Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

Pd(0)-Catalyzed Intramolecular Arylative Dearomatization of β-Naphthols

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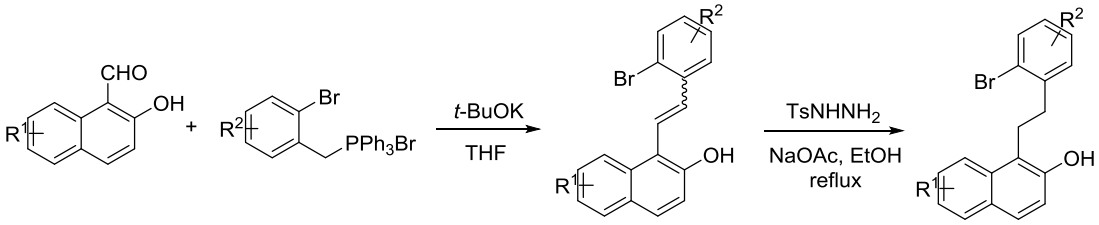
Table of Contents

General Methods. Unless stated otherwise, all reactions were carried out in flame-dried glassware under a dry argon atmosphere. All solvents were purified and dried according to standard methods prior to use. ^{1}H and ^{19}F NMR spectra were recorded on a Varian or Agilent instrument (400 MHz and 376 MHz, respectively) and internally referenced to tetramethylsilane signal or residual protio solvent signals and $CFCl_3$, respectively. ^{13}C NMR spectra were recorded on a Varian (100 MHz or 75 MHz) or Agilent instrument (100 MHz) and internally referenced to residual solvent signals. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant (s) in Hz, integration). Data for ^{13}C NMR and ^{19}F NMR are reported in terms of chemical shift (δ, ppm).

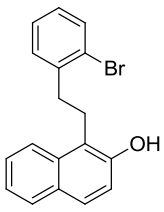
Substituted 2-bromobenzaldehydes and 2-hydroxy-1-naphthaldehyde were commercially available.

General procedure for the preparation of β-naphthols (1a-1o)

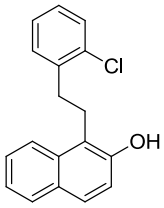


To a solution of the phosphonium salt[1] (13 mmol, 1.3 equiv.) in THF (60 mL), at 0 ℃ and under an argon atmosphere, was added *t*-BuOK (13 mmol, 1.3 equiv.). The mixture was stirred at 0 ℃ for 30 min before the aldehyde (10 mmol, 1.0 equiv.) was added. The resulting mixture was allowed to warm to room temperature and stirred for about 10 h. After completion (monitored by TLC), the reaction mixture was quenched with saturated NH_4Cl solution (20 mL) and THF was removed under reduced pressure. The mixture was diluted with H_2O (20 mL) and extracted with ethyl acetate (50 mL x 3). The combined ethyl acetate extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product was purified by silica gel column chromatography (PE : EtOAc = 50:1 - 20:1).

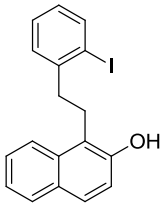
To a solution of the above obtained olefin (10 mmol, 1.0 equiv.) in EtOH (60 mL) were added NaOAc (20 mmol, 2.0 equiv.) and $TsNHNH_2$ (40 mmol, 4.0 equiv.). The resulting mixture was then refluxed for 2-6 h (monitored by ^1H NMR). After completion, the reaction mixture was quenched with saturated NH_4Cl solution (20 mL) and EtOH was removed under reduced pressure. The mixture was diluted with H_2O (20 mL) and extracted with ethyl acetate (50 mL x 3). The combined ethyl acetate extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product was purified by silica gel column chromatography (PE : EtOAc = 50:1 - 30:1) to afford the desired β-naphthol product.



White solid, m.p. = 91-93 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.54-7.50 (m, 1H), 7.37-7.33 (m, 1H), 7.26-7.22 (m, 2H), 7.12-7.09 (m, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 5.01 (s, 1H), 3.34-3.30 (m, 2H), 3.09-3.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 141.0 133.1, 132.8, 130.7, 129.4, 128.6, 128.1, 128.0, 127.7, 126.5, 124.2, 123.1, 122.7, 118.5, 117.7, 36.2, 25.7; IR (thin film): ν_{max} (cm^{-1}) = 3272, 2949, 2923, 1668, 1626, 1585, 1564, 1514, 1440, 1368, 1311, 1262, 1244, 1223, 1109, 1043, 1022, 926, 863, 810, 782, 743, 699, 656; Anal. calcd for $C_{18}H_{15}BrO$: C, 66.07; H, 4.62; Found: C, 66.06; H, 4.68.

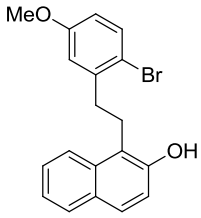


Colorless crystal solid, m.p. = 93-94 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.53-7.49 (m, 1H), 7.41-7.39 (m, 1H), 7.37-7.33 (m, 1H), 7.24-7.22 (m, 1H), 7.20-7.17 (m, 2H), 7.06 (d, *J* = 8.8 Hz, 1H), 4.97 (s, 1H), 3.34-3.30 (m, 2H), 3.08-3.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 139.3, 133.8, 133.1, 130.6, 129.5, 129.4, 128.6, 128.0, 127.7, 127.0, 126.5, 123.1, 122.7, 118.7, 117.7, 33.7, 25.5; IR (thin film): ν_{max} (cm^{-1}) = 3295, 3063, 1629, 1583, 1514, 1473, 1437, 1353, 1313, 1264, 1228, 1154, 1117, 1062, 1009, 946, 912, 854, 802, 776, 742, 698, 680; Anal. calcd for $C_{18}H_{15}ClO$: C, 76.46; H, 5.35; Found: C, 76.46; H, 5.29.

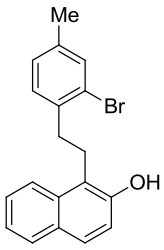


White solid, m.p. = 113-115 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H),

7.53-7.49 (m, 1H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.26-7.23 (m, 2H), 7.06 (d, *J* = 8.8 Hz, 1H), 6.93-6.89 (m, 1H), 5.05 (s, 1H), 3.31-3.27 (m, 2H), 3.07-3.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 144.3, 139.4, 133.1, 129.7, 129.4, 128.64, 128.58, 128.12, 128.07, 126.5, 123.1, 122.8, 118.2, 117.8, 100.2, 40.6, 26.0; IR (thin film): ν_{max}(cm^{-1}) = 3279, 3057, 2956, 2928, 1627, 1583, 1511, 1460, 1433, 1353, 1298, 1265, 1214, 1151, 1106, 1063, 1003, 945, 907, 876, 857, 803, 734, 695, 644; Anal. calcd for $C_{18}H_{15}IO$: C, 57.77; H, 4.04; Found: C, 57.65; H, 3.99.

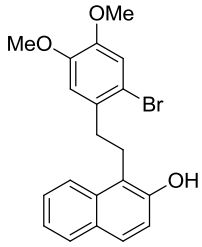


Light yellow solid, m.p. = 114-115 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.53-7.49 (m, 1H), 7.46 (d, *J* = 8.8 Hz, 1H), 7.36-7.32 (m, 1H), 7.07 (d, *J* = 8.8 Hz, 1H), 6.76 (d, *J* = 2.8 Hz, 1H), 6.66 (dd, *J* = 8.8, 3.2 Hz, 1H), 5.08 (s, 1H), 3.71 (s, 3H), 3.33-3.28 (m, 2H), 3.03-2.99 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 150.9, 141.9, 133.3, 133.1, 129.3, 128.6, 128.1, 126.5, 123.1, 122.7, 118.4, 117.7, 116.3, 114.6, 113.5, 55.4, 36.4, 25.6; IR (thin film): ν_{max}(cm^{-1}) = 3473, 3418, 3052, 2940, 1624, 1600, 1568, 1513, 1472, 1412, 1354, 1301, 1276, 1241, 1157, 1123, 1052, 1004, 910, 861, 807, 748, 726, 673; Anal. calcd for $C_{19}H_{17}BrO_2$: C, 63.88; H, 4.80; Found: C, 63.91; H, 4.76.

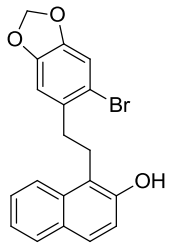


Light yellow solid, m.p. = 106-108 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.53-7.49 (m, 1H), 7.42 (s, 1H), 7.37-7.33 (m, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 8.8 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 5.04 (s, 1H), 3.30-3.26 (m, 2H), 3.04-3.00 (m, 2H), 2.31 (s, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ 150.9, 138.0, 137.8, 133.2, 133.1, 130.3, 129.4, 128.6, 128.5, 128.1, 126.5, 123.9, 123.1, 122.8, 118.5, 117.8, 35.7, 25.9, 20.6; IR (thin film): $\nu_{max}(cm^{-1})$ = 3253, 2964, 2922, 1628, 1584, 1514, 1489, 1439, 1358, 1322, 1300, 1266, 1215, 1164, 1126, 1064, 1039, 1014, 949, 910, 859, 806, 768, 739, 692, 672; Anal. calcd for $C_{19}H_{17}BrO$: C, 66.87; H, 5.02; Found: C, 66.70; H, 5.04.

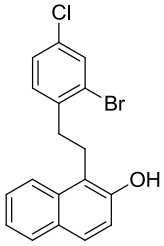


Light yellow solid, m.p. = 140-142 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.8 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.52-7.47 (m, 1H), 7.36-7.32 (m, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 7.04 (s, 1H), 6.55 (s, 1H), 5.23 (s, 1H), 3.85 (s, 3H), 3.69 (s, 3H), 3.32-3.28 (m, 2H), 3.02-2.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 148.2, 147.9, 133.1, 132.9, 129.2, 128.5, 127.9, 126.4, 123.0, 122.8, 118.6, 117.7, 115.4, 113.8, 113.2, 56.1, 55.9, 35.7, 25.6; IR (thin film): $\nu_{max}(cm^{-1})$ = 3446, 3160, 2963, 2936, 1604, 1502, 1458, 1436, 1382, 1354, 1311, 1253, 1212, 1155, 1061, 1026, 957, 911, 853, 809, 780, 746, 696; Anal. calcd for $C_{20}H_{19}BrO_3$: C, 62.03; H, 4.95; Found: C, 62.05; H, 4.91.

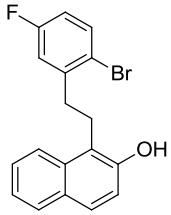


Light yellow solid, m.p. = 143-145 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 8.8 Hz, 1H), 7.04 (s, 1H), 6.73 (s, 1H), 5.95 (s, 2H), 4.99 (s, 1H), 3.28-3.24 (m, 2H), 2.99-2.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.8, 147.4, 146.9, 134.1, 133.1, 129.4, 128.6, 128.1, 126.5, 123.1, 122.7, 118.5, 117.7, 114.1, 112.7, 110.2, 101.6, 36.1, 25.9; IR (thin film): $\nu_{max}(cm^{-1})$ = 3538, 3445,

2891, 1622, 1600, 1583, 1501, 1472, 1438, 1389, 1355, 1308, 1272, 1229, 1199, 1148, 1109, 1041, 1013, 961, 936, 910, 851, 807, 770, 754, 699, 669, 646; Anal. calcd for $C_{19}H_{15}BrO_3$: C, 61.47; H, 4.07; Found: C, 61.45; H, 4.05.

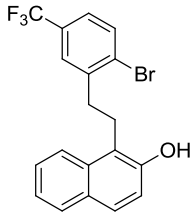


White solid, m.p. = 113-115 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.53-7.48 (m, 1H), 7.37-7.33 (m, 1H), 7.18 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 7.04 (d, *J* = 8.8 Hz, 1H), 4.93 (s, 1H), 3.32-3.28 (m, 2H), 3.06-3.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 139.6, 133.1, 132.5, 132.2, 131.3, 129.3, 128.7, 128.1, 127.7, 126.6, 124.4, 123.2, 122.6, 118.4, 117.6, 35.5, 25.5; IR (thin film): ν_{max}(cm^{-1}) = 3212, 2969, 1630, 1584, 1515, 1468, 1439, 1357, 1271, 1224, 1168, 1098, 1065, 1037, 1012, 912, 867, 841, 803, 780, 741, 688; Anal. calcd for $C_{18}H_{14}BrClO$: C, 59.78; H, 3.90; Found: C, 59.60; H, 3.85.

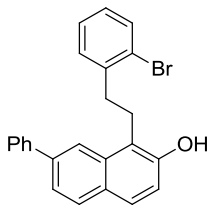


Light yellow solid, m.p. = 118-119 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.53-7.49 (m, 2H), 7.37-7.33 (m, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.98 (dd, *J* = 9.6, 3.2 Hz, 1H), 6.82 (td, *J* = 8.0, 2.8 Hz, 1H), 5.00 (s, 1H), 3.33-3.29 (m, 2H), 3.05-3.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, *J* = 245.6 Hz), 150.7, 143.2 (d, *J* = 7.3 Hz), 133.8 (d, *J* = 8.1 Hz), 133.1, 129.4, 128.7, 128.2, 126.6, 123.2, 122.6, 118.3, 118.27 (d, *J* = 3.1 Hz), 117.6, 117.4 (d, *J* = 22.2 Hz), 115.0 (d, *J* = 22.3 Hz), 36.2 (d, *J* = 1.1 Hz), 25.3; ^{19}F NMR (386 Hz, $CDCl_3$) δ -115.1(m); IR (thin film): ν_{max}(cm^{-1}) = 3557, 3499, 3450,

2986, 2950, 2927, 1623, 1576, 1512, 1469, 1406, 1356, 1258, 1231, 1196, 1153, 1103, 1063, 1014, 954, 910, 863, 808, 743, 693; Anal. calcd for $C_{18}H_{14}BrFO$: C, 62.63; H, 4.09; Found: C, 62.80; H, 4.08.

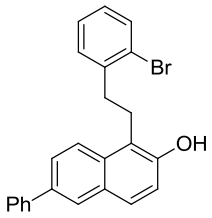


White solid, m.p. = 107-108 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.70-7.66 (m, 2H), 7.53-7.49 (m, 1H), 7.42 (d, *J* = 2.0 Hz, 1H), 7.37-7.31 (m, 2H), 7.04 (d, *J* = 8.8 Hz, 1H), 4.89 (s, 1H), 3.37-3.33 (m, 2H), 3.14-3.10 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 142.2, 133.2, 133.1, 130.0 (q, *J* = 33.9 Hz), 129.4, 128.7, 128.2, 128.15 (q, *J* = 1.5 Hz), 127.2 (q, *J* = 3.6 Hz), 126.6, 124.4 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 271.0 Hz), 123.2, 122.6, 118.3, 117.5, 36.0, 25.2; ^{19}F NMR (386 Hz, $CDCl_3$) δ -62.6 (s); IR (thin film): ν_{max}(cm^{-1}) = 3270, 2925, 1582, 1516, 1457, 1442, 1408, 1359, 1332, 1281, 1218, 1173, 1112, 1079, 1026, 1011, 954, 910, 893, 858, 823, 804, 757, 740, 702; Anal. calcd for $C_{19}H_{14}BrF_3O$: C, 57.74; H, 3.57; Found: C, 57.85; H, 3.72.

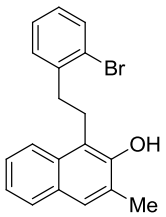


Colorless crystal solid, m.p. = 118-119 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.75-7.72 (m, 2H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.60 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.52-7.48 (m, 2H), 7.41-7.37 (m, 1H), 7.23-7.17 (m, 2H), 7.08-7.04 (m, 2H), 5.06 (s, 1H), 3.39-3.35 (m, 2H), 3.13-3.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.2, 141.6, 141.0, 139.2, 133.4, 132.7, 130.8, 129.1, 128.8, 128.5, 127.9, 127.8, 127.6, 127.5, 127.3, 124.2, 122.9, 121.1, 119.0, 117.7, 36.3, 25.7; IR (thin film): ν_{max}(cm^{-1}) = 3246, 3058, 3014, 2962, 1625, 1578,

1492, 1468, 1453, 1435, 1362, 1302, 1262, 1206, 1154, 1113, 1069, 1023, 1007, 928, 880, 831, 789, 748, 731, 690; Anal. calcd for $C_{24}H_{19}BrO$: C, 71.47; H, 4.75; Found: C, 71.54; H, 4.84.

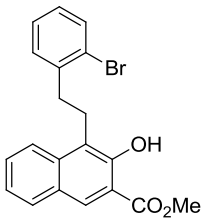


Light yellow solid, m.p. = 161-162 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.8 Hz, 1H), 7.99 (d, *J* = 2.0 Hz, 1H), 7.79 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.73-7.70 (m, 3H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.50-7.46 (m, 2H), 7.38-7.35 (m, 1H), 7.28-7.21 (m, 2H), 7.12-7.08 (m, 2H), 5.06 (s, 1H), 3.36-3.32 (m, 2H), 3.11-3.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 140.94, 140.93, 135.8, 132.8, 132.3, 130.7, 129.6, 128.8, 128.4, 128.0, 127.7, 127.2, 127.1, 126.5, 126.1, 124.3, 123.4, 118.5, 118.2, 36.2, 25.8; IR (thin film): ν_{max}(cm^{-1}) = 3311, 1628, 1571, 1492, 1468, 1445, 1365, 1325, 1270, 1223, 1191, 1151, 1112, 1072, 1023, 1008, 911, 894, 840, 806, 751, 728, 694, 655; Anal. calcd for $C_{24}H_{19}BrO$: C, 71.47; H, 4.75; Found: C, 71.52; H, 4.76.

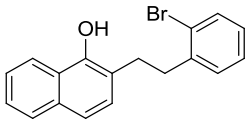


Yellow solid, m.p. = 104-105 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.8 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.52 (s, 1H), 7.47-7.43 (m, 1H), 7.34-7.30 (m, 1H), 7.27-7.22 (m, 2H), 7.12-7.07 (m, 1H), 5.15 (s, 1H), 3.31-3.27 (m, 2H), 3.06-3.02 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 140.9, 132.8, 131.8, 130.6, 129.2, 128.0, 127.9, 127.8, 127.7, 125.8, 125.6, 124.2, 123.1, 122.5, 117.7, 36.2, 26.0, 17.0; IR (thin film): ν_{max}(cm^{-1}) = 3569, 3064, 2920, 2872, 1628, 1505, 1468, 1435, 1397, 1254, 1219, 1196, 1177, 1157, 1097, 1023, 978, 886, 850, 740, 648, 622; HRMS (EI) calcd for $C_{19}H_{17}BrO$ $[M]^+$: 340.0463. Found:

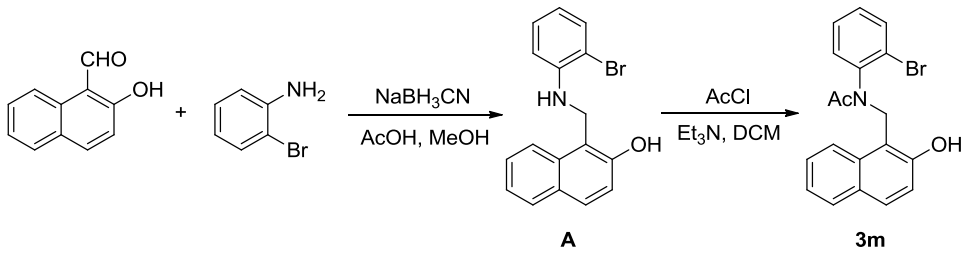
340.0462.



Yellow solid, m.p. = 123-125 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.75 (s, 1H), 8.42 (s, 1H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.58-7.52 (m, 2H), 7.34-7.30 (m, 2H), 7.23-7.20 (m, 1H), 7.08-7.04 (m, 1H), 4.03 (s, 3H), 3.40-3.36 (m, 2H), 3.08-3.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 153.7, 141.5, 136.3, 132.6, 130.74, 130.66, 130.0, 129.0, 127.6, 127.4, 126.9, 124.3, 123.3, 122.9, 121.4, 113.4, 52.5, 35.8, 25.4; IR (thin film): ν_{max}(cm^{-1}) = 3159, 3126, 2951, 1673, 1623, 1577, 1508, 1446, 1380, 1352, 1302, 1261, 1222, 1155, 1113, 1088, 1020, 998, 955, 931, 905, 861, 791, 764, 745, 726, 656; HRMS (ESI) calcd for $C_{20}H_{18}BrO_3$ $[M + H]^+$: 385.0434; Found: 385.0434.



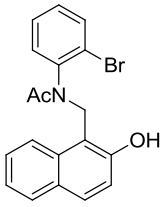
White solid, m.p. = 107-109 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H), 7.78 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.49-7.43 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.23-7.17 (m, 2H), 7.12-7.08 (m, 1H), 5.34 (s, 1H), 3.10-3.00 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 140.4, 133.5, 132.8, 130.6, 128.10, 128.07, 127.7, 127.6, 125.6, 125.3, 124.5, 124.2, 121.1, 120.4, 119.8, 37.1, 30.9; IR (thin film): ν_{max}(cm^{-1}) = 3371, 3050, 2943, 2872, 1902, 1805, 1572, 1506, 1464, 1388, 1253, 1197, 1170, 1070, 1022, 992, 921, 863, 793, 740, 657; Anal. calcd for $C_{18}H_{15}BrO$: C, 66.07; H, 4.62; Found: C, 66.05; H, 4.71.



A **3m**

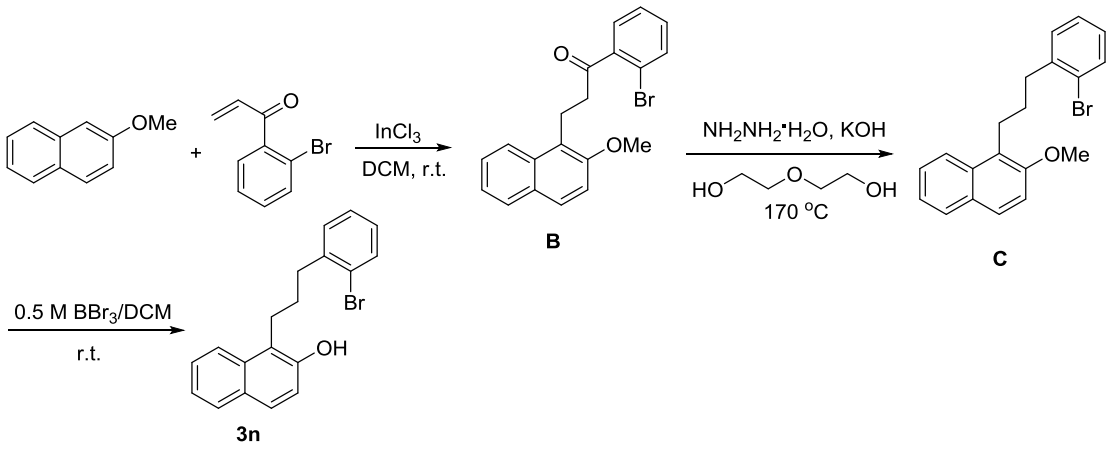
To a solution of the 2-bromoaniline (20 mmol, 1.0 equiv.) in MeOH (30 mL), under an argon atmosphere, was added 2-hydroxy-1-naphthaldehyde (20 mmol, 1.0 equiv.). The mixture was stirred for 2 h before adding sodium cyanoborohydride (22 mmol, 1.1 equiv.) and AcOH (0.8 mL). After completion (monitored by TLC), the reaction mixture was quenched with saturated $NaHCO_3$ solution (20 mL) and MeOH was removed under reduced pressure. The mixture was diluted with H_2O (20 mL) and extracted with ethyl acetate (50 mL x 3). The combined ethyl acetate extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product was purified by silica gel column chromatography (PE/EA = 10/1-4/1) to afford the desired product **A** (1.97 g, 30% yield).

To a solution of **A** (3.0 mmol, 1.0 equiv.) in DCM (20 mL), under an argon atmosphere, was added Et_3N (4.0 mmol, 1.3 equiv.). The mixture was stirred at rt when acetyl chloride (4.0 mmol, 1.3 equiv.) was added dropwise. After completion (monitored by TLC), the reaction mixture was quenched with saturated NH_4Cl solution (20 mL). The mixture was diluted with H_2O (20 mL) and extracted with DCM (50 mL x 3). The combined DCM extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product was purified by silica gel column chromatography (PE/EA = 20/1) to afford the desired product **3m** (0.61 g, 55% yield).



White solid, m.p. = 159-161 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H),

7.74-7.71 (m, 2H), 7.68 (d, J = 8.0 Hz, 1H), 7.29-7.23 (m, 2H), 7.18-7.13 (m, 2H), 7.02-6.97 (m, 1H), 6.85 (d, J = 7.6 Hz, 1H), 6.78 (d, J = 8.8 Hz, 1H), 5.48 (d, J_{AB} = 15.6 Hz, 1H), 4.93 (d, J_{BA} = 15.6 Hz, 1H), 1.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 155.1, 140.9, 134.0, 133.5, 131.0, 130.6, 130.4, 128.9, 128.6, 128.4, 126.0, 123.0, 122.4, 121.6, 119.9, 113.4, 43.7, 22.0; IR (thin film): ν_{max}(cm^{-1}) = 3071, 3038, 2965, 1624, 1579, 1522, 1476, 1456, 1416, 1375, 1292, 1239, 1201, 1158, 1073, 1034, 1018, 972, 860, 819, 796, 767, 746, 725, 705, 628; HRMS (ESI) calcd for $C_{19}H_{17}BrNO_2$ $[M + H]^+$: 370.0437; Found: 370.0439.

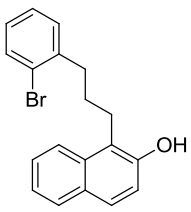


To a solution of the 2-methoxynaphthalene (10 mmol, 1.3 equiv.) in DCM (20 mL), under an argon atmosphere, was added 1-(2-bromophenyl)prop-2-en-1-one (7.7 mmol, 1.0 equiv.) and indium trichloride (0.77 mmol, 0.1 equiv.). The mixture was stirred at rt for about 20 h. After completion (monitored by TLC), the reaction mixture was quenched with saturated $NaHCO_3$ solution (10 mL). The mixture was diluted with H_2O (20 mL) and extracted with DCM (50 mL x 3). The combined DCM extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product (**B**) was obtained (1.4 g, 51% yield) and used in the following reaction without further purification.

To a 100 mL, round-bottomed flask were added **B** (3.8 mmol, 1.0 equiv.), hydrazine hydrate (1.8 ml, 10.0 equiv.), potassium hydroxide (13.3 mmol, 3.5 equiv.) and diethylene glycol (15 mL). The mixture was refluxed at 170 ^{o}C for about 2 h.

After completion (monitored by TLC), the reaction mixture was cooled to rt and quenched with saturated NH_4Cl solution (10 mL). The mixture was diluted with H_2O (20 mL) and extracted with ethyl acetate (50 mL x 3). The combined ethyl acetate extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product (**C**) was obtained (0.75 g, 56% yield) and used in the following reaction without further purification.

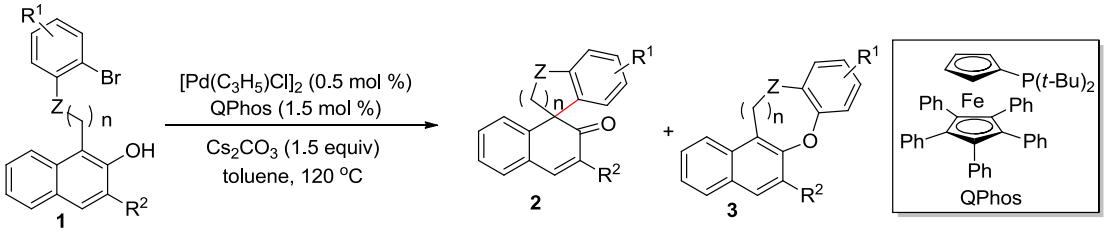
A flame-dried two-necked, round-bottomed flask was cooled down to room temperature under argon. To this flask were added **C** (2.11 mmol, 1.0 equiv.) and DCM (15 mL). The mixture was stirred at 0 ℃ while the 0.5 M BBr_3/DCM solution (6.4 mL, 1.5 equiv.) was added dropwise. Then the resulting mixture was allowed to warm to room temperature and stirred for about 2 h. After completion (monitored by TLC), the reaction mixture was quenched with saturated $NaHCO_3$ (20 mL). The mixture was diluted with H_2O (20 mL) and extracted with DCM (50 mL x 3). The combined DCM extract was washed with brine, dried over anhydrous Na_2SO_4 and filtrated. After the solvent was concentrated under reduced pressure, the crude product was purified by silica gel column chromatography (PE/EA = 30/1) to afford the desired product **3n** (0.67 g, 93% yield).



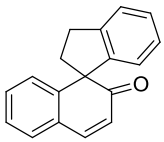
White solid, m.p. = 96-97 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.8 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.45 (m, 1H), 7.31 (m, 1H), 7.22 (m, 2H), 7.04 (m, 2H), 4.95 (s, 1H), 3.11 (t, *J* = 8.0 Hz, 2H), 2.91 (t, *J* = 8.0 Hz, 2H), 1.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 141.4, 133.1, 132.7, 130.2, 129.4, 128.6, 127.7, 127.5, 127.4, 126.4, 124.6, 123.0, 122.9, 119.8, 117.6, 36.2, 29.8, 24.7; IR (thin film): ν_{max}(cm^{-1}) = 3286, 3050, 2948, 1622, 1515, 1468, 1442, 1368, 1313, 1263, 1244, 1194, 1146, 1110, 1043, 1023, 926, 862, 812, 782, 743, 700, 657; Anal. calcd for $C_{19}H_{17}BrO$: C, 66.87; H, 5.02; Found: C,

66.97; H, 5.00.

General procedure for Pd-catalyzed arylative dearomatization reaction

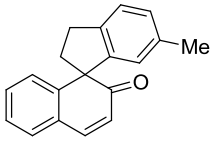


A flame-dried Schlenk tube was cooled down to room temperature under argon. To this tube were added $[Pd(C_3H_5)Cl]_2$ (1.5 mg, 0.004 mmol, 0.5 mol%), QPhos (8.6 mg, 0.012 mmol, 1.5 mol%), Cs_2CO_3 (391.0 mg, 1.2 mmol, 1.5 equiv.), β-naphthols (**1a-1o**) (0.8 mmol, 1.0 equiv.) and toluene (4.0 mL). Then the reaction mixture was stirred at 120 °C. After completion (monitored by TLC), the reaction mixture was cooled to room temperature and diluted with ethyl acetate (3mL). The mixture was filtered through celite, and the filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE : EtOAc = 50:1 - 30:1) to afford the desired products (**2a-2o**).



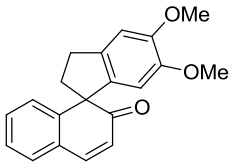
2a

Light yellow oil, 185.6 mg, 95% yield (from **1aa**); 180.2 mg, 92% yield (from **1ab**); 183.6 mg, 94% yield (from **1ac**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 10.0 Hz, 1H), 7.36-7.33 (m, 2H), 7.28-7.20 (m, 3H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.02-6.98 (m, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.18 (d, *J* = 10.0 Hz, 1H), 3.37-3.29 (m, 1H), 3.18-3.10 (m, 1H), 2.83-2.77 (m, 1H), 2.40-2.33 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.0, 146.4, 145.5, 145.1, 145.0, 129.9, 129.2, 129.0, 127.8, 127.5, 126.8, 126.7, 124.7, 124.3, 124.2, 64.9, 41.5, 31.4; IR (thin film): ν_{max} (cm^{-1}) = 3065, 3022, 2926, 2849, 1658, 1618, 1596, 1563, 1477, 1451, 1394, 1298, 1237, 1206, 1111, 1025, 955, 876, 826, 748, 666; HRMS (ESI) calcd for $C_{18}H_{15}O[M + H]^+$: 247.1111; Found: 247.1111.



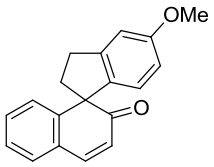
4b

Light yellow oil, 190.8 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 10.0 Hz, 1H), 7.35-7.33 (m, 1H), 7.26-7.20 (m, 3H), 7.04-6.99 (m, 2H), 6.56 (s, 1H), 6.18 (d, *J* = 10.0 Hz, 1H), 3.31-3.23 (m, 1H), 3.13-3.06 (m, 1H), 2.82-2.75 (m, 1H), 2.38-2.31 (m, 1H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4, 146.7, 145.7, 145.1, 142.0, 136.3, 130.0, 129.2, 129.1, 128.6, 127.9, 126.8, 124.8, 124.42, 124.41, 65.0, 42.0, 31.1, 21.1; IR (thin film): ν_{max} (cm^{-1}) = 3018, 2921, 2853, 1657, 1618, 1596, 1563, 1492, 1448, 1394, 1300, 1237, 1208, 1115, 1031, 976, 954, 876, 833, 812, 752, 665; HRMS (ESI) calcd for $C_{19}H_{17}O[M + H]^{+}$: 261.1274; Found: 2461.1273.



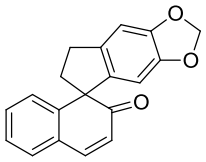
4c

White solid, m.p. = 152-154 ℃; 226.3 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 10.0 Hz, 1H), 7.37-7.35 (m, 1H), 7.28-7.26 (m, 2H), 7.00-6.98 (m, 1H), 6.87 (s, 1H), 6.28 (s, 1H), 6.21 (d, *J* = 10.0 Hz, 1H), 3.88 (s, 3H), 3.67 (s, 3H), 3.25-3.17 (m, 1H), 3.10-3.03 (m, 1H), 2.79-2.72 (m, 1H), 2.34-2.27 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 149.0, 148.3, 146.5, 145.0, 137.2, 136.5, 130.0, 129.1, 129.0, 127.8, 126.8, 124.4, 107.18, 107.16, 65.3, 55.8, 55.7, 42.9, 31.0; IR (thin film): ν_{max} (cm^{-1}) = 3053, 3003, 2933, 2897, 2833, 1658, 1624, 1564, 1502, 1447, 1403, 1330, 1303, 1266, 1247, 1211, 1188, 1166, 1115, 1078, 1032, 1002, 960, 875, 841, 823, 774, 741, 621; HRMS (ESI) calcd for $C_{20}H_{19}O_3[M + H]^{+}$: 307.1329; Found: 307.1327.



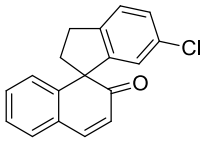
4d

Yellow oil, 208.3 mg, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 9.6 Hz, 1H), 7.34-7.32 (m, 1H), 7.28-7.23 (m, 2H), 7.03-7.01 (m, 1H), 6.87 (s, 1H), 6.66 (s, 2H), 6.17 (d, *J* = 10.0 Hz, 1H), 3.76 (s, 3H), 3.33-3.25 (m, 1H), 3.13-3.06 (m, 1H), 2.82-2.75 (m, 1H), 2.39-2.32 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5, 159.5, 146.75, 146.72, 145.0, 137.5, 130.0, 129.3, 129.0, 127.8, 126.8, 125.0, 124.3, 113.1, 109.6, 64.3, 55.2, 42.1, 31.5; IR (thin film): ν_{max} (cm^{-1}) = 3006, 2938, 2834, 1658, 1602, 1563, 1487, 1449, 1395, 1309, 1249, 1206, 1167, 1146, 1083, 1030, 960, 914, 835, 814, 752, 665; HRMS (ESI) calcd for $C_{19}H_{17}O_2[M + H]^+$: 277.1223; Found: 277.1222.



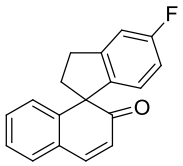
4e

Yellow oil, 218.3 mg, 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 10.0 Hz, 1H), 7.36-7.34 (m, 1H), 7.32-7.27 (m, 2H), 7.05-7.03 (m, 1H), 6.78 (s, 1H), 6.21 (s, 1H), 6.19 (d, *J* = 9.6 Hz, 1H), 5.90 (dd, *J* = 14.8, 0.8 Hz, 2H), 3.23-3.15 (m, 1H), 3.06-2.99 (m, 1H), 2.81-2.74 (m, 1H), 2.38-2.30 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 147.7, 146.9, 146.5, 145.1, 138.4, 137.8, 130.1, 129.3, 129.2, 127.9, 127.0, 124.5, 104.9, 104.8, 101.1, 64.9, 42.5, 31.2; IR (thin film): ν_{max} (cm^{-1}) = 2959, 2891, 2854, 1657, 1618, 1563, 1500, 1471, 1395, 1358, 1298, 1244, 1208, 1159, 1126, 1035, 935, 857, 820, 798, 756, 643; HRMS (ESI) calcd for $C_{19}H_{15}O_3[M + H]^+$: 291.1016; Found: 291.1015.



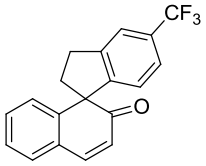
4f

Yellow oil, 210.1 mg, 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 10.0 Hz, 1H), 7.36-7.34 (m, 1H), 7.29-7.24 (m, 3H), 7.18 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.00-6.98 (m, 1H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.17 (d, *J* = 10.0 Hz, 1H), 3.31-3.23 (m, 1H), 3.12-3.05 (m, 1H), 2.83-2.77 (m, 1H), 2.41-2.34 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4, 147.4, 145.7, 145.4, 143.7, 132.3, 130.3, 129.3, 129.2, 127.89, 127.87, 127.2, 125.8, 124.6, 124.2, 64.9, 42.1, 30.9; IR (thin film): ν_{max} (cm^{-1}) = 3022, 2926, 2850, 1658, 1618, 1595, 1564, 1474, 1450, 1434, 1394, 1301, 1236, 1206, 1160, 1098, 1069, 984, 909, 870, 814, 751, 664; HRMS (ESI) calcd for $C_{18}H_{14}ClO$ $[M + H]^+$: 281.0728; Found: 281.0727.



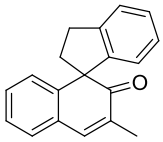
4g

Yellow oil, 200.3 mg, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 10.0 Hz, 1H), 7.36-7.33 (m, 1H), 7.29-7.24 (m, 2H), 7.02-6.98 (m, 2H), 6.78 (td, *J* = 8.8, 2.4 Hz, 1H), 6.69 (dd, *J* = 8.4, 5.2 Hz, 1H), 6.17 (d, *J* = 10.0 Hz, 1H), 3.33-3.25 (m, 1H), 3.13-3.05 (m, 1H), 2.83-2.76 (m, 1H), 2.41-2.34 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.9, 162.6 (d, *J* = 243.7 Hz), 147.5 (d, *J* = 8.2 Hz), 146.1, 145.2, 141.0 (d, *J* = 2.5 Hz), 130.1, 129.25, 129.19, 127.8, 127.0, 125.5 (d, *J* = 9.1 Hz), 124.2, 113.9 (d, *J* = 22.8 Hz), 111.6 (d, *J* = 22.0 Hz), 64.2, 42.3, 31.3 (d, *J* = 2.1 Hz); ^{19}F NMR (386 Hz, $CDCl_3$) δ -115.5 (m); IR (thin film): ν_{max} (cm^{-1}) = 3063, 3025, 2926, 2849, 1658, 1615, 1594, 1564, 1481, 1432, 1395, 1303, 1242, 1207, 1146, 1129, 1080, 961, 926, 862, 834, 813, 755, 665; HRMS (ESI) calcd for $C_{18}H_{14}FO$ $[M + H]^+$: 265.1023; Found: 265.1022.



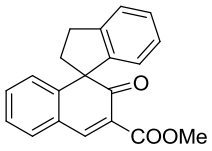
4h

Yellow oil, 215.1 mg, 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.54 (d, *J* = 10.0 Hz, 1H), 7.39-7.35 (m, 2H), 7.30-7.28 (m, 2H), 6.96-6.94 (m, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.19 (d, *J* = 9.6 Hz, 1H), 3.41-3.23 (m, 1H), 3.21-3.14 (m, 1H), 2.87-2.81 (m, 1H), 2.45-2.37 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4, 149.6, 146.2, 145.5, 133.0, 130.3 (q, *J* = 31.7 Hz), 129.5, 129.3, 127.9, 127.3, 124.3 (q, *J* = 270.9 Hz), 124.9, 124.14, 124.09 (q, *J* = 3.8 Hz), 121.8 (q, *J* = 3.8 Hz), 64.9, 42.1, 31.2; ^{19}F NMR (386 Hz, $CDCl_3$) δ -62.2 (s); IR (thin film): ν_{max} (cm^{-1}) = 3065, 3030, 2934, 2851, 1660, 1618, 1565, 1488, 1430, 1395, 1331, 1236, 1199, 1153, 1114, 1060, 956, 887, 825, 760, 687, 652; HRMS (ESI) calcd for $C_{19}H_{14}F_3O[M + H]^+$: 315.0991; Found: 315.0991.



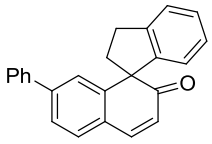
4i

White solid, m.p. = 64-66 ℃; 83.3 mg, 80% yield (0.4 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.32 (m, 2H), 7.29-7.20 (m, 4H), 7.07 (t, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 3.40-3.32 (m, 1H), 3.18-3.11 (m, 1H), 2.81-2.74 (m, 1H), 2.42-2.35 (m, 1H), 2.00 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4, 146.1, 146.0, 145.1, 141.7, 131.8, 130.0, 129.0, 128.2, 127.7, 127.5, 126.9, 126.7, 124.8, 124.3, 64.7, 41.6, 31.7, 16.0; IR (thin film): ν_{max} (cm^{-1}) = 3672, 2975, 2951, 2923, 1650, 1599, 1570, 1475, 1437, 1366, 1252, 1198, 1131, 1073, 1018, 976, 915, 888, 772, 755, 662, 612; HRMS (ESI) calcd for $C_{19}H_{17}O$ $[M + H]^+$: 261.1274; Found: 261.1272.



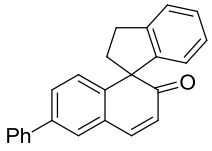
4j

Yellow solid, m.p. = 119-121 ℃; 198.6 mg, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.51 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.39-7.31 (m, 3H), 7.23 (td, *J* = 7.6, 0.8 Hz, 1H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.78 (d, *J* = 7.6 Hz, 1H), 3.85 (s, 3H), 3.37-3.29 (m, 1H), 3.16-3.09 (m, 1H), 2.93-2.87 (m, 1H), 2.43-2.36 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 165.2, 150.5, 147.7, 145.1, 143.9, 132.1, 131.2, 128.0, 127.9, 127.8, 127.3, 126.8, 125.1, 124.9, 124.6, 66.5, 52.3, 40.5, 31.4; IR (thin film): ν_{max} (cm^{-1}) = 2992, 2945, 1735, 1712, 1668, 1614, 1565, 1473, 1447, 1429, 1366, 1316, 1294, 1263, 1212, 1149, 1131, 1052, 988, 965, 944, 841, 798, 750, 621; HRMS (ESI) calcd for $C_{20}H_{17}O_3$ $[M + H]^+$: 305.1172; Found: 305.1171.



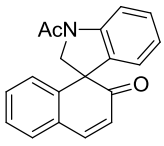
4k

Light yellow solid, m.p. = 83-85 ℃; 246.1 mg, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 9.6 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.45-7.39 (m, 3H), 7.37-7.33 (m, 3H), 7.31-7.27 (m, 1H), 7.24-7.19 (m, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.6 Hz, 1H), 6.19 (d, *J* = 9.6 Hz, 1H), 3.39-3.31 (m, 1H), 3.19-3.12 (m, 1H), 2.87-2.81 (m, 1H), 2.47-2.40 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.0, 147.1, 145.4, 145.2, 144.7, 142.8, 140.0, 129.6, 128.7, 128.5, 127.8, 127.7, 127.0, 126.8, 126.7, 125.7, 124.8, 124.4, 124.2, 65.3, 41.8, 31.5; IR (thin film): ν_{max} (cm^{-1}) = 3028, 2952, 2929, 1662, 1600, 1549, 1479, 1451, 1386, 1292, 1234, 1212, 1187, 1151, 1111, 1075, 1022, 982, 898, 850, 754, 718, 692, 647; HRMS (ESI) calcd for $C_{24}H_{19}O$ $[M + H]^+$: 323.1430; Found: 323.1429.



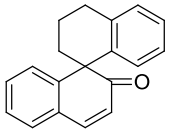
4l

Light yellow solid, m.p. = 149-151 ℃; 244.2 mg, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.55 (m, 4H), 7.47 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.37-7.33 (m, 2H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 1H), 6.22 (d, *J* = 9.6 Hz, 1H), 3.39-3.31 (m, 1H), 3.19-3.12 (m, 1H), 2.85-2.79 (m, 1H), 2.43-2.36 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.1, 145.5, 145.4, 145.2, 145.1, 140.0, 139.8, 129.7, 128.8, 128.7, 128.5, 127.73, 127.67, 127.6, 126.87, 126.85, 124.85, 124.81, 124.4, 64.9, 41.8, 31.5; IR (thin film): ν_{max} (cm^{-1}) = 2953, 2905, 1661, 1619, 1599, 1556, 1480, 1452, 1372, 1296, 1261, 1237, 1188, 1111, 1076, 1051, 1025, 926, 890, 841, 820, 757, 721, 693; HRMS (ESI) calcd for $C_{24}H_{19}O$ $[M + H]^+$: 323.1430; Found: 323.1430.



