Supporting information

Facile, highly efficient and environmentally friendly transesterification mediated by platinum dioxide and nickel oxide under essentially neutral conditions

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1. General methods

All manipulations were carried out in autoclave vessel or glass reaction tube equipped with a magnetic stir bar. Unless otherwise mentioned, solvents and reagents were purchased from commercial sources. The transformation progress was detected by TLC or HPLC. NMR spectra were acquired at 500 MHz for ^{1}H and 125 MHz for ^{13}C, respectively, on Varian INOVA 500 MHz (Bruker Corporation, Karlsruhe, Germany), in $CDCl_3$, with solvent peaks as references. ESI-MS and HR-ESI-MS data were measured using an AccuToFCS JMST100CS spectrometer (Agilent Technologies, Ltd, Santa Clara, CA, USA). Column chromatography (CC) was performed with silica gel (200-300 mesh, Qingdao Marine Chemical Inc. Qingdao, China). HPLC analysis was performed on an Agilent liquid chromatography 1260 (Agilent Technologies, Ltd, Santa Clara, CA, USA) with a YMC (250 × 5 mm i.d.) column packed with C18 (5 μM). TLC was carried out with glass precoated silica gel GF254 plates (Qingdao Marine Chemical, Inc., Qingdao, China). Spots were visualized under UV light or by spraying with 7% H_2SO_4 in 95% EtOH followed by heating.

2. General Procedures

2.1 General Procedure for the PtO_2/H_2-catalyzed transesterification of esters.

Methyl 3,5-dimethoxybenzoate (30 mg, 0.000153 mol), ethanol (10.0 mL), platinic oxide (35 mg, 0.000153 mol) were placed in an autoclave vessel. Autoclave was pressurized with 1–2 bar of nitrogen followed by 1–2 bar of hydrogen gas. The reaction mixtures were then warmed to 60 °C, stirred for 6 h at 500 rpm, and concentrated *in vacuo* to provide a residue. Whereafter, the residue was solved in acetone, filtered through microporous filtering film. The filtrate was concentrated *in vacuo* to give the products (Table 2, entry 1).

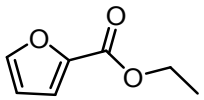
2.2 General Procedure for the PtO_2/NiO and H_2-catalyzed transesterification of esters.

Methyl 3,5-dimethoxybenzoate (30 mg, 0.000153 mol), ethanol (10.0 mL), platinic oxide (35 mg, 0.000153 mol) and nickel protoxide (13.7 mg, 0.000184 mol) were placed in an autoclave vessel. The autoclave was pressurized with 1-2 bar of nitrogen followed by 1-2 bar of hydrogen gas. Then the pressure was increased to the desired 6 bar. Subsequently, the reaction mixtures was warmed

to 95 °C with the pressure increased to 7-8 bar and stirred for 15 h at 680 rpm. Then, the reaction mixture was concentrated *in vacuo* to provide a residue. The residue was solved in acetone, filtered through microporous filtering film, and the filtrate was concentrated *in vacuo* to give the products (Table 8, entry 1).

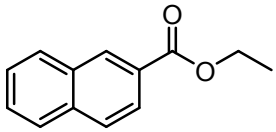
3. Products characterization

3.1 2-Furancaboxylic acid, ethyl ester.



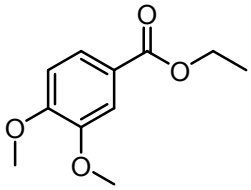
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, J = 0.9 Hz, 1H), 7.16 (dd, J = 3.5, 0.5 Hz, 1H), 6.49 (dd, J = 3.5, 1.7 Hz, 1H), 4.35 (q, J = 7.1 Hz, 2H), 1.37 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.88, 146.26, 145.02, 117.83, 111.90, 61.09, 14.45. (+)-ESI *m/z*: 163.2 $[M+Na]^+$. Spectral data were in agreement with those reported in the literature.[1]

3.2 2-Naphthalene carboxylic acid, ethyl ester.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.12 - 8.03 (m, 1H), 7.96 (d, J = 8.1 Hz, 1H), 7.88 (d, J = 8.6 Hz, 2H), 7.63 - 7.48 (m, 2H), 4.45 (q, J = 7.1 Hz, 2H), 1.45 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.92, 135.60, 132.63, 131.06, 129.45, 128.27, 128.20, 127.87, 127.87, 126.71, 125.38, 61.23, 14.53. (+)-ESI *m/z*: 223.2 $[M+Na]^+$. Spectral data were in agreement with those reported in the literature.[2]

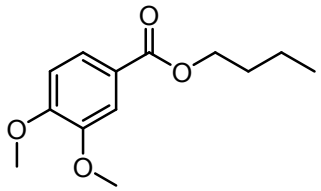
3.3 3,4-Dimethoxybenzoic acid, ethyl ester.



^{1} H NMR (500 MHz, $CDCl_3$) δ 7.68 (dd, J = 8.4, 1.9 Hz, 1H), 7.54 (d, J = 1.9 Hz, 1H), 6.87 (d, J = 8.4 Hz, 1H), 4.35 (q, J = 7.1 Hz, 2H), 3.92 (s, 6H), 1.38 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.52, 152.98, 148.69, 123.59, 123.16, 112.07, 110.31, 60.92, 56.11, 56.11,

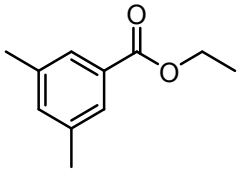
14.52. (+)-ESI *m/z*: 233.2 $[M+Na]^+$. Spectral data were in agreement with those reported in the literature.[3]

3.4 3,4-Dimethoxybenzoic acid, butyl ester.



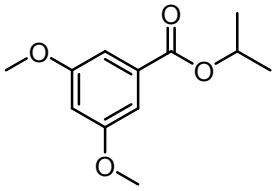
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (dd, J = 8.4, 1.9 Hz, 1H), 7.54 (d, J = 1.8 Hz, 1H), 6.87 (d, J = 8.4 Hz, 1H), 4.29 (t, J = 6.7 Hz, 2H), 3.92 (s, 3H), 1.79 - 1.68 (m, 2H), 1.46 (dt, J = 14.8, 7.4 Hz, 2H), 0.97 (t, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.57, 152.98, 148.70, 123.57, 123.18, 112.09, 110.32, 64.81, 56.10, 56.10, 30.96, 19.41, 13.90. (+)-ESI *m/z*: 261.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[4]

3.5 3,5-Dimethylbenzoic acid, ethyl ester.



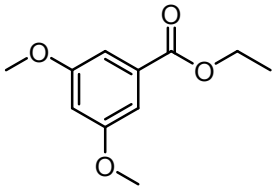
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (s, 2H), 7.18 (s, 1H), 4.36 (q, J = 7.1 Hz, 2H), 2.36 (s, 6H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.11, 138.08, 134.58, 134.56, 130.51, 127.38, 127.35, 60.94, 21.30, 21.27, 14.49. (+)-ESI *m/z*: 201.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[5]

3.6 3,5-Dimethoxybenzoic acid, 1-methylethyl ester.



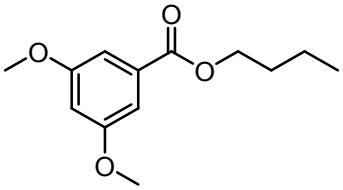
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, J = 2.2 Hz, 2H), 6.63 (t, J = 2.2 Hz, 1H), 5.23 (hept, J = 6.29 Hz, 1H), 3.83 (s, 6H), 1.36 (d, J = 6.3 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.98, 160.72 (2 × C), 132.98, 107.29 (2 × C), 105.49, 68.73, 55.72 (2 × C), 29.85, 22.06 (2 × C). (+)-ESI *m/z*: 247.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[6]

3.7 3,5-Dimethoxybenzoic acid, ethyl ester.



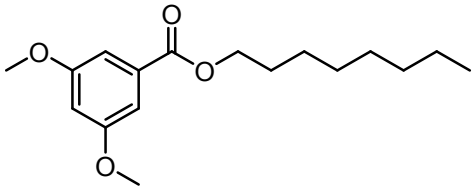
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (d, J = 2.4 Hz, 2H), 6.64 (t, J = 2.4 Hz, 1H), 4.37 (q, J = 7.1 Hz, 2H), 3.83 (s, 6H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.50, 160.74 (2 × C), 132.53, 107.26 (2 × C), 105.69, 61.27, 55.69 (2 × C), 14.44. (+)-ESI *m/z*: 233.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[7]

3.8 3,5-Dimethoxybenzoic acid, butyl ester.



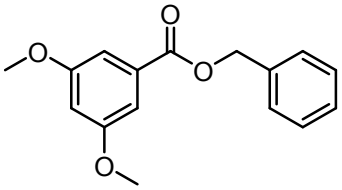
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (d, J = 2.3 Hz, 2H), 6.64 (t, J = 2.3 Hz, 1H), 4.31 (t, J = 6.6 Hz, 2H), 3.83 (s, 6H), 1.79 - 1.68 (m, 2H), 1.52 - 1.42 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.56, 160.75 (2 × C), 132.57, 107.31 (2 × C), 105.58, 65.17, 55.71 (2 × C), 30.90, 19.42, 13.91. (+)-ESI *m/z*: 261.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[8]

3.9 3,5-Dimethoxybenzoic acid, octyl ester.



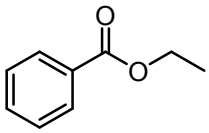
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (d, J = 2.3 Hz, 2H), 6.64 (t, J = 2.3 Hz, 1H), 4.30 (t, J = 6.7 Hz, 2H), 3.83 (s, 6H), 1.80 - 1.71 (m, 2H), 1.48 - 1.39 (m, 2H), 1.38 - 1.24 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.56, 160.75 (2 × C), 132.58, 107.31 (2 × C), 105.59, 65.48, 55.70 (2 × C), 31.94, 29.39, 29.34, 28.84, 26.18, 22.79, 14.23. (+)-ESI *m/z*: 317.3 $[M+Na]^+$.

3.10 3,5-Dimethoxybenzoic acid, phenylmethyl ester.



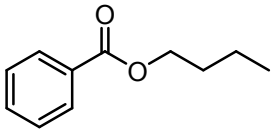
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, J = 6.7 Hz, 2H), 7.39 (t, J = 7.4 Hz, 2H), 7.35 (t, J = 7.1 Hz, 1H), 7.23 (d, J = 2.3 Hz, 2H), 6.65 (t, J = 2.3 Hz, 1H), 5.36 (s, 1H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.33, 160.78 (2 × C), 136.13, 132.14, 128.73 (2 × C), 128.37, 128.28 (2 × C), 107.47 (2 × C), 105.83, 66.97, 55.72 (2 × C). (+)-ESI *m/z*: 295.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[9]

3.11 Benzoic acid, ethyl ester.



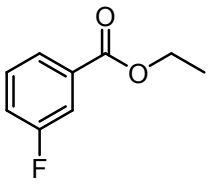
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 - 7.98 (m, 2H), 7.54 (tt, J = 10.6, 4.2 Hz, 1H), 7.43 (t, J = 7.7 Hz, 2H), 4.38 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.74, 132.89, 130.61, 129.63 (2 × C), 128.40 (2 × C), 61.05, 14.43. (+)-ESI *m/z*: 173.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[10]

3.12 Benzoic acid, butyl ester.



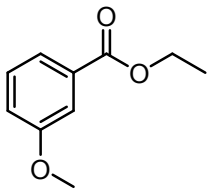
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 - 8.00 (m, 2H), 7.59 - 7.51 (m, 1H), 7.43 (t, J = 7.7 Hz, 2H), 4.33 (t, J = 6.6 Hz, 2H), 1.76 (dt, J = 14.5, 6.6 Hz, 2H), 1.48 (dt, J = 14.8, 7.4 Hz, 2H), 0.98 (t, J = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.80, 132.90, 130.67 (2 × C), 129.65 (2 × C), 128.43, 64.95, 30.92, 19.41, 13.89. (+)-ESI *m/z*: 201.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[11]

3.13 3-Fluorobenzoic acid, ethyl ester.



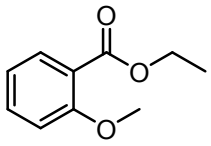
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dt, J = 7.7, 1.3 Hz, 1H), 7.72 (ddd, J = 9.4, 2.7, 1.5 Hz, 1H), 7.41 (td, J = 8.0, 5.5 Hz, 1H), 7.28 - 7.20 (m, 1H), 4.38 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.60, 162.67, 132.82, 130.06, 125.39, 119.98, 116.57, 61.47 , 14.40 . (+)-ESI *m/z*: 191.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[12]

3.14 3-Methoxybenzoic acid, ethyl ester.



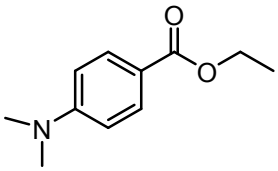
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (dt, J = 7.7, 1.3 Hz, 1H), 7.57 (dd, J = 2.7, 1.5 Hz, 1H), 7.34 (t, J = 7.9 Hz, 1H), 7.09 (ddd, J = 8.3, 2.7, 1.0 Hz, 1H), 4.38 (q, J = 7.1 Hz, 2H), 3.85 (s, 3H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.63, 159.67, 131.96, 129.46, 122.08, 119.45, 114.14, 61.19, 55.57, 14.47. (+)-ESI *m/z*: 203.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[12]

3.15 2-Methoxybenzoic acid, ethyl ester.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (dd, J = 7.9, 1.8 Hz, 1H), 7.42 - 7.48 (m, 1H), 6.98 - 6.93 (m, 2H), 4.34 (q, J = 7.1 Hz, 2H), 3.88 (s, 3H), 1.36 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.26, 159.17, 133.38, 131.52, 120.56, 120.16, 112.12, 60.84, 56.05, 14.38. (+)-ESI *m/z*: 203.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[12]

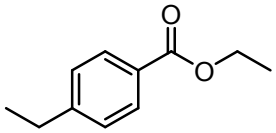
3.16 4-Dimethylaminobenzoic acid, ethyl ester.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, J = 8.9 Hz, 2H), 6.72 (d, J = 8.5 Hz, 2H), 4.32 (q, J = 7.1 Hz, 2H), 3.04 (s, 6H), 1.37 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.04, 152.97,

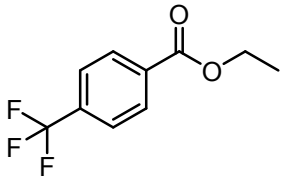
131.36 (2 × C), 131.36 (2 × C), 111.42, 60.35, 40.57 (2 × C), 14.62. (+)-ESI *m/z*: 216.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[10]

3.17 4-Ethylbenzoic acid, ethyl ester.



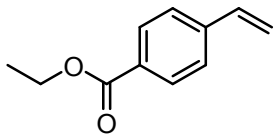
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, J = 7.8 Hz, 2H), 7.26 (d, J = 7.8 Hz, 2H), 4.36 (q, J = 7.2 Hz, 2H), 2.70 (q, J = 7.7 Hz, 2H), 1.38 (t, J = 7.2 Hz, 3H), 1.25 (t, J = 7.7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.86, 149.75, 129.80 (2 × C), 128.13, 127.96 (2 × C), 60.88, 29.10, 15.40, 14.50. (+)-ESI *m/z*: 201.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[13]

3.18 4-Trifluoromethylbenzoic acid, ethyl ester.



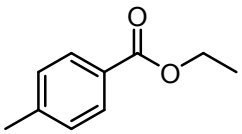
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, J = 8.1 Hz, 2H), 7.70 (d, J = 8.2 Hz, 2H), 4.42 (q, J = 7.1 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.53, 134.48, 133.86, 130.09, 125.50, 123.8, 61.70, 14.41. (-)-ESI *m/z*: 217.8 $[M-H]^-$. These data were in agreement with those reported in the literature.[12]

3.19 4-Ethenylbenzoic acid, ethyl ester.



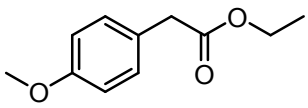
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.3 Hz, 2H), 6.75 (dd, J = 17.6, 10.9 Hz, 1H), 5.86 (d, J = 17.6 Hz, 1H), 5.38 (d, J = 10.9 Hz, 1H), 4.37 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.53, 141.95, 136.19, 129.98 (2 × C), 129.77, 126.19 (2 × C), 116.51, 61.06, 14.48. (+)-ESI *m/z*: 199.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[14]

3.20 4-Methylbenzoic acid, ethyl ester.



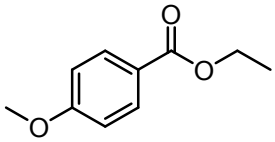
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, J = 8.2 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 4.36 (q, J = 7.1 Hz, 2H), 2.40 (s, 3H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.81, 143.51, 129.67 (2 × C), 129.13 (2 × C), 127.91, 60.86, 21.75, 14.47. (+)-ESI *m/z*: 187.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[12]

3.21 4-Methoxybenzene acetic acid, ethyl ester.



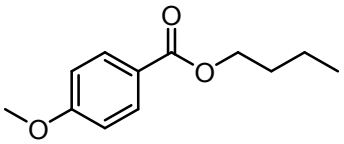
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, J = 8.7 Hz, 2H), 6.86 (d, J = 8.6 Hz, 2H), 4.14 (q, J = 7.1 Hz, 2H), 3.79 (s, 3H), 3.55 (s, 2H), 1.25 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.03, 158.77, 130.36 (2 × C), 126.35, 114.08 (2 × C), 60.88, 55.36, 40.64, 14.31. (+)-ESI *m/z*: 217.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[15]

3.22 4-Methoxybenzoic acid, ethyl ester.



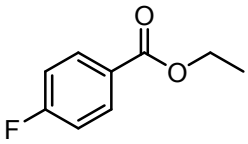
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, J = 8.9 Hz, 2H), 6.91 (d, J = 8.9 Hz, 2H), 4.35 (q, J = 7.1 Hz, 2H), 3.86 (s, 3H), 1.38 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.53, 163.38, 131.66 (2 × C), 123.10, 113.67 (2 × C), 60.77, 55.54, 14.52. (+)-ESI *m/z*: 203.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[12]

3.23 4-Methoxybenzoic acid, butyl ester.



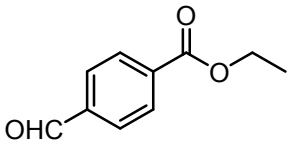
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, J = 8.8 Hz, 2H), 6.91 (d, J = 8.9 Hz, 2H), 4.29 (t, J = 6.6 Hz, 2H), 3.84 (s, 3H), 1.81 - 1.66 (m, 2H), 1.54 - 1.39 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.55, 163.35, 131.63 (2 × C), 123.10, 113.65 (2 × C), 64.63, 55.50, 30.96, 19.41, 13.89. (+)-ESI *m/z*: 231.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[16]

3.24 4-Fluorobenzoic acid, ethyl ester.



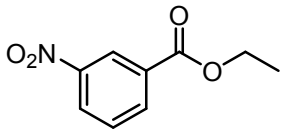
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 - 8.03 (m, 2H), 7.10 (t, J = 8.7 Hz, 2H), 4.36 (q, J = 7.1 Hz, 2H), 1.38 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $cdcl_3$) δ 166.29, 164.80, 132.18, 126.86, 115.55, 61.21, 14.44. (+)-ESI *m/z*: 191.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[12]

3.25 Ethyl 4-formylbenzoate.



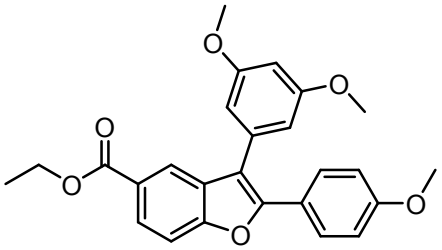
^{1}H NMR (500 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.20 (d, J = 8.3 Hz, 2H), 7.95 (d, J = 8.4 Hz, 2H), 4.42 (q, J = 7.1 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.80, 165.72, 139.23, 135.62, 130.29 (2 × C), 129.63 (2 × C), 61.76, 14.42. (+)-ESI *m/z*: 217.5 $[M+K]^+$. These data were in agreement with those reported in the literature.[12]

3.26 Ethyl 3-nitrobenzoate.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (t, J = 1.9 Hz, 1H), 8.43 – 8.38 (m, 1H), 8.36 (dd, J = 7.7, 1.4 Hz, 1H), 7.64 (t, J = 8.0 Hz, 1H), 4.44 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.58, 148.39, 135.38, 132.37, 129.69, 127.40, 124.66, 62.07, 14.39. (+)-ESI *m/z*: 218.2 $[M+Na]^+$. These data were in agreement with those reported in the literature.[17]

3.27 3-(3,5-Dimethoxyphenyl)-2-(4-methoxyphenyl)-5-Benzofuran carboxylic acid, ethyl ester



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 1.7 Hz, 1H), 8.04 (dd, J = 8.6, 1.8 Hz, 1H), 7.64 (d, J = 8.7 Hz, 2H), 7.54 (d, J = 8.6 Hz, 1H), 6.87 (d, J = 8.5 Hz, 2H), 6.64 (d, J = 2.4 Hz, 2H), 6.54 (t, J = 2.3 Hz, 1H), 4.38 (q, J = 7.1 Hz, 2H), 3.83 (s, 3H), 3.79 (s, 7H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.00, 161.45 (2 × C), 160.16, 156.42, 152.16, 134.38, 130.60, 128.71 (2 × C), 126.23, 125.78, 122.77, 122.30, 114.12 (2 × C), 110.86, 107.82 (2 × C), 100.35, 77.42, 77.16, 76.91, 61.07, 55.61, 55.46, 29.85. (+)-HRESI *m/z*: 455.1581 $[M+Na]^+$ (Calcd for $C_{26}H_{24}O_6Na$: 455.1473).

4. References

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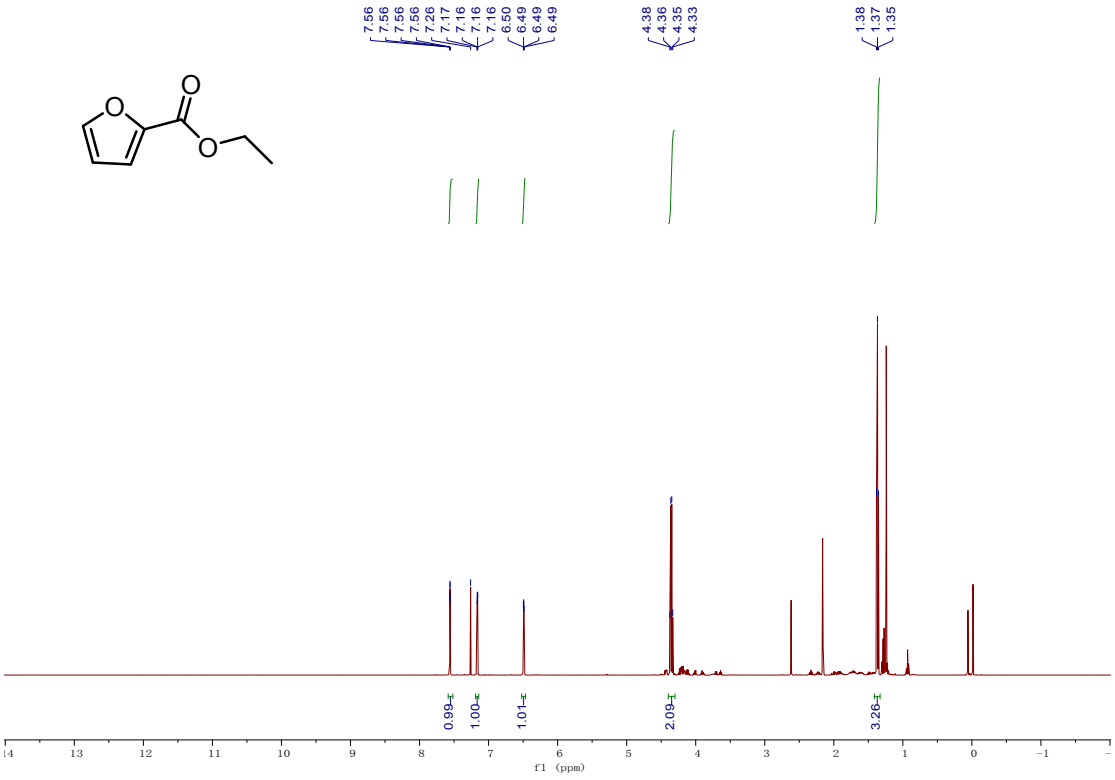
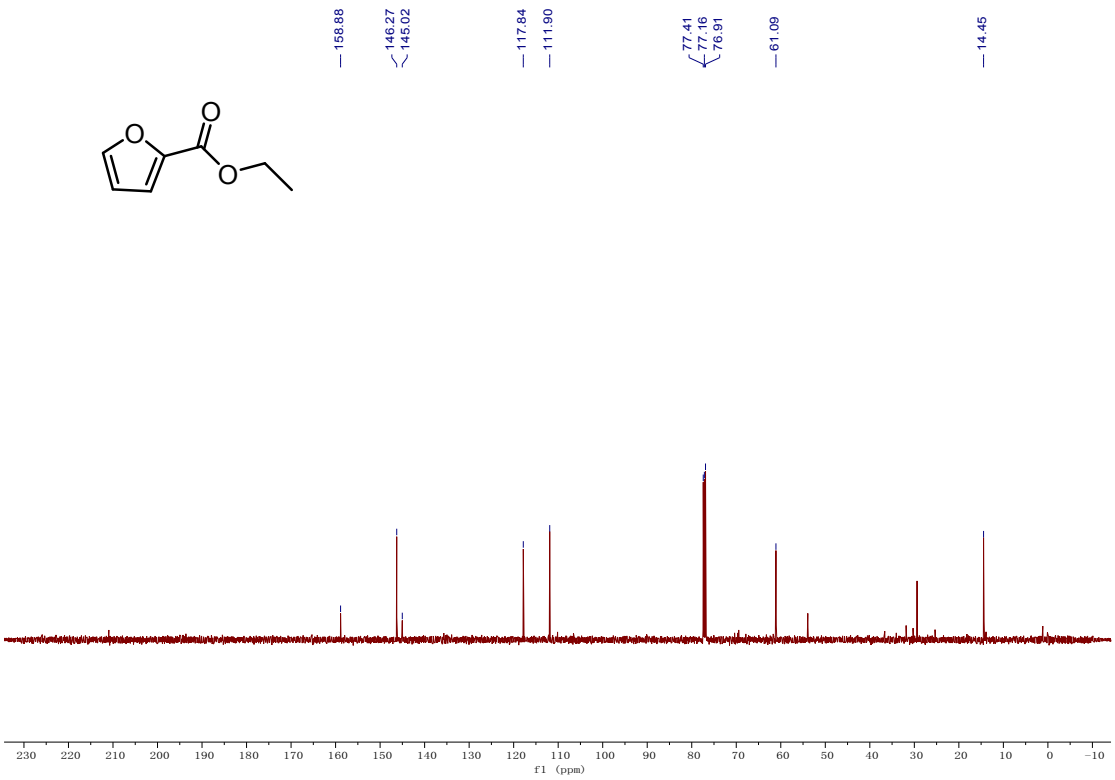
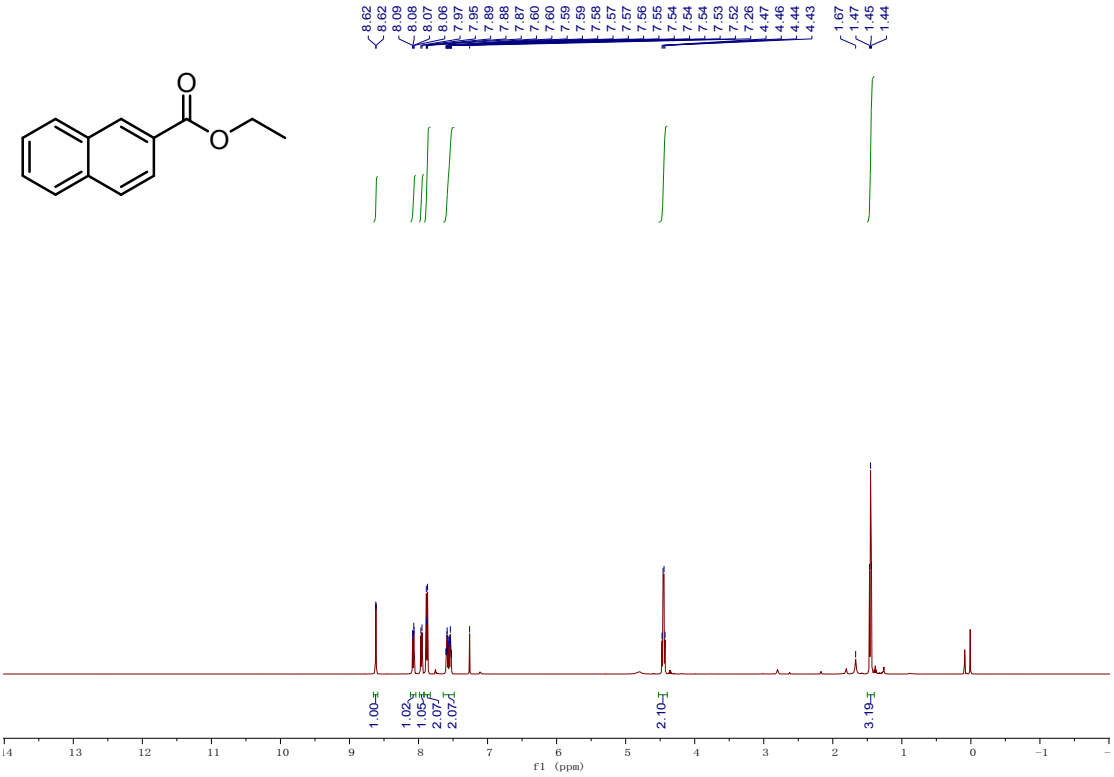
5. NMR spectra



