Supporting information

A systematic exploration of the effects of flexibility and basicity on sigma (σ) receptor binding in a series of substituted diamines

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The synthesis of intermediates **1A-1F**, conditions for potentiometric titrations and selected spectra of final compounds are reported here.

Synthesis of 2-benzofuranylmethanol **1A**

2-Benzofuranylmethanol was synthesised *via* an adaptation of the method reported by Wan *et al.*[1] To a solution of 2-benzofurancarboxaldehyde (1 mL, 8.3 mmol, 1 eq.) in CH_3OH (10 mL), sodium $NaBH_4$ (374 mg, 9.9 mmol, 1.2 eq.) was added portion-wise at - 4 °C. The reaction was then warmed to rt and stirred (8 h) before being quenched with HCl (1M, 2 mL) and then concentrated *in vacuo*. The residue was dissolved in CH_2Cl_2 (20 mL) and washed with H_2O (20 mL) and then brine (15 mL), dried over $MgSO_4$, filtered, reduced to dryness *in vacuo*. The resulting residue was purified by flash column chromatography on silica gel (EtOAc-Hexane, 15:85), yielding the titled compound as yellow oil (998 mg, 91%). **IR** (ZnSe cell): ν_{max} 3316, 2927, 2870, 1604, 1452, 1253, 1174, 1006, 936 cm^{-1}; **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.52-7.54 (1H, d, *J* = 7.6 Hz), 7.45-7.48 (1H, d, *J* = 15.6 Hz), 7.22-7.29 (2H, m), 6.59 (1H, s), 4.71-4.73 (2H, d, *J* =8.8 Hz), 3.93-3.98 (1H, t, *J* = 7.5 Hz) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$): δ 156.67 (C) ppm, 154.98 (C), 128.17 (C), 124.12 (CH), 122.64 (CH), 120.98 (CH), 111.08 (CH), 103.76 (CH), 57.61 (CH_2) ppm; **LRMS** (+ESI): m/z 149 $[M+H]^+$. Spectroscopic data matched that reported in literature.[2]

Synthesis of 2-(chloromethyl)benzofuran **1B**

2-(Chloromethyl)benzofuran was synthesised according to the method reported by Ferorelli *et al.*[3] To a solution of 2-benzofuranylmethanol **1A** (300 mg, 2.0 mmol, 1 *eq.*) in an anhydrous solution of DMF (0.5 mL) and THF (2 mL), $SOCl_2$ (200 µL, 2.7 mmol, 1.4 *eq.*) was added dropwise with stirring at rt. The reaction mixture was then heated at reflux for 2 h and then the THF was removed *in vacuo*. The residue was partitioned in H_2O (20 mL) and EtOAc (30 mL) with further extraction of the aqueous flayer with EtOAc (2×30 mL). The combined organic layers were then washed with brine (60 mL), dried over $MgSO_4$, filtered, and evaporated to dryness. The residue was purified by flash column chromatography on silica gel (100% hexane), yielding the titled compound as a colourless oil (247 mg, 73%). **IR** (ZnSe cell): ν_{max} 3063, 1586, 1452, 1283, 1253, 1191, 1151, 1123, 1007, 955, 824 cm^{-1}; **^{1}H NMR** (300 MHz, $CDCl_3$): 7.39-7.41 (1H, d, *J* = 7.5 Hz), 7.33-7.36 (1H, d, *J* =8.1 Hz), 7.17 (1H, t, *J* = 7.4 Hz), 7.09 (1H, t, *J* = 7.4 Hz), 6.56 (1H, s), 4.53 (2H, s) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$): δ 155.41 (C), 152.60 (C), 127.98 (C), 125.13 (CH), 123.16 (CH), 121.41 (CH), 111.46 (CH), 106.26 (CH), 37.82 (CH_2) ppm; **LRMS** m/z (+APCI): 131 $[M–Cl]^+$, 100), 167 $[M+H]^+$**.** Spectroscopic data matched that reported in literature.[4]

Synthesis of benzofuran-2-carboxamide **1C**

2-benzofurancarboxylic acid (1.50 g, 9.25 mmol) was converted to the acid chloride and reacted with ammonia (28% aq., 6.94 mmol) according to the general procedure A, and the product was purified by flash column chromatography on silica gel (eluent: 3:1 *v/v* EtOAc/hexane) to afford amide **1C** as a white solid (917 mg, 82%). **m.p.** 153-154 °C (lit. m.p. 158-159 °C);[5] **IR** (ZnSe cell): ν_{max} 3425, 3148, 1656, 1590, 1473, 1396, 1340, 1259, 1174, 1090, 938, 885, 840, 807 cm^{-1}; **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.56-7.58 (1H, d, *J* = 7.8 Hz,), 7.38-7.41 (2H, m), 7.29-7.34 (1H, t, *J* =7.8 Hz), 7.16-7.21 (1H, t, *J* = 7.4 Hz), 6.08 (2H, br s, NH_2) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$): δ 160.87 (C), 155.10 (C), 148.30 (C), 127.71 (C), 123.94 (CH), 122.99 (CH), 111.46 (CH), 110.66 (CH), ppm; **LRMS** (+ESI): m/z 162 $[M+H]^+$.

Synthesis of *N*-methylbenzofuran-2-carboxamide **1D**

2-benzofurancarboxylic acid (1.50 g, 9.25 mmol) was converted to the acid chloride and reacted with methylamine (2.0 M solution in THF, 6.94 mmol) according to the general procedure A, and the product was purified by flash column chromatography on silica gel (eluent: 3:1 *v/v* EtOAc/hexane) to afford amide **1D** as a pale yellow amorphous solid (1.07 g, 88%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65-7.62 (1H, d, *J* = 8.04 Hz); δ 7.46-7.43 (2H, m), 7.39-7.35 (1H, m); 7.28-7.24 (1H, m); 6.96 (1H, br s); 3.05-3.04 (3H, d, *J* = 5.06 Hz) ppm **^{13}C NMR** (400 MHz, $CDCl_3$) δ 159.7 (C), δ 154.7 (C), 148.8 (C), 127.6 (C), 126.8 (CH), 123.6 (CH) 122.7 (CH), 111.7 (CH), 110.1 (CH), 26.1 (CH_3) ppm; **LRMS** (+ESI): m/z 198 $[M+Na]^+$

Synthesis of benzofuran-2-ylmethanamine **1E**

Amide **1C** (800 mg, 4.96 mmol) was reduced according the general procedure C and purified by flash chromatography (eluent: 7% MeOH/CH_2Cl_2 + 1% Et_3N) to afford amine **1E** as a pale yellow oil (322 mg, 44%). **IR** (ZnSe cell): ν_{max} 3369, 3301, 3067, 2915, 2845, 1585, 1453, 1251, 1171, 1007, 943 cm^{-1}; **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.55-7.57 (1H, d, , *J* = 7.8 Hz), 7.47-7.50 (1H, d, *J* = 7.8 Hz), 7.22-7.31 (2H, m), 6.54 (1H, s), 3.98 (2H, s), 1.83 (2H, br s, NH_2) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$): δ 159.38 (C), 154.84 (C), 128.49 (C), 123.72 (CH), 122.62 (CH),

120.70 (CH), 110.95 (CH), 101.88 (CH), 39.72 (CH_2), ppm; **LRMS m/z** (+ESI): 148 $[M+H]^+$. The spectroscopic data matched that reported in the literature.[6]

1-(benzofuran-2-yl)-N-methylmethanamine **1F**

Amide **1D** (800 mg, 4.57 mmol) was reduced according the general procedure C and purified by flash column chromatography on silica gel (eluent: 5% MeOH/CH_2Cl_2 + 1% Et_2NH) to afford amine **1F** as a pale yellow oil (555 mg, 75%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.52-7.50 (1H, d *J* = 7.27 Hz), 7.44-7.42 (1H, d, *J* = 7.93 Hz), 7.26-7.18 (2H, m), 6.69 (1H, s), 5.34 (1H, br s), 4.00 (2H, s), 2.52 (3H, s) ppm, **LRMS** m/z (+ESI): 162 $[M+H]^+$

Experimental pK_a calculations

Experimental pK_a values were determined through potentiometric titrations. Liberated amines were dissolved in 40% ethanol and titrated with HCl solution. Titrations were carried out in triplicate at 18-20 °C. The pK_a values were determined from a plot of the titrated volume vs. the pH. The pK_a was calculated as the half-equivalence point of the pH from the sigmoid curve.

Calculated pK_a values from version 15 of MarvinSketch

Compound	**Predicted pK_a**		**N^1**	**N^2**	**Predicted microspecies distribution (%)**
	N^1	**N^2**			
1	7.74	2.01	N NH$^+$ N	N N NH$^+$	31.2 54.7 14.0
12a	7.79	--	N NH$^+$	N N	29.1 70.9
12b	--	8.58	N N	N NH$^+$	6.2 93.8
13a	7.80	--	N NH$^+$	N N	28.7 71.3
13b	--	7.8	N N	N NH$^+$	28.3 71.6
16a	7.82	--	N NH$^+$	N N	27.5 72.5
16b	--	8.60	N N	N NH$^+$	5.9 94.1
16c	7.84	--	N NH$^+$	N N	26.8 73.2
16d	--	7.93	N N	N NH$^+$	27.2 72.8

Compound	Predicted pK_a		N^1	N^2	Predicted microspecies distribution (%)
	N^1	N^2			
22a	13.02	7.86	N	N	25.5
			N	NH^+	74.5
22b	7.09	15.06	N	N	67.2
			NH^+	N	32.9
23a	--	7.90	N	N	24.1
			N	NH^+	75.9
23b	7.13	--	N	N	64.9
			NH^+	N	35.1
24a	13.07	6.89	N	N	76.3
			N	NH^+	23.7
24b	6.96	--	N	N	73.2
			NH^+	N	26.8
25a	--	5.93	N	N	74.6
			N	NH^+	25.4
25b	8.02	--	N	N	19.2
			NH^+	N	80.8

Compound	Predicted pK_a		N^1	N^2	Predicted microspecies distribution (%)
	N^1	N^2			
26a	5.43	8.69	N	N	5.6
			NH^+	N	12.9
			N	NH^+	80.4
			NH^+	NH^+	1.0
26b	8.40	4.34	N	N	9.2
			NH^+	N	57.9
			N	NH^+	32.9
			NH^+	NH^+	0.1
26c	5.86	9.02	N	N	2.3
			NH^+	N	8.1
			N	NH^+	86.9
			NH^+	NH^+	2.8
26d	8.79	4.80	N	N	4.3
			NH^+	N	48.4

	N	NH^+	47.2
	NH^+	NH^+	0.2

Figure 1. Average of three potentiometric titrations of benzylamine with HCl at 18-20 °C.

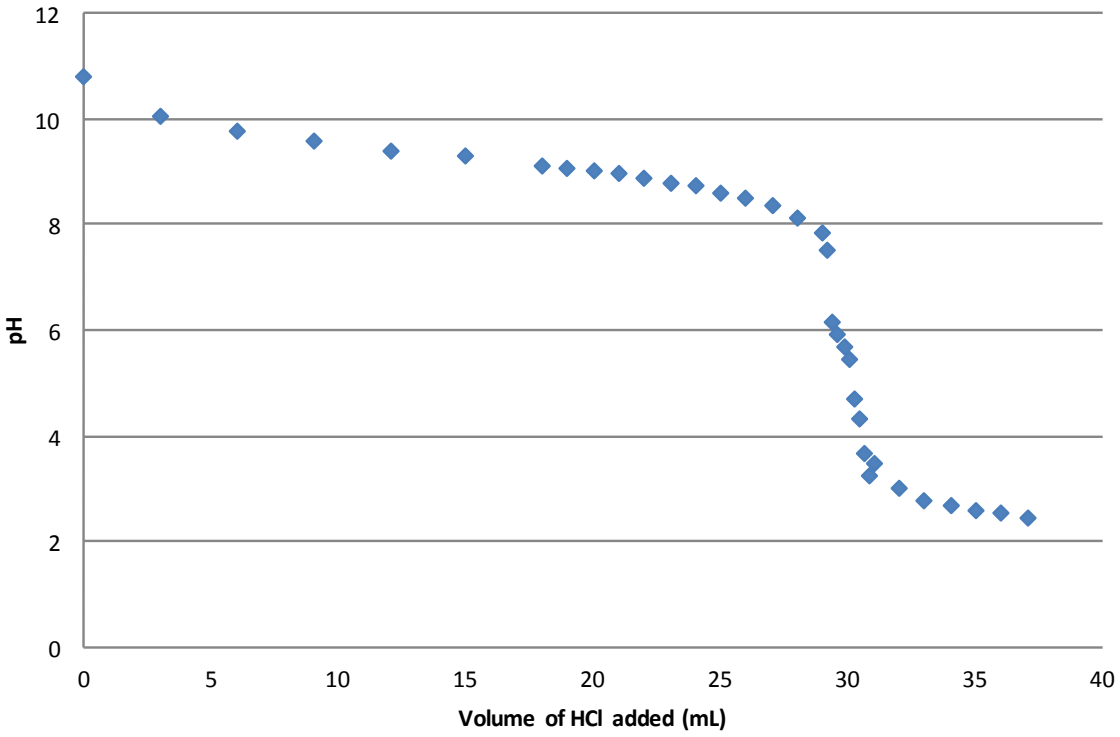


Figure 2. Average of three potentiometric titrations of **13b** with HCl at 18-20 °C.

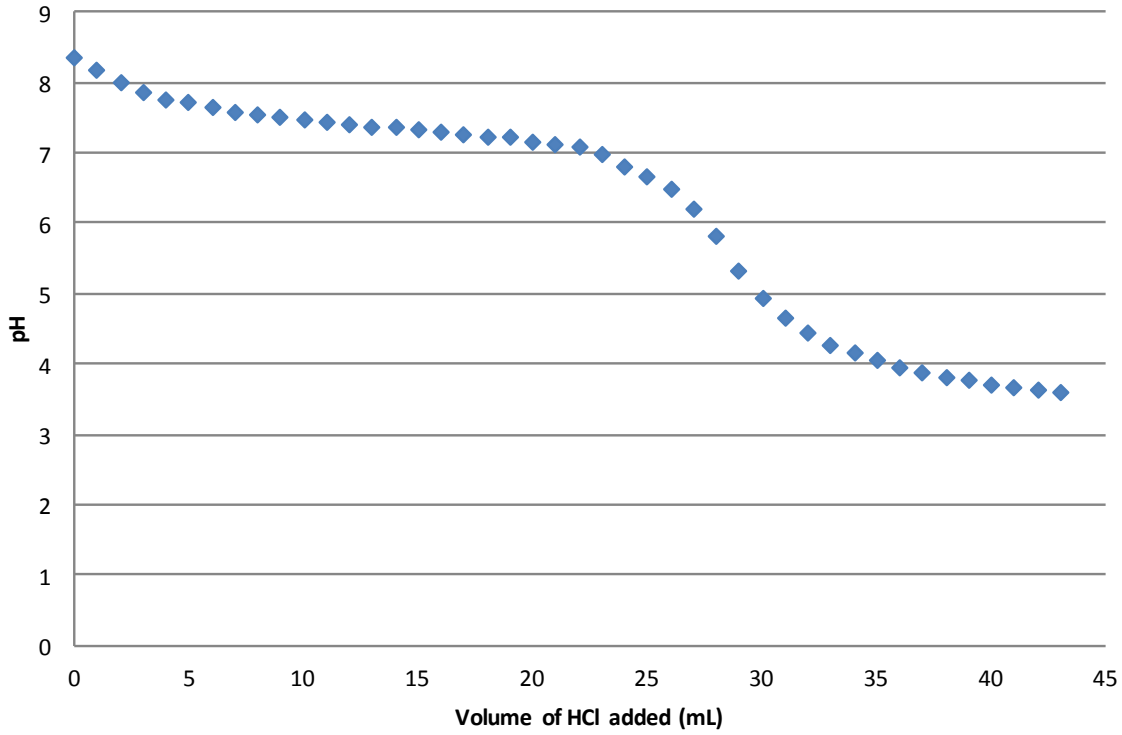
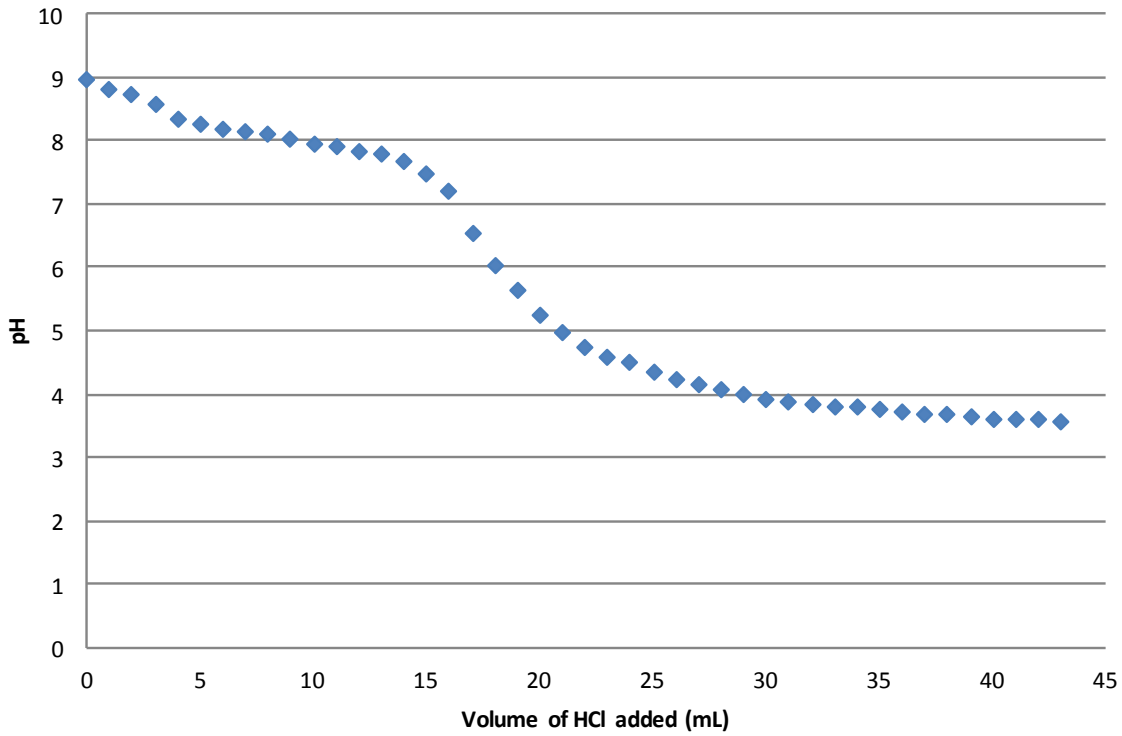
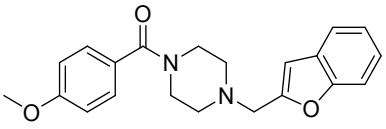
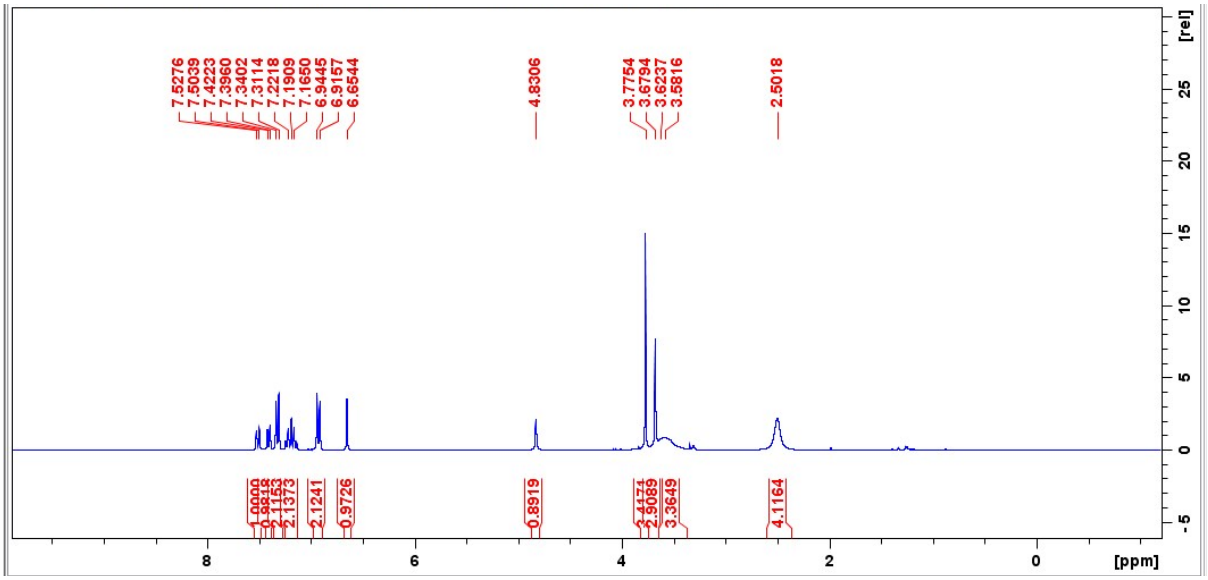


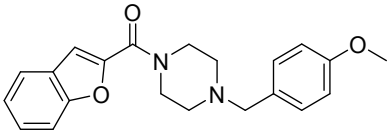
Figure 2. Average of three potentiometric titrations of **25b** with HCl at 18-20 °C.

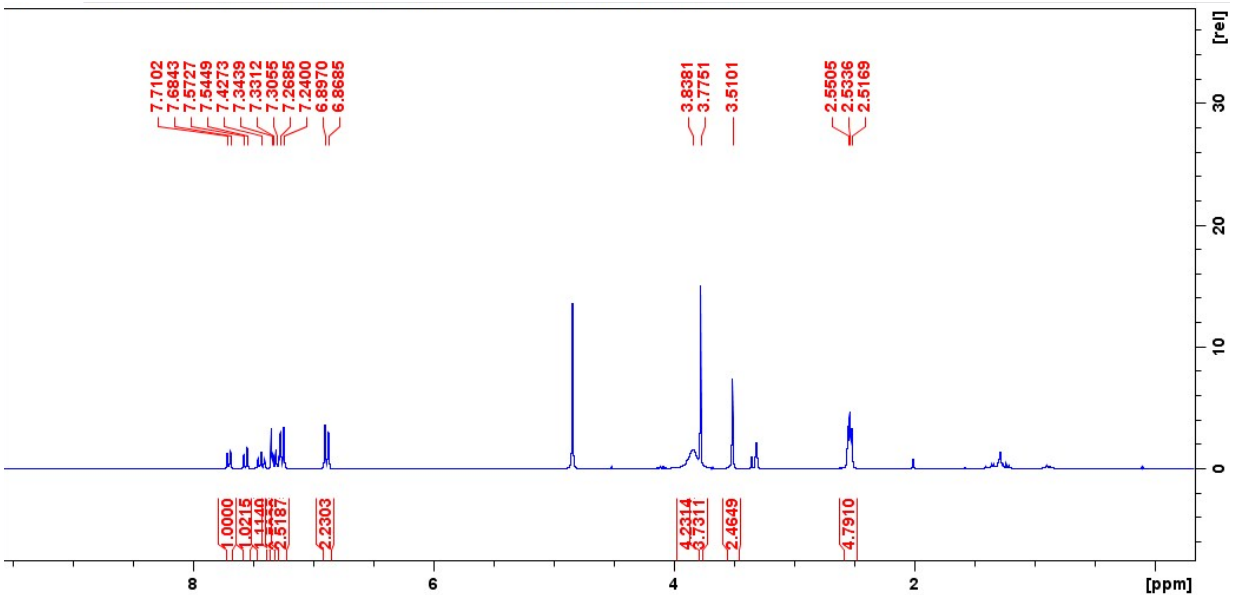


Spectra of compounds tested:

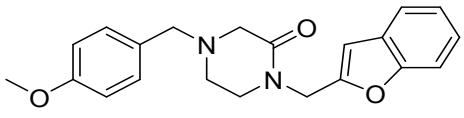
5a - $CDCl_3$ 

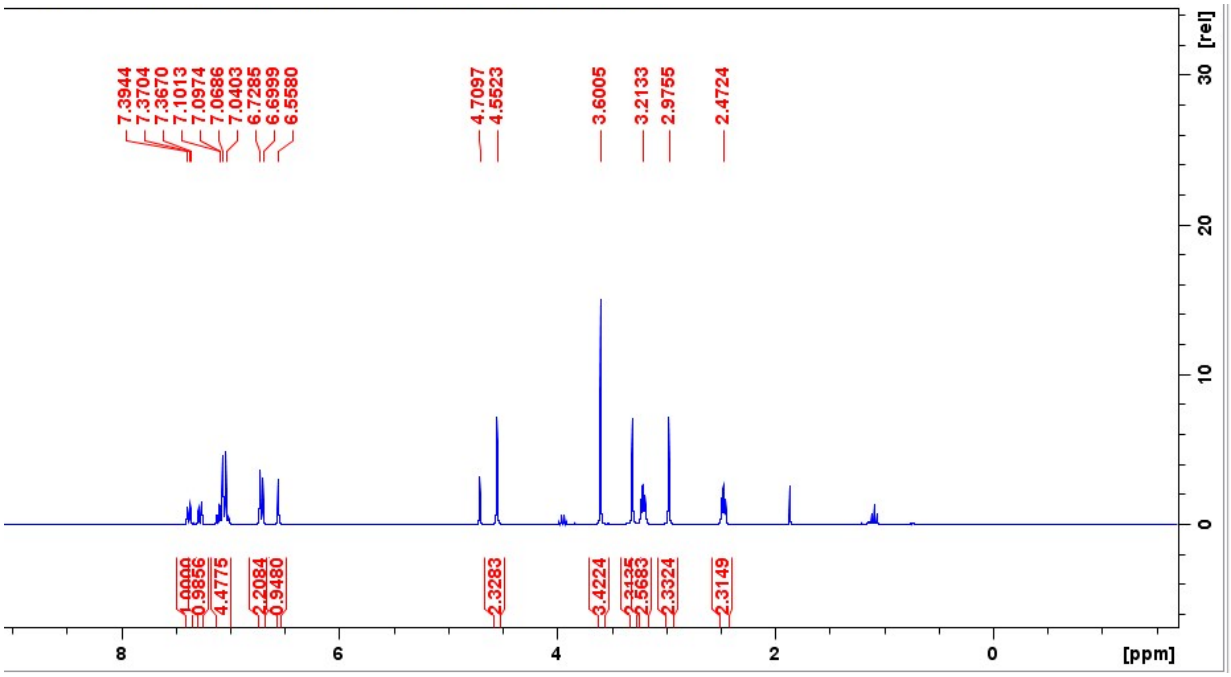


5b - $CDCl_3$ 



8a - $CDCl_3$





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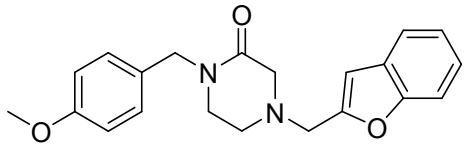

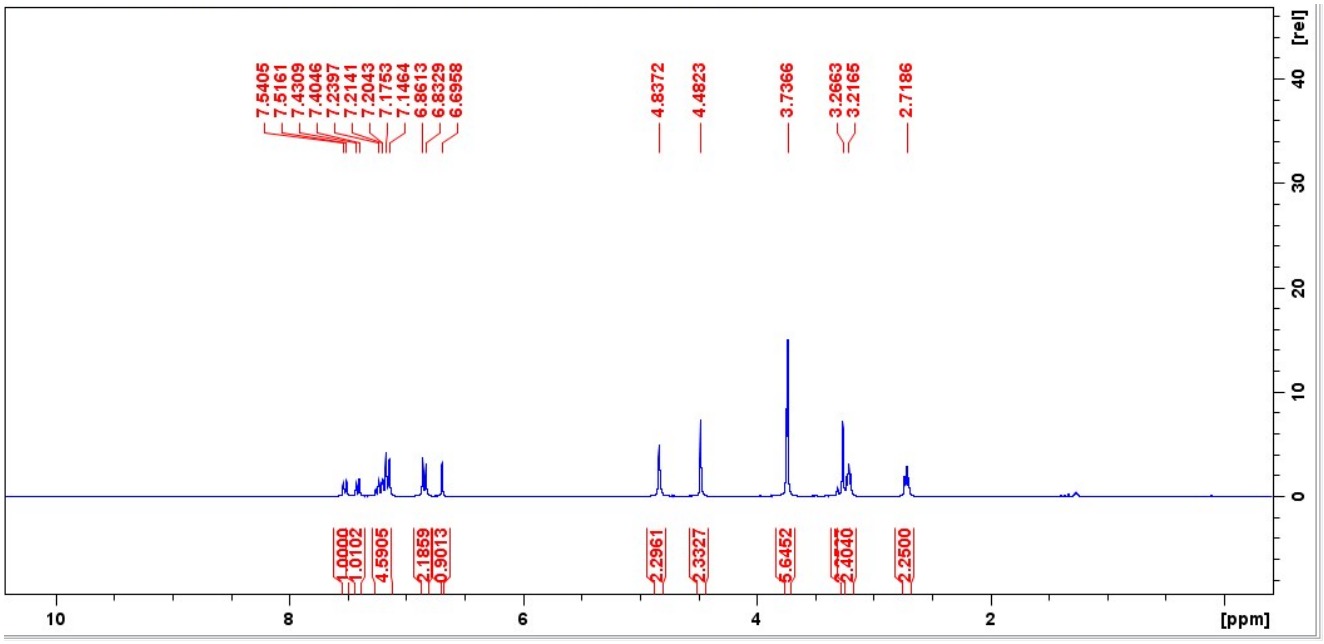

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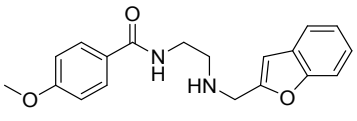
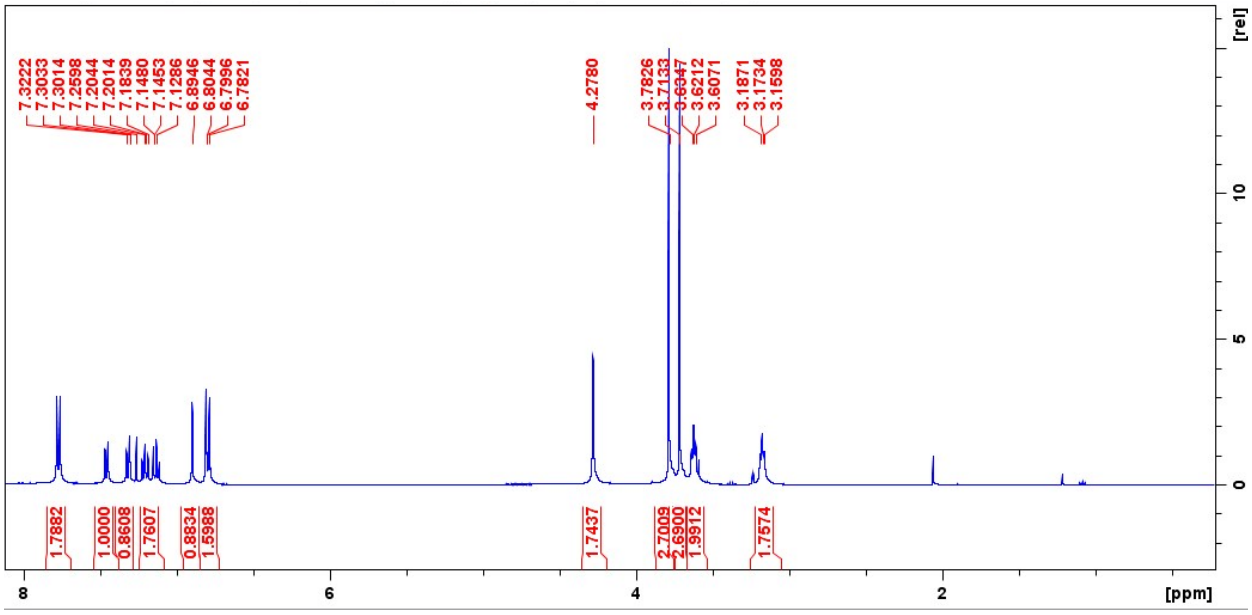
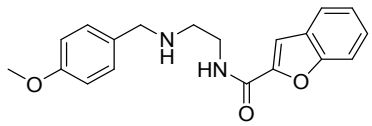
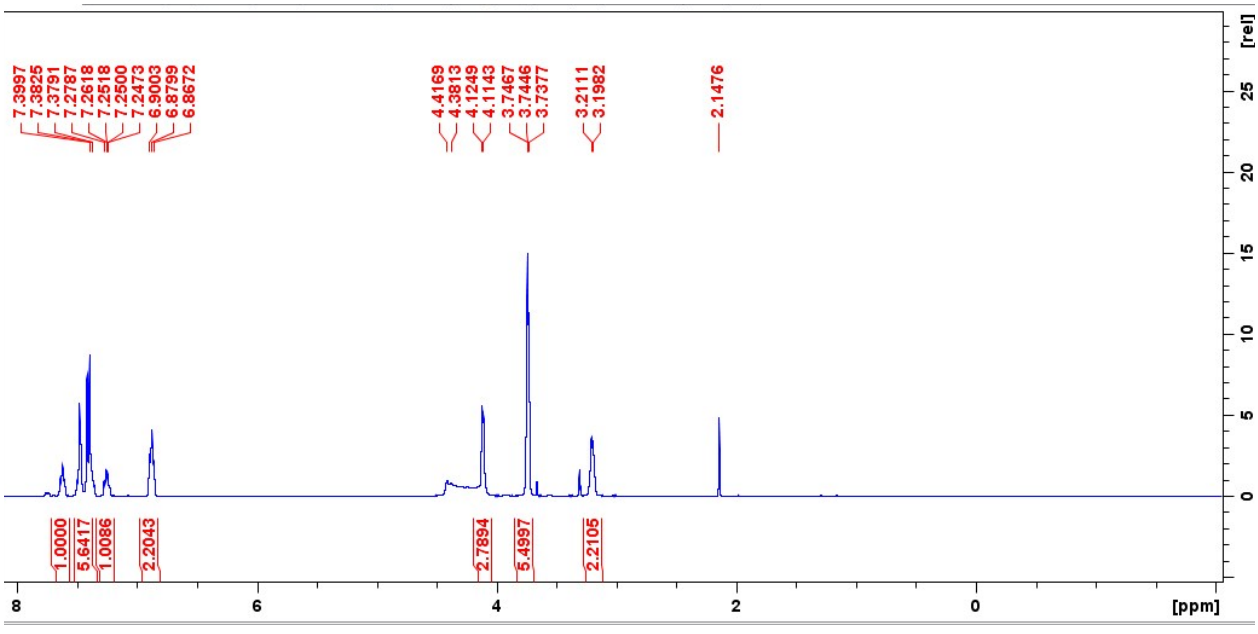
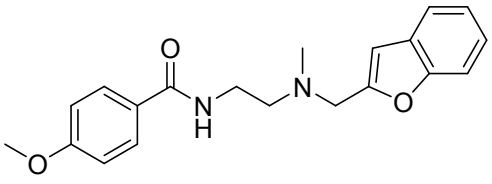




