Supporting Information

Palladium-Catalyzed Oxidative C-H Bond Coupling of Steered Acetanilides and Aldehydes: A Facile Access to *ortho*-Acylacetanilides

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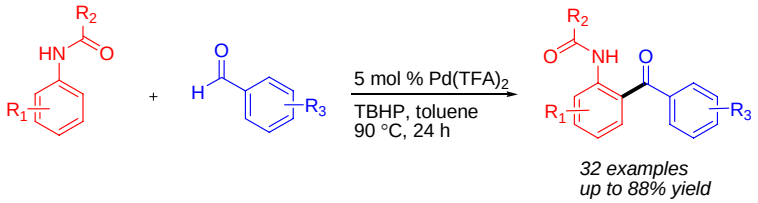

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1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All the reactions were performed in Rotaflo® (England) resealable screw-cap Schlenk flask (approx. 20 mL volume) in the presence of Teflon coated magnetic stirrer bar (4 mm × 10 mm). *N*,*N*-Dimethylformamide (DMF) was distilled under calcium hydride under reduced pressure. Dioxane and toluene were distilled from sodium under nitrogen. *tert*-Butanol was refluxing with sodium and the distillate was stored under CaH_2 and was distilled from calcium hydride under nitrogen prior to use. The concentration of *tert*-butyl hydroperoxide (TBHP) was determined by means of iodometric method which is generally used by commercial supplier (http://www.aladdin-reagent.com/thir.asp?Rea_SubID=15038).[1] *Note:* The TBHP concentration we applied to this study was 70.6%. Thin layer chromatography was performed on Merck precoated silica gel 60 F254 plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. ^{1}H NMR spectra were recorded on a Bruker (400 MHz) spectrometer. Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). Coupling constants (*J*) were reported in Hertz (Hz). High-resolution mass spectra (HRMS) were obtained on a Shimadzu LCMS-IT-TOF. MS spectra were recorded on an Agilent LC – MS 6120 with ESI or APCI. The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from Agilent 6890N GC-FID system. Compounds described in the literatures were characterized by

comparison of their ^{1}H, and/or ^{13}C NMR spectra to the previously reported data.

2. Preparation of substituted acetanilide substrates

All the substituted acetanilides in Table 3 were prepared from their corresponding precursors with Ac_2O in CH_2Cl_2 according to the literature method without modifications.[2]

N-phenylbenzamide, *N*-phenylpivalamide and *N*-phenylisobutyramide were prepared from phenylamine with their corresponding acyl chlorides in pyridine according to the literature method without modifications.[3]

3. General procedures for reaction condition screenings and coupling reactions

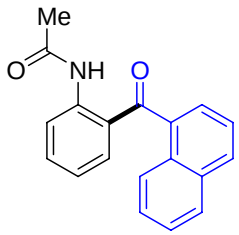
General procedures for screening: The acetanilide (0.135 g, 1.0 mmol) and the metal complex (5 mol% or as indicated in Table 1) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar under air atmosphere. The solvent (2.0 mL) was added into the tube. The solution was stirred for about 1 to 2 minutes until the solid had been dissolved. 4-Chlorobenzaldehyde (2.0 mmol), TBHP (4.0 mmol) were loaded into the tube. The tube was stirred at room temperature for ~5 minutes and then placed into a preheated oil bath (40-120 ^{o}C) for 24 hours. After completion of reaction, the reaction tube was allowed to cool to room temperature. Ethyl acetate (~10 mL), dodecane (114 μL, internal standard) and water (~3 ml) were added. The organic layer was subjected to GC analysis. The GC yield obtained was

previously calibrated by authentic sample/dodecane calibration curve.

General procedure for C-H bond coupling of steered acetanilides and aldehydes: Substituted acetanilide (1.0 mmol) and the $Pd(TFA)_2$ (16.1 mg, 0.05 mmol) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. Toluene (2.0 mL) was added into the tube. The solution was stirred for about 1 to 2 minutes until the solid was dissolved. Substituted benzaldehyde (2.0 mmol), TBHP (4.0 mmol) were loaded into the tube. The tube was stirred at room temperature for ~5 minutes and then placed into a preheated oil bath at 90 ^{o}C for 24 hours. After completion of reaction as judged by GC analysis, the reaction tube was allowed to cool to room temperature and quenched with saturated K_2CO_3 and diluted with EtOAc. The organic layer was separated and the aqueous layer was washed with EtOAc. The filtrate was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired oxidatively coupled product.

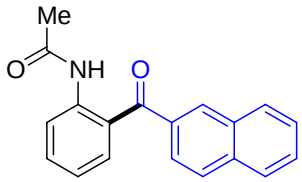
4. Characterization data of coupling products

_N_-(2-(1-Naphthoyl)phenyl)acetamide (3ab)[4]



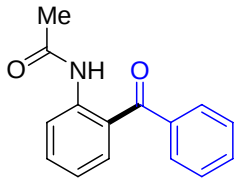
Hexane: EtOAc (1:5); R_f= 0. 4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.49 (s, 1H), 8.69 (d, *J* = 8.5 Hz, 1H), 7.91 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.86 – 7.79 (m, 2H), 7.50 – 7.43 (m, 2H), 7.43 – 7.38 (m, 3H), 7.32 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.92 – 6.79 (m, 1H), 2.20 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.16, 169.66, 141.54, 137.01, 135.39, 134.82, 133.63, 131.21, 130.63, 128.55, 127.41, 127.18, 126.62, 125.31, 124.43, 123.24, 122.19, 120.87, 25.56. ESI-MS $[M+H]^+$ 290.1.

_N_-(2-(2-Naphthoyl)phenyl)acetamide (3ac)[4]



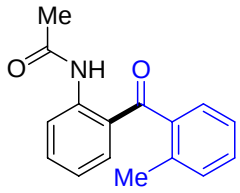
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.79 (s, 1H), 8.66 (d, *J* = 8.3 Hz, 1H), 8.18 (s, 1H), 7.94 (dd, *J* = 12.3, 8.7 Hz, 3H), 7.84 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.68 – 7.54 (m, 4H), 7.15 – 7.07 (m, 1H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ199.38, 172.01, 140.29, 135.94, 135.23, 134.20, 133.49, 132.45, 131.84, 129.55, 128.64, 128.31, 127.83, 127.05, 126.77, 125.42, 122.28, 121.78, 25.25. ESI-MS $[M+H]^+$ 290.1.

_N_-(2-Benzoylphenyl)acetamide(3ad) [5]



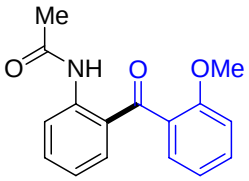
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.81 (s, 1H), 8.60 (d, *J* = 8.2 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.56 (dd, *J* = 15.8, 7.8 Hz, 3H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.33 (m, 1H), 7.08 (s, 1H), 2.21 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ199.75, 169.44, 140.35, 134.28, 133.53, 132.57, 129.92, 128.36, 126.97, 122.18, 121.60, 25.23. ESI-MS $[M+H]^+$ 240.1.

_N_-(2-(2-Methylbenzoyl)phenyl)acetamide (3ae) [4]



Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ11.56 (s, 1H), 8.75 (d, *J* = 8.5 Hz, 1H), 7.56 (dd, *J* = 11.4, 4.3 Hz, 1H), 7.39 (dd, *J* = 9.4, 2.6 Hz, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 2.29 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ202.92, 169.57, 141.54, 139.29, 135.90, 135.32, 134.52, 130.94, 130.25, 127.87, 125.38, 122.46, 122.17, 120.74, 25.55, 19.73. ESI-MS $[M+H]^+$ 254.1.

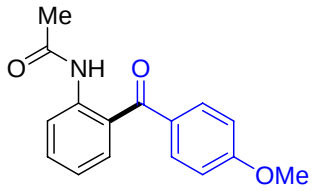
_N_-(2-(2-Methoxybenzoyl)phenyl)acetamide (3af) [6]



Hexane: EtOAc (1:5); R_f=0. 4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.61 (s, 1H), 8.75 (d, *J* = 8.5 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.52 – 7.44 (m, 2H), 7.32 – 7.28 (m, 1H), 7.06 (td,

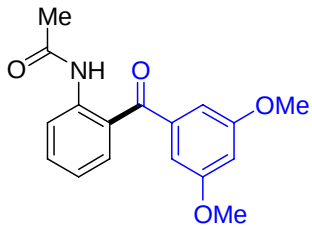
J = 7.5, 0.7 Hz, 1H), 7.04 – 6.97 (m, 2H), 3.77 (d, *J* = 3.4 Hz, 3H), 2.26 (d, *J* = 15.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.62, 169.64, 156.81, 141.29, 135.09, 134.55, 131.99, 129.09, 128.50, 126.95, 122.58, 120.49, 120.47, 111.44, 55.64, 25.55. ESI-MS $[M+H]^+$ 270.1.

_N_-(2-(4-Methoxybenzoyl)phenyl)acetamide (3ag)[4]



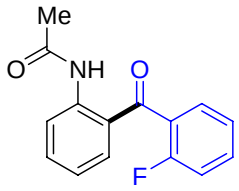
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.44 (s, 1H), 8.47 (d, *J* = 8.6 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.45 (dd, *J* = 10.1, 3.9 Hz, 2H), 7.01 (dd, *J* = 11.3, 3.8 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.89, 169.04, 163.45, 139.80, 133.51, 132.72, 132.61, 130.88, 124.27, 122.07, 121.72, 113.64, 55.52, 25.14. ESI-MS $[M+H]^+$ 270.0.

_N_-(2-(3,5-Dimethoxybenzoyl)phenyl)acetamide (3ah)



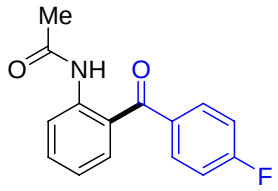
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.69 (s, 1H), 8.53 (d, *J* = 8.3 Hz, 1H), 7.58 – 7.38 (m, 2H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.73 (d, *J* = 2.2 Hz, 2H), 6.60 (t, *J* = 2.2 Hz, 1H), 3.74 (s, 6H), 2.16 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.40, 169.30, 160.55, 140.45, 140.38, 134.37, 133.51, 122.12, 121.54, 107.65, 104.81, 55.62, 25.26. HRMS: calcd. for $C_{17}H_{17}NO_4Na^+$: 322.1055, found 322.1051.

_N_-(2-(2-Fluorobenzoyl)phenyl)acetamide (3ai) [4]



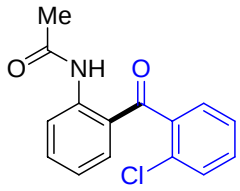
Hexane: EtOAc (1:5), R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ11.36 (s, 1H), 8.75 (d, *J* = 8.5 Hz, 1H), 7.62 – 7.57 (m, 1H), 7.54 (dd, *J* = 6.7, 1.4 Hz, 1H), 7.52 – 7.48 (m, 1H), 7.45 (d, *J* = 7.0 Hz, 1H), 7.31 – 7.25 (m, 1H), 7.20 (d, *J* = 9.4 Hz, 1H), 7.09 – 7.03 (m, 1H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.09, 169.48, 158.4,141.32, 135.57, 134.16, 133.04 (d, J_{CF} = 8.3 Hz), 130.19 (d, J_{CF} = 2.3 Hz), 127.61 (d, J_{CF} = 16.8 Hz), 124.28 (d, J_{CF} = 3.5 Hz), 122.27, 120.79, 116.37 (d, J_{CF} = 21.4 Hz), 25.52. ESI-MS [M+H]+ 258.1.

_N_-(2-(4-Fluorobenzoyl)phenyl)acetamide (3aj) [4]



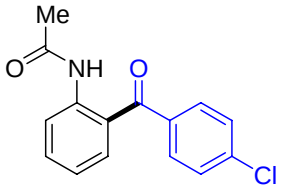
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.65 (s, 1H), 8.61 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.74 (m, 2H), 7.64 – 7.49 (m, 2H), 7.19 (t, *J* = 8.6 Hz, 2H), 7.11 (s, 1H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.81, 169.09, 166.53, 164.00, 140.06, 134.56 (d, J_{CF} = 3.1 Hz), 132.90, 132.49 (d, J_{CF} = 9.2 Hz), 127.57 (d, J_{CF} = 155.5 Hz), 123.30, 121.88 (d, J_{CF} = 43.1 Hz), 115.43 (d, J_{CF} = 22.0 Hz), 25.07. ESI-MS $[M+H]^+$ 258.1.

_N_-(2-(2-Chlorobenzoyl)phenyl)acetamide (3ak) [4]



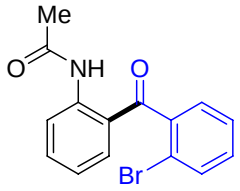
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ11.56 (s, 1H), 8.86 – 8.74 (m, 1H), 7.60 (s, 1H), 7.51 – 7.45 (m, 2H), 7.38 (ddd, *J* = 5.5, 3.3, 1.7 Hz, 2H), 7.33 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.06 – 6.99 (m, 1H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.27, 169.65, 141.92, 138.74, 135.95, 134.60, 131.20, 130.94, 130.14, 128.65, 126.75, 122.28, 121.27, 120.64, 25.63. ESI-MS $[M+H]^+$ 290.1.

_N_-(2-(4-Chlorobenzoyl)phenyl)acetamide (3al) [4]



Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.70 (s, 1H), 8.62 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.49 (dd, *J* = 13.5, 8.1 Hz, 3H), 7.10 (t, *J* = 7.6 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.92, 168.10, 138.62, 137.81, 135.07, 133.14, 131.21, 130.29, 127.94, 126.01, 123.24, 122.25, 23.99. ESI-MS $[M+H]^+$ 290.1.

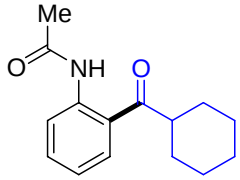
_N_-(2-(2-Bromobenzoyl)phenyl)acetamide (3am) [4]



Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.54 (s, 1H), 8.80 (d, *J* = 8.5 Hz, 1H), 7.65 (dd, *J* = 7.9, 0.9 Hz, 1H), 7.57 (dd, *J* = 11.4, 4.2 Hz, 1H), 7.39 –

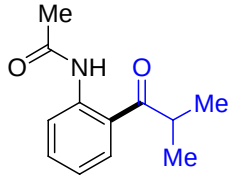
7.32 (m, 3H), 7.30 – 7.28 (m, 1H), 7.03 – 6.98 (m, 1H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ199.88, 169.63, 142.03, 140.83, 135.94, 134.68, 133.23, 131.23, 128.56, 127.28, 122.27, 120.98, 120.64, 119.25, 25.62. ESI-MS $[M+H]^+$ 318.0.

_N_-(2-(Cyclohexanecarbonyl)phenyl)acetamide (3an) [7]



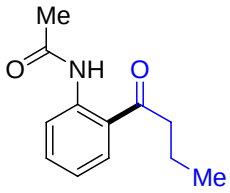
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ11.76 (s, 1H), 8.73 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.9 Hz, 1H), 7.12 (t, *J* = 7.7 Hz, 1H), 3.34 (t, *J* = 11.2 Hz, 1H), 2.23 (s, 3H), 1.88 (d, *J* = 6.8 Hz, 4H), 1.46 (ddd, *J* = 38.2, 20.3, 12.3 Hz, 4H), 1.32 – 1.20 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.62, 169.50, 141.41, 134.73, 130.49, 122.28, 121.09, 120.74, 46.67, 29.85, 25.89, 25.82, 25.58. ESI-MS $[M+H]^+$ 246.1.

_N_-(2-*iso*-Butyrylphenyl)acetamide (3ao)[4]



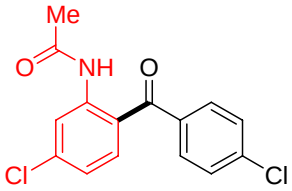
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.74 (s, 1H), 8.74 (dd, *J* = 8.5, 0.8 Hz, 1H), 7.93 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.64 – 7.47 (m, 1H), 7.18 – 7.03 (m, 1H), 3.75 – 3.57 (m, 1H), 2.24 (s, 3H), 1.23 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ209.28, 169.53, 141.45, 134.81, 130.55, 122.31, 121.11, 120.63, 36.26, 25.58, 19.52. ESI-MS $[M+H]^+$ 206.1.

_N_-(2-Butyrylphenyl)acetamide (3ap) [8]



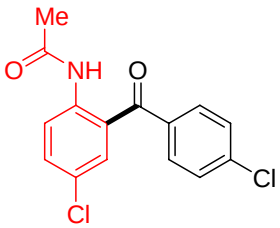
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.76 (s, 1H), 8.73 (d, *J* = 8.4 Hz, 1H), 7.92 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.61 – 7.48 (m, 1H), 7.15 – 7.03 (m, 1H), 3.00 (t, *J* = 7.3 Hz, 2H), 2.24 (s, 3H), 1.76 (dd, *J* = 14.7, 7.4 Hz, 2H), 1.02 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ205.11, 169.60, 140.95, 134.85, 130.74, 122.30, 121.57, 120.83, 41.88, 25.56, 17.98, 13.80. ESI-MS $[M+H]^+$ 206.1.

_N_-(5-Chloro-2-(4-chlorobenzoyl)phenyl)acetamide (3bl)



Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.87 (s, 1H), 8.75 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.07 (dd, *J* = 8.5, 2.0 Hz, 1H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ197.62, 169.28, 141.63, 141.03, 139.23, 136.65, 134.29, 131.15, 128.83, 122.36, 121.42, 120.79, 25.31. HRMS: calcd. for $C_{15}H_{11}NO_2Cl_2Na^+$: 330.0065, found 330.0059.

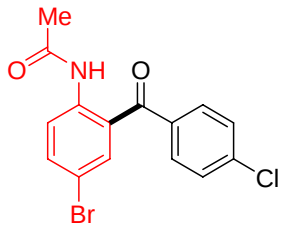
_N_-(4-Chloro-2-(4-chlorobenzoyl)phenyl)acetamide (3cl)[9]



Hexane: EtOAc (1:3); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.52 (s, 1H), 8.60 (d, *J* = 9.0 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.56 – 7.45 (m, 4H), 2.23 (s, 3H); ^{13}C

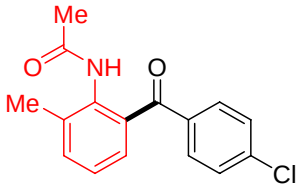
NMR (101 MHz, $CDCl_3$) δ195.92, 167.80, 139.06, 137.79, 135.35, 133.14, 131.21, 130.29, 127.94, 126.30, 123.31, 122.25, 24.19. ESI-MS $[M+H]^+$ 308.1.

_N_-(4-Bromo-2-(4-chlorobenzoyl)phenyl)acetamide (3dl)[10]



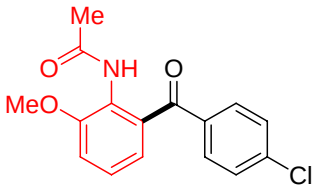
Hexane: EtOAc (1:3); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.52 (s, 1H), 8.54 (d, *J* = 9.0 Hz, 1H), 7.69 – 7.63 (m, 3H), 7.61 (d, *J* = 2.3 Hz, 1H), 7.53 – 7.49 (m, 2H), 2.22 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ196.94, 169.13, 139.65, 139.29, 137.06, 136.08, 135.12, 131.32, 128.97, 124.68, 123.51, 114.68, 25.24. ESI-MS $[M+H]^+$ 352.0.

_N_-(2-(4-Chlorobenzoyl)-6-methylphenyl)acetamide(3el)



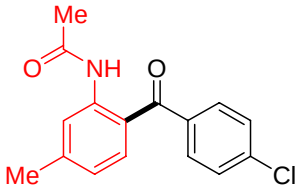
Hexane: EtOAc (1:3); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.89 – 7.82 (m, 2H), 7.44 – 7.37 (m, 2H), 7.16 (t, *J* = 8.0 Hz, 1H), 6.99 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.90 (dd, *J* = 7.7, 1.1 Hz, 1H), 3.84 (s, 3H), 2.03 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ193.87, 168.20, 151.78, 138.94, 135.41, 133.54, 131.76, 128.38, 124.91, 123.78, 120.92, 112.84, 55.93, 23.58. HRMS: calcd. for $C_{16}H_{14}NO_2ClNa^+$: 310.0611, found 310.0605.

_N_-(2-(4-Chlorobenzoyl)-6-methoxyphenyl)acetamide(3fl)



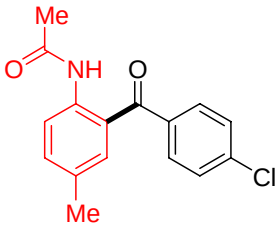
Hexane: EtOAc (1:3), R_f=0.4; 1H NMR (400 MHz, $CDCl_3$)δ 8.73 (s, 1H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.24 – 7.20 (m, 1H), 7.06 (d, *J* = 5.0 Hz, 2H), 2.12 (s, 3H), 1.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.39, 168.96, 139.61, 135.52, 135.39, 134.02, 133.89, 131.94, 128.58, 127.34, 125.30, 77.46, 77.14, 76.82, 23.18, 18.47. HRMS: calcd. for $C_{16}H_{14}NO_3ClNa^+$: 326.0560, found 326.0557.

_N_-(2-(4-Chlorobenzoyl)-5-methylphenyl)acetamide (3gl)



Hexane: EtOAc (1:2); R_f=0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.90 (s, 1H), 8.49 (s, 1H), 7.64 – 7.58 (m, 2H), 7.51 – 7.43 (m, 2H), 7.40 (d, *J* = 8.1 Hz, 1H), 6.89 (dd, *J* = 8.0, 0.8 Hz, 1H), 2.43 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ194.06, 168.08, 142.33, 137.12, 136.27, 131.21, 131.10, 130.12, 128.71, 128.19, 124.67, 123.50, 23.13, 21.04. HRMS: calcd. for $C_{16}H_{14}NO_2ClNa^+$: 310.0611, found 310.0613.

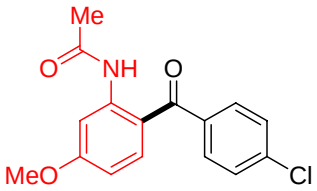
_N_-(2-(4-Chlorobenzoyl)-4-methylphenyl)acetamide (3hl)



Hexane: EtOAc (1:3), R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.74 (s, 1H), 8.61 (d, *J*

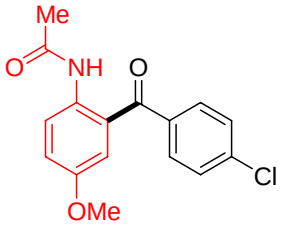
= 8.4 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.31 (s, 1H), 7.09 (t, *J* = 7.6 Hz, 1H), 2.46 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ199.36, 169.22, 143.53, 140.19, 135.82, 133.97, 133.29, 130.23, 129.04, 123.68, 122.05, 121.58, 25.27, 21.67. HRMS: calcd. for $C_{16}H_{14}NO_2ClNa^+$: 310.0611, found 310.0619.

_N_-(2-(4-Chlorobenzoyl)-5-methoxyphenyl)acetamide (3il)



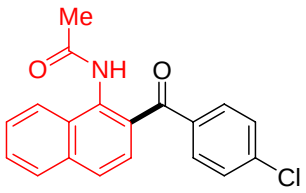
Hexane: EtOAc (1:3); R_f=0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.48 (s, 1H), 8.40 (d, *J* = 2.6 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.51 – 7.44 (m, 3H), 6.59 (dd, *J* = 8.9, 2.6 Hz, 1H), 3.92 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.62, 169.66, 164.84, 143.91, 138.10, 137.75, 135.93, 130.78, 128.59, 115.21, 109.11, 104.88, 55.71, 25.57. HRMS: calcd. for $C_{16}H_{14}NO_3ClNa^+$: 326.0560, found 326.0552.

_N_-(2-(4-Chlorobenzoyl)-4-methoxyphenyl)acetamide (3jl)



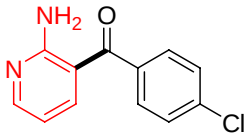
Hexane: EtOAc (1:3); R_f=0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.46 (d, *J* = 9.1 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.15 (dd, *J* = 9.1, 3.0 Hz, 1H), 6.99 (d, *J* = 3.0 Hz, 1H), 3.77 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ193.21, 167.89, 155.79, 137.38, 135.64, 132.73, 131.27, 131.10, 128.22, 125.77, 117.13, 113.84, 55.42, 22.57. HRMS: calcd. for $C_{16}H_{14}NO_3ClNa^+$: 326.0560, found 326.0563.

_N_-(2-(4-Chlorobenzoyl)naphthalen-1-yl)acetamide (3kl)



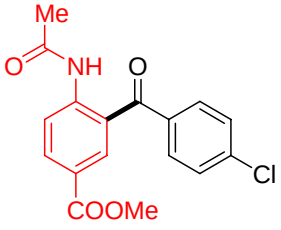
Hexane: EtOAc (1:3); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.95 (dd, *J* = 17.6, 8.3 Hz, 2H), 7.80 (d, *J* = 8.3 Hz, 3H), 7.59 (dd, *J* = 18.0, 6.1 Hz, 2H), 7.53 (s, 2H), 7.46 – 7.42 (m, 2H), 2.19 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ196.86, 169.80, 139.72, 135.35, 134.84, 131.92, 131.36, 130.38, 128.83, 128.65, 128.07, 127.77, 126.88, 125.70, 124.88, 124.18, 23.54. HRMS: calcd. for $C_{19}H_{14}NO_2ClNa^+$: 346.0611, found 346.0603.

(2-Aminopyridin-3-yl)(4-chlorophenyl)methanone (3ll)



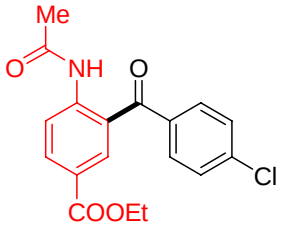
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ9.07 (s, 1H), 8.38 (d, *J* = 8.4 Hz, 1H), 8.19 (s, 1H), 7.91 – 7.84 (m, 2H), 7.81 – 7.70 (m, 1H), 7.45 (d, *J* = *8.6 Hz,* 2H), 7.06 (dd, *J* = 6.9, 5.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.84, 151.49, 147.82, 138.58, 132.71, 129.07, 128.75 120.09, 114.38. HRMS: calcd. for $C_{12}H_9N_2OClNa^+$: 255.0301, found 255.0299.

Methyl 4-acetamido-3-(4-chlorobenzoyl)benzoate (3ml)



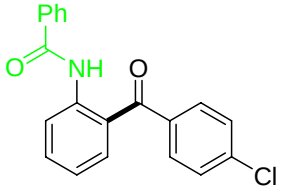
Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.86 (s, 1H), 8.69 (d, *J* = 9.4 Hz, 2H), 8.17 – 8.12 (m, 3H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 3.81 (s, 2H), 2.19 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ196.86, 168.40, 143.23, 138.54, 135.35, 134.41, 133.70, 130.31, 127.95, 127.65, 122.67, 121.09, 120.00, 51.30, 24.40. HRMS: calcd. for $C_{17}H_{14}NO_4ClNa^+$: 354.0509, found 354.0502.

Ethyl 4-acetamido-3-(4-chlorobenzoyl)benzoate (3nl)



Hexane: EtOAc (1:5), R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ10.93 (s, 1H), 8.76 (d, *J* = *9.4 Hz,* 1H), 8.23 (s, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.38 (s, 1H), 4.36 (d, *J* = 7.1 Hz, 2H), 2.27 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.85, 168.36, 143.13, 138.52, 135.36, 134.31, 133.69, 130.32, 127.91, 127.53, 123.05, 121.10, 119.93, 60.26, 24.38, 13.28. HRMS: calcd. for $C_{18}H_{16}NO_4ClNa^+$: 368.0666, found 368.0658.

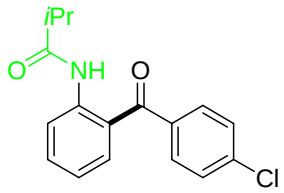
***N*-(2-(4-Chlorobenzoyl)phenyl)benzamide (5)[11]**



Hexane: EtOAc (1:5); R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ11.83 (s, 1H), 8.68 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.57 – 7.52 (m, 5H), 7.46 (d, *J* = 7.4 Hz, 1H), 7.36 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.30 (d, *J* = 4.4 Hz, 1H), 7.26 (d, *J* = 7.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.97, 190.95, 141.06, 138.99,

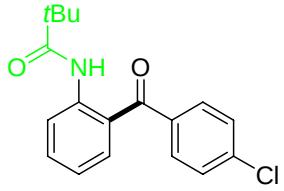
137.00, 134.87, 134.49, 133.70, 132.16, 130.92, 129.47, 128.88, 127.40, 122.86, 122.31, 121.64. ESI-MS $[M+H]^+$ 336.1

_N_-(2-(4-Chlorobenzoyl)phenyl)isobutyramide (6)



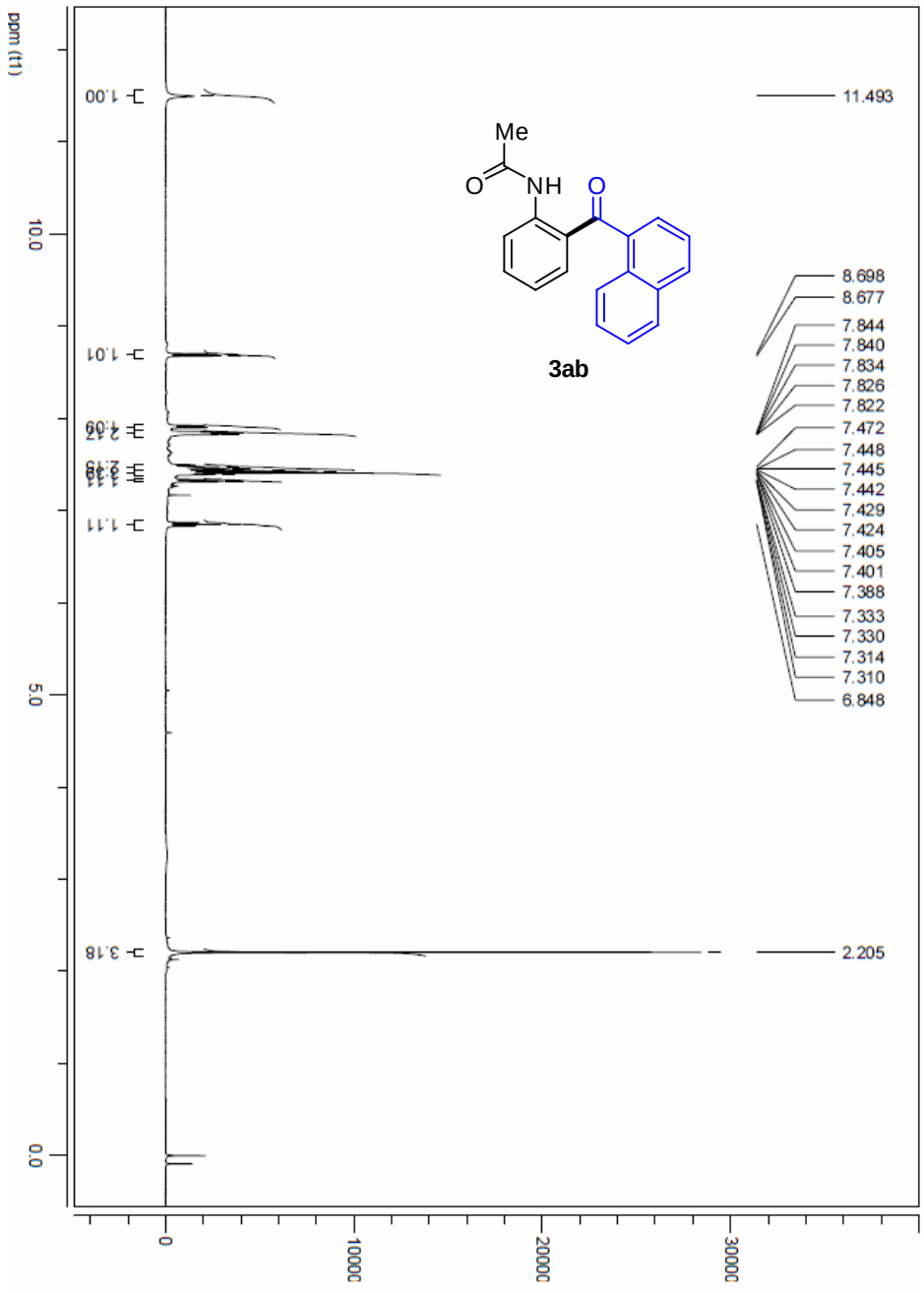
Hexane: EtOAc (1:10); R_f=0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.87 (s, 1H), 8.69 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.58 (s, 1H), 7.55 – 7.53 (m, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.08 (s, 1H), 1.30 (s, 3H), 1.28 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ198.54, 176.56, 140.93, 138.94, 137.03, 134.63, 133.39, 131.40, 128.99, 128.92, 121.98, 121.64, 37.09, 19.50. HRMS: calcd. for $C_{17}H_{16}NO_2ClNa^+$: 324.0767, found 324.0763.

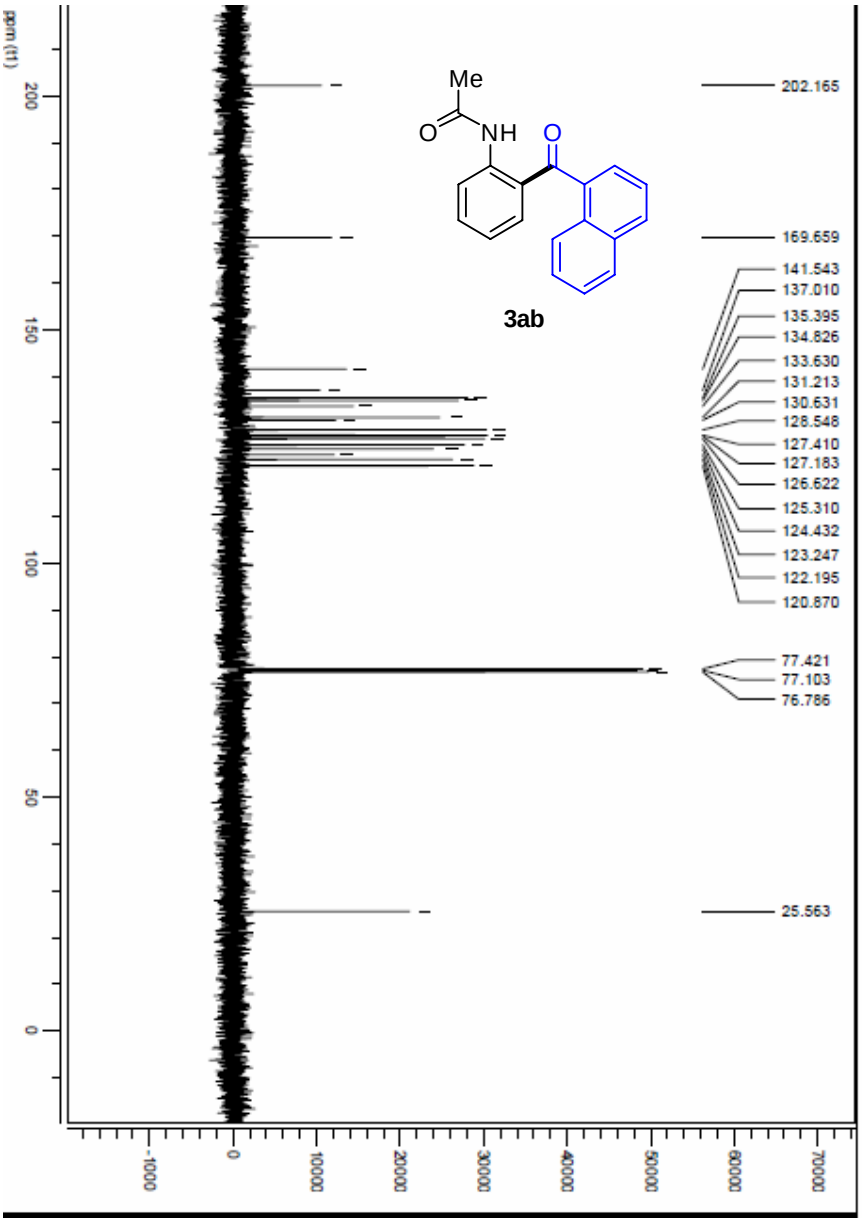
_N_-(2-(4-Chlorobenzoyl)phenyl)pivalamide (7)



Hexane: EtOAc (1:10); R_f=0.3; NMR (400 MHz, $CDCl_3$) δ 11.12 (s, 1H), 8.73 (s, 1H), 8.71 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.60 – 7.56 (m, 2H), 7.48 (s, 1H), 7.10 – 7.07 (m, 1H), 1.35 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.50, 177.74, 141.19, 138.84, 137.09, 134.65, 133.51, 131.29, 128.90, 128.65, 121.92, 121.55, 40.18, 27.79. HRMS: calcd. for $C_{18}H_{18}NO_2ClNa^+$: 338.0924, found 338.0918.

