Supporting Information

X-Ray Crystallographic Data and Modelling Figures/interaction maps

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Figure S1. Torsional Scanning of **1** and **13**

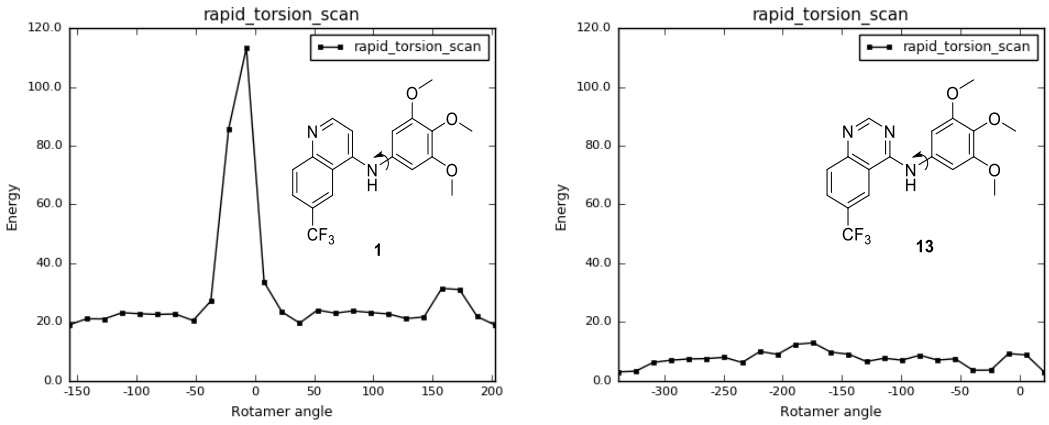


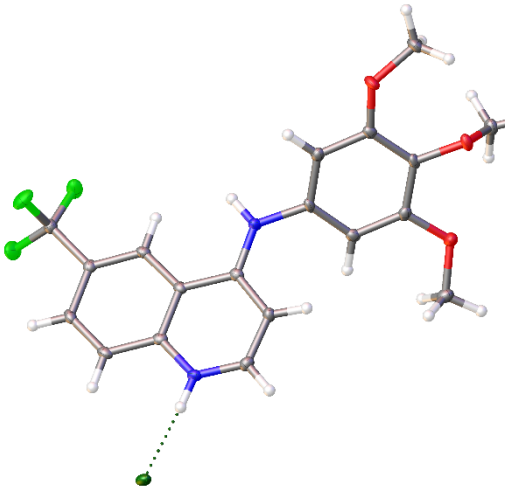
Table S1. Gas phase calculations of **1**, **13**, **9**, **49, 48**, **17** and **37**.

Compound	C-N-C angle	H-N-C-C torsion	Quin(az)oline-phenyl plane angle
1	128.54	149.21	57.24

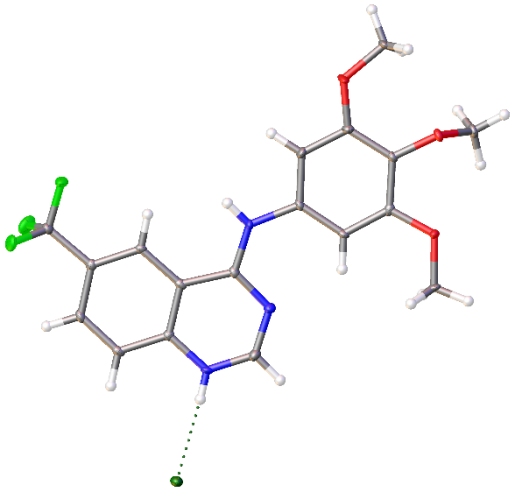
13	131.02	177.95	3.56
9	128.91	153.70	47.93
49	129.15	151.36	48.24
48	128.95	152.77	48.83
17	129.35	159.98	44.68
37	129.96	158.63	42.20

Figure S2. Crystal structures of **1**, **13**, **9**, **49, 48**, **17** and **37** (all ADP ellipsoids are shown at 50% probability)

1



13



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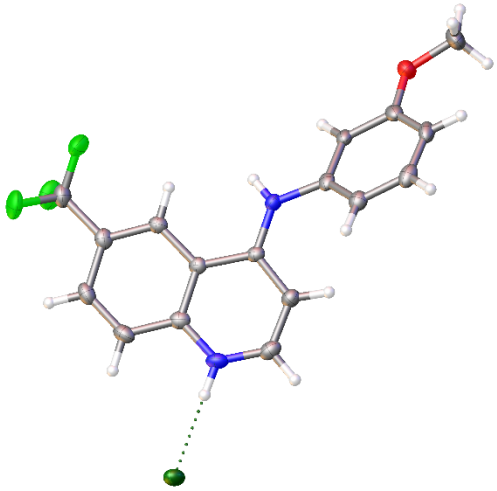
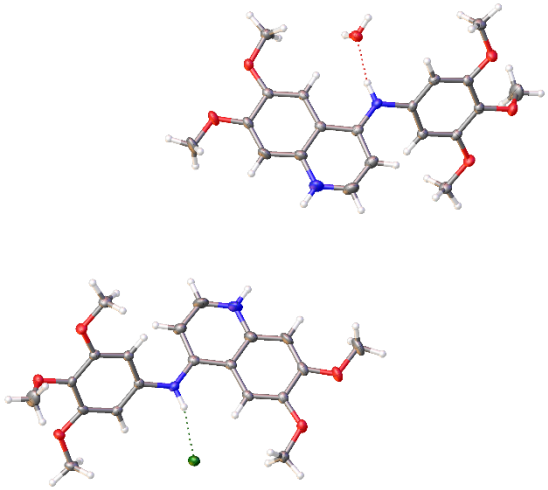
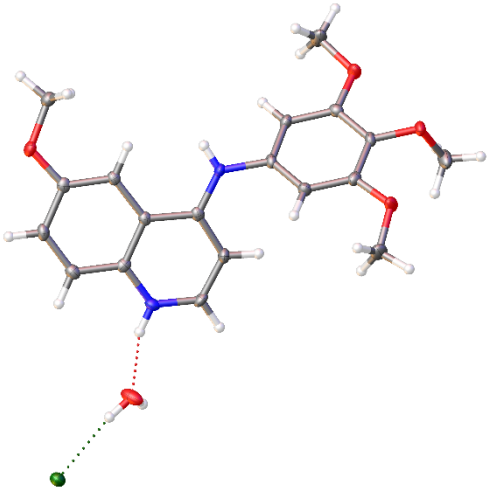


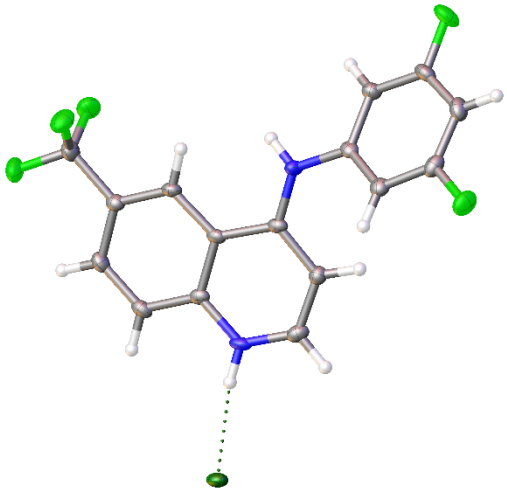
49



48



17



37

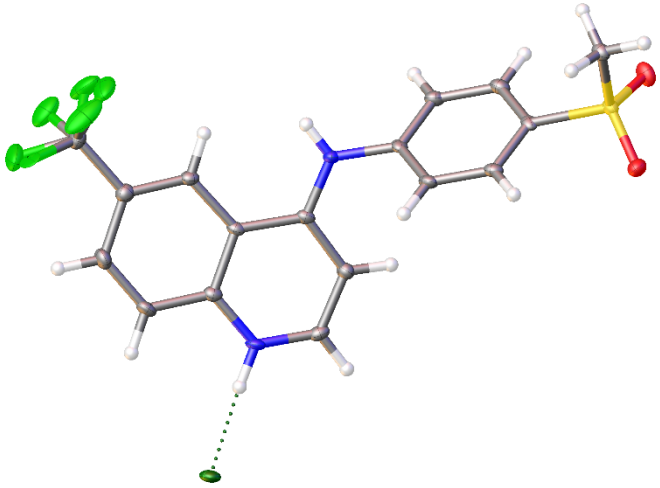


Table S2. Crystal structure data of **1**, **13**, **9**, **49, 48**, **17** and **37**.

Compound reference	**1** HCl	**13** HCl	**9** HCl	**49** HCl, H_2O	**48** HCl, H_2O	**17** HCl	**37** HCl
Chemical Formula	$C_{19}H_{18}ClF_3N_2O_3$	$C_{18}H_{17}ClF_3N_3O_3$	$C_{17}H_{14}ClF_3N_2O$	$C_{40}H_{47}ClN_4O_{11}$	$C_{19}H_{23}ClN_2O_5$	$C_{16}H_{10}ClF_5N_2$	$C_{17}H_{14}ClF_3N_2O_2S$
Formula Mass	414.80	415.79	354.75	795.26	394.84	360.71	402.81
Crystal System	monoclinic	triclinic	monoclinic	monoclinic	orthorhombic	monoclinic	triclinic
a/ Å	13.0547(4)	7.4430(4)	13.2992(6)	8.15904(9)	7.18960(10)	11.5664(5)	5.4737(2)
b/ Å	7.8338(2)	9.2967(5)	7.1675(3)	21.9132(2)	24.1253(4)	9.5134(4)	9.2142(3)
c/ Å	18.3234(5)	13.7306(6)	18.4659(11)	22.8051(2)	10.8297(2)	13.5408(6)	17.3243(7)
α/ °	90	102.723(4)	90	90	90	90	93.294(3)

β/ °	105.902(3)	96.290(4)	102.609(5)	96.4217(10)	90	101.823(4)	93.001(3)
γ/ °	90	111.251(4)	90	90	90	90	103.802(3)
Unit cell volume/ Å^3	1802.18(9)	844.80(8)	1717.75(15)	4051.74(7)	1878.43(5)	1458.36(11)	845.16(5)
Temperature/ K	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Space group	$P2_1/c$ (14)	$P\bar{1}$ (2)	$P2_1/c$ (14)	Ia (9)	$Pna2_1$ (33)	$P2_1/c$ (14)	$P\bar{1}$ (2)
No. of formula units per unit cell, Z	4	2	4	4	4	4	2
Radiation Type	MoK\α	MoK\α	MoK\α	MoK\α	MoK\α	MoK\α	MoK\α
Absorption coefficient, μ/ mm^{-1}	0.266	0.286	0.258	0.158	0.237	0.320	0.0396
No. of reflections measured	16094	10579	14254	54602	17624	13590	13815
No. of unique reflections	4096	3847	3914	9216	4215	3343	3836
No. of independent reflections, R_{int}	0.0344	0.0540	0.0678	0.0283	0.0375	0.0709	0.0474
Final R_1 values ($I>2\sigma(I)$)	0.0379	0.0444	0.0551	0.0327	0.0335	0.0487	0.0431
Final wR_2 values ($I>2\sigma(I)$)	0.0832	0.0912	0.1176	0.0870	0.0692	0.0849	0.1047
Final R_1 values (all data)	0.0538	0.0780	0.0948	0.0357	0.0394	0.0858	0.0579
Final wR_2 values (all data)	0.0891	0.1017	0.1310	0.0890	0.0722	0.0966	0.1118
Goodness of fit on F_2	1.035	1.016	1.037	1.044	1.044	1.026	1.045
CCDC ID	1534017	1534019	1534018	1534023	1534022	1534020	1534021

Table S3. Crystal structure analysis of **1**, **13**, **9**, **49, 48**, **17** and **37**.

Compound	C-N-C angle	H-N-C-C torsion	Quin(az)oline-phenyl plane angle	GAK K_i (μM)
1	127.14	136.46	52.06	0.0039
13	129.51	168.74	2.65	0.037
9	127.41	152.94	41.65	0.0057
49	126.13	137.89	48.74	0.00054
48	125.31	129.46	50.51	0.013
17	127.05	148.29	35.51	0.051
37	127.76	133.84	58.8	0.97

Figure S3. Watermap analysis of favourable docking poses showing that quinazoline ring system of **13** (left) leaves additional space to accommodation of water molecule (theoretical energy gain = 4.2 kcal/mol), whereas it is likely displaced by compound **1** (right) and other quinoline derivatives.

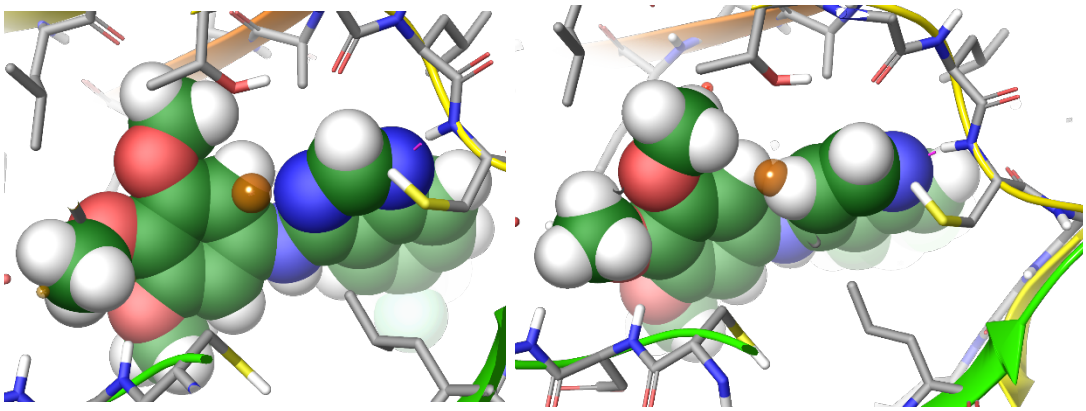
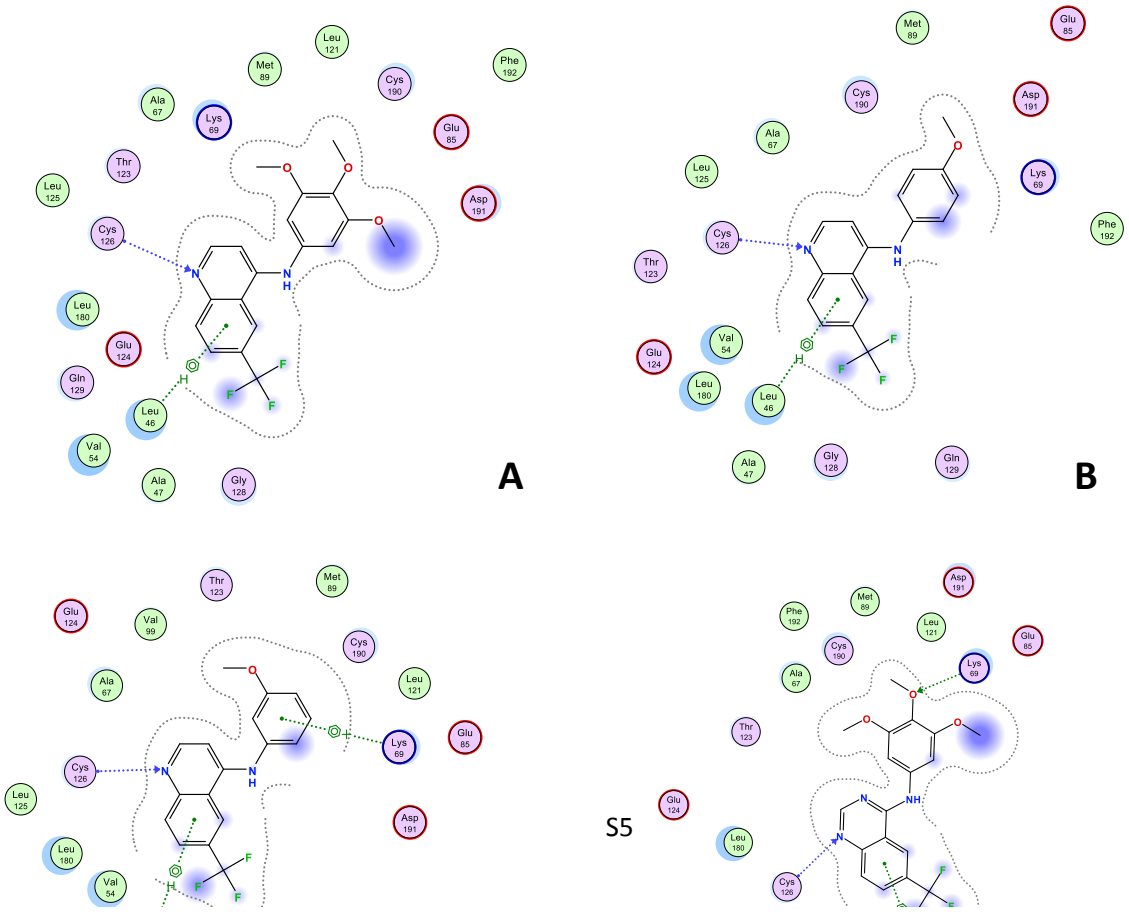
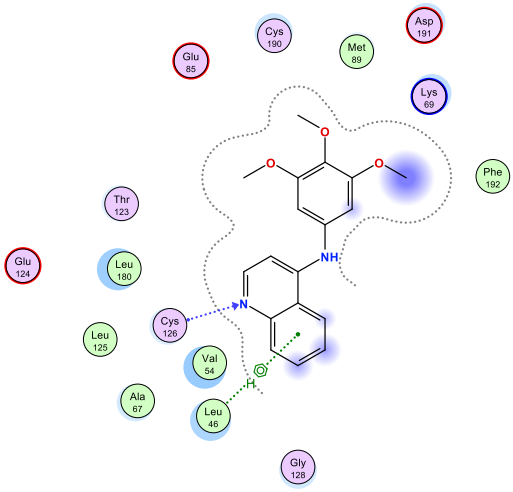


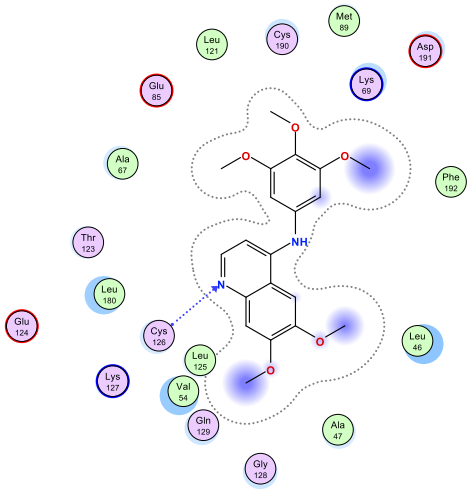
Figure S4. Ligand interaction diagrams in GAK active site. A - Compound **1**, B - Compound **8**, C - Compound **9**, D - Compound **13**, E - Compound **41**, F - Compound **49**.



C


Cys 190
Met 89
Asp 191
Glu 85
Lys 89
Phe 192
Thr 123
Glu 124
Leu 180
Leu 125
Cys 126
Val 54
Ala 67
Leu 46
Gly 128

D


Leu 121
Cys 190
Met 89
Asp 191
Glu 85
Lys 89
Ala 67
Phe 192
Thr 123
Leu 180
Glu 124
Cys 126
Leu 125
Leu 46
Lys 127
Val 54
Gln 129
Ala 47
Gly 128

E

F

Figure S5. Ligand interaction diagrams in AAK1 active site. A - Compound **1**, B - Compound **8**, C - Compound **9**, D - Compound **13**, E - Compound **41**, F - Compound **49**.

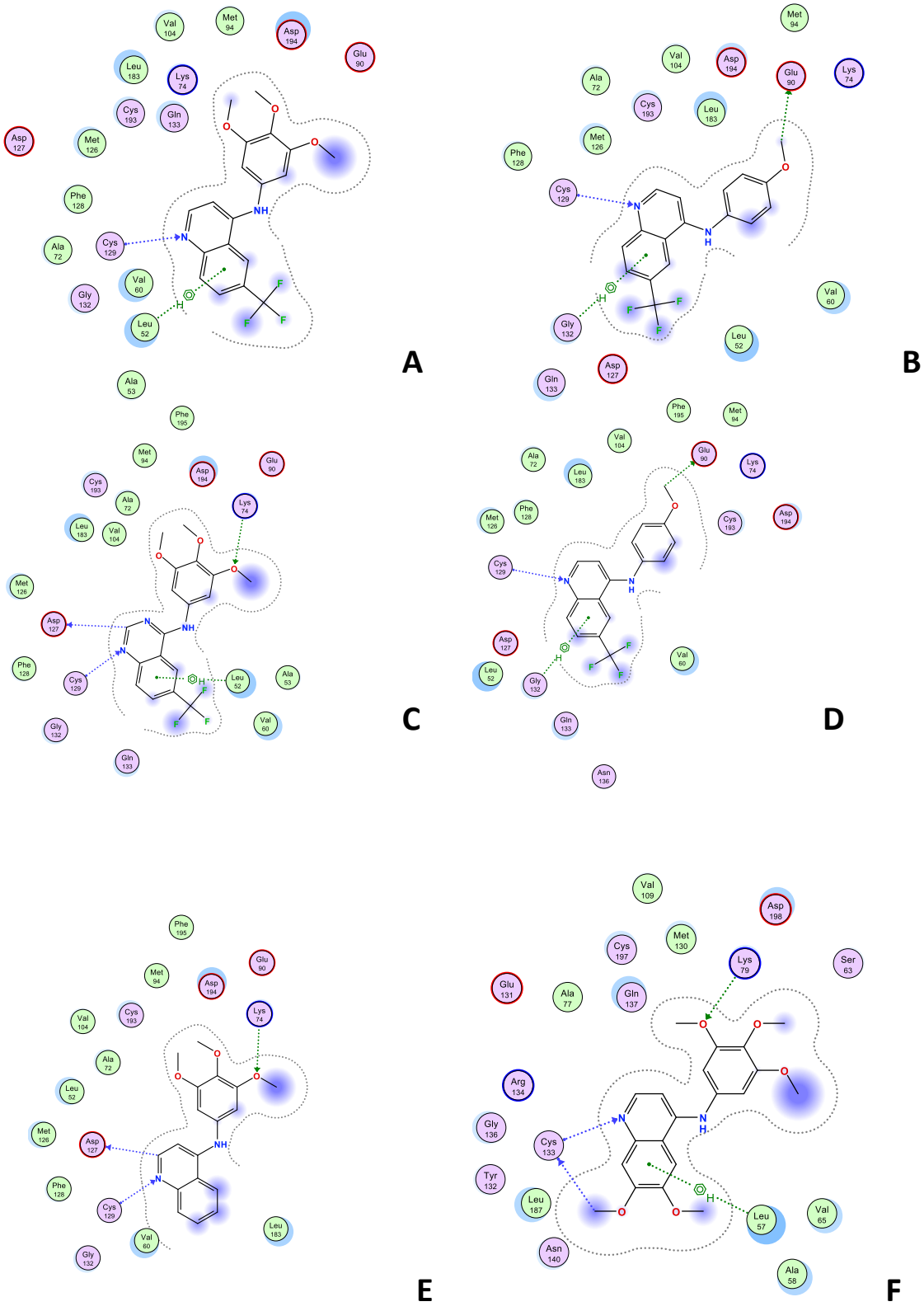


Figure S6. Ligand interaction diagrams in BMP2K active site. A - Compound **1**, B - Compound **8**, C - Compound **9**, D - Compound **13**, E - Compound **41**, F - Compound **49**.

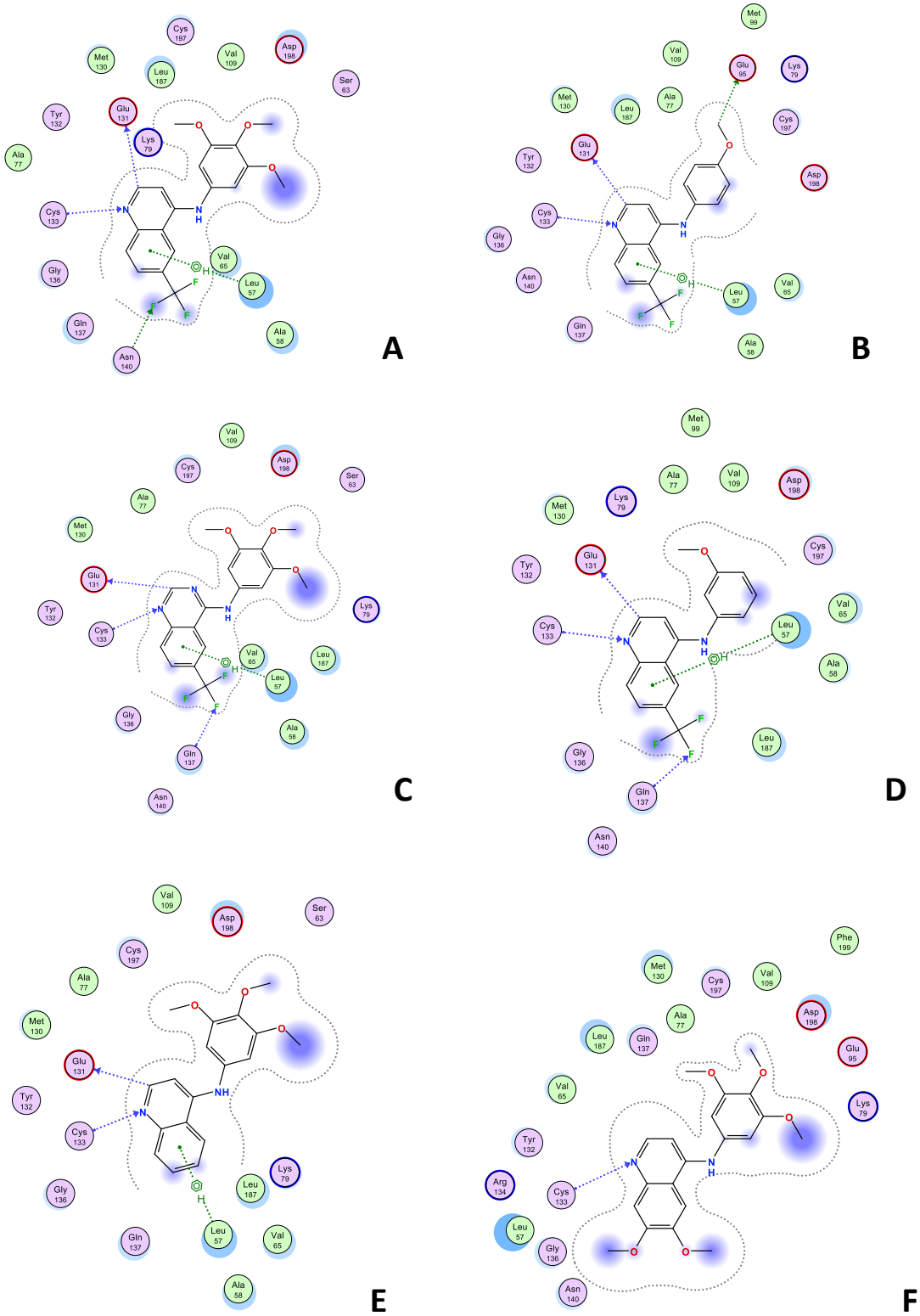


Figure S7. Ligand interaction diagrams in STK16 active site. A - Compound **1**, B - Compound **8**, C - Compound **9**, D - Compound **13**, E - Compound **41**, F - Compound **49**.

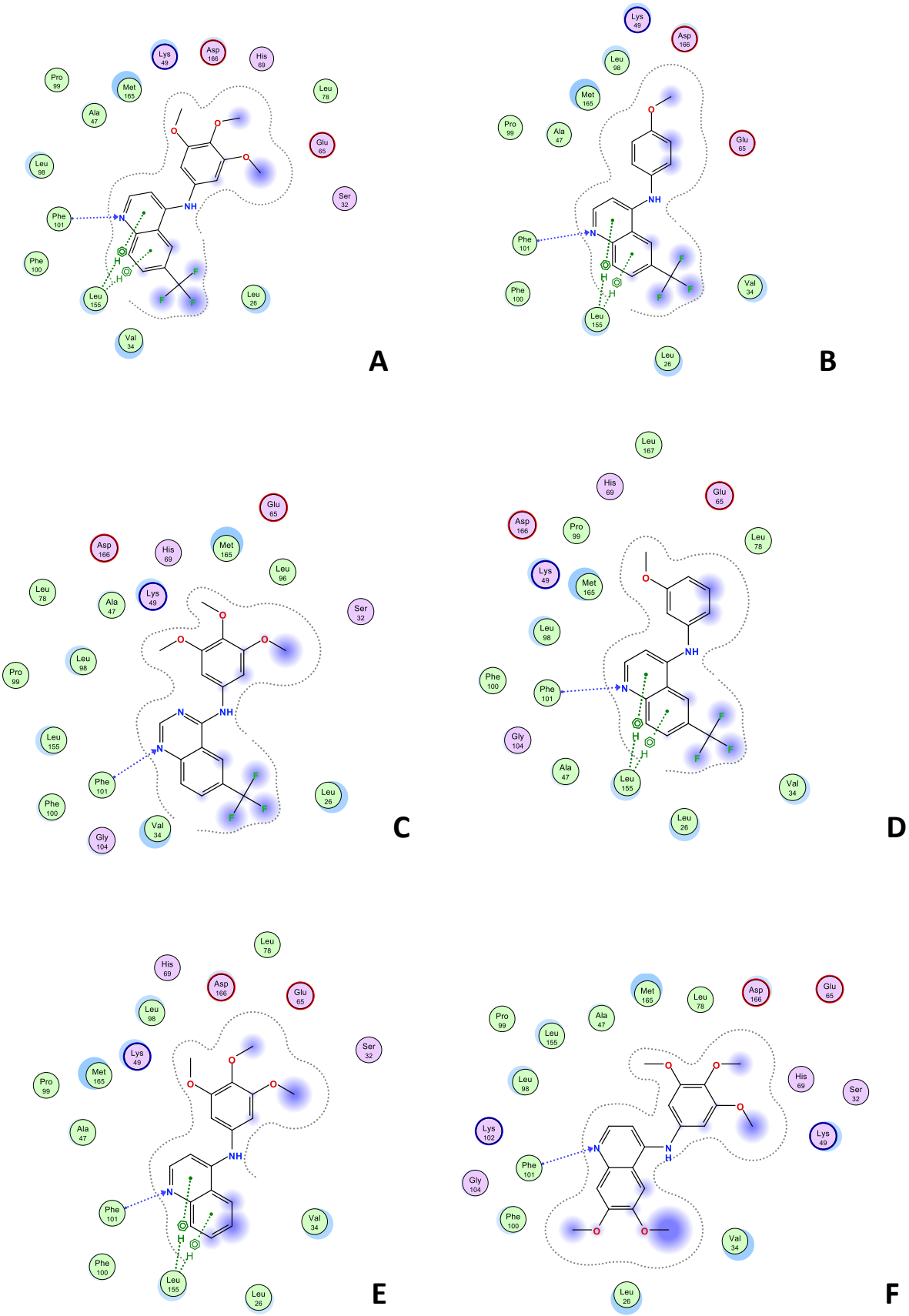
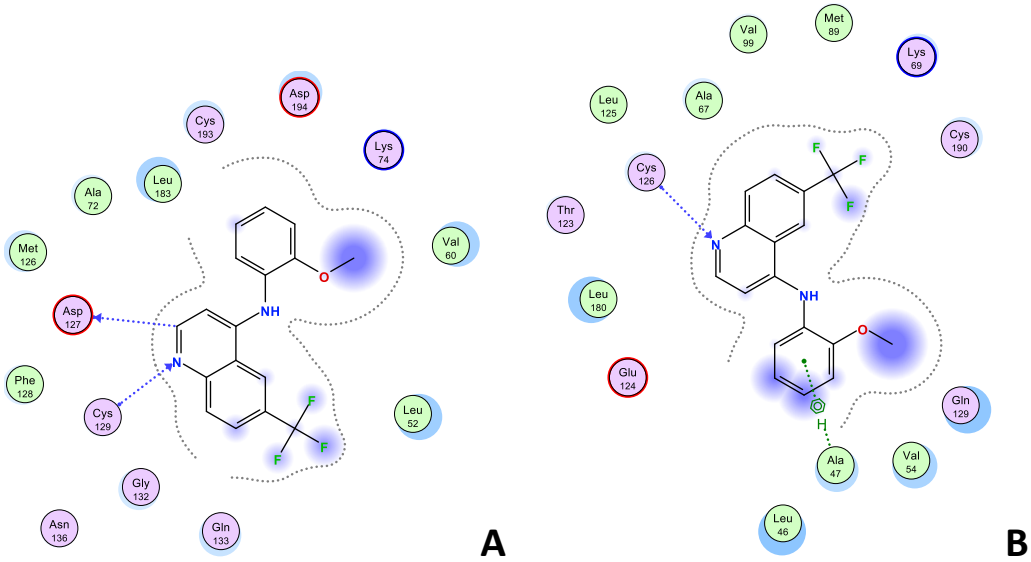
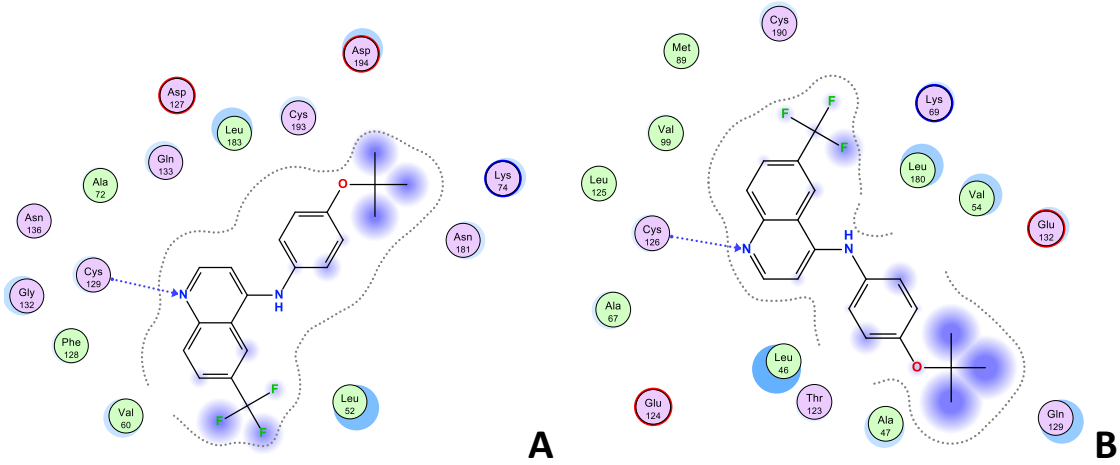


Figure S8. Ligand interaction diagrams of specific case studies - **10**, **39**, **40**, **49**, **31**, **37**, and **46**.

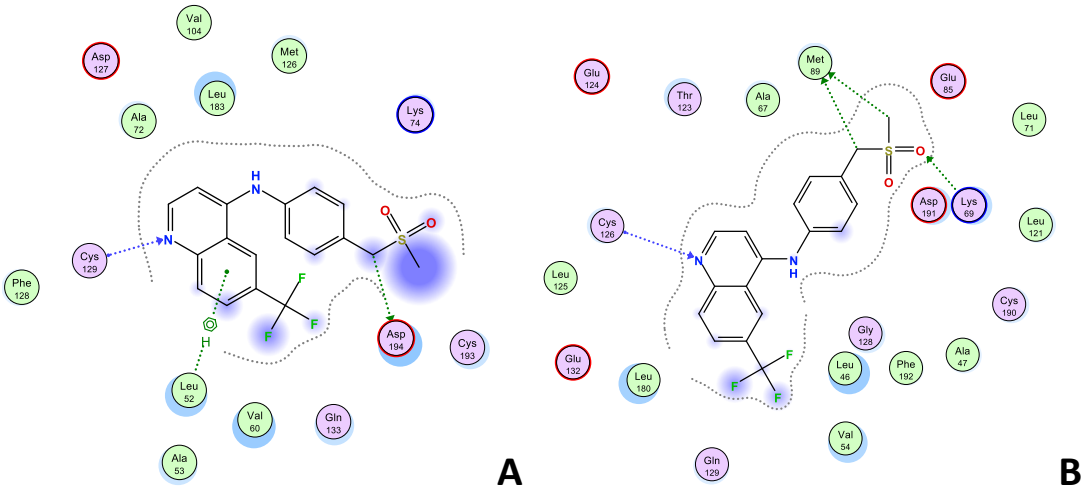
10 - AAK1 (**A**) vs GAK (**B**)



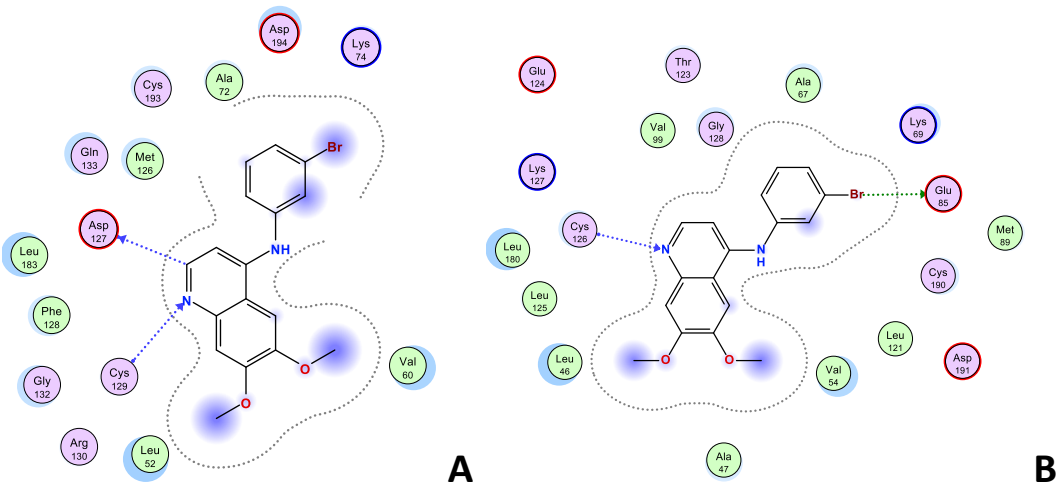
39 - AAK1 (**A**) vs GAK (**B**)



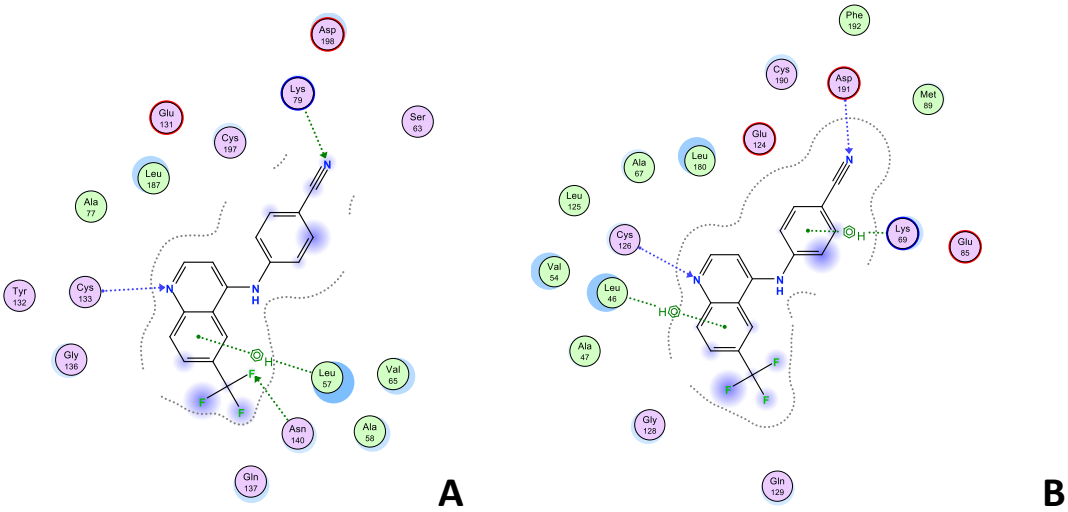
40 - AAK1 (**A**) vs GAK (**B**)



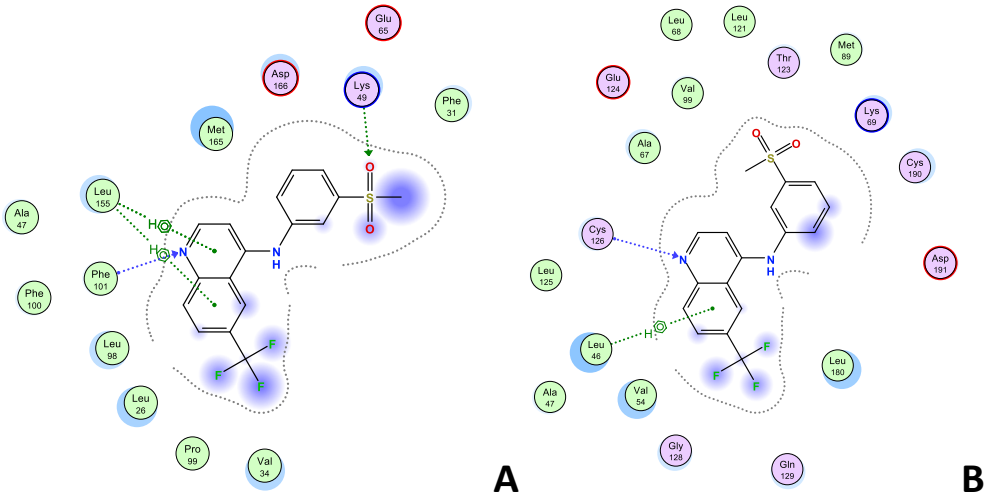
49 - AAK1 (**A**) vs GAK (**B**)



31 - BMP2K (**A**) vs GAK (**B**)



37 - STK16 (**A**) vs GAK (**B**)



46 - STK16 (**A**) vs GAK (**B**)

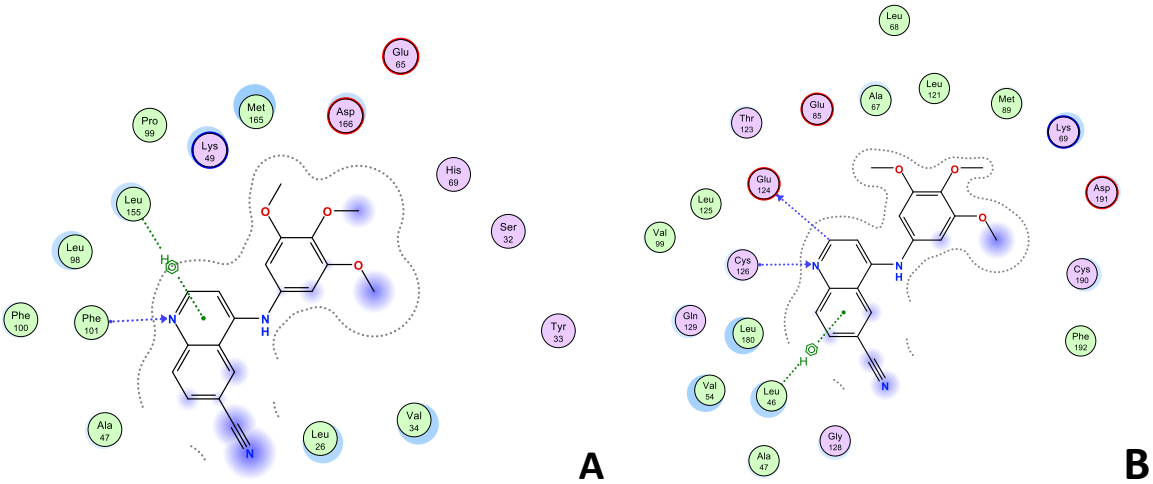
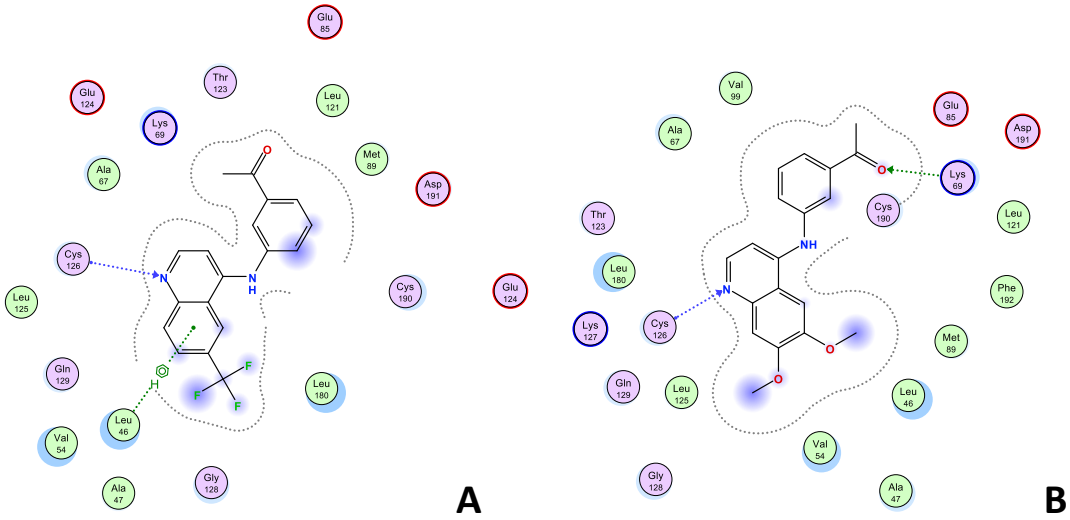
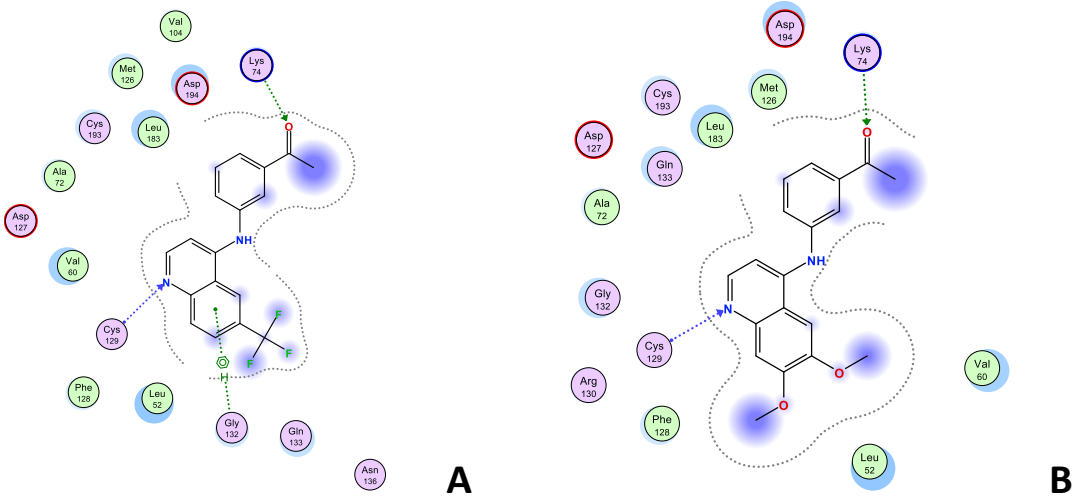


Figure S9. Pan-NAK compounds **36** - **A** and **56** - **B**

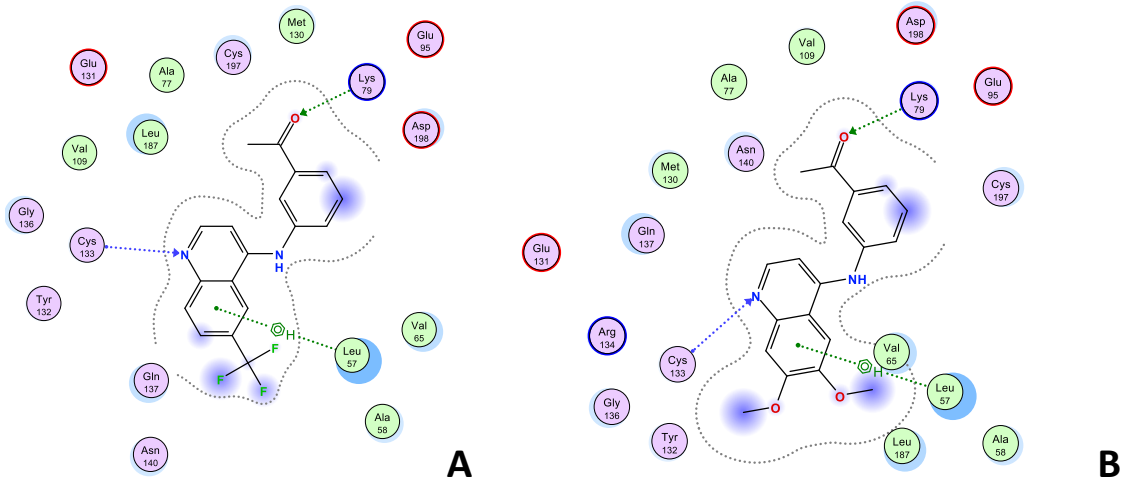
GAK



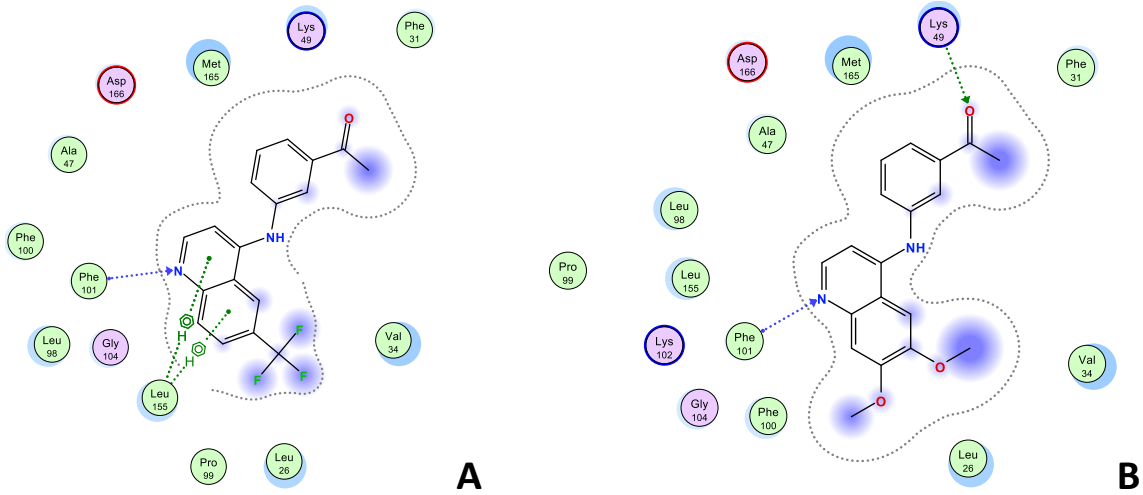
AAK1



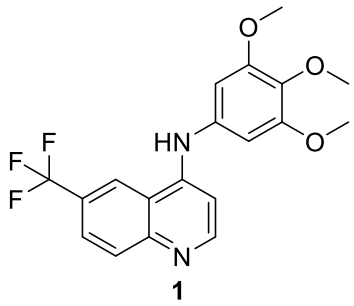
BMP2K/BIKE



STK16

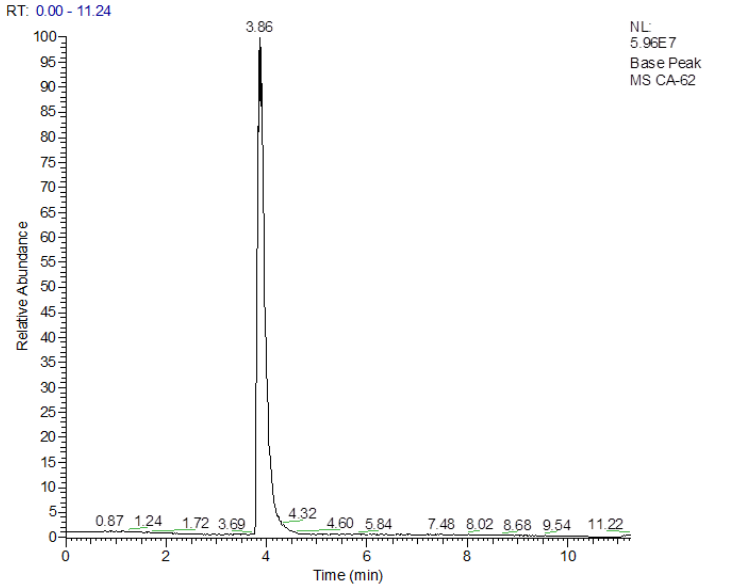


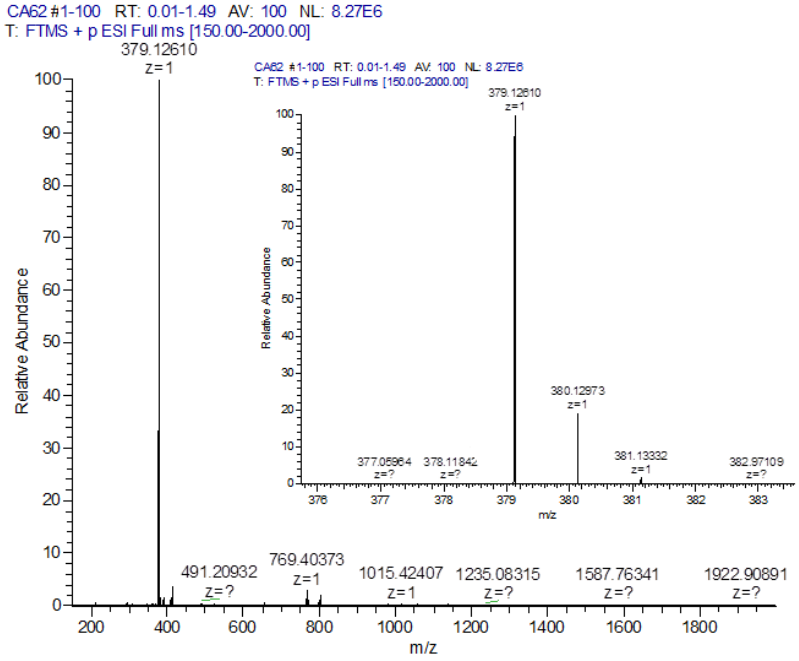
LCMS/HRMS and $^{1}H/^{13}C$ NMR anaylsis 1-57

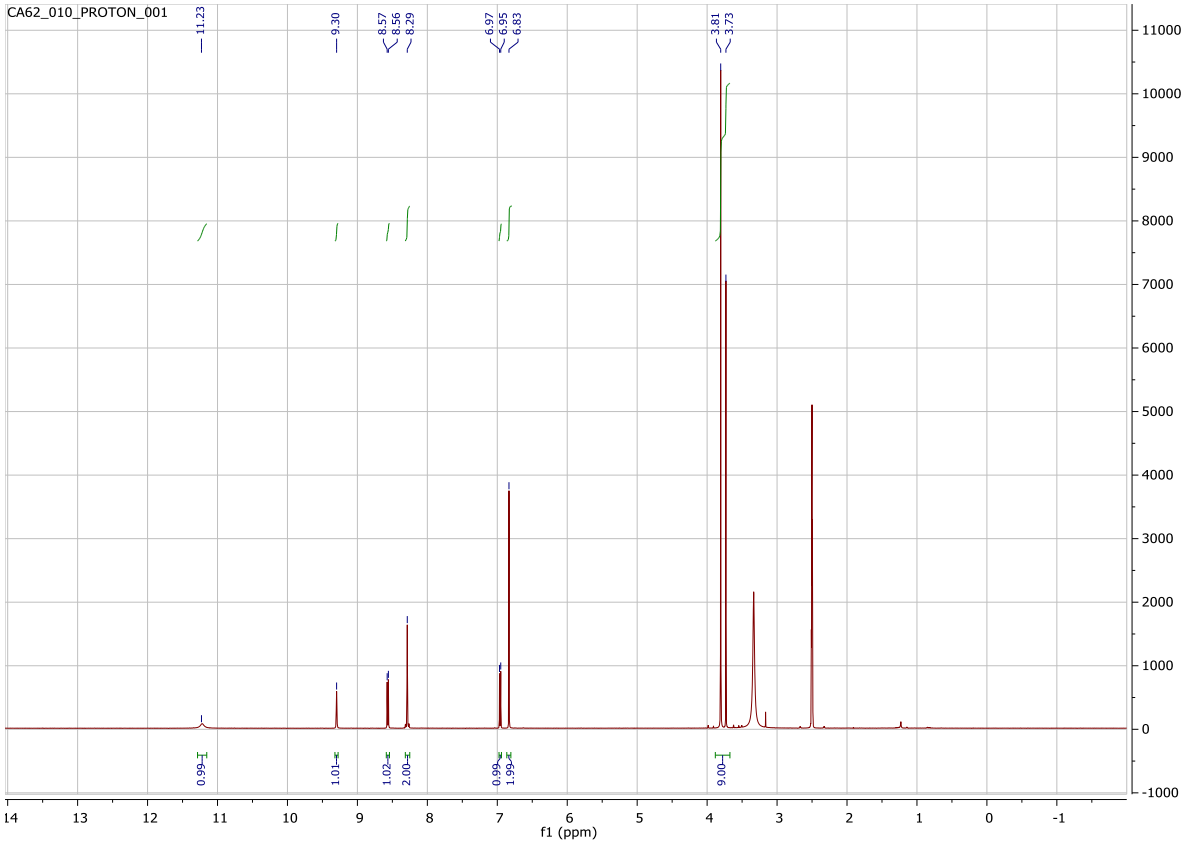


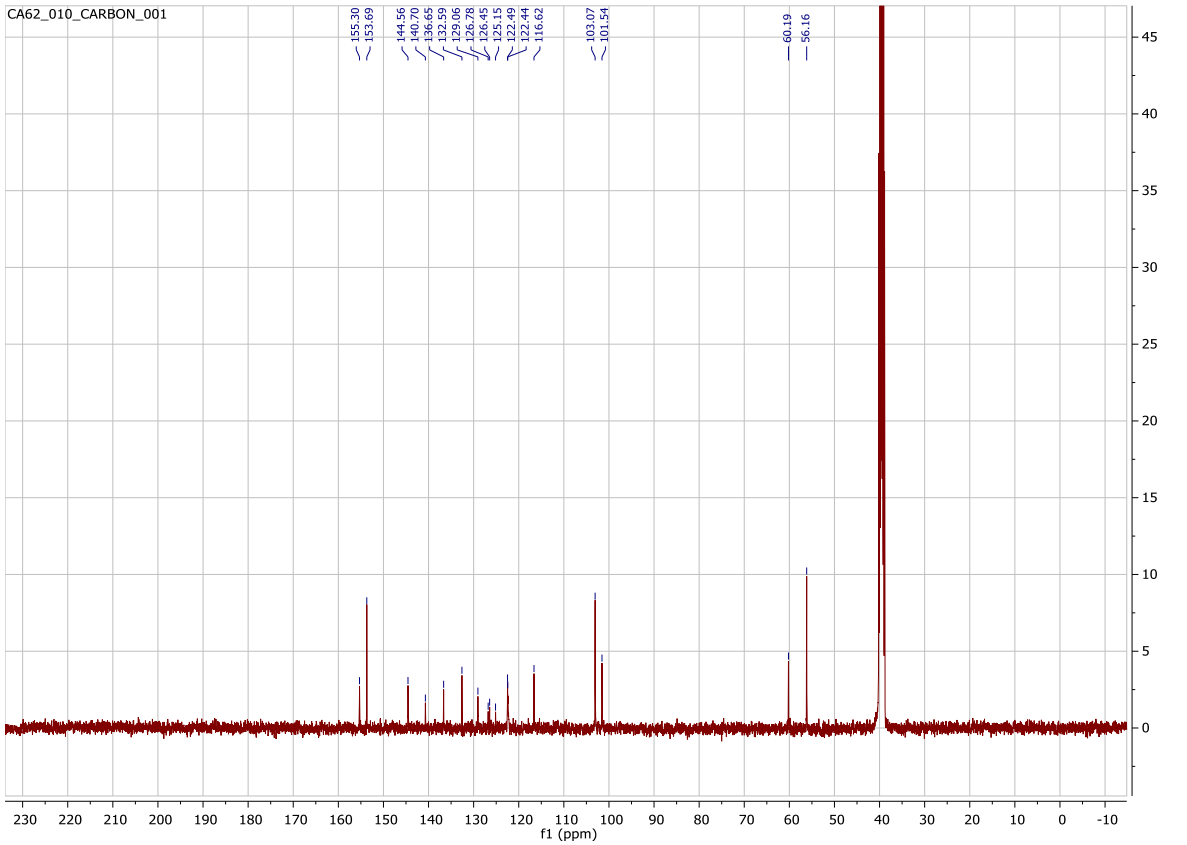
1

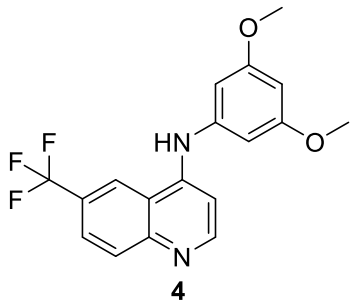
6-(Trifluoromethyl)-N-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**1**)





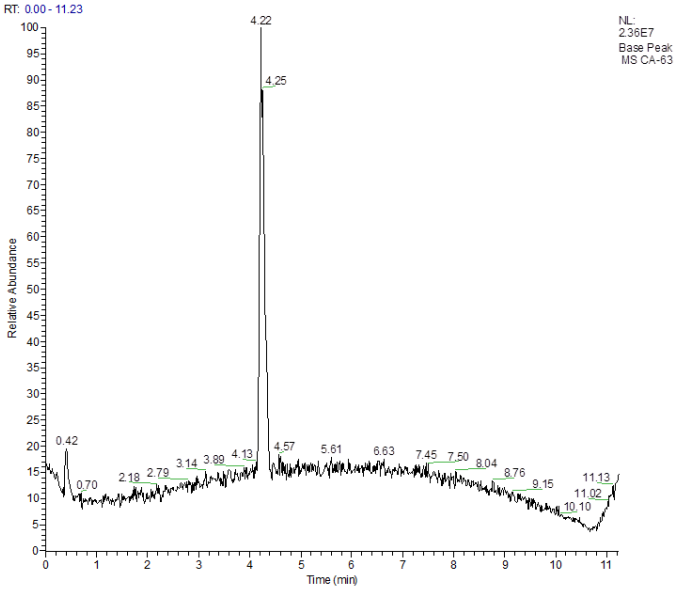

CA62_010_PROTON_001
11.23
9.30
8.57
8.56
8.29
6.97
6.95
6.83
3.81
3.73
0.99
1.01
1.02
2.00
0.99
1.99
9.00
f1 (ppm)

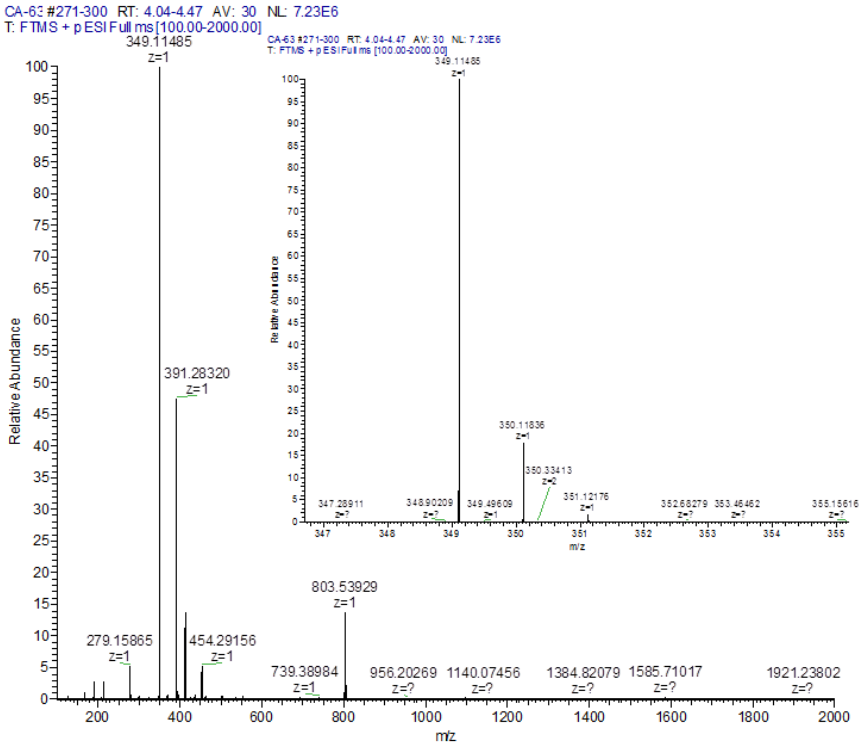

CA62_010_CARBON_001
155.30
153.69
144.56
140.70
136.65
132.59
129.06
126.78
126.45
125.15
122.49
122.44
116.62
103.07
101.54
60.19
56.16
f1 (ppm)

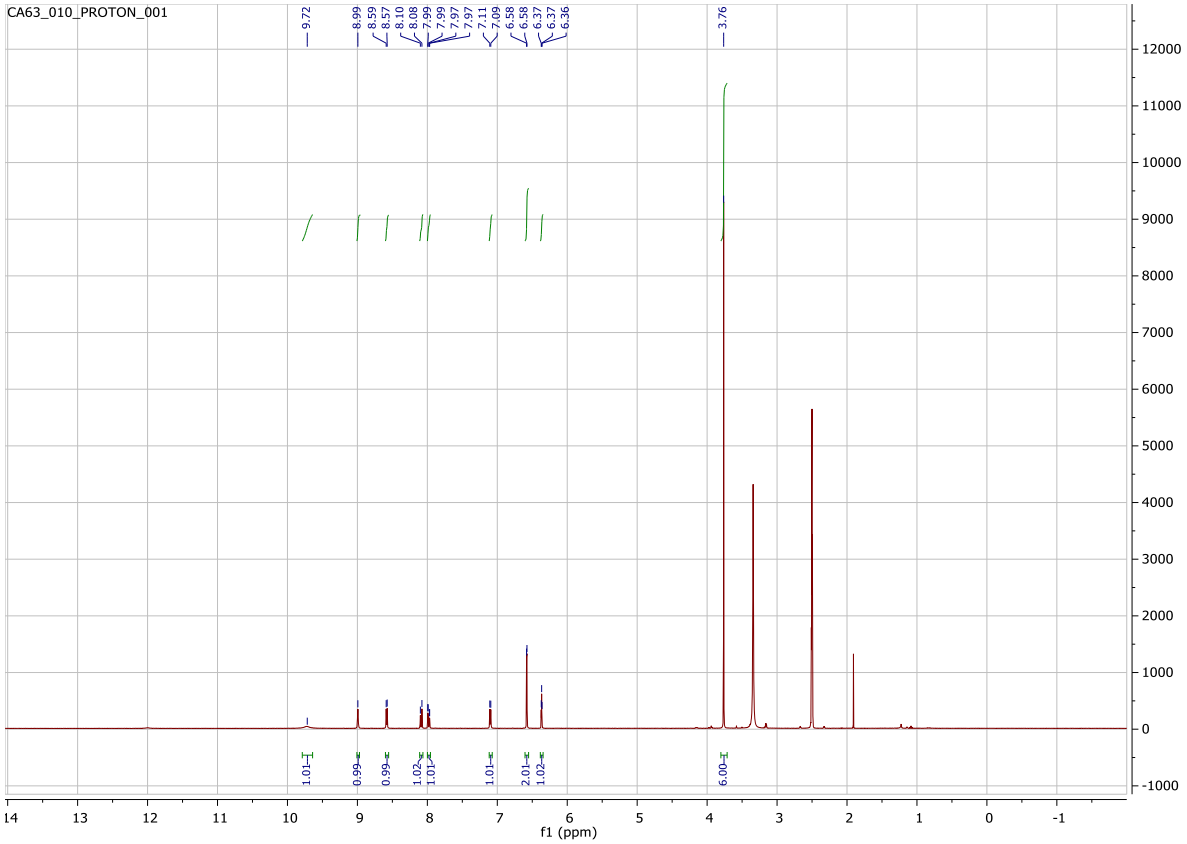


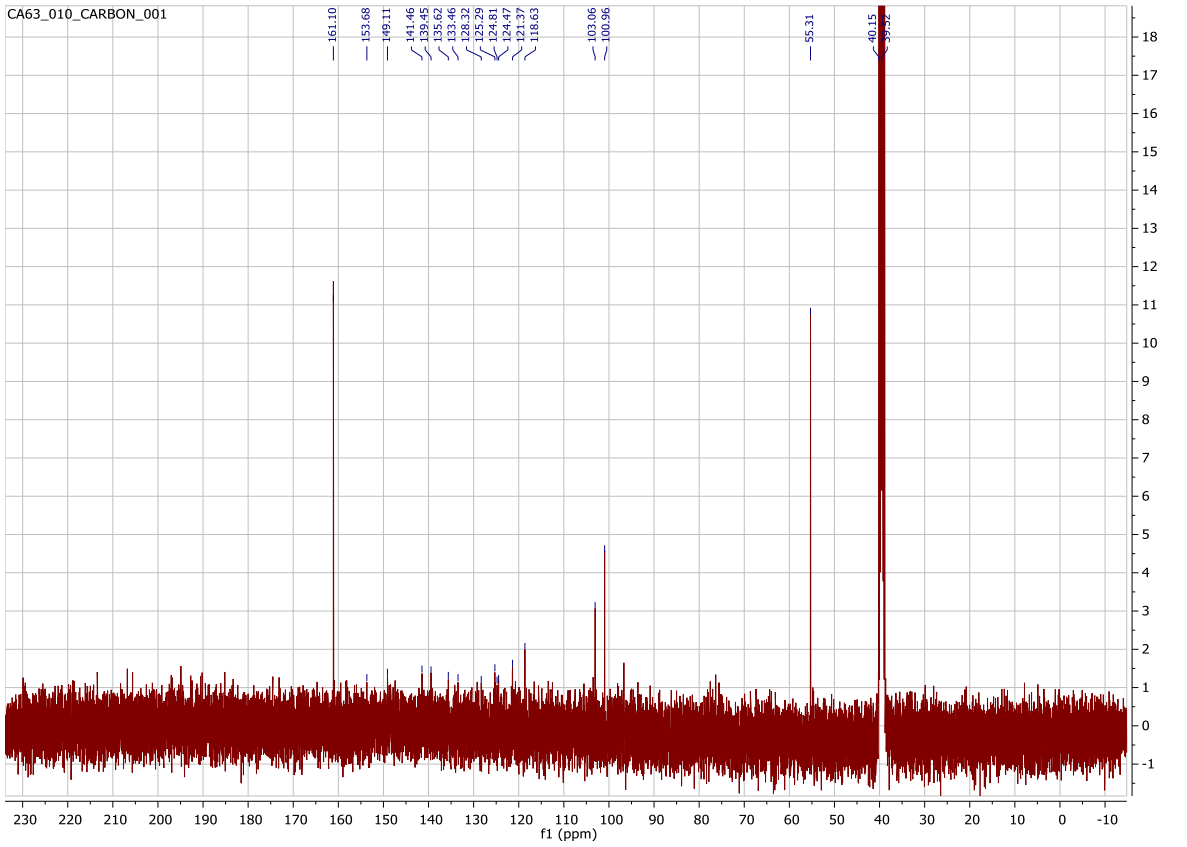
4

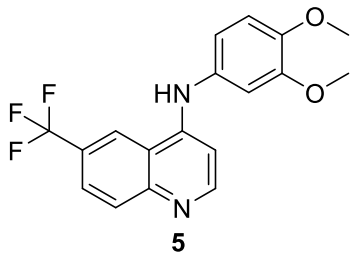
N-(3,5-Dimethoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**4**)





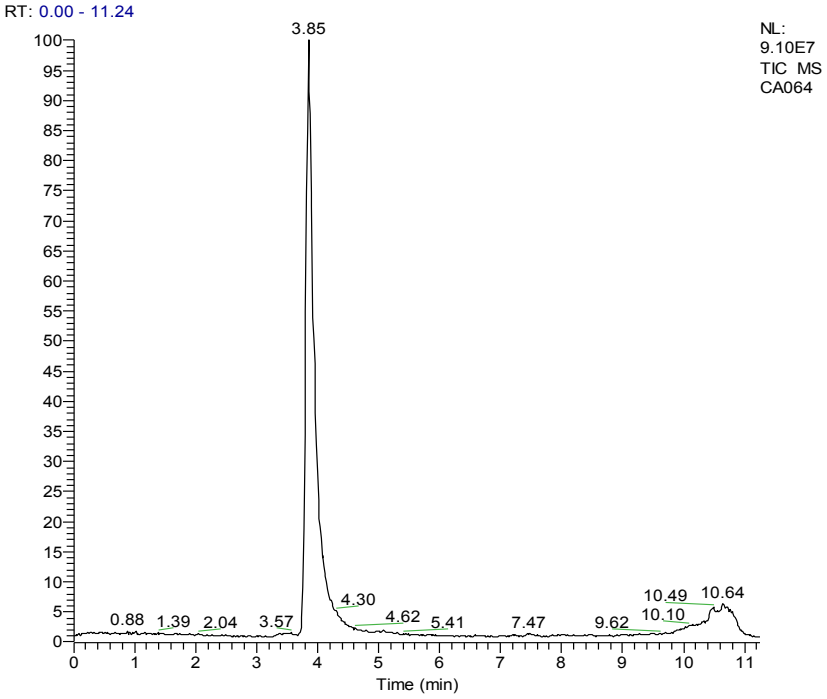

CA63_010_PROTON_001
9.72
8.99
8.59
8.57
8.10
8.08
7.99
7.99
7.97
7.97
7.11
7.09
6.58
6.58
6.37
6.37
6.36
3.76
1.01
0.99
0.99
1.02
1.01
1.01
2.01
1.02
6.00
f1 (ppm)

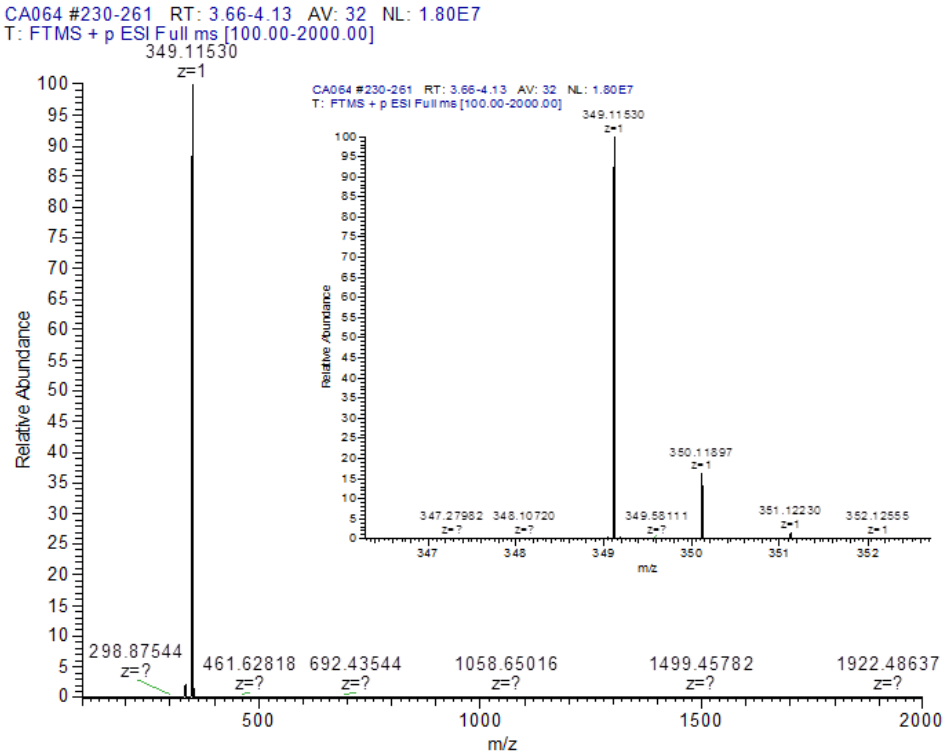

CA63_010_CARBON_001
161.10
153.68
149.11
141.46
139.45
135.62
133.46
128.32
125.29
124.81
124.47
121.37
118.63
103.06
100.96
55.31
40.15
39.92
f1 (ppm)

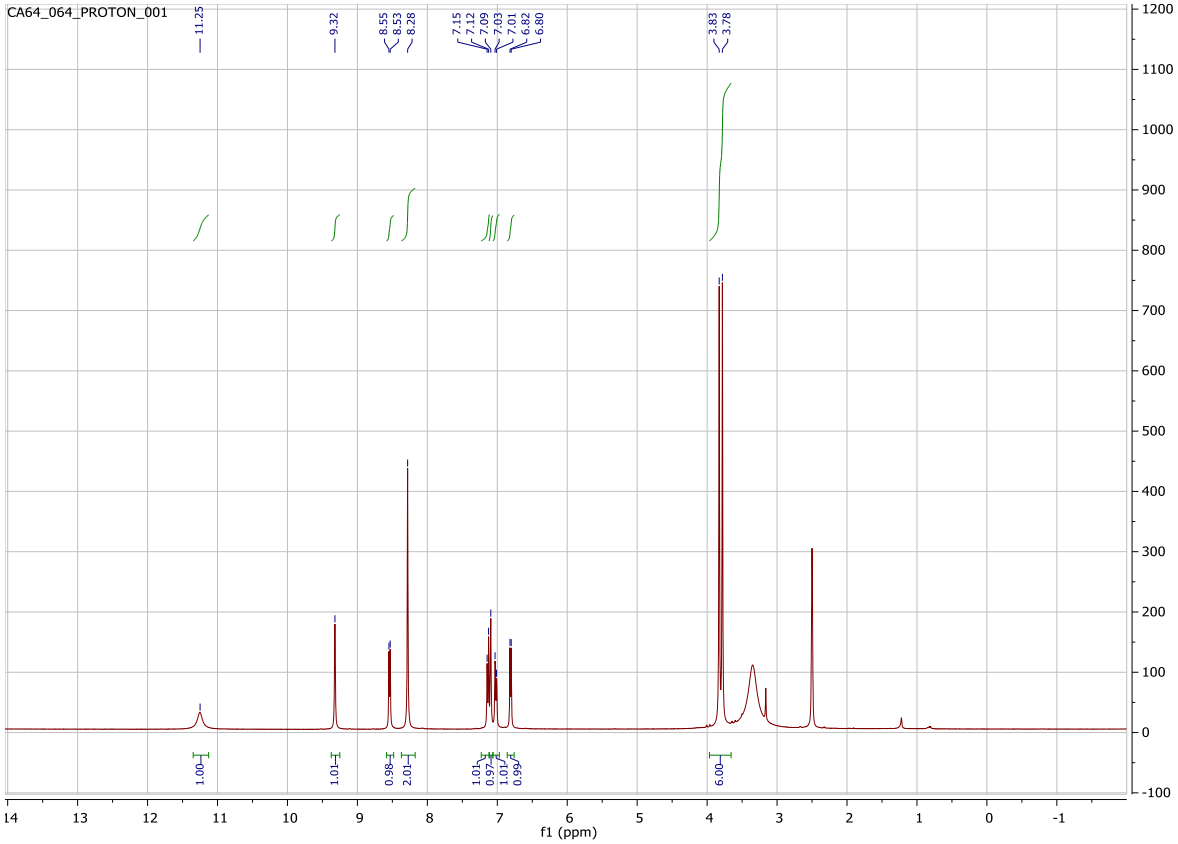


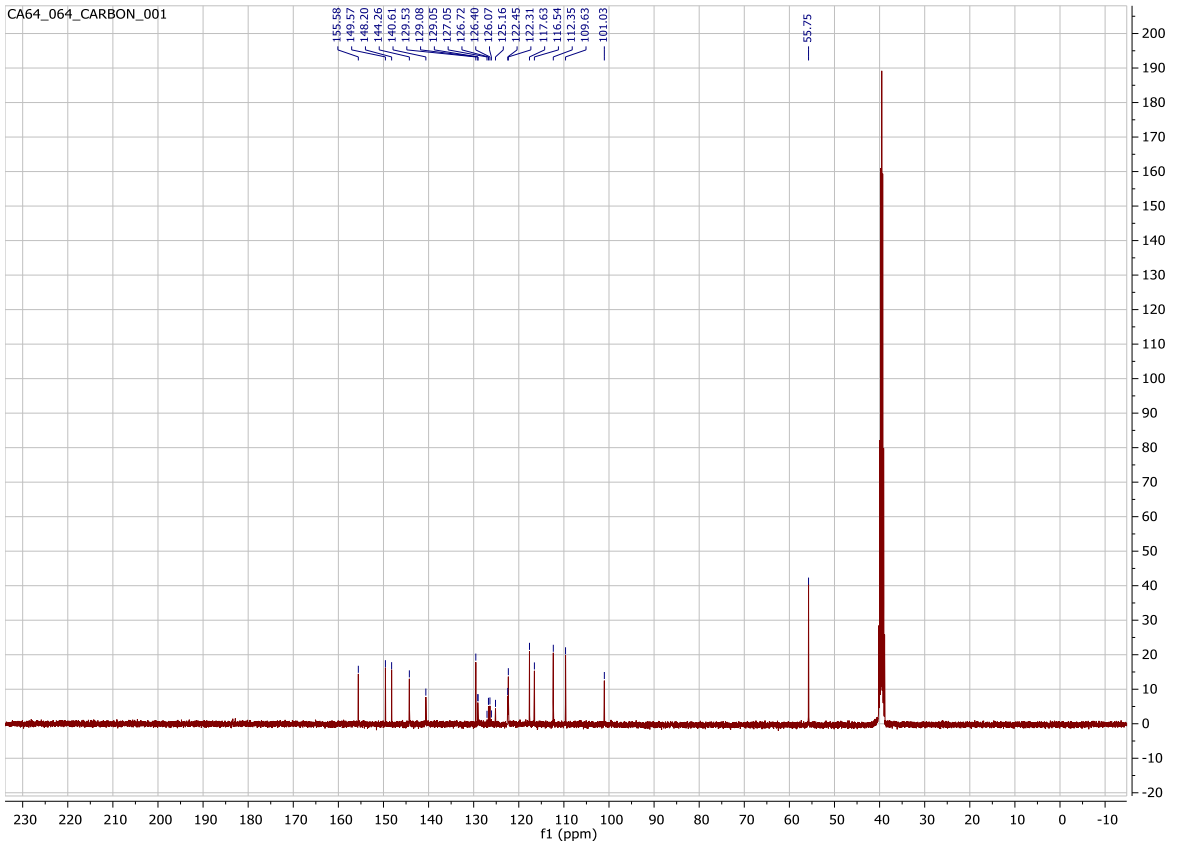
5

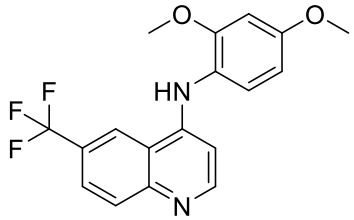
N-(3,4-Dimethoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**5**)





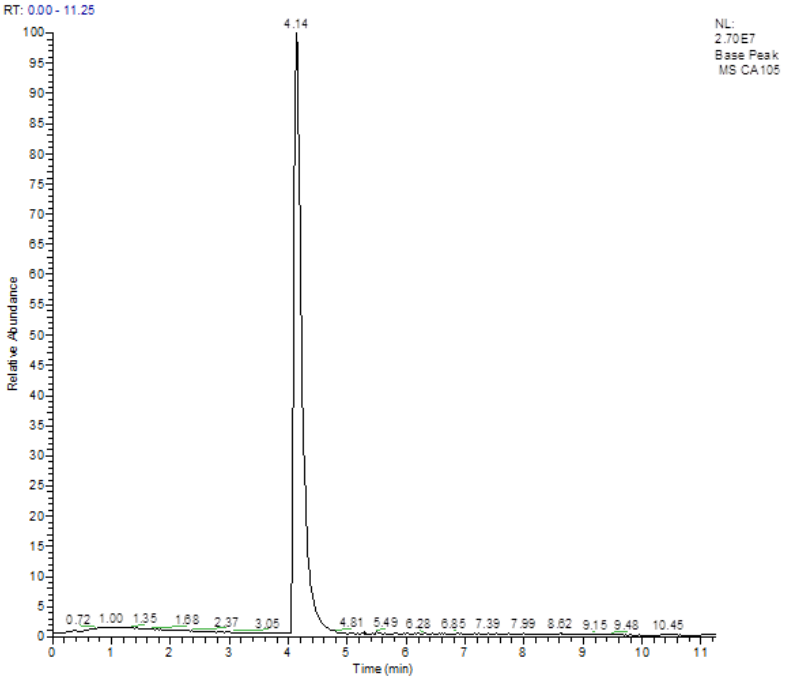

CA64_064_PROTON_001
11.25
9.32
8.55
8.53
8.28
7.15
7.12
7.09
7.03
7.01
6.82
6.80
3.83
3.78
1.00
1.01
0.98
2.01
1.01
0.97
1.01
0.99
6.00
f1 (ppm)

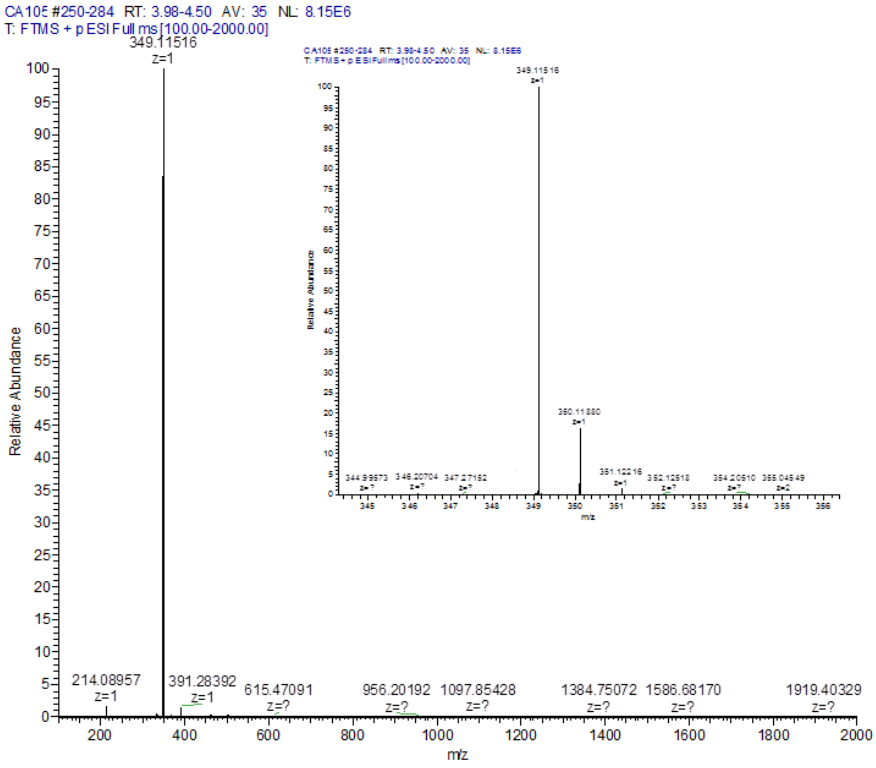

CA64_064_CARBON_001
155.58
149.57
148.20
144.26
140.61
129.53
129.08
129.05
127.05
126.72
126.40
126.07
125.16
122.45
122.31
117.63
116.54
112.35
109.63
101.03
55.75
f1 (ppm)

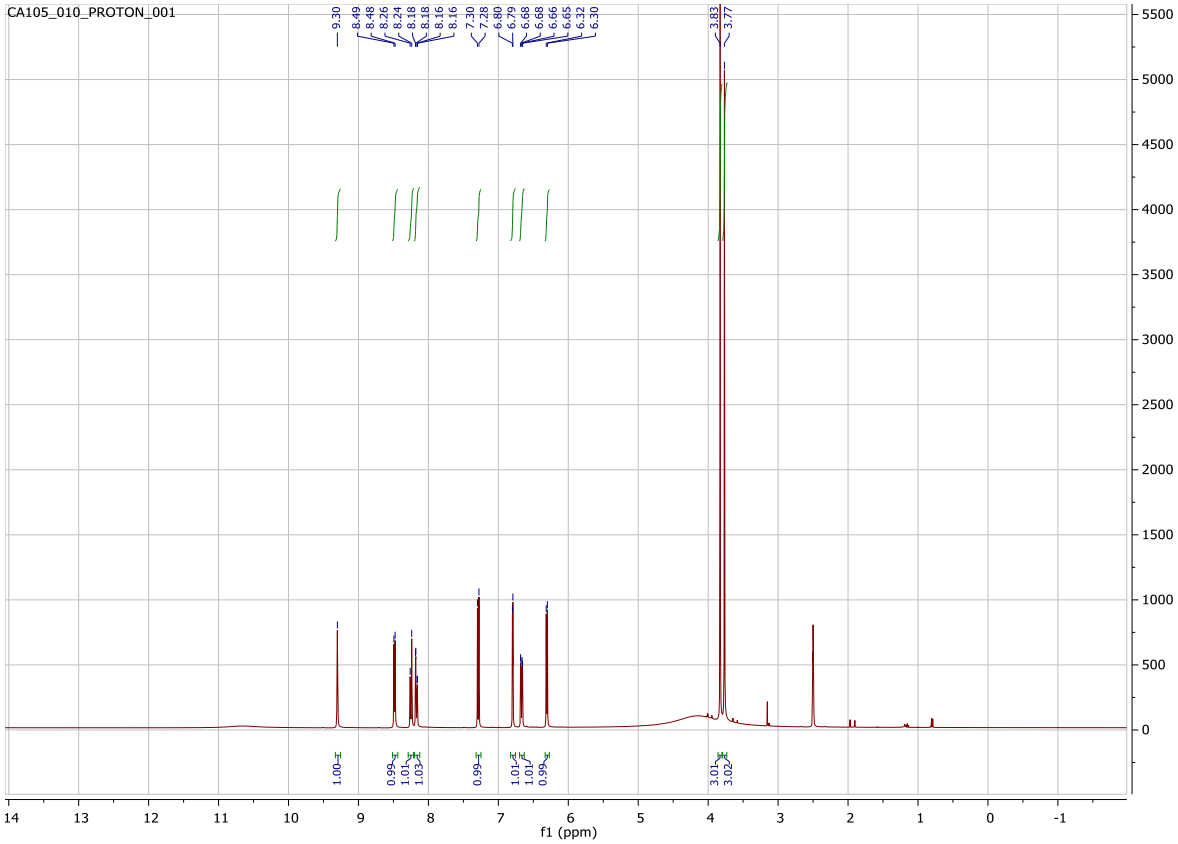


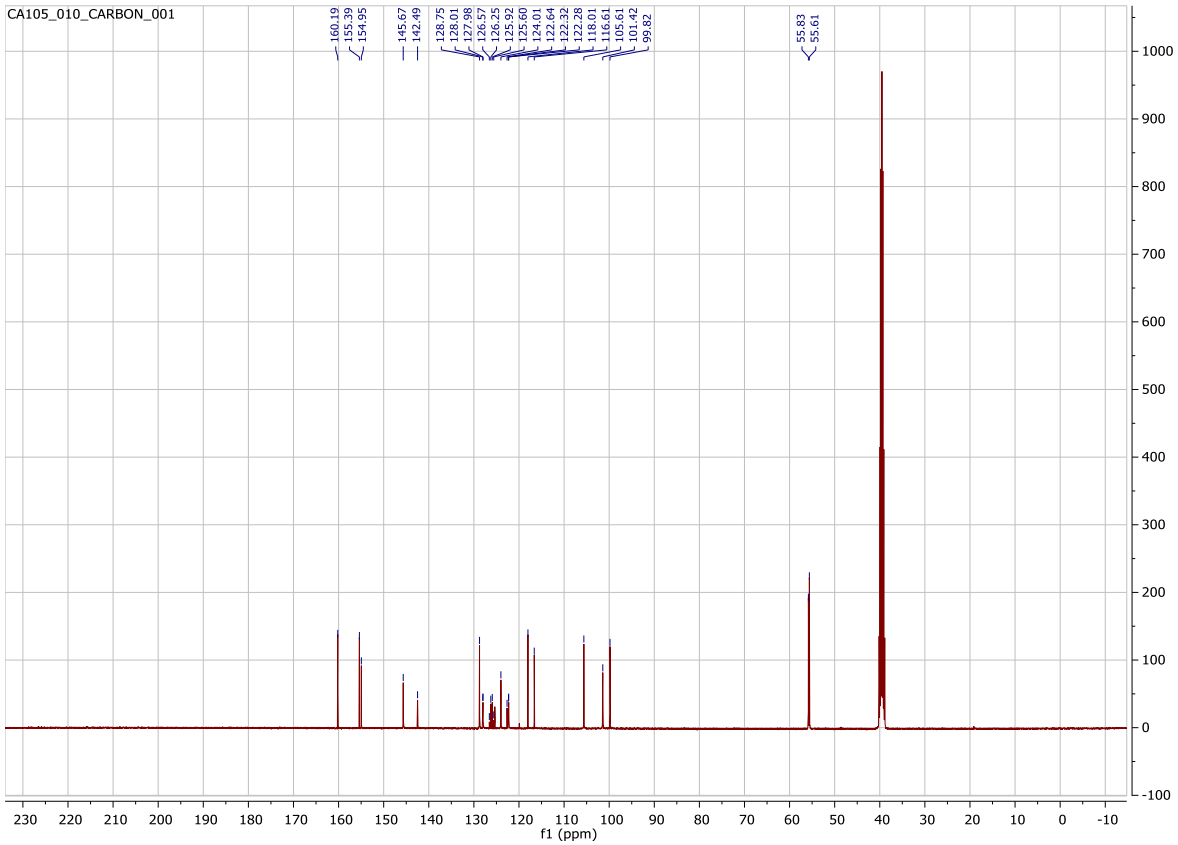
6

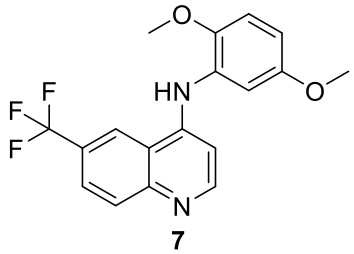
N-(2,4-Dimethoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**6**)





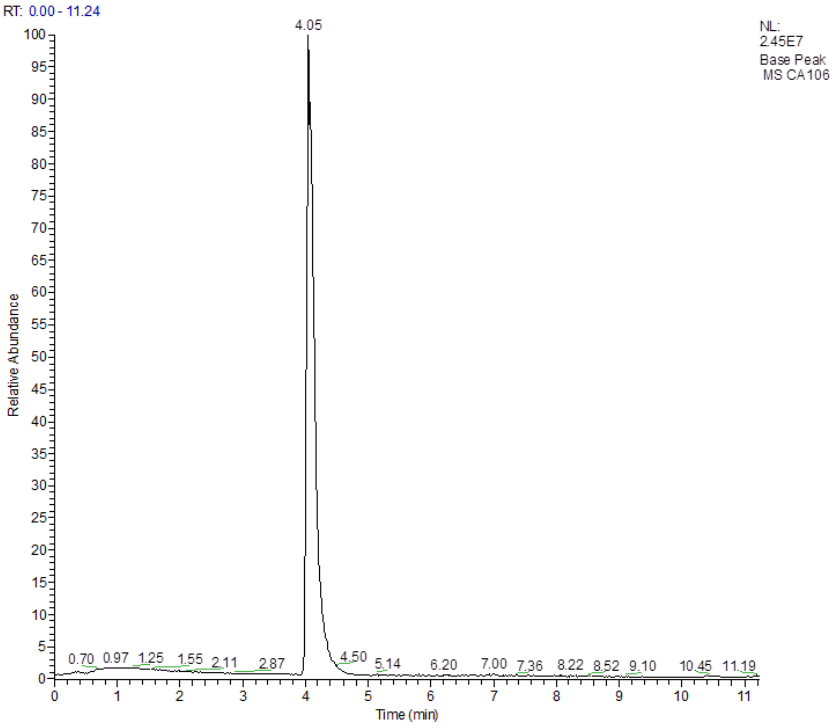

CA105_010_PROTON_001
9.30
8.49
8.48
8.26
8.24
8.18
8.18
8.16
8.16
7.30
7.28
6.80
6.79
6.68
6.68
6.66
6.65
6.32
6.30
3.83
3.77
1.00
0.99
1.01
1.03
0.99
1.01
1.01
0.99
3.01
3.02
f1 (ppm)

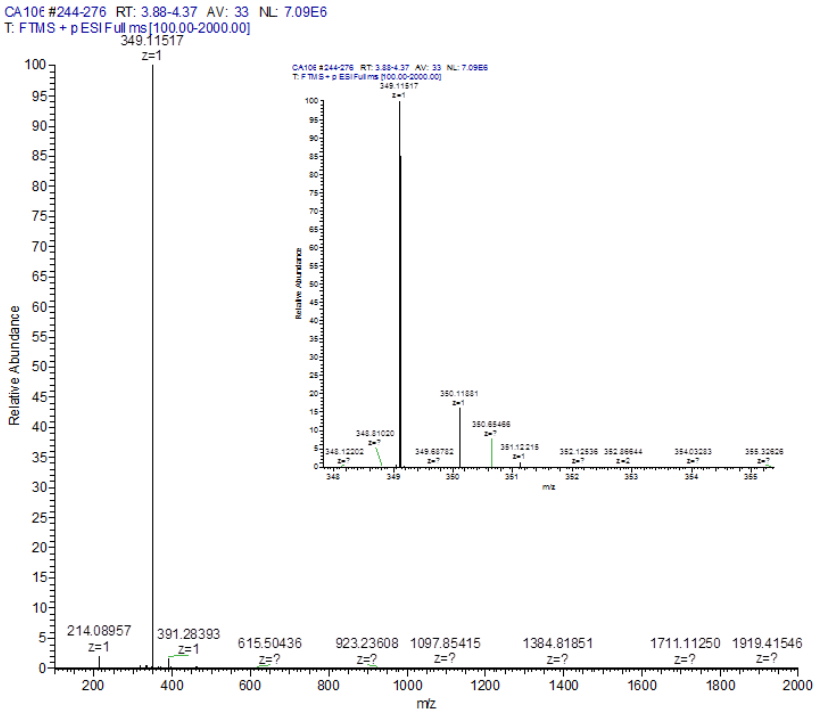

CA105_010_CARBON_001
160.19
155.39
154.95
145.67
142.49
128.75
128.01
127.98
126.57
126.25
125.92
125.60
124.01
122.64
122.32
122.28
118.01
116.61
105.61
101.42
99.82
55.83
55.61
f1 (ppm)

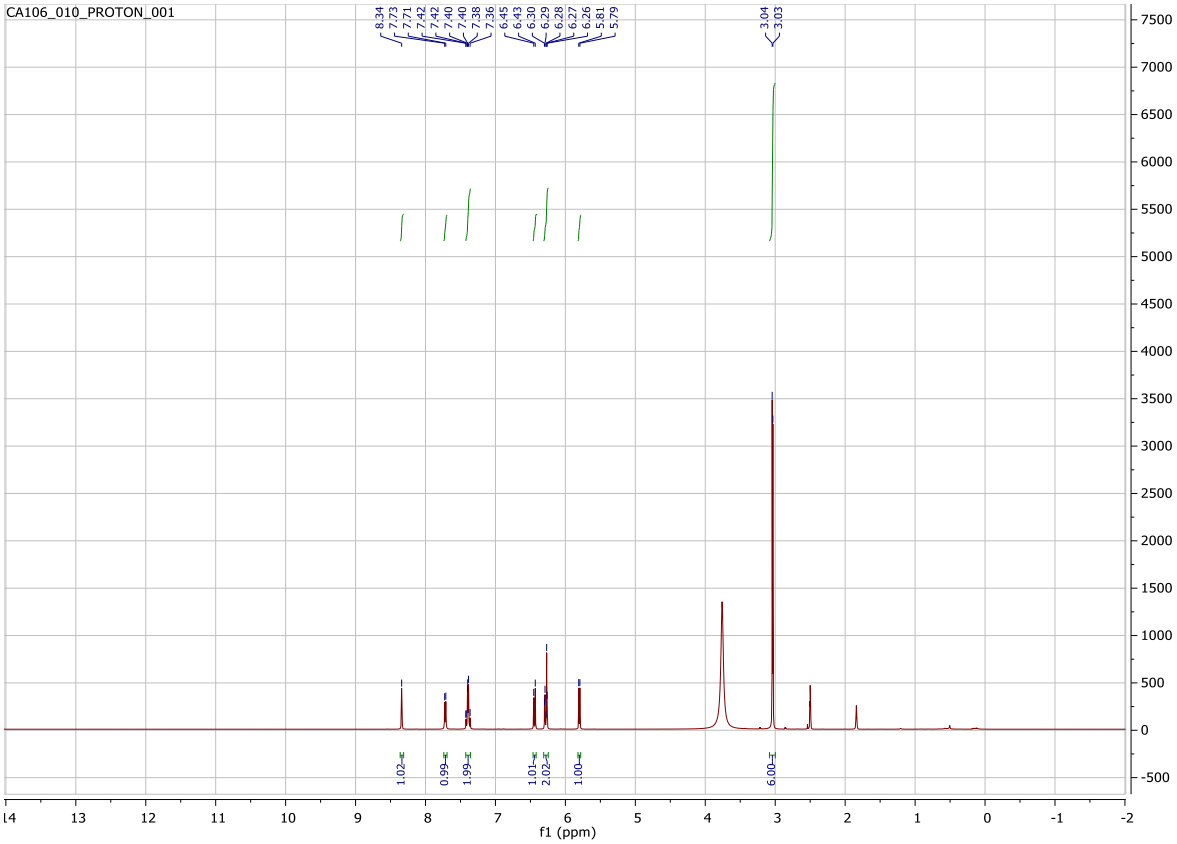


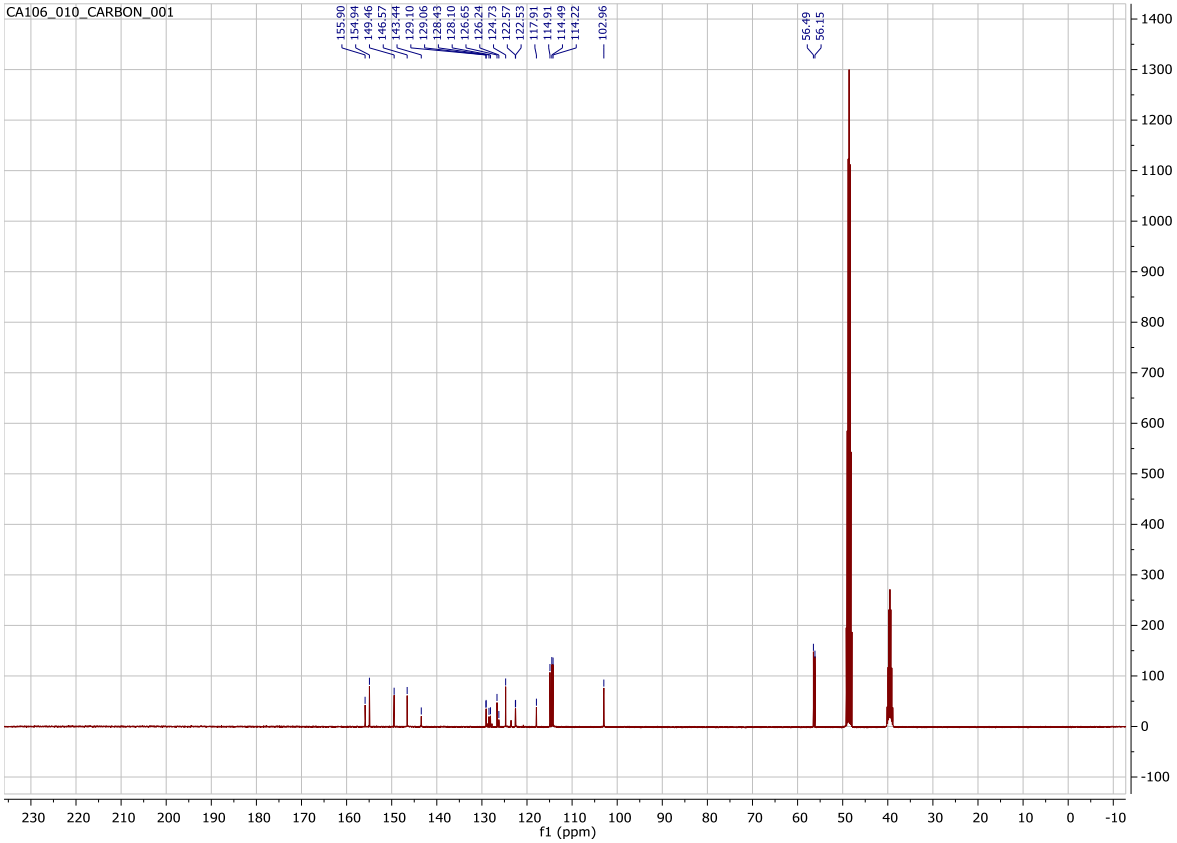
7

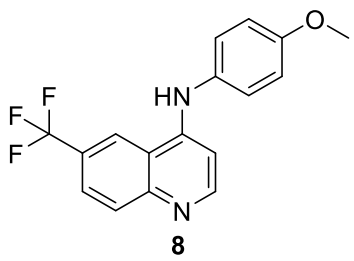
N-(2,5-Dimethoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**7**)