12b - CD_3OD







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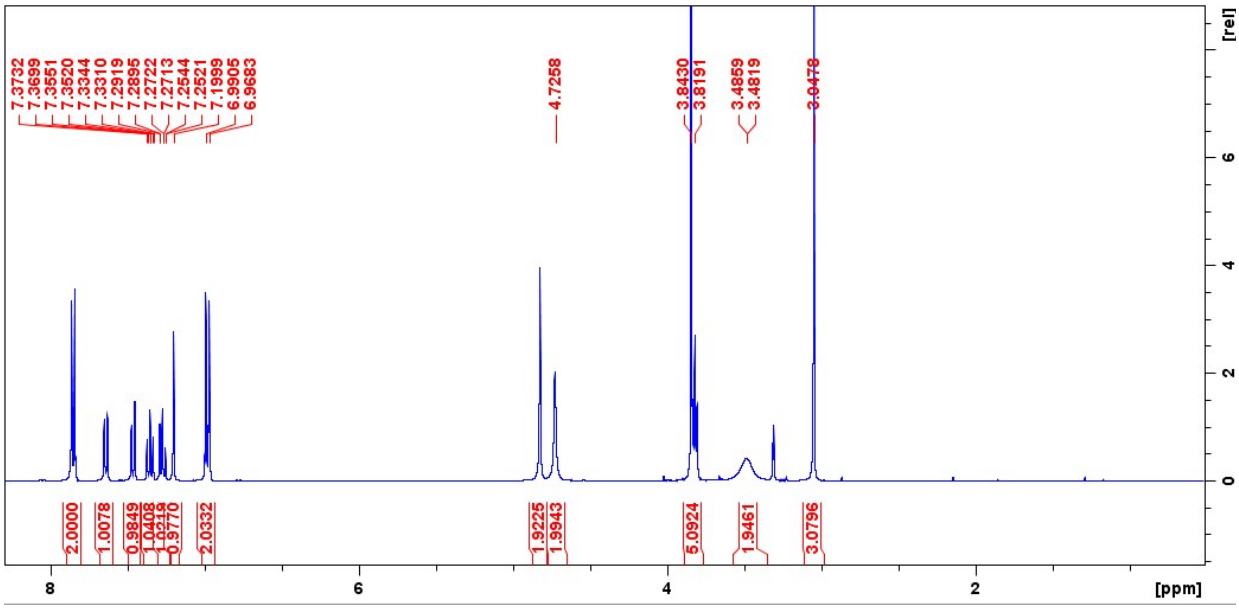
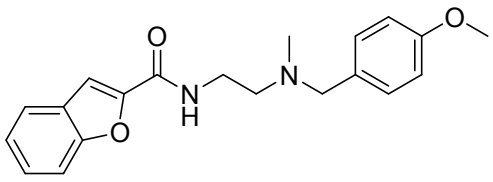
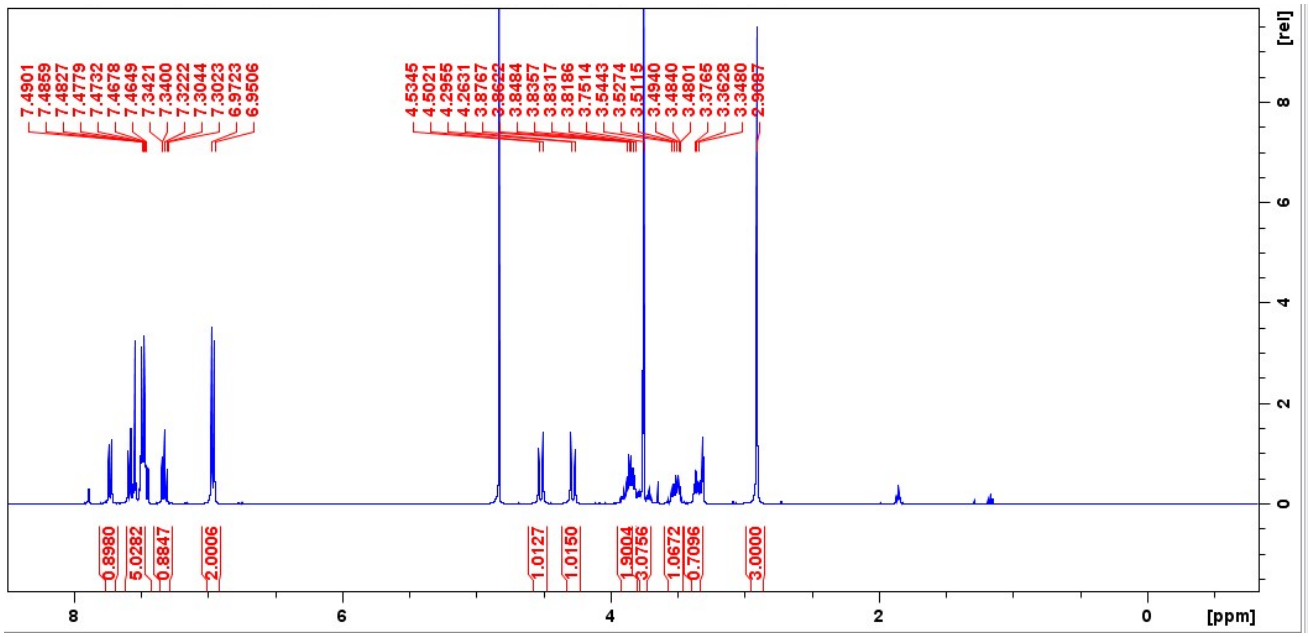
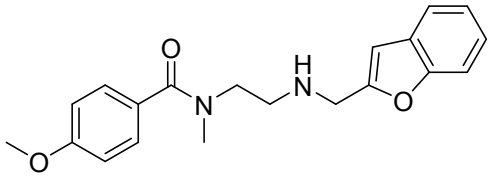


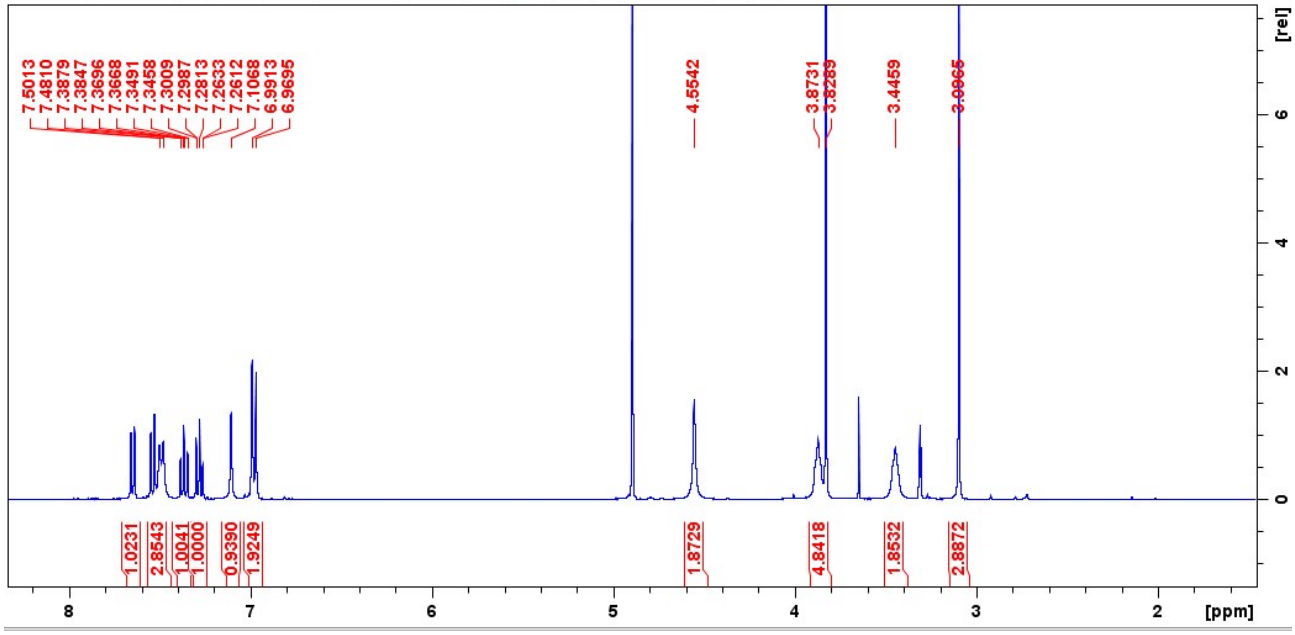


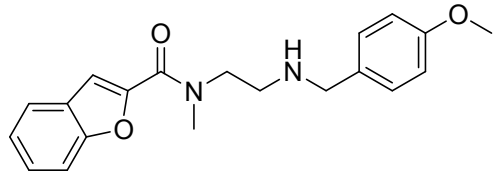
13b - CD_3OD



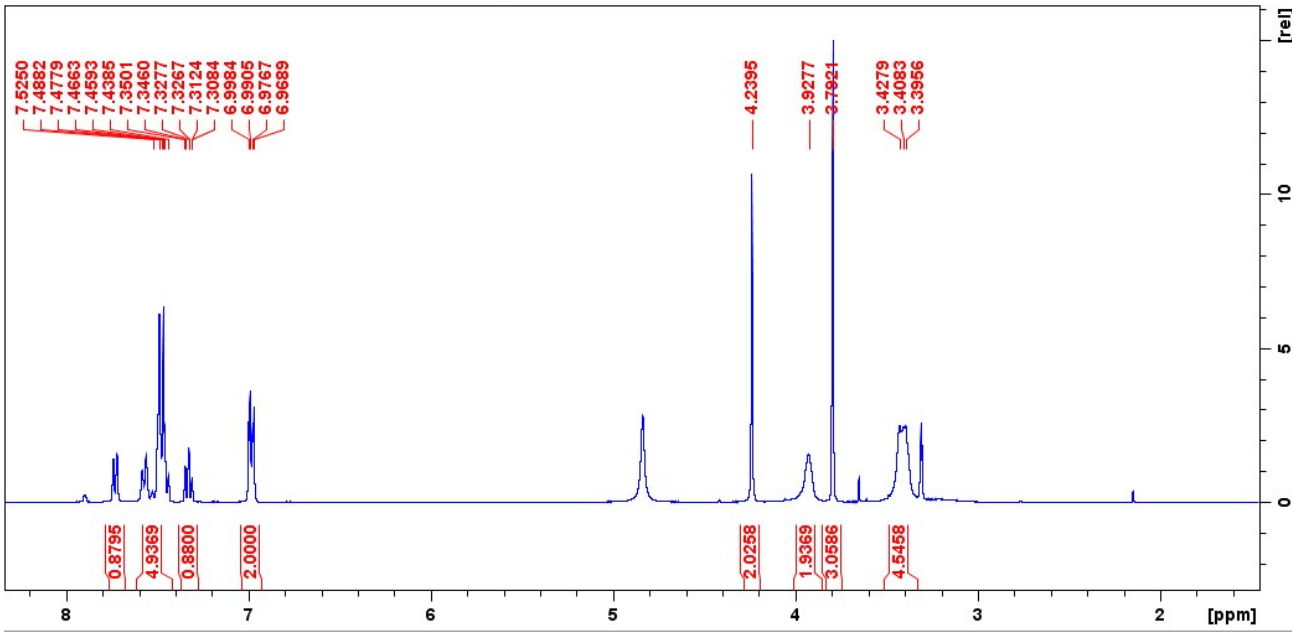


16a - CD_3OD

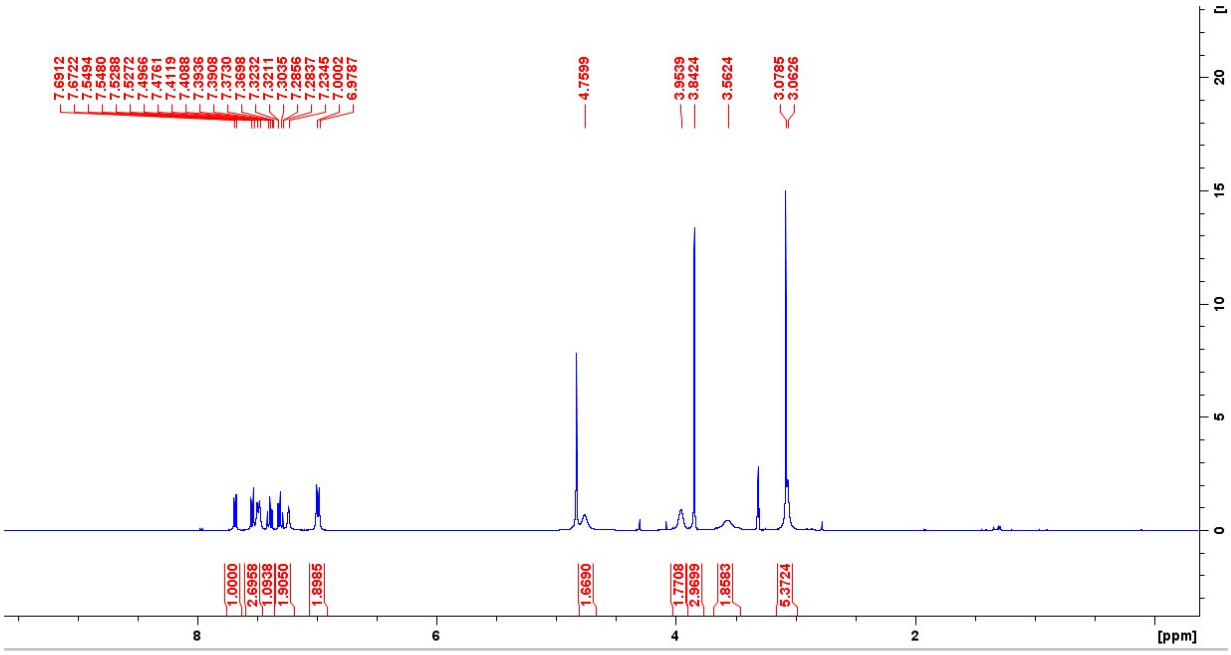




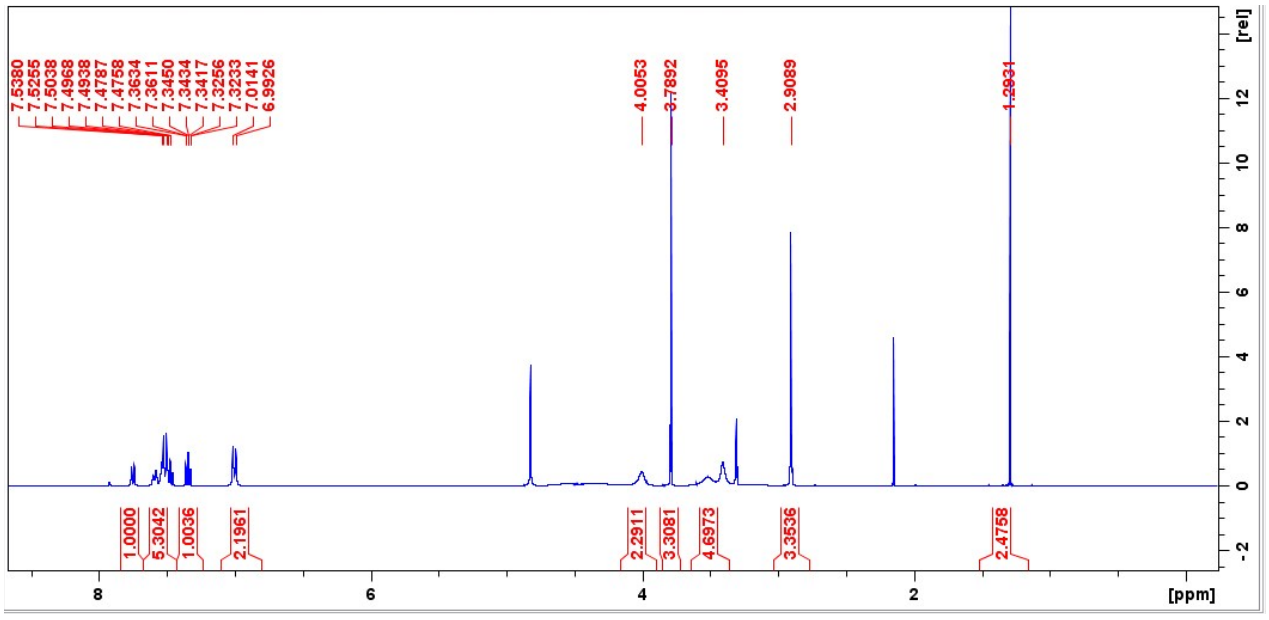
16b - CD_3OD



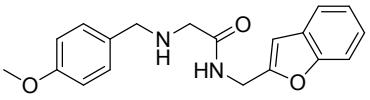
16c - CD_3OD

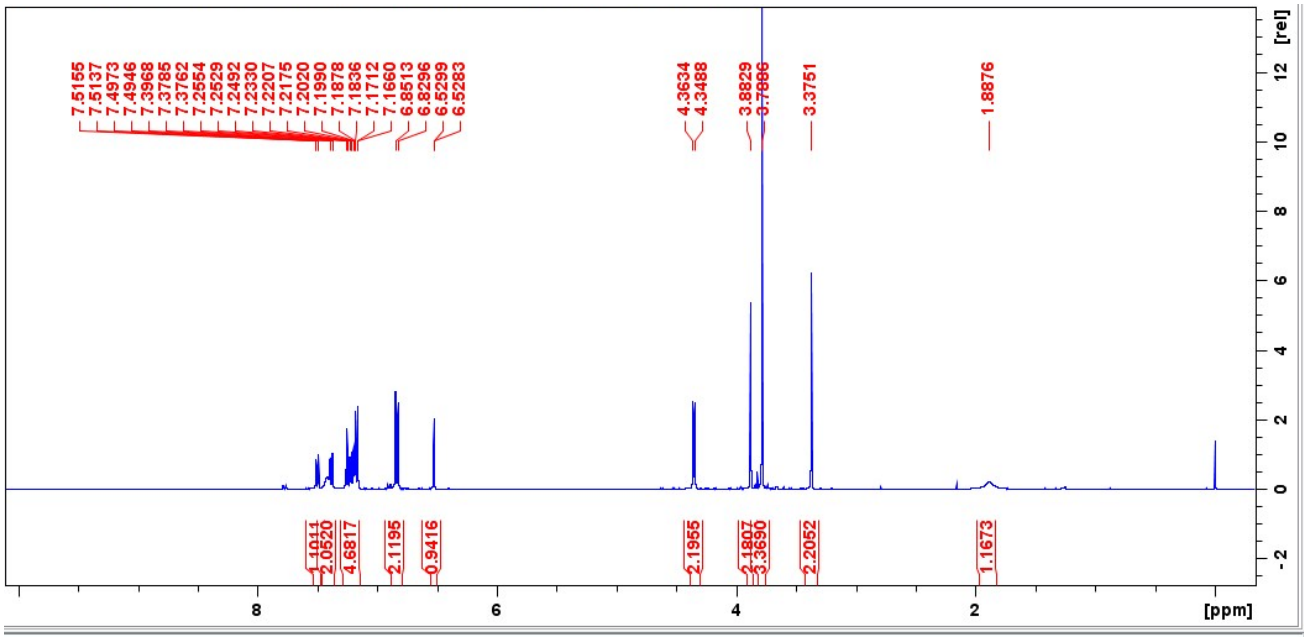


16d - CD_3OD

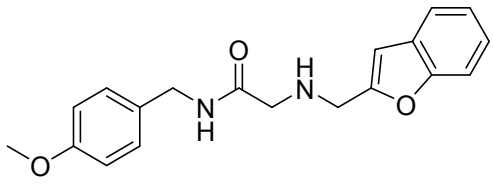


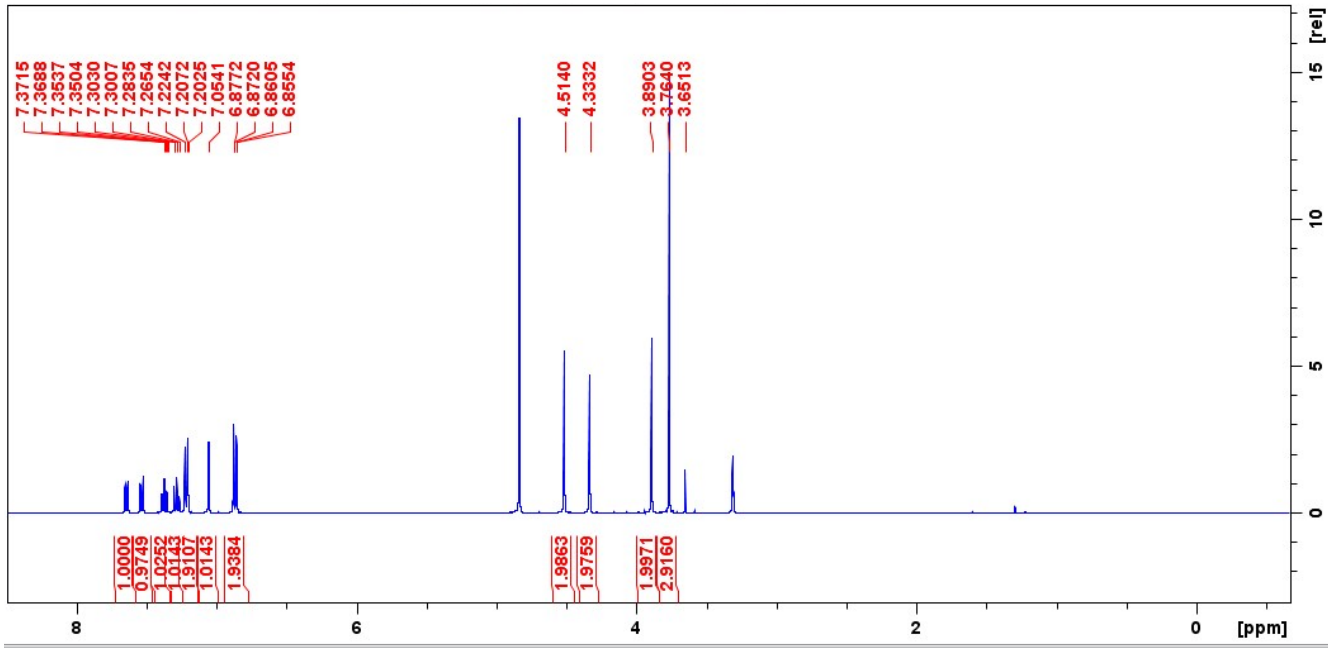
22a - $CDCl_3$

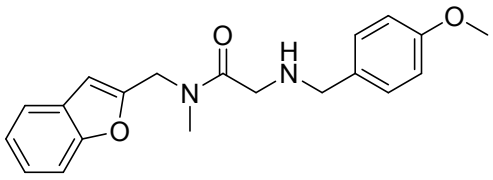




22b- CD_3OD







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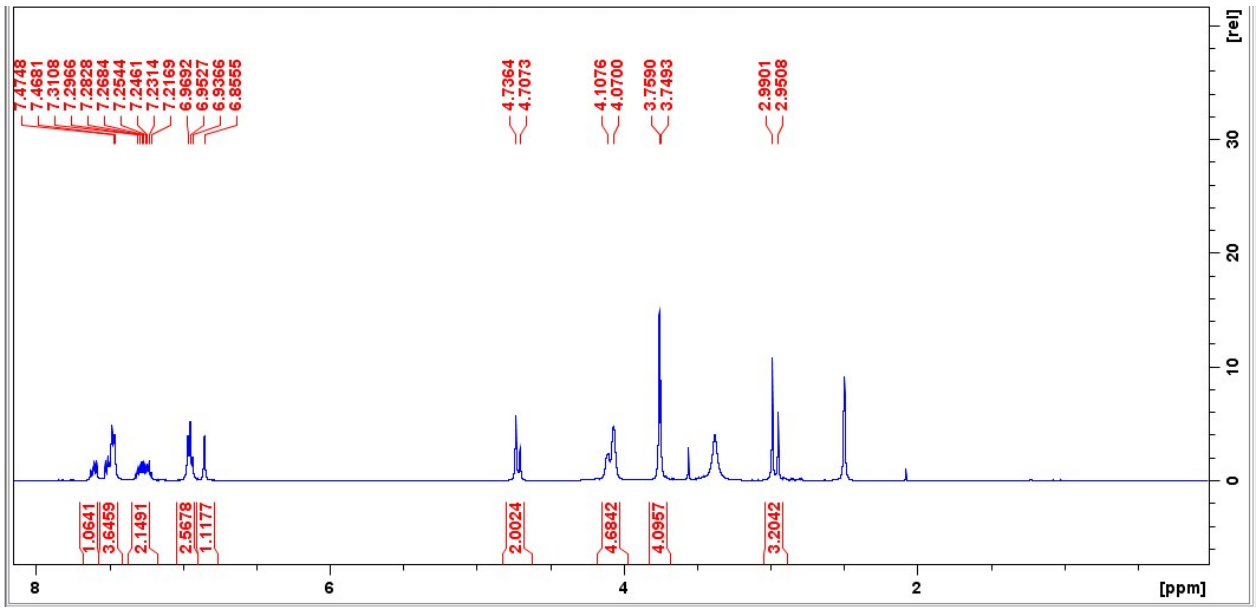
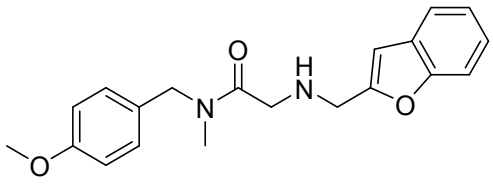
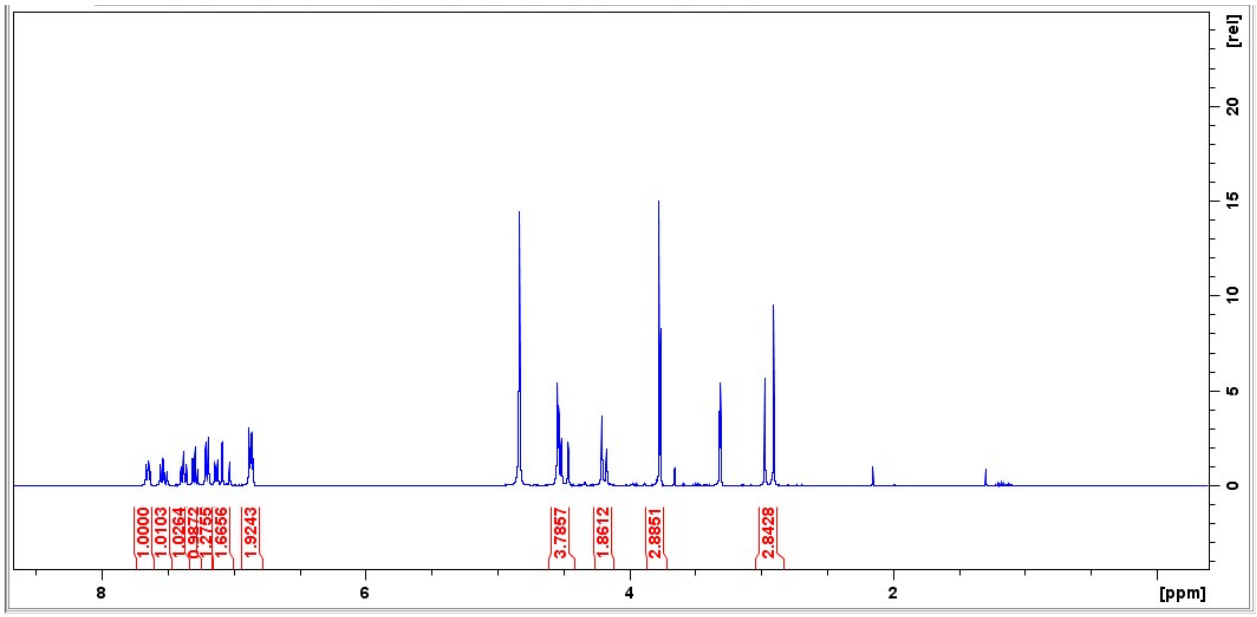
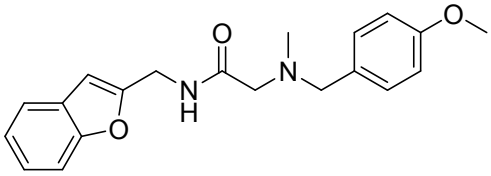


