Electronic Supporting Information

"Stereoselective Intramolecular Cyclopropanation through Catalytic Olefin Activation"

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Part I Experimental part

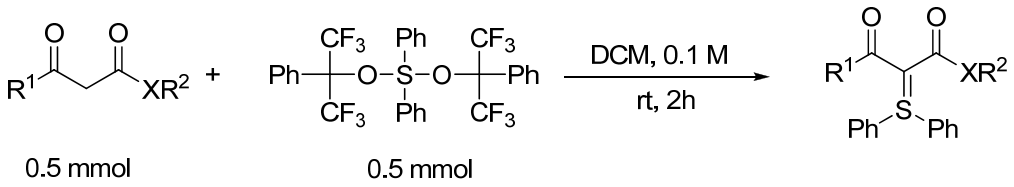
General information

Unless otherwise indicated, all glassware was oven dried by a heat gun before use and all reactions were performed under an atmosphere of Argon. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise stated. All the ylides were prepared according to the procedures reported by our group.[1] Reaction progress was monitored by thin layer chromatography (TLC) performed on plastic plates coated with kieselgel F_{254} with 0.2 mm thickness or GC-MS. Visualization was achieved by ultraviolet light (254 nm). Flash column chromatography was performed using silica gel 60 (230-400 mesh, Merck and co.). Neat infra-red spectra were recorded using a Perkin-Elmer Spectrum 100 FT-IR spectrometer. Wavelengths (ν) are reported in cm^{-1}. Mass spectra were obtained using a Finnigan MAT 8200 or (70 eV) or an Agilent 5973 (70 eV) spectrometer, using electrospray ionization (ESI). Melting points were recorded using a BÜCHI Melting Point thermometer (B-540). All ^{1}H NMR, ^{13}C NMR spectra were recorded on Bruker AV-500, AV-400 or AV-300 in $CDCl_3$. Chemical shifts were given in parts per million (ppm, δ), referenced to the peak of tetramethylsilane, defined at δ = 0.00 (^{1}H NMR), or the solvent peak of $CDCl_3$, defined at δ = 77.0 (^{13}C NMR). Coupling constants were quoted in Hz (*J*). ^{1}H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), sextet (se), septet (sep), octet (o). Splitting

[1] Huang, X.; Goddard, R.; Maulide, N. *Angew. Chem. Int. Ed.* **2010**, *49*, 8979.

patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br).

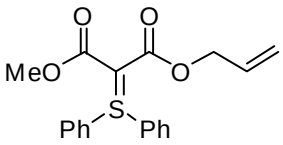
1.1 Preparation and characterisation of the sulfonium ylides



0.5 mmol 0.5 mmol

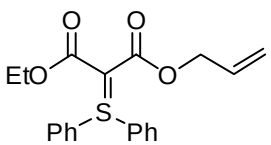
Typical procedure: A dry Schlenk tube was charged with Martin's sulfurane (0.5 mmol, 337mg), then dry dichloromethane (5 mL, 0.1 M) was added. To this solution was added the appropriate dicarbonyl compound (0.5 mmol). After stirring at room temperature for 2h, the solvent was evaporated, and the residue was purified by column chromatograph on silica gel, typically *iso*-hexane/ethyl acetate = ½, affording the desired ylide.

Allyl methyl 2-(diphenylsulfuranylidene) malonate



White solid, R_f = 0.37 (*iso*-hexane/ethyl acetate = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.4 Hz, 4H), 7.54-7.47 (m, 6H), 5.93-5.86 (m, 1H), 5.32 (d, *J* = 17.2 Hz, 1H), 5.14 (d, *J* = 10.5 Hz, 1H), 4.59 (s, 2H), 3.68 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.7, 165.6, 133.2, 131.2, 130.3, 129.4, 129.2, 116.7, 64.2, 60.0, 51.0; IR (neat) ν 1682, 1641, 1306, 1063, 738; EIMS *m/z* (%): 342 (1), 311 (4), 285 (10), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{18}O_4SNa$, 365.0818; found 365.0822.

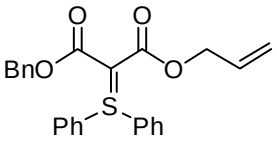
Allyl ethyl 2-(diphenylsulfuranylidene) malonate



White solid, R_f = 0.35 (*iso*-hexane/ethyl acetate = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.4 Hz, 4H), 7.45-7.38 (m, 6H),

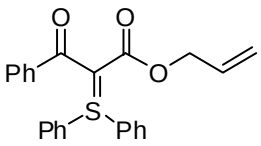
5.87-5.79 (m, 1H), 5.25 (dd, *J* = 15.5 Hz, *J* = 1.6 Hz ,1H), 5.06 (dd, *J* = 9.1 Hz, *J* = 1.2 Hz, 1H), 4.52 (d, *J* = 5.5 Hz, 2H), 4.04 (q, *J* = 7.1 Hz, 2H), 1.12 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.1, 165.8, 133.2, 131.2, 130.4, 129.3, 129.2, 116.7, 64.3, 60.1, 59.5, 14.5; IR (neat) ν 1715, 1682, 1621, 1272, 1055, 723; EIMS *m/z* (%): 356 (1), 311 (7), 299 (10), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{20}O_4SNa$, 375.0975; found 379.0973.

Allyl benzyl 2-(diphenylsulfuranylidene) malonate



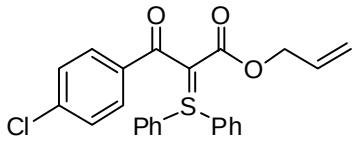
White solid, R_f = 0.24 (pentane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54-7.34 (m, 10H), 7.22-7.17 (m, 5H), 5.86-5.80 (m, 1H), 5.23-5.20 (m, 1H), 5.05 (br, 3H), 4.53 (t, *J* = 1.9 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.7, 137.1, 133.2, 131.2, 130.2, 129.4, 129.2, 128.20, 128.17, 127.72, 127.67, 127.4, 117.0, 65.3, 64.5, 60.4; IR (neat) ν 1719, 1683, 1630, 1273, 1049, 740; EIMS *m/z* (%): 418(1), 361 (3), 311 (4), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{22}O_4SNa$, 441.1131; found 441.1132.

Allyl 2-(diphenylsulfuranylidene) 3-oxo-3-phenylpropanoate



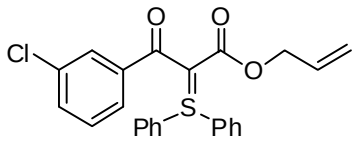
White solid, R_f = 0.25 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 4.6 Hz, 4H), 7.53 (d, *J* = 8.1 Hz, 8H), 7.35 (t, *J* = 8.1 Hz, 3H), 5.52-5.57 (m, 1H), 4.99 (d, *J* = 10.4 Hz, 1H), 4.93 (d, *J* = 17.2 Hz, 1H), 4.42 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.6, 165.9, 142.8, 132.7, 131.4, 129.8, 129.64, 129.57, 129.5, 127.7, 127.4, 116.7, 75.4, 64.3; IR (neat) ν 1674, 1561, 1039, 751; EIMS *m/z* (%): 388 (23), 331 (2), 285 (1), 283 (6), 186 (95), 105 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{20}O_3SNa$, 411.1025; found 411.1022.

Allyl 2-(diphenylsulfuranylidene) 3-(4-chlorophenyl)-3-oxo-propanoate



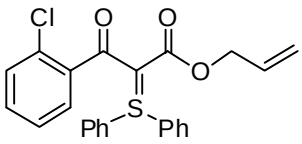
White solid, R_f = 0.26 (*iso*-hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74-7.71 (m, 4H), 7.57-7.48 (m, 8H), 7.32-7.28 (m, 2H), 5.69-5.61 (m, 1H), 5.05-4.96 (m, 2H), 4.44 (dt, *J* = 5.5 Hz, *J* = 1.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) one carbon overlapped δ 188.2, 165.7, 141.1, 135.4, 132.6, 131.5, 129.62, 129.55, 129.2, 127.6, 117.0, 75.5, 64.4; IR (neat) ν 1671, 1574, 1562, 1040, 741; EIMS *m/z* (%): 423 (4), 422 (4), 365 (5), 283 (10), 186 (100), 139 (81); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{19}O_3ClSNa$, 445.0636; found 445.0636.

Allyl 2-(diphenylsulfuranylidene) 3-(3-chlorophenyl)-3-oxo-propanoate



White solid, R_f = 0.38 (*iso*-hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64-7.62 (m, 4H), 7.48-7.41 (m, 7H), 7.32 (d, *J* = 7.4 Hz, 1H), 7.24 (dd, *J* = 6.9 Hz, *J* = 1.6 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 1H), 5.57-5.49 (m, 1H), 4.95-4.88 (m, 2H), 4.34 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) one carbon overlapped δ 187.7, 165.6. 144.5, 133.2, 132.5, 131.6, 129.6, 129.4, 129.2, 128.7, 127.8, 125.7, 117.1, 75.9, 64.4; IR (neat) ν 1676, 1584, 1573, 1561, 1329, 1041, 746; EIMS *m/z* (%): 423 (5), 422 (15), 365 (5), 283 (10), 186 (100), 139 (66); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{19}O_3ClSNa$, 445.0636; found 445.0637.

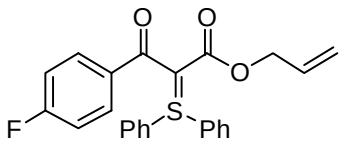
Allyl 2-(diphenylsulfuranylidene) 3-(2-chlorophenyl)-3-oxo-propanoate



Colorless oil, R_f = 0.24 (pentane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.4 Hz, 4H), 7.49-7.42 (m, 6H), 7.24-7.22 (m, 1H), 7.15-7.14 (m, 3H), 5.44 (d, *J* = 5.5 Hz,

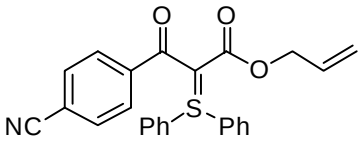
1H), 4.91-4.88 (m, 2H), 4.29 (d, J = 4.7 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) one carbon overlapped δ 186.0, 165.1, 142.9, 132.5, 131.4, 129.9, 129.6, 129.5, 128.8, 128.7, 127.3, 126.2, 116.8, 77.4, 64.4; IR (neat) ν 1682, 1661, 1563, 1060, 741; EIMS *m/z* (%): 423 (6), 422 (23), 387 (100), 283 (5), 186 (87), 139 (75); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{19}O_3ClSNa$, 445.0636; found 445.0636.

Allyl 2-(diphenylsulfuranylidene)-3-(4-fluorophenyl)-3-oxopropanoate



Off-white foam, R_f = 0.28 (*n*-pentane : EtOAc 1:1) ^{1}H (500 MHz, $CDCl_3$) δ = 7.75 – 7.68 (m, 4H), 7.61 – 7.45 (m, 8H), 7.00 (tt, J = 8.8, 2.1 Hz, 2H), 5.71 – 5.57 (m, 1H), 5.05 – 4.93 (m, 2H), 4.43 (dt, J = 5.5, 1.5 Hz, 2H); ^{13}C (100 MHz, $CDCl_3$) δ = 188.1, 165.6, 163.5 (d, J_{C-F} = 248.2 Hz), 138.7 (d, J_{C-F} = 3.22 Hz), 132.6, 131.4, 129.9 (d, J_{C-F} = 8.4 Hz), 129.7, 129.5, 129.5, 116.8, 114.1 (d, J_{C-F} = 21.6 Hz), 75.3, 64.2; IR (neat): ν = 3064, 2937, 1659, 1645, 1599, 1562, 1504, 1475, 1443, 1404, 1360, 1320, 1267, 1246, 1220, 1153, 1093, 1048, 998, 920, 843, 760, 741, 683; MS-(EI) m/z (%): 406(14), 228(13), 186(80), 123(100), 95(23), 77(14), 41(59); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{20}FO_3SNa$, 429.0931 ; found 429.0938 .

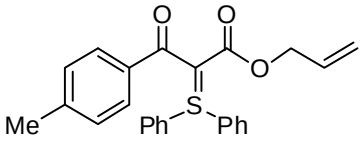
Allyl 2-(diphenylsulfuranylidene)-3-(4-cyanophenyl)-3-oxopropanoate



Orange solid (36%), R_f = 0.3 (*n*-pentane : EtOAc 1:1). ^{1}H (300 MHz, $CDCl_3$) δ = 7.66 – 7.60 (m, 4H), 7.54 – 7.39 (m, 10H), 5.58 – 5.43 (m, 1H), 4.97 – 4.84 (m, 2H), 4.30 (dt, J = 5.6, 1.4 Hz, 2H); ^{13}C (100 MHz, $CDCl_3$) δ = 187.4, 165.3, 147.3, 132.4, 131.7, 131.4, 129.7, 129.6, 129.2, 127.9, 118.8, 127.9, 118.8, 117.3, 112.4, 76.3, 64.5; IR (neat): ν = 3065, 2940, 2227, 1669, 1574, 1475, 1443, 1401, 1361, 1326, 1269, 1250, 1178, 1142, 1124, 1051, 1019, 998, 917, 838, 743, 683, 664; MS-(EI) m/z (%): 413(48), 283(12), 235(17), 219(16), 199(12), 186(100), 130(71), 121(19), 102(25), 77(15), 51(10),

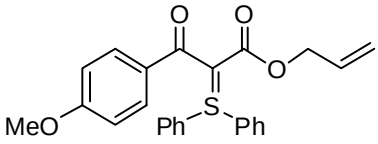
41(37); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{19}NO_3SNa$, 436.0977 ; found 436.0976.

Allyl 2-(diphenylsulfuranylidene) 3-oxo-3-p-tolylpropanoate



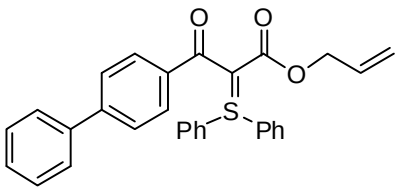
Colorless oil, R_f = 0.28 (*iso*-hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75-7.72 (m, 4H), 7.55-7.48 (m, 8H), 7.15 (d, *J* = 8.3 Hz, 2H), 5.69-5.61 (m, 1H), 5.02-4.94 (m, 2H), 4.44 (dt, *J* = 5.4 Hz, *J* = 1.4 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.4, 165.9, 139.8, 139.6, 132.8, 131.3, 129.9, 129.6, 129.5, 128.0, 127.9, 116.6, 74.8, 64.2, 21.4; IR (neat) ν 1672, 1561, 1325, 1039, 740; EIMS *m/z* (%): 402 (10), 345 (4), 365 (5), 283 (2), 186 (74), 119 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{22}O_3SNa$, 425.1182; found 425.1182.

Allyl 2-(diphenylsulfuranylidene)-3-(4-methoxyphenyl)-3-oxopropanoate



Colorless oil, R_f = 0.30 (pentane/ethyl acetate = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74-7.71 (m, 4H), 7.61-7.58 (m, 2H), 7.55-7.48 (m, 6H), 6.87-6.84 (m, 2H), 5.71-5.64 (m, 1H), 5.03-4.96 (m, 2H), 4.45 (dt, *J* = 5.4 Hz, *J* = 1.4 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.6, 165.9, 161.0, 134.9, 132.9, 131.3, 130.1, 130.0, 129.6, 129.5, 116.7, 112.6, 74.6, 64.2, 55.2; IR (neat) ν 1671, 1606, 1581, 1246, 1040, 743; EIMS *m/z* (%): 418 (12), 361 (3), 186 (52), 135(100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{22}O_4SNa$, 441.1131; found 441.1135.

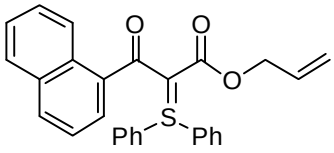
Allyl 2-(diphenylsulfuranylidene)-3-([1,1'-biphenyl]-4-yl)-3-oxopropanoate



Colorless solid, R_f = 0.40 (pentane/ethyl acetate = 1/1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.53 Hz,

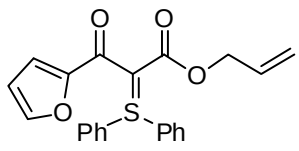
2H), 7.63 (d, *J* = 8.22 Hz, 2H), 7.59 (d, *J* = 8.22 Hz, 2H), 7.56 – 7.49 (m, 8H), 7.43 (t, *J* = 7.53 Hz, 2H), 7.34 (t, *J* = 6.85 Hz, 1H), 5.64 – 5.59 (m, 1H), 4.97 (d, *J* = 10.50 Hz, 1H), 4.92 (d, *J* = 17.30 Hz, 1H), 4.43 (d, *J* = 5.25 Hz, 2H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.3, 166.1, 142.5, 141.7, 141.1, 132.8, 131.6, 129.9, 129.8, 129.7, 128.8, 128.5, 127.5, 127.3, 126.4, 116.9, 75.5, 64.5; IR (neat) ν =3044, 2929, 1894, 1737, 1669, 1554, 1475, 1443, 1362, 1326, 1251, 1125, 1039, 924, 836, 739, 717, 696, 681; MS-(EI) m/z (%): 464 (100), 354 (17), 337 (21), 314 (27), 286 (81), 270 (35), 252 (10), 241 (24), 186 (28), 181 (90), 165 (19), 152 (25), 77 (11), 41 (57); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{30}H_{24}O_3SNa$, 487.1338; found 487.1338.

Allyl 2-(diphenylsulfuranylidene)-3-(naphtalen-1-yl)-3-oxopropanoate



Yellowish foam, R_f = 0.39 (*n*-pentane : EtOAc 1:1). ^{1}H (500 MHz, $CDCl_3$) δ = 7.92 (d, *J* = 7.8 Hz, 1H), 7.82 – 7.37 (m, 6H), 7.58 – 7.50 (m, 7H), 7.43 – 7.36 (m, 4H), 5.21 (s, br, 1H), 4.79 (d, br, *J* = 10.5 Hz, 1H), 4.72 (d, br, *J* = 14.8 Hz, 1H), 4.17 (s, br, 1H) ; ^{13}C (100 MHz, $CDCl_3$) δ = 189.4, 165.6, 141.8, 133.6, 132.5, 131.7, 130.6, 129.8, 129.8, 128.3, 128.2, 126.1, 125.6, 125.3, 125.0, 123.6, 116.8, 78.7, 64.5; IR (neat): ν = 3058, 2932, 1680, 1644, 1558, 1474, 1442, 1359, 1313, 1269, 1209, 1150, 1099, 1051, 998, 924, 779, 741, 682; MS-(EI) m/z (%): 438 (15), 194(13), 186(100), 155 (17), 127 (20); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{28}H_{22}O_3SNa$, 461.1181 ; found 461.1183 .

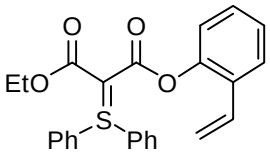
Allyl -(diphenylsulfuranylidene)-3-(furan-2-yl)-3-oxopropanoate



Colourless solid, R_f = 0.23 (*iso*-hexane/ethyl acetate = 1/1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 – 7.65, (m, 4H), 7.5 – 7-41 (m, 7H), 7.08 (dd, *J* = 3.5 Hz, *J* = 0.7 Hz, 1H), 6.40 (dd, *J* = 3.5 Hz, *J* = 1.7 Hz, 1H), 5.82 – 5.70 (m, 1H), 5.15 – 5.04 (m, 2H), 4.52 (dt, *J* = 5.5 Hz, *J* = 1.4

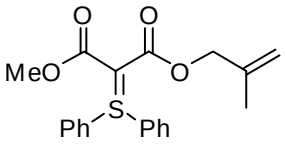
Hz, 2H); ^{13}C NMR(125 MHz, $CDCl_3$) δ 175.9, 165.5, 153.5, 143.3, 132.9, 131.3, 129.7, 129.6, 129.5, 116.9, 114.6, 110.9, 74.38, 64.4; IR (neat) ν 3062, 2933, 1659, 1644, 1571, 1553, 1473, 1443, 1387, 1319, 1266, 1178, 1050, 998, 927, 884, 814, 742, 684; MS-(EI) m/z (%): 378 (3), 186 (100), 95 (36) 41 (10); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{18}O_4SNa$, 401.0818; found 401.0819.

Ethyl 2-(diphenylsulfuranylidene)-2-vinylphenyl malonate



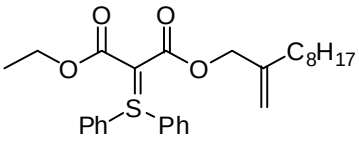
Colorless oil, R_f = 0.36 (*n*-pentane/ethyl acetate = 2/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60-7.58 (m, 4H), 7.45-7.38 (m, 6H), 7.11-7.08 (m, 1H), 7.02 (t, *J* = 7.3 Hz, 1H), 6.90 (d, *J* = 7.9 Hz, 1H), 6.69 (dd, *J* = 17.7 Hz, *J* = 11.1 Hz, 1H), 5.61 (dd, *J* = 17.7 Hz, *J* = 0.9 Hz, 1H), 5.18 (s, 1H), 5.08 (dd, *J* = 11.1 Hz, *J* = 0.9 Hz, 1H), 4.10 (q, *J* = 7.1 Hz, 2H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.1, 164.0, 148.7, 131.4, 131.1, 130.5, 130.3, 129.5, 129.3, 128.1, 125.7, 125.0, 123.3, 115.0, 60.6, 59.8, 14.4.

Methyl 2-(diphenylsulfuranylidene)-2-methylallyl malonate



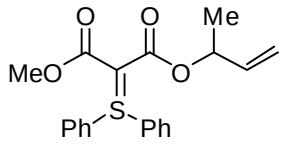
Colorless oil, R_f = 0.37 (*iso*-hexane/ethyl acetate = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55-7.53 (m, 4H), 7.45-7.37 (m, 6H), 4.92 (s, 1H), 4.77 (s, 1H), 4.42 (s, 2H), 3.59 (s, 3H), 1.62 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.6, 165.5, 140.8, 131.2, 130.2, 129.3, 129.2, 111.5, 66.7, 60.0, 50.9, 19.4; IR (neat) ν 1681, 1639, 1223, 1065, 738; EIMS *m/z* (%): 356 (1), 325 (2), 285 (10), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{20}O_4SNa$, 379.0975; found 379.0973.

Ethyl 2-(diphenylsulfuranylidene)-(2-methylenedecyl) malonate



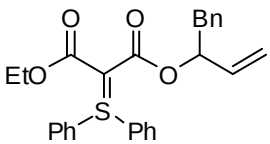
Colourless oil (316 mg, 0.67 mmol. 67%) R_f = 028 (*n*-pentane/ethyl acetate 1/1). ^{1}H (300 MHz, $CDCl_3$) δ = 7.58 – 7.51 (m, 4H), 7.47 – 7.35 (m, 6H), 5.00 (s, 1H), 4.78 (s, 1H), 4.46 (s, 2H), 4.04 (q, *J* = 7.1 Hz, 2H), 1.98 – 1.89 (m, 2H), 1.41, - 1.29 (m, 2H), 1.25 – 1.09 (m, 13H), 0.80 (t, *J* = 6.7 Hz, 3H); ^{13}C (75 MHz, $CDCl_3$) δ = 166.2, 165.9, 144.9, 131.2, 130.5, 129.4, 129.3, 110.6, 66.0, 59.6, 33.3, 31.8, 29.4, 29.4, 29.2, 27.5, 22.6, 14.6, 14.1; IR (neat): ν = 3064, 2925, 2854, 1720, 1687, 1630, 1475, 1443, 1387, 1365, 1275, 1221, 1179, 1065, 1023, 999, 901, 768, 742, 684; MS-(EI) m/z (%): 468(1), 186(100), 55(10); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C28H_{36}O_4SNa$, 491.2226; found 491.2228.

But-3-en-2-yl 2-(diphenylsulfuranylidene) methyl malonate



Colorless oil, R_f = 0.18 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54-7.52 (m, 4H), 7.46-7.39 (m, 6H), 5.70-5.64 (m, 1H), 5.32-5.27 (m, 1H), 5.11 (d, *J* = 17.1 Hz, 1H), 4.94 (d, *J* = 10.6 Hz, 1H), 3.61 (s, 3H), 1.12 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 165.0, 138.6, 131.22, 131.19, 130.5, 130.4, 129.40, 129.38, 129.3, 129.2, 114.7, 69.8, 60.0, 51.1, 20.1; IR (neat) ν 1717, 1683, 1628, 1294, 1051, 741; EIMS *m/z* (%): 356 (3), 325 (4), 285 (19), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{20}O_4SNa$, 379.0975; found 379.0973.

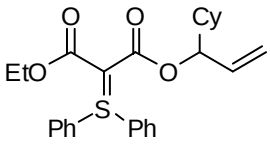
Ethyl 1-phenylbut-3-en-2-yl 2-(diphenylsulfuranylidene) malonate



Colorless oil, R_f = 0.33 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.49 (m, 2H), 7.43-7.34 (m, 8H),

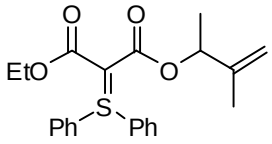
7.12-7.06 (m, 6H), 5.72-5.65 (m, 1H), 5.48 (q, *J* = 6.4 Hz, 1H), 5.13-5.5.09 (m, 1H), 4.98-4.95 (m, 1H), 4.03 (q, *J* = 7.1 Hz, 2H), 2.89 (dd, *J* = 13.7 Hz, *J* = 7.1 Hz, 1H), 2.74 (dd, *J* = 13.7 Hz, *J* = 6.5 Hz, 1H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.2, 165.0, 137.5, 136.7, 131.2, 131.0, 130.44, 130.39, 129.6, 129.30, 129.27, 129.16, 129.1, 127.9, 126.0, 115.8, 73.8, 59.8, 59.5, 41.0, 14.5; IR (neat) ν 1683, 1627, 1276, 1049, 742; EIMS *m/z* (%): 446 (1), 401 (2), 299 (20), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{26}O_4SNa$, 469.1444; found 469.1443.

1-Cyclohexylallyl ethyl-2-(diphenylsulfuranylidene) malonate



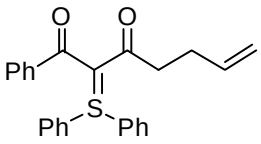
Colorless oil, R_f = 0.34 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65-7.61 (m, 4H), 7.55-7.44 (m, 6H), 5.78-5.67 (m, 1H), 5.23-5.07 (m, 3H), 4.17-4.09 (m, 2H), 1.70-1.48 (m, 6H), 1.27-0.98 (m, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 165.5, 136.1, 131.14, 131.09, 130.7, 129.4, 129.3, 129.2, 116.3, 77.7, 60.3, 59.6, 41.8, 28.6, 28.4, 26.4, 26.1, 14.5; IR (neat) ν 1685, 1628, 1274, 1063, 742.

Ethyl 3-methylbut-3-en-2-yl2-(diphenylsulfuranylidene) malonate



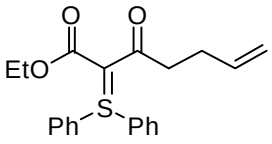
Colorless oil, R_f = 0.26 (*iso*- hexane/ethyl acetate = 2/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55-7.52 (m, 4H), 7.45-7.37 (m, 6H), 5.24 (q, *J* = 6.5 Hz, 1H), 4.88 (s, 1H), 4.69 (s, 1H), 4.06-4.01 (m, 2H), 1.61 (s, 3H), 1.17 (d, *J* = 6.5 Hz, 3H), 1.13 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.4, 165.4, 145.6, 131.2, 131.1, 130.6, 130.5, 129.33, 129.28, 129.2, 128.3, 110.6, 72.4, 60.4, 59.6, 19.4, 18.6, 14.5; IR (neat) ν 1683, 1628, 1274, 1056, 743; EIMS *m/z* (%): 384 (1), 339 (1), 299 (6), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{24}O_4SNa$, 407.1288; found 407.1286.

1-Phenyl-2-(diphenylsulfuranylidene)hept-6-ene-1,3-dione



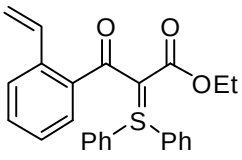
Colorless oil, R_f = 0.50 (*iso*-hexane/ethyl acetate = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53-7.52 (m, 4H), 7.45-7.27 (m, 11H), 5.69-5.61 (m, 1H), 4.84-4.76 (m, 2H), 2.68 (t, *J* = 7.6 Hz, 2H), 2.21 (q, *J* = 7.1 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.8, 189.9, 143.0, 138.2, 131.4, 129.8, 129.6, 129.51, 129.47, 128.2, 127.3, 114.3, 90.1, 40.8, 29.5; IR (neat) ν 1605, 1585, 1567, 1322; EIMS *m/z* (%): 386 (1), 331 (5), 186 (100), 105 (35); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{22}O_2SNa$, 409.1233; found 409.1230.

Ethyl 2-(diphenylsulfuranylidene)-3-oxohept-6-enoate



Colorless oil, R_f = 0.43 (*iso*-hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51-7.50 (m, 4H), 7.43-7.35 (m, 6H), 5.82-5.74 (m, 1H), 4.95-4.82 (m, 2H), 4.02 (q, *J* = 7.1 Hz, 2H), 2.94-2.91 (m, 2H), 2.31-2.27 (m, 2H), 1.09 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.8, 166.2, 138.6, 131.1, 129.9, 129.3, 124.7, 114.1, 75.6, 59.3, 39.9, 29.8, 14.4; IR (neat) ν 1660, 1596, 1050, 740; EIMS *m/z* (%): 354 (2), 309 (3), 299 (8), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{22}O_3SNa$, 377.1182; found 377.1181.

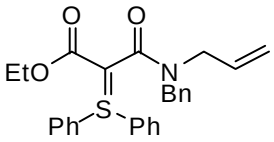
Ethyl 2-(diphenylsulfuranylidene)-3-oxo-3-(2-vinylphenyl)propanoate



Colorless oil, R_f = 0.28 (pentane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.3 Hz, 4H), 7.44-7.38 (m, 7H), 7.18-7.09 (m, 3H), 6.71 (dd, *J* = 17.5 Hz, *J* = 11.0 Hz, 1H), 5.53 (d, *J* = 17.4 Hz, 1H), 5.05 (d, *J* = 11.1 Hz, 1H), 3.72 (d, *J* = 6.3 Hz, 2H), 0.66 (bs, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) one carbon overlapped δ 189.3, 165.5, 142.9, 134.5, 134.0, 131.3, 129.5, 129.4, 127.6, 126.8, 126.0, 124.5, 114.5, 78.3, 59.2, 13.5; IR (neat) ν 1679,

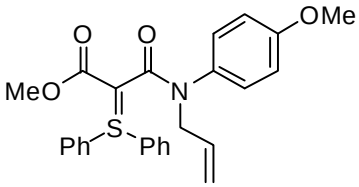
1654, 1561, 1273, 1061, 743; EIMS *m/z* (%): 402 (1), 357 (1), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{22}O_3SNa$, 425.1182; found 425.1181.

Ethyl 3-(allyl(benzyl)amino)-2-(diphenylsulfuranylidene)-3-oxopropanoate



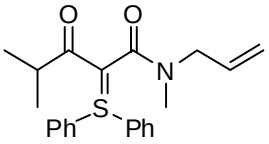
Colorless oil, R_f = 0.27 (pentane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64-7.57 (m, 4H), 7.45-7.36 (m, 6H), 7.14-7.08 (m, 3H), 6.95 (d, *J* = 6.4 Hz, 2H), 5.69-5.61 (m, 1H), 5.00-4.94 (m, 2H), 4.54 (s, 2H), 3.99 (q, *J* = 7.1 Hz, 2H), 3.85 (d, *J* = 5.5 Hz, 2H), 1.04 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) ylide cabon missing δ 168.7, 165.5, 138.2, 134.6, 131.6, 130.9, 129.6, 129.3, 128.3, 128.2, 127.6, 126.6, 116.8, 59.5, 59.0, 14.7; IR (neat) ν 1642, 1589, 1575, 1063, 684; EIMS *m/z* (%): 444 (1), 400 (1), 299 (3), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{27}NO_3SNa$, 468.1604; found 468.1606.

Methyl 3-(allyl(4-methoxyphenyl)amino)- 2-(diphenylsulfuranylidene)-3-oxopropanoate



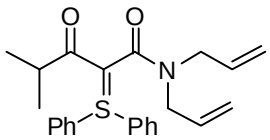
Colorless oil, R_f = 0.30 (*iso*-Hexane/ethyl acetate = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.4 Hz, 4H), 7.42-7.35 (m, 6H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.63 (d, *J* = 8.7 Hz, 2H), 5.79-5.72 (m, 1H), 5.00-4.91 (m, 2H), 4.25 (d, *J* = 5.6 Hz, 2H), 3.67 (s, 3H), 3.20 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.5, 165.4, 156.9, 138.3, 134.5, 131.4, 130.9, 129.5, 129.2, 128.1, 116.2, 113.2, 60.2, 55.2, 53.7, 50.1; IR (neat) ν 1640, 1592, 1574, 1509, 1077, 742; EIMS *m/z* (%): 447 (3), 416 (2), 285 (100), 186 (77); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{26}H_{25}NO_4SNa$, 470.1397; found 470.1395.

_N_-Allyl-_N_,4-dimethyl 2-(diphenylsulfuranylidene)-3-oxopentanamide



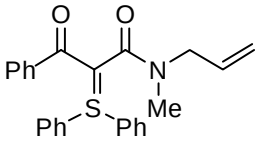
White solid. R_f = 0.16 (ethyl acetate) as a mixture of rotamers. ^{1}H (300 MHz, $CDCl_3$) δ 7.67 (d, br, J = 5.9 Hz, 4H), 7.51 – 7.40 (m, 6H), 5.47 – 5.30 (m, br, 1H), 5.05 – 4.59 (m, 2H), 3.91 and 3.80 (2s, br, 2H), 2.87 (br, 3H), 2.82 – 2.68 (m 1H), 1.17 – 1.00 (m, br, 6H); ^{13}C (75 MHz, $CDCl_3$) δ 191.8, 168.1, 133.0 131.1, 130.9, 130.6, 129.8, 129.3, 117.1, 72.9, 52.0, 35.5, 35.0, 19.8; IR (neat) ν 3078, 3061, 3018, 2981, 2956, 2926, 2865, 2295, 1979, 1737, 1646, 1569, 1474, 1442, 1421, 1385, 1303, 1385, 1268, 1224, 1124, 1088, 1021, 948, 920, 911, 820, 757, 743, 688, 660; MS-(EI) m/z (%): 367 (1), 206 (25), 186 (100), 138 (12), 110 (11), 70 (18), 43 (20); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{25}NO_2SNa$, 390.1498; found 390.1500.

***N*,*N*-diallyl-2-(diphenylsulfuranylidene)-4-methyl-3-oxopentanamide**



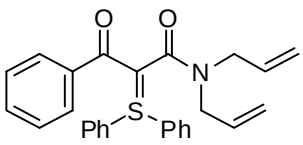
Colourless solid (247 mg, 0.63 mmol, 63%). R_f = 0.22 (*i*-Hexan/ethyl acetate 1/1) as a mixture of rotamers. ^{1}H (500 MHz, $CDCl_3$) δ = 7.74 – 7.65 (m, 4H), 7.53 – 7.41 (m, 6H), 5.28 – 5.39 (m, 2H), 5.09 – 4.72 (m, 4H), 4.00 – 3.72 (m, 4H), 3.35 – 2.87 (m, 1H), 1.17 – 1.03 (m, 6H); ^{13}C (125 MHz, $CDCl_3$) δ = 191.8, 168.1, 165.9, 133.3, 131.9, 131.1, 130.9, 130.5, 129.9, 129.6, 129.4, 129.1, 127.1, 117.6, 72.7, 71.2, 49.4, 46.6, 34.9, 33.7, 20.2, 19.8; IR (neat): ν = 3062, 2962, 2927, 2868, 2300, 1737, 1640, 1590, 1569, 1475, 1442, 1399, 1381, 1355, 1261, 1231, 1180, 1081, 1064, 1023, 998, 921, 829, 745, 687, 663; MS-(EI) m/z (%): 393(1), 232(29), 186(100), 96(11), 41(23); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{27}NO_2SNa$, 416.1654; found 416.1651.

_N_-Allyl-_N_-methyl 2-(diphenylsulfuranylidene)-3-oxo-3-phenylpropanamide



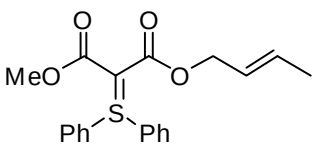
Colourless oil, R_f = 0.16 (ethyl acetate) as a mixture of rotamers. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (s, br, 4H), 7.58 (s, br, 2H), 7.51 – 7.42 (m, 6H), 7.36 – 7.27 (m, 3H). 5.20 (s, br, 1H), 4.86 (d, *J* = 10.1 Hz, 1H), 4.72 (d, *J* = 17.0 Hz. 1H), 3.59 (br, 2H), 2.44 (br, 3H); ^{13}C (125 MHz, $CDCl_3$) δ 183.7 (br), 168.2 (br), 141.8, 133.0 (br), 131.3, 130.9, 129.9, 129.6, 129.4, 127.7, 127.5, 116.7 (br), 75.2, 51.3 (br), 35.0 (br); IR (neat) ν 3083, 3055, 3019, 2981, 2921, 1586, 1540, 1474, 1440, 1426, 1393, 1363, 1349, 1265, 1243, 1122, 1065, 1020, 999, 959, 918, 909, 833, 777, 757, 744, 698, 689; MS-(EI) m/z (%): 401 (33), 331 (13), 308 (26), 292 (16), 278 (17), 223 (21), 215 (11), 194 (52), 186 (100), 165 (27), 129 (10), 105 (53), 77 (35), 51 (10), 41(35); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{23}NO_2SNa$, 424.1341; found 424.1338.

_N,N_-diallyl-2-(diphenylsulfuranylidene)-3-oxo-3-phenylpropanamide



Yellowish solid (341 mg, 0.79 mmol, 80%). R_f = 0,41 (ethyl acetate) as a mixture of roatmers. ^{1}H (500 MHz, $CDCl_3$) δ = 7.77 (d, J = 6.3 Hz, 4H, br), 7.61 (d, J = 5.9 Hz, 2H, br), 7.54 – 7.41 (m, 6H), 7.41 – 7.27 (m, 3H), 5.25 – 4.72 (m, 5H, br), 3.68 (s, 4H, br) ;^{13}C (125 MHz, $CDCl_3$) δ = 183.99 (br), 141.7, 133.4, 131.3, 129.9, 129.4, 127.8, 127.7, 117.1, 74.9, 49.3; IR (neat): ν = 3060, 2233, 1959, 1639, 1584, 1535, 1474, 1442, 1399, 1327, 1246, 1178, 1134, 1067, 1024, 998, 957, 919, 785, 728, 685, 659.

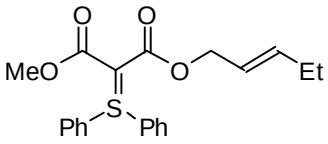
(_E_)-But-2-enyl methyl 2-(diphenylsulfuranylidene) malonate



Colorless oil,R_f = 0.37 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.4 Hz, 4H), 7.45-

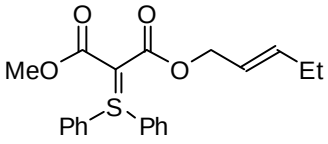
7.37 (m, 6H), 5.67-5.60 (m, 1H), 5.49-5.44 (m, 1H), 4.42 (d, *J* = 6.1 Hz, 2H), 3.59 (s, 3H), 1.58 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.6, 165.7, 131.1, 130.3, 129.4, 129.3, 129.2, 126.1, 64.2, 59.8, 50.9, 17.7; IR (neat) ν 1682, 1629, 1274, 1048, 742; EIMS *m/z* (%): 356 (0.3), 325 (2), 285 (9), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{20}O_4SNa$, 379.0974; found 379.0975.

(*E*)-methyl pent-2-enyl 2-(diphenylsulfuranylidene) malonate



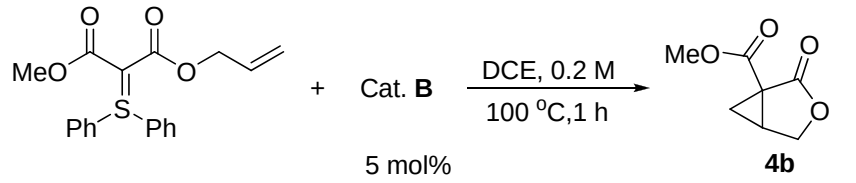
Colorless oil,R_f = 0.20 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54-7.42 (m, 4H), 7.45-7.38 (m, 6H), 5.70-5.64 (m, 1H), 5.46-5.40 (m, 1H), 4.43 (dd, *J* = 6.1 Hz, *J* = 0.9 Hz, 2H), 3.60 (s, 3H), 1.97-1.92 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.7, 165.7, 136.2, 131.2, 130.4, 129.3, 129.2, 123.8, 64.3, 59.9, 51.0, 25.2, 13.1; IR (neat) ν 1684, 1630, 1273, 1050, 742; EIMS *m/z* (%): 370 (0.2), 339 (1), 285 (9), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{22}O_4SNa$, 393.1131; found 393.1134.

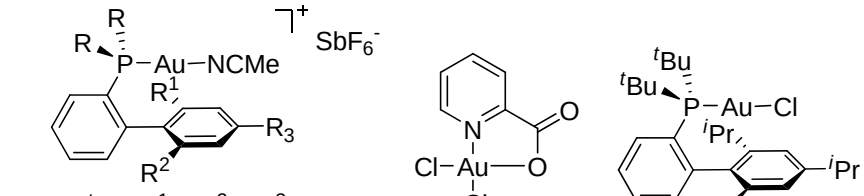
(*Z*)-methyl pent-2-enyl 2-(diphenylsulfuranylidene) malonate



Colorless oil,R_f = 0.20 (*iso*- hexane/ethyl acetate = 1/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54-7.51 (m, 4H), 7.45-7.37 (m, 6H), 5.46-5.42 (m, 1H), 5.38-5.33 (m, 1H), 4.53 (d, *J* = 6.7 Hz, 2H), 3.59 (s, 3H), 2.01-1.96 (m, 2H), 0.85 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.7, 165.7, 135.5, 131.2, 130.3, 129.3, 129.2, 123.9, 59.8, 59.4, 51.0, 20.7, 14.0; EIMS *m/z* (%): 370 (0.2), 339 (1), 285 (8), 186 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{22}O_4SNa$, 393.1131; found 393.1133.

1.2 Optimization of the gold-catalyzed cyclopropanation



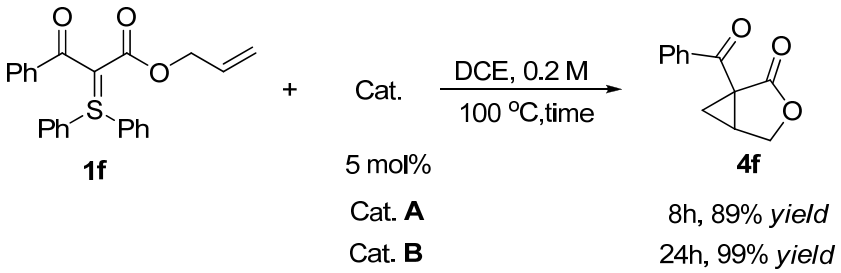


As illustrated in Table S1, the structure of the gold pre-catalyst employed played a crucial role. Compared to the catalysts bearing bulky electron-rich ligand (entries 1 and 5), a gold complex of triphenylphosphine led to lower conversions (entry 2). The strong σ-donation provided by an NHC ligand also resulted in lower catalytic activity (entry 3), and the use of PicAu(III) dichloride afforded only sluggish conversion under similar conditions (entry 4). Control experiments revealed that the use of either gold(I) chloride complex **E** or $AgSbF_6$ alone was ineffective for this cyclopropanation reaction (entries 5 and 6).

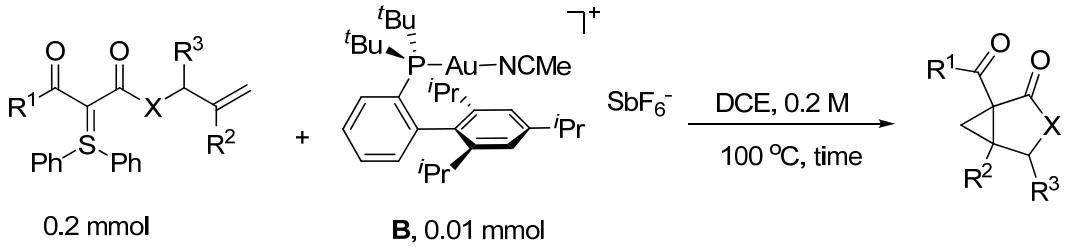
Entry	Conditions	Conversion (%)[a]
1	as described	99 (91)
2	$Ph_3PAuCl/AgSbF_6$ instead of **B**	56
3	**C** instead of **B**	56
4	**D** instead of **B**	17
5	**A** instead of **B**	99
6	**E** instead of **B**	-[b]
7	$AgSbF_6$ instead of **B**	3

[a] Determined by ^1H NMR; numbers between brackets refer to isolated yields of pure product. [b] Full recovery of ylide **5** was observed.

In contrast to the ylides derived from malonates, in the reaction of ylides derived from ketoesters catalysts and **A** and **B** showed different activities. Employing ligand **A**, the reaction was complete in 8 hours and cyclopropane **4f** was isolated in 89% yield. When ligand **B** is considered, a longer reaction time was required but cyclopropane **4f** was isolated in quantitative yield.

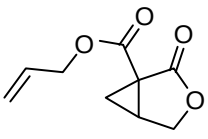


1.3 Gold (I) catalyzed cyclopropanation of sulfonium ylides



Take the procedure of preparation of 4a as typical procedure: A dry Schlenk tube was charged with sulfonium ylide (0.2 mmol, 73.6 mg) and catalyst **B** (0.01 mmol, 9.0 mg). The tube was evacuated and back filled with argon, and this was repeated three times. The mixture was dissolved by dry dichloroethane (1 mL, 0.2 M). The tube was placed on a preheated bath (100 ^{o}C), and stirred for 1h. The mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The residue was purified by column chromatography on silica gel, pentane/ethyl acetate from 2/1 to 1/1, providing **4a** as colorless oil, 35.0 mg, 96% yield.

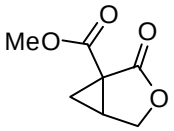
Allyl 2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4a) [2]



Compound **4a** was obtained as colorless oil, 35.0 mg, in 96% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.91-5.83 (m, 1H), 5.33 (dd, *J* = 17.2 Hz, *J* = 1.3 Hz, 1H), 5.21 (dd, *J* = 10.3 Hz, *J* = 0.6 Hz, 1H), 4.63 (d, *J* = 5.7 Hz, 2H), 4.31 (q, *J* = 4.7 Hz, 1H), 4.13 (d, *J* = 9.5 Hz, 1H), 2.72-2.68 (m, 1H), 2.03 (dd, *J* = 8.1 Hz, *J* = 4.8 Hz, 1H), 1.34 (t, *J* = 5.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 166.4, 131.2, 119.0, 67.0, 66.4, 29.3, 28.0, 20.8.

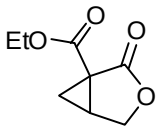
[2] a) Kitaori, K.; Mikami, M.; Furukawa, Y.; Yoshimoto, H.; Otera, J. *Synlett* **1998**, 499-500. b) Oumar-Mahamat, H.; Moustrou, C.; Surzur, J.-M.; Bertrand, M. P. *J. Org. Chem.* **1989**, *54*, 5684-5688.

Methyl 2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4b) [2a]



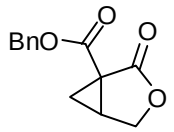
Compound **4b** was obtained as colorless oil, 28.5 mg, in 86% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.31 (q, *J* = 4.8 Hz, 1H), 4.13 (d, *J* = 9.5 Hz, 1H), 3.75 (s, 3H), 2.71-2.68 (m, 1H), 2.03 (dd, *J* = 8.0 Hz, *J* = 4.7 Hz, 1H), 1.34 (t, *J* = 5.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.5, 167.2, 67.0, 52.9, 29.2, 28.0, 20.9.

Ethyl 2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4c) [2a]



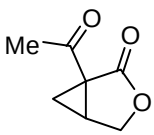
Compound **4c** was obtained as colorless oil, 33.4 mg, in 98% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.30 (q, *J* = 4.7 Hz, 1H), 4.23-4.16 (m, 2H), 4.13 (d, *J* = 9.5 Hz, 1H), 2.70-2.66 (m, 1H), 2.02 (dd, *J* = 8.1 Hz, *J* = 4.8 Hz, 1H), 1.32 (t, *J* = 5.2 Hz, 1H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.5, 166.6, 66.9, 61.9, 29.3, 27.9, 20.7, 14.0.

Benzyl 2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4d) [2a]



Compound **4d** was obtained as white solid, 41.0 mg, in 88% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.35 (m, 5H), 5.28-5.22 (m, 2H), 4.36 (t, *J* = 4.9 Hz, 1H), 4.19 (d, *J* = 9.2 Hz, 1H), 2.77 (d, *J* = 4.0 Hz, 1H), 2.11 (t, *J* = 4.0 Hz, 1H), 1.42 (d, *J* = 3.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 166.5, 135.1, 128.6, 128.3, 128.0, 67.3, 66.9, 29.3, 28.0, 20.8.

1-Acetyl-3-oxabicyclo[3.1.0]hexan-2-one (4e) [3]

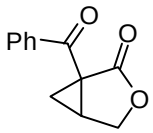


Compound **4e** was obtained as a white solid, 20.0 mg, in 71% yield, and 15.0 mg sulfonium ylide was recovered. ^{1}H NMR (500 MHz, $CDCl_3$) δ

[3] a) Tong, X.; Beller, M.; Tse, M. K. *J. Am. Chem. Soc.* **2007**, *129*, 4906-4907. b) Welbes, L. L.; Lyons, T. W.; K. A. Cychosz, K. A.; Sanford, M. S. *J. Am. Chem. Soc.* **2007**, *129*, 5836-5837. c) Tsujihara, T.; Takenaka, K.; Onitsuka, K.; Hatanaka, M.; Sasai, H. *J. Am. Chem. Soc.* **2009**, *131*, 3452-3453.

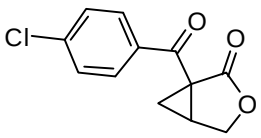
4.28 (q, *J* = 4.8 Hz, 1H), 4.13 (d, *J* = 9.5 Hz, 1H), 2.76-2.72 (m, 1H), 2.52 (s, 3H), 2.00 (dd, *J* = 8.0 Hz, *J* = 4.1 Hz, 1H), 1.36 (dd, *J* = 5.5 Hz, *J* = 4.3 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.5, 172.8, 67.2, 36.5, 29.8, 29.3, 24.2.

1-Benzoyl-3-oxabicyclo[3.1.0]hexan-2-one (4f) [5]



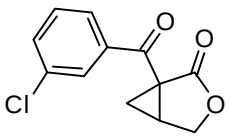
Compound **4f** was obtained as a white solid, 42.0 mg, in 99% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.4 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 2H), 4.51 (q, *J* = 4.8 Hz, 1H), 4.29 (d, *J* = 9.7 Hz, 1H), 2.79-2.75 (m, 1H), 2.06 (dd, *J* = 7.9 Hz, *J* = 4.8 Hz, 1H), 1.38 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.1, 172.7, 135.5, 133.7, 129.2, 128.5, 67.9, 35.8, 27.1, 19.2.

1-(4-Chlorobenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4g)



Compound **4g** was obtained as a white solid, 36.0 mg, in 76% yield. R_f = 0.32 (pentane/ethyl acetate = 2/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78-7.75 (m, 2H), 7.39-7.36 (m, 2H), 4.47 (dd, *J* = 9.7 Hz, *J* = 4.8 Hz, 1H), 2.79 (dt, *J* = 8.0 Hz, *J* = 4.9 Hz, 1H), 2.00 (dt, *J* = 8.0 Hz, *J* = 4.8 Hz, 1H), 1.40 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.9, 172.4, 140.1, 133.8, 130.6, 128.8, 67.9, 35.8, 26.8, 19.8; IR (neat) ν 1760, 1675, 1088, 993; EIMS *m/z* (%): 236 (39), 178 (11), 139 (100); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{12}H_9O_3ClNa$, 259.0132; found 259.0132.

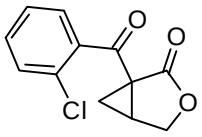
1-(3-Chlorobenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4h)



Compound **4h** was obtained as white solid, 38.5 mg, in 81% yield. R_f = 0.50 (pentane/ethyl acetate = 3/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (t, *J* = 1.9 Hz, 1H), 7.68 (dt, *J* = 7.8 Hz, *J* = 1.3 Hz, 1H), 7.49

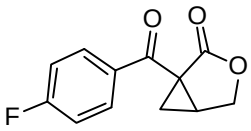
(ddd, *J* = 8.0 Hz, *J* = 2.1 Hz, *J* = 1.0 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H), 4.49 (dd, *J* = 9.7 Hz, *J* = 4.8 Hz, 1H), 4.27 (d, *J* = 9.7 Hz, 1H), 2.81 (dt, *J* = 8.0 Hz, *J* = 4.8 Hz, 1H), 2.02 (dt, *J* = 8.0 Hz, *J* = 4.8 Hz, 1H), 1.42 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.1, 172.3, 137.1, 134.8, 133.5, 129.7, 129.0, 127.3, 67.9, 35.8, 27.1, 19.8; IR (neat) ν 1760, 1675, 1089, 995, 729; EIMS *m/z* (%): 236 (31), 178 (10), 139 (100), 111 (44); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{12}H_9O_3ClNa$, 259.0132; found 259.0133.

1-(2-Chlorobenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4i)



The reaction was run in toluene (1.0M). Compound **4i** was obtained as yellow solid, 36.0 mg, in 76% yield. R_f = 0.27 (pentane/ethyl acetate = 2/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42-7.36 (m, 4H), 4.48 (dd, *J* = 9.5 Hz, *J* = 4.6 Hz, 1H), 4.29 (d, *J* = 9.5 Hz, *J* = 4.0 Hz, 1H), 2.97 (dt, *J* = 8.0 Hz, *J* = 5.2 Hz, 1H), 2.46 (dt, *J* = 8.0 Hz, *J* = 4.2 Hz, 1H), 1.55 (dd, *J* = 5.6 Hz, *J* = 4.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.4, 172.1, 138.0, 132.2, 130.3, 129.7, 129.4, 127.2, 67.5, 37.6, 32.5, 22.3; IR (neat) ν 1768, 1676, 1073, 996, 734; EIMS *m/z* (%): 201 (100), 139 (47), 111 (27); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{12}H_9O_3ClNa$, 259.0132; found 259.0132.

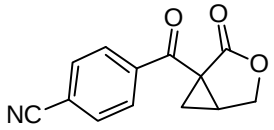
1-(4-Fluorobenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4j)



The reaction was run in toluene (0.2M). Compound **4j** was obtained as colourless solid, 43.7 mg, in 99% yield, R_f = 0.36 (n-pentane/ethyl acetate = 1/1) ^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.05 – 7.92 (m, 2H), 7.22 – 7.12 (m, 2H), 4.57 (dd, *J* = 9.6, 4.6 Hz, 1H), 4.36 (d, *J* = 9.6 Hz, 1H), 2.92 – 2.84 (m, 1H), 2.08 (dd, *J* = 7.9, 4.7 Hz, 1H), 1.49 (t, *J* = 5.0 Hz, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ = 190.4, 172.5, 166.0 (d, J_{C-F} 257.0 Hz), 132.0 (d, J_{C-F} 9.5 Hz), 131.9

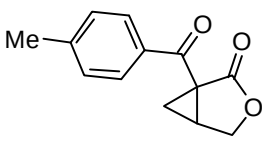
(d, $J_{C\text{-}F}$ 3.17 Hz), 115.7 (d, $J_{C\text{-}F}$ 22.1 Hz), 67.9, 35.77, 26.6, 19.7; IR (neat): ν = 3513, 3078, 2976, 2912, 2371, 2326, 2299, 2000, 1961, 1763, 1671, 1597, 1506, 1443, 1409, 1379, 1294, 1266, 1229, 1156, 1112, 1089, 1046, 995, 966, 902, 877, 845, 803, 767, 746, 705, 653; MS-(EI) m/z (%): 220(20), 123(100), 95(34); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{12}H_9FO_3Na$, 243.0427; found 243.0424.

1-(4-Cyanobenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4k)



The reaction was run in toluene (0.2M). Compound **4k** was obtained as yellow solid, 43 mg, in 95% yield, R_f = 0.32 (n-pentane/ethyl acetate = 1/1) ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.99 (d, *J* = 8.7 Hz, 2h); 7.79 (d, *J* = 8.7 Hz, 2H), 4.57 (dd, *J* = 9.7, 4.8 Hz, 1H), 4.37 (d, *J* = 9.6 Hz, 1H), 3.02 – 2.94 (m, 1H), 2.15 (dd, *J* = 8.1, 4.8 Hz, 1H), 1.58 (t, *J* = 5.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 191.6, 171.9, 138.8, 132.2, 129.6, 117.8, 116.7, 67.8, 36.0, 27.4, 20.9; IR (neat): ν = 3094, 2974, 2912, 2231, 1762, 1679, 1606, 1477, 1443, 1405, 1379, 1365, 1311, 1288, 1267, 1210, 1175, 1113, 1092, 1048, 994, 968, 994, 909, 875, 845, 824, 767, 731, 706, 686; MS-(EI) m/z (%): 227(26), 169(12), 130(100), 102(44); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{13}H_9NO_3Na$, 250.0474; found 250.0472.

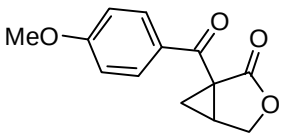
1-(4-Methylbenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4l)



Compound **4l** was obtained as a white solid, 38.0 mg, in 87% yield. R_f = 0.53 (pentane/ethyl acetate = 2/1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 8.2 Hz, 2H), 4.48 (dd, *J* = 9.6 Hz, *J* = 4.7 Hz, 1H), 4.25 (d, *J* = 9.6 Hz, 1H), 2.72 (dt, *J* = 8.1 Hz, *J* = 4.8 Hz, 1H), 2.34 (s, 3H), 2.01 (dd, *J* = 8.0 Hz, *J* = 4.8 Hz, 1H), 1.33 (t, *J* = 5.0 Hz, 1H); ^{13}C

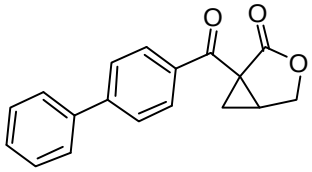
NMR (125 MHz, $CDCl_3$) δ 191.4, 172.9, 144.7, 132.9, 129.3, 129.2, 67.9, 35.7, 26.8, 21.7, 18.9; IR (neat) ν 1761, 1672, 1091, 994; EIMS *m/z* (%): 216 (29), 119 (100), 91 (32); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{13}H_{12}O_3Na$, 239.0679; found 239.0678.

1-(4-Methoxybenzoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4m)



Compound **4m** was obtained as a white solid, 40.0 mg, in 86% yield. R_f = 0.43 (pentane/ethyl acetate = 1/1); ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.9 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 4.47 (dd, *J* = 9.6 Hz, *J* = 4.7 Hz, 1H), 4.25 (d, *J* = 9.6 Hz, 1H), 3.79 (s, 3H), 2.71 (dt, *J* = 8.0 Hz, *J* = 4.8 Hz, 1H), 1.96 (dd, *J* = 7.9 Hz, *J* = 4.8 Hz, 1H), 1.33 (t, *J* = 4.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.9, 173.0, 164.0, 131.7, 128.3, 113.7, 68.0, 55.5, 35.5, 26.2, 18.9; IR (neat) ν 1760, 1663, 1597, 1255, 1091, 843; EIMS *m/z* (%): 216 (29), 119 (100), 91 (32); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{13}H_{12}O_4Na$, 255.0628; found 255.0628.