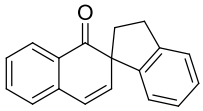
4m

Light yellow solid, m.p. = 159-161 ℃; 42.7 mg, 74% yield (0.2 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 10.0 Hz, 1H), 7.41-7.38 (m, 1H), 7.35-7.31 (m, 2H), 7.23-7.17 (m, 2H), 6.87-6.83 (m, 1H), 6.78 (d, *J* = 7.2 Hz, 1H), 6.28 (d, *J* = 10.0 Hz, 1H), 4.86 (d, *J* = 10.8 Hz, 1H), 4.34 (d, *J* = 10.8 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8, 168.3, 146.2, 144.8, 142.0, 134.6, 131.0, 129.7, 128.9, 128.2, 127.8, 127.2, 124.1, 123.8, 122.7, 117.7, 60.6, 59.4, 24.3; IR (thin film): ν_{max} (cm^{-1}) = 3295, 3028, 2924, 2853, 1662, 1560, 1478, 1404, 1337, 1283, 1238, 1215, 1193, 1163, 1133, 1094, 1024, 950, 861, 839, 811, 763, 695, 618; HRMS (ESI) calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$: 290.1176; Found: 290.1174.



4n

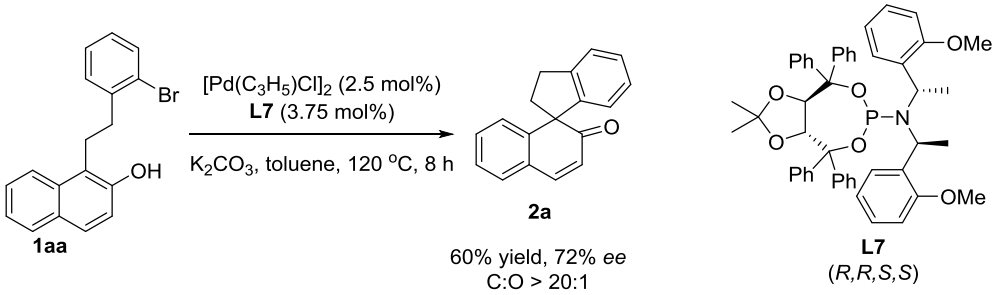
Light yellow oil, 200.4 mg, 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 10.0 Hz, 1H), 7.33-7.31 (m, 1H), 7.24-7.13 (m, 4H), 7.00 (t, *J* = 6.4 Hz, 1H), 6.81 (d, *J* = 8.4 Hz, 1H), 6.54 (d, *J* = 7.6 Hz, 1H), 6.15 (d, *J* = 9.6 Hz, 1H), 2.91-2.90 (m, 2H), 2.21-2.16 (m, 1H), 2.00-1.89 (m, 2H), 1.80-1.73 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.3, 148.8, 144.2, 138.7, 137.2, 130.6, 129.64, 129.56, 129.1, 129.0, 126.9, 126.7, 126.1, 123.8, 58.3, 39.0, 29.6, 17.8; IR (thin film): ν_{max} (cm^{-1}) = 3060, 3018, 2927, 2855, 1657, 1618, 1563, 1487, 1446, 1395, 1287, 1261, 1228, 1124, 1097, 1065, 1038, 1001, 964, 876, 823, 747, 665; HRMS (ESI) calcd for $C_{19}H_{17}O$ $[M + H]^+$: 261.1274; Found: 261.1273.



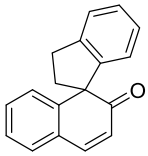
4o

Light yellow oil, 40.6 mg, 88% yield (0.2 mmol scale). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.6 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.37-7.29 (m, 3H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 9.6 Hz, 1H), 6.22 (d, *J* = 9.6 Hz, 1H), 3.49-3.41 (m, 1H), 3.13-3.06 (m, 1H), 2.77-2.71 (m, 1H), 2.26-2.19 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.3, 145.1, 143.5, 138.9, 138.6, 134.4, 128.5, 128.1, 127.9, 127.3, 127.1, 126.5, 125.5, 123.9, 123.4, 62.2, 37.7, 32.2; IR (thin film): ν_{max} (cm^{-1}) = 3063, 3026, 2930, 2852, 1668, 1593, 1455, 1390, 1284, 1227, 1152, 1073, 1023, 968, 881, 759, 688; HRMS (ESI) calcd for $C_{19}H_{17}O$ $[M + H]^+$: 247.1117; Found: 247.1120.

Palladium-catalyzed asymmetric arylative dearomatization reaction



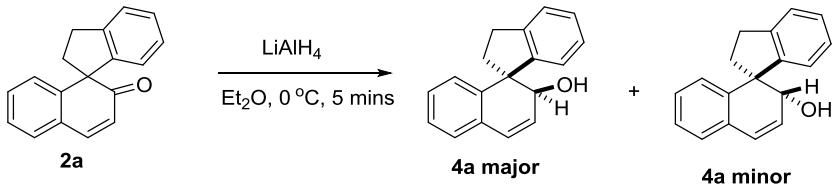
A flame-dried Schlenk tube was cooled down to room temperature under argon. To this tube were added $[Pd(C_3H_5)Cl]_2$ (1.8 mg, 0.005 mmol, 2.5 mol %), (*R*,*R*,*S*,*S*)-**L7** (5.9 mg, 0.0075 mmol, 3.75 mol %), K_2CO_3 (41.5 mg, 0.3 mmol, 1.5 equiv.) and toluene (1.0 mL). After the reaction was stirred at room temperature for 30 minutes, **1aa** (65.5 mg, 0.2 mmol) was added. Then the reaction was stirred at 120 ^oC. After 10 h, the reaction mixture was cooled to room temperature and diluted with ethyl acetate (3mL). The mixture was filtered through celite, and the filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE/EtOAc = 30/1) to afford the desired product **2a**.



2a

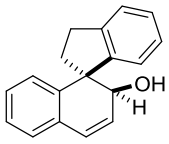
Light yellow oil, 29.5 mg, 60% yield, 72% *ee* [Daicel Chiralpak AD-H, *n*-hexane/2-propanol =99/1, v = 1.0 mL·min^{-1}, λ = 254 nm, t (minor) = 12.96 min, t (major) = 15.57 min]; $[\alpha]_D^{20}$ = + 129.3 (c = 0.4, $CHCl_3$).

Transformations of 2a.



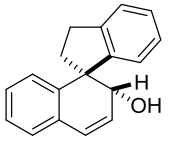
2a **4a major** **4a minor**

A flame-dried Schlenk tube was cooled down to room temperature under argon. To this tube were added **2a** (98.4 mg, 0.40 mmol) and Et_2O (3.0 mL). Then the reaction mixture was cooled to 0 ℃ followed by adding $LiAlH_4$ (15.2 mg, 0.40 mmol). After completion (5 minutes), the reaction was quenched by adding H_2O (1.0 mL). The mixture was filtered and the filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE/EtOAc = 30/1) to afford **4a major** (80.4 mg, 81% yield) and **4a minor** (11.6 mg, 12% yield).



4a major

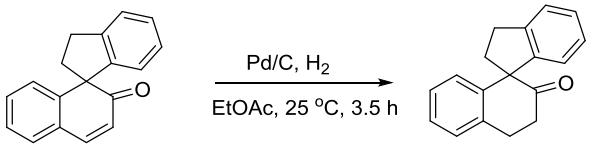
Colorless oil, 80.4 mg, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) 7.31-7.22 (m, 4H), 7.17-7.09 (m, 2H), 7.01 (td, *J* = 7.6, 1.6 Hz, 1H), 6.57 (d, *J* = 7.6 Hz, 1H), 6.48 (dd, *J* = 10.0, 2.8 Hz, 1H), 5.99 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.99 (t, *J* = 2.4 Hz, 1H), 2.97-2.81 (m, 3H), 1.92-1.84 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 145.0, 142.2, 132.5, 131.4, 127.7, 127.58, 127.56, 126.83, 126.78, 126.6, 126.2, 124.8, 124.2, 74.5, 59.2, 31.7, 30.6; IR (thin film): ν_{max} (cm^{-1}) = 3538, 3431, 3023, 2932, 2845, 1952, 1917, 1811, 1633, 1596, 1478, 1365, 1221, 1164, 1111, 1066, 1016, 956, 912, 871, 829, 751; HRMS (ESI) calcd for $C_{18}H_{15}$ $[M - OH]^+$: 231.1168; Found: 231.1169.



4a minor

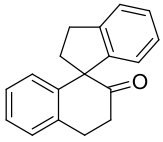
Colorless oil, 11.6 mg, 12% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.30 (td, *J* = 7.2, 1.2 Hz, 1H), 7.26-7.24 (m, 1H), 7.2-7.12 (m, 3H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 9.6 Hz, 1H), 6.22 (dd, *J* = 9.6,

5.6 Hz, 1H), 4.07 (d, *J* = 5.6 Hz, 1H), 3.06-2.98 (m, 1H), 2.95-2.88 (m, 1H), 2.51-2.45(m, 1H), 1.96-1.89 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 143.9, 141.1, 131.8, 130.3, 128.4, 127.6, 127.4, 127.23, 127.19, 127.0, 126.8, 126.3, 124.9, 69.1, 57.7, 37.8, 30.2; IR (thin film): ν_{max} (cm^{-1}) = 3552, 3431, 3024, 2931, 2853, 1950, 1918, 1810, 1727, 1632, 1594, 1479, 1400, 1272, 1215, 1159, 1038, 956, 917, 867, 751; HRMS (ESI) calcd for $C_{18}H_{15}$ $[M - OH]^+$: 231.1168; Found: 231.1170.



2a **5a**
83% yield

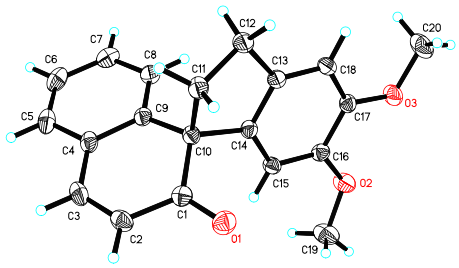
A flame-dried Schlenk tube was cooled down to room temperature under argon. To this tube were added **2a** (49.2 mg, 0.20 mmol), EtOAc (2.0 mL) and Pd/C (20 mg). Then the reaction mixture was subjected to hydrogen (1 atm.). The mixture was stirred at room temperature for 3.5 h. After completion, the mixture was filtered and the filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE/EtOAc = 30/1) to afford **5a** (40.9 mg, 83% yield).



5a

Colorless oil, 40.9 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 7.2 Hz, 1H), 7.24-7.20 (m, 2H), 7.29-7.11 (m, 3H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 1H), 3.31-3.12 (m, 3H), 3.07-3.00 (m, 1H), 2.82 (dd, *J* = 8.4, 5.2 Hz, 2H), 2.78-2.71 (m, 1H), 2.31-2.24 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.7, 145.7, 145.0, 142.6, 136.0, 128.4, 127.7, 127.6, 127.0, 126.7, 126.5, 125.4, 124.5, 65.5, 41.0, 37.6, 31.4, 28.9; IR (thin film): ν_{max} (cm^{-1}) = 3659, 3548, 3020, 2931, 2851, 1955, 1708, 1605, 1480, 1445, 1347, 1298, 1263, 1228, 1162, 1120, 1092, 1027, 748; HRMS (ESI) calcd for $C_{18}H_{20}$ NO $[M + NH_4]^+$: 266.1539; Found: 266.1542.

X-Ray of 2c (CCDC 1534422)



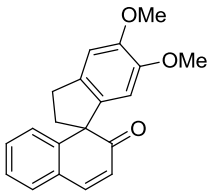


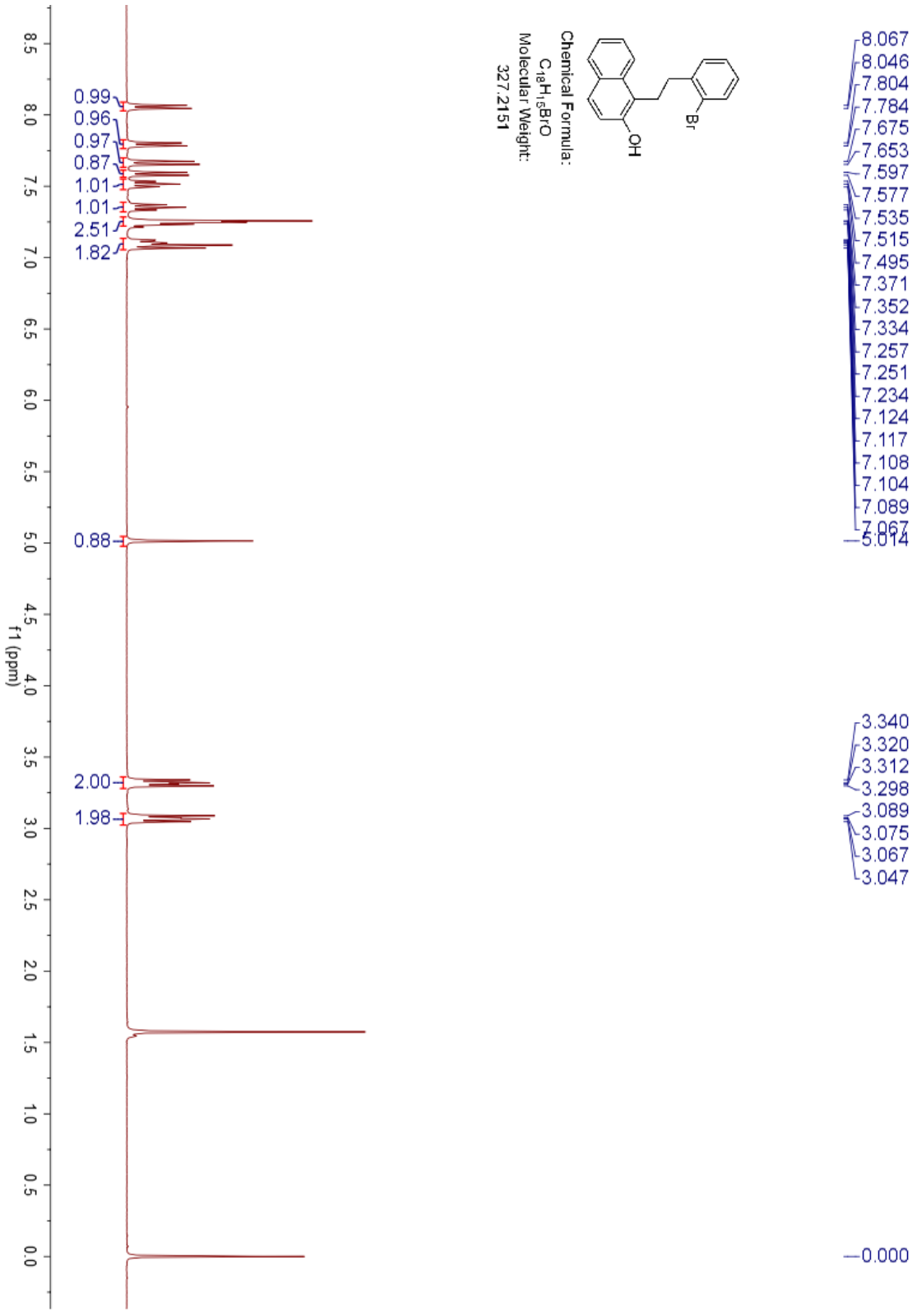
Table 1. Crystal data and structure refinement for cd214584.

Identification code	cd214584	
Empirical formula	C20 H18 O3	
Formula weight	306.34	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 27.179(3) Å	a= 90 °.
	b = 6.7881(7) Å	b= 127.703(2) °.
	c = 20.759(2) Å	g = 90 °.
Volume	3030.2(5) $Å^3$	
Z	8	
Density (calculated)	1.343 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	1296	
Crystal size	0.211 x 0.165 x 0.123 mm^3	
Theta range for data collection	1.998 to 25.991 °.	
Index ranges	-33<=h<=33, -4<=k<=8, -25<=l<=25	
Reflections collected	8734	
Independent reflections	2978 [R(int) = 0.0307]	
Completeness to theta = 25.242 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6484	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2978 / 0 / 210	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.1083	
R indices (all data)	R1 = 0.0482, wR2 = 0.1145	
Extinction coefficient	n/a	