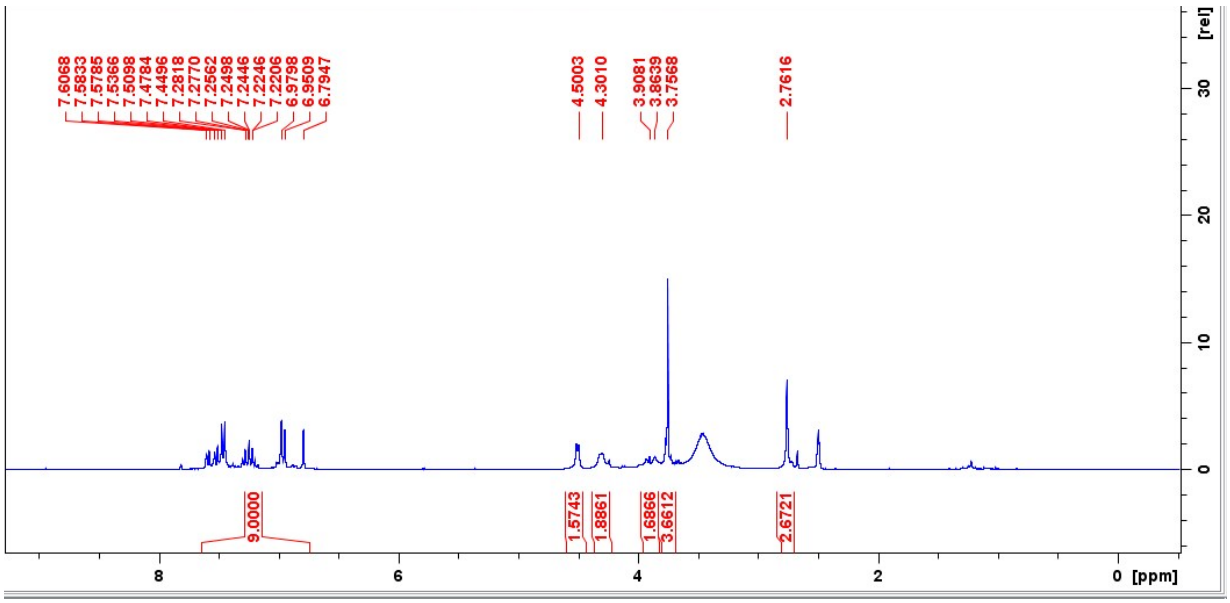


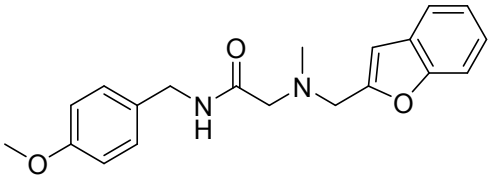
23b - CD_3OD



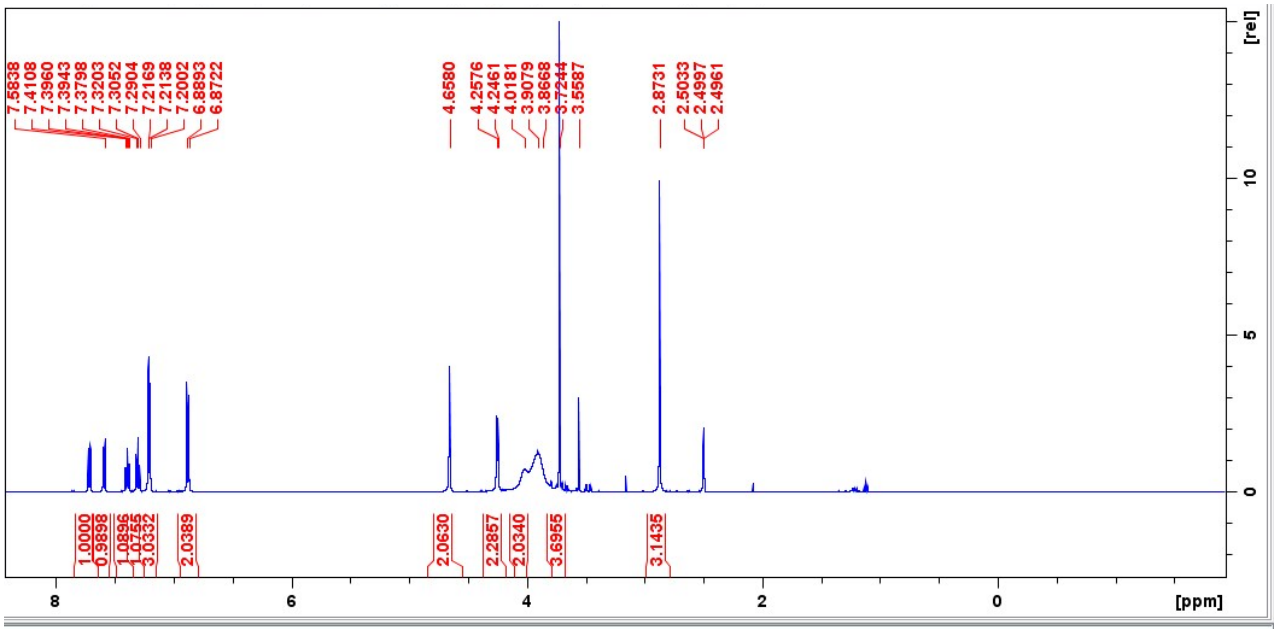


24a - d_6-DMSO

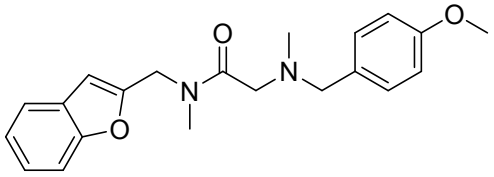


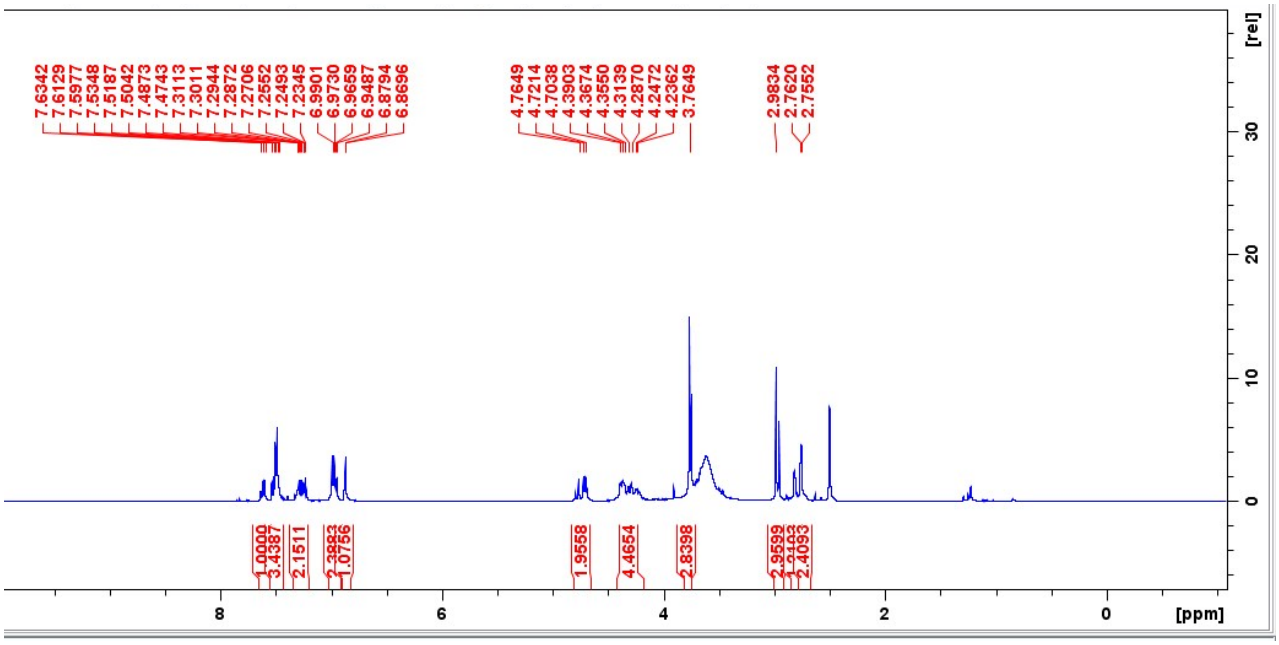


24b - d_6-DMSO

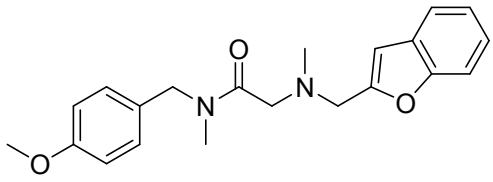


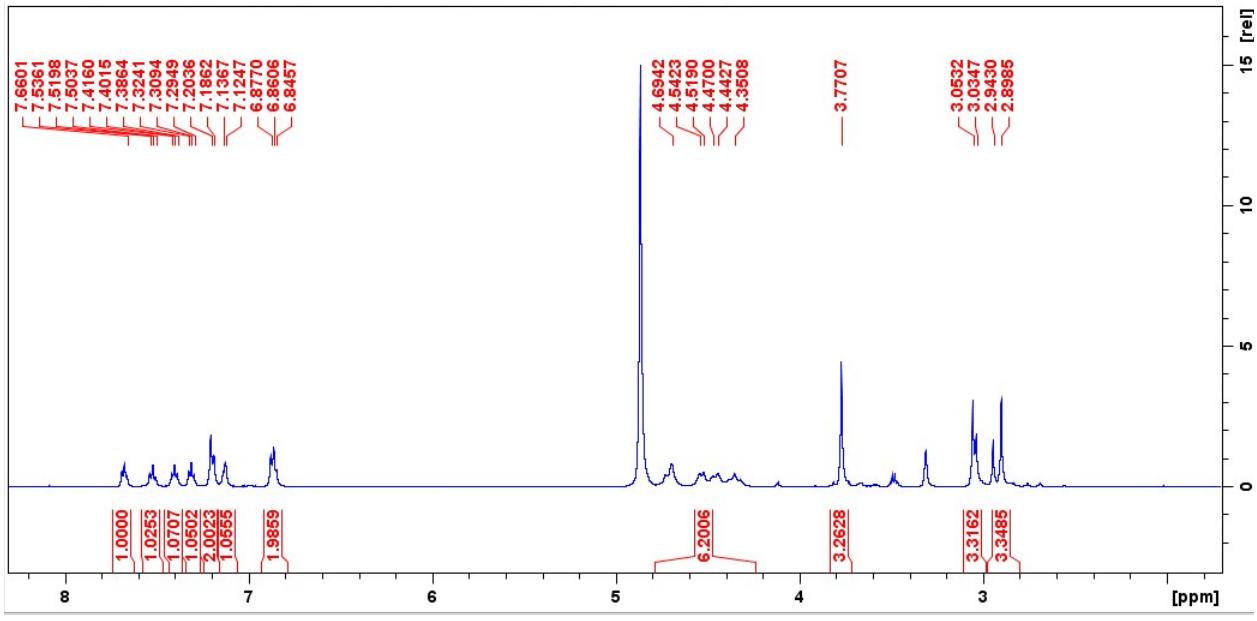
25a - d_6-DMSO

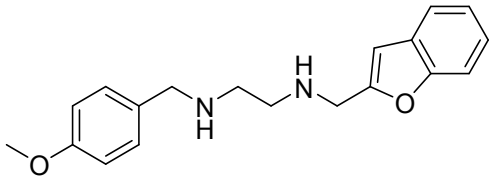




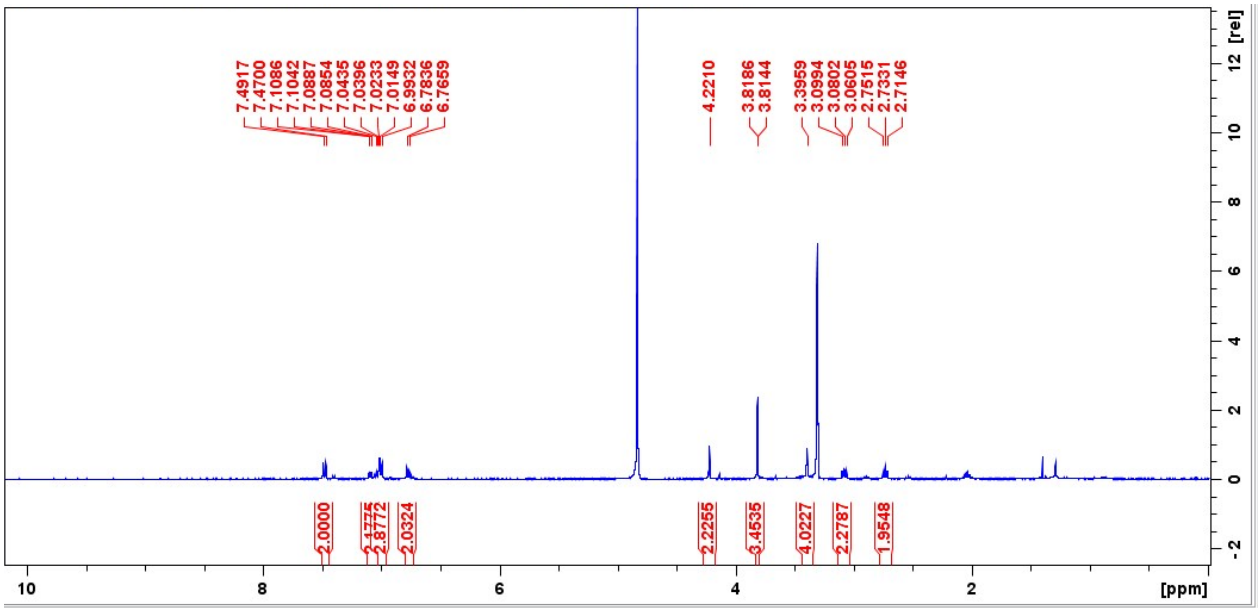
25b - CD_3OD

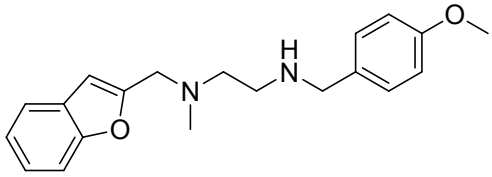




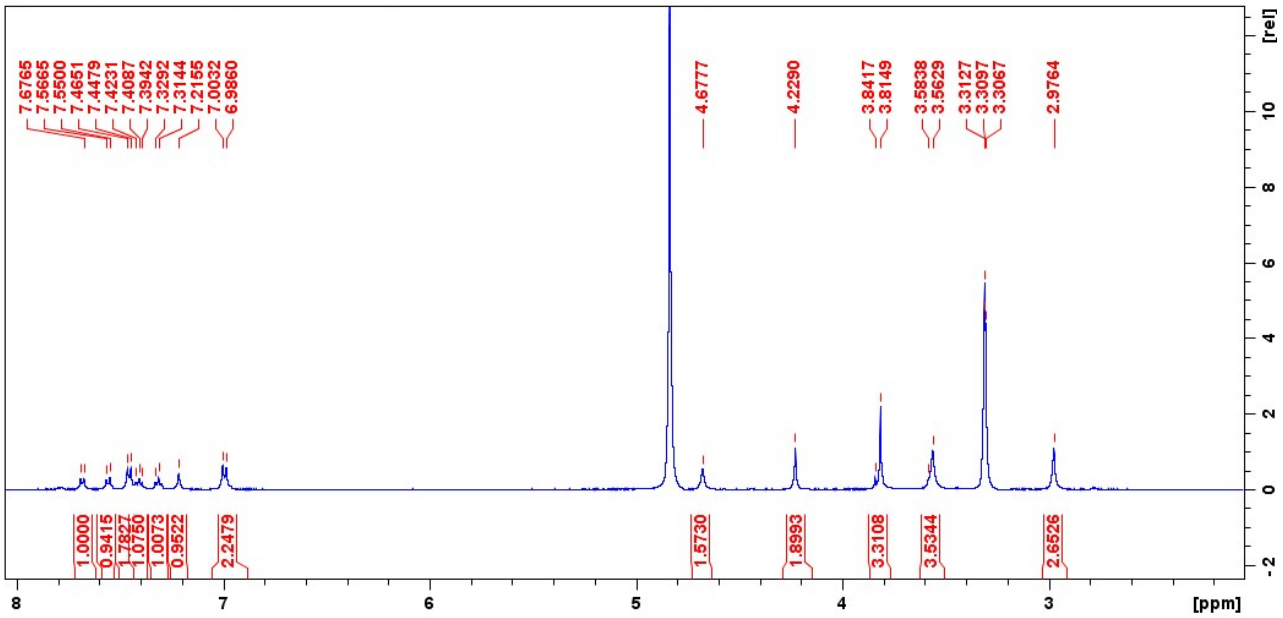


26a - CD_3OD

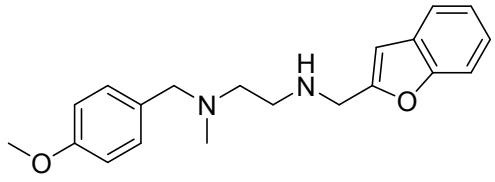


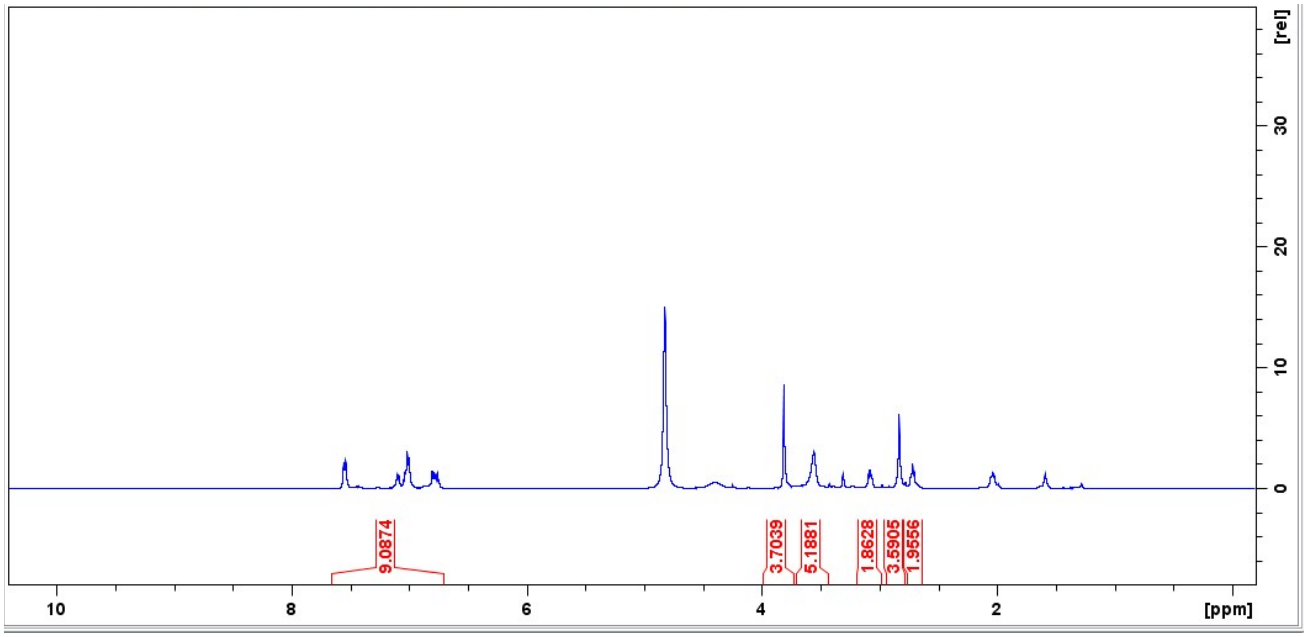


26b - CD_3OD

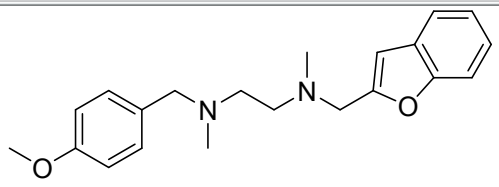


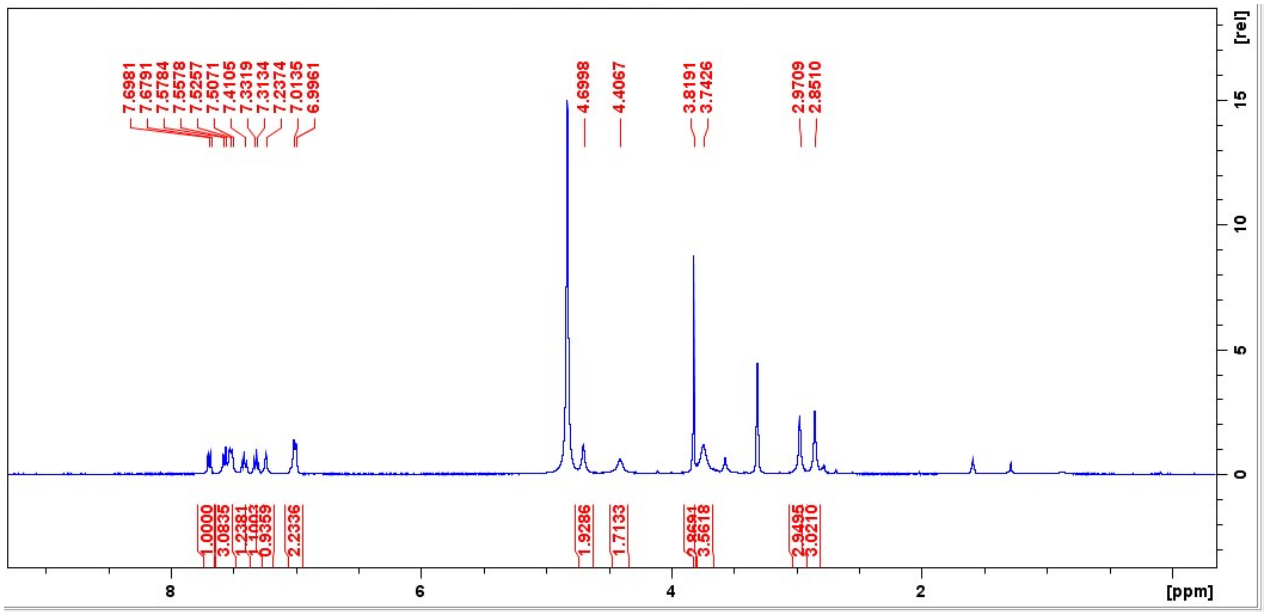
26c - CD_3OD



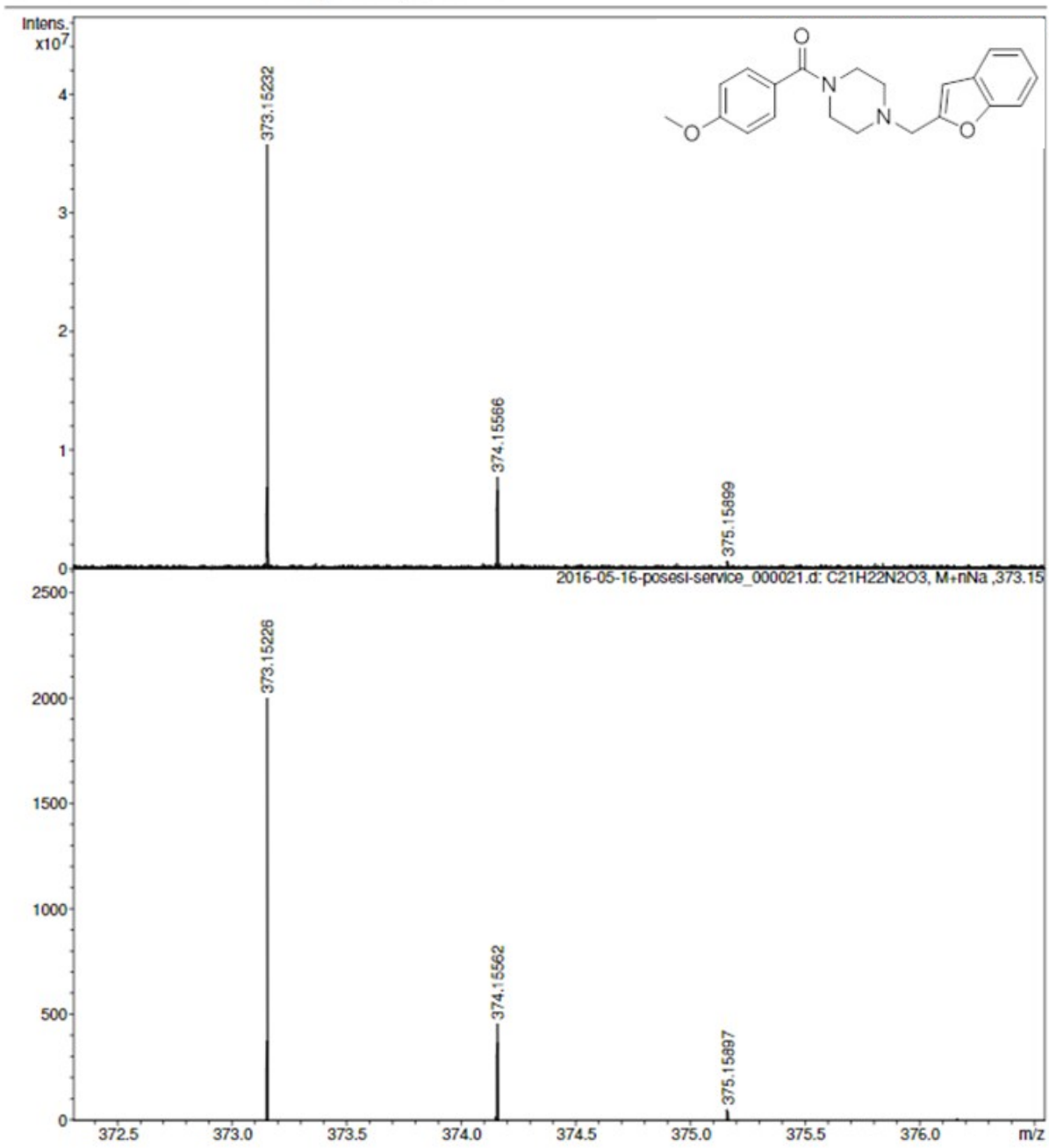


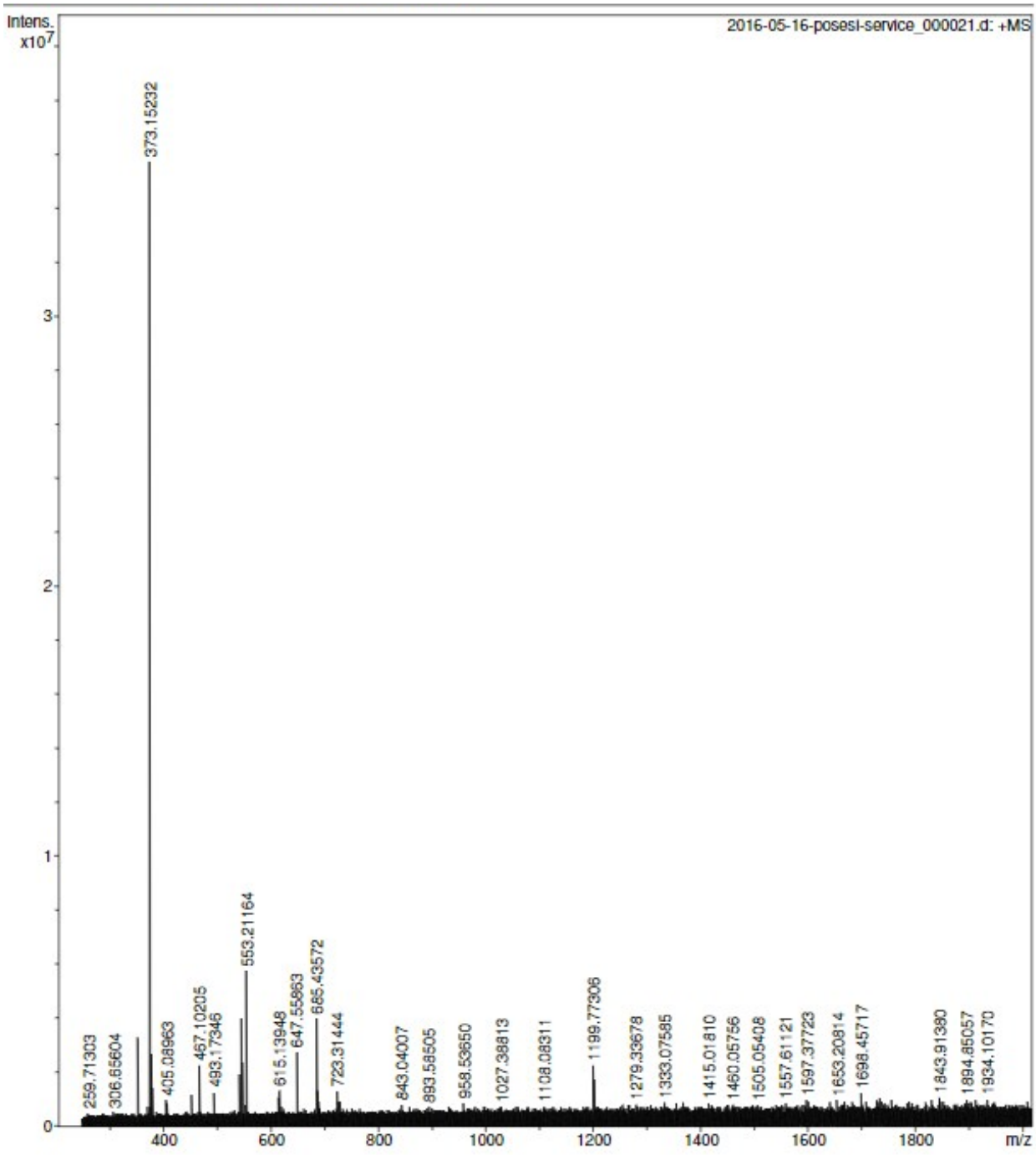
26d- CD_3OD



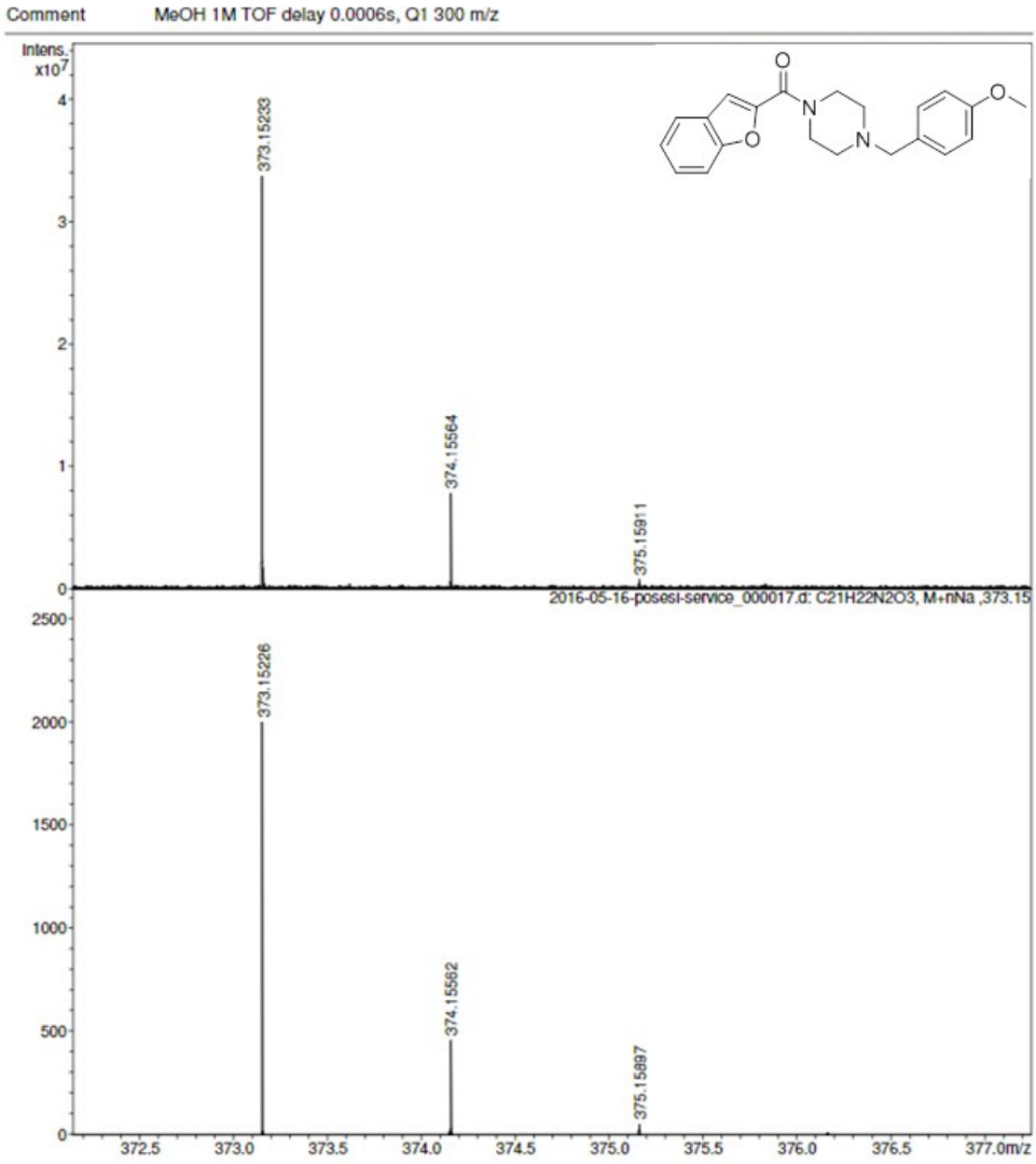


5a - HRMS

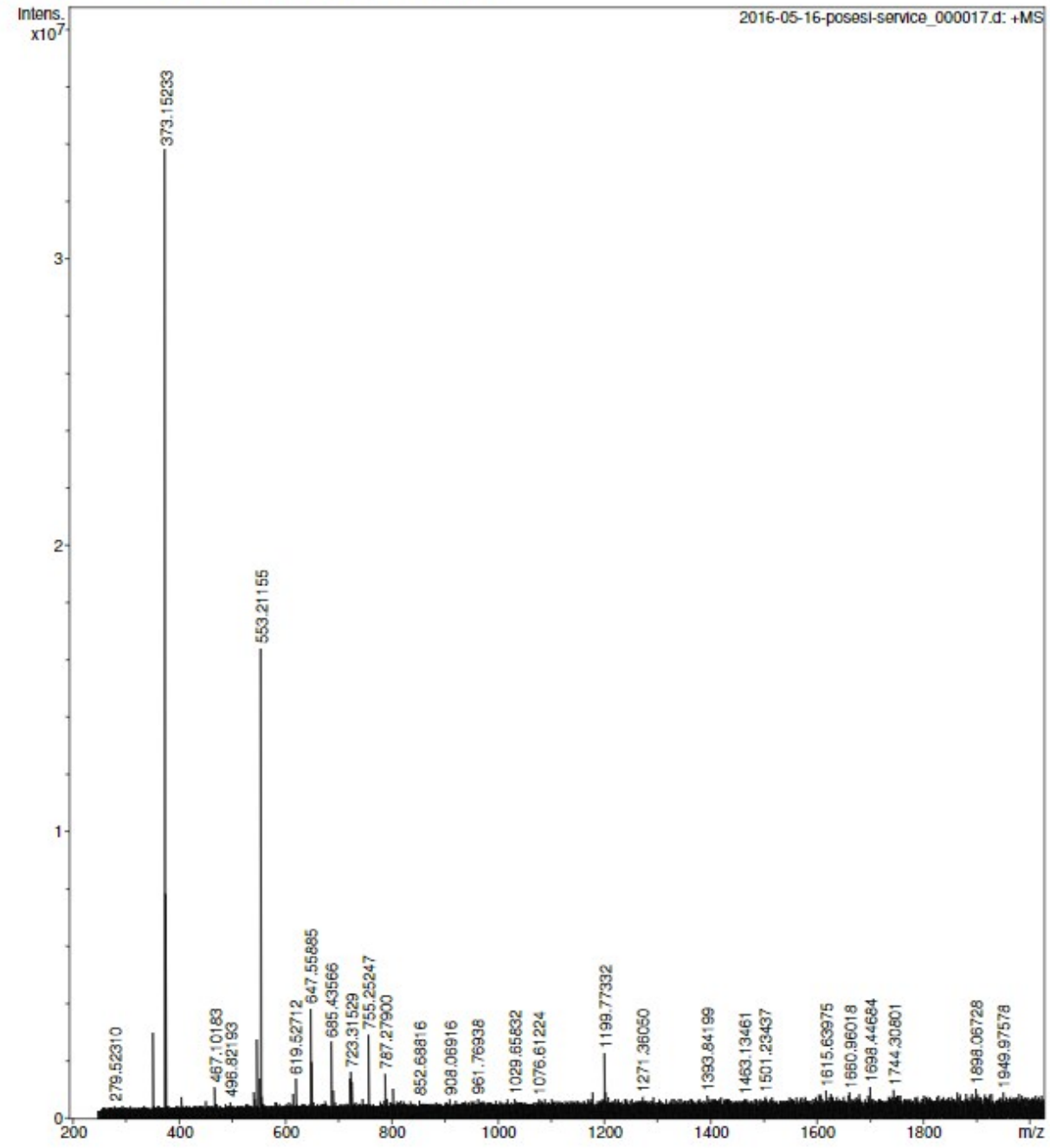

Intens.
x10^7
373.15232
374.15566
375.15899
2016-05-16-posesi-service_000021.d: C21H22N2O3, M+nNa ,373.15
373.15226
374.15562
375.15897
372.5
373.0
373.5
374.0
374.5
375.0
375.5
376.0
m/z


Intens.
x10^7
2016-05-16-posesi-service_000021.d: +MS
373.15232
553.21164
685.43572
647.55863
615.13948
467.10205
493.17346
405.08963
306.65604
259.71303
723.31444
843.04007
893.58505
958.53650
1027.38813
1108.08311
1199.77306
1279.33678
1333.07585
1415.01810
1460.05756
1505.05408
1557.61121
1597.37723
1653.20814
1698.45717
1843.91380
1894.85057
1934.10170
0
1
2
3
400
600
800
1000
1200
1400
1600
1800
m/z

