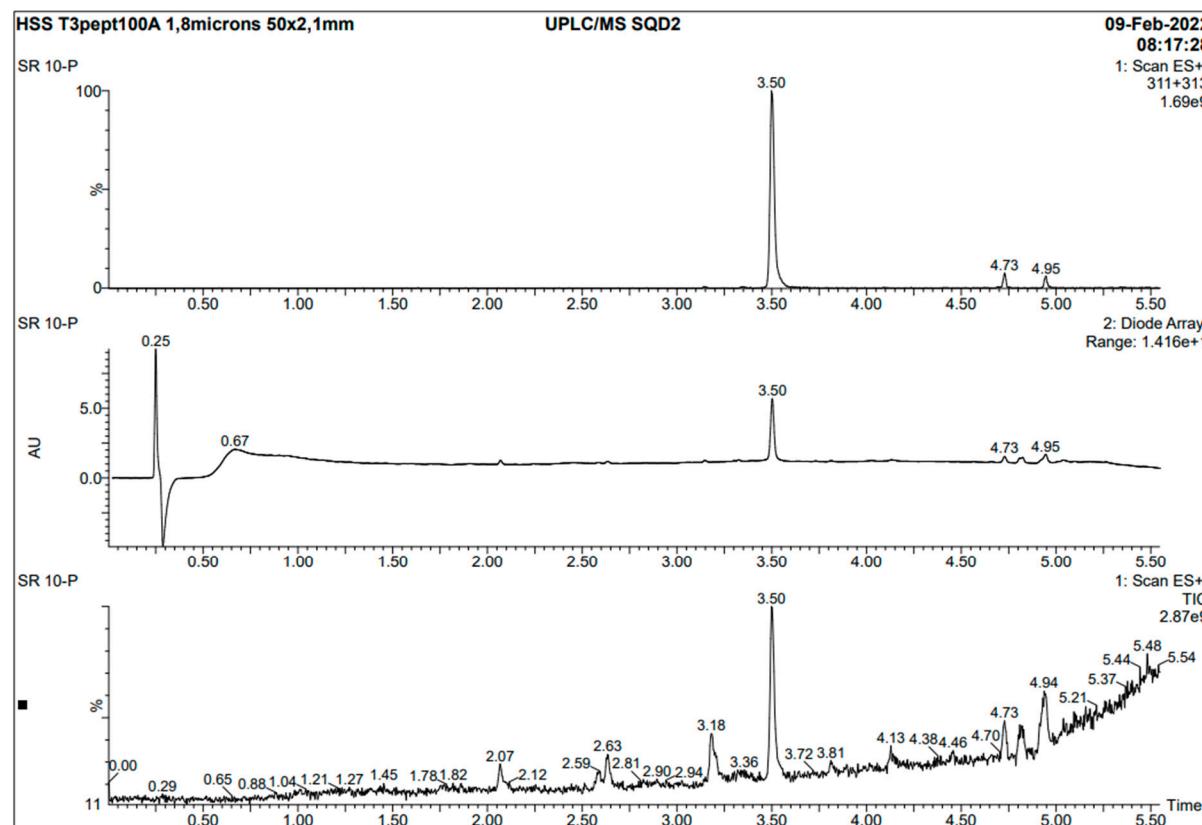
S11.

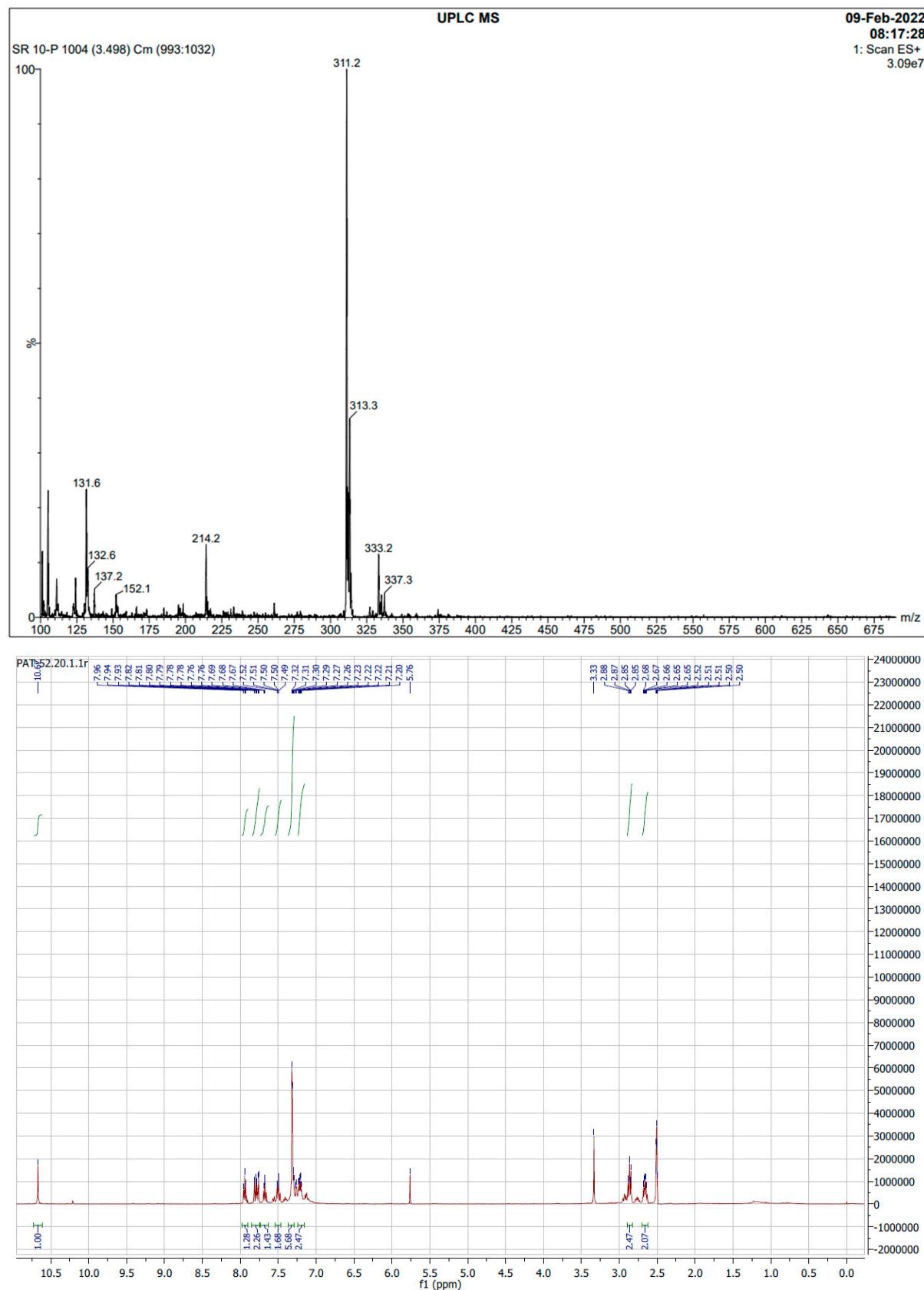
2-chloro-3-(2-(pyridin-3-ylmethylene)hydrazinyl)quinoxaline (14e).

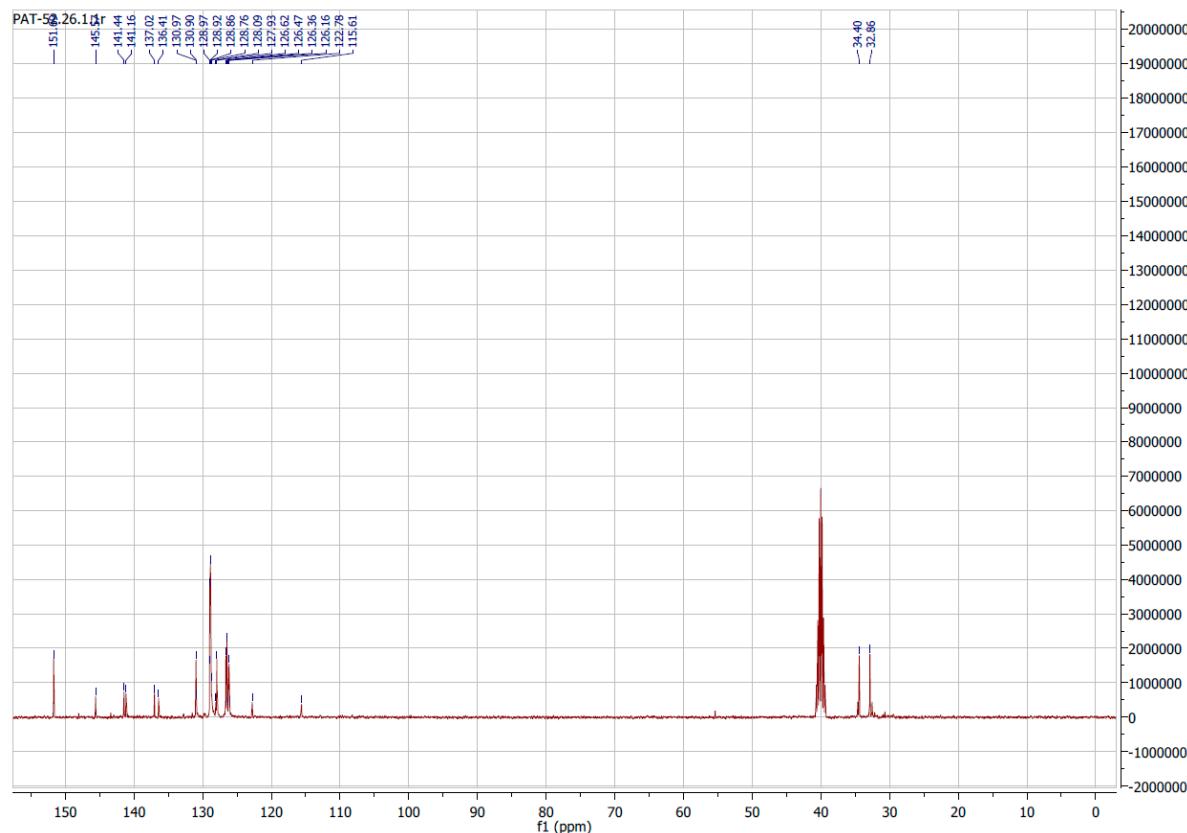




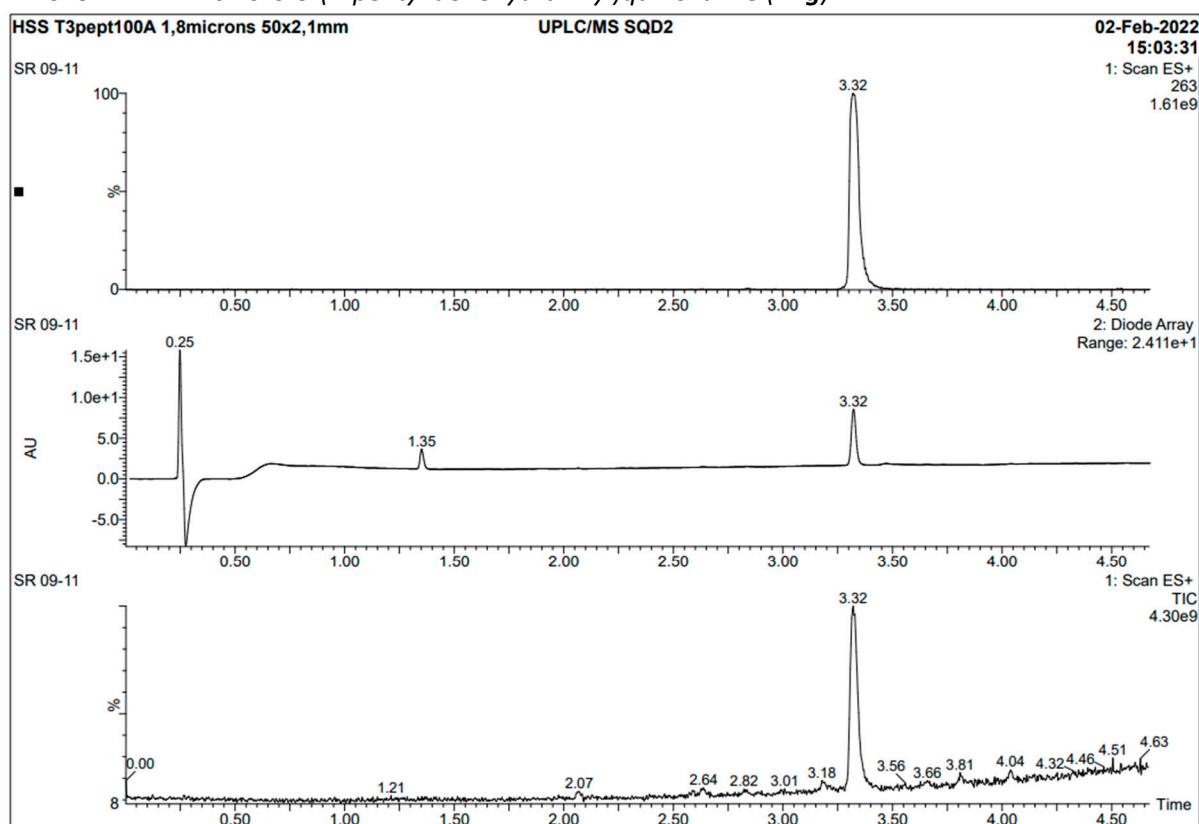
S12. 2-chloro-3-(2-(3-phenylpropylidene)hydrazinyl)quinoxaline (**14f**).

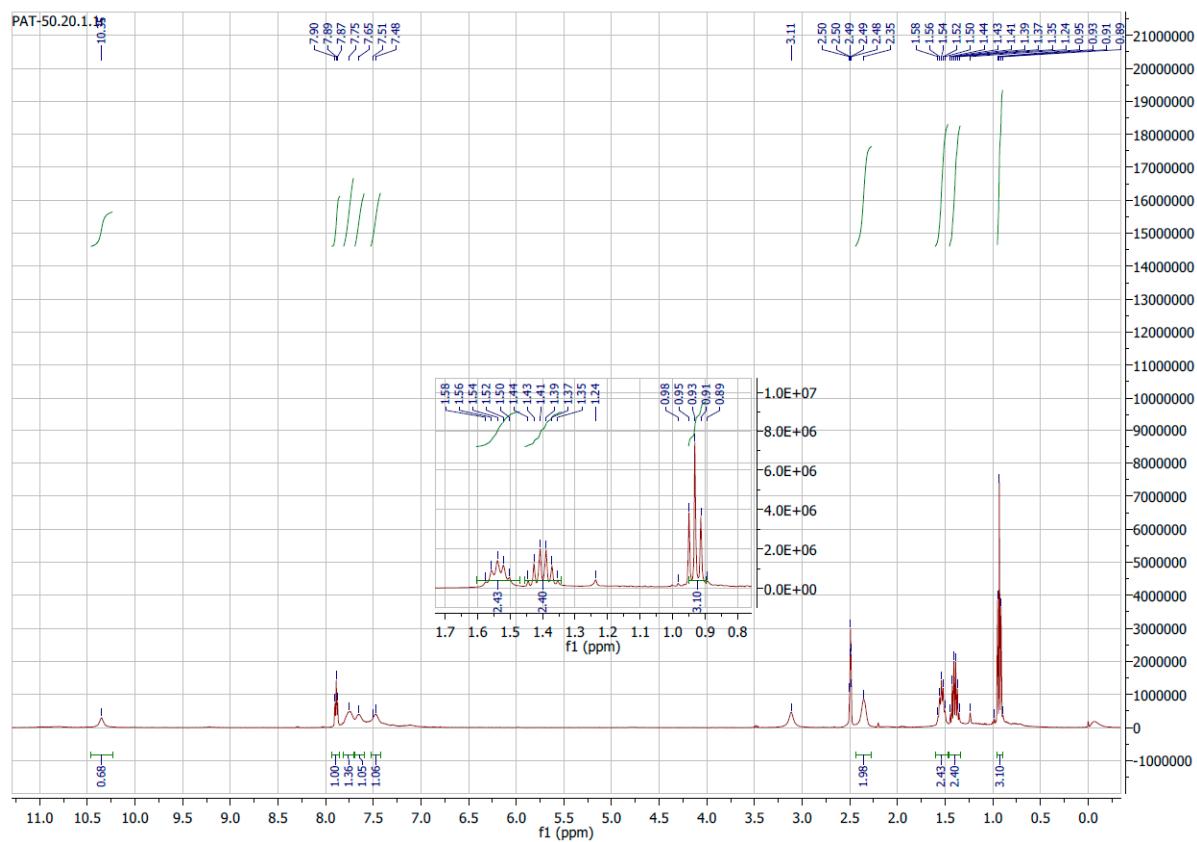
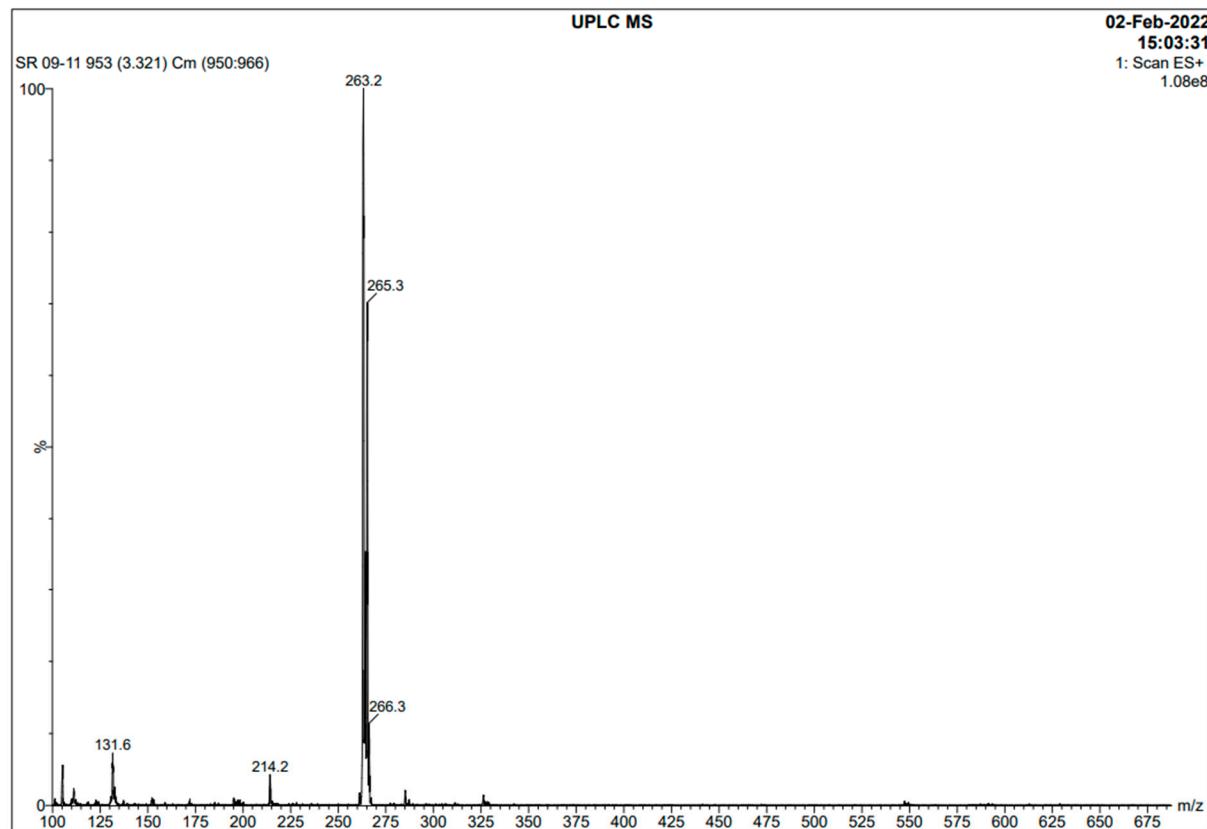


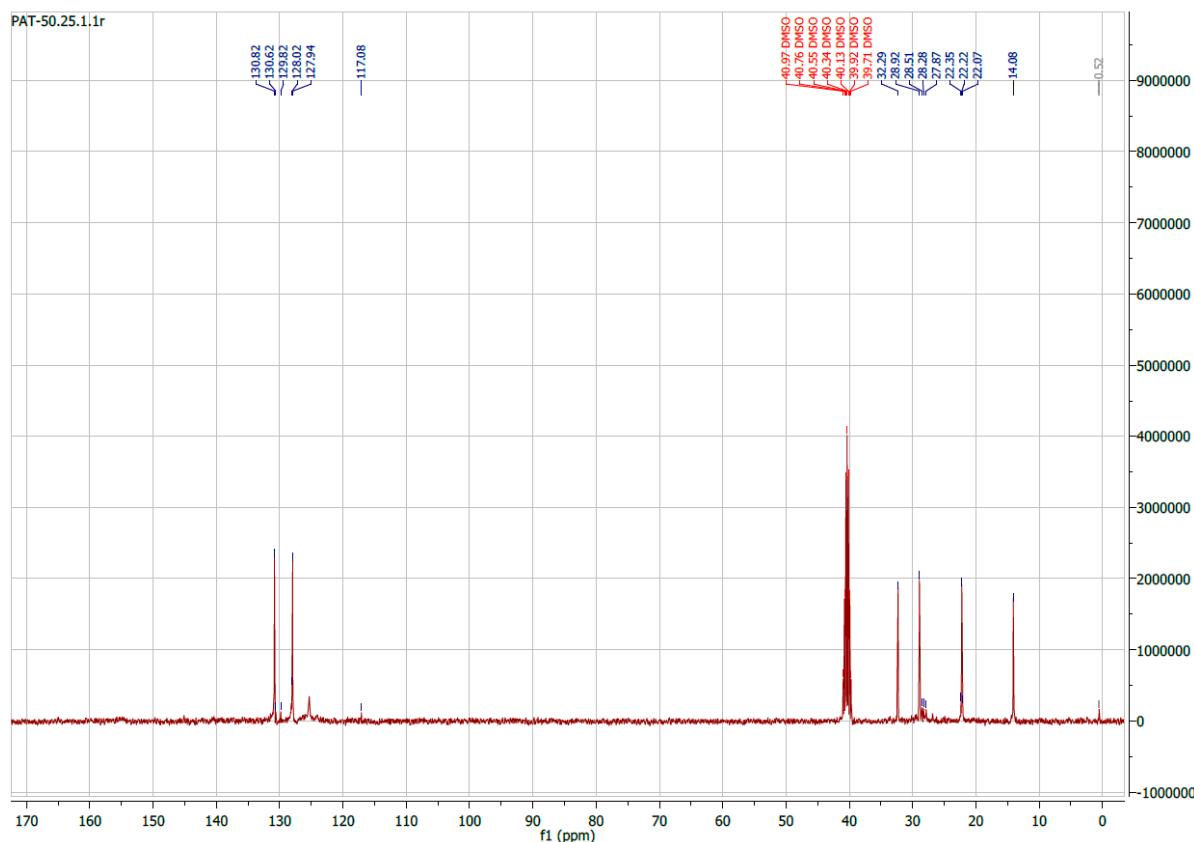




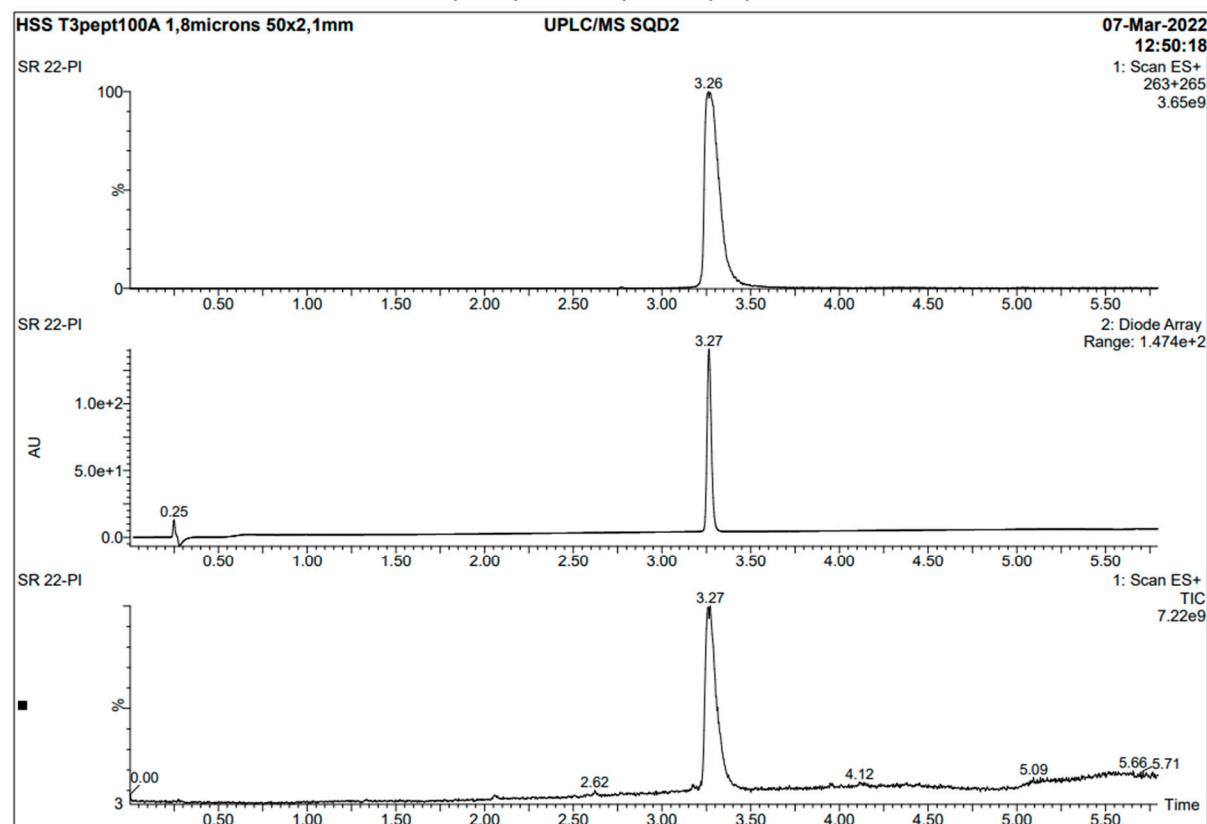
S13. 2-chloro-3-(2-pentylidenehydrazinyl)quinoxaline (**14g**).

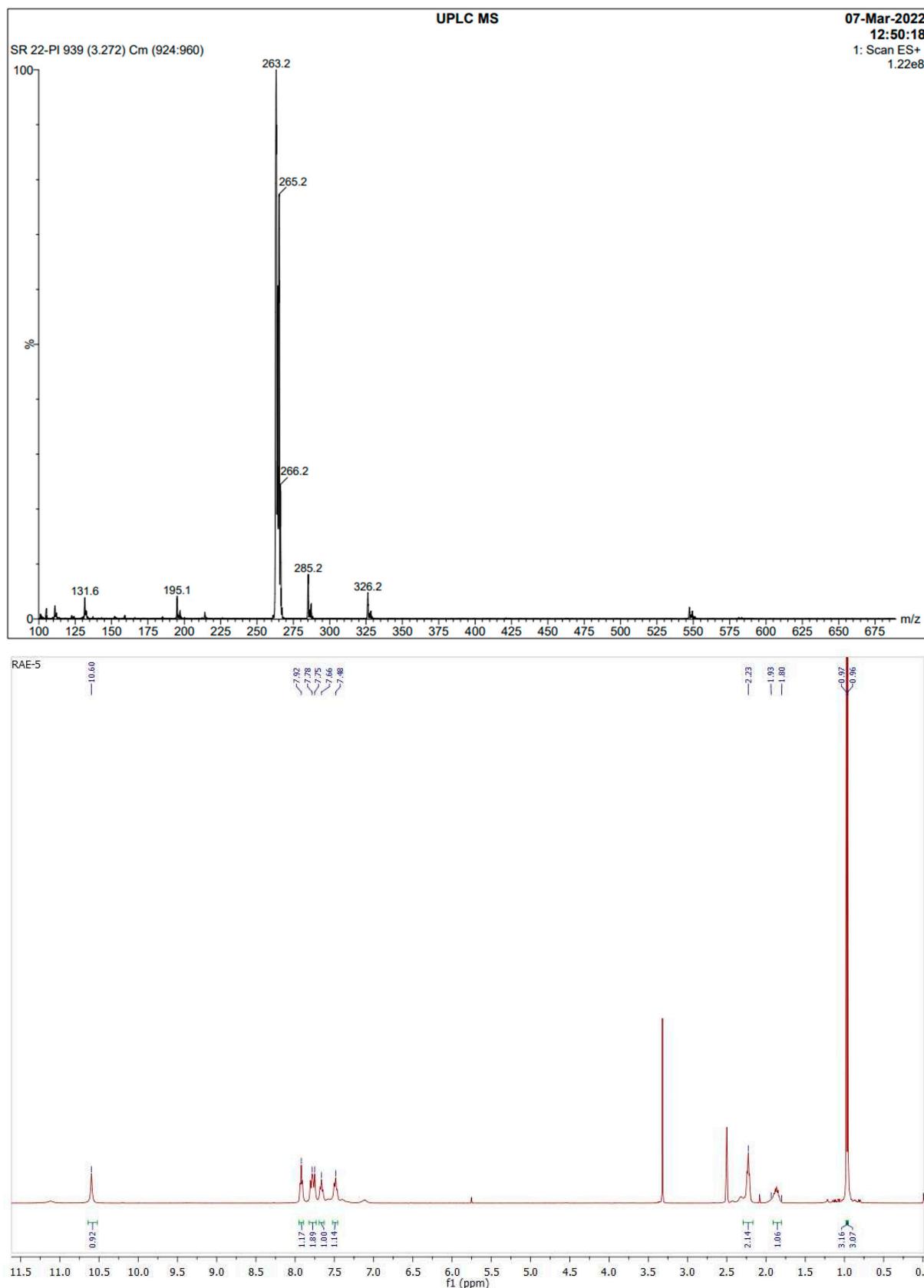


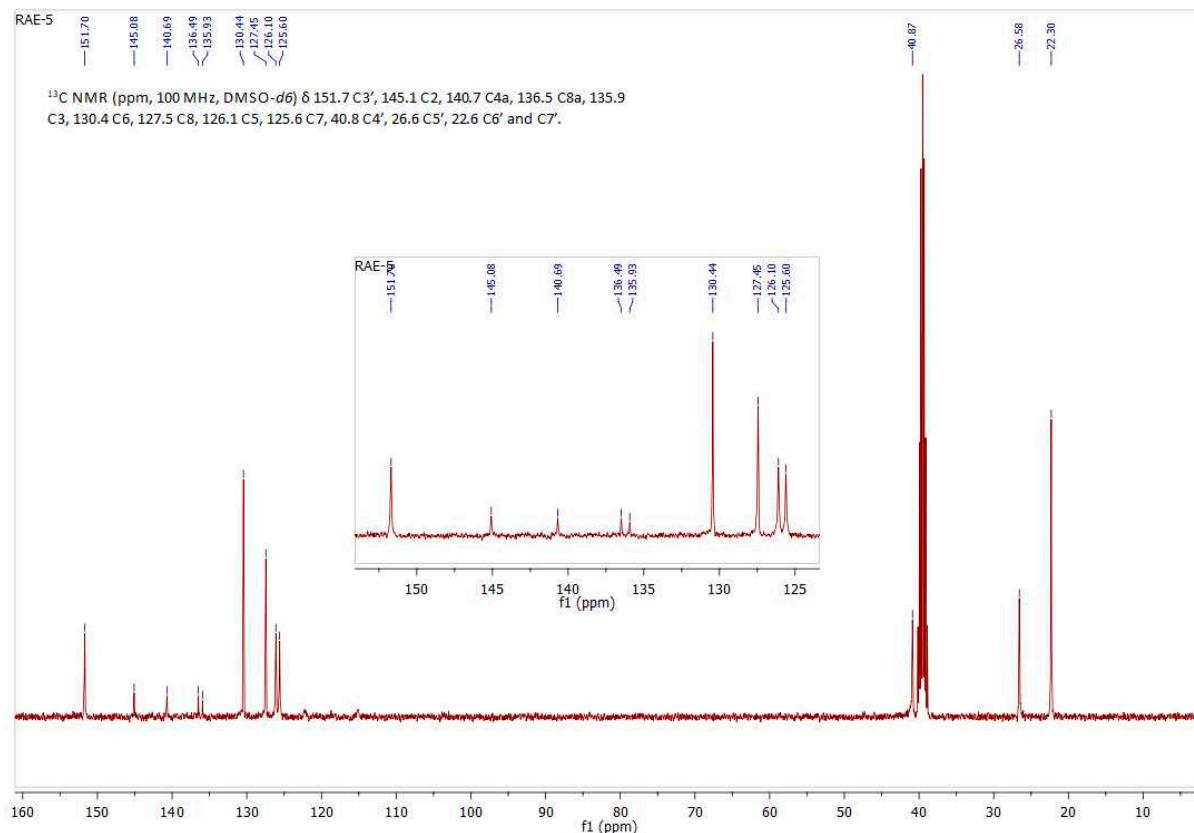




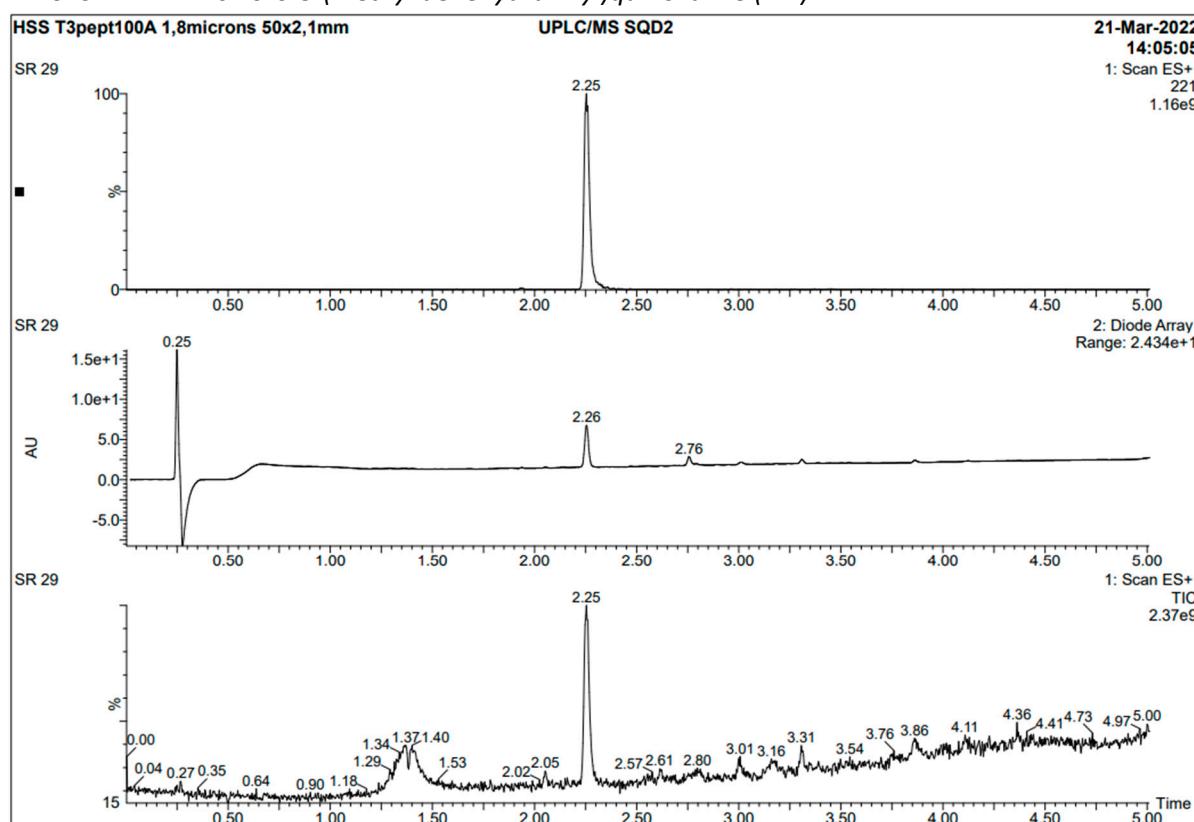
S14. 2-chloro-3-(2-(3-methylbutylidene)hydrazinyl)quinoxaline (**14h**).