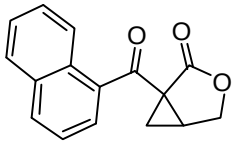
1-([1,1'-Biphenyl]-4-carbonyl)-3-oxabicyclo[3.1.0]hexan-2-one (4n)



The reaction was run in toluene (0.2M). Compound **4n** was obtained as colorless solid, 55.0 mg, in 99% yield, R_f = 0.44 (*n*-pentane/ethyl acetate 1/1) ^1H (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.63 (d, *J* = 7.0 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 2H), 7.41 (t, *J* = 7.0 Hz, 1H), 4.61 (dd, *J* = 9.4 Hz, *J* = 4.7 Hz, 1H), 4.38 (d, *J* = 9.7 Hz, 1H), 2.88 – 2.85 (m, 1H), 2.16 – 2.13 (m, 1H), 1.48 (t, *J* = 4.9 Hz, 1H); ^{13}C (125 MHz, $CDCl_3$) δ 191.5, 172.8, 146.5, 139.8, 134.2, 129.9, 128.9, 128.4, 127.3, 127.2, 68.0, 35.9, 26.9, 19.3; IR (neat) ν 3059, 2983, 2917, 1760, 1669, 1602, 1559, 1486, 1448, 1404, 1383, 1313, 1290, 1266, 1220, 1182, 1109, 1100, 998, 963, 899, 842, 775, 737, 695; MS-

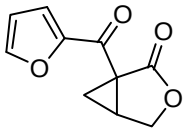
(EI) m/z (%): 278 (85), 181 (100), 152 (32); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{14}O_3Na$, 301.0835; found 301.0834.

1-(1-Naphthoyl)-3-oxabicyclo[3.1.0]hexan-2-one (4o)



Compound **4o** was obtained as a colourless solid, 47.0 mg, in 93% yield, R_f = 0.42 (*n*-pentane : EtOAc 1:1) ^{1}H (500 MHz, $CDCl_3$) δ = 8.35 (d, J = 8.1 Hz, 1H), 8.02 (d, J = 8.2 Hz, 1H), 7.89 (d, J = 8.1 Hz, 1H), 7.81 (d, J = 6.5 Hz, 1H), 7.60 – 7.57 (m, 1H), 7.55 – 7.51 (m, 2H), 4.58 (dd, J = 9.8, 4.7 Hz, 1H), 4.35 (d, J = 9.6 Hz, 1H), 3.04 – 2.99 (m, 1H), 2.35 (dd, J = 8.1, 4.5 Hz, 1H), 1.56 (t, J = 4.6 Hz, 1H) ; ^{13}C (100 MHz, $CDCl_3$) δ = 195.5, 172.2, 133.9, 133.1, 130.2, 128.6, 128.3, 127.9, 126.6, 125.1, 124.1, 67.4, 37.3, 29.5, 21.3; IR (neat): ν = 3060, 2964, 2909, 1767, 1671, 1508, 1376, 1295, 1255, 1209, 1113, 1094, 1046, 993, 908, 792, 781, 734; MS-(EI) m/z (%): 252(59), 155(100), 127(67); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{12}O_3Na$, 275.0678; found 275.0677.

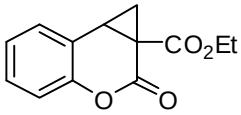
1-(Furan-2-carbonyl)-3-oxabicyclo[3.1.0]hexan-2-one (4p)



Compound **4p** was obtained as a reddish solid, 38.2 mg, in 99% yield, R_f = 0.31 (*i*-hexane/ethyl acetate = 1/1) ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 1.6 Hz, *J* = 0.6 Hz, 1H), 7.45 (dd, *J* = 3.7 Hz, *J* = 0.6 Hz, 1H), 6.58 (dd, *J* = 3.6 Hz, *J* = 16.0 Hz, 1H), 4.52 (dd, *J* = 9.5 Hz, *J* = 4.6 Hz, 1H), 4.31 (d, *J* = 9.5 Hz, 1H), 2.77 – 2.70 (m, 1H), 2.21 (dd, *J* = 7.9 Hz, *J* = 4.9 Hz, 1H), 1.36 (t, *J* = 4.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 178.8, 172.4, 151.4, 147.2, 119.9, 112.7, 68.0, 35.6, 28.1, 18.2; IR (neat) ν 3517, 3136, 2974, 2911, 1762, 1659, 1566, 1463, 1396, 1380, 1298, 1276, 1228, 1208, 1157, 1113, 1096, 1048, 1018, 998, 974, 925, 884, 874, 797, 766,

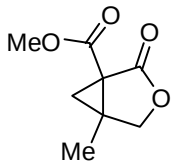
703; MS-(EI) m/z (%): 192 (41), 162 (15), 134 (20), 95 (100), 39 (26); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{10}H_8O_4Na$, 215.0314; found 215.0315.

Ethyl 2-oxo-1,1*a*,2,7*b*-tetrahydrocyclopropa[*c*]chromene-1*a*-carboxylate (4q)[4]



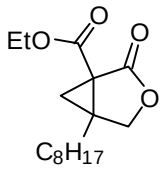
The reaction was run in 0.1 mmol scale, use toluene (0.2M) as solvent. Compound **4q** was obtained colorless oil, 16.0 mg, in 69% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 7.5, *J* = 1.0 Hz, 1H), 7.25-7.17 (m, 1H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 8.2 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 2H), 2.82 (dd, *J* = 9.0, *J* = 6.5 Hz, 1H), 2.39 (dd, *J* = 9.0, *J* = 5.0 Hz, 1H), 1.31-1.28 (m, *J* = 1H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.4, 162.4, 149.4, 128.5, 127.7, 124.6, 120.1, 117.2, 62.4, 28.9, 28.7, 21.0, 14.0.

Methyl 5-methyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4r) [5]



Compound **4r** was obtained as colorless oil, 29.5 mg, in 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.17 (d, *J* = 9.3 Hz, 1H), 4.04 (d, *J* = 9.3 Hz, 1H), 3.76 (s, 3H), 1.93 (d, *J* = 4.8 Hz, 1H), 1.39 (d, *J* = 4.8 Hz, 1H), 1.38 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.4, 166.3, 71.9, 52.8, 35.7, 34.1, 25.3, 14.0.

Ethyl 5-octyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4s)

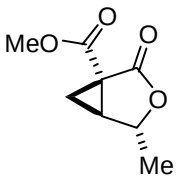


The reaction was run in 0.13mmol scale and used toluene (0.2M) as solvent, Compound **4s** was obtained as colorless oil, 36.4 mg, in 99% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.23-4.18 (m, 2H), 4.13 (s, 2H), 1.93 (d, *J* = 4.8 Hz, 1H), 1.68-1.87 (m, 2H), 1.39-1.34 (m, 2H), 1.26-1.19 (m, 14H), 0.81 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.6, 165.9, 70.7, 61.9, 39.8, 34.1, 31.7, 29.4, 29.3, 29.1, 28.7, 26.8, 24.7, 22.6, 14.1, 14.0; MS-(EI) m/z (%): 282 (1), 237 (6),

[4] Yamashita, M.; Okuyama, K.; Kawajiri, T.; Takada, A.; Inagaki, Y.; Nakano, H.; Tomiyama, M.; Ohnaka, A.; Terayama, I.; Kawasaki, I.; Ohta, S. *Tetrahedron* **2002**, *58*, 1497.
[5] Ando, W.; Imai, I.; Migita, T. *J. Org. Chem.* **1972**, *37*, 3596-3600.

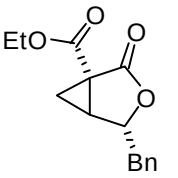
183 (4), 99 (20), 29 (100). HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{26}O_4Na$, 305.1723; found 305.1721.

Methyl 4-methyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4t) [6]



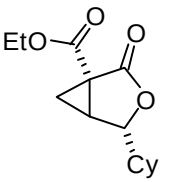
Compound **4t** was obtained as a mixture of diastereo-isomers, white solid, 30.0 mg, in 88% yield, dr >12/1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.38 (q, *J* = 6.4 Hz, 1H), 3.75 (s, 3H), 2.46 (dd, *J* = 8.0 Hz, *J* = 5.6 Hz, 1H), 1.98 (dd, *J* = 8.1 Hz, *J* = 4.7 Hz, 1H), 1.38 (d, *J* = 6.4 Hz, 3H), 1.34 (t, *J* = 5.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.9, 167.4, 75.2, 52.9, 33.9, 29.7, 22.0, 21.2.

Ethyl 4-benzyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4u)



The reaction was run in toluene (0.2M). Compound **4u** was obtained as colorless oil, 42.0 mg, in 81% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.21 (m, 5H), 4.58 (t, *J* = 5.3 Hz, 1H), 4.18-4.04 (m, 2H), 3.05 (d, *J* = 5.3 Hz, 2H), 2.54 (dd, *J* = 8.1 Hz, *J* = 5.5 Hz, 1H), 1.96 (dd, *J* = 8.1 Hz, *J* = 4.7 Hz, 1H), 1.37-1.32 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.7, 166.5, 134.1, 129.8,128.7, 127.1, 78.1, 61.8, 41.4, 31.8, 29.8, 20.7, 13.9; IR (neat) ν 1776, 1719, 1088, 1044, 726, 700; EIMS *m/z* (%): 260 (23), 215 (5), 169 (100), 91 (40); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{16}O_4Na$, 283.0941; found 283.0940.

Ethyl 4-cyclohexyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4v)

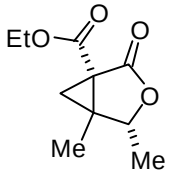


The reaction was run in toluene (0.2M). Compound **4v** was obtained as colorless oil, 34.0 mg, in 67% yield. R_f = 0.59 (pentane/ethyl acetate = 1/1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.26-4.14 (m, 2H), 4.04 (d, *J* = 5.1 Hz, 1H), 2.46 (dd, *J* = 8.2 Hz, *J* = 5.5 Hz, 1H), 1.96 (dd, *J* = 8.1 Hz, *J* = 4.7 Hz, 1H), 1.73-1.62 (m, 5H), 1.58-1.51 (m, 1H), 1.28-0.97 (m, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ

[6] Romo, D.; Romine, J. L.; Midura, W.; Meyers, A. I. *Tetradedron* **1990**, *46*, 4951.

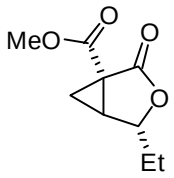
170.4, 166.8, 82.7, 61.9, 42.5, 30.5, 29.8, 27.5, 26.7, 26.0, 25.6, 25.5, 20.5, 14.1; IR (neat) ν 1775, 1723, 1191, 1088, 1042, 729; EIMS *m/z* (%): 260 (23), 215 (5), 169 (100), 91 (40); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{20}O_4Na$, 275.1254; found 275.1254.

Ethyl 4,5-dimethyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4w)



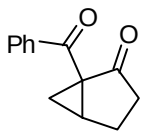
The reaction was run in toluene (0.2M). Compound **4w** was obtained as colorless oil, 30.0 mg, in 76% yield. R_f = 0.51 (iso-Hexane/ethyl acetate = 1/1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.42 (q, *J* = 6.4 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 2H), 1.84 (d, *J* = 4.7 Hz, 1H), 1.35 (d, *J* = 4.7 Hz, 1H), 1.33 (d, *J* = 6.5 Hz, 3H), 1.30 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.0, 166.0, 78.7, 61.9, 38.7, 34.7, 26.0, 19.3, 14.2, 12.3; IR (neat) ν 1773, 1722, 1037, 674; EIMS *m/z* (%): 260 (23), 215 (5), 169 (100), 91 (40); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{10}H_{14}O_4Na$, 221.0784; found 221.0784.

Methyl 4-ethyl-2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxylate (4x)



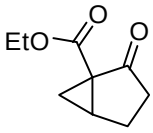
Compound **4w** was obtained as colorless oil. From (***E***)-**8b**, **4x** obtained as a mixture of isomers (dr >17:1), 35.2 mg in 96% yield, and from (***Z***)-**8b**, **4w** obtained as a mixture of isomers (dr >17:1), 32.3 mg in 87% yield, R_f = 0.49 (Pentane/ethyl acetate = 1/1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.21 (t, *J* = 6.0 Hz, 1H), 3.75 (s, 3H), 2.47 (dd, *J* = 8.1 Hz, *J* = 5.5 Hz, 1H), 1.98 (dd, *J* = 8.1 Hz, *J* = 4.8 Hz, 1H), 1.69 (p, *J* = 7.1 Hz, 1H), 1.33 (t, *J* = 5.1 Hz, 1H), 0.94 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.1, 167.3, 79.8, 52.9, 32.2, 29.6, 28.8, 20.9, 8.2; EIMS *m/z* (%): 260 (23), 215 (5), 169 (100), 91 (40); HRMS-(EI) (*m/z*): $[M]^+$ calcd for $C_9H_{12}O_4$, 184.0736; found 184.0734.

1-Benzoylbicyclo[3.1.0]hexan-2-one (6a) [7]



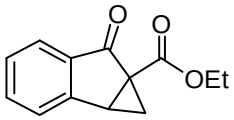
Compound **6a** was obtained pale yellow oil, 31.0 mg, in 78% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72-7.70 (m, 2H), 7.47 (tt, *J* = 3.7 Hz, *J* = 1.4 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 2H), 2.59 (dt, *J* = 8.0 Hz, *J* = 5.1 Hz, 1H), 2.37-2.27 (m, 3H), 2.12-2.08 (m, 1H), 2.00 (dd, *J* = 7.9 Hz, *J* = 5.0 Hz, 1H), 1.43 (t, *J* = 5.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 209.7, 195.1, 136.3, 133.1, 129.0, 128.3, 45.1, 33.1, 31.7, 21.6, 19.8.

Ethyl 2-oxobicyclo[3.1.0]hexane-1-carboxylate (6b) [8]



Compound **6b** was obtained colorless oil, 26.0 mg, in 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.17-4.10 (m, 2H), 2.53 (dt, *J* = 8.1 Hz, *J* = 5.3 Hz, 1H), 2.23-2.10 (m, 3H), 1.99-1.92 (m, 2H), 2.00 (dd, *J* = 7.9 Hz, *J* = 5.0 Hz, 1H), 1.32 (t, *J* = 5.2 Hz, 1H), 1.22 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.0, 168.2, 61.1, 37.6, 33.6, 32.9, 22.0, 20.8, 14.1.

Ethyl 6-Oxo-1a,6-dihydro-1*H*-cyclopropa[*a*]indene-6a-carboxylate (6c) [9]



Compound **6c** was obtained colorless oil, 37.4 mg, in 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.7 Hz, 1H), 7.43 (tt, *J* = 3.7 Hz, *J* = 1.0 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.26 (tt, *J* = 7.5 Hz, *J* = 0.8 Hz, 1H), 4.22 (qd, *J* = 7.1 Hz, *J* = 1.9 Hz, 2H), 3.29 (dd, *J* = 7.5 Hz, *J* = 4.6 Hz, 1H), 2.31 (dd, *J* = 7.5 Hz, *J* = 4.2 Hz, 1H), 1.67 (t, *J* = 4.4 Hz, 1H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.5, 168.5, 151.4, 134.10, 134.09, 127.6, 125.3, 124.4, 61.6, 39.8, 38.6, 32.1, 14.1.

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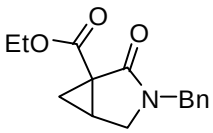
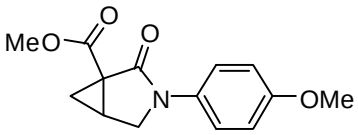
Ethyl 3-benzyl-2-oxo-3-azabicyclo[3.1.0]hexane-1-carboxylate (6d) [10]



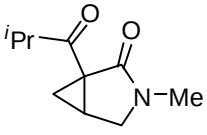
The reaction was run in 0.1 mmol scale, compound **6d** was obtained colorless oil, 20.3 mg, in 78% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26-7.19 (m, 3H), 7.12 (d, *J* = 7.6 Hz, 2H), 4.43 (d , *J* = 14.7 Hz, 1H), 4.18 (q , *J* = 7.2 Hz, 3H), 3.37 (dd, *J* = 10.5 Hz, *J* = 5.9 Hz, 1H), 3.03 (d, *J* = 10.5 Hz, 1H), 2.23 (q, *J* = 6.4 Hz, 1H), 1.84 (dd, *J* = 8.0 Hz, *J* = 4.6 Hz, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 0.98 (t, *J* = 4.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.2, 168.7, 136.3, 128.7, 128.2, 127.7, 61.5, 46.43, 46.37, 31.6, 22.7, 20.7, 14.2.

Methyl 3-(4-methoxyphenyl)-2-oxo-3-azabicyclo[3.1.0]hexane-1-carboxylate (**6e)**



Compound **6e** was obtained as a white solid, 42.0 mg, in 80% yield. R_f = 0.45 (*iso*-hexane/ethyl acetate = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37-7.34 (m, 2H), 6.82-6.79 (m, 2H), 3.95 (dd, *J* = 10.3 Hz, *J* = 5.9 Hz, 1H), 3.74 (s, 3H), 3.71 (s, 3H), 3.61 (d, *J* = 10.3 Hz, 1H), 2.39 (dt, *J* = 7.9 Hz, *J* = 5.6 Hz, 1H), 1.95 (dd, *J* = 8.3 Hz, *J* = 4.6 Hz, 1H), 1.22 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.0, 168.0, 156.7, 131.9, 122.0, 114.0, 55.4, 52.6, 48.8, 32.5, 22.3, 21.0; IR (neat) ν 1748, 1710, 1686, 1512, 1092, 1075, 832; EIMS *m/z* (%): 261 (100), 202 (3), 59 (5); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{15}NO_4Na$, 284.0893; found 284.0895.

1-Isobutyryl-3-methyl-3-azabicyclo[3.1.0]hexan-2-one (6f)



Compound **6f** was obtained as colorless oil, 30.0 mg, in 83% yield, R_f = 0.21 (*iso*-hexane/ethyl acetate = 1/1). ^{1}H (300 MHz, $CDCl_3$) δ 3.71 (sep, *J* = 6.7 Hz, 1H), 3.54 (dd, *J* = 10.4 Hz, *J* = 5.8 Hz, 1H), 3.22 (d, *J* = 10.0 Hz, 1H), 2.79 (s, 3H), 2.32 – 2.26 (m, 1H), 1.88 (dd, *J* = 8.0 Hz, *J* = 3.8 Hz, 1H),

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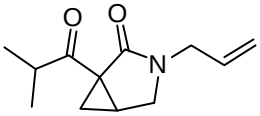
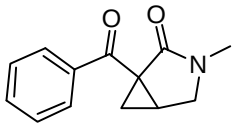
1.14 (d, *J* = 6.28 Hz, 3H), 1.07 – 1.00 (m, 4H); ^{13}C (75 MHz, $CDCl_3$) δ 209.2, 171.1, 49.2, 38.3, 37.6, 29.6, 24.5, 23.5, 18.3, 17.9; IR (neat) ν 3506, 2970, 2932, 2874, 1677, 1496, 1464, 1444, 1402, 1385, 1316, 1284, 1224, 1089, 1064, 1044, 983, 967, 881, 816, 757, 655; MS-(EI) m/z (%): 181 (100), 166 (31), 138 (61), 110 (44), 95 (20), 70 (32), 53 (29), 42 (32), 27 (22).

3-Allyl-1-isobutyryl-3-azabicyclo[3.1.0]hexan-2-one (6g)



Compound **6g** was obtained as colourless oil, 41 mg, in 99% yield, R_f = 0.51 (*n*-pentane/ethyl acetate = 1/1) ^{1}H NMR (300 MHz, $CDCl_3$) δ = 5.79 – 5.61 (m, 1H), 5.25 – 5.21 (m, 2H), 3.84 (dd, *J* = 6.2, 1.2 Hz, 2H), 3.74 (sep, *J* = 6.9 Hz, 1H), 3.53 (dd, *J* = 10.4, 5.7 Hz, 1H), 3.23 (d, *J* = 10.4 Hz, 1H), 3.27 – 3.28 (m, 1H), 1.92 (dd, *J* = 7.8, 4.0 Hz, 1H), 1.17 (d, *J* = 6.7 Hz, 3H), 1.10 – 1.05 (m, 4H) ;^{13}C NMR (75 MHz, $CDCl_3$) δ = 209.1, 170.9, 132.2, 118.3, 46.7, 45.1, 38.3, 37.7, 24.6, 23.4, 18.3, 17.8; IR (neat): ν = 3687, 3083, 2971, 2932, 2874, 1679, 1645, 1486, 1444, 1415, 1385, 1362, 1346, 1302, 1250, 1218, 1115, 1095, 1076, 1023, 986, 930, 880, 817, 759, 695; MS-(EI) m/z (%): 207(100), 192(24), 164(50), 136(10), 95(11), 53(12), 41(28); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{12}H_{17}NO_2Na$, 230.1151; found 230.1150.

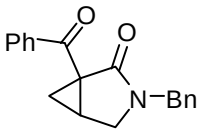
1-Benzoyl-3-methyl-3-azabicyclo[3.1.0]hexan-2-one (6h)



Compound **6h** was obtained as colourless oil, 20.0 mg, in 46% yield, R_f = 0.13 (*i*-hexane/ethyl acetate = 1/1) ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.91 – 7.84 (m, 2H), 7.55 (tt, *J* = 7.4, 2.0 Hz, 1H), 7.48 – 7.41 (m, 2H), 3.78 (dd, *J* = 10.8, 5.8 Hz, 1H), 3.41 (d, *J* = 10.9 Hz, 1H), 2.84 and 2.82 (5:1, s, 3H), 2.46 – 2.39 (m, 1H), 1.99 (dd, *J* = 7.9, 4.6 Hz, 1H), 1.14 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR

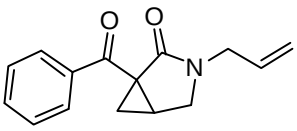
(75 MHz, $CDCl_3$) δ = 194.7, 171.5, 136.6, 133.1, 129.1, 128.3, 49.9, 38.5, 29.7, 22.1, 19.4; IR (neat): ν = 3060, 2922, 2876, 1671, 1897, 1579, 1493, 1448, 1402, 1370, 1319, 1264, 1229, 1208, 1039, 965, 902, 782, 715, 661; MS-(EI) m/z (%): 215(48), 136(14), 110(12), 105(100), 77(72), 57(26), 51(19), 42(16); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{13}H_{13}NO_2Na$, 238.0838; found 238.0839**.**

1-Benzoyl-3-benzyl-3-azabicyclo[3.1.0]hexan-2-one (6i)



Compound **6i** was obtained as colorless oil, 46.6 mg, in 80% yield, R_f = 0,36 (*iso*-hexane/ethyl acetate = 1/1) ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 – 7.83 (m, 2H), 7.56 (tt, *J* = 7.3, 1.5 Hz, 1H), 7.49 – 7.31 (m, 5H), 7.28 – 7.22 (m, 2H), 4.24 (d, *J* = 14.2 Hz,, 1H), 4.27 (d, *J* = 14.2 Hz, 1H), 3.64 (dd, *J* = 10.8 Hz, *J* = 5.7 Hz, 1H), 3.29 (d, *J* = 10.5 Hz, 1H), 2.39 – 2.33 (m, 1H), 2.01 (dd, *J* = 8.1 Hz, *J* = 4.5 Hz, 1H), 1.13 (t, *J* = 4.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.7, 171.3, 136.6, 136.4, 133.1, 129.1, 128.8, 128.4, 128.3, 127.9, 47.2, 16.6, 38.6, 22.3, 18.8; IR (neat) ν 3062, 3030, 2919, 1671, 1597, 1448, 1422, 1371, 1297, 1270, 1223, 1208, 1177, 1061, 1026, 998, 901, 781, 749, 710, 701, 664; MS-(EI) m/z (%): 291 (77), 158 (18), 118 (28), 109 (13), 105 (100), 91 (95), 77 (78), 65 (20), 51 (17).

3-Allyl-1-benzoyl-3-azabicyclo[3.1.0]hexan-2-one (6j)

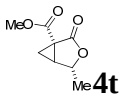


Compound **6j** was obtained as colourless solid, 47 mg, in 97% yield, R_f = 0.43 (*n*-pentane/ethyl acetate = 1/1) ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.92 – 7.89 (m, 2H), 7.57 (tt, J = 7.4, 1.7 Hz, 1H), 7.47 (t, J = 7.92 Hz, 2H), 5.77 – 5.69 (m, 1H), 5.28 – 5.21 (m, 2H), 3.93 – 3.83 (m, 2H), 3.76 (dd, J = 10.6, 5.7 Hz, 1H), 3.40 (d, J = 10.8 Hz, 1H), 2.49 – 2.43 (m, 1H), 2.03 (dd, J = 7.8, 4.4 Hz, 1H), 1.17 (t, J = 4.7 Hz, 1H);^{13}C NMR (75 MHz, $CDCl_3$) δ = 194.7, 171.2, 136.6, 133.1, 132.2,

129.1, 128.3, 118.6, 47.3, 45.2, 38.7, 22.1, 19.3; IR (neat): ν = 3062, 2917, 1669, 1597, 1579, 1485, 1448, 1415, 1371, 1321, 1271, 1210, 1175, 1118, 1060, 1024, 999, 967, 932, 901, 782, 713, 687; MS-(EI) m/z (%): 241(35), 105(100), 77(80), 68(12), 51(20), 41(28); HRMS-(ESIpos) (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{15}NO_2Na$, 264.0995; found 265.0997.

1.4 X-ray crystal structure of cyclopropane 4t

The crystal was prepared by slow diffusion of pentane to the solution of **4t** in diethyl ether, and was suitable for X-ray crystallographic analysis. CCDC 885364.



4t

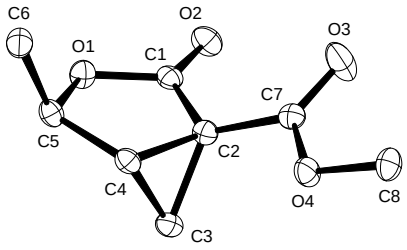


Figure S1. Solid state structure of **4t.**

Part II Computational details

All calculations were performed using the GAUSSIAN 03 software package,[1] and the PBE0 functional, without symmetry constraints. That functional uses a hybrid generalized gradient approximation (GGA), including 25 % mixture of Hartree-Fock[2] exchange with DFT[3] exchange-correlation, given by Perdew, Burke and Ernzerhof functional (PBE).[4] The optimized geometries were obtained with the relativistic Stuttgart Effective Core Potentials and associated basis set[5] augmented with a f-polarization function[6] for Au, and a standard 6-31G(d,p)[7] for the remaining elements (basis b1). Transition state optimizations were performed with the Synchronous Transit-Guided Quasi-Newton Method (STQN) developed by Schlegel *et al*,[8] following extensive searches of the Potential Energy Surface. Frequency calculations were performed to confirm the nature of the stationary points, yielding one imaginary frequency for the transition states and none for the minima. Each transition state was further confirmed by following its vibrational mode downhill on both sides and obtaining the minima presented on the energy profile. The electronic energies (E_{b1}) obtained at the PBE0/b1 level of theory were converted to free energy at 298.15 K and 1 atm (G_{b1}) by using zero point energy and thermal energy corrections based on structural and vibration frequency data calculated at the same level.

Single point energy calculations were performed using a improved basis set (basis b2) and the geometries optimized at the PBE0/b1 level. Basis b2 consisted of the same bases (b1) for Au atoms and a standard 6-311++G(d,p)[9] for the remaining elements. Solvent effects (dichloroethane) were considered in the PBE0/b2//PBE0/b1 energy calculations using the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers[10] as implemented on Gaussian 03.[11] The molecular cavity was based on the united atom topological model applied on UAHF radii, optimized for the HF/6-31G(d) level.

The free energy values presented along the text (G_{b2}^{soln}) were derived from the electronic energy values obtained at the PBE0/b2//PBE0/b1 level, including solvent effects (E_{b2}^{soln}), according to the following expression:

$$G_{b2}^{soln} = E_{b2}^{soln} + G_{b1} - E_{b1}$$

References for computational part

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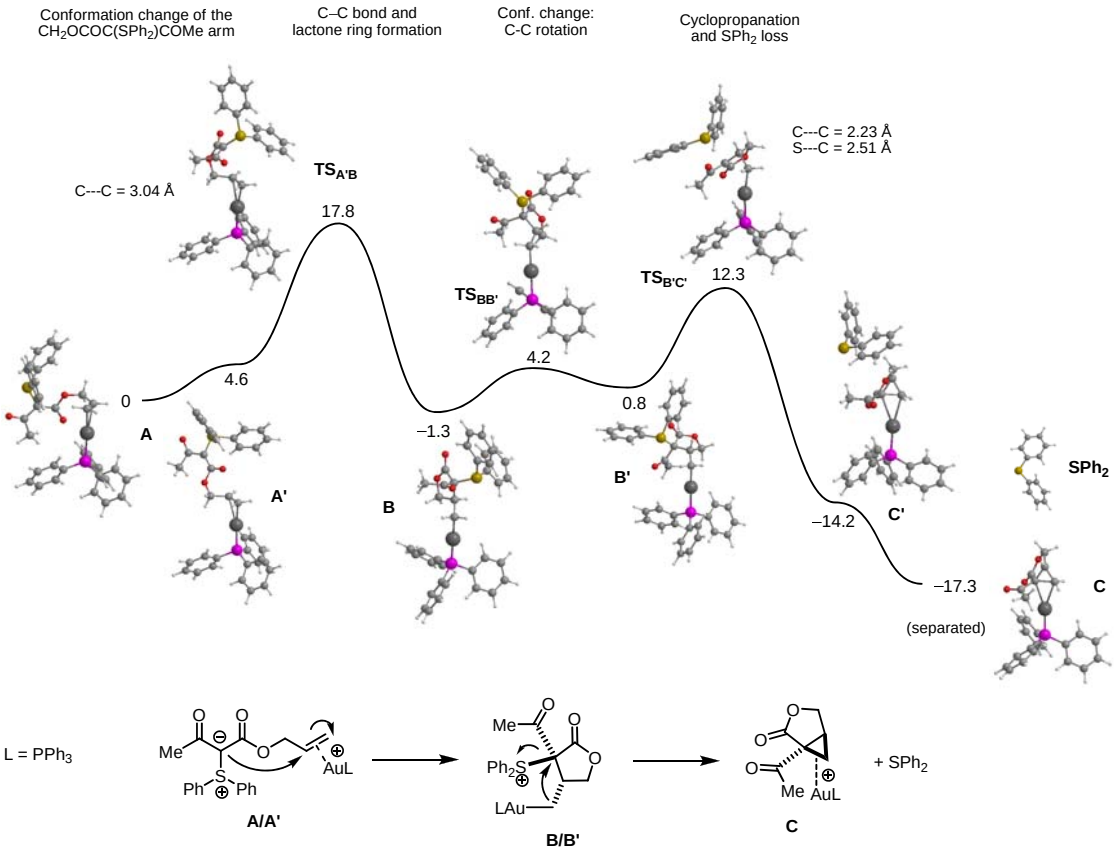

Figure S2. Free energy profile (PBE0) for the formation of lactone **4e** from sulfonium ylide **1e**. The minima and the transition states were optimised and the structures obtained are presented with the more relevant bond distances, in each step. Free energy values (kcal/mol) are referred to the initial intermediate (**A**)..

Atomic Coordinates for all the optimized molecules (PBE0/b1)

1g

C	-2.939929	3.578477	-1.773293
S	-1.037864	0.008170	-1.975397
O	-2.920764	1.656423	-3.171626
H	-3.490489	3.554575	-0.829093
C	-2.481798	2.190528	-2.154094
H	-3.578897	3.948300	-2.576391
O	-1.464310	2.985681	0.567864
C	-1.521255	1.512845	-1.289200
O	-0.379738	1.000260	0.678598
H	-2.093659	4.249159	-1.607311
C	-1.154648	1.932250	0.039127
H	-0.392390	2.275293	2.287500
H	1.167993	1.488505	1.936794
C	0.084059	1.335154	1.989191
C	0.641484	-0.418969	3.673614
C	-0.253896	0.228803	2.931929
C	0.744753	-0.157638	-1.842411
H	1.702596	-0.187895	3.611379
C	1.527238	0.989727	-1.761158
H	1.050679	1.960337	-1.668369
C	2.912580	0.870017	-1.803099
H	3.526559	1.762950	-1.734564
C	3.508310	-0.381611	-1.930433
C	2.713754	-1.520534	-2.026448
H	4.590076	-0.469304	-1.960422
H	3.171372	-2.499331	-2.133815
C	1.326771	-1.415105	-1.992121
C	-1.681600	-1.385516	-1.040670
H	0.709612	-2.304245	-2.073398
H	-1.288869	-3.350048	1.681607
C	-1.728748	-2.950767	0.772488
H	-0.196920	-1.453086	0.520930
C	-1.105681	-1.889448	0.124236
H	-3.293929	-1.500074	-2.461955
C	-2.862999	-1.918506	-1.556656
H	-4.399347	-3.393622	-1.285079
C	-3.478925	-2.973843	-0.891147
H	-3.389899	-4.318390	0.784973
C	-2.910666	-3.491413	0.269319
H	0.348858	-1.190100	4.379829
H	-1.311874	-0.020311	3.005474

4g

H	-1.556319	-0.926399	0.555852
H	-0.341352	0.353445	-2.881008
H	0.913986	1.592363	-3.131815
O	2.273343	0.513199	-1.328698
H	-0.468422	1.902870	-2.046408
O	1.801367	-1.743463	0.637230
O	0.643847	-0.581751	2.168679
H	-1.742873	0.264050	-0.819874
C	0.341422	0.082783	-0.054132
C	1.065282	0.569745	-1.272808
C	0.241250	1.146448	-2.399164
H	-0.945249	0.477671	2.905621
C	1.047425	-0.852415	0.892300
H	0.558099	1.410383	2.688879
C	-0.085095	0.640206	2.248771
C	-0.478888	1.000747	0.833358
C	-1.167910	-0.049019	0.045124
H	-0.609312	2.046938	0.576193

SPh_2

S	-0.378120	2.178890	1.826410
C	1.072381	1.961829	0.820239
C	2.285096	2.456587	1.305425
H	2.327913	2.889540	2.300502
C	3.431457	2.385014	0.518780

H	4.369697	2.774333	0.903537
C	3.381280	1.801101	-0.742921
C	2.172788	1.298650	-1.221761
H	4.278572	1.735805	-1.350950
H	2.124403	0.845160	-2.207754
C	1.017977	1.387901	-0.453415
C	-1.252931	0.643887	1.620141
H	0.074686	1.009034	-0.834315
H	-0.841717	-2.725681	1.662785
C	-1.348701	-1.766896	1.600801
H	0.465235	-0.633997	1.853200
C	-0.609842	-0.594640	1.707628
H	-3.132096	1.657487	1.361020
C	-2.637144	0.694316	1.442198
H	-4.449186	-0.436768	1.225132
C	-3.372617	-0.485204	1.361138
H	-3.304907	-2.636831	1.359190
C	-2.731624	-1.717616	1.433590

A

Au	-1.510505	-0.495780	1.585733
C	1.222916	0.709258	-2.382190
S	-1.379945	-1.894536	-4.114719
O	1.196239	-0.888643	-4.140754
P	0.244424	0.707872	2.537661
H	0.613237	1.615557	-2.357443
C	0.484068	0.341487	4.300398
C	0.576914	-0.365325	-3.221980
H	-1.624691	0.036379	4.650862
H	2.203569	0.916574	-2.811926
C	-0.633738	0.068095	5.097835
O	-1.290436	0.546363	-1.013531
H	-1.345116	-0.376839	7.075145
C	-0.795361	-0.785208	-2.916336
C	-0.476383	-0.165730	6.459186
O	-2.752825	-1.044100	-1.661811
H	0.918172	-0.329693	8.089697
H	1.336181	0.378815	-1.345146
C	0.795674	-0.138899	7.027830
C	-1.574650	-0.345232	-1.812954
H	2.901873	0.141328	6.678795
H	-4.670748	-0.726071	-1.126946
C	1.910546	0.125329	6.236434
H	-3.561710	0.587696	-0.681851
H	2.632017	0.569379	4.258434
C	-3.669062	-0.500140	-0.738516
C	1.760027	0.367776	4.873943
C	-2.844586	-2.225445	0.937994
H	-0.691523	2.322717	0.325785
C	-3.564988	-1.102604	0.632276
C	-0.046611	2.495055	2.386802
H	-1.046167	4.755503	0.057074
C	-1.582760	-3.521541	-3.378567
C	-0.499896	2.996511	1.158039
C	-0.948563	-3.802976	-2.173331
H	-0.623754	6.296884	1.954631
H	-0.405324	-3.015963	-1.657367
C	-0.699001	4.364601	1.008764
C	-1.000300	-5.099866	-1.667707
H	0.164763	5.402665	4.128632
H	-0.499823	-5.332038	-0.732111
C	-0.460864	5.230084	2.075465
C	-1.674993	-6.098625	-2.364589
H	0.535725	2.975350	4.411948
C	-2.287693	-5.806941	-3.581418
C	-0.018344	4.729653	3.296609
H	-1.711152	-7.108534	-1.968166
H	2.478975	2.402356	1.610473
H	-2.800446	-6.586964	-4.135539
C	0.191861	3.362511	3.457422
C	-2.234945	-4.518366	-4.103712

H	4.620119	1.848031	0.502468
C	-3.036939	-1.407298	-4.602547
C	1.817376	0.349406	1.700940
H	-2.700614	-4.296265	-5.059317
H	5.167588	-0.507667	-0.043386
H	-6.347624	-1.905361	-4.117817
C	2.719319	1.368515	1.380891
C	-5.431993	-1.494685	-4.533004
H	3.572078	-2.318205	0.529176
C	3.923325	1.054613	0.754658
H	-4.149574	-2.675337	-3.261611
C	-4.202872	-1.932487	-4.049463
H	1.426163	-1.775325	1.634225
H	-2.163497	-0.079487	-6.062072
C	4.230442	-0.268227	0.449750
C	-3.082689	-0.462428	-5.627650
C	3.333706	-1.286792	0.770090
H	-4.362617	0.715648	-6.884596
C	2.128088	-0.980850	1.390070
C	-4.319248	-0.020456	-6.088149
H	-6.455256	-0.201856	-5.915746
C	-5.491862	-0.537395	-5.544294
H	-2.990057	-2.737247	1.885608
H	-2.282253	-2.740138	0.161842
H	-4.265884	-0.700939	1.365678

A’

Au	1.275142	-1.845522	-0.329072
H	2.797618	4.006071	-2.343279
H	2.344917	5.685330	-2.776186
O	2.816664	6.568383	-0.542306
S	3.084438	5.318170	1.876464
H	1.140442	4.545248	-2.116673
O	1.759840	2.567758	1.655521
O	1.641452	2.566753	-0.575391
P	1.382914	-3.566194	-1.898836
C	2.502622	4.487951	0.460901
C	0.600509	-3.096455	-3.470402
C	2.525121	5.386210	-0.694276
C	2.184148	4.868704	-2.071880
H	-1.086419	-2.169699	-2.483436
H	-0.099256	1.578126	-0.024137
C	1.952873	3.190524	0.605428
H	0.848728	0.926041	-1.381488
C	-0.628355	-2.423881	-3.436911
C	0.916173	1.369492	-0.383167
C	1.606703	0.434181	0.572546
H	-2.221734	-1.569119	-4.595065
C	-1.267992	-2.087018	-4.623718
C	0.965686	-0.471960	1.387409
H	2.694467	0.478461	0.582723
H	-1.179451	-2.138362	-6.773578
C	-0.681621	-2.408559	-5.847291
H	0.999846	-3.319028	-6.836076
C	0.541960	-3.070803	-5.883529
H	2.141072	-3.934391	-4.731096
C	1.185882	-3.418801	-4.698556
H	1.209852	-4.774869	0.731389
C	0.524965	-5.051149	-1.301010
H	0.111947	-6.824296	1.570665
C	4.032026	4.122225	2.822161
C	0.638655	-5.401932	0.050423
C	4.035404	4.160939	4.213121
H	-1.202437	-8.252608	0.025526
H	3.377075	4.834027	4.751502
C	0.022408	-6.554779	0.522879
C	4.895520	3.315393	4.910253
H	-1.412928	-7.630103	-2.364974
H	4.897376	3.337389	5.995665
C	-0.715524	-7.356287	-0.346507
C	5.747449	2.455249	4.225430

H	-0.316139	-5.585161	-3.218083
C	5.746730	2.442857	2.832152
C	-0.834834	-7.007501	-1.689108
H	6.418522	1.802663	4.775288
H	2.715274	-6.170011	-2.301073
H	6.421142	1.784806	2.292216
C	-0.216318	-5.857235	-2.171399
C	4.893976	3.280189	2.121941
H	5.047390	-6.757618	-2.872731
C	1.729609	5.786565	2.946678
C	3.094719	-4.043568	-2.273616
H	4.894414	3.283455	1.036118
H	6.745449	-4.975374	-3.168524
H	-0.825410	4.643767	4.843149
C	3.454803	-5.385620	-2.432460
C	-0.159862	5.345048	4.348738
H	6.108536	-2.593995	-2.888873
C	4.769070	-5.715061	-2.753568
H	1.048847	3.800990	3.427129
C	0.884691	4.863805	3.567766
H	3.782510	-1.993464	-2.307626
H	2.205413	7.855523	2.575449
C	5.721514	-4.713589	-2.919654
C	1.542053	7.161887	3.083326
C	5.365190	-3.375036	-2.762145
H	0.330086	8.692349	3.979383
C	4.057235	-3.038294	-2.434590
C	0.487226	7.624426	3.865834
H	-1.178491	7.081113	5.110076
C	-0.358287	6.718009	4.498016
H	1.530642	-0.981517	2.165284
H	-0.112275	-0.413320	1.527239

$TS_{A'B}$

Au	1.178310	-1.025270	-0.917598
H	2.664195	4.399029	-1.787655
H	1.682141	5.769055	-1.270308
O	0.284131	4.079032	0.449441
S	2.303289	3.970510	2.517130
H	0.880659	4.405591	-2.044906
O	4.908556	3.234727	0.966595
O	3.834679	2.489655	-0.816126
P	0.837411	-2.960808	-2.178724
C	2.594011	3.753157	0.824267
C	0.907124	-2.614194	-3.959182
C	1.432592	4.117258	0.015713
C	1.695339	4.677673	-1.369104
H	-0.198932	-0.765039	-3.762990
H	1.892473	2.246572	-1.581052
C	3.842391	3.199512	0.381599
H	3.111905	1.027144	-1.956356
C	0.288457	-1.455763	-4.447765
C	2.730052	1.677992	-1.160763
C	2.257941	0.842225	0.003836
H	-0.188898	-0.293025	-6.188601
C	0.292715	-1.190024	-5.811850
C	0.957156	0.771263	0.433154
H	3.045652	0.381586	0.602984
H	0.929903	-1.857429	-7.755897
C	0.921262	-2.070594	-6.691323
H	2.034463	-3.902203	-6.892653
C	1.542153	-3.218741	-6.207784
H	2.024440	-4.391641	-4.469247
C	1.536527	-3.496374	-4.843224
H	-0.647105	-3.292569	0.291968
C	-0.788024	-3.690229	-1.829445
H	-2.826746	-4.335011	0.813851
C	3.277910	5.313145	3.199574
C	-1.247629	-3.722914	-0.506384
C	2.734352	5.904451	4.341508
H	-4.205563	-5.310286	-1.003048

H	1.802614	5.537339	4.762641
C	-2.472179	-4.310483	-0.211901
C	3.396307	6.977773	4.927068
H	-3.397802	-5.247095	-3.346084
H	2.983263	7.444333	5.815855
C	-3.245675	-4.858516	-1.234019
C	4.572857	7.462100	4.360255
H	-1.217810	-4.210863	-3.881718
C	5.092418	6.872738	3.210107
C	-2.793517	-4.823015	-2.550159
H	5.083137	8.306732	4.813128
H	0.709364	-5.882418	-1.797866
H	6.008361	7.253983	2.769196
C	-1.565458	-4.241077	-2.853294
C	4.450252	5.789042	2.616607
H	2.466320	-7.568371	-1.371221
C	2.858558	2.523357	3.410572
C	2.091980	-4.222523	-1.819303
H	4.857018	5.304604	1.736372
H	4.835387	-6.871286	-1.149241
H	5.566143	0.882238	4.595850
C	1.746119	-5.572741	-1.704544
C	4.524984	1.098213	4.376828
H	5.450163	-4.475980	-1.353484
C	2.736805	-6.521009	-1.463062
H	4.970063	2.946842	3.349985
C	4.200423	2.261631	3.684235
H	3.703898	-2.780034	-1.772529
H	0.805087	1.908333	3.646311
C	4.066548	-6.128506	-1.339058
C	1.845952	1.660362	3.836475
C	4.413682	-4.783031	-1.453167
H	1.407658	-0.168138	4.878011
C	3.430296	-3.829480	-1.687667
C	2.187681	0.500679	4.526342
H	3.791821	-0.679215	5.341388
C	3.526657	0.219561	4.792650
H	0.724405	0.294600	1.382790
H	0.186530	1.399760	-0.010484

B

Au	0.701188	-0.798299	-0.725147
H	1.406765	5.464832	-0.677778
H	-0.300192	5.154183	-0.247188
O	0.465694	3.928279	1.821259
S	2.899732	2.893968	2.490001
H	0.595816	4.027585	-1.302789
O	4.168324	4.704094	0.021407
O	3.514850	3.063128	-1.338671
P	0.452483	-2.844500	-1.862832
C	2.407187	3.135001	0.723744
C	1.291253	-2.856116	-3.483659
C	1.096387	3.944159	0.789508
C	0.668784	4.691607	-0.435734
H	0.539521	-0.892202	-3.975400
H	1.724147	2.241861	-1.963187
C	3.474217	3.744240	-0.197010
H	3.081397	1.108061	-1.804472
C	1.135064	-1.737503	-4.313365
C	2.585558	1.965210	-1.346743
C	2.198023	1.707319	0.107789
H	1.602130	-0.841544	-6.208893
C	1.732630	-1.708520	-5.568085
C	0.860698	1.023569	0.290700
H	2.993452	1.082183	0.536777
H	2.972022	-2.763207	-6.977879
C	2.501027	-2.788696	-5.999755
H	3.265662	-4.739960	-5.509792
C	2.666346	-3.898082	-5.176160
H	2.194036	-4.805790	-3.283408
C	2.062271	-3.936700	-3.921169

H	-1.978140	-2.324537	-0.396461
C	-1.287486	-3.254104	-2.217824
H	-4.352095	-2.909587	-0.782537
C	2.930554	4.441288	3.377111
C	-2.264513	-2.877586	-1.288116
C	2.413231	4.343821	4.670580
H	-5.009893	-4.146689	-2.830356
H	2.008228	3.405527	5.036616
C	-3.598699	-3.204239	-1.506804
C	2.413354	5.475391	5.478547
H	-3.287353	-4.802251	-4.489669
H	2.016121	5.413298	6.486453
C	-3.967032	-3.898185	-2.657342
C	2.904968	6.681943	4.987863
H	-0.912986	-4.230398	-4.107163
C	3.397944	6.764530	3.687220
C	-3.000444	-4.266664	-3.589668
H	2.895716	7.565232	5.618906
H	-0.364278	-5.691230	-1.602906
H	3.769292	7.709762	3.303966
C	-1.662766	-3.947507	-3.373705
C	3.418937	5.642723	2.864304
H	0.645801	-7.590327	-0.384550
C	4.574877	2.281039	2.431343
C	1.126295	-4.273095	-0.951282
H	3.789284	5.700906	1.846389
H	2.702753	-7.256492	0.959639
H	7.822114	3.119315	2.020552
C	0.539461	-5.540800	-1.019561
C	6.947647	2.503459	2.204339
H	3.746954	-5.010365	1.090397
C	1.108064	-6.609231	-0.331348
H	5.577022	4.149815	2.000115
C	5.687388	3.089841	2.193513
H	2.729280	-3.098053	-0.115768
H	3.828522	0.309227	2.912732
C	2.262754	-6.420890	0.423491
C	4.704694	0.914223	2.696760
C	2.849668	-5.159372	0.497083
H	6.087874	-0.714575	2.901274
C	2.281244	-4.087000	-0.181780
C	5.974216	0.344902	2.695856
H	8.081591	0.694053	2.457666
C	7.091127	1.138429	2.449686
H	0.678274	0.825714	1.353931
H	0.043564	1.668481	-0.058061

$TS_{BB'}$

Au	-0.657855	-0.885004	-0.606759
H	0.586546	2.798755	-3.345916
H	-1.173359	3.106046	-3.491994
O	-1.442982	3.894865	-1.102627
S	0.374739	4.313364	0.852439
H	-0.585719	1.610055	-2.738738
O	2.613990	4.456486	-1.568526
O	2.675124	2.228521	-1.505591
P	-1.034013	-2.973331	-1.626841
C	0.754555	3.187032	-0.569274
C	-0.118936	-3.148567	-3.196851
C	-0.456966	3.325840	-1.513362
C	-0.388104	2.682338	-2.864556
H	-0.882797	-1.271088	-3.941513
H	1.313443	0.715941	-1.896338
C	2.110619	3.407845	-1.260593
H	2.506511	0.380270	-0.624176
C	-0.245554	-2.127977	-4.149207
C	1.848866	1.142869	-1.043936
C	0.903639	1.744704	-0.000207
H	0.317651	-1.424834	-6.099432
C	0.427552	-2.214482	-5.361959
C	-0.370116	0.966044	0.330586

H	1.516278	1.858078	0.906182
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C	1.243507	-3.313157	-5.629945
H	2.010896	-5.183315	-4.892124
C	1.377364	-4.325894	-4.685676
H	0.801235	-5.045242	-2.740834
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C	0.311270	7.982620	-0.945129
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C	-3.151337	-4.004541	-3.184624
C	0.689768	6.670172	-0.679599
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C	1.882771	4.372528	1.805183
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H	1.474960	6.188711	-1.251494
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C	1.863520	3.608953	2.976417
C	0.993548	-5.279126	1.065548
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C	2.985420	3.607693	3.799201
H	4.968152	4.378039	4.106269
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H	-1.263504	1.563475	0.112776

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O	3.647027	2.873161	-1.487434
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C	1.937764	0.152240	-2.735791
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H	1.805505	-0.141864	0.336824
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C	0.355898	-3.360661	-6.075172
H	1.025750	-5.345705	-5.580101
C	0.540596	-4.443347	-5.220091
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H	-3.347360	-2.513693	0.054598
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H	-5.746742	-3.120477	0.032097
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C	-5.623671	-4.177104	-1.841289
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H	-2.803201	-4.554594	-3.697235
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H	-1.887989	-5.893918	-1.149402
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C	-3.443652	-4.246633	-2.875500
C	2.224448	4.305402	-3.820953
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C	1.123853	4.981617	-0.485040
C	-0.352642	-4.421069	-0.783638
H	3.032338	3.844335	-3.263044
H	1.466389	-7.236195	1.167948
H	3.757064	6.944773	0.306471
C	-0.925863	-5.693465	-0.686629
C	2.774718	6.488148	0.371713
H	2.484964	-4.979450	1.010544
C	-0.269390	-6.701396	0.014478
H	3.065189	5.287240	-1.390113
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C	1.531804	-5.181356	0.531055
H	-0.033690	6.537726	2.293899
C	0.876502	-4.169638	-0.162258
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O	-1.700023	2.681313	-3.271886
S	0.646771	4.173239	-1.471475
H	-0.081768	0.197890	-3.674795
O	1.419316	0.711283	-0.928273
O	0.178917	1.483880	0.775760
P	-1.166747	-2.750809	-1.973020

C	-0.612352	2.007186	-1.326241
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C	-0.784851	2.015569	-2.826710
C	0.185035	1.261554	-3.682621
H	-2.591355	-1.544676	-4.177510
H	-1.575171	1.917193	1.750943
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C	-1.773688	-2.119590	-4.607712
C	-0.954271	2.352429	0.965870
C	-1.669397	2.445865	-0.386020
H	-2.298625	-1.620930	-6.629258
C	-1.609266	-2.161159	-5.987430
C	-2.604694	1.276359	-0.652660
H	-2.102166	3.428104	-0.585196
H	-0.426468	-2.916478	-7.619801
C	-0.557825	-2.889701	-6.542242
H	1.145161	-4.145456	-6.147111
C	0.324634	-3.579664	-5.716335
H	0.850785	-4.091027	-3.692890
C	0.159950	-3.550537	-4.333218
H	-2.864854	-3.051879	0.340399
C	-2.538867	-3.895364	-1.622837
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C	1.644563	4.239686	-2.942742
C	-3.174793	-3.808054	-0.377671
C	0.968243	4.623190	-4.107429
H	-5.406757	-6.341539	-0.724256
H	-0.090147	4.863447	-4.074808
C	-4.199200	-4.690343	-0.054932
C	1.669269	4.699424	-5.305891
H	-4.292752	-6.493279	-2.934185
H	1.149996	5.003241	-6.209442
C	-4.602144	-5.656885	-0.974891
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H	-2.462398	-4.936146	-3.513467
C	3.695947	4.037320	-4.175772
C	-3.977735	-5.742427	-2.215932
H	3.576825	4.480247	-6.278103
H	-0.452298	-5.496480	-1.174281
H	4.759366	3.820144	-4.199810
C	-2.945555	-4.866353	-2.543185
C	3.008889	3.943642	-2.970467
H	1.592521	-6.446895	-0.164233
C	1.757890	4.400908	-0.097337
C	0.304178	-3.471720	-1.184028
H	3.535980	3.667617	-2.064607
H	3.500271	-4.970104	0.411533
H	4.201118	2.954050	1.749236
C	0.384018	-4.846855	-0.932788
C	3.482971	3.699677	1.422641
H	3.355298	-2.530025	-0.025556
C	1.534870	-5.380727	-0.361305
H	2.763542	2.484534	-0.199165
C	2.681048	3.435437	0.316734
H	1.323726	-1.567063	-1.028689
H	0.898463	6.347375	0.266254
C	2.605617	-4.550201	-0.038575
C	1.621223	5.607832	0.597345
C	2.526353	-3.181677	-0.284379
H	2.331045	6.792658	2.239426
C	1.378469	-2.637895	-0.852104
C	2.429090	5.854564	1.702331
H	3.987407	5.097647	2.977138
C	3.359565	4.903057	2.113116
H	-3.107606	0.929744	0.257232
H	-3.292079	1.510357	-1.467444

C'

Au	-0.827968	-1.239048	-1.258545
H	0.944649	2.426458	-3.752028

H	-0.516614	1.885021	-4.644037
O	-1.709845	1.419045	-2.446747
S	2.234175	4.918587	-3.109198
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O	2.138121	-0.325736	-2.277327
O	2.532448	1.005786	-0.515673
P	-1.433622	-3.292026	-2.039527
C	0.362338	1.073984	-1.373924
C	-2.212949	-3.123972	-3.668920
C	-0.503021	1.369598	-2.584440
C	0.207824	1.622245	-3.873265
H	-3.120959	-1.217004	-3.194294
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C	1.753990	0.490487	-1.481778
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H	-4.267390	-1.020454	-5.372158
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H	-0.111323	3.004806	-0.329180
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C	4.241194	6.532498	-2.124244
H	-5.051389	-5.945480	1.449926
H	3.641051	7.360238	-2.489373
C	-3.190993	-4.876561	1.279102
C	5.468878	6.763015	-1.511406
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H	5.828311	7.780793	-1.393421
C	-4.367002	-5.435586	0.778750
C	6.240683	5.692102	-1.064708
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H	7.202748	5.875811	-0.595947
H	-1.074050	-6.188280	-1.749060
H	6.390322	3.550664	-0.891545
C	-3.793303	-4.683484	-1.441777
C	4.552570	4.147989	-1.832139
H	0.887765	-7.652914	-2.092305
C	1.004610	5.223600	-1.860729
C	0.010284	-4.373414	-2.207250
H	4.198635	3.130445	-1.972860
H	3.076316	-6.674621	-2.725530
H	0.498816	6.081202	1.386218
C	-0.119251	-5.757112	-2.036445
C	0.259990	5.783284	0.368995
H	3.305241	-4.219887	-3.012930
C	0.986541	-6.580195	-2.226968
H	2.326101	5.748241	-0.238551
C	1.296094	5.592747	-0.544529
H	1.360265	-2.742509	-2.672678
H	-0.570288	4.801056	-3.278572
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C	-0.331968	5.061726	-2.250435
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C

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H	4.122626	3.275860	-1.298686
O	3.052251	0.024815	2.470474
O	3.375632	2.026204	3.424545
P	-0.130780	-0.773474	-0.624395
C	3.355275	2.008614	1.081305
C	0.533688	-1.442644	-2.173105
C	4.163853	1.464860	-0.084756
C	4.081329	2.187181	-1.405117
H	0.545094	0.490603	-3.148876
H	3.103763	4.049786	3.596897
C	3.263835	1.201279	2.369227
H	4.784790	3.524146	3.313524
C	0.770614	-0.569346	-3.244658
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H	1.457840	-0.387939	-5.270238
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C	0.818945	-2.804620	-2.302842
H	-1.830143	1.055994	0.845223
C	-1.787927	-0.123831	-0.966259
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H	-4.341694	-0.364053	-3.192055
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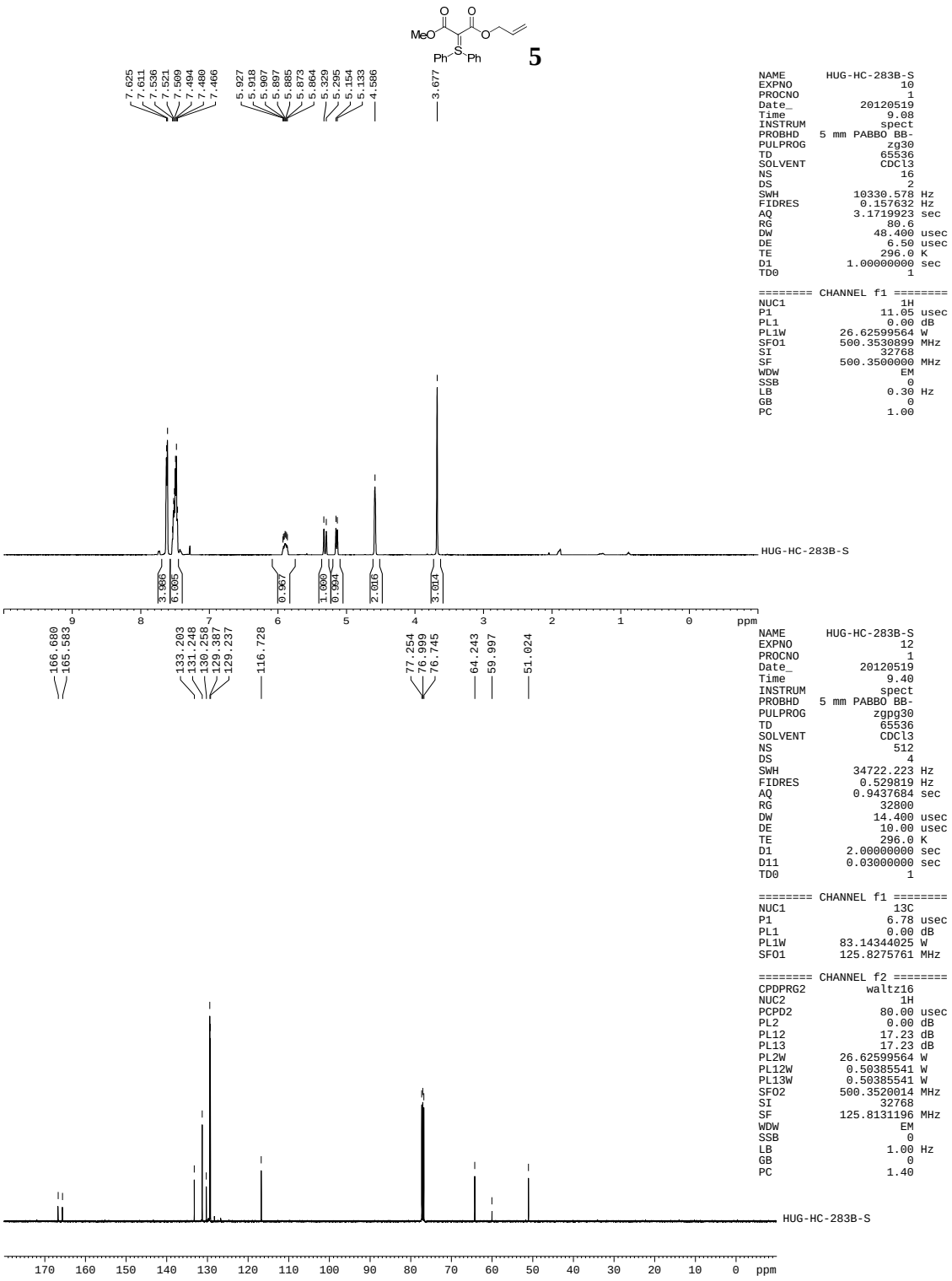
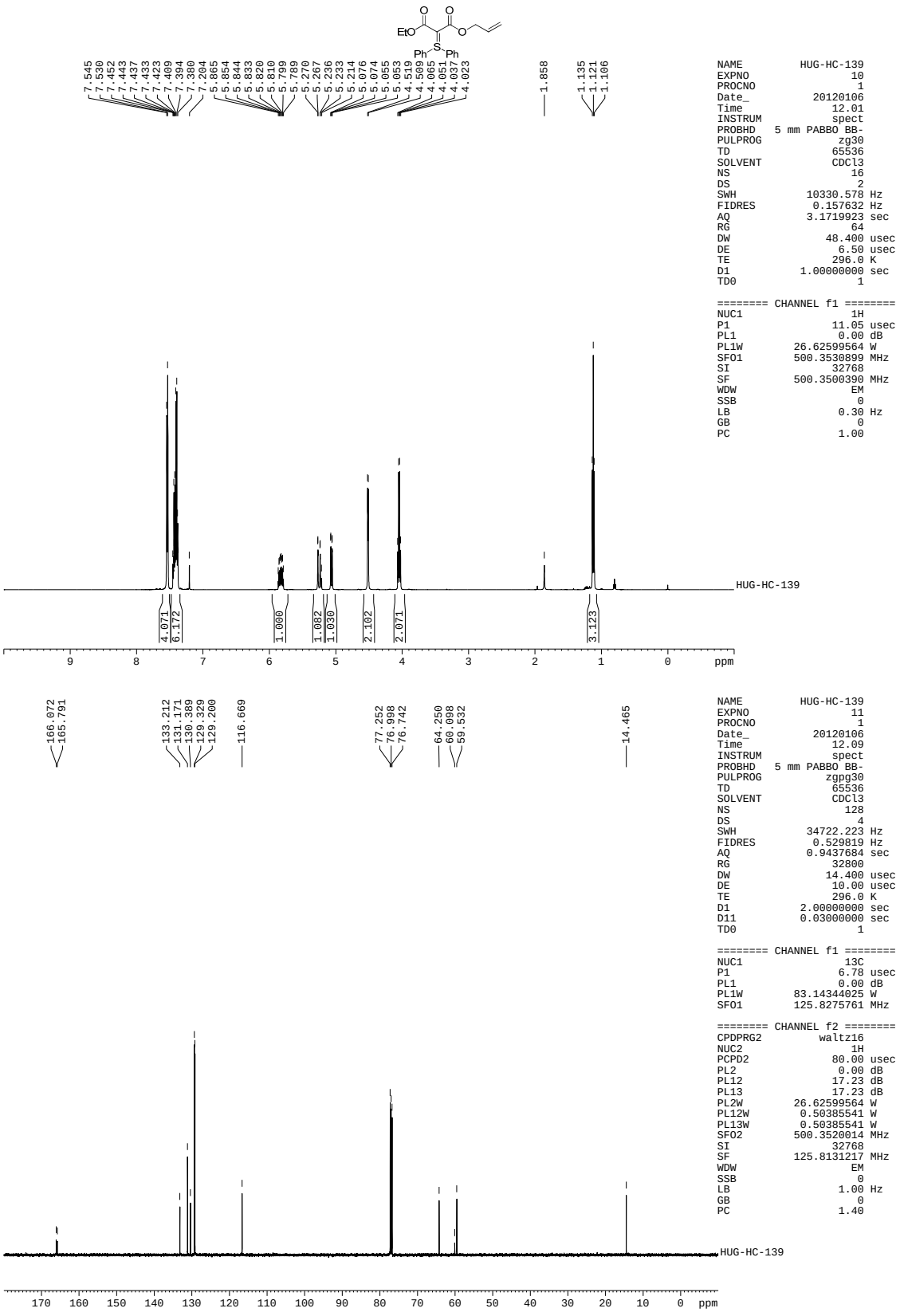
C	-2.497209	-0.523952	-2.103801
H	-2.410349	-4.623403	1.447305
C	-0.286229	-2.123246	0.570331
H	-0.561915	-5.091026	3.032434
C	-1.431212	-2.930543	0.562656
H	1.457776	-3.648289	3.051104
C	-1.522772	-3.998327	1.448525
H	1.637278	-1.742931	1.497391
C	-0.482724	-4.259298	2.338898
C	0.652590	-3.452387	2.350129
C	0.756254	-2.380140	1.469679
H	1.382721	3.049329	1.700626
H	1.971203	3.521878	0.016820