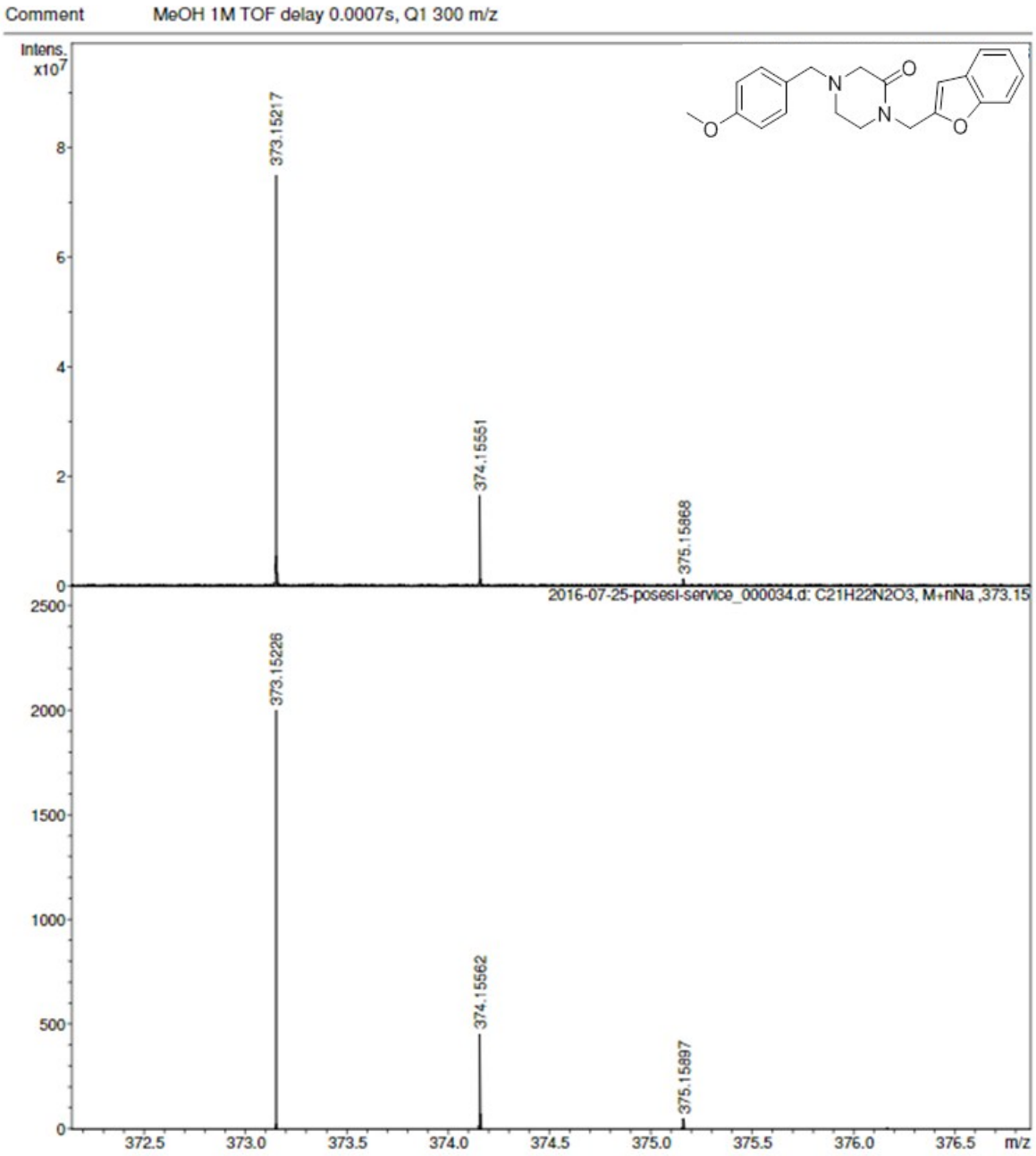
5b - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
373.15233
374.15564
375.15911
2016-05-16-posesi-service_000017.d: C21H22N2O3, M+nNa ,373.15
373.15226
374.15562
375.15897
372.5
373.0
373.5
374.0
374.5
375.0
375.5
376.0
376.5
377.0m/z

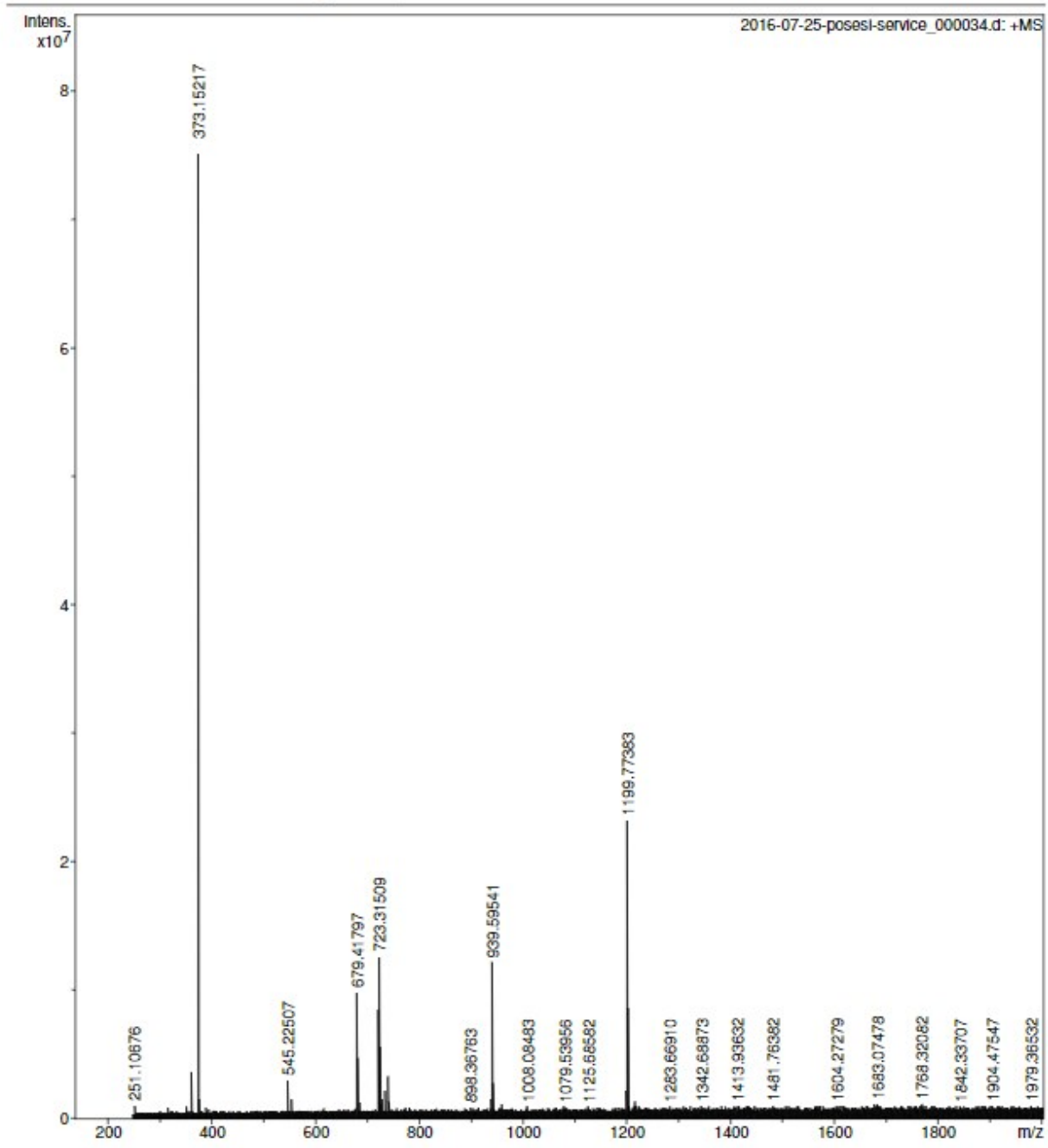
Comment MeOH 1M TOF delay 0.0006s, Q1 300 m/z



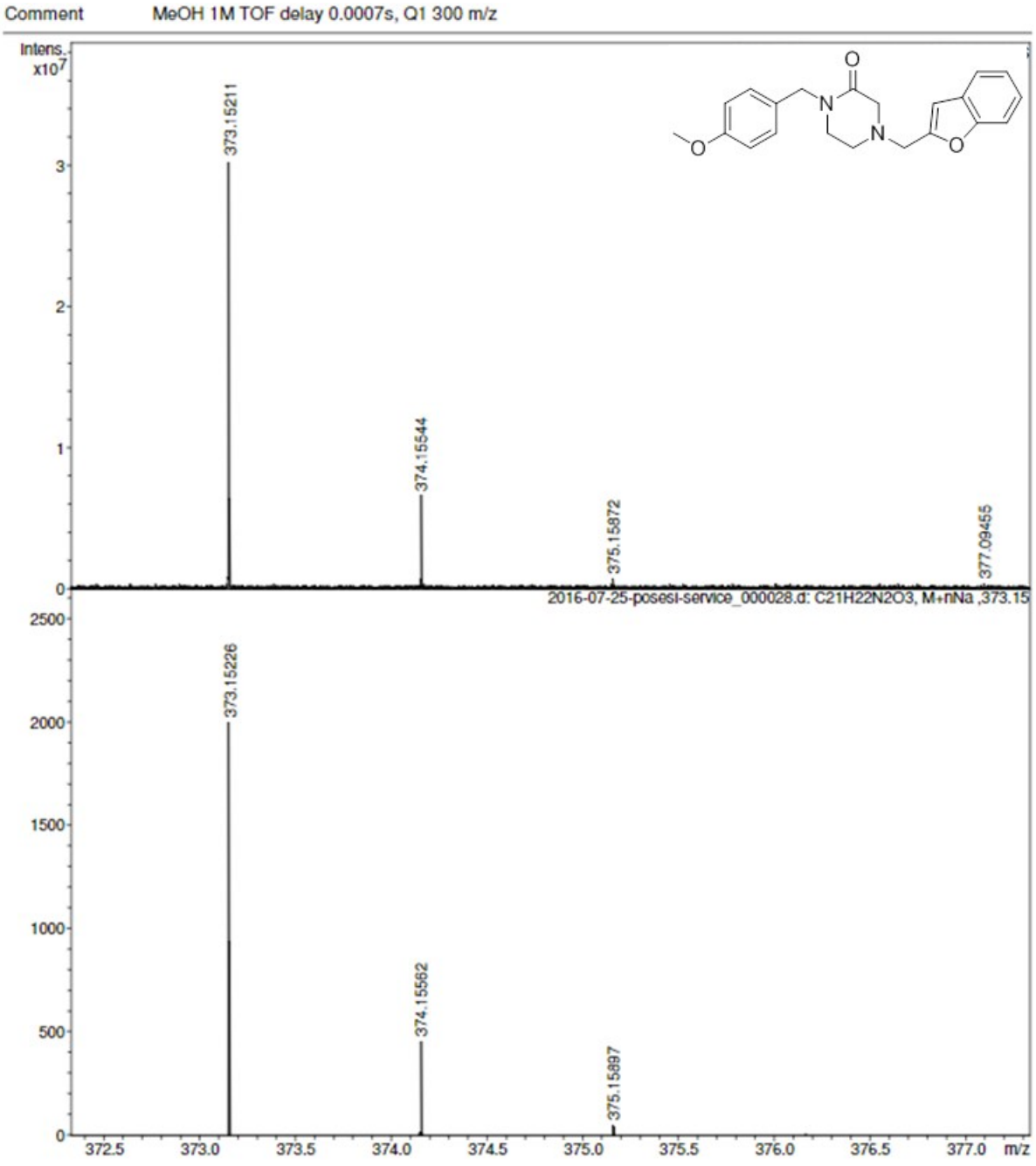
8a - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
373.15217
374.15551
375.15868
2016-07-25-posesi-service_000034.d: C21H22N2O3, M+nNa ,373.15
373.15226
374.15562
375.15897
m/z

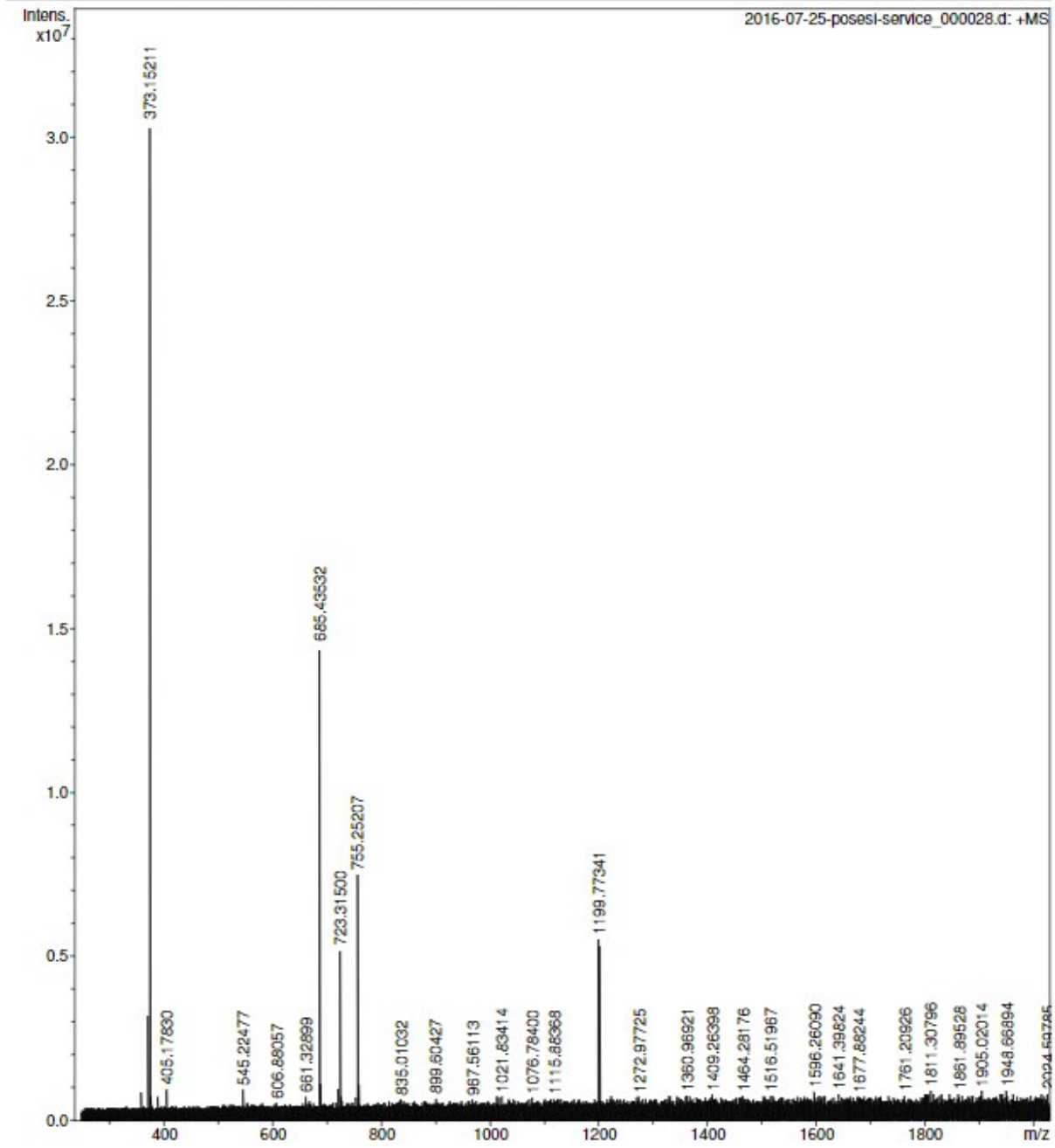
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



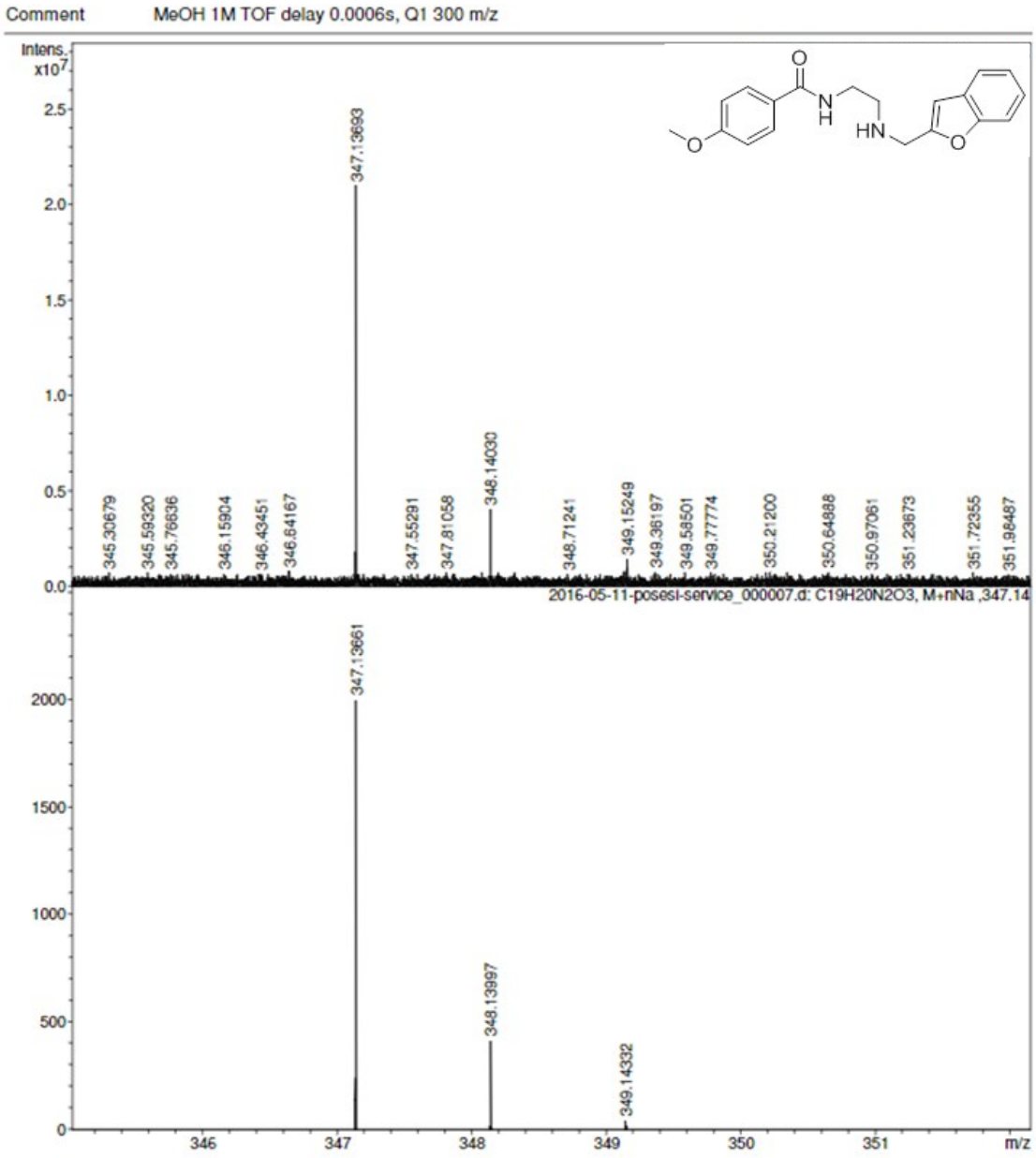
8b - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
373.15211
374.15544
375.15872
377.09455
2016-07-25-posesi-service_000028.d: C21H22N2O3, M+nNa ,373.15
373.15226
374.15562
375.15897
372.5
373.0
373.5
374.0
374.5
375.0
375.5
376.0
376.5
377.0
m/z

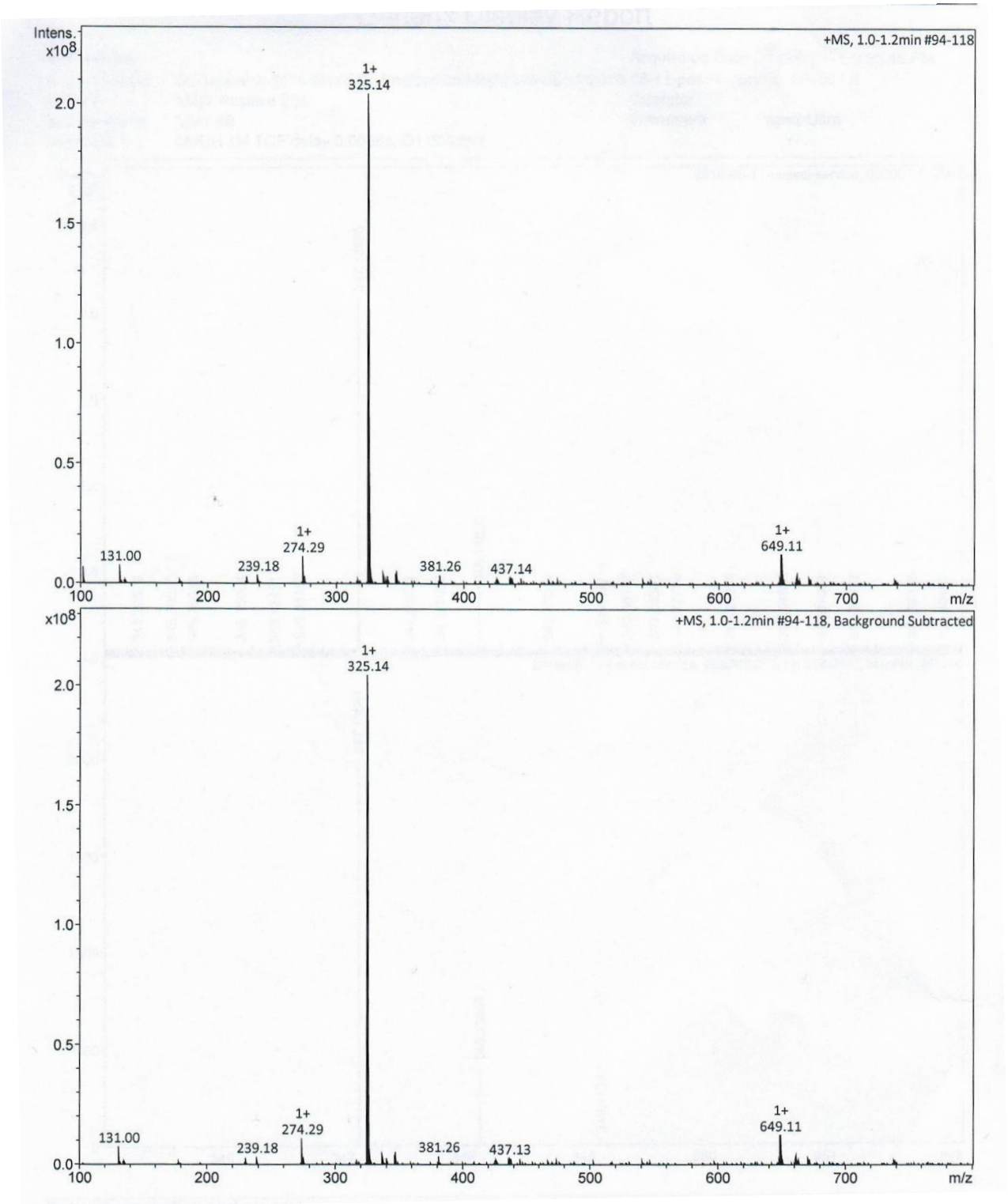
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



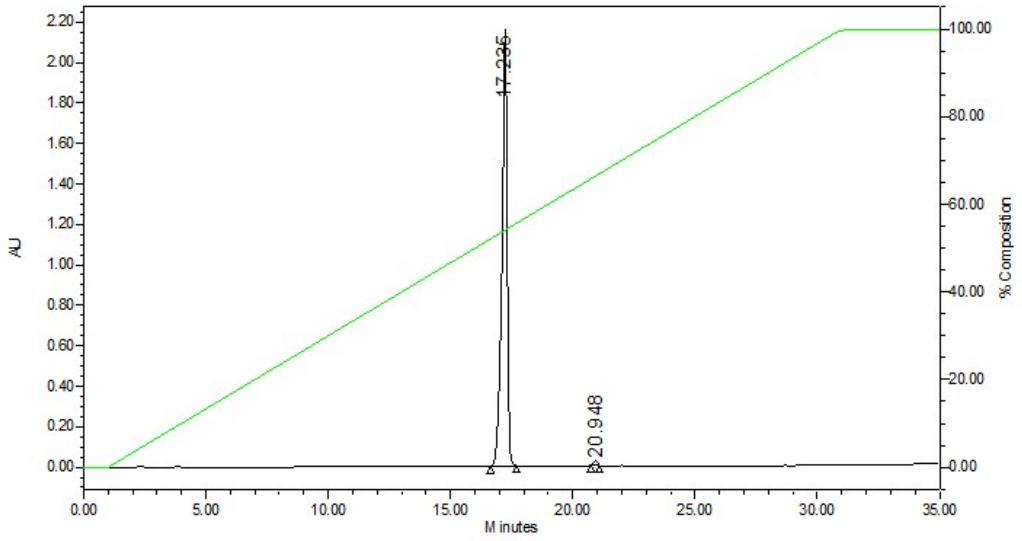
12a - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
2.5
2.0
1.5
1.0
0.5
0.0
347.13693
348.14030
345.30679
345.59320
345.76636
346.15904
346.43451
346.64167
347.55291
347.81058
348.71241
349.15249
349.36197
349.58501
349.77774
350.21200
350.64888
350.97061
351.23673
351.72355
351.98487
O
N
H
HN
O
O
2016-05-11-posesi-service_000007.d: C19H20N2O3, M+nNa ,347.14
2000
1500
1000
500
0
347.13661
348.13997
349.14332
346
347
348
349
350
351
m/z

12a - LRMS


Intens.
x10^8
+MS, 1.0-1.2min #94-118
1+
325.14
2.0
1.5
1.0
0.5
0.0
1+
274.29
131.00
239.18
381.26
437.14
1+
649.11
100
200
300
400
500
600
700
m/z
x10^8
+MS, 1.0-1.2min #94-118, Background Subtracted
1+
325.14
2.0
1.5
1.0
0.5
0.0
1+
274.29
131.00
239.18
381.26
437.13
1+
649.11
100
200
300
400
500
600
700
m/z

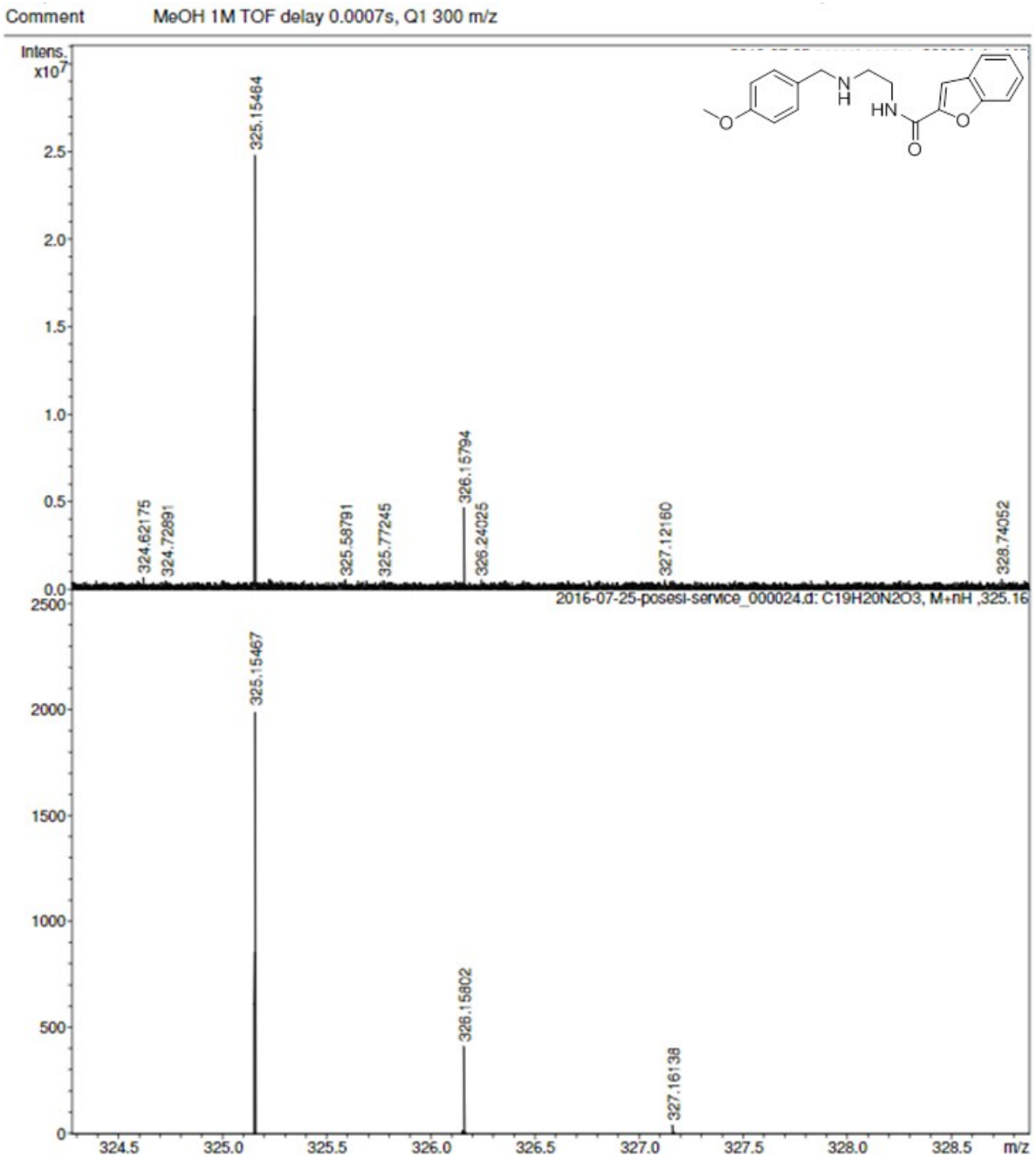
12a - HPLC



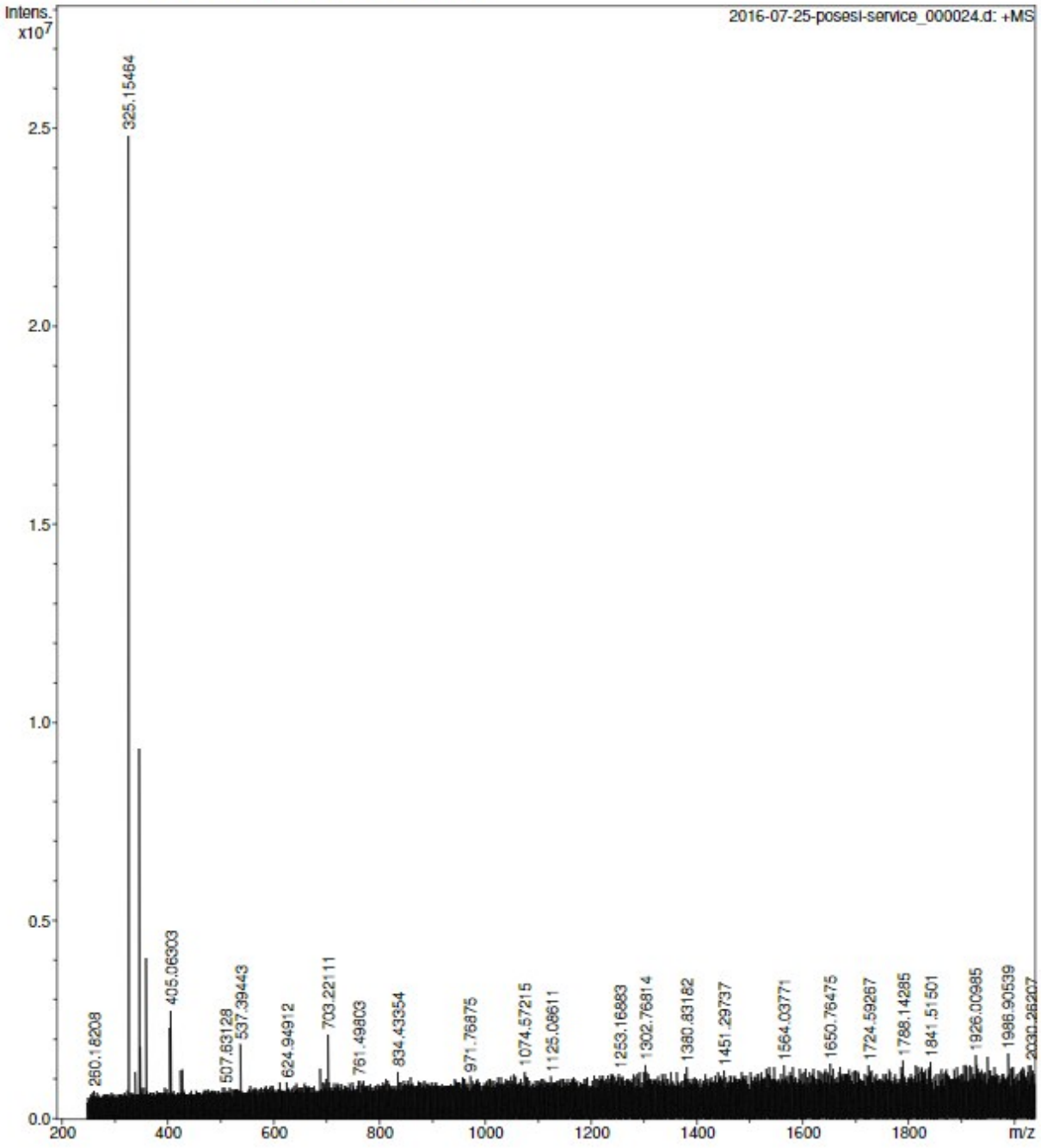
Peak information

	RT	Area	% Area
1	17.235	31917559	99.27
2	20.948	235600	0.73

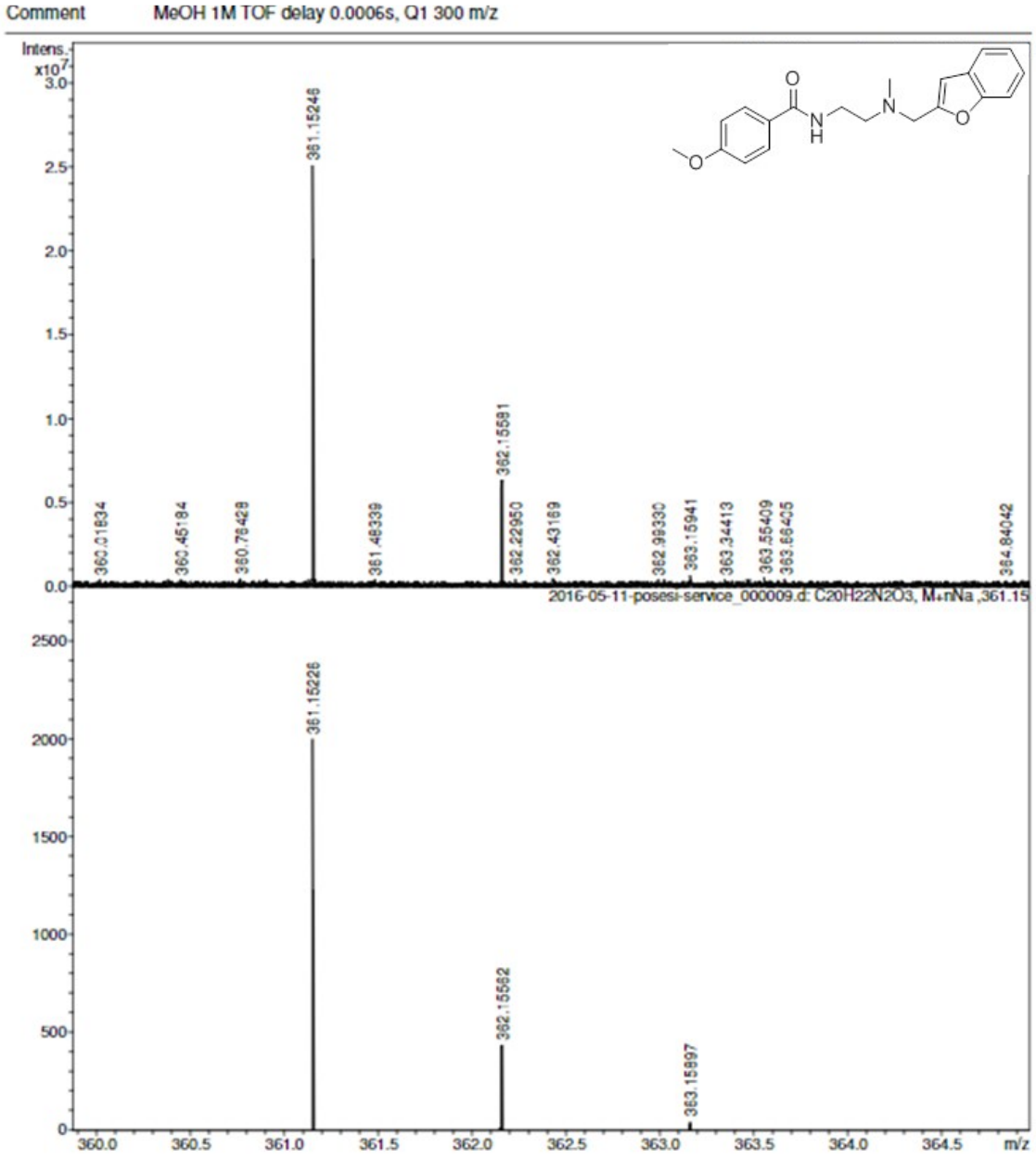
12b - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
325.15464
324.62175
324.72891
325.58791
325.77245
326.15794
326.24025
327.12160
328.74052
2016-07-25-posesi-service_000024.d: C19H20N2O3, M+nH ,325.16
325.15467
326.15802
327.16138
m/z