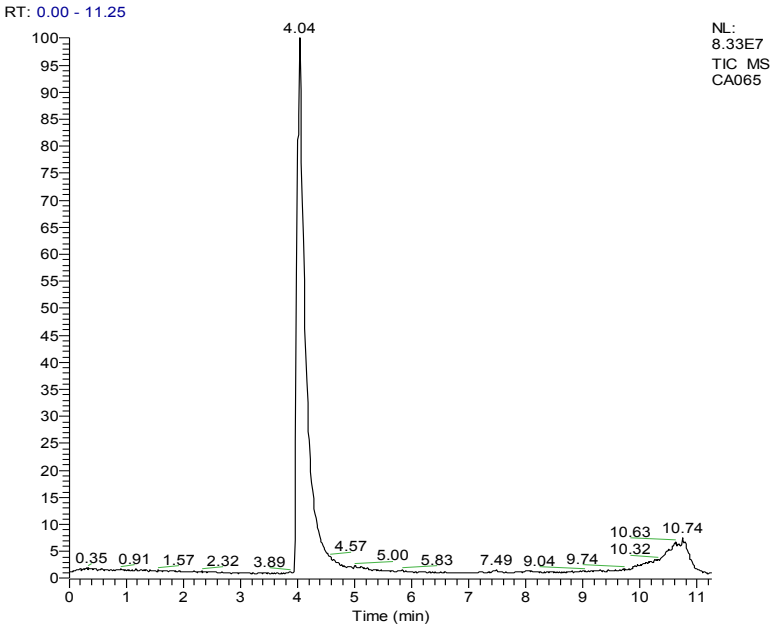

CA106_010_PROTON_001
8.34
7.73
7.71
7.42
7.42
7.40
7.40
7.38
7.36
6.45
6.43
6.30
6.29
6.28
6.27
6.26
5.81
5.79
3.04
3.03
1.02
0.99
1.99
1.01
2.02
1.00
6.00
f1 (ppm)

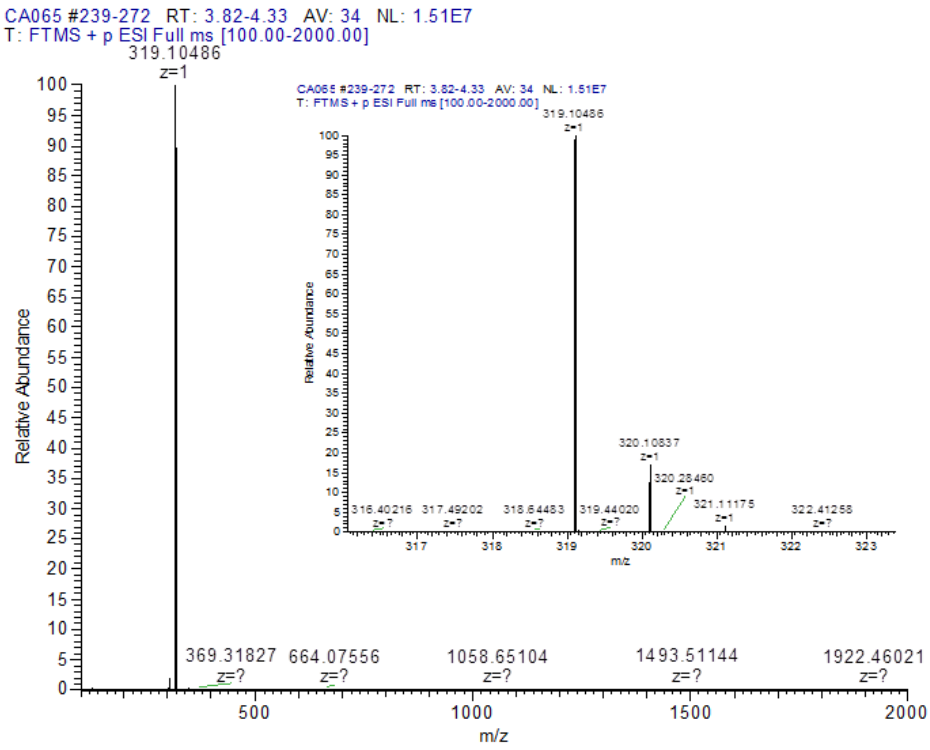

CA106_010_CARBON_001
155.90
154.94
149.46
146.57
143.44
129.10
129.06
128.43
128.10
126.65
126.24
124.73
122.57
122.53
117.91
114.91
114.49
114.22
102.96
56.49
56.15
f1 (ppm)

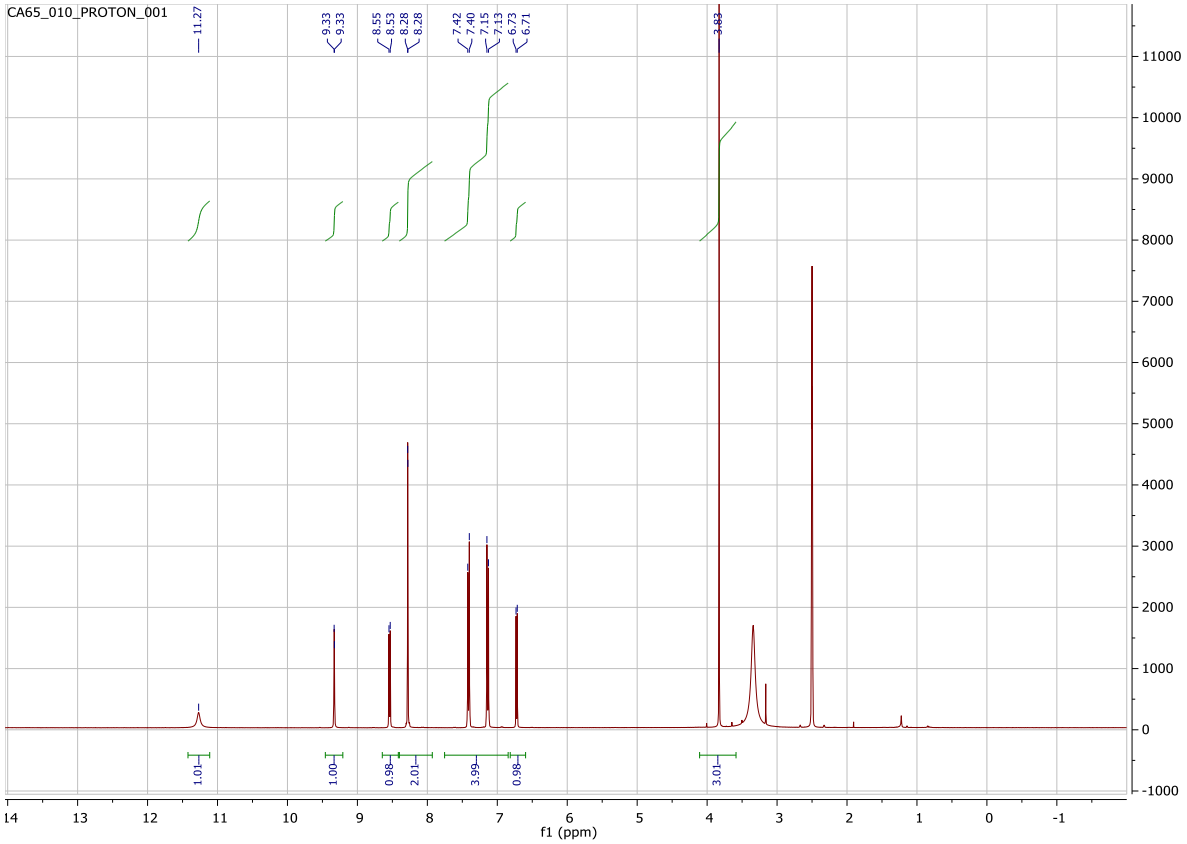


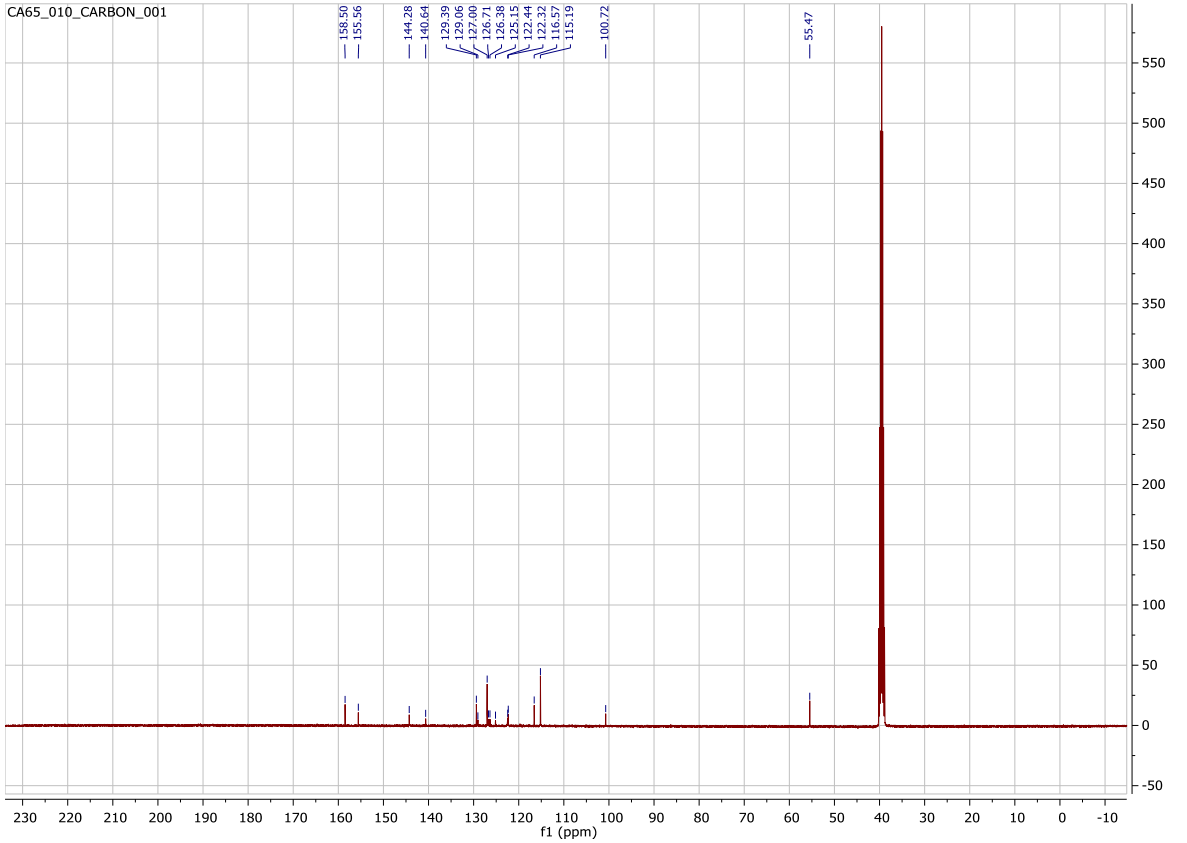
8

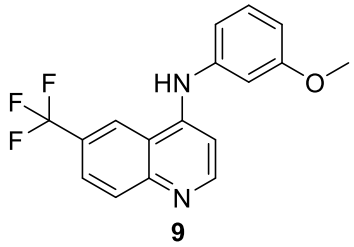
N-(4-Methoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**8**)





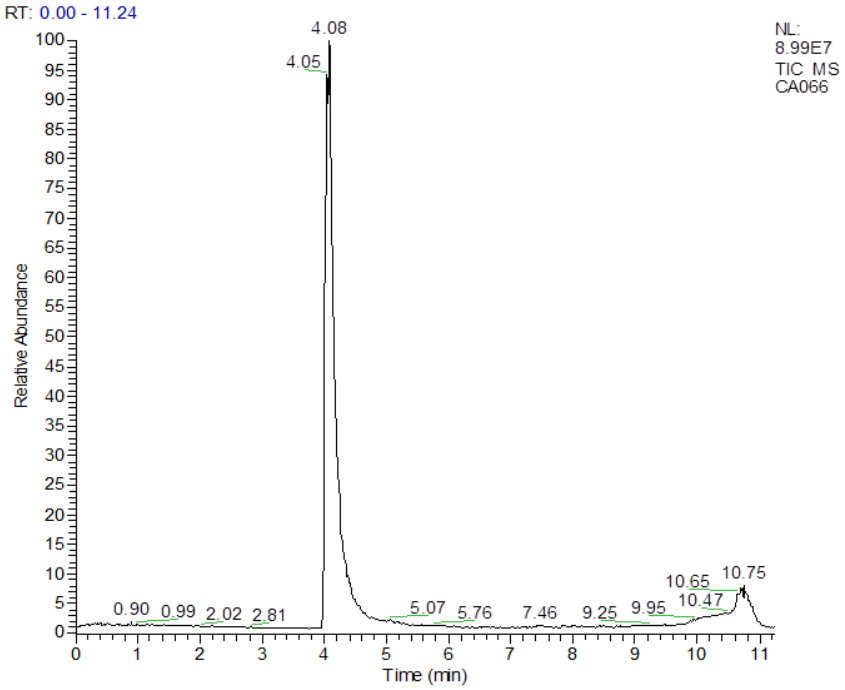

CA65_010_PROTON_001
11.27
9.33
9.33
8.55
8.53
8.28
8.28
7.42
7.40
7.15
7.13
6.73
6.71
3.83
1.01
1.00
0.98
2.01
3.99
0.98
3.01
f1 (ppm)

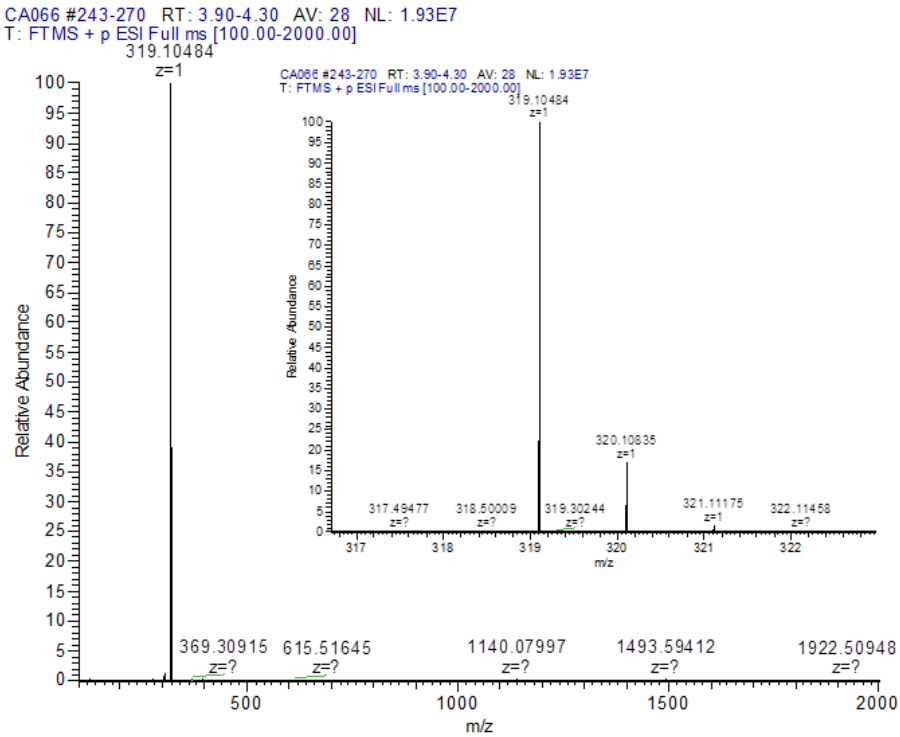

CA65_010_CARBON_001
158.50
155.56
144.28
140.64
129.39
129.06
127.00
126.71
126.38
125.15
122.44
122.32
116.57
115.19
100.72
55.47
f1 (ppm)

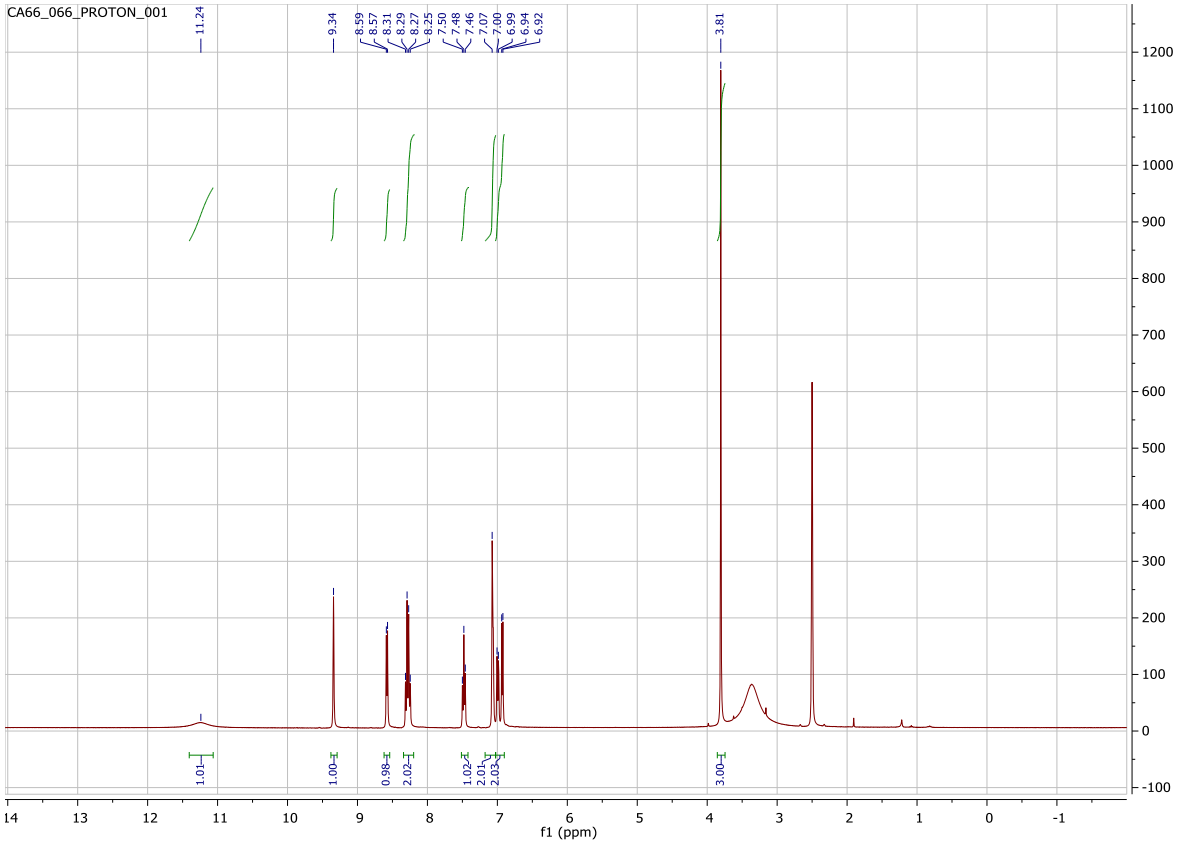


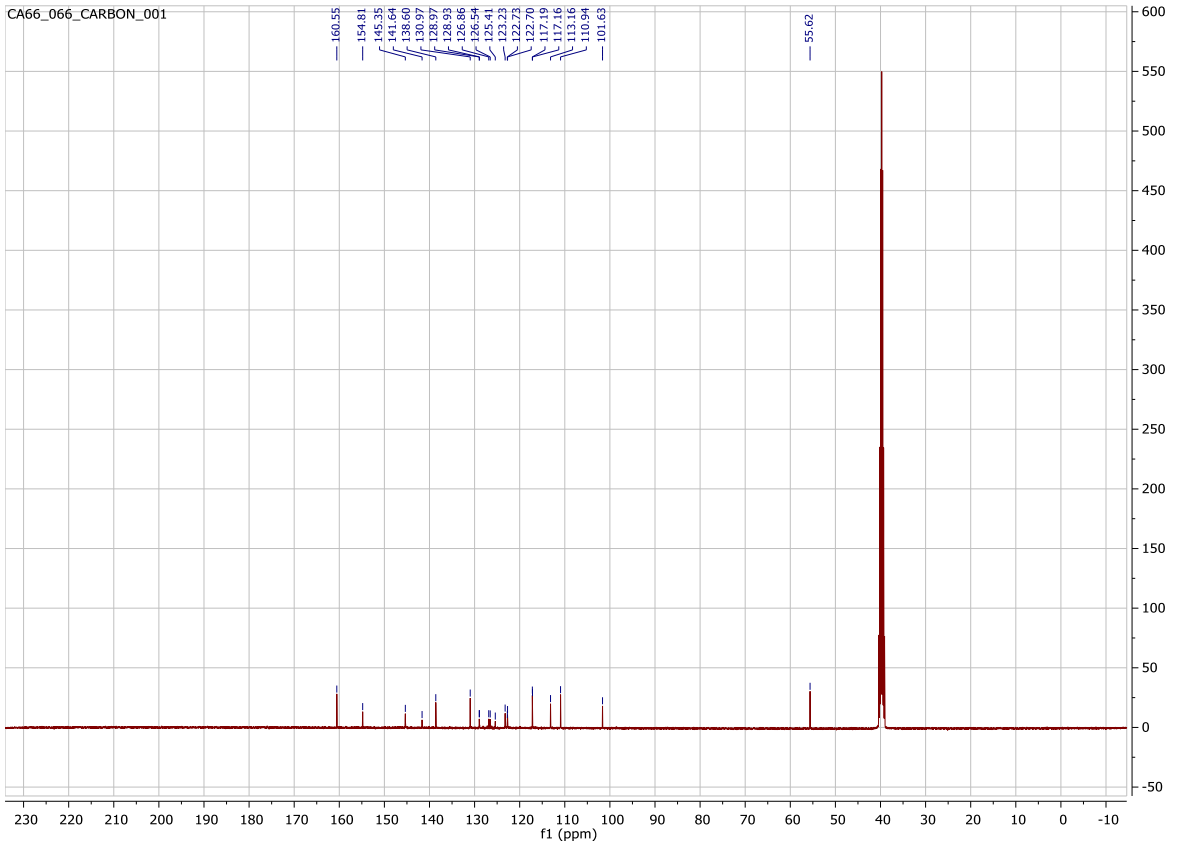
9

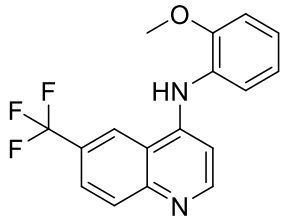
N-(3-Methoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**9**)





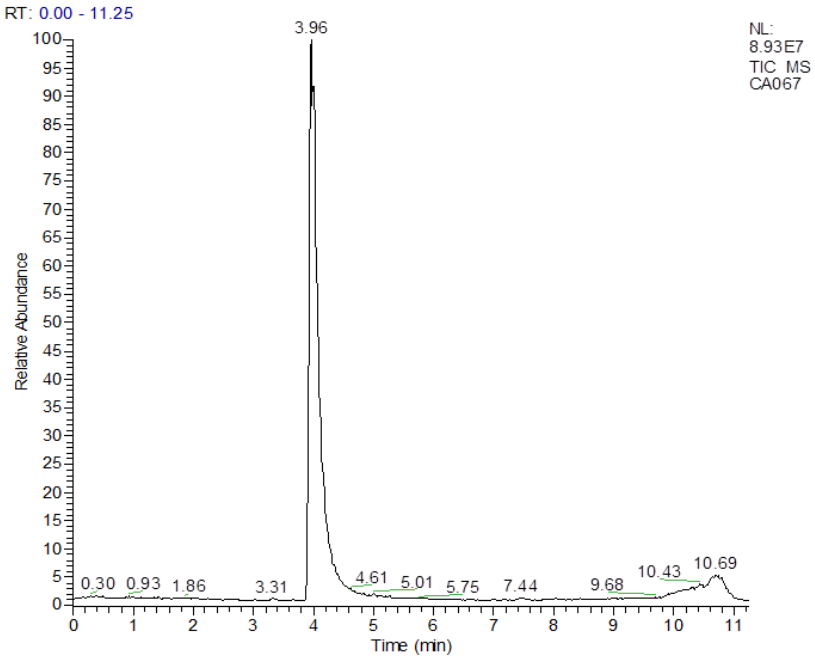

CA66_066_PROTON_001
11.24
9.34
8.59
8.57
8.31
8.29
8.27
8.25
7.50
7.48
7.46
7.07
7.00
6.99
6.94
6.92
3.81
1.01
1.00
0.98
2.02
1.02
2.01
2.03
3.00
f1 (ppm)

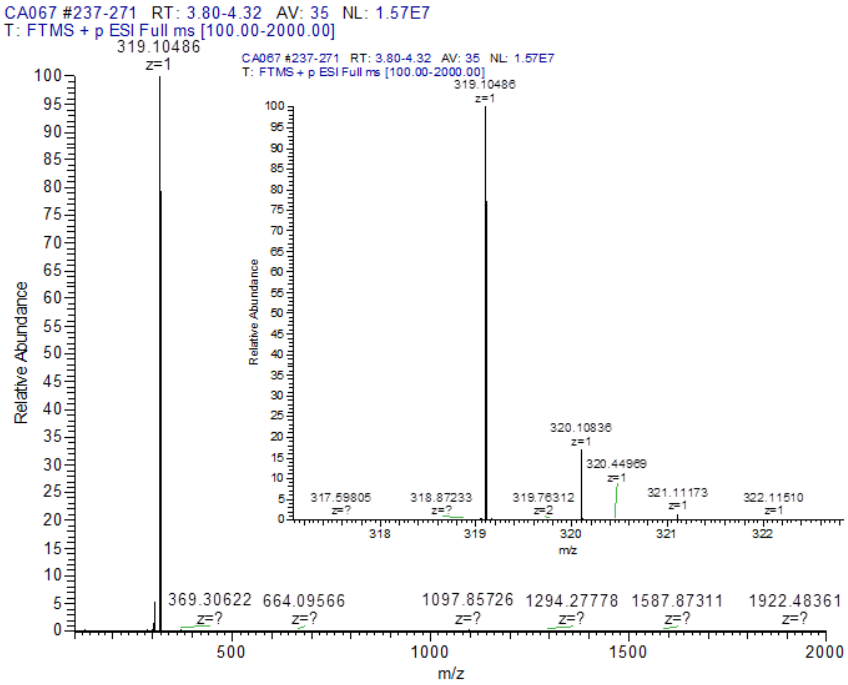

CA66_066_CARBON_001
160.55
154.81
145.35
141.64
138.60
130.97
128.97
128.93
126.86
126.54
125.41
123.23
122.73
122.70
117.19
117.16
113.16
110.94
101.63
55.62
f1 (ppm)

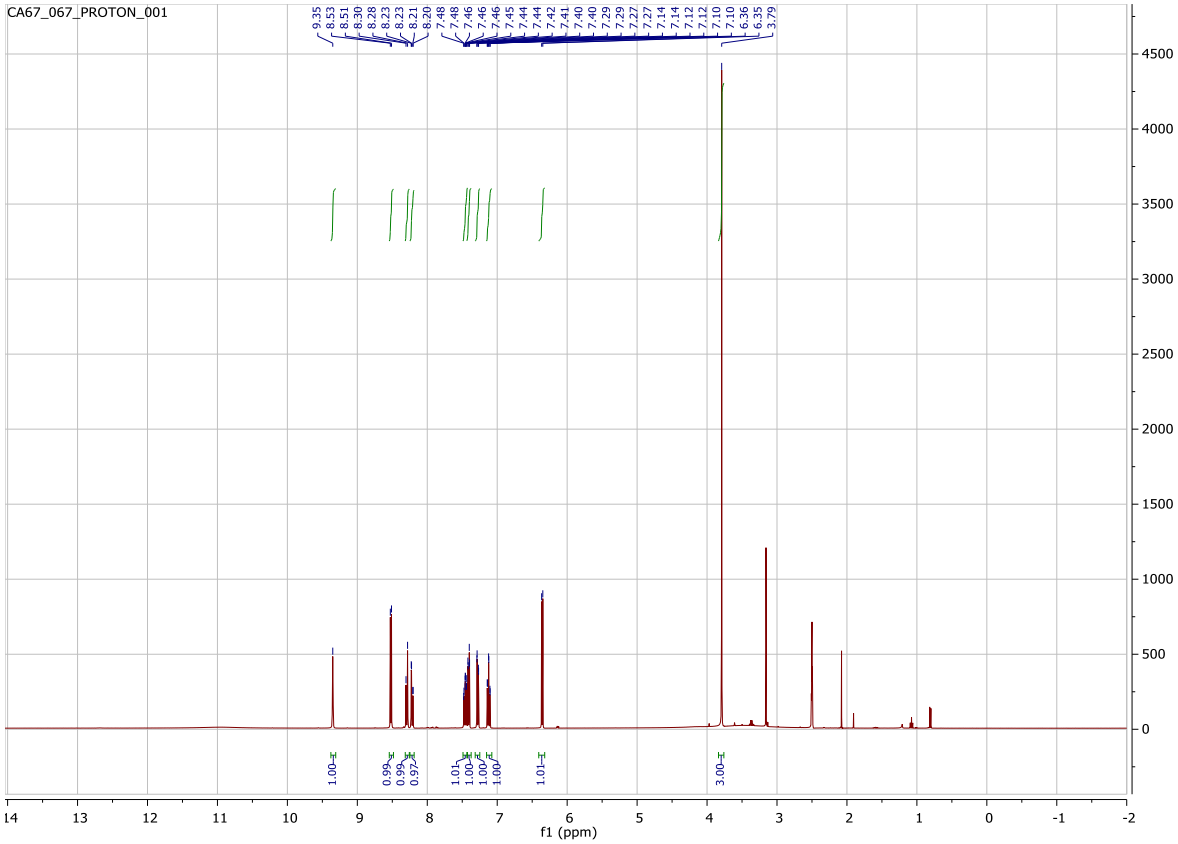


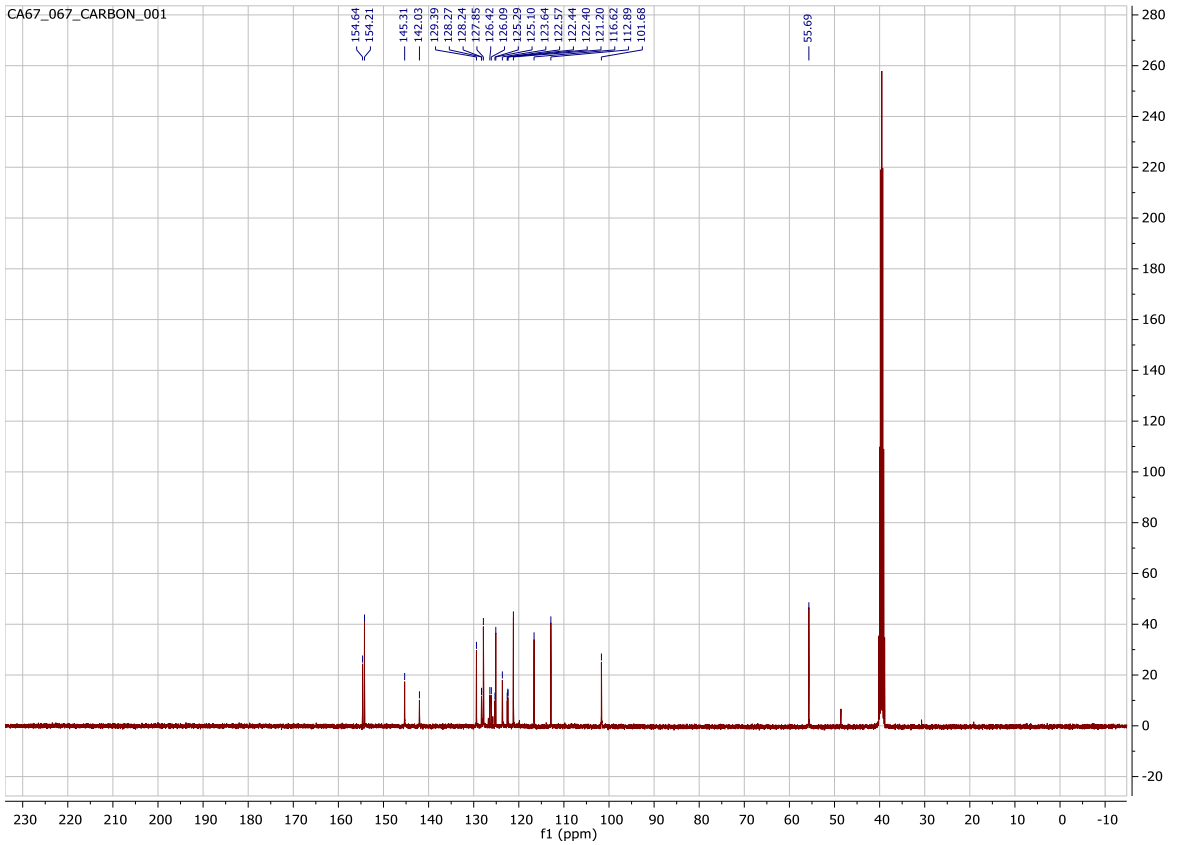
10

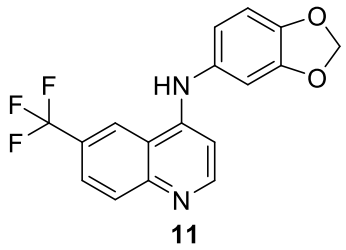
N-(2-Methoxyphenyl)-6-(trifluoromethyl)quinolin-4-amine (**10**)





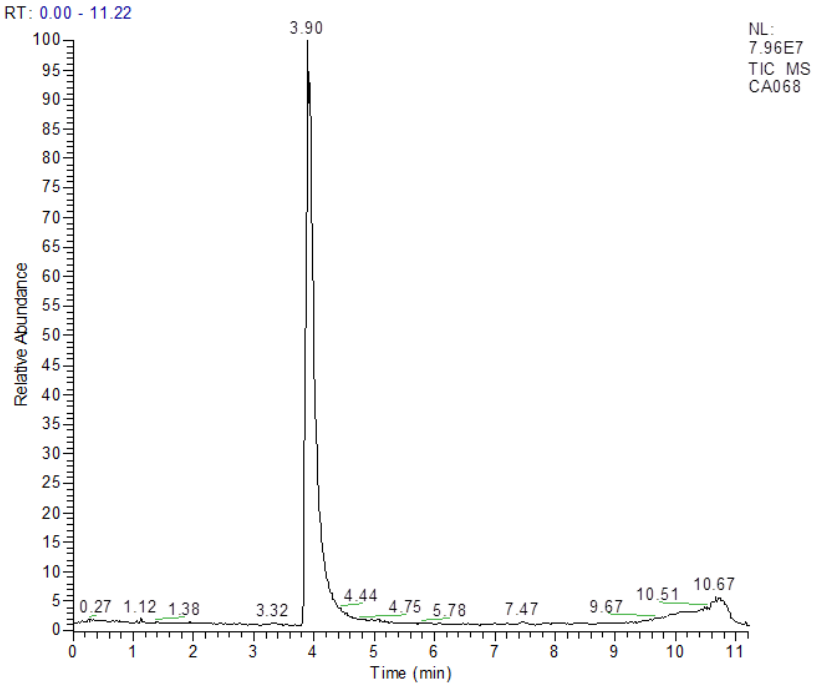

CA67_067_PROTON_001
9.35
8.53
8.51
8.30
8.28
8.23
8.23
8.21
8.20
7.48
7.48
7.46
7.46
7.46
7.45
7.44
7.44
7.42
7.41
7.40
7.40
7.29
7.29
7.27
7.27
7.14
7.14
7.12
7.12
7.10
7.10
6.36
6.35
3.79
1.00
0.99
0.99
0.97
1.01
1.00
1.00
1.00
1.01
3.00
f1 (ppm)

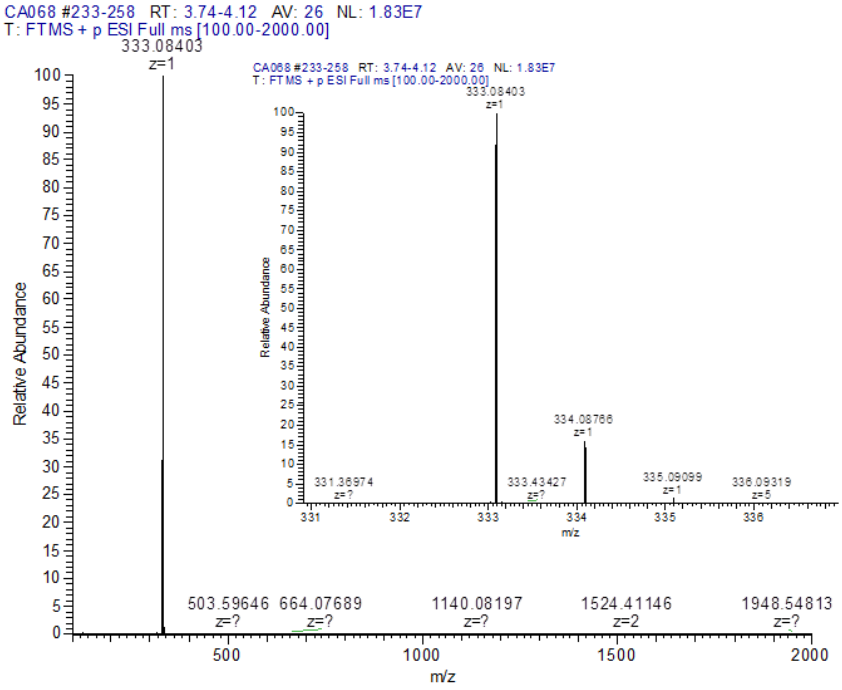

CA67_067_CARBON_001
154.64
154.21
145.31
142.03
129.39
128.27
128.24
127.85
126.42
126.09
125.29
125.10
123.64
122.57
122.44
122.40
121.20
116.62
112.89
101.68
55.69
f1 (ppm)

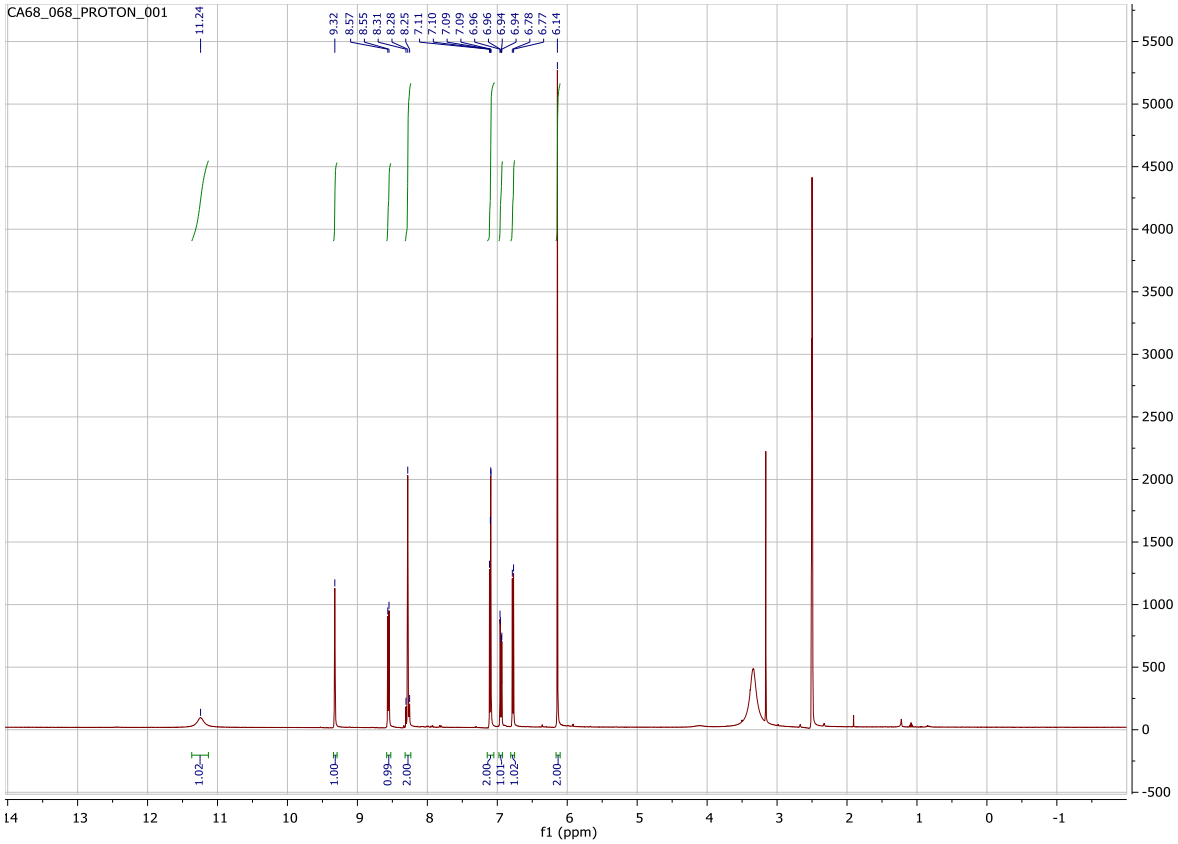


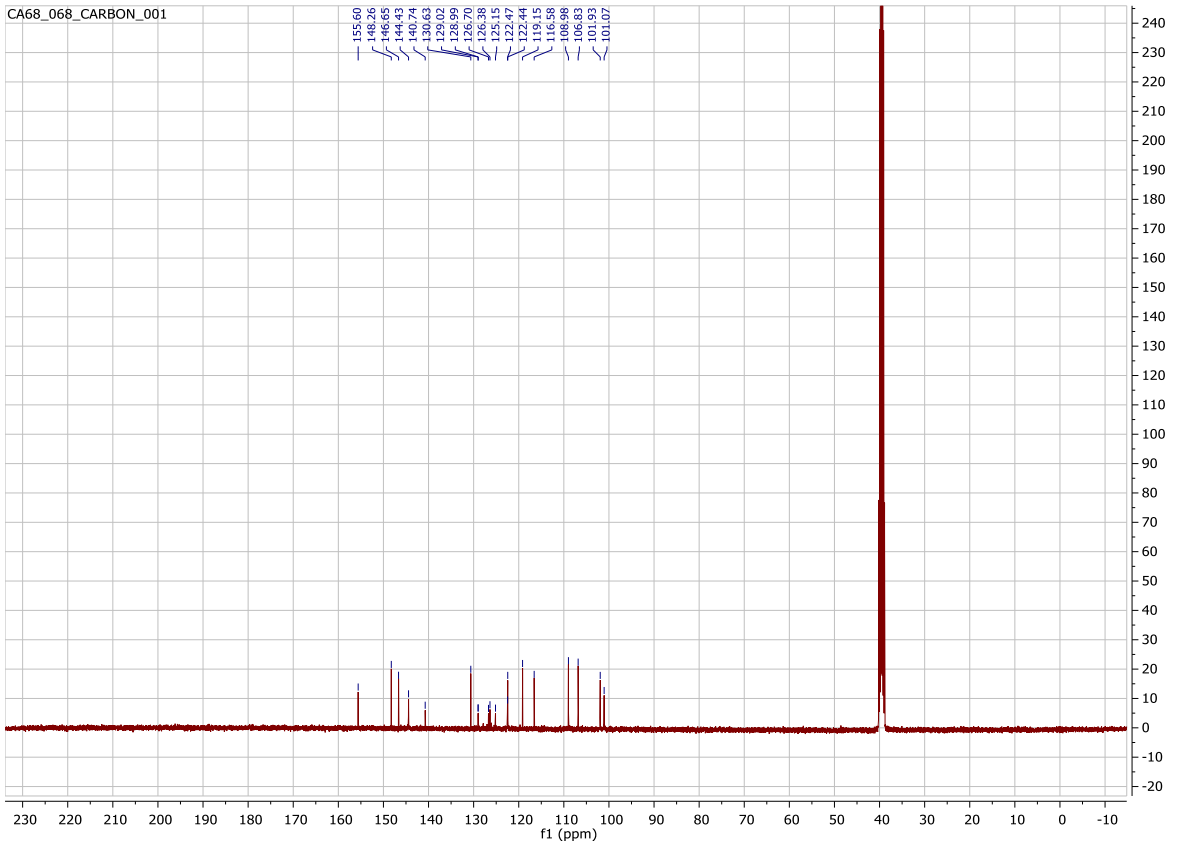
11

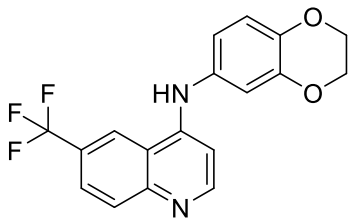
N-(Benzo[*d*][1,3]dioxol-5-yl)-6-(trifluoromethyl)quinolin-4-amine (**11**)





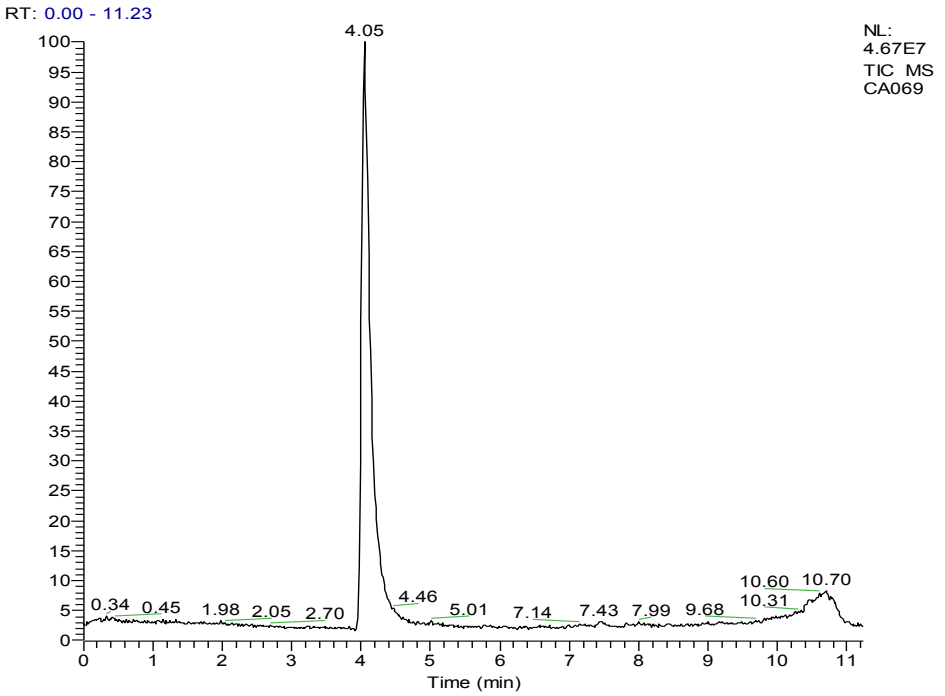

CA68_068_PROTON_001
11.24
9.32
8.57
8.55
8.31
8.28
8.25
7.11
7.10
7.09
7.09
6.96
6.96
6.94
6.94
6.78
6.77
6.14
1.02
1.00
0.99
2.00
2.00
1.01
1.02
2.00
f1 (ppm)

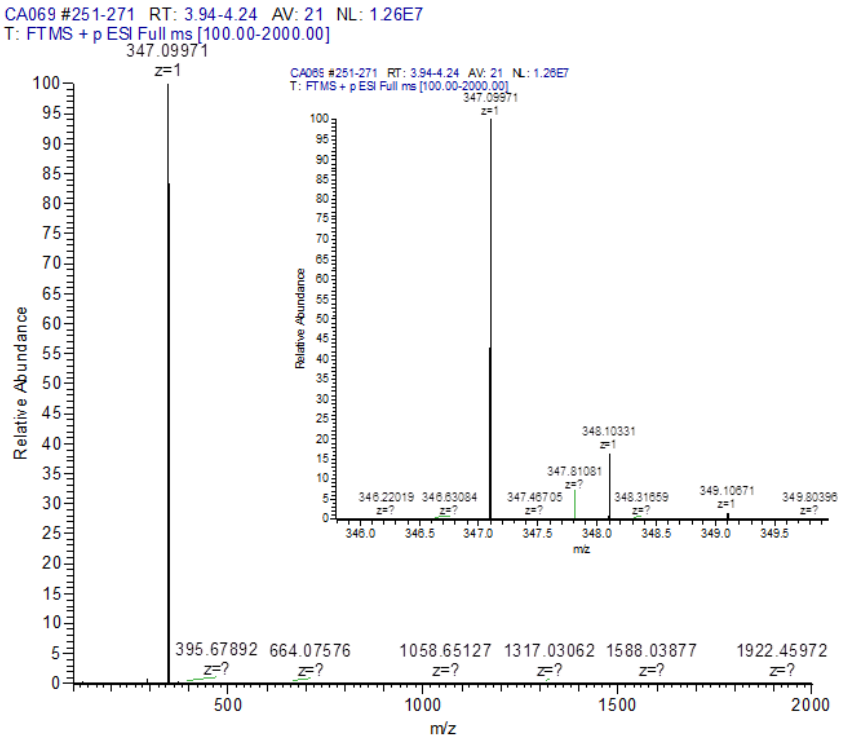

CA68_068_CARBON_001
155.60
148.26
146.65
144.43
140.74
130.63
129.02
128.99
126.70
126.38
125.15
122.47
122.44
119.15
116.58
108.98
106.83
101.93
101.07
f1 (ppm)

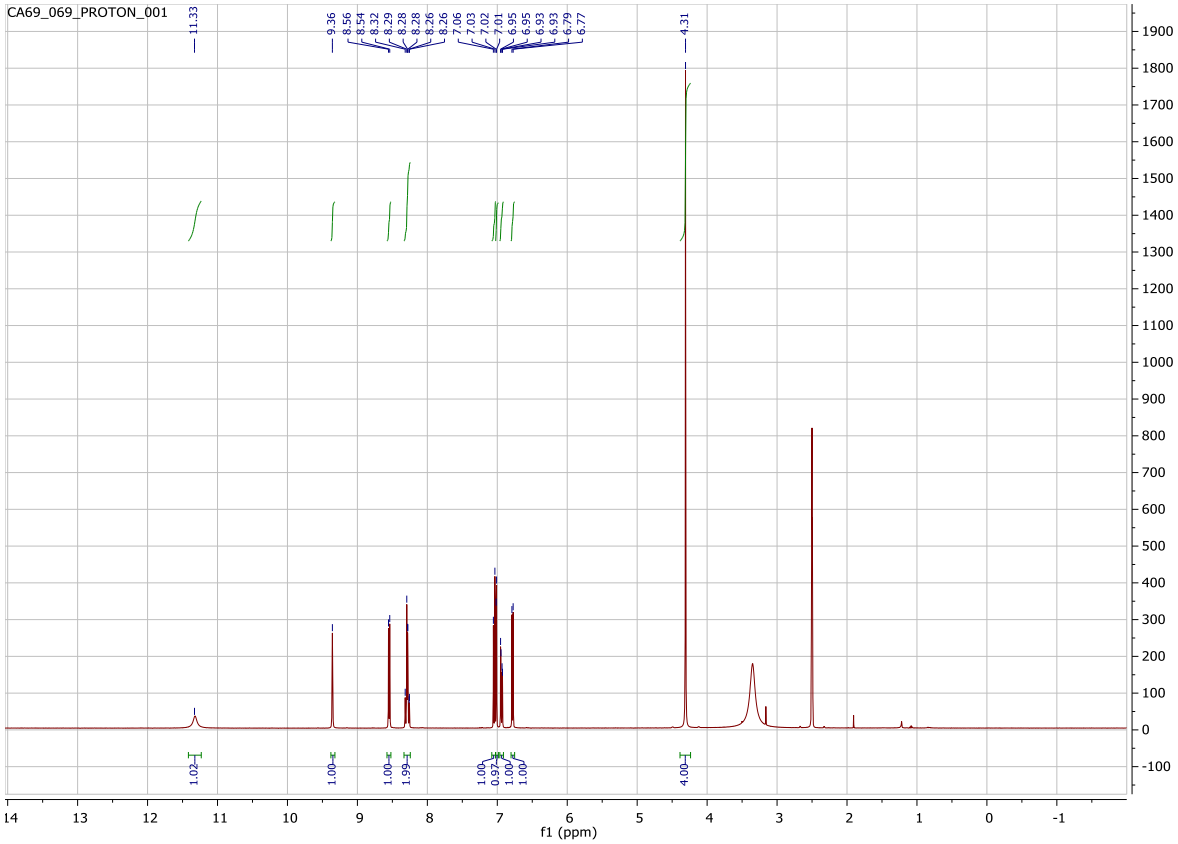


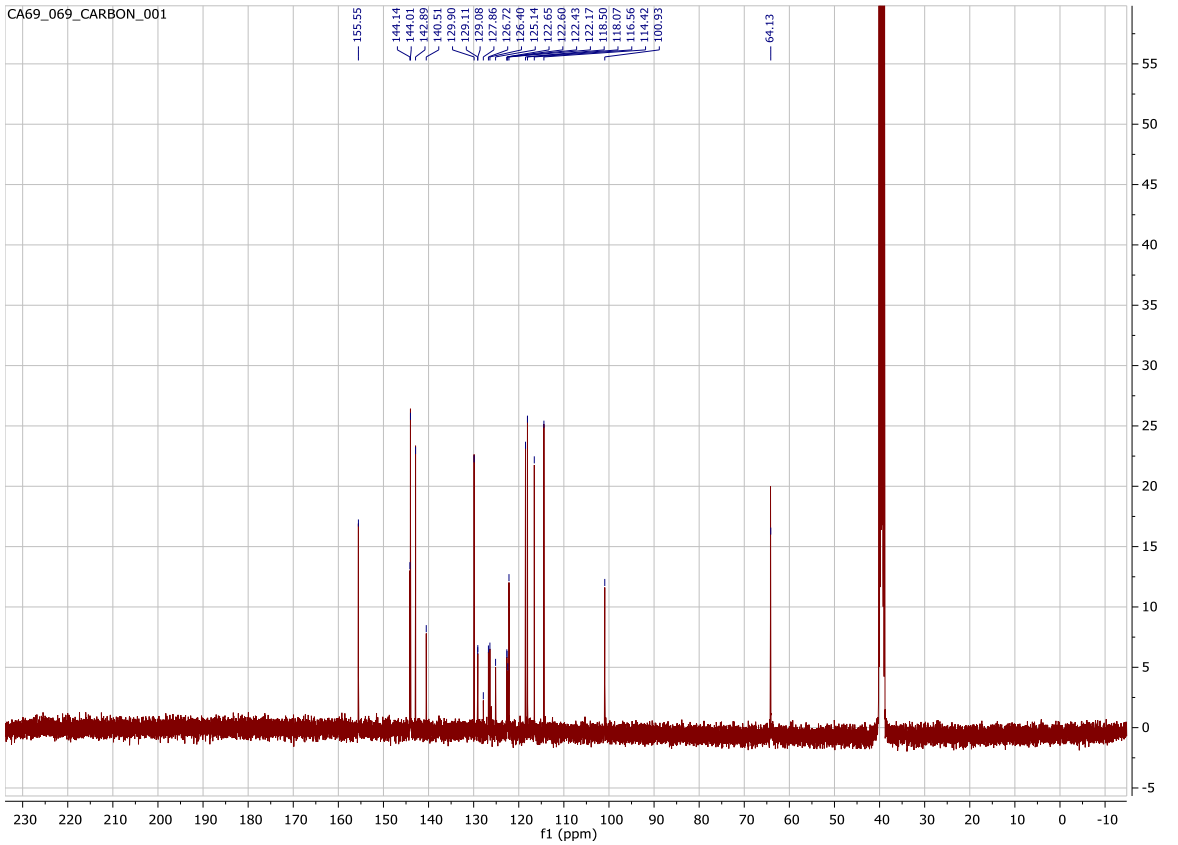
12

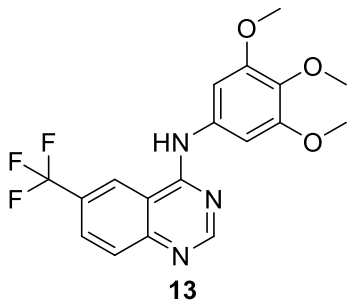
N-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-6-(trifluoromethyl)quinolin-4-amine (**12**)





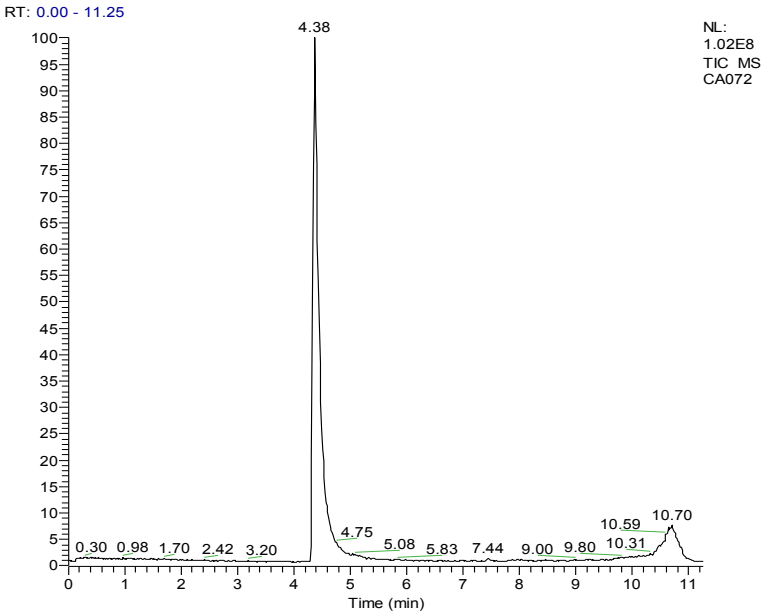

CA69_069_PROTON_001
11.33
9.36
8.56
8.54
8.32
8.29
8.28
8.28
8.26
8.26
7.06
7.03
7.02
7.01
6.95
6.95
6.93
6.93
6.79
6.77
4.31
1.02
1.00
1.00
1.99
1.00
0.97
1.00
1.00
4.00
f1 (ppm)

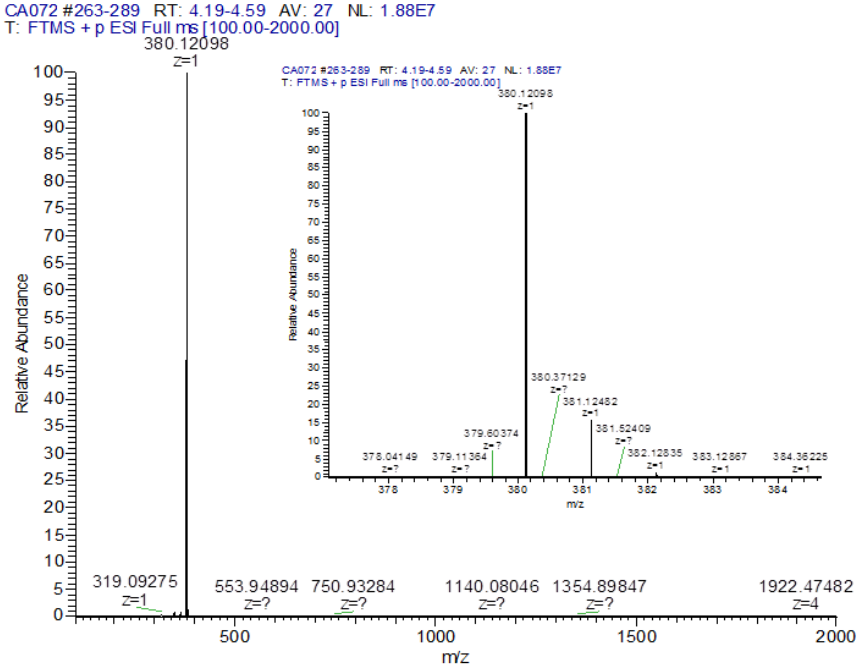

CA69_069_CARBON_001
155.55
144.14
144.01
142.89
140.51
129.90
129.11
129.08
127.86
126.72
126.40
125.14
122.65
122.60
122.43
122.17
118.50
118.07
116.56
114.42
100.93
64.13
f1 (ppm)

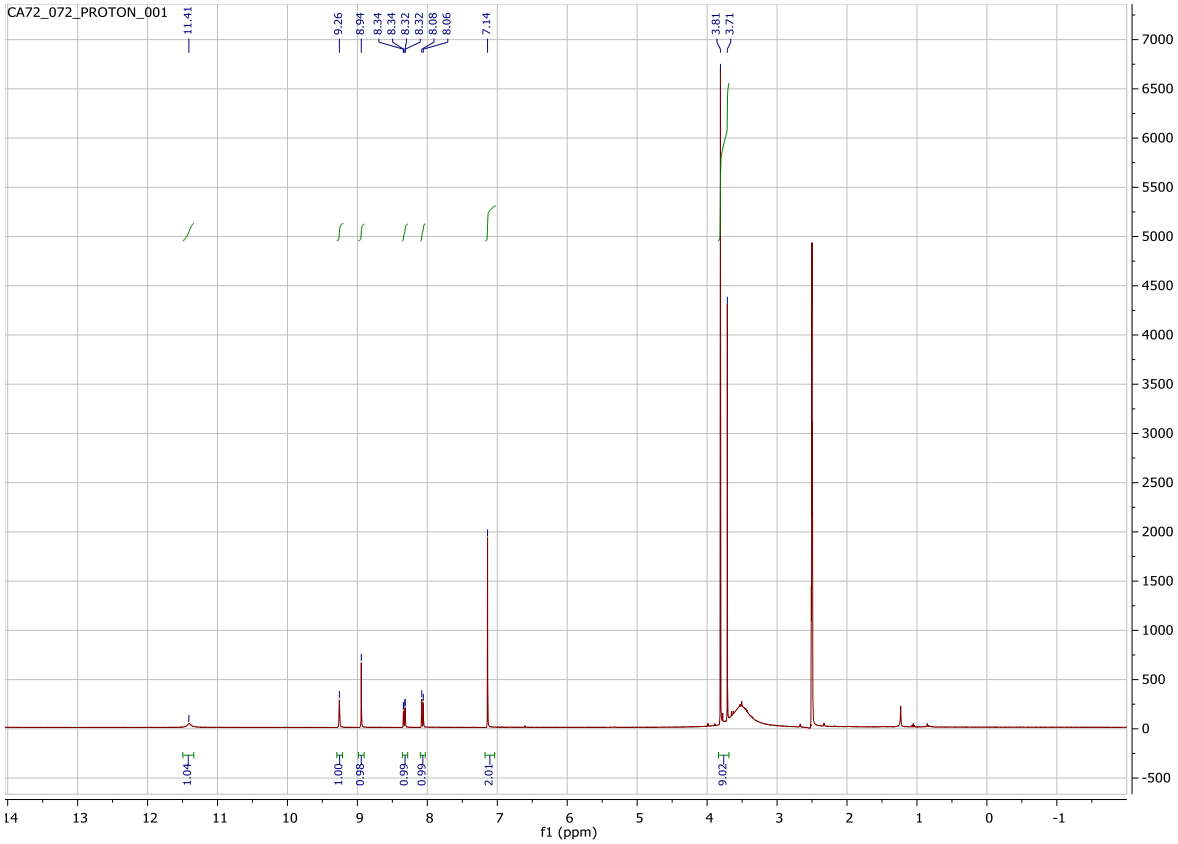


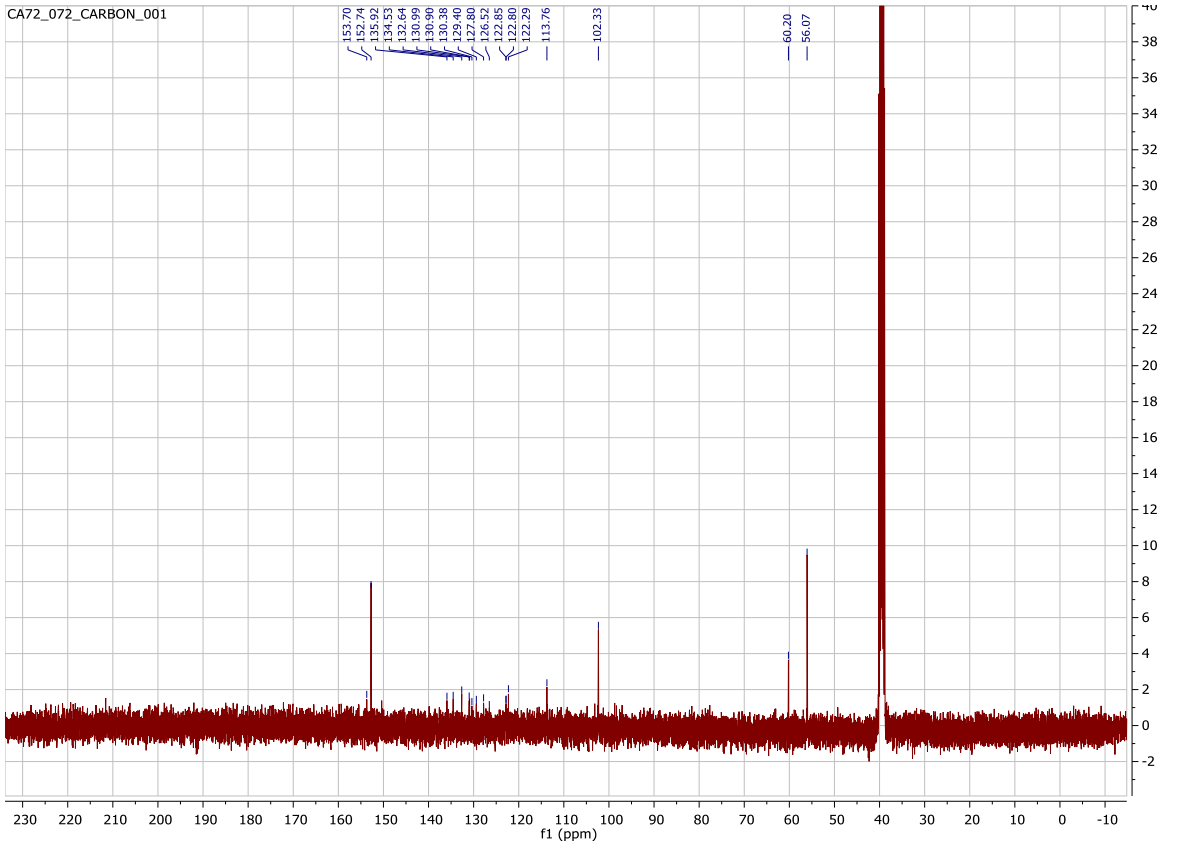
13

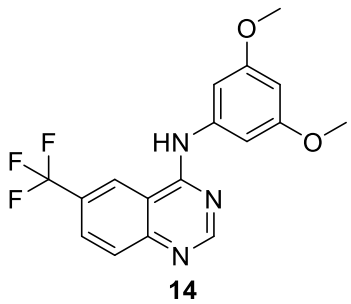
6-(Trifluoromethyl)-*N*-(3,4,5-trimethoxyphenyl)quinazolin-4-amine (**13**)





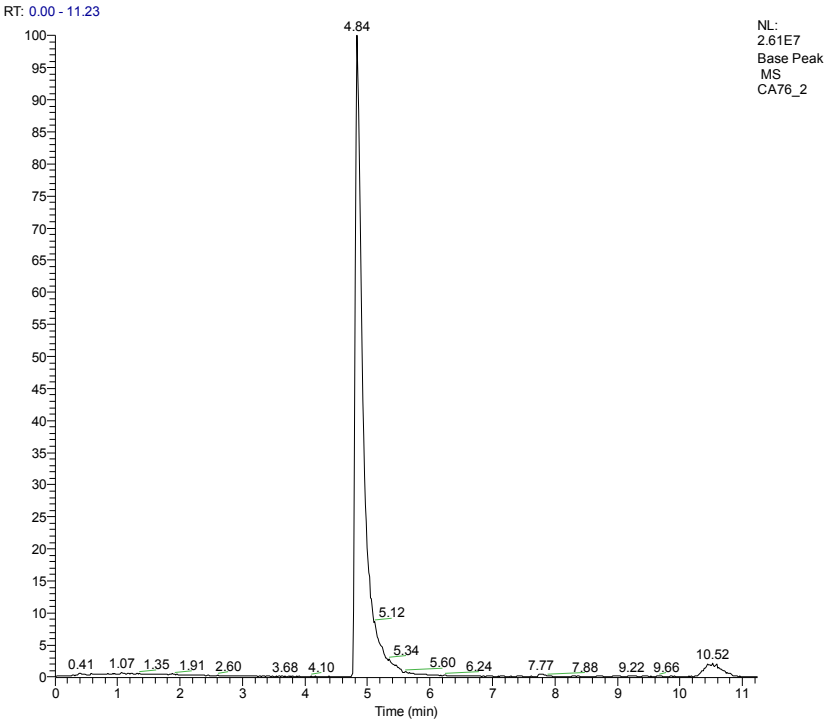

CA72_072_PROTON_001
11.41
9.26
8.94
8.34
8.34
8.32
8.32
8.08
8.06
7.14
3.81
3.71
1.04
1.00
0.98
0.99
0.99
2.01
9.02
f1 (ppm)

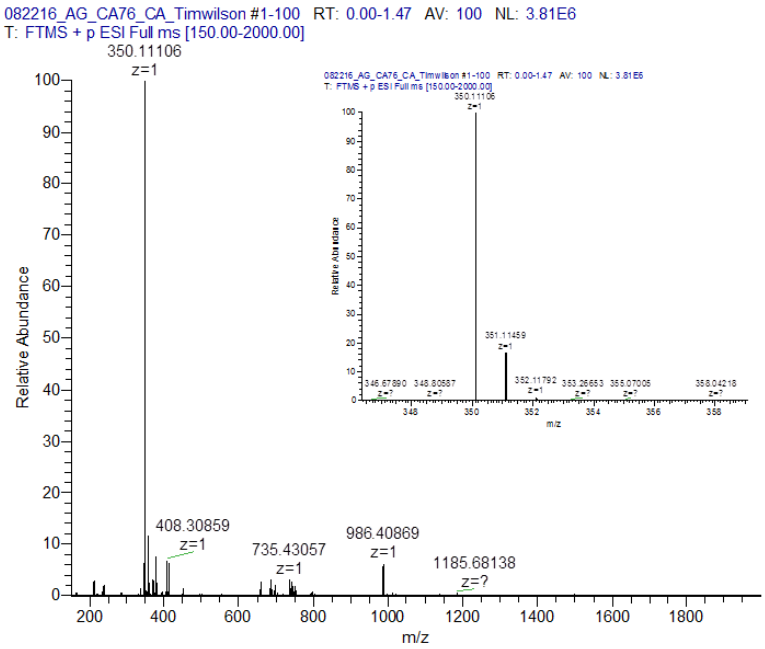

CA72_072_CARBON_001
153.70
152.74
135.92
134.55
132.64
130.99
130.90
130.38
129.40
127.80
126.52
122.85
122.80
122.29
113.76
102.33
60.20
56.07
f1 (ppm)

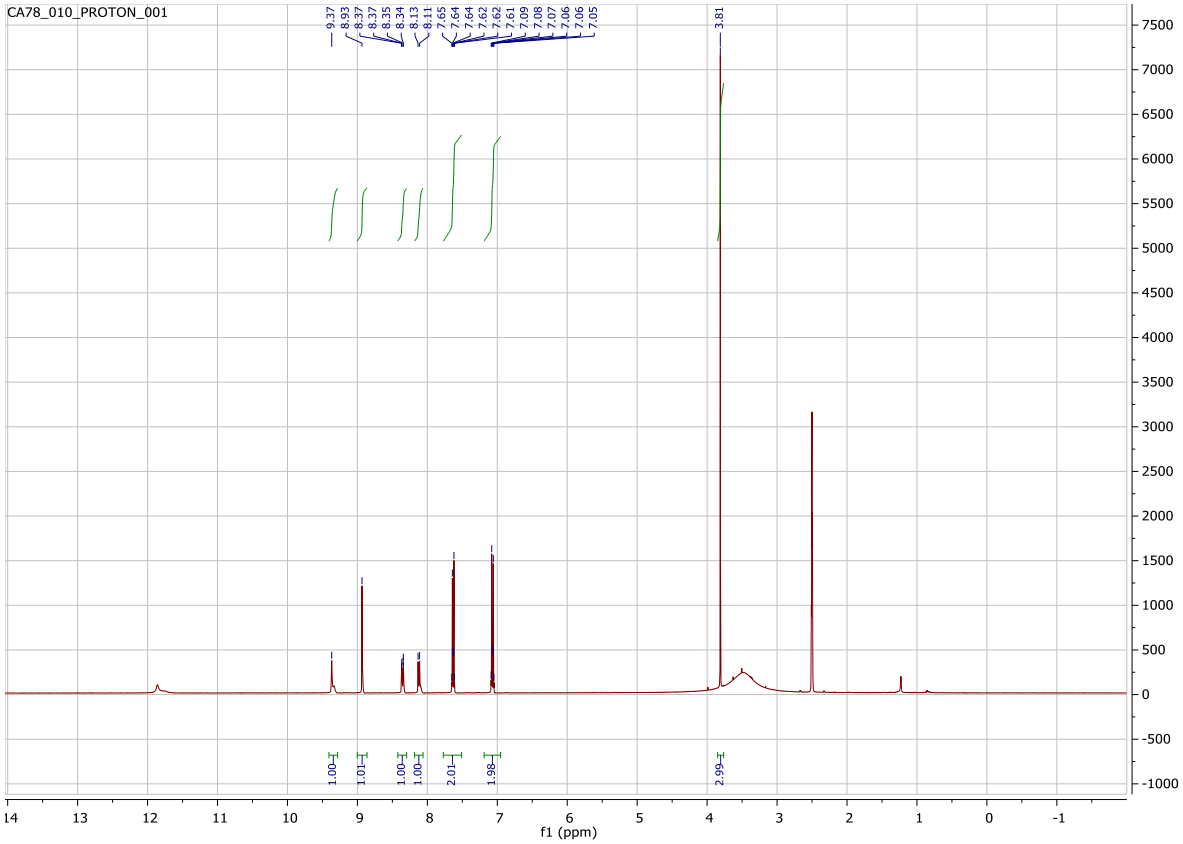


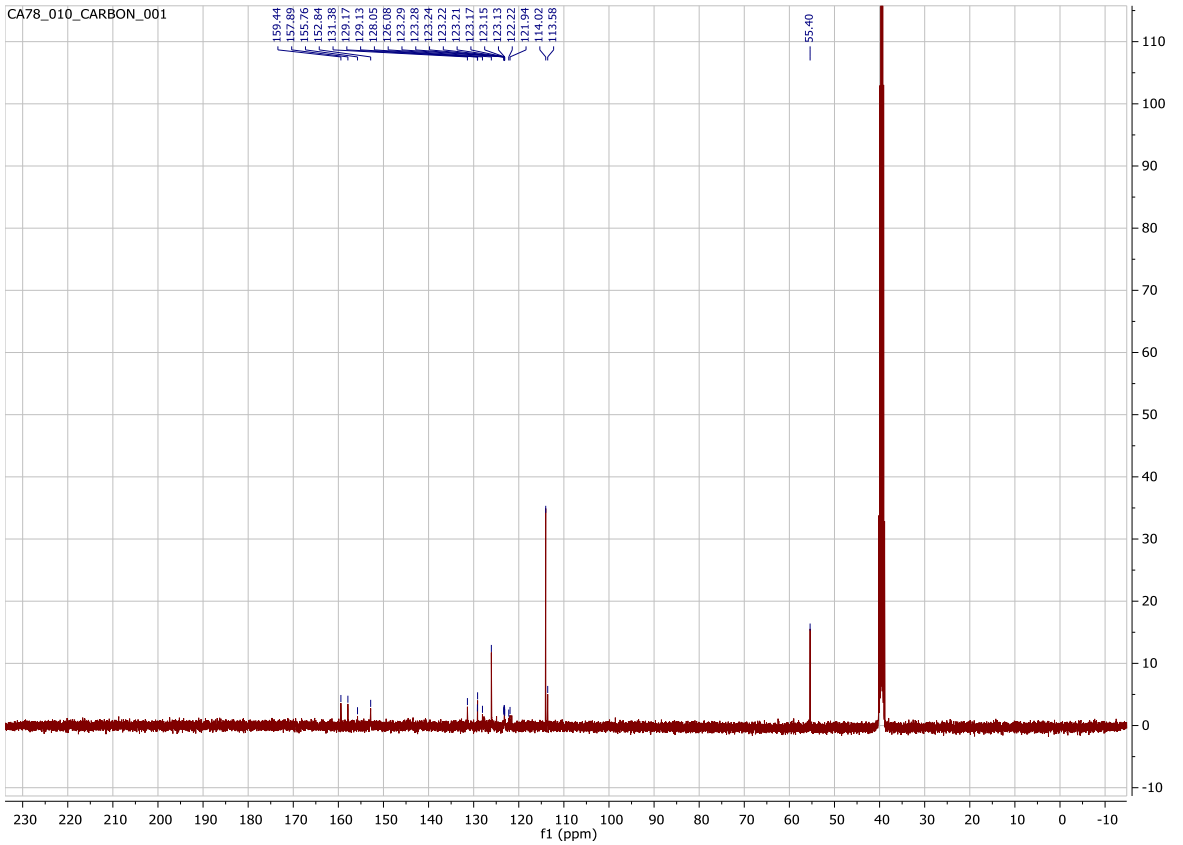
14

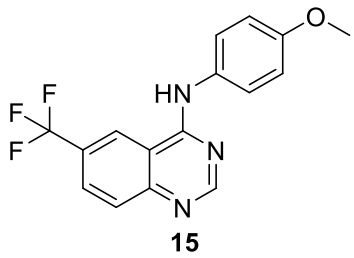
N-(3,5-Dimethoxyphenyl)-6-(trifluoromethyl)quinazolin-4-amine (**14**)





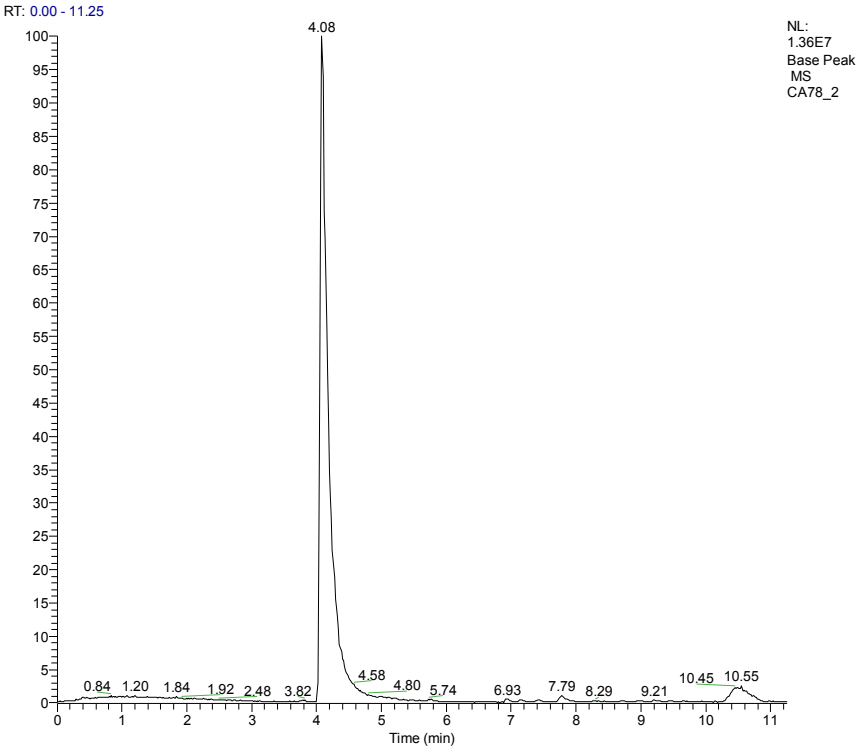

CA78_010_PROTON_001
9.37
8.93
8.37
8.37
8.35
8.34
8.13
8.11
7.65
7.64
7.64
7.62
7.62
7.61
7.09
7.08
7.07
7.06
7.06
7.05
3.81
1.00
1.01
1.00
1.00
2.01
1.98
2.99
f1 (ppm)

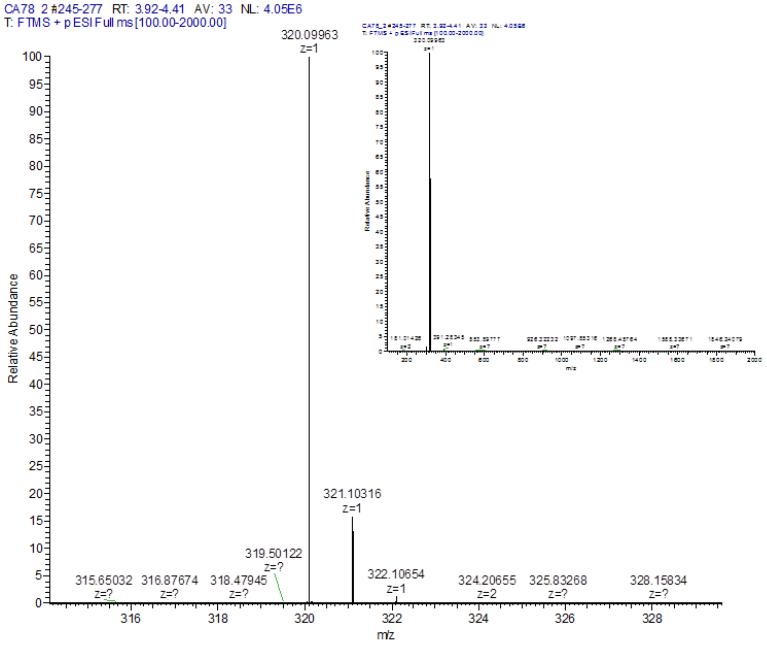

CA78_010_CARBON_001
159.44
157.89
155.76
152.84
131.38
129.17
129.13
128.65
126.08
123.28
123.24
123.22
123.21
123.17
123.15
123.13
122.22
121.94
114.02
113.58
55.40
f1 (ppm)

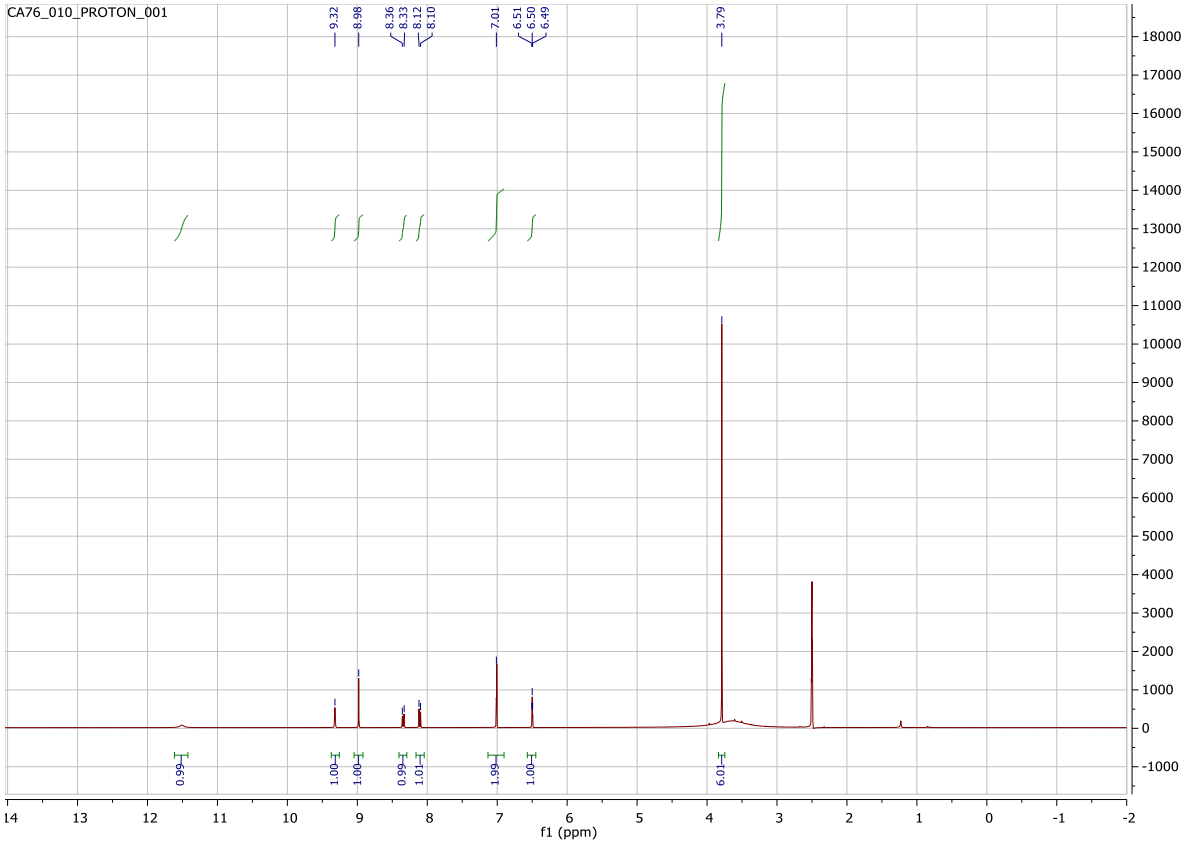


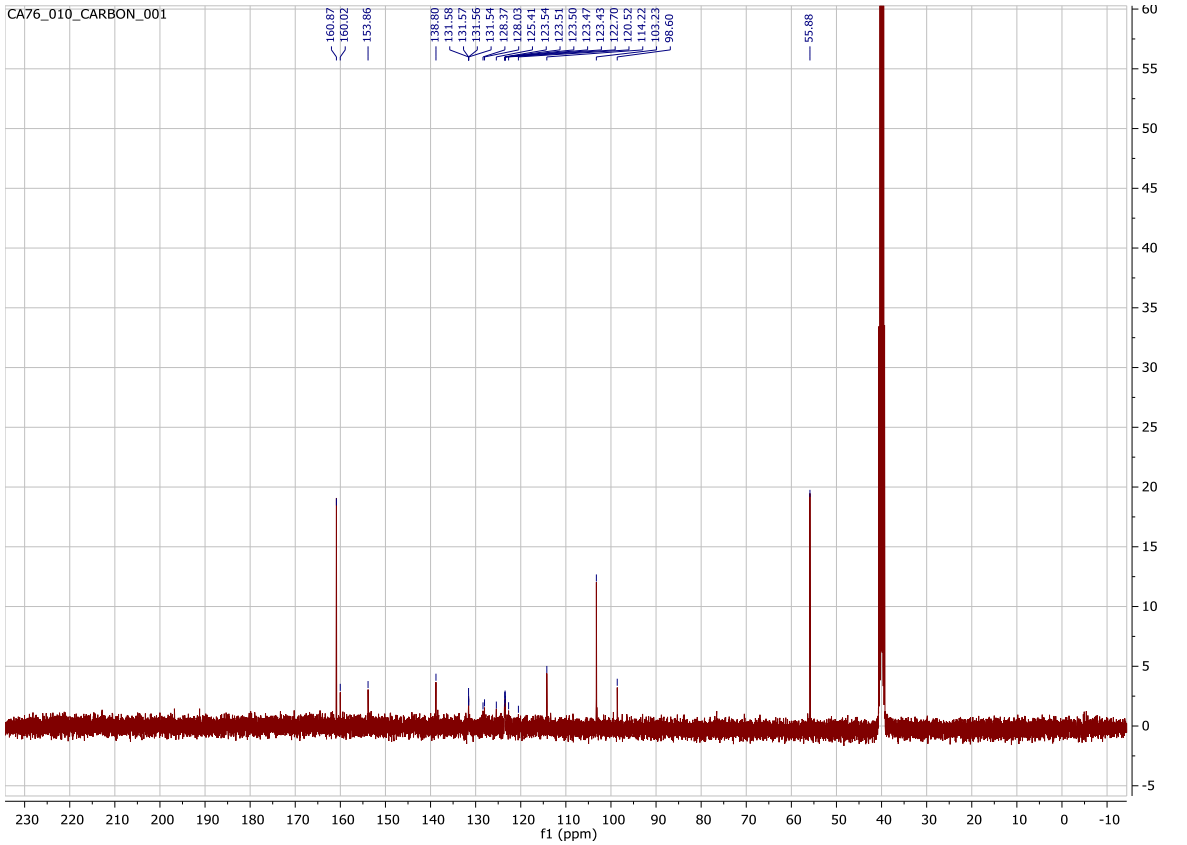
15

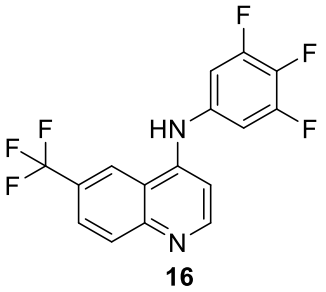
N-(4-Methoxyphenyl)-6-(trifluoromethyl)quinazolin-4-amine (**15**)





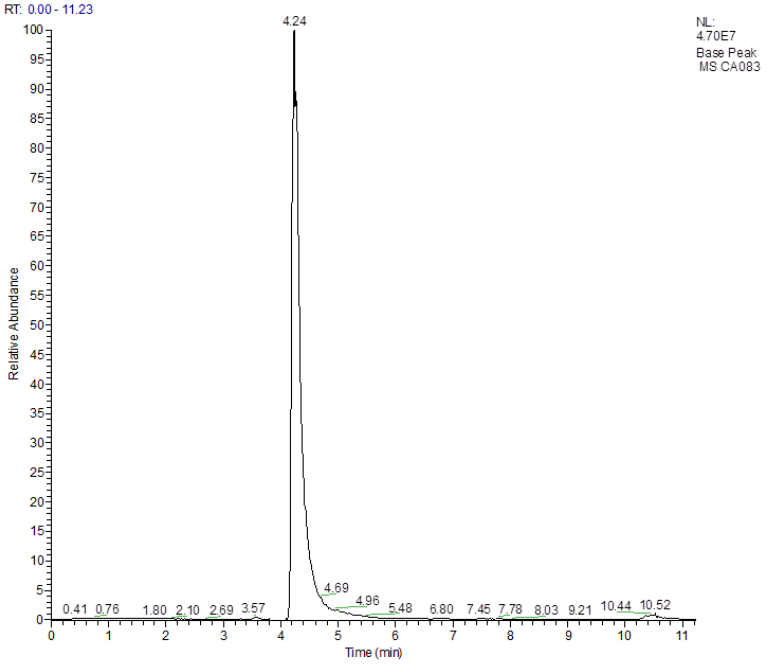

CA76_010_PROTON_001
9.32
8.98
8.36
8.33
8.12
8.10
7.01
6.51
6.50
6.49
3.79
0.99
1.00
1.00
0.99
1.01
1.99
1.00
6.01
f1 (ppm)

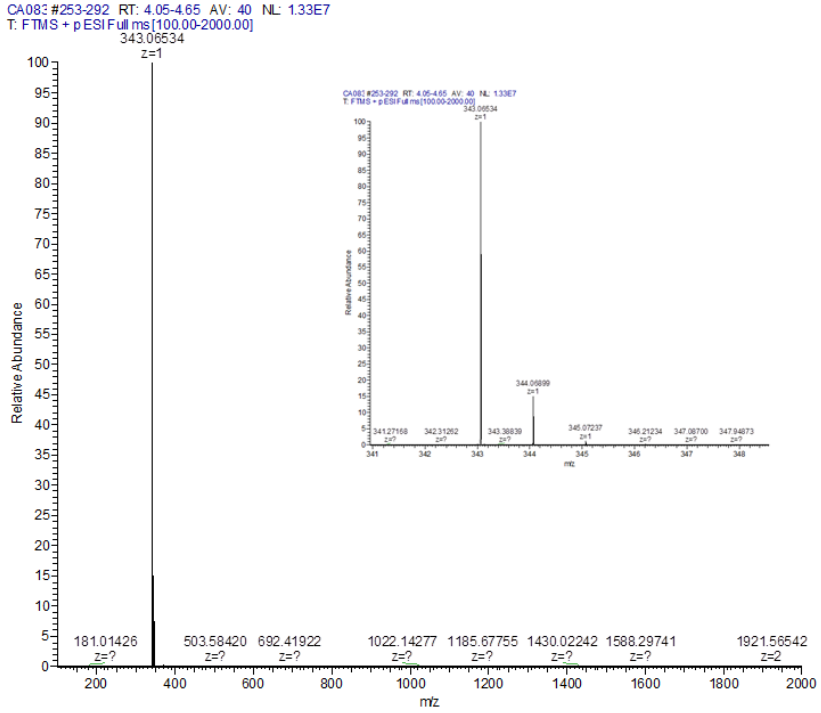

CA76_010_CARBON_001
160.87
160.02
153.86
138.80
131.58
131.57
131.56
131.54
128.37
128.03
125.41
123.54
123.51
123.50
123.47
123.43
122.70
120.52
114.22
103.23
98.60
55.88
f1 (ppm)

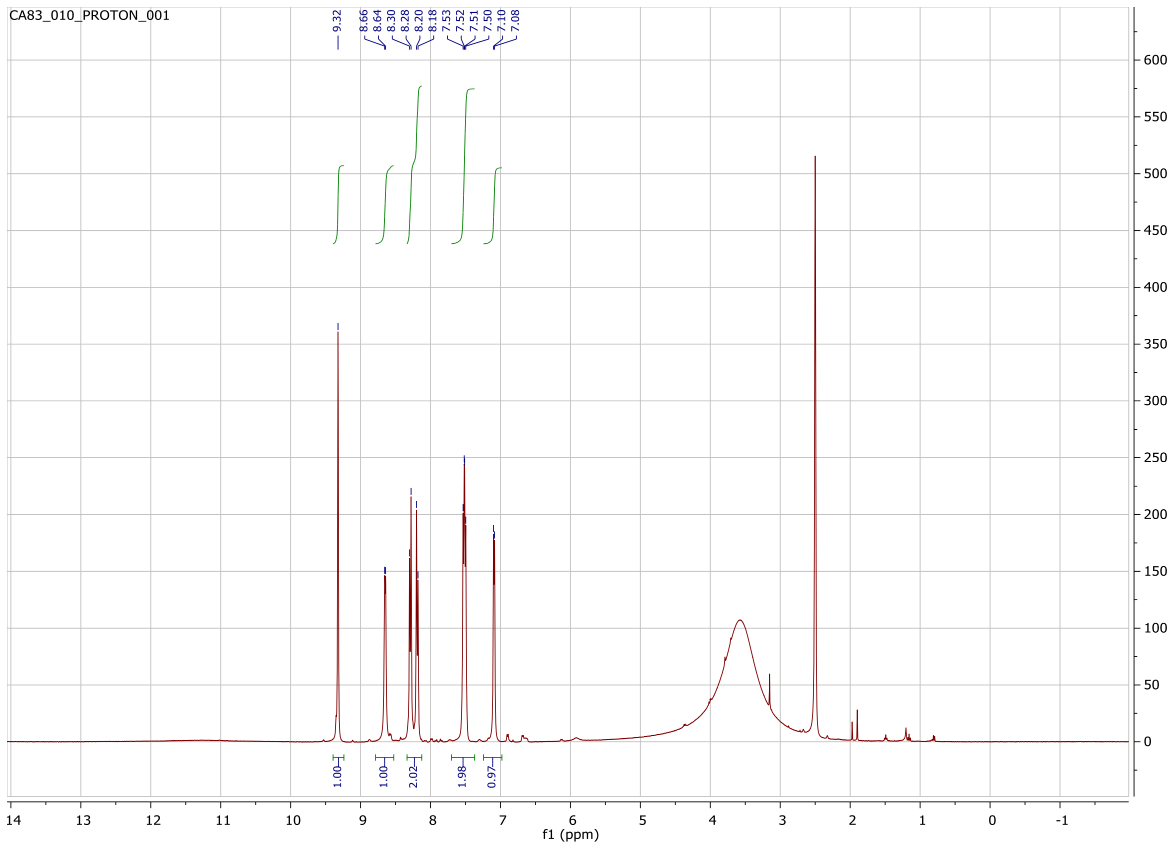


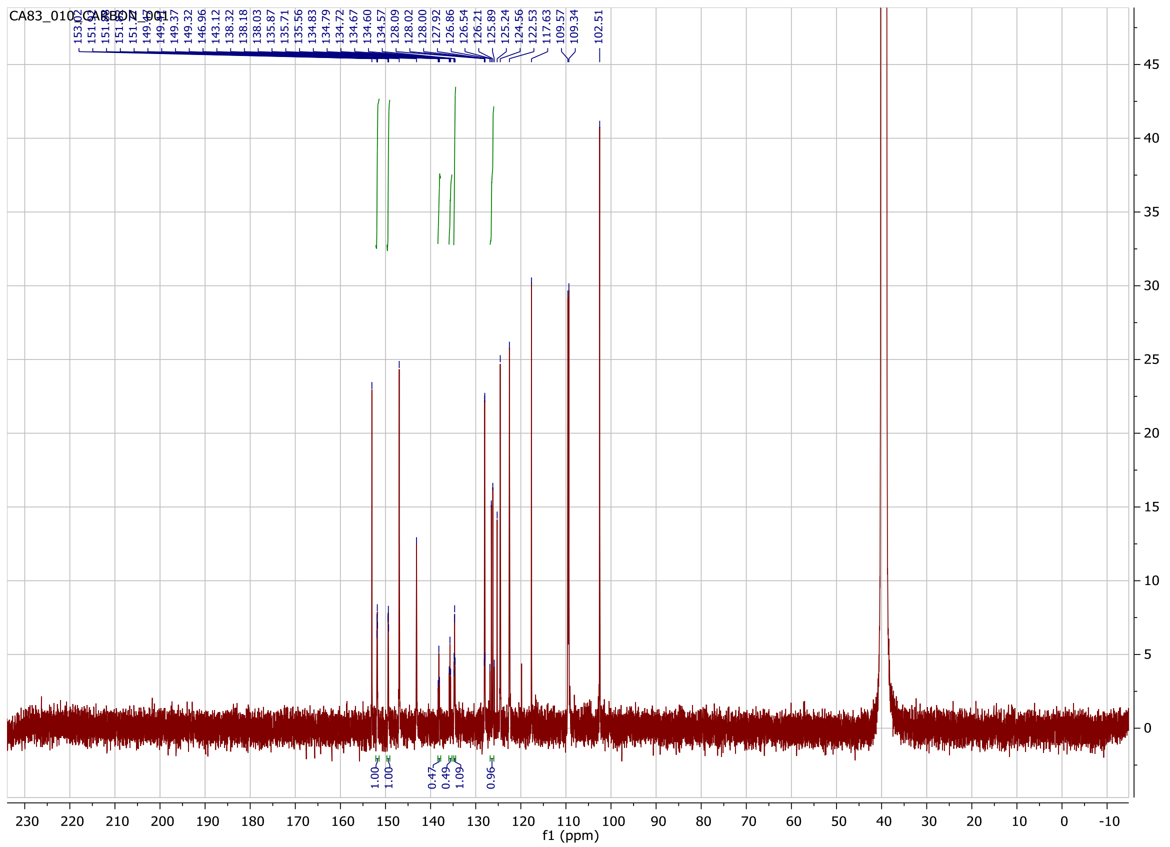
16

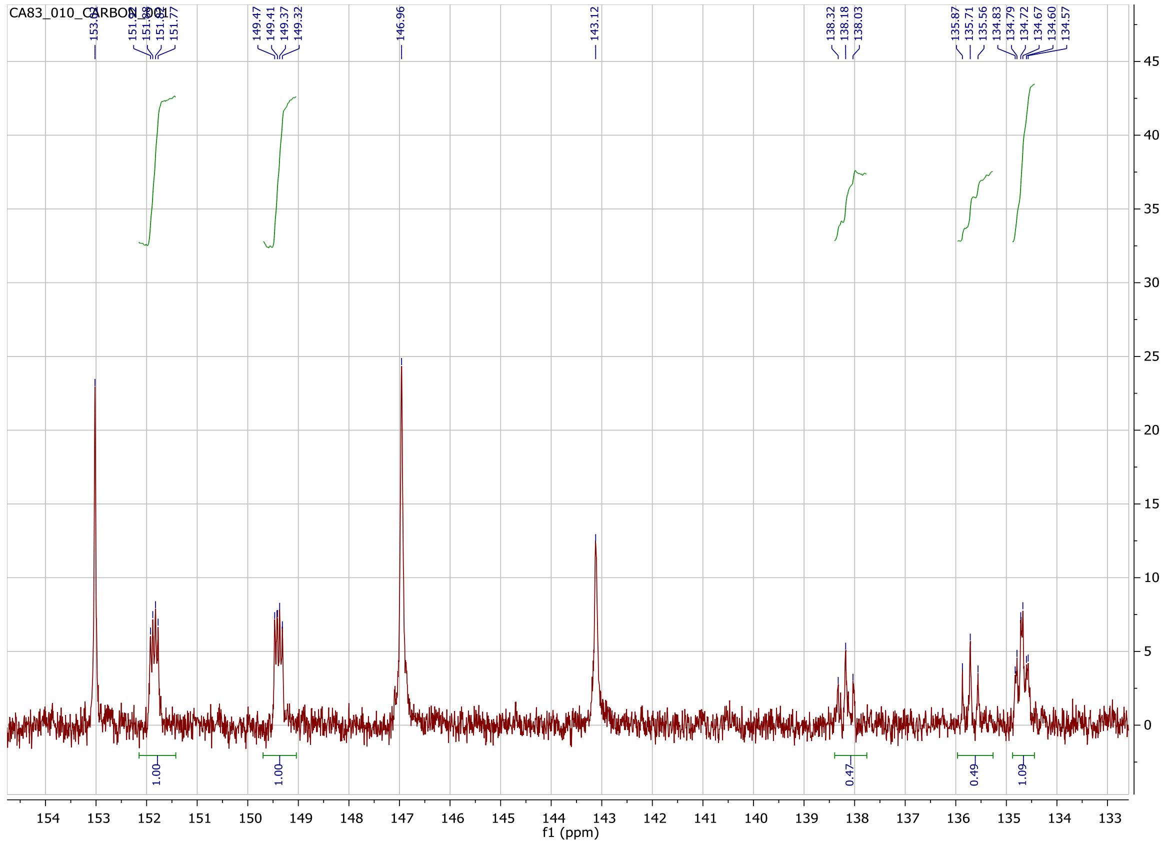
6-(Trifluoromethyl)-*N*-(3,4,5-trifluorophenyl)quinolin-4-amine (**16**)