Part III NMR spectra



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PROCNO                 1
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Time               12.01
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TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                    64
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
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PL1                0.00 dB
PL1W         26.62599564 W
SFO1        500.3530899 MHz
SI                 32768
SF          500.3500390 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
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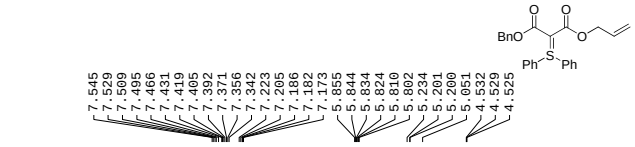
Time               12.09
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

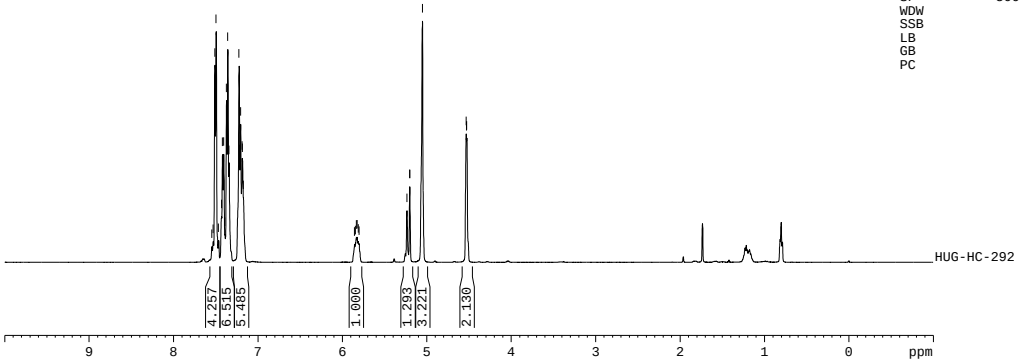
======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1        125.8275761 MHz

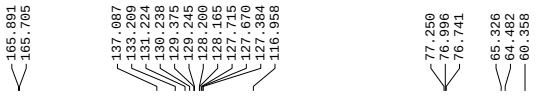
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2        500.3520014 MHz
SI                 32768
SF          125.8131217 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```




```
NAME          HUG-HC-292
EXPNO                 10
PROCNO                 1
Date_           20120520
Time               12.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                  71.8
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1        500.3530899 MHz
SI                 32768
SF          500.3500501 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

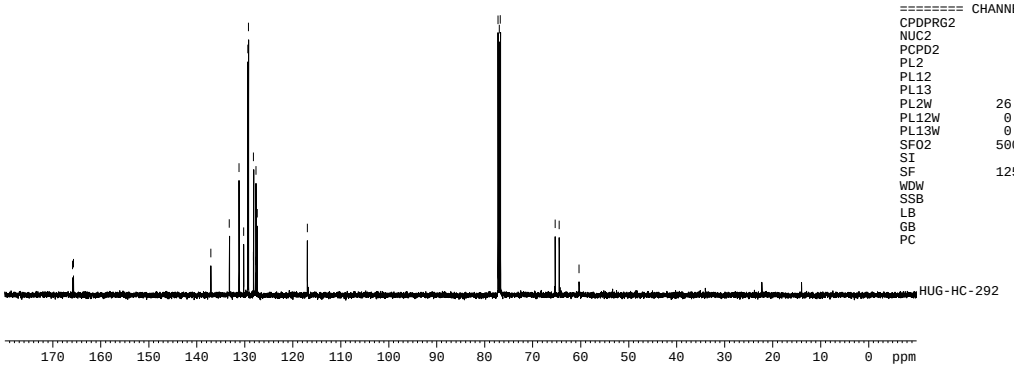


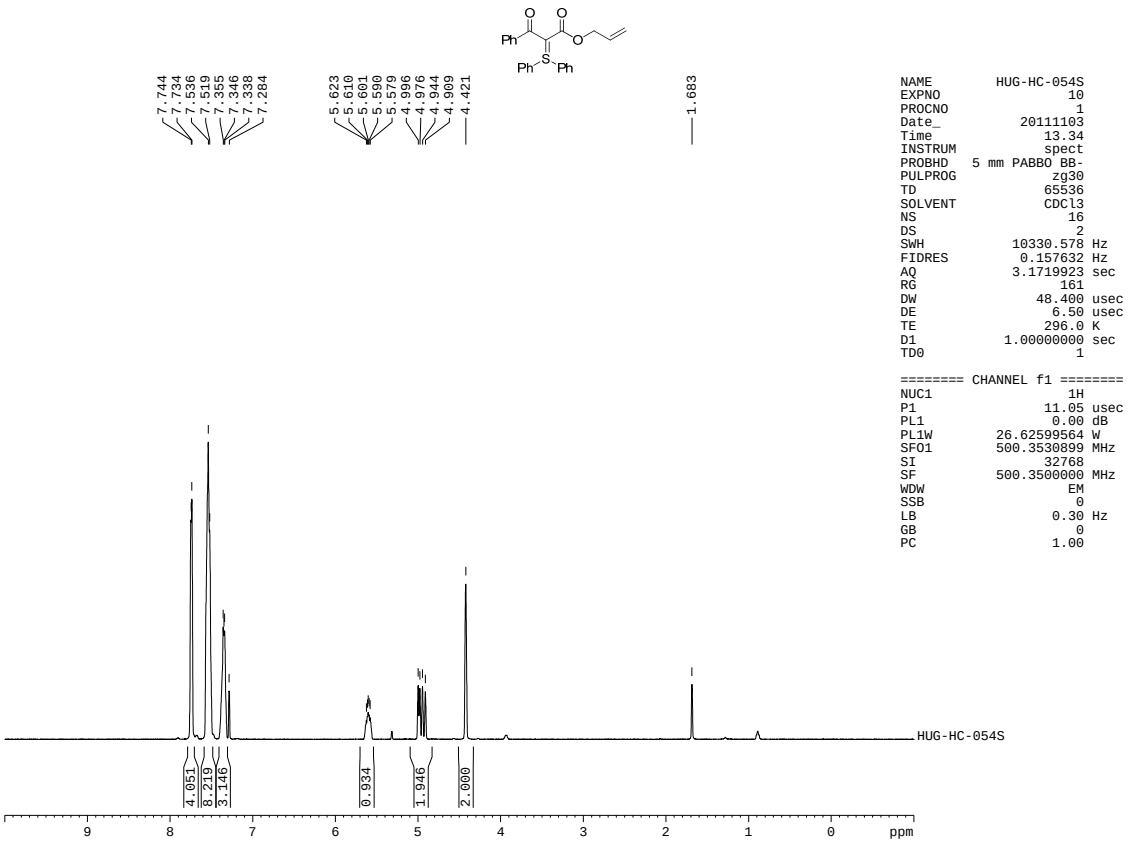



```
NAME          HUG-HC-292
EXPNO                 11
PROCNO                 1
Date_           20120520
Time               12.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1        125.8275761 MHz

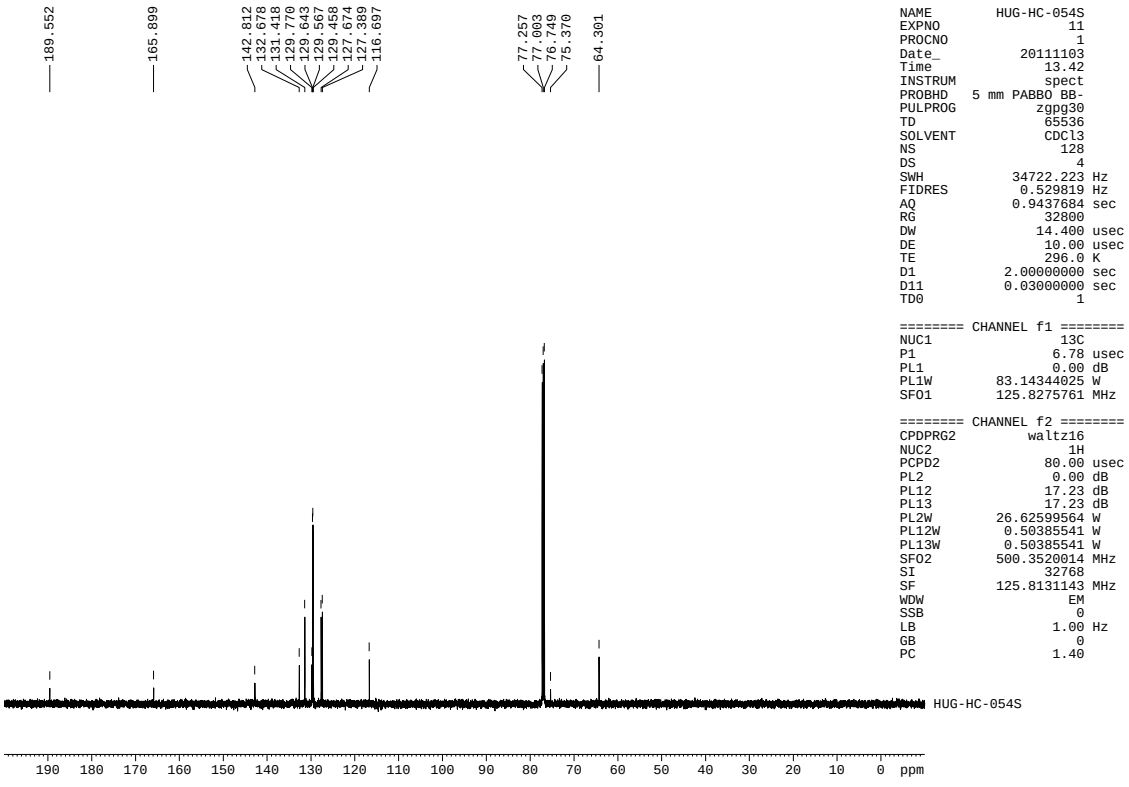
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2        500.3520014 MHz
SI                 32768
SF          125.8131206 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```






```
NAME          HUG-HC-054S
EXPNO                  10
PROCNO                  1
Date_           20111103
Time               13.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1

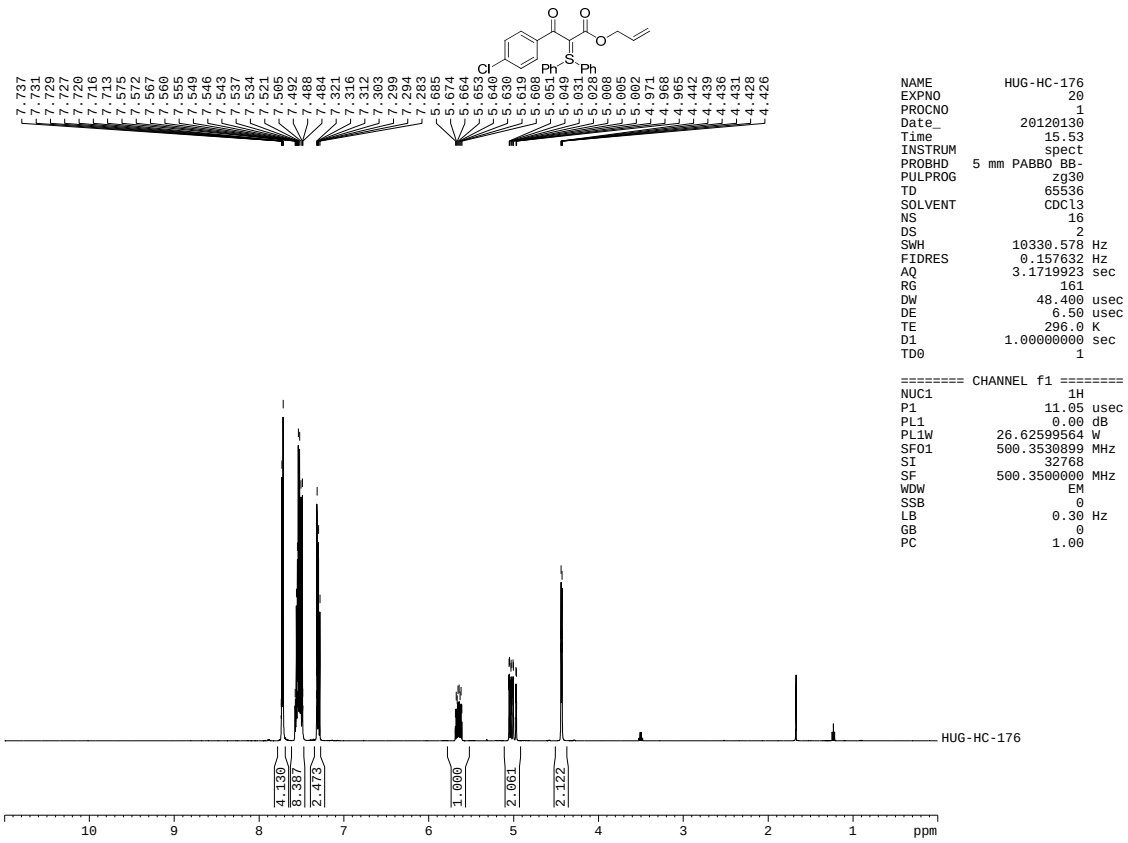
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W          26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME          HUG-HC-054S
EXPNO                  11
PROCNO                  1
Date_           20111103
Time               13.42
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

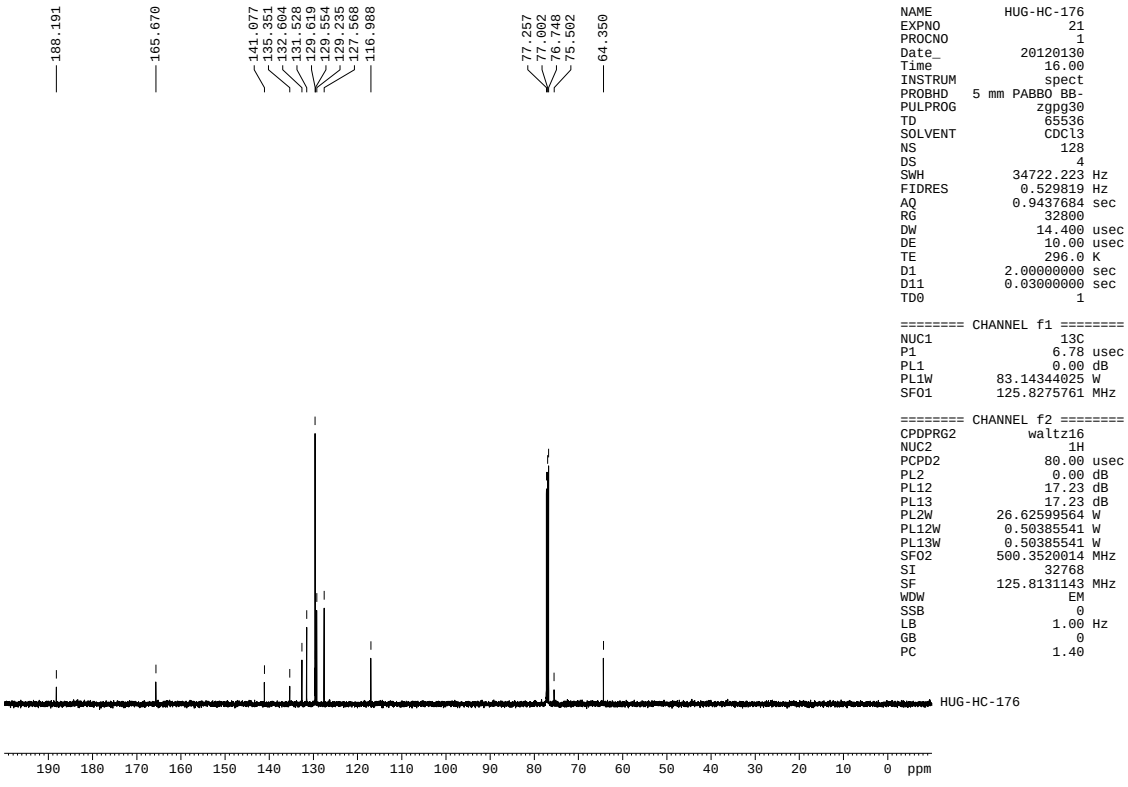
======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W          83.14344025 W
SFO1         125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W          26.62599564 W
PL12W          0.50385541 W
PL13W          0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131143 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
NAME          HUG-HC-176
EXPNO                 20
PROCNO                 1
Date_           20120130
Time               15.53
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

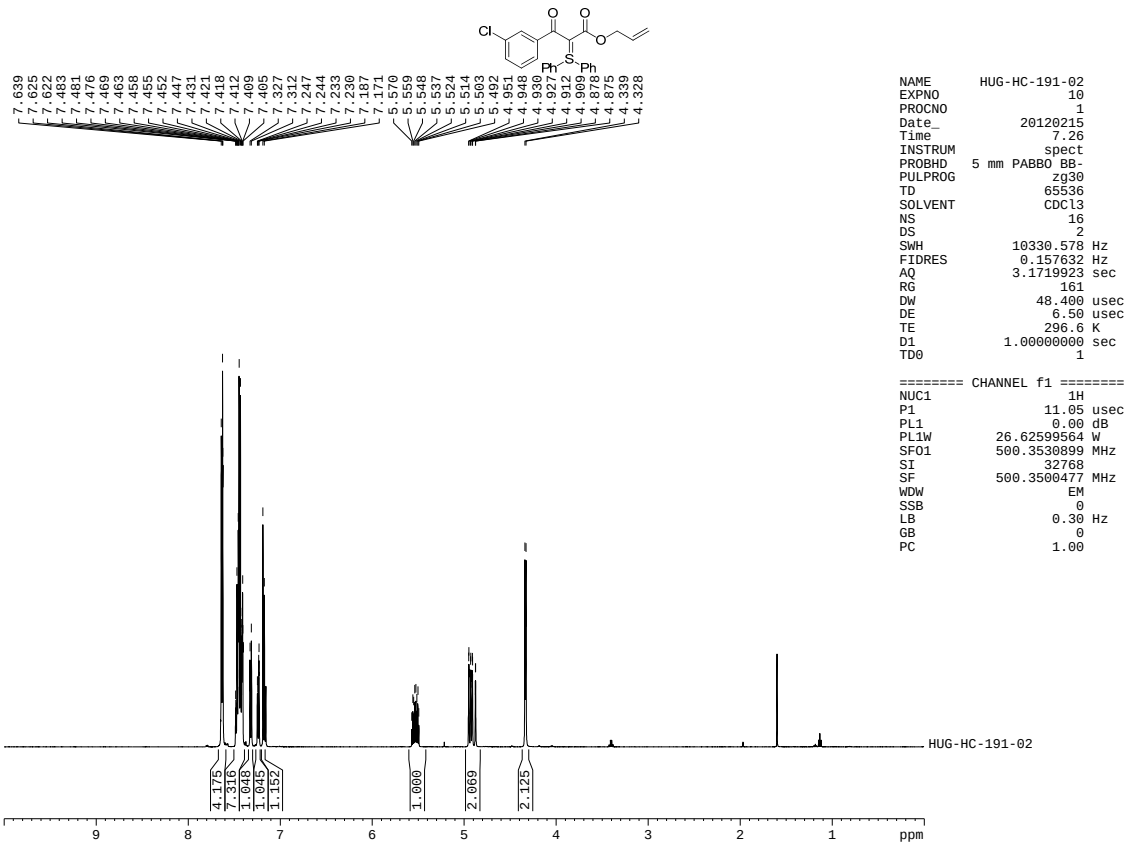
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

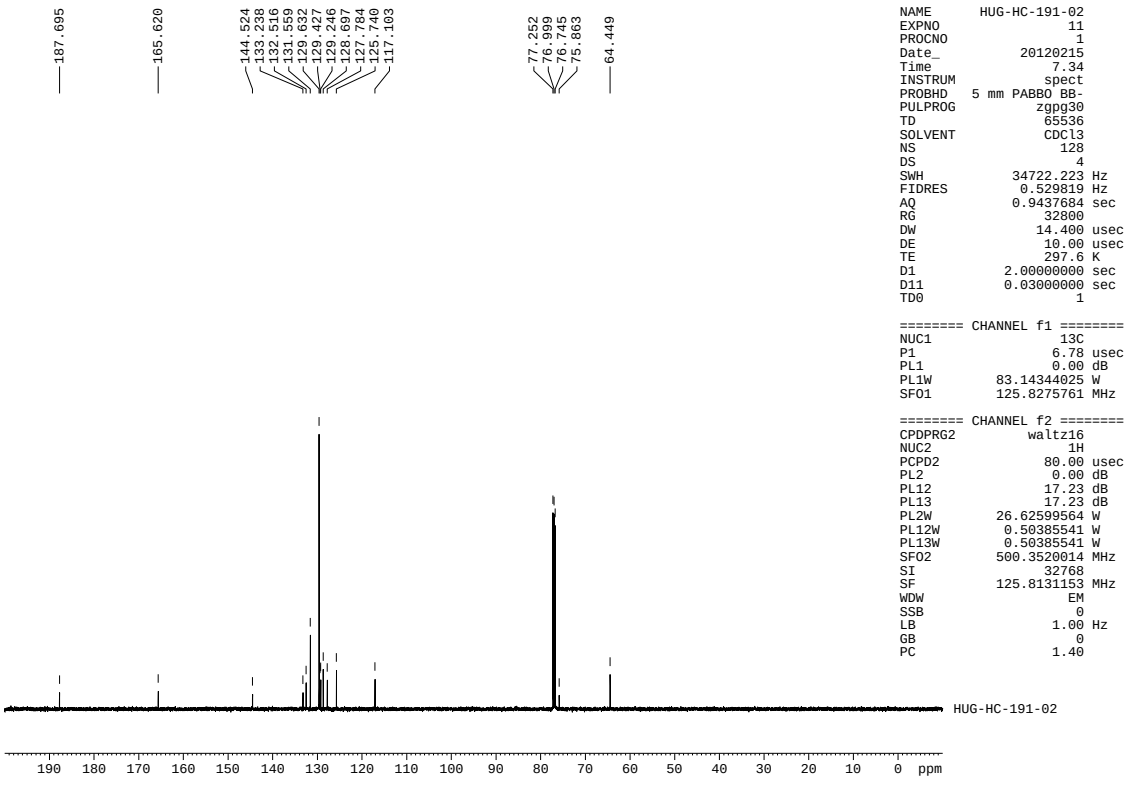


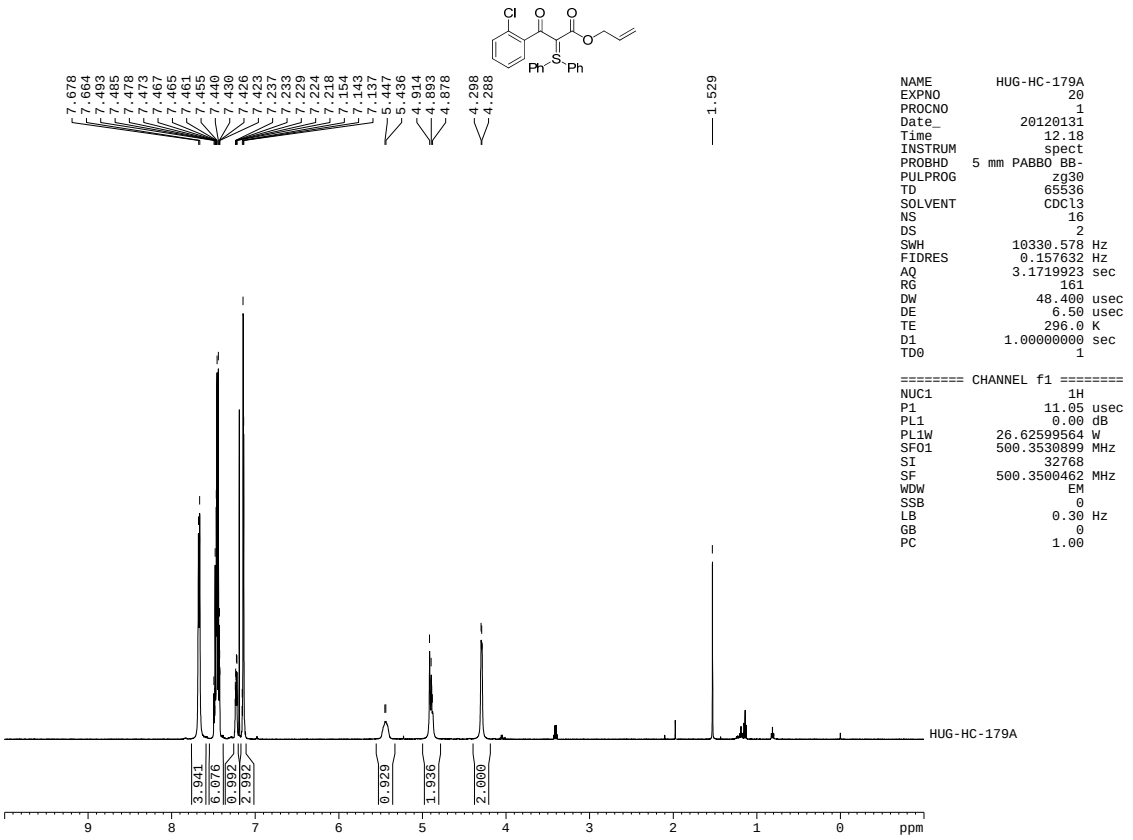

```
NAME          HUG-HC-176
EXPNO                 21
PROCNO                 1
Date_           20120130
Time               16.00
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1        125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131143 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

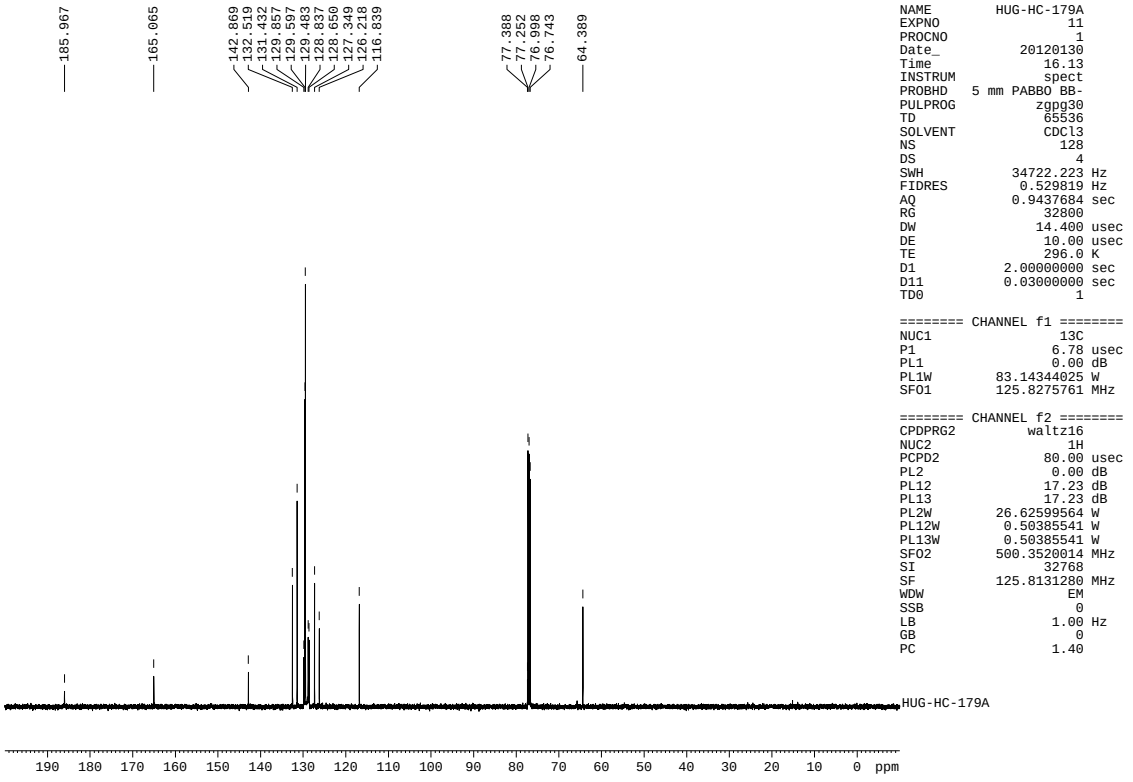

Cl
O
O
O
Ph
S
Ph
7.639
7.625
7.622
7.483
7.481
7.476
7.469
7.463
7.458
7.455
7.452
7.447
7.431
7.421
7.418
7.412
7.409
7.405
7.327
7.312
7.247
7.244
7.233
7.230
7.187
7.171
5.570
5.559
5.548
5.537
5.524
5.514
5.503
5.492
4.951
4.948
4.930
4.927
4.912
4.909
4.878
4.875
4.339
4.328
NAME HUG-HC-191-02
EXPNO 10
PROCNO 1
Date_ 20120215
Time 7.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500477 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-191-02
4.175
7.316
1.048
1.045
1.152
1.000
2.069
2.125
9
8
7
6
5
4
3
2
1
ppm


187.695
165.620
144.524
133.238
132.516
131.559
129.632
129.427
129.246
128.697
127.784
125.740
117.103
77.252
76.999
76.745
75.863
64.449
NAME HUG-HC-191-02
EXPNO 11
PROCNO 1
Date_ 20120215
Time 7.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131153 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-191-02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm




```
NAME          HUG-HC-179A
EXPNO                  20
PROCNO                  1
Date_           20120131
Time               12.18
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ              3.1719923 sec
RG                    161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                     1

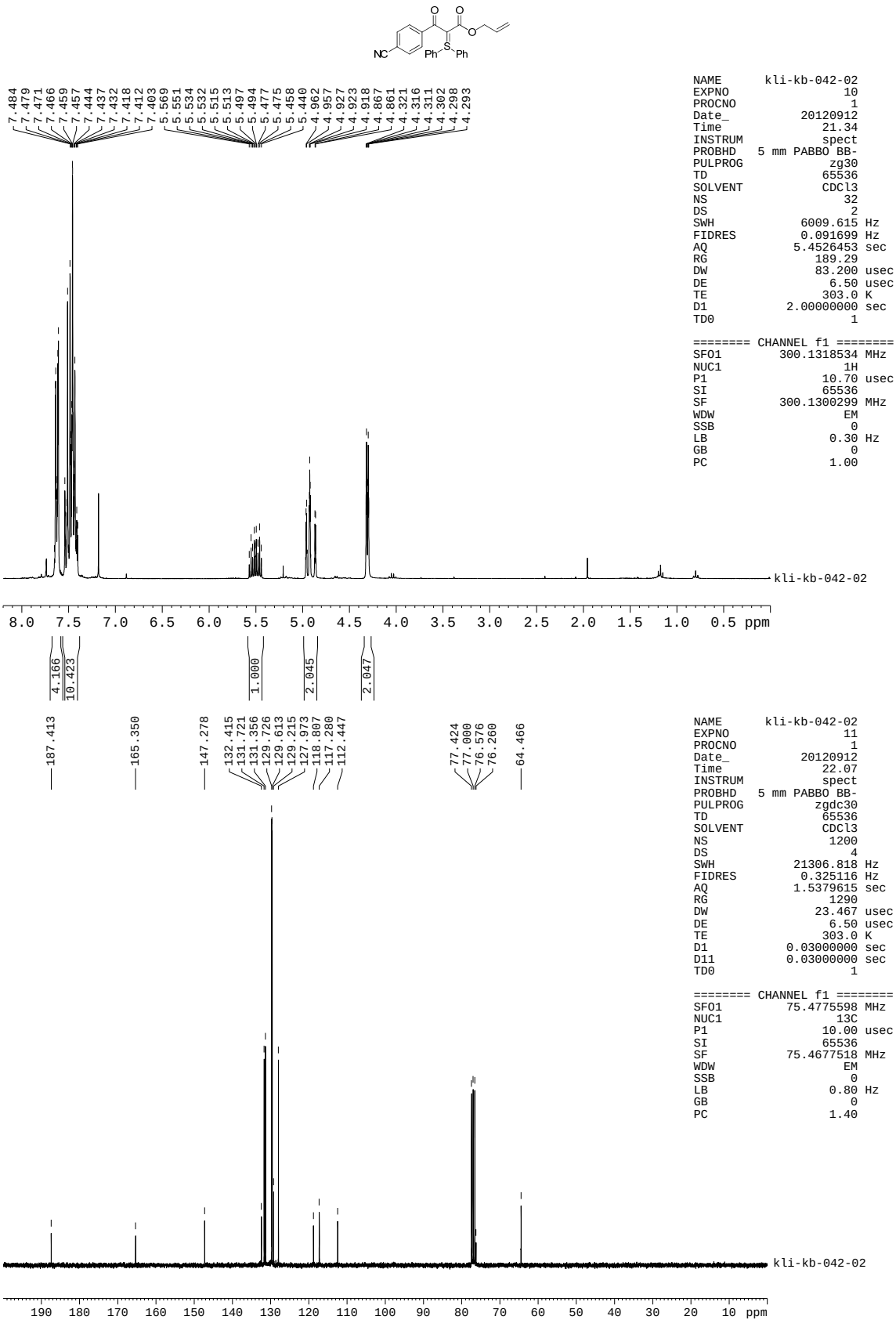
======== CHANNEL f1 ========
NUC1                   1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W          26.62599564 W
SFO1          500.3530899 MHz
SI                  32768
SF            500.3500462 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

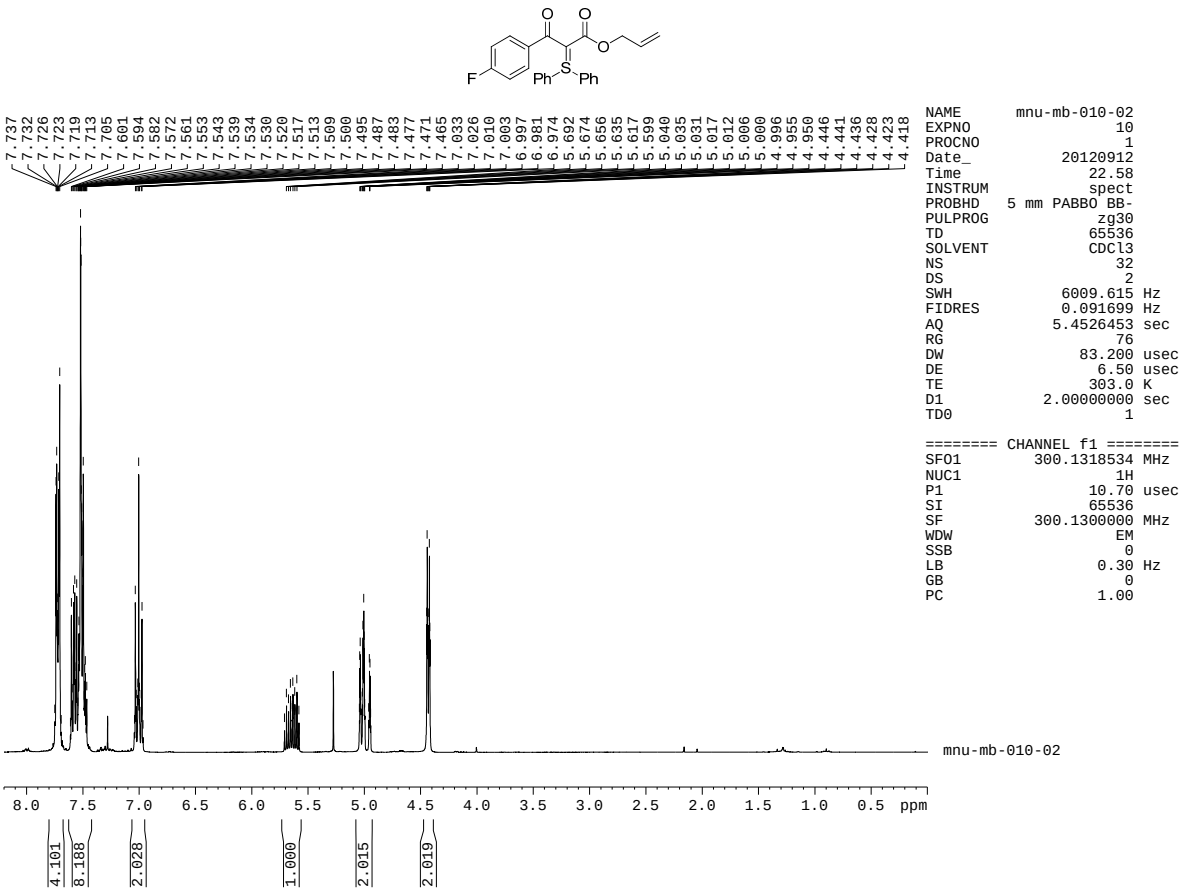


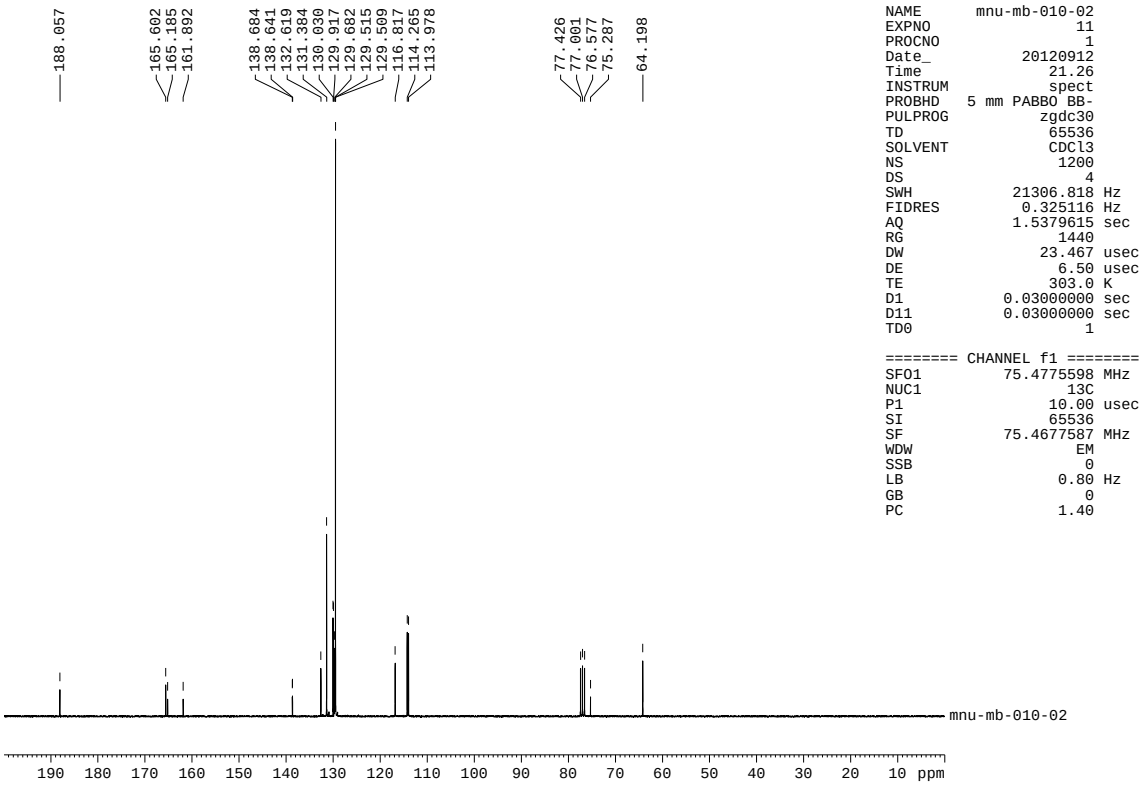

```
NAME          HUG-HC-179A
EXPNO                  11
PROCNO                  1
Date_           20120130
Time               16.13
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      4
SWH            34722.223 Hz
FIDRES          0.529819 Hz
AQ              0.9437684 sec
RG                  32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

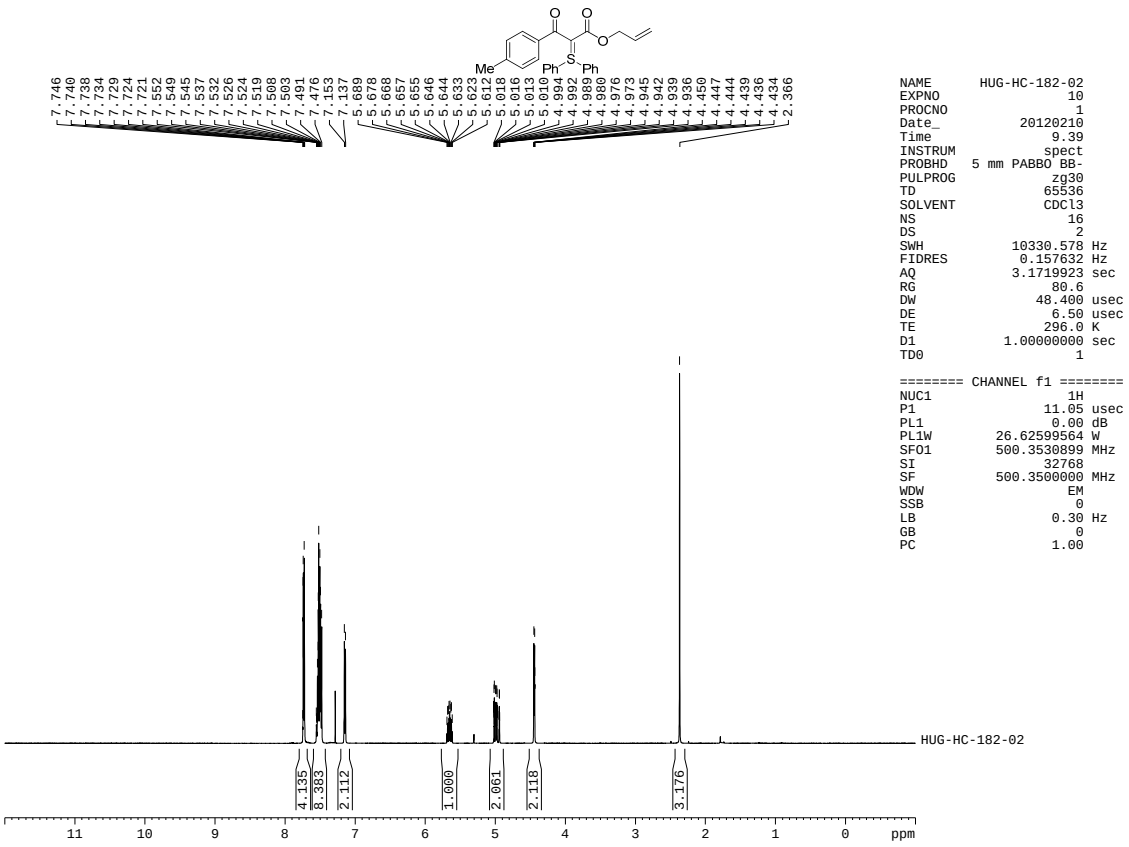
======== CHANNEL f1 ========
NUC1                   13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W          83.14344025 W
SFO1          125.8275761 MHz