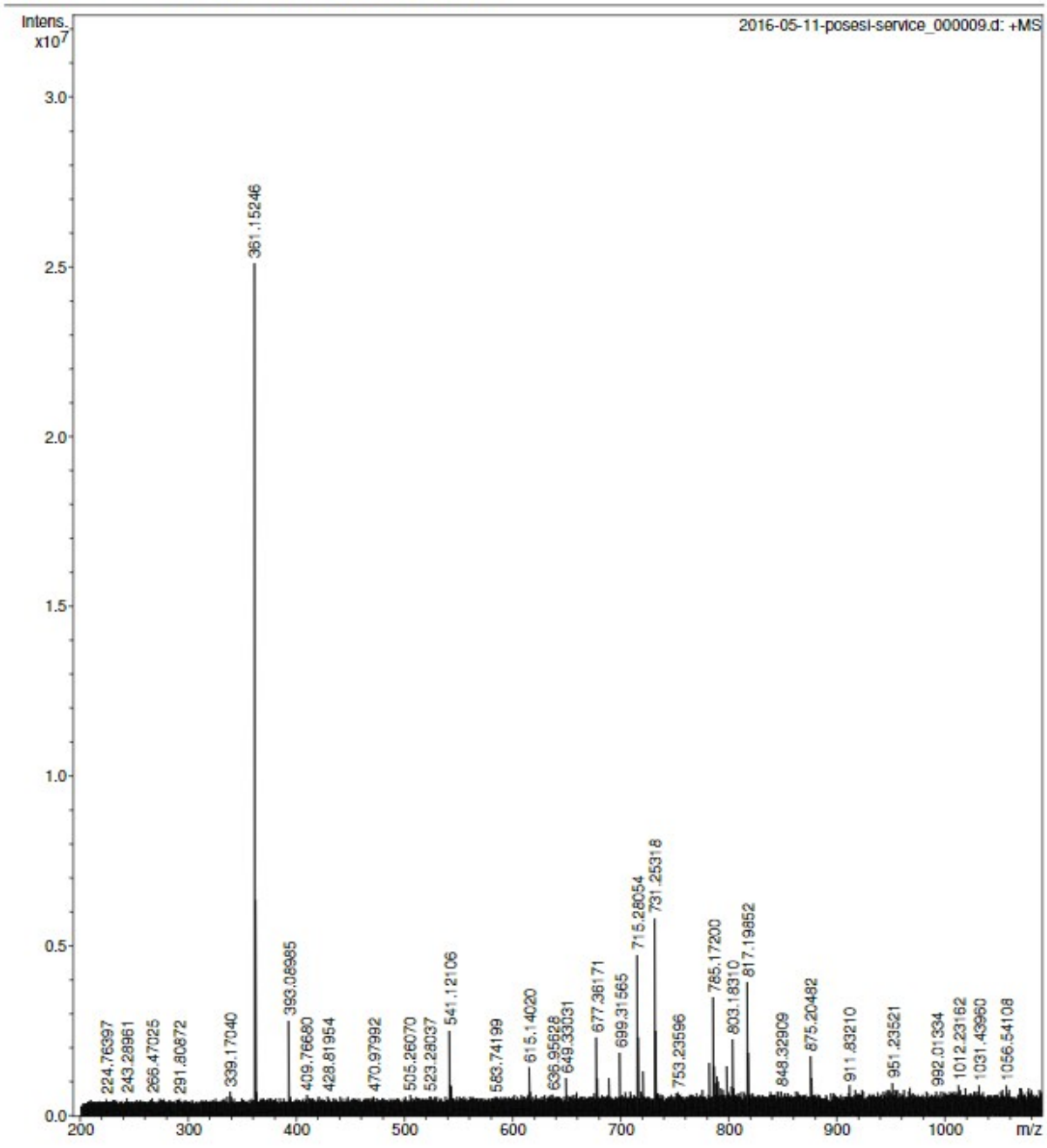
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



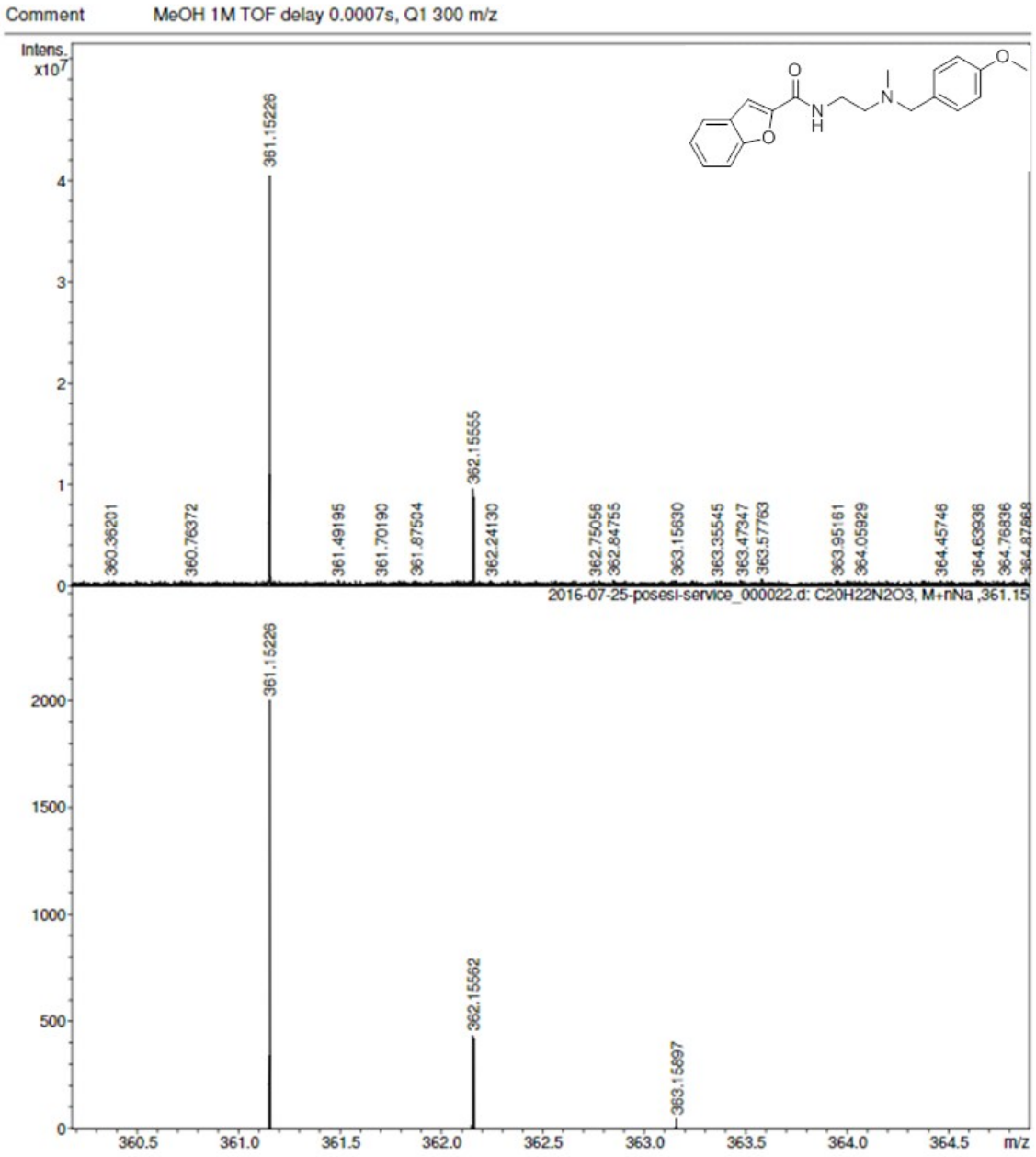
13a - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
361.15246
362.15581
360.01834
360.45184
360.78428
361.48339
362.22950
362.43169
362.98330
363.15941
363.34413
363.55409
363.68405
364.84042
2016-05-11-posesi-service_000009.d: C20H22N2O3, M+Na ,361.15
361.15226
362.15582
363.15897
m/z

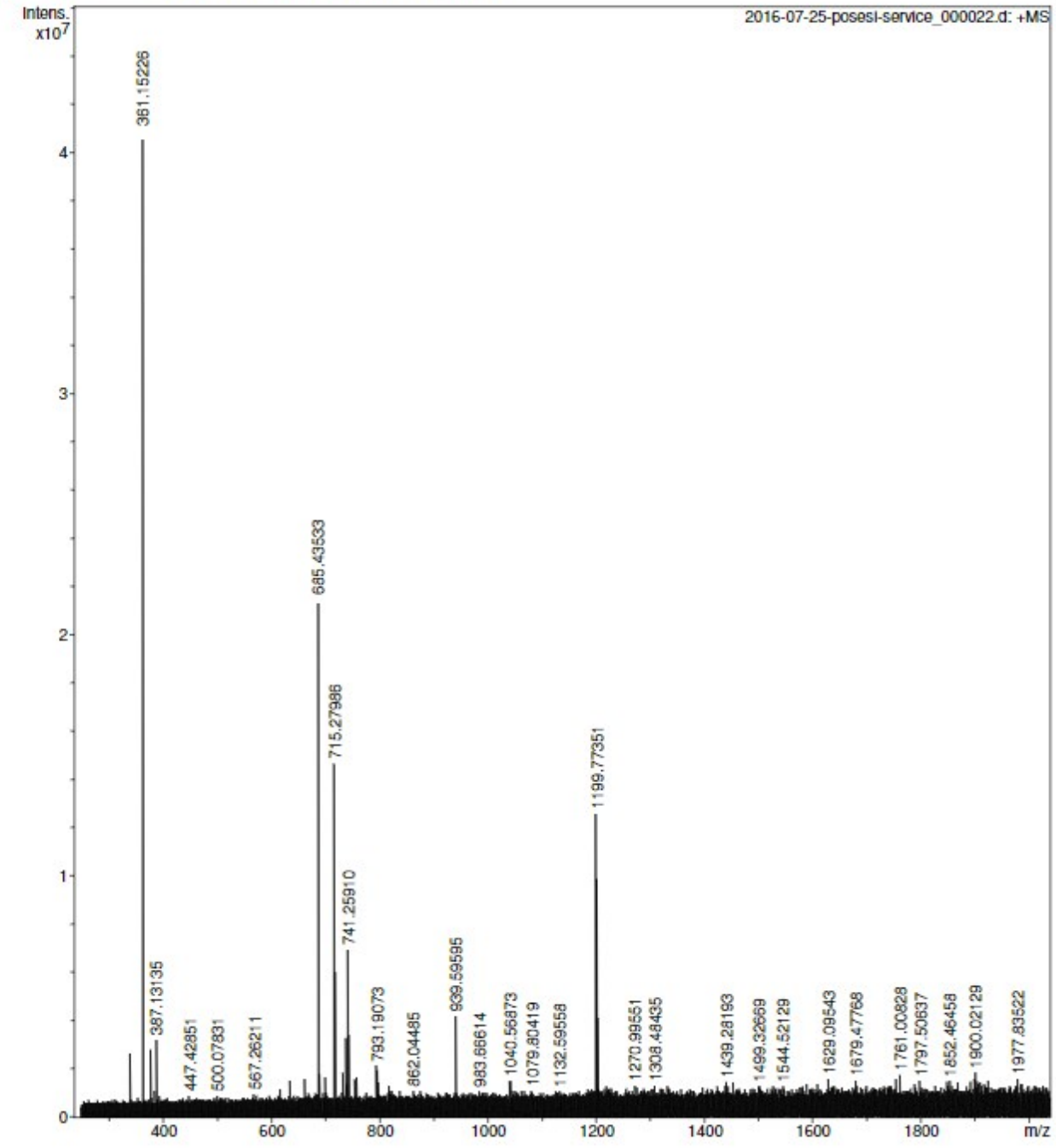
Comment MeOH 1M TOF delay 0.0006s, Q1 300 m/z



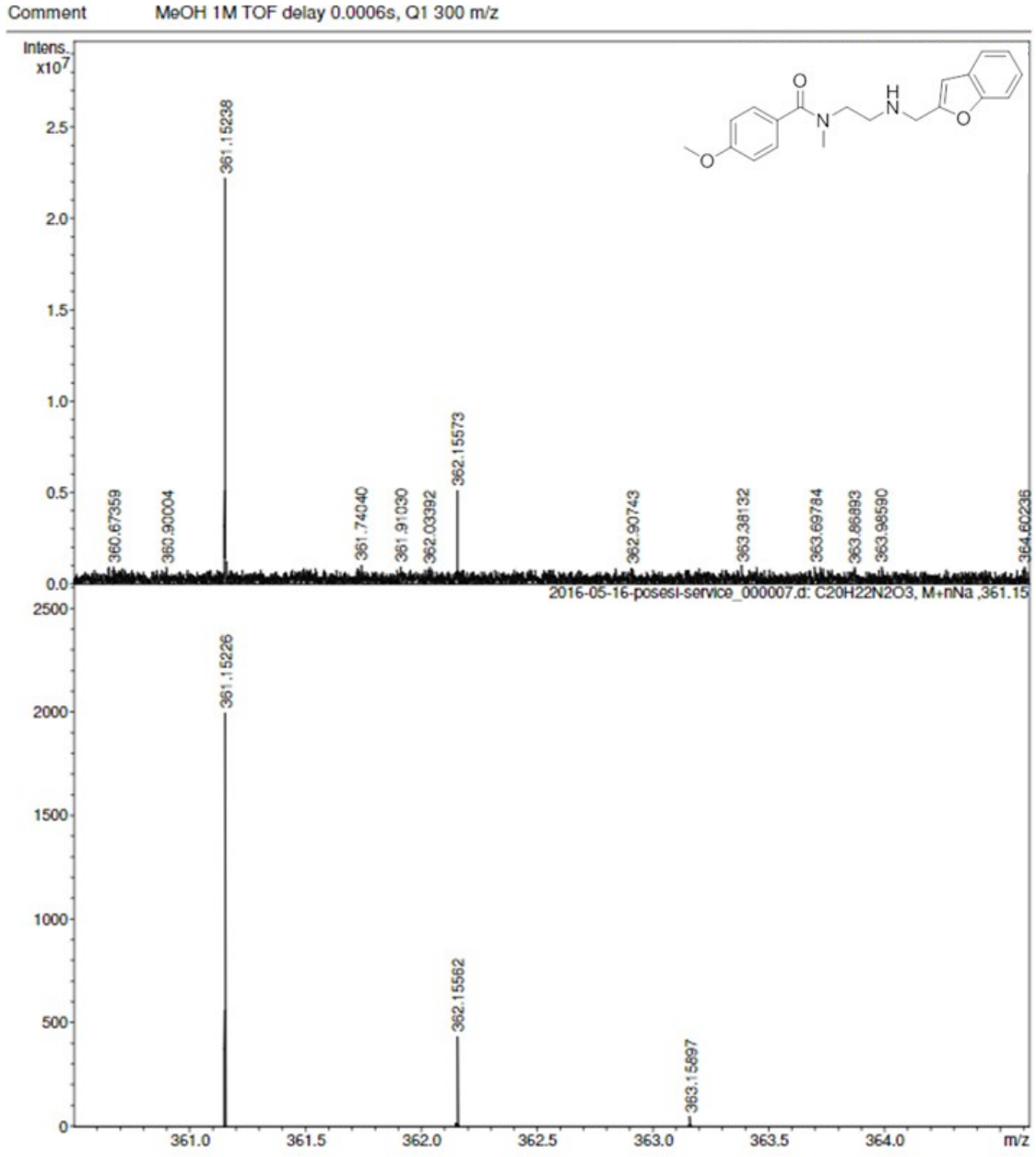
13b - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
361.15226
362.15555
360.36201
360.76372
361.49195
361.70190
361.87504
362.24130
362.75056
362.84755
363.15630
363.35545
363.47347
363.57763
363.95161
364.05929
364.45746
364.63936
364.76836
364.87868
2016-07-25-posesi-service_000022.d: C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15897
m/z

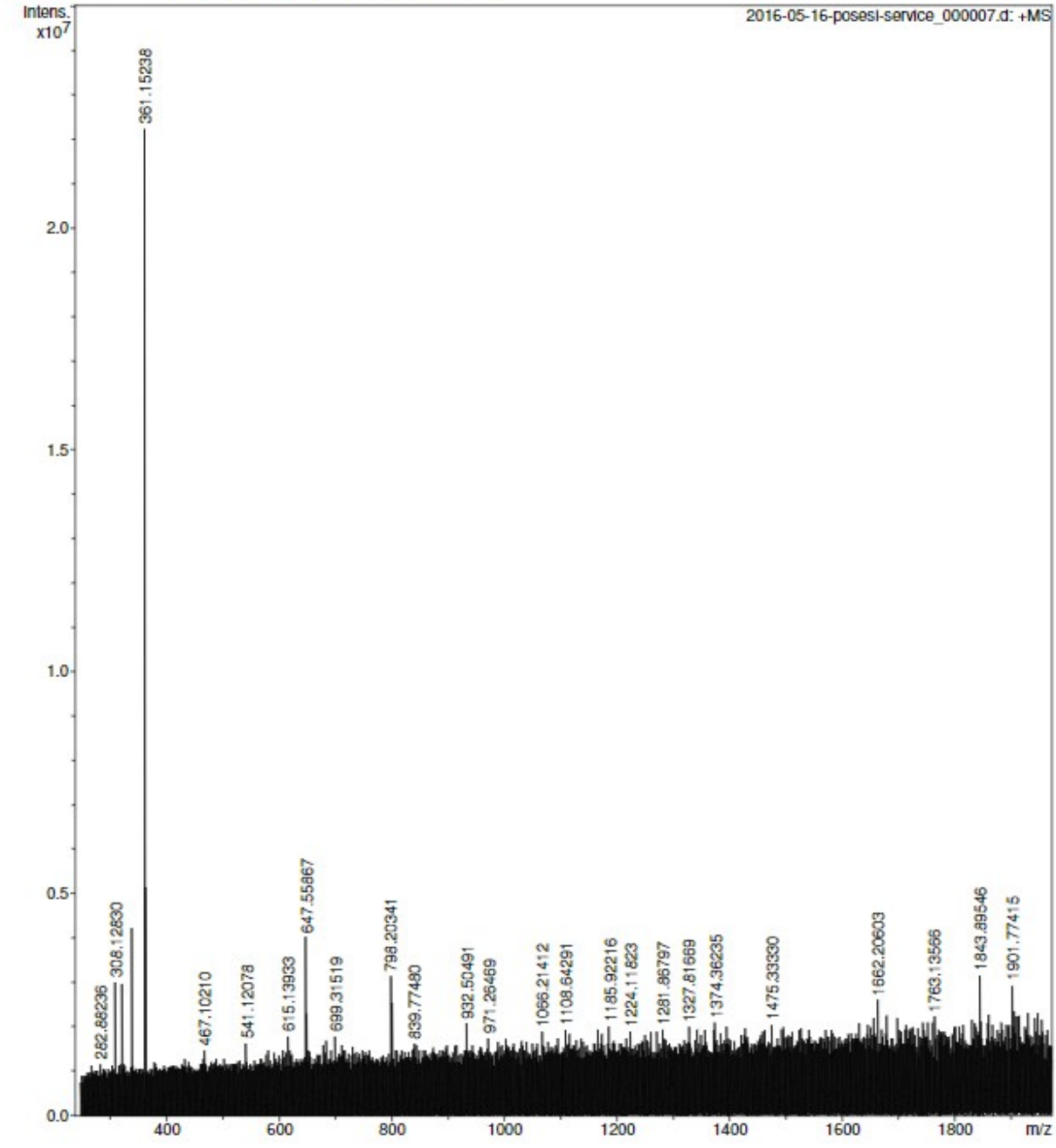
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



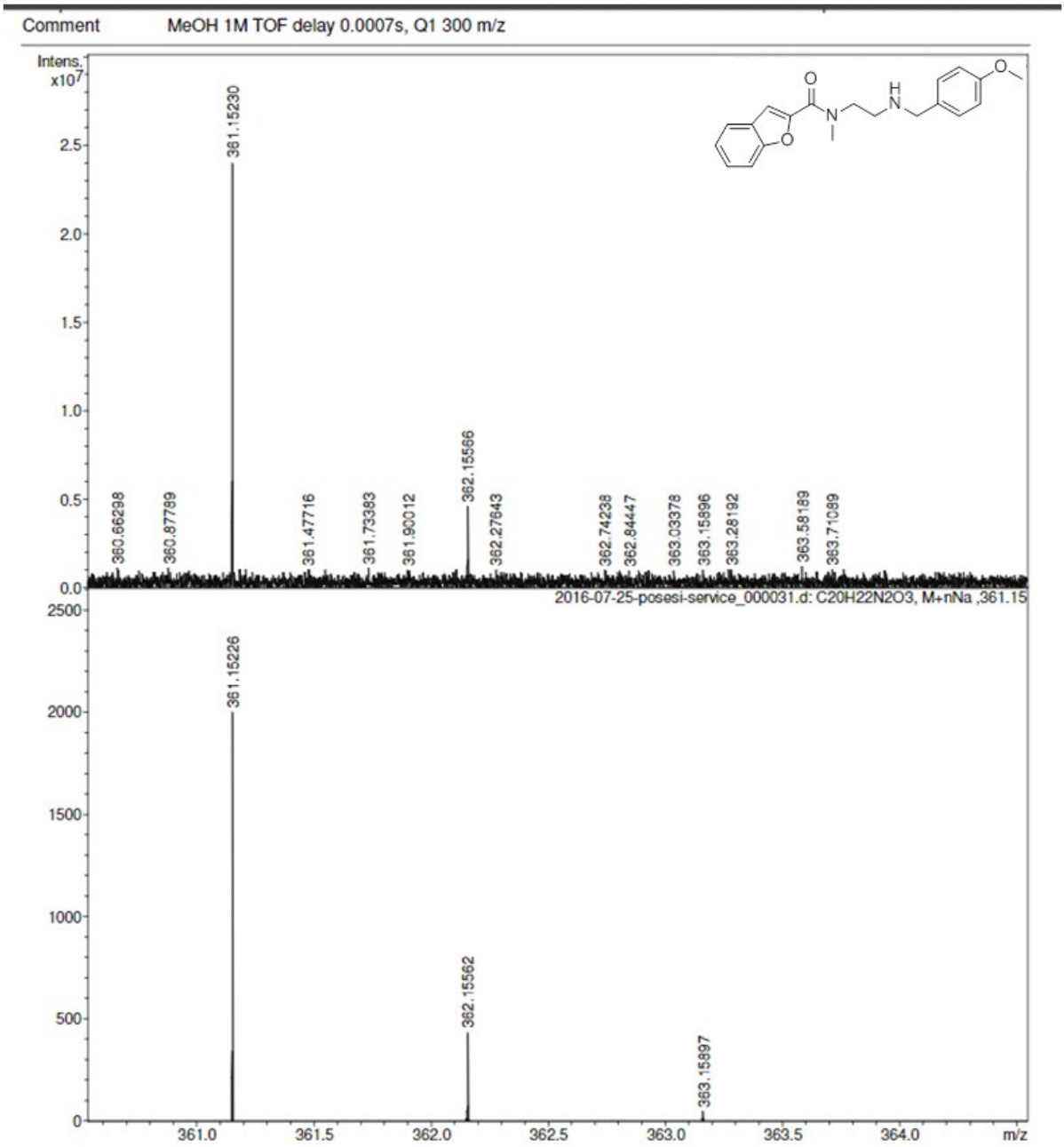
16a - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
361.15238
360.67359
360.90004
361.74040
361.91030
362.03392
362.15573
362.90743
363.38132
363.69784
363.86893
363.98590
364.60236
2016-05-16-posesi-service_000007.d: C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15697
m/z

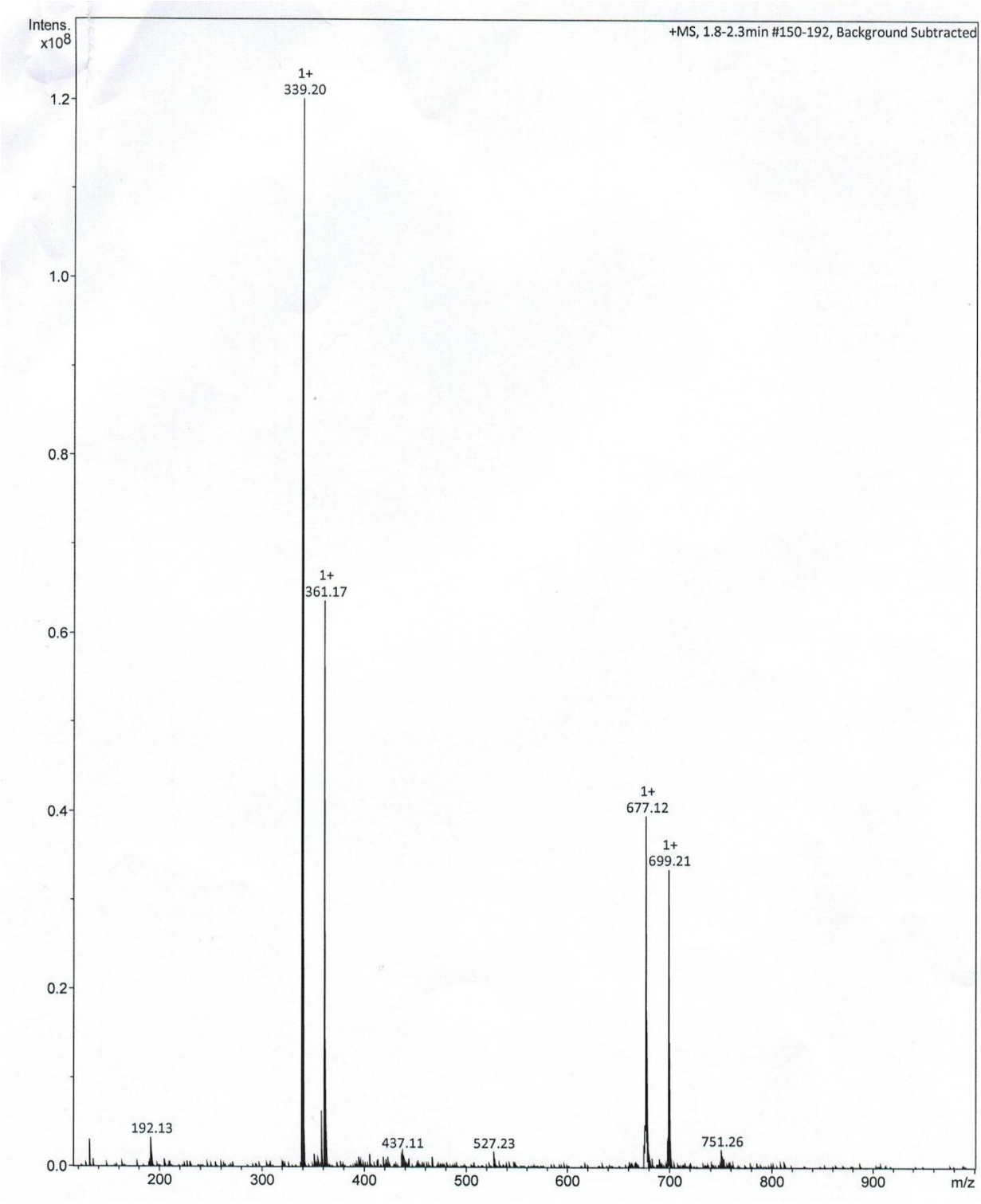
Comment MeOH 1M TOF delay 0.0006s, Q1 300 m/z



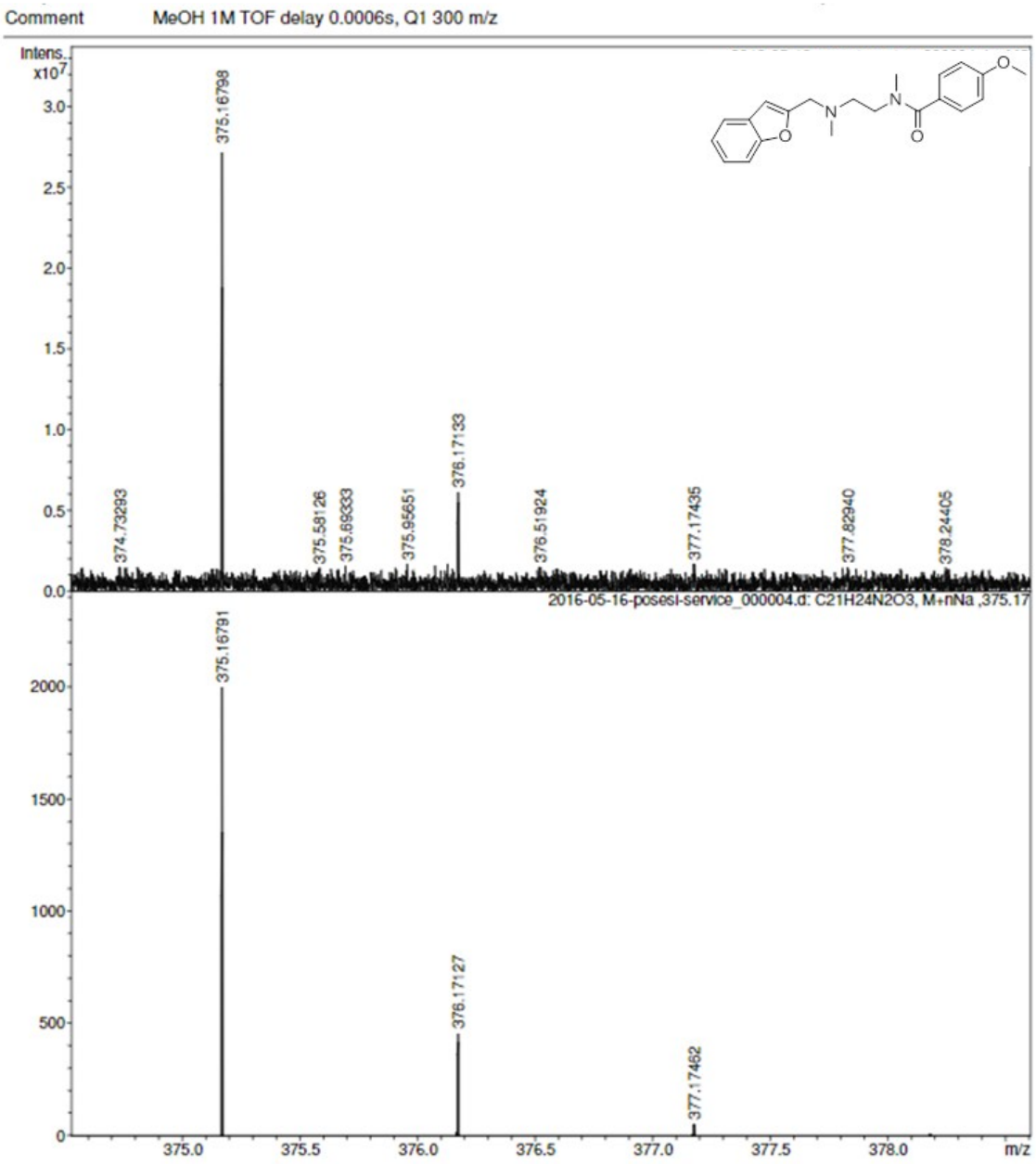
16b - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
361.15230
360.66298
360.87789
361.47716
361.73383
361.90012
362.15566
362.27643
362.74238
362.84447
363.03378
363.15896
363.28192
363.58189
363.71089
2016-07-25-posesi-service_000031.d: C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15897
m/z