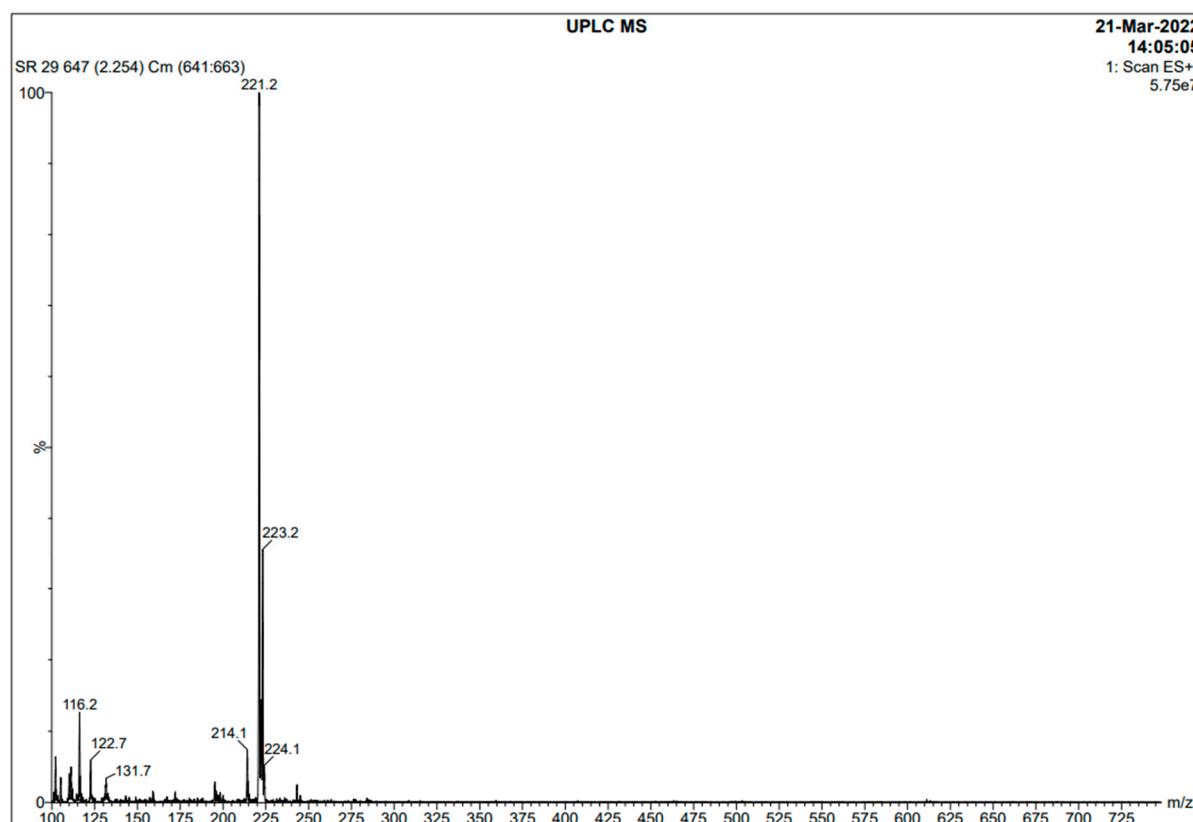




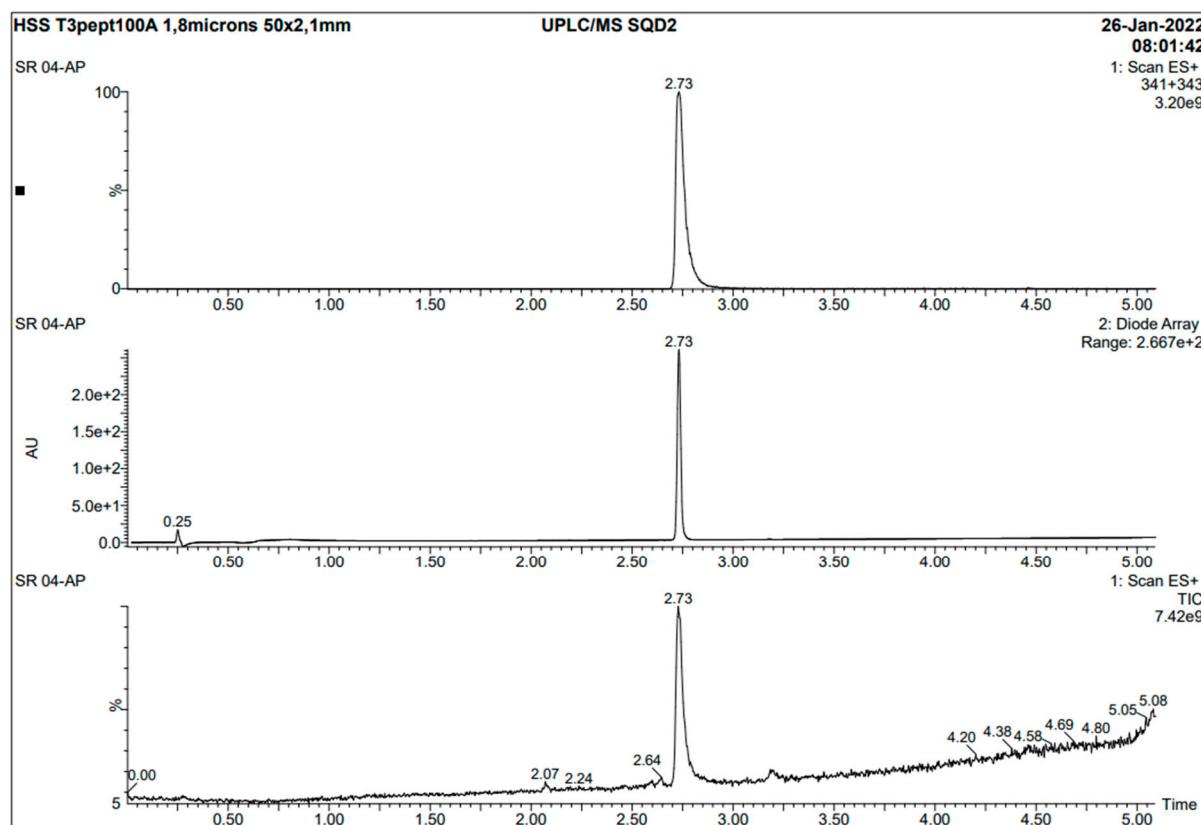


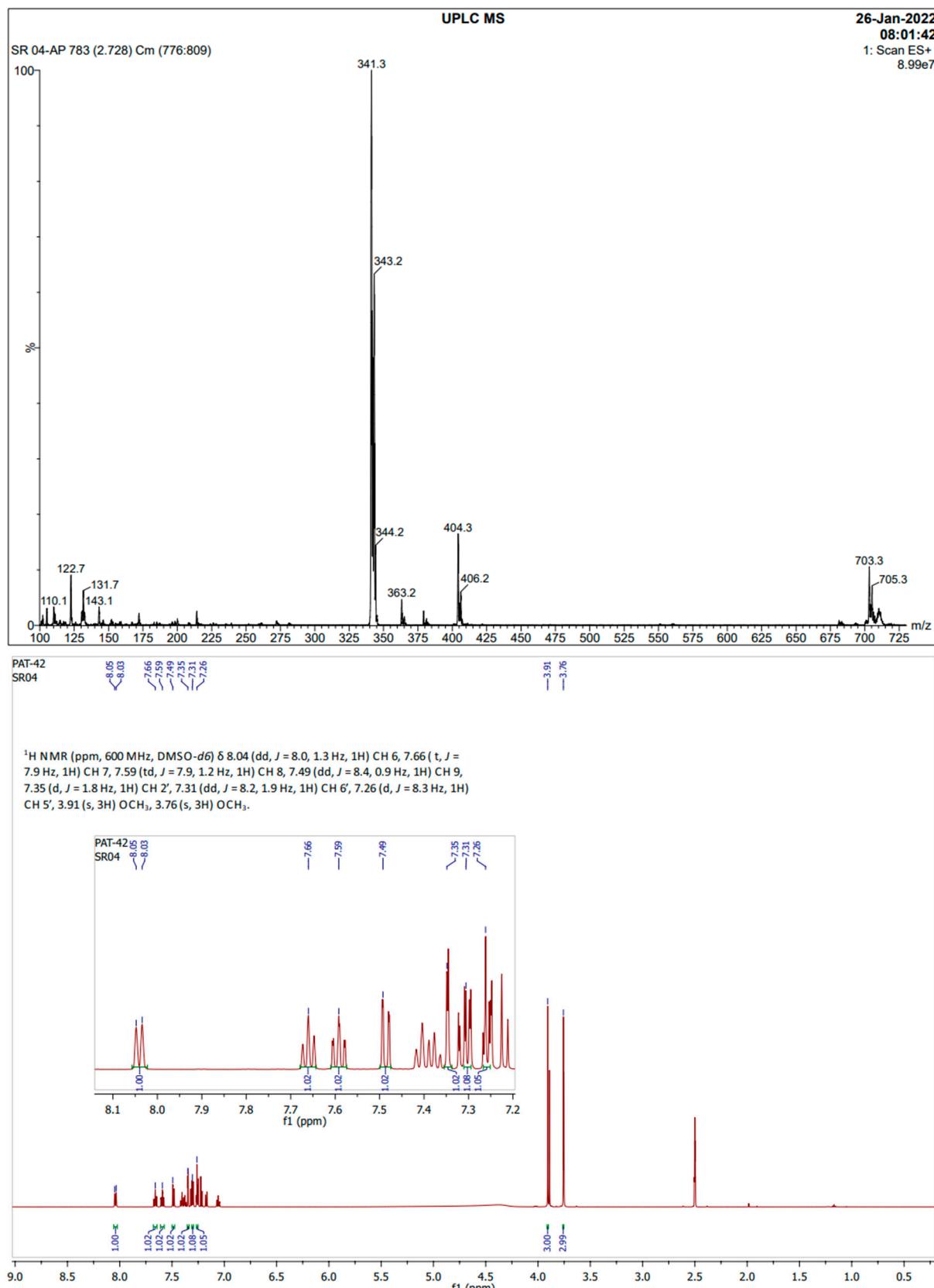
S15. 2-chloro-3-(2-ethylidenehydrazinyl)quinoxaline (**14i**).

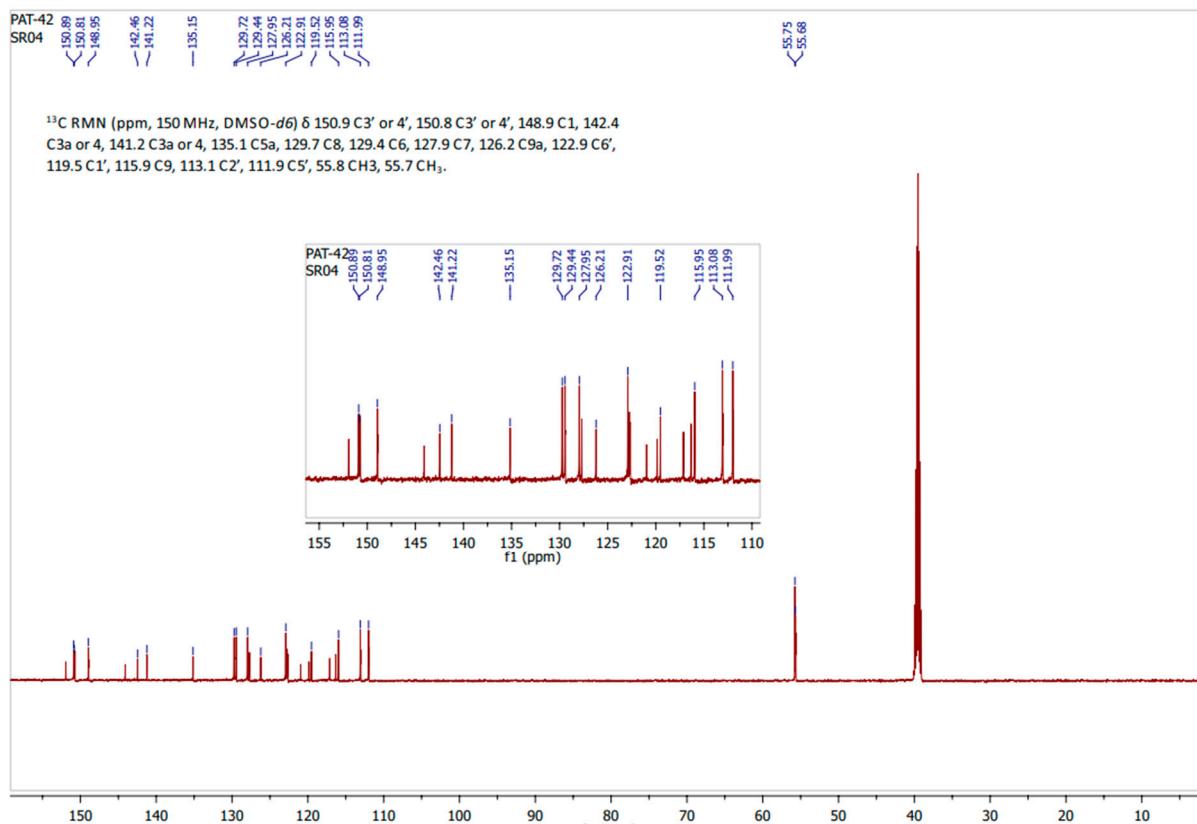




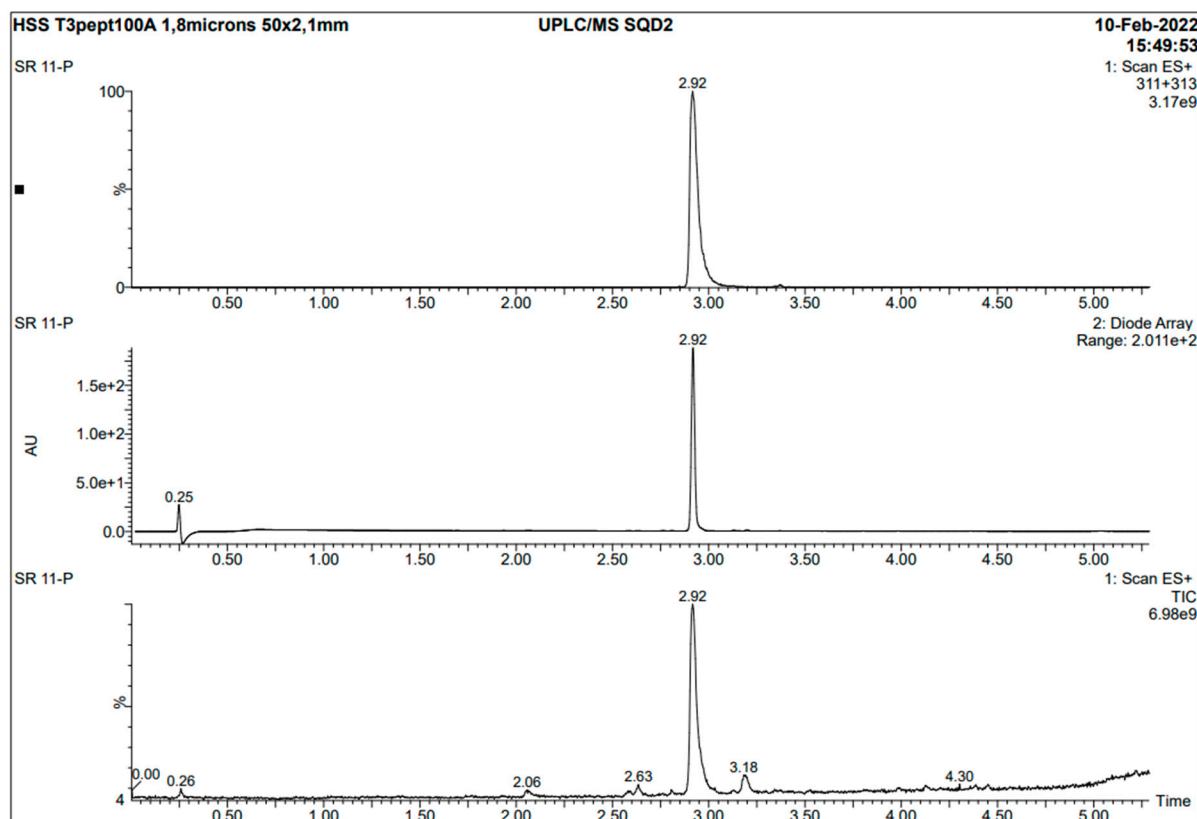
S16. 4-chloro-1-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxaline (**15a**).

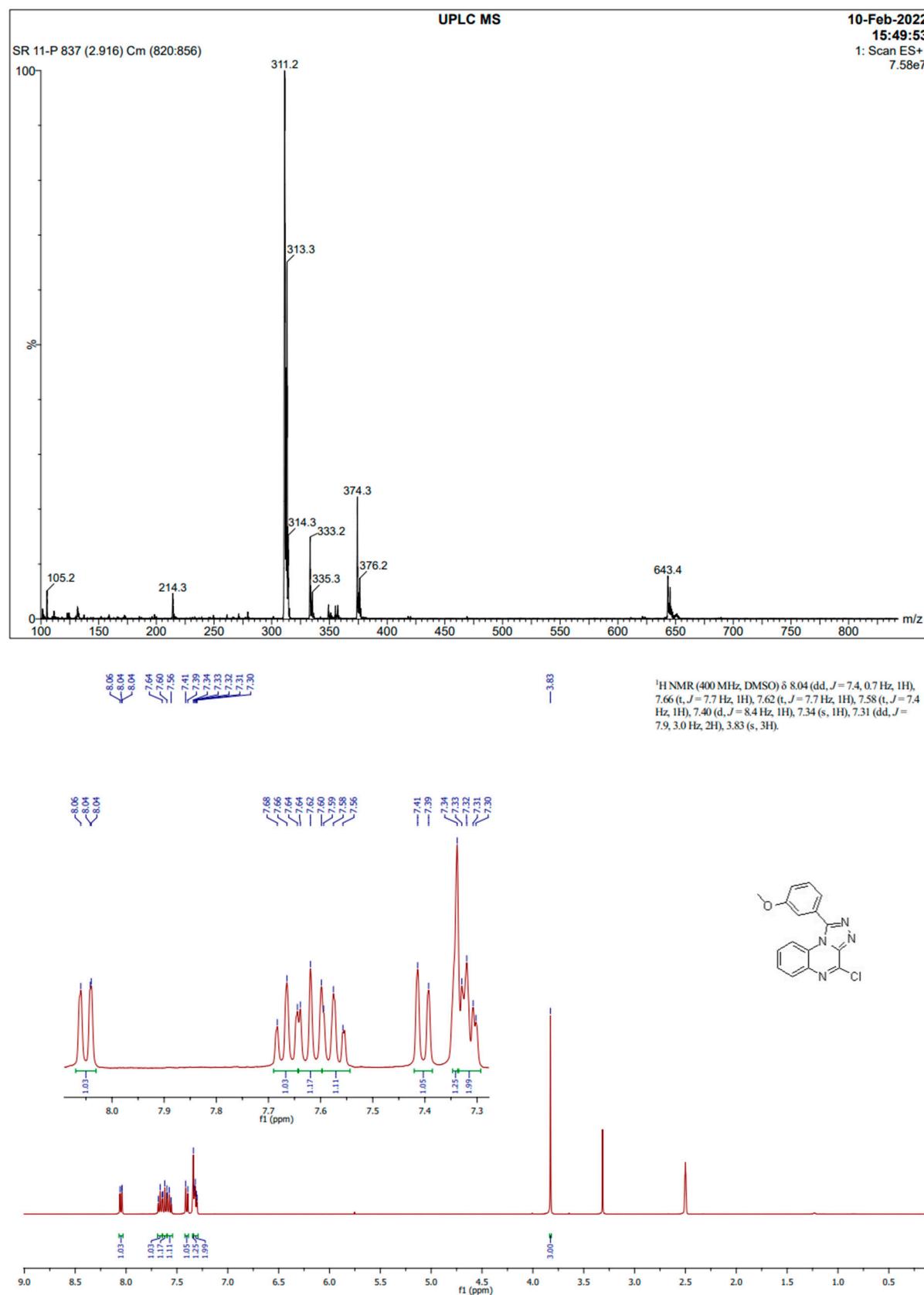


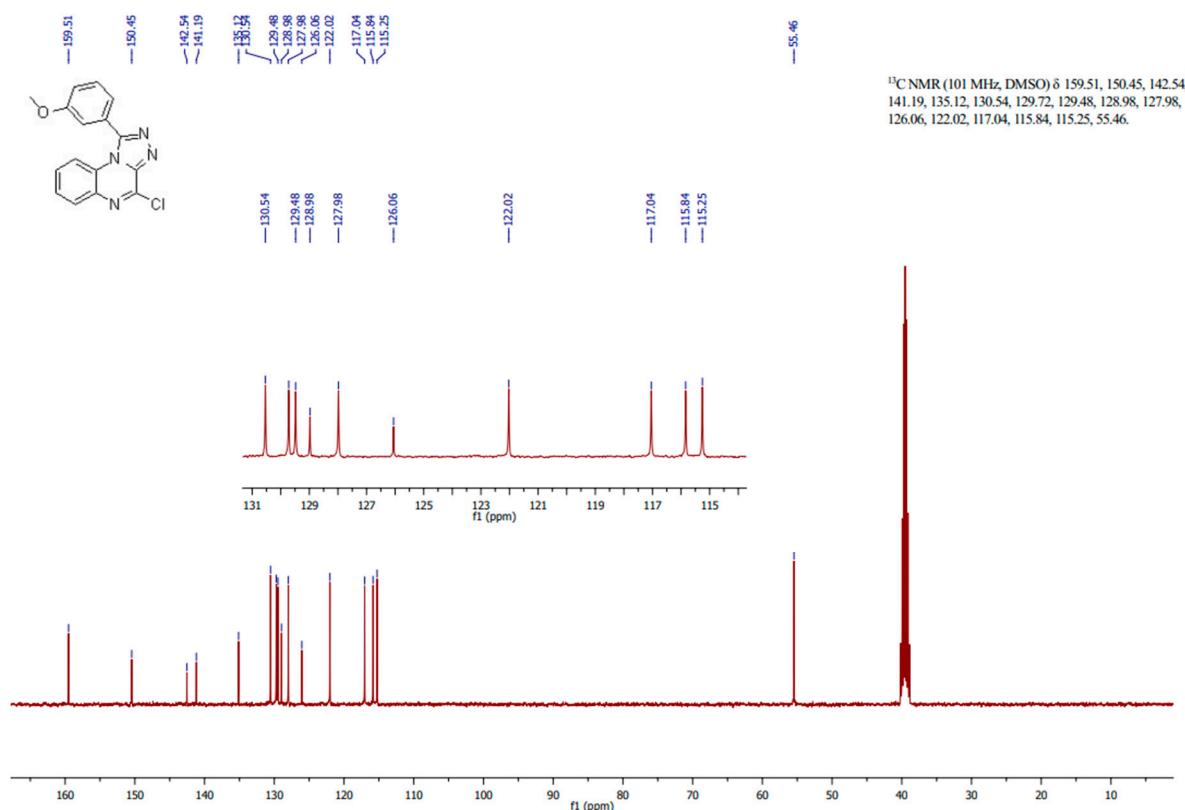




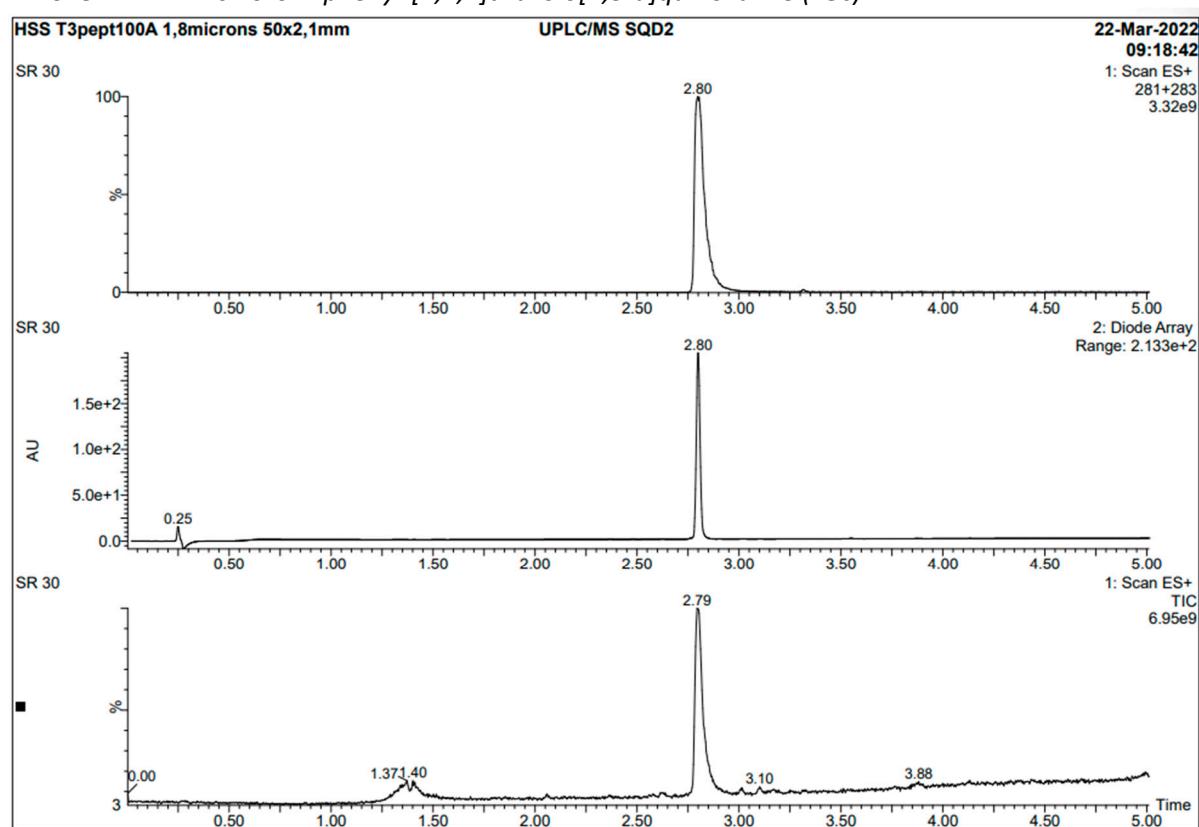
S17. 4-chloro-1-(3-methoxyphenyl)-[1,2,4]triazolo[4,3-*a*]quinoxaline (**15b**).

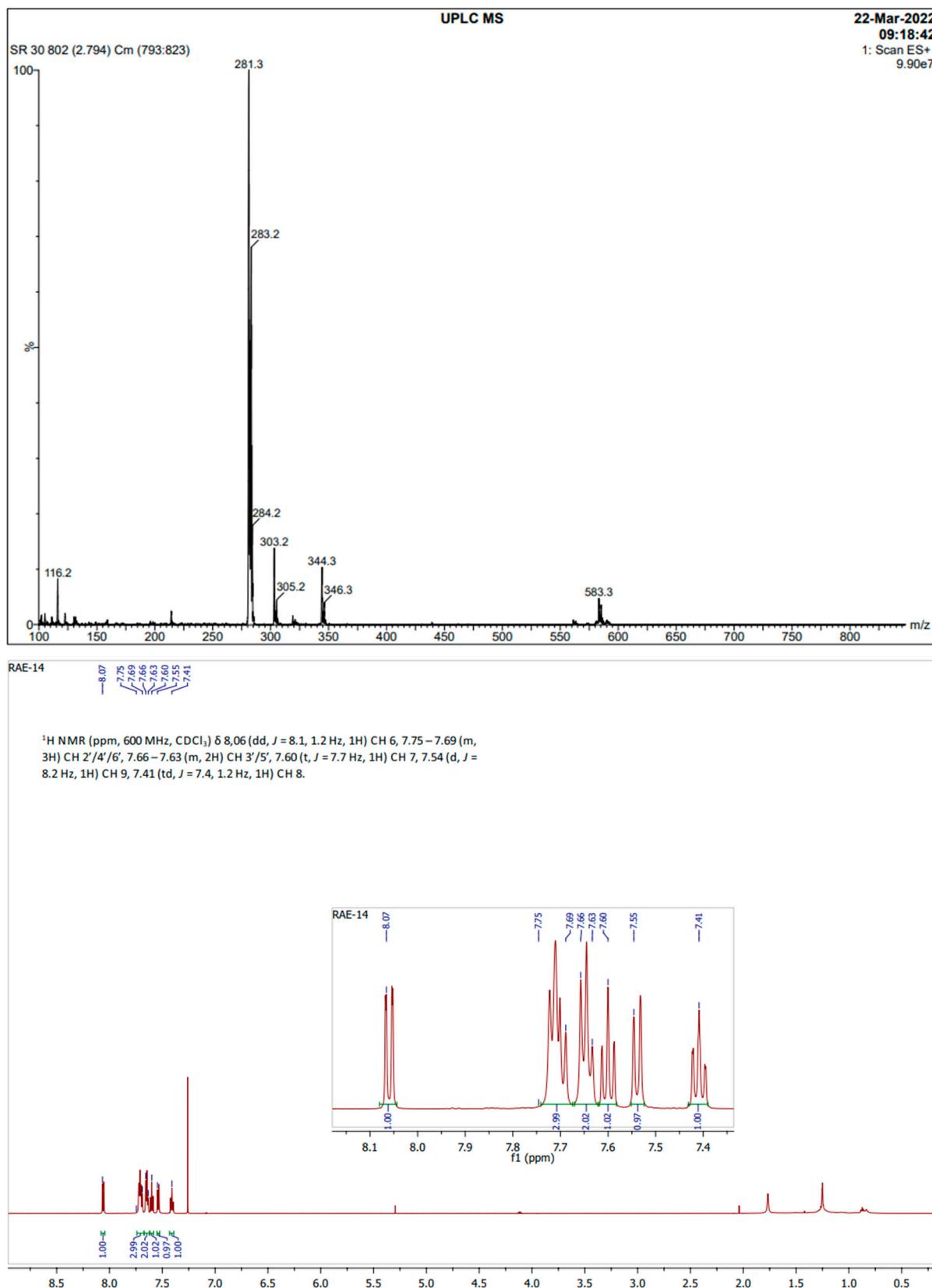


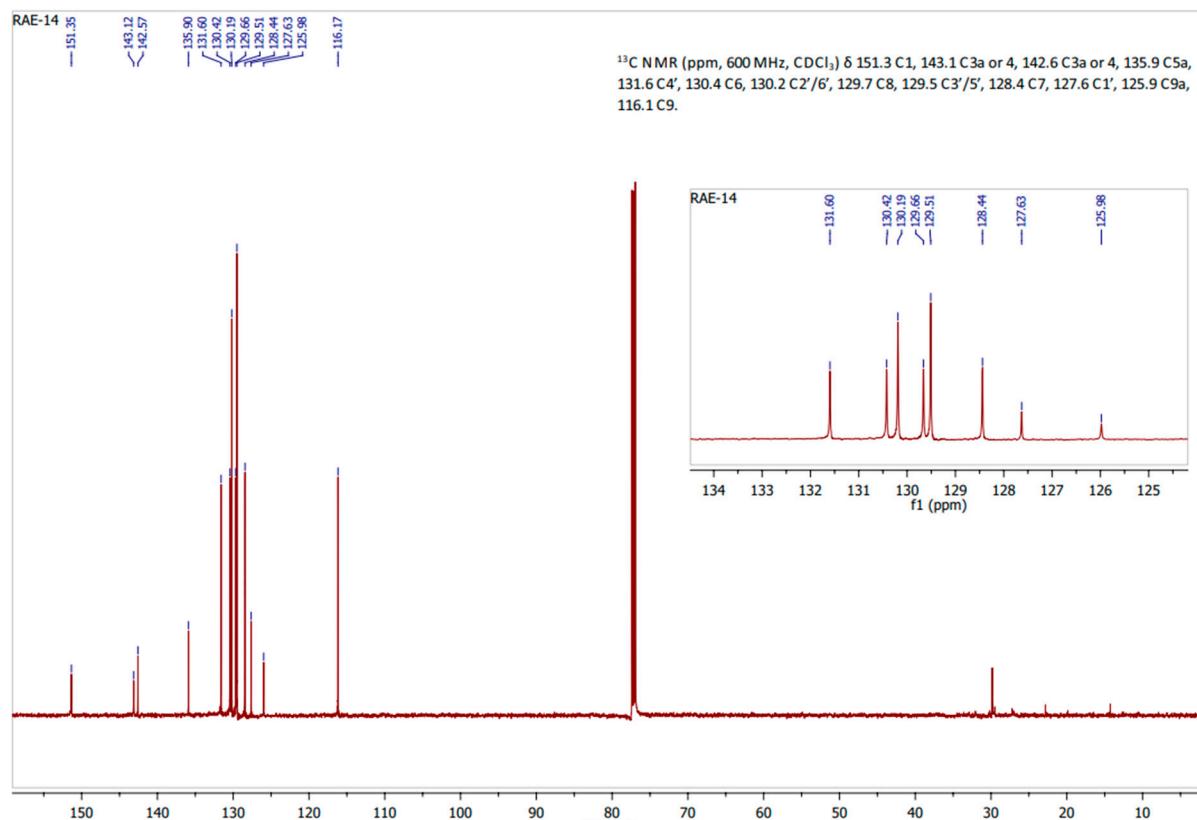




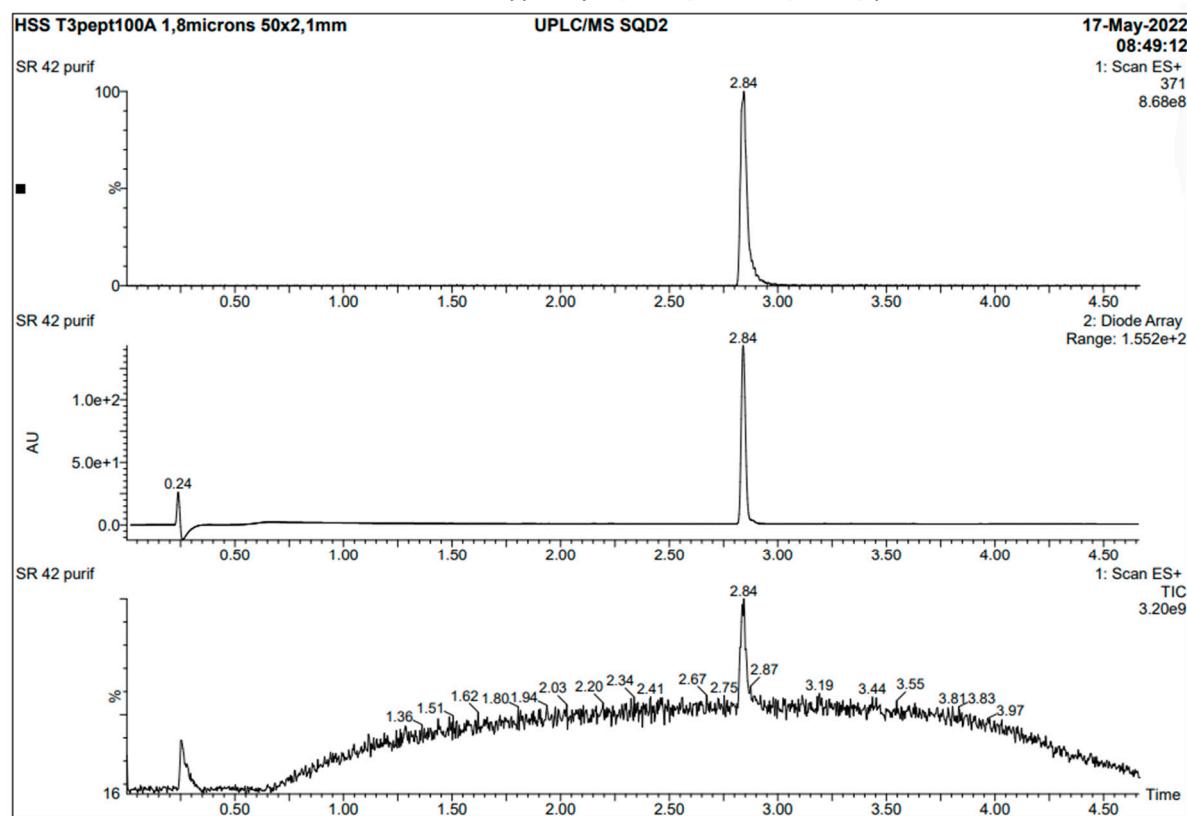
S18. 4-chloro-1-phenyl-[1,2,4]triazolo[4,3-a]quinoxaline (**15c**).