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7.58
7.57
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7.53
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7.26
4.47
4.46
4.44
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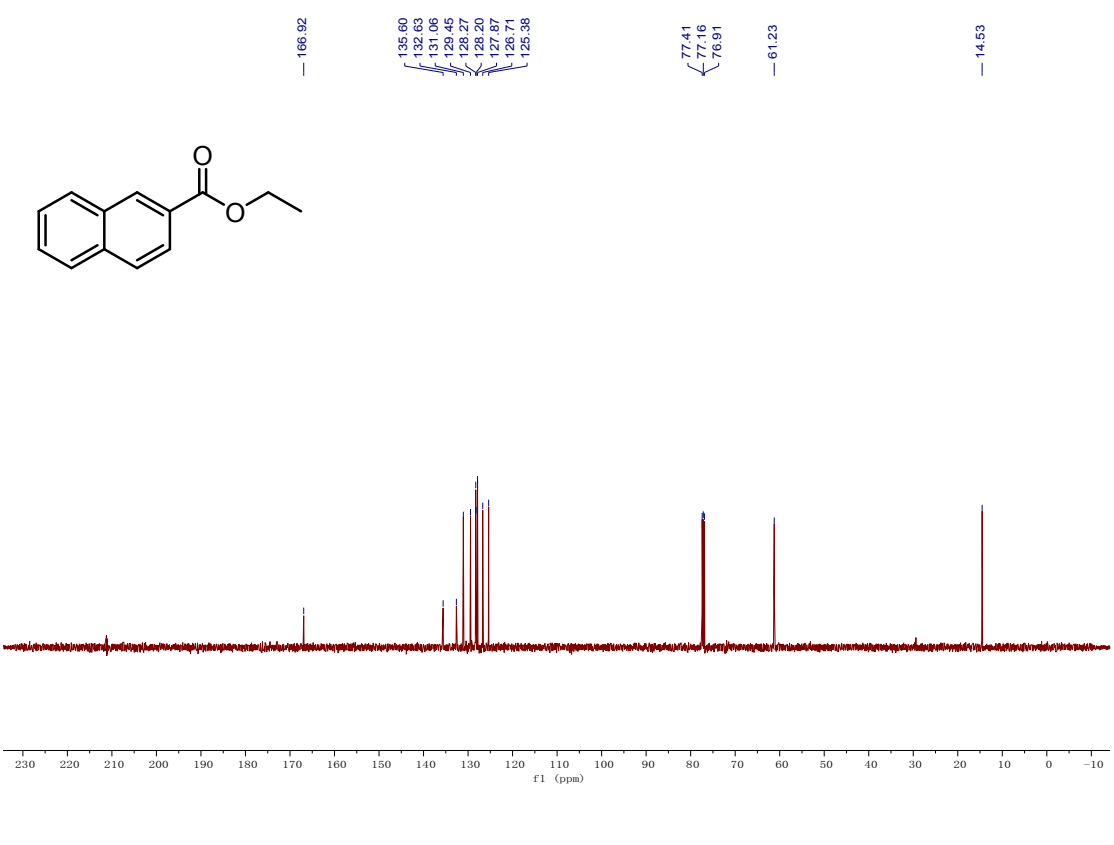
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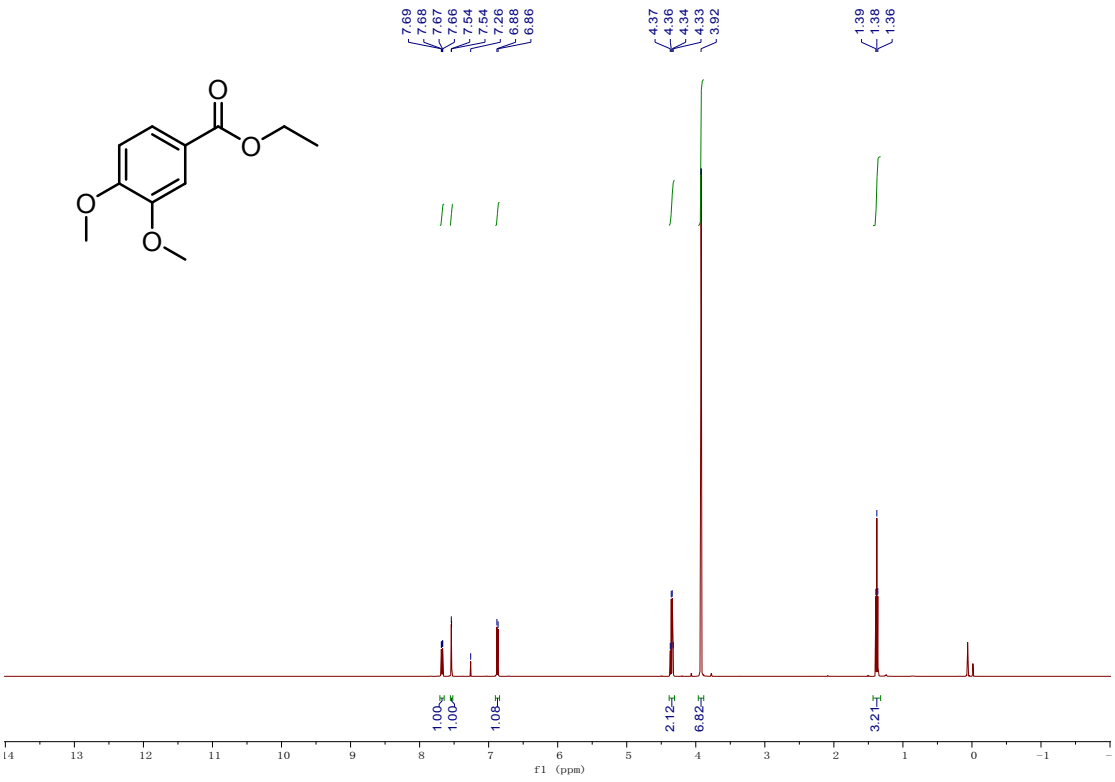
f1 (ppm)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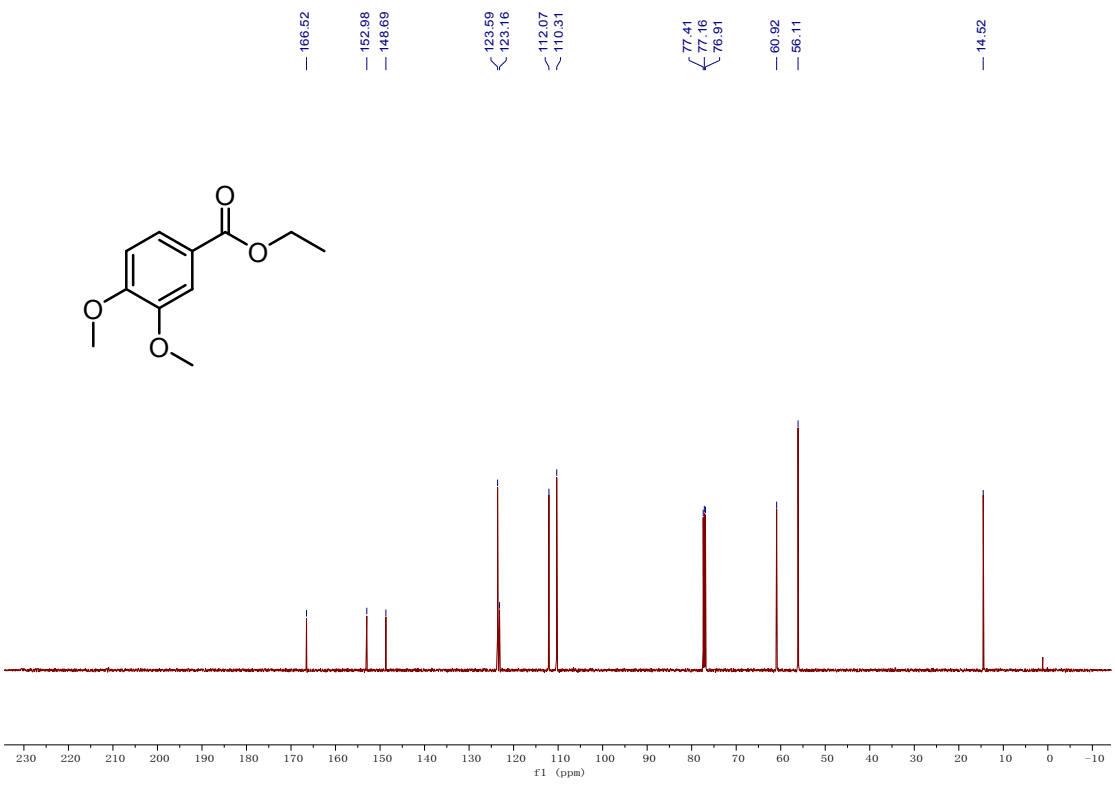
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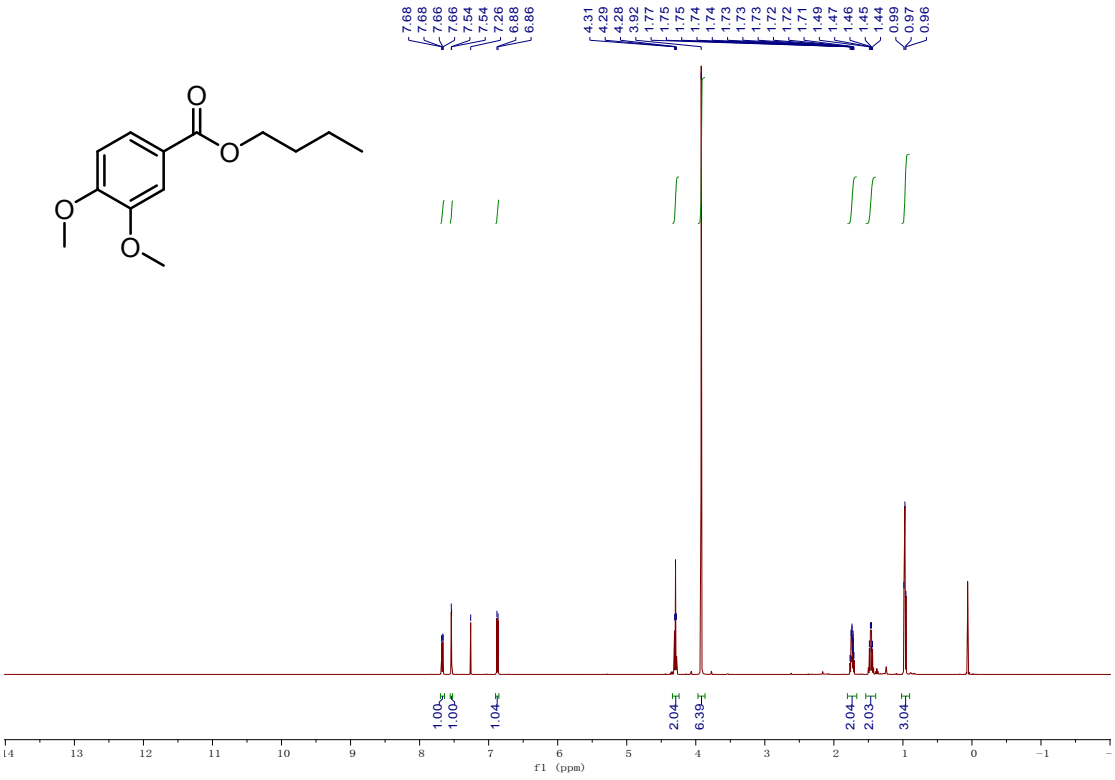
f1 (ppm)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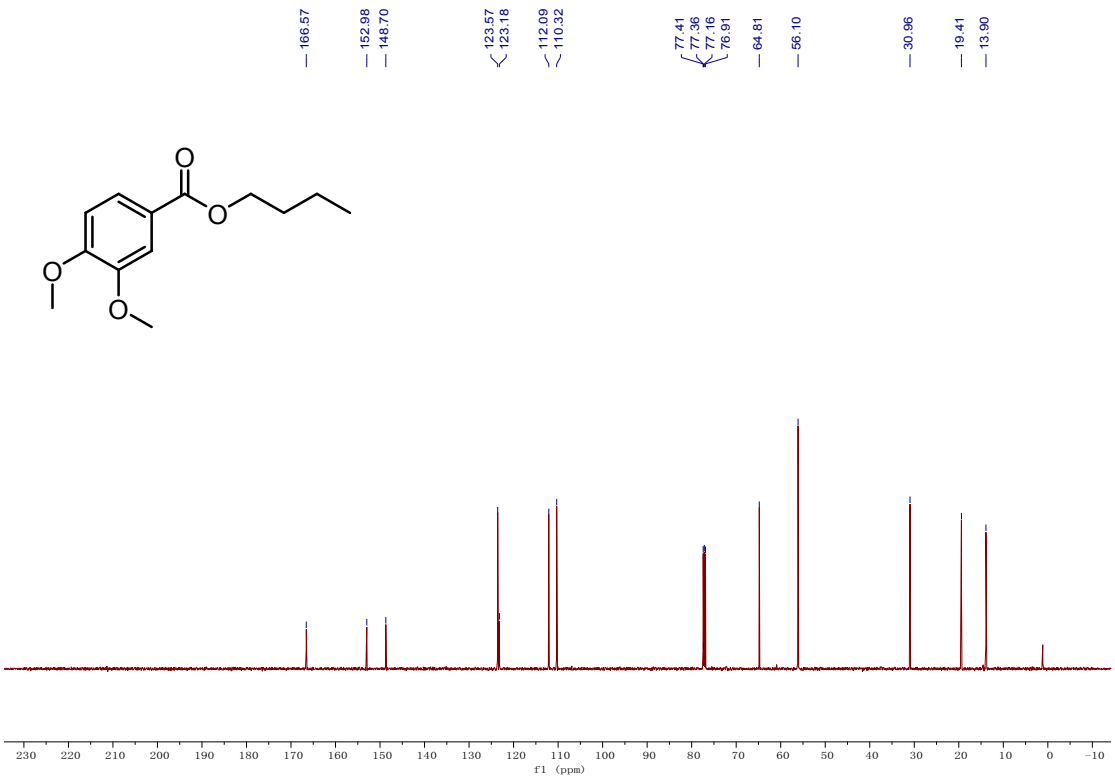
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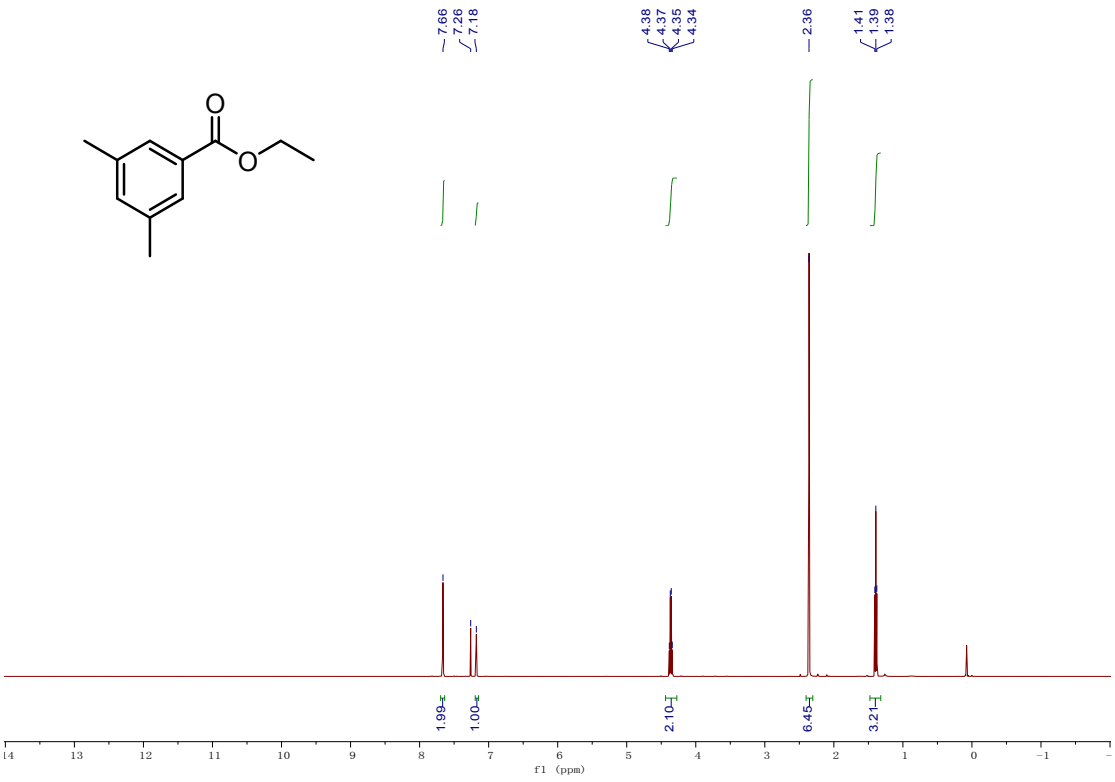
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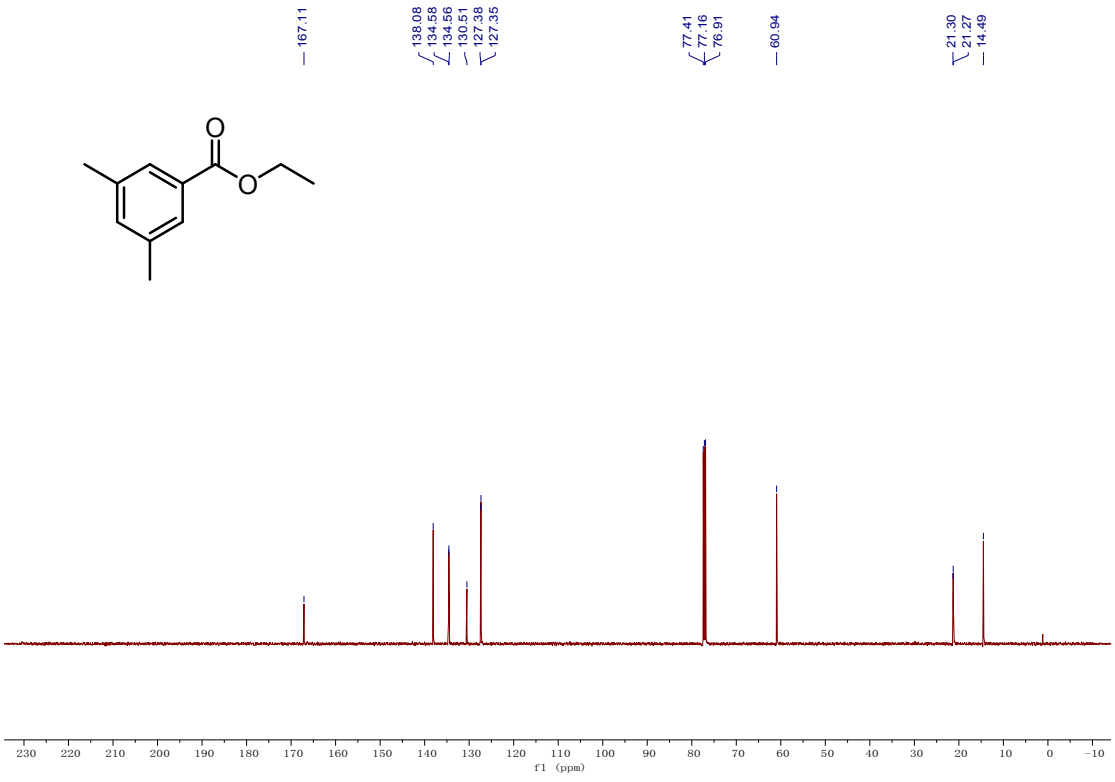
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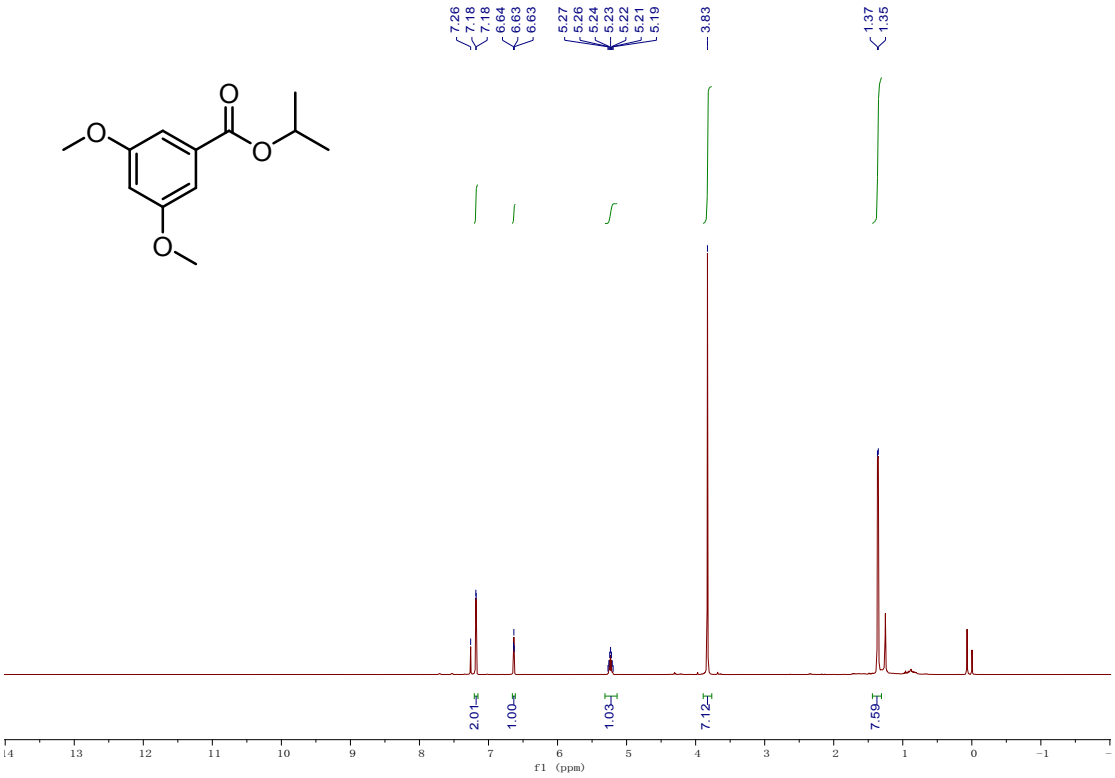
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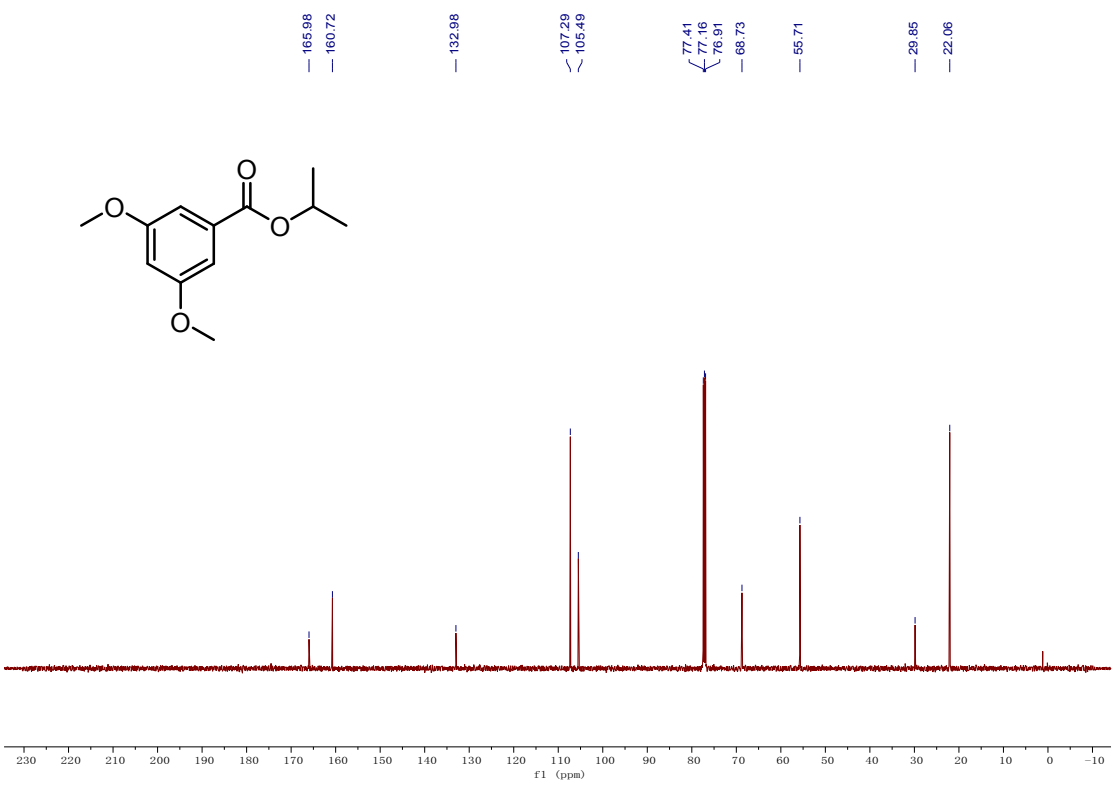
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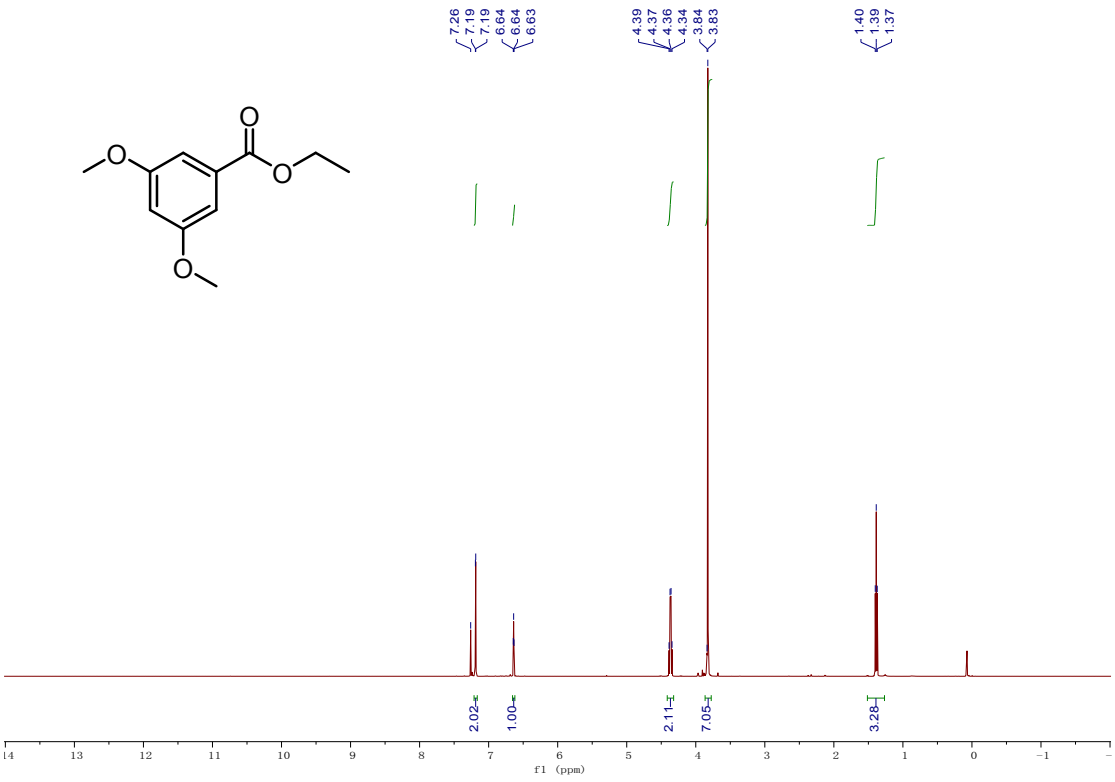
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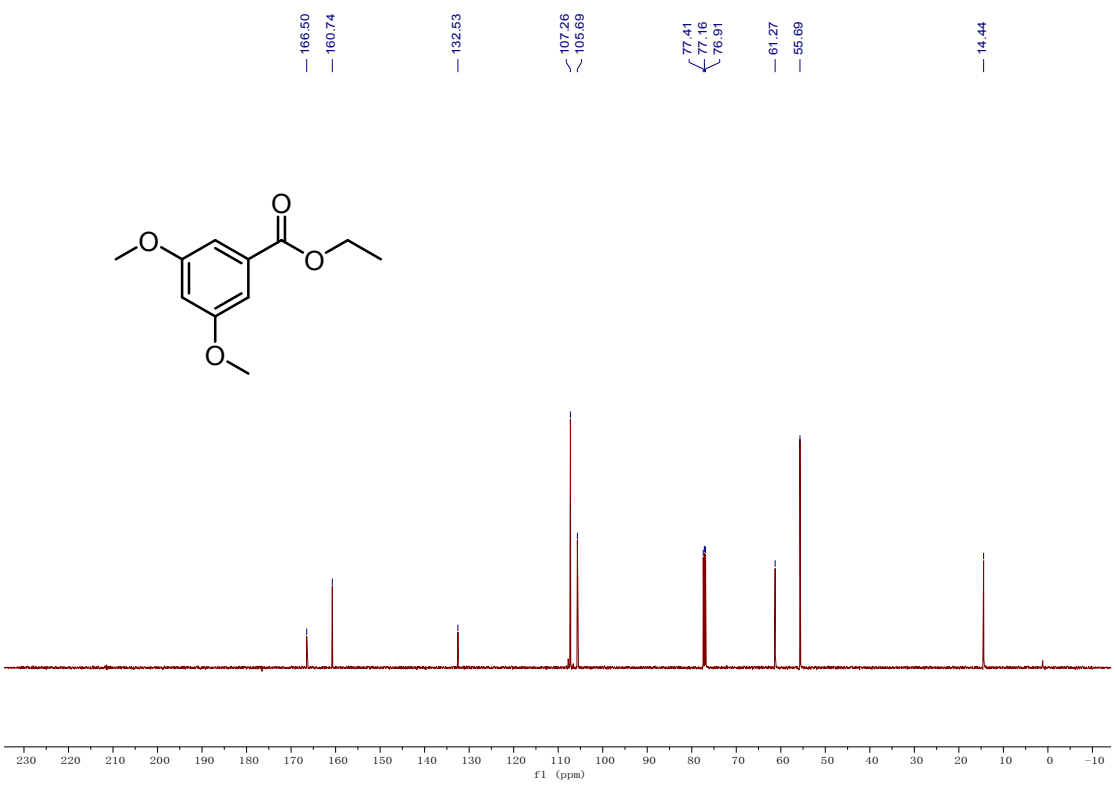
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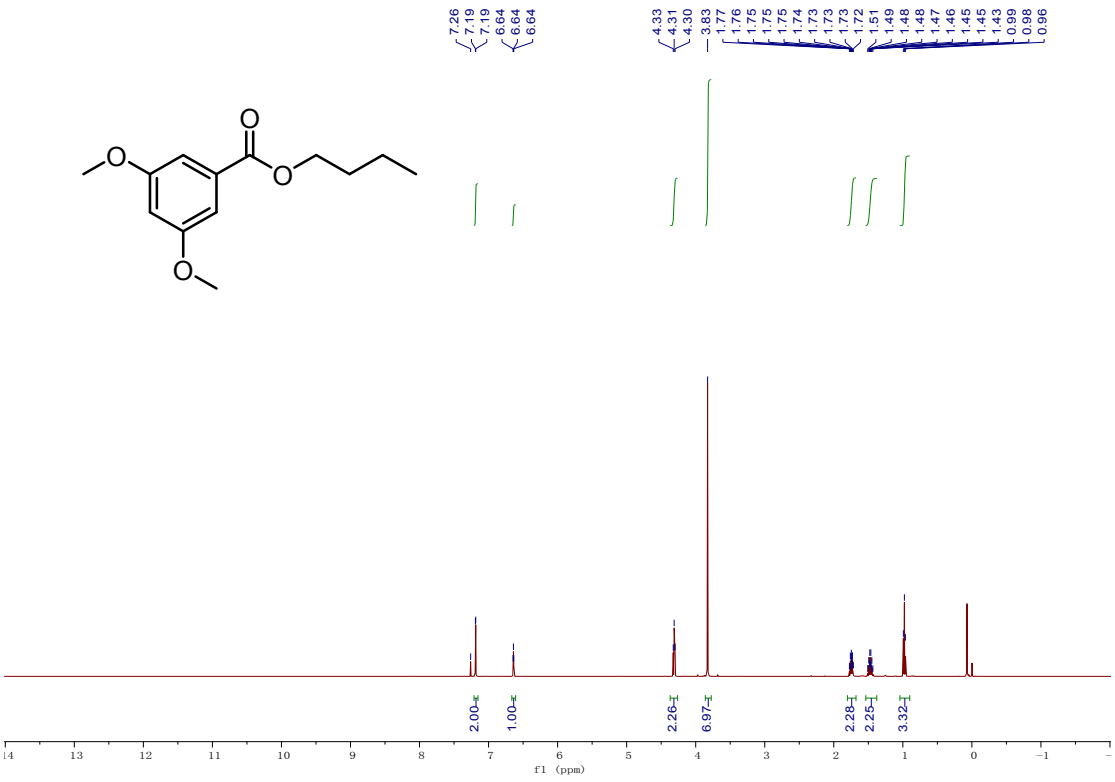
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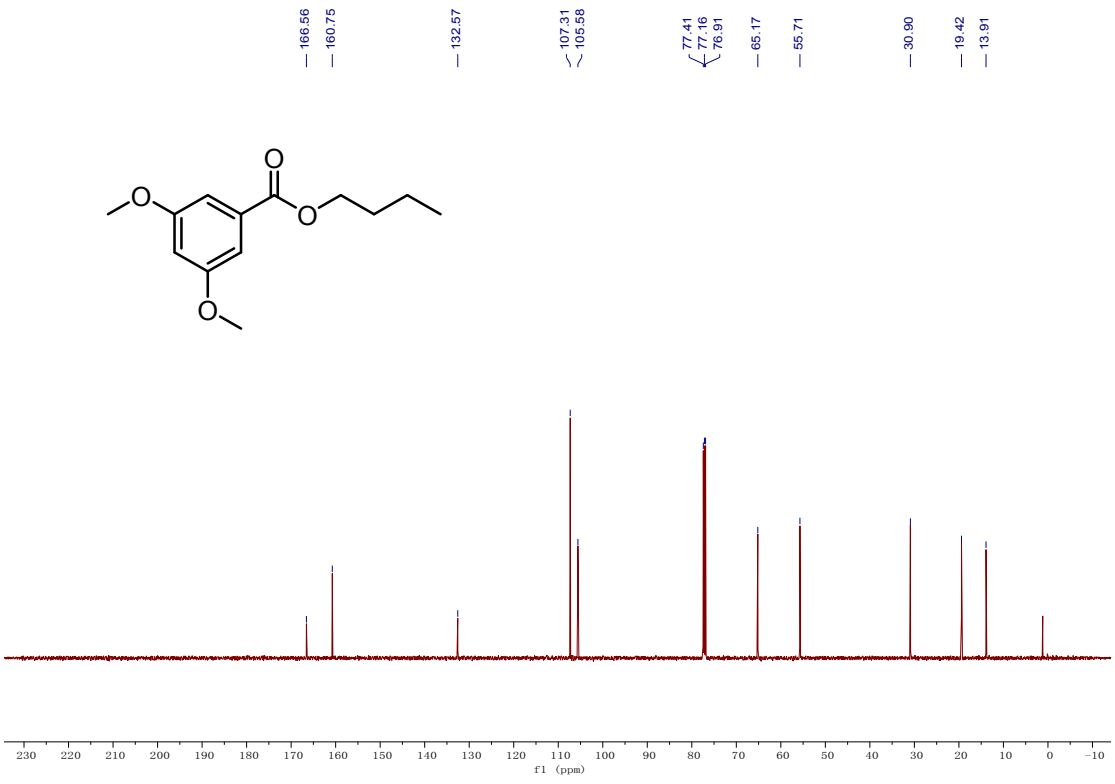
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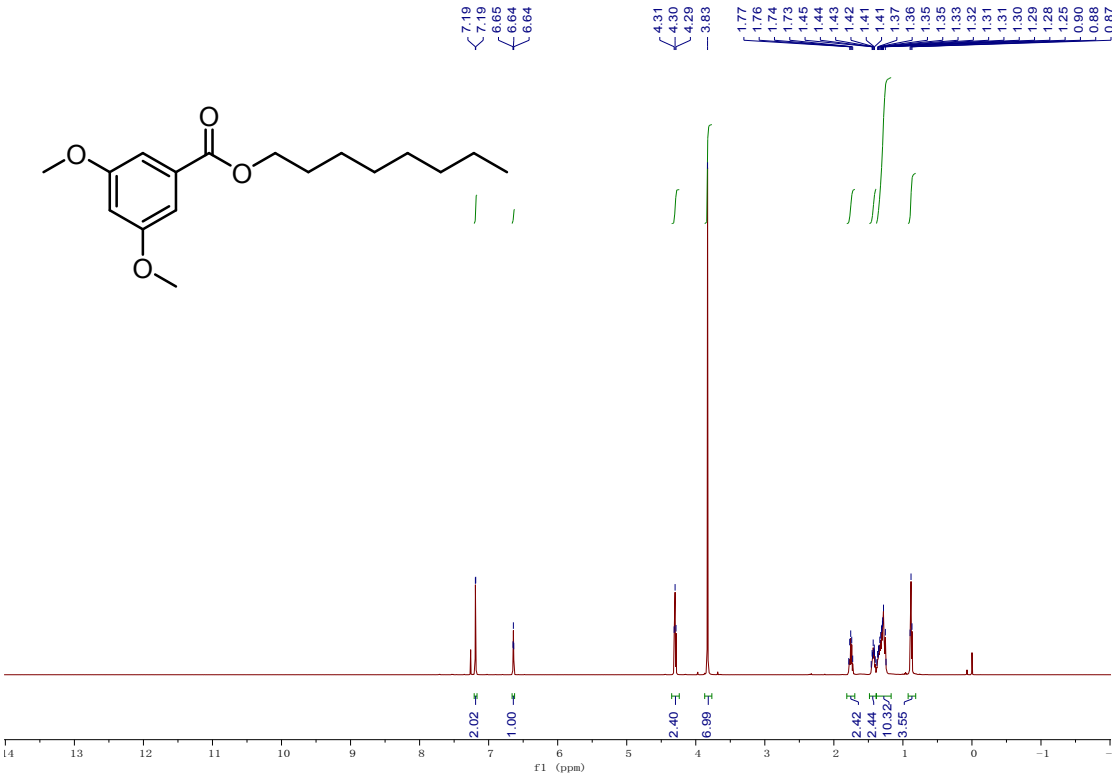
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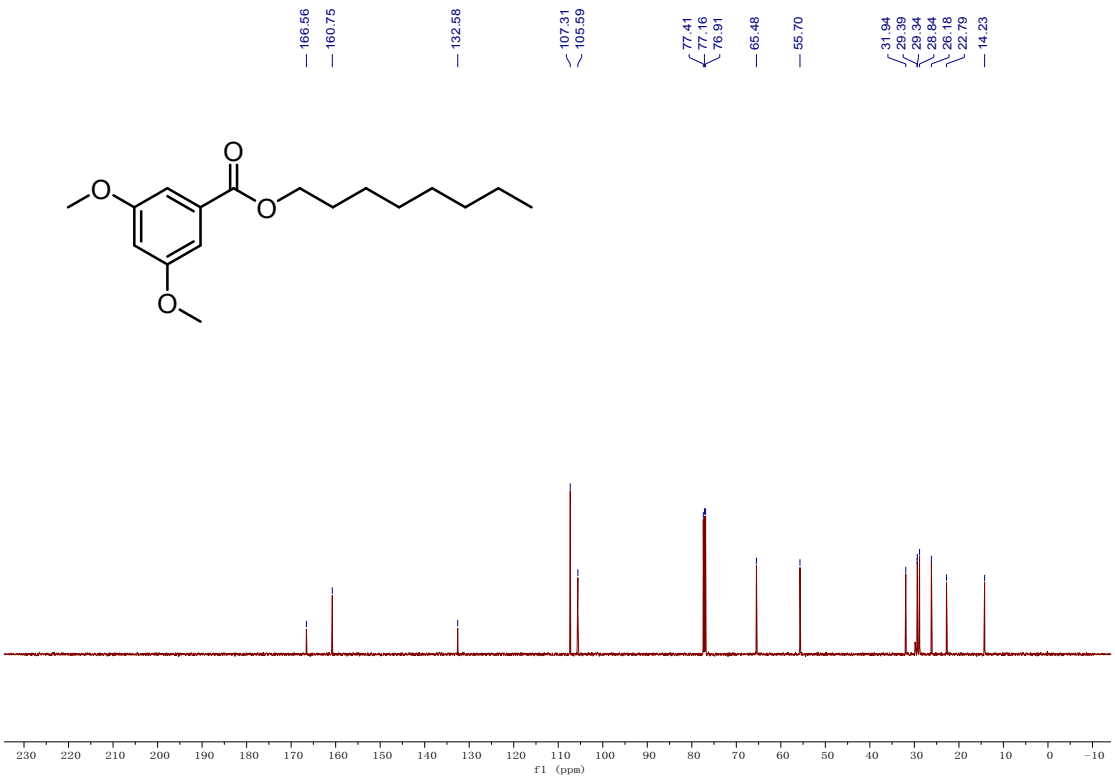
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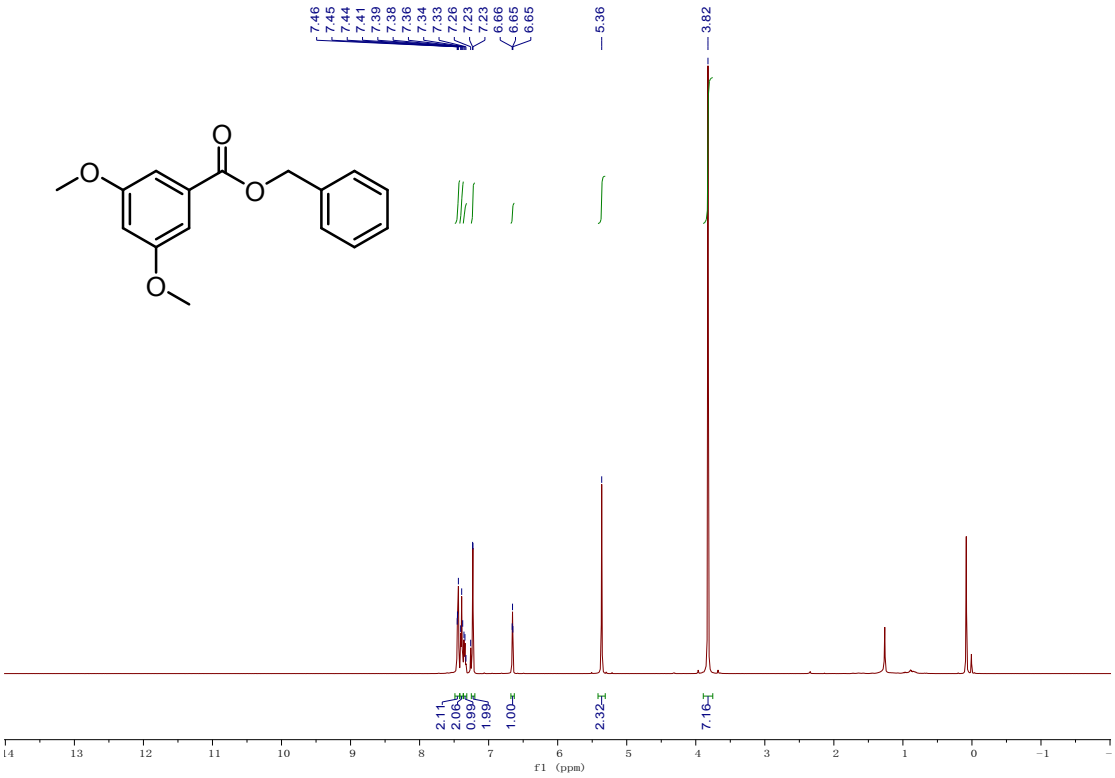
f1 (ppm)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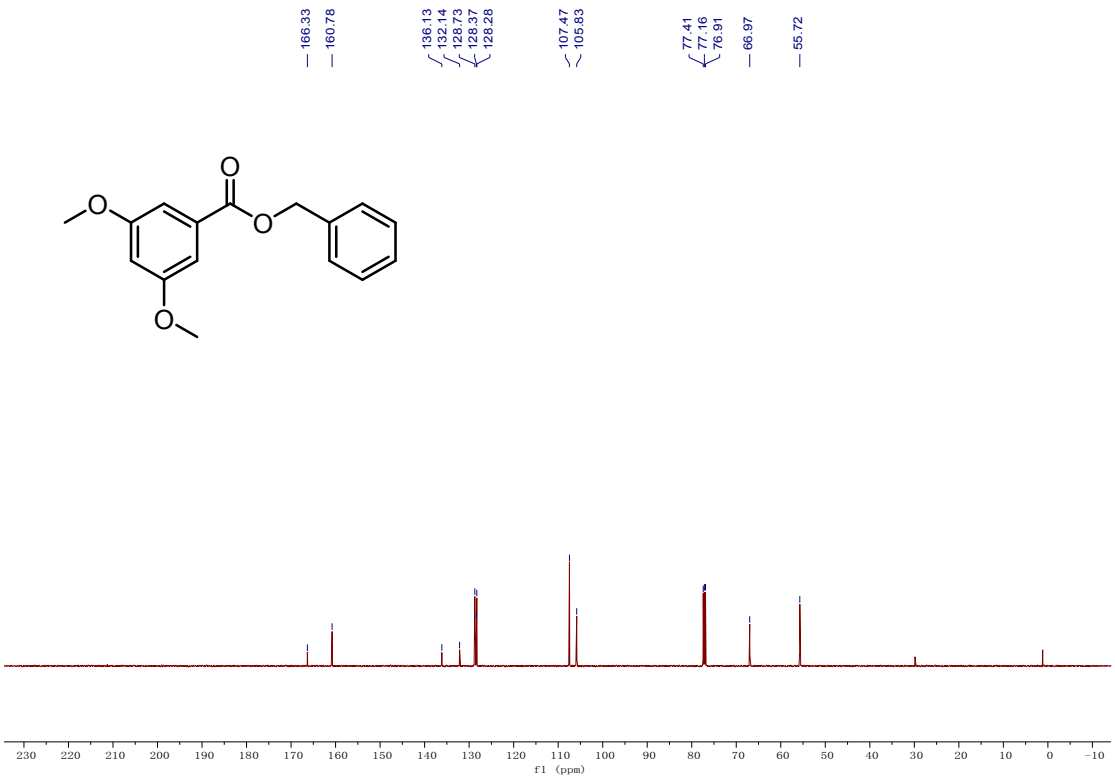
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O
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O