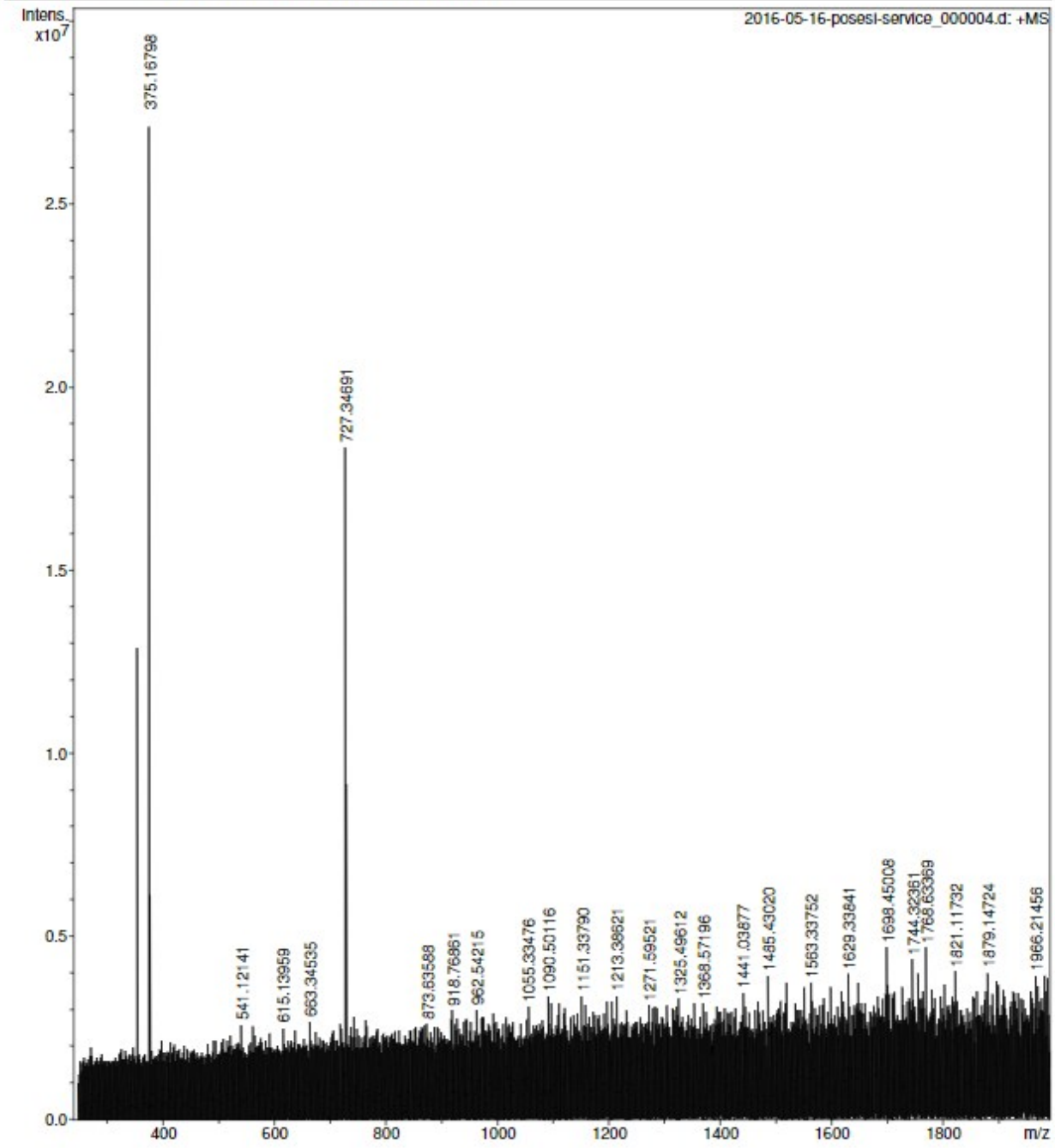
16b - LRMS


Intens.
x10^8
+MS, 1.8-2.3min #150-192, Background Subtracted
1+
339.20
1+
361.17
1+
677.12
1+
699.21
192.13
437.11
527.23
751.26
1.2
1.0
0.8
0.6
0.4
0.2
0.0
200
300
400
500
600
700
800
900
m/z

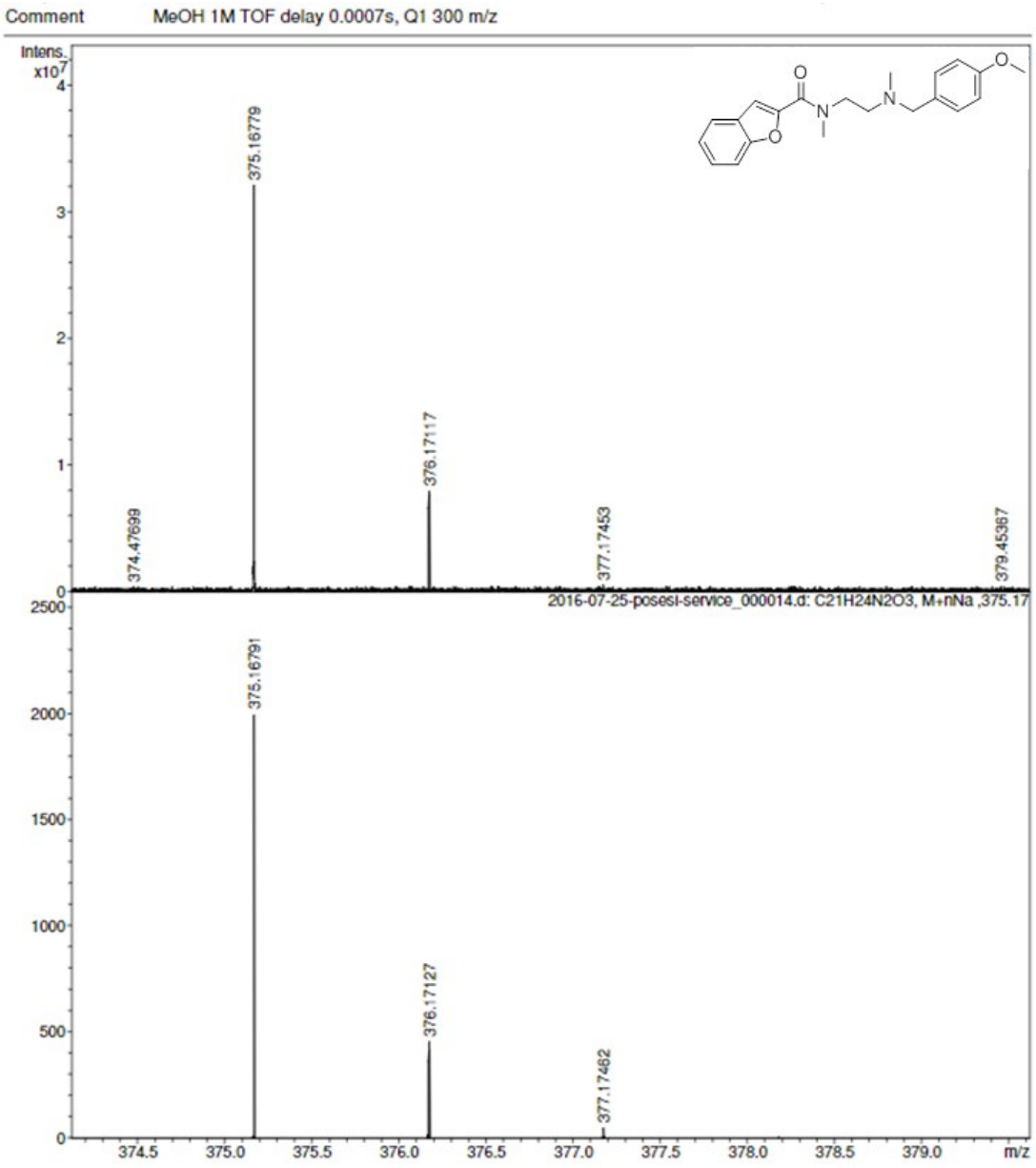
16c - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
3.0
2.5
2.0
1.5
1.0
0.5
0.0
375.16798
374.73293
375.58126
375.69333
375.95651
376.17133
376.51924
377.17435
377.82940
378.24405
2016-05-16-posesi-service_000004.d: C21H24N2O3, M+nNa ,375.17
2000
1500
1000
500
0
375.16791
376.17127
377.17462
375.0
375.5
376.0
376.5
377.0
377.5
378.0
m/z

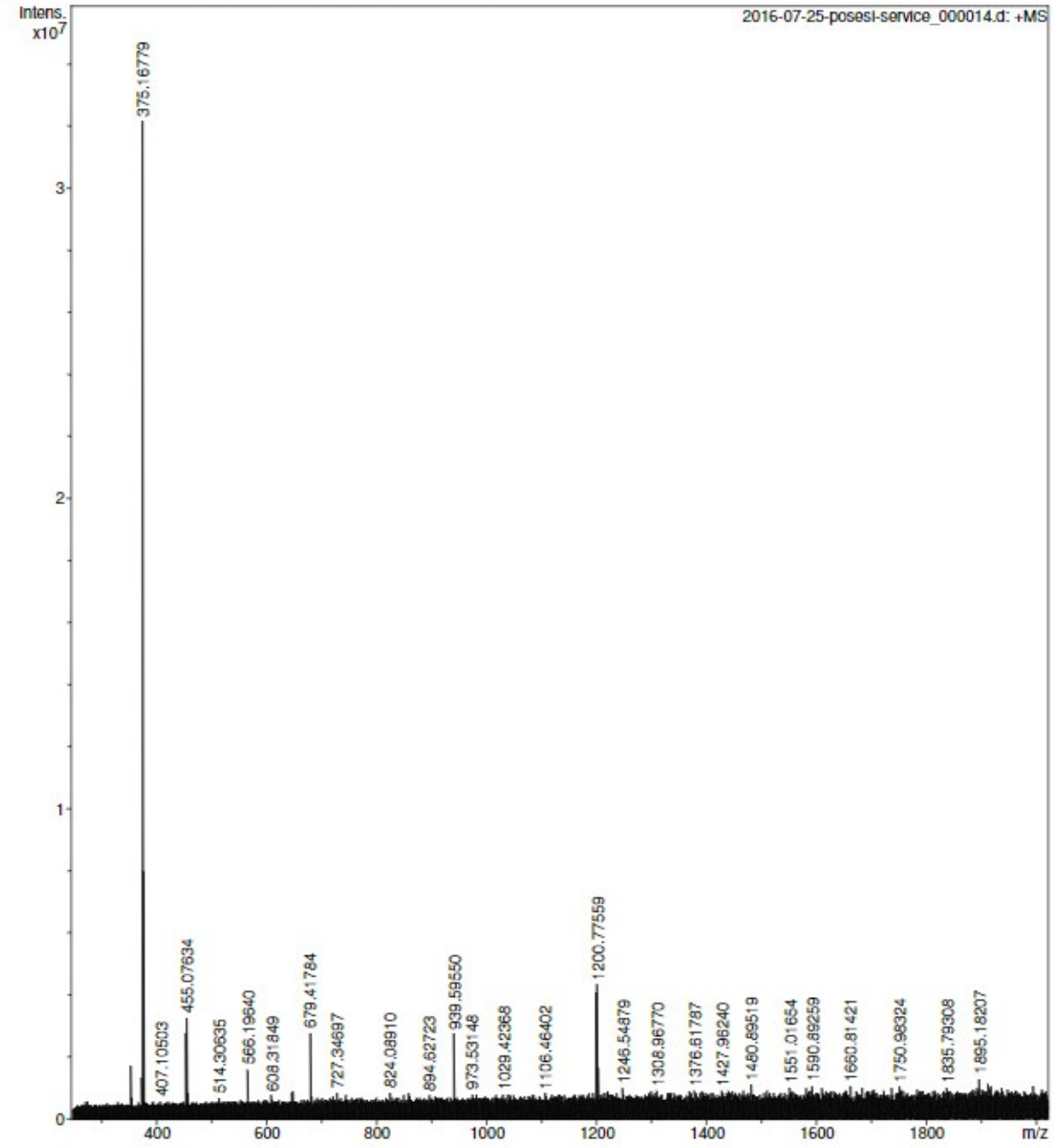
Comment MeOH 1M TOF delay 0.0006s, Q1 300 m/z



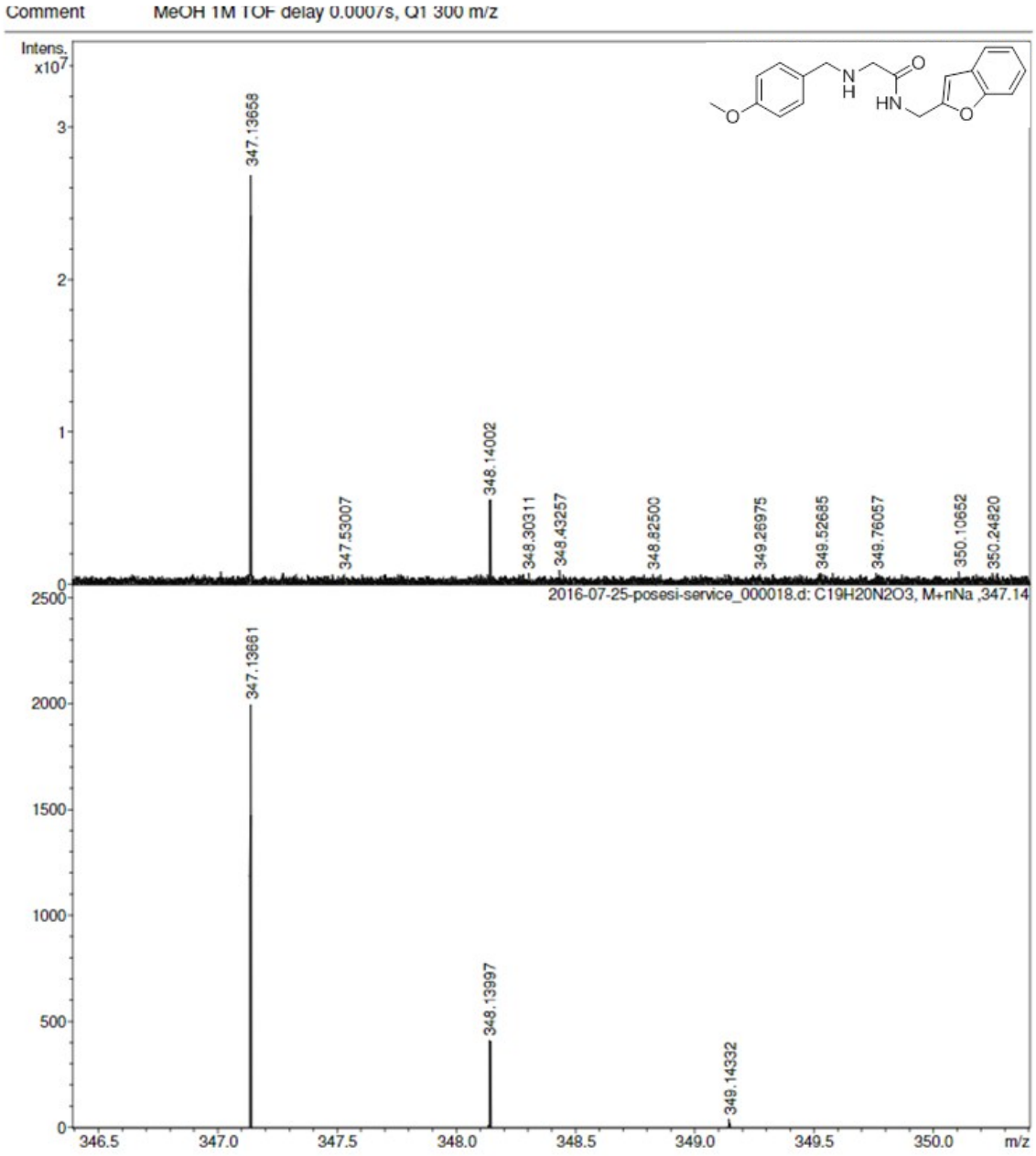
16d - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
375.16779
376.17117
374.47699
377.17453
379.45367
2016-07-25-posesi-service_000014.d: C21H24N2O3, M+nNa ,375.17
375.16791
376.17127
377.17462
m/z

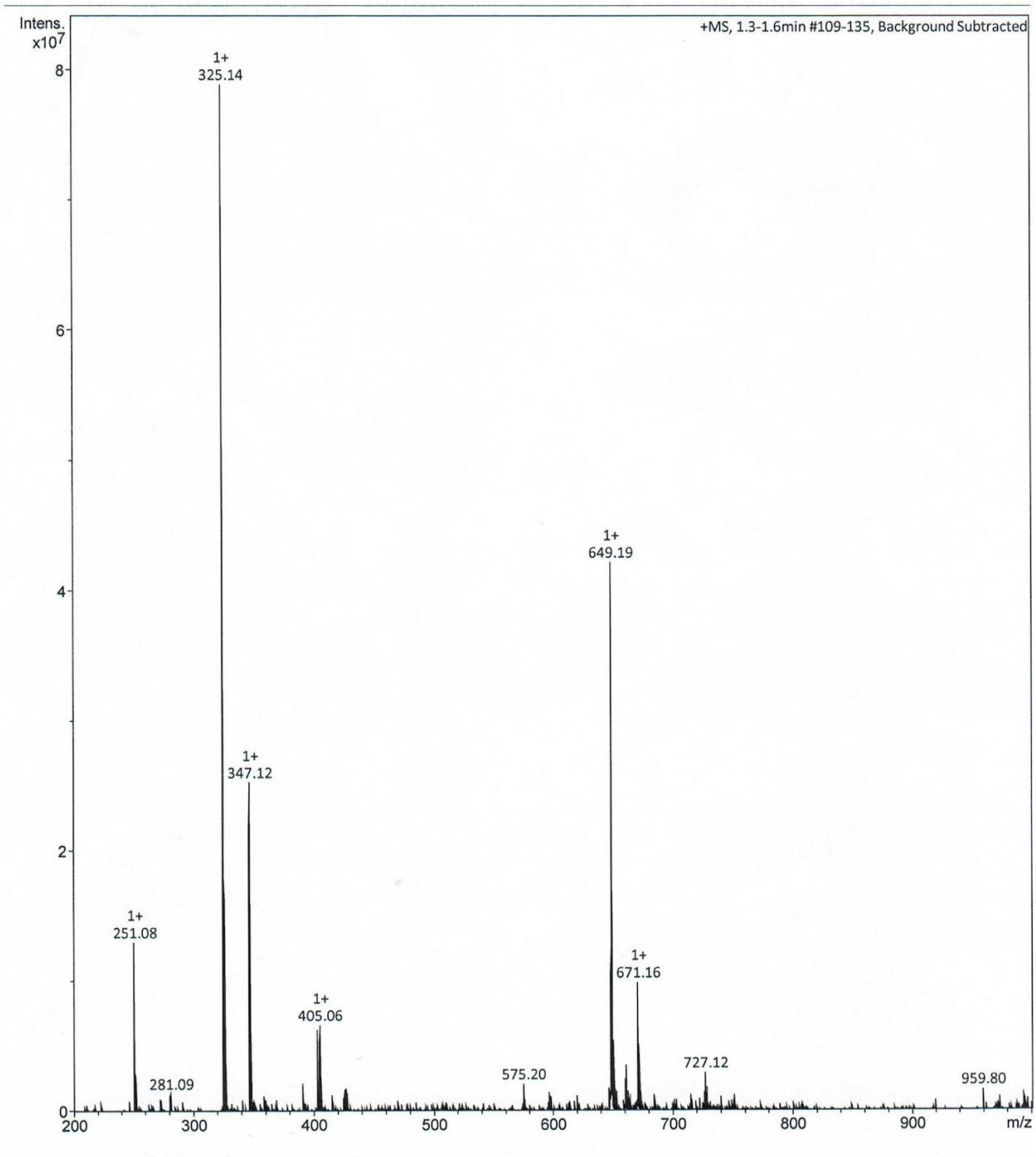
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



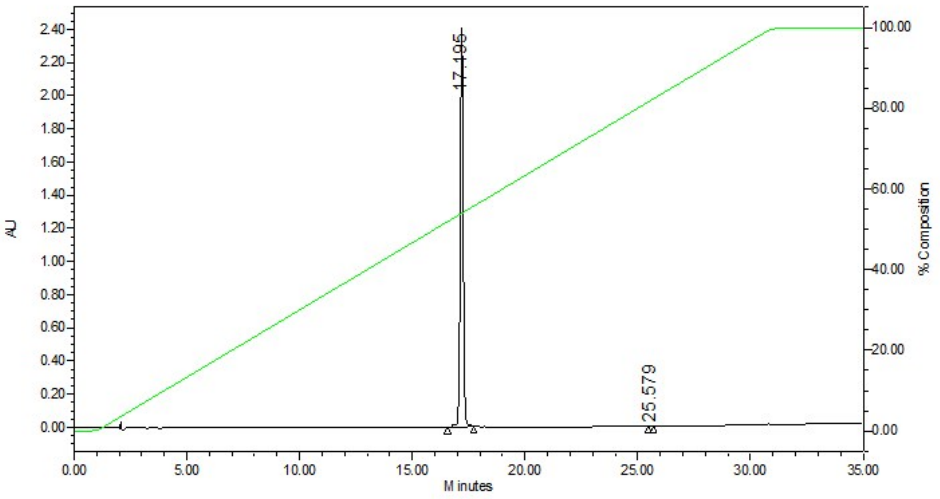
22a - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
347.13658
348.14002
347.53007
348.30311
348.43257
348.82500
349.26975
349.52685
349.76057
350.10652
350.24820
2016-07-25-posesi-service_000018.d: C19H20N2O3, M+nNa ,347.14
347.13661
348.13997
349.14332
346.5
347.0
347.5
348.0
348.5
349.0
349.5
350.0
m/z

22a - LRMS


Intens.
x10^7
+MS, 1.3-1.6min #109-135, Background Subtracted
1+
325.14
1+
649.19
1+
347.12
1+
251.08
1+
671.16
1+
405.06
281.09
575.20
727.12
959.80
8
6
4
2
0
200
300
400
500
600
700
800
900
m/z

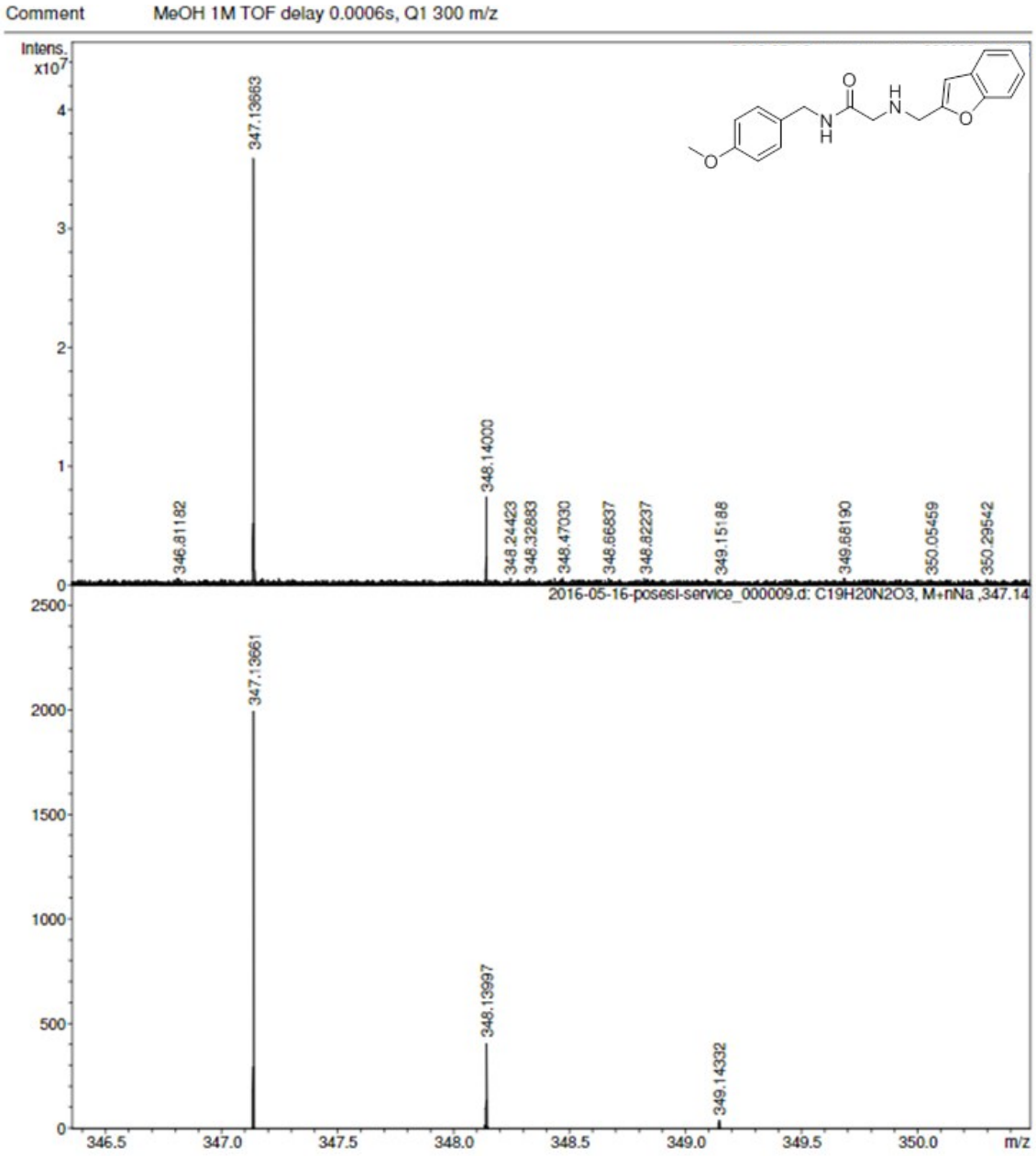
22a - HPLC



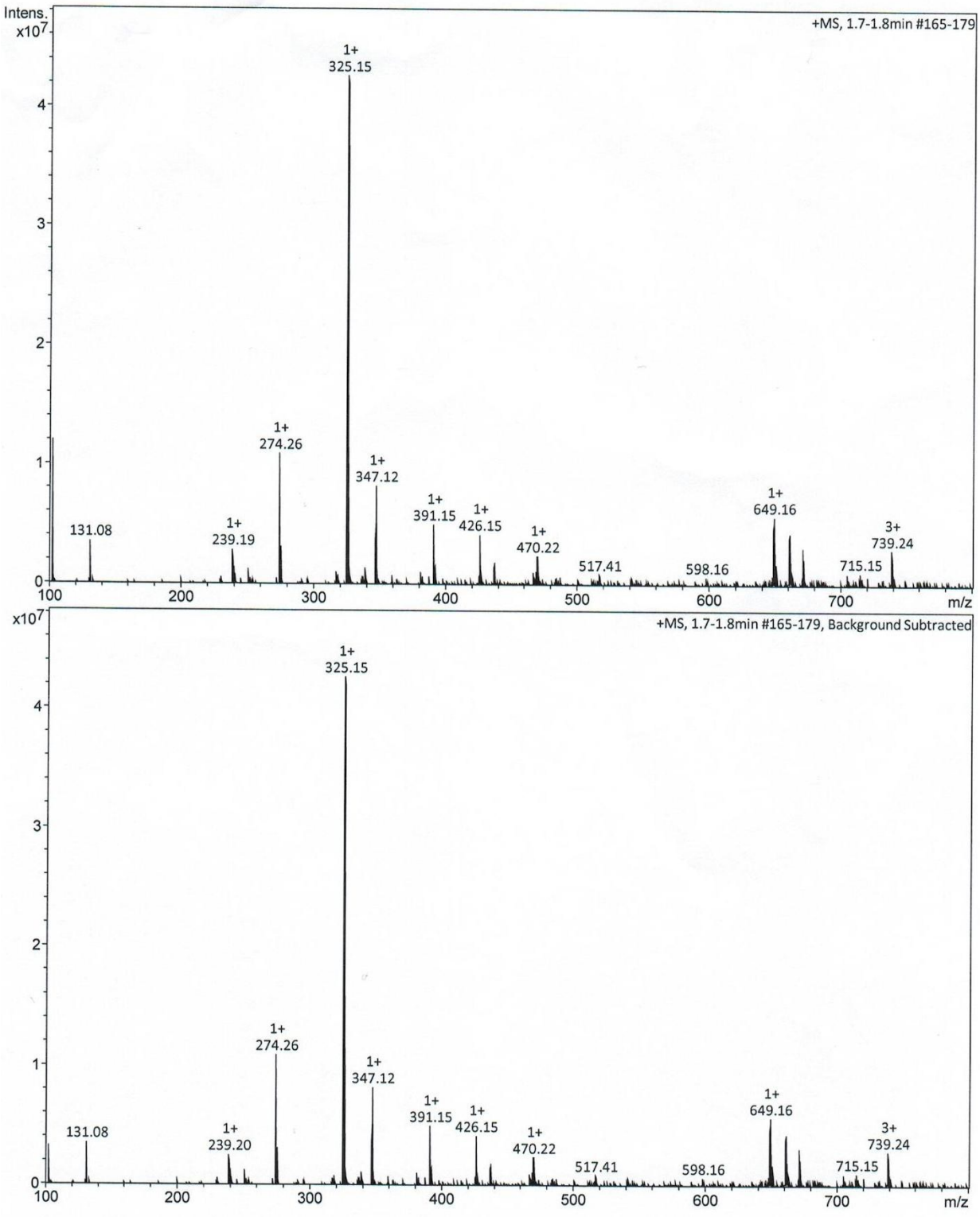
Peak information

	RT	Area	% Area
1	17.195	21988933	99.89
2	25.579	23964	0.11

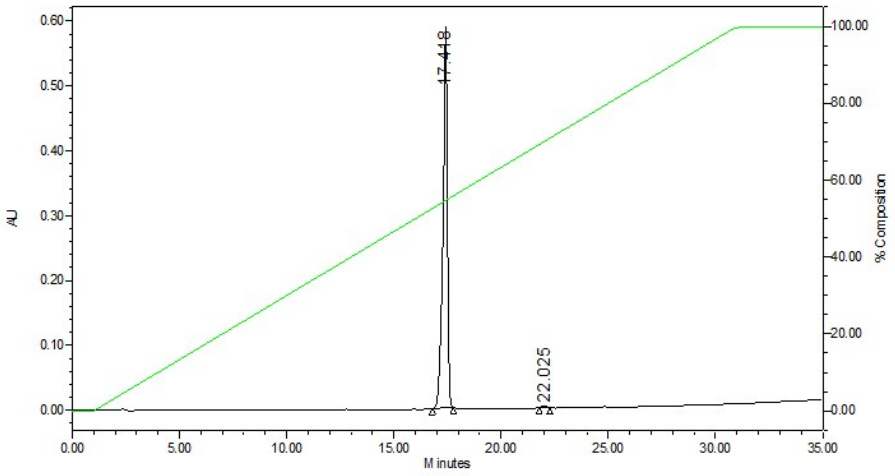
22b - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
347.13663
348.14000
346.81182
348.24423
348.32883
348.47030
348.66837
348.82237
349.15188
349.68190
350.05459
350.29542
2016-05-16-posesi-service_000009.d: C19H20N2O3, M+nNa ,347.14
347.13661
348.13997
349.14332
m/z

22b - LRMS


Intens.
x10^7
+MS, 1.7-1.8min #165-179
1+ 325.15
1+ 274.26
1+ 347.12
1+ 391.15
1+ 426.15
1+ 470.22
1+ 649.16
3+ 739.24
131.08
1+ 239.19
517.41
598.16
715.15
m/z
+MS, 1.7-1.8min #165-179, Background Subtracted
1+ 325.15
1+ 274.26
1+ 347.12
1+ 391.15
1+ 426.15
1+ 470.22
1+ 649.16
3+ 739.24
131.08
1+ 239.20
517.41
598.16
715.15
m/z

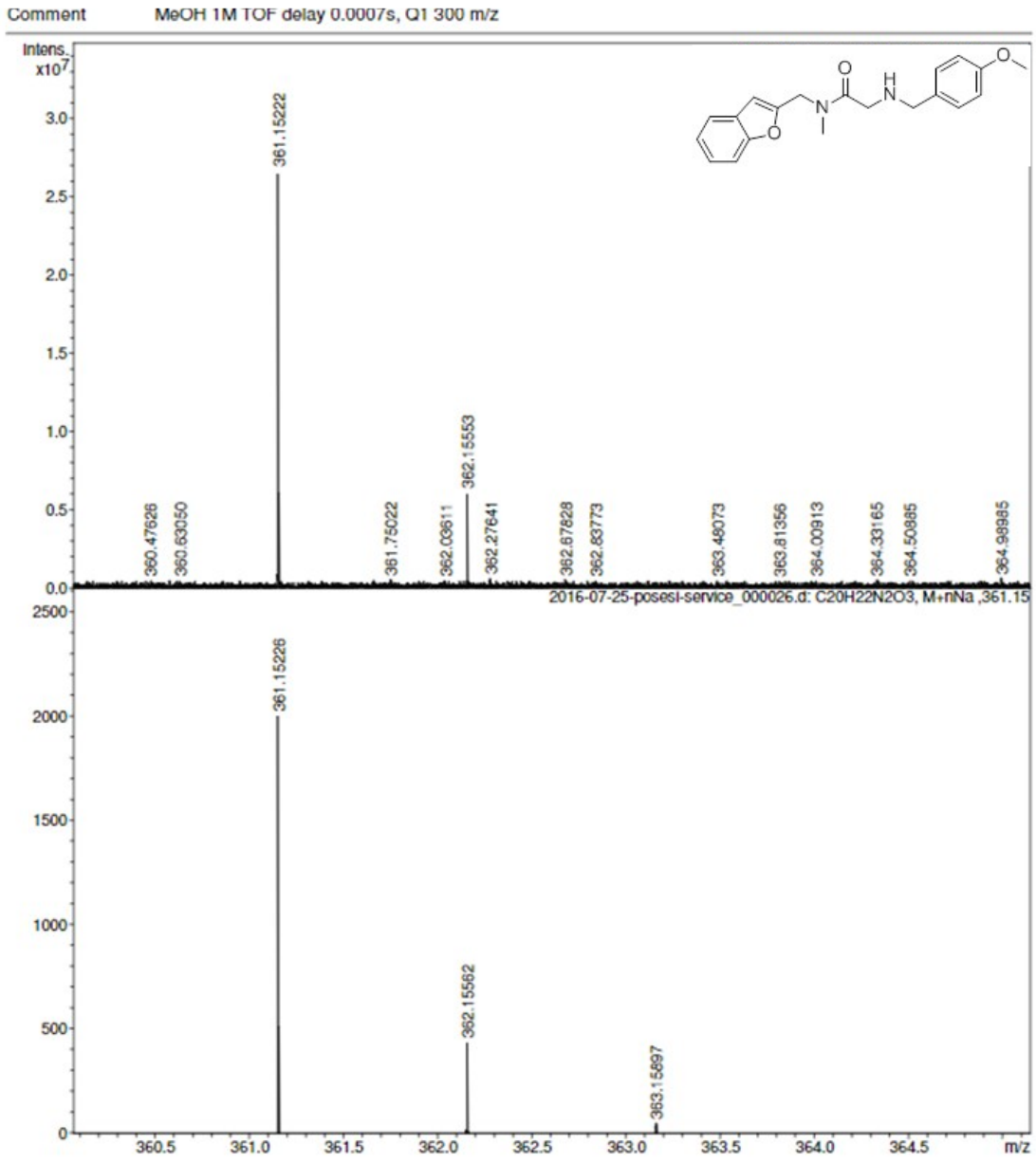
22b - HPLC



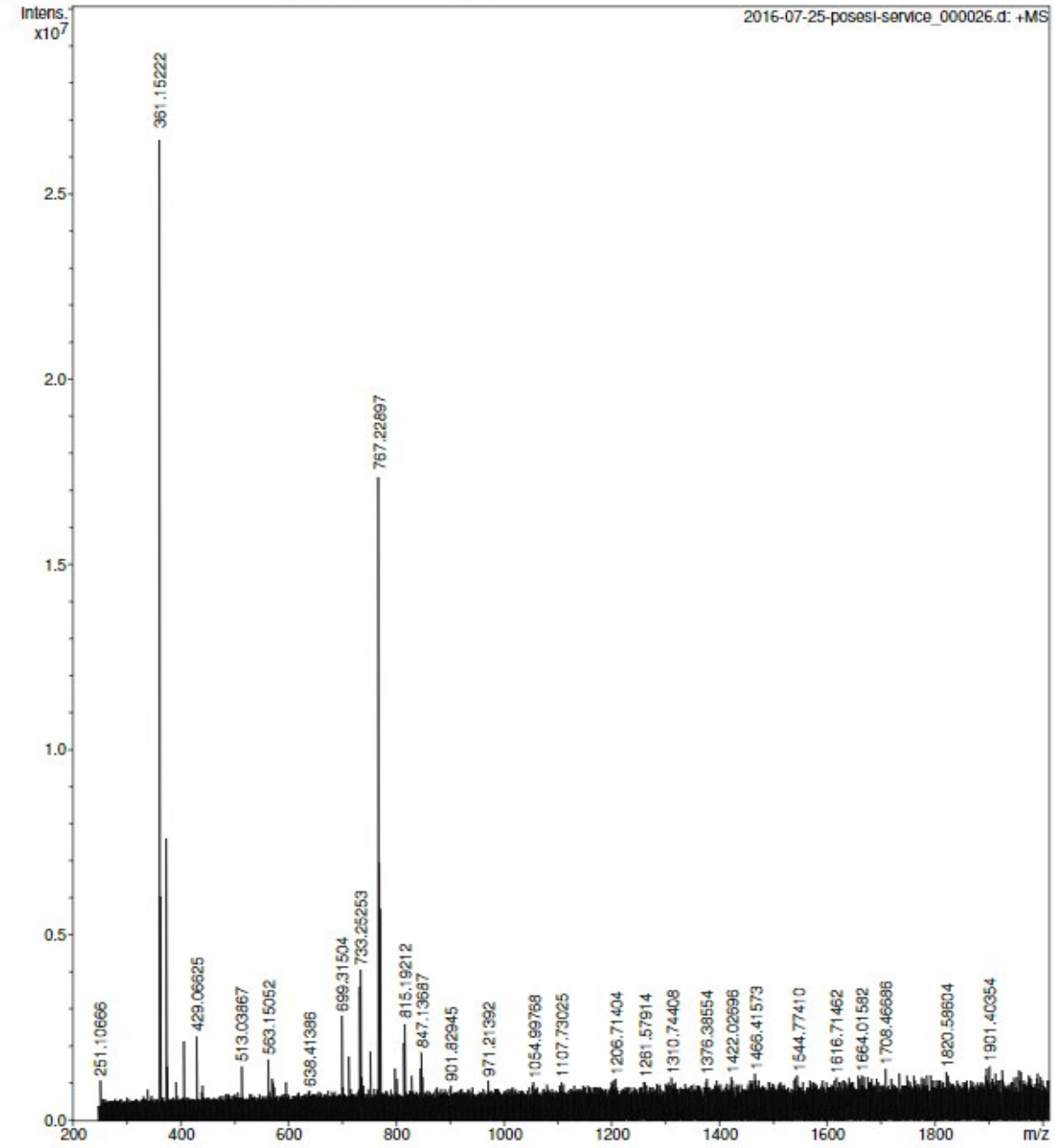
Peak information

	RT	Area	% Area
1	17.418	8361008	99.49
2	22.025	42512	0.51

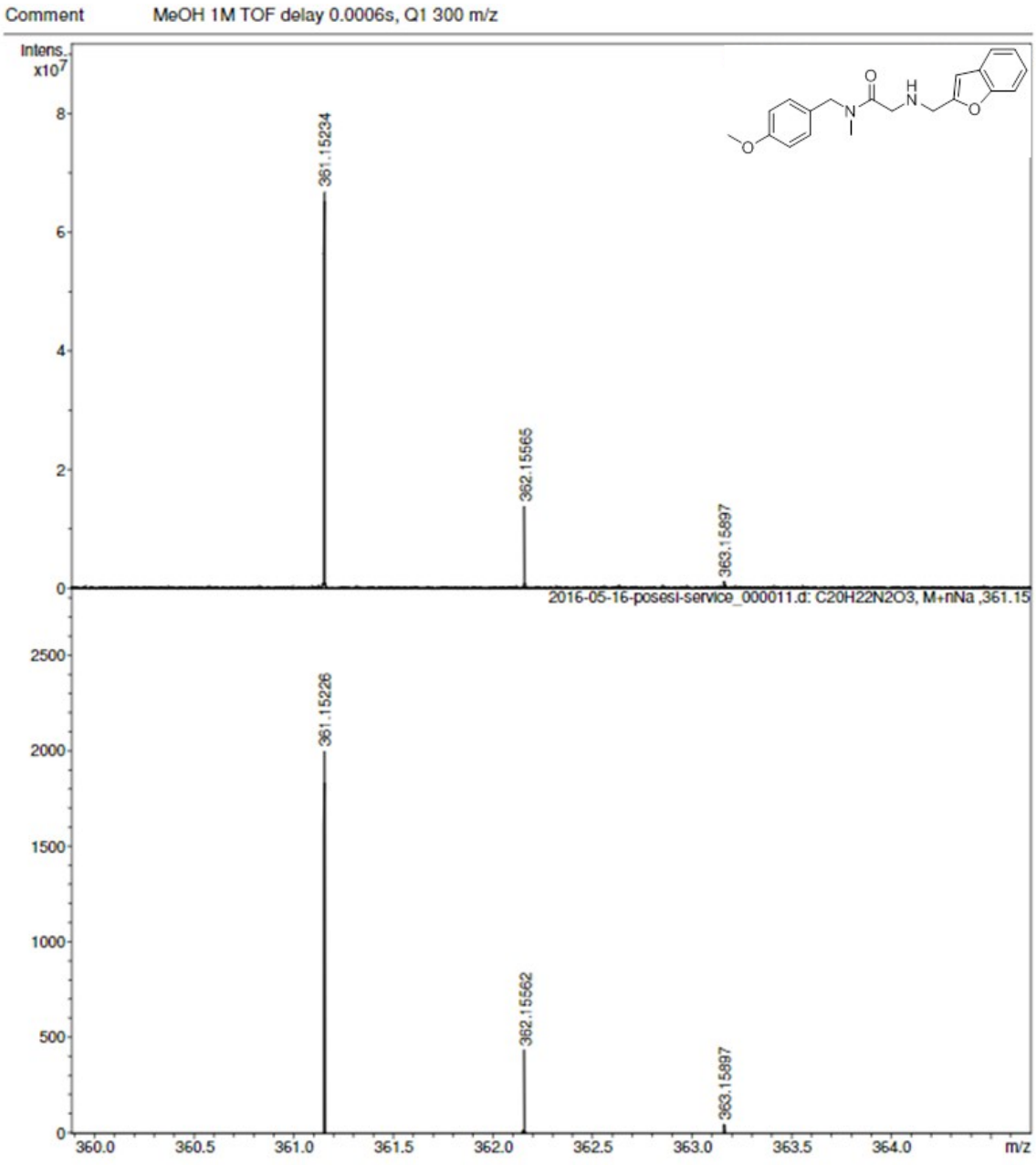
23a - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
361.15222
360.47626
360.63050
361.75022
362.03611
362.15553
362.27641
362.67828
362.83773
363.48073
363.81356
364.00913
364.33165
364.50885
364.99985
2016-07-25-posesi-service_000026.d: C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15897
m/z

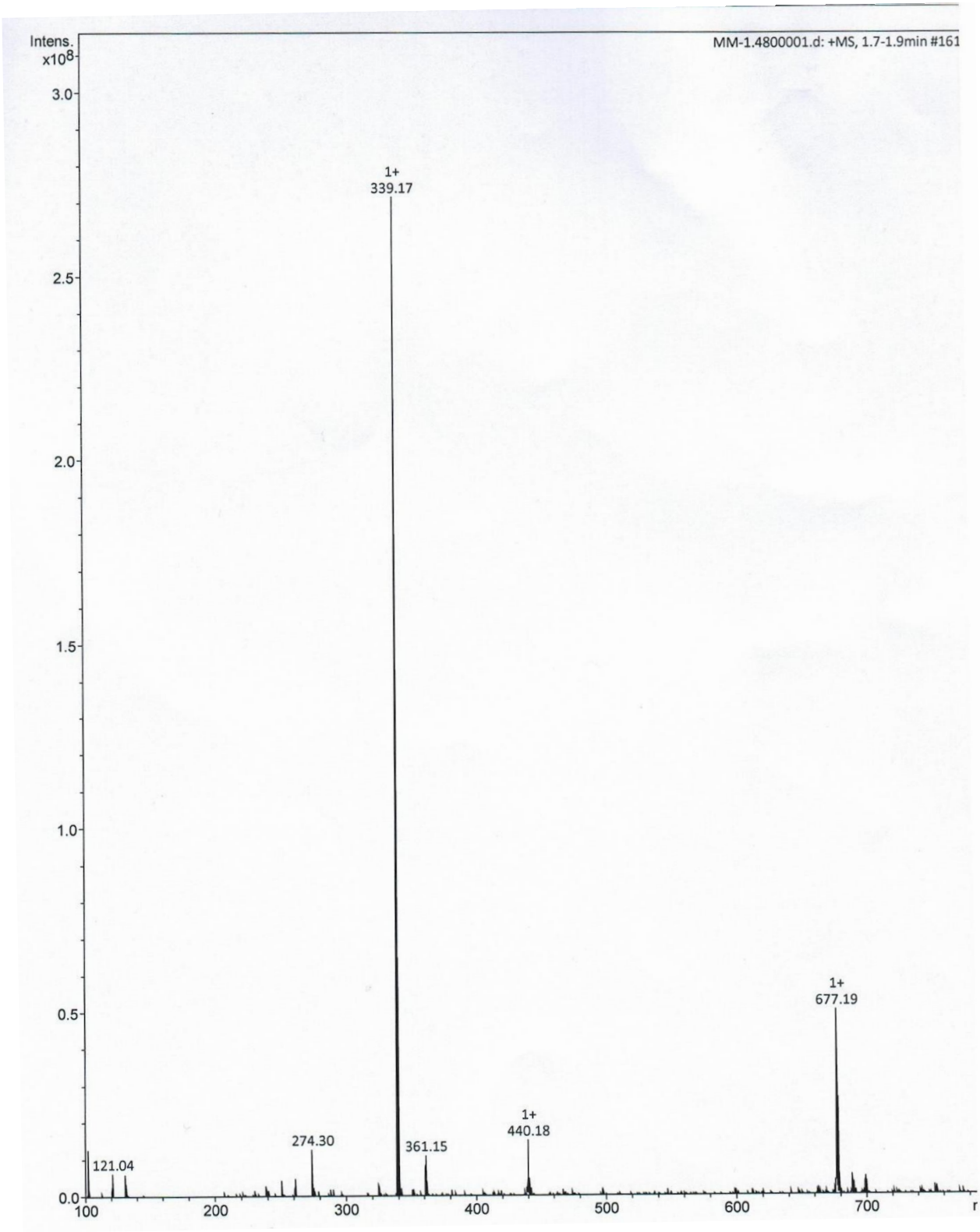
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



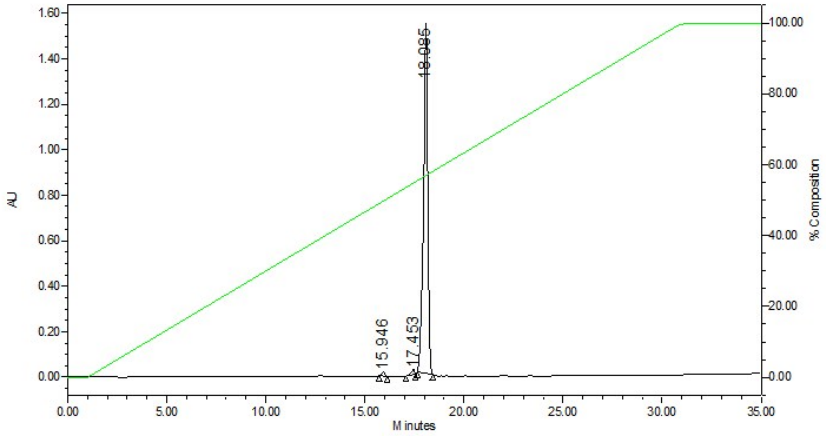
23b - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
361.15234
362.15565
363.15897
2016-05-16-posesi-service_000011.d: C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15897
m/z

23b - LRMS


Intens.
x10^8
MM-1.4800001.d: +MS, 1.7-1.9min #161
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1+
339.17
1+
677.19
1+
440.18
274.30
361.15
121.04
100
200
300
400
500
600
700

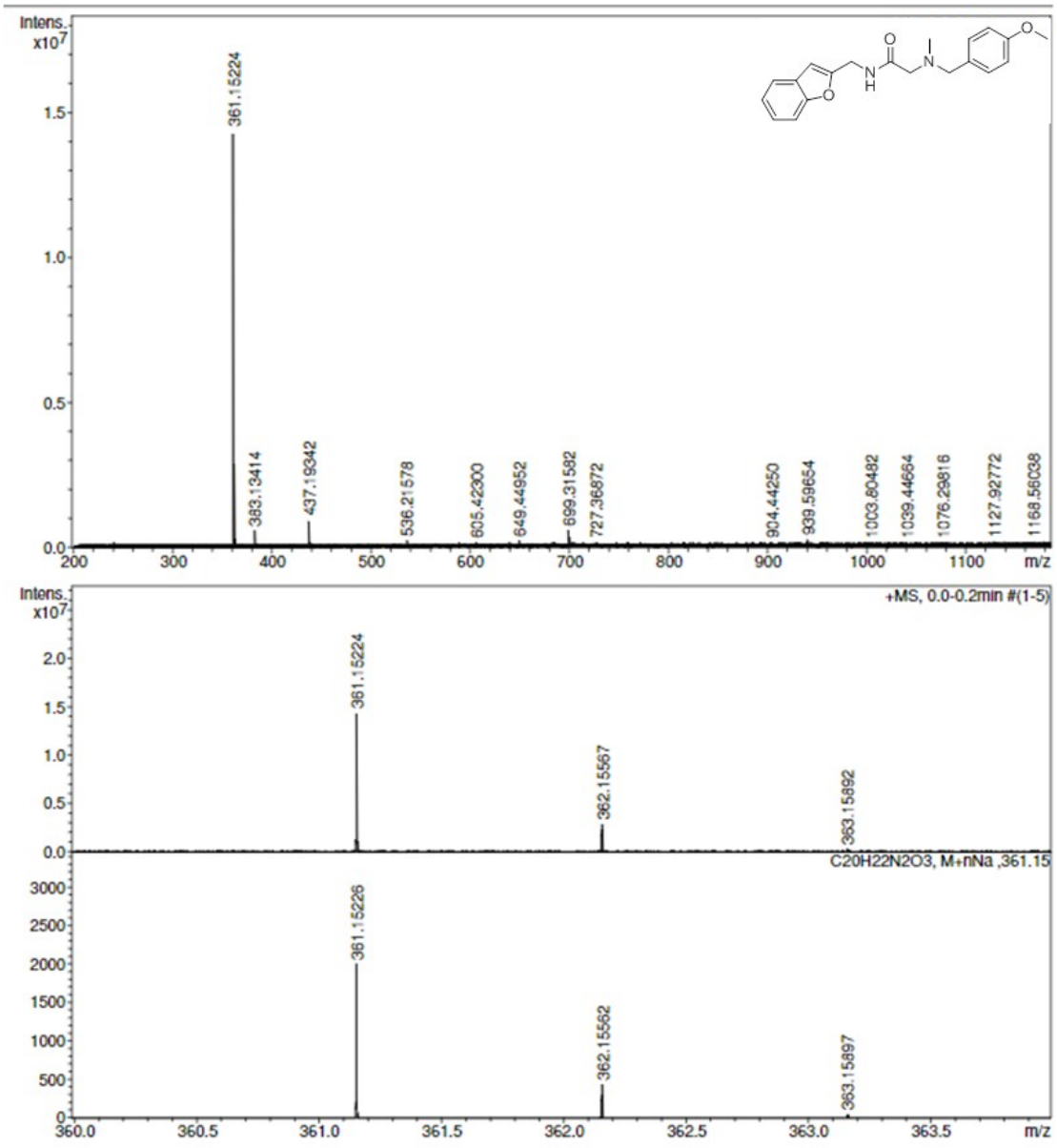
23b - HPLC



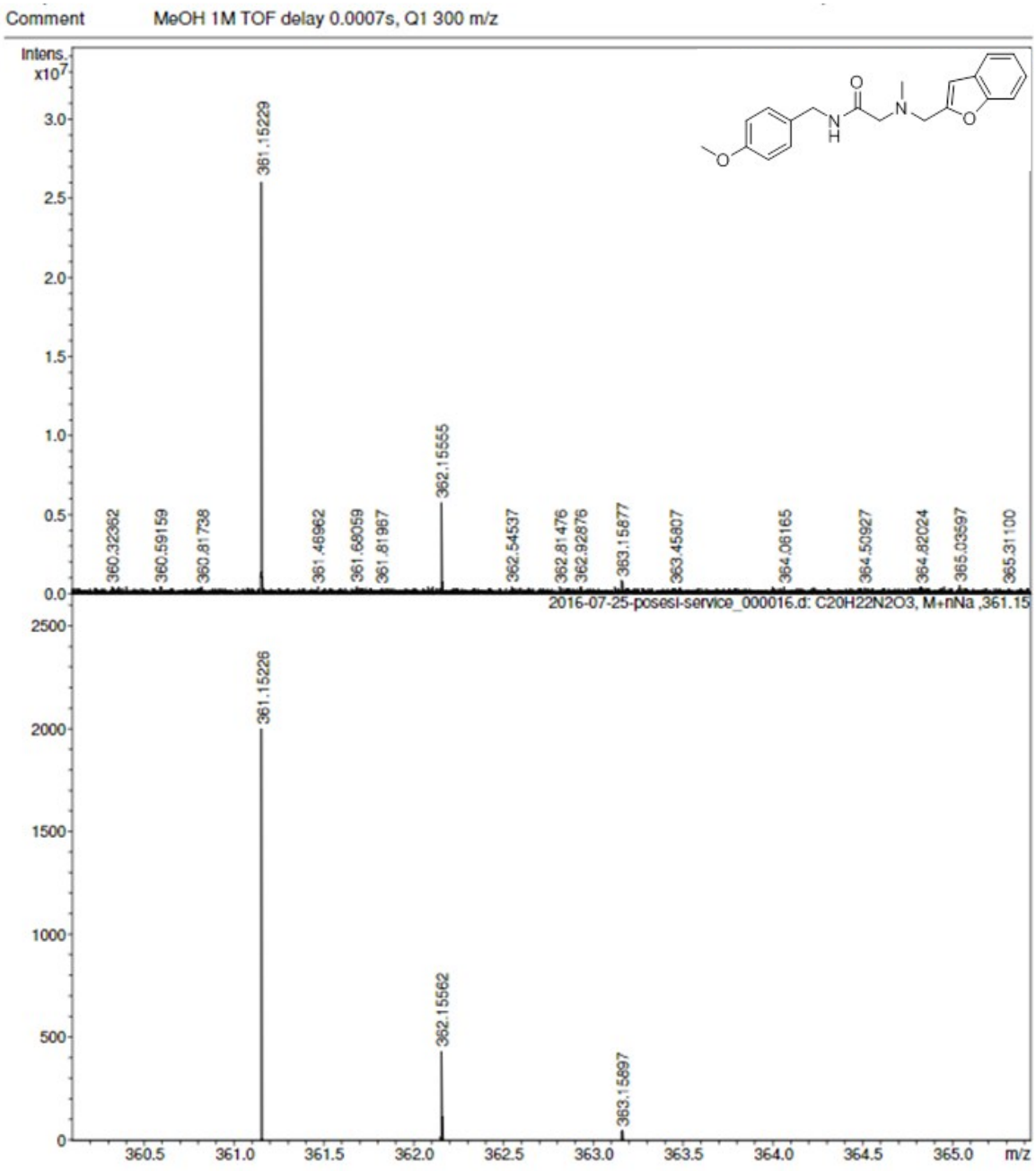
Peak information

	RT	Area	% Area
1	15.946	200526	0.86
2	17.453	246565	1.05
3	18.085	22966760	98.09

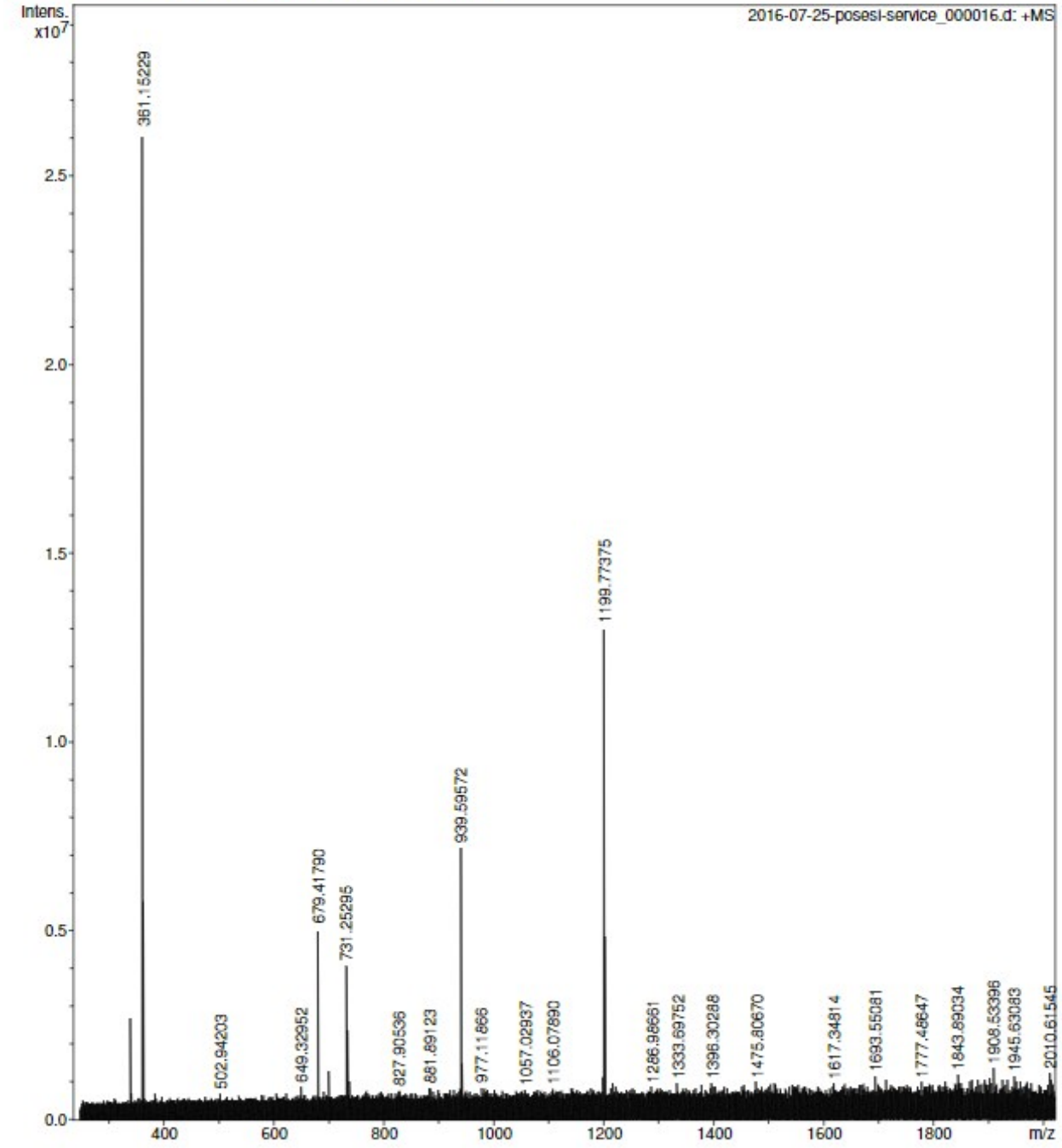
24a - HRMS


Intens.
x10^7
361.15224
383.13414
437.19342
536.21578
605.42300
649.44952
699.31582
727.36872
904.44250
939.59654
1003.60492
1039.44664
1076.29816
1127.92772
1168.56038
m/z
+MS, 0.0-0.2min #(1-5)
362.15567
363.15892
C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15897

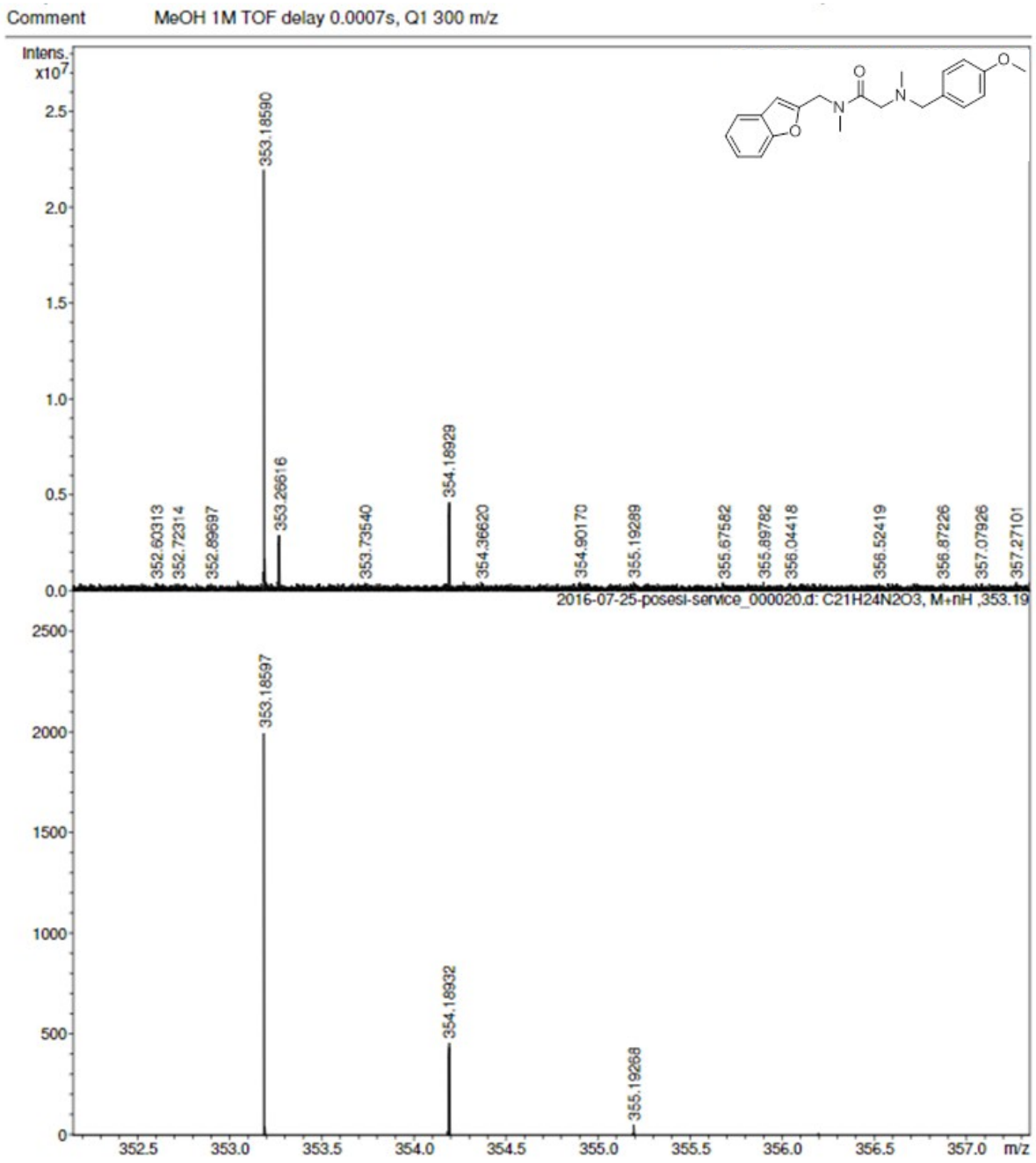
24b - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
361.15229
362.15555
2016-07-25-posesi-service_000016.d: C20H22N2O3, M+nNa ,361.15
361.15226
362.15562
363.15897
m/z

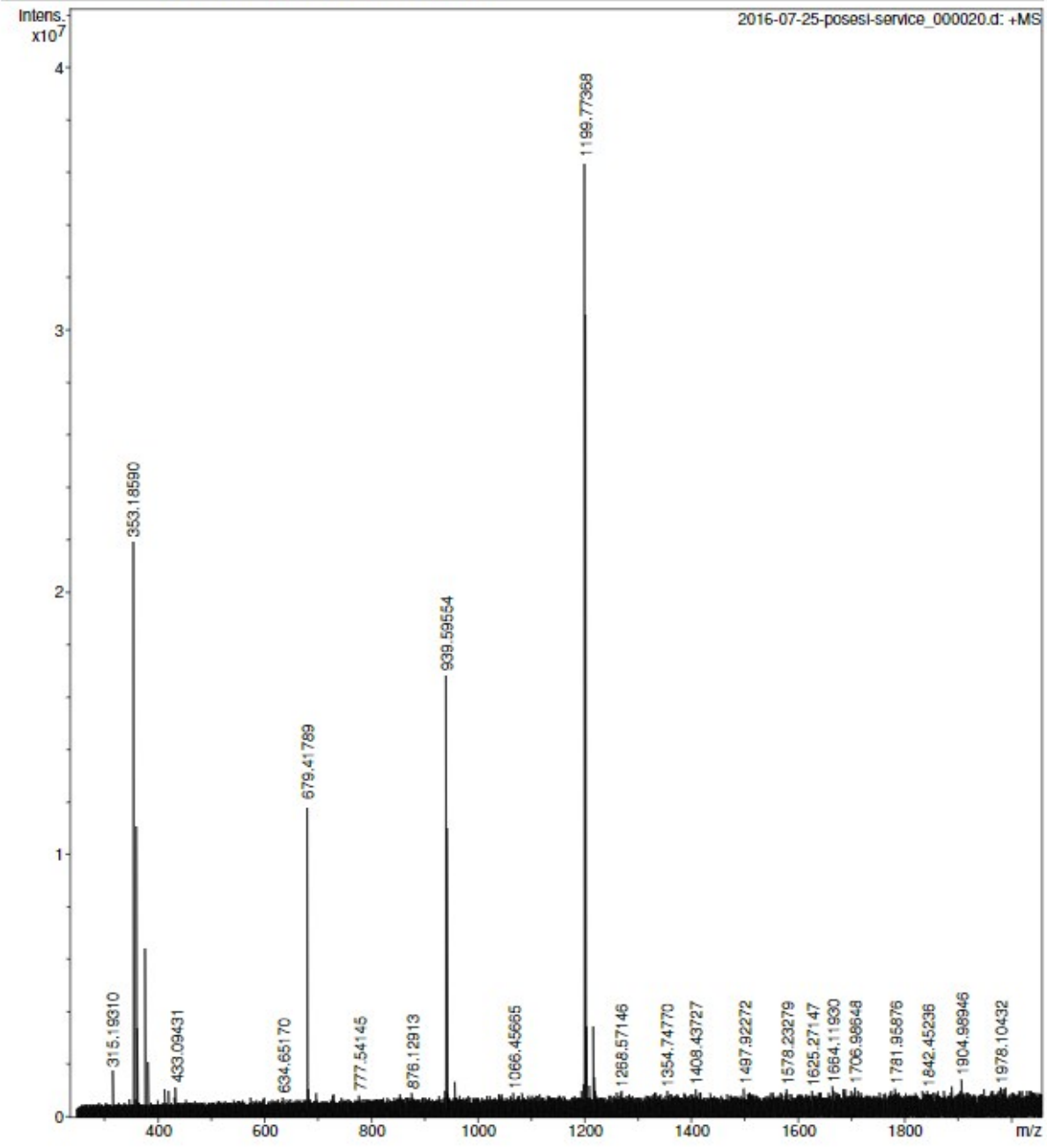
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



