Supplementary Information

Pd(II)-Catalyzed Decarboxylative Acylation of Phenylacetamides with α-Oxocarboxylic Acids via C–H Bond Activation

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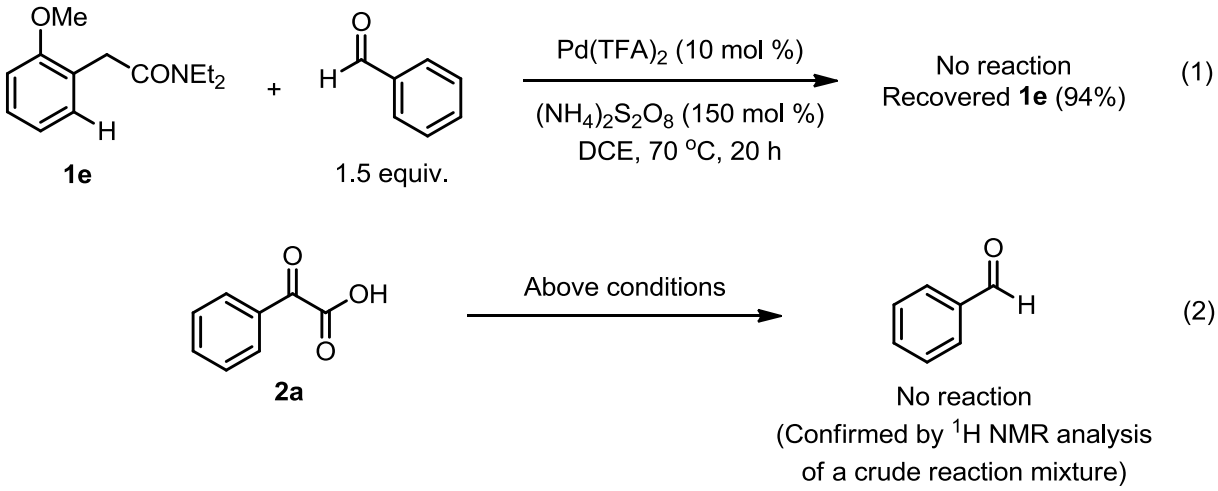
General methods

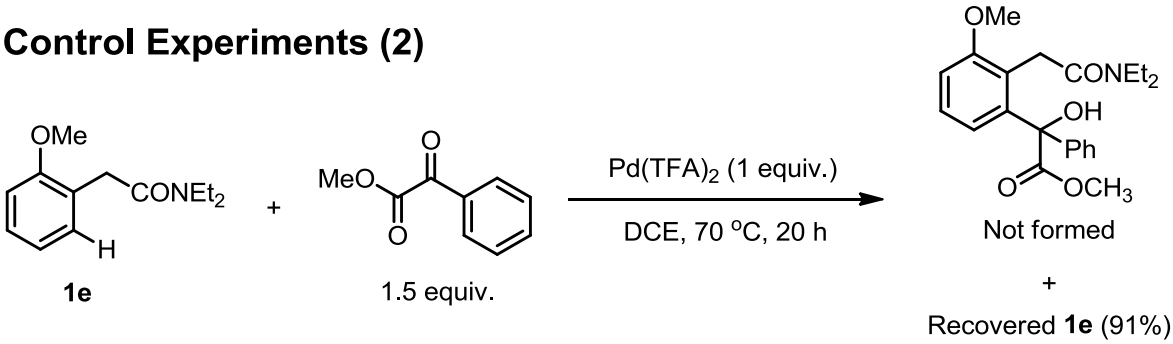
Commercially available reagents were used without additional purification, unless otherwise stated. Sealed tubes (13 x100 mm^2) were purchased from Fischer Scientific and dried in oven for overnight and cooled at room temperature prior to use. Thin layer chromatography was carried out using plates coated with Kieselgel $60F_{254}$ (Merck). For flash column chromatography, E. Merck Kieselgel 60 (230-400 mesh) was used. Nuclear magnetic resonance spectra (^1H and ^{13}C NMR) were recorded on a Bruker Unity 400, 500 and 700 MHz spectrometer for $CDCl_3$ and CD_3OD solutions and chemical shifts are reported as parts per million (ppm). Resonance patterns are reported with the notations s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). In addition, the notation br is used to indicate a broad signal. Coupling constants (*J*) are reported in hertz (Hz). IR spectra were recorded on a Varian 2000 Infrared spectrophotometer and are reported as cm^{-1}. High-resolution mass spectra (HRMS) were recorded on a JEOL JMS-600 spectrometer.

Control Experiments (1)



As the control experiment for a decarboxylation of α-oxocarboxylic acids followed by a C-H functionalization of the resulting aldehyde, we examined the coupling of 2-methoxyphenylacetamide **1e** and benzaldehyde instead of phenylglyoxylic acid (**2a**) under standard reaction conditions ($Pd(TFA)_2$ (10 mol %), $(NH_4)_2S_2O_8$ (1.5 equiv.), DCE (0.3 M)). However, this reaction did not provide any acylated product and most of starting material **1e** was recovered. Also, phenylglyoxylic acid (**2a**) was added to standard reaction conditions in the absence of 2-methoxyphenylacetamide **1e**. As a result, phenylglyoxylic acid (**2a**) was not converted to benzaldehyde. Thus it is not possible mechanism that a decarboxylation of α-oxocarboxylic acids under palladium catalysis can provide the corresponding aldehyde, which can be inserted to palladacycle intermediate.

Control Experiments (2)



As the control experiment for a Heck type addition to a C=O bond of α-oxocarboxylic acids followed by decarboxylation rather than β-hydride elimination, we examined the coupling of 2-

methoxyphenylacetamide **1e** and methyl benzoylformate, which cannot participate in a decarboxylation process, in the presence of 1 equiv. of $Pd(TFA)_2$, to obtain Heck type addition compound to a C=O bond. However, we did not obtain any Heck type addition compound and most of starting compounds were recovered.

General procedure for the synthesis of *N*,*N*-diethylphenylacetamides 1a–j

To a stirred solution of phenylacetic acids (7.30 mmol, 100 mol %) in anhydrous CH_2Cl_2 (37 mL) was added $SOCl_2$ (11.0 mmol, 150 mol %) at 0 ^oC under N_2. The reaction mixture was stirred for 2 h at 80 ^oC. After cooling to room temperature, diethylamine (21.9 mmol, 300 mol %) was added to the reaction mixture, which was stirred for 2 h at room temperature. The reaction mixture was quenched with H_2O (50 mL) and the aqueous layer was extracted with CH_2Cl_2 (50 mL). The organic layer was washed with H_2O and brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (*n*-hexanes/EtOAc) to afford the corresponding *N*,*N*-diethylphenylacetamides.

General procedure for the synthesis of α-oxocarboxylic acids

α-Oxocarboxylic acids were prepared from corresponding aryl methyl ketones with SeO_2 and pyridine, according to the reported procedure.[1]

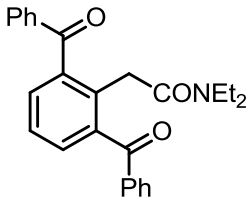
(1) Wadhwa, K.; Yang, C.-X.; West, P. R.; Deming, K. C.; Chemburkar, S. R.; Reddy, R. E. *Synth. Commun.* **2008**, *38*, 4434.

Typical procedure for the synthesis of acylation products (3a–j and 4b–j)

To an oven-dried sealed tube charged with *N*,*N*-diethyl-2-(2-methoxyphenyl)acetamide (**1e**) (66.4 mg, 0.30 mmol, 100 mol %), $Pd(TFA)_2$ (10 mg, 0.03 mmol, 10 mol %), and $(NH_4)_2S_2O_8$ (102.7 mg, 0.45 mmol, 150 mol %) in DCE (1 mL) was added phenylglyoxylic acid (**2a**) (67.6 mg, 0.45 mmol, 150 mol %). The reaction mixture was allowed to stir for 20 h at 70 ^oC. The reaction mixture was diluted with EtOAc (5 mL) and washed with sodium carbonate solution. The aqueous layer was extracted with EtOAc (10 mL × 3). The combined organic layer was dried over Mg_2SO_4 and concentrated in vacuo. The residue was purified by flash column chromatography (*n*-hexanes/EtOAc = 2:1) to afford the acylated product **3e** (69.2 mg) in 71% yield.

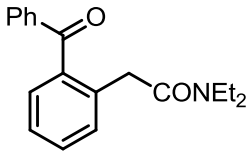
Characterization data for acylation products (3a–j and 4b–j)

2-(2,6-Dibenzoylphenyl)-*N*,*N*-diethylacetamide (3a)



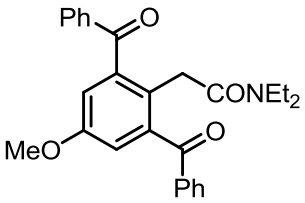
R_f = 0.62 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 4H), 7.55-7.51 (m, 2H), 7.44-7.40 (m, 6H), 7.31 (t, *J* = 8.3 Hz, 1H), 4.03 (s, 2H), 3.12 (q, *J* = 7.2 Hz, 2H), 3.07 (q, *J* = 7.1 Hz, 2H), 0.96 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 162.6, 140.7, 137.5, 134.4, 133.1, 130.5, 129.9, 128.3, 125.1, 42.1, 40.6, 33.3, 13.8, 12.7; IR (KBr) υ 2976, 2933, 1717, 1665, 1598, 1448, 1381, 1261, 1140, 1037, 921, 853 cm^{-1}; HRMS (EI) Calcd for $C_{26}H_{25}NO_3$ $[M]^+$ 399.1834, found 399.1833.

2-(2-Benzoylphenyl)-*N*,*N*-diethylacetamide (3aa)



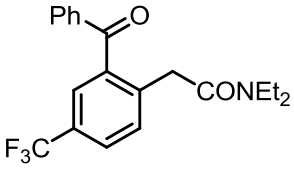
R_f = 0.41 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, CD_3OD) δ 7.86 (d, *J* = 7.1 Hz, 2H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.60-7.55 (m, 3H), 7.47-7.44 (m, 3H), 4.02 (s, 2H), 3.46 (q, *J* = 7.2 Hz, 2H), 3.34 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.04 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 200.0, 172.1, 139.8, 139.1, 136.8, 134.2, 132.9, 131.9, 131.4, 130.8, 129.5, 127.4, 43.7, 41.9, 38.7, 14.2, 13.1; IR (KBr) υ 2973, 2930, 1713, 1642, 1453, 1314, 1271, 1136, 1074, 946 cm^{-1}; HRMS (EI) Calcd for $C_{19}H_{21}NO_2$ $[M]^+$ 295.1572, found 295.1566.

2-(2,6-Dibenzoyl-4-methoxyphenyl)-*N*,*N*-diethylacetamide (3b)



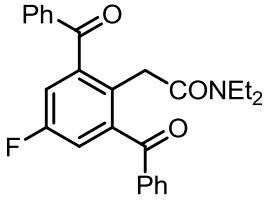
R_f = 0.55 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.4 Hz, 4H), 7.53 (t, *J* = 7.2 Hz, 2H), 7.44-7.41 (m, 4H), 6.95 (s, 2H), 3.89 (s, 2H), 3.72 (s, 3H), 3.06 (q, *J* = 6.7 Hz, 4H), 0.83 (br s, 6H); ^{13}C NMR (125 MHz, CD_3OD) δ 199.3, 171.1, 158.5, 143.3, 138.6, 134.6, 131.5, 129.6, 126.4, 117.3, 56.1, 43.4, 41.9, 33.9, 14.0, 13.1; IR (KBr) υ 2974, 2934, 1717, 1666, 1598, 1450, 1333, 1249, 1132, 1018, 925, 862 cm^{-1}; HRMS (EI) Calcd for $C_{27}H_{27}NO_4$ $[M]^+$ 429.1940, found 429.1943.

2-(2-Benzoyl-4-(trifluoromethyl)phenyl)-*N*,*N*-diethylacetamide (3c)



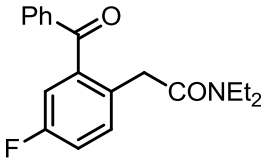
R_f = 0.48(*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.57-7.56 (m, 2H), 7.49-7.43 (m, 3H), 3.92 (s, 2H), 3.28-3.23 (m, 4H), 1.12 (br s, 3H), 0.94 (br s, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 198.2, 171.1, 141.4, 140.7, 138.3, 134.6, 134.1, 131.3, 130.7, 129.6, 129.4, 128.2 (q, $J_{C\text{-}F}$ = 3.6 Hz), 126.9 (q, $J_{C\text{-}F}$ = 3.6 Hz), 125.2 (q, $J_{C\text{-}F}$ = 270.2 Hz), 43.6, 41.9, 38.5, 14.2, 13.1; IR (KBr) υ 2978, 2935, 1716, 1644, 1451, 1334, 1257, 1173, 1080, 1021, 959, 865 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{20}F_3NO_2$ $[M]^+$ 363.1446, found 363.1431.

2-(2,6-Dibenzoyl-4-fluorophenyl)-*N*,*N*-diethylacetamide (3d)



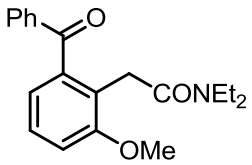
R_f = 0.73 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.4 Hz, 4H), 7.58 (t, *J* = 7.2 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 4H), 7.16 (d, *J* = 8.2 Hz, 2H), 3.98 (s, 2H), 3.09 (br s, 4H), 0.96 (br s, 3H), 0.76 (br s, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 197.9, 170.5, 161.2 (d, J_{C-F} = 247.5 Hz), 144.1 (d, J_{C-F} = 5.8 Hz), 138.1, 134.9, 131.5, 129.7, 129.4, 118.5 (d, J_{C-F} = 22.6 Hz), 43.5, 41.9, 34.1, 14.0, 13.1; IR (KBr) υ 2781, 1718, 1669, 1597, 1450, 1328, 1252, 1177, 1098, 927 cm^{-1}; HRMS (EI) Calcd for $C_{26}H_{24}FNO_3$ $[M]^+$ 417.1740, found 417.1737.

2-(2-Benzoyl-4-fluorophenyl)-*N*,*N*-diethylacetamide (3dd)



R_f = 0.45 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.4 Hz, 4H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.35-7.32 (m, 1H), 7.16-7.14 (m, 1H), 7.05 (dd, *J* = 8.7, 2.6 Hz, 1H), 3.82 (s, 2H), 3.27 (q, *J* = 6.9 Hz, 4H), 1.10 (br s, 3H), 0.97 (br s, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 198.5, 171.9, 162.2 (d, J_{C-F} = 245.6 Hz), 141.7, 138.5, 135.1 (d, J_{C-F} = 7.6 Hz), 134.6, 132.8, 131.5, 129.7, 118.4 (d, J_{C-F} = 20.7 Hz), 117.4 (d, J_{C-F} = 23.5 Hz), 43.7, 42.0, 37.9, 14.3, 13.2; IR (KBr) υ 2975, 2932, 1743, 1644, 1588, 1484, 1381, 1286, 1177, 1084, 1026, 979, 866 cm^{-1}; HRMS (EI) Calcd for $C_{19}H_{20}FNO_2$ $[M]^+$ 313.1478, found 313.1490.

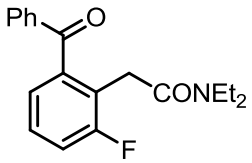
2-(2-Benzoyl-6-methoxyphenyl)-*N*,*N*-diethylacetamide (3e)



R_f = 0.34 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.21 (t, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 3.85 (s, 2H), 3.80 (s, 3H), 3.30-3.22 (m, 4H), 1.12 (br s, 3H), 0.91 (br s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 169.6, 158.0, 140.5, 137.9, 132.8, 130.5, 128.1, 126.8, 124.5, 121.3, 112.6, 55.8, 42.2, 40.5, 30.1, 14.1, 13.0; IR (KBr) υ 2973, 2933, 2838,

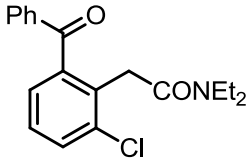
1661, 1580, 1461, 1321, 1278, 1138, 1080, 1040, 984, 854 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{23}NO_3$ $[M]^+$ 325.1678, found 325.1676.

2-(2-Benzoyl-6-fluorophenyl)-*N*,*N*-diethylacetamide (3f)



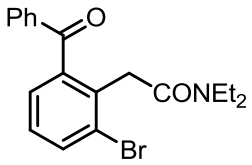
R_f = 0.59 (*n*-hexanes/EtOAc = 1:1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.0 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.25-7.17 (m, 2H), 7.13 (d, *J* = 7.4 Hz, 1H), 3.93 (s, 2H), 3.33-3.25 (m, 4H), 1.17 (br s, 3H), 0.94 (br s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 168.2, 161.5 (d, J_{C-F} = 244.8 Hz), 140.8 (d, J_{C-F} = 3.3 Hz), 137.5, 132.9, 130.4, 128.2, 127.2 (d, J_{C-F} = 8.7 Hz), 125.1 (d, J_{C-F} = 3.1 Hz), 123.3 (d, J_{C-F} = 16.1 Hz), 117.4 (d, J_{C-F} = 23.4 Hz), 42.1, 40.6, 29.3, 14.1, 12.9; IR (KBr) υ 2975, 2933, 1662, 1579, 1459, 1318, 1276, 1129, 1074, 922, 848 cm^{-1}; HRMS (EI) Calcd for $C_{19}H_{20}FNO_2$ $[M]^+$ 313.1478, found 313.1478.

2-(2-Benzoyl-6-chlorophenyl)-*N*,*N*-diethylacetamide (3g)



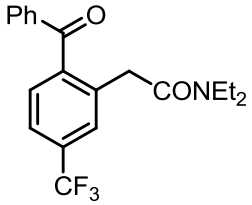
R_f = 0.68 (*n*-hexanes/EtOAc = 1:1); ^1H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.4 Hz, 2H), 7.56-7.50 (m, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.23-7.20 (m, 2H), 4.06 (s, 2H), 3.32-3.27 (m, 4H), 1.18 (br s, 3H), 0.94 (br s, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 197.4, 169.1, 141.1, 137.2, 136.3, 133.2, 133.1, 131.1, 130.1, 128.1, 127.4, 127.2, 42.2, 40.5, 33.9, 12.8, 11.7; IR (KBr) υ 2975, 2933, 1664, 1596, 1446, 1380, 1271, 1176, 1097, 1027, 971, 852 cm^{-1}; HRMS (EI) Calcd for $C_{19}H_{20}ClNO_2$ $[M]^+$ 329.1183, found 329.1181.

2-(2-Benzoyl-6-bromophenyl)-*N*,*N*-diethylacetamide (3h)



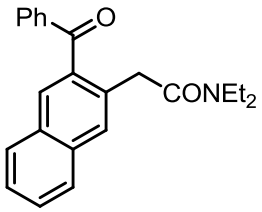
R_f = 0.67 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (700 MHz, CD_3OD) δ 7.82-7.80 (m, 3H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.33-7.29 (m, 2H), 4.12 (s, 2H), 3.42 (q, *J* = 7.1 Hz, 2H), 3.26 (q, *J* = 7.1 Hz, 2H), 1.21 (t, *J* = 7.1 Hz, 3H), 0.97 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 197.4, 168.8, 141.2, 137.1, 134.8, 134.6, 133.2, 130.2, 128.1, 127.9, 127.4, 127.3, 42.2, 40.5, 36.7, 12.8, 11.8; IR (KBr) υ 2974, 2932, 1662, 1596, 1558, 1433, 1380, 1318, 1269, 1222, 1138, 1109, 1074, 922, 850 cm^{-1}; HRMS (EI) Calcd for $C_{19}H_{20}BrNO_2$ $[M]^+$ 373.0677, found 373.0679.

2-(2-Benzoyl-5-(trifluoromethyl)phenyl)-*N*,*N*-diethylacetamide (3i)



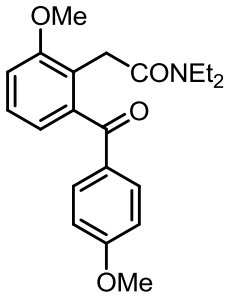
R_f = 0.72 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 2H), 7.59-7.54 (m, 3H), 7.43 (t, *J* = 7.8 Hz, 3H), 3.91 (s, 2H), 3.25 (br s, 4H), 1.11 (br s, 3H), 0.94 (br s, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 198.7, 171.3, 143.6, 138.2 (d, $J_{C\text{-}F}$ = 27.5 Hz), 134.6, 133.2 (d, $J_{C\text{-}F}$ = 31.4 Hz), 131.6, 130.9, 129.9 (d, $J_{C\text{-}F}$ = 3.9 Hz), 129.7, 125.2 (q, $J_{C\text{-}F}$ = 270.0 Hz), 124.43 (d, $J_{C\text{-}F}$ = 3.7 Hz), 43.8, 42.1, 38.4, 14.3, 13.2; IR (KBr) υ 2977, 2935, 1667, 1645, 1598, 1449, 1364, 1287, 1221, 1129, 1077, 1026, 942, 842 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{20}F_3NO_2$ $[M]^+$ 363.1446, found 363.1433.

2-(3-Benzoylnaphthalen-2-yl)-*N*,*N*-diethylacetamide (3j)



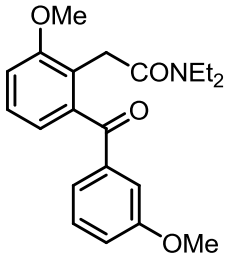
R_f = 0.51 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.75 (m, 7H), 7.56-7.50 (m, 2H), 7.47-7.42 (m, 4H), 4.08 (s, 2H), 3.34 (q, *J* = 7.2 Hz, 2H), 3.27 (q, *J* = 7.1 Hz, 2H), 1.18 (t, *J* = 7.1 Hz, 3H), 0.95 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 169.8, 138.2, 136.5, 134.2, 132.7, 132.4, 131.0, 130.6, 130.5, 130.1, 128.3, 128.2, 127.7, 127.4, 126.3, 42.3, 40.4, 38.0, 14.2, 12.9; IR (KBr) υ 2975, 2931, 1657, 1590, 1449, 1431, 1380, 1316, 1285, 1212, 1139, 1095, 919, 878 cm^{-1}; HRMS (EI) Calcd for $C_{23}H_{23}NO_2$ $[M]^+$ 345.1729, found 345.1730.

_N,N_-Diethyl-2-(2-methoxy-6-(4-methoxybenzoyl)phenyl)acetamide (4b)



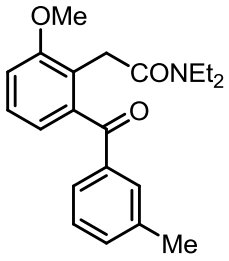
R_f = 0.28 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.8 Hz, 2H), 7.19 (t, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 1H), 6.82 (d, *J* = 8.7 Hz, 3H), 3.78 (s, 8H), 3.24 (br s, 4H), 1.01-0.97 (m, 6H); ^{13}C NMR (175 MHz, CD_3OD) δ 199.1, 172.1, 165.7, 159.8, 142.4, 134.2, 133.5, 131.7, 129.2, 128.6, 124.7, 121.8, 116.1, 115.2, 114.8, 113.6, 109.3, 56.4, 56.2, 43.8, 42.0, 31.7, 14.3, 13.4; IR (KBr) υ 2973, 2933, 2839, 1653, 1509, 1461, 1380, 1281, 1223, 1159, 1139, 1079, 984, 922, 847 cm^{-1}; HRMS (EI) Calcd for $C_{21}H_{25}NO_4$ $[M]^+$ 355.1784, found 355.1788.

_N,N_-Diethyl-2-(2-methoxy-6-(3-methoxybenzoyl)phenyl)acetamide (4c)



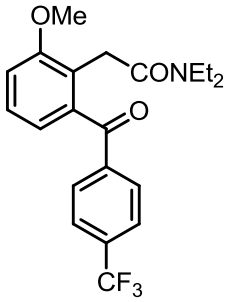
R_f = 0.27 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.39 (m, 2H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 8.2 Hz, 1H), 7.00 (d, *J* = 8.2 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 3.89 (s, 2H), 3.85 (s, 3H), 3.81 (s, 3H), 3.32 (br s, 4H), 1.06 (br s, 6H); ^{13}C NMR (175 MHz, CD_3OD) δ 199.9, 172.1, 161.2, 159.7, 141.7, 140.6, 130.6, 128.5, 125.2, 124.3, 122.4, 120.7, 115.8, 114.1, 56.5, 56.0, 43.7, 42.0, 31.6, 14.3, 14.4; IR (KBr) υ 2972, 2936, 2837, 1716, 1660, 1583, 1463, 1433, 1321, 1280, 1220, 1141, 1077, 993, 877 cm^{-1}; HRMS (EI) Calcd for $C_{21}H_{25}NO_4$ $[M]^+$ 355.1784, found 355.1776.

_N,N_-Diethyl-2-(2-methoxy-6-(4-(trifluoromethyl)benzoyl)phenyl)acetamide (4d)



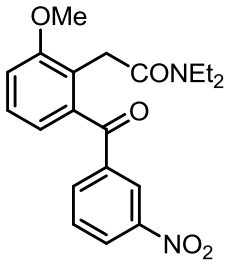
R_f = 0.35 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, CD_3OD) δ 7.59 (t, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.35-7.32 (m, 2H), 7.15 (d, *J* = 8.2 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 3.87 (s, 3H), 3.83 (s, 2H), 3.38 (q, *J* = 7.2 Hz, 2H), 3.24 (q, *J* = 7.1 Hz, 2H), 2.36 (s, 3H), 1.14 (t, *J* = 7.2 Hz, 3H), 0.97 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 200.2, 172.0, 159.6, 141.8, 139.5, 139.2, 135.1, 132.0, 129.3, 128.7, 128.4, 125.0, 122.2, 113.9, 56.4, 43.6, 41.9, 31.5, 21.3, 14.2, 13.3; IR (KBr) υ 2973, 2934, 2837, 1714, 1647, 1602, 1584, 1462, 1321, 1282, 1259, 1138, 1081, 985, 821 cm^{-1}; HRMS (EI) Calcd for $C_{21}H_{25}NO_3$ $[M]^+$ 339.1834, found 339.1833.

_N,N_-Diethyl-2-(2-methoxy-6-(4-(trifluoromethyl)benzoyl)phenyl)acetamide (4e)



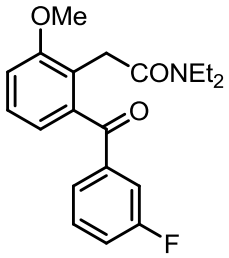
R_f = 0.48 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (400 MHz, CD_3OD) δ 7.98 (d, *J* = 8.1 Hz, 2H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.22 (d, *J* = 8.3 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 3.96 (s, 2H), 3.90 (s, 3H), 3.46 (q, *J* = 7.1 Hz, 2H), 3.26 (q, *J* = 7.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H), 0.98 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD) δ 198.6, 172.0, 159.6, 142.4, 140.7, 135.0 (q, J_{C-F} = 32.2 Hz), 131.9, 128.5, 126.3 (q, J_{C-F} = 3.8 Hz), 125.5, 125.2 (q, J_{C-F} = 270.0 Hz), 122.5, 114.5, 56.4, 43.6, 30.9, 14.2, 13.2; IR (KBr) υ 2975, 2936, 2839, 1719, 1643, 1582, 1463, 1380, 1325, 1278, 1169, 1132, 1065, 986, 947, 862 cm^{-1}; HRMS (EI) Calcd for $C_{21}H_{22}F_3NO_3$ $[M]^+$ 393.1552, found 393.1554.

_N,N_-Diethyl-2-(2-methoxy-6-(3-nitrobenzoyl)phenyl)acetamide (4f)



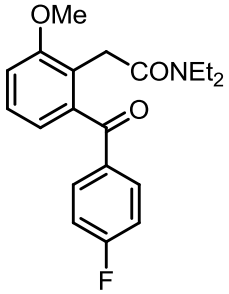
R_f = 0.29 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.37 (d, *J* = 8.2 Hz, 1H), 8.17 (d, *J* = 7.7 Hz, 1H), 7.60 (t, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.2 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 4.01 (s, 2H), 3.87 (s, 3H), 3.33 (br s, 4H), 1.10 (br s, 6H); ^{13}C NMR (100 MHz, CD_3OD) δ 197.3, 172.1, 159.7, 149.6, 140.7, 140.3, 137.1, 130.9, 128.6, 128.2, 125.8, 125.6, 122.5, 114.7, 56.5, 43.7, 41.9, 30.7, 14.3, 13.3; IR (KBr) υ 2975, 2935, 2839, 2237, 1581, 1532, 1463, 1380, 1321, 1297, 1273, 1141, 1075, 1000, 913, 827 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{22}N_2O_5$ $[M]^+$ 370.1529, found 370.1524.

_N,N_-Diethyl-2-(2-(3-fluorobenzoyl)-6-methoxyphenyl)acetamide (4g)



R_f = 0.38 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62-7.56 (m, 2H), 7.39-7.38 (m, 1H), 7.28-7.22 (m, 2H), 7.01 (d, *J* = 8.2 Hz, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 3.93 (s, 2H), 3.86 (s, 3H), 3.33 (br s, 4H), 1.12 (br s, 6H); ^{13}C NMR (100 MHz, CD_3OD) δ 198.4 (d, J_{C-F} = 2.1 Hz), 172.0, 163.6 (d, J_{C-F} = 244.9 Hz), 159.6, 141.4 (d, J_{C-F} = 6.2 Hz), 141.0, 131.3 (d, J_{C-F} = 7.5 Hz), 128.5, 127.6, 127.5, 125.3, 122.3, 121.0 (d, J_{C-F} = 21.6 Hz), 117.6 (d, J_{C-F} = 22.5 Hz), 114.3, 56.4, 43.6, 41.9, 31.1, 14.2, 13.3; IR (KBr) υ 2973, 2934, 2838, 1718, 1644, 1586, 1440, 1380, 1323, 1272, 1136, 1051, 994, 884 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{22}FNO_3$ $[M]^+$ 343.1584, found 343.1577.

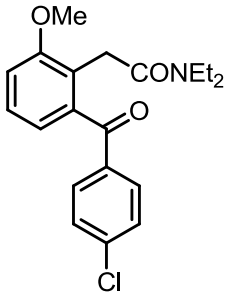
_N,N_-Diethyl-2-(2-(4-fluorobenzoyl)-6-methoxyphenyl)acetamide (4h)



R_f = 0.40 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, CD_3OD) δ 7.94-7.91 (m, 2H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.26-7.21 (m, 3H), 6.95 (d, *J* = 7.7 Hz, 1H), 3.93 (s, 3H), 3.92 (s, 2H), 3.46 (q, *J* = 7.2 Hz, 2H), 3.30 (q, *J* = 7.1 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H), 1.02 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 196.9, 170.6, 165.8 (d, J_{C-F} = 251.9 Hz), 158.2, 140.0, 134.2, 133.0 (d, J_{C-F} = 9.4 Hz), 127.1, 123.6, 120.6, 114.9 (d, J_{C-F} = 22.0 Hz), 112.6, 55.0, 42.2,

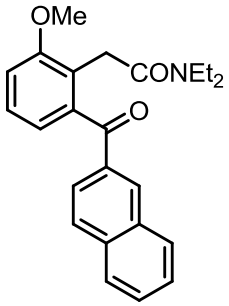
40.5, 29.8, 12.5, 11.8; IR (KBr) υ 2974, 2935, 2838, 1713, 1644, 1598, 1462, 1380, 1279, 1226, 1153, 1079, 986, 922, 856 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{22}FNO_3$ $[M]^+$ 343.1584, found 343.1584.

2-(2-(4-Chlorobenzoyl)-6-methoxyphenyl)-*N*,*N*-diethylacetamide (4i)



R_f = 0.41 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (500 MHz, CD_3OD) δ 7.87 (d, *J* = 8.6 Hz, 2H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.26 (d, *J* = 8.2 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 3.97 (s, 2H), 3.96 (s, 3H), 3.51 (q, *J* = 7.2 Hz, 2H), 3.34 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.06 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 197.2, 170.6, 158.2, 139.8, 139.1, 136.2, 131.7, 128.2, 127.1, 123.8, 120.8, 112.6, 54.9, 42.2, 40.5, 29.7, 12.8, 11.8; IR (KBr) υ 2973, 2934, 2837, 1644, 1584, 1462, 1323, 1277, 1138, 1078, 985, 921, 846 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{22}ClNO_3$ $[M]^+$ 359.1288, found 359.1284.

2-(2-(2-Naphthoyl)-6-methoxyphenyl)-*N*,*N*-diethylacetamide (4j)

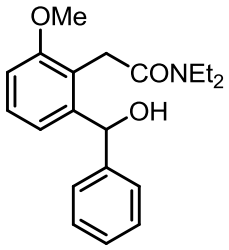


R_f = 0.35 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.04 (d, *J* = 8.6 Hz, 1H), 7.94-7.87 (m, 3H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 1H), 7.34-7.28

(m, 1H), 7.07 (d, *J* = 8.1 Hz, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 3.94 (s, 2H), 3.90 (s, 3H), 3.29 (br s, 4H), 1.16-0.93 (m, 6H); ^{13}C NMR (175 MHz, CD_3OD) δ 200.1, 172.0, 159.8, 142.1, 137.3, 136.4, 134.8, 133.8, 131.0, 130.0, 129.4, 128.9, 128.7, 128.0, 126.0, 125.1, 122.3, 114.0, 56.5, 43.6, 41.9, 31.7, 14.3, 13.3; IR (KBr) υ 2972, 2933, 1655, 1581, 1463, 1321, 1238, 1139, 1076, 989, 921 cm^{-1}; HRMS (EI) Calcd for $C_{24}H_{25}NO_3$ $[M]^+$ 375.1834, found 375.1831.

Experimental procedure and characterization data for the synthesis of 3-isochromanone 6

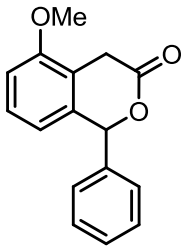
N,*N*-Diethyl-2-(2-(hydroxy(phenyl)methyl)-6-methoxyphenyl)acetamide (5)



To a stirred solution of **3e** (79 mg, 0.243 mmol, 100 mol %) in EtOH (1.2 mL) was added $NaBH_4$ (13.8 mg, 150 mol %) at room temperature. The reaction mixture was stirred for 30 min at 50 ^{o}C, and quenched with a saturated solution of NH_4Cl (1.2 mL). The aqueous layer was extracted with EtOAc (15 mL × 2). The organic layer was washed with H_2O, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (*n*-hexanes/EtOAc = 1:1) to afford 59.8 mg of **5** in 75% yield.

R_f = 0.37 (*n*-hexanes/EtOAc = 1:1); ^{1}H NMR (700 MHz, CD_3OD) δ 7.35-7.31 (m, 4H), 7.26-7.22 (m, 2H), 6.91 (t, *J* = 8.2 Hz, 2H), 5.96 (s, 1H), 3.86 (d, *J* = 16.0 Hz, 1H), 3.81 (s, 3H), 3.71 (d, *J* = 16.0 Hz, 1H), 3.51 (q, *J* = 7.1 Hz, 2H), 3.38 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (175 MHz, CD_3OD) δ 171.6, 157.8, 144.0, 143.4, 127.8, 127.4, 126.8, 126.6, 122.8, 120.1, 109.4, 72.7, 54.7, 42.4, 40.7, 29.7, 13.0, 11.9; IR (KBr) υ 3270, 2974, 2934, 1615, 1469, 1321, 1264, 1144, 1070, 1038, 949, 859 cm^{-1}; HRMS (EI) Calcd for $C_{20}H_{25}NO_3$ $[M]^+$ 327.1834, found 327.1832.

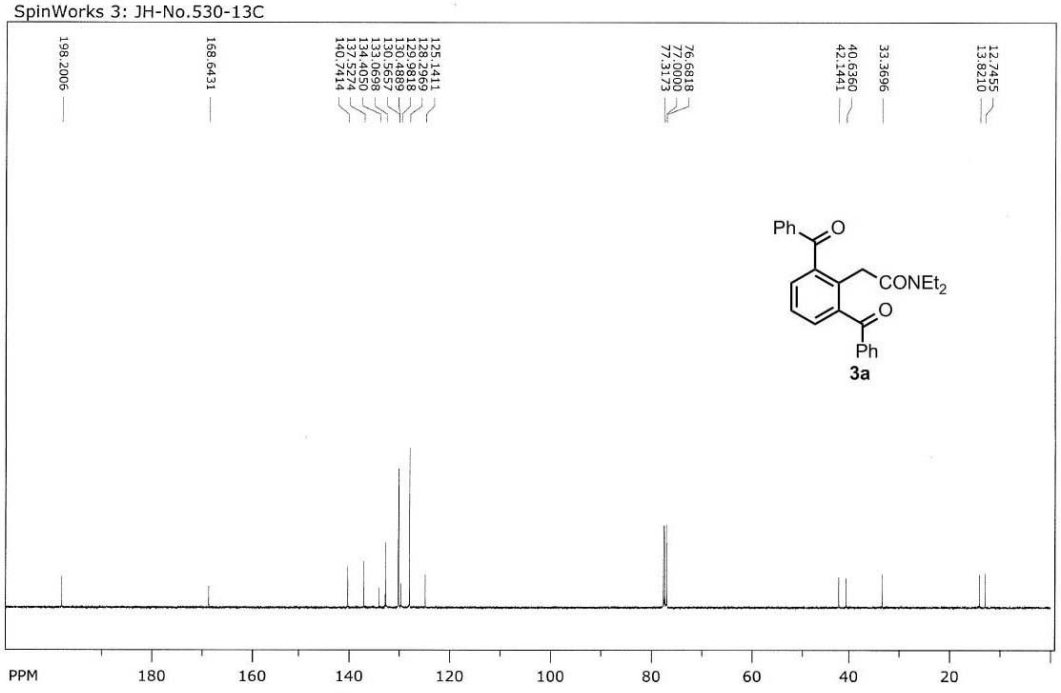
5-Methoxy-1-phenylisochroman-3-one (6)



To a stirred solution of **5** (41 mg, 0.161 mmol, 100 mol %) in THF (0.8 mL) was added 1 M HCl (0.8 mL) at room temperature. The reaction mixture was stirred for 12 h at 100 ^{o}C, and quenched with a saturated solution of Na_2CO_3 (1.2 mL). The aqueous layer was extracted with EtOAc (10 mL × 2). The organic layer was washed with H_2O, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (*n*-hexanes/EtOAc = 4:1) to afford 39.3 mg of **6** in 96% yield.

R_f = 0.36 (*n*-hexanes/EtOAc = 3:1); ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.41-7.37 (m, 3H), 7.31-7.25 (m, 3H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.63 (d, *J* = 7.6 Hz, 1H), 6.41 (s, 1H), 3.89 (s, 3H), 3.79 (d, *J* = 19.4 Hz, 1H), 3.62 (d, *J* = 19.4 Hz, 1H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 170.7, 156.0, 137.5, 135.5, 128.8, 128.7, 128.0, 127.4, 119.0, 118.1, 110.2, 82.0, 55.6, 29.6; IR (KBr) υ 2938, 2839, 1740, 1958, 1480, 1367, 1329, 1267, 1230, 1151, 1078, 1015, 974, 845 cm^{-1}; HRMS (EI) Calcd for $C_{16}H_{14}O_3$ $[M]^+$ 254.0943, found 254.0941.

SpinWorks 3: JH-No.530-13C



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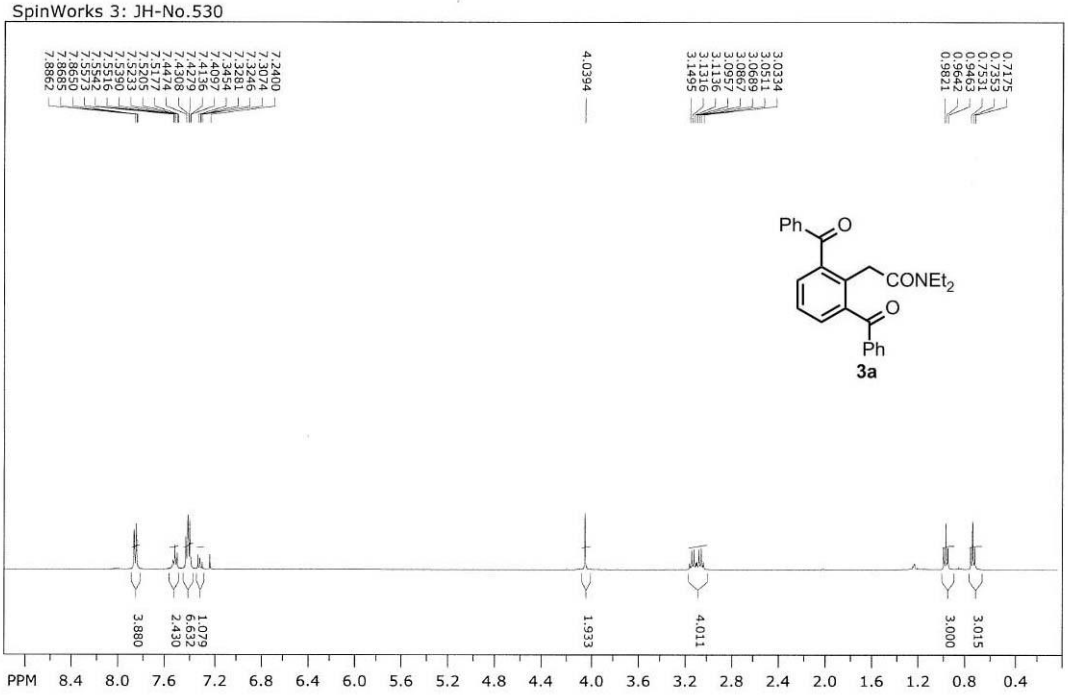
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.612776 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 845.265 ppm/cm: 8.40033

SpinWorks 3: JH-No.530



file: ...ator\바탕 화면\SKK_KIS (24)\116H\1\fid expt: <zg30>
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number of scans: 16

freq. of 0 ppm: 400.130019 MHz
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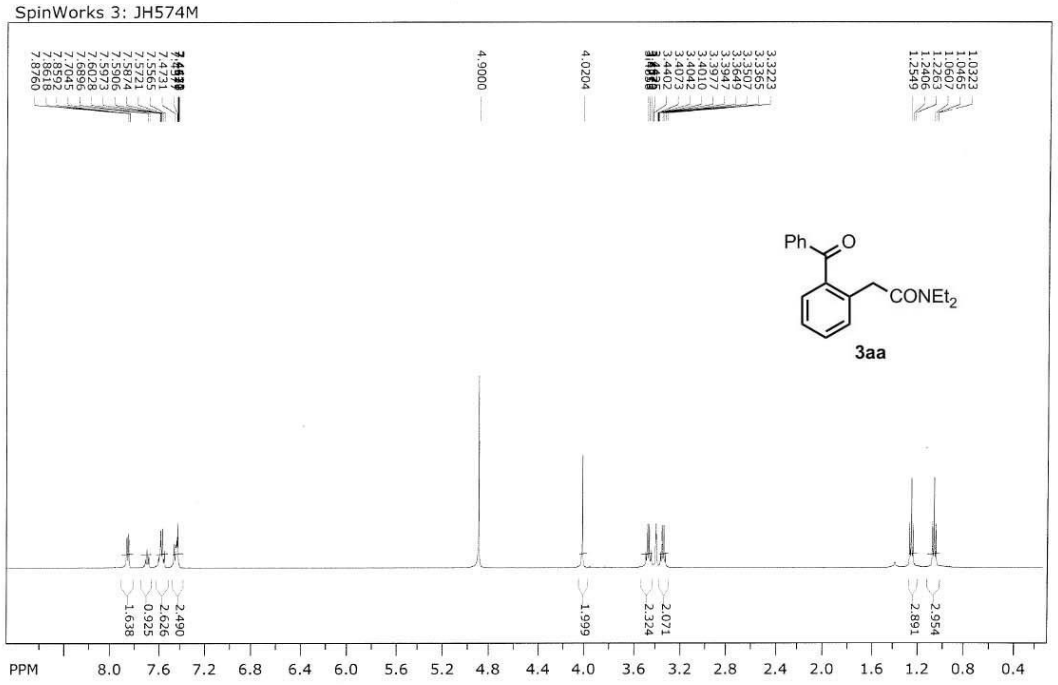
LB: 0.000 GF: 0.0000
Hz/cm: 143.926 ppm/cm: 0.35970



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time domain size: 36372 points
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number of scans: 36

freq. of 0 ppm: 499.958943 MHz
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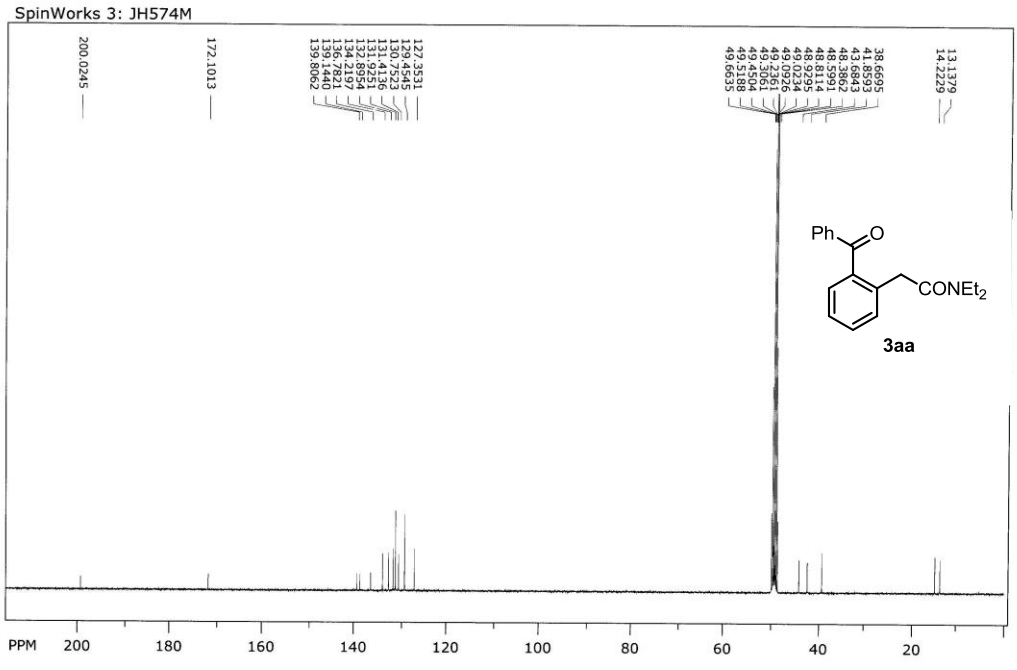
Hz/cm: 175.503 ppm/cm: 0.35103



file: ...gs\PC\바탕 화면\SKK_KIS (2)\173c\1\fid expt: <zgpg30>
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time domain size: 65536 points
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number of scans: 1024

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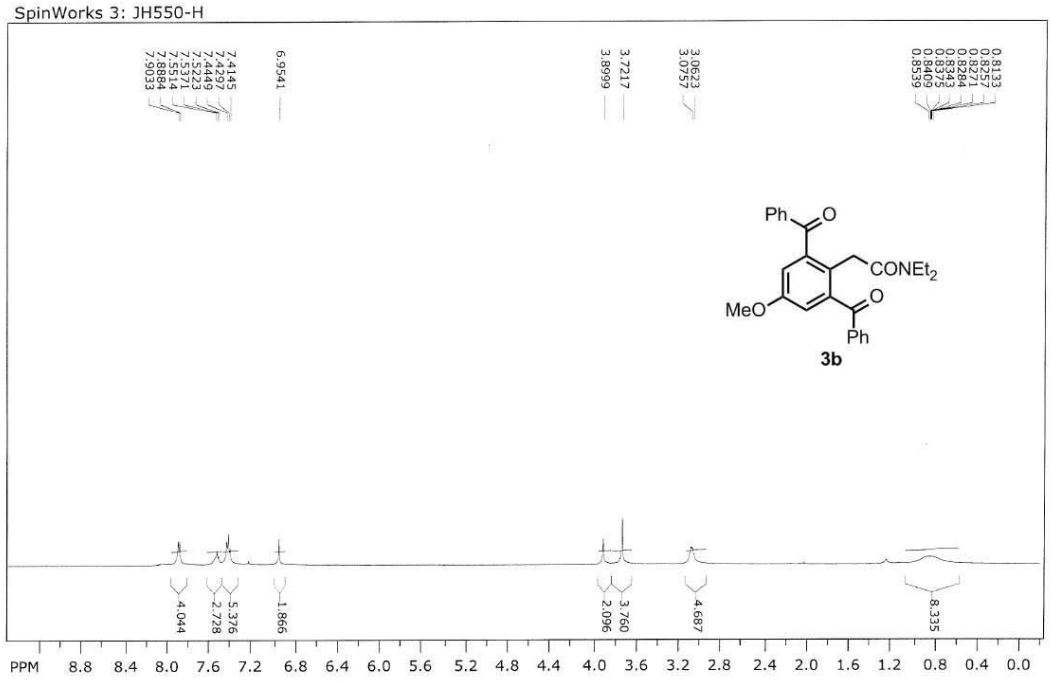

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number of scans: 32

freq. of 0 ppm: 499.957031 MHz
processed size: 65536 complex points
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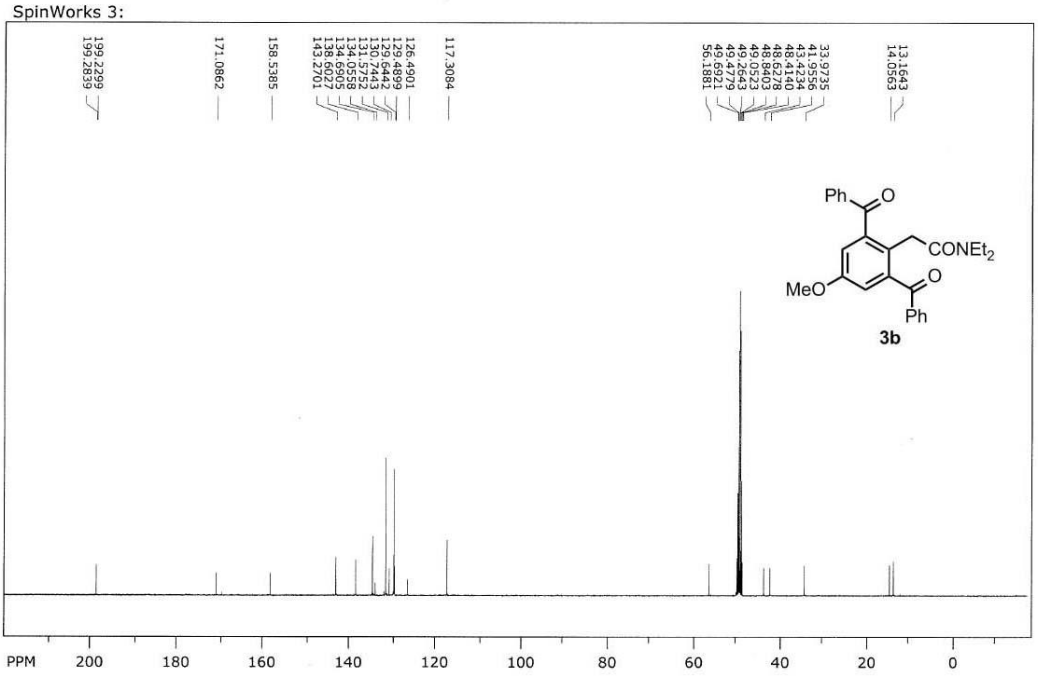
Hz/cm: 194.813 ppm/cm: 0.38966



file: ...strator\바탕 화면\SKK_KIS\149c-1\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
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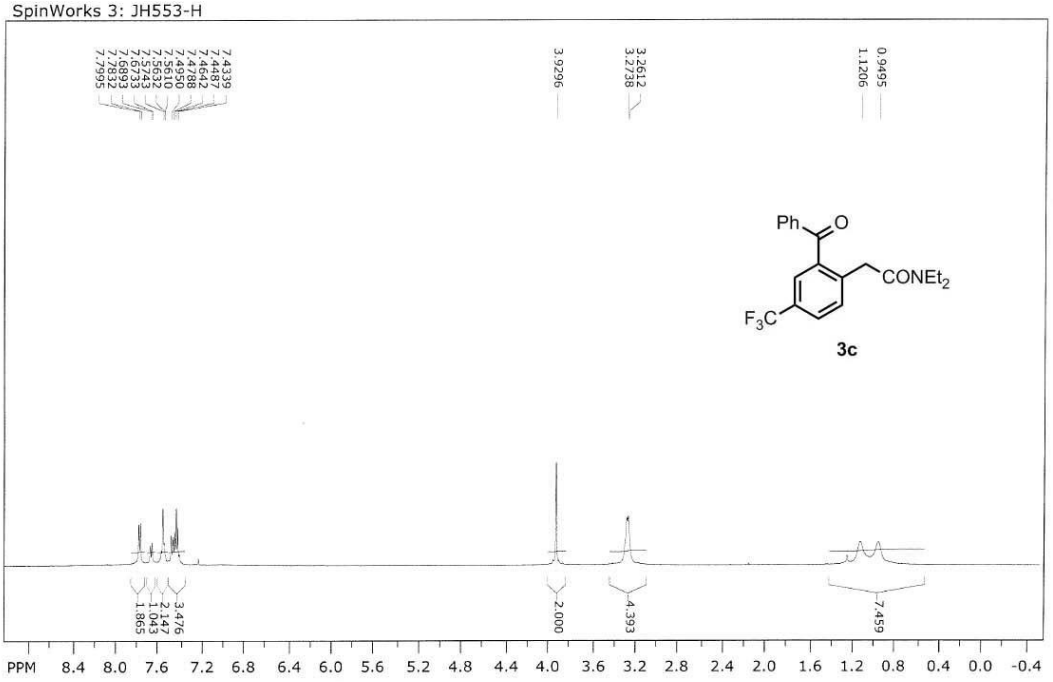
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55587

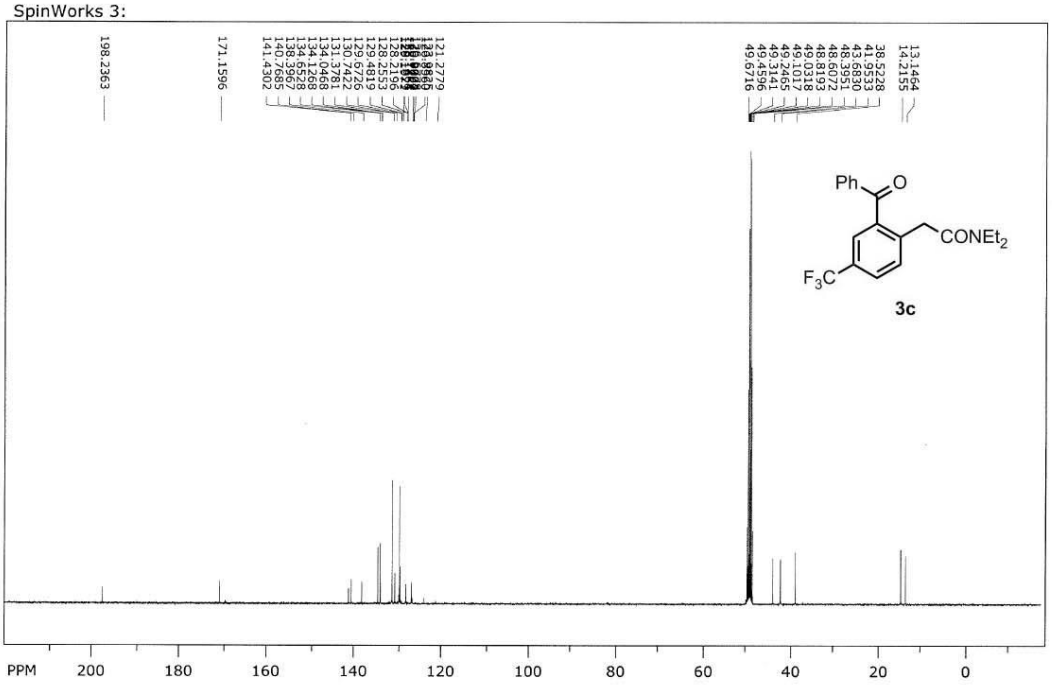
SpinWorks 3: JH553-H



file: F:\JH553-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

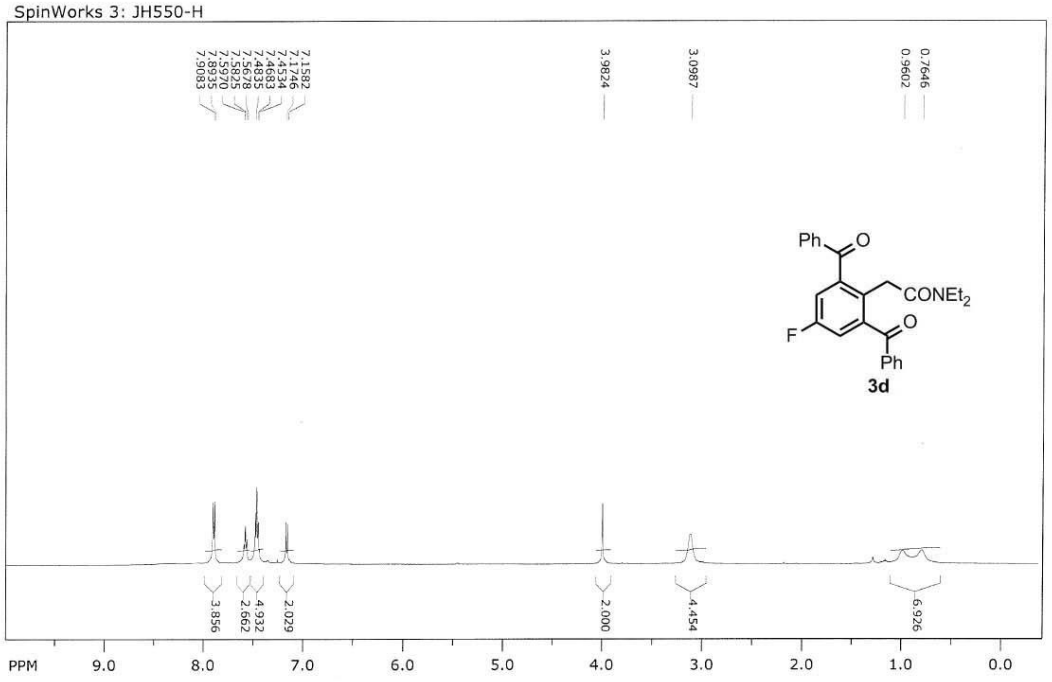
freq. of 0 ppm: 499.957029 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 192.024 ppm/cm: 0.38408

SpinWorks 3:



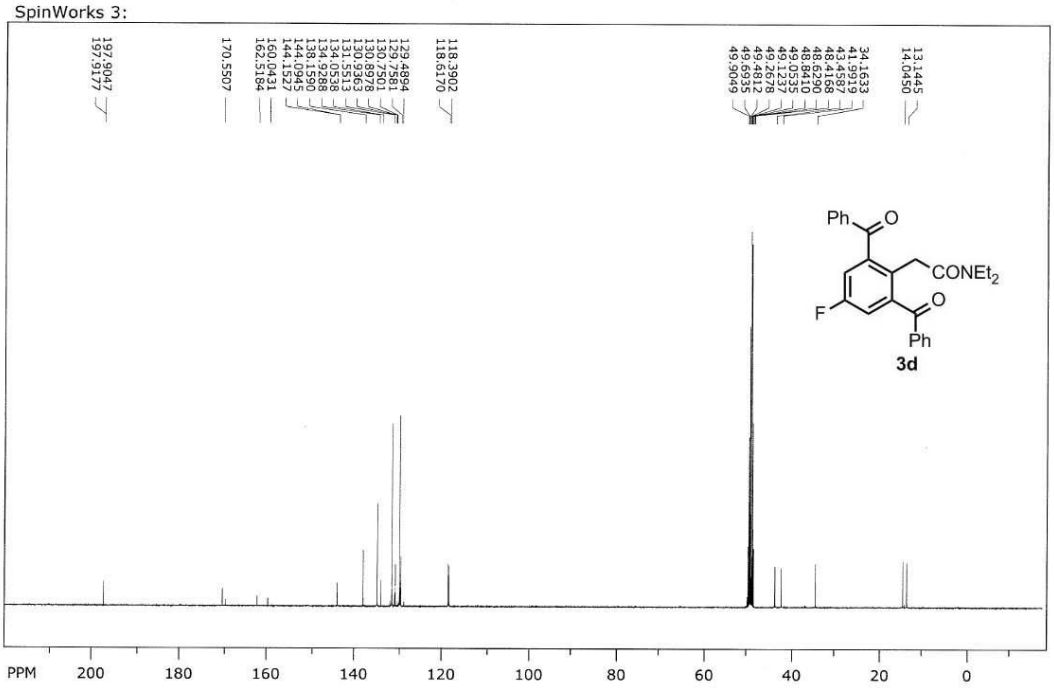
file: ...strator\바탕 화면\SKK_KIS\152c-1\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55587



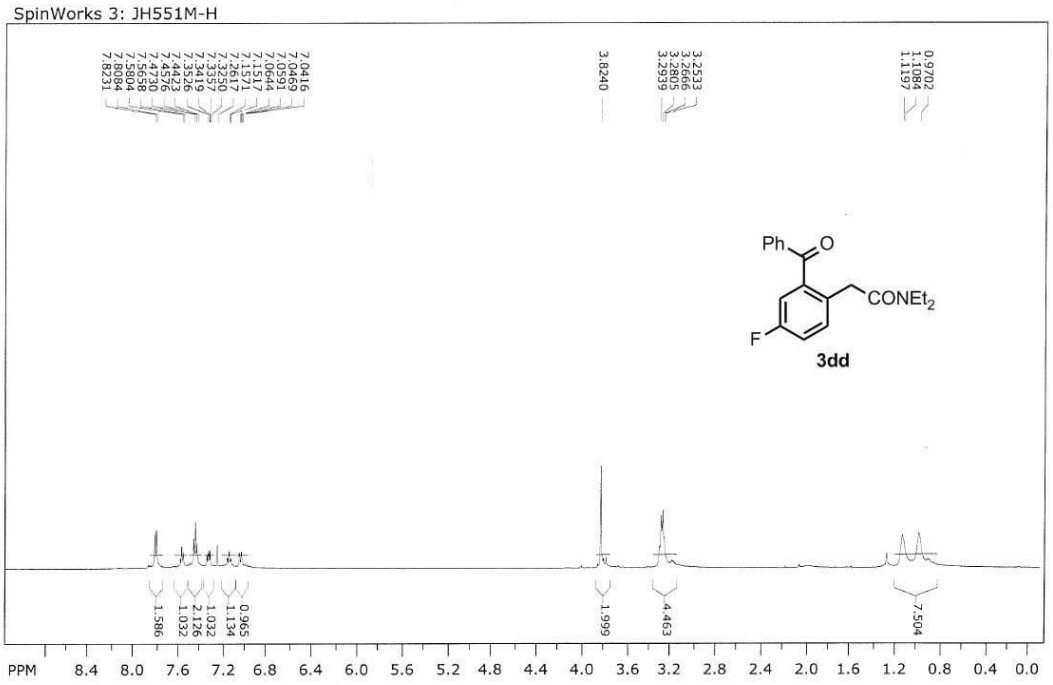
file: F:\JH551D-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

freq. of 0 ppm: 499.957020 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 208.544 ppm/cm: 0.41712



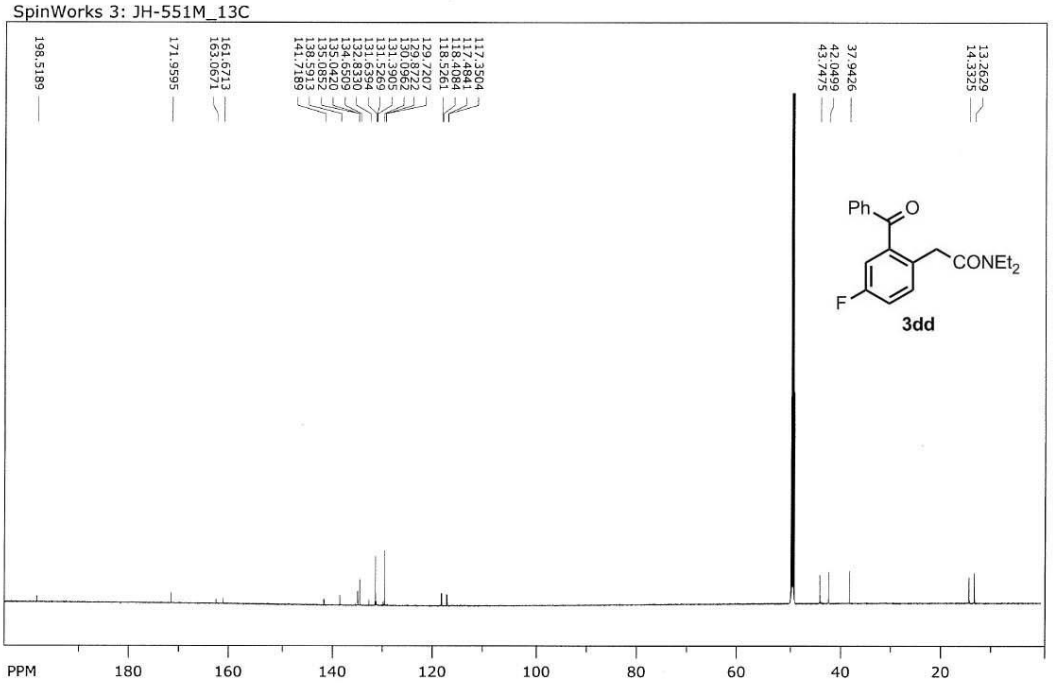
file: ...strator\바탕 화면\SKK_KIS\151c-1\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55587



file: F:\JH551M-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

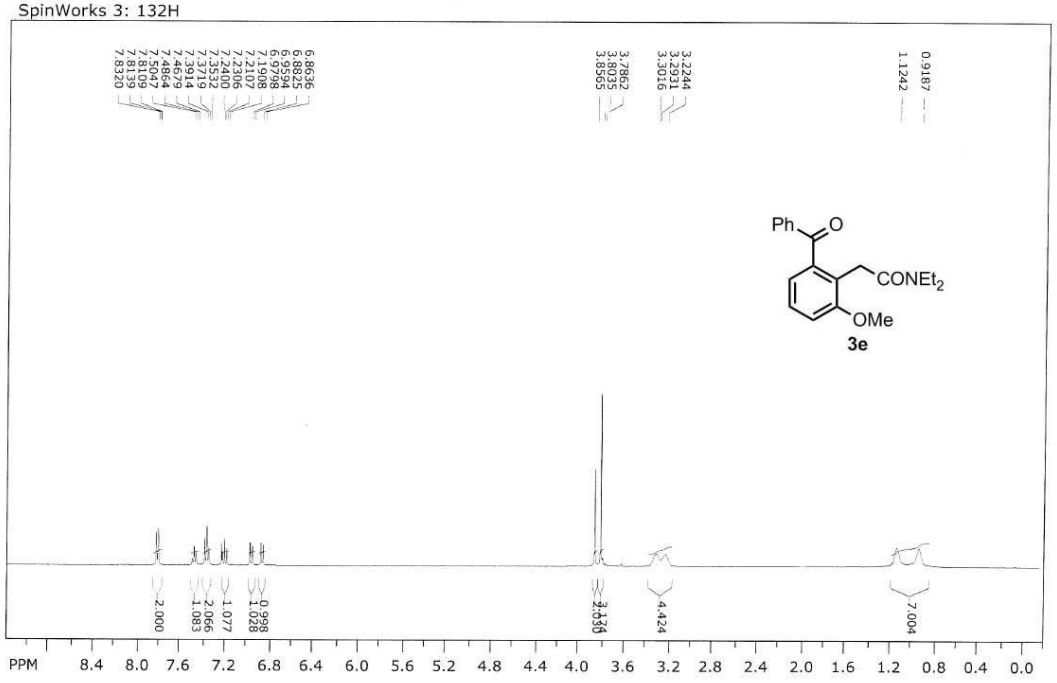
freq. of 0 ppm: 499.957020 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 186.016 ppm/cm: 0.37206



file: ...r1\SU_20121107\13C\JH-551M_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 256

freq. of 0 ppm: 176.148134 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1443.614 ppm/cm: 8.19462

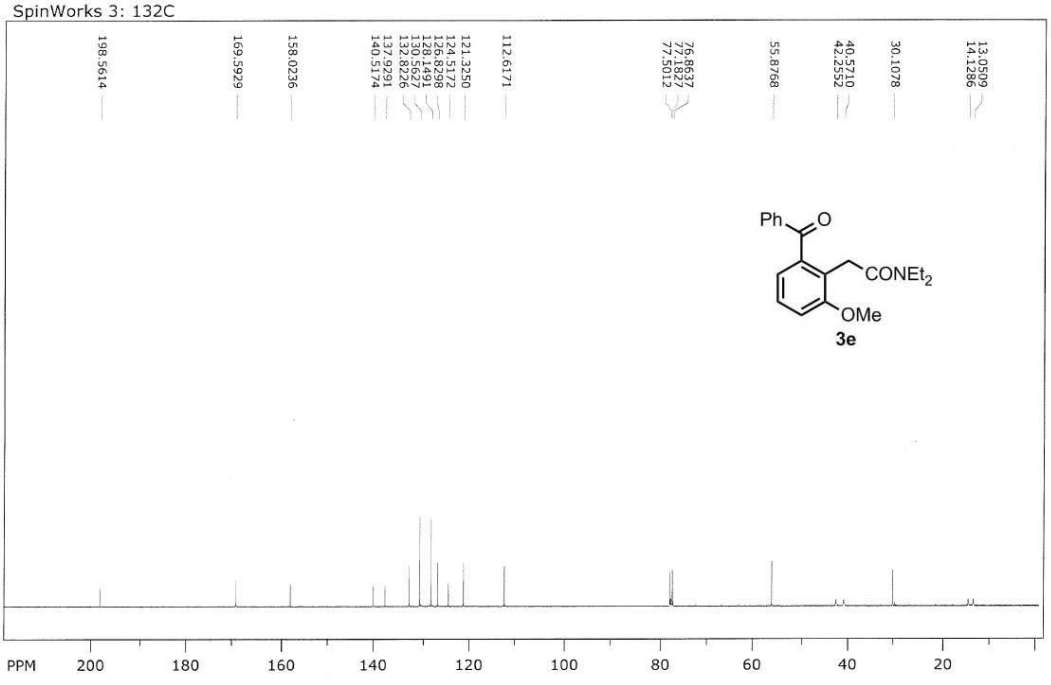
SpinWorks 3: 132H



file: ...ttings\PC\바탕 화면\SKK_KIS\132H\1\fid expt: <zg30>
transmitter freq.: 400.131601 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.0255 ppm = 0.122266 Hz/pt
number of scans: 16

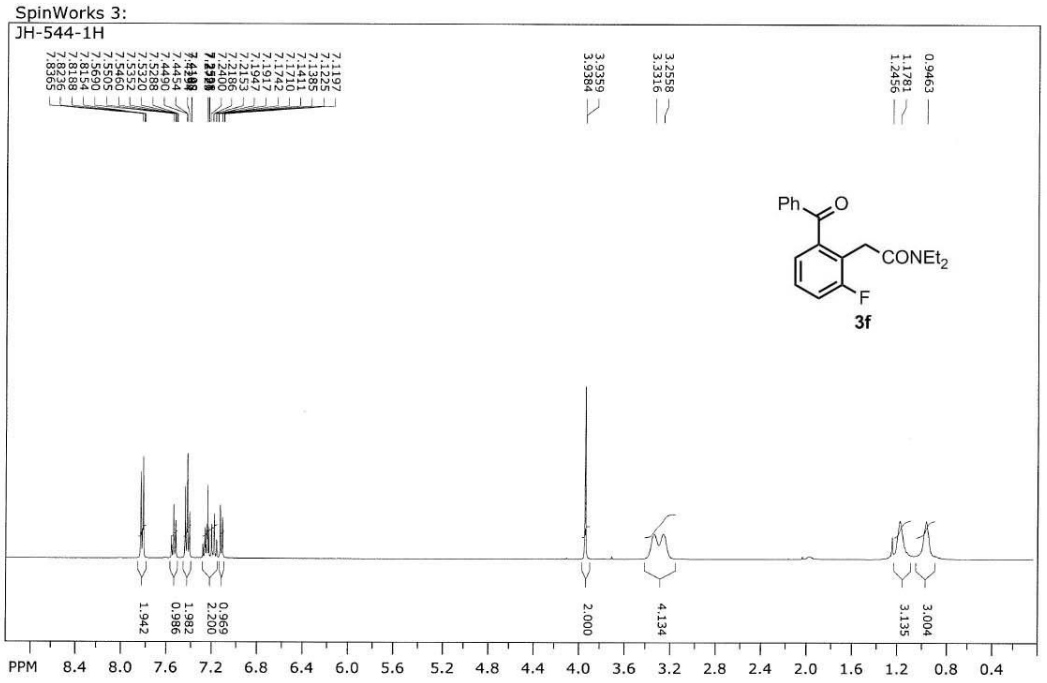
freq. of 0 ppm: 400.130019 MHz
processed size: 131072 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 150.062 ppm/cm: 0.37503

SpinWorks 3: 132C



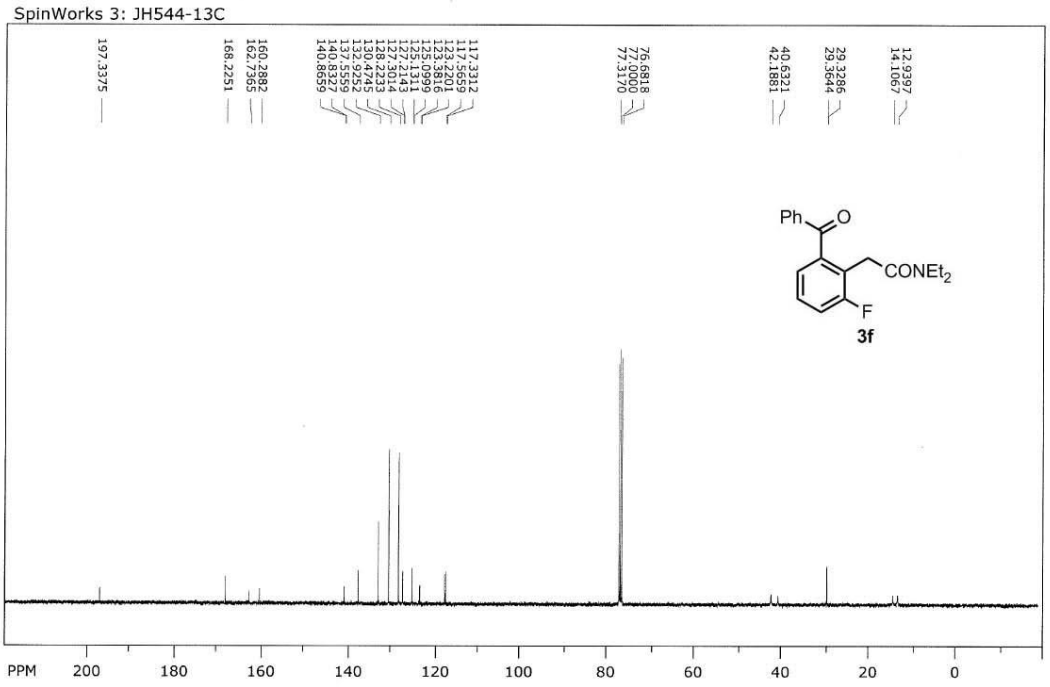
file: ...ttings\PC\바탕 화면\SKK_KIS\132C\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 885.345 ppm/cm: 8.79865



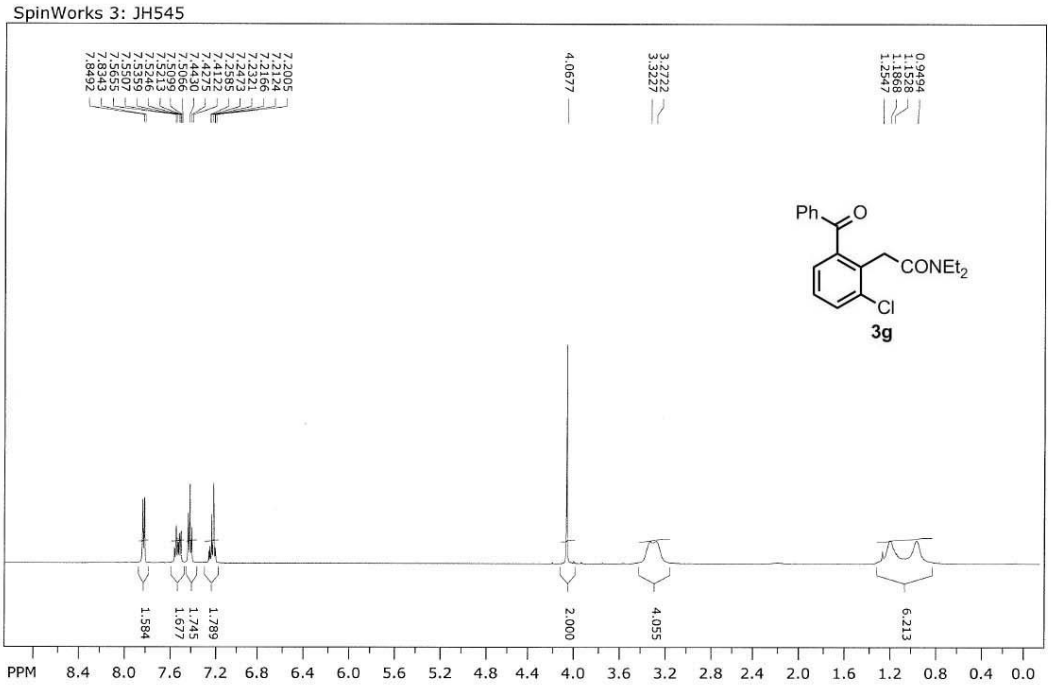
file: ...ettings\aj\Desktop\nmr1\142H\1\fid expt: <zg30>
transmitter freq.: 400.131601 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.0255 ppm = 0.122266 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130014 MHz
processed size: 131072 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 144.361 ppm/cm: 0.36078



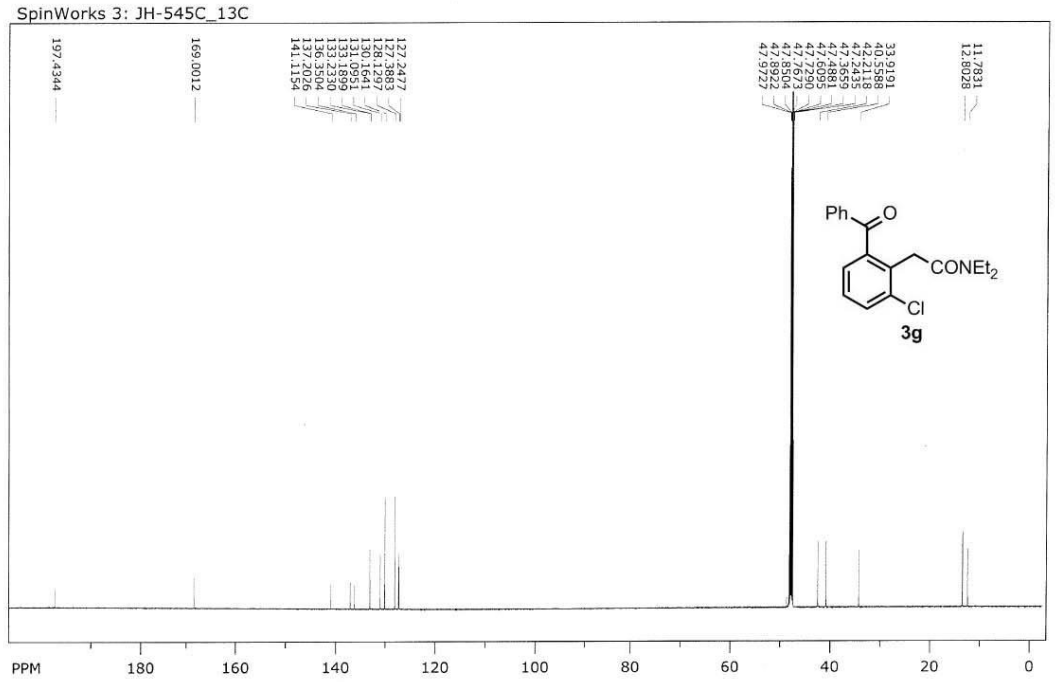
file: ...ettings\aj\Desktop\nmr1\142C\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.612772 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55587



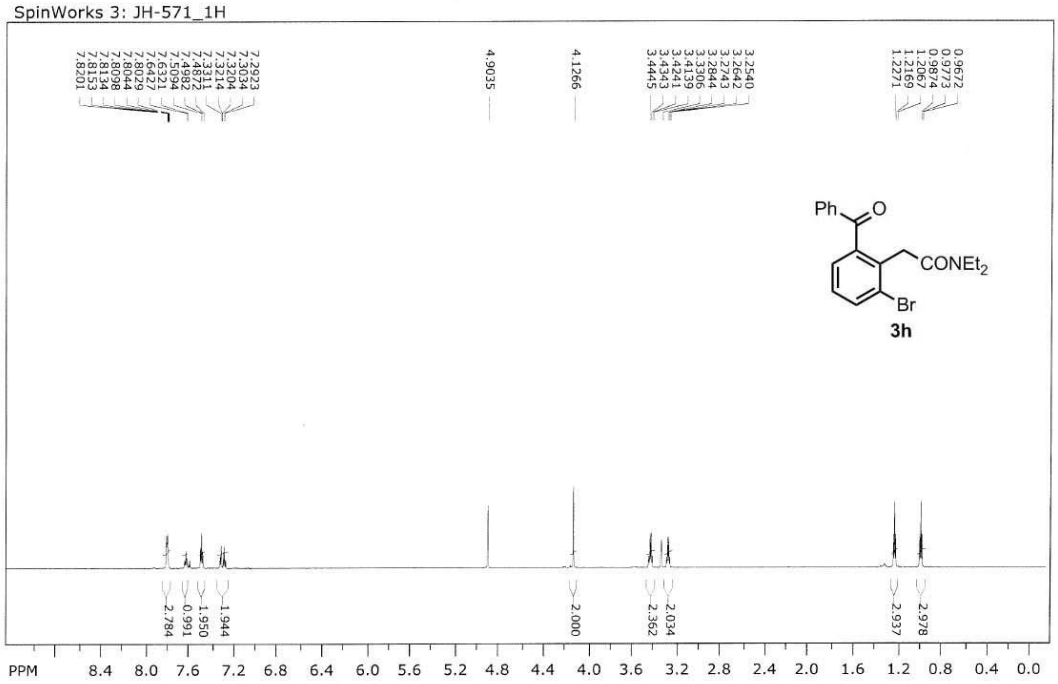
file: G:\JH545.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

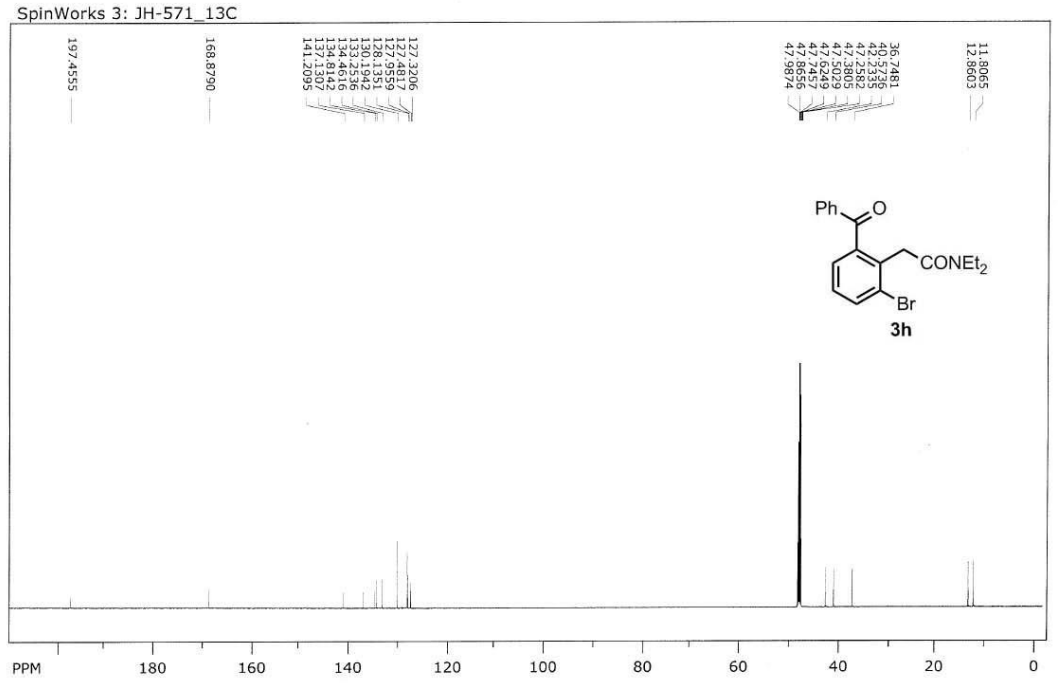
freq. of 0 ppm: 499.957020 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 184.664 ppm/cm: 0.36936

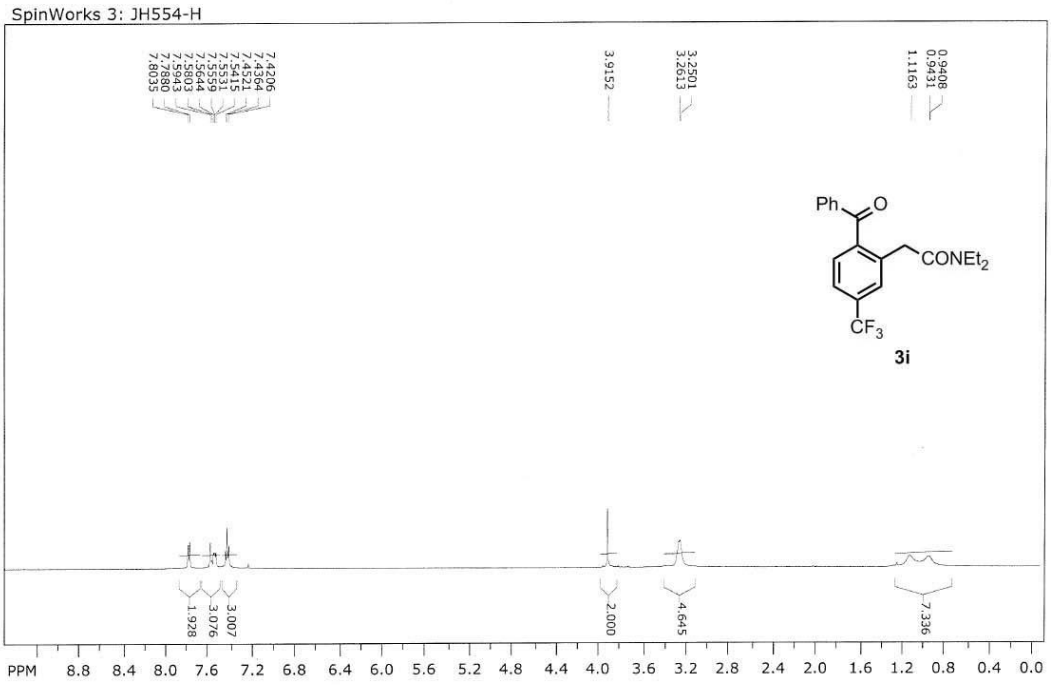


file: F:\SU_20121108\JH-545_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 60

freq. of 0 ppm: 176.148409 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1481.585 ppm/cm: 8.41016

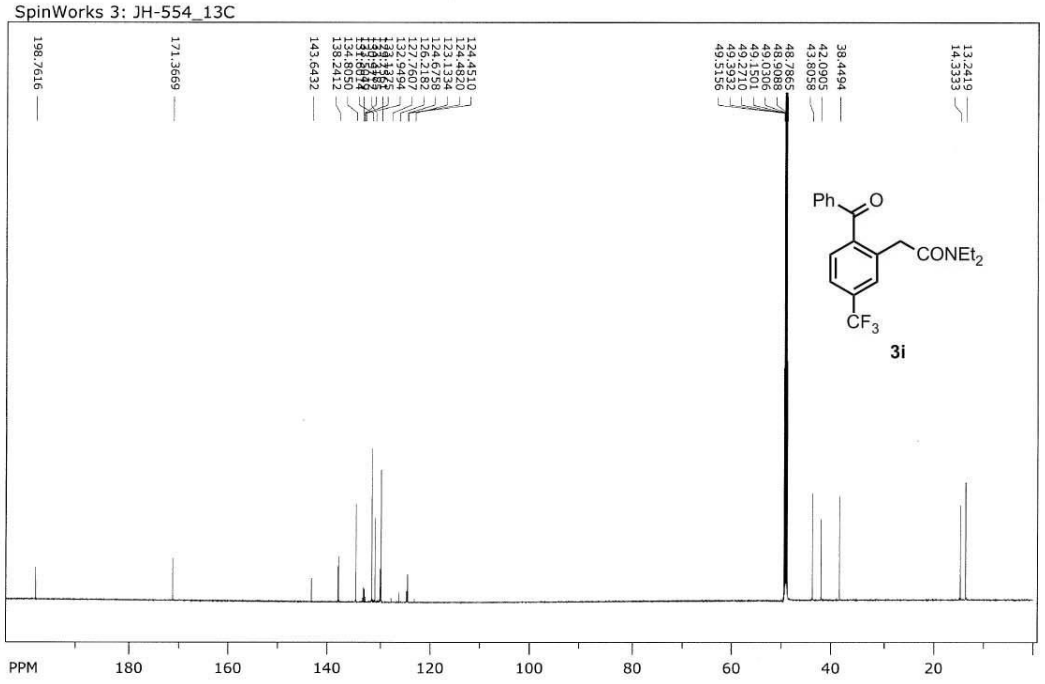

SpinWorks 3: JH-571_1H
Ph
O
CONEt2
Br
3h
PPM
file: F:\SU_20121108\JH-571_1H\fid expt: <zg30>
transmitter freq.: 700.534326 MHz
time domain size: 65536 points
width: 14423.08 Hz = 20.5887 ppm = 0.220079 Hz/pt
number of scans: 16
freq. of 0 ppm: 700.530000 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 264.638 ppm/cm: 0.37777


SpinWorks 3: JH-571_13C
Ph
O
CONEt2
Br
3h
PPM
file: F:\SU_20121108\JH-571_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 72
freq. of 0 ppm: 176.148409 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1498.326 ppm/cm: 8.50519



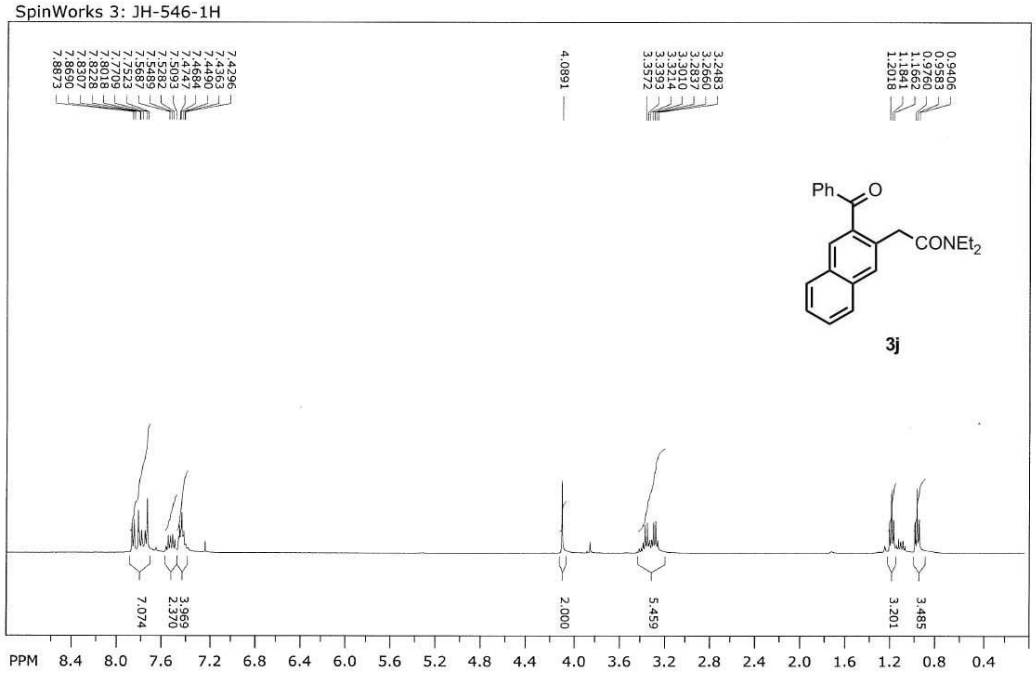
file: F:\JH554-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

freq. of 0 ppm: 499.957029 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 192.024 ppm/cm: 0.38408



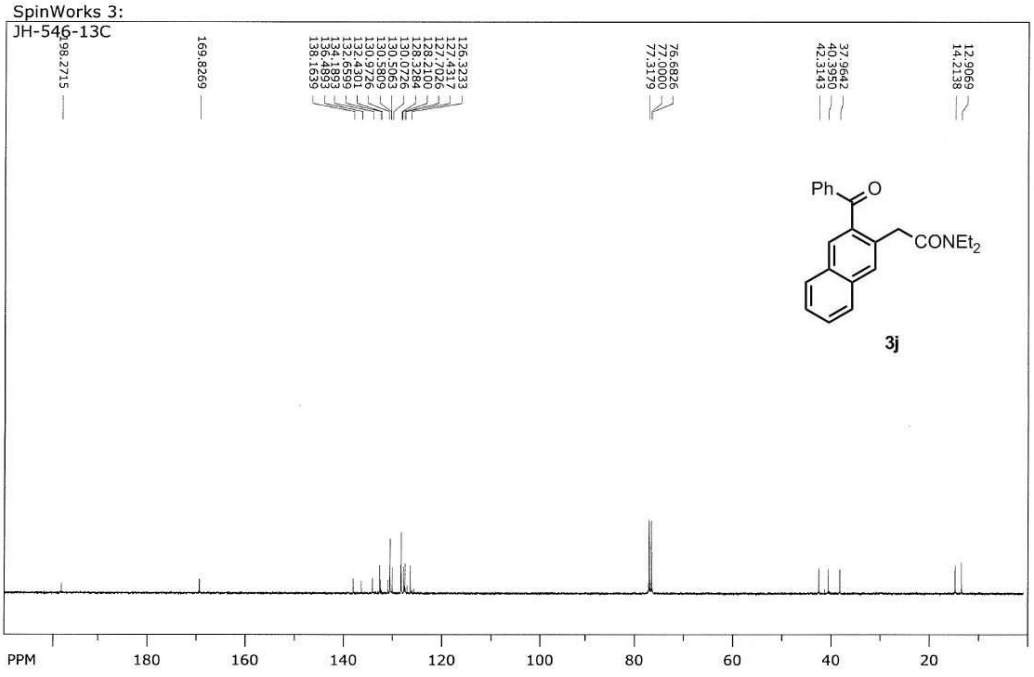
file: ...mr1\SU_20121107\13C\JH-554_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 128

freq. of 0 ppm: 176.148135 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1443.614 ppm/cm: 8.19462



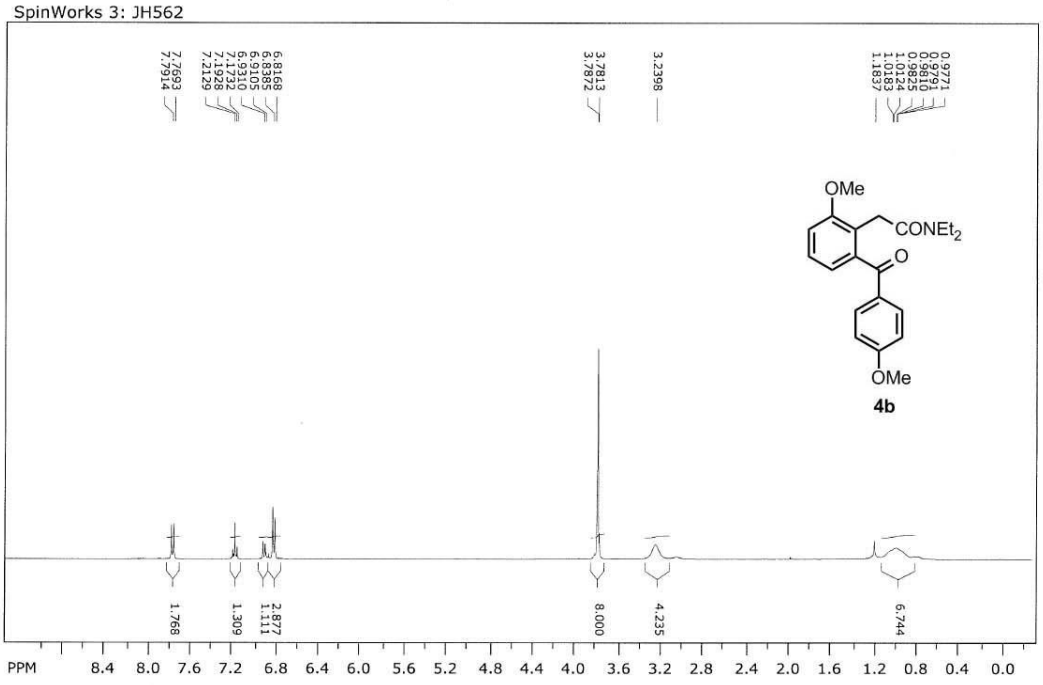
file: ...ettings\aj\Desktop\nmr1\143H\1\fid expt: <zg30>
transmitter freq.: 400.131601 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.0255 ppm = 0.122266 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130019 MHz
processed size: 131072 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 143.926 ppm/cm: 0.35970



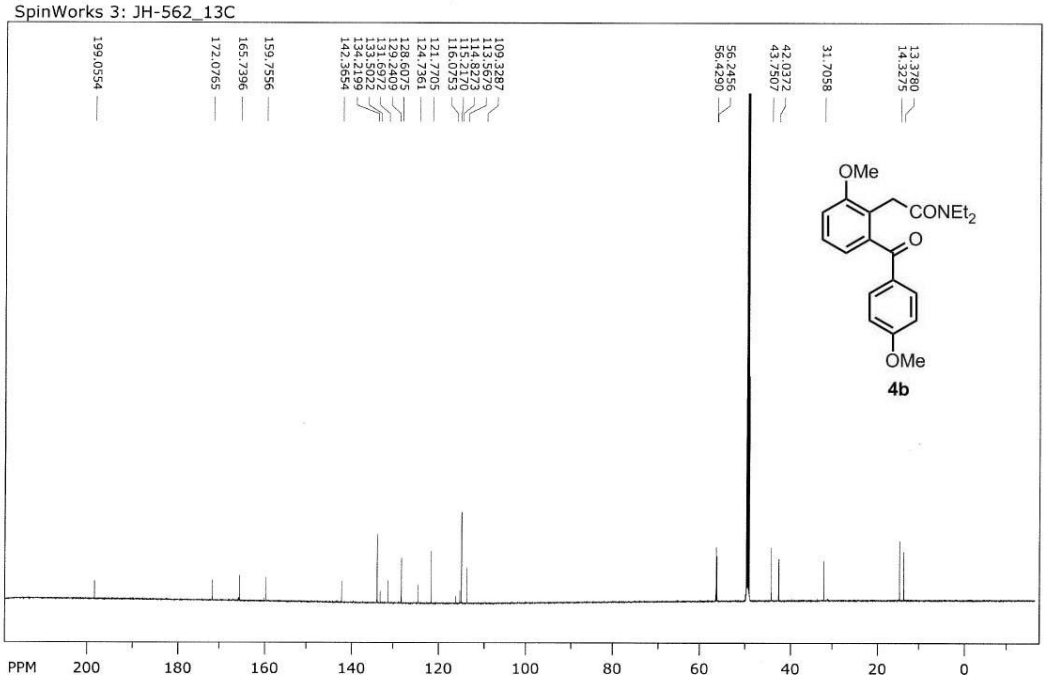
file: ...ettings\aj\Desktop\nmr1\143C\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.612775 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 845.265 ppm/cm: 8.40033



file: ...inistrator\바탕 화면\지혜\NMR\158H\1\fid expt: <zg30>
transmitter freq.: 400.131601 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.0255 ppm = 0.122266 Hz/pt
number of scans: 16

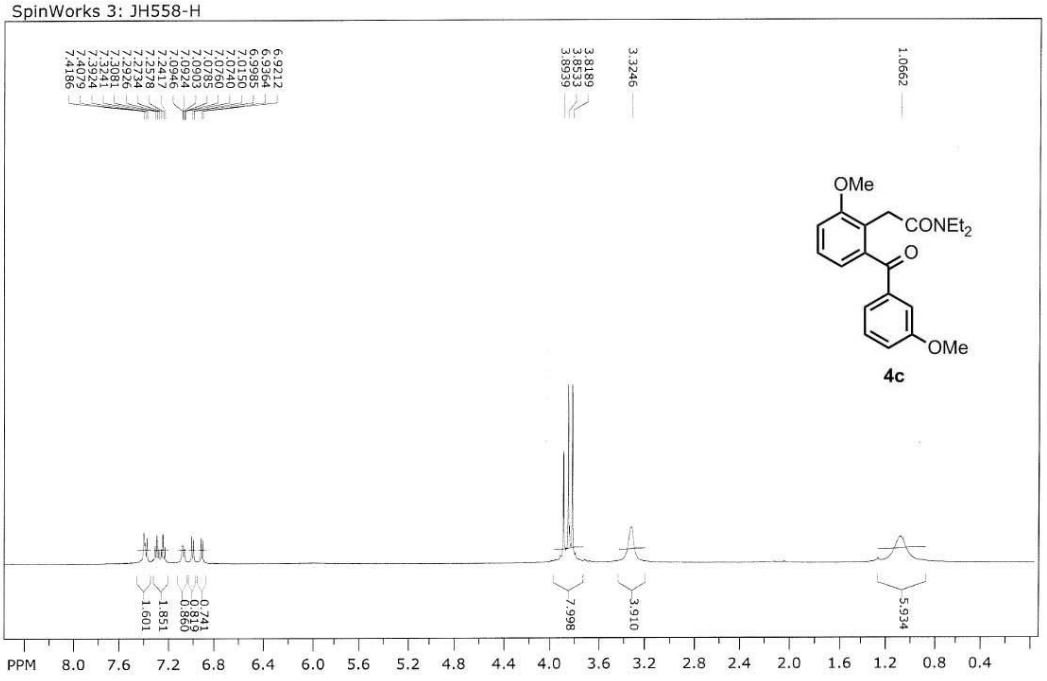
freq. of 0 ppm: 400.130038 MHz
processed size: 131072 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 154.595 ppm/cm: 0.38636



file: ...mr1\SU_20121107\13C\JH-562_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 136

freq. of 0 ppm: 176.148135 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1666.667 ppm/cm: 9.46077

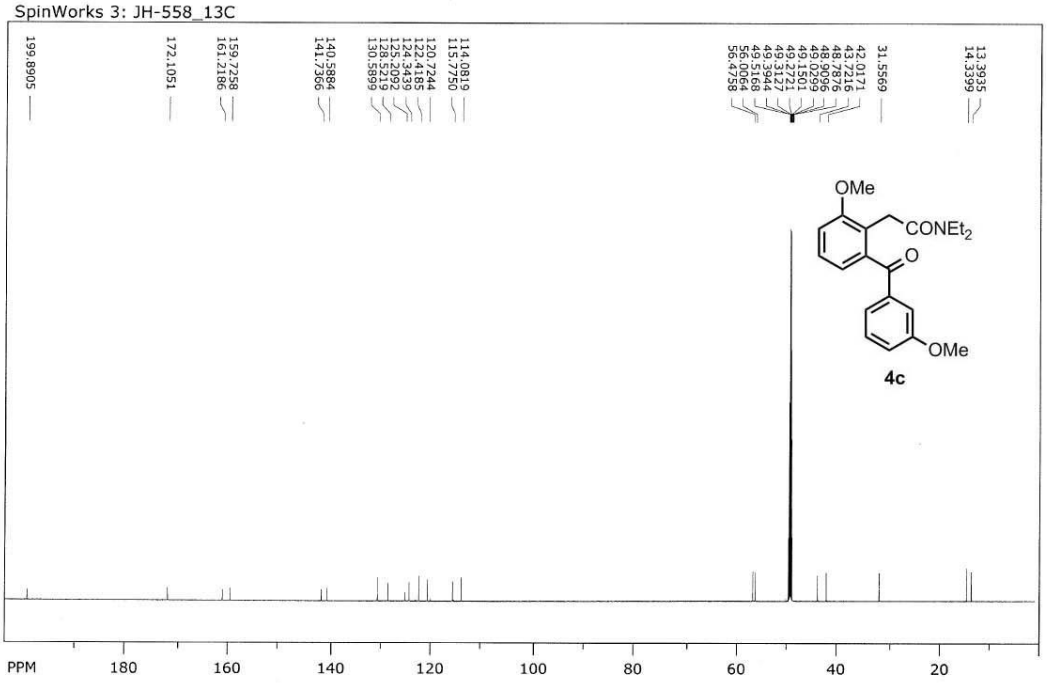
SpinWorks 3: JH558-H



file: F:\JH558-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

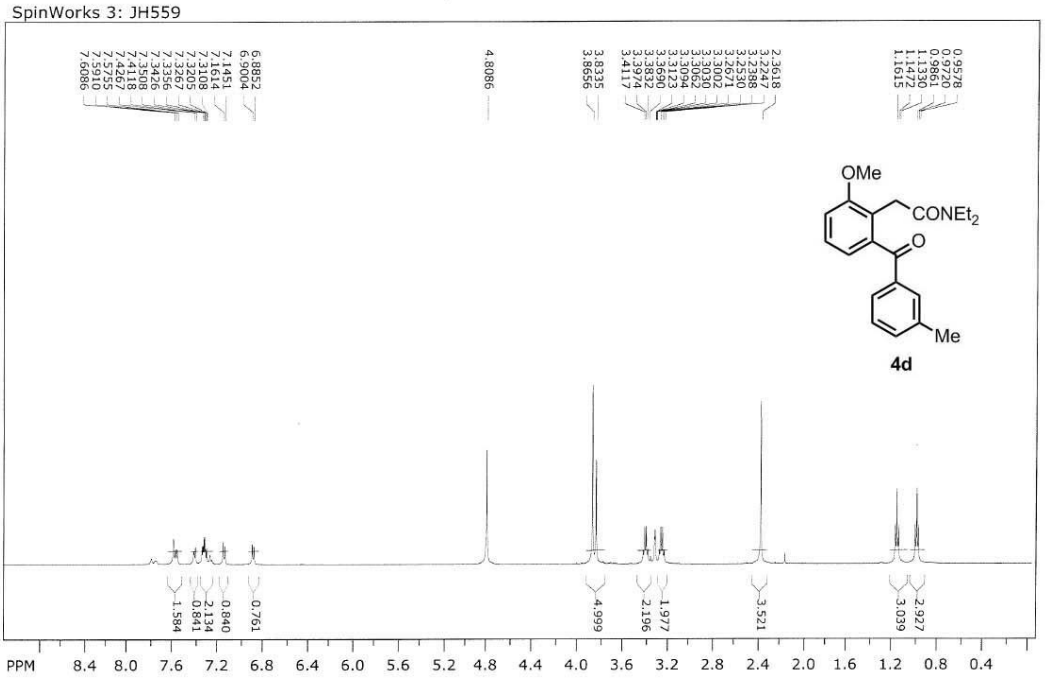
freq. of 0 ppm: 499.957020 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 173.244 ppm/cm: 0.34652

SpinWorks 3: JH-558_13C



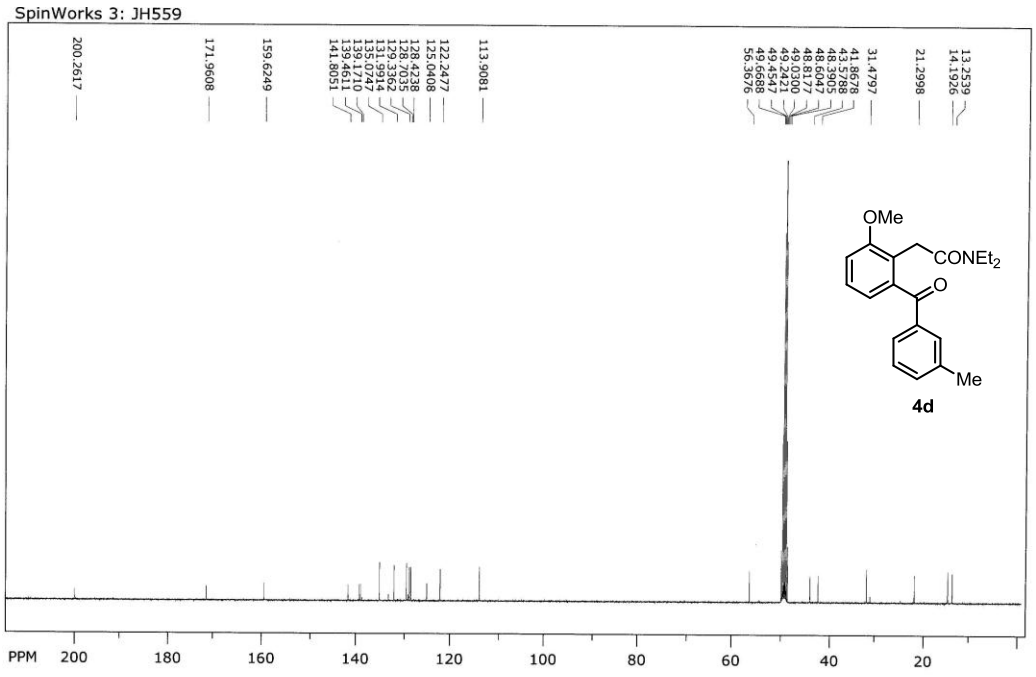
file: ...mr1\SU_20121107\13C\JH-558_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 80

freq. of 0 ppm: 176.148136 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1434.556 ppm/cm: 8.14321



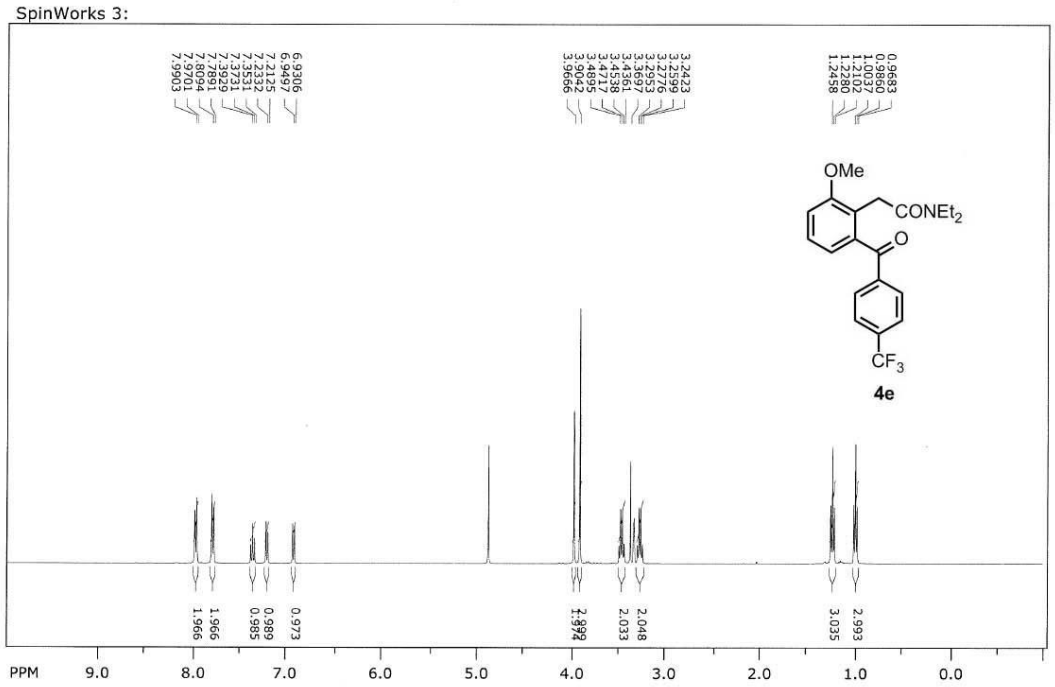
file: ...탕 화면\20121109\JH559-121109.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.962180 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2253 ppm = 0.264267 Hz/pt
number of scans: 32

freq. of 0 ppm: 499.958990 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 183.871 ppm/cm: 0.36777



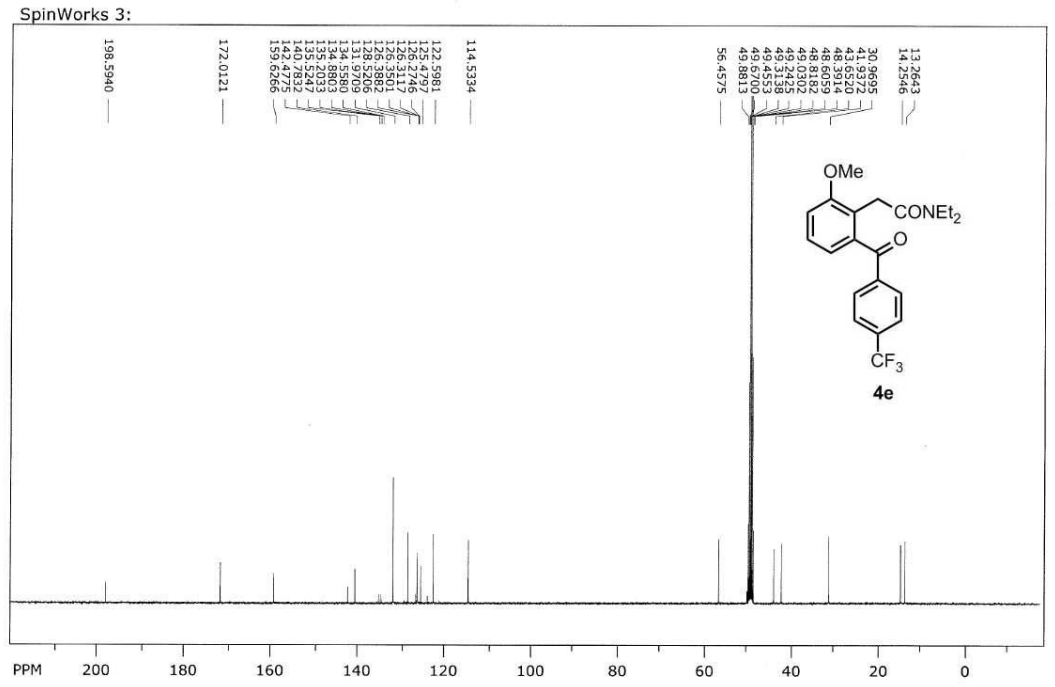
file: ...gs\PC\바탕 화면\SKK_KIS (2)\172c\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 871.394 ppm/cm: 8.66001



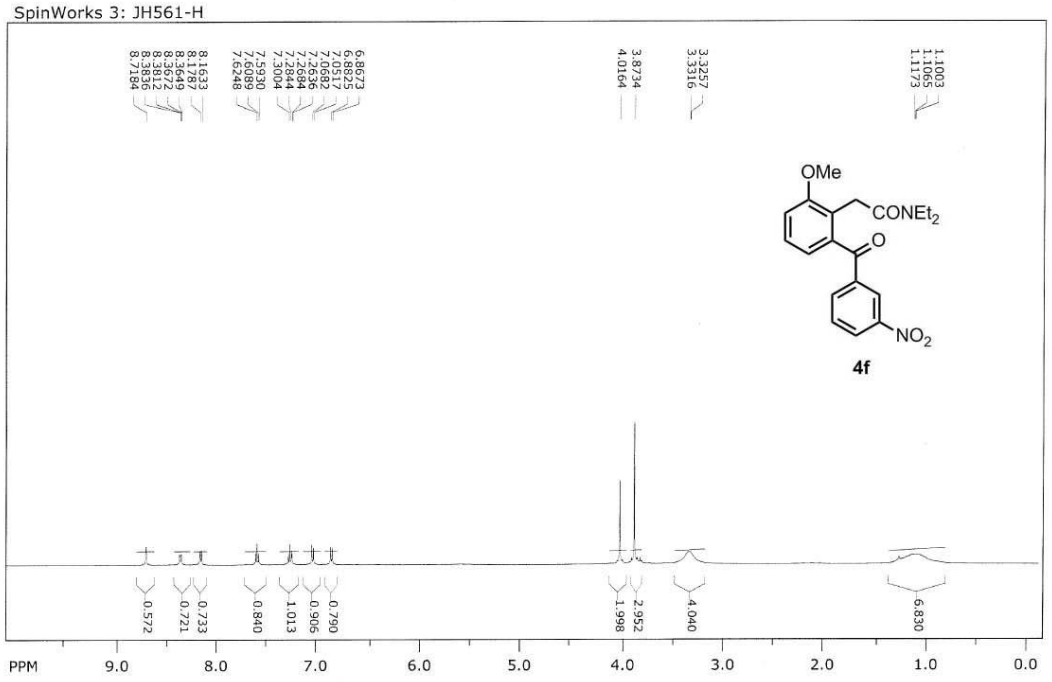
file: ...strator\바탕 화면\SKK_KIS\155h-1\1\fid expt: <zg30>
transmitter freq.: 400.131601 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.0255 ppm = 0.122266 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130000 MHz
processed size: 131072 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 175.934 ppm/cm: 0.43969



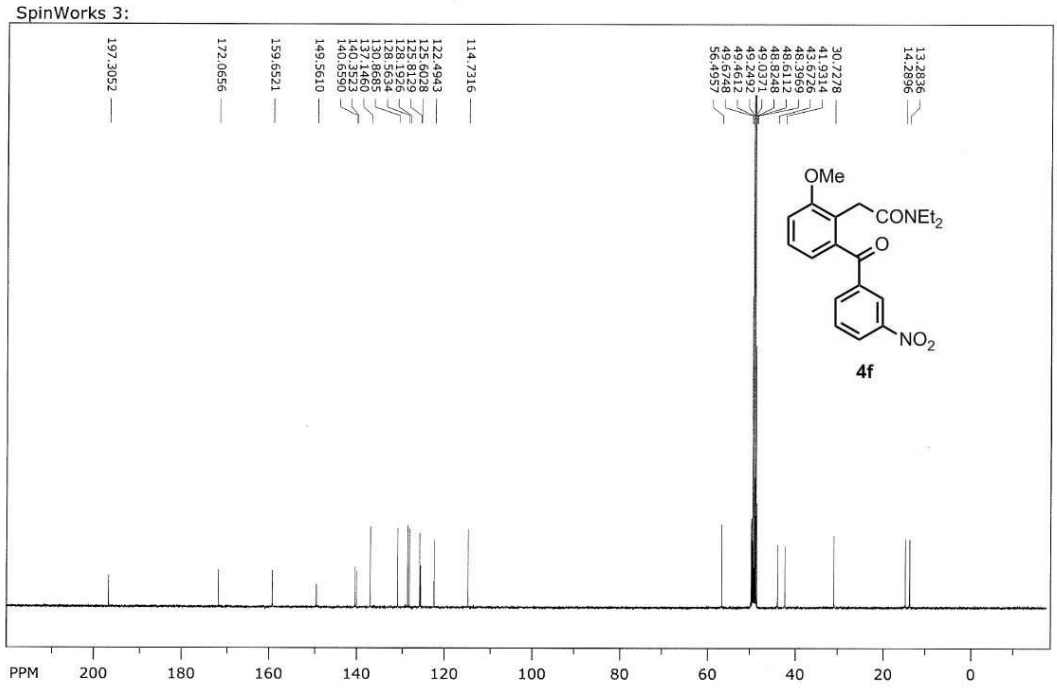
file: ...strator\바탕 화면\SKK_KIS\155c-1\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55587



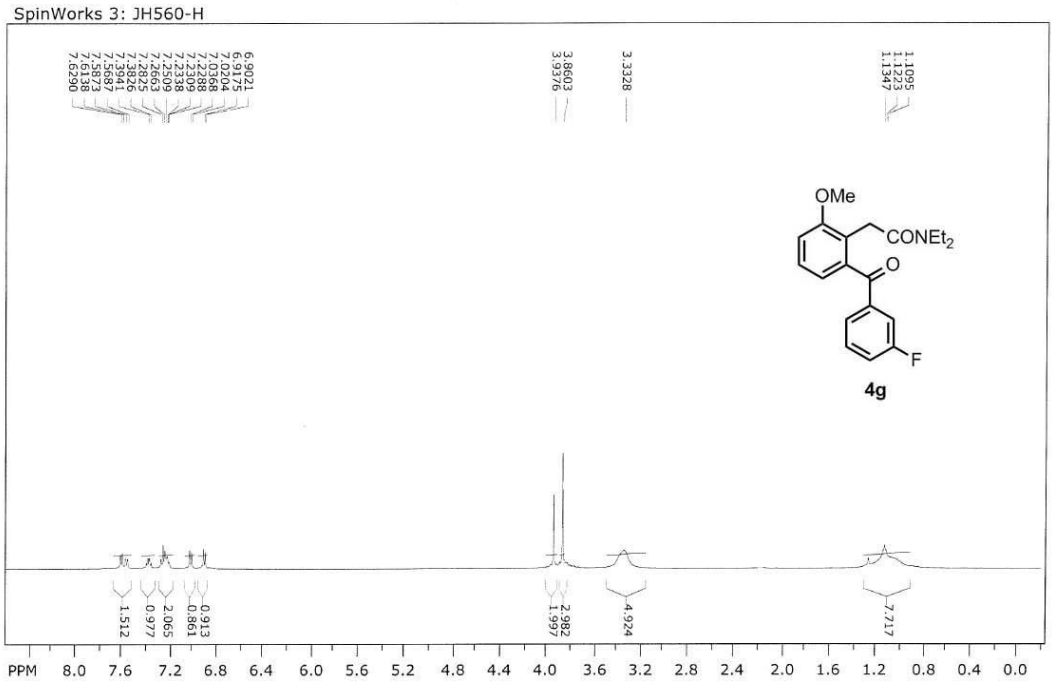
file: F:\JH561-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

freq. of 0 ppm: 499.957020 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 204.897 ppm/cm: 0.40983



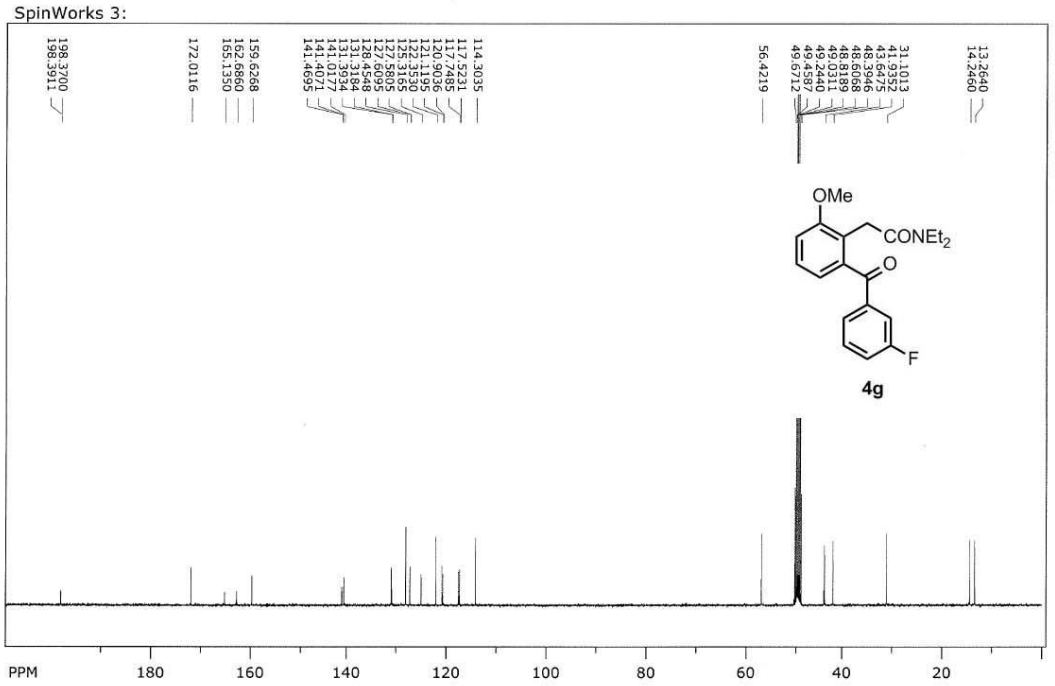
file: ...strator\바탕 화면\SKK_KIS\153c-1\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55587



file: F:\JH560-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.960210 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2254 ppm = 0.264267 Hz/pt
number of scans: 32

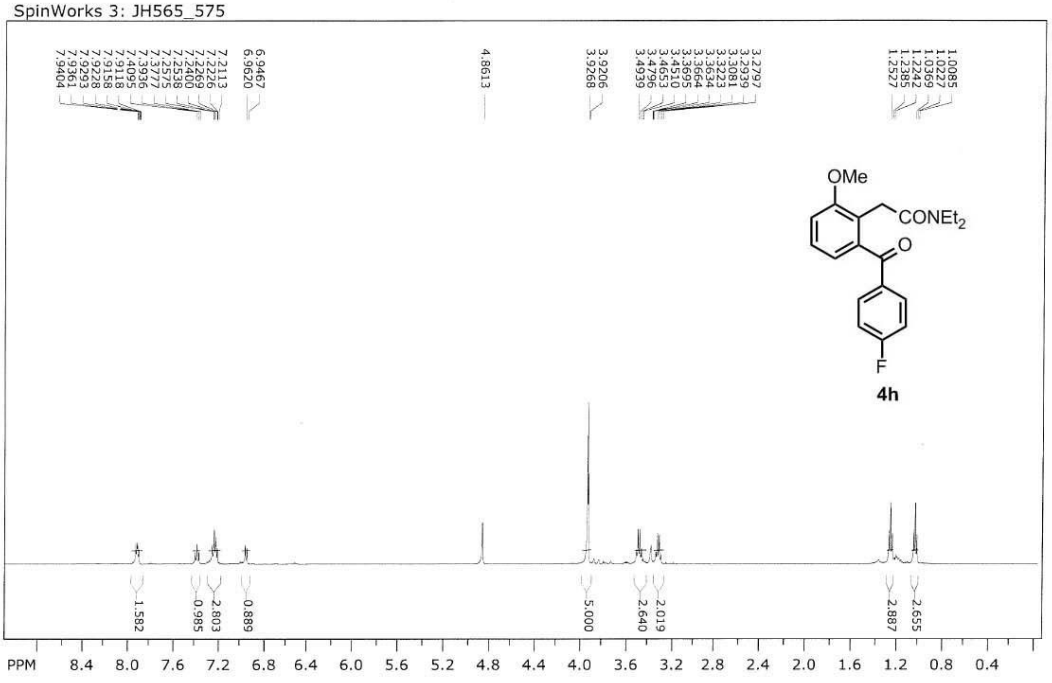
freq. of 0 ppm: 499.957020 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 176.720 ppm/cm: 0.35347



file: ...strator\바탕 화면\SKK_KIS\154c-1\1\fid expt: <zgpg30>
transmitter freq.: 100.622829 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8967 ppm = 0.366798 Hz/pt
number of scans: 1024

freq. of 0 ppm: 100.612626 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 845.265 ppm/cm: 8.40033

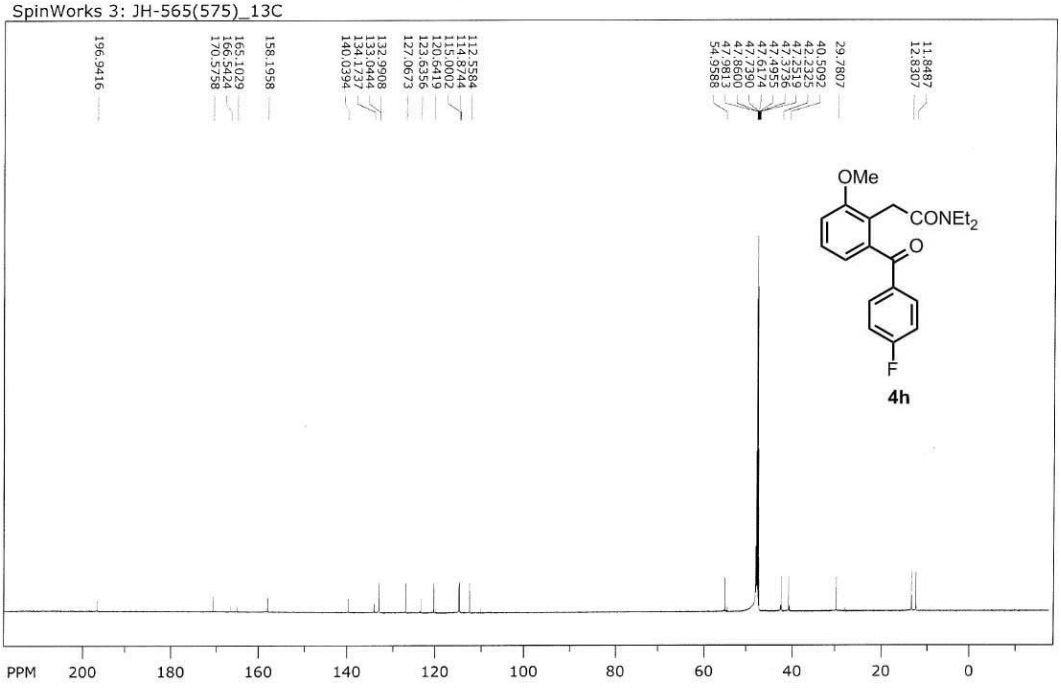
SpinWorks 3: JH565_575



file: ...C\바탕 화면\20121109\JH565_575.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.962585 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2253 ppm = 0.264267 Hz/pt
number of scans: 28

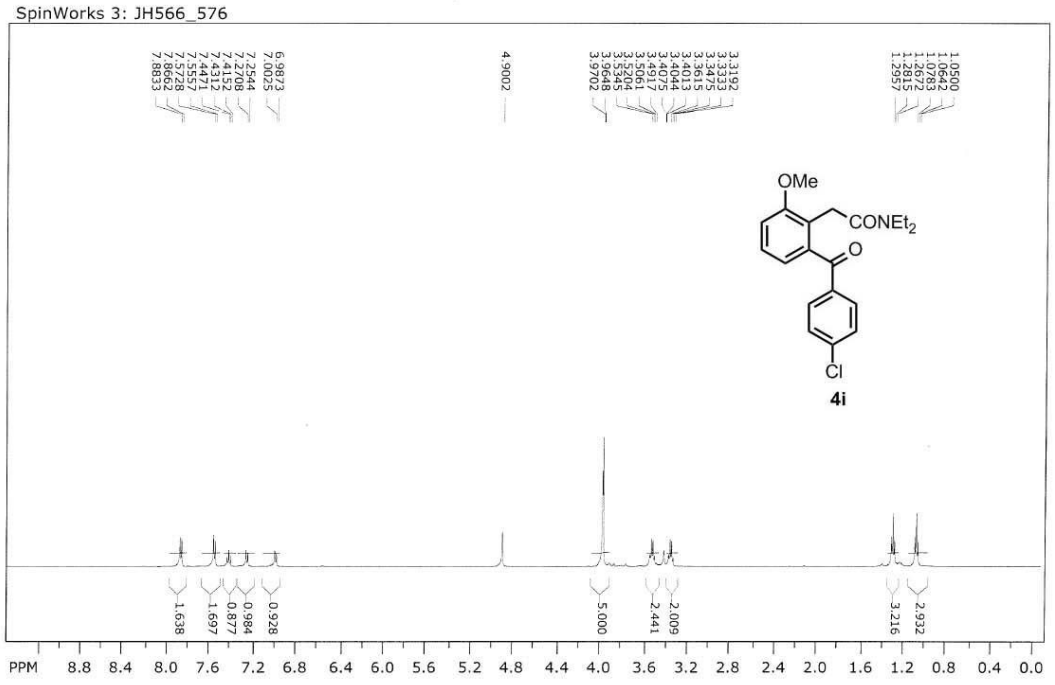
freq. of 0 ppm: 499.958960 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 183.656 ppm/cm: 0.36734

SpinWorks 3: JH-565(575)_13C



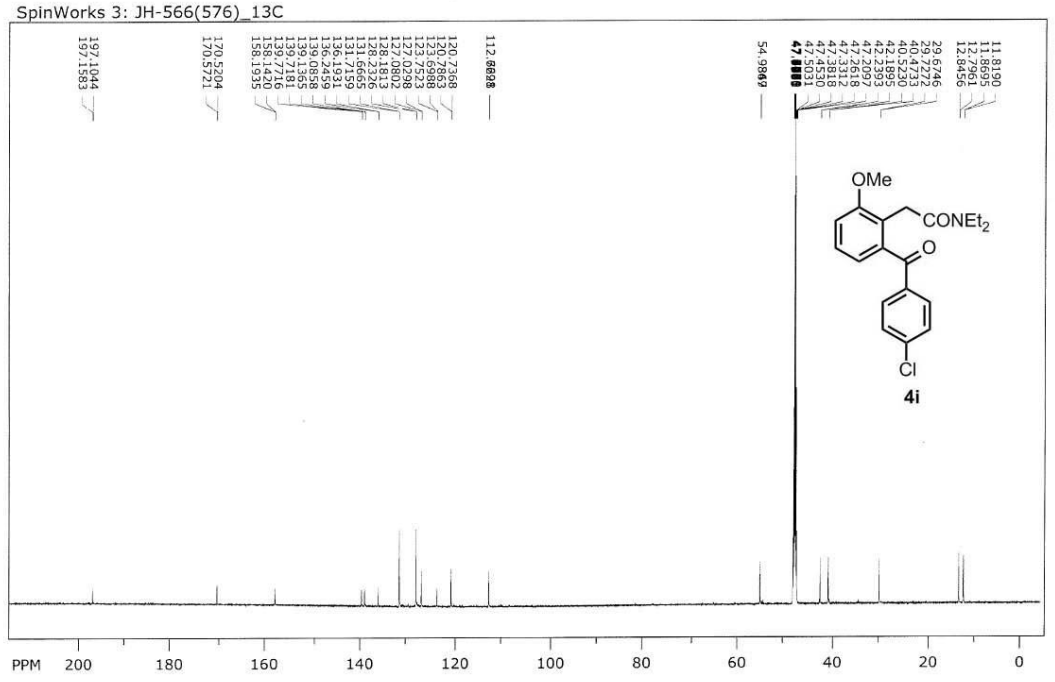
file: F:\SU_20121108\JH565(575)_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 152

freq. of 0 ppm: 176.148409 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1666.667 ppm/cm: 9.46077



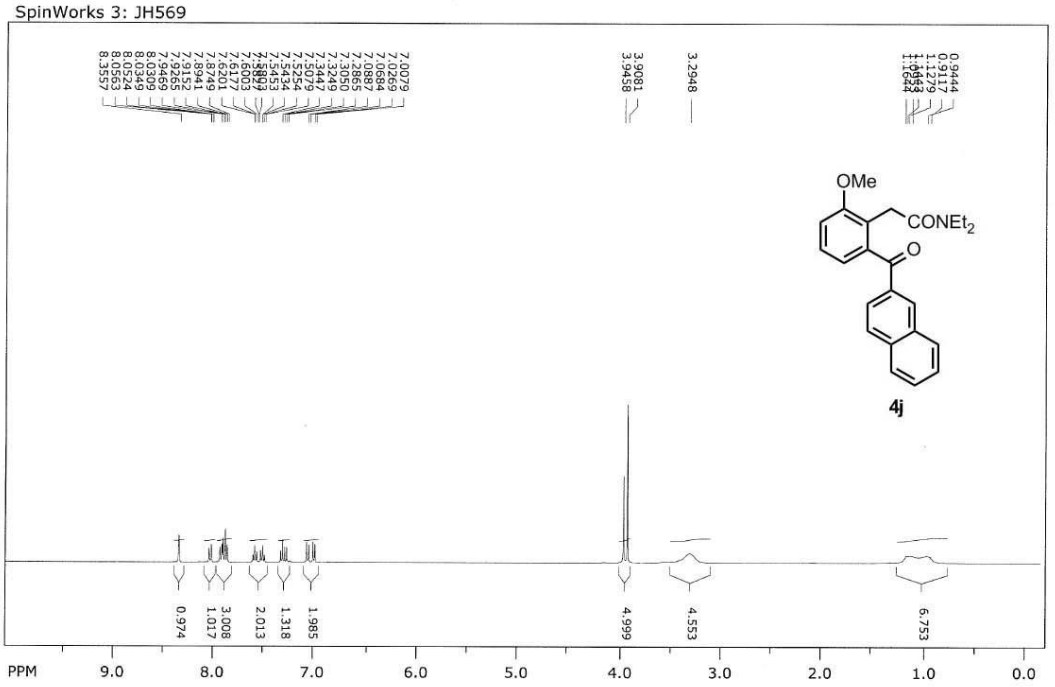
file: ...C\바탕 화면\20121109\JH566_576.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.962585 MHz
time domain size: 36372 points
width: 9611.92 Hz = 19.2253 ppm = 0.264267 Hz/pt
number of scans: 32

freq. of 0 ppm: 499.958941 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 191.809 ppm/cm: 0.38365



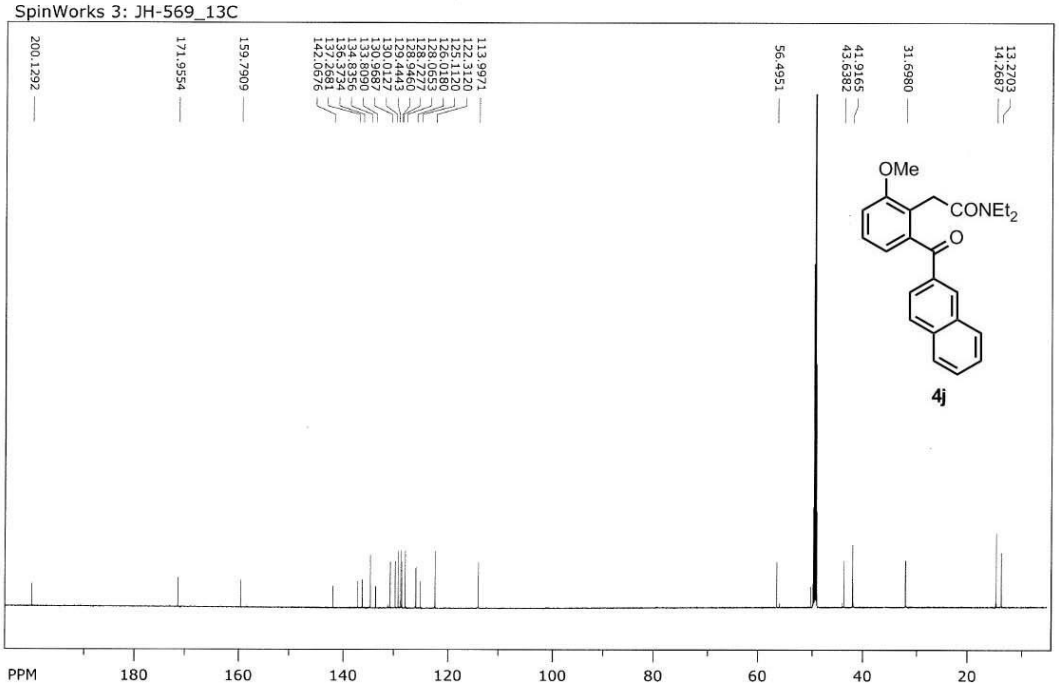
file: F:\SU_20121108\JH566(576)_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 129

freq. of 0 ppm: 176.148409 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1547.619 ppm/cm: 8.78500



file: ...inistrator\바탕 화면\지혜\NMR\159H\1\fid expt: <zg30>
transmitter freq.: 400.131601 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.0255 ppm = 0.122266 Hz/pt
number of scans: 16

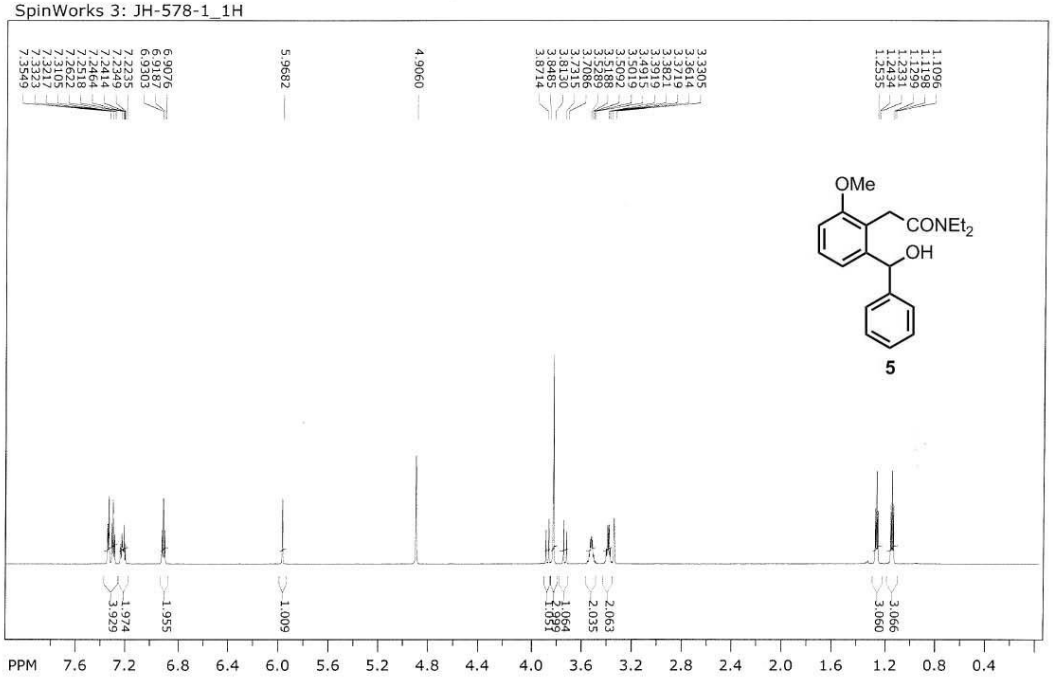
freq. of 0 ppm: 400.130000 MHz
processed size: 131072 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 164.393 ppm/cm: 0.41085



file: ...mr1\SU_20121107\13C\JH-569_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 72

freq. of 0 ppm: 176.148137 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1415.308 ppm/cm: 8.03394

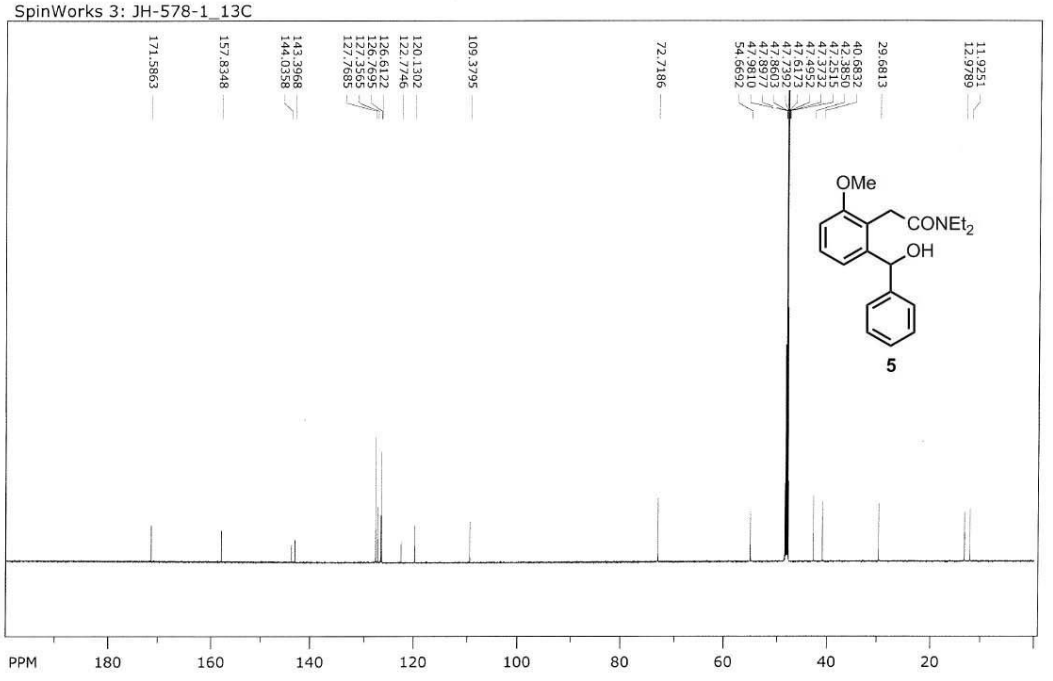
SpinWorks 3: JH-578-1_1H



file: F:\SU_20121108\JH-578-1_1H\fid expt: <zg30>
transmitter freq.: 700.534326 MHz
time domain size: 65536 points
width: 14423.08 Hz = 20.5887 ppm = 0.220079 Hz/pt
number of scans: 16

freq. of 0 ppm: 700.530000 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 230.834 ppm/cm: 0.32951

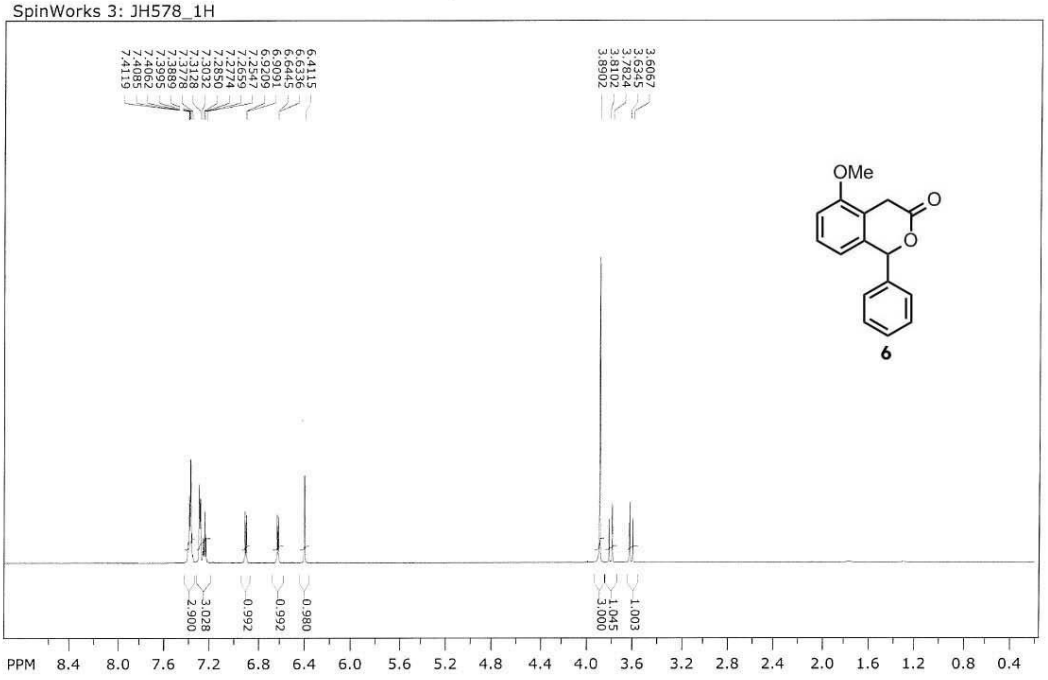
SpinWorks 3: JH-578-1_13C



file: F:\SU_20121108\JH-578-1_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 49

freq. of 0 ppm: 176.148409 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1414.621 ppm/cm: 8.03004

SpinWorks 3: JH578_1H



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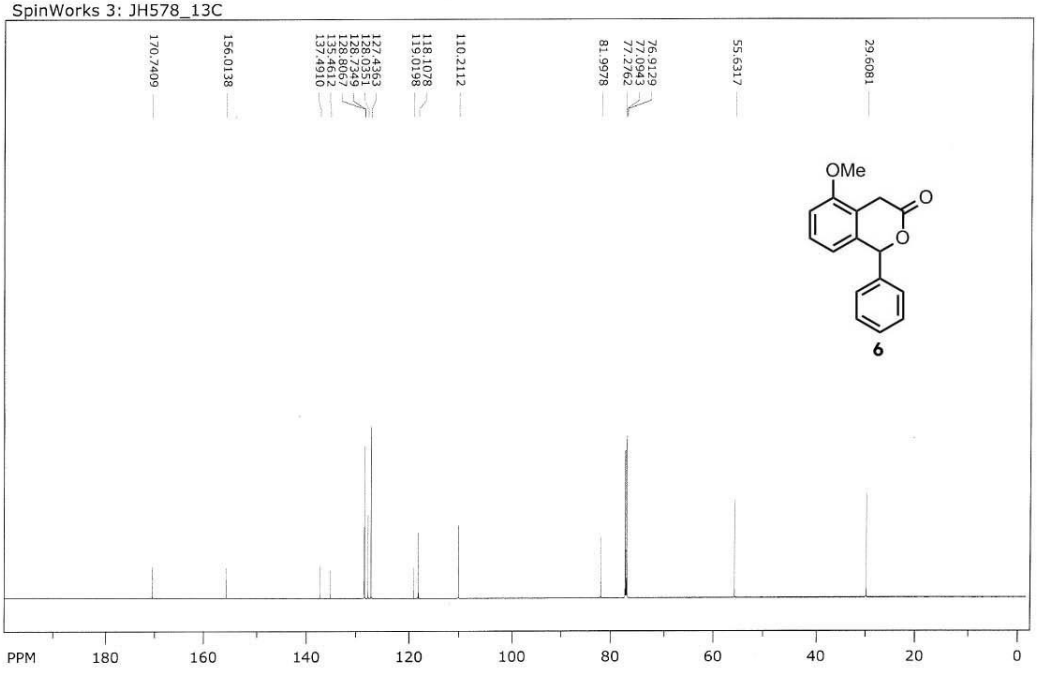
file: F:\SU_20121108\JH578_1H\fid expt: <zg30>
transmitter freq.: 700.534326 MHz
time domain size: 65536 points
width: 14423.08 Hz = 20.5887 ppm = 0.220079 Hz/pt
number of scans: 16

freq. of 0 ppm: 700.530000 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 247.422 ppm/cm: 0.35319

SpinWorks 3: JH578_13C



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file: F:\SU_20121108\JH578_13C\fid expt: <zgpg30>
transmitter freq.: 176.166023 MHz
time domain size: 65536 points
width: 41666.67 Hz = 236.5193 ppm = 0.635783 Hz/pt
number of scans: 36

freq. of 0 ppm: 176.148409 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1424.851 ppm/cm: 8.08812