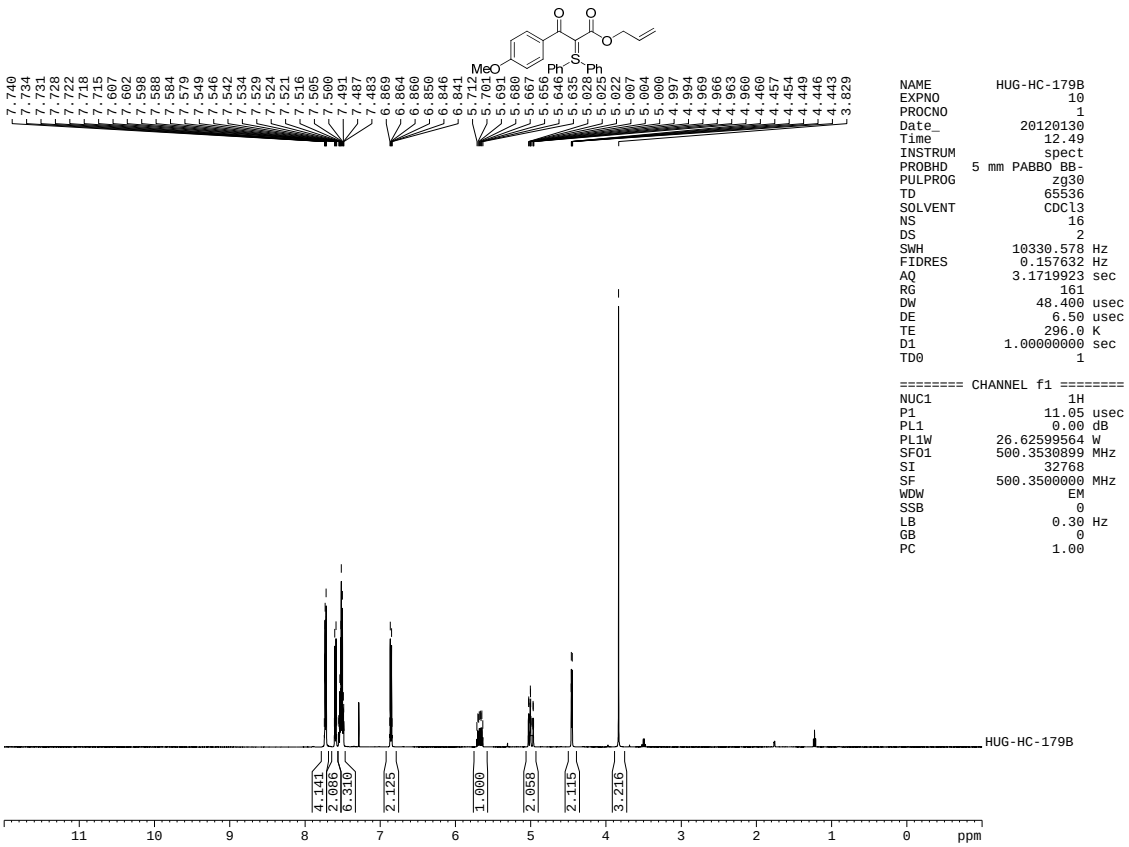
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W          26.62599564 W
PL12W          0.50385541 W
PL13W          0.50385541 W
SFO2          500.3520014 MHz
SI                  32768
SF            125.8131280 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 1.40
```

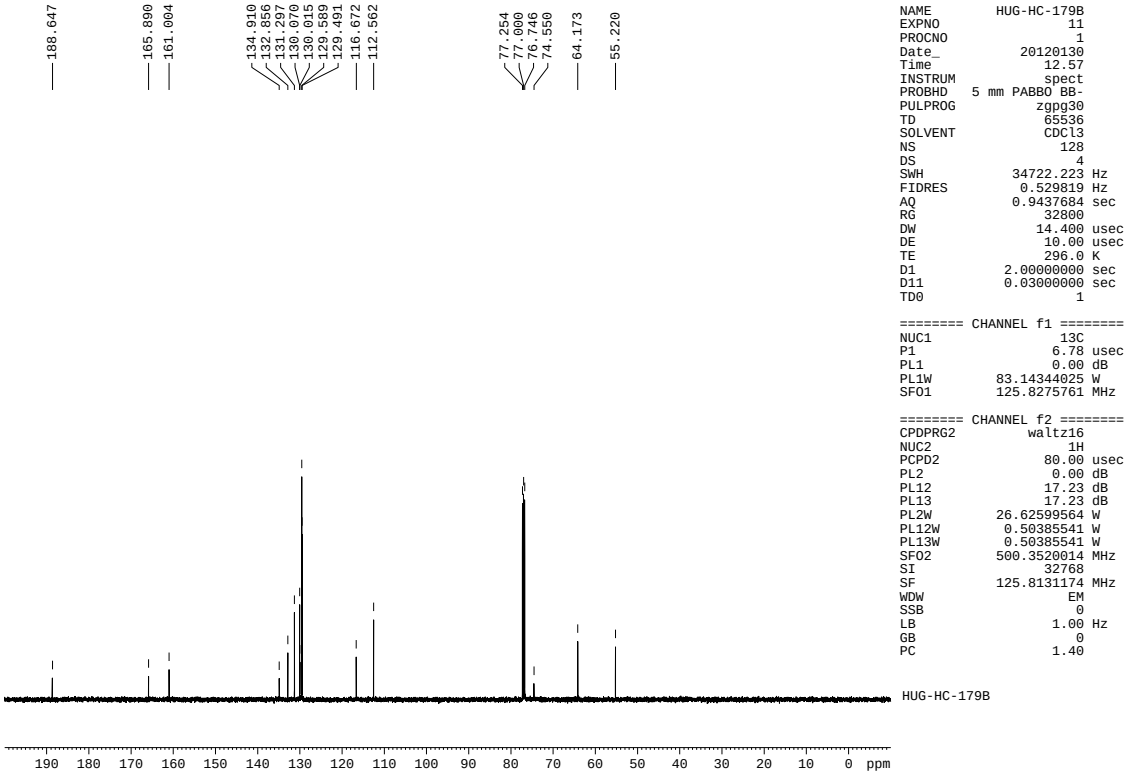

NC
Ph
S
Ph
O
O
O
7.484
7.479
7.471
7.466
7.459
7.457
7.444
7.437
7.432
7.418
7.412
7.403
5.569
5.551
5.534
5.532
5.515
5.513
5.497
5.494
5.477
5.475
5.458
5.440
4.962
4.957
4.927
4.923
4.918
4.867
4.861
4.321
4.316
4.311
4.302
4.298
4.293
NAME kli-kb-042-02
EXPNO 10
PROCNO 1
Date_ 20120912
Time 21.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 189.29
DW 83.200 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.70 usec
SI 65536
SF 300.1300299 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
kli-kb-042-02
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 ppm
4.166
10.423
1.000
2.045
2.047
187.413
165.350
147.278
132.415
131.721
131.356
129.726
129.613
129.215
127.973
118.807
117.280
112.447
77.424
77.000
76.576
76.260
64.466
NAME kli-kb-042-02
EXPNO 11
PROCNO 1
Date_ 20120912
Time 22.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 21306.818 Hz
FIDRES 0.325116 Hz
AQ 1.5379615 sec
RG 1290
DW 23.467 usec
DE 6.50 usec
TE 303.0 K
D1 0.03000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4775598 MHz
NUC1 13C
P1 10.00 usec
SI 65536
SF 75.4677518 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.40
kli-kb-042-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

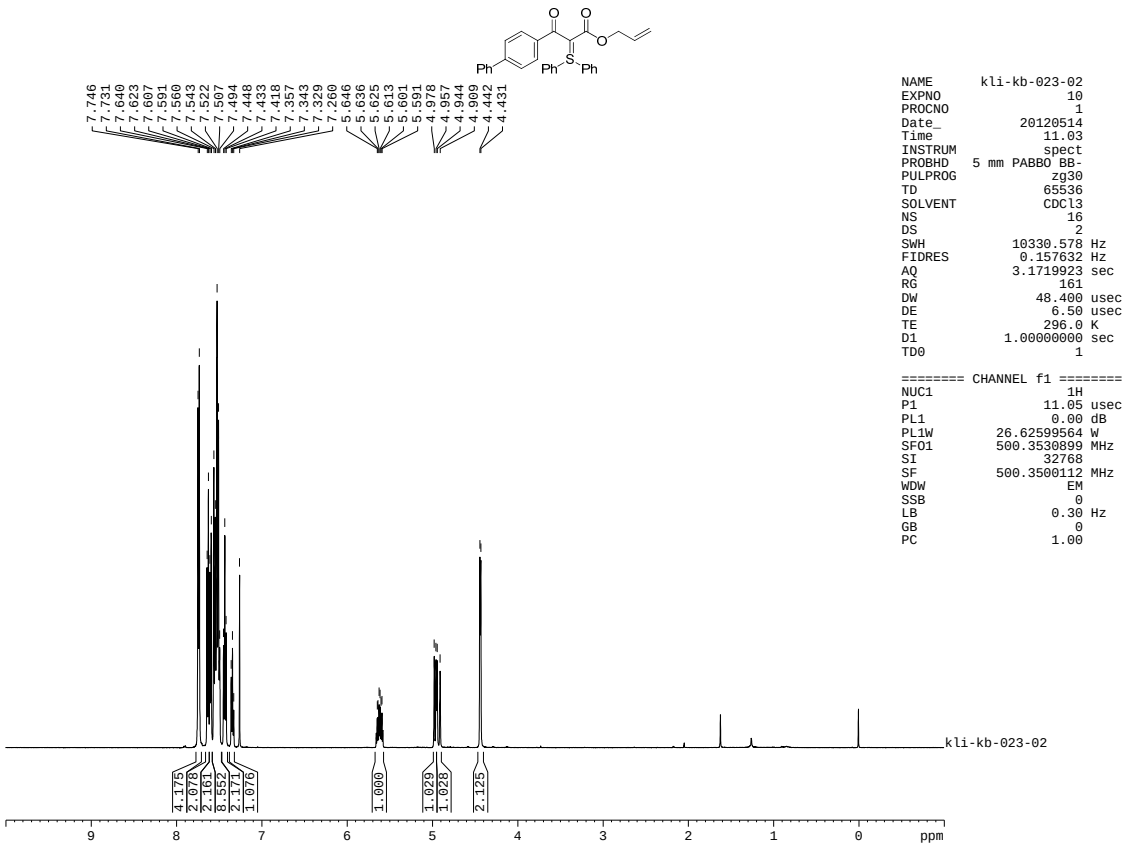

7.737 7.732 7.726 7.723 7.719 7.713 7.705 7.601 7.594 7.582 7.572 7.561 7.553 7.543 7.539 7.534 7.530 7.520 7.517 7.513 7.509 7.500 7.495 7.487 7.483 7.477 7.471 7.465 7.033 7.026 7.010 7.003 6.997 6.981 6.974 6.692 5.674 5.656 5.635 5.617 5.599 5.040 5.035 5.031 5.017 5.012 5.006 5.000 4.996 4.955 4.950 4.446 4.441 4.436 4.428 4.423 4.418
NAME mnu-mb-010-02
EXPNO 10
PROCNO 1
Date_ 20120912
Time 22.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4526453 sec
RG 76
DW 83.200 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.70 usec
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
mnu-mb-010-02
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 ppm
4.101 8.188 2.028 1.000 2.015 2.019

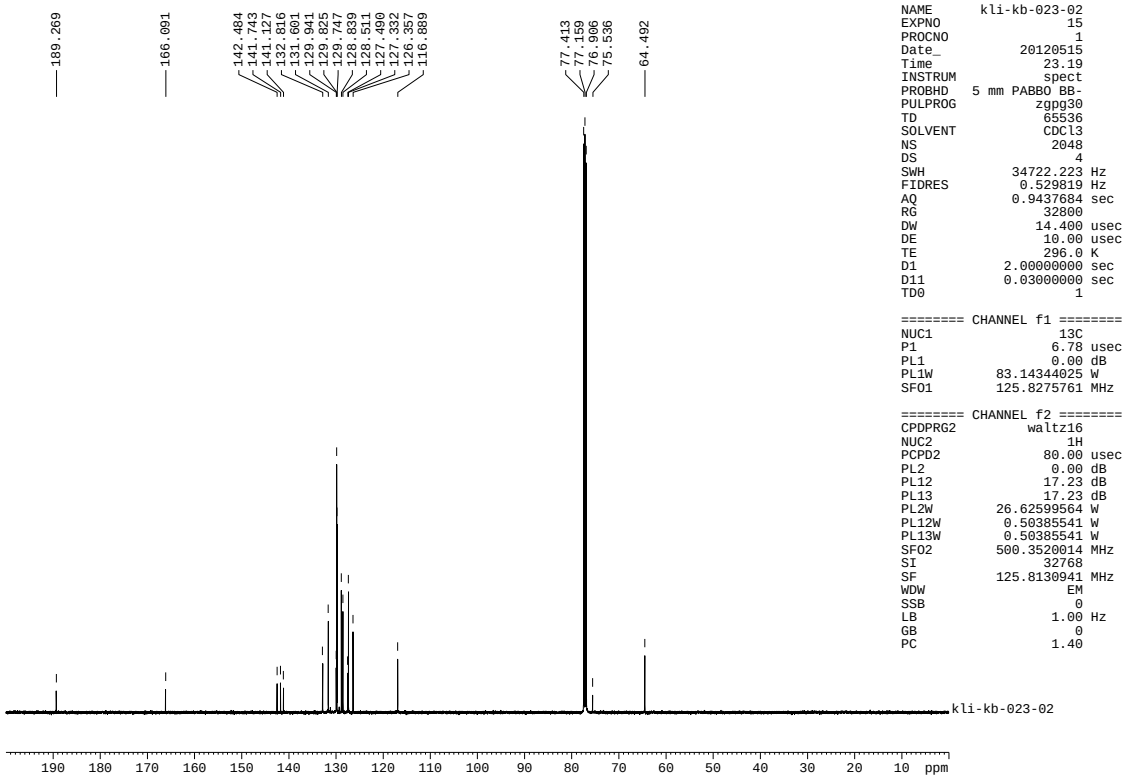

188.057 165.602 165.185 161.892 138.684 138.641 132.619 131.384 130.030 129.917 129.682 129.515 129.509 116.817 114.265 113.978 77.426 77.001 76.577 75.287 64.198
NAME mnu-mb-010-02
EXPNO 11
PROCNO 1
Date_ 20120912
Time 21.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 21306.818 Hz
FIDRES 0.325116 Hz
AQ 1.5379615 sec
RG 1440
DW 23.467 usec
DE 6.50 usec
TE 303.0 K
D1 0.03000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4775598 MHz
NUC1 13C
P1 10.00 usec
SI 65536
SF 75.4677587 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.40
mnu-mb-010-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

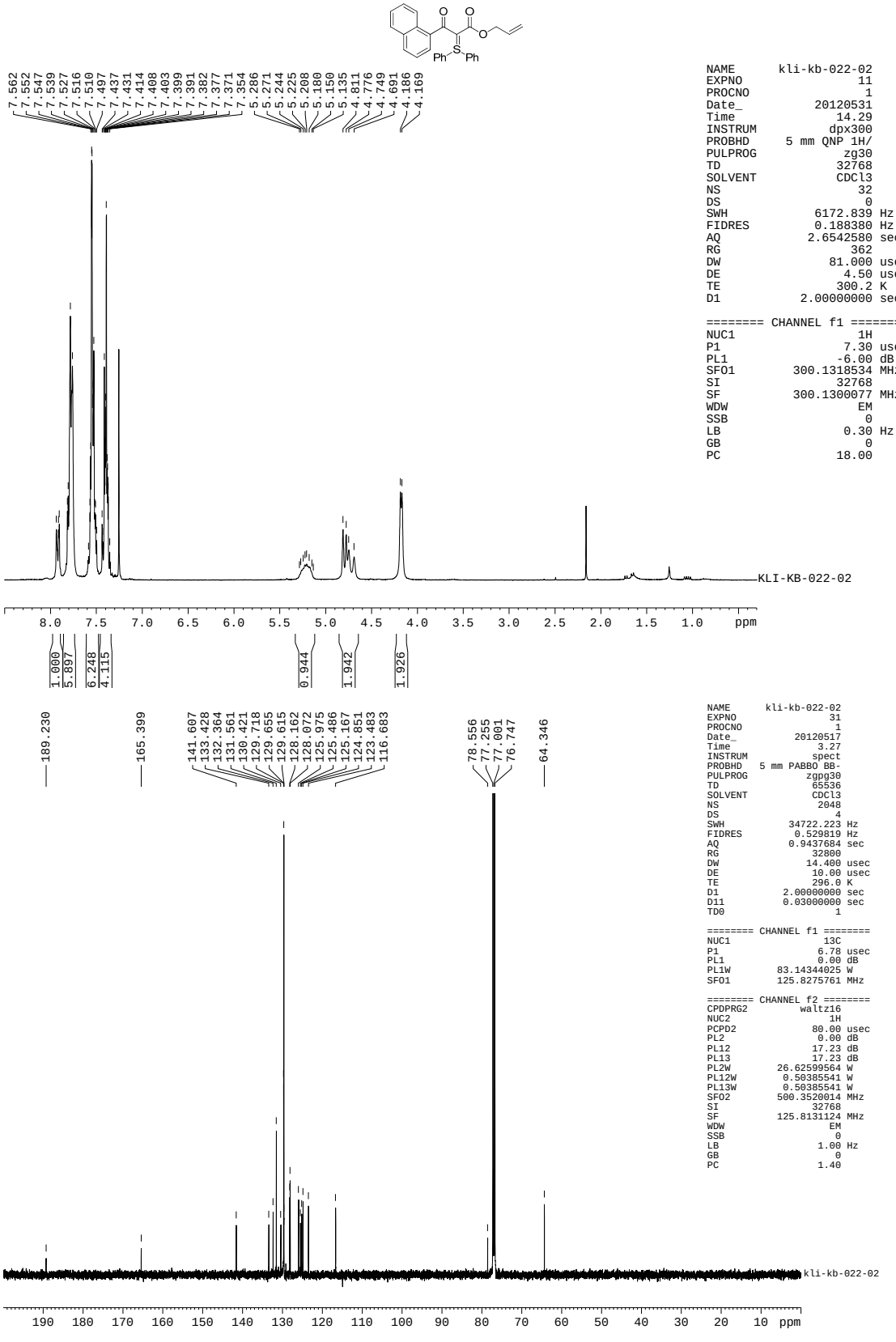

Me
Ph
S
Ph
O
O
O
7.746 7.740 7.738 7.734 7.729 7.724 7.721 7.552 7.549 7.545 7.537 7.532 7.526 7.524 7.519 7.508 7.503 7.491 7.476 7.153 7.137 5.689 5.678 5.668 5.657 5.655 5.646 5.644 5.633 5.623 5.612 5.018 5.016 5.013 5.010 4.994 4.992 4.989 4.980 4.976 4.973 4.945 4.942 4.939 4.936 4.450 4.447 4.444 4.439 4.436 4.434 2.366
NAME HUG-HC-182-02
EXPNO 10
PROCNO 1
Date_ 20120210
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-182-02
4.135
8.383
2.112
1.000
2.061
2.118
3.176
11 10 9 8 7 6 5 4 3 2 1 0 ppm
189.423
165.863
139.794
139.607
132.789
131.306
129.901
129.582
129.487
127.984
127.894
116.585
77.252
76.998
76.744
74.825
64.156
21.396
NAME HUG-HC-182-02
EXPNO 11
PROCNO 1
Date_ 20120210
Time 9.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131196 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-182-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

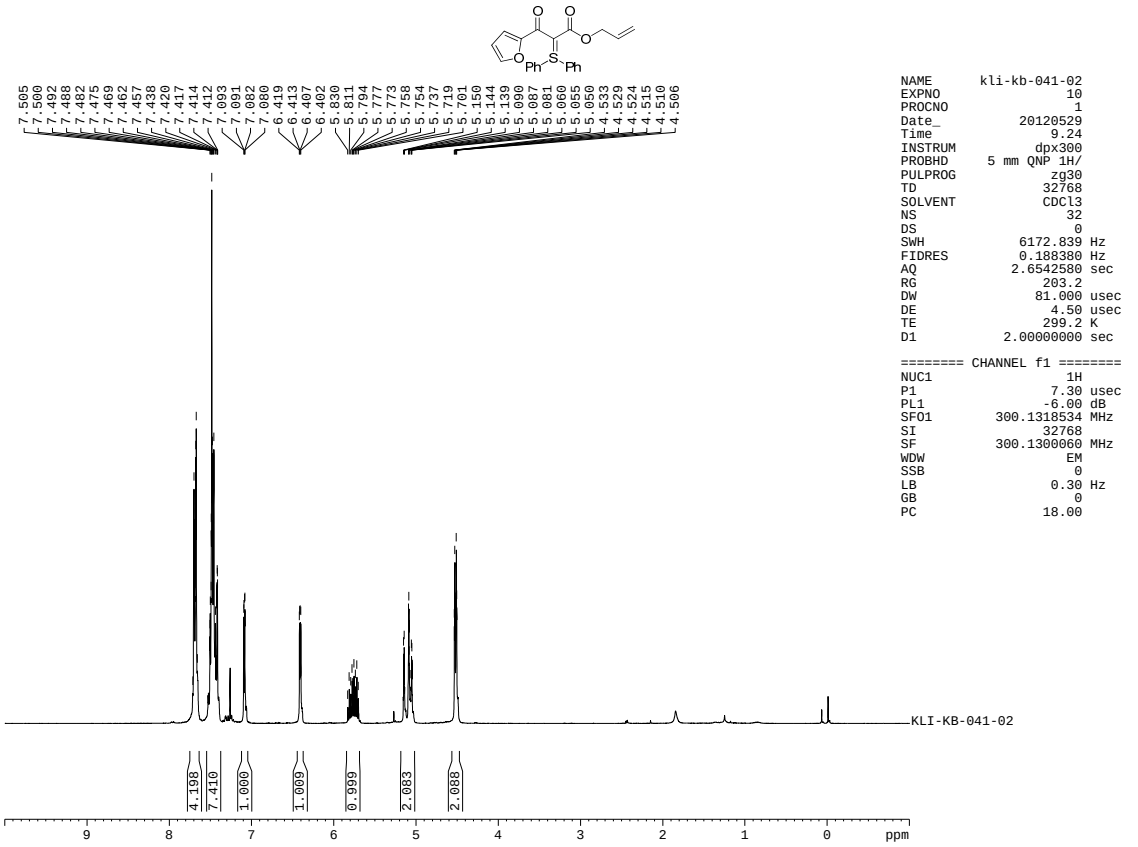

7.740 7.734 7.731 7.728 7.722 7.718 7.715 7.607 7.602 7.598 7.588 7.584 7.579 7.549 7.546 7.542 7.534 7.529 7.524 7.521 7.516 7.505 7.500 7.491 7.487 7.483 6.869 6.864 6.860 6.850 6.846 6.841 5.712 5.701 5.691 5.680 5.667 5.656 5.646 5.635 5.028 5.025 5.022 5.007 5.004 5.000 4.997 4.994 4.969 4.966 4.963 4.960 4.460 4.457 4.454 4.449 4.446 4.443 3.829
MeO
Ph
Ph
NAME HUG-HC-179B
EXPNO 10
PROCNO 1
Date_ 20120130
Time 12.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-179B
4.141 2.086 6.310 2.125 1.000 2.058 2.115 3.216
11 10 9 8 7 6 5 4 3 2 1 0 ppm

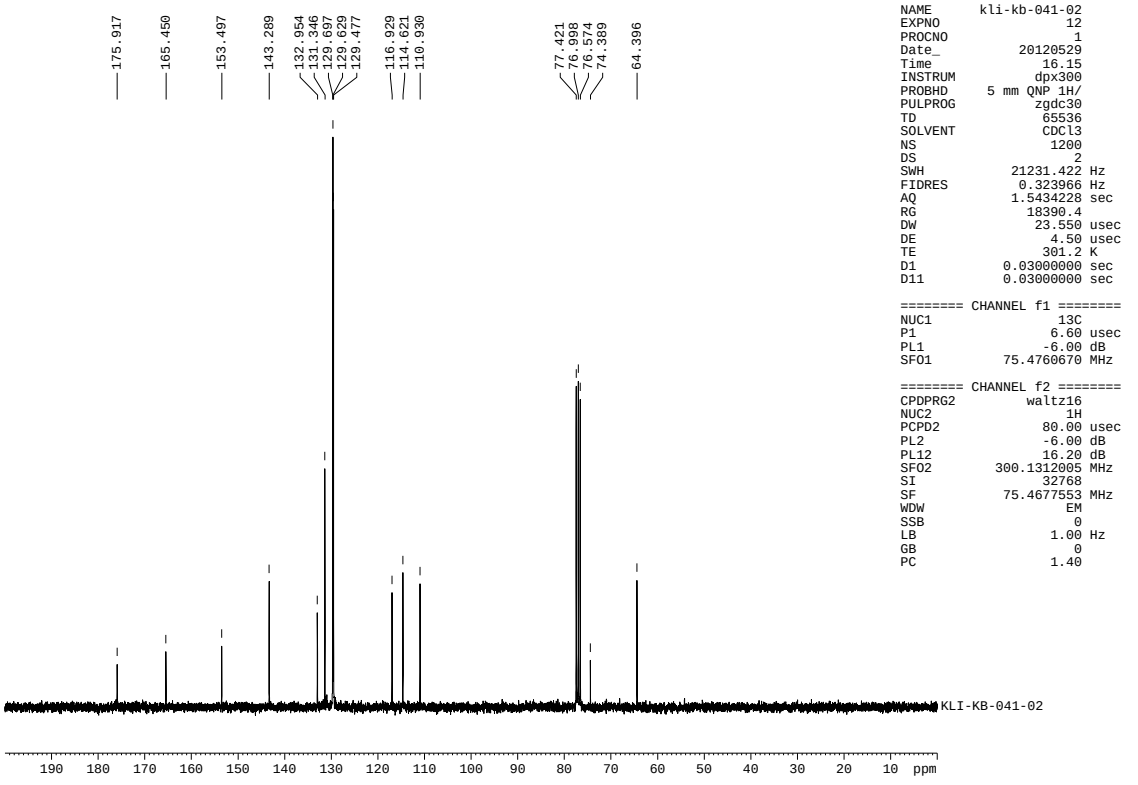

188.647 165.890 161.004 134.910 132.856 131.297 130.070 130.015 129.589 129.491 116.672 112.562 77.254 77.000 76.746 74.550 64.173 55.220
NAME HUG-HC-179B
EXPNO 11
PROCNO 1
Date_ 20120130
Time 12.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131174 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-179B
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

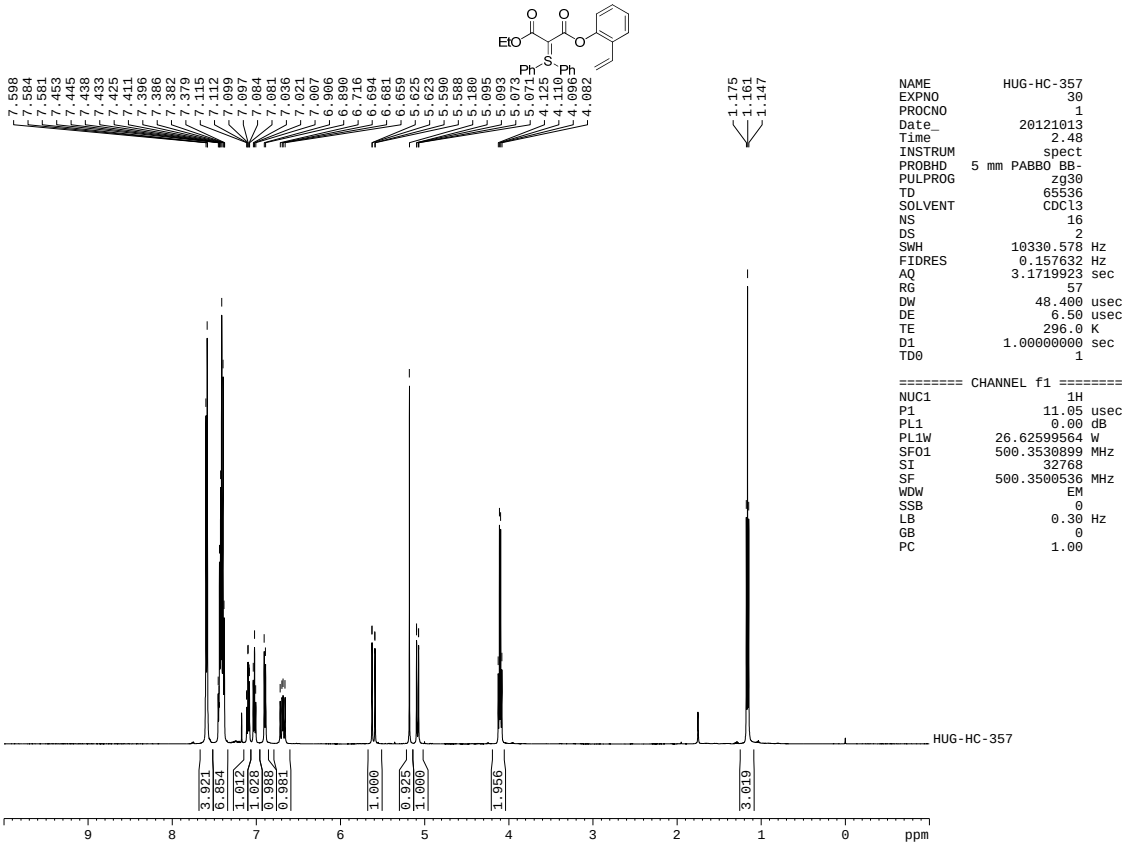

7.746
7.731
7.640
7.623
7.607
7.591
7.560
7.543
7.522
7.507
7.494
7.448
7.433
7.418
7.357
7.343
7.329
7.260
5.646
5.636
5.625
5.613
5.601
5.591
4.978
4.957
4.944
4.909
4.442
4.431
NAME kli-kb-023-02
EXPNO 10
PROCNO 1
Date_ 20120514
Time 11.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
kli-kb-023-02
4.175
2.078
2.161
8.552
2.171
1.076
1.000
1.029
1.028
2.125
9
8
7
6
5
4
3
2
1
0
ppm


189.269
166.091
142.484
141.743
141.127
132.816
131.601
129.941
129.825
129.747
128.839
128.511
127.490
127.332
126.357
116.889
77.413
77.159
76.906
75.536
64.492
NAME kli-kb-023-02
EXPNO 15
PROCNO 1
Date_ 20120515
Time 23.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8130941 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-023-02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.562
7.552
7.547
7.539
7.527
7.516
7.510
7.497
7.437
7.431
7.414
7.408
7.403
7.399
7.391
7.382
7.377
7.371
7.354
5.286
5.271
5.244
5.225
5.208
5.180
5.150
5.135
4.811
4.776
4.749
4.691
4.186
4.169
NAME kli-kb-022-02
EXPNO 11
PROCNO 1
Date_ 20120531
Time 14.29
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 362
DW 81.000 usec
DE 4.50 usec
TE 300.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
KLI-KB-022-02
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 ppm
1.000
5.897
6.248
4.115
0.944
1.942
1.926
189.230
165.399
141.607
133.428
132.364
131.561
130.421
129.718
129.655
129.615
128.162
128.072
125.975
125.486
125.167
124.851
123.483
116.683
78.556
77.255
77.001
76.747
64.346
NAME kli-kb-022-02
EXPNO 31
PROCNO 1
Date_ 20120517
Time 3.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131124 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-022-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

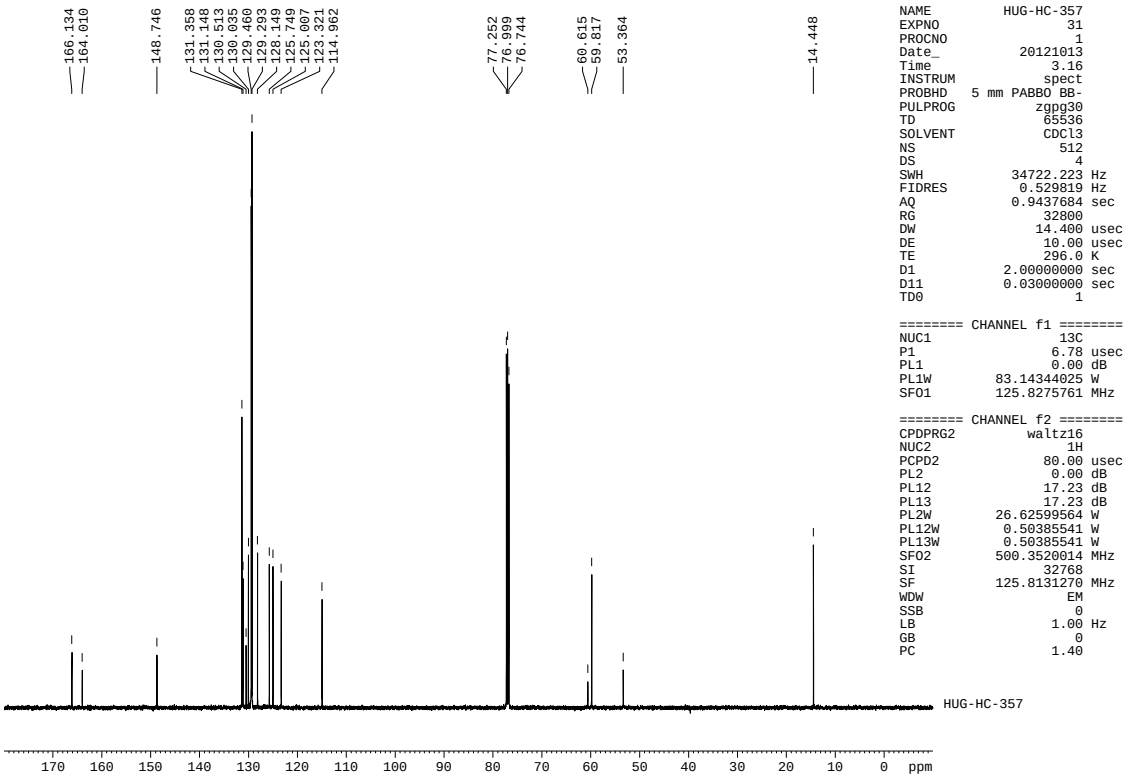

7.505
7.500
7.492
7.488
7.482
7.475
7.469
7.462
7.457
7.438
7.420
7.417
7.414
7.412
7.093
7.091
7.082
7.080
6.419
6.413
6.407
6.402
5.830
5.811
5.794
5.777
5.773
5.758
5.754
5.737
5.719
5.701
5.150
5.144
5.139
5.090
5.087
5.081
5.060
5.055
5.050
4.533
4.529
4.524
4.515
4.510
4.506
NAME kli-kb-041-02
EXPNO 10
PROCNO 1
Date_ 20120529
Time 9.24
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 203.2
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
KLI-KB-041-02
4.198
7.410
1.000
1.009
0.999
2.083
2.008
9
8
7
6
5
4
3
2
1
0
ppm


175.917
165.450
153.497
143.289
132.954
131.346
129.697
129.629
129.477
116.929
114.621
110.930
77.421
76.998
76.574
74.389
64.396
NAME kli-kb-041-02
EXPNO 12
PROCNO 1
Date_ 20120529
Time 16.15
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 18390.4
DW 23.550 usec
DE 4.50 usec
TE 301.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677553 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
KLI-KB-041-02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm




```
NAME          HUG-HC-357
EXPNO             30
PROCNO             1
Date_          20121013
Time               2.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                16
DS                 2
SWH          10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG                57
DW              48.400 usec
DE               6.50 usec
TE              296.0 K
D1           1.00000000 sec
TD0                1

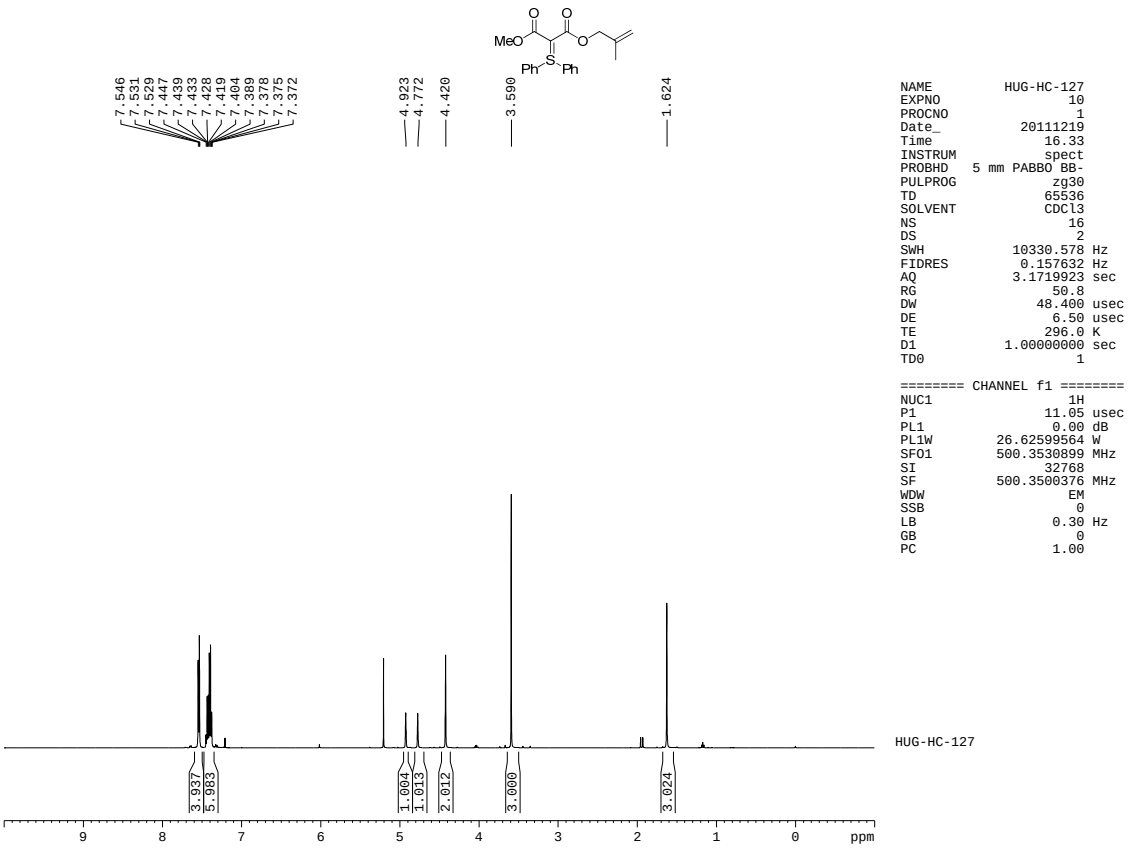
======== CHANNEL f1 ========
NUC1               1H
P1              11.05 usec
PL1              0.00 dB
PL1W       26.62599564 W
SFO1       500.3530899 MHz
SI              32768
SF         500.3500536 MHz
WDW                EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```




```
NAME          HUG-HC-357
EXPNO             31
PROCNO             1
Date_          20121013
Time               3.16
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                512
DS                 4
SWH          34722.223 Hz
FIDRES        0.529819 Hz
AQ            0.9437684 sec
RG                32800
DW              14.400 usec
DE              10.00 usec
TE              296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                1

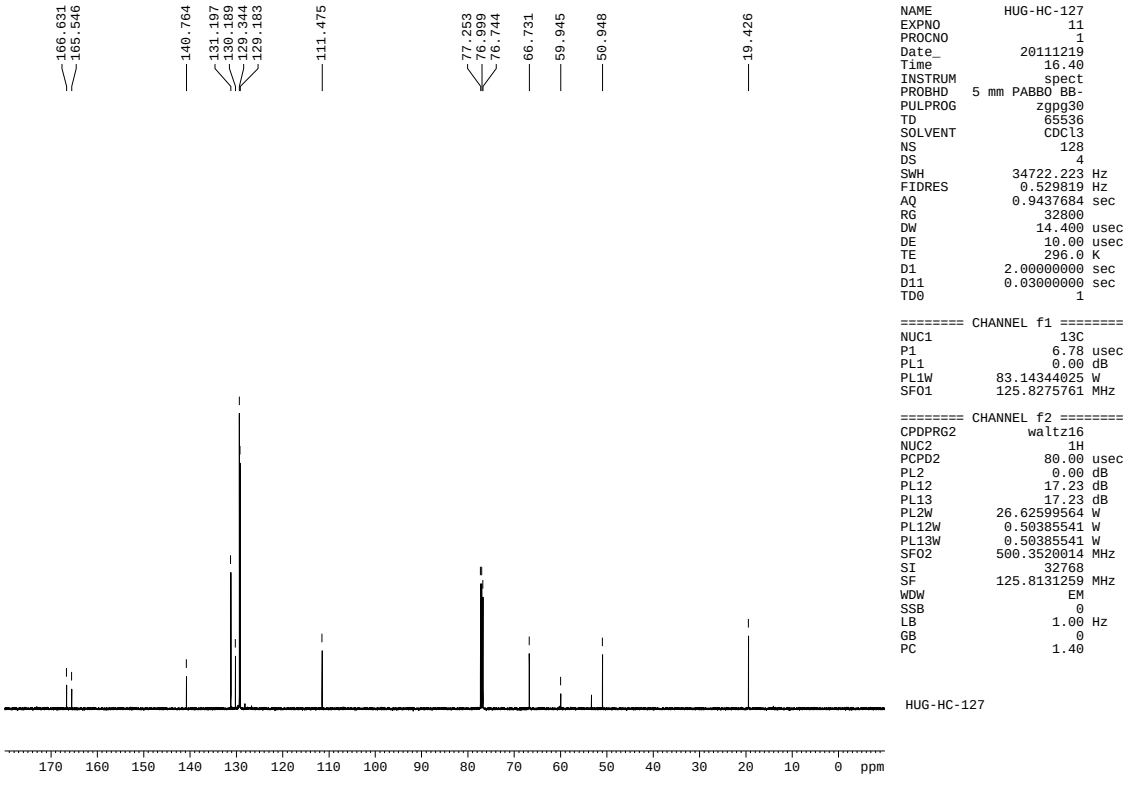
======== CHANNEL f1 ========
NUC1               13C
P1               6.78 usec
PL1              0.00 dB
PL1W       83.14344025 W
SFO1       125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2           80.00 usec
PL2              0.00 dB
PL12            17.23 dB
PL13            17.23 dB
PL2W       26.62599564 W
PL12W       0.50385541 W
PL13W       0.50385541 W
SFO2       500.3520014 MHz
SI              32768
SF         125.8131270 MHz
WDW                EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```




```
NAME          HUG-HC-127
EXPNO                 10
PROCNO                 1
Date_           20111219
Time               16.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                  50.8
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

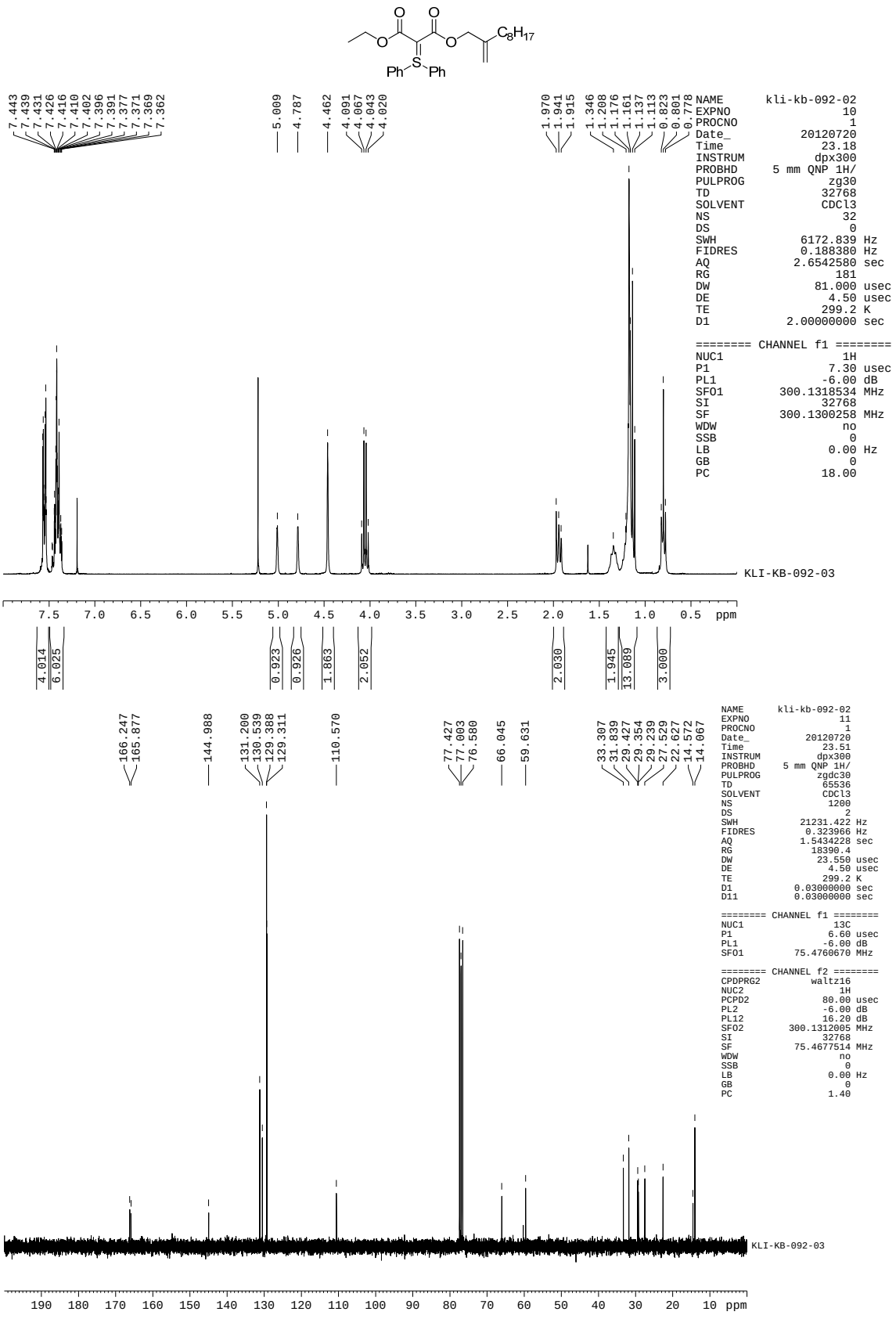
======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500376 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

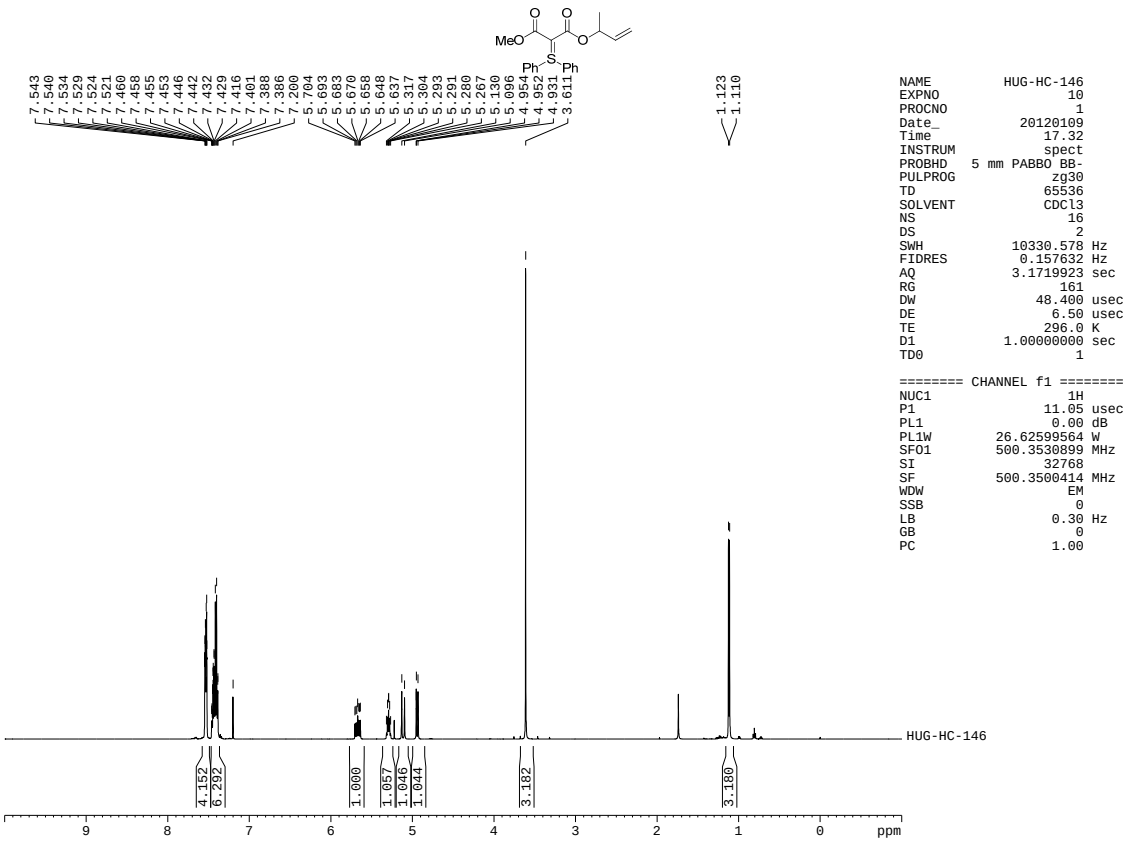



```
NAME          HUG-HC-127
EXPNO                 11
PROCNO                 1
Date_           20111219
Time               16.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131259 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```


O
O
O
O
C_8H_{17}
Ph
S
Ph
7.443
7.439
7.431
7.426
7.416
7.410
7.402
7.396
7.391
7.377
7.371
7.369
7.362
5.009
4.787
4.462
4.091
4.067
4.043
4.020
1.970
1.941
1.915
1.346
1.208
1.176
1.161
1.137
1.113
0.823
0.801
0.778
NAME kli-kb-092-02
EXPNO 10
PROCNO 1
Date_ 20120720
Time 23.18
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 181
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300258 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 18.00
KLI-KB-092-03
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 ppm
4.014
6.025
0.923
0.926
1.863
2.052
2.030
1.945
13.089
3.000
166.247
165.877
144.988
131.200
130.539
129.388
129.311
110.570
77.427
77.003
76.580
66.045
59.631
33.307
31.839
29.427
29.354
29.239
27.529
22.627
14.572
14.067
NAME kli-kb-092-02
EXPNO 11
PROCNO 1
Date_ 20120720
Time 23.51
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 18390.4
DW 23.550 usec
DE 4.50 usec
TE 299.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677514 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
KLI-KB-092-03
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


MeO
O
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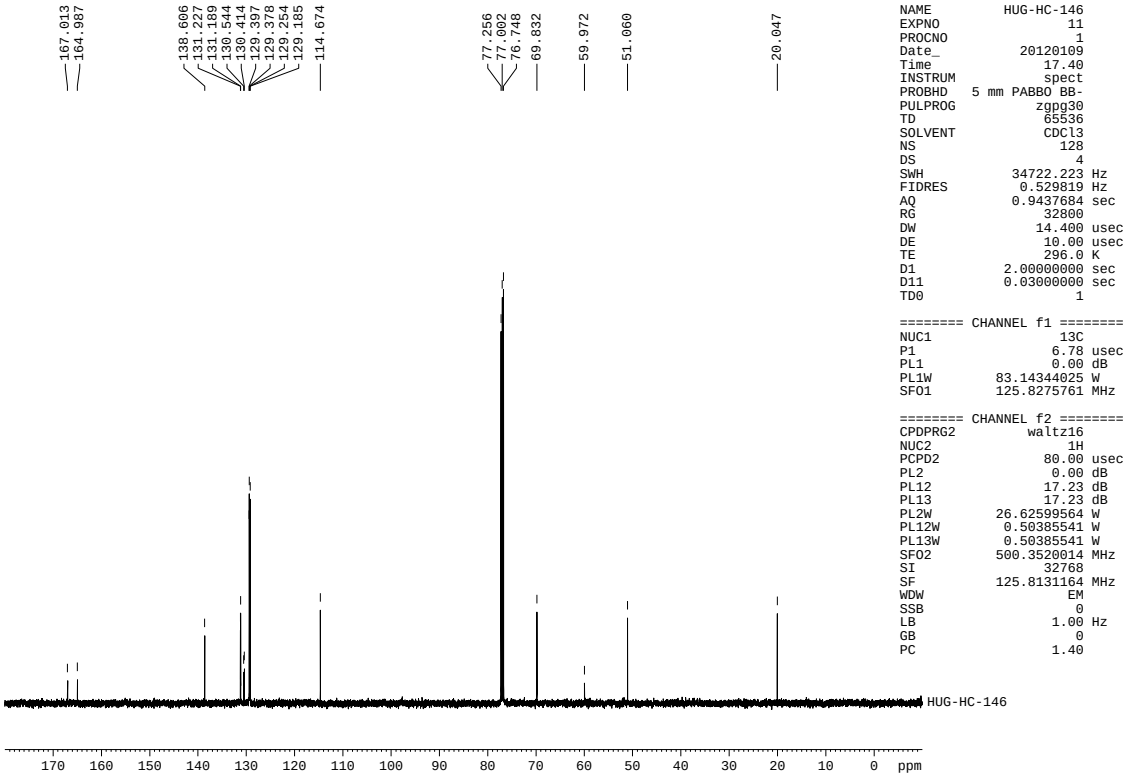
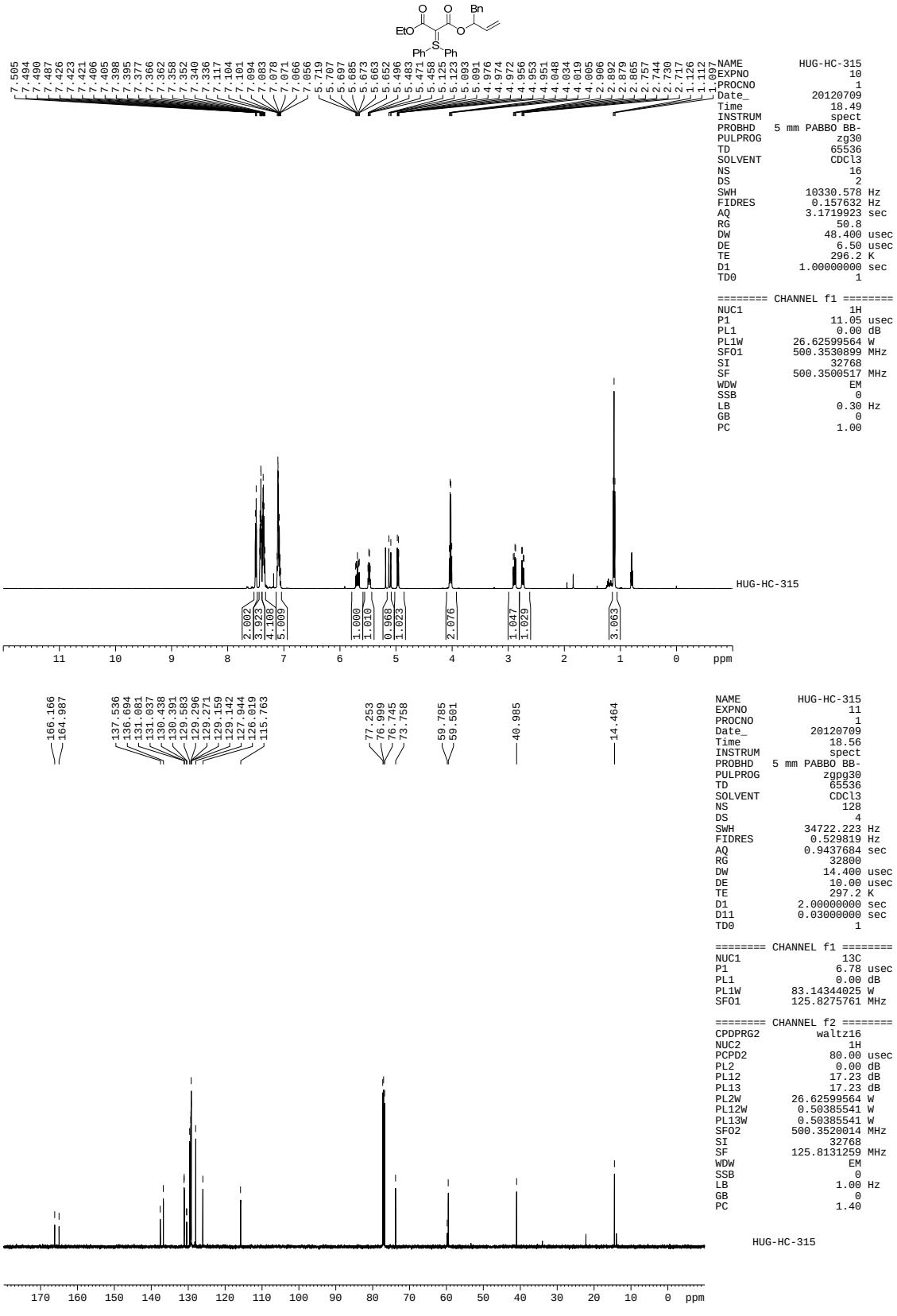
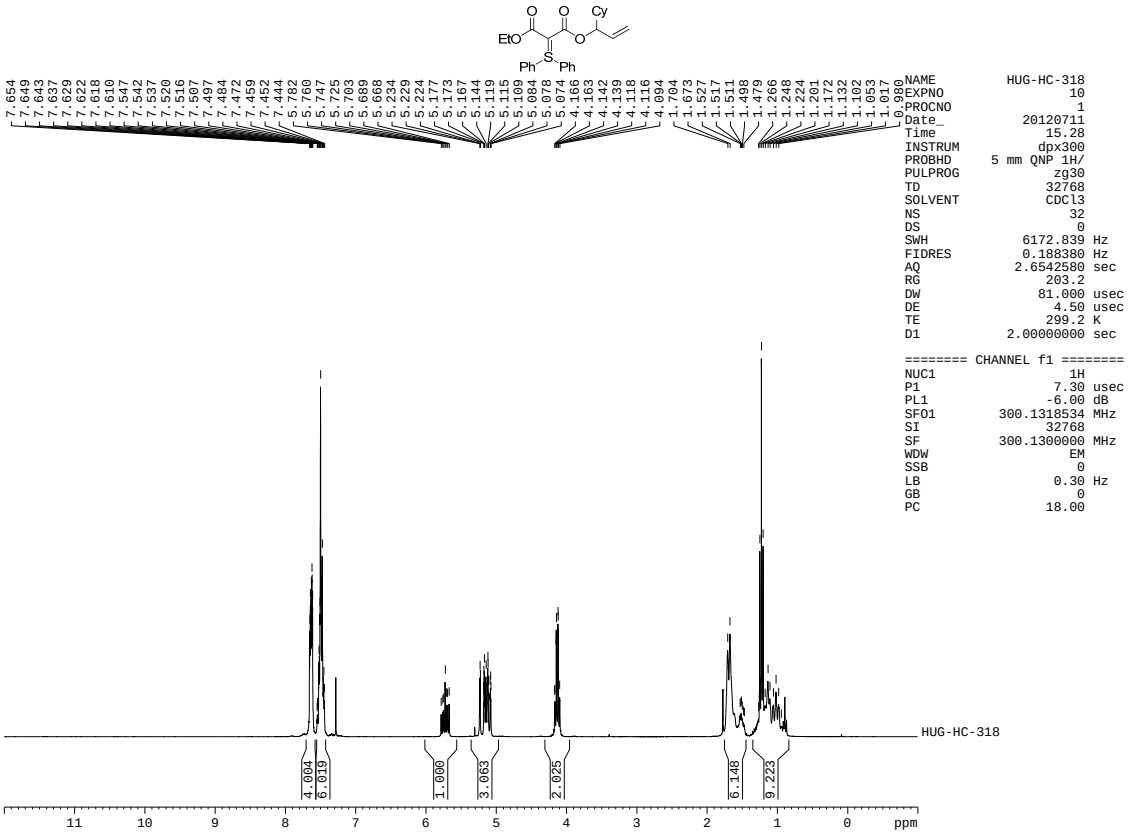
O
Si
Ph
Ph
7.543
7.540
7.534
7.529
7.524
7.521
7.460
7.458
7.455
7.453
7.446
7.442
7.432
7.429
7.416
7.401
7.388
7.386
7.200
5.704
5.693
5.683
5.670
5.658
5.648
5.637
5.317
5.304
5.293
5.291
5.280
5.267
5.130
5.096
4.954
4.952
4.931
3.611
1.123
1.110
NAME HUG-HC-146
EXPNO 10
PROCNO 1
Date_ 20120109
Time 17.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500414 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-146
4.152
6.292
1.000
1.057
1.046
1.044
3.182
3.180
9
8
7
6
5
4
3
2
1
0
ppm

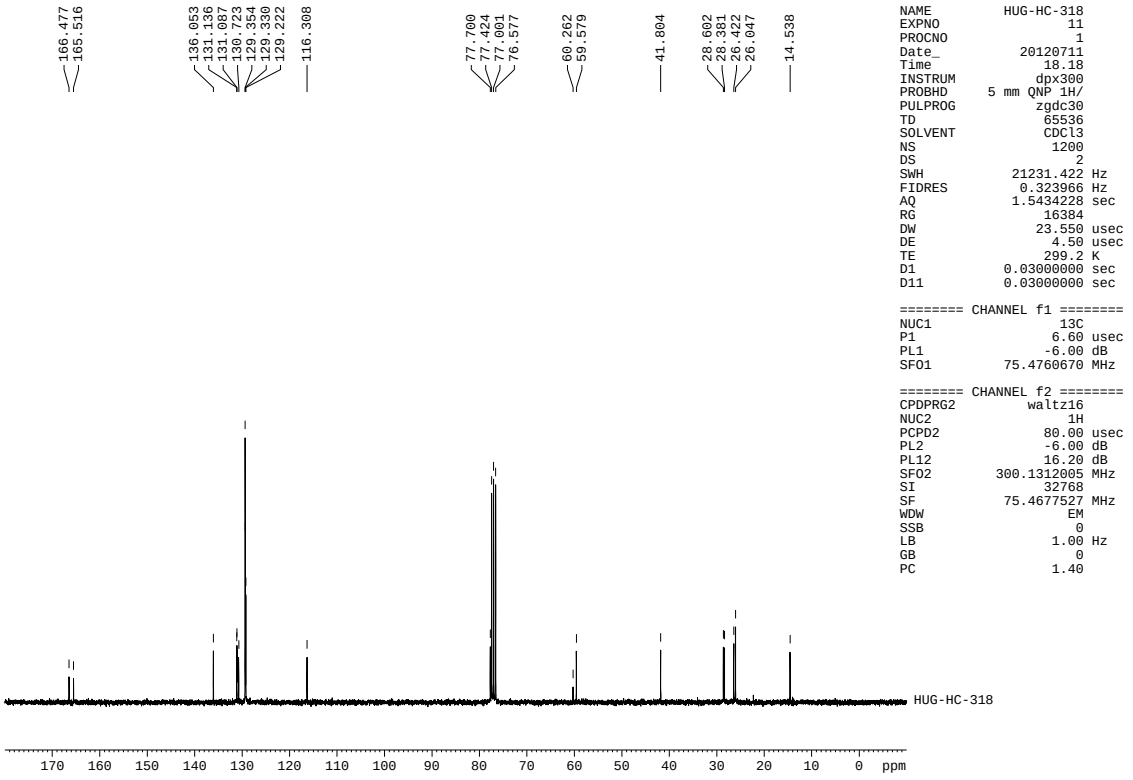

167.013
164.987
138.606
131.227
131.189
130.544
130.414
129.397
129.378
129.254
129.185
114.674
77.256
77.002
76.748
69.832
59.972
51.060
20.047
NAME HUG-HC-146
EXPNO 11
PROCNO 1
Date_ 20120109
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131164 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-146
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


EtO
O
O
Bn
S
Ph
Ph
HUG-HC-315
ppm
HUG-HC-315
ppm




```
NAME          HUG-HC-318
EXPNO                 10
PROCNO                 1
Date_           20120711
Time               15.28
INSTRUM            dpx300
PROBHD     5 mm QNP 1H/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             6172.839 Hz
FIDRES          0.188380 Hz
AQ              2.6542580 sec
RG                 203.2
DW                81.000 usec
DE                 4.50 usec
TE                 299.2 K
D1              2.00000000 sec

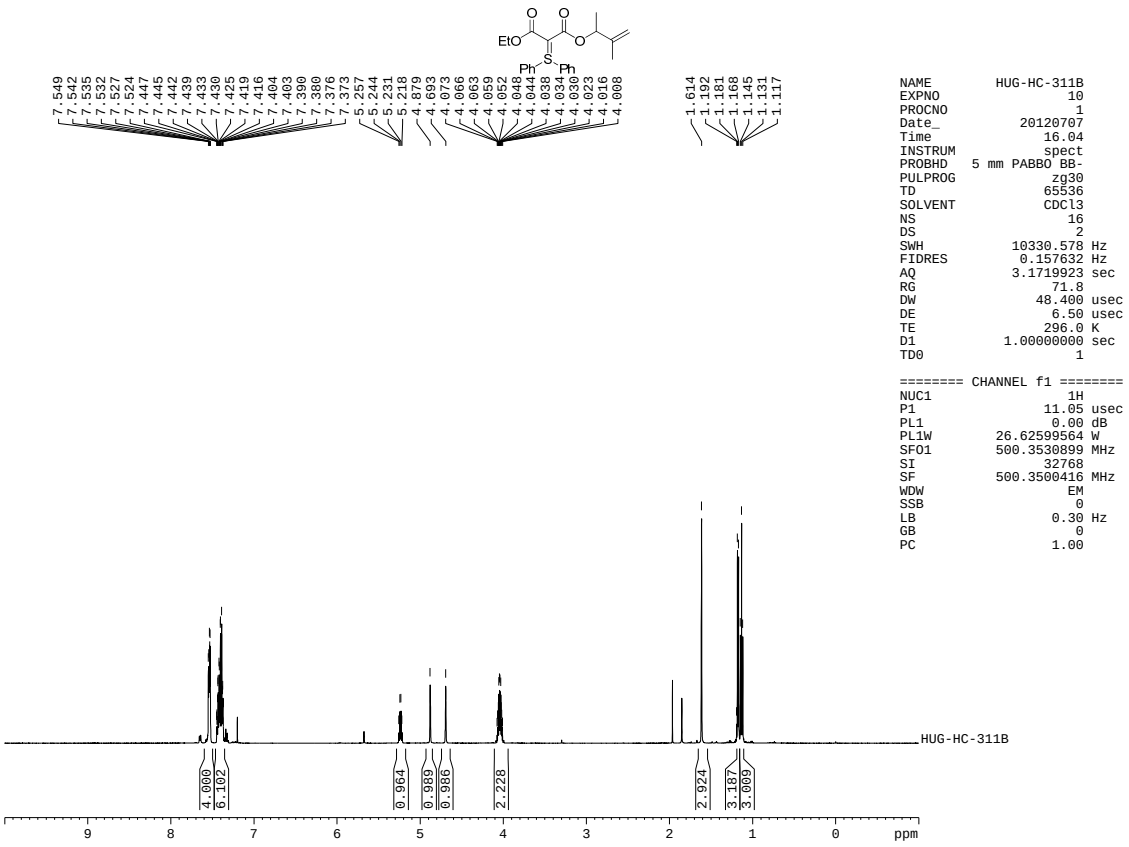
======== CHANNEL f1 ========
NUC1                1H
P1                 7.30 usec
PL1                -6.00 dB
SFO1         300.1318534 MHz
SI                 32768
SF           300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                 18.00
```

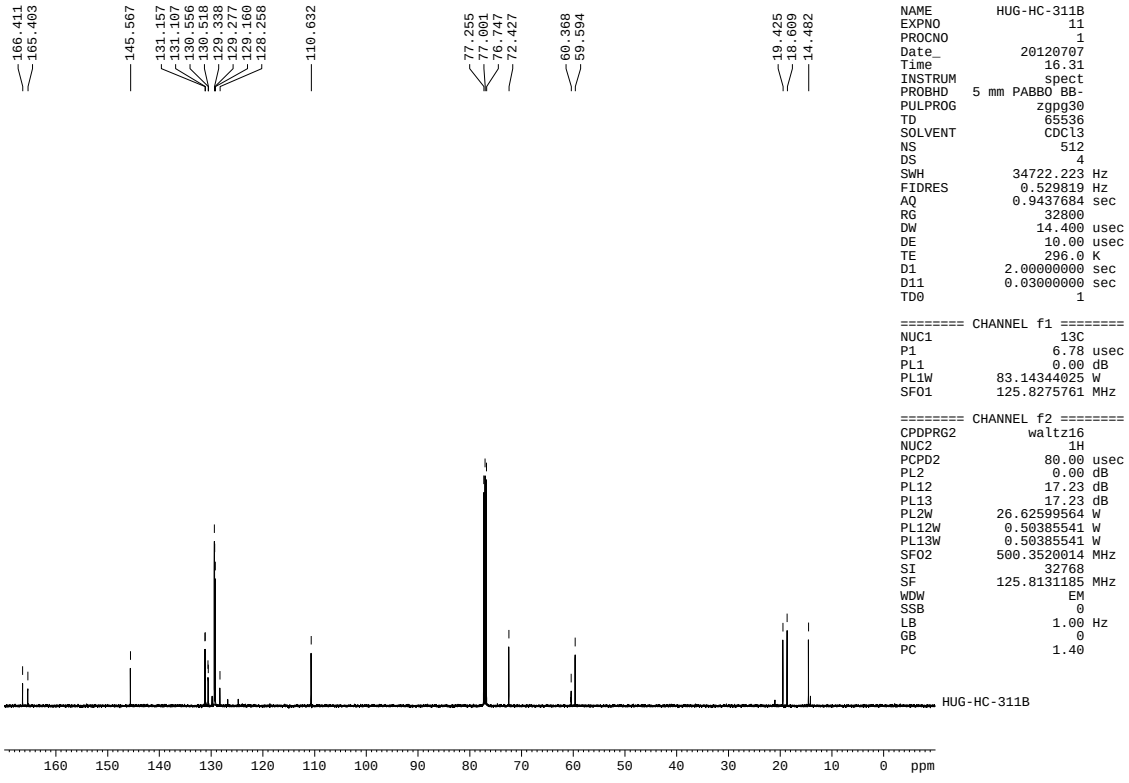


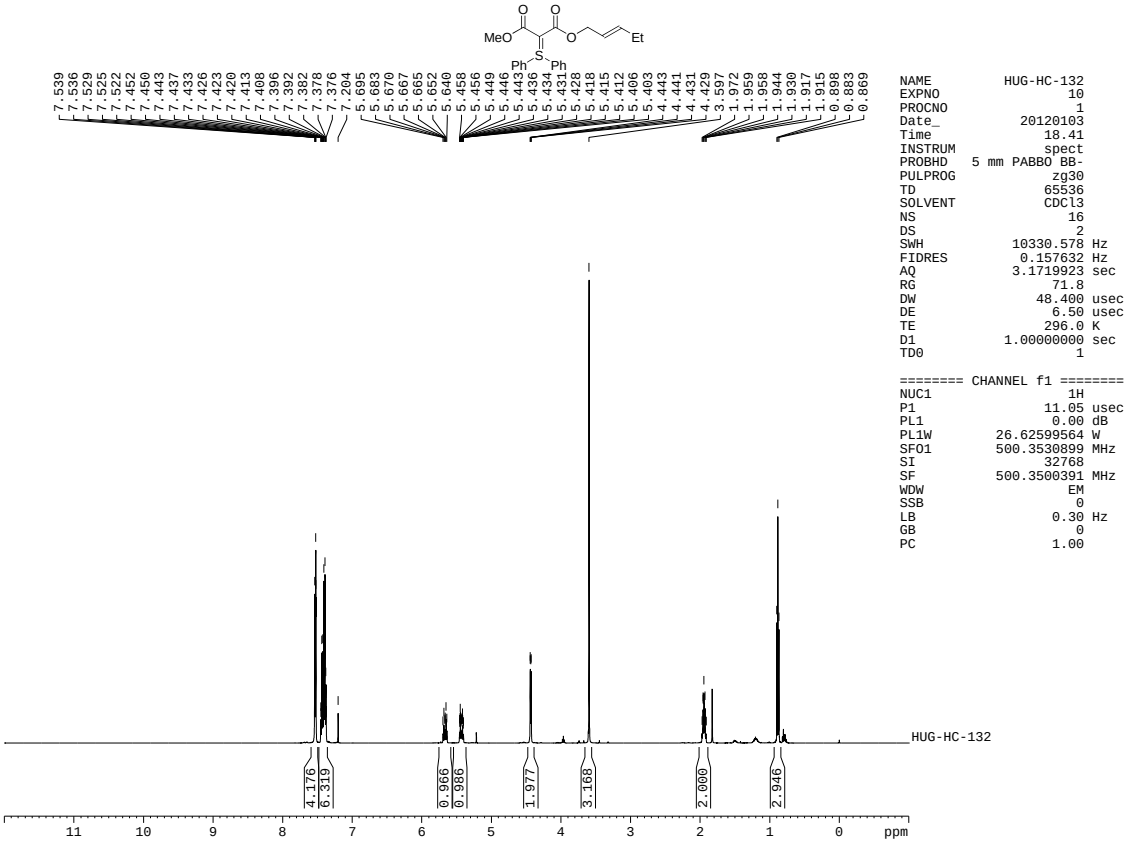

```
NAME          HUG-HC-318
EXPNO                 11
PROCNO                 1
Date_           20120711
Time               18.18
INSTRUM            dpx300
PROBHD     5 mm QNP 1H/
PULPROG           zgdc30
TD                 65536
SOLVENT            CDCl3
NS                  1200
DS                     2
SWH            21231.422 Hz
FIDRES          0.323966 Hz
AQ              1.5434228 sec
RG                 16384
DW                23.550 usec
DE                 4.50 usec
TE                 299.2 K
D1              0.03000000 sec
D11             0.03000000 sec