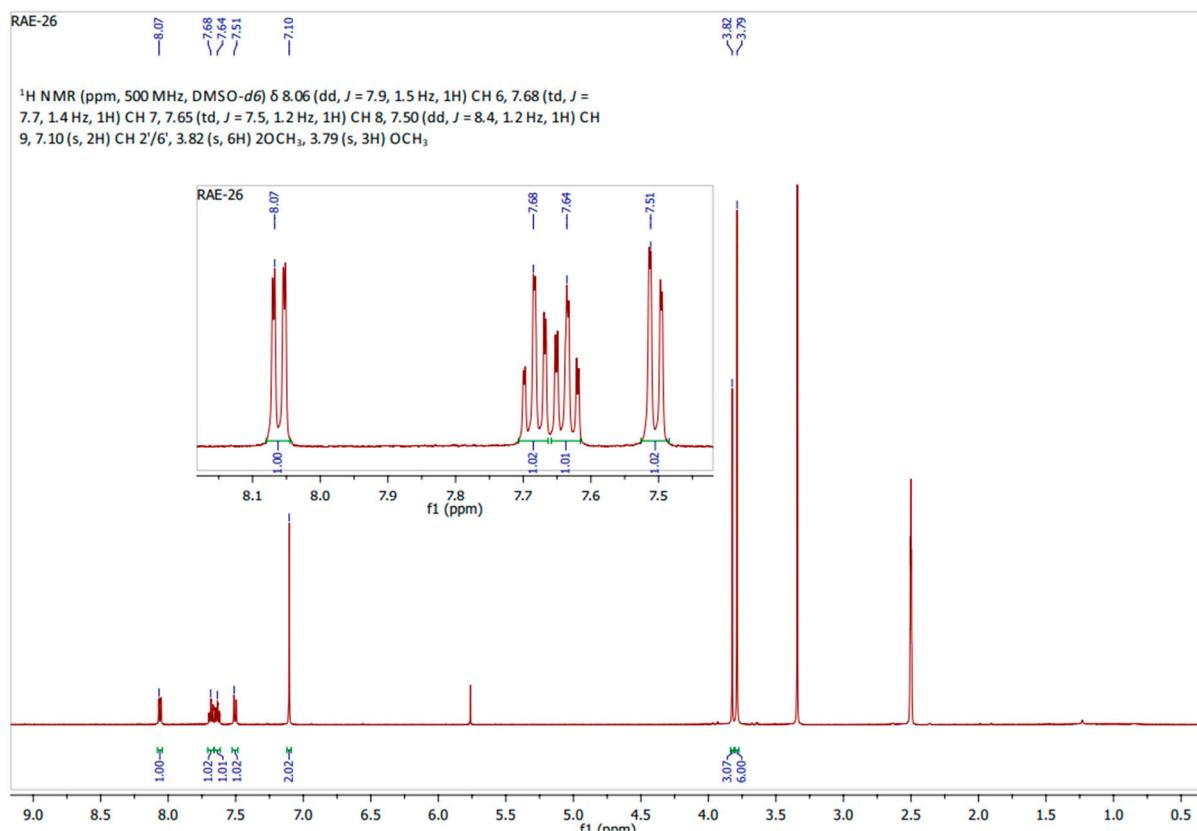
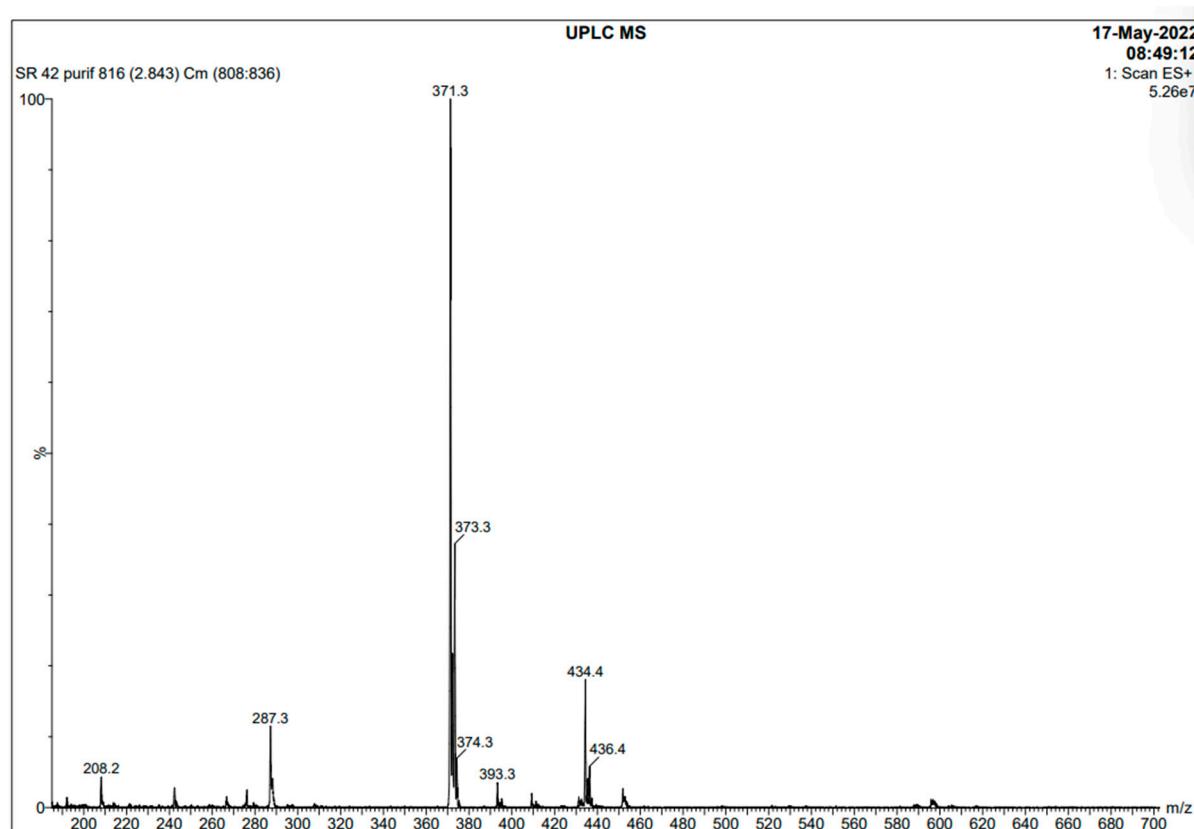


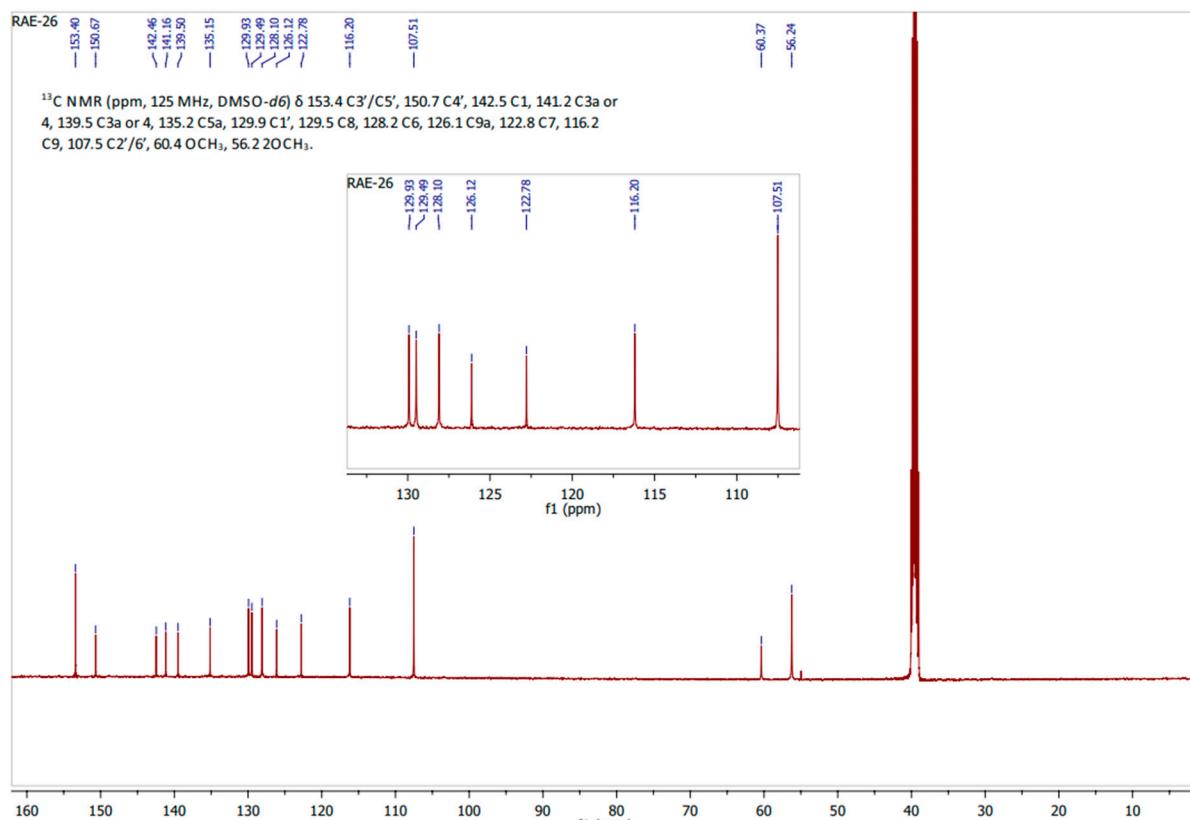




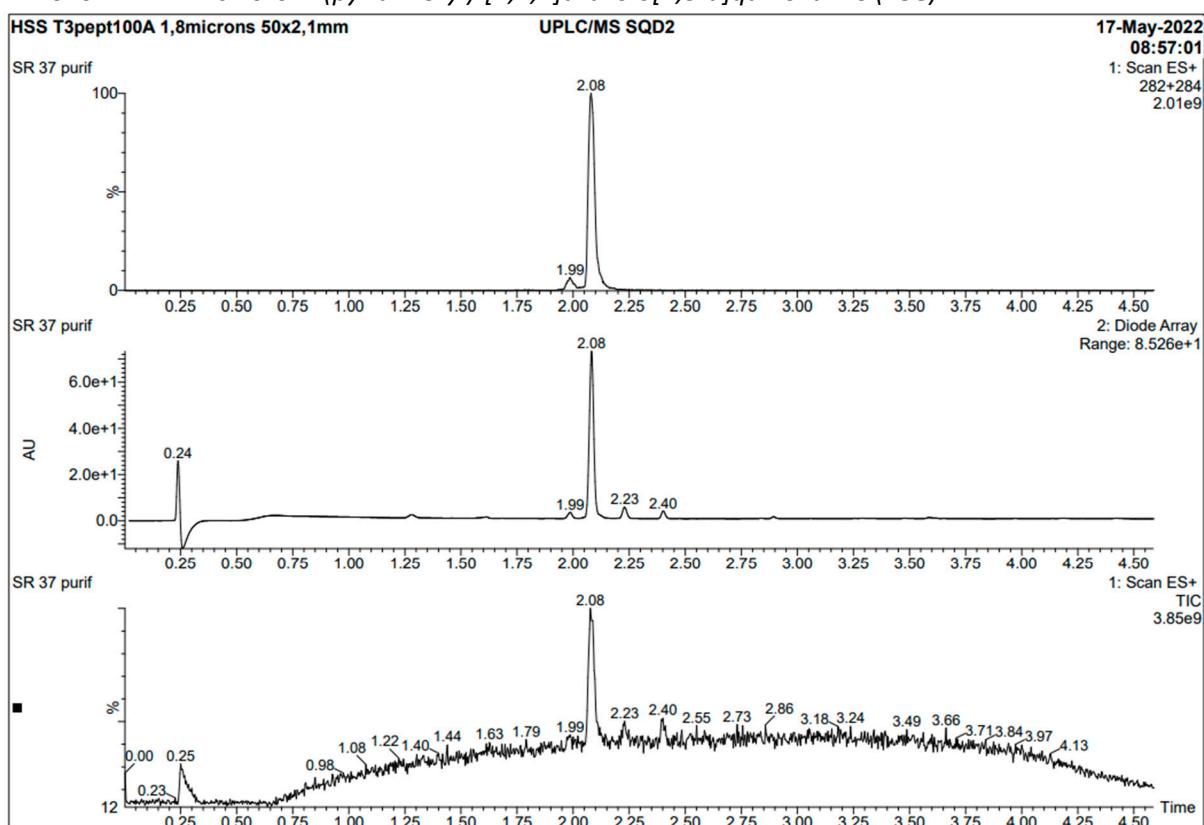
S19. 4-chloro-1-(3,4,5-trimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxaline (**15d**).

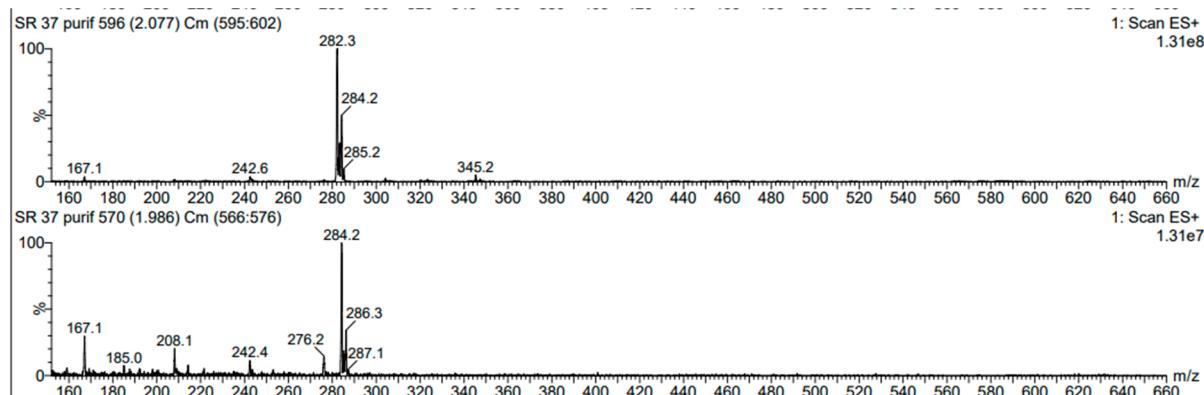




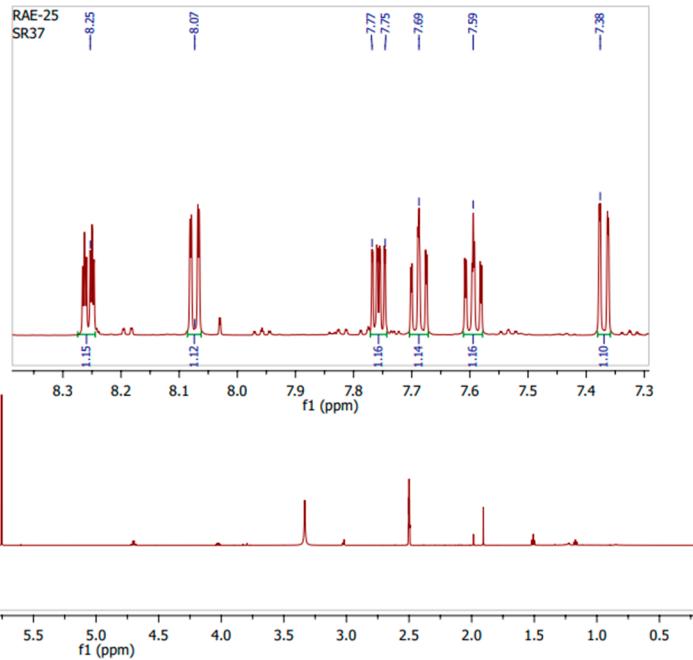


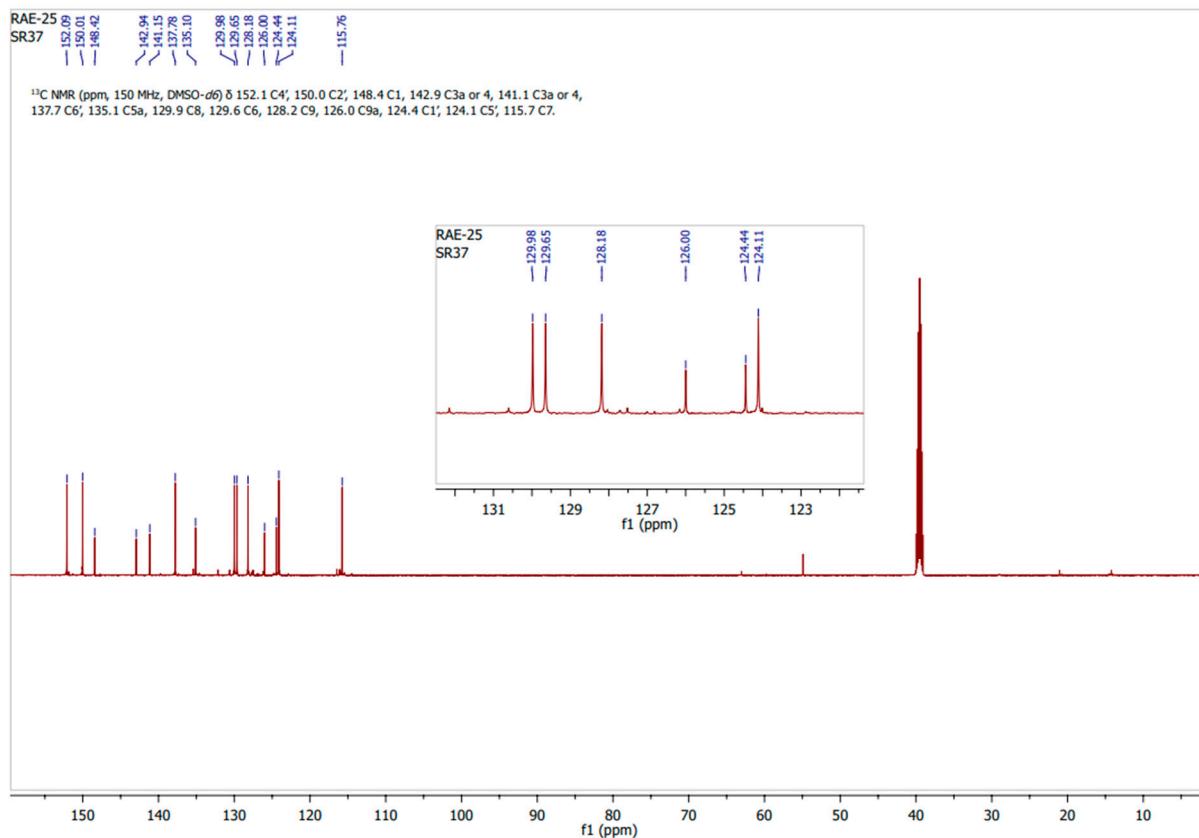
S20. *4-chloro-1-(pyridin-3-yl)-[1,2,4]triazolo[4,3-*a*]quinoxaline (15e).*



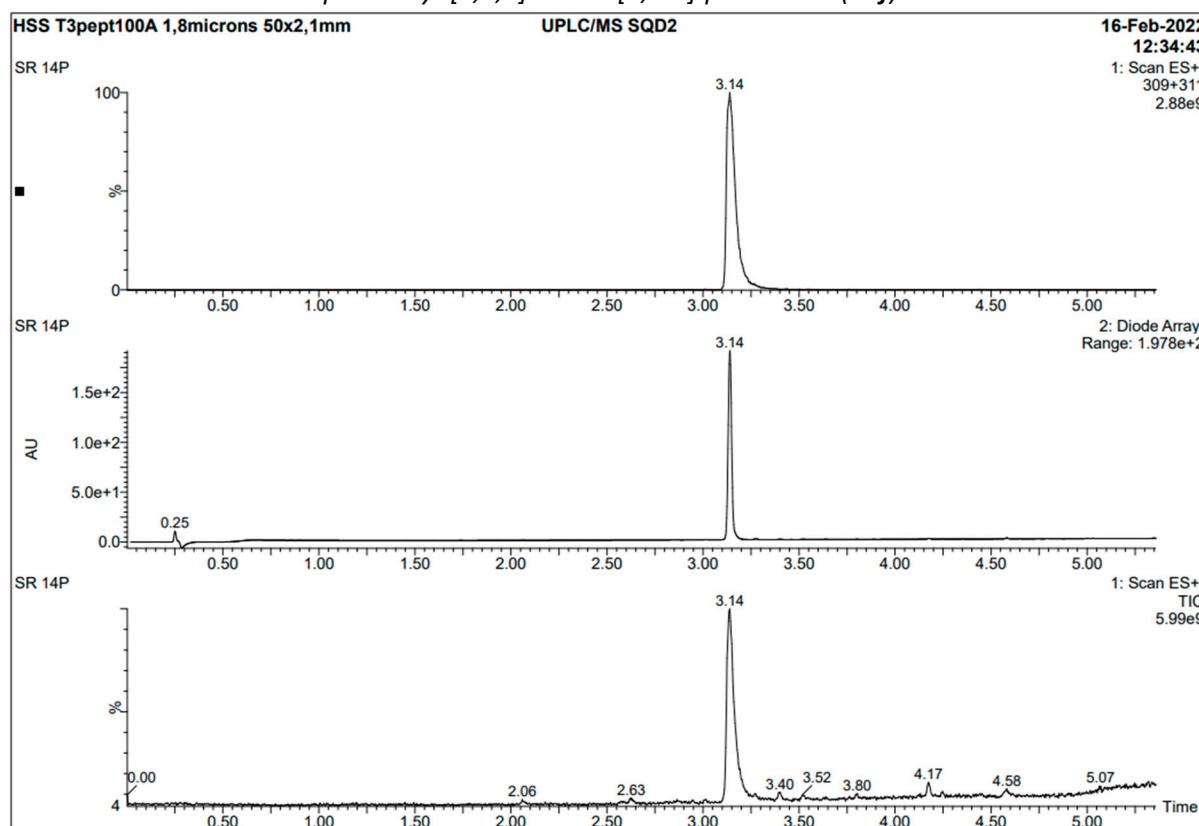
RAE-25
SR37
8.97
8.94
—8.25
—8.07
7.77
7.75
7.69
7.59
7.38

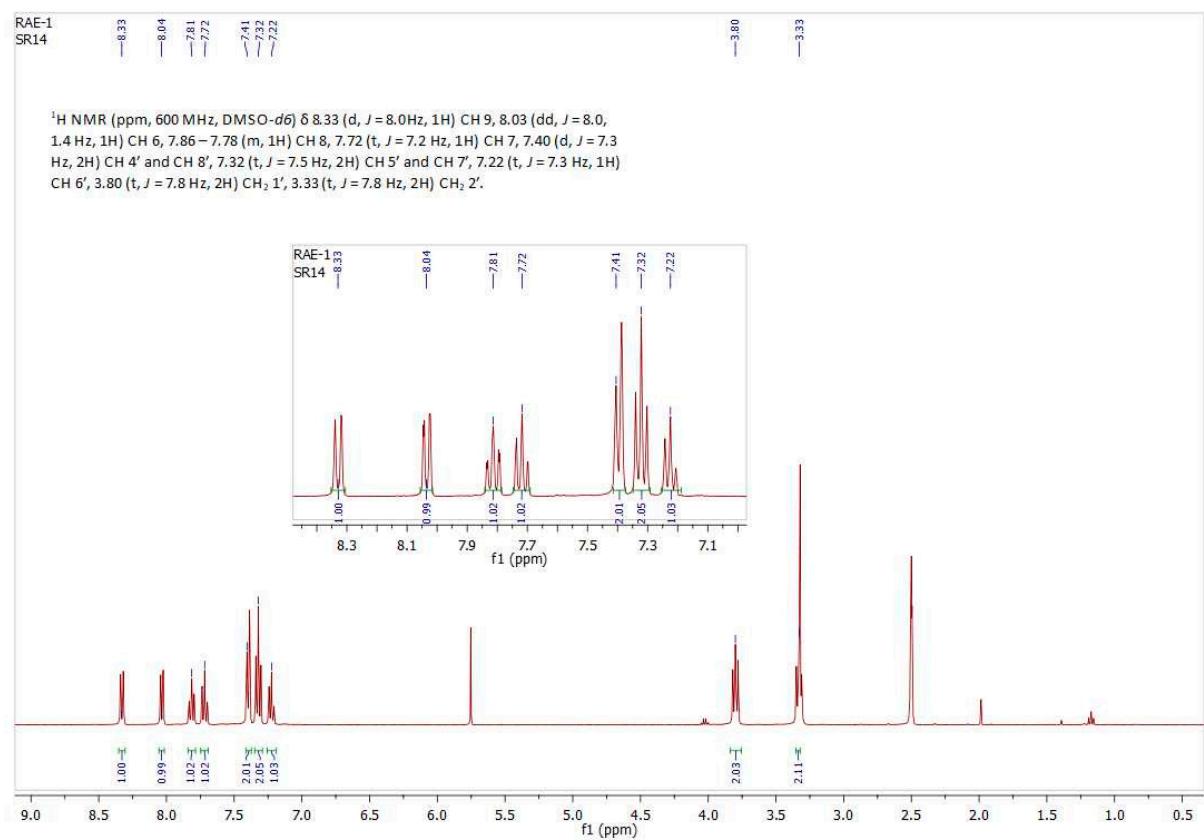
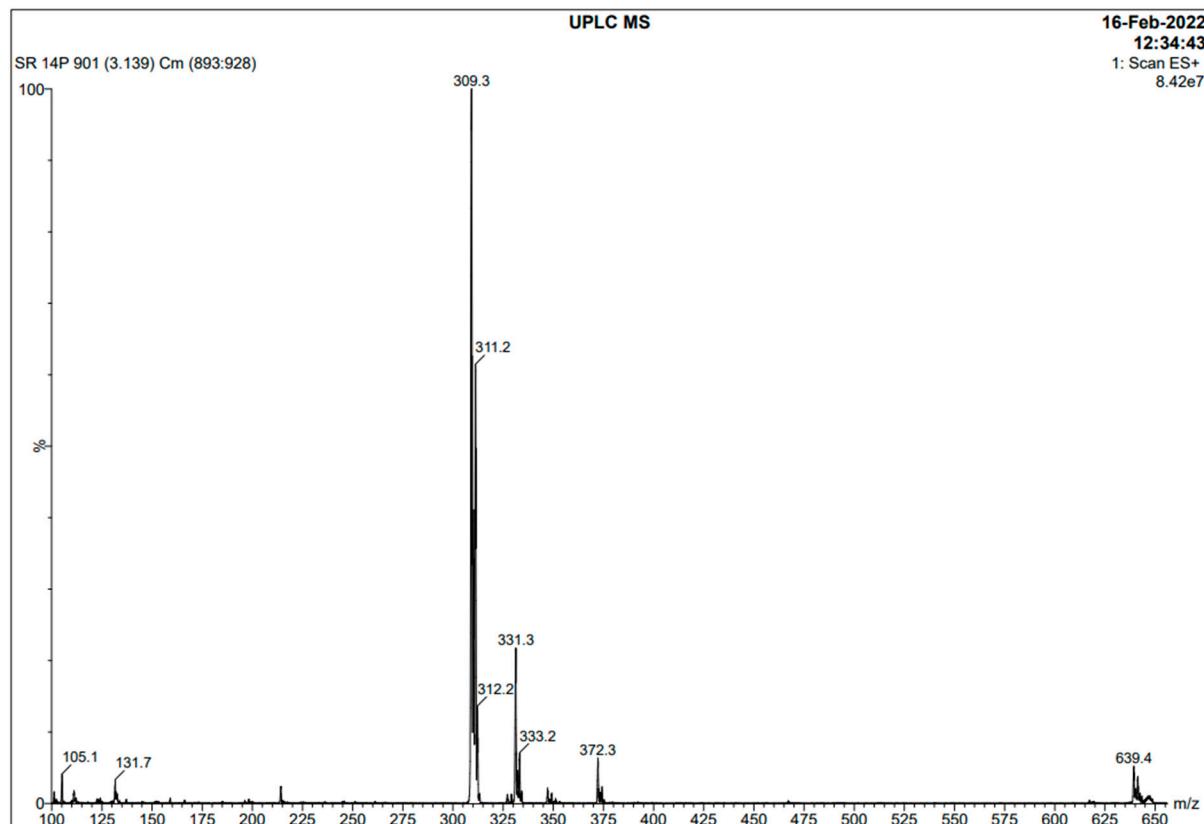
¹H NMR (ppm, 600 MHz, DMSO-*d*6) δ 8.97 (dd, *J* = 4.6, 2.3 Hz, 1H) CH 2', 8.94 (dd, *J* = 4.9, 1.7 Hz, 1H) CH 4', 8.25 (ddd, *J* = 6.7, 4.4, 2.3 Hz, 1H) CH 6', 8.07 (dd, *J* = 8.1, 1.4 Hz, 1H) CH 6, 7.77 – 7.74 (m, 1H) CH 5', 7.69 (td, *J* = 7.8, 1.2 Hz, 1H) CH 7, 7.59 (ddd, *J* = 8.7, 7.4, 1.5 Hz, 1H) CH 8, 7.37 (dd, *J* = 8.5, 1.0 Hz, 1H) CH 9.