5. ^{1}H and ^{13}C NMR, and HRMS spectra

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141.543
137.010
135.395
134.826
133.630
131.213
130.631
128.548
127.410
127.183
126.622
125.310
124.432
123.247
122.195
120.870
77.421
77.103
76.786
25.563
ppm (t1)
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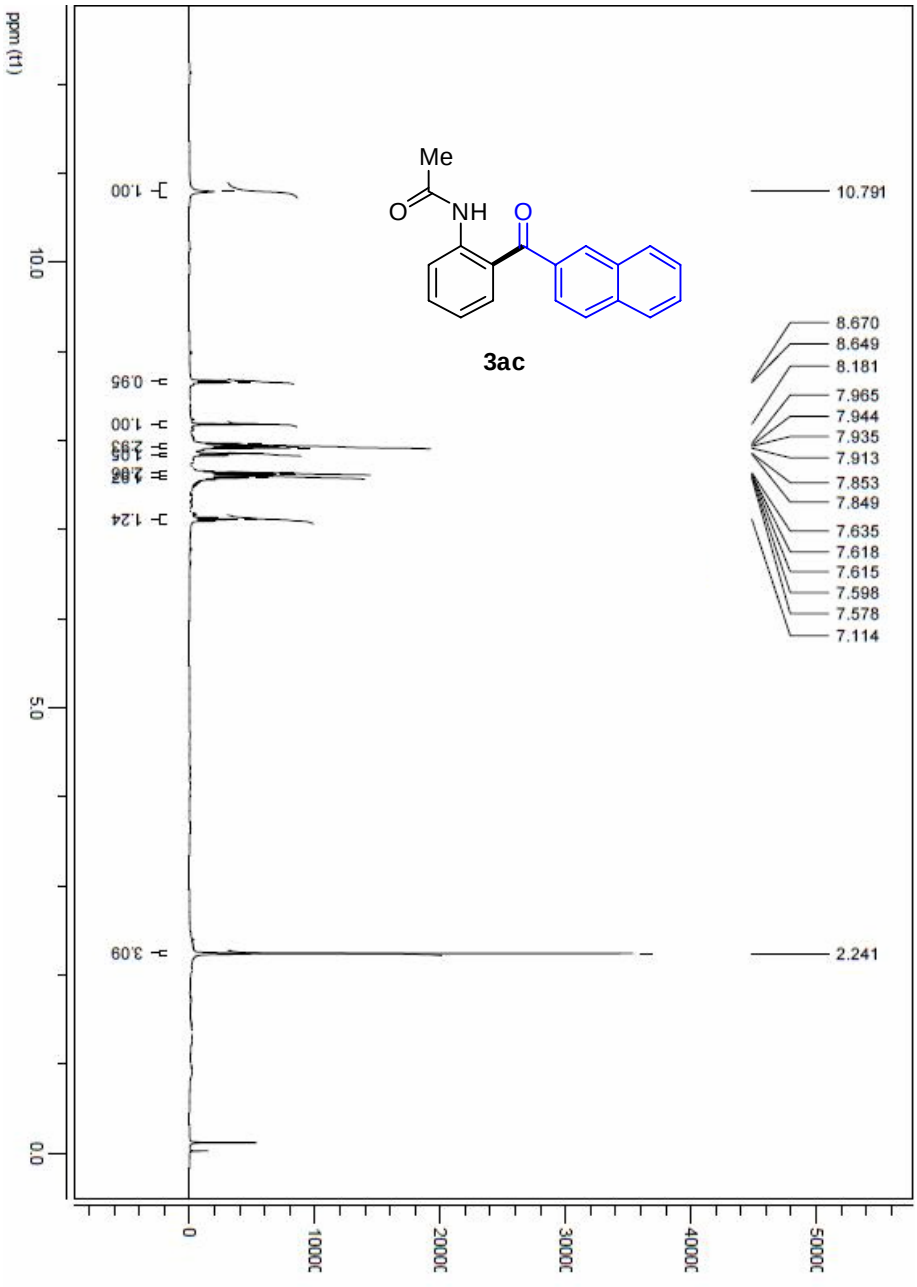
100
50
0
-1000
0
10000
20000
30000
40000
50000
60000
70000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7.849
7.635
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7.615
7.598
7.578
7.114
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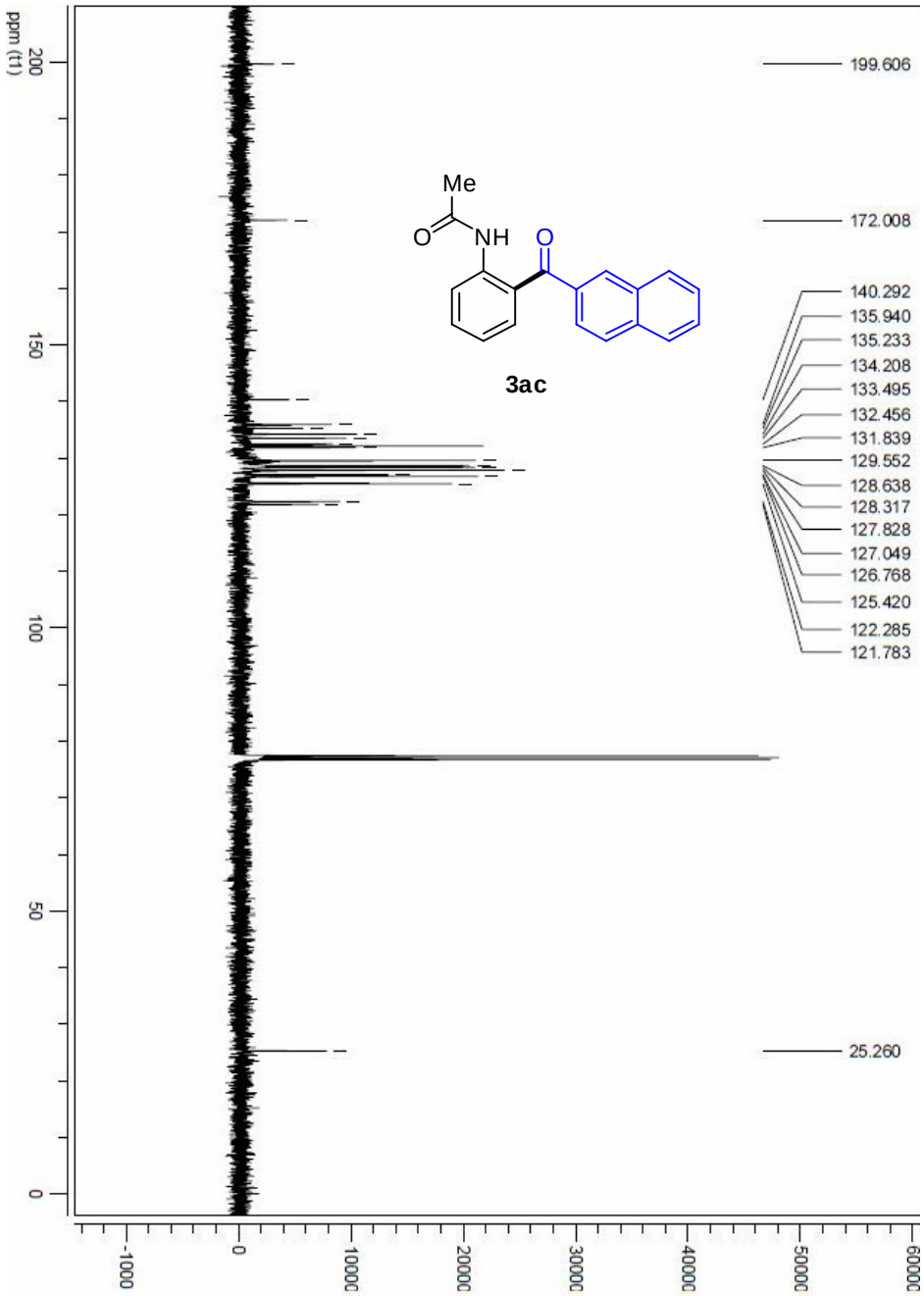
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50000
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135.940
135.233
134.208
133.495
132.456
131.839
129.552
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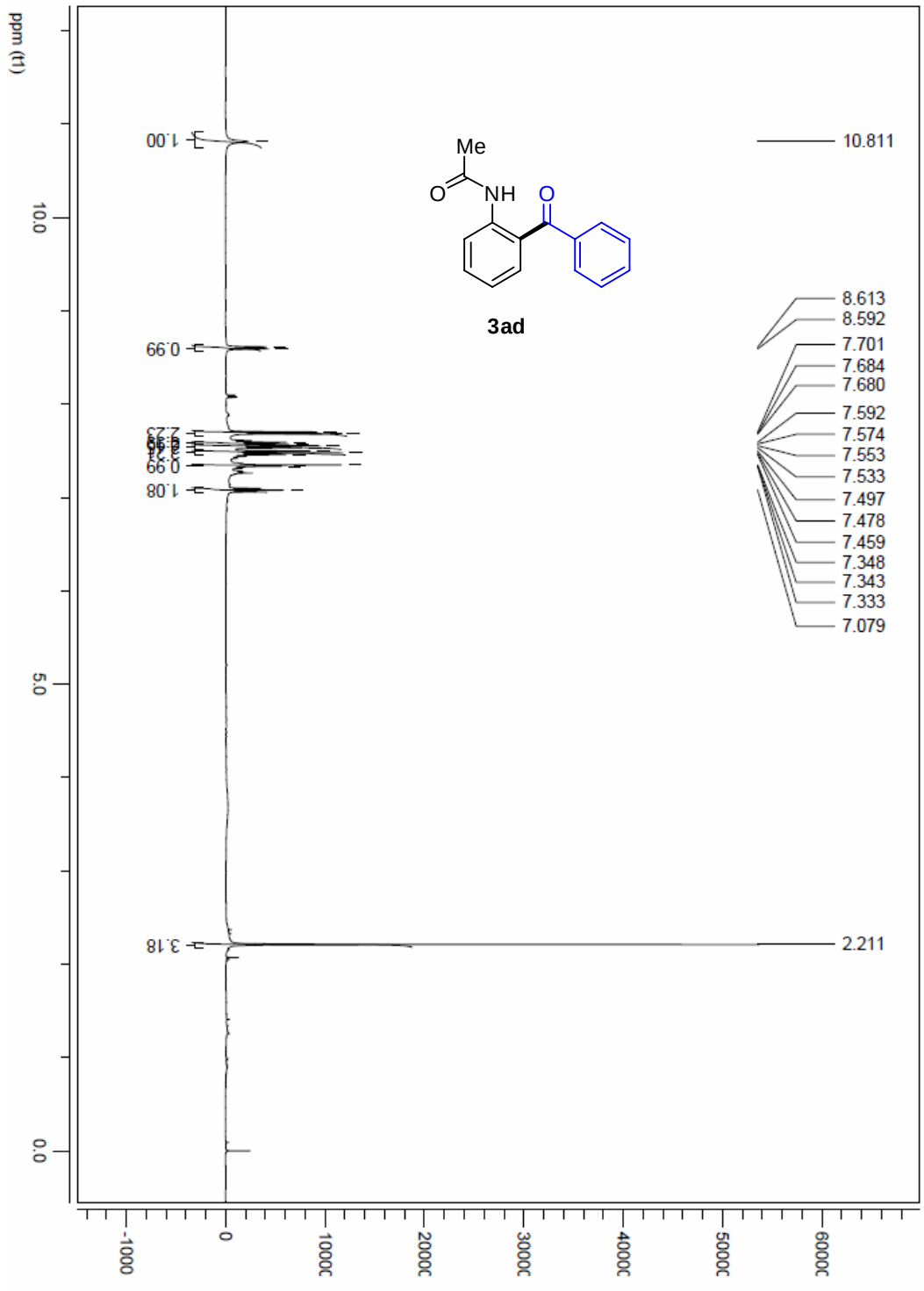
125.420
122.285
121.783
25.260
Me
O
NH
O

3ac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8.592
7.701
7.684
7.680
7.592
7.574
7.553
7.533
7.497
7.478
7.459
7.348
7.343
7.333
7.079
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NH
O
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0
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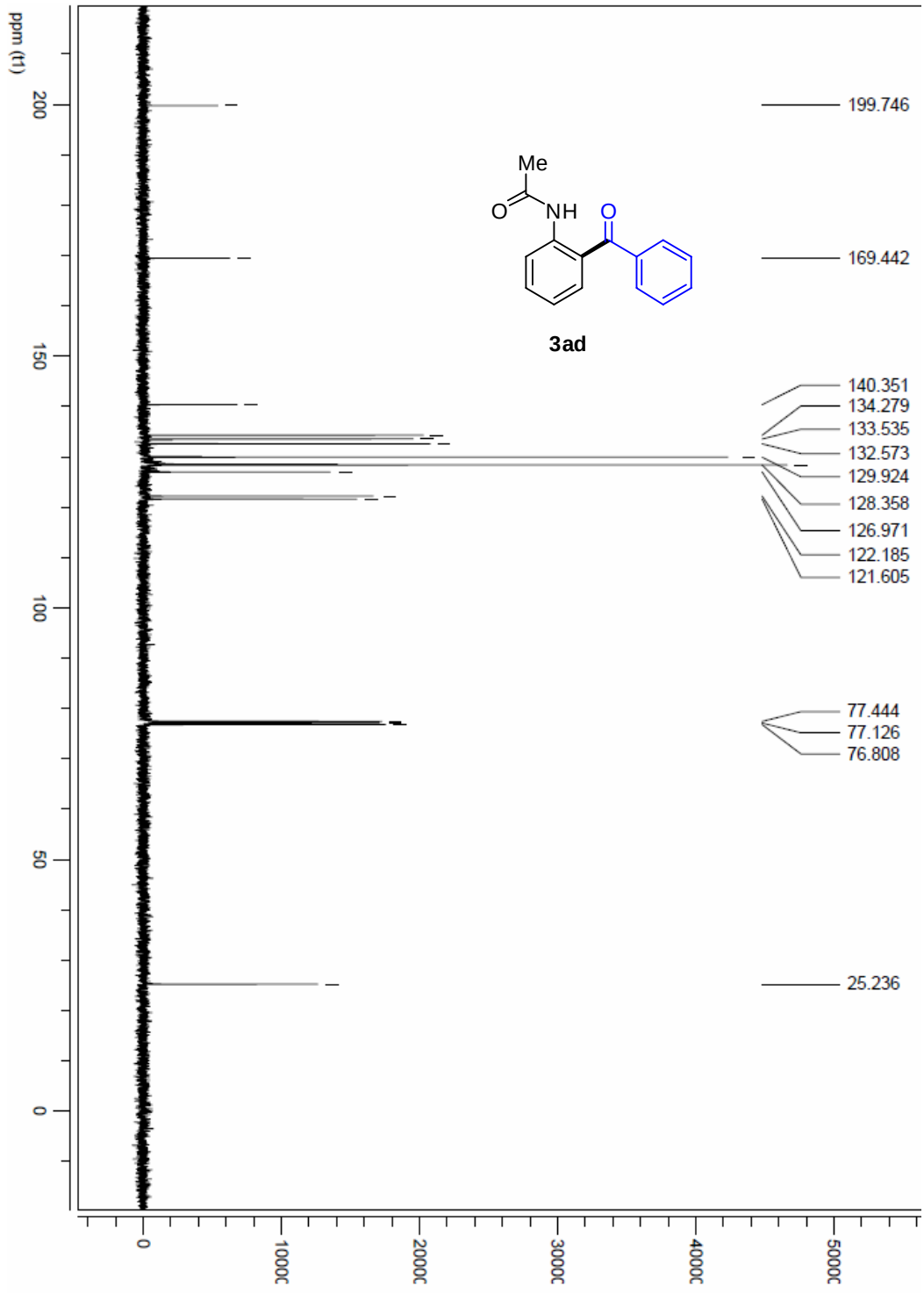
2000
3000
4000
5000
6000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133.535
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126.971
122.185
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76.808
25.236
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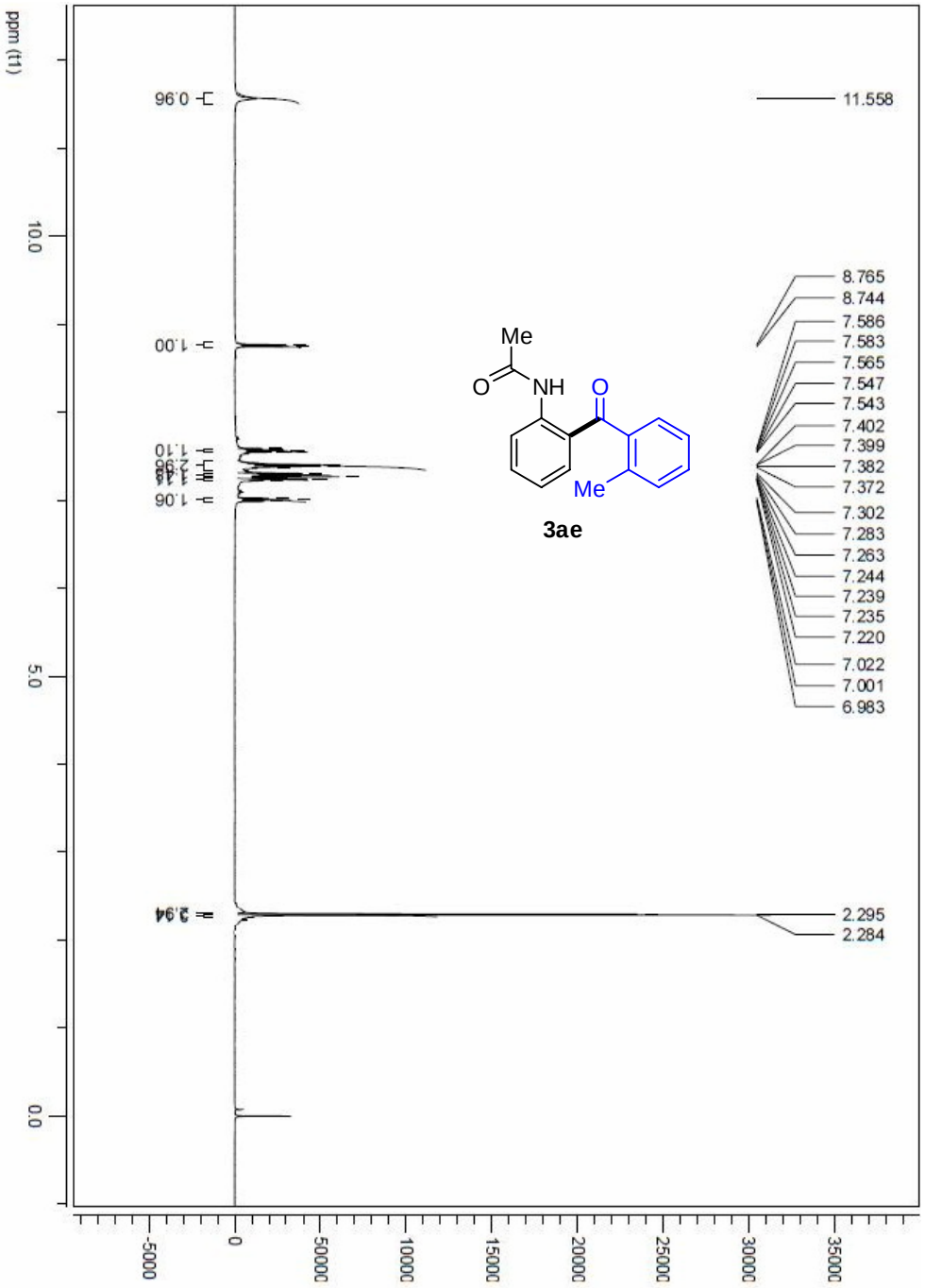
30000
40000
50000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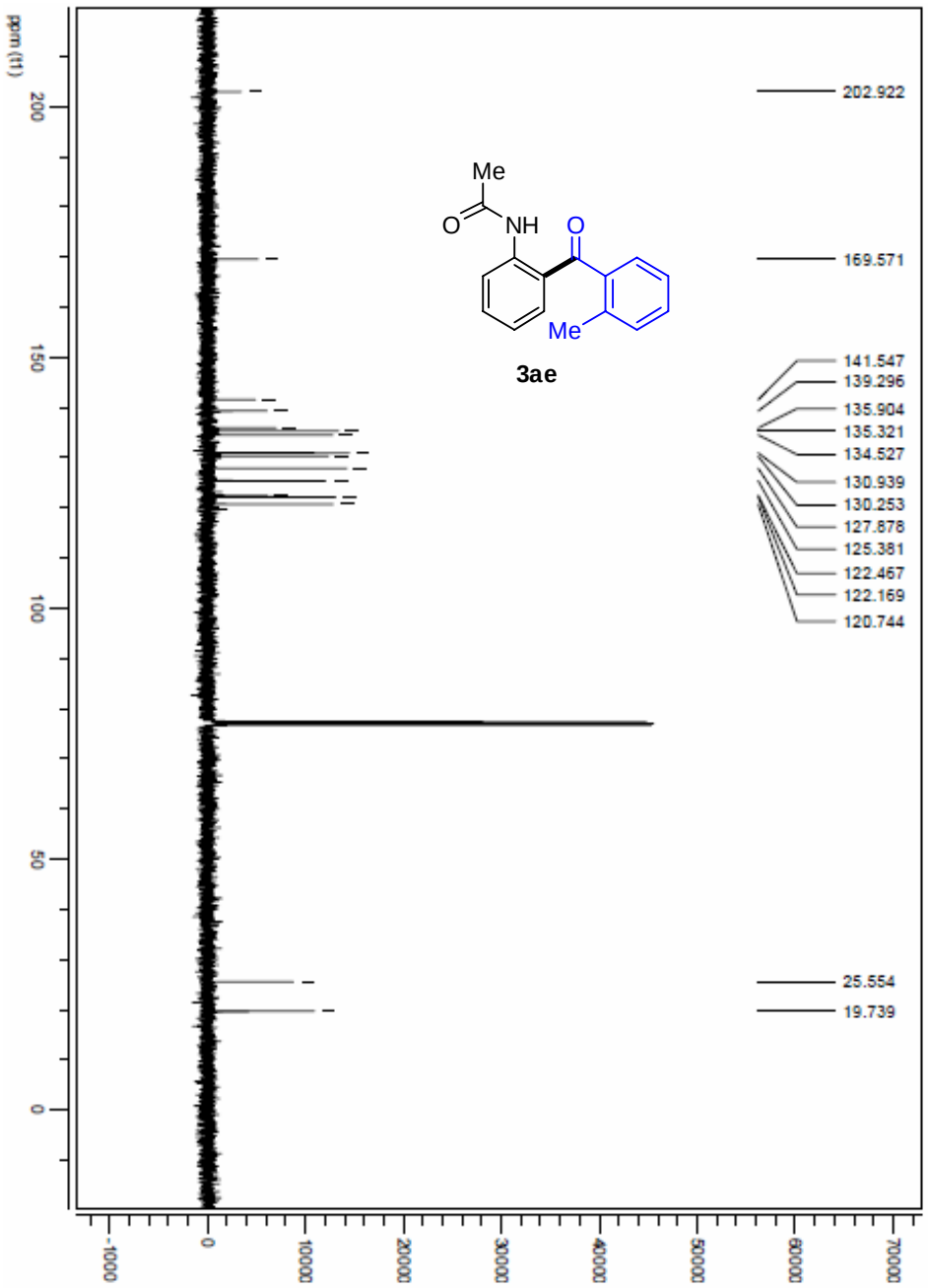
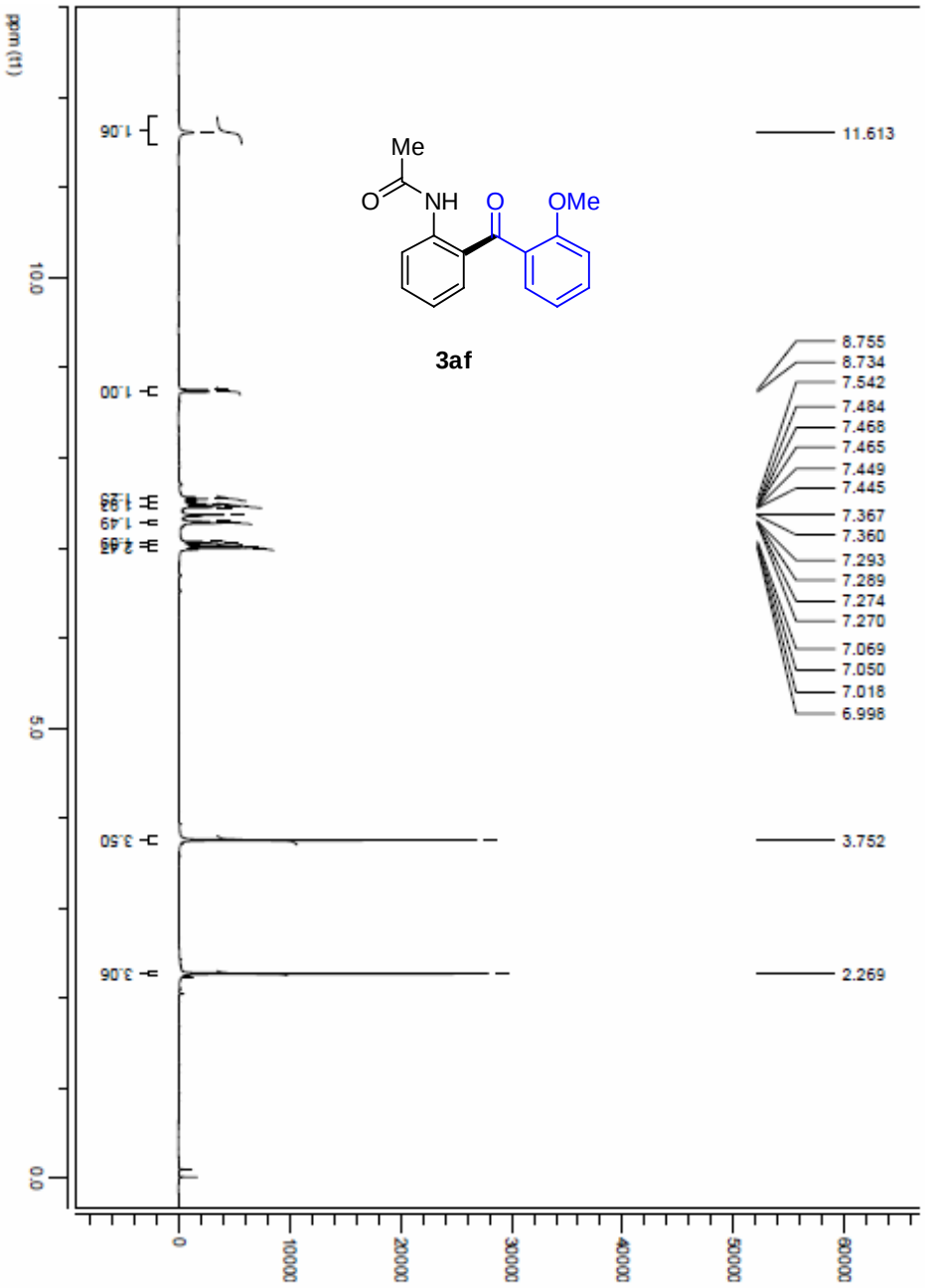
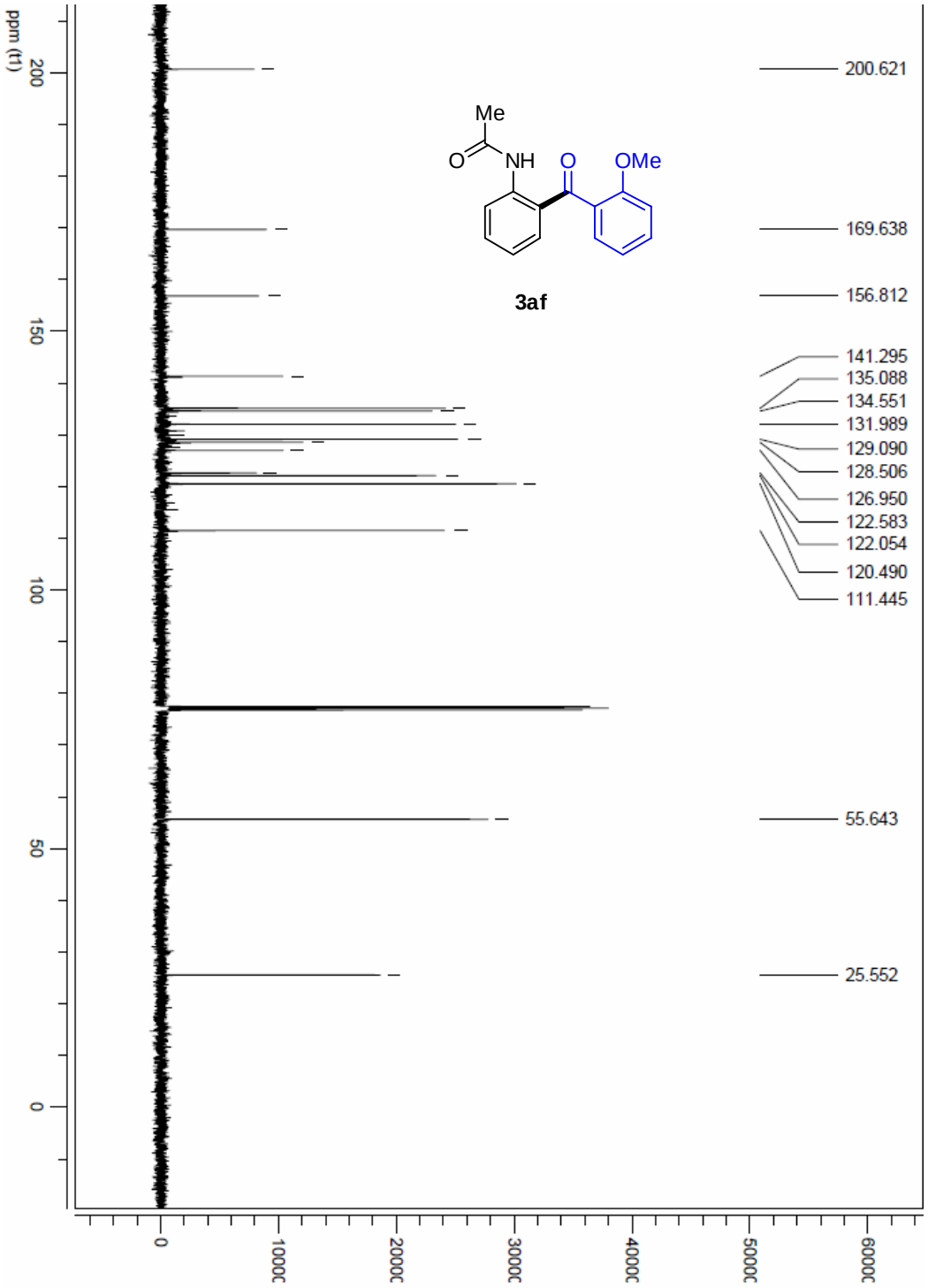
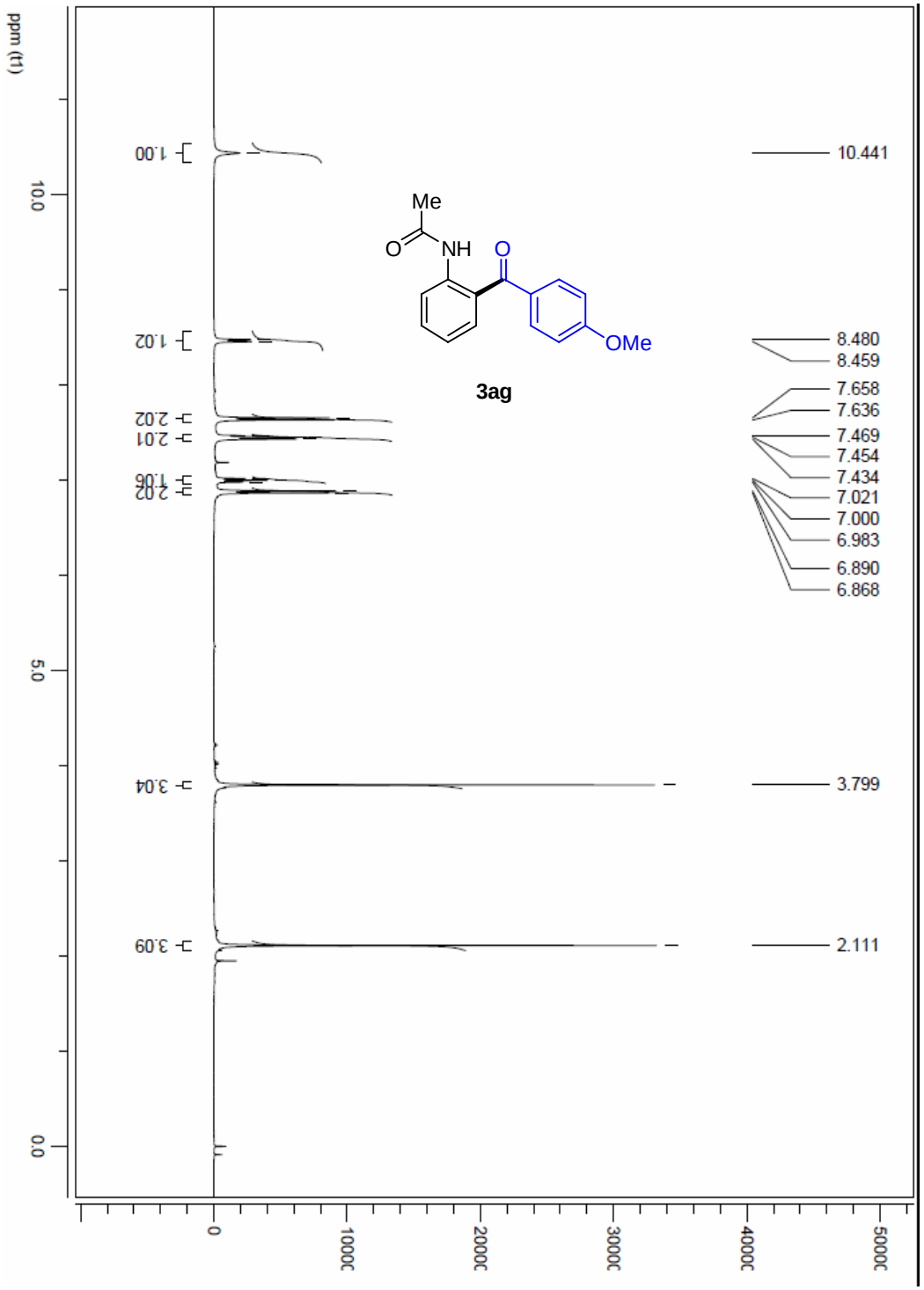
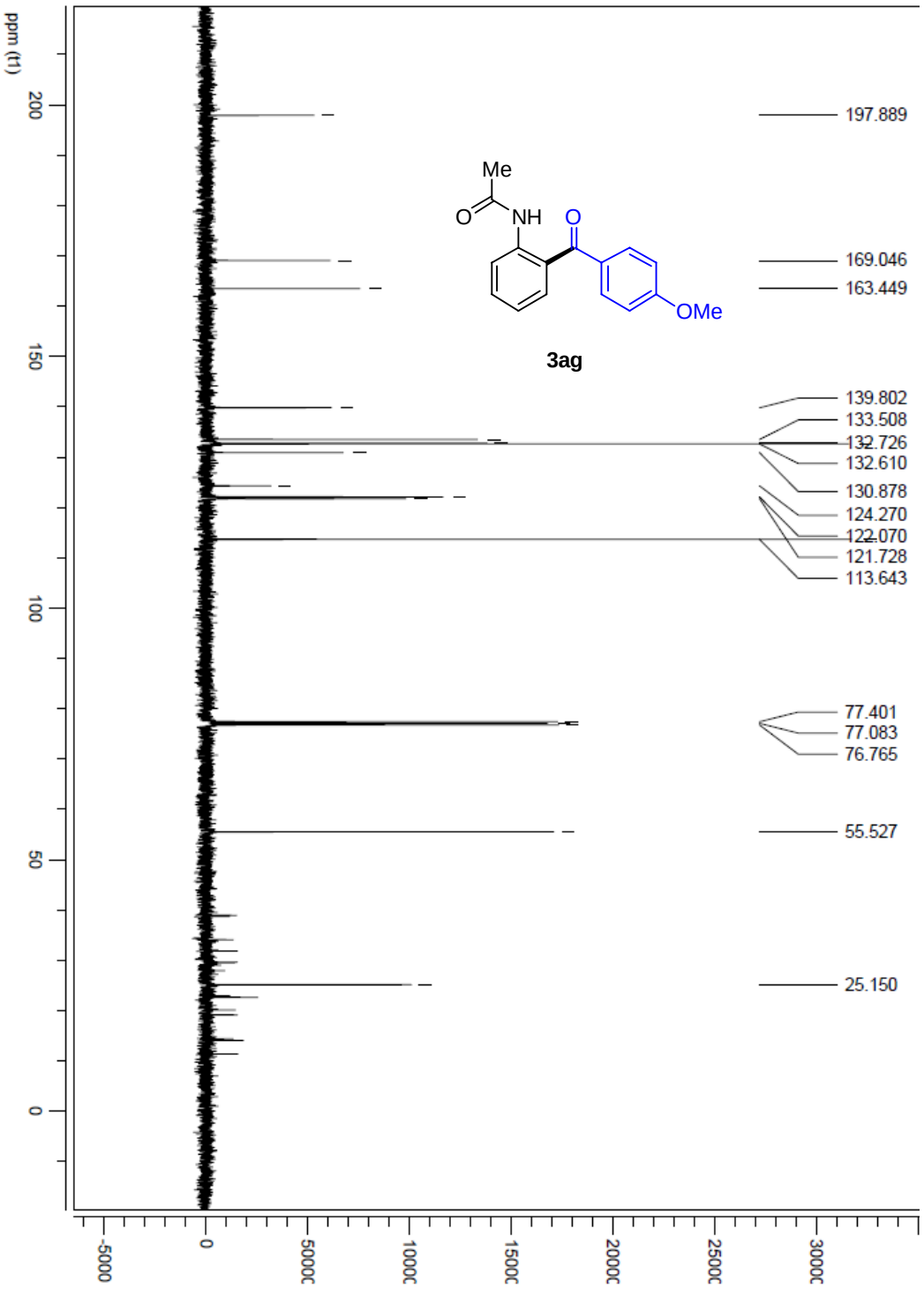
7.547
7.543
7.402
7.399
7.382
7.372
7.302
7.283
7.263
7.244
7.239
7.235
7.220
7.022
7.001
6.983
2.295
2.284
Me
O
NH
O
Me
3ae
-5000
0
50000
10000
15000
20000
25000
30000
35000


ppm (t1)
200
150
100
50
0
-10000
0
10000
20000
30000
40000
50000
60000
70000
Me
O
NH
O
Me
3ae
202.922
169.571
141.547
139.296
135.904
135.321
134.527
130.939
130.253
127.878
125.381
122.467
122.169
120.744
25.554
19.739

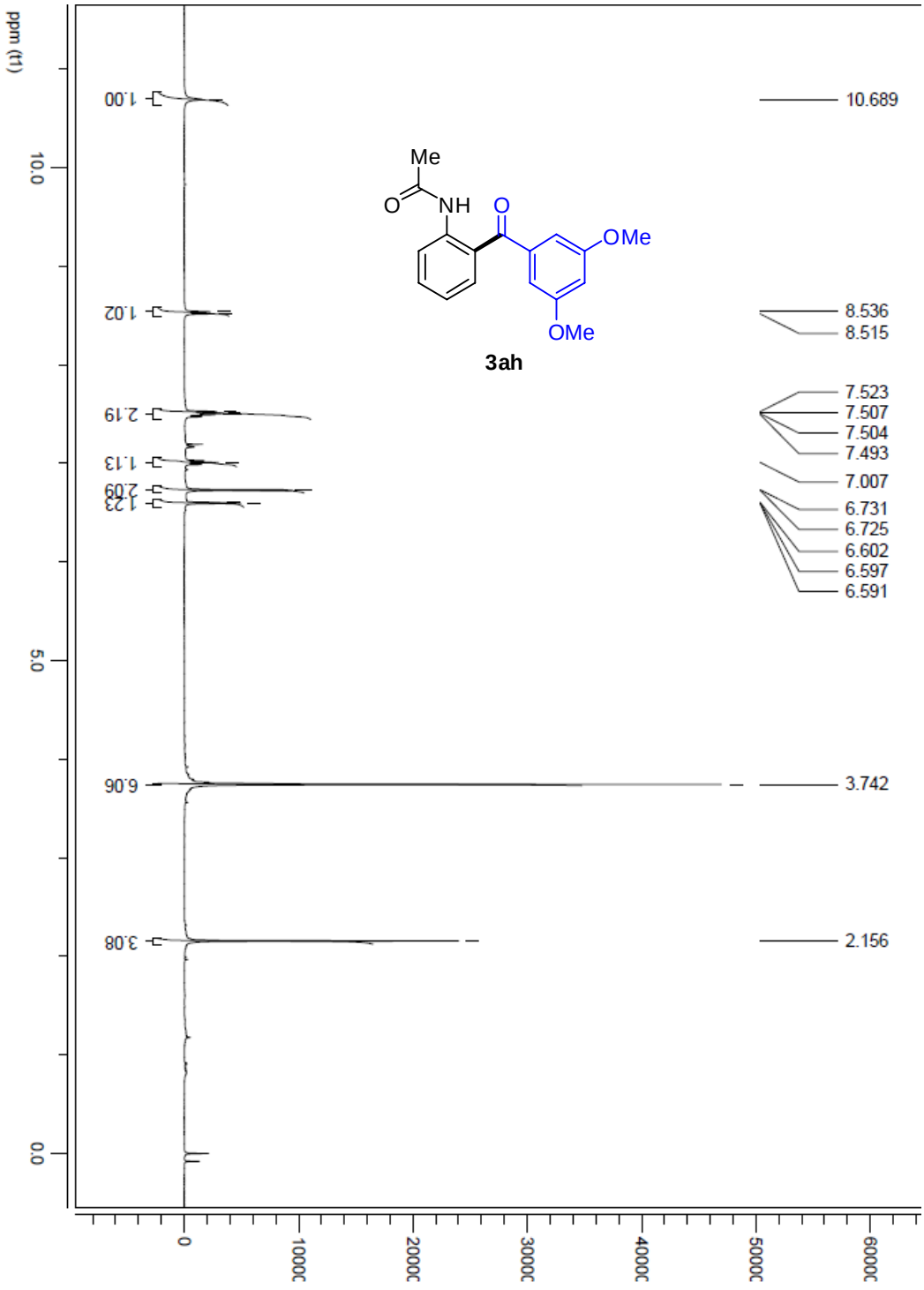

Me
O
NH
O
OMe
3af
11.613
8.755
8.734
7.542
7.484
7.468
7.465
7.449
7.445
7.367
7.360
7.293
7.289
7.274
7.270
7.069
7.050
7.018
6.998
3.752
2.269
1.06
1.00
3.50
3.06
ppm (t1)
10.0
5.0
0.0
0
10000
20000
30000
40000
50000
60000