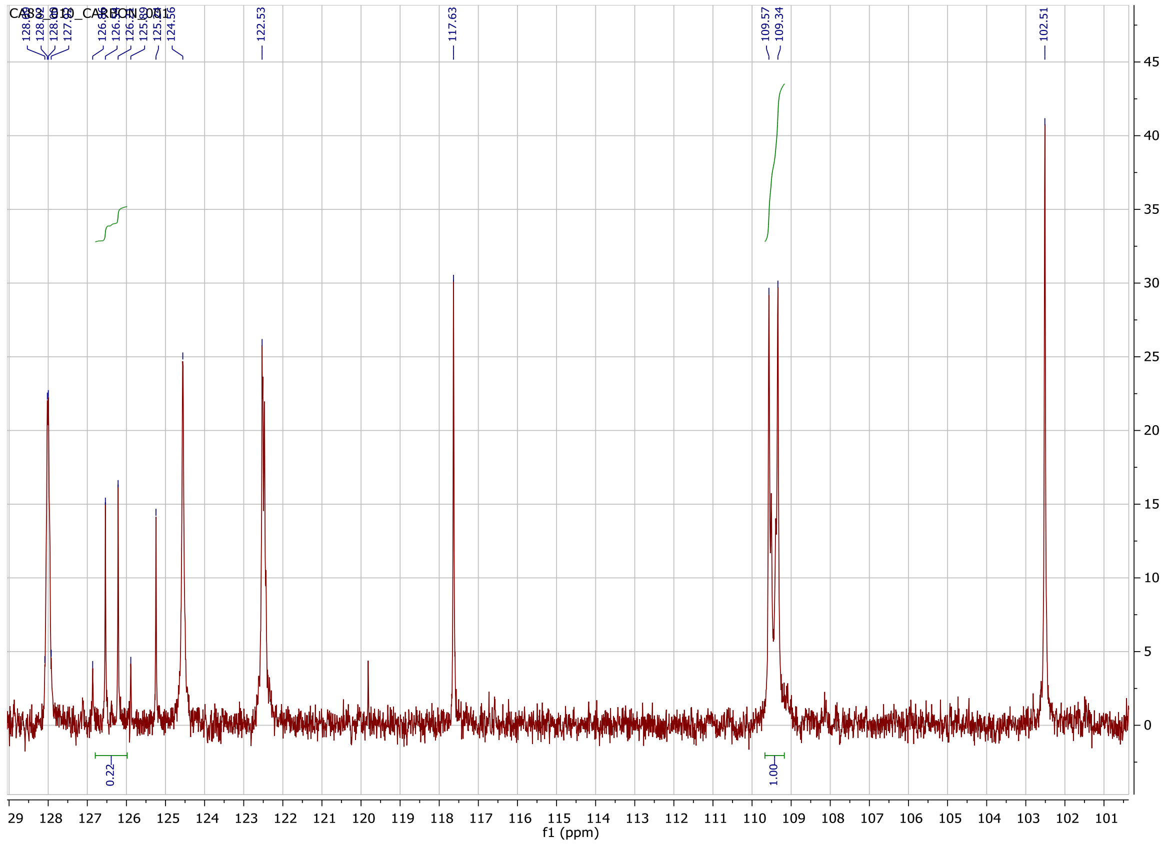


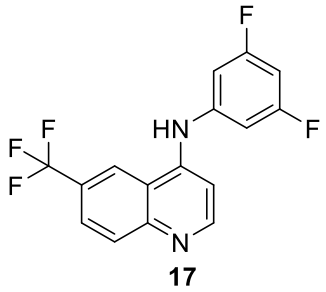



CA83_010_PROTON_001
f1 (ppm)


CA83_010_CARBON_001
f1 (ppm)

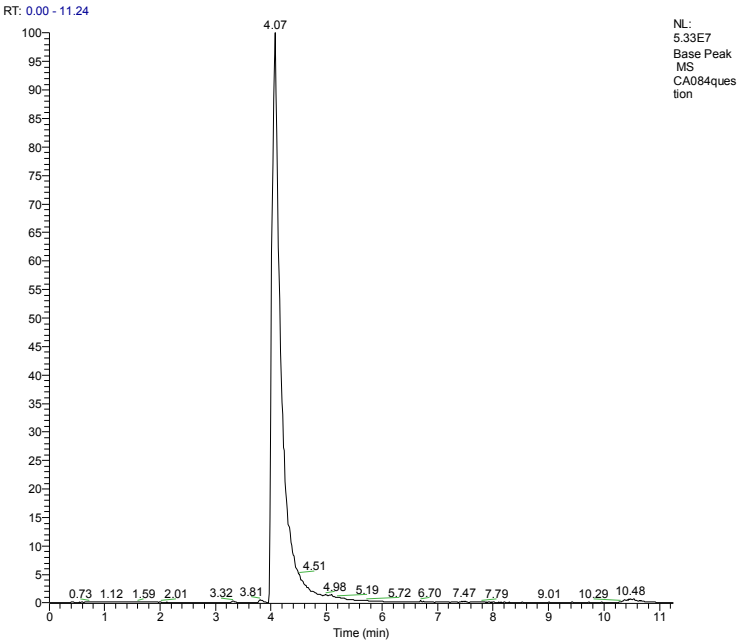

CA83_010_CARBON_001
153.0
151.77
149.47
149.41
149.37
149.32
146.96
143.12
138.32
138.18
138.03
135.87
135.71
135.56
134.83
134.79
134.72
134.67
134.60
134.57
1.00
1.00
0.47
0.49
1.09
f1 (ppm)

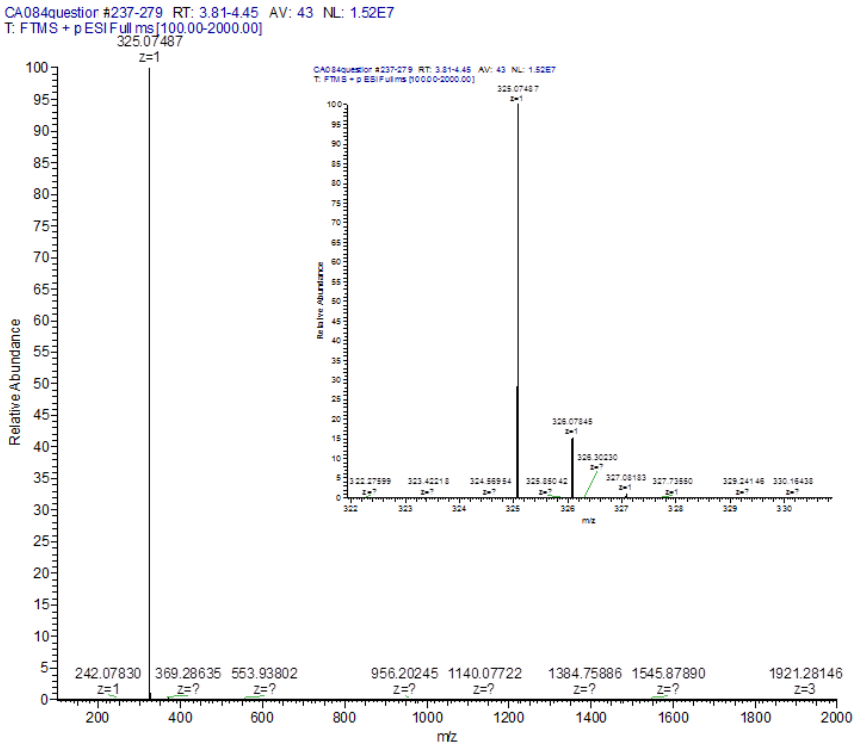

CA83_010_CARBON_001
124.56
122.53
117.63
109.57
109.34
102.51
0.22
1.00
f1 (ppm)

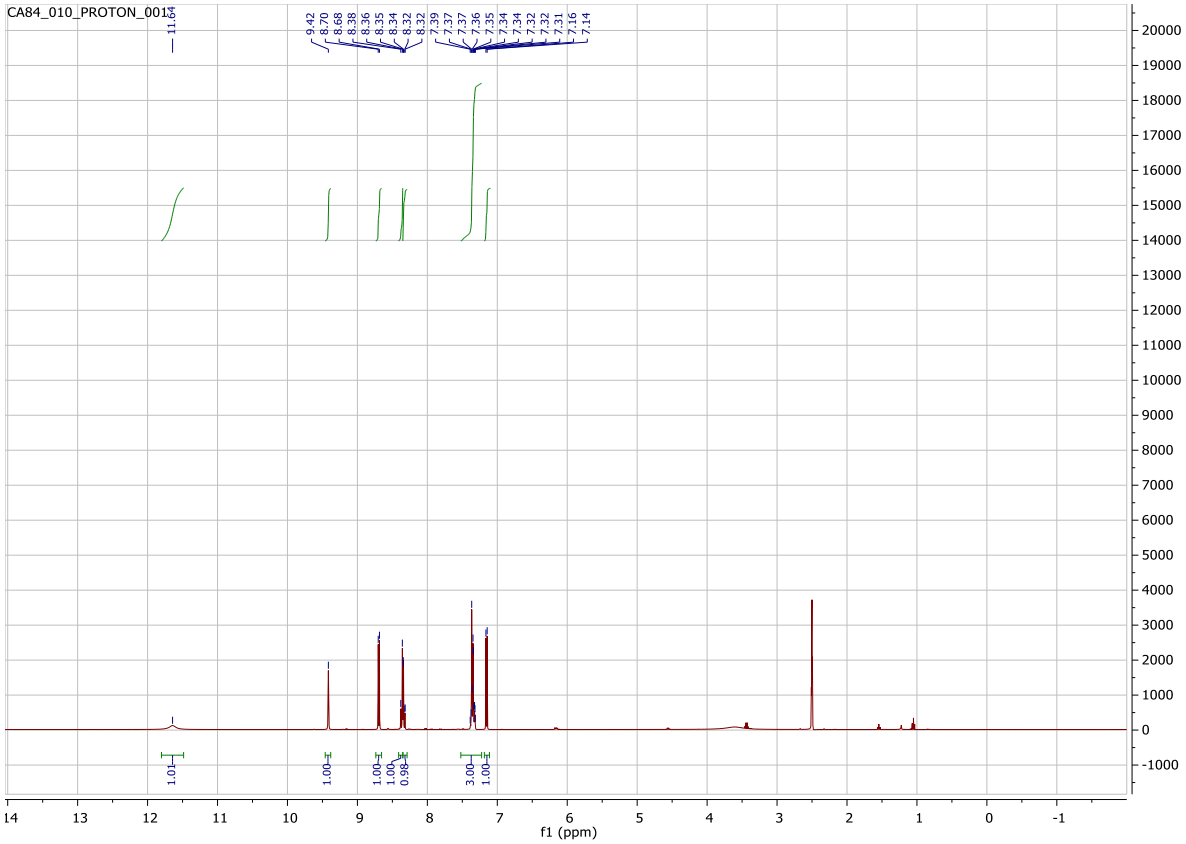


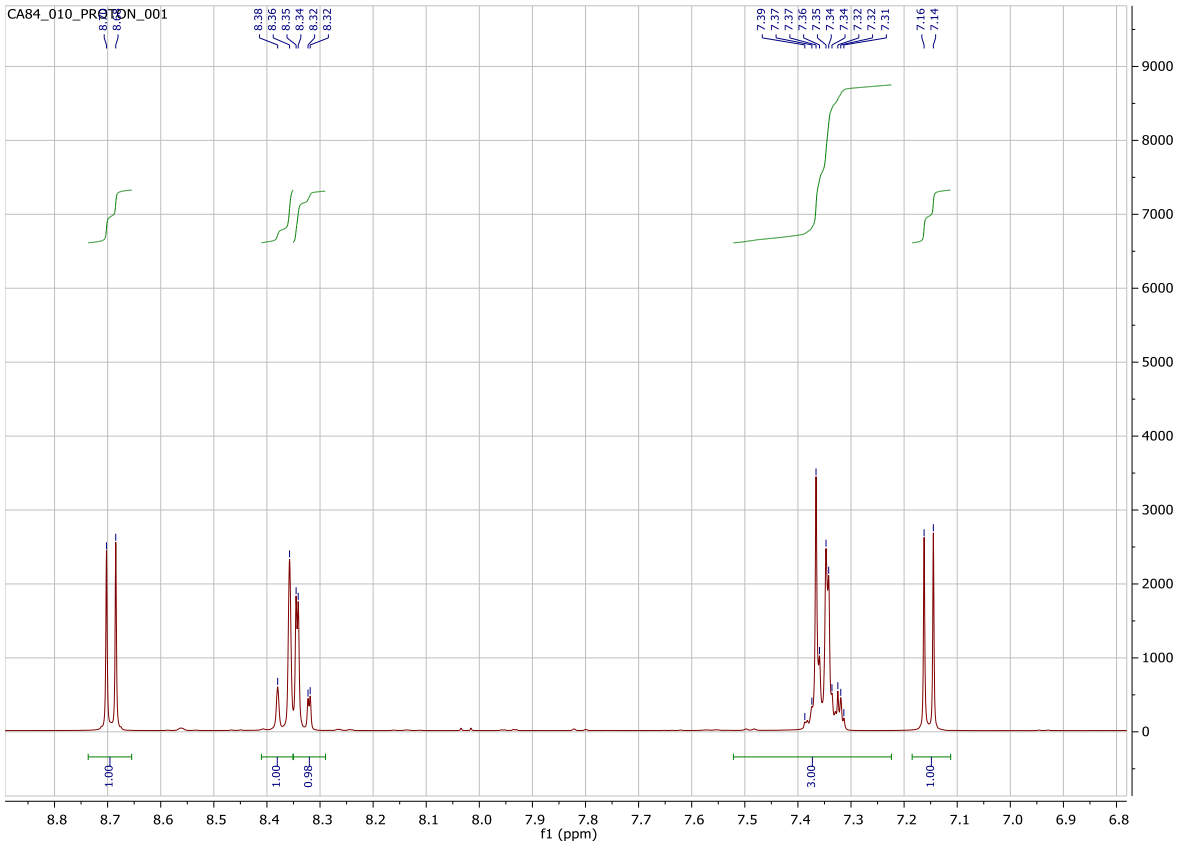
17

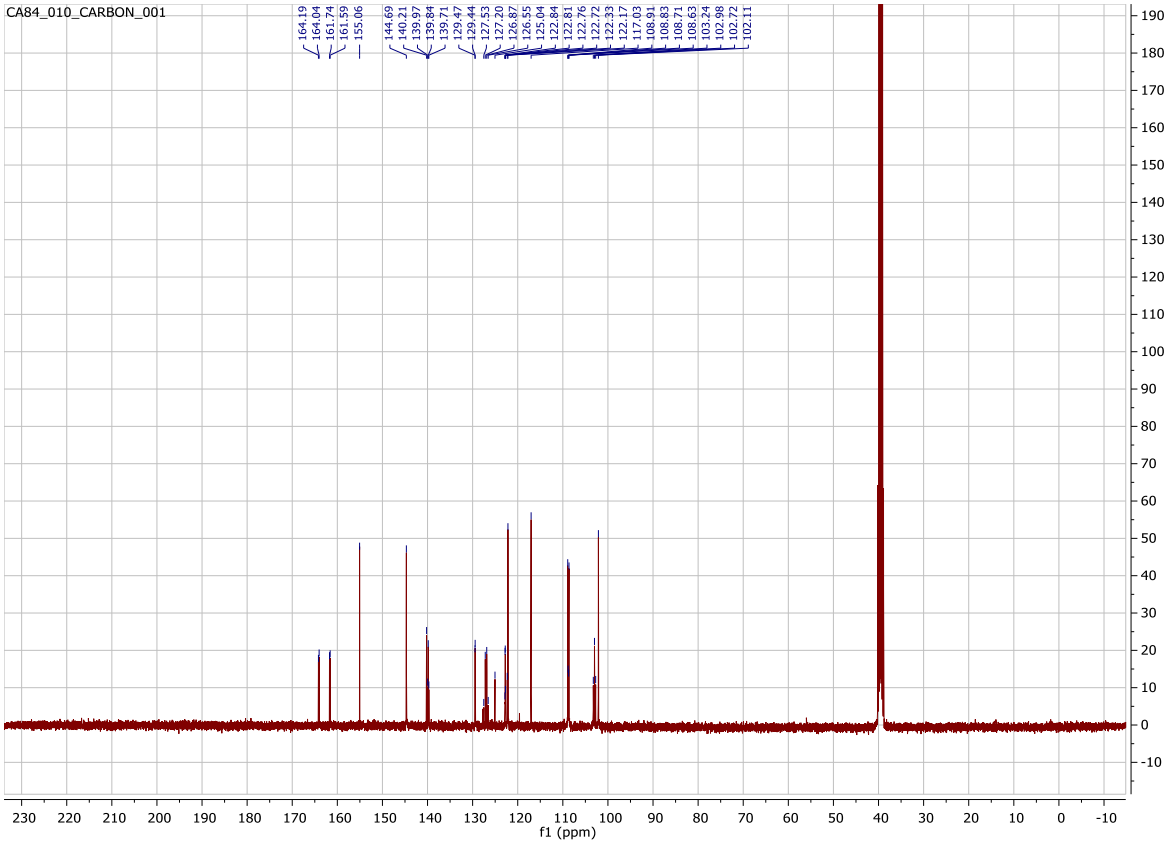
N-(3,5-Difluorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**17**)

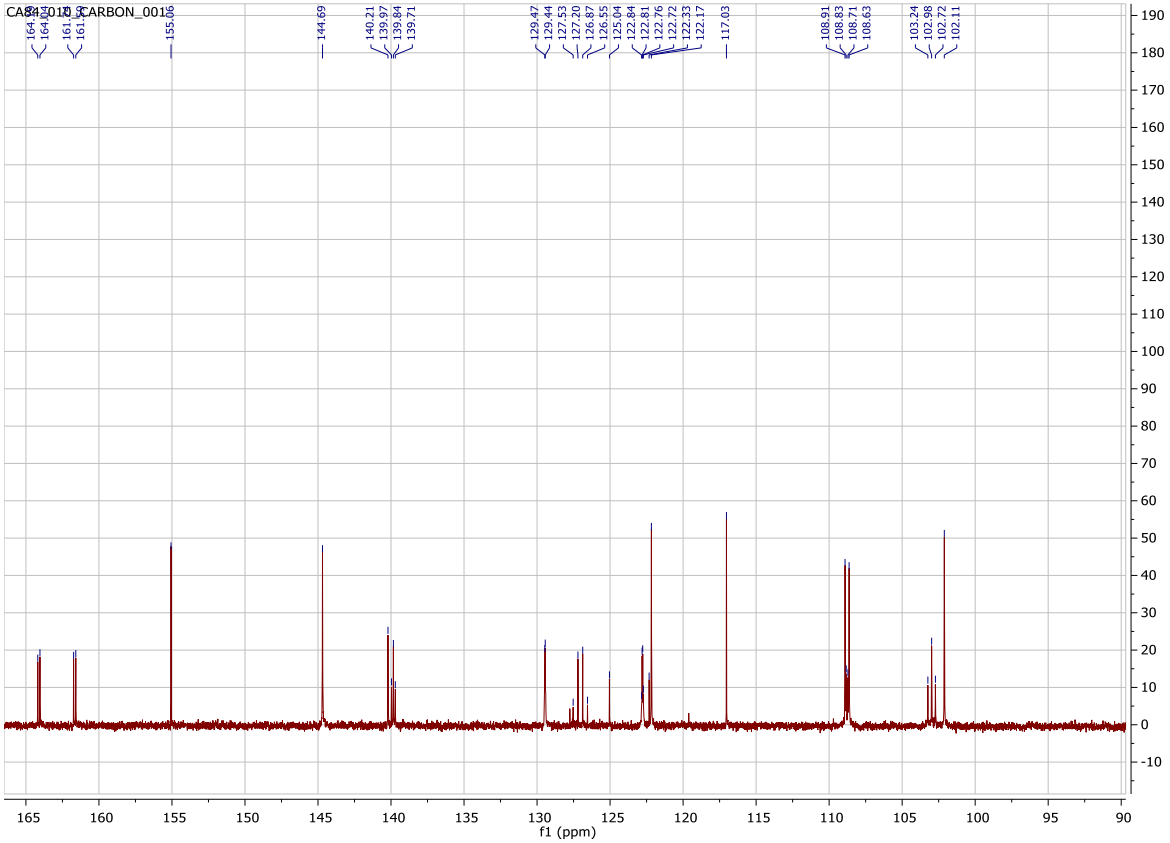


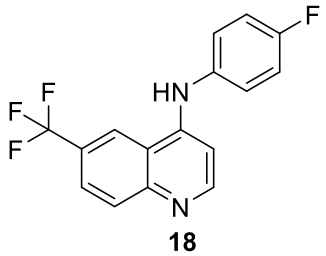



CA84_010_PROTON_001
11.64
9.42
8.70
8.68
8.38
8.36
8.35
8.34
8.32
8.32
7.39
7.37
7.37
7.36
7.35
7.34
7.34
7.32
7.32
7.31
7.16
7.14
1.01
1.00
1.00
1.00
0.98
3.00
1.00
f1 (ppm)


CA84_010_PROTON_001
8.38
8.36
8.35
8.34
8.32
8.32
7.39
7.37
7.37
7.36
7.35
7.34
7.34
7.32
7.32
7.31
7.16
7.14
1.00
1.00
0.98
3.00
1.00
f1 (ppm)

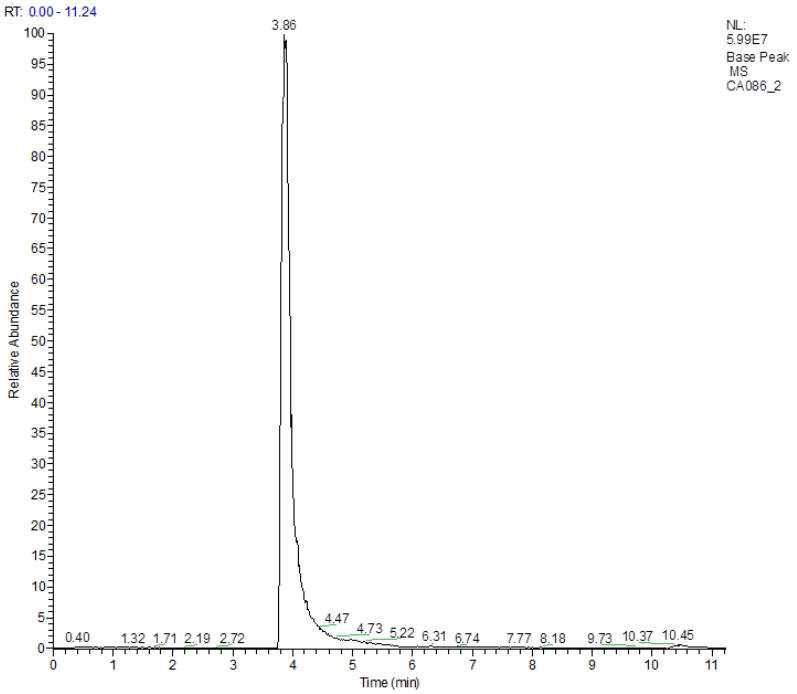

CA84_010_CARBON_001
164.19
164.04
161.74
161.59
155.06
144.69
140.21
139.97
139.84
139.71
129.47
129.44
127.53
127.20
126.87
126.55
125.04
122.84
122.81
122.76
122.72
122.33
122.17
117.03
108.91
108.83
108.71
108.63
103.24
102.98
102.72
102.11
f1 (ppm)

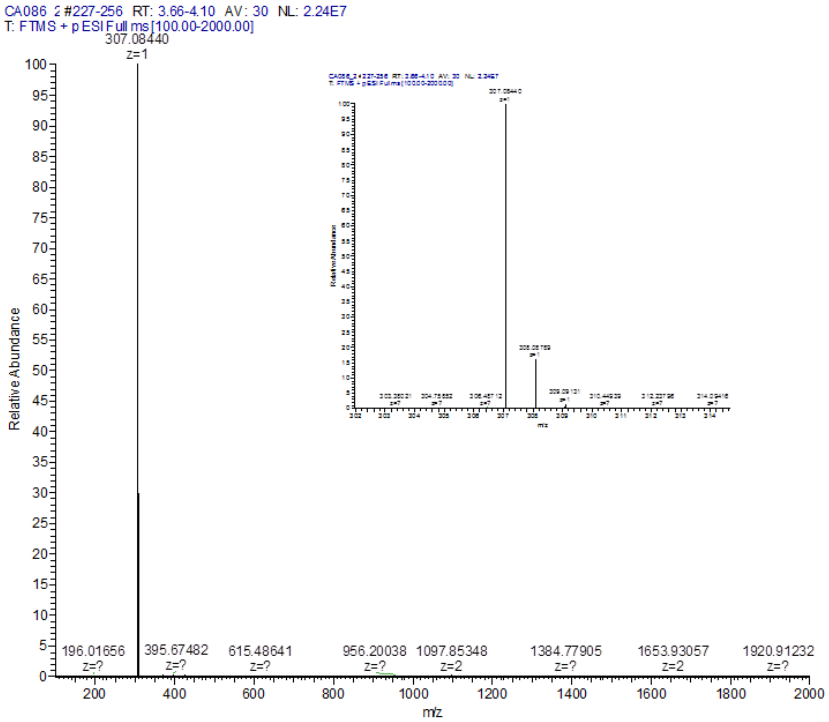

CA84_010_CARBON_001
155.06
144.69
140.21
139.97
139.84
139.71
129.47
129.44
127.53
127.20
126.87
126.55
125.04
122.84
122.81
122.76
122.72
122.33
122.17
117.03
108.91
108.83
108.71
108.63
103.24
102.98
102.72
102.11
f1 (ppm)

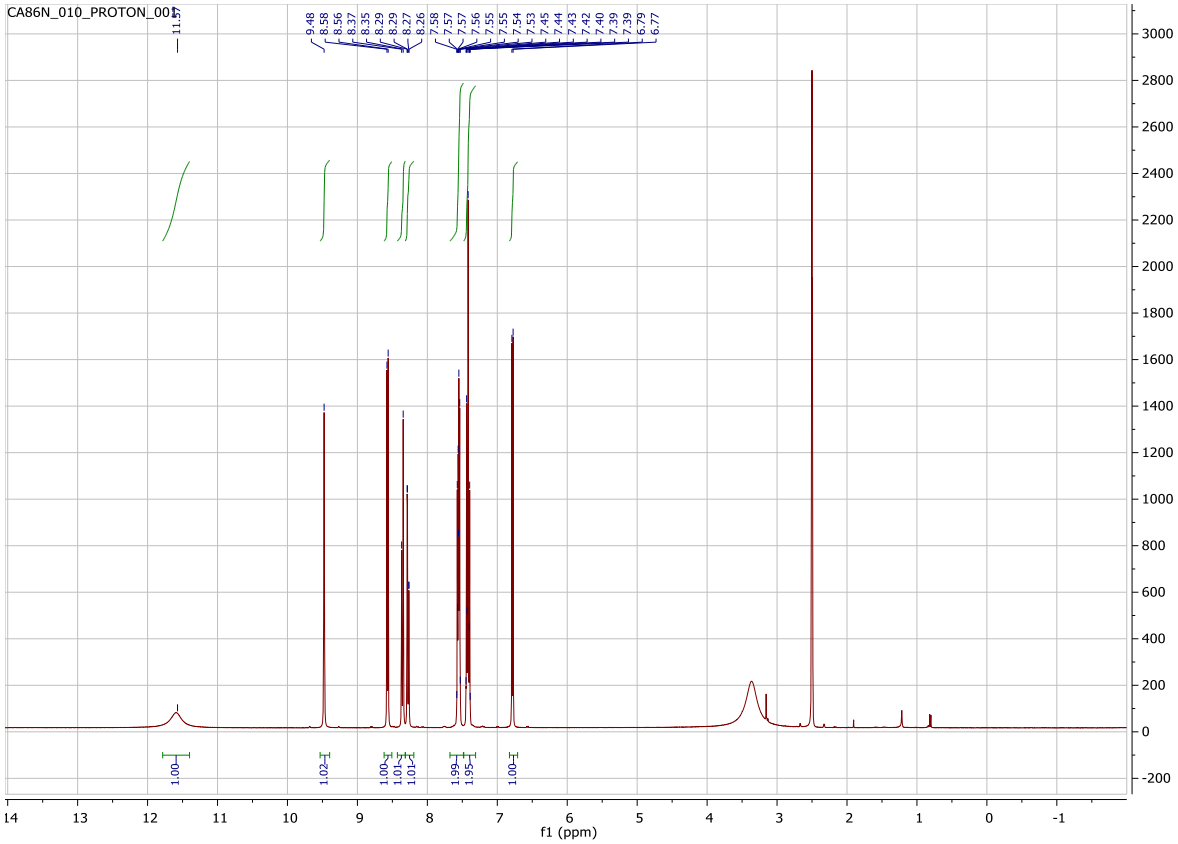


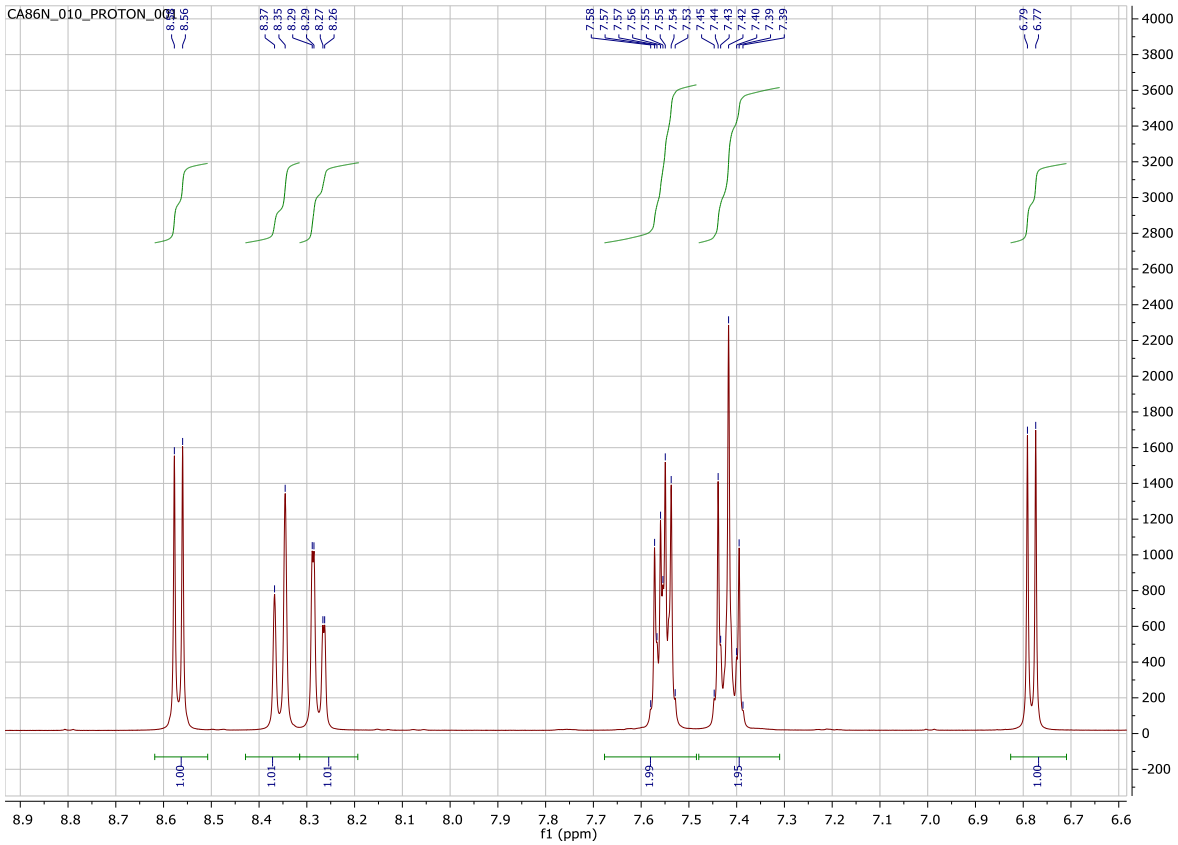
18

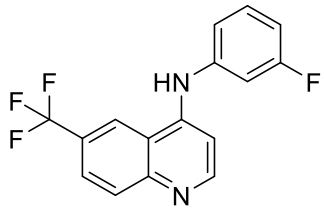
N-(4-Fluorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**18**)





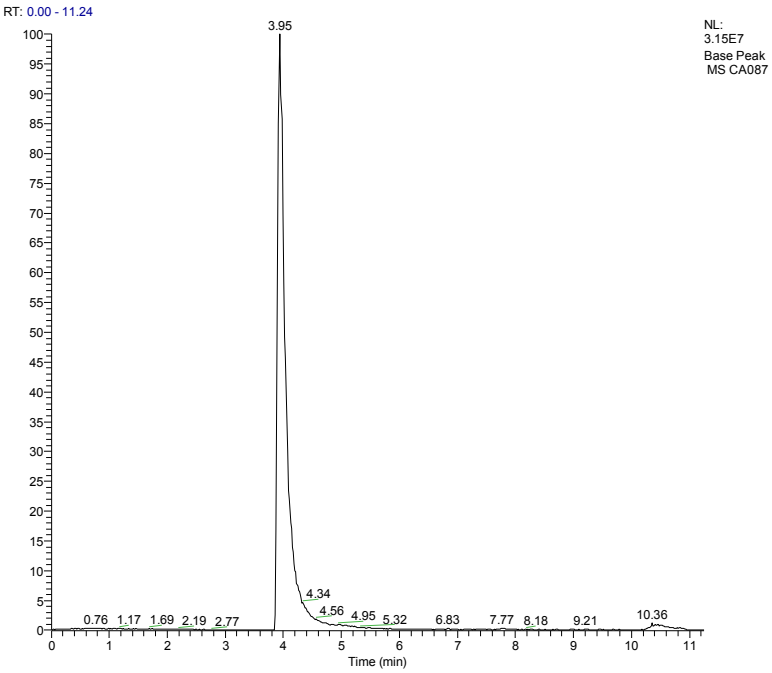

CA86N_010_PROTON_001
11.57
9.48
8.58
8.56
8.37
8.35
8.29
8.29
8.27
8.26
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.45
7.44
7.43
7.42
7.40
7.39
7.39
6.79
6.77
1.00
1.02
1.00
1.01
1.01
1.99
1.95
1.00
f1 (ppm)

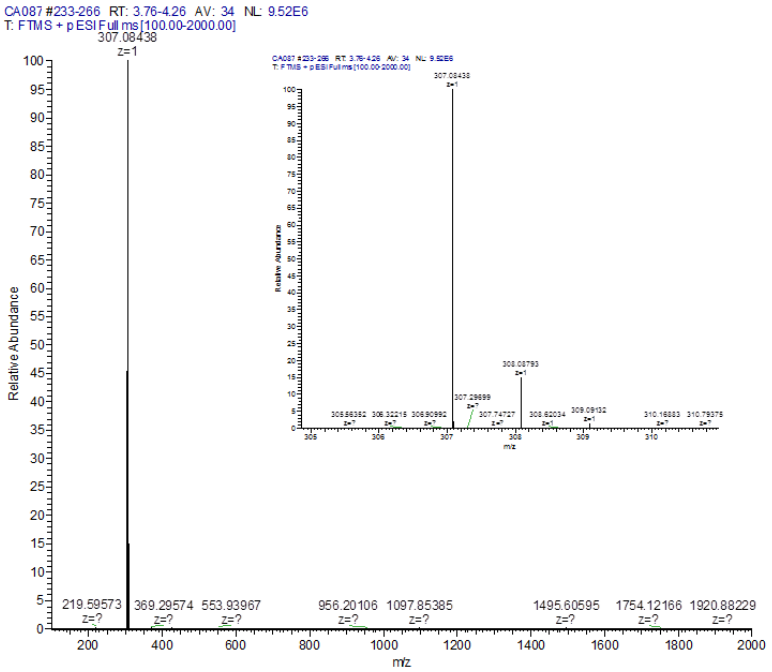

CA86N_010_PROTON_001
8.58
8.56
8.37
8.35
8.29
8.29
8.27
8.26
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.45
7.44
7.43
7.42
7.40
7.39
7.39
6.79
6.77
1.00
1.01
1.01
1.99
1.95
1.00
f1 (ppm)

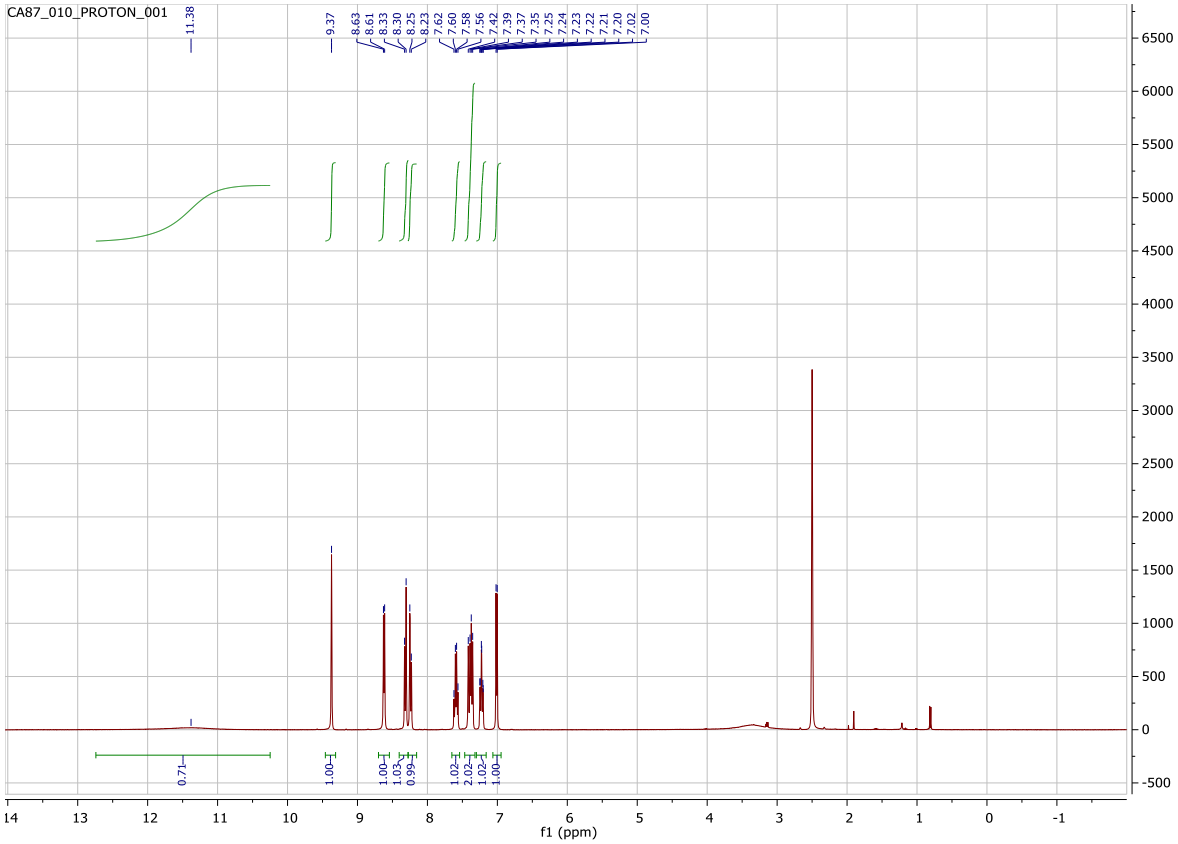


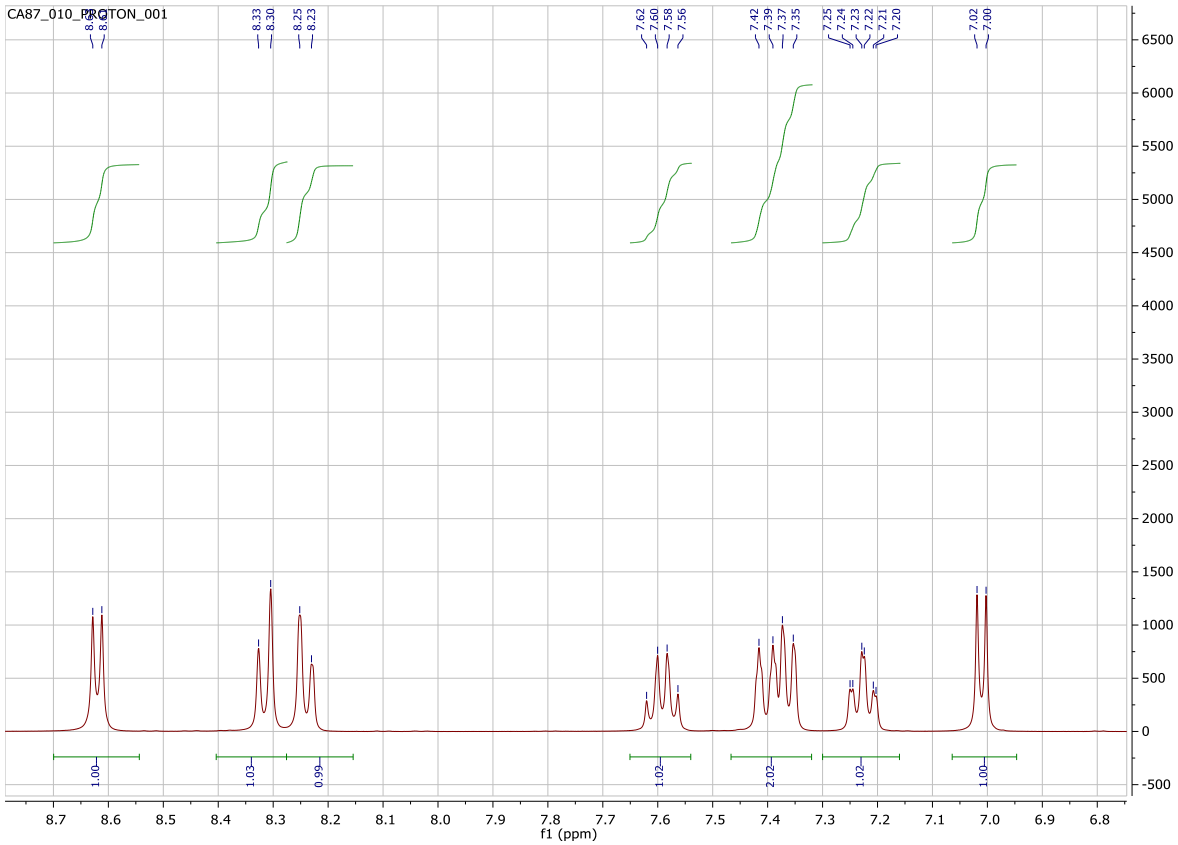
19

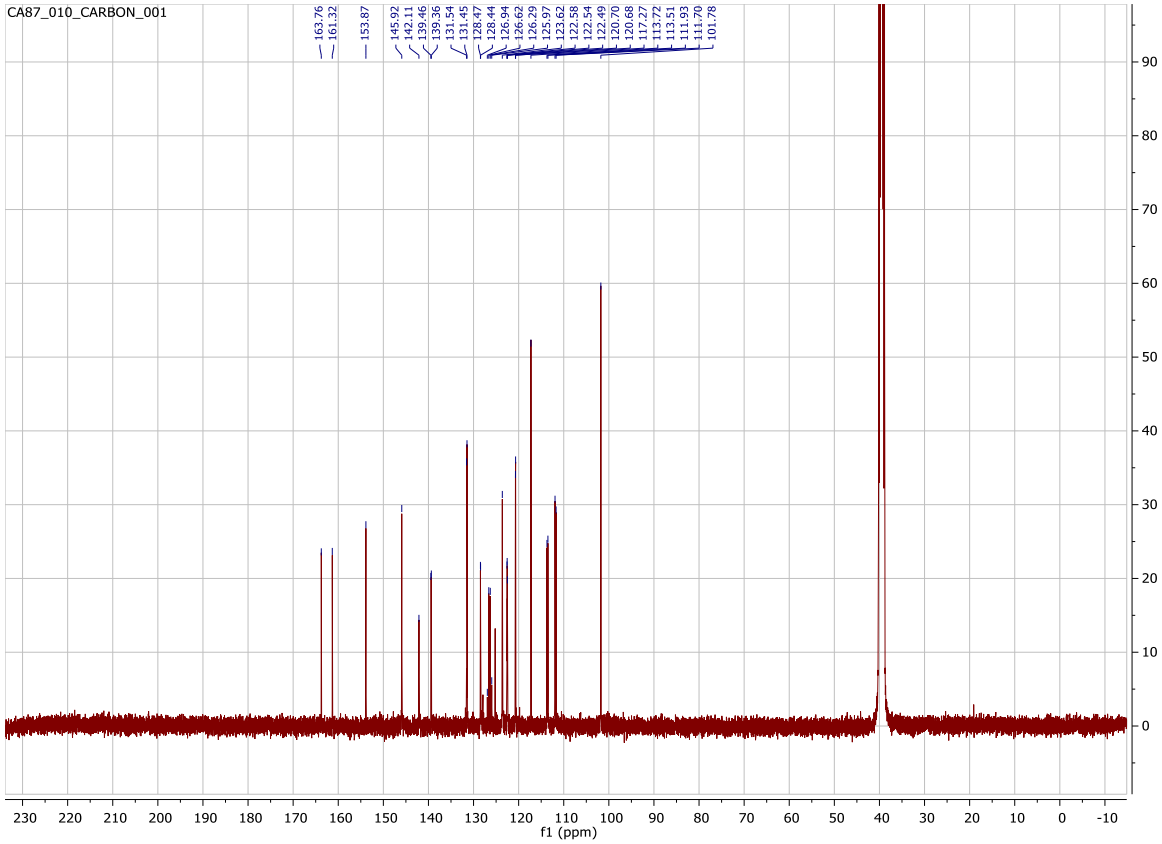
N-(3-Fluorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**19**)

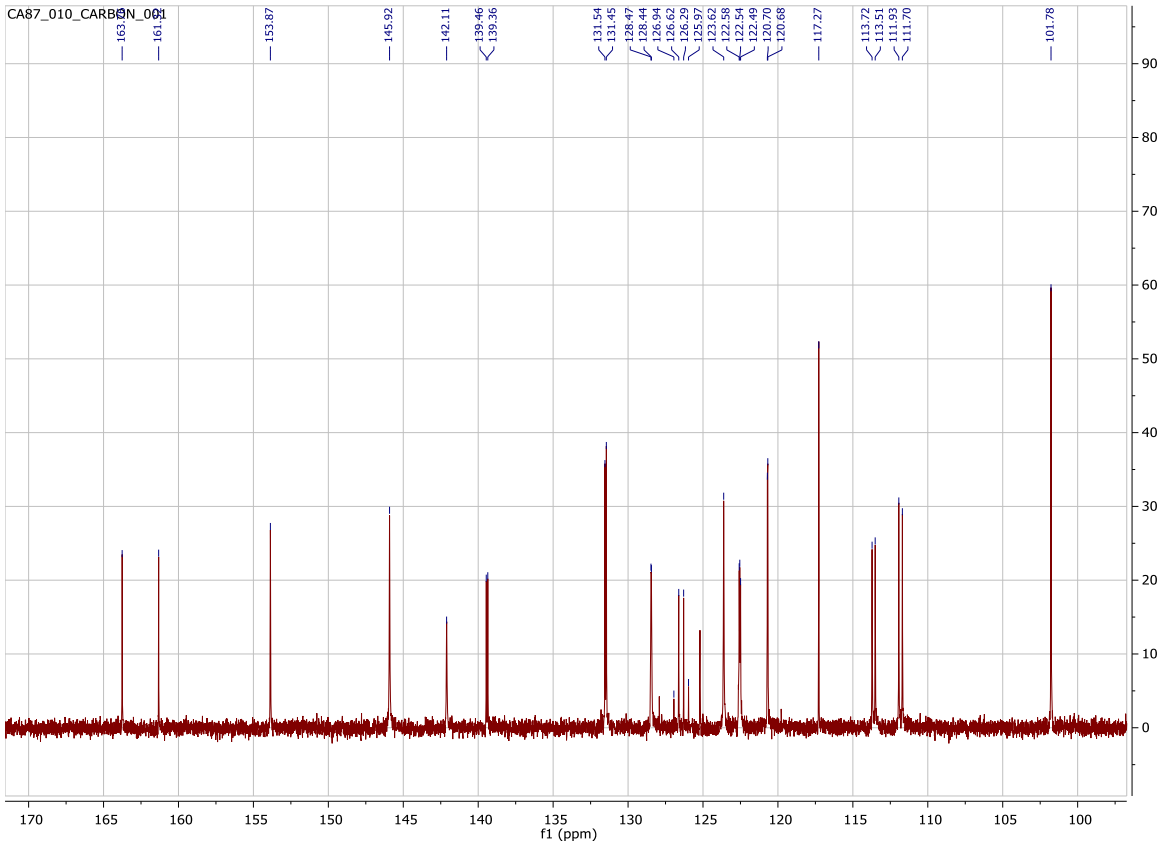


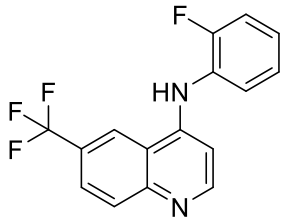



CA87_010_PROTON_001
11.38
9.37
8.63
8.61
8.33
8.30
8.25
8.23
7.62
7.60
7.58
7.56
7.42
7.39
7.37
7.35
7.25
7.24
7.23
7.22
7.21
7.20
7.02
7.00
0.71
1.00
1.00
1.03
0.99
1.02
2.02
1.02
1.00
f1 (ppm)


CA87_010_PROTON_001
8.33
8.30
8.25
8.23
7.62
7.60
7.58
7.56
7.42
7.39
7.37
7.35
7.25
7.24
7.23
7.22
7.21
7.20
7.02
7.00
1.00
1.03
0.99
1.02
2.02
1.02
1.00
f1 (ppm)

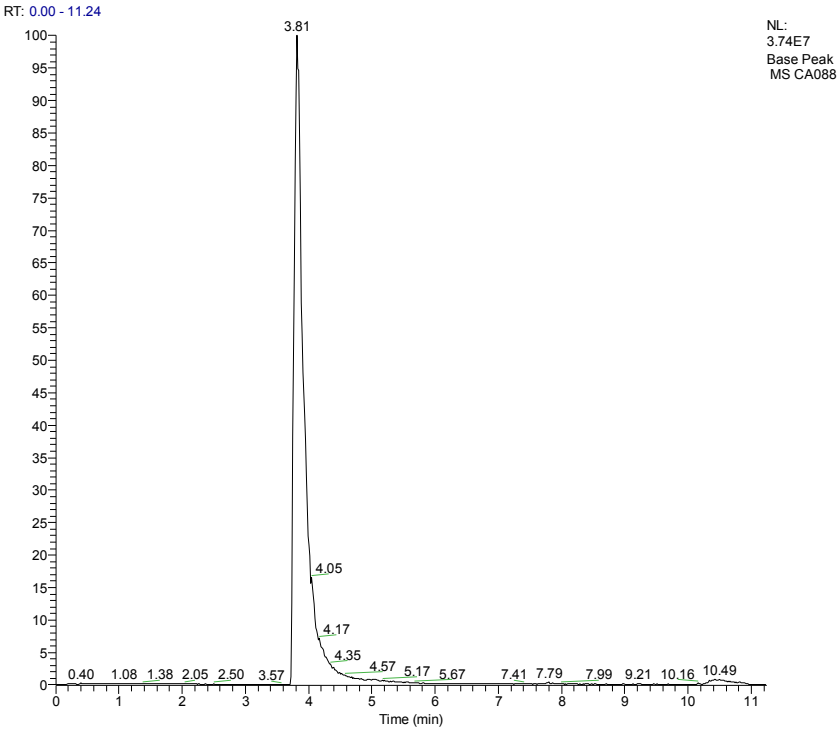

CA87_010_CARBON_001
163.76
161.32
153.87
145.92
142.11
139.46
139.36
131.54
131.45
128.47
128.44
126.94
126.62
126.29
125.97
123.62
122.58
122.54
122.49
120.70
120.68
117.27
113.72
113.51
111.93
111.70
101.78
f1 (ppm)

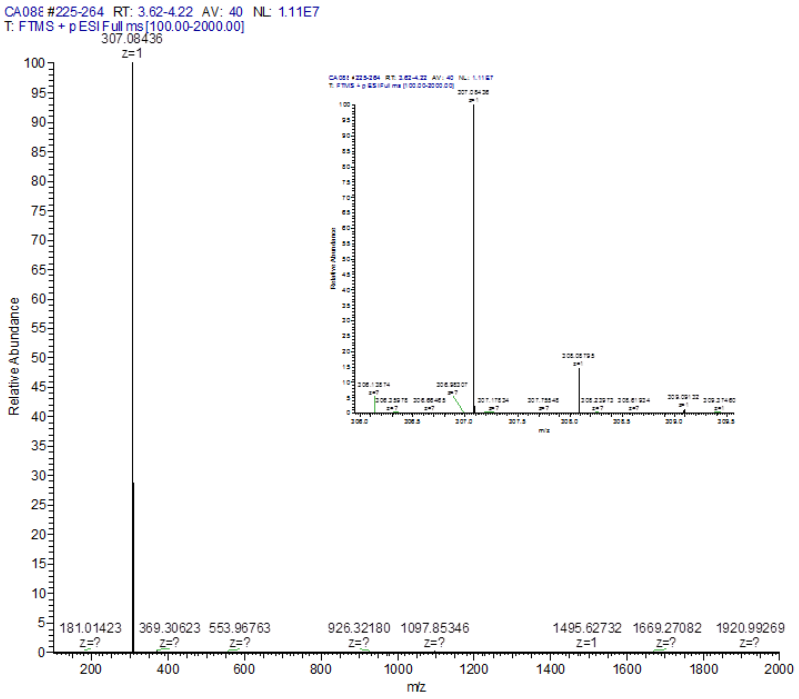

CA87_010_CARBON_001
153.87
145.92
142.11
139.46
139.36
131.54
131.45
128.47
128.44
126.94
126.62
126.29
125.97
123.62
122.58
122.54
122.49
120.70
120.68
117.27
113.72
113.51
111.93
111.70
101.78
f1 (ppm)

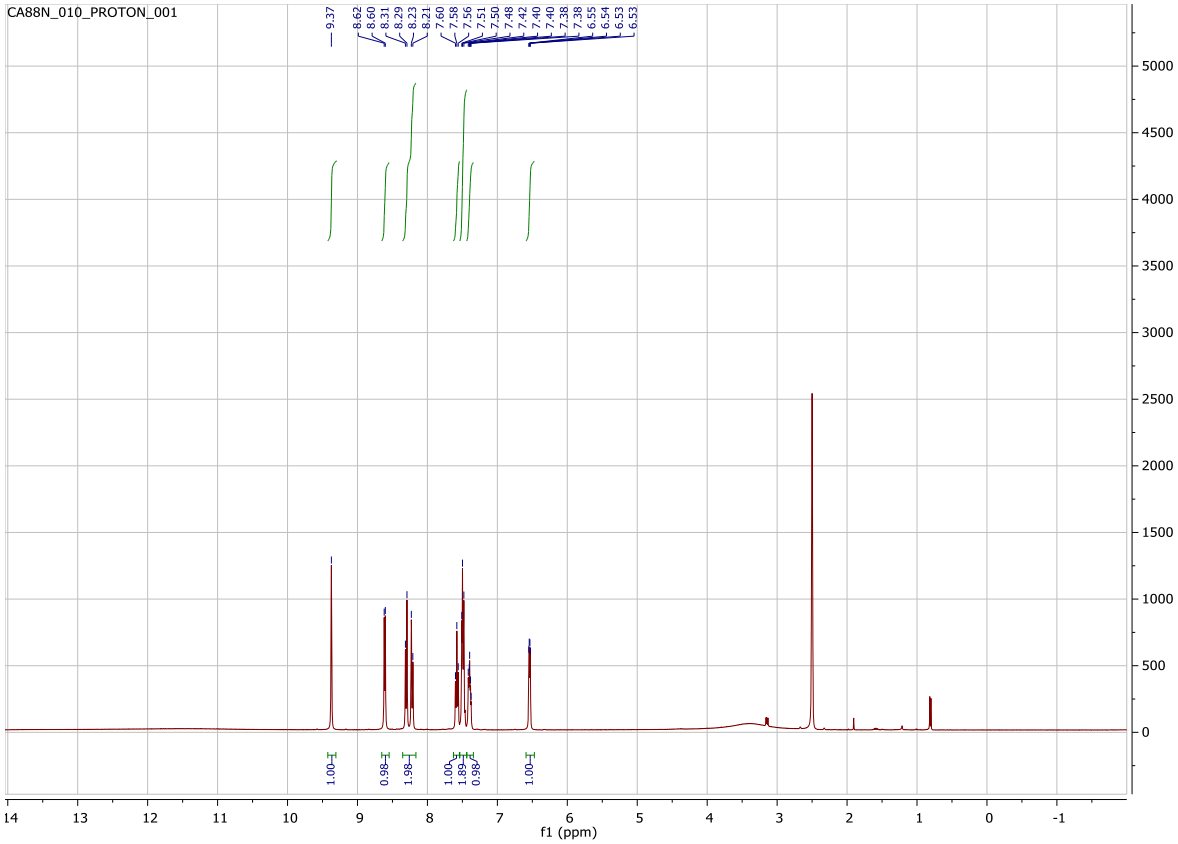


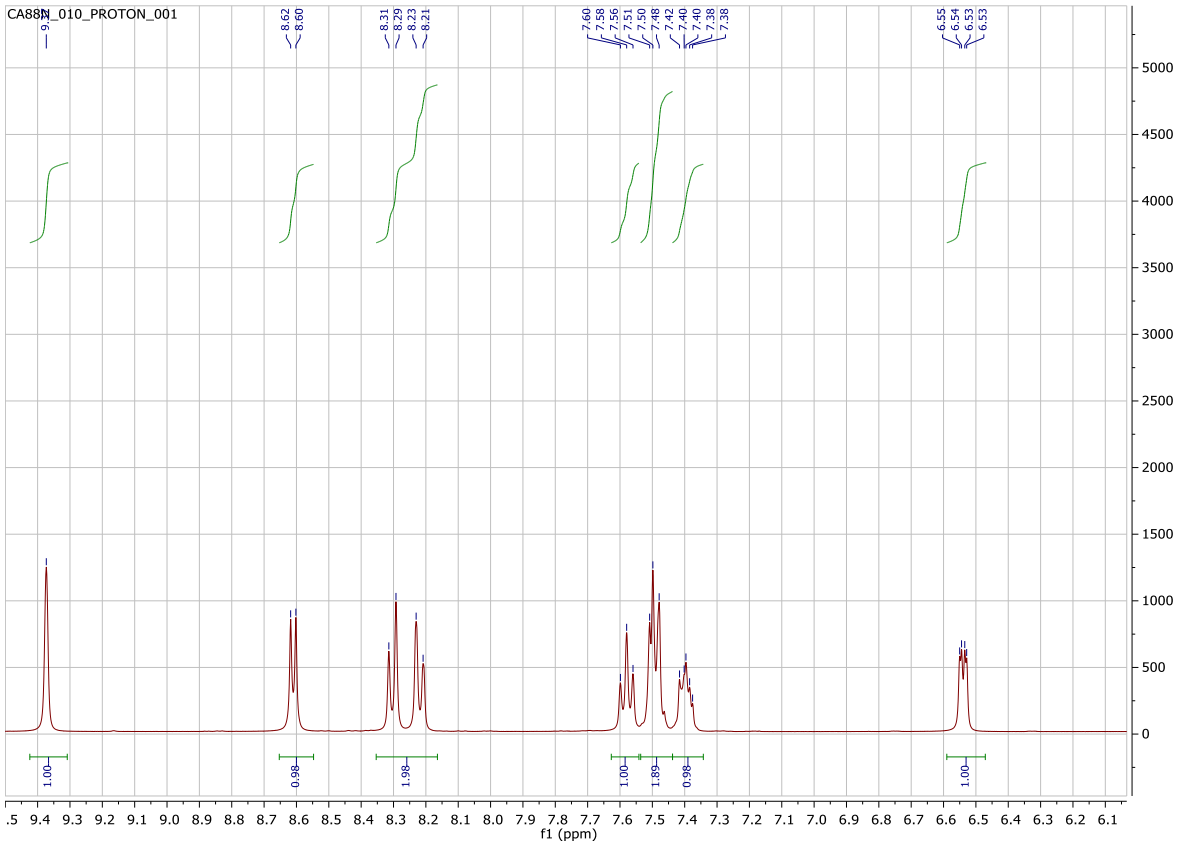
20

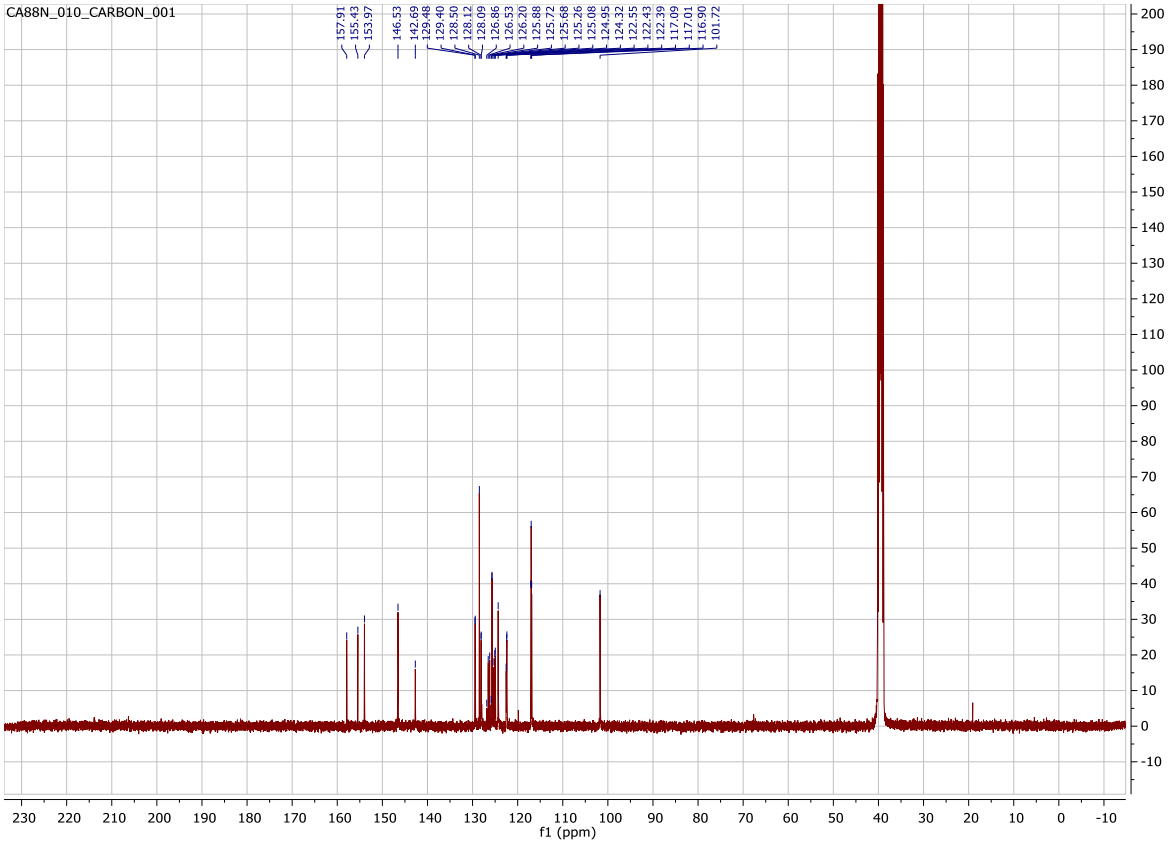
N-(2-Fluorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**20**)

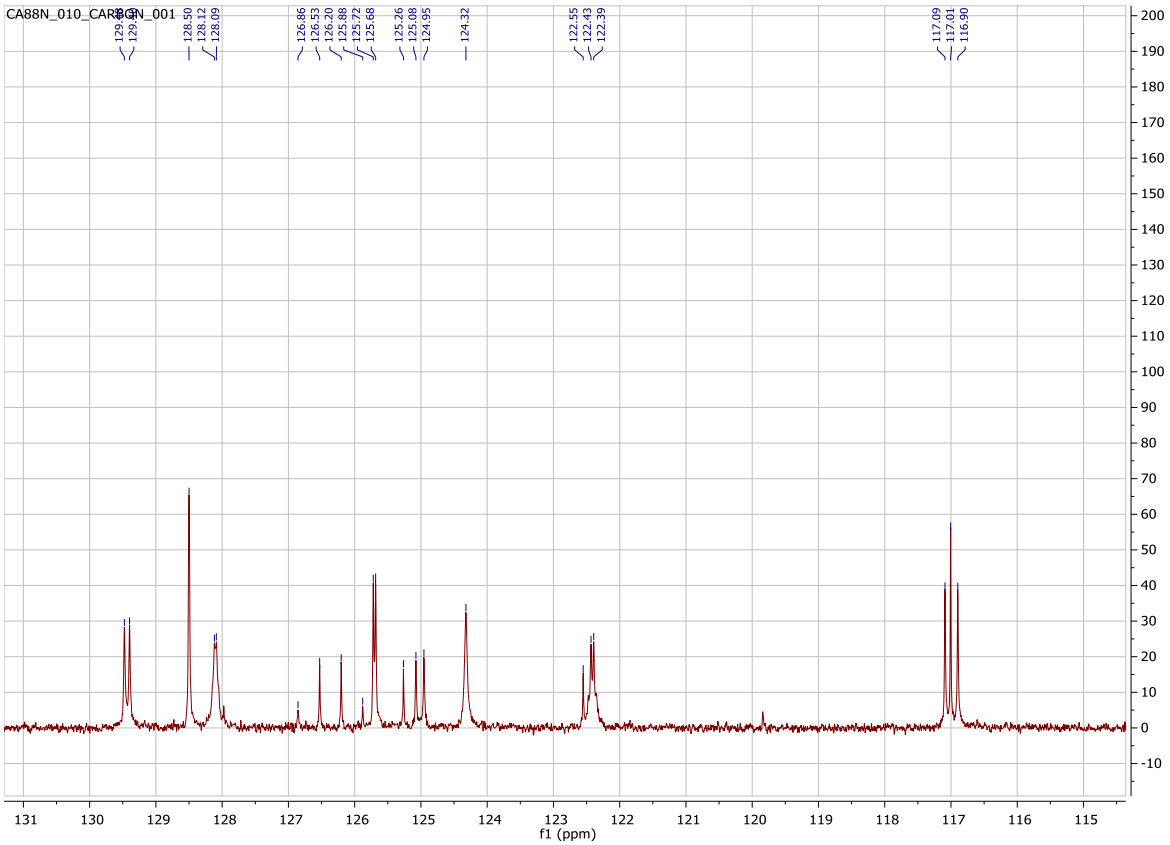


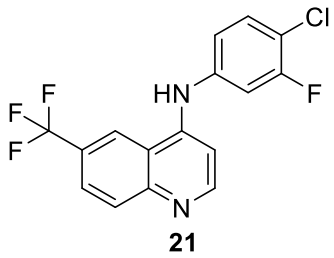



CA88N_010_PROTON_001
9.37
8.62
8.60
8.31
8.29
8.23
8.21
7.60
7.58
7.56
7.51
7.50
7.48
7.42
7.40
7.40
7.38
6.55
6.54
6.53
6.53
1.00
0.98
1.98
1.00
1.89
0.98
1.00
f1 (ppm)


CA88N_010_PROTON_001
9.37
8.62
8.60
8.31
8.29
8.23
8.21
7.60
7.58
7.56
7.51
7.50
7.48
7.42
7.40
7.40
7.38
6.55
6.54
6.53
6.53
1.00
0.98
1.98
1.00
1.89
0.98
1.00
f1 (ppm)

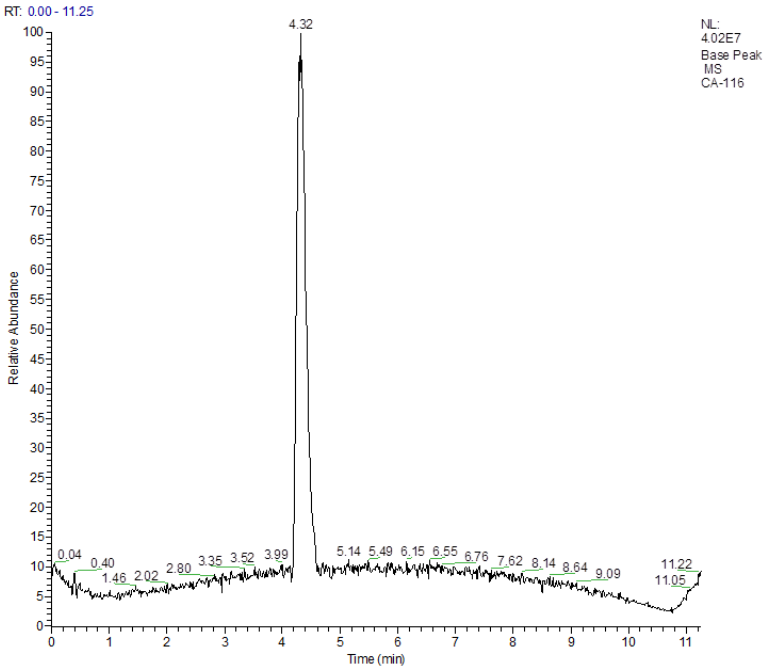

CA88N_010_CARBON_001
157.91
155.43
153.97
146.53
142.69
129.48
129.40
128.50
128.12
128.09
126.86
126.53
126.20
125.88
125.72
125.68
125.26
125.08
124.95
124.32
122.55
122.43
122.39
117.09
117.01
116.90
101.72
f1 (ppm)

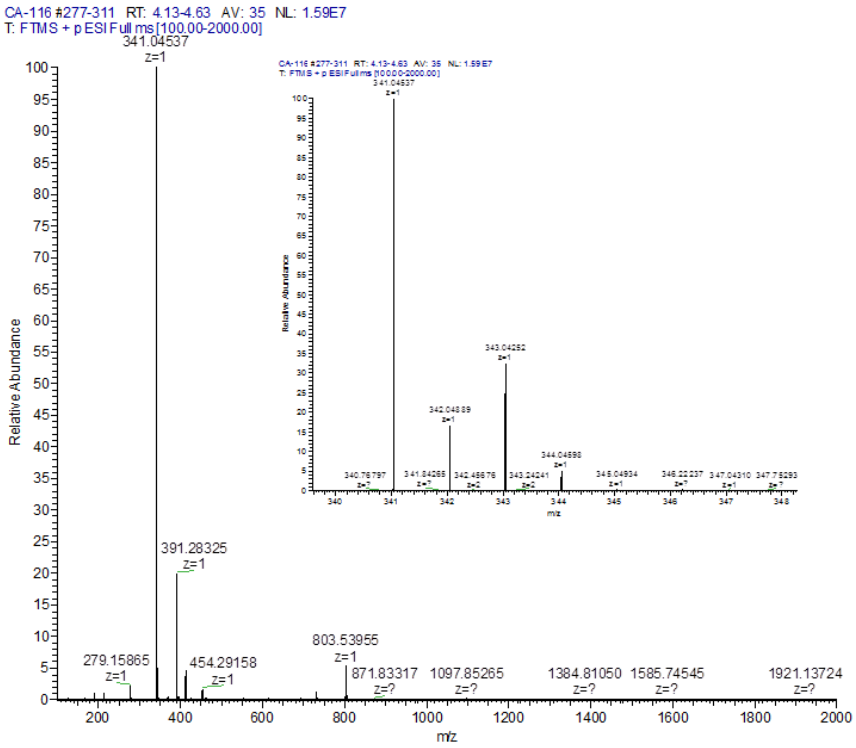

CA88N_010_CARBON_001
129.91
129.71
128.50
128.12
128.09
126.86
126.53
126.20
125.88
125.72
125.68
125.26
125.08
124.95
124.32
122.55
122.43
122.39
117.09
117.01
116.90
f1 (ppm)

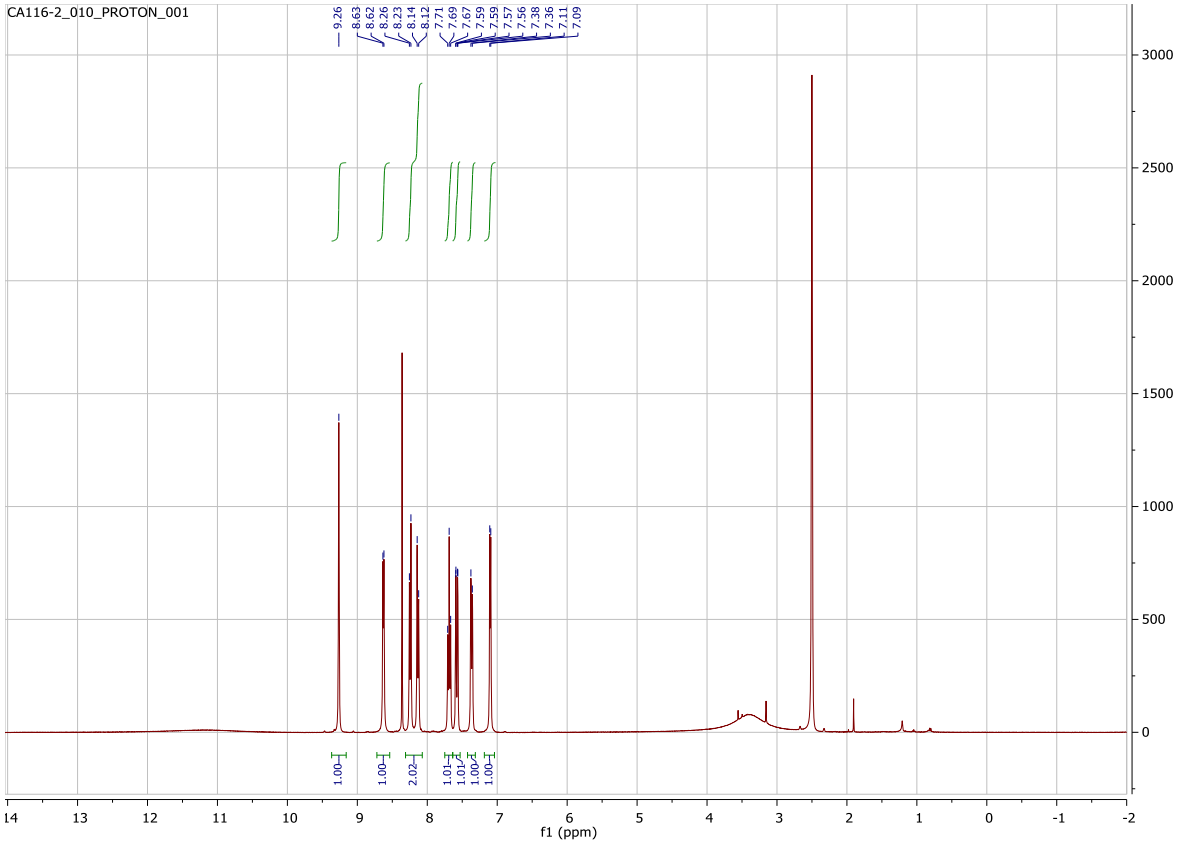


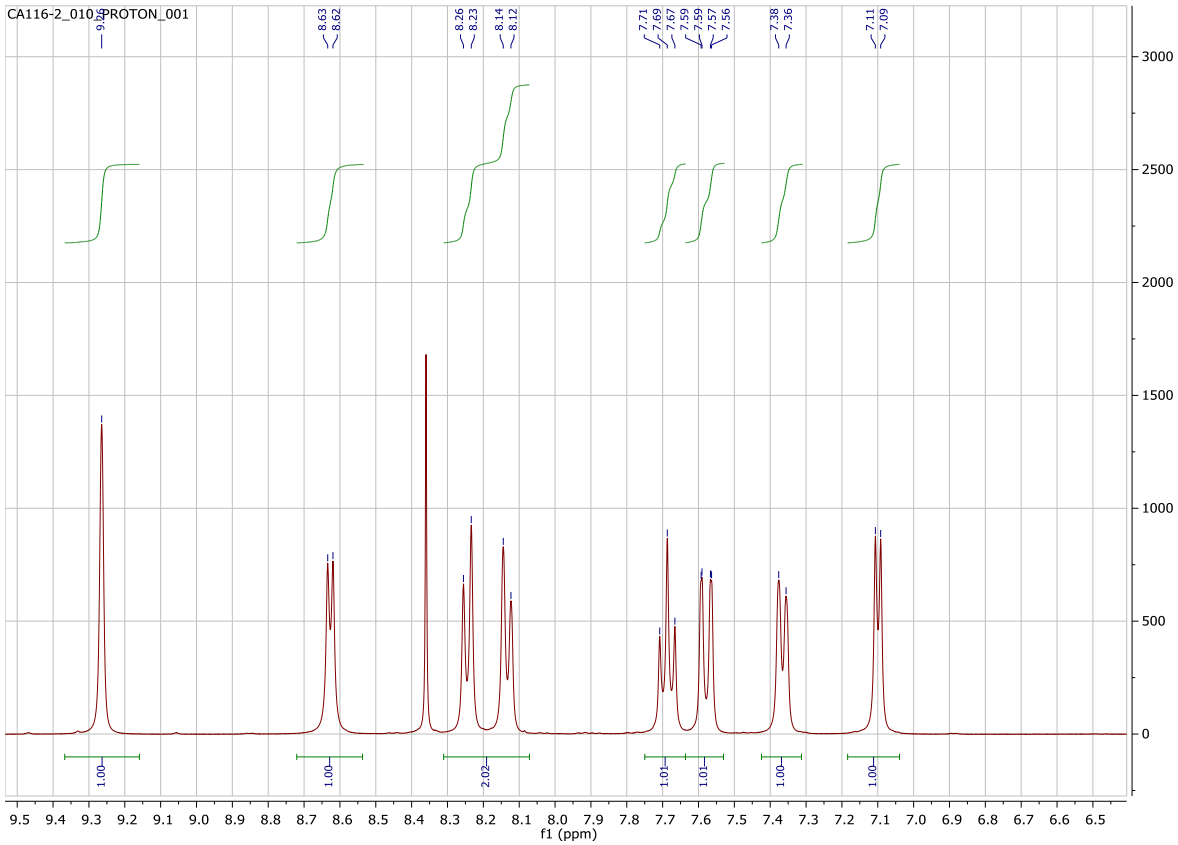
21

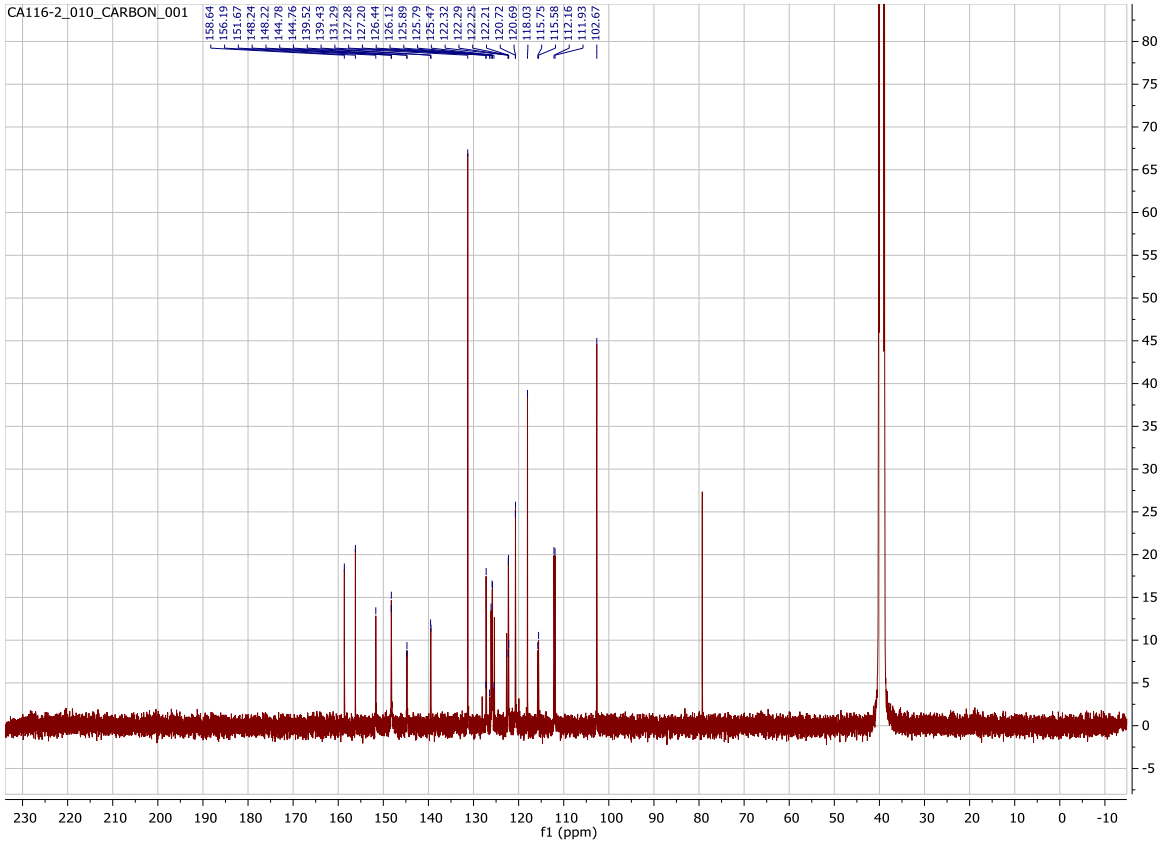
N-(4-Chloro-3-fluorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**21**)

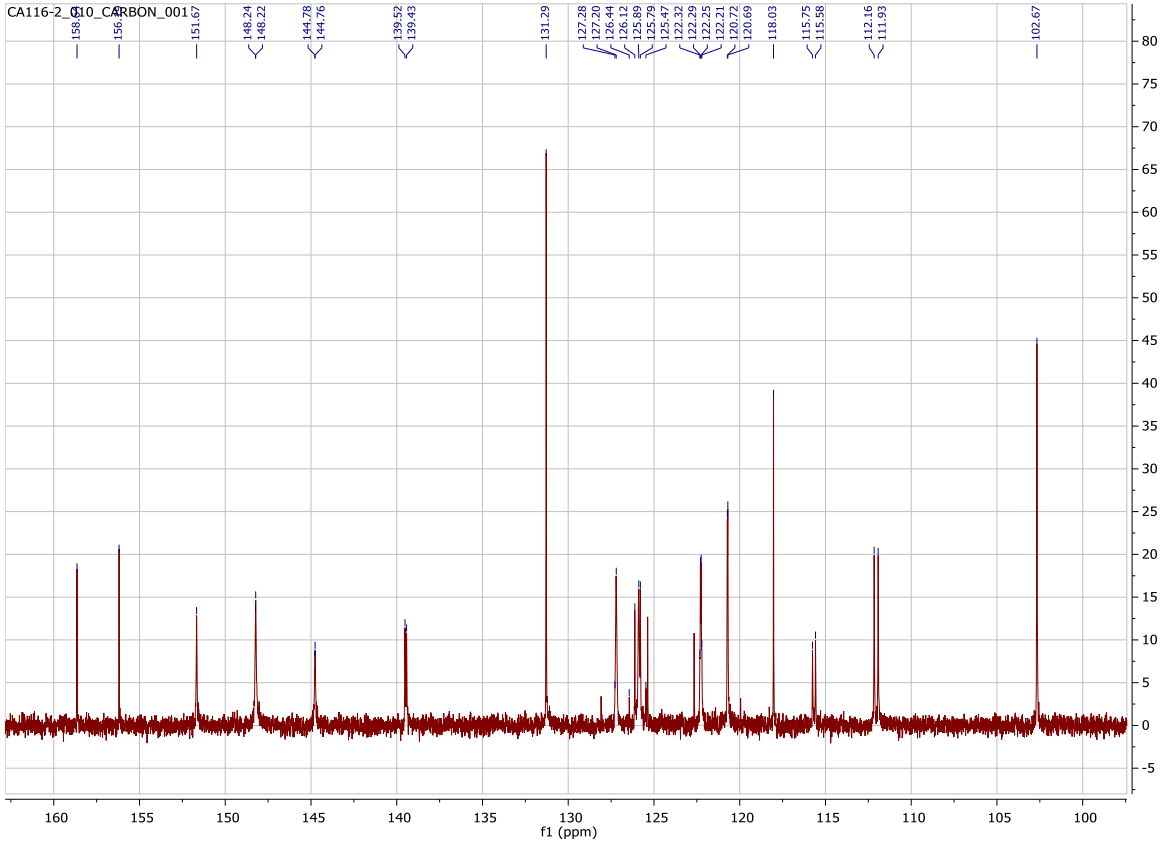


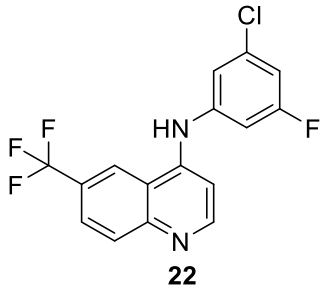



CA116-2_010_PROTON_001
9.26
8.63
8.62
8.26
8.23
8.14
8.12
7.71
7.69
7.67
7.59
7.59
7.57
7.56
7.38
7.36
7.11
7.09
1.00
1.00
2.02
1.01
1.01
1.00
1.00
f1 (ppm)


CA116-2_010_PROTON_001
9.26
8.63
8.62
8.26
8.23
8.14
8.12
7.71
7.69
7.67
7.59
7.59
7.57
7.56
7.38
7.36
7.11
7.09
1.00
1.00
2.02
1.01
1.01
1.00
1.00
f1 (ppm)

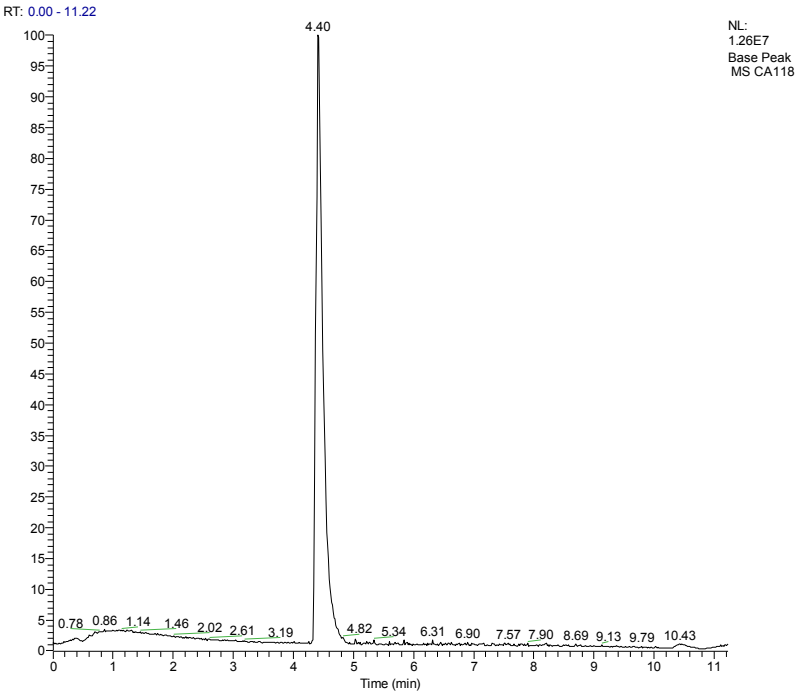

CA116-2_010_CARBON_001
158.64
156.19
151.67
148.24
148.22
144.78
144.76
139.52
139.43
131.29
127.28
127.20
126.44
126.12
125.89
125.79
125.47
122.32
122.29
122.25
122.21
120.72
120.69
118.03
115.75
115.58
112.16
111.93
102.67
f1 (ppm)

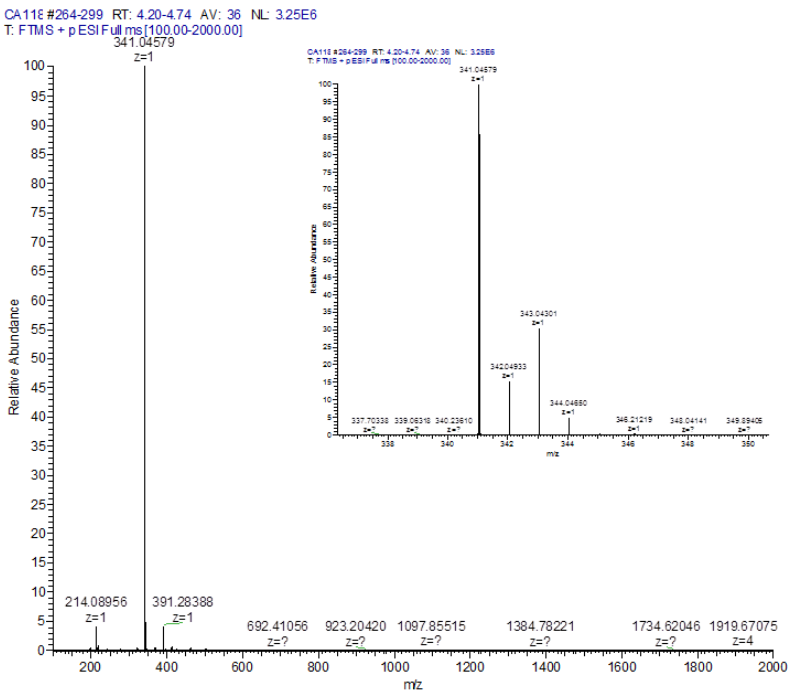

CA116-2_010_CARBON_001
151.67
148.24
148.22
144.78
144.76
139.52
139.43
131.29
127.28
127.20
126.44
126.12
125.89
125.79
125.47
122.32
122.29
122.25
122.21
120.72
120.69
118.03
115.75
115.58
112.16
111.93
102.67
f1 (ppm)

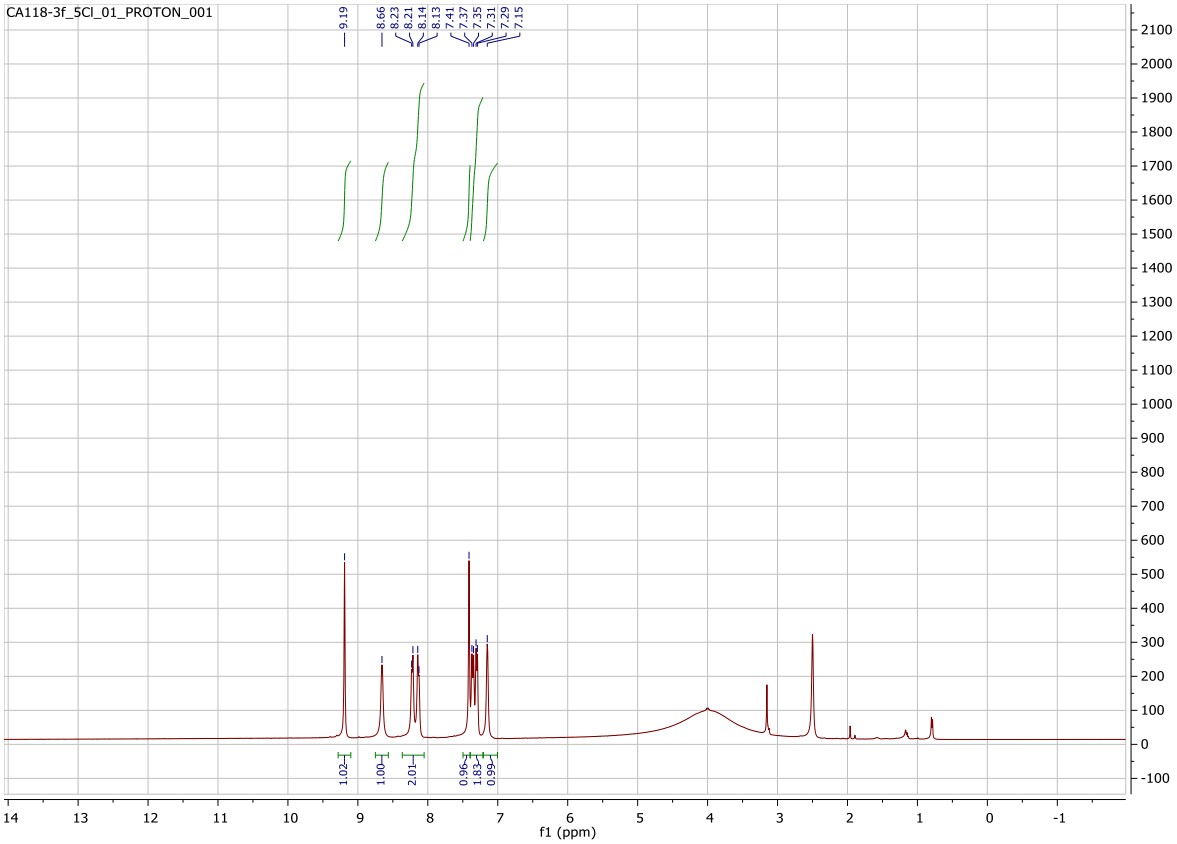


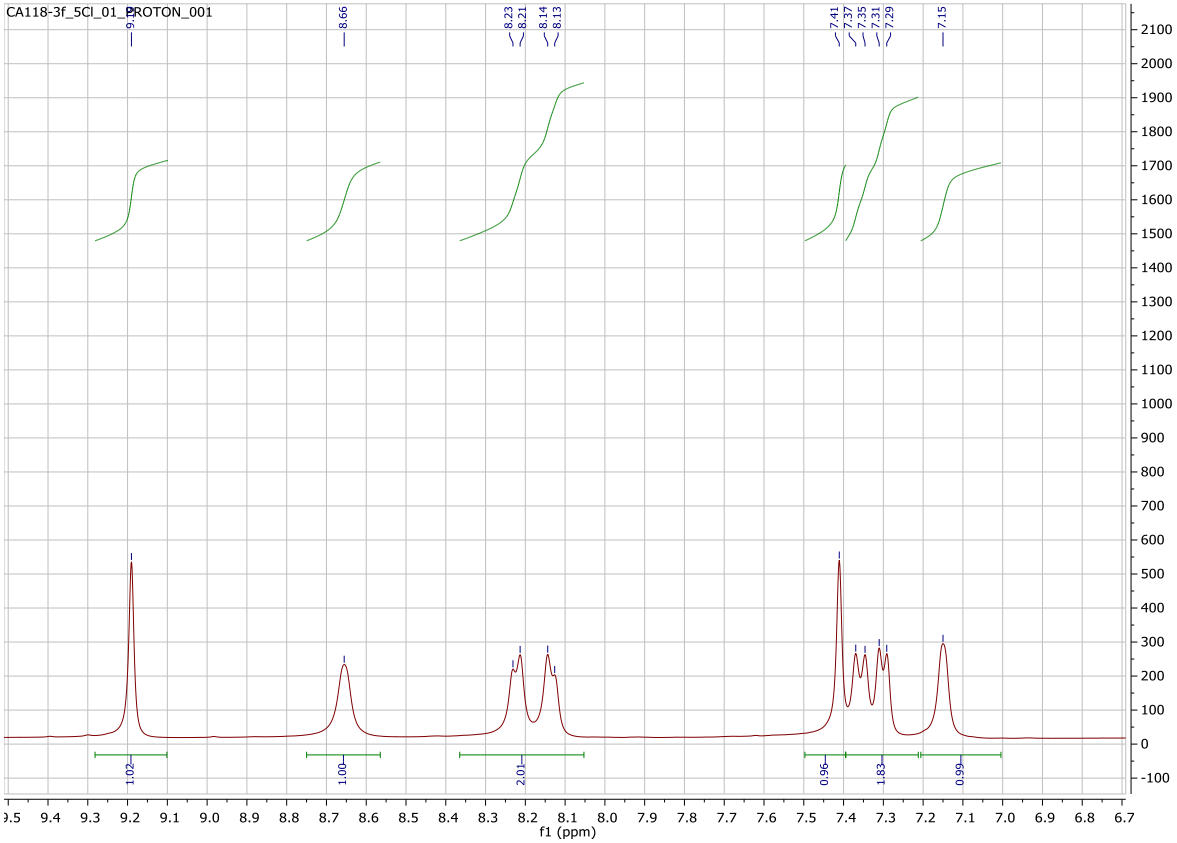
22

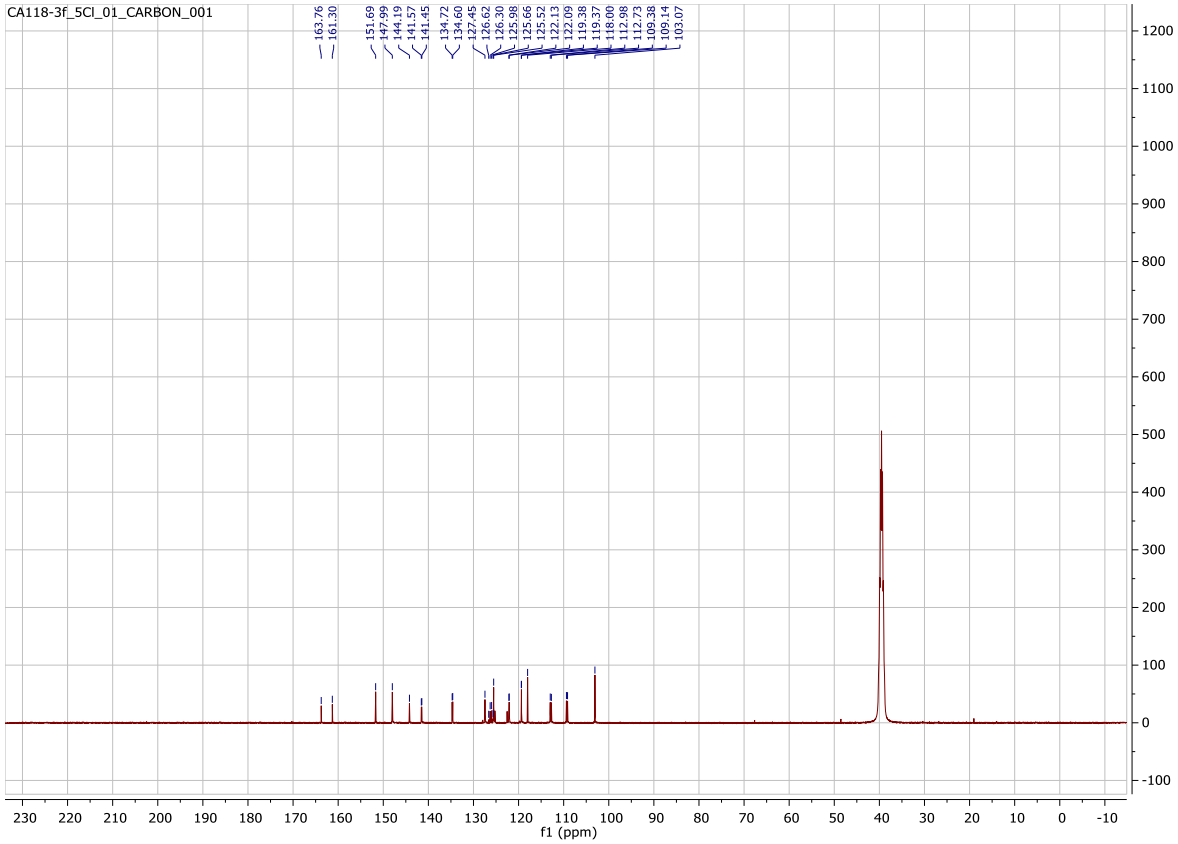
N-(3-Chloro-5-fluorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**22**)

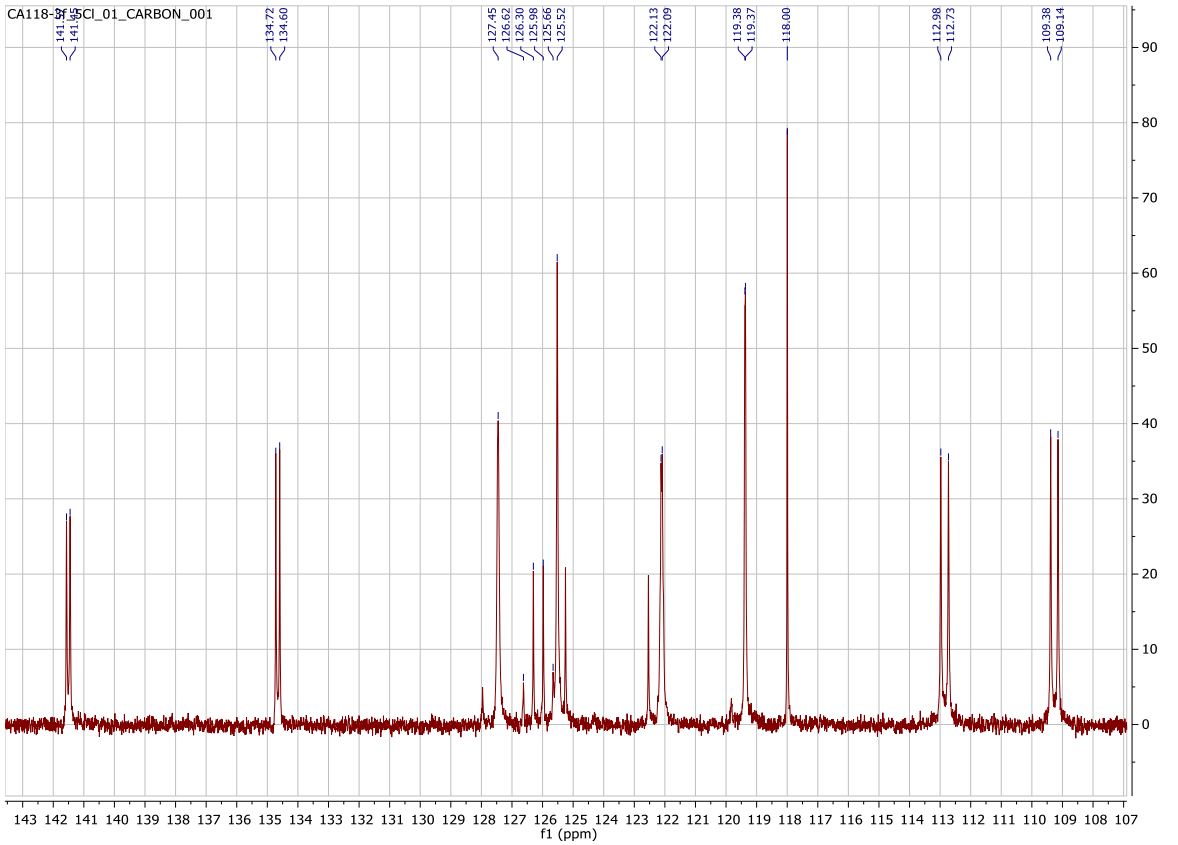


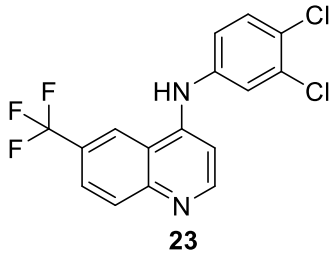



CA118-3f_5Cl_01_PROTON_001
9.19
8.66
8.23
8.21
8.14
8.13
7.41
7.37
7.35
7.31
7.29
7.15
1.02
1.00
2.01
0.96
1.83
0.99
f1 (ppm)


CA118-3f_5Cl_01_PROTON_001
9.19
8.66
8.23
8.21
8.14
8.13
7.41
7.37
7.35
7.31
7.29
7.15
1.02
1.00
2.01
0.96
1.83
0.99
f1 (ppm)