Largest diff. peak and hole	0.192 and -0.221 e.Å^{-3}

References

(1) Nina, B., Igor, O., Bogdan A, Š. *Synlett* **2013**, *24*, 49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7.577
7.535
7.515
7.495
7.371
7.352
7.334
7.257
7.251
7.234
7.124
7.117
7.108
7.104
7.089
7.067
5.014
3.340
3.320
3.312
3.298
3.089
3.075
3.067
3.047
0.000
0.99
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0.97
0.87
1.01
1.01
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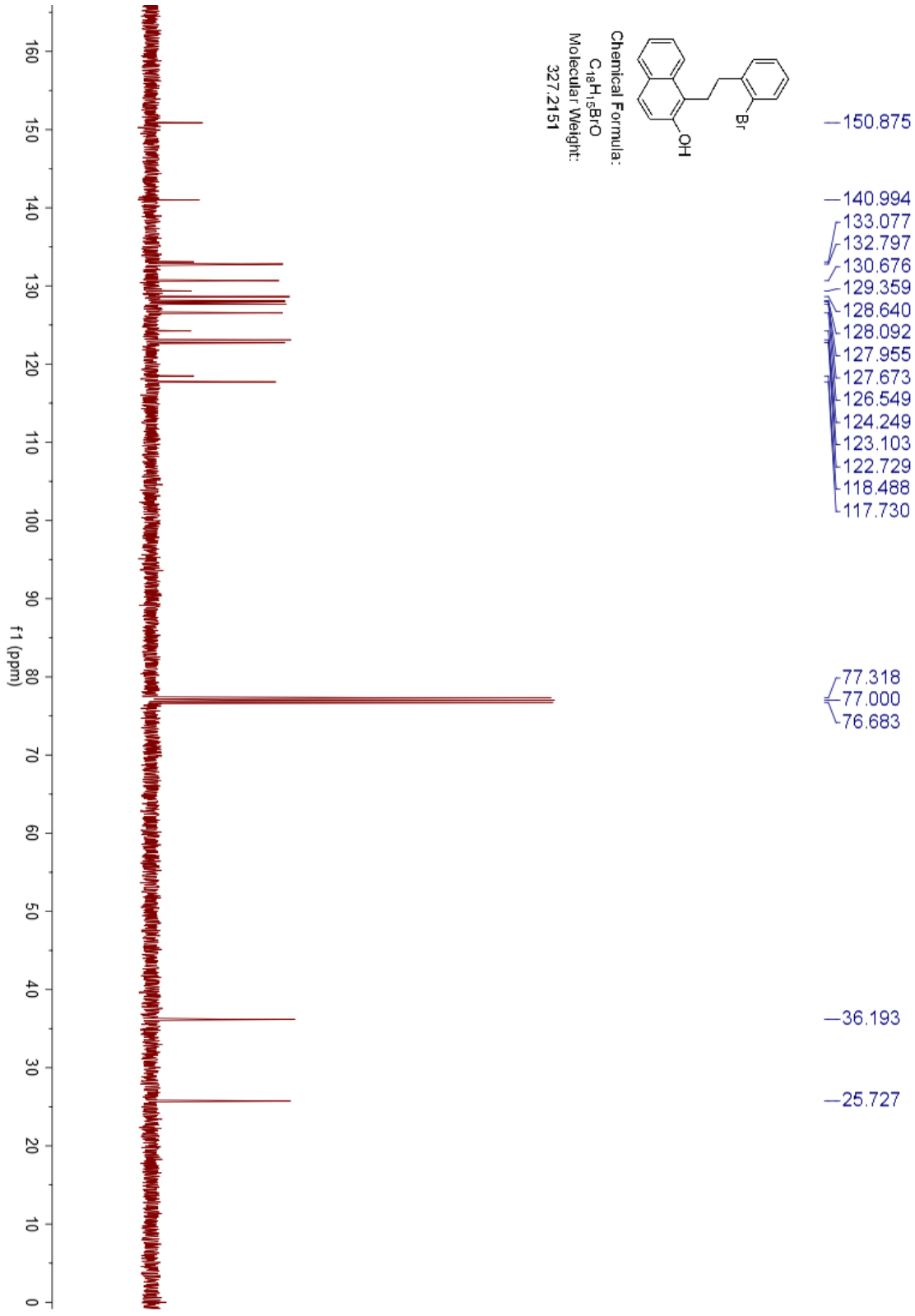
2.00
1.98
f1 (ppm)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128.640
128.092
127.955
127.673
126.549
124.249
123.103
122.729
118.488
117.730
77.318
77.000
76.683
36.193
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f1 (ppm)
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10
20
30
40
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60
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80
90
100
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120
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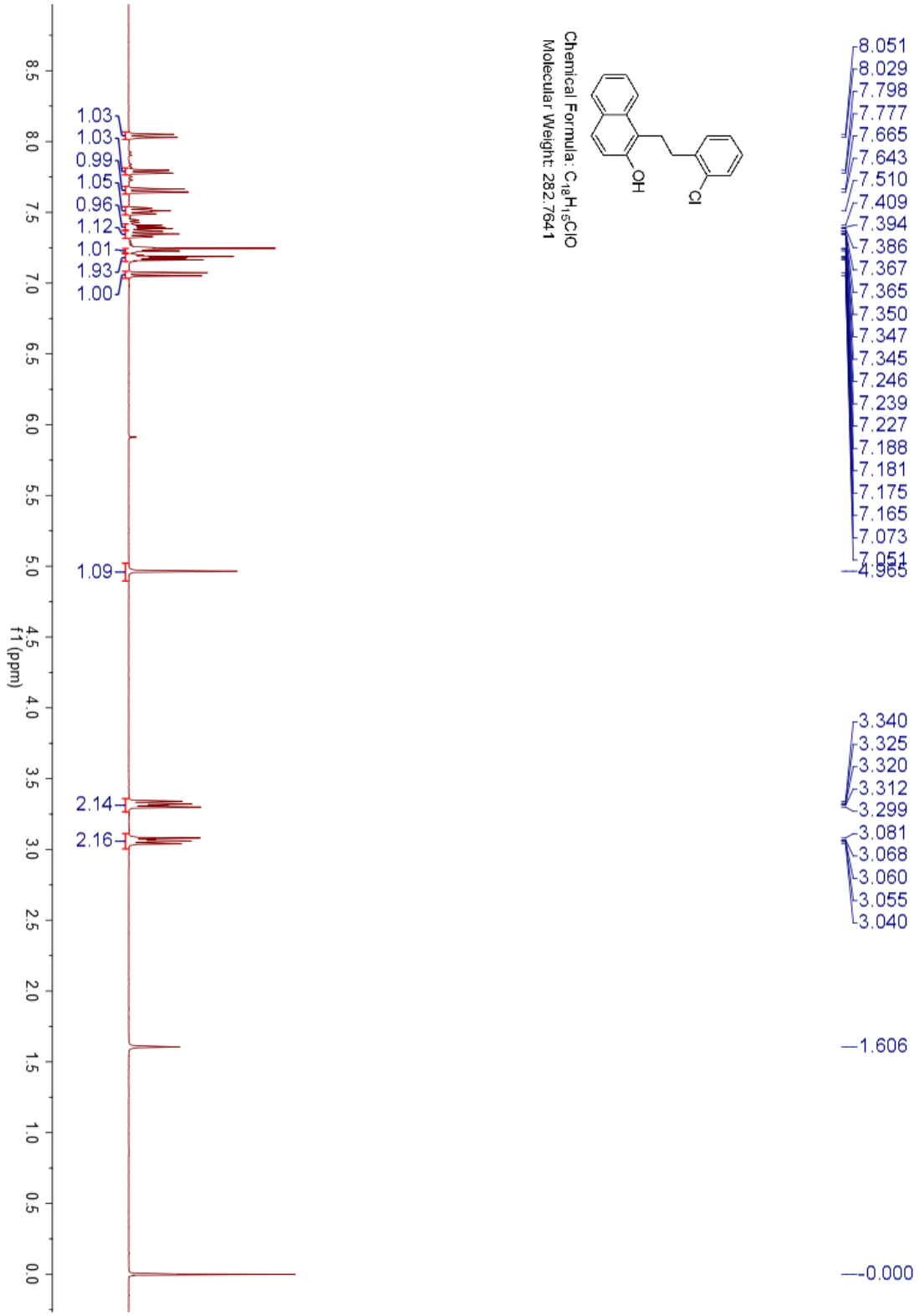
140
150
160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Molecular Weight: 282.7641
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7.394
7.386
7.367
7.365
7.350
7.347
7.345
7.246
7.239
7.227
7.188
7.181
7.175
7.165
7.073
7.051
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3.325
3.320
3.312
3.299
3.081
3.068
3.060
3.055
3.040
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0.000
1.03
1.03
0.99
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0.96
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1.01
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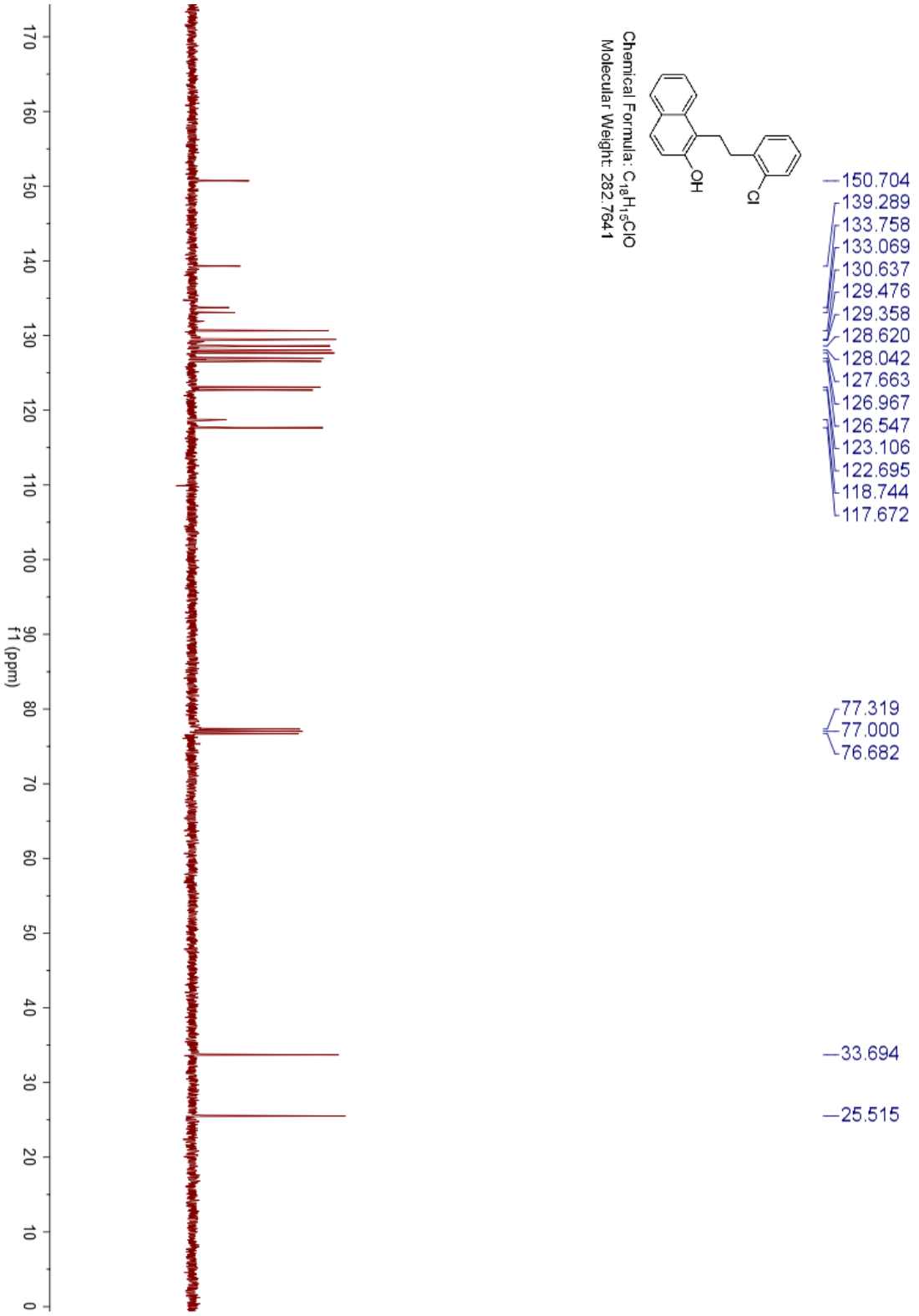
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128.042
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126.967
126.547
123.106
122.695
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77.000
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33.694
25.515
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60
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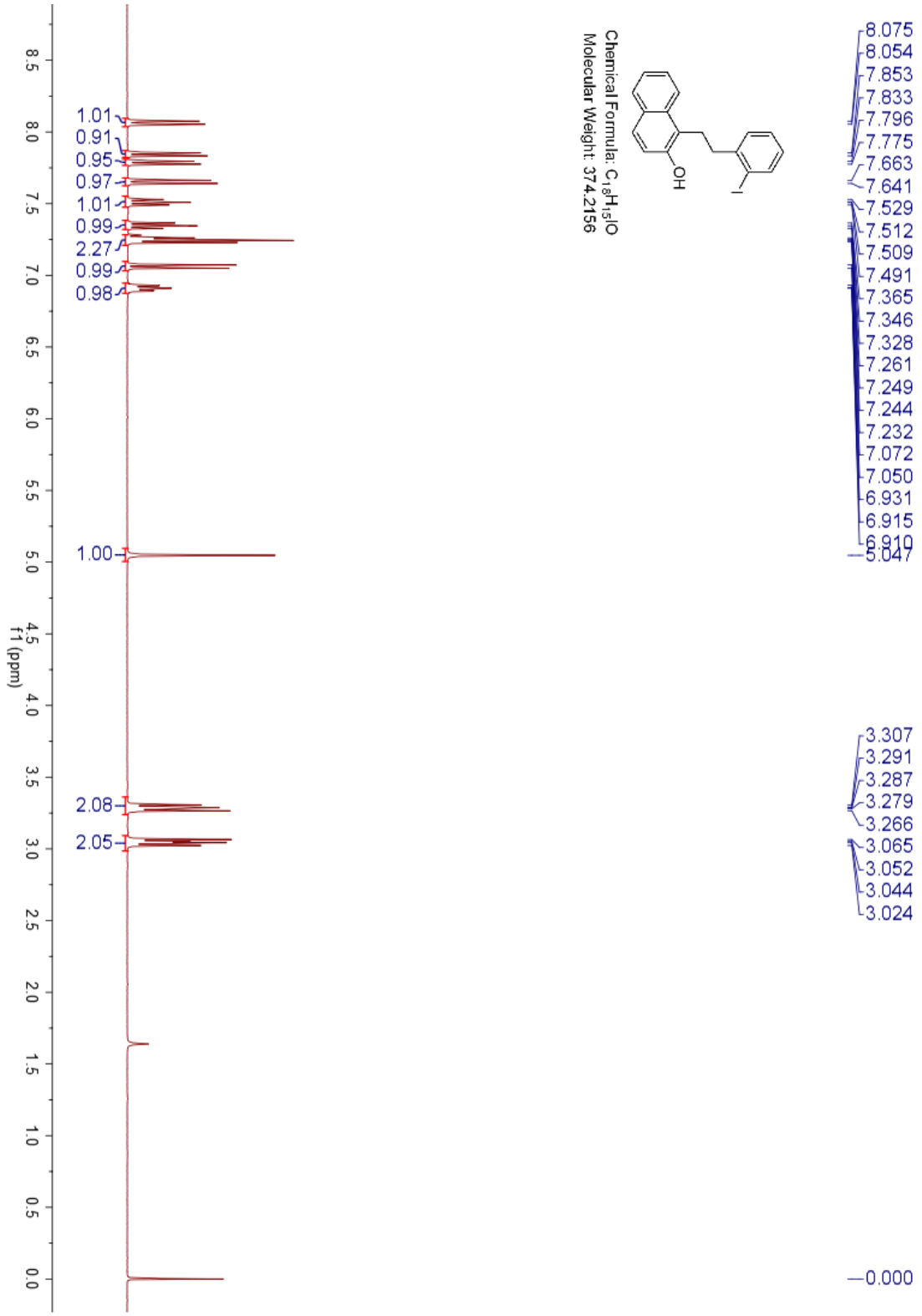
40
30
20
10
0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7.346
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7.249
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7.232
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6.910
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3.287
3.279
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3.052
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0.99
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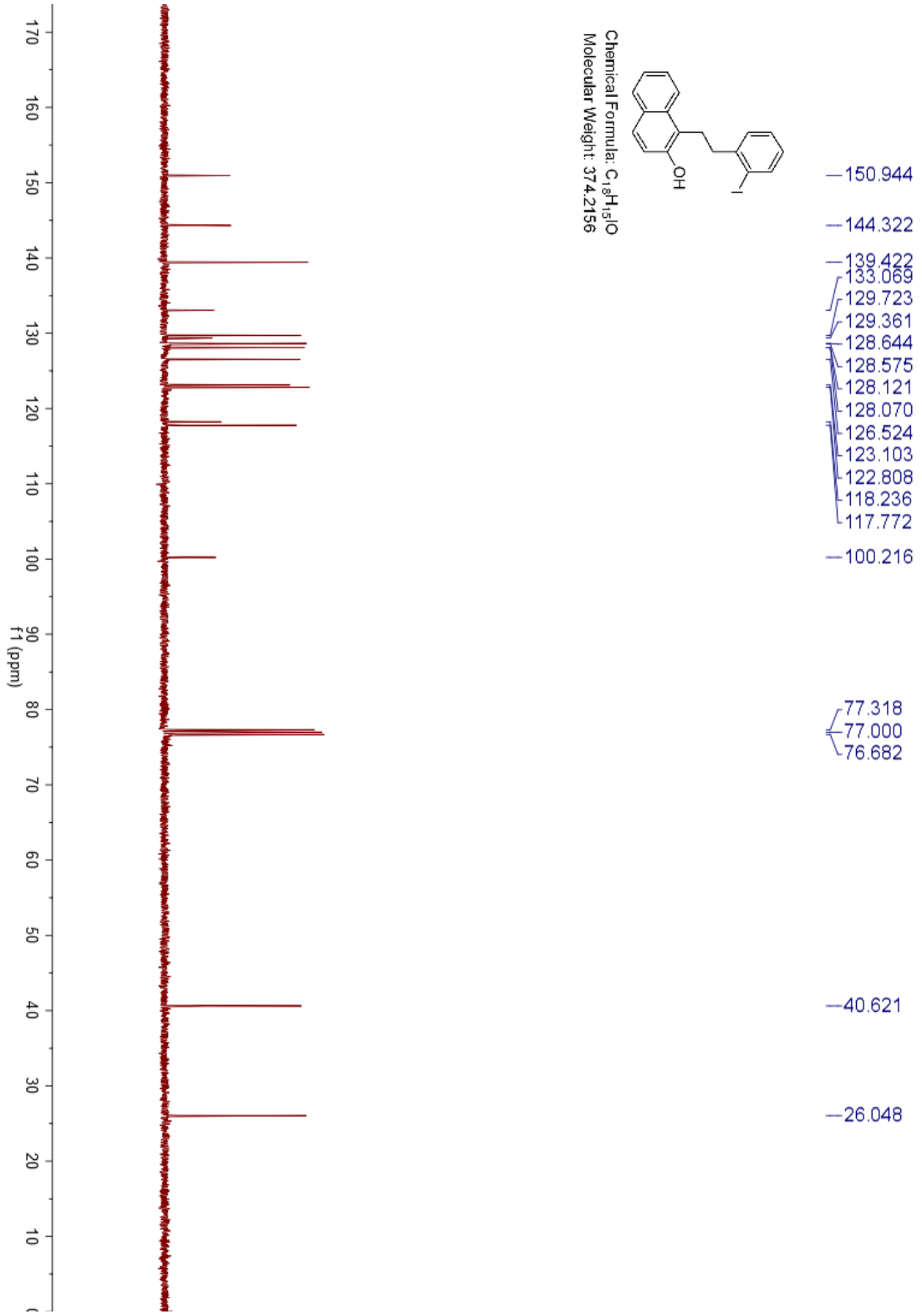
f1 (ppm)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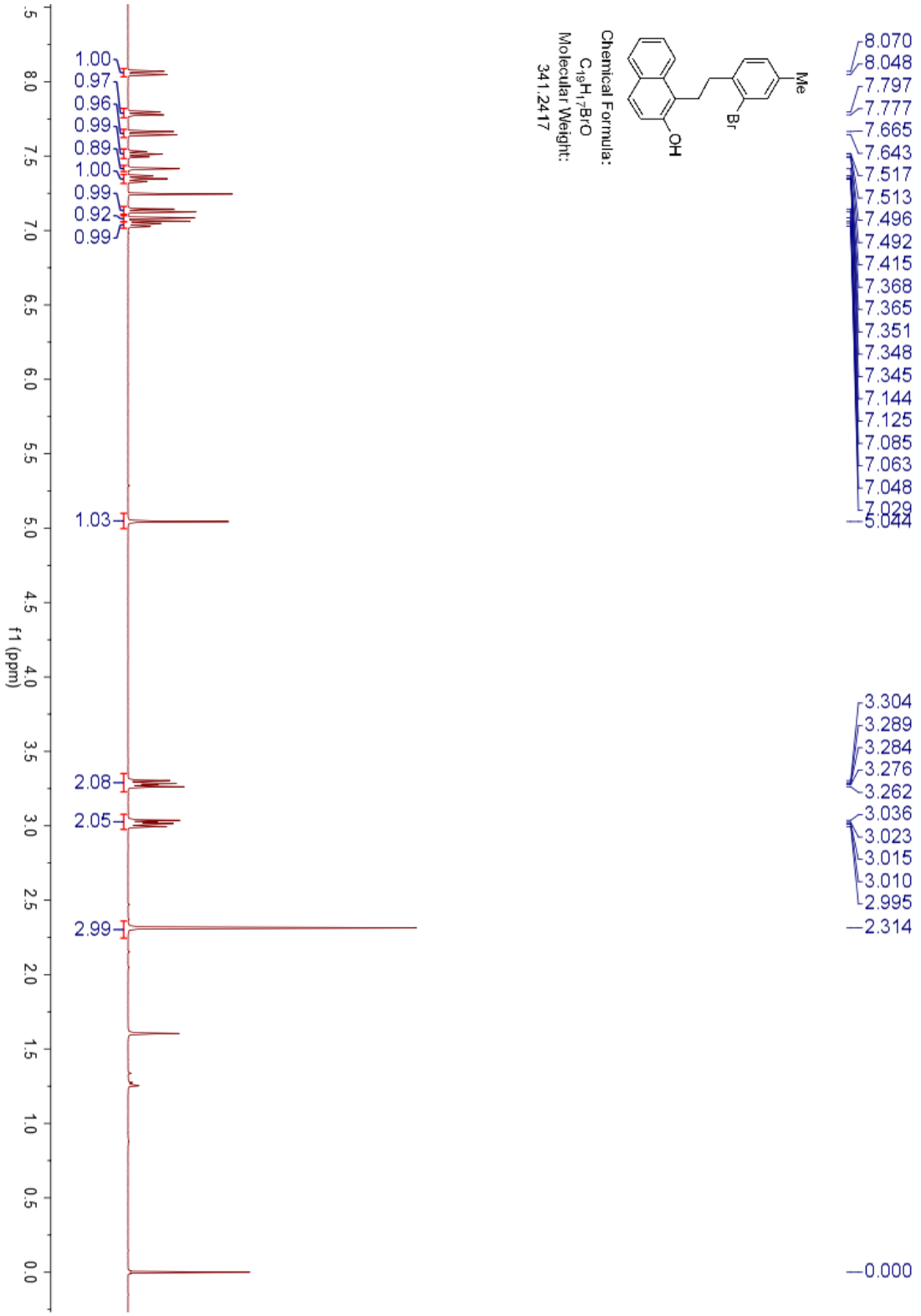
f1 (ppm)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7.513
7.496
7.492
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7.368
7.365
7.351
7.348
7.345
7.144
7.125
7.085
7.063
7.048
7.029
5.044
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3.284
3.276
3.262
3.036
3.023
3.015
3.010
2.995
2.314
0.000
1.00
0.97
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0.99
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0.99
0.92
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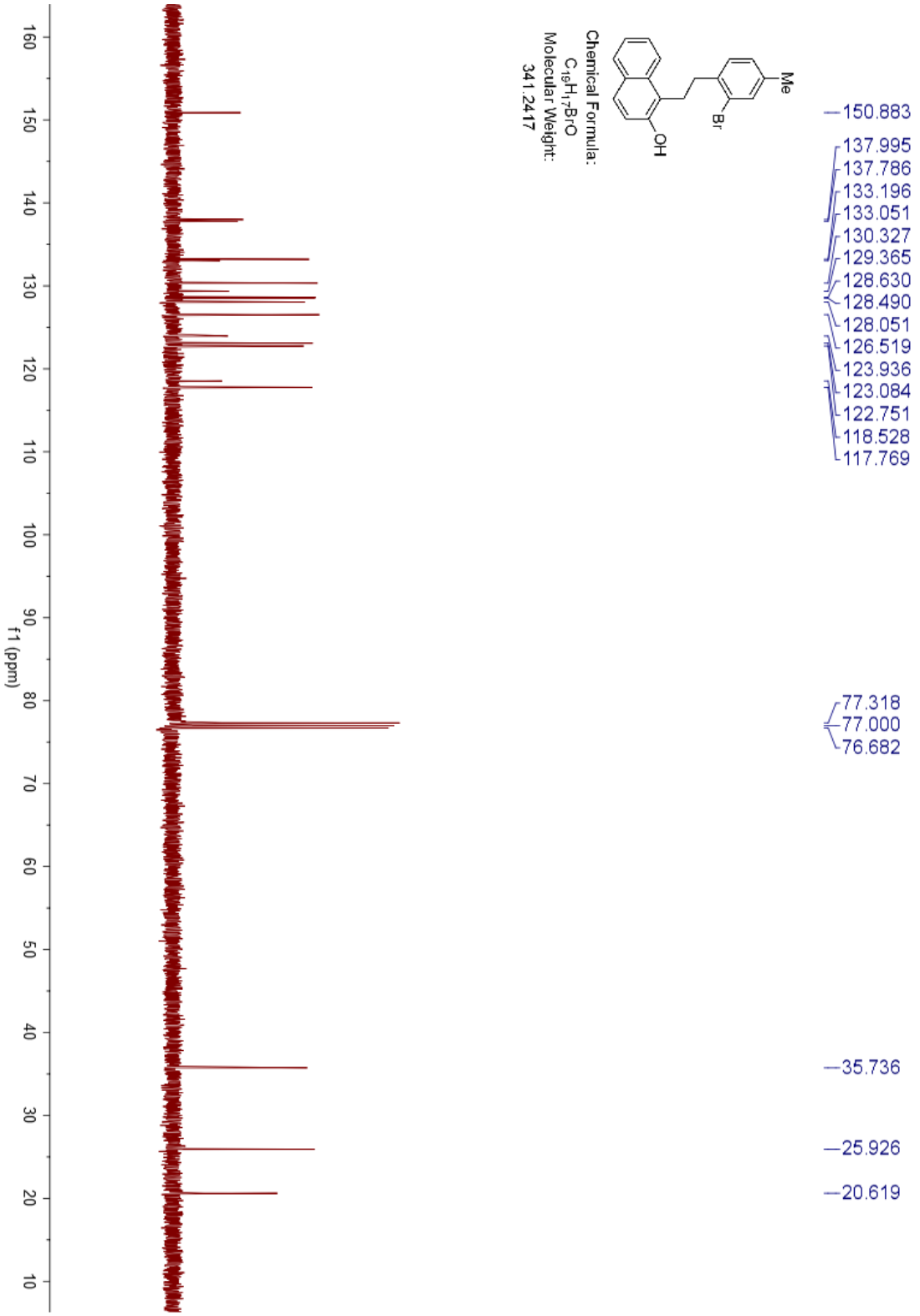
2.05
2.99
f1 (ppm)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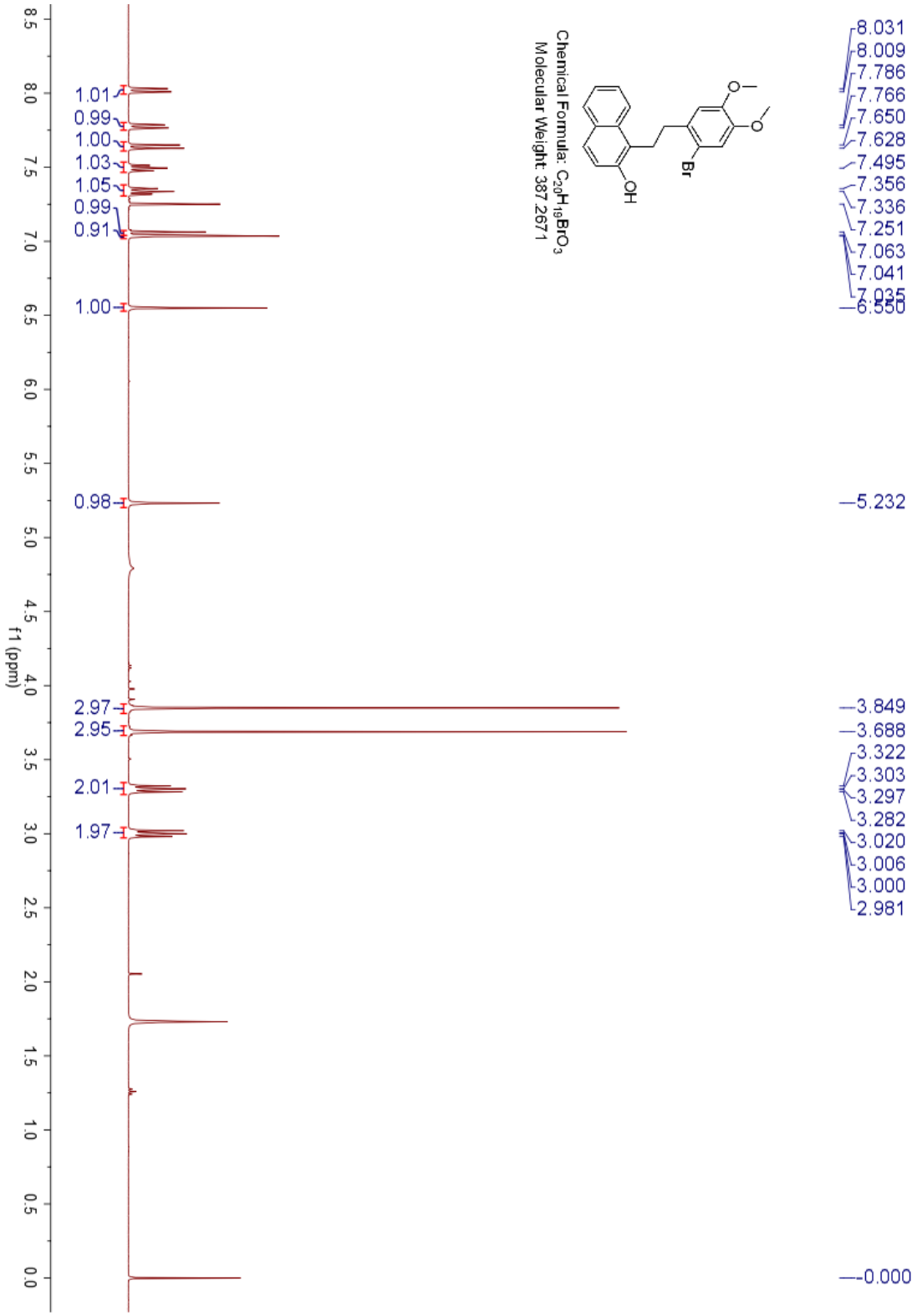
f1 (ppm)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1.05
0.99
0.91
1.00
0.98
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2.95
2.01
1.97
8.031
8.009
7.786
7.766
7.650
7.628
7.495
7.356
7.336
7.251
7.063
7.041
7.035
6.550
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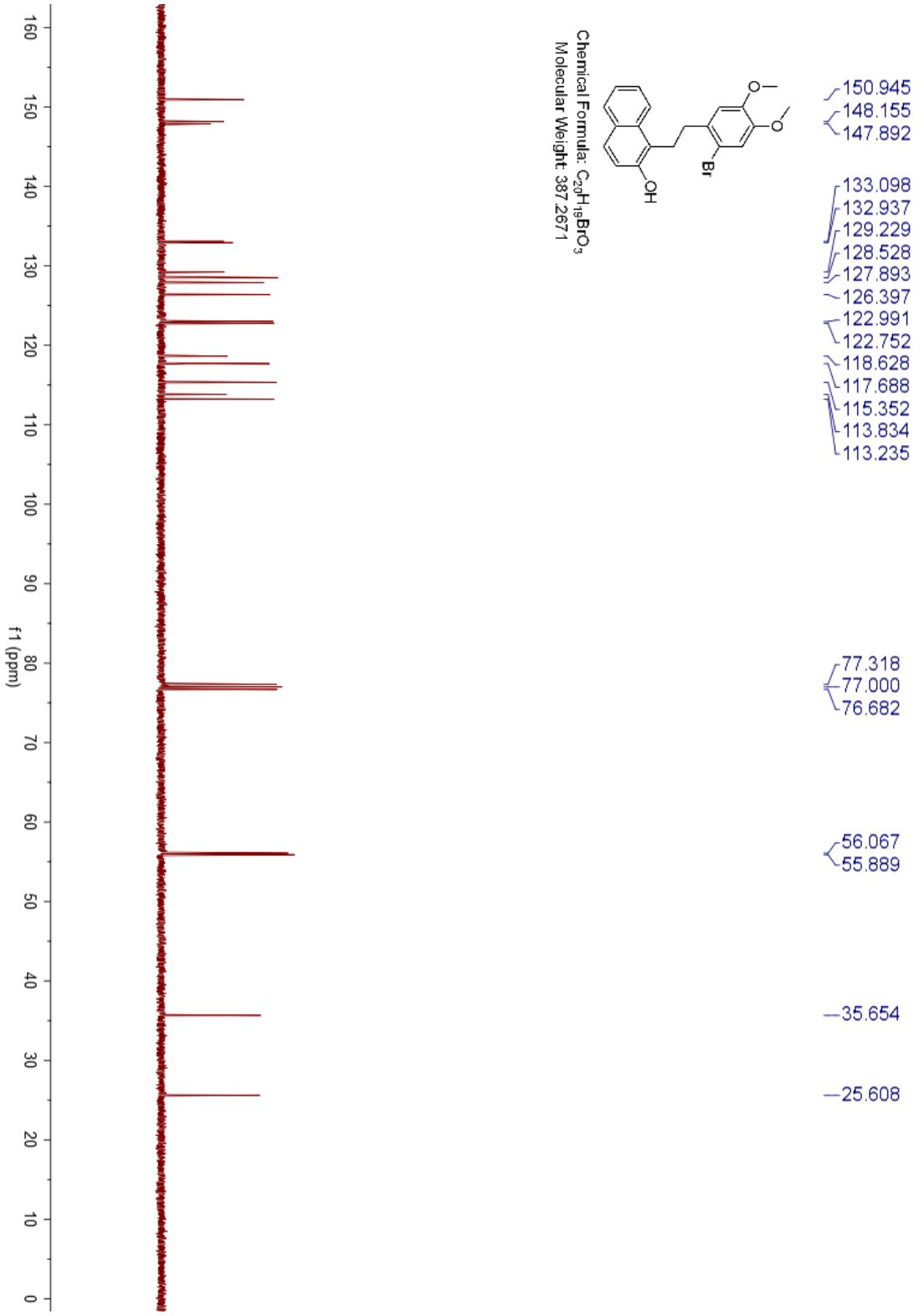
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Molecular Weight: 387.2671
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Br
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O
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118.628
117.688
115.352
113.834
113.235
77.318
77.000
76.682
56.067
55.889
35.654
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f1 (ppm)
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140
130
120
110
100
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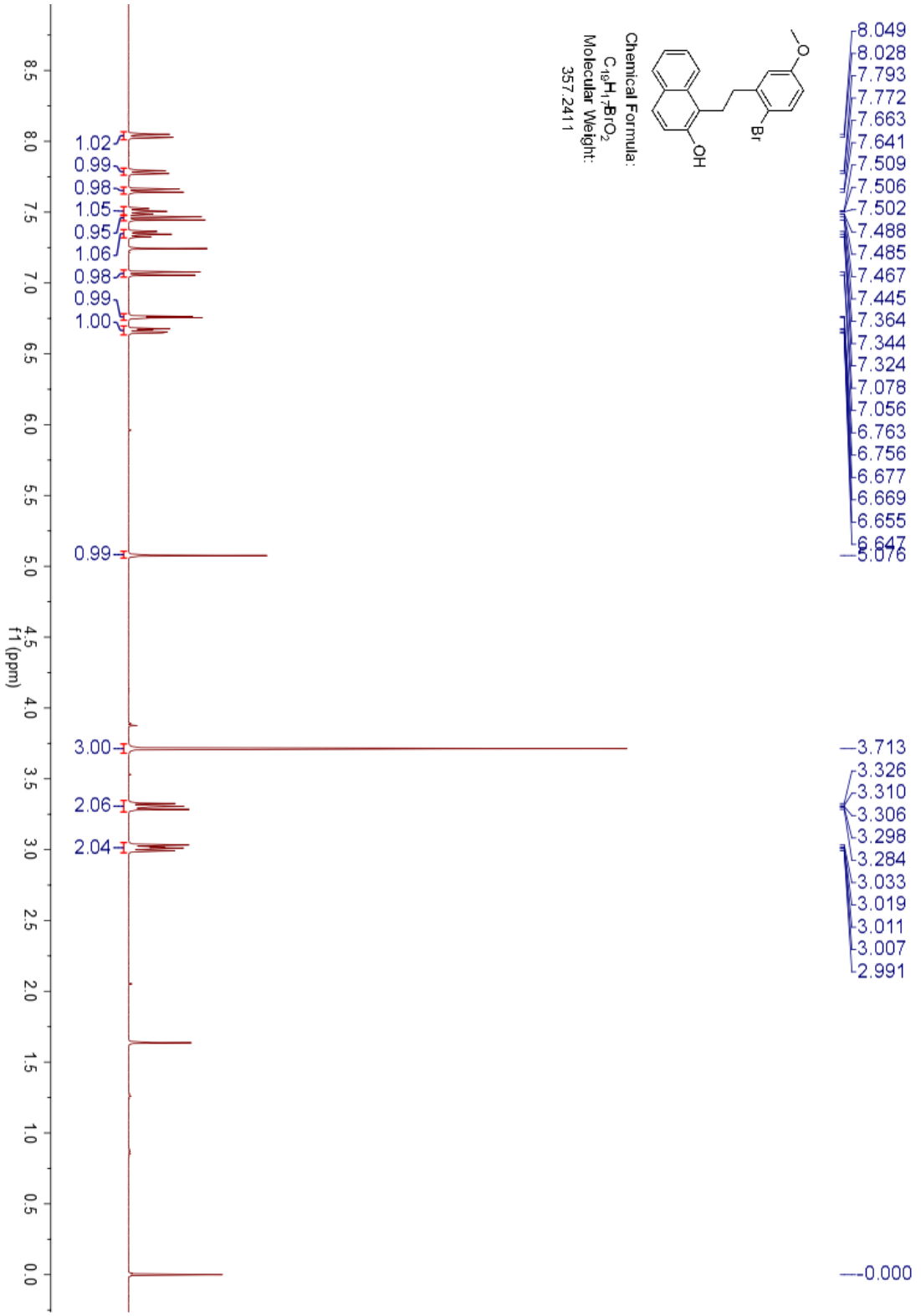
80
70
60
50
40
30
20
10
0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Molecular Weight: 357.2411
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0.98
0.99
1.00
0.99
3.00
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2.04
8.049
8.028
7.793
7.772
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7.324
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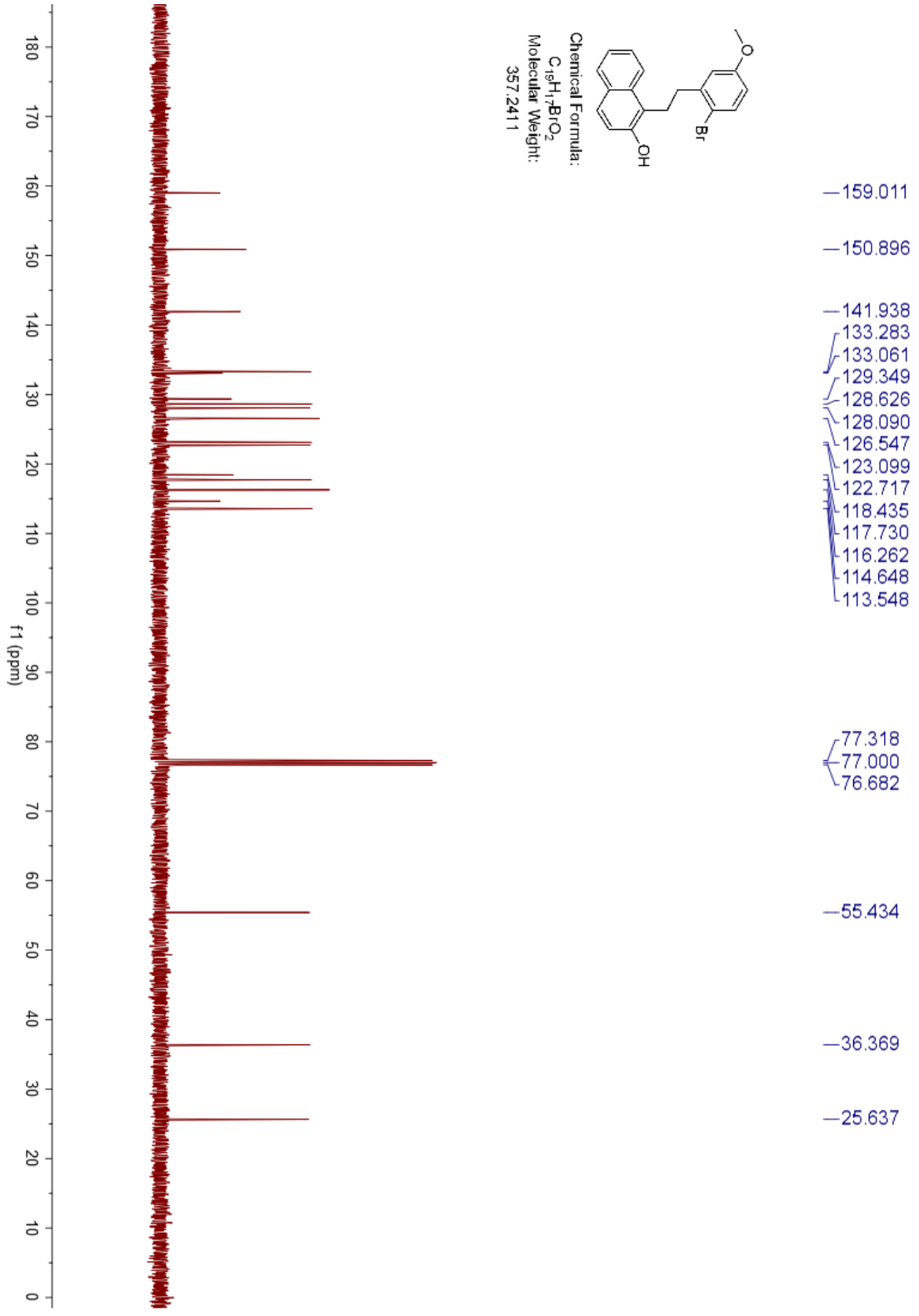
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116.262
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77.000
76.682
55.434
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25.637
f1 (ppm)
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140
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120
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60
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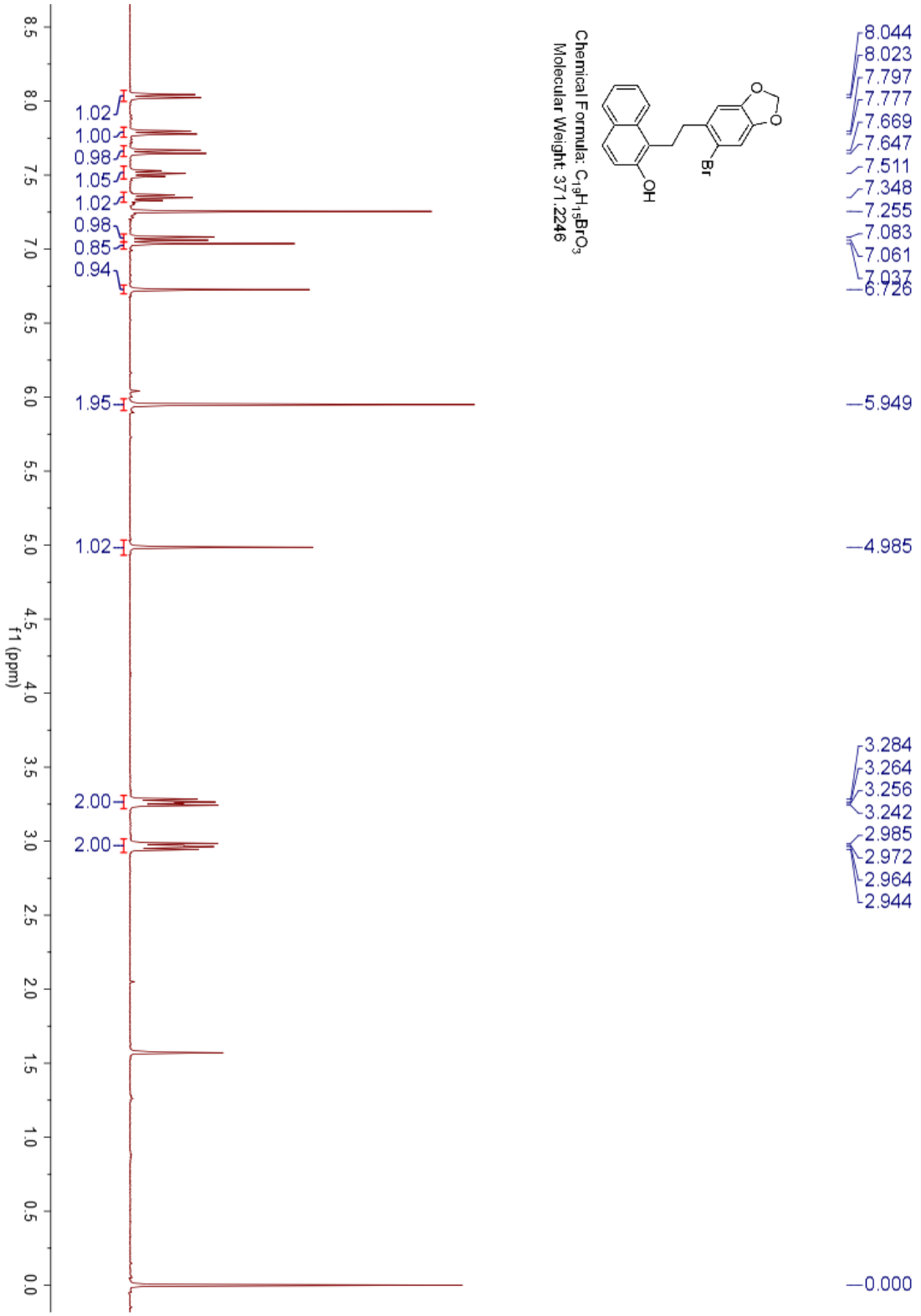
10
0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4.985
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3.264
3.256
3.242
2.985
2.972
2.964
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1.02
1.00
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0.85
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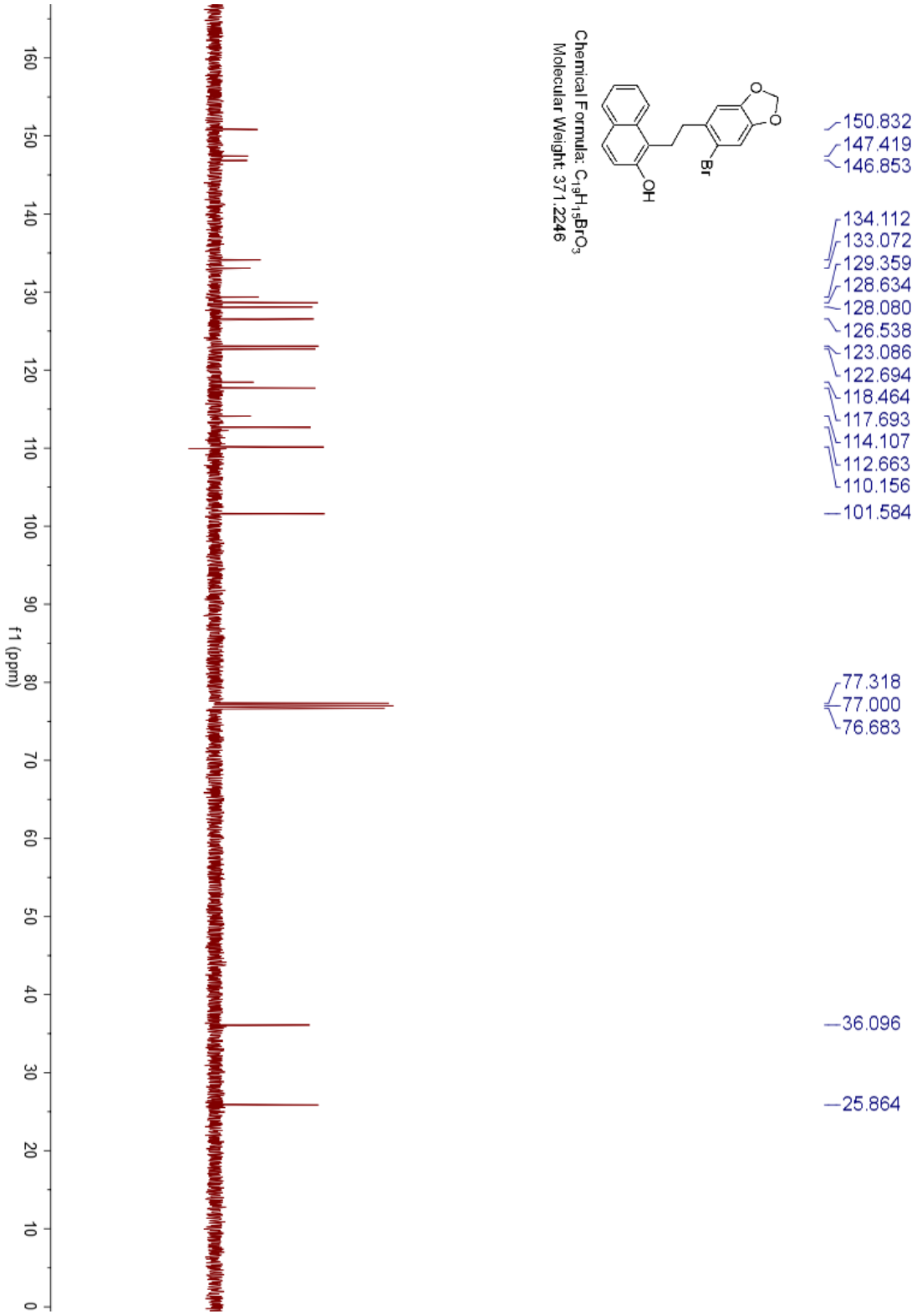
2.00
f1 (ppm)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122.694
118.464
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114.107
112.663
110.156
101.584
77.318
77.000
76.683
36.096
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140
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30
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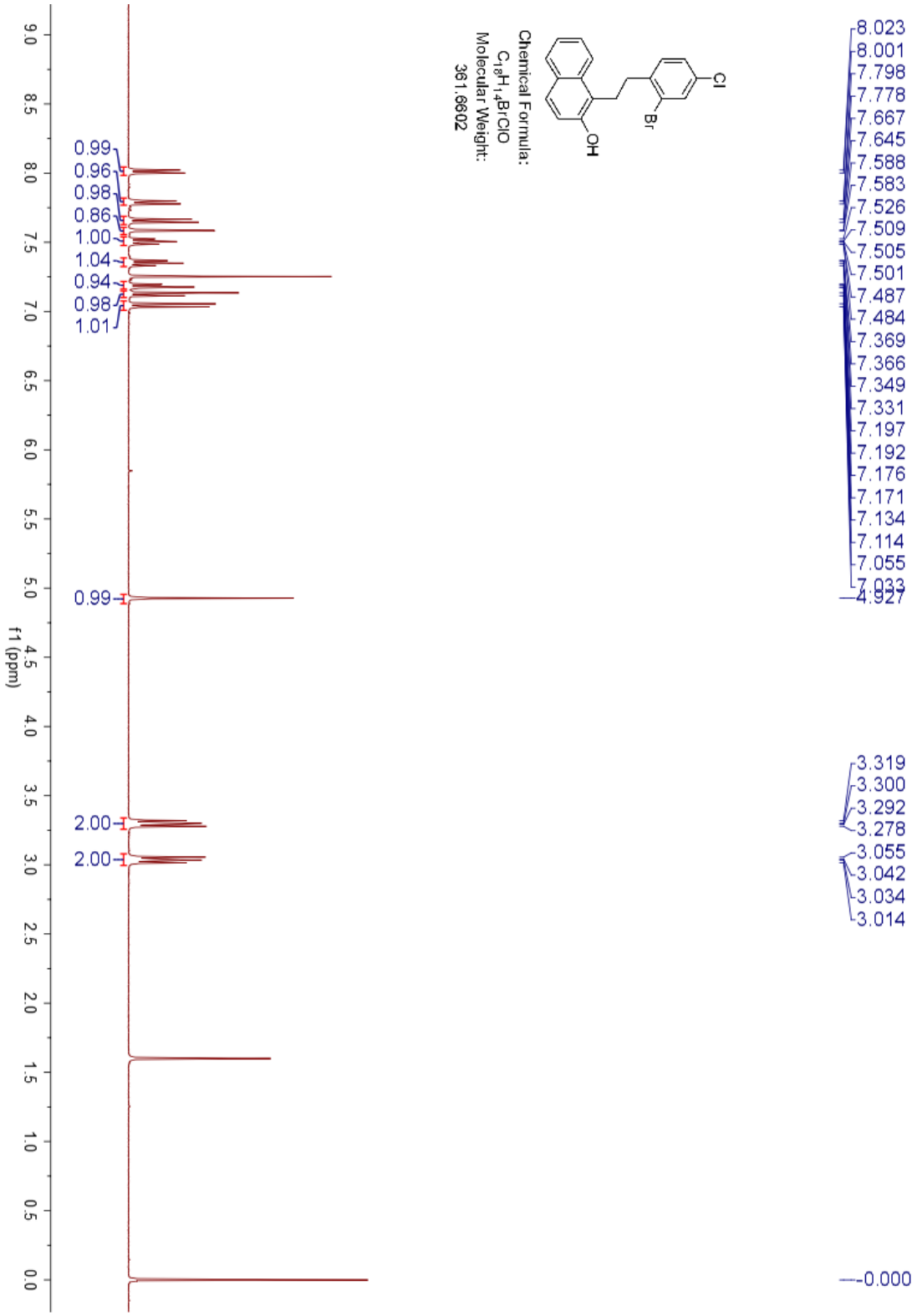
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7.509
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7.501
7.487
7.484
7.369
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7.349
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7.176
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7.134
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3.300
3.292
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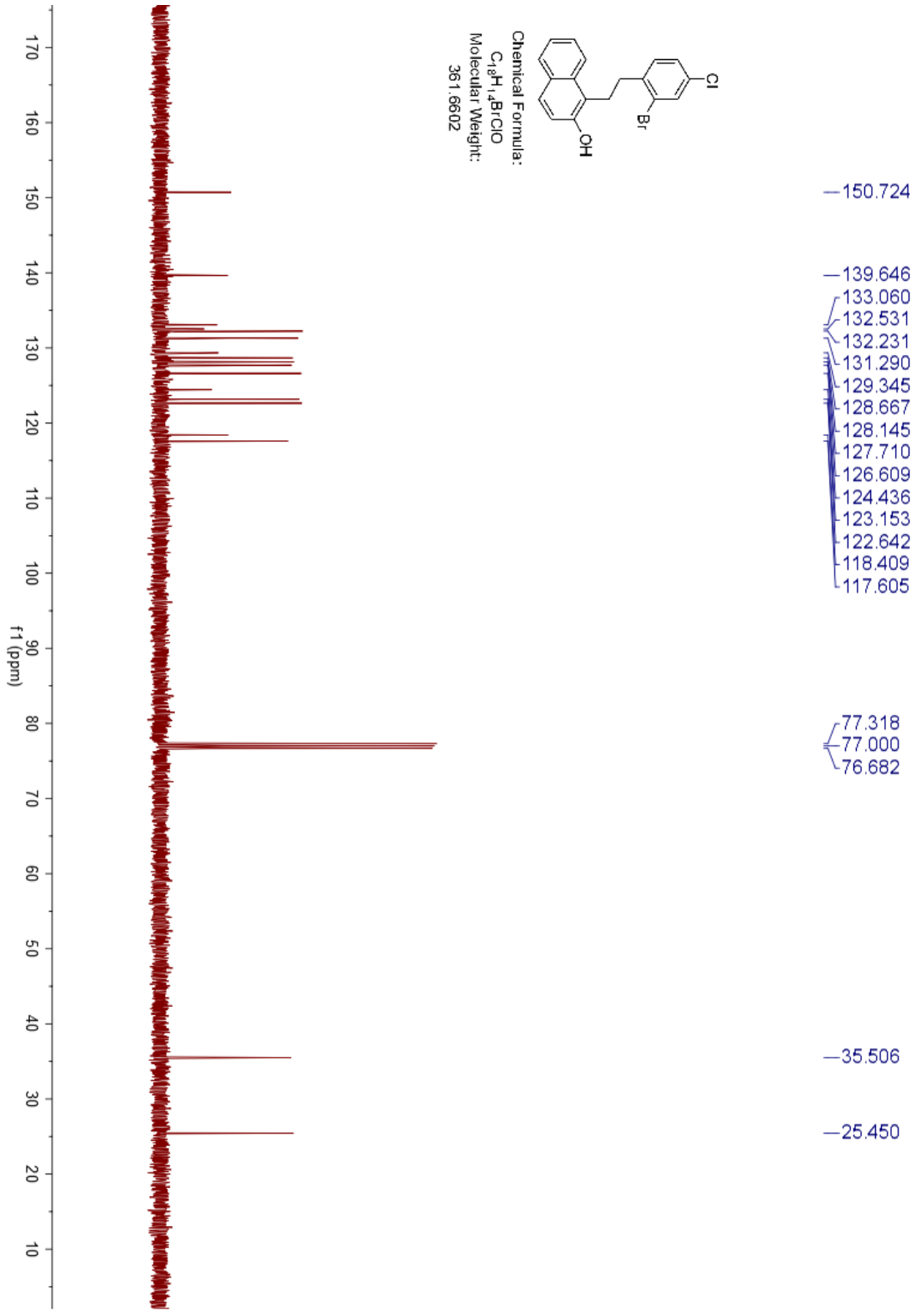
2.00
f1 (ppm)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117.605
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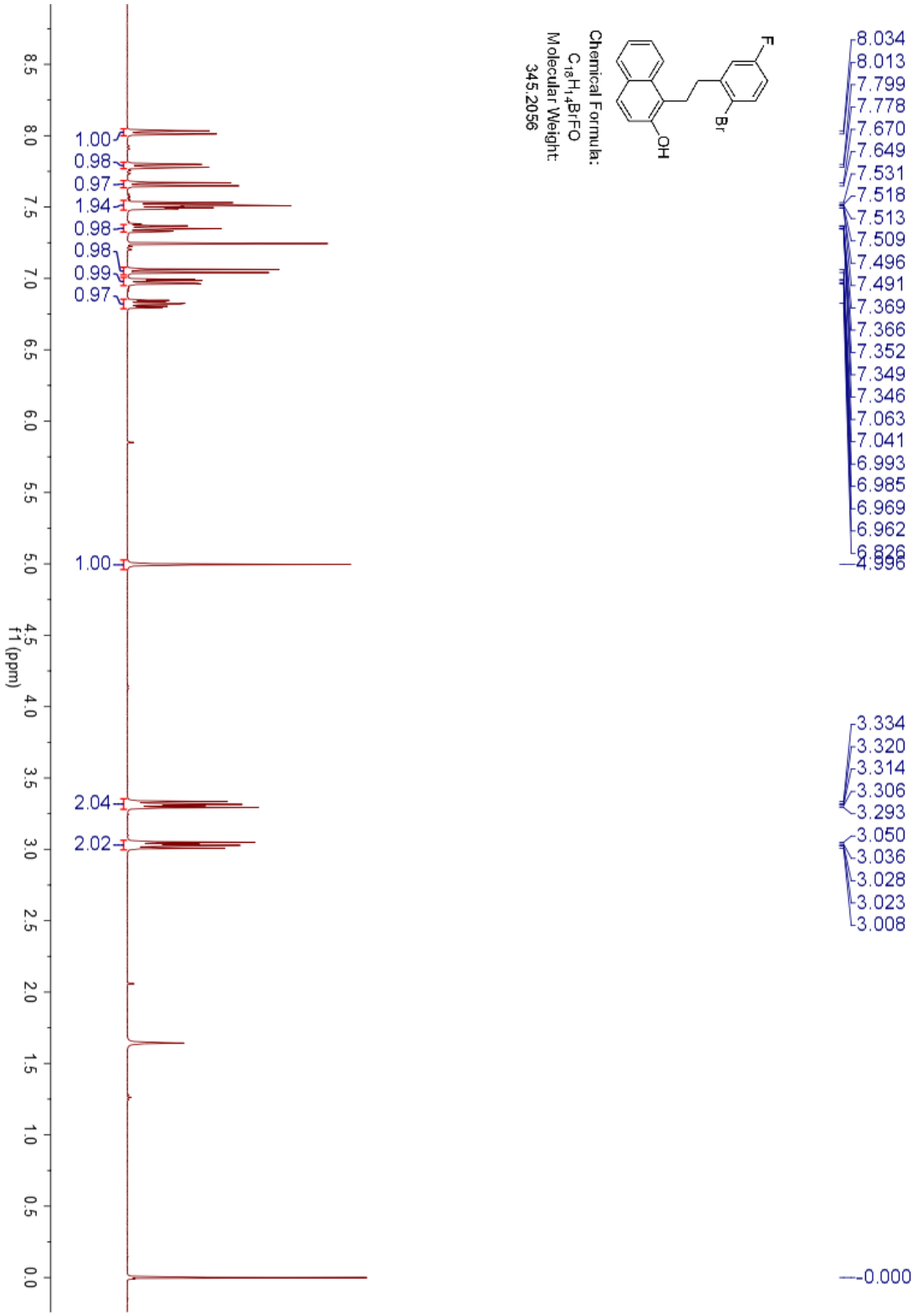
25.450
f1 (ppm)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Molecular Weight:
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7.496
7.491
7.369
7.366
7.352
7.349
7.346
7.063
7.041
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6.985
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6.962
4.996
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3.320
3.314
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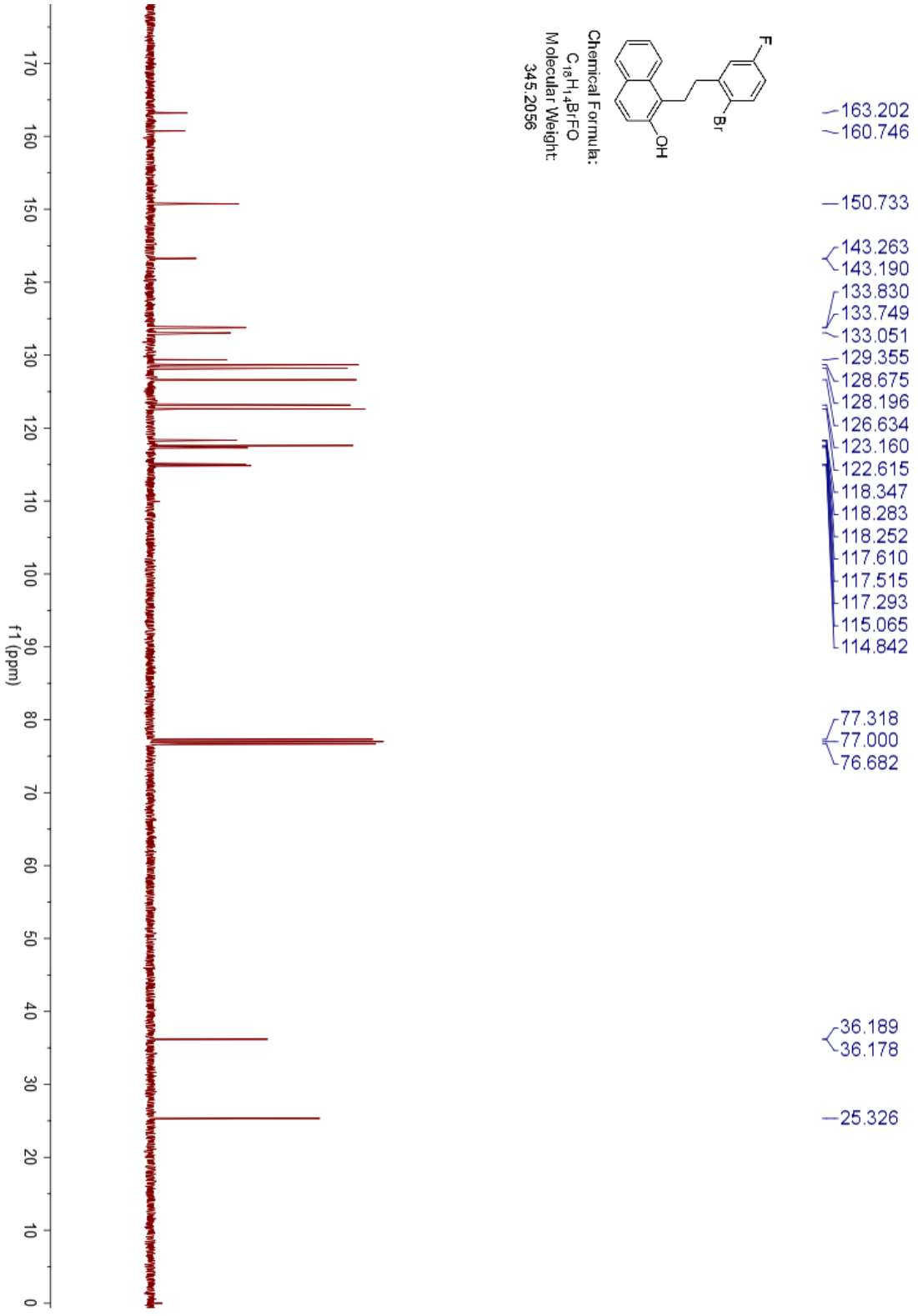
2.02
f1 (ppm)


Chemical Formula:
$C_{18}H_{14}BrFO$
Molecular Weight:
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Br
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133.749
133.051
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128.675
128.196
126.634
123.160
122.615
118.347
118.283
118.252
117.610
117.515
117.293
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25.326
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70
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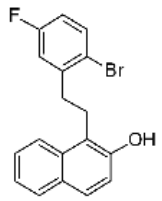

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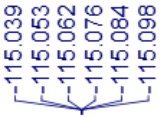
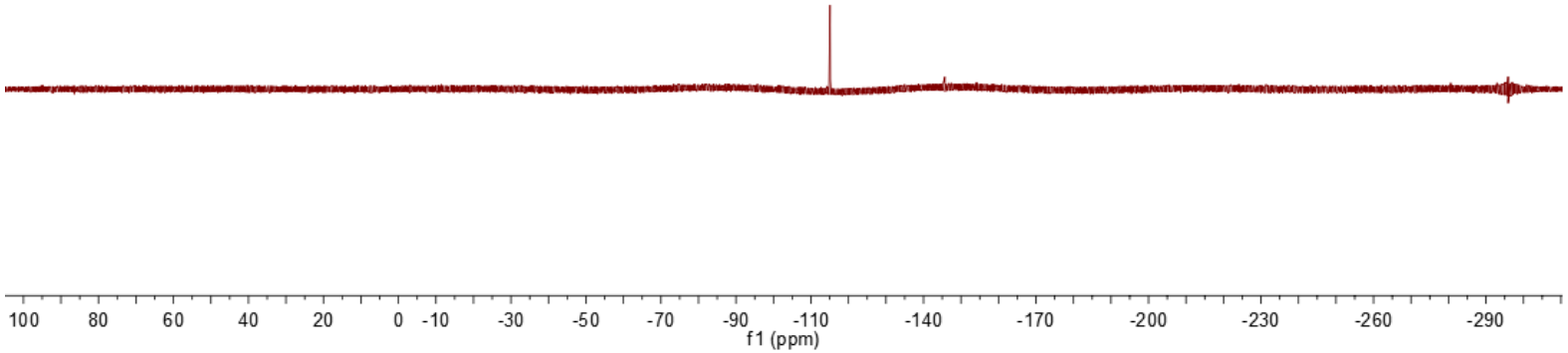
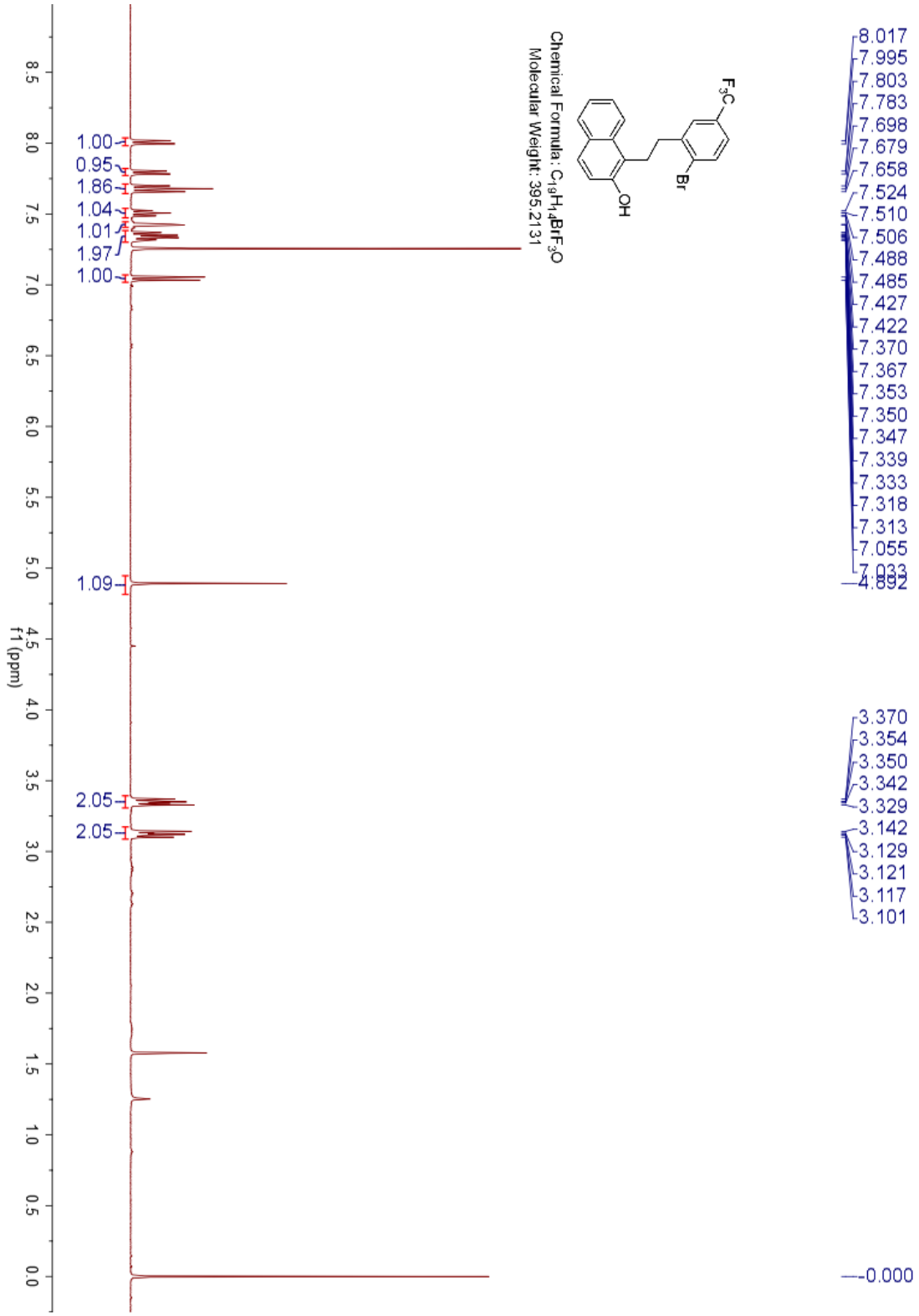
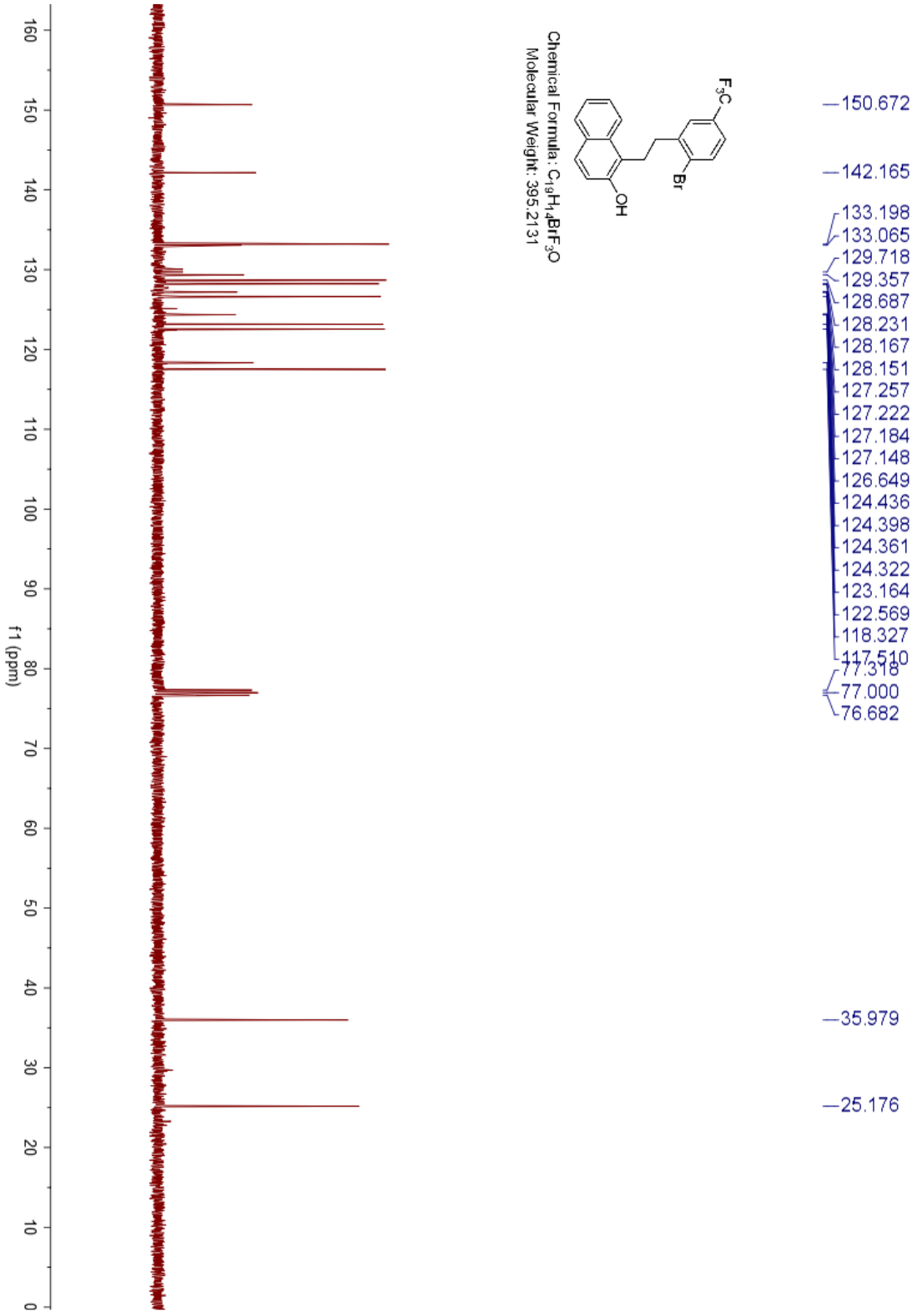
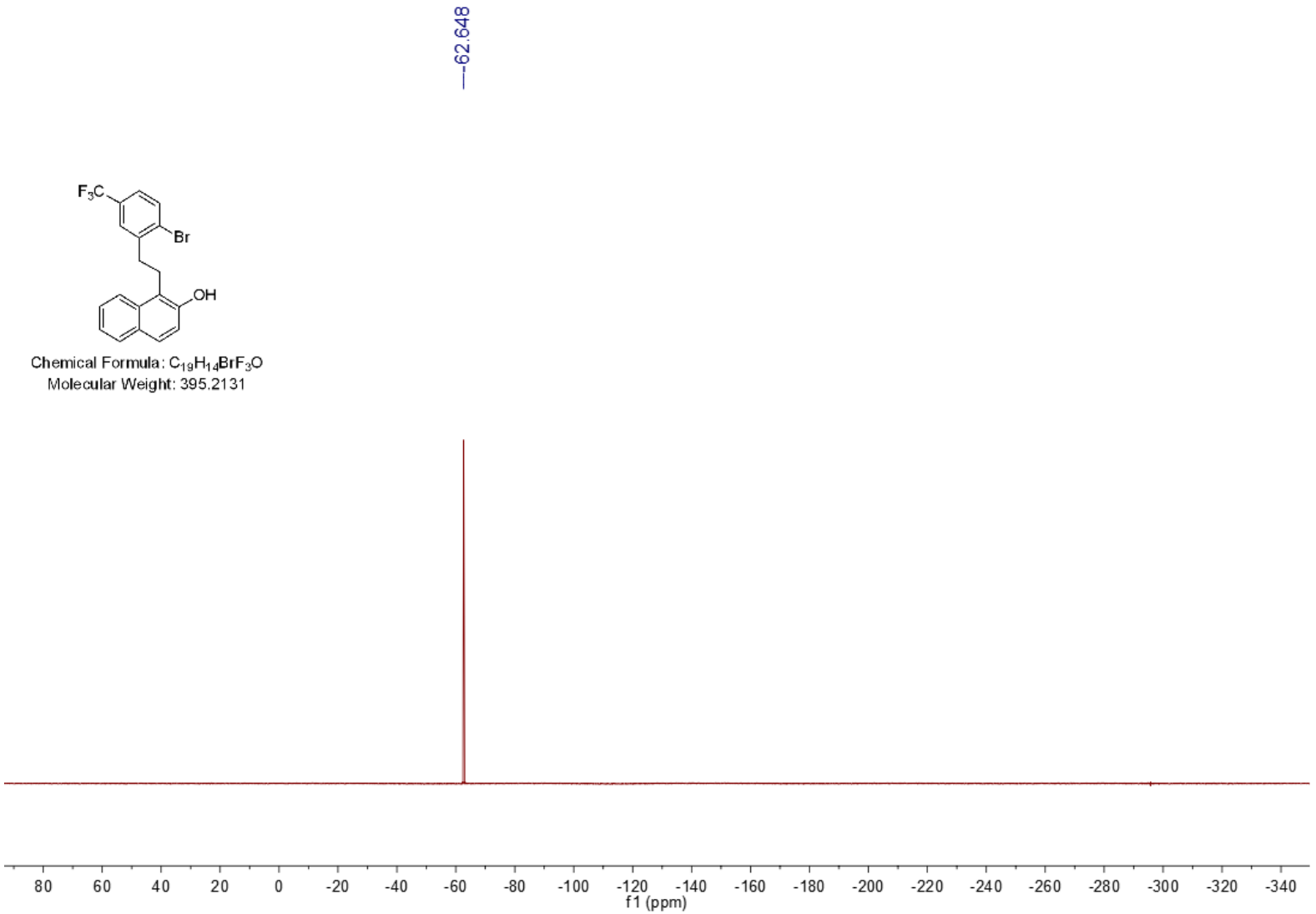
Molecular Weight:
345.2056