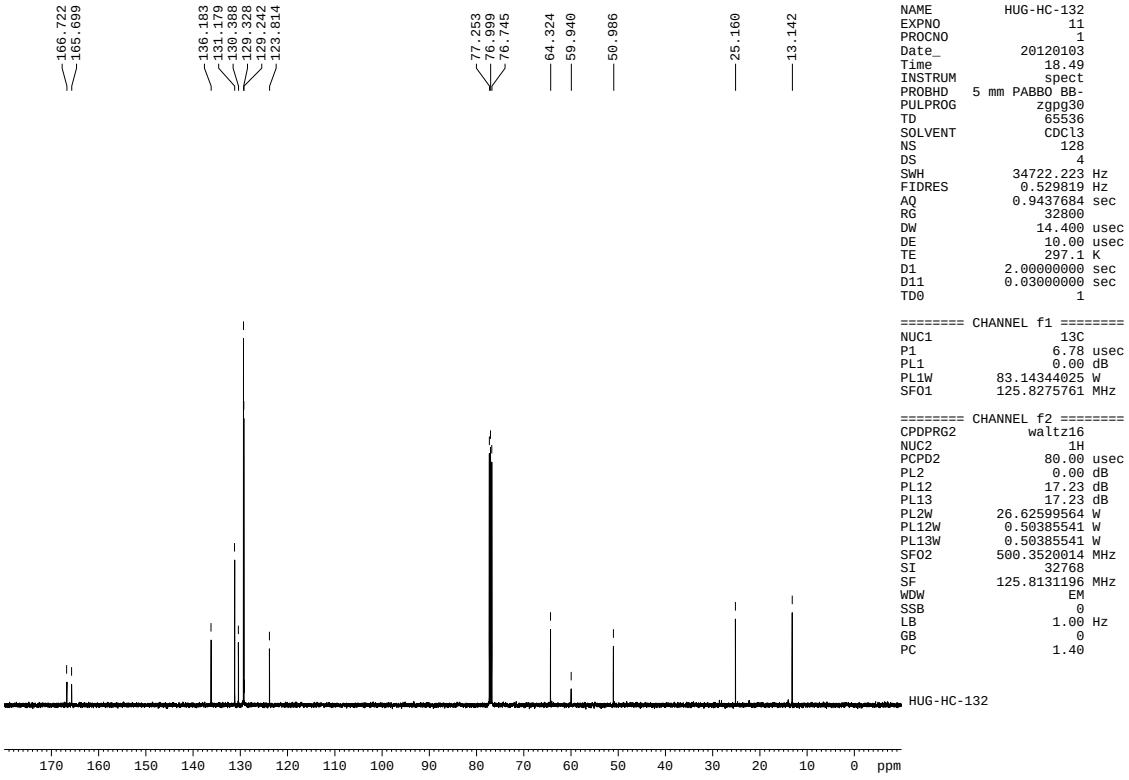
======== CHANNEL f1 ========
NUC1                13C
P1                 6.60 usec
PL1                -6.00 dB
SFO1         75.4760670 MHz

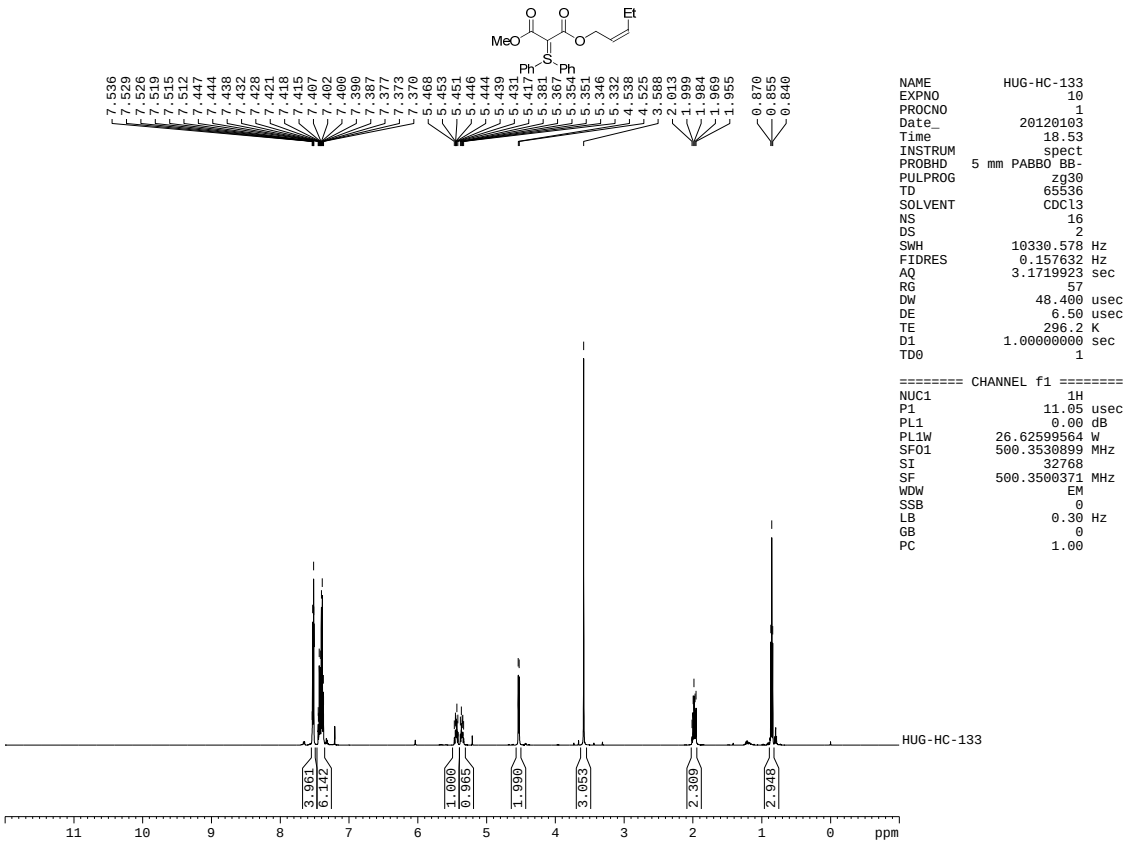
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                -6.00 dB
PL12               16.20 dB
SFO2         300.1312005 MHz
SI                 32768
SF           75.4677527 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                 1.40
```

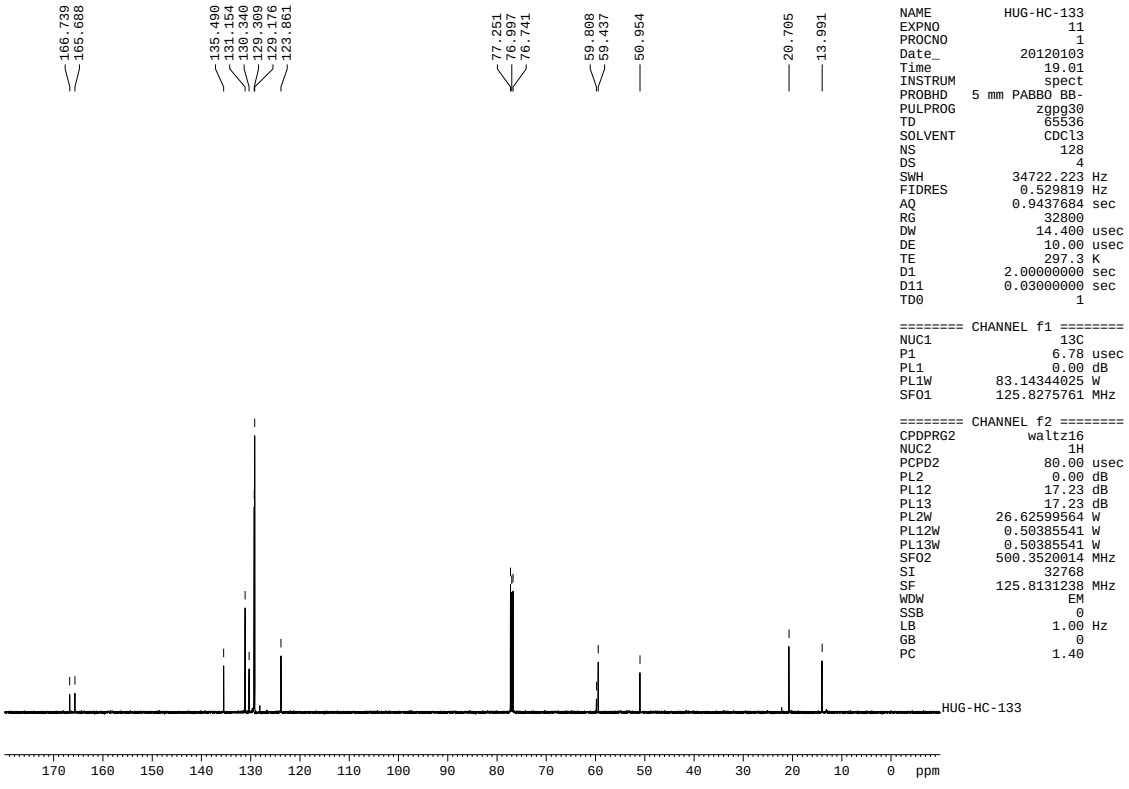

EtO
O
O
O
S
Ph
Ph
7.549 7.542 7.535 7.532 7.527 7.524 7.447 7.445 7.442 7.439 7.433 7.430 7.425 7.419 7.416 7.404 7.403 7.390 7.380 7.376 7.373
5.257 5.244 5.231 5.218 4.879 4.693 4.073 4.066 4.063 4.059 4.052 4.048 4.044 4.038 4.034 4.030 4.023 4.016 4.008
1.614 1.192 1.181 1.168 1.145 1.131 1.117
NAME HUG-HC-311B
EXPNO 10
PROCNO 1
Date_ 20120707
Time 16.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500416 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-311B
4.000 6.102 0.964 0.989 0.986 2.228 2.924 3.187 3.009
9 8 7 6 5 4 3 2 1 0 ppm


166.411 165.403
145.567
131.157 131.107 130.556 130.518 129.338 129.277 129.160 128.258
110.632
77.255 77.001 76.747 72.427
60.368 59.594
19.425 18.609 14.482
NAME HUG-HC-311B
EXPNO 11
PROCNO 1
Date_ 20120707
Time 16.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131185 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-311B
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


MeO
O
O
O
Et
S
Ph
Ph
7.539 7.536 7.529 7.525 7.522 7.452 7.450 7.443 7.437 7.433 7.426 7.423 7.420 7.413 7.408 7.396 7.392 7.382 7.378 7.376 7.204 5.695 5.683 5.670 5.667 5.665 5.652 5.640 5.458 5.456 5.449 5.446 5.443 5.436 5.434 5.431 5.428 5.418 5.415 5.412 5.406 5.403 4.443 4.441 4.431 4.429 3.597 1.972 1.959 1.958 1.944 1.930 1.917 1.915 0.898 0.883 0.869
NAME HUG-HC-132
EXPNO 10
PROCNO 1
Date_ 20120103
Time 18.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500391 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-132
4.176 6.319 0.966 0.986 1.977 3.168 2.000 2.946
11 10 9 8 7 6 5 4 3 2 1 0 ppm


166.722 165.699 136.183 131.179 130.388 129.328 129.242 123.814 77.253 76.999 76.745 64.324 59.940 50.986 25.160 13.142
NAME HUG-HC-132
EXPNO 11
PROCNO 1
Date_ 20120103
Time 18.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131196 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-132
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


MeO
O
O
O
Et
S
Ph
Ph
7.536 7.529 7.526 7.519 7.515 7.512 7.447 7.444 7.438 7.432 7.428 7.421 7.418 7.415 7.407 7.402 7.400 7.390 7.387 7.377 7.373 7.370 7.468 5.453 5.451 5.446 5.444 5.439 5.431 5.417 5.381 5.367 5.354 5.351 5.346 5.332 4.538 4.525 3.588 2.013 1.999 1.984 1.969 1.955 0.870 0.855 0.840
NAME HUG-HC-133
EXPNO 10
PROCNO 1
Date_ 20120103
Time 18.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500371 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-133
3.961 6.142 1.000 0.965 1.990 3.053 2.309 2.948
11 10 9 8 7 6 5 4 3 2 1 0 ppm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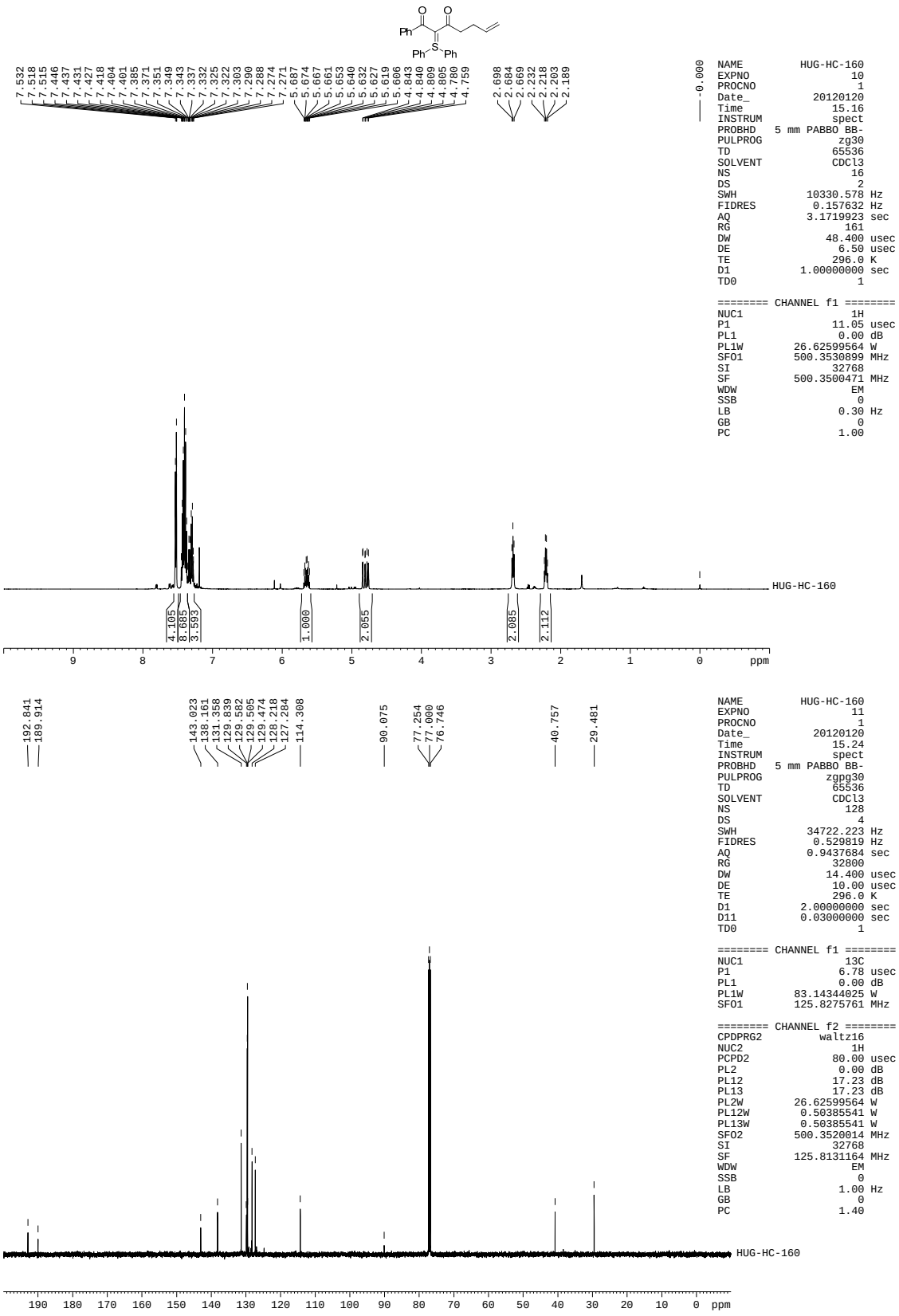
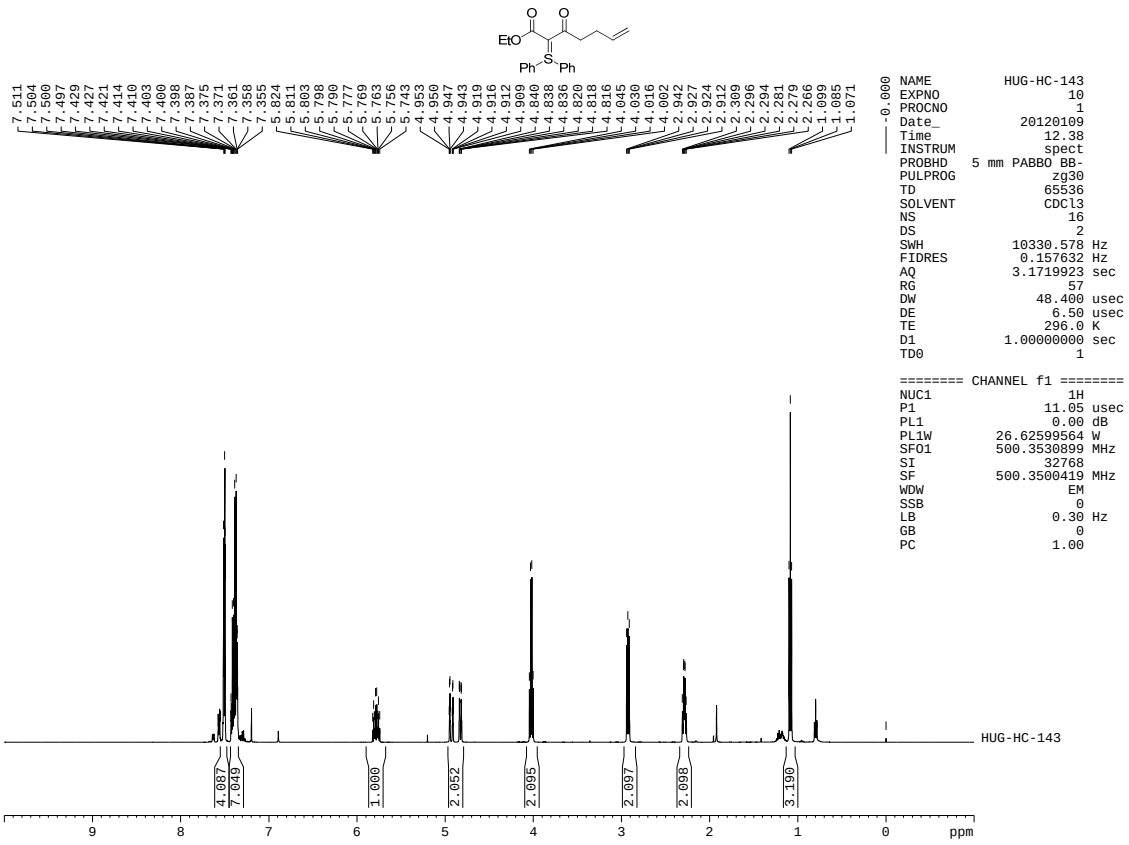
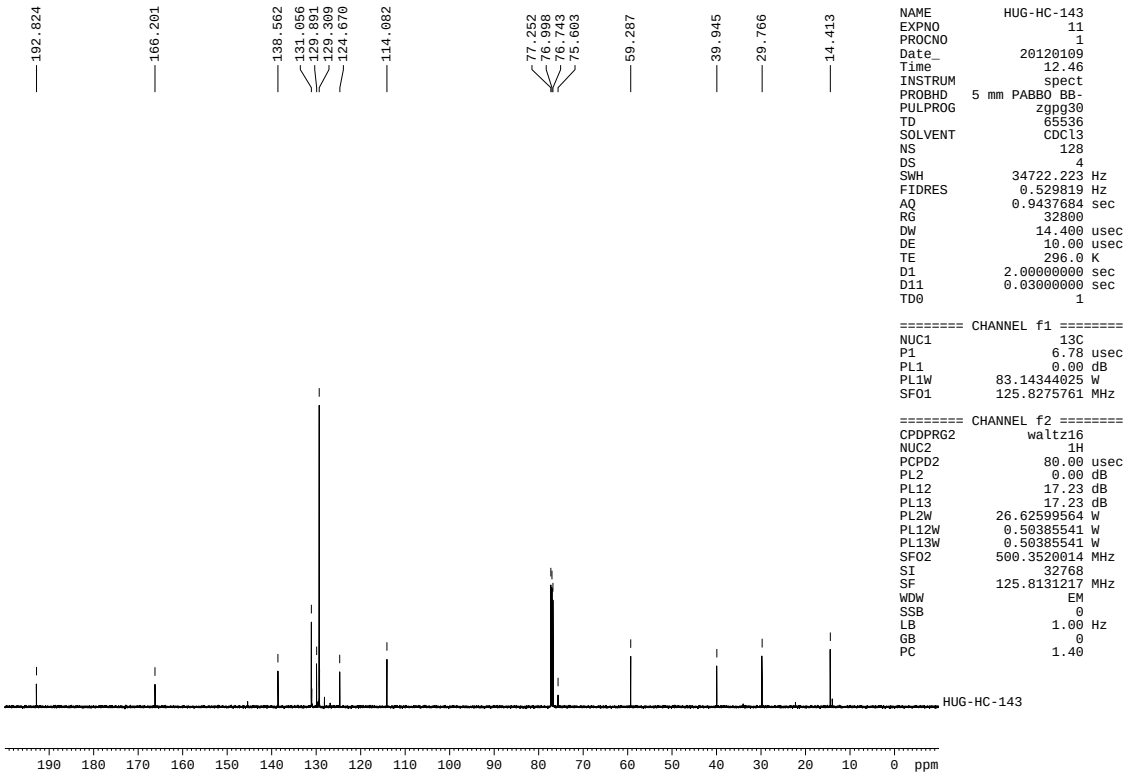
NAME HUG-HC-133
EXPNO 11
PROCNO 1
Date_ 20120103
Time 19.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131238 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-133
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ph
O
O
Ph
S
Ph
7.532 7.518 7.515 7.446 7.437 7.431 7.427 7.418 7.404 7.401 7.385 7.371 7.351 7.349 7.343 7.337 7.332 7.325 7.322 7.303 7.290 7.288 7.274 7.271 5.687 5.674 5.667 5.661 5.653 5.640 5.632 5.627 5.619 5.606 4.843 4.840 4.809 4.805 4.780 4.759 2.698 2.684 2.669 2.232 2.218 2.203 2.189
-0.000
NAME HUG-HC-160
EXPNO 10
PROCNO 1
Date_ 20120120
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500471 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-160
4.105 8.685 3.593 1.000 2.055 2.085 2.112
9 8 7 6 5 4 3 2 1 0 ppm
192.841 189.914 143.023 138.161 131.358 129.839 129.582 129.505 129.474 128.218 127.284 114.308 90.075 77.254 77.000 76.746 40.757 29.481
NAME HUG-HC-160
EXPNO 11
PROCNO 1
Date_ 20120120
Time 15.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131164 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-160
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



NAME HUG-HC-143
EXPNO 10
PROCNO 1
Date_ 20120109
Time 12.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

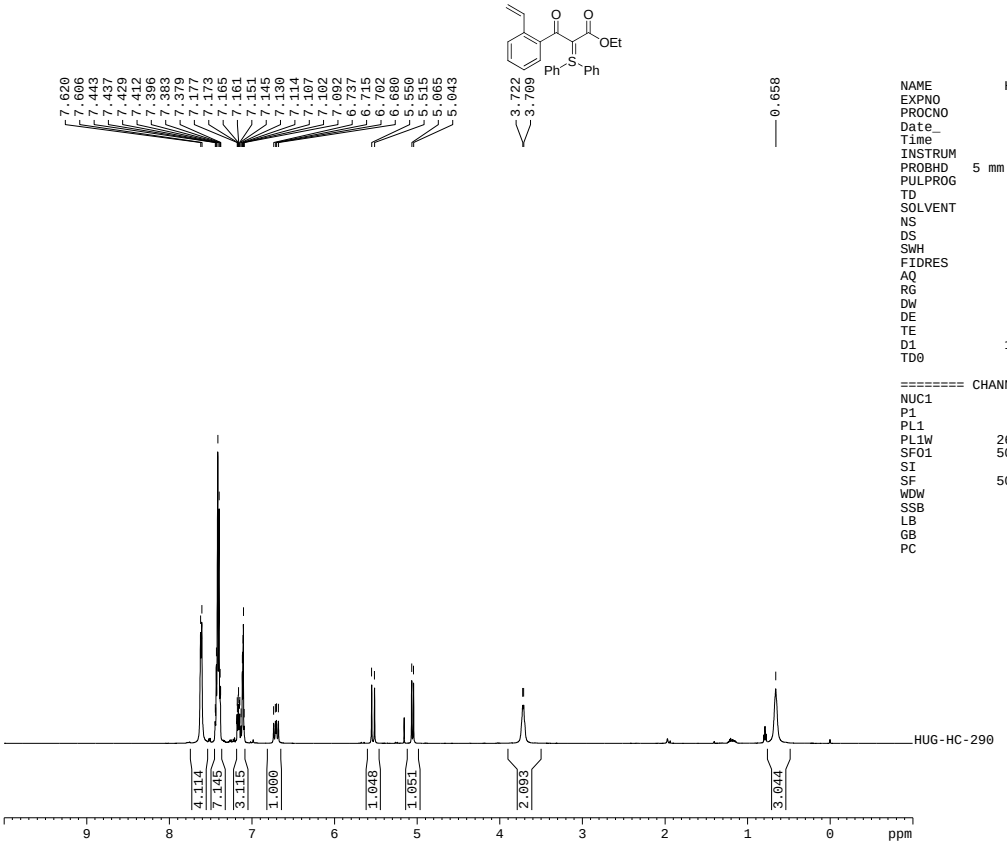
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500419 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME HUG-HC-143
EXPNO 11
PROCNO 1
Date_ 20120109
Time 12.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

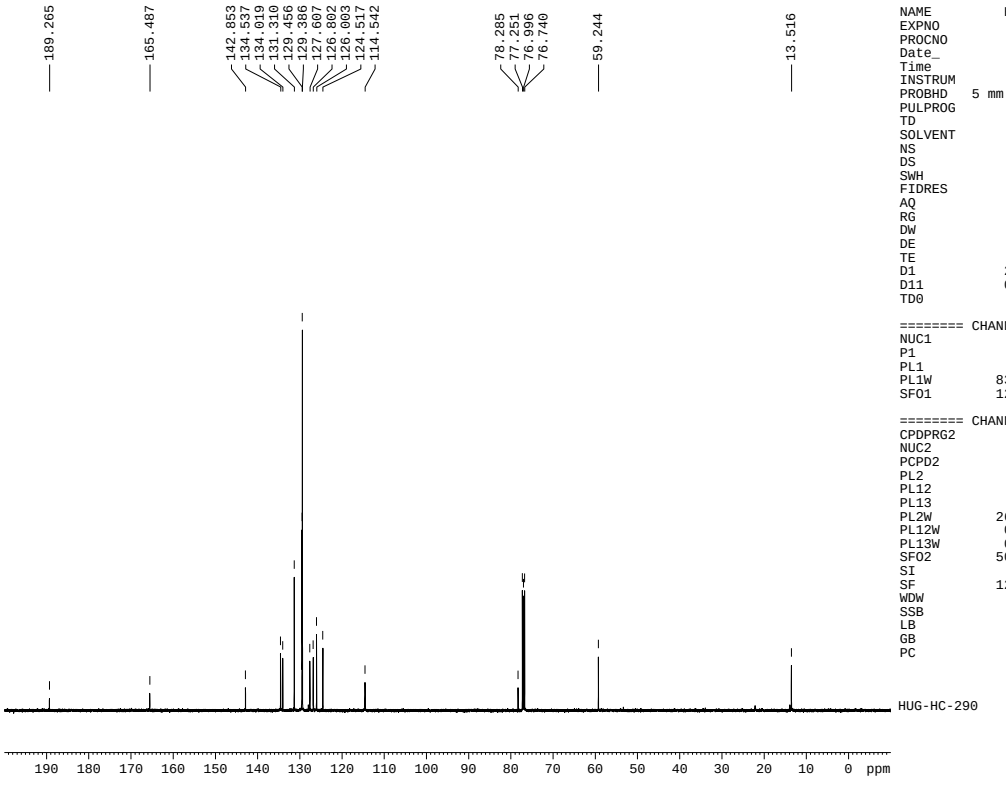
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131217 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
NAME          HUG-HC-290
EXPNO                 10
PROCNO                 1
Date_           20120517
Time                17.34
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ              3.1719923 sec
RG                    36
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

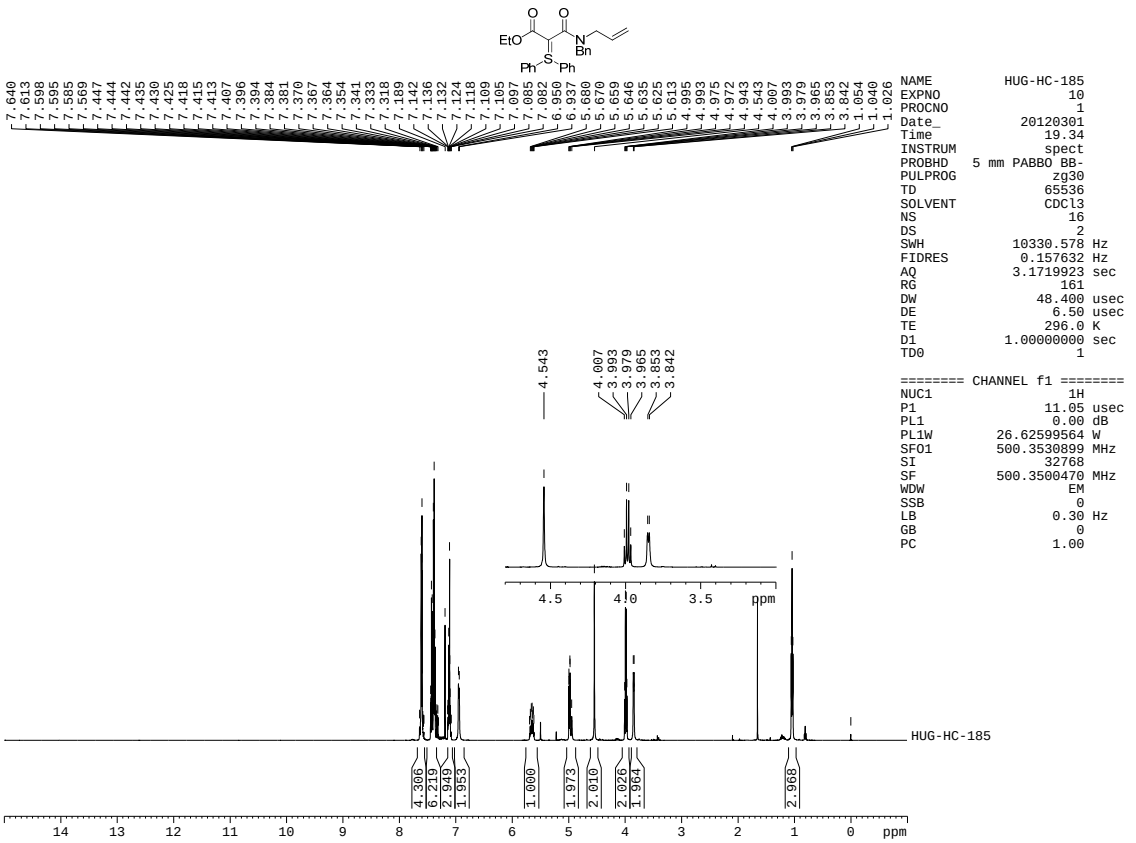
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W          26.62599564 W
SFO1          500.3530899 MHz
SI                 32768
SF            500.3500527 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```




```
NAME          HUG-HC-290
EXPNO                 11
PROCNO                 1
Date_           20120517
Time                17.41
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH            34722.223 Hz
FIDRES          0.529819 Hz
AQ              0.9437684 sec
RG                 32800
DW                14.400 usec
DE                 10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

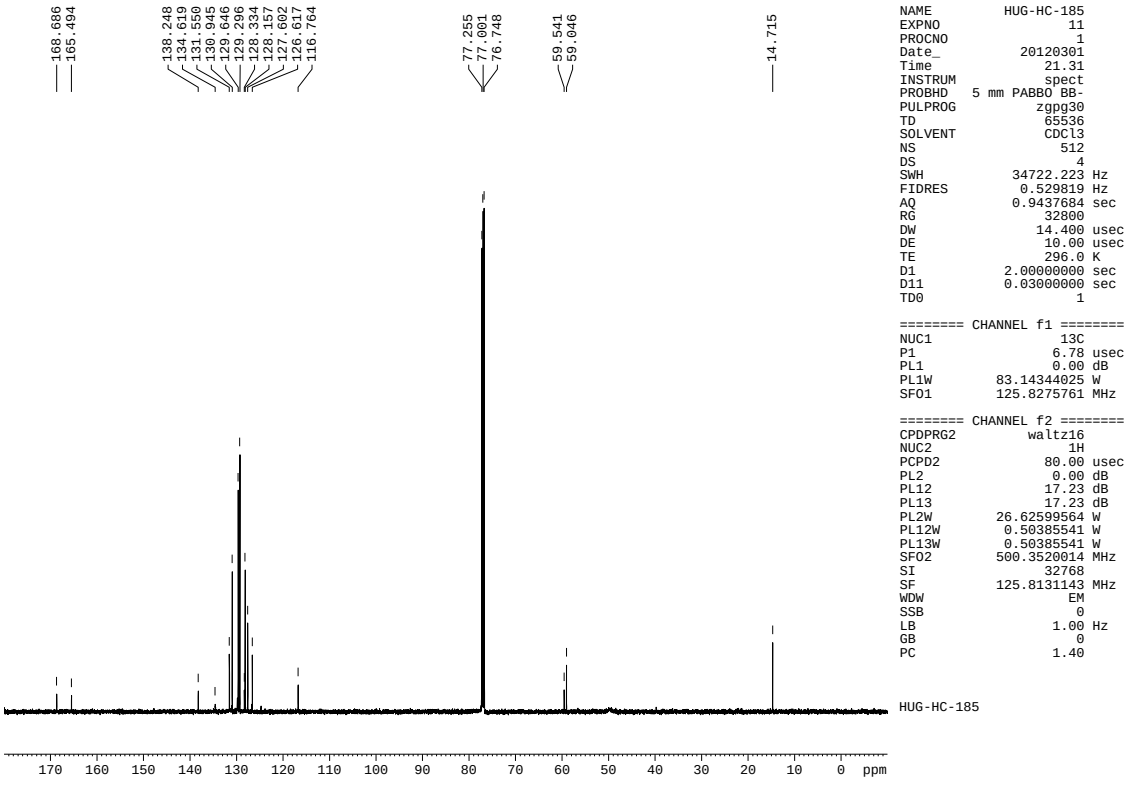
======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W          83.14344025 W
SFO1          125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W          26.62599564 W
PL12W          0.50385541 W
PL13W          0.50385541 W
SFO2          500.3520014 MHz
SI                 32768
SF            125.8131365 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```




```
NAME          HUG-HC-185
EXPNO                 10
PROCNO                 1
Date_           20120301
Time               19.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

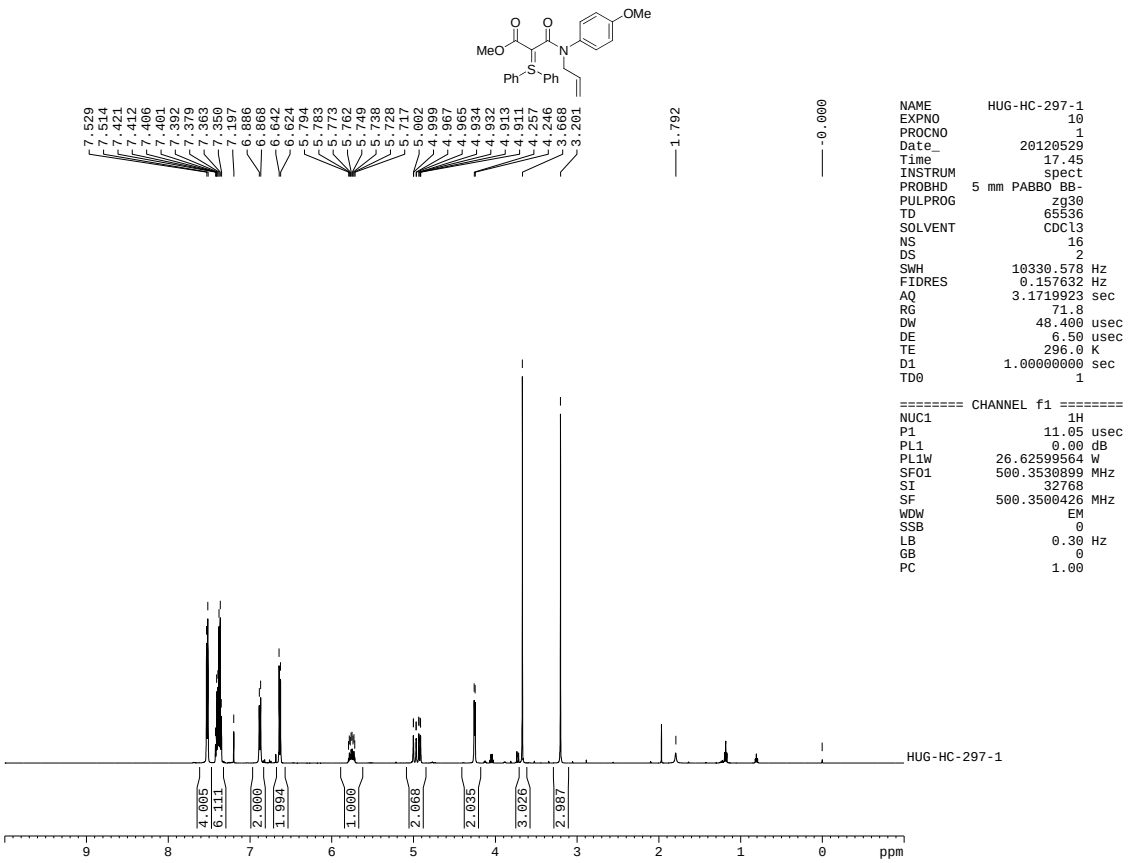
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1        500.3530899 MHz
SI                 32768
SF          500.3500470 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

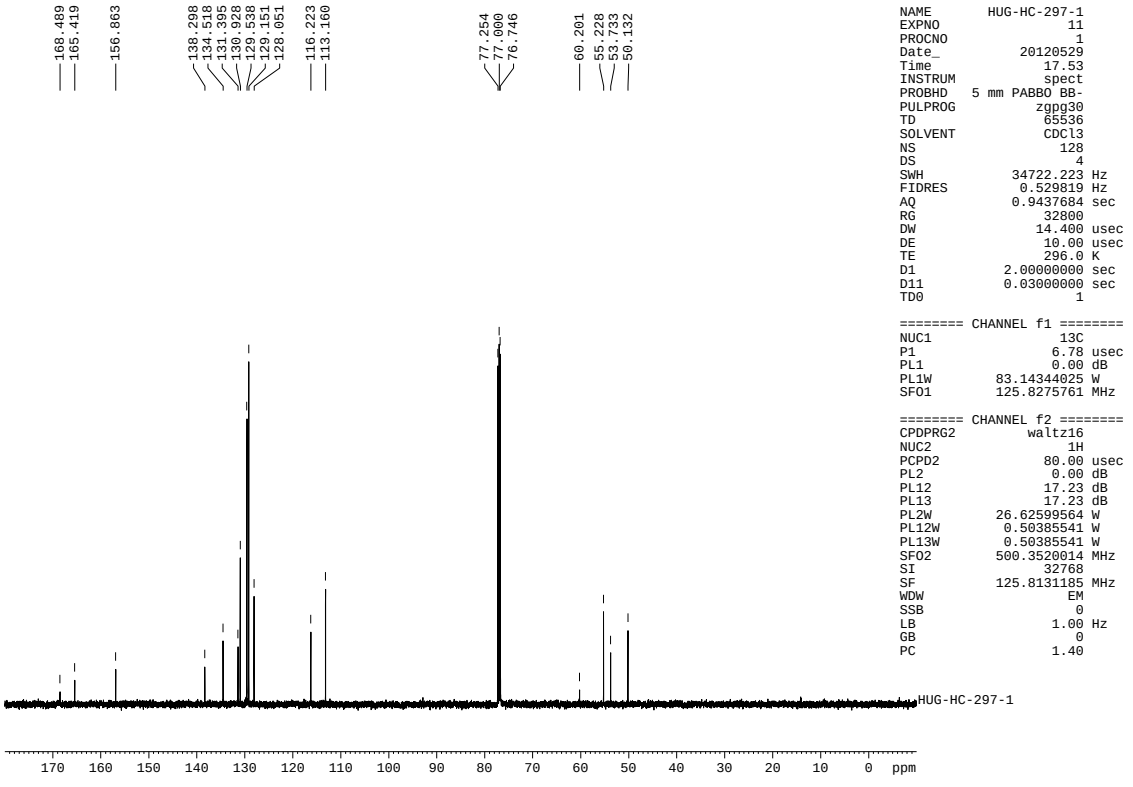


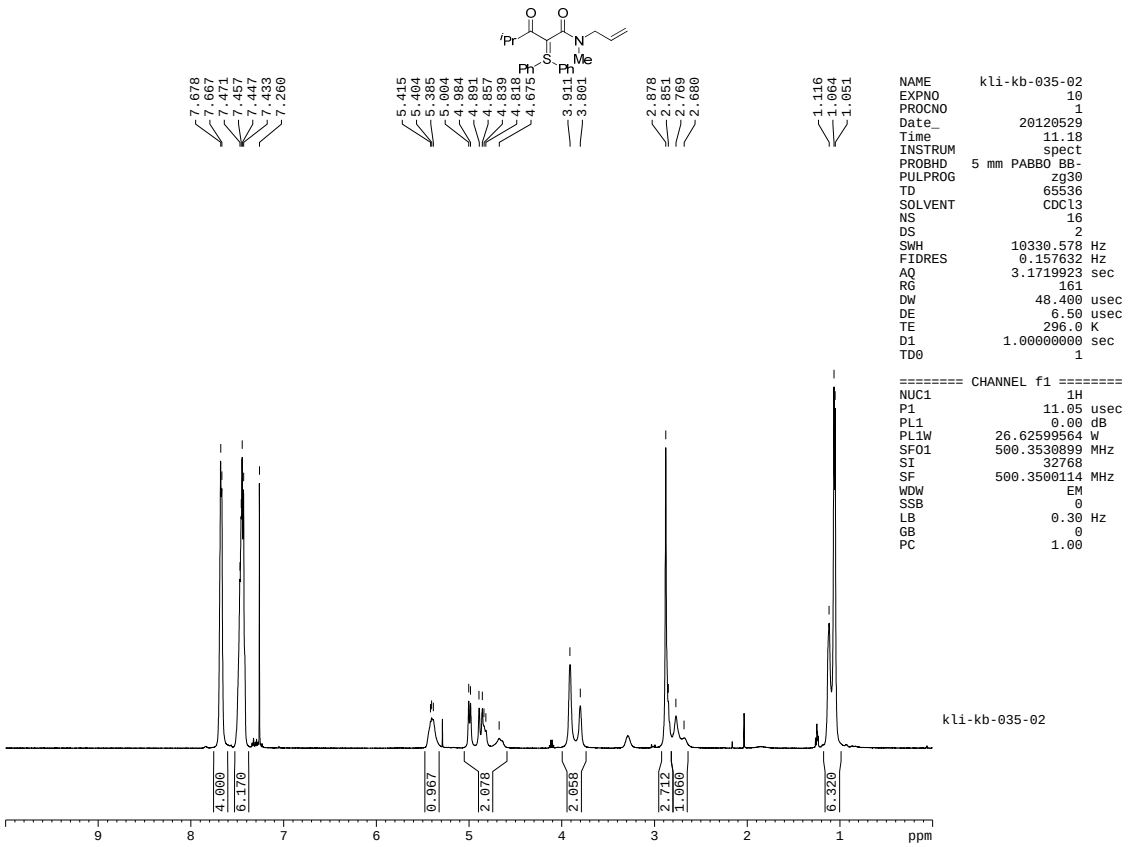

```
NAME          HUG-HC-185
EXPNO                 11
PROCNO                 1
Date_           20120301
Time               21.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1        125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2        500.3520014 MHz
SI                 32768
SF          125.8131143 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

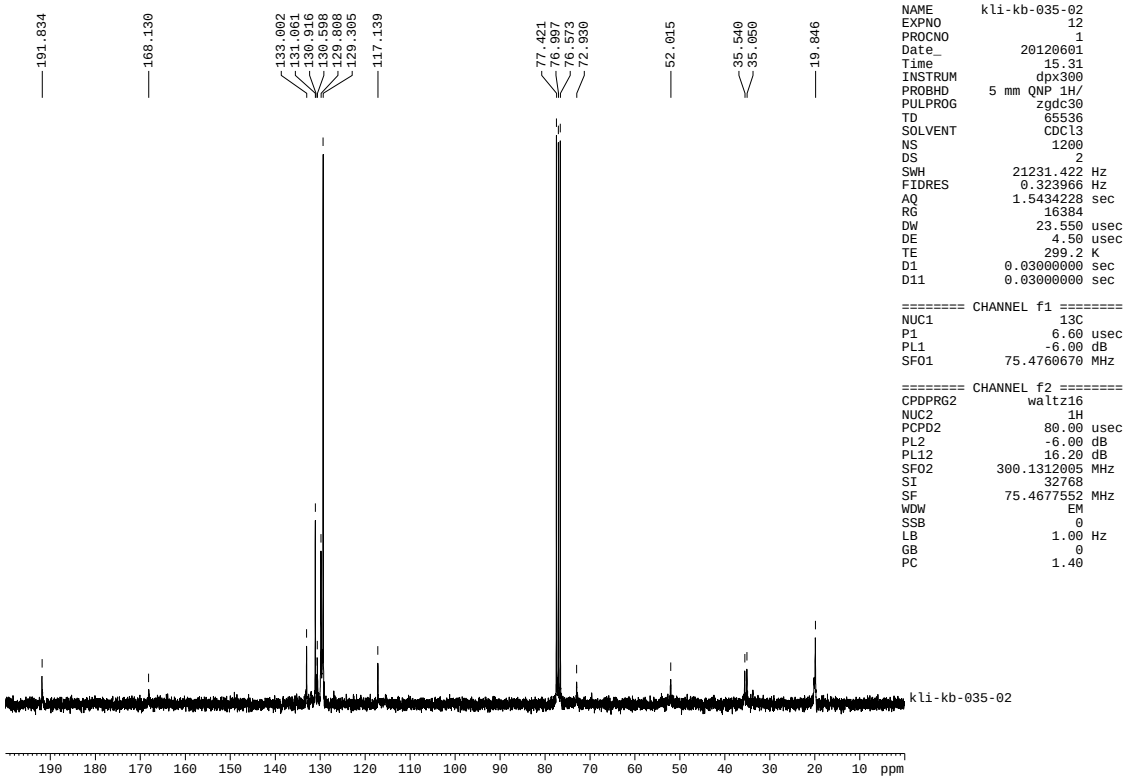

OMe
O
O
MeO
N
S
Ph
Ph
7.529
7.514
7.421
7.412
7.406
7.401
7.392
7.379
7.363
7.350
7.197
6.886
6.868
6.642
6.624
5.794
5.783
5.773
5.762
5.749
5.738
5.728
5.717
5.002
4.999
4.967
4.965
4.934
4.932
4.913
4.911
4.257
4.246
3.668
3.201
1.792
-0.000
NAME HUG-HC-297-1
EXPNO 10
PROCNO 1
Date_ 20120529
Time 17.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500426 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-297-1
4.005
6.111
2.000
1.994
1.000
2.068
2.035
3.026
2.987
9
8
7
6
5
4
3
2
1
0
ppm


168.489
165.419
156.863
138.298
134.518
131.395
130.928
129.538
129.151
128.051
116.223
113.160
77.254
77.000
76.746
60.201
55.228
53.733
50.132
NAME HUG-HC-297-1
EXPNO 11
PROCNO 1
Date_ 20120529
Time 17.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131185 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-297-1
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm




```
NAME          kli-kb-035-02
EXPNO                    10
PROCNO                    1
Date_              20120529
Time                  11.18
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH              10330.578 Hz
FIDRES            0.157632 Hz
AQ                3.1719923 sec
RG                      161
DW                   48.400 usec
DE                    6.50 usec
TE                   296.0 K
D1                1.00000000 sec
TD0                       1

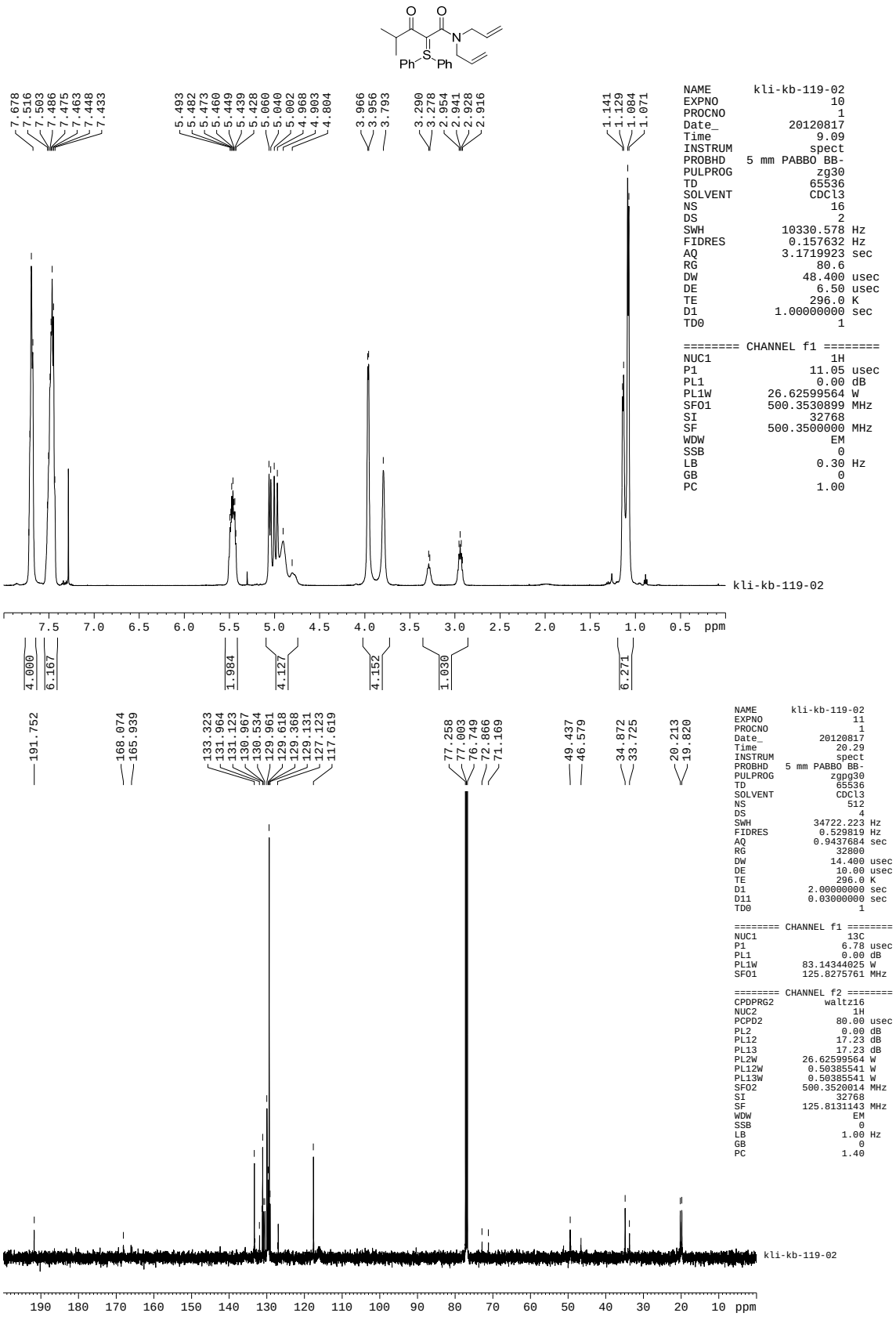
======== CHANNEL f1 ========
NUC1                    1H
P1                   11.05 usec
PL1                   0.00 dB
PL1W             26.62599564 W
SFO1             500.3530899 MHz
SI                      32768
SF               500.3500114 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                    1.00
```

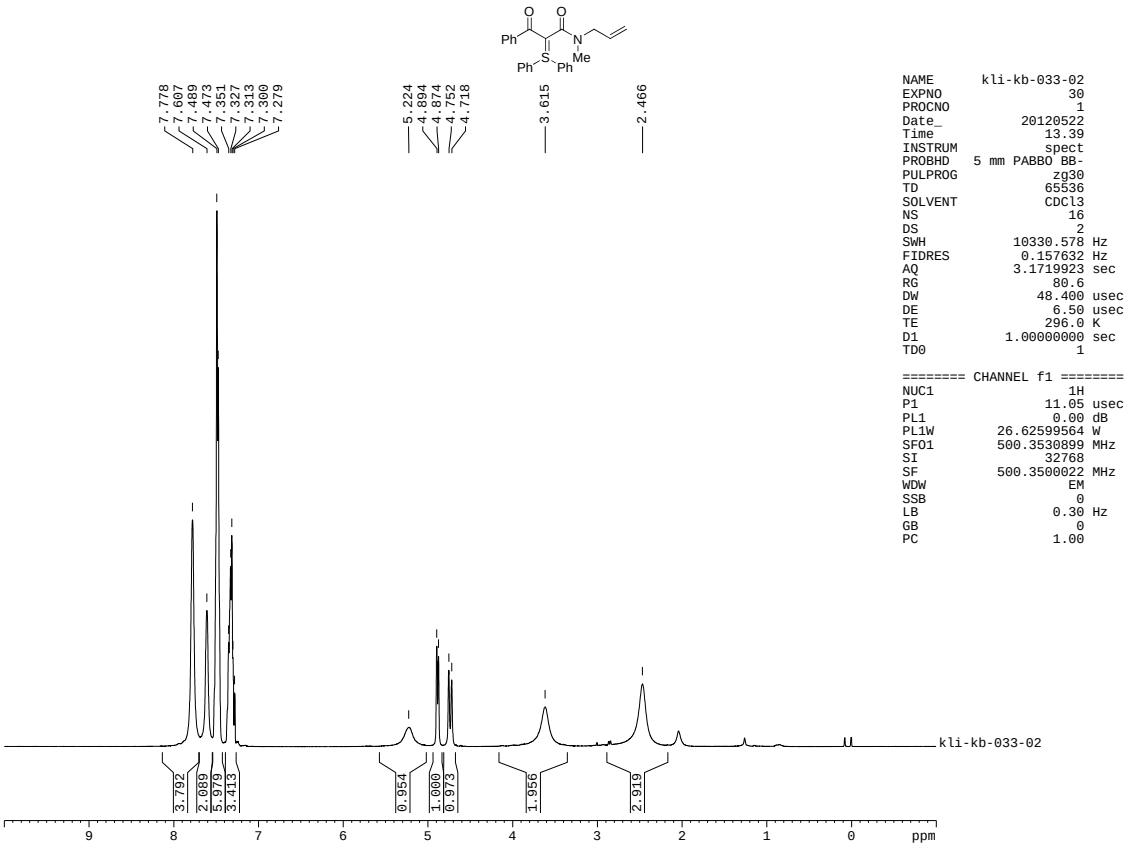



```
NAME          kli-kb-035-02
EXPNO                    12
PROCNO                    1
Date_              20120601
Time                  15.31
INSTRUM             dpx300
PROBHD     5 mm QNP 1H/
PULPROG             zgdc30
TD                    65536
SOLVENT               CDCl3
NS                     1200
DS                        2
SWH              21231.422 Hz
FIDRES            0.323966 Hz
AQ                1.5434228 sec
RG                    16384
DW                   23.550 usec
DE                    4.50 usec
TE                   299.2 K
D1                0.03000000 sec
D11               0.03000000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                    6.60 usec
PL1                  -6.00 dB
SFO1             75.4760670 MHz

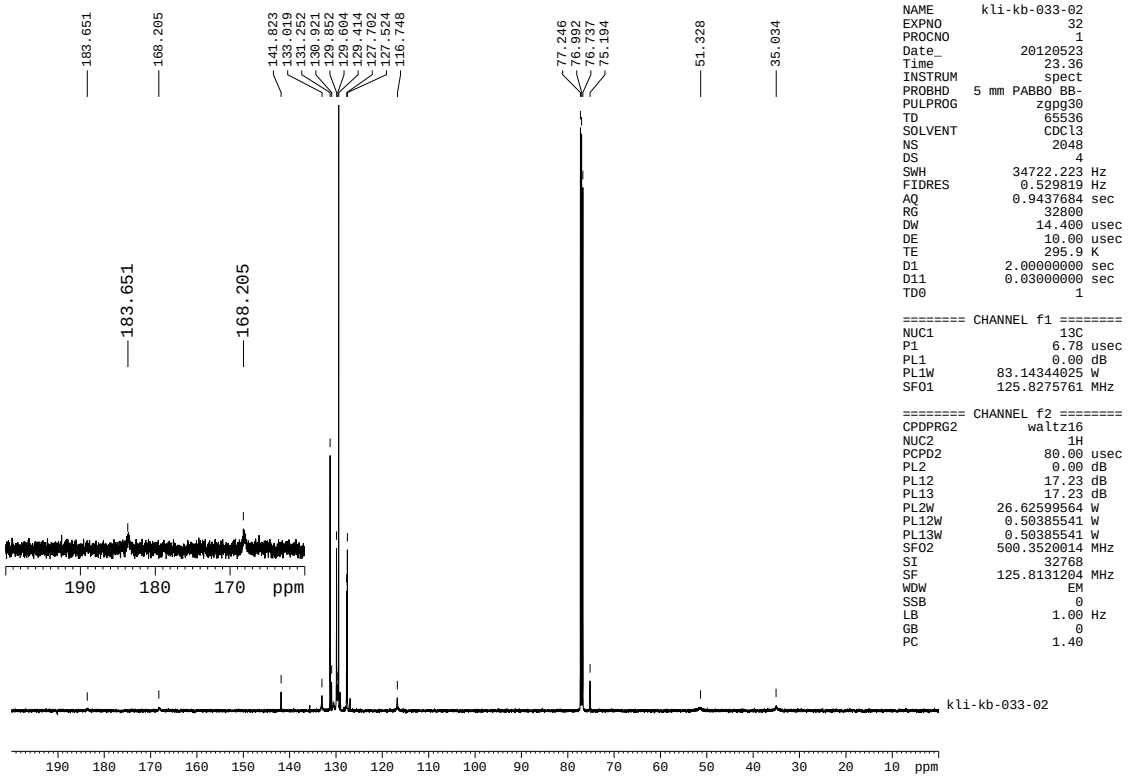
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -6.00 dB
PL12                 16.20 dB
SFO2            300.1312005 MHz
SI                      32768
SF               75.4677552 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```


7.678 7.516 7.503 7.486 7.475 7.463 7.448 7.433
5.493 5.482 5.473 5.460 5.449 5.439 5.428 5.060 5.040 5.002 4.968 4.903 4.804
3.966 3.956 3.793
3.290 3.278 2.954 2.941 2.928 2.916
1.141 1.129 1.084 1.071
NAME kli-kb-119-02
EXPNO 10
PROCNO 1
Date_ 20120817
Time 9.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
kli-kb-119-02
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 ppm
4.000 6.167 1.984 4.127 4.152 1.030 6.271
191.752
168.074 165.939
133.323 131.964 131.123 130.967 130.534 129.961 129.618 129.368 129.131 127.123 117.619
77.258 77.003 76.749 72.866 71.169
49.437 46.579
34.872 33.725
20.213 19.820
NAME kli-kb-119-02
EXPNO 11
PROCNO 1
Date_ 20120817
Time 20.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131143 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-119-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm




```
NAME        kli-kb-033-02
EXPNO                  30
PROCNO                  1
Date_            20120522
Time                13.39
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10330.578 Hz
FIDRES           0.157632 Hz
AQ               3.1719923 sec
RG                    80.6
DW                  48.400 usec
DE                   6.50 usec
TE                  296.0 K
D1              1.00000000 sec
TD0                     1