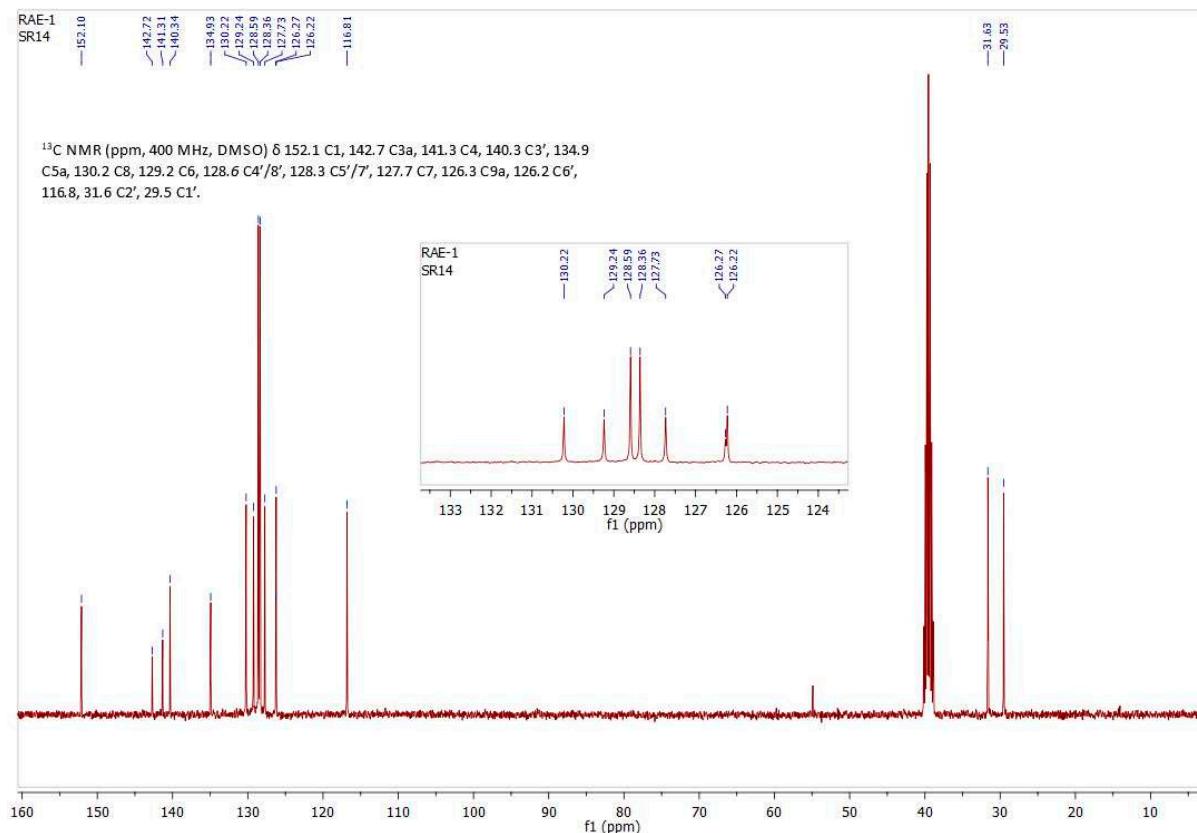




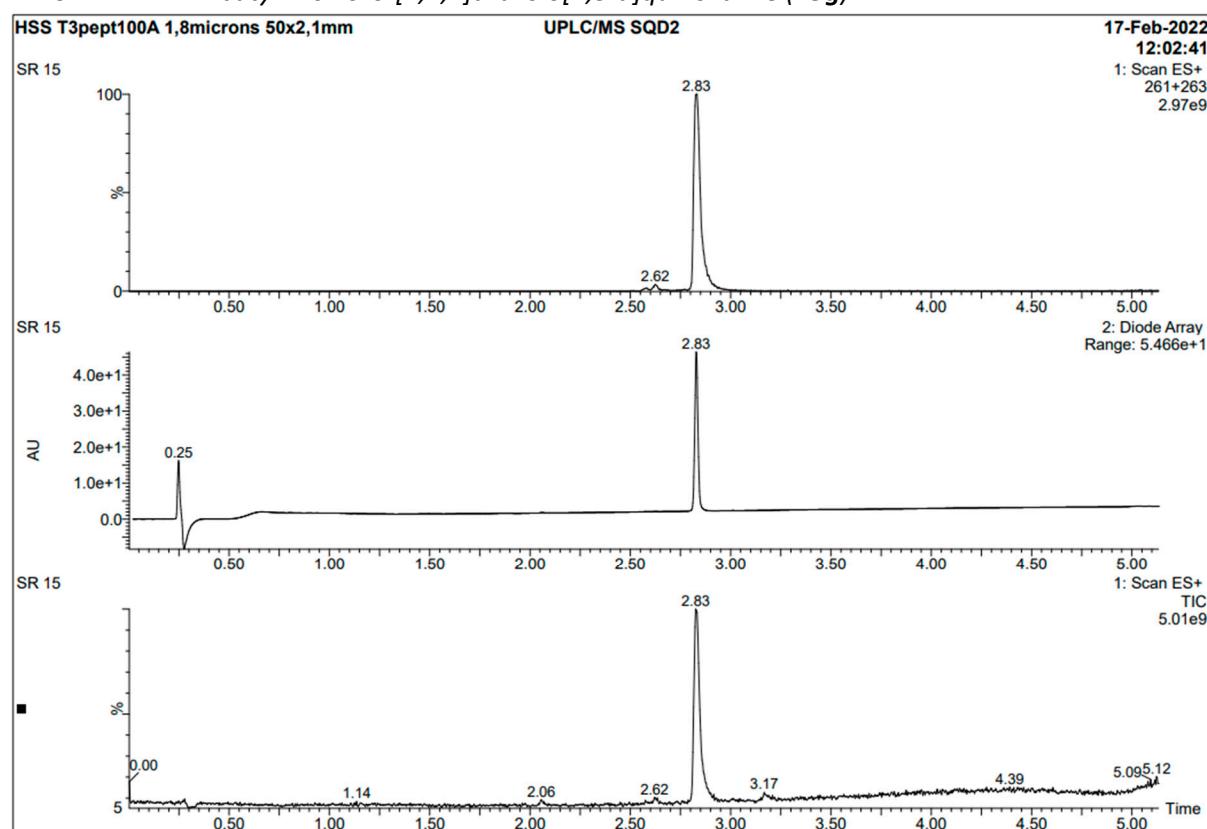
S21. 4-chloro-1-phenethyl-[1,2,4]triazolo[4,3-*a*]quinoxaline (**15f**).

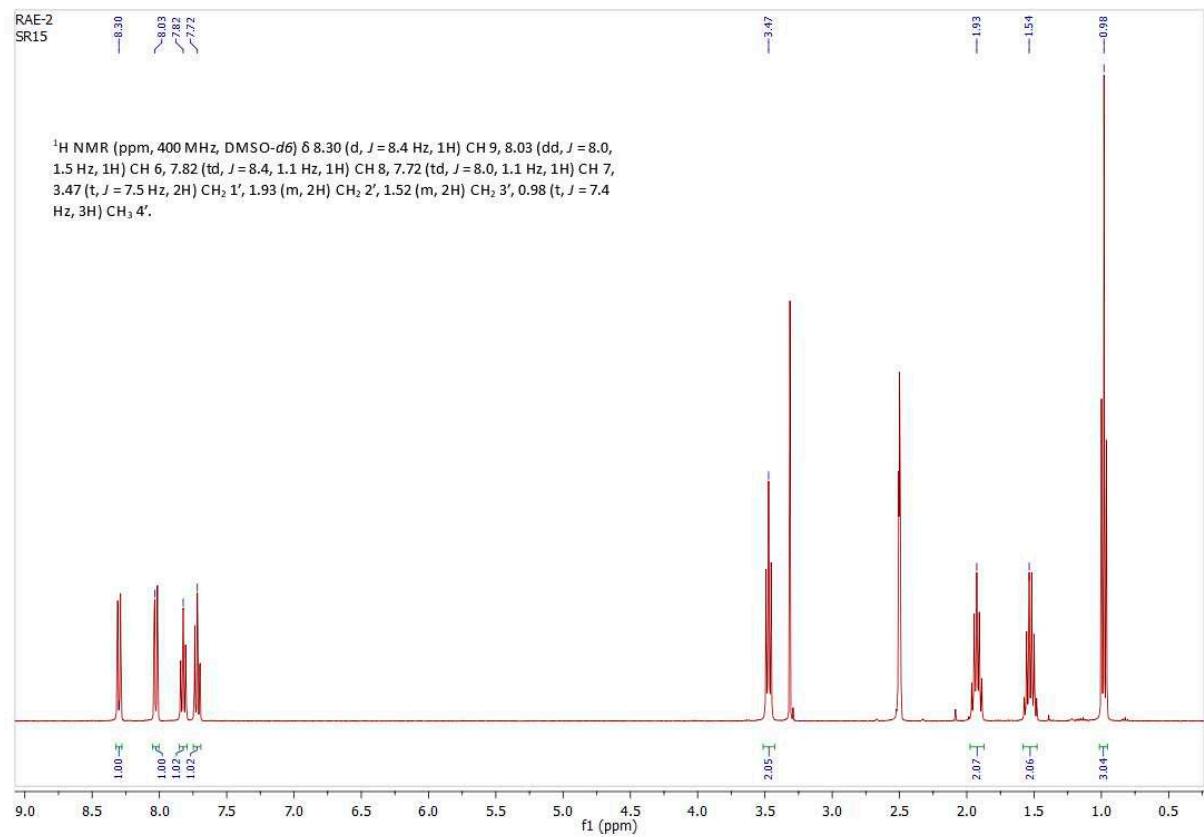
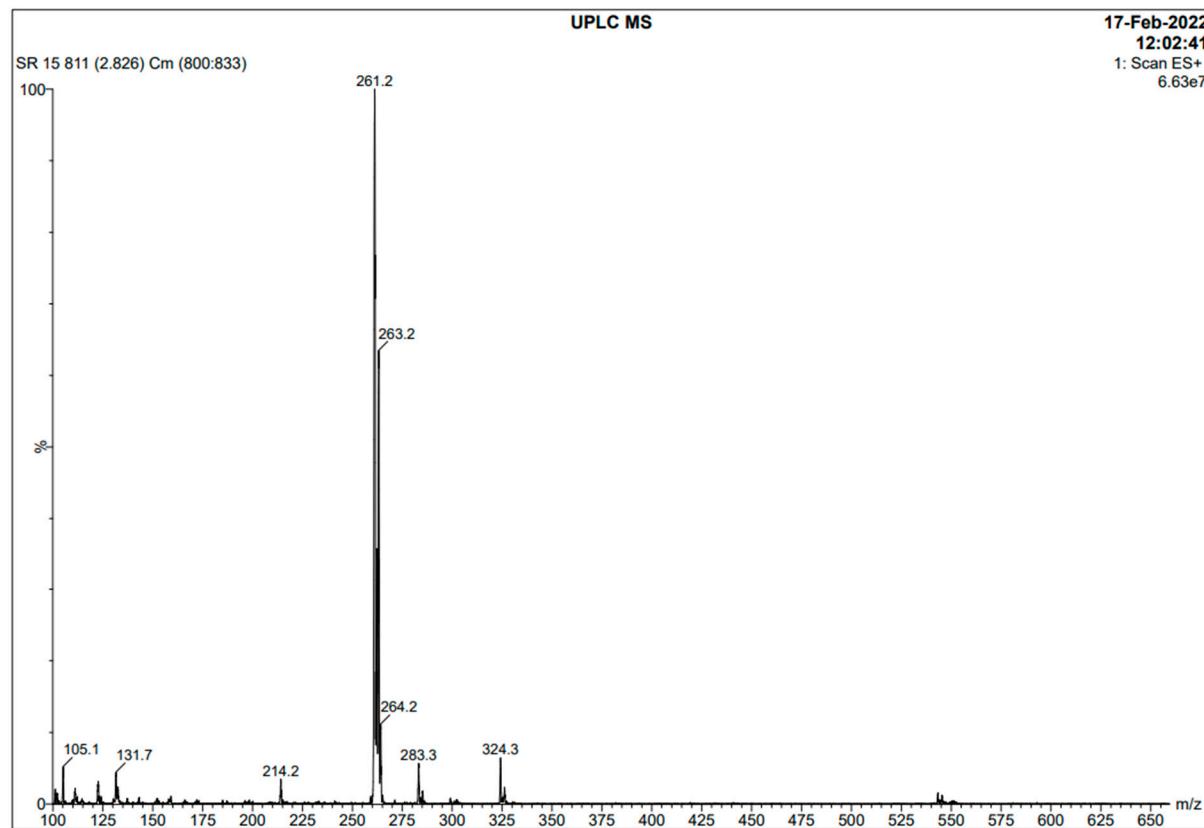


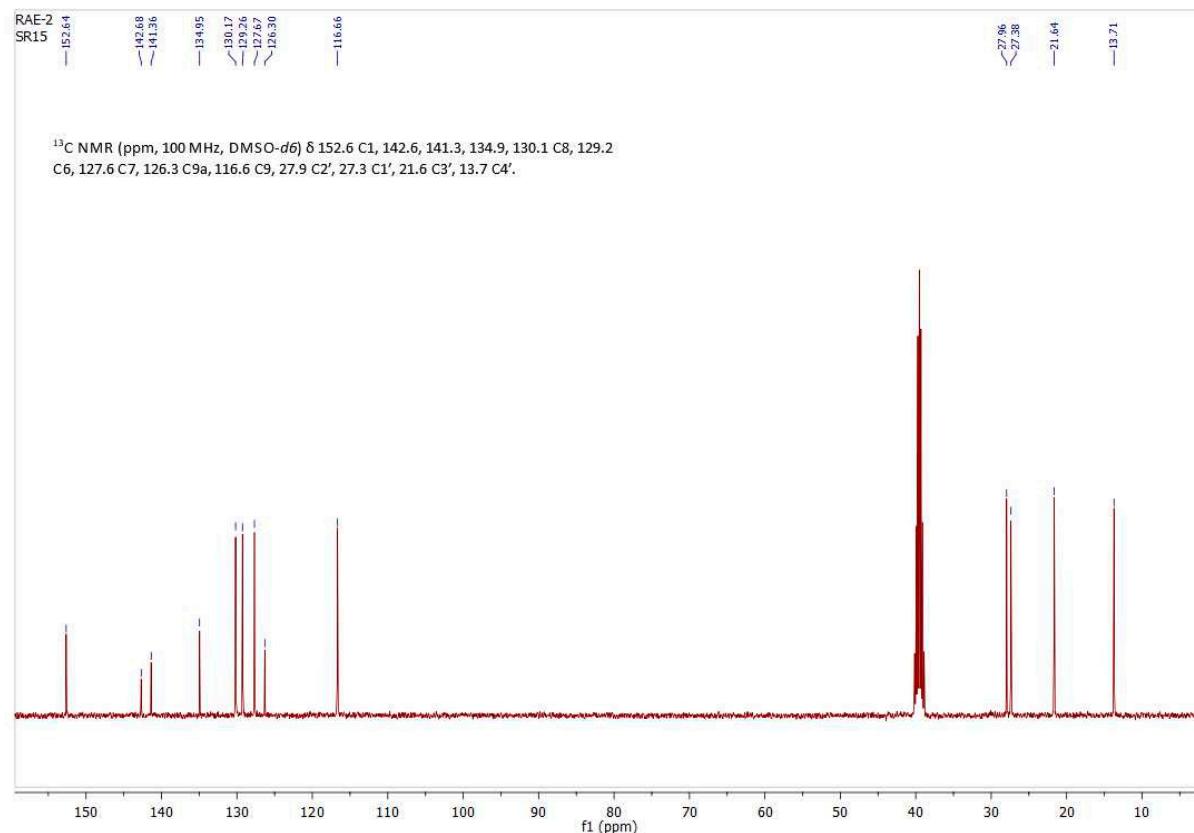




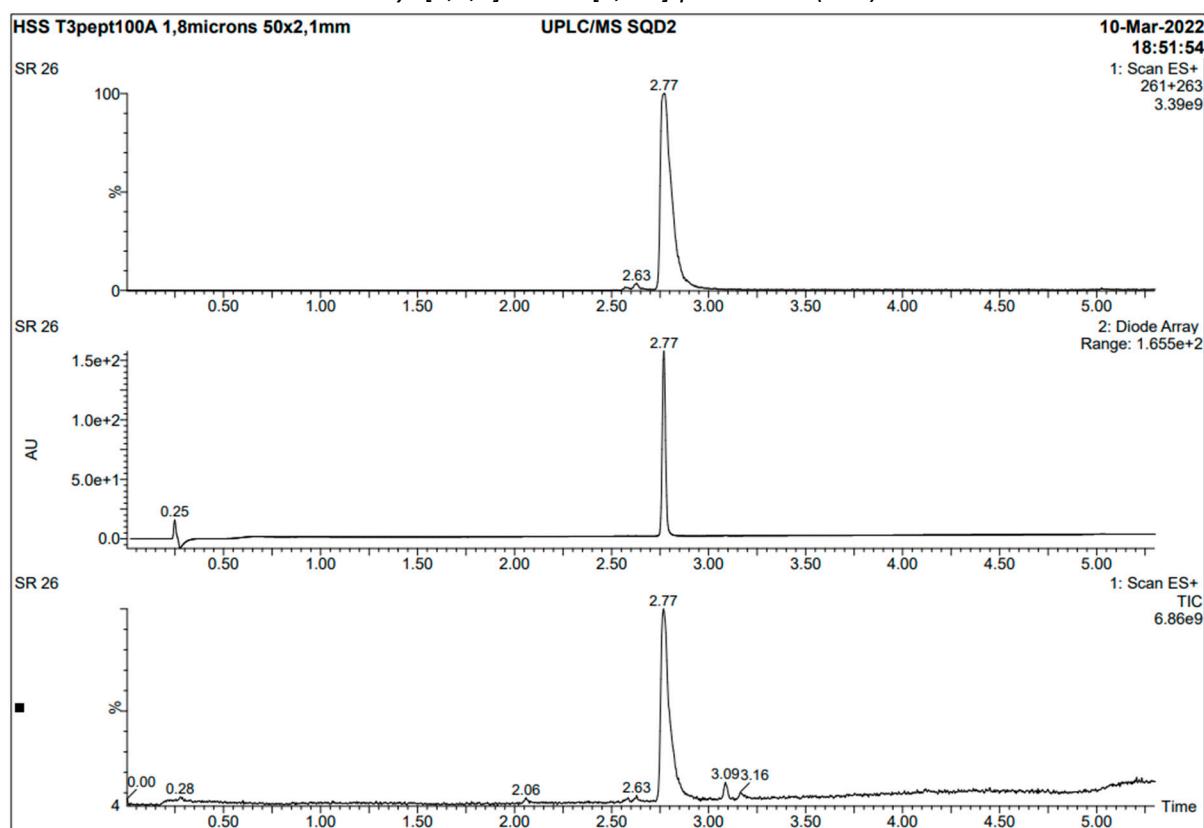
S22. *1-butyl-4-chloro-[1,2,4]triazolo[4,3-*a*]quinoxaline (15g).*

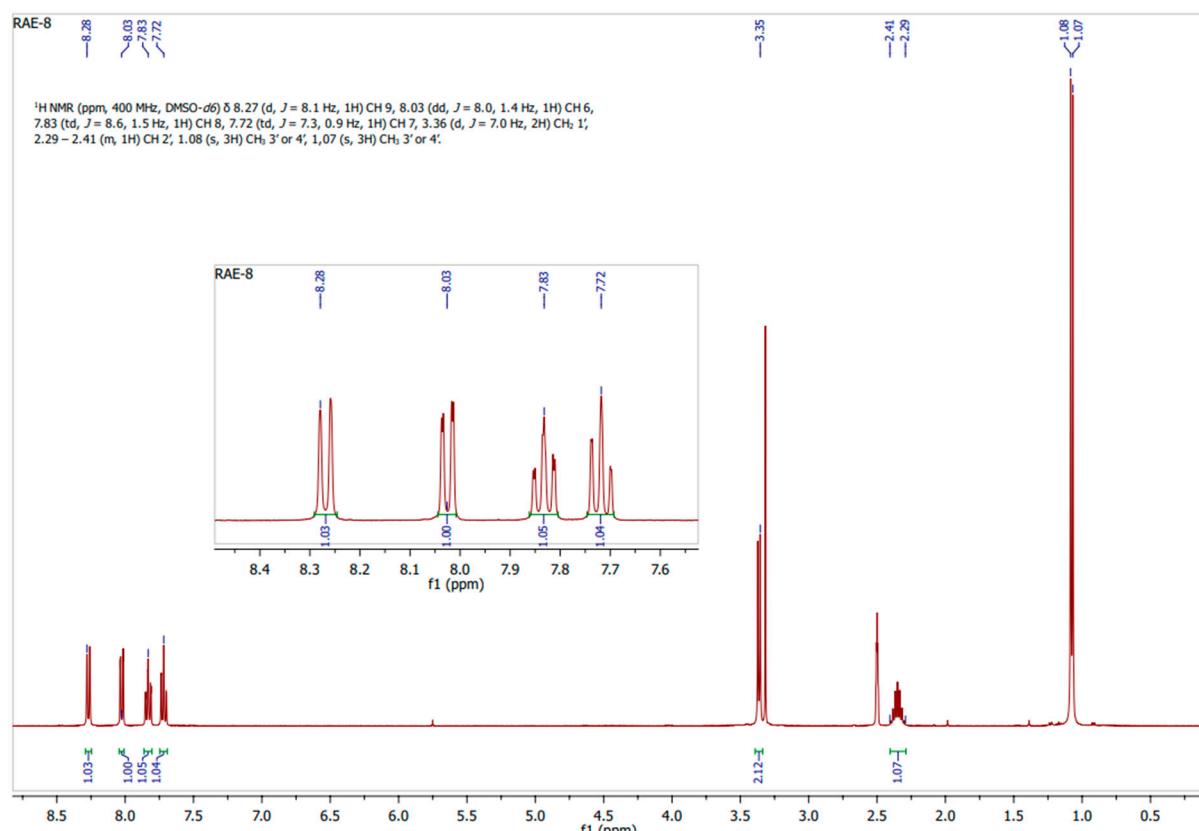
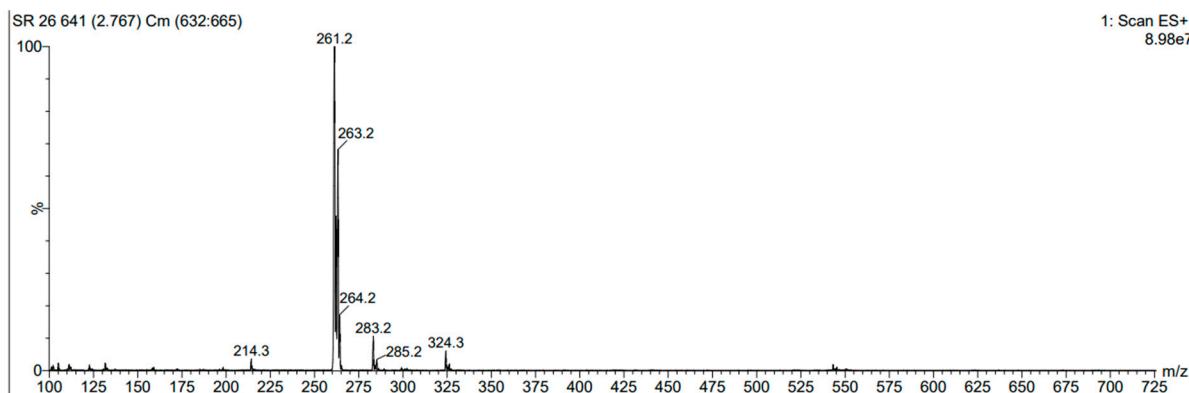


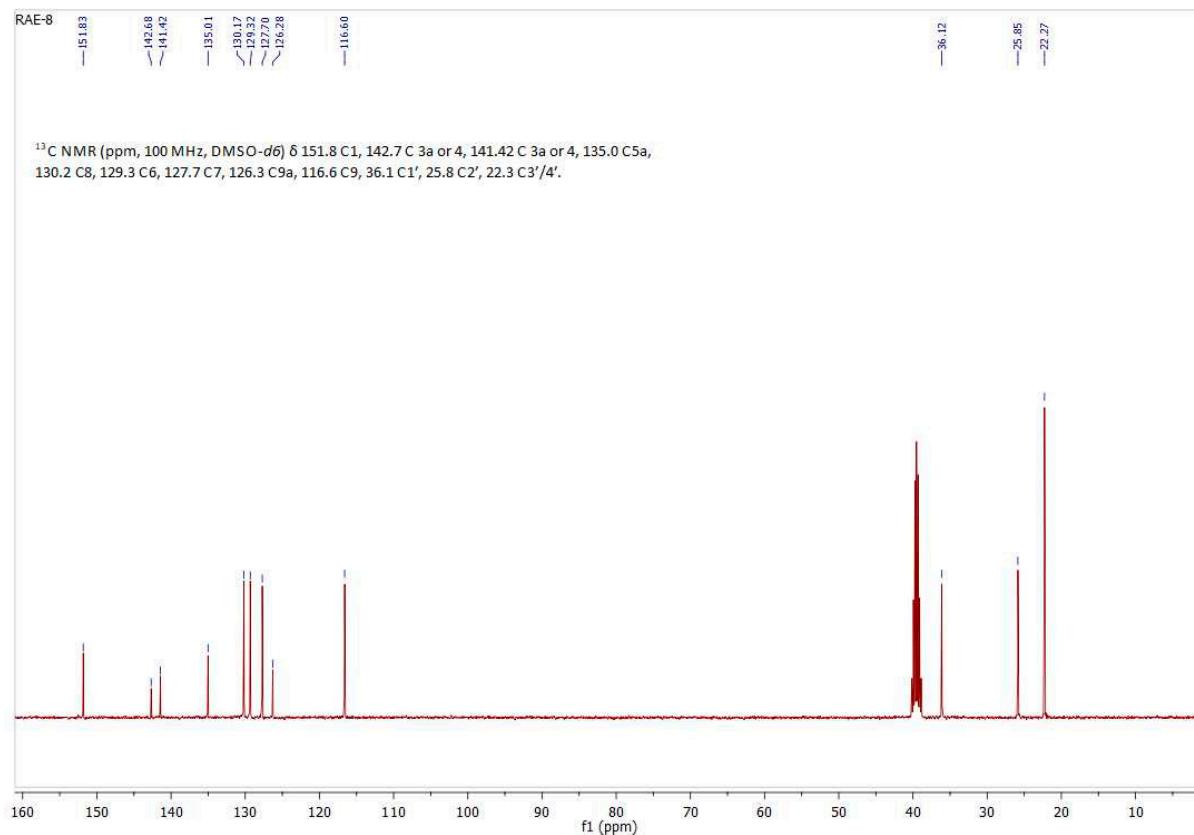




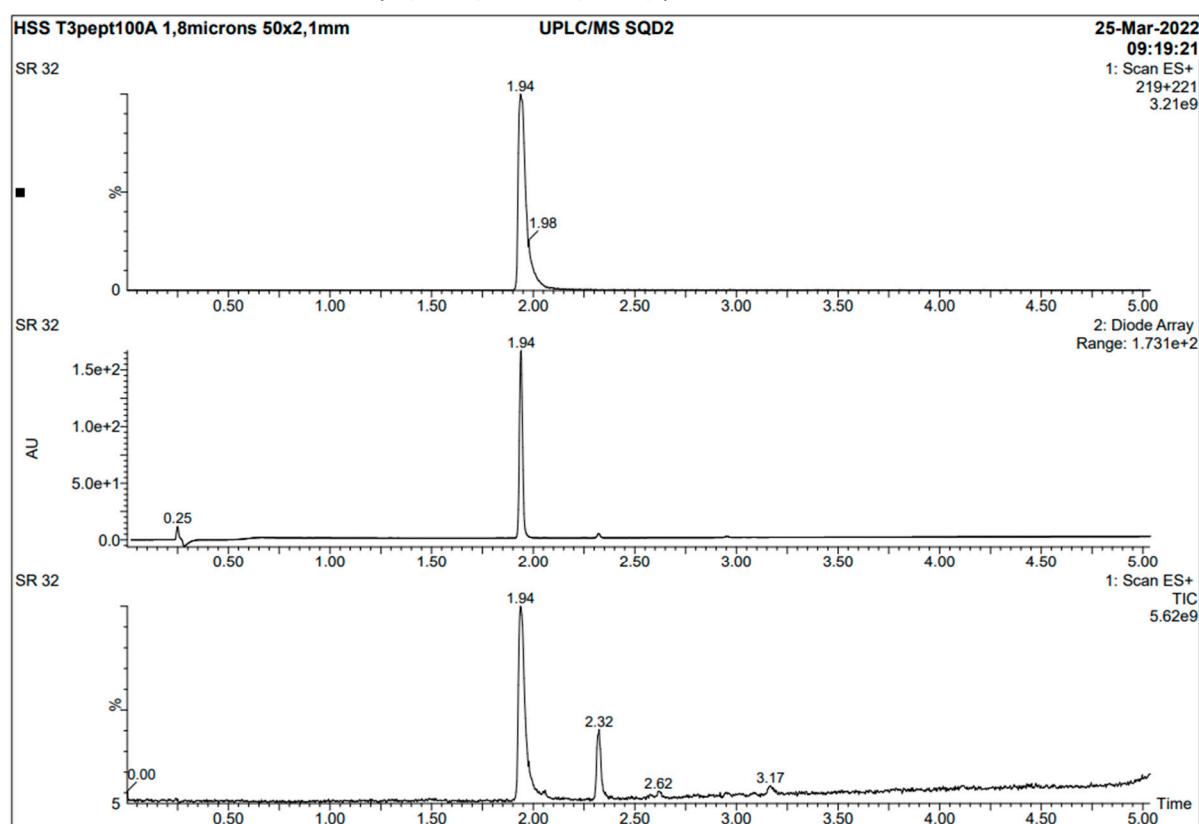
S23. *4-chloro-1-isobutyl-[1,2,4]triazolo[4,3-*a*]quinoxaline (15h).*

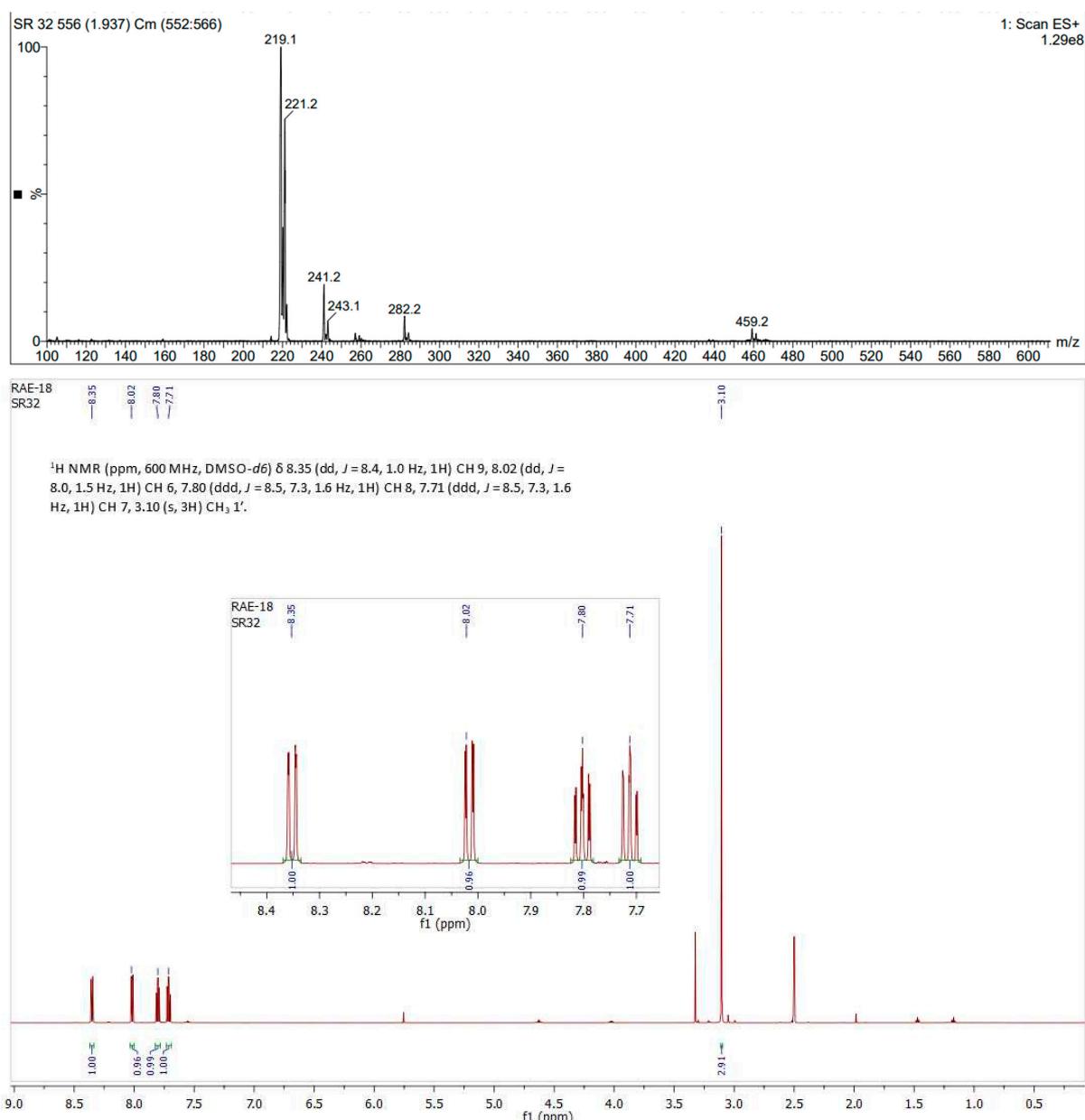


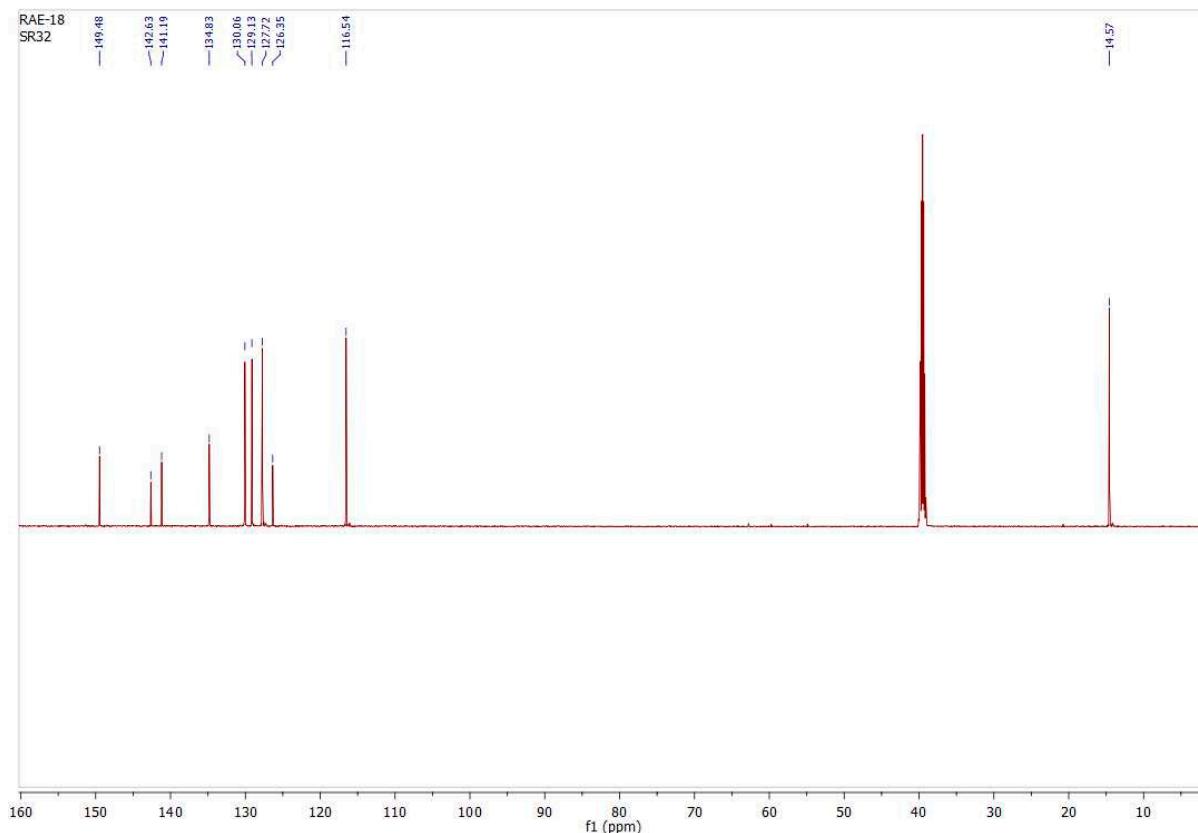




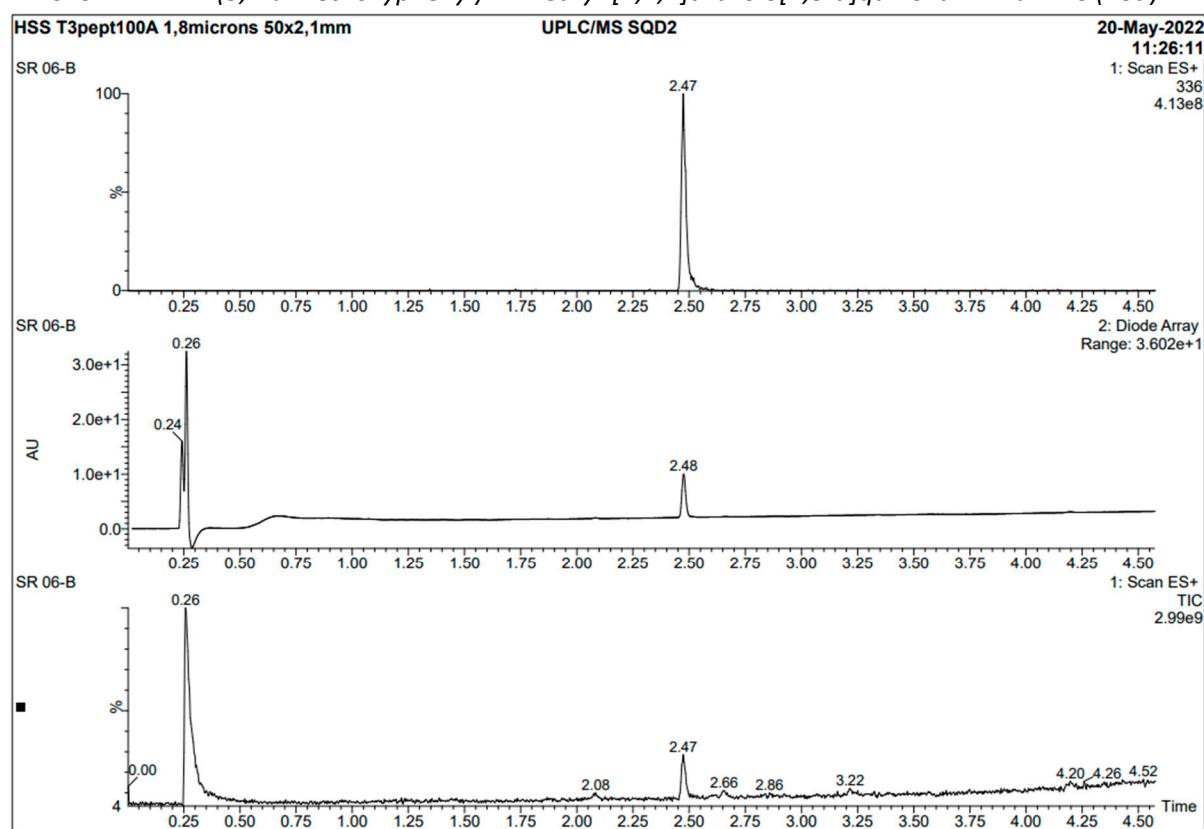
S24. 4-chloro-1-methyl-[1,2,4]triazolo[4,3-a]quinoxaline (15i).

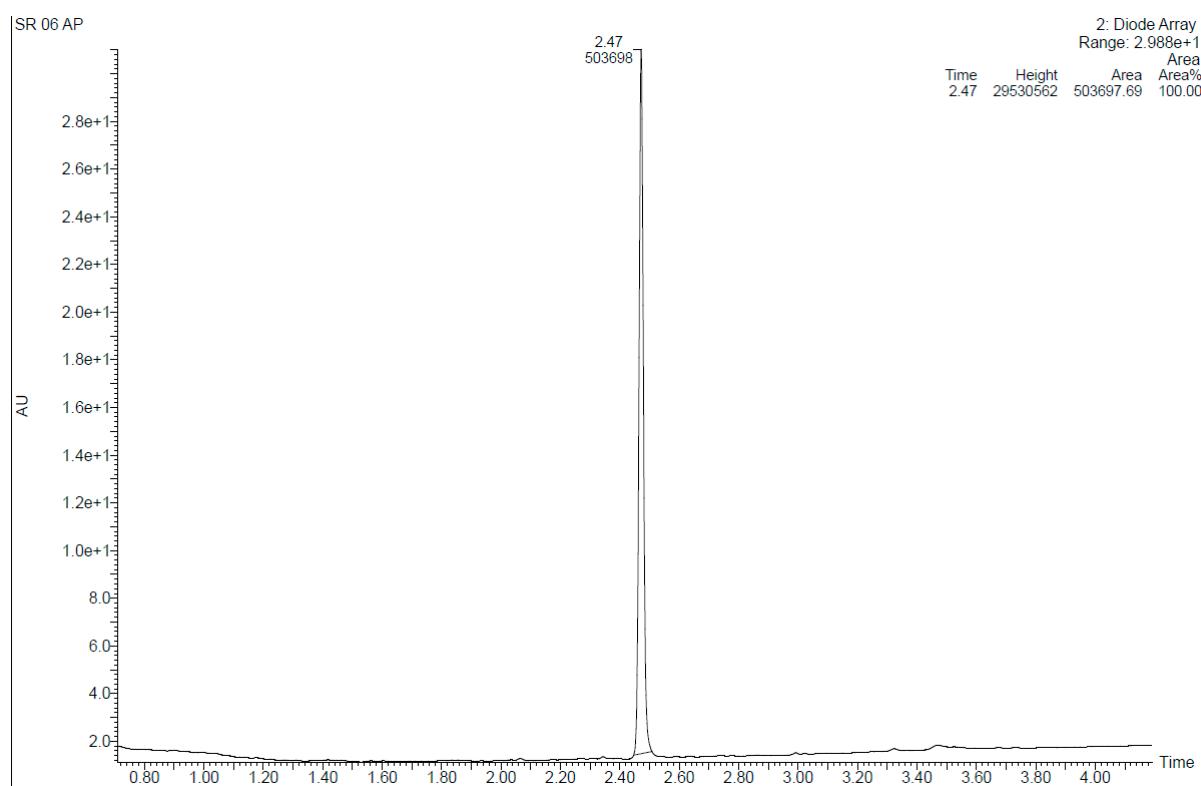
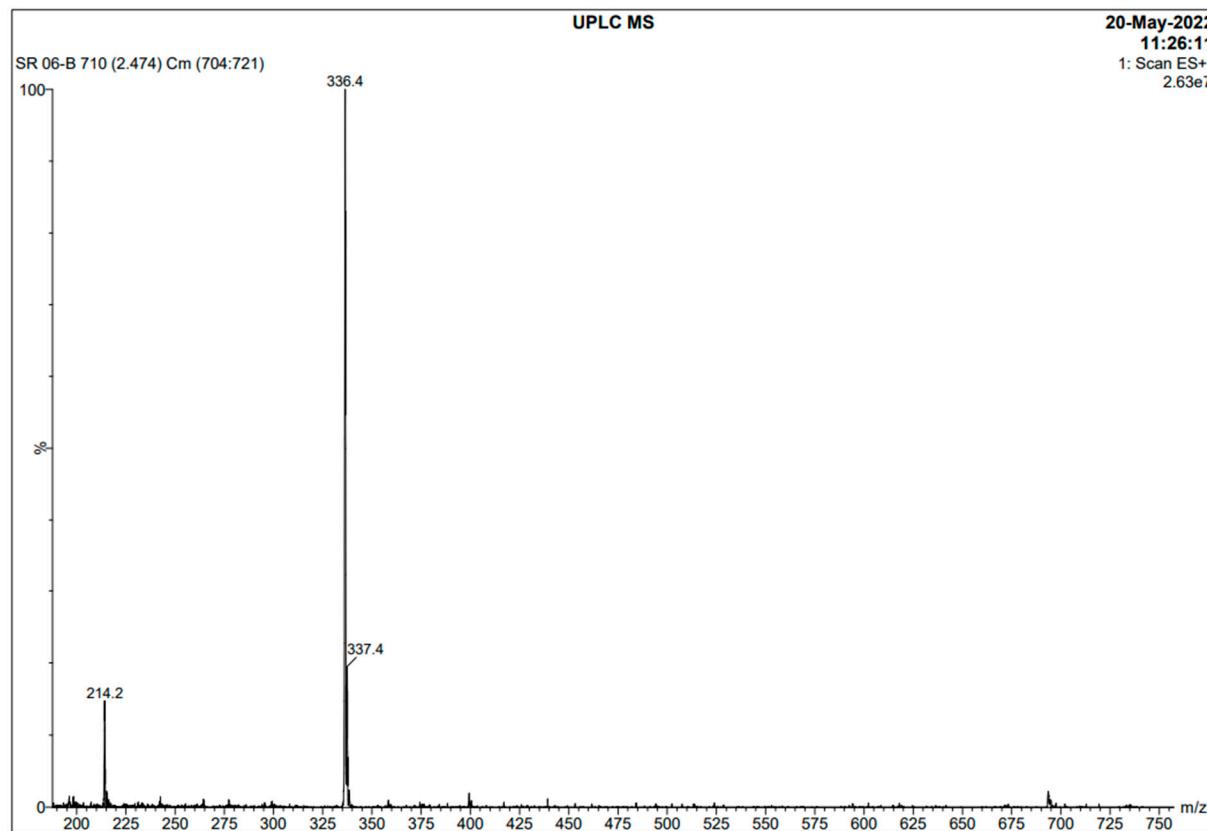






S25. 1-(3,4-dimethoxyphenyl)-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16a**).





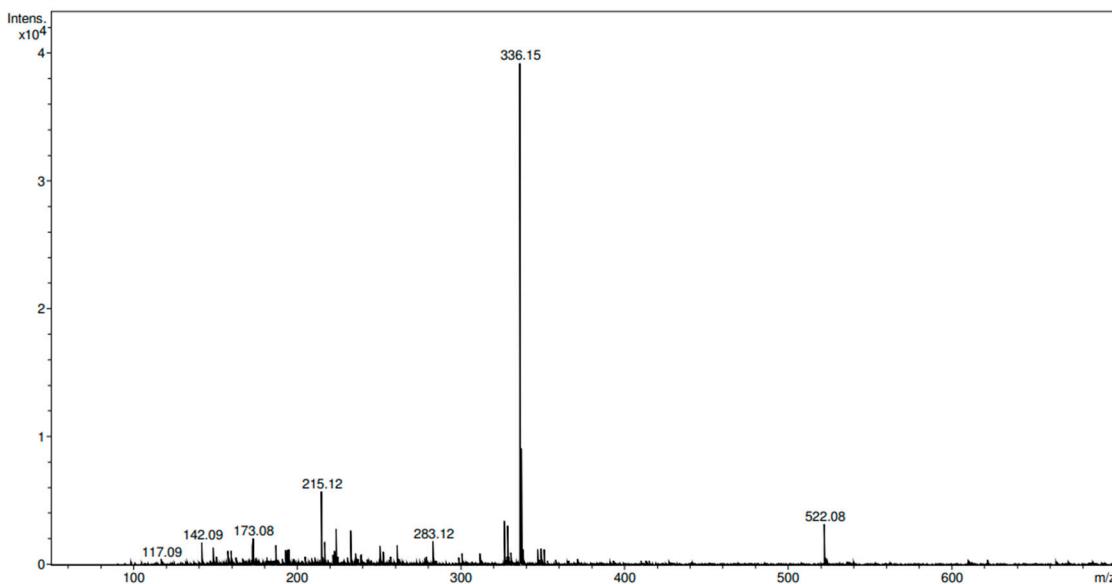
Acquisition Parameter

Source Type ESI

Ion Polarity Positive

Scan Begin 50 m/z

Scan End 2200 m/z

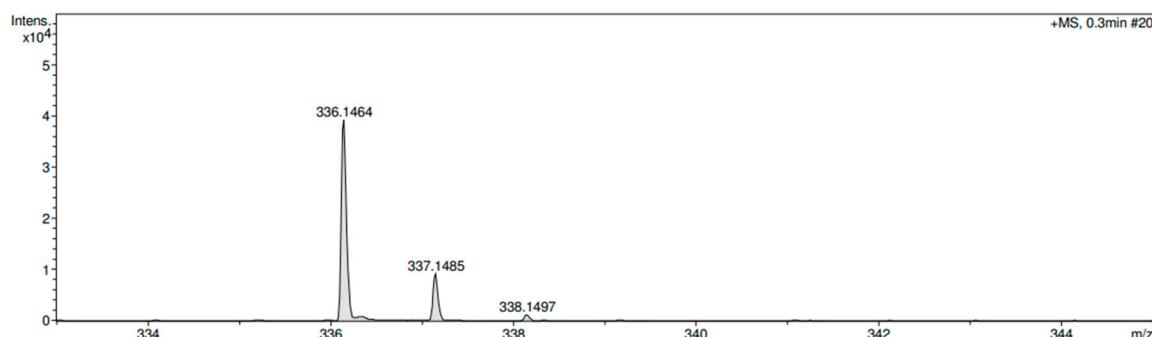

Acquisition Parameter

Source Type ESI

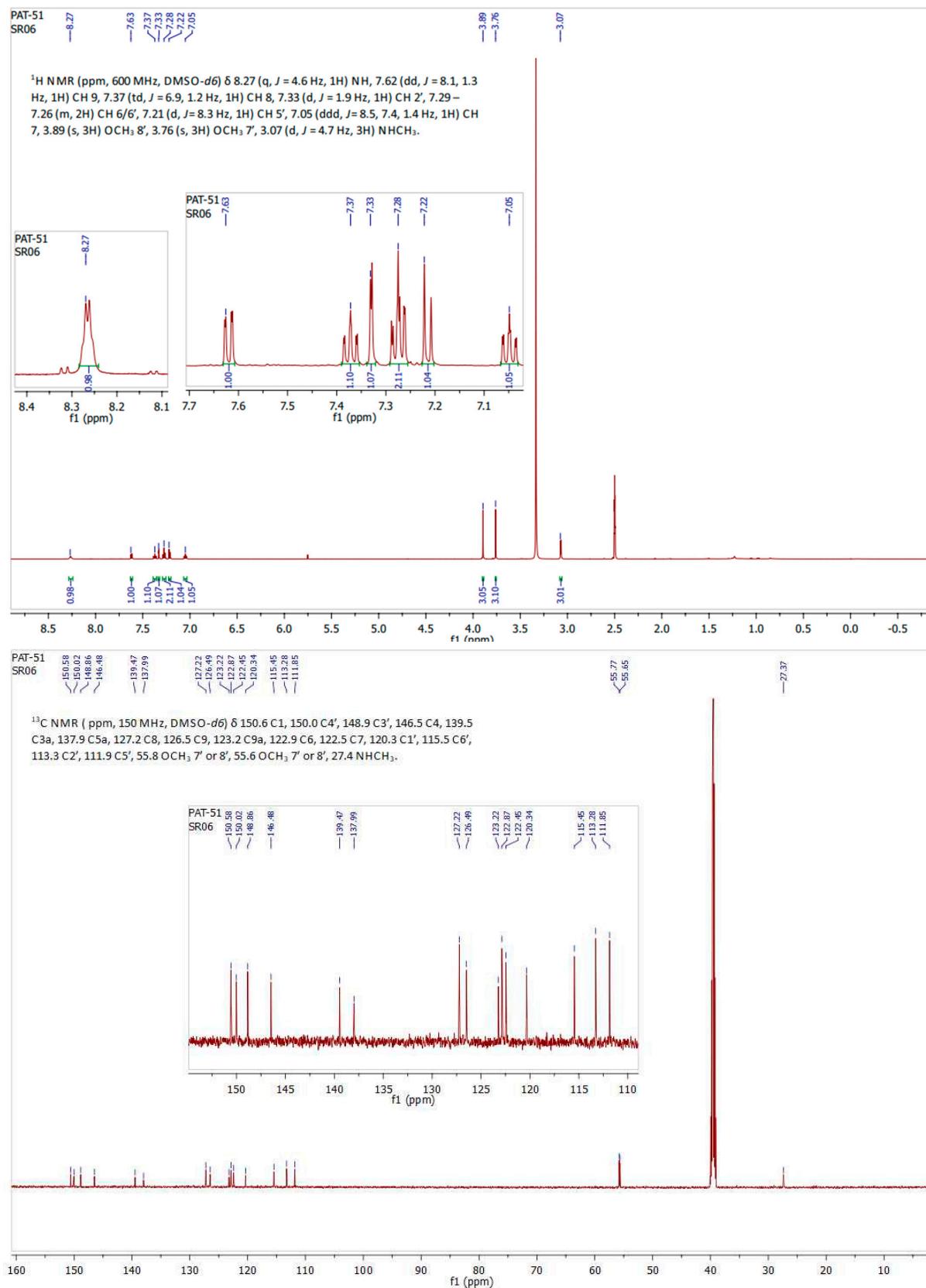
Ion Polarity Positive

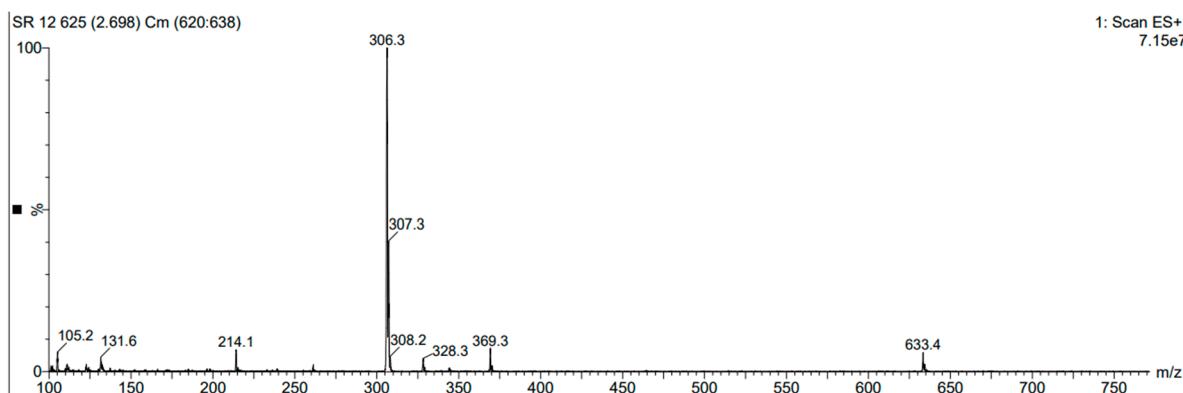
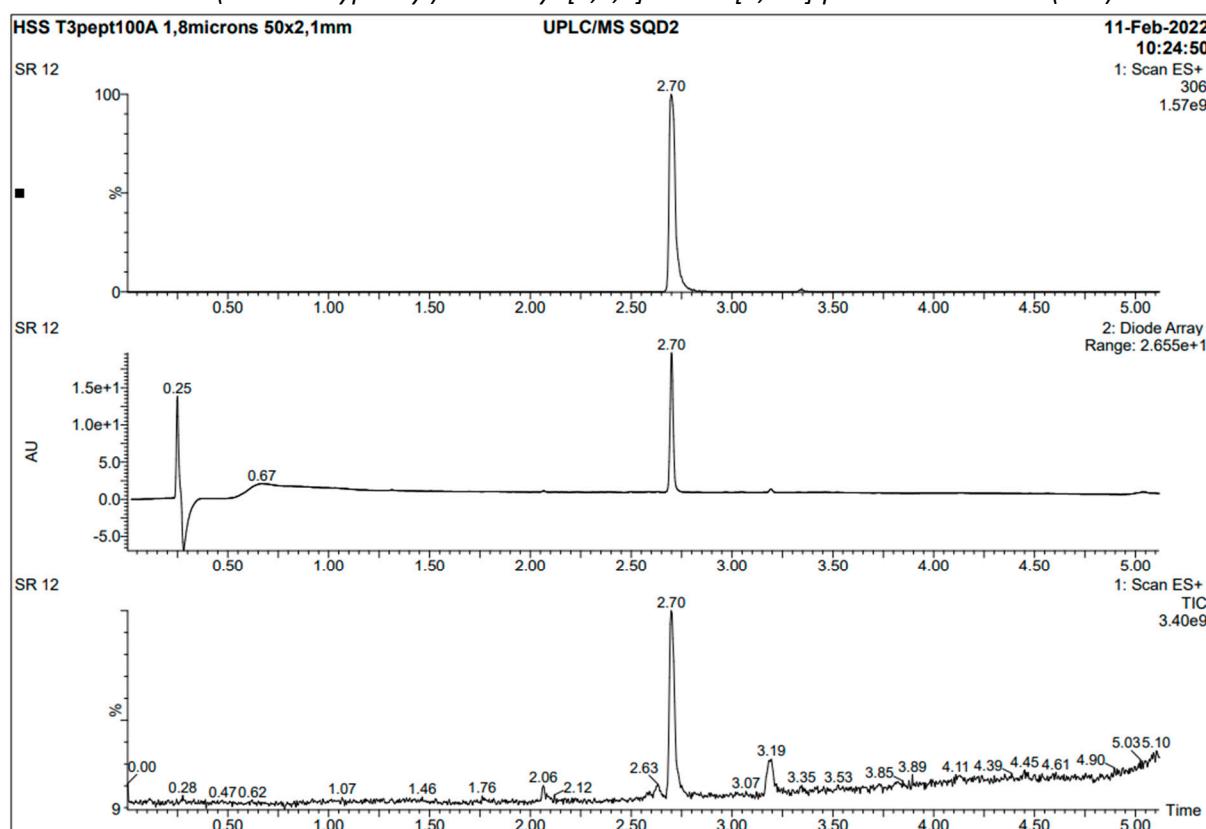
Scan Begin 50 m/z

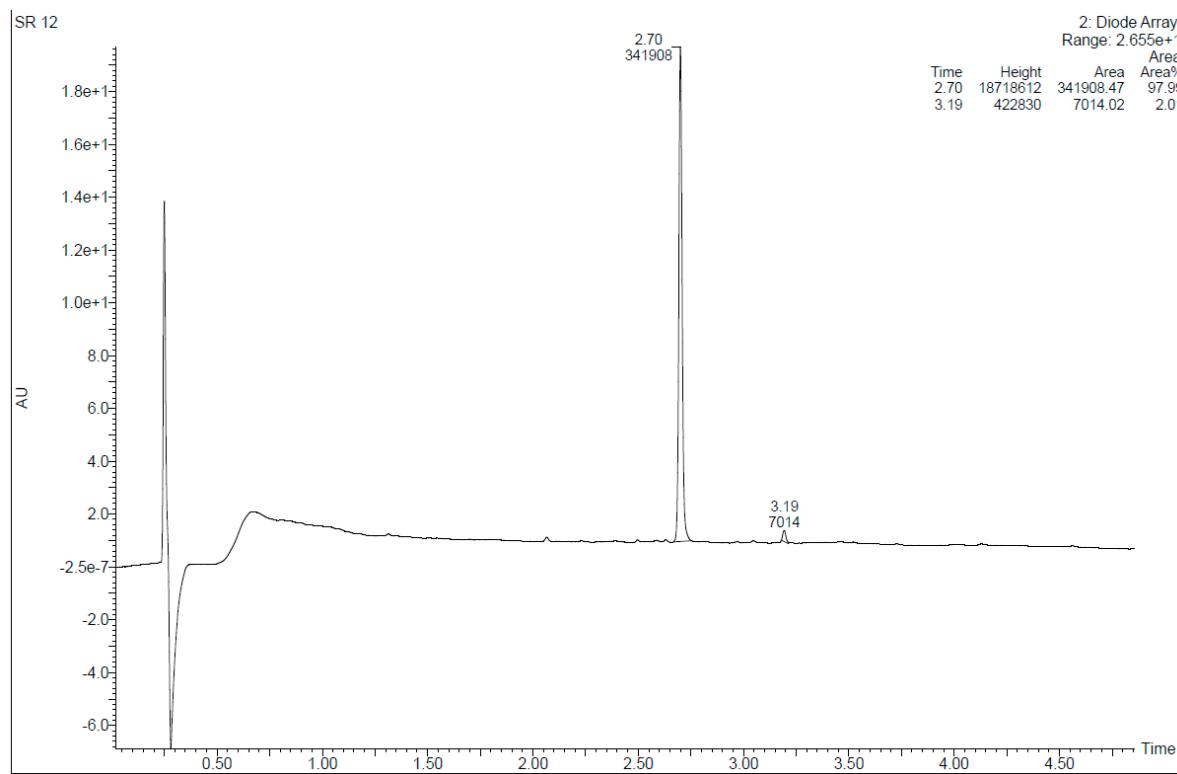
Scan End 2200 m/z



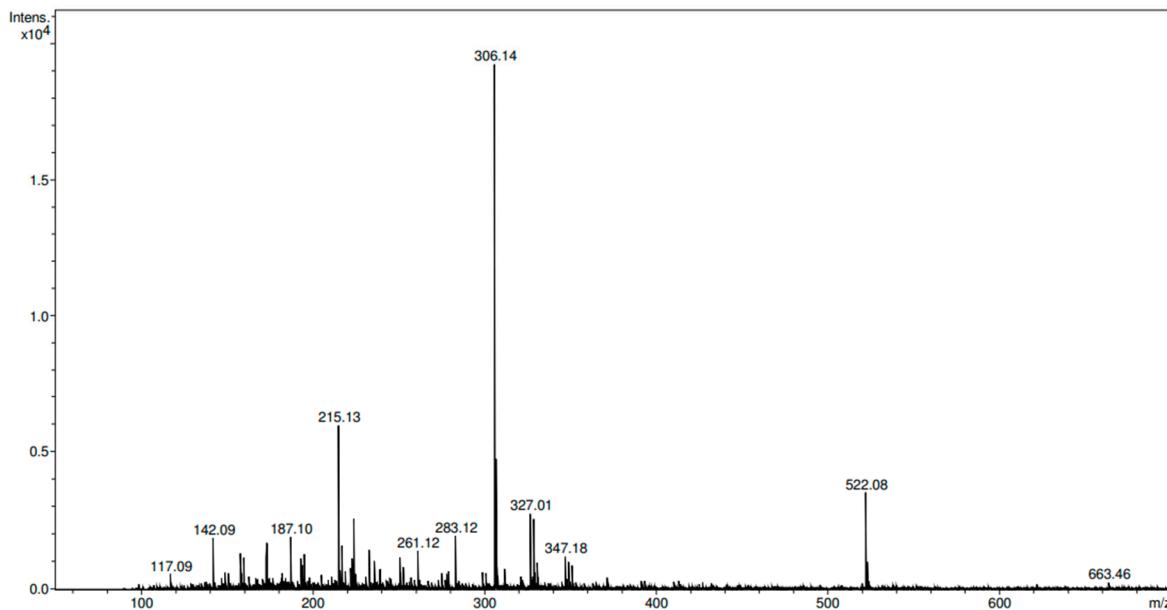
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
336.1464	1	C ₁₈ H ₁₈ N ₅ O ₂	336.1455	-2.6	9.8	1	100.00	12.5	even		ok



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

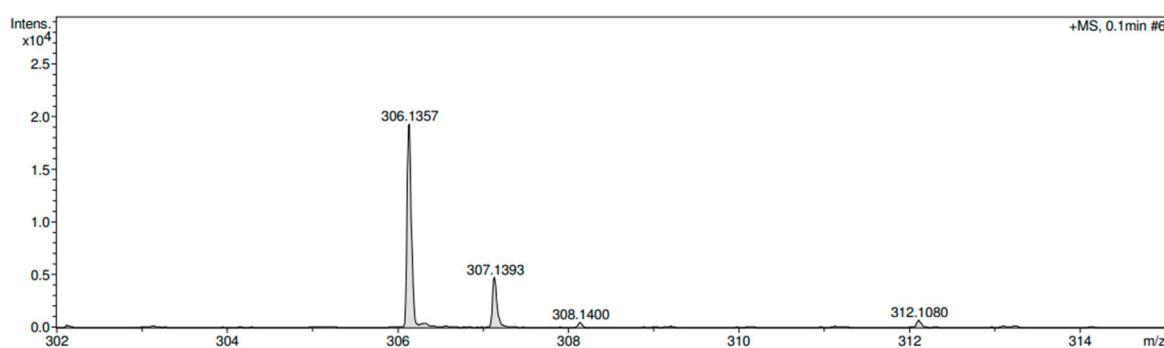
**Acquisition Parameter**

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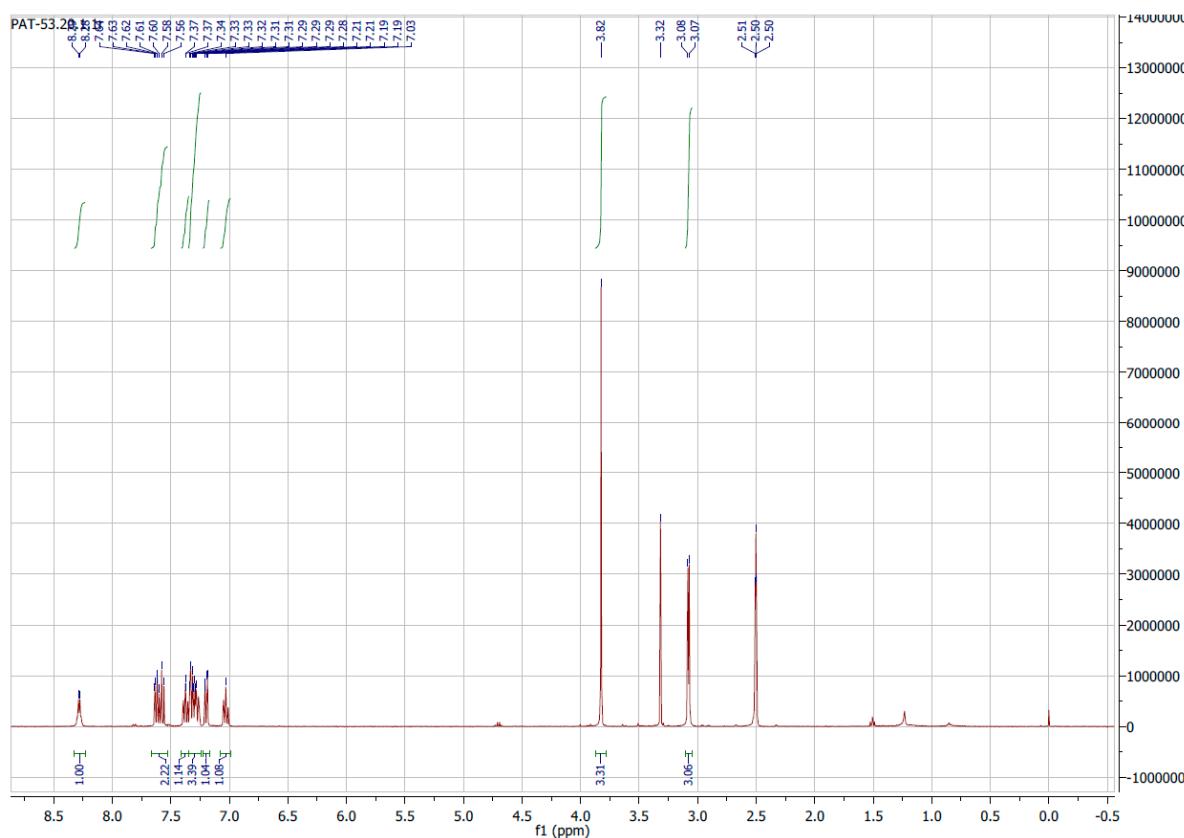