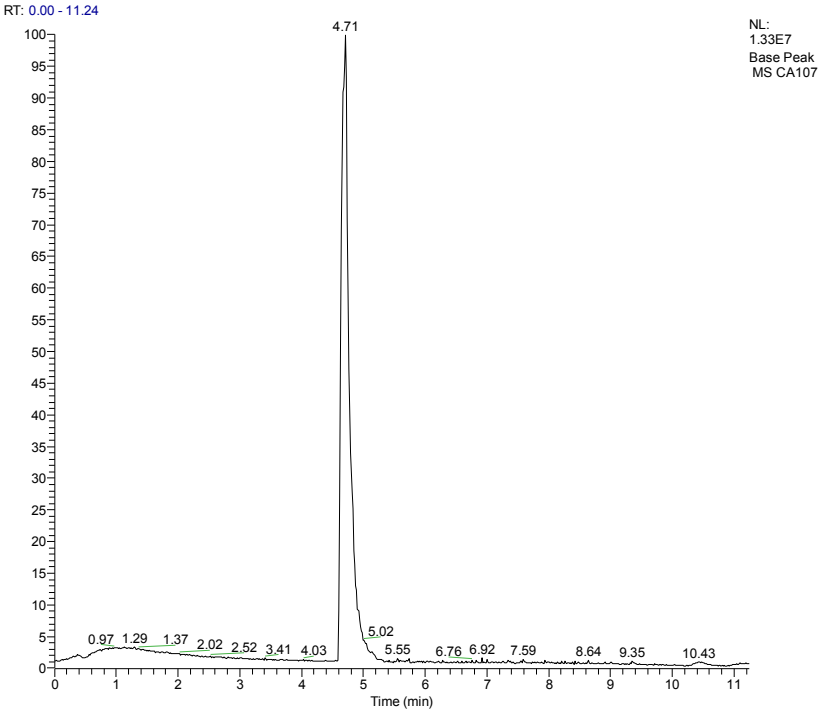

CA118-3f_5Cl_01_CARBON_001
163.76
161.30
151.69
147.99
144.19
141.57
141.45
134.72
134.60
127.45
126.62
126.30
125.98
125.66
125.52
122.13
122.09
119.38
119.37
118.00
112.98
112.73
109.38
109.14
103.07
f1 (ppm)

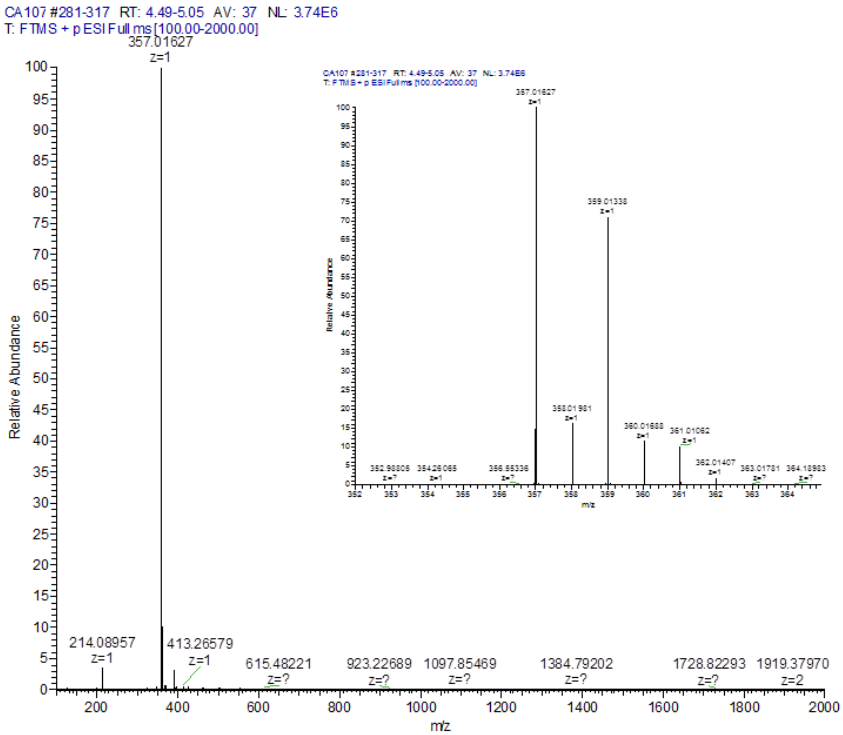

CA118-3f_5Cl_01_CARBON_001
141.45
134.72
134.60
127.45
126.62
126.30
125.98
125.66
125.52
122.13
122.09
119.38
119.37
118.00
112.98
112.73
109.38
109.14
f1 (ppm)

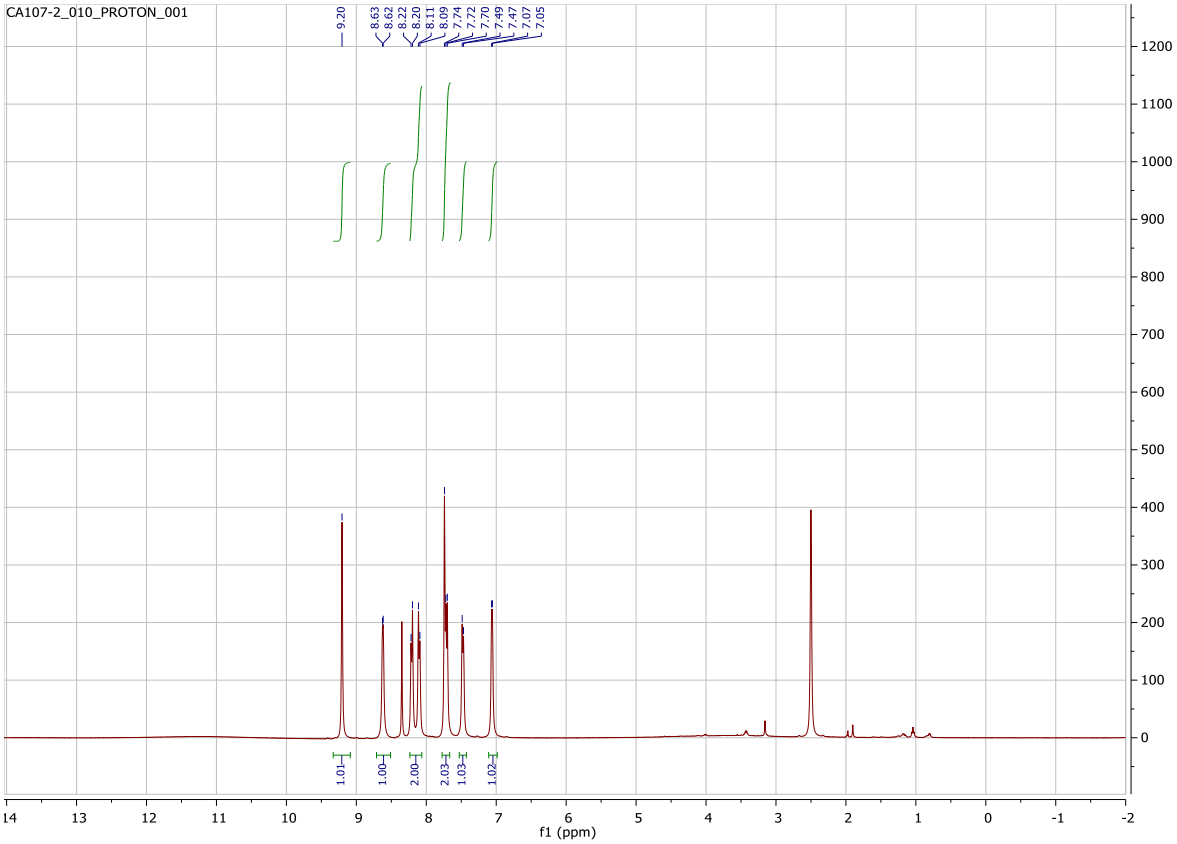


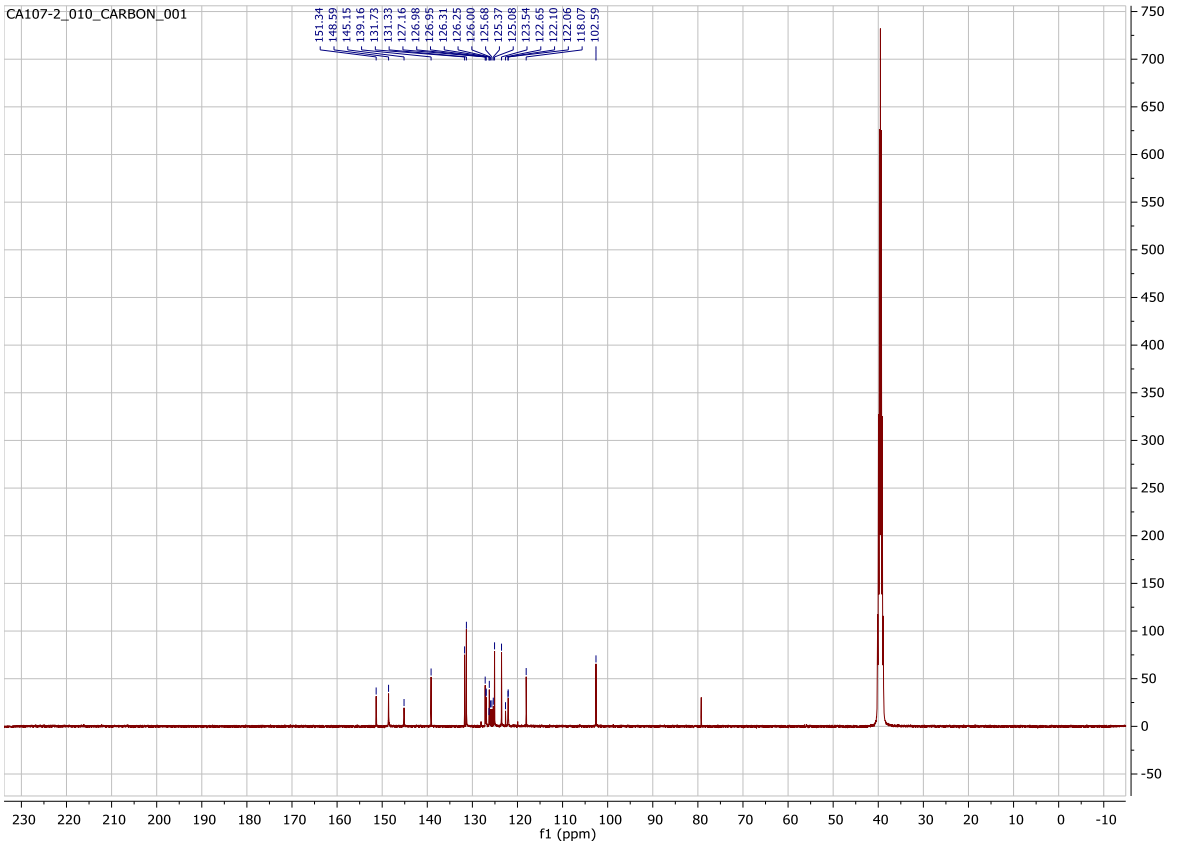
23

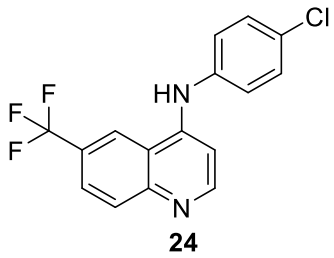
N-(3,4-Dichlorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**23**)





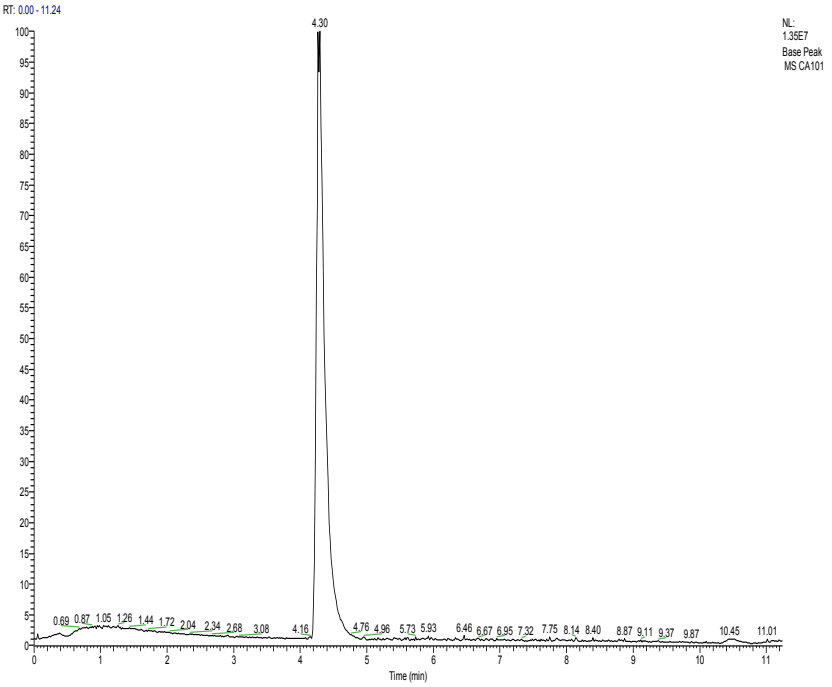

CA107-2_010_PROTON_001
9.20
8.63
8.62
8.22
8.20
8.11
8.09
7.74
7.72
7.70
7.49
7.47
7.07
7.05
1.01
1.00
2.00
2.03
1.03
1.02
f1 (ppm)

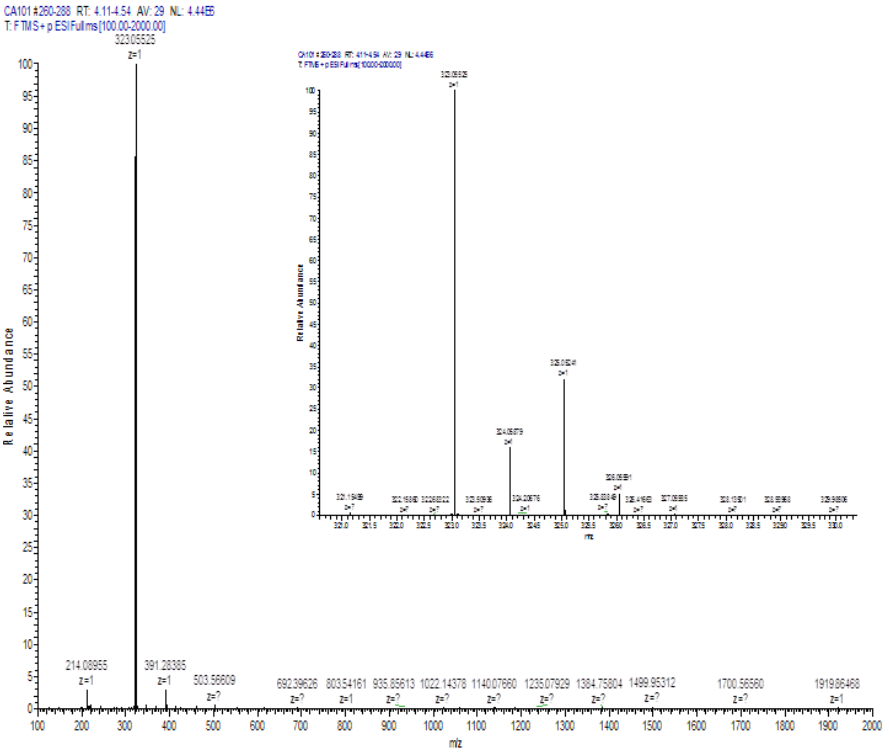

CA107-2_010_CARBON_001
151.34
148.59
145.15
139.16
131.73
131.33
127.16
126.98
126.95
126.31
126.25
126.00
125.68
125.37
125.08
123.54
123.45
122.10
122.06
118.07
102.59
f1 (ppm)

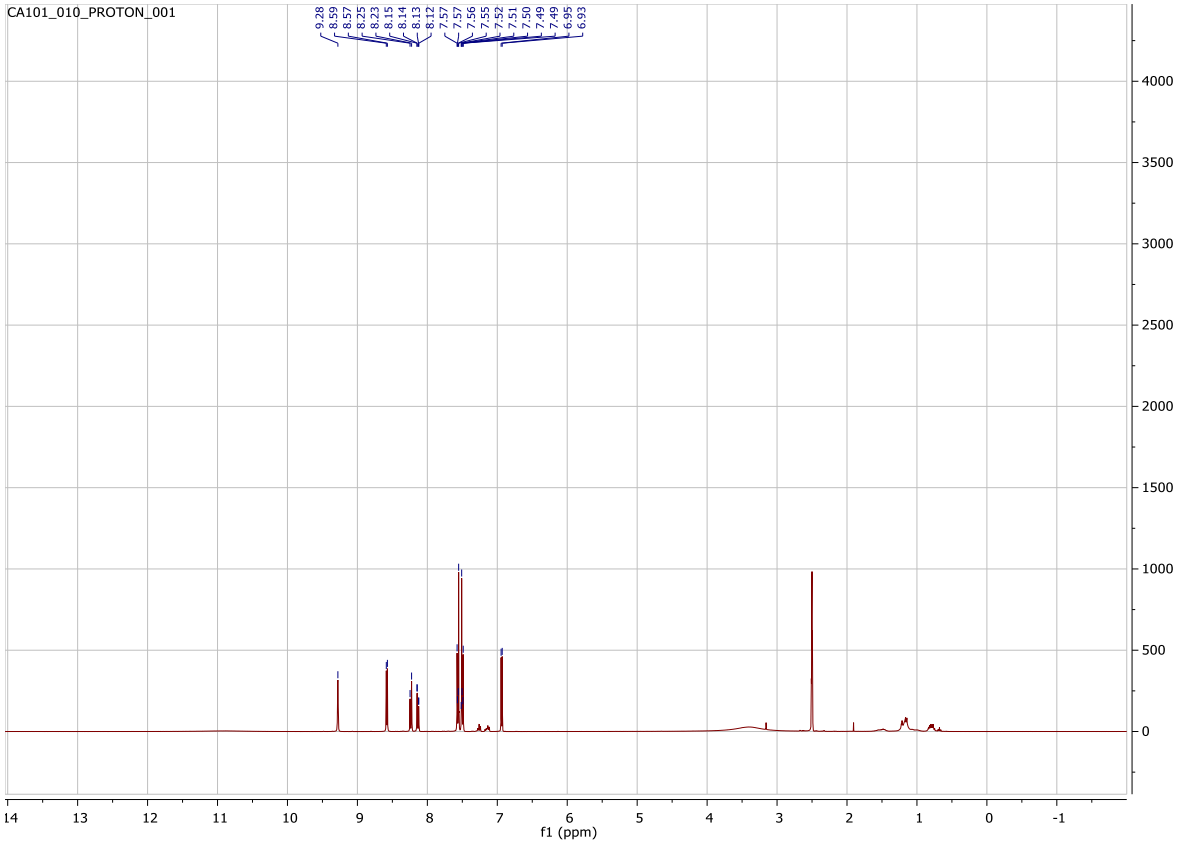


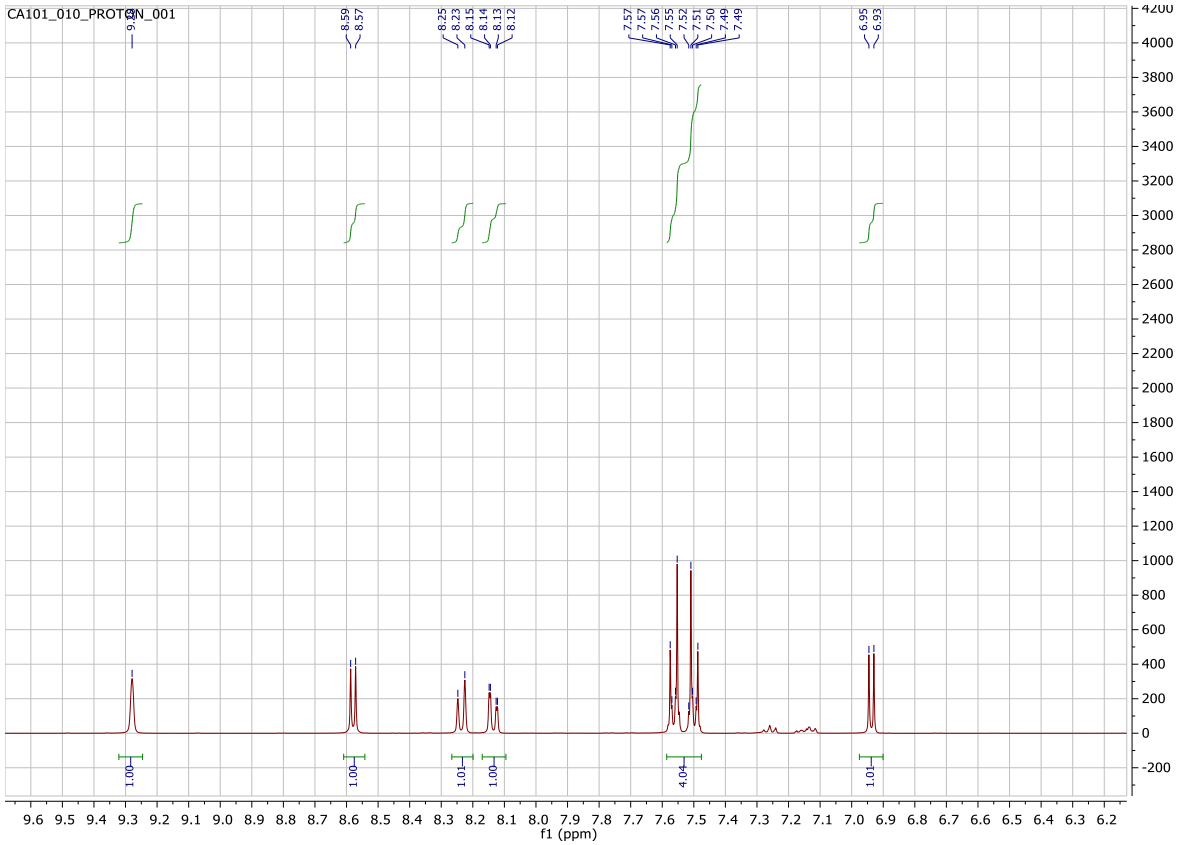
24

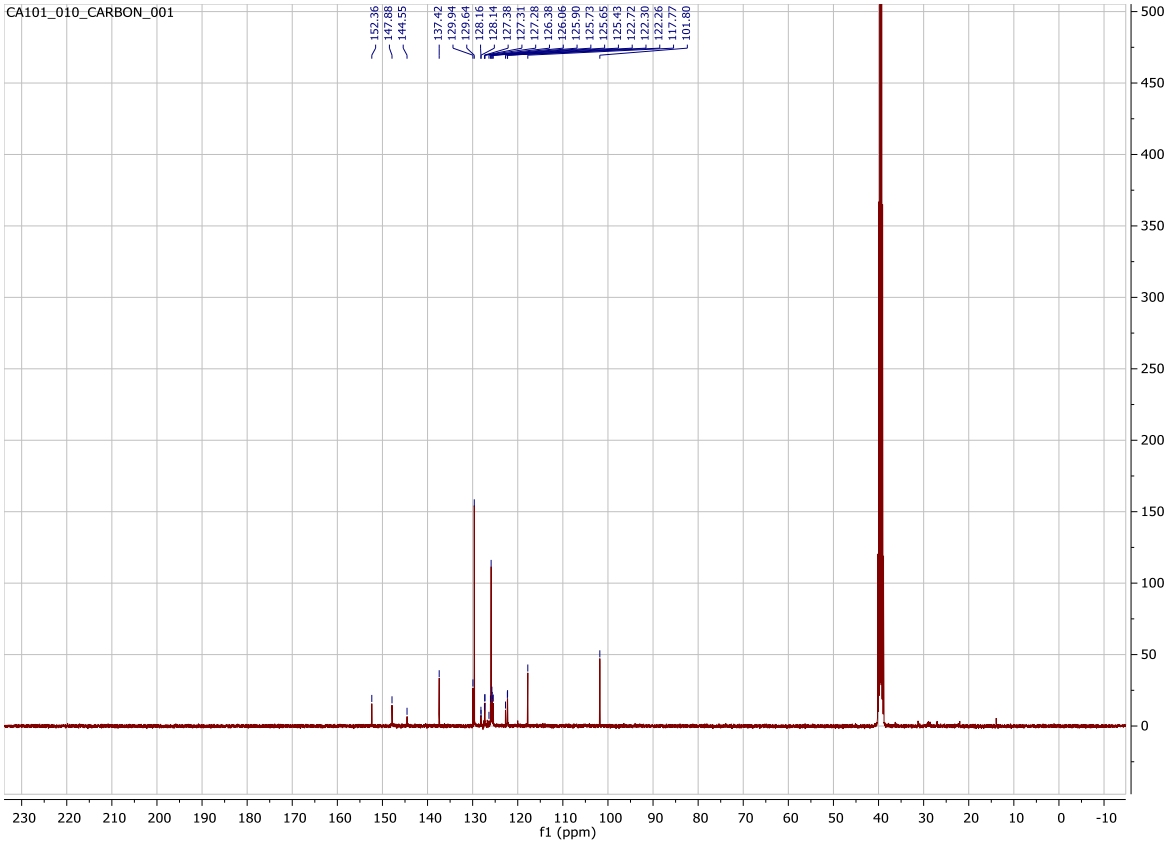
N-(4-Chlorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**24**)

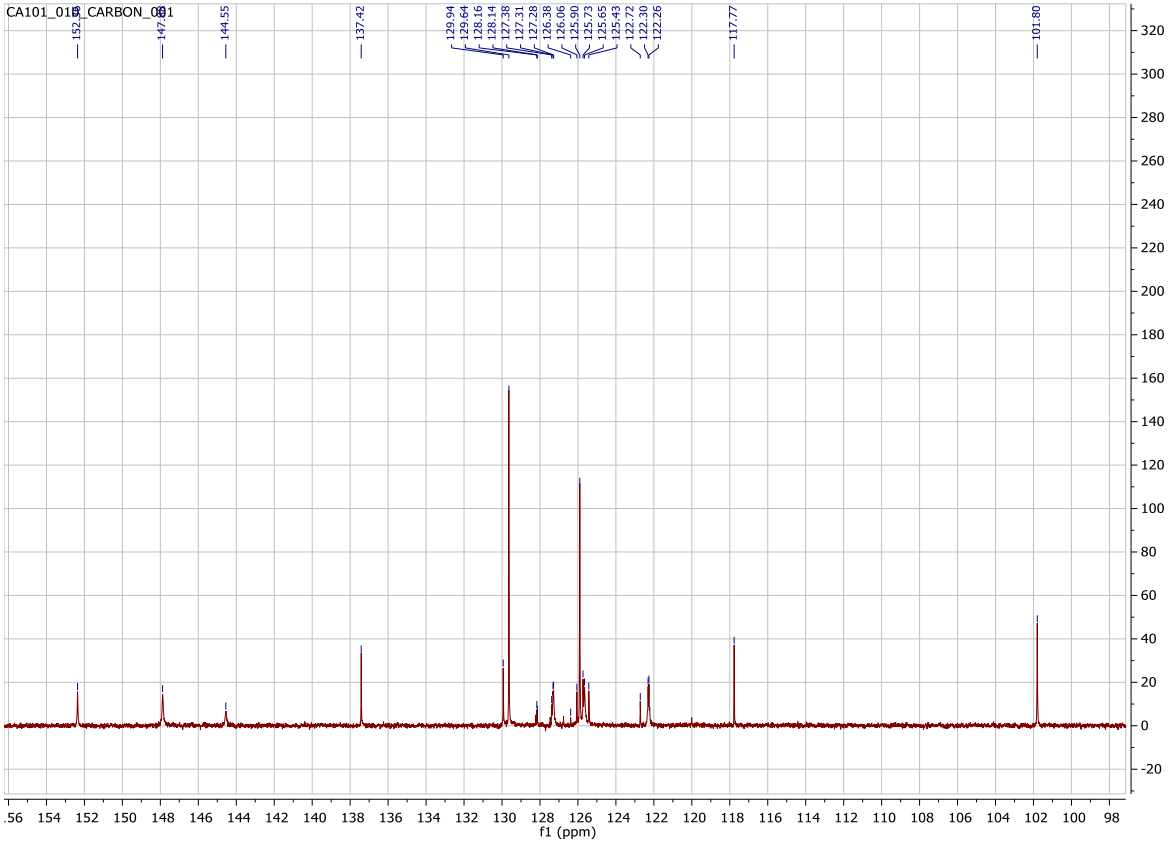


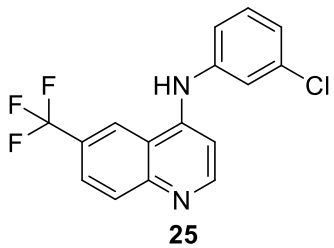



CA101_010_PROTON_001
9.28
8.59
8.57
8.25
8.23
8.15
8.14
8.13
8.12
7.57
7.57
7.56
7.55
7.52
7.51
7.50
7.49
7.49
6.95
6.93
f1 (ppm)


CA101_010_PROTON_001
9.28
8.59
8.57
8.25
8.23
8.15
8.14
8.13
8.12
7.57
7.57
7.56
7.55
7.52
7.51
7.50
7.49
7.49
6.95
6.93
1.00
1.00
1.01
1.00
4.04
1.01
f1 (ppm)

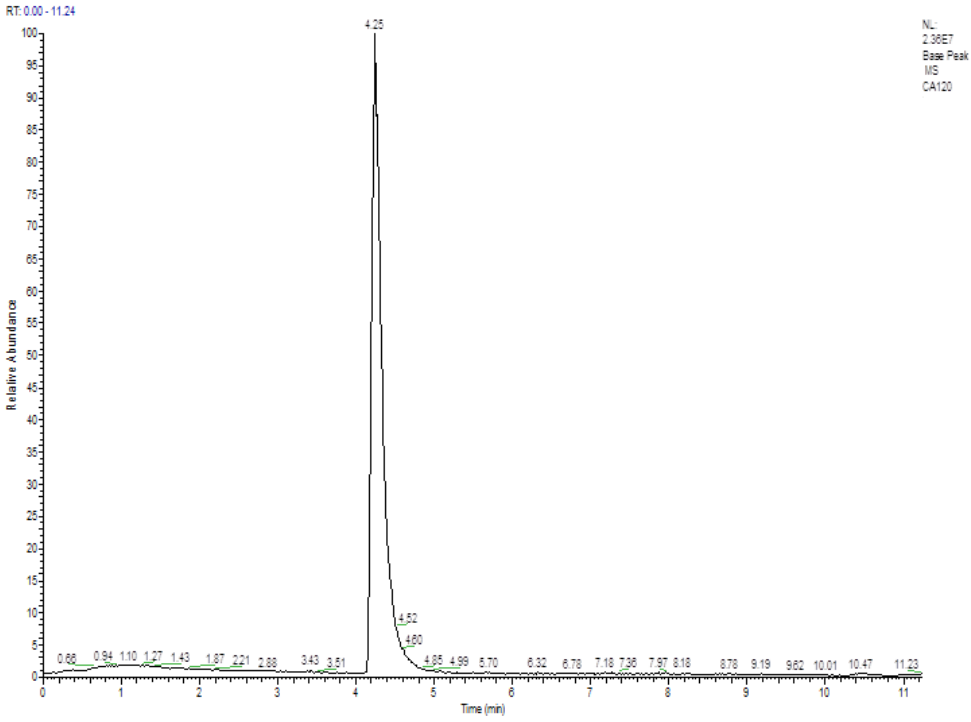

CA101_010_CARBON_001
152.36
147.88
144.55
137.42
129.94
129.64
128.16
128.14
127.38
127.31
127.28
126.38
126.06
125.90
125.73
125.65
125.43
122.72
122.30
122.26
117.77
101.80
f1 (ppm)

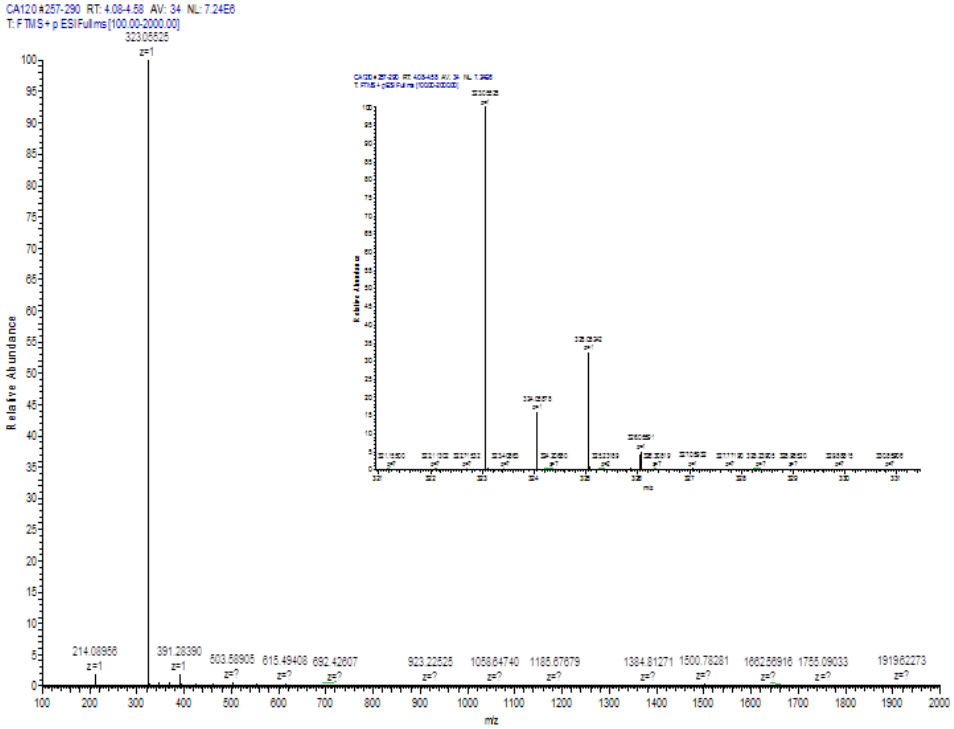

CA101_010_CARBON_001
152.36
147.88
144.55
137.42
129.94
129.64
128.16
128.14
127.38
127.31
127.28
126.38
126.06
125.90
125.73
125.65
125.43
122.72
122.30
122.26
117.77
101.80
f1 (ppm)

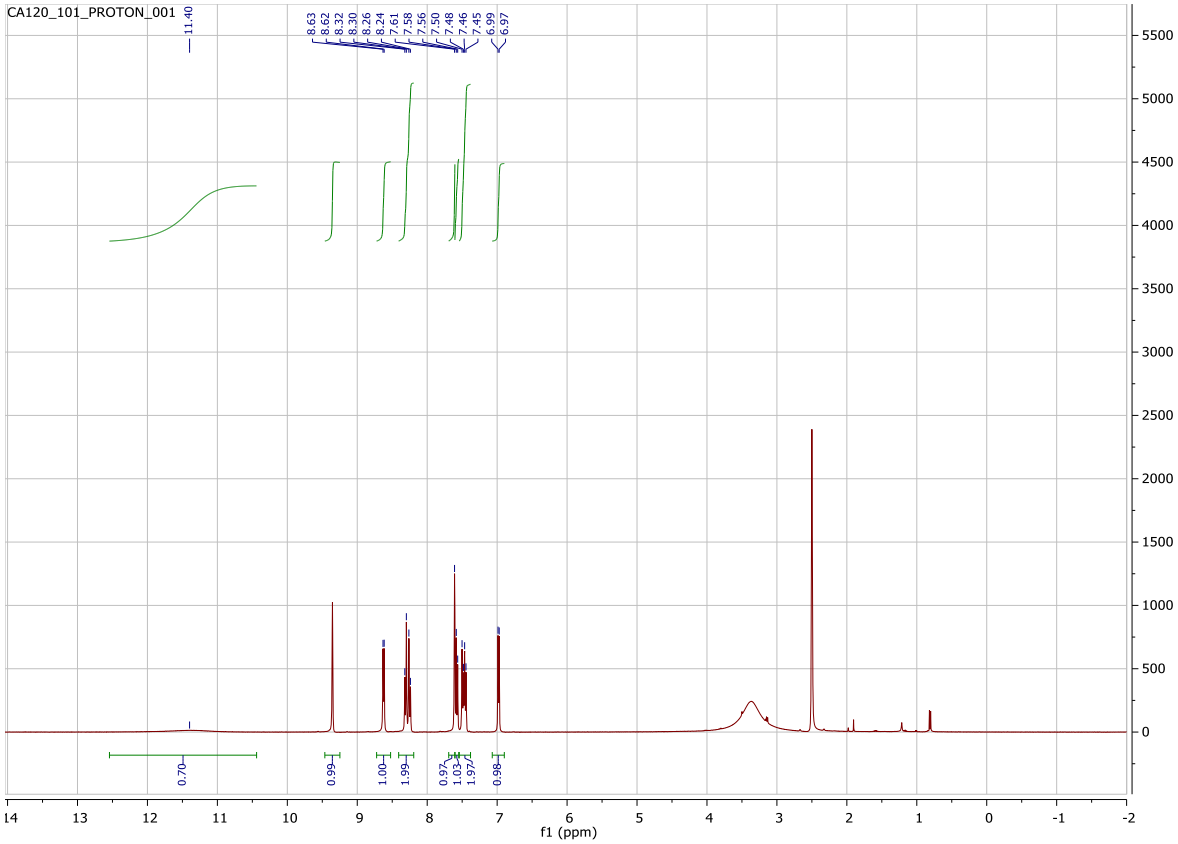


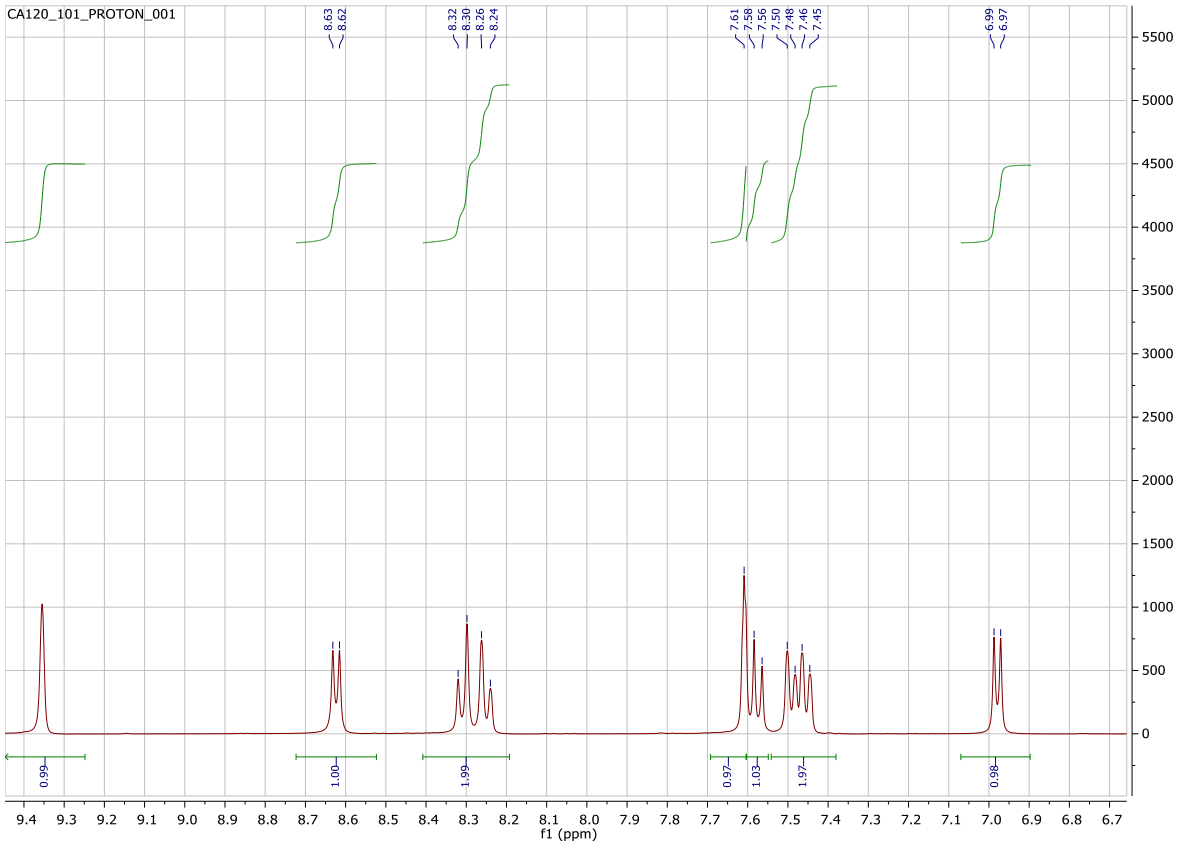
25

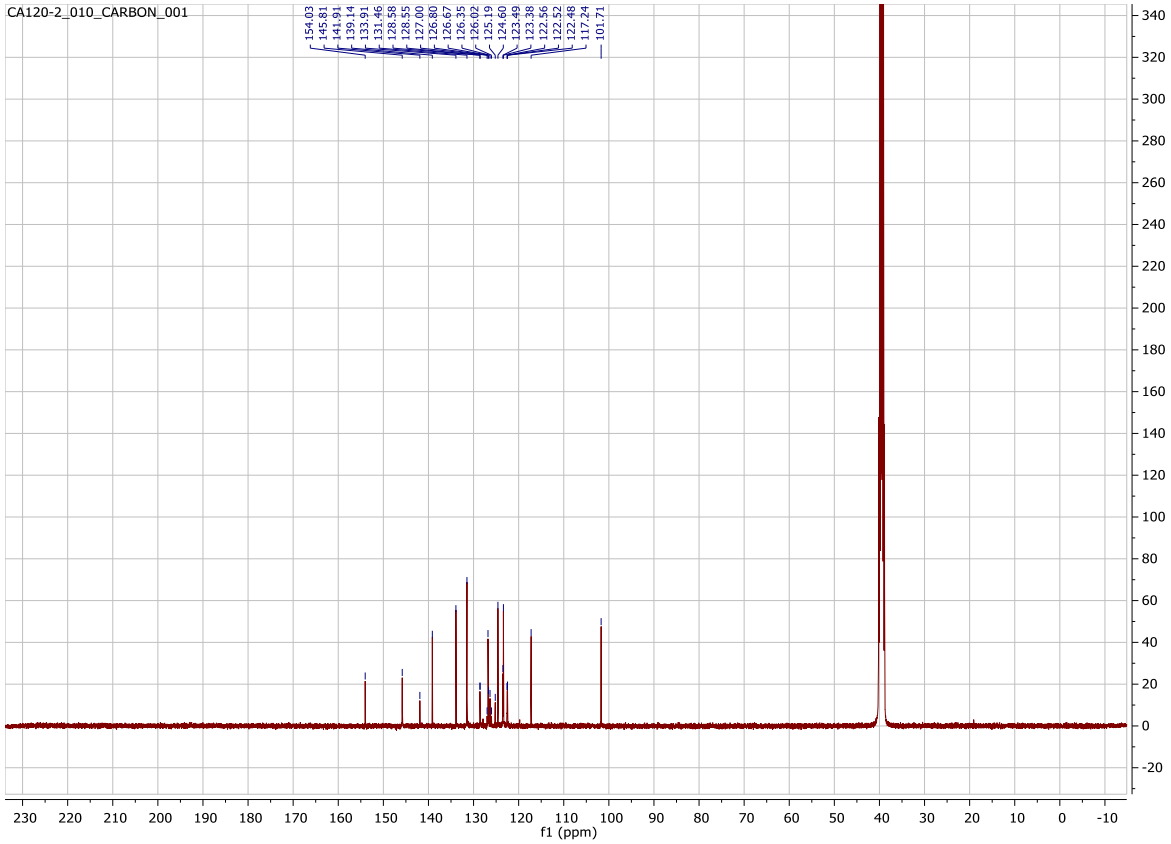
N-(3-Chlorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**25**)

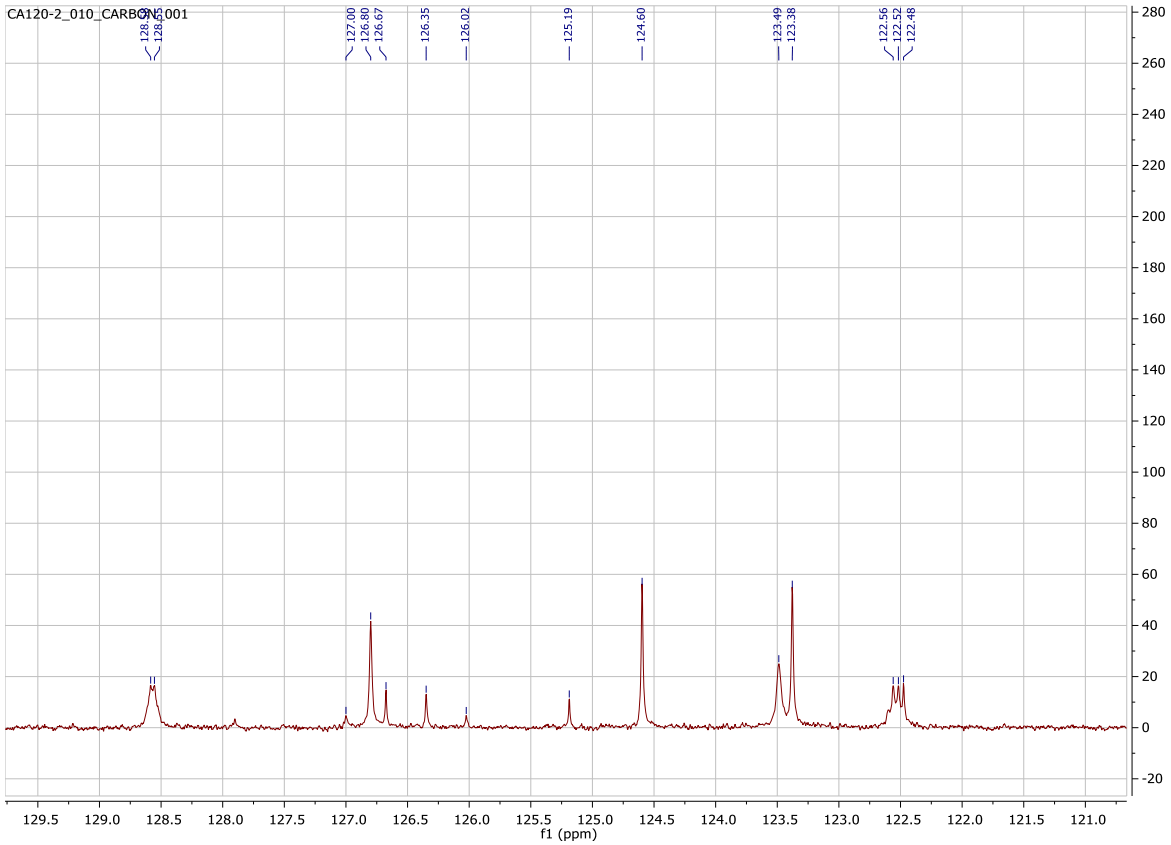


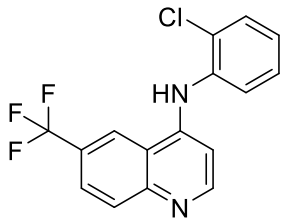



CA120_101_PROTON_001
11.40
8.63
8.62
8.32
8.30
8.26
8.24
7.61
7.58
7.56
7.50
7.48
7.46
7.45
6.99
6.97
0.70
0.99
1.00
1.99
0.97
1.03
1.97
0.98
f1 (ppm)


CA120_101_PROTON_001
8.63
8.62
8.32
8.30
8.26
8.24
7.61
7.58
7.56
7.50
7.48
7.46
7.45
6.99
6.97
0.99
1.00
1.99
0.97
1.03
1.97
0.98
f1 (ppm)

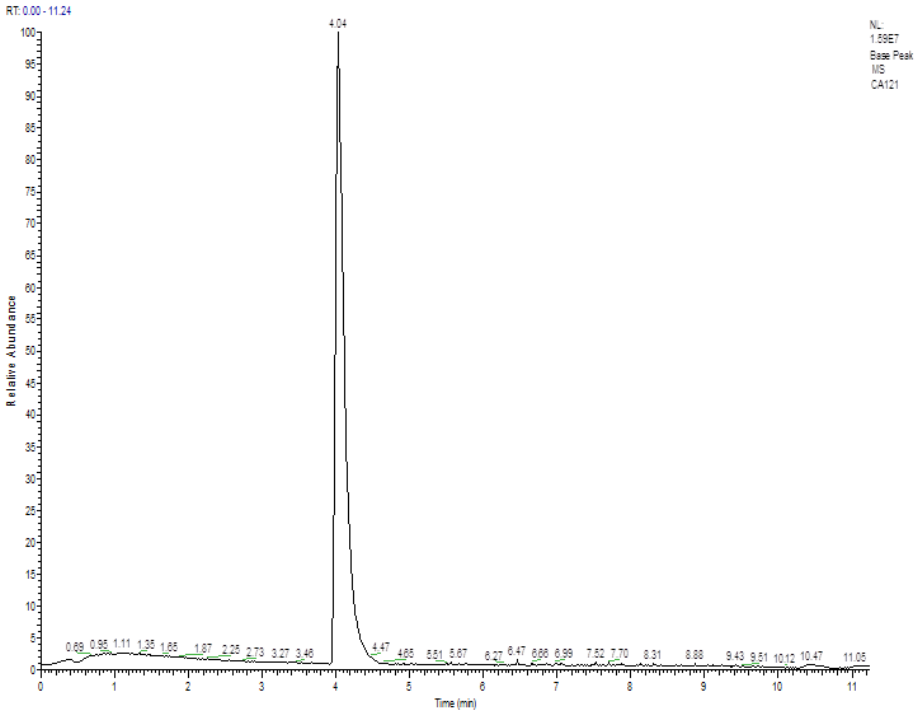

CA120-2_010_CARBON_001
154.03
145.81
141.91
139.14
133.91
131.46
128.58
128.55
127.00
126.80
126.67
126.35
126.02
125.19
124.60
123.49
123.38
122.56
122.52
122.48
117.24
101.71
f1 (ppm)

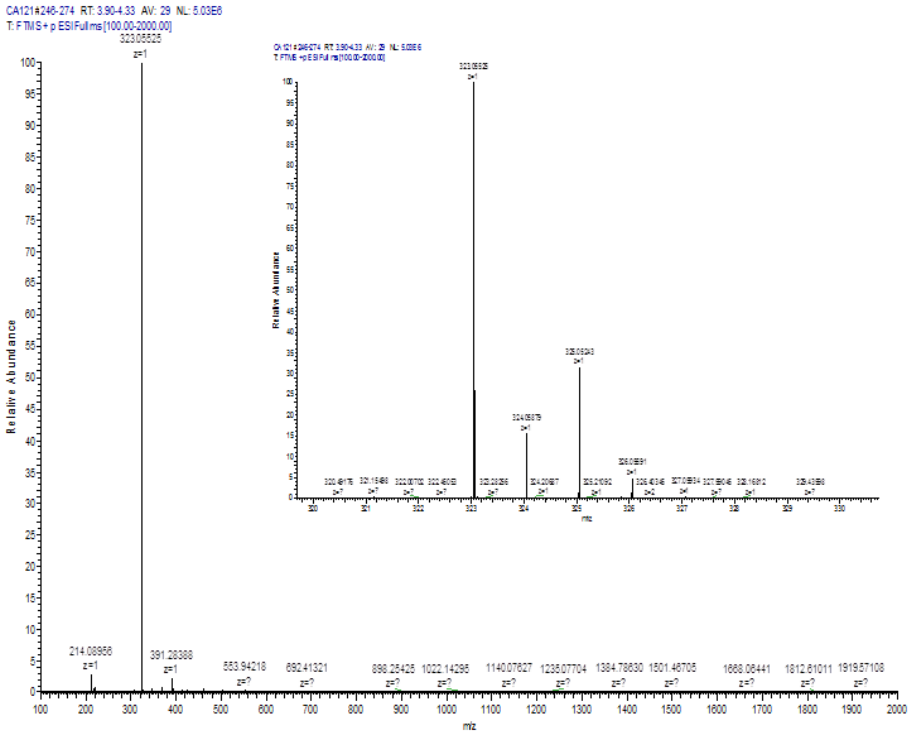

CA120-2_010_CARBON_001
128.58
128.55
127.00
126.80
126.67
126.35
126.02
125.19
124.60
123.49
123.38
122.56
122.52
122.48
f1 (ppm)

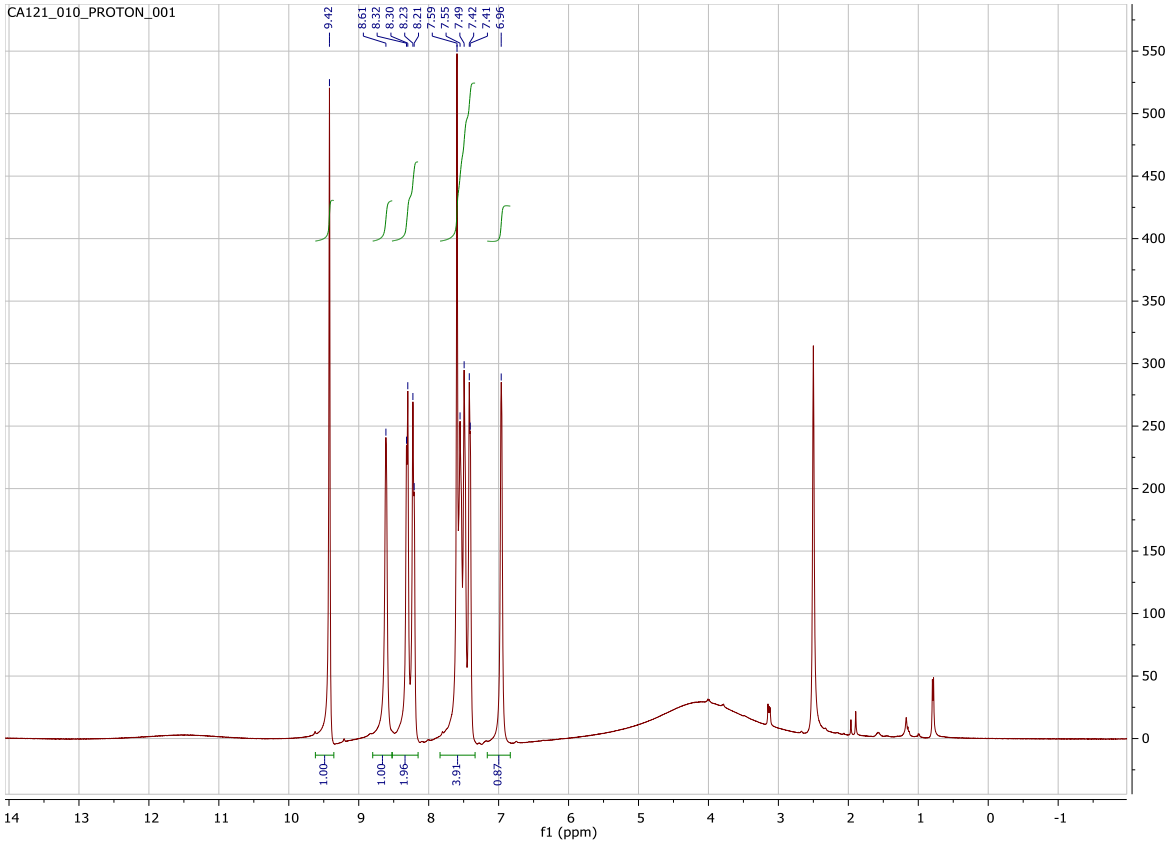


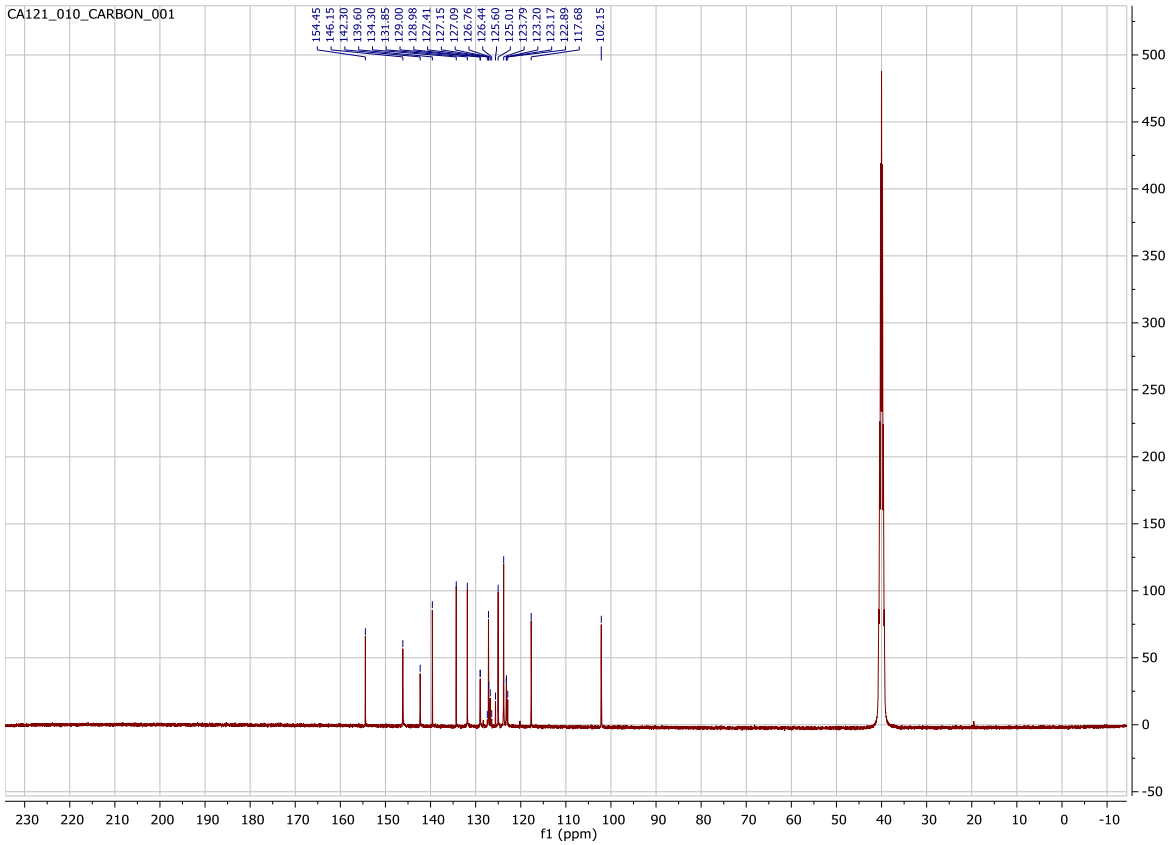
26

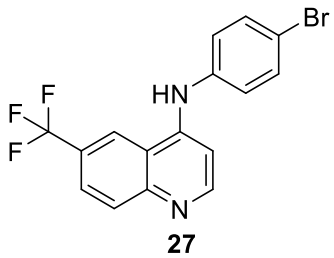
N-(2-Chlorophenyl)-6-(trifluoromethyl)quinolin-4-amine (**26**)





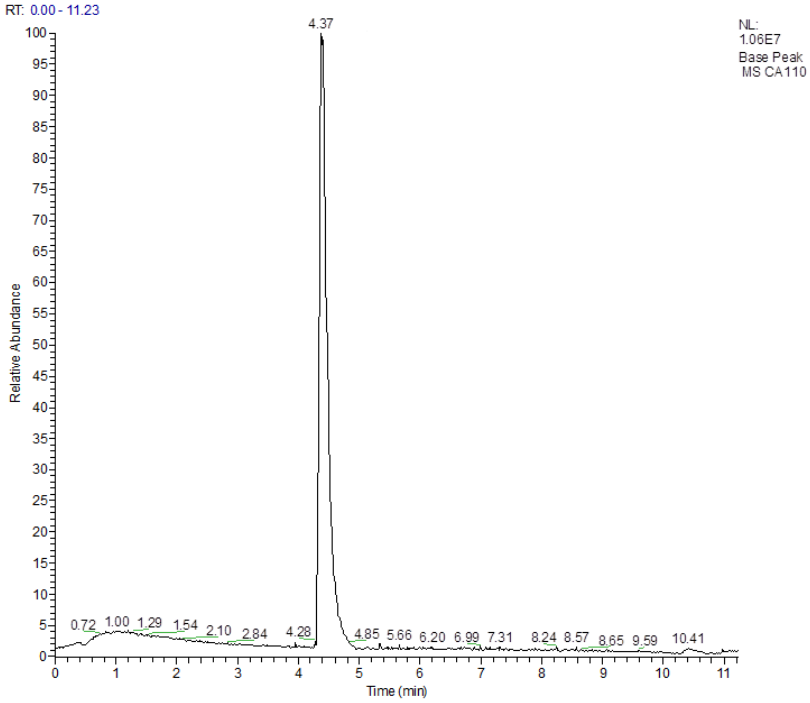

CA121_010_PROTON_001
9.42
8.61
8.32
8.30
8.23
8.21
7.59
7.55
7.49
7.42
7.41
6.96
1.00
1.00
1.96
3.91
0.87
f1 (ppm)

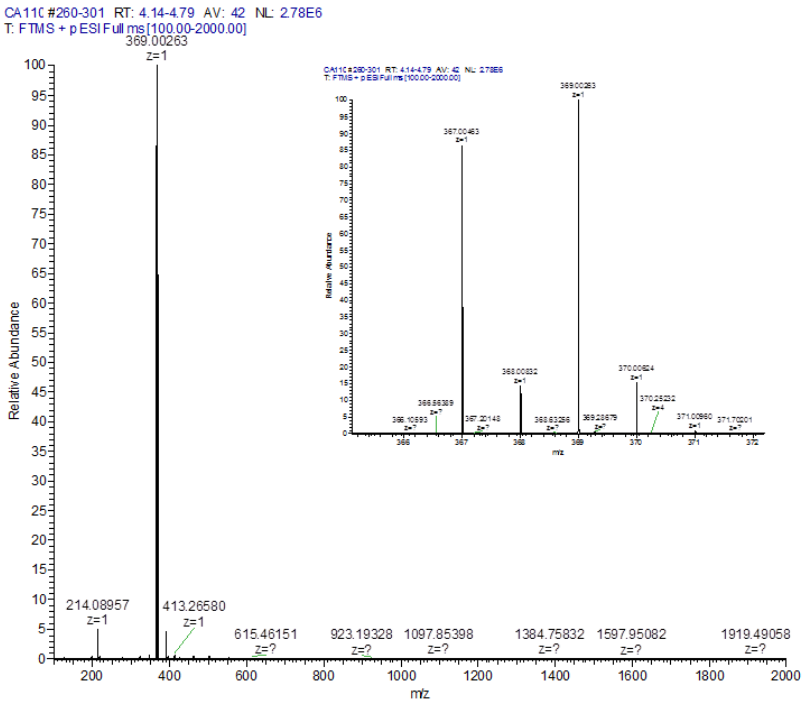

CA121_010_CARBON_001
154.45
146.15
142.30
139.60
134.30
131.85
129.00
128.98
127.41
127.15
127.09
126.76
126.44
125.60
125.01
123.79
123.20
123.17
122.89
117.68
102.15
f1 (ppm)

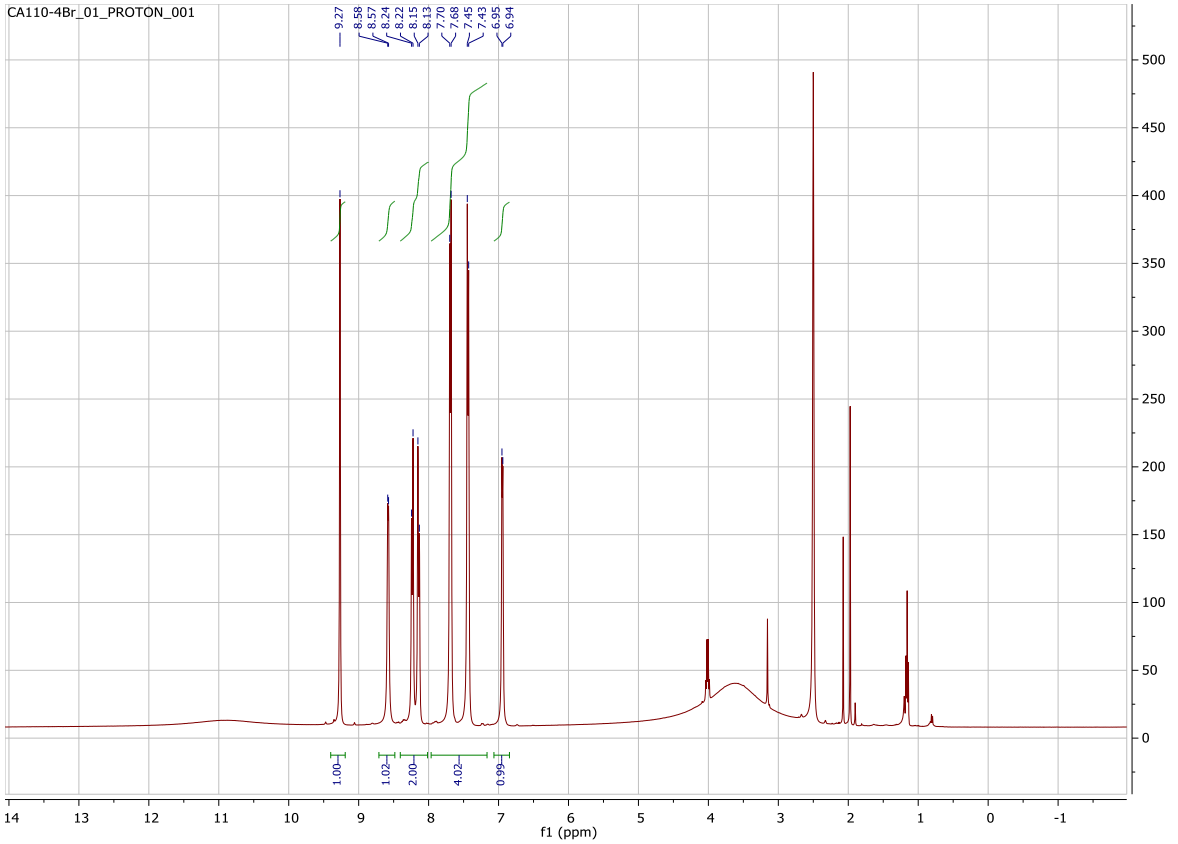


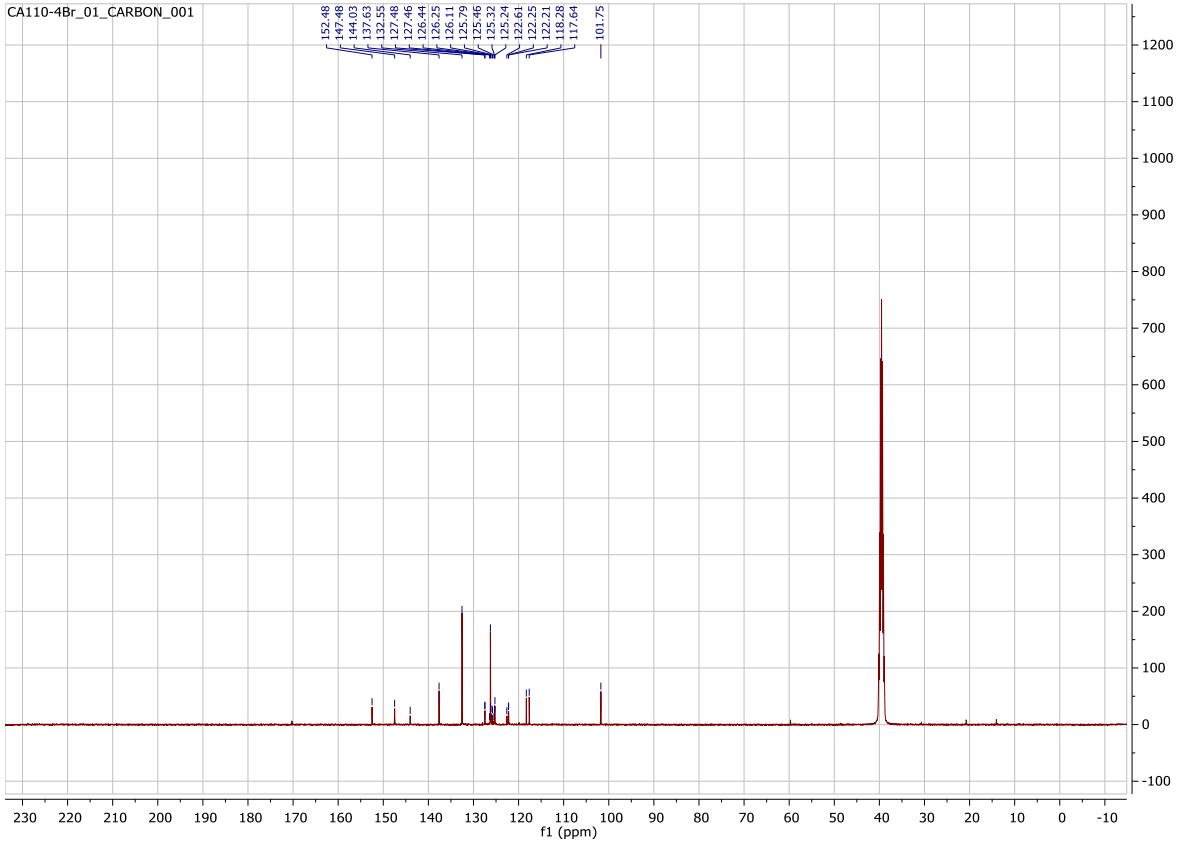
27

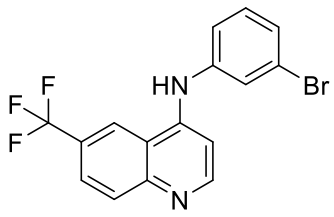
N-(4-Bromophenyl)-6-(trifluoromethyl)quinolin-4-amine (**27**)





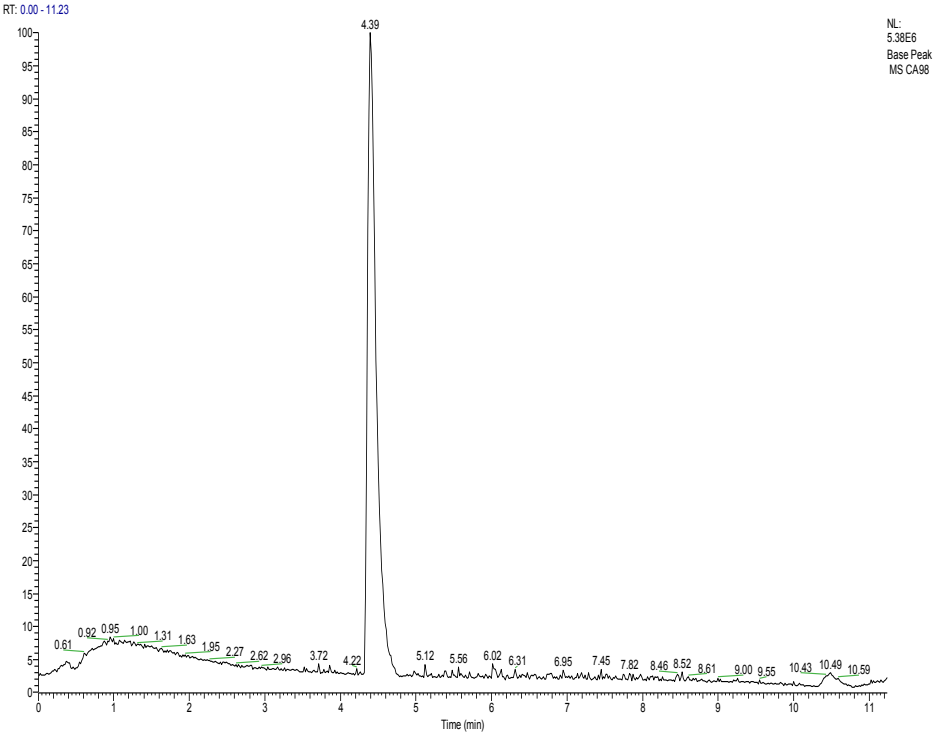

CA110-4Br_01_PROTON_001
9.27
8.58
8.57
8.24
8.22
8.15
8.13
7.70
7.68
7.45
7.43
6.95
6.94
1.00
1.02
2.00
4.02
0.99
f1 (ppm)

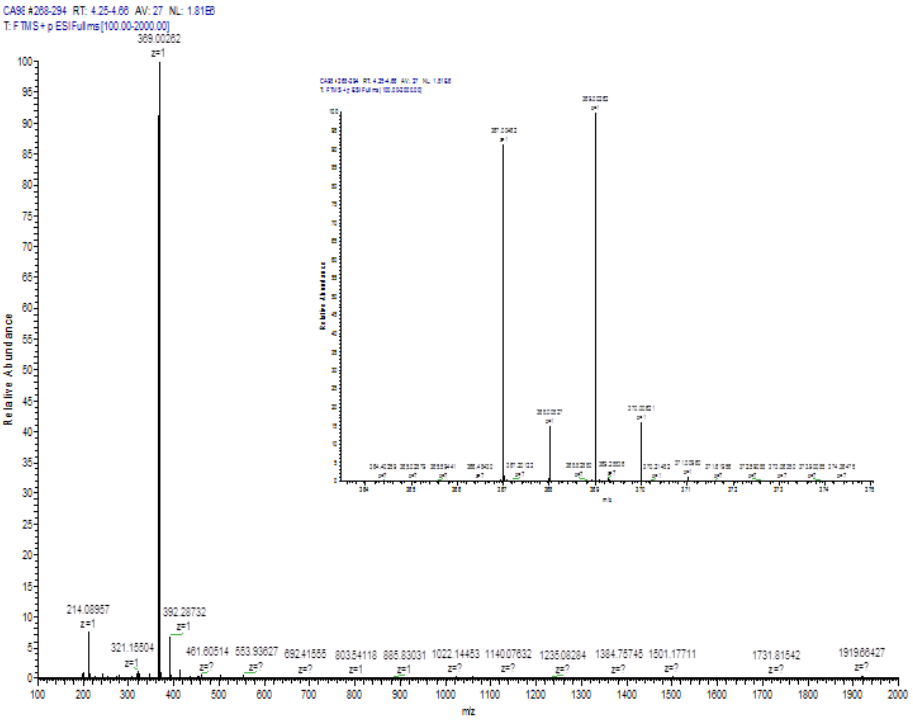

CA110-4Br_01_CARBON_001
152.48
147.48
144.03
137.63
132.55
127.48
127.46
126.44
126.25
126.11
125.79
125.46
125.32
125.24
122.61
122.25
122.21
118.28
117.64
101.75
f1 (ppm)

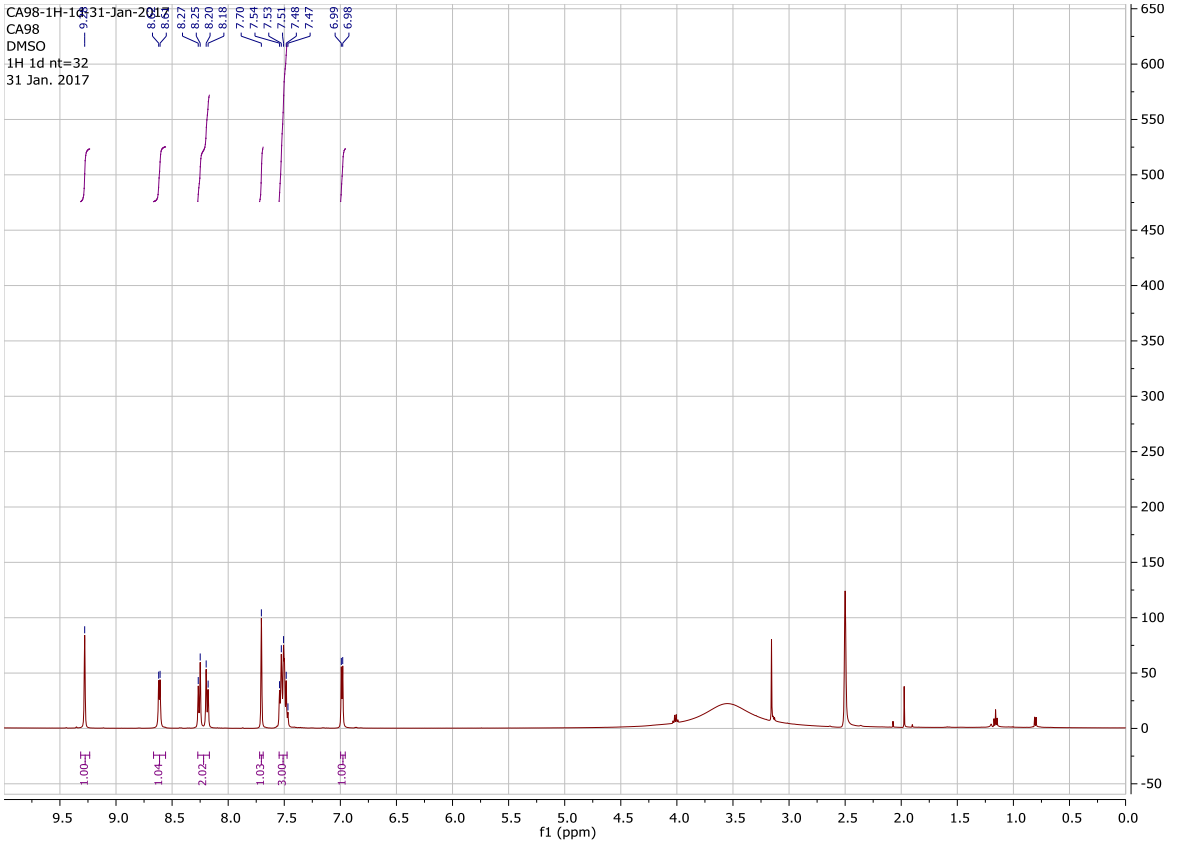


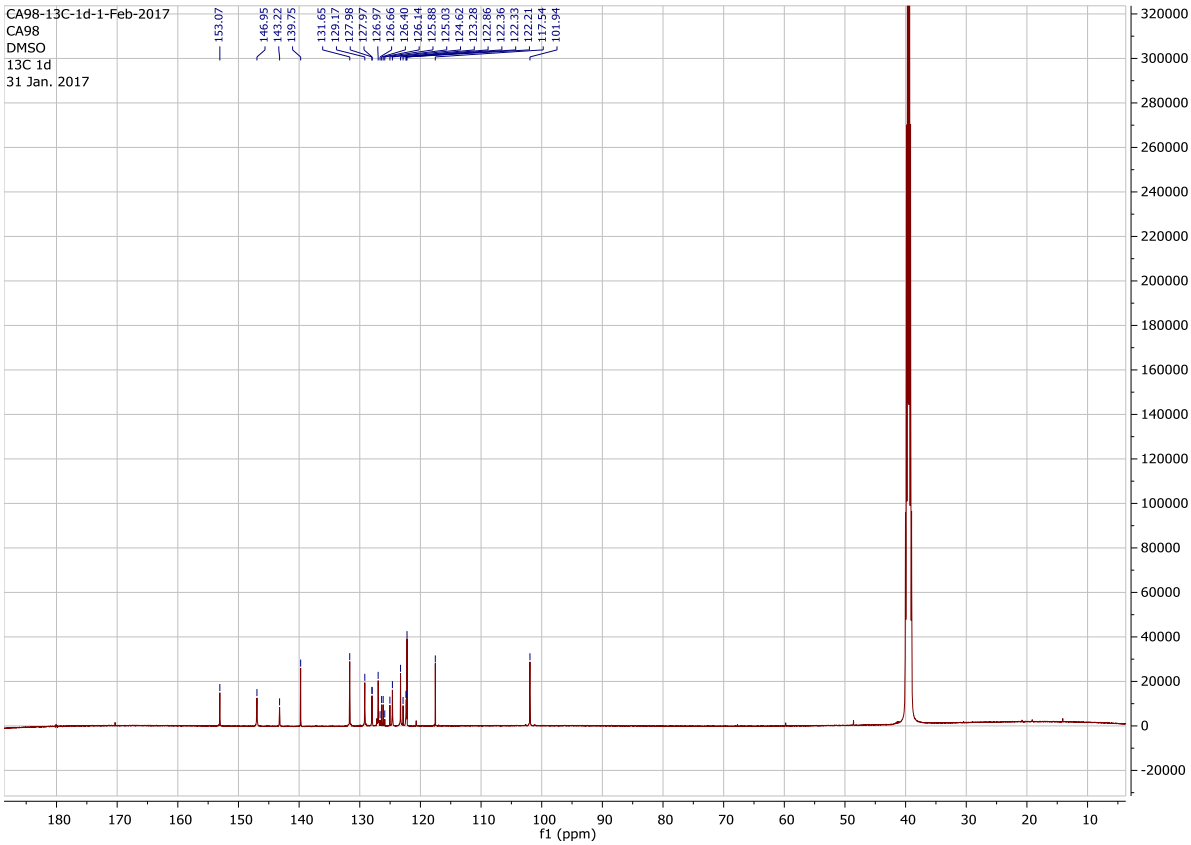
28

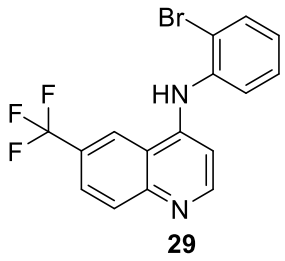
N-(3-Bromophenyl)-6-(trifluoromethyl)quinolin-4-amine (**28**)





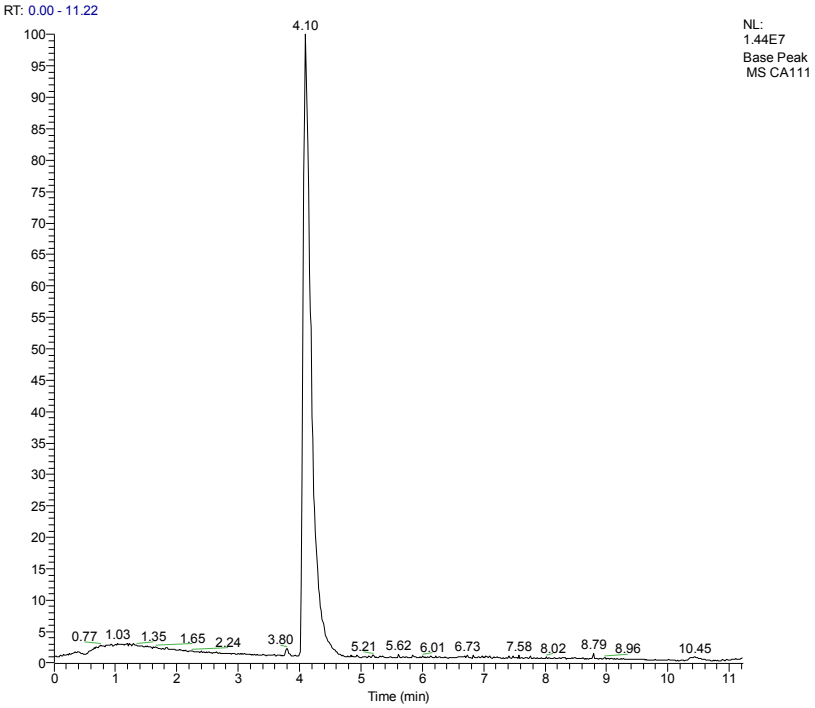

CA98-1H-1d-31-Jan-2017
CA98
DMSO
1H 1d nt=32
31 Jan. 2017
9.13
8.62
8.27
8.25
8.20
8.18
7.70
7.54
7.53
7.51
7.48
7.47
6.99
6.98
1.00
1.04
2.02
1.03
3.00
1.00
f1 (ppm)

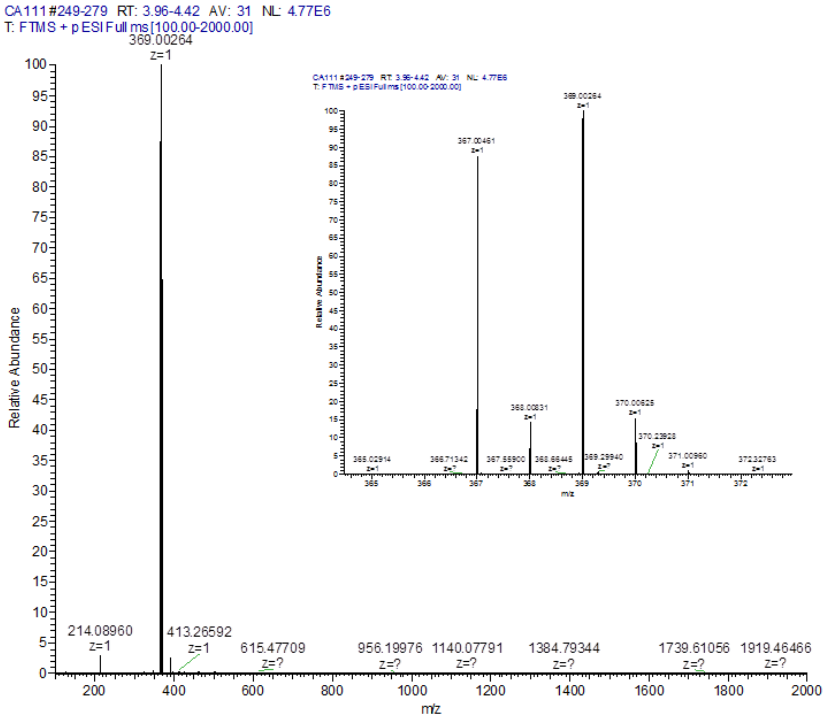

CA98-13C-1d-1-Feb-2017
CA98
DMSO
13C 1d
31 Jan. 2017
153.07
146.95
143.22
139.75
131.65
129.17
127.98
127.97
126.97
126.66
126.40
126.14
125.88
125.03
124.62
123.28
122.86
122.36
122.33
122.21
117.54
101.94
f1 (ppm)

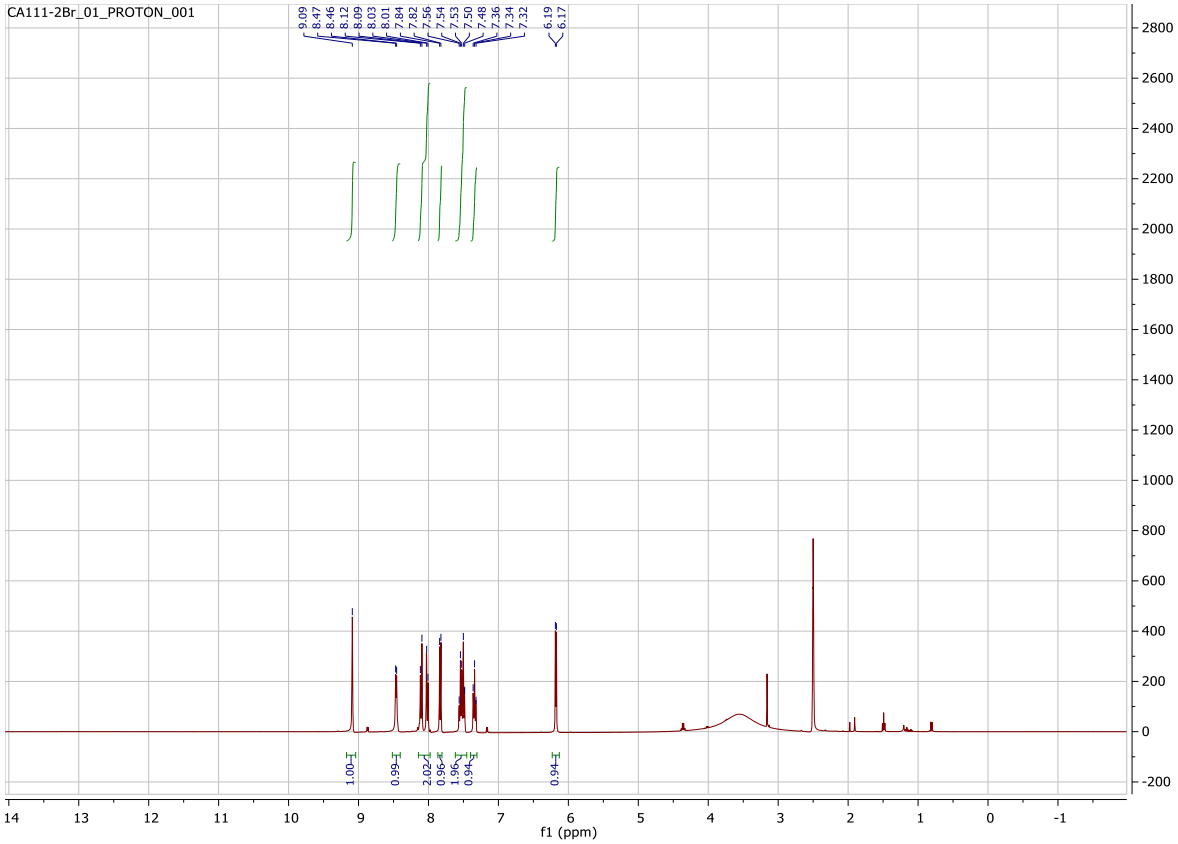


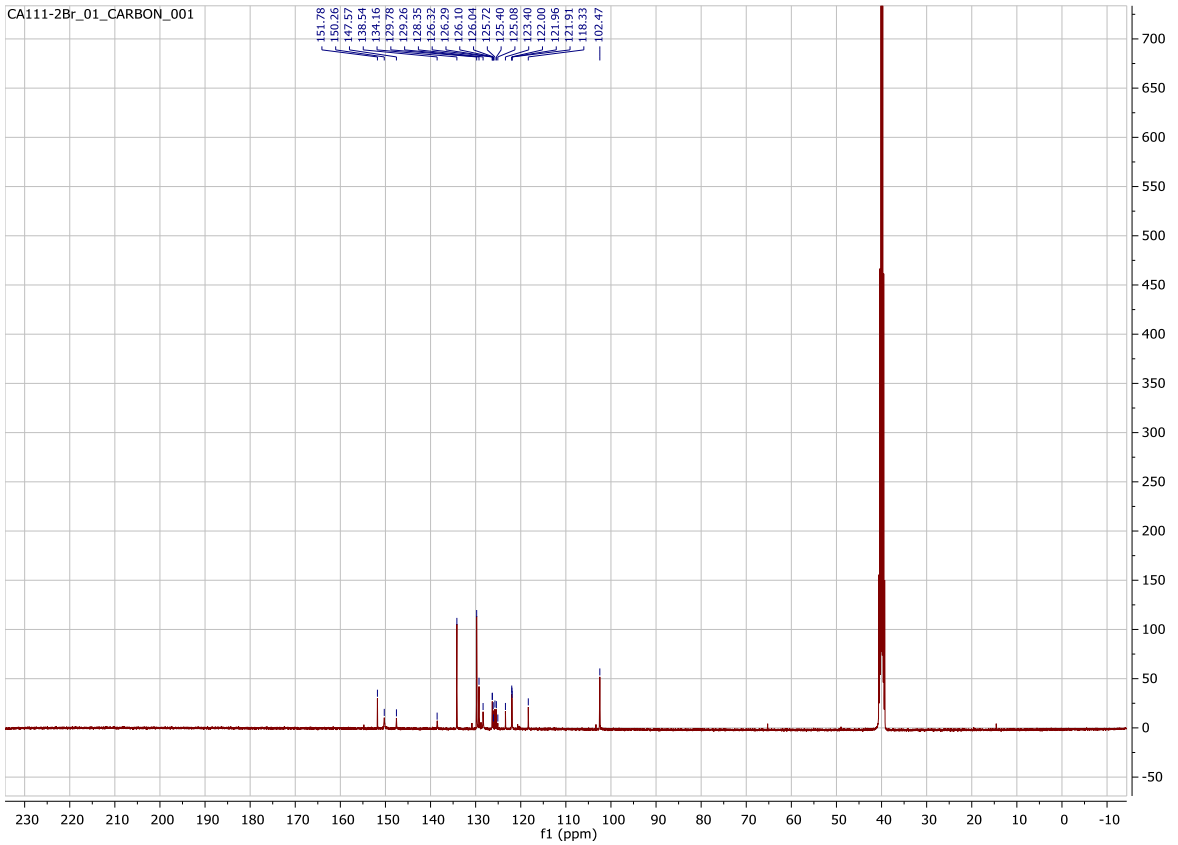
29

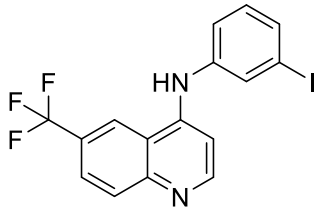
N-(2-Bromophenyl)-6-(trifluoromethyl)quinolin-4-amine (**29**)





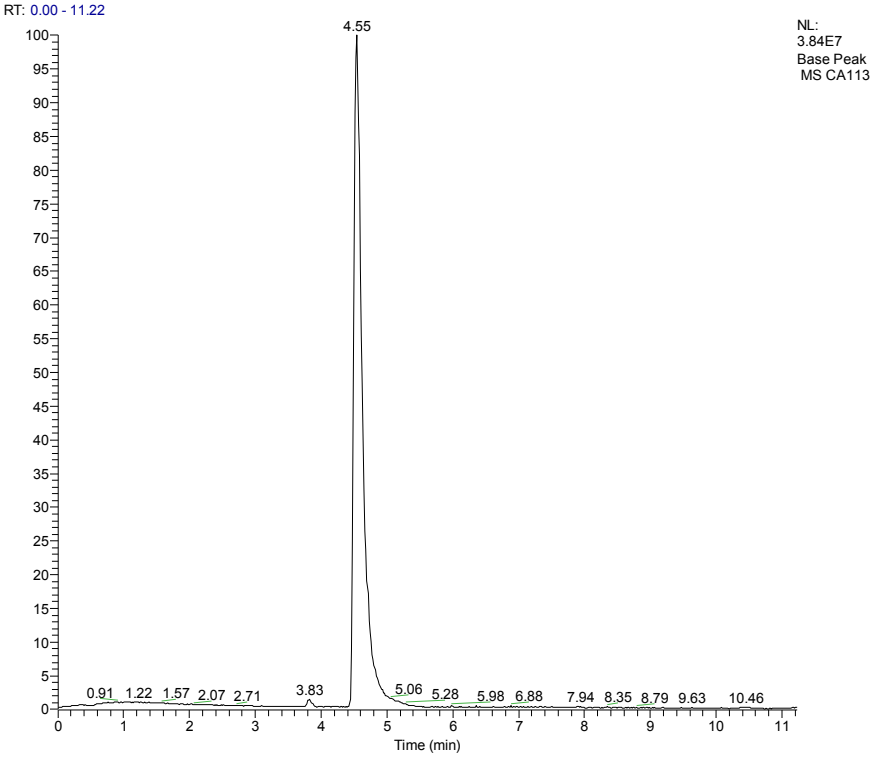

CA111-2Br_01_PROTON_001
9.09
8.47
8.46
8.12
8.09
8.03
8.01
7.84
7.82
7.56
7.54
7.53
7.50
7.48
7.36
7.34
7.32
6.19
6.17
1.00
0.99
2.02
0.96
1.96
0.94
0.94
f1 (ppm)

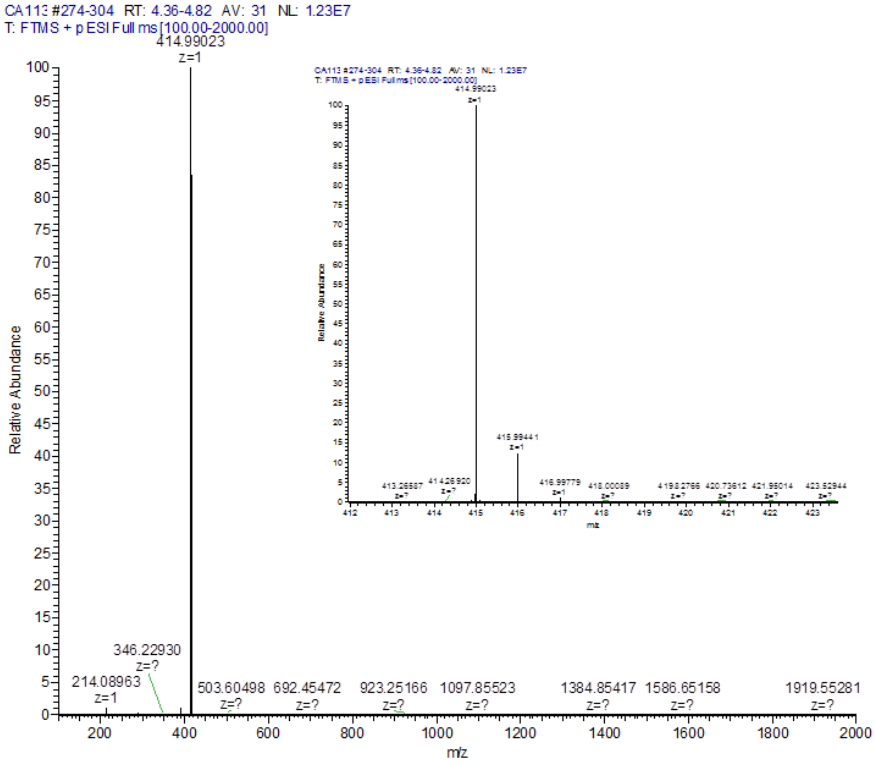

CA111-2Br_01_CARBON_001
151.78
150.26
147.57
138.54
134.16
129.78
129.26
128.35
126.32
126.29
126.10
126.04
125.72
125.40
125.08
123.40
122.00
121.96
121.91
118.33
102.47
f1 (ppm)

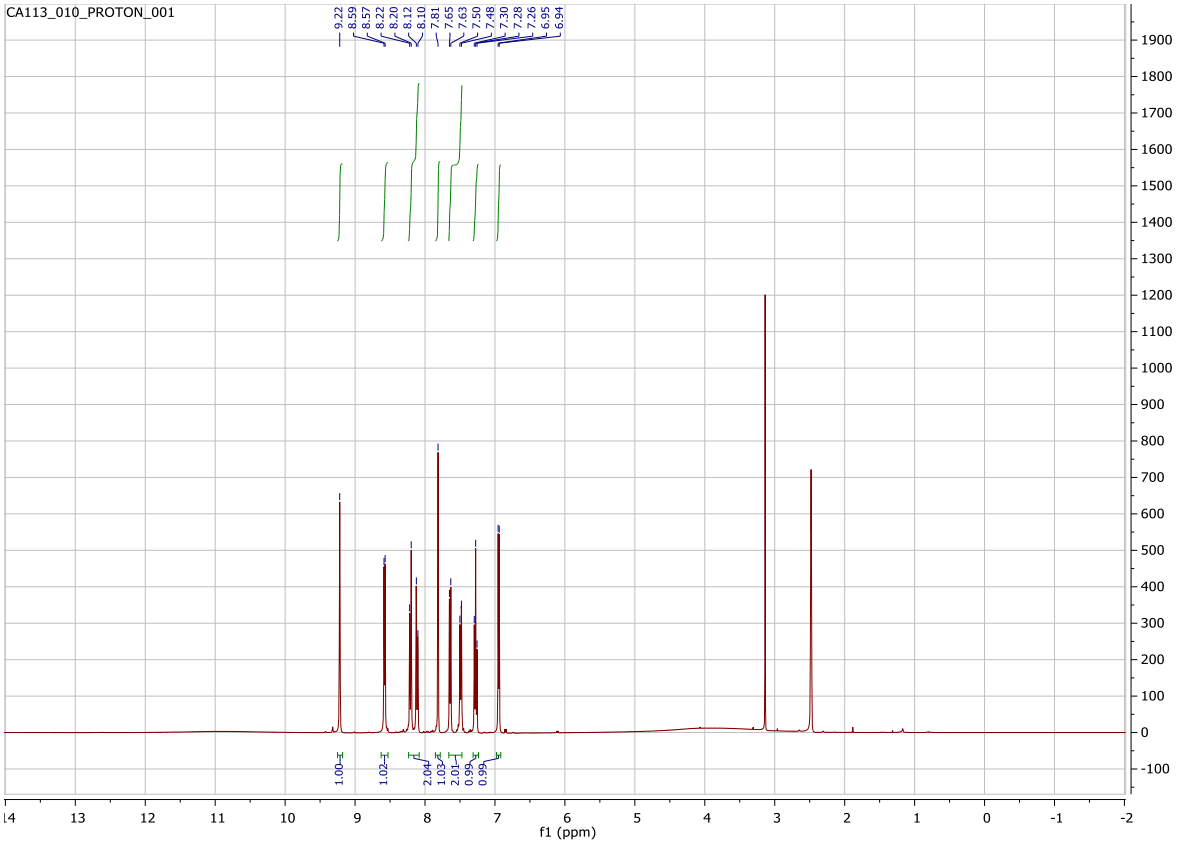


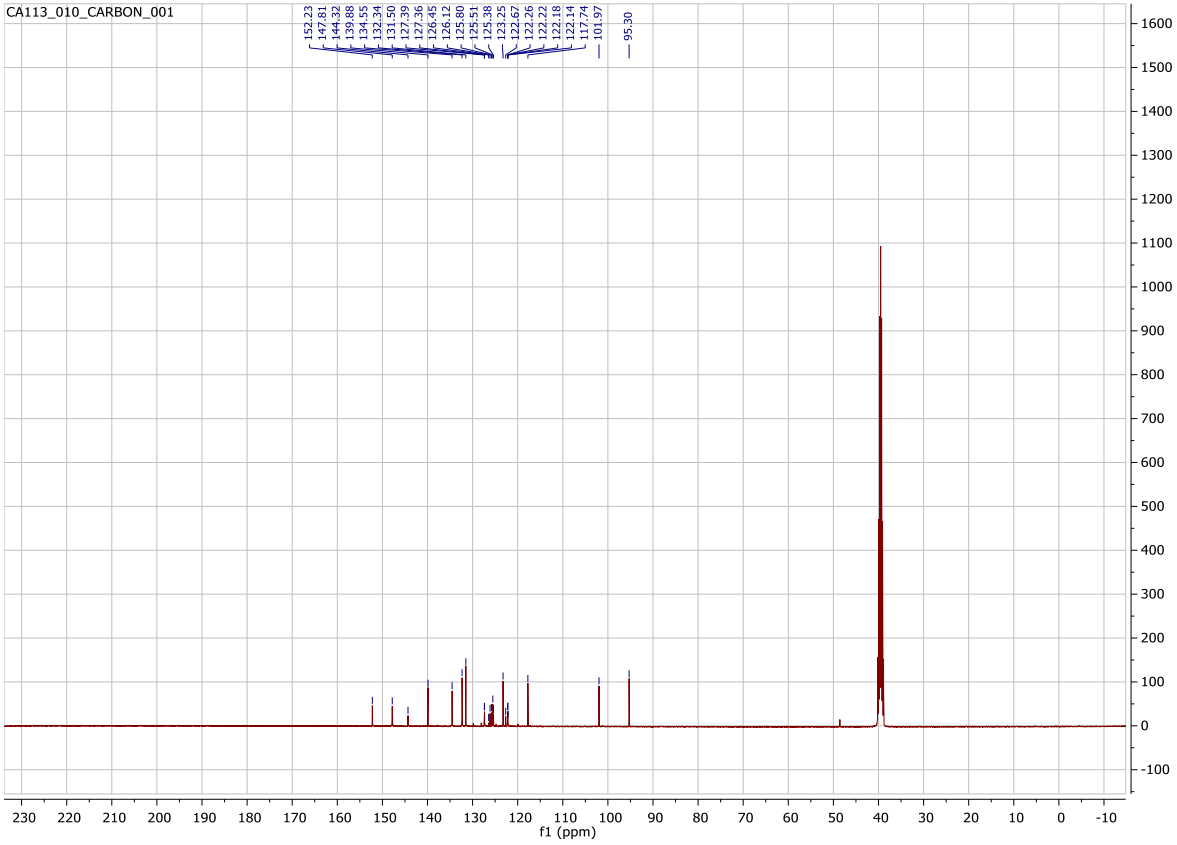
30

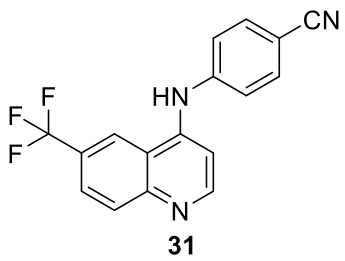
N-(3-Iodophenyl)-6-(trifluoromethyl)quinolin-4-amine (**30**)