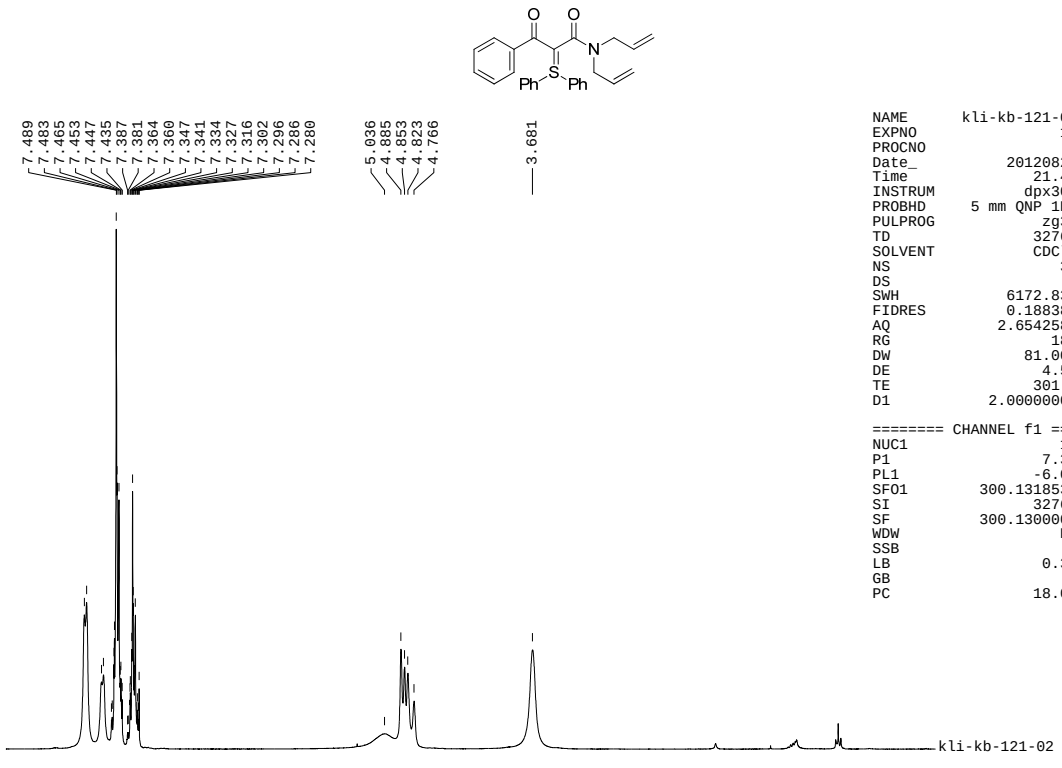
======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  0.00 dB
PL1W           26.62599564 W
SFO1           500.3530899 MHz
SI                   32768
SF             500.3500022 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

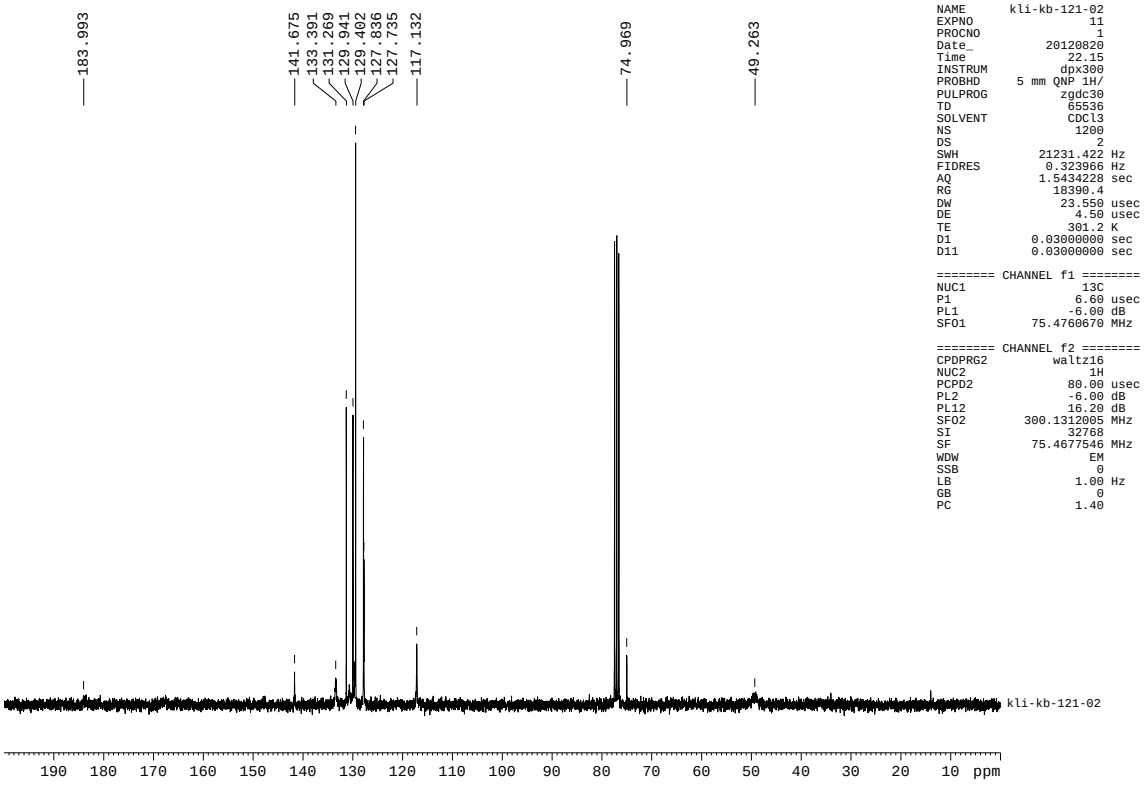


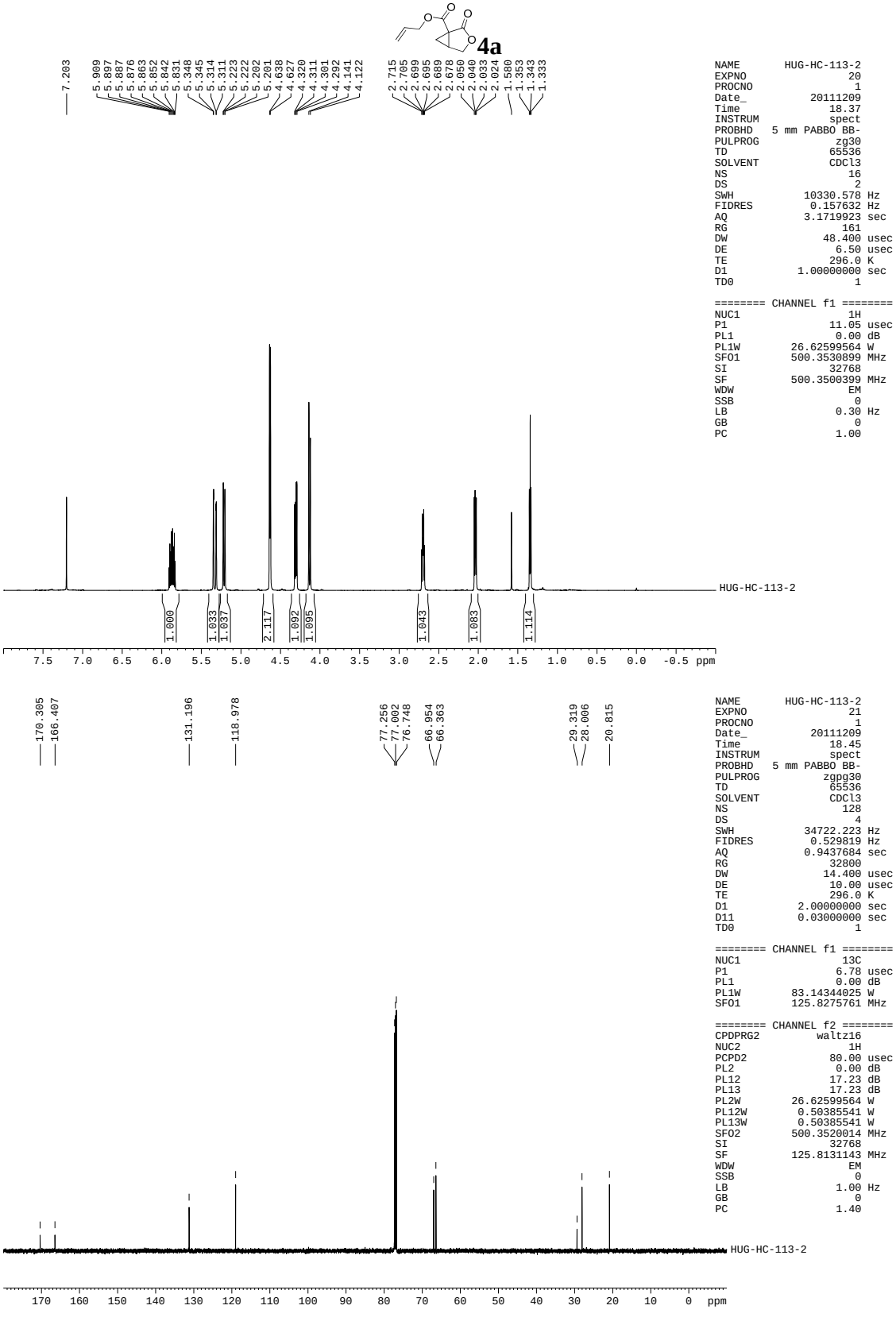

```
NAME        kli-kb-033-02
EXPNO                  32
PROCNO                  1
Date_            20120523
Time                23.36
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2048
DS                      4
SWH             34722.223 Hz
FIDRES           0.529819 Hz
AQ               0.9437684 sec
RG                  32800
DW                  14.400 usec
DE                  10.00 usec
TE                  295.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

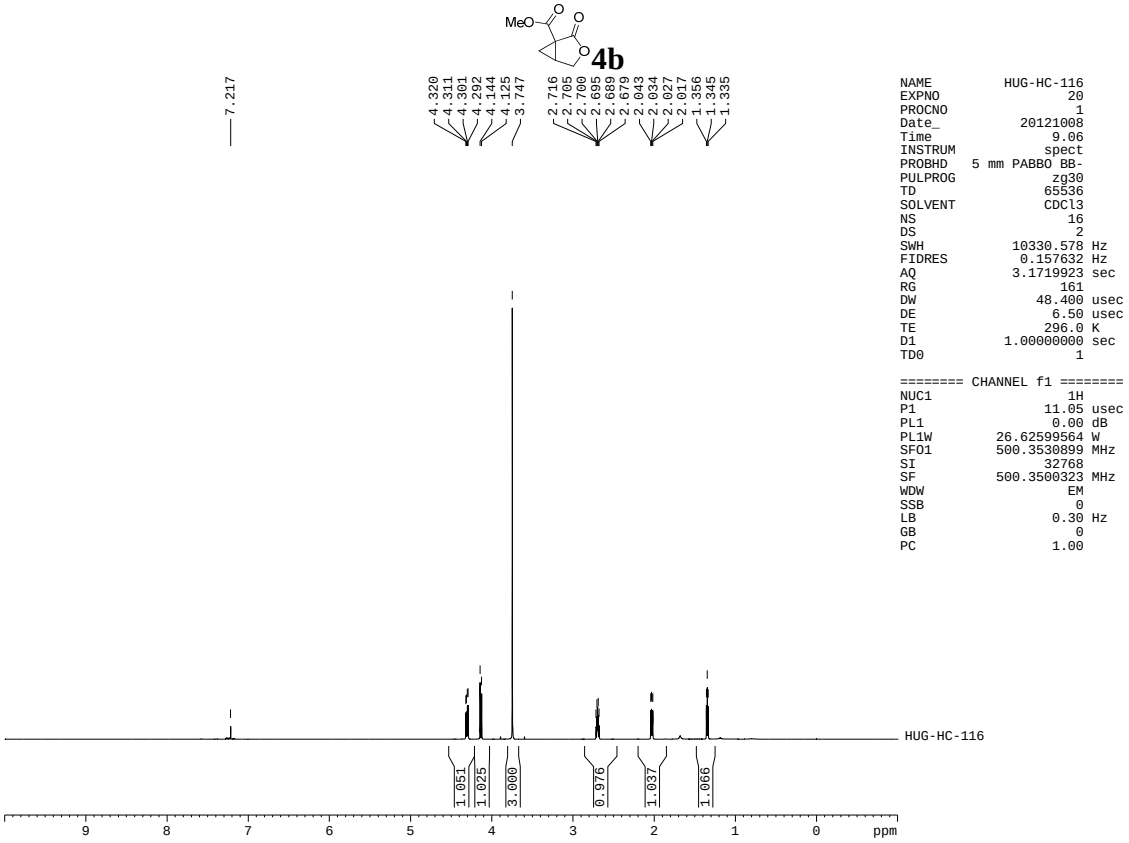
======== CHANNEL f1 ========
NUC1                  13C
P1                   6.78 usec
PL1                  0.00 dB
PL1W           83.14344025 W
SFO1           125.8275761 MHz

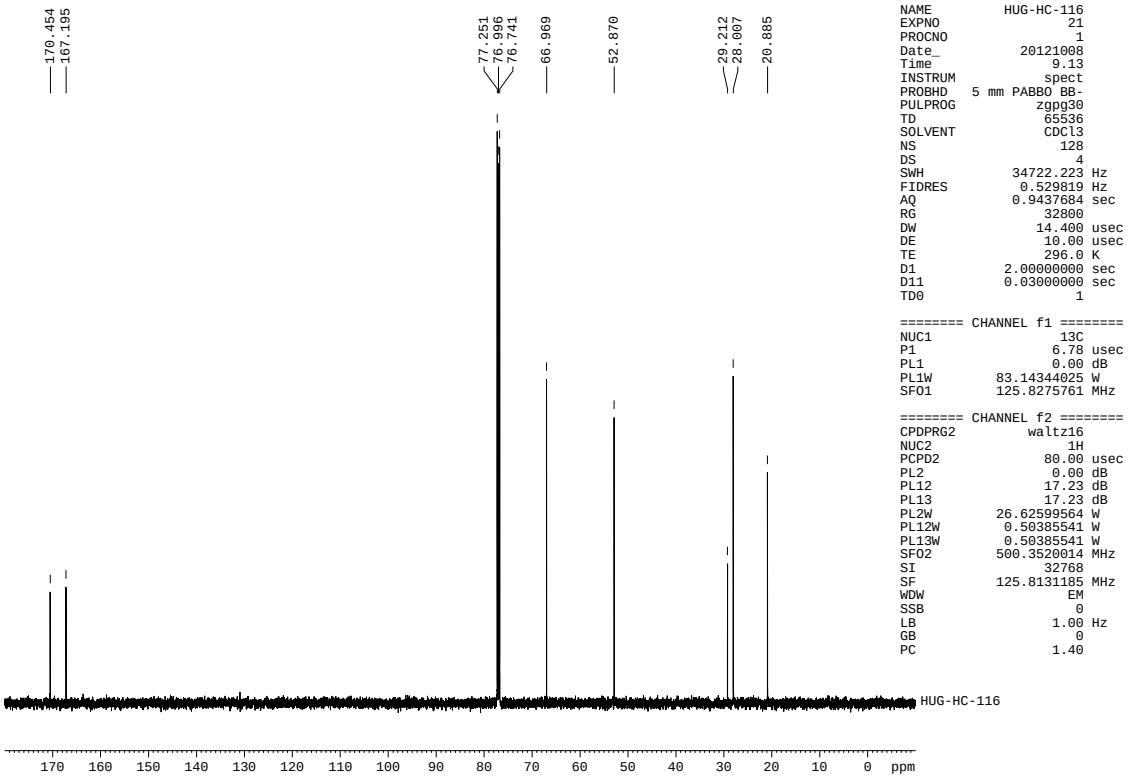
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                17.23 dB
PL13                17.23 dB
PL2W           26.62599564 W
PL12W           0.50385541 W
PL13W           0.50385541 W
SFO2           500.3520014 MHz
SI                   32768
SF             125.8131204 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

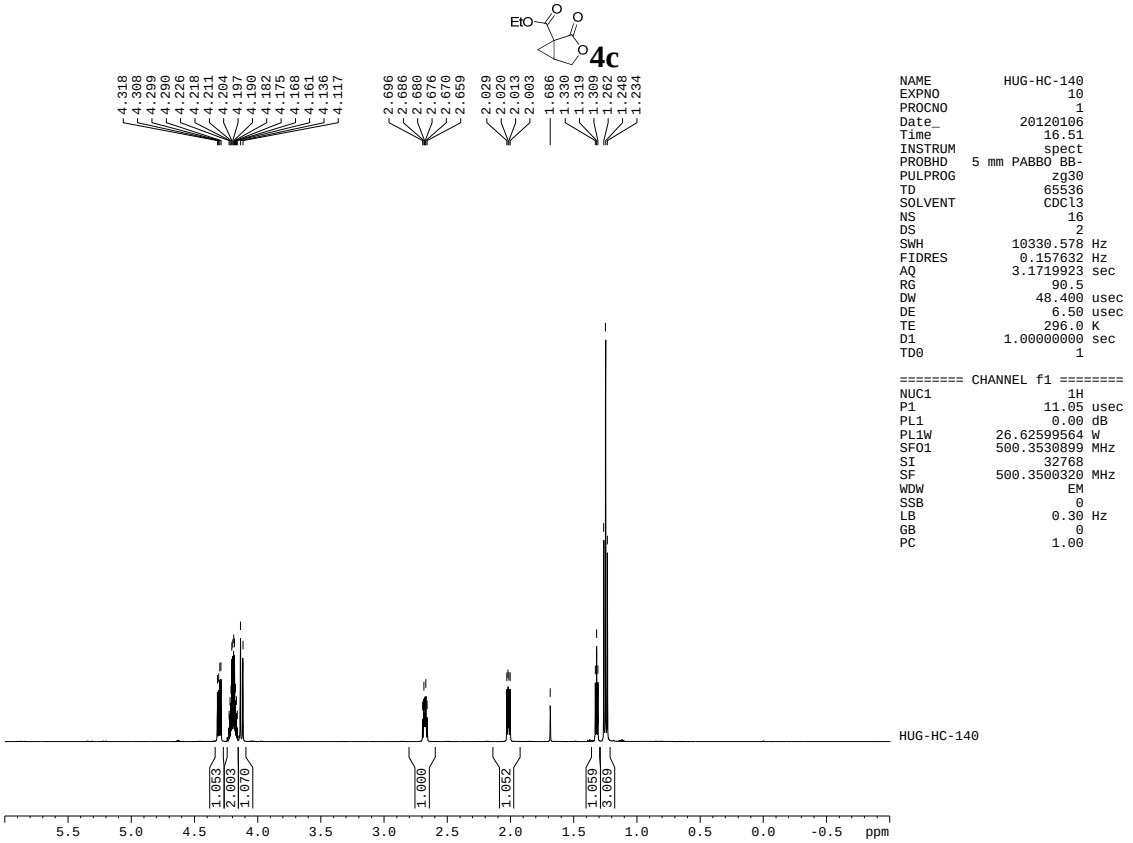





4a
7.203
5.909
5.897
5.887
5.876
5.863
5.852
5.842
5.831
5.348
5.345
5.314
5.311
5.223
5.222
5.202
5.201
4.638
4.627
4.320
4.311
4.301
4.292
4.141
4.122
2.715
2.705
2.699
2.695
2.689
2.678
2.650
2.040
2.033
2.024
1.580
1.353
1.343
1.333
NAME HUG-HC-113-2
EXPNO 20
PROCNO 1
Date_ 20111209
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500399 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-113-2
1.000
1.033
1.037
2.117
1.092
1.095
1.043
1.083
1.114
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 -0.5 ppm
170.305
166.407
131.196
118.978
77.256
77.002
76.748
66.954
66.363
29.319
28.006
20.815
NAME HUG-HC-113-2
EXPNO 21
PROCNO 1
Date_ 20111209
Time 18.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131143 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-113-2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

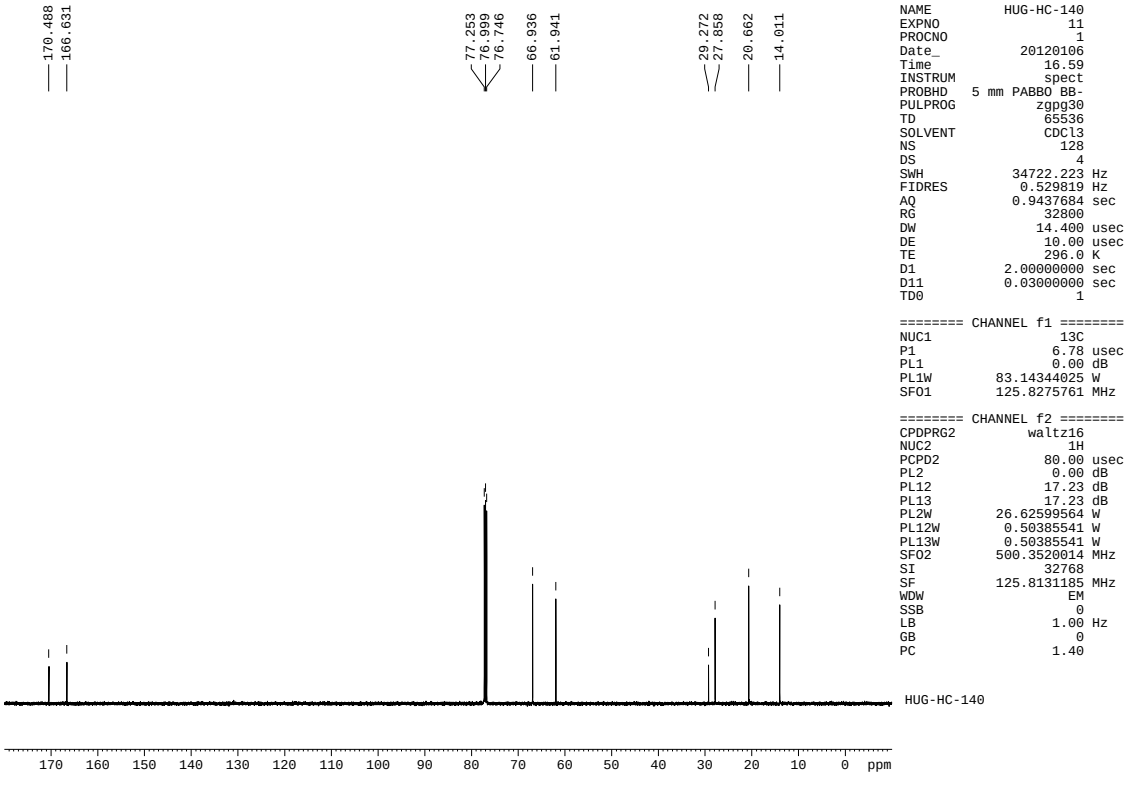

MeO
O
O
O
4b
7.217
4.320
4.311
4.301
4.292
4.144
4.125
3.747
2.716
2.705
2.700
2.695
2.689
2.679
2.043
2.034
2.027
2.017
1.356
1.345
1.335
NAME HUG-HC-116
EXPNO 20
PROCNO 1
Date_ 20121008
Time 9.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500323 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-116
1.051
1.025
3.000
0.976
1.037
1.066
9
8
7
6
5
4
3
2
1
0
ppm


170.454
167.195
77.251
76.996
76.741
66.969
52.870
29.212
28.007
20.885
NAME HUG-HC-116
EXPNO 21
PROCNO 1
Date_ 20121008
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131185 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-116
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm




```
NAME          HUG-HC-140
EXPNO                 10
PROCNO                 1
Date_           20120106
Time                16.51
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                  90.5
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

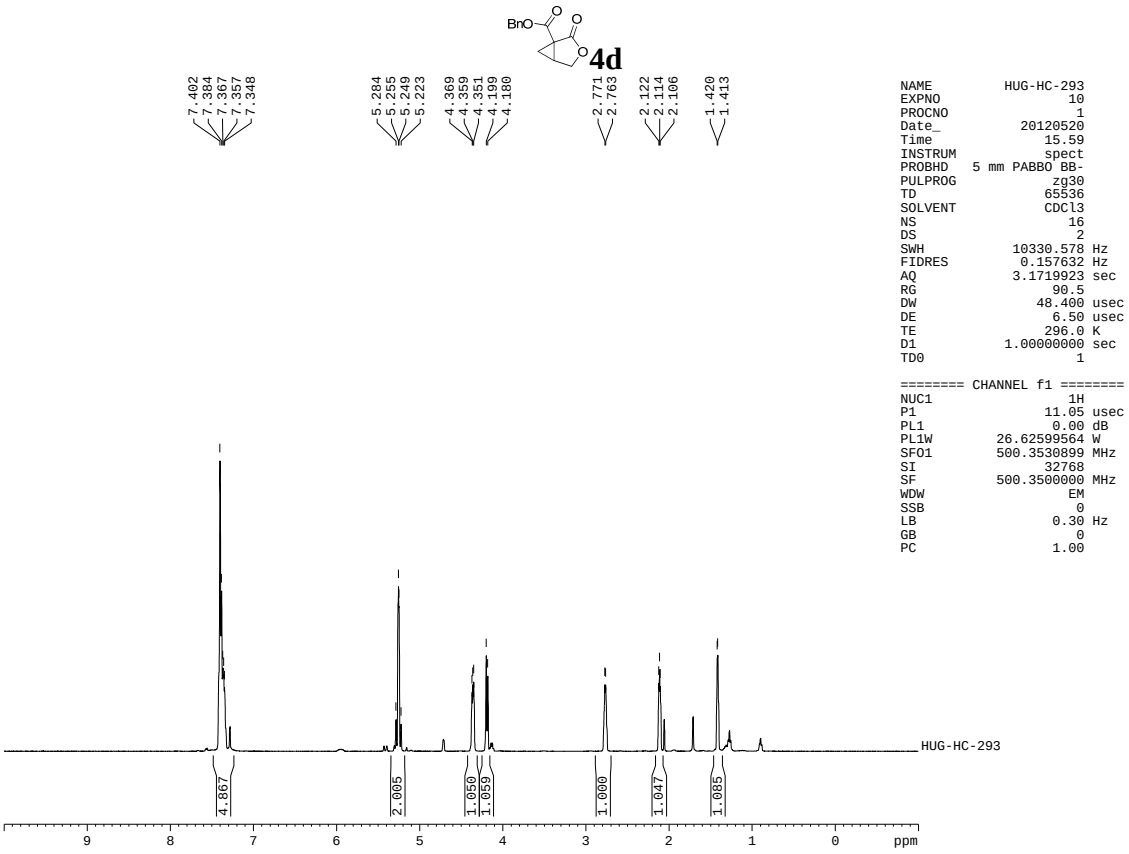
======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500320 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

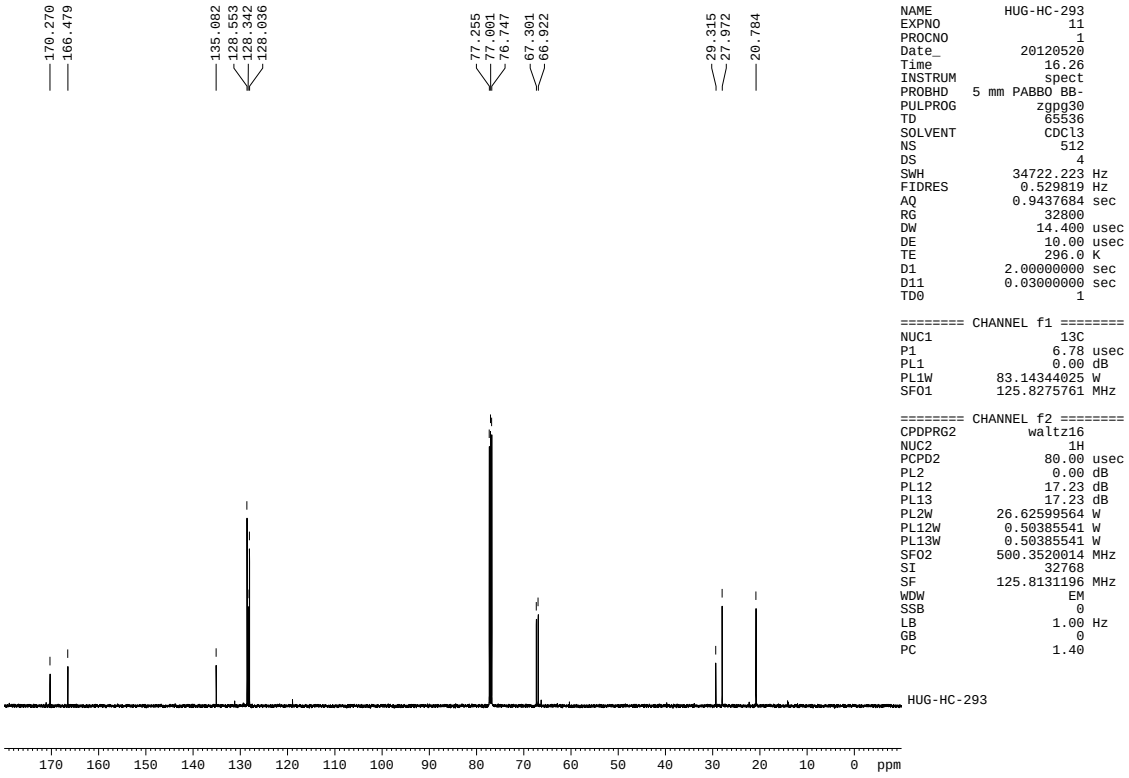


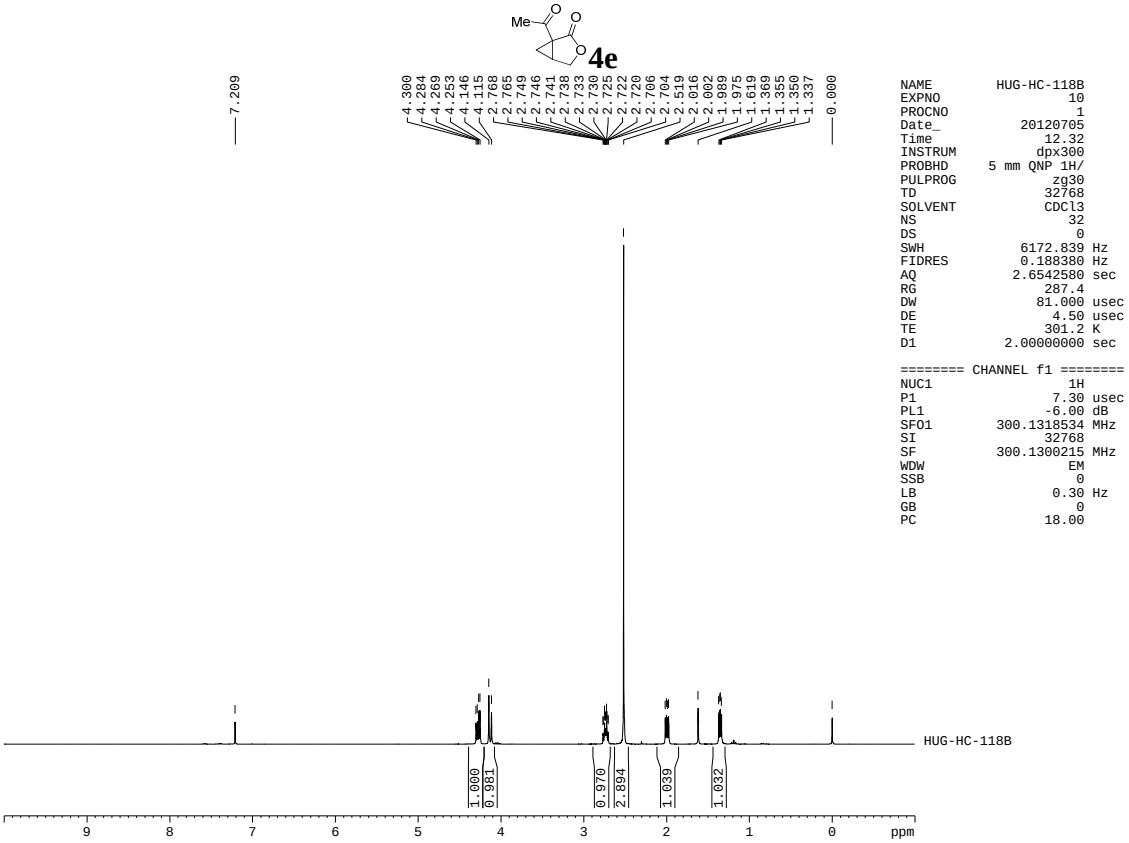

```
NAME          HUG-HC-140
EXPNO                 11
PROCNO                 1
Date_           20120106
Time                16.59
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

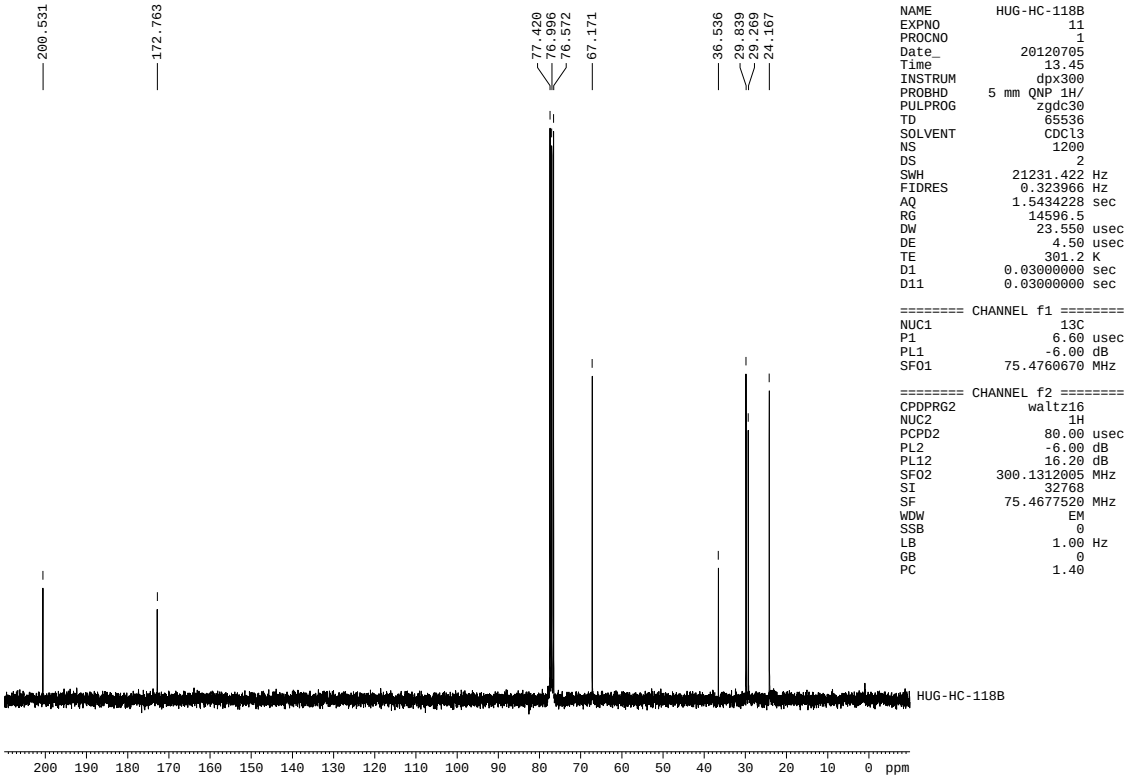
======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.8275761 MHz

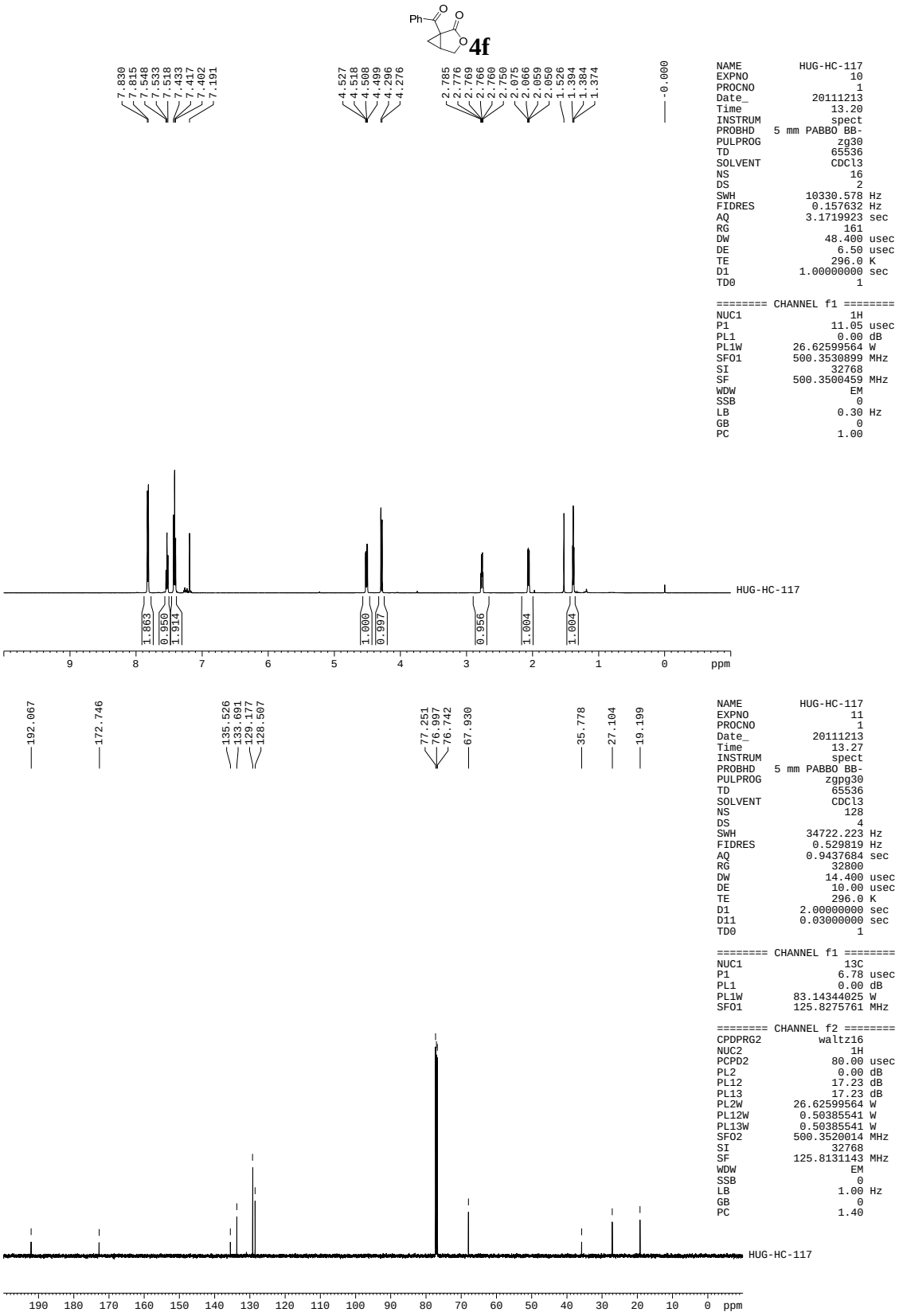
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131185 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

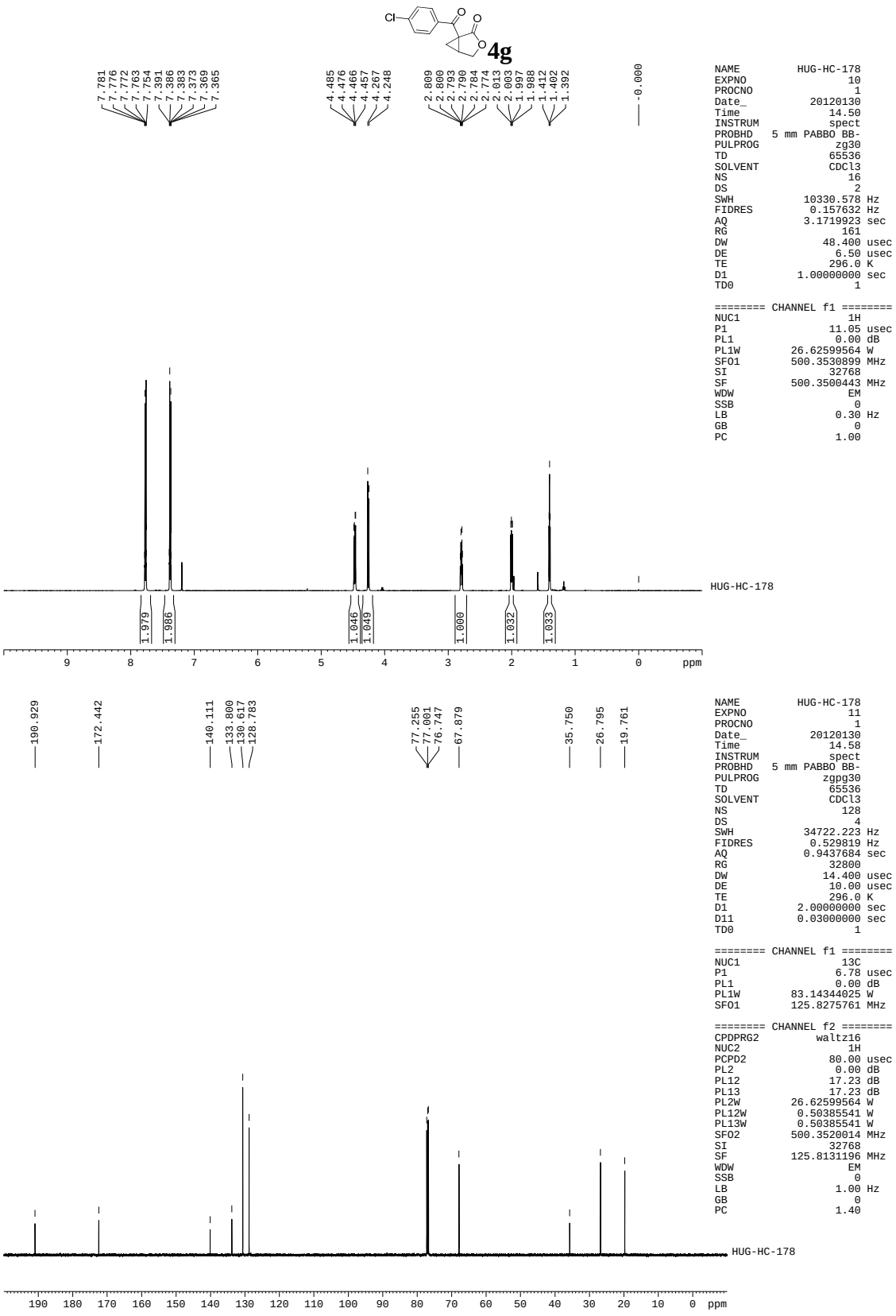

BnO
4d
7.402
7.384
7.367
7.357
7.348
5.284
5.255
5.249
5.223
4.369
4.359
4.351
4.199
4.180
2.771
2.763
2.122
2.114
2.106
1.420
1.413
NAME HUG-HC-293
EXPNO 10
PROCNO 1
Date_ 20120520
Time 15.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-293
4.867
2.005
1.050
1.059
1.000
1.047
1.085
9
8
7
6
5
4
3
2
1
0
ppm

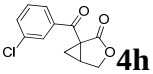

170.270
166.479
135.082
128.553
128.342
128.036
77.255
77.001
76.747
67.301
66.922
29.315
27.972
20.784
NAME HUG-HC-293
EXPNO 11
PROCNO 1
Date_ 20120520
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131196 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-293
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


Me
4e
7.269
4.300
4.284
4.269
4.253
4.146
4.115
2.768
2.765
2.749
2.746
2.741
2.738
2.733
2.730
2.725
2.722
2.720
2.706
2.704
2.519
2.016
2.002
1.989
1.975
1.619
1.369
1.355
1.350
1.337
0.000
NAME HUG-HC-118B
EXPNO 10
PROCNO 1
Date_ 20120705
Time 12.32
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 287.4
DW 81.000 usec
DE 4.50 usec
TE 301.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300215 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
HUG-HC-118B
1.000
0.981
0.970
2.894
1.039
1.032
9
8
7
6
5
4
3
2
1
0
ppm


200.531
172.763
77.420
76.996
76.572
67.171
36.536
29.839
29.269
24.167
NAME HUG-HC-118B
EXPNO 11
PROCNO 1
Date_ 20120705
Time 13.45
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 14596.5
DW 23.550 usec
DE 4.50 usec
TE 301.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-118B
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


Ph
4f
7.830
7.815
7.548
7.533
7.518
7.433
7.417
7.402
7.191
4.527
4.518
4.508
4.499
4.296
4.276
2.785
2.776
2.769
2.766
2.760
2.750
2.075
2.066
2.059
2.050
1.526
1.394
1.384
1.374
-0.000
NAME HUG-HC-117
EXPNO 10
PROCNO 1
Date_ 20111213
Time 13.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500459 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-117
1.863
0.950
1.914
1.000
0.997
0.956
1.004
1.004
9
8
7
6
5
4
3
2
1
0
ppm
192.067
172.746
135.526
133.691
129.177
128.507
77.251
76.997
76.742
67.930
35.778
27.104
19.199
NAME HUG-HC-117
EXPNO 11
PROCNO 1
Date_ 20111213
Time 13.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131143 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-117
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

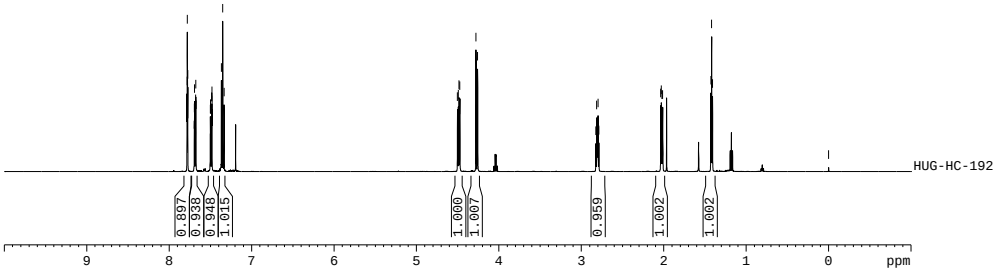

4g
7.781
7.776
7.772
7.763
7.754
7.391
7.386
7.383
7.373
7.369
7.365
4.485
4.476
4.466
4.457
4.267
4.248
2.809
2.800
2.793
2.790
2.784
2.774
2.013
2.003
1.997
1.988
1.412
1.402
1.392
-0.000
NAME HUG-HC-178
EXPNO 10
PROCNO 1
Date_ 20120130
Time 14.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500443 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-178
1.979
1.986
1.046
1.049
1.000
1.032
1.033
9 8 7 6 5 4 3 2 1 0 ppm
190.929
172.442
140.111
133.800
130.617
128.783
77.255
77.001
76.747
67.879
35.750
26.795
19.761
NAME HUG-HC-178
EXPNO 11
PROCNO 1
Date_ 20120130
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131196 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-178
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

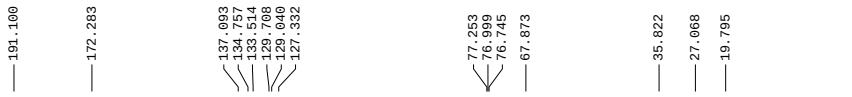


4h


```
NAME          HUG-HC-192
EXPNO                 10
PROCNO                 1
Date_           20120216
Time                14.01
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ              3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1        500.3530899 MHz
SI                 32768
SF          500.3500442 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

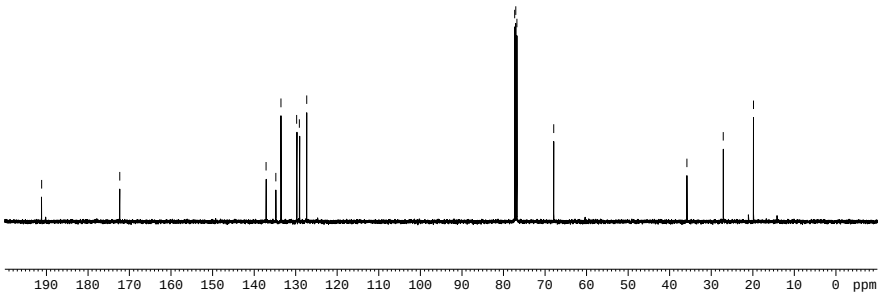


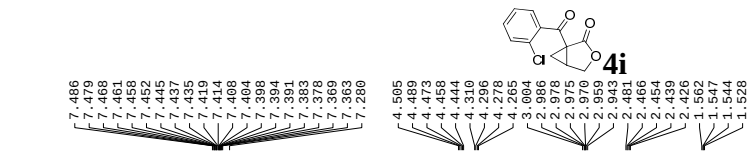



```
NAME          HUG-HC-192
EXPNO                 11
PROCNO                 1
Date_           20120216
Time                14.09
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH            34722.223 Hz
FIDRES          0.529819 Hz
AQ              0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1        125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2        500.3520014 MHz
SI                 32768
SF          125.8131185 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

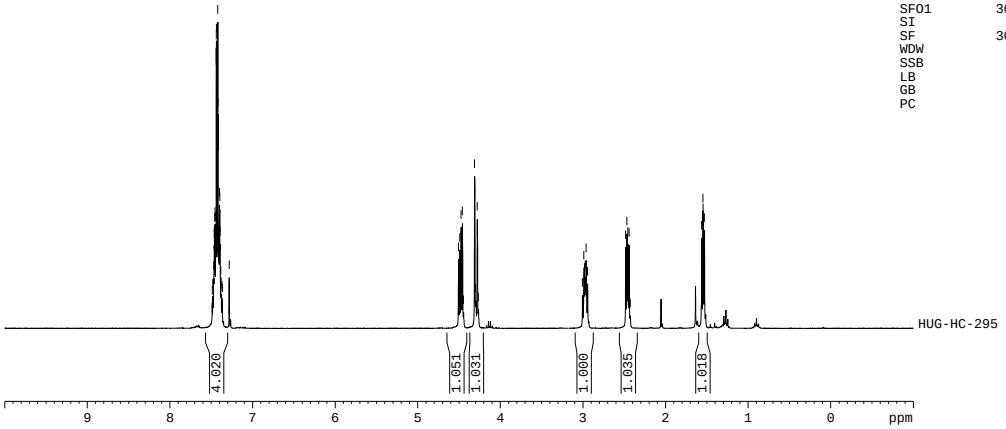


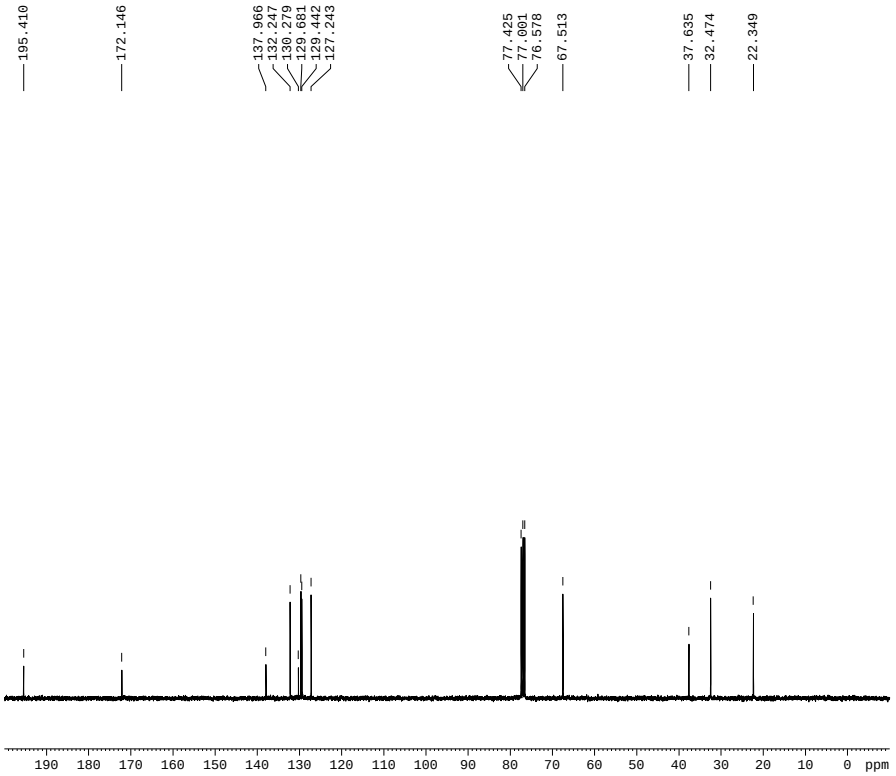


4i

```
NAME          HUG-HC-295
EXPNO                 10
PROCNO                 1
Date_           20120525
Time               14.12
INSTRUM           dpx300
PROBHD     5 mm QNP 1H/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH            6172.839 Hz
FIDRES         0.188380 Hz
AQ             2.6542580 sec
RG                287.4
DW               81.000 usec
DE                4.50 usec
TE                300.2 K
D1            2.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                7.30 usec
PL1              -6.00 dB
SFO1        300.1318534 MHz
SI                32768
SF          300.1300000 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC              18.00
```

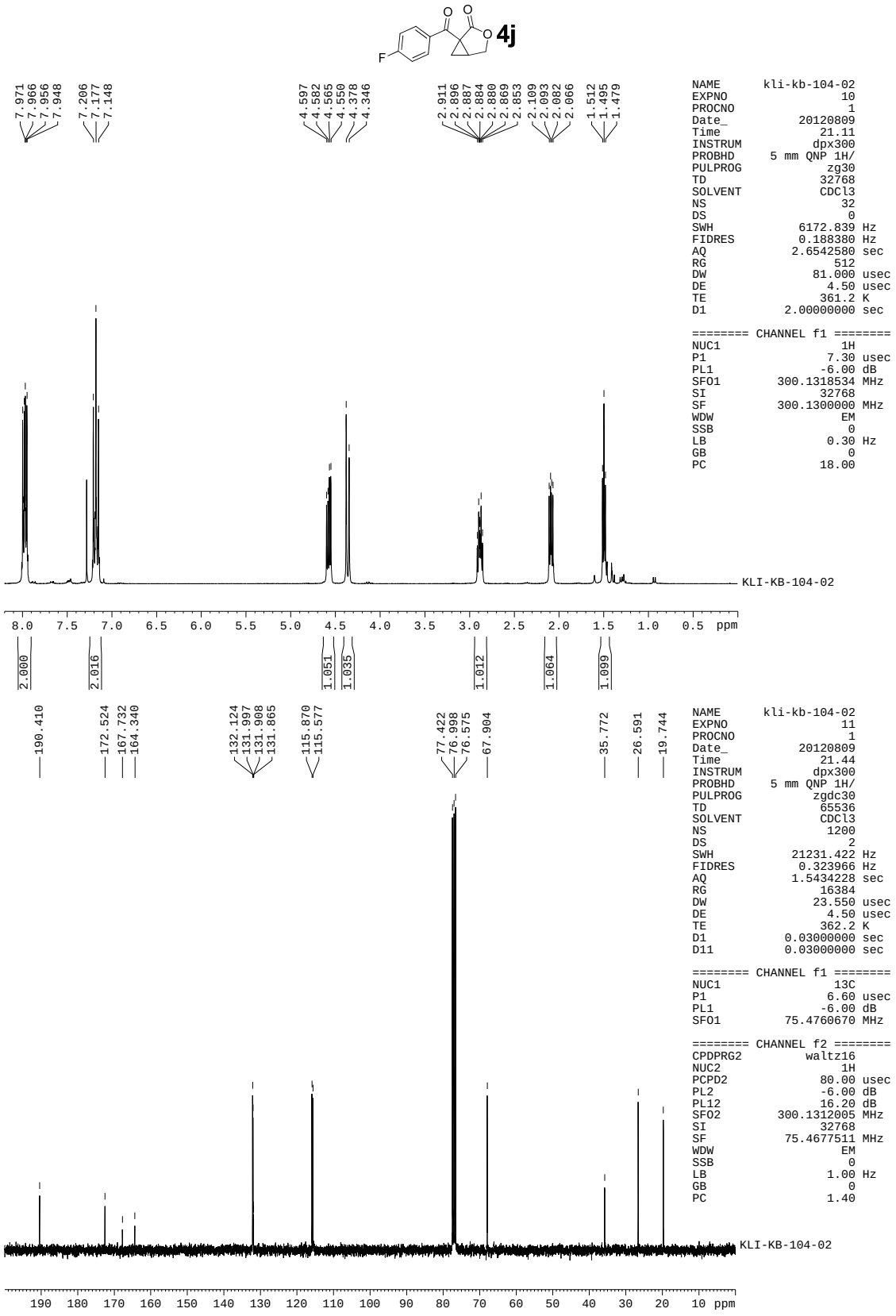


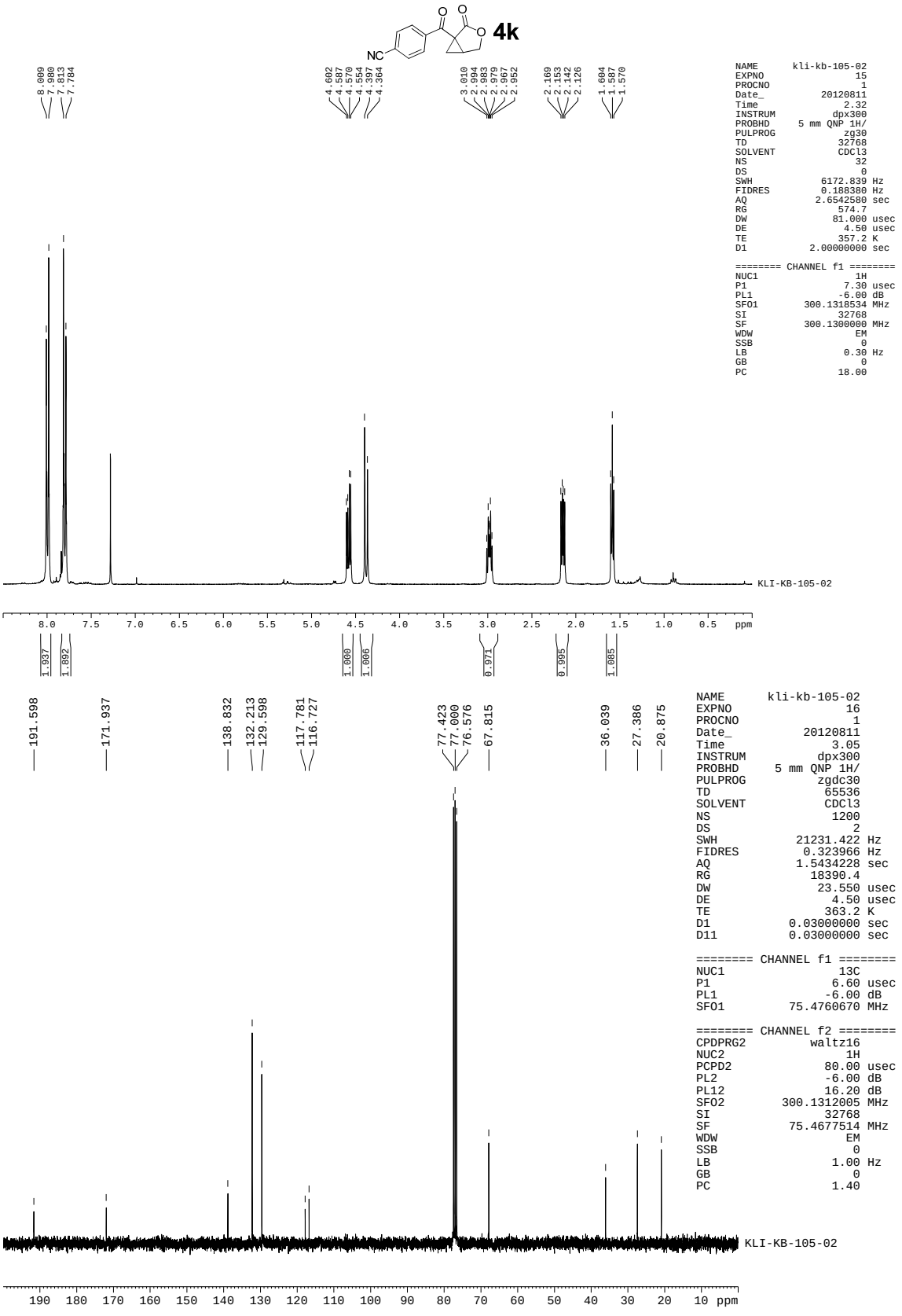


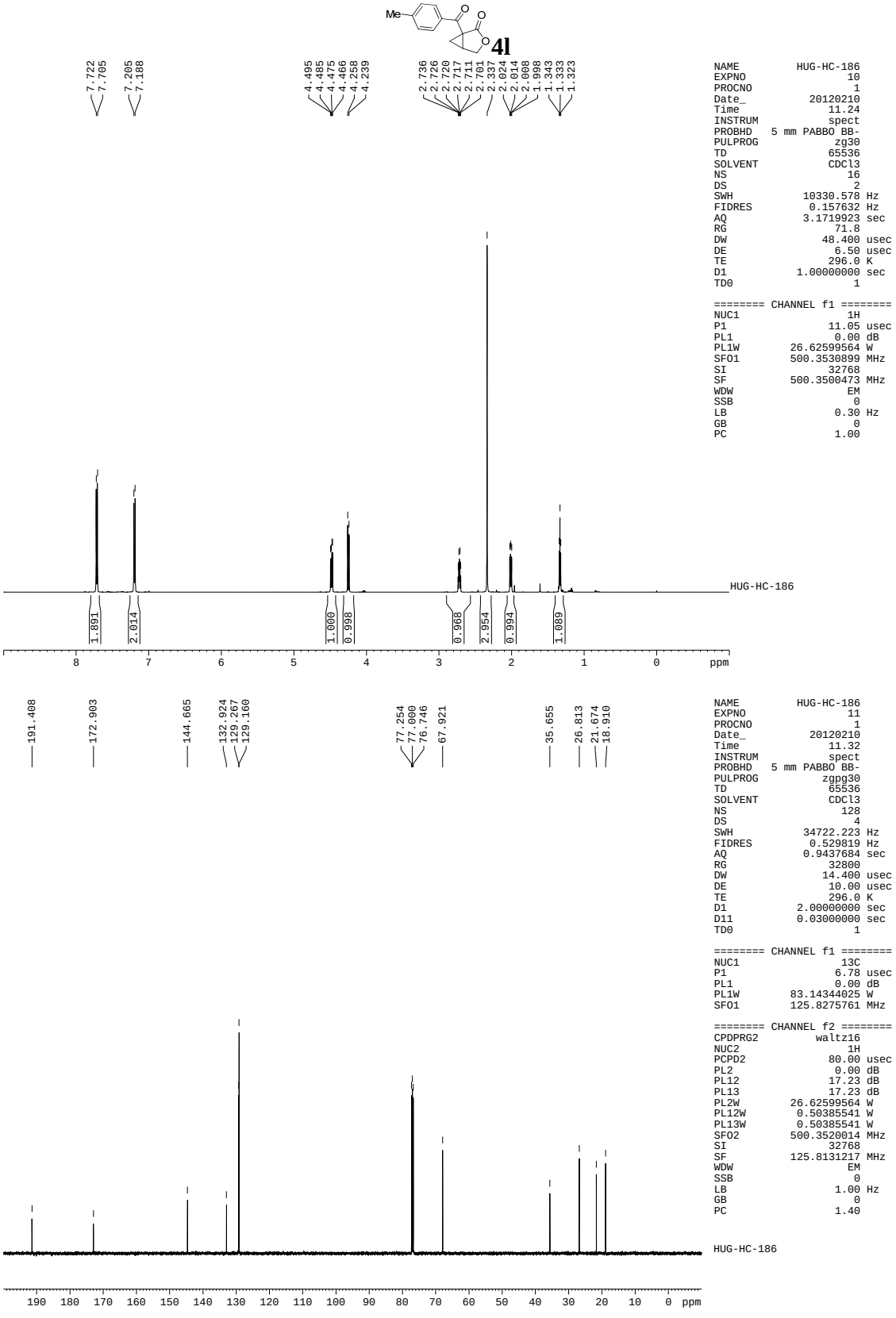