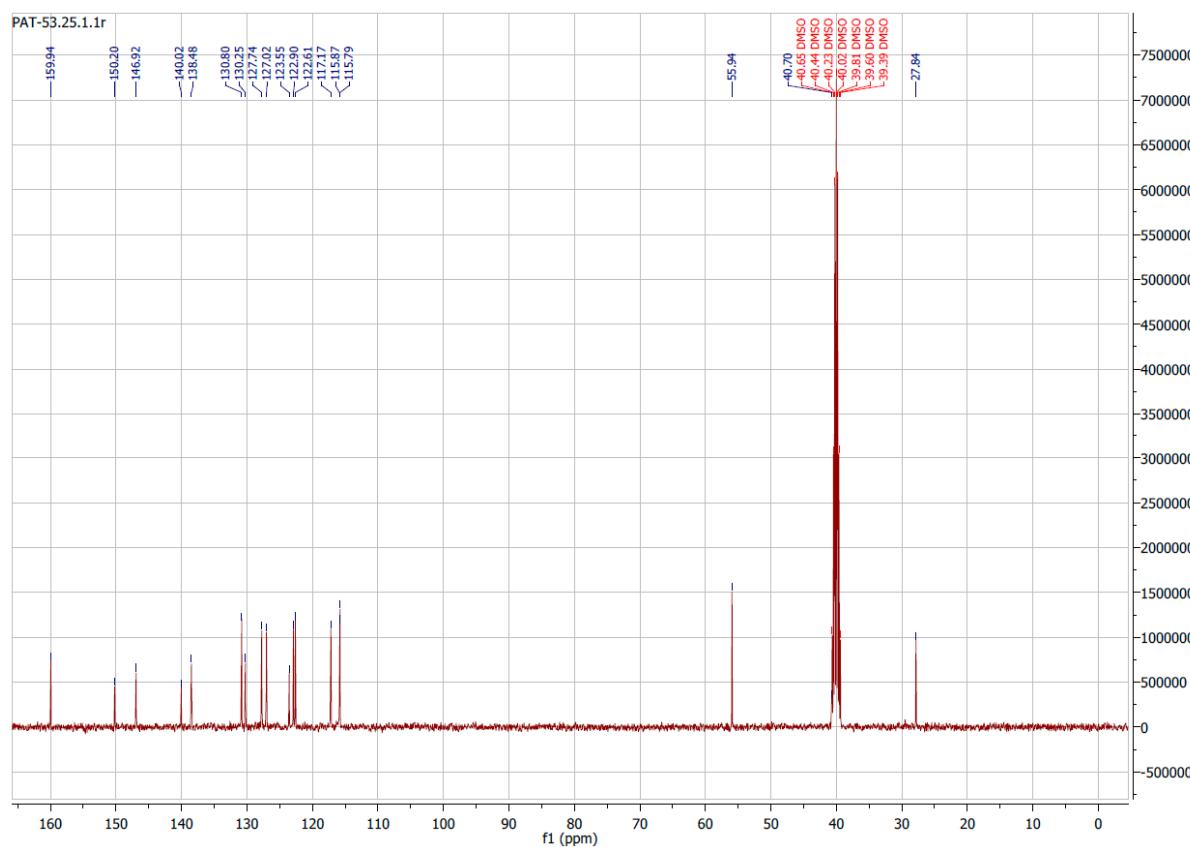
**Acquisition Parameter**

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

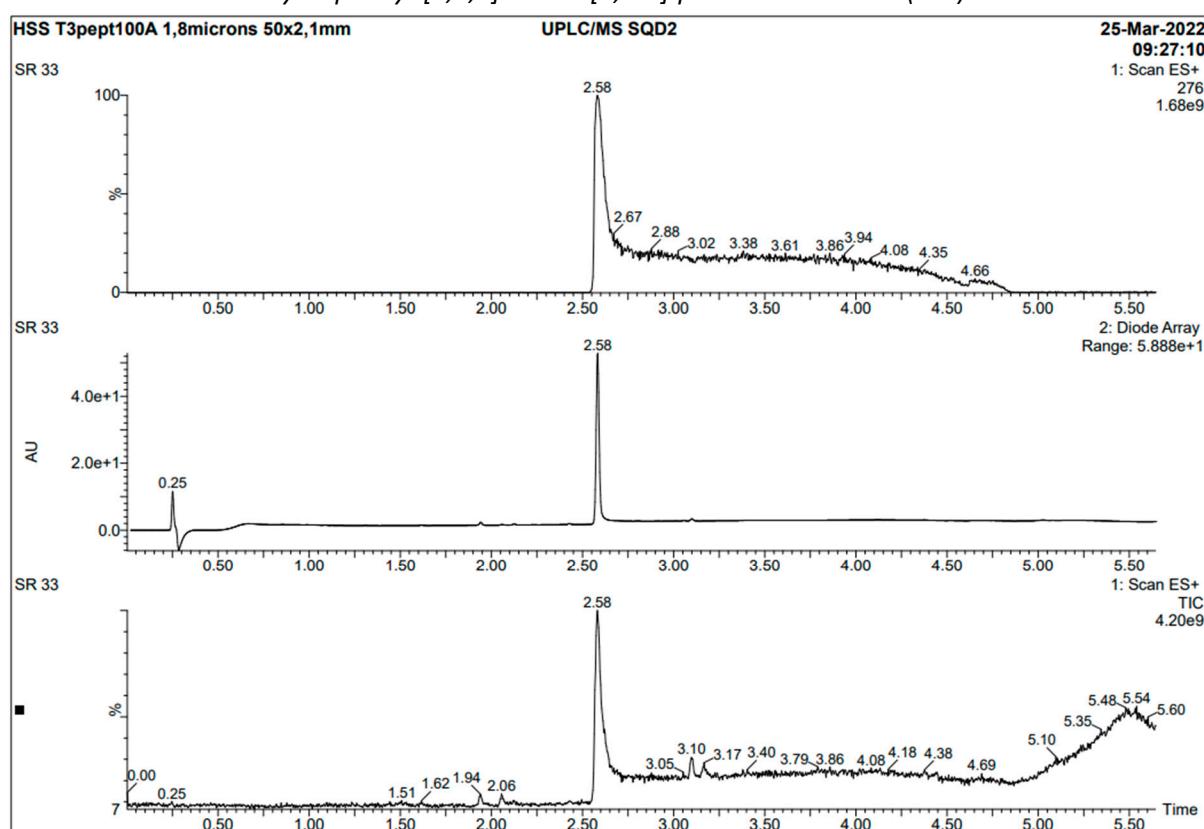


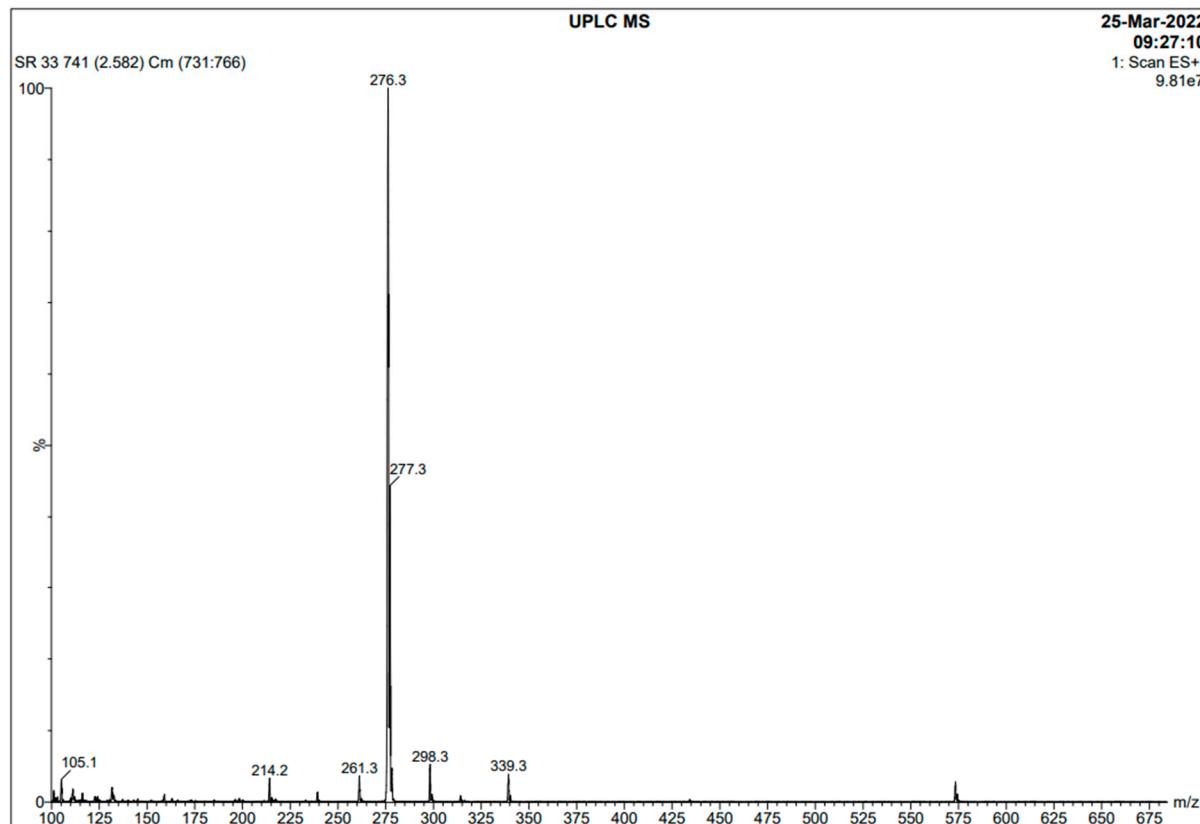
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
306.1357	1	C17H16NO	306.1349	-2.4	24.3	1	100.00	12.5	even	ok
	2	C16H20NO5	306.1336	-6.7	37.7	2	30.36	7.5	even	ok



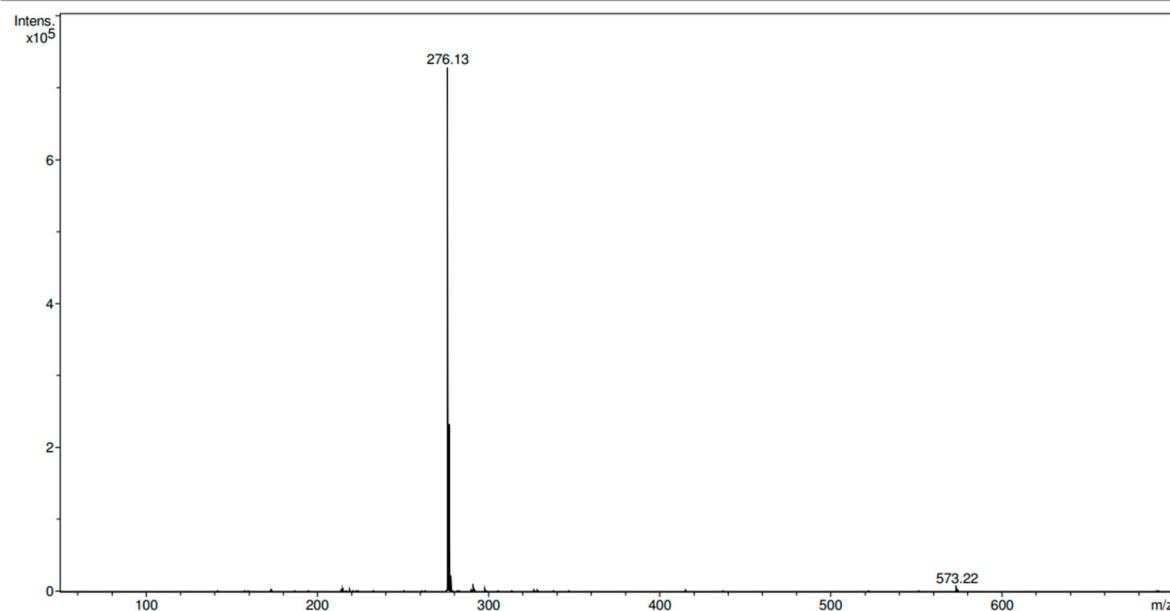


S27. *N-methyl-1-phenyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16c).*




Acquisition Parameter

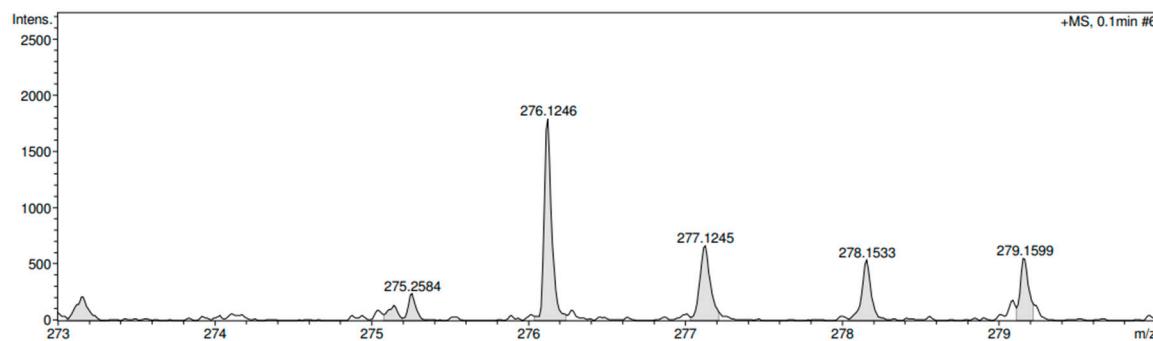
Source Type	ESI	Ion Polarity	Positive	Scan Begin	50 m/z	Scan End	2200 m/z
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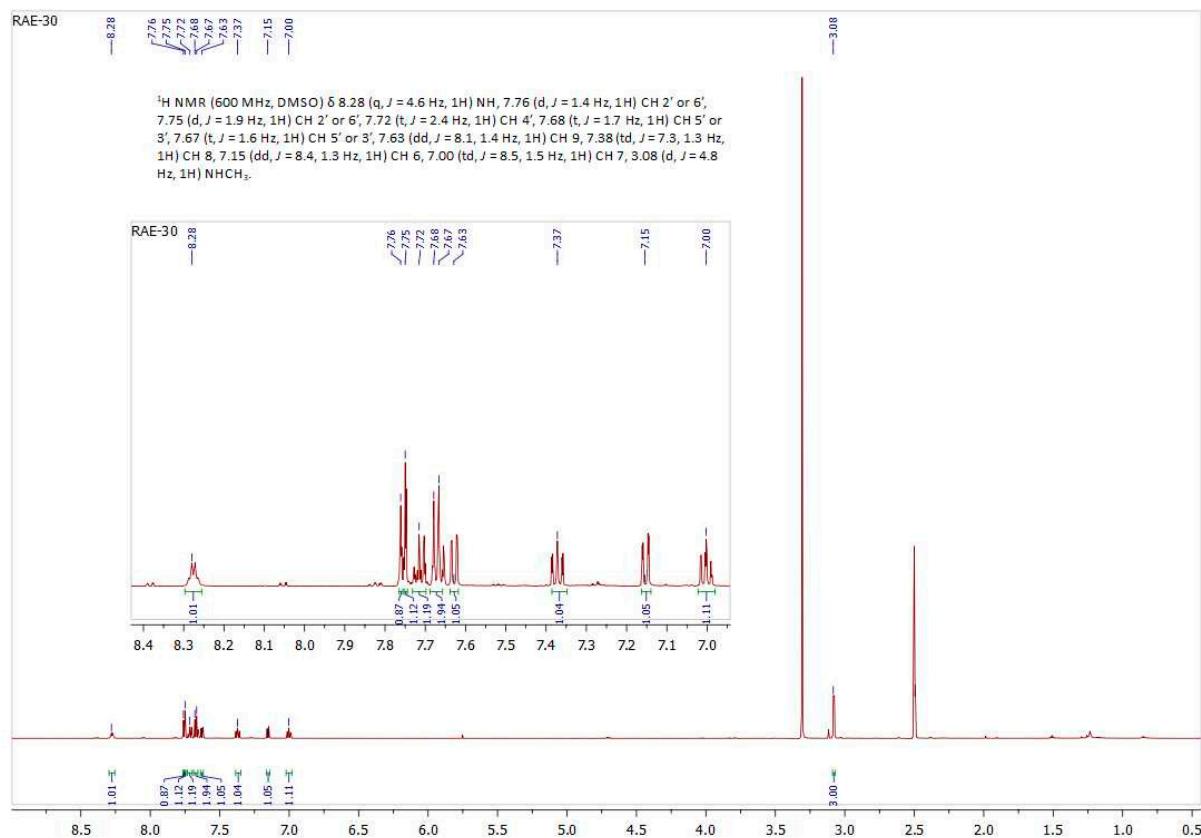


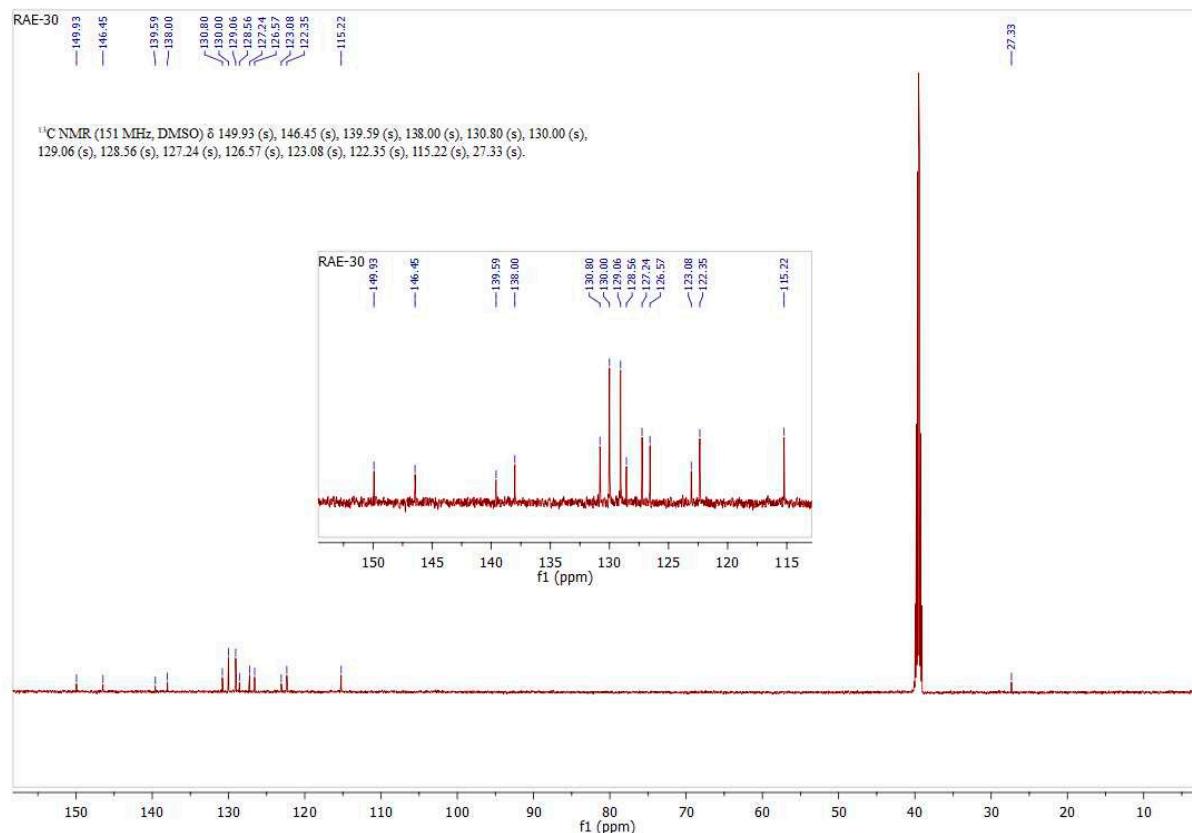
Acquisition Parameter

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

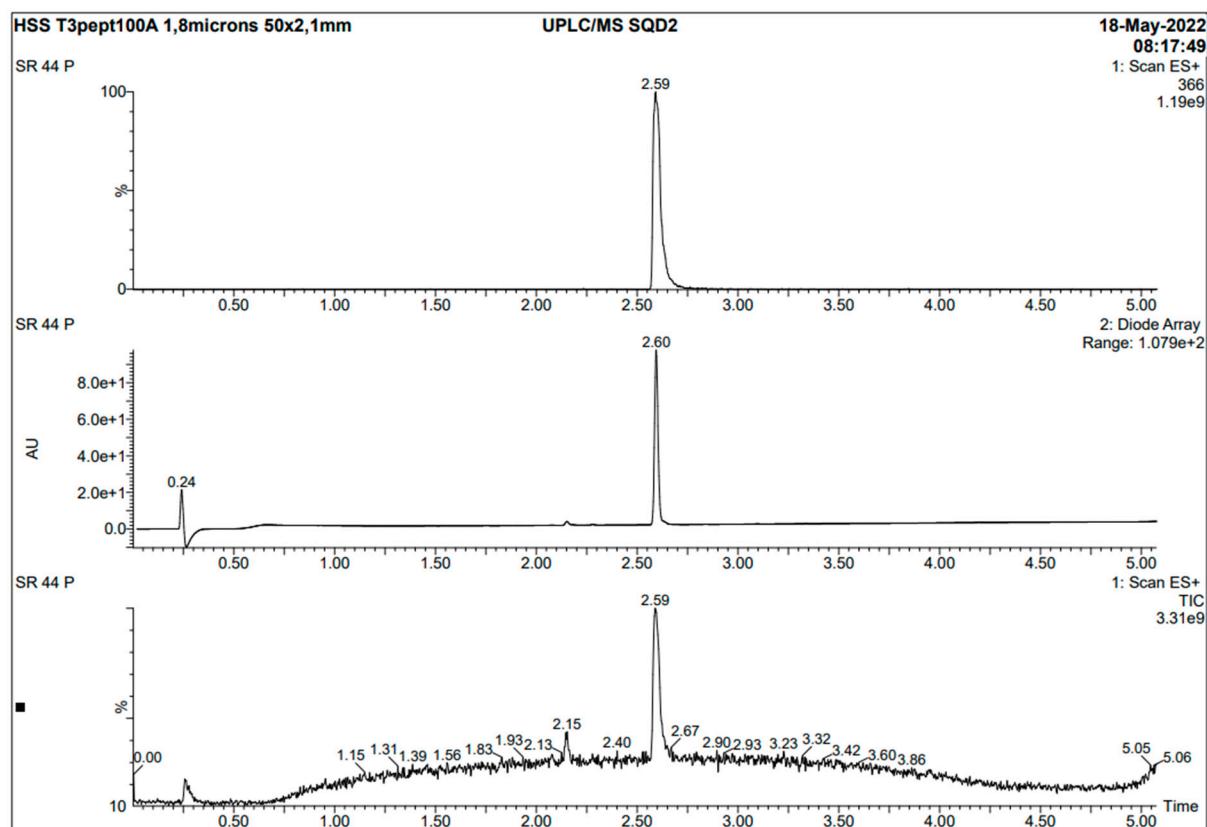


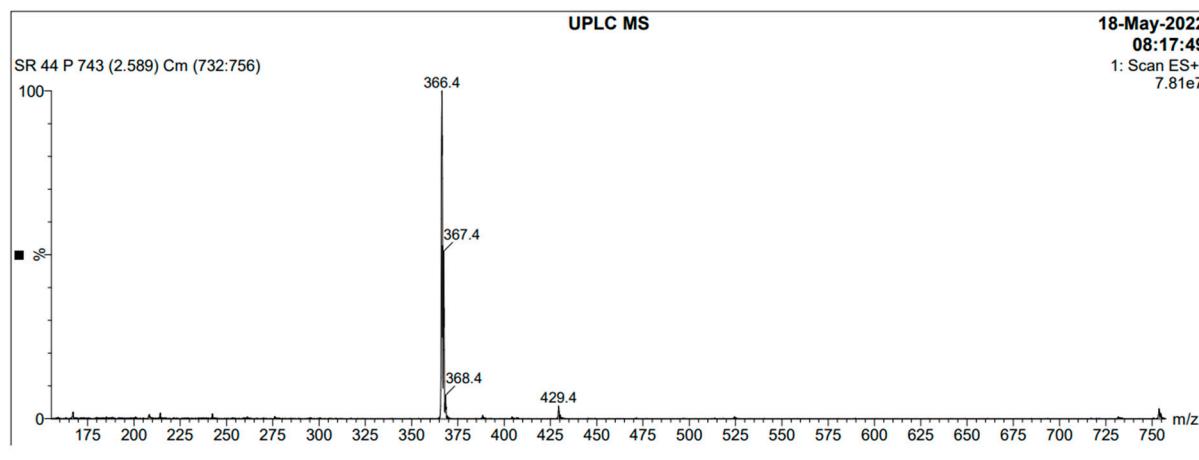
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
276.1246	1	C16H14N5	276.1244	-0.7	193.1	1	100.00	12.5	even	ok
	2	C15H18NO4	276.1230	-5.6	198.9	2	29.82	7.5	even	ok



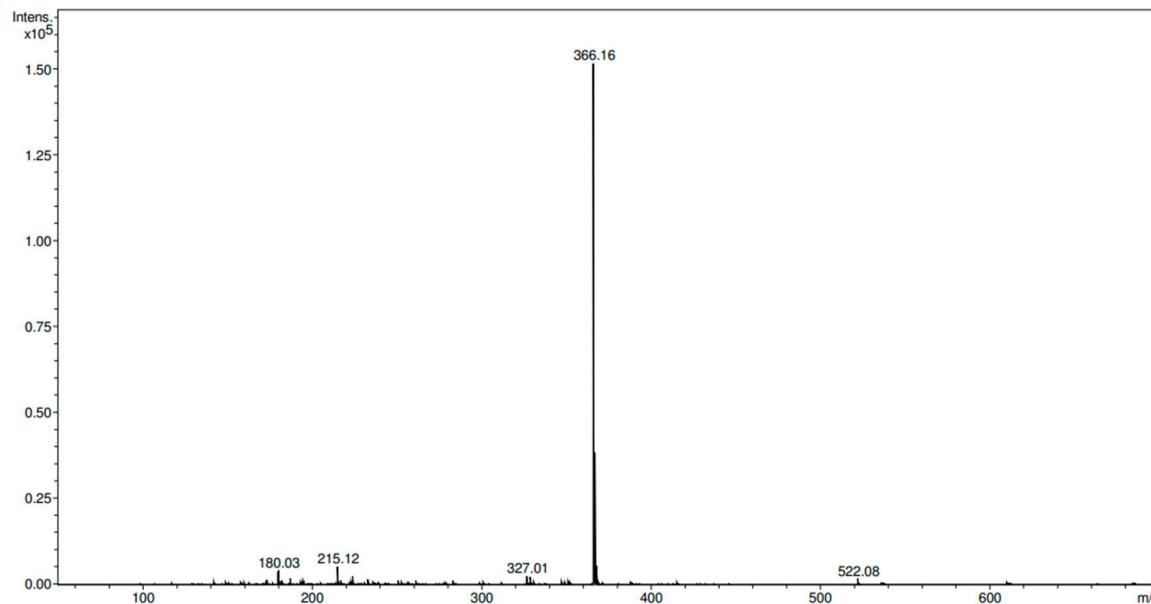


S28. *N-methyl-1-(3,4,5-trimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16d).*

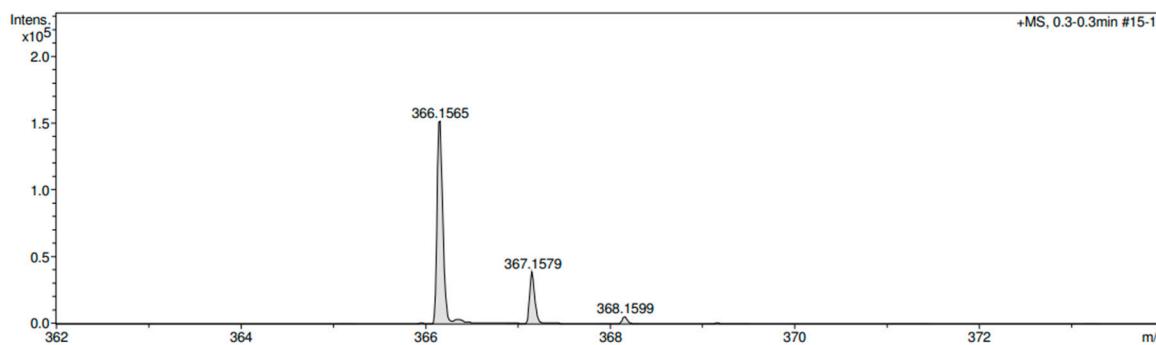


**Acquisition Parameter**

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 ⁻ Conf	N-Rule
366.1565	1	C ₁₉ H ₂₀ N ₅ O ₃	366.1561	1.1	15.8	1	100.00	12.5	even	ok

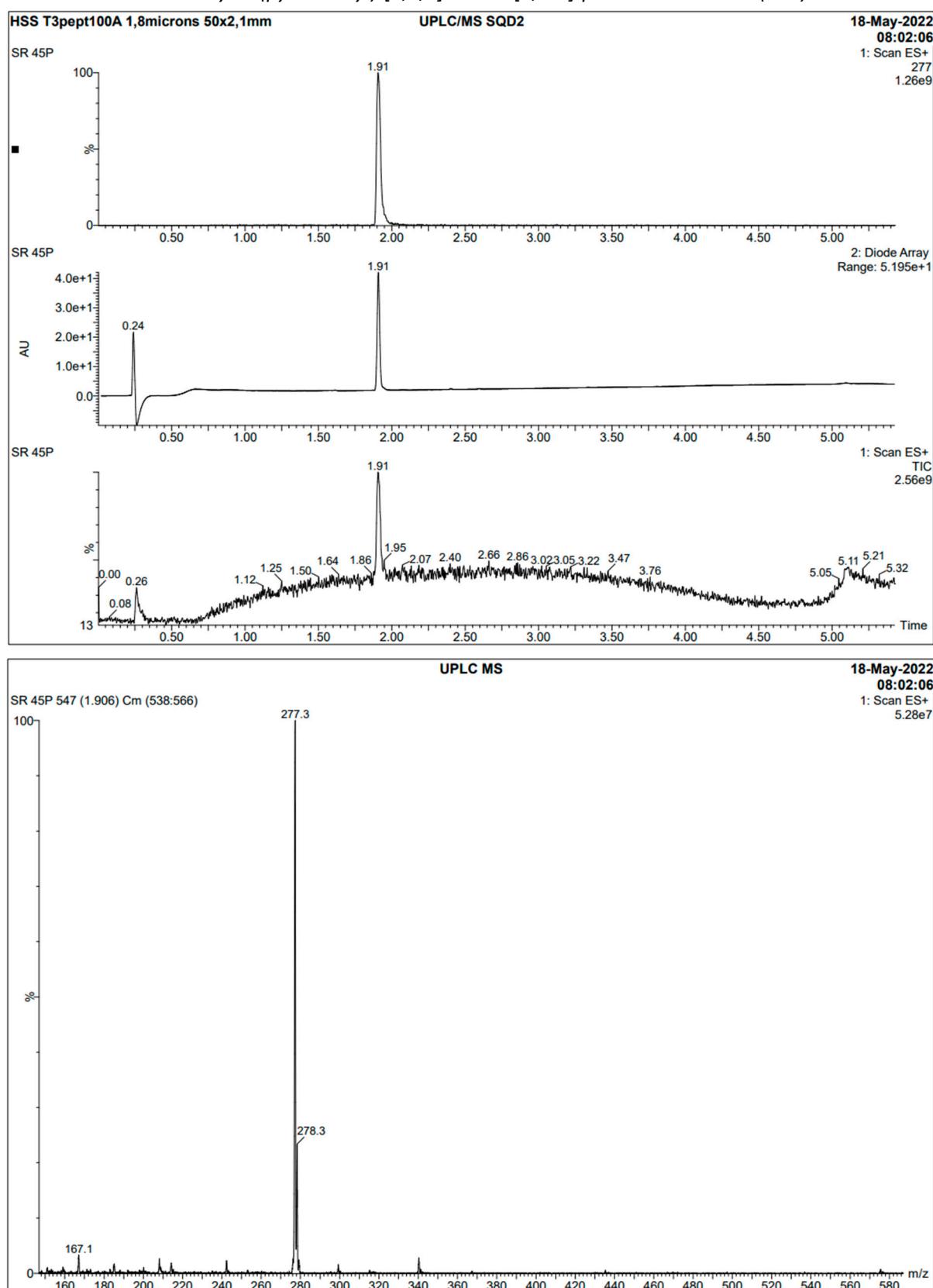
RAE-35
SR44

¹H NMR (600 MHz, DMSO) δ 8.28 (d, *J* = 3.4 Hz, 1H) NH, 7.63 (d, *J* = 7.6 Hz, 1H) CH9, 7.39 (t, *J* = 7.4 Hz, 1H) CH8, 7.28 (d, *J* = 8.1 Hz, 1H) CH6, 7.12 – 7.05 (m, 3H) CH7/2'/6'; 3.81 (s, 3H) OCH₃, 3.79 (s, 6H) 2^oOCH₃, 3.07 (s, *J* = 3.2 Hz, 3H) NHCH₃.

RAE-35
SR44RAE-35
SR44

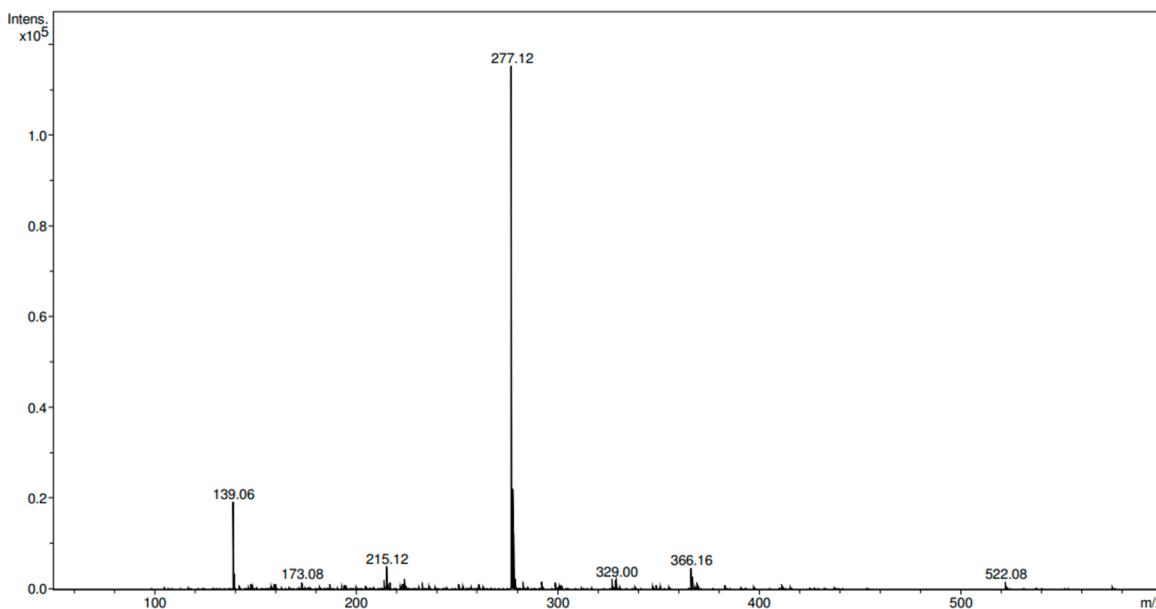
¹³C NMR (151 MHz, DMSO) δ 153.3 C4', 149.9 C1, 146.4 C4, 139.4 C3a, 139.2 C1', 138.0 C9a, 127.3 C8, 126.5 C9, 123.6 C3' or 5', 123.1 C3' or 5', 122.5 C7, 115.62 C6, 107.6 C2'/6', 60.3 OCH₃, 56.2 2^oOCH₃, 27.4 NHCH₃.

RAE-35
SR44

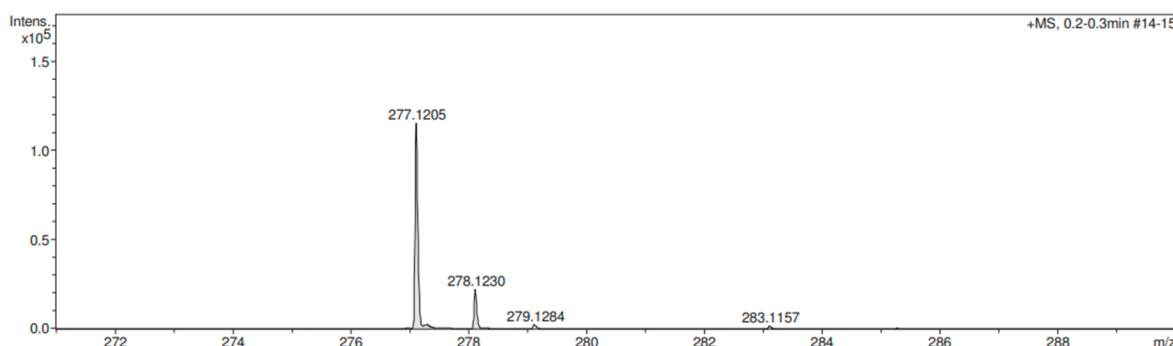
S29. *N*-methyl-1-(pyridin-3-yl)-[1,2,4]triazolo[4,3-*a*]quinoxalin-4-amine (**16e**).

**Acquisition Parameter**

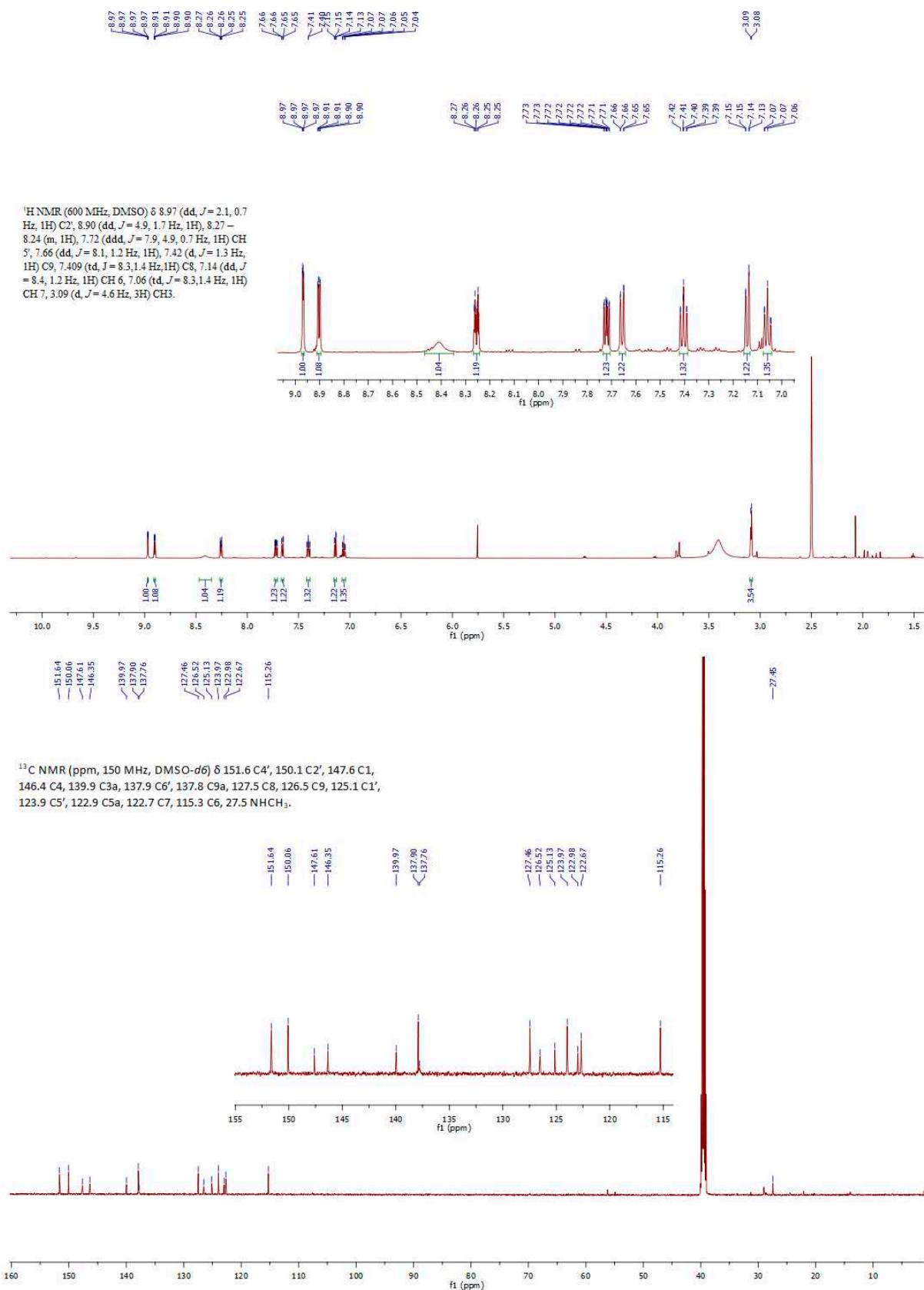
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

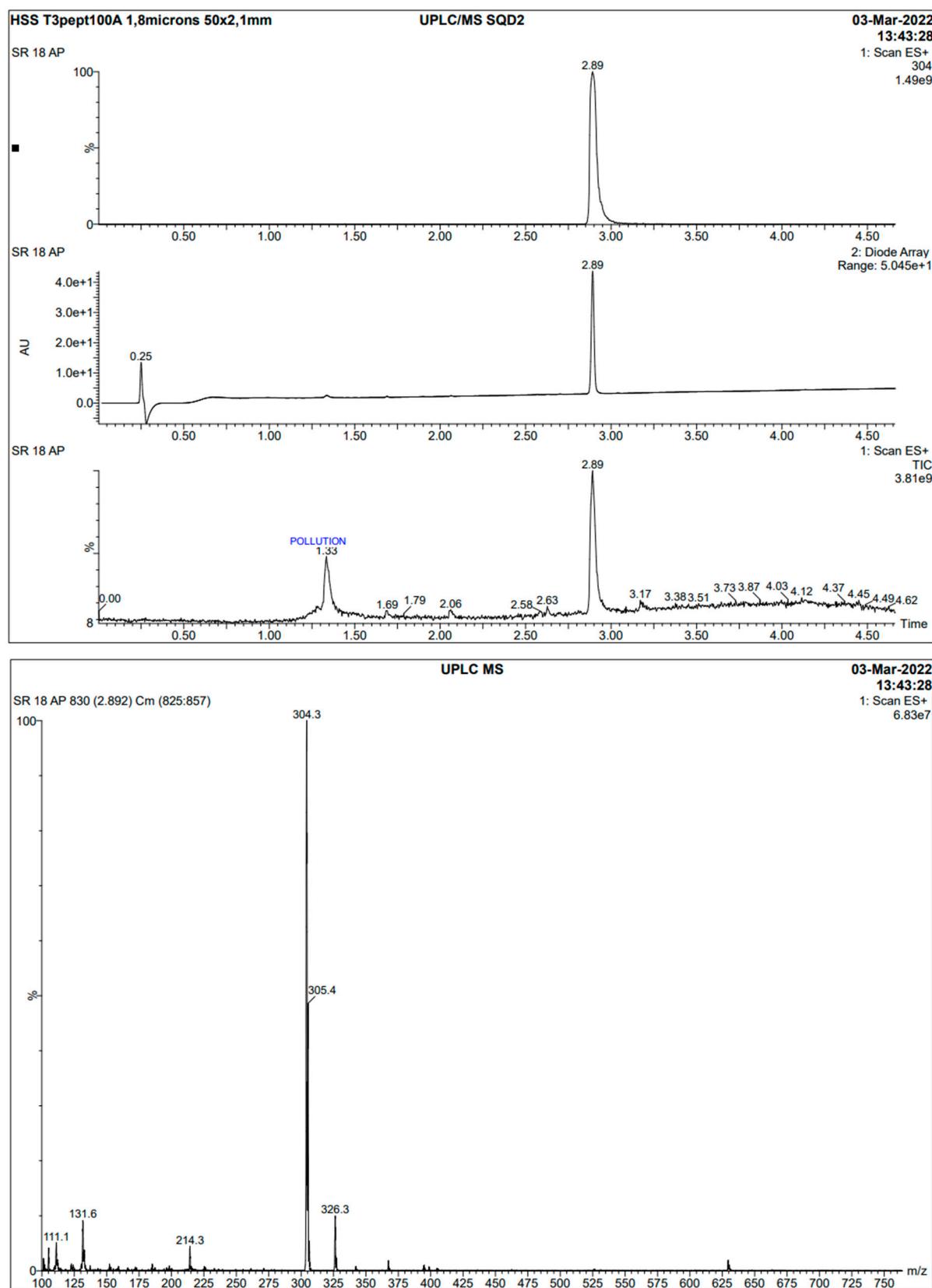
**Acquisition Parameter**

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



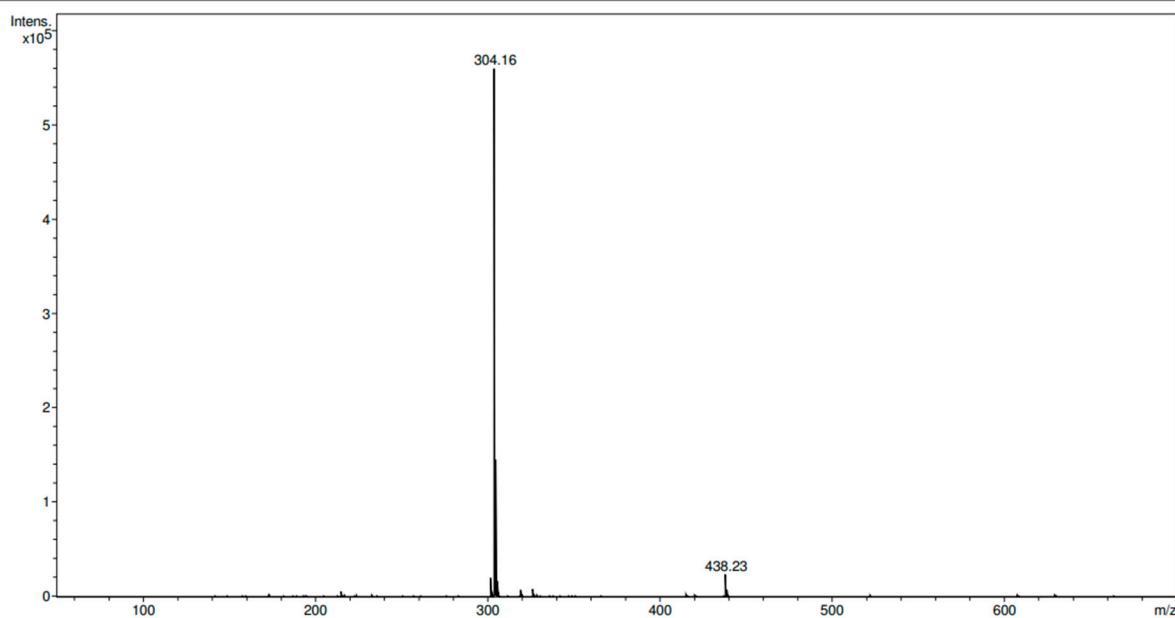
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
277.1205	1	C15H13N6	277.1196	3.0	4.1	1	100.00	12.5	even	ok



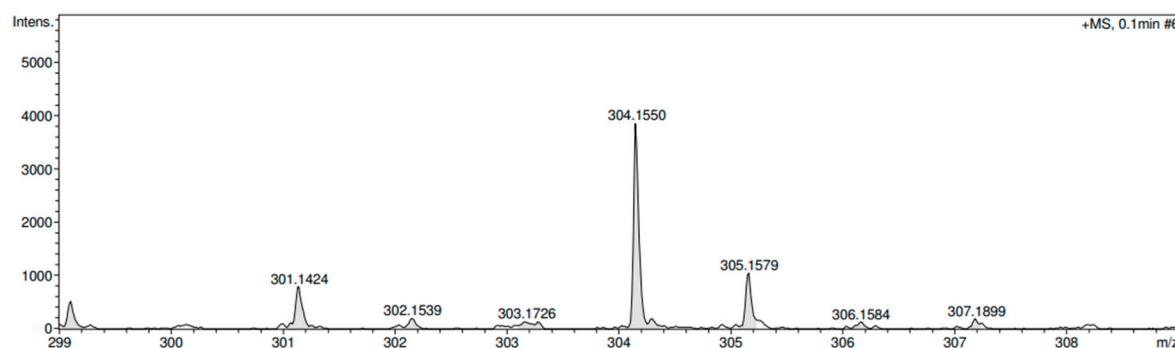
S30. *N-methyl-1-phenethyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16f).*

**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 ⁻ Conf	N-Rule
304.1550	1	C ₁₈ H ₁₈ N ₅	304.1557	2.1	32.5	1	100.00	12.5	even	ok



RAE-6

—8.16
—8.07
—7.65
—7.45
—7.37
—7.32
—7.23

¹H NMR (ppm, 600 MHz, DMSO-*d*6) δ 8.15 (d, *J* = 3.9 Hz, 1H) NH, 8.07 (d, *J* = 8.1 Hz, 1H) CH 9, 7.64 (d, *J* = 7.9 Hz, 1H) CH 6, 7.45 (t, *J* = 7.7 Hz, 1H) CH 7, 7.38 (d, *J* = 7.3 Hz, 2H) CH 4'/8', 7.34 – 7.30 (m, 3H) CH 8/5'/7', 7.23 (t, *J* = 7.2 Hz, 1H) CH 6', 3.72 (t, *J* = 7.9 Hz, 2H) CH₂ 1', 3.29 (t, *J* = 7.9 Hz, 2H) CH₂ 2', 3.04 (d, *J* = 4.3 Hz, 3H) CH₃.

RAE-6

—8.16
—8.07

—7.65
—7.45
—7.37
—7.32
—7.23

RAE-6

—150.99
—146.44
—140.52
—139.70
—137.81
—128.49
—128.34
—127.01
—126.31
—126.15
—123.37
—122.99
—116.02

—31.84
—29.54
—27.21

¹³C NMR (ppm, 150 MHz, DMSO-*d*6) δ 150.9 C1, 146.4 C4, 140.5 C3', 139.7 C3a, 137.8 C5a, 128.4 C4/8', 128.3 C5/8', 127.0 C7, 126.3 C6, 126.1 C6', 123.3 C9a, 122.9 C8, 116.0 C9, 31.84 C2, 29.5 C1', 27.2 CH₃.

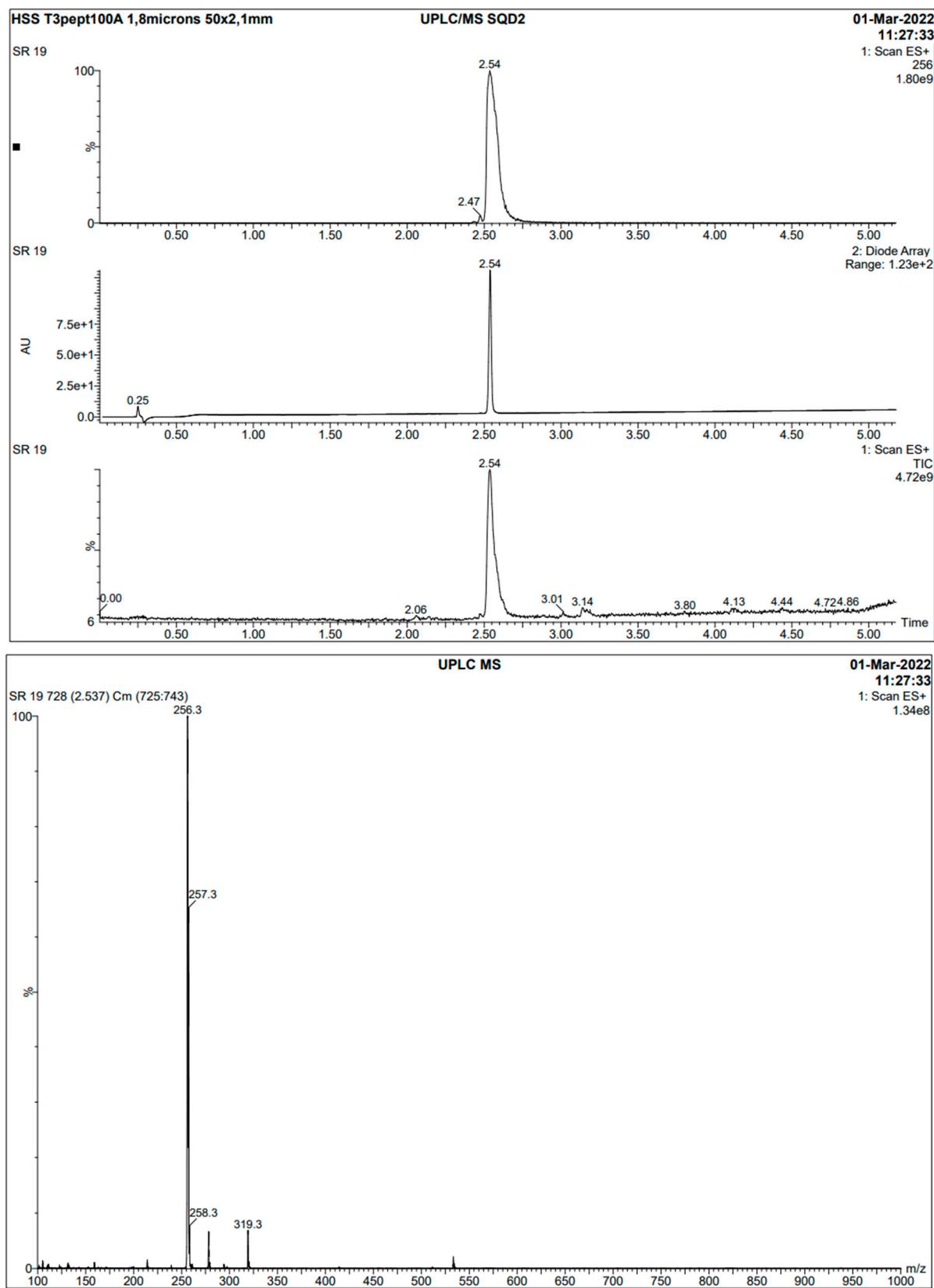
RAE-6

—150.99
—146.44
—140.52
—139.70
—137.81
—128.49
—128.34
—127.01
—126.31
—126.15
—123.37
—122.99
—116.02

—31.84
—29.54
—27.21

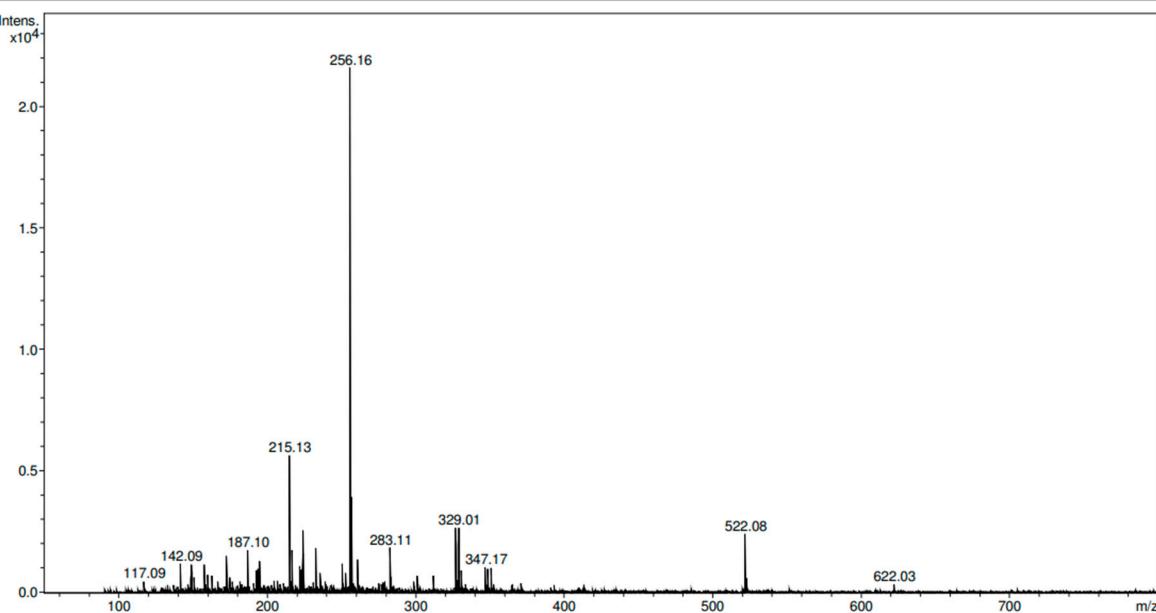
RAE-6

f1 (ppm)

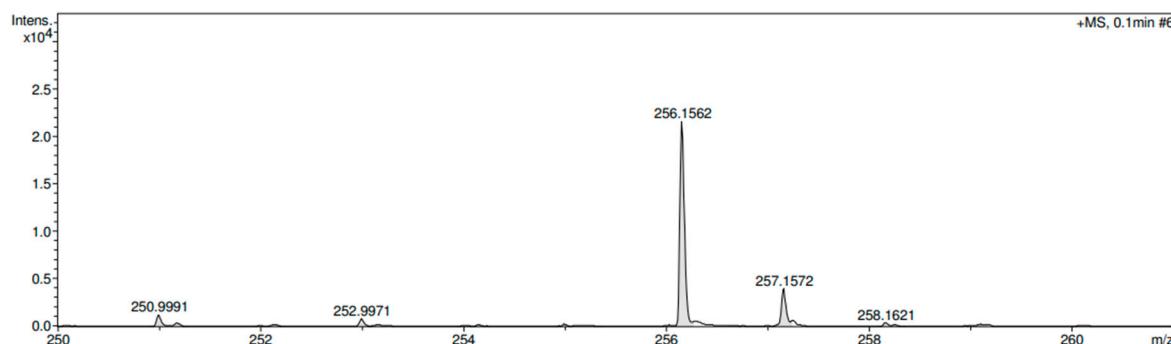
S31. 1-butyl-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16g**).

**Acquisition Parameter**

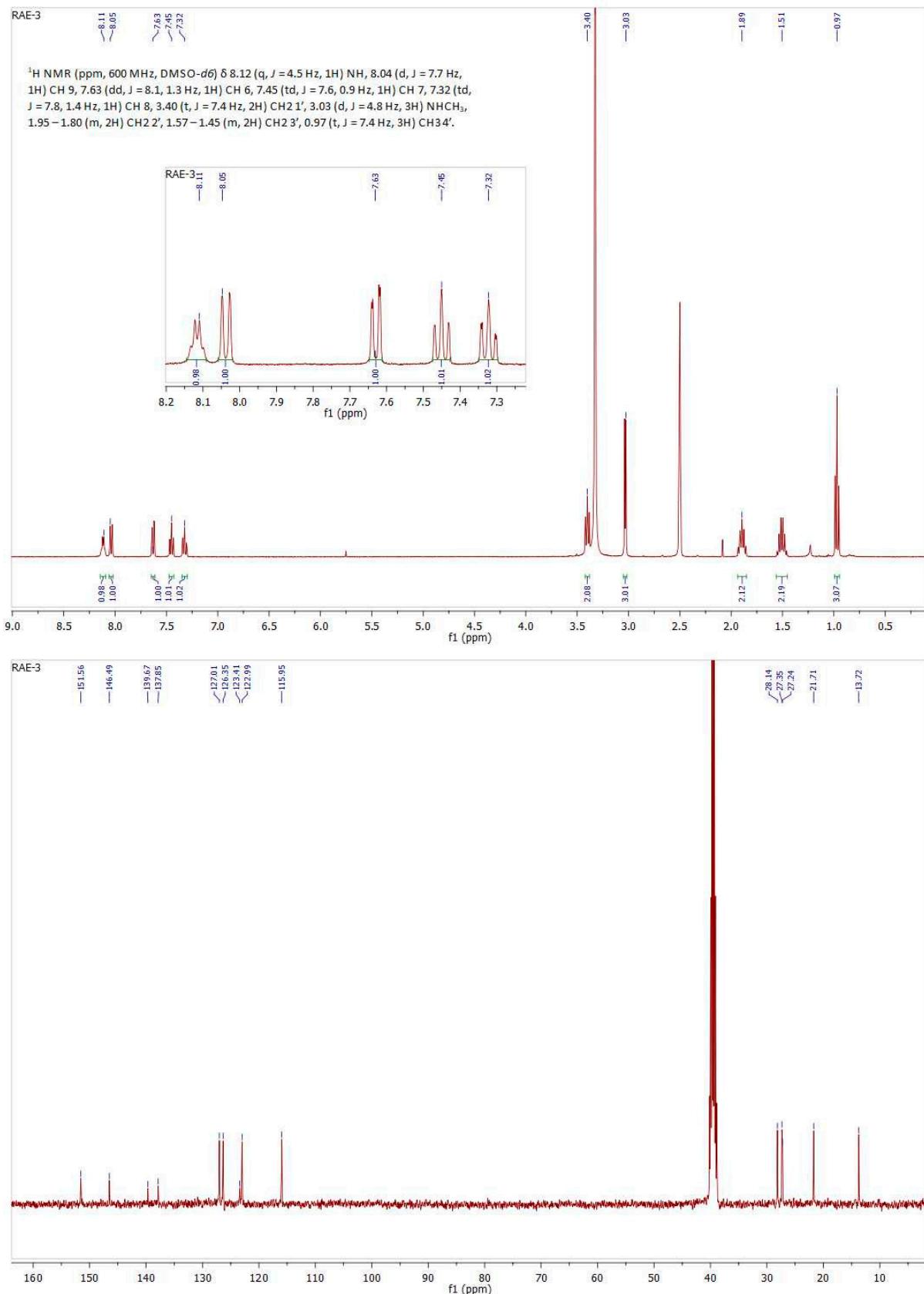
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

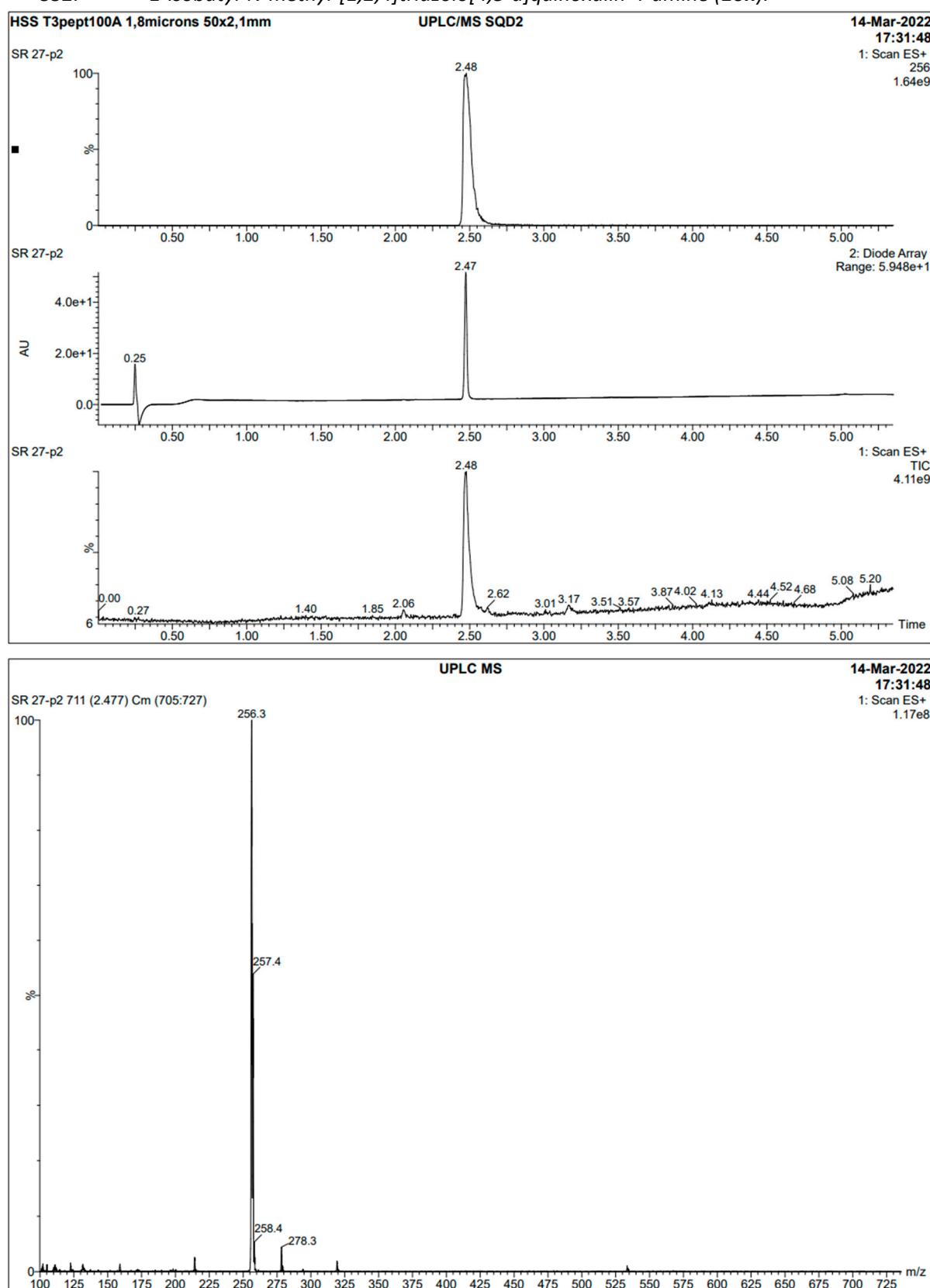
**Acquisition Parameter**

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



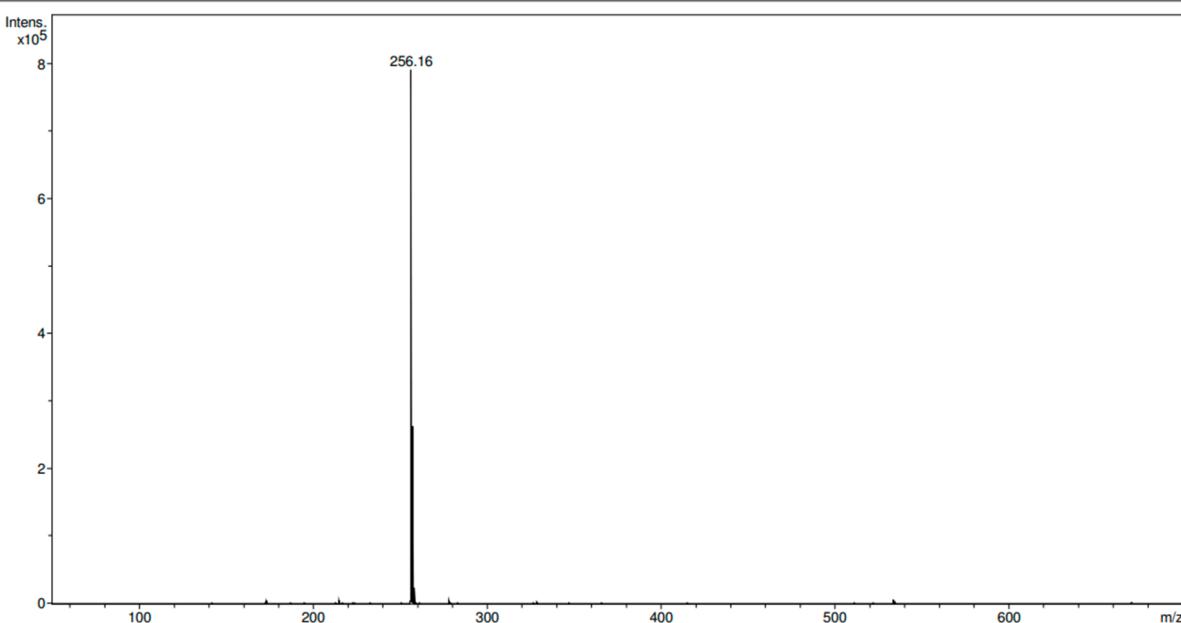
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
256.1562	1	C ₁₄ H ₁₈ N ₅	256.1557	2.1	6.6	1	100.00	8.5	even	ok



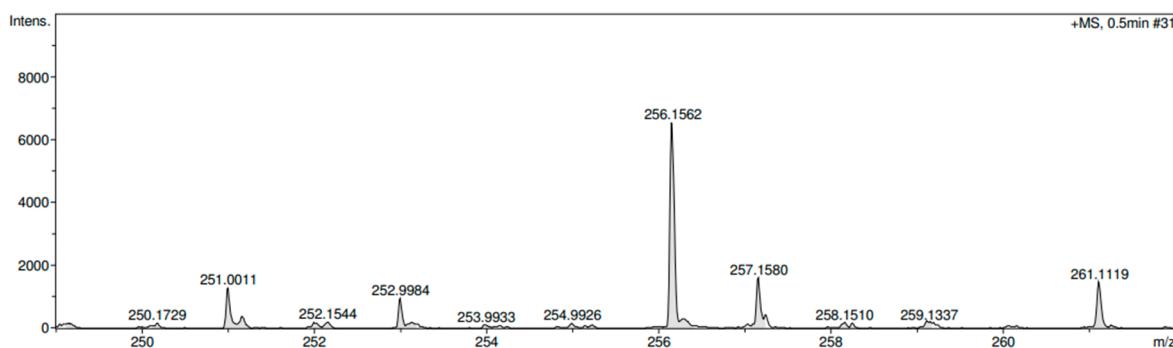
S32. *1-isobutyl-N-methyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16h).*

**Acquisition Parameter**

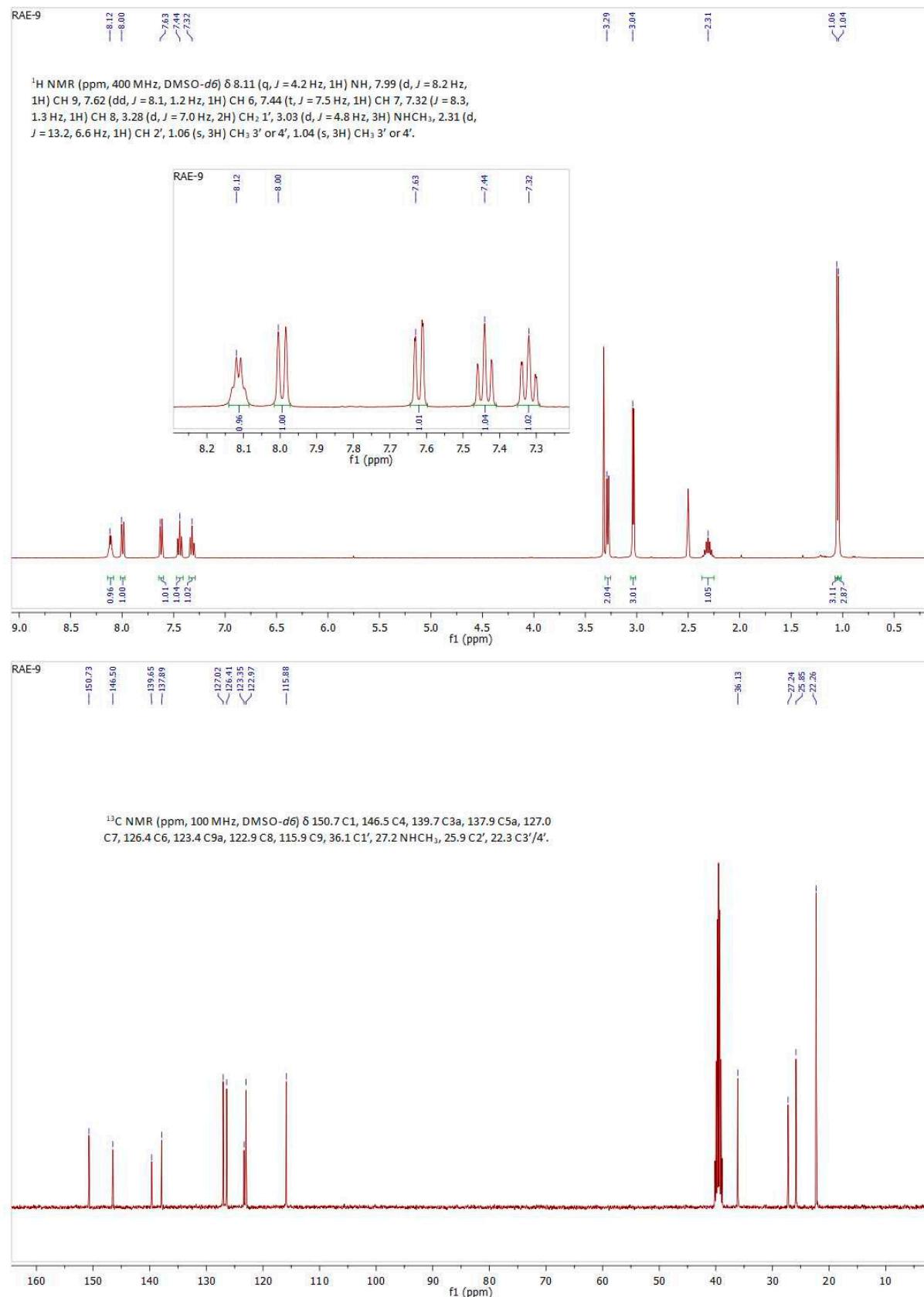
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

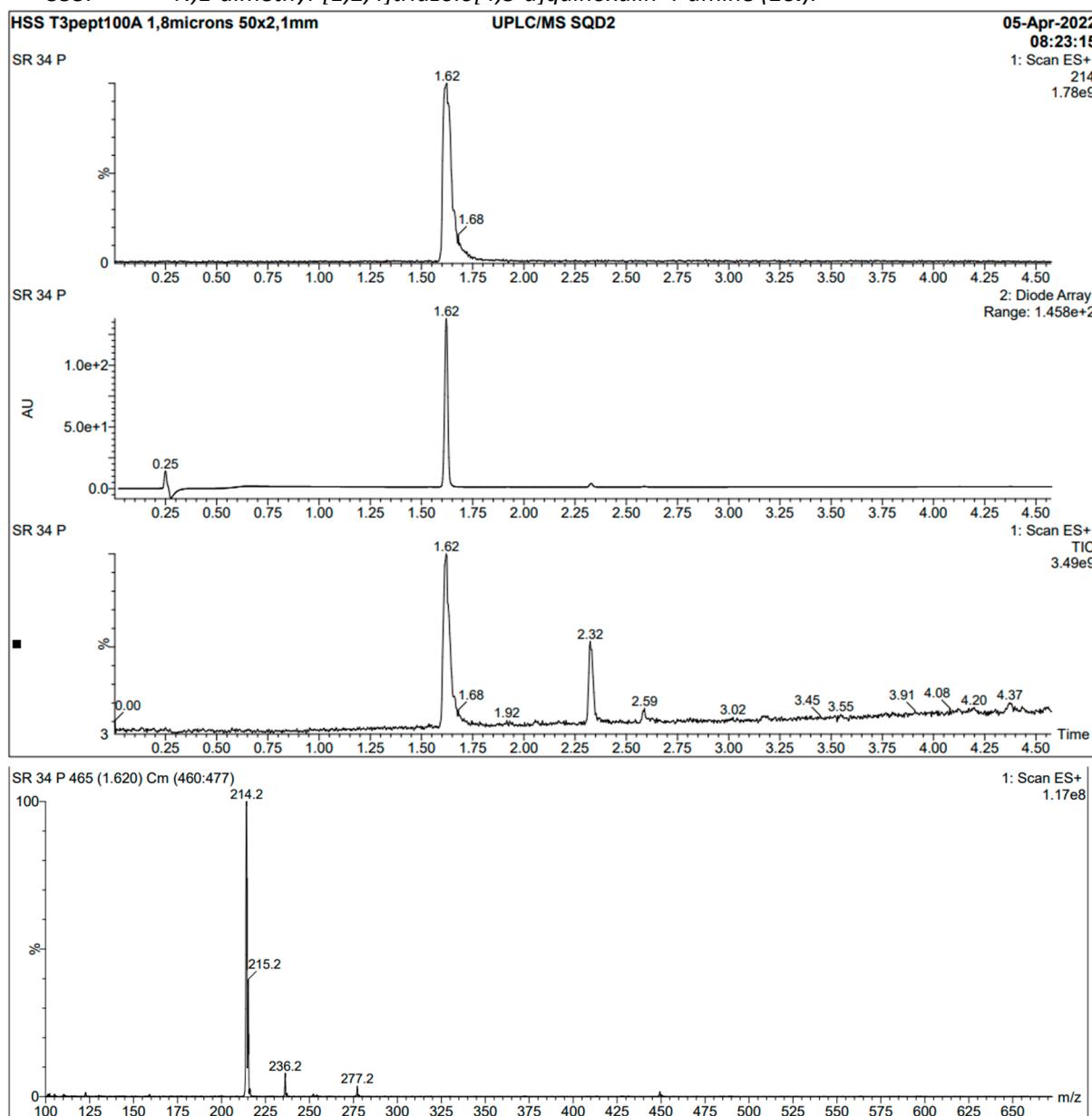
**Acquisition Parameter**

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



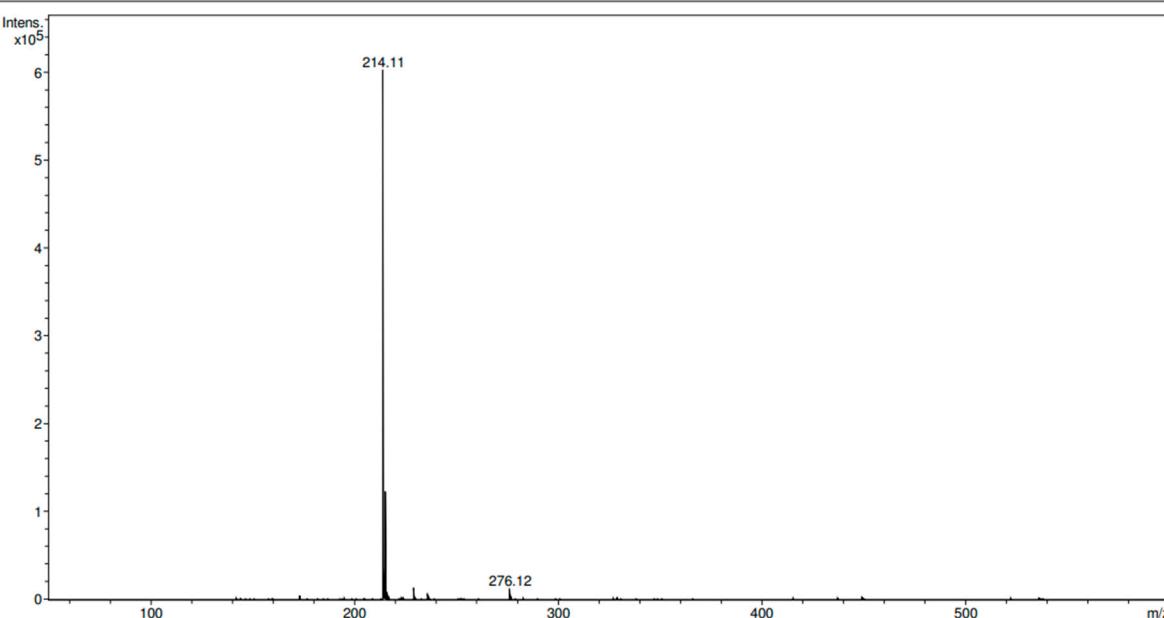
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
256.1562	1	C ₁₄ H ₁₈ N ₅	256.1557	2.0	43.7	1	100.00	8.5	even	ok
	2	C ₁₃ H ₂₂ NO ₄	256.1543	-7.2	56.7	2	29.86	3.5	even	ok



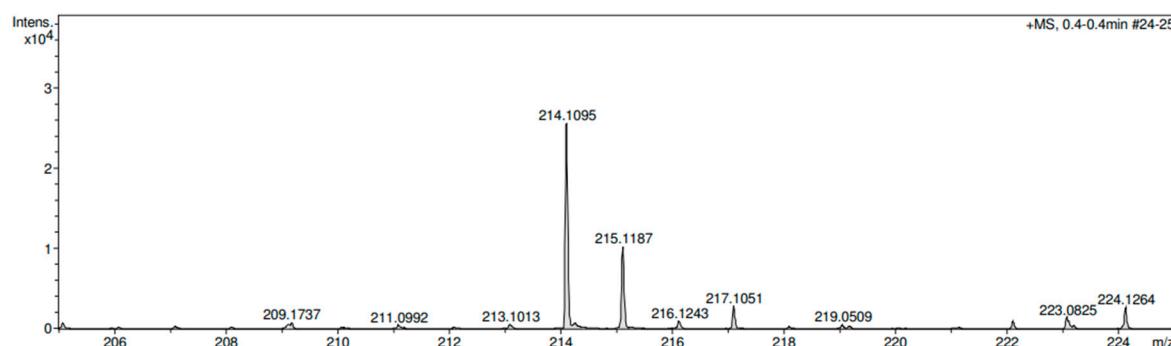
S33. *N,1-dimethyl-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (16i).*

Acquisition Parameter

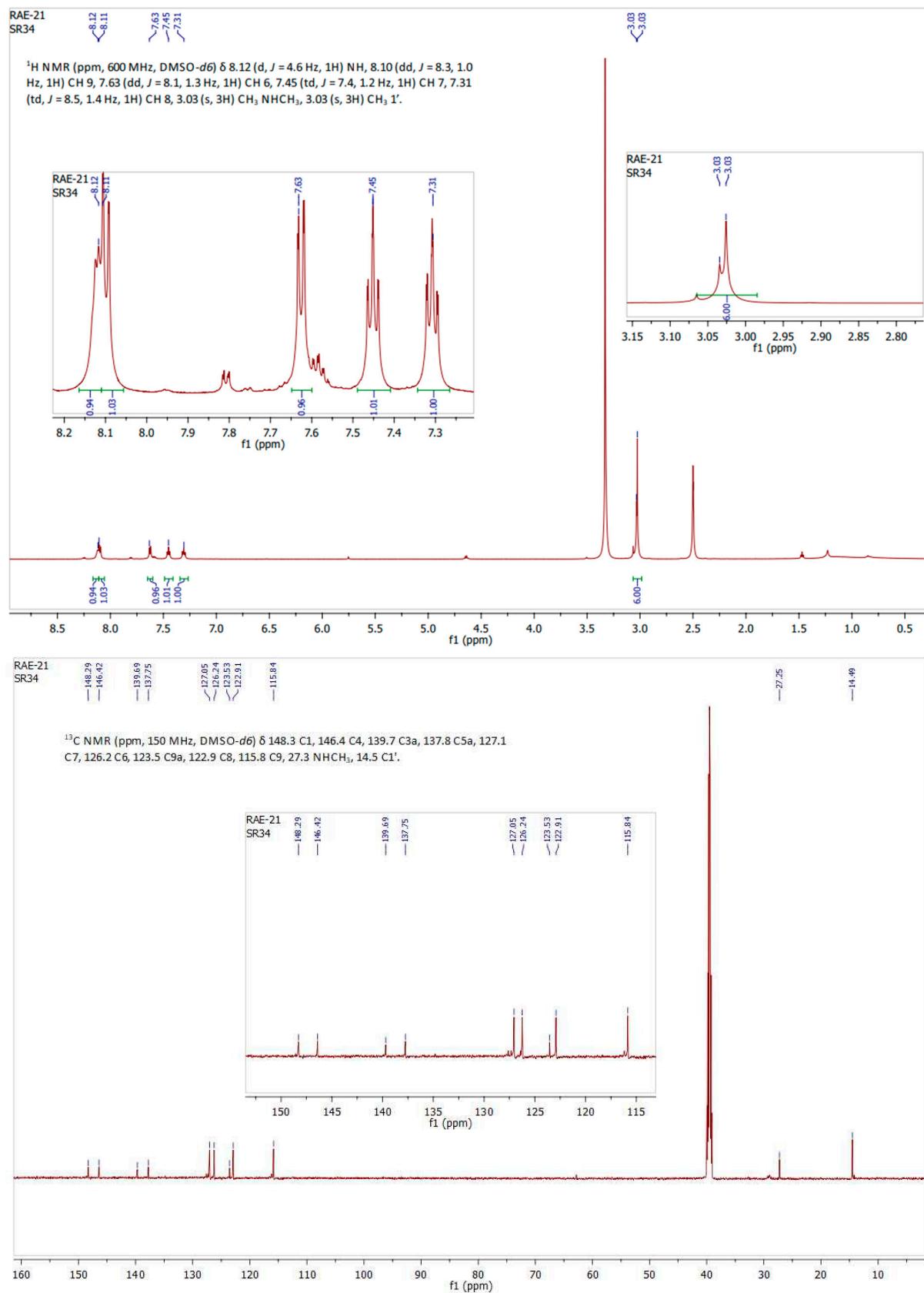
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

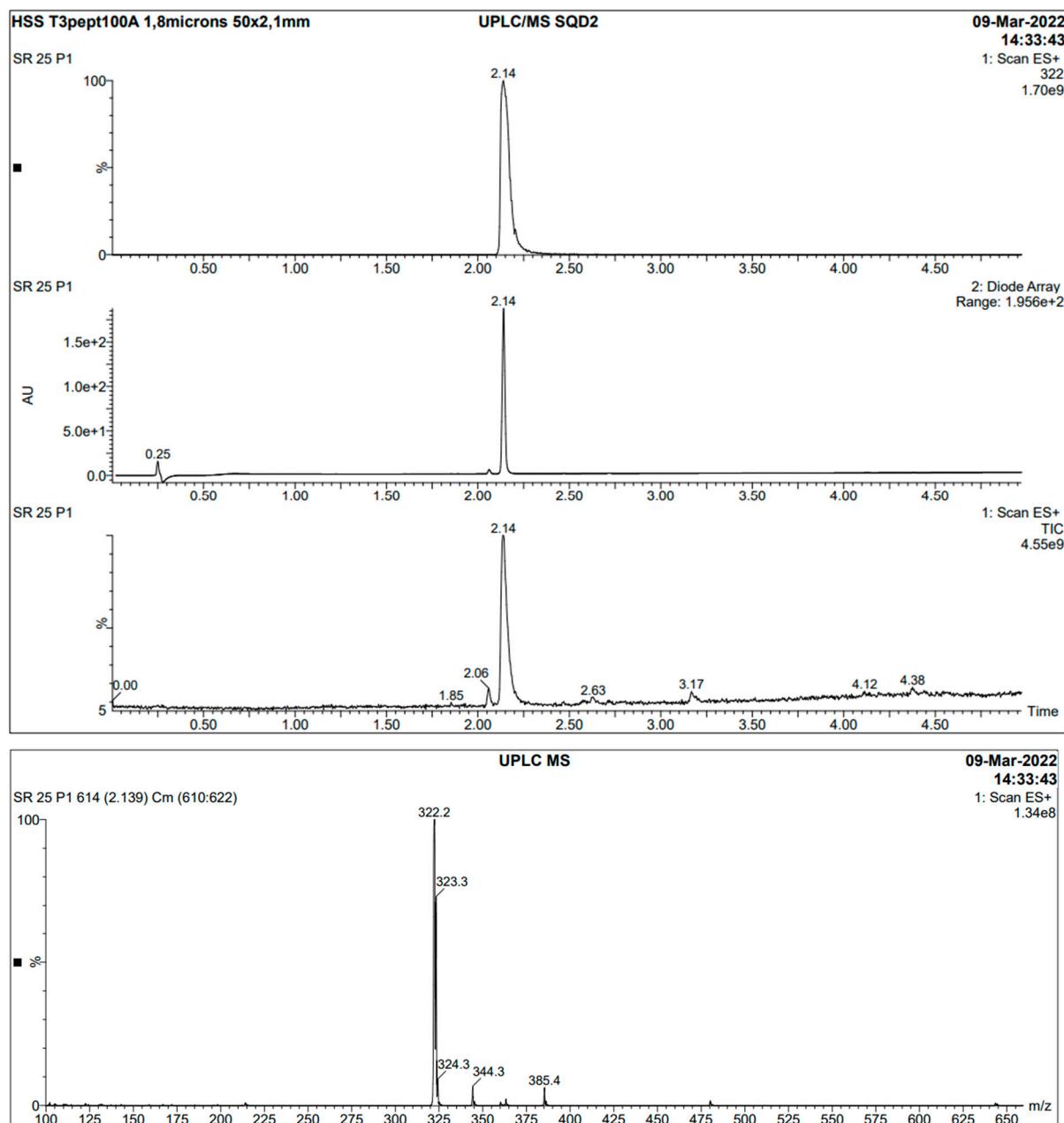

Acquisition Parameter

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



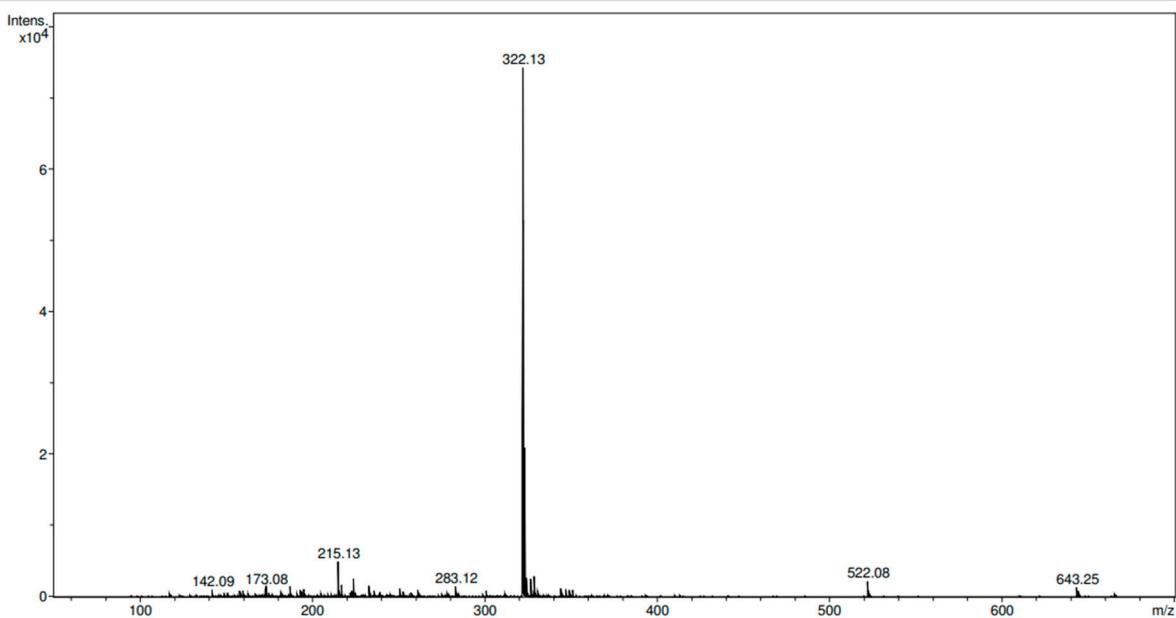
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
214.1095	1	C ₁₁ H ₁₂ N ₅	214.1087	3.8	153.8	1	100.00	8.5	even	ok



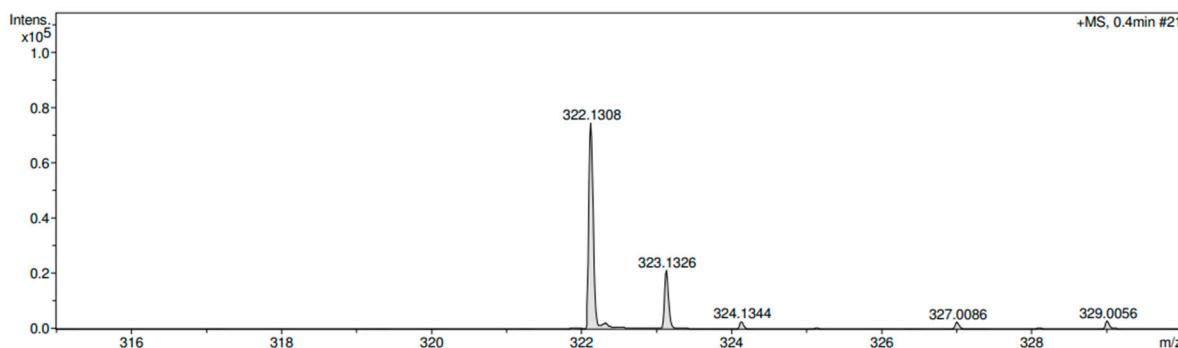
S34. 1-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[4,3-a]quinoxalin-4-amine (**16j**).

**Acquisition Parameter**

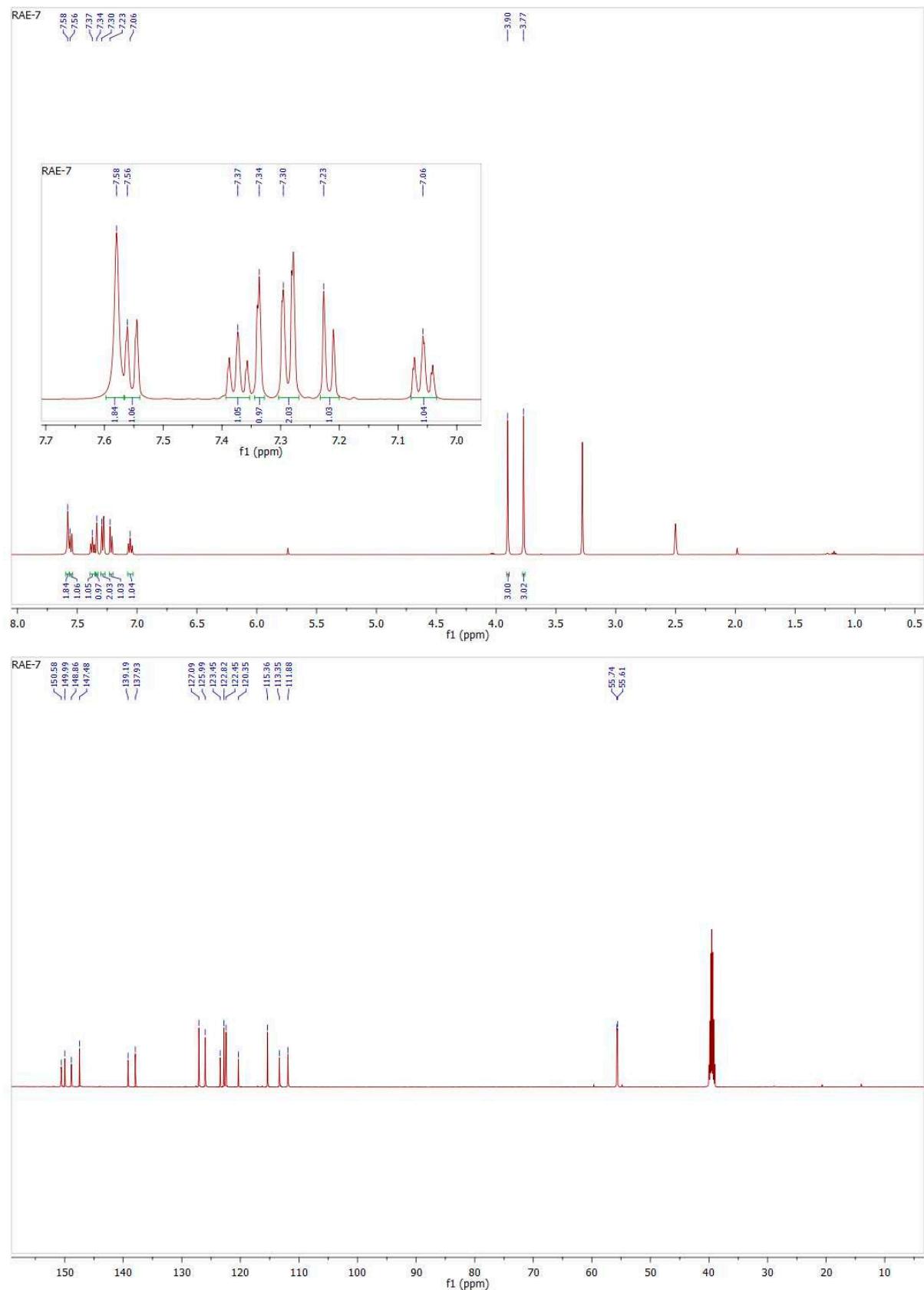
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z

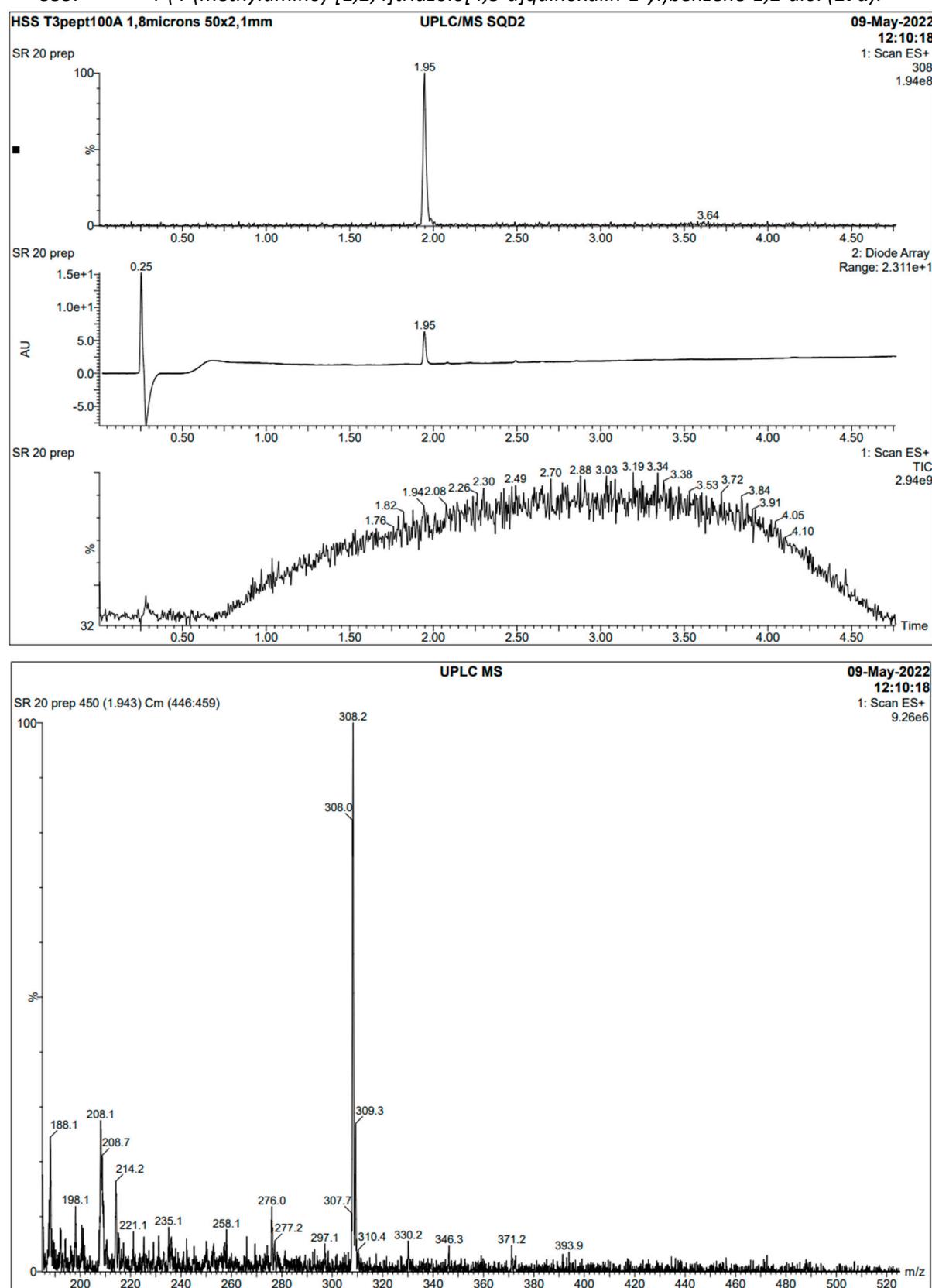
**Acquisition Parameter**

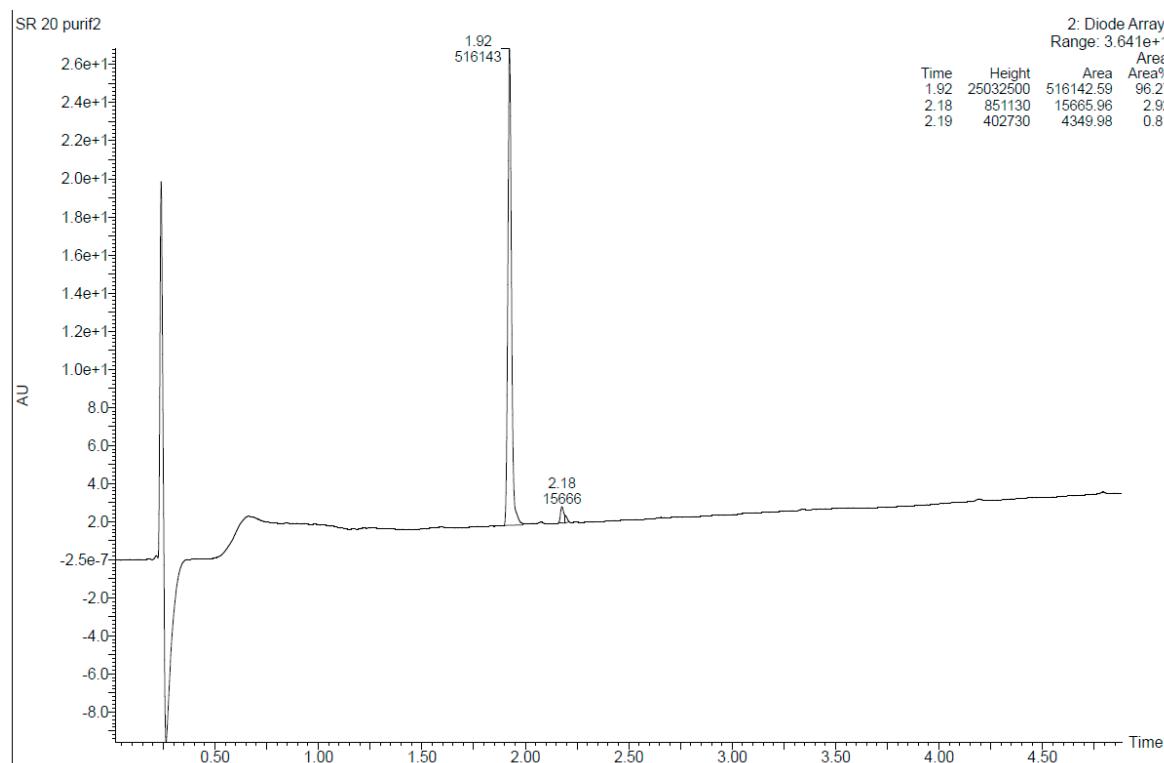
Source Type ESI Ion Polarity Positive Scan Begin 50 m/z Scan End 2200 m/z



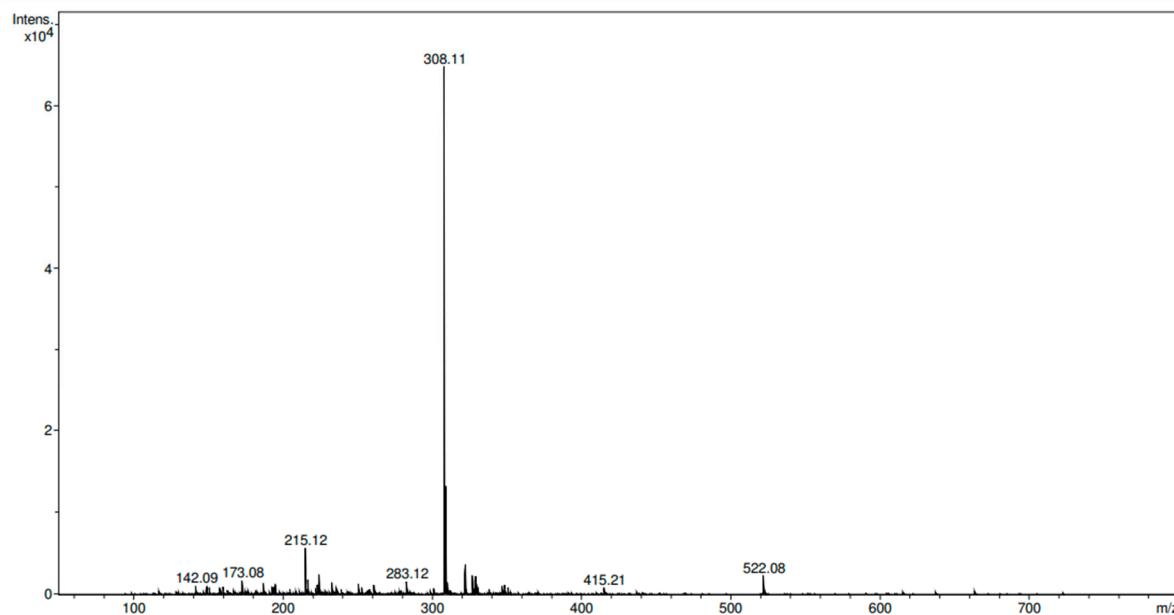
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule ok
322.1308	1	C17H16N5O2	322.1299	-3.0	45.8	2	100.00	12.5	even	ok
	2	C16H20NO6	322.1285	7.2	59.0	3	26.15	7.5	even	



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
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Acquisition Parameter

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