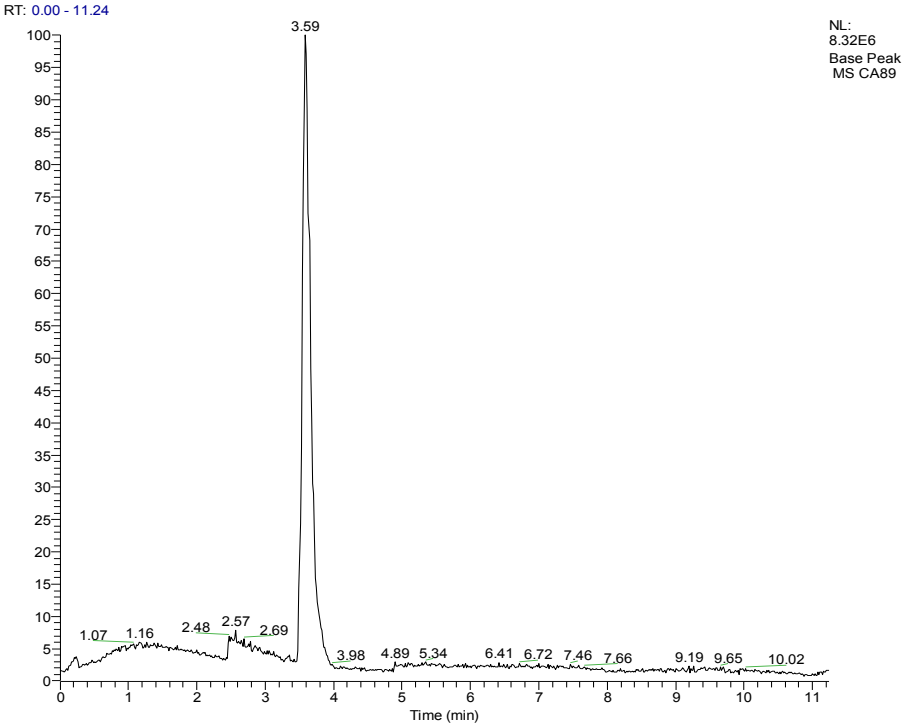

CA113_010_PROTON_001
9.22
8.59
8.57
8.22
8.20
8.12
8.10
7.81
7.65
7.63
7.50
7.48
7.30
7.28
7.26
6.95
6.94
1.00
1.02
2.04
1.03
2.01
0.99
0.99
f1 (ppm)

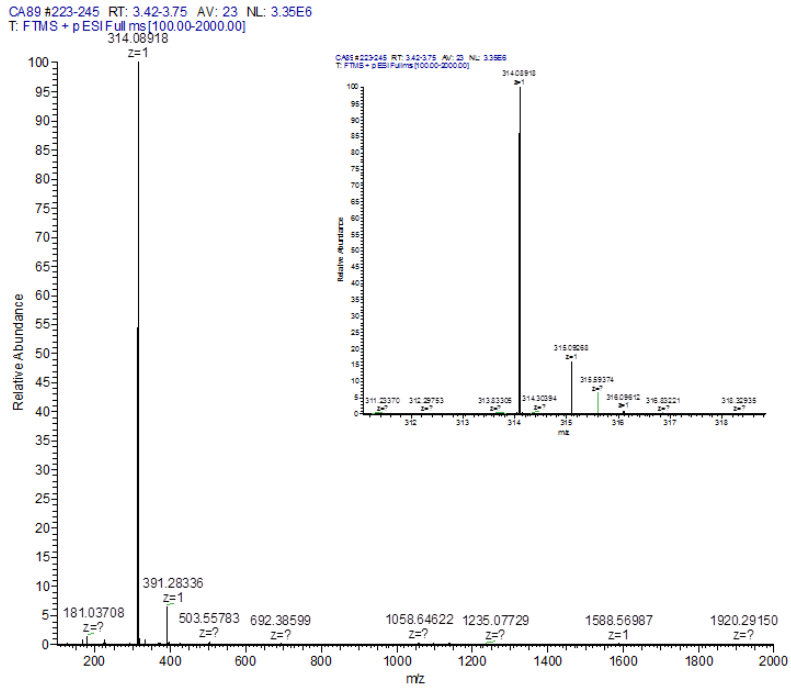

CA113_010_CARBON_001
152.23
147.81
144.32
139.88
134.55
132.34
131.50
127.39
127.36
126.45
126.12
125.80
125.51
125.38
123.25
122.67
122.26
122.22
122.18
122.14
117.74
101.97
95.30
f1 (ppm)

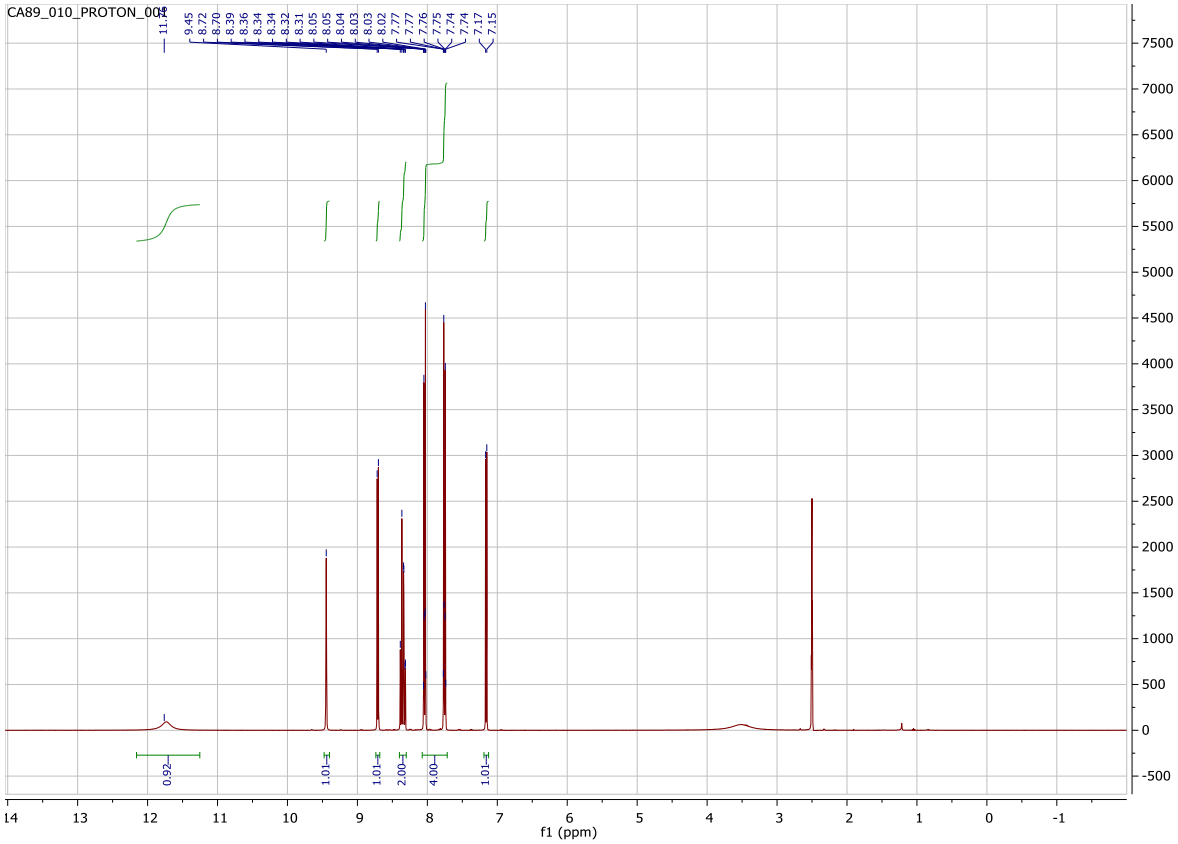


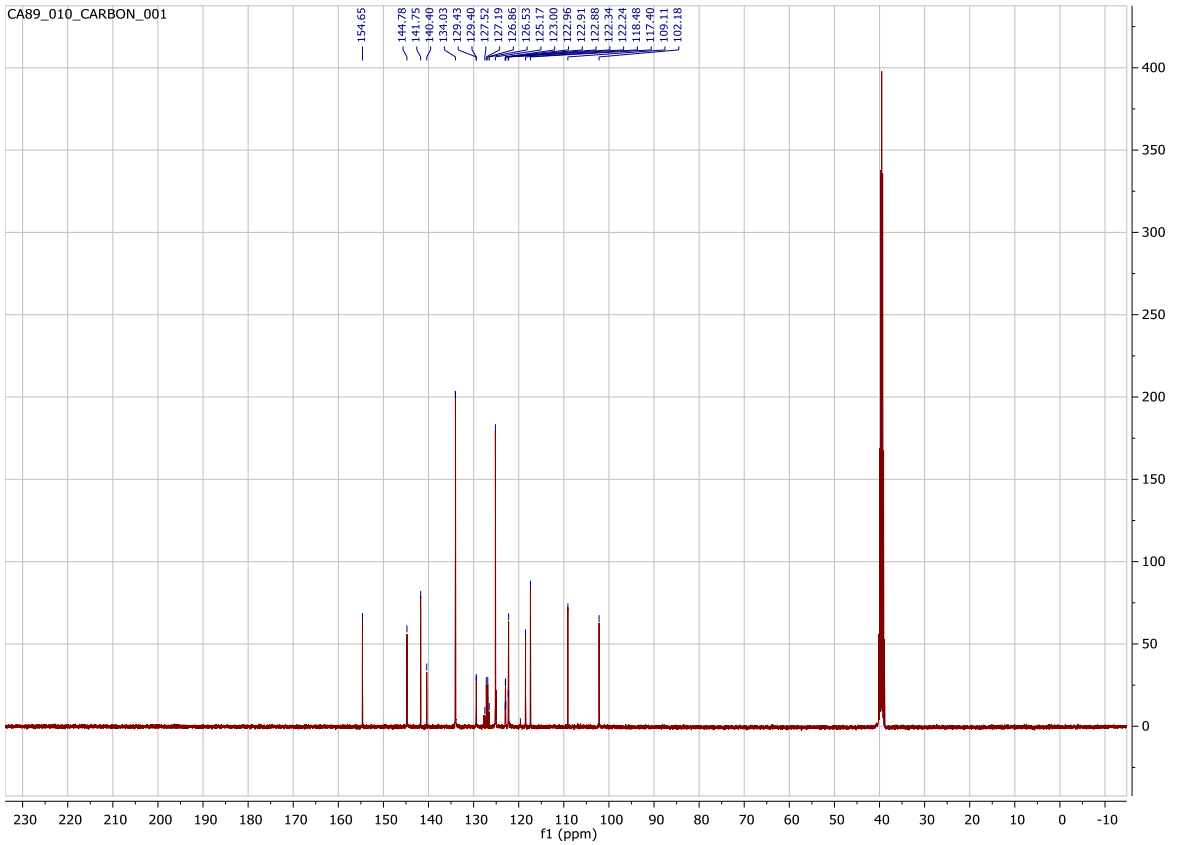
31

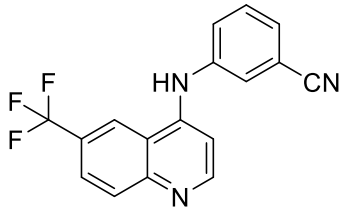
4-((6-(Trifluoromethyl)quinolin-4-yl)amino)benzonitrile (**31**)





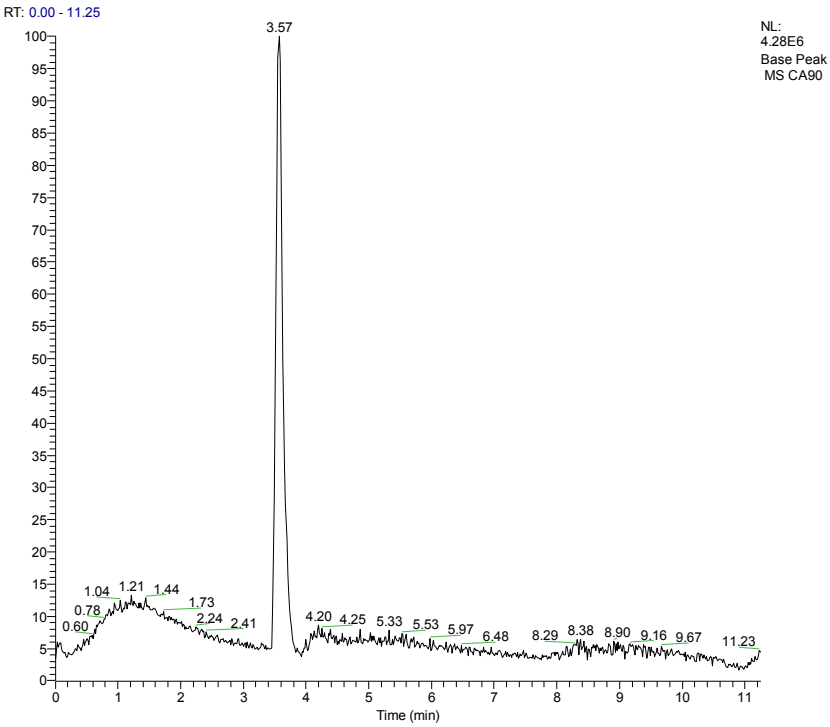

CA89_010_PROTON_001
11.14
9.45
8.72
8.70
8.39
8.36
8.34
8.34
8.32
8.31
8.05
8.05
8.04
8.03
8.03
8.02
7.77
7.77
7.76
7.75
7.74
7.74
7.17
7.15
0.92
1.01
1.01
2.00
4.00
1.01
f1 (ppm)

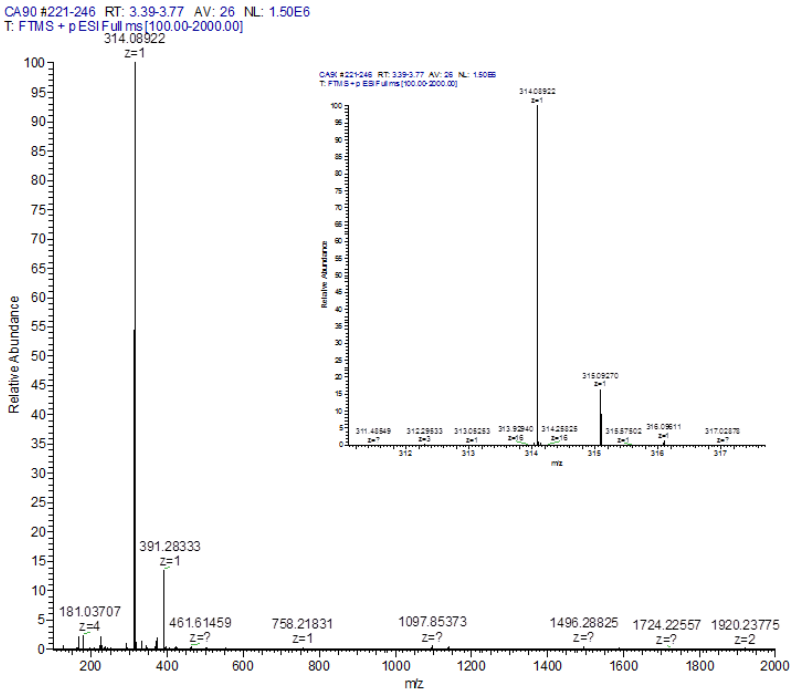

CA89_010_CARBON_001
154.65
144.78
141.75
140.40
134.03
129.43
128.40
127.52
127.19
126.86
126.53
125.17
123.00
122.96
122.91
122.88
122.34
122.24
118.48
117.40
109.11
102.18
f1 (ppm)

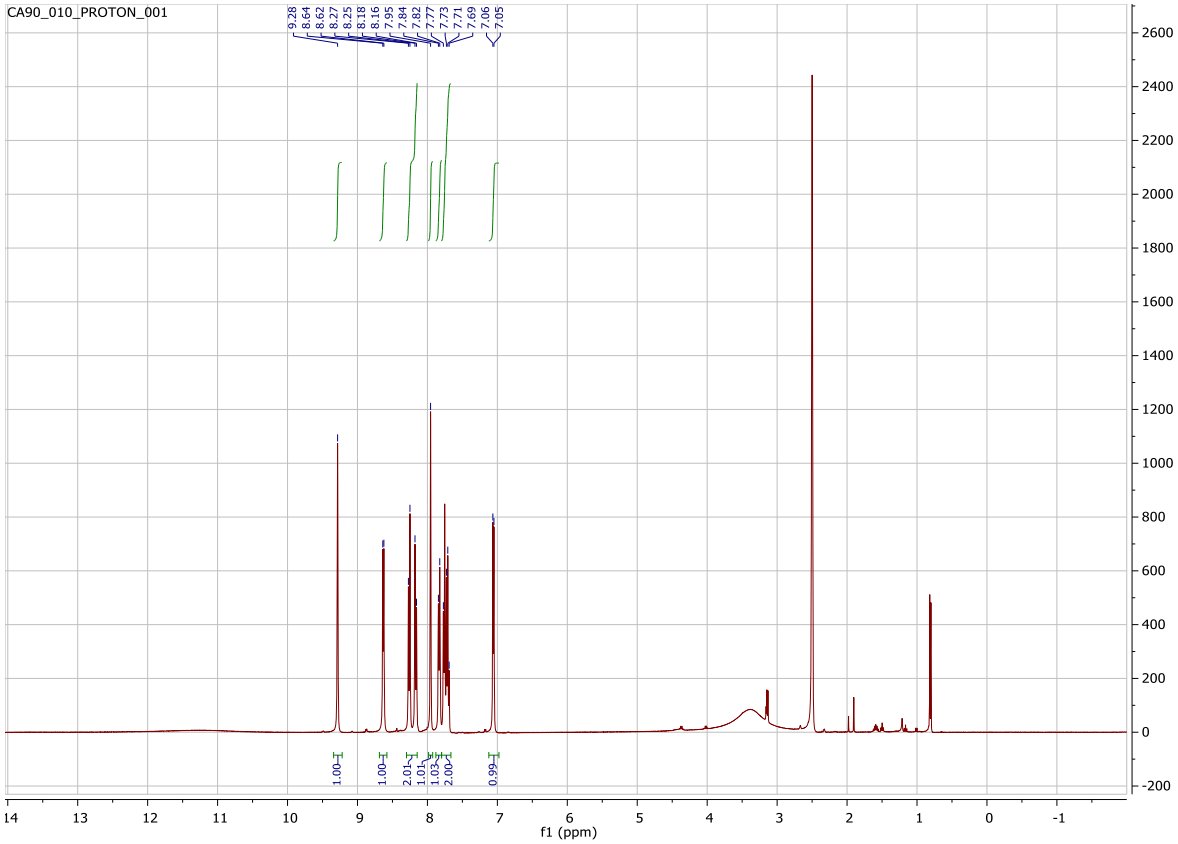


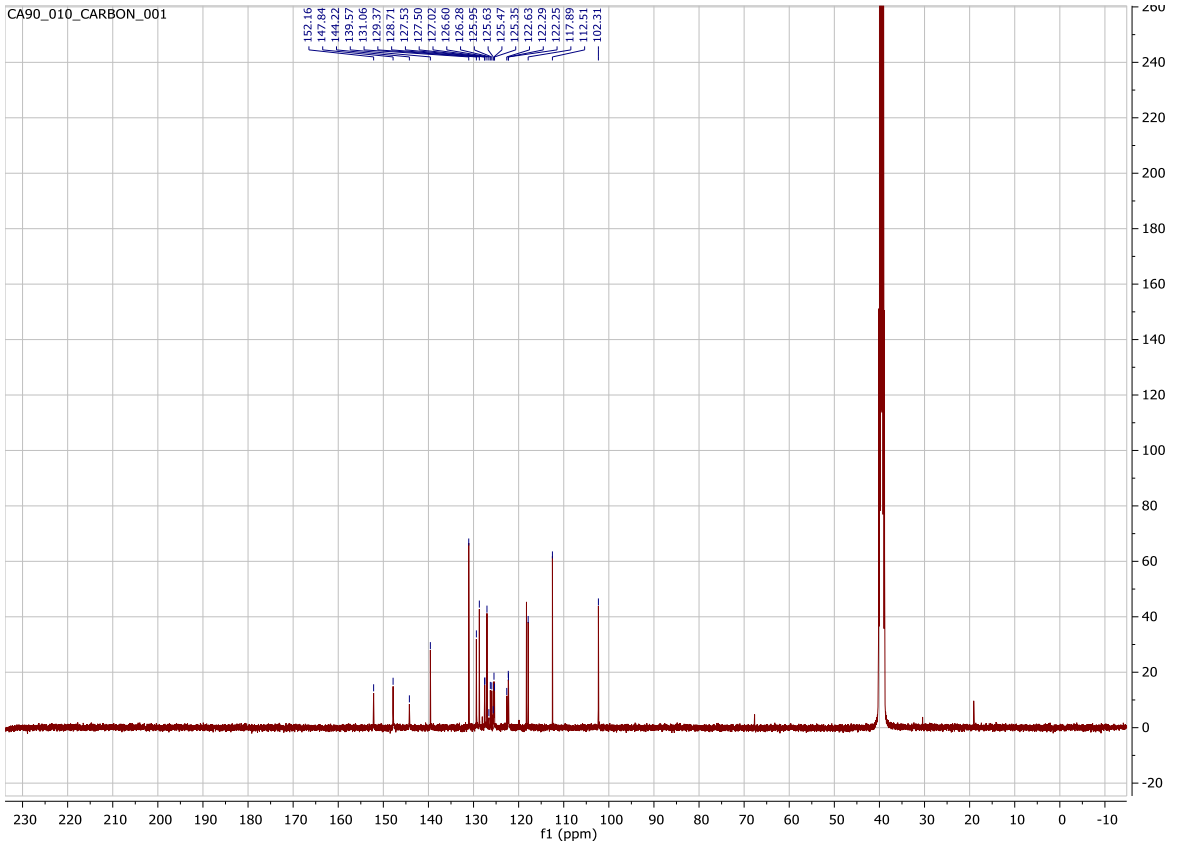
32

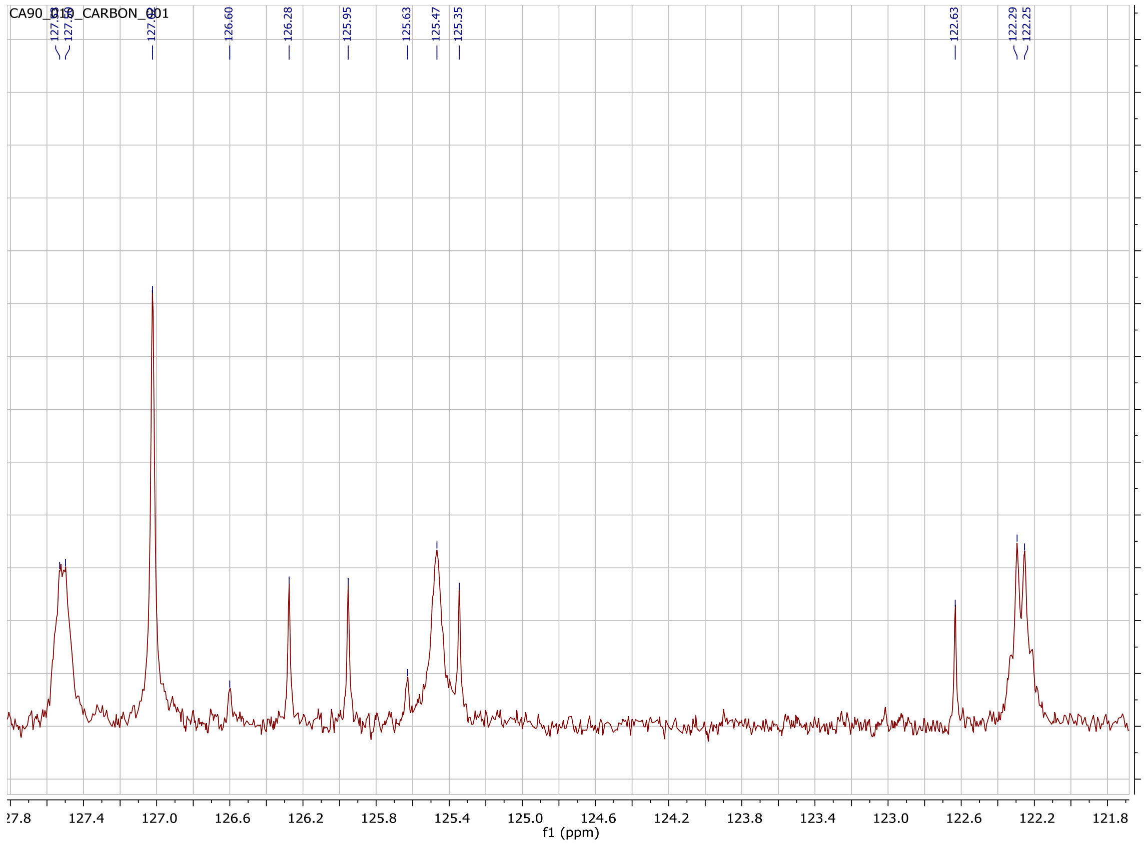
3-((6-(Trifluoromethyl)quinolin-4-yl)amino)benzonitrile (**32**)

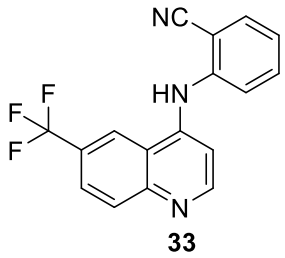





CA90_010_PROTON_001
9.28
8.64
8.62
8.27
8.25
8.18
8.16
7.95
7.84
7.82
7.77
7.73
7.71
7.69
7.06
7.05
1.00
1.00
2.01
1.01
1.03
2.00
0.99
f1 (ppm)

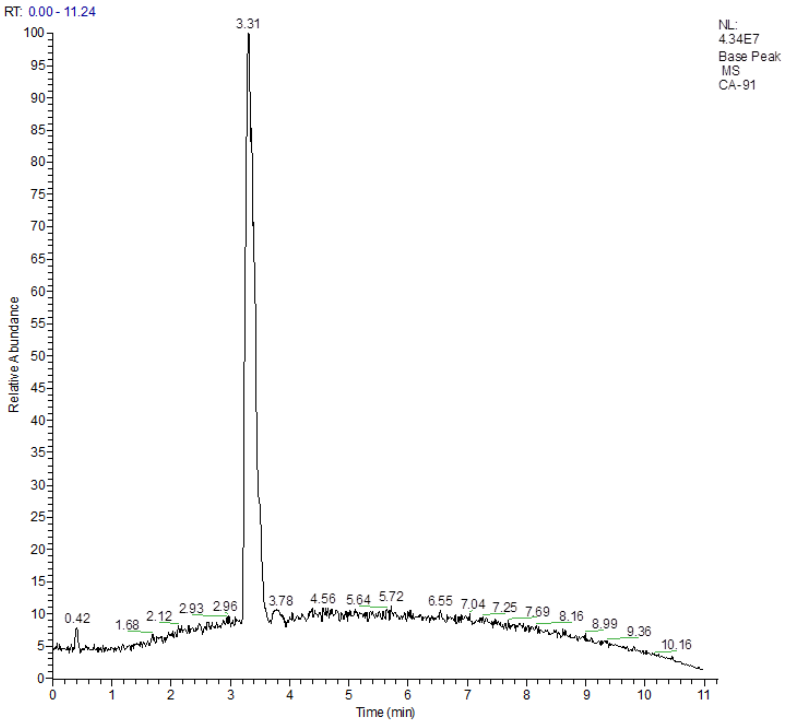

CA90_010_CARBON_001
152.16
147.84
144.22
139.57
131.06
129.37
128.71
127.53
127.50
127.02
126.60
126.28
125.95
125.63
125.47
125.35
122.63
122.29
122.25
117.89
112.51
102.31
f1 (ppm)

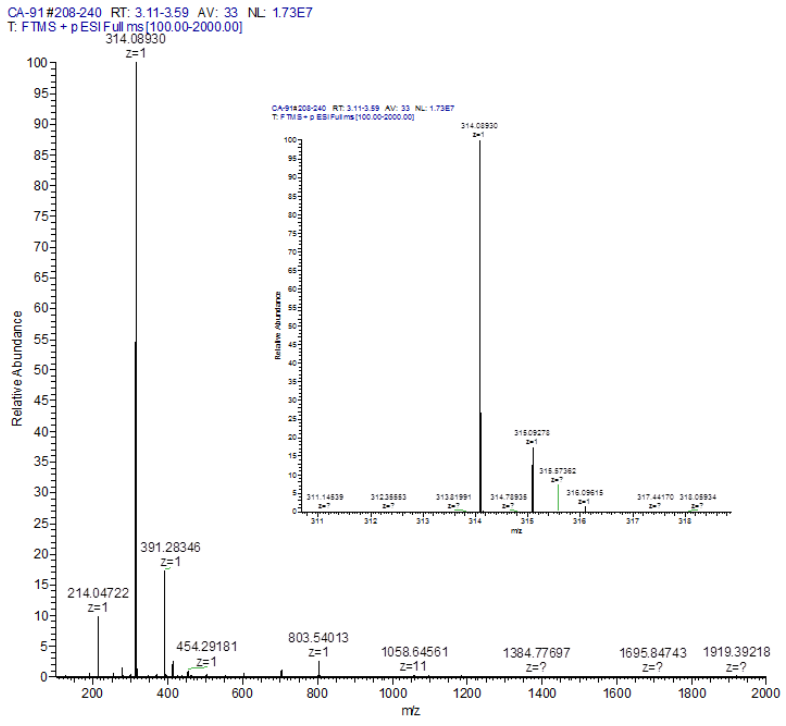

CA90_019_CARBON_001
126.60
126.28
125.95
125.63
125.47
125.35
122.63
122.29
122.25
f1 (ppm)

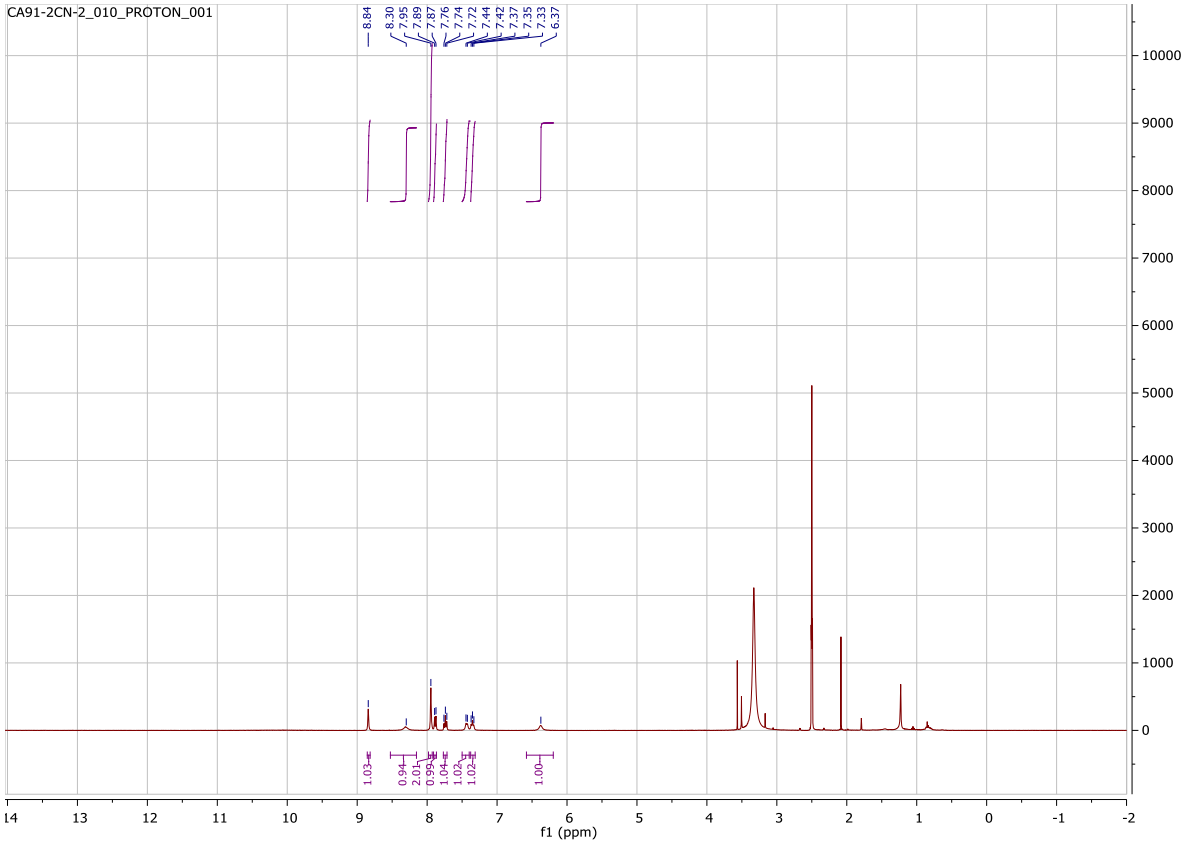


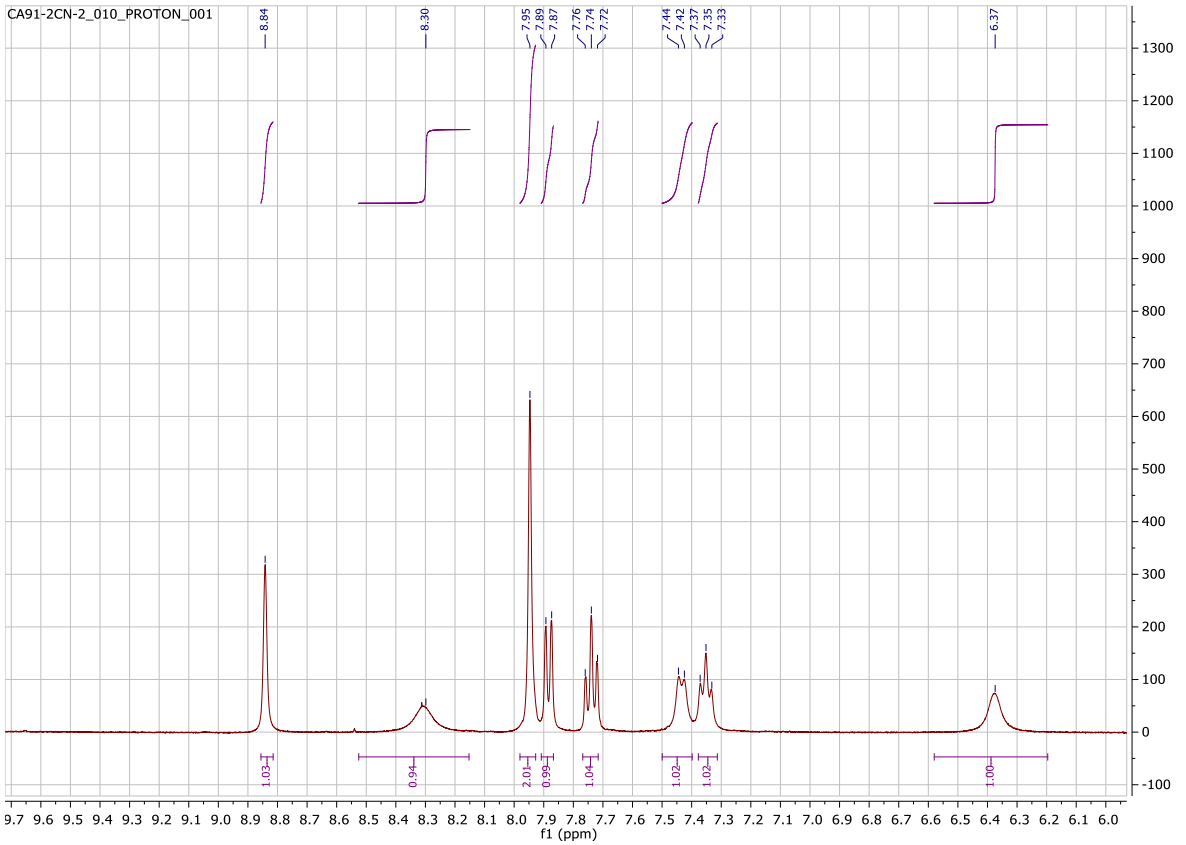
33

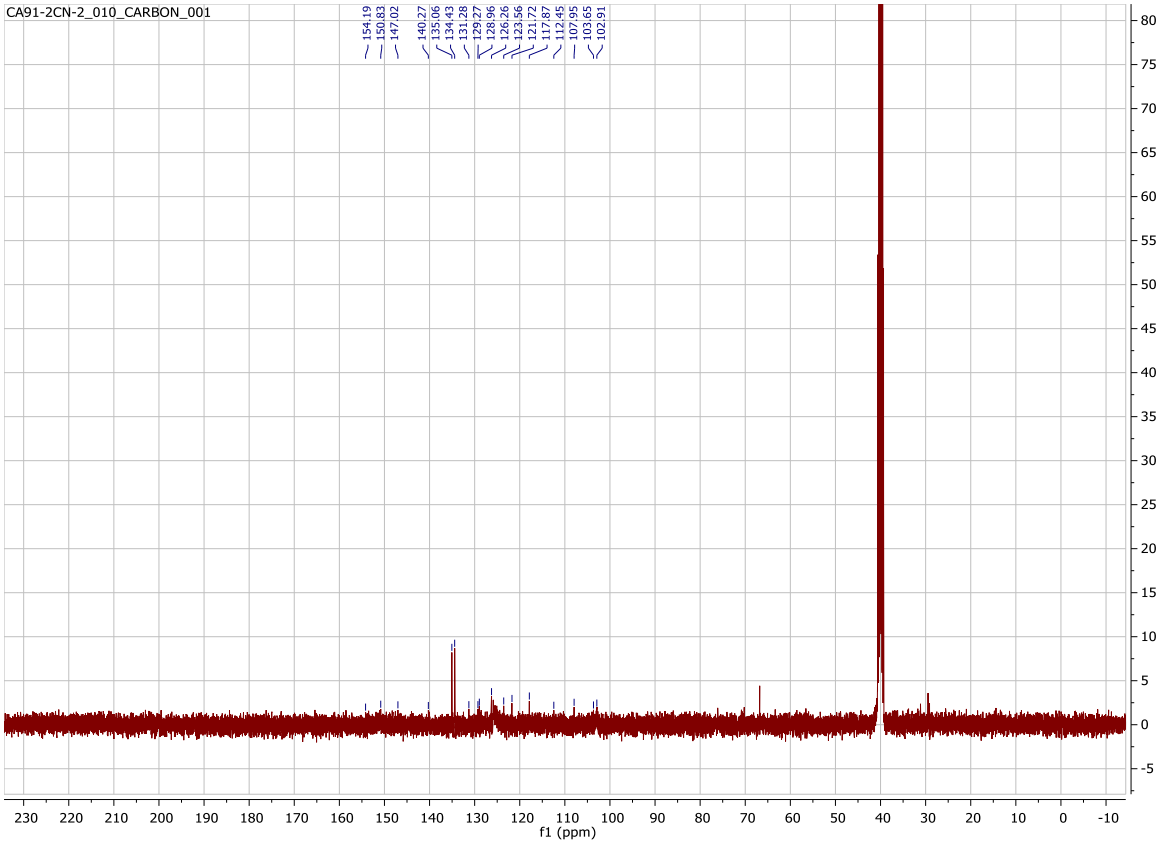
2-((6-(Trifluoromethyl)quinolin-4-yl)amino)benzonitrile (**33**)

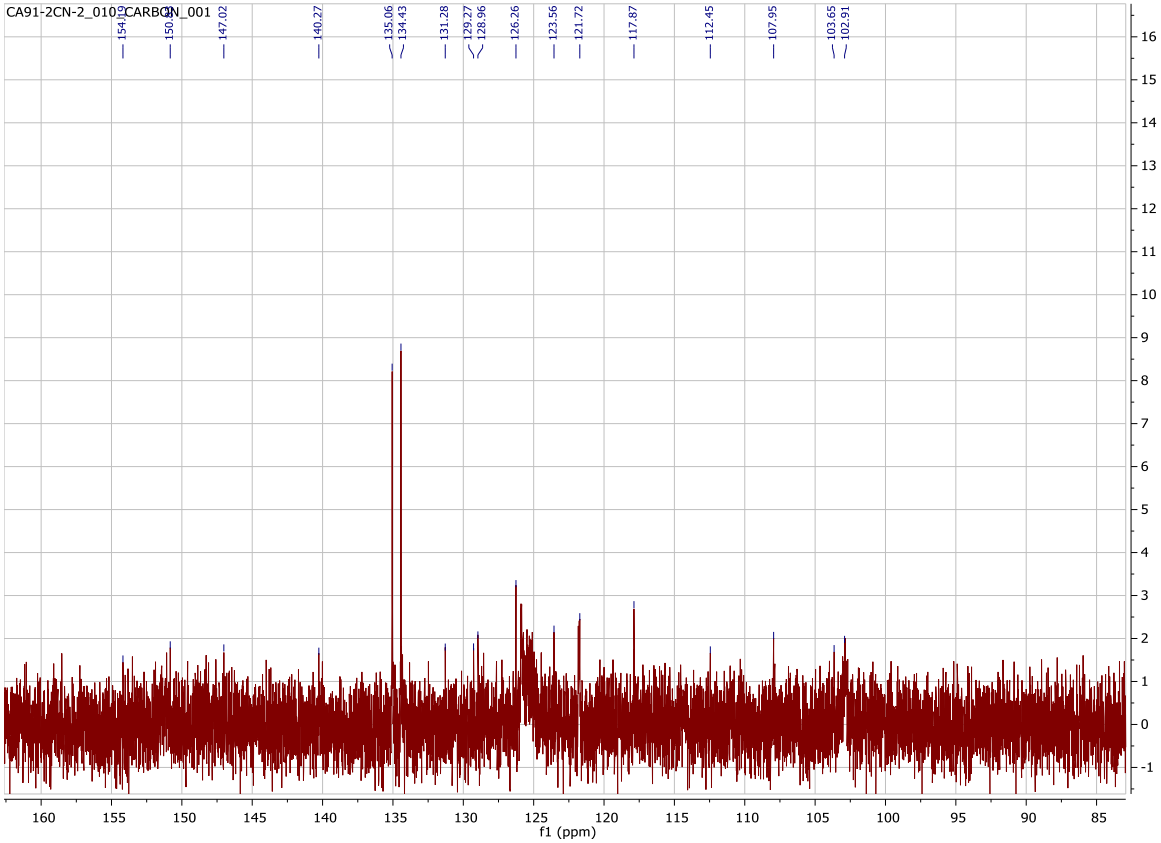


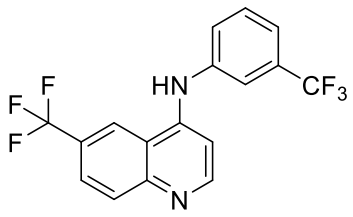



CA91-2CN-2_010_PROTON_001
8.84
8.30
7.95
7.89
7.87
7.76
7.74
7.72
7.44
7.42
7.37
7.35
7.33
6.37
1.03
0.94
2.01
0.99
1.04
1.02
1.02
1.00
f1 (ppm)


CA91-2CN-2_010_PROTON_001
8.84
8.30
7.95
7.89
7.87
7.76
7.74
7.72
7.44
7.42
7.37
7.35
7.33
6.37
1.03
0.94
2.01
0.99
1.04
1.02
1.02
1.00
f1 (ppm)

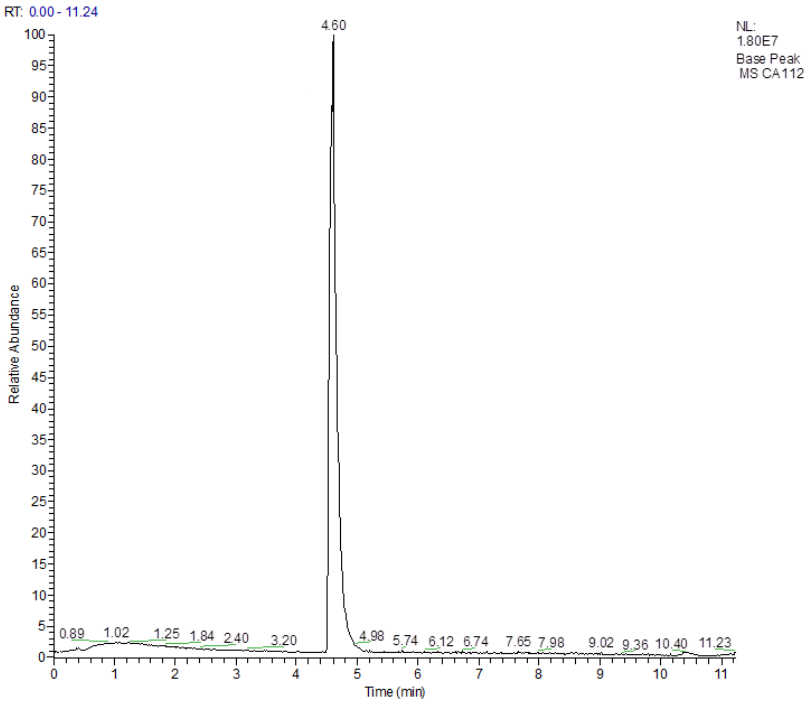

CA91-2CN-2_010_CARBON_001
154.19
150.83
147.02
140.27
135.06
134.43
131.28
129.27
128.96
126.26
123.56
121.72
117.87
112.45
107.95
103.65
102.91
f1 (ppm)

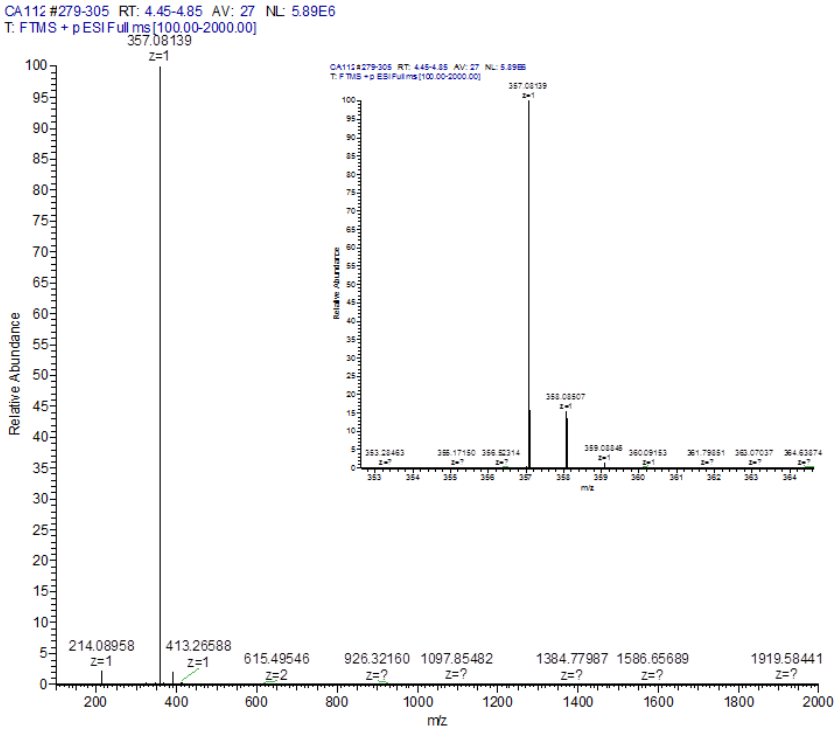

CA91-2CN-2_010_CARBON_001
154.19
150.83
147.02
140.27
135.06
134.43
131.28
129.27
128.96
126.26
123.56
121.72
117.87
112.45
107.95
103.65
102.91
f1 (ppm)

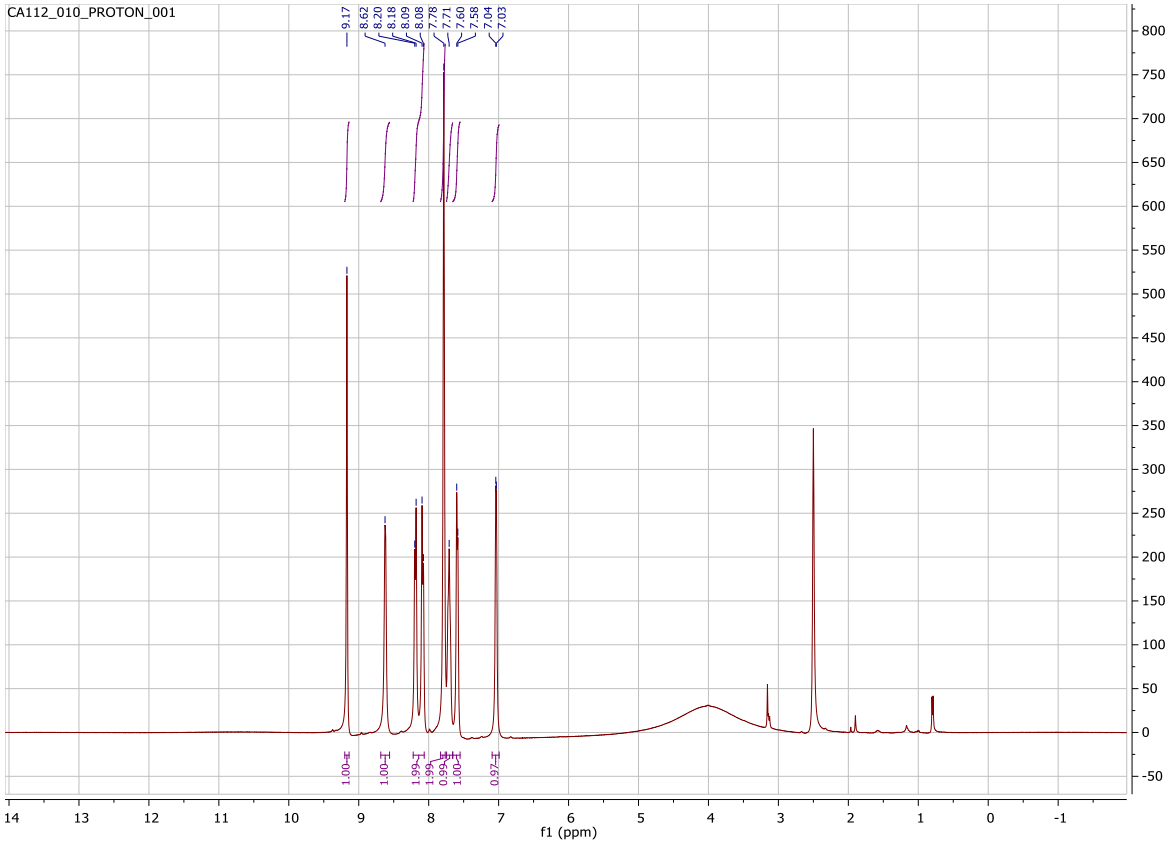


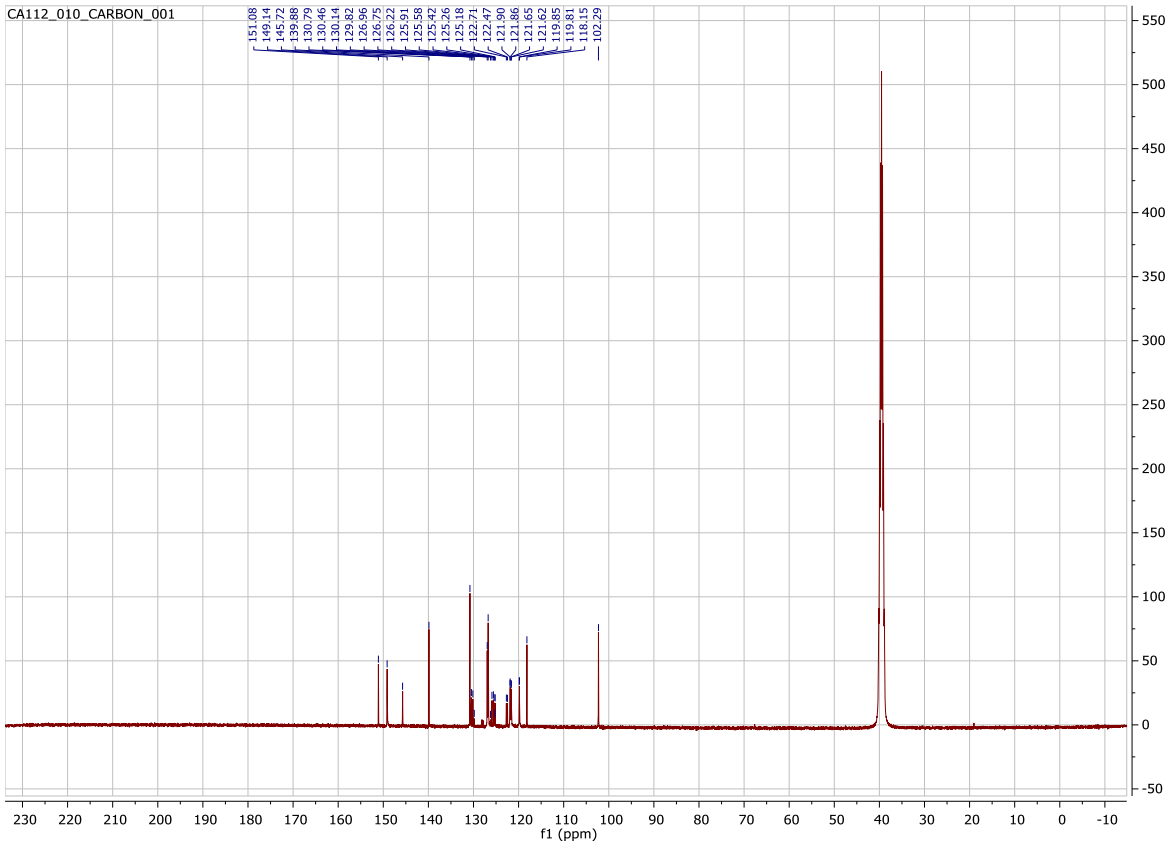
34

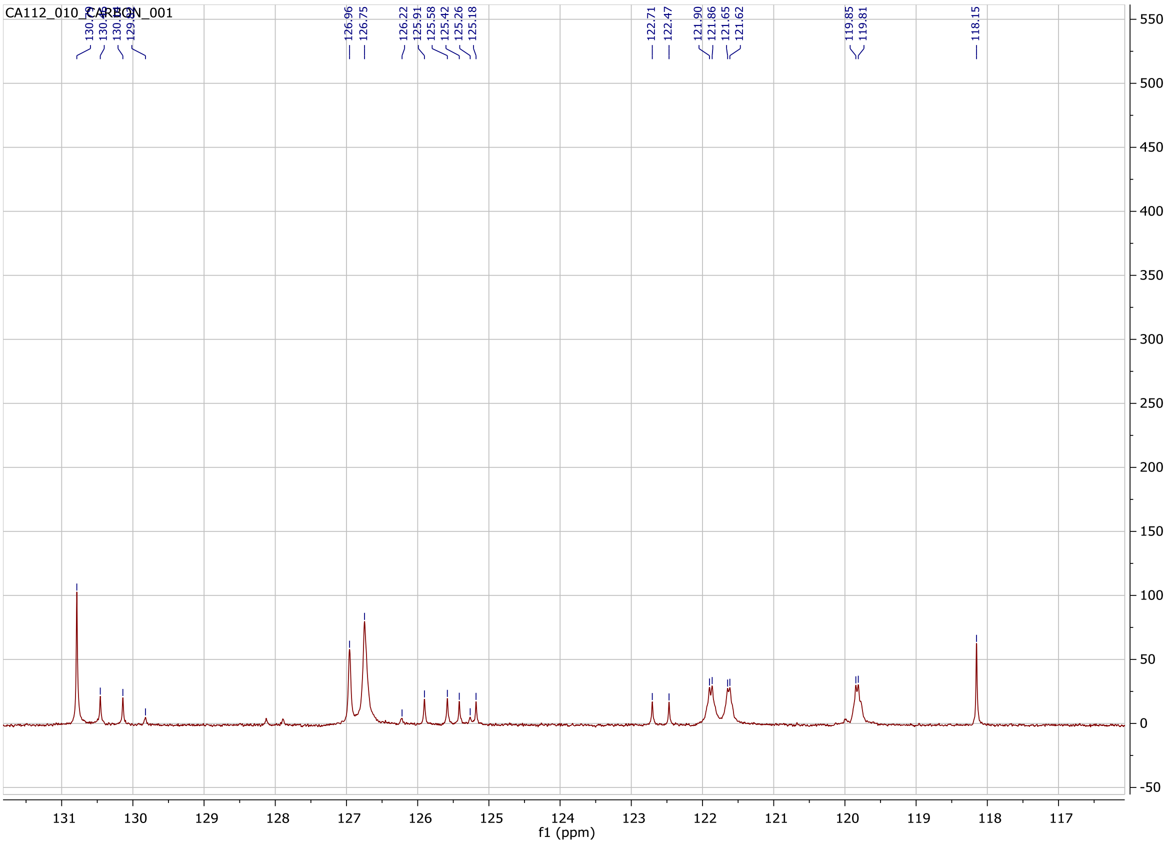
6-(Trifluoromethyl)-*N*-(3-(trifluoromethyl)phenyl)quinolin-4-amine (**34**)



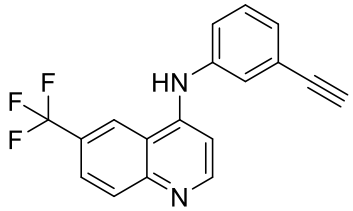



CA112_010_PROTON_001
9.17
8.62
8.20
8.18
8.09
8.08
7.78
7.71
7.60
7.58
7.04
7.03
1.00
1.00
1.99
1.99
0.99
1.00
0.97
f1 (ppm)


CA112_010_CARBON_001
151.08
149.14
145.72
139.88
130.79
130.46
130.14
129.82
126.96
126.75
126.22
125.91
125.58
125.42
125.26
125.18
122.71
122.47
121.90
121.86
121.65
121.62
119.85
119.81
118.15
102.29
f1 (ppm)

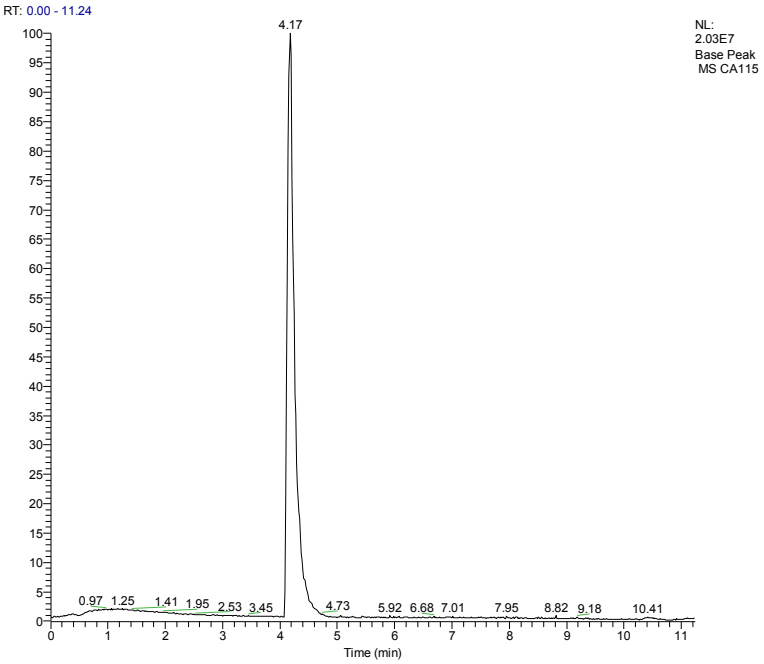


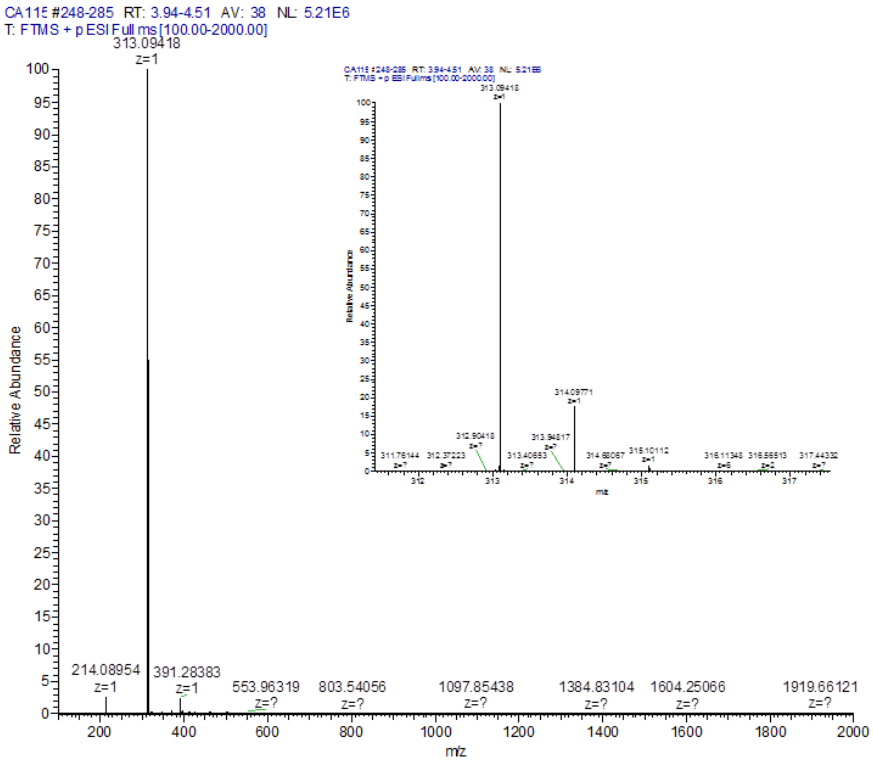
CA112_010_CARBON_001
126.96
126.75
126.22
125.91
125.58
125.42
125.26
125.18
122.71
122.47
121.90
121.86
121.65
121.62
119.85
119.81
118.15
f1 (ppm)

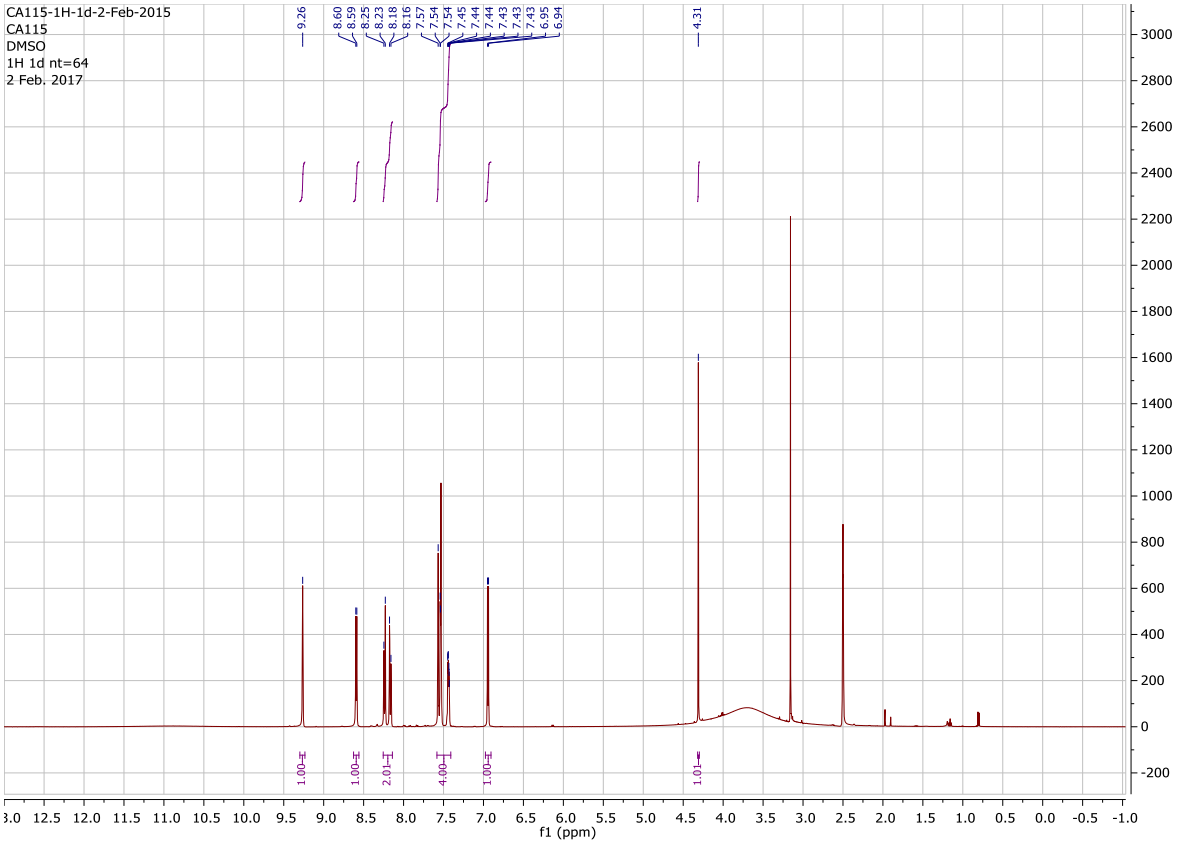


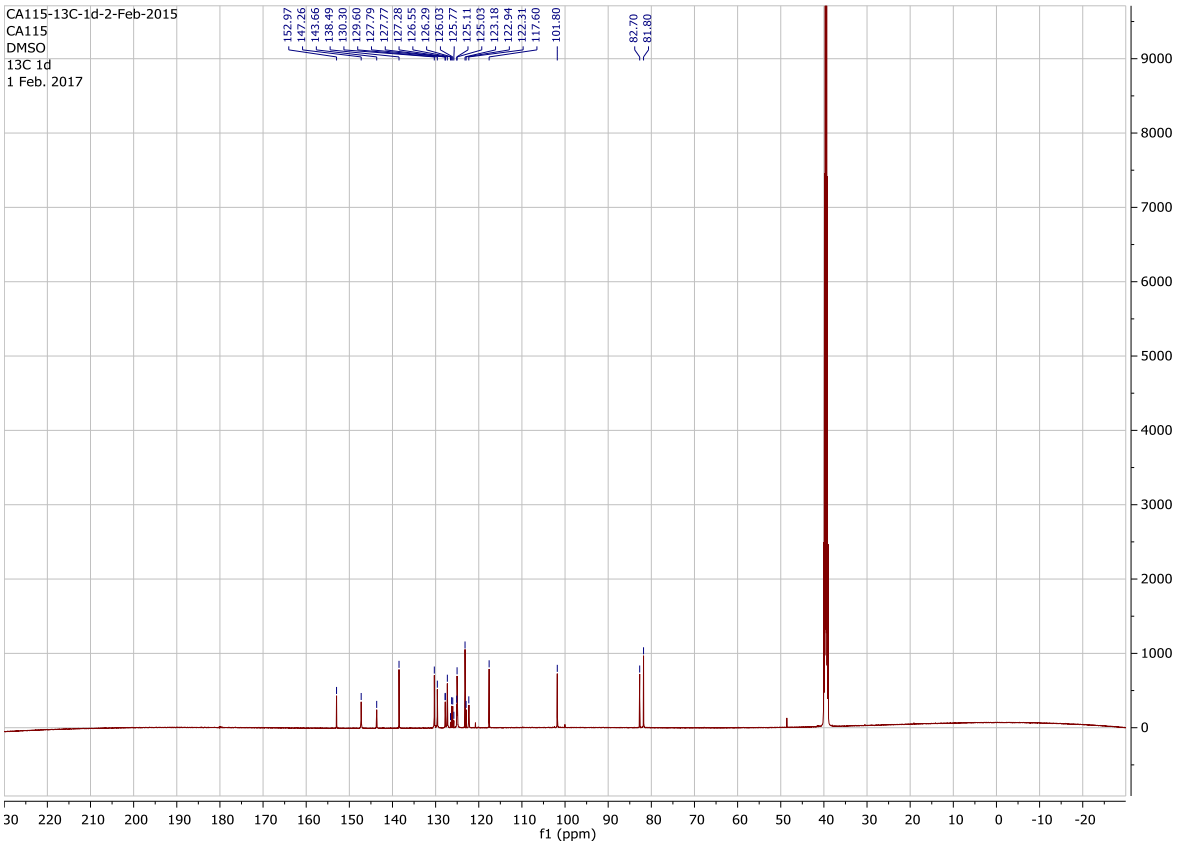
35

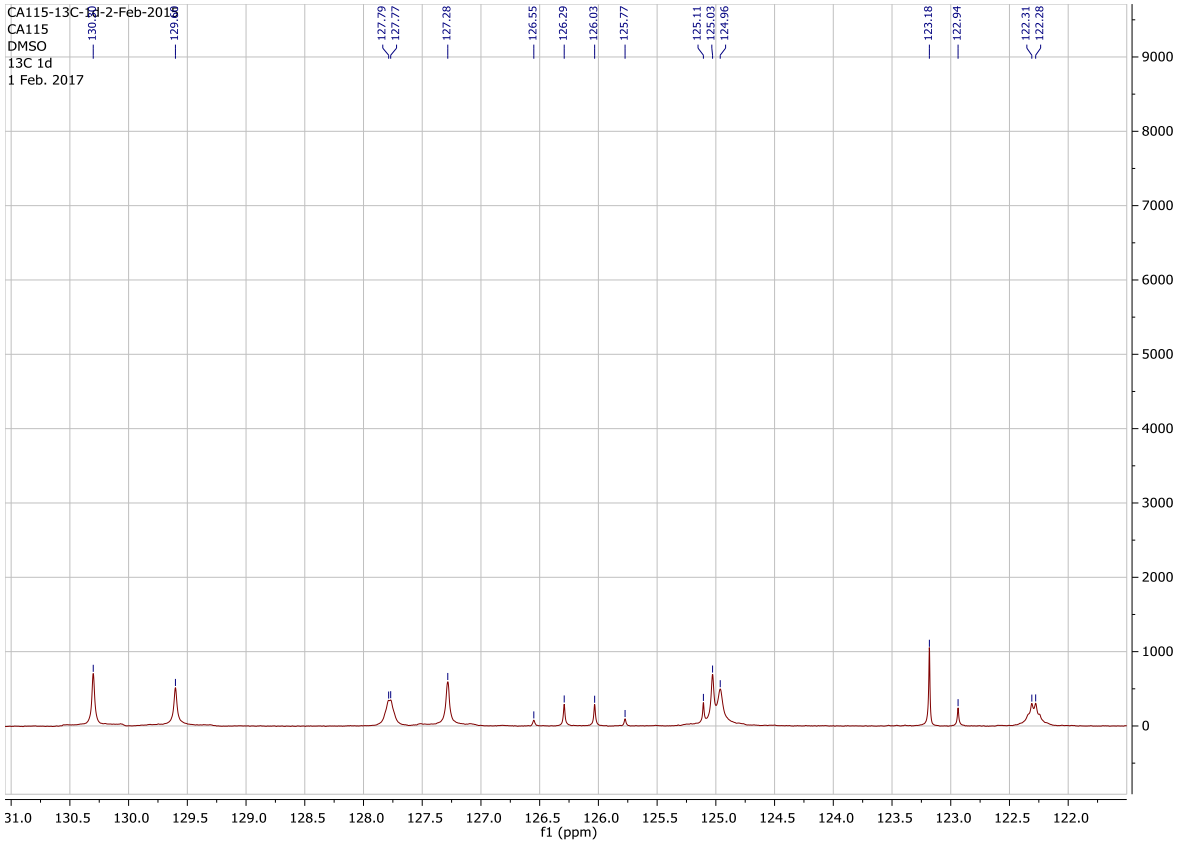
N-(3-Ethynylphenyl)-6-(trifluoromethyl)quinolin-4-amine (**35**)

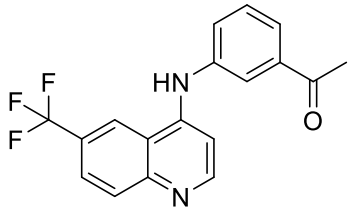





CA115-1H-1d-2-Feb-2015
CA115
DMSO
1H 1d nt=64
2 Feb. 2017
9.26
8.60
8.59
8.25
8.23
8.18
8.16
7.57
7.54
7.54
7.45
7.44
7.44
7.43
7.43
7.43
6.95
6.94
4.31
1.00
1.00
2.01
4.00
1.00
1.01
f1 (ppm)

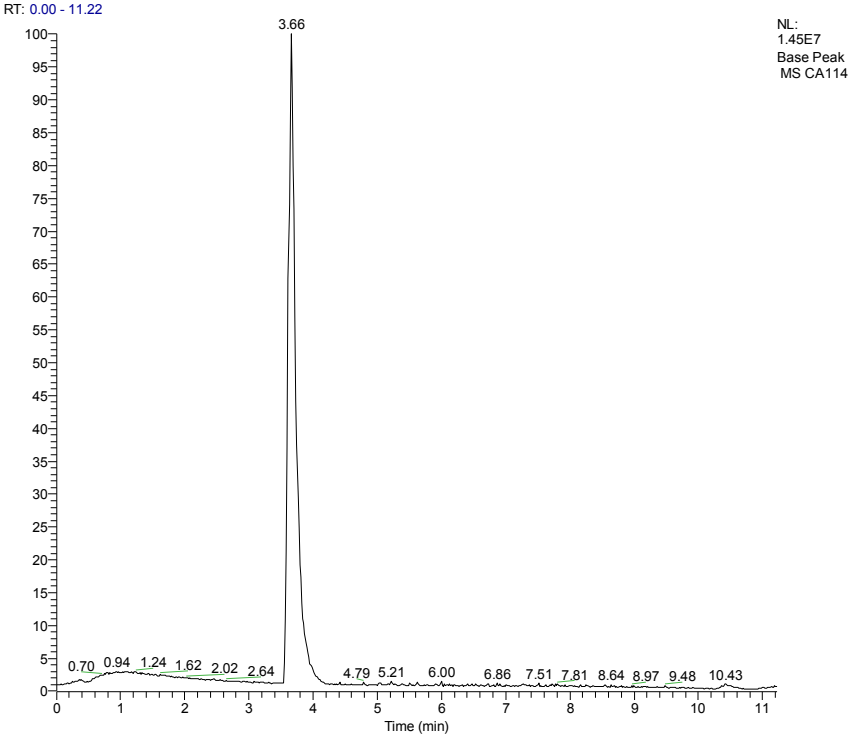

CA115-13C-1d-2-Feb-2015
CA115
DMSO
13C 1d
1 Feb. 2017
152.97
147.26
143.66
138.49
130.30
129.60
127.79
127.77
127.28
126.55
126.29
126.03
125.77
125.11
125.03
123.18
122.94
122.31
117.60
101.80
82.70
81.80
f1 (ppm)

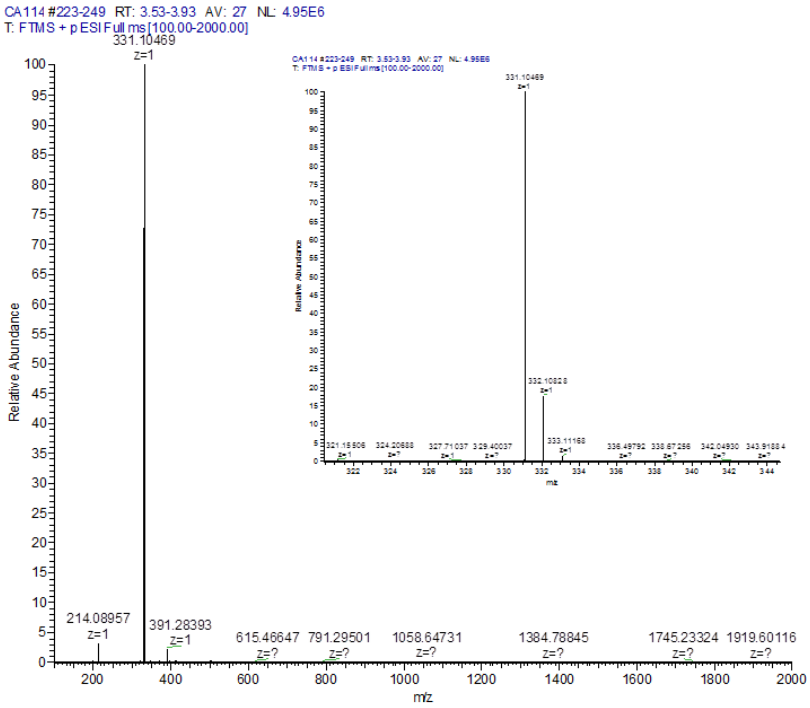

CA115-13C-1d-2-Feb-2017
CA115
DMSO
13C 1d
1 Feb. 2017
130.71
129.48
127.79
127.77
127.28
126.55
126.29
126.03
125.77
125.11
125.03
124.96
123.18
122.94
122.31
122.28
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
31.0
130.5
130.0
129.5
129.0
128.5
128.0
127.5
127.0
126.5
126.0
125.5
125.0
124.5
124.0
123.5
123.0
122.5
122.0
f1 (ppm)

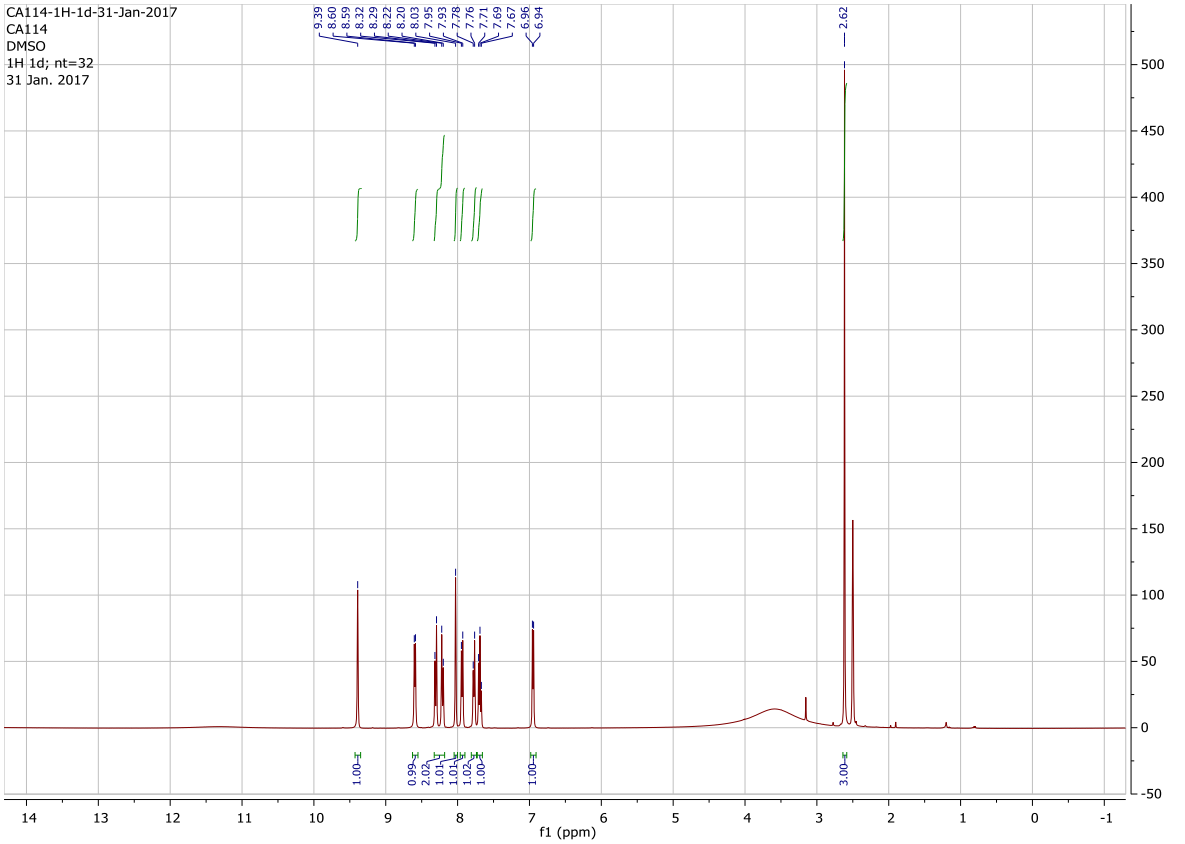


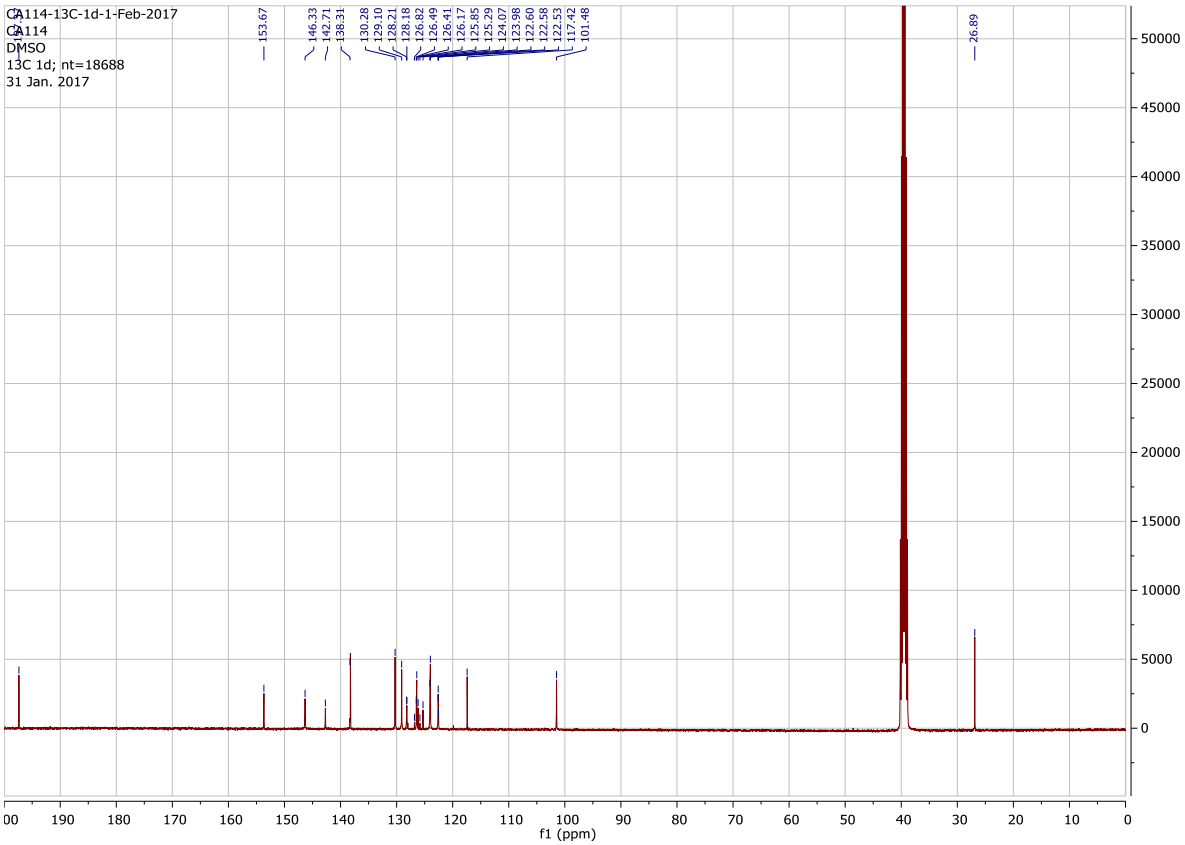
36

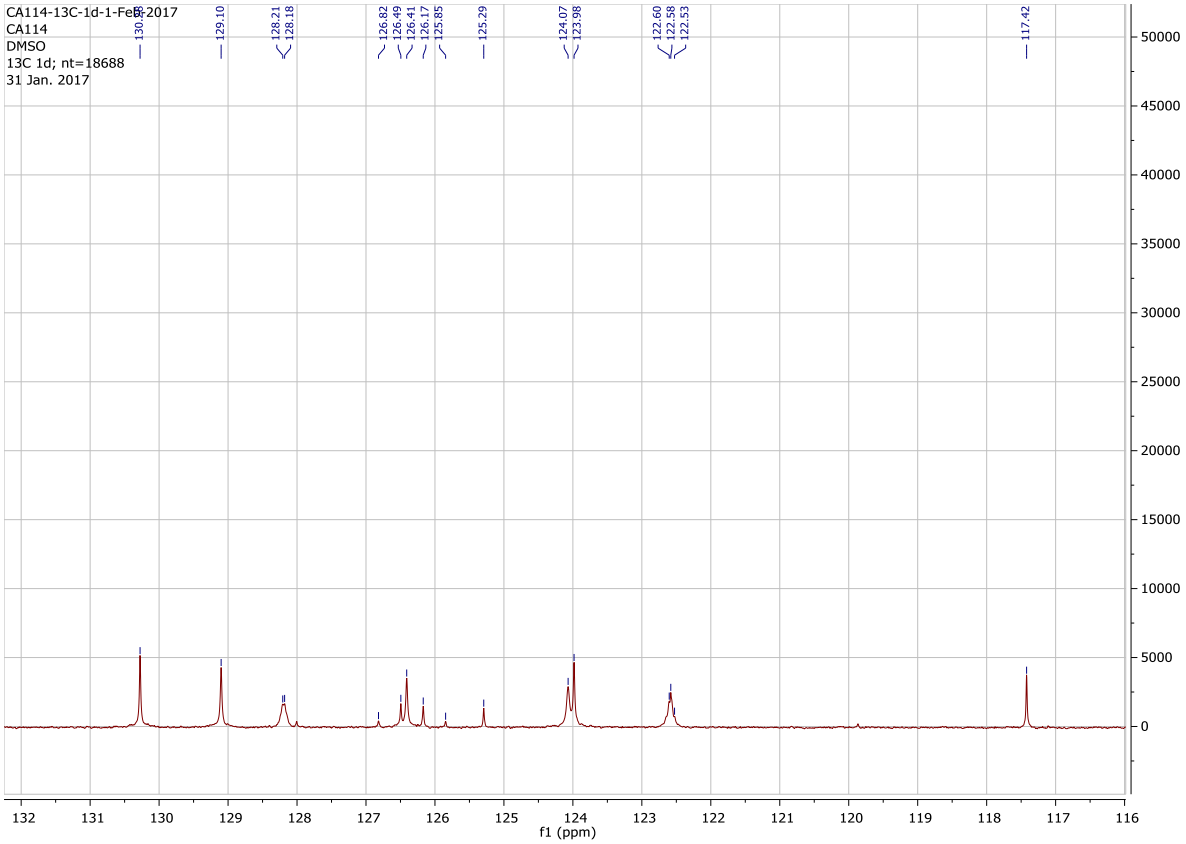
1-(3-((6-(Trifluoromethyl)quinolin-4-yl)amino)phenyl)ethan-1-one (**36**)

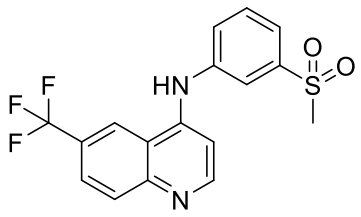





CA114-1H-1d-31-Jan-2017
CA114
DMSO
1H 1d; nt=32
31 Jan. 2017
9.39
8.60
8.59
8.32
8.29
8.22
8.20
8.03
7.95
7.93
7.78
7.76
7.71
7.69
7.67
6.96
6.94
2.62
1.00
0.99
2.02
1.01
1.01
1.02
1.00
1.00
3.00
f1 (ppm)

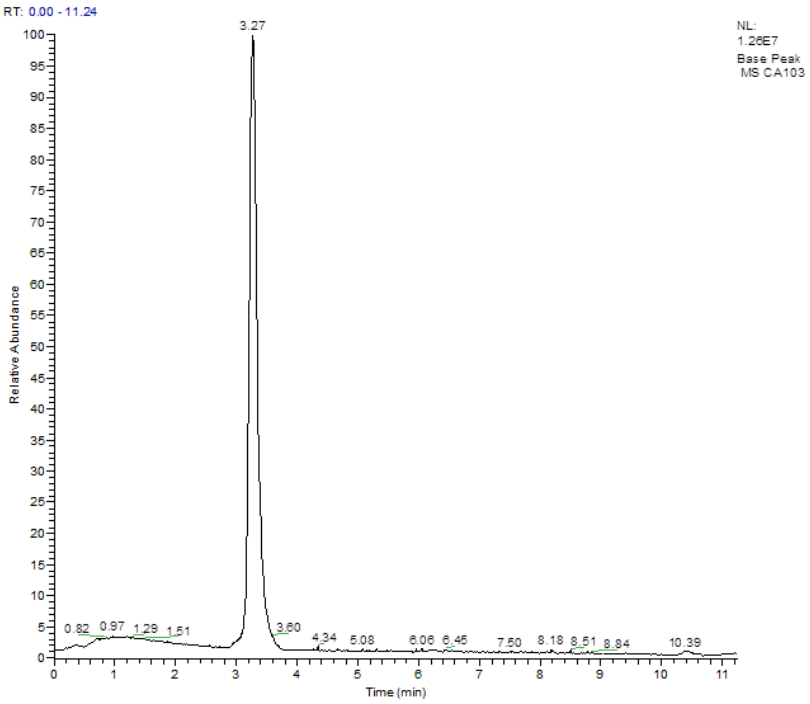

CA114-13C-1d-1-Feb-2017
CA114
DMSO
13C 1d; nt=18688
31 Jan. 2017
153.67
146.33
142.71
138.31
130.28
129.10
128.21
128.18
126.82
126.49
126.41
126.17
125.85
125.29
124.07
123.98
122.60
122.58
122.53
117.42
101.48
26.89
f1 (ppm)

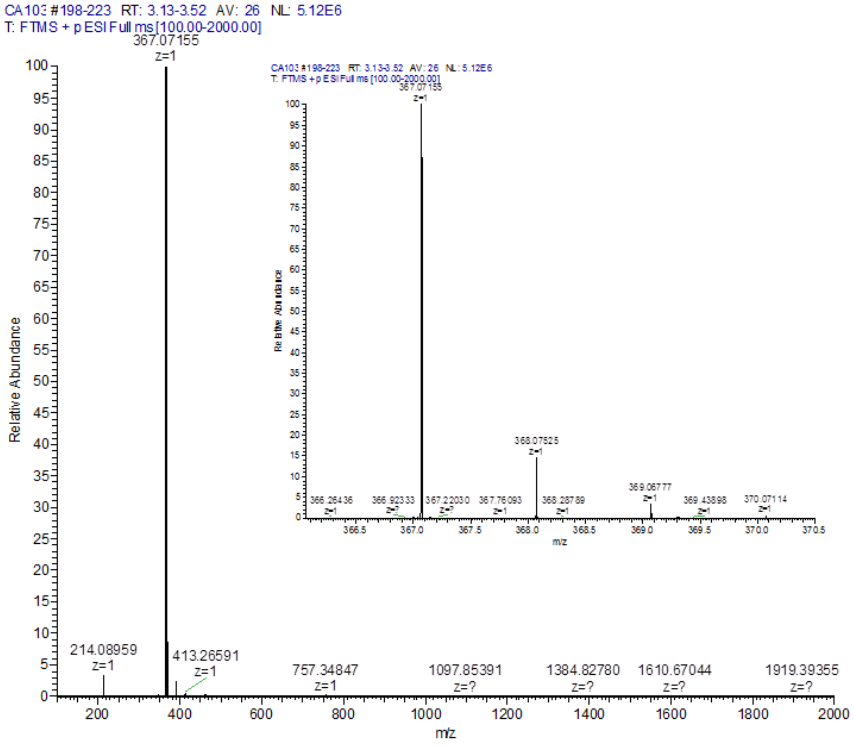

CA114-13C-1d-1-Feb-2017
CA114
DMSO
13C 1d; nt=18688
31 Jan. 2017
130.68
129.10
128.21
128.18
126.82
126.49
126.41
126.17
125.85
125.29
124.07
123.98
122.60
122.58
122.53
117.42
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
132
131
130
129
128
127
126
125
124
123
122
121
120
119
118
117
116
f1 (ppm)

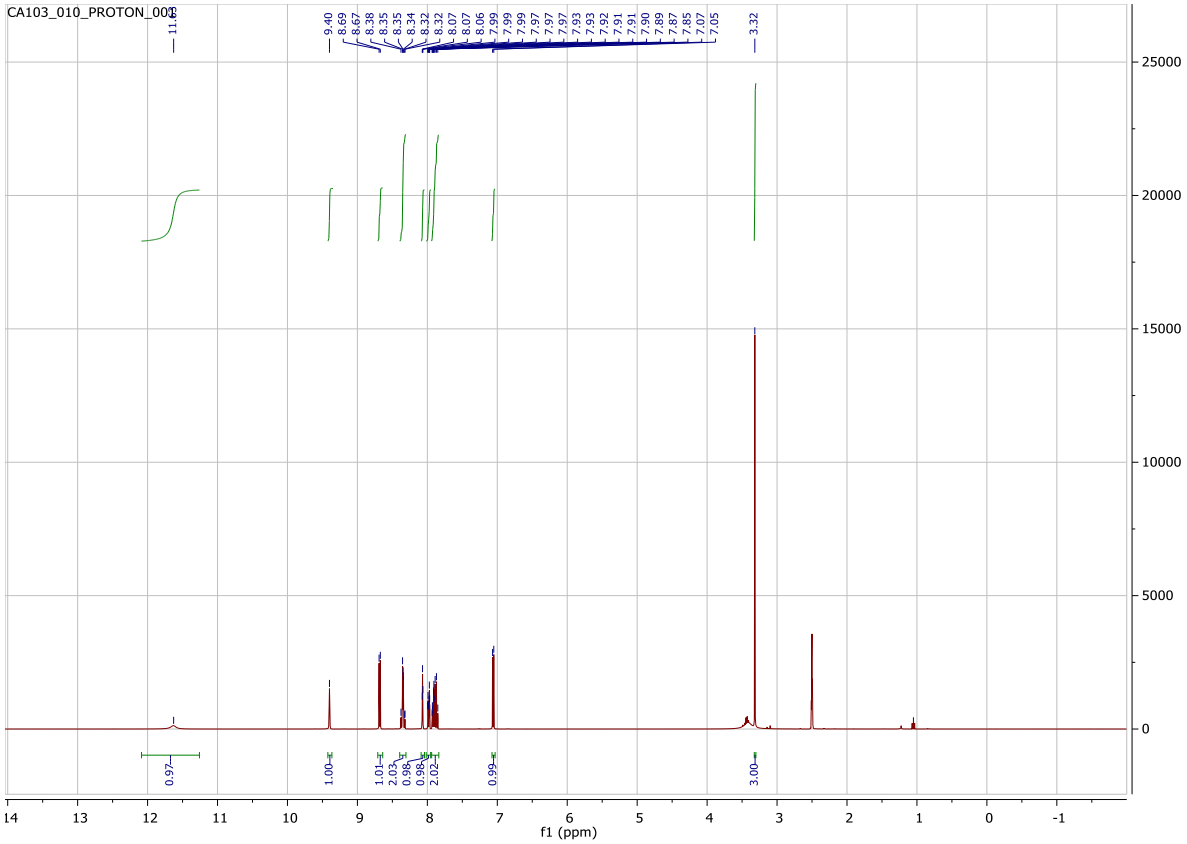


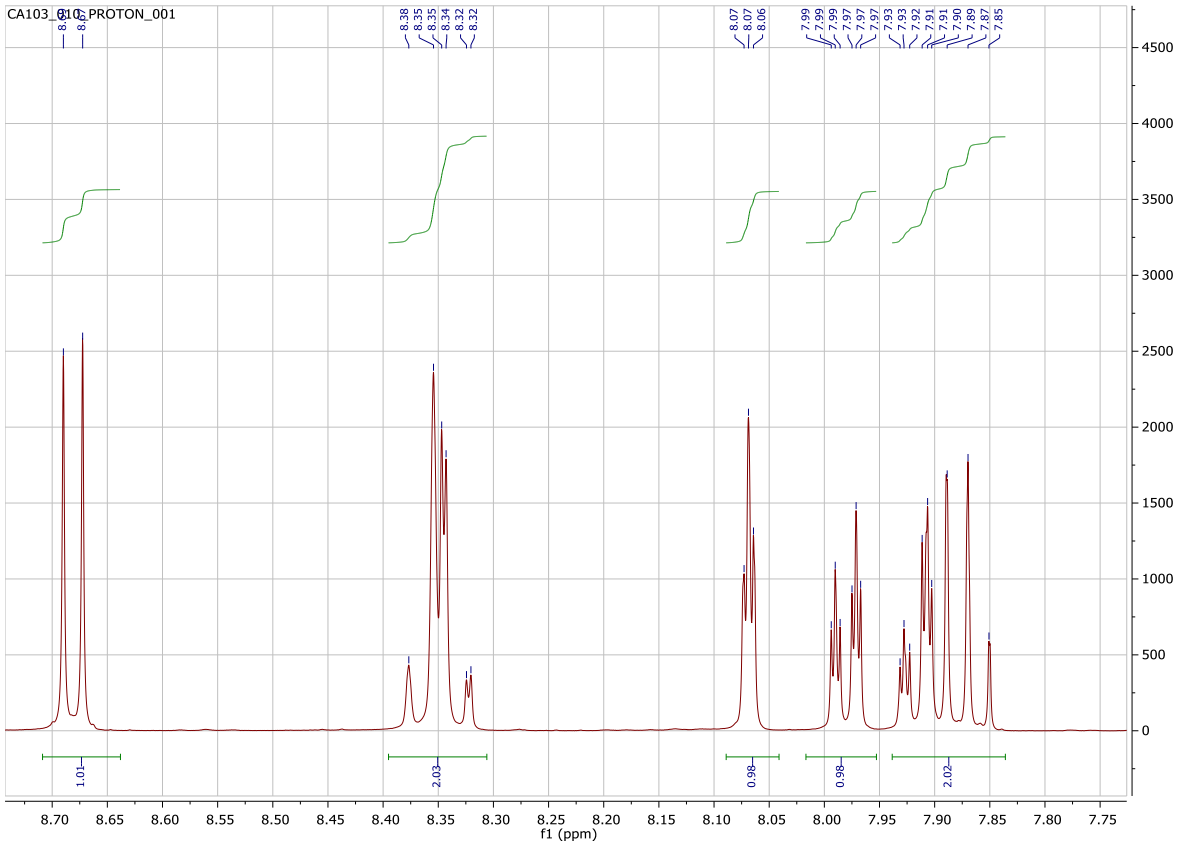
37

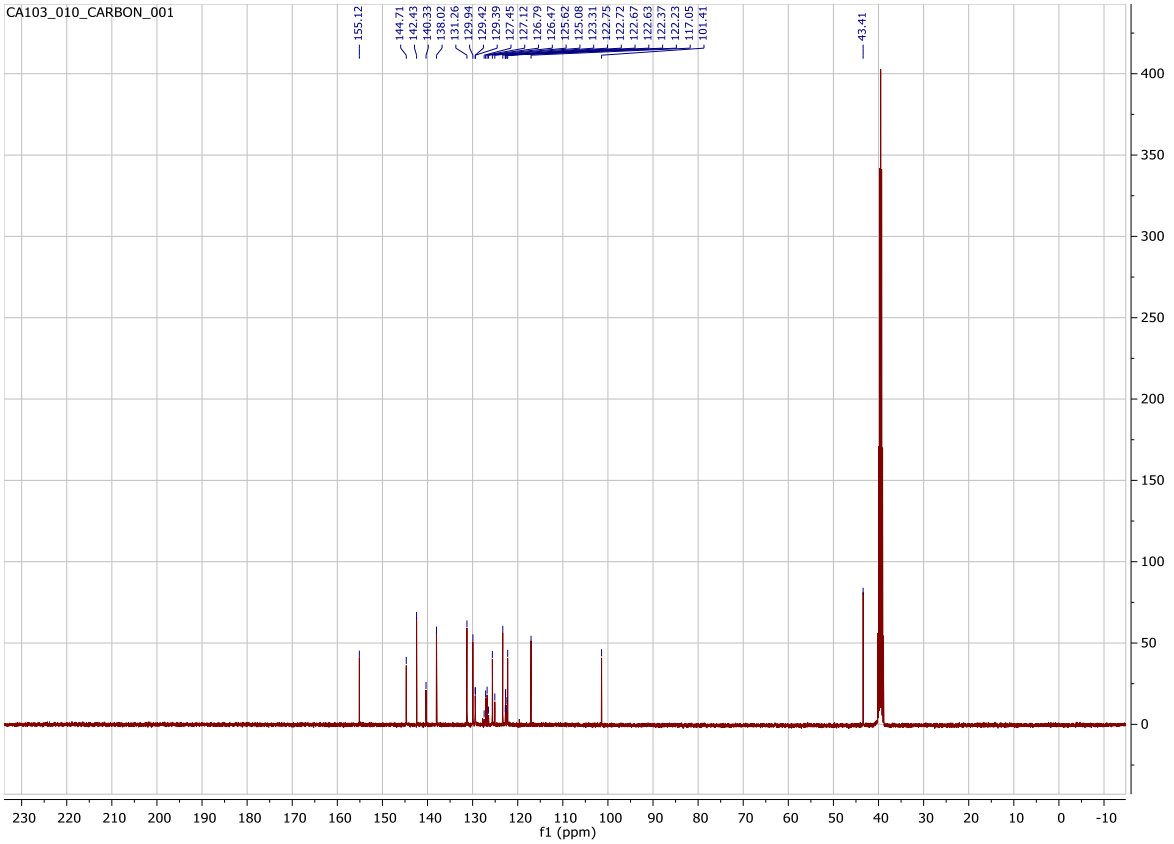
N-(3-(Methylsulfonyl)phenyl)-6-(trifluoromethyl)quinolin-4-amine (**37**)

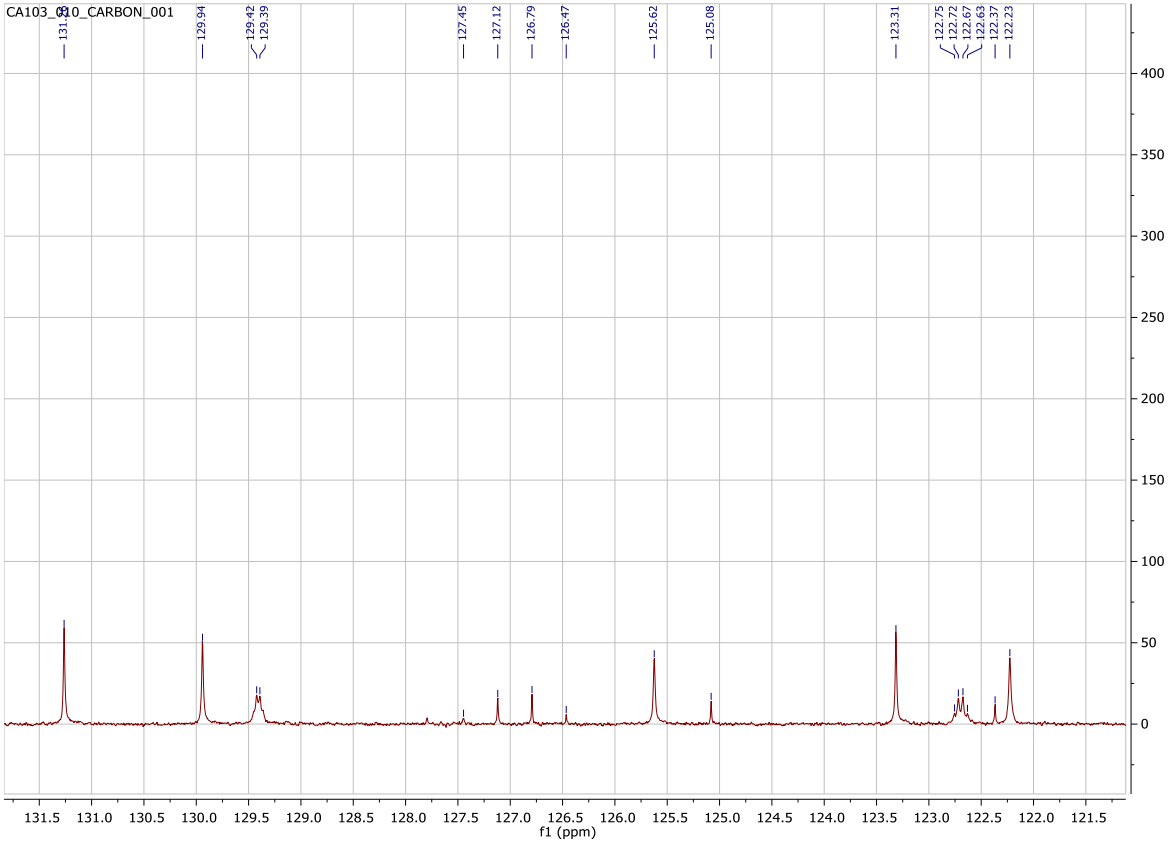


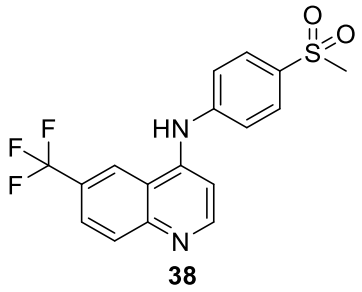



CA103_010_PROTON_001
11.68
9.40
8.69
8.67
8.38
8.35
8.35
8.34
8.32
8.32
8.07
8.07
8.06
7.99
7.99
7.99
7.97
7.97
7.97
7.93
7.93
7.92
7.91
7.91
7.90
7.89
7.87
7.85
7.07
7.05
3.32
0.97
1.00
1.01
2.03
0.98
0.98
2.02
0.99
3.00
f1 (ppm)


CA103_010_PROTON_001
8.38
8.35
8.35
8.34
8.32
8.32
8.07
8.07
8.06
7.99
7.99
7.99
7.97
7.97
7.97
7.93
7.93
7.92
7.91
7.91
7.90
7.89
7.87
7.85
1.01
2.03
0.98
0.98
2.02
f1 (ppm)

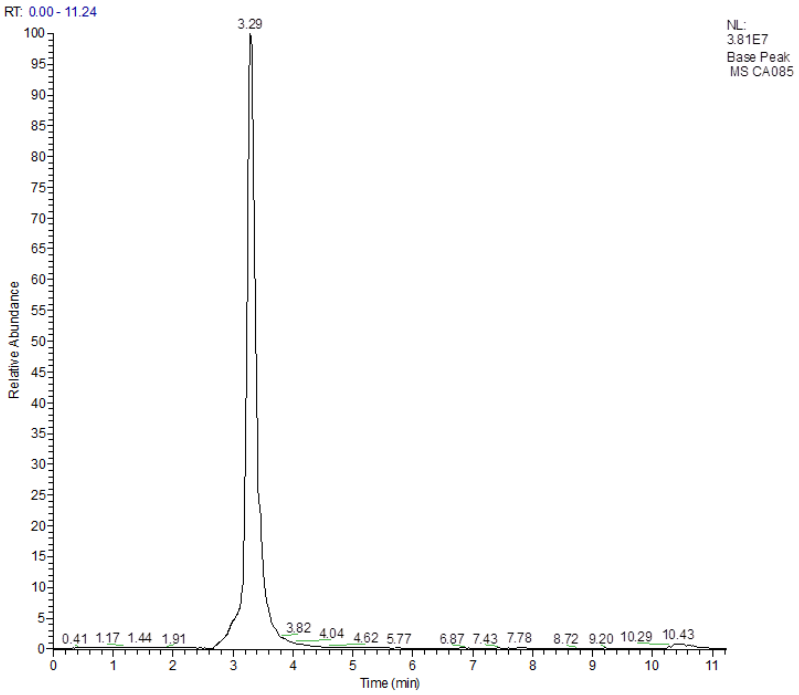

CA103_010_CARBON_001
155.12
144.71
142.43
140.33
138.02
131.26
129.94
129.42
129.39
127.45
127.12
126.79
126.47
125.62
125.08
123.31
122.75
122.72
122.67
122.63
122.37
122.23
117.05
101.41
43.41
f1 (ppm)

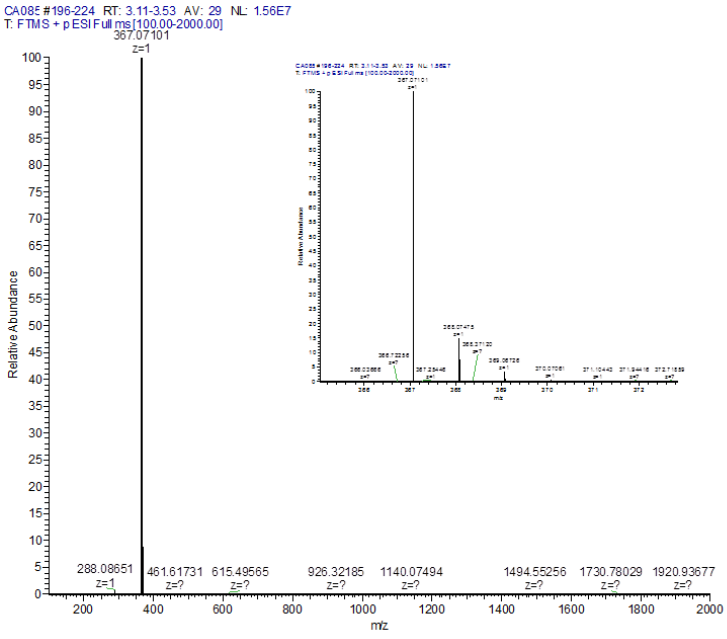

CA103_010_CARBON_001
131.94
129.94
129.42
129.39
127.45
127.12
126.79
126.47
125.62
125.08
123.31
122.75
122.72
122.67
122.63
122.37
122.23
f1 (ppm)

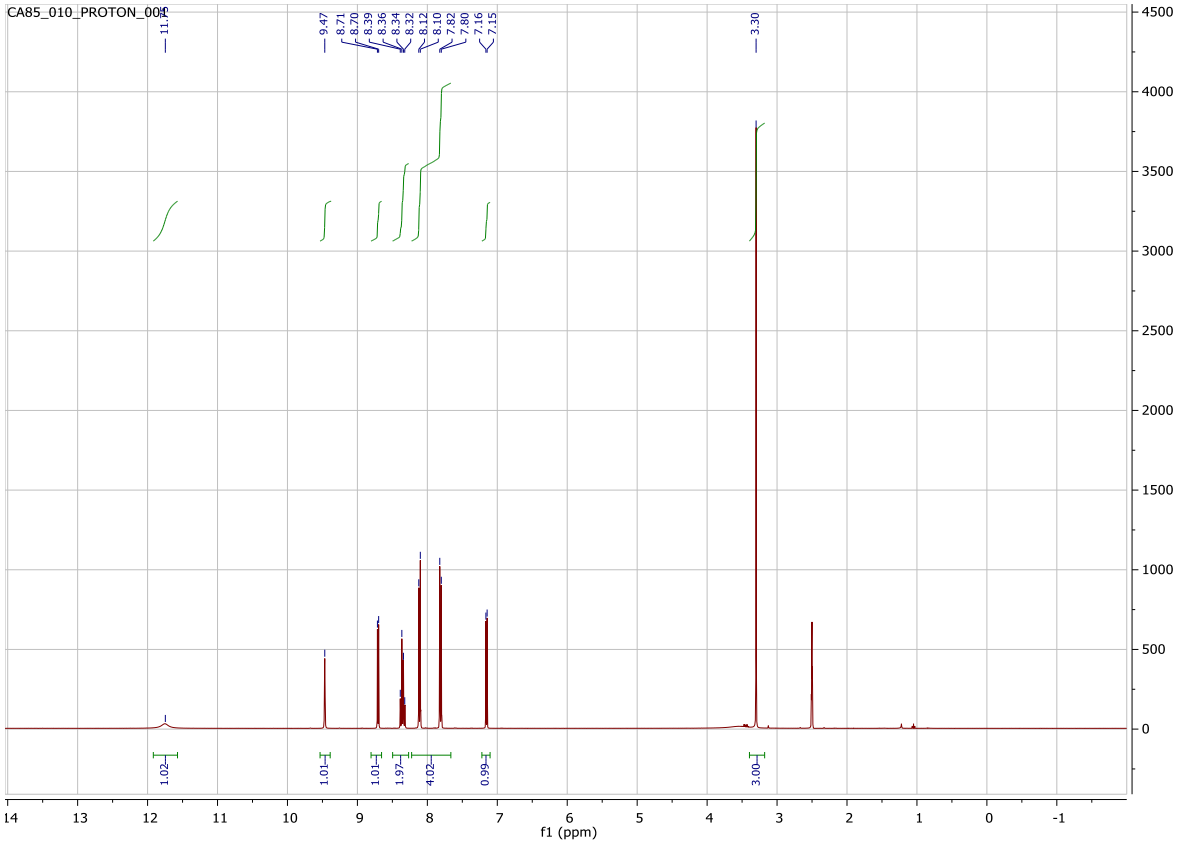


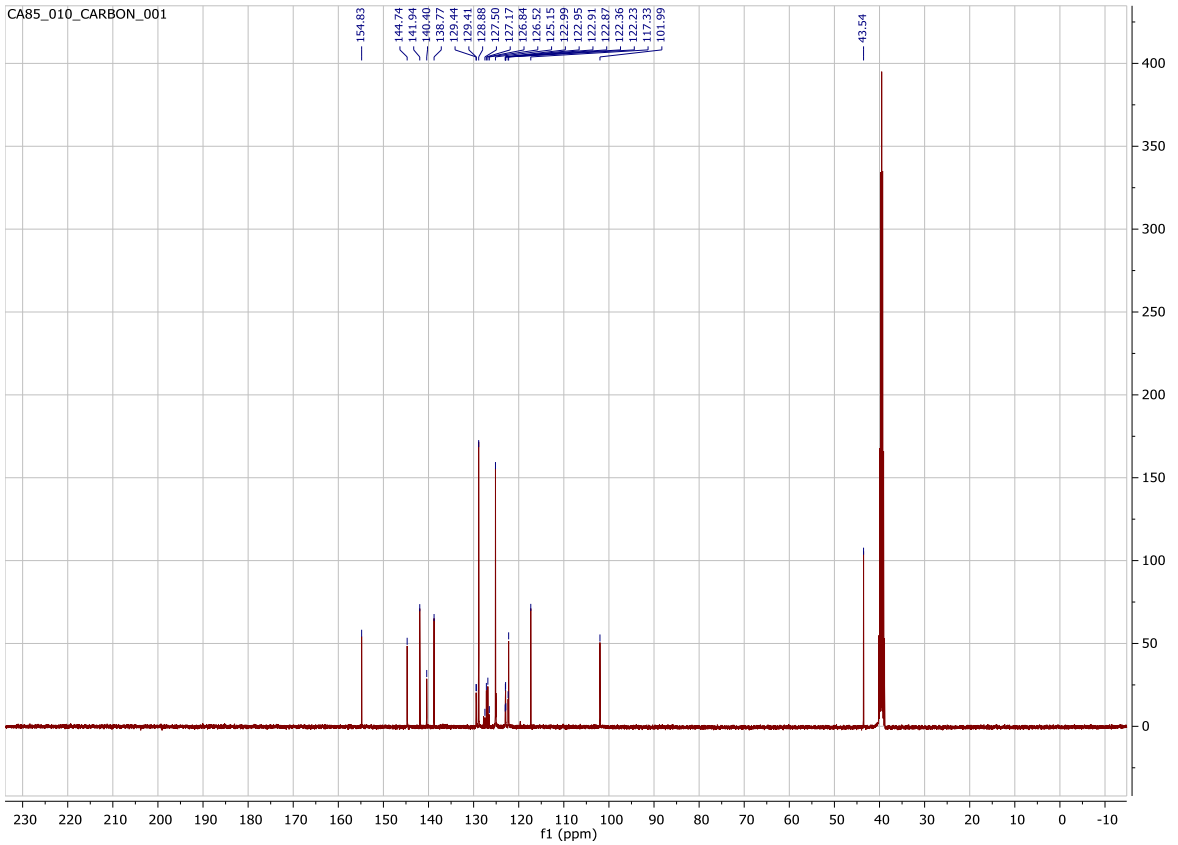
38

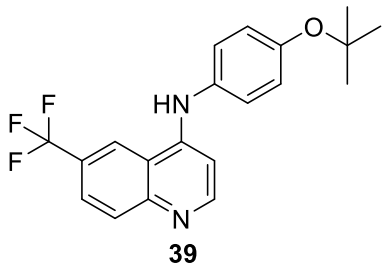
N-(4-(Methylsulfonyl)phenyl)-6-(trifluoromethyl)quinolin-4-amine (**38**)





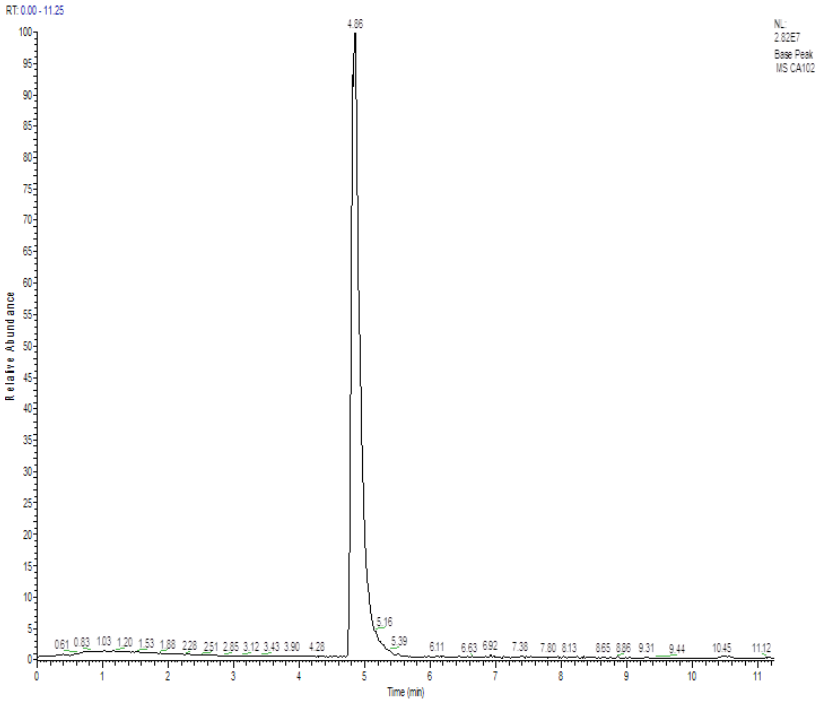

CA85_010_PROTON_001
11.75
9.47
8.71
8.70
8.39
8.36
8.34
8.32
8.12
8.10
7.82
7.80
7.16
7.15
3.30
1.02
1.01
1.01
1.97
4.02
0.99
3.00
f1 (ppm)

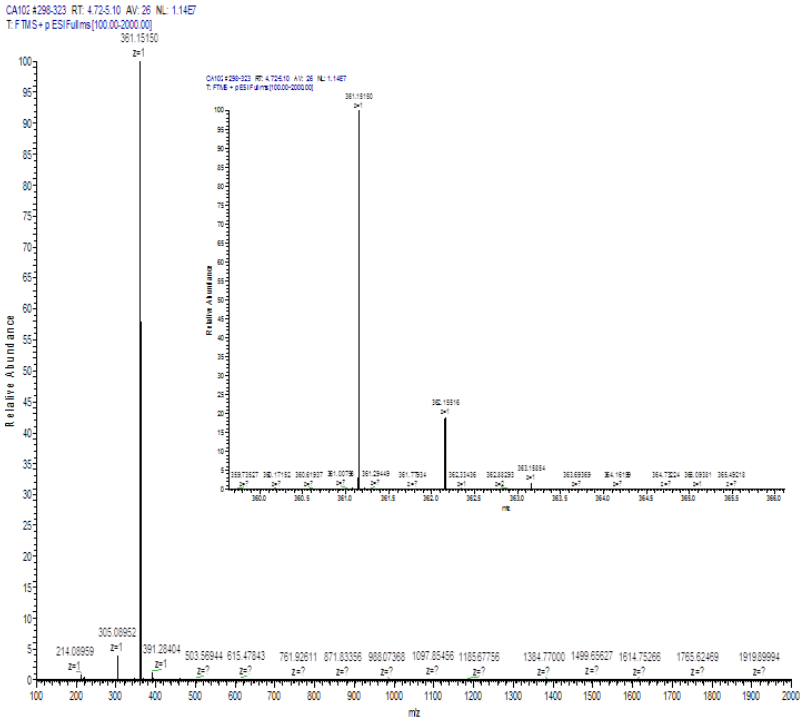

CA85_010_CARBON_001
154.83
144.74
141.94
140.40
138.77
129.44
129.41
128.88
127.50
127.17
126.84
126.52
125.15
122.99
122.95
122.91
122.87
122.36
122.23
117.33
101.99
43.54
f1 (ppm)

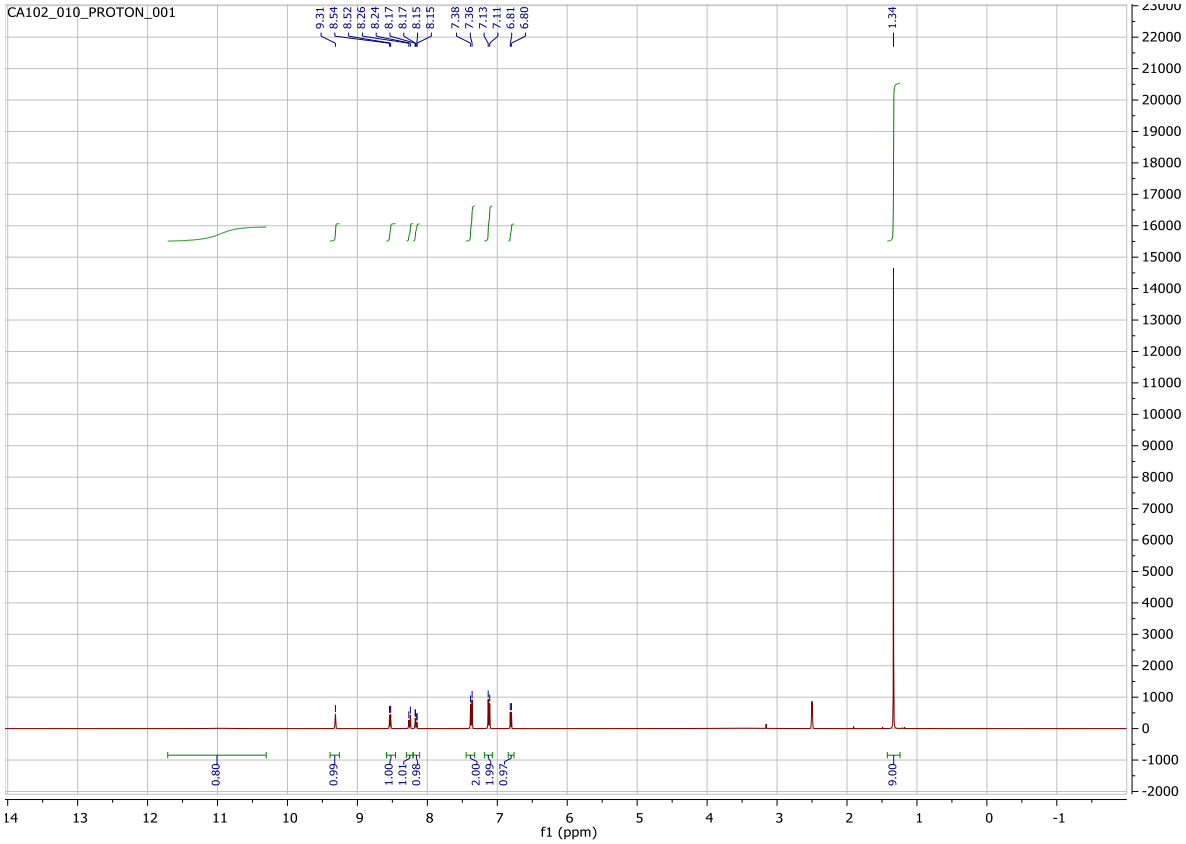


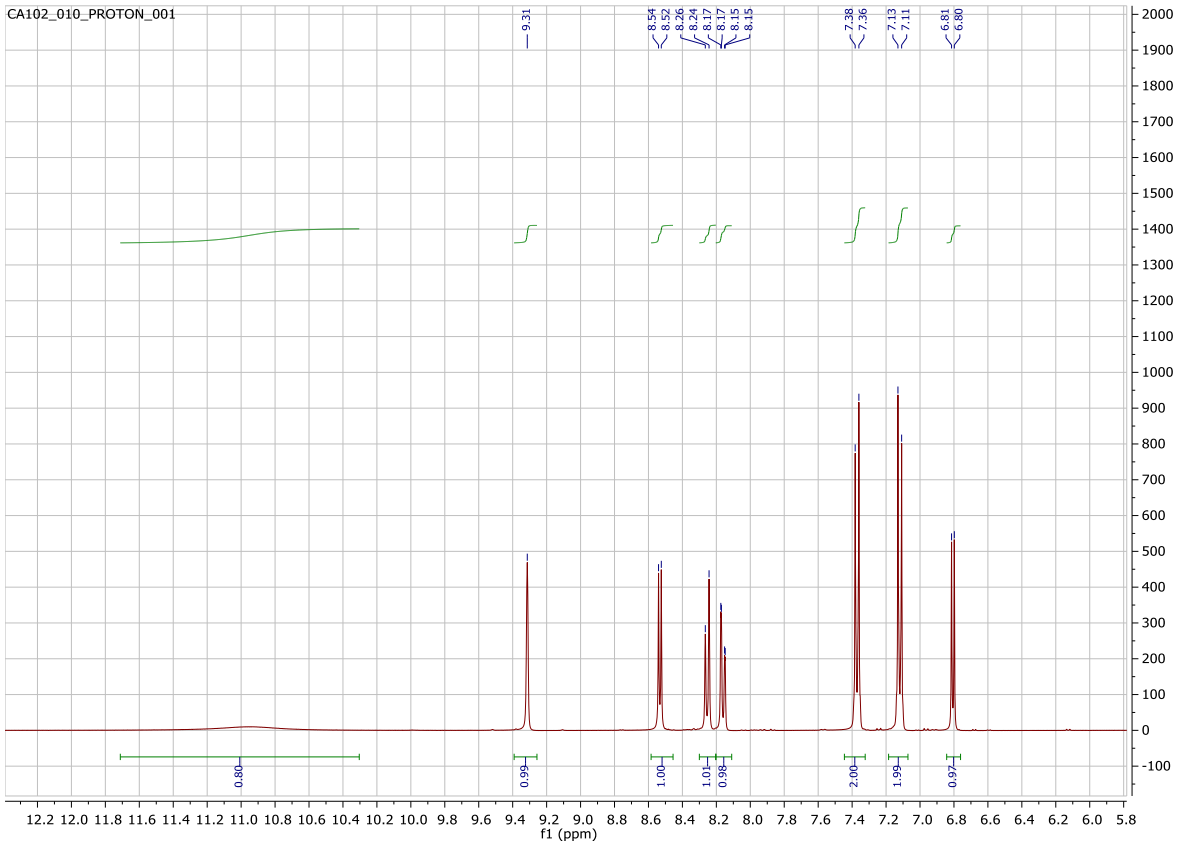
39

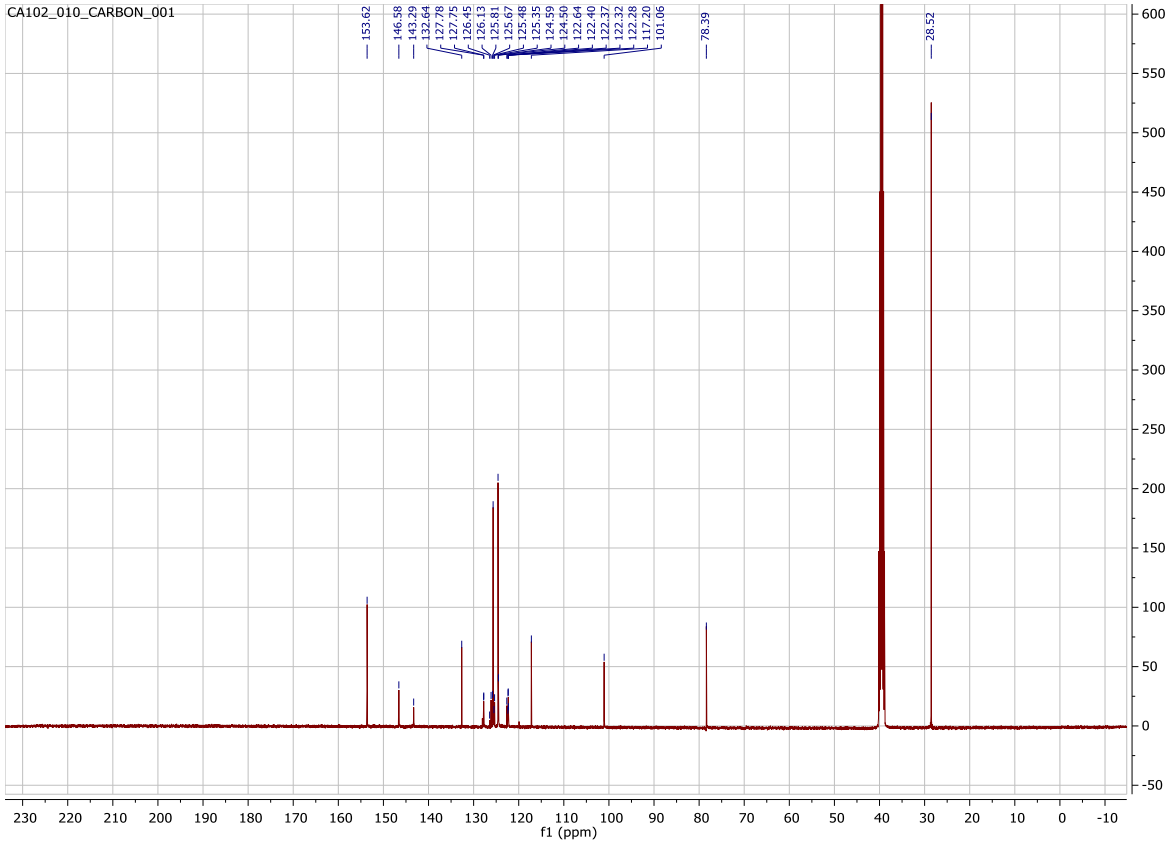
N-(4-(*tert*-Butoxy)phenyl-6-(trifluoromethyl)quinolin-4-amine (**39**)

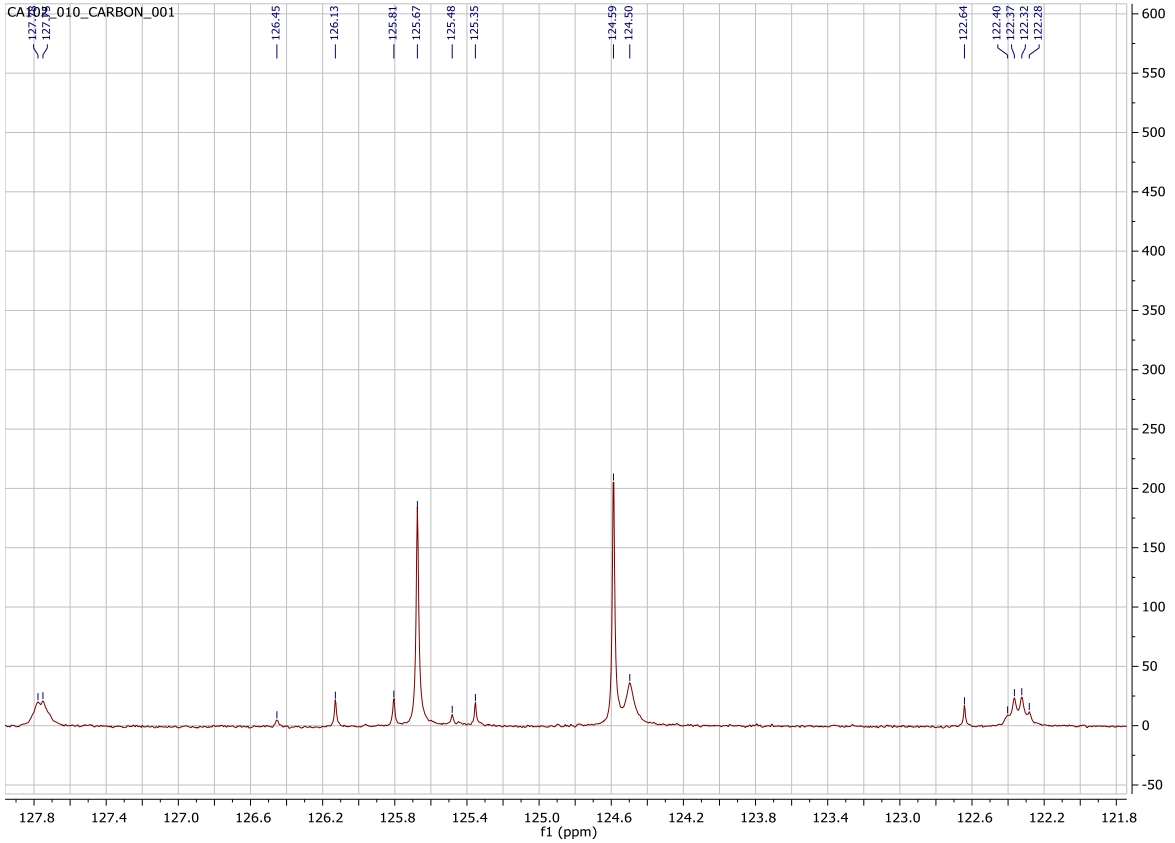


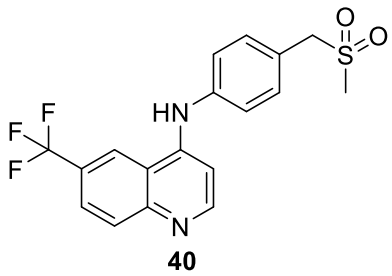



CA102_010_PROTON_001
9.31
8.54
8.52
8.26
8.24
8.17
8.17
8.15
8.15
7.38
7.36
7.13
7.11
6.81
6.80
1.34
0.80
0.99
1.00
1.01
0.98
2.00
1.99
0.97
9.00
f1 (ppm)


CA102_010_PROTON_001
9.31
8.54
8.52
8.26
8.24
8.17
8.17
8.15
8.15
7.38
7.36
7.13
7.11
6.81
6.80
0.80
0.99
1.00
1.01
0.98
2.00
1.99
0.97
f1 (ppm)

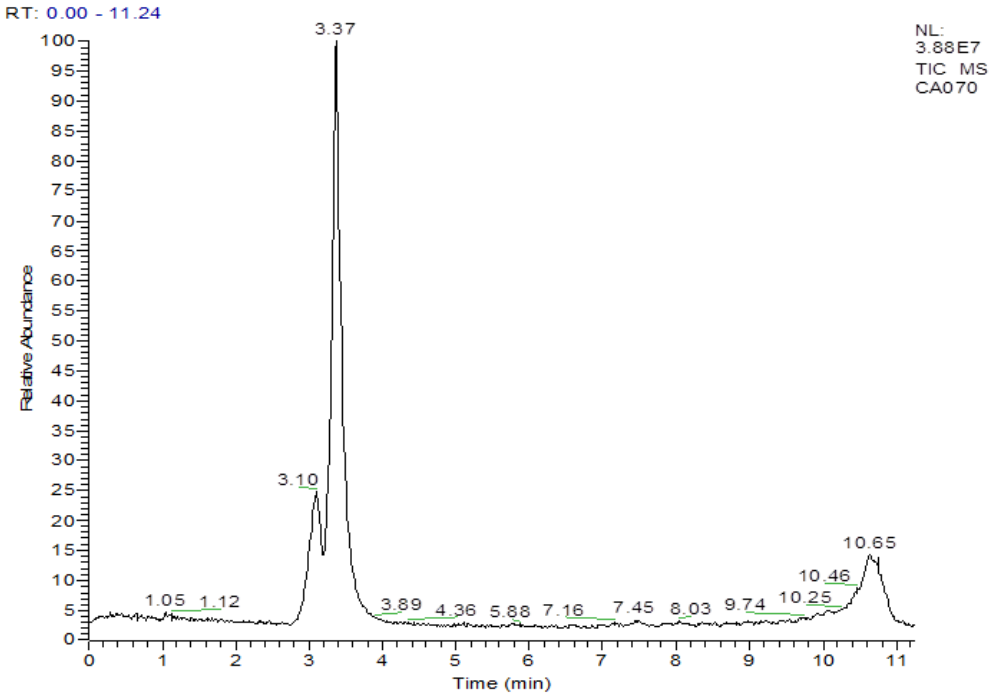

CA102_010_CARBON_001
153.62
146.58
143.29
132.64
127.78
127.75
126.45
126.13
125.81
125.67
125.48
125.35
124.59
124.50
122.64
122.40
122.37
122.32
122.28
117.20
101.06
78.39
28.52
f1 (ppm)

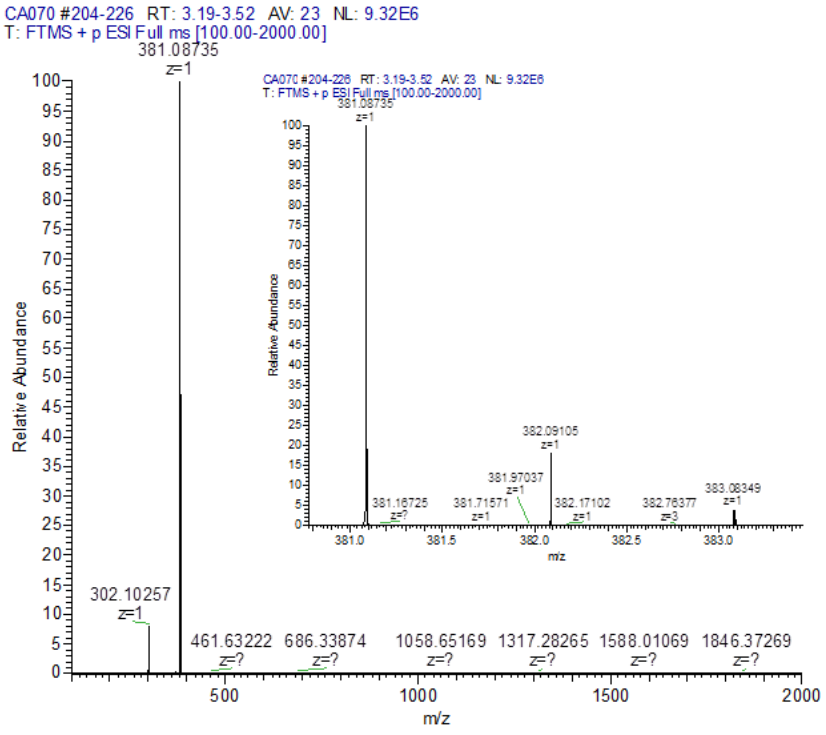

CA102_010_CARBON_001
127.92
127.84
126.45
126.13
125.81
125.67
125.48
125.35
124.59
124.50
122.64
122.40
122.37
122.32
122.28
f1 (ppm)

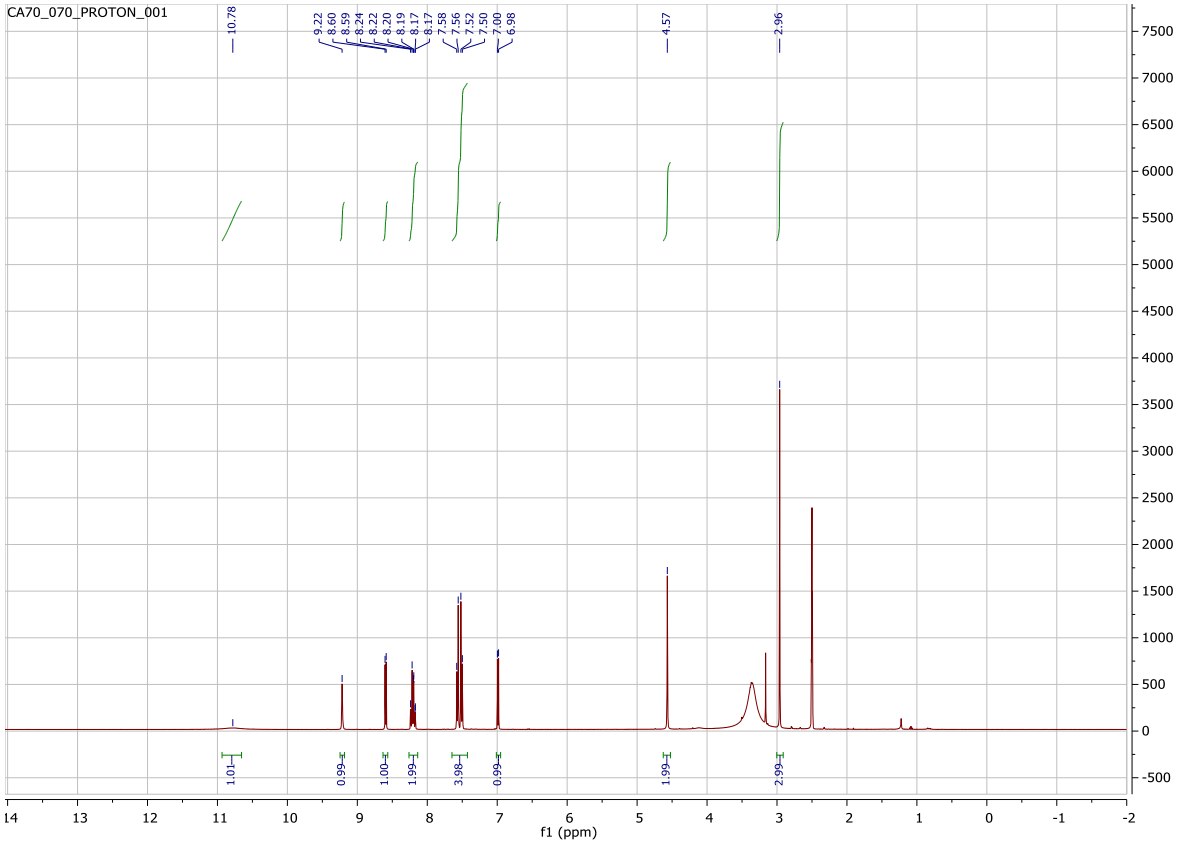


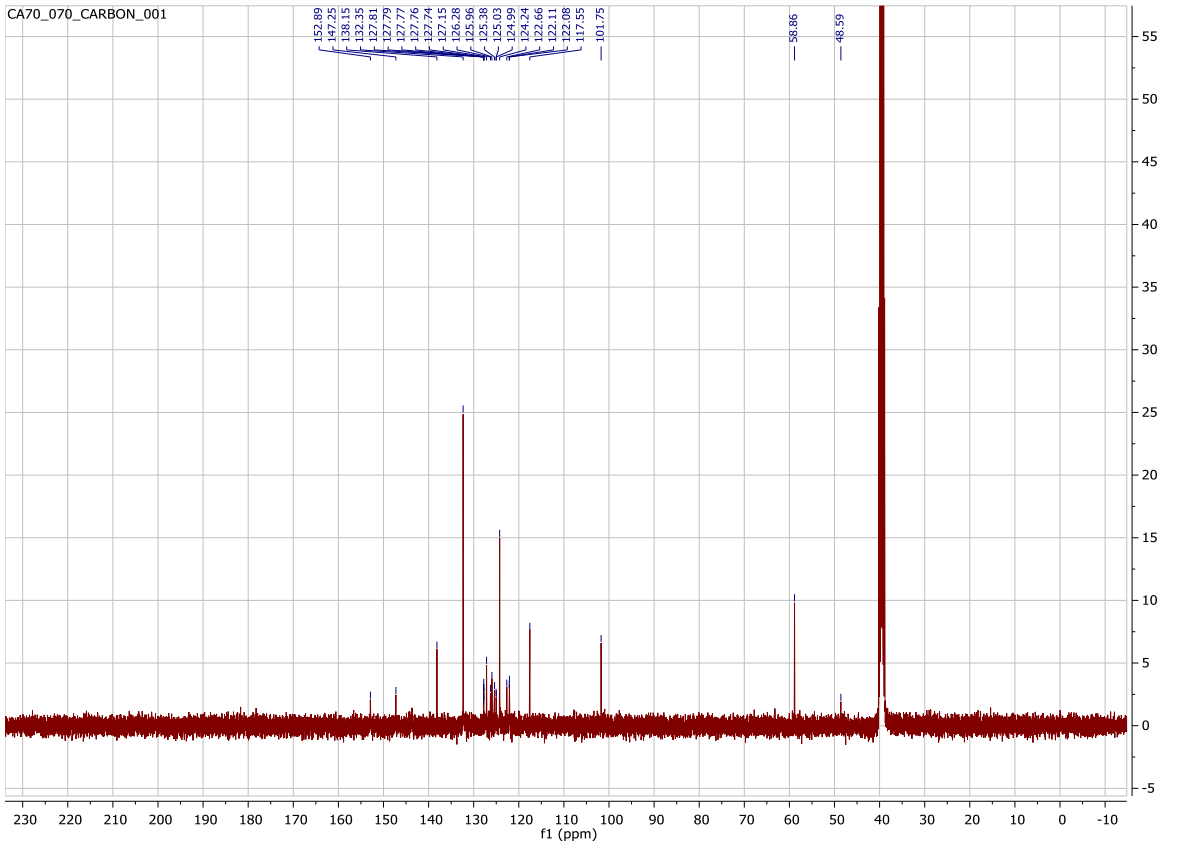
40

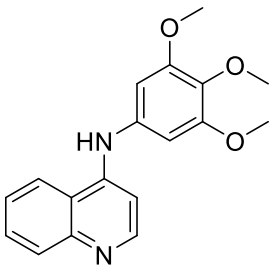
N-(4-((Methylsulfonyl)methyl)phenyl)-6-(trifluoromethyl)quinolin-4-amine (**40**)





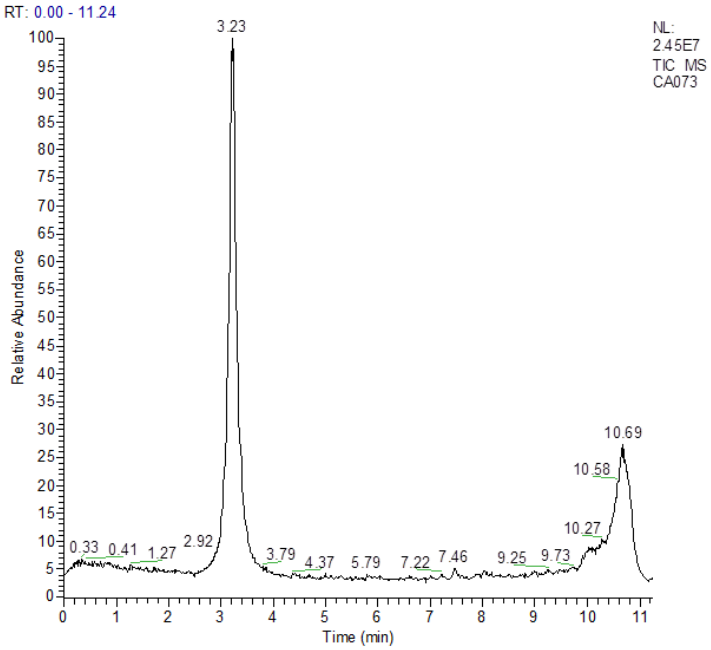

CA70_070_PROTON_001
10.78
9.22
8.60
8.39
8.24
8.22
8.20
8.19
8.17
7.58
7.56
7.52
7.50
7.00
6.98
4.57
2.96
1.01
0.99
1.00
1.99
3.98
0.99
1.99
2.99
f1 (ppm)

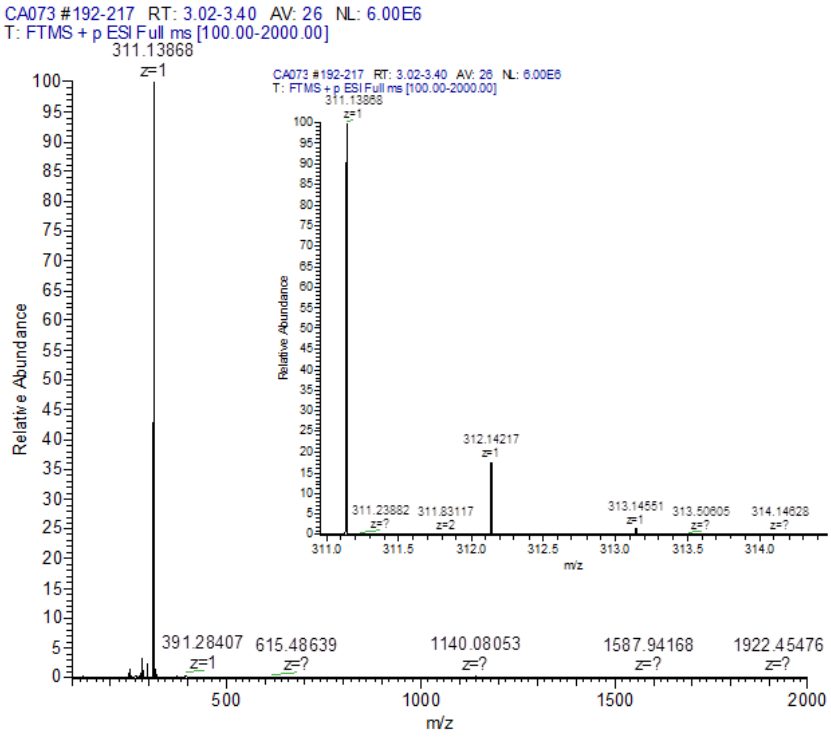

CA70_070_CARBON_001
152.89
147.25
138.15
132.35
127.81
127.79
127.77
127.76
127.74
127.15
126.28
125.96
125.38
125.03
124.99
124.24
122.66
122.11
122.08
117.55
101.75
58.86
48.59
f1 (ppm)

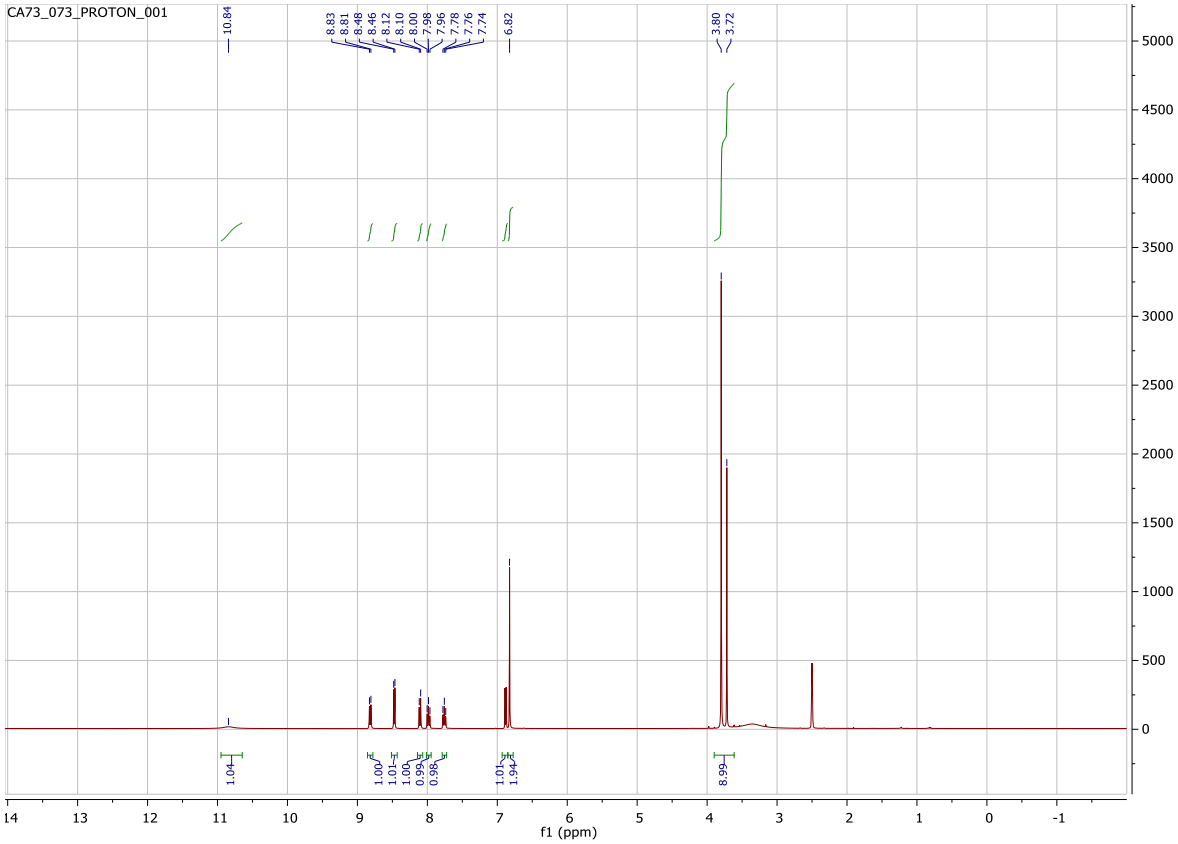


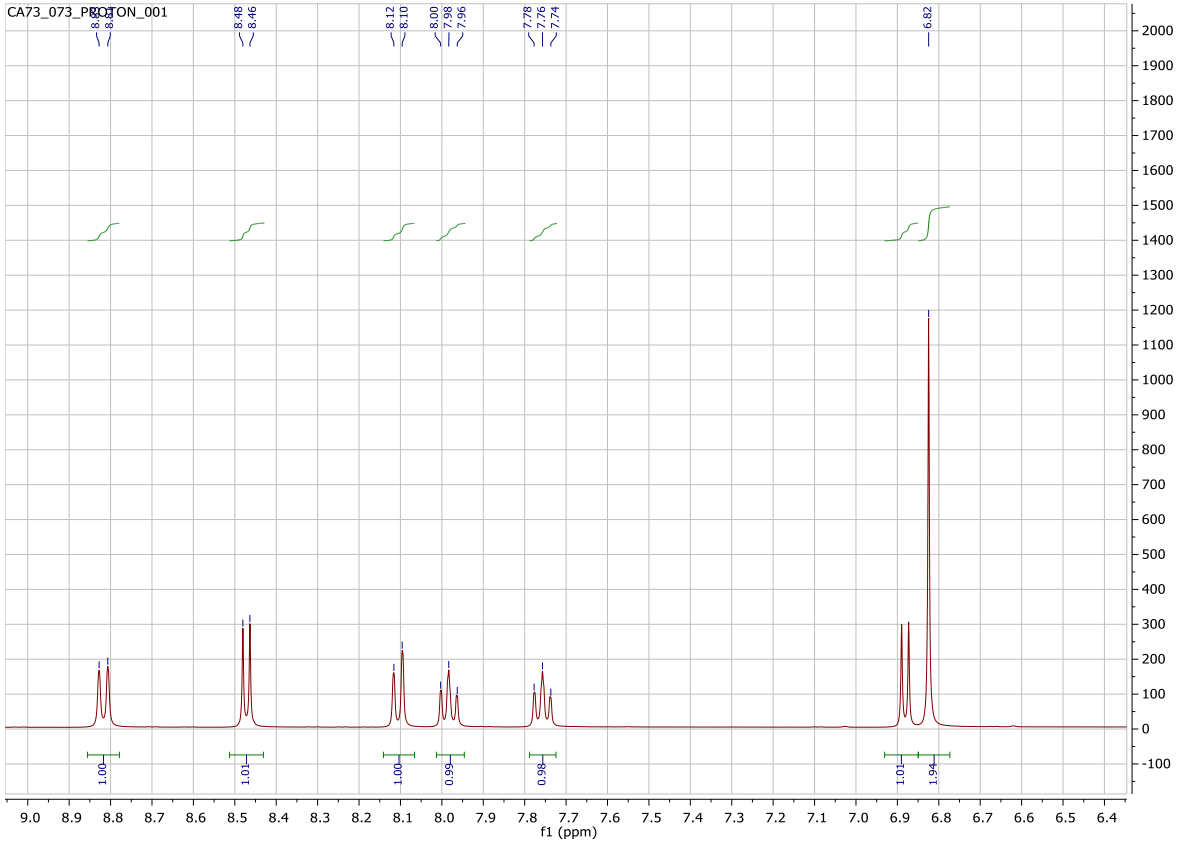
41

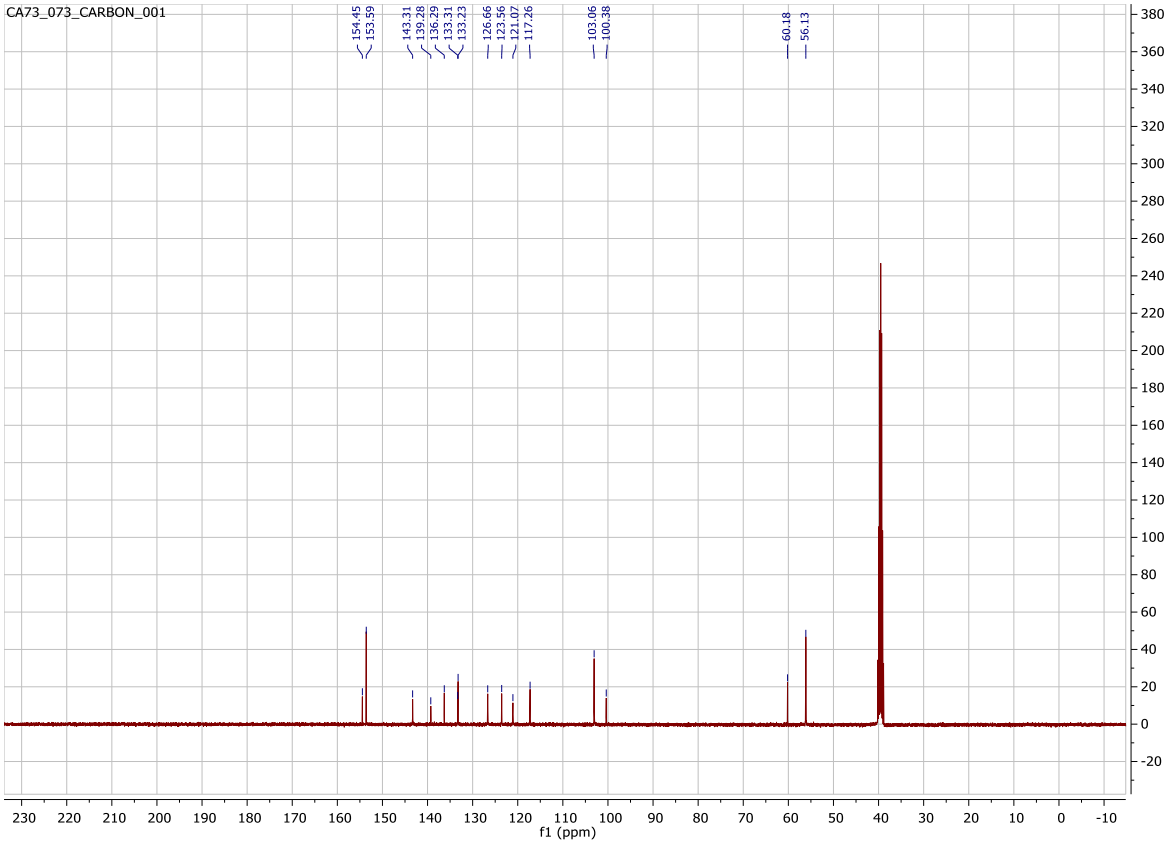
N-(3,4,5-Trimethoxyphenyl)quinolin-4-amine (**41**)

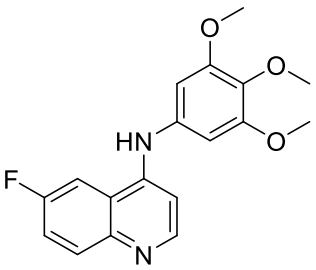





CA73_073_PROTON_001
10.84
8.83
8.81
8.48
8.46
8.12
8.10
8.00
7.98
7.96
7.78
7.76
7.74
6.82
3.80
3.72
1.04
1.00
1.01
1.00
0.99
0.98
1.01
1.94
8.99
f1 (ppm)

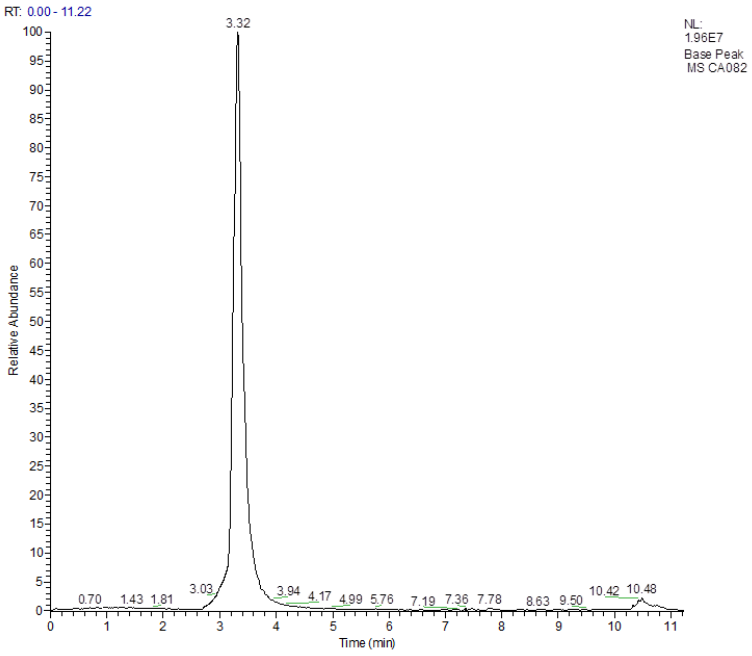

CA73_073_PROTON_001
8.48
8.46
8.12
8.10
8.00
7.98
7.96
7.78
7.76
7.74
6.82
1.00
1.01
1.00
0.99
0.98
1.01
1.94
f1 (ppm)

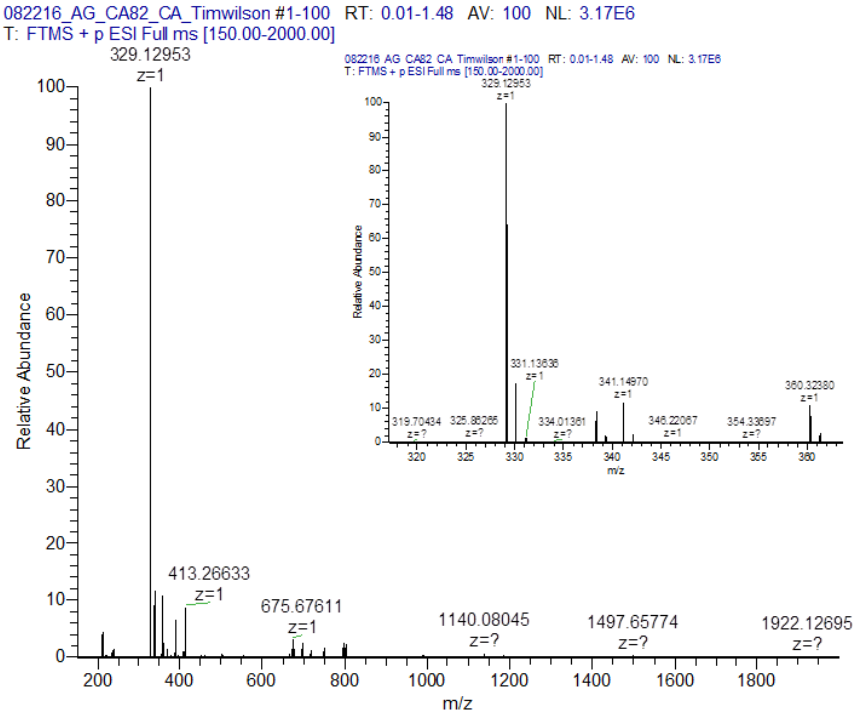

CA73_073_CARBON_001
154.45
153.59
143.31
139.28
136.29
133.31
133.23
126.66
123.56
121.07
117.26
103.06
100.38
60.18
56.13
f1 (ppm)

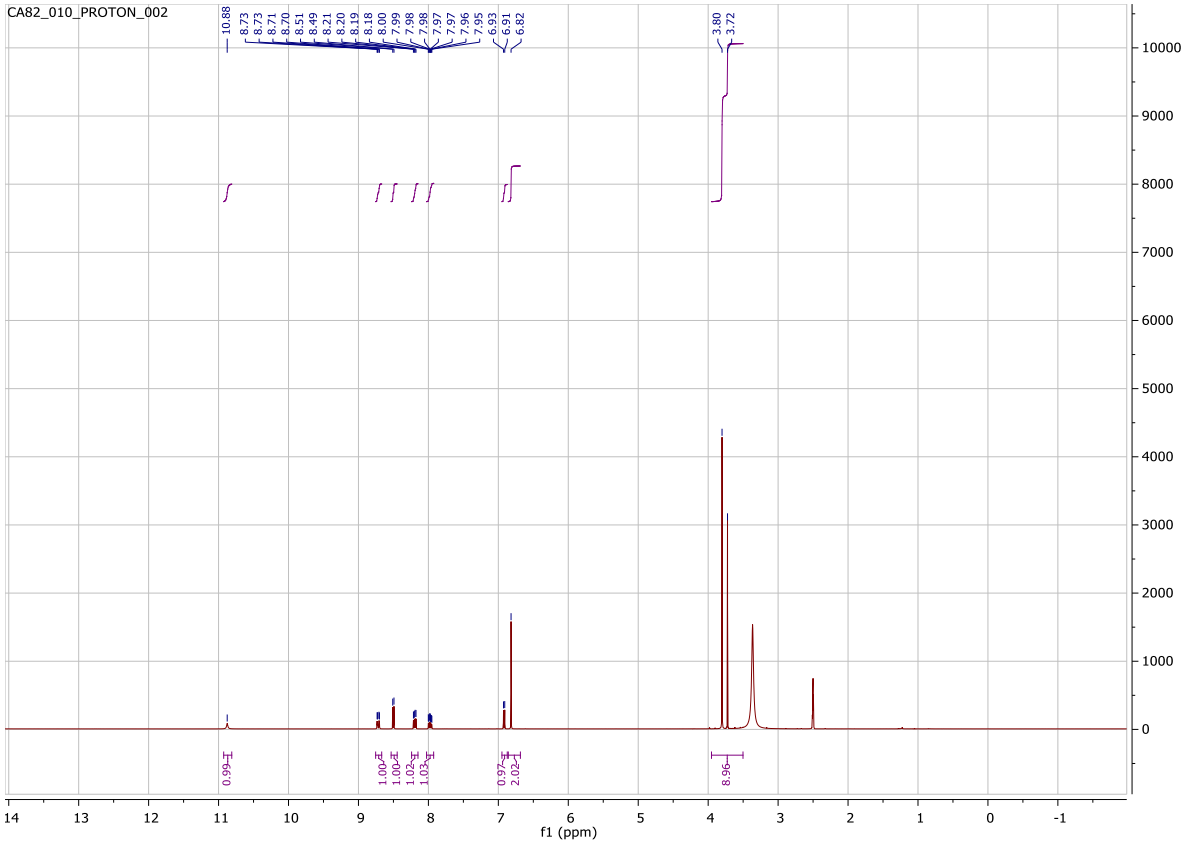


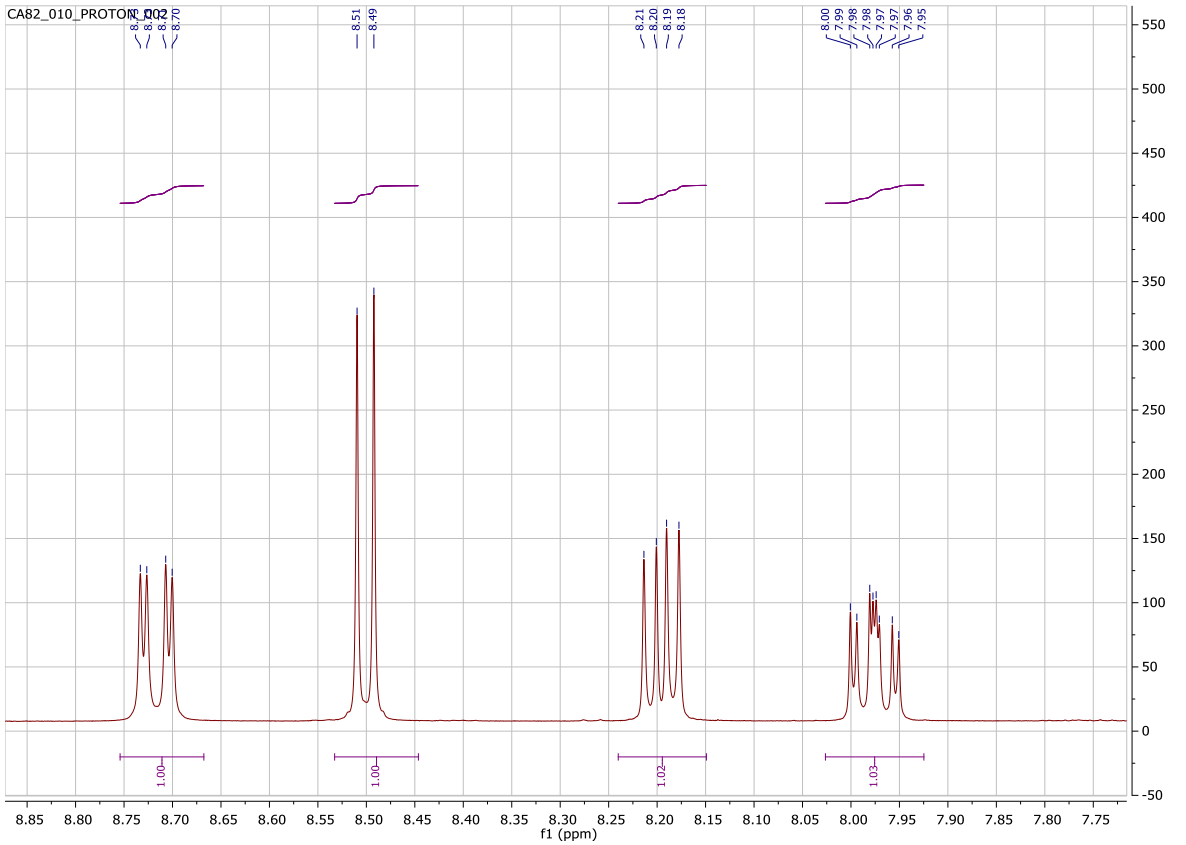
42

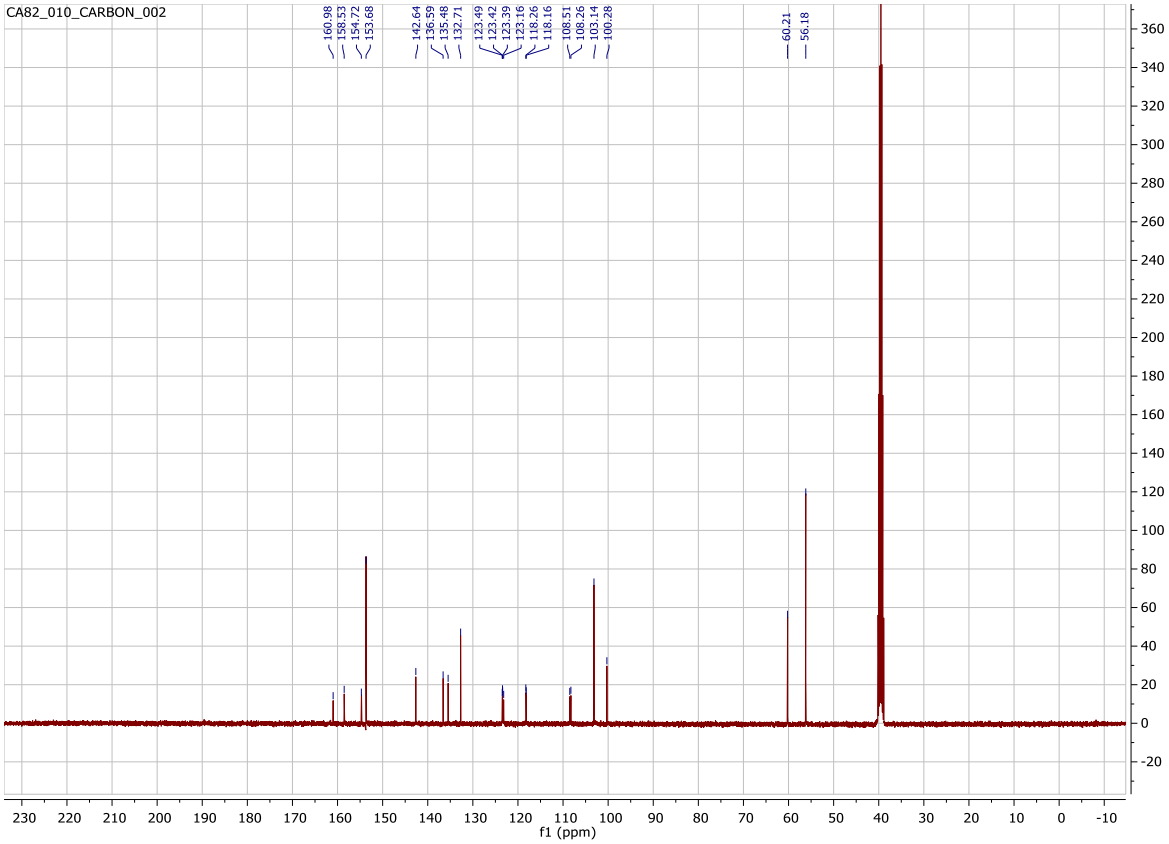
6-Fluoro-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**42**)

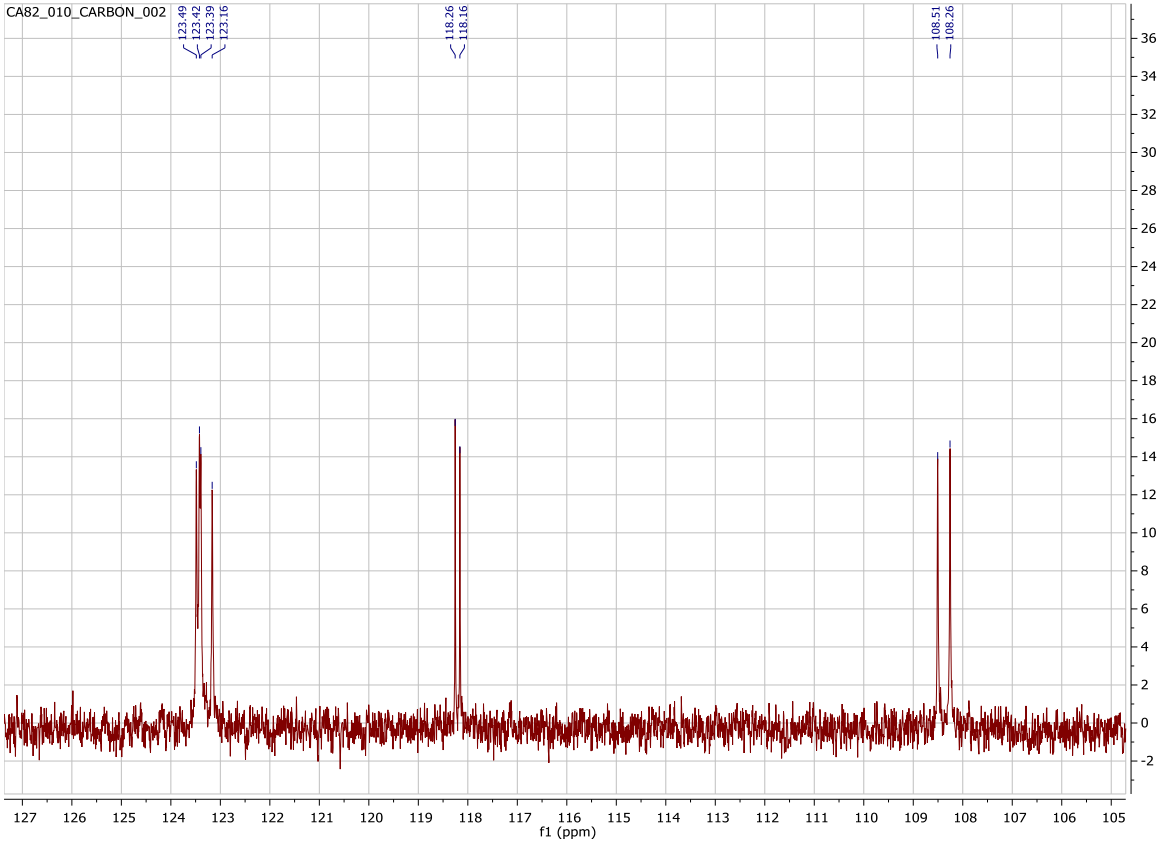


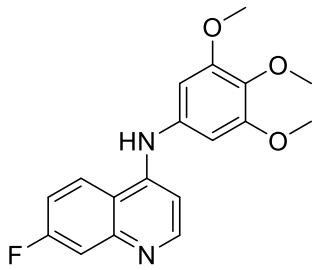



CA82_010_PROTON_002
10.88
8.73
8.73
8.71
8.70
8.51
8.49
8.21
8.20
8.19
8.18
8.00
7.99
7.98
7.98
7.97
7.97
7.96
7.95
6.93
6.91
6.82
3.80
3.72
0.99
1.00
1.00
1.02
1.03
0.97
2.02
8.96
f1 (ppm)


CA82_010_PROTON_002
8.70
8.51
8.49
8.21
8.20
8.19
8.18
8.00
7.99
7.98
7.98
7.97
7.97
7.96
7.95
1.00
1.00
1.02
1.03
f1 (ppm)

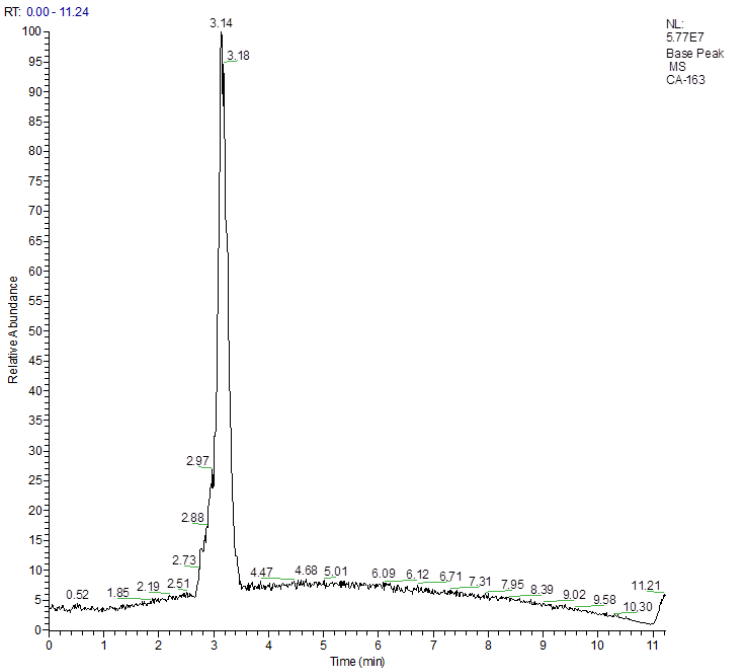

CA82_010_CARBON_002
160.98
158.53
154.72
153.68
142.64
136.59
135.48
132.71
123.49
123.42
123.39
123.16
118.26
118.16
108.51
108.26
103.14
100.28
60.21
56.18
f1 (ppm)

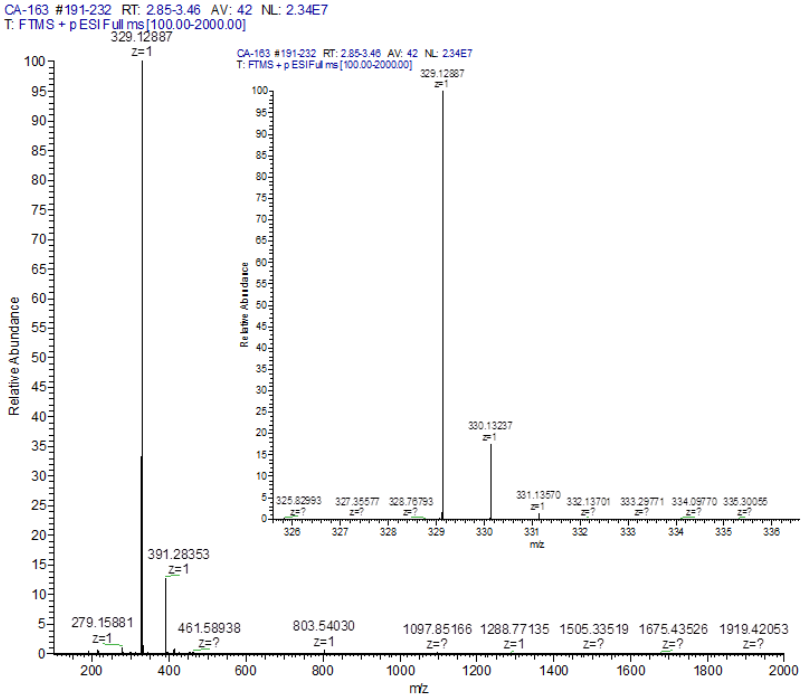

CA82_010_CARBON_002
123.49
123.42
123.39
123.16
118.26
118.16
108.51
108.26
f1 (ppm)

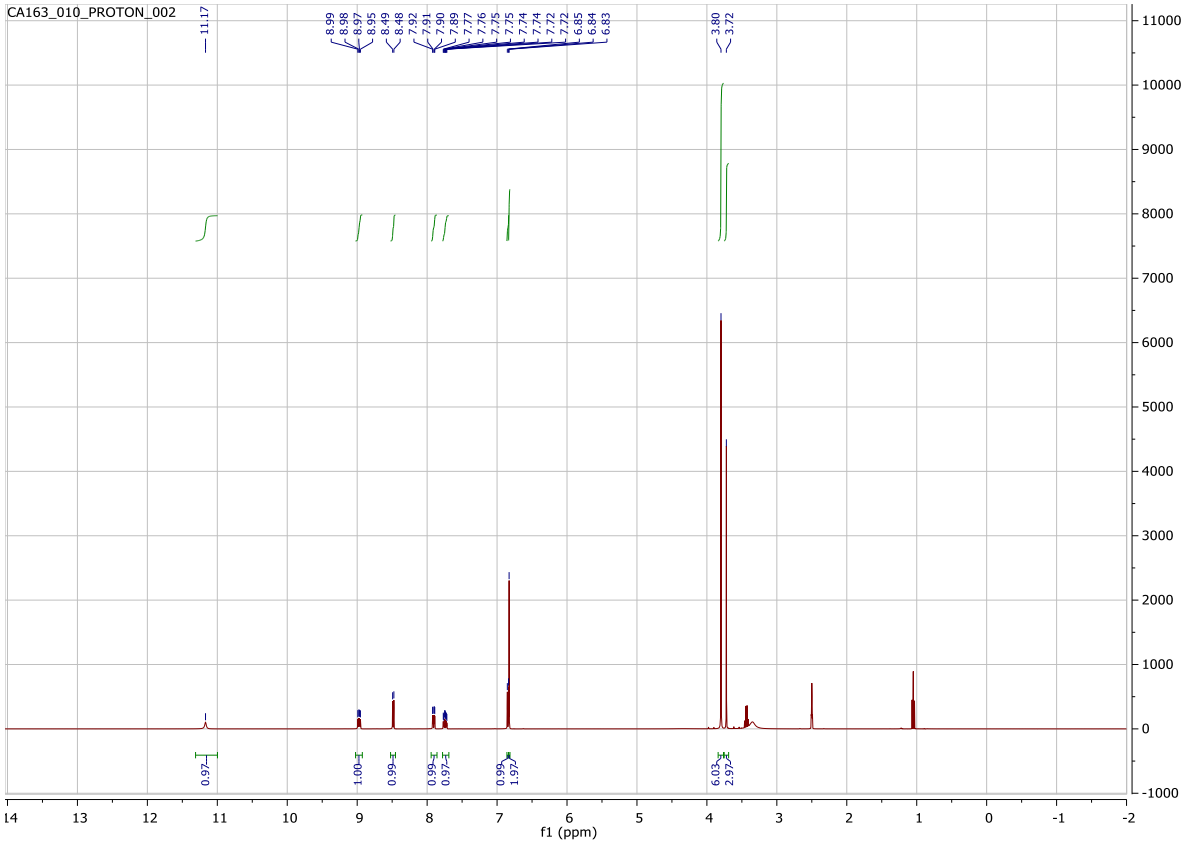


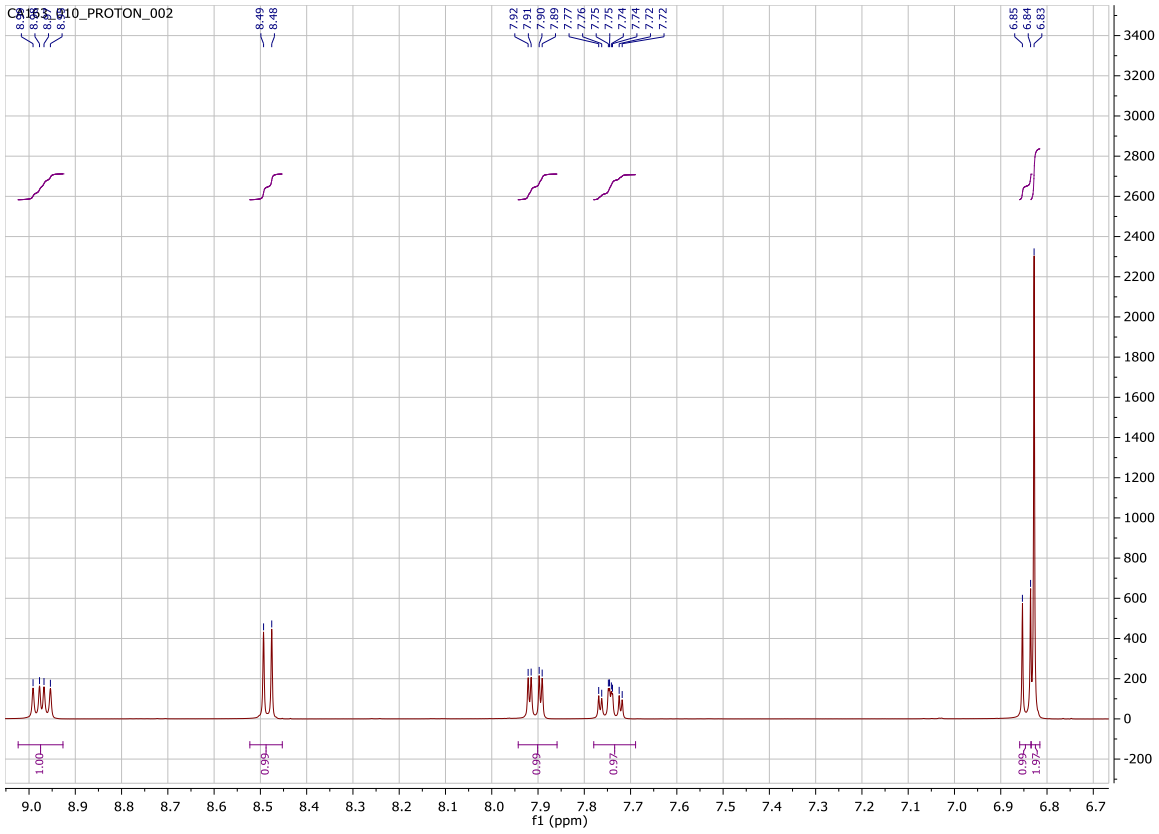
43

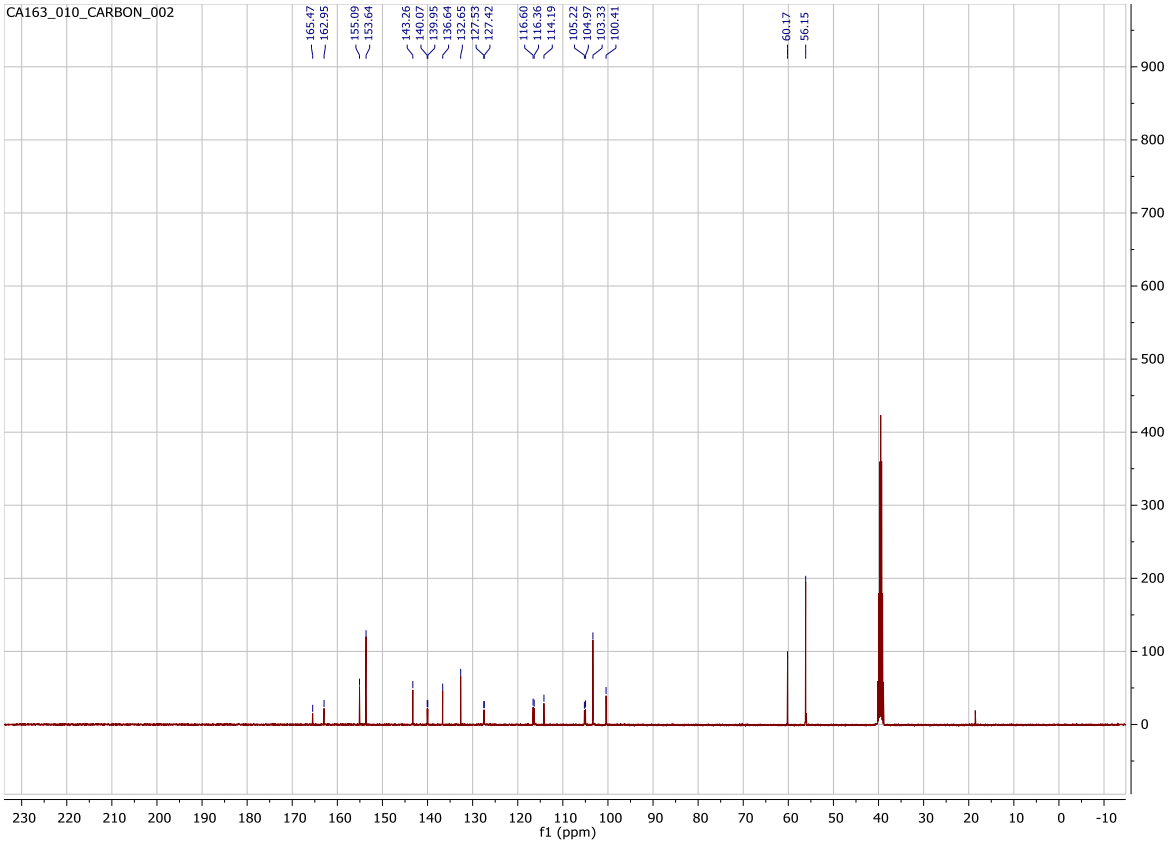
7-Fluoro-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**43**)

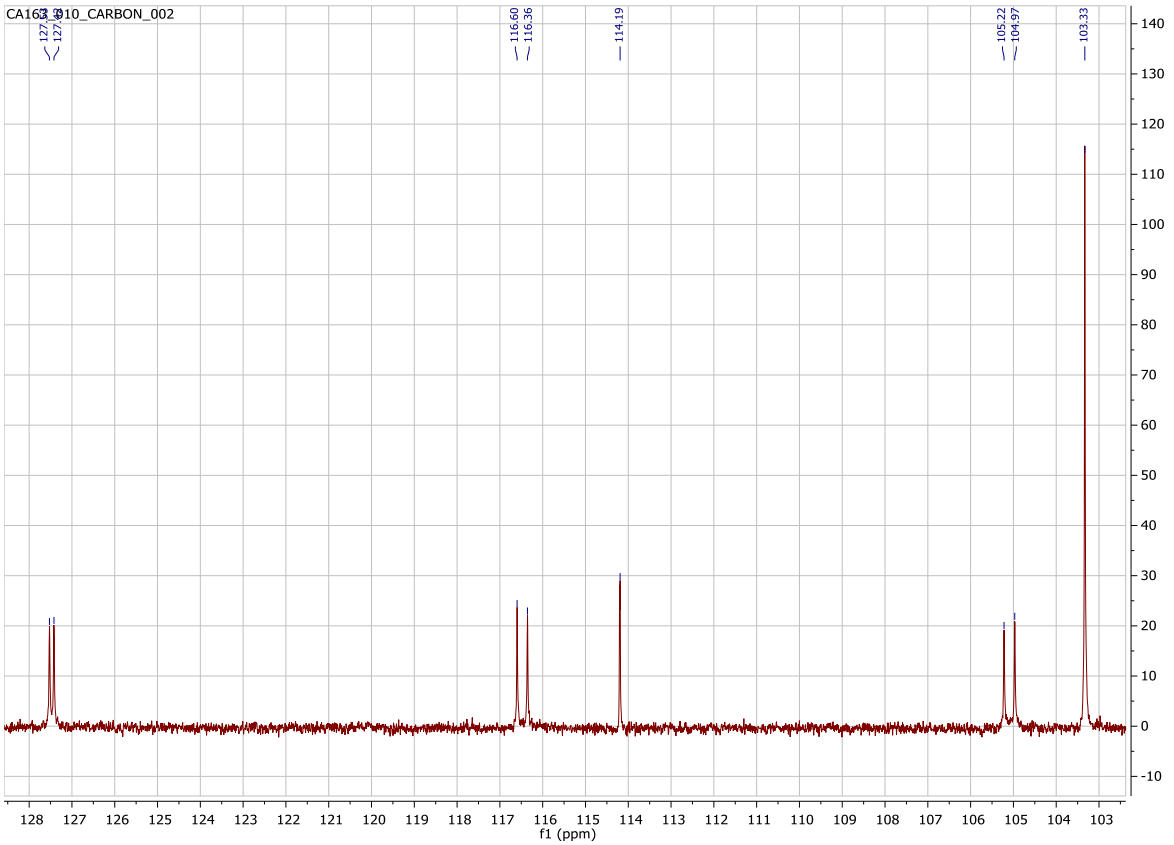


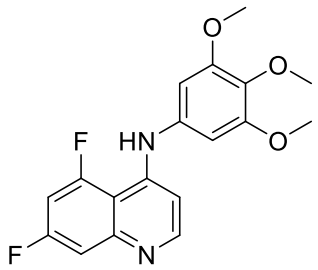



CA163_010_PROTON_002
11.17
8.99
8.98
8.97
8.95
8.49
8.48
7.92
7.91
7.90
7.89
7.77
7.76
7.75
7.75
7.74
7.74
7.72
7.72
6.85
6.84
6.83
3.80
3.72
0.97
1.00
0.99
0.99
0.97
0.99
1.97
6.03
2.97
f1 (ppm)


CA163_010_PROTON_002
8.49
8.48
7.92
7.91
7.90
7.89
7.77
7.76
7.75
7.75
7.74
7.74
7.72
7.72
6.85
6.84
6.83
1.00
0.99
0.99
0.97
0.99
1.97
f1 (ppm)

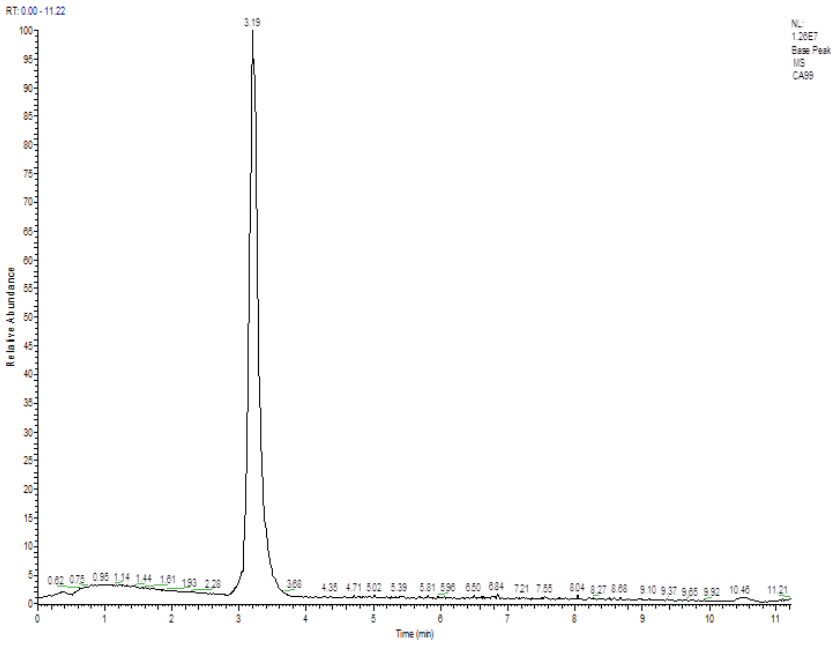

CA163_010_CARBON_002
165.47
162.95
155.09
153.64
143.26
140.07
139.95
136.64
132.65
127.53
127.42
116.60
116.36
114.19
105.22
104.97
103.33
100.41
60.17
56.15
f1 (ppm)

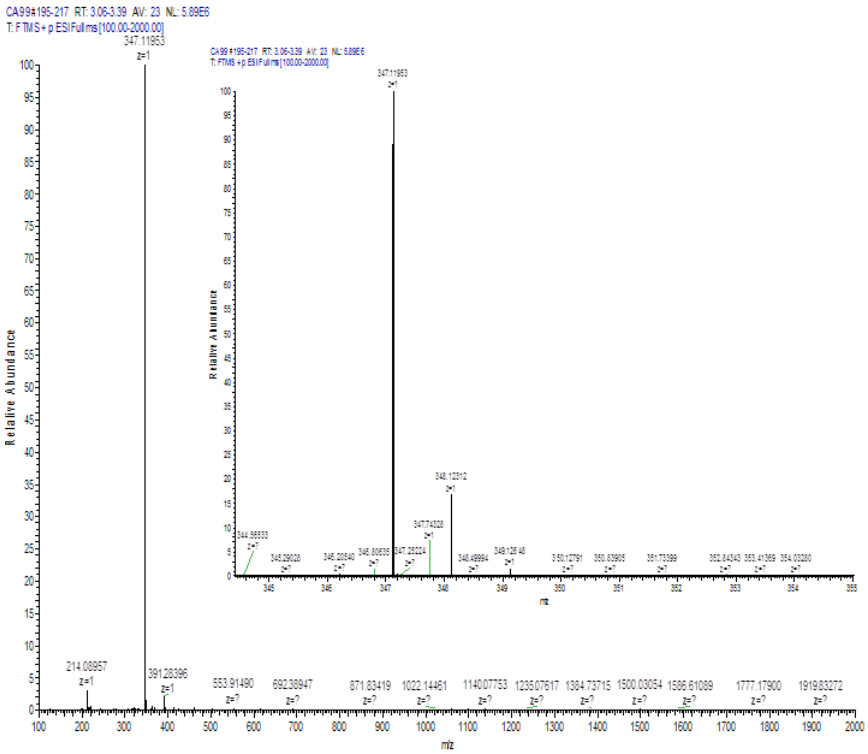

CA163_010_CARBON_002
127.53
127.42
116.60
116.36
114.19
105.22
104.97
103.33
f1 (ppm)

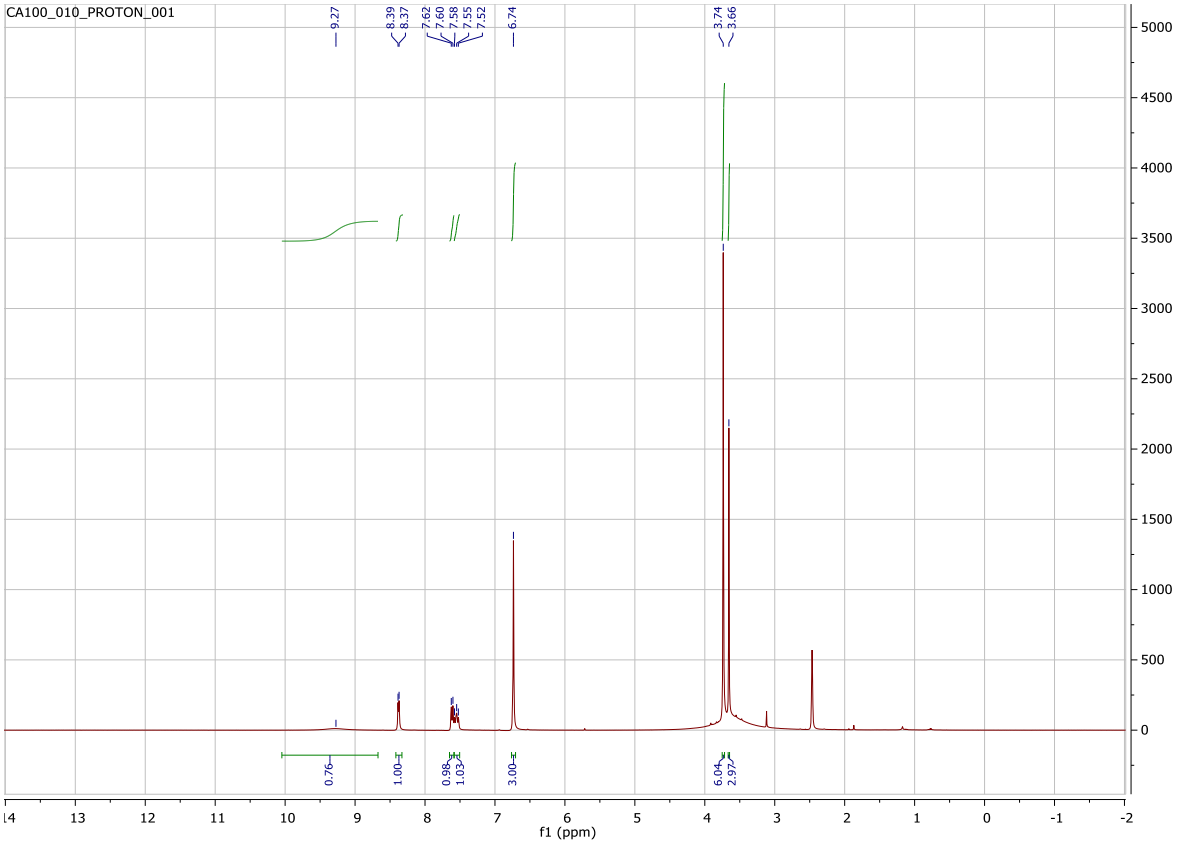


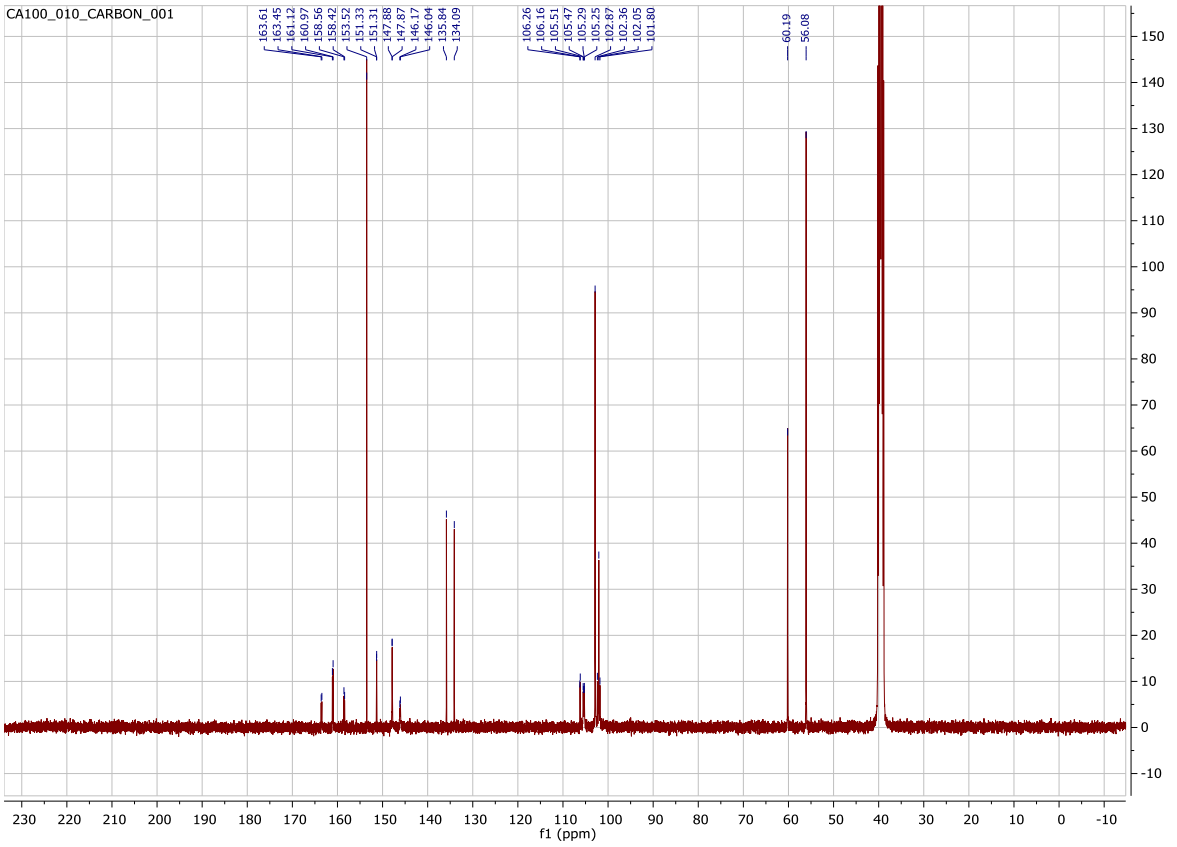
44

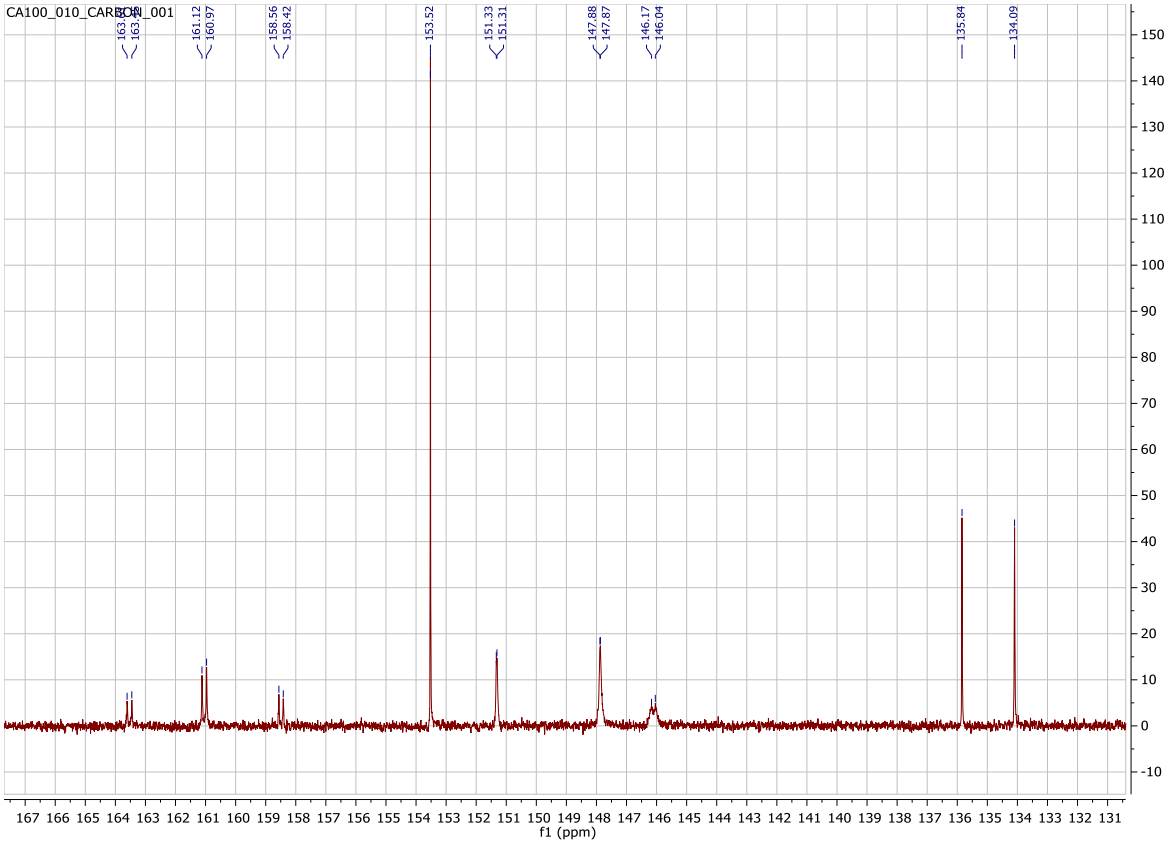
5,7-Difluoro-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**44**)

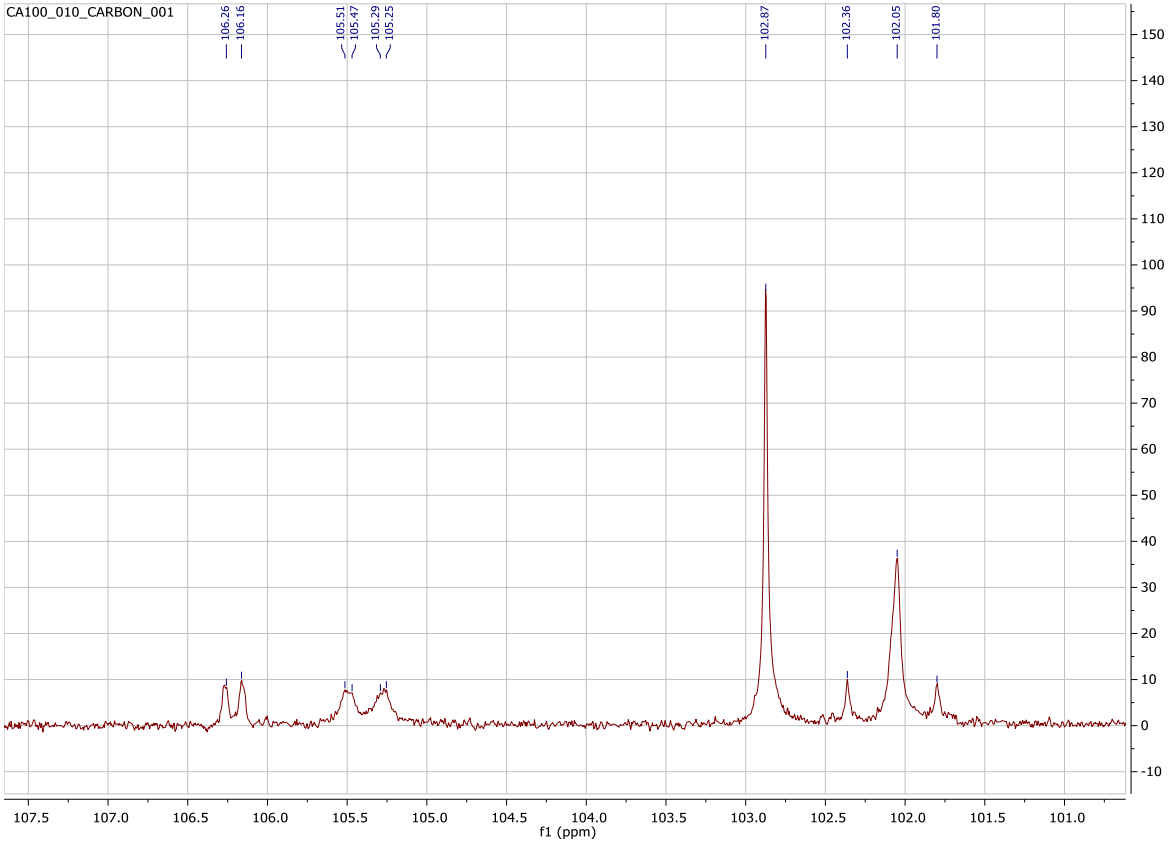


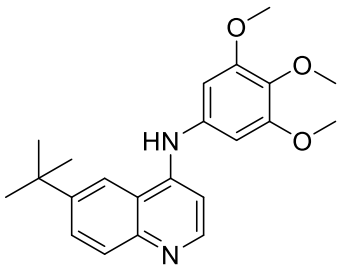



CA100_010_PROTON_001
9.27
8.39
8.37
7.62
7.60
7.58
7.55
7.52
6.74
3.74
3.66
0.76
1.00
0.98
1.03
3.00
6.04
2.97
f1 (ppm)


CA100_010_CARBON_001
163.61
163.45
161.12
160.97
158.56
158.42
153.52
151.33
147.88
147.87
146.17
146.04
135.84
134.09
106.26
106.16
105.51
105.47
105.29
105.25
102.87
102.36
102.05
101.80
60.19
56.08
f1 (ppm)

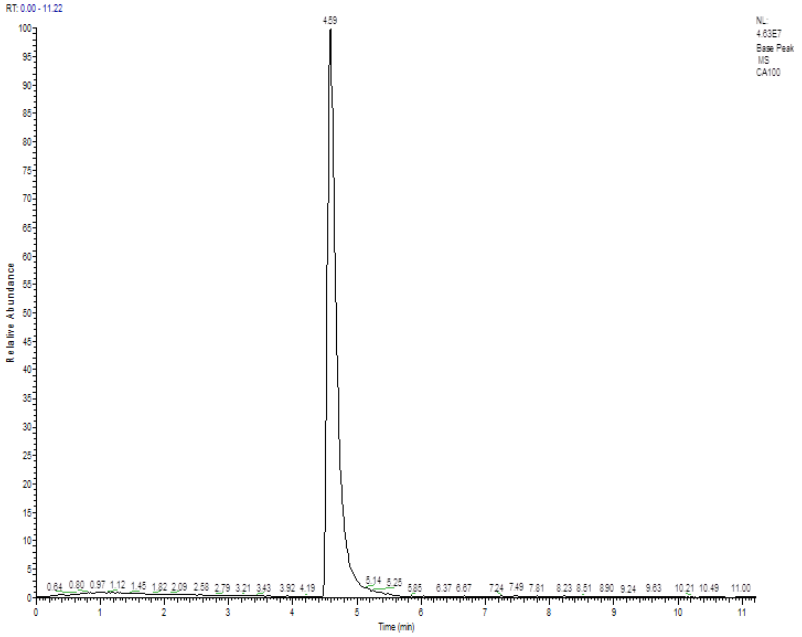

CA100_010_CARBON_001
163.84
163.47
161.12
160.97
158.56
158.42
153.52
151.33
151.31
147.88
147.87
146.17
146.04
135.84
134.09
f1 (ppm)

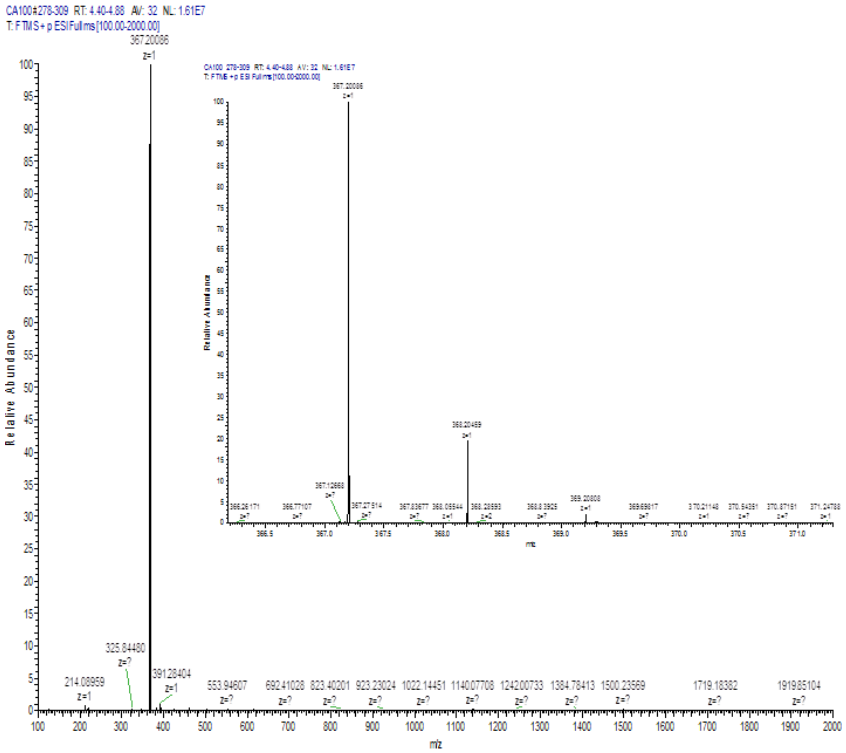

CA100_010_CARBON_001
106.26
106.16
105.51
105.47
105.29
105.25
102.87
102.36
102.05
101.80
f1 (ppm)

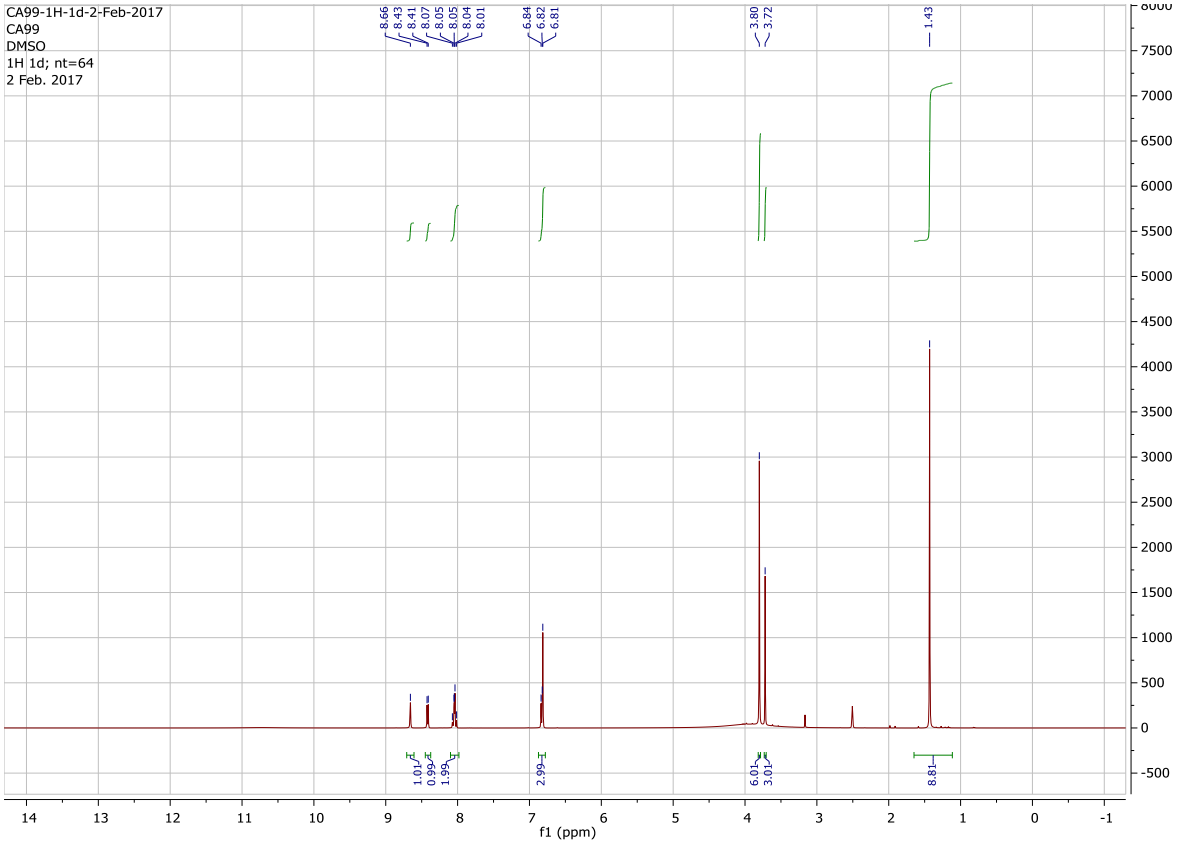


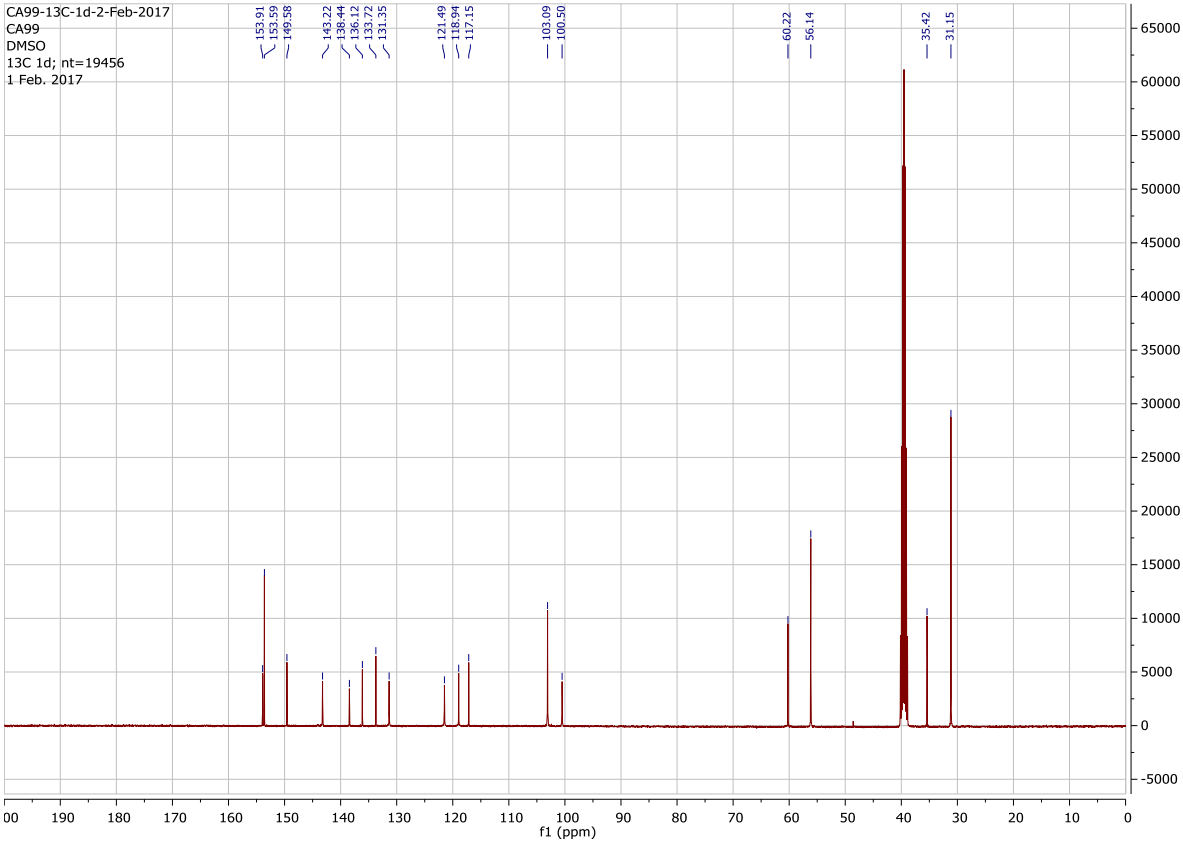
45

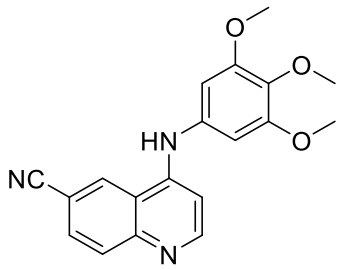
6-(*tert*-Butyl)-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**45**)





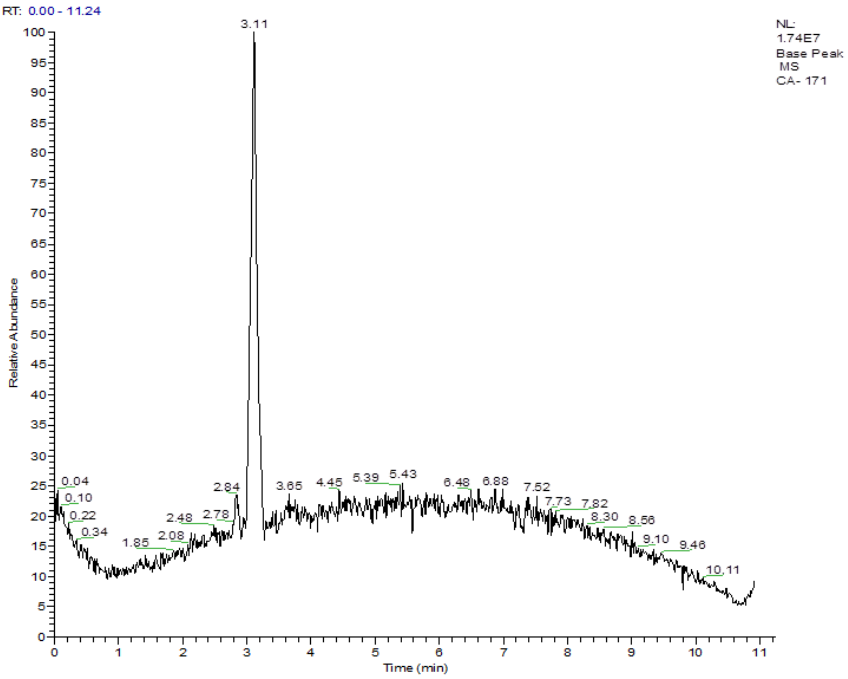

CA99-1H-1d-2-Feb-2017
CA99
DMSO
1H 1d; nt=64
2 Feb. 2017
8.66
8.43
8.41
8.07
8.05
8.05
8.04
8.01
6.84
6.82
6.81
3.80
3.72
1.43
1.01
0.99
1.99
2.99
6.01
3.01
8.81
f1 (ppm)

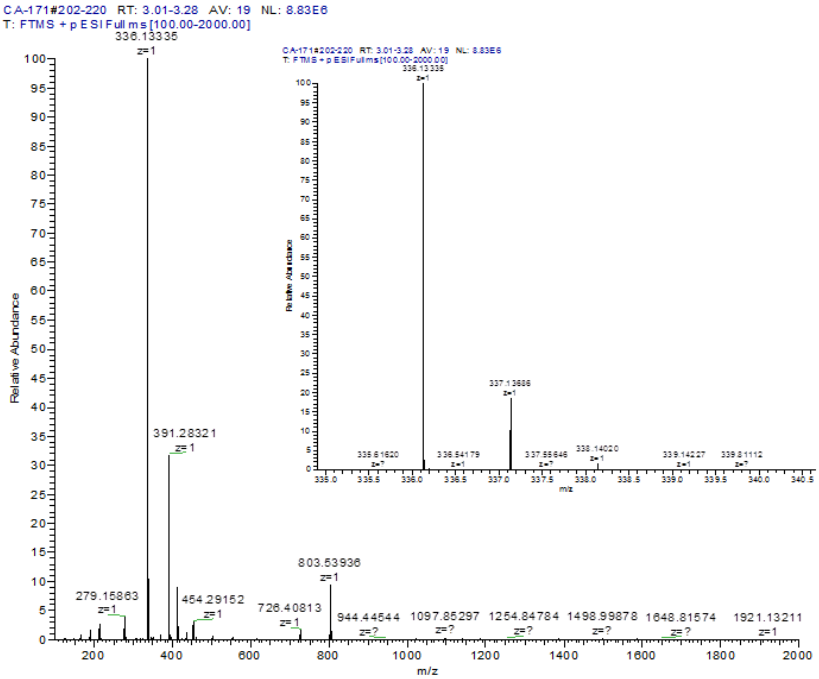

CA99-13C-1d-2-Feb-2017
CA99
DMSO
13C 1d; nt=19456
1 Feb. 2017
153.91
153.59
149.58
143.22
138.44
136.12
133.72
131.35
121.49
118.94
117.15
103.09
100.50
60.22
56.14
35.42
31.15
f1 (ppm)

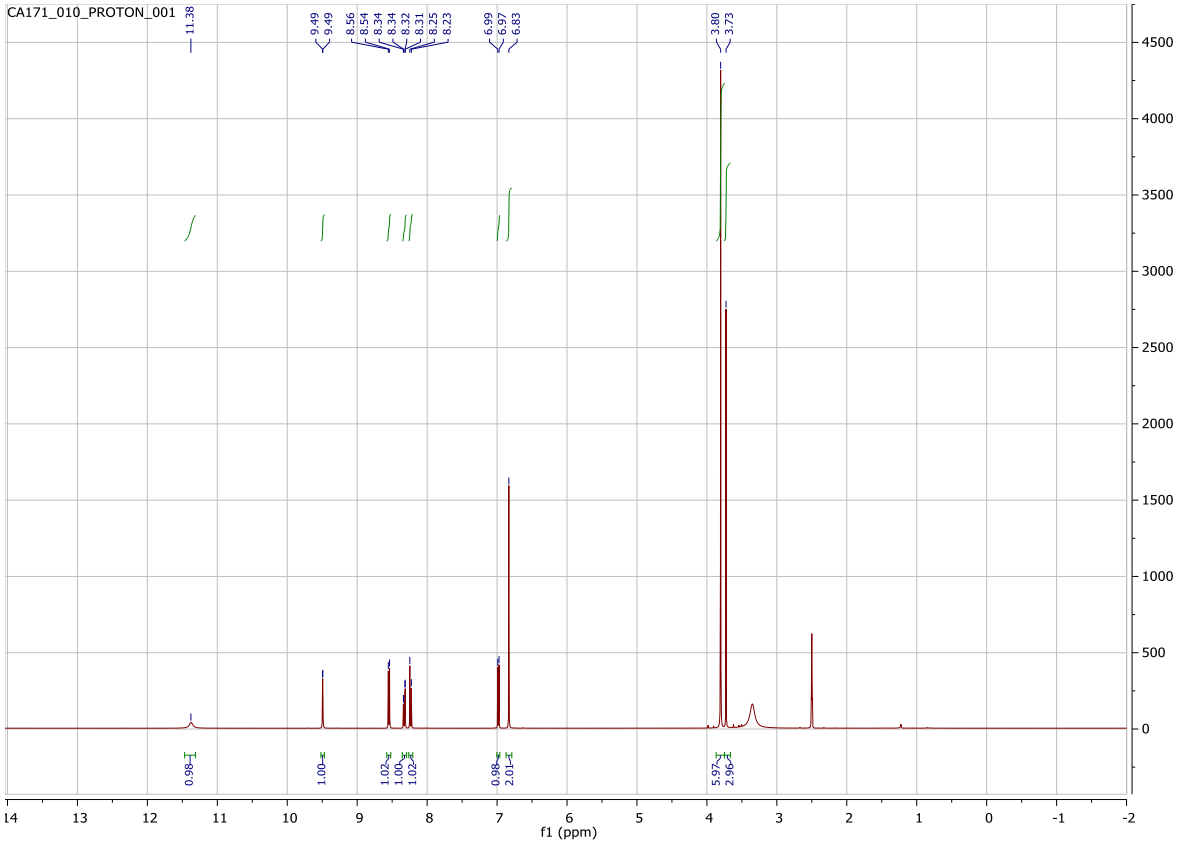


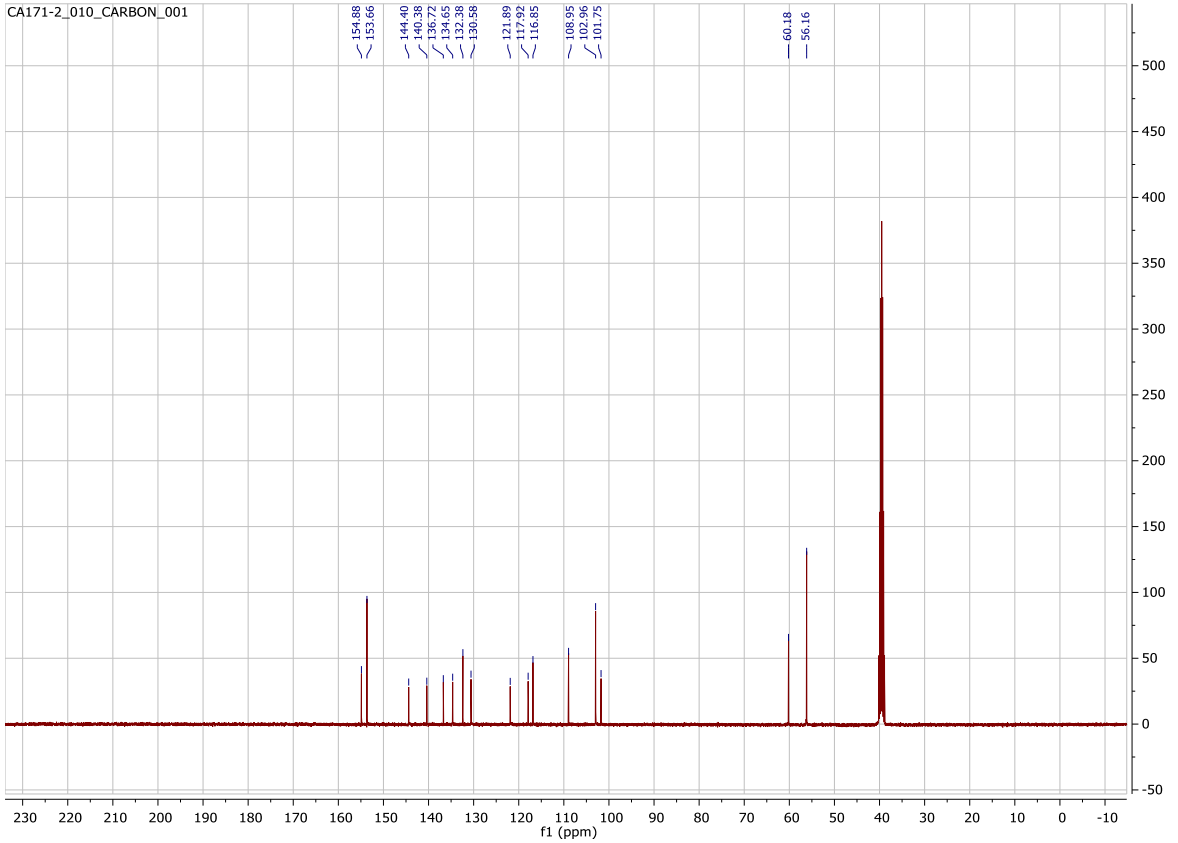
46

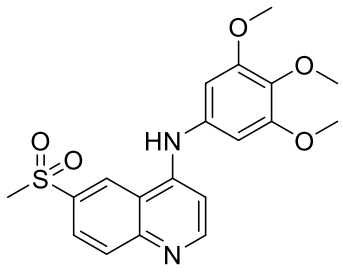
4-((3,4,5-Trimethoxyphenyl)amino)quinoline-6-carbonitrile (**46**)





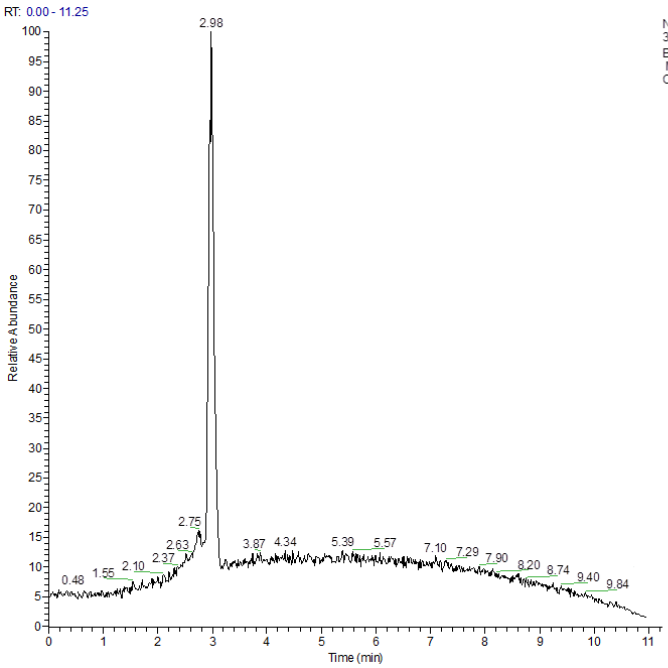

CA171_010_PROTON_001
11.38
9.49
9.49
8.56
8.54
8.34
8.34
8.32
8.31
8.25
8.23
6.99
6.97
6.83
3.80
3.73
0.98
1.00
1.02
1.00
1.02
0.98
2.01
5.97
2.96
f1 (ppm)

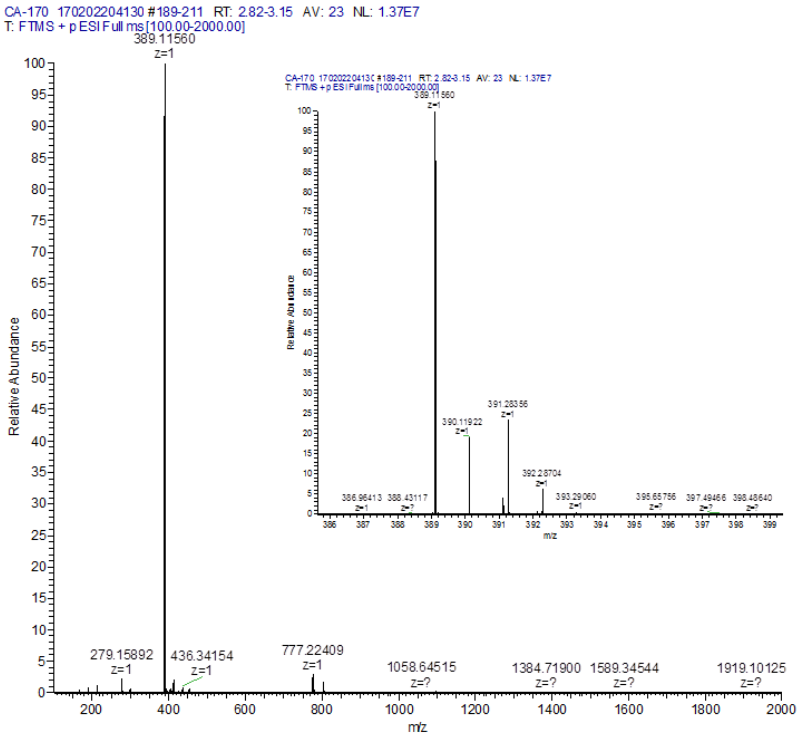

CA171-2_010_CARBON_001
154.88
153.66
144.40
140.38
136.72
134.65
132.38
130.58
121.89
117.92
116.85
108.95
102.96
101.75
60.18
56.16
f1 (ppm)

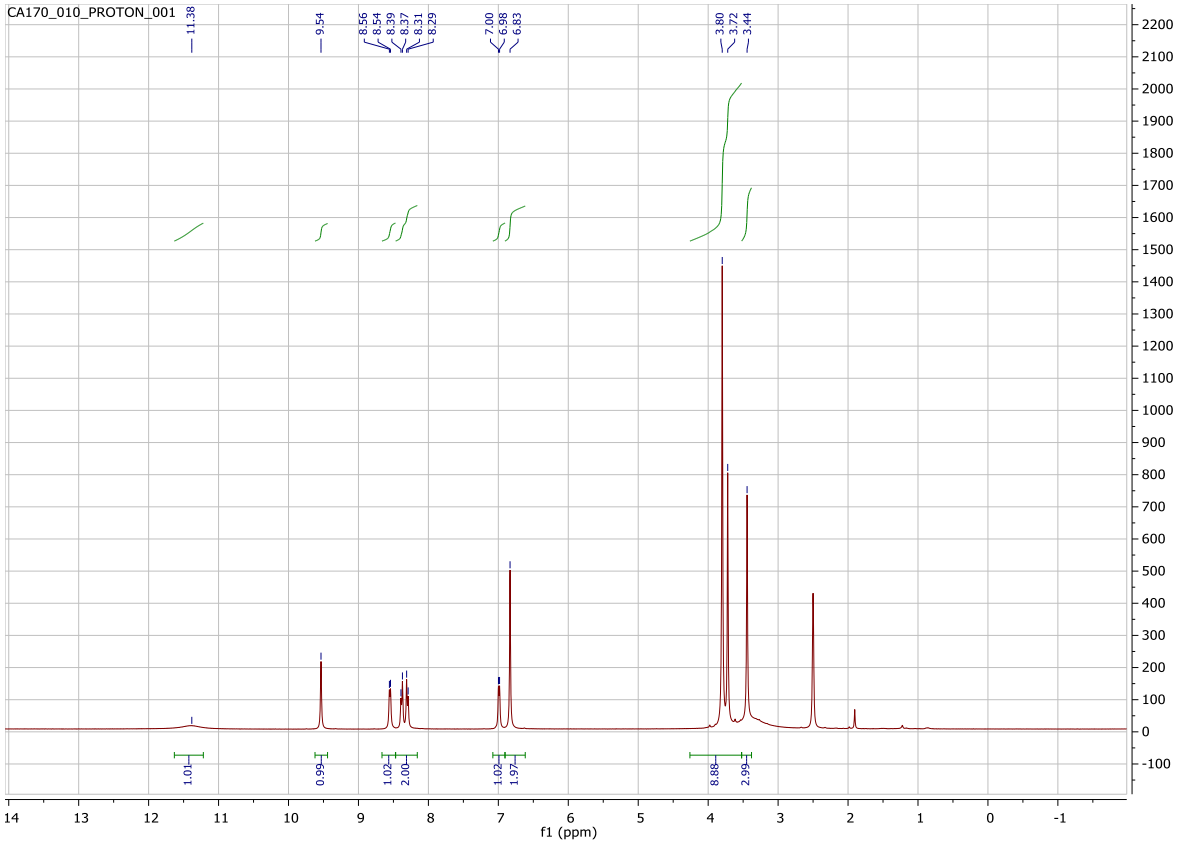


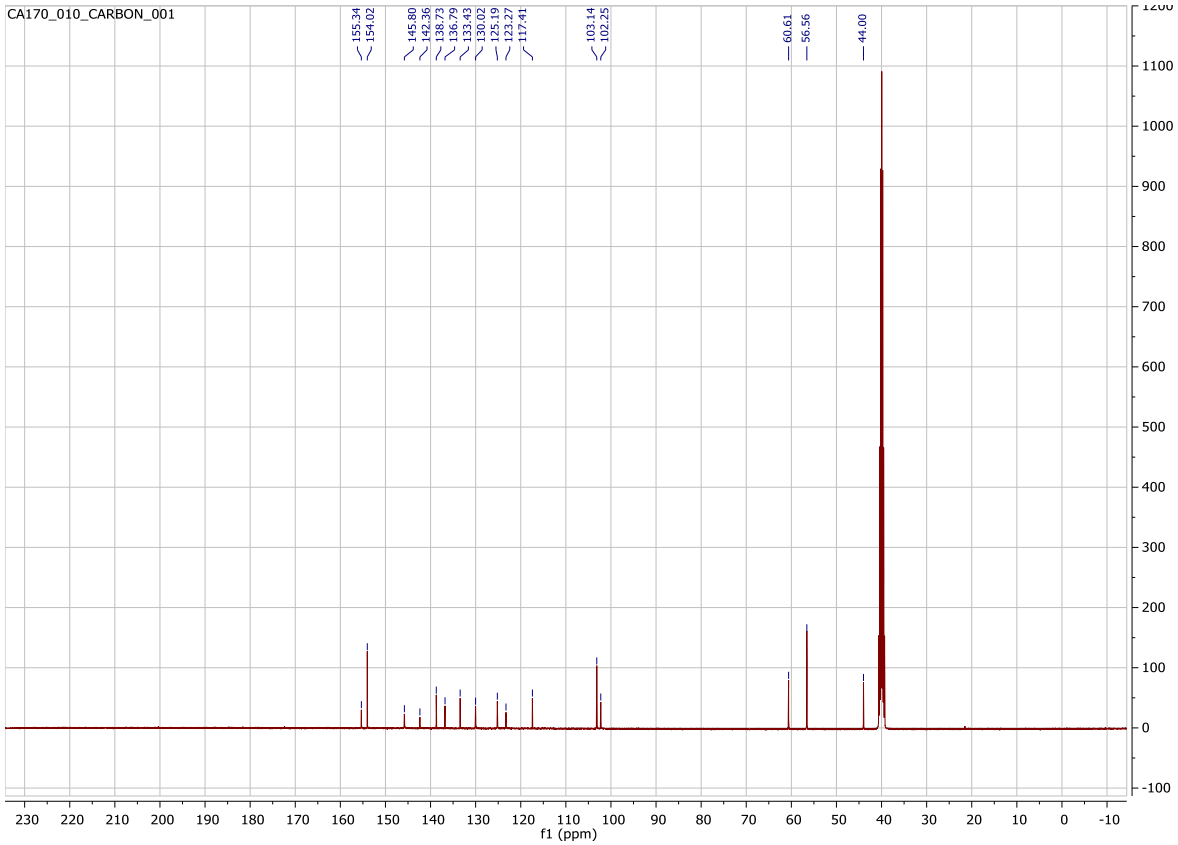
47

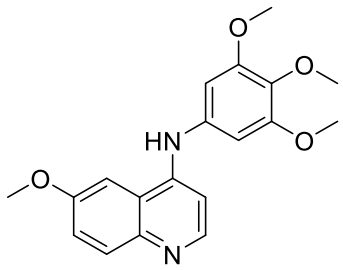
6-(Methylsulfonyl)-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**47**)





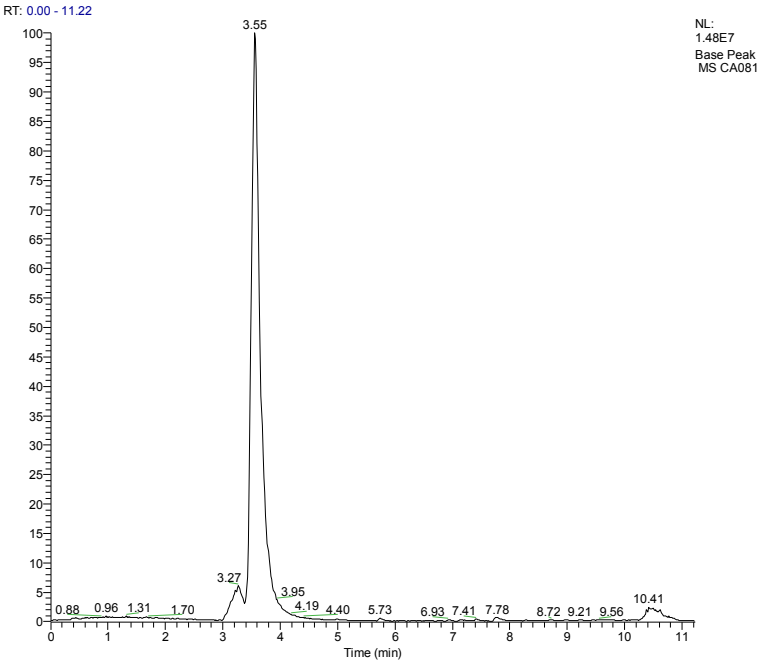

CA170_010_PROTON_001
11.38
9.54
8.56
8.54
8.39
8.37
8.31
8.29
7.00
6.98
6.83
3.80
3.72
3.44
1.01
0.99
1.02
2.00
1.02
1.97
8.88
2.99
f1 (ppm)

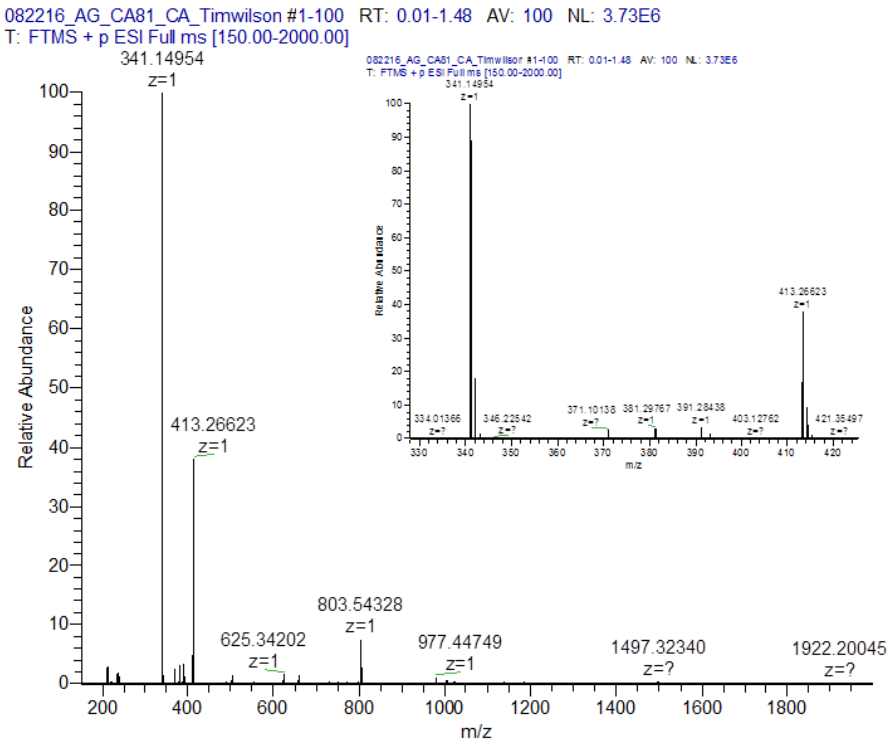

CA170_010_CARBON_001
155.34
154.02
145.80
142.36
138.73
136.79
133.43
130.02
125.19
123.27
117.41
103.14
102.25
60.61
56.56
44.00
f1 (ppm)

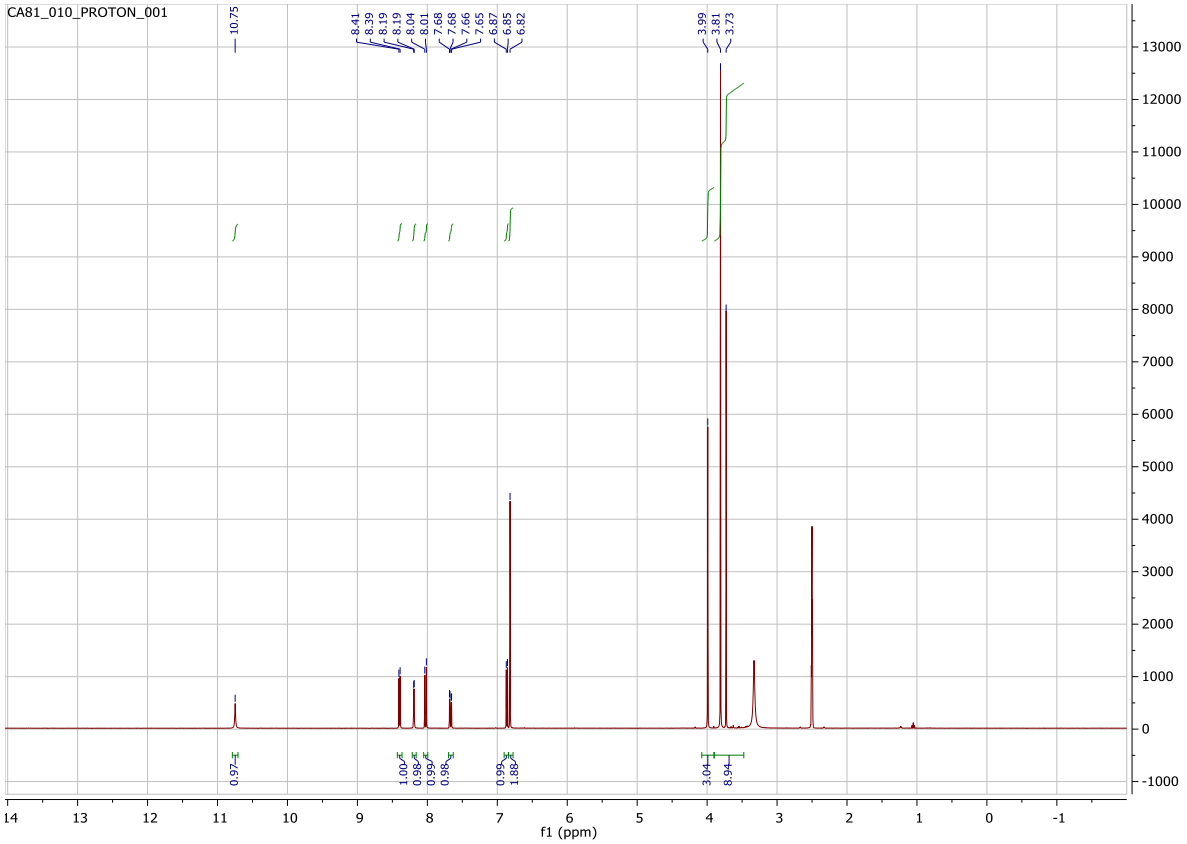


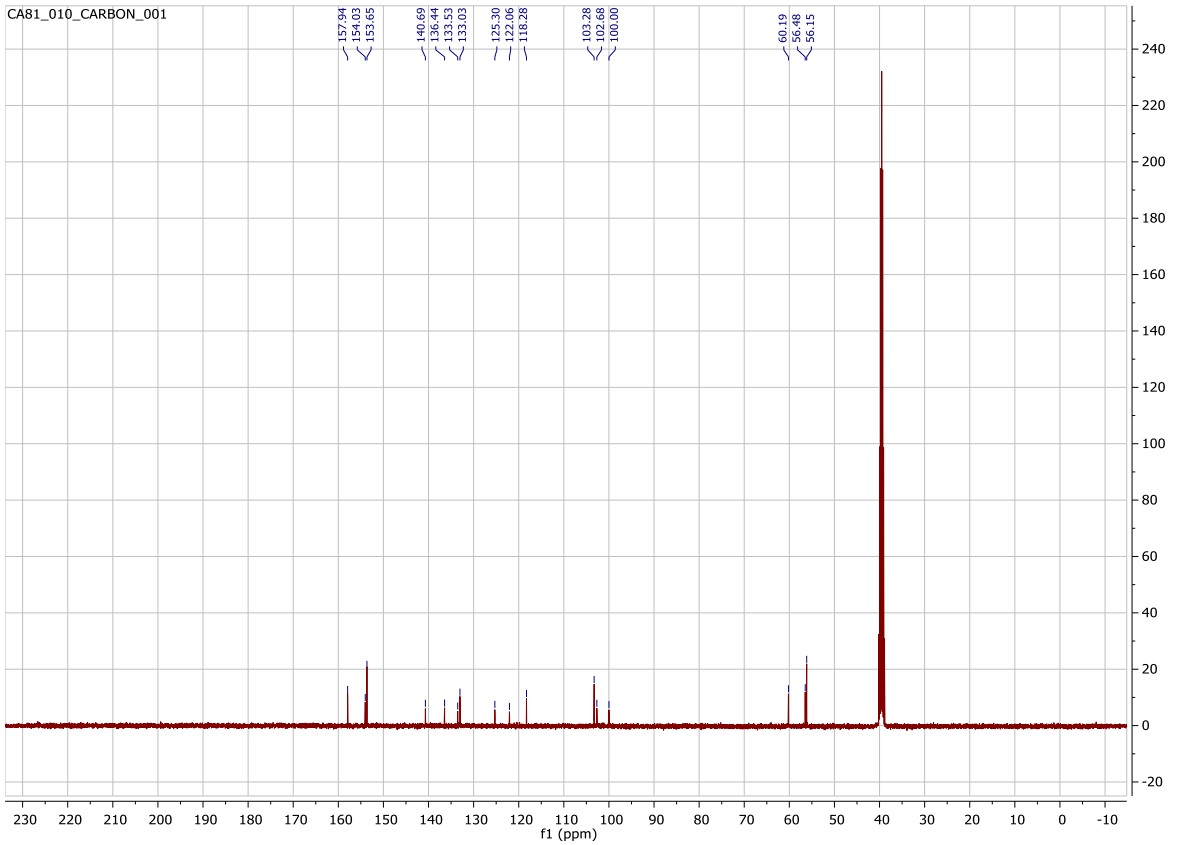
48

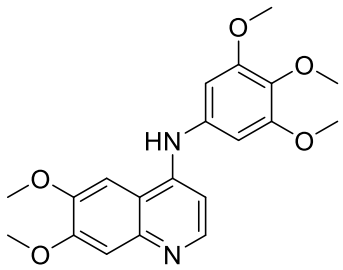
6-Methoxy-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**48**)





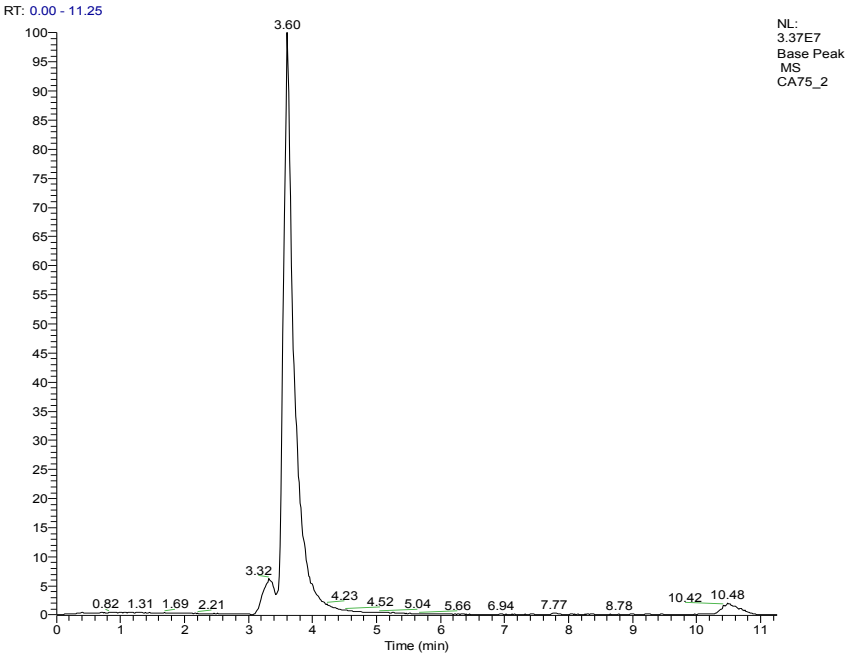

CA81_010_PROTON_001
10.75
8.41
8.39
8.19
8.19
8.04
8.01
7.68
7.68
7.66
7.65
6.87
6.85
6.82
3.99
3.81
3.73
0.97
1.00
0.98
0.99
0.98
0.99
1.88
3.04
8.94
f1 (ppm)

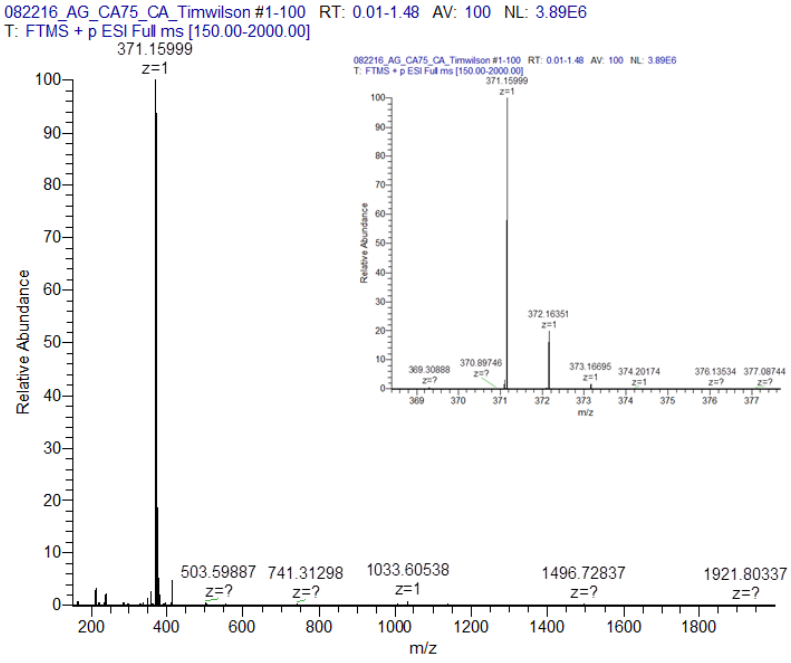

CA81_010_CARBON_001
157.94
154.03
153.65
140.69
136.44
133.53
133.03
125.30
122.06
118.28
103.28
102.68
100.00
60.19
56.48
56.15
f1 (ppm)

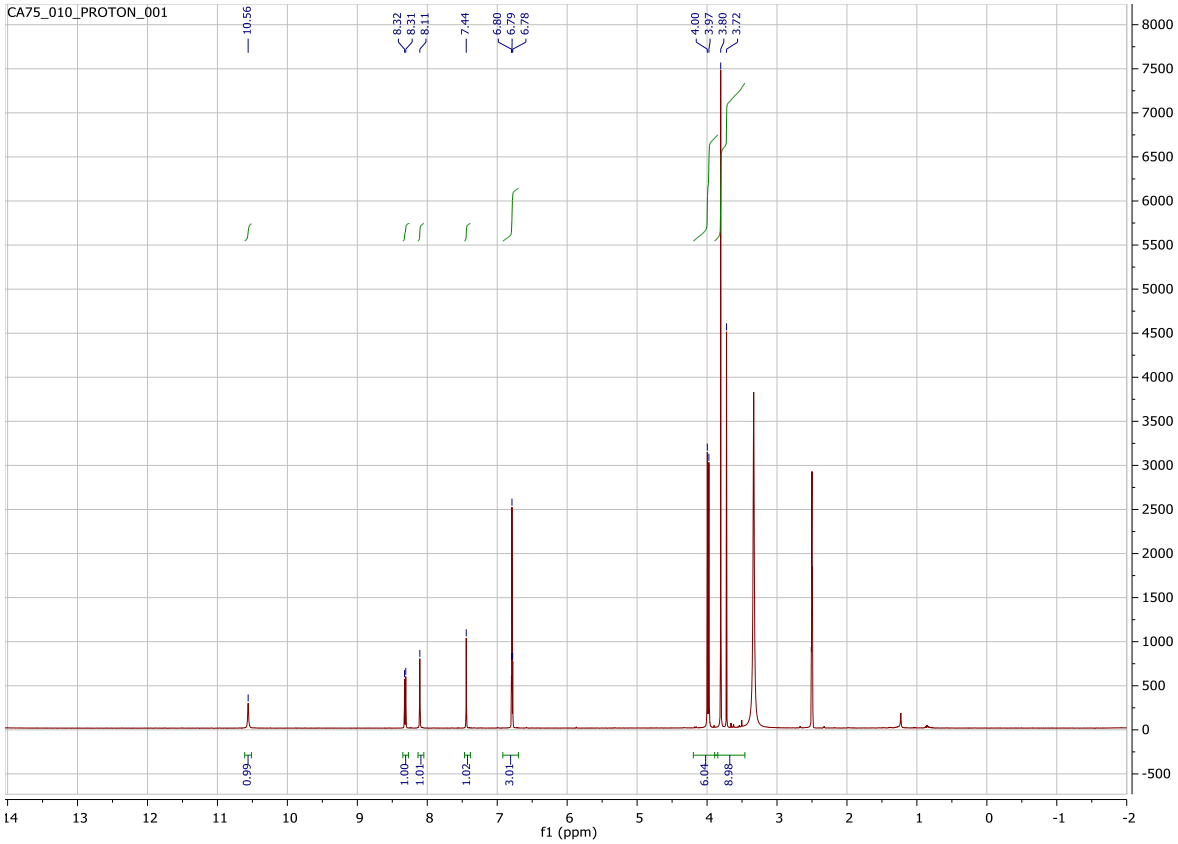


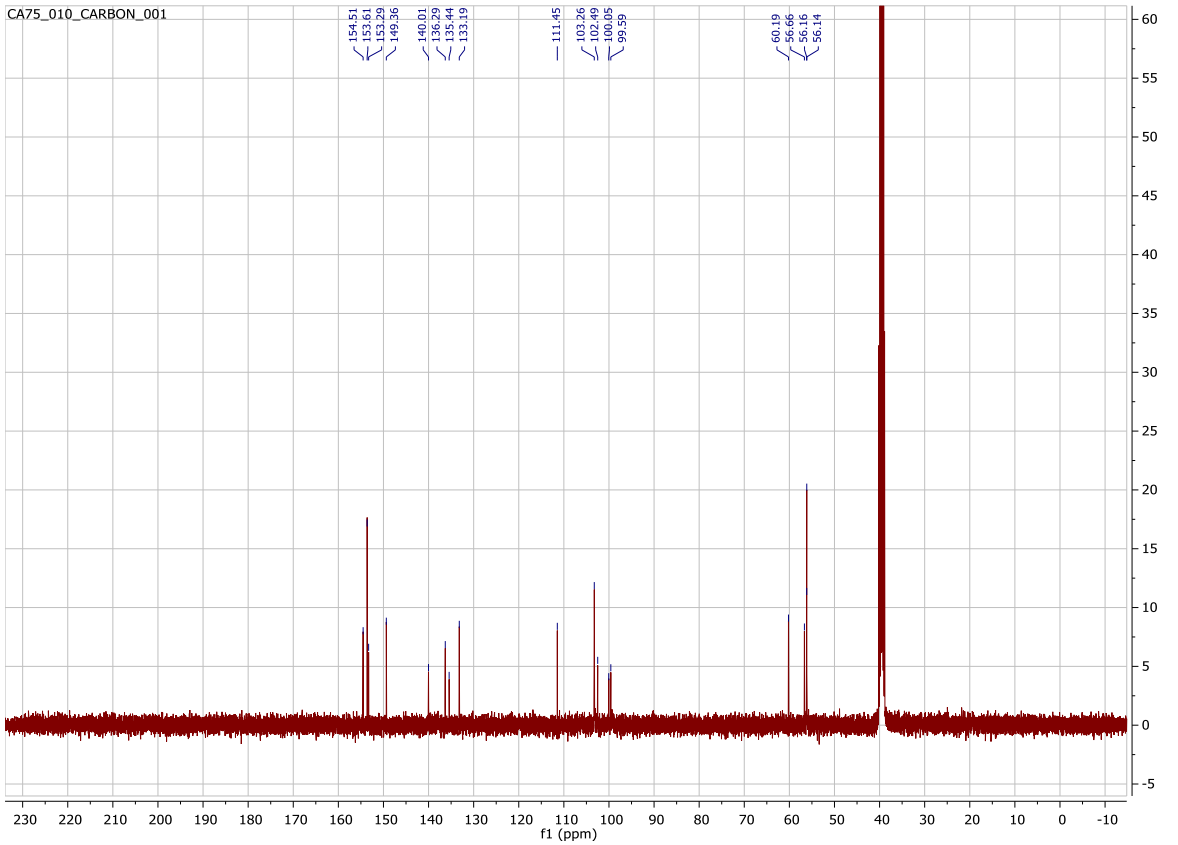
49

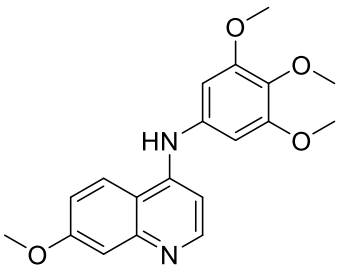
6,7-Dimethoxy-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**49**)





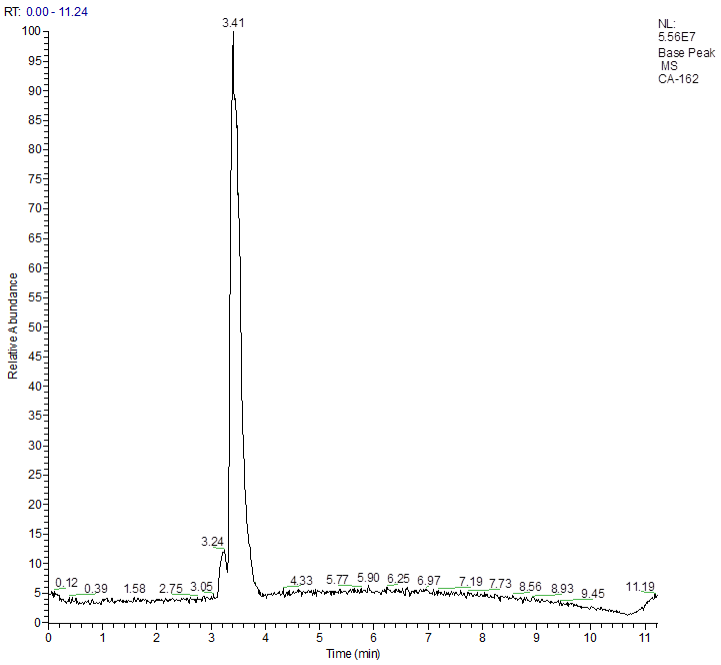

CA75_010_PROTON_001
10.56
8.32
8.31
8.11
7.44
6.80
6.79
6.78
4.00
3.97
3.90
3.72
0.99
1.00
1.01
1.02
3.01
6.04
8.98
f1 (ppm)

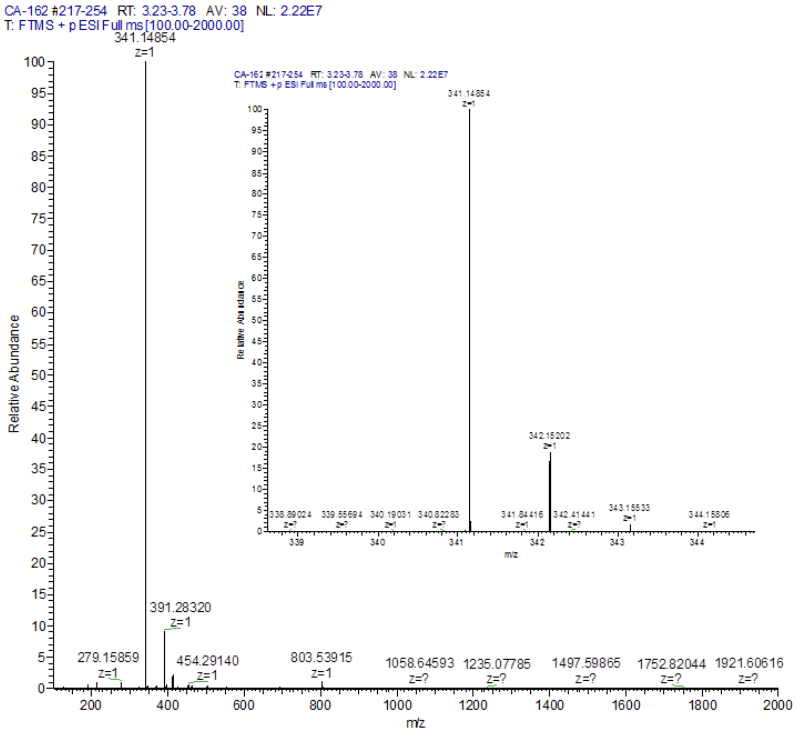

CA75_010_CARBON_001
154.51
153.61
153.29
149.36
140.01
136.29
135.44
133.19
111.45
103.26
102.49
100.05
99.59
60.19
56.66
56.16
56.14
f1 (ppm)

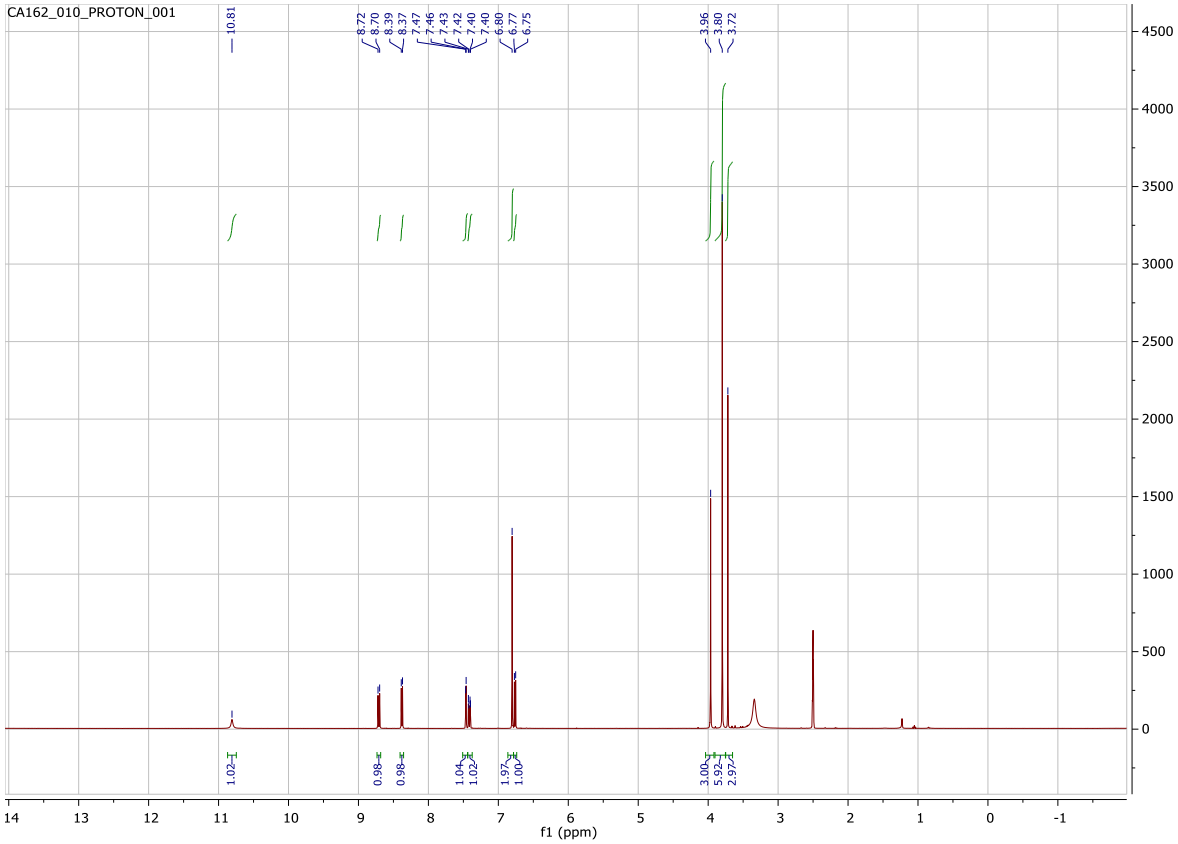


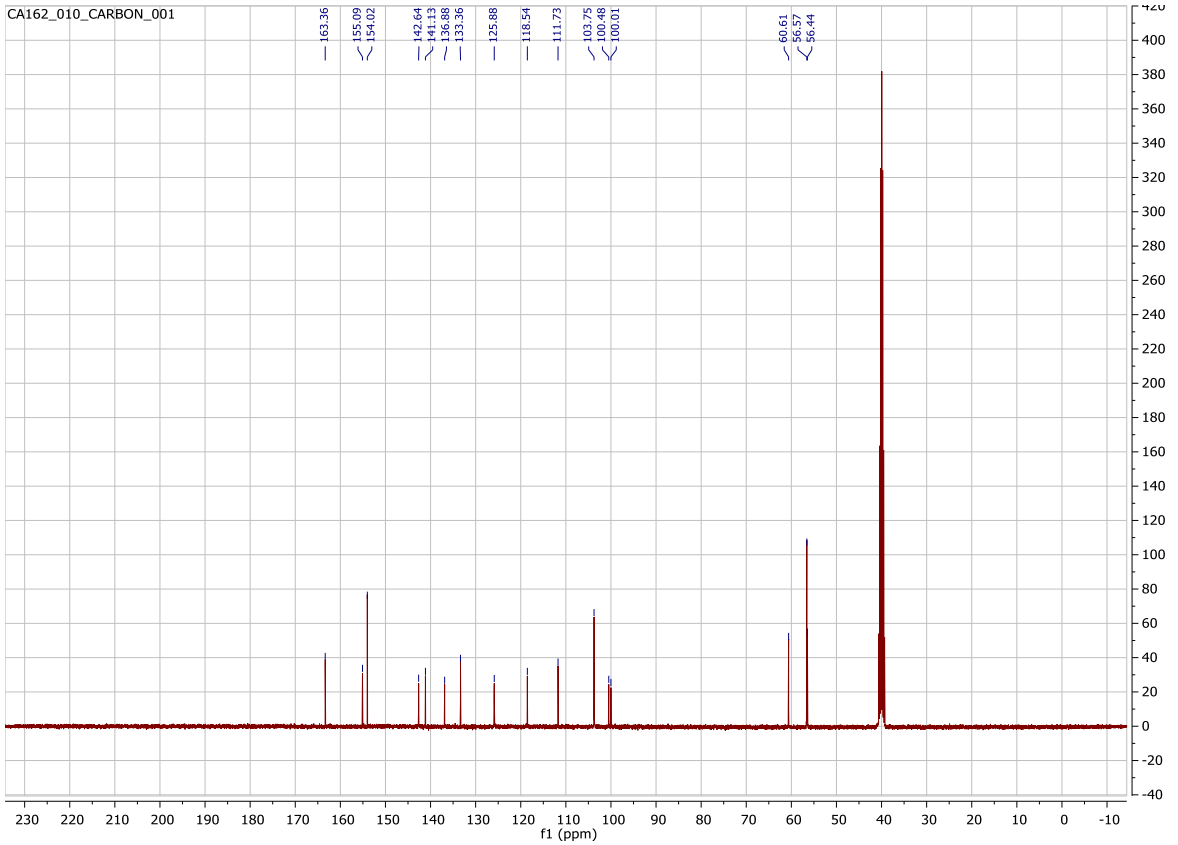
50

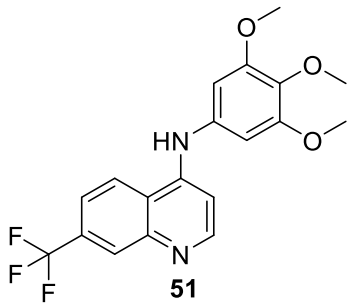
7-Methoxy-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**50**)





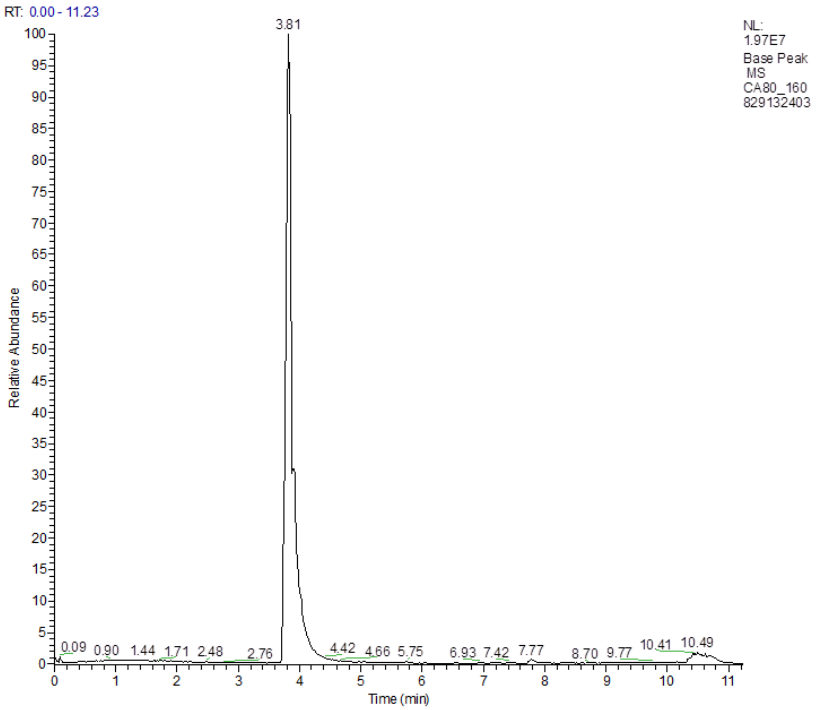

CA162_010_PROTON_001
10.81
8.72
8.70
8.39
8.37
7.47
7.46
7.43
7.42
7.40
7.40
6.80
6.77
6.75
3.96
3.80
3.72
1.02
0.98
0.98
1.04
1.02
1.97
1.00
3.00
5.92
2.97
f1 (ppm)

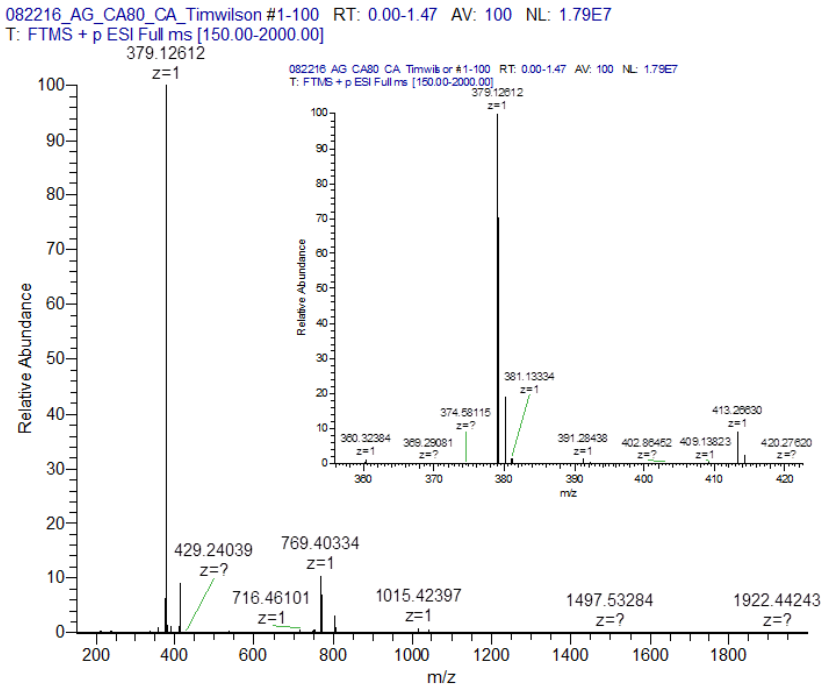

CA162_010_CARBON_001
163.36
155.09
154.02
142.64
141.13
136.88
133.36
125.88
118.54
111.73
103.75
100.48
100.01
60.61
56.57
56.44
f1 (ppm)

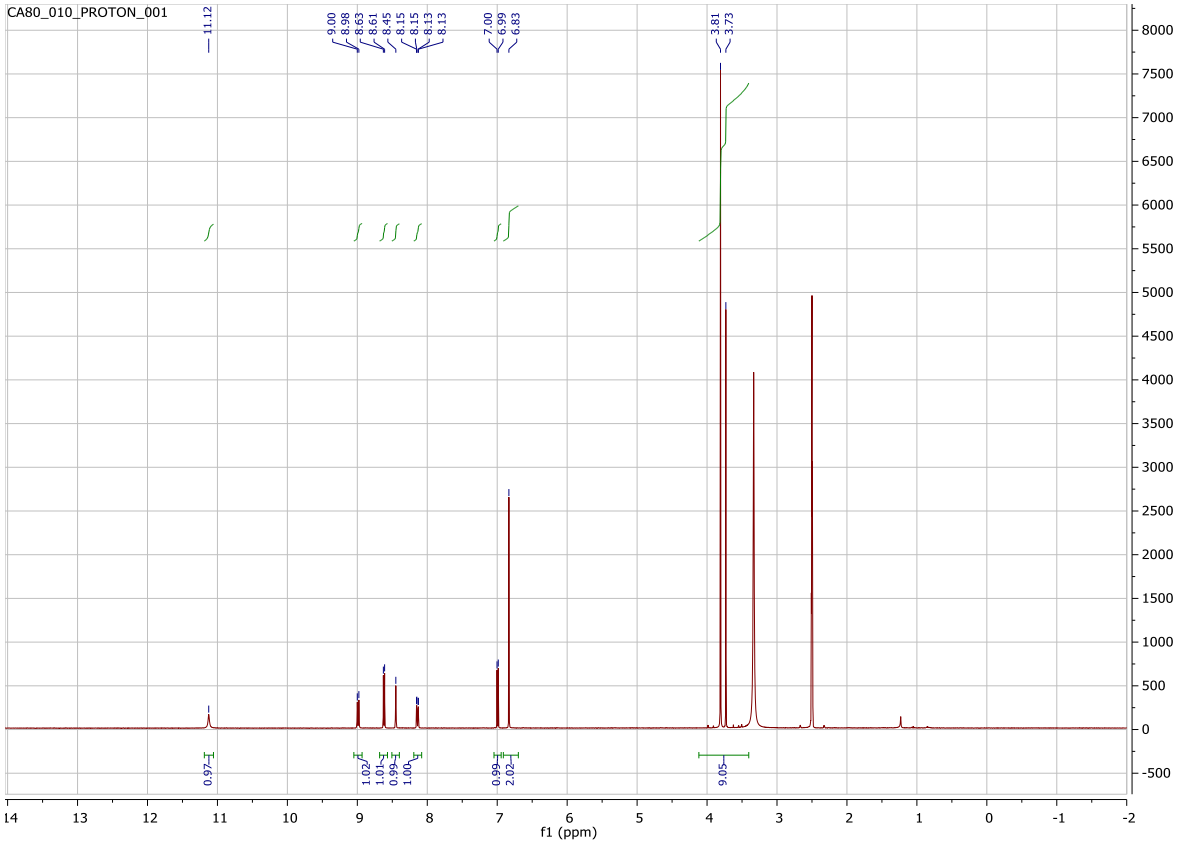


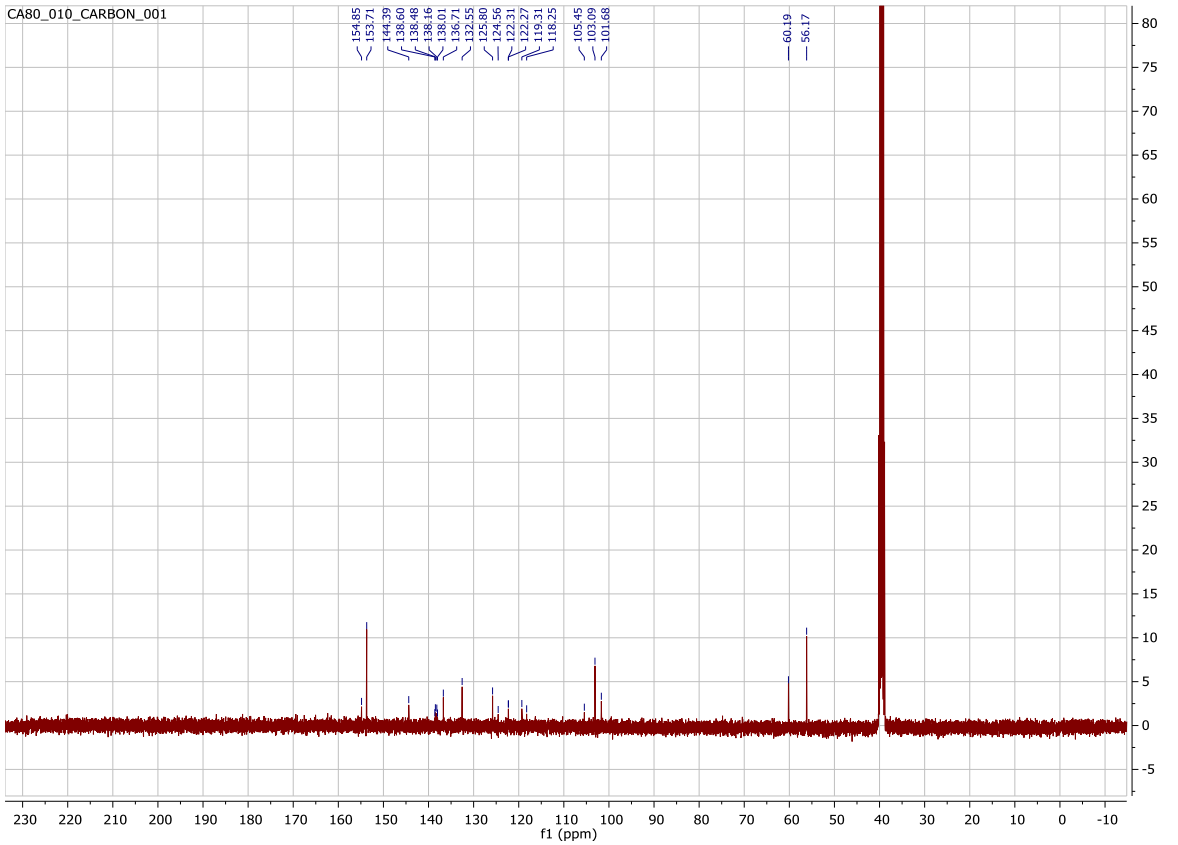
51

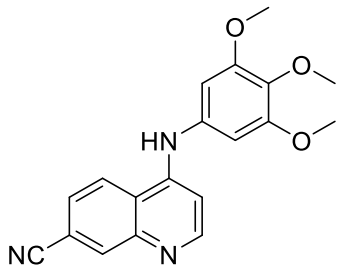
7-(Trifluoromethyl)-*N*-(3,4,5-trimethoxyphenyl)quinolin-4-amine (**51**)





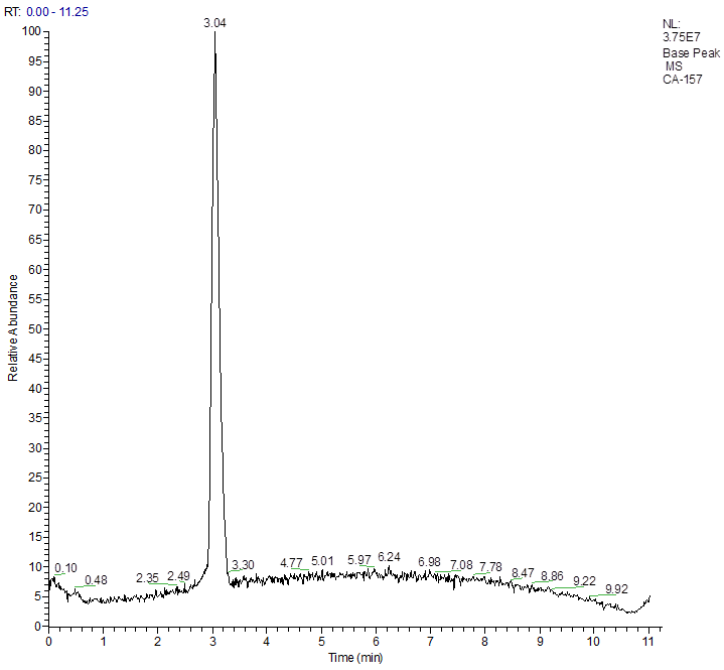

CA80_010_PROTON_001
11.12
9.00
8.98
8.63
8.61
8.45
8.15
8.13
8.13
7.00
6.99
6.83
3.81
3.73
0.97
1.02
1.01
0.99
1.00
0.99
2.02
9.05
f1 (ppm)

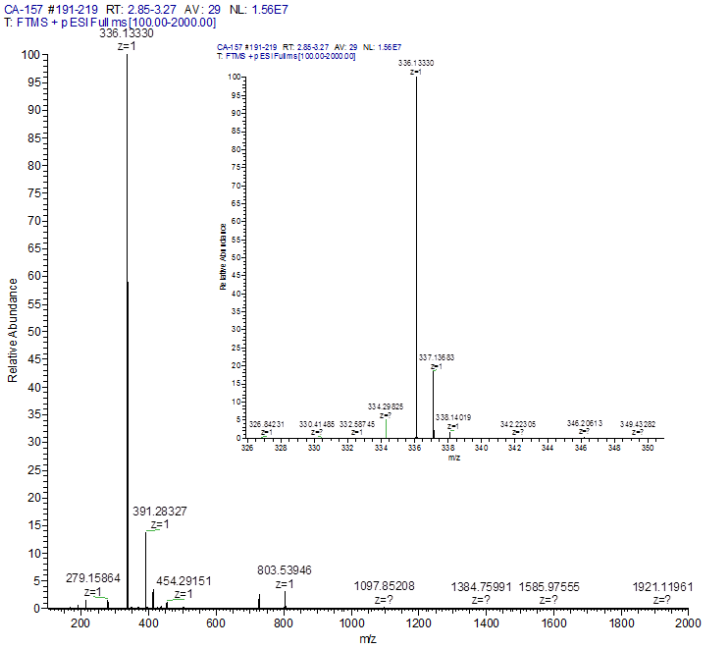

CA80_010_CARBON_001
154.85
153.71
144.39
138.60
138.48
138.16
138.01
136.71
132.55
125.80
124.56
122.31
122.27
119.31
118.25
105.45
103.09
101.68
60.19
56.17
f1 (ppm)

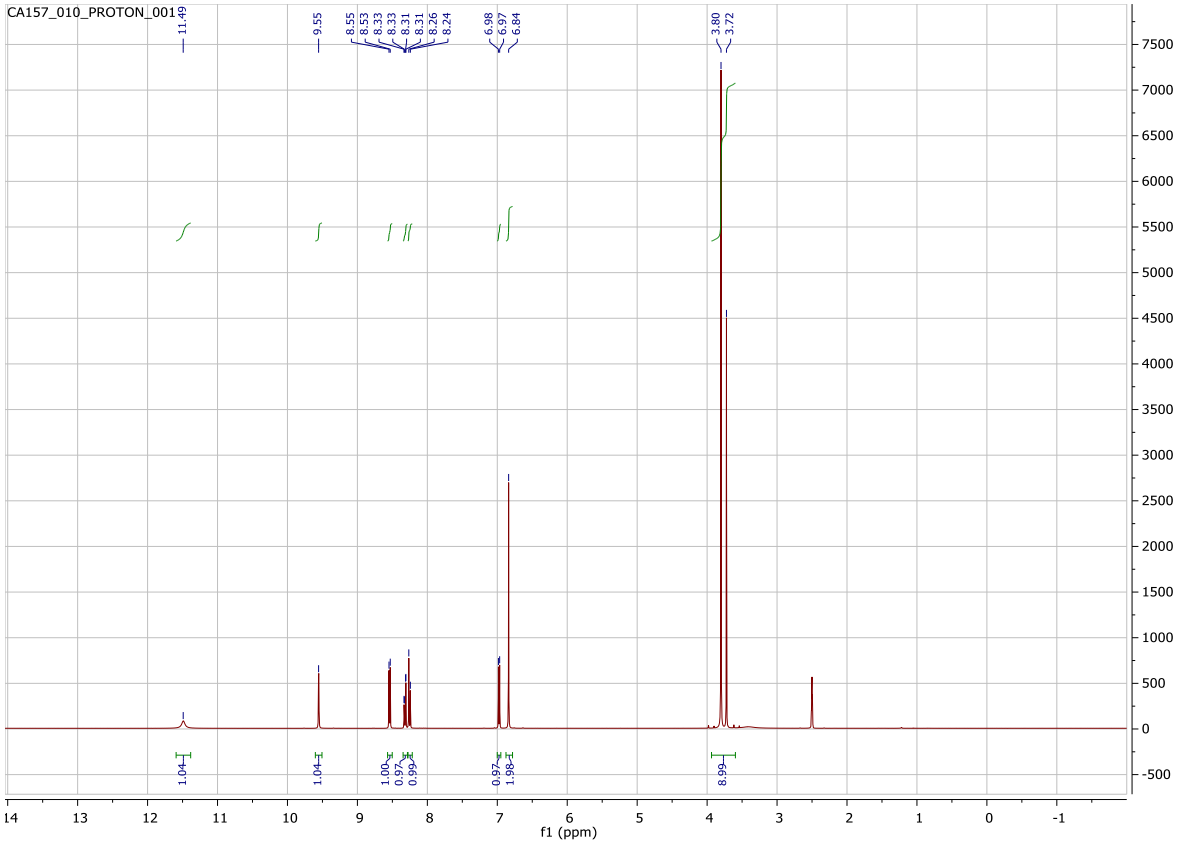


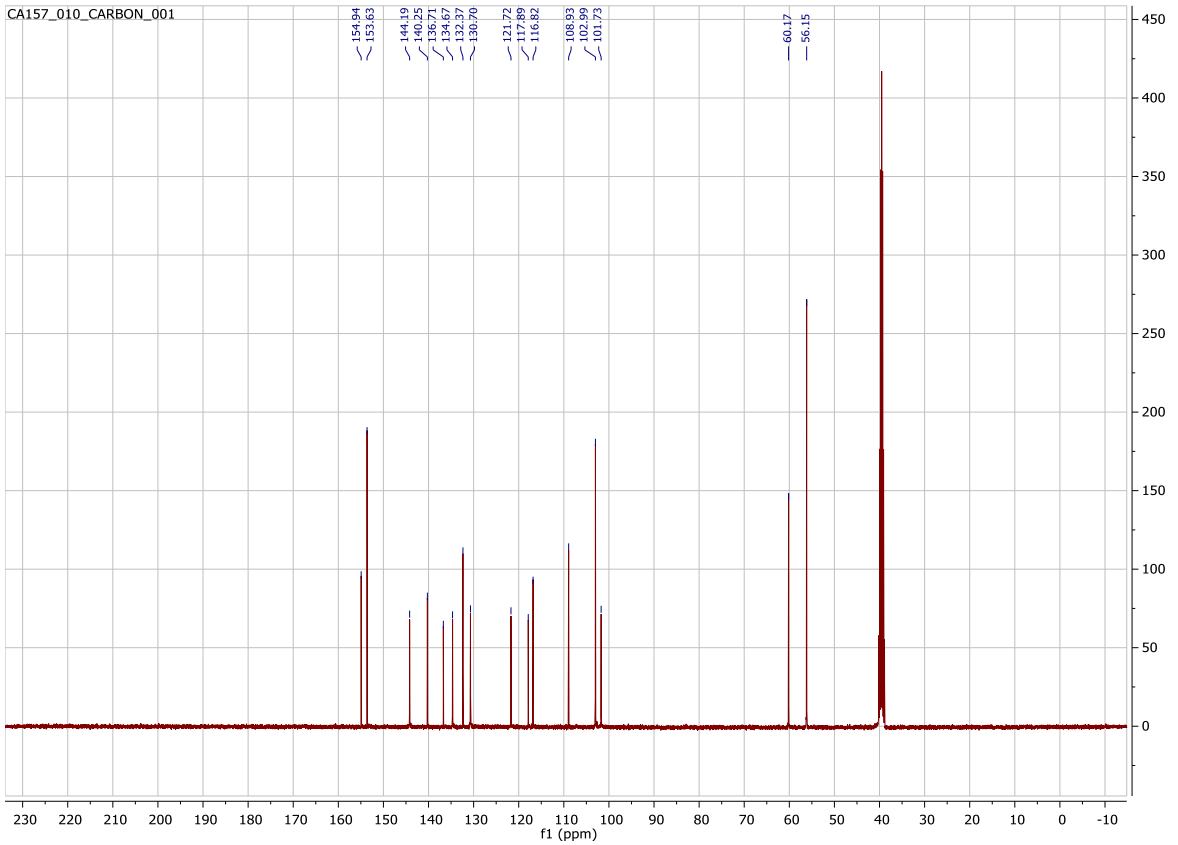
52

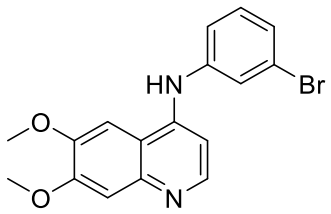
4-((3,4,5-Trimethoxyphenyl)amino)quinoline-7-carbonitrile (**52**)





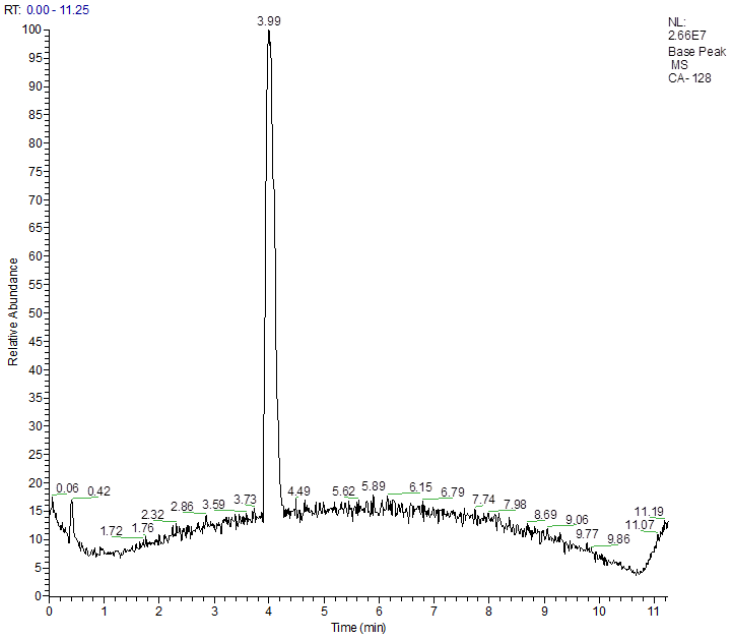

CA157_010_PROTON_001
11.49
9.55
8.55
8.53
8.33
8.33
8.31
8.31
8.26
8.24
6.98
6.97
6.84
3.80
3.72
1.04
1.04
1.00
0.97
0.99
0.97
1.98
8.99
f1 (ppm)

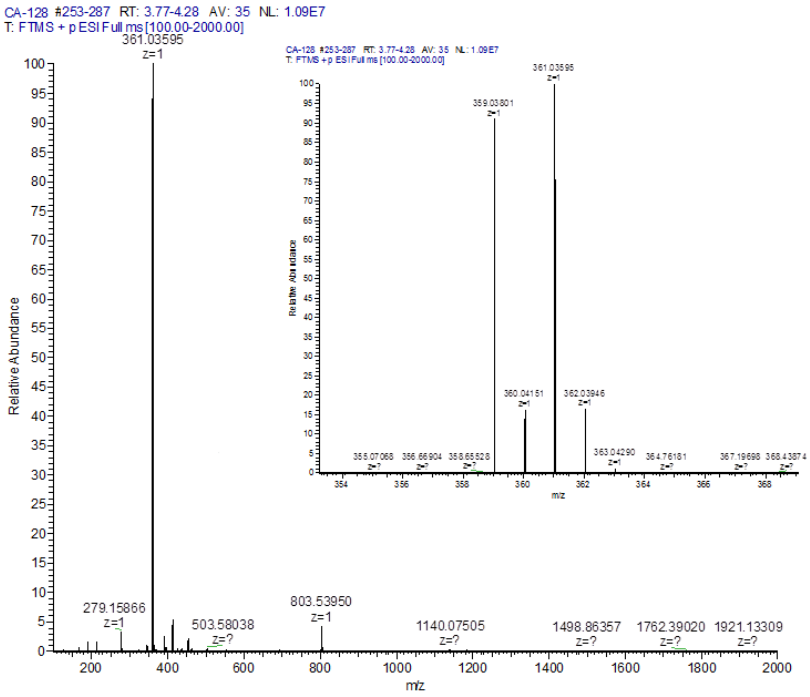

CA157_010_CARBON_001
154.94
153.63
144.19
140.25
136.71
134.67
132.37
130.70
121.72
117.89
116.82
108.93
102.99
101.73
60.17
56.15
f1 (ppm)

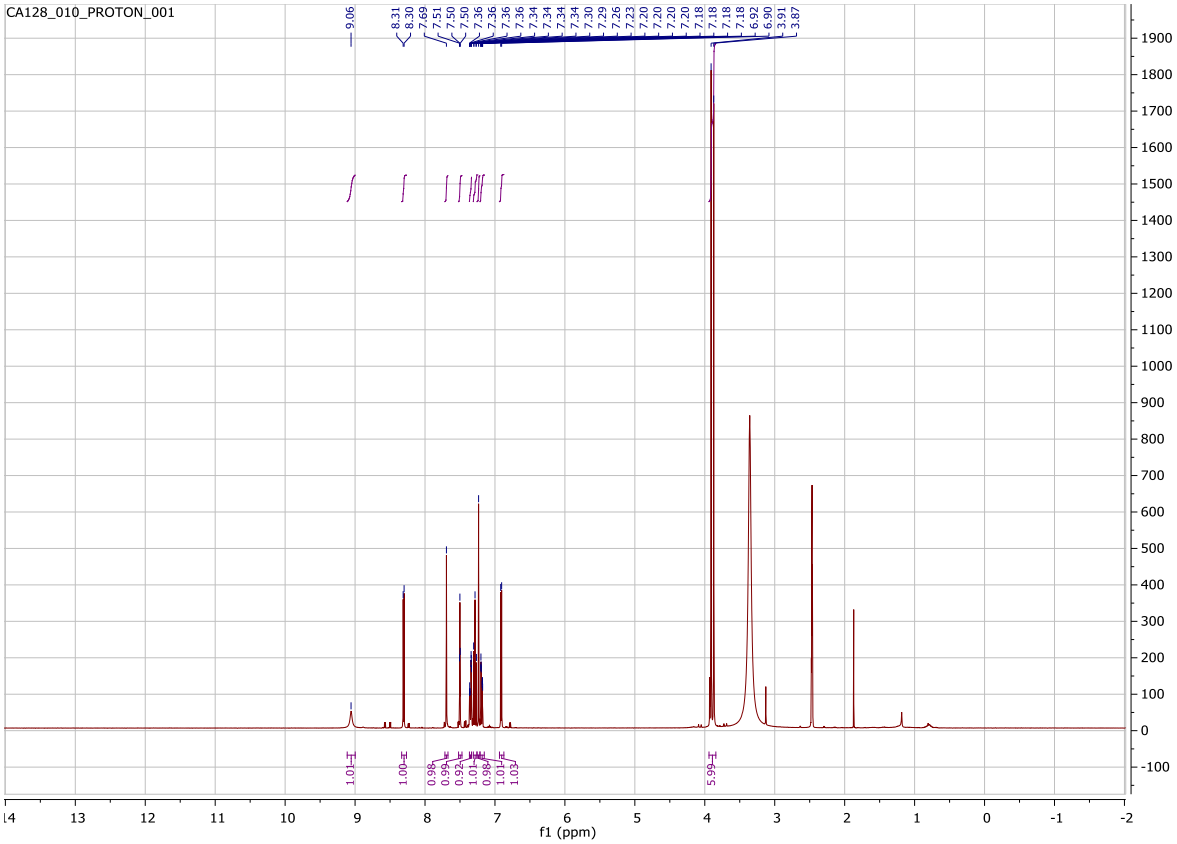


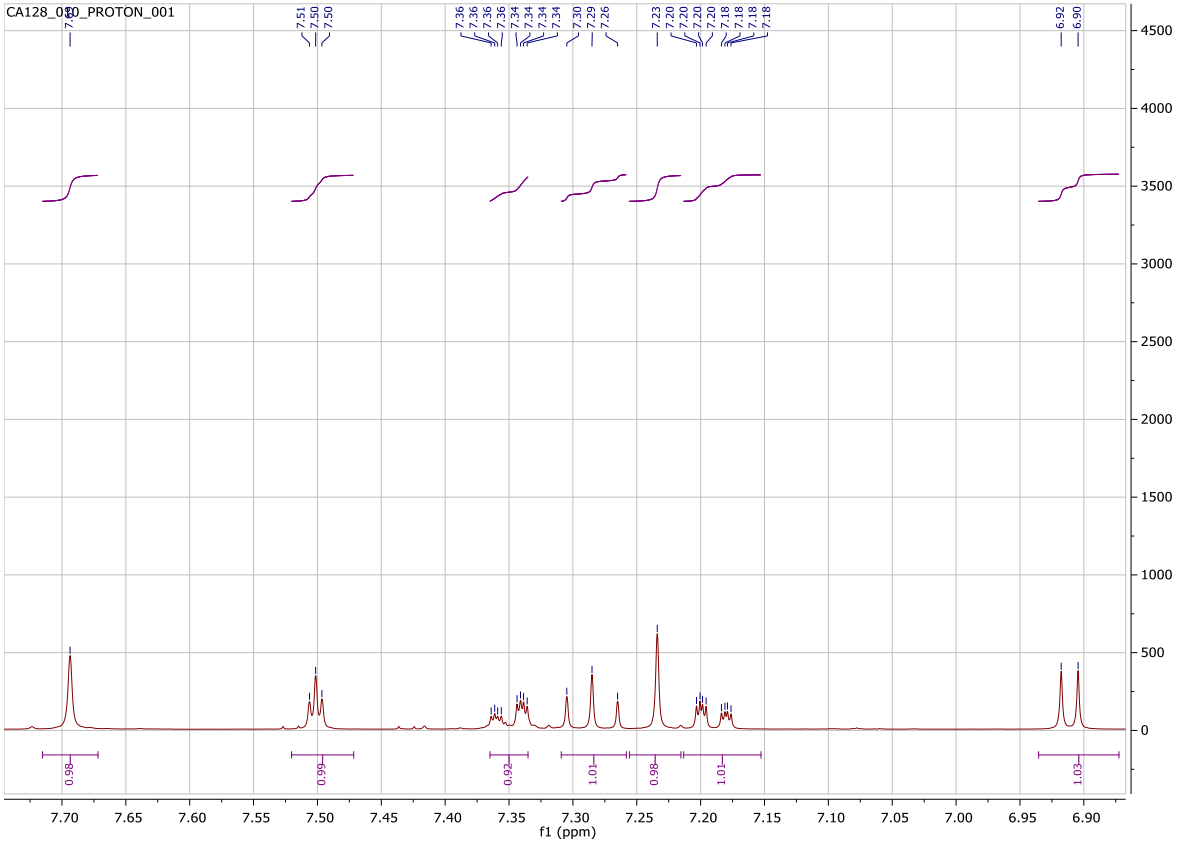
53

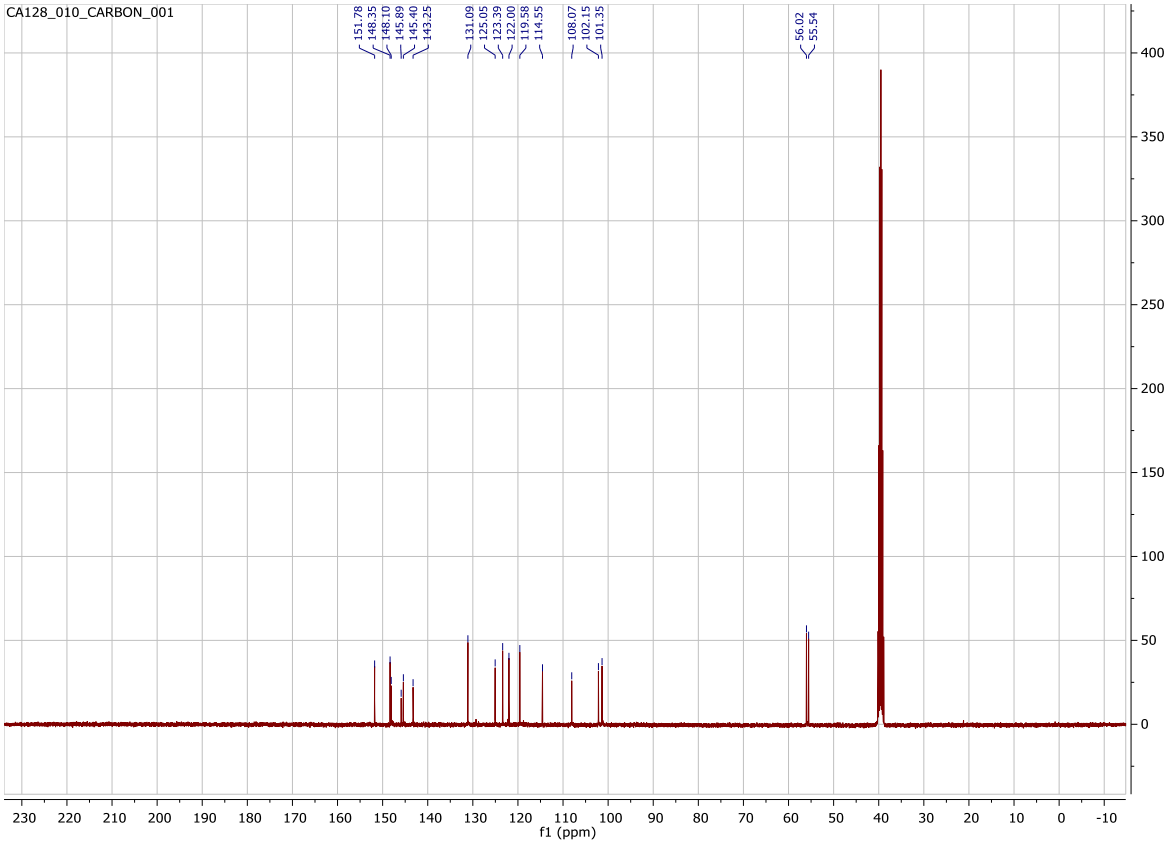
N-(3-Bromophenyl)-6,7-dimethoxyquinolin-4-amine (**53**)

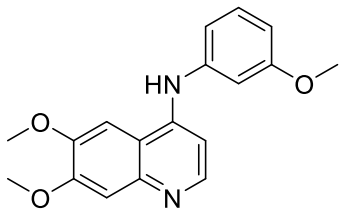





CA128_010_PROTON_001
f1 (ppm)

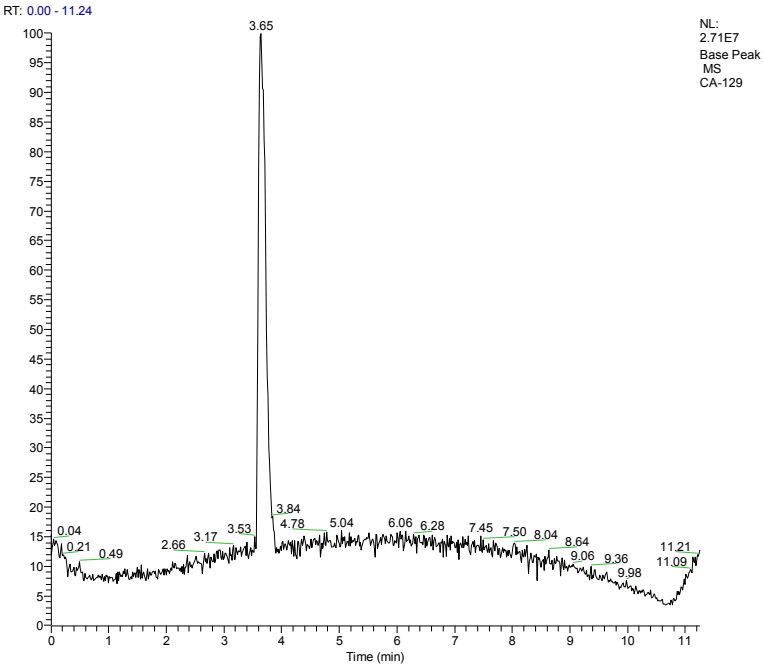

CA128_010_PROTON_001
f1 (ppm)

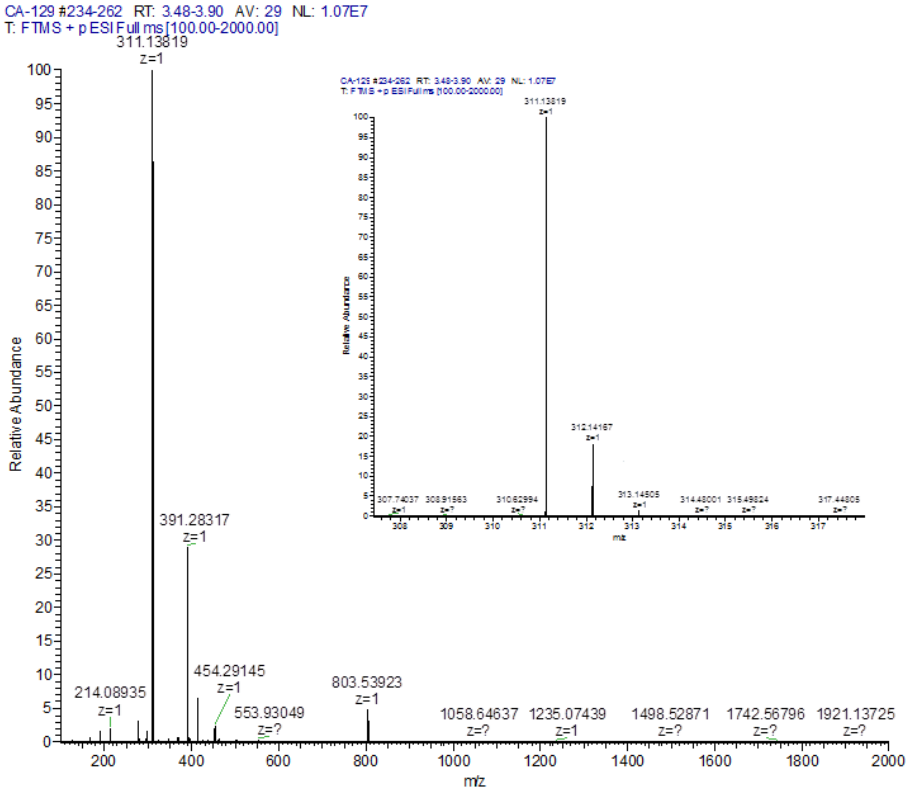

CA128_010_CARBON_001
151.78
148.35
148.10
145.89
145.40
143.25
131.09
125.05
123.39
122.00
119.58
114.55
108.07
102.15
101.35
56.02
55.54
f1 (ppm)

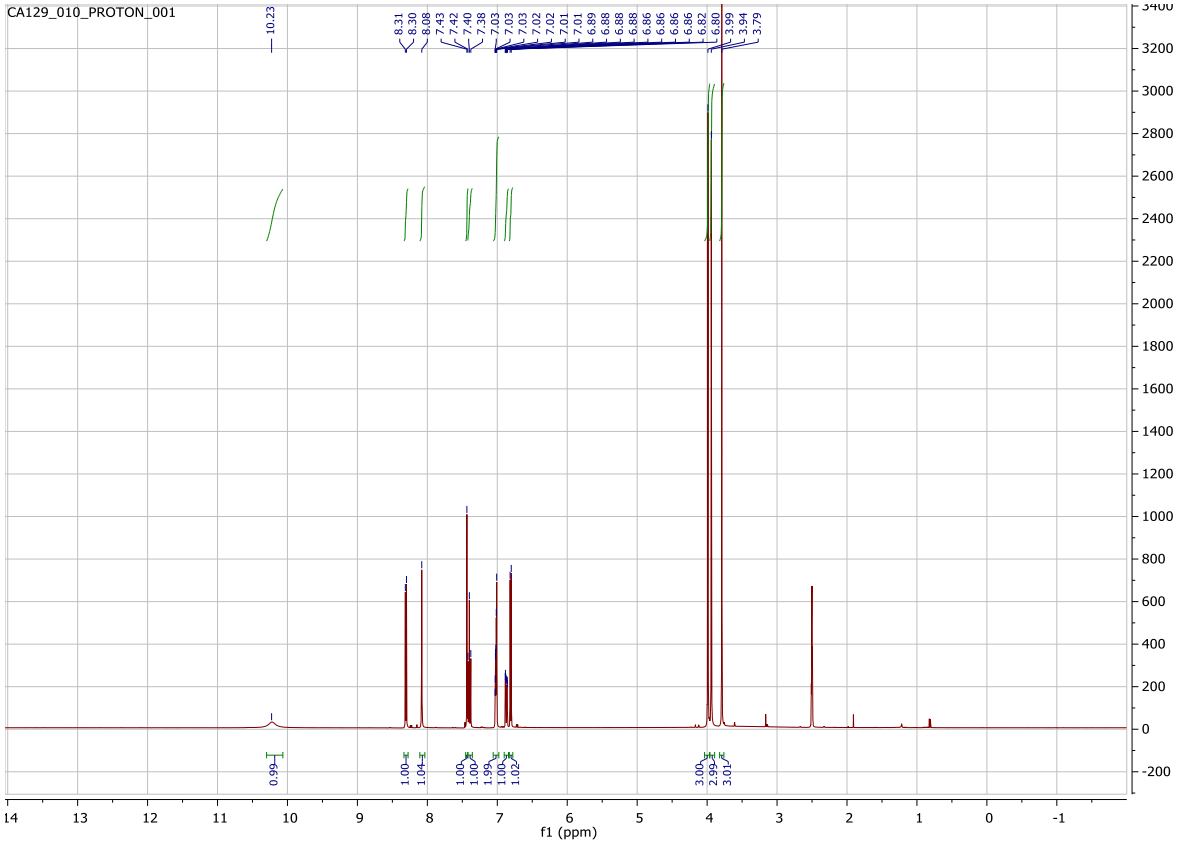


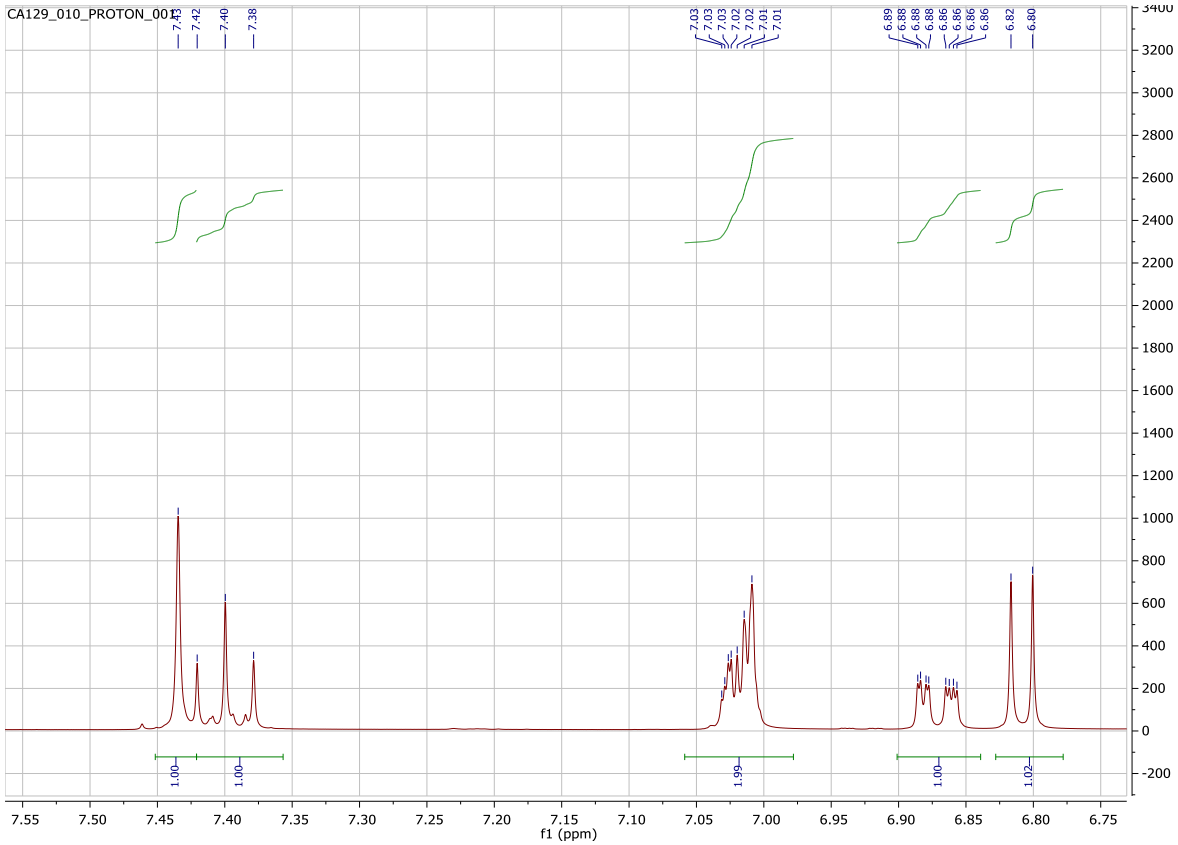
54

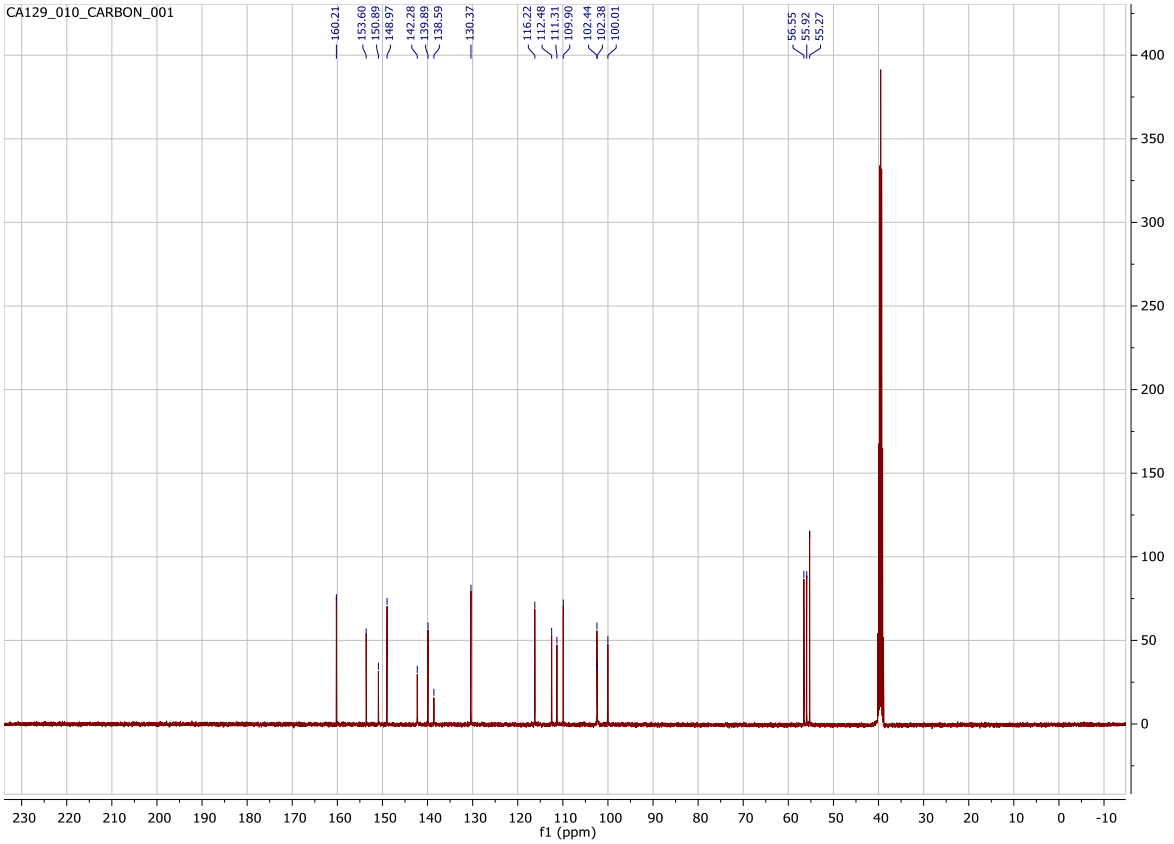
6,7-Dimethoxy-*N*-(3-methoxyphenyl)quinolin-4-amine (**54**)

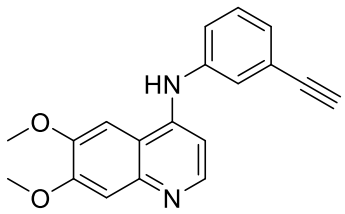





CA129_010_PROTON_001
f1 (ppm)

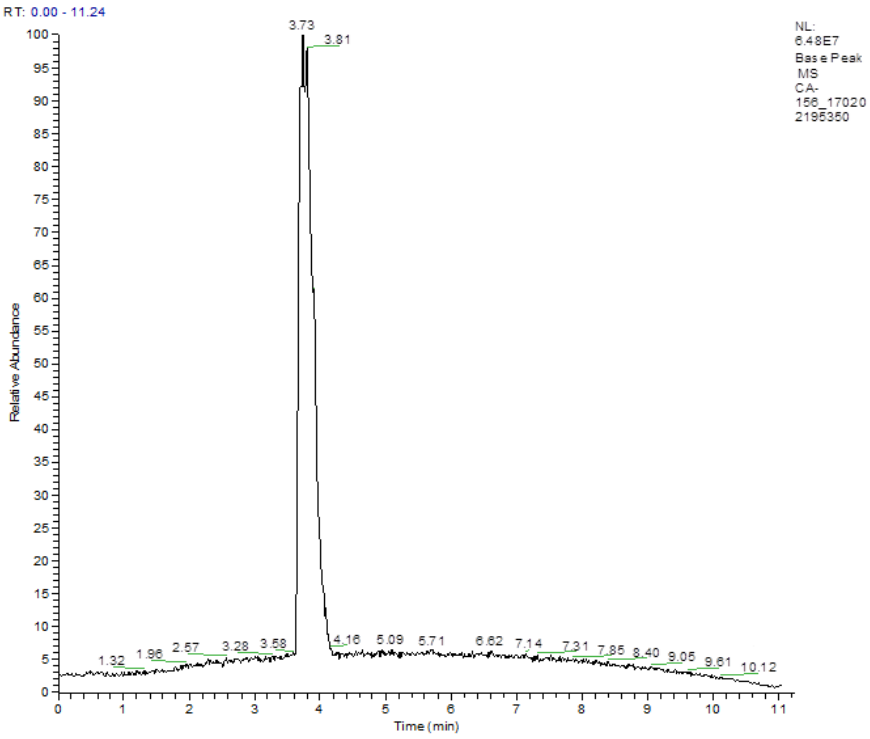

CA129_010_PROTON_001
f1 (ppm)

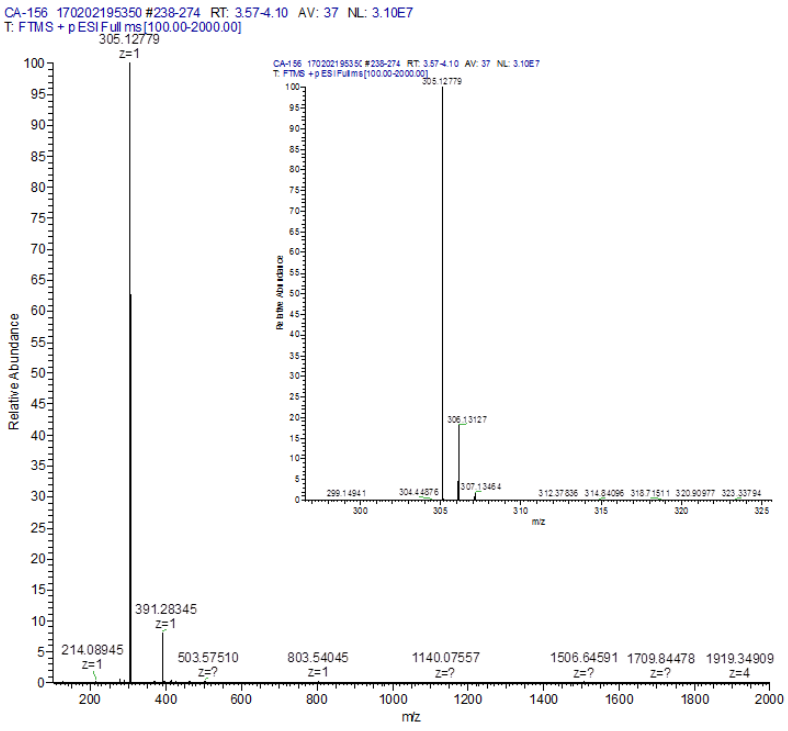

CA129_010_CARBON_001
160.21
153.60
150.89
148.97
142.28
139.89
138.59
130.37
116.22
112.46
111.31
109.90
102.44
102.38
100.01
56.55
55.32
55.27
f1 (ppm)

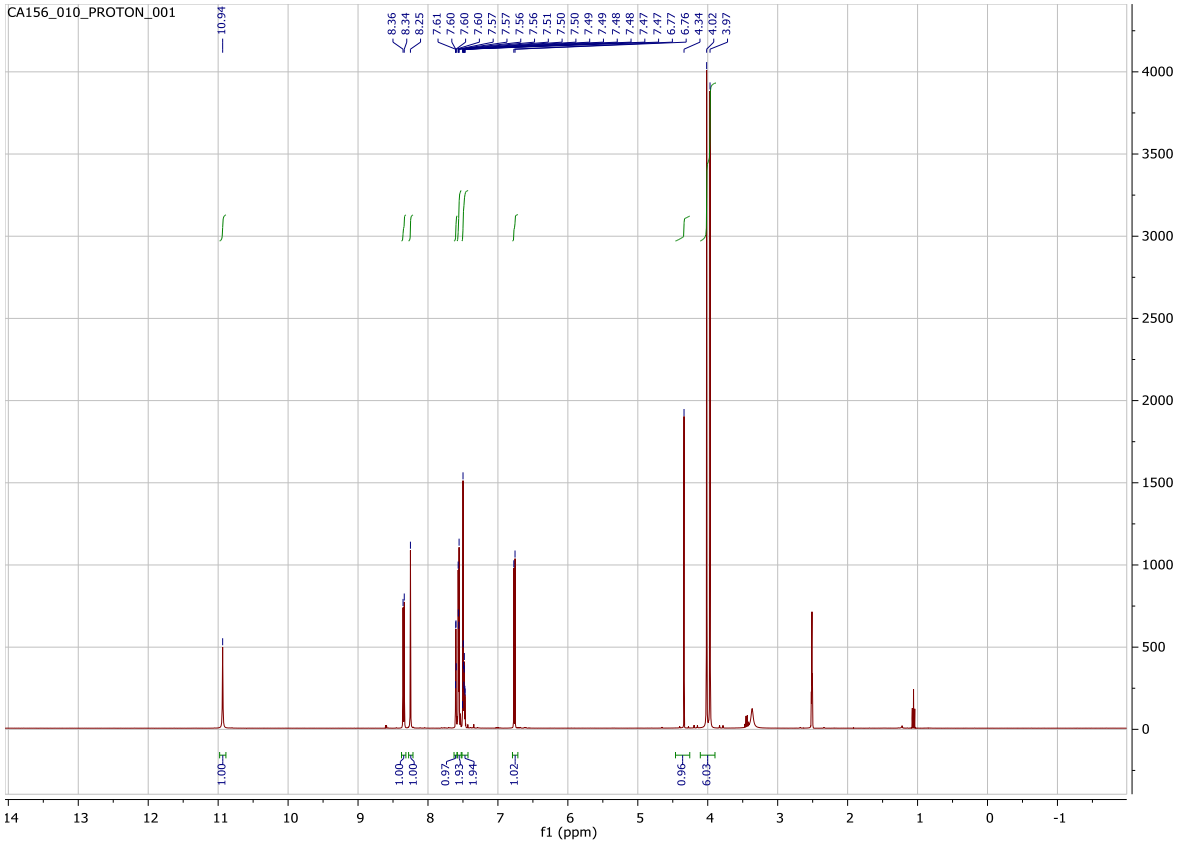


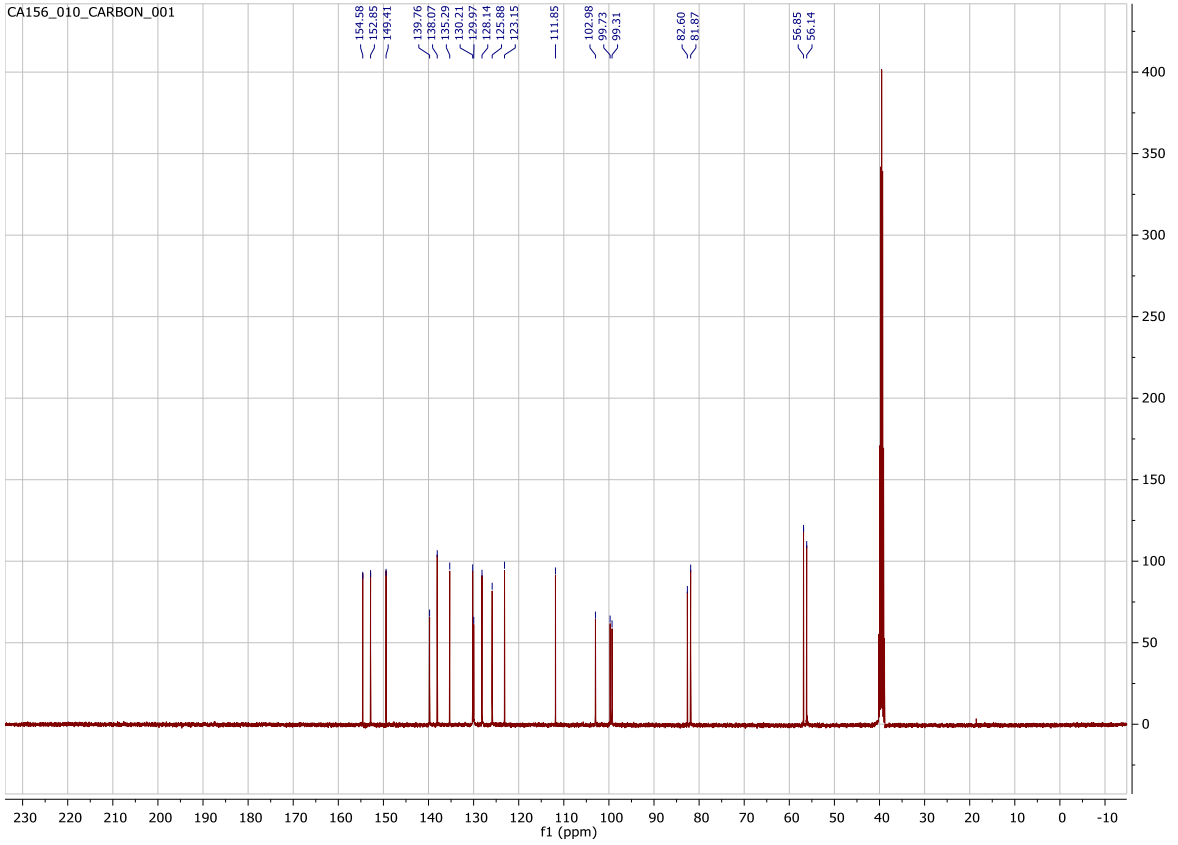
55

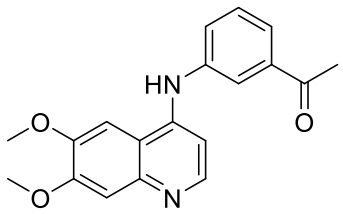
N-(3-Ethynylphenyl)-6,7-dimethoxyquinolin-4-amine (**55**)





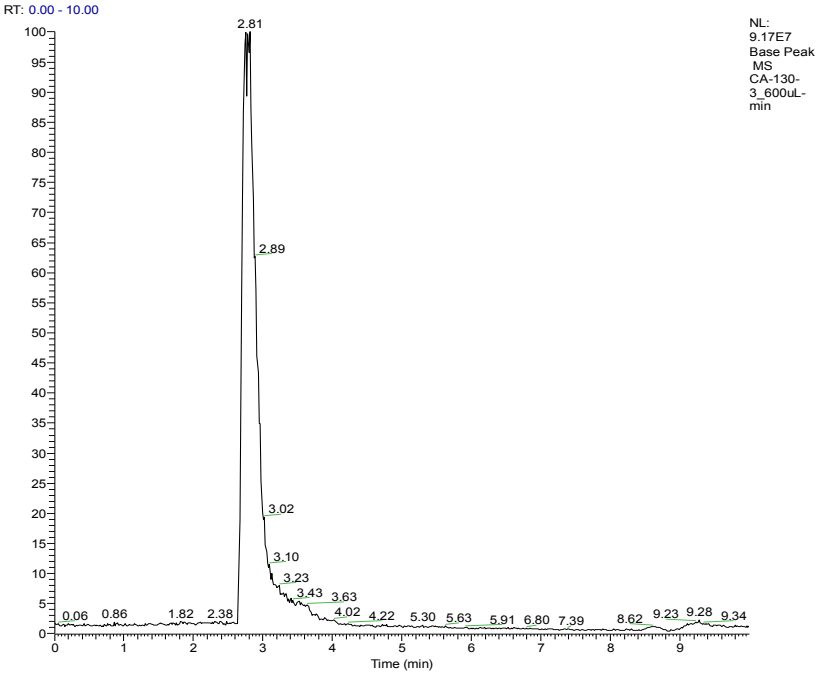

CA156_010_PROTON_001
10.94
8.36
8.34
8.25
7.61
7.60
7.60
7.60
7.57
7.57
7.56
7.56
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.47
6.77
6.76
4.34
4.02
3.97
1.00
1.00
1.00
0.97
1.93
1.94
1.02
0.96
6.03
f1 (ppm)

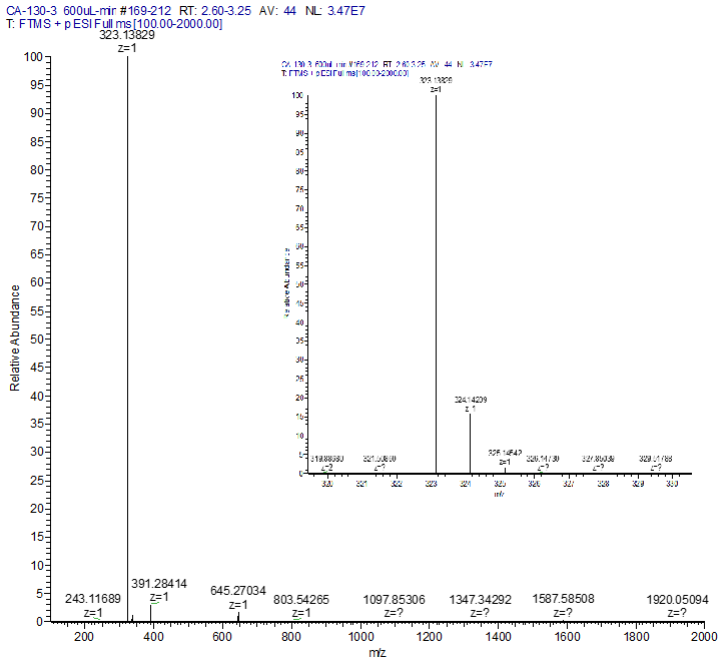

CA156_010_CARBON_001
154.58
152.85
149.41
139.76
138.07
135.29
130.21
129.97
128.14
125.88
123.15
111.85
102.98
99.73
99.31
82.60
81.87
56.85
56.14
f1 (ppm)

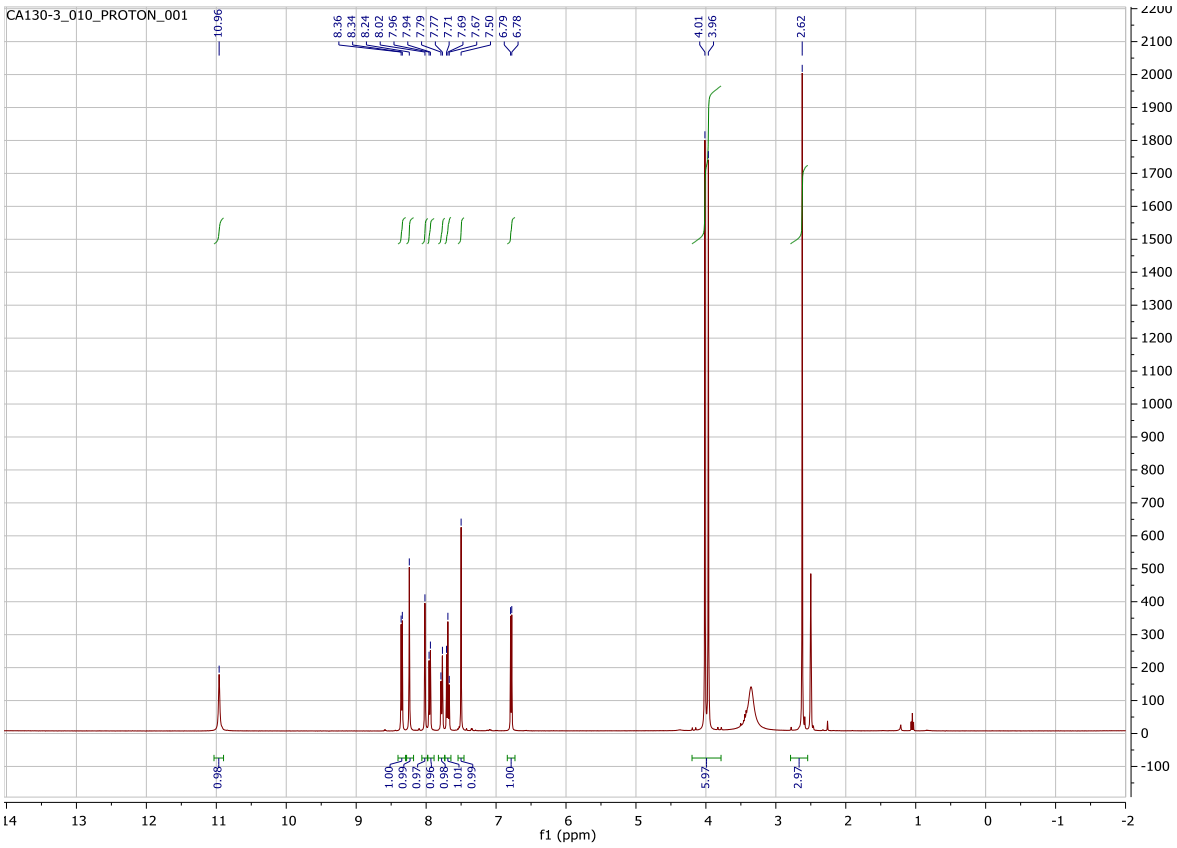


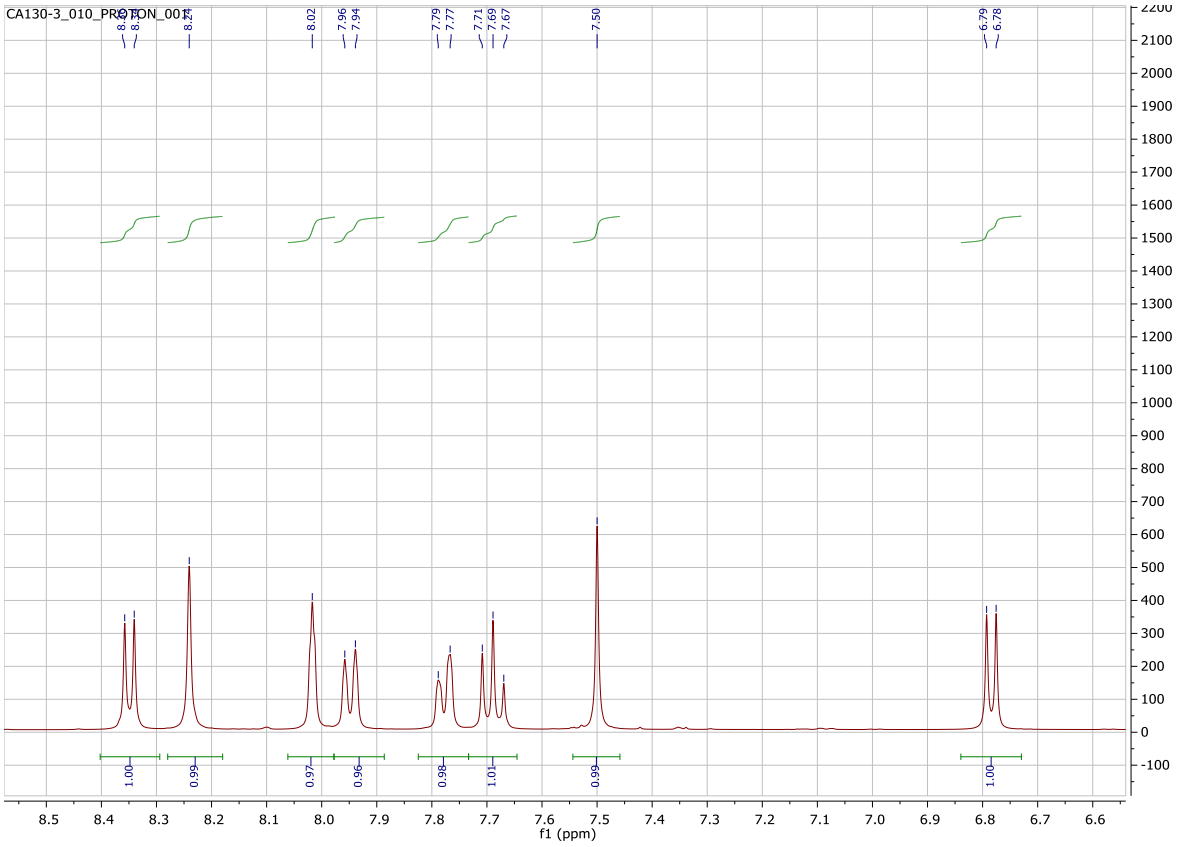
56

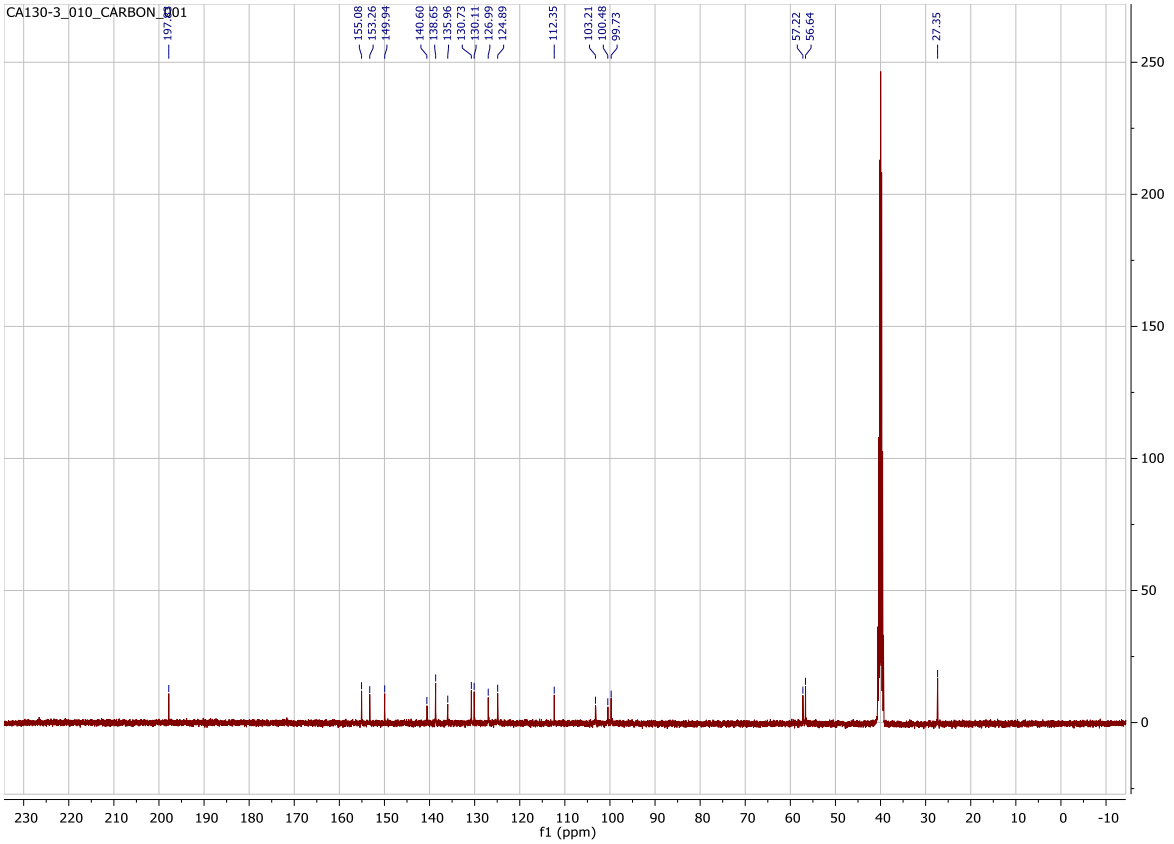
1-(3-((6,7-dimethoxyquinolin-4-yl)amino)phenyl)ethan-1-one (**56**)

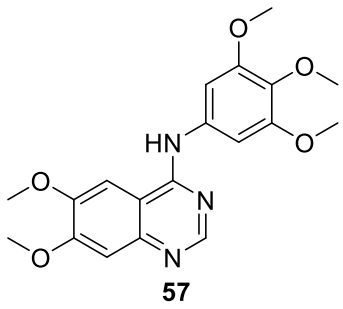





CA130-3_010_PROTON_001
10.96
8.36
8.34
8.24
8.02
7.96
7.94
7.79
7.77
7.71
7.69
7.67
7.50
6.79
6.78
4.01
3.96
2.62
0.98
1.00
0.99
0.97
0.96
0.98
1.01
0.99
1.00
5.97
2.97
f1 (ppm)

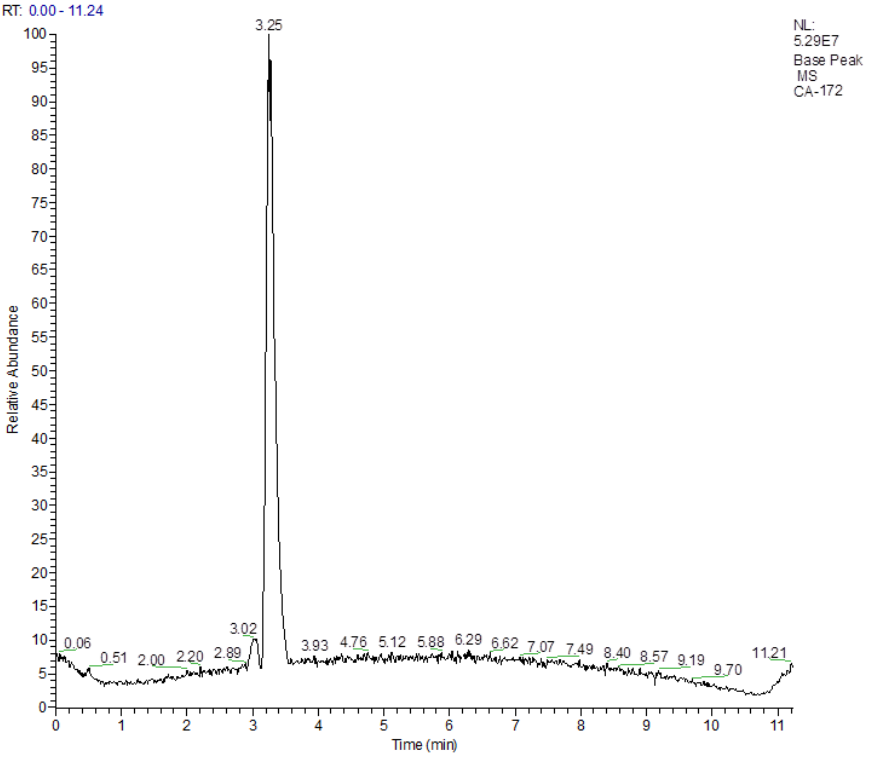

CA130-3_010_PROTON_001
8.24
8.02
7.96
7.94
7.79
7.77
7.71
7.69
7.67
7.50
6.79
6.78
1.00
0.99
0.97
0.96
0.98
1.01
0.99
1.00
f1 (ppm)

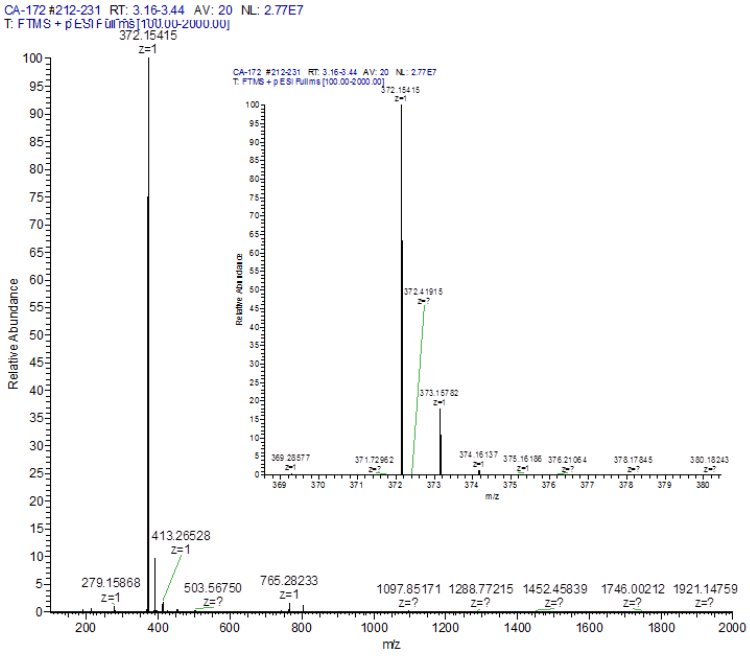

CA130-3_010_CARBON_001
197.70
155.08
153.26
149.94
140.60
138.65
135.96
130.73
130.11
126.99
124.89
112.35
103.21
100.48
99.73
57.22
56.64
27.35
f1 (ppm)

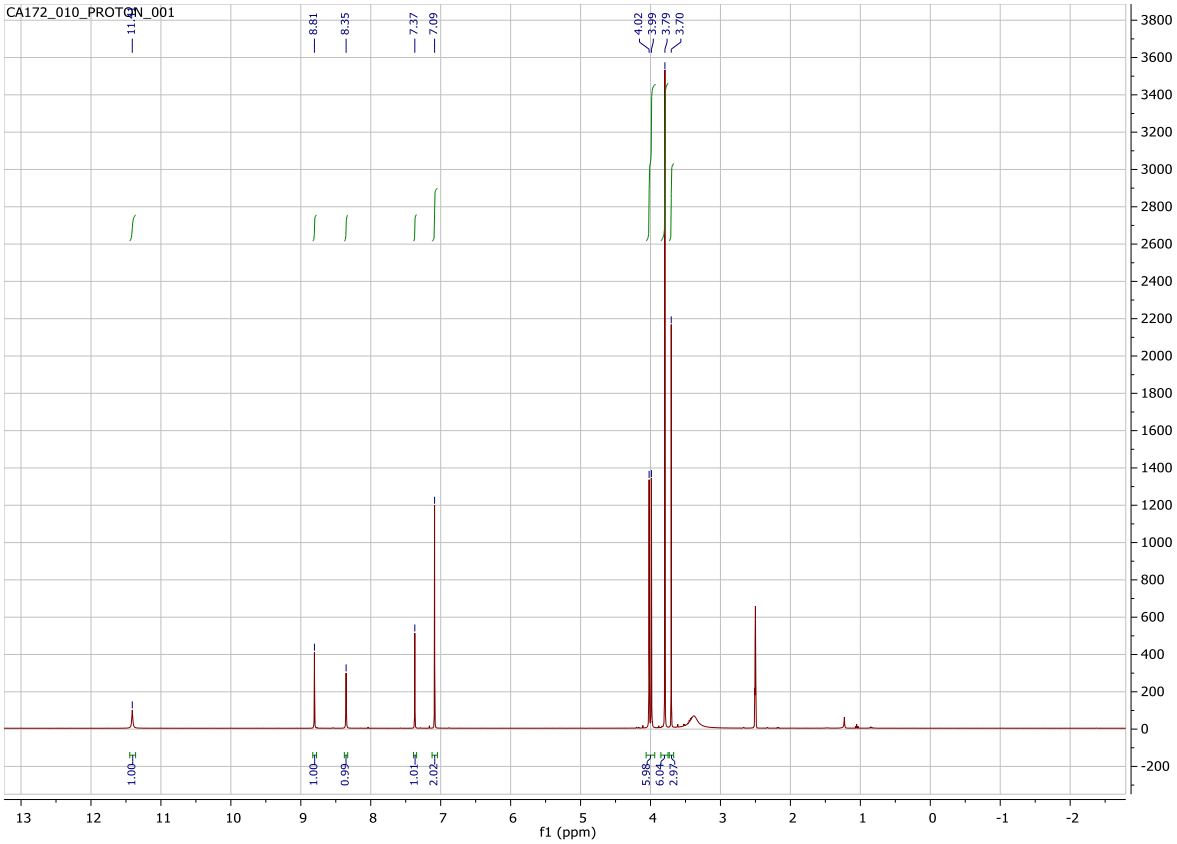


57

6,7-Dimethoxy-*N*-(3,4,5-trimethoxyphenyl)quinazolin-4-amine (**57**)






CA172_010_PROTON_001
11.47
8.81
8.35
7.37
7.09
4.02
3.99
3.79
3.70
1.00
1.00
0.99
1.01
2.02
5.98
6.04
2.97
f1 (ppm)

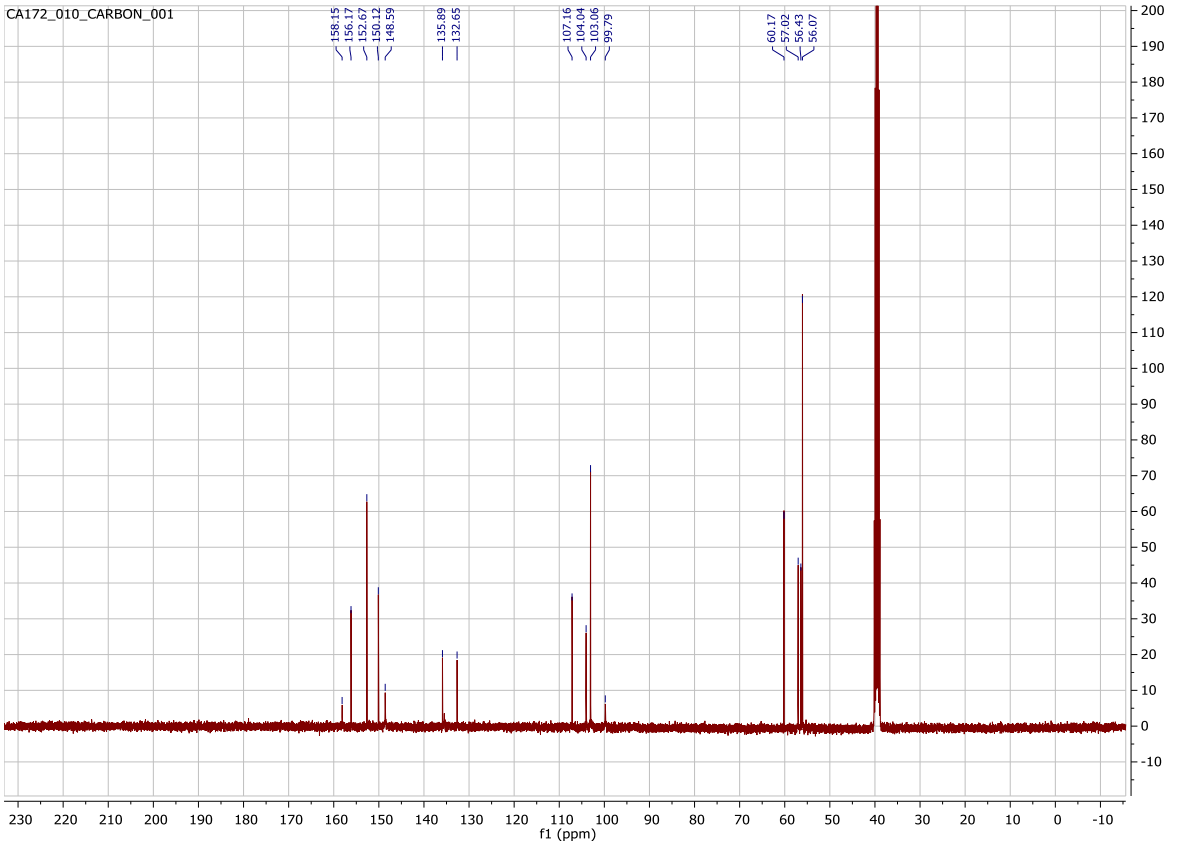

CA172_010_CARBON_001
158.15
156.17
152.67
150.12
148.59
135.89
132.65
107.16
104.04
103.06
99.79
60.17
57.02
56.43
56.07
f1 (ppm)

Table S4 - Annotations, reference numbers and smiles

Paper	Lab-book	Annotation	Smiles
1	**CA62**	3,4,5-OMe	COC(C=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C(C(OC)=C1)OC
2	-	**GW494610**	COC1=C(OC)C(OC)=CC(NC2=C3C(C=C(C4=CC=NC=C4)C=C3)=NC=C2)=C1
3	-	**GI230329**	BrC1=CC(NC2=C3C(C=C(OC)C(OC)=C3)=NC=N2)=CC=C1
4	**CA63**	3,5-OMe	COC1=CC(OC)=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
5	**CA64**	3,4-OMe	COC1=C(OC)C=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
6	**CA105**	2,4-OMe	COC(C=C1)=CC(OC)=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
7	**CA106**	2,5-OMe	COC(C=CC(OC)=C1)=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
8	**CA65**	4-OMe	FC(C1=CC2=C(NC3=CC=C(OC)C=C3)C=CN=C2C=C1)(F)F
9	**CA66**	3-OMe	FC(C1=CC2=C(NC3=CC(OC)=CC=C3)C=CN=C2C=C1)(F)F
10	**CA67**	2-OMe	FC(C1=CC2=C(NC3=C(OC)C=CC=C3)C=CN=C2C=C1)(F)F
11	**CA68**	3,4-OCH_2O-	FC(C1=CC2=C(NC3=CC=C(OCO4)C4=C3)C=CN=C2C=C1)(F)F
12	**CA69**	3,4-OCH_2CH_2O-	FC(C1=CC2=C(NC3=CC=C(OCCO4)C4=C3)C=CN=C2C=C1)(F)F
13	**CA72**	3,4,5-OMe-Q	FC(C1=CC2=C(NC3=CC(OC)=C(C(OC)=C3)OC)N=CN=C2C=C1)(F)F
14	**CA76**	3,5-OMe-Q	COC1=CC(OC)=CC(NC2=C3C(C=CC=C3)=NC=N2)=C1
15	**CA78**	4-OMe-Q	COC(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=N2
16	**CA83**	3,4,5-F	FC1=C(F)C(F)=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
17	**CA84**	3,5-F	FC1=CC(F)=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
18	**CA86**	4-F	FC(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
19	**CA87**	3-F	FC1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
20	**CA88**	2-F	FC(C=CC=C1)=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
21	**CA116**	3-F, 4-Cl	ClC(C=C1)=C(F)C=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
22	**CA118**	3-F, 5-Cl	ClC1=CC(F)=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
23	**CA107**	3,4-Cl	ClC(C=C1)=C(Cl)C=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
24	**CA101**	4-Cl	ClC(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
25	**CA120**	3-Cl	ClC1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
26	**CA121**	2-Cl	ClC(C=CC=C1)=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
27	**CA110**	4-Br	BrC(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
28	**CA98**	3-Br	BrC1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
29	**CA111**	2-Br	BrC(C=CC=C1)=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
30	**CA113**	3-I	IC1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
31	**CA89**	4-CN	FC(C1=CC2=C(NC3=CC=C(C#N)C=C3)C=CN=C2C=C1)(F)F
32	**CA90**	3-CN	FC(C1=CC2=C(NC3=CC(C#N)=CC=C3)C=CN=C2C=C1)(F)F
33	**CA91**	2-CN	FC(C1=CC2=C(NC3=C(C#N)C=CC=C3)C=CN=C2C=C1)(F)F
34	**CA112**	3-CF_3	FC(C1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1)(F)F
35	**CA115**	3-C≡C	C#CC1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1
36	**CA114**	3-Ac	CC(C1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1)=O
37	**CA103**	3-SO_2Me	O=S(C1=CC=CC(NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)=C1)(C)=O
38	**CA85**	4-SO_2Me	O=S(C(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)(C)=O
39	**CA102**	4-O^{t}Bu	CC(C)(C)OC(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2
40	**CA70**	4-$CH_2SO_2CH_3$	O=S(CC(C=C1)=CC=C1NC2=C3C(C=CC(C(F)(F)F)=C3)=NC=C2)(C)=O

41	**CA73**	6-H	COC(C=C1NC2=C3C(C=CC=C3)=NC=C2)=C(C(OC)=C1)OC
42	**CA82**	6-F	COC(C=C1NC2=C3C(C=CC(F)=C3)=NC=C2)=C(C(OC)=C1)OC
43	**CA163**	7-F	COC1=C(OC)C(OC)=CC(NC2=C3C(C=C(F)C=C3)=NC=C2)=C1
44	**CA99**	5,7-F	COC(C=C1NC2=C3C(C=C(F)C=C3F)=NC=C2)=C(C(OC)=C1)OC
45	**CA100**	6-^{t}Bu	COC(C=C1NC2=C3C(C=CC(C(C)(C)C)=C3)=NC=C2)=C(C(OC)=C1)OC
46	**CA171**	6-CN	COC1=C(OC)C(OC)=CC(NC2=C3C(C=CC(C#N)=C3)=NC=C2)=C1
47	**CA170**	6-SO_2Me	COC1=C(OC)C(OC)=CC(NC2=C3C(C=CC(S(=O)(C)=O)=C3)=NC=C2)=C1
48	**CA81**	6-OMe	COC1=C(OC)C(OC)=CC(NC2=C3C(C=CC(OC)=C3)=NC=C2)=C1
49	**CA75**	6,7-OMe	COC(C=C1NC2=C3C(C=C(OC)C(OC)=C3)=NC=C2)=C(C(OC)=C1)OC
50	**CA162**	7-OMe	COC1=C(OC)C(OC)=CC(NC2=C3C(C=C(OC)C=C3)=NC=C2)=C1
51	**CA80**	7-CF_3	COC(C=C1NC2=C3C(C=C(C(F)(F)F)C=C3)=NC=C2)=C(C(OC)=C1)OC
52	**CA157**	7-CN	COC1=C(OC)C(OC)=CC(NC2=C3C(C=C(C#N)C=C3)=NC=C2)=C1
53	**CA128**	3-Br	BrC1=CC=CC(NC2=C3C(C=C(OC)C(OC)=C3)=NC=C2)=C1
54	**CA129**	3-OMe	COC1=CC=CC(NC2=C3C(C=C(OC)C(OC)=C3)=NC=C2)=C1
55	**CA156**	3-C≡C	COC1=CC2=C(NC3=CC(C#C)=CC=C3)C=CN=C2C=C1OC
56	**CA130**	3-Ac	COC1=CC2=C(NC3=CC(C(C)=O)=CC=C3)C=CN=C2C=C1OC
57	**CA172**	3,4,5-OMe-Q	COC1=C(OC)C(OC)=CC(NC2=C3C(C=C(OC)C(OC)=C3)=NC=N2)=C1

Figure S10 - K_i curves for GAK – previously identified

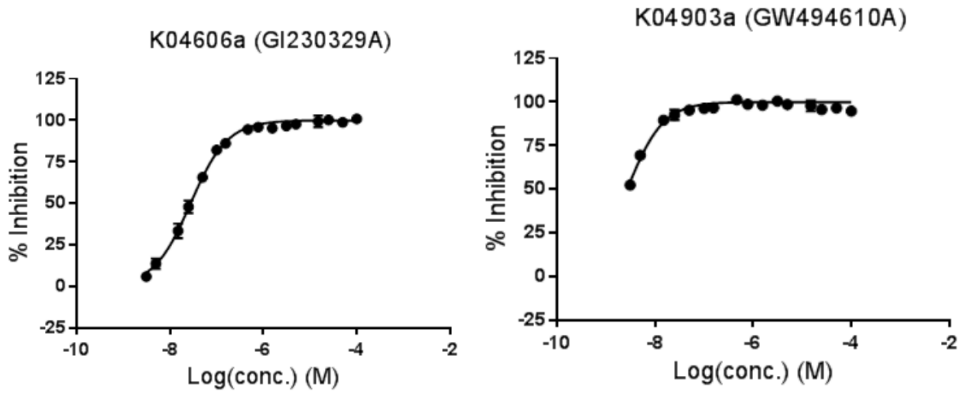
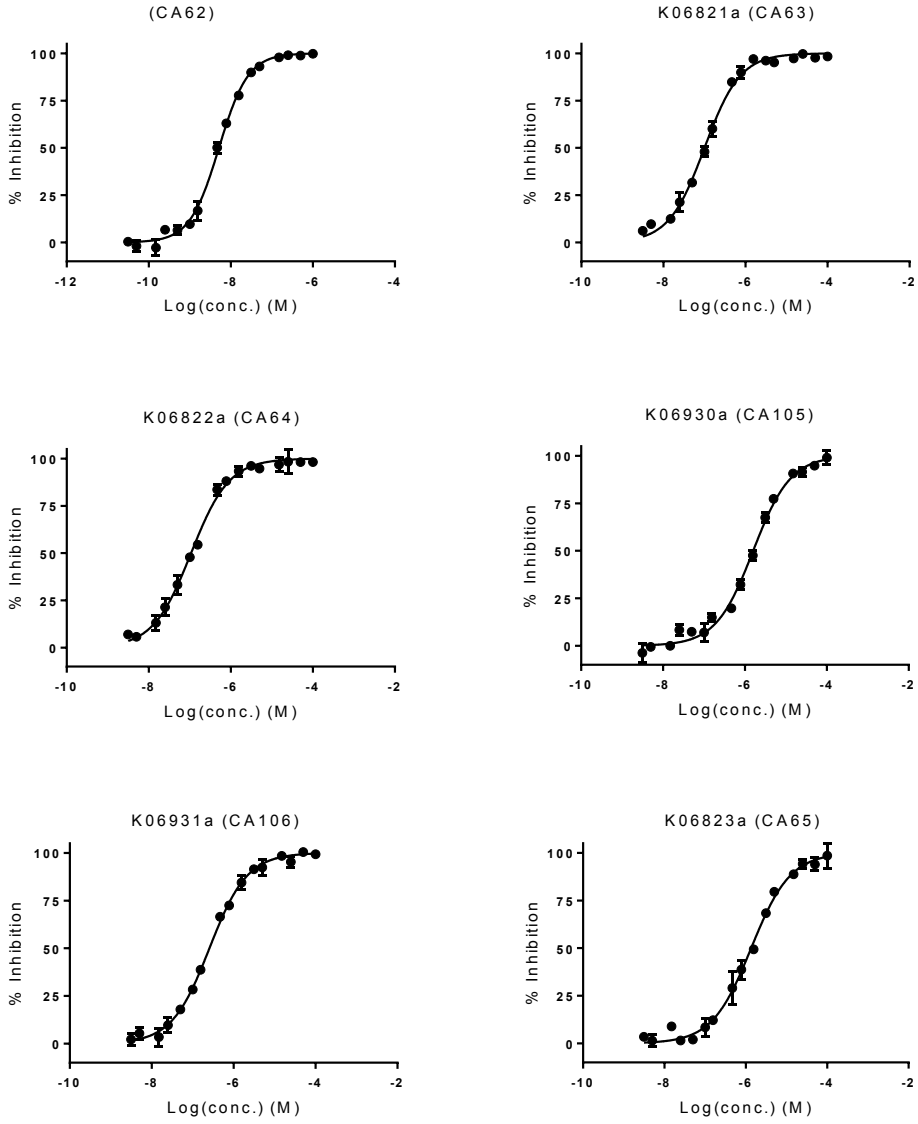
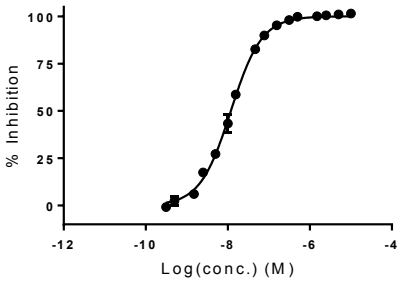


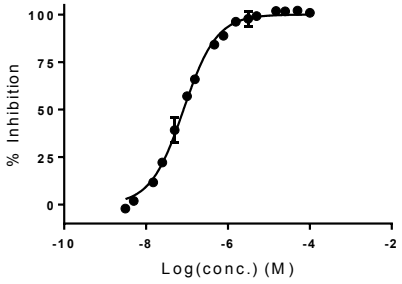
Figure S11 - K_i curves for GAK



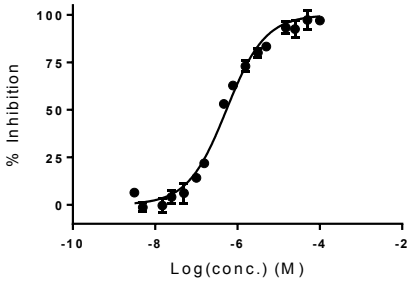
(CA66)



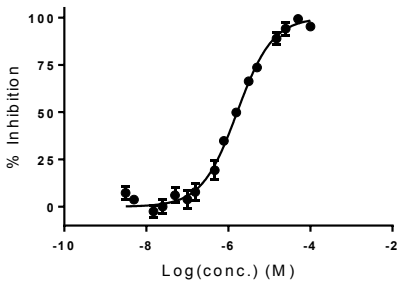
K62827a (CA67)



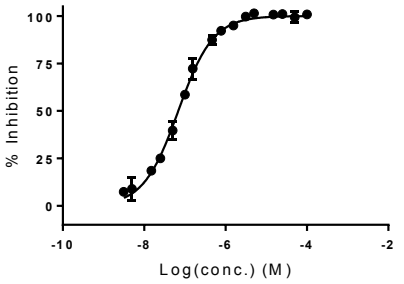
K06848a (CA68)



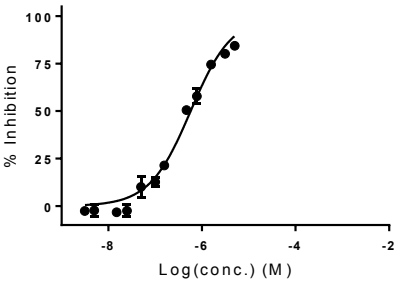
K06825a (CA69)



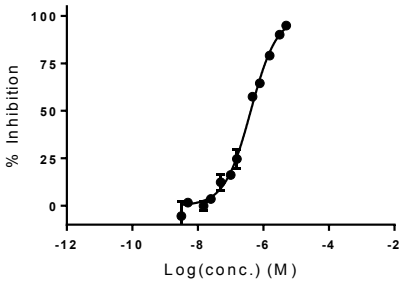
K06828a (CA72)



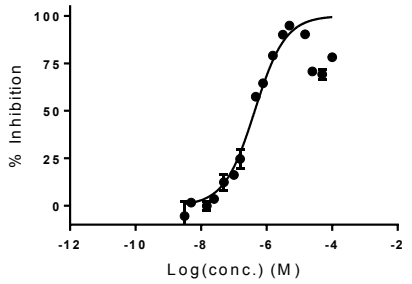
K06852a (CA76)

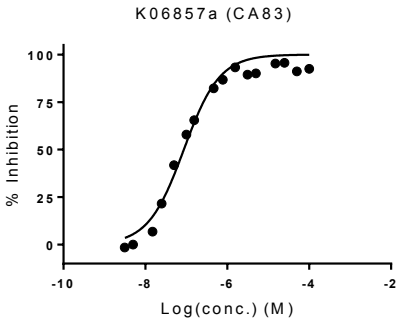


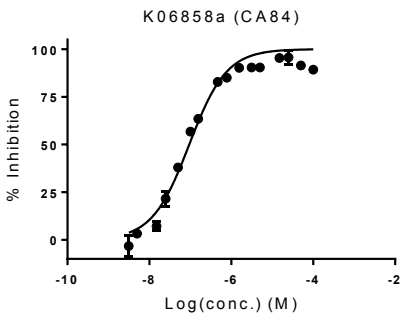
(CA76)

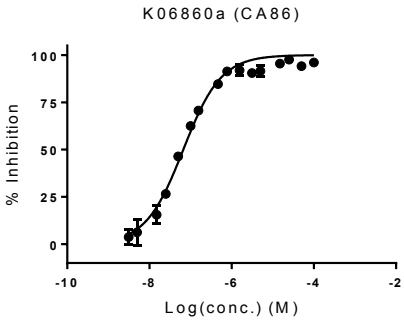


(CA76)




K06857a (CA83)
% Inhibition
100
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06858a (CA84)
% Inhibition
100
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06860a (CA86)
% Inhibition
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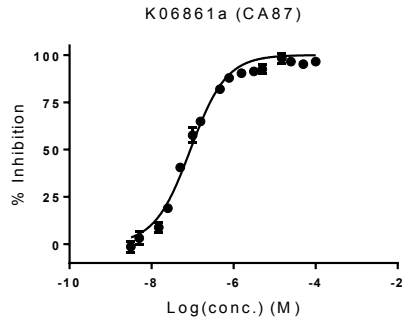
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06861a (CA87)
% Inhibition
100
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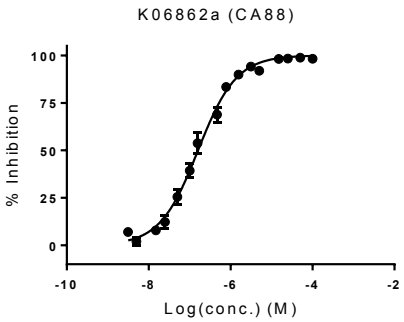
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06862a (CA88)
% Inhibition
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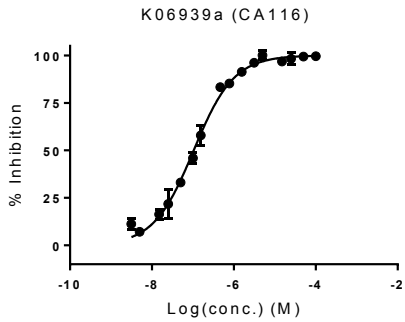
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06939a (CA116)
% Inhibition
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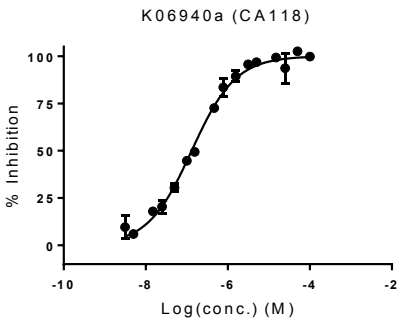
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06940a (CA118)
% Inhibition
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0
-10
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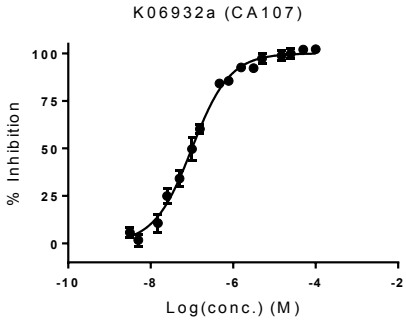
-6
-4
-2
Log(conc.) (M)


K06932a (CA107)
% Inhibition
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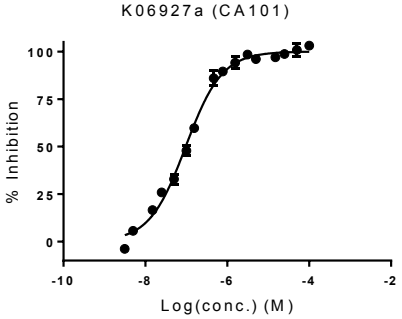
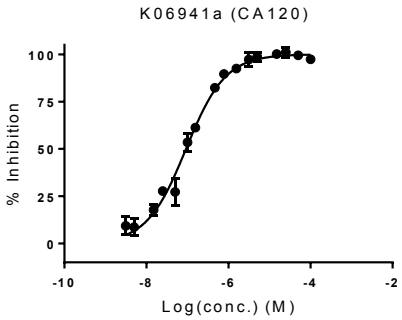
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06927a (CA101)
% Inhibition
100
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06941a (CA120)
% Inhibition
100
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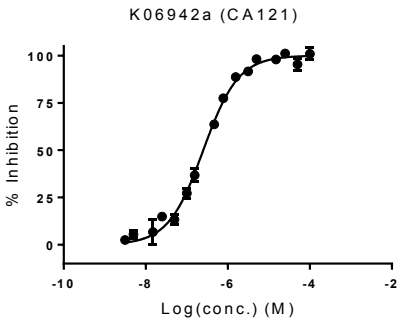
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06942a (CA121)
% Inhibition
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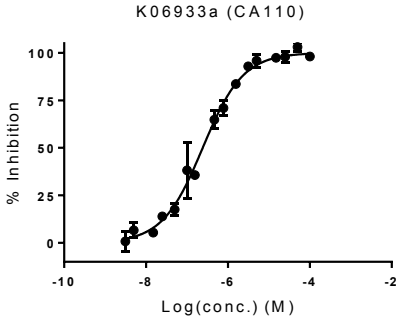
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06933a (CA110)
% Inhibition
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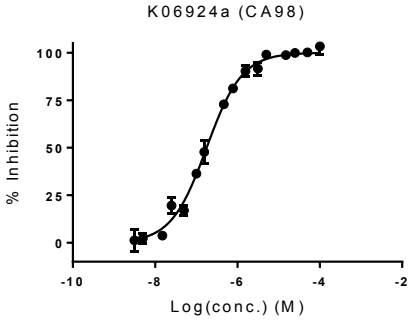
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06924a (CA98)
% Inhibition
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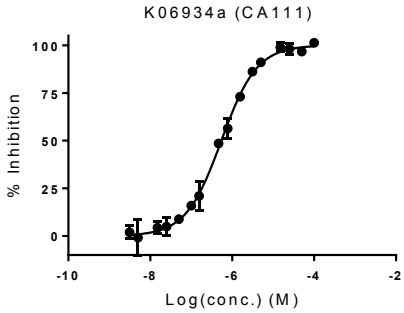
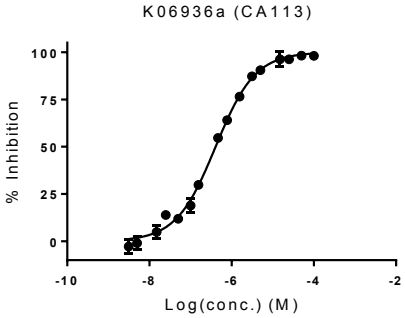
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06934a (CA111)
% Inhibition
100
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06936a (CA113)
% Inhibition
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-10
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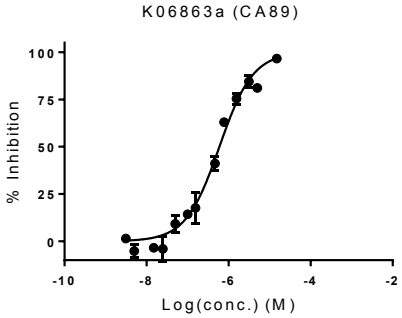
-6
-4
-2
Log(conc.) (M)


K06863a (CA89)
% Inhibition
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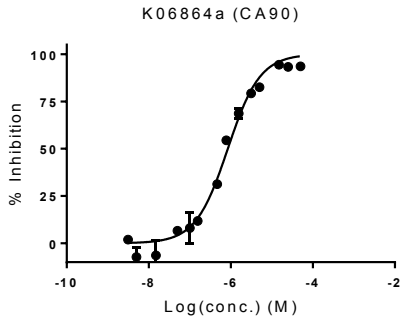
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06864a (CA90)
% Inhibition
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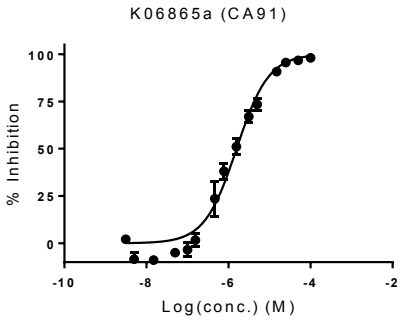
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06865a (CA91)
% Inhibition
100
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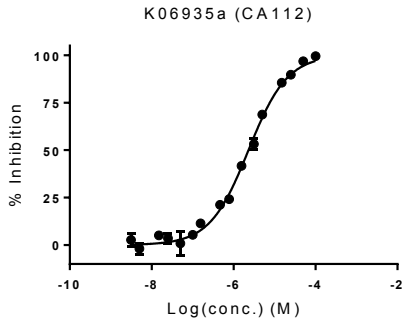
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06935a (CA112)
% Inhibition
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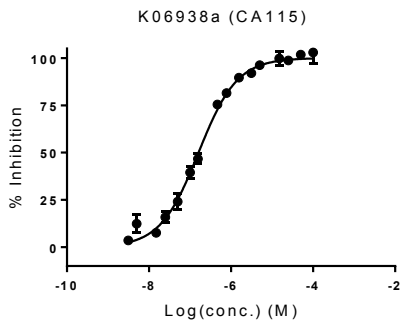
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06938a (CA115)
% Inhibition
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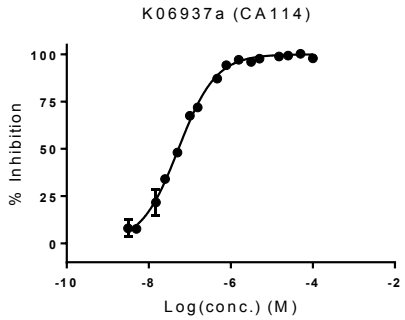
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06937a (CA114)
% Inhibition
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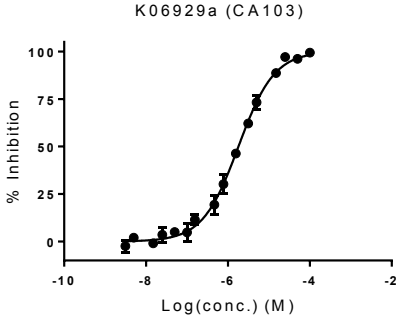
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06929a (CA103)
% Inhibition
100
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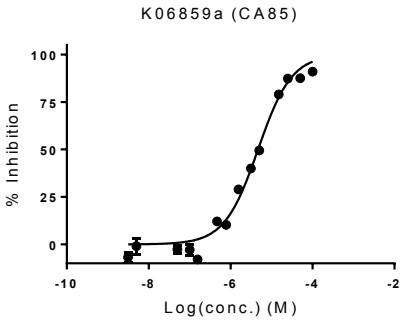
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)


K06859a (CA85)
% Inhibition
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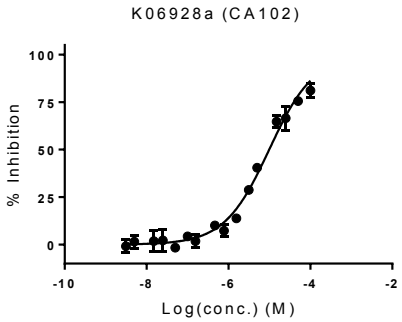
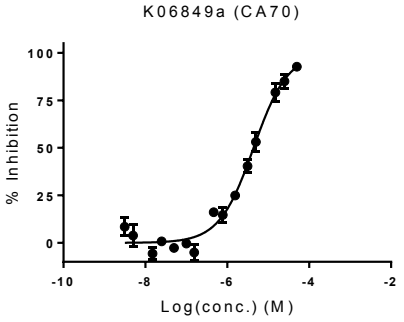
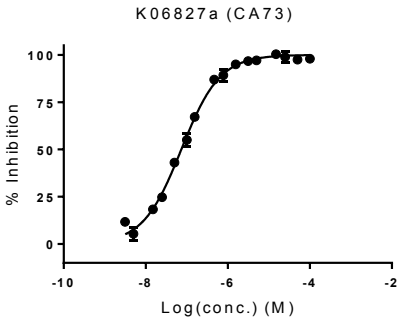
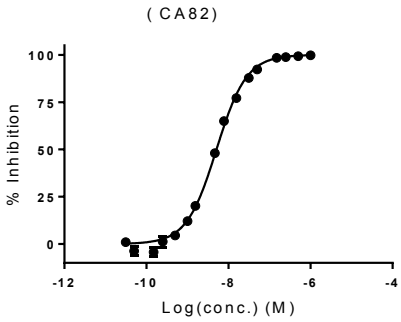
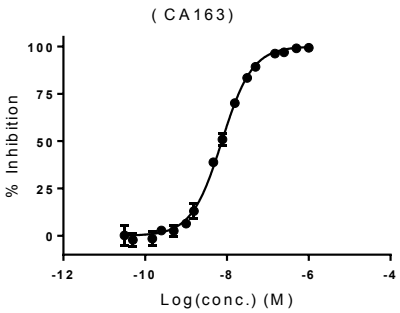
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)

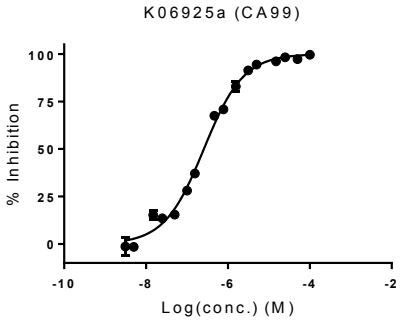

K06928a (CA102)
% Inhibition
100
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)

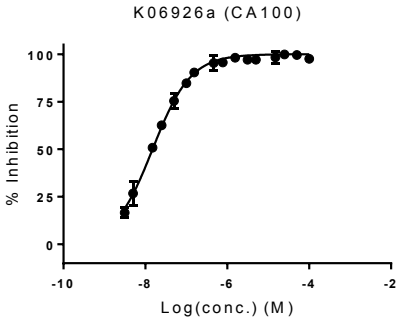

K06849a (CA70)
% Inhibition
100
75
50
25
0
-10
-8
-6
-4
-2
Log(conc.) (M)

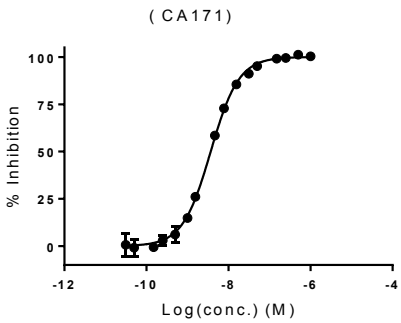

K06827a (CA73)
% Inhibition
Log(conc.) (M)

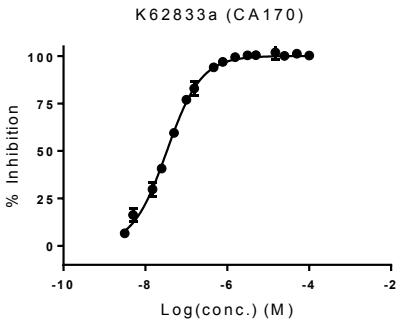

(CA82)
% Inhibition
Log(conc.) (M)

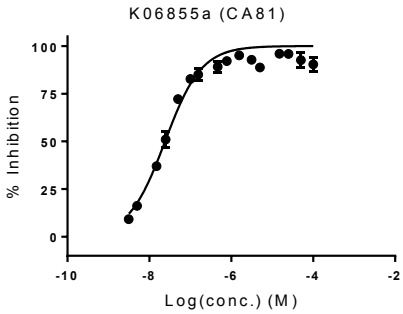

(CA163)
% Inhibition
Log(conc.) (M)

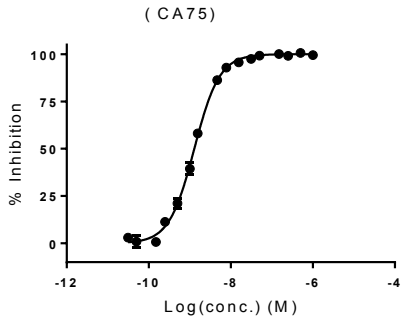

K06925a (CA99)
% Inhibition
Log(conc.) (M)


K06926a (CA100)
% Inhibition
Log(conc.) (M)


(CA171)
% Inhibition
Log(conc.) (M)


K62833a (CA170)
% Inhibition
Log(conc.) (M)


K06855a (CA81)
% Inhibition
Log(conc.) (M)


(CA75)
% Inhibition
100
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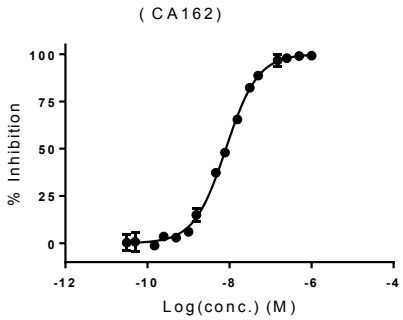
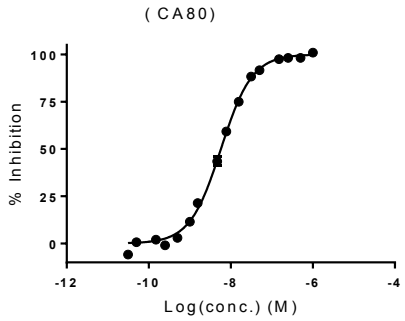
50
25
0
-12
-10
-8
-6
-4
Log(conc.) (M)


(CA162)
% Inhibition
100
75
50
25
0
-12
-10
-8
-6
-4
Log(conc.) (M)


(CA80)
% Inhibition
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75
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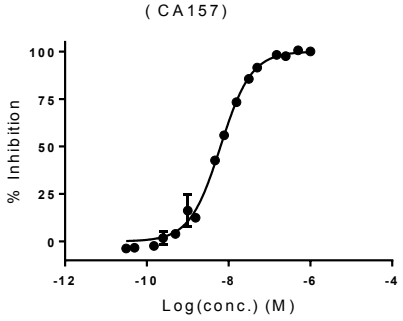
25
0
-12
-10
-8
-6
-4
Log(conc.) (M)


(CA157)
% Inhibition
100
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50
25
0
-12
-10
-8
-6
-4
Log(conc.) (M)

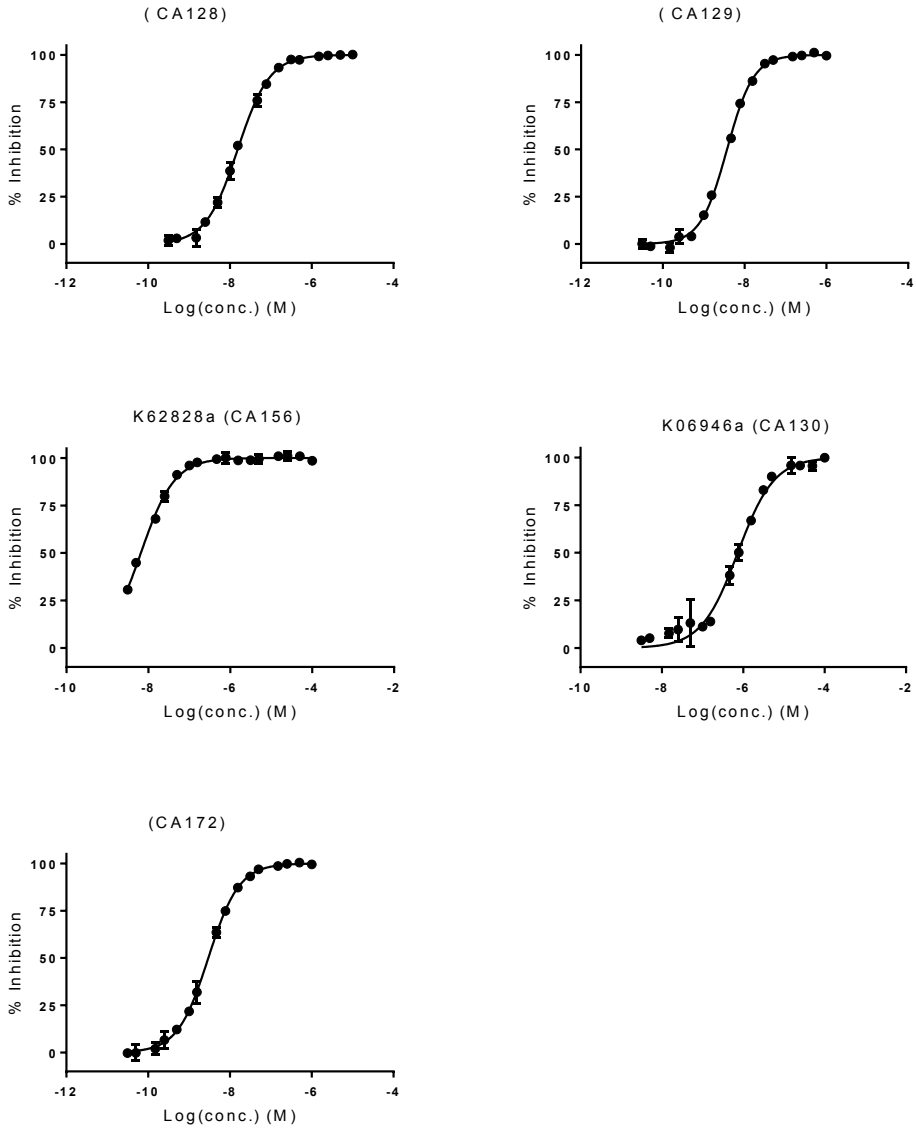


Table S4 - Hill slopes for GAK K_i measurement in ligand binding displacement assay

Paper	Lab-book	Annotation	Hill Slope
1	**CA62**	3,4,5-OMe	1.03
2	-	**GW494610**	1.18
3	-	**GI230329**	1.10
4	**CA63**	3,5-OMe	1.00
5	**CA64**	3,4-OMe	0.93
6	**CA105**	2,4-OMe	0.95
7	**CA106**	2,5-OMe	0.94
8	**CA65**	4-OMe	0.90
9	**CA66**	3-OMe	0.93

10	**CA67**	2-OMe	1.07
11	**CA68**	3,4-OCH_2O-	0.92
12	**CA69**	3,4-OCH_2CH_2O-	1.00
13	**CA72**	3,4,5-OMe-Q	1.02
14	**CA76**	3,5-OMe-Q	0.99
15	**CA78**	4-OMe-Q	1.12
16	**CA83**	3,4,5-F	1.00
17	**CA84**	3,5-F	0.95
18	**CA86**	4-F	0.94
19	**CA87**	3-F	0.99
20	**CA88**	2-F	0.93
21	**CA116**	3-F, 4-Cl	0.89
22	**CA118**	3-F, 5-Cl	0.81
23	**CA107**	3,4-Cl	0.95
24	**CA101**	4-Cl	0.98
25	**CA120**	3-Cl	0.90
26	**CA121**	2-Cl	1.02
27	**CA110**	4-Br	0.88
28	**CA98**	3-Br	1.01
29	**CA111**	2-Br	1.00
30	**CA113**	3-I	0.90
31	**CA89**	4-CN	1.06
32	**CA90**	3-CN	1.11
33	**CA91**	2-CN	1.11
34	**CA112**	3-CF_3	0.92
35	**CA115**	3-C≡C	0.93
36	**CA114**	3-Ac	0.95
37	**CA103**	3-SO_2Me	0.99
38	**CA85**	4-SO_2Me	1.06
39	**CA102**	4-O^{t}Bu	0.79
40	**CA70**	4-$CH_2SO_2CH_3$	1.04
41	**CA73**	6-H	1.05
42	**CA82**	6-F	0.76
43	**CA163**	7-F	1.18
44	**CA99**	5,7-F	0.90
45	**CA100**	6-^{t}Bu	0.93
46	**CA171**	6-CN	1.04
47	**CA170**	6-SO_2Me	1.04
48	**CA81**	6-OMe	0.98
49	**CA75**	6,7-OMe	0.44
50	**CA162**	7-OMe	1.10
51	**CA80**	7-CF_3	0.86
52	**CA157**	7-CN	1.10
53	**CA128**	3-Br	0.76
54	**CA129**	3-OMe	1.02
55	**CA156**	3-C≡C	1.06

56	**CA130**	3-Ac	0.97
57	**CA172**	3,4,5-OMe-Q	1.13

Figure S12 - K_d curves for compound **13** (CA72) on EGFR and GAK

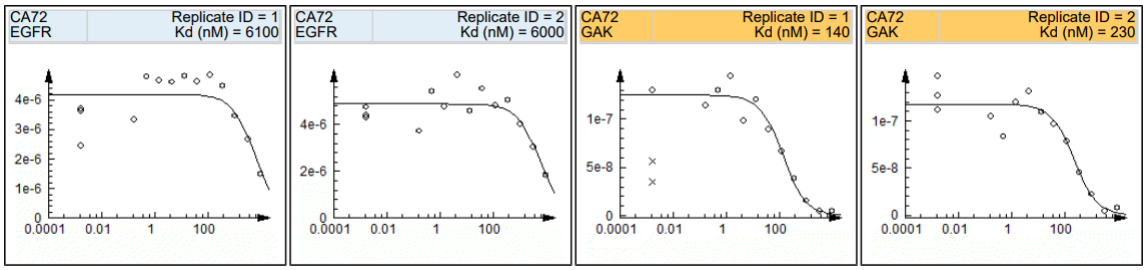
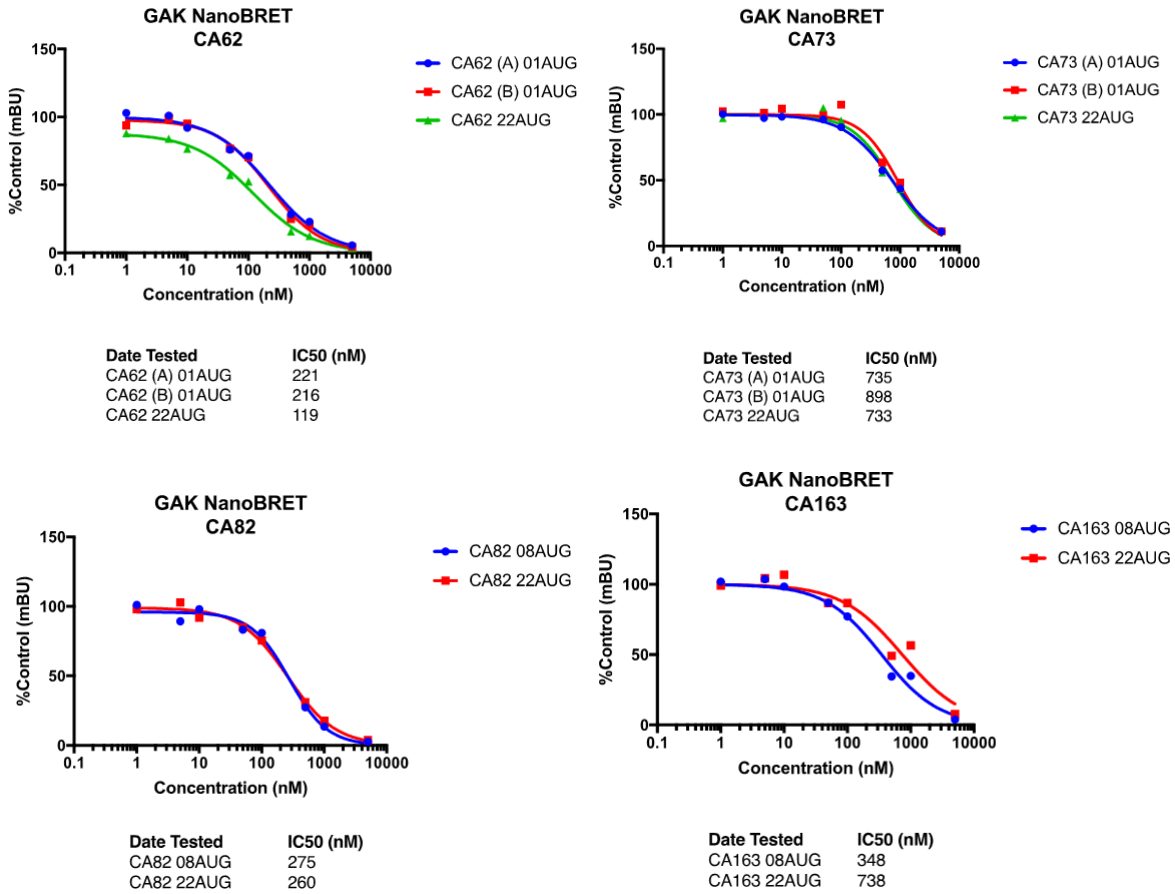


Figure S13 - IC_{50} curves for GAK

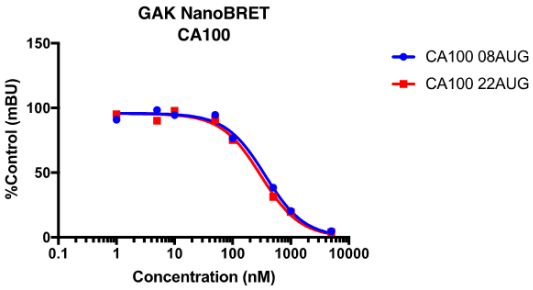


Date Tested	IC50 (nM)
CA62 (A) 01AUG	221
CA62 (B) 01AUG	216
CA62 22AUG	119

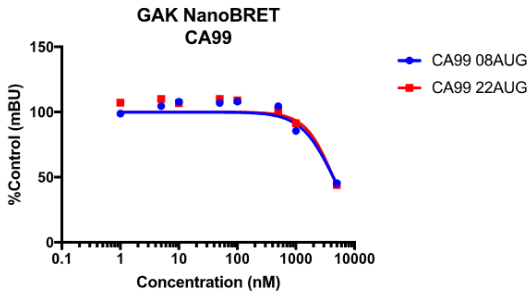
Date Tested	IC50 (nM)
CA73 (A) 01AUG	735
CA73 (B) 01AUG	898
CA73 22AUG	733

Date Tested	IC50 (nM)
CA82 08AUG	275
CA82 22AUG	260

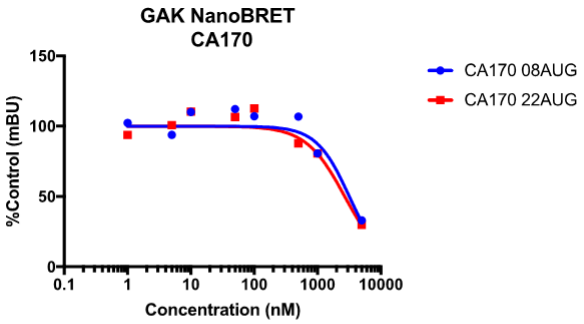
Date Tested	IC50 (nM)
CA163 08AUG	348
CA163 22AUG	738



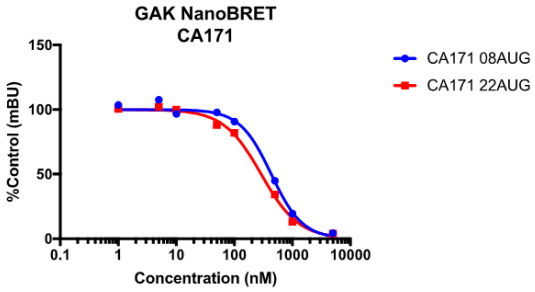
Date Tested	IC50 (nM)
CA100 08AUG	363
CA100 22AUG	305



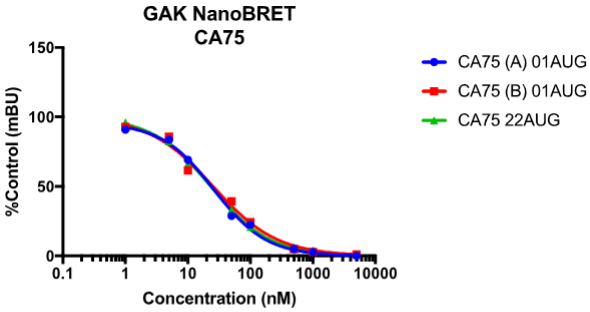
Date Tested	IC50 (nM)
CA99 08AUG	~4400
CA99 22AUG	~4400



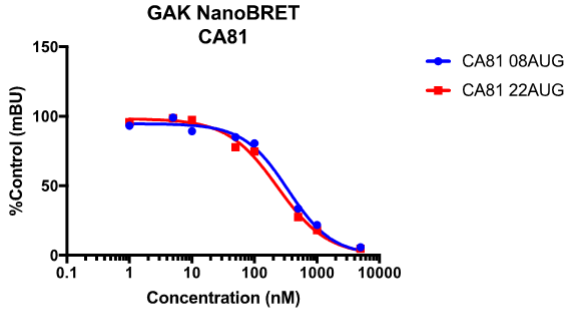
Date Tested	IC50 (nM)
CA170 08AUG	~3200
CA170 22AUG	~2700



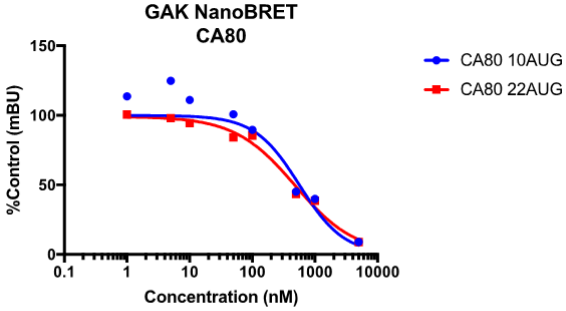
Date Tested	IC50 (nM)
CA171 08AUG	432
CA171 22AUG	290



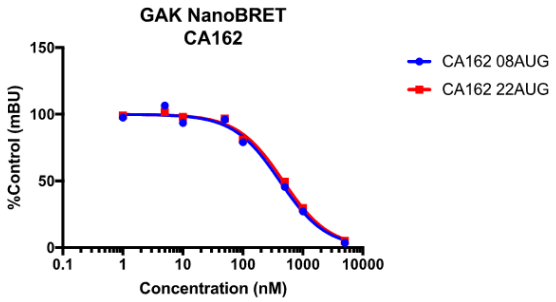
Date Tested	IC50 (nM)
CA75 (A) 01AUG	26
CA75 (B) 01AUG	26
CA75 22AUG	23



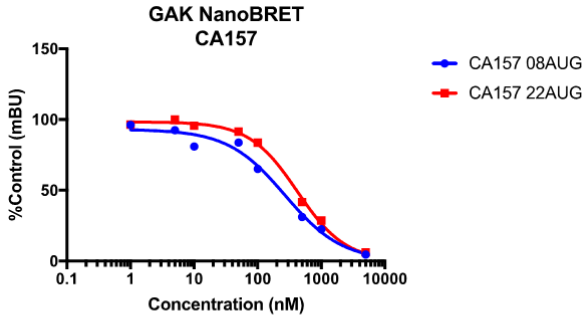
Date Tested	IC50 (nM)
CA81 08AUG	342
CA81 22AUG	234



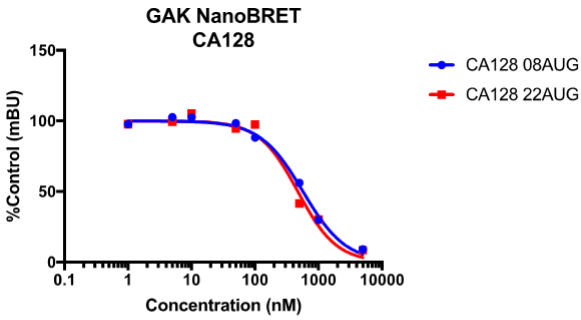
Date Tested	IC50 (nM)
CA80 10AUG	564



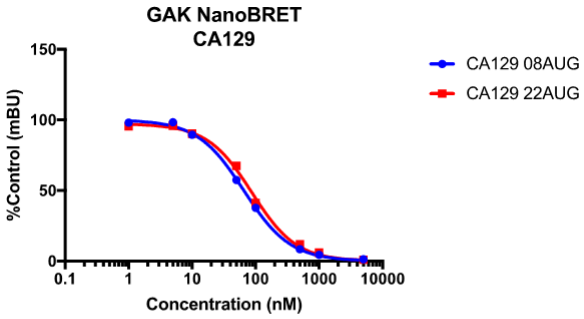
Date Tested	IC50 (nM)
CA162 08AUG	411
CA162 22AUG	469



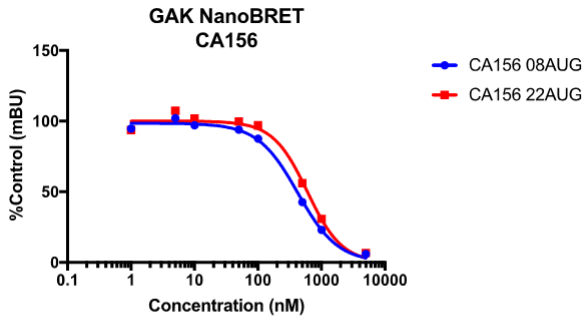
Date Tested	IC50 (nM)
CA157 08AUG	269
CA157 22AUG	420



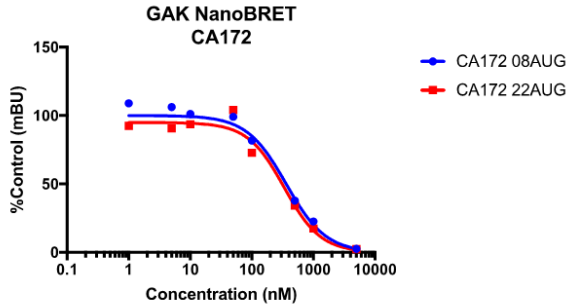
Date Tested	IC50 (nM)
CA128 08AUG	570
CA128 22AUG	474



Date Tested	IC50 (nM)
CA129 08AUG	65
CA129 22AUG	88



Date Tested	IC50 (nM)
CA156 08AUG	423
CA156 22AUG	600



Date Tested	IC50 (nM)
CA172 08AUG	361
CA172 22AUG	336