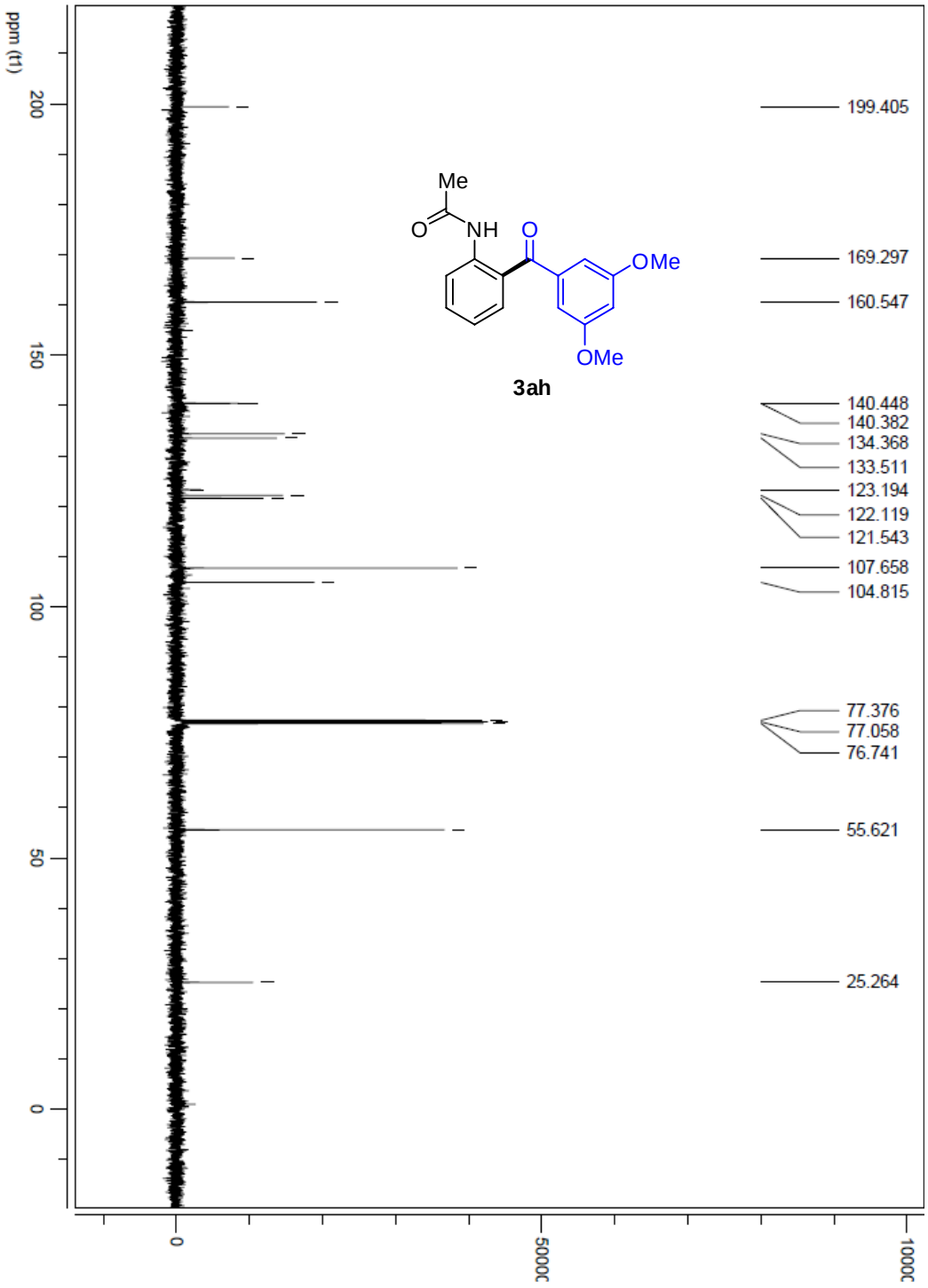

ppm (t1)
200
150
100
50
0
Me
O
NH
O
OMe
3af
200.621
169.638
156.812
141.295
135.088
134.551
131.989
129.090
128.506
126.950
122.583
122.054
120.490
111.445
55.643
25.552
0
10000
20000
30000
40000
50000
60000

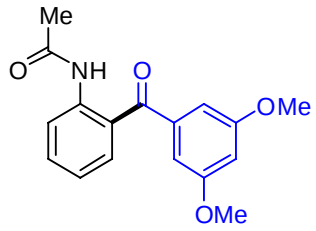

ppm (t1)
10.0
5.0
0.0
1.00
1.02
2.02
2.01
1.06
2.02
3.04
3.09
10.441
8.480
8.459
7.658
7.636
7.469
7.454
7.434
7.021
7.000
6.983
6.890
6.868
3.799
2.111
Me
O
NH
O
OMe
3ag
0
10000
20000
30000
40000
50000


ppm (t1)
200
150
100
50
0
-5000
0
5000
10000
15000
20000
25000
30000
197.889
169.046
163.449
139.802
133.508
132.726
132.610
130.878
124.270
122.070
121.728
113.643
77.401
77.083
76.765
55.527
25.150
Me
O
NH
O
OMe

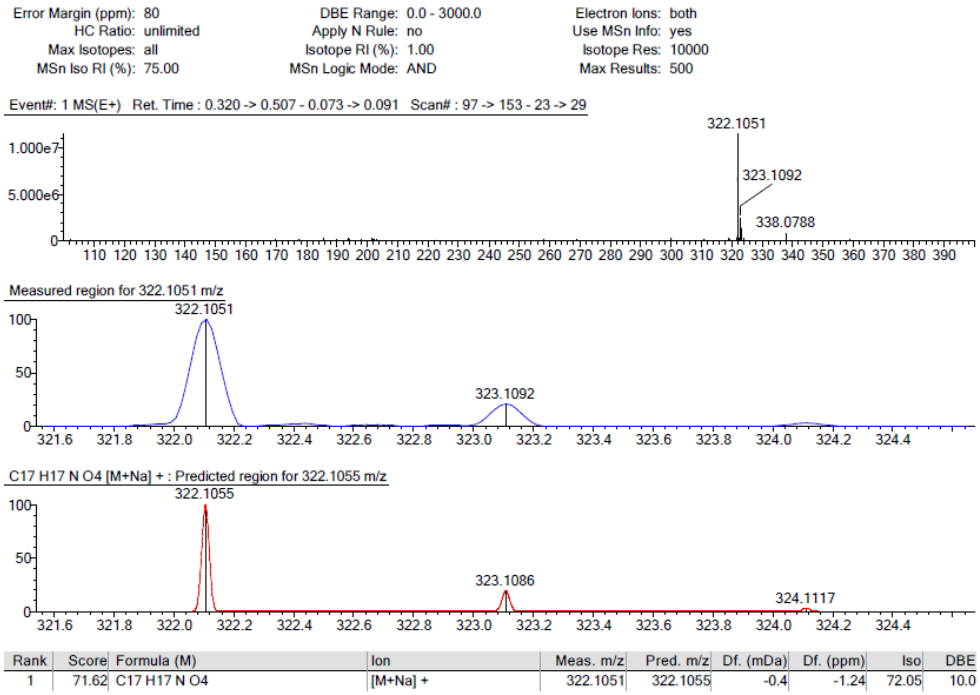
3ag


ppm (t1)
10.0
5.0
0.0
1.00
1.02
2.19
1.13
2.09
1.23
6.06
3.08
0
10000
20000
30000
40000
50000
60000
Me
O
NH
O
OMe
OMe
3ah
10.689
8.536
8.515
7.523
7.507
7.504
7.493
7.007
6.731
6.725
6.602
6.597
6.591
3.742
2.156

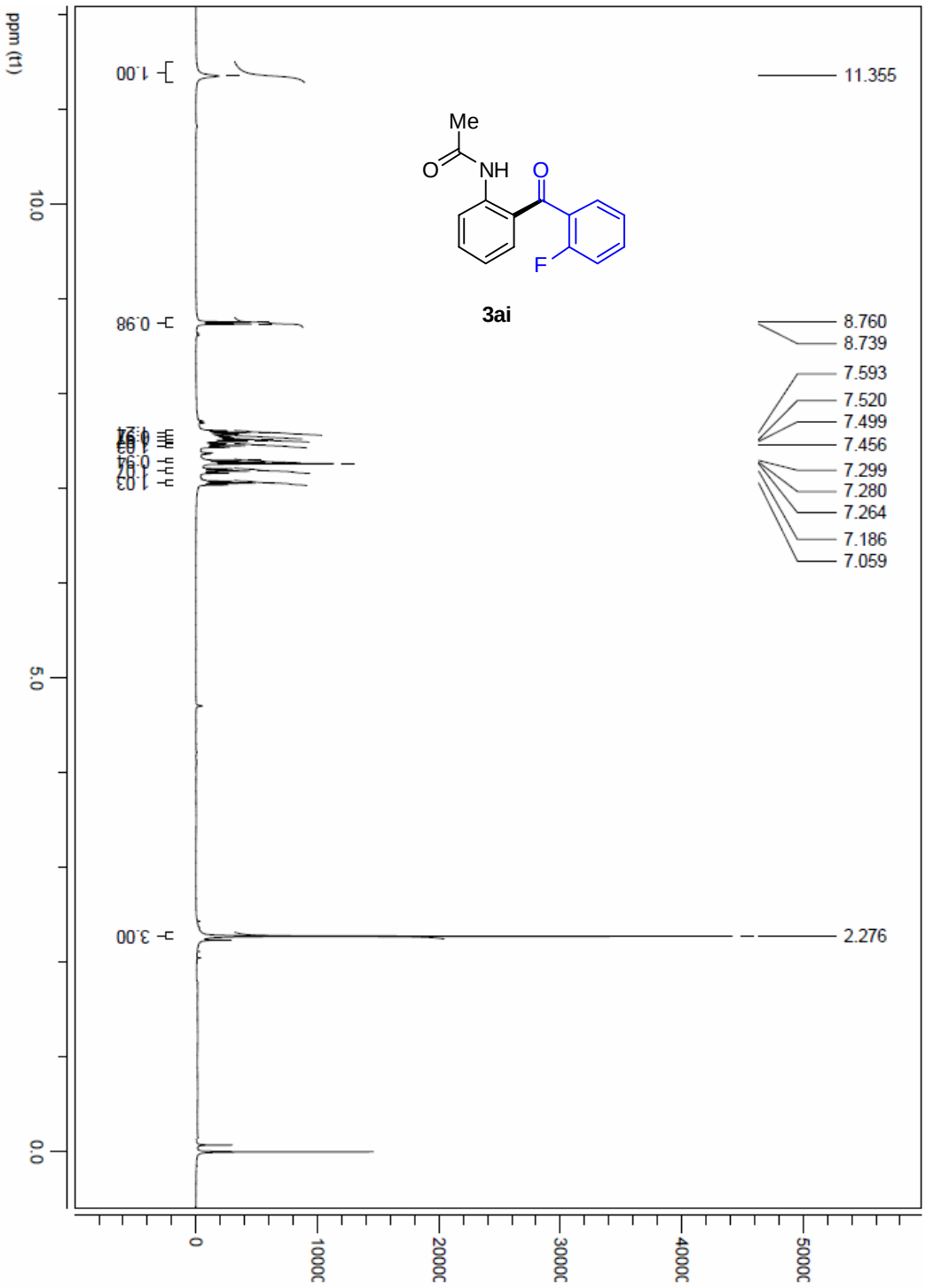

ppm (t1)
200
150
100
50
0
0
5000
10000
199.405
169.297
160.547
140.448
140.382
134.368
133.511
123.194
122.119
121.543
107.658
104.815
77.376
77.058
76.741
55.621
25.264
Me
O
NH
O
OMe
OMe
3ah

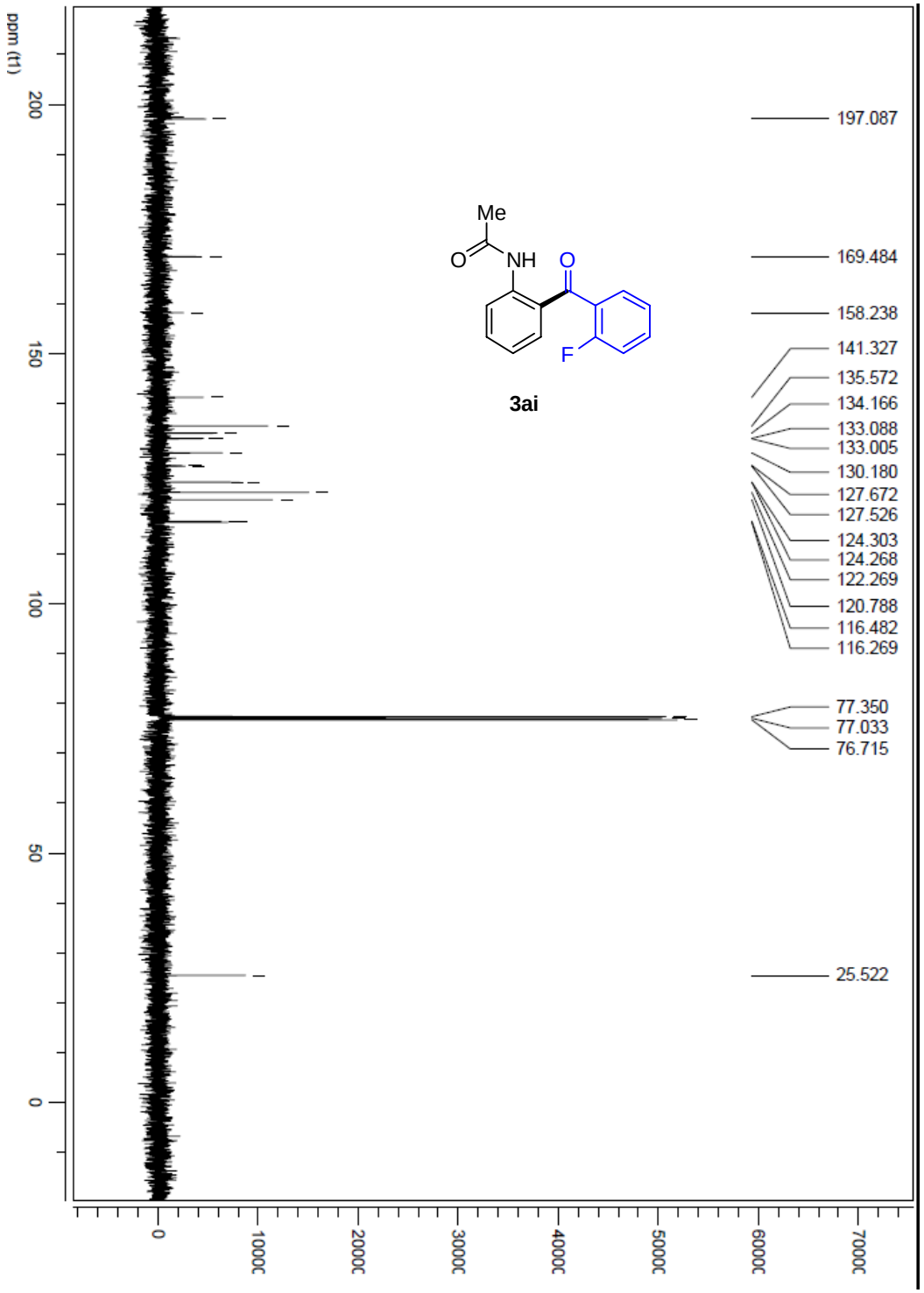


3ah

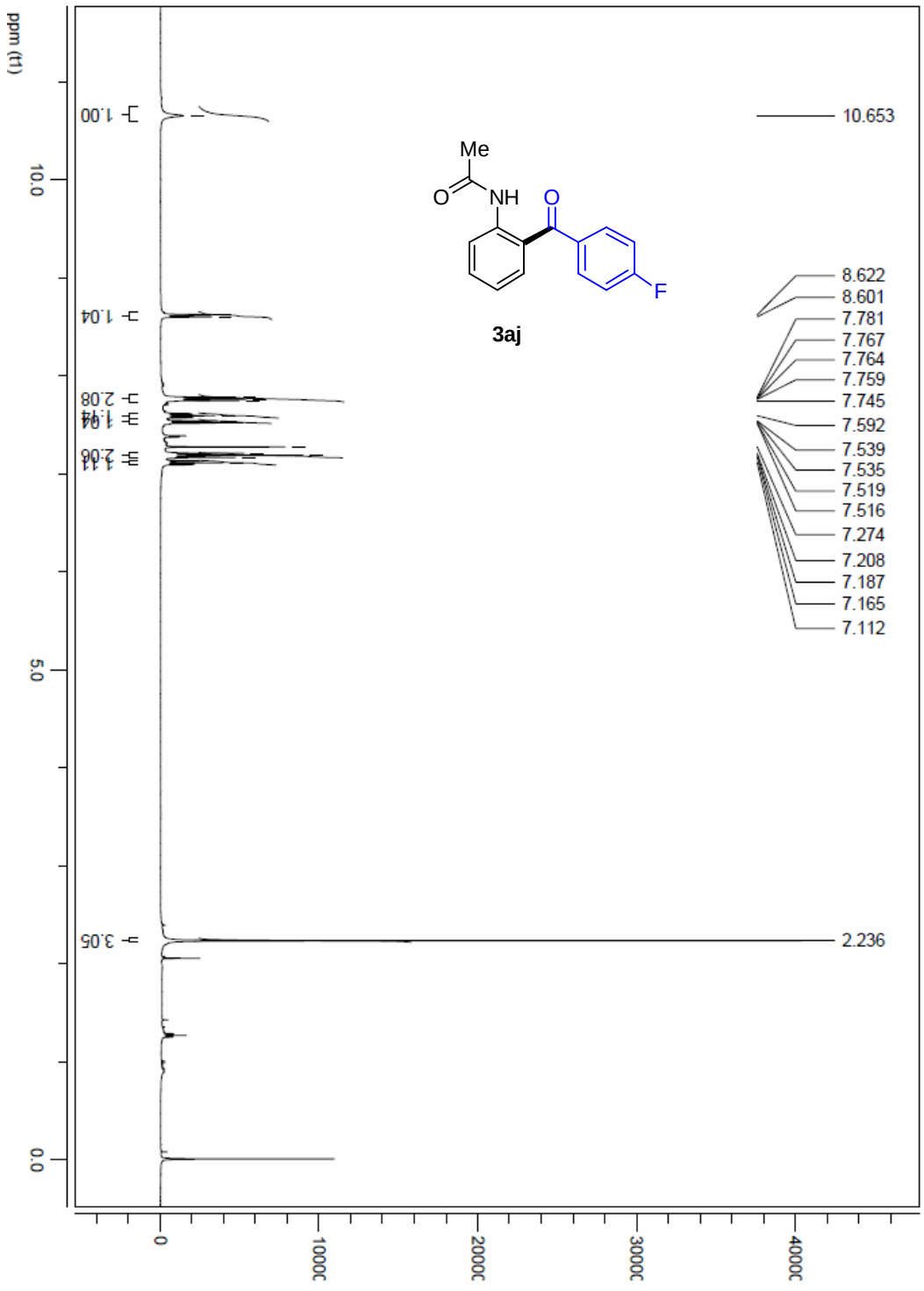


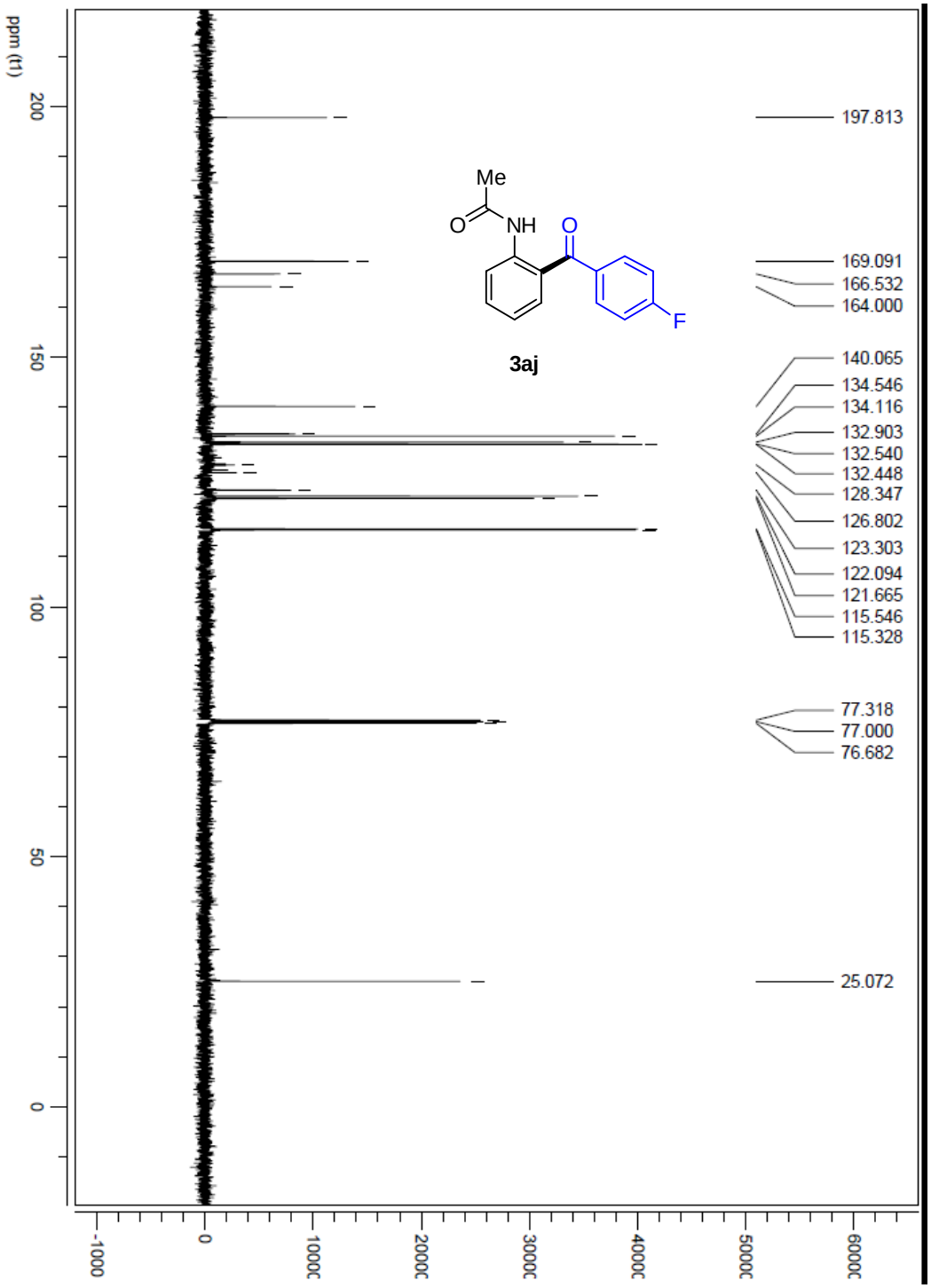
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.62	C17 H17 N O4	[M+Na] +	322.1051	322.1055	-0.4	-1.24	72.05	10.0

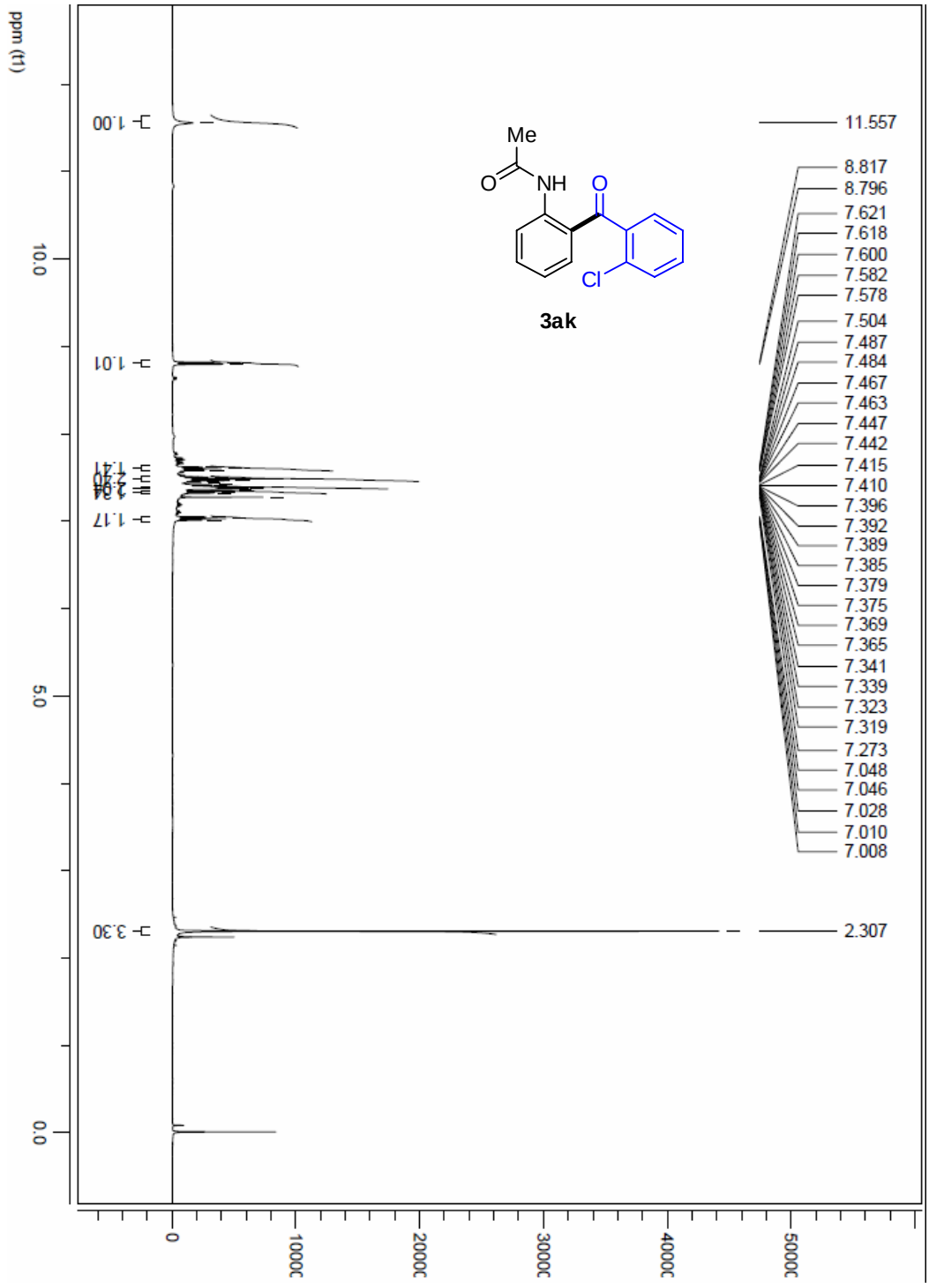

ppm (t1)
10.0
5.0
0.0
1.00
0.98
3.00
11.355
8.760
8.739
7.593
7.520
7.499
7.456
7.299
7.280
7.264
7.186
7.059
2.276
Me
O
NH
O
F
3ai
0
10000
20000
30000
40000
50000

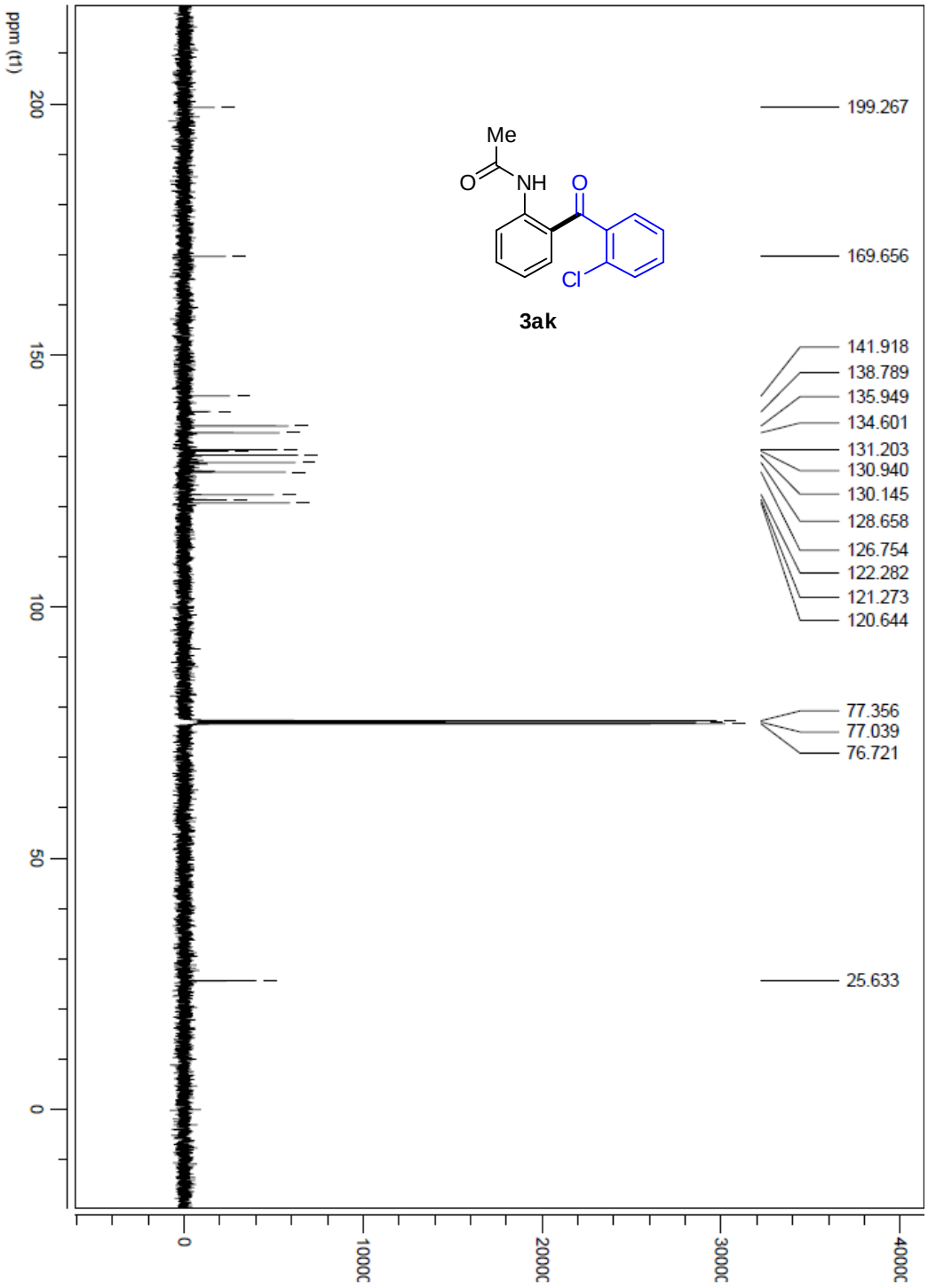

ppm (t1)
200
150
100
50
0
0
1000
2000
3000
4000
5000
6000
7000
197.087
169.484
158.238
141.327
135.572
134.166
133.088
133.005
130.180
127.672
127.526
124.303
124.268
122.269
120.788
116.482
116.269
77.350
77.033
76.715
25.522
Me
O
NH
O
F

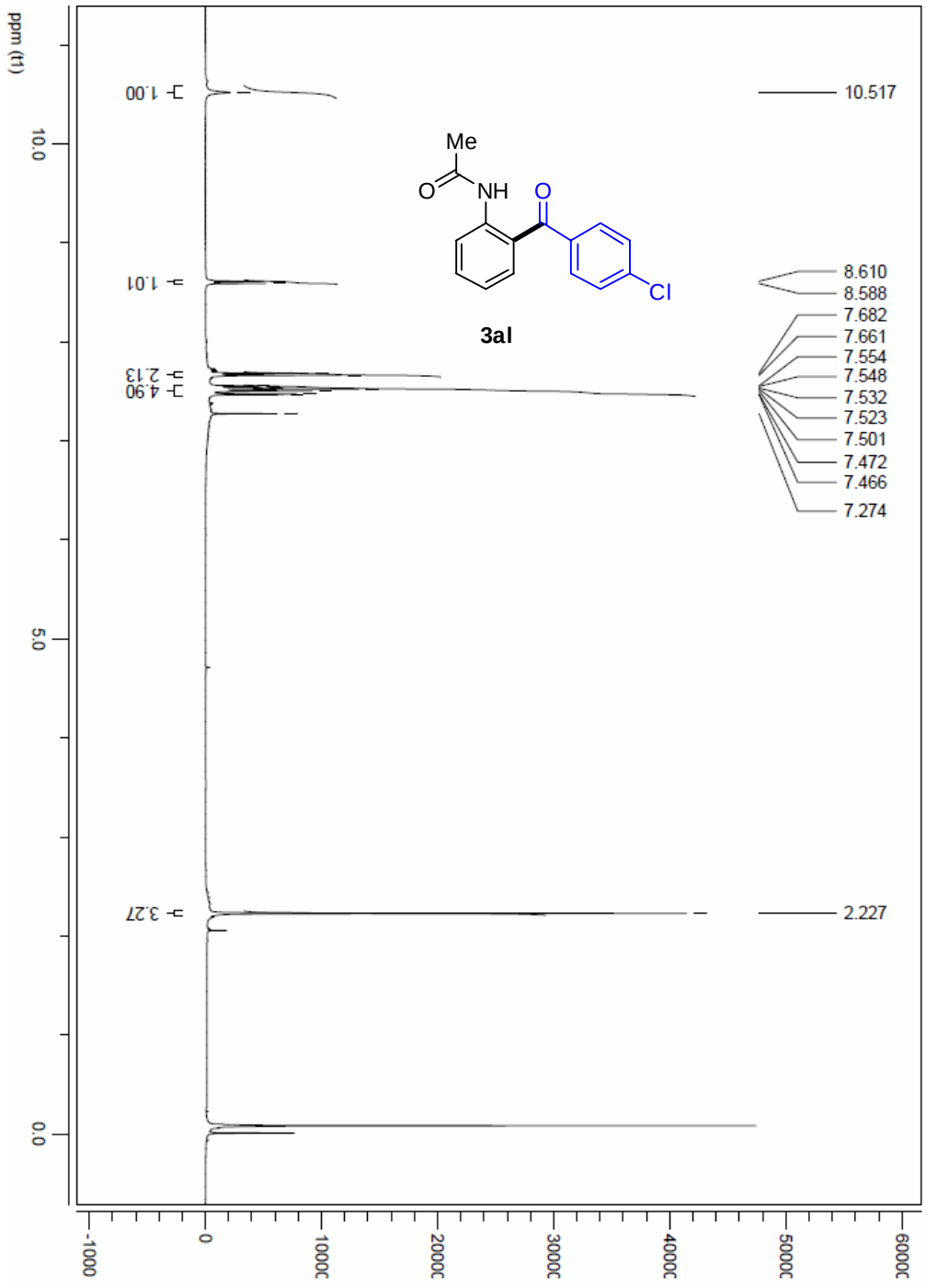
3ai

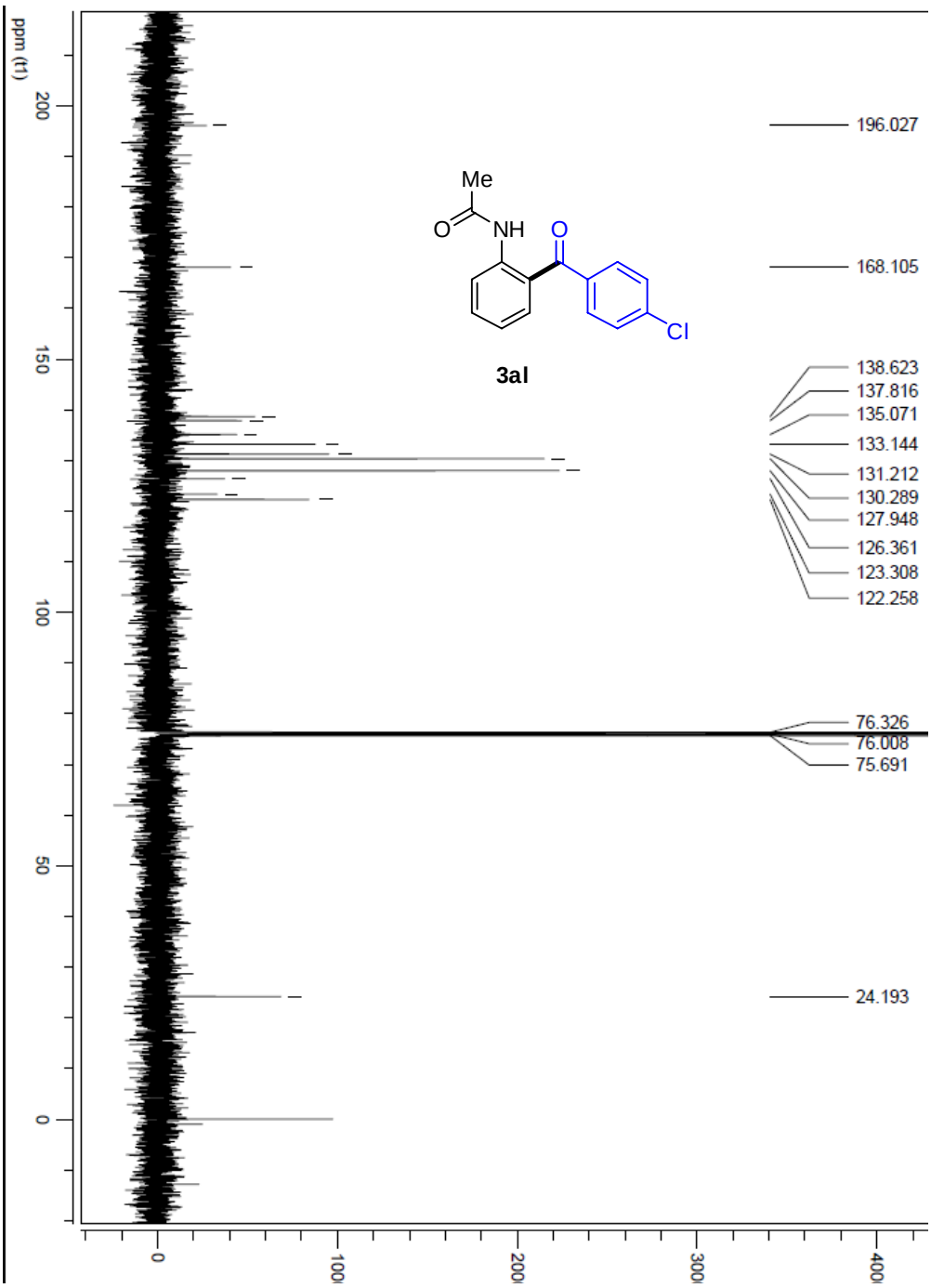

ppm (t1)
10.0
5.0
0.0
1.00
1.04
2.08
1.84
2.06
1.11
3.05
10.653
8.622
8.601
7.781
7.767
7.764
7.759
7.745
7.592
7.539
7.535
7.519
7.516
7.274
7.208
7.187
7.165
7.112
2.236
Me
O
NH
O
F
3aj
0
10000
20000
30000
40000