```
NAME          HUG-HC-295
EXPNO                 11
PROCNO                 1
Date_           20120525
Time               15.44
INSTRUM           dpx300
PROBHD     5 mm QNP 1H/
PULPROG          zgdc30
TD                65536
SOLVENT           CDCl3
NS                 1200
DS                    2
SWH           21231.422 Hz
FIDRES         0.323966 Hz
AQ             1.5434228 sec
RG              18390.4
DW               23.550 usec
DE                4.50 usec
TE                300.2 K
D1            0.03000000 sec
D11           0.03000000 sec

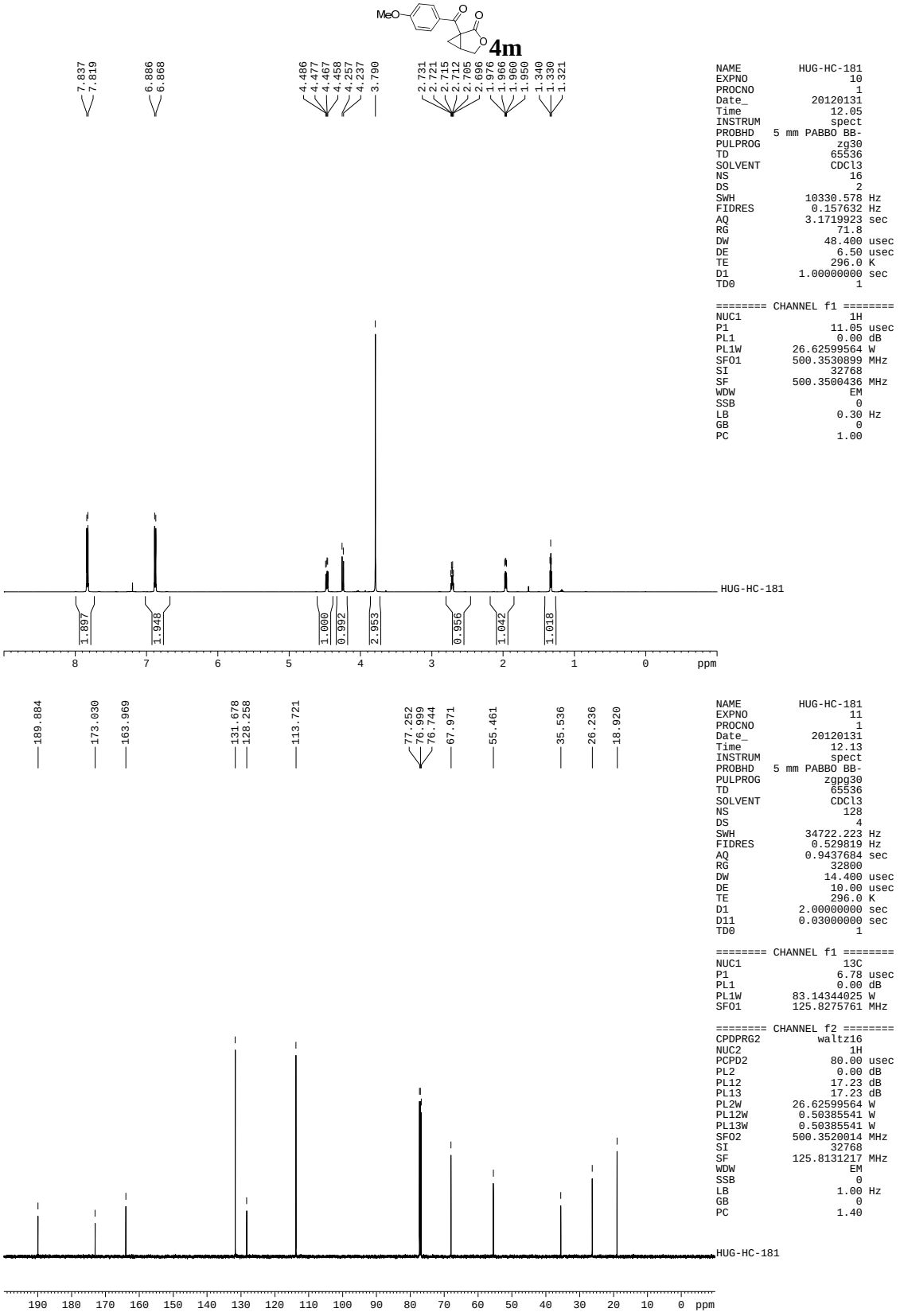
======== CHANNEL f1 ========
NUC1                13C
P1                6.60 usec
PL1              -6.00 dB
SFO1        75.4760670 MHz

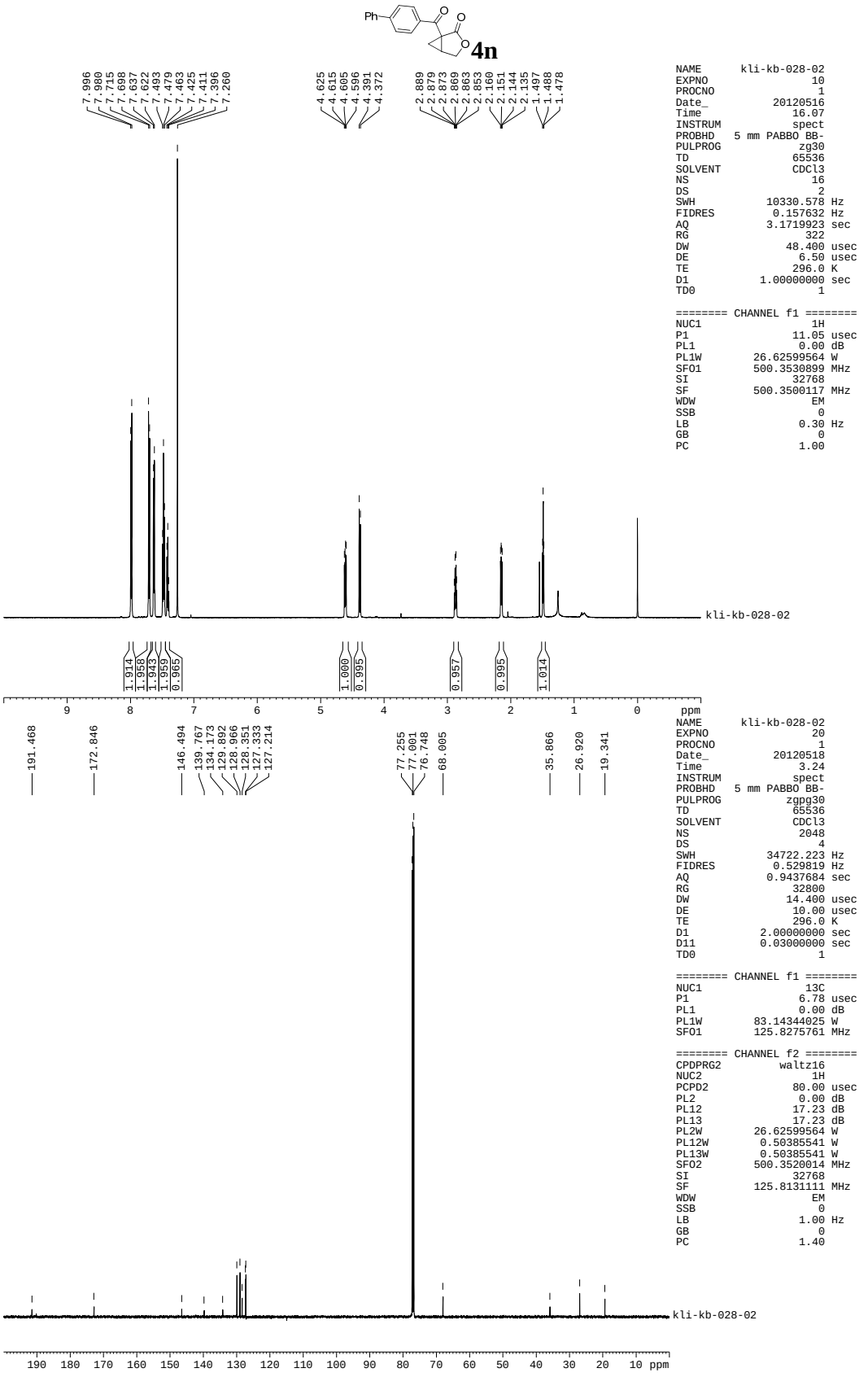
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -6.00 dB
PL12             16.20 dB
SFO2        300.1312005 MHz
SI                32768
SF          75.4677540 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC              1.40
```

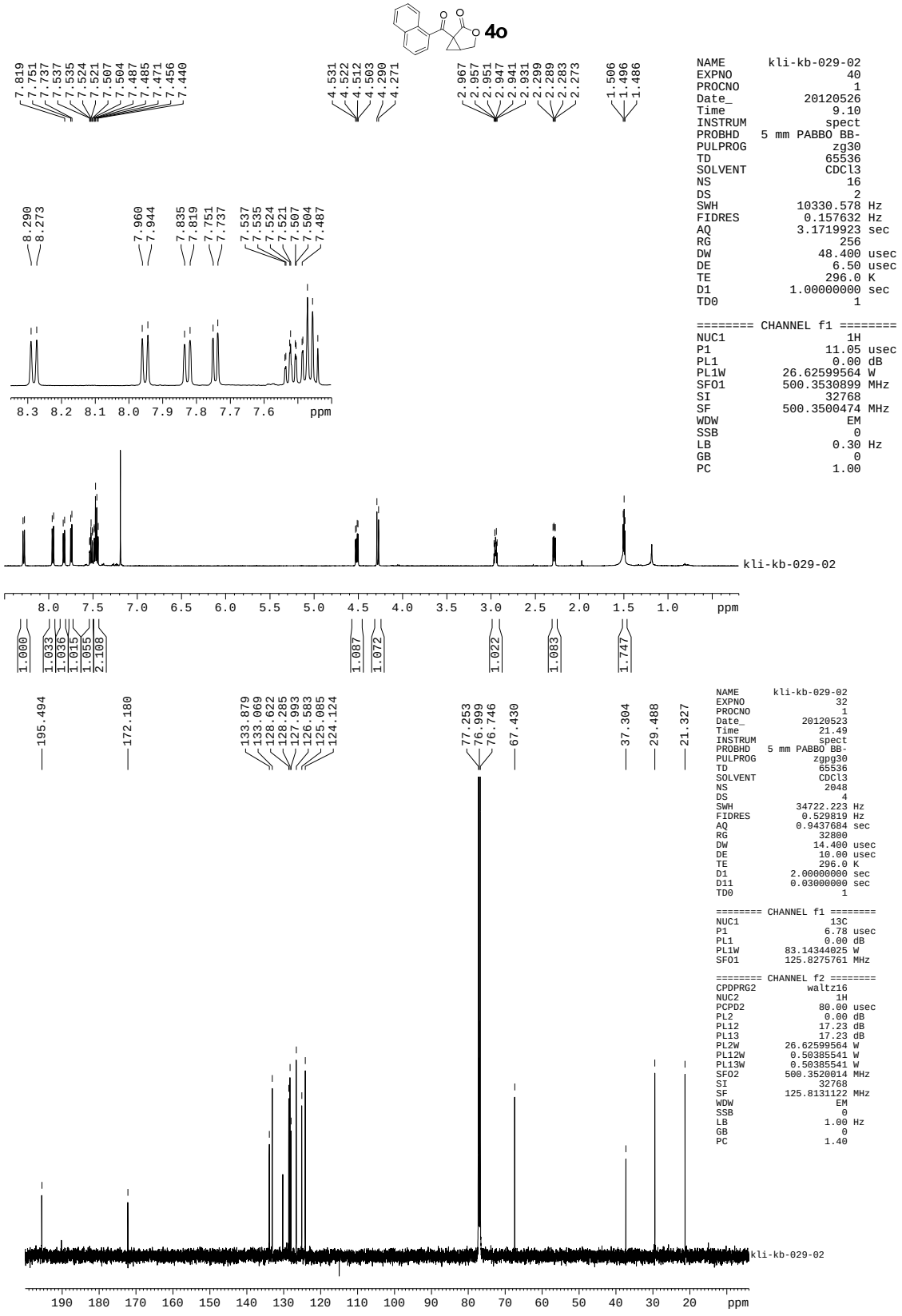

4j
F
7.971
7.966
7.956
7.948
7.206
7.177
7.148
4.597
4.582
4.565
4.550
4.378
4.346
2.911
2.896
2.887
2.884
2.880
2.869
2.853
2.109
2.093
2.082
2.066
1.512
1.495
1.479
NAME kli-kb-104-02
EXPNO 10
PROCNO 1
Date_ 20120809
Time 21.11
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 512
DW 81.000 usec
DE 4.50 usec
TE 361.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
KLI-KB-104-02
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 ppm
2.000
2.016
1.051
1.035
1.012
1.064
1.099
190.410
172.524
167.732
164.340
132.124
131.997
131.908
131.865
115.870
115.577
77.422
76.998
76.575
67.904
35.772
26.591
19.744
NAME kli-kb-104-02
EXPNO 11
PROCNO 1
Date_ 20120809
Time 21.44
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 16384
DW 23.550 usec
DE 4.50 usec
TE 362.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677511 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
KLI-KB-104-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

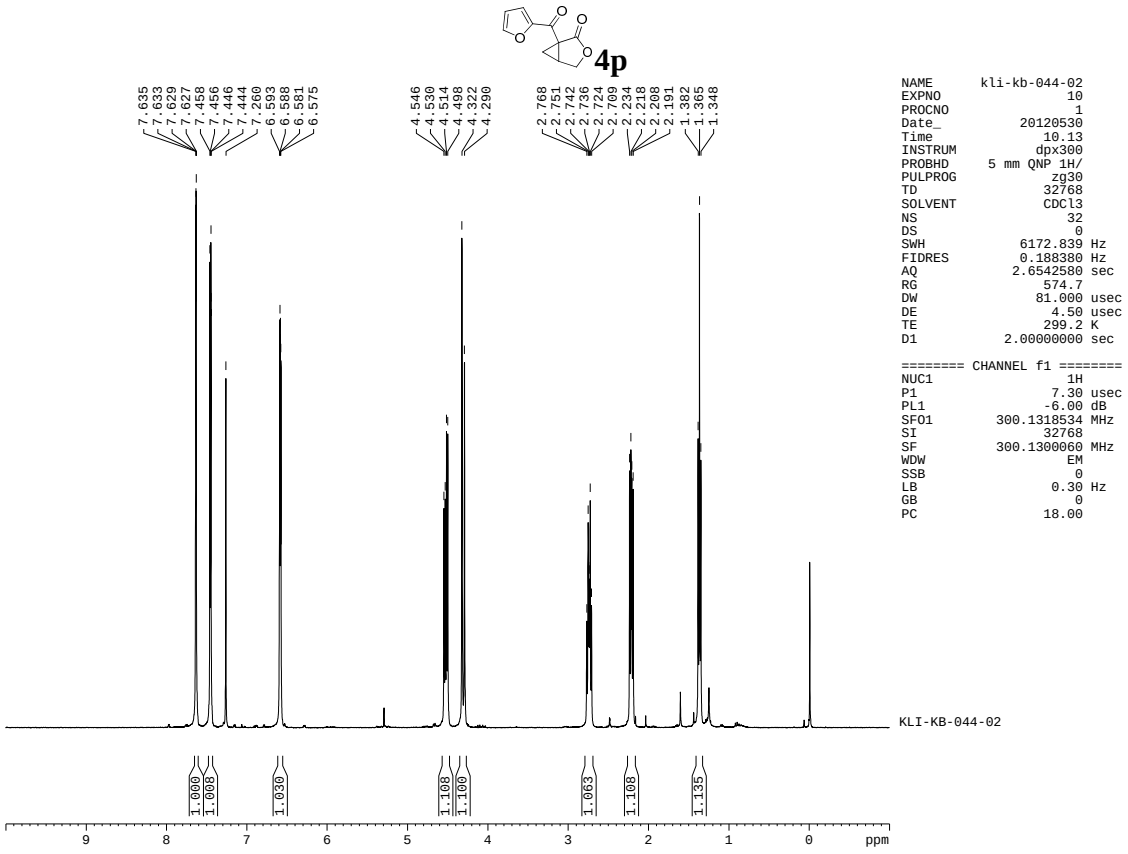

4k
NC
O
O
O
8.009
7.900
7.843
7.784
4.602
4.587
4.570
4.554
4.537
4.384
3.010
2.994
2.983
2.979
2.967
2.952
2.169
2.153
2.142
2.126
1.604
1.587
1.570
NAME kli-kb-105-02
EXPNO 15
PROCNO 1
Date_ 20120811
Time 2.32
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 574.7
DW 81.000 usec
DE 4.50 usec
TE 357.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
KLI-KB-105-02
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 ppm
1.937
1.892
1.000
1.006
0.971
0.995
1.085
191.598
171.937
138.832
132.213
129.598
117.781
116.727
77.423
77.000
76.576
67.815
36.039
27.386
20.875
NAME kli-kb-105-02
EXPNO 16
PROCNO 1
Date_ 20120811
Time 3.05
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 18390.4
DW 23.550 usec
DE 4.50 usec
TE 363.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
KLI-KB-105-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

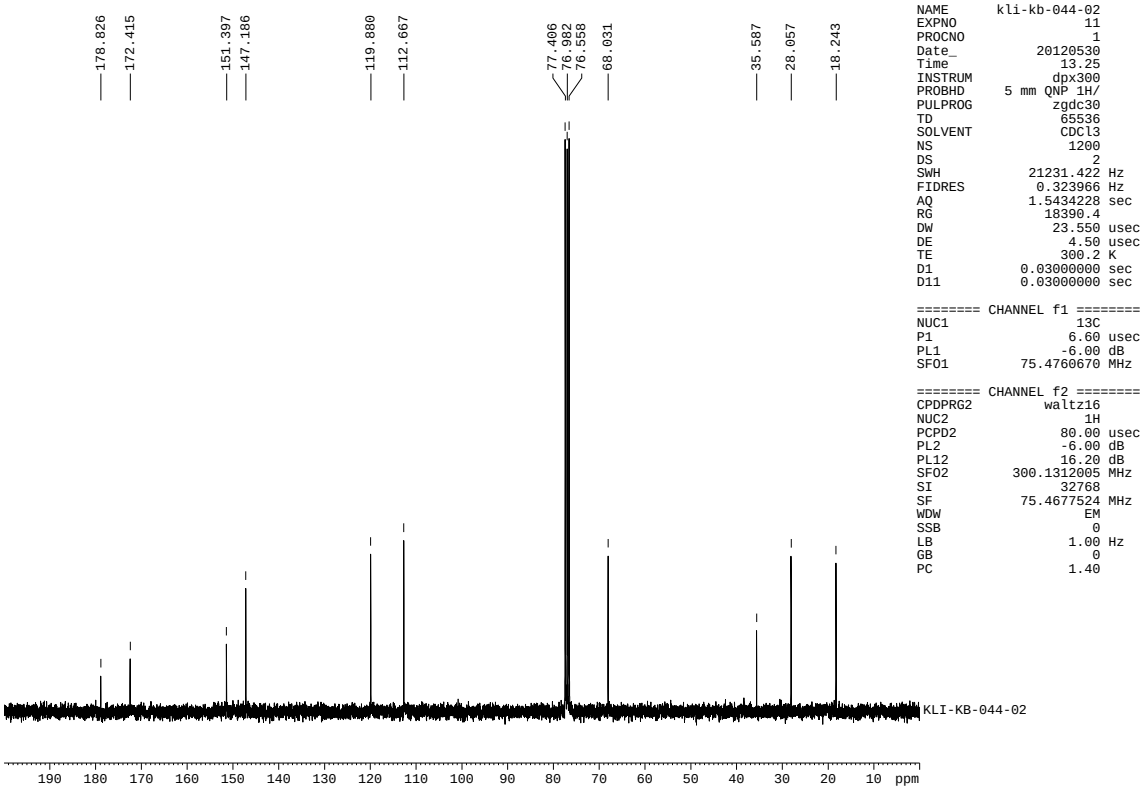

Me
O
O
O
4l
7.722
7.705
7.205
7.188
4.495
4.485
4.475
4.466
4.258
4.239
2.736
2.726
2.720
2.717
2.711
2.701
2.337
2.024
2.014
2.008
1.998
1.343
1.333
1.323
NAME HUG-HC-186
EXPNO 10
PROCNO 1
Date_ 20120210
Time 11.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500473 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-186
1.891
2.014
1.000
0.998
0.968
2.954
0.994
1.089
8
7
6
5
4
3
2
1
0
ppm
191.408
172.903
144.665
132.924
129.267
129.160
77.254
77.000
76.746
67.921
35.655
26.813
21.674
18.910
NAME HUG-HC-186
EXPNO 11
PROCNO 1
Date_ 20120210
Time 11.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131217 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-186
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

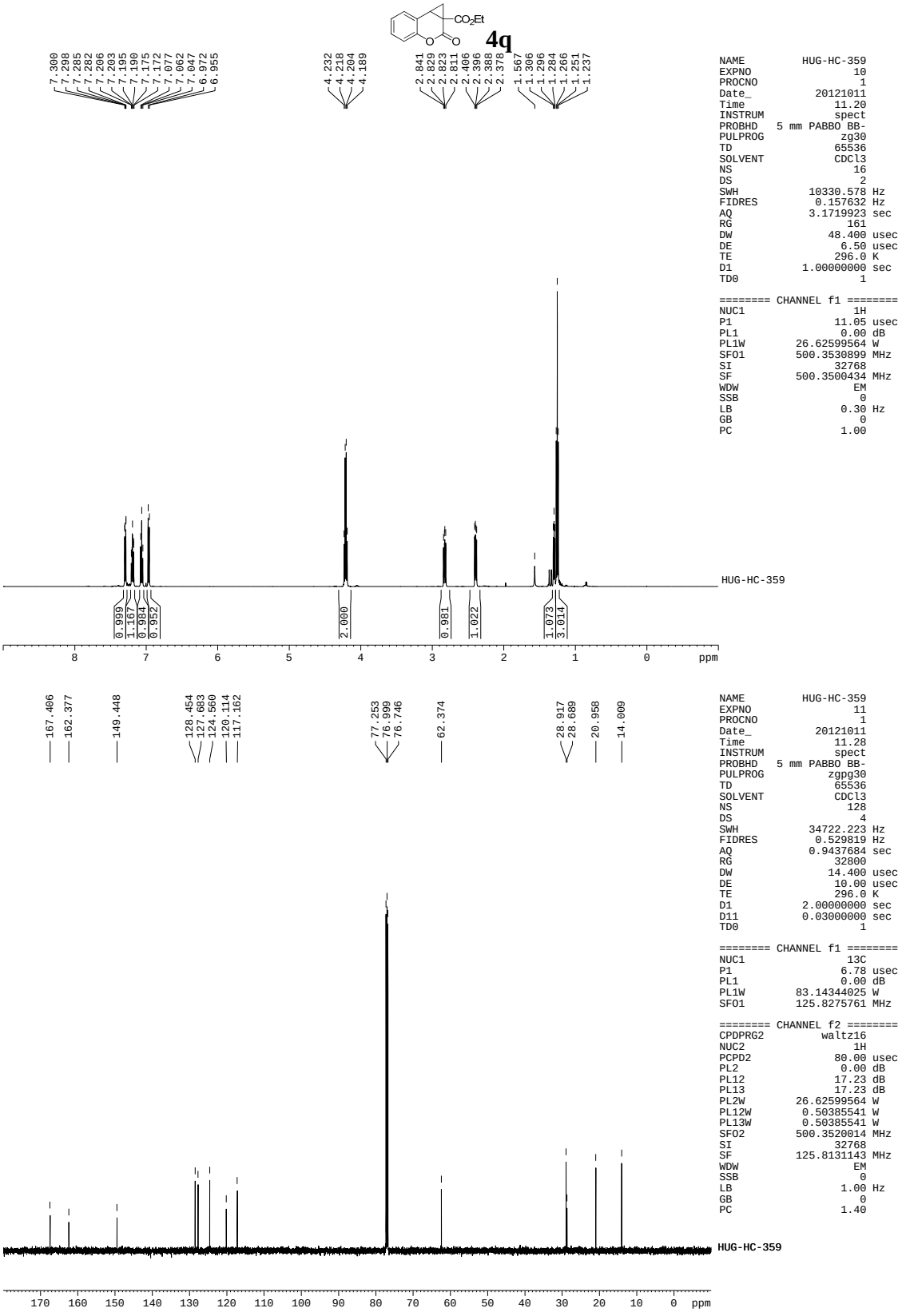

MeO
4m
7.837
7.819
6.886
6.868
4.486
4.477
4.467
4.458
4.257
4.237
3.790
2.731
2.721
2.715
2.712
2.705
2.696
1.976
1.966
1.960
1.950
1.340
1.330
1.321
NAME HUG-HC-181
EXPNO 10
PROCNO 1
Date_ 20120131
Time 12.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500436 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-181
1.897
1.948
1.000
0.992
2.953
0.956
1.042
1.018
8
7
6
5
4
3
2
1
0
ppm
189.884
173.030
163.969
131.678
128.258
113.721
77.252
76.999
76.744
67.971
55.461
35.536
26.236
18.920
NAME HUG-HC-181
EXPNO 11
PROCNO 1
Date_ 20120131
Time 12.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131217 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-181
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

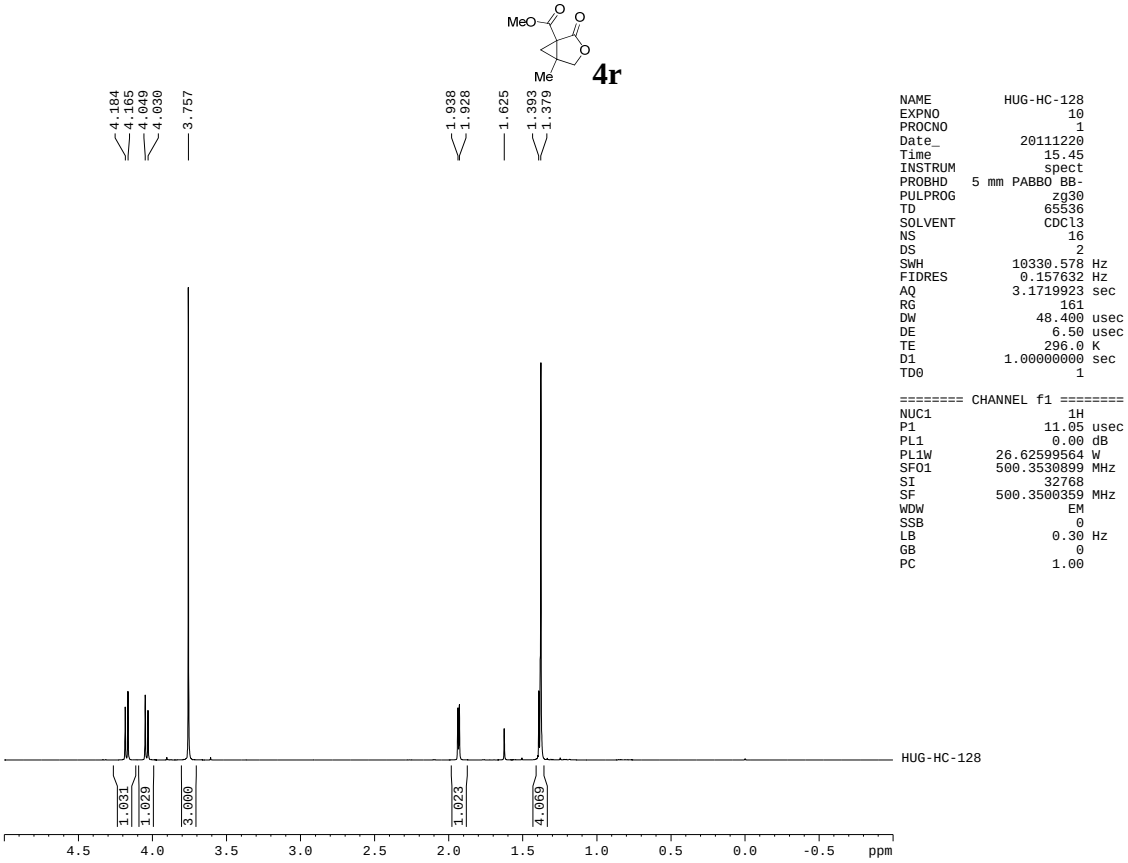

Ph
O
O
O
4n
7.996
7.980
7.715
7.698
7.637
7.622
7.493
7.479
7.463
7.425
7.411
7.396
7.260
4.625
4.615
4.605
4.596
4.391
4.372
2.889
2.879
2.873
2.869
2.863
2.853
2.160
2.151
2.144
2.135
2.497
1.488
1.478
NAME kli-kb-028-02
EXPNO 10
PROCNO 1
Date_ 20120516
Time 16.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 322
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
kli-kb-028-02
1.914
1.958
1.943
1.959
0.965
1.000
0.995
0.957
0.995
1.014
9 8 7 6 5 4 3 2 1 0 ppm
191.468
172.846
146.494
139.767
134.173
129.892
128.966
128.351
127.333
127.214
77.255
77.001
76.748
68.005
35.866
26.920
19.341
NAME kli-kb-028-02
EXPNO 20
PROCNO 1
Date_ 20120518
Time 3.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131111 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-028-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


4o
7.819 7.751 7.737 7.537 7.535 7.524 7.521 7.507 7.504 7.487 7.485 7.471 7.456 7.440
4.531 4.522 4.512 4.503 4.290 4.271
2.967 2.957 2.951 2.947 2.941 2.931 2.299 2.289 2.283 2.273
1.506 1.496 1.486
NAME kli-kb-029-02
EXPNO 40
PROCNO 1
Date_ 20120526
Time 9.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 256
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500474 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.290 8.273
7.960 7.944
7.835 7.819 7.751 7.737
7.537 7.535 7.524 7.521 7.507 7.504 7.487
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 ppm
kli-kb-029-02
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 ppm
1.000 1.033 1.036 1.015 1.055 2.108 1.087 1.072 1.022 1.083 1.747
195.494 172.180 133.879 133.069 128.622 128.285 127.993 126.583 125.085 124.124 77.253 76.999 76.746 67.430 37.304 29.488 21.327
NAME kli-kb-029-02
EXPNO 32
PROCNO 1
Date_ 20120523
Time 21.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131122 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-029-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


4p
7.635
7.633
7.629
7.627
7.458
7.456
7.446
7.444
7.260
6.593
6.588
6.581
6.575
4.546
4.530
4.514
4.498
4.322
4.290
2.768
2.751
2.742
2.736
2.724
2.709
2.234
2.218
2.208
2.191
1.382
1.365
1.348
NAME kli-kb-044-02
EXPNO 10
PROCNO 1
Date_ 20120530
Time 10.13
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 574.7
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
KLI-KB-044-02
1.000
1.008
1.030
1.108
1.100
1.063
1.108
1.135
9
8
7
6
5
4
3
2
1
0
ppm

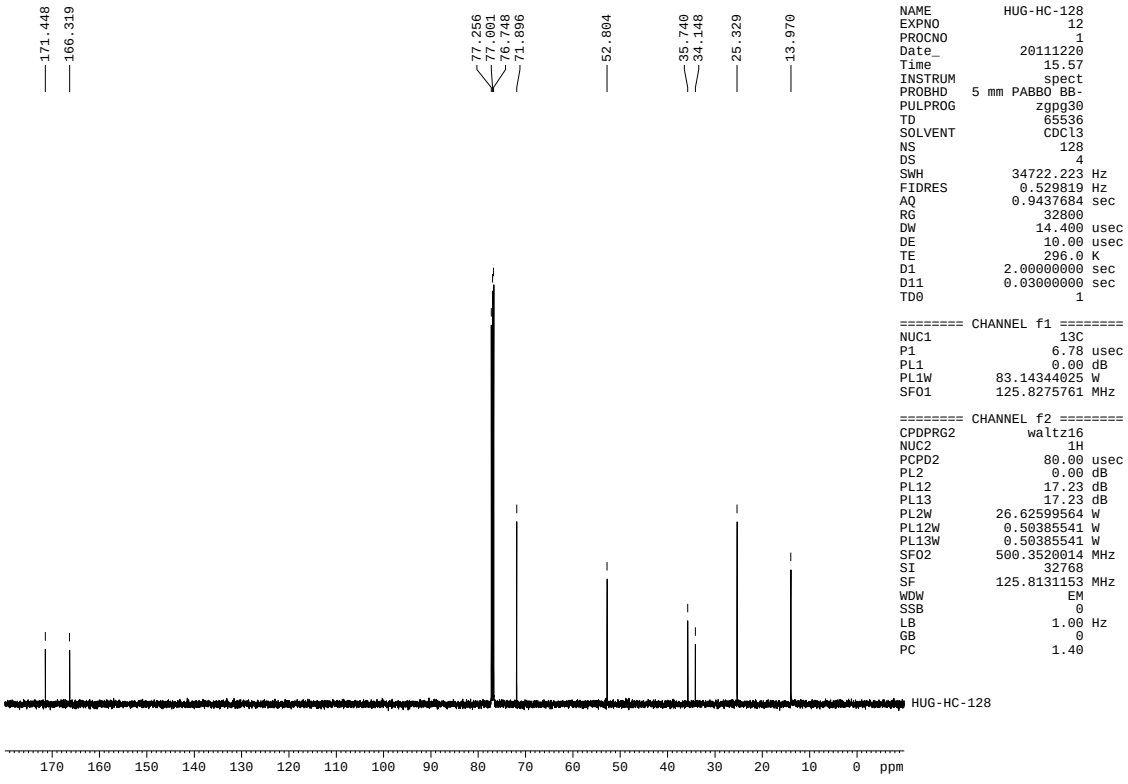

178.826
172.415
151.397
147.186
119.880
112.667
77.406
76.982
76.558
68.031
35.587
28.057
18.243
NAME kli-kb-044-02
EXPNO 11
PROCNO 1
Date_ 20120530
Time 13.25
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 18390.4
DW 23.550 usec
DE 4.50 usec
TE 300.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
KLI-KB-044-02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


CO2Et
4q
7.300
7.298
7.285
7.282
7.206
7.203
7.195
7.190
7.175
7.172
7.077
7.062
7.047
6.972
6.955
4.232
4.218
4.204
4.189
2.841
2.829
2.823
2.811
2.406
2.396
2.388
2.378
1.567
1.306
1.296
1.284
1.266
1.251
1.237
NAME HUG-HC-359
EXPNO 10
PROCNO 1
Date_ 20121011
Time 11.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500434 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-359
0.999
1.167
0.984
0.952
2.000
0.981
1.022
1.073
3.014
8
7
6
5
4
3
2
1
0
ppm
167.406
162.377
149.448
128.454
127.683
124.560
120.114
117.162
77.253
76.999
76.746
62.374
28.917
28.689
20.958
14.009
NAME HUG-HC-359
EXPNO 11
PROCNO 1
Date_ 20121011
Time 11.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131143 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-359
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm




```
NAME          HUG-HC-128
EXPNO                 10
PROCNO                 1
Date_           20111220
Time               15.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
TD0                    1

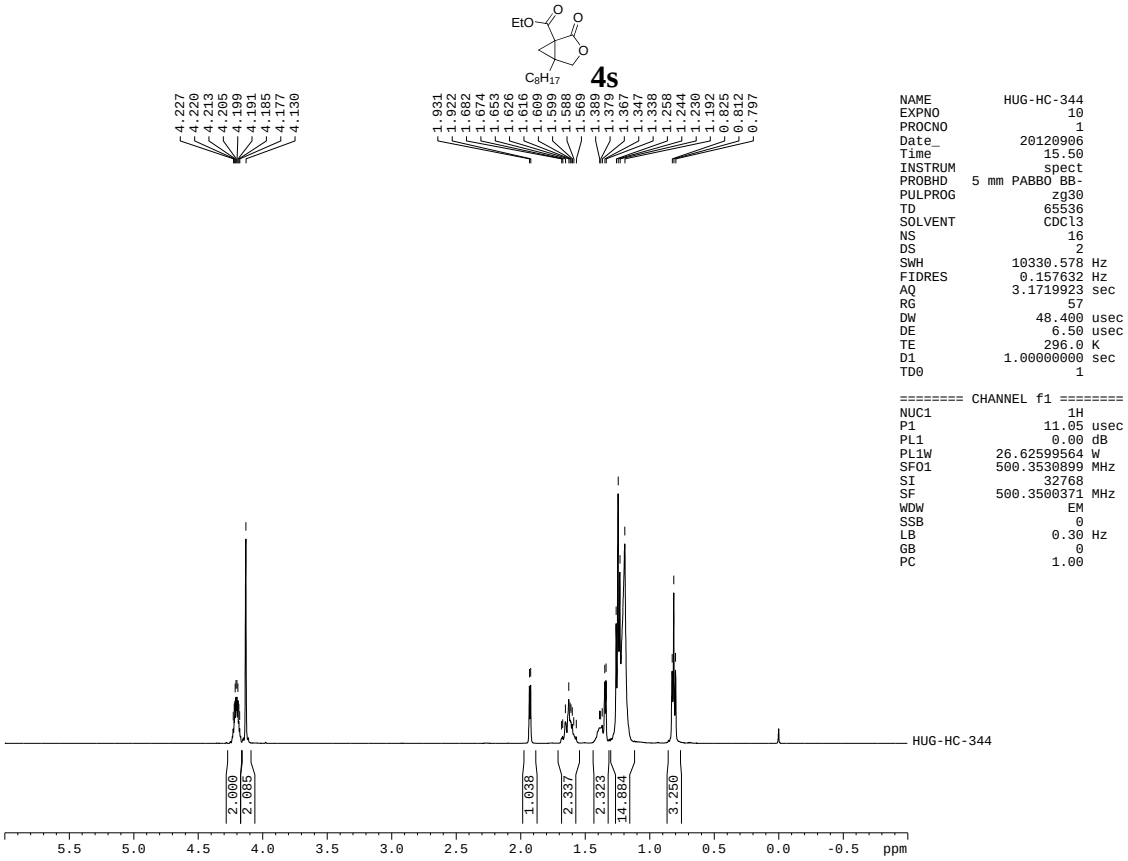
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500359 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

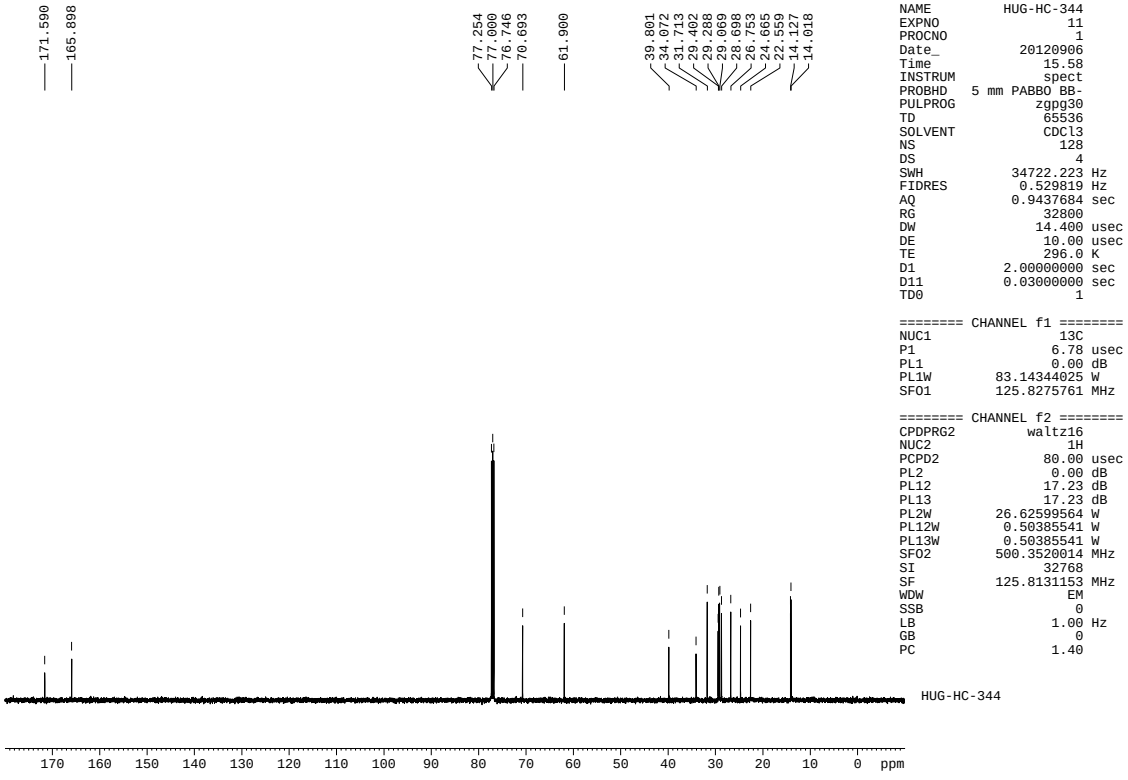


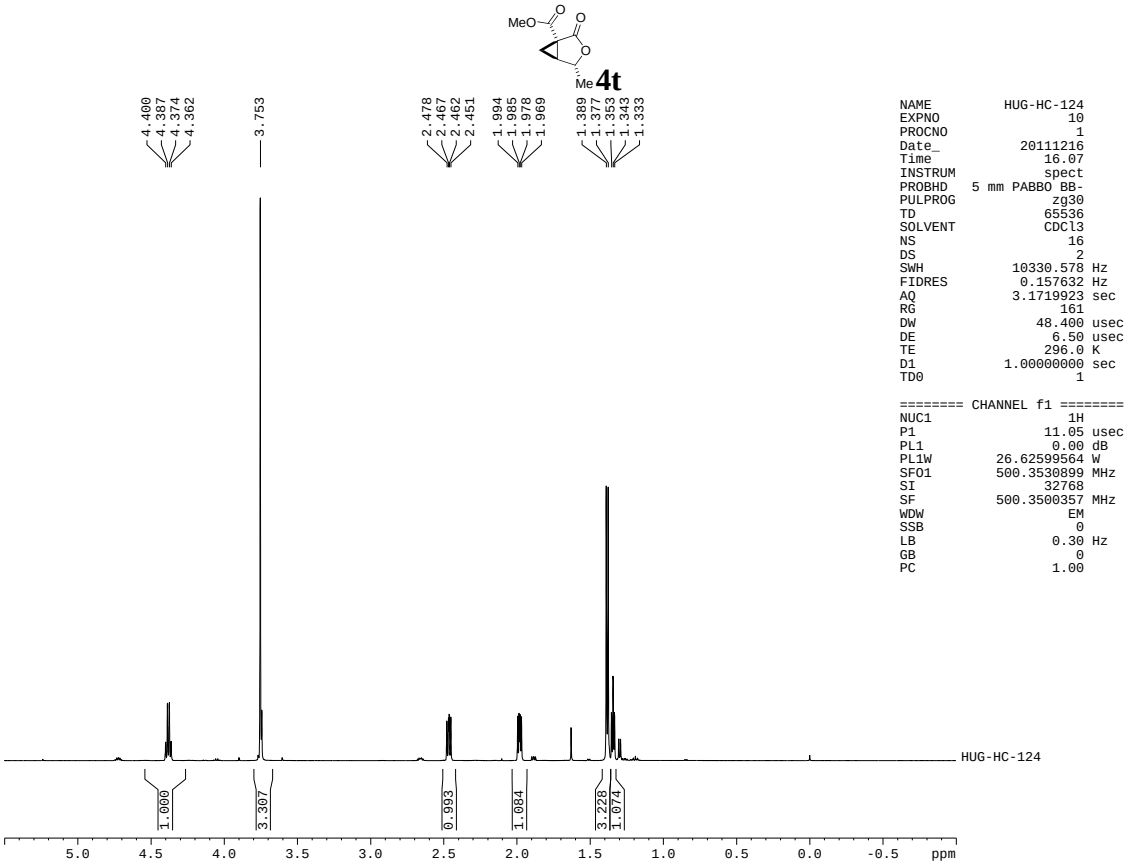

```
NAME          HUG-HC-128
EXPNO                 12
PROCNO                 1
Date_           20111220
Time               15.57
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                 10.00 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131153 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

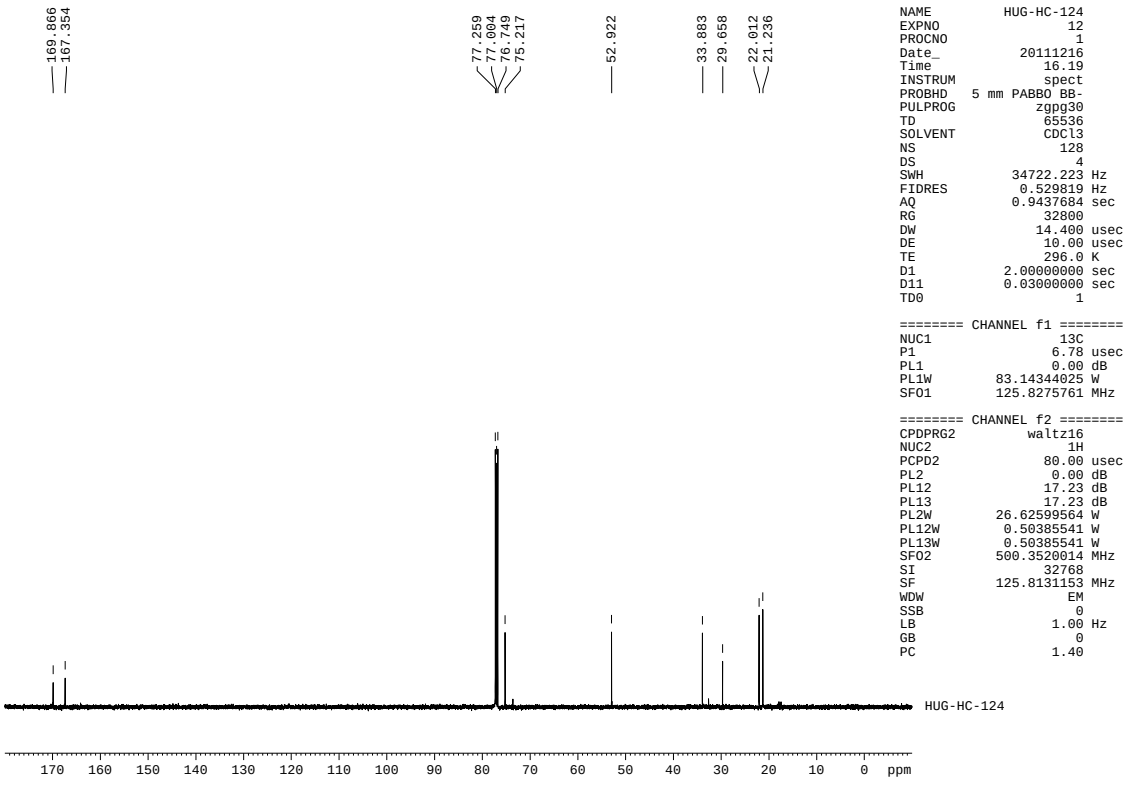

EtO
O
O
O
C8H17
4s
4.227
4.220
4.213
4.205
4.199
4.191
4.185
4.177
4.130
1.931
1.922
1.682
1.674
1.653
1.626
1.616
1.609
1.599
1.588
1.569
1.389
1.379
1.367
1.347
1.338
1.258
1.244
1.230
1.192
0.825
0.812
0.797
NAME HUG-HC-344
EXPNO 10
PROCNO 1
Date_ 20120906
Time 15.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500371 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-344
2.000
2.085
1.038
2.337
2.323
14.684
3.250
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm


171.590
165.898
77.254
77.000
76.746
70.693
61.900
39.801
34.072
31.713
29.402
29.288
29.069
28.698
28.753
24.665
22.559
14.127
14.018
NAME HUG-HC-344
EXPNO 11
PROCNO 1
Date_ 20120906
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131153 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-344
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm




```
NAME          HUG-HC-124
EXPNO                 10
PROCNO                 1
Date_           20111216
Time               16.07
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ              3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

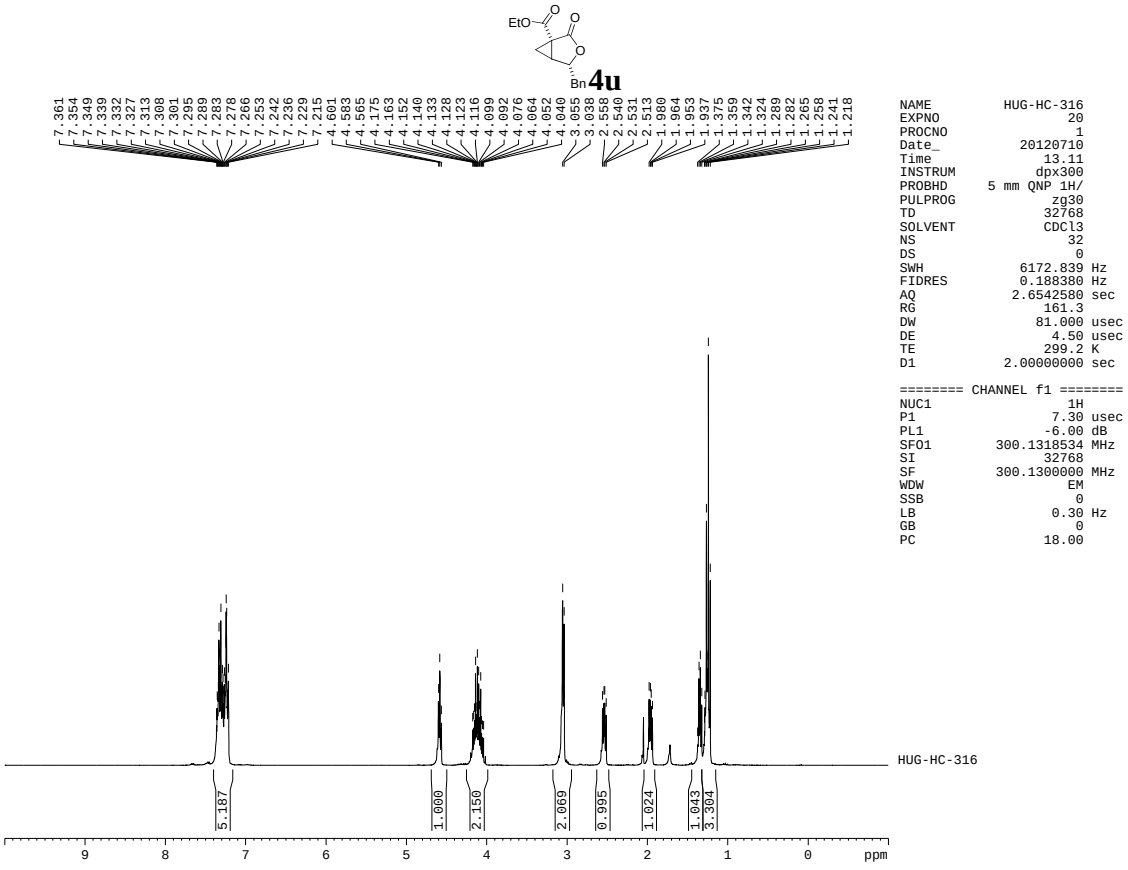
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500357 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