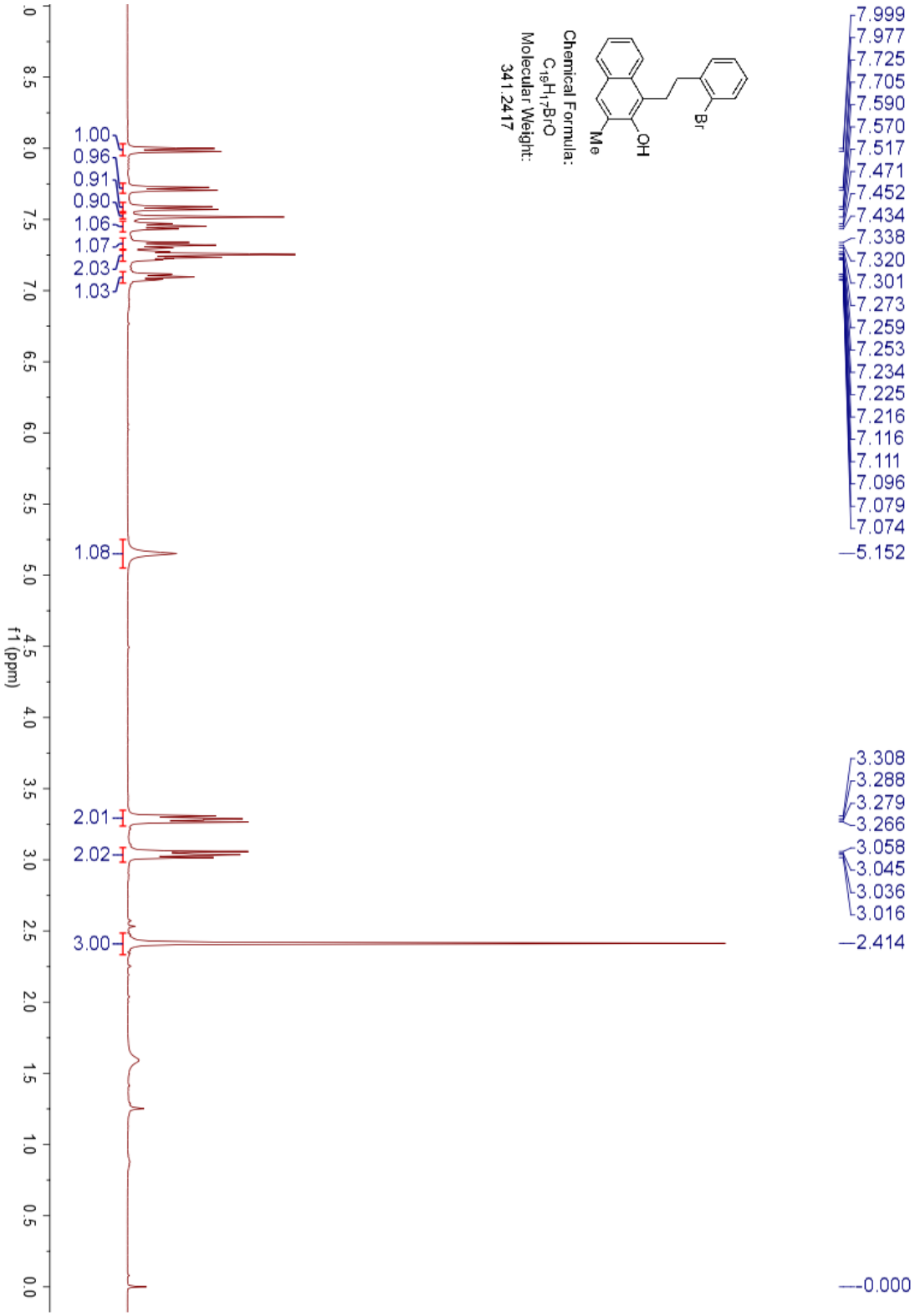


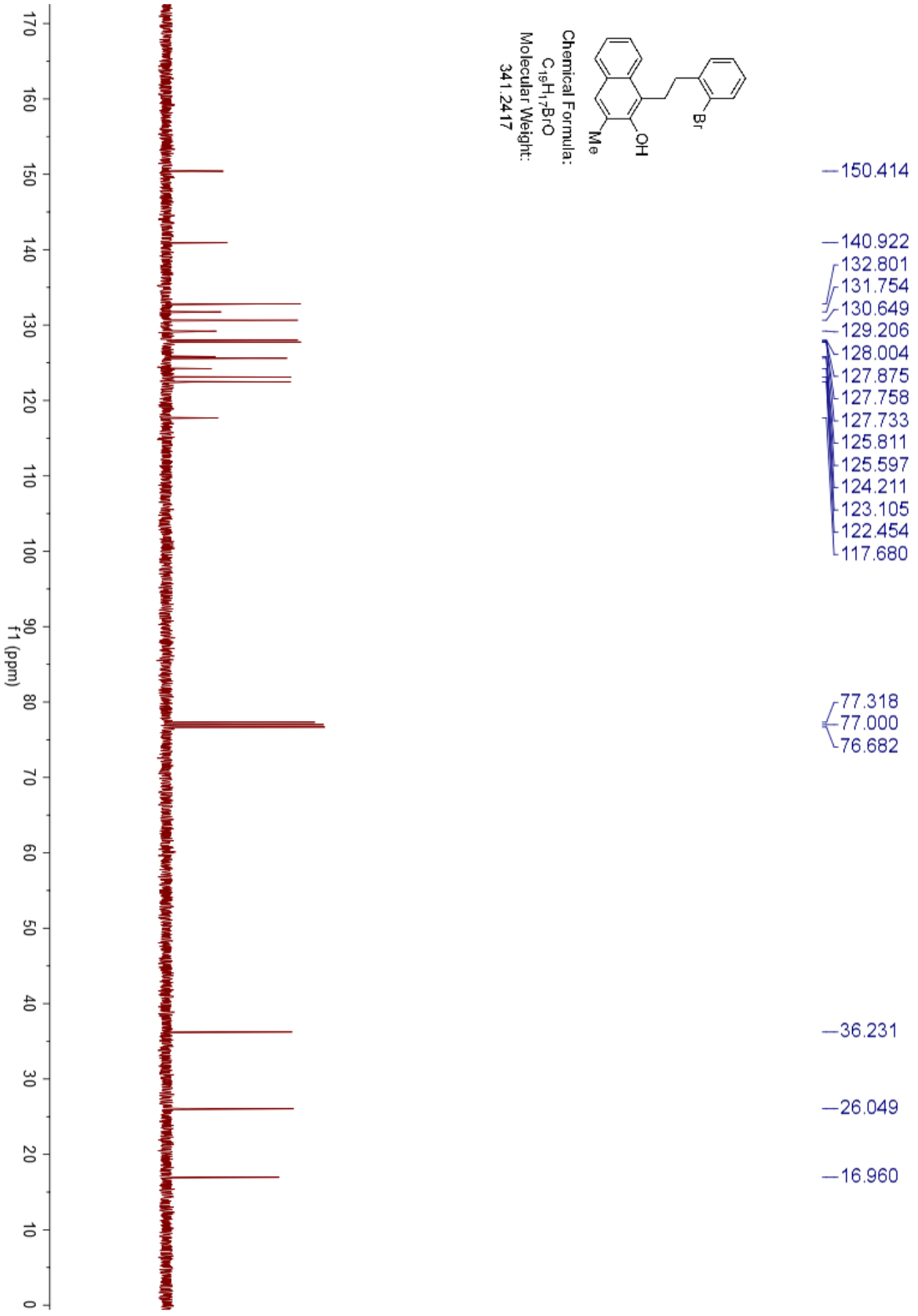


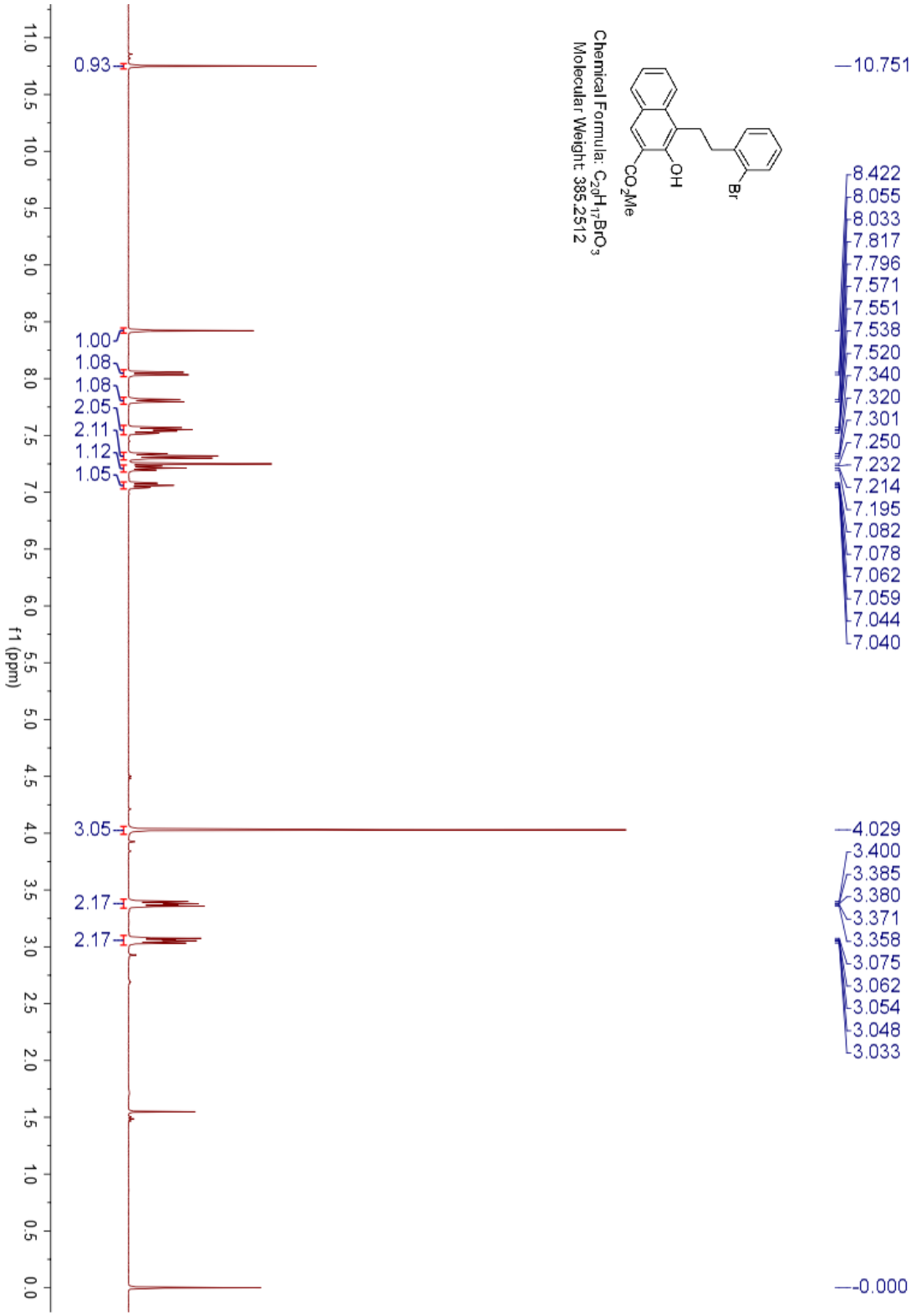

Chemical Formula: $C_{13}H_{14}BrF_3O$
Molecular Weight: 395.2131
F_3C
Br
OH
f1 (ppm)
1.00
0.95
1.86
1.04
1.01
1.97
1.00
1.09
2.05
2.05
8.017
7.995
7.803
7.783
7.698
7.679
7.658
7.524
7.510
7.506
7.488
7.485
7.427
7.422
7.370
7.367
7.353
7.350
7.347
7.339
7.333
7.318
7.313
7.055
7.033
4.892
3.370
3.354
3.350
3.342
3.329
3.142
3.129
3.121
3.117
3.101
0.000

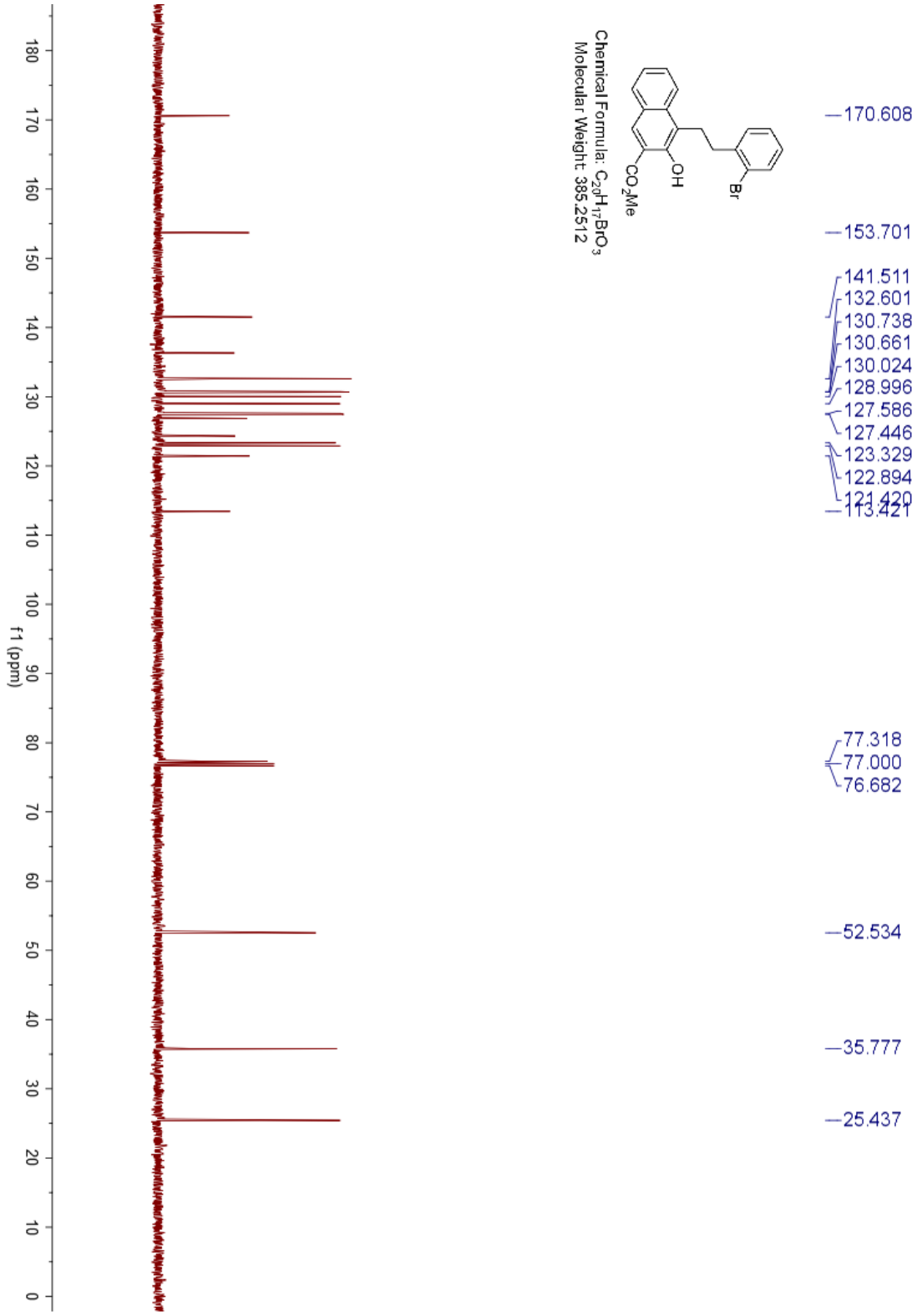

Chemical Formula: $C_{19}H_{14}BrF_3O$
Molecular Weight: 395.2131
F_3C
Br
OH
150.672
142.165
133.198
133.065
129.718
129.357
128.687
128.231
128.167
128.151
127.257
127.222
127.184
127.148
126.649
124.436
124.398
124.361
124.322
123.164
122.569
118.327
117.510
77.318
77.000
76.682
35.979
25.176
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

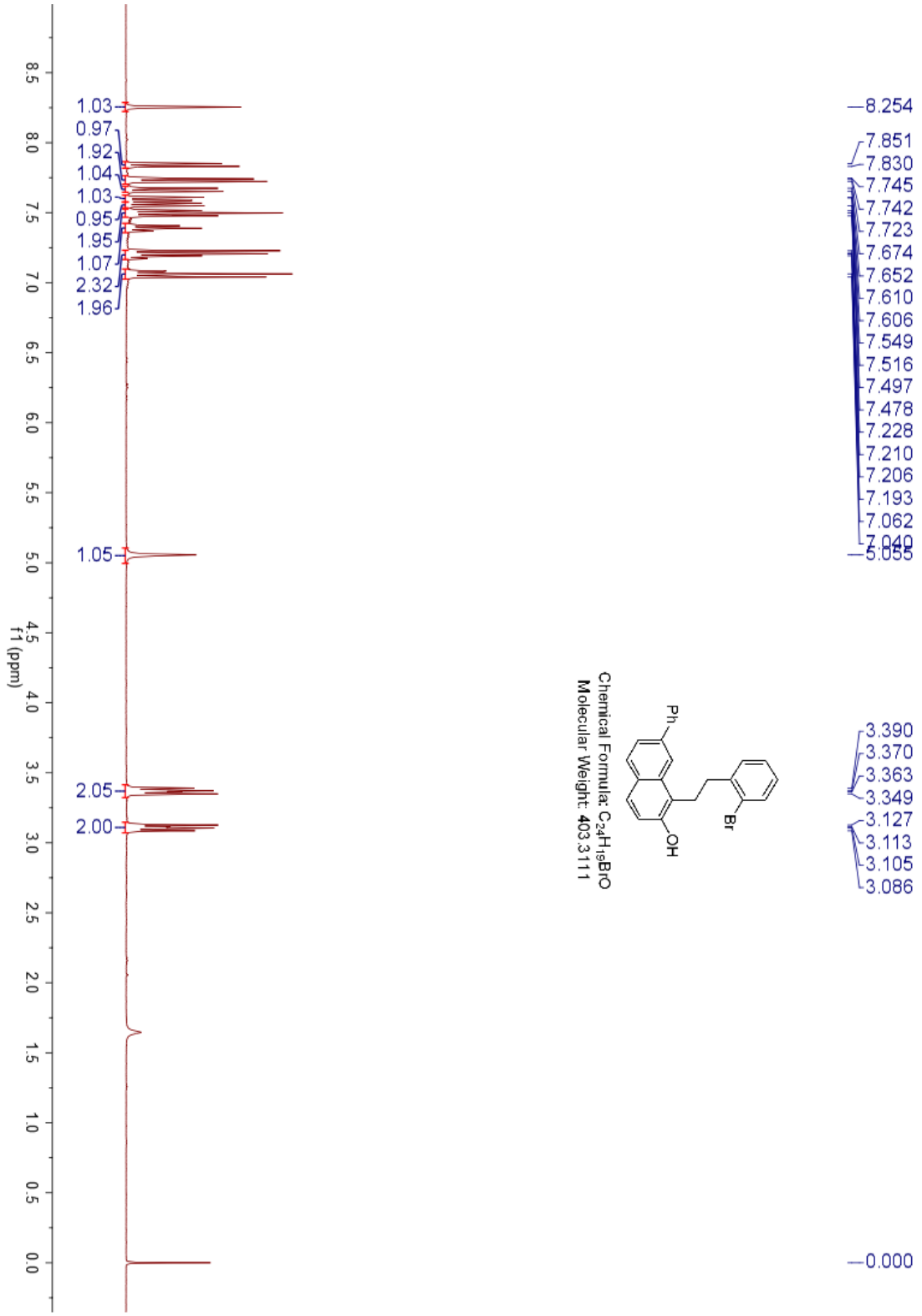

-62.648
F3C
Br
OH
Chemical Formula: C19H14BrF3O
Molecular Weight: 395.2131
80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300 -320 -340
f1 (ppm)

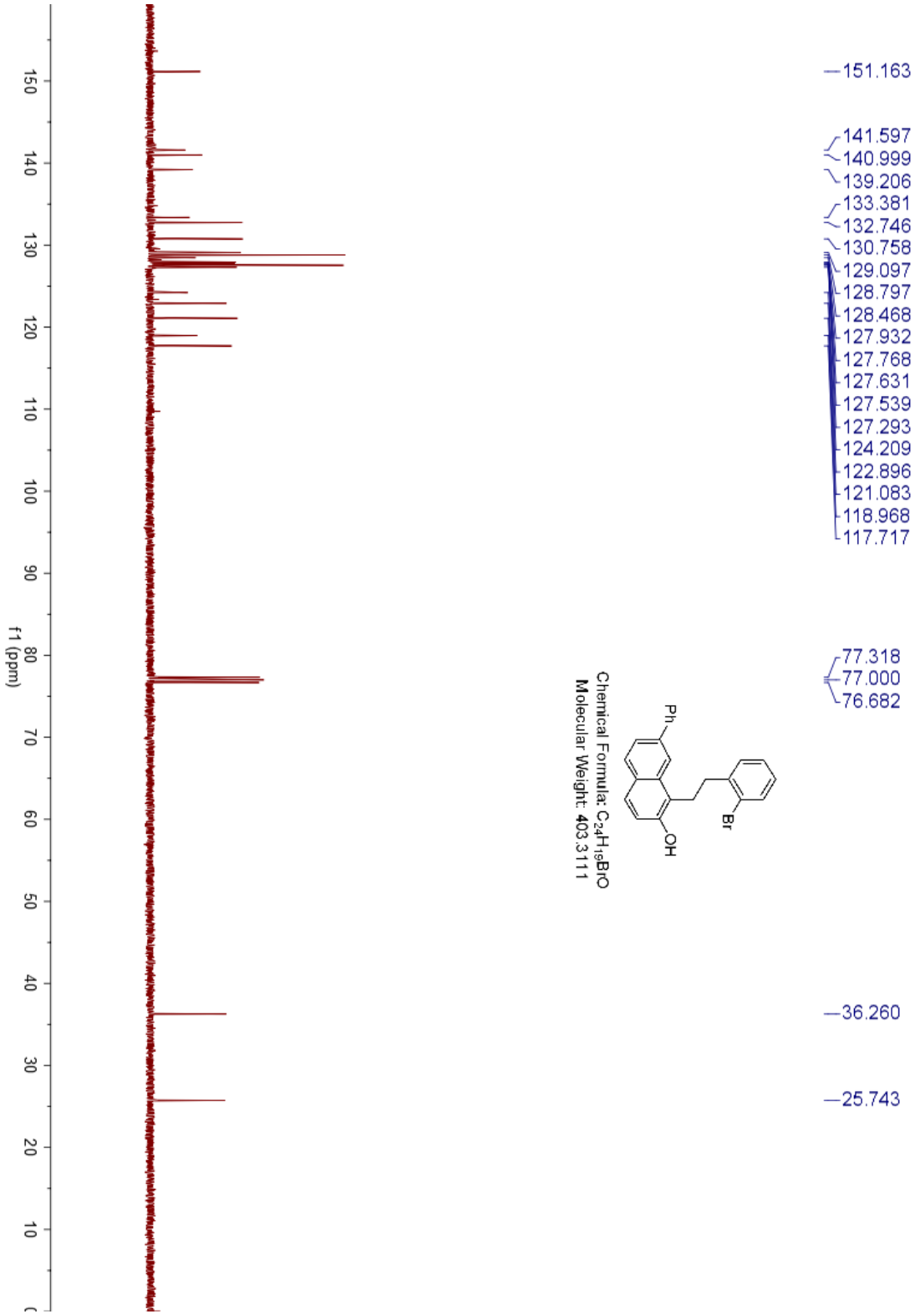

Chemical Formula:
$C_{18}H_{17}BrO$
Molecular Weight:
341.2417
Me
OH
Br
7.999
7.977
7.725
7.705
7.590
7.570
7.517
7.471
7.452
7.434
7.338
7.320
7.301
7.273
7.259
7.253
7.234
7.225
7.216
7.116
7.111
7.096
7.079
7.074
5.152
3.308
3.288
3.279
3.266
3.058
3.045
3.036
3.016
2.414
0.000
1.00
0.96
0.91
0.90
1.06
1.07
2.03
1.03
1.08
2.01
2.02
3.00
f1 (ppm)

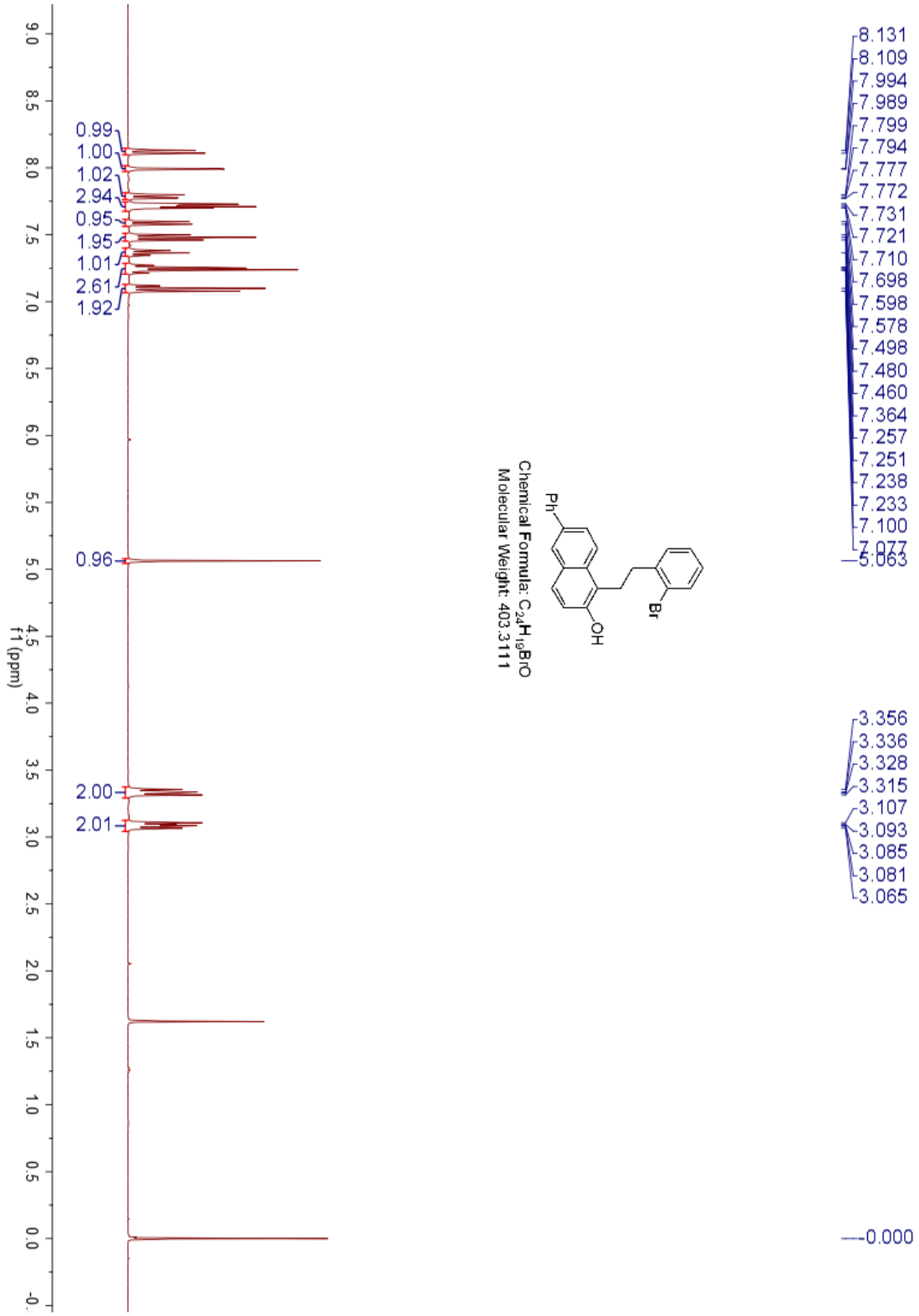

Chemical Formula:
$C_{18}H_{17}BrO$
Molecular Weight:
341.2417
Me
OH
Br
150.414
140.922
132.801
131.754
130.649
129.206
128.004
127.875
127.758
127.733
125.811
125.597
124.211
123.105
122.454
117.680
77.318
77.000
76.682
36.231
26.049
16.960
f1 (ppm)

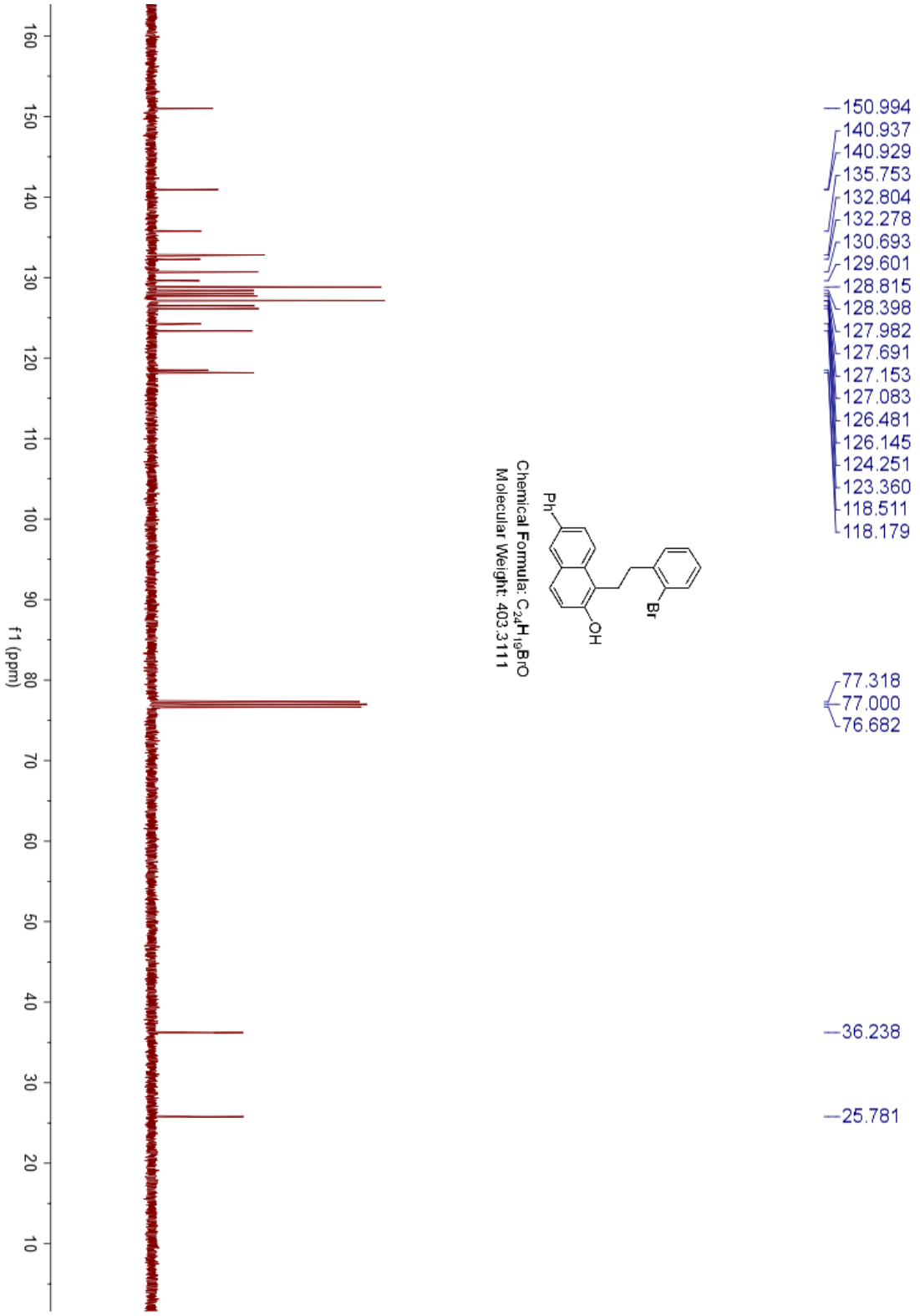

Chemical Formula: $C_{20}H_{17}BrO_3$
Molecular Weight: 385.2512
CO_2Me
OH
Br
0.93
1.00
1.08
1.08
2.05
2.11
1.12
1.05
3.05
2.17
2.17
10.751
8.422
8.055
8.033
7.817
7.796
7.571
7.551
7.538
7.520
7.340
7.320
7.301
7.250
7.232
7.214
7.195
7.082
7.078
7.062
7.059
7.044
7.040
4.029
3.400
3.385
3.380
3.371
3.358
3.075
3.062
3.054
3.048
3.033
-0.000
f1 (ppm)

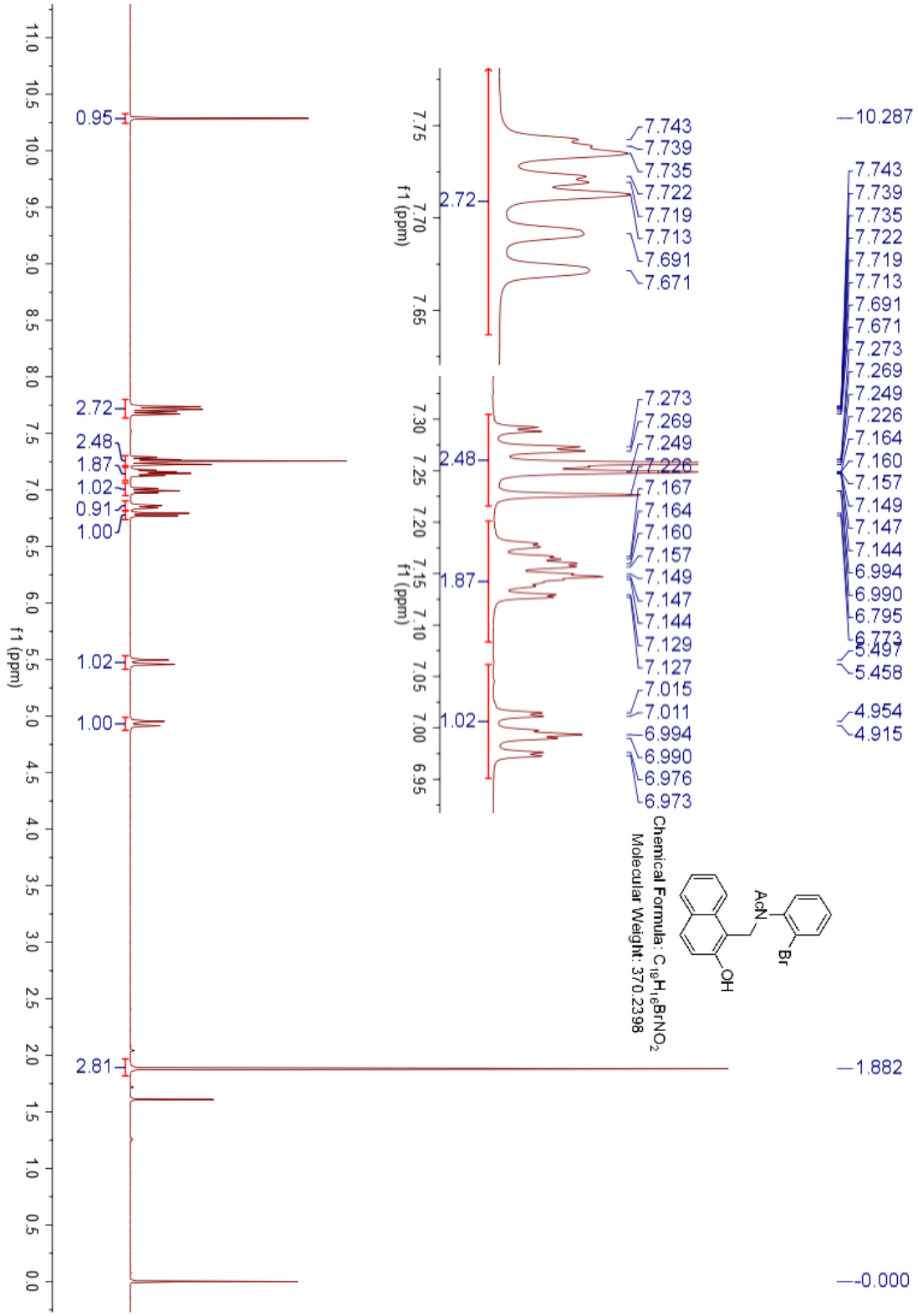

Chemical Formula: $C_{20}H_{17}BrO_3$
Molecular Weight: 385.2512
CO_2Me
OH
Br
170.608
153.701
141.511
132.601
130.738
130.661
130.024
128.996
127.586
127.446
123.329
122.894
121.420
113.421
77.318
77.000
76.682
52.534
35.777
25.437
f1 (ppm)

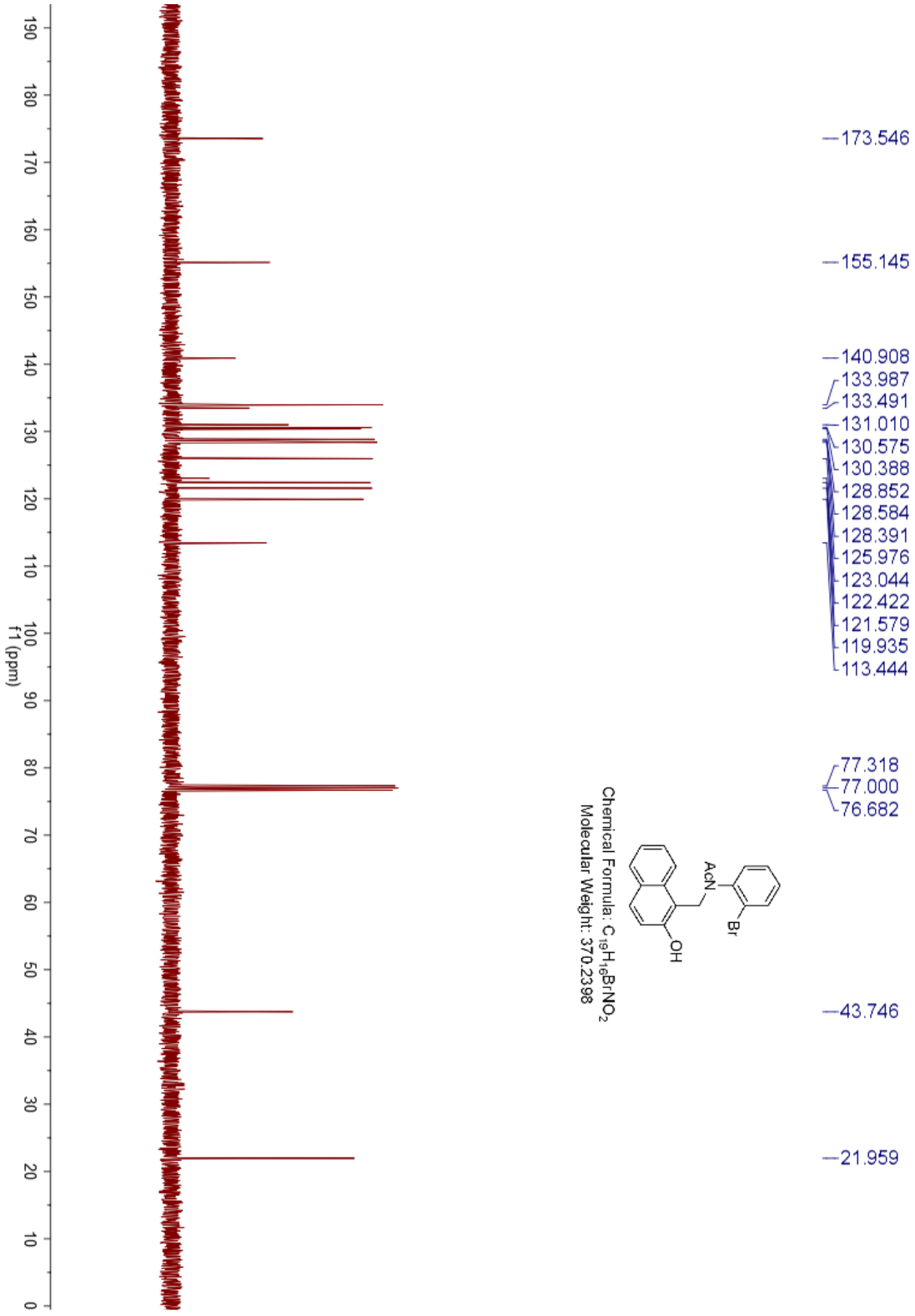

1.03
0.97
1.92
1.04
1.03
0.95
1.95
1.07
2.32
1.96
1.05
2.05
2.00
f1 (ppm)
8.254
7.851
7.830
7.745
7.742
7.723
7.674
7.652
7.610
7.606
7.549
7.516
7.497
7.478
7.228
7.210
7.206
7.193
7.062
7.040
5.055
3.390
3.370
3.363
3.349
3.127
3.113
3.105
3.086
0.000
Chemical Formula: C24H19BrO
Molecular Weight: 403.3111
Ph
OH
Br

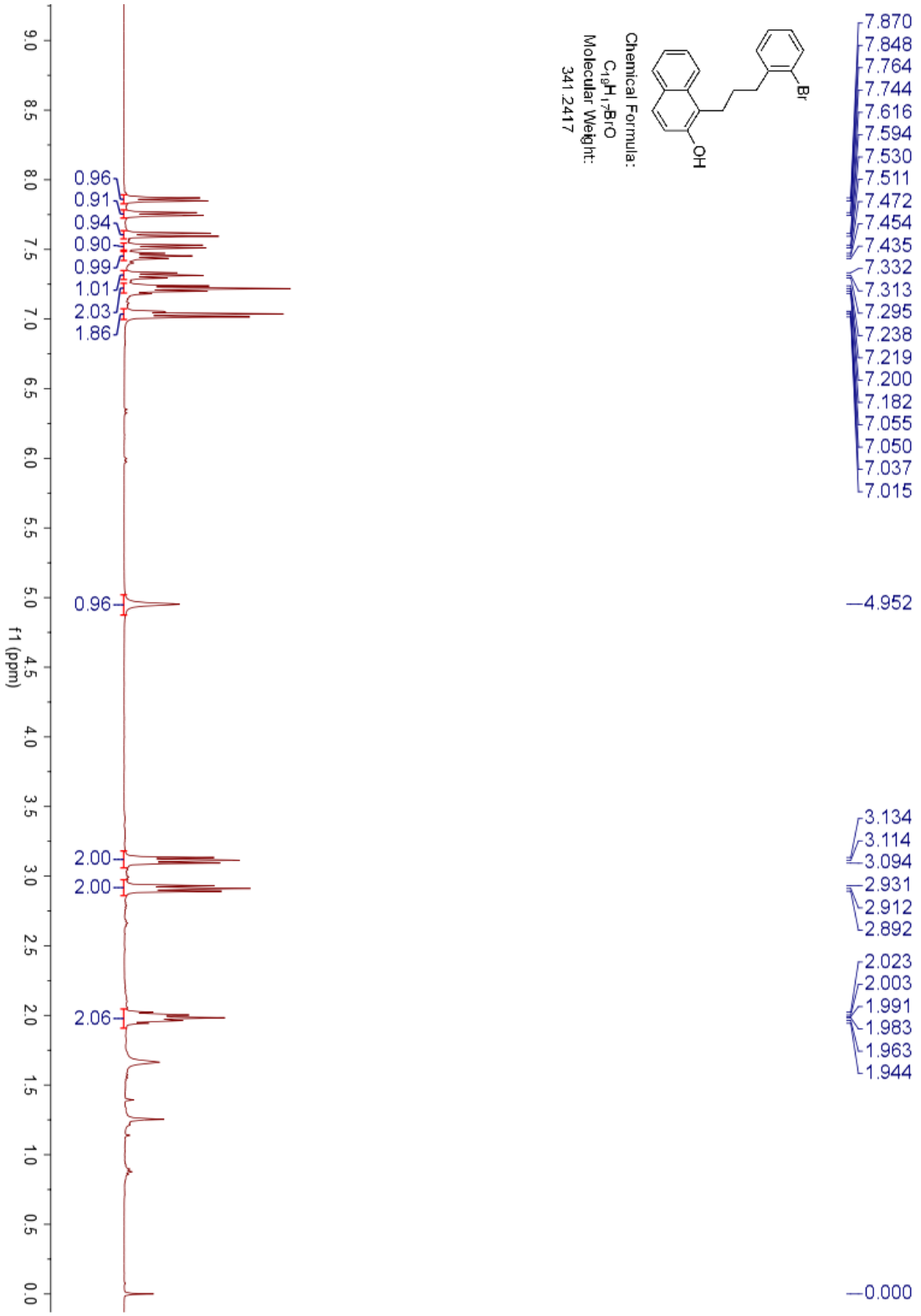

151.163
141.597
140.999
139.206
133.381
132.746
130.758
129.097
128.797
128.468
127.932
127.768
127.631
127.539
127.293
124.209
122.896
121.083
118.968
117.717
77.318
77.000
76.682
36.260
25.743
Chemical Formula: C24H19BrO
Molecular Weight: 403.3111
Ph
OH
Br
f1 (ppm)

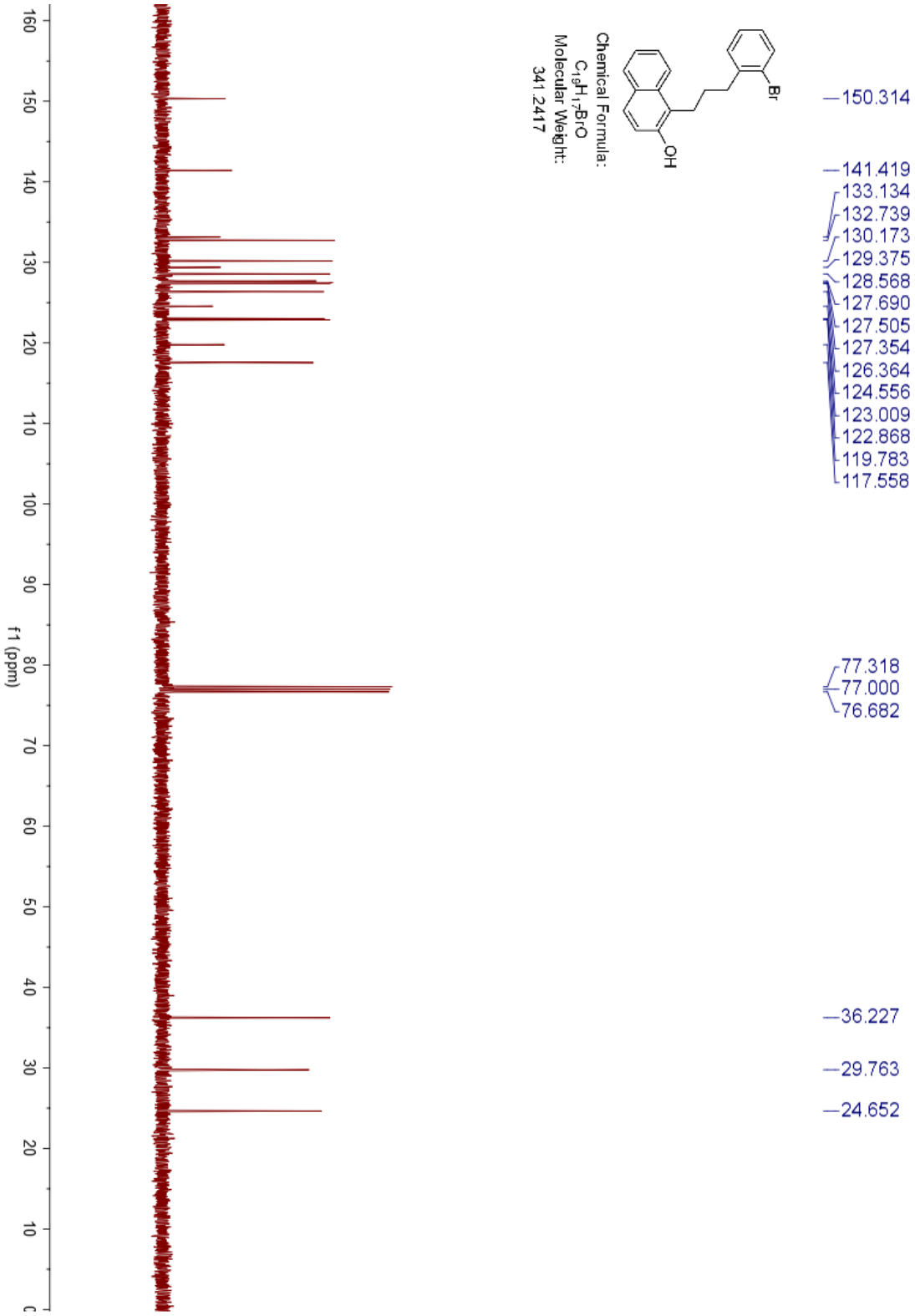

f1 (ppm)
0.99
1.00
1.02
2.94
0.95
1.95
1.01
2.61
1.92
0.96
2.00
2.01
Chemical Formula: C24H19BrO
Molecular Weight: 403.3111
Ph
OH
Br
8.131
8.109
7.994
7.989
7.799
7.794
7.777
7.772
7.731
7.721
7.710
7.698
7.598
7.578
7.498
7.480
7.460
7.364
7.257
7.251
7.238
7.233
7.100
7.077
5.063
3.356
3.336
3.328
3.315
3.107
3.093
3.085
3.081
3.065
0.000

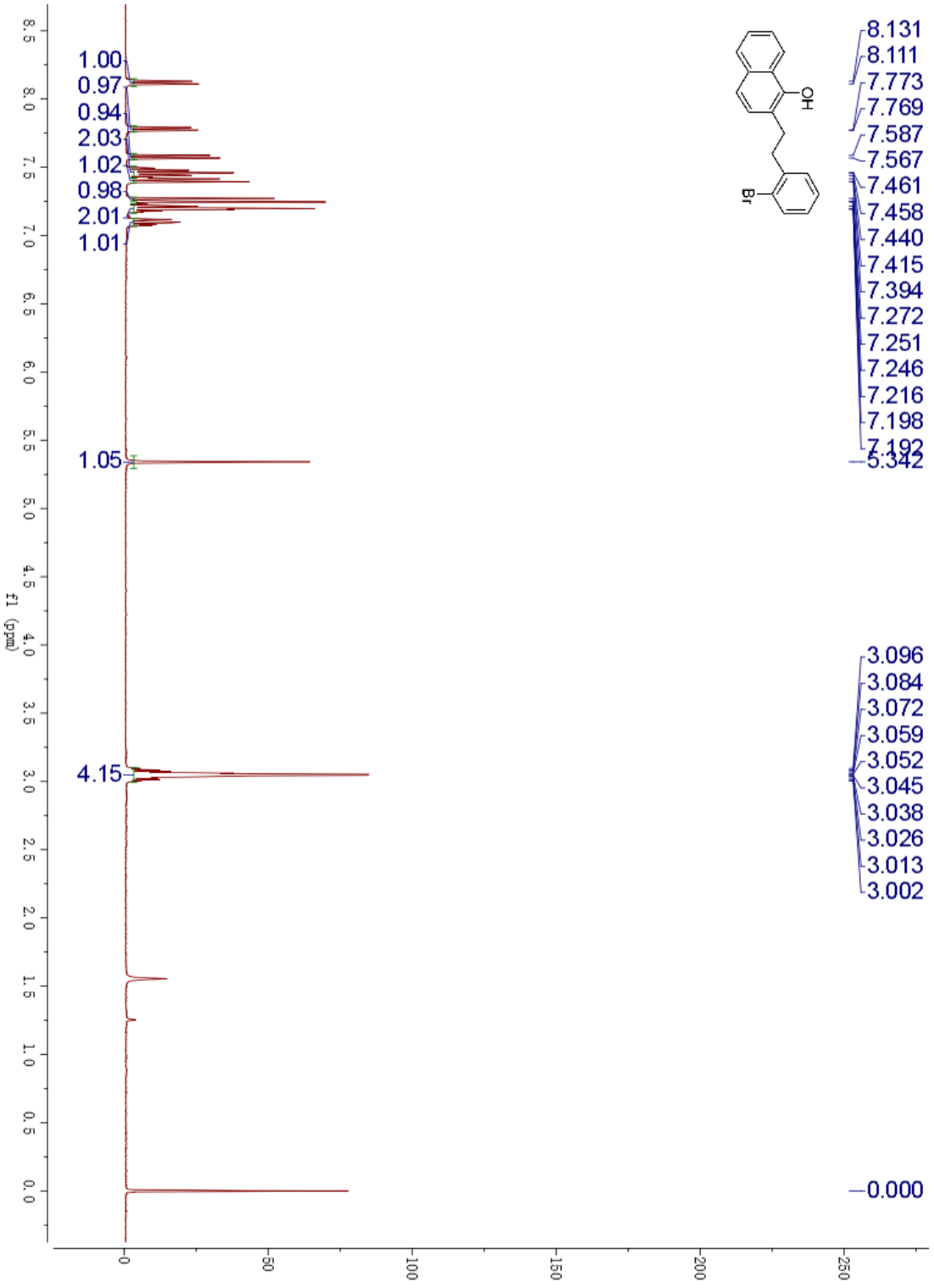

150.994
140.937
140.929
135.753
132.804
132.278
130.693
129.601
128.815
128.398
127.982
127.691
127.153
127.083
126.481
126.145
124.251
123.360
118.511
118.179
77.318
77.000
76.682
36.238
25.781
Chemical Formula: C24H19BrO
Molecular Weight: 403.3111
Ph
OH
Br
f1 (ppm)

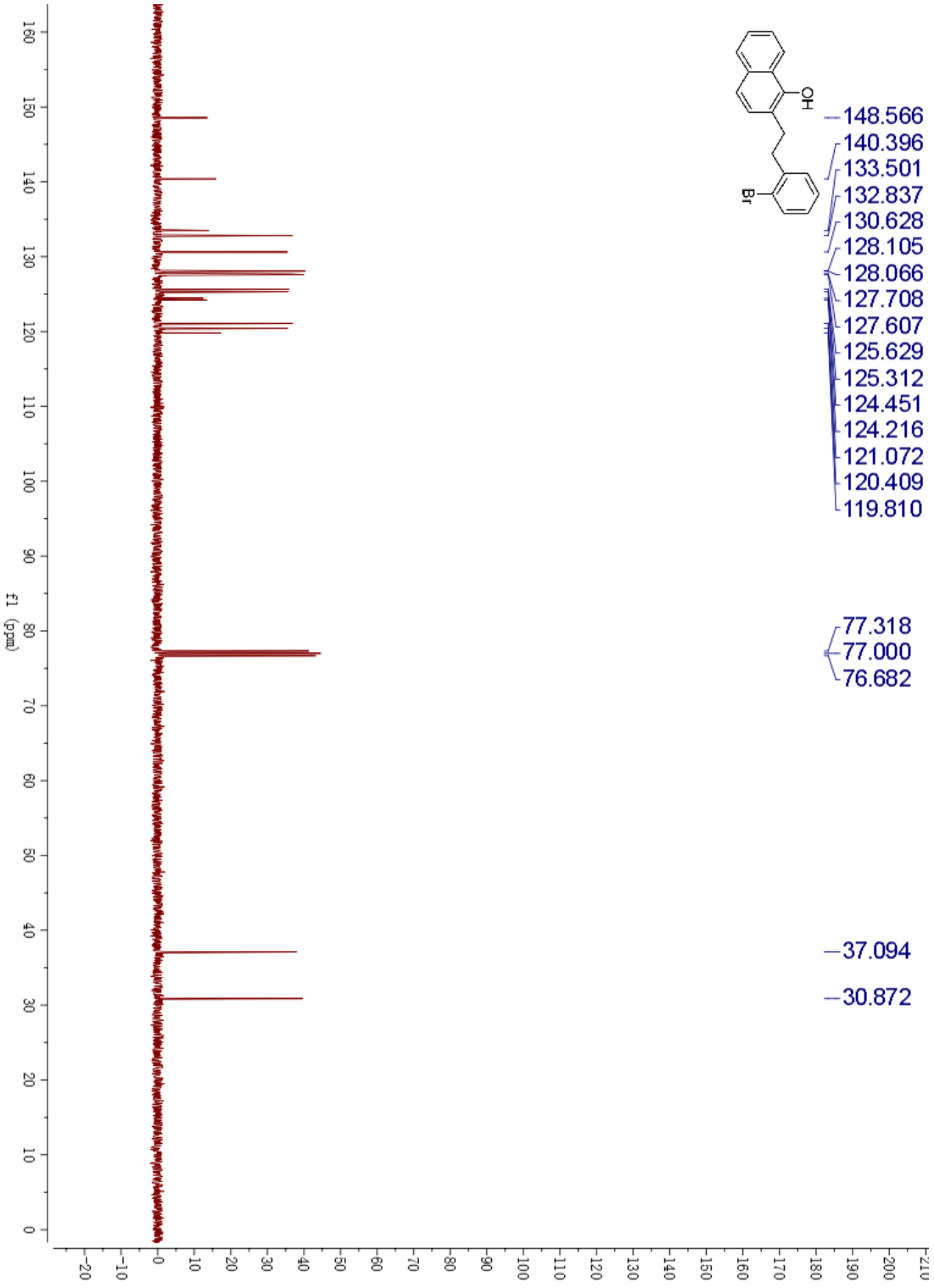

0.95
2.72
2.48
1.87
1.02
0.91
1.00
1.02
1.00
2.81
f1 (ppm)
2.72
2.48
1.87
1.02
7.743
7.739
7.735
7.722
7.719
7.713
7.691
7.671
7.273
7.269
7.249
7.226
7.167
7.164
7.160
7.157
7.149
7.147
7.144
7.129
7.127
7.015
7.011
6.994
6.990
6.976
6.973
10.287
7.743
7.739
7.735
7.722
7.719
7.713
7.691
7.671
7.273
7.269
7.249
7.226
7.164
7.160
7.157
7.149
7.147
7.144
6.994
6.990
6.795
5.497
5.458
4.954
4.915
1.882
0.000
Chemical Formula: C18H14BrNO2
Molecular Weight: 370.2318
AcN
Br
OH

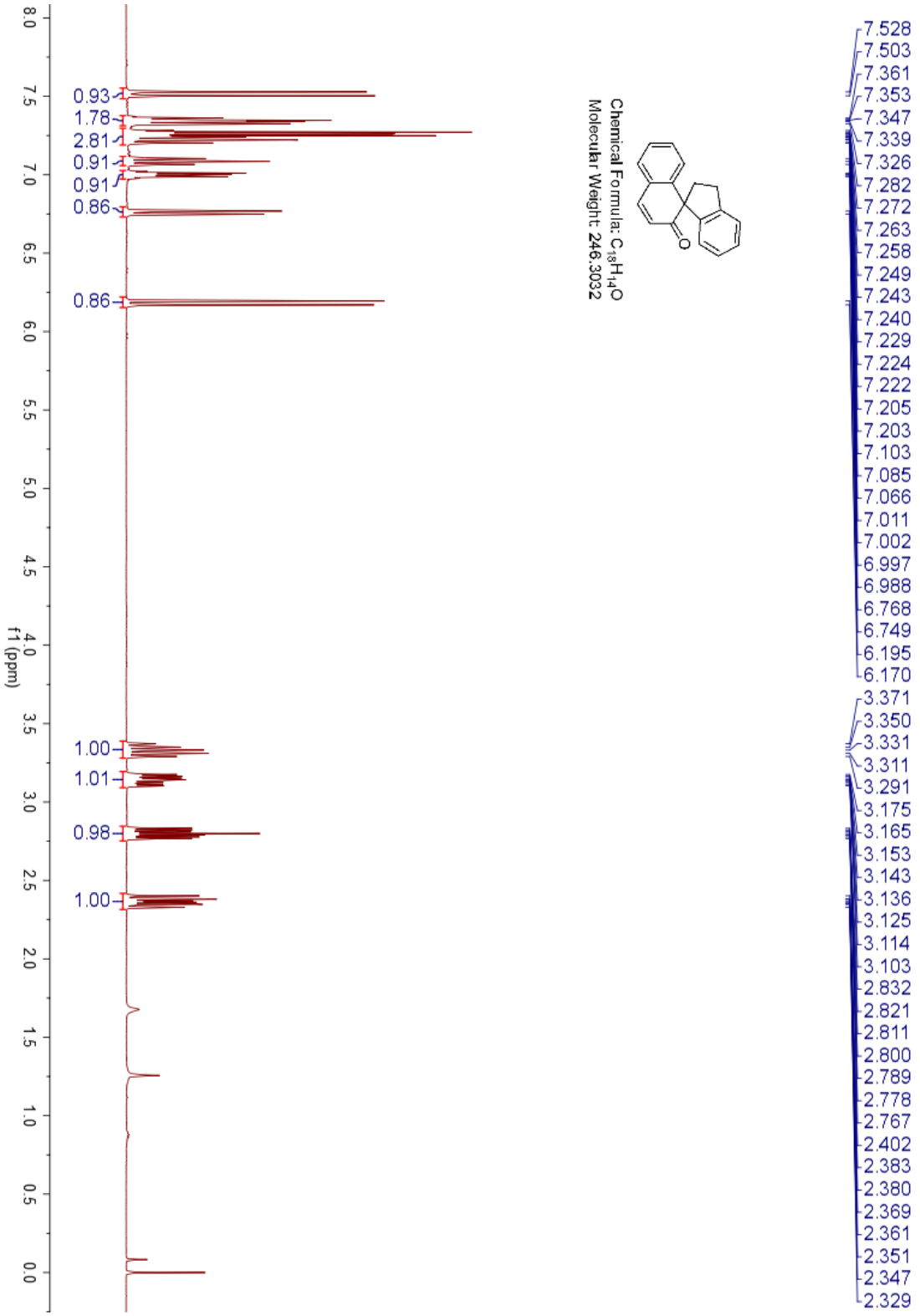

f1 (ppm)
173.546
155.145
140.908
133.987
133.491
131.010
130.575
130.388
128.852
128.584
128.391
125.976
123.044
122.422
121.579
119.935
113.444
77.318
77.000
76.682
43.746
21.959
Chemical Formula: C18H16BrNO2
Molecular Weight: 370.2398
AcN
Br
OH

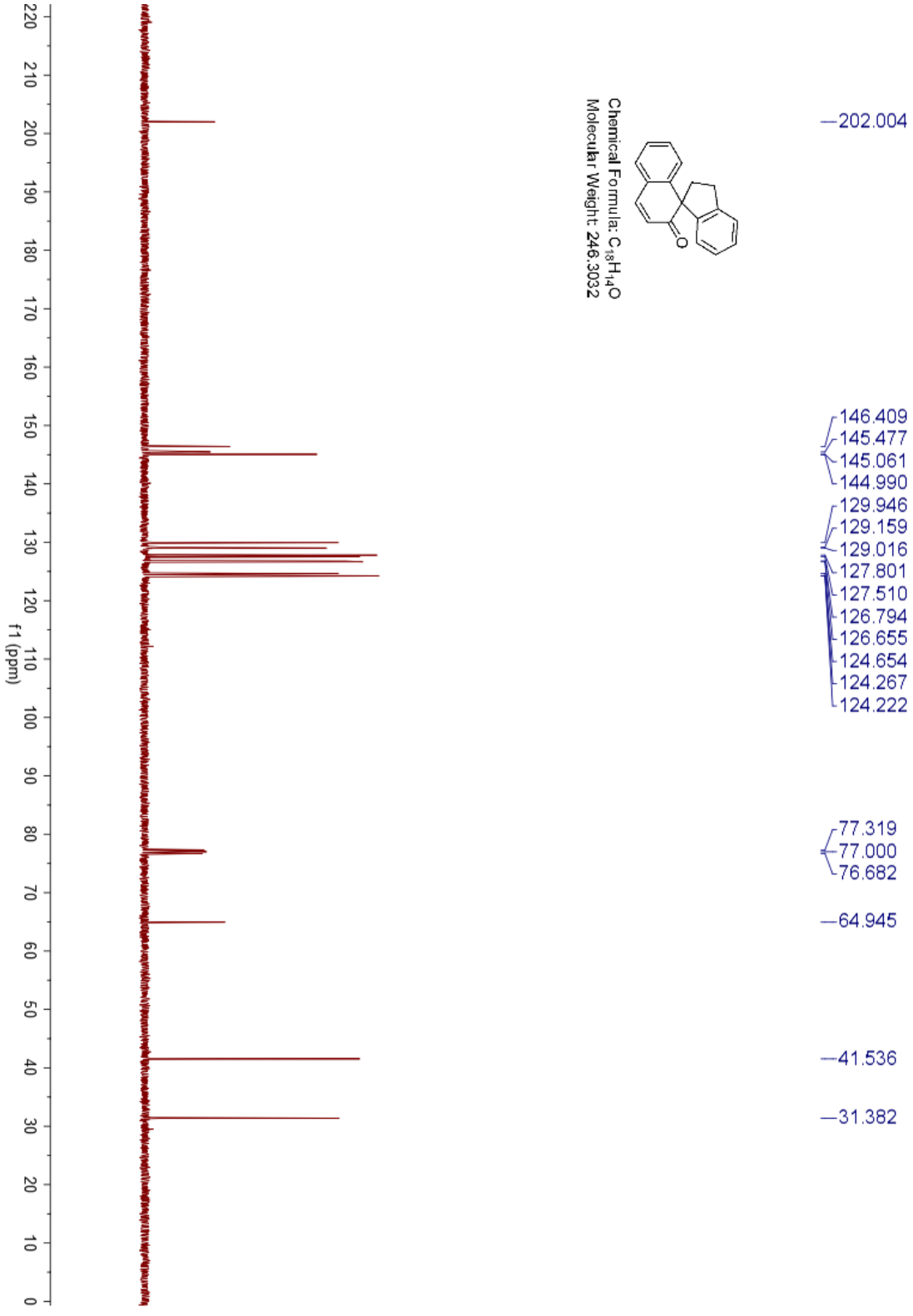

Chemical Formula:
$C_{19}H_{17}BrO$
Molecular Weight:
341.2417
Br
OH
7.870
7.848
7.764
7.744
7.616
7.594
7.530
7.511
7.472
7.454
7.435
7.332
7.313
7.295
7.238
7.219
7.200
7.182
7.055
7.050
7.037
7.015
4.952
3.134
3.114
3.094
2.931
2.912
2.892
2.023
2.003
1.991
1.983
1.963
1.944
0.000
0.96
0.91
0.94
0.90
0.99
1.01
2.03
1.86
0.96
2.00
2.00
2.06
f1 (ppm)


Chemical Formula:
$C_{18}H_{17}BrO$
Molecular Weight:
341.2417
Br
OH
150.314
141.419
133.134
132.739
130.173
129.375
128.568
127.690
127.505
127.354
126.364
124.556
123.009
122.868
119.783
117.558
77.318
77.000
76.682
36.227
29.763
24.652
f1 (ppm)

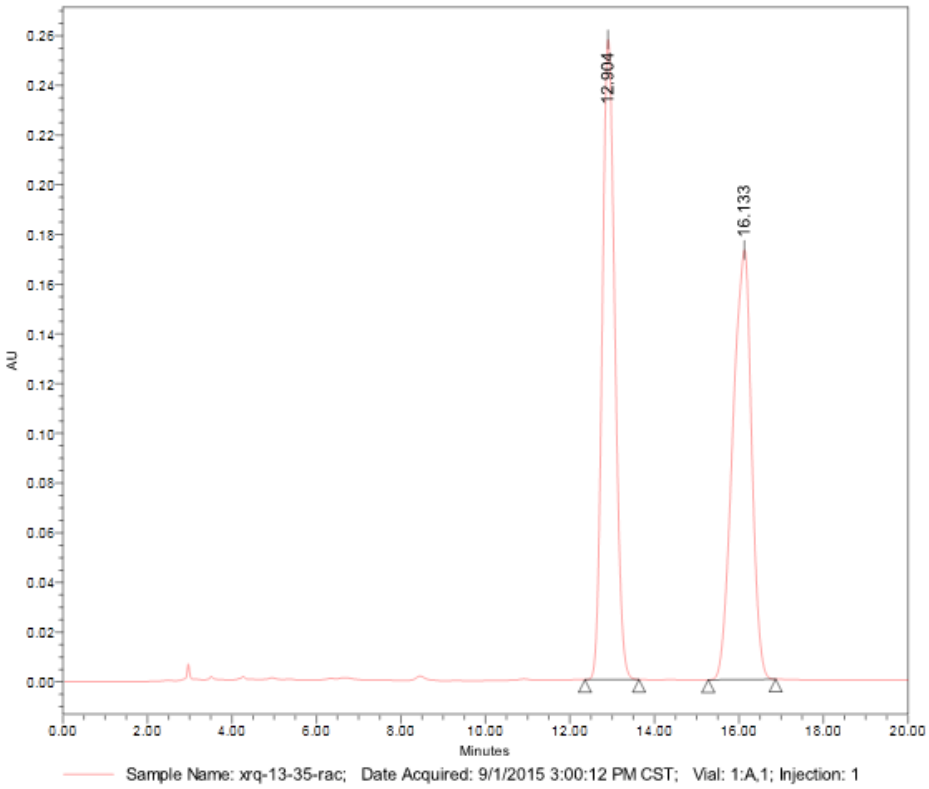

1.00
0.97
0.94
2.03
1.02
0.98
2.01
1.01
1.05
4.15
f1 (ppm)
OH
Br
8.131
8.111
7.773
7.769
7.587
7.567
7.461
7.458
7.440
7.415
7.394
7.272
7.251
7.246
7.216
7.198
7.192
5.342
3.096
3.084
3.072
3.059
3.052
3.045
3.038
3.026
3.013
3.002
0.000


148.566
140.396
133.501
132.837
130.628
128.105
128.066
127.708
127.607
125.629
125.312
124.451
124.216
121.072
120.409
119.810
77.318
77.000
76.682
37.094
30.872
OH
Br
f1 (ppm)


Chemical Formula: C18H14O
Molecular Weight: 246.3032
f1 (ppm)
0.93
1.78
2.81
0.91
0.91
0.86
0.86
1.00
1.01
0.98
1.00
7.528
7.503
7.361
7.353
7.347
7.339
7.326
7.282
7.272
7.263
7.258
7.249
7.243
7.240
7.229
7.224
7.222
7.205
7.203
7.103
7.085
7.066
7.011
7.002
6.997
6.988
6.768
6.749
6.195
6.170
3.371
3.350
3.331
3.311
3.291
3.175
3.165
3.153
3.143
3.136
3.125
3.114
3.103
2.832
2.821
2.811
2.800
2.789
2.778
2.767
2.402
2.383
2.380
2.369
2.361
2.351
2.347
2.329


Chemical Formula: C18H14O
Molecular Weight: 246.3032
202.004
146.409
145.477
145.061
144.990
129.946
129.159
129.016
127.801
127.510
126.794
126.655
124.654
124.267
124.222
77.319
77.000
76.682
64.945
41.536
31.382
f1 (ppm)

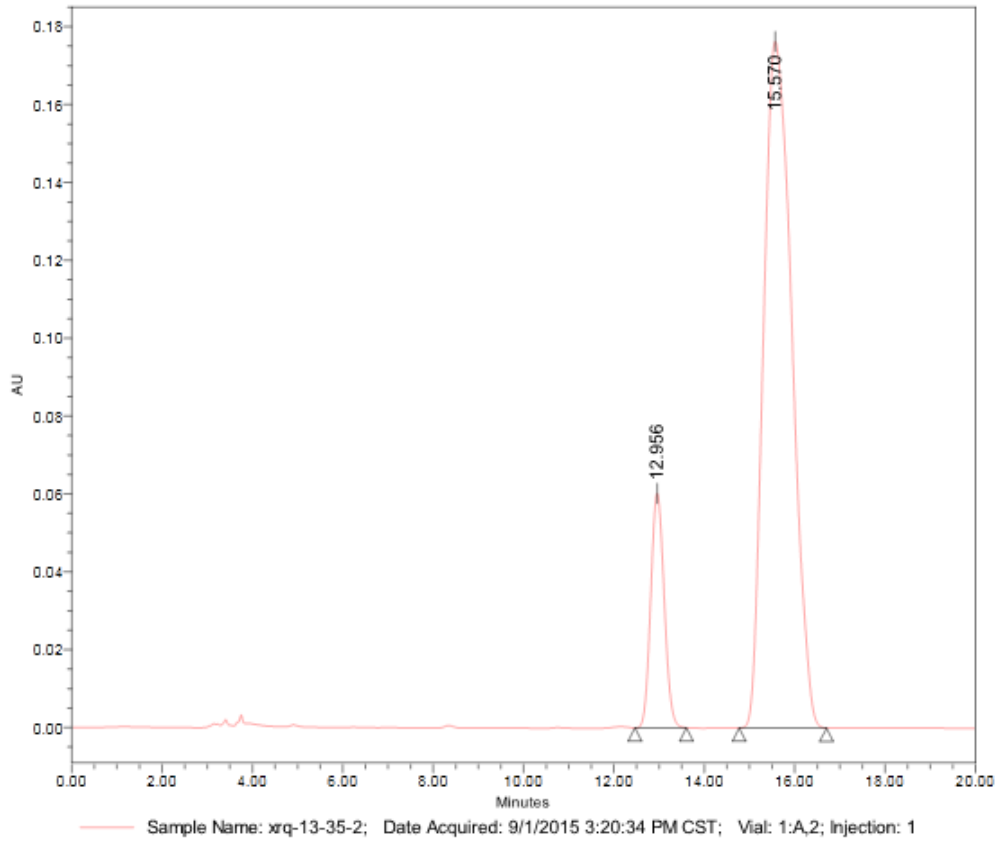
Racemic sample



Peak Summary with Statistics
Name:

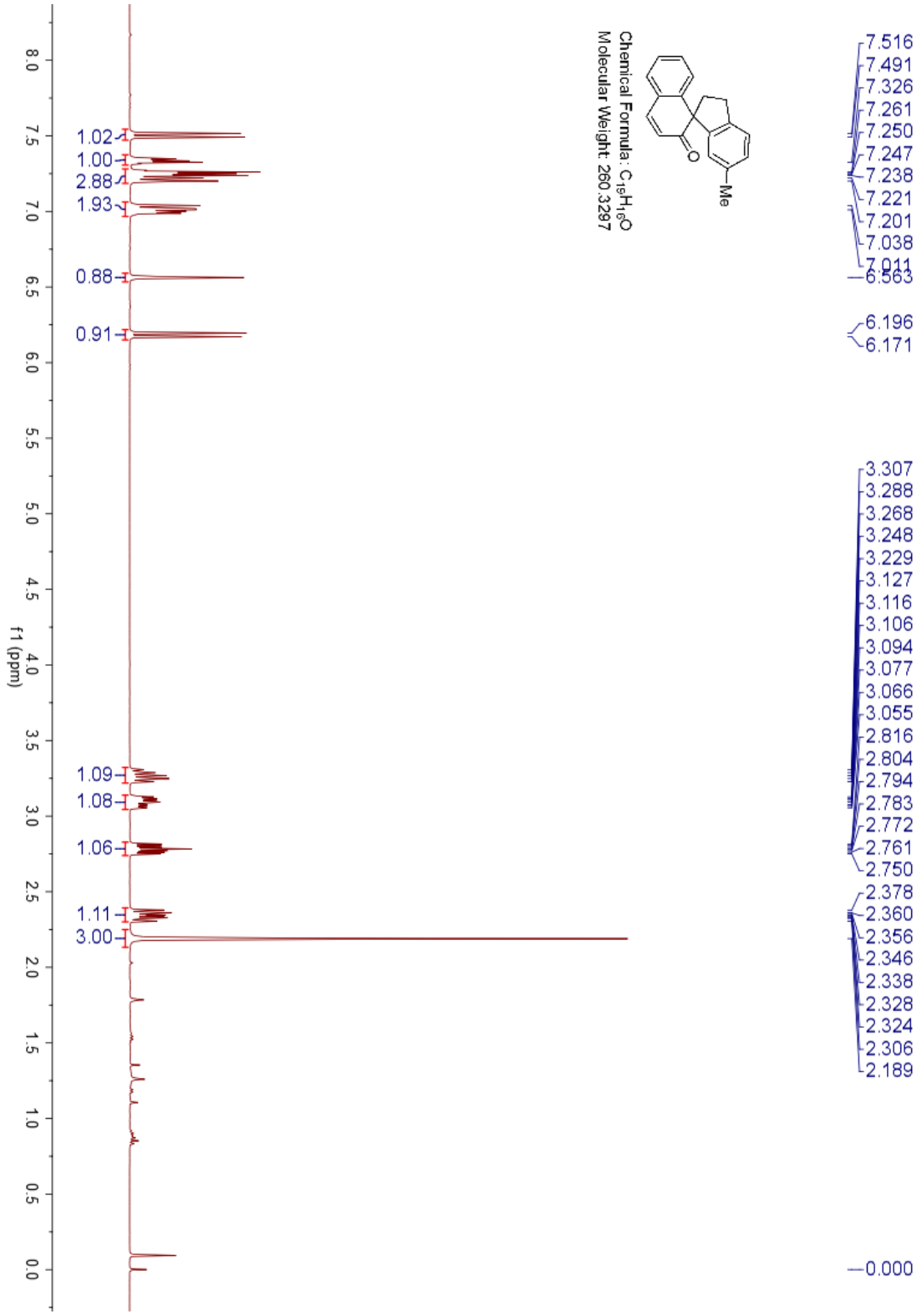
	Sample Name	Vial	Inj	Retention Time (min)	Area	% Area	Height
1	xrq-13-35-rac	1:A,1	1	16.133	5357651	50.04	172896
2	xrq-13-35-rac	1:A,1	1	12.904	5350142	49.96	257584
Mean				14.518			
Std. Dev.				2.283			

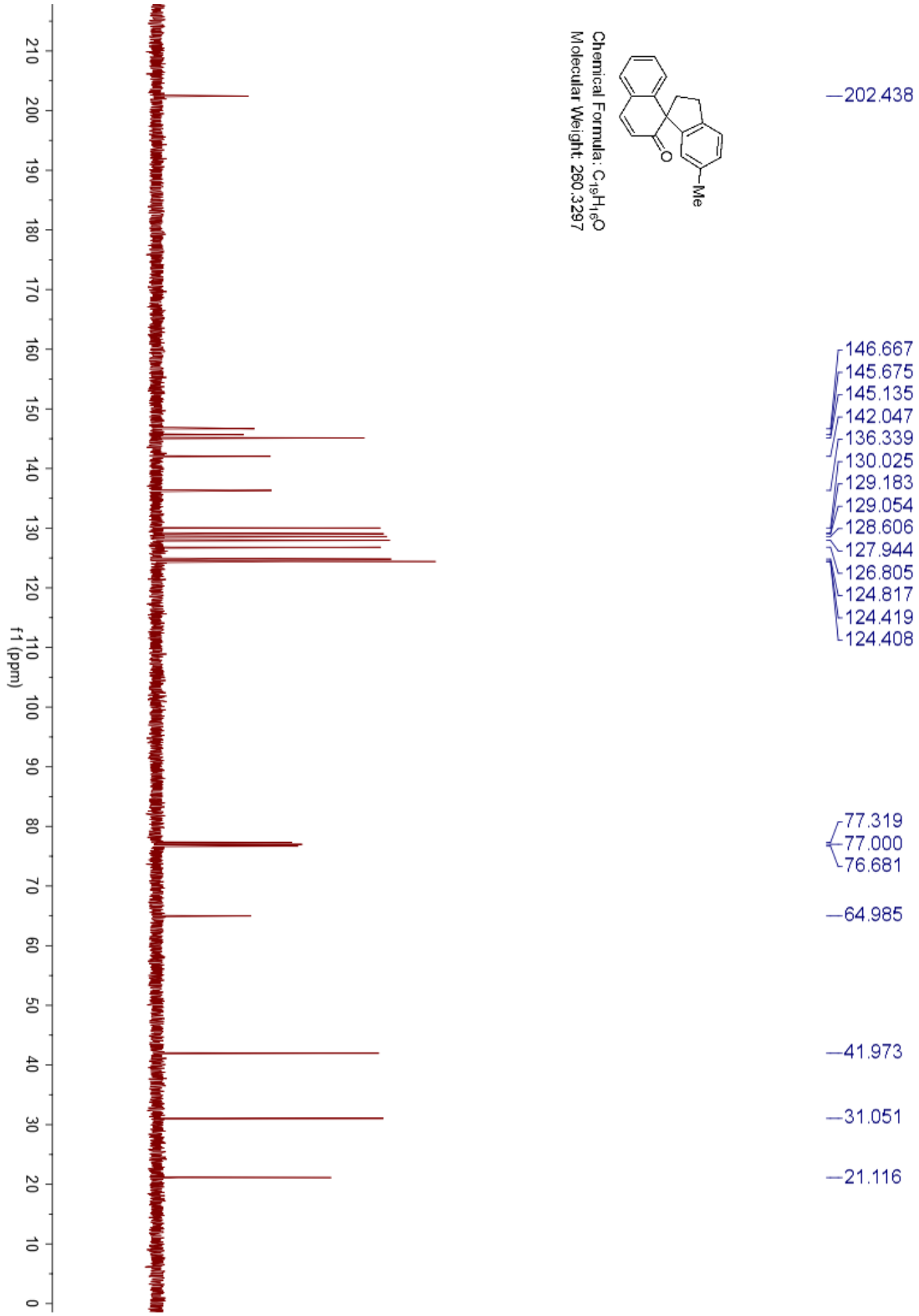
Enantioenriched sample

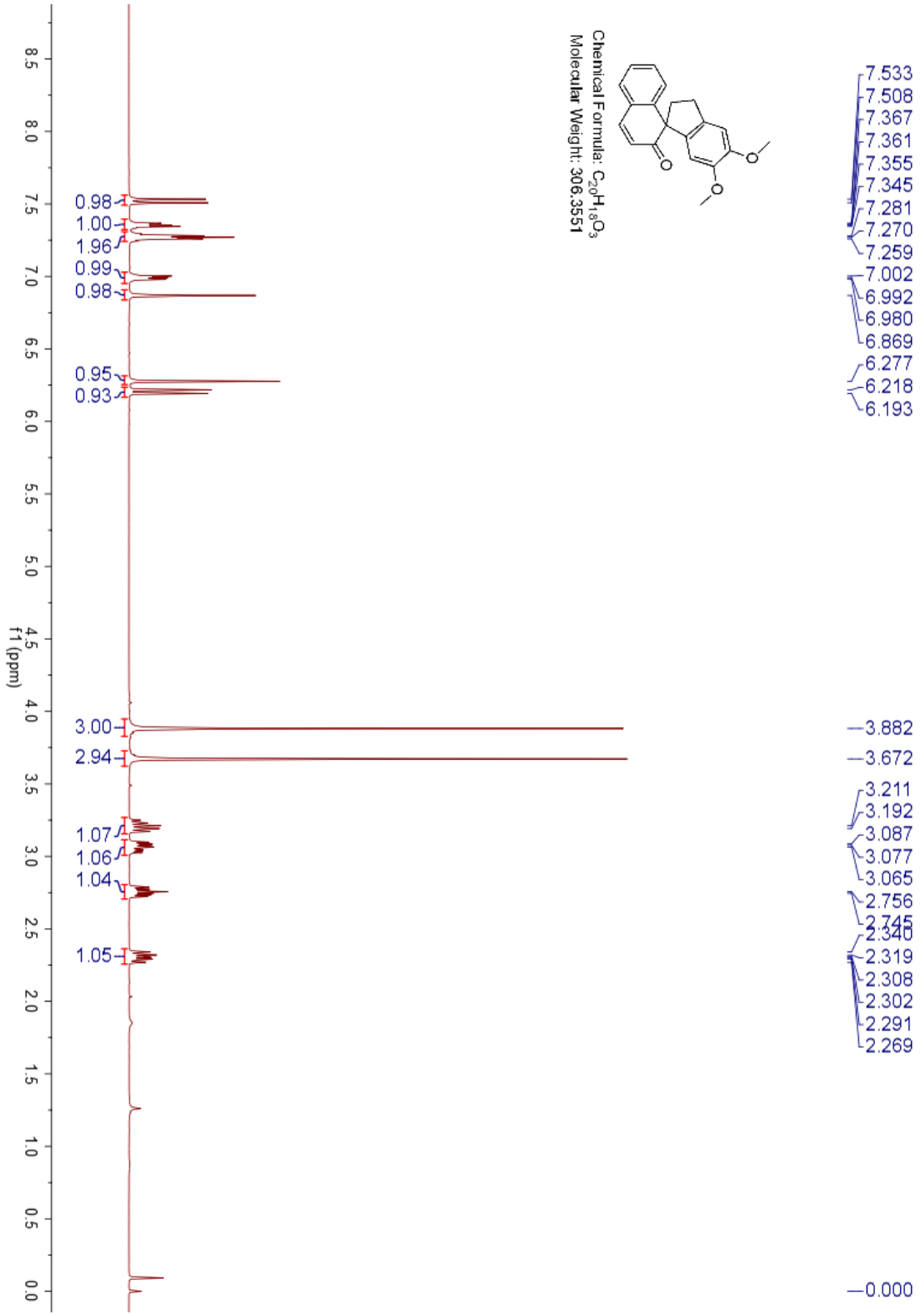


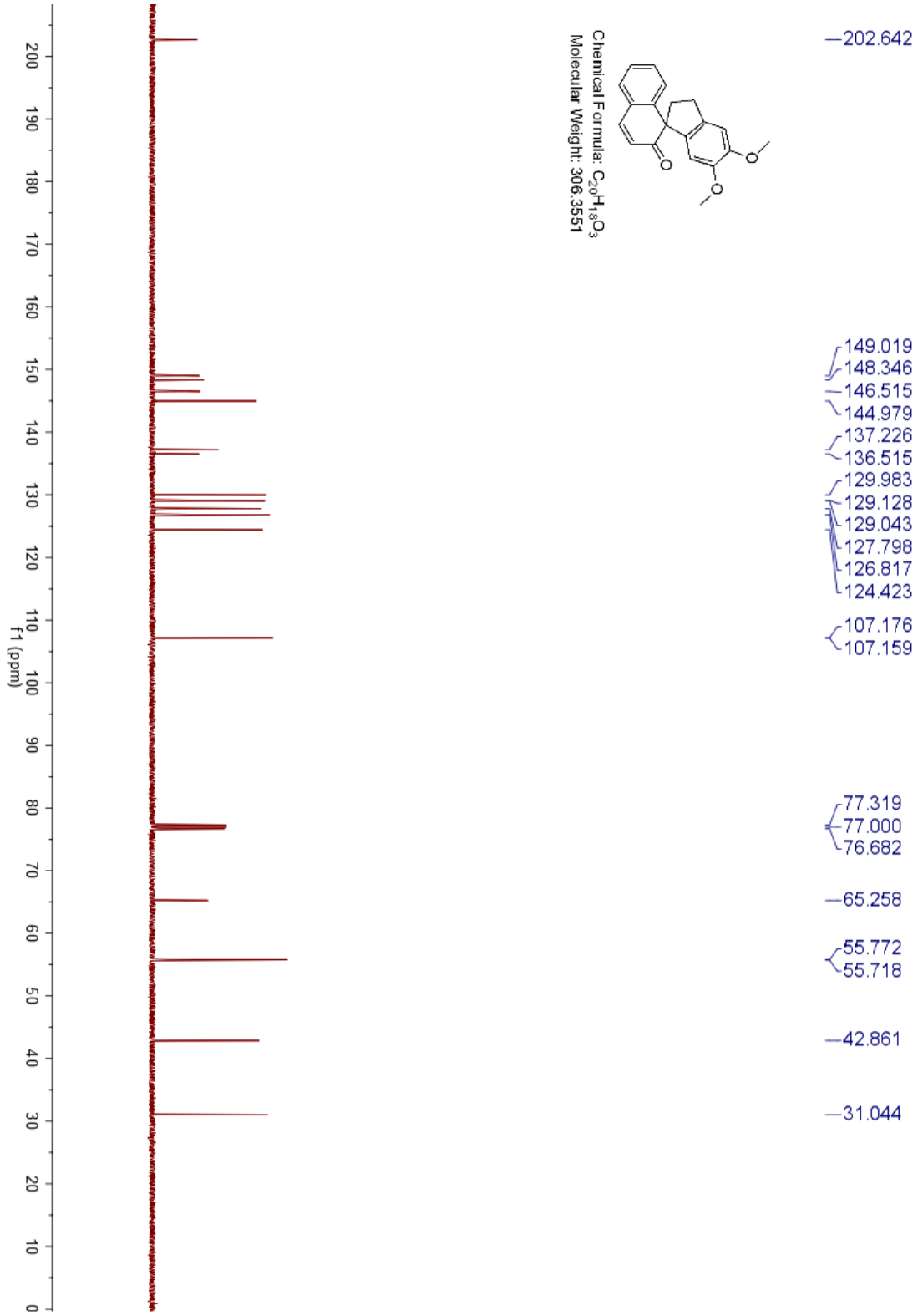
Peak Summary with Statistics
Name:

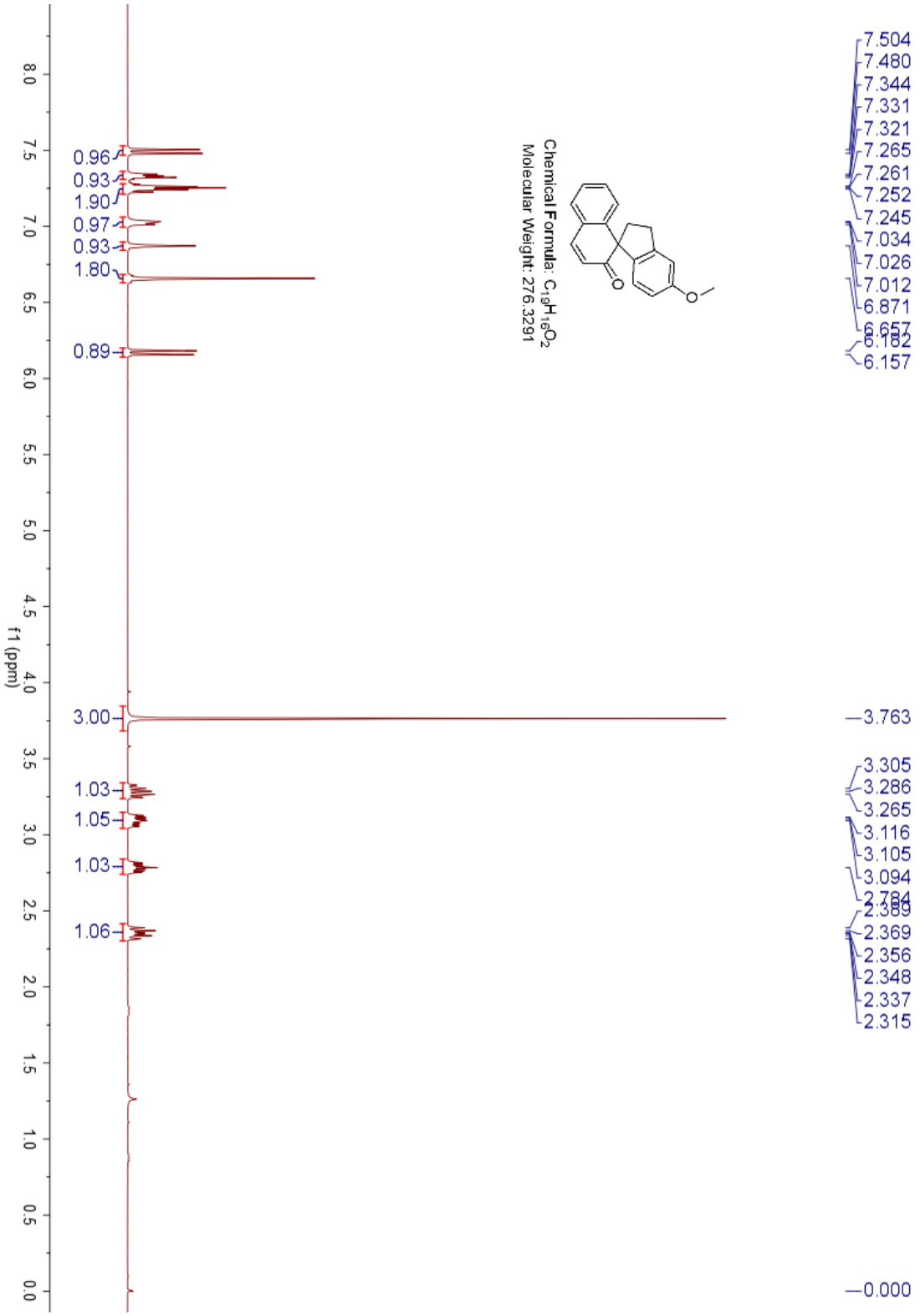
	Sample Name	Vial	Inj	Retention Time (min)	Area	% Area	Height
1	xrq-13-35-2	1:A,2	1	15.570	7637168	85.96	176295
2	xrq-13-35-2	1:A,2	1	12.956	1247475	14.04	60234
Mean				14.263			
Std. Dev.				1.848			

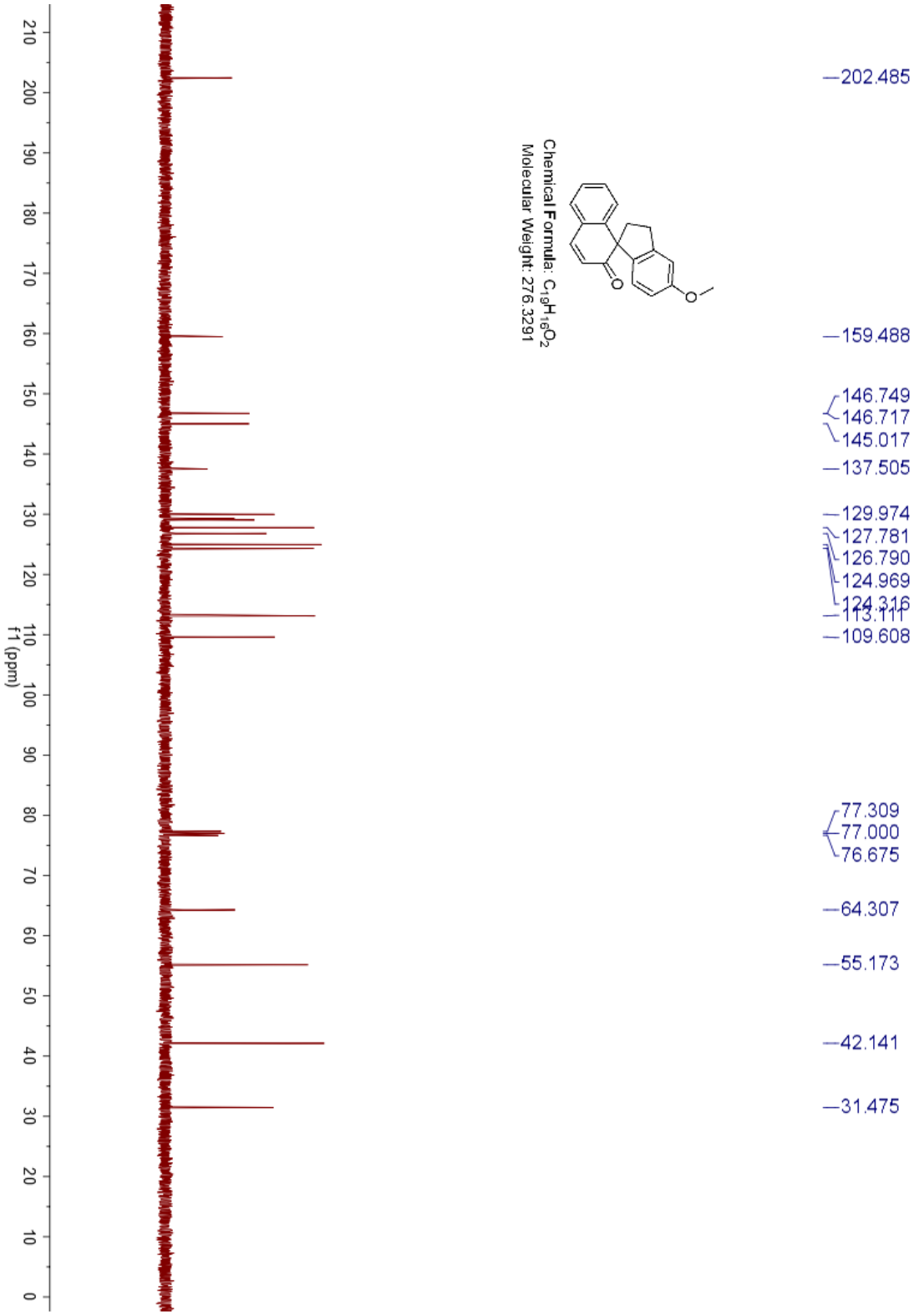

Chemical Formula: C19H16O
Molecular Weight: 260.3297
O
Me
f1 (ppm)
1.02
1.00
2.88
1.93
0.88
0.91
1.09
1.08
1.06
1.11
3.00
7.516
7.491
7.326
7.261
7.250
7.247
7.238
7.221
7.201
7.038
7.011
6.563
6.196
6.171
3.307
3.288
3.268
3.248
3.229
3.127
3.116
3.106
3.094
3.077
3.066
3.055
2.816
2.804
2.794
2.783
2.772
2.761
2.750
2.378
2.360
2.356
2.346
2.338
2.328
2.324
2.306
2.189
0.000

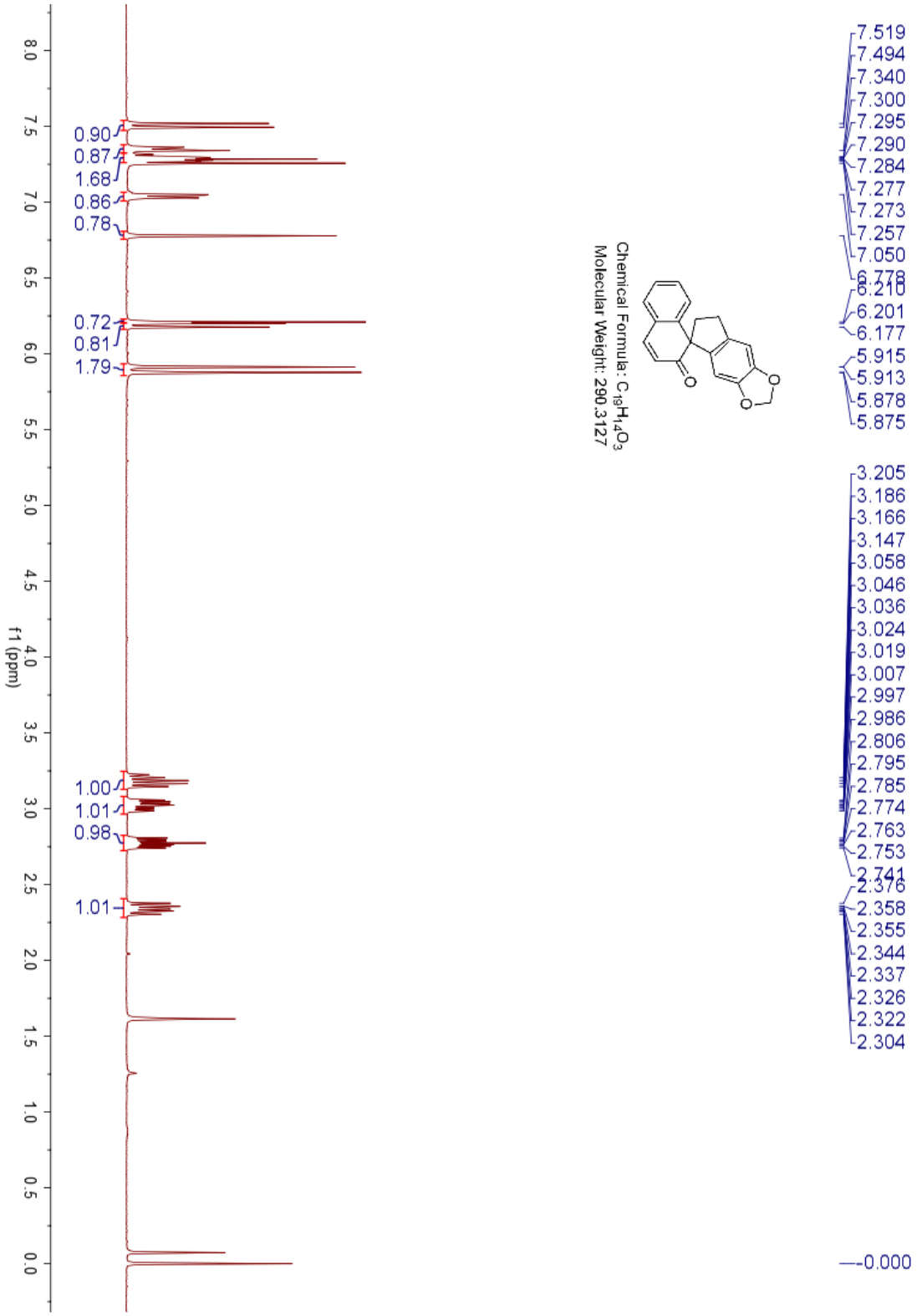

Chemical Formula: C15H16O
Molecular Weight: 260.3297
Me
O
202.438
146.667
145.675
145.135
142.047
136.339
130.025
129.183
129.054
128.606
127.944
126.805
124.817
124.419
124.408
77.319
77.000
76.681
64.985
41.973
31.051
21.116
f1 (ppm)

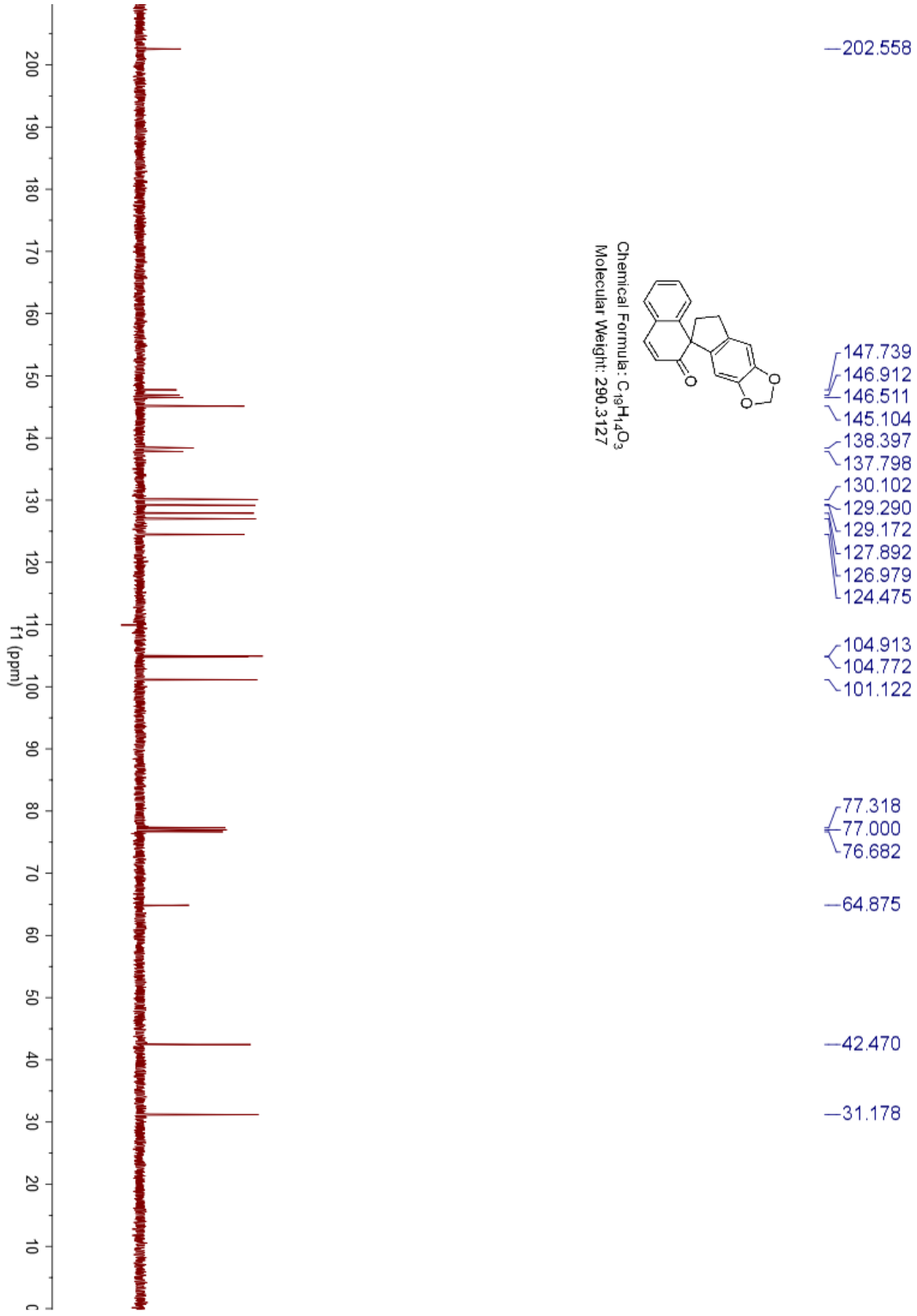

Chemical Formula: C20H18O3
Molecular Weight: 306.3551
7.533
7.508
7.367
7.361
7.355
7.345
7.281
7.270
7.259
7.002
6.992
6.980
6.869
6.277
6.218
6.193
3.882
3.672
3.211
3.192
3.087
3.077
3.065
2.756
2.745
2.340
2.319
2.308
2.302
2.291
2.269
0.000
0.98
1.00
1.96
0.99
0.98
0.95
0.93
3.00
2.94
1.07
1.06
1.04
1.05
f1 (ppm)

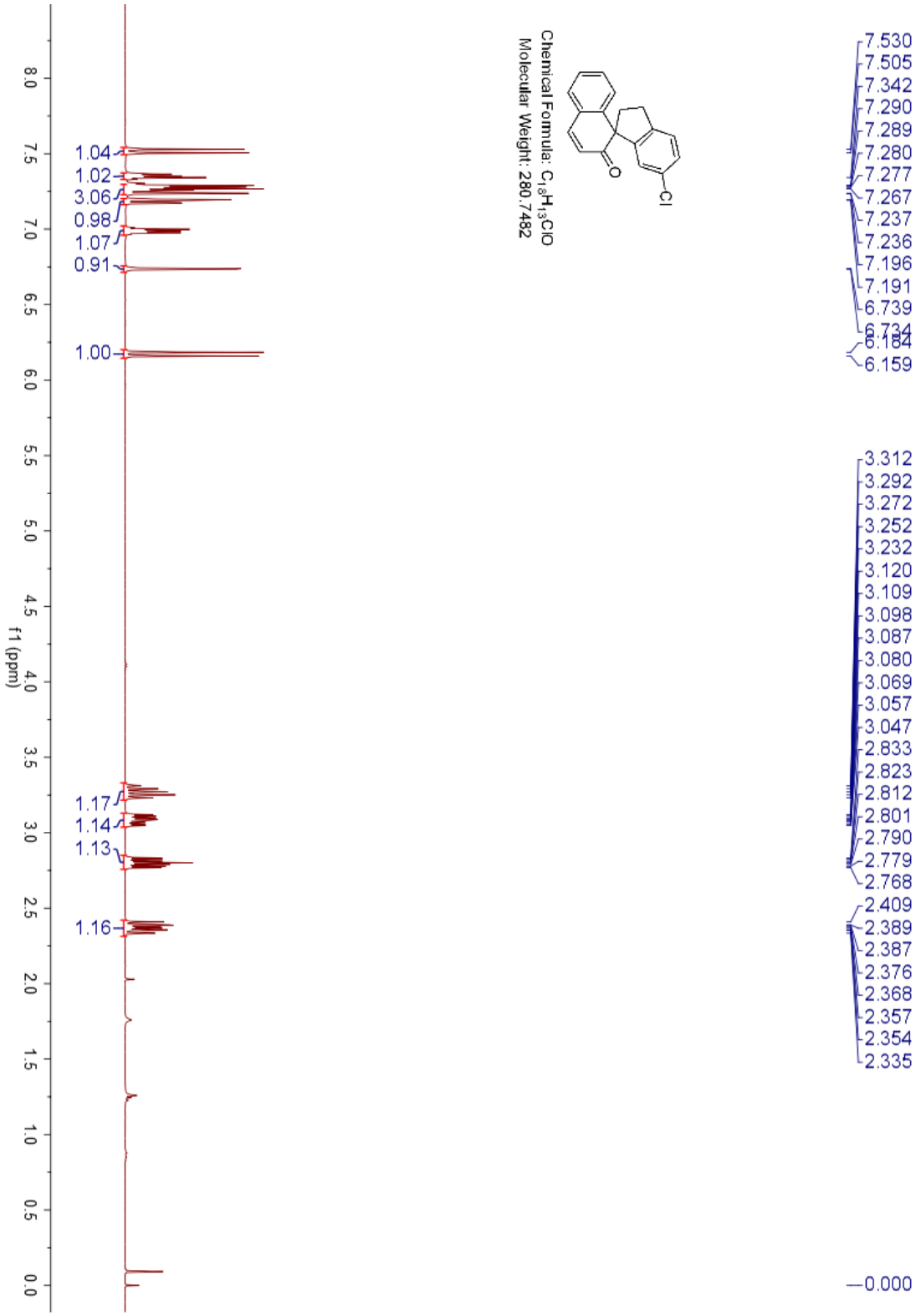

Chemical Formula: C20H18O3
Molecular Weight: 306.3551
202.642
149.019
148.346
146.515
144.979
137.226
136.515
129.983
129.128
129.043
127.798
126.817
124.423
107.176
107.159
77.319
77.000
76.682
65.258
55.772
55.718
42.861
31.044
f1 (ppm)

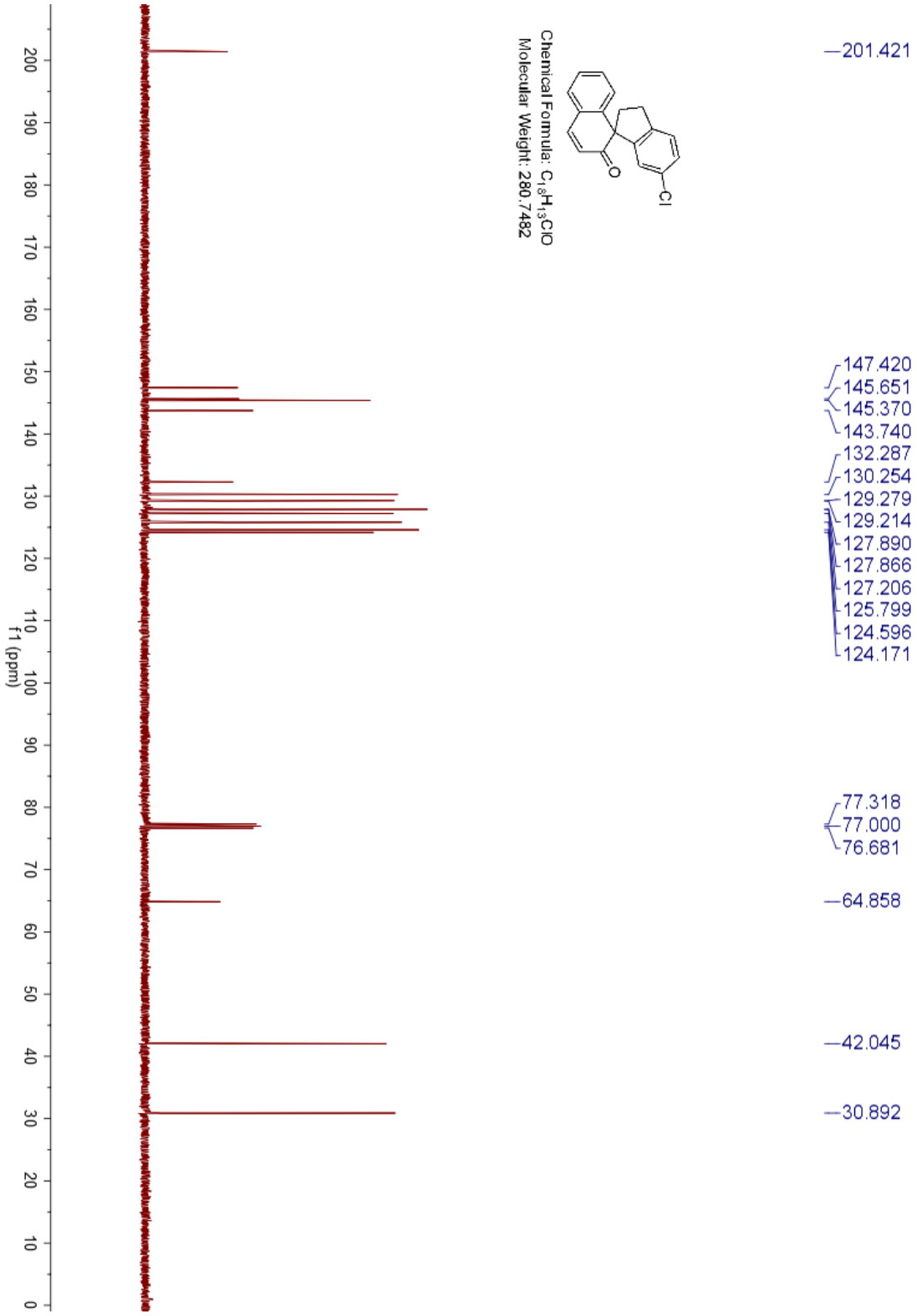

Chemical Formula: C19H16O2
Molecular Weight: 276.3291
f1 (ppm)
0.96
0.93
1.90
0.97
0.93
1.80
0.89
3.00
1.03
1.05
1.03
1.06
7.504
7.480
7.344
7.331
7.321
7.265
7.261
7.252
7.245
7.034
7.026
7.012
6.871
6.657
6.182
6.157
3.763
3.305
3.286
3.265
3.116
3.105
3.094
2.784
2.369
2.356
2.348
2.337
2.315
0.000

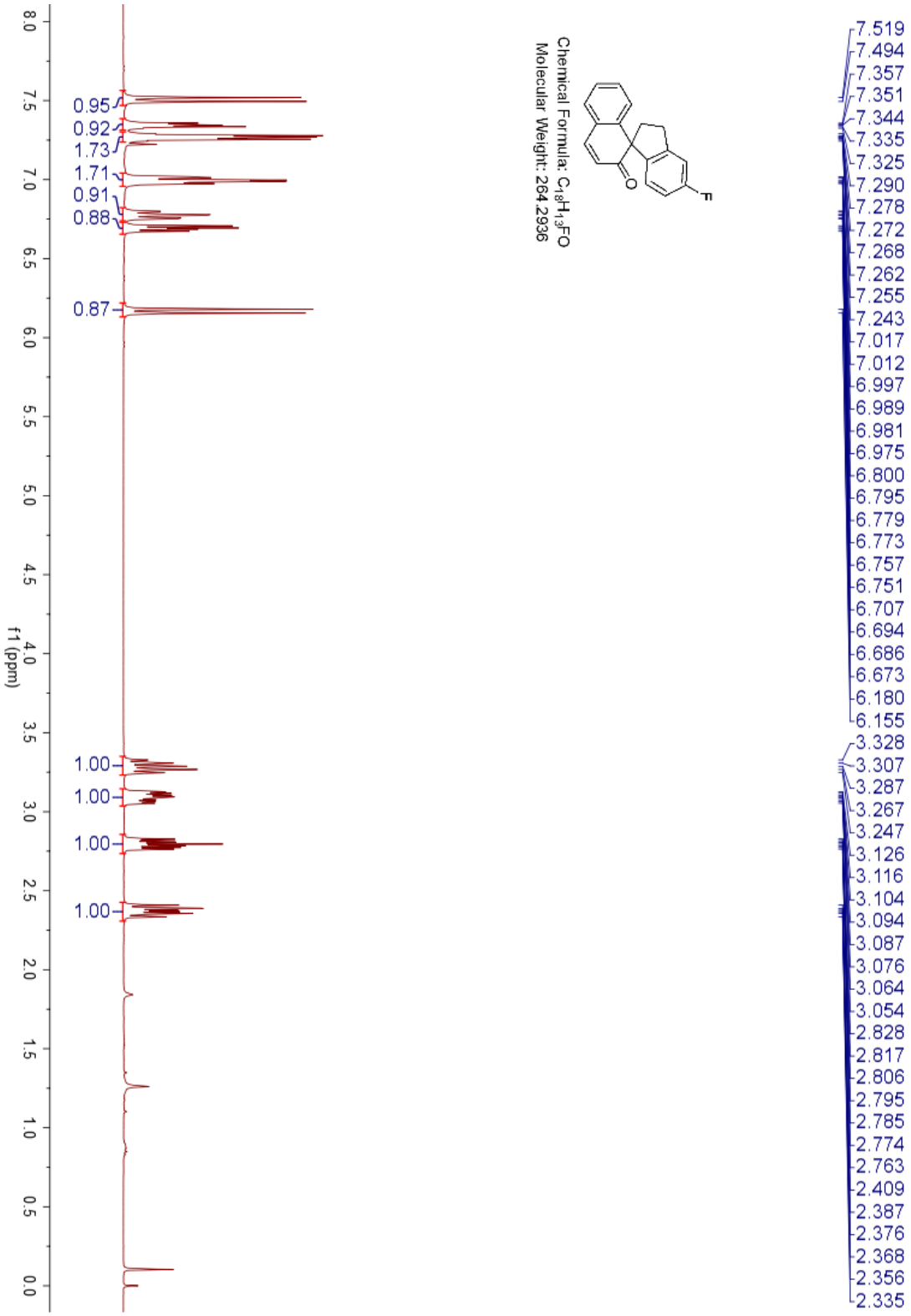

Chemical Formula: C19H16O2
Molecular Weight: 276.3291
O
O
202.485
159.488
146.749
146.717
145.017
137.505
129.974
127.781
126.790
124.969
124.316
113.111
109.608
77.309
77.000
76.675
64.307
55.173
42.141
31.475
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

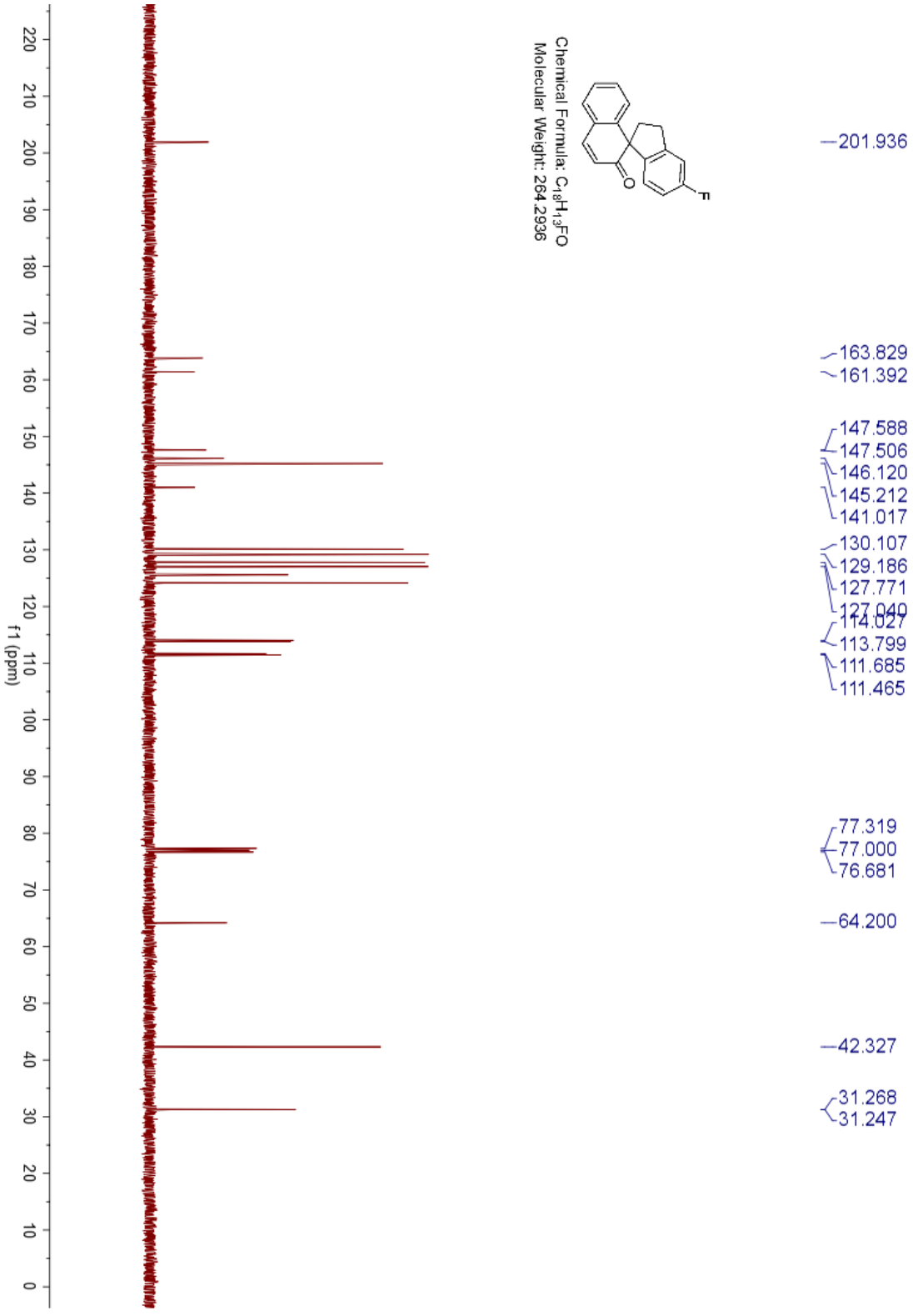

f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.90
0.87
1.68
0.86
0.78
0.72
0.81
1.79
1.00
1.01
0.98
1.01
Chemical Formula: C19H14O3
Molecular Weight: 290.3127
7.519
7.494
7.340
7.300
7.295
7.290
7.284
7.277
7.273
7.257
7.050
6.778
6.210
6.201
6.177
5.915
5.913
5.878
5.875
3.205
3.186
3.166
3.147
3.058
3.046
3.036
3.024
3.019
3.007
2.997
2.986
2.806
2.795
2.785
2.774
2.763
2.753
2.741
2.376
2.358
2.355
2.344
2.337
2.326
2.322
2.304
0.000

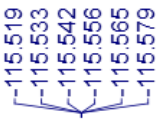

Chemical Formula: C19H14O3
Molecular Weight: 290.3127
202.558
147.739
146.912
146.511
145.104
138.397
137.798
130.102
129.290
129.172
127.892
126.979
124.475
104.913
104.772
101.122
77.318
77.000
76.682
64.875
42.470
31.178
f1 (ppm)

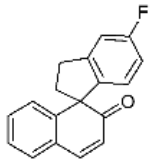

Chemical Formula: C18H13ClO
Molecular Weight: 280.7482
Cl
O
7.530
7.505
7.342
7.290
7.289
7.280
7.277
7.267
7.237
7.236
7.196
7.191
6.739
6.734
6.184
6.159
3.312
3.292
3.272
3.252
3.232
3.120
3.109
3.098
3.087
3.080
3.069
3.057
3.047
2.833
2.823
2.812
2.801
2.790
2.779
2.768
2.409
2.389
2.387
2.376
2.368
2.357
2.354
2.335
0.000
1.04
1.02
3.06
0.98
1.07
0.91
1.00
1.17
1.14
1.13
1.16
f1 (ppm)


Chemical Formula: $C_{18}H_{13}ClO$
Molecular Weight: 280.7482
O
Cl
201.421
147.420
145.651
145.370
143.740
132.287
130.254
129.279
129.214
127.890
127.866
127.206
125.799
124.596
124.171
77.318
77.000
76.681
64.858
42.045
30.892
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

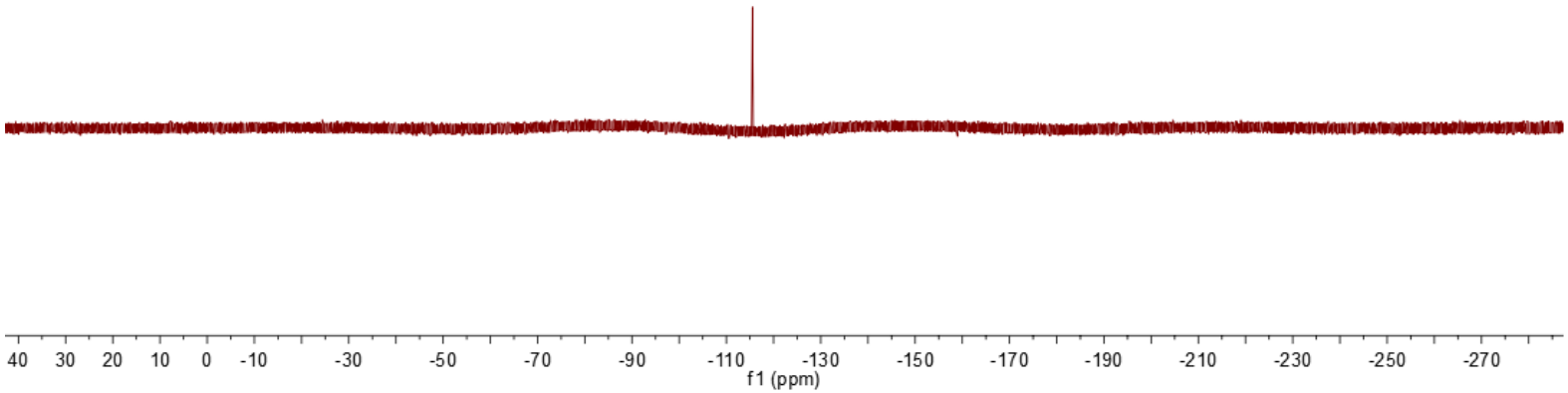

Chemical Formula: C18H13FO
Molecular Weight: 264.2936
F
O
f1 (ppm)
0.95
0.92
1.73
1.71
0.91
0.88
0.87
1.00
1.00
1.00
1.00
7.519
7.494
7.357
7.351
7.344
7.335
7.325
7.290
7.278
7.272
7.268
7.262
7.255
7.243
7.017
7.012
6.997
6.989
6.981
6.975
6.800
6.795
6.779
6.773
6.757
6.751
6.707
6.694
6.686
6.673
6.180
6.155
3.328
3.307
3.287
3.267
3.247
3.126
3.116
3.104
3.094
3.087
3.076
3.064
3.054
2.828
2.817
2.806
2.795
2.785
2.774
2.763
2.409
2.387
2.376
2.368
2.356
2.335

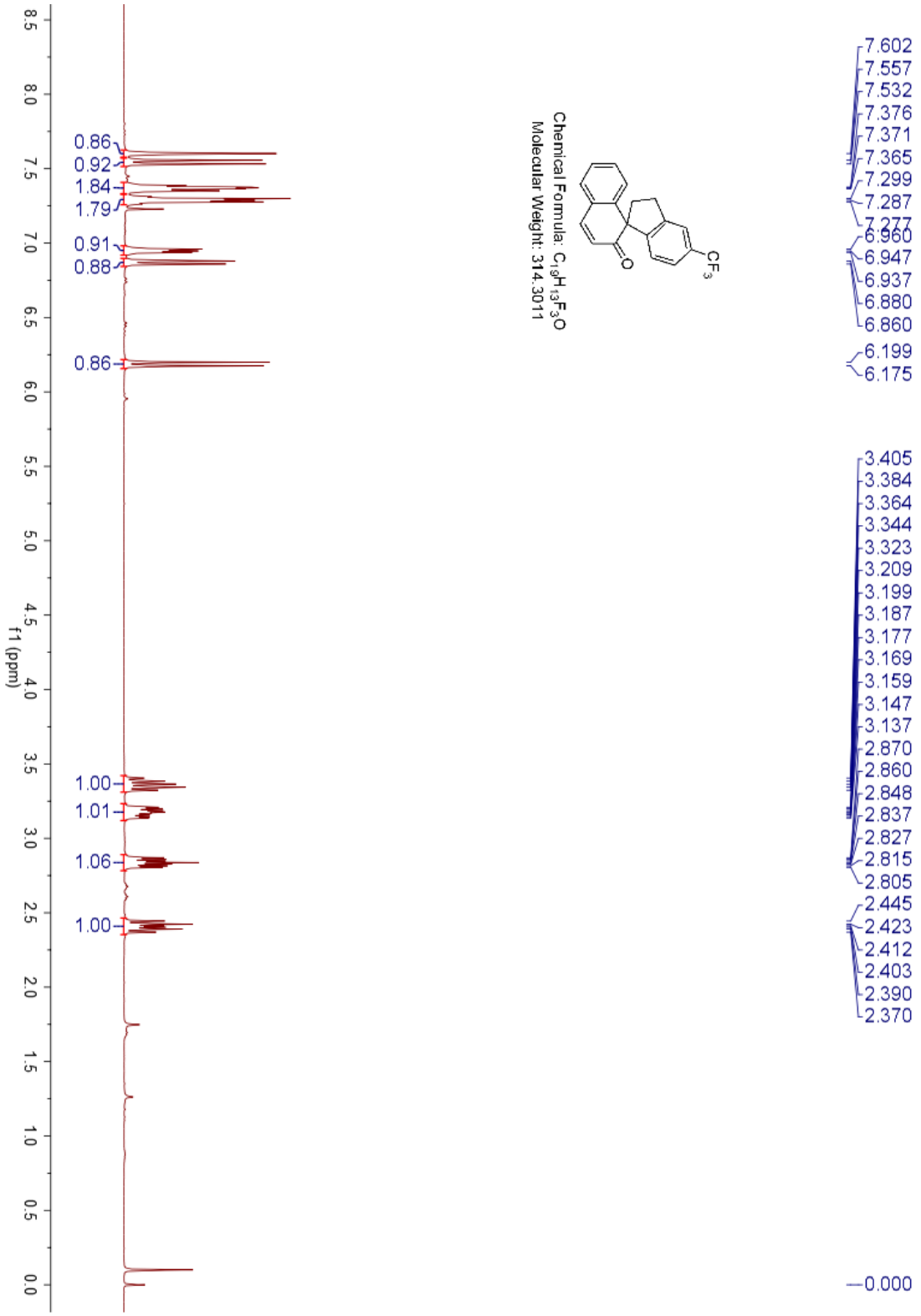

Chemical Formula: $C_{18}H_{13}FO$
Molecular Weight: 264.2936
F
O
201.936
163.829
161.392
147.588
147.506
146.120
145.212
141.017
130.107
129.186
127.771
127.040
114.027
113.799
111.685
111.465
77.319
77.000
76.681
64.200
42.327
31.268
31.247
f1 (ppm)

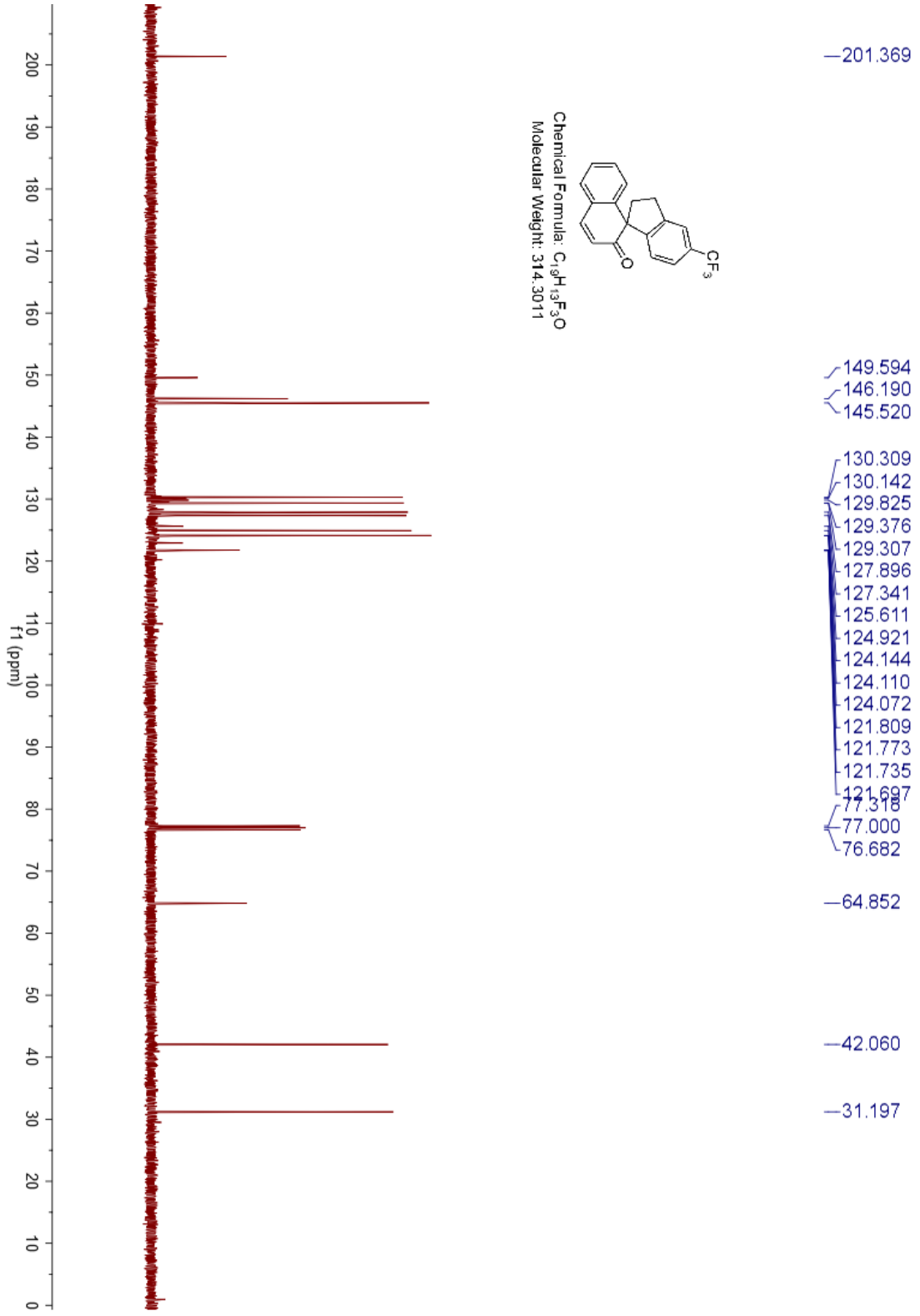


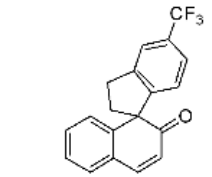


Chemical Formula: $C_{18}H_{13}FO$
Molecular Weight: 264.2936

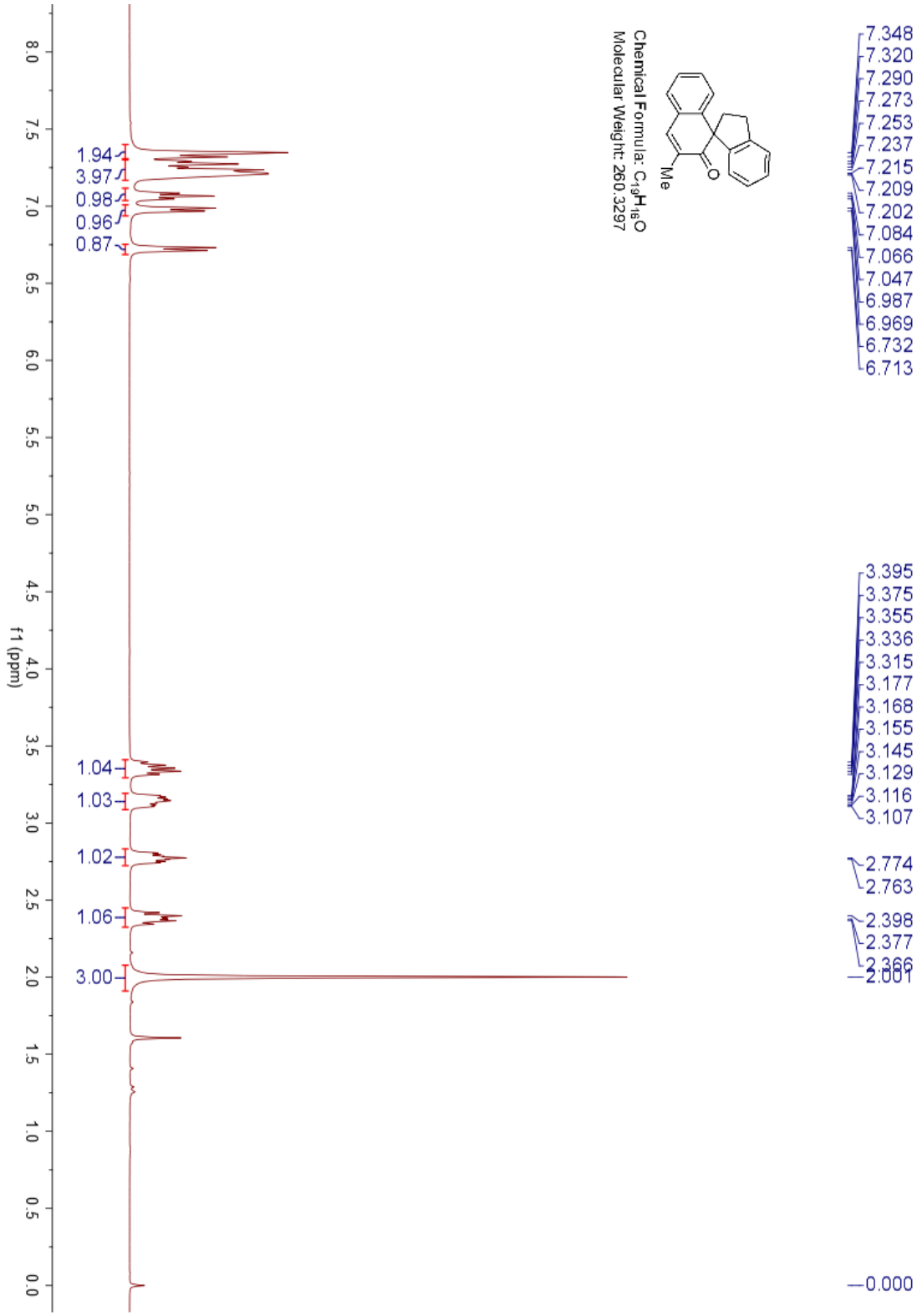


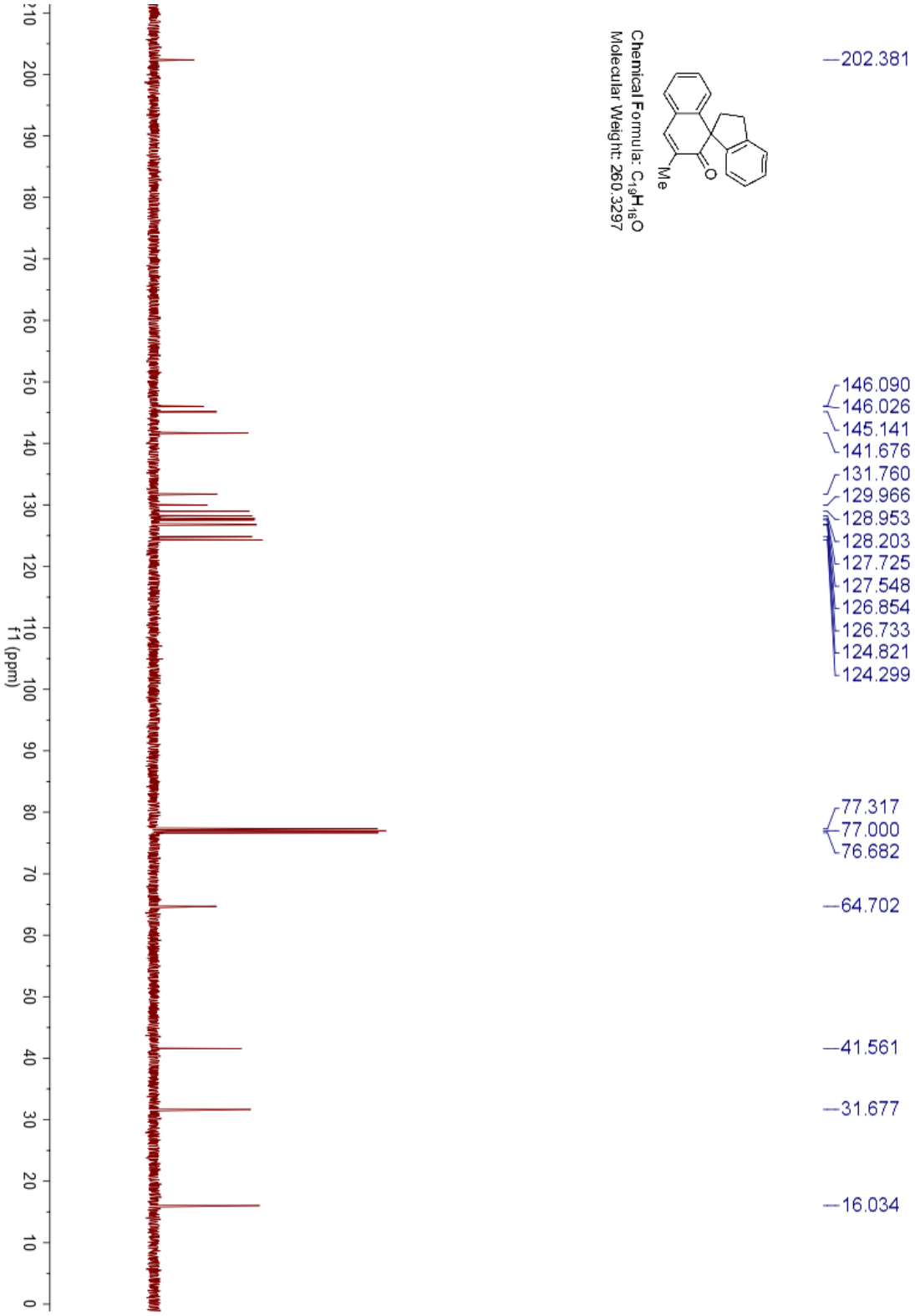

Chemical Formula: C19H13F3O
Molecular Weight: 314.3011
CF3
O
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.86
0.92
1.84
1.79
0.91
0.88
0.86
1.00
1.01
1.06
1.00
7.602
7.557
7.532
7.376
7.371
7.365
7.299
7.287
7.277
6.960
6.947
6.937
6.880
6.860
6.199
6.175
3.405
3.384
3.364
3.344
3.323
3.209
3.199
3.187
3.177
3.169
3.159
3.147
3.137
2.870
2.860
2.848
2.837
2.827
2.815
2.805
2.445
2.423
2.412
2.403
2.390
2.370
0.000

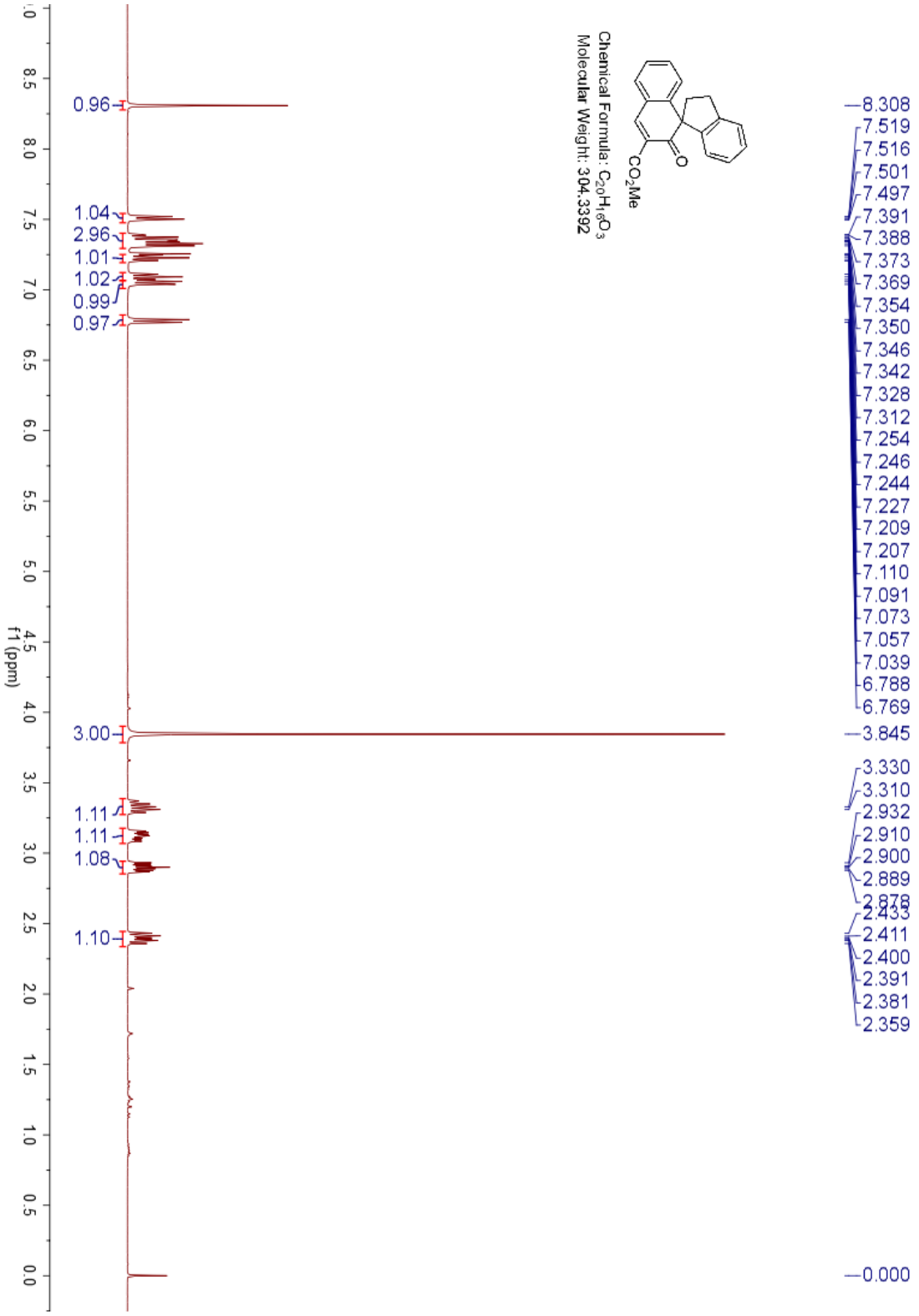

Chemical Formula: $C_{19}H_{13}F_3O$
Molecular Weight: 314.3011
O
CF_3
201.369
149.594
146.190
145.520
130.309
130.142
129.825
129.376
129.307
127.896
127.341
125.611
124.921
124.144
124.110
124.072
121.809
121.773
121.735
121.697
77.318
77.000
76.682
64.852
42.060
31.197
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

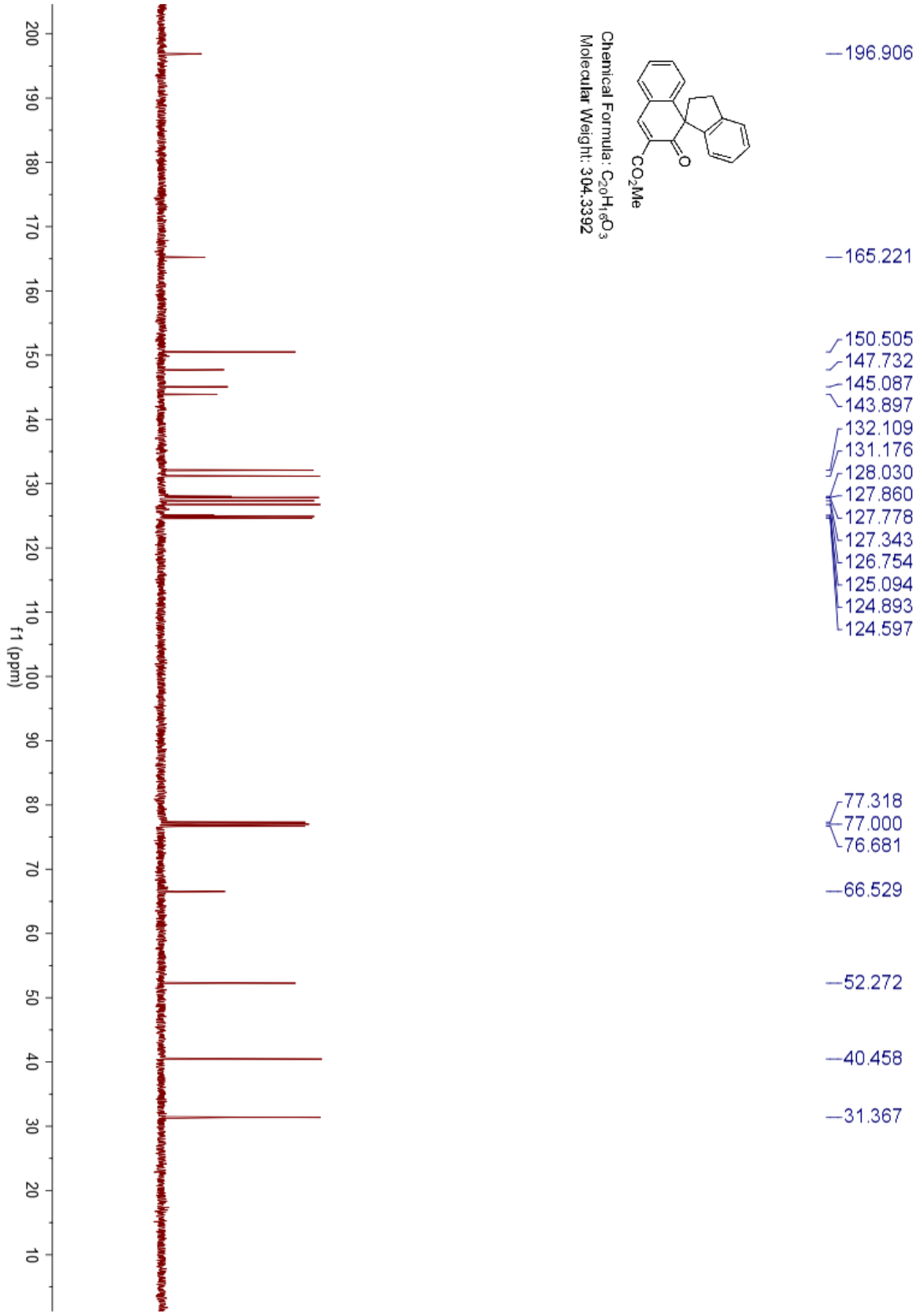


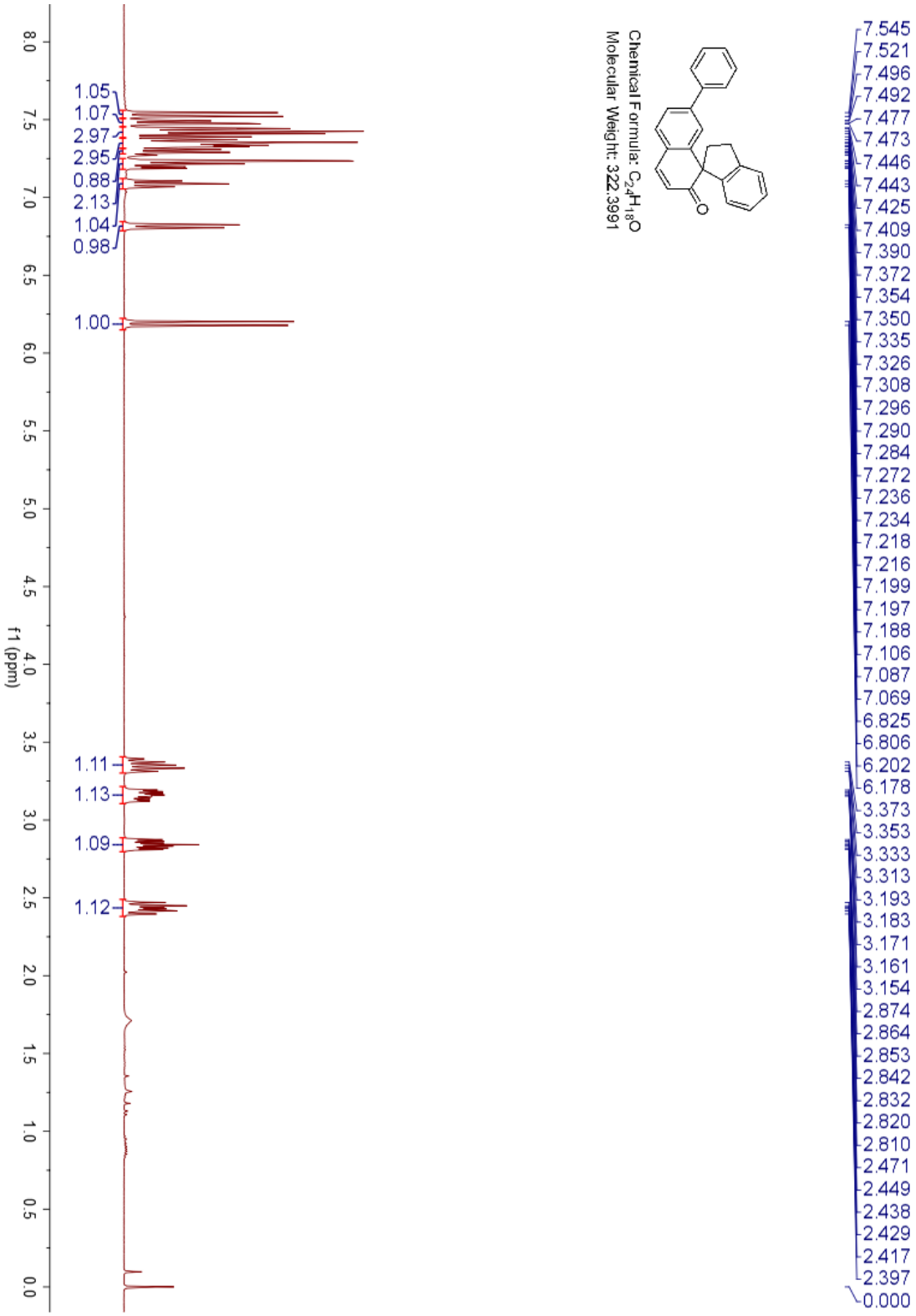
Chemical Formula: $C_{19}H_{13}F_3O$
Molecular Weight: 314.3011


Chemical Formula: C19H16O
Molecular Weight: 260.3297
Me
O
7.348
7.320
7.290
7.273
7.253
7.237
7.215
7.209
7.202
7.084
7.066
7.047
6.987
6.969
6.732
6.713
3.395
3.375
3.355
3.336
3.315
3.177
3.168
3.155
3.145
3.129
3.116
3.107
2.774
2.763
2.398
2.377
2.366
2.001
0.000
1.94
3.97
0.98
0.96
0.87
1.04
1.03
1.02
1.06
3.00
f1 (ppm)


Chemical Formula: C19H16O
Molecular Weight: 260.3297
Me
O
202.381
146.090
146.026
145.141
141.676
131.760
129.966
128.953
128.203
127.725
127.548
126.854
126.733
124.821
124.299
77.317
77.000
76.682
64.702
41.561
31.677
16.034
f1 (ppm)


Chemical Formula: $C_{20}H_{16}O_3$
Molecular Weight: 304.3392
CO_2Me
O
f1 (ppm)
0.96
1.04
2.96
1.01
1.02
0.99
0.97
3.00
1.11
1.11
1.08
1.10
8.308
7.519
7.516
7.501
7.497
7.391
7.388
7.373
7.369
7.354
7.350
7.346
7.342
7.328
7.312
7.254
7.246
7.244
7.227
7.209
7.207
7.110
7.091
7.073
7.057
7.039
6.788
6.769
3.845
3.330
3.310
2.932
2.910
2.900
2.889
2.878
2.433
2.411
2.400
2.391
2.381
2.359
0.000


Chemical Formula: $C_{20}H_{16}O_3$
Molecular Weight: 304.3392
CO_2Me
O
196.906
165.221
150.505
147.732
145.087
143.897
132.109
131.176
128.030
127.860
127.778
127.343
126.754
125.094
124.893
124.597
77.318
77.000
76.681
66.529
52.272
40.458
31.367
f1 (ppm)


Chemical Formula: $C_{24}H_{18}O$
Molecular Weight: 322.3991
1.05
1.07
2.97
2.95
0.88
2.13
1.04
0.98
1.00
1.11
1.13
1.09
1.12
f1 (ppm)
7.545
7.521
7.496
7.492
7.477
7.473
7.446
7.443
7.425
7.409
7.390
7.372
7.354
7.350
7.335
7.326
7.308
7.296
7.290
7.284
7.272
7.236
7.234
7.218
7.216
7.199
7.197
7.188
7.106
7.087
7.069
6.825
6.806
6.202
6.178
3.373
3.353
3.333
3.313
3.193
3.183
3.171
3.161
3.154
2.874
2.864
2.853
2.842
2.832
2.820
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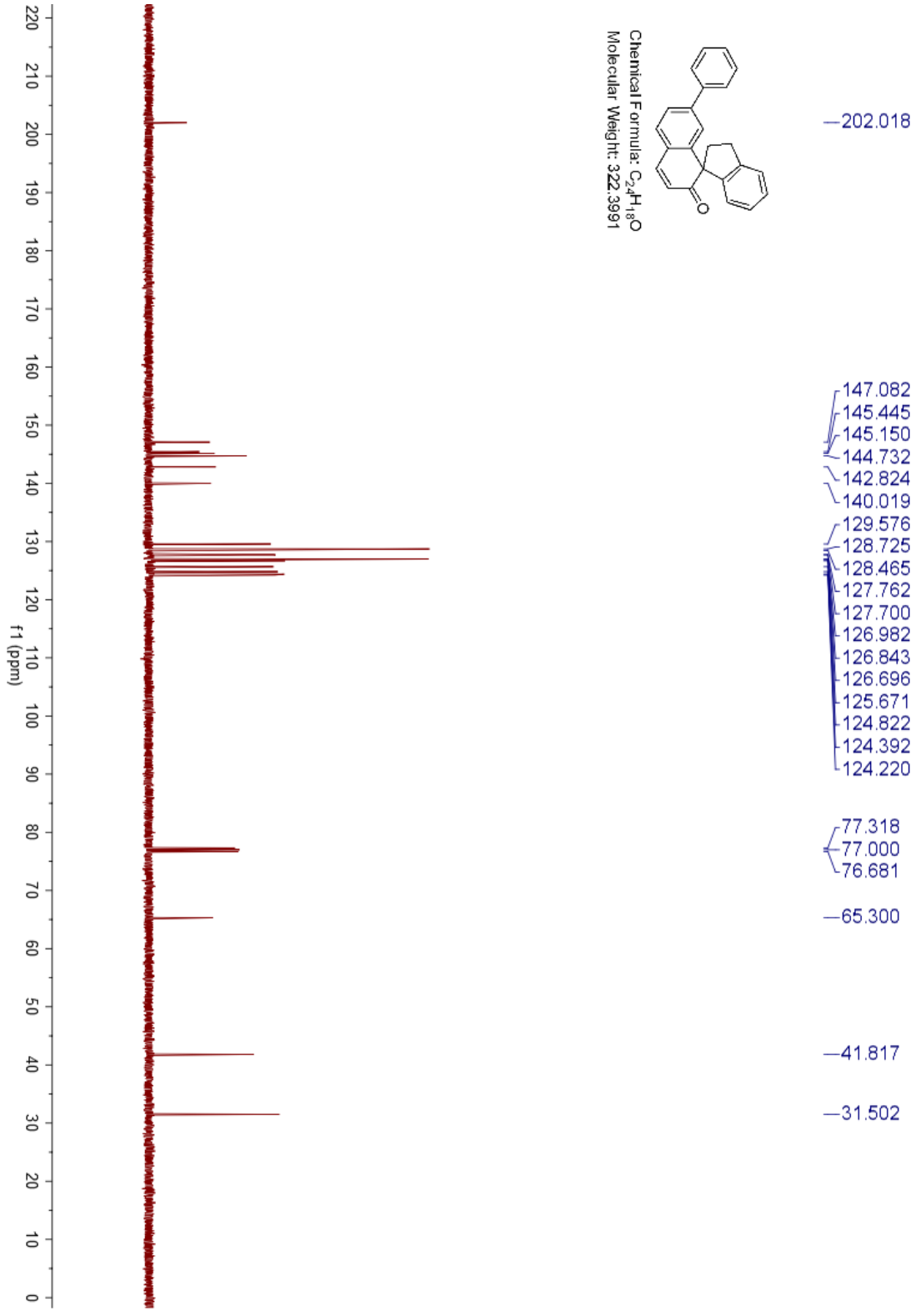
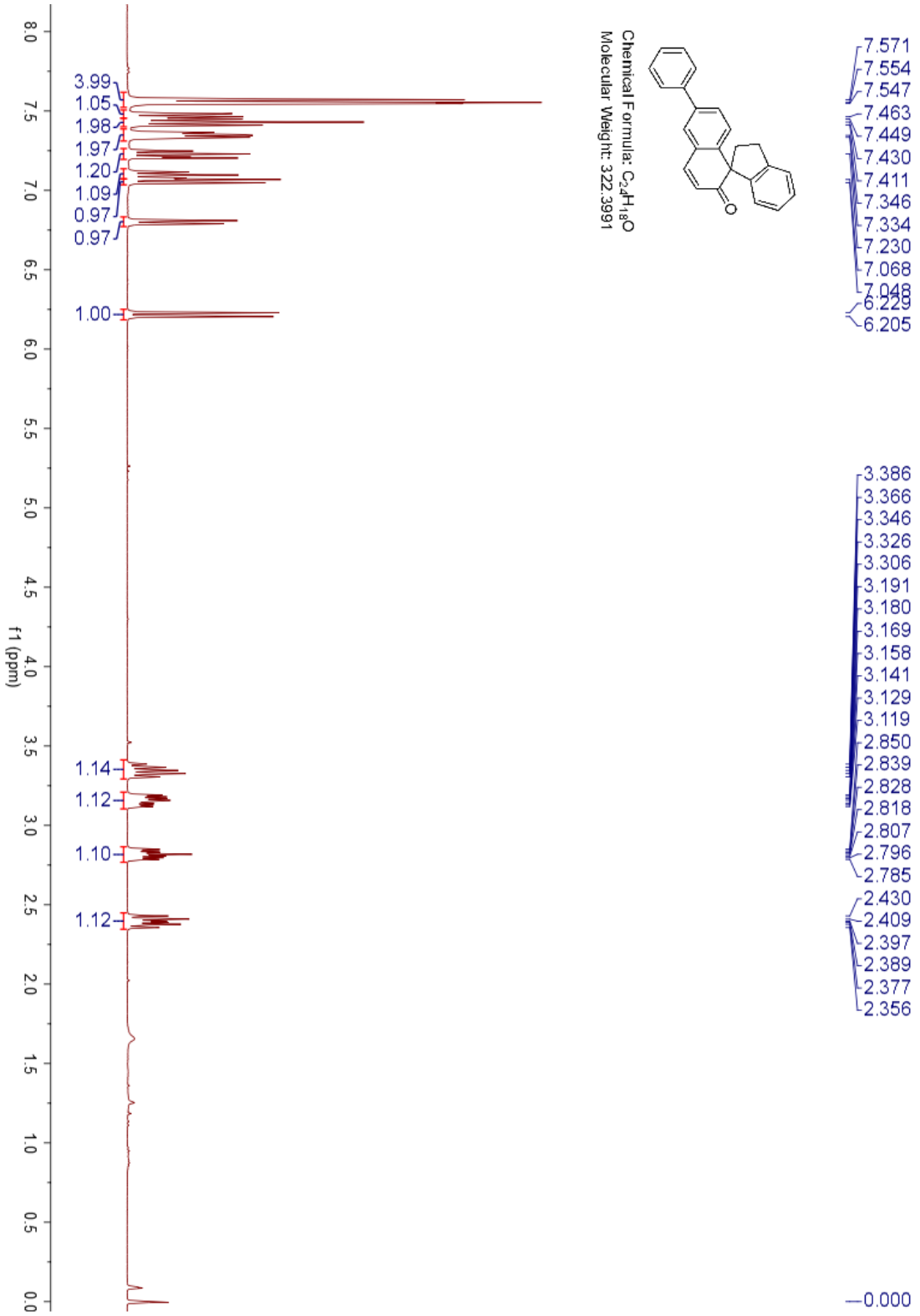
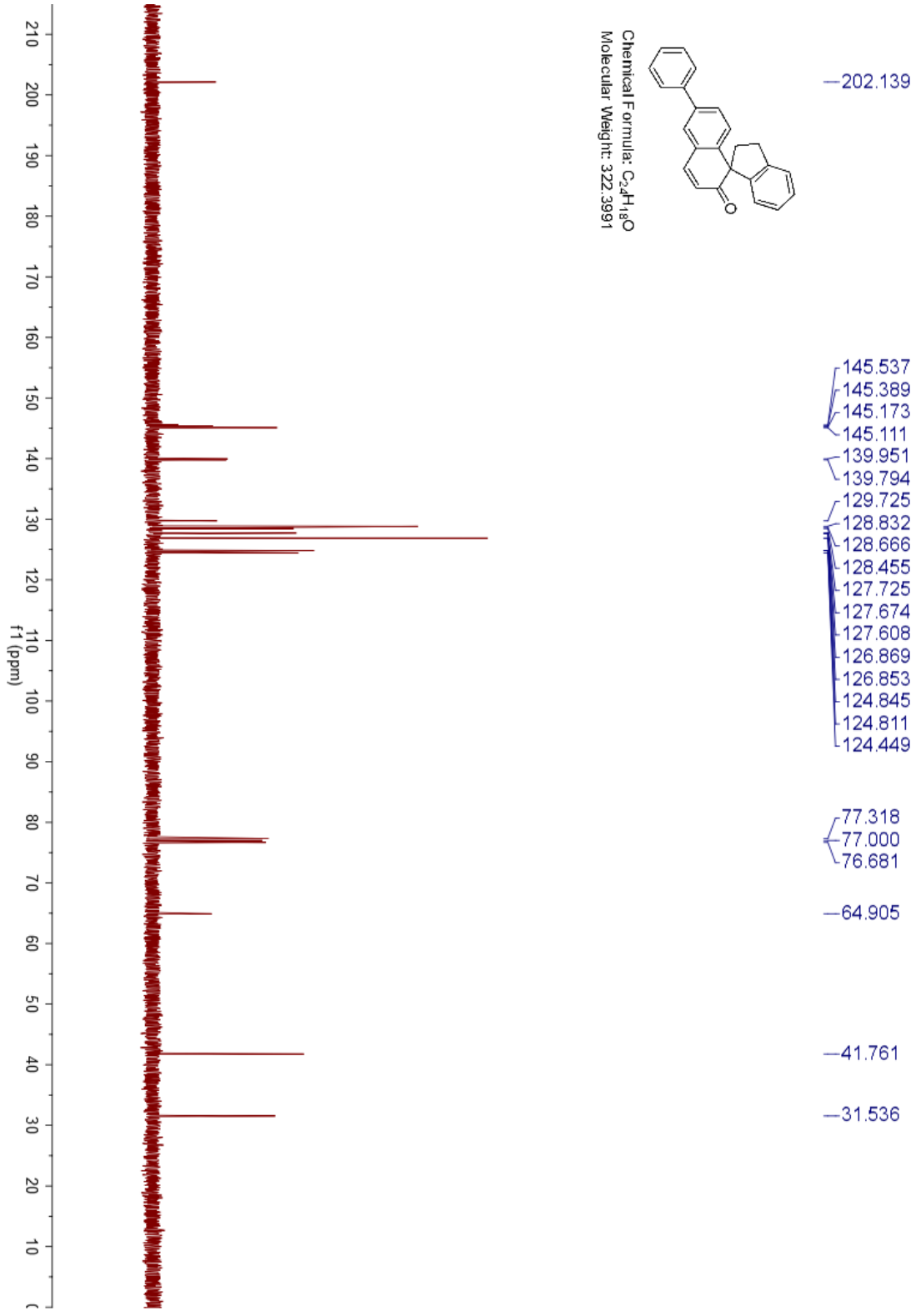
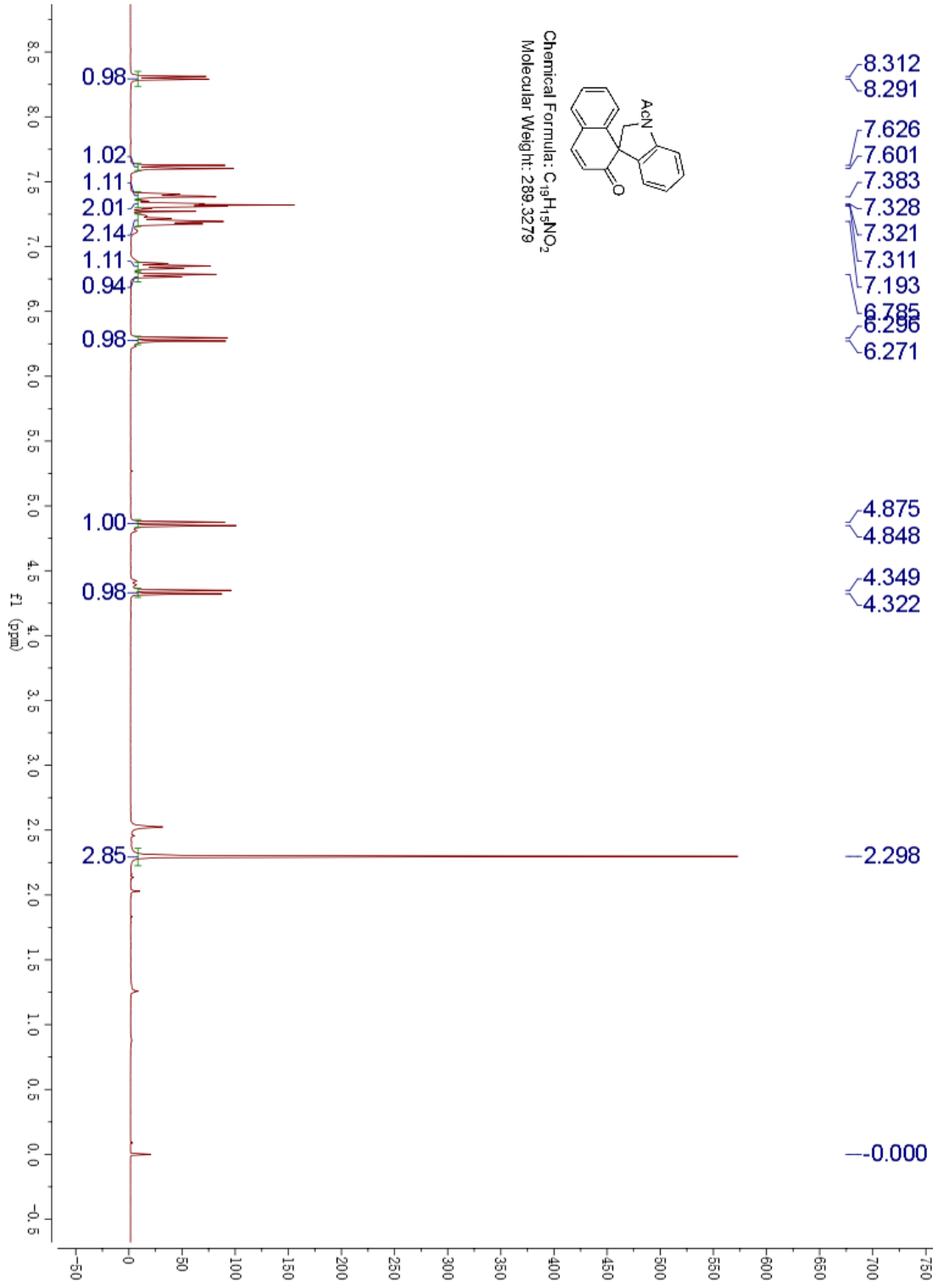
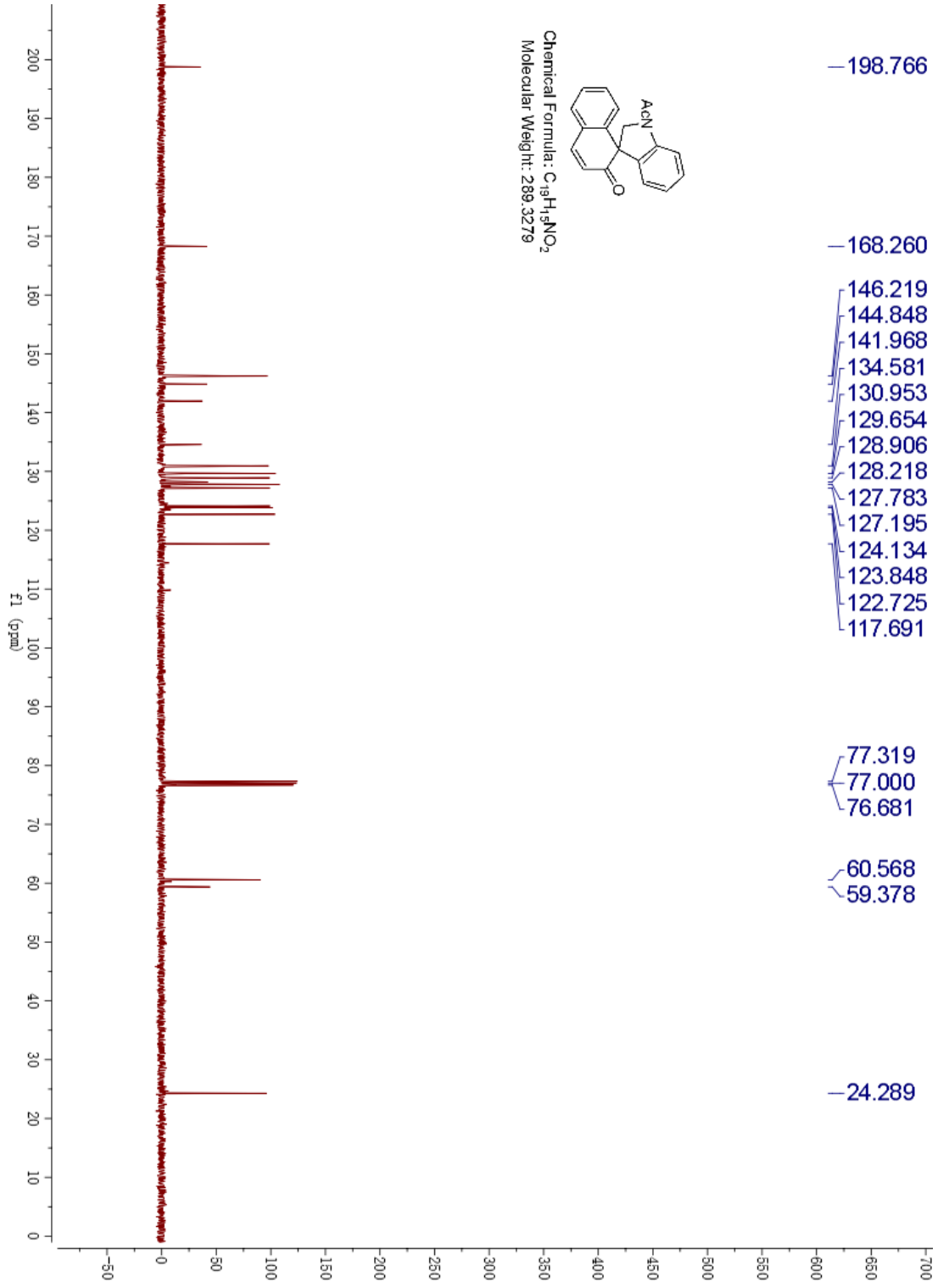
2.471
2.449
2.438
2.429
2.417
2.397
0.000

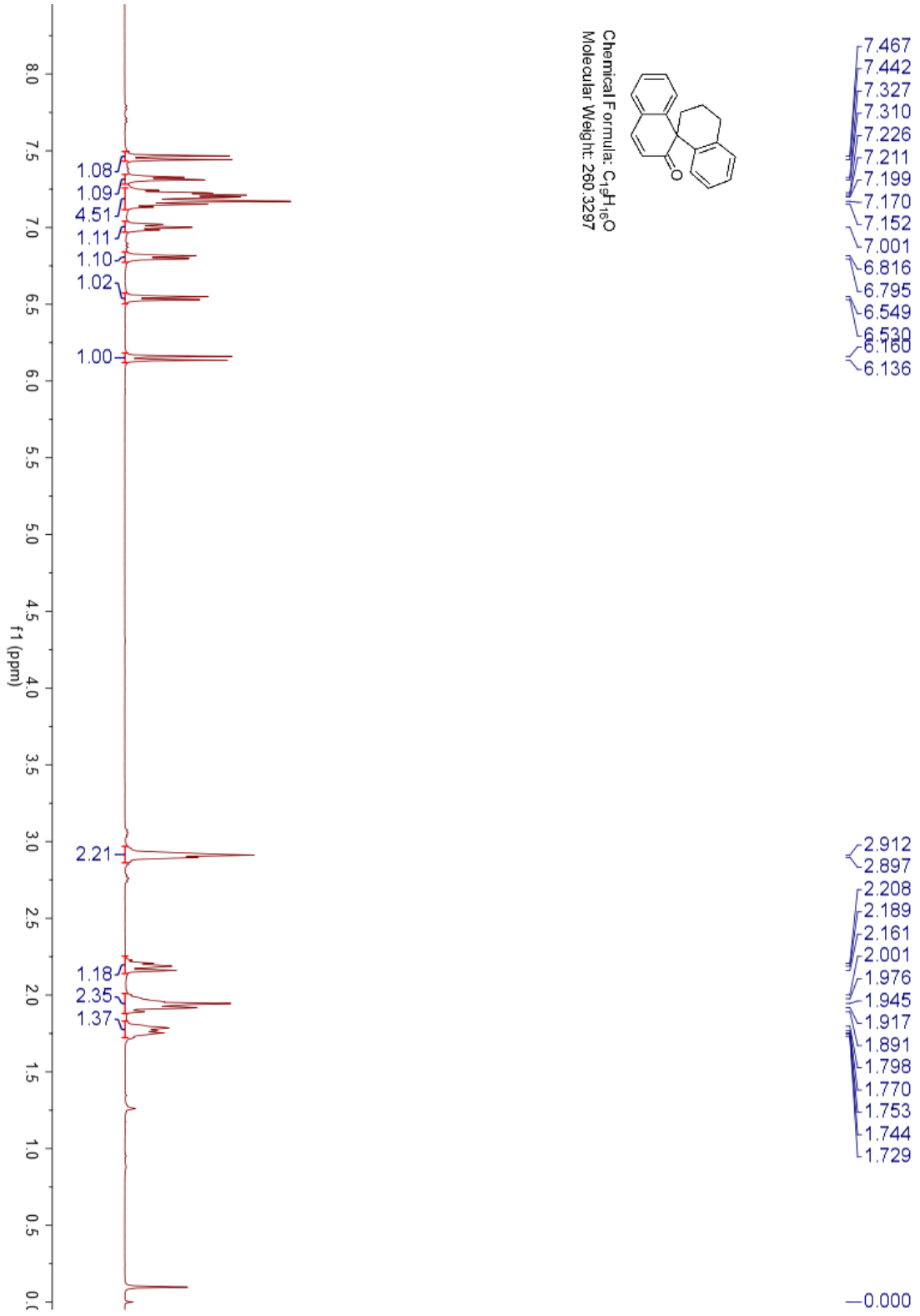

Chemical Formula: $C_{24}H_{18}O$
Molecular Weight: 322.3991
202.018
147.082
145.445
145.150
144.732
142.824
140.019
129.576
128.725
128.465
127.762
127.700
126.982
126.843
126.696
125.671
124.822
124.392
124.220
77.318
77.000
76.681
65.300
41.817
31.502
f1 (ppm)

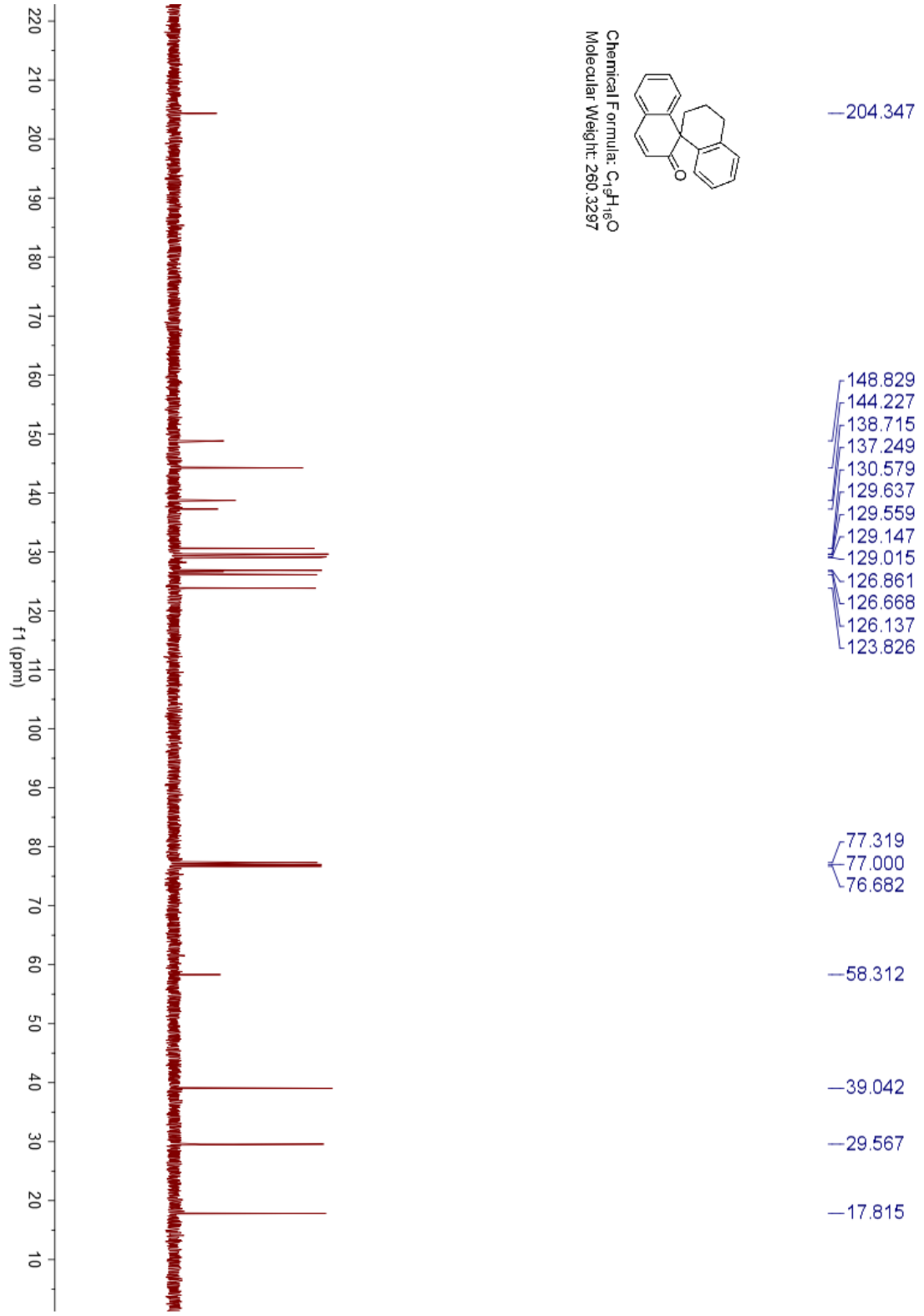

Chemical Formula: C24H18O
Molecular Weight: 322.3991
7.571
7.554
7.547
7.463
7.449
7.430
7.411
7.346
7.334
7.230
7.068
7.048
6.229
6.205
3.386
3.366
3.346
3.326
3.306
3.191
3.180
3.169
3.158
3.141
3.129
3.119
2.850
2.839
2.828
2.818
2.807
2.796
2.785
2.430
2.409
2.397
2.389
2.377
2.356
0.000
3.99
1.05
1.98
1.97
1.20
1.09
0.97
0.97
1.00
1.14
1.12
1.10
1.12
f1 (ppm)

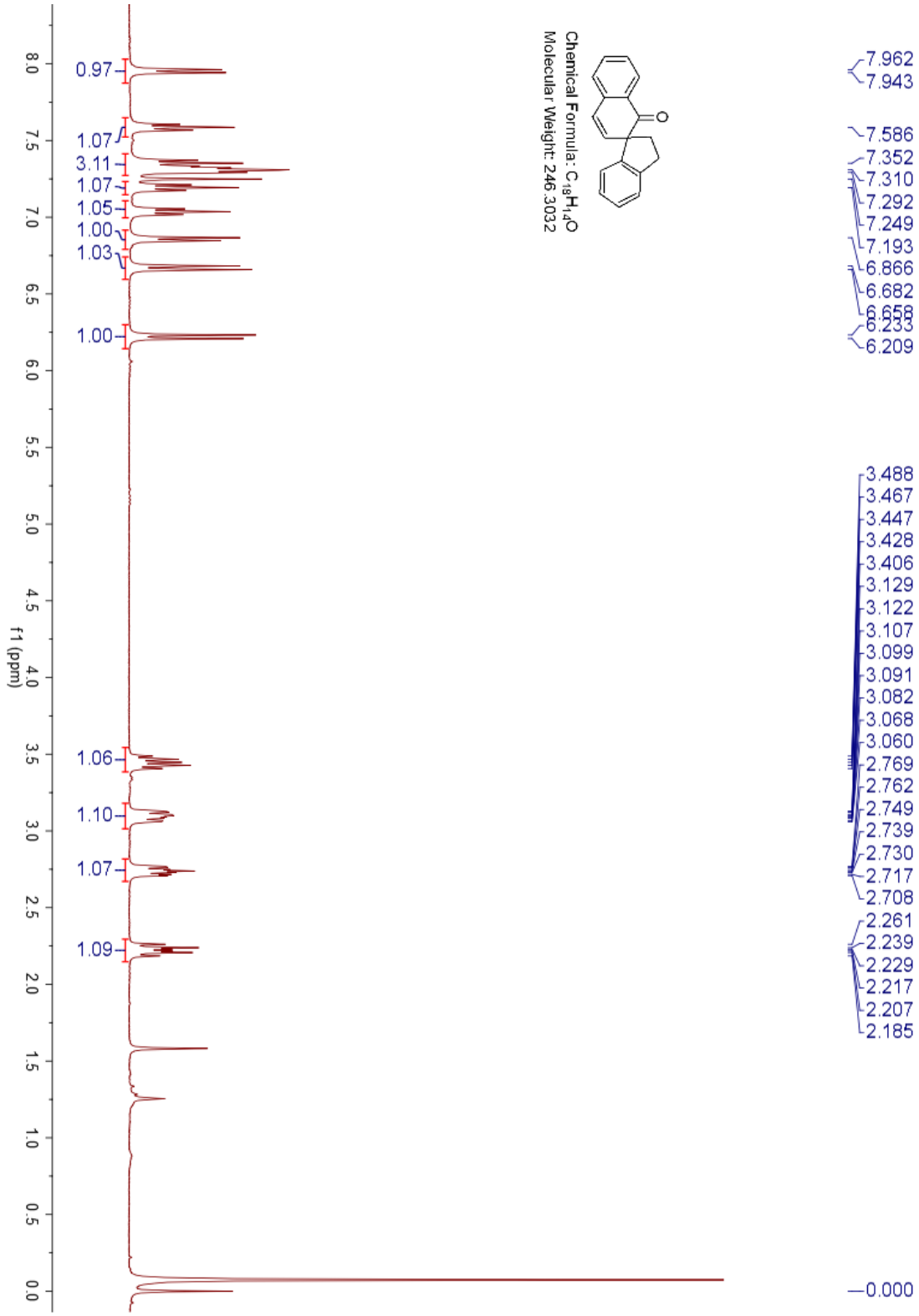

Chemical Formula: C24H18O
Molecular Weight: 322.3991
202.139
145.537
145.389
145.173
145.111
139.951
139.794
129.725
128.832
128.666
128.455
127.725
127.674
127.608
126.869
126.853
124.845
124.811
124.449
77.318
77.000
76.681
64.905
41.761
31.536
f1 (ppm)

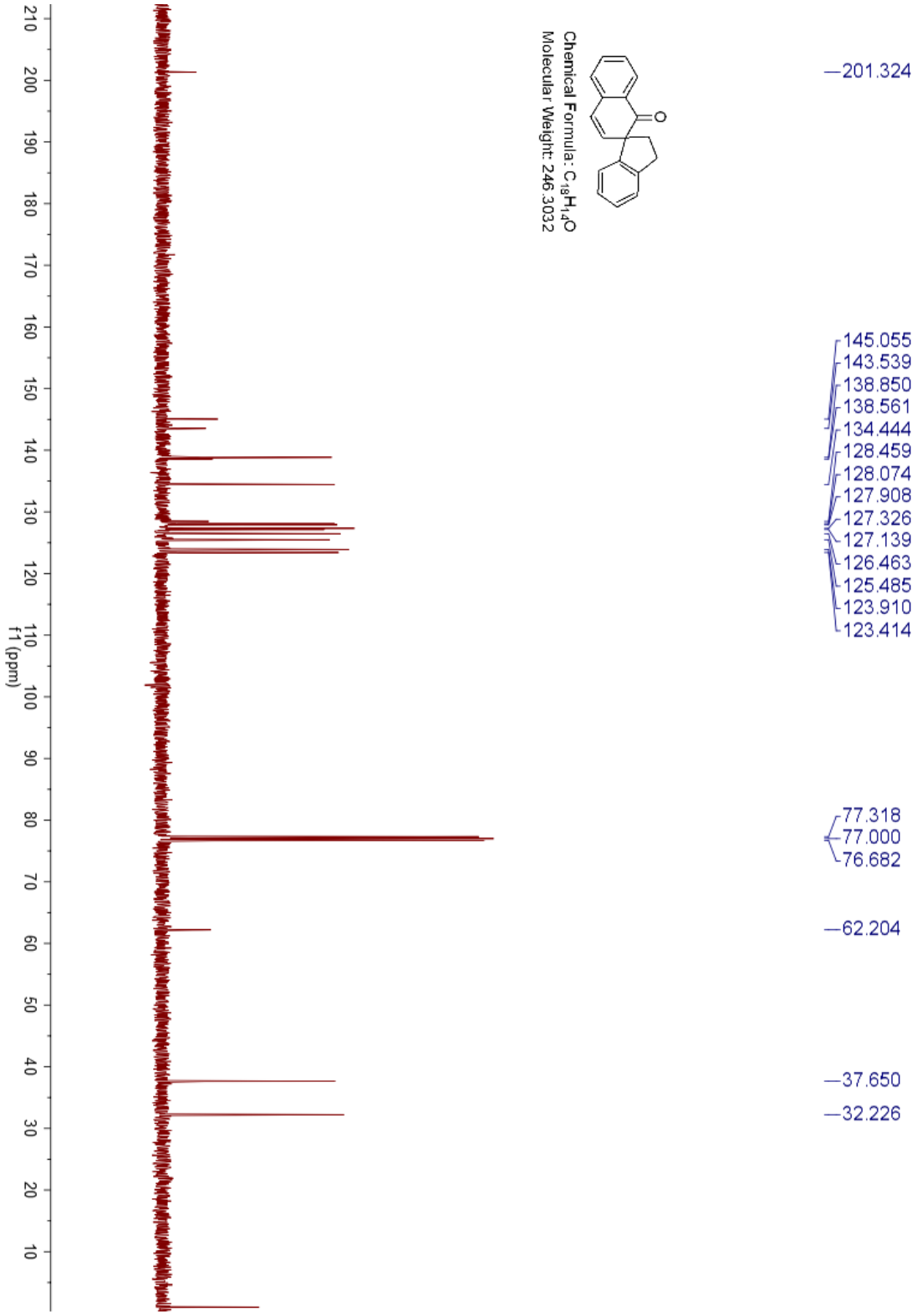

Chemical Formula: $C_{19}H_{15}NO_2$
Molecular Weight: 289.3279
AcN
O
8.312
8.291
7.626
7.601
7.383
7.328
7.321
7.311
7.193
6.785
6.296
6.271
4.875
4.848
4.349
4.322
2.298
-0.000
0.98
1.02
1.11
2.01
2.14
1.11
0.94
0.98
1.00
0.98
2.85
f1 (ppm)

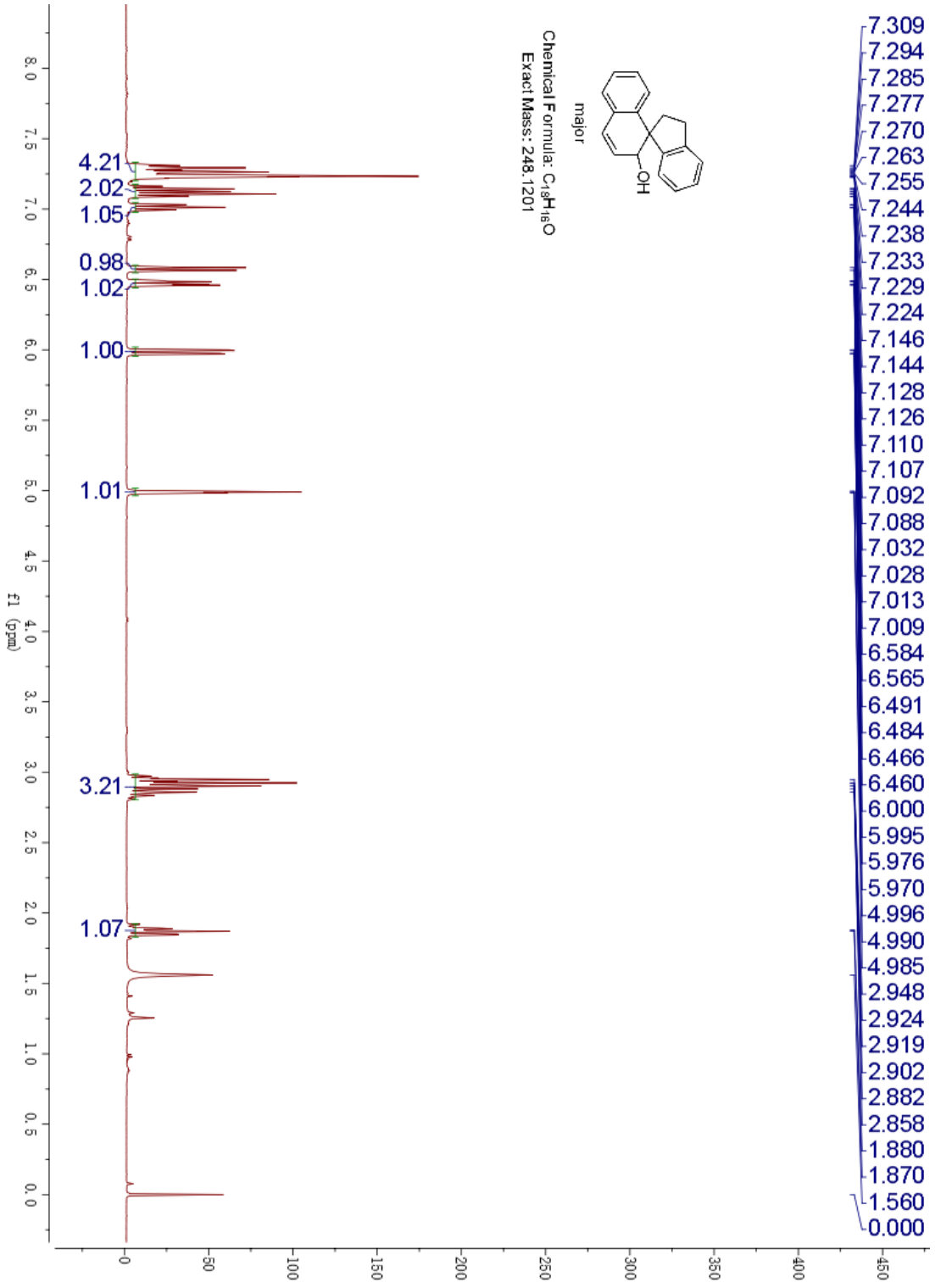

Chemical Formula: $C_{19}H_{15}NO_2$
Molecular Weight: 289.3279
AcN
O
198.766
168.260
146.219
144.848
141.968
134.581
130.953
129.654
128.906
128.218
127.783
127.195
124.134
123.848
122.725
117.691
77.319
77.000
76.681
60.568
59.378
24.289
f1 (ppm)

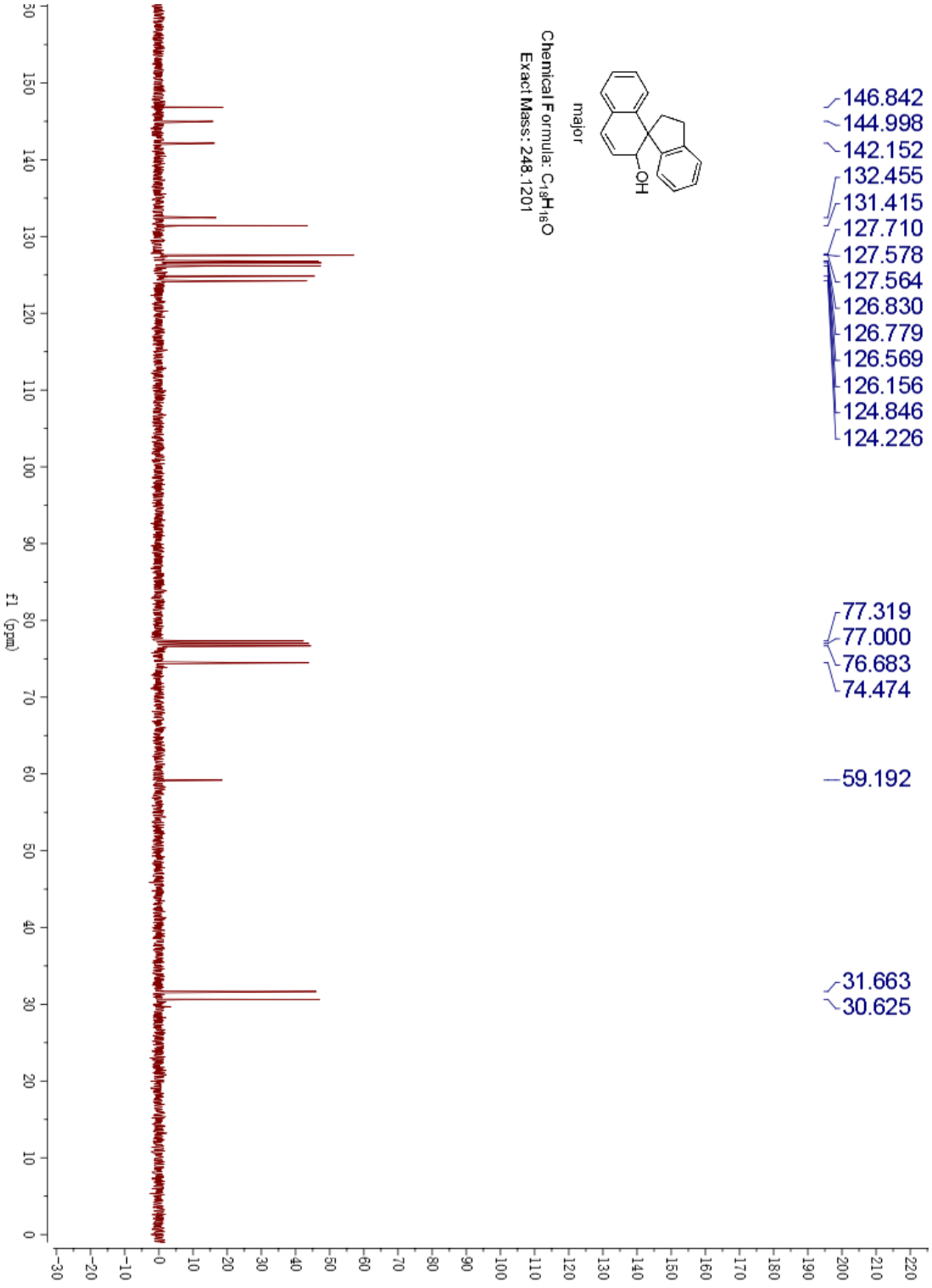

Chemical Formula: C15H16O
Molecular Weight: 260.3297
7.467
7.442
7.327
7.310
7.226
7.211
7.199
7.170
7.152
7.001
6.816
6.795
6.549
6.530
6.160
6.136
2.912
2.897
2.208
2.189
2.161
2.001
1.976
1.945
1.917
1.891
1.798
1.770
1.753
1.744
1.729
0.000
1.08
1.09
4.51
1.11
1.10
1.02
1.00
2.21
1.18
2.35
1.37
f1 (ppm)

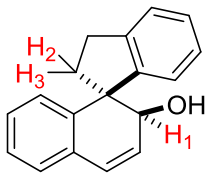

Chemical Formula: C19H16O
Molecular Weight: 260.3297
O
204.347
148.829
144.227
138.715
137.249
130.579
129.637
129.559
129.147
129.015
126.861
126.668
126.137
123.826
77.319
77.000
76.682
58.312
39.042
29.567
17.815
f1 (ppm)


Chemical Formula: C18H14O
Molecular Weight: 246.3032
f1 (ppm)
0.97
1.07
3.11
1.07
1.05
1.00
1.03
1.00
1.06
1.10
1.07
1.09
7.962
7.943
7.586
7.352
7.310
7.292
7.249
7.193
6.866
6.682
6.658
6.233
6.209
3.488
3.467
3.447
3.428
3.406
3.129
3.122
3.107
3.099
3.091
3.082
3.068
3.060
2.769
2.762
2.749
2.739
2.730
2.717
2.708
2.261
2.239
2.229
2.217
2.207
2.185
0.000

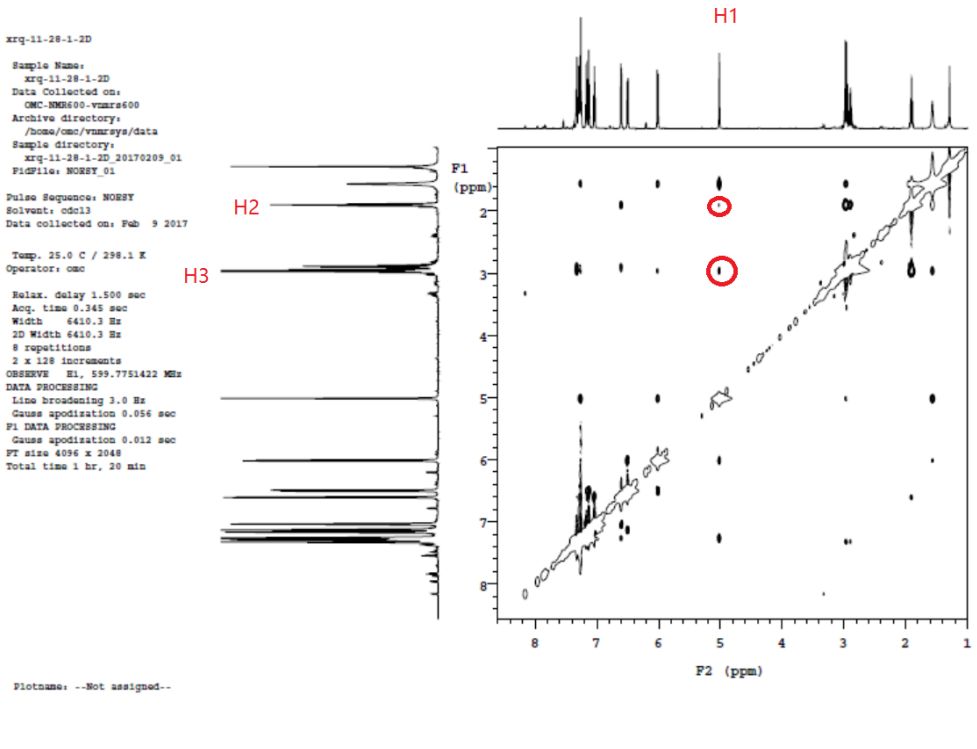

Chemical Formula: C18H14O
Molecular Weight: 246.3032
O
201.324
145.055
143.539
138.850
138.561
134.444
128.459
128.074
127.908
127.326
127.139
126.463
125.485
123.910
123.414
77.318
77.000
76.682
62.204
37.650
32.226
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

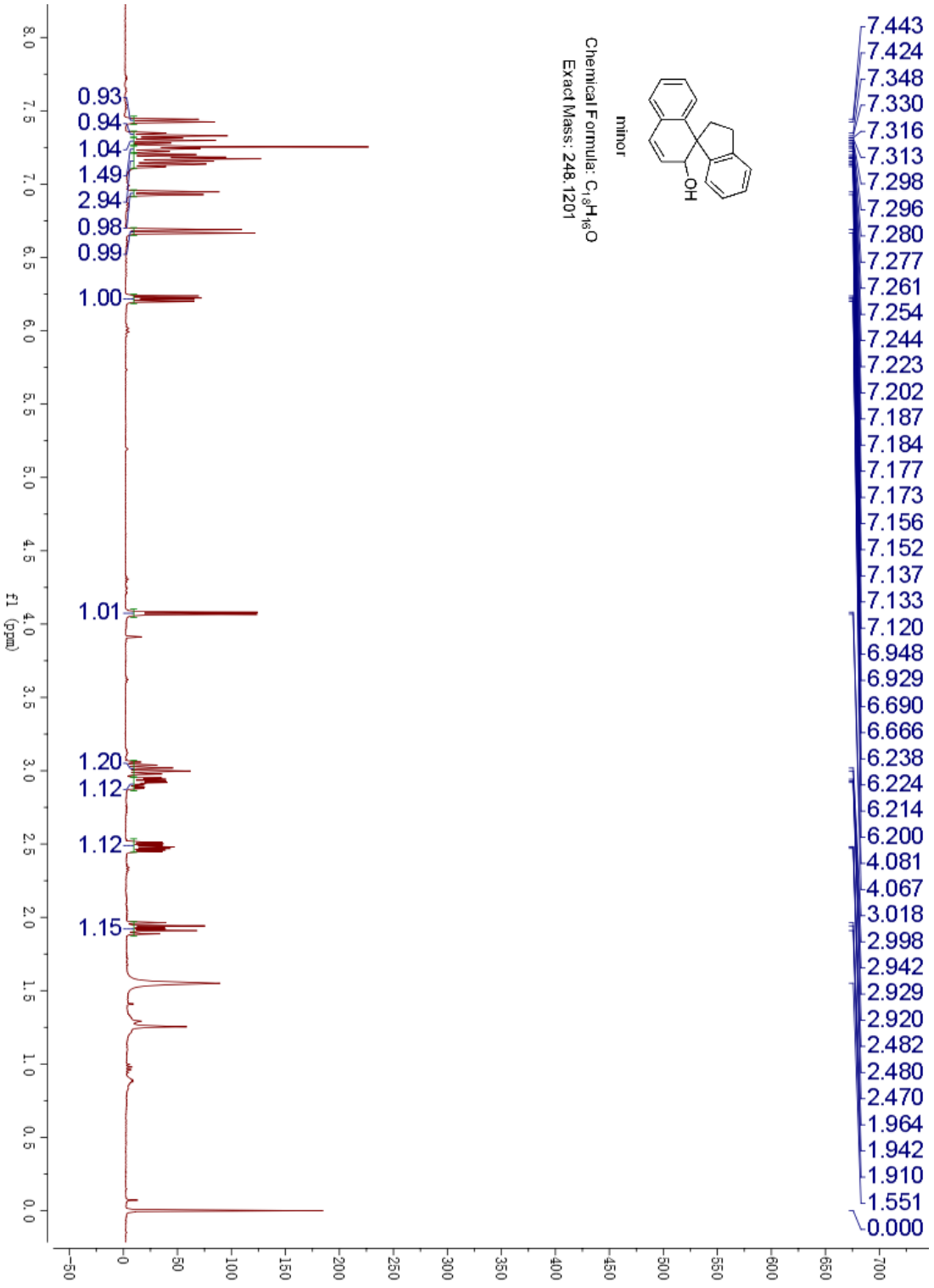

major
Chemical Formula: C18H16O
Exact Mass: 248.1201
OH
4.21
2.02
1.05
0.98
1.02
1.00
1.01
3.21
1.07
f1 (ppm)
7.309
7.294
7.285
7.277
7.270
7.263
7.255
7.244
7.238
7.233
7.229
7.224
7.146
7.144
7.128
7.126
7.110
7.107
7.092
7.088
7.032
7.028
7.013
7.009
6.584
6.565
6.491
6.484
6.466
6.460
6.000
5.995
5.976
5.970
4.996
4.990
4.985
2.948
2.924
2.919
2.902
2.882
2.858
1.880
1.870
1.560
0.000


Chemical Formula: C18H16O
Exact Mass: 248.1201
major
OH
146.842
144.998
142.152
132.455
131.415
127.710
127.578
127.564
126.830
126.779
126.569
126.156
124.846
124.226
77.319
77.000
76.683
74.474
59.192
31.663
30.625
f1 (ppm)


H2
H3
OH
H1

4a major


xrq-11-28-1-2D
Sample Name:
xrq-11-28-1-2D
Data Collected on:
OMC-NMR600-vnmrs600
Archive directory:
/home/omc/vnmrsys/data
Sample directory:
xrq-11-28-1-2D_20170209_01
FidFile: NOESY_01
Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Feb 9 2017
Temp. 25.0 C / 298.1 K
Operator: omc
Relax. delay 1.500 sec
Acq. time 0.345 sec
Width 6410.3 Hz
2D Width 6410.3 Hz
8 repetitions
2 x 128 increments
OBSERVE H1, 599.7751422 MHz
DATA PROCESSING
Line broadening 3.0 Hz
Gauss apodization 0.056 sec
F1 DATA PROCESSING
Gauss apodization 0.012 sec
FT size 4096 x 2048
Total time 1 hr, 20 min
Plotname: --Not assigned--
H1
H2
H3
F1
(ppm)
F2 (ppm)


minor
Chemical Formula: C18H16O
Exact Mass: 248.1201
OH
f1 (ppm)
0.93
0.94
1.04
1.49
2.94
0.98
0.99
1.00
1.01
1.20
1.12
1.12
1.15
7.443
7.424
7.348
7.330
7.316
7.313
7.298
7.296
7.280
7.277
7.261
7.254
7.244
7.223
7.202
7.187
7.184
7.177
7.173
7.156
7.152
7.137
7.133
7.120
6.948
6.929
6.690
6.666
6.238
6.224
6.214
6.200
4.081
4.067
3.018
2.998
2.942
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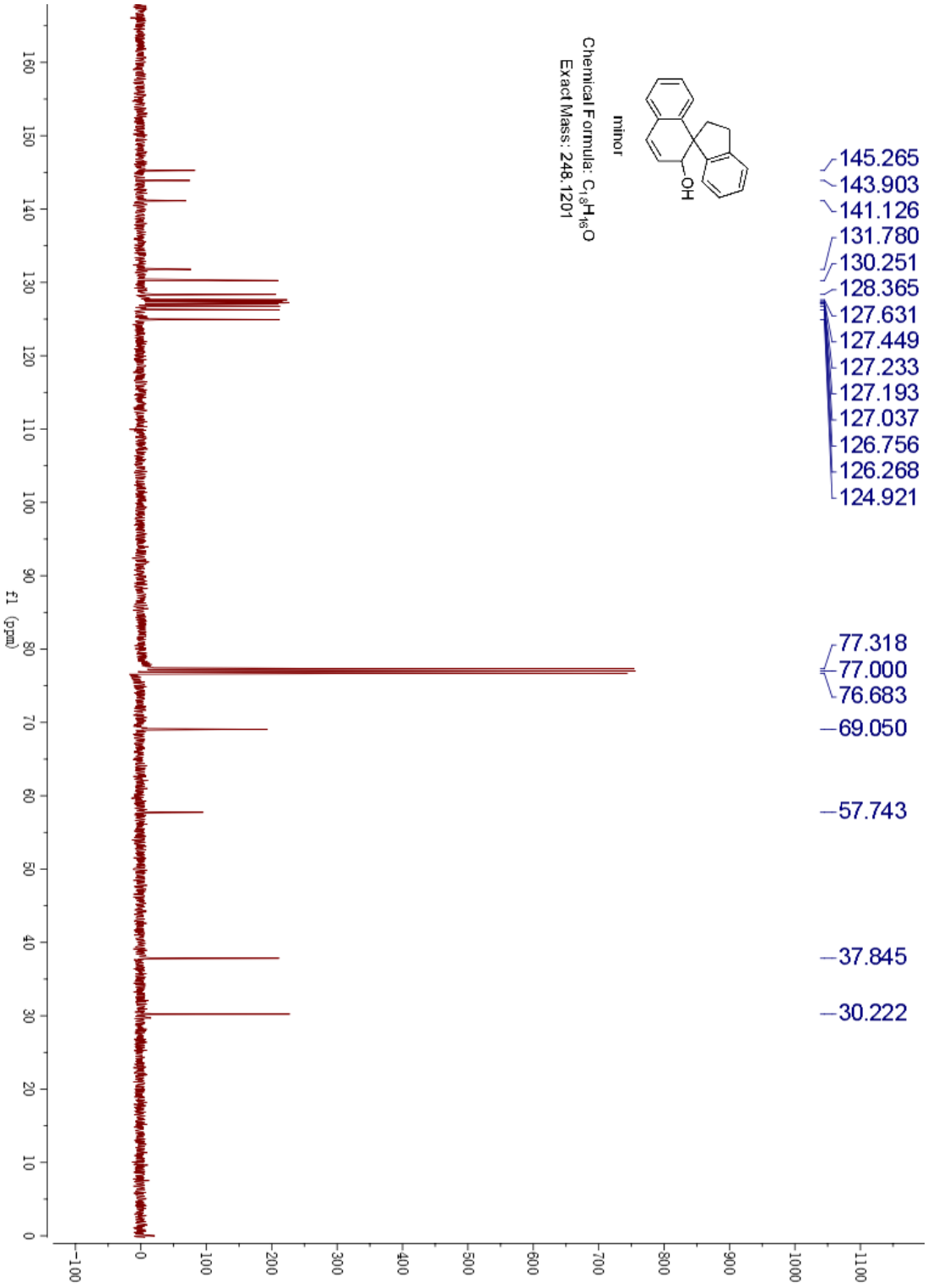
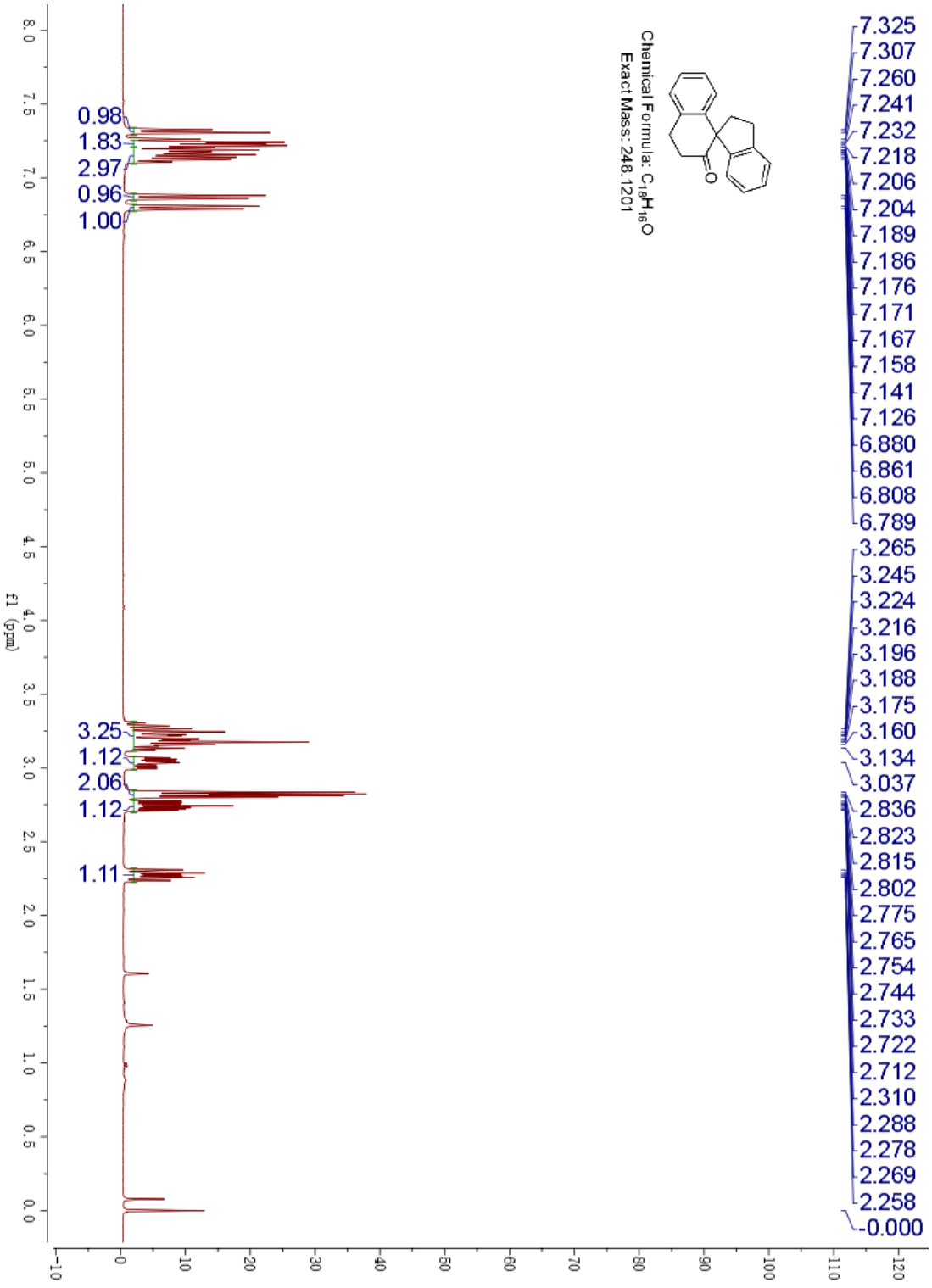
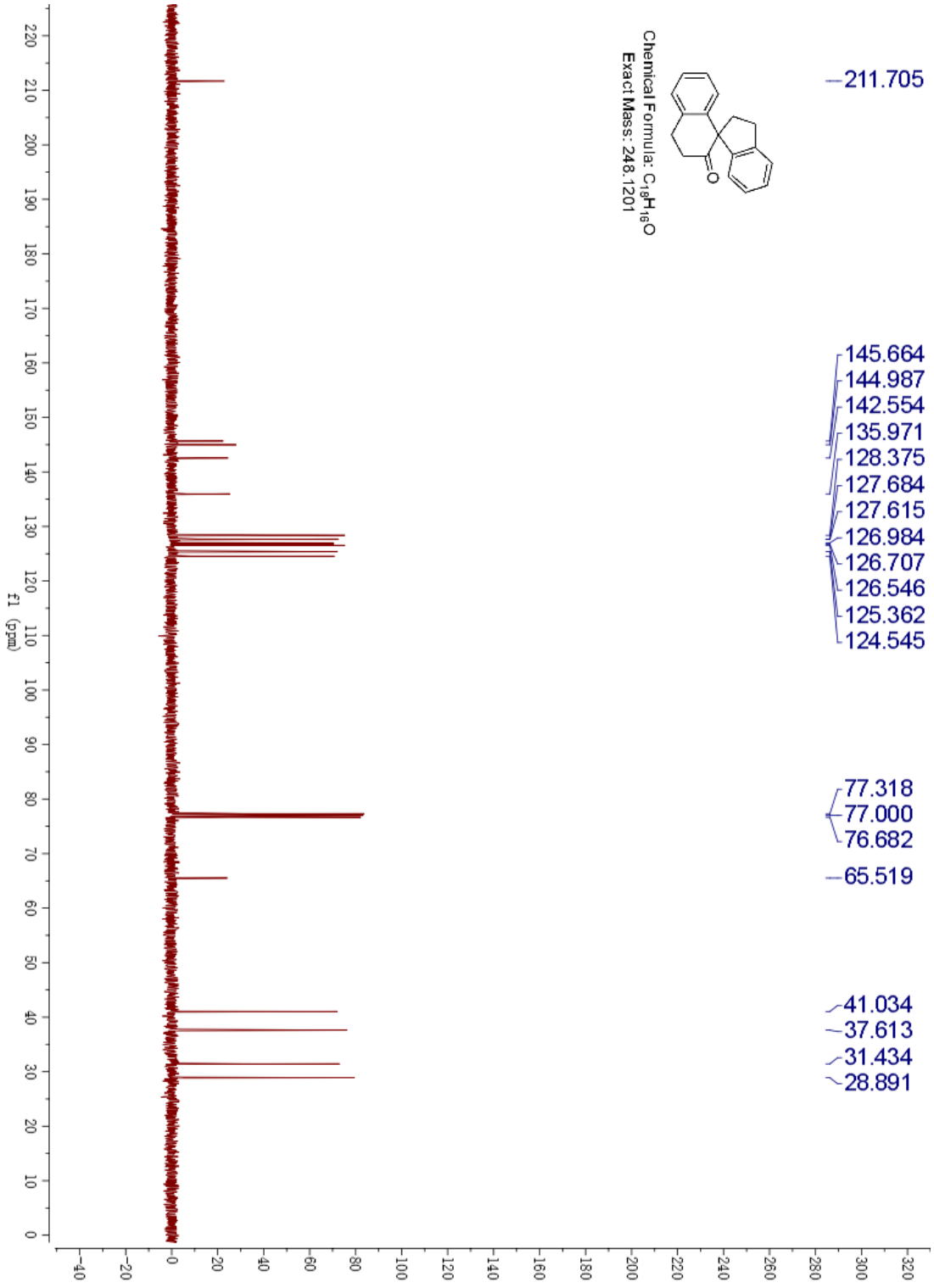
2.920
2.482
2.480
2.470
1.964
1.942
1.910
1.551
0.000


minor
Chemical Formula: C18H16O
Exact Mass: 248.1201
OH
145.265
143.903
141.126
131.780
130.251
128.365
127.631
127.449
127.233
127.193
127.037
126.756
126.268
124.921
77.318
77.000
76.683
69.050
57.743
37.845
30.222
f1 (ppm)


Chemical Formula: C18H16O
Exact Mass: 248.1201
O
0.98
1.83
2.97
0.96
1.00
3.25
1.12
2.06
1.12
1.11
f1 (ppm)
7.325
7.307
7.260
7.241
7.232
7.218
7.206
7.204
7.189
7.186
7.176
7.171
7.167
7.158
7.141
7.126
6.880
6.861
6.808
6.789
3.265
3.245
3.224
3.216
3.196
3.188
3.175
3.160
3.134
3.037
2.836
2.823
2.815
2.802
2.775
2.765
2.754
2.744
2.733
2.722
2.712
2.310
2.288
2.278
2.269
2.258
-0.000


Chemical Formula: C18H16O
Exact Mass: 248.1201
211.705
145.664
144.987
142.554
135.971
128.375
127.684
127.615
126.984
126.707
126.546
125.362
124.545
77.318
77.000
76.682
65.519
41.034
37.613
31.434
28.891
f1 (ppm)