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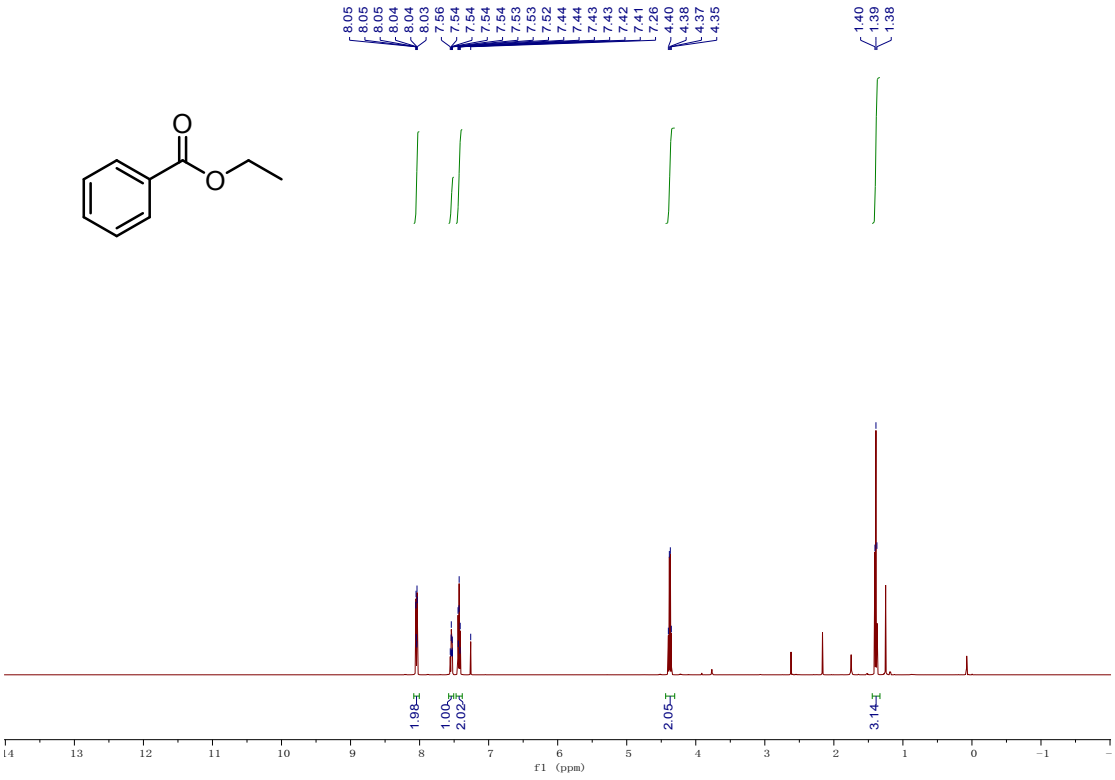
f1 (ppm)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7.42
7.41
7.26
4.40
4.38
4.37
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1.39
1.38
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O
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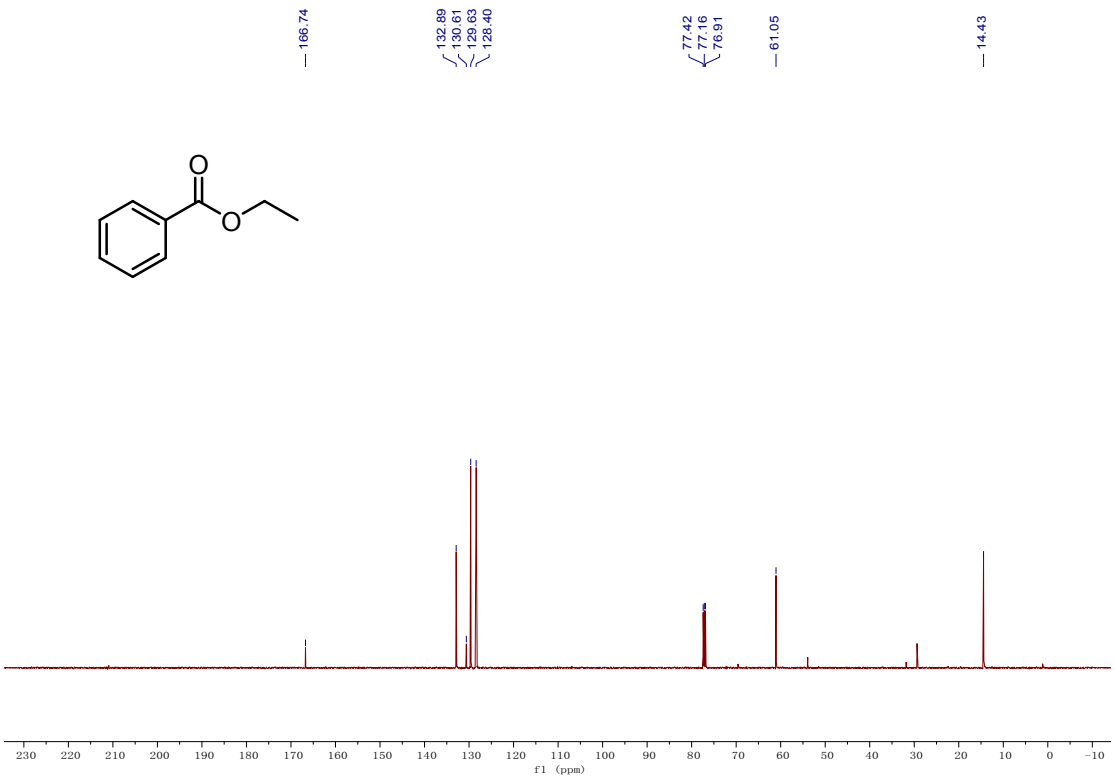
2.02
2.05
3.14
f1 (ppm)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76.91
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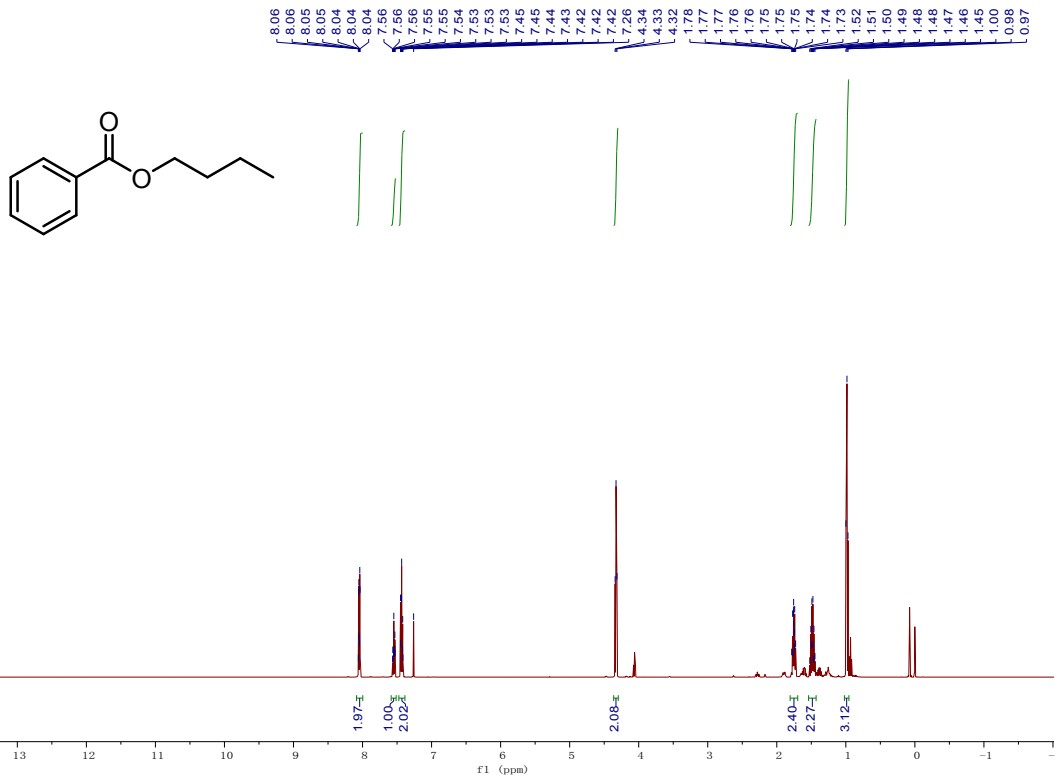
O
f1 (ppm)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7.42
7.42
7.26
4.34
4.33
4.32
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1.77
1.76
1.76
1.75
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1.75
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1.74
1.73
1.52
1.51
1.50
1.49
1.48
1.48
1.47
1.46
1.45
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O
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1.00
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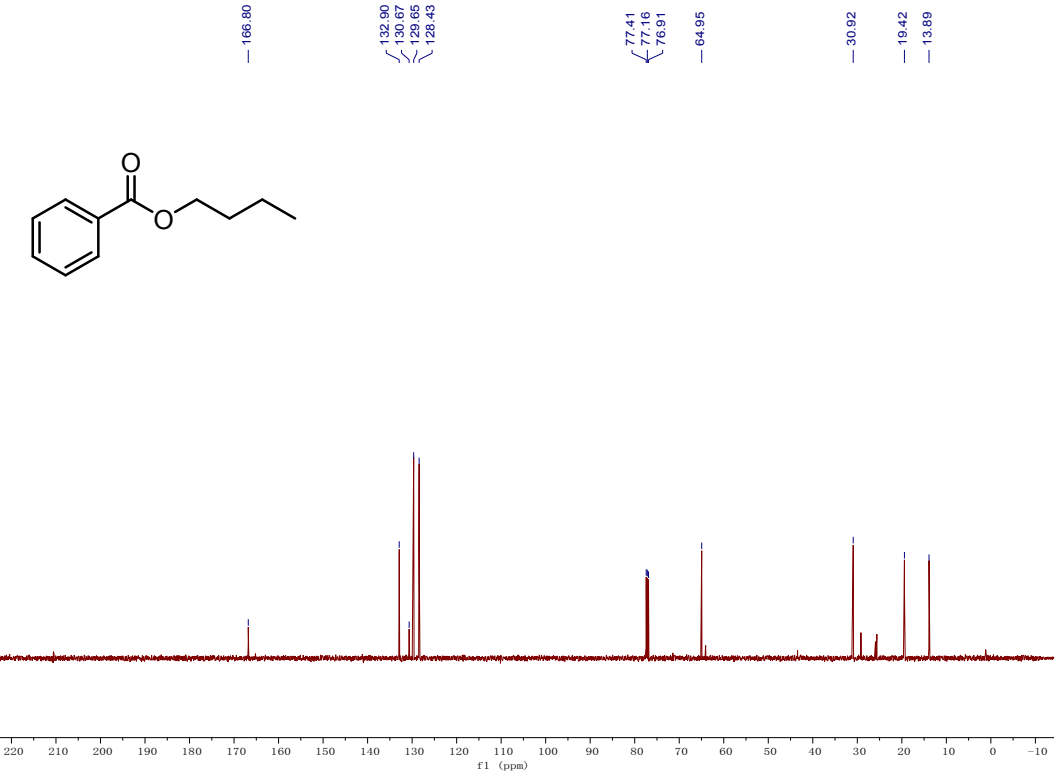
2.40
2.27
3.12
f1 (ppm)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76.91
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19.42
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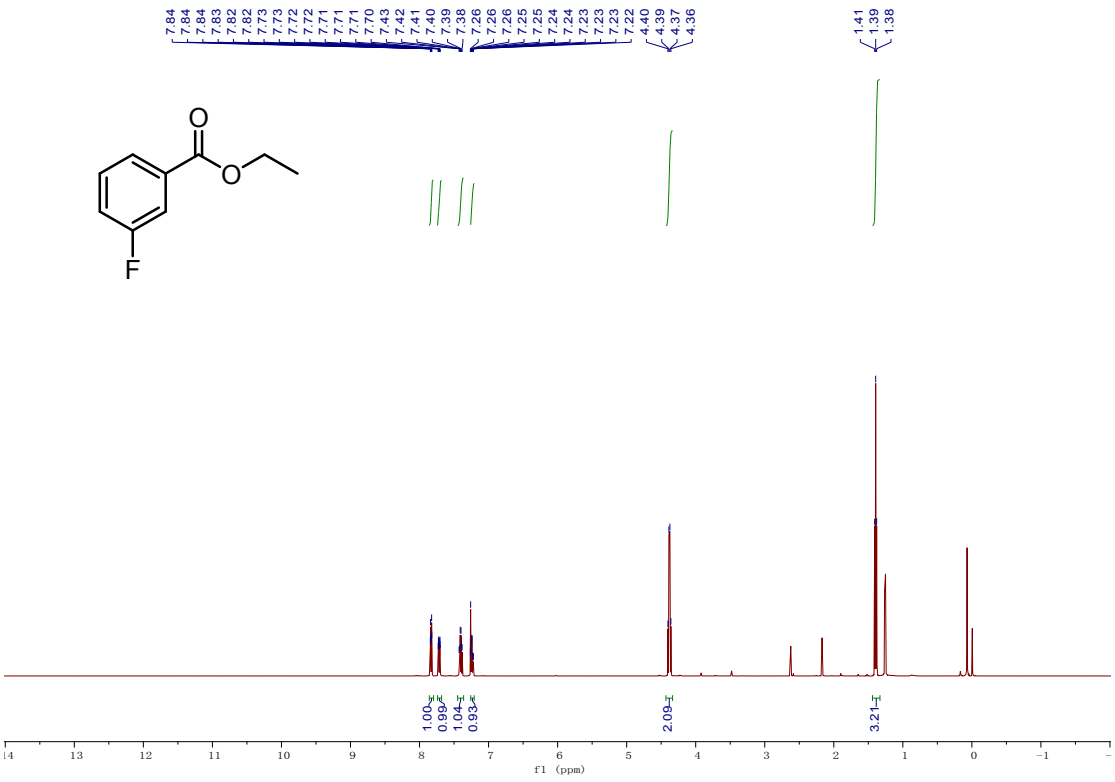
O
O
f1 (ppm)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7.40
7.39
7.38
7.26
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7.24
7.24
7.23
7.23
7.23
7.22
4.40
4.39
4.37
4.36
1.41
1.39
1.38
O
O
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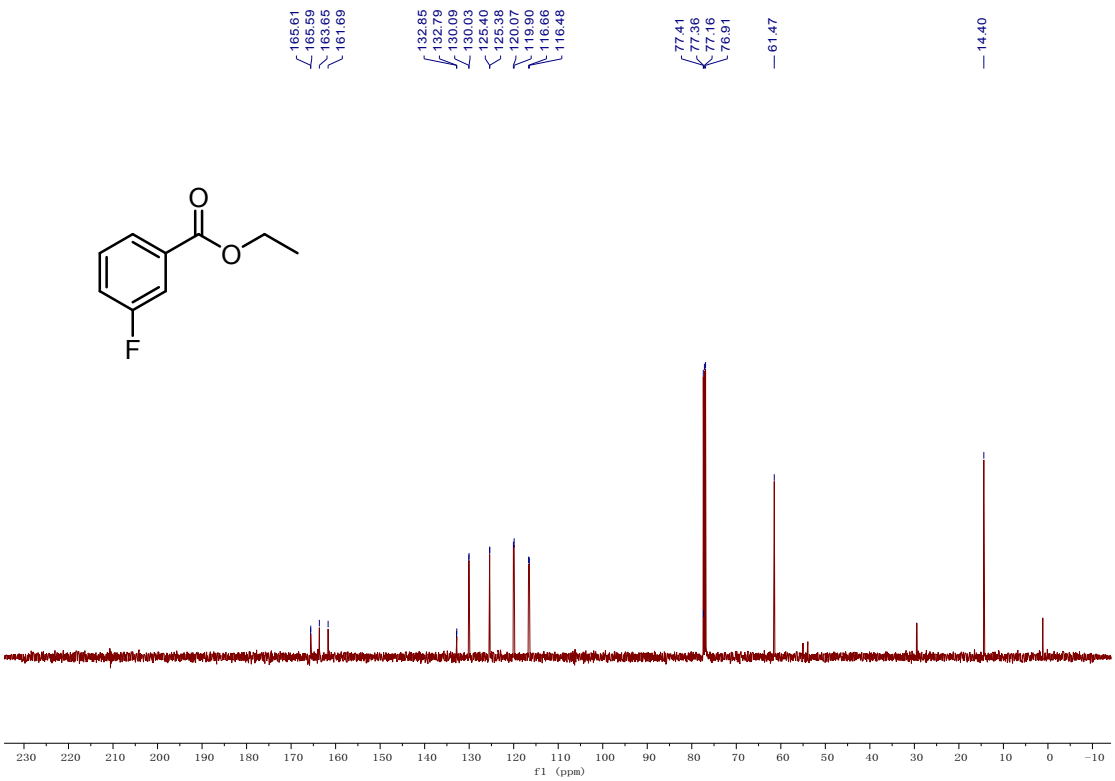
0.99
1.04
0.93
2.09
3.21
f1 (ppm)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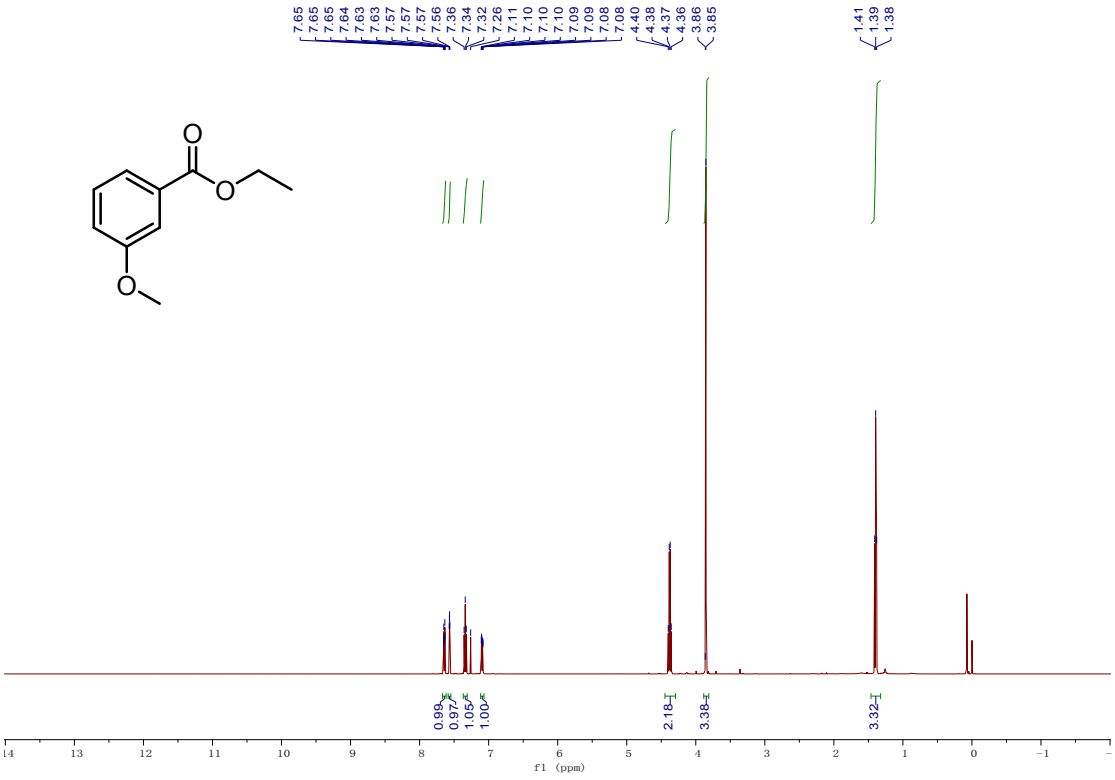
77.16
76.91
61.47
14.40
O
O
F
f1 (ppm)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7.10
7.09
7.09
7.08
7.08
4.40
4.38
4.37
4.36
3.86
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1.41
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1.38
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0.97
1.05
1.00
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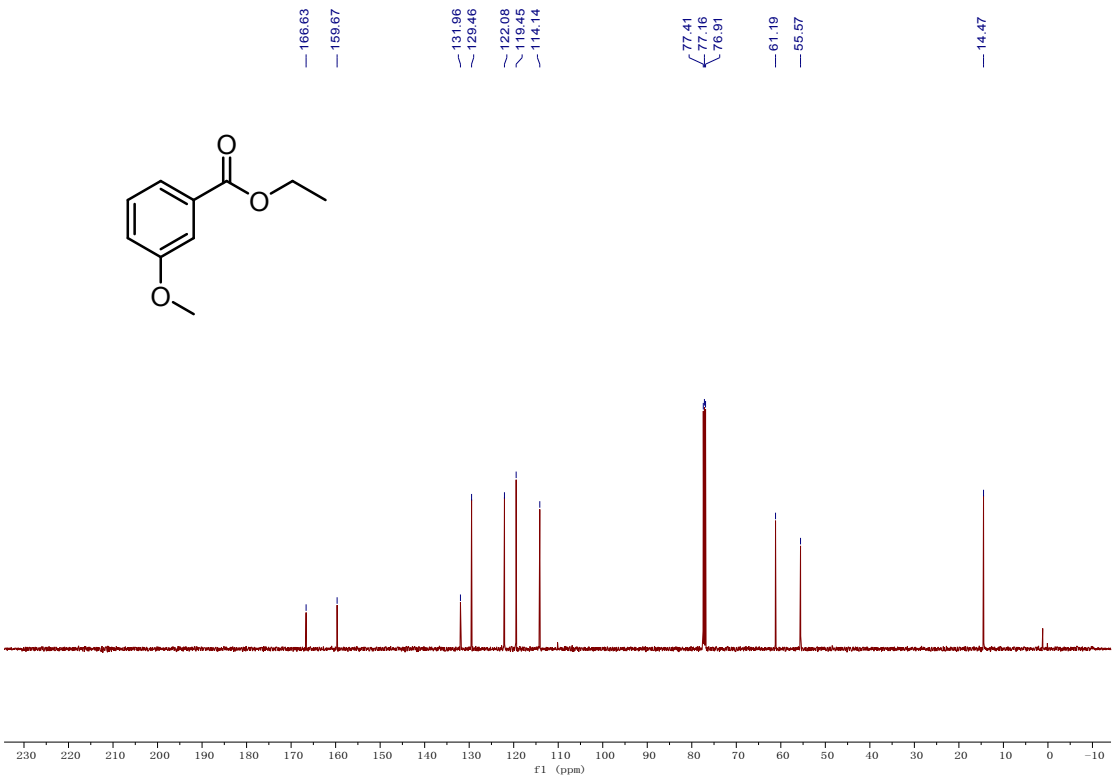
3.38
3.32
f1 (ppm)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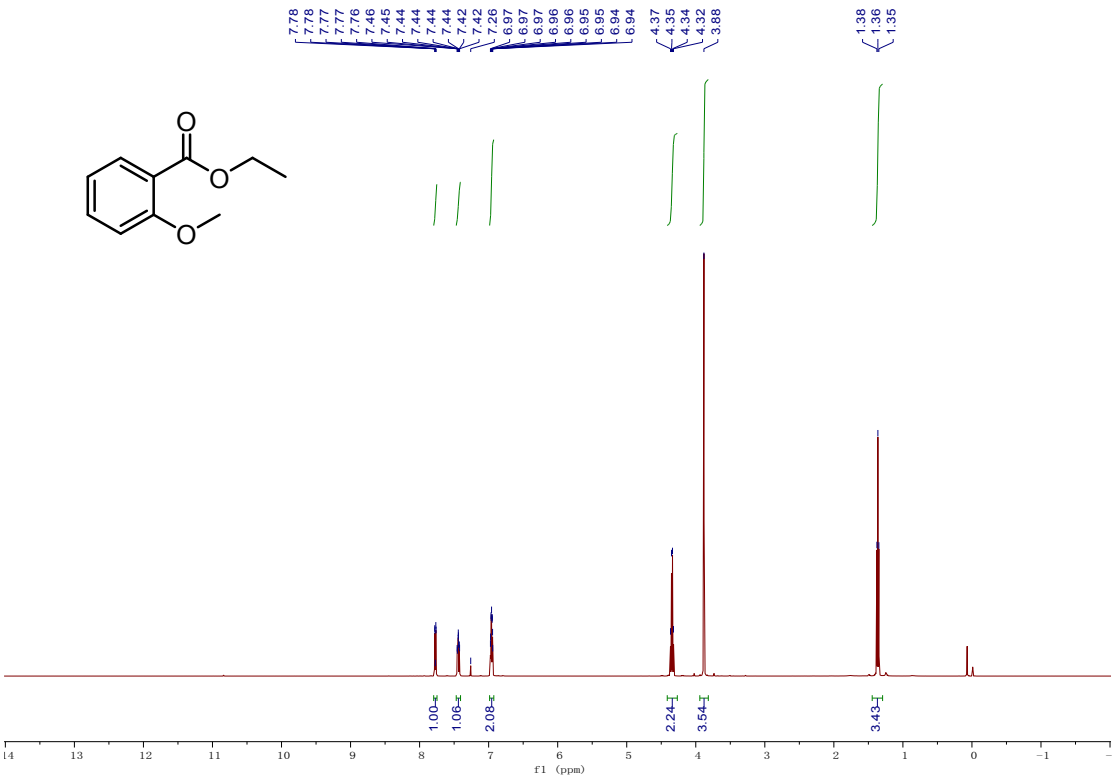
119.45
114.14
77.41
77.16
76.91
61.19
55.57
14.47
f1 (ppm)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7.26
6.97
6.97
6.96
6.96
6.95
6.95
6.94
6.94
4.37
4.35
4.34
4.32
3.88
1.38
1.36
1.35
O
O
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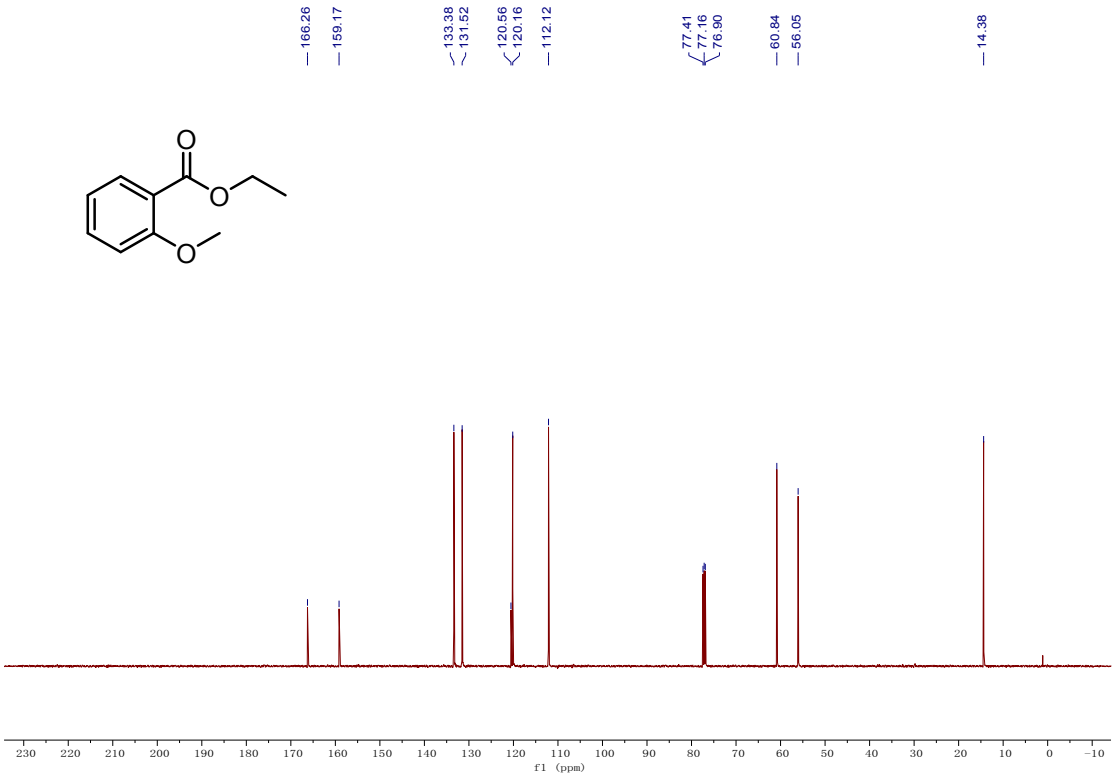
1.00
1.06
2.08
2.24
3.54
3.43
f1 (ppm)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133.38
131.52
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77.41
77.16
76.90
60.84
56.05
14.38
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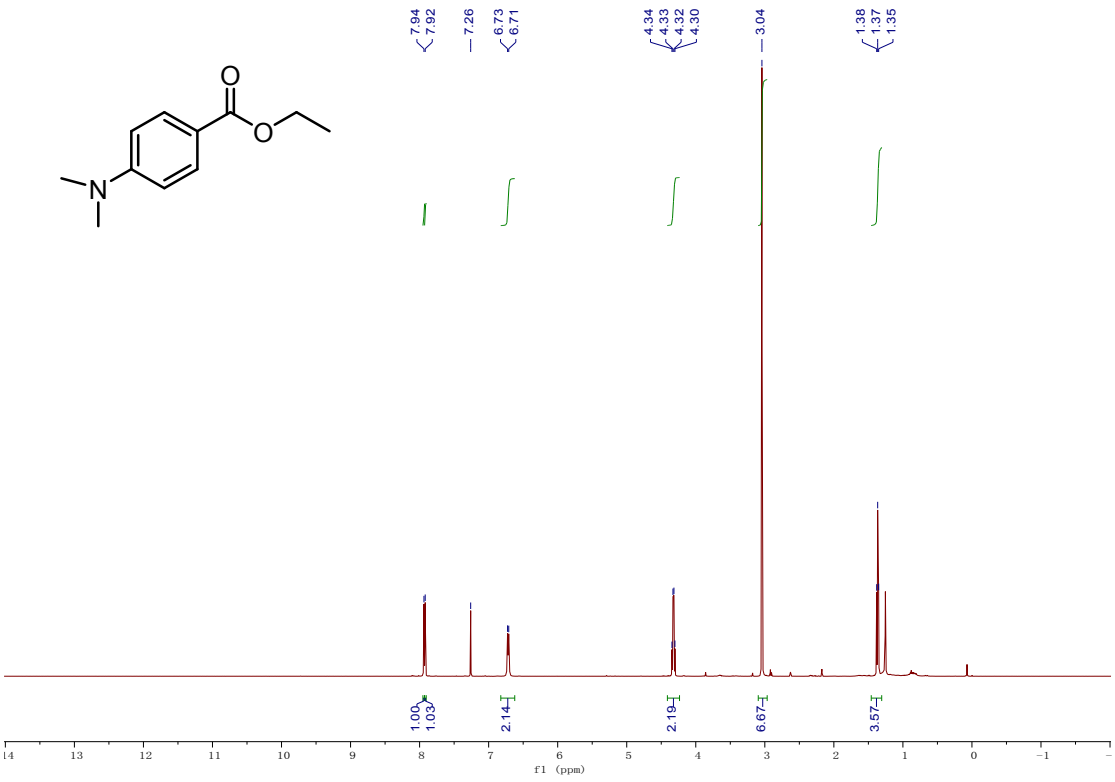
O
O
f1 (ppm)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4.34
4.33
4.32
4.30
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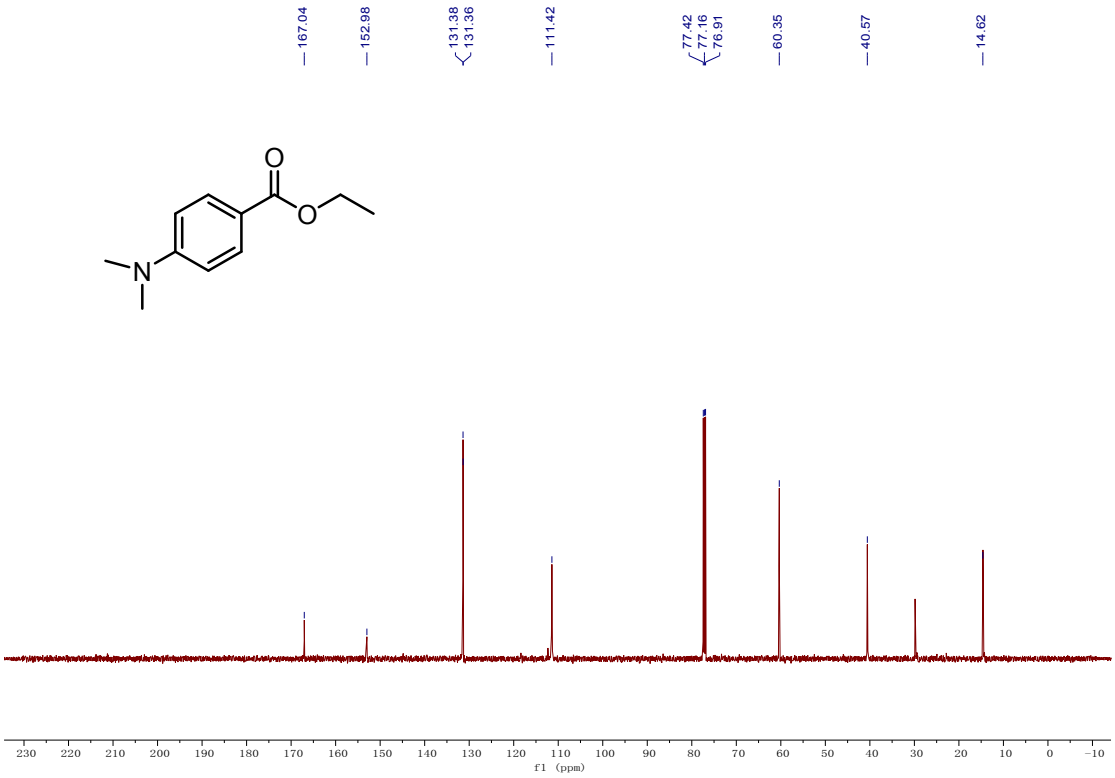
1.37
1.35
1.00
1.03
2.14
2.19
6.67
3.57
f1 (ppm)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76.91
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14.62
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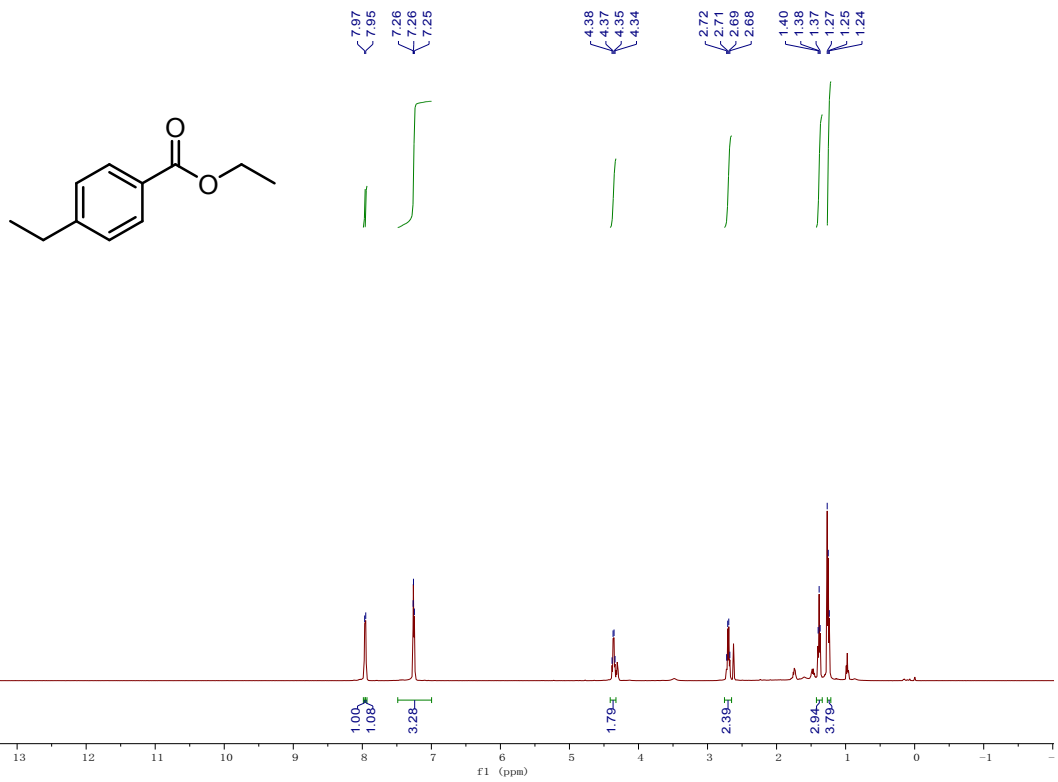
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4.38
4.37
4.35
4.34
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2.71
2.69
2.68
1.40
1.38
1.37
1.27
1.25
1.24
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O
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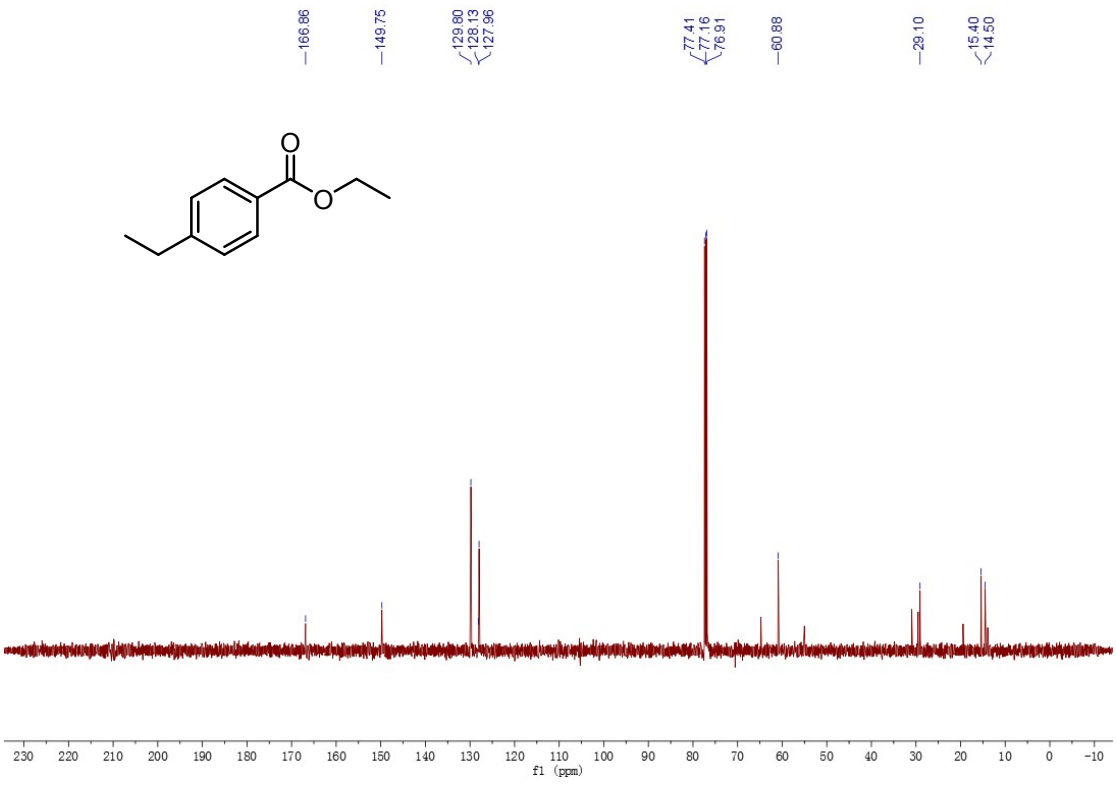
1.08
3.28
1.79
2.39
2.94
3.79
f1 (ppm)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76.91
60.88
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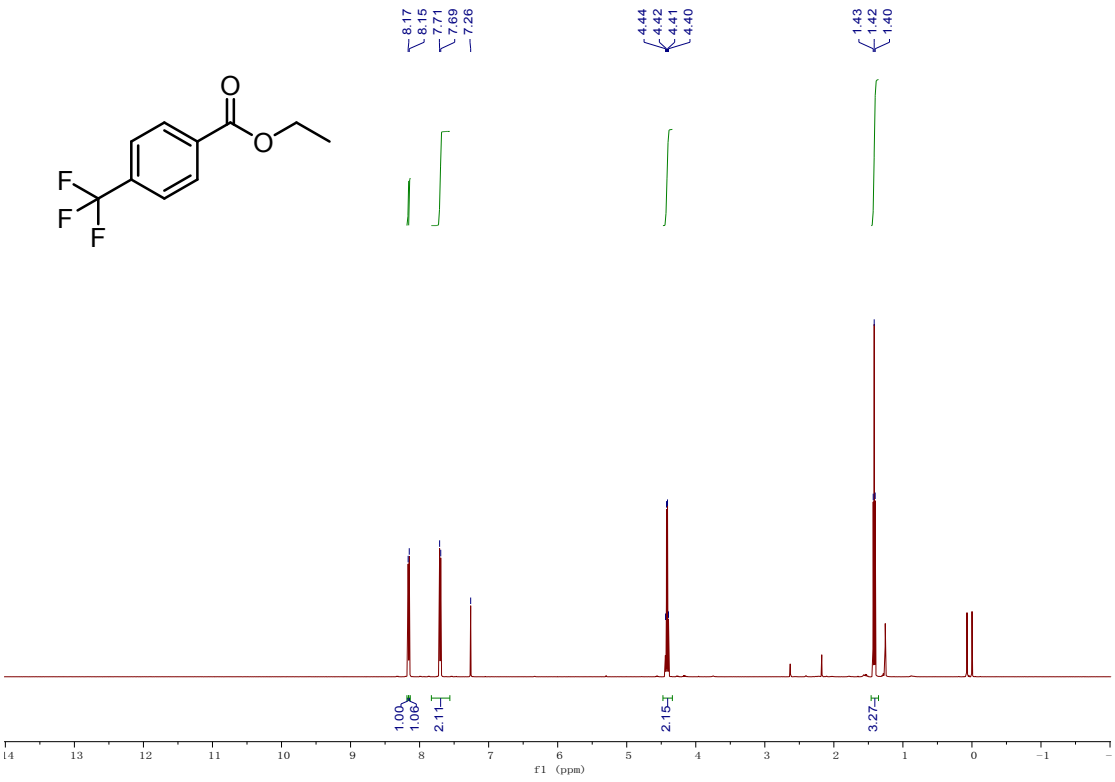
15.40
14.50
O
O
f1 (ppm)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4.41
4.40
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1.42
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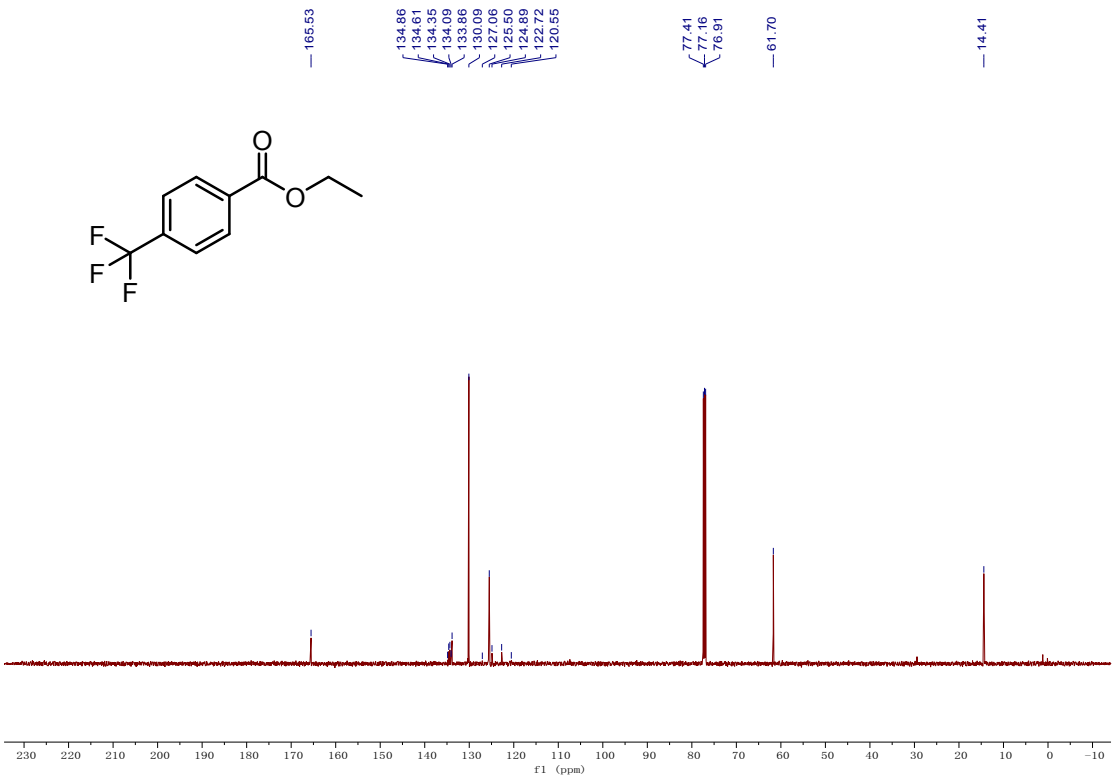
2.11
2.15
3.27
f1 (ppm)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134.09
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130.09
127.06
125.50
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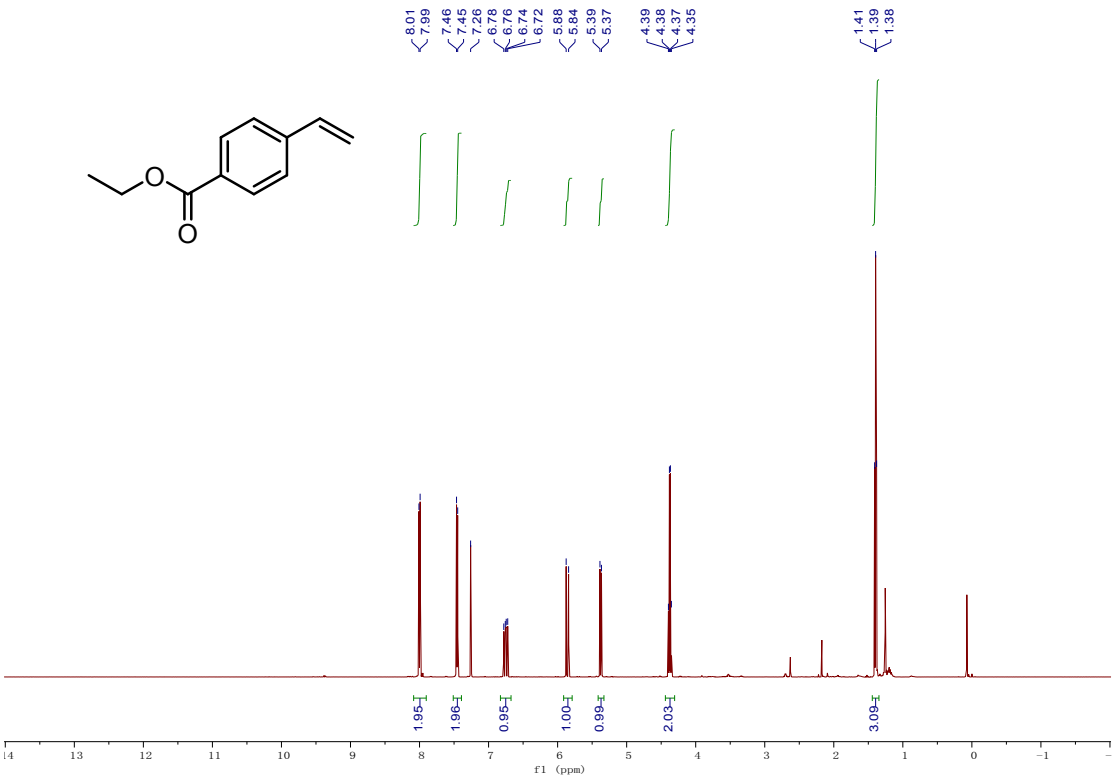
77.41
77.16
76.91
61.70
14.41
O
O
F
F
F
f1 (ppm)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5.84
5.39
5.37
4.39
4.38
4.37
4.35
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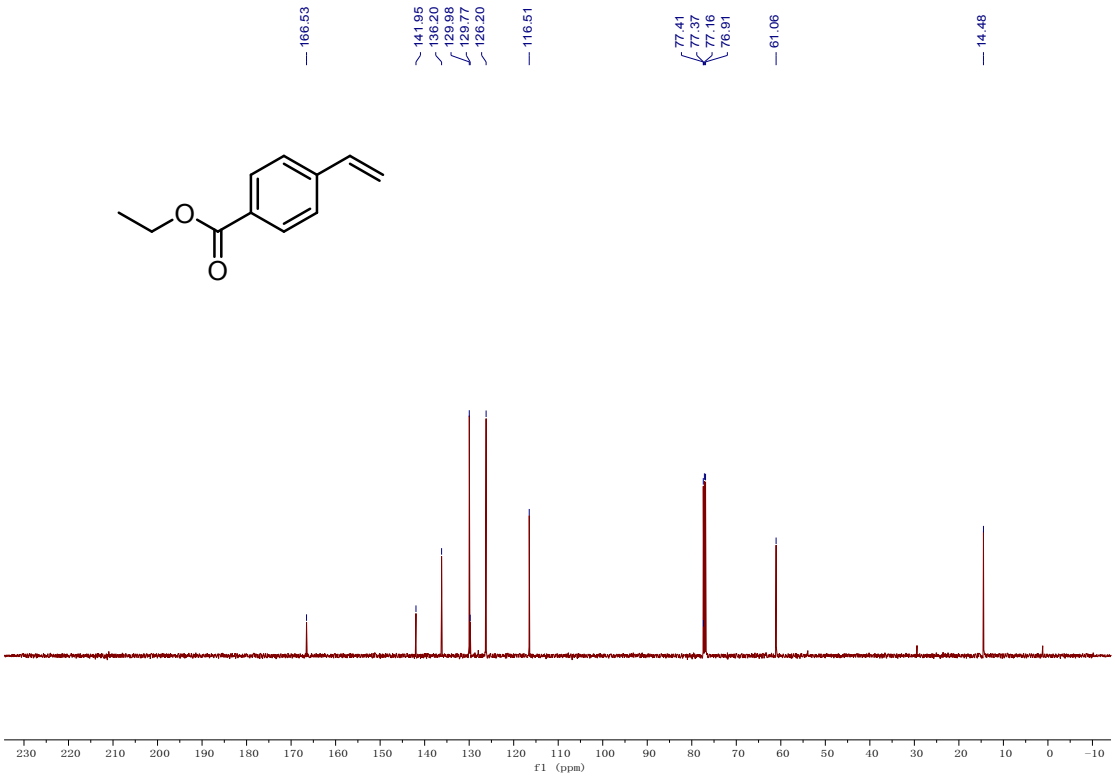
1.38
1.95
1.96
0.95
1.00
0.99
2.03
3.09
f1 (ppm)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77.41
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76.91
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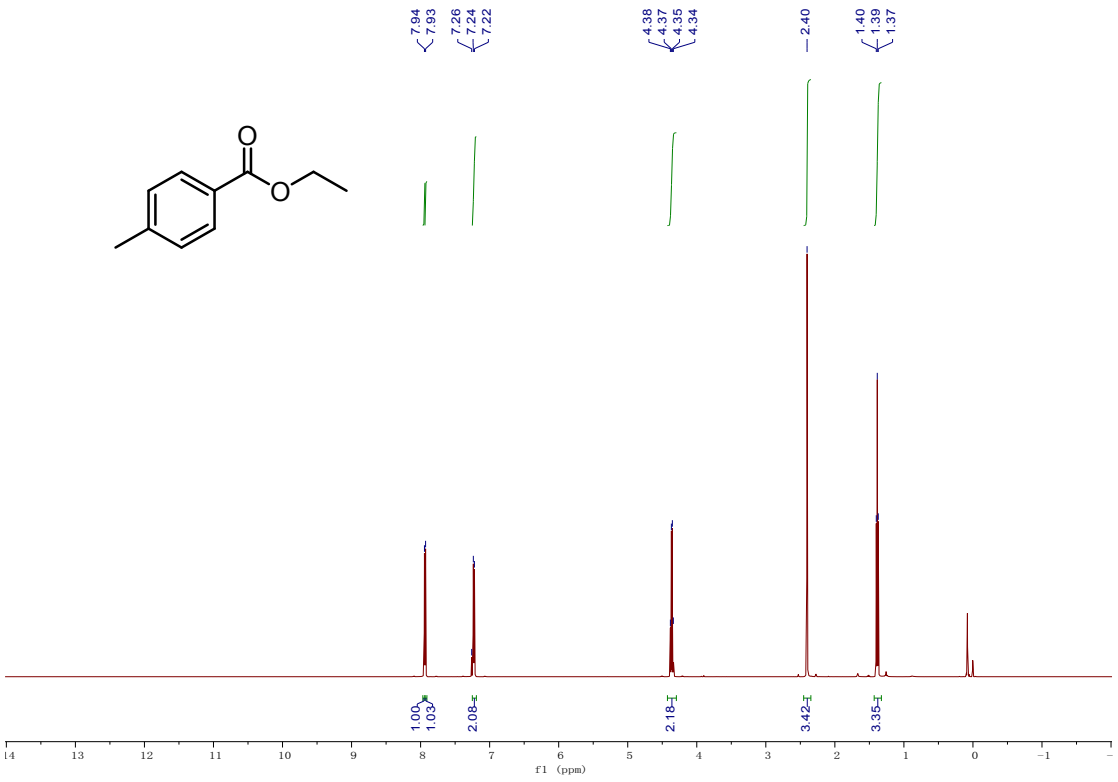
14.48
f1 (ppm)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4.37
4.35
4.34
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1.39
1.37
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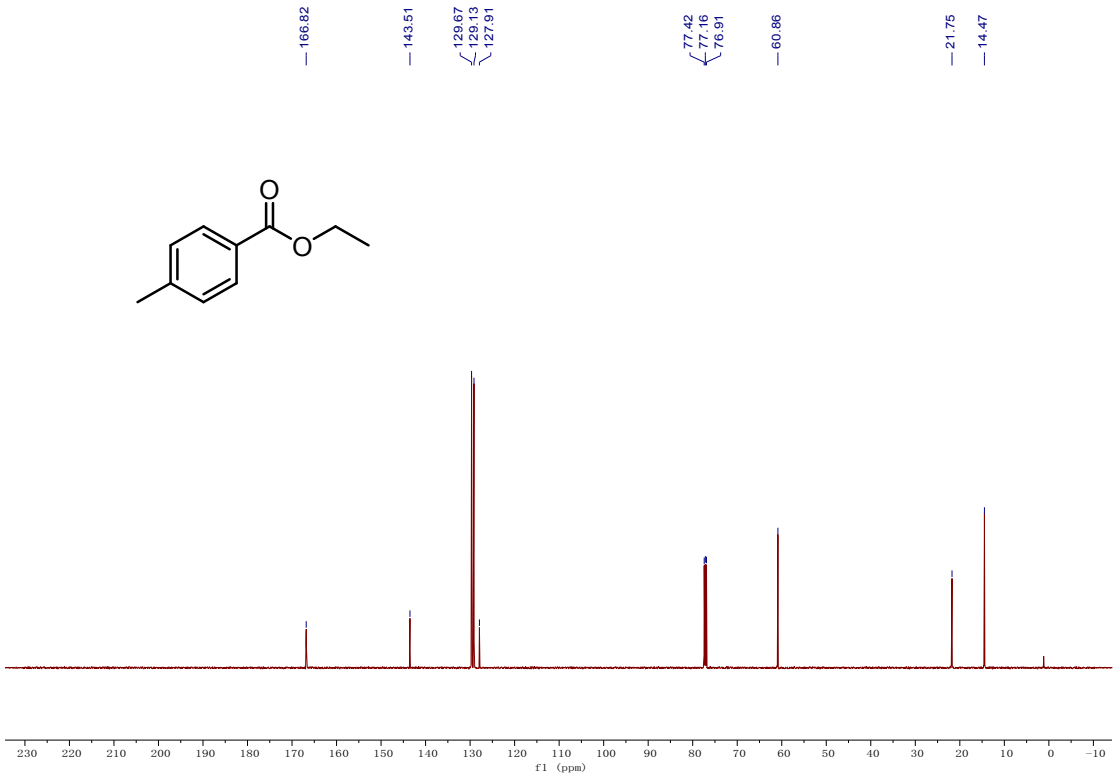
1.03
2.08
2.18
3.42
3.35
f1 (ppm)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76.91
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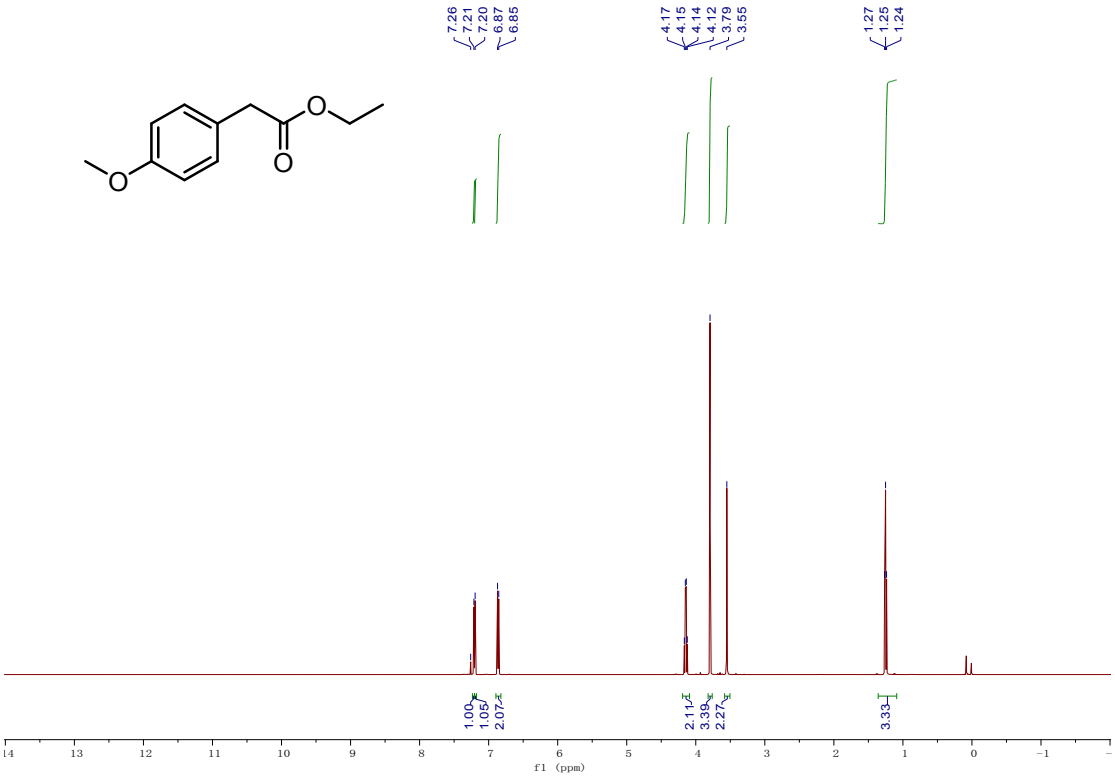
14.47
f1 (ppm)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4.17
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4.14
4.12
3.79
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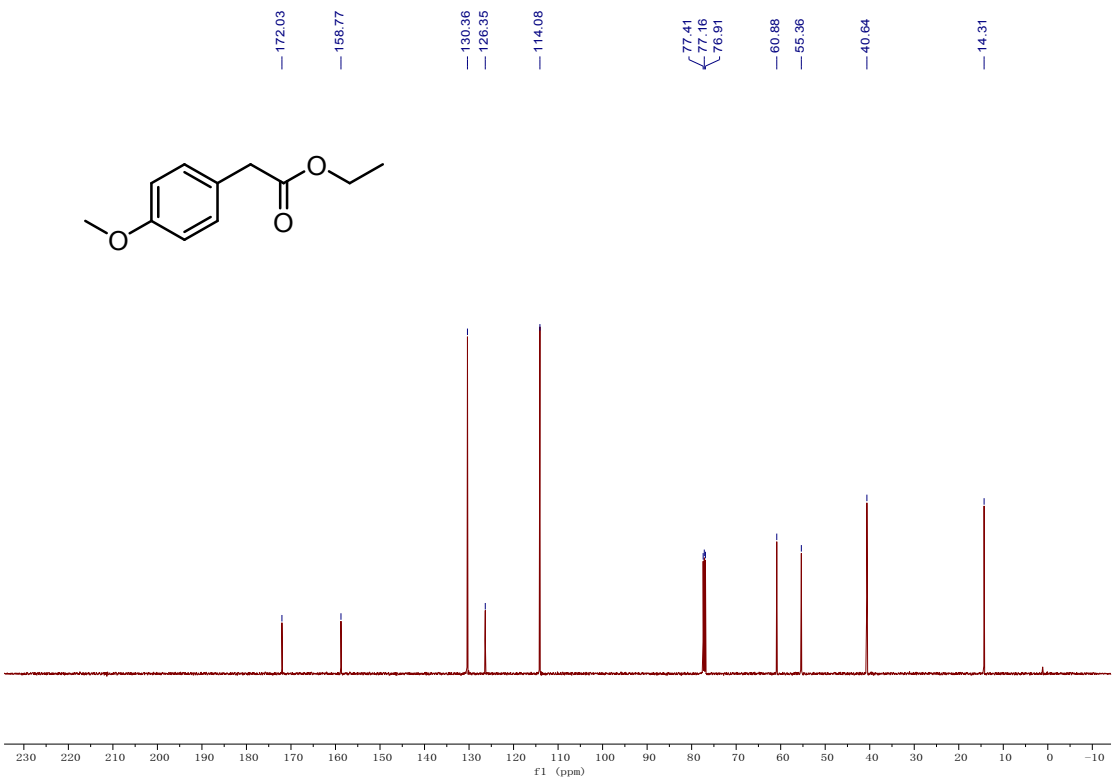
1.24
1.00
1.05
2.07
2.11
3.39
2.27
3.33
f1 (ppm)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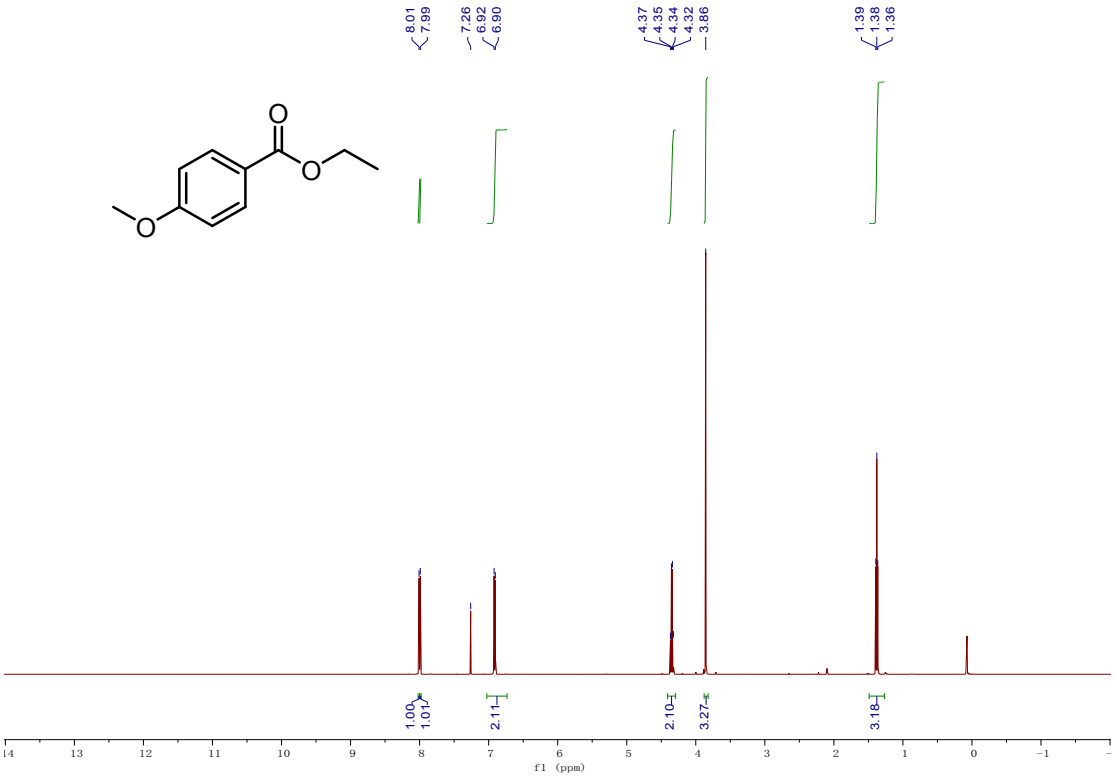
14.31
f1 (ppm)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4.35
4.34
4.32
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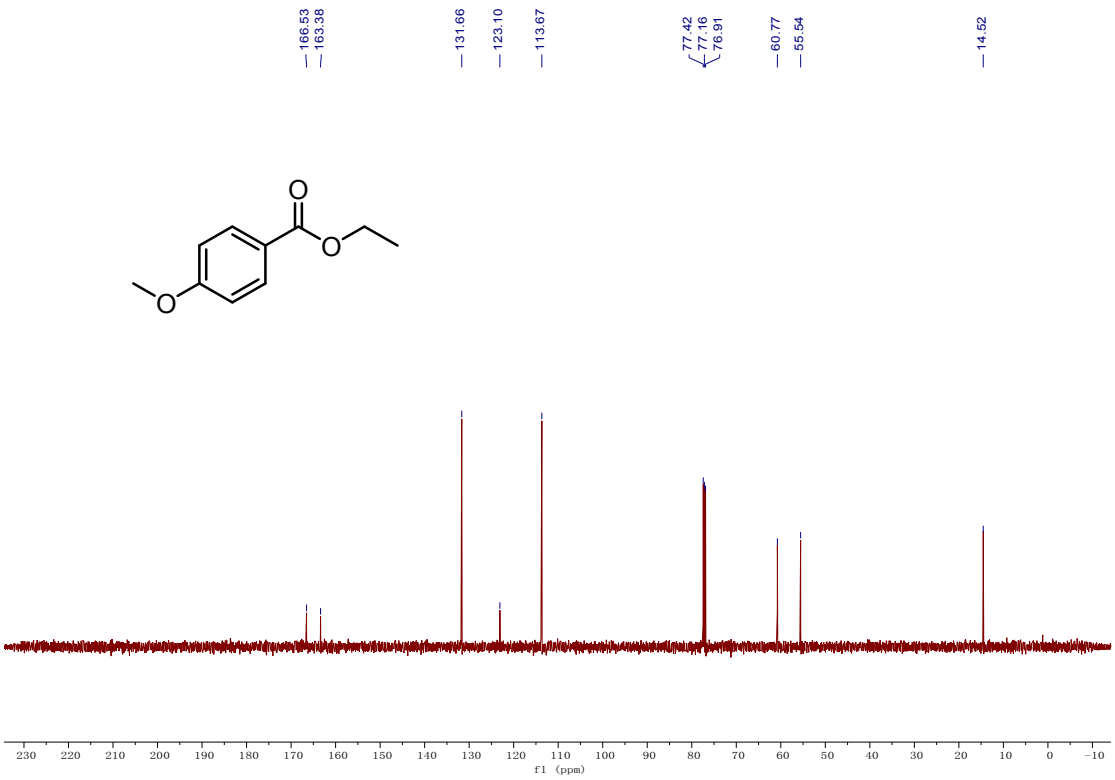
1.38
1.36
1.00
1.01
2.11
2.10
3.27
3.18
f1 (ppm)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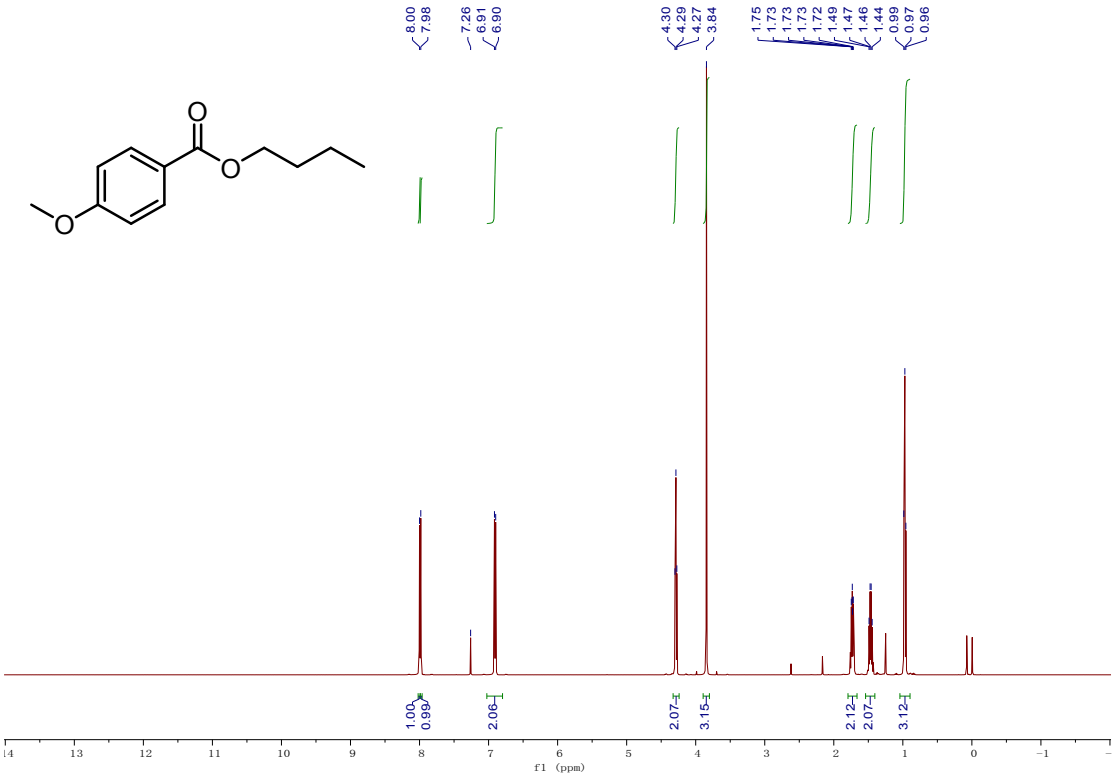
77.16
76.91
60.77
55.54
14.52
f1 (ppm)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1.73
1.73
1.72
1.49
1.47
1.46
1.44
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0.97
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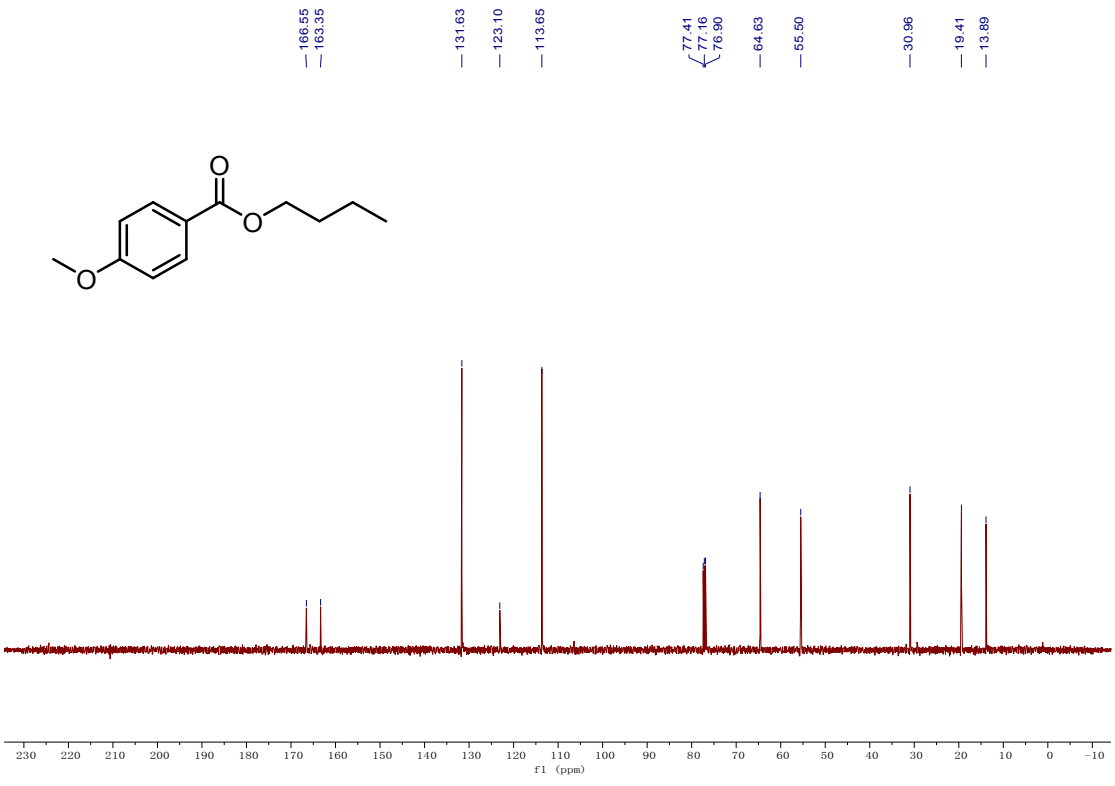
1.00
0.99
2.06
2.07
3.15
2.12
2.07
3.12
f1 (ppm)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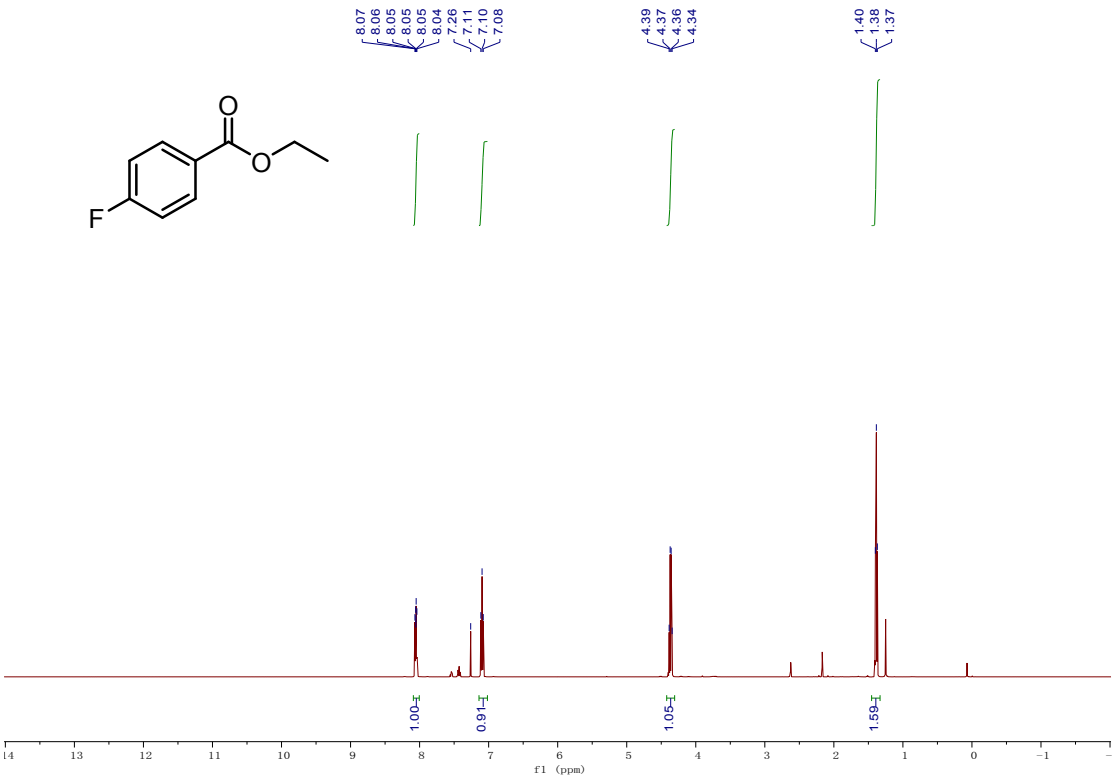
30.96
19.41
13.89
f1 (ppm)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7.08
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1.38
1.37
O
O
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0.91
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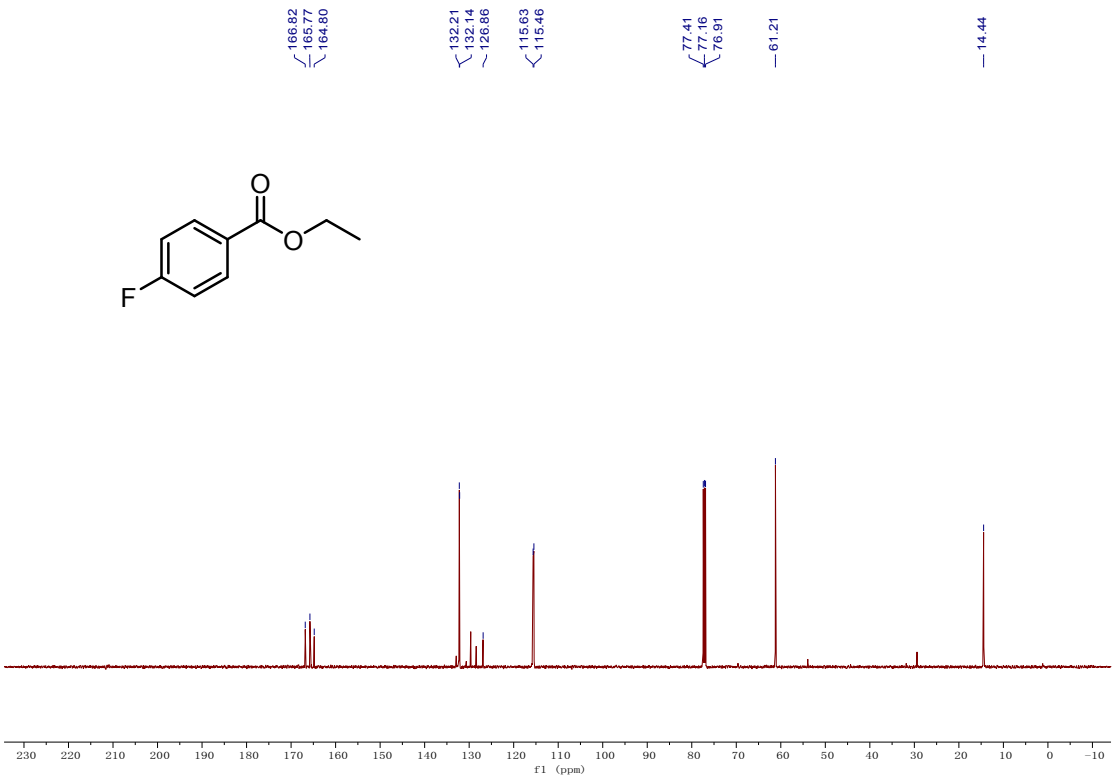
1.59
f1 (ppm)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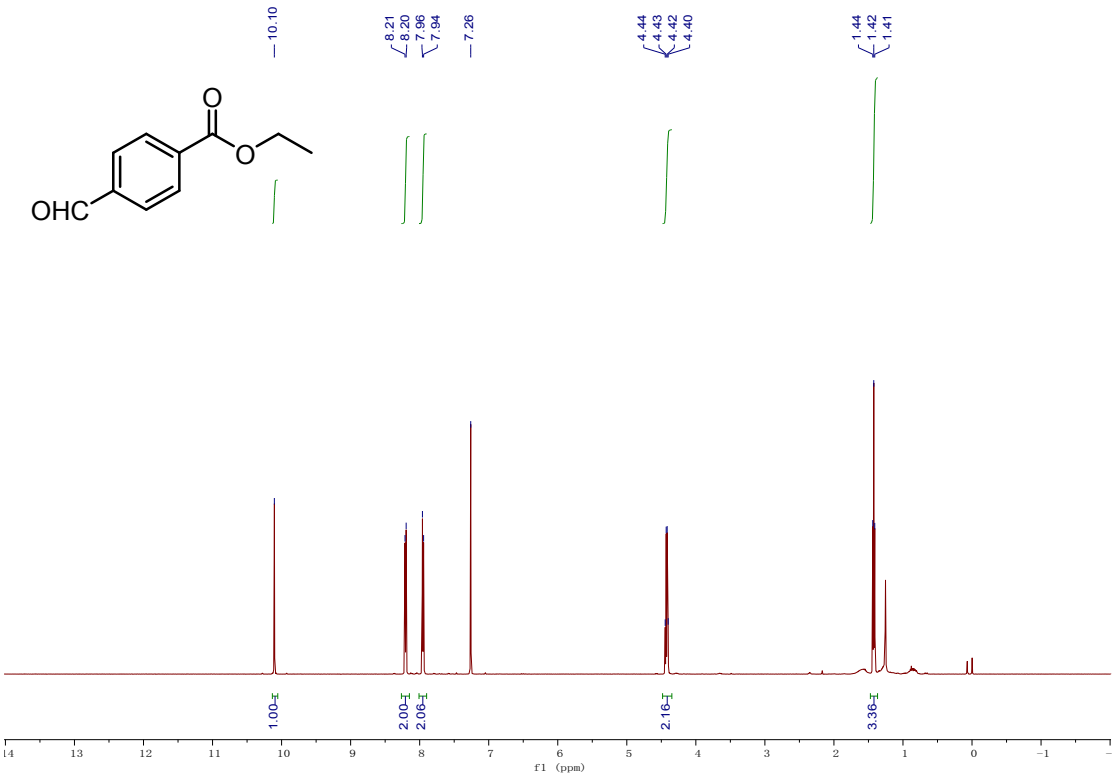
77.16
76.91
61.21
14.44
O
O
F
f1 (ppm)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4.42
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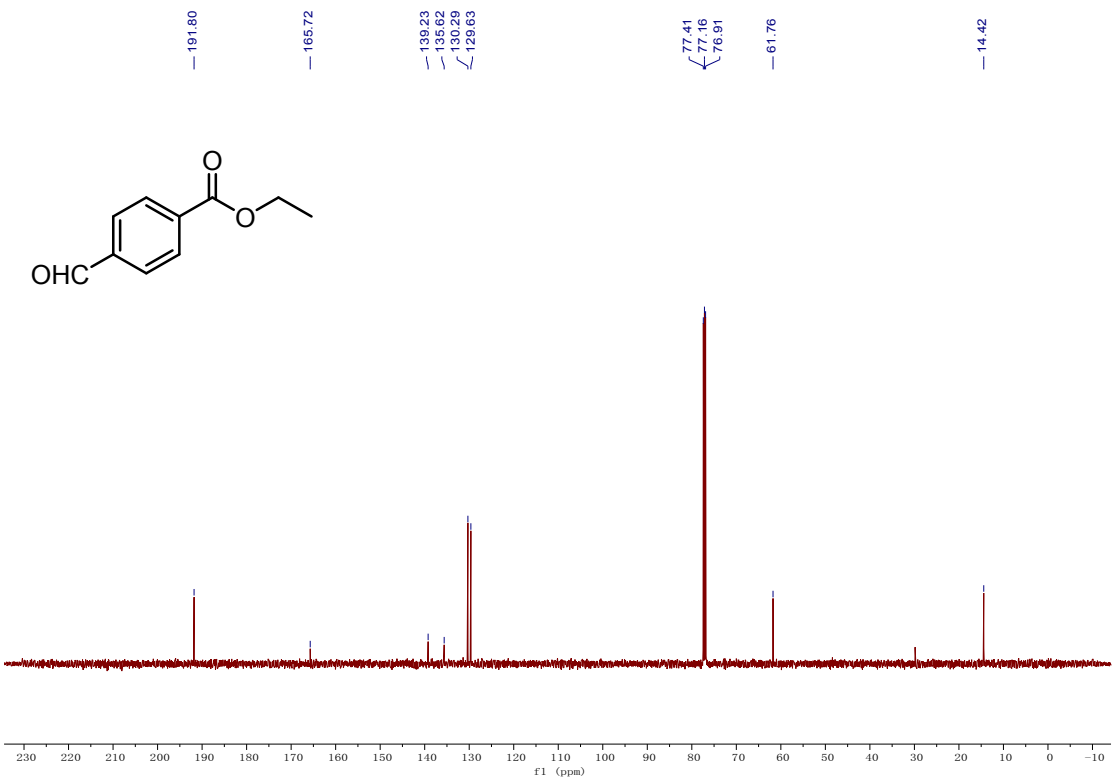
1.41
O
O
OHC
1.00
2.00
2.06
2.16
3.36
f1 (ppm)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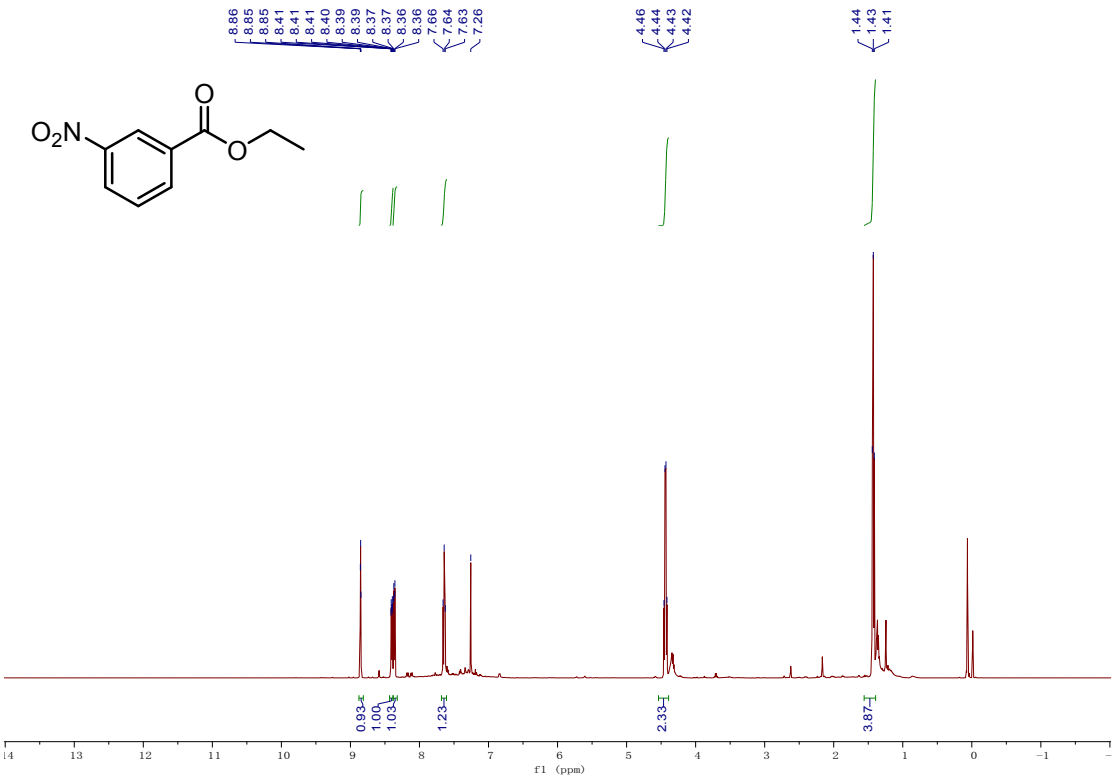
76.91
61.76
14.42
O
O
OHC
f1 (ppm)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7.66
7.64
7.63
7.26
4.46
4.44
4.43
4.42
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O2N
O
O
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1.23
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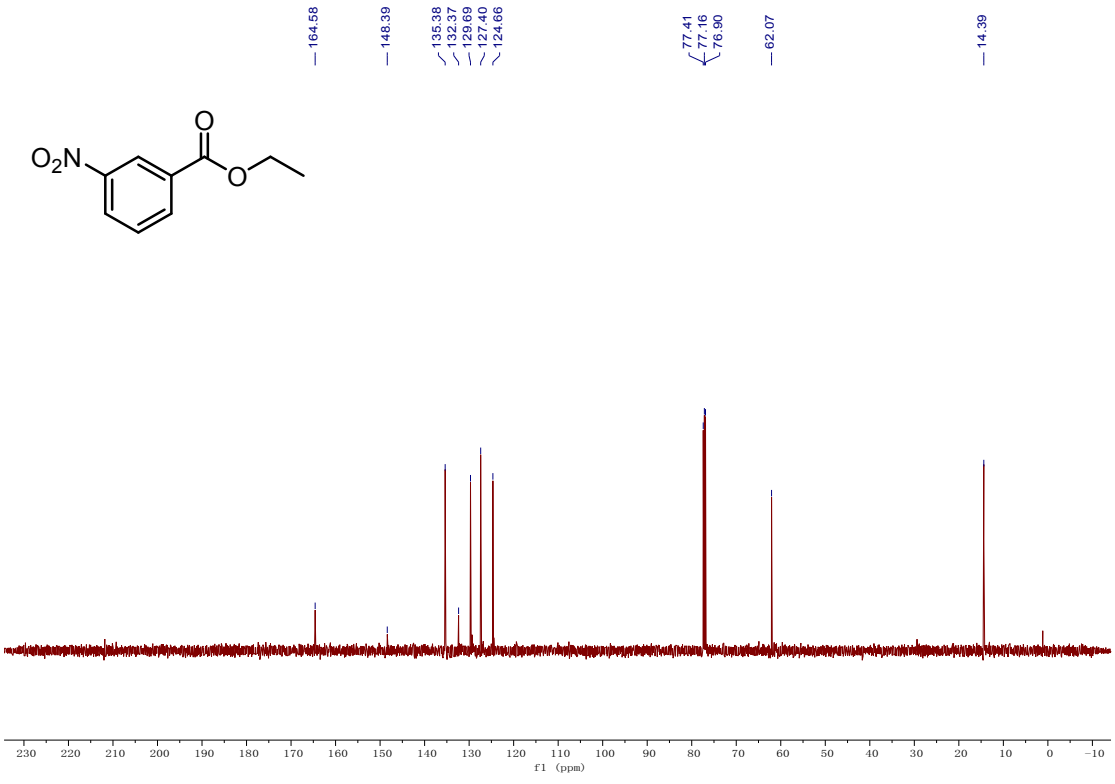
3.87
f1 (ppm)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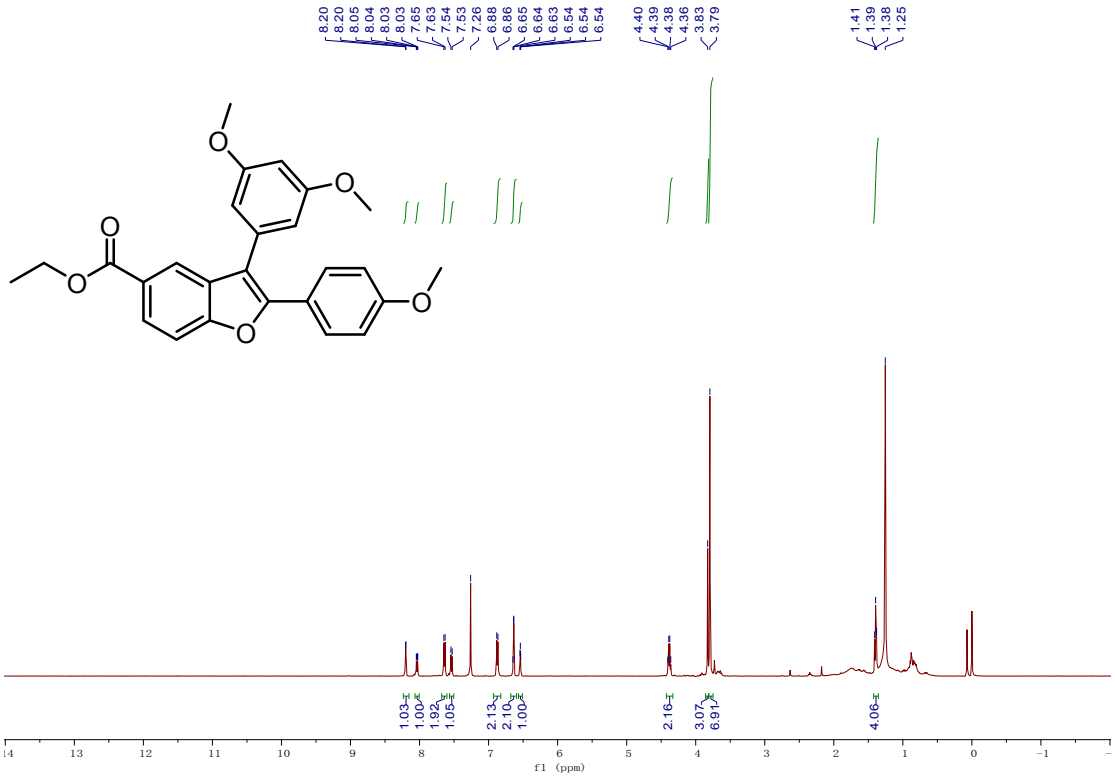
76.90
62.07
14.39
O2N
O
O
f1 (ppm)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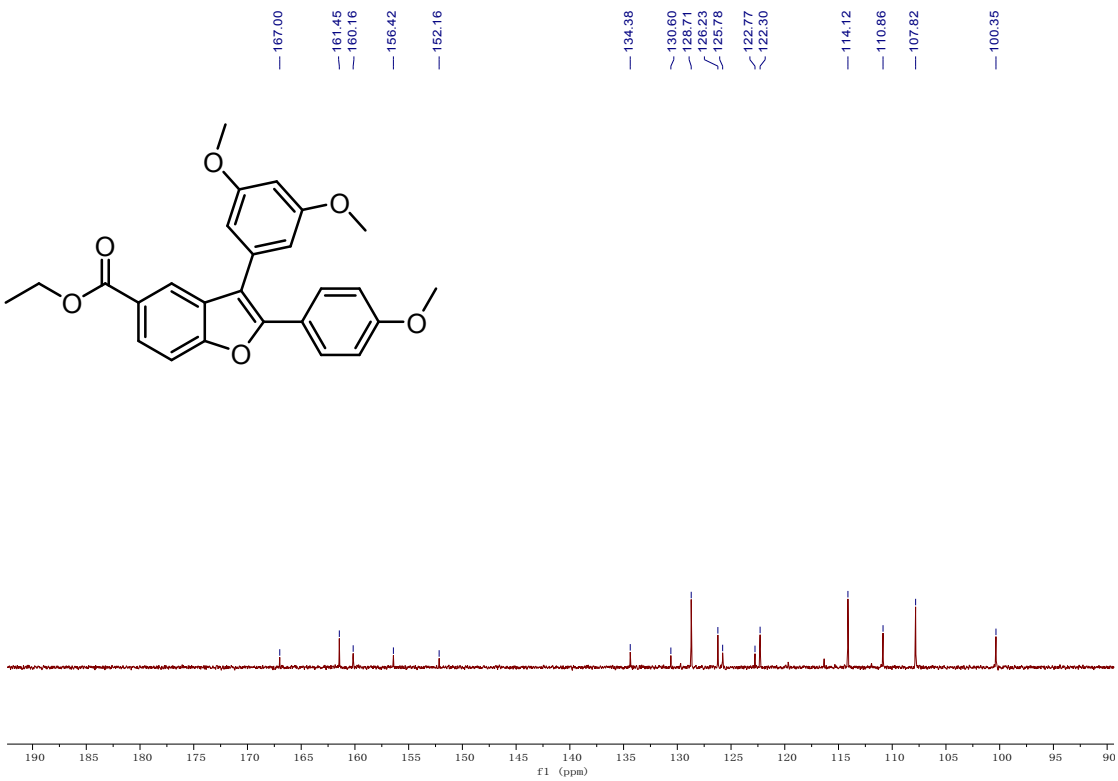
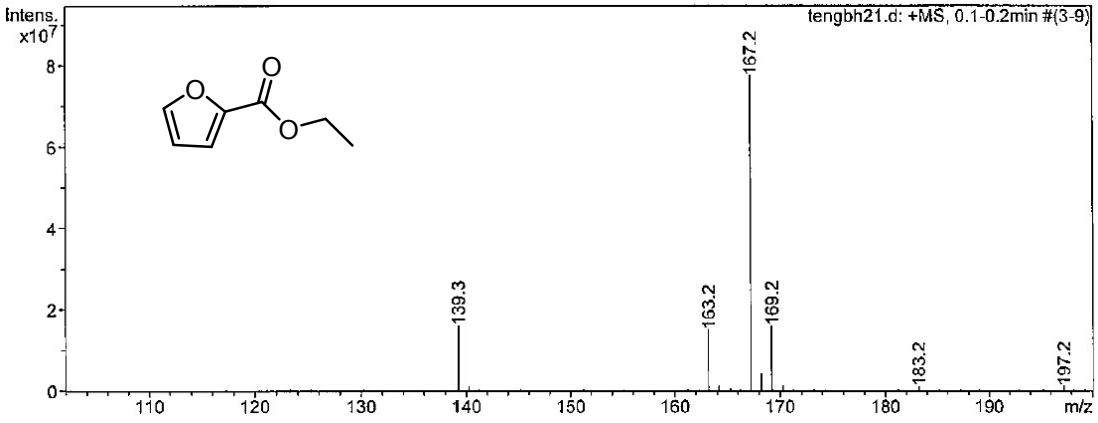
1.39
1.38
1.25
1.03
1.00
1.92
1.05
2.13
2.10
1.00
2.16
3.07
6.91
4.06
f1 (ppm)


167.00
161.45
160.16
156.42
152.16
134.38
130.60
128.71
126.23
125.78
122.77
122.30
114.12
110.86
107.82
100.35
f1 (ppm)

6. ESI MS spectra

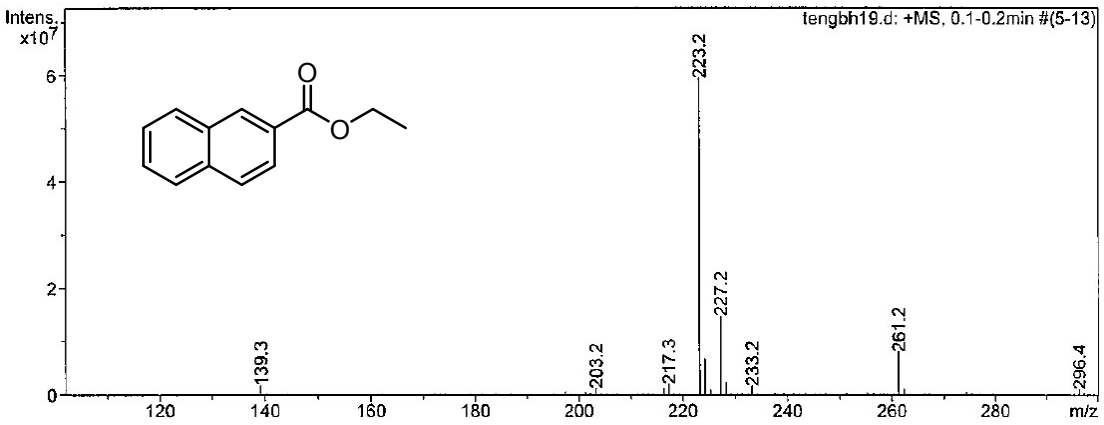
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh21.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:09:24 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:08:05 AM
Sample Name: E56
Analysis Info:



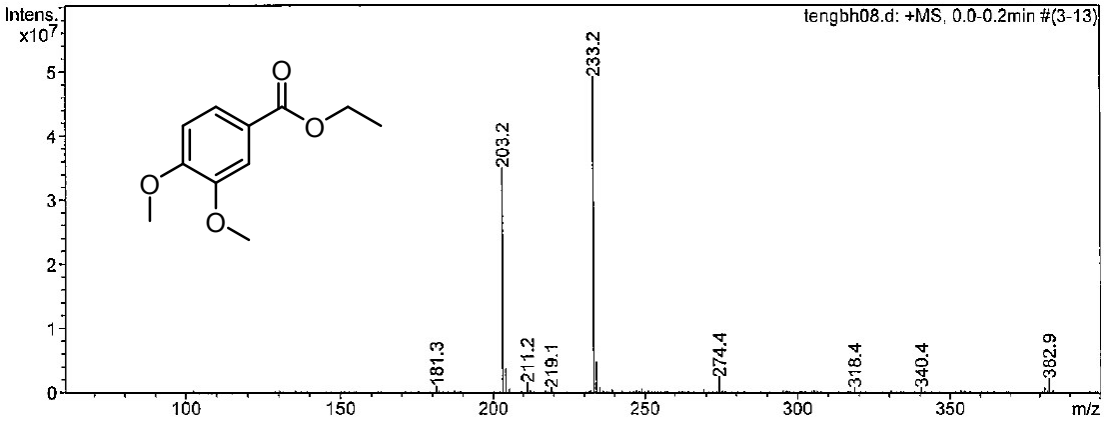
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh19.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:10:23 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:57:18 AM
Sample Name: E54
Analysis Info:



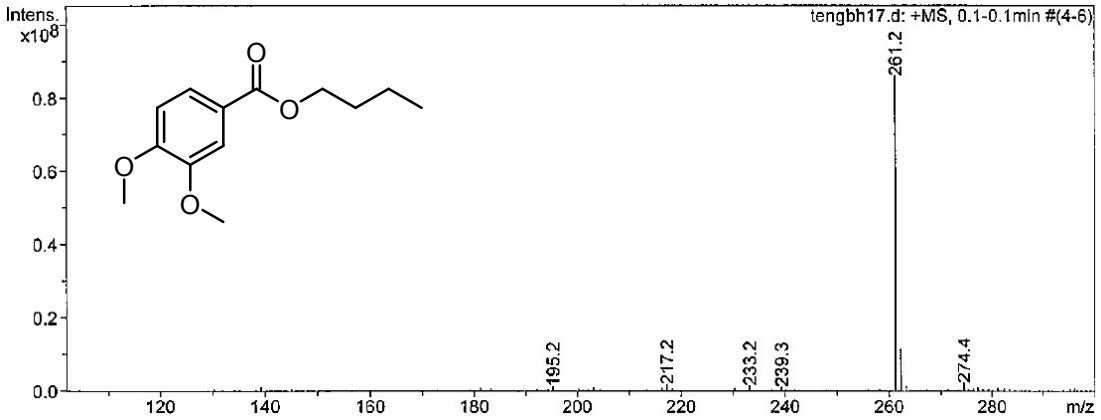
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh08.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:39:51 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:10:55 AM
Sample Name: E28
Analysis Info:



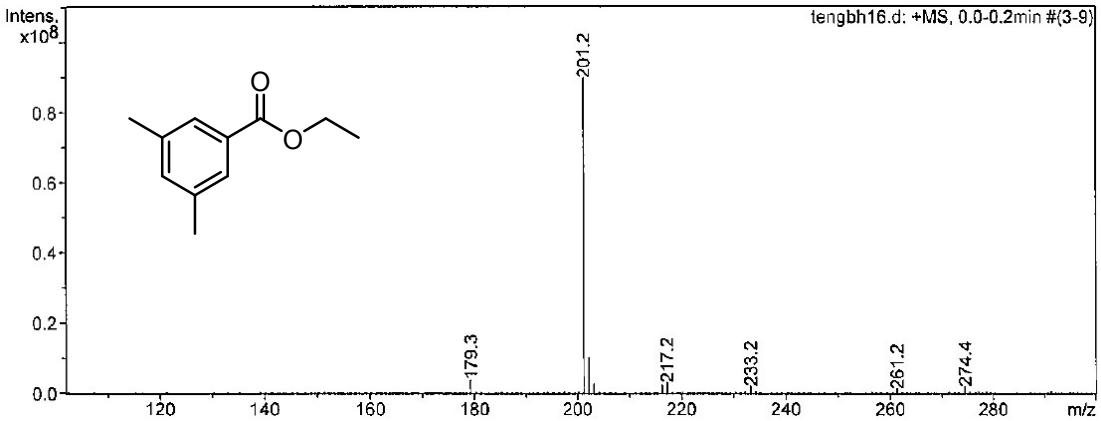
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh17.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:55:35 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:49:49 AM
Sample Name: E48
Analysis Info:



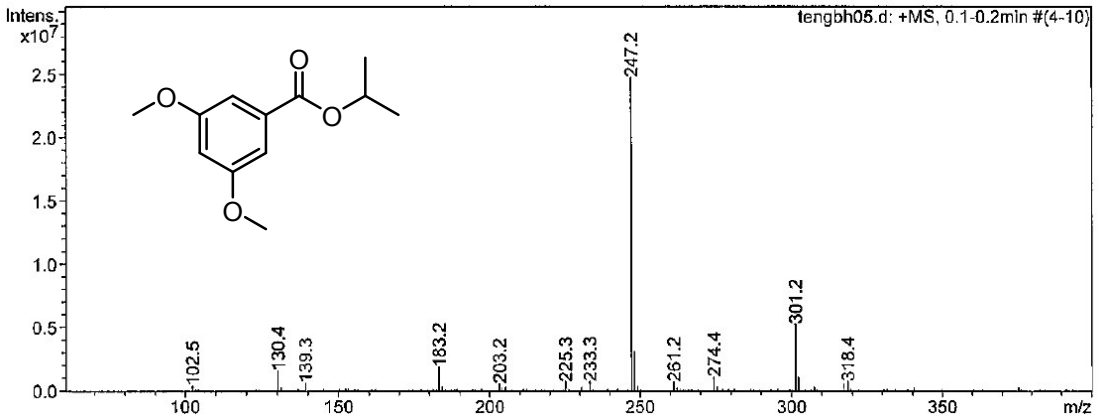
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh16.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:52:10 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:46:09 AM
Sample Name: E37
Analysis Info:



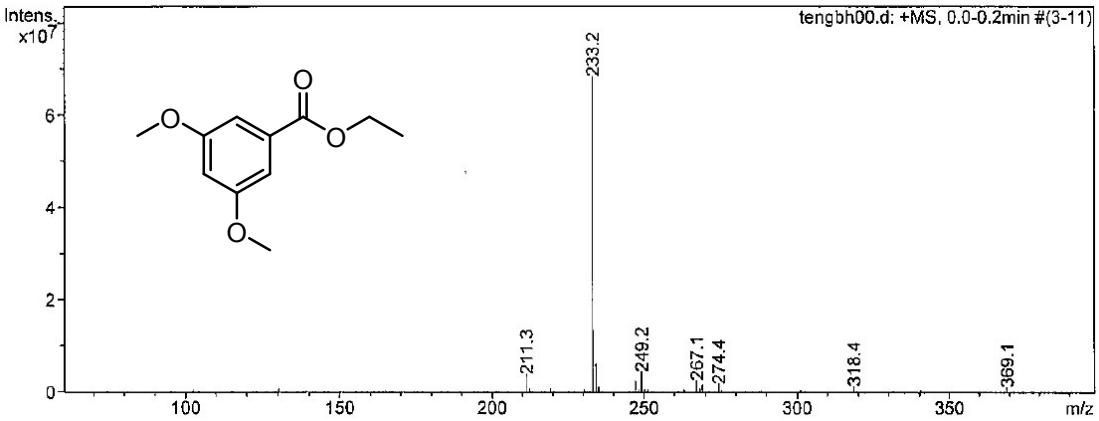
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh05.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:03:53 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 9:58:01 AM
Sample Name: E20
Analysis Info:



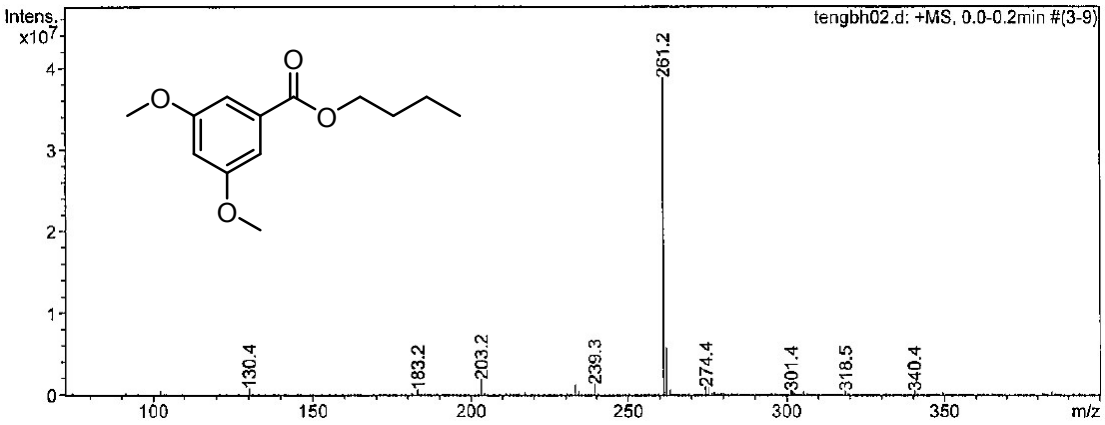
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh00.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 9:48:48 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 9:32:45 AM
Sample Name: E7
Analysis Info:



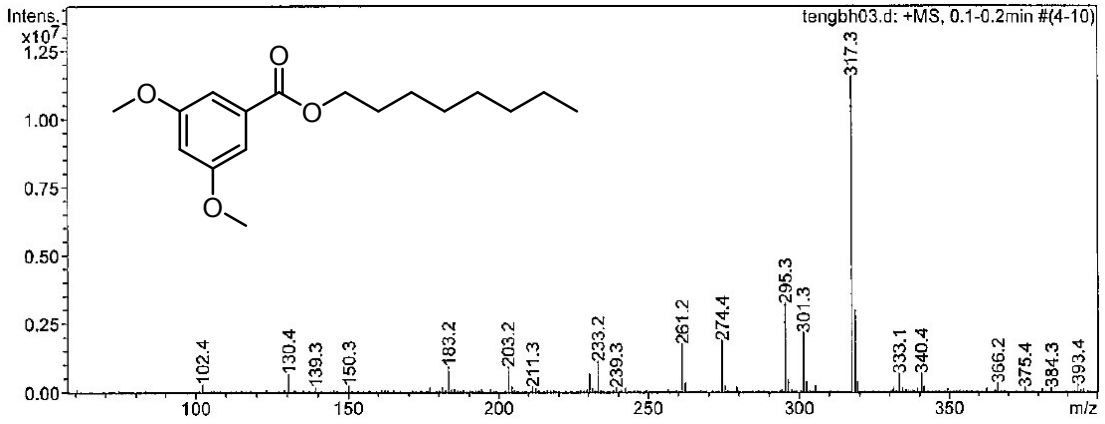
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh02.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 9:52:55 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 9:45:52 AM
Sample Name: E17
Analysis Info:



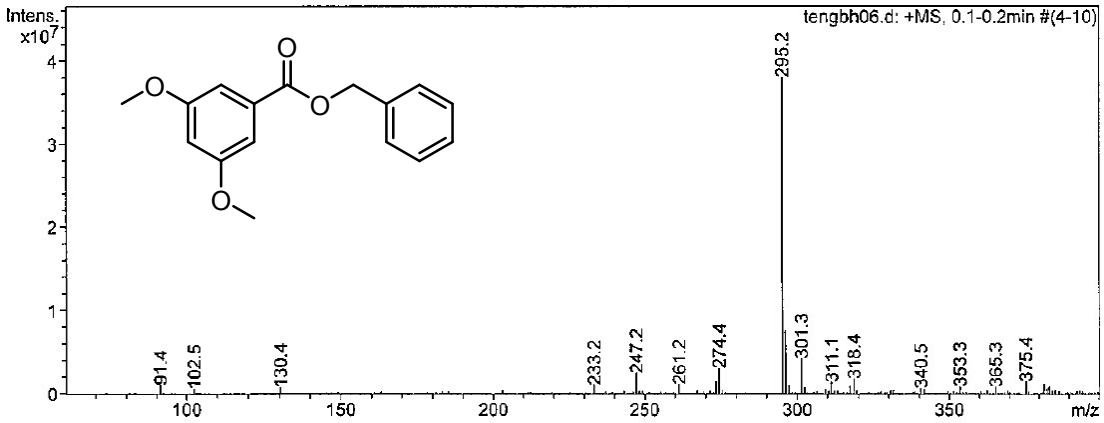
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh03.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:00:20 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 9:49:50 AM
Sample Name: E18
Analysis Info:



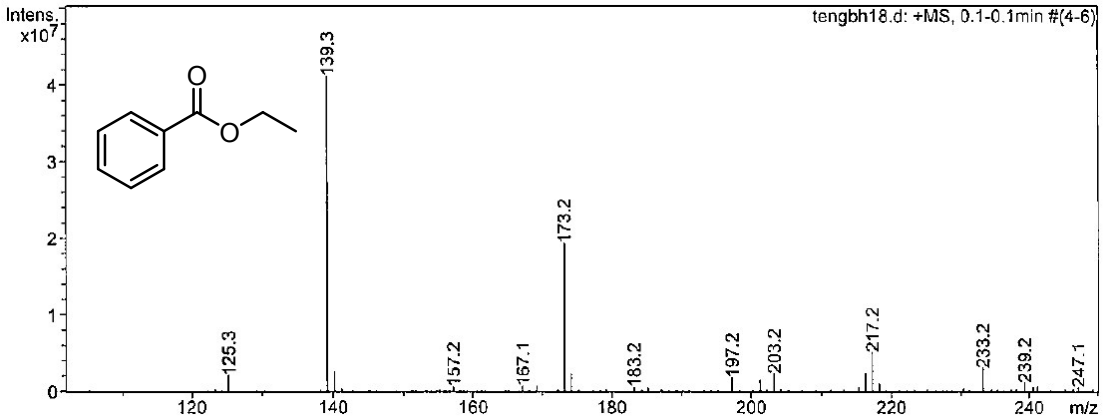
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh06.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:25:06 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:01:58 AM
Sample Name: E22
Analysis Info:



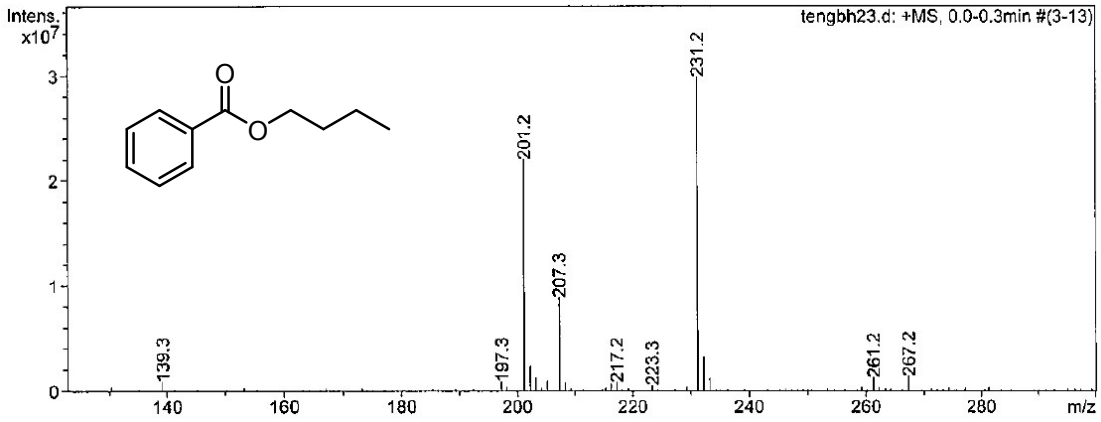
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh18.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:55:52 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:53:22 AM
Sample Name: E49
Analysis Info:



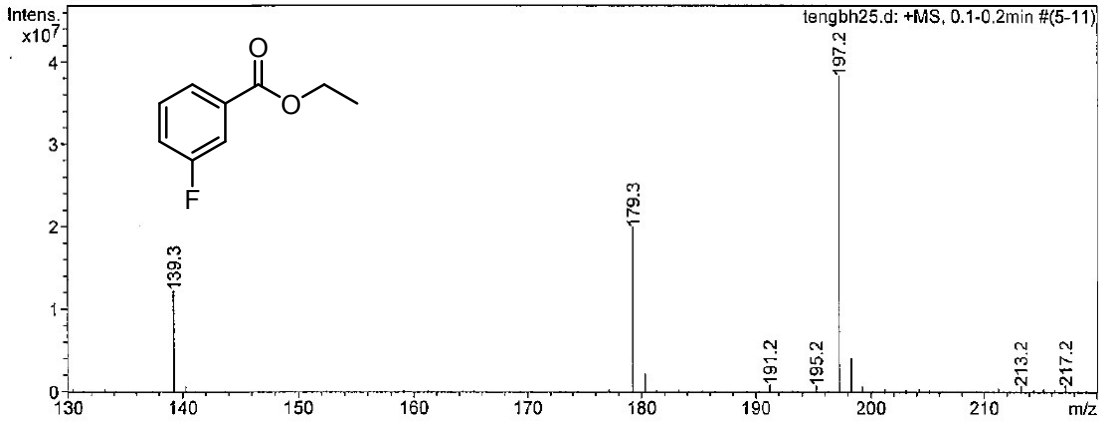
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh23.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:41:57 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:16:27 AM
Sample Name: E58
Analysis Info:



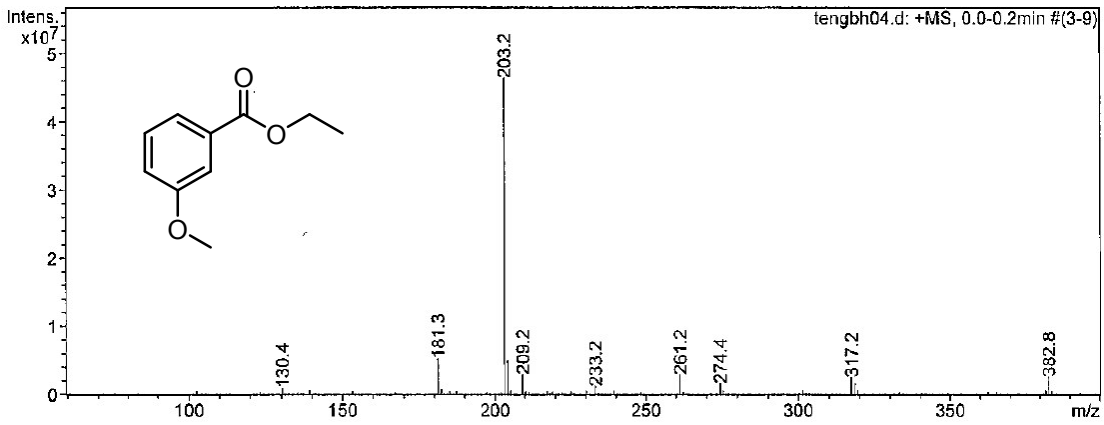
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh25.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:27:40 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:25:21 AM
Sample Name: E66
Analysis Info:



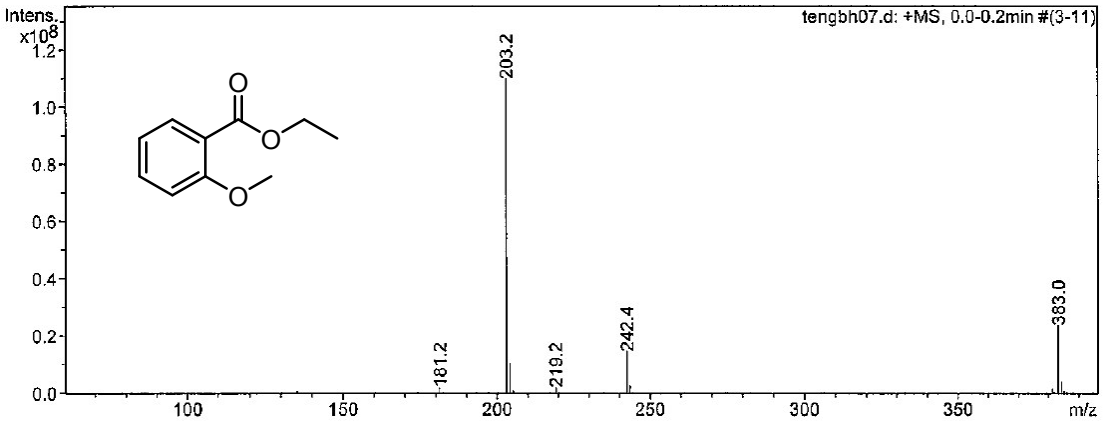
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh04.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:00:44 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 9:53:47 AM
Sample Name: E19
Analysis Info:



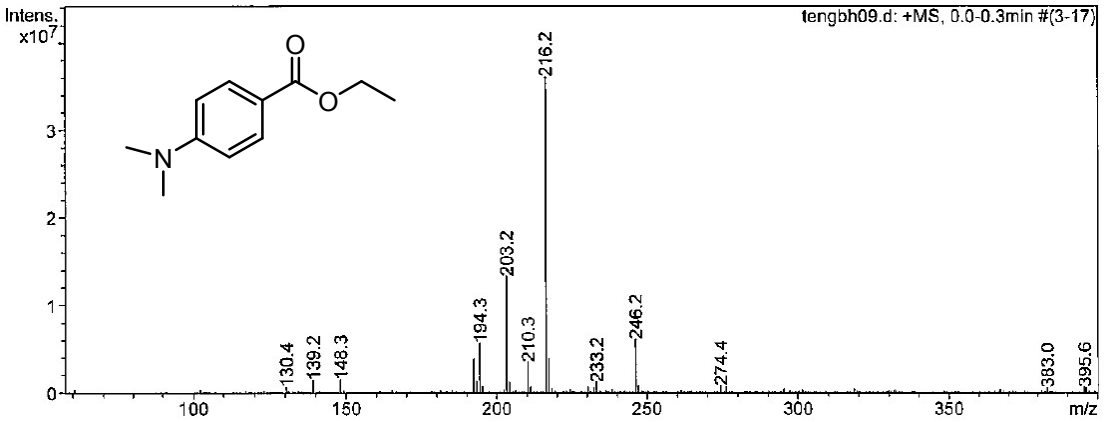
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh07.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:34:29 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:06:38 AM
Sample Name: E26
Analysis Info:



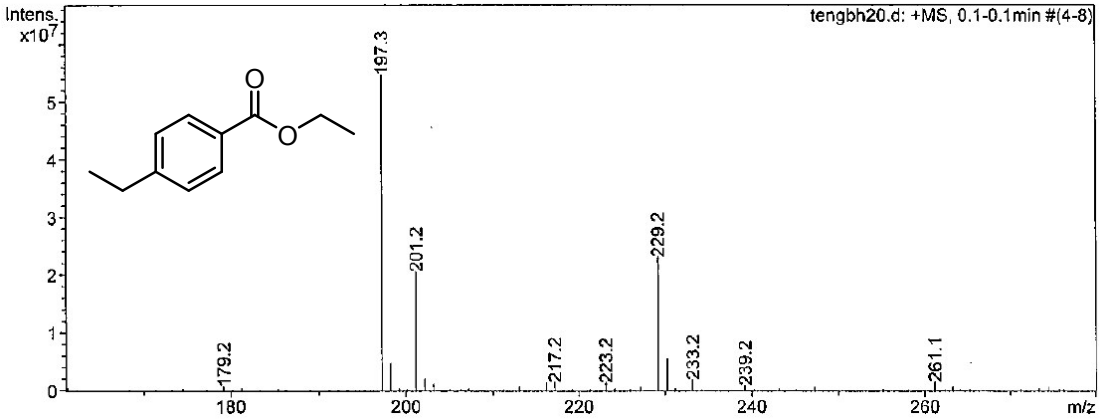
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh09.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:43:54 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:15:03 AM
Sample Name: E29
Analysis Info:



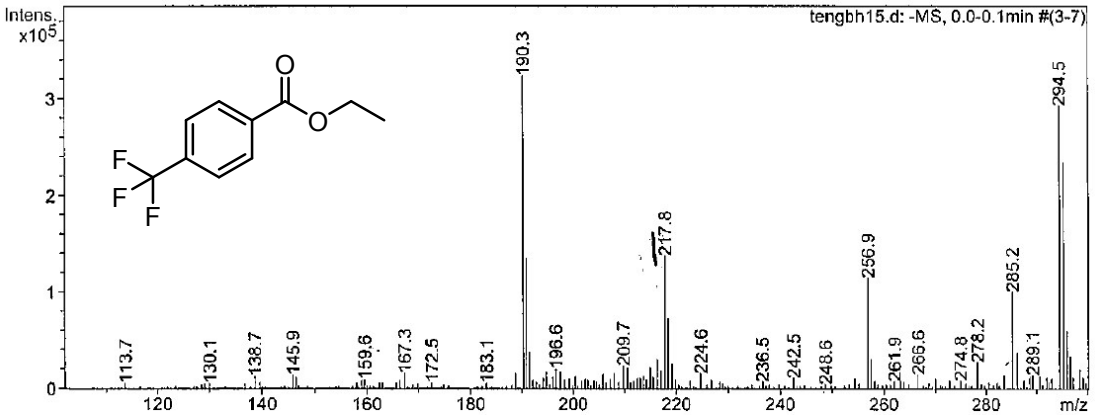
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh20.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:05:04 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:03:12 AM
Sample Name: E55-2
Analysis Info:



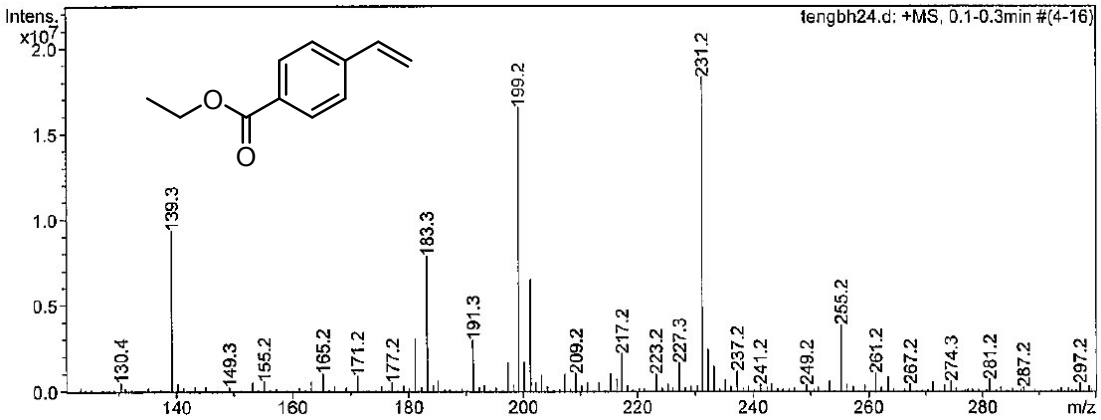
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh15.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:51:45 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:42:29 AM
Sample Name: E36
Analysis Info:



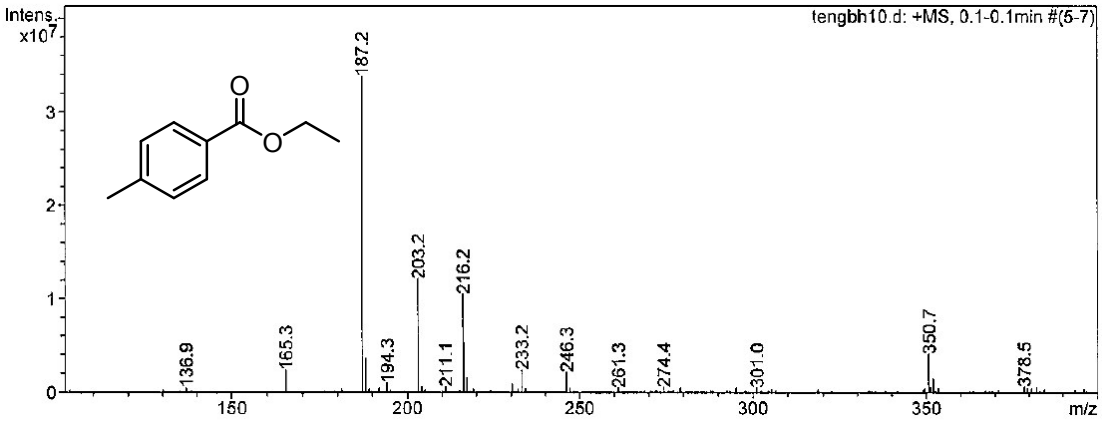
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh24.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:42:15 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:20:13 AM
Sample Name: E59
Analysis Info:



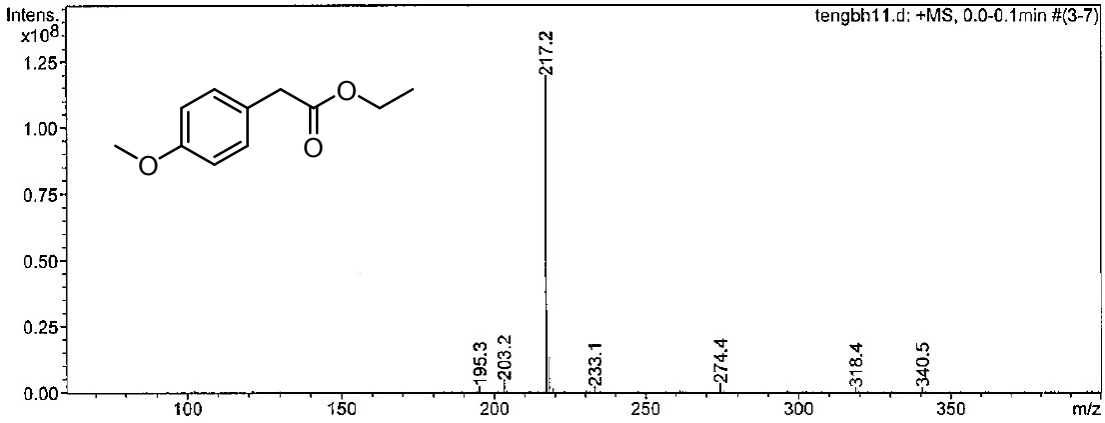
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh10.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:44:13 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:19:16 AM
Sample Name: E30
Analysis Info:



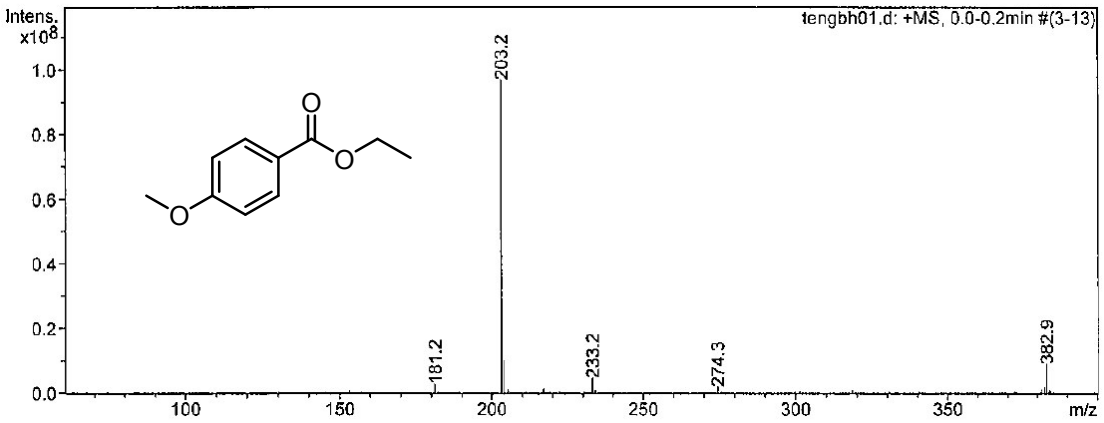
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh11.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:44:31 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:23:45 AM
Sample Name: E32
Analysis Info:



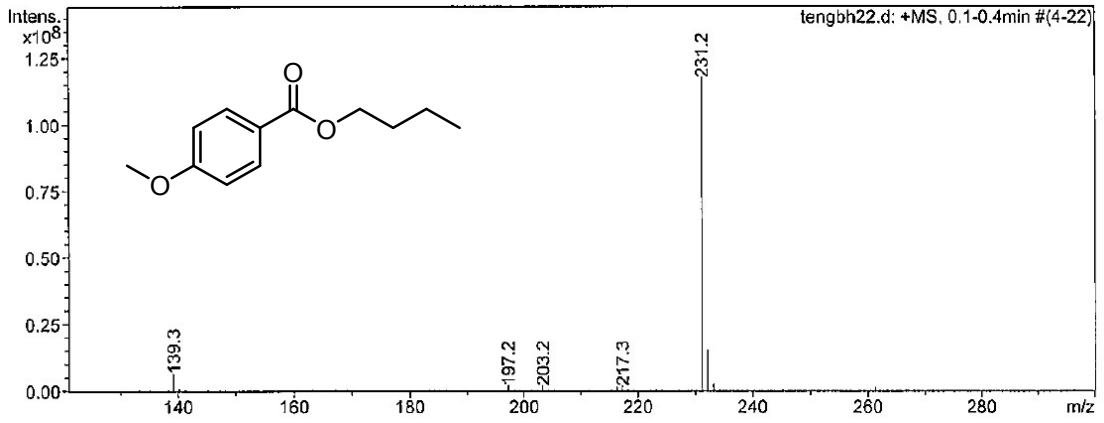
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh01.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 9:51:49 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 9:38:42 AM
Sample Name: E16
Analysis Info:



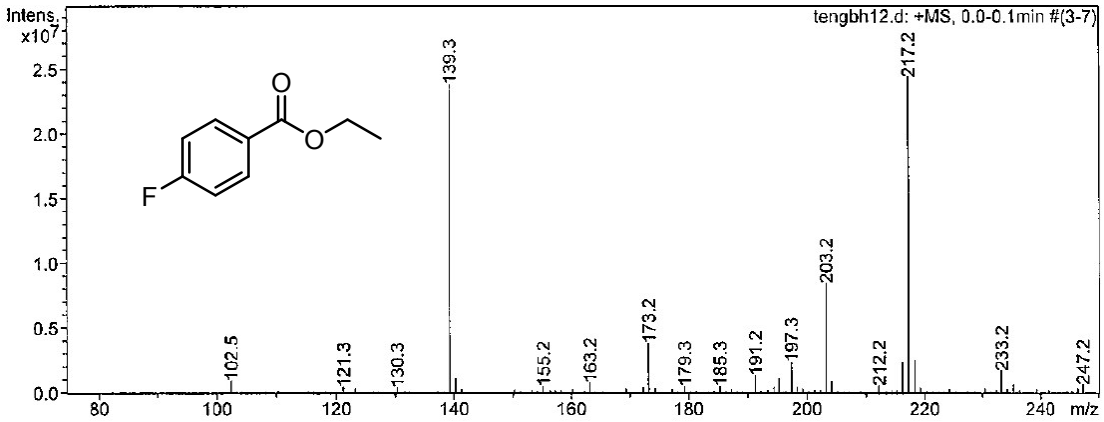
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh22.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:22:48 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:12:15 AM
Sample Name: E57
Analysis Info:



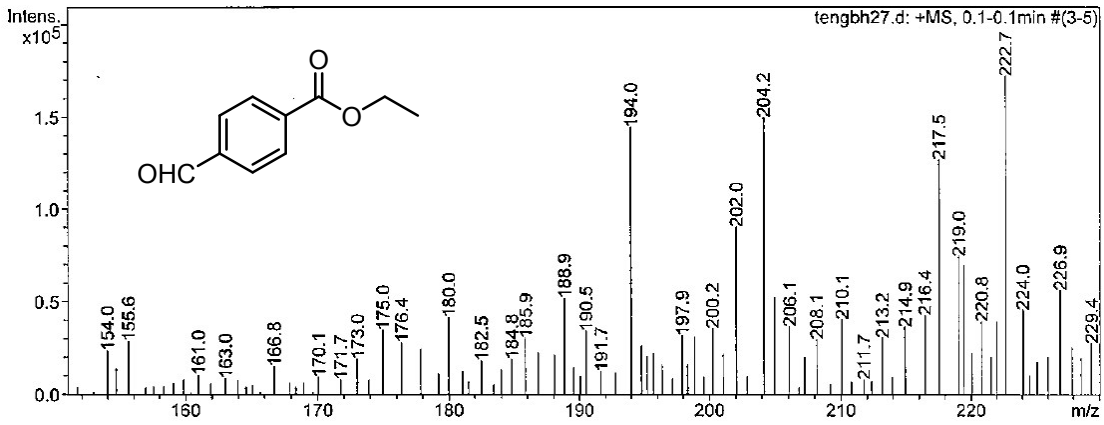
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh12.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 10:47:35 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 10:29:49 AM
Sample Name: E34
Analysis Info:



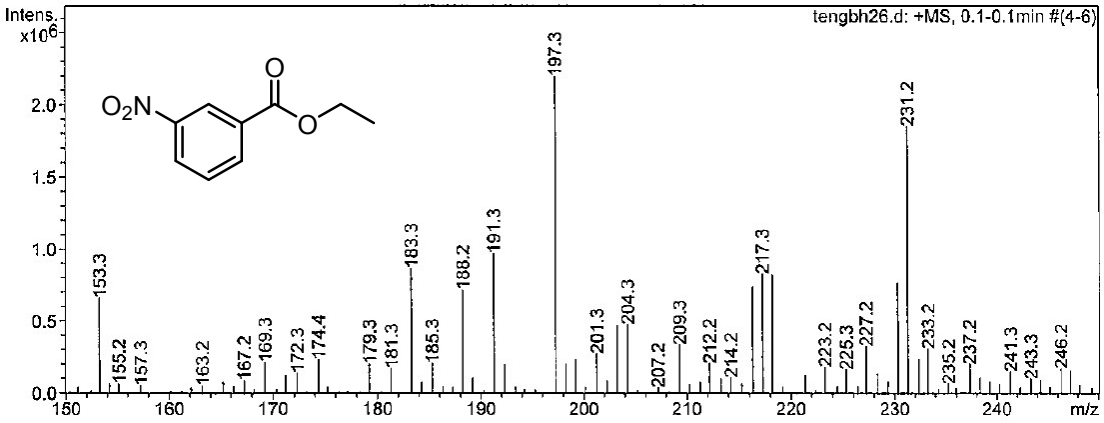
Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh27.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:46:59 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:36:47 AM
Sample Name: E68
Analysis Info:



Single Mass Spectrum Deconvolution Report

Analysis Name: tengbh26.d **Instrument:** LC-MSD-Trap-SL **Print Date:** 1/3/2018 11:45:40 AM
Method: TEST.M **Operator:** Operator **Acq. Date:** 1/3/2018 11:31:07 AM
Sample Name: E67
Analysis Info:

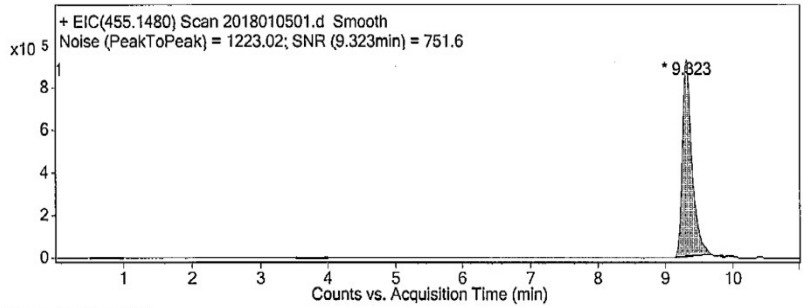

tengbh26.d: +MS, 0.1-0.1min #(4-6)
Intens.
x10^6
2.0
1.5
1.0
0.5
0.0
150
160
170
180
190
200
210
220
230
240
m/z
O2N
O
O
153.3
155.2
157.3
163.2
167.2
169.3
172.3
174.4
179.3
181.3
183.3
185.3
188.2
191.3
197.3
201.3
204.3
207.2
209.3
212.2
214.2
217.3
223.2
225.3
227.2
231.2
233.2
235.2
237.2
241.3
243.3
246.2

Qualitative Analysis Report

Data Filename	2018010501.d	**Sample Name**	HTBCC
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Some Ions Missed
DA Method	TEST LCMS.m	**Comment**	

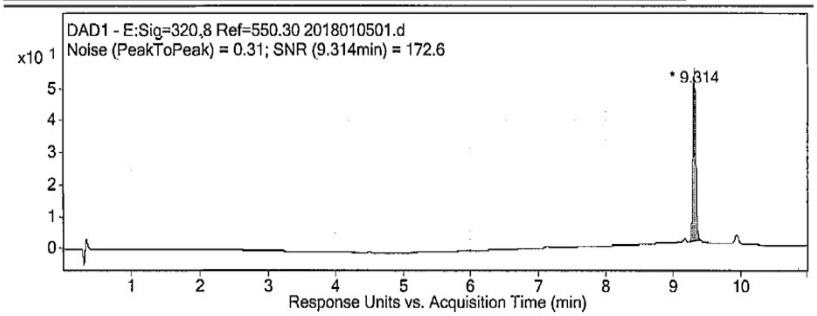
User Chromatograms

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	9.146	9.323	9.678	919204	9084400	100	751.6



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	9.243	9.314	9.406	54.07	157.65	100	172.6

User Spectra

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Esi