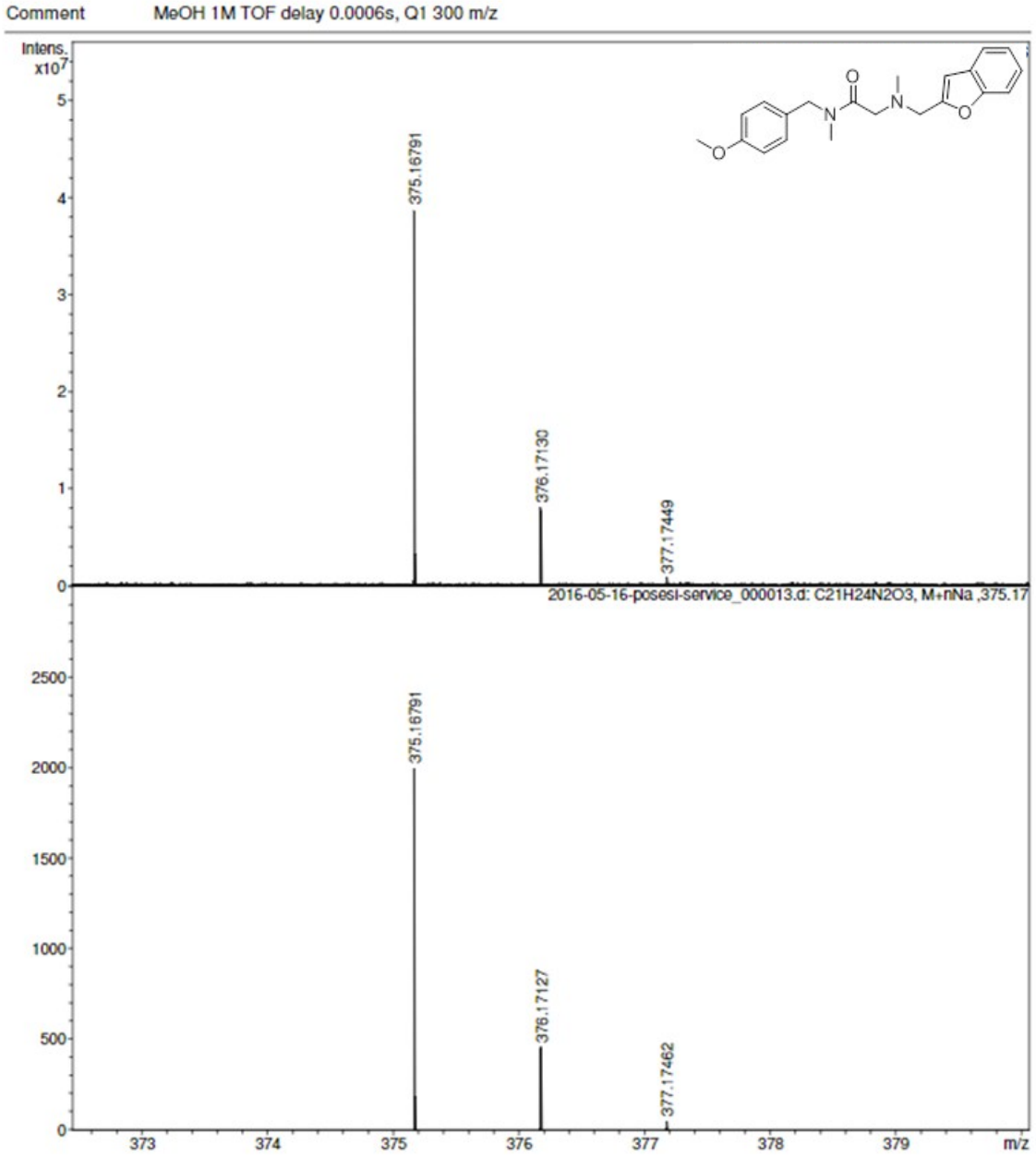
25a - HRMS


Comment
MeOH 1M TOF delay 0.0007s, Q1 300 m/z
Intens.
x10^7
353.18590
354.18929
353.26616
352.60313
352.72314
352.89697
353.73540
354.36620
354.90170
355.19289
355.67562
355.89782
356.04418
356.52419
356.87226
357.07926
357.27101
2016-07-25-posesi-service_000020.d: C21H24N2O3, M+nH ,353.19
353.18597
354.18932
355.19268
m/z

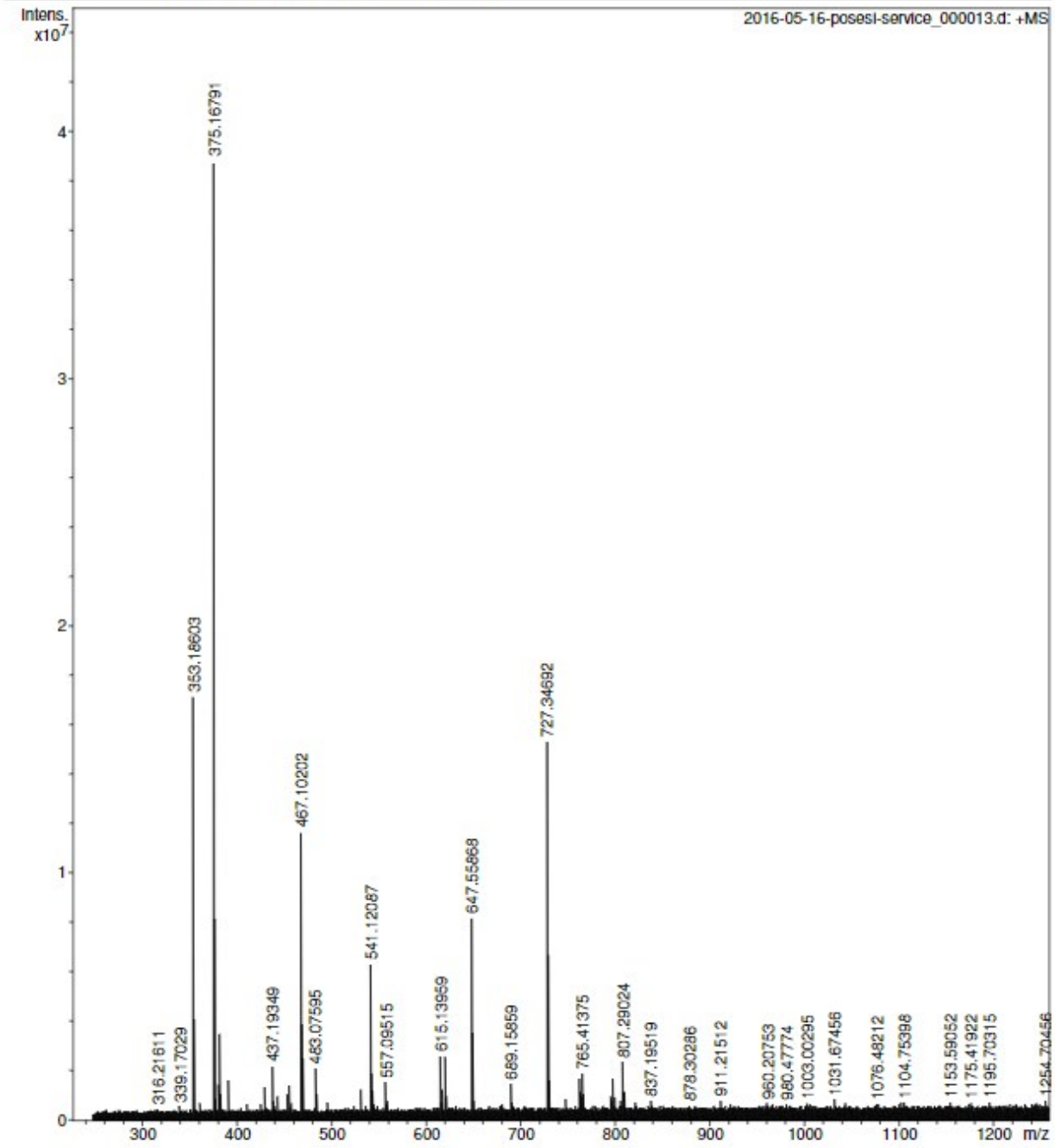
Comment MeOH 1M TOF delay 0.0007s, Q1 300 m/z



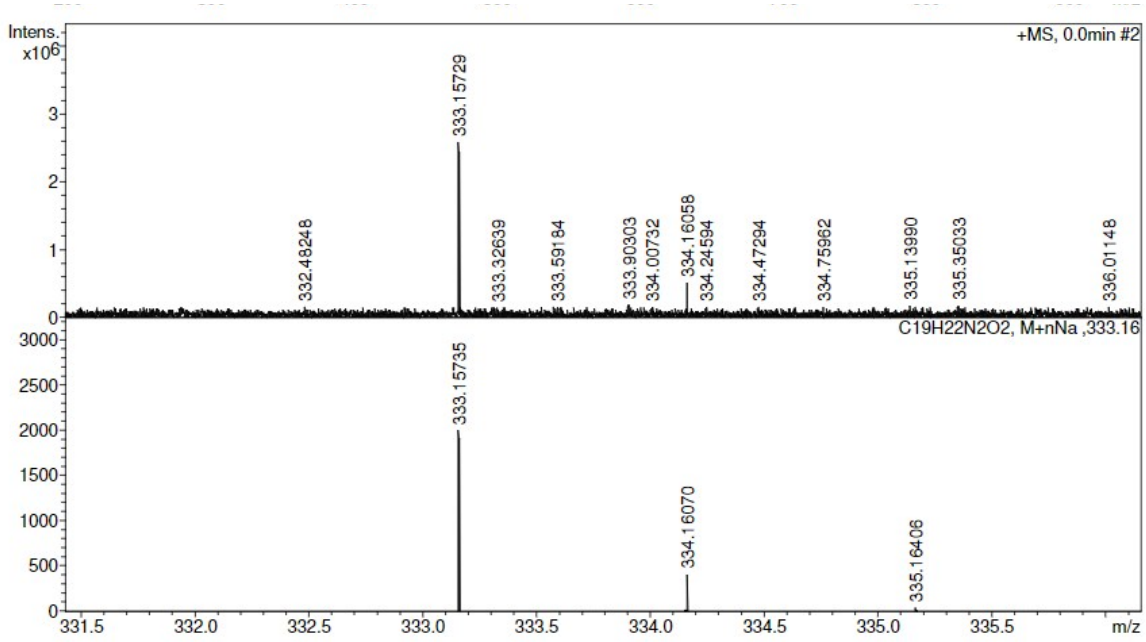
25b - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
375.16791
376.17130
377.17449
2016-05-16-posesi-service_000013.d: C21H24N2O3, M+nNa ,375.17
375.16791
376.17127
377.17462
m/z

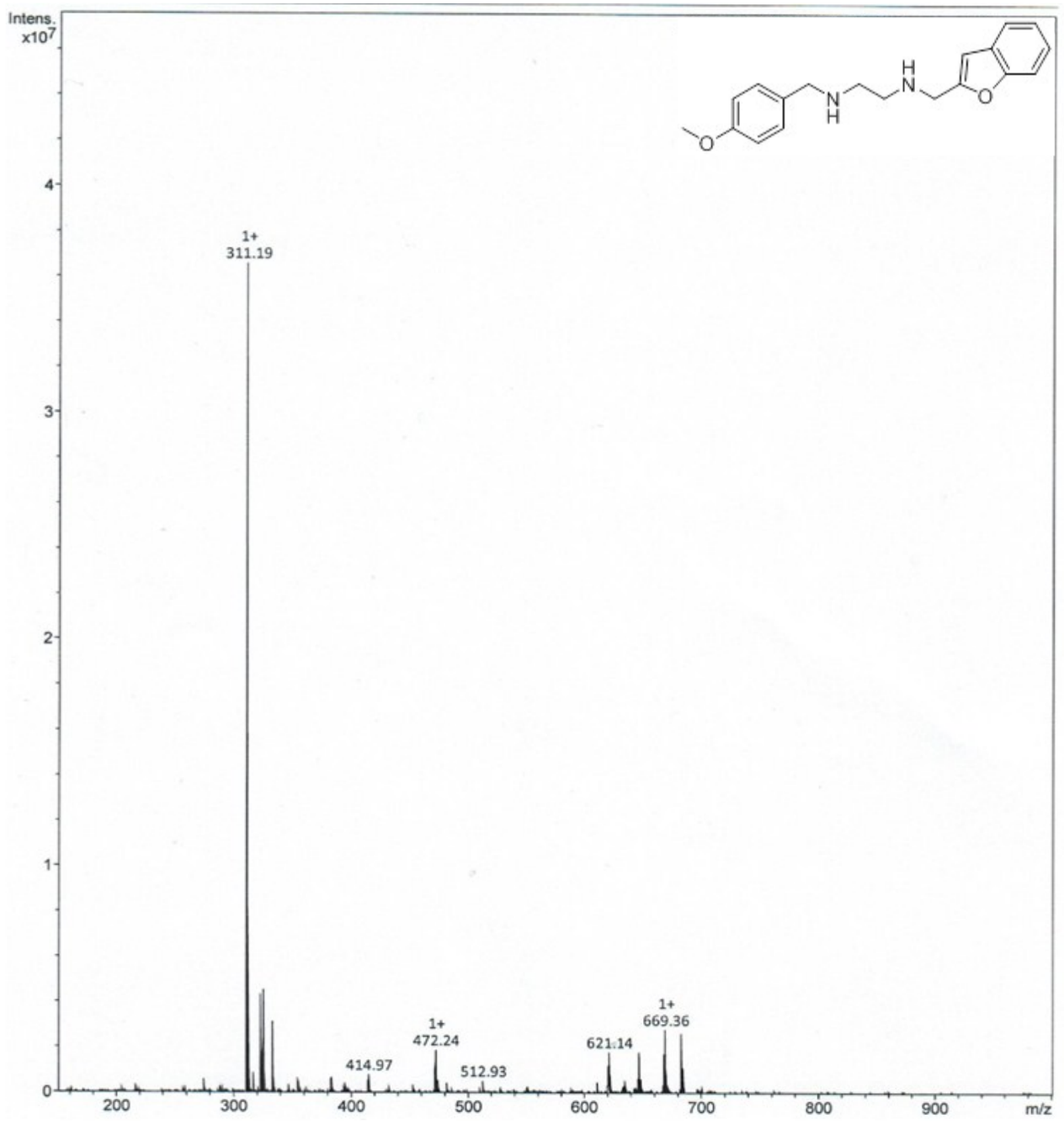
Comment MeOH 1M TOF delay 0.0006s, Q1 300 m/z



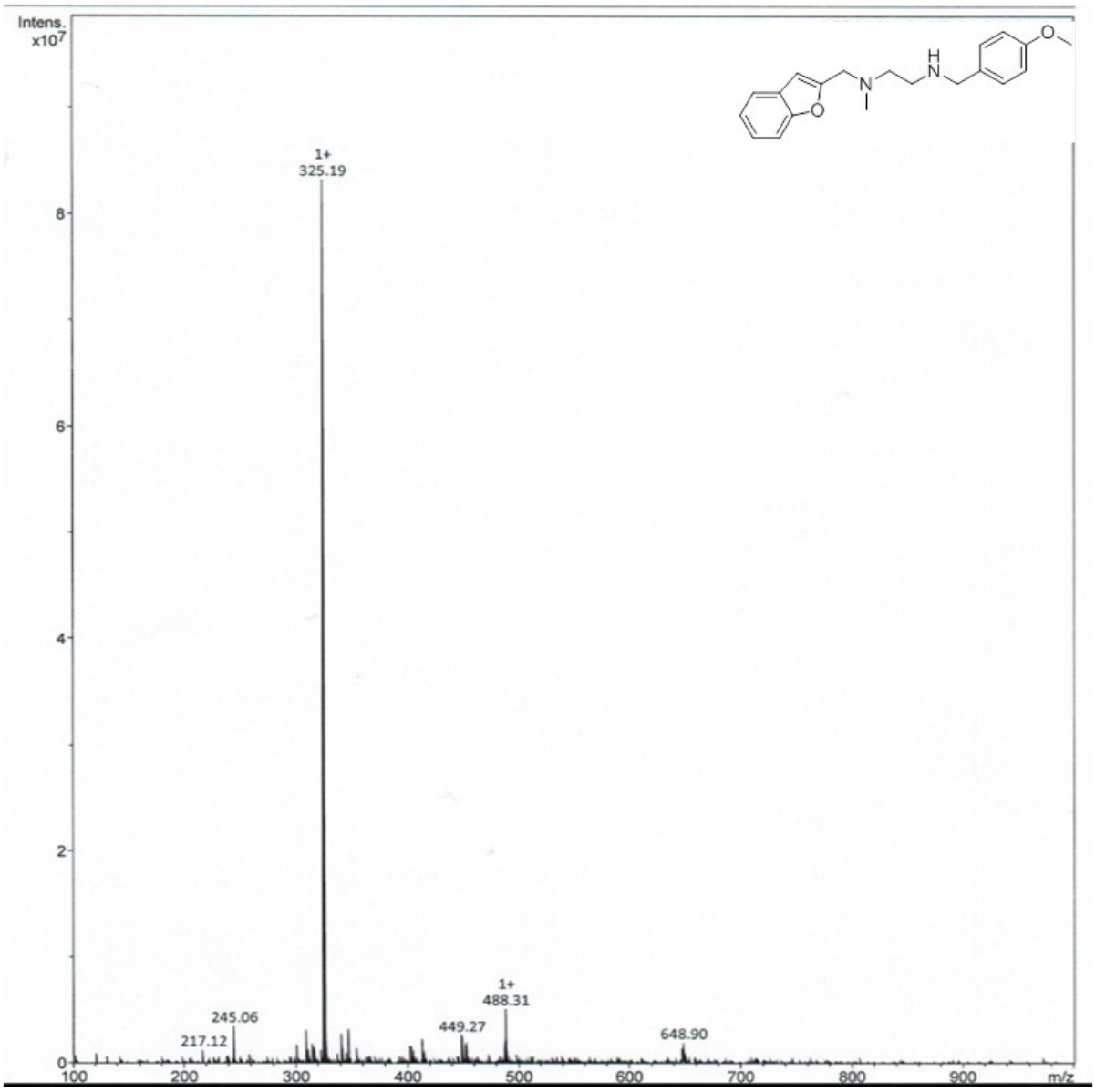
26a -HRMS


Intens.
x10^6
+MS, 0.0min #2
333.15729
332.48248
333.32639
333.59184
333.90303
334.00732
334.16058
334.24594
334.47294
334.75962
335.13990
335.35033
336.01148
C19H22N2O2, M+nNa ,333.16
333.15735
334.16070
335.16406
m/z

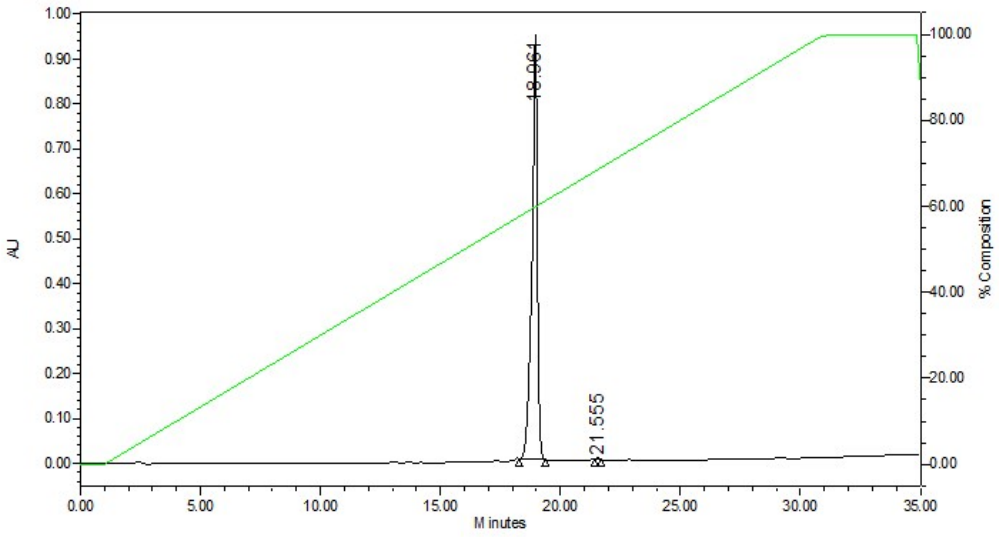
26a - LRMS


Intens.
x10^7
4
3
2
1
0
1+
311.19
1+
472.24
414.97
512.93
621.14
1+
669.36
200
300
400
500
600
700
800
900
m/z
O
N
H
N
H
O

26b - LRMS


Intens.
x10^7
1+
325.19
8
6
4
2
0
245.06
217.12
449.27
1+
488.31
648.90
100
200
300
400
500
600
700
800
900
m/z
O
N
H
N
O

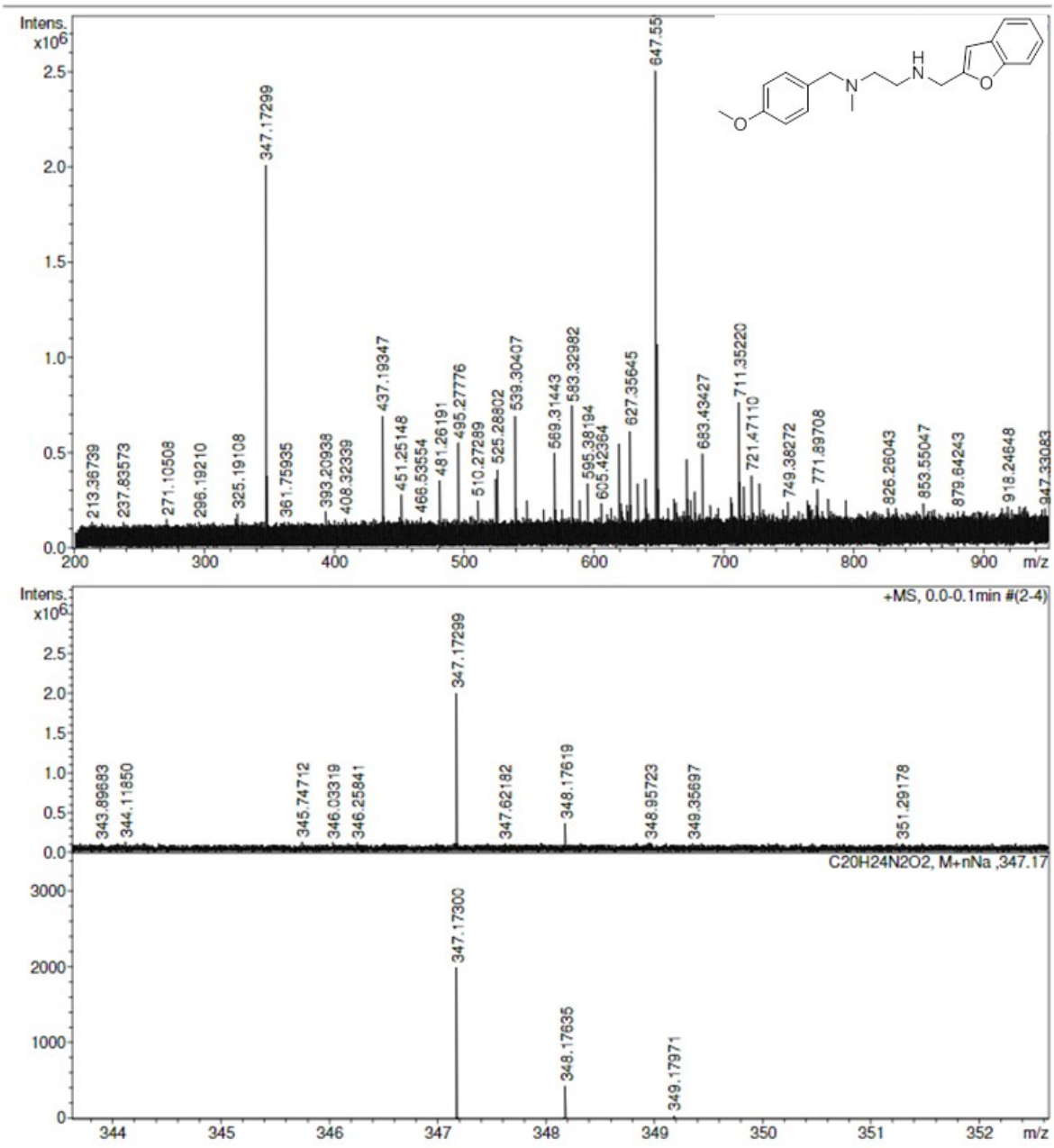
26b - HPLC



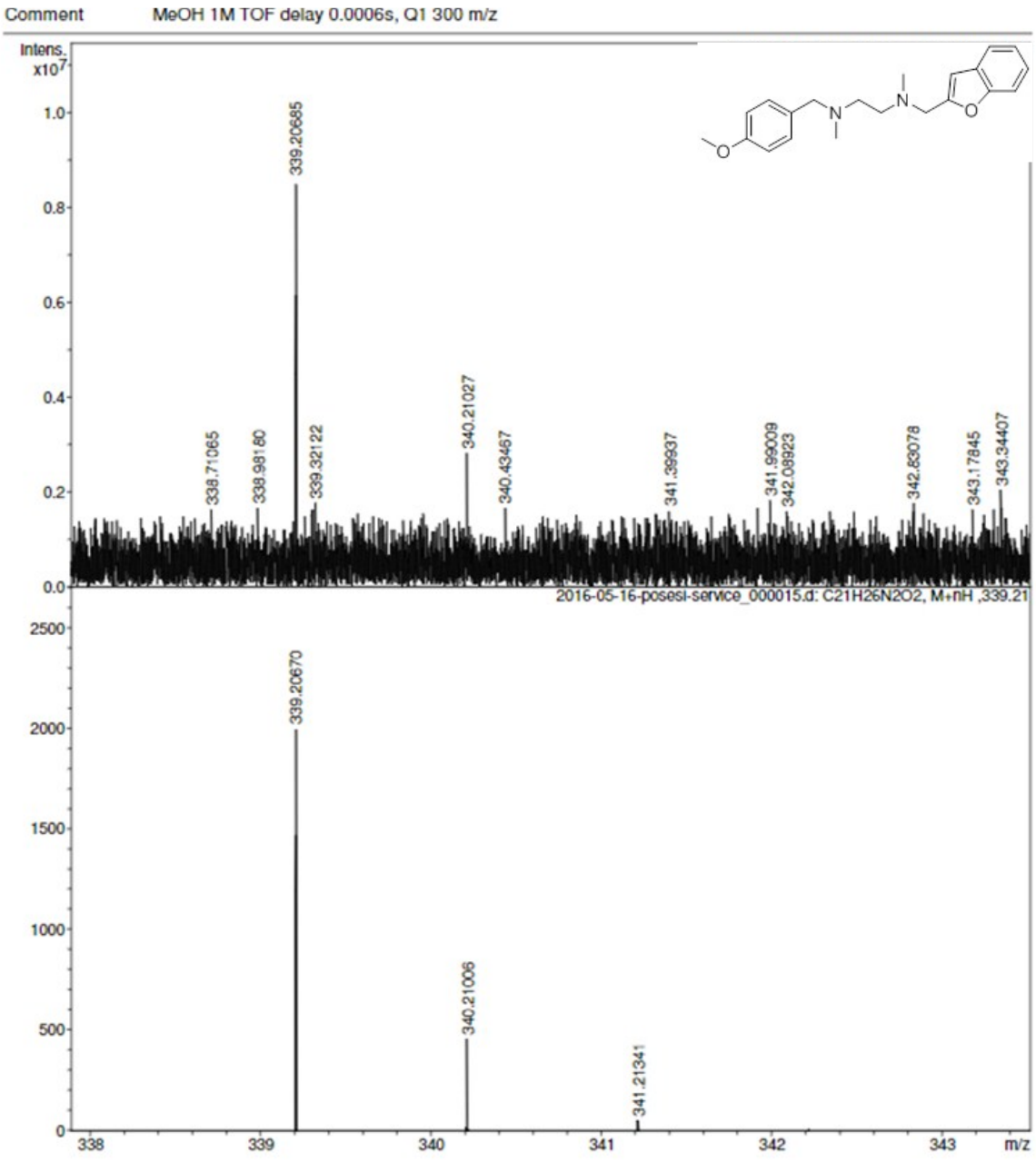
Peak information

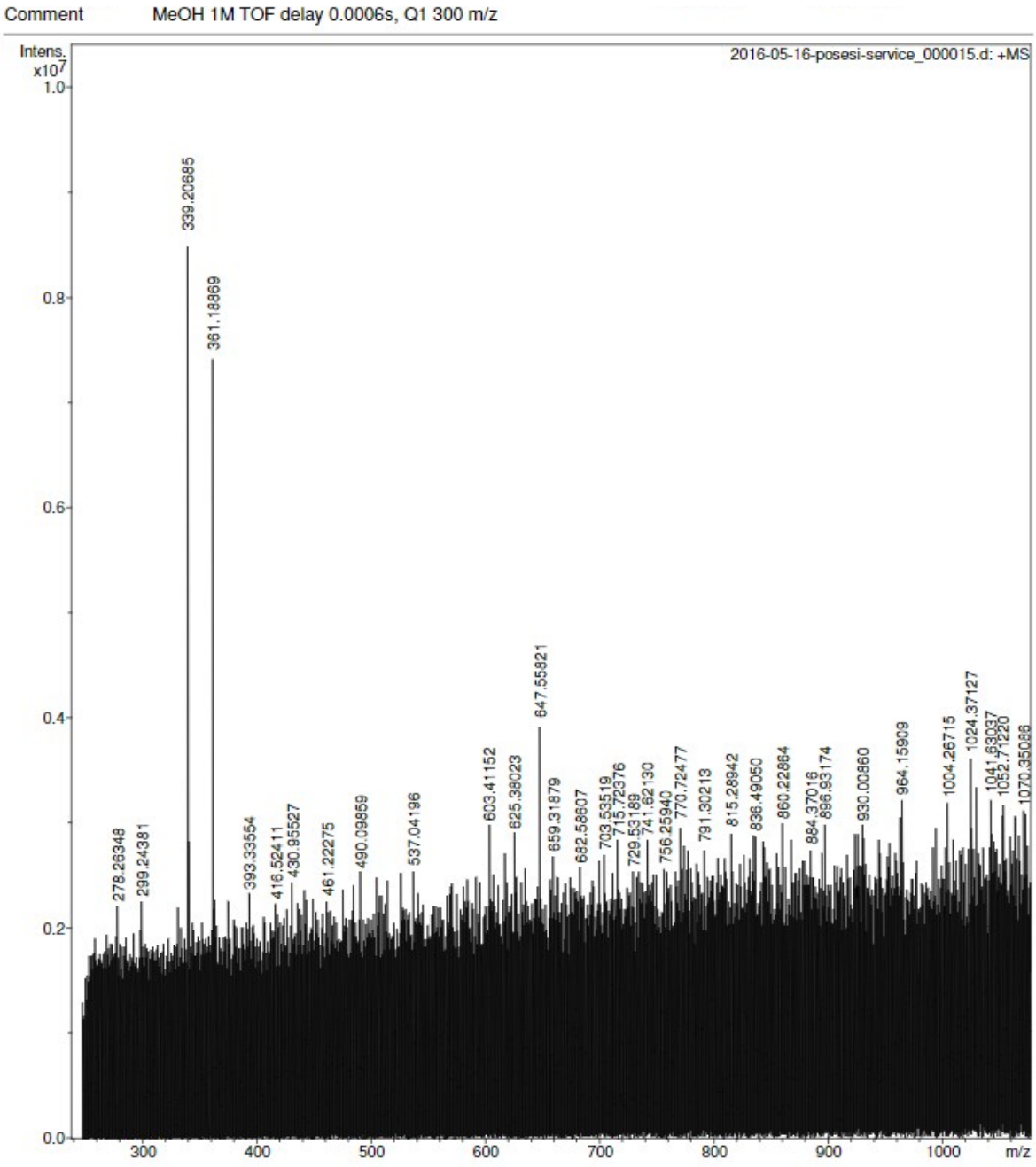
	RT	Area	% Area
1	18.961	14768109	99.83
2	21.555	25625	0.17

26c - HRMS


Intens.
x10^6
2.5
2.0
1.5
1.0
0.5
0.0
347.17299
647.55
213.36739
237.83573
271.10508
296.19210
325.19108
361.75935
393.20938
408.32339
437.19347
451.25148
466.53554
481.26191
495.27776
510.27289
525.28802
539.30407
569.31443
583.32982
595.38194
605.42364
627.35645
683.43427
711.35220
721.47110
749.38272
771.89708
826.26043
853.55047
879.64243
918.24648
947.33083
200
300
400
500
600
700
800
900
m/z
+MS, 0.0-0.1min #(2-4)
343.89683
344.11850
345.74712
346.03319
346.25841
347.17299
347.62182
348.17619
348.95723
349.35697
351.29178
C20H24N2O2, M+nNa ,347.17
3000
2000
1000
0
347.17300
348.17635
349.17971
344
345
346
347
348
349
350
351
352
m/z

26d - HRMS


Comment
MeOH 1M TOF delay 0.0006s, Q1 300 m/z
Intens.
x10^7
339.20685
338.71065
338.98180
339.32122
340.21027
340.43467
341.39937
341.99009
342.08923
342.83078
343.17845
343.34407
2016-05-16-posesi-service_000015.d: C21H26N2O2, M+nH ,339.21
339.20670
340.21006
341.21341
m/z



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