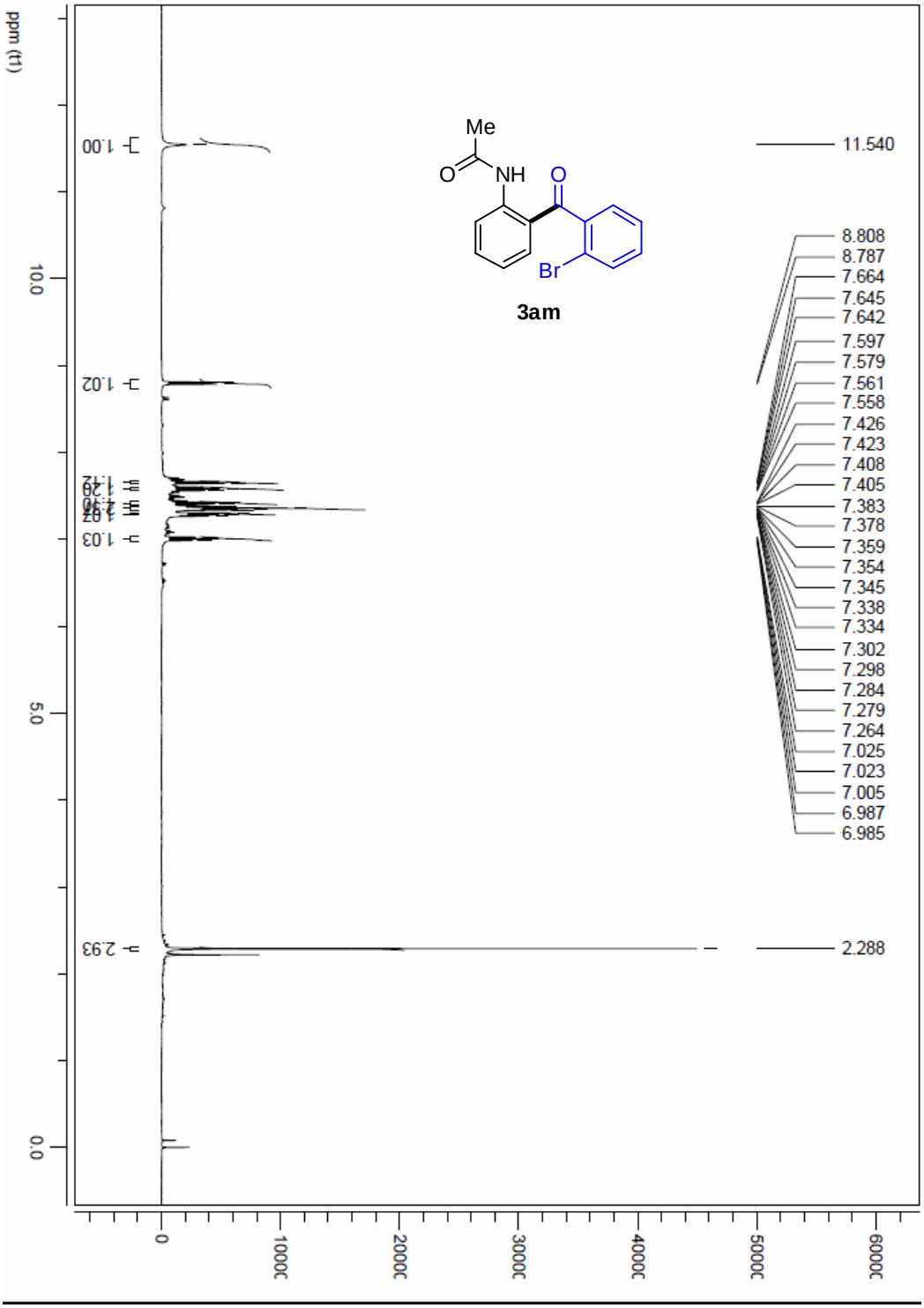

ppm (t1)
200
150
100
50
0
-1000
0
1000
2000
3000
4000
5000
6000
Me
O
NH
O
F
3aj
197.813
169.091
166.532
164.000
140.065
134.546
134.116
132.903
132.540
132.448
128.347
126.802
123.303
122.094
121.665
115.546
115.328
77.318
77.000
76.682
25.072

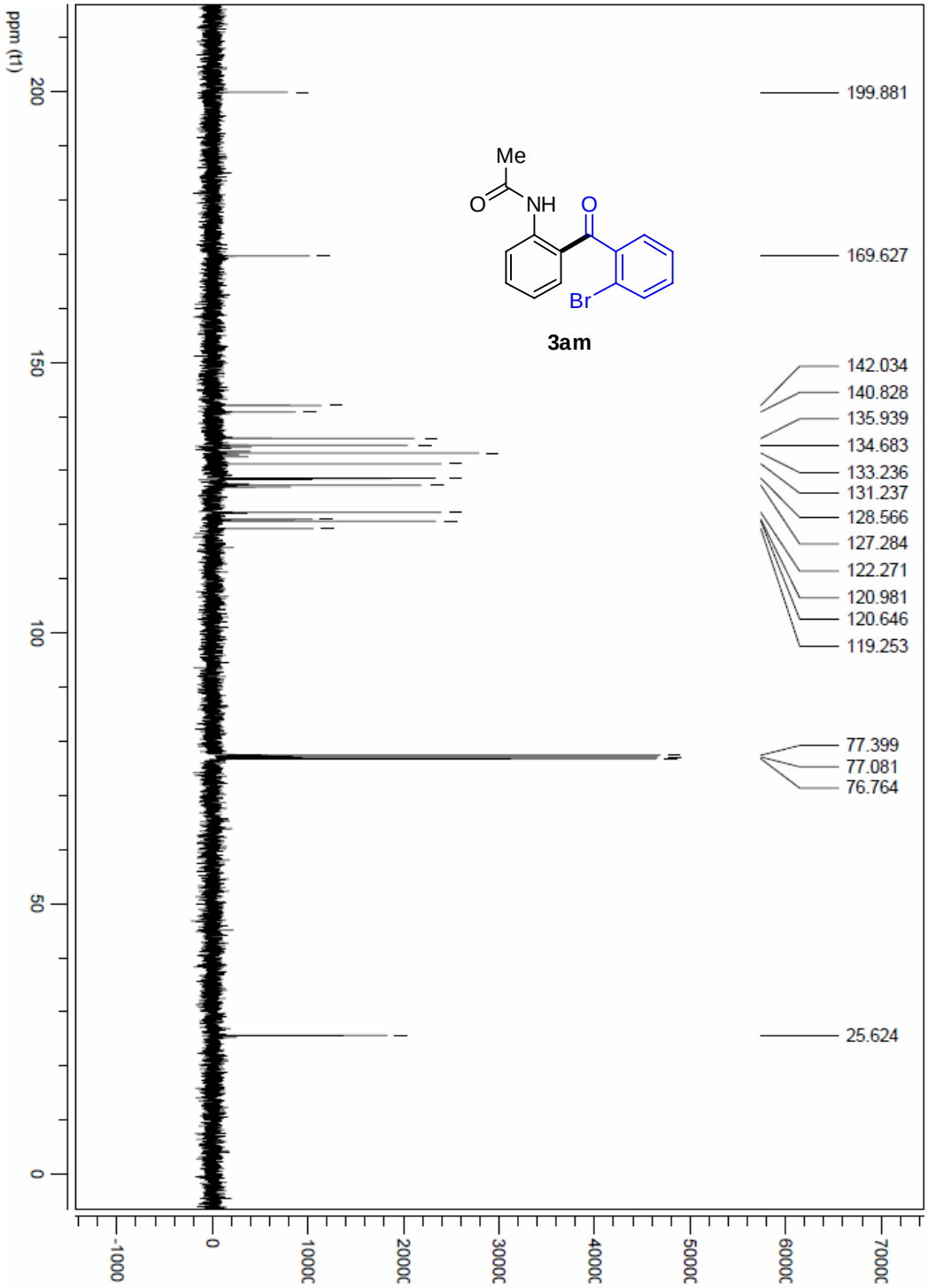

ppm (t1)
10.0
5.0
0.0
1.00
1.01
1.41
2.30
2.34
1.17
3.30
11.557
8.817
8.796
7.621
7.618
7.600
7.582
7.578
7.504
7.487
7.484
7.467
7.463
7.447
7.442
7.415
7.410
7.396
7.392
7.389
7.385
7.379
7.375
7.369
7.365
7.341
7.339
7.323
7.319
7.273
7.048
7.046
7.028
7.010
7.008
2.307
Me
O
NH
O
Cl
3ak
0
10000
20000
30000
40000
50000


ppm (t1)
200
150
100
50
0
0
10000
20000
30000
40000
Me
O
NH
O
Cl
3ak
199.267
169.656
141.918
138.789
135.949
134.601
131.203
130.940
130.145
128.658
126.754
122.282
121.273
120.644
77.356
77.039
76.721
25.633

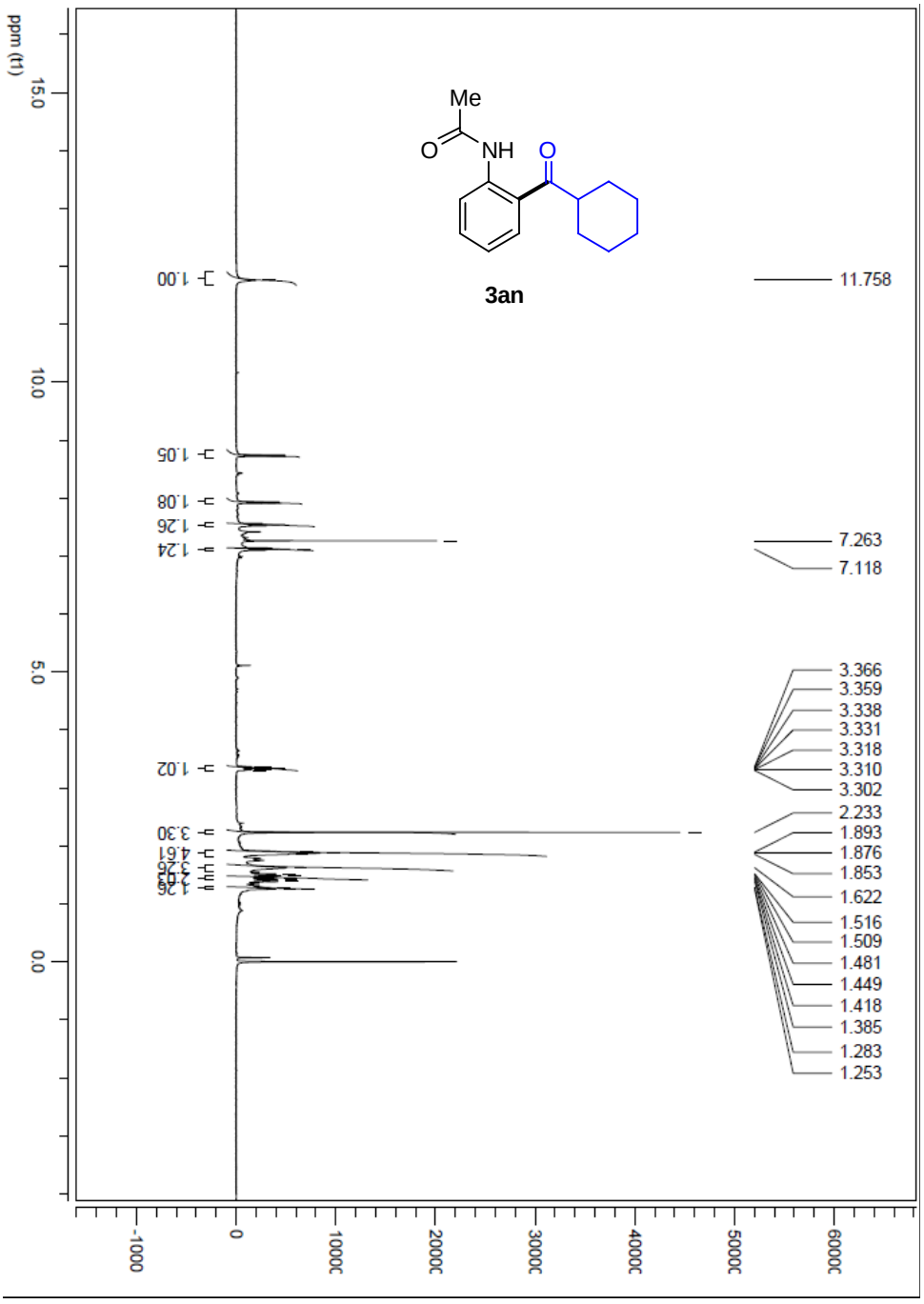

ppm (t1)
10.0
5.0
0.0
1.00
1.01
2.13
4.90
3.27
10.517
8.610
8.588
7.682
7.661
7.554
7.548
7.532
7.523
7.501
7.472
7.466
7.274
2.227
Me
O
NH
O
Cl
3aI
-1000
0
1000
2000
3000
4000
5000
6000

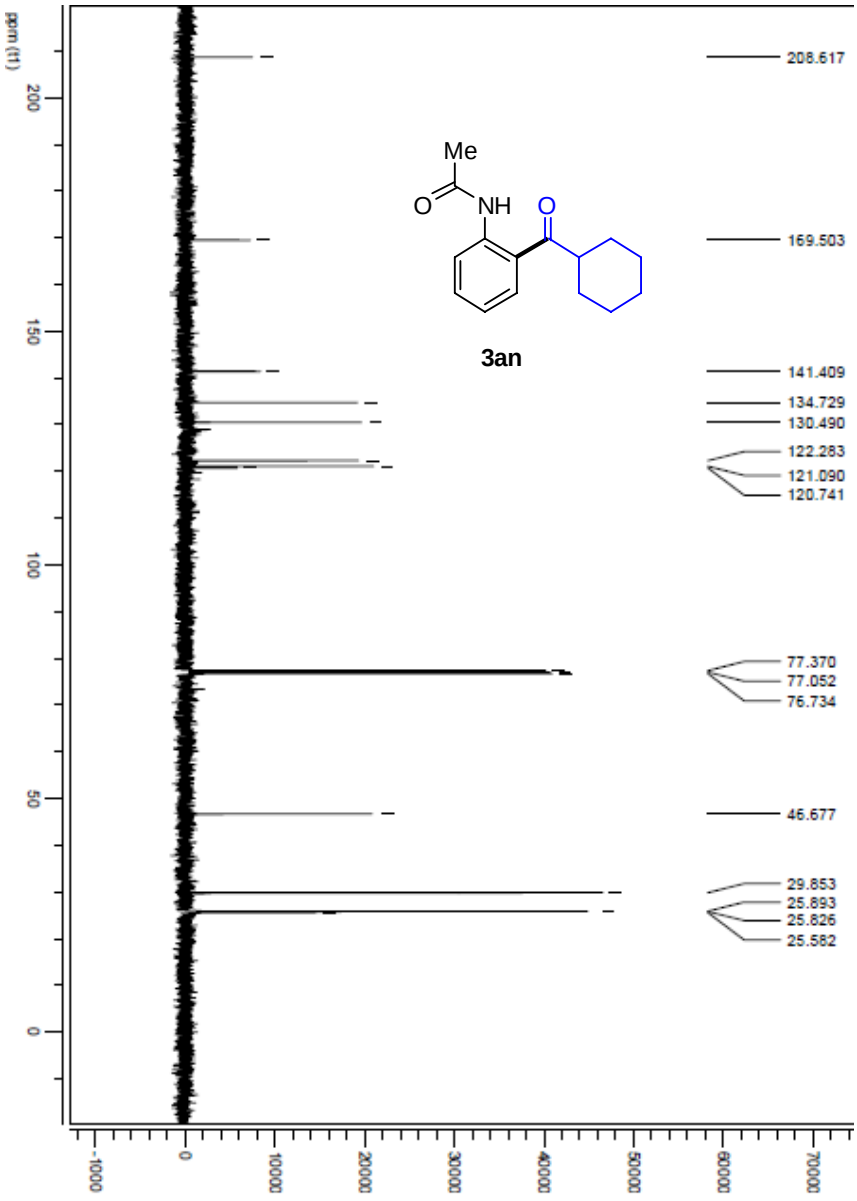

ppm (t1)
200
150
100
50
0
0
100
200
300
400
196.027
168.105
138.623
137.816
135.071
133.144
131.212
130.289
127.948
126.361
123.308
122.258
76.326
76.008
75.691
24.193
Me
O
NH
O
Cl
3al


Me
O
NH
O
Br
3am
11.540
8.808
8.787
7.664
7.645
7.642
7.597
7.579
7.561
7.558
7.426
7.423
7.408
7.405
7.383
7.378
7.359
7.354
7.345
7.338
7.334
7.302
7.298
7.284
7.279
7.264
7.025
7.023
7.005
6.987
6.985
2.288
1.00
1.02
1.03
2.93
ppm (t1)
10.0
5.0
0.0
0
1000
2000
3000
4000
5000
6000

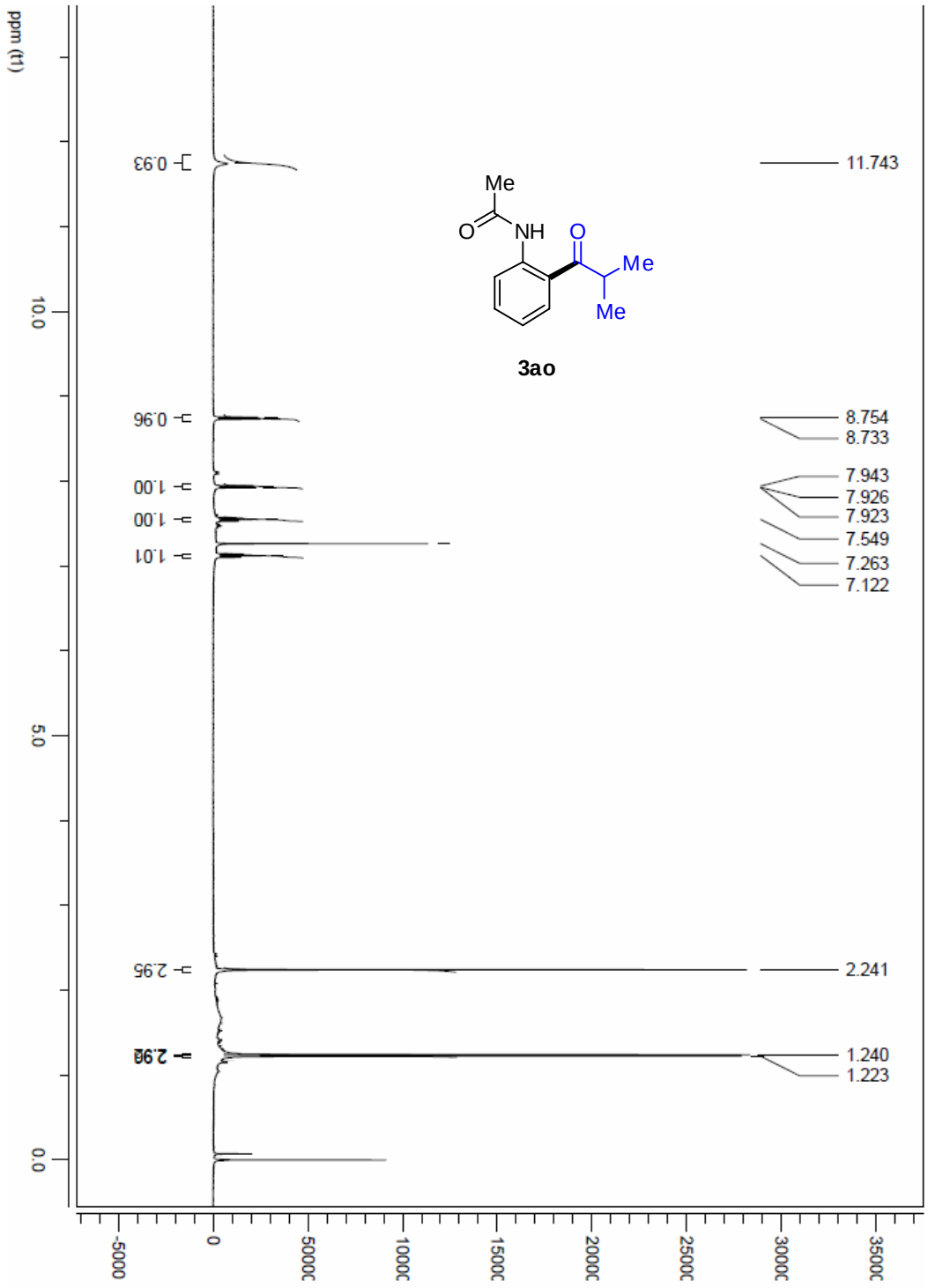

ppm (t1)
200
150
100
50
0
-1000
0
1000
2000
3000
4000
5000
6000
7000
199.881
169.627
142.034
140.828
135.939
134.683
133.236
131.237
128.566
127.284
122.271
120.981
120.646
119.253
77.399
77.081
76.764
25.624
Me
O
NH
O
Br

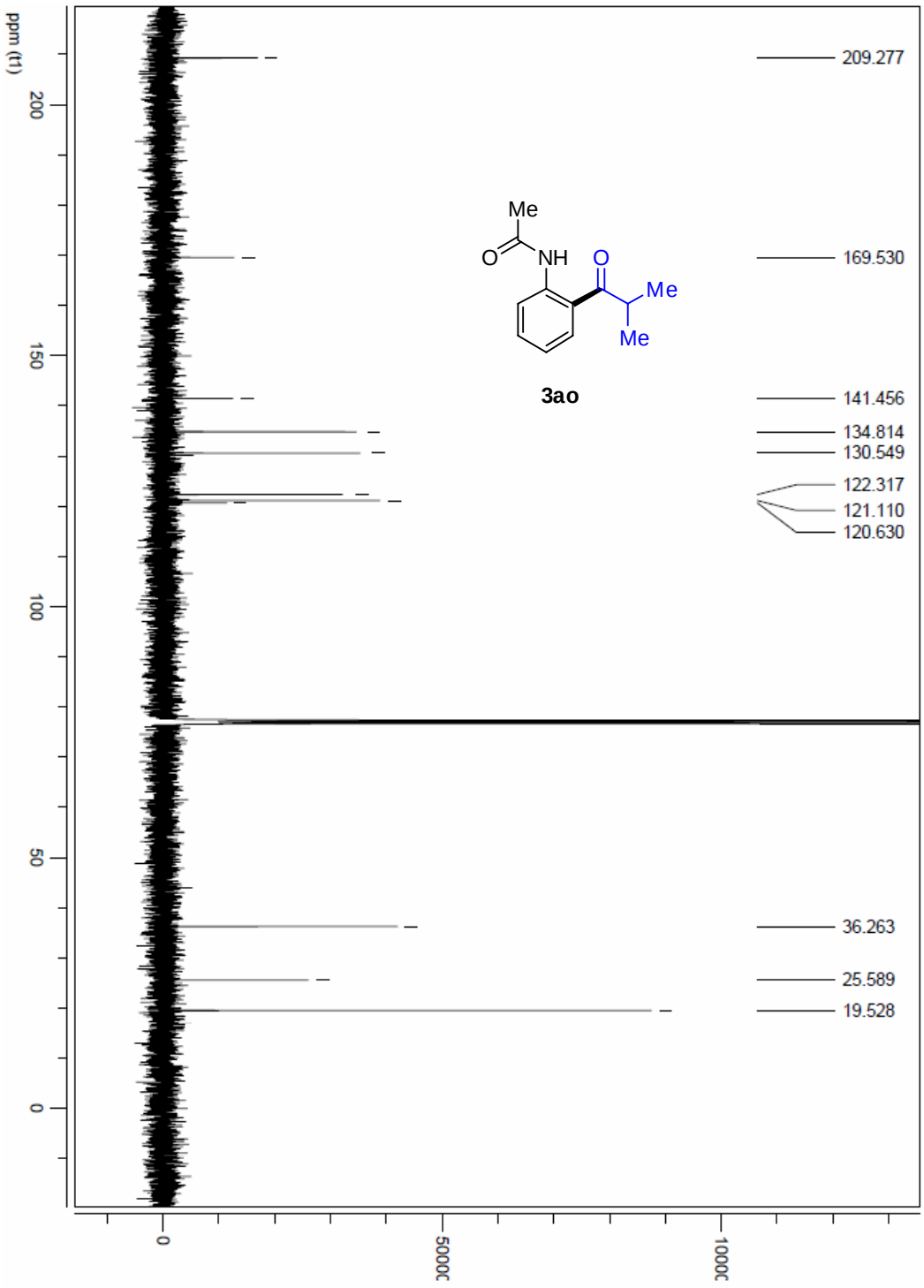
3am

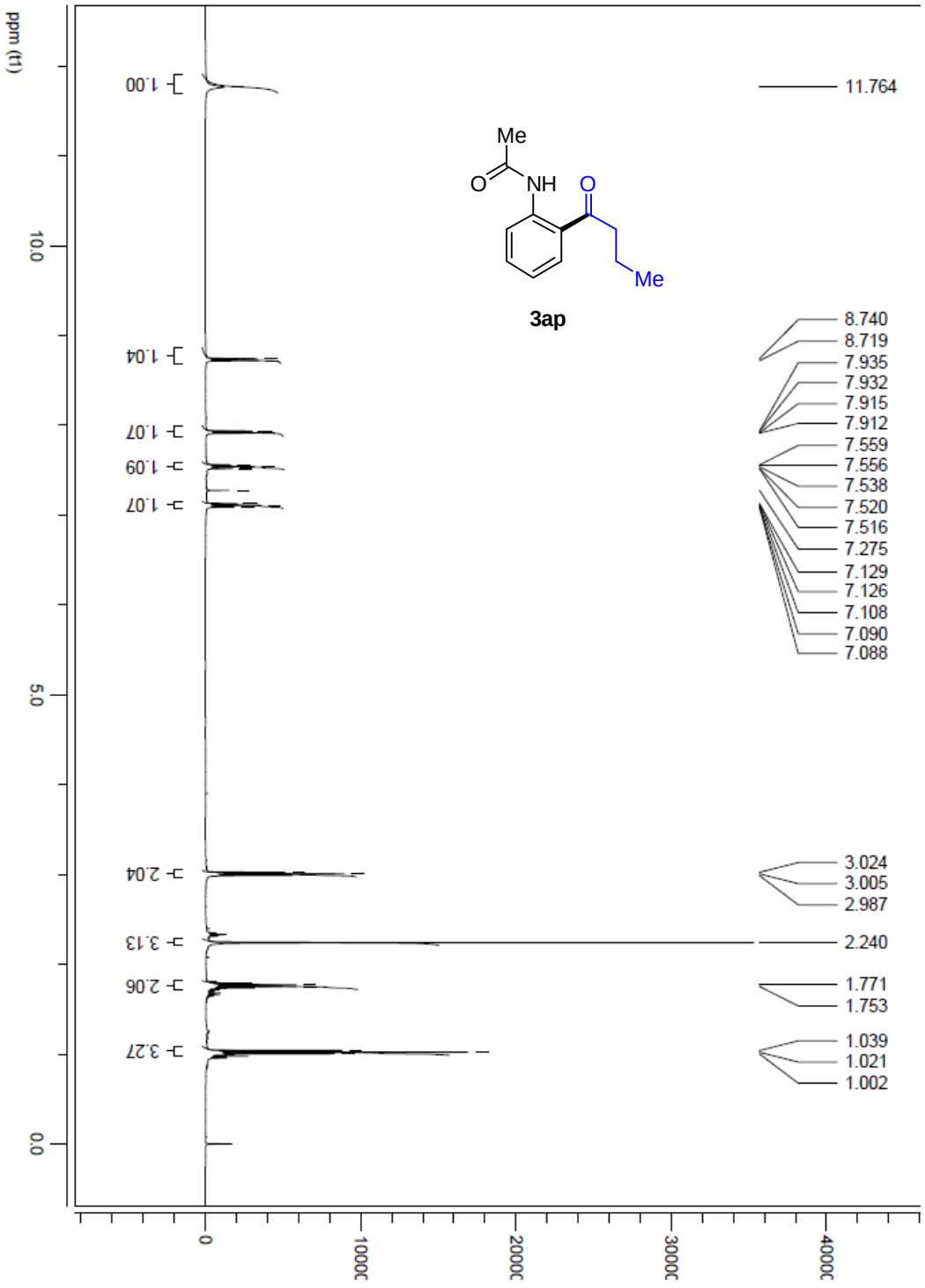

Me
O
NH
O
3an
ppm (t1)
15.0
10.0
5.0
0.0
1.00
1.05
1.08
1.26
1.24
1.02
3.30
4.61
11.758
7.263
7.118
3.366
3.359
3.338
3.331
3.318
3.310
3.302
2.233
1.893
1.876
1.853
1.622
1.516
1.509
1.481
1.449
1.418
1.385
1.283
1.253
-1000
0
1000
2000
3000
4000
5000
6000

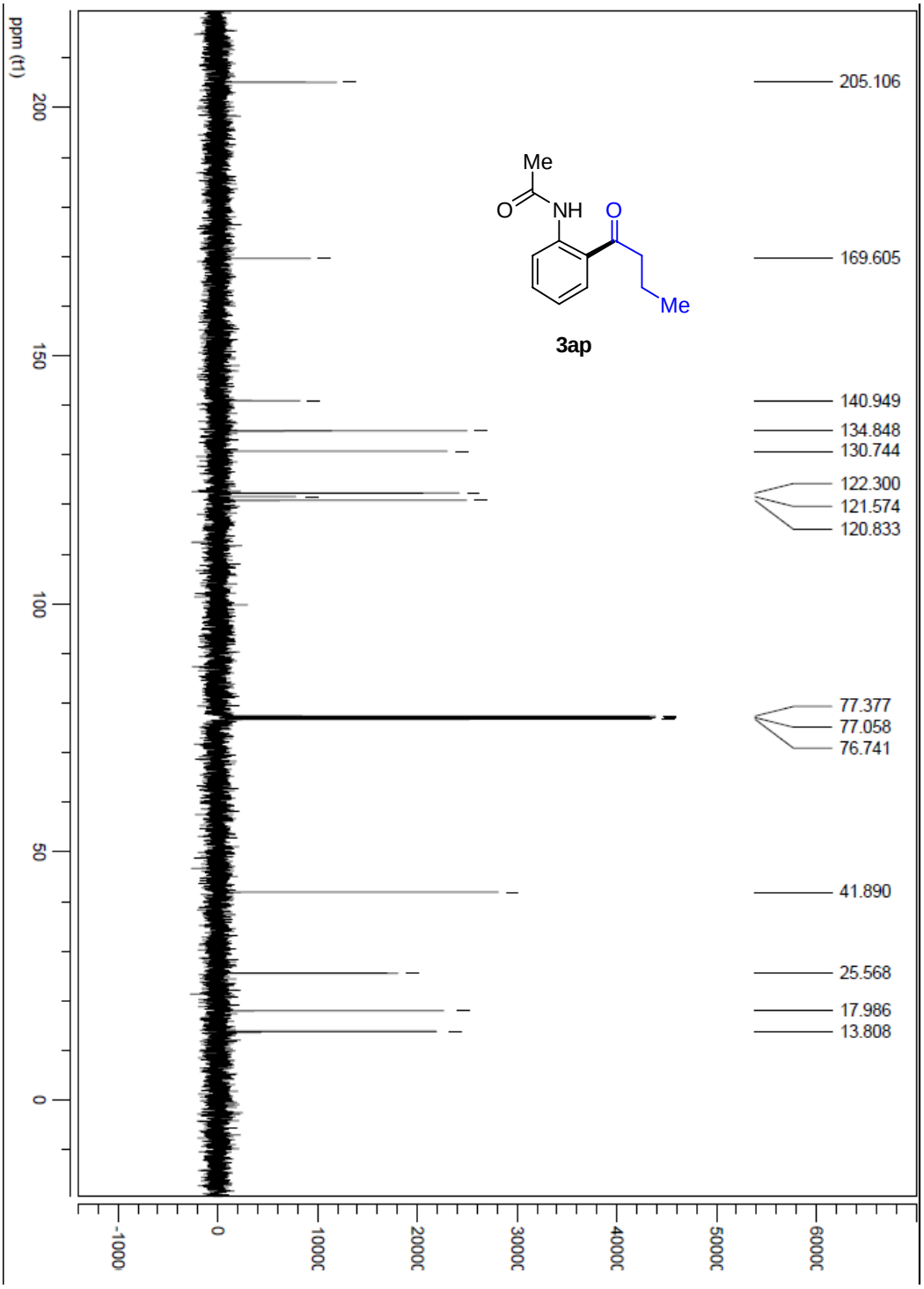

ppm (t1)
200
150
100
50
0
-10000
0
10000
20000
30000
40000
50000
60000
70000
208.617
169.503
141.409
134.729
130.490
122.283
121.090
120.741
77.370
77.052
76.734
46.677
29.853
25.893
25.826
25.582
Me
O
NH
O

3an

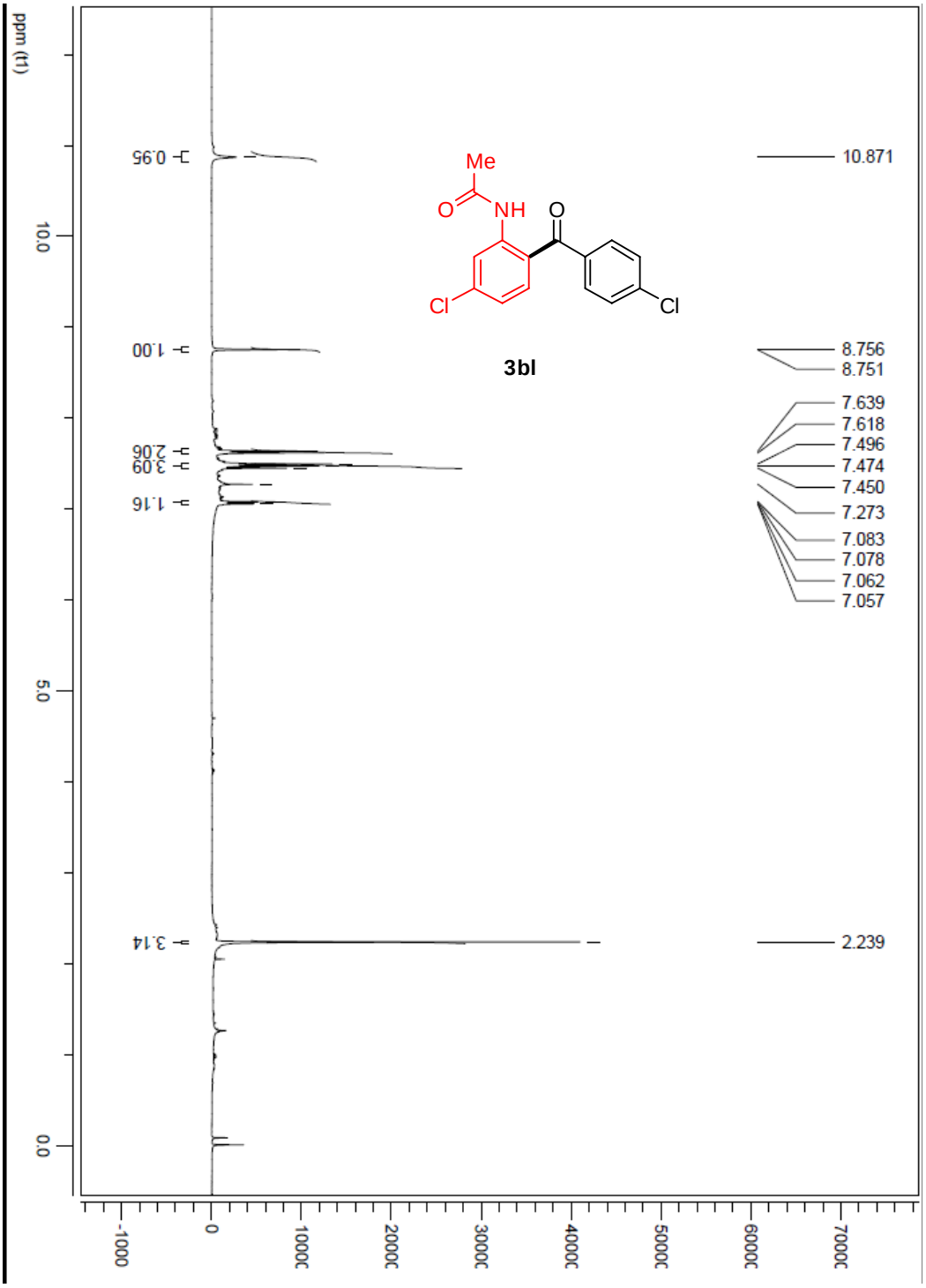

ppm (t1)
10.0
5.0
0.0
0.93
0.96
1.00
1.00
1.01
2.95
2.98
11.743
8.754
8.733
7.943
7.926
7.923
7.549
7.263
7.122
2.241
1.240
1.223
Me
O
NH
O
Me
Me
3ao
-5000
0
5000
10000
15000
20000
25000
30000
35000

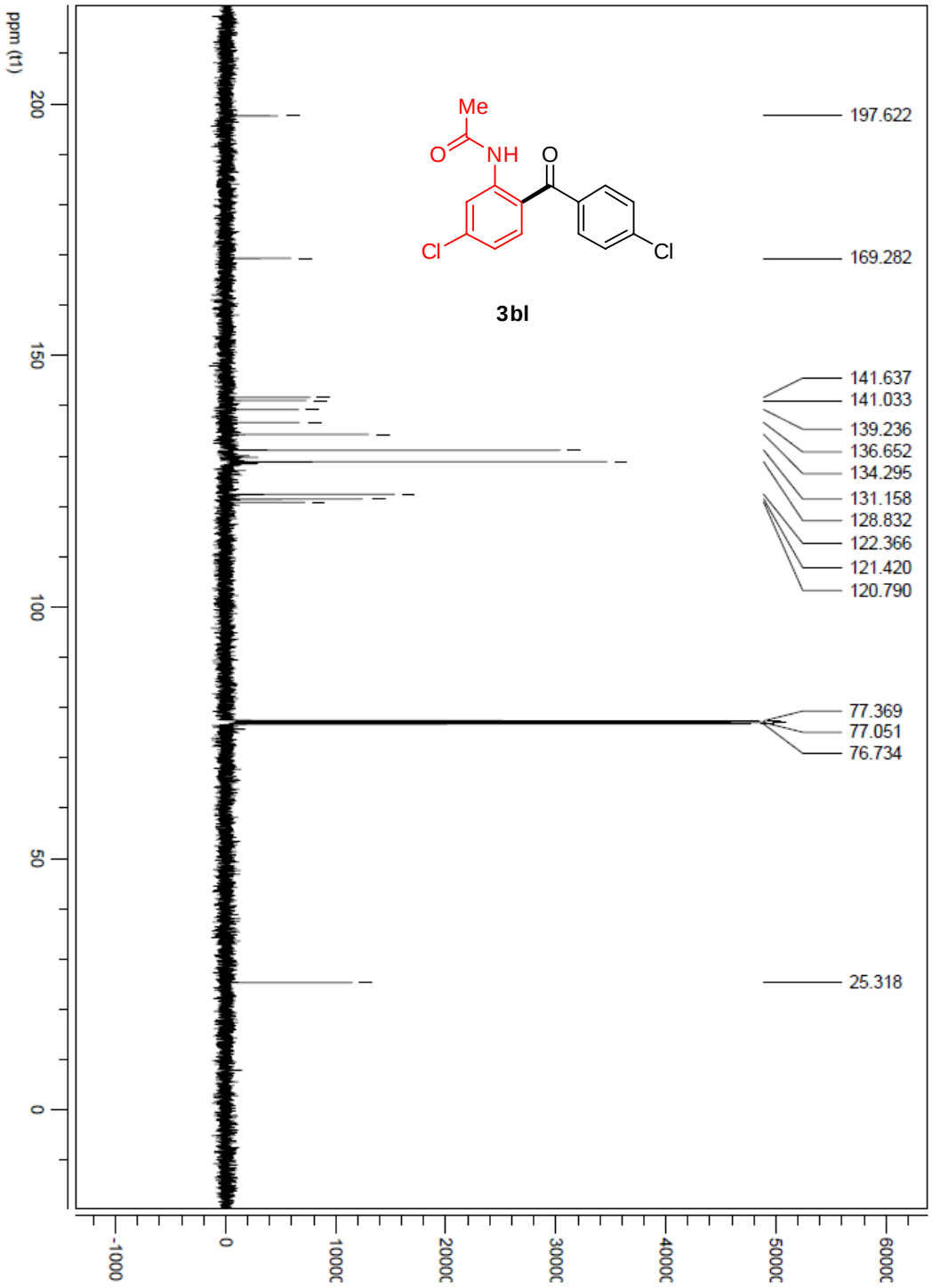

ppm (t1)
200
150
100
50
0
209.277
169.530
141.456
134.814
130.549
122.317
121.110
120.630
36.263
25.589
19.528
Me
O
NH
O
Me
Me
3ao
0
50000
100000


ppm (t1)
10.0
5.0
0.0
1.00
1.04
1.07
1.09
1.07
2.04
3.13
2.06
3.27
11.764
8.740
8.719
7.935
7.932
7.915
7.912
7.559
7.556
7.538
7.520
7.516
7.275
7.129
7.126
7.108
7.090
7.088
3.024
3.005
2.987
2.240
1.771
1.753
1.039
1.021
1.002
Me
O
NH
O
Me
3ap
0
10000
20000
30000
40000

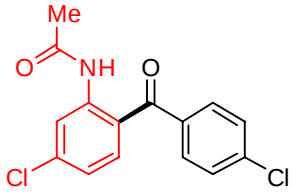

ppm (t1)
200
150
100
50
0
-1000
0
1000
2000
3000
4000
5000
6000
205.106
169.605
140.949
134.848
130.744
122.300
121.574
120.833
77.377
77.058
76.741
41.890
25.568
17.986
13.808
Me
O
NH
O
Me

3ap

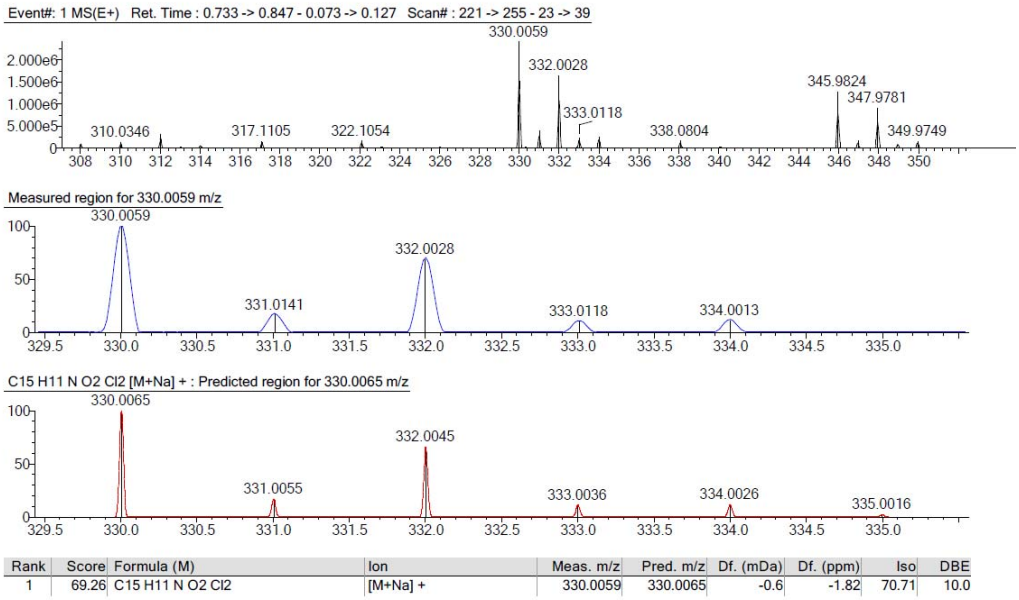

ppm (t1)
10.0
5.0
0.0
0.95
1.00
2.06
3.09
1.16
3.14
Me
O
NH
O
Cl
Cl
3bl
10.871
8.756
8.751
7.639
7.618
7.496
7.474
7.450
7.273
7.083
7.078
7.062
7.057
2.239
-1000
0
1000
2000
3000
4000
5000
6000
7000


ppm (t1)
200
150
100
50
0
-1000
0
1000
2000
3000
4000
5000
6000
Me
O
NH
O
Cl
Cl
197.622
169.282
141.637
141.033
139.236
136.652
134.295
131.158
128.832
122.366
121.420
120.790
77.369
77.051
76.734
25.318

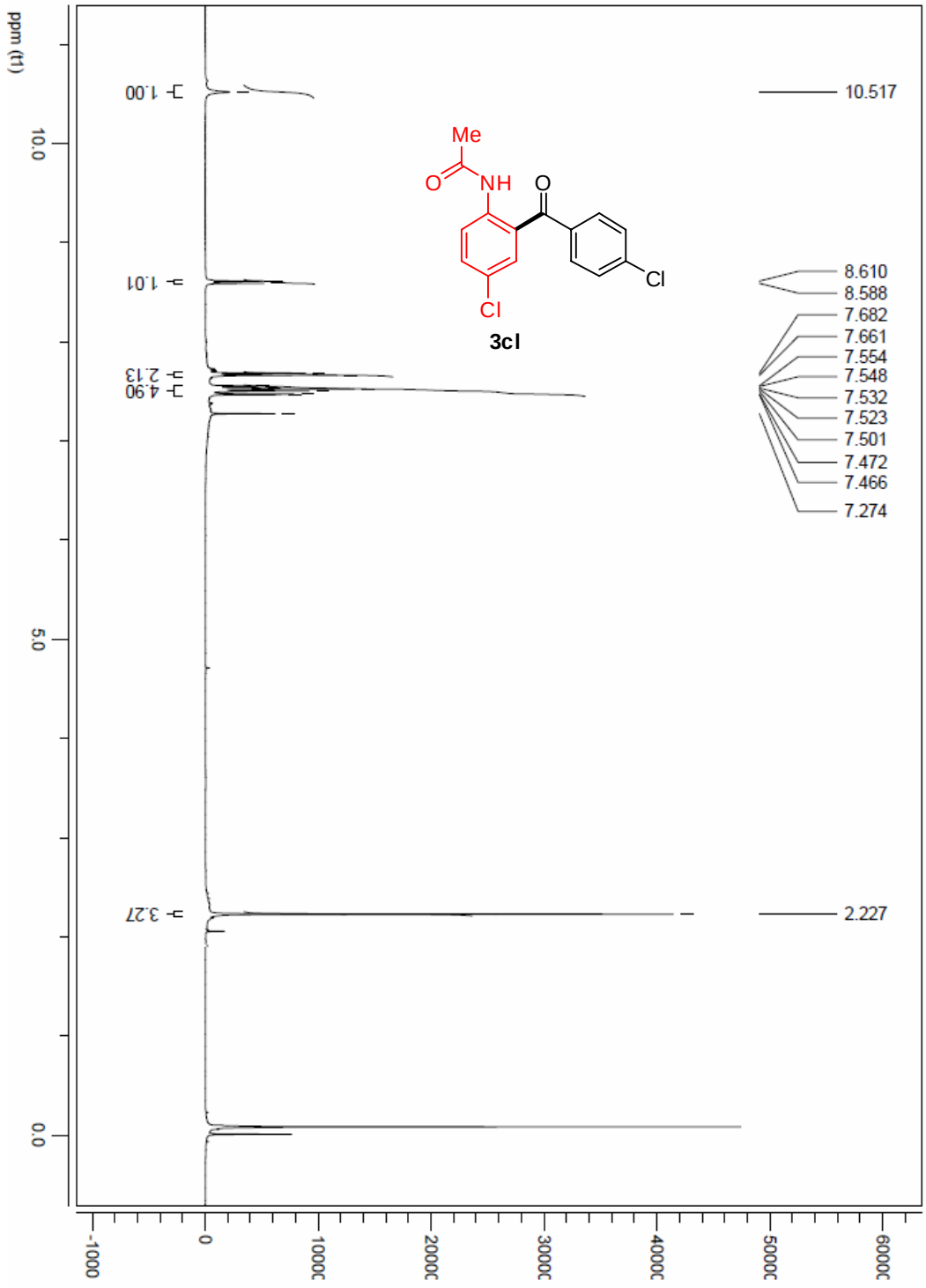
3bl

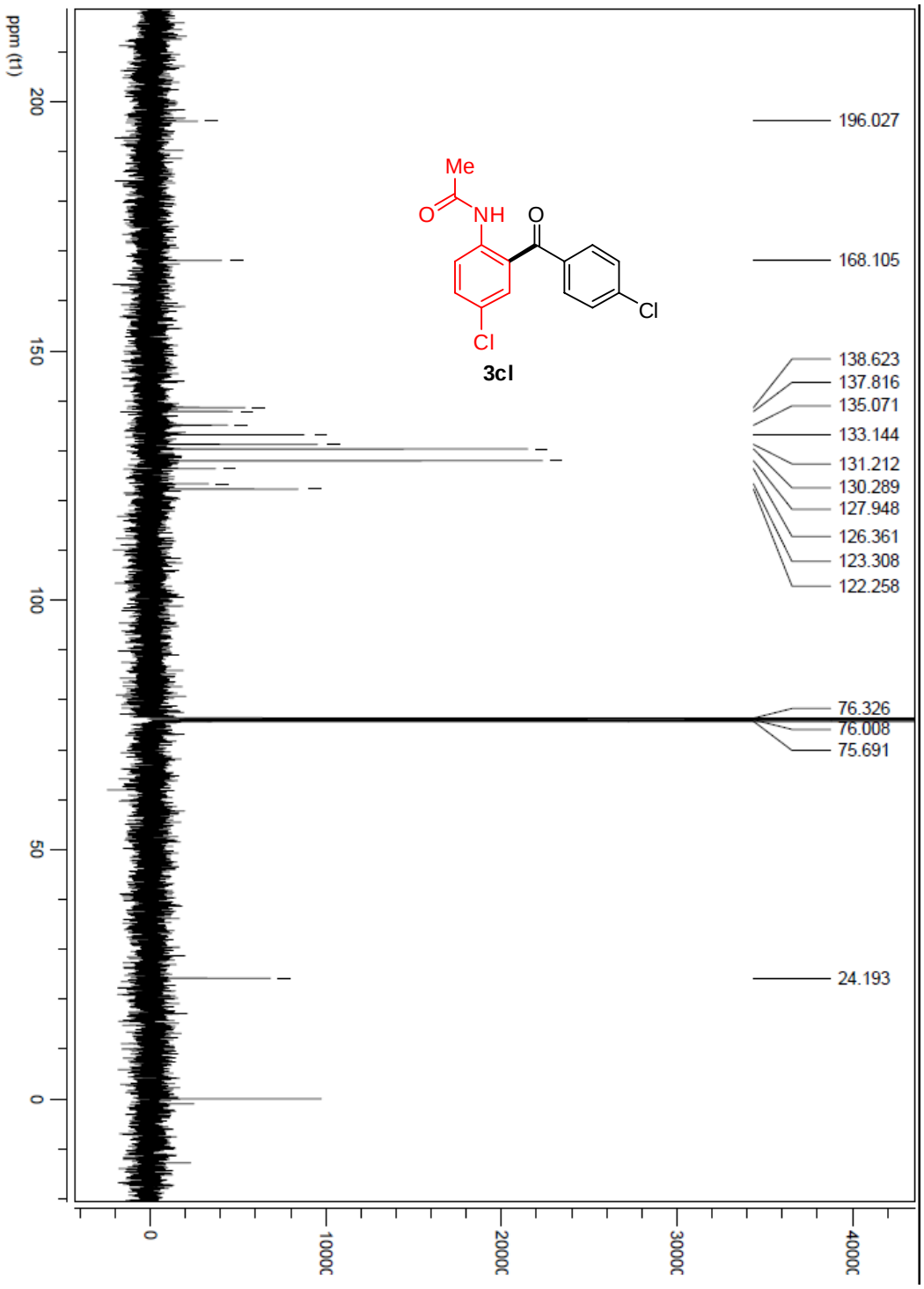


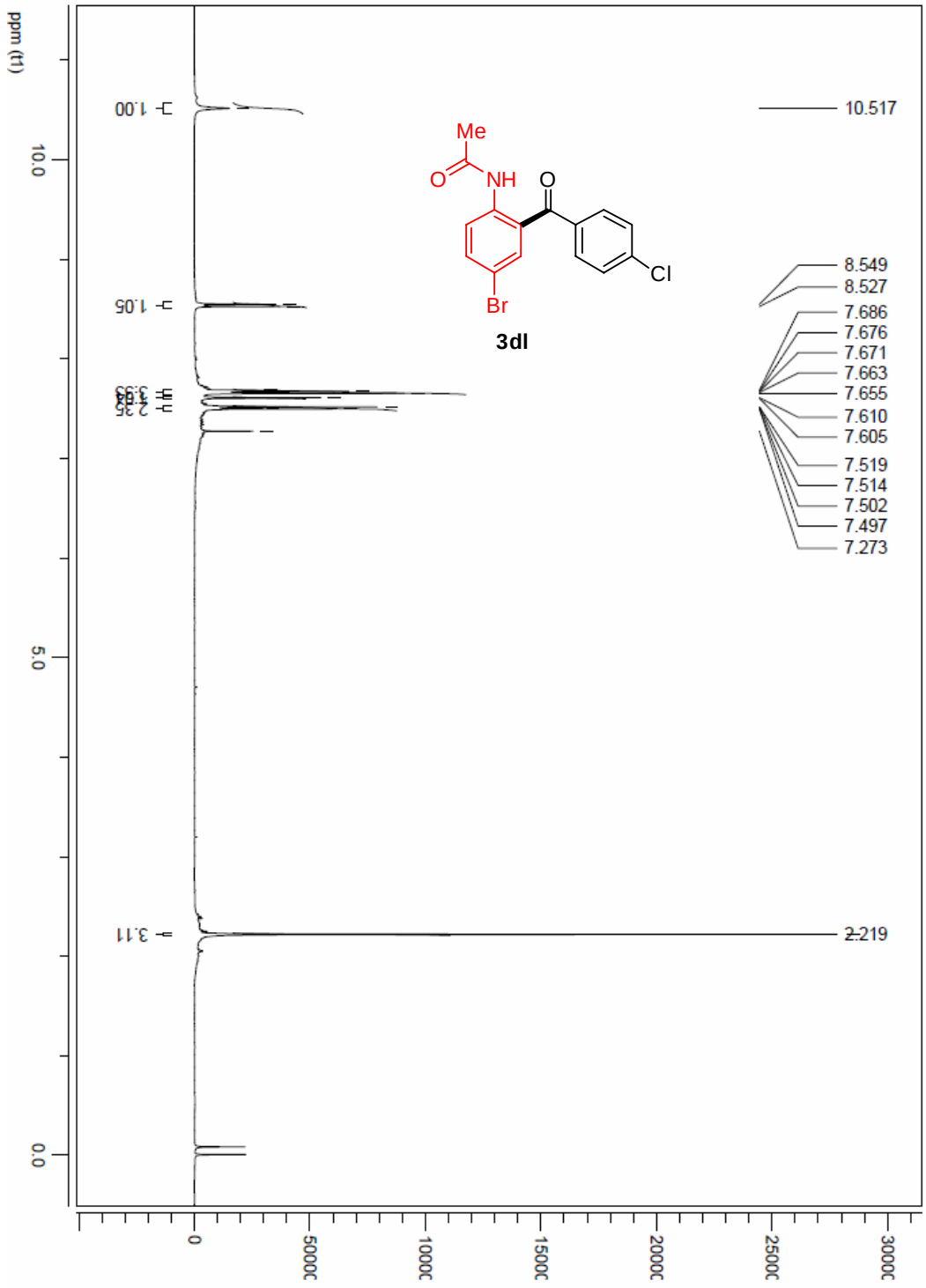
3bl

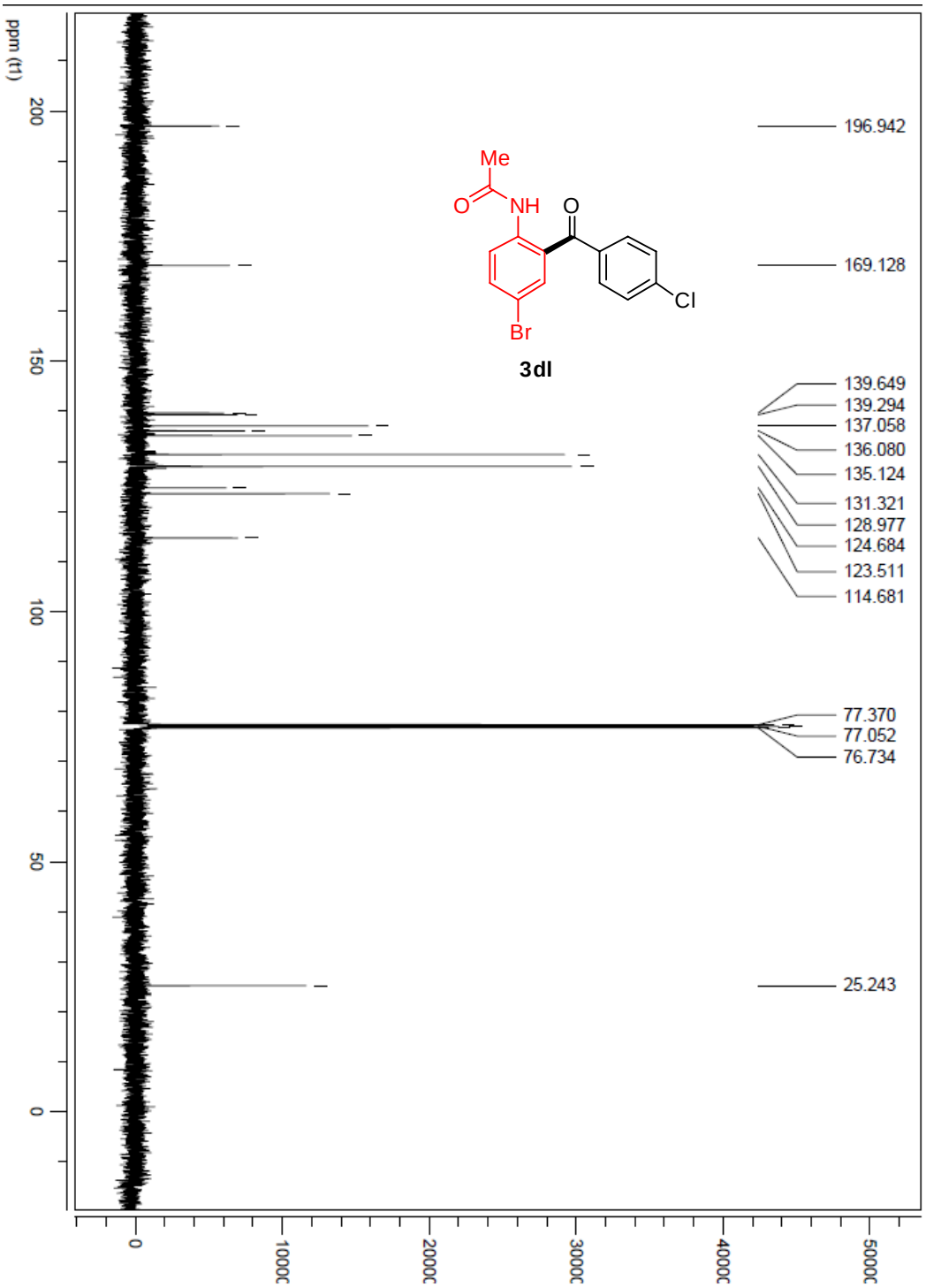


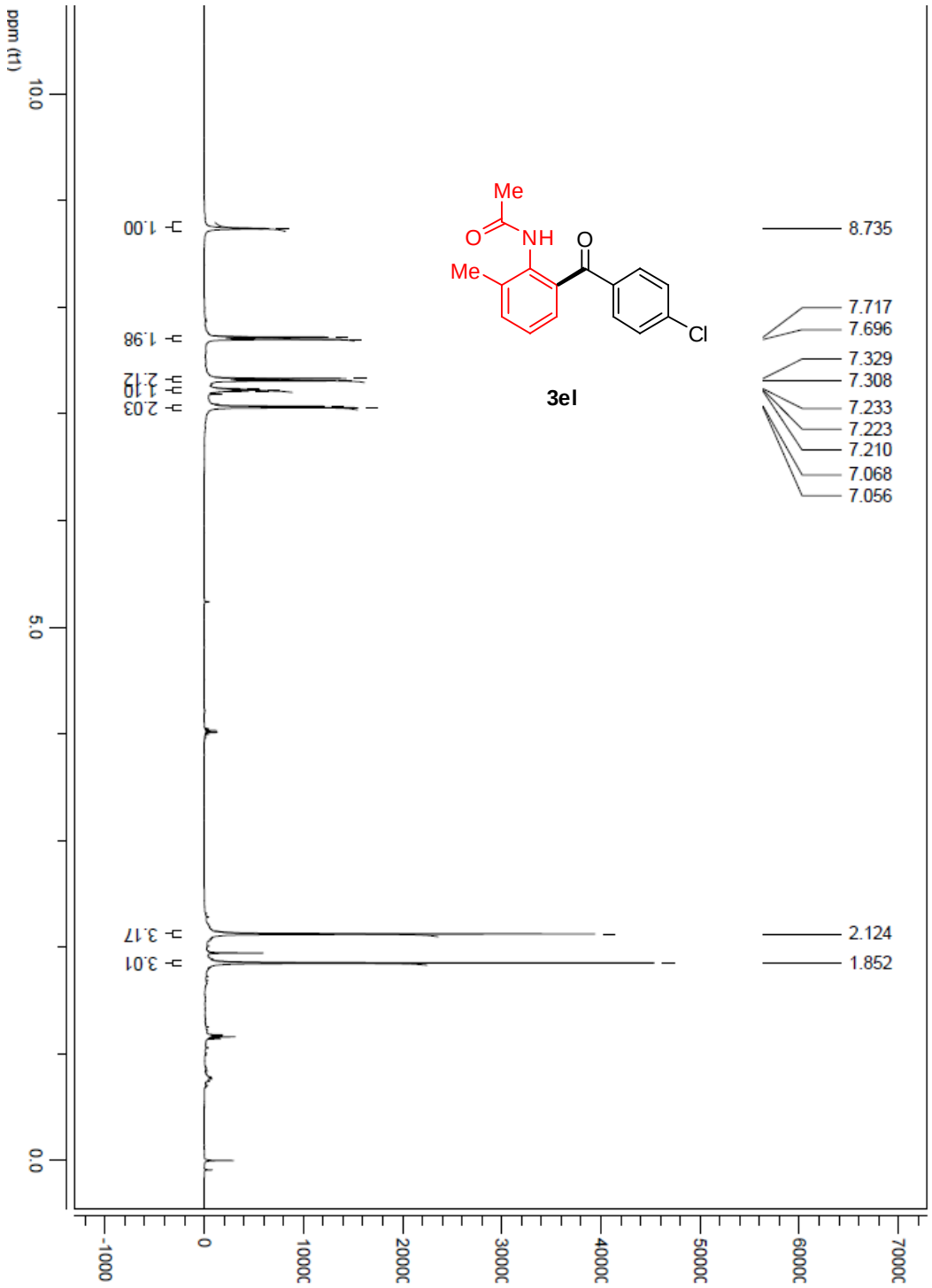
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.26	C15 H11 N O2 Cl2	[M+Na] +	330.0059	330.0065	-0.6	-1.82	70.71	10.0

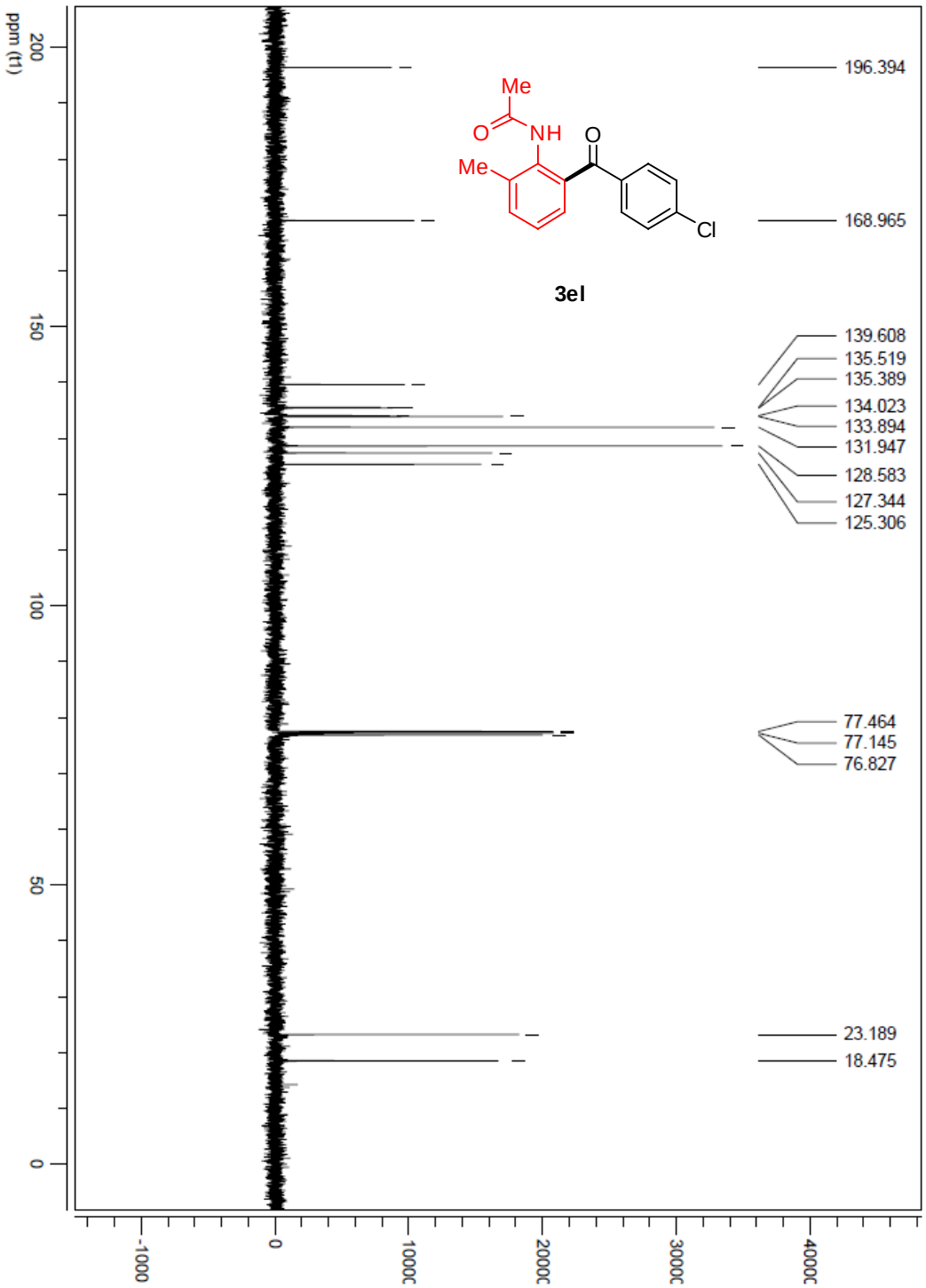

ppm (t1)
10.0
5.0
0.0
1.00
1.01
2.13
4.90
3.27
Me
O
NH
O
Cl
Cl
3cl
10.517
8.610
8.588
7.682
7.661
7.554
7.548
7.532
7.523
7.501
7.472
7.466
7.274
2.227
-1000
0
1000
2000
3000
4000
5000
6000

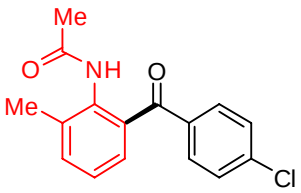

ppm (t1)
200
150
100
50
0
0
1000
2000
3000
4000
196.027
168.105
138.623
137.816
135.071
133.144
131.212
130.289
127.948
126.361
123.308
122.258
76.326
76.008
75.691
24.193
Me
O
NH
O
Cl
Cl
3cl


ppm (t1)
10.0
5.0
0.0
1.00
1.05
2.35
3.11
2.19
0
5000
10000
15000
20000
25000
30000
Me
O
NH
O
Cl
Br
3dl
10.517
8.549
8.527
7.686
7.676
7.671
7.663
7.655
7.610
7.605
7.519
7.514
7.502
7.497
7.273


ppm (t1)
200
150
100
50
0
0
10000
20000
30000
40000
50000
Me
O
NH
O
Br
Cl
3dl
196.942
169.128
139.649
139.294
137.058
136.080
135.124
131.321
128.977
124.684
123.511
114.681
77.370
77.052
76.734
25.243


ppm (t1)
10.0
5.0
0.0
1.00
1.98
2.12
1.10
2.03
3.17
3.01
Me
O
NH
O
Me
Cl
3el
8.735
7.717
7.696
7.329
7.308
7.233
7.223
7.210
7.068
7.056
2.124
1.852
-1000
0
1000
2000
3000
4000
5000
6000
7000

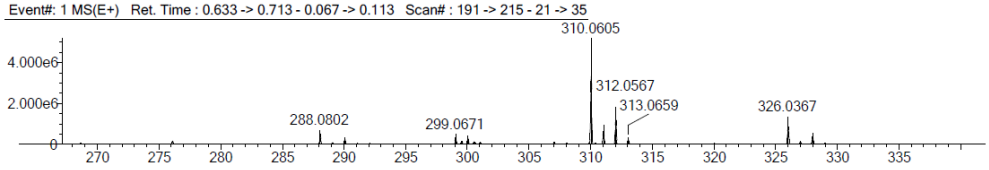

ppm (t1)
200
150
100
50
0
-1000
0
1000
2000
3000
4000
196.394
168.965
139.608
135.519
135.389
134.023
133.894
131.947
128.583
127.344
125.306
77.464
77.145
76.827
23.189
18.475
Me
O
NH
O
Me
Cl
3el



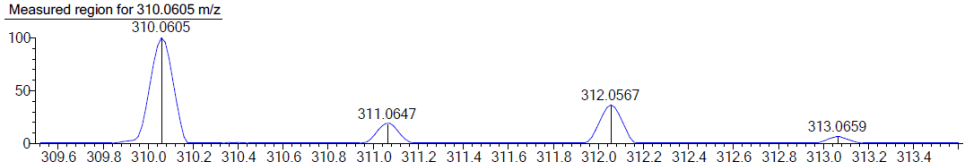
3el

Error Margin (ppm):	80	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

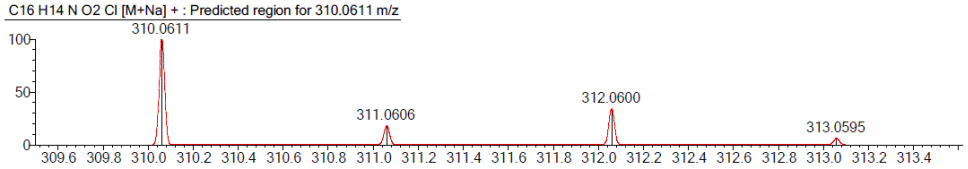
Event#: 1 MS(E+) Ret. Time : 0.633 -> 0.713 - 0.067 -> 0.113 Scan# : 191 -> 215 - 21 -> 35



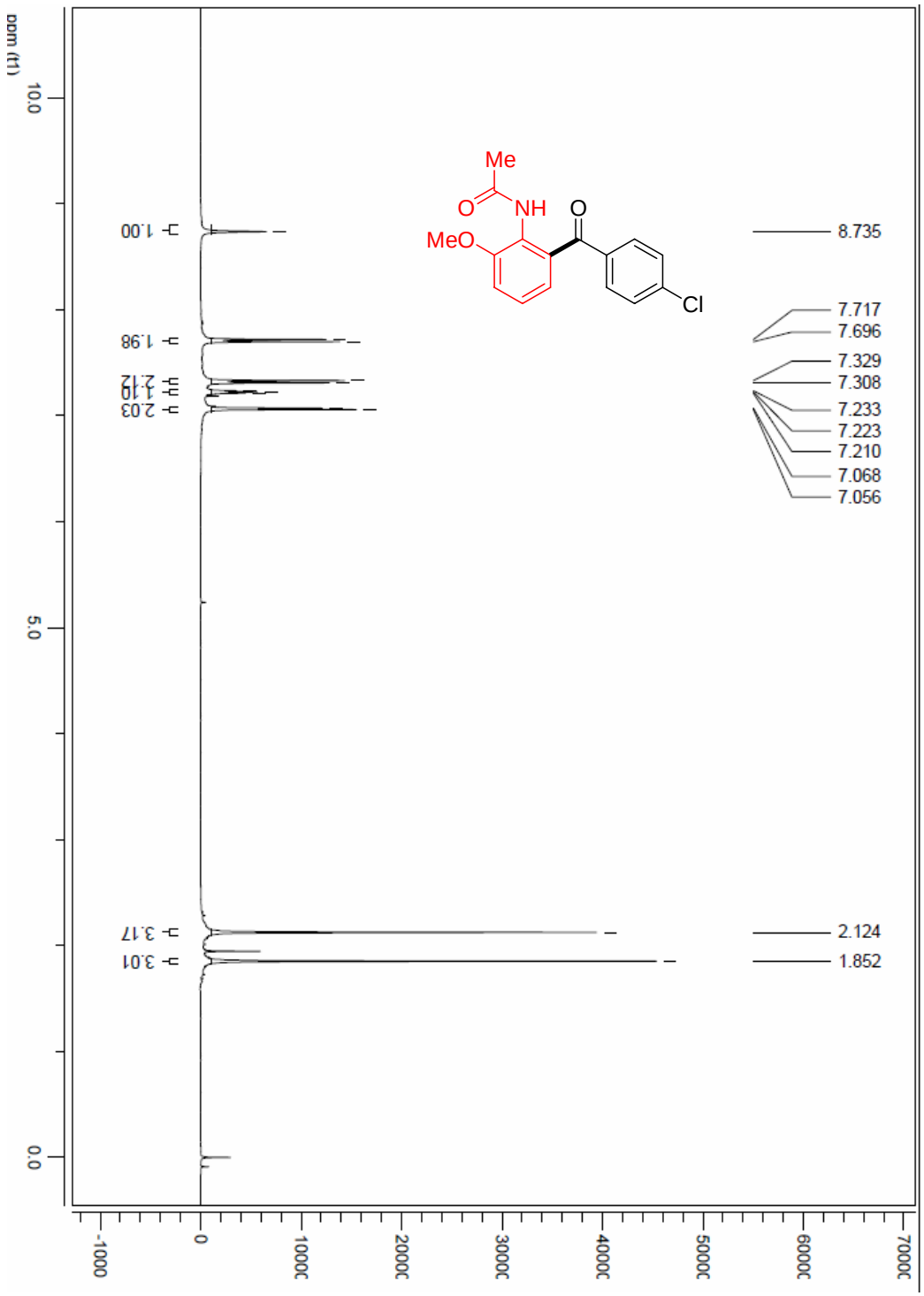
Measured region for 310.0605 m/z

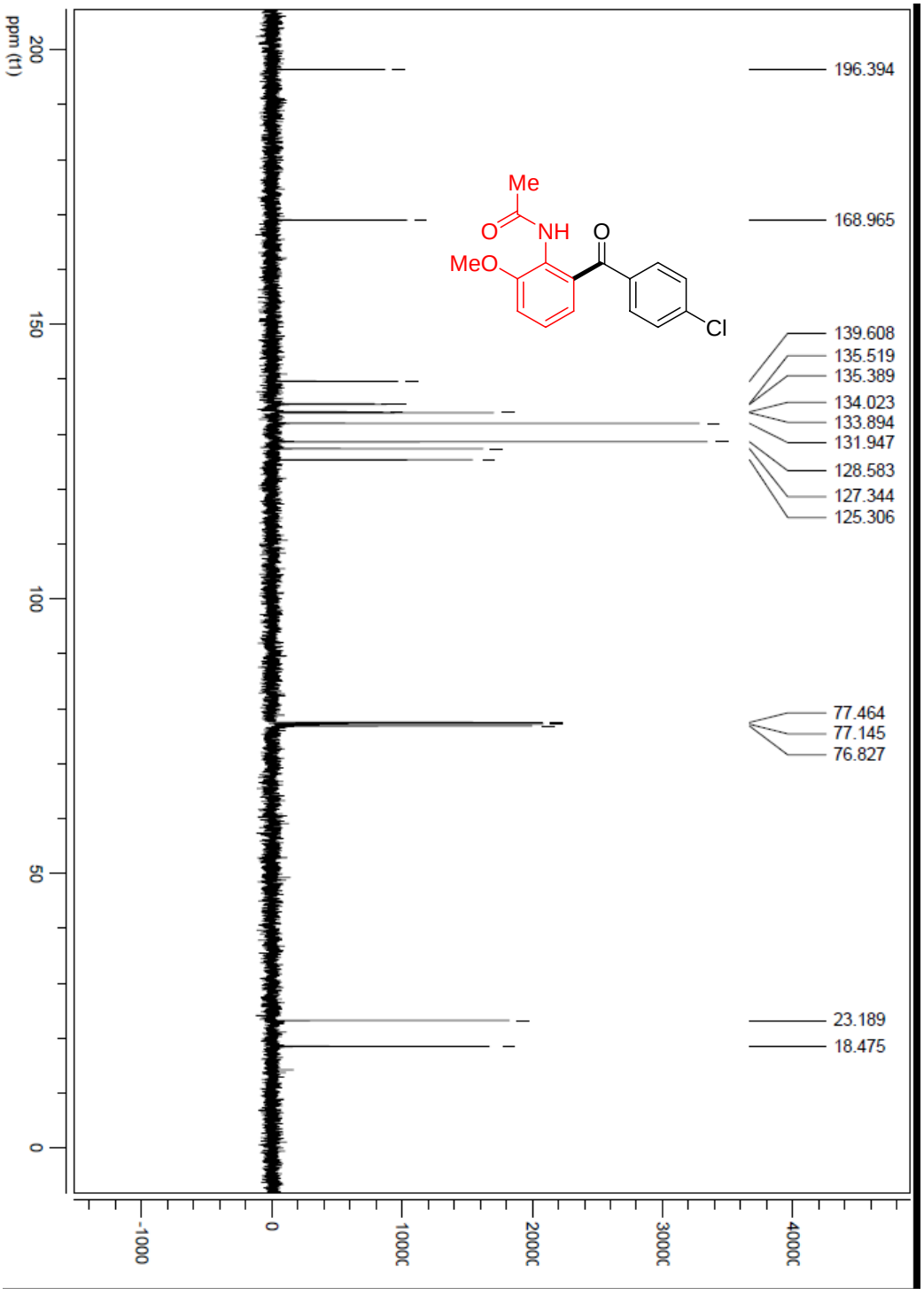


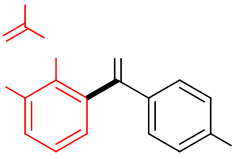
C16 H14 N O2 Cl [M+Na] + : Predicted region for 310.0611 m/z



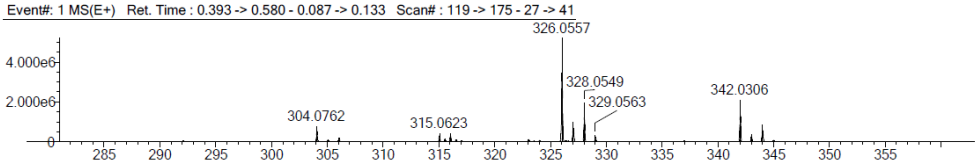
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.97	C16 H14 N O2 Cl	[M+Na] +	310.0605	310.0611	-0.6	-1.94	74.72	10.0

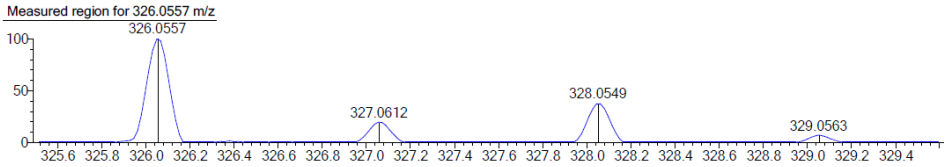

Me
O
NH
O
MeO
Cl
8.735
7.717
7.696
7.329
7.308
7.233
7.223
7.210
7.068
7.056
2.124
1.852
1.00
1.98
2.12
1.10
2.03
3.17
3.01
ppm (f1)
10.0
5.0
0.0
-1000
0
1000
2000
3000
4000
5000
6000
7000

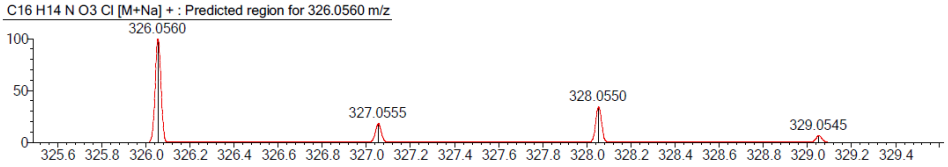

ppm (t1)
200
150
100
50
0
-1000
0
1000
2000
3000
4000
196.394
168.965
139.608
135.519
135.389
134.023
133.894
131.947
128.583
127.344
125.306
77.464
77.145
76.827
23.189
18.475
Me
O
NH
O
MeO
Cl



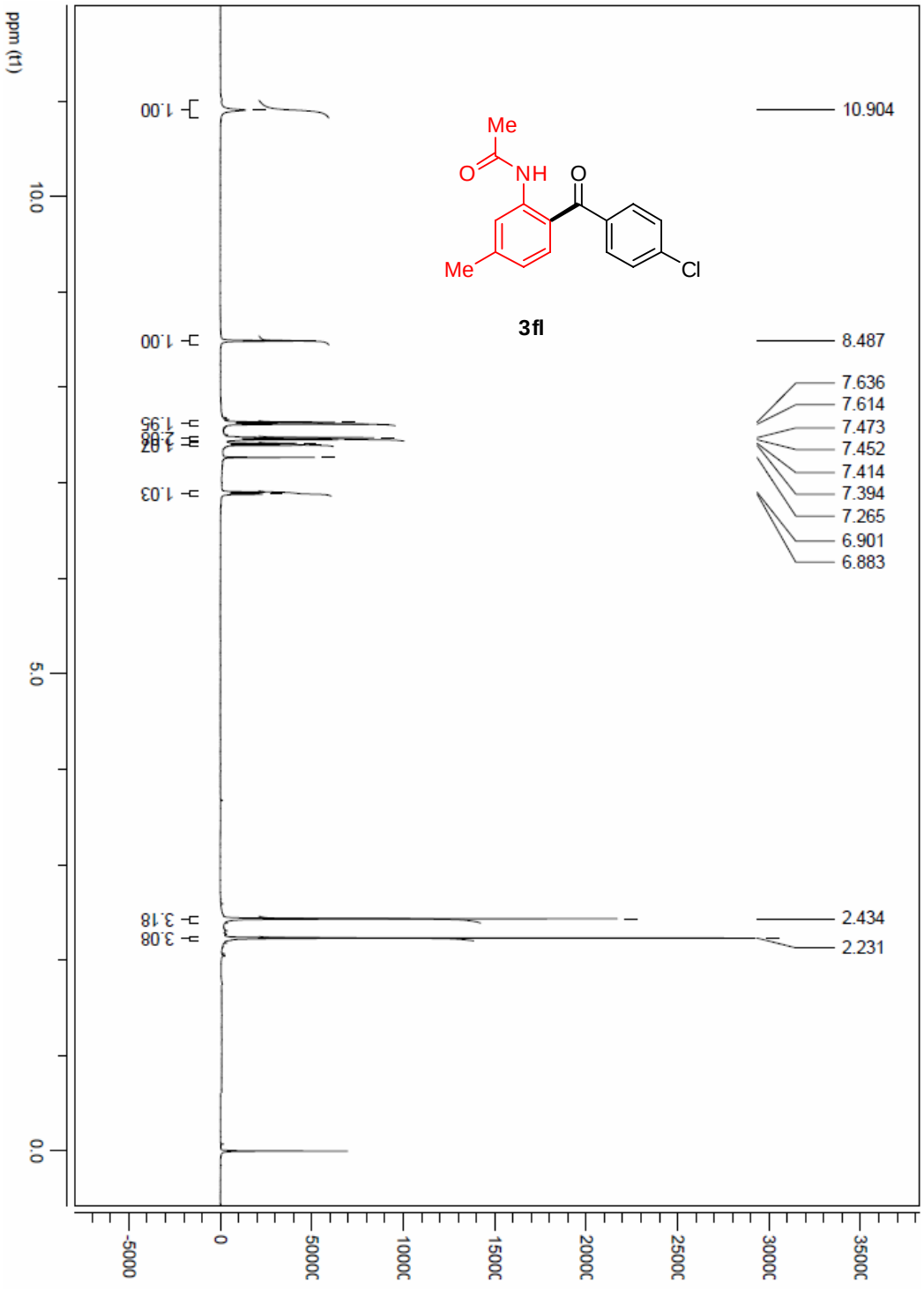
Error Margin (ppm):	80	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

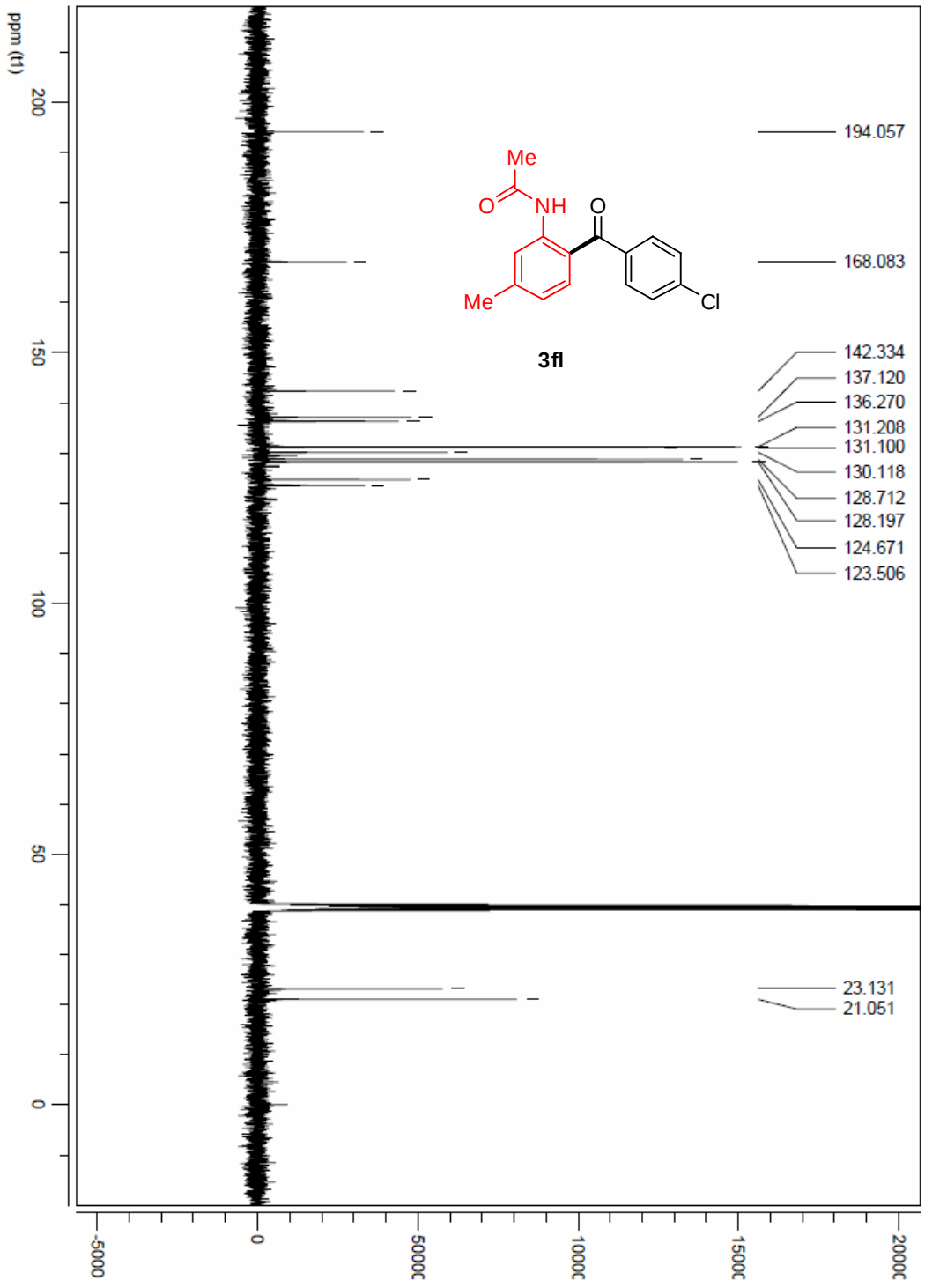


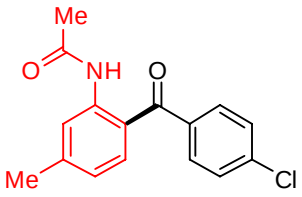




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.69	C16 H14 N O3 Cl	[M+Na] +	326.0557	326.0560	-0.3	-0.92	72.69	10.0


ppm (t1)
10.0
5.0
0.0
1.00
1.00
1.95
2.08
2.02
1.03
3.18
3.08
10.904
8.487
7.636
7.614
7.473
7.452
7.414
7.394
7.265
6.901
6.883
2.434
2.231
Me
O
NH
O
Me
Cl
3fl
-5000
0
5000
10000
15000
20000
25000
30000
35000

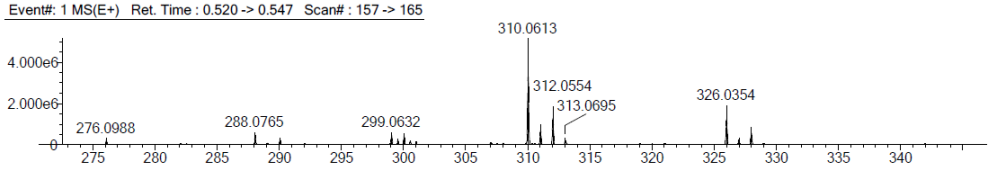

ppm (t1)
200
150
100
50
0
-5000
0
5000
10000
15000
20000
194.057
168.083
142.334
137.120
136.270
131.208
131.100
130.118
128.712
128.197
124.671
123.506
23.131
21.051
Me
O
NH
O
Me
Cl
3fl



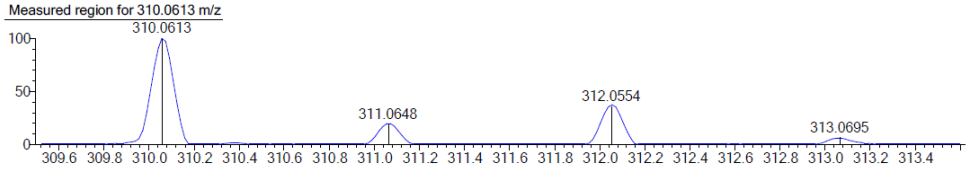
3fl

Error Margin (ppm):	100	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

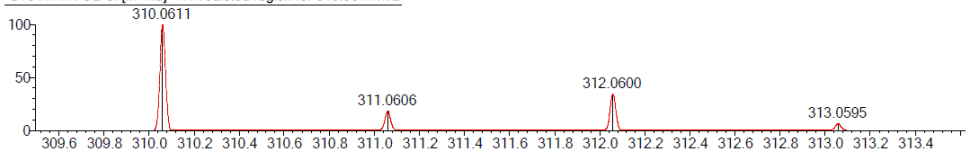
Event#: 1 MS(E+) Ret. Time : 0.520 -> 0.547 Scan# : 157 -> 165



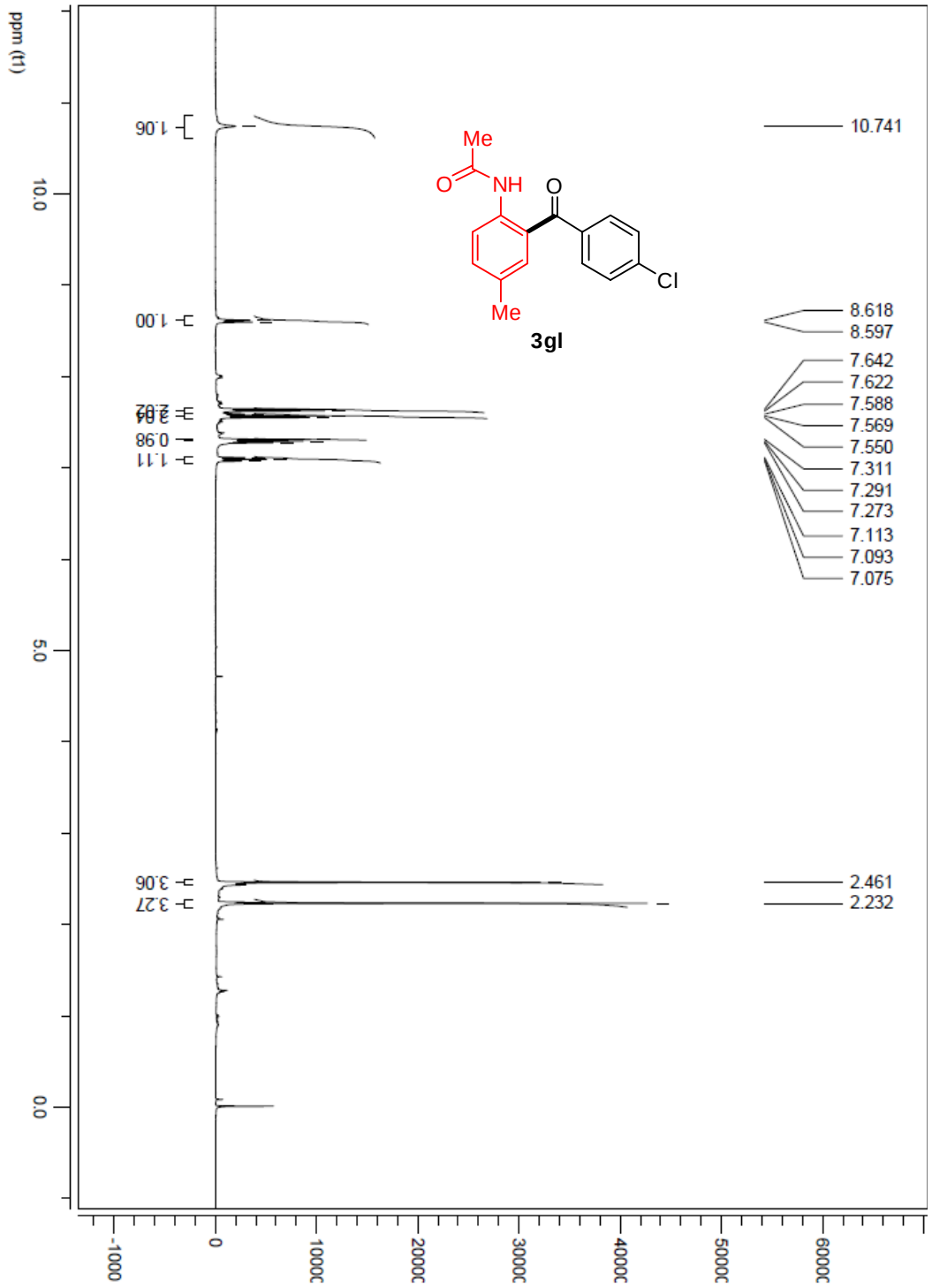
Measured region for 310.0613 m/z

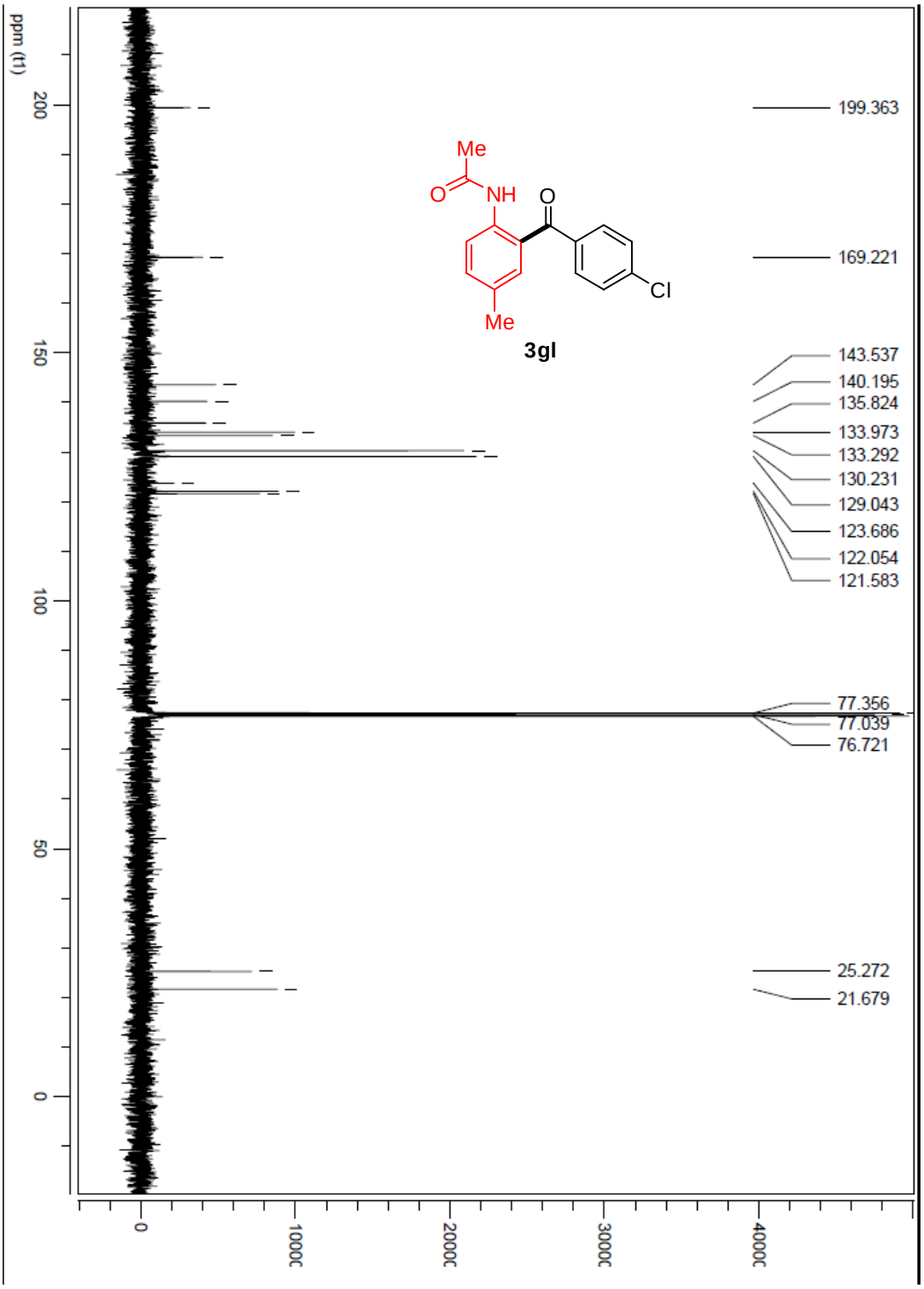


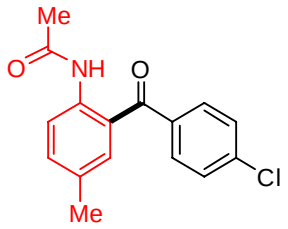
C16 H14 N O2 Cl [M+Na] + : Predicted region for 310.0611 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.94	C16 H14 N O2 Cl	[M+Na] +	310.0613	310.0611	0.2	0.65	72.94	10.0


ppm (t1)
10.0
5.0
0.0
1.06
1.00
2.04
0.98
1.11
3.06
3.27
Me
O
NH
O
Cl
Me
3gl
10.741
8.618
8.597
7.642
7.622
7.588
7.569
7.550
7.311
7.291
7.273
7.113
7.093
7.075
2.461
2.232
-1000
0
1000
2000
3000
4000
5000
6000

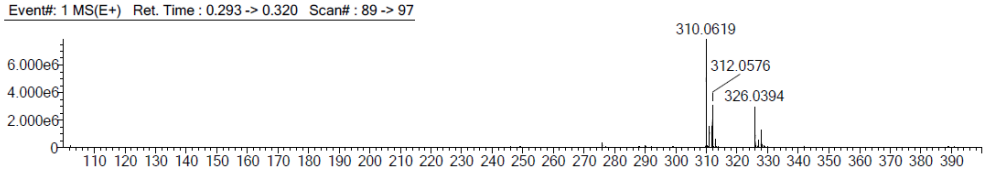

ppm (t1)
200
150
100
50
0
0
10000
20000
30000
40000
Me
O
NH
O
Cl
Me
3gl
199.363
169.221
143.537
140.195
135.824
133.973
133.292
130.231
129.043
123.686
122.054
121.583
77.356
77.039
76.721
25.272
21.679



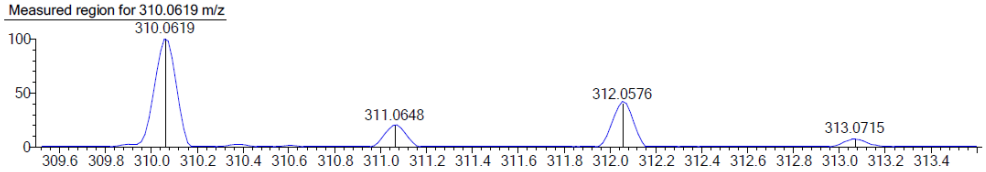
3gl

Error Margin (ppm):	100	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

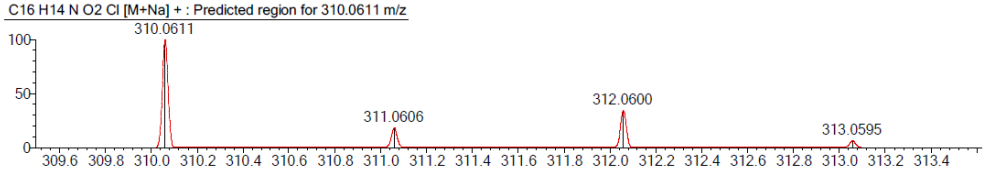
Event#: 1 MS(E+) Ret. Time : 0.293 -> 0.320 Scan# : 89 -> 97



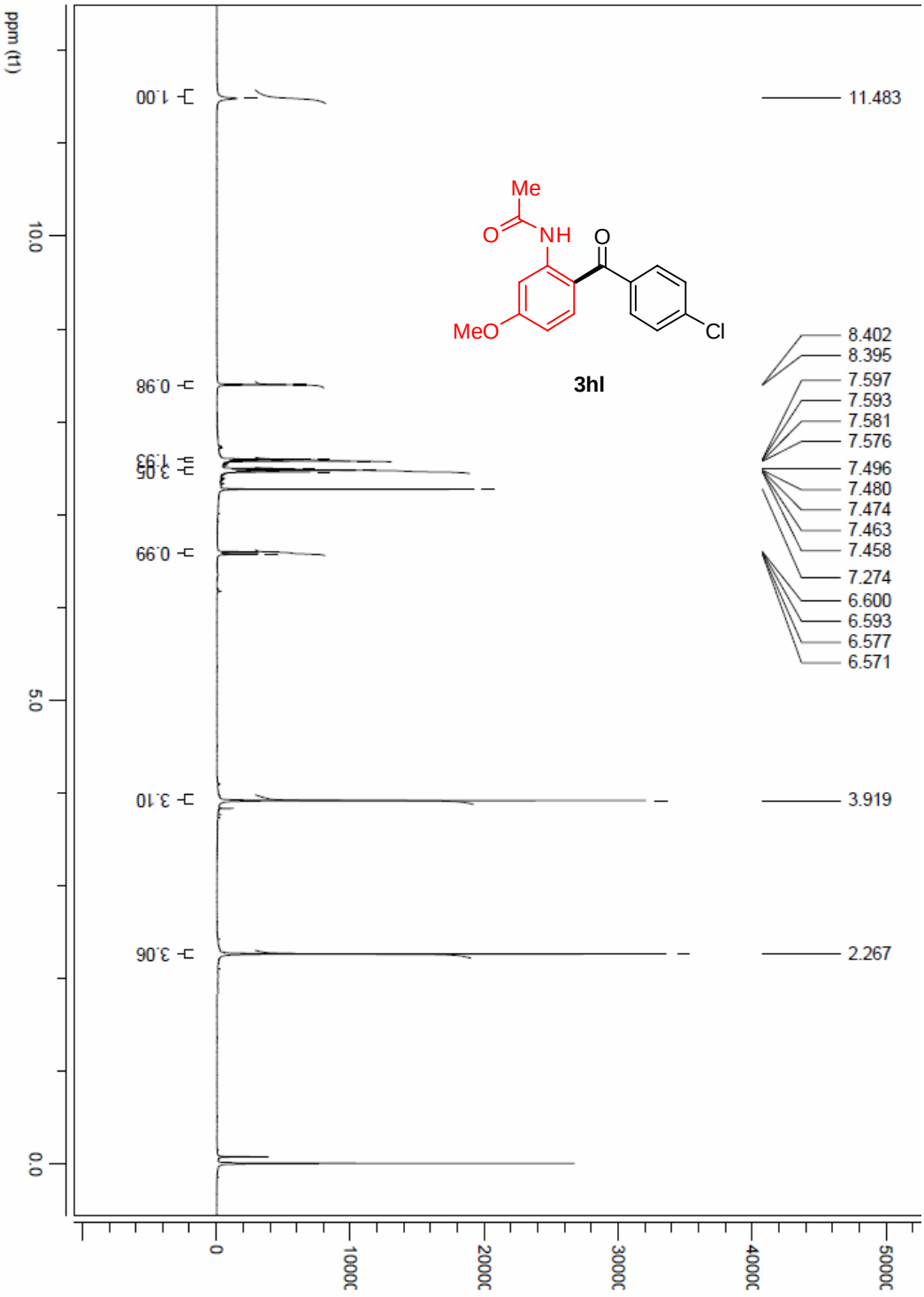
Measured region for 310.0619 m/z

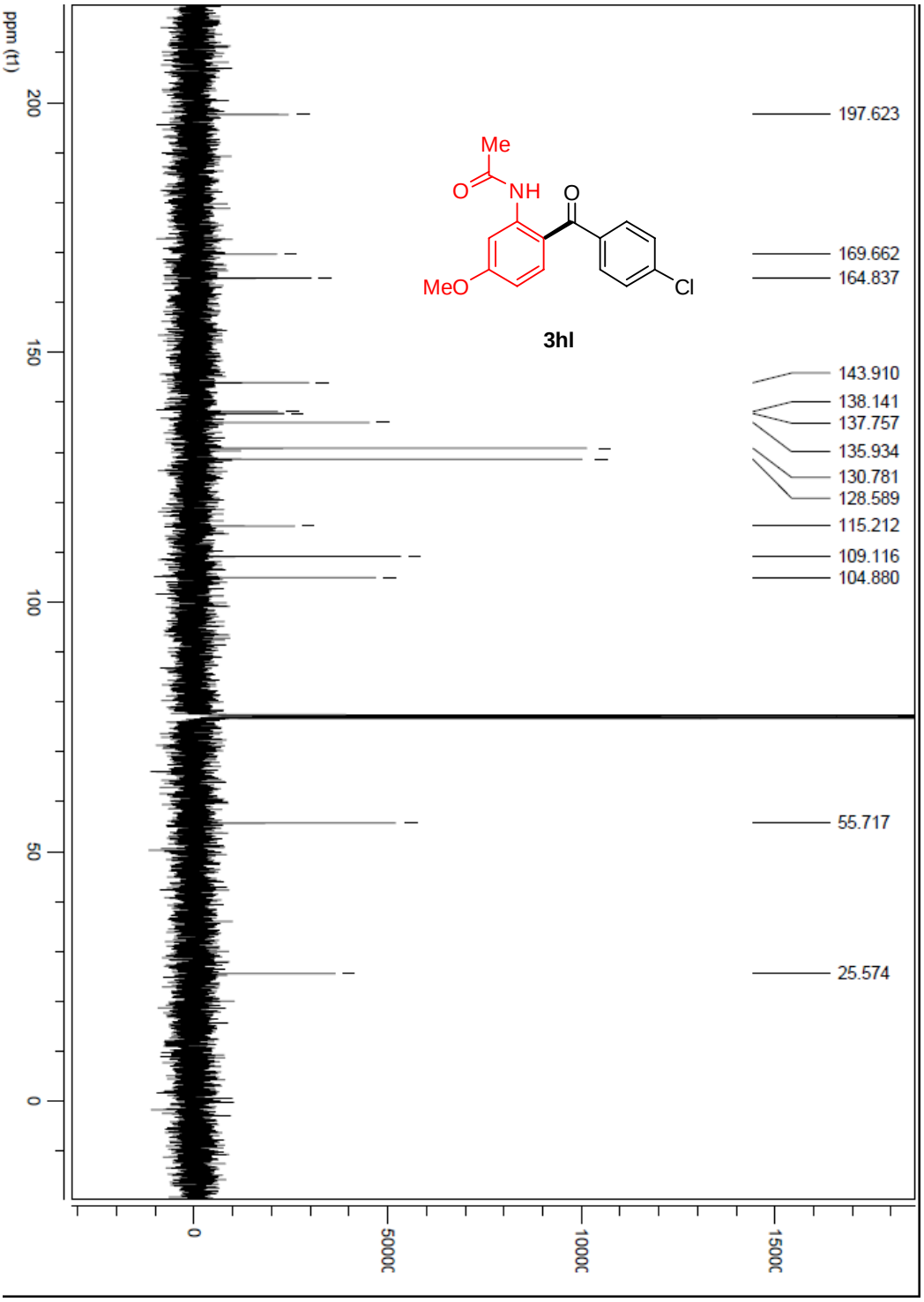


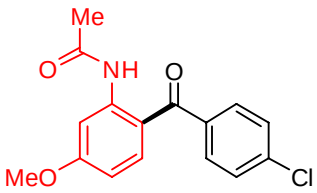
C16 H14 N O2 Cl [M+Na] + : Predicted region for 310.0611 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.15	C16 H14 N O2 Cl	[M+Na] +	310.0619	310.0611	0.8	2.58	53.25	10.0


ppm (t1)
10.0
5.0
0.0
1.00
0.98
1.93
3.05
0.99
3.10
3.06
11.483
8.402
8.395
7.597
7.593
7.581
7.576
7.496
7.480
7.474
7.463
7.458
7.274
6.600
6.593
6.577
6.571
3.919
2.267
Me
O
NH
O
MeO
Cl
3hl
0
10000
20000
30000
40000
50000

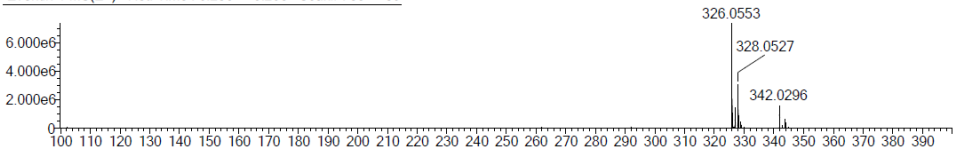

ppm (t1)
200
150
100
50
0
0
50000
100000
150000
Me
O
NH
O
MeO
Cl
3hl
197.623
169.662
164.837
143.910
138.141
137.757
135.934
130.781
128.589
115.212
109.116
104.880
55.717
25.574



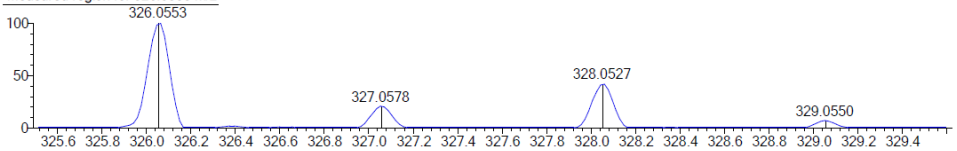
3hl

Error Margin (ppm):	100	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

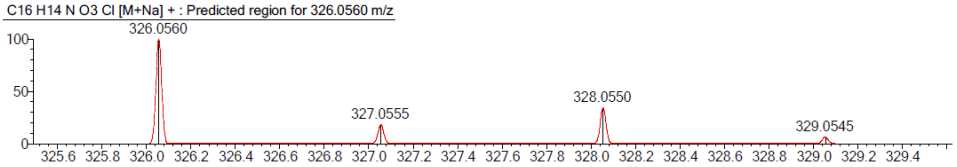
Event#: 1 MS(E+) Ret. Time : 0.280 -> 0.293 Scan# : 85 -> 89



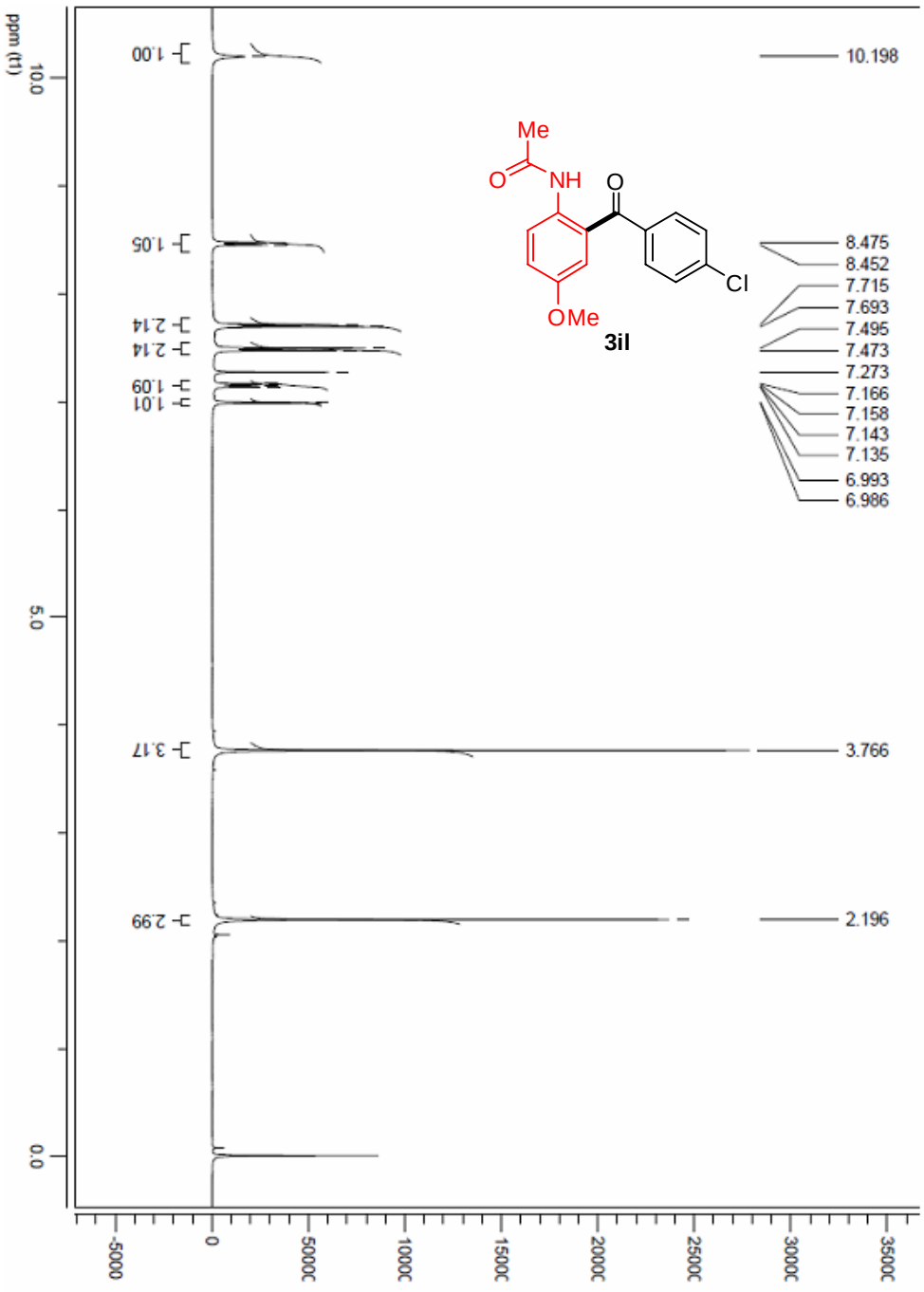
Measured region for 326.0553 m/z

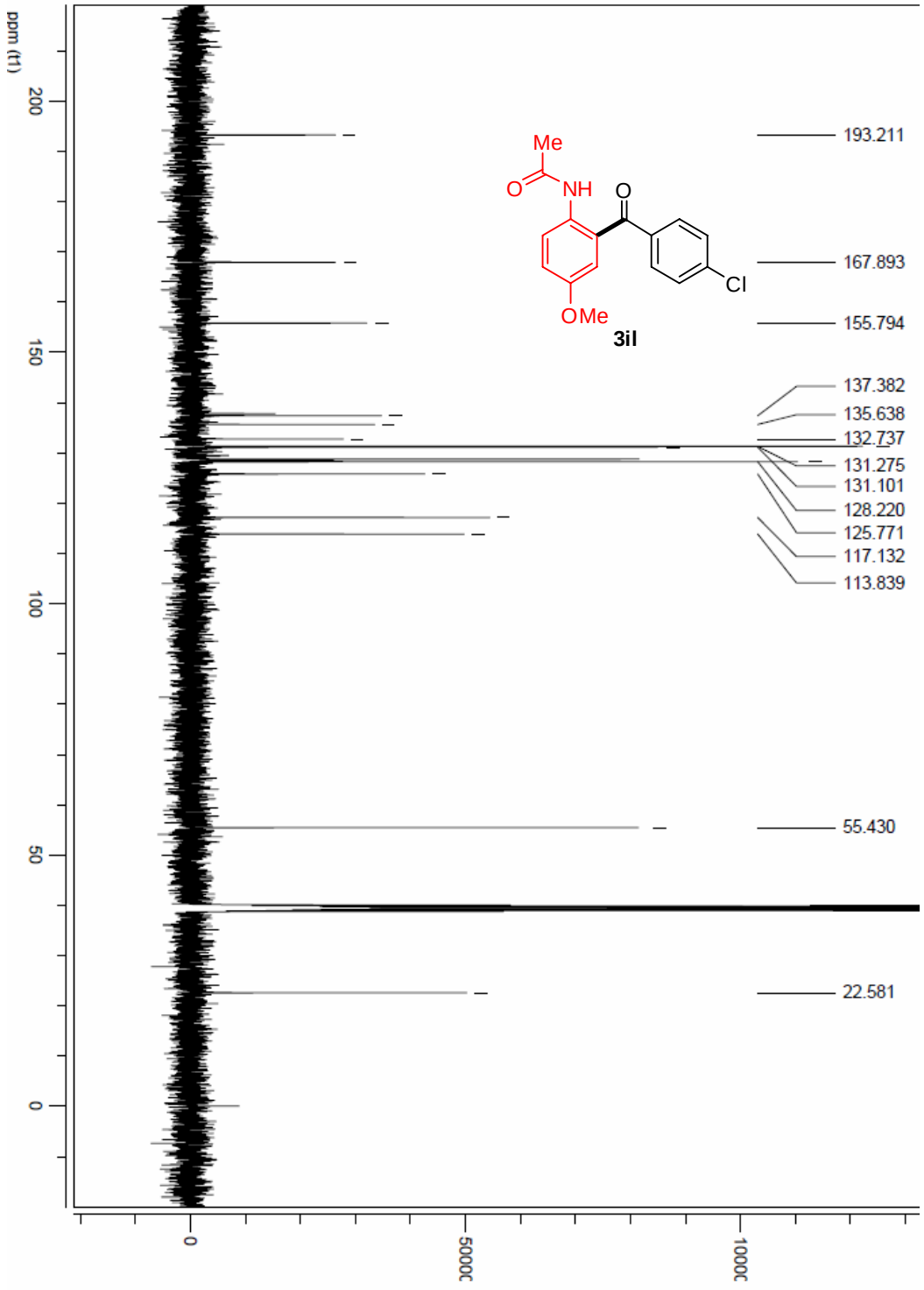


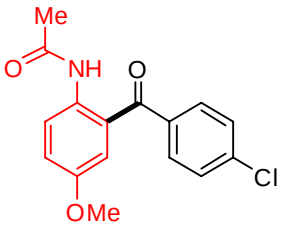
C16 H14 N O3 Cl [M+Na] + : Predicted region for 326.0560 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	54.69	C16 H14 N O3 Cl	[M+Na] +	326.0553	326.0560	-0.7	-2.15	56.31	10.0


ppm (t1)
10.0
5.0
0.0
1.00
1.05
2.14
2.14
1.09
1.01
3.17
2.99
10.198
8.475
8.452
7.715
7.693
7.495
7.473
7.273
7.166
7.158
7.143
7.135
6.993
6.986
3.766
2.196
Me
O
NH
O
Cl
OMe
3il
-5000
0
5000
10000
15000
20000
25000
30000
35000

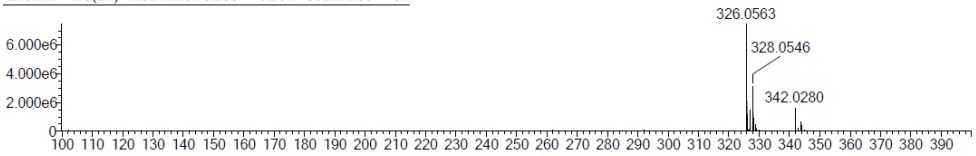

ppm (t1)
200
150
100
50
0
0
50000
100000
193.211
167.893
155.794
137.382
135.638
132.737
131.275
131.101
128.220
125.771
117.132
113.839
55.430
22.581
Me
O
NH
O
Cl
OMe
3il



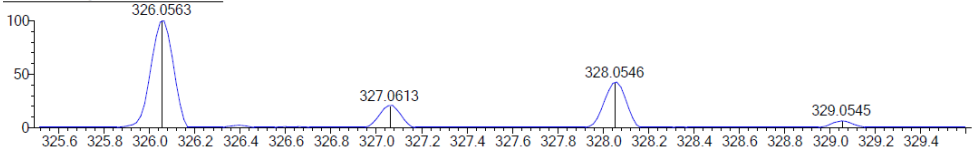
3il

Error Margin (ppm):	100	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

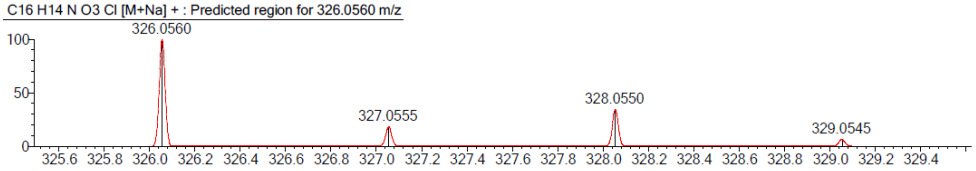
Event#: 1 MS(E+) Ret. Time : 0.280 -> 0.287 Scan# : 85 -> 87



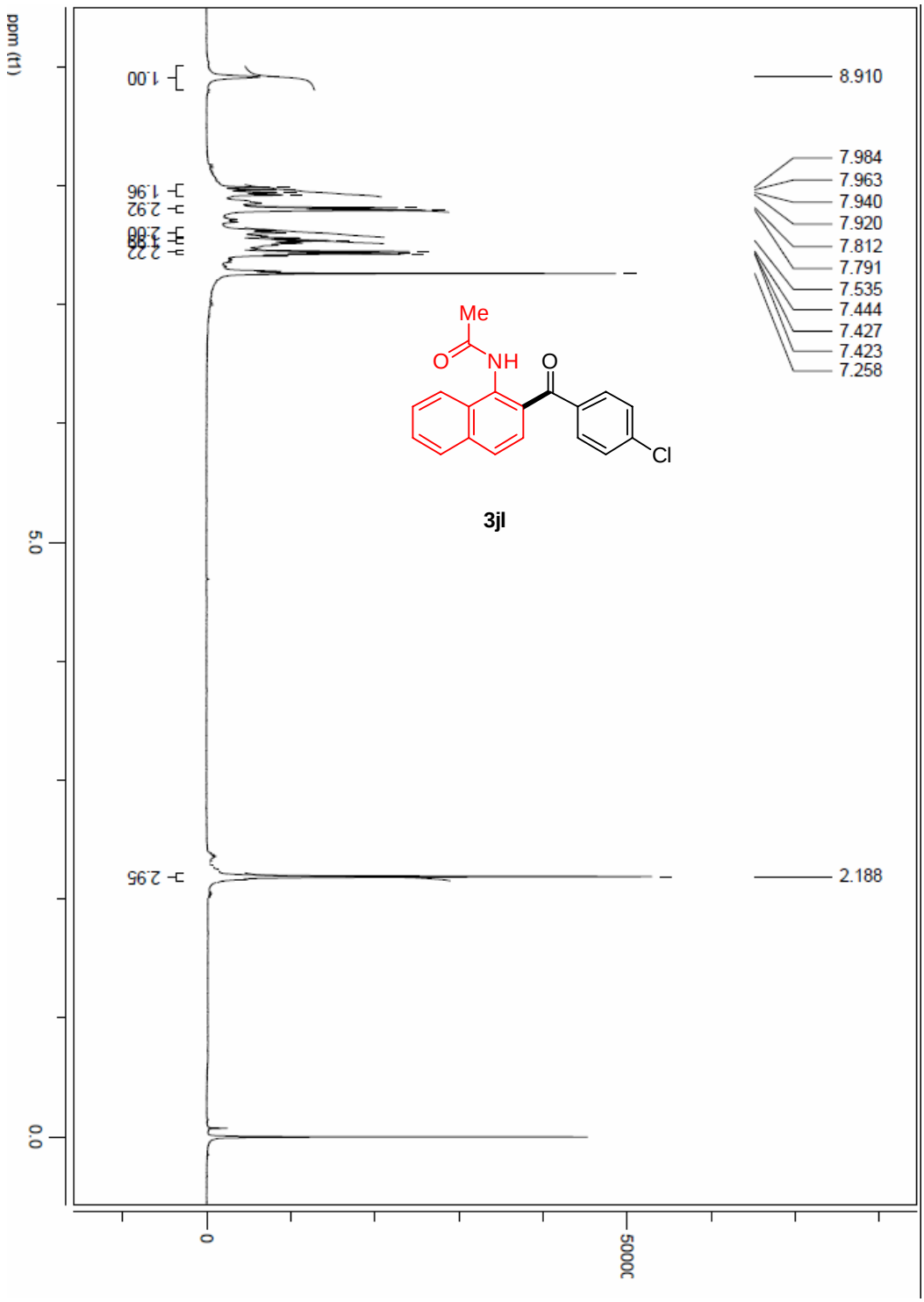
Measured region for 326.0563 m/z



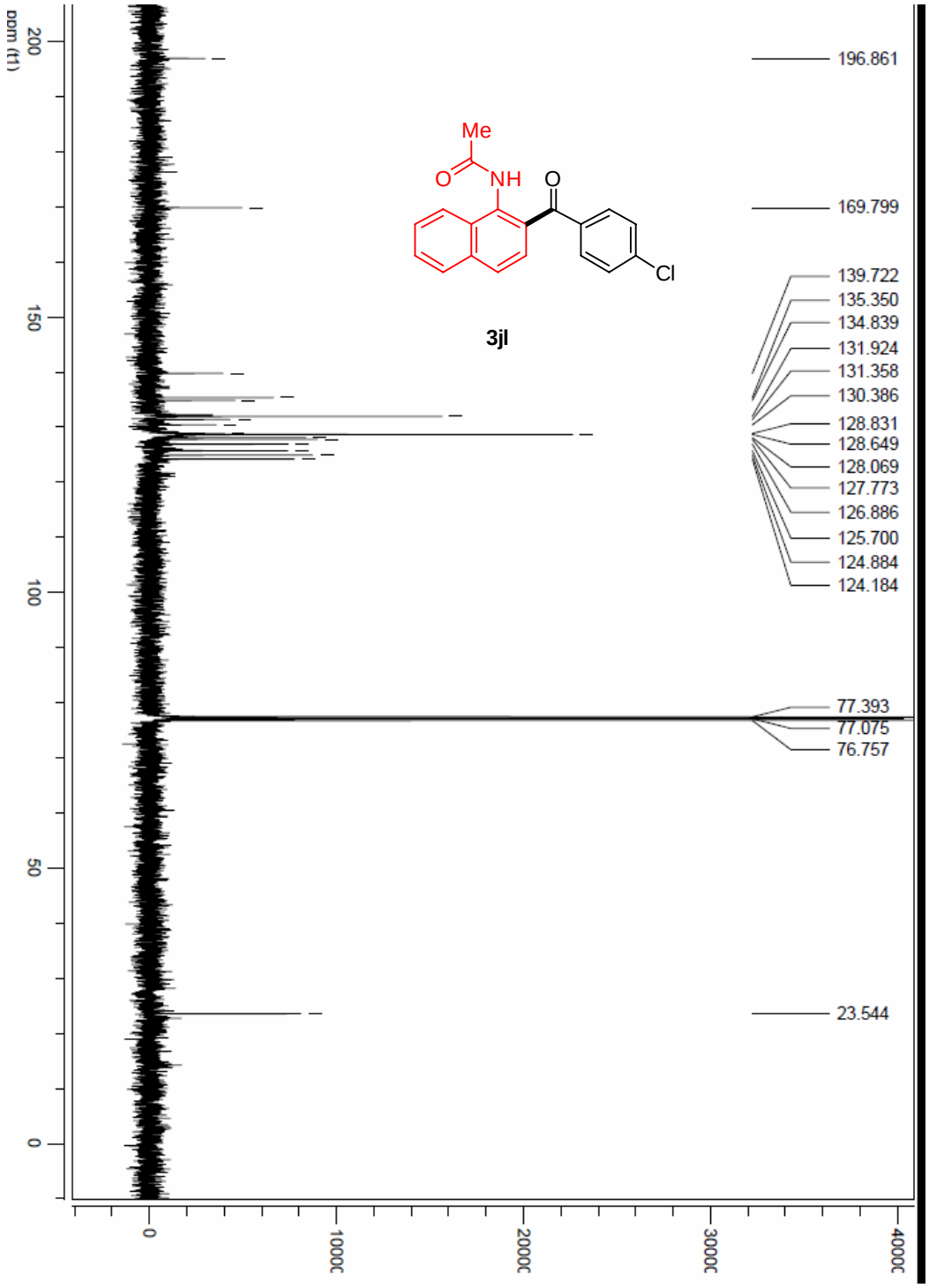
C16 H14 N O3 Cl [M+Na] + : Predicted region for 326.0560 m/z

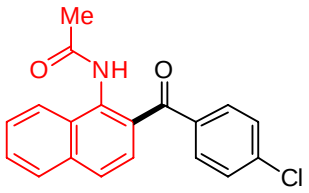


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	53.66	C16 H14 N O3 Cl	[M+Na] +	326.0563	326.0560	0.3	0.92	53.66	10.0


ppm (t1)
5.0
0.0
1.00
1.96
2.92
2.00
3.88
2.22
2.95
8.910
7.984
7.963
7.940
7.920
7.812
7.791
7.535
7.444
7.427
7.423
7.258
2.188
Me
O
NH
O
Cl
0
50000

3jl

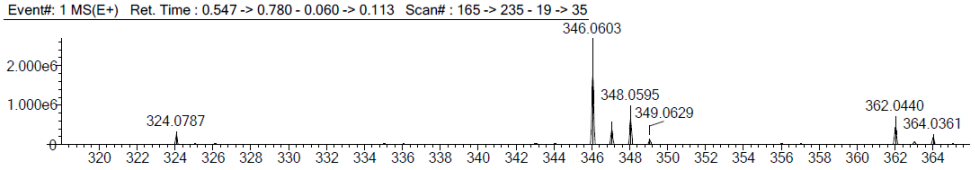

ppm (t1)
200
150
100
50
0
0
10000
20000
30000
40000
Me
O
NH
O
Cl
3jl
196.861
169.799
139.722
135.350
134.839
131.924
131.358
130.386
128.831
128.649
128.069
127.773
126.886
125.700
124.884
124.184
77.393
77.075
76.757
23.544



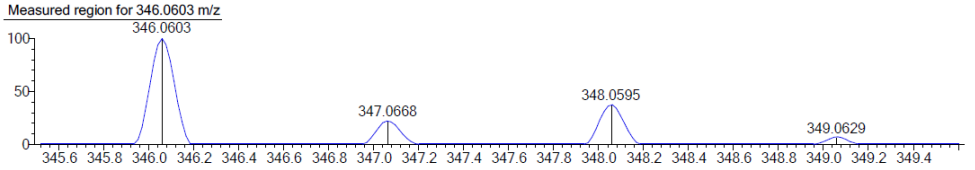
3jl

Error Margin (ppm):	80	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

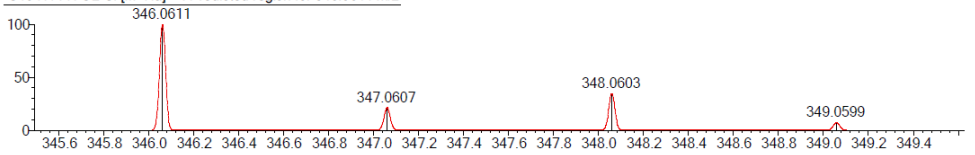
Event#: 1 MS(E+) Ret. Time : 0.547 -> 0.780 - 0.060 -> 0.113 Scan# : 165 -> 235 - 19 -> 35



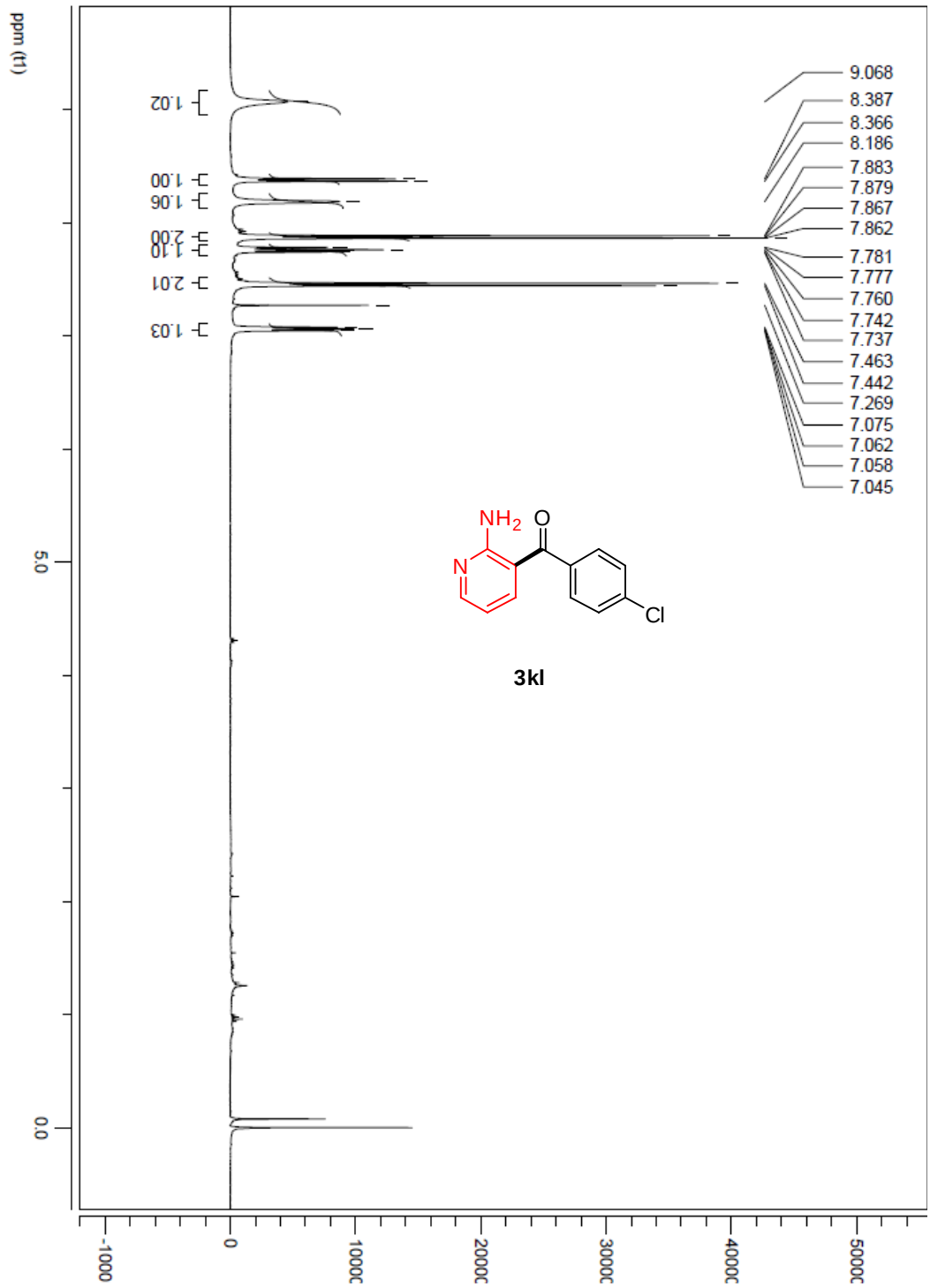
Measured region for 346.0603 m/z



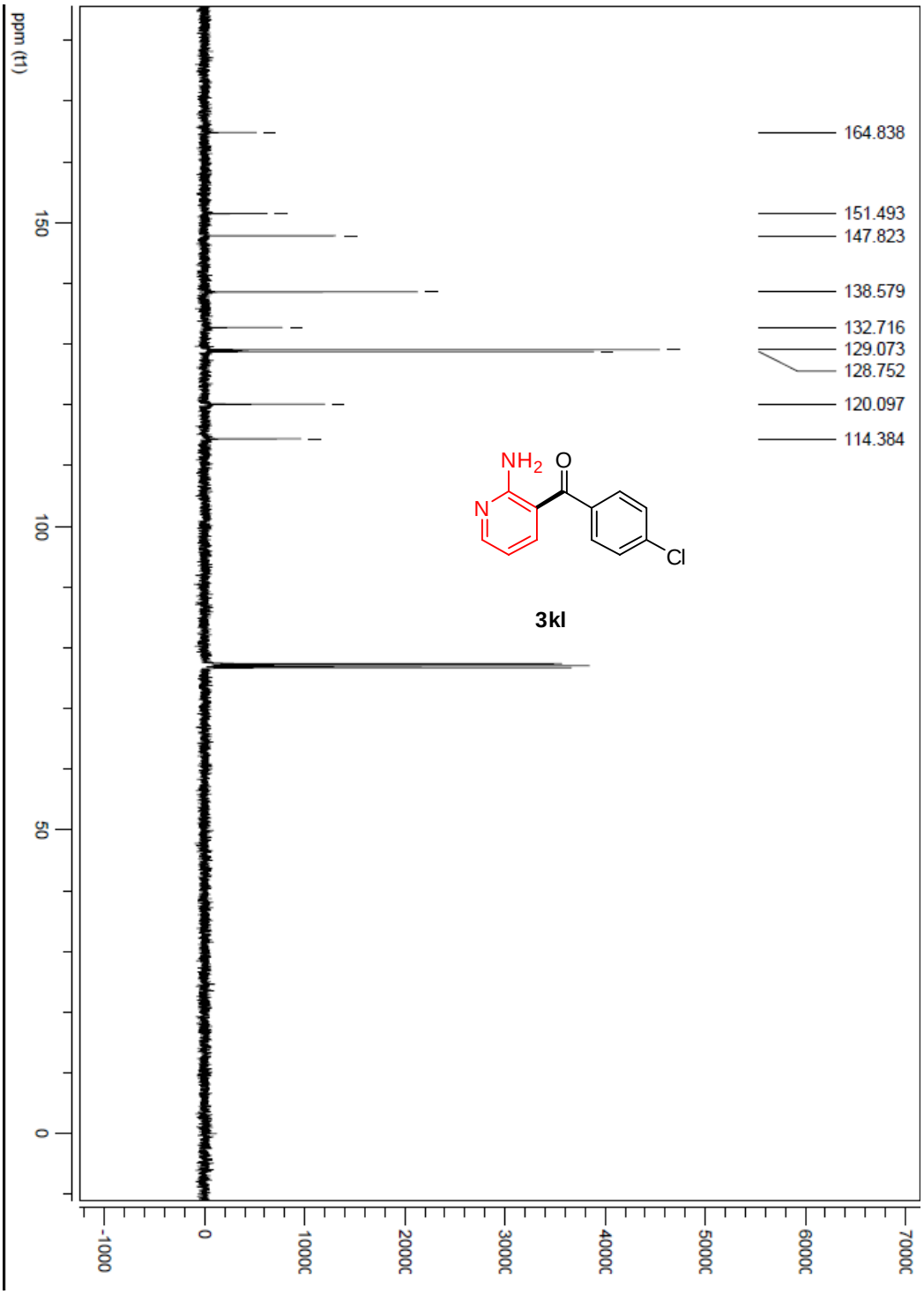
C19 H14 N O2 Cl [M+Na] + : Predicted region for 346.0611 m/z

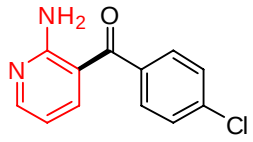


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	75.58	C19 H14 N O2 Cl	[M+Na] +	346.0603	346.0611	-0.8	-2.31	78.14	13.0

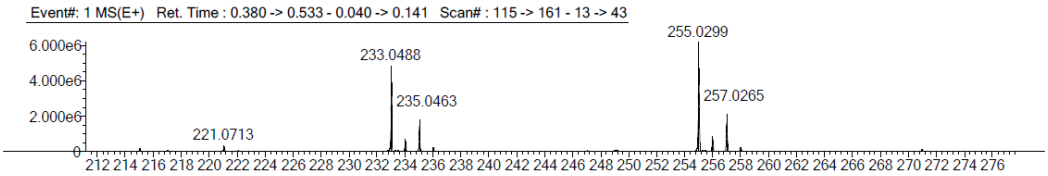

ppm (t1)
5.0
0.0
1.02
1.00
1.06
2.00
1.10
2.01
1.03
9.068
8.387
8.366
8.186
7.883
7.879
7.867
7.862
7.781
7.777
7.760
7.742
7.737
7.463
7.442
7.269
7.075
7.062
7.058
7.045
NH2
O
N
Cl
-1000
0
1000
2000
3000
4000
5000

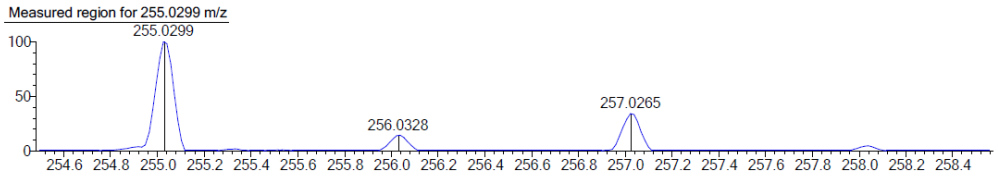
3kl

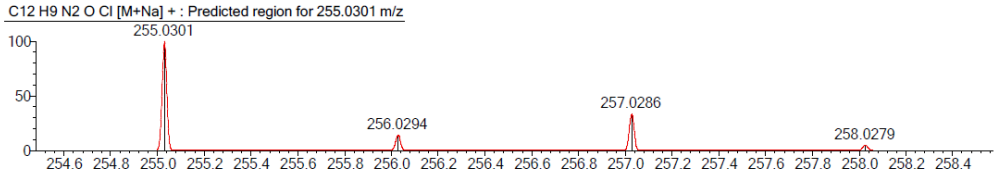

ppm (f1)
150
100
50
0
-1000
0
1000
2000
3000
4000
5000
6000
7000
164.838
151.493
147.823
138.579
132.716
129.073
128.752
120.097
114.384
NH2
O
N
Cl
3kl



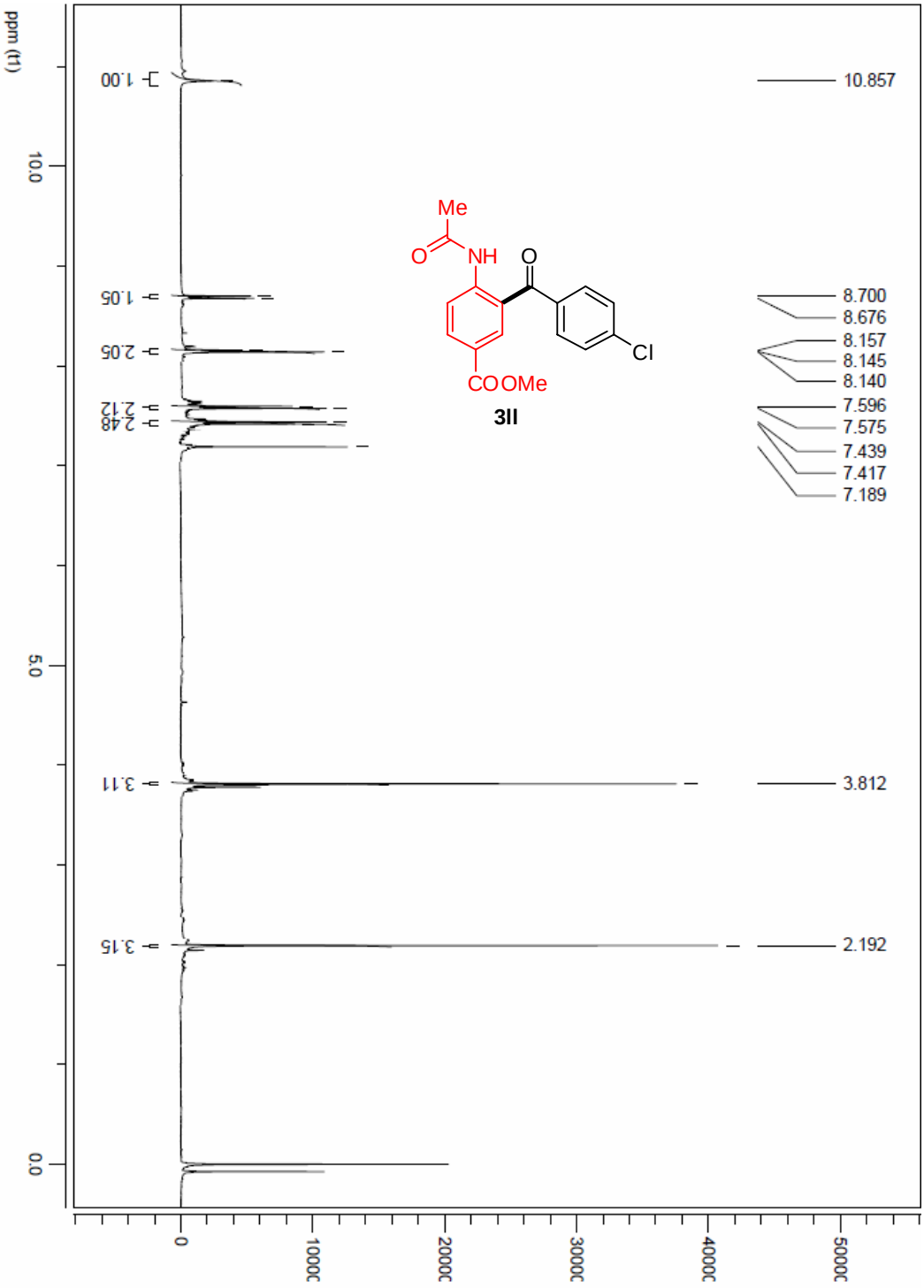
3kl



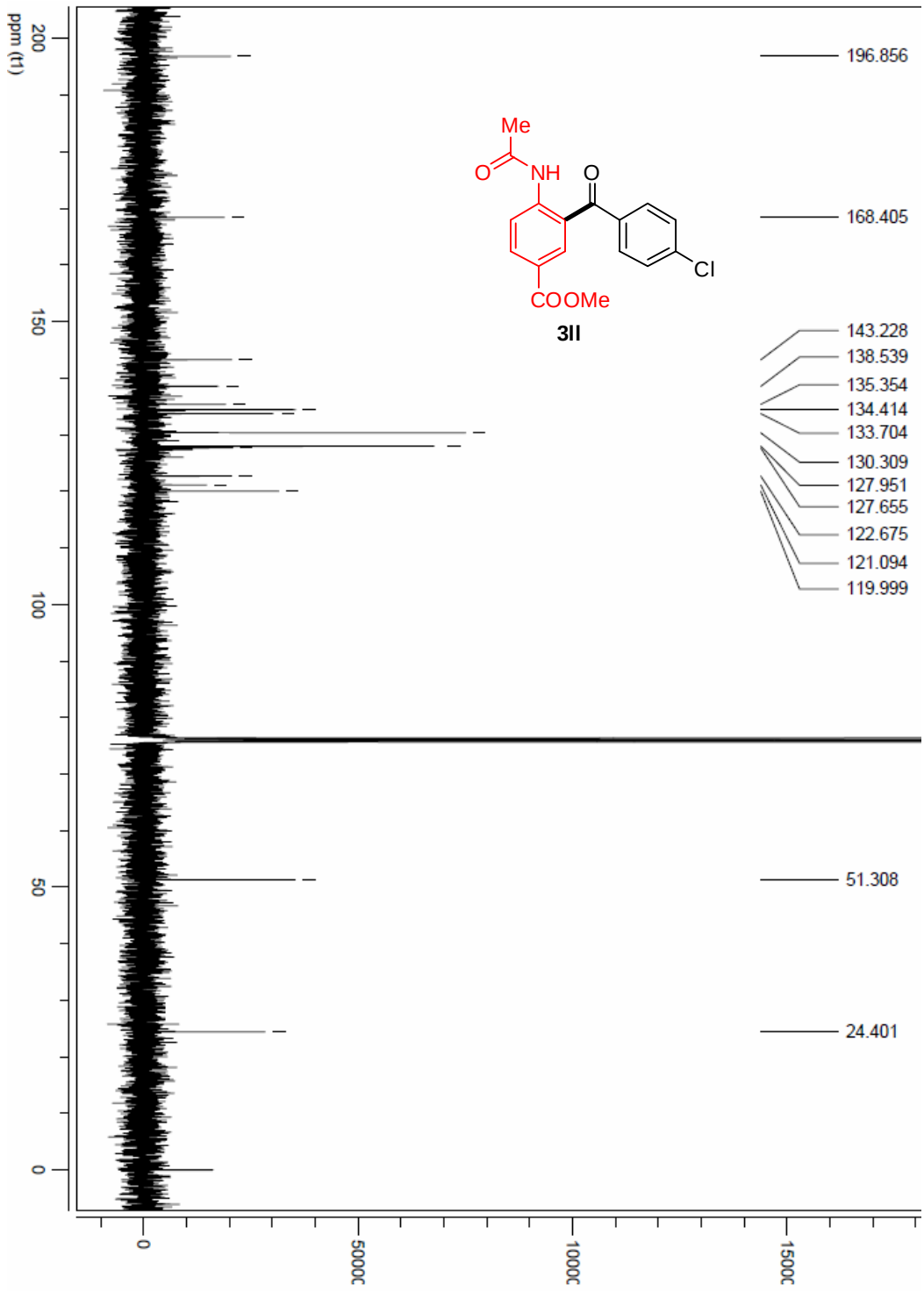


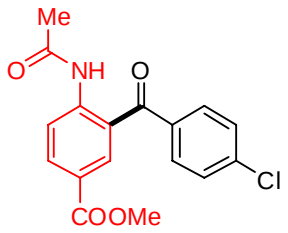


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	75.67	C12 H9 N2 O Cl	[M+Na] +	255.0299	255.0301	-0.2	-0.78	75.67	9.0


ppm (t1)
10.0
5.0
0.0
1.00
1.05
2.05
2.12
2.48
3.11
3.15
10.857
8.700
8.676
8.157
8.145
8.140
7.596
7.575
7.439
7.417
7.189
3.812
2.192
Me
O
NH
O
Cl
COOMe
0
10000
20000
30000
40000
50000

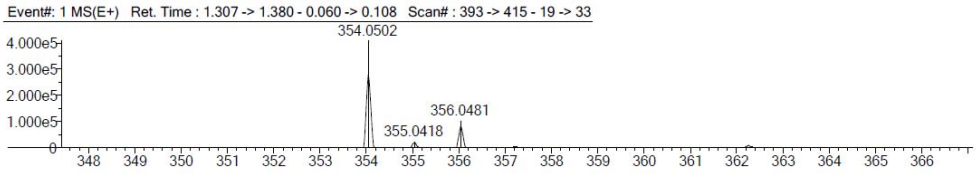
3ll

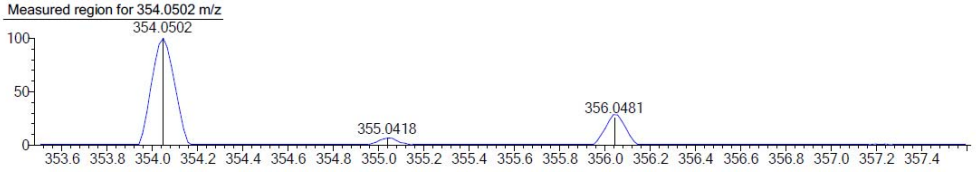

ppm (t1)
200
150
100
50
0
0
5000
10000
15000
196.856
168.405
143.228
138.539
135.354
134.414
133.704
130.309
127.951
127.655
122.675
121.094
119.999
51.308
24.401
Me
O
NH
O
Cl
COOMe
3ll

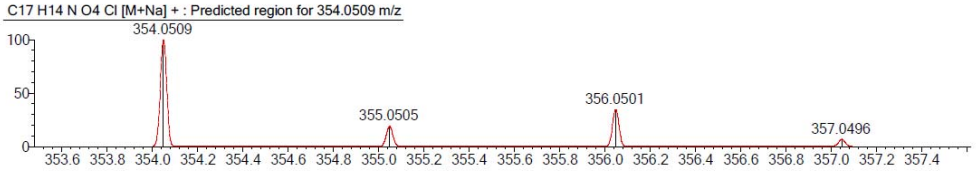


3ll

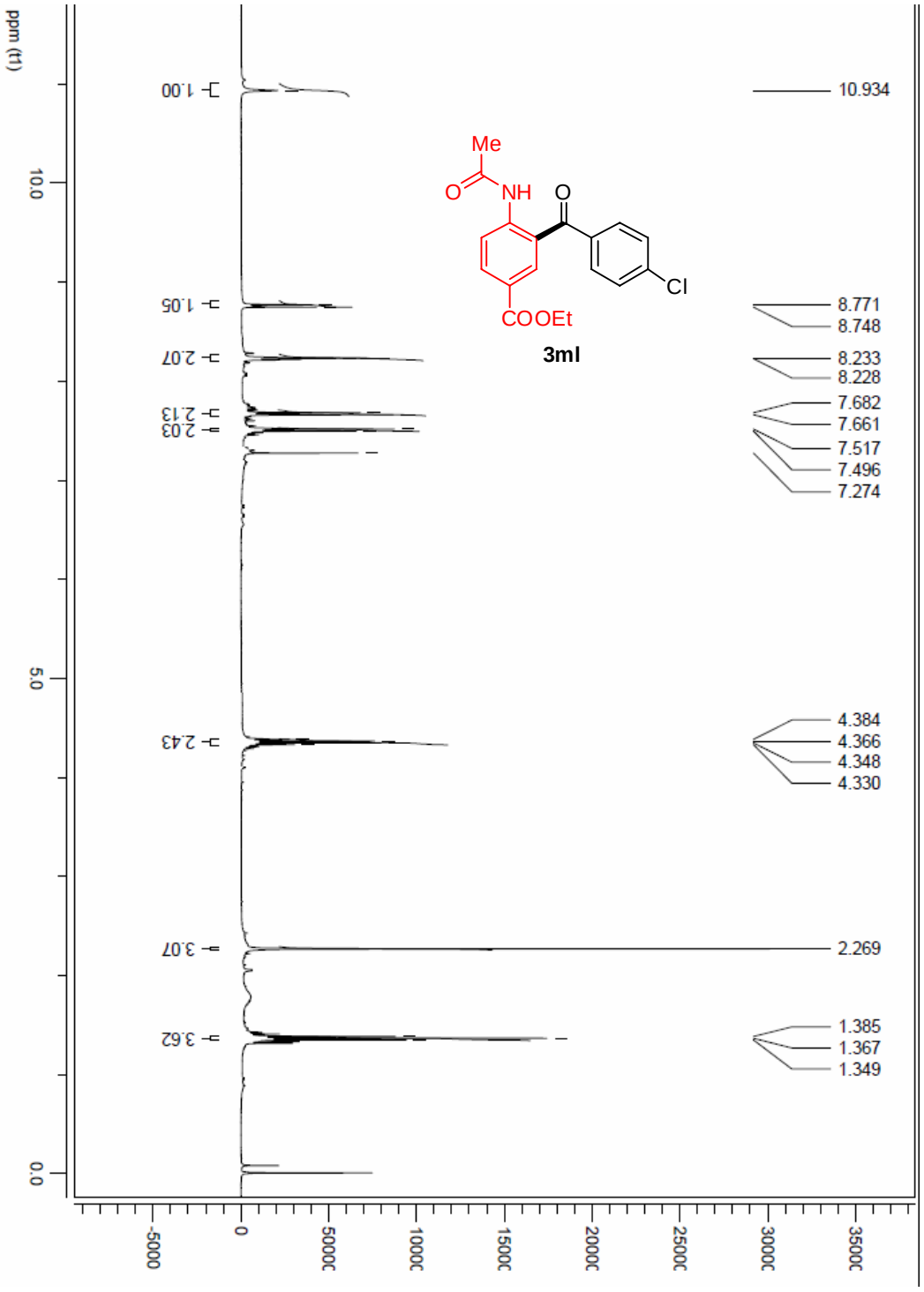
Error Margin (ppm):	80	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

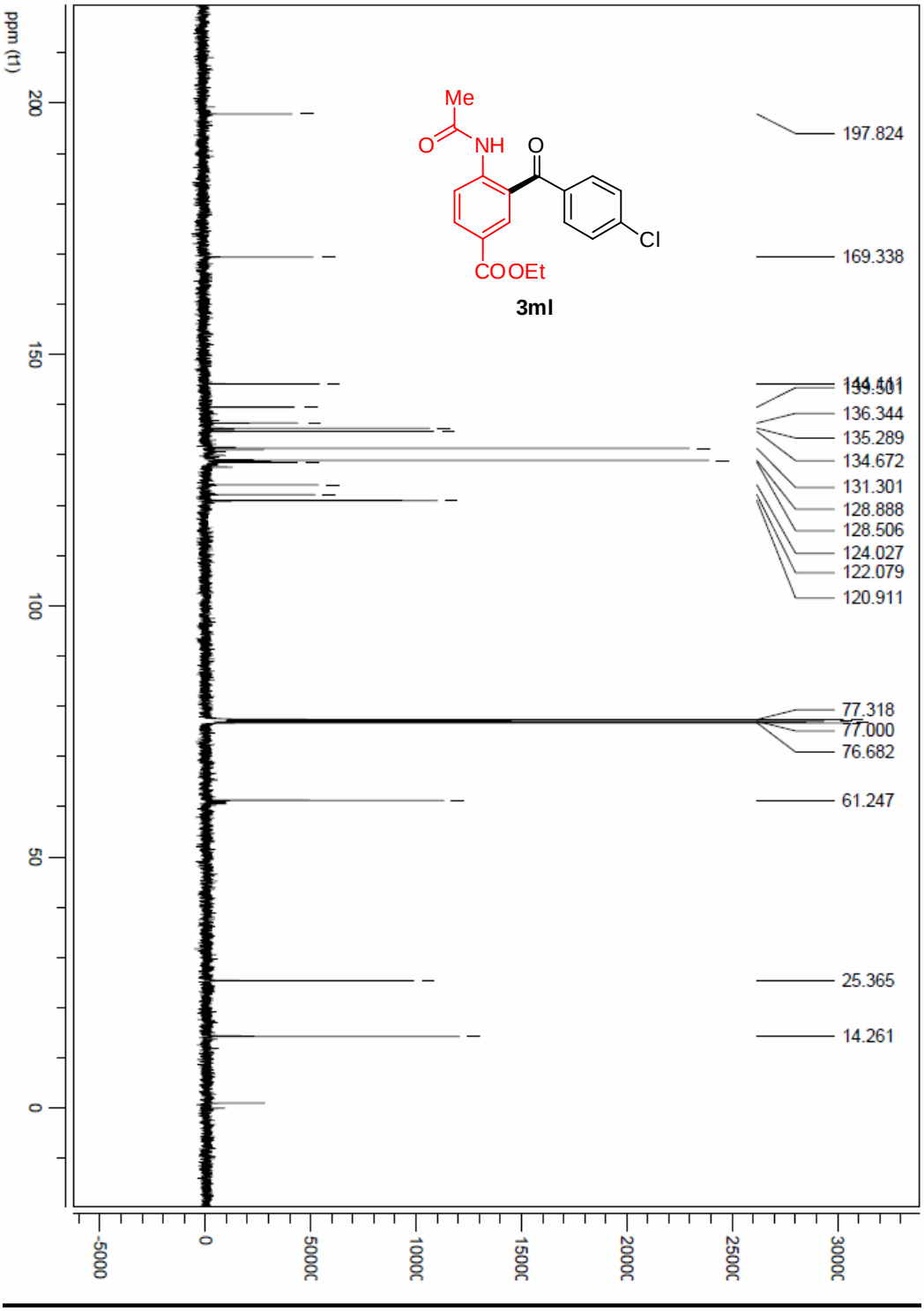


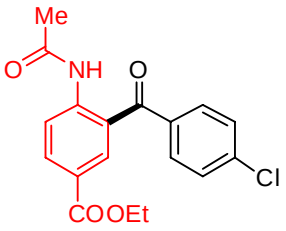




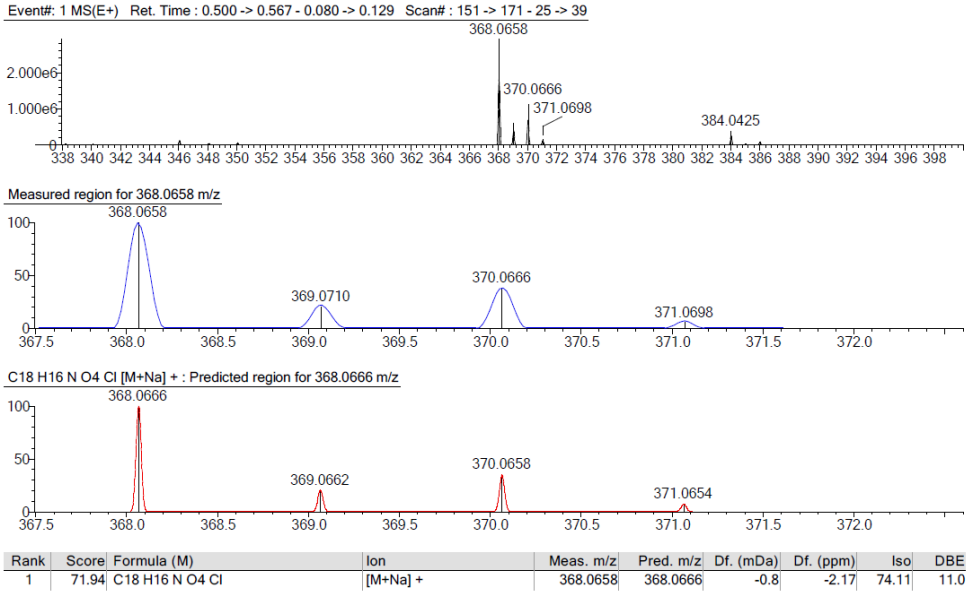
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	43.63	C17 H14 N O4 Cl	[M+Na] +	354.0502	354.0509	-0.7	-1.98	44.72	11.0


ppm (t1)
10.0
5.0
0.0
1.00
1.05
2.07
2.13
2.03
2.43
3.07
3.62
10.934
8.771
8.748
8.233
8.228
7.682
7.661
7.517
7.496
7.274
4.384
4.366
4.348
4.330
2.269
1.385
1.367
1.349
Me
O
NH
O
Cl
COOEt
3ml
-5000
0
5000
10000
15000
20000
25000
30000
35000

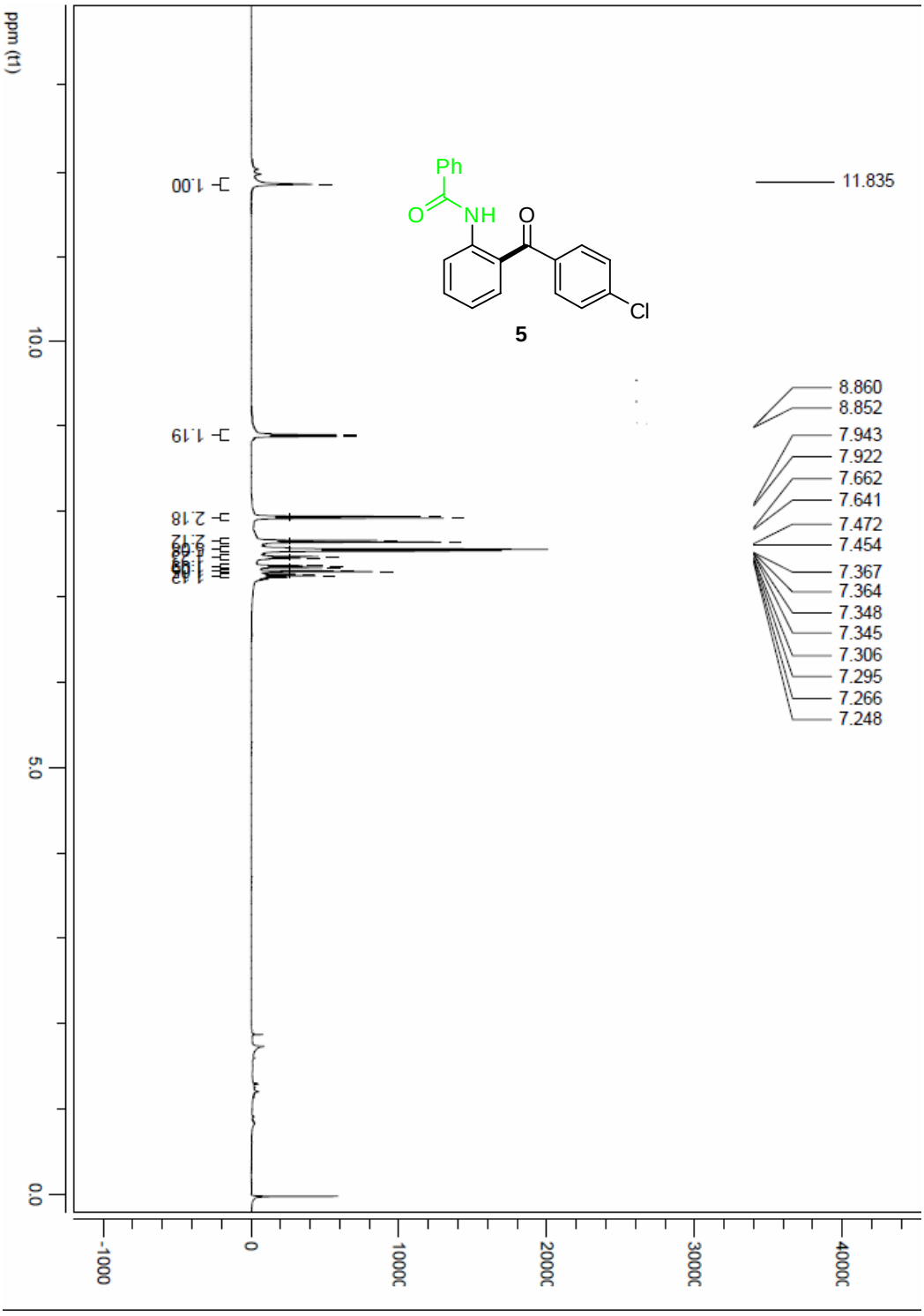

ppm (t1)
200
150
100
50
0
-5000
0
5000
10000
15000
20000
25000
30000
Me
O
NH
O
Cl
COOEt
3ml
197.824
169.338
144.141
139.501
136.344
135.289
134.672
131.301
128.888
128.506
124.027
122.079
120.911
77.318
77.000
76.682
61.247
25.365
14.261

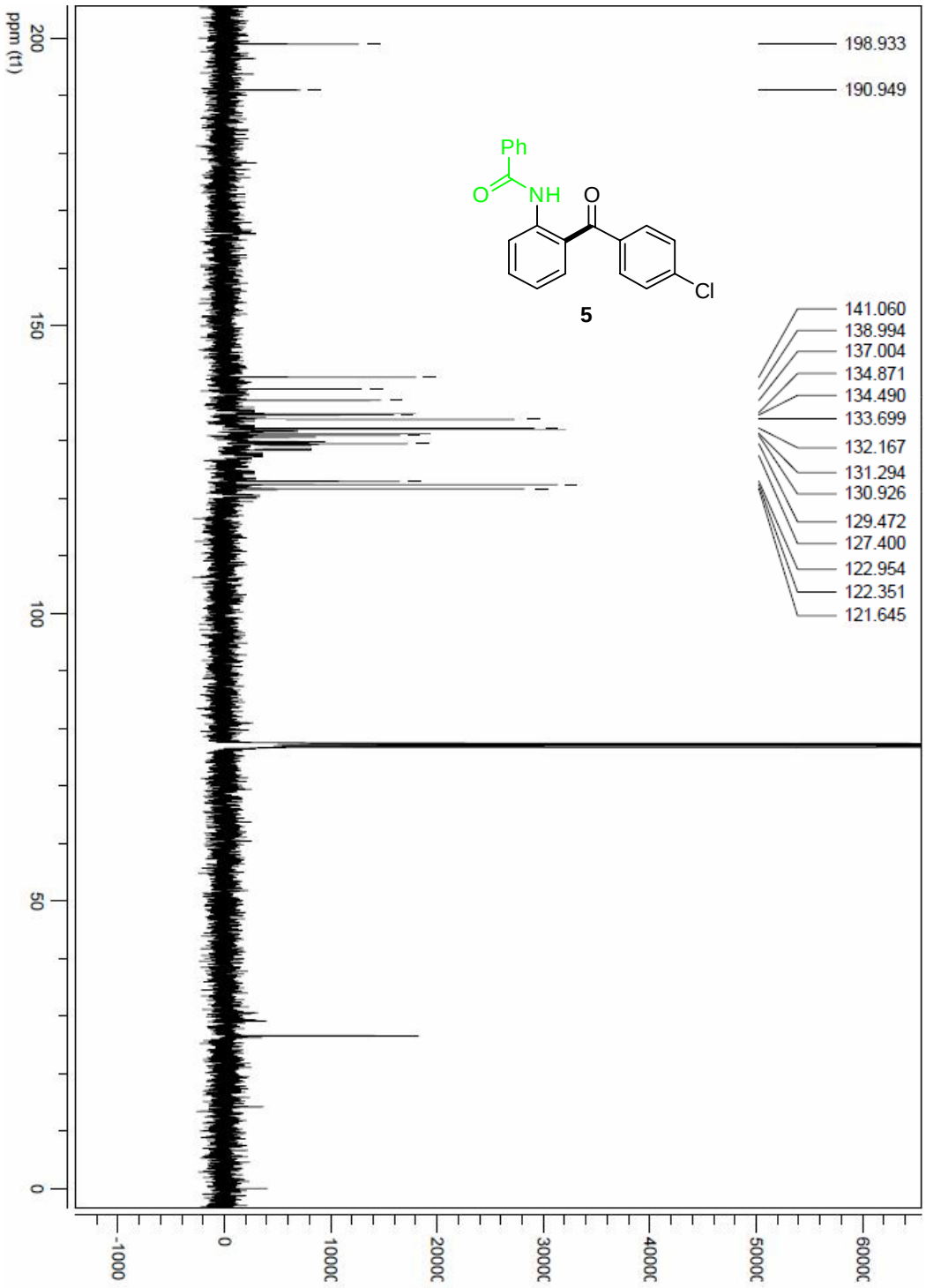


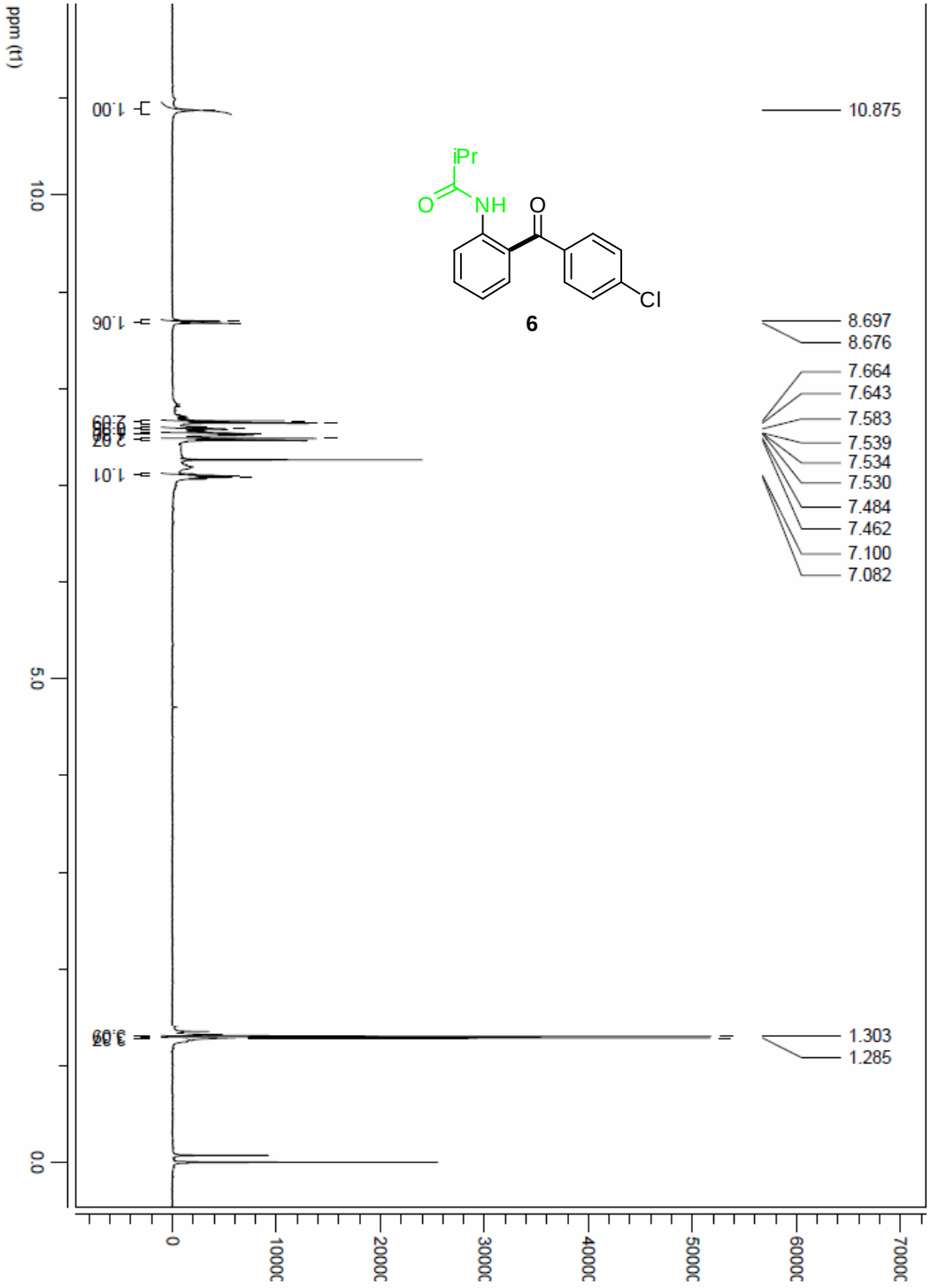
3ml

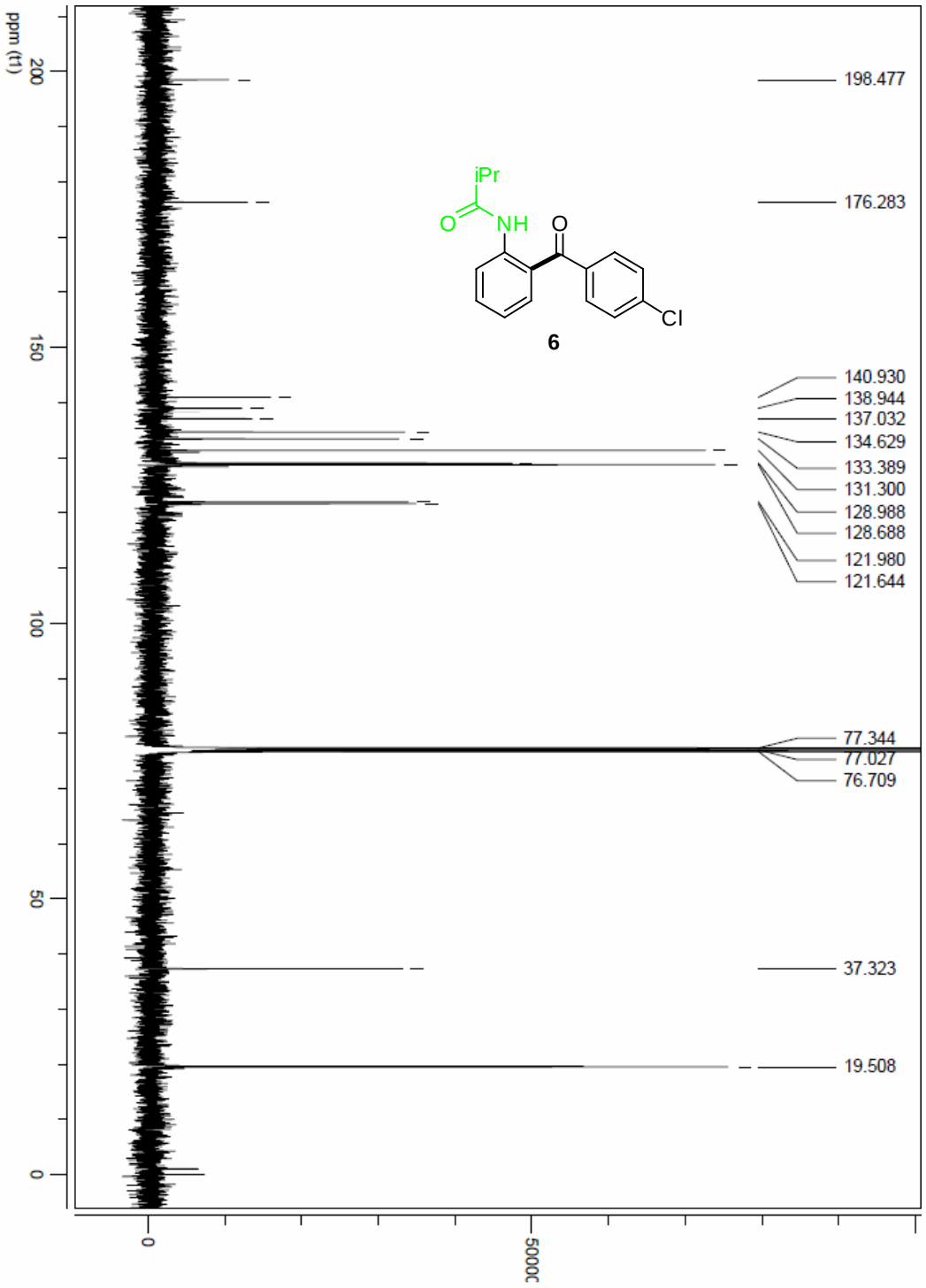


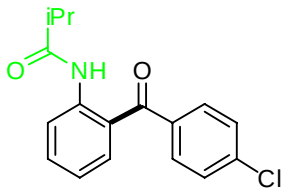
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.94	C18 H16 N O4 Cl	[M+Na] +	368.0658	368.0666	-0.8	-2.17	74.11	11.0


ppm (t1)
10.0
5.0
0.0
-1000
0
1000
2000
3000
4000
1.00
1.19
2.18
11.835
8.860
8.852
7.943
7.922
7.662
7.641
7.472
7.454
7.367
7.364
7.348
7.345
7.306
7.295
7.266
7.248
Ph
O
NH
O
Cl
5


ppm (t1)
200
150
100
50
0
-1000
0
10000
20000
30000
40000
50000
60000
198.933
190.949
Ph
O
NH
O
Cl
5
141.060
138.994
137.004
134.871
134.490
133.699
132.167
131.294
130.926
129.472
127.400
122.954
122.351
121.645


ppm (t1)
10.0
5.0
0.0
1.00
1.06
1.01
10.875
8.697
8.676
7.664
7.643
7.583
7.539
7.534
7.530
7.484
7.462
7.100
7.082
1.303
1.285
iPr
O
NH
O
Cl
6
0
1000
2000
3000
4000
5000
6000
7000

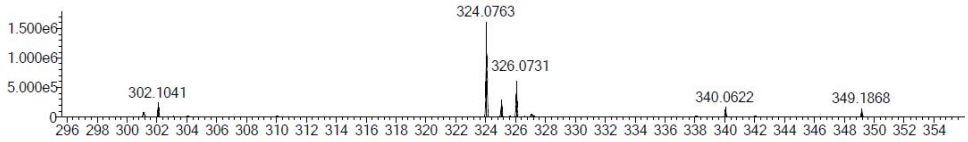

ppm (t1)
200
150
100
50
0
198.477
176.283
iPr
O
NH
O
Cl
6
140.930
138.944
137.032
134.629
133.389
131.300
128.988
128.688
121.980
121.644
77.344
77.027
76.709
37.323
19.508
0
50000



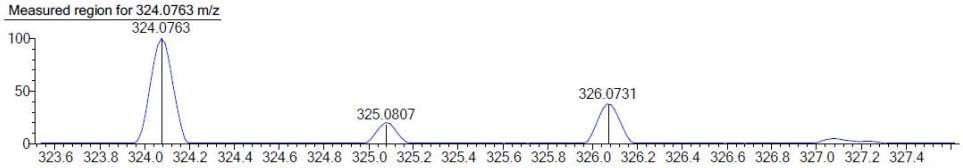
6

Error Margin (ppm):	80	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

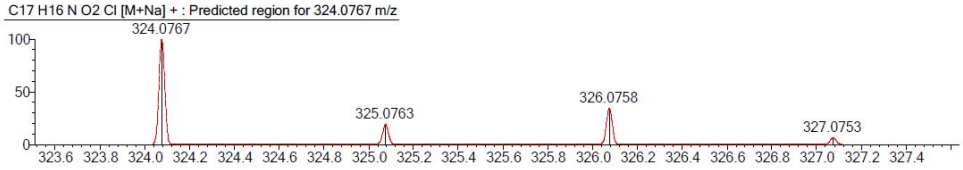
Event#: 1 MS(E+) Ret. Time : 1.053 -> 1.280 - 0.067 -> 0.128 Scan# : 317 -> 385 - 21 -> 39



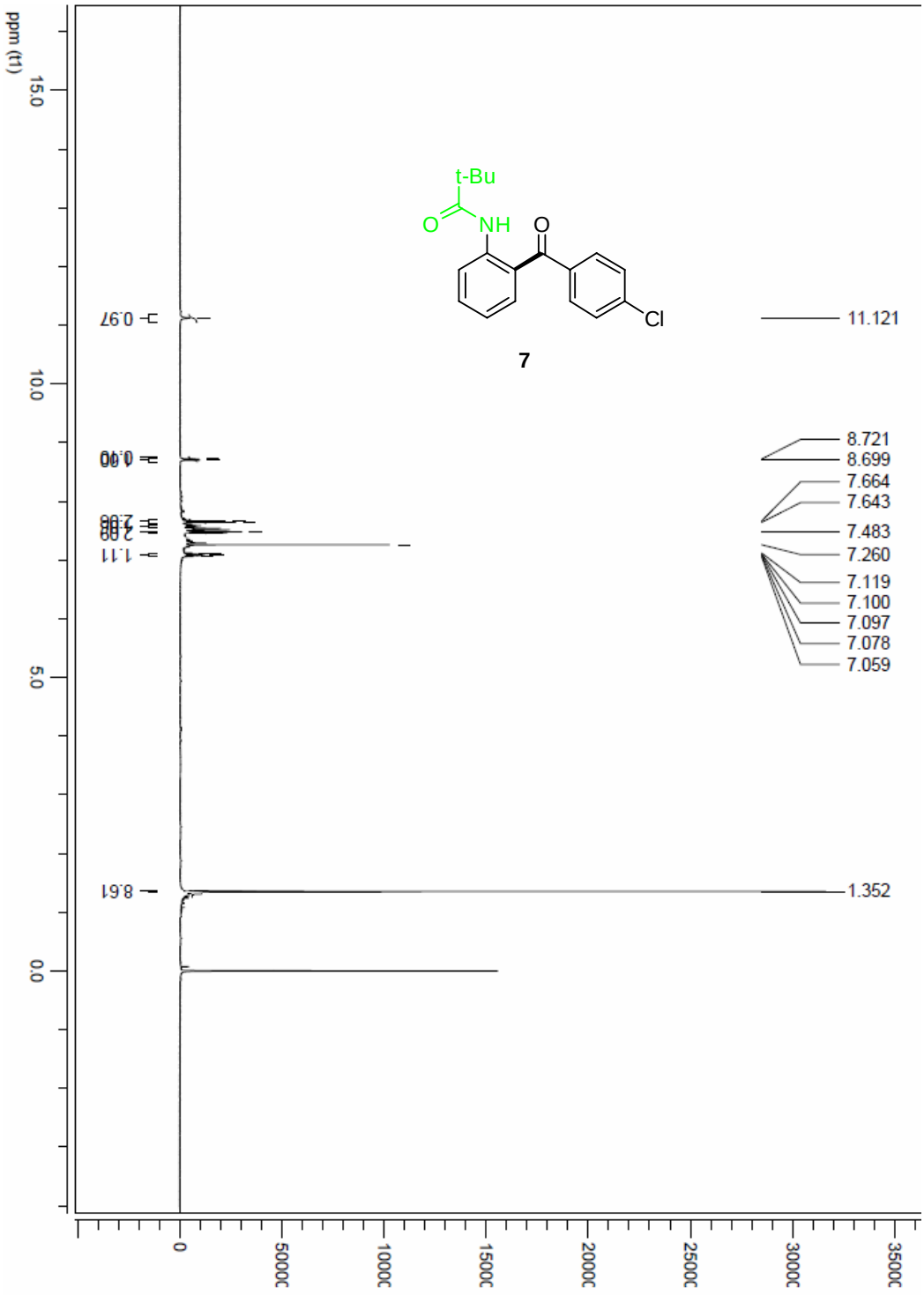
Measured region for 324.0763 m/z

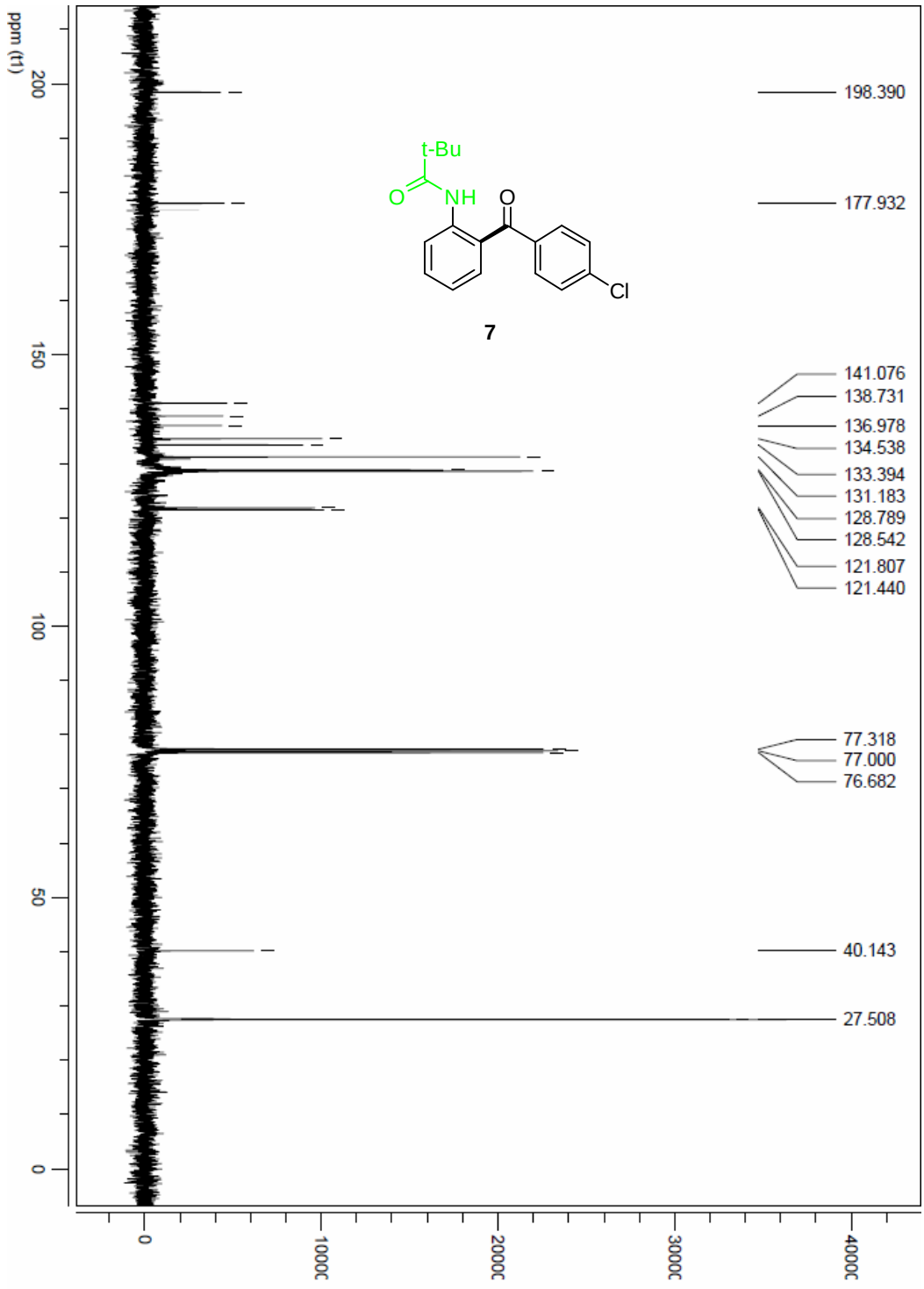


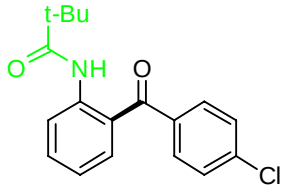
C17 H16 N O2 Cl [M+Na] + : Predicted region for 324.0767 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.29	C17 H16 N O2 Cl	[M+Na] +	324.0763	324.0767	-0.4	-1.23	69.69	10.0


ppm (t1)
15.0
10.0
5.0
0.0
t-Bu
O
NH
O
Cl
7
11.121
8.721
8.699
7.664
7.643
7.483
7.260
7.119
7.100
7.097
7.078
7.059
1.352
0
5000
10000
15000
20000
25000
30000
35000

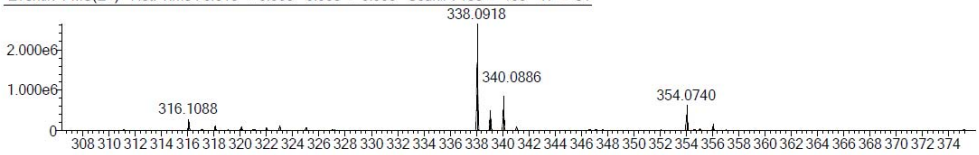

ppm (t1)
200
150
100
50
0
0
10000
20000
30000
40000
198.390
177.932
141.076
138.731
136.978
134.538
133.394
131.183
128.789
128.542
121.807
121.440
77.318
77.000
76.682
40.143
27.508
t-Bu
O
NH
O
Cl
7



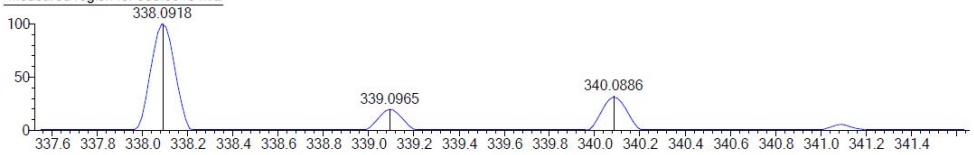
7

Error Margin (ppm):	80	DBE Range:	0.0 - 3000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	no	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

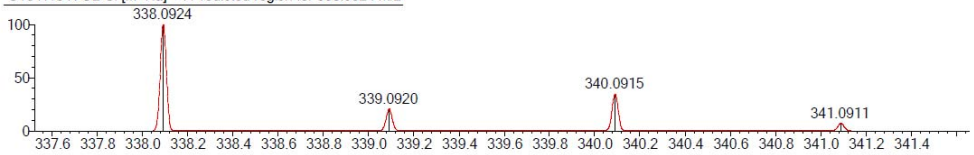
Event#: 1 MS(E+) Ret. Time : 0.613 -> 0.660 - 0.053 -> 0.099 Scan# : 185 -> 199 - 17 -> 31



Measured region for 338.0918 m/z



C18 H18 N O2 Cl [M+Na] + : Predicted region for 338.0924 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	68.42	C18 H18 N O2 Cl	[M+Na] +	338.0918	338.0924	-0.6	-1.77	69.76	10.0

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