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De novo synthesis of alkyne substituted tryptophans as chemical probes for protein profiling studies

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Supporting Information

Table of Contents

General experimental: All reagents and solvents were obtained from commercial suppliers and were used as-is without further purification. Anhydrous solvents were obtained from our in-house solvent purification system wherever necessary. NMR spectra were recorded on a 500 MHz ^{1}H, 125 MHz ^{13}C NMR spectrometer at 25 °C. Chemical shifts are reported in ppm (δ) referenced to the NMR solvent residual peak, and coupling constants (*J*) are in hertz. Silica gel flash column chromatography was used to purify all compounds. All reactions were monitored using TLC and LTQ-MS. Reactions were carried out under N_2 atmosphere wherever necessary. $Pd(PPh_3)_4$ was obtained from Strem Chemicals, and $PdCl_2$(dppf) was obtained from Acros Organics. For characterization of new compounds, ^{1}H, ^{13}C NMR and LTQ-MS data has been included, whereas for known compounds only ^{1}H NMR data is reported along with appropriate literature reference.

General procedure for 9-BBN protection of tryptophan:-

Appropriate tryptophan (1eq) was suspended in anhydrous THF (20 mL) and vigorously stirred for 5 min. A solution of 9-BBN in THF (0.5 M, 2.2 eq) was added via syringe and the resulting suspension was stirred under N_2 at ambient temperature until all materials had dissolved (~12 h). The solvents were evaporated to obtain a crude oil from which the product was precipitated by addition of cyclohexane, filtered, and recrystallized from CH_3CN-water to yield corresponding –bicyclononylboronate tryptophan in near quantitative yields.

(1R,5S)-4'-((5-bromo-1H-indol-3-yl)methyl)-9l4-boraspiro[bicyclo[3.3.1]nonane-9,2'-[1,3,2]oxazaborolidin]-5'-one (1): Buff solid. ^{1}H NMR (*d_6*-DMSO, 500 MHz) δ 11.13 (s, 1H), 7.74 (s, 1H), 7.37 (s, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 1H), 6.50-6.46 (br m, 1H), 5.55-5.51 (br m, 1H), 3.84-3.82 (br s, 1H), 3.23-3.19, br m, 1H), 3.10-3.06 (br m, 1H), 1.76-1.39 (br, 12H), 0.40 (d, *J* = 58.0 Hz, 2H) ppm ; ^{13}C NMR (*d_6*-DMSO, 125 MHz) δ 173.8, 135.4, 129.5, 126.6, 123.8, 121.1, 113.8, 111.6, 109.6, 55.5, 31.7, 31.6, 26.8, 26.5, 24.6, 24.3, 22.2 ppm; LTQ-MS Calcd for $C_{19}H_{24}BBrN_2O_2$ – 403.13; found 403.21.

(1R,5S)-4'-((6-bromo-1H-indol-3-yl)methyl)-9l4-boraspiro[bicyclo[3.3.1]nonane-9,2'-[1,3,2]oxazaborolidin]-5'-one (2): Pale yellow solid. ^{1}H NMR (*d_6*-DMSO, 500 MHz) δ 11.11 (s, 1H), 7.54 (s, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.35 (s, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 5.55-5.51 (br m, 1H), 3.84-3.82 (br s, 1H), 3.25-3.21, br m, 1H), 3.12-3.07 (br m, 1H), 1.71-1.32 (br, 12H), 0.40 (d, *J* = 58.0 Hz, 2H) ppm ; ^{13}C NMR (*d_6*-DMSO, 125 MHz) δ 173.8, 137.5, 126.6, 125.9, 121.7, 120.5, 114.3, 114.2, 110.0, 55.4, 31.7, 31.6, 31.1, 26.8, 26.5, 24.6, 24.3 ppm; LTQ-MS Calcd for $C_{19}H_{24}BBrN_2O_2$ – 403.13; found 403.26.

(1R,5S)-4'-((5-hydroxy-1H-indol-3-yl)methyl)-9l4-boraspiro[bicyclo[3.3.1]nonane-9,2'-[1,3,2]oxazaborolidin]-5'-one (5): Off-white crystalline solid. ^{1}H NMR (*d_6*-DMSO, 500 MHz) δ 10.61 (s, 1H), 8.63 (s, 1H), 7.19 (s, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 6.84 (s, 1H), 6.60 (d, *J* = 8.4 Hz, 1H), 6.53-6.49 (br m, 1H), 5.37-5.33 (br m, 1H), 3.81-3.78 (br s, 1H), 3.19-3.15, (br m, 1H), 3.04-2.99 (br m, 1H), 1.73-1.23 (br, 12 H), 0.42 (d, *J* = 43.5 Hz, 1H) ppm ; ^{13}C NMR (*d_6*-DMSO, 125 MHz) δ 173.8, 15.8, 131.2, 128.2, 125.2, 112.2, 111.8, 108.4, 102.5, 55.4, 31.7, 31.6, 31.1, 31.0, 26.9, 24.6, 24.3 ppm: LTQ-MS Calcd for $C_{19}H_{25}BN_2O_3$ – 340.23; found 339.23.

General procedure for BOC protection of bicyclonylboronate tryptophan:-

To a stirred solution of bicyclononylboronate tryptophan (1 eq) in anhydrous DCM (25 mL) was added Boc-anydride (2.5 eq) and cat. dimethylamino pyridine (0.1 eq). The resultant reaction mixture was allowed to stir for 12 h following which the reaction was quenched with sat. NH_4Cl solution and extracted with DCM. The organic layer was washed with water followed by brine, dried over Na_2SO_4, filtered and evaporated solvents over a rotatory evaporator to give corresponding BOC protected tryptophan moieties.

tert-butyl-5-bromo-3-(((1R,5S)-5'-oxo-9l4-boraspiro[bicyclo[3.3.1]nonane-9,2'-[1,3,2]oxazaborolidin]-4'-yl)methyl)-1H-indole-1-carboxylate (3): off-white solid. ^{1}H NMR (*d*$_6$-DMSO, 500 MHz) δ 7.97 (d, *J* = 8.4 Hz, 1H), 7.84 (s, 1H), 7.74 (s, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 6.44-6.40 (Br m, 1H), 5.86-5.82 (br m, 1H), 3.93-3.89 (br s, 1H), 3.26-3.20, br m, 1H), 3.05-3.00 (br m, 1H), 1.74-1.53 (br, 21 H), 0.47 (s, 2H) ppm ; ^{13}C NMR (*d*$_6$-DMSO, 125 MHz) δ 173.5, 149.9, 134.1, 132.6, 127.3, 126.6, 122.3, 116.9, 115.8, 115.6, 84.6, 54.6, 31.7, 31.1, 31.0, 28.1, 28.0, 25.9, 24.6, 24.3 ppm; LTQ-MS Calcd for $C_{24}H_{32}BBrN_2O_4$ – 503.24; found 503.29.

tert-butyl-6-bromo-3-(((1R,5S)-5'-oxo-9l4-boraspiro[bicyclo[3.3.1]nonane-9,2'-[1,3,2]oxazaborolidin]-4'-yl)methyl)-1H-indole-1-carboxylate (4): light brown solid. ^{1}H NMR (*d*$_6$-DMSO, 500 MHz) δ 8.20 (s, 1H), 7.71 (s, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 6.44-6.41 (br m, 1H), 5.87-5.85 (br m, 1H), 3.89-3.87 (br s, 1H), 3.25-3.21 (br m, 1H), 3.06-3.01 (br m, 1H), 1.76-1.51 (br, 21 H), 0.46 (s, 2H) ppm ; ^{13}C NMR (*d*$_6$-DMSO, 125 MHz) δ 173.4, 149.2, 129.7, 125.9, 125.8, 121.5, 117.8, 117.5, 116.4, 84.7, 69.5, 54.6, 32.3, 31.7, 31.1, 31.0, 28.1, 28.0, 26.5, 26.0, 24.6, 24.3, 22.2 ppm; LTQ-MS Calcd for $C_{24}H_{32}BBrN_2O_4$ – 503.24; found 503.19.

NMR data and literature references for intermediate compounds in Scheme 4:

3-benzyl-1H-indole (7)[1]: brown oil. ^{1}H NMR (C*D*Cl$_3$, 500 MHz) δ 8.13 (br s, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.33-7.26 (br m, 4 H), 7.22-7.16 (obscured t, 2 H), 7.06 (t, *J* = 7.5 Hz, 1H), 7.02 (br s, 1H), 4.14 (s, 2H) ppm.

3-(prop-2-yn-1-yl)-1H-indole (8)[2]: light yellow oil. ^{1}H NMR (C*D*Cl$_3$, 500 MHz) δ 7.95 (br s, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.24 (t, *J* = 6.5 Hz, 1H), 7.19-7.16 (obscured t, 1 H), 3.73 (s, 2H), 2.17 (s, 1H) ppm.

methyl 2-((diphenylmethylene)amino)-3-hydroxypropanoate (9)[3]: white crystalline solid. ^{1}H NMR (*d*$_6$-DMSO, 500 MHz) δ 7.54-7.18 (m, 10H), 4.93 (br, 0.5H), 4.01-3.97 (m, 0.5H), 3.91 (d, *J* = 16.5 Hz, 1H), 3.86-3.82 (m, 0.5H), 3.65 (s, 3H), 3.56 (d, *J* = 9.5 Hz, 0.5H) ppm: LTQ-MS Calcd for $C_{17}H_{17}NO_3$ – 283.33; found 284.14.

Synthesis procedures and NMR data for intermediate compounds in Table 3:

5-ethynyl-1H-indole: brown solid. ^{1}H NMR (*d*$_6$-DMSO, 500 MHz) δ 11.28 (s, 1H), 7.69 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.44 (s, 1H), 3.87 (s, 1H) ppm.

5-(prop-2-yn-1-yloxy)-1H-indole (14)[4, 5]: light brown solid. ^{1}H NMR (*d*$_6$-DMSO, 500 MHz) δ 10.94 (s, 1H), 7.28 (s, 1H), 7.11 (s, 1H), 6.76 (d, J = 10.5 Hz, 1H), 6.33 (s, 1H), 4.73 (s, 2H), 3.48 (s, 1H) ppm; LTQ-MS Calcd for $C_{11}H_9NO$ – 171.20; found 172.17 (M + H).

1-(prop-2-yn-1-yl)-5-(prop-2-yn-1-yloxy)-1H-indole (15): During the o-alkylation process of 5-hydroxy indole, **15** was obtained as a minor product (~15% yield) during flash chromatography purification. ^{1}H NMR (*d*$_6$-DMSO, 500 MHz) δ 7.41 (d, *J* = 8.4 Hz, 1H), 7.35 (s, 1H), 7.14(s,

1H), 6.87(s, 1H), 5.04 (s, 2H), 4.76 (s, 2H), 3.49 (s, 1H), 3.36 (s, 1H) ppm; ^{13}C NMR (d_6-DMSO, 125 MHz) δ 152.1, 131.6, 129.5, 129.1, 112.4, 111.1, 104.8, 101.5, 80.3, 79.7, 78.2, 75.8, 56.5, 35.6 ppm; LTQ-MS Calcd for $C_{14}H_{11}NO$ – 209.25; found 208.37 (M – H).

6-iodohex-1-yne[6]: light brown oil. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 3.21 (br s, 2H), 2.22 (br s, 2H), 1.96 (s, 2H), 1.94 (merged s, 1H), 1.65 (br s, 2H) ppm

5-(hex-5-yn-1-yloxy)-1H-indole (16): To a clean and dry flask with stir bar and acetone (20 mL), 5-hydroxyindole (1 eq), 6-iodohex-1-yne (1.5 eq) and Cs_2CO_3 (3 eq) were added and set for reflux. After 2h, an LTQ MS analysis confirmed the formation of desired product. The reaction mixture was allowed to cool to room temperature, quenched with NH_4Cl and extracted with DCM. The organic layer was washed with water and brine, dried over Na_2SO_4, filtered and solvents were evaporated on a rotatory evaporator. The crude was then purified by flash chromatography using 2:1 Hexanes:Ethyl Acetate system to give **16** as a pure white solid. ^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.86 (s, 1H), 7.24 (s, 1H), 7.02 (s, 1H), 6.70 (br s, 1H), 6.30 (s, 1H), 3.93 (br s, 2H), 2.76 (s, 1H), 2.23 (br, 2H), 1.80-1.78 (br m, 2H), 1.62-1.59 (br m, 2H) ppm; ^{13}C NMR (d_6-DMSO, 125 MHz) δ 152.9, 131.5, 128.4, 126.1, 112.3, 112.0, 103.2, 101.2, 84.8, 71.7, 67.8, 28.5, 25.2, 17.9 ppm; LTQ-MS Calcd for $C_{14}H_{16}NO$ – 213.28; found 214.19 + Na (236.09)

1H-indol-5-yl hex-5-ynoate (17): Standard EDC coupling conditions were used to synthesize compound **17**. After purification, white solid was obtained. ^{1}H NMR (d_6-DMSO, 500 MHz) δ 11.15 (s, 1H), 7.38 (s, 1H), 7.24 (s, 1H), 6.81 (br s, 1H), 6.41 (s, 1H), 2.85 (s, 1H), 2.67-2.65 (t, J = 6.5 Hz, 2H), 2.29 (br m, 2H), 1.84-1.81 (m, 2H) ppm; ^{13}C NMR (d_6-DMSO, 125 MHz) δ 172.5, 143.9, 134.1, 128.1, 127.1, 115.7, 112.4, 101.6, 84.1, 72.3, 32.9, 23.9, 17.6 ppm; LTQ-MS Calcd for $C_{14}H_{13}NO_2$ – 227.26; found 226.15 (M – H).

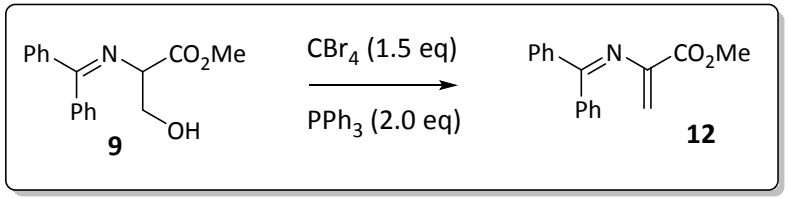
Synthesis of methyl 2-((diphenylmethylene)amino)acrylate (12) using Appel Reaction:

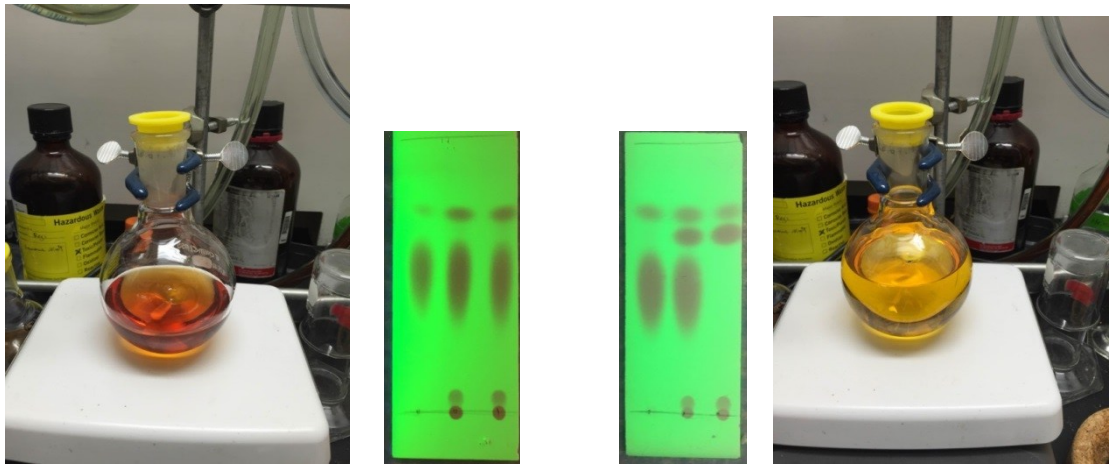
To a clean and dry 500 mL flask with stir bar under a N_2 purge was added **9** (1.0 g, 3.53 mmol, 1 eq) dissolved in DCM (250 mL). This was followed by the addition of CBr_4 (1.76 g, 5.29 mmol, 1.5 eq) and the reaction mixture was allowed to stir for 20 mins. PPh_3 (1.85 g, 7.06 mmol, 2.0 eq) was added slowly over a period of 10 mins making sure that the reaction is under a constant flow of N_2. During the addition of PPh_3, a dark brown coloration is observed which disappears on the addition of additional DCM (100 mL). A TLC at this point (30 mins) confirms the disappearance of **9**, following which the solvents are evaporated over a rotatory evaporator, contents are transferred to a separatory funnel and washed with $NaHCO_3$, followed by sat. $Na_2S_2O_3$. The organic layer is finally washed with brine, Na_2SO_4, filtered and solvents were evaporated on a rotatory evaporator. The crude was then purified by flash chromatography using 2:1 Hexanes:Ethyl Acetate system to give **12** as a pale yellow oil (1.23g, 69%). ^{1}H NMR (d_6-DMSO, 500 MHz) δ 7.79 (br, 0.5H), 7.71 (s, 2H), 7.57-755 (br, 2H), 7.45 (s, 4H), 7.23 (s, 1.5H), 5.44 (s, 1H), 4.82 (s, 1H), 3.63 (s, 3H) ppm; LTQ-MS Calcd for $C_{17}H_{15}NO_2$ – 265.31; found 265.21.

Important Notes for this protocol:

1. During the addition of PPh_3, if the brown color persists, add DCM until the color turn bight pale yellow.
2. Washing with bicarbonate and thiosulfate is very important.

3. Compound **12** has been found to dimerize (compd **13**) on standing, so it is safer to store in DCM solution at -80 °C or use immediately.
4. The reaction image below shows the course of reaction monitored via TLC.





General synthesis procedure for substituted tryptophan moieties in Table 3[7]:

To a clean and dry flask with stir bar was added corresponding indole compound (1 eq), **12** (1 eq) dissolved in DCM. The reaction mixture was cooled in an ice bath and purged with N_2 for 20 mins. $AlCl_3$ (2.0 eq) was added and allowed to stir for 2h. After confirming the completion of reaction by TLC, the reaction mixture was quenched with $NaHCO_3$, filtered over a bed of Celite, washed the organic layer with water and brine, dried over Na_2SO_4, filtered and evaporated the solvents over a rotatory evaporator. The crude obtained from this process was then subjected to flash purification using 2:1 Hexane:Ethyl Acetate.

Methyl-2-((diphenylmethylene)amino)-3-(1H-indol-3-yl)propanoate (11): ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.91 (br s, 1H), 7.59 (br, 2H), 7.32-7.28 (m, 3H), 7.21 (d, J = 7.5 Hz, 1H), 7.15-7.10 (m, 3H), 6.97 (br, 1H), 6.92 (t, J = 7.5 Hz, 1H), 6.59 (br, 2H), 4.42 (br, 1H), 3.72 (s, 3H), 3.47 (obscured br d, 1H), 3.24 (br s, 1H) ppm; LTQ-MS Calcd for $C_{25}H_{22}N_2O_2$ – 382.46; found 383.22 (M + H).

Methyl-2-((diphenylmethylene)amino)-3-(5-ethynyl-1H-indol-3-yl)propanoate (18): LTQ-MS Calcd for $C_{27}H_{22}N_2O_2$ – 406.49; found 407.21 (M + H).

Methyl-2-((diphenylmethylene)amino)-3-(5-(prop-2-yn-1-yloxy)-1H-indol-3-yl)propanoate (21): ^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.66 (s, 1H), 7.47 (d, *J* = 7.5 Hz, 2H), 7.44-7.41 (obscured t, 1H), 7.35 (t, *J* = 7.5 Hz, 3H), 7.27 (t, *J* = 7.5 Hz, 2H), 7.19 (br d, *J* = 15 Hz, 1H), 6.95 (br, 1H), 6.69 (br, 2H), 6.67 (br, 2H), 4.51 (s, 1H), 4.21 (t, *J* = 7.0 Hz, 1H), 3.60 (s, 3H), 3.49 (s, 1H), 3.26 (dd, *J* = 14.0, 5.5 Hz, 1H), 3.03 (dd, *J* = 14.0, 8.0 Hz, 1H) ppm; ^{13}C (d_6-DMSO, 125 MHz) δ 172.2, 169.6, 151.4, 139.3, 135.7, 132.0, 130.8, 128.8, 128.7, 128.6, 127.6, 125.1, 112.1, 110.1, 102.7, 80.3, 78.0, 66.6, 56.8, 52.2, 29.5 ppm; LTQ-MS Calcd for $C_{28}H_{24}N_2O_3$ – 436.51; found 437.22 (M + H).

Methyl-2-((diphenylmethylene)amino)-3-(1-(prop-2-yn-1-yl)-5-(prop-2-yn-1-yloxy)-1H-indol-3-yl)propanoate (22): ^{1}H NMR (d_6-DMSO, 500 MHz) δ 7.47-7.41(m, 4H), 7.35-7.28 (m, 6H), 7.01 (s, 1H), 6.78 (br, 2H), 6.70 (br s, 1H), 4.94 (s, 2H), 4.53 (s, 2H), 4.20 (br s, 1H), 3.61 (s, 3H), 3.50 (s, 1H), 3.24 (obscured dd, 1H), 3.05-3.01 (obscured dd, 1H) ppm; ^{13}C (d_6-DMSO, 125 MHz) δ 172.2, 169.6, 151.4, 139.3, 135.7, 132.1, 130.8, 128.8, 128.7, 128.6, 128.0, 127.6, 125.1, 112.2, 112.1, 110.1, 102.7, 80.3, 78.0, 66.6, 56.8, 52.3, 29.2 ppm; LTQ-MS Calcd for $C_{31}H_{26}N_2O_3$ – 474.56; found 475.20 (M + H).

Methyl-2-((diphenylmethylene)amino)-3-(5-(hex-5-yn-1-yloxy)-1H-indol-3-yl)propanoate (23): ^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.60 (s, 1H), 7.46 (d, *J* = 7.5 Hz, 2H), 7.43-7.40 (m, 1H), 7.35 (br s, 3H), 7.29-7.26 (obscured t, 2H), 7.15 (d, *J* = 9.0 Hz, 1H), 6.92 (s, 1H), 6.67-6.62 (m, 3H), 6.58 (s, 1H), 4.21 (s, 1H), 3.71-3.68 (obscured dd, 2H), 3.59 (s, 3H), 3.25 (obscured dd, 1H), 3.04-3.01 (obscured dd, 1H) 2.79 (s, 1H), 2.23 (br s, 2H), 1.75 (br s, 2H), 1.63-1.58 (br m, 2H) ppm; ^{13}C (d_6-DMSO, 125 MHz) δ 172.2, 169.6, 152.6, 139.3, 135.8, 131.6, 130.8, 128.8, 128.7, 128.6, 128.5, 127.6, 125.1, 112.0, 110.0, 101.5, 84.8, 71.8, 67.7, 66.8, 52.2, 29.6, 28.5, 25.3, 17.9 ppm; LTQ-MS Calcd for $C_{31}H_{30}N_2O_3$ – 478.59; found 479.27 (M + H).

3-(2-((diphenylmethylene)amino)-3-methoxy-3-oxopropyl)-1H-indol-5-yl hex-5-ynoate (24): ^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.87 (s, 1H), 7.48 (d, *J* = 7.5 Hz, 2H), 7.44-7.41 (m, 1H), 7.36 (br d, 3H), 7.34-7.31 (obscured t, 2H), 7.27 (d, *J* = 9.0 Hz, 1H), 6.78-6.75 (m, 2H), 6.73 (s, 1H), 4.19 (s, 1H), 3.57 (s, 3H), 3.27-3.24 (obscured dd, 1H), 3.00-2.96 (obscured dd, 1H) 2.88 (s, 1H), 2.67-2.64 (br t, 2H), 2.32 (br s, 2H), 1.84-1.81 (br t, 2H) ppm; ^{13}C (d_6-DMSO, 125 MHz) δ 172.2, 169.8, 143.6, 139.1, 135.8, 134.2, 128.9, 128.8, 128.6, 128.5, 127.6, 125.7, 115.8, 111.9, 110.5, 84.1, 72.3, 66.8, 52.2, 32.8, 29.5, 23.9, 17.6 ppm; LTQ-MS Calcd for $C_{31}H_{28}N_2O_4$ – 492.58; found 493.27 (M + H).

Deprotection of compound 19 to amine 23 and amino acid 24 (Scheme 4): Protocol as listed in *Org. Lett.* **2012**, *14*, 600-603

Compound **19** (1 eq) was dissolved in THF, to it was added HCl (1N, 5 eq) and the reaction mixture was allowed to stir for 6 h. After confirming the completion of reaction by TLC, the contents were diluted with water and extracted with Et_2O. The organic layer, which would now consist of benzophenone protecting group was separated using a separatory funnel. The aqueous layer was neutralized to pH 7.0 using 1N NaOH following which the aqueous content were evaporated via a rotatory evaporator to reduce the contents to minimum. Finally the crude layer was purified

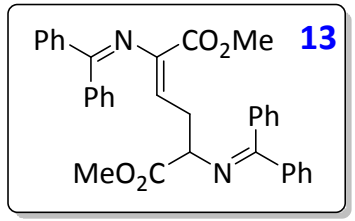
using flash chromatography using 10% MeOH in DCM, collecting fractions corresponding to desired product, evaporated the solvents to give amine **23** as a brown solid. After characterizing by ^{1}H NMR and LTQ-MS, **23** was subjected to ester deprotection. **23** was added to a flask containing THF:H_2O (1:1) and to it was added LiOH (5 eq). The reaction mixture was allowed to stir overnight and analyzed by LTQ-MS to confirm formation of product. The contents were lyophilized to give **24** as a light brown solid.

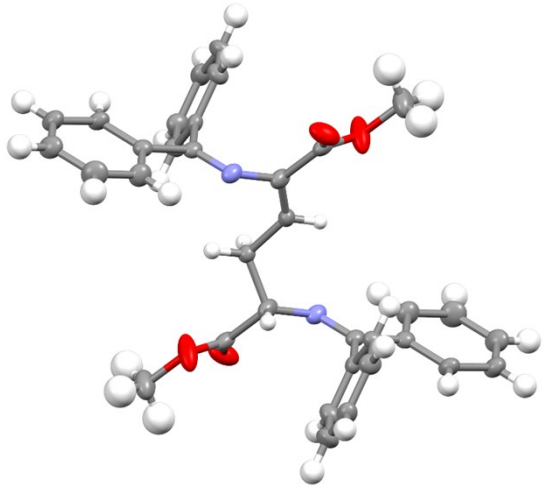
Methyl-2-amino-3-(5-(prop-2-yn-1-yloxy)-1H-indol-3-yl)propanoate (23): ^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.86 (s, 1H), 7.26 (d, J = 9.0 Hz, 1H), 7.15 (s, 1H), 7.08 (s, 1H), 6.78 (d, J = 8.5 Hz, 1H), 6.02 (br, 2H for NH_2), 4.74 (s, 2H), 4.01 (br, 1H), 3.63 (s, 3H), 3.11-3.08 (br t, 2H) ppm; LTQ-MS Calcd for $C_{28}H_{24}N_2O_3$ – 272.20; found 273.19 (M + H).

2-amino-3-(5-(prop-2-yn-1-yloxy)-1H-indol-3-yl)propanoic acid (24): LTQ-MS – m/z 258.1

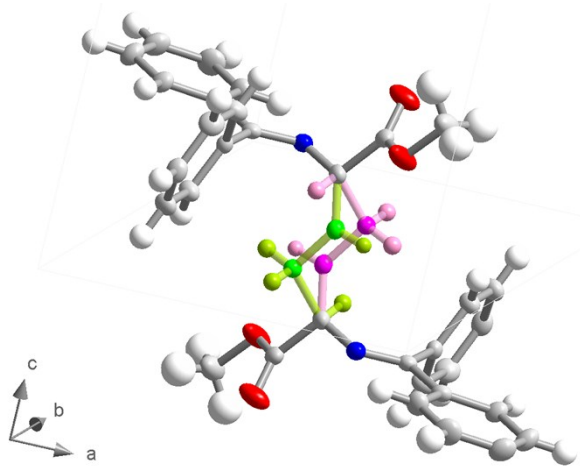
Dimethyl (E)-2,5-bis((diphenylmethylene)amino)hex-2-enedioate (13): During the process of *de novo* tryptophan synthesis from corresponding substituted indoles and compound **12**, a side product is also obtained. After flash chromatography purification, the fractions corresponding to an unknown compound were isolated and evaporated to dryness to give a yellow solid. ^{1}H NMR (d_6-DMSO, 500 MHz) δ 7.74 (br m, 2H), 7.58-7.46 (br m, 12H), 7.38-7.29 (br m, 5H), 7.11-7.03 (br d, 4H), 5.78 (br s, 1H), 4.03 (br s, 1H), 3.62 (s, 3H), 3.47 (s, 3H), 2.53 (merged with dmso reference, 2H) ppm; ^{13}C (d_6-DMSO, 125 MHz) δ 171.6, 170.6, 170.5, 163.8, 141.1, 139.2, 138.4, 137.5, 136.6, 135.8, 133.1, 131.7, 130.1, 129.6, 129.3, 129.2, 129.0, 128.8, 128.7, 128.5, 127.9, 127.7, 121.4, 64.0, 52.5, 52.1, 31.5 ppm; LTQ-MS Calcd for $C_{34}H_{30}N_2O_4$ – 530.22; found 531.23 (M + H). The solid was redissolved in DCM and allowed to crystallize via buffer diffusion using Hexanes to give X-ray quality crystals enabling X-ray crystallography data.

The structure was solved in space group $P\bar{1}$. The two $(Ph)_2C{=}N\text{-}C\text{-}CO_2Me$ portions were related through the inversion center, resulting in 2 bridging –CH-CH_2- moieties. Each of these refined to approximately equal occupancy and so were set to 50% for the final refinements. The final R-factor of 6.19% indicated that this is an excellent description of the structure.





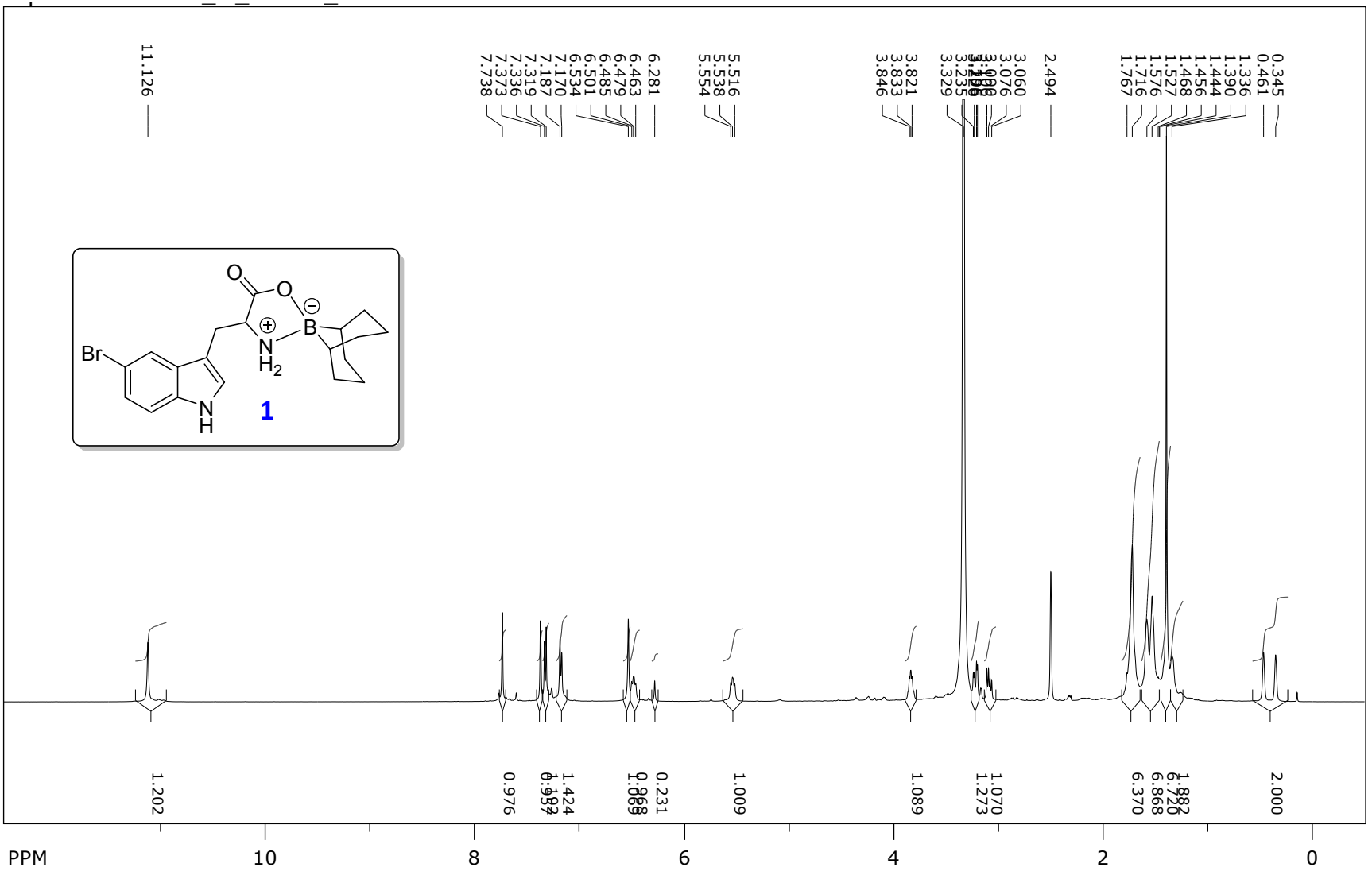
Ellipsoid view of crystal structure of **13**. The space group symmetry results in two linking –CH-CH_2- moieties, each with 50% occupancy. One of these has been removed for clarity.



Crystal structure of **13** showing the two half-occupied linking groups colored in green and pink respectively.

Experimental procedure for Protein synthesis studies:

The cells were washed once with PBS (pH=7.4), resuspended in PBS in the presence of EDTA free protease inhibitor (Roche), sonicated (Fisher Scientific, model FB120) using a total of 72, 2-second pulses at 60% amplitude followed by a 21,000 *g* spin. Protein concentration was measured using the BCA reagent (ThermoFisher), and normalized to 1 µg/µL with PBS for click chemistry. Click chemistry was performed using, 3 µM azido-tetramethylrhodamine (LumiProbe) in the presence of 500 µM copper sulfate, 50 µM TBTA (tris[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl])-amine) in a 4:1 solution of t-butanol/DMSO, and 500 µM TCEP (tris(2-carboxyethyl)phosphine). After click chemistry, 2× SDS and reducing agent was added to the samples and incubated at 95°C for 5 min. 15 µg of protein was run on a 10-20% Tris-Glycine Gel (ThermoFisher) with the ECL Ranibow Ladder (Amersham). Rhodamine-labeled proteins were detected using a FluorChemQ fluorescence imager (Protein Simple).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6.479
6.463
6.281
5.554
5.538
5.516
3.846
3.833
3.821
3.329
3.235
3.076
3.060
2.494
1.767
1.716
1.576
1.527
1.468
1.456
1.444
1.390
1.336
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0.345
1.202
0.976
1.424
1.089
0.231
1.009
1.089
1.070
1.273
6.370
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8
6
4
2
0
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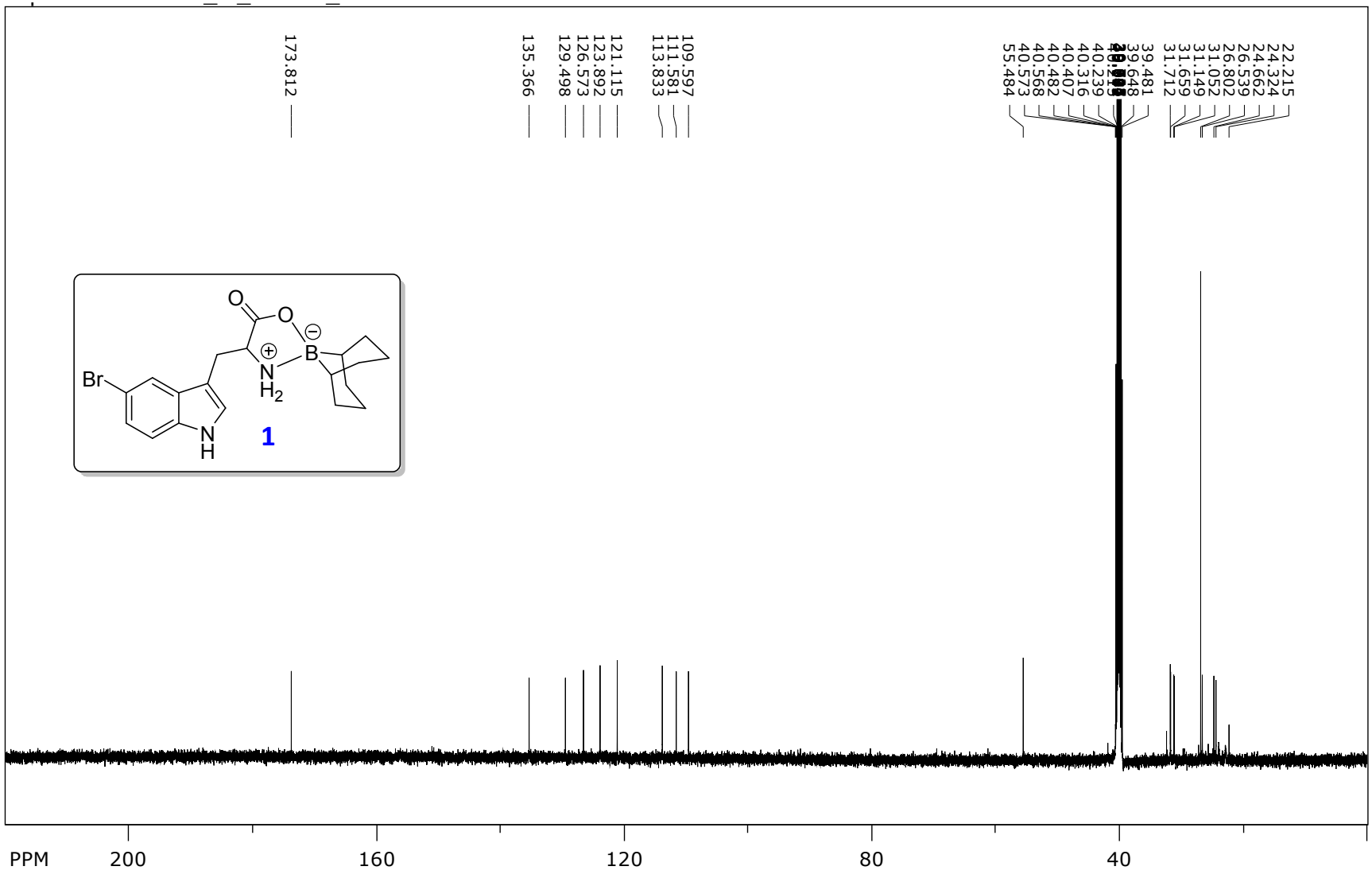
N
H
O
O
B
N
H2
1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40.316
40.239
39.648
39.481
31.712
31.659
31.149
31.052
26.802
26.539
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H
O
O
B
N
H2
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PPM
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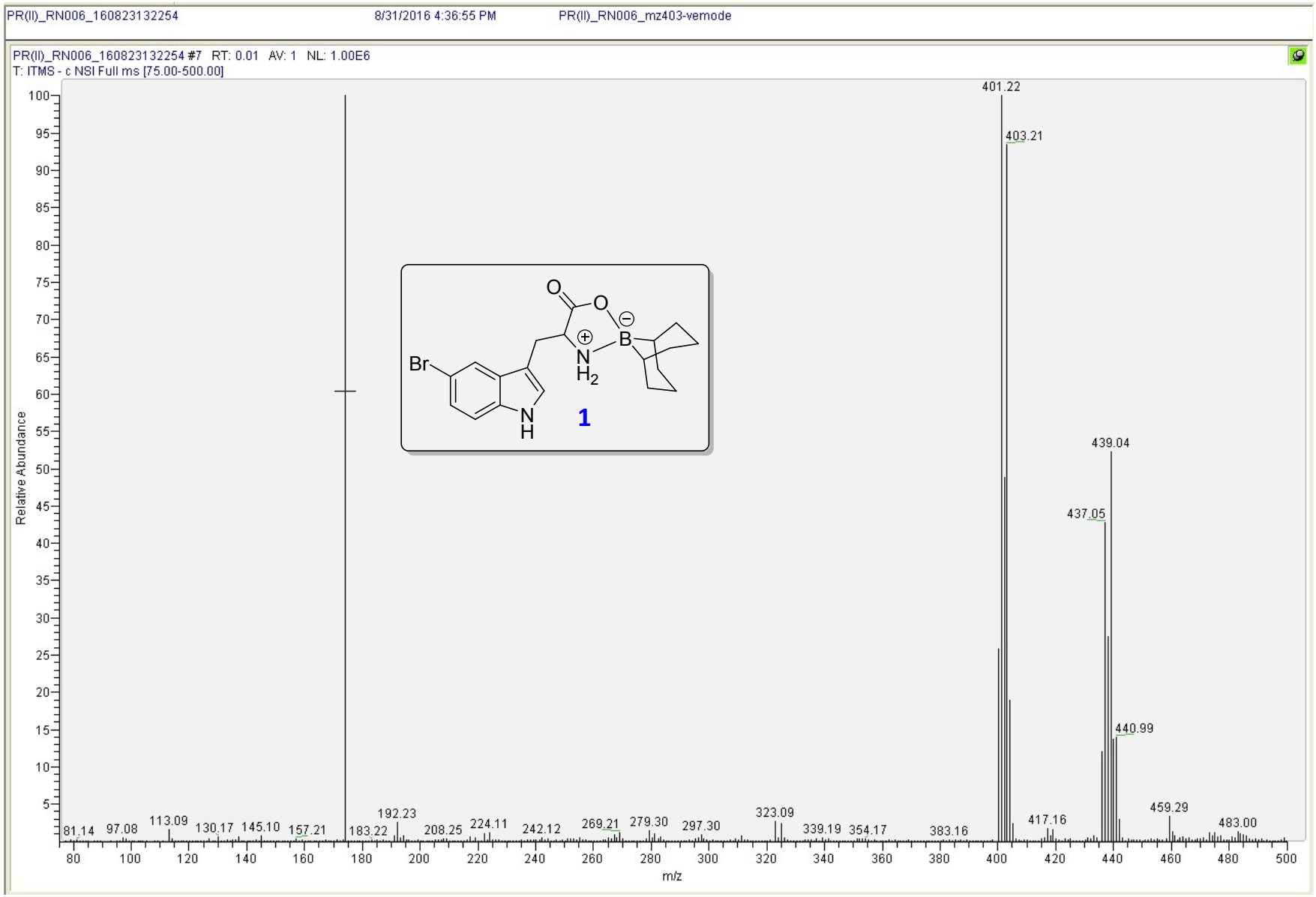
160
120
80
40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8/31/2016 4:36:55 PM
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437.05
440.99
459.29
483.00
417.16
323.09
192.23
113.09
81.14
97.08
130.17
145.10
157.21
183.22
208.25
224.11
242.12
269.21
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297.30
339.19
354.17
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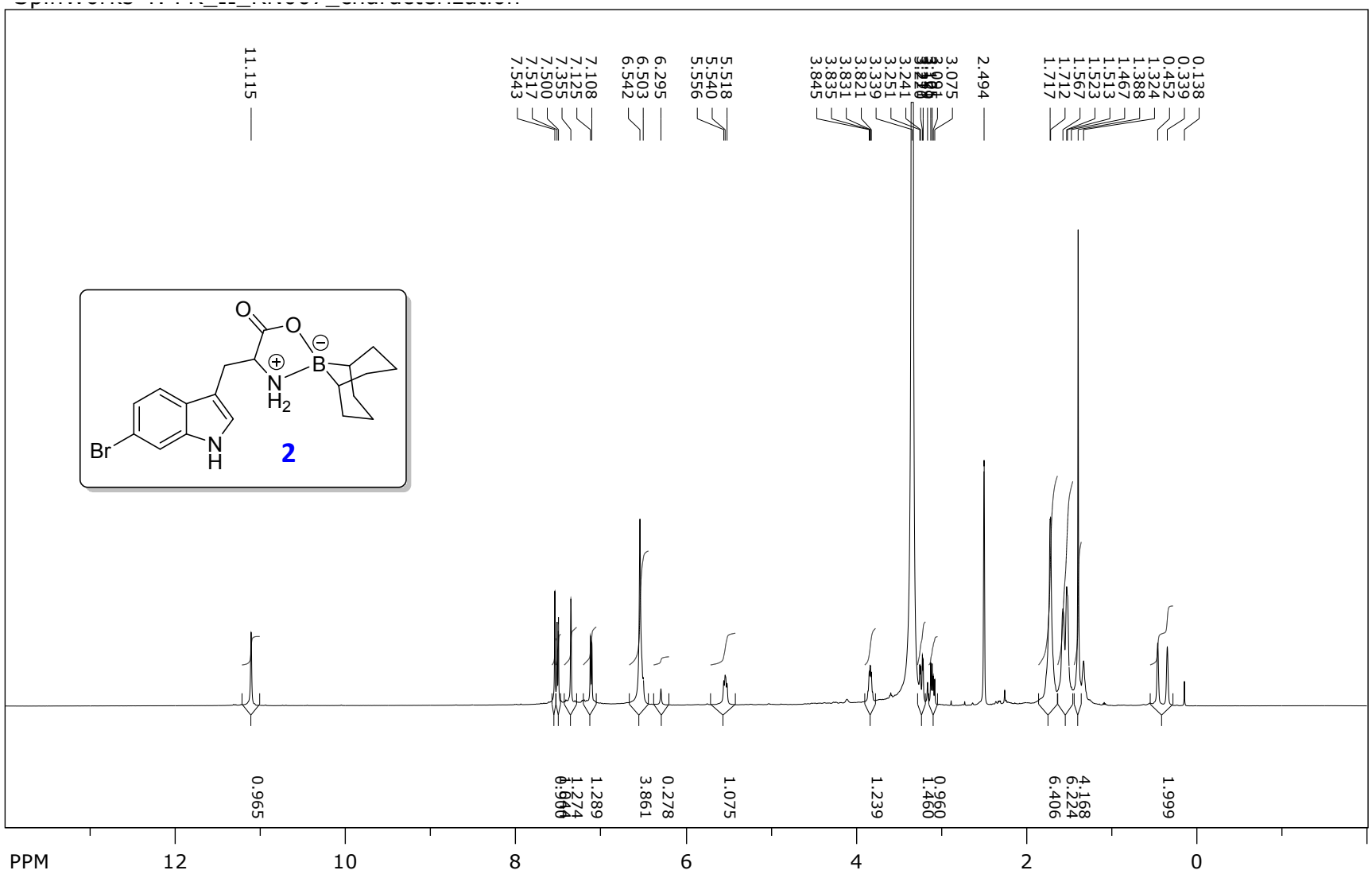
O
O
B
N
H2
N
H
1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6.542
6.503
6.295
5.556
5.540
5.518
3.845
3.835
3.821
3.339
3.251
3.241
3.075
2.494
1.717
1.712
1.567
1.523
1.513
1.467
1.388
1.324
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0.339
0.138
Br
N
H
O
O
B
N
H2
2
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1.274
0.278
3.861
1.075
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PPM
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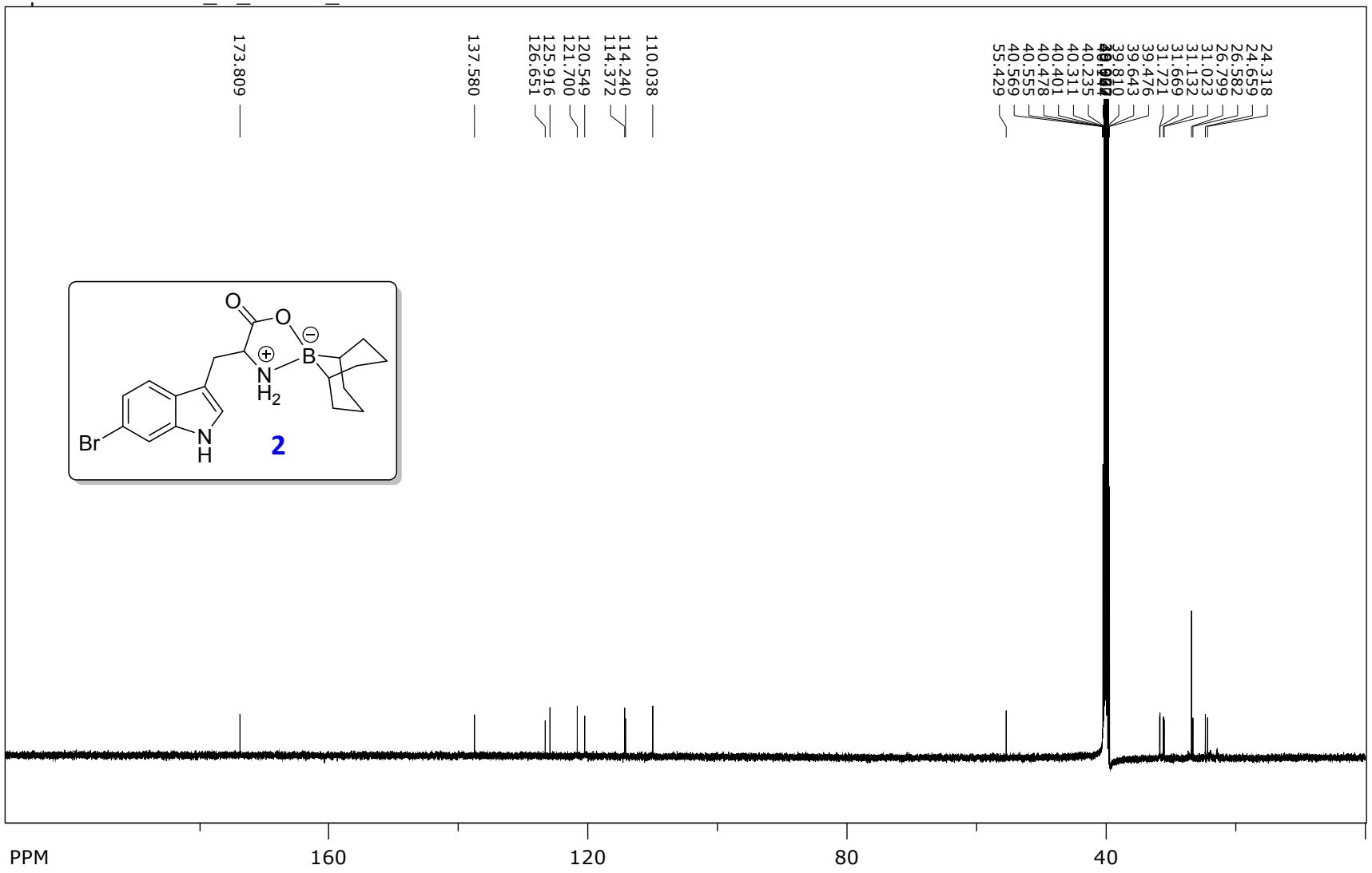
8
6
4
2
0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55.429
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40.478
40.401
40.311
40.235
39.810
39.643
39.476
31.721
31.669
31.132
31.023
26.799
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24.318
O
O
B
N
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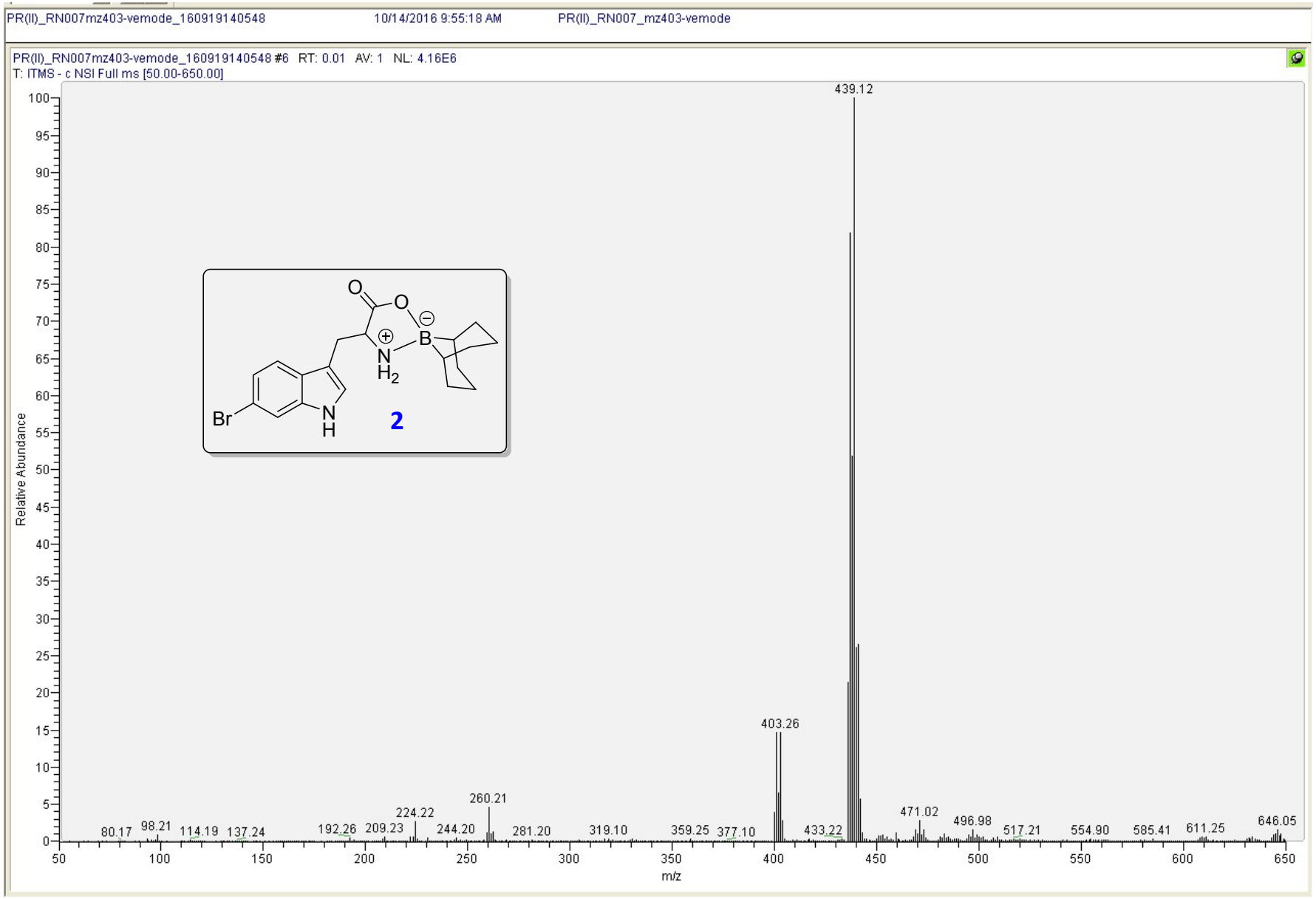
Br
N
H
2
PPM
160
120
80
40


PR(II)_RN007mz403-vemode_160919140548 10/14/2016 9:55:18 AM PR(II)_RN007_mz403-vemode
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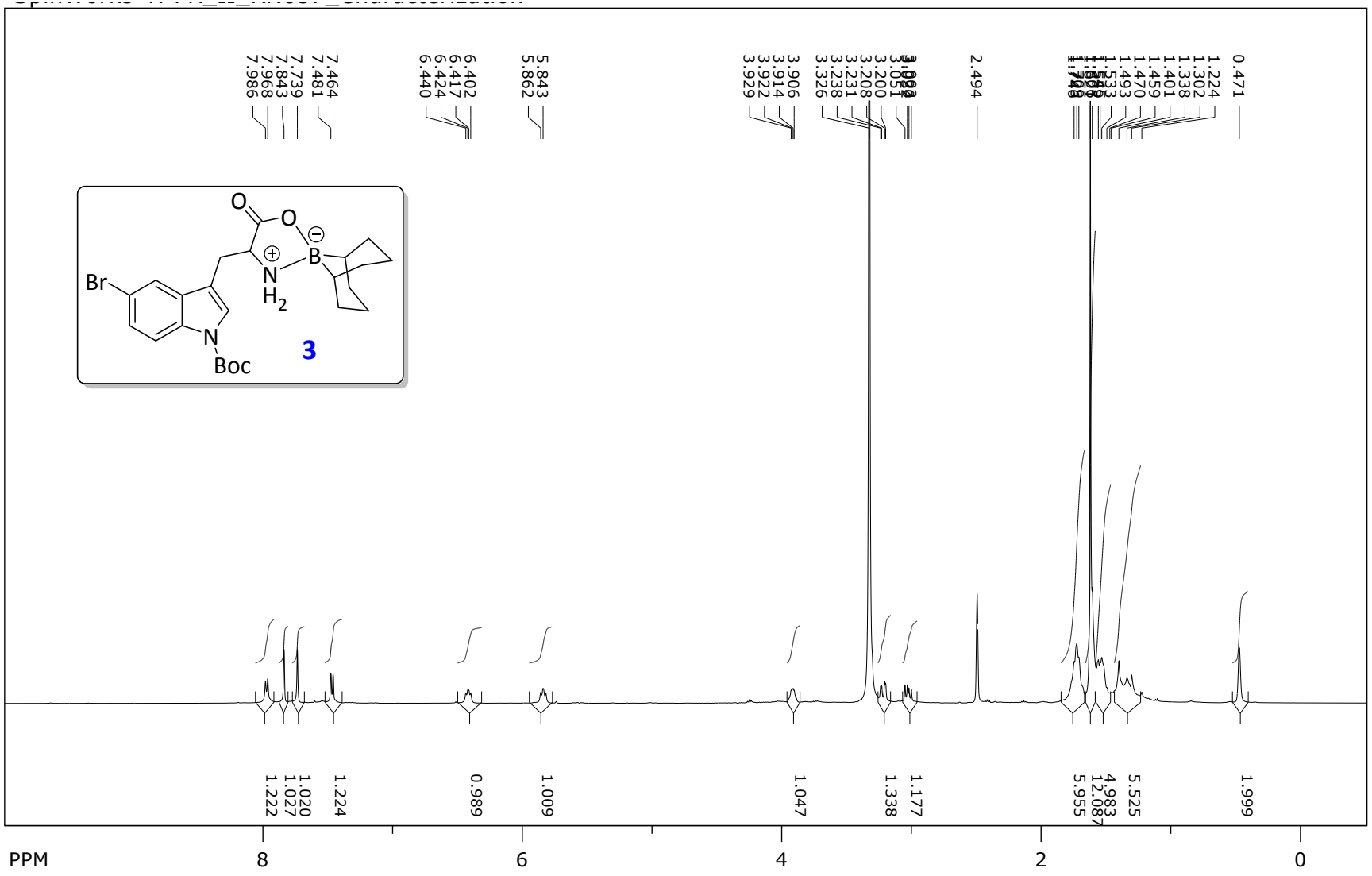
224.22
471.02
496.98
517.21
554.90
585.41
611.25
646.05
80.17
98.21
114.19
137.24
192.26
209.23
244.20
281.20
319.10
359.25
377.10
433.22
Br
2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7.481
7.464
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6.417
6.402
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5.843
3.929
3.922
3.914
3.906
3.326
3.238
3.231
3.208
3.200
3.051
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1.302
1.338
1.401
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1.470
1.493
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Boc
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O
B
N
H2
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1.020
1.027
1.224
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1.009
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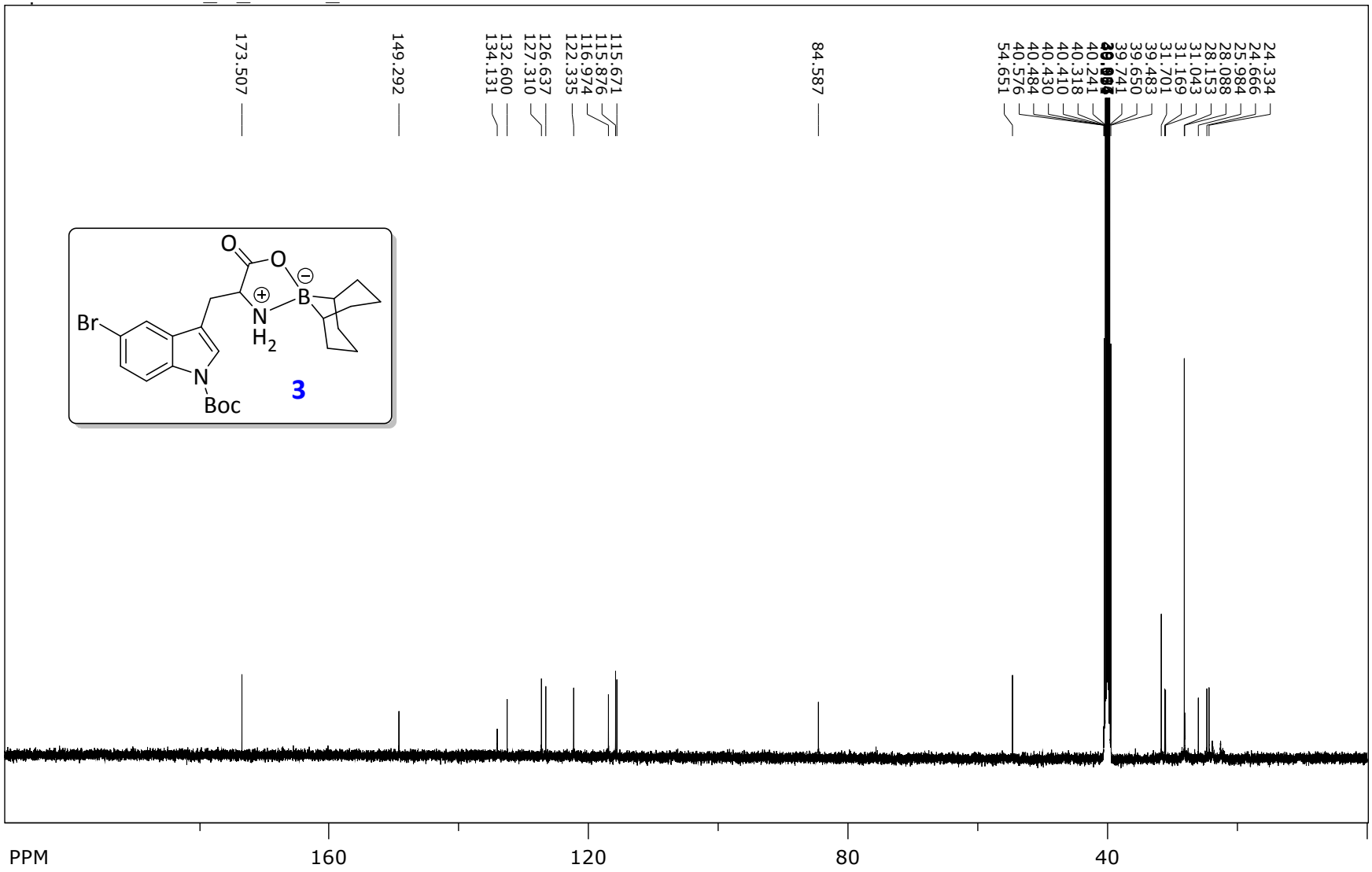
4
2
0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40.576
40.484
40.430
40.410
40.318
40.241
39.741
39.650
39.483
31.701
31.169
31.043
28.153
28.088
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24.334
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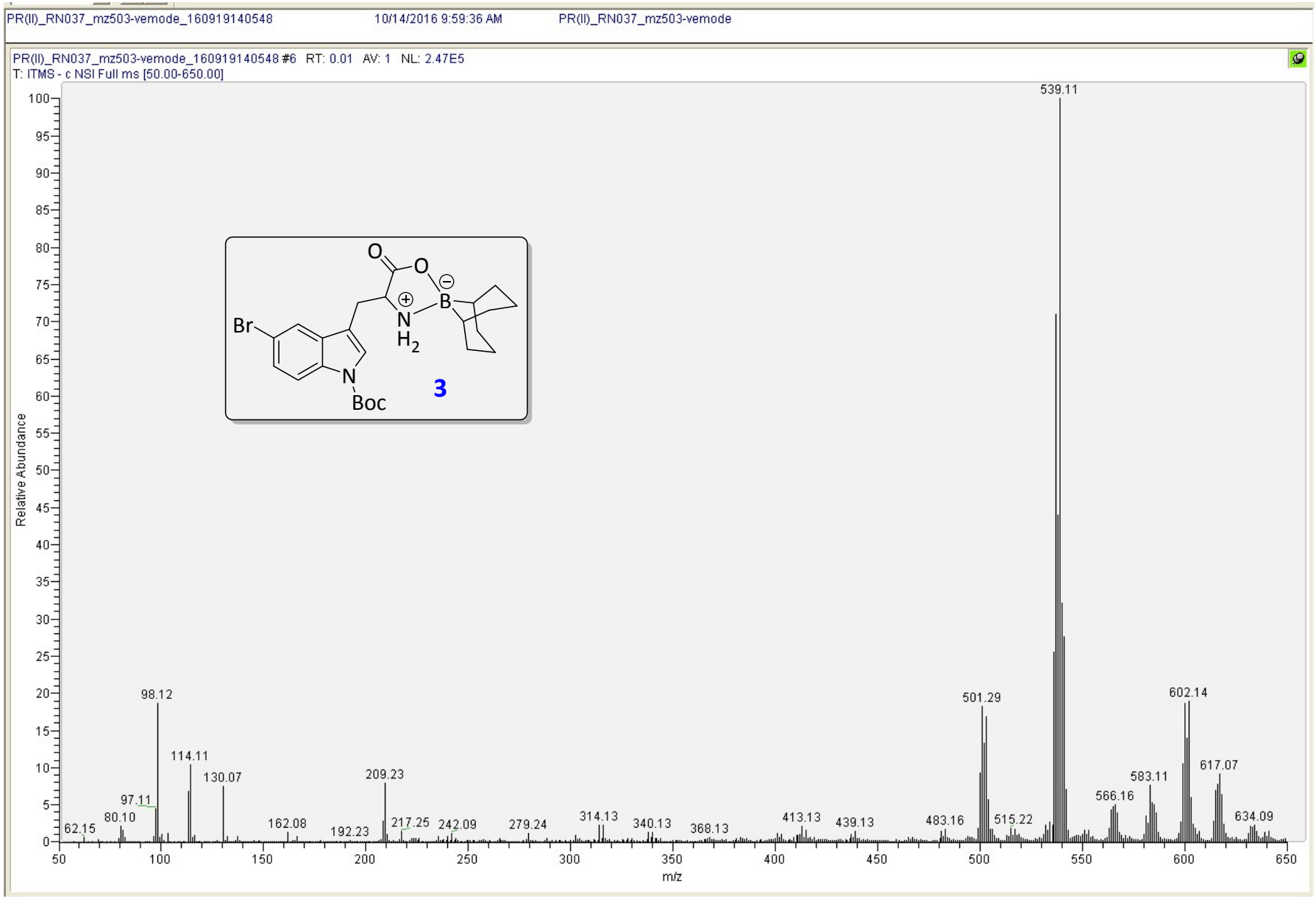
Boc
O
O
B
N
H2
3
PPM
160
120
80
40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T: ITMS - c NSI Full ms [50.00-650.00]
Br
N
Boc
O
O
B
N
H2
3
Relative Abundance
m/z
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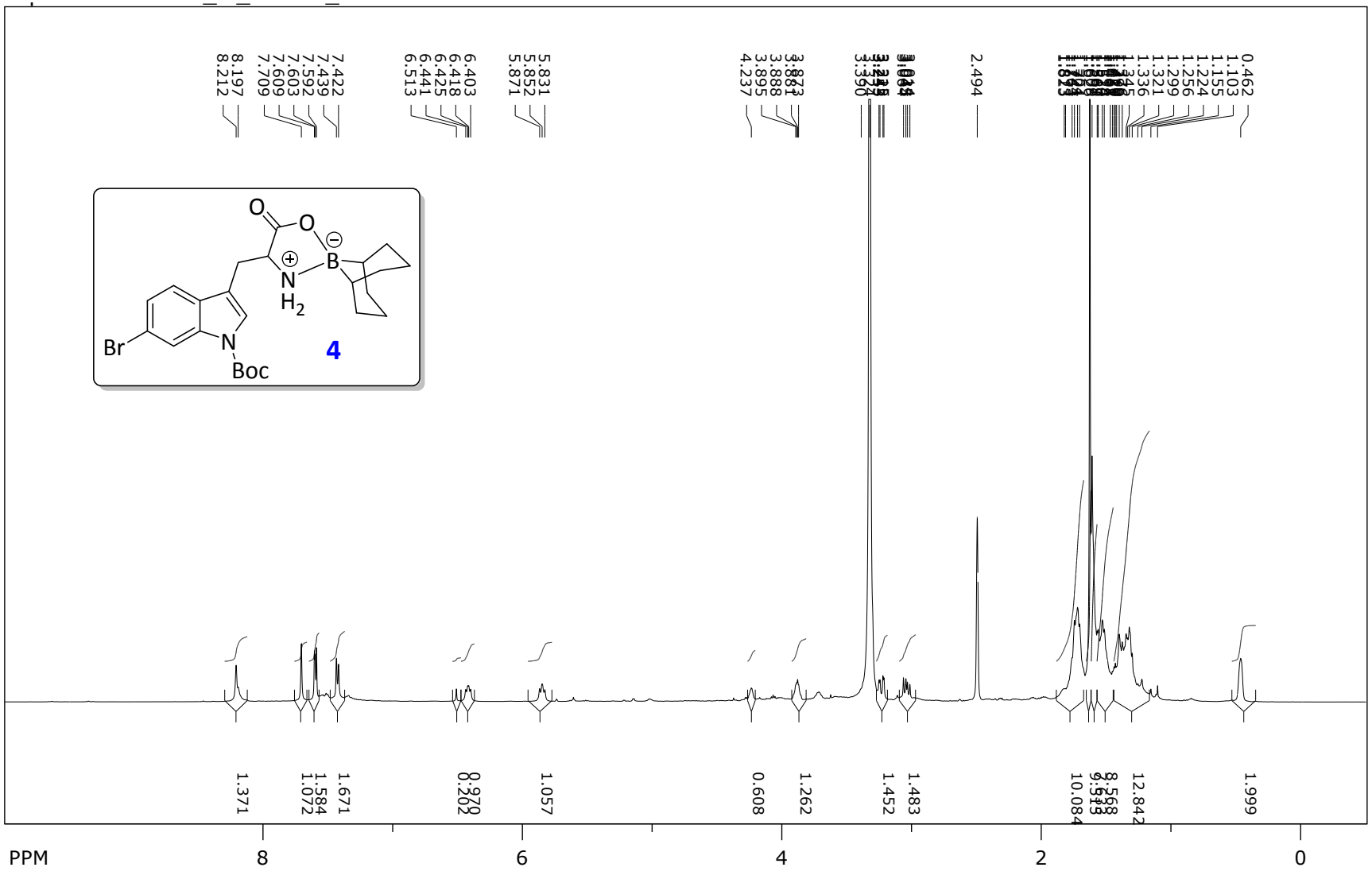
501.29
602.14
617.07
583.11
566.16
634.09
515.22
483.16
439.13
413.13
368.13
340.13
314.13
279.24
242.09
217.25
209.23
192.23
162.08
130.07
114.11
98.12
97.11
80.10
62.15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6.403
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5.852
5.831
4.237
3.895
3.888
3.881
3.873
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2.494
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1.321
1.299
1.256
1.224
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1.103
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1.072
1.671
0.979
0.262
1.057
0.608
1.262
1.452
1.483
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PPM
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2
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Br
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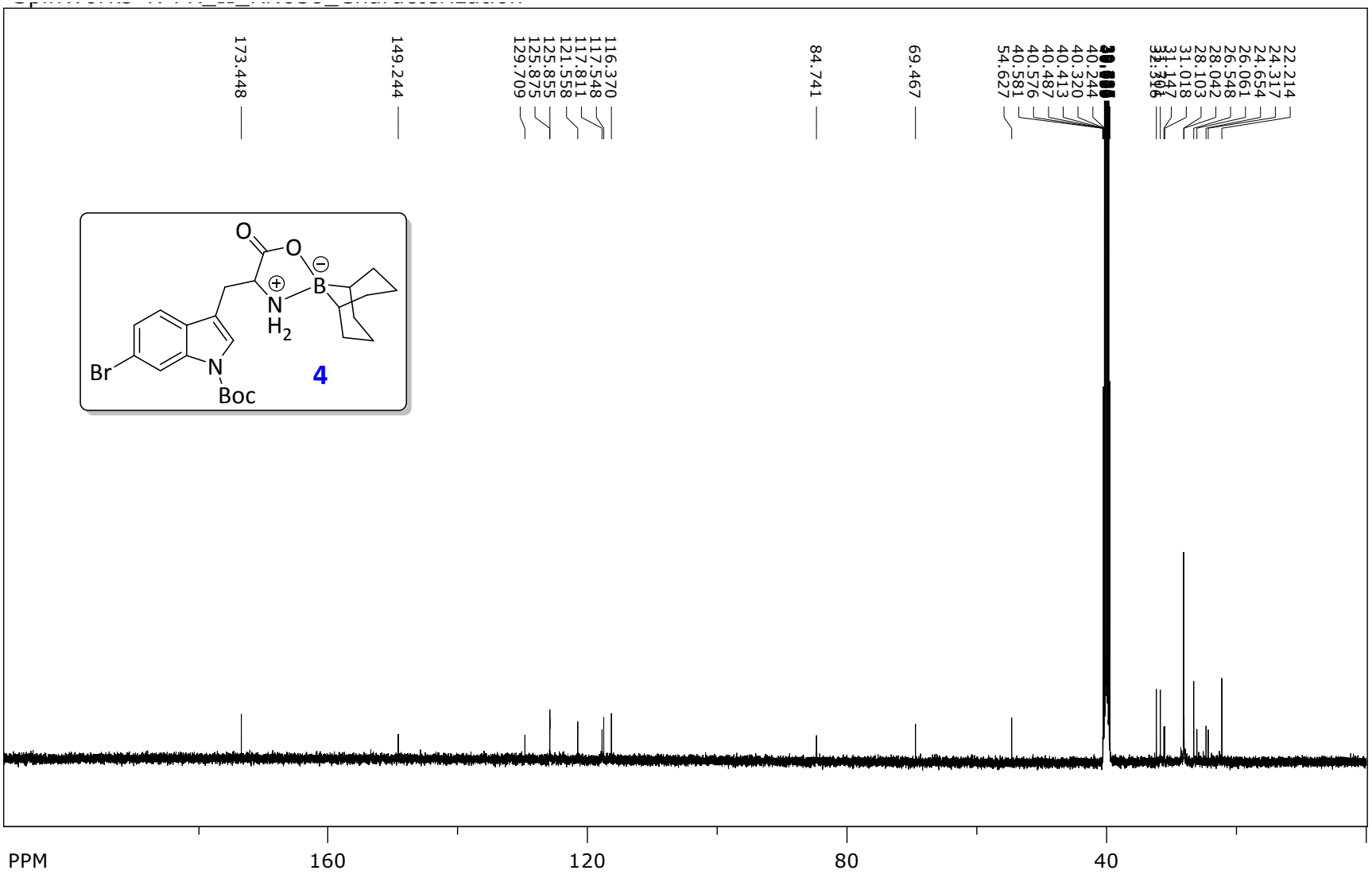
Boc
O
O
B
N
H2
4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40.576
40.487
40.413
40.320
40.244
31.018
28.103
28.042
26.548
26.061
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Br
N
Boc
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PPM
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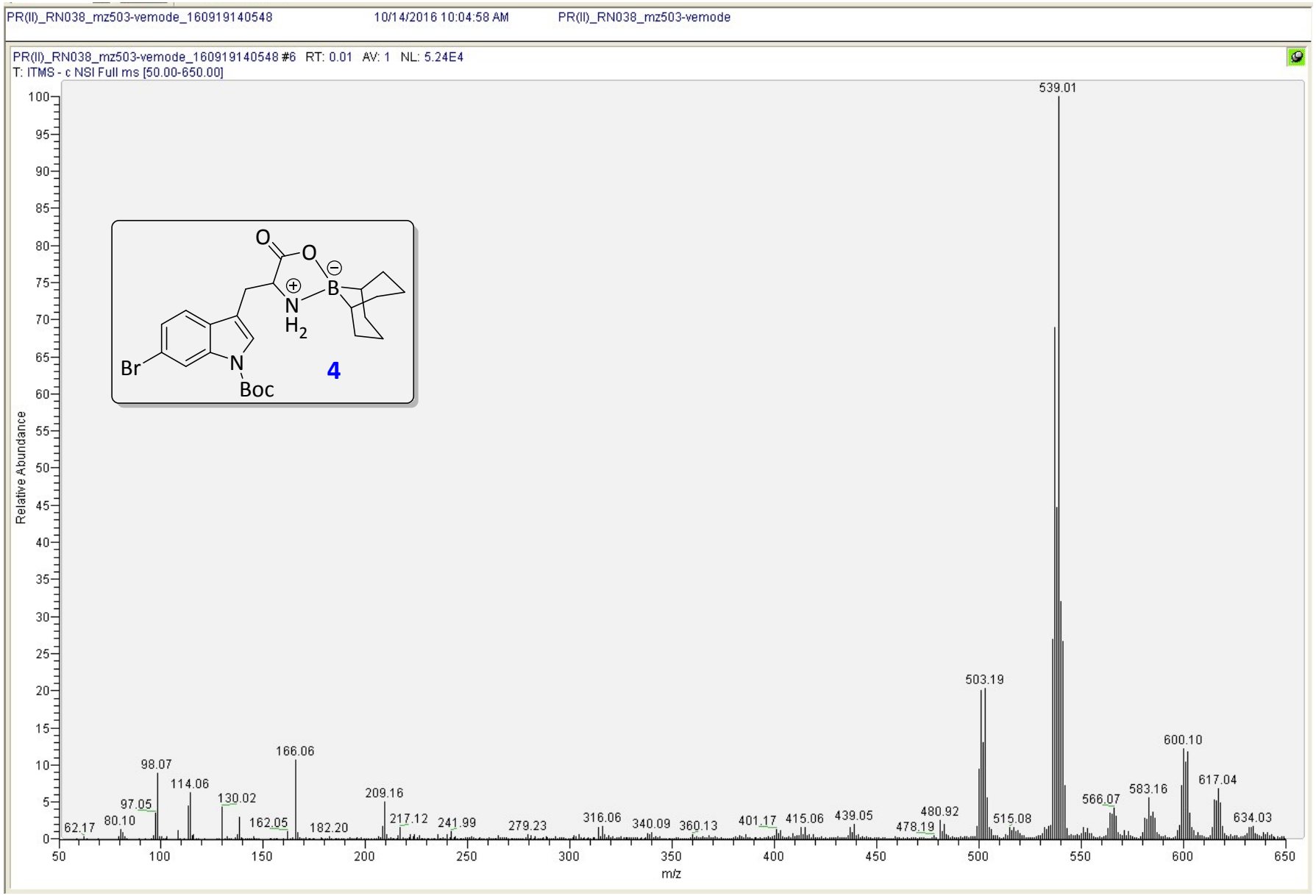
120
80
40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PR(II)_RN038_mz503-vemode_160919140548 #6 RT: 0.01 AV: 1 NL: 5.24E4
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617.04
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566.07
634.03
515.08
480.92
478.19
439.05
415.06
401.17
360.13
340.09
316.06
279.23
241.99
217.12
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162.05
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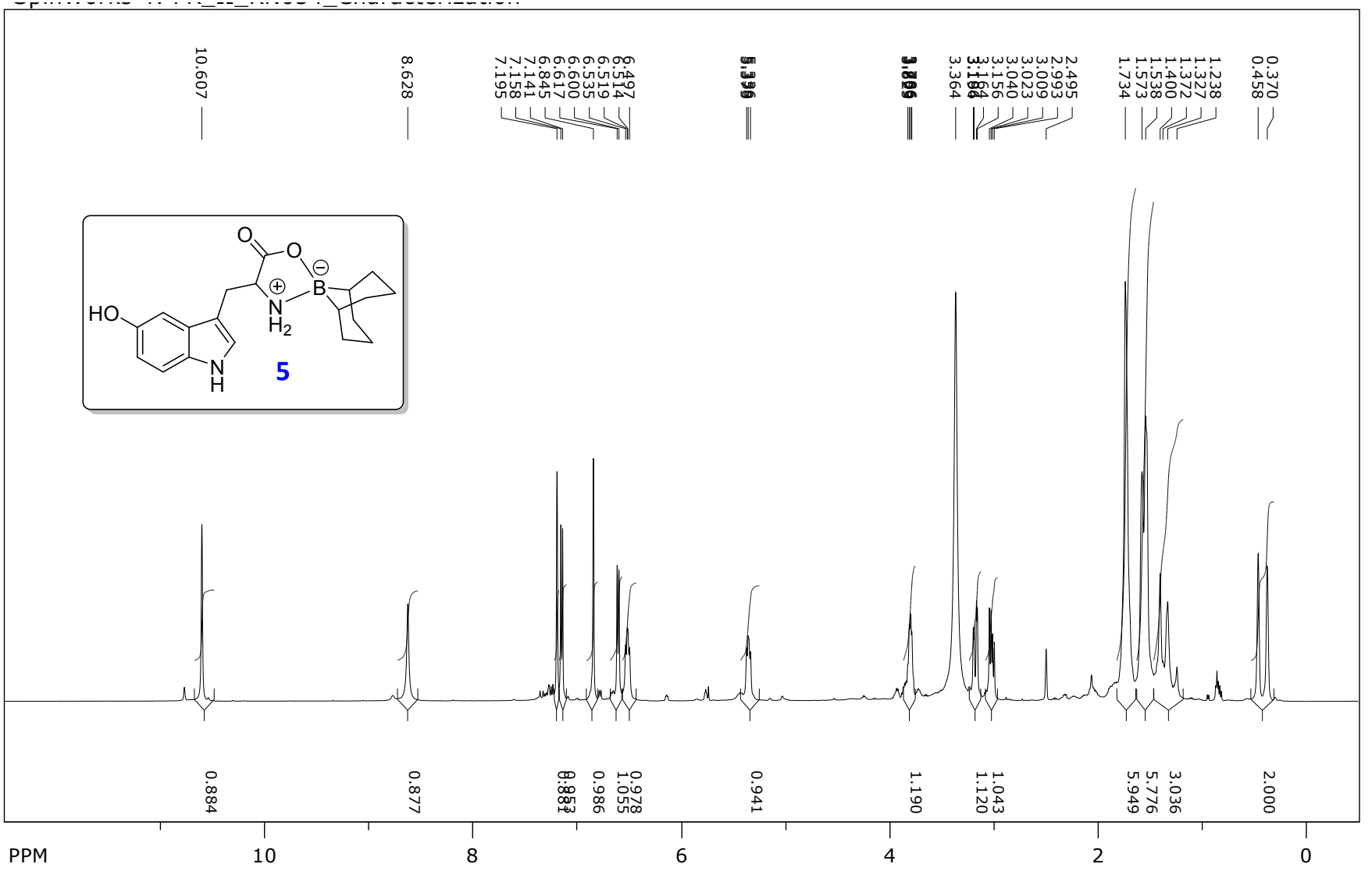
114.06
98.07
97.05
80.10
62.17
Br
N
Boc
4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1.327
1.238
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0.370
HO
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H
N
H2
B
O
O
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2
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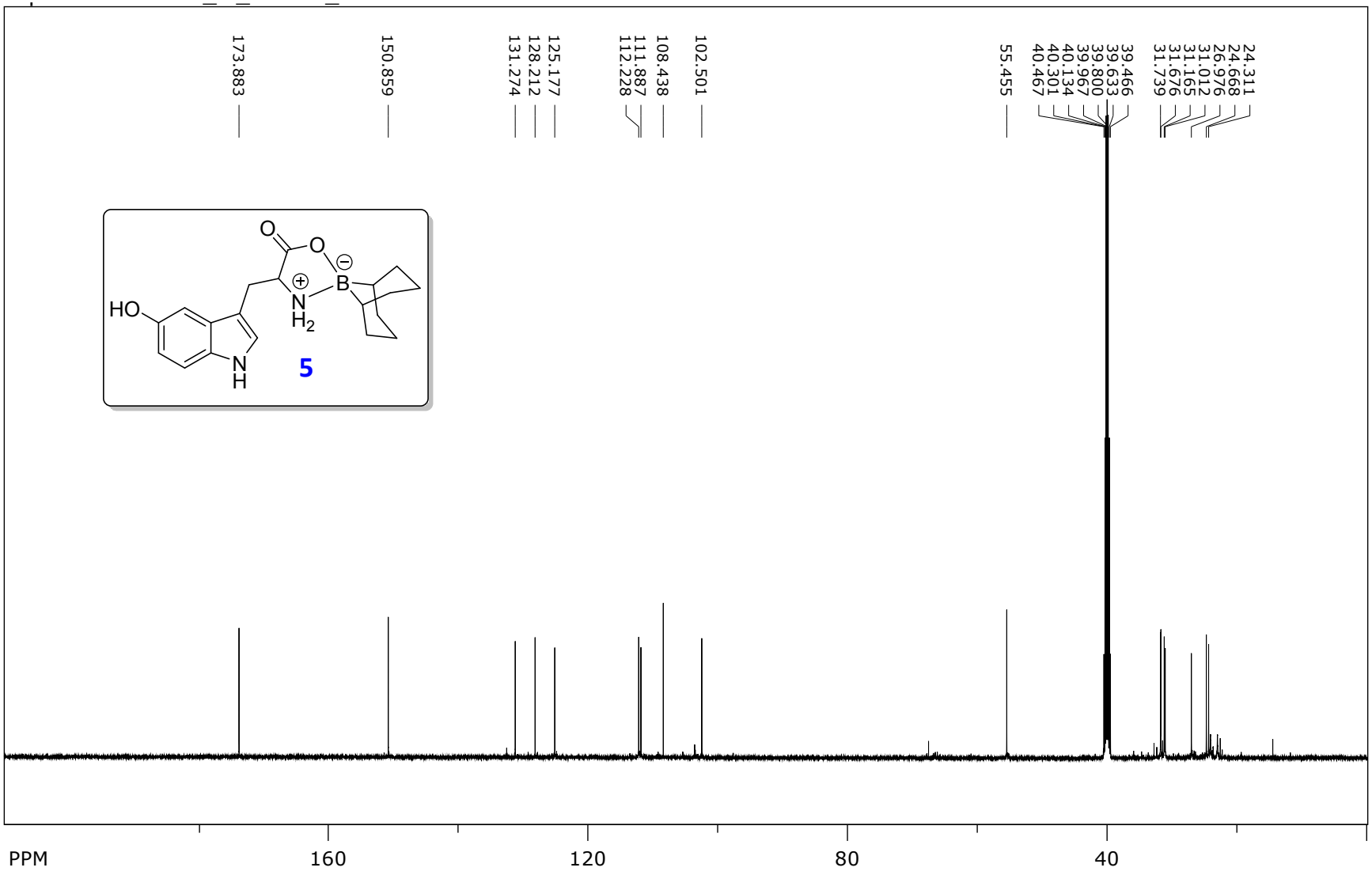
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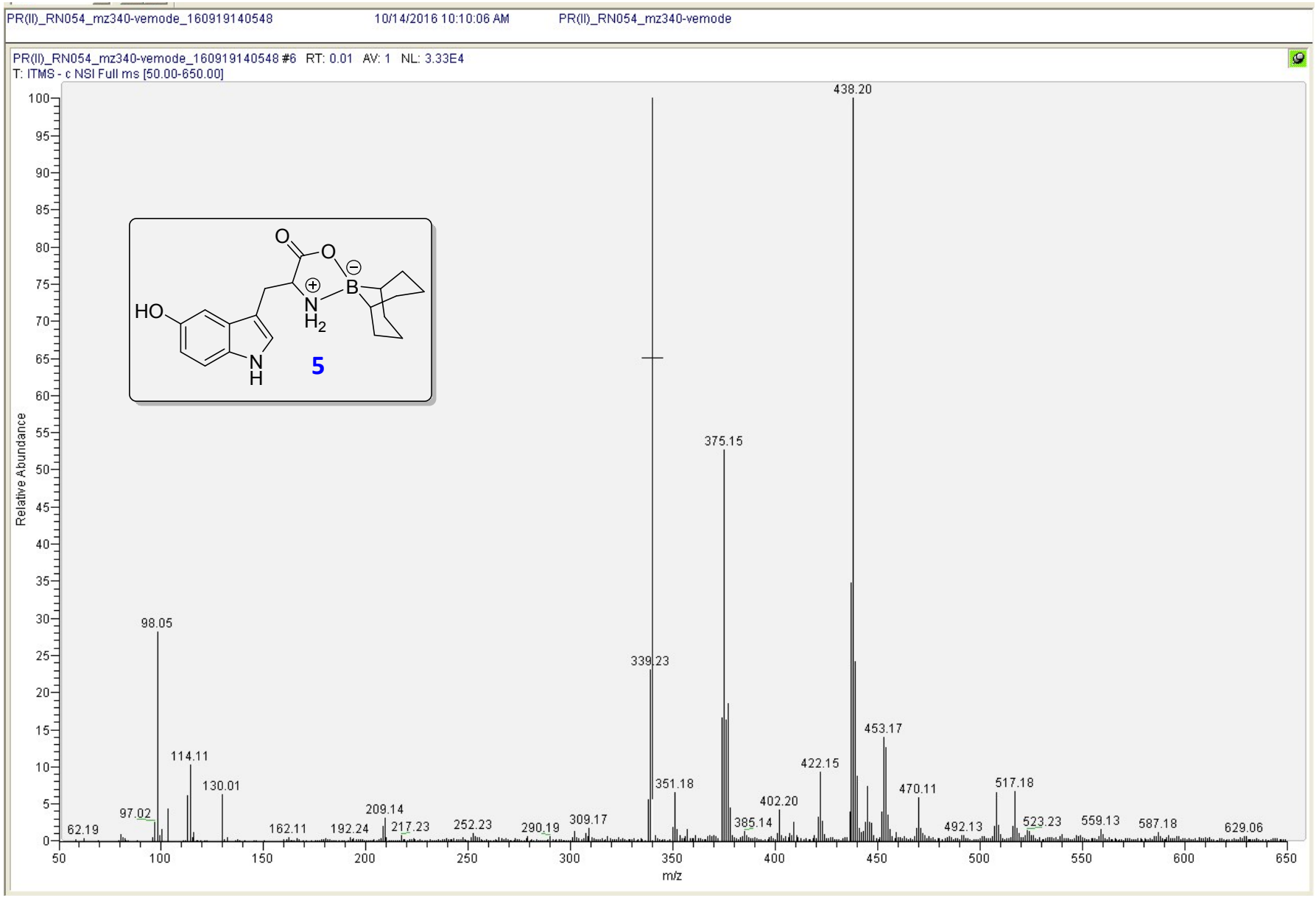
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H
O
O
B
N
H2
5
Relative Abundance
m/z
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375.15
339.23
98.05
453.17
422.15
114.11
130.01
351.18
470.11
517.18
402.20
97.02
209.14
62.19
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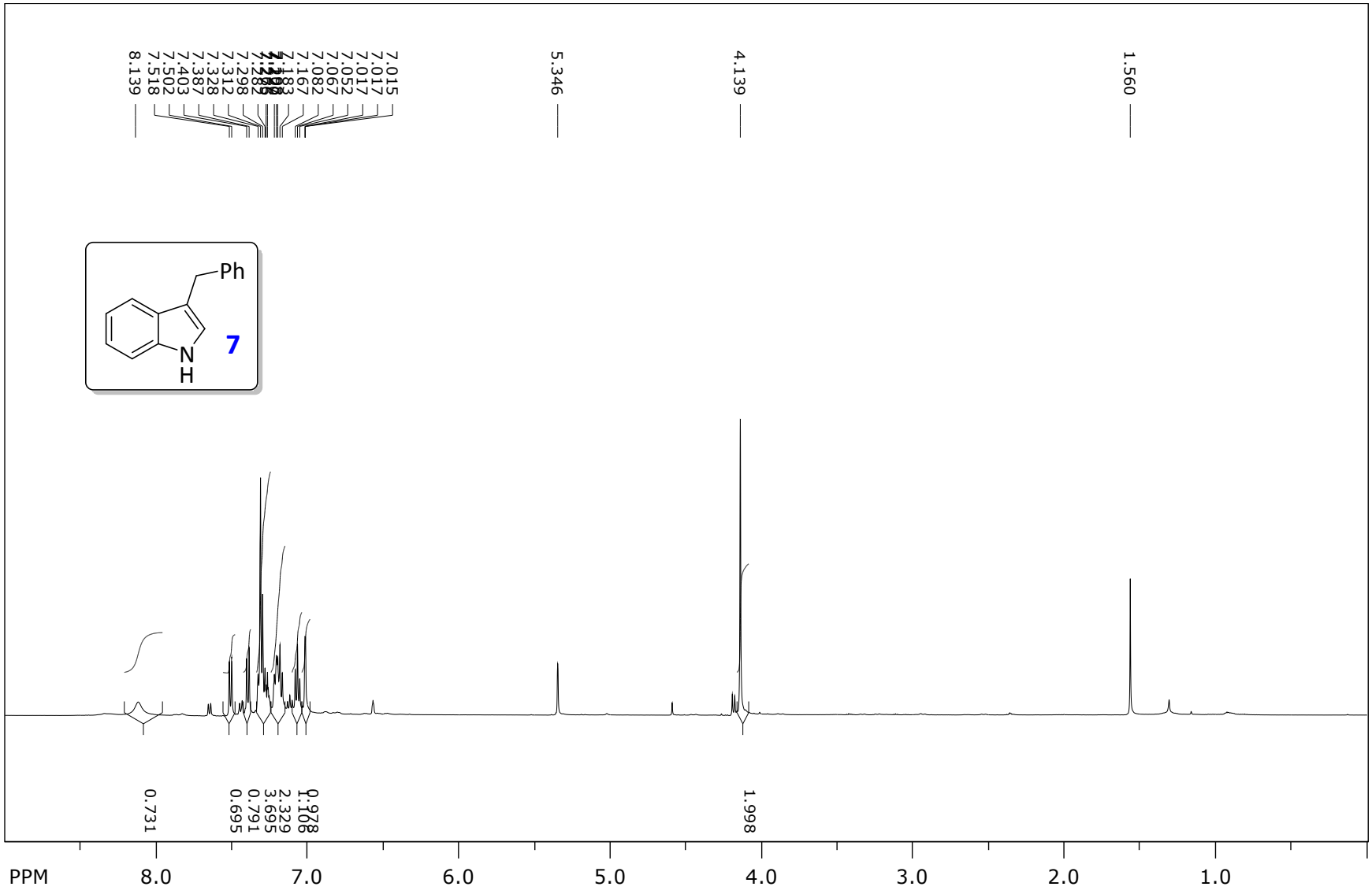
629.06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7.015
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PPM
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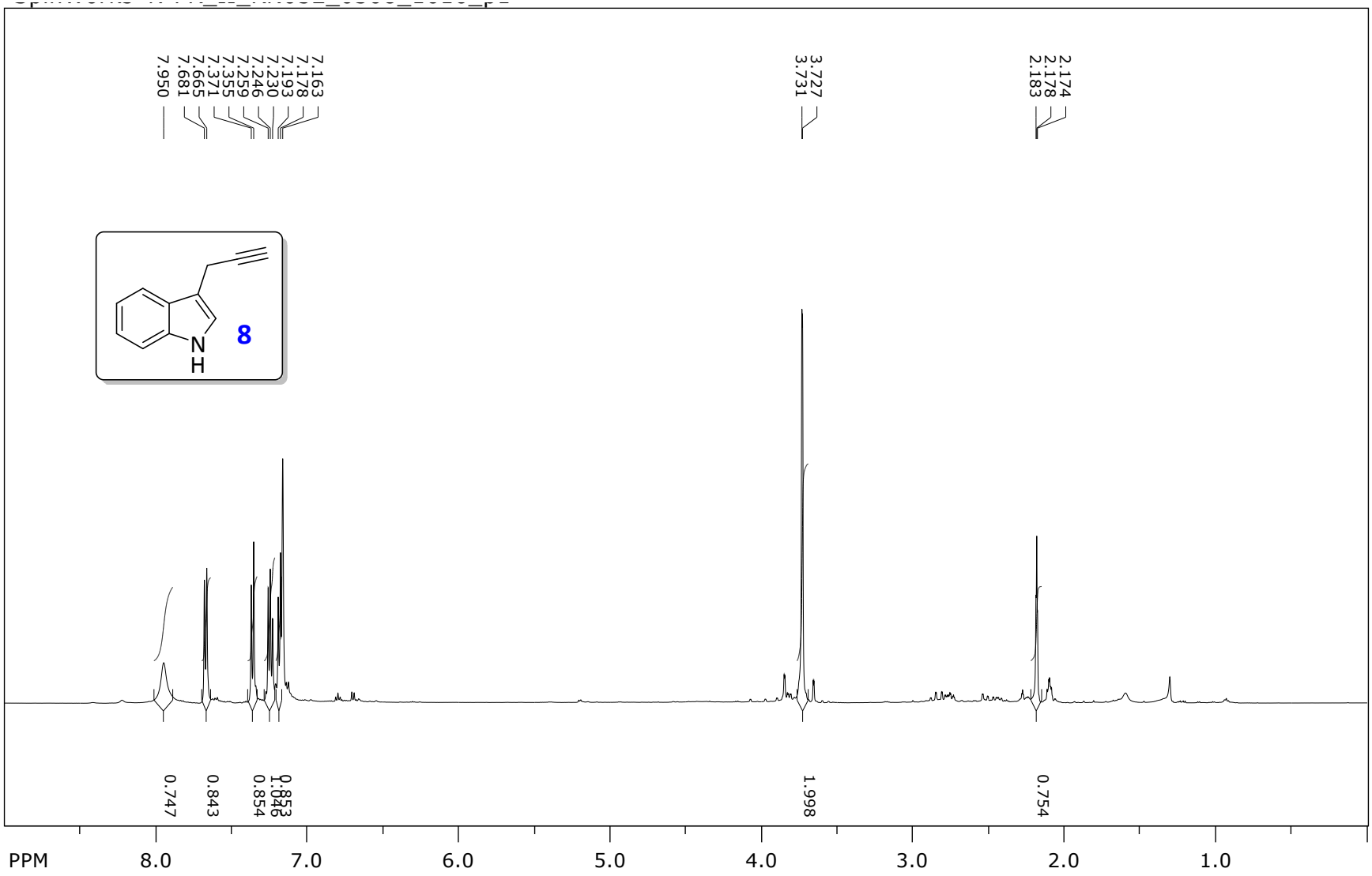
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0.854
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PPM
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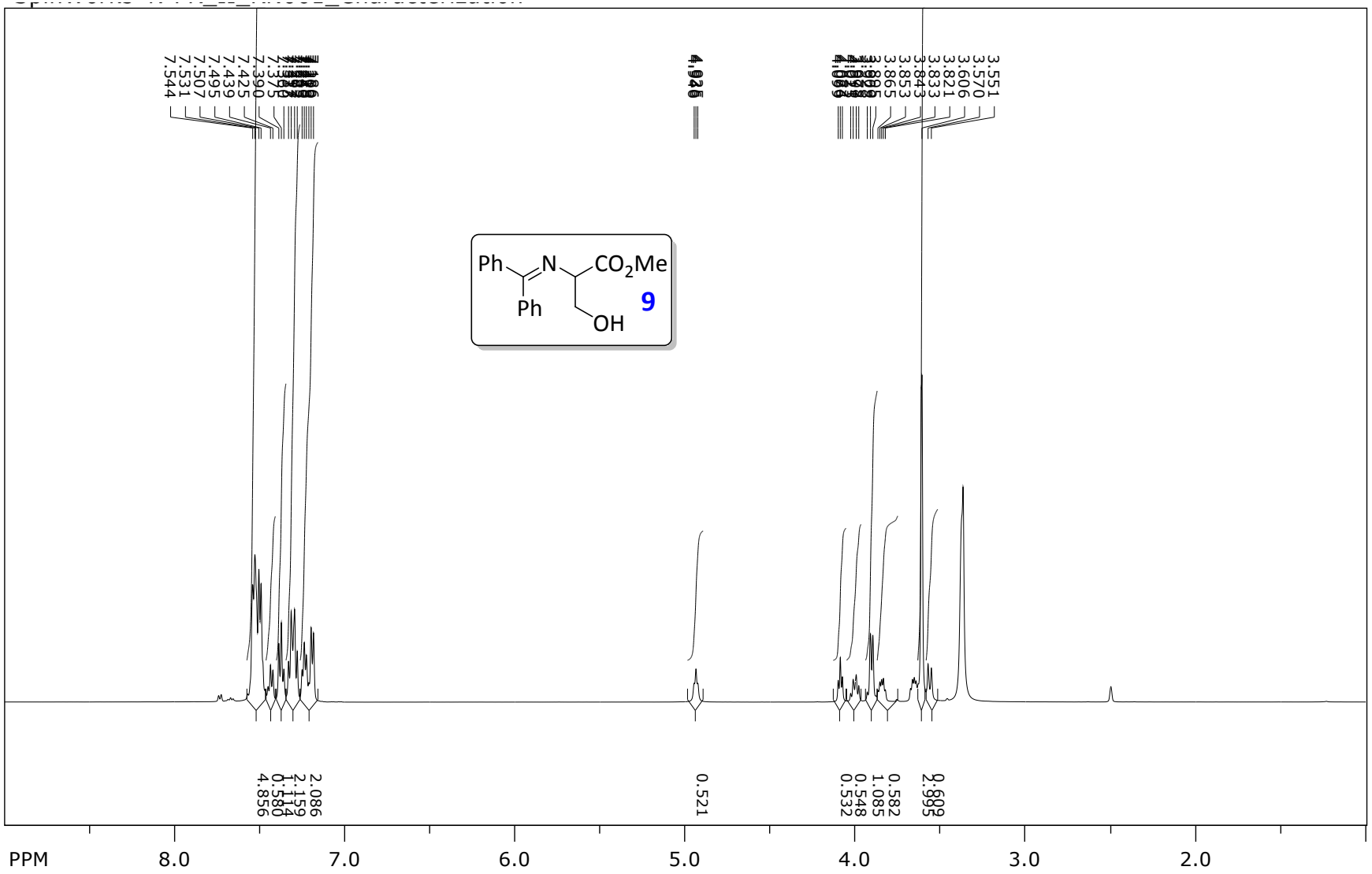
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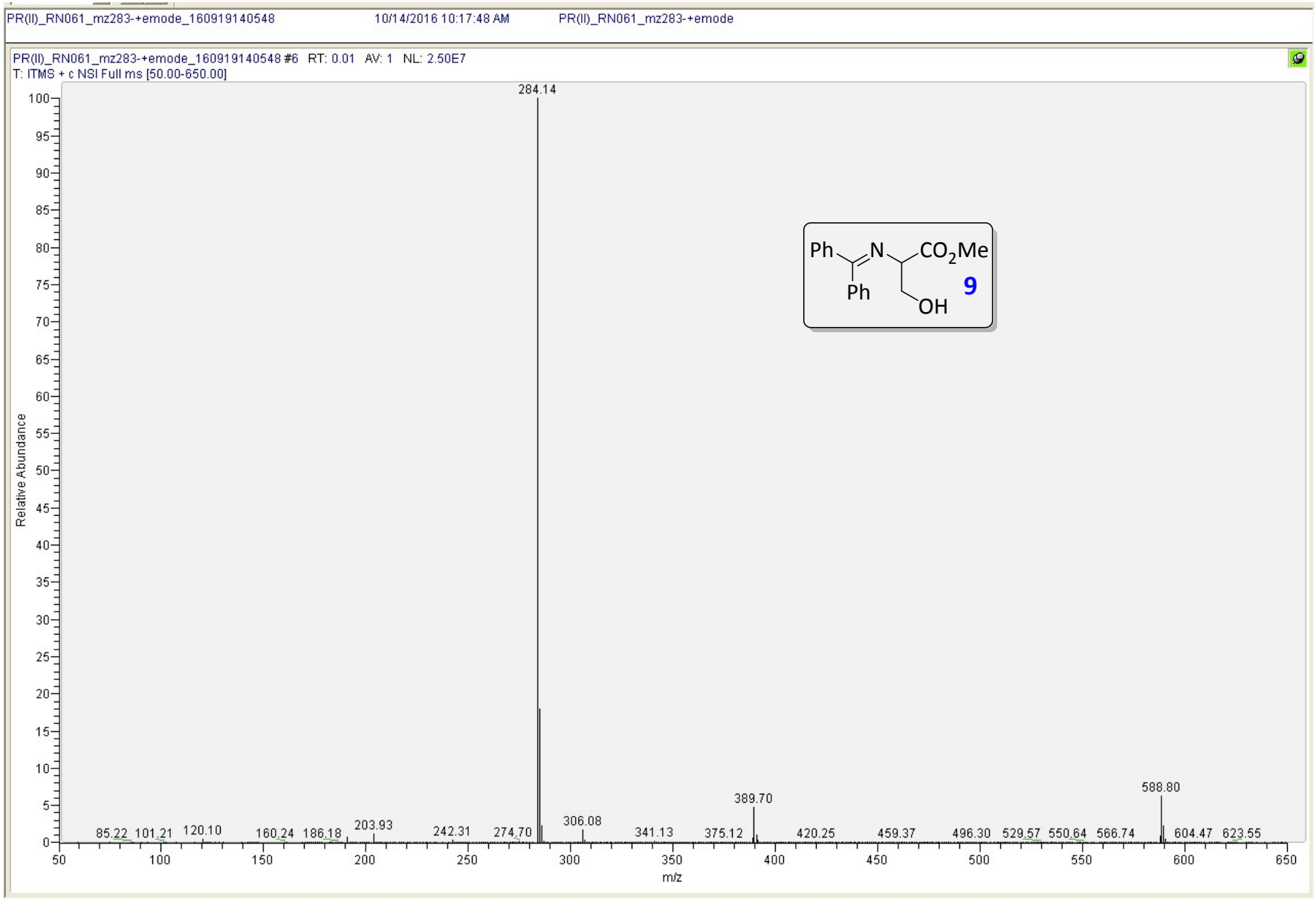
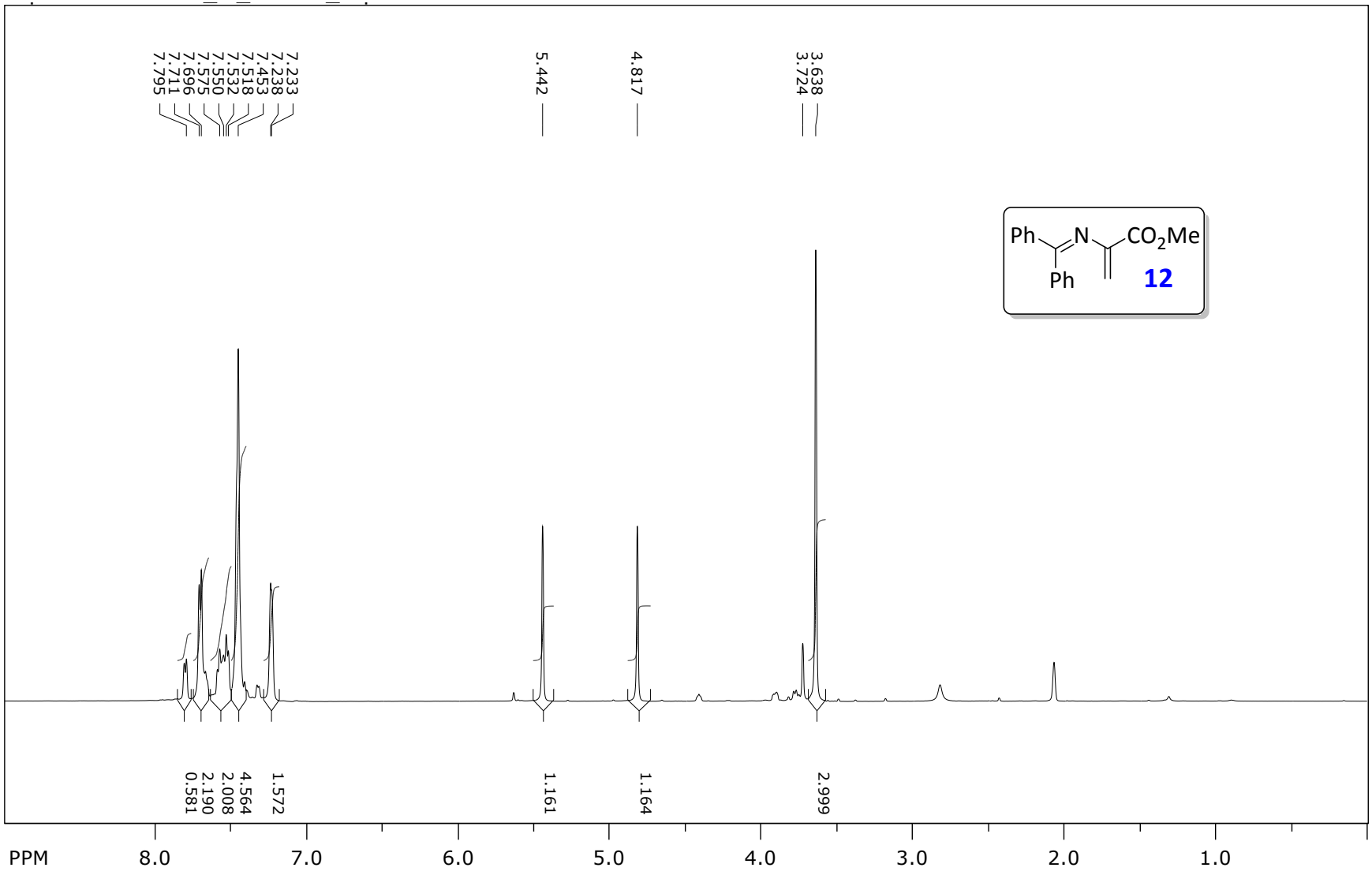
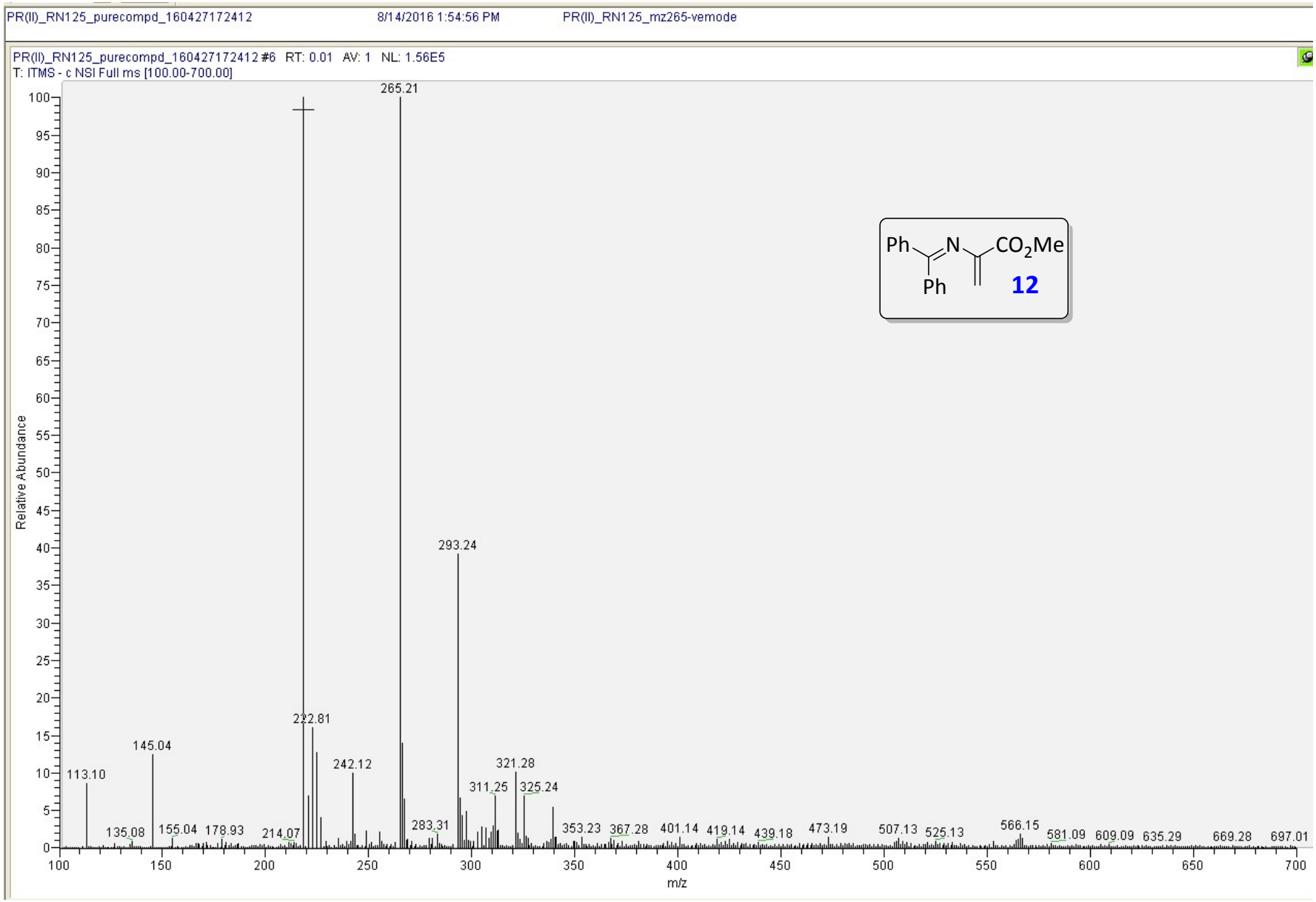
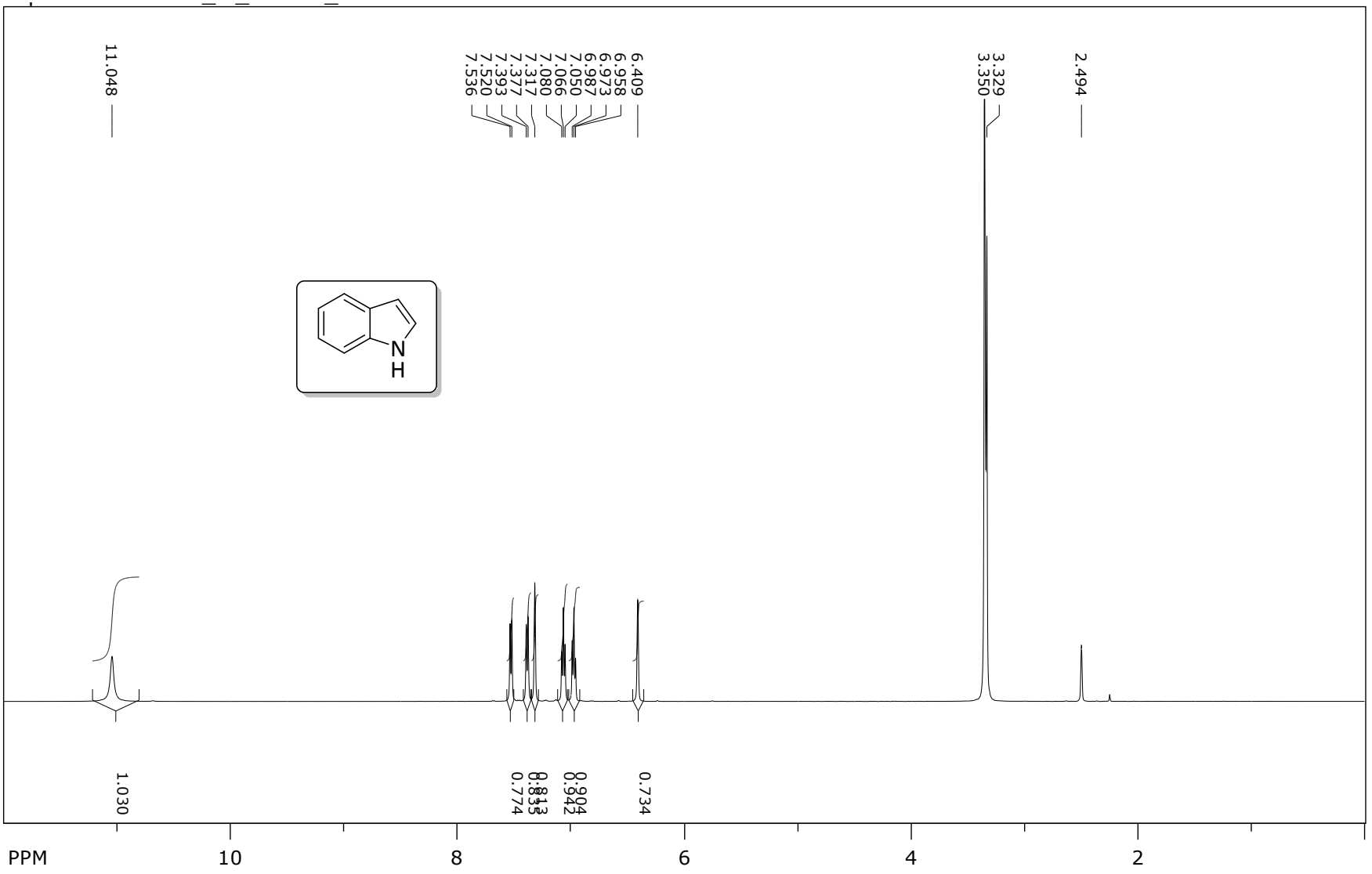
3.843
3.833
3.821
3.606
3.570
3.551
Ph
N
CO2Me
Ph
OH
9
2.086
0.521
0.582
1.085
0.548
0.532
2.995
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0

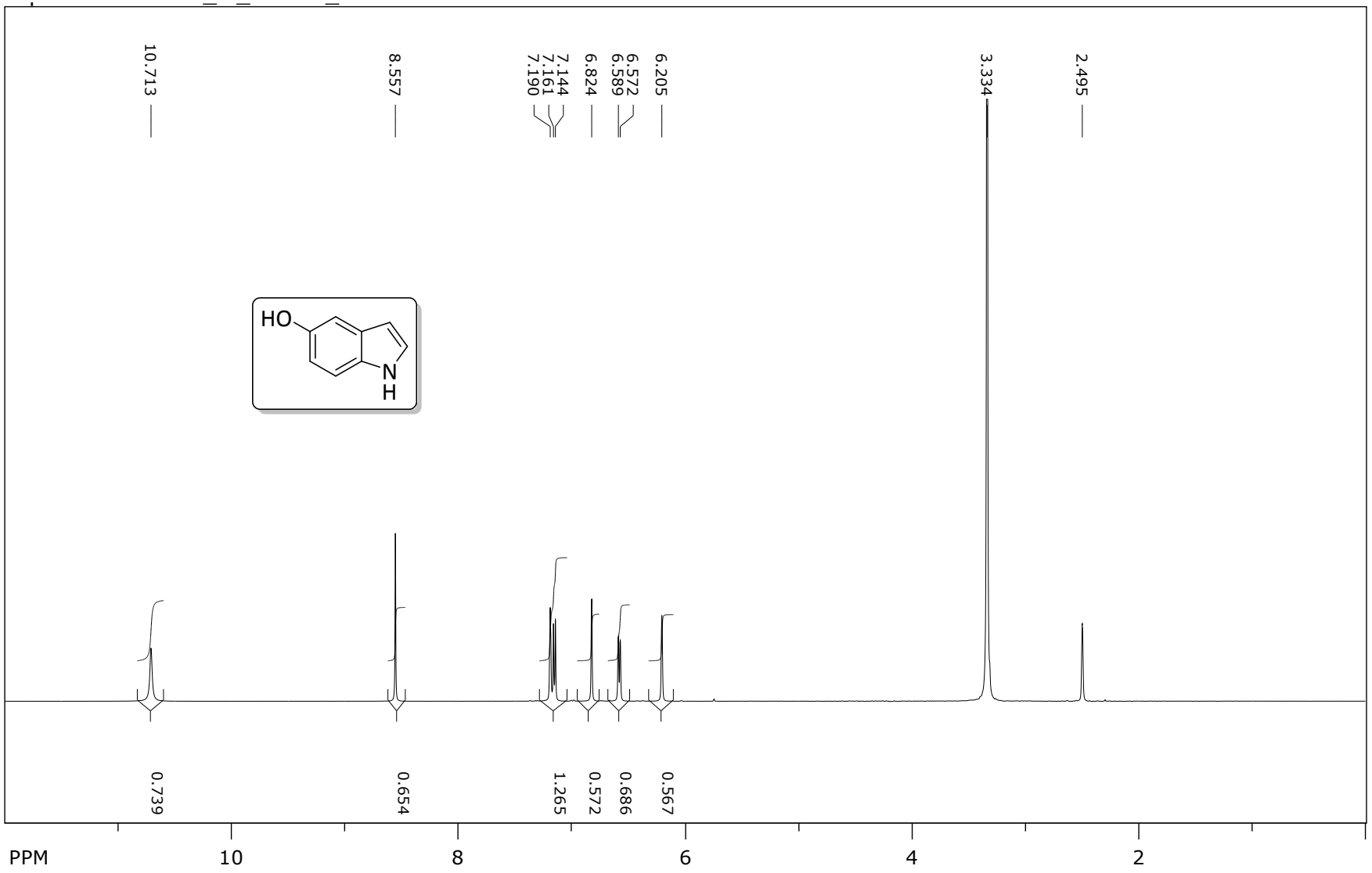

PR(II)_RN061_mz283-+emode_160919140548 10/14/2016 10:17:48 AM PR(II)_RN061_mz283-+emode
PR(II)_RN061_mz283-+emode_160919140548 #6 RT: 0.01 AV: 1 NL: 2.50E7
T: ITMS + c NSI Full ms [50.00-650.00]
Relative Abundance
m/z
284.14
389.70
588.80
306.08
203.93
85.22
101.21
120.10
160.24
186.18
242.31
274.70
341.13
375.12
420.25
459.37
496.30
529.57
550.64
566.74
604.47
623.55
Ph
N
CO2Me
Ph
OH
9


7.795
7.711
7.696
7.575
7.550
7.532
7.518
7.453
7.238
7.233
5.442
4.817
3.724
3.638
Ph
N
CO2Me
Ph
12
0.581
2.190
2.008
4.564
1.572
1.161
1.164
2.999
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0

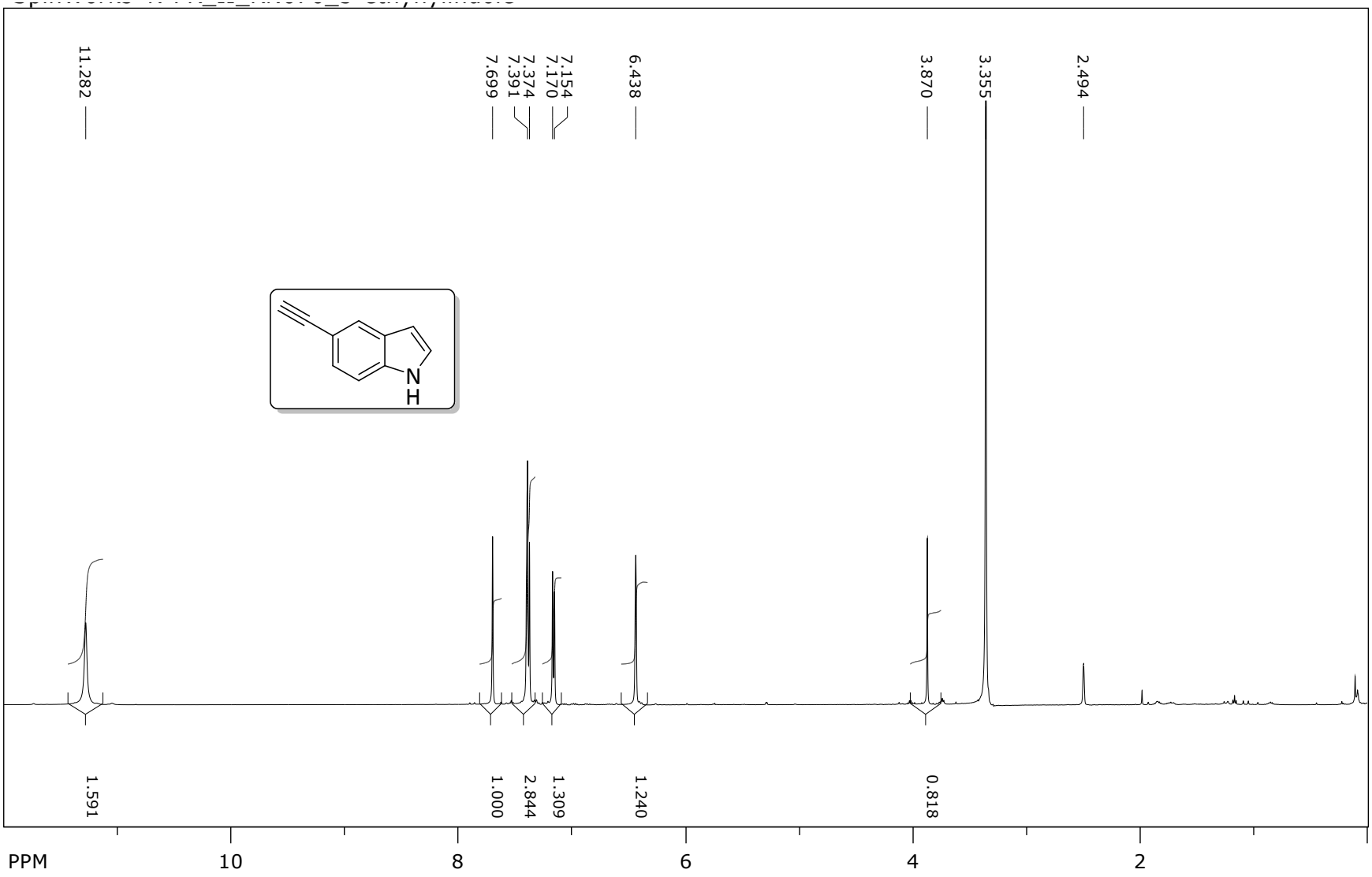

PR(II)_RN125_purecompd_160427172412 8/14/2016 1:54:56 PM PR(II)_RN125_mz265-vemode
PR(II)_RN125_purecompd_160427172412 #6 RT: 0.01 AV: 1 NL: 1.56E5
T: ITMS - c NSI Full ms [100.00-700.00]
Relative Abundance
m/z
265.21
293.24
222.81
145.04
242.12
321.28
311.25
325.24
113.10
135.08
155.04
178.93
214.07
283.31
353.23
367.28
401.14
419.14
439.18
473.19
507.13
525.13
566.15
581.09
609.09
635.29
669.28
697.01
Ph
N
CO2Me
Ph
12

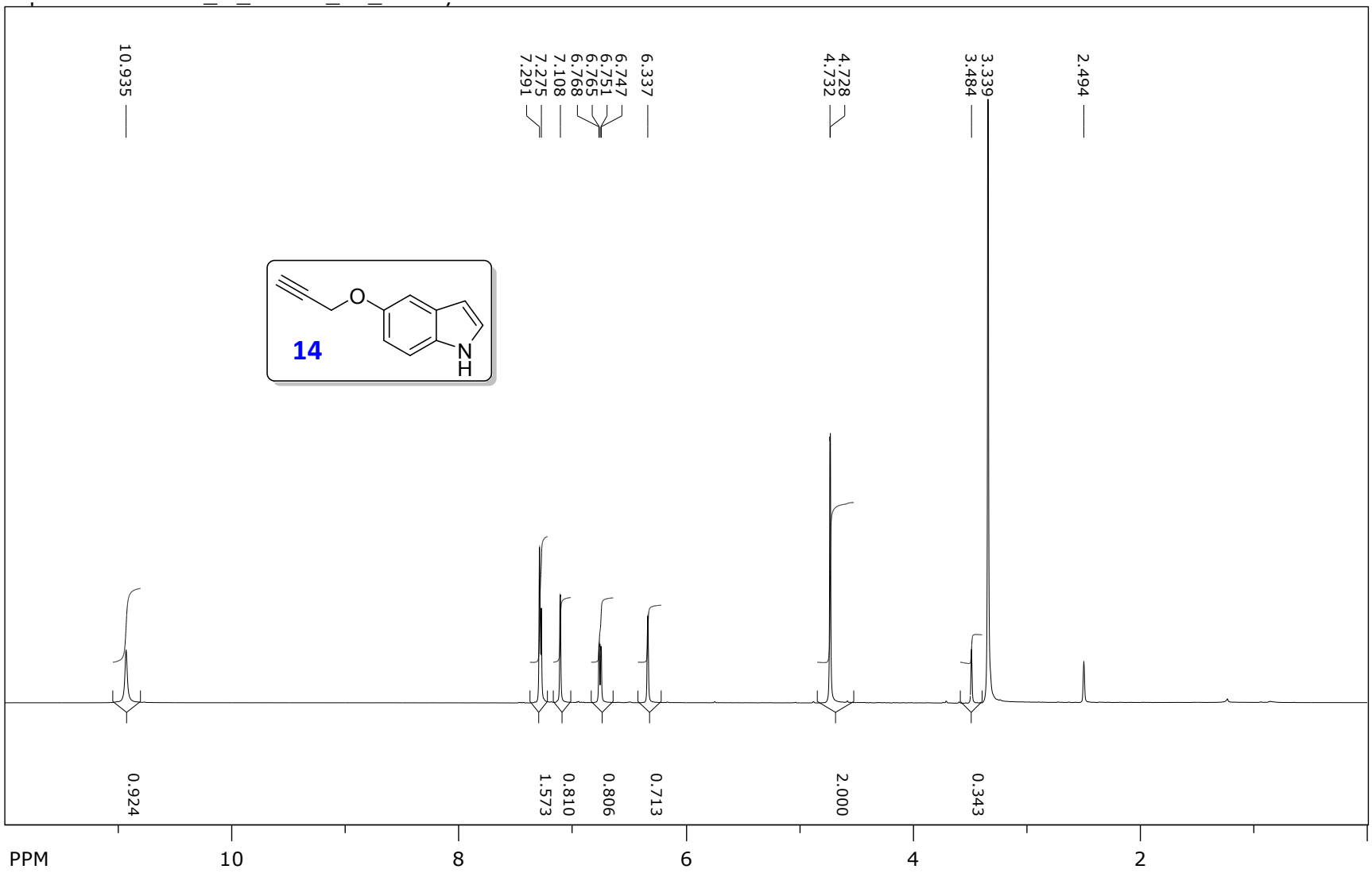


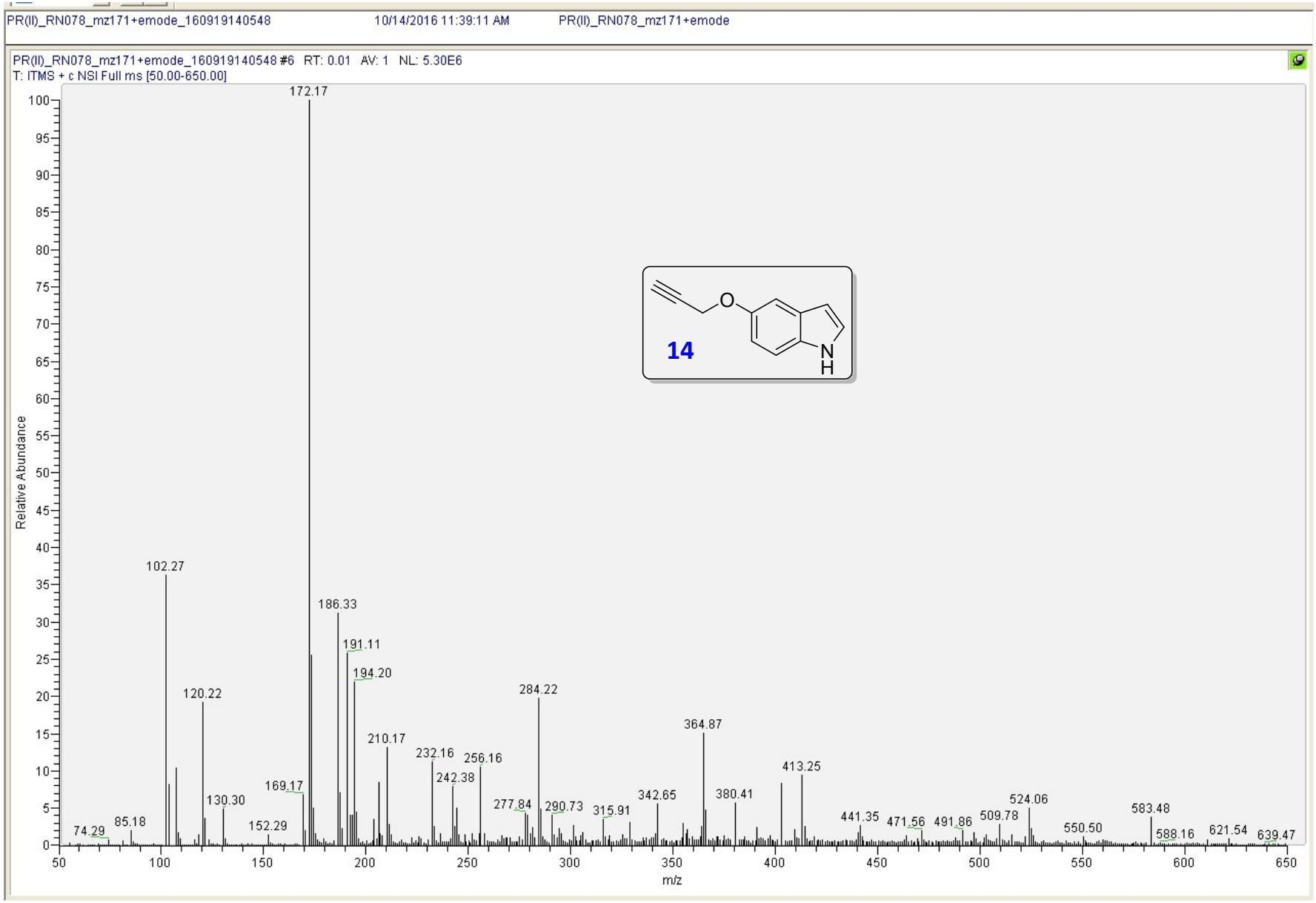
Indole NH peak at 11.0 ppm.

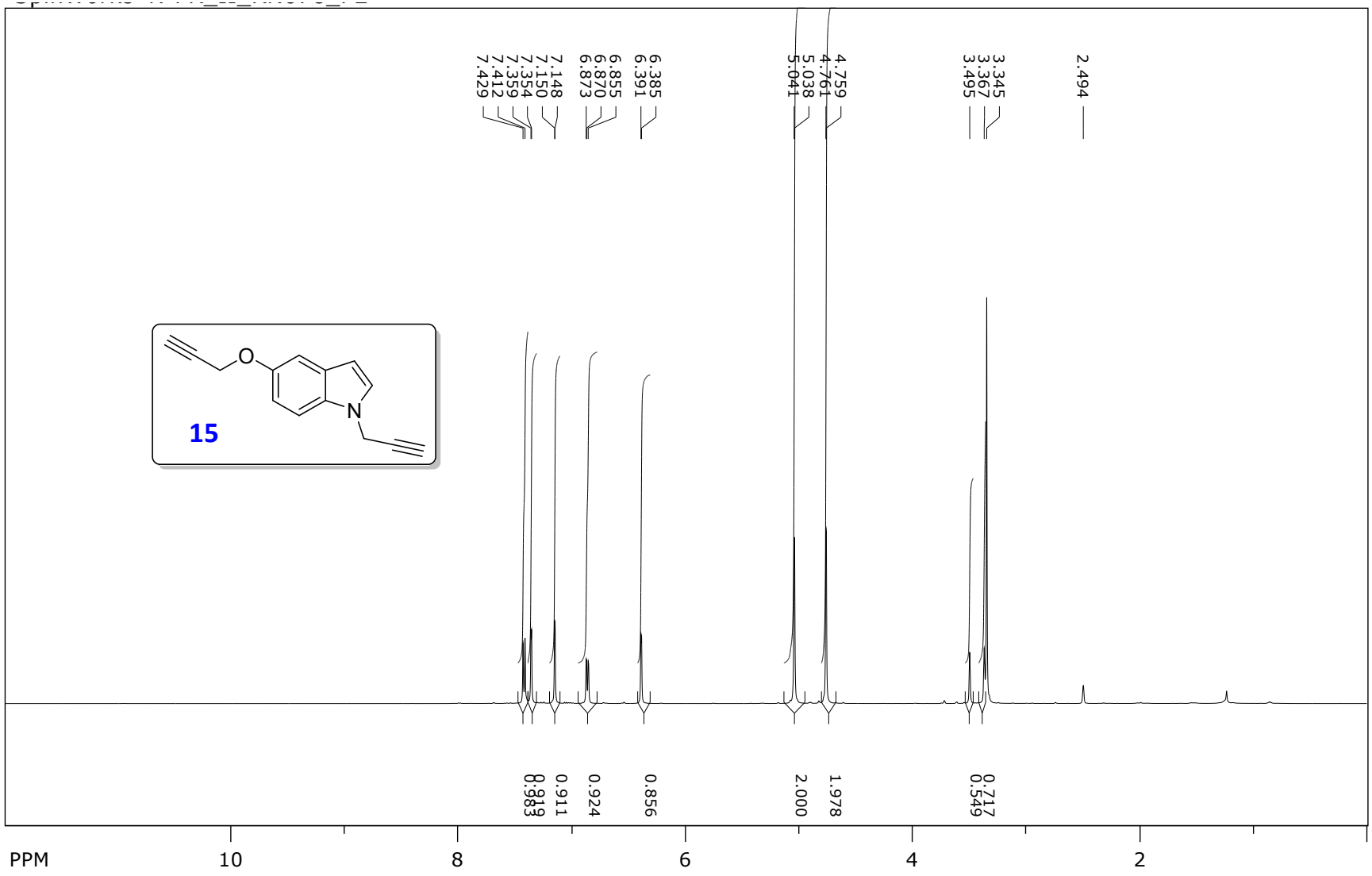


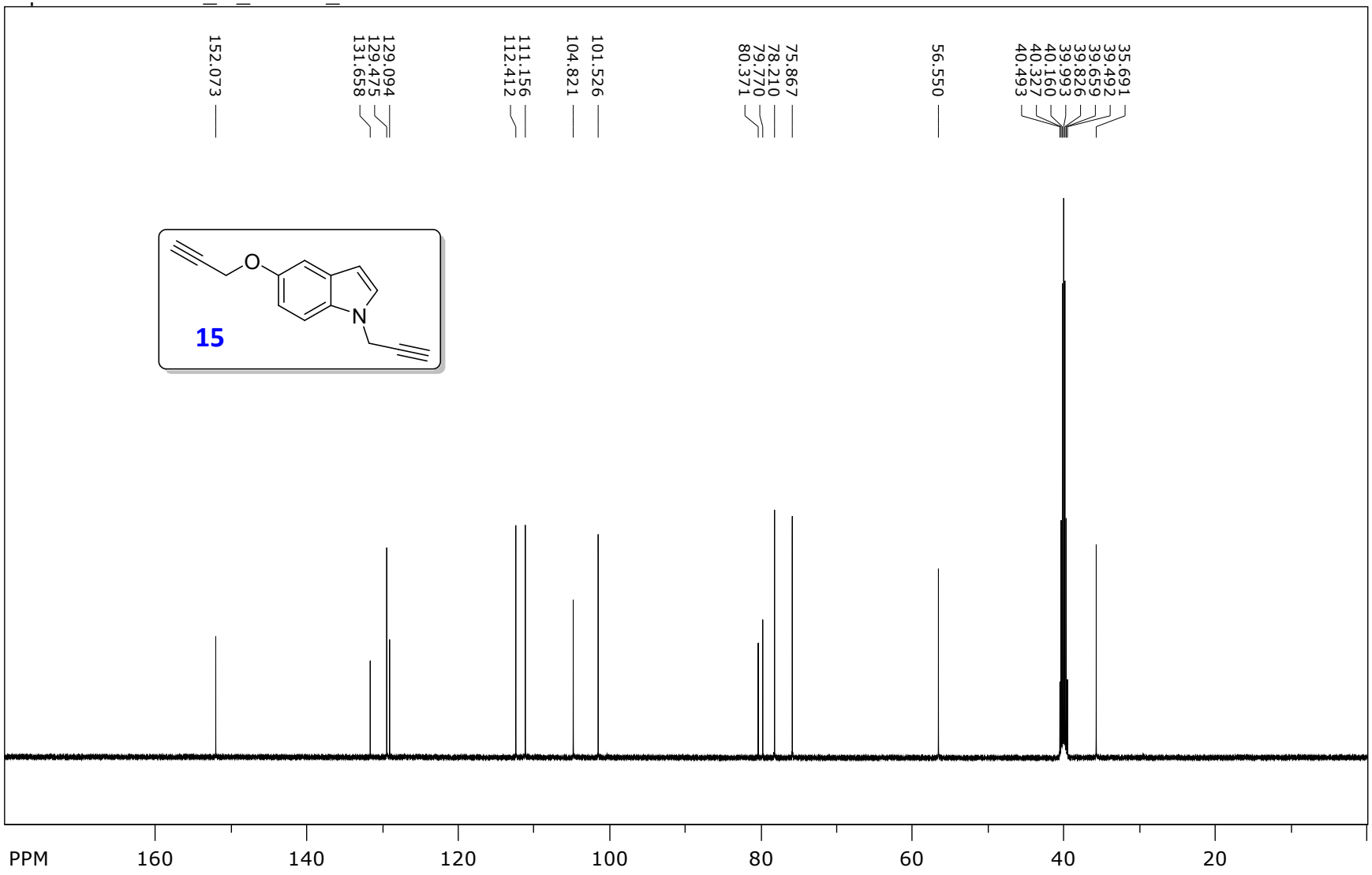
Indole NH peak @ 10.71 ppm; OH peak @ 8.55 ppm

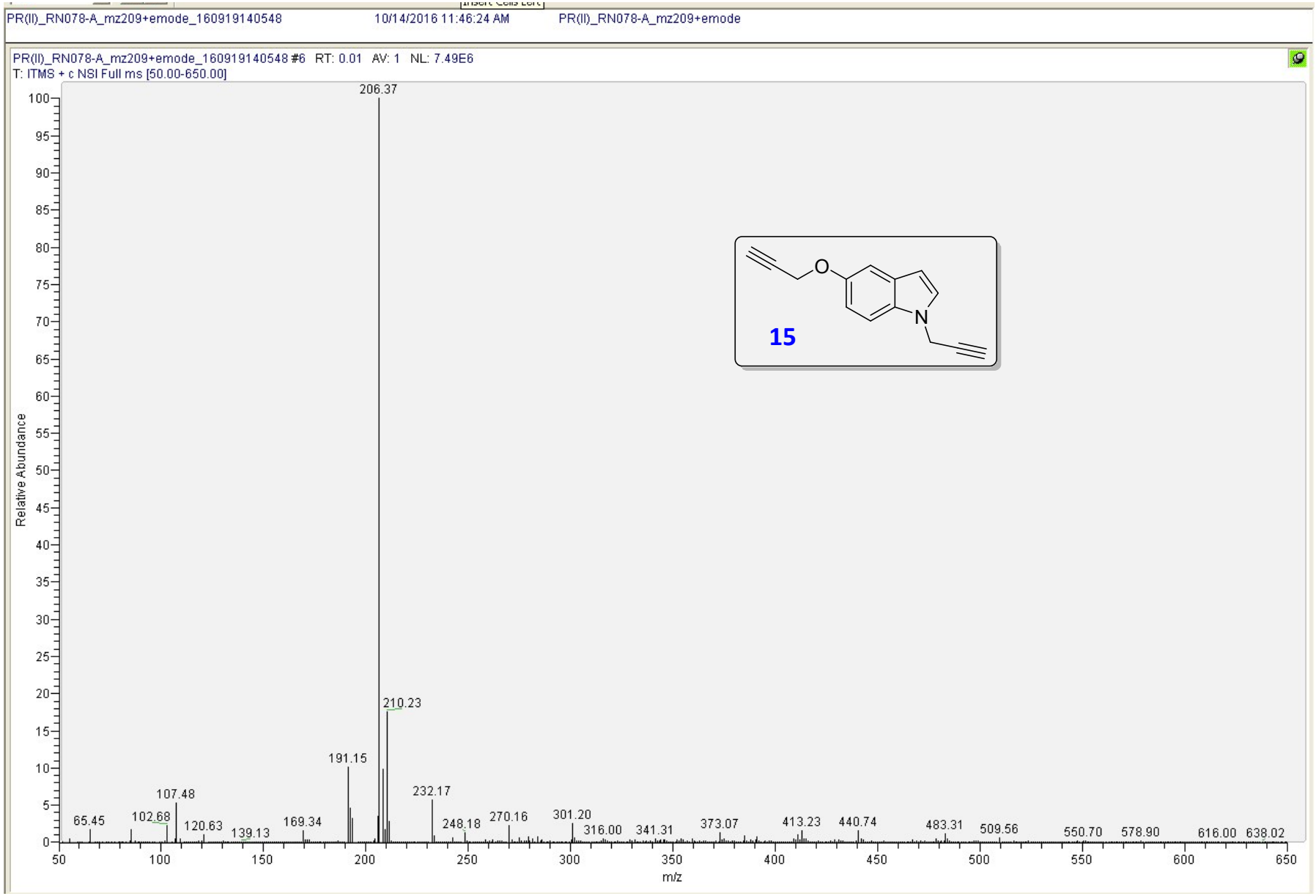

11.282
7.699
7.391
7.374
7.170
7.154
6.438
3.870
3.355
2.494
N
H
1.591
1.000
2.844
1.309
1.240
0.818
PPM
10
8
6
4
2

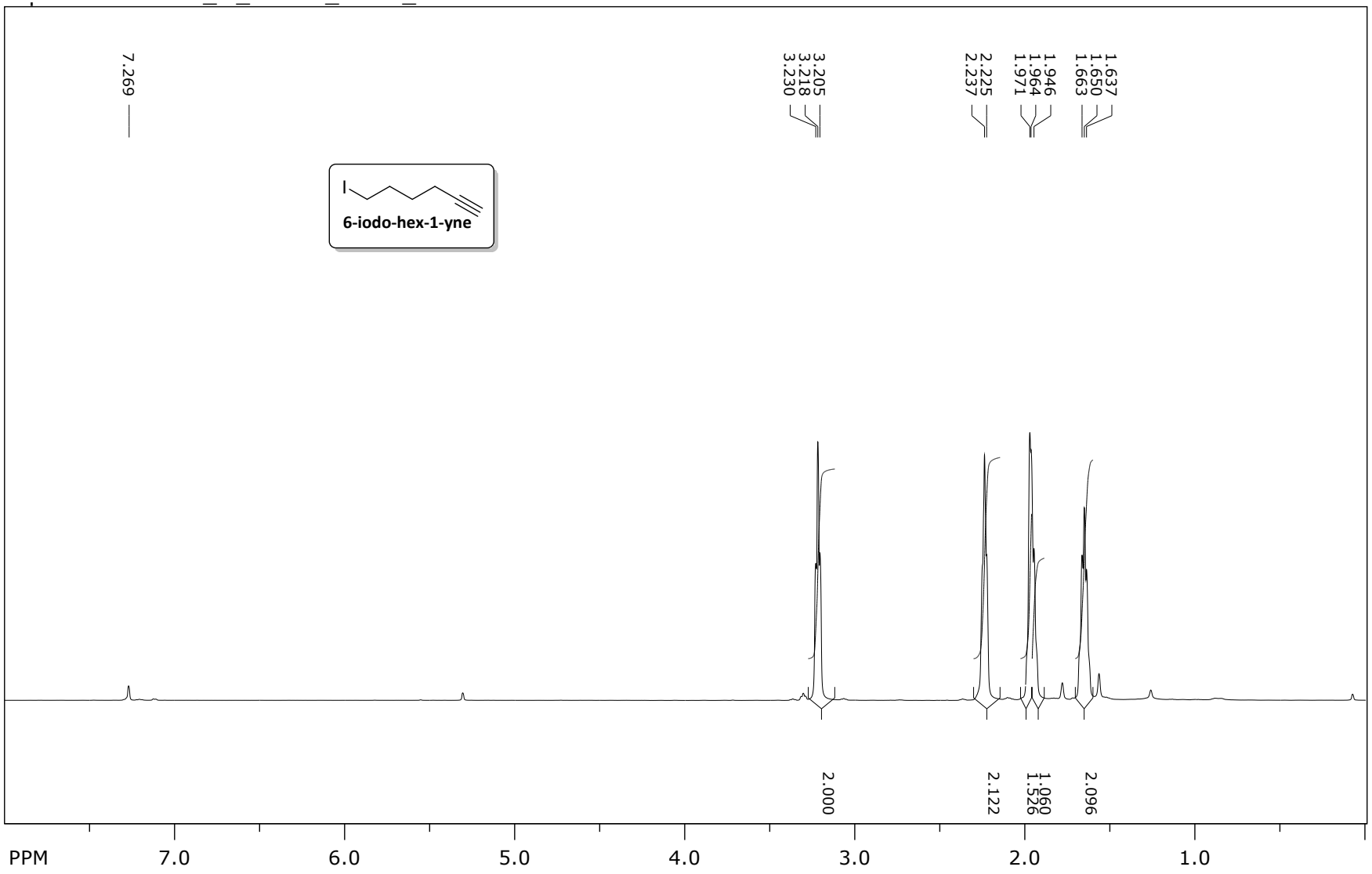

10.935
7.291
7.275
7.108
6.768
6.765
6.751
6.747
6.337
4.732
4.728
3.484
3.339
2.494
14
O
N
H
0.924
1.573
0.810
0.806
0.713
2.000
0.343
PPM
10
8
6
4
2

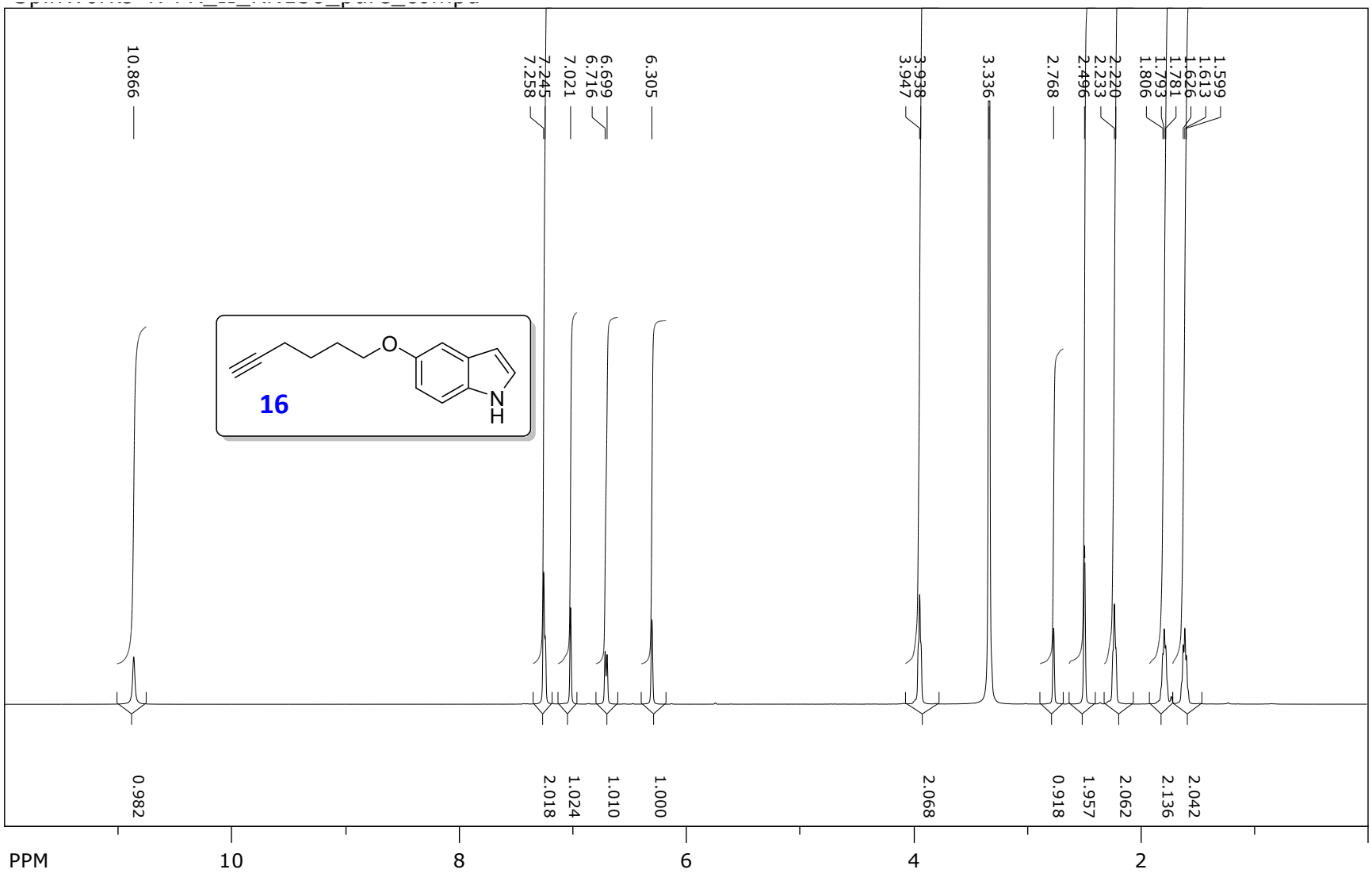

PR(II)_RN078_mz171+emode_160919140548 10/14/2016 11:39:11 AM PR(II)_RN078_mz171+emode
PR(II)_RN078_mz171+emode_160919140548 #6 RT: 0.01 AV: 1 NL: 5.30E6
T: ITMS + c NSI Full ms [50.00-650.00]
14
Relative Abundance
m/z
172.17
102.27
186.33
191.11
194.20
120.22
284.22
364.87
210.17
232.16
256.16
242.38
413.25
130.30
169.17
380.41
277.84
290.73
315.91
342.65
524.06
583.48
74.29
85.18
152.29
441.35
471.56
491.86
509.78
550.50
588.16
621.54
639.47

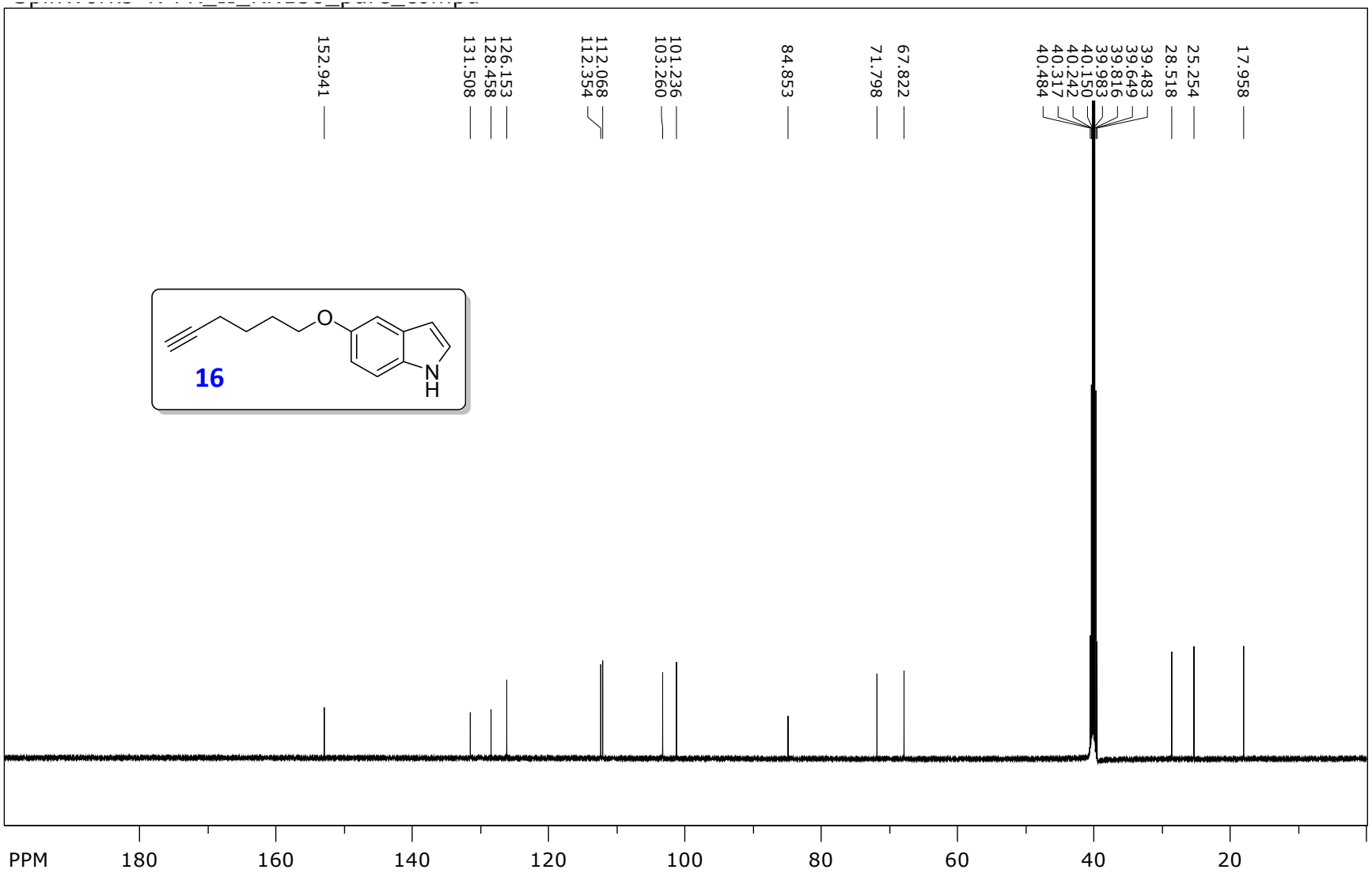

7.429
7.412
7.359
7.354
7.150
7.148
6.873
6.870
6.855
6.391
6.385
5.041
5.038
4.761
4.759
3.495
3.367
3.345
2.494
15
0.983
0.919
0.911
0.924
0.856
2.000
1.978
0.717
0.549
PPM
10
8
6
4
2

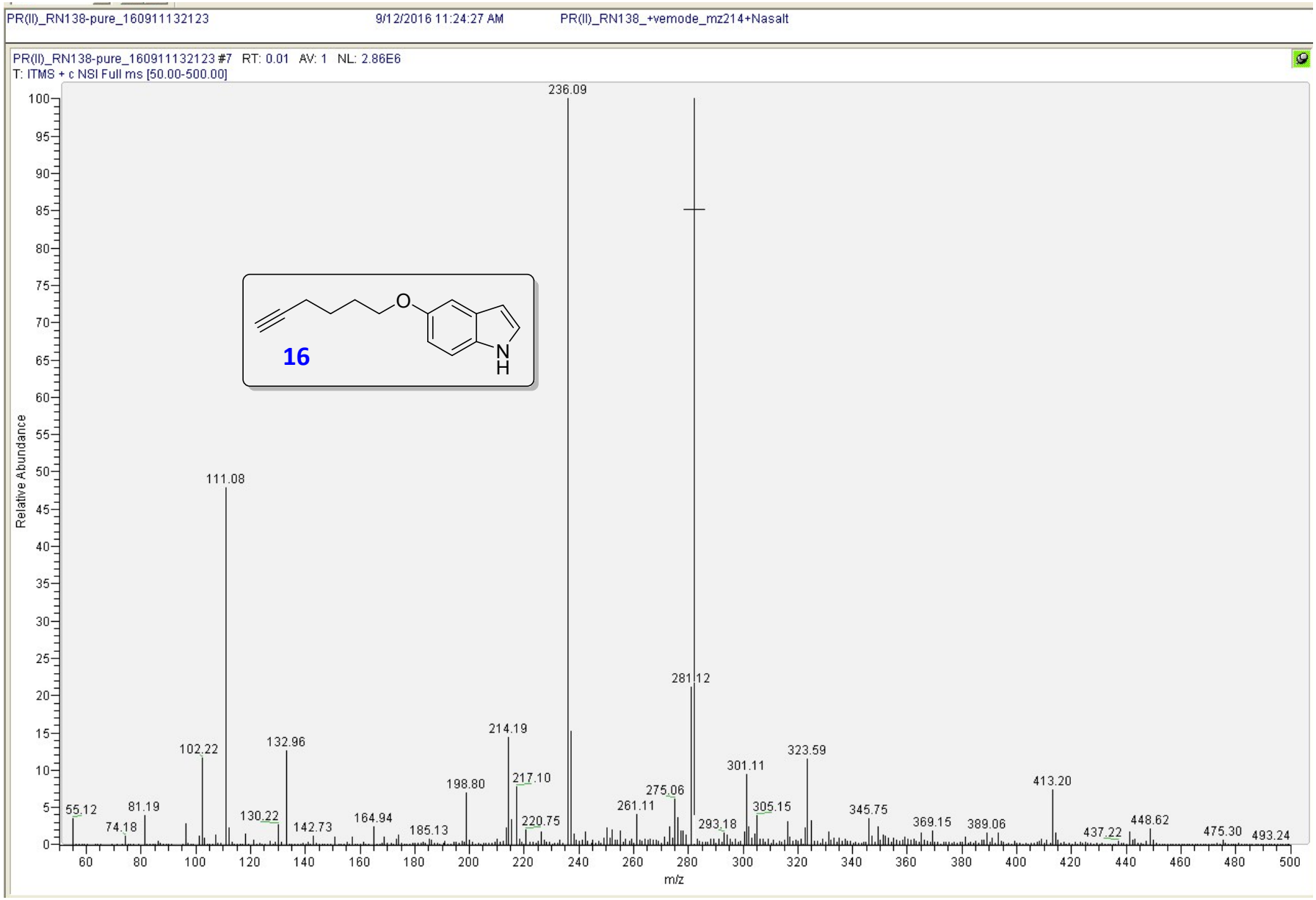

152.073
131.658
129.475
129.094
112.412
111.156
104.821
101.526
80.371
79.770
78.210
75.867
56.550
40.493
40.327
40.160
39.993
39.826
39.659
39.492
35.691
O
N
15
PPM
160
140
120
100
80
60
40
20

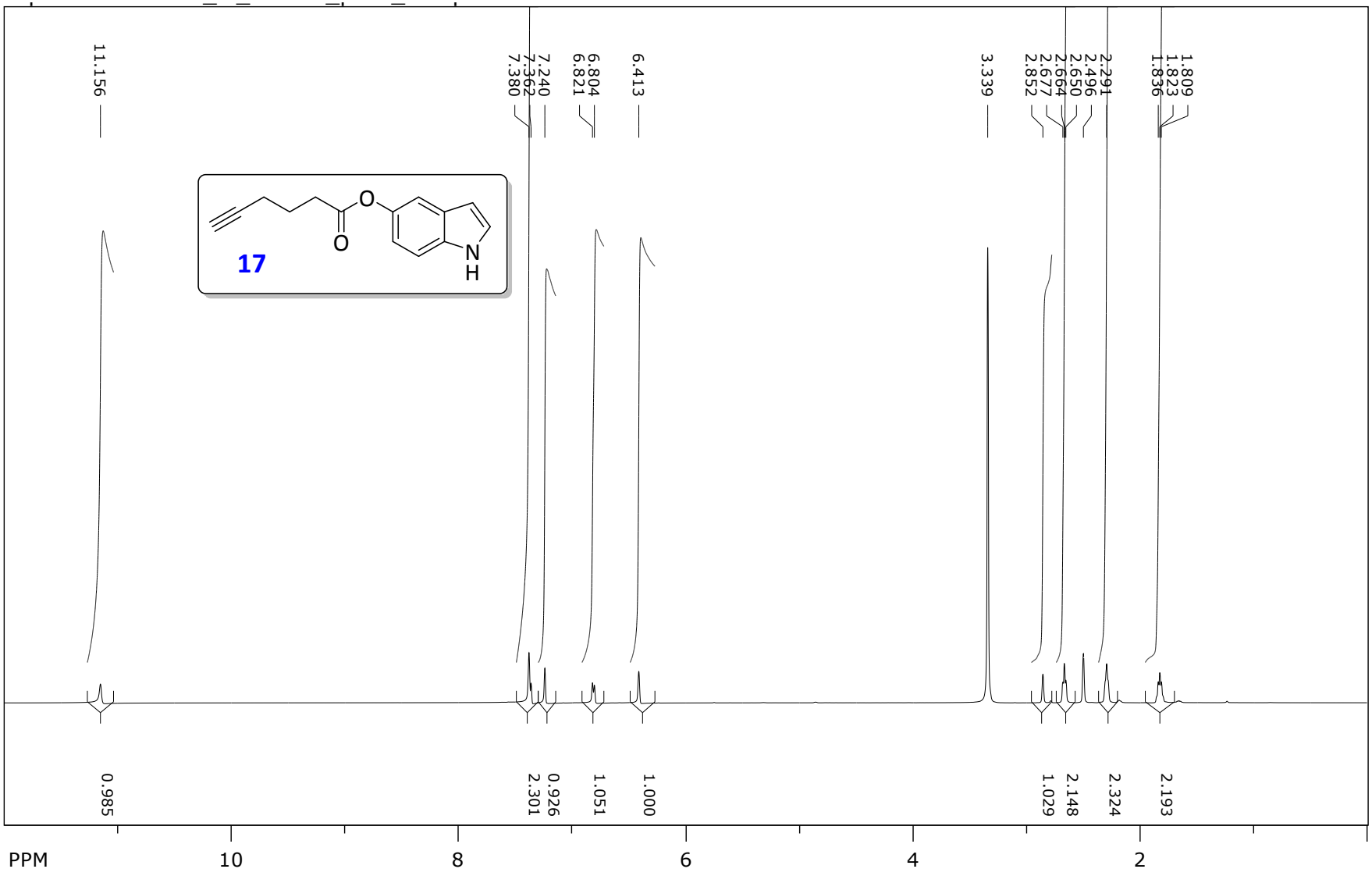

PR(II)_RN078-A_mz209+emode_160919140548 10/14/2016 11:46:24 AM PR(II)_RN078-A_mz209+emode
PR(II)_RN078-A_mz209+emode_160919140548 #6 RT: 0.01 AV: 1 NL: 7.49E6
T: ITMS + c NSI Full ms [50.00-650.00]
Relative Abundance
m/z
206.37
210.23
191.15
107.48
232.17
65.45
102.68
120.63
139.13
169.34
248.18
270.16
301.20
316.00
341.31
373.07
413.23
440.74
483.31
509.56
550.70
578.90
616.00
638.02
O
N
15

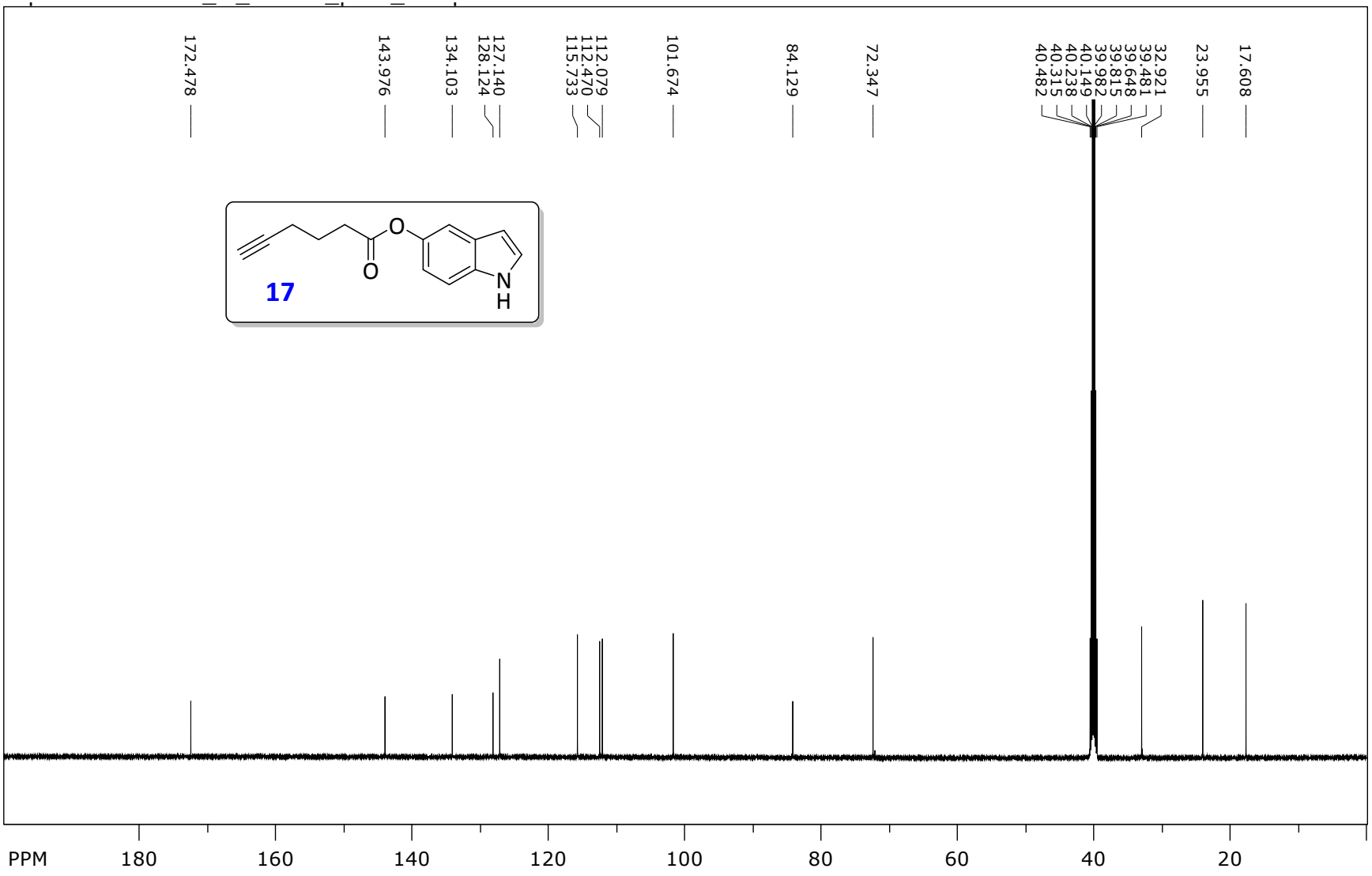

7.269
3.205
3.218
3.230
2.225
2.237
1.946
1.964
1.971
1.637
1.650
1.663
6-iodo-hex-1-yne
2.000
2.122
1.060
1.526
2.096
PPM
7.0
6.0
5.0
4.0
3.0
2.0
1.0

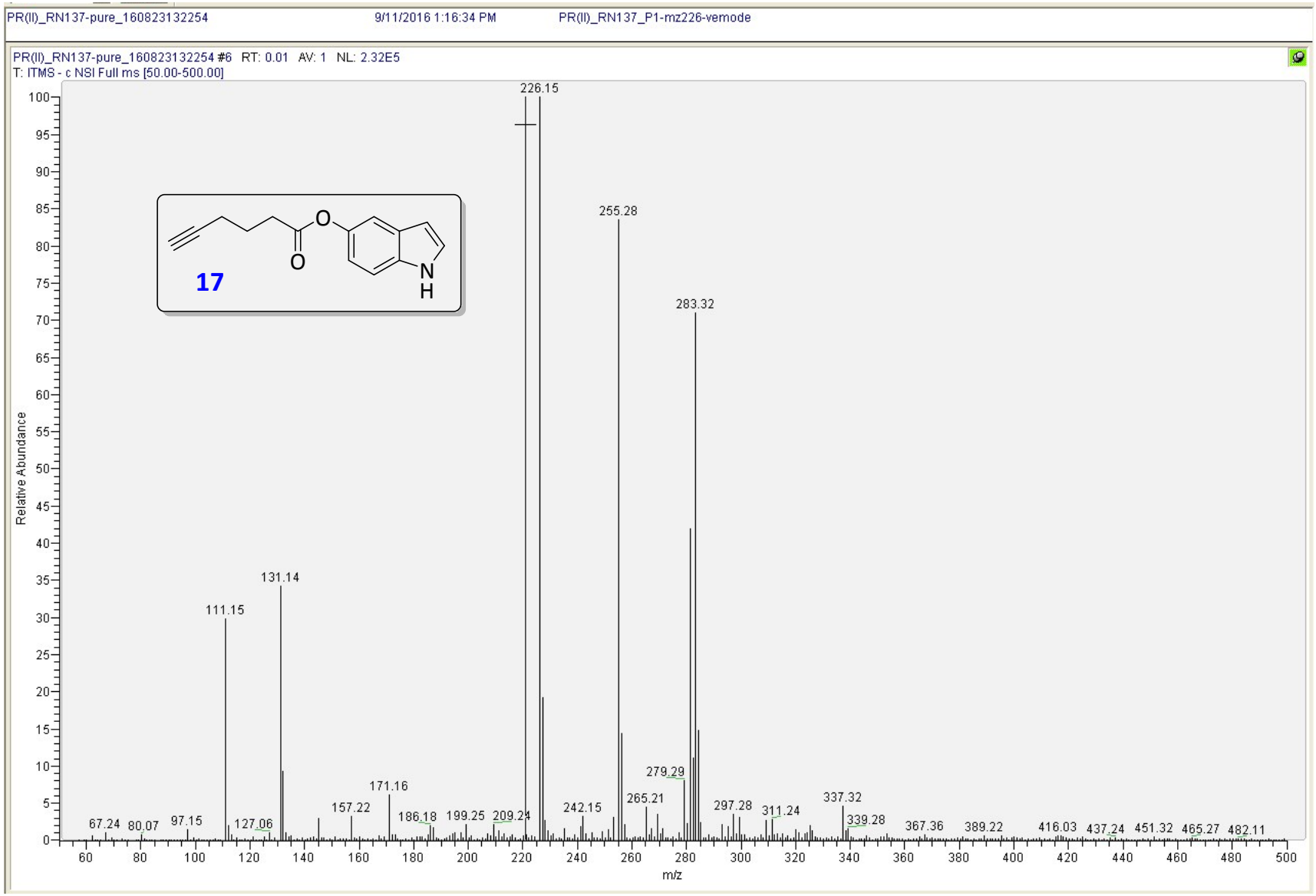

10.866
7.258
7.245
7.021
6.716
6.699
6.305
3.947
3.938
3.336
2.768
2.496
2.233
2.220
1.806
1.793
1.781
1.626
1.613
1.599
16
O
N
H
0.982
2.018
1.024
1.010
1.000
2.068
0.918
1.957
2.062
2.136
2.042
PPM
10
8
6
4
2

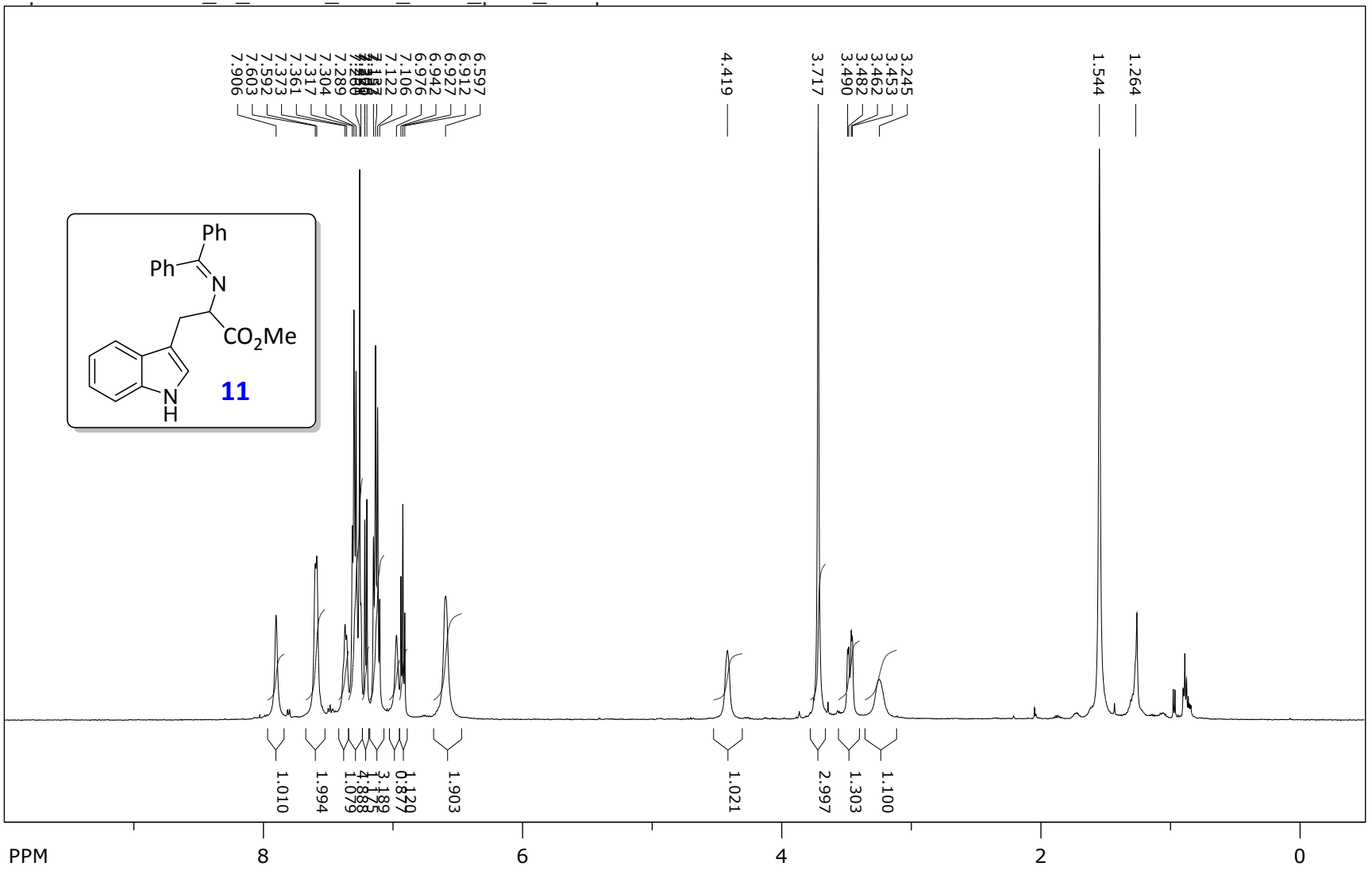

152.941
131.508
128.458
126.153
112.354
112.068
103.260
101.236
84.853
71.798
67.822
40.484
40.317
40.242
40.150
39.983
39.816
39.649
39.483
28.518
25.254
17.958
O
N
H
16
PPM
180
160
140
120
100
80
60
40
20

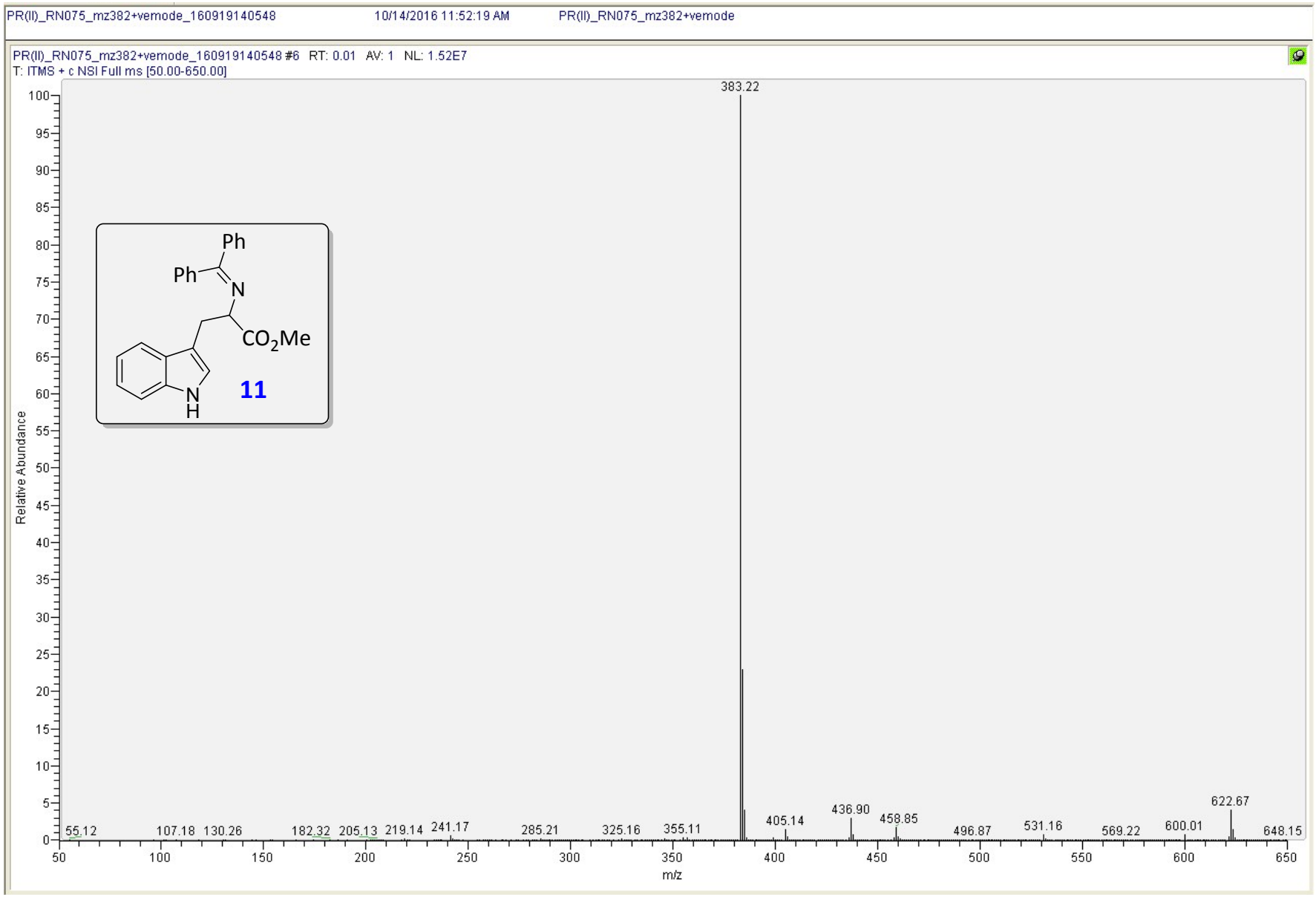

PR(II)_RN138-pure_160911132123
9/12/2016 11:24:27 AM
PR(II)_RN138_+vemode_mz214+Nasalt
PR(II)_RN138-pure_160911132123 #7 RT: 0.01 AV: 1 NL: 2.86E6
T: ITMS + c NSI Full ms [50.00-500.00]
16
Relative Abundance
m/z
236.09
111.08
281.12
214.19
102.22
132.96
323.59
301.11
217.10
198.80
275.06
413.20
261.11
305.15
345.75
55.12
81.19
74.18
130.22
142.73
164.94
185.13
220.75
293.18
369.15
389.06
437.22
448.62
475.30
493.24

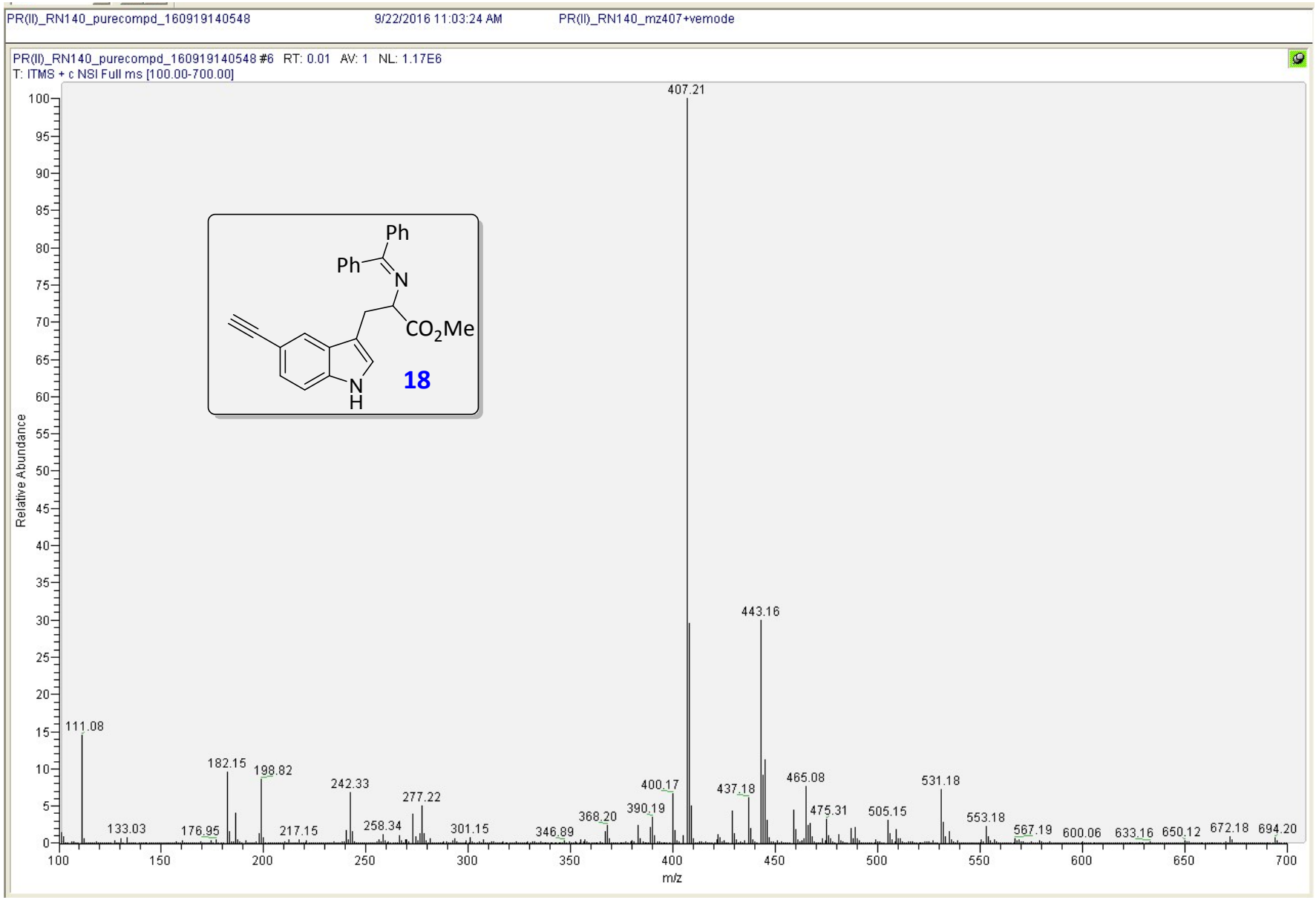

11.156
7.380
7.362
7.240
6.821
6.804
6.413
3.339
2.852
2.677
2.664
2.650
2.496
2.291
1.836
1.823
1.809
17
O
O
N
H
0.985
2.301
0.926
1.051
1.000
1.029
2.148
2.324
2.193
PPM
10
8
6
4
2

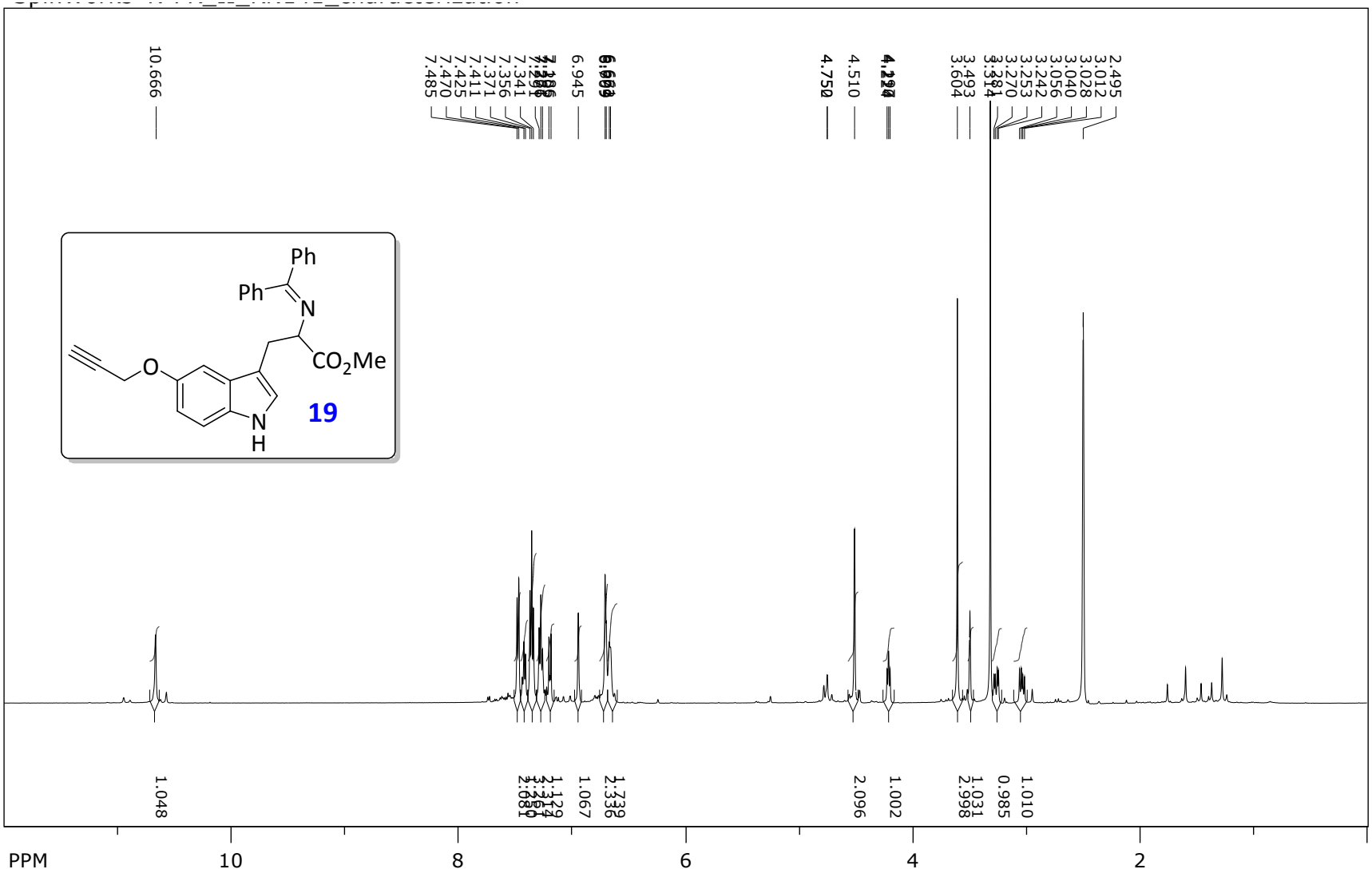

172.478
143.976
134.103
127.140
128.124
115.733
112.470
112.079
101.674
84.129
72.347
40.482
40.315
40.238
40.149
39.982
39.815
39.648
39.481
32.921
23.955
17.608
O
O
N
H
17
PPM
180
160
140
120
100
80
60
40
20

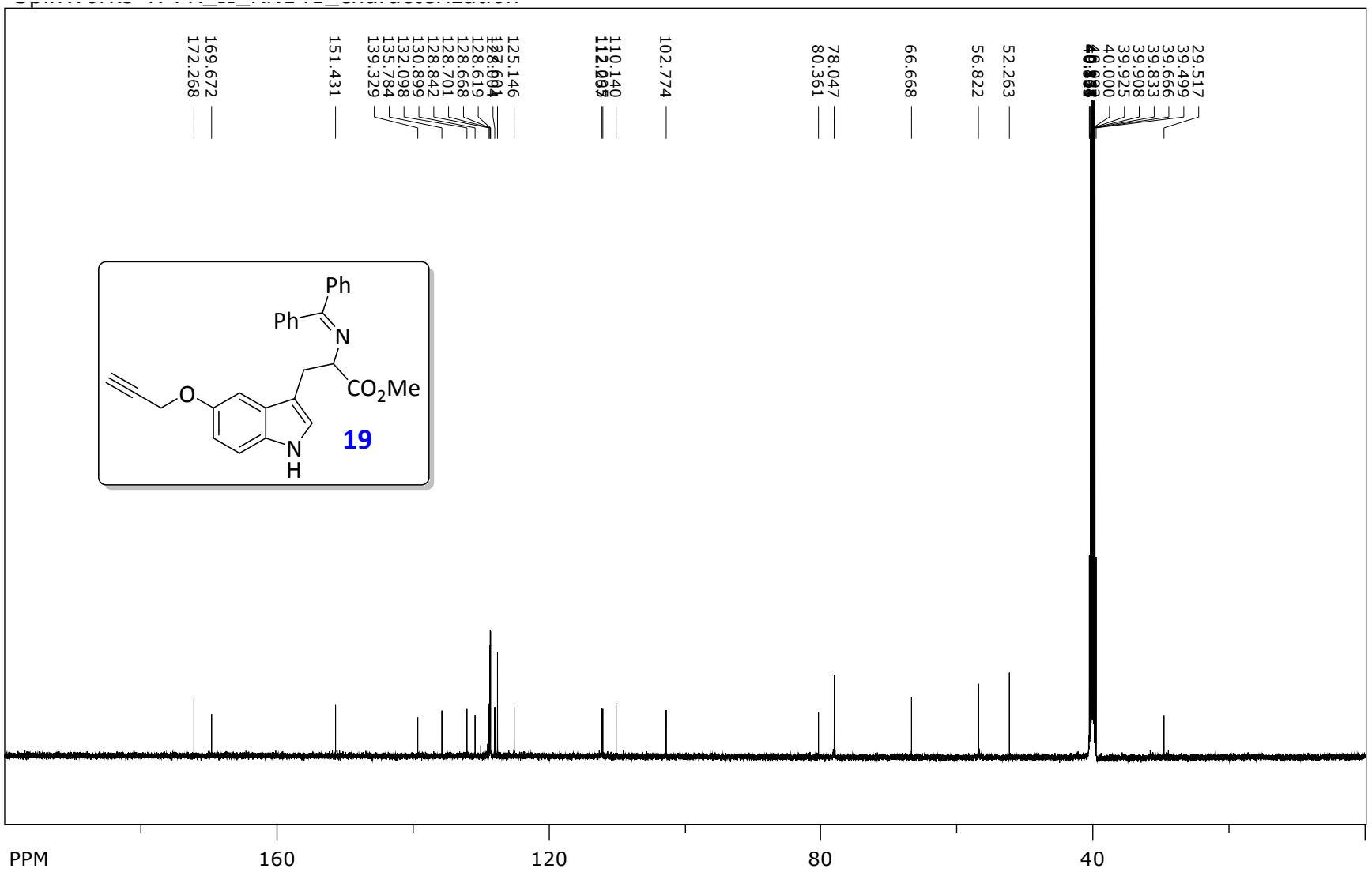

PR(II)_RN137-pure_160823132254
9/11/2016 1:16:34 PM
PR(II)_RN137_P1-mz226-vemode
PR(II)_RN137-pure_160823132254 #6 RT: 0.01 AV: 1 NL: 2.32E5
T: ITMS - c NSI Full ms [50.00-500.00]
17
O
O
N
H
Relative Abundance
m/z
226.15
255.28
283.32
131.14
111.15
171.16
157.22
279.29
265.21
297.28
311.24
337.32
339.28
242.15
186.18
199.25
209.24
67.24
80.07
97.15
127.06
367.36
389.22
416.03
437.24
451.32
465.27
482.11

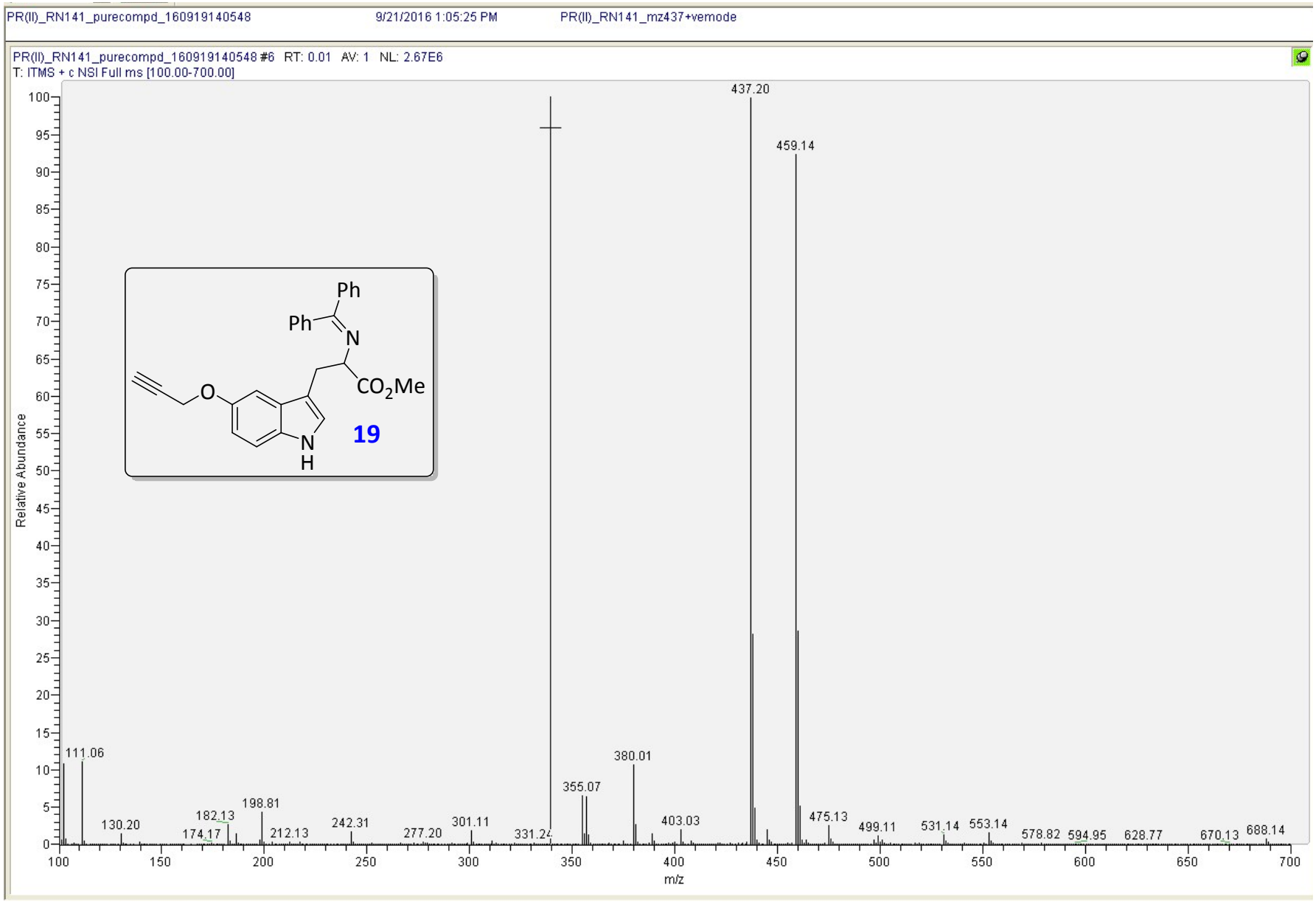

Ph
Ph
N
CO2Me
N
H
11
7.906
7.603
7.592
7.373
7.361
7.317
7.304
7.289
6.597
6.912
6.927
6.942
6.976
7.106
7.122
4.419
3.717
3.490
3.482
3.462
3.453
3.245
1.544
1.264
1.010
1.994
1.079
1.903
1.021
2.997
1.303
1.100
PPM
8
6
4
2
0

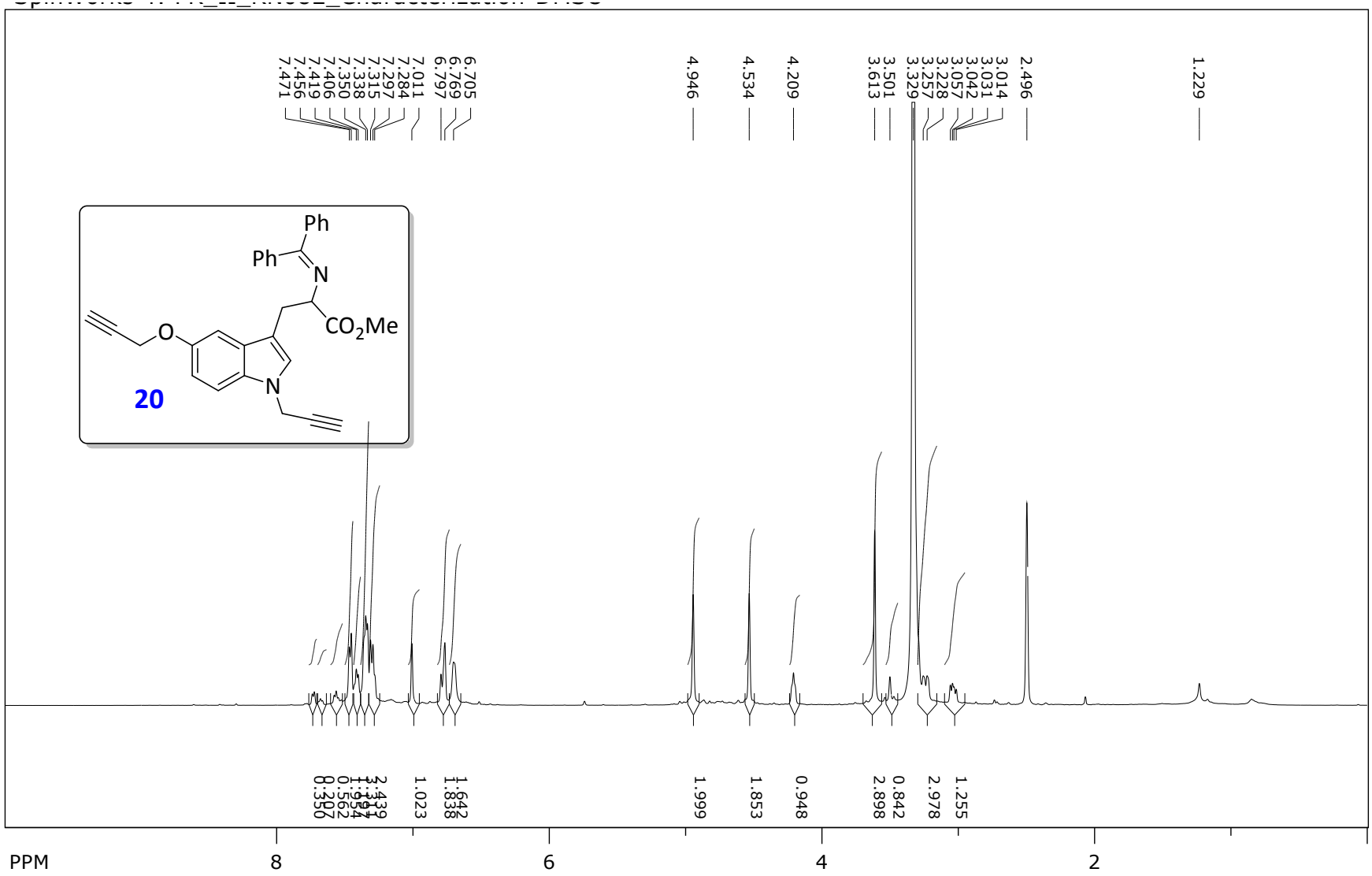

PR(II)_RN075_mz382+vemode_160919140548 10/14/2016 11:52:19 AM PR(II)_RN075_mz382+vemode
PR(II)_RN075_mz382+vemode_160919140548 #6 RT: 0.01 AV: 1 NL: 1.52E7
T: ITMS + c NSI Full ms [50.00-650.00]
Ph
Ph
N
CO2Me
N
H
11
Relative Abundance
m/z
383.22
622.67
436.90
458.85
405.14
55.12
107.18
130.26
182.32
205.13
219.14
241.17
285.21
325.16
355.11
496.87
531.16
569.22
600.01
648.15

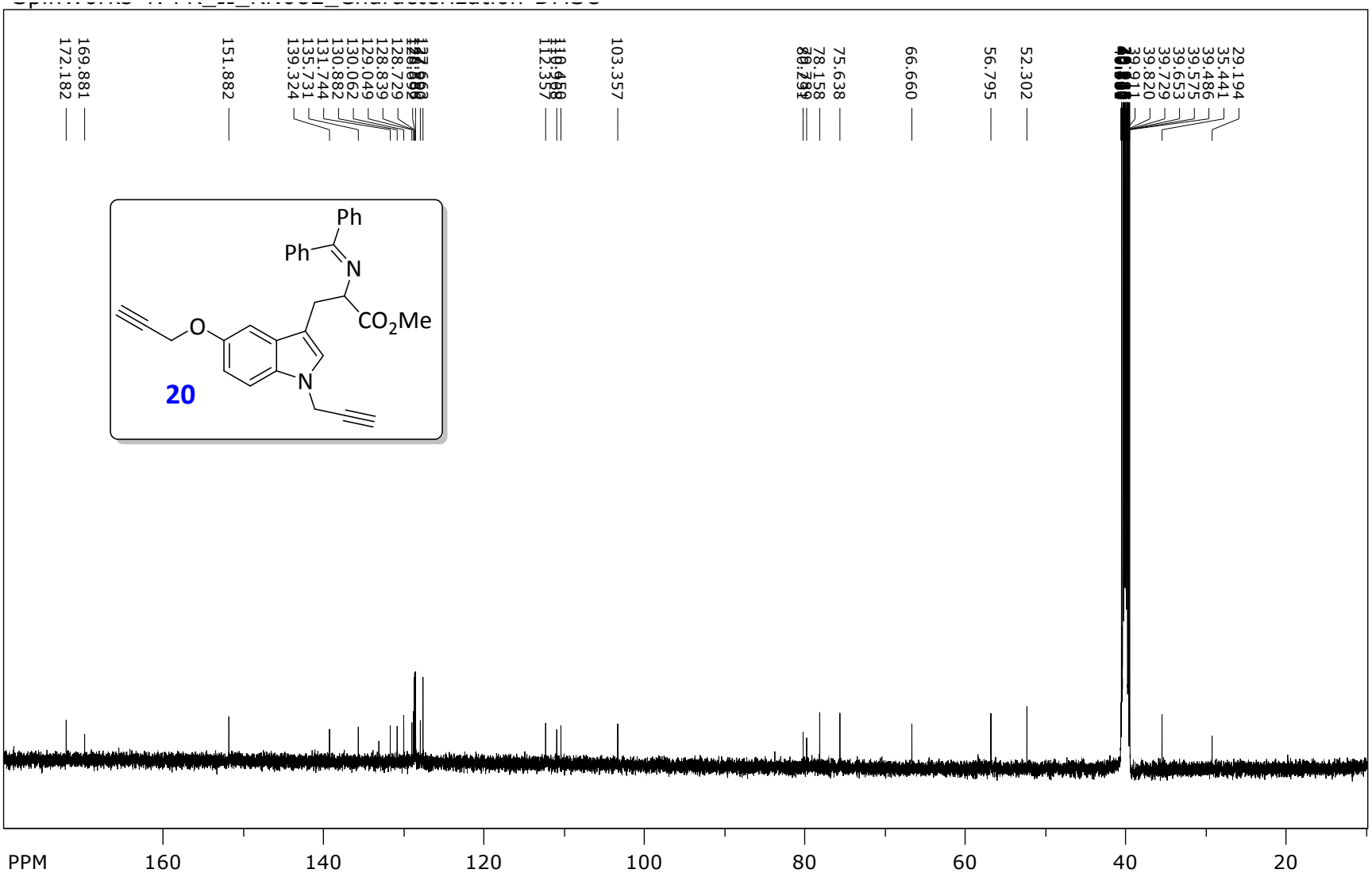

PR(II)_RN140_purecompd_160919140548 9/22/2016 11:03:24 AM PR(II)_RN140_mz407+vemode
PR(II)_RN140_purecompd_160919140548 #6 RT: 0.01 AV: 1 NL: 1.17E6
T: ITMS + c NSI Full ms [100.00-700.00]
Ph
Ph
N
CO2Me
N
H
18
Relative Abundance
m/z
407.21
443.16
111.08
182.15
198.82
242.33
277.22
400.17
390.19
368.20
437.18
465.08
475.31
505.15
531.18
553.18
133.03
176.95
217.15
258.34
301.15
346.89
567.19
600.06
633.16
650.12
672.18
694.20

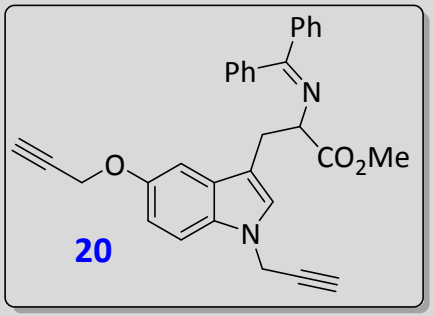

10.666
7.485
7.470
7.425
7.411
7.371
7.356
7.341
6.945
4.750
4.510
3.604
3.493
3.314
3.270
3.253
3.242
3.056
3.040
3.028
3.012
2.495
Ph
Ph
N
CO2Me
O
N
H
19
1.048
2.096
1.002
2.998
1.031
0.985
1.010
1.067
PPM
10
8
6
4
2

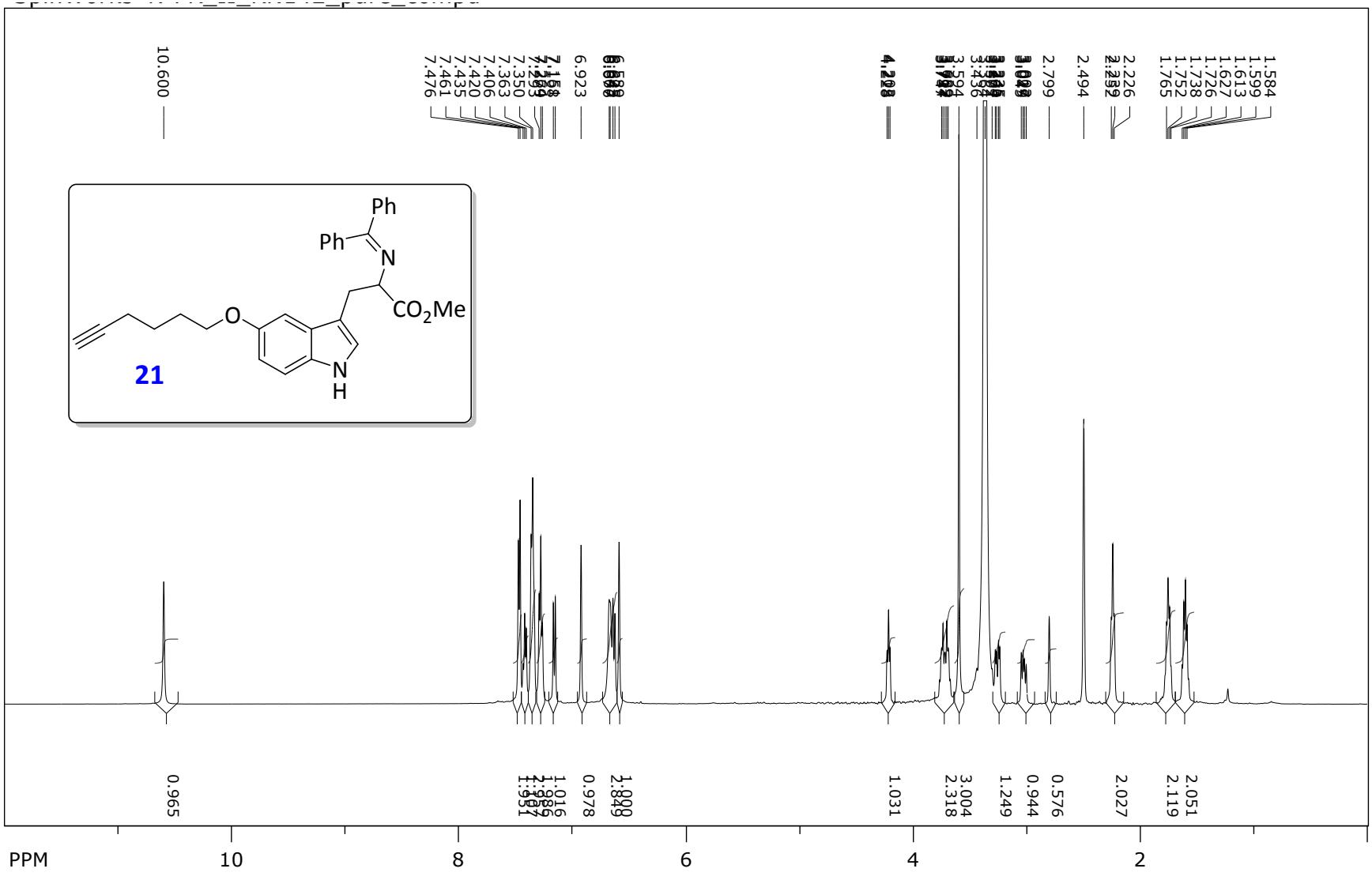

172.268
169.672
151.431
139.329
135.784
132.098
130.899
128.842
128.701
128.668
128.619
125.146
110.140
102.774
80.361
78.047
66.668
56.822
52.263
40.000
39.925
39.908
39.833
39.666
39.499
29.517
Ph
Ph
N
CO2Me
O
N
H
19
PPM
160
120
80
40

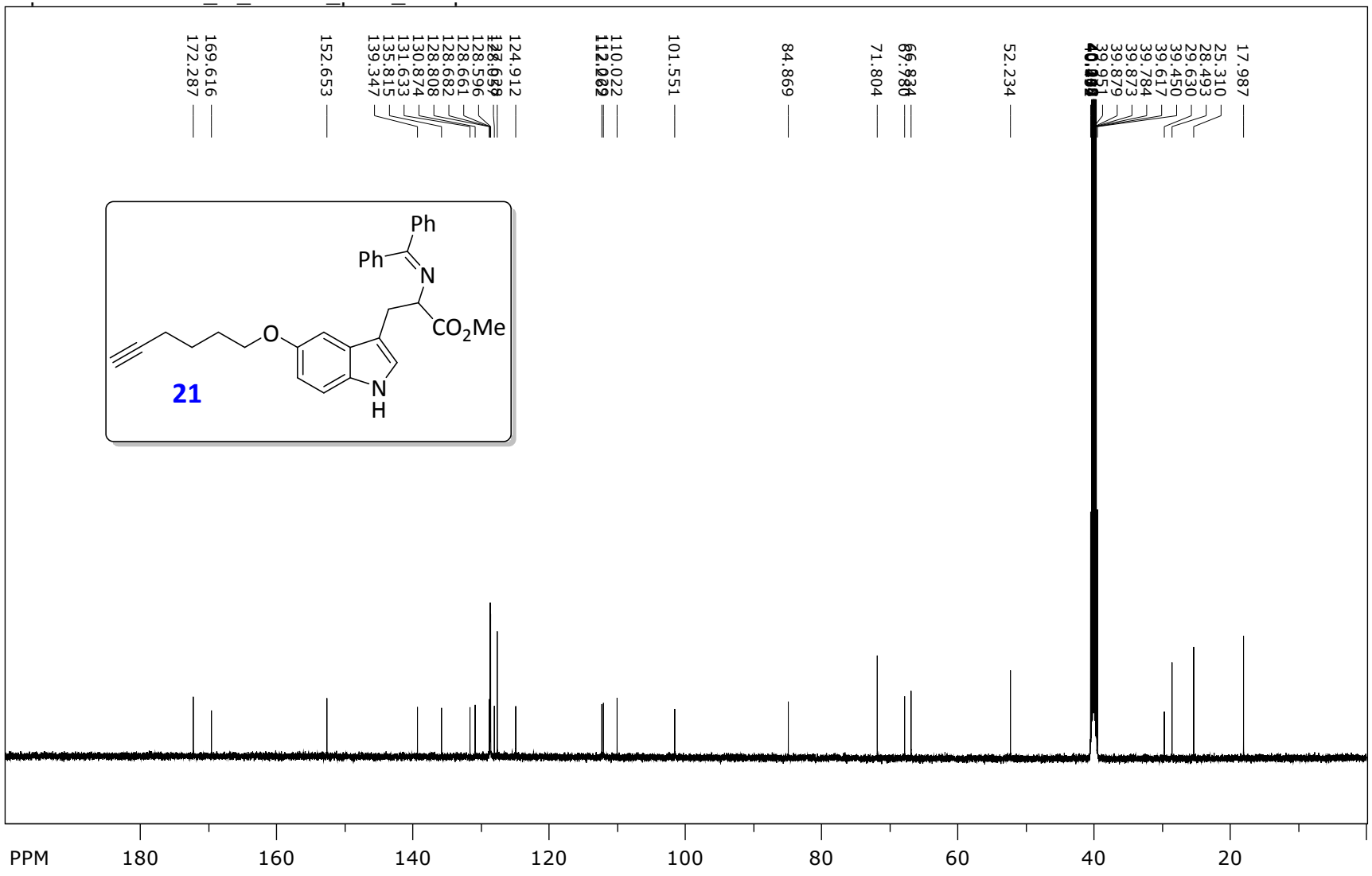

PR(II)_RN141_purecompd_160919140548 9/21/2016 1:05:25 PM PR(II)_RN141_mz437+vemode
PR(II)_RN141_purecompd_160919140548 #6 RT: 0.01 AV: 1 NL: 2.67E6
T: ITMS + c NSI Full ms [100.00-700.00]
Relative Abundance
m/z
437.20
459.14
111.06
130.20
182.13
174.17
198.81
212.13
242.31
277.20
301.11
331.24
355.07
380.01
403.03
475.13
499.11
531.14
553.14
578.82
594.95
628.77
670.13
688.14
Ph
Ph
N
CO2Me
O
N
H
19

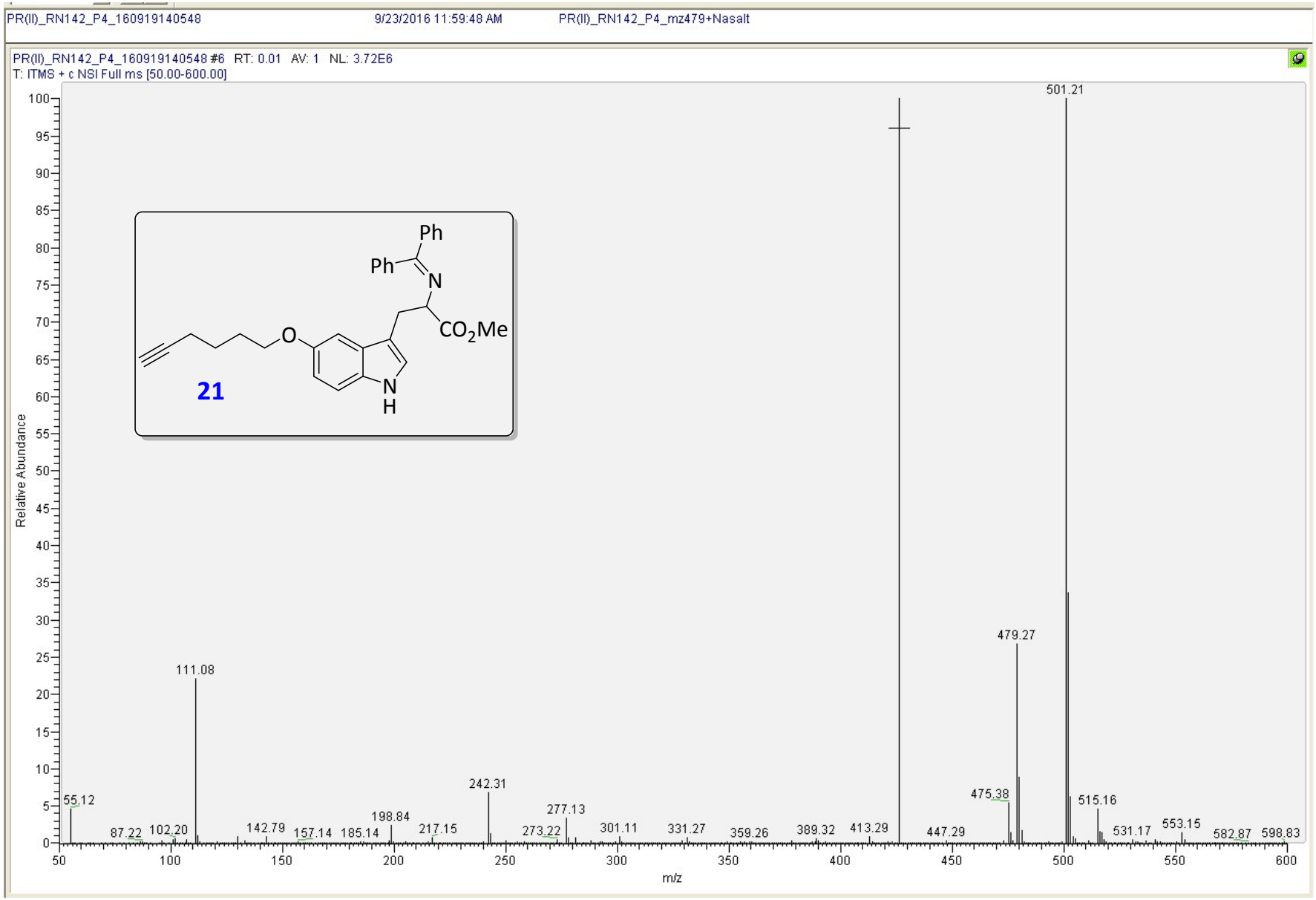

7.471
7.456
7.419
7.406
7.350
7.338
7.315
7.297
7.284
7.011
6.797
6.769
6.705
4.946
4.534
4.209
3.613
3.501
3.329
3.257
3.228
3.057
3.042
3.031
3.014
2.496
1.229
Ph
Ph
N
CO2Me
O
N
20
0.350
0.307
1.023
1.838
1.642
1.999
1.853
0.948
2.898
0.842
2.978
1.255
PPM
8
6
4
2

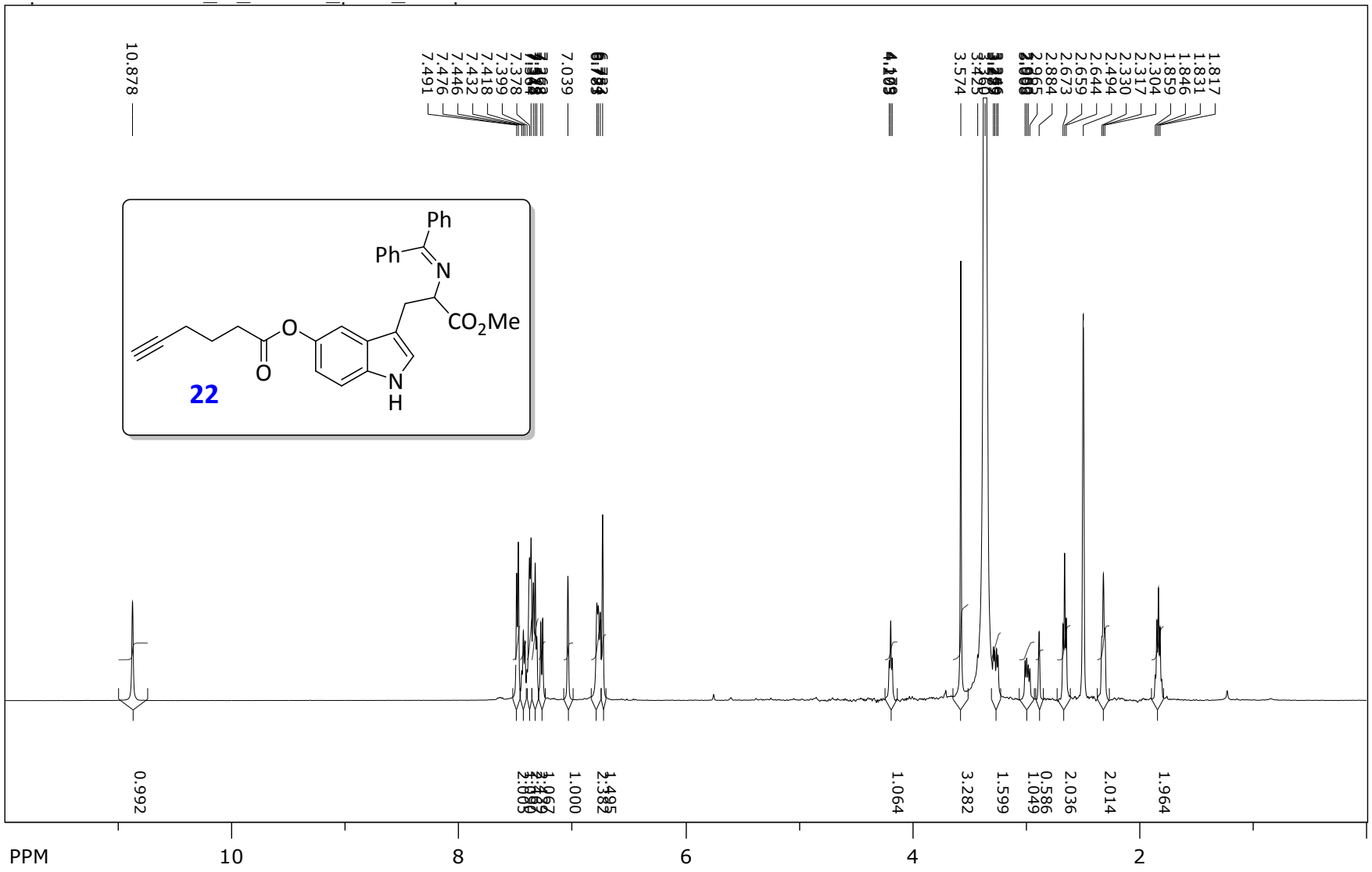

169.881
172.182
151.882
139.324
135.731
131.744
130.882
130.062
129.049
128.839
128.729
112.357
103.357
80.291
78.158
75.638
66.660
56.795
52.302
39.820
39.729
39.653
39.575
39.486
35.441
29.194
Ph
Ph
N
CO2Me
O
N
20
PPM
160
140
120
100
80
60
40
20

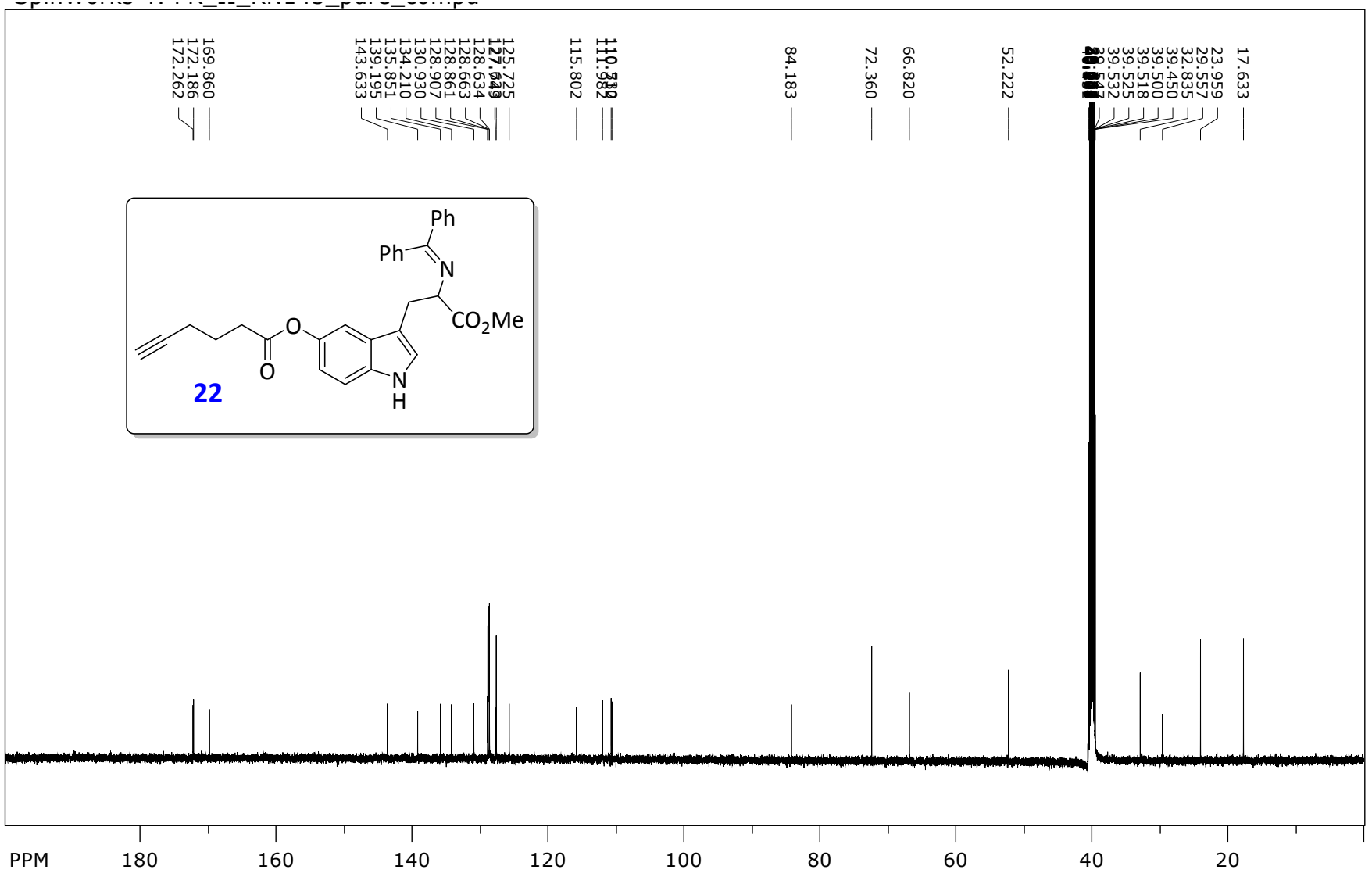

Ph
Ph
N
O
CO2Me
N
20

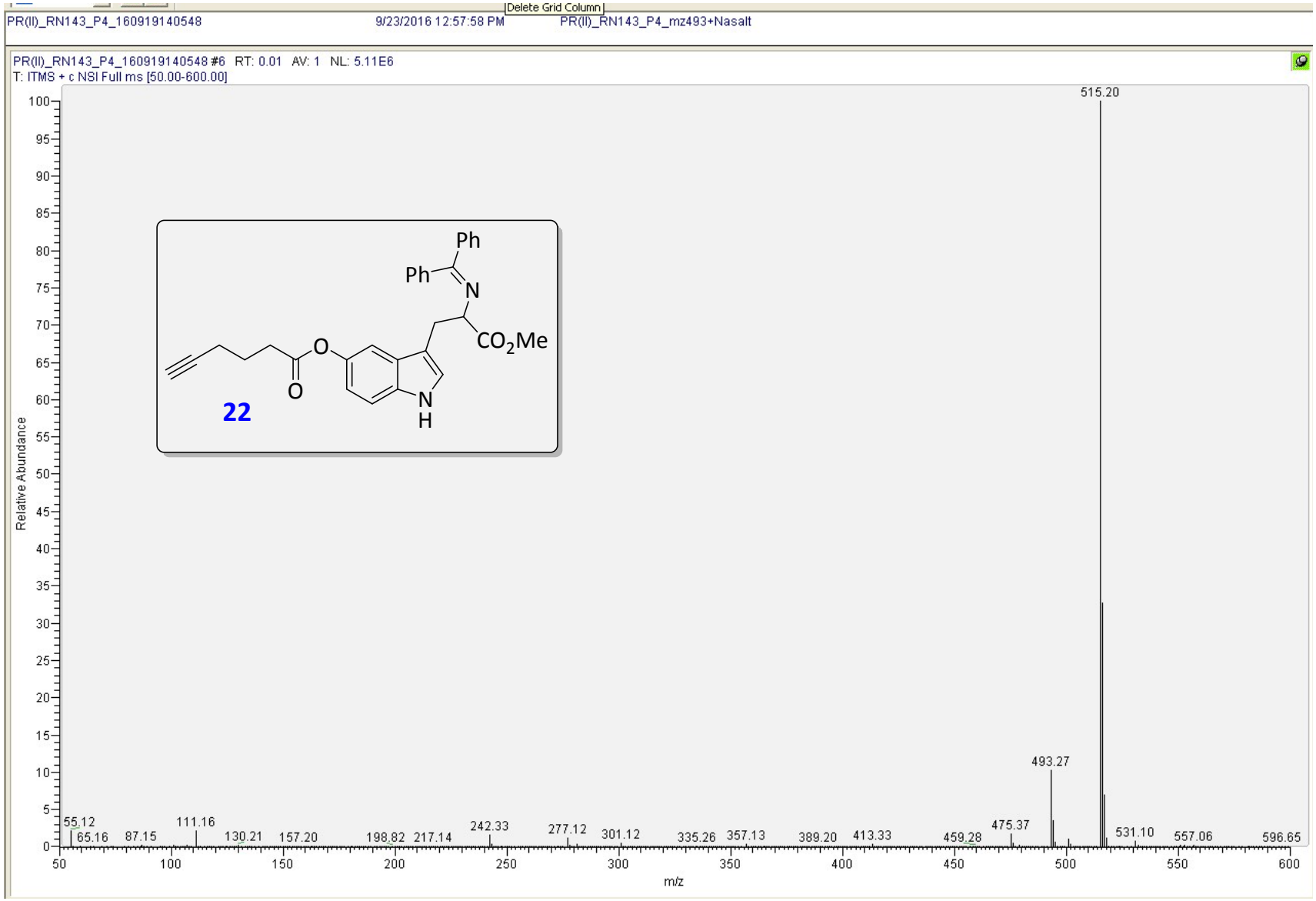

21
Ph
Ph
N
CO2Me
O
N
H
PPM
10
8
6
4
2

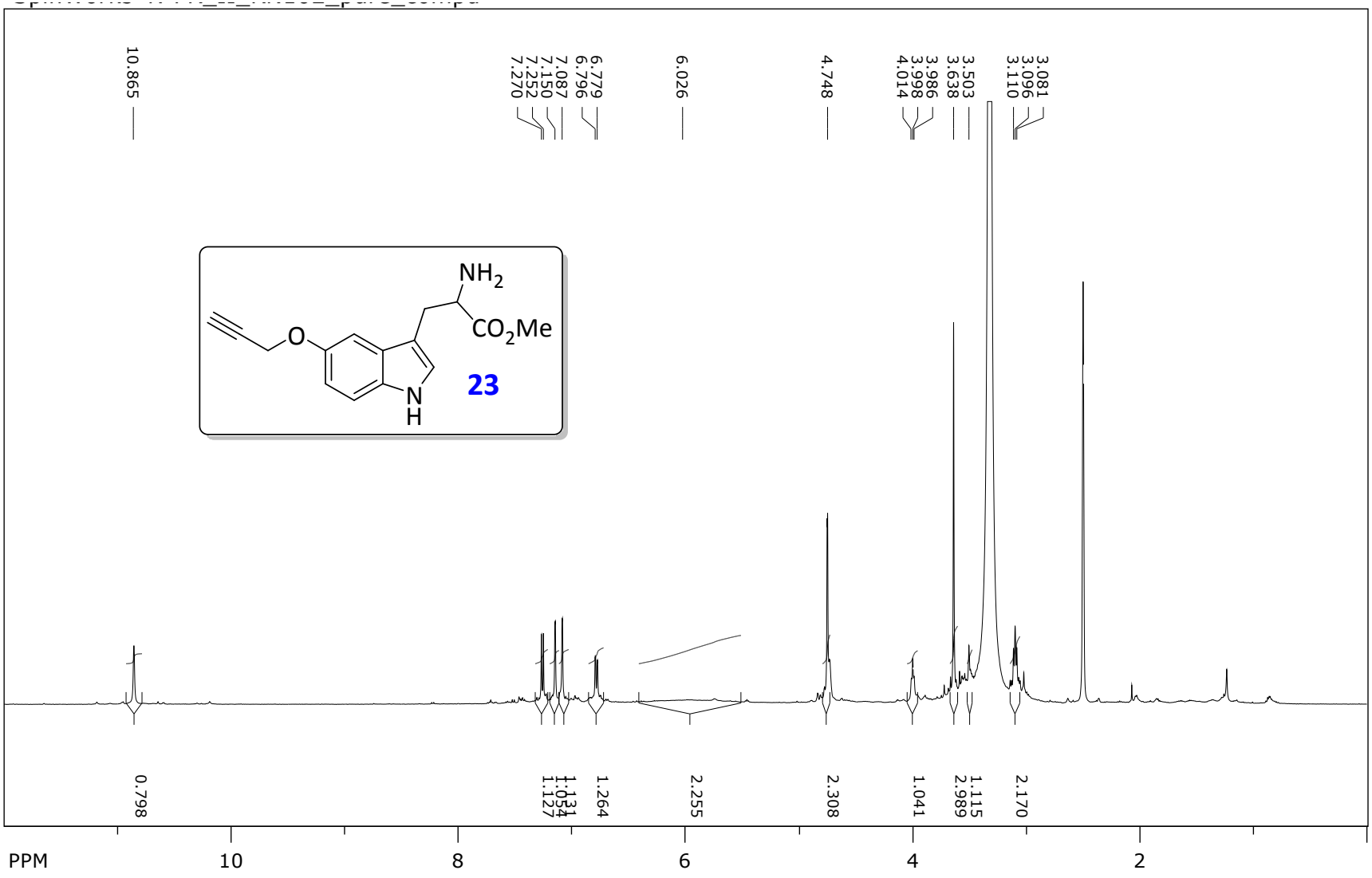

172.287
169.616
152.653
139.347
135.815
131.633
130.874
128.808
128.682
128.661
128.596
124.912
110.022
101.551
84.869
71.804
52.234
39.784
39.617
39.450
29.630
28.493
25.310
17.987
Ph
Ph
N
CO2Me
O
N
H
21
PPM
180
160
140
120
100
80
60
40
20

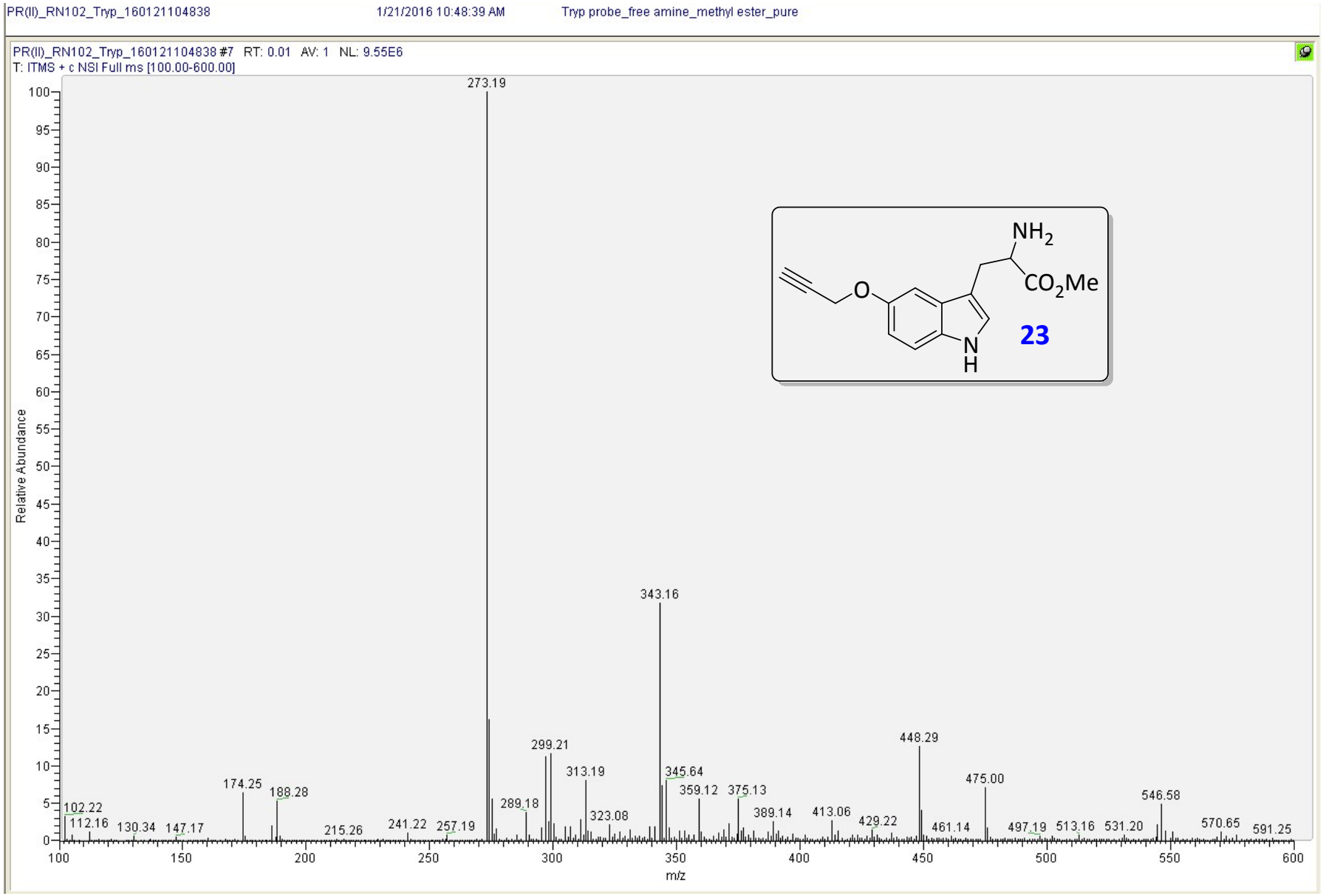

PR(II)_RN142_P4_160919140548
9/23/2016 11:59:48 AM
PR(II)_RN142_P4_mz479+Nasalt
PR(II)_RN142_P4_160919140548 #6 RT: 0.01 AV: 1 NL: 3.72E6
T: ITMS + c NSI Full ms [50.00-600.00]
Ph
Ph
N
CO2Me
O
N
H
21
Relative Abundance
m/z
501.21
479.27
111.08
242.31
277.13
475.38
515.16
55.12
87.22
102.20
142.79
157.14
185.14
198.84
217.15
273.22
301.11
331.27
359.26
389.32
413.29
447.29
531.17
553.15
582.87
598.83

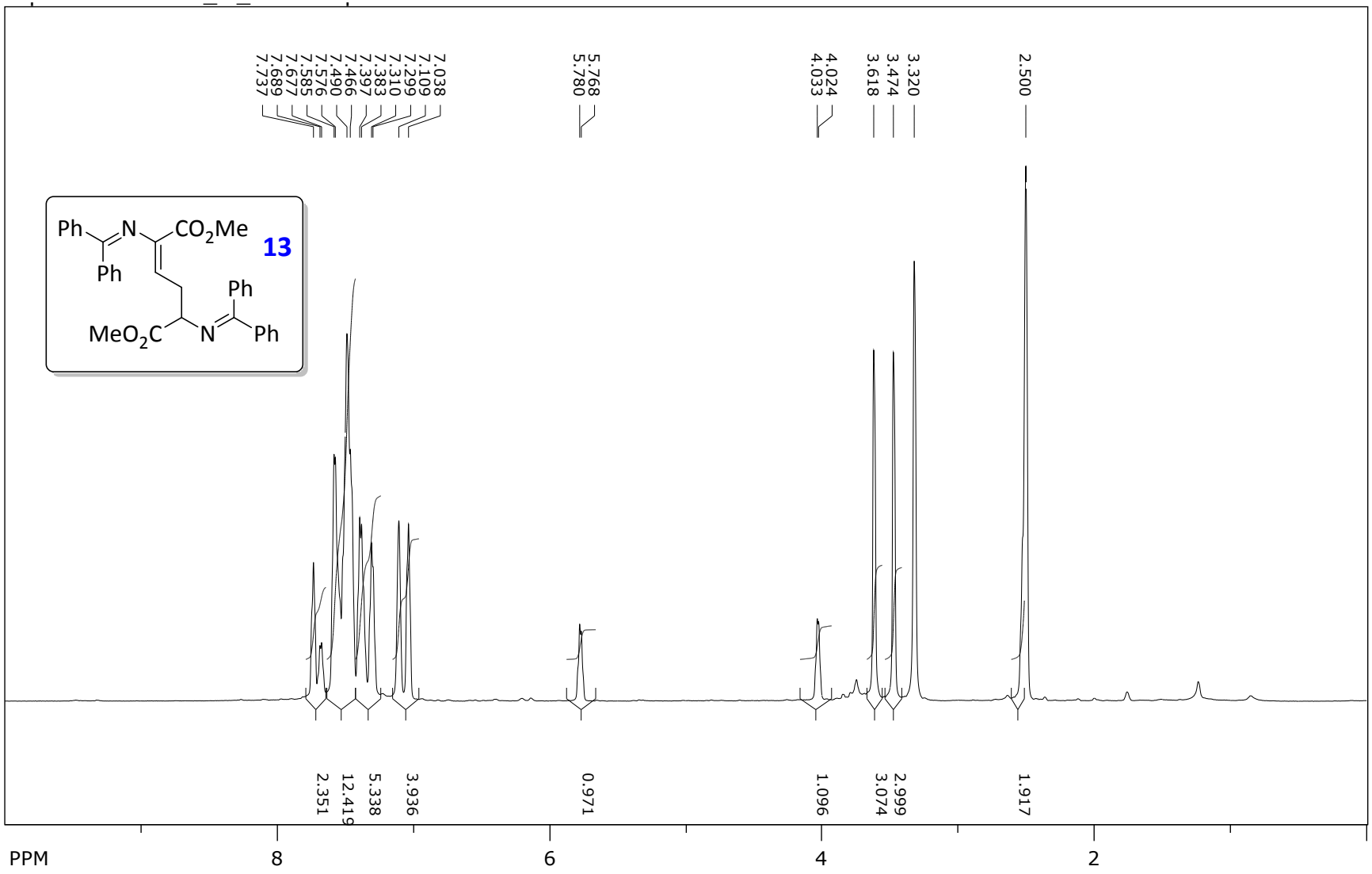

10.878
7.491
7.476
7.446
7.432
7.418
7.399
7.378
7.039
3.574
1.817
1.831
1.846
1.859
2.304
2.317
2.330
2.494
2.644
2.659
2.673
2.884
Ph
Ph
N
CO2Me
O
O
N
H
22
0.992
1.000
1.064
3.282
1.599
0.586
1.049
2.036
2.014
1.964
PPM
10
8
6
4
2

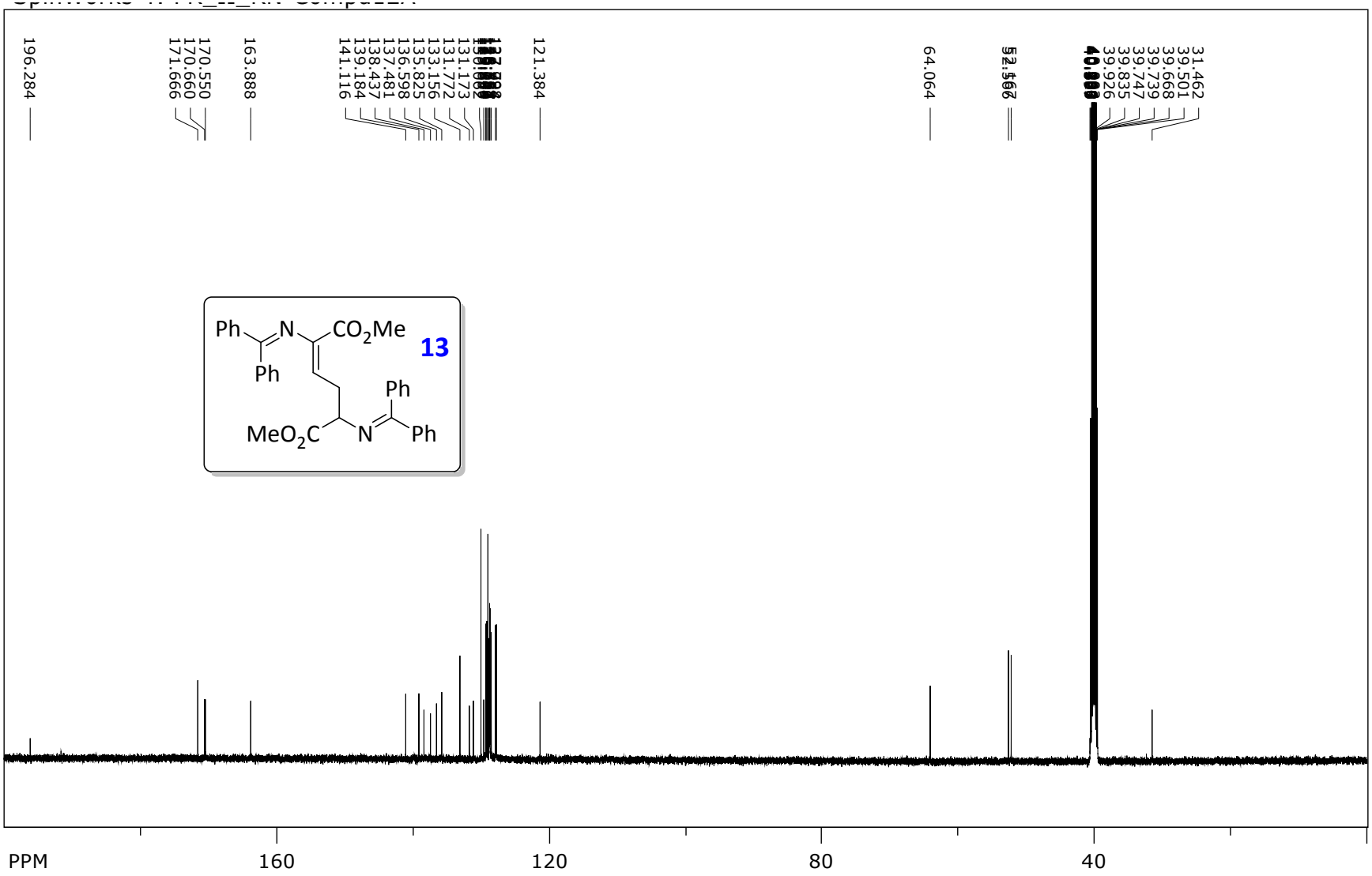

172.262
169.860
172.186
143.633
139.195
135.851
134.210
130.930
128.907
128.861
128.663
128.634
125.725
115.802
84.183
72.360
66.820
52.222
39.532
39.525
39.518
39.500
39.450
32.835
29.557
23.959
17.633
Ph
Ph
N
CO2Me
O
O
N
H
22
PPM
180
160
140
120
100
80
60
40
20

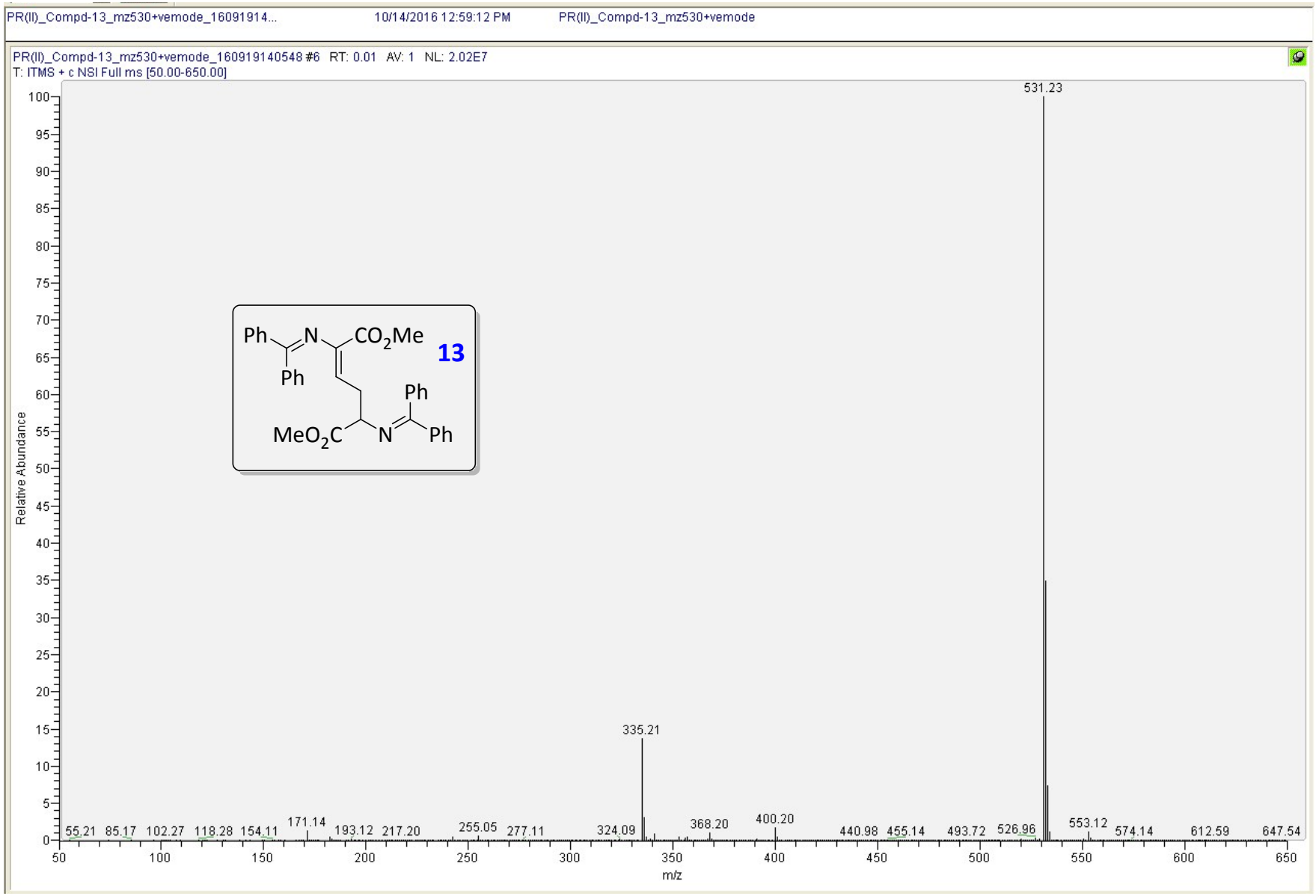

Delete Grid Column
PR(II)_RN143_P4_160919140548
9/23/2016 12:57:58 PM
PR(II)_RN143_P4_mz493+Nasalt
PR(II)_RN143_P4_160919140548 #6 RT: 0.01 AV: 1 NL: 5.11E6
T: ITMS + c NSI Full ms [50.00-600.00]
Ph
Ph
N
CO2Me
O
O
N
H
22
Relative Abundance
m/z
515.20
493.27
55.12
65.16
87.15
111.16
130.21
157.20
198.82
217.14
242.33
277.12
301.12
335.26
357.13
389.20
413.33
459.28
475.37
531.10
557.06
596.65


10.865
7.270
7.252
7.150
7.087
6.796
6.779
6.026
4.748
4.014
3.998
3.986
3.638
3.503
3.110
3.096
3.081
NH2
CO2Me
O
N
H
23
0.798
1.127
1.054
1.031
1.264
2.255
2.308
1.041
2.989
1.115
2.170
PPM
10
8
6
4
2


PR(II)_RN102_Tryp_160121104838 1/21/2016 10:48:39 AM Tryp probe_free amine_methyl ester_pure
PR(II)_RN102_Tryp_160121104838 #7 RT: 0.01 AV: 1 NL: 9.55E6
T: ITMS + c NSI Full ms [100.00-600.00]
Relative Abundance
m/z
273.19
343.16
299.21
448.29
174.25
188.28
313.19
345.64
359.12
375.13
475.00
546.58
102.22
112.16
130.34
147.17
215.26
241.22
257.19
289.18
323.08
389.14
413.06
429.22
461.14
497.19
513.16
531.20
570.65
591.25
NH2
CO2Me
O
N
H
23


7.737
7.689
7.677
7.585
7.576
7.490
7.466
7.397
7.383
7.310
7.299
7.109
7.038
5.780
5.768
4.033
4.024
3.618
3.474
3.320
2.500
Ph
N
CO2Me
Ph
Ph
MeO2C
N
Ph
13
2.351
12.419
5.338
3.936
0.971
1.096
2.999
3.074
1.917
PPM
8
6
4
2


196.284
171.666
170.660
170.550
163.888
141.116
139.184
138.437
137.481
136.598
135.825
133.156
131.772
131.173
121.384
64.064
52.167
52.156
40.000
39.926
39.835
39.747
39.739
39.668
39.501
31.462
Ph
N
CO2Me
Ph
13
Ph
MeO2C
N
Ph
PPM
160
120
80
40


PR(II)_Compd-13_mz530+vemode_16091914...
10/14/2016 12:59:12 PM
PR(II)_Compd-13_mz530+vemode
PR(II)_Compd-13_mz530+vemode_160919140548 #6 RT: 0.01 AV: 1 NL: 2.02E7
T: ITMS + c NSI Full ms [50.00-650.00]
Ph
N
CO2Me
Ph
13
Ph
MeO2C
N
Ph
Relative Abundance
m/z
531.23
335.21
55.21
85.17
102.27
118.28
154.11
171.14
193.12
217.20
255.05
277.11
324.09
368.20
400.20
440.98
455.14
493.72
526.96
553.12
574.14
612.59
647.54

References

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