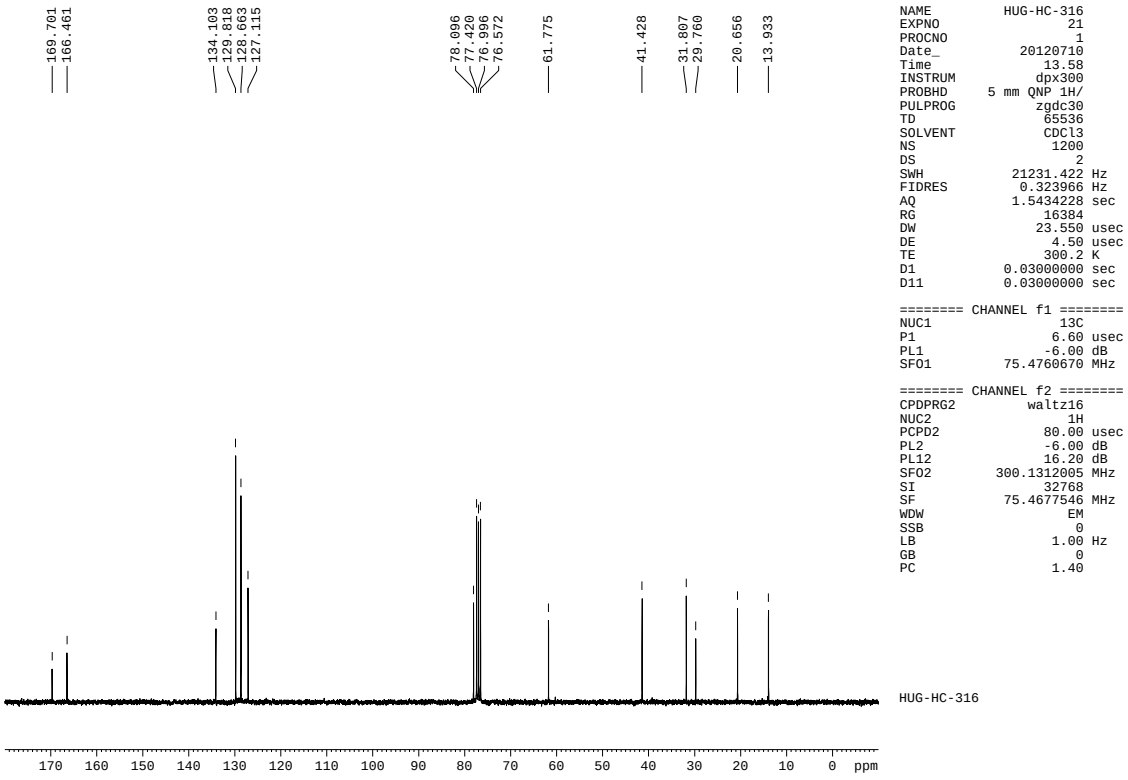


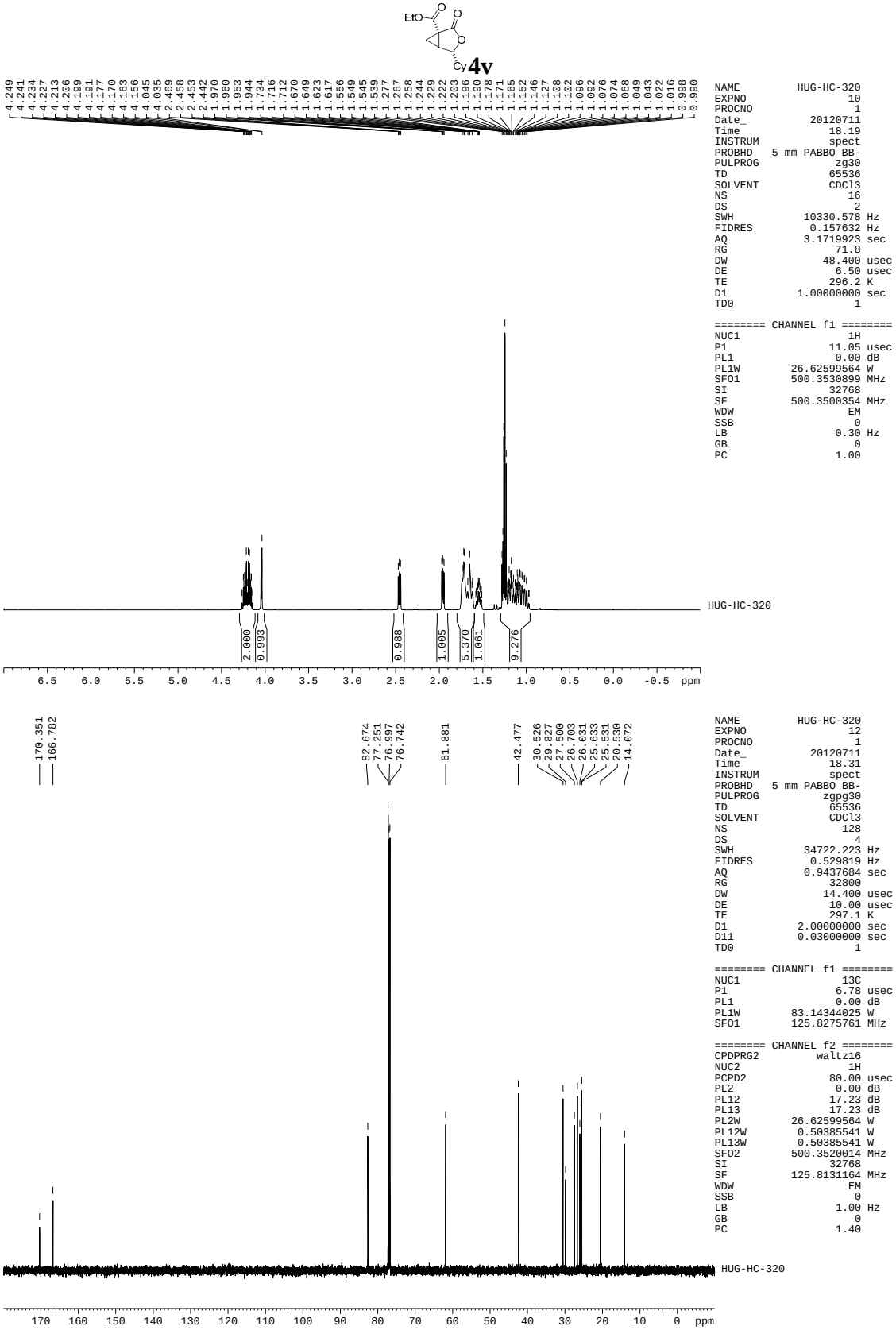

```
NAME          HUG-HC-124
EXPNO                 12
PROCNO                 1
Date_           20111216
Time               16.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH            34722.223 Hz
FIDRES          0.529819 Hz
AQ              0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

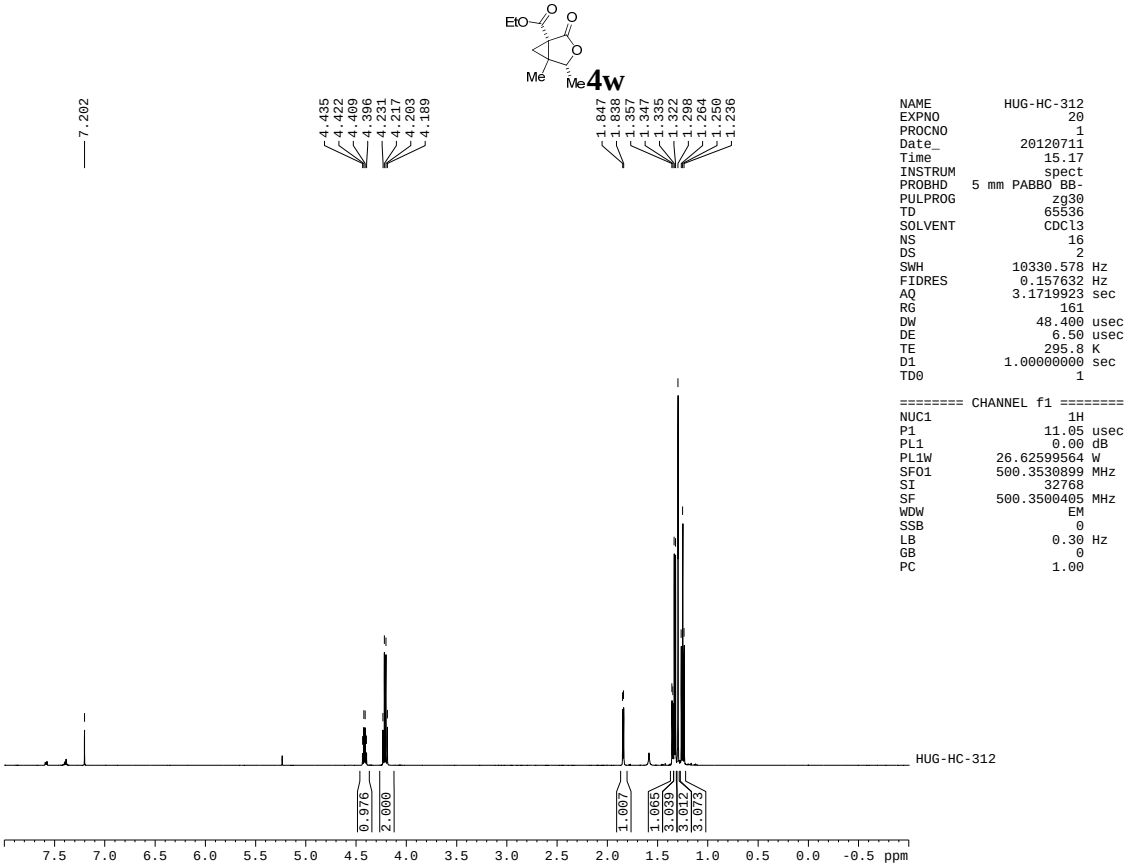
======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1         125.8275761 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131153 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```


EtO
O
O
O
Bn
4u
7.361 7.354 7.349 7.339 7.332 7.327 7.313 7.308 7.301 7.295 7.289 7.283 7.278 7.266 7.253 7.242 7.236 7.229 7.215
4.601 4.583 4.565 4.175 4.163 4.152 4.140 4.133 4.128 4.123 4.116 4.099 4.092 4.076 4.064 4.052 4.040
3.055 3.038 2.558 2.540 2.531 2.513 1.980 1.964 1.953 1.937 1.375 1.359 1.342 1.324 1.289 1.282 1.265 1.258 1.241 1.218
NAME HUG-HC-316
EXPNO 20
PROCNO 1
Date_ 20120710
Time 13.11
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 161.3
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
HUG-HC-316
5.187 1.000 2.150 2.069 0.995 1.024 1.043 3.304
9 8 7 6 5 4 3 2 1 0 ppm

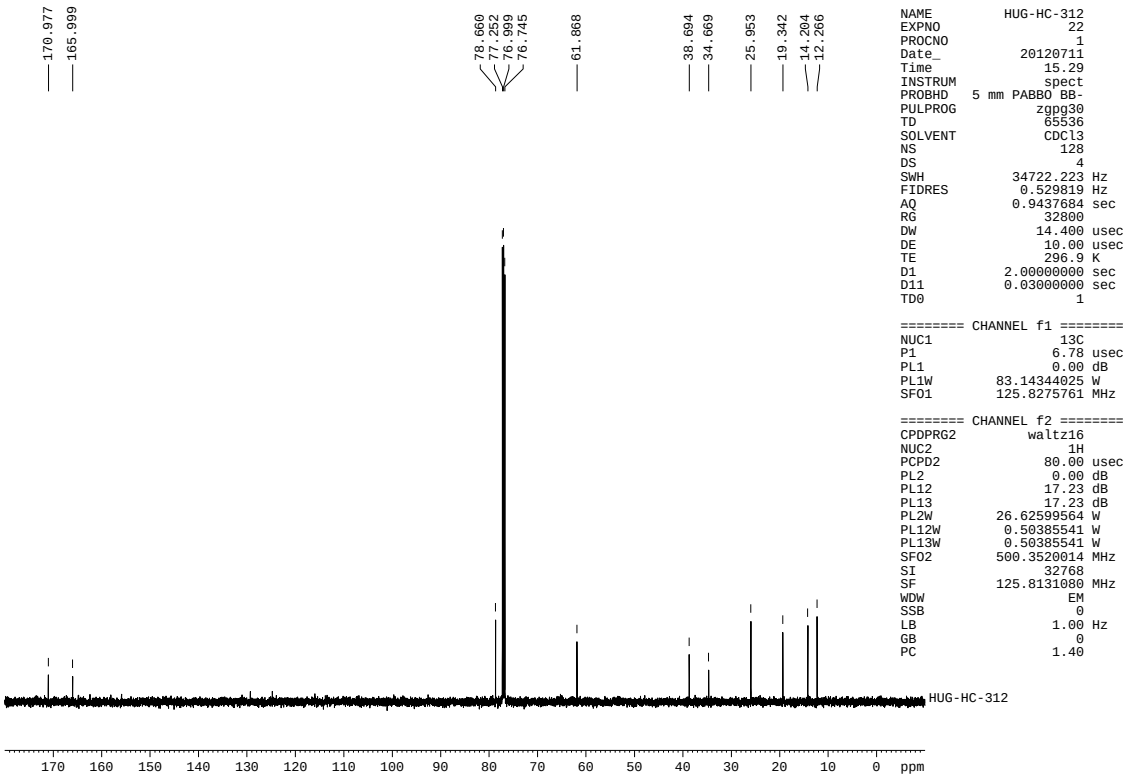

169.701
166.461
134.103
129.818
128.663
127.115
78.096
77.420
76.996
76.572
61.775
41.428
31.807
29.760
20.656
13.933
NAME HUG-HC-316
EXPNO 21
PROCNO 1
Date_ 20120710
Time 13.58
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 16384
DW 23.550 usec
DE 4.50 usec
TE 300.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677546 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-316
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


EtO
O
O
O
Cy
4v
4.249 4.241 4.234 4.227 4.213 4.206 4.199 4.191 4.177 4.170 4.163 4.156 4.045 4.035 2.469 2.458 2.453 2.442 1.970 1.960 1.953 1.944 1.734 1.716 1.712 1.670 1.649 1.623 1.617 1.556 1.549 1.545 1.539 1.277 1.267 1.258 1.244 1.229 1.222 1.203 1.196 1.190 1.178 1.171 1.165 1.152 1.146 1.127 1.108 1.102 1.096 1.092 1.076 1.074 1.068 1.049 1.043 1.022 1.016 0.998 0.990
NAME HUG-HC-320
EXPNO 10
PROCNO 1
Date_ 20120711
Time 18.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500354 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-320
2.000
0.993
0.988
1.005
5.370
1.061
9.276
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 -0.5 ppm
170.351 166.782 82.674 77.251 76.997 76.742 61.881 42.477 30.526 29.827 27.500 26.703 26.031 25.633 25.531 20.530 14.072
NAME HUG-HC-320
EXPNO 12
PROCNO 1
Date_ 20120711
Time 18.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131164 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-320
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm




```
NAME          HUG-HC-312
EXPNO                 20
PROCNO                 1
Date_           20120711
Time               15.17
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   161
DW                48.400 usec
DE                 6.50 usec
TE                295.8 K
D1           1.00000000 sec
TD0                    1

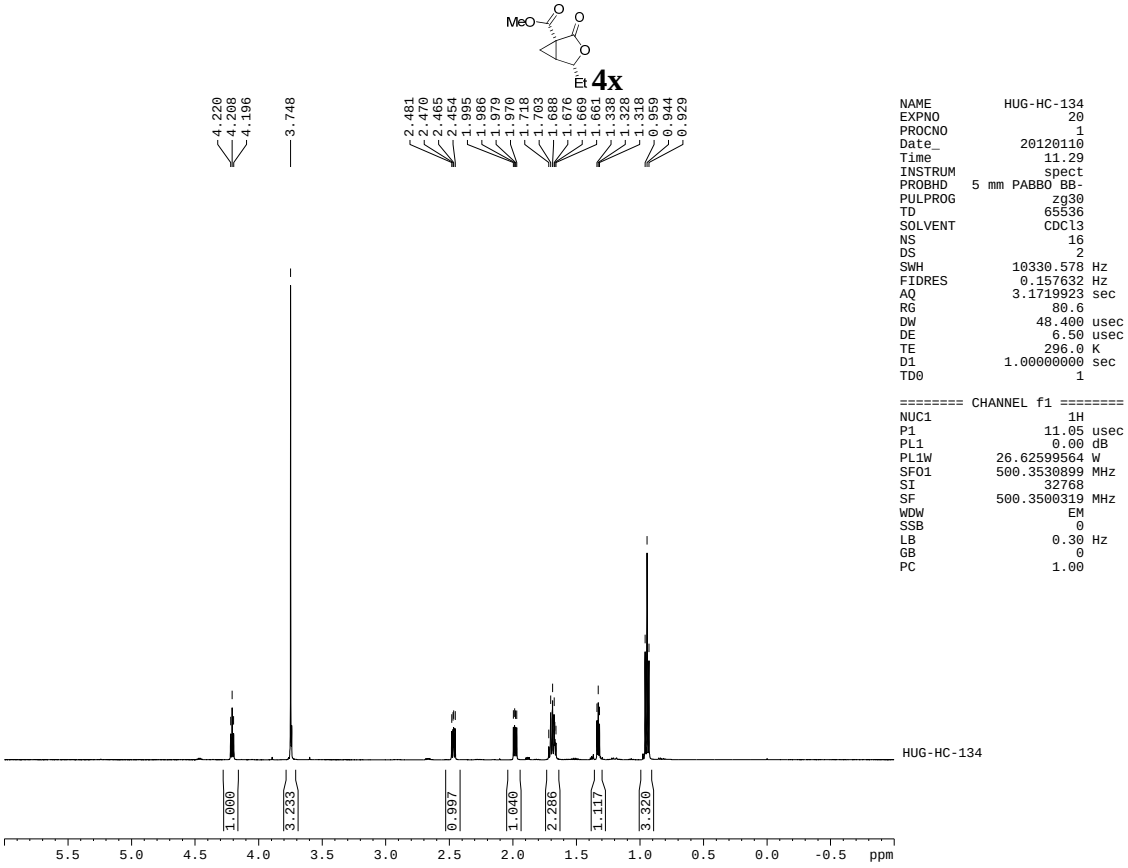
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1        500.3530899 MHz
SI                 32768
SF          500.3500405 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

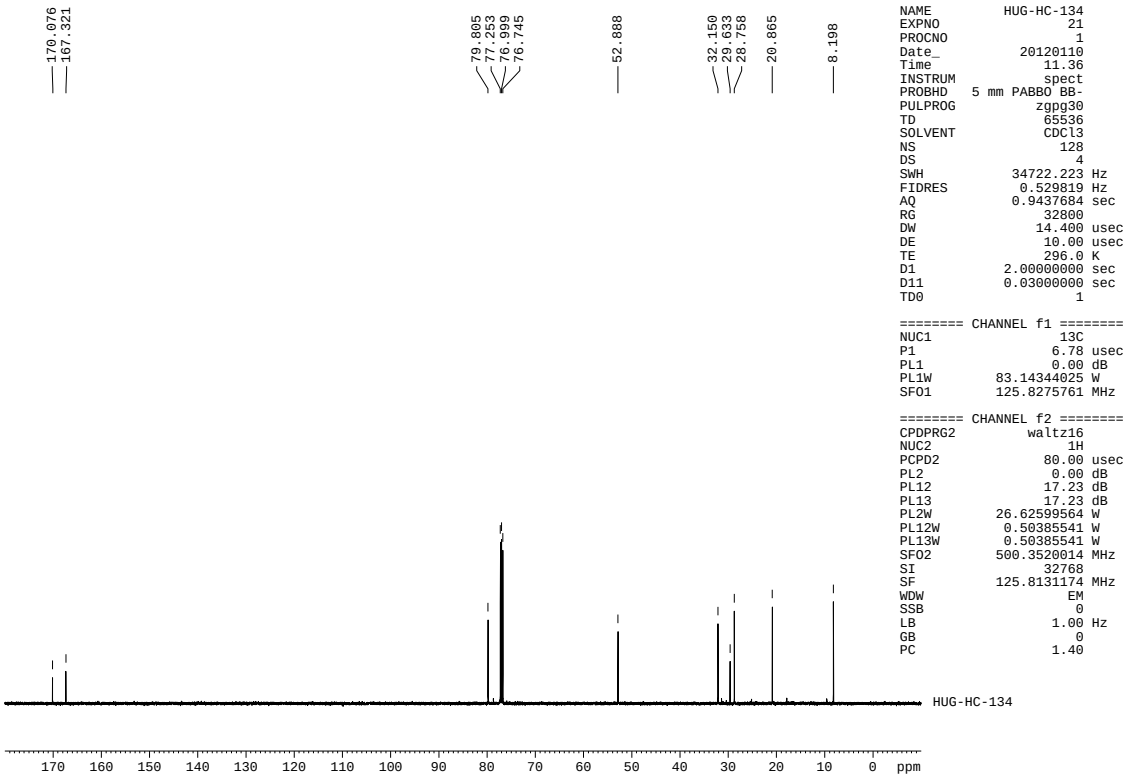


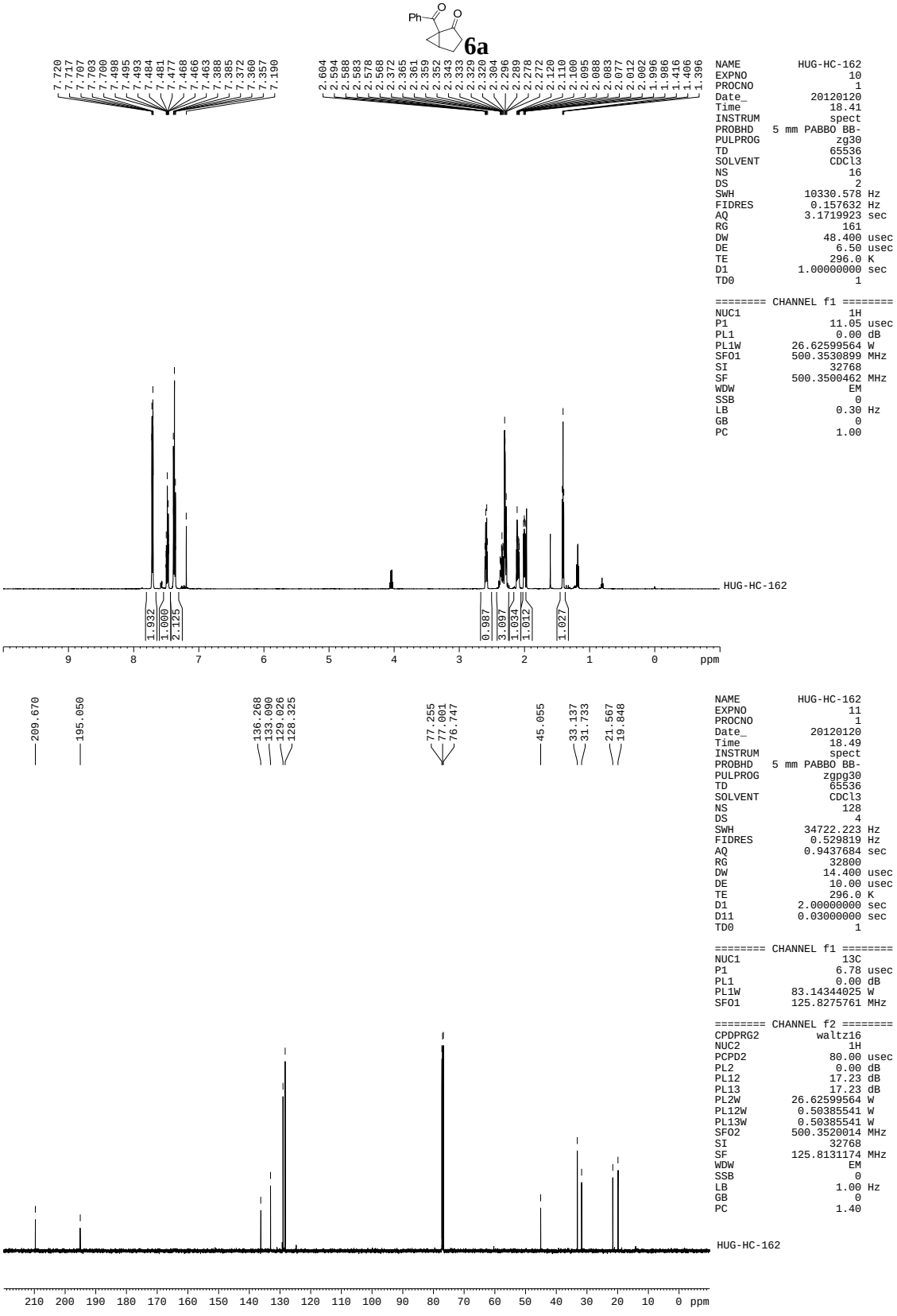

```
NAME          HUG-HC-312
EXPNO                 22
PROCNO                 1
Date_           20120711
Time               15.29
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

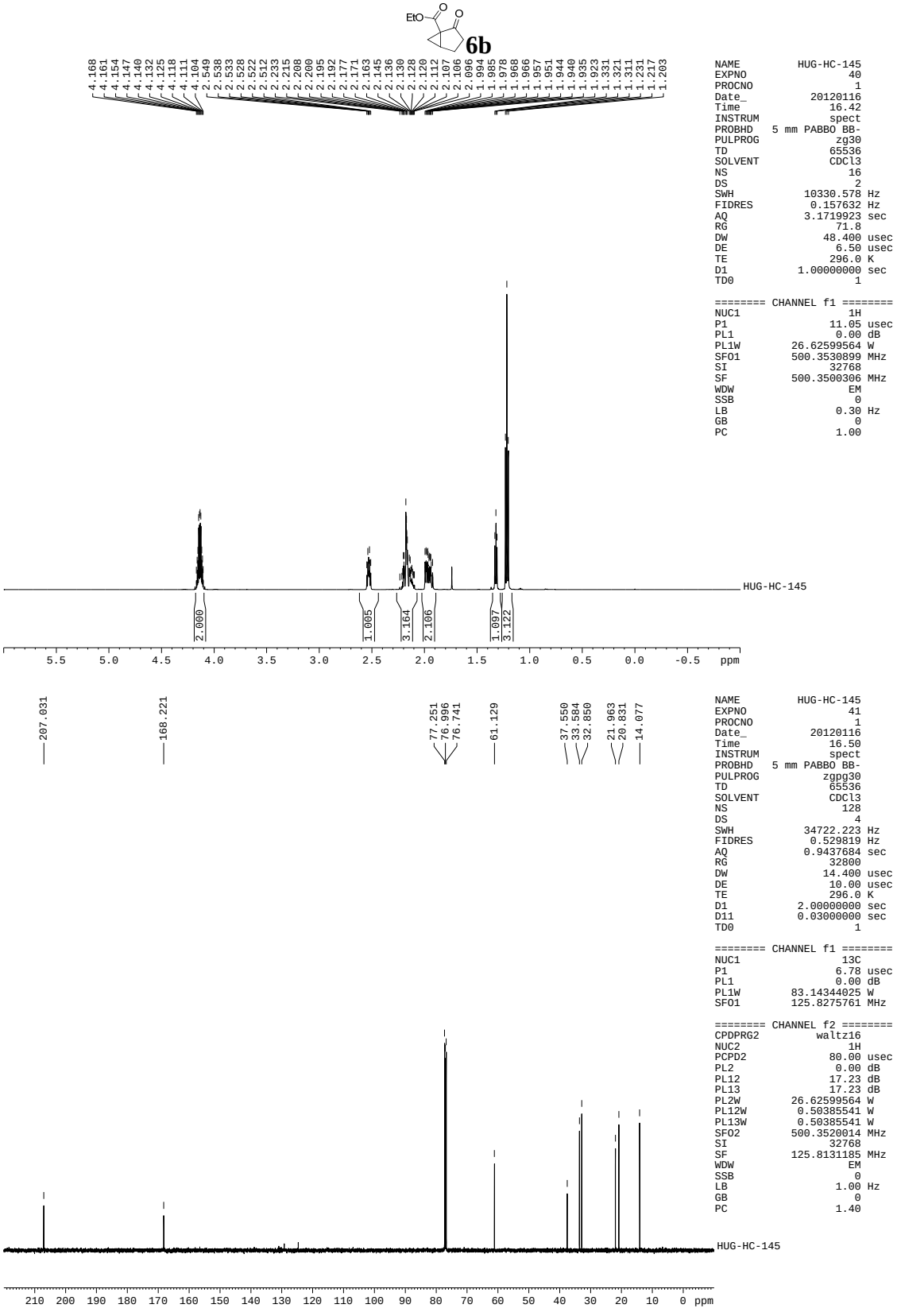
======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1        125.8275761 MHz

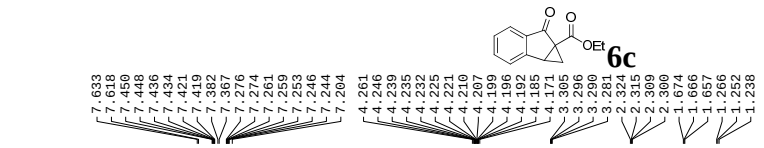
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2        500.3520014 MHz
SI                 32768
SF          125.8131080 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```


MeO
Et
4x
4.220
4.208
4.196
3.748
2.481
2.470
2.465
2.454
1.995
1.986
1.979
1.970
1.718
1.703
1.688
1.676
1.669
1.651
1.338
1.328
1.318
0.959
0.944
0.929
NAME HUG-HC-134
EXPNO 20
PROCNO 1
Date_ 20120110
Time 11.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500319 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-134
1.000
3.233
0.997
1.040
2.286
1.117
3.320
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm


170.076
167.321
79.805
77.253
76.999
76.745
52.888
32.150
29.633
28.758
20.865
8.198
NAME HUG-HC-134
EXPNO 21
PROCNO 1
Date_ 20120110
Time 11.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131174 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-134
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

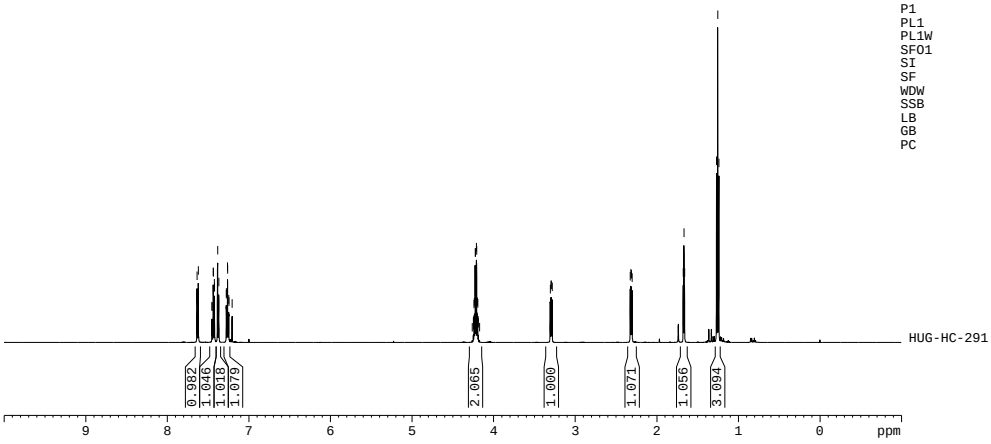

Ph
O
O
6a
7.720
7.717
7.707
7.703
7.700
7.498
7.495
7.493
7.484
7.481
7.477
7.468
7.466
7.463
7.388
7.385
7.372
7.360
7.357
7.190
2.604
2.594
2.588
2.583
2.578
2.568
2.372
2.365
2.361
2.359
2.352
2.343
2.333
2.329
2.320
2.304
2.296
2.289
2.278
2.272
2.120
2.110
2.100
2.095
2.088
2.083
2.077
2.012
2.002
1.996
1.986
1.416
1.406
1.396
NAME HUG-HC-162
EXPNO 10
PROCNO 1
Date_ 20120120
Time 18.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500462 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-162
1.932
1.000
2.125
0.987
3.097
1.034
1.012
1.027
9
8
7
6
5
4
3
2
1
0
ppm
209.670
195.050
136.268
133.090
129.026
128.325
77.255
77.001
76.747
45.055
33.137
31.733
21.567
19.848
NAME HUG-HC-162
EXPNO 11
PROCNO 1
Date_ 20120120
Time 18.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131174 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-162
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

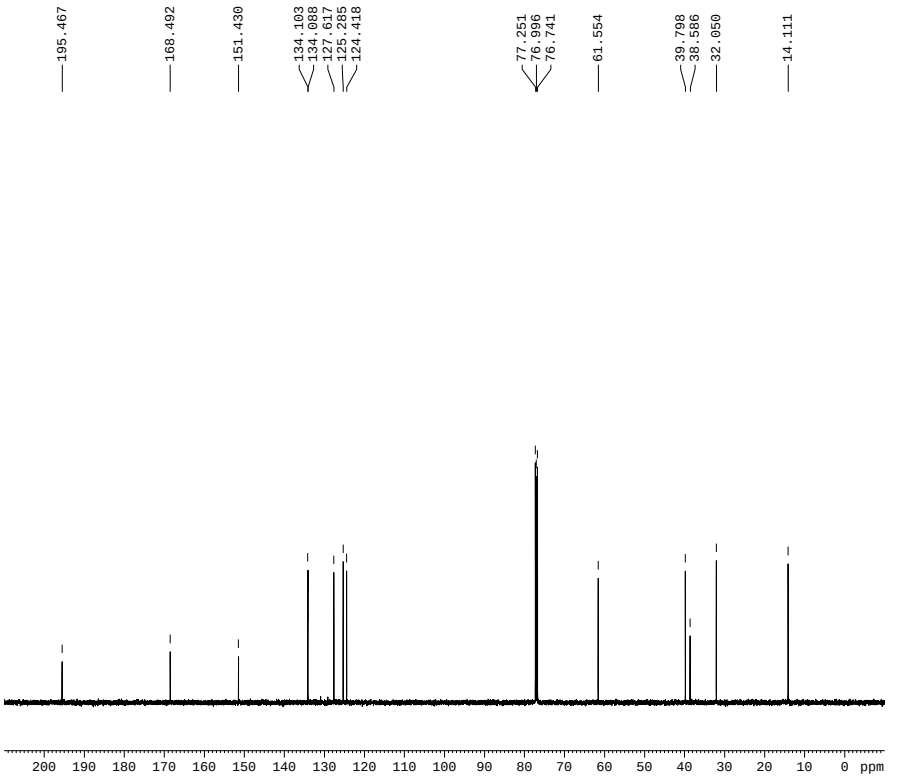

EtO
O
O
6b
4.168 4.161 4.154 4.147 4.140 4.132 4.125 4.118 4.111 4.104 4.549 2.538 2.533 2.528 2.522 2.512 2.233 2.215 2.208 2.200 2.195 2.192 2.177 2.171 2.163 2.145 2.136 2.130 2.128 2.120 2.112 2.107 2.106 2.096 1.994 1.985 1.978 1.968 1.966 1.957 1.951 1.944 1.940 1.935 1.923 1.331 1.321 1.311 1.231 1.217 1.203
NAME HUG-HC-145
EXPNO 40
PROCNO 1
Date_ 20120116
Time 16.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500306 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-145
2.000 1.005 3.164 2.106 1.097 3.122
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
207.031 168.221 77.251 76.996 76.741 61.129 37.550 33.584 32.850 21.963 20.831 14.077
NAME HUG-HC-145
EXPNO 41
PROCNO 1
Date_ 20120116
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131185 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-145
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm




```
NAME          HUG-HC-291
EXPNO                 10
PROCNO                 1
Date_           20120518
Time                4.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                  80.6
DW                48.400 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1         500.3530899 MHz
SI                 32768
SF           500.3500394 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

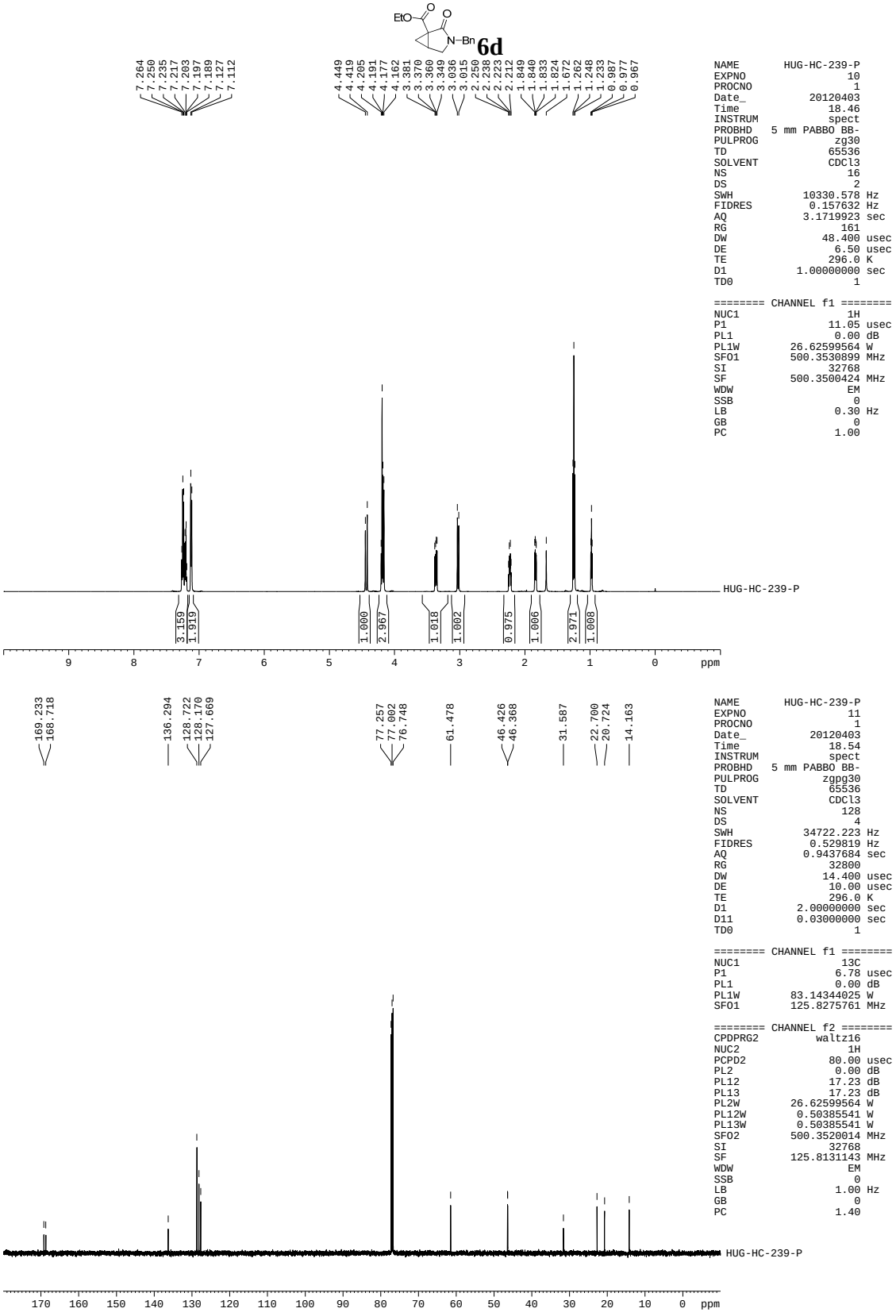


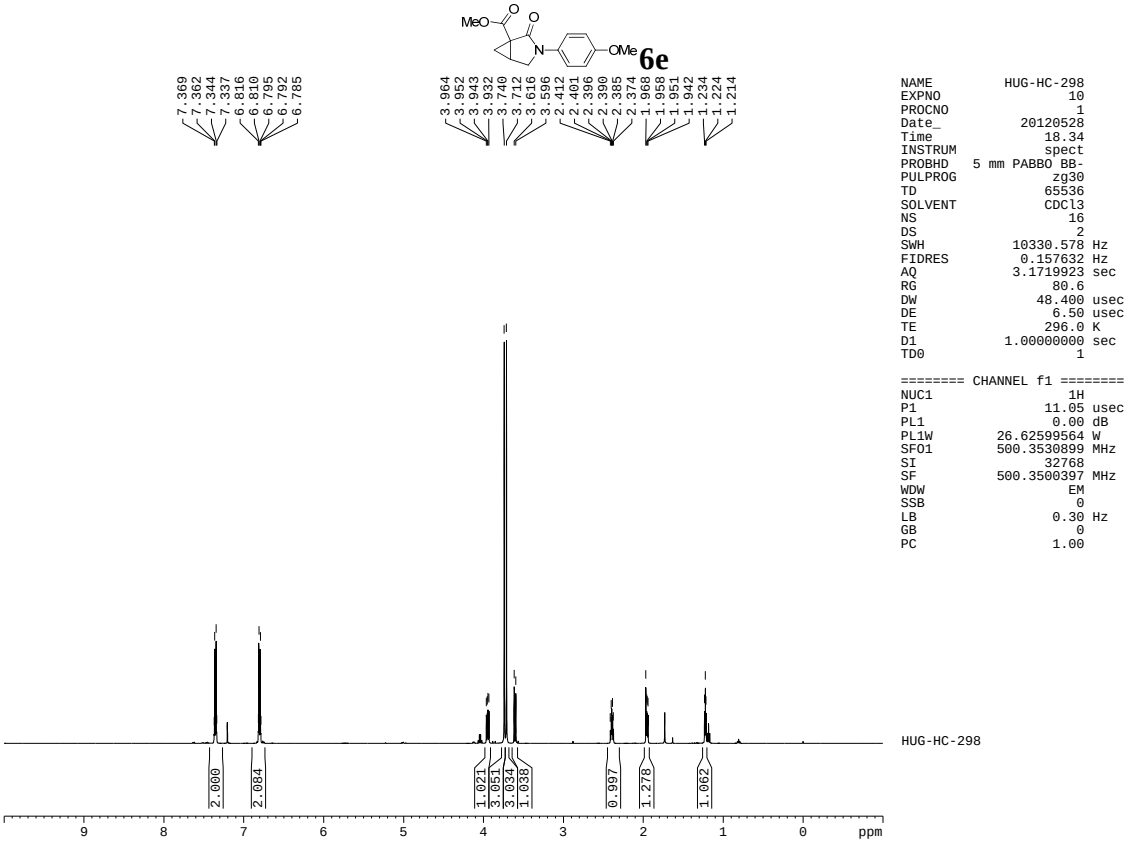


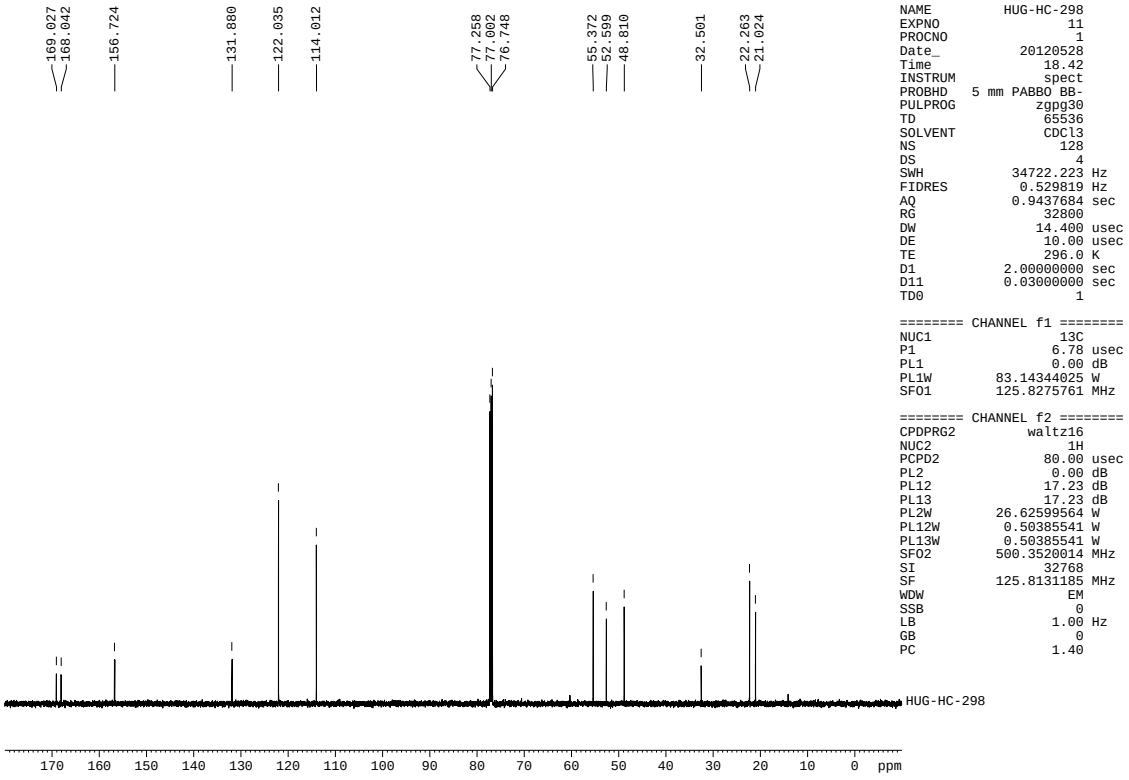

```
NAME          HUG-HC-291
EXPNO                 11
PROCNO                 1
Date_           20120518
Time                5.07
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

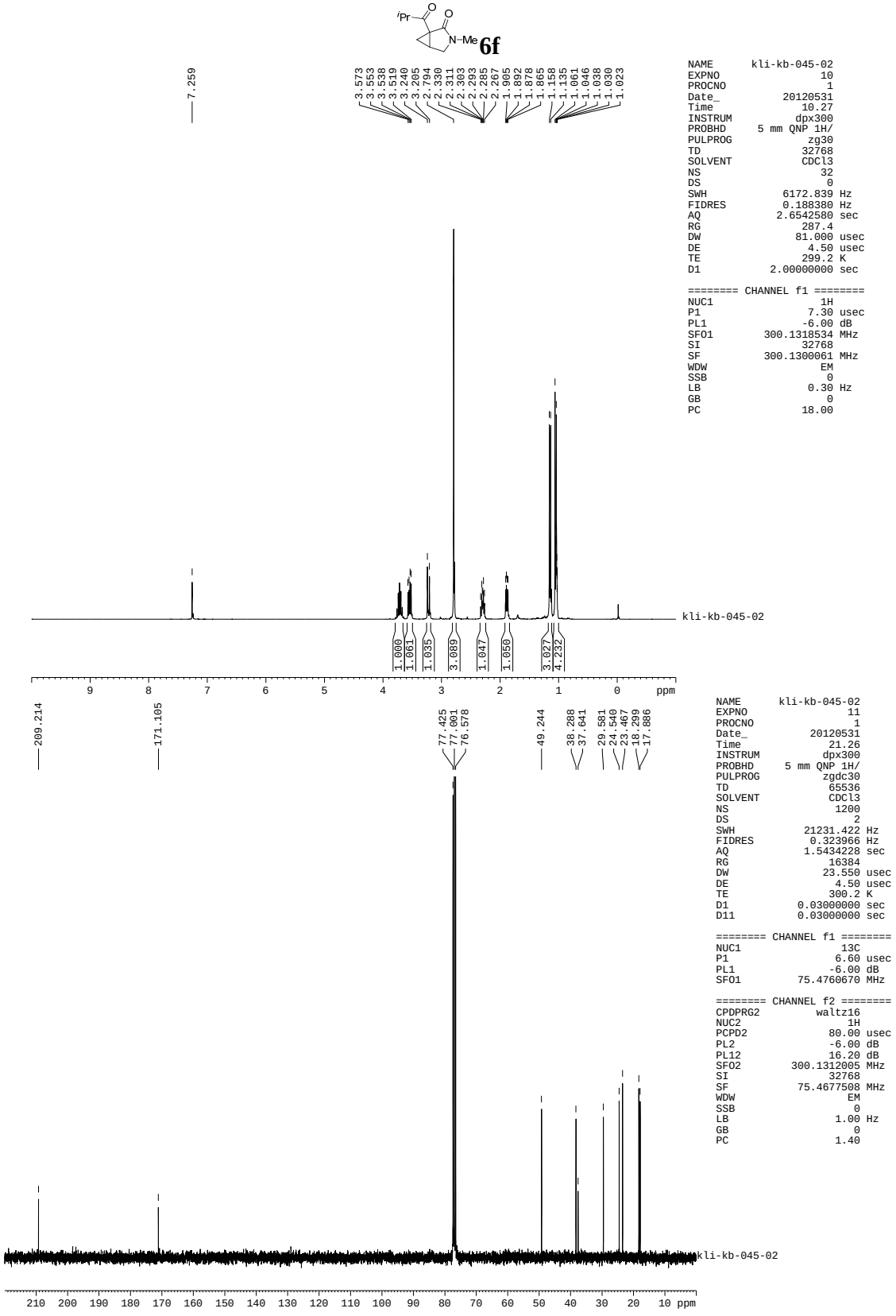
======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1         125.8275761 MHz

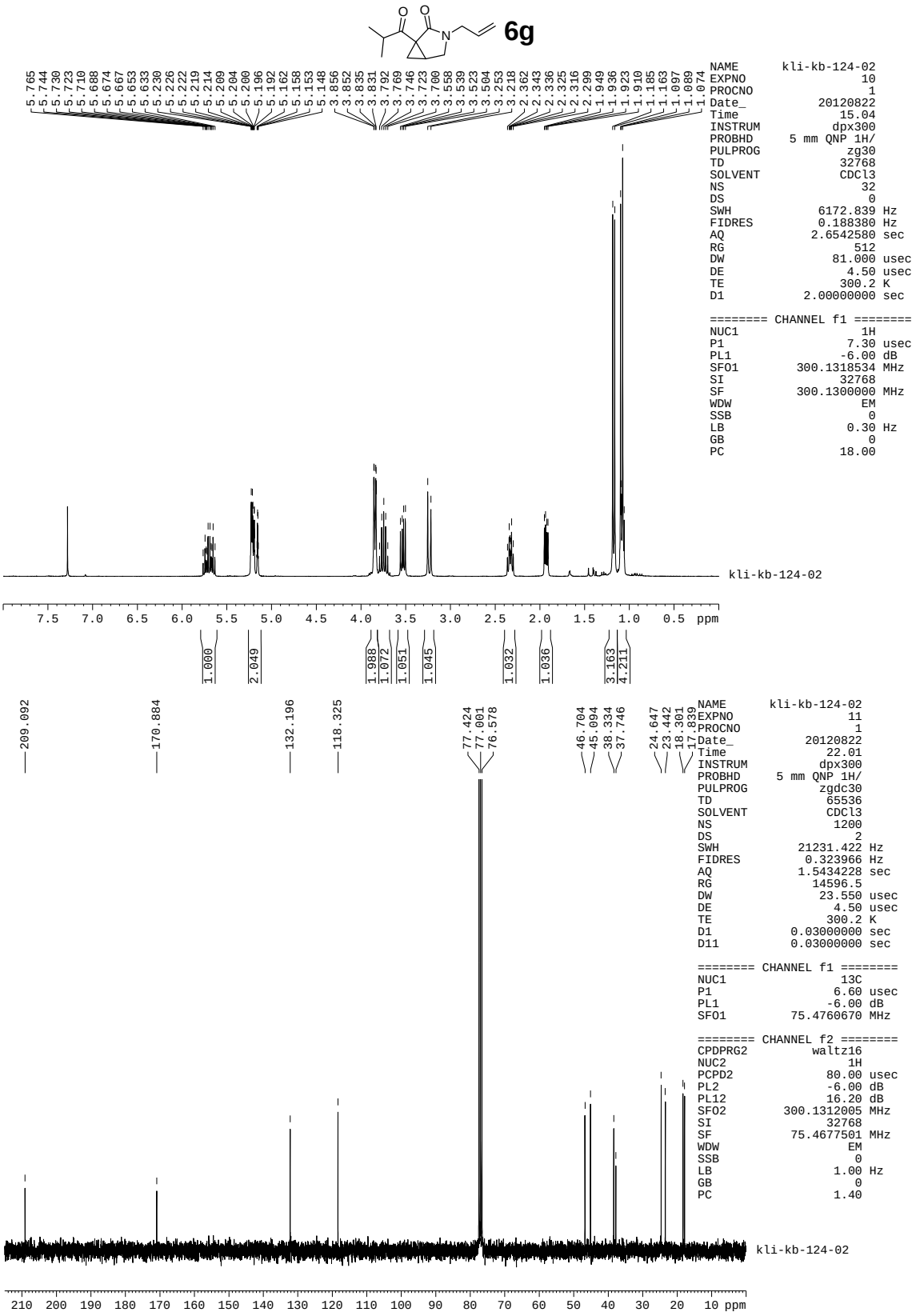
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.3520014 MHz
SI                 32768
SF           125.8131185 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

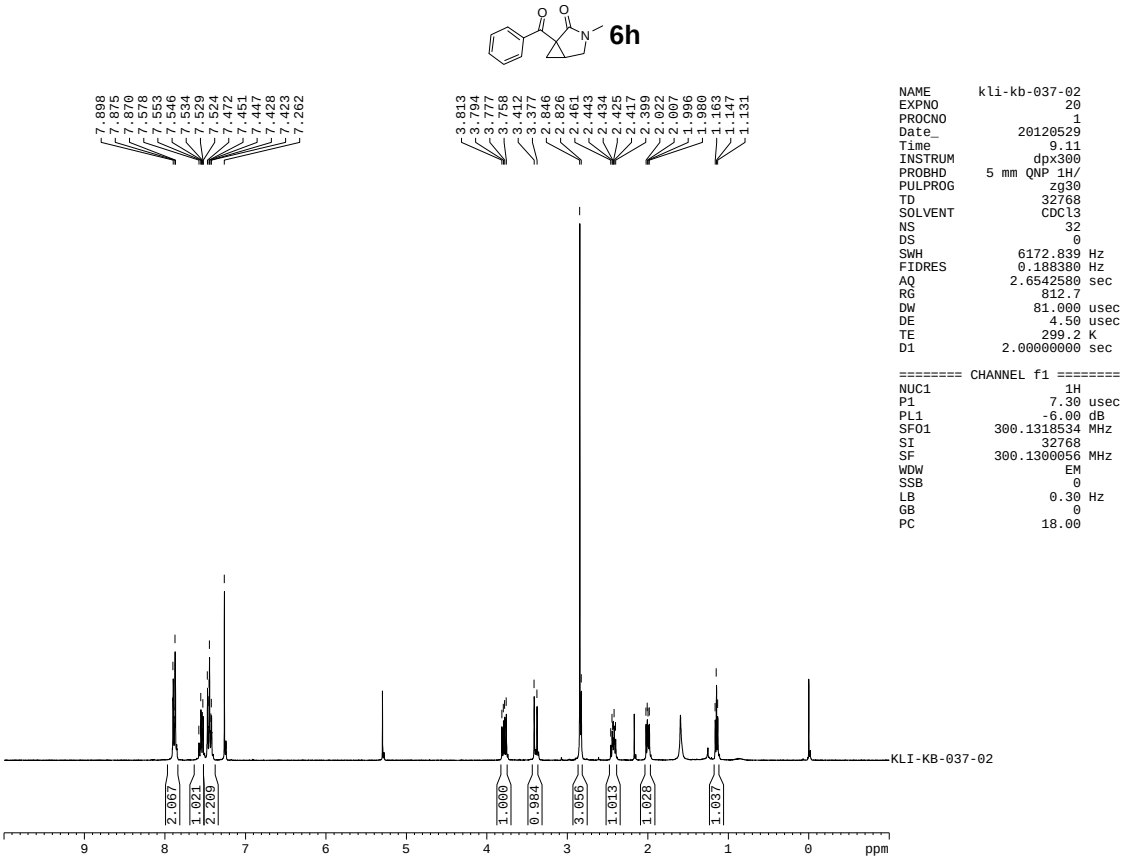


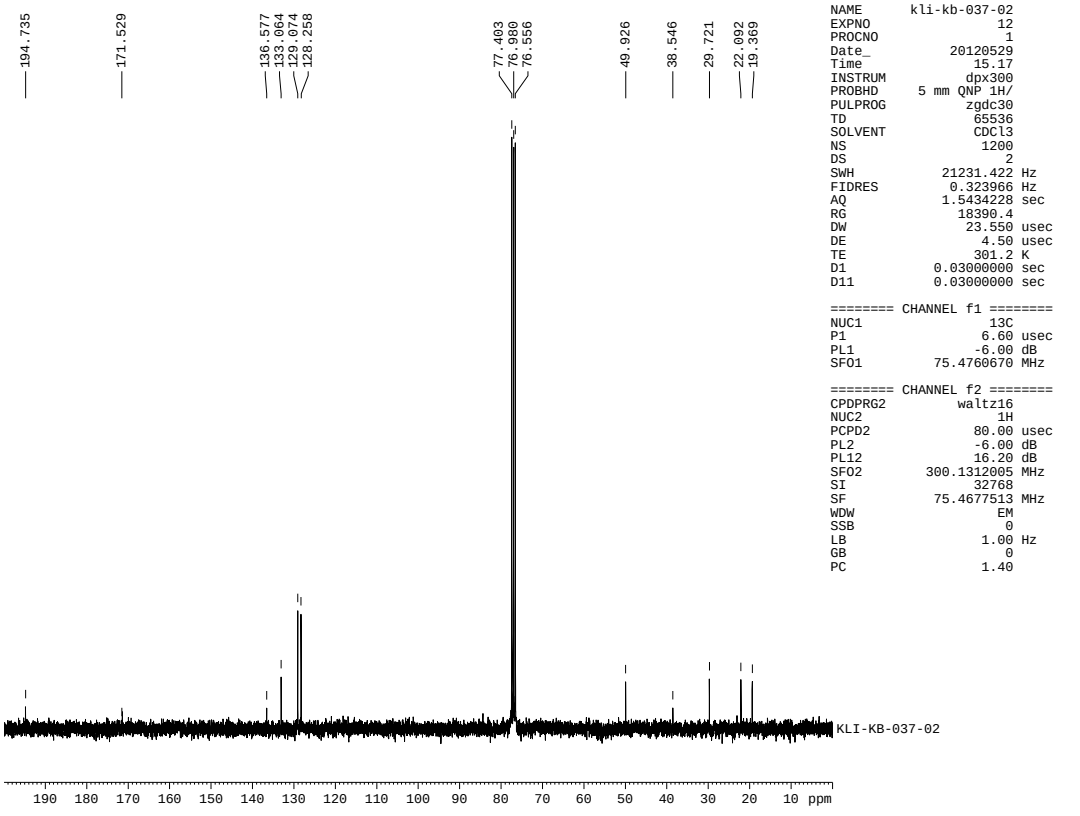

MeO
O
O
N
OMe
6e
7.369
7.362
7.344
7.337
6.816
6.810
6.795
6.792
6.785
3.964
3.952
3.943
3.932
3.740
3.712
3.616
3.596
2.412
2.401
2.396
2.390
2.385
2.374
1.968
1.958
1.951
1.942
1.234
1.224
1.214
NAME HUG-HC-298
EXPNO 10
PROCNO 1
Date_ 20120528
Time 18.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500397 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HC-298
2.000
2.084
1.021
3.051
3.034
1.038
0.997
1.278
1.062
9
8
7
6
5
4
3
2
1
0
ppm

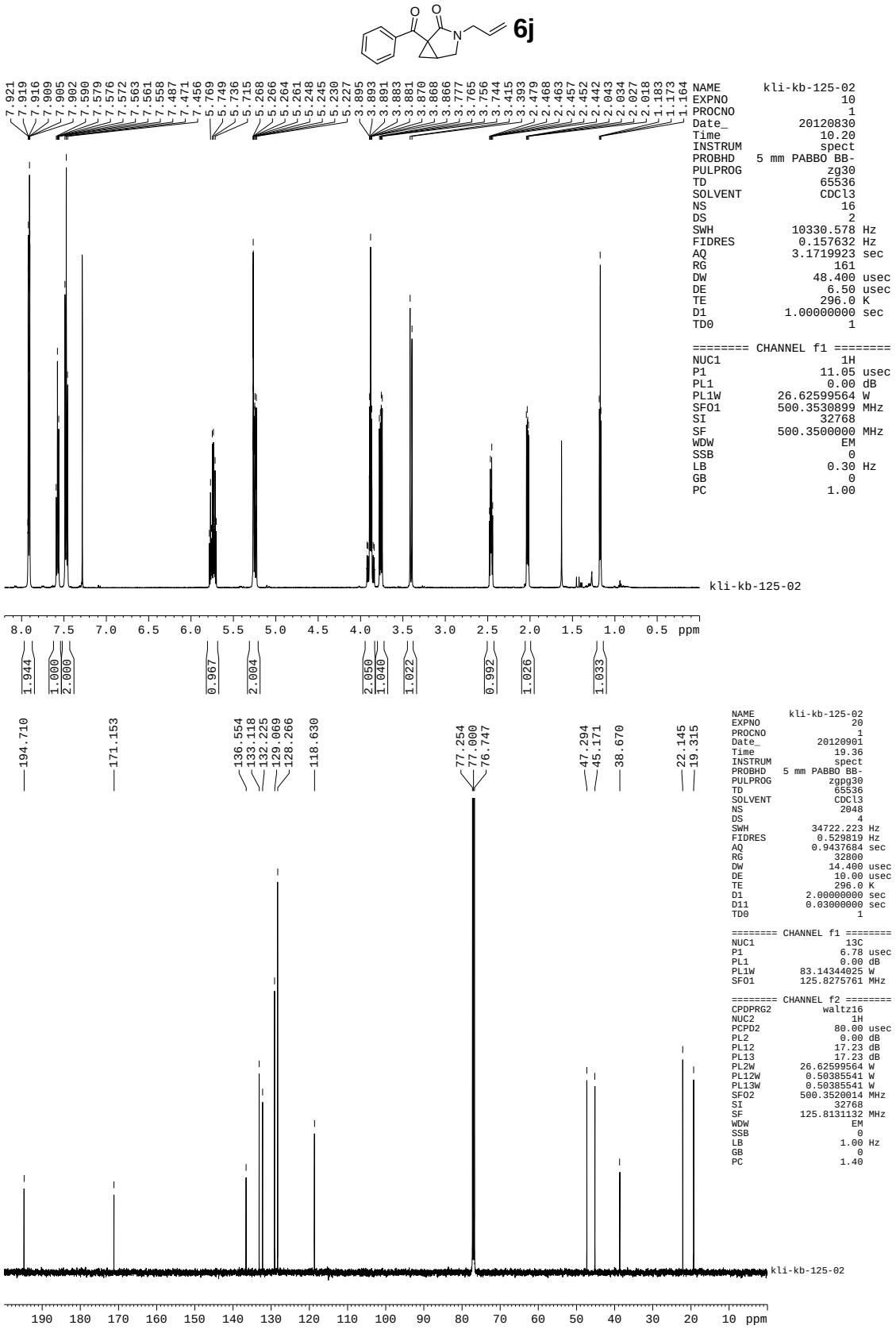

169.027
168.042
156.724
131.880
122.035
114.012
77.258
77.002
76.748
55.372
52.599
48.810
32.501
22.263
21.024
NAME HUG-HC-298
EXPNO 11
PROCNO 1
Date_ 20120528
Time 18.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131185 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HC-298
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


6f
7.259
3.573
3.553
3.538
3.519
3.240
3.205
2.794
2.330
2.311
2.303
2.293
2.285
2.267
2.005
1.892
1.878
1.865
1.158
1.135
1.061
1.046
1.038
1.030
1.023
NAME kli-kb-045-02
EXPNO 10
PROCNO 1
Date_ 20120531
Time 10.27
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 287.4
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
kli-kb-045-02
1.000
1.061
1.035
3.089
1.047
1.050
3.027
4.232
9 8 7 6 5 4 3 2 1 0 ppm
209.214
171.105
77.425
77.001
76.578
49.244
38.288
37.641
29.581
24.540
23.467
18.299
17.886
NAME kli-kb-045-02
EXPNO 11
PROCNO 1
Date_ 20120531
Time 21.26
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 16384
DW 23.550 usec
DE 4.50 usec
TE 300.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677508 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-045-02
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


6g
kli-kb-124-02
ppm
kli-kb-124-02
ppm


6h
7.898
7.875
7.870
7.578
7.553
7.546
7.534
7.529
7.524
7.472
7.451
7.447
7.428
7.423
7.262
3.813
3.794
3.777
3.758
3.412
3.377
2.846
2.826
2.461
2.443
2.434
2.425
2.417
2.399
2.022
2.007
1.996
1.980
1.163
1.147
1.131
NAME kli-kb-037-02
EXPNO 20
PROCNO 1
Date_ 20120529
Time 9.11
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 812.7
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
KLI-KB-037-02
2.067
1.021
2.209
1.000
0.984
3.056
1.013
1.028
1.037
9
8
7
6
5
4
3
2
1
0
ppm


194.735
171.529
136.577
133.064
129.074
128.258
77.403
76.980
76.556
49.926
38.546
29.721
22.092
19.369
NAME kli-kb-037-02
EXPNO 12
PROCNO 1
Date_ 20120529
Time 15.17
INSTRUM dpx300
PROBHD 5 mm QNP 1H/
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 18390.4
DW 23.550 usec
DE 4.50 usec
TE 301.2 K
D1 0.03000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677513 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
KLI-KB-037-02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


6j
7.921 7.919 7.916 7.909 7.905 7.902 7.590 7.579 7.576 7.572 7.563 7.561 7.558 7.487 7.471 7.456 5.769 5.749 5.736 5.715 5.268 5.266 5.264 5.261 5.248 5.245 5.230 5.227 3.895 3.893 3.891 3.883 3.881 3.870 3.868 3.866 3.777 3.765 3.756 3.744 3.415 3.393 2.479 2.468 2.463 2.457 2.452 2.442 2.043 2.034 2.027 2.018 1.183 1.173 1.164
NAME kli-kb-125-02
EXPNO 10
PROCNO 1
Date_ 20120830
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.3530899 MHz
SI 32768
SF 500.3500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
kli-kb-125-02
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 ppm
1.944 1.000 2.000 0.967 2.004 2.050 1.040 1.022 0.992 1.026 1.033
194.710 171.153 136.554 133.118 132.225 129.069 128.266 118.630 77.254 77.000 76.747 47.294 45.171 38.670 22.145 19.315
NAME kli-kb-125-02
EXPNO 20
PROCNO 1
Date_ 20120901
Time 19.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.8275761 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.3520014 MHz
SI 32768
SF 125.8131132 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
kli-kb-125-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm