Supporting Information

Strategy for Catalytic Chemoselective Cross-Enolate Coupling Reaction via a Transient Homocoupling Dimer

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1. General

All reactions were carried out using heat gun dried glassware under a positive pressure of dry argon unless otherwise noted. Catalytic reactions were run under argon atmosphere. Air- and moisture-sensitive liquids were transferred via a syringe and a stainless-steel needle. Reactions were magnetically stirred and monitored by thin layer chromatography using Merck Silica Gel 60 F254 plates. All work-up and purification procedures were carried out with reagent-grade solvents under ambient atmosphere. Flash chromatography was performed using silica gel 60N (spherical neutral, particle size 40–50μm) purchased from Kanto Chemical Co. Ltd.

2. Instrumentation

NMR was recorded on 500 MHz Bruker Advanced III. Chemical shifts for proton are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26 ppm). For ^{13}C NMR, chemical shifts were reported in the scale relative to NMR solvent ($CDCl_3$: δ 77.0 ppm) as an internal reference. NMR data are reported as follows: chemical shifts, multiplicity (s: singlet, d: doublet, dd: doublet of doublets, t: triplet, q: quartet, quin: quintet, sep: septet, m: multiplet, br: broad signal), coupling constant (Hz), and integration. Infrared (IR) spectra were recorded on with Shimadzu FTIR-8400. High-resolution mass spectroscopy (HRMS) was obtained with Waters ACQUITY UPLC®–LCT-Premier™ XE system and Bruker MicrOTOF II. Ultraviolet and visible absorption spectrum was recorded on with Shimadzu UV-2600.

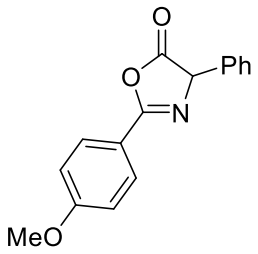
3. Materials

Chlorobenzene was distilled from MS4A and stored in schlenk flask. Toluene, benzene and THF were distilled from MS4A. Acetonitrile and 1,2-dichloroethane were distilled from MS3A. $FeCl_3$ was purchased from Aldrich and used as received (sublimed grade, ≥99.9% trace metals basis). $FeCl_3$ was stored in a dry box. DMAP was purchased from Wako Pure Chemical Industries, Ltd. and used after recrystallization. DTBP was purchased from TCI and used as received. Molecular Sieves 4A was purchased from Nacalai Tesque, Inc. All other commercially available reagents were used as received. All other commercially available reagents were used as received.

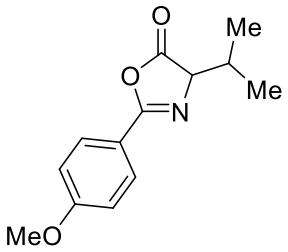
4. Substrate Syntheses and Characterization

General procedure for synthesis of 1a, and 1h[1]

To a solution of DL-2-(4-methoxybenzamido)-2-phenylacetic acid, (4-methoxybenzoyl)alanine or (4-methoxybenzoyl)valine (12 mmol, 1.0 equiv.) in CH_2Cl_2 (167 mL, 0.072 M) under argon atmosphere was added 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (16 mmol, 1.3 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 1 h, the reaction mixture was washed with H_2O, sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4 and filtered. After removal of solvent under reduced pressure, desired product (**1a, 1h and 1i**) was obtained as a solid which was used after recrystallization (Diethyl ether/*n*-Hexane).

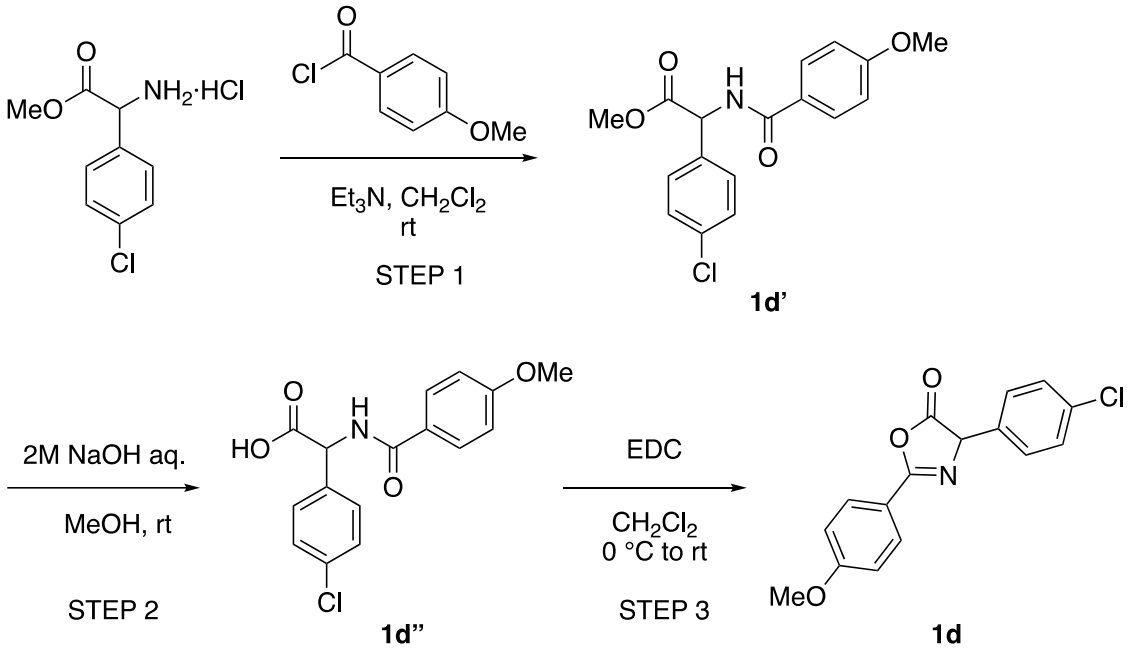


2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (1a): CAS Registry Number 28172-58-9; (Yellow solid, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.45-7.34 (m, 5H, *Ph*), 7.01 (d, *J* = 9.0 Hz, 2H, Ar*H*), 5.49 (s, 1H, COC*H*), 3.89 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.5, 163.5, 162.3, 133.8, 130.0, 129.0, 128.7, 126.9, 118.0, 114.3, 68.1, 55.5.



4-isopropyl-2-(4-methoxyphenyl)oxazol-5(4*H*)-one (1h): CAS Registry Number 79137-48-7; (White solid, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 9.0 Hz, 2H, Ar*H*), 6.98 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.27 (d, *J* = 4.0 Hz, 1H, COC*H*), 3.88 (s, 3H, OCH_3), 2.41-2.32 (m, 1H, C*H*$(CH_3)_2$), 1.14 (d, *J* = 7.0 Hz, 3H, CH(CH_3)$_2$), 1.01 (d, *J* = 7.0 Hz, 3H, CH(CH_3)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.1, 163.1, 161.4, 129.8, 118.2, 114.2, 70.6, 55.5, 31.3, 18.8, 17.6.

General procedure for synthesis of 4-(4-chlorophenyl)-2-(4-methoxyphenyl)oxazol-5(4*H*)-one (1d)[2]



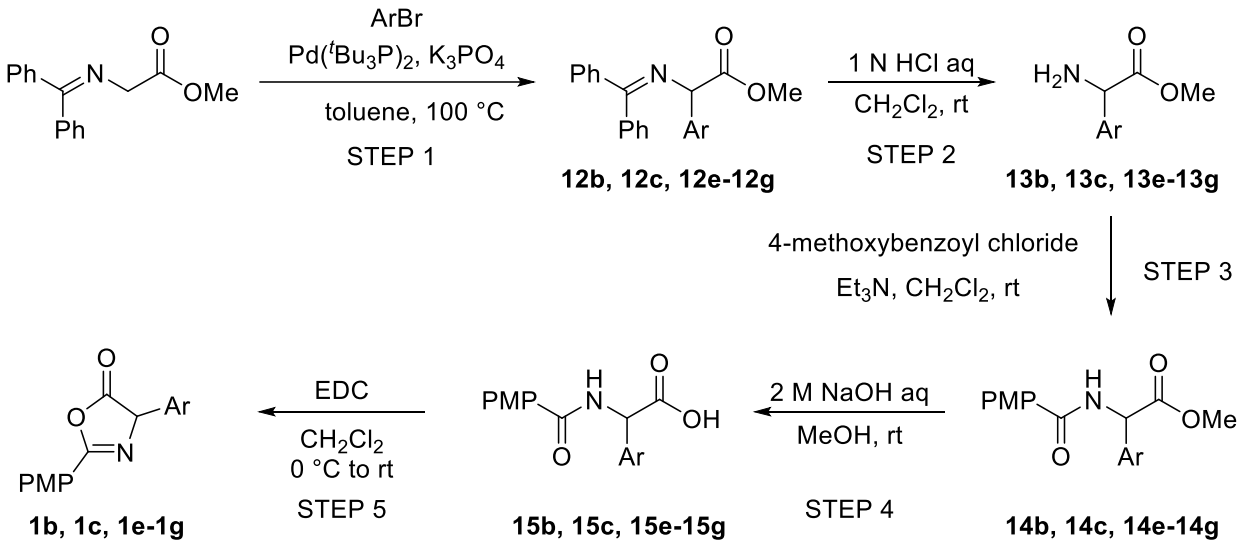
STEP 1: To a solution of DL-methyl 2-amino-2-(4-chlorophenyl)acetate hydrochloride (4.8 mmol, 1.0 equiv.) and Et_3N (14 mmol, 3.0 equiv.) in CH_2Cl_2 (10 mL, 0.25 M) was added dropwise 4-methoxybenzoyl chloride (5.3 mmol, 1.1 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 5 h, the reaction mixture was washed with 1 N HCl aq, sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4, filtered and concentrated to obtain the crude **1d'**, which was used in the next step without further purification.

STEP 2: To a solution of **1d'** (5.0 mmol, 1.0 equiv.) in MeOH (8.5 mL, 0.57 M) was added 2.0 M NaOH aq (2.7 mL, 5.4 mmol) and stirred for 0.5 h. After volatile was removed, H_2O was added to the residue and the resulting aqueous solution was washed with CH_2Cl_2. The aqueous layer was acidified with 1 N HCl aq until precipitate was generated. The white precipitate was filtered and washed with diethyl ether. It was used in the next step without further purification.

STEP 3: To a solution of **1d"** (4.6 mmol, 1.0 equiv.) in CH_2Cl_2 (70 mL, 0.072 M) was added dropwise 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (6.0 mmol, 1.3 equiv.) at 0 °C under argon atmosphere. The cooling bath was removed and the reaction mixture was stirred for 1 h. The reaction

mixture was washed with H_2O, sat. $NaHCO_3$ aq and brine. The organic layer was dried over Na_2SO_4, filtered and concentrated. The pure 4-(4-chlorophenyl)-2-(4-methoxyphenyl)oxazol-5(4*H*)-one (**1d**) was obtained by recrystallization (Diethyl ether/*n*-Hexane). : CAS Registry Number 1356585-06-2; (Yellow solid, 91% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.42-7.37 (m, 4H, Ar*H*), 7.01 (d, *J* = 8.5 Hz, 2H, Ar*H*), 5.46 (s, 1H, COC*H*), 3.90 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.1, 163.4, 162.5, 134.7, 132.3, 130.1, 129.1, 128.2, 117.8, 114.4, 67.3, 55.6.

General procedure for synthesis of azlactones (1b, 1c, 1e-1g)[2, 3]



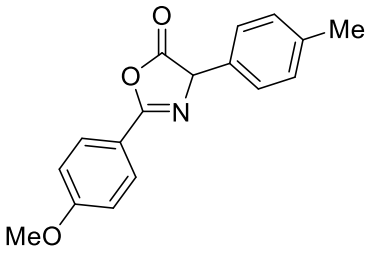
STEP 1: A flame-dried 25 mL round-bottom flask equipped with a magnetic stirring bar was filled with argon, and charged with methyl *N*-(diphenylmethylene)glycinate (1.1 equiv.), Pd(^{t}Bu$_3$P)$_2$ (1.0 mol%), K_3PO_4 (3.0 equiv.), toluene (0.33 M) and aryl chloride(1.0 equiv.). The mixture was stirred at 100 °C for 20 h, and the reaction mixture was filtered through plug of Celite. After evaporation of the organic solvent under reduced pressure, the residue was purified by silica gel flash chromatography.

STEP 2: To a solution of **12** (1.0 equiv.) in CH_2Cl_2 (0.40 M) was added 1 N HCl aq (0.40 M). After stirring for 12 h, sat. $NaHCO_3$ aq was added and the resultant mixture was extracted with CH_2Cl_2 several times. The combined organic layers were dried over Na_2SO_4, filtered and concentrated to obtain the crude **13**, which was used in the next step without further purification.

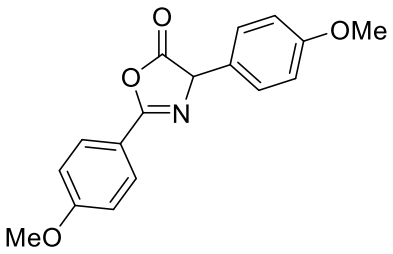
STEP 3: To a solution of **13** (1.0 equiv.) and Et_3N (3.0 equiv.) in CH_2Cl_2 (0.25 M) was added dropwise 4-methoxybenzoyl chloride (1.1 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 5 h, the reaction mixture was washed with 1 N HCl aq, sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4, filtered and concentrated to obtain the crude **14**, which was used in the next step without further purification.

STEP 4: To a solution of **14** (1.0 equiv.) in THF (0.57 M) was added 2.0 M NaOH (1.9 M) and stirred for 0.5 h. After volatile was removed, H_2O was added to the residue and washed with CH_2Cl_2. The aqueous layer was acidified with 1 N HCl aq until precipitate was generated. The white precipitate was filtered and washed with diethyl ether. It was used in the next step without further purification.

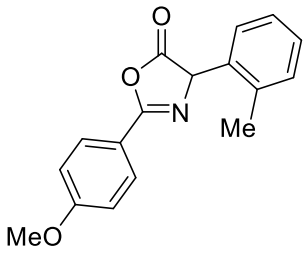
STEP 5: To a solution of **15** (1.0 equiv.) in CH_2Cl_2 (0.072 M) was added dropwise 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.3 equiv.) at 0 °C under argon atmosphere. The cooling bath was removed and the reaction mixture was stirred for 1 h. The reaction mixture was washed with H_2O, sat. $NaHCO_3$ aq and brine. The organic layers were dried over Na_2SO_4, filtered and concentrated. The pure azlactones were obtained by recrystallization (Diethyl ether/*n*-Hexane).



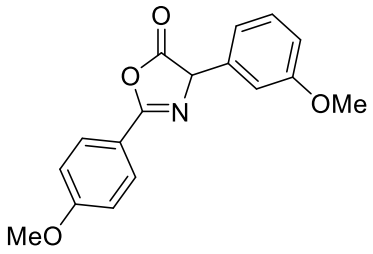
2-(4-methoxyphenyl)-4-(*p*-tolyl)oxazol-5(4*H*)-one (1b): CAS Registry Number 142312-20-7; (Yellow solid, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.31 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.20 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.01 (d, *J* = 9.0 Hz, 2H, Ar*H*), 5.45 (s, 1H, COC*H*), 3.89 (s, 3H, OCH_3), 2.53 (s, 3H, ArCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.7, 163.4, 162.1, 138.5, 130.8, 130.0, 129.7, 126.8, 118.0, 114.3, 68.1, 55.3, 21.2.



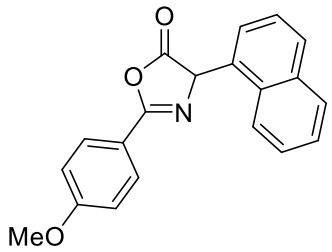
2,4-bis(4-methoxyphenyl)oxazol-5(4*H*)-one (1c): CAS Registry Number 1356585-03-9; (Yellow solid, 61% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.34 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.00 (d, *J* = 8.5 Hz, 2H, Ar*H*), 6.92 (d, *J* = 9.0 Hz, 2H, Ar*H*), 5.43 (s, 1H, COC*H*), 3.89 (s, 3H, OCH_3), 3.80 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.8, 163.4, 162.1, 159.9, 130.0, 128.1, 125.9, 118.0, 114.4, 114.3, 67.8, 55.5, 55.4.



2-(4-methoxyphenyl)-4-(*o*-tolyl)oxazol-5(4*H*)-one (1e): (Yellow solid, 91% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.26-7.17 (m, 4H, Ar*H*), 7.01 (d, *J* = 8.5 Hz, 2H, Ar*H*), 5.70 (s, 1H, COC*H*), 3.90 (s, 3H, OCH_3), 2.53 (s, 3H, ArCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.5, 163.4, 162.4, 136.7, 132.4, 131.1, 130.0, 128.8, 126.9, 126.5, 118.0, 114.3, 66.5, 55.5, 19.5; IR (KBr) 2974, 2943, 2843, 1809, 1786, 1655, 1609, 1578, 1512, 1462, 1424, 1312, 1261, 1180, 1138, 1115, 1057, 1034, 999, 941, 903, 841, 752 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{17}H_{16}NO_3$ $(M + H)^+$ 282.1125, found 282.1126.



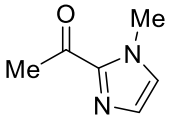
4-(3-methoxyphenyl)-2-(4-methoxyphenyl)oxazol-5(4*H*)-one (1f): CAS Registry Number 1356585-01-7 (Yellow solid, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.32 (t, *J* = 8.0 Hz, 1H, Ar*H*), 7.05-6.97 (m, 4H, Ar*H*), 6.91-6.89 (m, 1H, Ar*H*), 5.46 (s, 1H, COC*H*), 3.90 (s, 3H, OCH_3), 3.82 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.3, 163.5, 162.3, 160.0, 135.2, 130.1, 130.0, 119.1, 118.0, 114.3, 114.2, 112.5, 68.0, 55.5, 55.3.



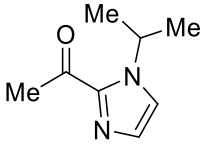
2-(4-methoxyphenyl)-4-(naphthalen-1-yl)oxazol-5(4*H*)-one (1g): (Yellow solid, 85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.5 Hz, 1H, Ar*H*), 8.07 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.91 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.87 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.64 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.56 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.46-7.41 (m, 2H, Ar*H*), 7.02 (d, *J* = 8.5 Hz, 2H, Ar*H*), 5.30 (s, 1H, COC*H*) 3.90 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.1, 163.5, 162.5, 134.2, 131.1, 130.1, 129.8, 129.6, 128.9, 126.9, 126.2, 125.3, 124.8, 123.7, 118.0, 114.3, 65.9, 55.6; IR (KBr) 2959, 2936, 2835, 1829, 1651, 1609, 1578, 1512, 1466, 1420, 1323, 1308, 1258, 1227, 1173, 1138, 1115, 1069, 1026, 988, 895, 841, 791, 772, 741 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{20}H_{16}NO_3$ $(M + H)^+$ 318.1125, found 318.1125.

General procedure for synthesis of acylimidazoles[4,5,6]: To a solution of 1-methylimidazole, 1-isopropylimidazole or 1-phenylimidazole (1.0 equiv.) in dry THF (0.70 M) under argon atmosphere was added dropwise 2.6 M *n*-BuLi in *n*-hexane (1.1 equiv.) at –78 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 0.5 h, the mixture was again cooled to –78 °C

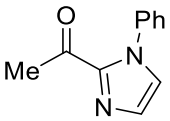
and indicated ester (2.5 equiv.) was added. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 3 h, it was quenched by sat. NH_4Cl aq and volatiles were removed *in vacuo*. To the resultant residude was added sat. $NaHCO_3$ aq and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4 and filtered. After removal of solvent under reduced pressure, the residue was purified by silica gel flash chromatography to afford the desired acylimidazole, which was used without further purification unless otherwise noted.



1-(1-methyl-1*H*-imidazol-2-yl)ethan-1-one (2a): CAS Registry Number 85692-37-1; (Colorless liquid, 68% yield); Following the general procedure using ethyl acetate and performing the distillation after silica gel flash chromatography. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (s, 1H, *imidazole*), 7.03 (s, 1H, *imidazole*), 4.00 (s, 3H, NCH_3), 2.66 (s, 3H, COCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.6, 143.3, 129.0, 126.9, 36.2, 27.1.

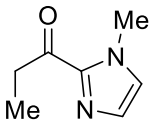


1-(1-isopropyl-1*H*-imidazol-2-yl)ethan-1-one (2c): CAS Registry Number 1378459-89-2; (Colorless liquid, 54% yield); Following the general procedure using ethyl acetate and performing the distillation after silica gel flash chromatography. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (s, 1H, *imidazole*), 7.17 (s, 1H, *imidazole*), 5.57 (sep, *J* = 6.5 Hz, 1H, C*H*$(CH_3)_2$), 2.68 (s, 3H, COCH_3), 1.43 (d, *J* = 6.5 Hz, 6H, CH(CH_3)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.8, 142.5, 129.5, 121.1, 49.2, 27.9, 23.6.

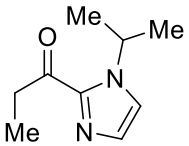


1-(1-phenyl-1*H*-imidazol-2-yl)ethan-1-one (2d): CAS Registry Number 66869-82-7; (White solid, 43% yield); Following the general procedure using ethyl acetate. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47-7.45 (m,

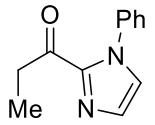
3H, *Ph*), 7.29-7.26 (m, 3H, *Ph, imidazole*), 7.17 (s, 1H, *imidazole*), 2.66 (s, 3H, COCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.9, 143.2, 138.4, 129.6, 129.0, 128.7, 127.1, 125.9, 27.3.



1-(1-methyl-1*H*-imidazol-2-yl)propan-1-one (2b): CAS Registry Number 138536-16-0; (Colorless liquid, 48% yield); Following the general procedure using methyl propionate and performing the distillation after silica gel flash chromatography. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.02 (s, 1H, *imidazole*), 4.01 (s, 3H, NCH_3), 3.15 (q, *J* = 6.0 Hz, 2H, COCH_2), 1.20 (t, *J* = 6.0 Hz, 3H, CH_2CH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.9, 143.0, 128.9, 126.7, 36.2, 32.3, 8.1.

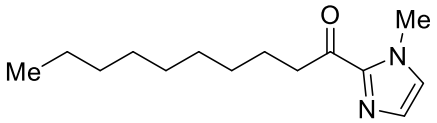


1-(1-isopropyl-1*H*-imidazol-2-yl)propan-1-one (2e): (Colorless liquid, 61% yield); Following the general procedure using methyl propionate and performing the distillation after silica gel flash chromatography. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (s, 1H, *imidazole*), 7.16 (s, 1H, *imidazole*), 5.57 (sep, *J* = 7.0 Hz, 1H, C*H*$(CH_3)_2$), 3.17 (q, *J* = 7.5 Hz, 2H, COCH_2), 1.44 (d, *J* = 7.0 Hz, 6H, CH(CH_3)$_2$), 1.19 (t, *J* = 7.5 Hz, 3H, CH_2CH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.0, 142.2, 129.3, 120.8, 49.1, 32.9, 23.6, 8.2; IR (thin film, NaCl) 3020, 2982, 2940, 2878, 1678, 1545, 1408, 1393, 1312, 1254, 1215, 1150, 1088, 1011, 945, 914, 756, 706 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_9H_{15}N_2O$ $(M + H)^+$ 167.1179, found 167.1178.

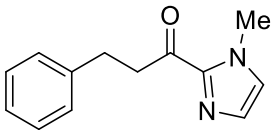


1-(1-phenyl-1*H*-imidazol-2-yl)propan-1-one (2f): CAS Registry Number 1233735-48-2; (White solid, 65% yield); Following the general procedure using methyl propionate. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46-7.45 (m, 3H, *Ph*), 7.29-7.26 (m, 3H, *Ph, imidazole*), 7.16 (s, 1H, *imidazole*), 3.17 (q, *J* = 7.5 Hz, 2H, COCH_2), 1.13

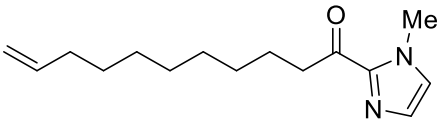
(t, *J* = 7.5 Hz, 3H, CH_2CH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.1, 143.0, 138.5, 129.4, 129.0, 128.7, 126.9, 126.0, 32.5, 7.8.



1-(1-methyl-1*H*-imidazol-2-yl)decan-1-one (2g): CAS Registry Number 1491692-48-8; (Colorless liquid, 36% yield); Following the general procedure using ethyl decanoate and performing the distillation after silica gel flash chromatography. ^1H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.01 (s, 1H, *imidazole*), 4.00 (s, 3H, NCH_3), 3.11 (t, *J* = 7.5 Hz, 2H, $COCH_2$), 1.72 (quin, *J* = 7.5 Hz, 2H, $COCH_2CH_2$), 1.40-1.26 (m, 12H, $COCH_2CH_2(CH_2)_6$), 0.88 (t, *J* = 7.0 Hz, 3H, CH_2CH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.5, 143.1, 128.9, 126.8, 39.1, 36.2, 31.9, 29.5, 29.5, 29.3, 29.3, 24.3, 22.7, 14.1.

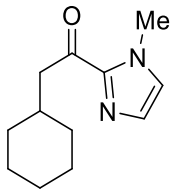


1-(1-methyl-1*H*-imidazol-2-yl)-3-phenylpropan-1-one (2h): CAS Registry Number 1179358-90-7; (Pale yellow liquid, 22% yield); Following the general procedure using ethyl 3-phenylpropionate and performing the distillation after silica gel flash chromatography. ^1H NMR (500 MHz, $CDCl_3$) δ 7.29-7.26 (m, 4H, *Ph*), 7.19-7.18 (m, 1H, *Ph*), 7.12 (s, 1H, *imidazole*), 7.01 (s, 1H, *imidazole*), 4.00 (s, 3H, NCH_3), 3.48 (t, *J* = 7.5 Hz, 2H, $COCH_2$), 3.04 (t, *J* = 7.5 Hz, 2H, $PhCH_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.1, 143.0, 141.1, 129.1, 128.5, 128.4, 126.9, 126.0, 40.4, 36.2, 30.0.

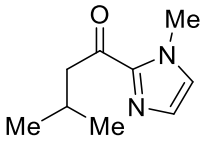


1-(1-methyl-1*H*-imidazol-2-yl)undec-10-en-1-one (2i): (Colorless liquid, 14% yield); Following the general procedure using methyl undec-10-enoate and performing the distillation after silica gel flash chromatography. ^1H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.01 (s, 1H, *imidazole*), 5.85-5.77

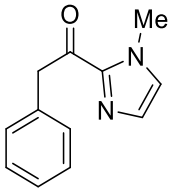
(m, 1H, C*H*CH_2), 5.01-4.91 (m, 2H, CHC*H*$_2$), 4.00 (s, 3H, NC*H*$_3$), 3.11 (t, *J* = 7.5 Hz, 2H, COC*H*$_2$), 2.05-2.01 (m, 2H, C*H*$_2$CH), 1.73-1.67 (m, 2H, $COCH_2$C*H*$_2$), 1.38-1.29 (m, 10H, (C*H*$_2$)$_5$$CH_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.5, 143.2, 139.3, 128.9, 126.8, 114.1, 39.1, 36.2, 33.8, 29.4, 29.4, 29.3, 29.1, 28.9, 24.3; IR (neat) 2924, 2853, 2359, 2342, 1672, 1639, 1464, 1406, 1288, 1153, 993, 976, 912, 764, 696 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{15}H_{25}N_2O$ $(M + H)^+$ 249.1961, found 249.1967.



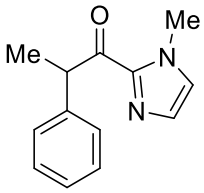
2-cyclohexyl-1-(1-methyl-1*H*-imidazol-2-yl)ethan-1-one (2l): CAS Registry Number 69393-33-5; (White solid, 26% yield); Following the general procedure using methyl cyclohexylacetate. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.01 (s, 1H, *imidazole*), 4.00 (s, 3H, NC*H*$_3$), 2.99 (d, *J* = 7.0 Hz, 2H, COC*H*$_2$), 2.03-1.95 (m, 1H, *cyclohexyl*), 1.75-1.62 (m, 5H, *cyclohexyl*), 1.33-1.24 (m, 2H, *cyclohexyl*), 1.21-1.14 (m, 1H, *cyclohexyl*), 1.09-1.01 (m, 2H, *cyclohexyl*); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.1, 143.5, 128.9, 126.8, 46.5, 36.3, 34.5, 33.3, 26.3, 26.2.



3-methyl-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (2m): CAS Registry Number 1119410-05-7; (Colorless liquid, 19% yield); Following the general procedure using methyl isovalerate and performing the distillation after silica gel flash chromatography. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.02 (s, 1H, *imidazole*), 4.01 (s, 3H, NC*H*$_3$), 3.00 (d, *J* = 7.0 Hz, 2H, COC*H*$_2$), 2.30 (sep, *J* = 6.5 Hz, 1H, C*H*$(CH_3)_2$), 0.99 (d, *J* = 6.5 Hz, 6H, CH(C*H*$_3$)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.0, 143.4, 128.8, 126.8, 47.8, 36.2, 25.1, 22.6.

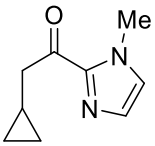


1-(1-methyl-1*H*-imidazol-2-yl)-2-phenylethan-1-one (2n): CAS Registry Number 1339495-68-9; (Brown solid, 62% yield); Following the general procedure using ethyl phenylacetate. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.30 (m, 4H, *Ph*), 7.61 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.19 (s, 1H, *imidazole*), 7.04 (s, 1H, *imidazole*) 4.43 (s, 2H, $COCH_2$), 3.97 (s, 3H, NCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.1, 142.8, 134.6, 129.9, 129.3, 128.5, 127.4, 126.8,45.4, 36.2.



1-(1-methyl-1*H*-imidazol-2-yl)-2-phenylpropan-1-one (2p): CAS Registry Number 1702873-91-3; (Brown solid, 67% yield); Following the general procedure using (±)-methyl 2-phenylpropanoate. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.0 Hz, 2H, *Ph*), 7.29 (t, *J* = 8.0 Hz, 2H, *Ph*), 7.20 (t, *J* = 8.0 Hz, 1H, *Ph*), 7.14 (s, 1H, *imidazole*), 6.98 (s, 1H, *imidazole*) 5.28 (q, *J* = 7.0 Hz, 1H, COC*H*), 3.94(s, 3H, NCH_3), 1.54(d, *J* = 7.0 Hz, 3H,$CHCH_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.3, 142.6, 140.8, 129.2, 128.5, 128.3, 127.3, 126.8, 46.7, 36.2, 18.1.

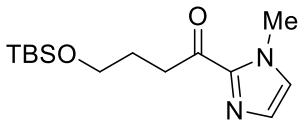
Procedure for synthesis of 2-cyclopropyl-1-(1-methyl-1*H*-imidazol-2-yl)ethan-1-one (2k)[5,6]



To a solution of 1-methylimidazole (17 mmol, 1.0 equiv.) in dry THF (26 mL, 0.70 M) under argon atmosphere was added dropwise 2.6 M *n*-BuLi in *n*-hexane (18 mmol, 1.1 equiv.) at –78°C. After 0.5 h, 2-cyclopropyl-*N*-methoxy-*N*-methylacetamide (18 mmol, 1.1 equiv.) was added. After stirring for 17 h, it was quenched by acetic acid, and added sat. $NaHCO_3$ aq. The volatiles were removed in *vacuo*. To the resultant mixture was added sat. $NaHCO_3$ aq and extracted with CH_2Cl_2. The combined organic layers

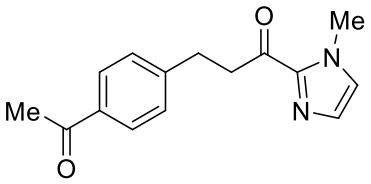
were dried over Na_2SO_4 and filtered. After removal of solvent under reduced pressure, the resulting residue was purified by silica gel flash chromatography to afford **2j**. : CAS Registry Number 1509675-93-7; (Colorless liquid, 1.1 g, 38% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (s, 1H, *imidazole*), 7.02 (s, 1H, *imidazole*), 4.02 (s, 3H, NC*H*$_3$), 3.01 (d, *J* = 7.0 Hz, 2H, COC*H*$_2$), 1.58-1.14 (m, 1H, C*H*$(CH_2)_2$), 0.58-0.54 (m, 2H, CH(C*H*$_2)_2$), 0.23-0.22 (m, 2H, CH(C*H*$_2)_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.9, 143.1, 129.0, 126.9, 44.1, 36.2, 6.5, 4.3.

Procedure for synthesis of 4-((*tert*-butyldimethylsilyl)oxy)-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (2j)



To a solution of 1-methylimidazole (0.10 mol, 1.0 equiv.) in dry THF (143 mL, 0.70 M) under argon atmosphere was added dropwise 2.6 M *n*-BuLi in *n*-hexane (0.11 mol, 1.1 equiv.) at –78 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 0.5 h, the mixture was again cooled to –78°C and γ-butyrolactone (0.13 mol, 1.3 equiv.) was added. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 3 h, it was quenched by sat. NH_4Cl aq and volatiles were removed *in vacuo*. The resultant mixture was added sat. $NaHCO_3$ aq and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4, filtered and concentrated. To the crude mixture (4-hydroxy-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one, 12 mmol, 1.0 equiv.) was added CH_2Cl_2 (26 mL, 0.45 M), TBSCl (15 mmol, 1.3 equiv.) and 1-methylimidazole (15 mmol, 1.3 equiv.) under argon atmosphere at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 3 h, it was quenched by sat. NH_4Cl aq and volatiles were removed *in vacuo*. To the resultant mixture was added sat. $NaHCO_3$ aq and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4 and filtered. The residue was purified by the distillation after silica gel flash chromatography to afford **2i**. : (Colorless liquid, 2.5 g, 33% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.01 (s, 1H, *imidazole*), 4.00 (s, 3H, NC*H*$_3$), 3.70 (t, *J* = 7.0 Hz, 2H, C*H*$_2$OTBS), 3.18 (t, *J* = 7.0 Hz, 2H, COC*H*$_2$), 1.94 (quin, *J* = 7.0 Hz, 2H, $COCH_2CH_2$), 0.87 (s, 9H, SiC(C*H*$_3)_3$), 0.30 (s, 6H, Si(C*H*$_3)_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.0, 143.1, 128.9, 126.7, 62.5, 36.2, 35.5, 27.4, 25.9, 18.3, −5.3; IR (thin film, NaCl) 3021, 2955, 2931, 2859, 1674, 1416, 1254, 1215, 1103, 837, 772 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{14}H_{27}N_2O_2Si$ $(M + H)^+$ 283.1836, found 283.1836.

Procedure for synthesis of 3-(4-acetylphenyl)-1-(1-methyl-1*H*-imidazol-2-yl)propan-1-one (2o)

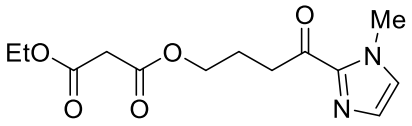


To a solution of $AlCl_3$ (50 mmol, 3.3 equiv.) in dry CH_2Cl_2 (75 mL, 0.20 M) under argon atmosphere was added acetyl chloride (15 mmol, 1.0 equiv.) and 1-(1-methyl-1*H*-imidazol-2-yl)-3-phenylpropan-1-one (**2h**, 15 mmol, 1.0 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 13 h, it was quenched by H_2O. To the mixture was added sat. $NaHCO_3$ aq and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4, filtered and concentrated. The residue was purified by the recrystallization after silica gel flash chromatography. : (Brown solid, 1.7 g, 44% yield) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.36 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.13 (s, 1H, *imidazole*), 7.03 (s, 1H, *imidazole*), 4.00 (s, 3H, NCH_3), 3.51 (t, *J* = 7.5 Hz, 2H, COCH_2), 3.10 (t, *J* = 7.5 Hz, 2H, PhCH_2), 2.58 (s, 3H, COCH_3); ^{13}C NMR (125MHz, $CDCl_3$) δ 197.9, 191.4, 146.9, 142.8, 135.2, 129.1, 128.7, 128.6, 127.1, 39.7, 36.2, 29.8, 26.6; IR (KBr) 3117, 1670, 1605, 1570, 1404, 1362, 1269, 1180, 1150, 1072, 980, 957, 914, 826, 787 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{15}H_{17}N_2O_2$ $(M + H)^+$ 257.1285, found 257.1285.

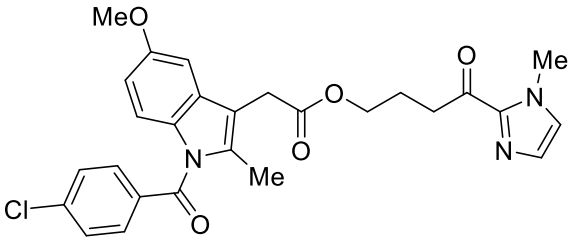
Procedure for synthesis of ethyl (4-(1-methyl-1H-imidazol-2-yl)-4-oxobutyl) malonate (2s), 4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (2q) and 4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (2r)

To a solution of 1-methylimidazole (30 mmol, 1.0 equiv.) in dry THF (30 mL, 1.0 M) under argon atmosphere was added dropwise 2.6 M *n*-BuLi in *n*-hexane (36 mmol, 1.2 equiv.) at –78 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 0.5 h, the mixture was again cooled to –78°C and γ-butyrolactone (60 mol, 2.0 equiv.) was added. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 3 h, it was quenched by NH_4Cl. The mixture was filtrated through a short plug of Celite. After evaporation of the

organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain (4-hydroxy-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one. To the crude mixture (4-hydroxy-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one, (5.0 mmol, 1.0 equiv.) was added CH_2Cl_2 (25 mL, 0.20 M), monoethyl malonate or indometacin (6.0 mmol, 1.3 equiv.), triethylamine (7.0 mmol, 1.4 equiv.), DMAP (0.50 mmol, 0.10 equiv.) and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (6.5 mmol, 1.3 equiv.) under argon atmosphere at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. The mixture was stirred for 14 h and diluted with EtOAc. The mixture was washed with sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4 and filtered. The residue was purified by silica gel flash chromatography to afford **2p** and **2r**.

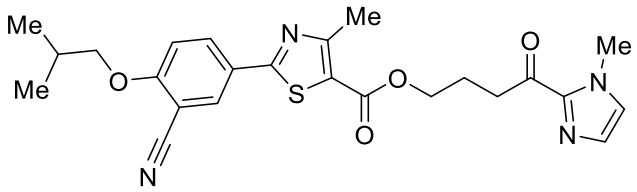


ethyl (4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl) malonate (2s): (Colorless liquid, 0.86 g, 61% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 1H, *imidazole*), 7.04 (s, 1H, *imidazole*), 4.25-4.18 (m, 4H, OC*H*$_2$CH$_3$, OC*H*$_2$CH$_2$), 4.01 (s, 3H, NC*H*$_3$), 3.36 (s, 2H, COC*H*$_2$CO), 3.23 (t, *J* = 7.5 Hz, 2H, COC*H*$_2$CH$_2$), 2.08 (quin, *J* = 7.5 Hz, 2H, COCH$_2$C*H*$_2$), 1.28 (t, *J* = 9.0 Hz, 3H, COCH$_2$C*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.7, 166.6, 166.5, 142.8, 129.1, 127.0, 64.8, 61.6, 41.6, 36.2, 35.2, 22.9, 14.1; IR (neat) 1744, 1726, 1672, 1464, 1408, 1368, 1331, 1288, 1267, 1182, 1150, 1098, 1030, 997, 970, 914, 779, 696, 685 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{13}H_{19}N_2O_5$ $(M + H)^+$283.1288, found 283.1288.



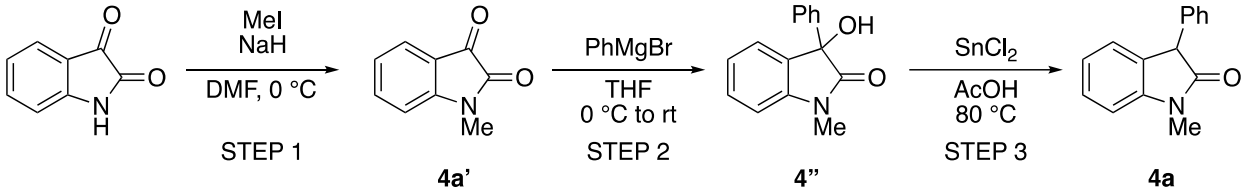
4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (2q): (Yellow solid, 1.6 g, 61% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.47 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.10 (s, 1H, *imidazole*), 7.03 (s, 1H, *imidazole*), 6.96 (d, *J* = 2.5 Hz, 1H, Ar*H*), 6.87 (d, *J* = 9.0 Hz, 1H, Ar*H*), 6.65 (dd, *J* = 9.0 Hz, 2.5 Hz, 1H, Ar*H*), 4.19 (t, *J* = 7.0 Hz, 2H, COC*H*$_2$), 3.99 (s,

3H, NC*H*$_3$), 3.83 (s, 3H, OC*H*$_3$), 3.65 (s, 2H, ArC*H*$_2$), 3.19 (t, *J* = 7.0 Hz, 2H, OC*H*$_2$), 2.37 (s, 3H, ArC*H*$_3$), 2.06 (quin, *J* = 7.0 Hz, 2H, COCH$_2$C*H*$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.7, 170.8, 168.3, 156.0, 142.8, 139.2, 135.9, 133.9. 131.2, 130.8, 130.6, 129.1, 129.1, 127.0, 115.0, 112.6, 111.8, 101.0, 64.4, 55.7, 36.2, 35.3, 30.3, 23.0, 13.4; IR (neat) 1732, 1672, 1589, 1476, 1456, 1437, 1402, 1356, 1314, 1288, 1260, 1219, 1163, 1142, 1111, 1088, 1067, 1034, 1013, 991, 926, 914, 831, 799, 773, 752, 739, 691, 667, 648, 631, 602, 592, 561, 546, 480, 432, 419 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{27}H_{27}ClN_3O_5$ (M + H)$^+$508.1634, found 508.1634.



4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (2r): (White solid, 76% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 2.5 Hz, 1H, Ar*H*), 8.08 (dd, *J* = 9.0, 2.5 Hz, 1H, Ar*H*), 7.14 (s, 1H, *imidazole*), 7.04 (s, 1H, *imidazole*), 7.01 (d, *J* = 9.0 Hz, 1H, Ar*H*), 4.39 (t, *J* = 6.5 Hz, 2H, OC*H*$_2$CH$_2$), 4.00 (s, 3H, NC*H*$_3$), 3.90 (d, *J* = 6.5 Hz, 2H, OC*H*$_2$CH), 3.31 (t, *J* = 7.5 Hz, 2H, COC*H*$_2$), 2.75 (s, 3H, ArC*H*$_3$), 2.20 (m, 3H, COCH$_2$C*H*$_2$, C*H*(CH$_3$)$_2$), 1.09 (d, *J* = 7.0 Hz, 6H, CH(*CH*$_3$)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.6, 167.2, 162.5, 161.9, 161.3, 142.8, 132.5, 132.1, 129.1, 127.1, 126.0, 121.7, 115.4, 112.6, 102.9, 75.7, 64.7, 36.2, 35.3, 28.1, 23.1, 19.1, 17.5; IR (neat) 1682, 1603, 1431, 1414, 1350, 1329, 1300, 1292, 1275, 1132, 1111, 1043, 1013, 982, 914, 797 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{24}H_{27}N_4O_4S$ (M + H)$^+$ 467.1748, found 467.1748.

Procedure for synthesis of 1-methyl-3-phenylindolin-2-one (4a)



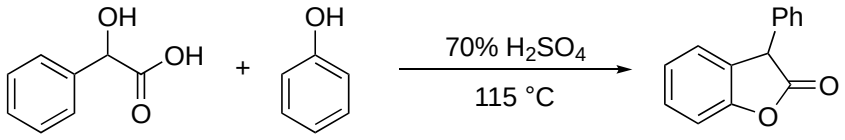
STEP 1: To a solution of isatine (20 mmol, 1.0 equiv.) in DMF (80 mL, 0.25 M) was added dropwise sodium hydride (60%, dispersion in Paraffin Liquid, 24 mmol, 1.2 equiv.) at 0 °C. After 5 min, the mixture

was added iodomethane (30 mmol, 1.5 equiv.). After stirring for 30 min, it was quenched by sat. NH_4Cl aq. The reaction mixture was added EtOAc and washed with H_2O, sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4, filtered and concentrated to obtain the crude **4a'**, which was used in the next step without further purification.

STEP 2: To a solution of crude **4a'** (20 mmol, 1.0 equiv.) in THF (60 mL, 0.33 M) was added dropwise phenylmagnesium bromide (1.0 M in THF, 24 mmol, 1.2 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 3 h, it was quenched by sat. NH_4Cl aq. The reaction mixture was added EtOAc and washed with H_2O and brine. The combined organic layers were dried over Na_2SO_4, filtered and concentrated to obtain the crude **4a''**, which was used in the next step without further purification.

STEP 3: To a solution of crude **4a''** (5 mmol, 1.0 equiv.) in AcOH (30 mL, 0.17 M) was added $SnCl_2$ (10 mmol, 2.0 equiv.). The mixture was stirred at 60 °C for 2 h and diluted with EtOAc. The reaction mixture was washed with H_2O, sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4 and filtered. The residue was purified by silica gel flash chromatography to afford **4a**.: CAS Registry Number 3335-97-5; (White solid, 35% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.27 (m, 4H, Ar*H*), 7.21-7.16 (m, 3H, Ar*H*), 7.07 (t, *J* = 7.5 Hz, 1H, Ar*H*), 6.90 (d, *J* = 8.0 Hz, 1H, Ar*H*), 4.61 (s, 1H, COC*H*), 3.26 (s, 3H, NC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.0, 144.5, 136.6, 128.9, 128.8, 128.4, 128.4, 127.6, 125.1, 122.7, 108.2, 52.0, 26.5.

Procedure for synthesis of 3-phenylbenzofuran-2(3*H*)-one (4b)



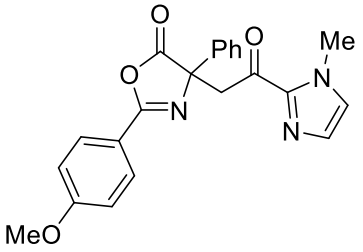
4b

To a solution of DL-mandelic acid (20 mmol, 1.0 equiv.) in 70% H_2SO_4 (7.8 mL, 2.6 M) was added phenol (27 mmol, 1.4 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at 115 °C. After stirring for 1 h, it was quenched by H_2O. To the mixture was added sat. $NaHCO_3$ aq and extracted withEtOAc. The combined organic layers were dried over Na_2SO_4, filtered and concentrated.

The residue was purified by the recrystallization after silica gel flash chromatography to afford **4b**.: CAS Registry Number 3117-37-1; (White solid, 31% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39-7.32 (m, 4H, Ar*H*), 7.26-7.16 (m, 5H, Ar*H*), 4.90 (s, 1H, COC*H*); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.2, 154.0, 135.1, 129.4, 129.2, 128.3, 128.3, 127.1, 125.4, 124.5, 110.9, 49.7.

5. General Procedure and Characterization of the Products

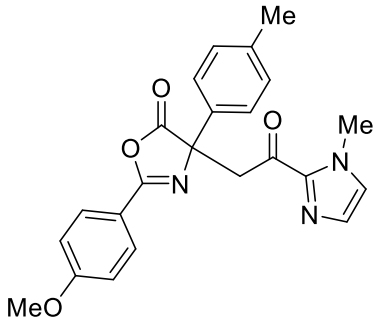
General procedure for catalytic oxidative cross enolate coupling reaction (Table 2): A 20 mL shlenk flask equipped with a magnetic stirring bar and 3-way glass stopcock was charged with 4A crushed molecular sieves (MA 4A 100.0 mg) and flamed-dried under vacumm. After cooling down to room temperature, azlactone (0.20 mmol, 1.0 equiv.), $FeCl_3$ (20 µmol, 10 mol%), DMAP (20 µmol, 10 mol%) were added followed by the addition of chlorobenzene (0.40 mL, 0.50 M) and acylimidazole (0.40 mmol, 2.0 equiv.). Then DTBP (60 µL, 1.6 equiv.) was added to the reaction mixture. The mixture was stirred under Ar at 60 °C for 2 h and diluted with EtOAc. The diluted solution was filtered through silica short column and washed with EtOAc. After evaporation of the organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain cross coupling product.



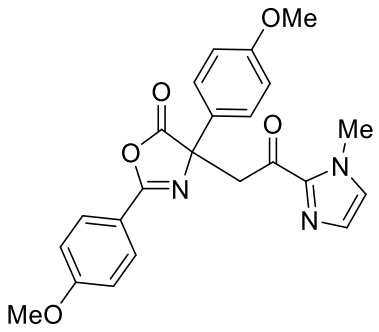
2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-4-phenyloxazol-5(4*H*)-one (3aa): (Yellow solid, *n*-Hexane/Acetone = 9/1 to 4/1, 74% yield, 57.6 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.70 (d, *J* =8.0 Hz, 2H, *Ph*), 7.37 (t, *J* = 8.0 Hz, 2H, *Ph*), 7.32 (t, *J* = 8.0 Hz, 1H, *Ph*), 7.10 (s, 1H, *imidazole*), 7.00-6.97 (m, 3H, *imidazole*, Ar*H*), 4.49 (d, *J* = 19 Hz, 1H, COCH_2), 3.93 (d, *J* = 19 Hz, 1H, COCH_2), 3.90 (s, 3H, NCH_3), 3.87 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ187.6, 179.0, 163.2, 161.5, 142.0, 138.1, 130.1, 129.5, 128.8, 128.4, 127.3, 125.7, 118.6, 114.1, 70.6, 55.5, 49.4, 36.0; IR (KBr) 1817, 1686, 1651, 1608, 1512, 1416, 1308, 1265, 1173, 1099, 1072, 988, 845 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for

$C_{22}H_{20}N_3O_4$ $(M + H)^+$ 390.1448, found 390.1448.

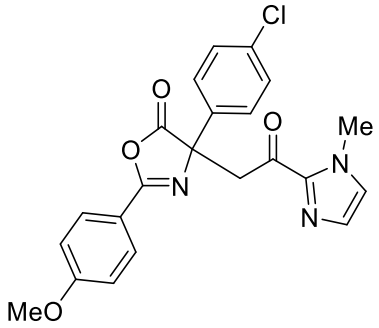
Gram scale (4.0 mmol) procedure for catalytic oxidative cross enolate coupling reaction: A 50 mL flask equipped with a magnetic stirring bar and 3-way glass stopcock was charged with 4A crushed molecular sieves (MA 4A 2.0 g) and flamed-dried under vacumm. After cooling down to room temperature, azlactone **1a** (1.07 g, 4.0 mmol, 1.0 equiv.), $FeCl_3$ (64.9 mg, 0.4 mmol, 10 mol%), DMAP (48.9 mg, 0.4 mmol, 10 mol%) were added followed by the addition of chlorobenzene (8.0 mL, 0.50 M) and acylimidazole **2a** (0.992 mL, 8.0 mmol, 2.0 equiv.). Then DTBP (1.2 mL, 1.6 equiv.) was added to the reaction mixture. The mixture was stirred under Ar at 60 °C for 7 h and diluted with EtOAc. The diluted solution was filtered through silica short column and washed with EtOAc. After evaporation of the organic solvent under reduced pressure (70% NMR yield), the resultant mixture was purified by silica gel flash chromatography (*n*-Hexane/Acetone 9/1 to 8/1) to obtain cross coupling product **3aa** (904.9 mg, 58% yield).



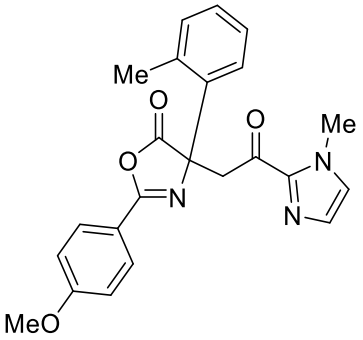
2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-4-(*p*-tolyl)oxazol-5(4*H*)-one (3ba): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 62% yield, 50.0 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.56 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.13 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.13 (s, 1H, *imidazole*), 6.99-6.97 (m, 3H, *imidazole*, Ar*H*), 4.48 (d, *J* = 19 Hz, 1H, COCH_2), 3.92 (d, *J* = 19 Hz, 1H, COCH_2), 3.89 (s, 3H, NCH_3), 3.87 (s, 3H, OCH_3), 2.33 (s, 3H, ArCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.8, 179.2, 163.2, 161.4, 142.0, 138.2, 135.1, 130.1, 129.5, 129.4, 127.3, 125.6, 118.6, 114.1, 70.5, 55.5, 49.2, 36.0, 21.1; IR (KBr) 1817, 1678, 1651, 1609, 1512, 1458, 1412, 1308, 1261, 1173, 1080, 999, 956, 895, 880, 841, 822, 741 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{23}H_{22}N_3O_4$ $(M + H)^+$ 404.1605, found 404.1605.



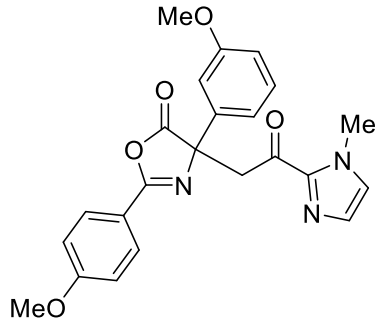
2,4-bis(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)oxazol-5(4*H*)-one (3ca): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 57% yield, 47.8 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.60 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.10 (s, 1H, *imidazole*), 6.99-6.97 (m, 3H, *imidazole*, Ar*H*), 6.89 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.46 (d, *J* = 19 Hz, 1H, COCH_2), 3.92-3.87 (m, 7H, COCH_2, NCH_3, OCH_3), 3.80 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.8, 179.2, 163.2, 161.4, 159.6, 142.0, 130.1, 130.1, 129.5, 127.3, 126.9, 118.6, 114.1, 114.1, 70.2, 55.5, 55.3, 49.3, 36.0; IR (KBr) 1813, 1674, 1651, 1609, 1512, 1412, 1308, 1258, 1173, 1080, 1030, 999, 837 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{23}H_{22}N_3O_5$ $(M + H)^+$ 420.1554, found 420.1554.



4-(4-chlorophenyl)-2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)oxazol-5(4*H*)-one (3da): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 68% yield, 57.8 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.64 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.33 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.10 (s, 1H, *imidazole*), 7.01-6.98 (m, 3H, *imidazole,* Ar*H*), (d, *J* = 19 Hz, 1H, COCH_2), 3.89-3.85 (m, 7H, COCH_2, NCH_3, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.3, 178.7, 163.3, 161.8, 141.9, 136,7, 134.4, 130.2, 129.6, 128.9, 127.4, 127.2, 118.3, 114.2, 70.2, 55.5, 49.2, 36.1; IR (KBr) 1817, 1678, 1651, 1609, 1574, 1512, 1489, 1466, 1412, 1308, 1261, 1173, 1080, 999, 957, 895, 880, 841, 748 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{22}H_{19}ClN_3O_4$ $(M + H)^+$ 424.1059, found 424.1059.

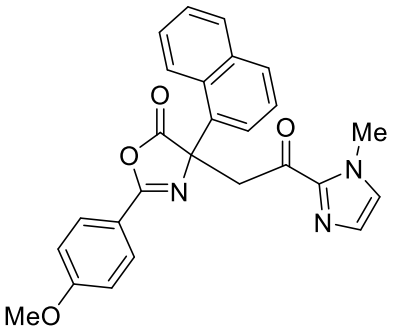


2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-4-(*o*-tolyl)oxazol-5(4*H*)-one (3ea): (White solid, Reaction time = 5 h, *n*-Hexane/Acetone = 9/1 to 4/1, 48% yield, 38.4 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.65 (d, *J* = 7.5 Hz, 1H, Ar*H*), 7.22-7.16 (m, 3H, Ar*H*), 7.11 (s, 1H, *imidazole*), 6.99 (s, 1H, *imidazole*), 6.96 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.73 (d, *J* = 19 Hz, 1H, COC*H*$_2$), 3.89 (s, 3H, NC*H*$_3$), 3.86 (s, 3H, OC*H*$_3$), 3.82 (d, *J* = 19 Hz, 1H, COC*H*$_2$), 2.78 (s, 3H, ArC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.9, 179.1, 163.1, 160.7, 142.1, 137.6, 134.9, 133.2, 130.0, 129.5, 128.2, 127.3, 126.1, 125.5, 118.7, 114.1, 72.8, 55.5, 46.9, 36.1, 22.4; IR (KBr) 2222, 1817, 1682, 1651, 1609, 1574, 1512, 1466, 1411, 1312, 1261, 1242, 1177, 1157, 1096, 1061, 999, 953, 899, 845, 772, 725 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{23}H_{22}N_3O_4$ $(M + H)^+$ 404.1605, found 404.1605.

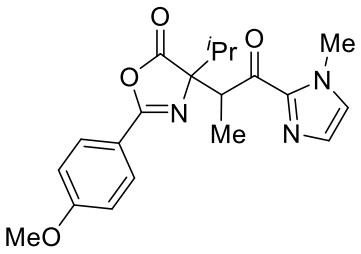


4-(3-methoxyphenyl)-2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)oxazol-5(4*H*)-one (3fa): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 44% yield, 37.0 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.30-7.26 (m, 3H, Ar*H*), 7.10 (s, 1H, *imidazole*), 7.00-6.97 (m, 3H, *imidazole*, Ar*H*), 6.87-6.84 (m, 1H, Ar*H*), 4.49 (d, *J* = 19 Hz, 1H, COC*H*$_2$), 3.92 (d, *J* = 19 Hz, 1H, COC*H*$_2$), 3.89 (s, 3H, NC*H*$_3$), 3.88 (s, 3H, OC*H*$_3$), 3.81 (s, 3H, OC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.6, 178.9, 163.2, 161.5, 159.8, 142.0, 139.6, 130.1, 129.8, 129.5, 127.3, 118.6, 118.0, 114.1, 113.9, 111.6, 70.5, 55.5, 55.3, 49.5, 36.0; IR (KBr) 1817, 1674, 1651, 1609, 1512, 1411, 1261, 999, 968 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for

$C_{23}H_{22}N_3O_5$ $(M + H)^+$ 420.1554, found 420.1555.

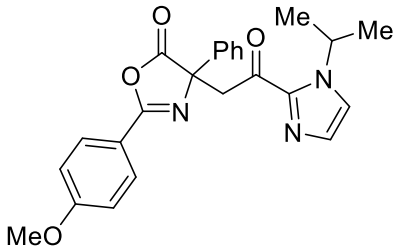


2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-4-(naphthalen-1-yl)oxazol-5(4*H*)-one (3ga): (White solid, Reaction time = 7 h, *n*-Hexane/Acetone = 9/1 to 4/1, 37% yield, 32.3 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.21 (d, *J* = 9.0 Hz, 1H, Ar*H*), 8.03 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.86 (d, *J* = 7.5 Hz, 1H, Ar*H*), 7.81 (t, *J* = 8.0 Hz, 2H, Ar*H*), 7.60 (t, *J* = 8.0 Hz, 1H, Ar*H*), 7.51 (t, *J* = 8.0 Hz, 1H, Ar*H*), 7.41 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.07 (s, 1H, *imidazole*), 7.00 (s, 1H, *imidazole*), 6.95 (d, *J* = 9.0 Hz, 2H, Ar*H*), 5.05 (d, *J* = 19 Hz, 1H, COC*H*$_2$), 3.98 (d, *J* = 19 Hz, 1H, COC*H*$_2$), 3.92 (s, 3H, NC*H*$_3$), 3.85 (s, 3H, OC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.0, 178.8, 163.1, 161.0, 142.1, 135.1, 132.8, 131.1, 130.1, 129.8, 129.5, 129.0, 127.3, 127.2, 126.1, 125.7, 124.9, 123.3, 118.6, 114.0, 73.2, 55.5, 47.7, 36.1; IR (KBr) 1813, 1674, 1655, 1609, 1578, 1512, 1412, 1292, 1258, 1173, 1099, 1080, 1022, 984, 902, 841, 779, 737 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{26}H_{22}N_3O_4$ $(M + H)^+$ 440.1605, found 440.1605.

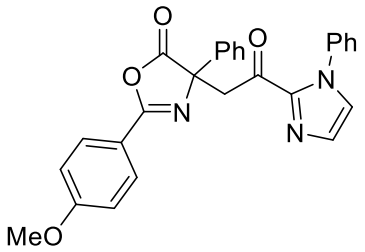


4-isopropyl-2-(4-methoxyphenyl)-4-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxopropan-2-yl)oxazol-5(4*H*)-one (3hb): (White solid, *n*-Hexane/Acetone = 4/1 to 2/1, 18% yield, 14.7 mg, single diastereomer); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.16 (s, 1H, *imidazole*), 6.99 (s, 1H, *imidazole*), 6.93 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.71 (q, *J* = 7.5 Hz, 1H, COC*H*$_2$), 3.85 (s, 3H, NC*H*$_3$), 3.81 (s, 3H, OC*H*$_3$), 2.37 (sep, *J* = 7.0 Hz, 1H, C*H*$(CH_3)_2$), 1.55 (d, *J* = 7.5 Hz, 3H, CHC*H*$_3$), 1.23 (d, *J* = 7.0 Hz, 3H, CH(C*H*$_3)_2$), 0.81 (d, *J* = 7.0 Hz,

3H, CH(C*H*$_3$)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.8, 180.8, 162.9, 160.8, 141.5, 129.9, 129.5, 127.5, 118.5, 113.9, 74.8, 55.5, 47.4, 36.3, 32.4, 16.8, 16.6, 12.1; IR (neet) 1817, 1678, 1645, 1607, 1576, 1512, 1456, 1423, 1410, 1304, 1265, 1173, 1165, 1155, 1107, 1016, 1007, 995, 964, 924, 914, 880, 843, 820, 789, 743, 691, 658, 615, 602, 552, 525, 511, 494 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{20}H_{24}N_3O_4$ (M + H)$^+$370.1761, found 370.1760.

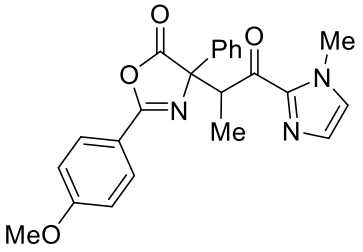


4-(2-(1-isopropyl-1*H*-imidazol-2-yl)-2-oxoethyl)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (3ac): (White solid, Reaction time = 4.5 h, *n*-Hexane/Acetone = 9/1 to 4/1, 72% yield, 60.1 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.70 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.37 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.31 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.23 (s, 1H, *imidazole*), 7.13 (s, 1H, *imidazole*), 6.98 (d, *J* = 9.0 Hz,2H, Ar*H*), 5.41 (sep, *J* = 6.5 Hz, 1H, NC*H*), 4.52 (d, *J* = 18 Hz, 1H, COC*H*$_2$), 3.94 (d, *J* = 18 Hz, 1H, COC*H*$_2$), 3.88 (s, 3H, OC*H*$_3$), 1.34 (dd, *J* = 30 Hz, 6.5 Hz, 6H, CH(C*H*$_3$)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.7, 179.0, 163.2, 161.5, 141.2, 138.2, 130.1, 130.0, 128.7, 128.3, 125.7, 121.6, 118.6, 114.1, 70.7, 55.5, 50.1, 49.2, 23.6, 23.5; IR (KBr) 1817, 1678, 1651, 1609, 1512, 1400, 1308, 1258, 1173, 1069, 980 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{24}H_{24}N_3O_4$ (M + H)$^+$ 418.1761, found 418.1762.

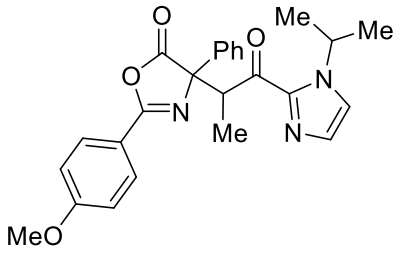


2-(4-methoxyphenyl)-4-(2-oxo-2-(1-phenyl-1*H*-imidazol-2-yl)ethyl)-4-phenyloxazol-5(4*H*)-one (3ad): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 44% yield, 39.7 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.69 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.39-7.31 (m, 4H, *Ph*), 7.26-7.23 (m, 3H, *Ph*, *imidazole*),

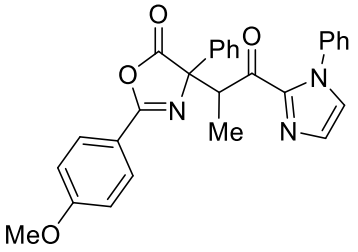
7.15-7.13 (m, 3H, *Ph*, *imidazole*), 6.96 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.55 (d, *J* = 18 Hz, 1H, COC*H*$_2$), 3.90 (d, *J* = 18 Hz, 1H, COC*H*$_2$), 3.88 (s, 3H, OC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 186.2, 178.6, 163.1, 161.5, 142.0, 138.2, 137.7, 130.1, 130.0, 128.9, 128.8, 128.6, 128.4, 127.4, 125.7, 125.6, 118.6, 114.0, 70.9, 55.5, 49.5, ; IR (KBr) 1813, 1686, 1651, 1609, 1493, 1447, 1408, 1312, 1261, 1177, 1103, 1022, 964, 845, 764 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{27}H_{22}N_3O_4$ $(M + H)^+$ 452.1605, found 452.1605.



2-(4-methoxyphenyl)-4-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxopropan-2-yl)-4-phenyloxazol-5(4*H*)-one (3ab): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 85% yield, 68.5 mg, dr = 85/15); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.95 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.79 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.38 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.31 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.15 (s, 1H, *imidazole*), 6.99 (s, 1H, *imidazole*), 6.92 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.79 (q, *J* = 7.5 Hz, 1H, COC*H*), 3.85 (s, 3H, NC*H*$_3$), 3.84 (s, 3H, OC*H*$_3$), 1.37 (d, *J* = 7.5 Hz, 3H, CHC*H*$_3$); minor : δ 8.12 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.75 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.38-7.30 (m, 3H, *Ph*), 7.14 (s, 1H, *imidazole*), 7.01 (d, *J* = 9.0 Hz, 2H, Ar*H*), 6.99 (s, 1H, *imidazole*), 4.59 (q, *J* = 7.5 Hz, 1H, COC*H*), 3.90 (s, 3H, NC*H*$_3$), 3.89 (s, 3H, OC*H*$_3$), 1.51 (d, *J* = 7.5 Hz, 3H, CHC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 192.6, 177.6, 163.0, 160.6, 141.7, 136.4, 130.0, 129.5, 128.5, 128.2, 127.4, 126.9, 118.5, 113.9, 74.1, 55.4, 52.9, 36.2, 13.0; minor : δ 193.0, 179.7, 163.1, 160.6, 141.6, 138.2,130.1, 129.3, 128.5, 128.3, 127.0, 126.4, 119.0, 114.1, 74.0, 55.5, 52.6, 36.2, 13.7; IR (KBr) 1802, 1670, 1655, 1605, 1574, 1512, 1451, 1408, 1304, 1261, 1173, 1157, 1099, 1022, 1003, 968, 930, 910, 845, 745, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{23}H_{22}N_3O_4$ $(M + H)^+$ 404.1605, found 404.1604.

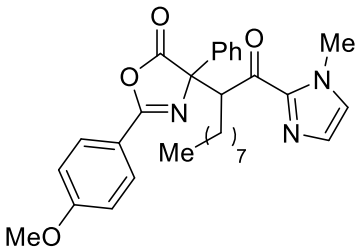


4-(1-(1-isopropyl-1*H*-imidazol-2-yl)-1-oxopropan-2-yl)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (3ae): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 81% yield, 69.9 mg, dr = 81/19); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.94 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.80 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.38 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.30 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.23 (s, 1H, *imidazole*), 7.18 (s, 1H, *imidazole*), 6.90 (d, *J* = 9.0 Hz,2H, Ar*H*), 4.79 (sep, *J* = 6.5 Hz, 1H, NC*H*), 4.84 (q, *J* = 6.5 Hz, 1H, COC*H*), 3.84 (s, 3H, OCH_3), 1.39-1.35 (m, 6H, CH(CH_3)$_2$), 1.18 (d, *J* = 6.5 Hz, 3H, CHCH_3); minor : δ 8.11 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.75 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.36 (t, *J* = 7.0 Hz, 2H, *Ph*), 7.31 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.22 (s, 1H, *imidazole*), 7.17 (s, 1H, *imidazole*), 7.01 (d, *J* = 9.0 Hz,2H, Ar*H*), 5.39 (sep, *J* = 7.0 Hz, 1H, NC*H*), 4.65 (q, *J* = 7.5 Hz, 1H, COC*H*), 3.89 (s, 3H, OCH_3), 1.49 (d, *J* = 7.5 Hz, 3H, CHCH_3), 1.37 (dd, *J* = 16.5 Hz, 7.0 Hz, 6H, CH(CH_3)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 192.9, 177.5, 163.0, 160.6, 141.0, 136.4, 130.0, 128.5, 128.2, 126.9, 121.7, 118.5, 113.9, 74.3, 55.4, 53.4, 49.3, 23.5, 23.4, 13.0; minor : δ 193.2, 179.7, 163.1, 160.5, 140.9, 138.3, 130.1, 129.7, 128.5, 128.3, 126.4, 121.1, 119.1, 114.1, 74.1, 55.5, 53.0, 49.1, 23.7, 23.6, 13.8; IR (KBr) 2982, 2940, 1809, 1670, 1651, 1609, 1578, 1512, 1454, 1400, 1373, 1308, 1258, 1173, 1150, 1099, 1038, 1003, 964, 910, 887, 841, 745, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{25}H_{26}N_3O_4$ $(M + H)^+$ 432.1918, found 432.1918.

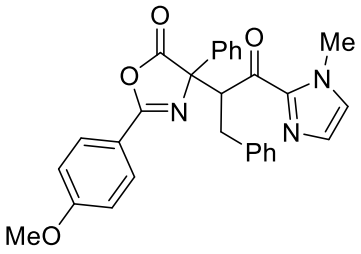


2-(4-methoxyphenyl)-4-(1-oxo-1-(1-phenyl-1*H*-imidazol-2-yl)propan-2-yl)-4-phenyloxazol-5(4*H*)-one (3af): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 76% yield, 69.9 mg, dr = 80/20); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.99 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.74 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.37-7.30 (m, 6H, *Ph*), 7.26 (s, 1H, *imidazole*), 7.21-7.19 (m, 2H, *Ph*), 7.14 (s, 1H, *imidazole*), 6.95 (d, *J* = 9.0 Hz,2H, Ar*H*), 4.68 (q, *J* = 8.0 Hz, 1H, COC*H*), 3.87 (s, 3H, OCH_3), 1.48 (d, *J* = 8.0 Hz, 3H, CHCH_3); minor : δ 7.95 (d, *J* = 9.0 Hz, 2H, Ar*H*),

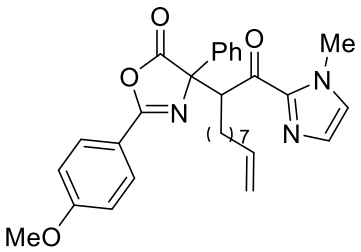
7.81 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.39 (t, *J* = 8.0 Hz, 2H, *Ph*), 7.33-7.26 (m, 3H, *Ph*, *imidazole*), 7.14 (s, 1H, *imidazole*), 7.07 (t, *J* = 7.5 Hz, 2H, *Ph*), 6.99-6.94 (m, 4H, *Ph*, Ar*H*), 4.82 (q, *J* = 7.5 Hz, 1H, COC*H*), 3.87 (s, 3H, OCH_3), 1.39 (d, *J* = 7.5 Hz, 3H, CHCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 191.4, 179.4, 163.0, 160.3, 141.8, 138.2, 138.0, 130.0, 129.7, 129.0, 128.5, 128.2, 127.3, 126.9, 125.3, 118.5, 114.0, 74.4, 55.5, 53.1, 12.7. minor : δ 191.3, 179.4, 163.0, 160.3, 141.8, 138.2, 138.0, 130.0, 129.7, 129.0, 128.5, 128.5, 128.3, 127.1, 126.4, 125.6, 118.9, 114.0, 74.0, 55.5, 52.2, 13.4.; IR (KBr) 1809, 1682, 1651, 1609, 1512, 1493, 1447, 1404, 1308, 1261, 1173, 1034, 953, 910, 760 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{28}H_{23}N_3O_4$ $(M + H)^+$ 466.1761, found 466.1761.



2-(4-methoxyphenyl)-4-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxodecan-2-yl)-4-phenyloxazol-5(4*H*)-one (3ag): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 76% yield, 76.2 mg, dr = 68/32); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.91 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.80 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.33 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.28-7.25 (m, 1H, *Ph*), 7.15 (s, 1H, *imidazole*), 6.95 (s, 1H, *imidazole*), 6.90 (d, *J* = 8.5 Hz,2H, Ar*H*), 4.88 (dd, *J* = 10 Hz, 3.5 Hz, 1H, COC*H*), 3.84 (s, 3H, NCH_3), 3.77 (s, 3H, OCH_3), 2.01-1.94 (m, 1H, C_8H_{17}), 1.64-1.57 (m, 2H, C_8H_{17}), 1.22-1.07 (m, 12H, C_8H_{17}), 0.82 (t, *J* = 7.0 Hz, 3H, C_8H_{17}); minor : δ 8.06 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.78 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.35 (t, *J* = 7.0 Hz, 2H, *Ph*), 7.30 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.15 (s, 1H, *imidazole*), 7.01-6.99 (m, 3H, *imidazole,* Ar*H*), 4.81 (dd, *J* = 7.0 Hz, 4.5 Hz, 1H, COC*H*), 3.89 (s, 3H, NCH_3), 3.89 (s, 3H, OCH_3), 1.96-1.84 (m, 2H, C_8H_{17}), 1.34-1.09 (m, 12H, C_8H_{17}), 1.06 (t, *J* = 8.0 Hz, 3H, C_8H_{17}); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 193.2, 177.4, 163.0, 160.1, 143.7, 136.4, 130.0, 129.5, 128.3, 128.1, 127.3, 126.0, 118.3, 114.0, 75.2, 56.4, 55.4, 36.1, 31.7, 29.5, 29.1, 29.1, 27.7, 27.6, 22.6, 14.1; minor : δ 193.2, 179.0, 163.1, 159.9, 143.1, 138.1, 130.1, 129.4, 128.4, 128.2, 127.2, 126.6, 118.8, 114.1, 74.6, 55.6, 55.5, 36.2, 31.8, 29.6, 29.1, 29.1, 28.6, 27.5, 22.6, 14.1; IR (KBr) 2928, 2854, 1813, 1651, 1608, 1512, 1408, 1258, 1030, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{30}H_{36}N_3O_4$ $(M + H)^+$ 516.2857, found 516.2856.

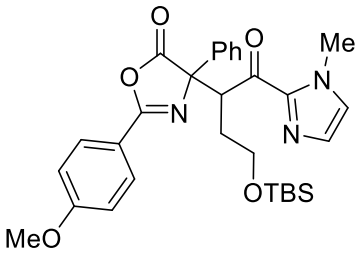


2-(4-methoxyphenyl)-4-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxo-3-phenylpropan-2-yl)-4-phenyloxazol-5(4*H*)-one (3ah): (Diastereomixture, White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 82% yield, 78.2 mg, dr = 80/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.5 Hz, 2H, Ar*H,* minor), 7.93 (d, *J* = 8.5 Hz, 2H, Ar*H,* major), 7.83 (d, *J* = 7.5 Hz, 2H, *Ph,* major), 7.77 (d, *J* = 7.0 Hz, 2H, *Ph,* minor), 7.35-7.25 (m, 6H, *diastereomers*), 7.96-6.75 (m, 16H, *diastereomers*), 6.86 (s, 1H, *imidazole,* minor), 6.75 (s, 1H, *imidazole,* major), 5,32-5.25 (m, 2H, *diastereomers*), 3.90 (s, 3H, NCH_3, major), 3.84 (s, 3H, NCH_3, minor), 3.74 (s, 3H, OCH_3, minor), 3.63 (s, 3H, OCH_3, major), 3.35-2.92 (m, 2H, CH_2Ph, *diastereomers*), 3.14 (dd, *J* = 13 Hz, 6.0 Hz, 1H, CH_2Ph, minor), 2.94 (dd, *J* = 14 Hz, 5.0 Hz, 1H, CH_2Ph, major); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.1, 192.0, 178.4, 177.4, 163.2, 163.1, 160.3, 160.1, 143.6, 143.3, 138.4, 137.6, 137.5, 136.2, 130.1, 129.4, 129.4, 129.3, 129.2, 128.4, 128.3, 127.9, 127.8, 127.0, 126.9, 126.9, 126.6, 126.1, 125.9, 118.7, 118.3, 114.2, 114.0, 74.9, 74.4, 57.0, 56.3, 55.5, 55.5, 35.9, 35.7, 34.3, 33.7; IR (KBr) 1809, 1651, 1609, 1512, 1497, 1451, 1408, 1308, cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{29}H_{26}N_3O_4$ $(M + H)^+$ 480.1918, found 480.1917.



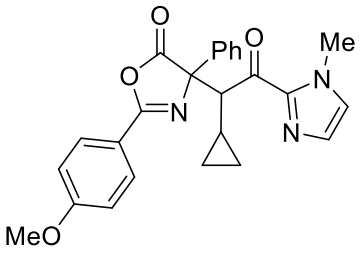
2-(4-methoxyphenyl)-4-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxoundec-10-en-2-yl)-4-phenyloxazol-5(4*H*)-one (3ai): (Colorless liquid, *n*-Hexane/Acetone = 9/1, 81% yield, 82.8 mg, dr = 70/30); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.91 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.80 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.34 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.29-7.28 (m, 1H, *Ph*), 7.16 (s, 1H, *imidazole*), 6.96 (s, 1H, *imidazole*), 6.91 (d, *J* = 9.0 Hz, 2H, Ar*H*), 5.80-5.72 (m, 1H, C*H*CH_2CH_2), 4.97-4.87 (m, 3H, COC*H*, CHCH_2CH_2), 3.84 (s, 3H, NCH_3), 3.77 (s, 3H, OCH_3), 2.01-1.93 (m, 3H, $CHCH_2CH_2$, $COCHCH_2$), 1.63-1.59 (m, 1H, $CHCH_2CH_2$), 1.28-1.05 (m, 10H, C_5H_{10}); minor : δ 8.07 (d,

J = 9.0 Hz, 2H, Ar*H*), 7.78 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.36 (t, *J* = 7.0 Hz, 2H, *Ph*), 7.30 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.15 (s, 1H, *imidazole*), 7.02-6.99 (m, 3H, *imidazole*, Ar*H*), 5.80-5.73 (m, 1H, C*H*CH_2CH_2), 4.98-4.89 (m, 2H, CHC*H*$_2$$CH_2$), 4.81 (dd, *J* = 7.0 Hz, 5.5Hz, 1H, COC*H*), 3.89 (s, 3H, NC*H*$_3$), 3.89 (s, 3H, OC*H*$_3$), 1.99-1.87 (m, 4H, $CHCH_2$C*H*$_2$, COCHC*H*$_2$), 1.31-1.09 (m, 10H, C_5H_{10}); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 193.2, 177.4, 163.1, 160.1, 143.6, 139.2, 136.4, 130.0, 129.6, 128.4, 128.2, 127.4, 126.9, 118.3, 114.1, 114.0, 75.2, 56.4, 55.5, 36.1, 33.7, 29.5, 29.0, 28.9, 28.8, 27.6, 27.6; minor : δ 193.2, 179.0, 163.1, 160.0, 143.1, 139.3, 138.1, 130.1, 129.4, 128.4, 128.3, 127.3, 126.6, 118.8, 114.1, 114.1, 74.5, 55.6, 55.5, 36.2, 33.8, 29.6, 29.0, 28.9, 28.8, 28.6, 27.5; IR (neat) 1809, 1667, 1651, 1609, 1512, 1406, 1258, 1171, 1155, 907, 889, 841, 729, 700, 648, 604, 563 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{31}H_{36}N_3O_4$ $(M + H)^+$ 514.2700, found 514.2688.

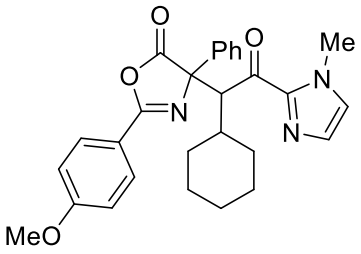


4-(4-((tert-butyldimethylsilyl)oxy)-1-(1-methyl-1*H*-imidazol-2-yl)-1-oxobutan-2-yl)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (3aj): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 77% yield, 84.6 mg, dr = 84/16); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.87 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.81 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.35 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.28 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.14 (s, 1H, *imidazole*), 6.93 (s, 1H, *imidazole*), 6.89 (d, *J* = 8.5 Hz,2H, Ar*H*), 4.91 (dd, *J* = 10 Hz, 3.0 Hz, 1H, COC*H*), 3.83 (s, 3H, NC*H*$_3$), 3.75 (s, 3H, OC*H*$_3$), 3.53-3.40 (m, 2H, OC*H*$_2$), 2.28-2.21 (m, 1H, CHC*H*$_2$), 1.93-1.87 (m, 1H, CHC*H*$_2$), 0.70 (s, 9H, C(C*H*$_3$)$_3$), −0.16 (s, 3H, SiC*H*$_3$), −0.24 (s, 3H, SiC*H*$_3$); minor : δ 8.06 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.77 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.36 (t, *J* = 7.0 Hz, 2H, *Ph*), 7.30 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.13 (s, 1H, *imidazole*), 7.00 (d, *J* = 9.0 Hz,2H, Ar*H*), 6.97 (s, 1H, *imidazole*), 4.78 (dd, *J* = 6.5 Hz, 5.0 Hz, 1H, COC*H*), 3.89 (s, 3H, NC*H*$_3$), 3.87 (s, 3H, OC*H*$_3$), 3.71-3.41 (m, 1H, OC*H*$_2$), 3.45-3.41 (m, 1H, OC*H*$_2$), 2.29-2.23 (m, 1H, CHC*H*$_2$), 2.15-2.09 (m, 1H, CHC*H*$_2$), 0.73 (s, 9H, C(C*H*$_3$)$_3$), −0.14 (s, 3H, SiC*H*$_3$), −0.19 (s, 3H, SiC*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 192.2, 177.2, 163.0, 160.2, 143.4, 136.3, 130.0, 129.4, 128.5, 128.2, 127.1, 127.0, 118.3, 113.9, 75.2, 61.6, 55.4, 54.5, 36.0, 31.0, 25.7, 18.1, −5.7, −5.7; minor : δ 192.2, 178.3, 163.1, 160.2, 142.7, 138.0, 130.1, 129.3, 128.5, 128.4, 127.0, 126.6, 118.8, 114.1, 74.3, 61.7, 55.5, 53.6, 36.1, 31.8, 25.8,

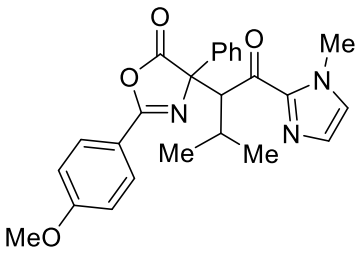
18.2, −5.5, −5.5; IR (KBr) 2955, 2932, 2859, 1813, 1674, 1651, 1609, 1512, 1466, 1408, 1308, 1258, 1173, 1092, 1042, 891, 841, 779, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{30}H_{37}N_3NaO_5Si$ $(M + Na)^+$ 570.2395, found 570.2394.



4-(1-cyclopropyl-2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (3ak): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 79% yield, 67.9 mg, dr = 62/38); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.98 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.84 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.31 (t, *J* = 7.0 Hz, 2H, *Ph*), 7.27 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.12 (s, 1H, *imidazole*), 6.97 (s, 1H, *imidazole*), 6.93 (d, *J* = 9.0 Hz,2H, Ar*H*), 4.09 (d, *J* = 10.5 Hz, 1H, COC*H*), 3.84 (s, 3H, NCH_3), 3.82 (s, 3H, OCH_3), 1.44-1.36 (m, 1H, *cyclopropyl*), 0.40-0.34 (m, 2H, *cyclopropyl*), 0.32-0.27 (m, 1H, *cyclopropyl*), −0.19-−0.24 (m, 1H, *cyclopropyl*); minor : δ 8.09 (d, *J* = 9.0 Hz, 2H, Ar*H*), 8.82 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.35-7.27 (m, 3H, *Ph*), 7.13 (s, 1H, *imidazole*), 7.02-7.00 (m, 3H, *imidazole,* Ar*H*), 4.14 (d, *J* = 10.5 Hz, 1H, COC*H*), 3.91 (s, 3H, NCH_3), 3.89 (s, 3H, OCH_3), 1.37-1.33 (m, 1H, *cyclopropyl*), 0.47-0.35 (m, 2H, *cyclopropyl*), 0.29-0.24 (m, 1H, *cyclopropyl*), −0.21-−0.26 (m, 1H, *cyclopropyl*); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 191.6, 177.7, 163.1, 160.4, 143.2, 136.8, 130.1, 129.4, 128.1, 128.3, 127.6, 127.0, 118.4, 114.0, 74.7, 60.7, 55.5, 36.2, 8.9, 6.2, 2.9; minor : δ 192.5, 178.9, 163.1, 159.9, 143.3, 138.4, 130.1, 129.3, 128.1, 128.1, 127.5, 126.7, 118.9, 114.1, 75.0, 59.1, 55.5, 36.2, 10.3, 5.8, 2.7; IR (KBr) 3445, 3422, 1809, 1651, 1609, 1512, 1408, 1323, 1261, 1173, 1057, 1026, 937, 841, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{25}H_{24}N_3O_4$ $(M + H)^+$ 430.1761, found 430.1760.

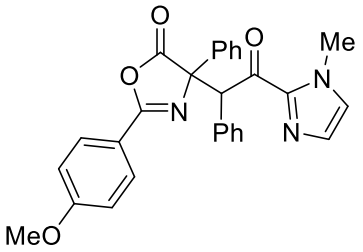


4-(1-cyclohexyl-2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (3al): (White solid, Reaction time = 24 h, *n*-Hexane/Acetone = 9/1 to 4/1, 32% yield, 30.2 mg, dr = 71/29); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.95 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.74 (d, *J* = 8.5 Hz, 2H, *Ph*), 7.30-7.21 (m, 3H, *Ph*), 7.16 (s, 1H, *imidazole*), 6.93-6.91 (m, 3H, *imidazole,* Ar*H*), 4.87 (d, *J* = 6.5 Hz, 1H, COC*H*), 3.85 (s, 3H, NCH_3), 3.72 (s, 3H, OCH_3), 2.16-2.09 (m, 1H, *cyclohexyl*), 1.66-1.61 (m, 1H, *cyclohexyl*), 1.56-1.50 (m, 2H, *cyclohexyl*), , 1.28-1.16 (m, 4H, *cyclohexyl*), 1.06-0.93 (m, 2H, *cyclohexyl*), 0.87-0.78 (m, 1H, *cyclohexyl*); minor : δ 8.11 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.77 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.36 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.30 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.21 (s, 1H, *imidazole*), 7.03-7.02 (m, 3H, *imidazole,* Ar*H*), 4.92 (d, *J* = 5.0 Hz, 1H, COC*H*), 3.91 (s, 3H, NCH_3), 3.90 (s, 3H, OCH_3), 2.23-2.17 (m, 1H, *cyclohexyl*), 1.72-1.70 (m, 1H, *cyclohexyl*), 1.60-1.52 (m, 3H, *cyclohexyl*), , 1.26-1.07 (m, 4H, *cyclohexyl*), 0.96-0.82 (m, 2H, *cyclohexyl*); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 192.6, 178.0, 163.1, 160.1, 144.3, 136.8, 130.0, 129.3, 128.2, 128.1, 127.1, 127.0, 118.4, 114.0, 74.6, 61.1, 55.4, 37.1, 36.0, 33.1, 31.2, 26.6, 26.5, 25.8; minor : δ 194.5, 179.6, 163.1, 160.1, 144.1, 139.1, 130.1, 129.4, 128.5, 128.2, 127.4, 126.5, 119.0, 114.2, 75.0, 60.4, 55.5, 39.1, 36.3, 33.1, 31.3, 26.8, 26.7, 26.0; IR (KBr) 2928, 1813, 1651, 1609, 1512, 1411, 1258 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{28}H_{30}N_3O_4$ $(M + H)^+$ 472.2231, found 472.2231.

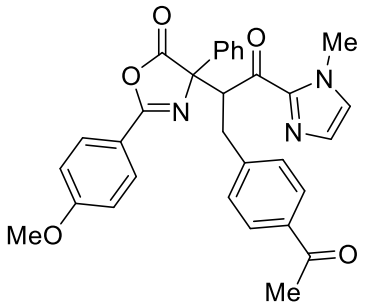


2-(4-methoxyphenyl)-4-(3-methyl-1-(1-methyl-1*H*-imidazol-2-yl)-1-oxobutan-2-yl)-4-phenyloxazol-5(4*H*)-one (3am): (White solid, Reaction time = 6 h, *n*-Hexane/Acetone = 9/1 to 4/1, 63% yield, 54.4 mg, dr = 68/32); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.97 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.73 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.29-7.20 (m, 3H, *Ph*), 7.15 (s, 1H, *imidazole*), 6.94-6.92 (m, 3H, *imidazole,* Ar*H*), 4.89 (d, *J* = 6.5 Hz, 1H,

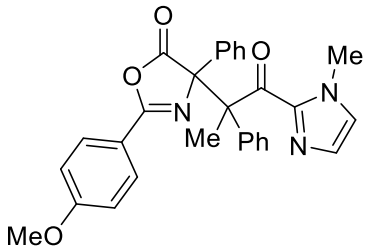
COC*H*), 3.85 (s, 3H, NCH_3), 3.71 (s, 3H, OCH_3), 2.47-2.38 (m, 1H, C*H*(CH_3)$_2$), 0.83 (dd, *J* = 15.0 Hz, 6.5 Hz, 6H, CH(CH_3)$_2$); minor : δ 8.11 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.78 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.36-7.30 (m, 3H, *Ph*), 7.20 (s, 1H, *imidazole*), 7.03-7.01 (m, 3H, *imidazole,* Ar*H*), 4.92 (d, *J* = 4.5 Hz, 1H, COC*H*), 3.91 (s, 3H, NCH_3), 3.90 (s, 3H, OCH_3), 2.55-2.49 (m, 1H, C*H*(CH_3)$_2$), 0.90 (dd, *J* = 20.5 Hz, 7.0 Hz, 6H, CH(CH_3)$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 192.6, 178.1, 163.1, 160.1, 144.4, 136.2, 130.1, 129.3, 128.2, 128.1, 127.1, 127.0, 118.4, 114.0, 74.9, 61.3, 55.5, 36.0, 27.7, 22.8, 21.2; minor : δ 194.3, 179.6, 163.1, 160.1, 144.0, 139.1, 130.1, 129.4, 128.5, 128.2, 127.3, 126.6, 119.0, 114.2, 75.0, 60.7, 55.5, 36.2, 29.3, 23.2, 20.9; IR (KBr) 1809, 1667, 1647, 1609, 1512, 1408, 1261, 1173, 1049, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{25}H_{26}N_3O_4$ $(M + H)^+$ 432.1918, found 432.1918.



2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxo-1-phenylethyl)-4-phenyloxazol-5(4*H*)-one (3an): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 68% yield, 63.3 mg, dr = 71/29); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 8.00 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.56-7.54 (m, 2H, *Ph*), 7.22-7.15 (m, 8H, *Ph*), 7.04 (s, 1H, *imidazole*), 6.94 (d, *J* = 9.0 Hz, 2H, Ar*H*), 6.04 (s, 1H, *imidazole*), 6.04 (s, 1H, COC*H*), 3.86 (s, 3H, NCH_3), 3.84 (s, 3H, OCH_3); minor : δ 8.09 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.54-7.52 (m, 2H, *Ph*), 7.25-7.24 (m, 3H, *Ph*), 7.17-7.13 (m, 3H, *Ph*), 7.08-7.06 (m, 2H, *Ph*), 7.02-7.00 (m, 3H, Ar*H, imidazole*), 6.84 (s, 1H, *imidazole*), 5.82 (s, 1H, COC*H*), 3.89 (s, 3H, NCH_3), 3.87 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 188.2, 177.0, 163.1, 160.6, 142.3, 136.4, 132.0, 130.8, 130.1, 129.7, 128.1, 128.0, 128.0, 127.9, 127.3, 126.9, 118.4, 114.0, 74.1, 63.4, 55.5, 36.1; minor : δ 189.6, 179.4, 163.1, 160.1, 142.0, 137.6, 133.3, 130.9, 130.1, 129.6, 128.2, 128.2, 127.6, 127.4, 126.9, 126.6, 119.1, 114.1, 74.3, 62.9, 55.5, 36.1; IR (KBr) 1813, 1651, 1609, 1404, 1323, 1308, 1258, 1173, 1157, 1057, 1022, 984, 953, 891, 841 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{28}H_{24}N_3O_4$ $(M + H)^+$ 466.1761, found 466.1762.

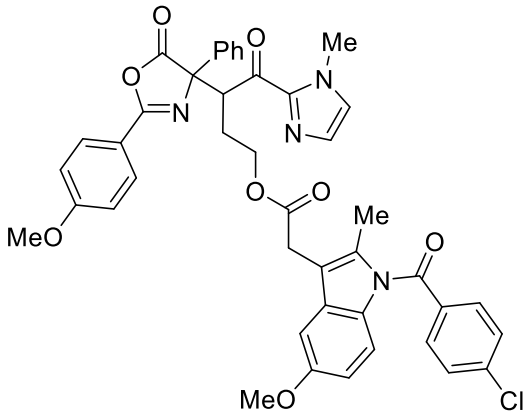


4-(3-(4-acetylphenyl)-1-(1-methyl-1*H*-imidazol-2-yl)-1-oxopropan-2-yl)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4*H*)-one (3ao): (White solid, *n*-Hexane/Acetone = 4/1 to 2/1, 70% yield, 72.9 mg, dr = 82/18); ^{1}H NMR (500 MHz, $CDCl_3$) (ppm) major : δ 7.93 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.82 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.64 (d, *J* = 8.0 Hz, 2H, Ar*H*, 7.33 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.27 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.12 (d, *J* = 8.0 Hz, 2H, Ar*H*), 6.94 (s, 1H, *imidazole*), 6.92 (d, *J* = 9.0 Hz, 2H, Ar*H*), 6.79 (s, 1H, *imidazole*), 5.31 (q, *J* = 5.0 Hz, 1H, COC*H*), 3.85 (s, 3H, NCH_3), 3.66 (s, 3H, OCH_3), 3.37 (dd, *J* = 14 Hz, 5.0 Hz, 1H, CHCH_2), 3.01 (dd, *J* = 14 Hz, 5.0 Hz, 1H, CHCH_2), 2.48 (s, 3H, COCH_3); minor : δ 8.07 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.72 (d, *J* = 6.5 Hz, 2H, *Ph*), 7.62 (d, *J* = 8.0 Hz, 2H, Ar*H*), 7.29-7.24 (m, 3H, *Ph*), 7.17 (d, *J* = 8.0 Hz, 2H, Ar*H*), 7.17 (s, 1H, *imidazole*), 7.02 (d, *J* = 9.0 Hz, 2H, Ar*H*), 6.91 (s, 1H, *imidazole*), 5.27 (dd, *J* = 7.0 Hz, 6.5 Hz, 1H, COC*H*), 3.90 (s, 3H, NCH_3), 3.78 (s, 3H, OCH_3), 3.37 (dd, *J* = 14 Hz, 6.5 Hz, 1H, CHCH_2), 3.22 (dd, *J* = 14 Hz, 7.0 Hz, 1H, CHCH_2), 2.48 (s, 3H, COCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 197.9, 191.5, 177.3, 163.2, 160.5, 143.7, 143.2, 135.9, 135.1, 130.1, 129.5, 129.4, 128.5, 128.4, 128.1, 127.3, 126.9, 118.0, 114.0, 74.8, 56.8, 55.5, 35.9, 33.6, 26.6; minor : δ 198.0, 191.4, 178.4, 163.3, 160.3, 144.5, 142.8, 137.3, 134.9, 130.1, 129.6, 129.5, 128.4, 128.3, 127.9, 127.3, 126.6, 118.5, 114.2, 74.1, 56.2, 55.6, 36.0, 34.4, 26.6; IR (KBr) 1813, 1678, 1651, 1609, 1512, 1447, 1408, 1308, 1261, 1157, 1069, 1030, 984, 907, 841, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{31}H_{28}N_3O_5$ $(M + H)^+$ 522.2023, found 522.2022.



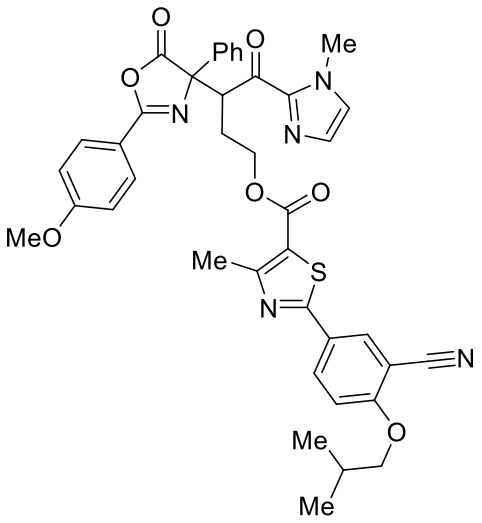
2-(4-methoxyphenyl)-4-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxo-2-phenylpropan-2-yl)-4-phenyloxazol-5(4*H*)-one (3ap): (Diastereomixture, Temperature = 80 °C, White solid, *n*-Hexane/Acetone = 9/1 to 4/1,

47% yield, 47.7 mg, dr = 53/47); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 6.5 Hz, 2H, Ar*H*, minor), 8.00 (d, *J* = 7.0 Hz, 2H, Ar*H*, major), 7.25-7.06 (m, 16H, *diastereomers*), 6.99-6.94 (m, 8H, *diastereomers*), 6.90 (s, 1H, *imidazole*, major), 6.83-6.82 (m, 2H, *diastereomers*), 6.78 (s, 1H, *imidazole*, minor), 3.90-3.86 (m, 12H, *diastereomers*), 2.37 (s, 3H, COCC*H*$_3$, major), 2.23 (s, 3H, COCC*H*$_3$, minor); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.3, 192.3, 178.6, 178.0, 162.9, 162.8, 159.8, 159.6, 141.0, 140.8, 138.4, 137.4, 135.7, 134.6, 129.9, 129.8, 129.1, 129.0, 129.0, 128.9, 128.0, 127.9, 127.5, 127.2, 127.0, 126.9, 126.8, 126.5, 126.1, 125.8, 119.4, 119.3, 114.0, 114.0, 76.3, 75.6, 65.3, 64.6, 55.5, 55.5, 37.0, 36.9, 20.5, 18.8; IR (KBr) 1802, 1659, 1609, 1578, 1512, 1393, 1308, 1258, 1153, 1107, 1030, 968, 914, 891, 841, 733, 706 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{29}H_{26}N_3O_4$ $(M + H)^+$ 480.1918, found 480.1917.



3-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (3aq): (yellow solid, *n*-Hexane/Acetone = 4/1 to 3/1, 64% yield, 98.8 mg, dr = 82/18); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.88 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.77 (d, *J* = 7.0 Hz, 2H, Ar*H*), 7.67 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.47 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.34 (t, *J* = 7.0 Hz, 2H, Ar*H*), 7.28 (t, *J* = 7.0 Hz, 1H, Ar*H*), 7.06 (s, 1H, *imidazole*), 6.95 (s, 1H, *imidazole*), 6.91--6.88 (m, 4H, Ar*H*), 6.66 (dd, *J* = 9.0 Hz, 2.5 Hz, 1H, Ar*H*), 5.01 (dd, *J* = 11 Hz, 3.5 Hz, 1H, COC*H*), 3.91 (t, *J* = 6.5 Hz, 2H, OC*H*$_2$CH$_2$), 3.84 (s, 3H, NC*H*$_3$), 3.83 (s, 3H, OC*H*$_3$), 3.76 (s, 3H, OC*H*$_3$), 3.45 (d, *J* = 4.0 Hz, 2H, COC*H*$_2$), 2.41-2.34 (m, 1H, CHC*H*$_2$), 2.28 (s, 3H, ArC*H*$_3$), 2.07-2.03 (m, 1H, CHC*H*$_2$); minor : δ 8.05 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.75 (d, *J* = 6.5 Hz, 2H, Ar*H*), 7.65 (d, *J* = 8.5 Hz, 2H, Ar*H*), 7.45 (d, *J* = 7.5 Hz, 2H, Ar*H*), 7.37-7.30 (m, 3H, Ar*H*), 7.10 (s, 1H, *imidazole*), 7.00-6.97 (m, 3H, Ar*H*), 6.87-6.85 (m, 3H, *imidazole*, Ar*H*), 6.64 (dd, *J* = 9.0 Hz, 2.5 Hz, 1H, Ar*H*), 4.89 (dd, *J* = 7.0 Hz, 4.5 Hz, 1H, COC*H*), 4.14-4.04 (m, 2H, OC*H*$_2$CH$_2$), 3.90 (s, 3H, NC*H*$_3$), 3.88 (s, 3H, OC*H*$_3$), 3.79 (s, 3H, OC*H*$_3$), 3.42 (d, *J* = 4.0 Hz, 2H,

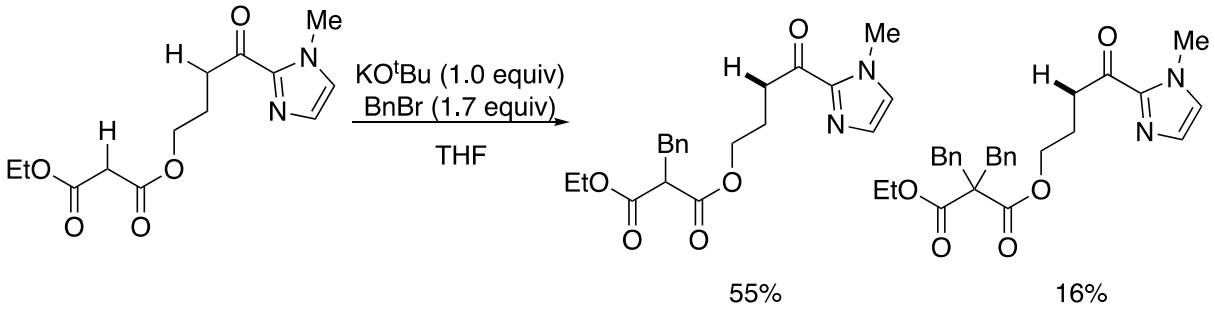
COC*H*$_2$), 2.46-2.39 (m, 1H, CHC*H*$_2$), 2.29-2.22 (m, 4H, ArC*H*$_3$, CHC*H*$_2$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 191.9, 177.1, 170.3, 168.3, 163.2, 160.5, 156.1, 143.3, 139.2, 135.9, 135.8, 134.0, 131.2, 130.8, 130.7, 130.0, 129.8, 129.1, 128.6, 128.5, 127.8, 126.9, 118.1, 114.9, 114.0, 112.5, 111.9, 101.2, 74.9, 62.7, 55.8, 55.5, 53.5, 36.1, 30.0, 26.7, 13.3; minor : δ191.9, 178.8, 170.4, 168.3, 163.2, 160.5, 156.0, 142.5, 139.2, 137.7, 135.9, 133.9, 131.2, 130.7, 130.7, 130.1, 129.6, 129.1, 128.7, 128.6, 127.6, 126.5, 118.5, 114.9, 114.2, 112.5, 111.8, 101.1, 74.1, 63.0, 55.7, 55.5, 53.1, 36.3, 29.9, 27.8, 13.4; IR (neat) 2361, 1809, 1712, 1668, 1647, 1607, 1510, 1431, 1408, 1323, 1292, 1256, 1171, 1092, 1045, 1013, 991, 908, 889, 841, 727, 702, 648 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{43}H_{38}ClN_4O_8$ $(M + H)^+$ 773.2373, found773.2220.



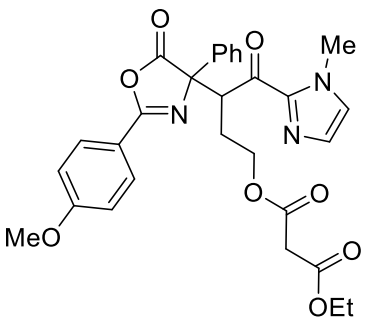
3-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl 2-(3-cyano-4-isobutoxyphenyl)-5-methylthiazole-4-carboxylate (3ar): (white solid, *n*-Hexane/Acetone = 9/1 to 4/1, 69% yield, 97.8 mg, dr = 84/16); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 8.13 (d, *J* = 2.5 Hz, 1H, Ar*H*), 8.05 (dd, *J* = 7.0 Hz, 2.0 Hz, 1H, Ar*H*), 7.88 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.83 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.39 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.32 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.08 (s, 1H, *imidazole*), 7.01 (d, *J* = 9.0 Hz, 1H, Ar*H*), 6.91-6.89 (m, 3H, Ar*H*, *imidazole*), 5.07 (dd, *J* = 11 Hz, 8.5 Hz, 1H, COC*H*), 4.19-4.10 (m, 2H, ArOC*H*$_2$), 3.90 (d, *J* = 6.5 Hz, 2H, CO_2CH_2), 3.84 (s, 3H, NC*H*$_3$), 3.71 (s, 3H, OC*H*$_3$), 2.64 (s, 3H, ArC*H*$_3$), 2.54-2.47 (m, 1H, COCHC*H*$_2$), 2.24-2.15 (m, 2H, COCHC*H*$_2$, C*H*$(CH_3)_2$), 1.10 (d, *J* = 6.5 Hz, 6H, CH(C*H*$_3$)$_2$); minor : δ 8.13 (d, *J* = 2.0 Hz, 1H, Ar*H*), 8.09 (d, *J* = 9.0 Hz, 2H, Ar*H*), 8.05 (dd, *J* = 9.0 Hz, 2.5 Hz, 1H, Ar*H*), 7.80 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.38 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.32 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.11 (s, 1H, *imidazole*), 7.03-7.00 (m, 3H, Ar*H*), 6.97 (s, 1H, *imidazole*), 4.95 (dd, *J* = 6.5 Hz, 5.0 Hz, 1H, COC*H*), 4.33-4.24 (m, 2H, ArOC*H*$_2$),

3.91-3.89 (m, 5H, CO_2CH_2, NCH_3), 3.85 (s, 3H, OCH_3), 2.65 (s, 3H, $ArCH_3$), 2.57-2.51 (m, 1H, $COCHCH_2$), 2.42-2.17 (m, 1H, $COCHCH_2$), 2.21 (seq, *J* = 6.5 Hz, 1H, $CH(CH_3)_2$), 1.09 (d, *J* = 6.5 Hz, 6H, $CH(CH_3)_2$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 191.8, 177.0, 167.0, 163.2, 162.5, 161.3, 161.1, 160.5, 143.2, 136.0, 132.4, 132.0, 130.0, 129.9, 128.7, 128.5, 127.7, 126.9, 126.0, 121.6, 118.1, 115.4, 114.0, 112.7, 103.0, 75.7, 75.0, 63.2, 55.5, 54.0, 36.0, 28.2, 26.8, 19.1, 17.4; minor : δ 191.8, 178.8, 167.0, 163.3, 162.5, 161.5, 161.0, 160.5, 142.6, 137.7, 132.4, 132.0, 130.1, 129.7, 128.7, 128.6, 127.4, 126.5, 126.0, 121.7, 118.6, 115.4, 114.2, 112.6, 103.0, 75.7, 74.2, 63.4, 55.5, 53.2, 36.2, 28.2, 27.9, 19.1, 17.4; IR (neat) 1809, 1734, 1668, 1647, 1607, 1512, 1477, 1406, 1319, 1258, 1223, 1169, 1088, 1067, 1030, 1015, 908, 839, 727, 702 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{40}H_{38}N_5O_7S$ $(M + H)^+$ 732.2486, found732.2365.

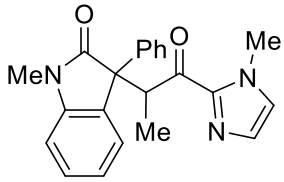
Benzylation of 2s using KO^{t}Bu and Benzyl bromide



To a solution of ethyl (4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl) malonate (**2s**) (1.0 equiv.) in dry THF (0.20 M) under argon atmosphere was added potassium *tert*-butoxide (1.0 equiv.) in dry THF (0.20 M) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 2 h, the mixture was again cooled to 0 °C and benzyl bromide (1.7 equiv.) was added. The cooling bath was removed and the reaction mixture was stirred for 1 h at room temperature. After removal of solvent under reduced pressure, the residue was purified by silica gel flash chromatography.

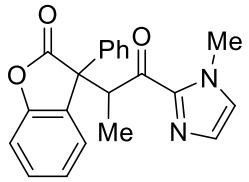


Ethyl(3-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutyl) malonate (3as): (White solid, *n*-Hexane/Acetone = 9/1 to 4/1, 74% yield, 81.0 mg, dr = 83/17); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.89 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.80 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.39 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.33 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.15 (s, 1H, *imidazole*), 7.00 (s, 1H, *imidazole*), 6.91 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.97 (dd, *J* = 10 Hz, 2.5 Hz, 1H, COC*H*), 4.15 (q, *J* = 7.0 Hz, 2H, OC*H*$_2$CH$_3$), 3.99-3.90 (m, 2H, OC*H*$_2$CH$_2$), 3.84 (s, 3H, NC*H*$_3$), 3.80 (s, 3H, OC*H*$_3$), 3.14 (s, 2H, COC*H*$_2$CO), 2.39-2.32 (m, 1H, CHC*H*$_2$), 2.10-2.04 (m, 1H, CHC*H*$_2$), 1.24 (t, *J* = 7.0 Hz, 3H, OCH$_2$C*H*$_3$); minor : δ 8.08 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.77 (d, *J* = 7.0 Hz, 2H, *Ph*), 7.38 (t, *J* = 7.0 Hz, 2H, *Ph*), 7.34 (t, *J* = 7.0 Hz, 1H, *Ph*), 7.15 (s, 1H, *imidazole*), 7.05-7.00 (m, 3H, *imidazole*, Ar*H*), 4.83 (dd, *J* = 6.5 Hz, 4.5 Hz, 1H, COC*H*), 4.22-4.08 (m, 4H, OC*H*$_2$CH$_3$, OC*H*$_2$CH$_2$), 3.91 (s, 3H, NC*H*$_3$), 3.90 (s, 3H, OC*H*$_3$), 3.12 (d, *J* = 2.0 Hz, 2H, COC*H*$_2$CO), 2.50-2.43 (m, 1H, CHC*H*$_2$), 2.27-2.20 (m, 1H, CHC*H*$_2$), 1.23 (t, *J* = 7.0 Hz, 3H, OCH$_2$C*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) major : δ 191.7, 177.1, 166.4, 166.2, 163.1, 160.5, 143.0, 135.9, 130.1, 129.9, 128.7, 128.5, 127.9, 126.9, 118.1, 114.0, 74.7, 63.3, 61.5, 55.5, 53.6, 41.3, 36.2, 26.5, 14.1; minor : δ 191.7, 178.9, 166.4, 166.2, 163.2, 160.5, 142.3, 137.7, 130.1, 129.6, 128.7, 128.6, 127.5, 126.5, 118.6, 114.2, 74.0, 63.5, 61.4, 55.5, 53.2, 41.3, 36.2, 27.6, 14.0; IR (neat) 1811, 1749, 1730, 1667, 1647, 1607, 1512, 1406, 1325, 1256, 1171, 1150, 1028, 912, 889, 841, 731, 702, 648, 604, 563 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{29}H_{30}N_3O_8$ $(M + H)^+$ 548.2027, found 548.1988.



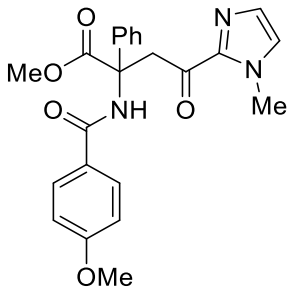
1-methyl-3-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxopropan-2-yl)-3-phenylindolin-2-one (5ab): (White solid, *n*-Hexane/Acetone = 4/1 to 2/1, 57% yield, 41.0 mg, dr = 68/32); ^{1}H NMR (500 MHz, $CDCl_3$) major : δ 7.58 (d, *J* = 7.5 Hz, 2H, Ar*H*), 7.49 (d, *J* = 7.5 Hz, 1H, Ar*H*), 7.41 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.31-7.23 (m, 3H, Ar*H*), 7.17 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.15 (s, 1H, *imidazole*), 6.95 (d, *J* = 7.5 Hz, 1H, Ar*H*), 6.93 (s, 1H, *imidazole*), 5.13 (q, *J* = 7.5 Hz, 1H, COC*H*), 3.77 (s, 3H, NC*H*$_3$), 3.14 (s, 3H, NC*H*$_3$), 1.52 (d, *J* = 7.5 Hz, 3H, CHC*H*$_3$); minor : δ 7.78 (d, *J* = 7.0 Hz, 1H, Ar*H*), 7.52 (d, *J* = 7.5 Hz, 2H, Ar*H*), 7.26-7.22 (m, 3H, Ar*H*), 7.18-7.14 (m, 2H, Ar*H*, *imidazole*), 7.04 (t, *J* = 7.5 Hz, 1H, Ar*H*), 6.93 (s, 1H, *imidazole*), 6.84 (d, *J* = 8.0 Hz, 1H, Ar*H*), 5.34 (q, *J* = 7.0 Hz, 1H, COC*H*), 3.74 (s, 3H, NC*H*$_3$), 3.29 (s, 3H, NC*H*$_3$), 1.24 (d, *J* = 7.0 Hz, 3H, CHC*H*$_3$);

^{13}C NMR (125 MHz, $CDCl_3$) major : δ 193.2, 178.3, 144.6, 142.0, 138.1, 130.5, 129.1, 128.5, 128.1, 127.7, 127.6, 126.8, 126.4, 121.7, 108.5, 57.1, 50.6, 36.2, 26.5, 14.6; minor : δ 193.5 177.8, 144.0, 142.7, 138.9, 130.8, 129.1, 128.4, 128.4, 128.1, 127.2, 127.1, 126.7, 122.2, 107.9, 57.6, 48.8, 36.0, 26.5, 14.1; IR (KBr) 1692, 1678, 1674, 1611, 1493, 1470, 1404, 1366, 1356, 1157, 1138, 1078, 974, 914, 908, 795, 758, 746, 729, 721, 700, 687, 660, 646, 621, 613, 598, 544, 532, 498, 488 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{22}H_{22}N_3O_2$ $(M + H)^+$ 360.1707, found 360.1707.

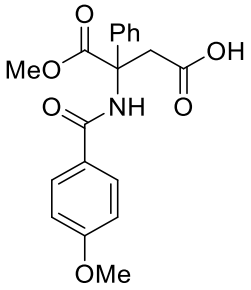


3-(1-(1-methyl-1*H*-imidazol-2-yl)-1-oxopropan-2-yl)-3-phenylbenzofuran-2(3*H*)-one (5bb): (Diastereomixture, White solid, *n*-Hexane/EtOAc = 20/1 to 9/1 to 4/1, 48% yield, 33.3 mg, dr = 51/49); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.5 Hz, 1H, Ar*H*, minor), 7.57-7.53 (m, 5H, *diastereomers*), 7.44 (t, *J* = 7.5 Hz, 1H, Ar*H*, minor), 7.35-7.23 (m, 9H, *diastereomers*), 7.16-7.15 (m, 2H, *diastereomers*), 7.13-7.07 (m, 2H, *diastereomers*), 6.98-6.97 (m, 2H, *diastereomers*), 5.24 (q, *J* = 7.5 Hz, 1H, COC*H*, major), 5.02 (q, *J* = 7.5 Hz, 1H, COC*H*, minor), 3.83 (s, 3H, NCH_3, minor), 3.78 (s, 3H, NCH_3, major), 1.59 (d, *J* = 7.5 Hz, 3H, CHCH_3, minor), 1.37 (d, *J* = 7.5 Hz, 3H, CHCH_3, major); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.8, 192.5, 178.0, 176.9, 154.0, 153.2, 141.9, 141.6, 137.4, 136.7, 130.3, 129.4, 129.3, 128.9, 128.9, 128.8, 128.8, 128.8, 128.2, 127.7, 127.6, 127.5, 127.2, 126.8, 126.6, 125.5, 124.0, 123.5, 111.1, 110.7, 56.1, 56.0, 52.6, 50.3, 36.3, 36.1, 14.3, 14.2; IR (KBr) 1794, 1670, 1618, 1497, 1476, 1460, 1402, 1369, 1288, 1233, 1155, 1138, 1115, 1063, 1036, 1020, 974, 908, 872, 775, 754, 731, 696, 669, 658, 646, 638, 629, 619, 592, 575, 525, 498, 488, 449 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{21}H_{19}N_2O_3$ $(M + H)^+$347.1390, found 347.1390.

6. Transformation of the Products

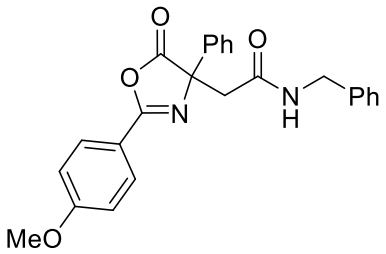


methyl 2-(4-methoxybenzamido)-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxo-2-phenylbutanoate (6aa)[7]: A flame-dried Schlenk equipped with a magnetic stirring bar was filled with argon, and charged with 2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-4-phenyloxazol-5(4H)-one (**3aa**, 0.10 mmol, 1.0 equiv.), (+)-10-camphorsulfonic acid (10 μmol, 0.10 equiv.), MeOH (0.15 mmol, 1.5 equiv.) and dichloromethane (0.50 mL, 0.20 M). The mixture was stirred at room temperature for 24 h, and diluted with EtOAc. Then the diluted solution was washed with sat. $NaHCO_3$ aq and brine. After evaporation of the organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain **6aa**. (White solid, *n*-Hexane/EtOAc = 2/1, 37.0 mg, 88% yield); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.06 (s, 1H, N*H*), 7.80 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.60 (d, *J* = 8.5 Hz, 2H, *Ph*), 7.34 (t, *J* = 8.5 Hz, 2H, *Ph*), 7.28 (t, *J* = 8.5 Hz, 1H, *Ph*), 7.16 (s, 1H, *imidazole*), 6.99 (s, 1H, *imidazole*), 6.91 (d, *J* = 9.0 Hz, 2H, Ar*H*), 5.20 (d, *J* = 19 Hz, 1H, COCH_2), 4.39 (d, *J* = 19 Hz, 1H, COCH_2), 3.91 (s, 3H, NCH_3), 3.84 (s, 3H, OCH_3), 3.73 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.5, 173.3, 165.1, 162.3, 142.5, 138.5, 129.5, 129.0, 128.6, 128.0, 127.1, 126.9, 126.0, 113.7, 62.5, 55.4, 53.4, 43.3, 36.0; IR (KBr) 3421, 1740, 1674, 1605, 1524, 1489, 1447, 1412, 1296, 1258, 1215, 1180, 1157, 1026, 999, 768 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{23}H_{24}N_3O_5$ $(M + H)^+$ 422.1710, found 422.1710.



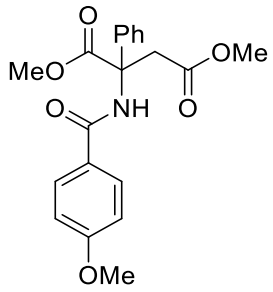
4-methoxy-3-(4-methoxybenzamido)-4-oxo-3-phenylbutanoic acid (7aa)[5,6]: A flame-dried Schlenk equipped with a magnetic stirring bar was filled with argon, and charged with methyl 2-(4-methoxybenzamido)-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxo-2-phenylbutanoate (**6aa**, 0.20 mmol, 1.0

equiv.), activated MS4A (100.0 mg) and CH_3CN (2.0 mL, 0.10 M). The suspension was stirred for 2h and then methyl trifluoromethanesulfonate (0.30 mmol, 1.5 equiv.) was added. After stirring for 0.5 h, H_2O (20 mmol, 100 equiv.) and DBU (0.30 mmol, 1.5 equiv.) were added. After stirring for 1 h, the mixture was filtrated through a short plug of Celite. After evaporation of the organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain **7aa**. (White solid, *n*-Hexane/EtOAc/AcOH = 16/4/1, 49.0 mg, 68% yield); ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.36 (s, 1H, N*H*), 7.82 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.53 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.37 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.31 (t, *J* = 7.5 Hz, 1H, *Ph*), 7.03 (d, *J* = 9.0 Hz, 2H, Ar*H*), 3.83 (s, 3H, OCH_3), 3.71 (d, *J* = 17 Hz, 1H, COCH_2), 3.62-3,59 (m, 4H, COCH_2, OCH_3); ^{13}C NMR (125 MHz, DMSO-d_6) δ 172.3, 171.9, 165.4, 162.4, 138.9, 129.6, 128.8, 128.2, 126.6, 126.5, 114.2, 63.1, 55.9, 53.4, 39.1; IR (KBr) 3403, 3017, 2963, 2920, 2839, 1740, 1609, 1574, 1535, 1501, 1439, 1331, 1308, 1258, 1242, 1200, 1165, 1134, 1069, 1030, 899, 853, 768, 729, 702cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{19}H_{20}NO_6$ $(M + H)^+$ 358.1285, found 358.1285.



***N*-benzyl-2-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)acetamide (8aa)**[5,6]: To a solution of 4-methoxy-3-(4-methoxybenzamido)-4-oxo-3-phenylbutanoic acid (**7aa**, 0.10 mmol, 1.0 equiv.) in THF (2.5 mL, 0.040 M) under argon atmosphere was added benzylamine (0.18 mmol, 1.8 equiv.), 1-hydroxybenzotriazole monohydrate (0.12 mmol, 1.2 equiv.) and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (0.18 mmol, 1.8 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 20 h, the reaction mixture was added EtOAc and, the mixture washed with 1 N HCl aq, sat. $NaHCO_3$ aq and brine. The combined organic layers were dried over Na_2SO_4 and filtered. After evaporation of the organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain **8aa**. (White solid, *n*-Hexane/EtOAc =2/1, 24.0 mg, 57% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.42-7.37 (m, 5H, *Ph*), 7.34-7.25 (m, 5H, *Ph*), 6.93 (d, *J* = 9.0 Hz, 2H, Ar*H*), 6.71 (s, 1H, N*H*), 4.83 (d, *J* = 14 Hz, 1H, COCH_2), 4.76 (d, *J* = 14 Hz, 1H, COCH_2), 3.85 (s, 3H, OCH_3), 3.67 (d, *J* = 18 Hz, 1H, PhCH_2), 3.38 (d, *J* = 18 Hz, 1H, PhCH_2); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.0, 173.7, 166.7, 162.9, 138.0, 135.4, 129.6, 129.3, 129.1, 128.6, 128.2, 127.8, 125.6, 124.9, 113.9, 63.0, 55.5, 42.8, 42.5; IR (KBr) 1709, 1632, 1497,

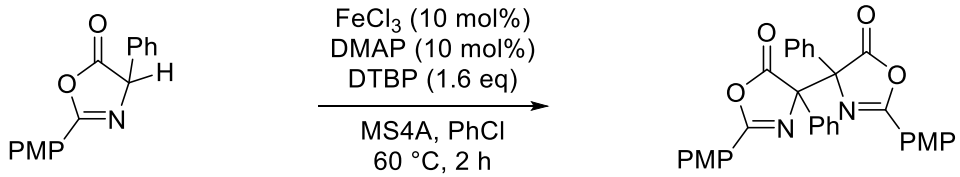
1397, 1258, 1177 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{25}H_{23}N_2O_4$ $(M + H)^+$ 415.1652, found 415.1652.



dimethyl 2-(4-methoxybenzamido)-2-phenylsuccinate (9aa)[5,6]: A flame-dried Schlenk equipped with a magnetic stirring bar was filled with argon, and charged with 2-(4-methoxyphenyl)-4-(2-(1-methyl-1*H*-imidazol-2-yl)-2-oxoethyl)-4-phenyloxazol-5(4*H*)-one (**3aa**, 0.10 mmol, 1.0 equiv.), activated MS4A (50.0 mg) and CH_3CN (1.0 mL, 1.0 M). The suspension was stirred for 2h and then methyl trifluoromethanesulfonate (0.15 mmol, 1.5 equiv.) was added. After stirring for 0.5 h, MeOH (1.0 mmol, 10 equiv.) and DBU (0.3 mmol, 3.0 equiv.) were added. After stirring for 1h, the mixture was filtrated through a short plug of Celite. After evaporation of the organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain **9aa**. (White solid, *n*-Hexane/EtOAc = 2/1, 33.0 mg, 89% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 1H, N*H*), 7.80 (d, *J* = 9.0 Hz, 2H, Ar*H*), 7.47 (d, *J* = 7.5 Hz, 2H, *Ph*), 7.35 (t, *J* = 7.5 Hz, 2H, *Ph*), 7.30 (t, *J* = 7.5 Hz, 1H, *Ph*), 6.93 (d, *J* = 9.0 Hz, 2H, Ar*H*), 4.21 (d, *J* = 17 Hz, 1H, COCH_2), 3.85 (s, 3H, OCH_3), 3.75 (s, 3H, OCH_3), 3.73 (d, *J* = 17 Hz, 1H, COCH_2), 3.64 (s, 3H, OCH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.6, 171.4, 165.4, 162.4, 138.1, 129.0, 128.8, 128.2, 126.5, 125.6, 113.8, 62.9, 55.5, 53.4, 51.9, 38.1; IR (KBr) 3421, 2955, 1740, 1659, 1605, 1578, 1524, 1489, 1439, 1343, 1300, 1258, 1238, 1184, 1157, 1107, 1069, 1030, 976, 895, 852, 802, 768, 729 cm^{-1}; HRMS (ESI, H) *m/z* calc'd for $C_{20}H_{22}NO_6$ $(M + H)^+$ 372.1442, found 372.1442.

7.Mechanistic Study

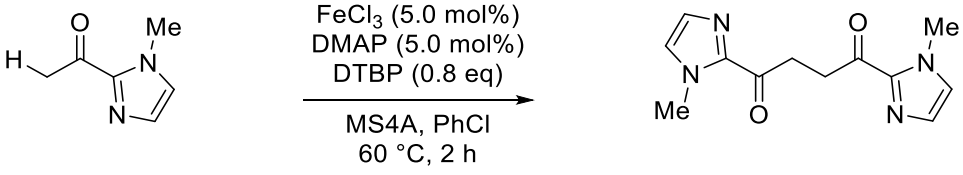
Homo-Coupling Dimer Formation (Scheme 6)



1a **10a**: 96% yield

A 20 mL shlenk flask equipped with a magnetic stirring bar and 3-way glass stopcock was charged with 4A crushed molecular sieves (MA 4A 100.0 mg) and flamed-dried under vacumm. After cooling down to room temperature, azlactone **1a** (0.10 mmol, 1.0 equiv.), $FeCl_3$ (10 μmol, 10 mol%), DMAP (10 μmol, 10 mol%) were added followed by the addition of chlorobenzene (0.20 mL, 0.50 M). Then DTBP (30 μL, 1.6 equiv.) was added to the reaction mixture. The mixture was stirred under Ar at 60 °C for 2 h and diluted with EtOAc. The diluted solution was filtered through silica short column and washed with EtOAc. After evaporation of the organic solvent under reduced pressure, the resultant mixture was purified by silica gel flash chromatography to obtain homo-coupling dimer (**10a**).

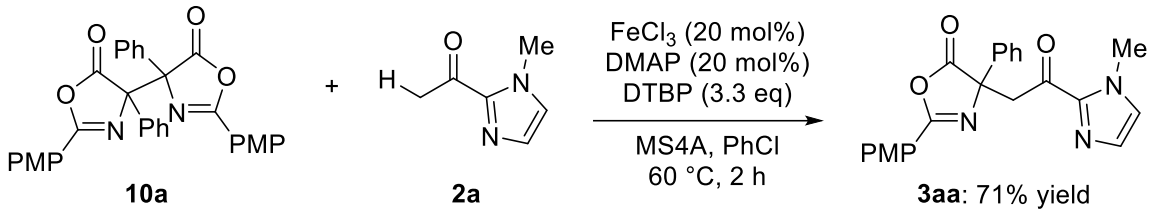
2,2'-bis(4-methoxyphenyl)-4,4'-diphenyl-[4,4'-bioxazole]-5,5'(4*H*,4'*H*)-dione (10a): CAS Registry Number 99553-83-0; (Diastereomixture dr = 3/1, Brown solid, *n*-Hexane/EtOAc = 4/1, 51.0 mg, 96% yield); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 9.0 Hz, 4H, Ar*H*, minor), 7.83 (d, *J* = 9.0 Hz, 4H, Ar*H*, major), 7.69 (d, *J* = 7.0 Hz, 4H, *Ph*, minor), 7.44 (d, *J* = 7.5 Hz, 4H, *Ph*, major), 7.35-7.22 (m, 12H, *diastereomers*), 6.95 (d, *J* = 9.0 Hz, 4H, Ar*H*, minor), 6.84 (d, *J* = 9.0 Hz, 4H, Ar*H*, major), 3.87 (s, 6H, OC*H*$_3$, minor), 3.81 (s, 6H, OC*H*$_3$, major); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.2, 173.6, 163.45, 163.37, 162.1, 161.1, 132.0, 131.3, 130.2, 130.0, 128.97, 128.92, 128.7, 128.5, 128.2, 127.5, 127.3, 117.8, 117.5, 114.14, 114.07, 55.5, 55.4.



2a **11a**: not detected

A 20 mL shlenk flask equipped with a magnetic stirring bar and 3-way glass stopcock was charged with 4A crushed molecular sieves (MA 4A 100.0 mg) and flamed-dried under vacumm. After cooling down to

room temperature, $FeCl_3$ (10 µmol, 5 mol%), DMAP (10 µmol, 5 mol%) were added followed by the addition of chlorobenzene (0.20 mL, 1.0 M) and acylimidazole **2a** (0.20 mmol. 1.0 equiv). Then DTBP (30 µL, 0.8 equiv.) was added to the reaction mixture. The mixture was stirred under Ar at 60 °C for 2 h and diluted with EtOAc. The diluted solution was filtered through silica short column and washed with EtOAc. After evaporation of the organic solvent under reduced pressure, TLC and ^{1}H-NMR analysis were conducted. However, no homo-coupling dimer (**11a**) was detected.

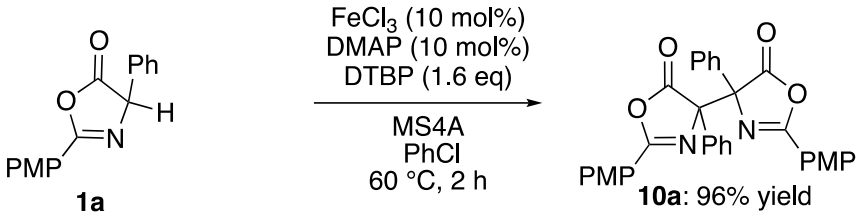


10a **2a** **3aa**: 71% yield

A 20 mL shlenk flask equipped with a magnetic stirring bar and 3-way glass stopcock was charged with 4A crushed molecular sieves (MA 4A 100.0 mg) and flamed-dried under vacumm. After cooling down to room temperature, homo-coupling dimer (**10a**) (0.050 mmol, 1.0 equiv.), $FeCl_3$ (10 µmol, 20 mol%), DMAP (10 µmol, 20 mol%) were added followed by the addition of chlorobenzene (0.20 mL, 0.25 M) and acylimidazole (0.20 mmol, 4.0 equiv.). Then DTBP (30 µL, 3.3 equiv.) was added to the reaction mixture. The mixture was stirred under Ar at 60 °C for 2 h and diluted with EtOAc. The diluted solution was filtered through silica short column and washed with EtOAc. After evaporation of the organic solvent under reduced pressure, yield of **3aa** was determined by ^{1}H NMR analysis using 1,2,4,5-tetramethylbenzene as an internal standard.

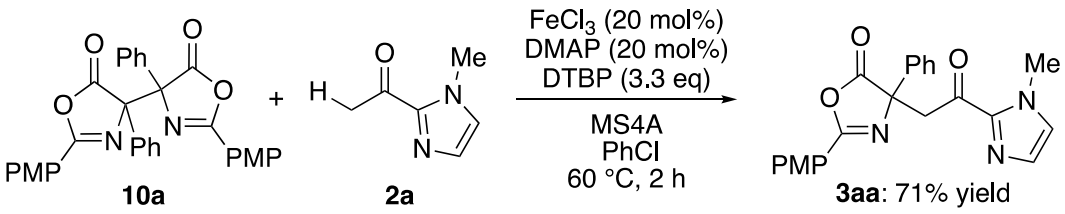
Control Experiments

We performed a series of control experiments to gain preliminary mechanistic insight. In the absence of DTBP, coupling product **10a** was obtained in only an equimolar amount of the catalyst. On the other hand, 100 mol% of $FeCl_3$ and DMAP delivered **10a** in quantitative yield, suggesting that $FeCl_3$/DMAP catalyzes the formation of **10a** and DTBP serves as an oxidant of the iron catalyst for the participation in the catalytic cycle. When $FeCl_3$ and DMAP were omitted, **10a** was not produced. A similar tendency was observed in the control experiments using **10a** with **2a**.



1a **10a**: 96% yield

without DTBP:	10% yield
100 mol% $FeCl_3$/DMAP, without DTBP:	99% yield
without $FeCl_3$/DMAP:	trace

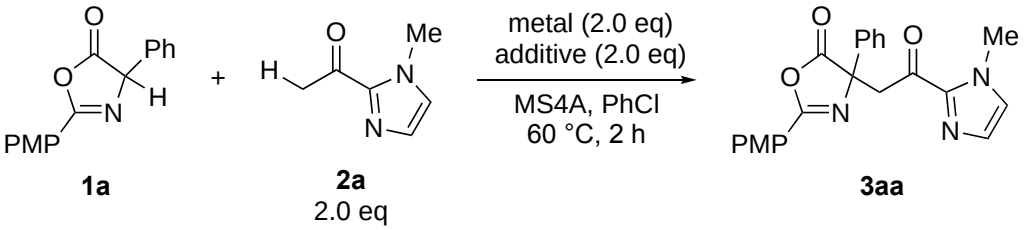


10a **2a** **3aa**: 71% yield

without DTBP:	17% yield
200 mol% $FeCl_3$/DMAP, without DTBP:	55% yield
without $FeCl_3$/DMAP:	Not detected

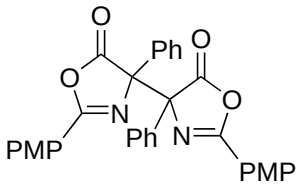
8. Full Optimization Study

Table S1. Initial Study using Stoichiometric Amount of Metal



1a **2a** 2.0 eq **3aa**

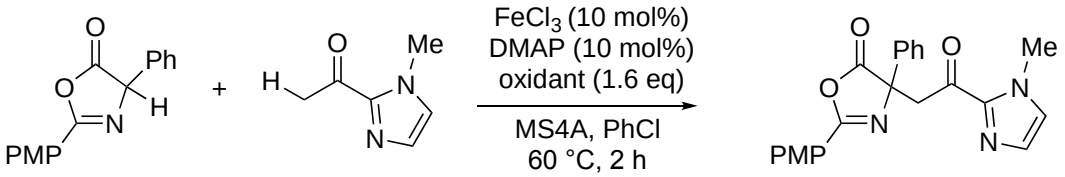
entry[a]	metal	additive	**3aa**	**4aa**
1	$CuCl_2$	none	N.D.	88%
2	CuCl	none	N.D.	46%
3	$FeCl_3$	none	3%	71%
4	$FeCl_2$	none	N.D.	43%
5	$FeCl_3$	DMAP	43%	27%
6	$FeCl_3$	PPh_3	N.D.	78%



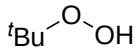
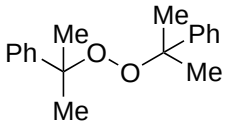
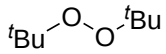
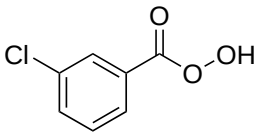
4aa

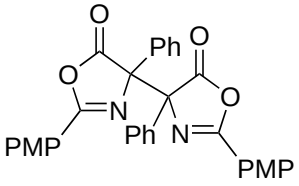
[a]Determined by ^1H NMR analysis and intertnal standard substance 1,2,4,5-tetramethylbenzene.
PMP = *p*-methoxyphenyl, N.D. = not detected.

Table S2. Screening of Oxidant

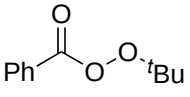


1a **2a** 3.0 eq **3aa**

entry[a]	oxidant	**3aa**	**4aa**
1	 TBHP	9%	— [b]
2	 DCP	19%	56%
3	 DTBP	72%	N.D.
4	 *m*CPBA	N.D.	60%

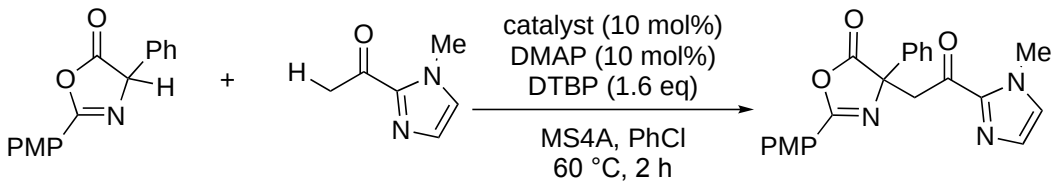


4aa

entry[a]	oxidant	**3aa**	**4aa**
5	 TBPB	N.D.	— [b]
6	O_2	N.D.	— [b]
7	H_2O_2	N.D.	59%

[a]Determined by ^{1}H NMR analysis and intertnal standard substance 1,2,4,5-tetramethylbenzene.
[b]Yield could not be calculated.

Table S3. Screening of Catalyst

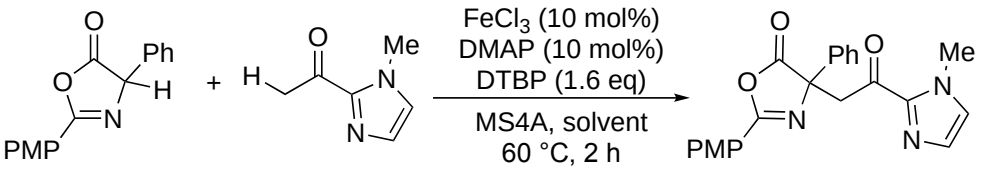


1a **2a** 3.0 eq **3aa**

entry[a]	catalyst	**3aa**	**4aa**	entry[a]	catalyst	**3aa**	**4aa**
1	$FeCl_3$	72% 74%[b]	N.D.	8	$Fe(OAc)_2$	N.D.	56%
2[c]	$FeCl_2$	11%	64%	9	$CuCl_2$	N.D.	50%
3[c]	$FeBr_3$	5%	80%	10	CuCl	N.D.	68%
4	$Fe(acac)_3$	2%	—[d]	11	$NiCl_2$	N.D.	—[d]
5	$Fe(acac)_2$	17%	—[d]	12	$Ni(acac)_2$	N.D.	—[d]
6	$Fe(OTf)_3$	12%	75%	13	$Ni(OAc)_2 \cdot 4H_2O$	N.D.	—[d]
7	$Fe(OTf)_2$	13%	48%	14	$CoCl_2$	N.D.	trace

[a]Determined by ^1H NMR analysis and intertnal standard substance 1,2,4,5-tetramethylbenzene. [b]Isolated yield. [c]Determined by ^1H NMR analysis and intertnal standard substance 1,1,2,2-tetrachloroethane. [d]Yield could not be calculated.

Table S4. Screening of Solvent

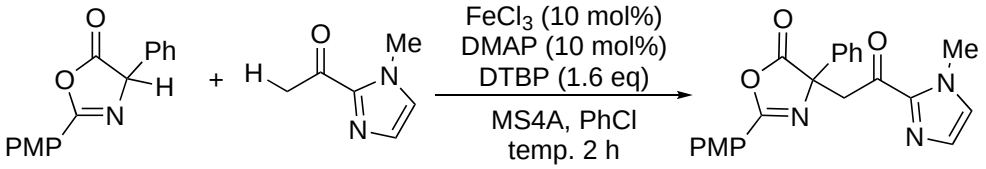


1a **2a** 3.0 eq **3aa**

entry	solvent	**3aa**	**4aa**	entry	solvent	**3aa**	**4aa**
1	toluene	15%	— [b]	5	CH_3CN	26%	48%
2	benzene	60%	20%	6	PhCl	72%	N.D.
3	$C_2H_4Cl_2$	69%	N.D.	7[c]	PhCl	8%	64%
4	THF	19%	40%				

[a]Determined by ^{1}H NMR analysis and intertnal standard substance 1,2,4,5-tetramethylbenzene. [b]Yield could not be calculated. [c]Without MS4A.

Table S5. Screening of Temperature

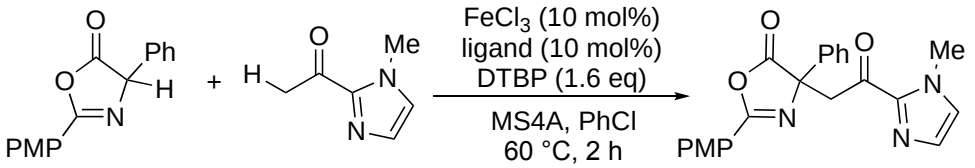


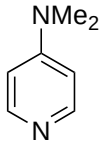
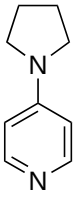
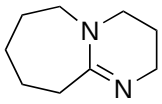
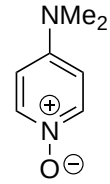
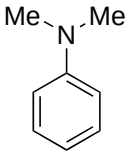
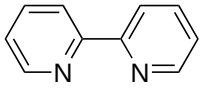
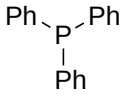
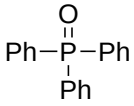
1a **2a** 2.0 eq **3aa**

entry[a]	temp.	**3aa**	**4aa**
1[b]	rt	6%	42%
2	60 °C	72%	N.D.
3	80 °C	70%	N.D.
4	100 °C	59%	N.D.
5	120 °C	41%	N.D.

[a]Determined by ^{1}H NMR analysis and intertnal standard substance1,2,4,5-tetramethylbenzene. [b]Reaction time was 24 h. rt = room temperature.

Table S6. Screening of Ligand



entry[a]	ligand	3aa	4aa
1	 DMAP	72%	N.D.
2	 4-pyrrolidinopyridine	69%	N.D.
3	 pyridine	25%	56%
4	 DBU	28%	— [b]
5	 DMAPO	13%	56%
6	 *N,N*-dimethylaniline	N.D.	60%
7	 2,2'-bipyridine	N.D.	34%
8	 triphenylphosphine	9%	78%
9	 triphenylphosphine oxide	35%	48%

[a]Determined by ^{1}H NMR analysis and intertnal standard substance 1,2,4,5-tetramethylbenzene.
[b]Yield could not be calculated.

9. Determination of the Relative Configuration of the Product

The relative configuration of **3af** was determined by X-ray crystallographic analysis. Suitable crystals were grown by diffusion of *n*-hexane into the methanol solution for **3af**. The crystals were mounted on the CryoLoop with a layer of liquid paraffin and placed in a nitrogen stream at 90 K. All X-ray data were collected on a Bruker AXS APEX II diffractometer with graphite-monochromated MoKα radiation (λ = 0.71073 Å). The reflection data were collected using the program APEX II below 146 K. Molecular structure of **3af** with thermal ellipsoids at 50% probability was shown Figure S6. The crystal data and data collection parameters for **3af** were summarized in Table S4. The relative configuration of the other products was deduced by analogy.

The C-C bond length of **3af** was found to be 1.529(6) Å. On the other hand, the C-C bond length of **10a** was much more longer (1.608(3) Å).[8] These results suggested that cross-coupling product would be more thermodynamically stable than homo-coupling dimer. We also confirmed that no retro-reaction was observed under standard conditions.

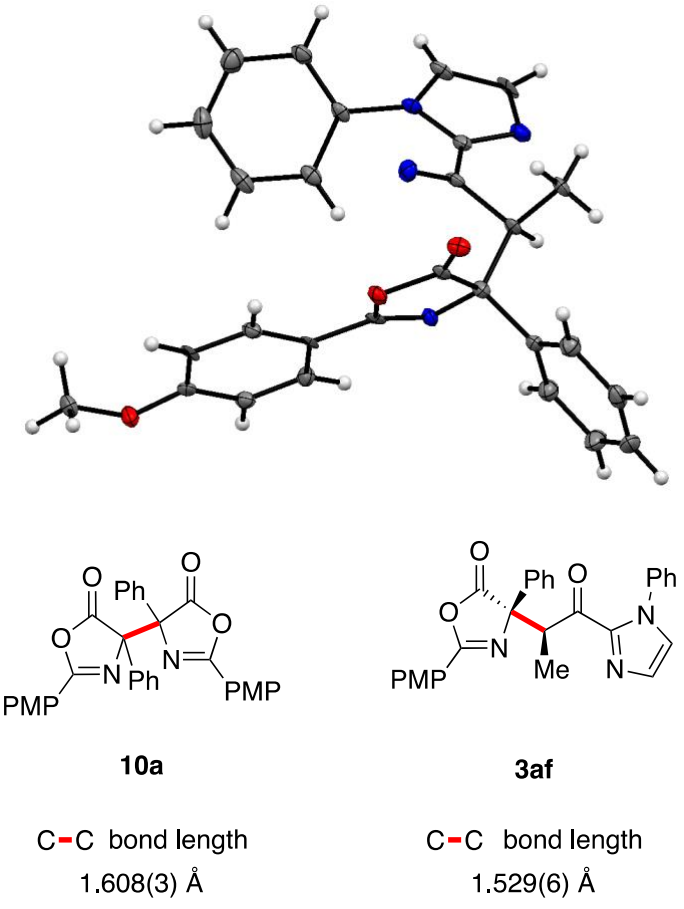


Figure S1. X-ray crystallographic structure of 3af and bond length.

Table S7. Crystal Data and Data Collection Parameters for 3af

empirical formula	$C_{28}H_{23}N_3O_4$
formula weight	465.49
crystal system	monoclinic
space group	P 2_1/n
a, Å	9.7467(14)
b, Å	13.847(2)
c, Å	17.025(3)
α, deg.	90
β, deg.	91.185(2)
γ, deg.	90
V, $Å_3$	2297.25
Z	4
D_{calcd}, g cm_{-3}	1.346
μ [Mo-*K*α], mm^{-1}	0.71073
T, K	90
θ for data collection, deg.	0.869- 0.964
no. of reflections	5176
unique data (R_{int})	0.0227
data / restraints / parameters	5176/0/318
*R*1 (*I*>2.0σ(*I*))	0.0866
w*R*2 (*I*>2.0σ(*I*))	0.2531
*R*1 (all data)	0.0925
w*R*2 (all data)	0.2549
GOF on F^2	1.332
Δρ, e Å-3	0.964-0.869

10. References

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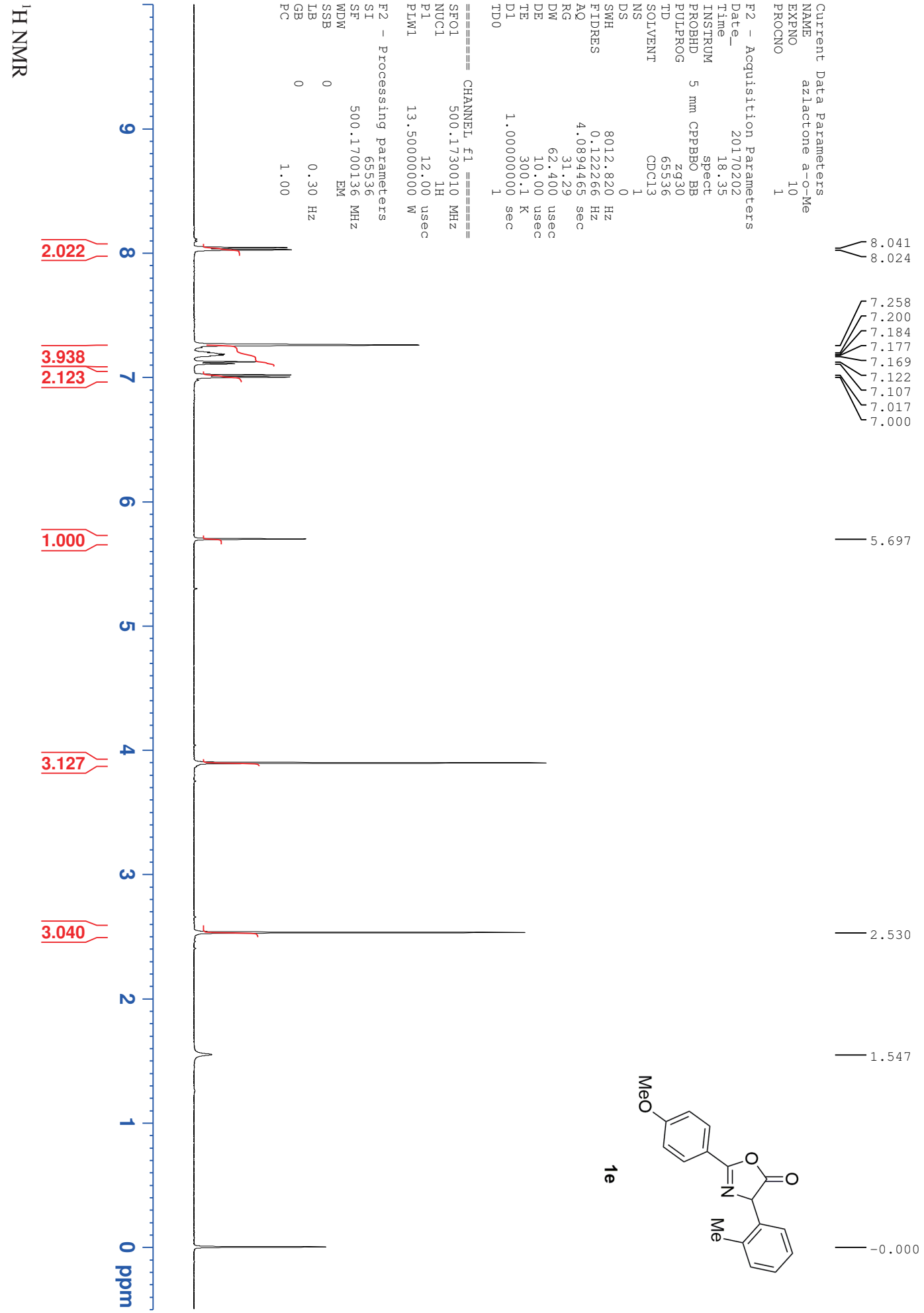
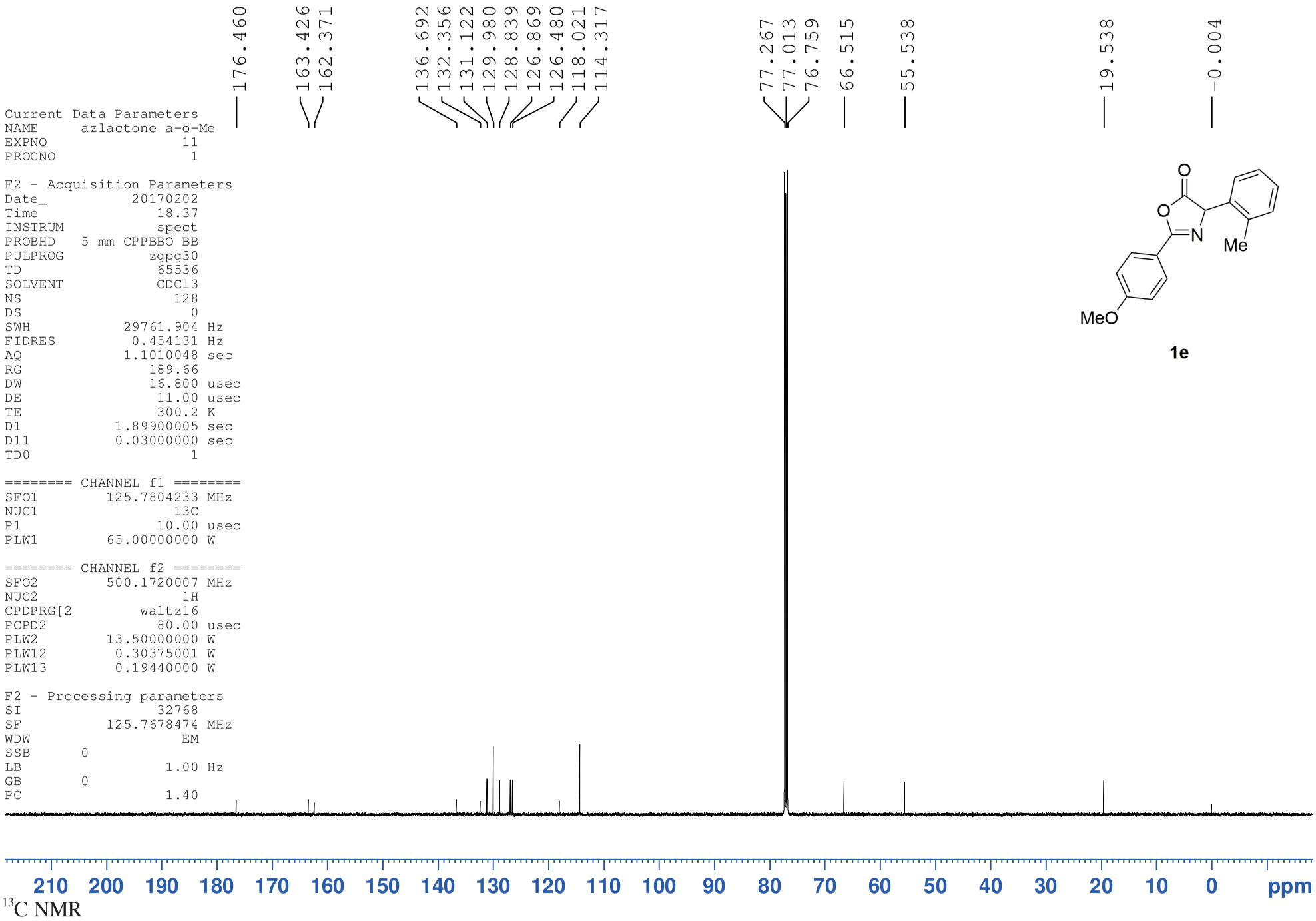
8. Curto, J. M.; Kozlowski, M. C. *J. Am. Chem. Soc*. **2015**, *137*, 18.

11. NMR Spectra of New Compounds

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163.426
162.371
136.692
132.356
131.122
129.980
128.839
126.869
126.480
118.021
114.317
77.267
77.013
76.759
66.515
55.538
19.538
-0.004
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PROCNO 1
F2 - Acquisition Parameters
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678474 MHz
WDW EM
SSB 0
LB 1.00 Hz
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O
N
Me
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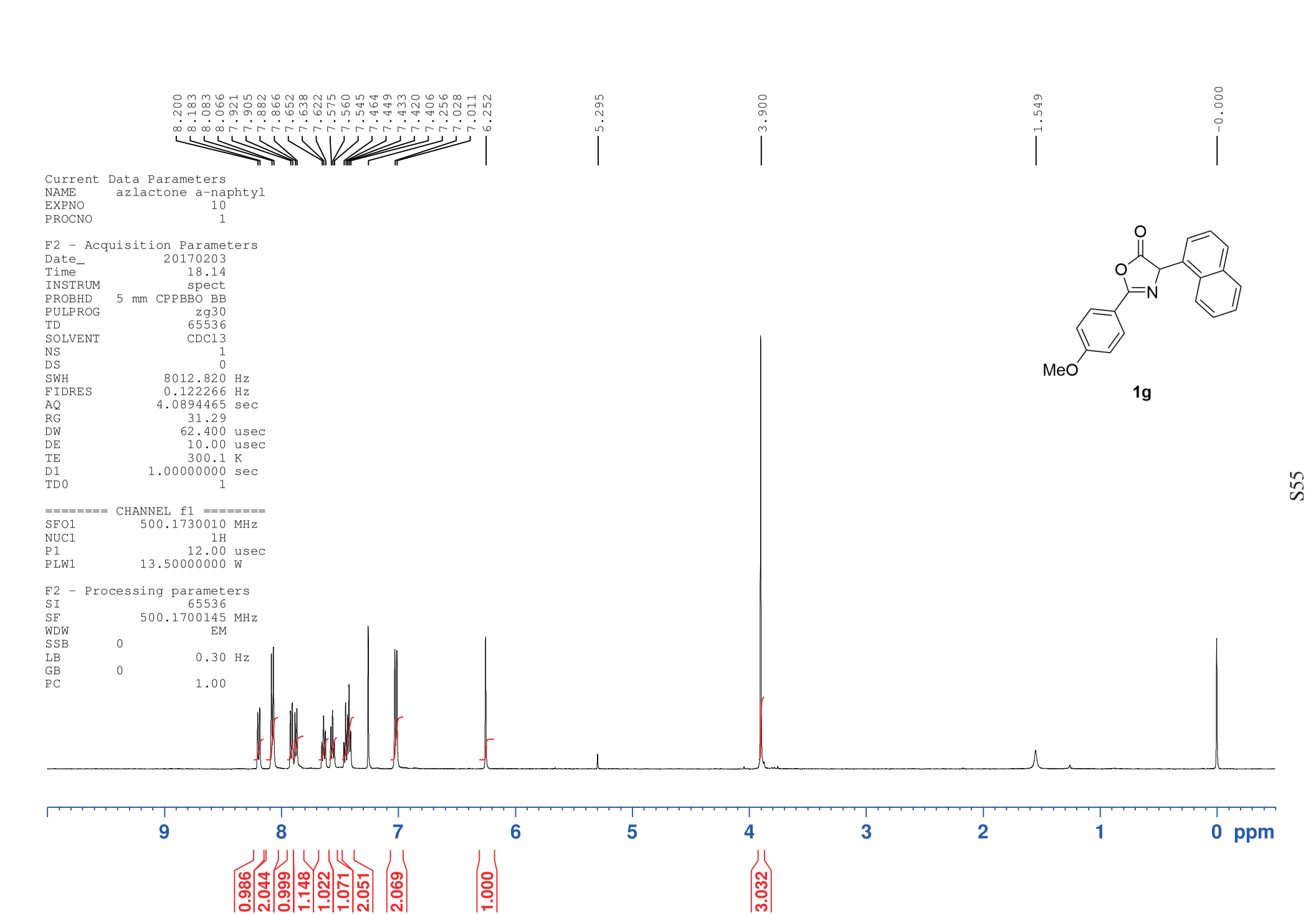
^{13}C NMR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8.183
8.083
8.066
7.921
7.905
7.882
7.866
7.652
7.638
7.622
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7.560
7.545
7.464
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7.420
7.406
7.256
7.028
7.011
6.252
5.295
3.900
1.549
-0.000
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PROCNO 1
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TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
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NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
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SF 500.1700145 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
MeO
1g
9
8
7
6
5
4
3
2
1
0 ppm
0.986
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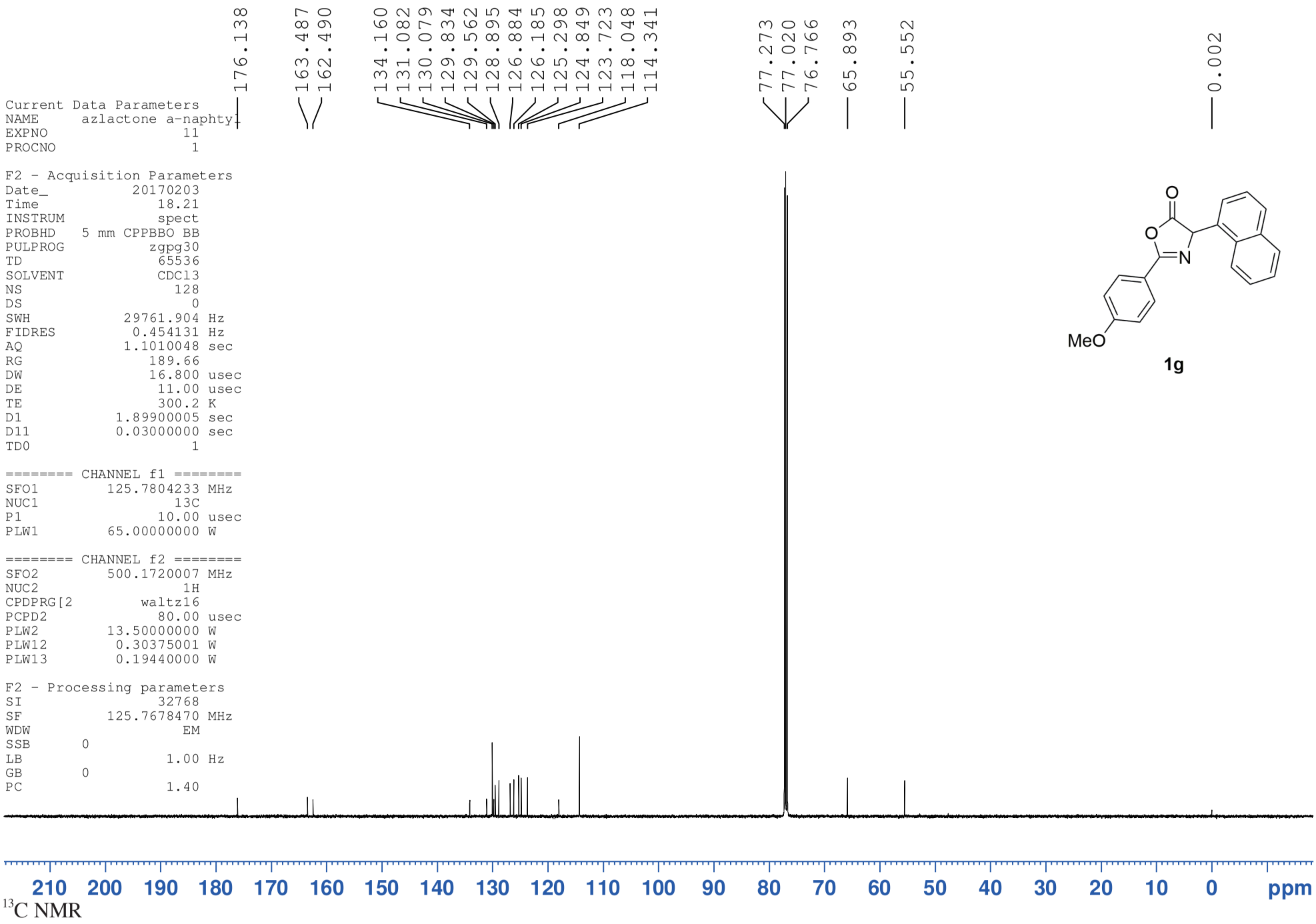
1.022
1.071
2.051
2.069
1.000
3.032

^{1}H NMR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130.079
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129.562
128.895
126.884
126.185
125.298
124.849
123.723
118.048
114.341
77.273
77.020
76.766
65.893
55.552
0.002
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
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NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
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WDW EM
SSB 0
LB 1.00 Hz
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N
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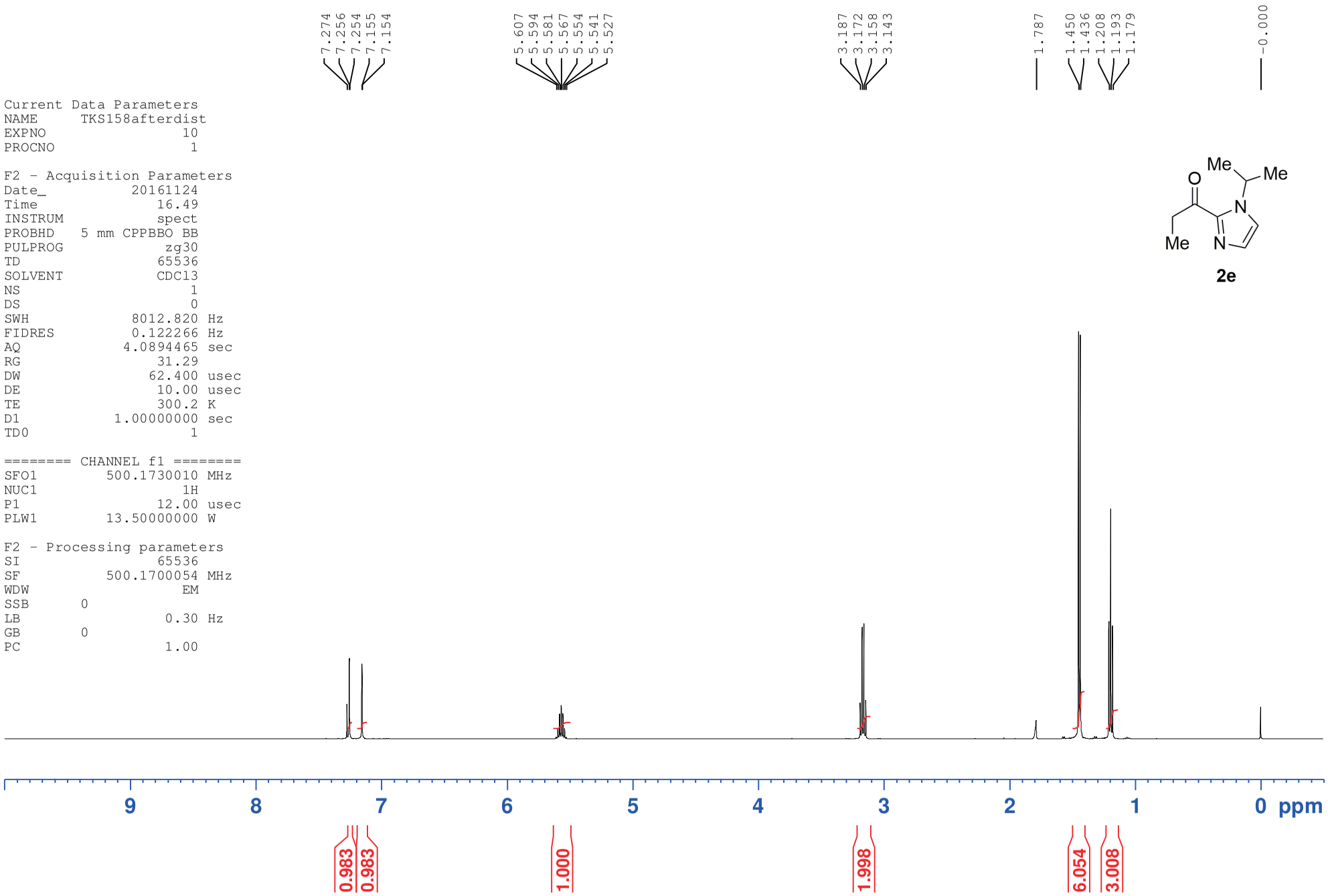
^{13}C NMR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3.187
3.172
3.158
3.143
1.787
1.450
1.436
1.208
1.193
1.179
0.000
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FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
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DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
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Me
O
N
Me
N
2e
9
8
7
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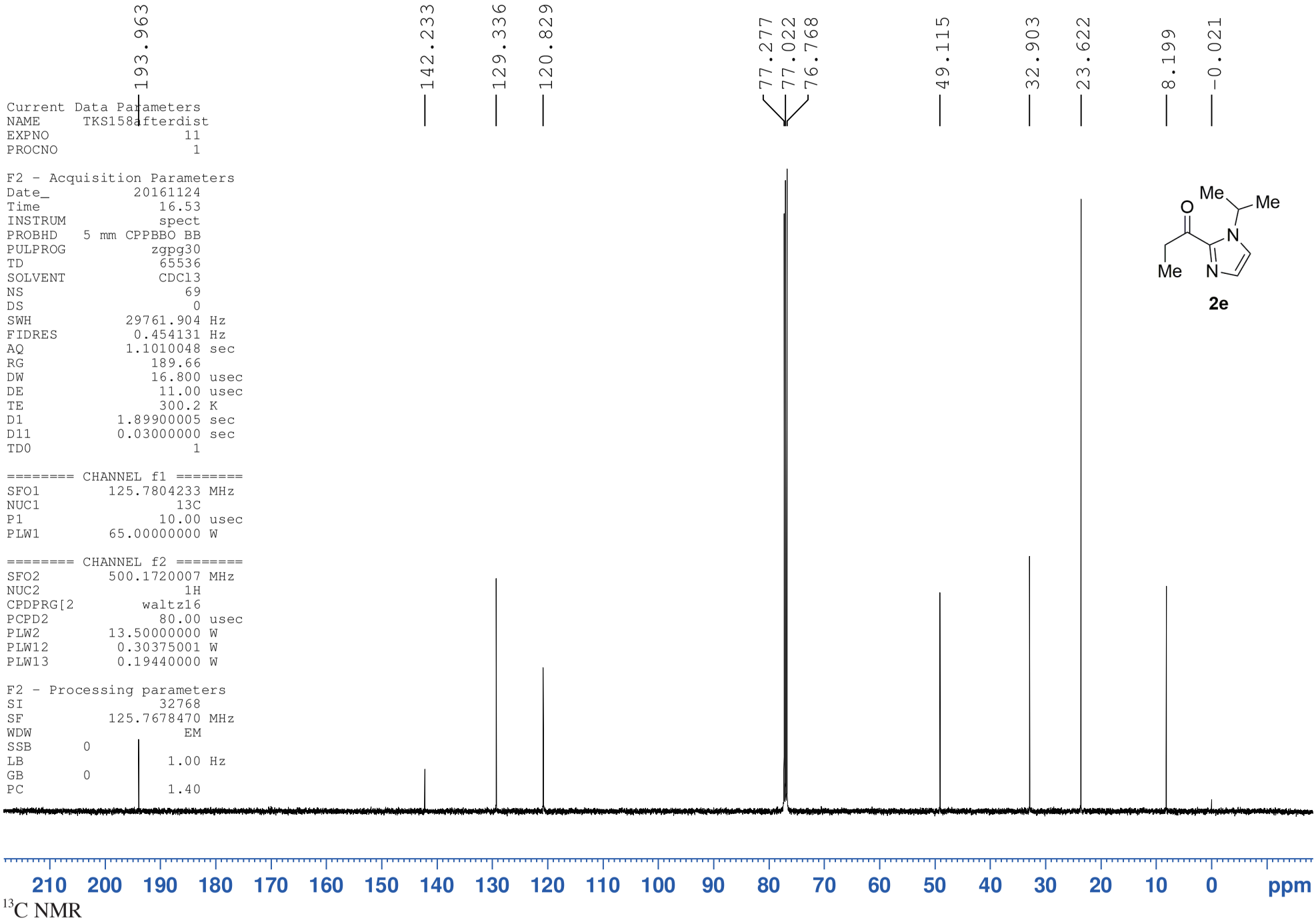
6.054
3.008

^{1}H NMR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PROCNO 1
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FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
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NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
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SSB 0
LB 1.00 Hz
GB 0
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O
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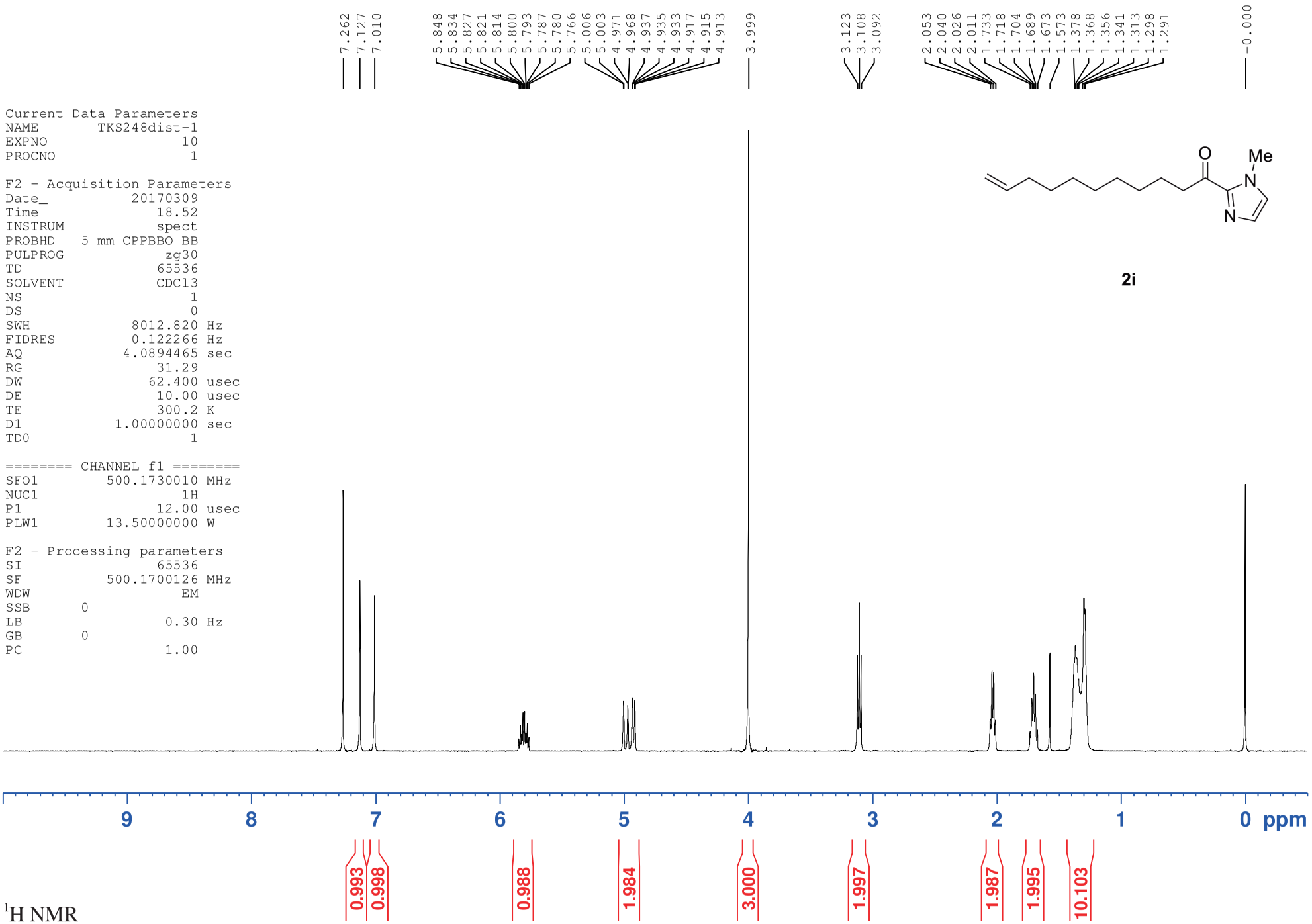
^{13}C NMR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5.780
5.766
5.006
5.003
4.971
4.968
4.937
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4.933
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4.915
4.913
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3.092
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2.026
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1.733
1.718
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1.573
1.378
1.368
1.356
1.341
1.313
1.298
1.291
-0.000
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FIDRES 0.122266 Hz
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RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
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SSB 0
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GB 0
PC 1.00
O
Me
N
N
2i
9
8
7
6
5
4
3
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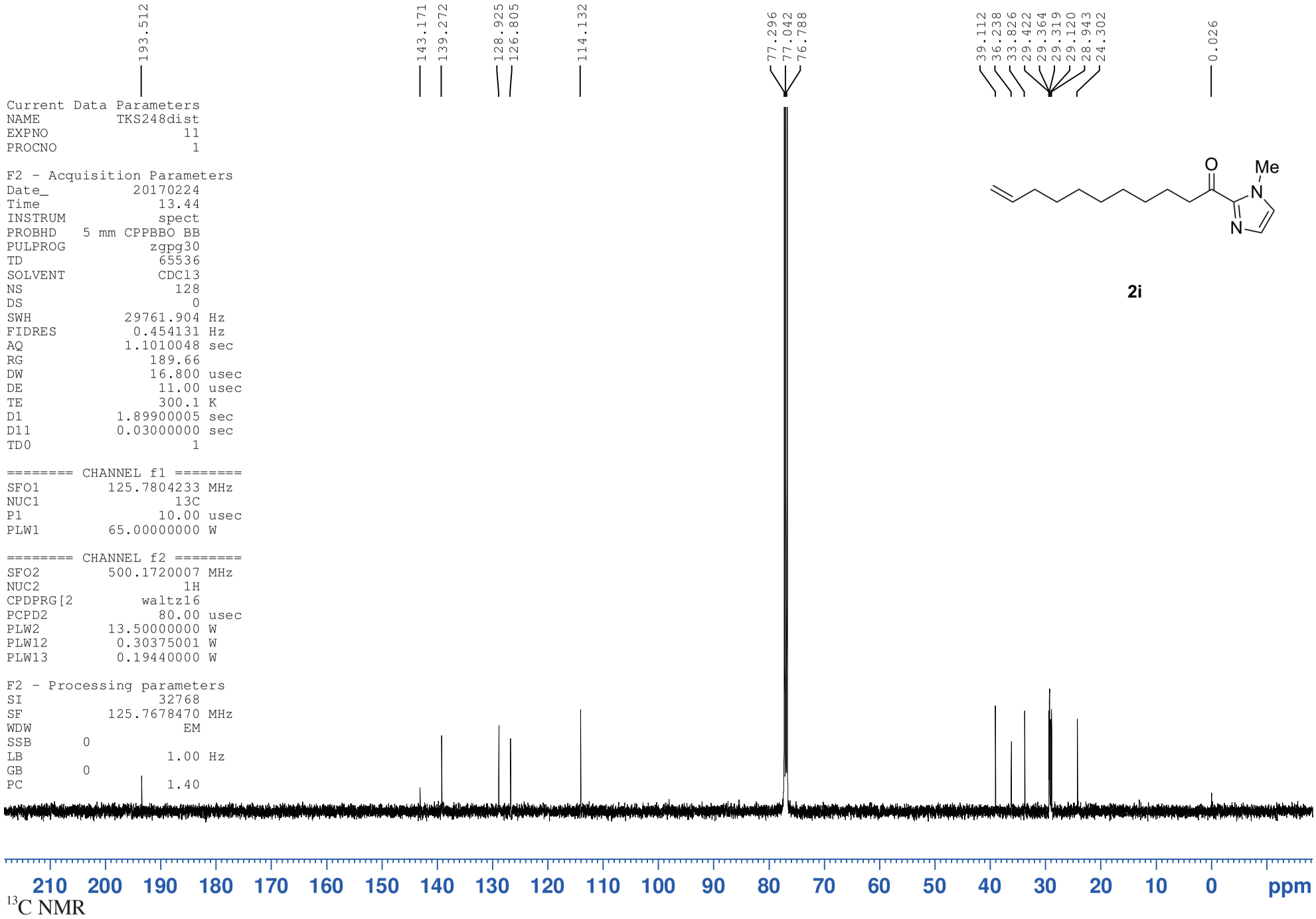
1.987
1.995
10.103

^{1}H NMR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29.319
29.120
28.943
24.302
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PROCNO 1
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Time 13.44
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PULPROG zgpg30
TD 65536
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SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
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SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
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Me
N
N
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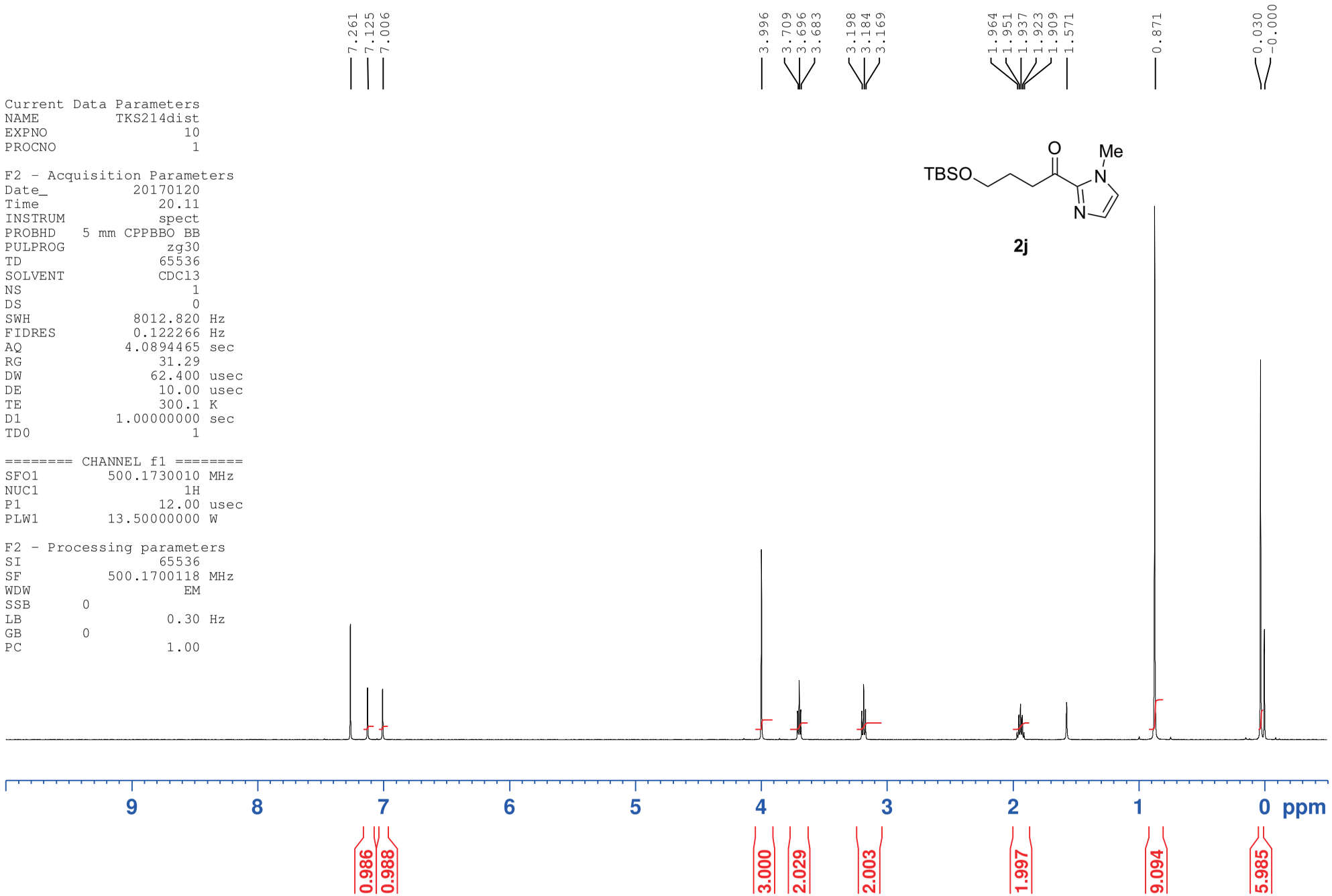
^{13}C NMR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1.909
1.571
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0.030
-0.000
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PROCNO 1
F2 - Acquisition Parameters
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Time 20.11
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PULPROG zg30
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SOLVENT CDCl3
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DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TBSO
O
Me
N
N
2j
9
8
7
6
5
4
3
2
1
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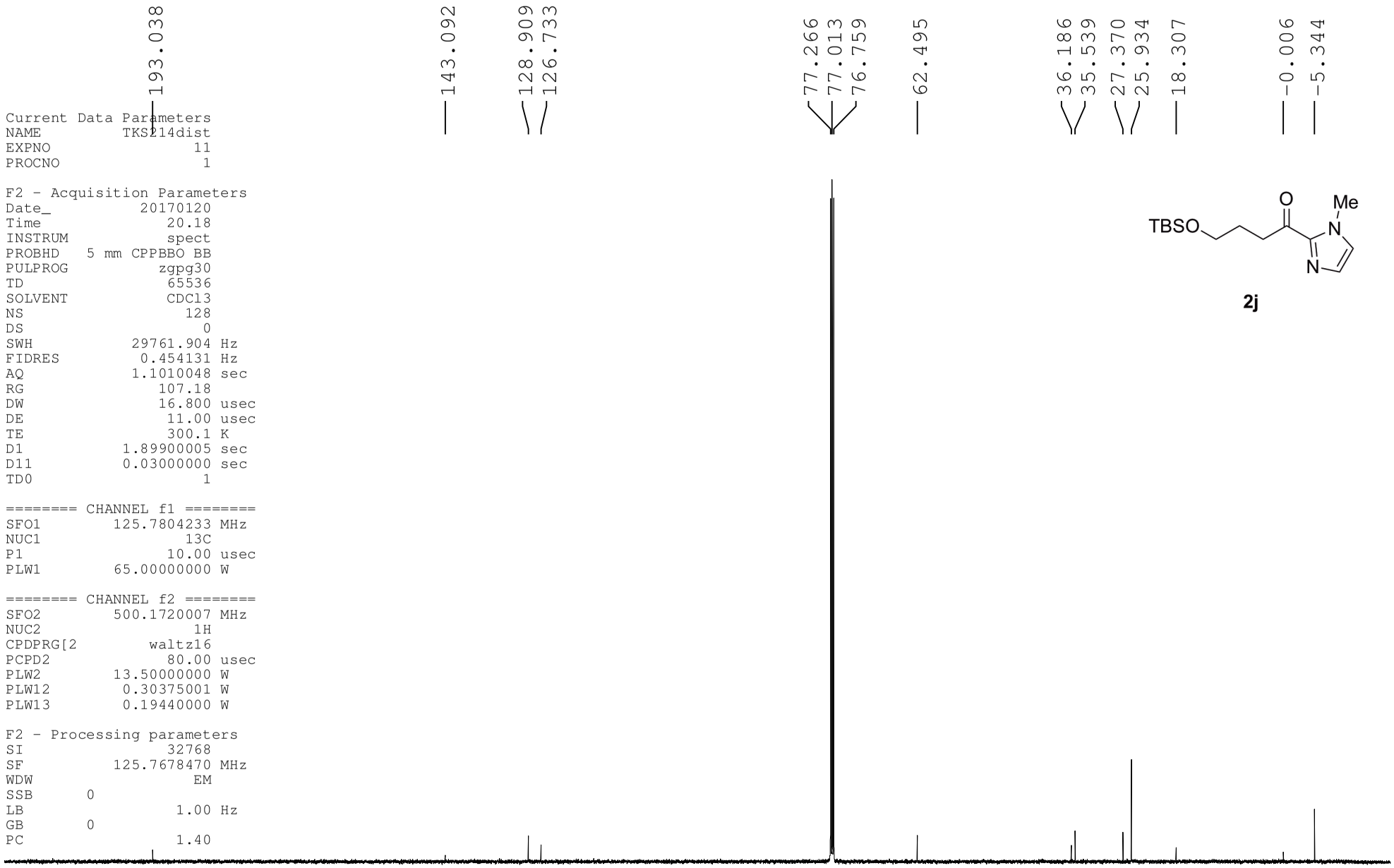
1.997
9.094
5.985

^{1}H NMR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FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
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NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TBSO
O
Me
N
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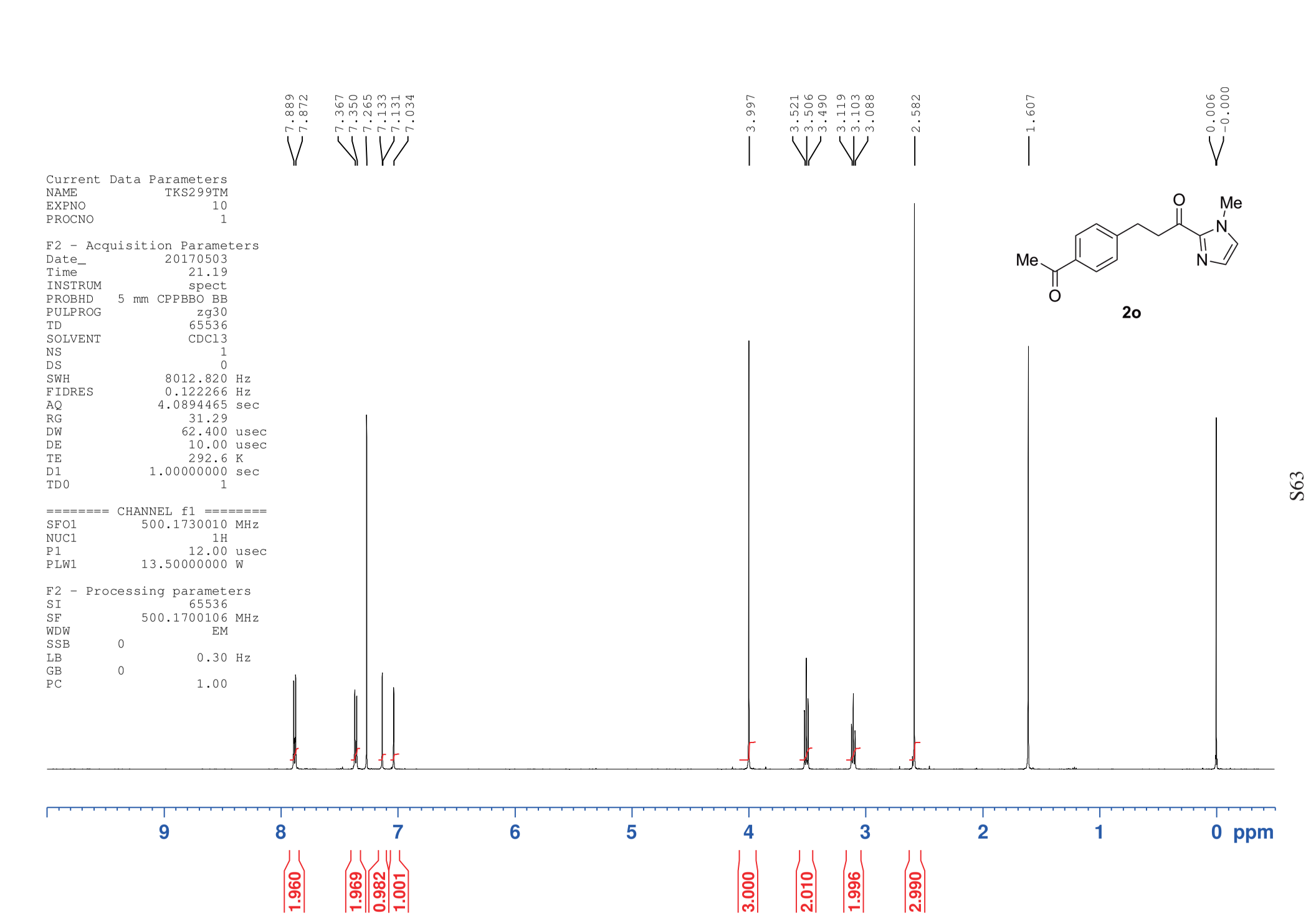
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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7.265
7.133
7.131
7.034
3.997
3.521
3.506
3.490
3.119
3.103
3.088
2.582
1.607
0.006
-0.000
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PROCNO 1
F2 - Acquisition Parameters
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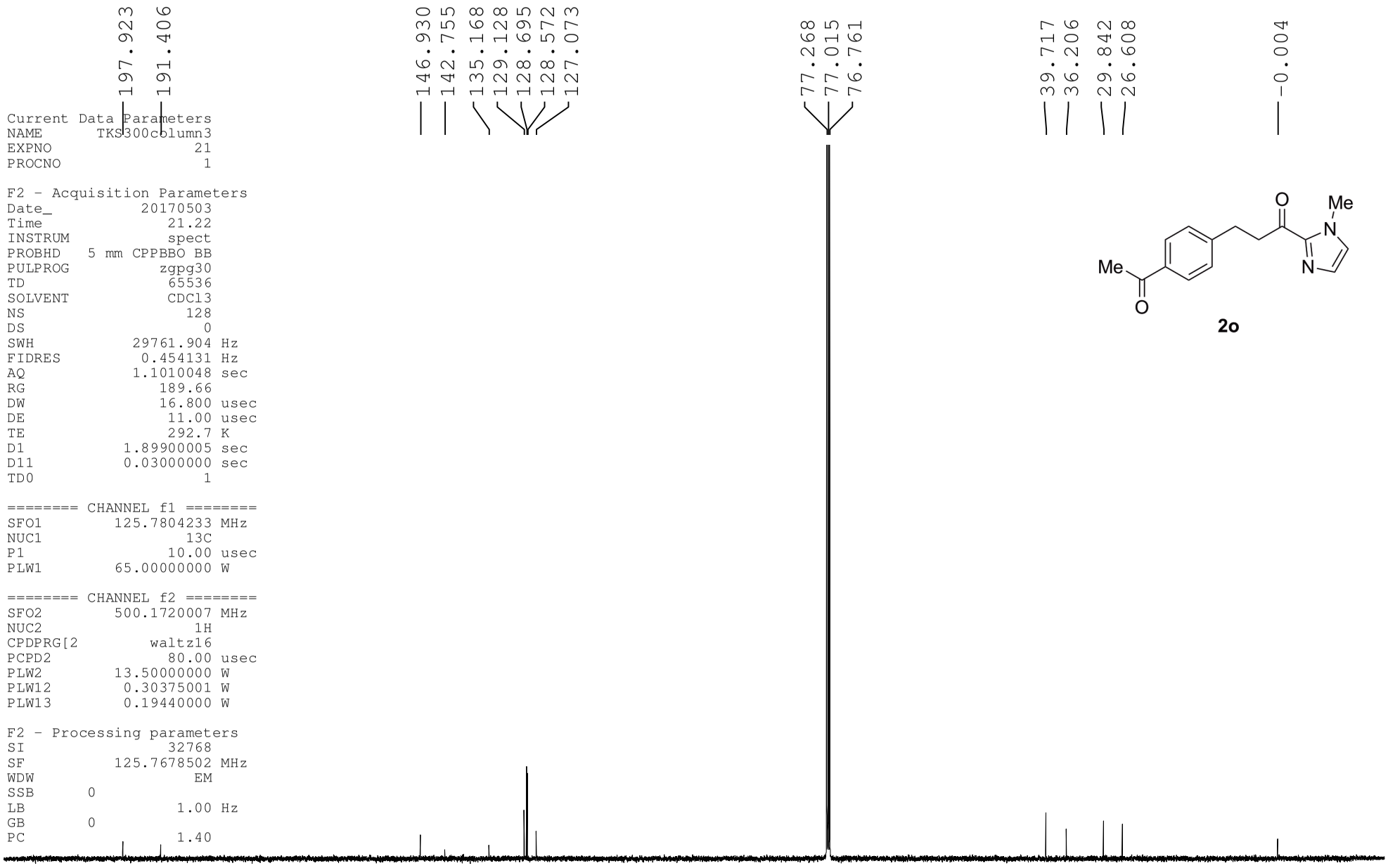
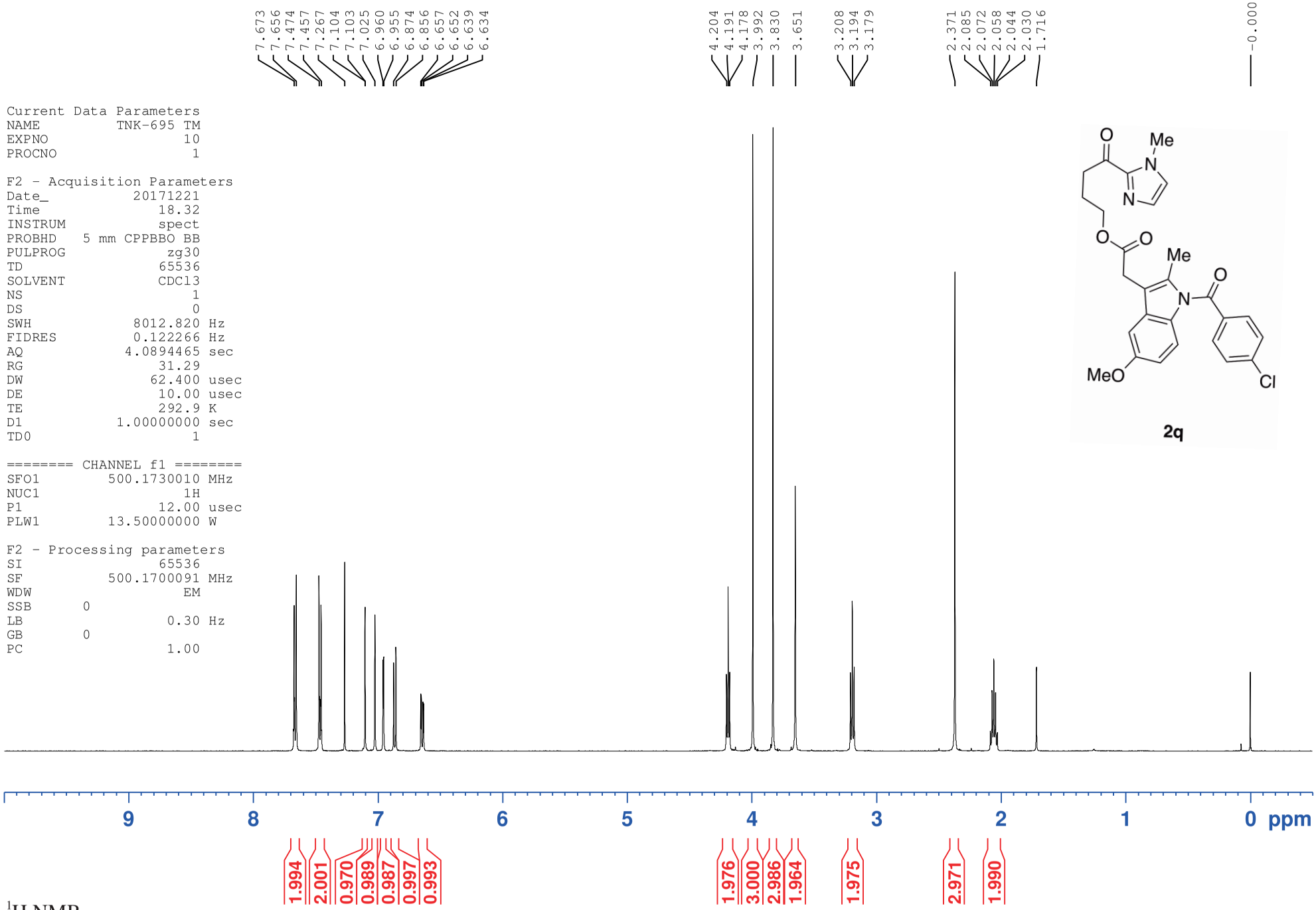
Time 21.19
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
N
Me
N
O
2o
9
8
7
6
5
4
3
2
1
0 ppm
1.960
1.969
0.982
1.001
3.000
2.010
1.996
2.990

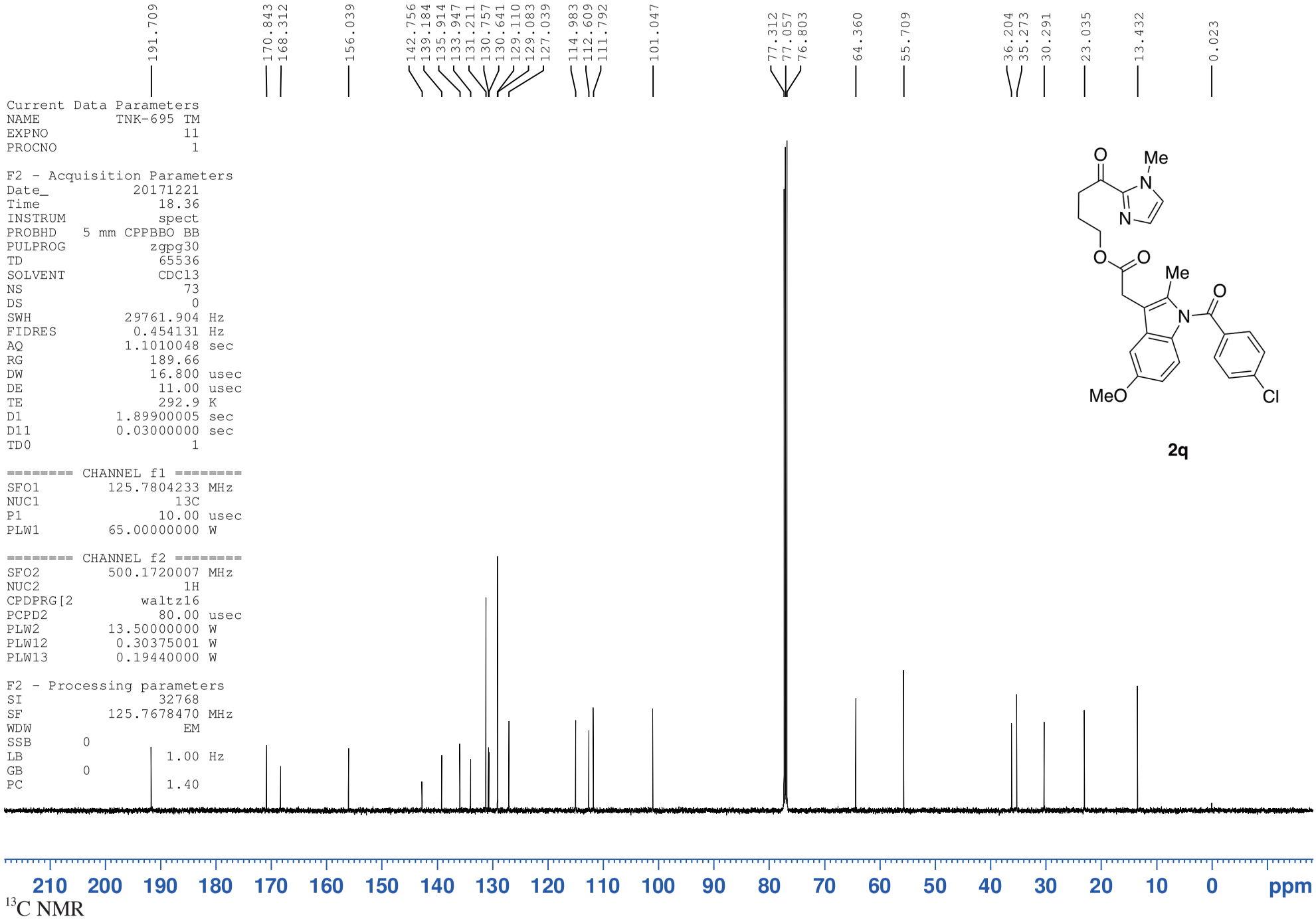
^{1}H NMR


197.923
191.406
146.930
142.755
135.168
129.128
128.695
128.572
127.073
77.268
77.015
76.761
39.717
36.206
29.842
26.608
-0.004
Current Data Parameters
NAME TKS300column3
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170503
Time 21.22
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.7 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678502 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Me
N
N
Me
O
2o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

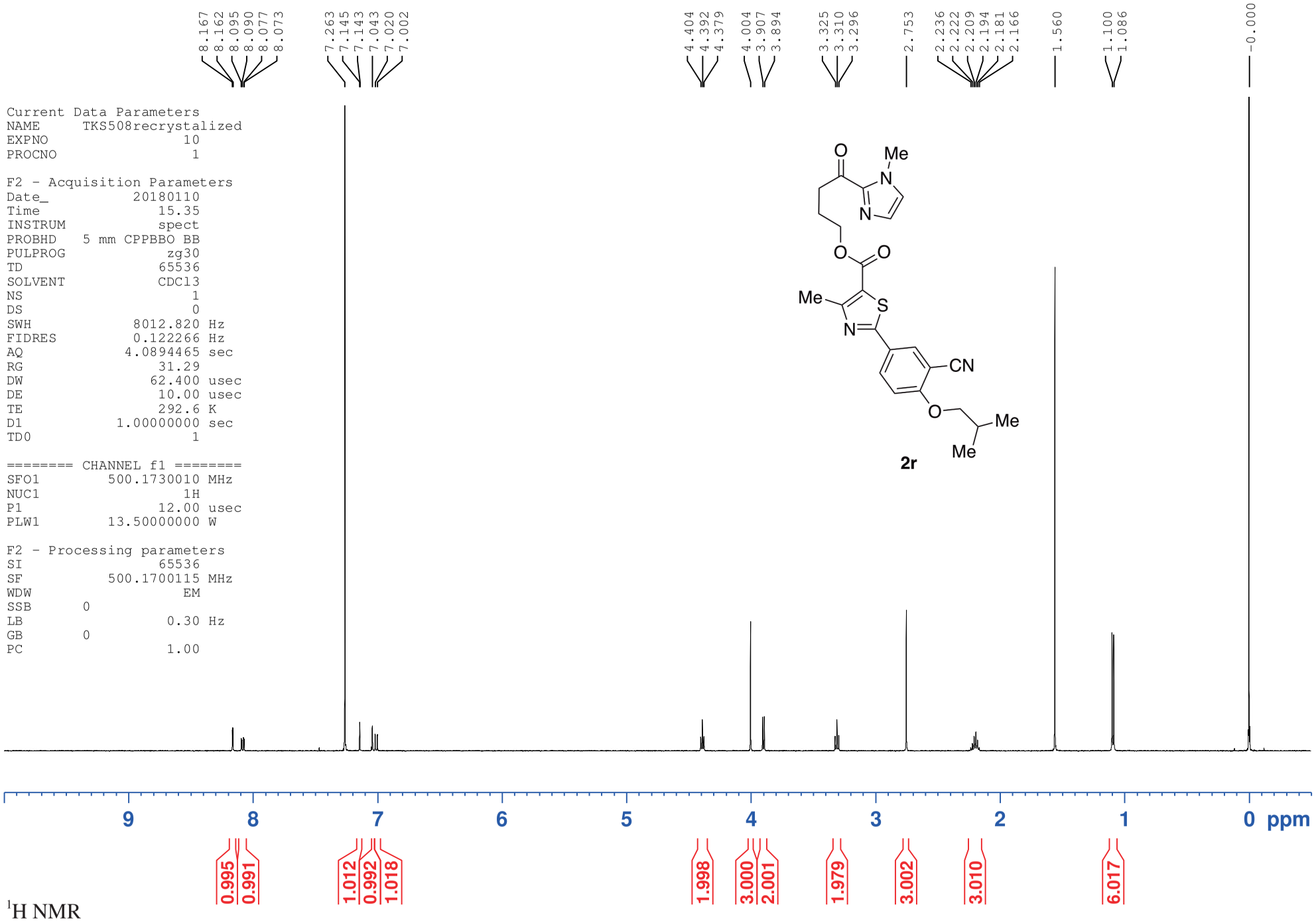
^{13}C NMR


7.673
7.656
7.474
7.457
7.267
7.104
7.103
7.025
6.960
6.955
6.874
6.856
6.657
6.652
6.639
6.634
4.204
4.191
4.178
3.992
3.830
3.651
3.208
3.194
3.179
2.371
2.085
2.072
2.058
2.044
2.030
1.716
-0.000
Current Data Parameters
NAME TNK-695 TM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time 18.32
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
N
N
O
O
O
Me
N
O
MeO
Cl
2q
9
8
7
6
5
4
3
2
1
0 ppm
1.994
2.001
0.970
0.989
0.987
0.997
0.993
1.976
3.000
2.986
1.964
1.975
2.971
1.990

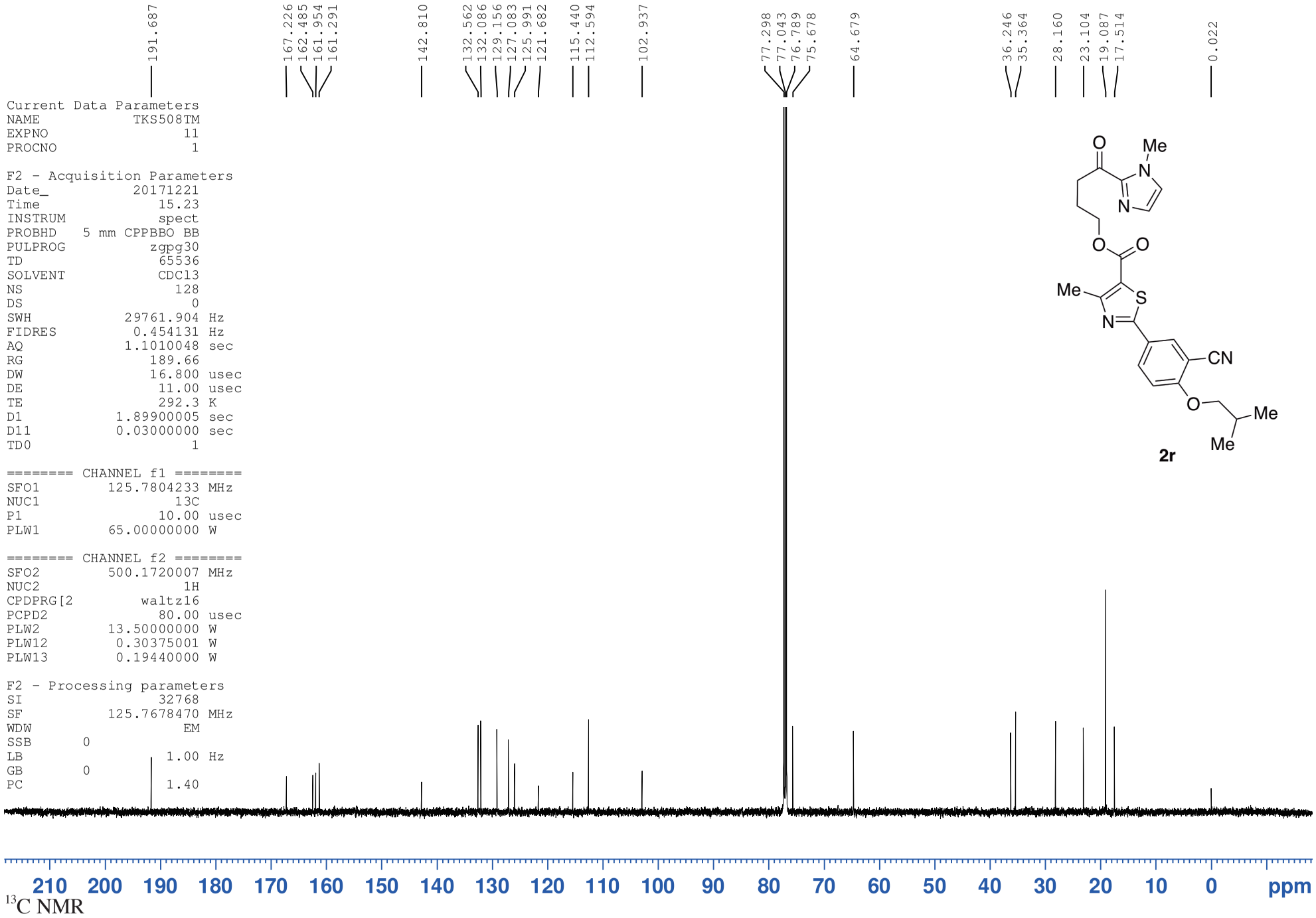
^{1}H NMR


191.709
170.843
168.312
156.039
142.756
139.184
135.914
133.947
131.211
130.757
130.641
129.110
129.083
127.039
114.983
112.609
111.792
101.047
77.312
77.057
76.803
64.360
55.709
36.204
35.273
30.291
23.035
13.432
0.023
Current Data Parameters
NAME TNK-695 TM
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time 18.36
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 73
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.9 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Me
N
N
O
O
Me
O
N
MeO
Cl
2q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

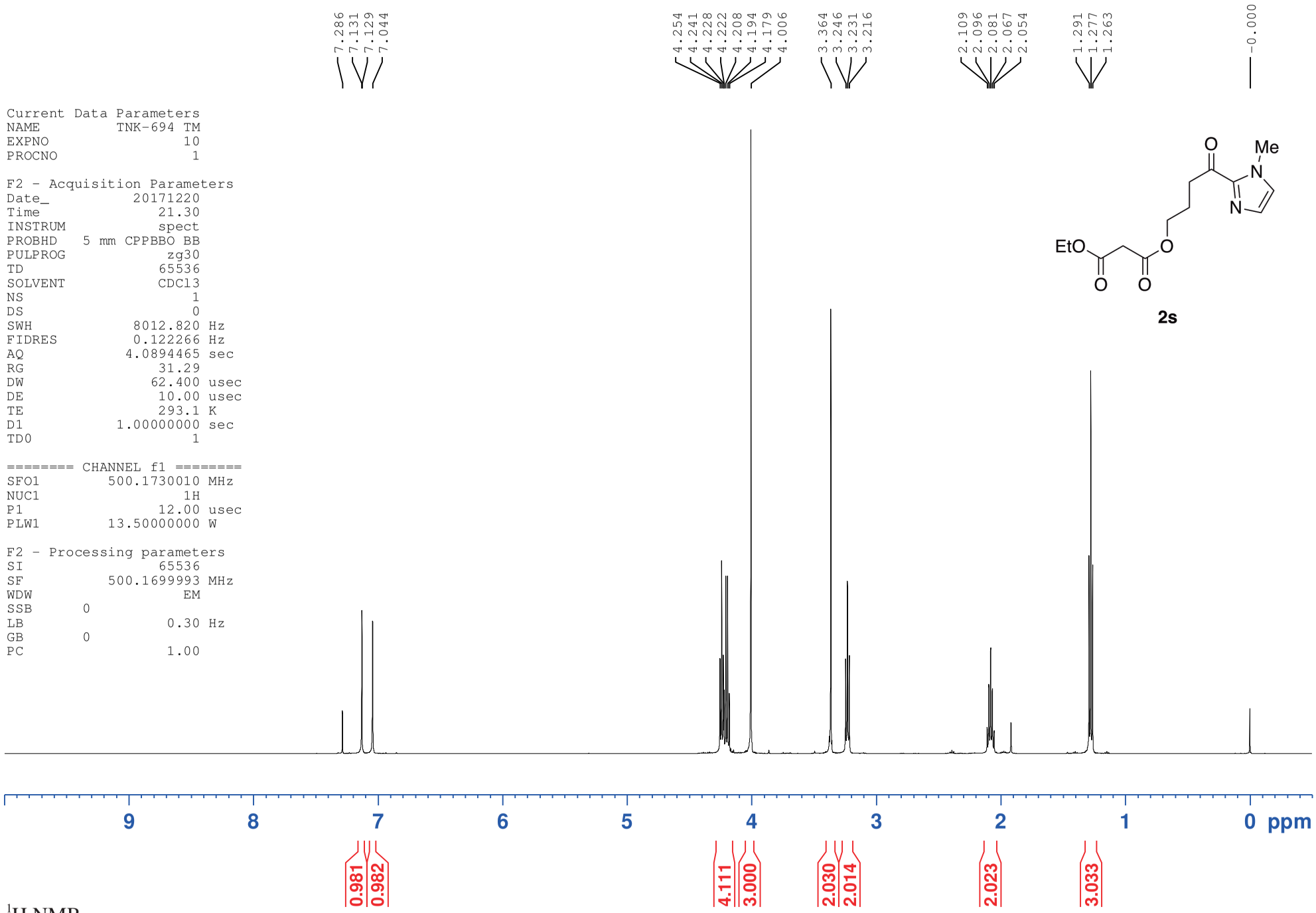
^{13}C NMR


8.167
8.162
8.095
8.090
8.077
8.073
7.263
7.145
7.143
7.043
7.020
7.002
4.404
4.392
4.379
4.004
3.907
3.894
3.325
3.310
3.296
2.753
2.236
2.222
2.209
2.194
2.181
2.166
1.560
1.100
1.086
0.000
Current Data Parameters
NAME TKS508recrystalized
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180110
Time 15.35
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
N
N
O
O
Me
S
N
CN
O
Me
Me
2r
9
8
7
6
5
4
3
2
1
0 ppm
0.995
0.991
1.012
0.992
1.018
1.998
3.000
2.001
1.979
3.002
3.010
6.017

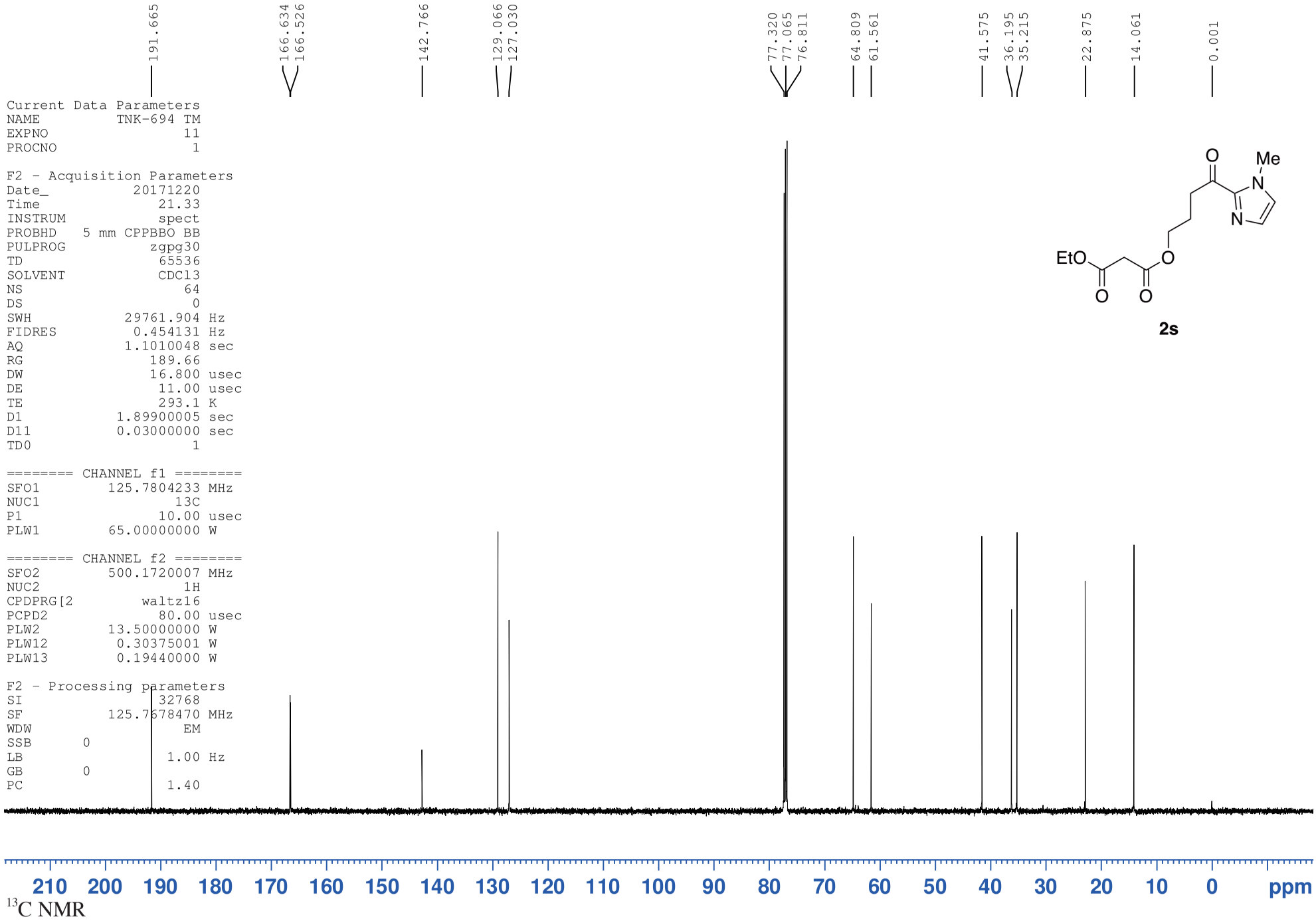
^{1}H NMR


191.687
167.226
162.485
161.954
161.291
142.810
132.562
132.086
129.156
127.083
125.991
121.682
115.440
112.594
102.937
77.298
77.043
76.789
75.678
64.679
36.246
35.364
28.160
23.104
19.087
17.514
0.022
Current Data Parameters
NAME TKS508TM
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time 15.23
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.3 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Me
N
N
O
O
Me
S
N
CN
O
Me
Me
2r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

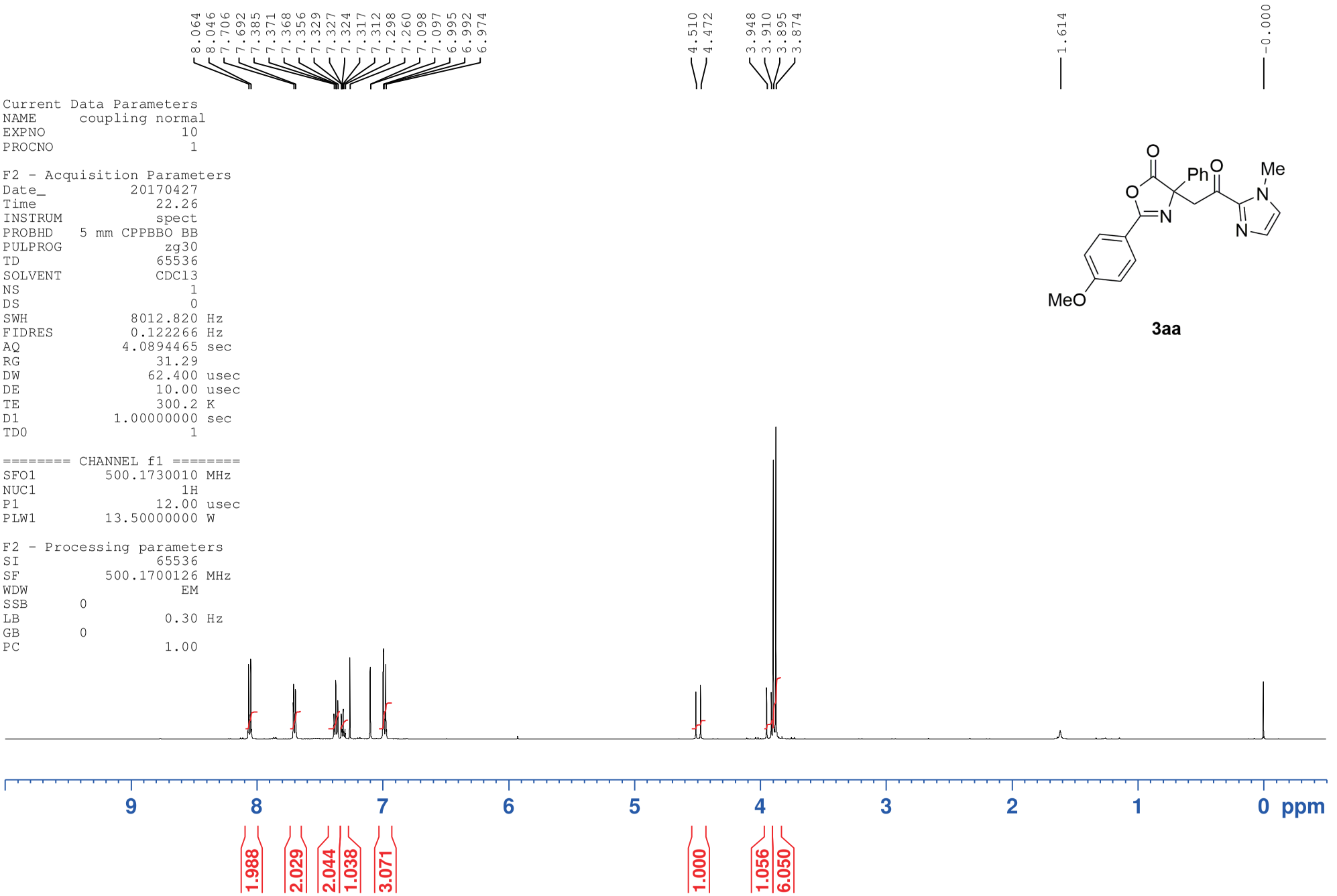
^{13}C NMR


7.286
7.131
7.129
7.044
4.254
4.241
4.228
4.222
4.208
4.194
4.179
4.006
3.364
3.246
3.231
3.216
2.109
2.096
2.081
2.067
2.054
1.291
1.277
1.263
-0.000
Current Data Parameters
NAME TNK-694 TM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171220
Time 21.30
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1699993 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
N
N
EtO
O
O
O
2s
9
8
7
6
5
4
3
2
1
0 ppm
0.981
0.982
4.111
3.000
2.030
2.014
2.023
3.033

^{1}H NMR

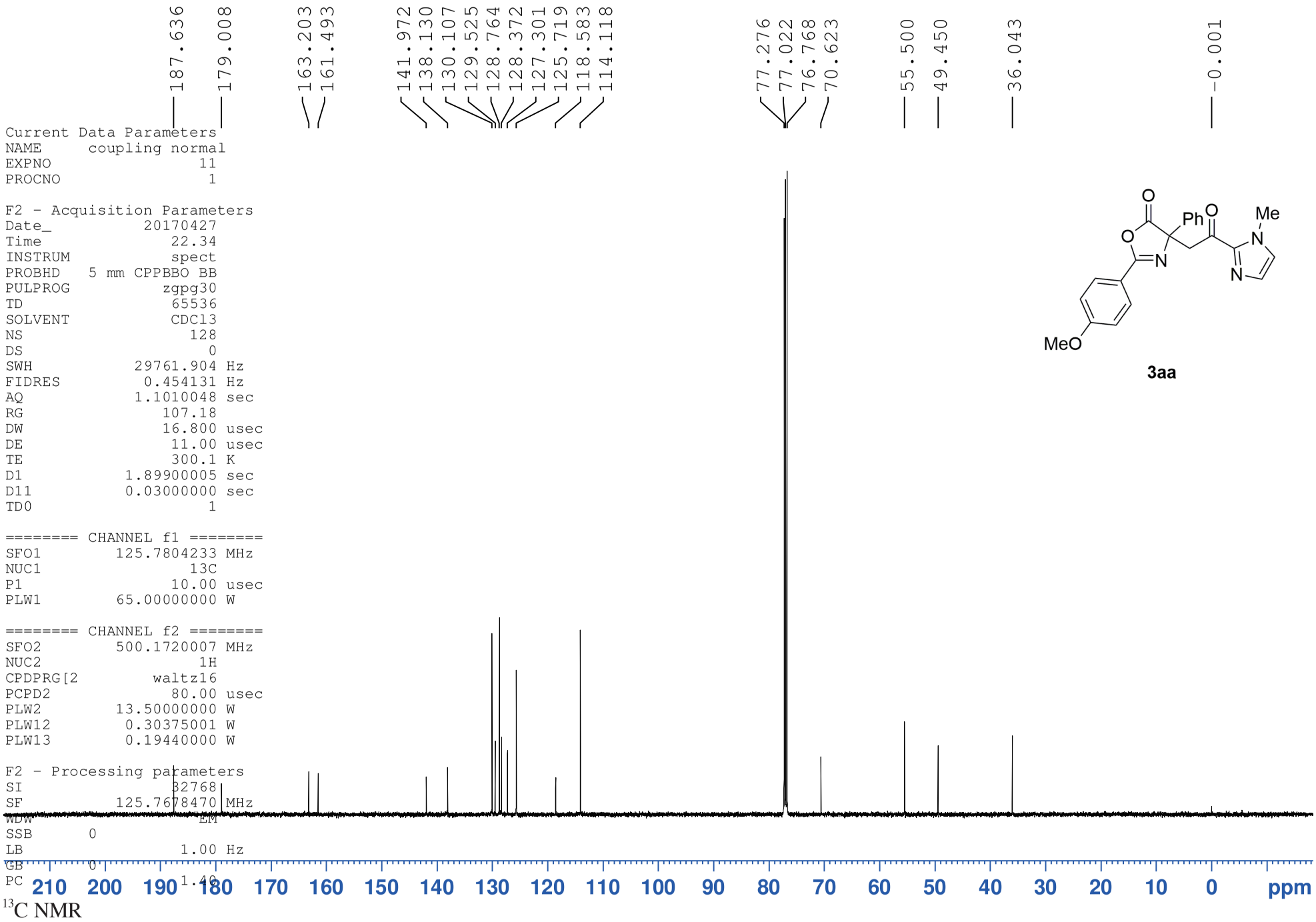

191.665
166.634
166.526
142.766
129.066
127.030
77.320
77.065
76.811
64.809
61.561
41.575
36.195
35.215
22.875
14.061
0.001
Current Data Parameters
NAME TNK-694 TM
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171220
Time 21.33
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 293.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Me
N
N
EtO
O
O
O
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR

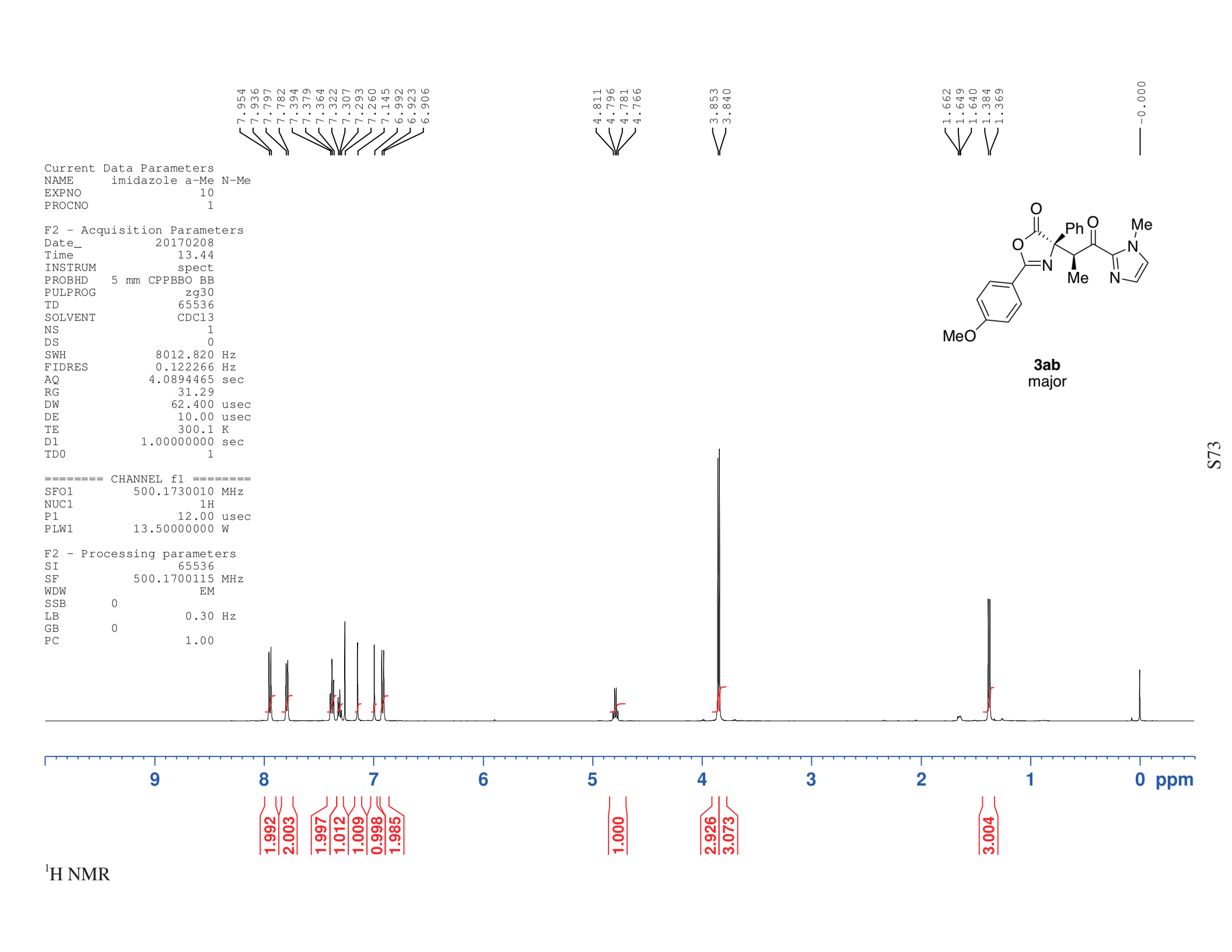

8.064
8.046
7.706
7.692
7.385
7.371
7.368
7.356
7.329
7.327
7.324
7.317
7.312
7.298
7.260
7.098
7.097
6.995
6.992
6.974
4.510
4.472
3.948
3.910
3.895
3.874
1.614
-0.000
Current Data Parameters
NAME coupling normal
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170427
Time 22.26
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
N
MeO
9
8
7
6
5
4
3
2
1
0 ppm
1.988
2.029
2.044
1.038
3.071
1.000
1.056
6.050

3aa

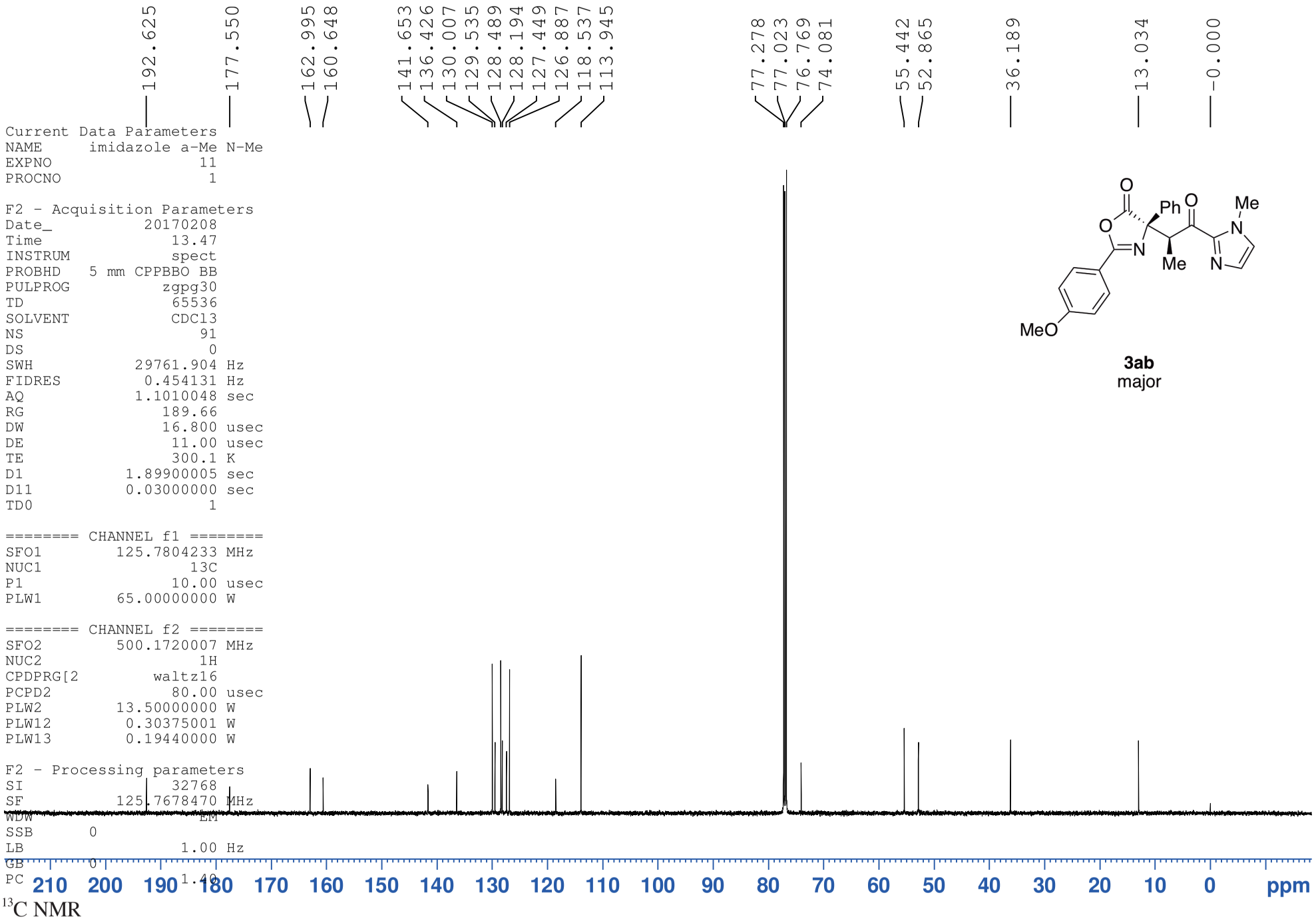
^{1}H NMR


187.636
179.008
163.203
161.493
141.972
138.130
130.107
129.525
128.764
128.372
127.301
125.719
118.583
114.118
77.276
77.022
76.768
70.623
55.500
49.450
36.043
-0.001
Current Data Parameters
NAME coupling normal
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170427
Time 22.34
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
N
MeO
3aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

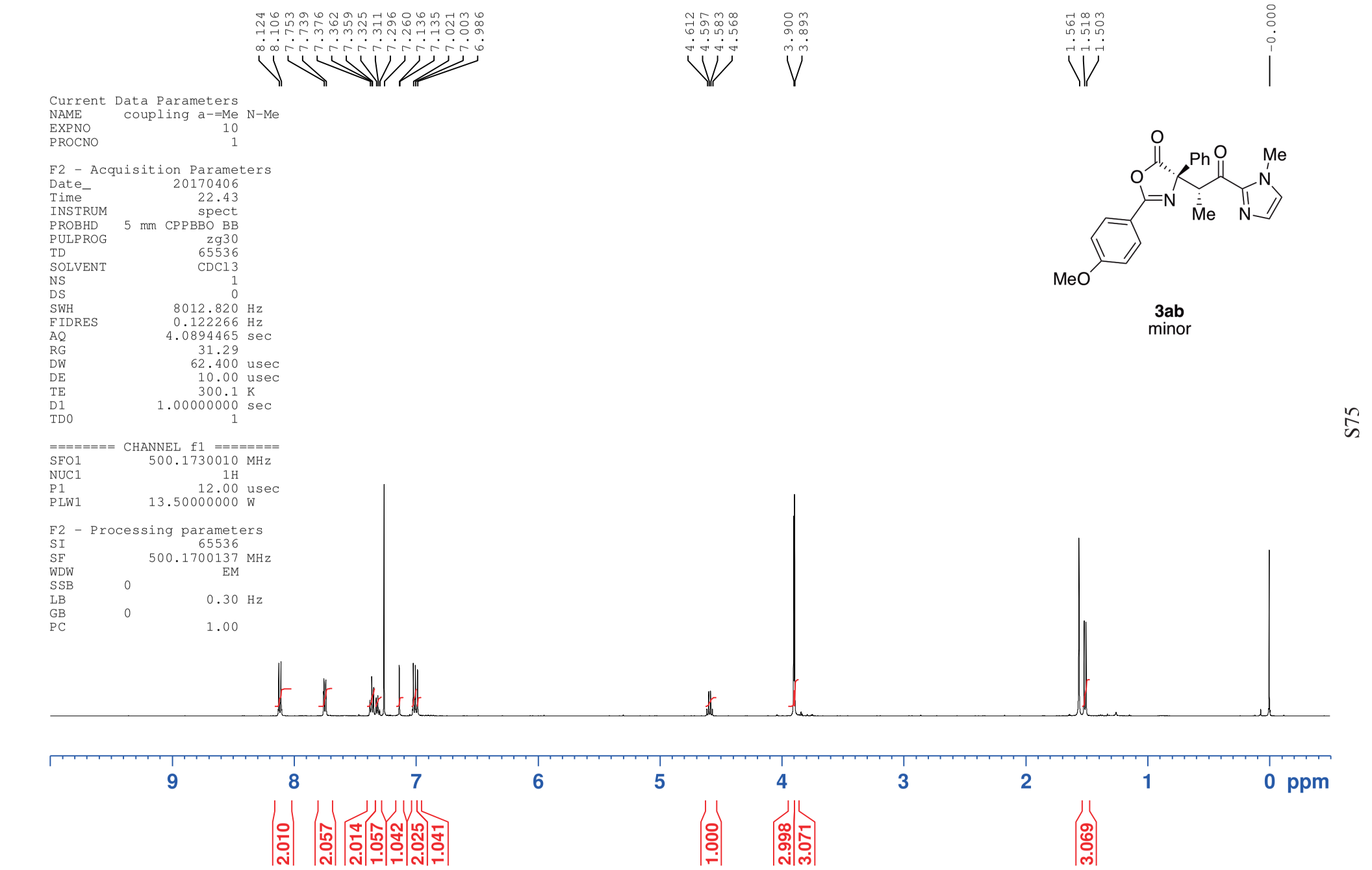
^{13}C NMR


7.954
7.936
7.797
7.782
7.394
7.379
7.364
7.322
7.307
7.293
7.260
7.145
6.992
6.923
6.906
4.811
4.796
4.781
4.766
3.853
3.840
1.662
1.649
1.640
1.384
1.369
-0.000
Current Data Parameters
NAME imidazole a-Me N-Me
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170208
Time 13.44
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
Me
N
MeO
3ab
major
9
8
7
6
5
4
3
2
1
0 ppm
1.992
2.003
1.997
1.012
1.009
0.998
1.985
1.000
2.926
3.073
3.004

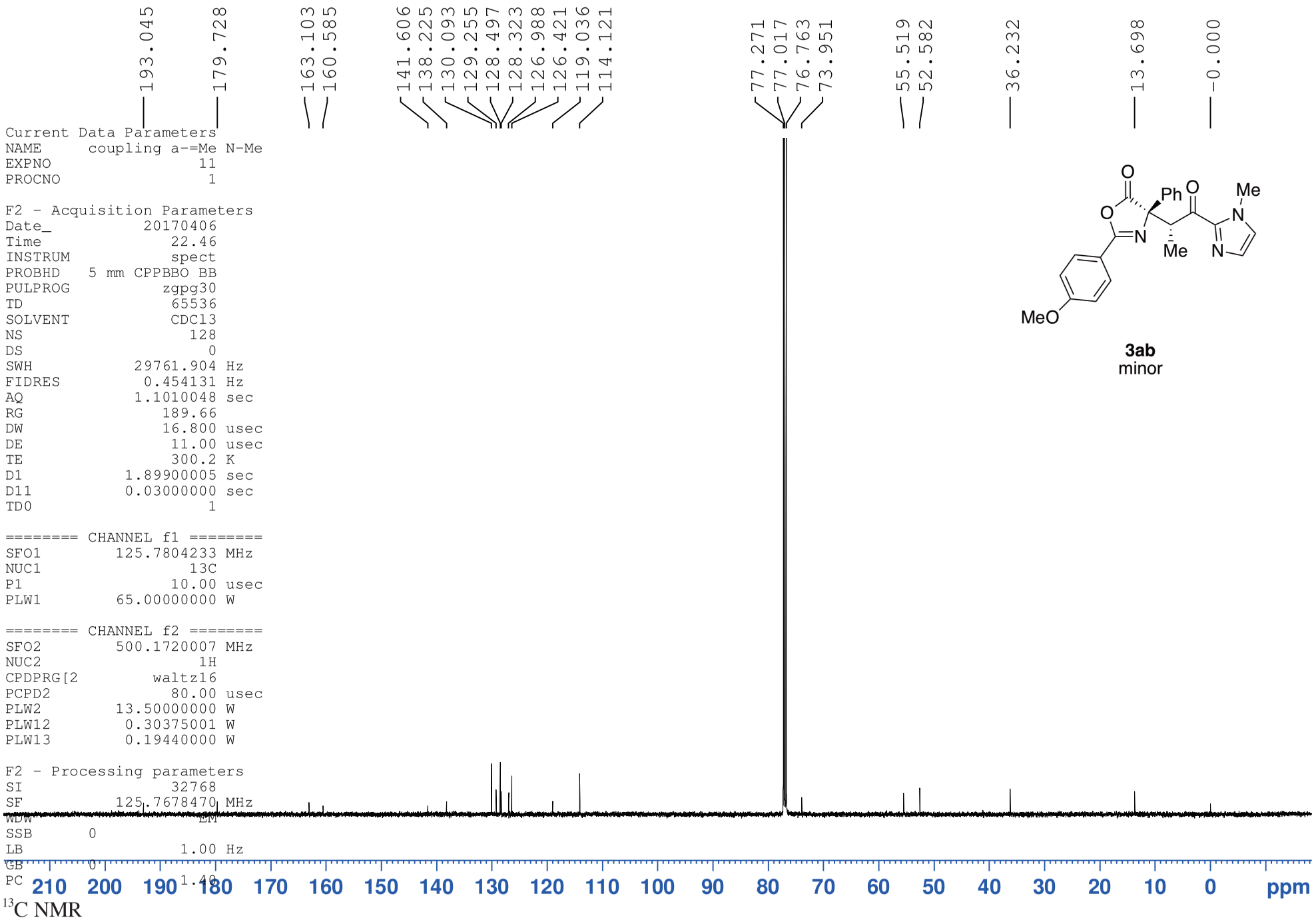
^{1}H NMR


192.625
177.550
162.995
160.648
141.653
136.426
130.007
129.535
128.489
128.194
127.449
126.887
118.537
113.945
77.278
77.023
76.769
74.081
55.442
52.865
36.189
13.034
-0.000
Current Data Parameters
NAME imidazole a-Me N-Me
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170208
Time 13.47
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 91
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
N
O
N
Me
N
MeO
3ab
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

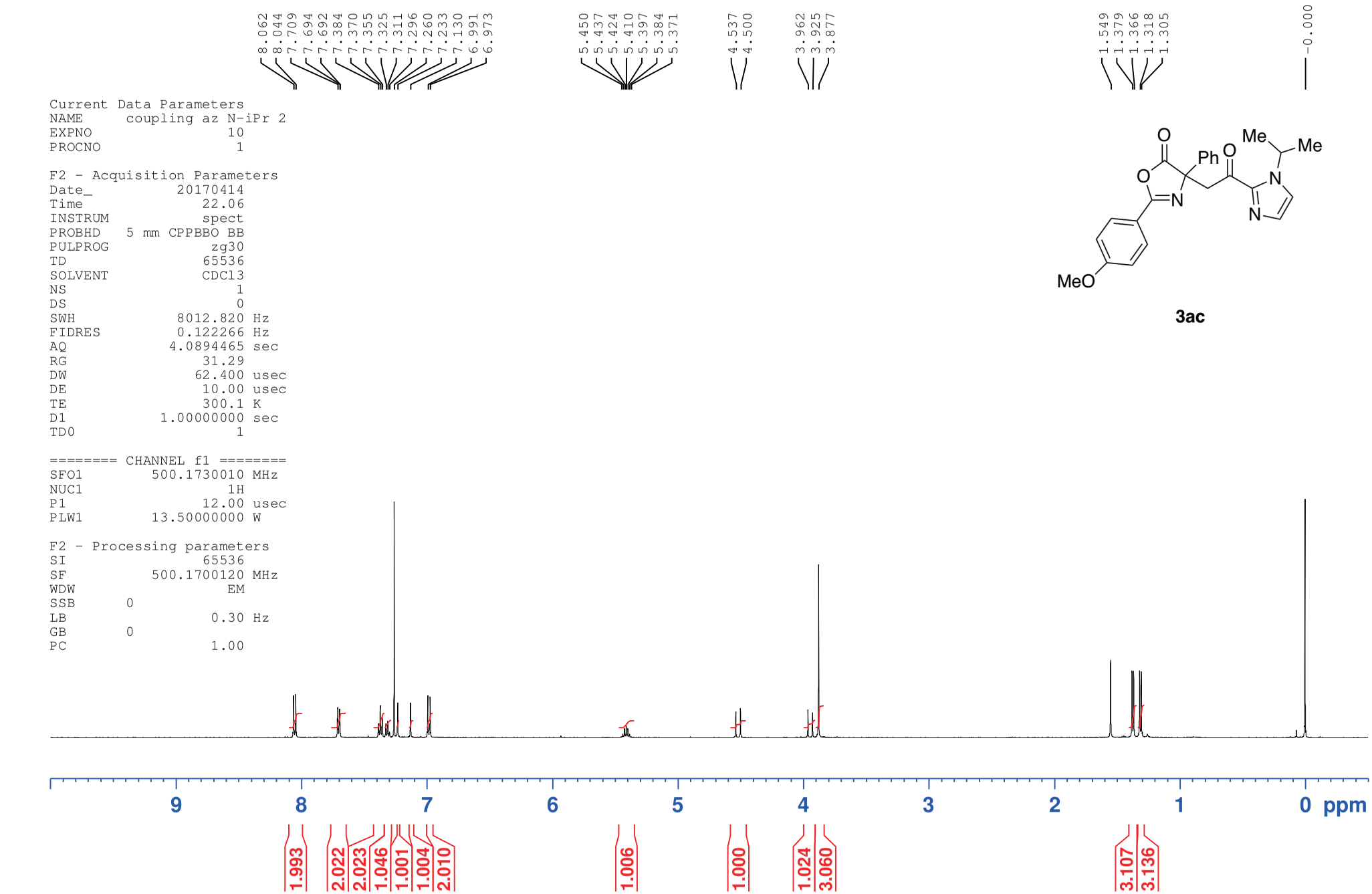
^{13}C NMR


8.124
8.106
7.753
7.739
7.376
7.362
7.359
7.325
7.311
7.296
7.260
7.136
7.135
7.021
7.003
6.986
4.612
4.597
4.583
4.568
3.900
3.893
1.561
1.518
1.503
0.000
Current Data Parameters
NAME coupling a-=Me N-Me
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170406
Time 22.43
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
Me
N
MeO
3ab
minor
9
8
7
6
5
4
3
2
1
0 ppm
2.010
2.057
2.014
1.057
1.042
2.025
1.041
1.000
2.998
3.071
3.069

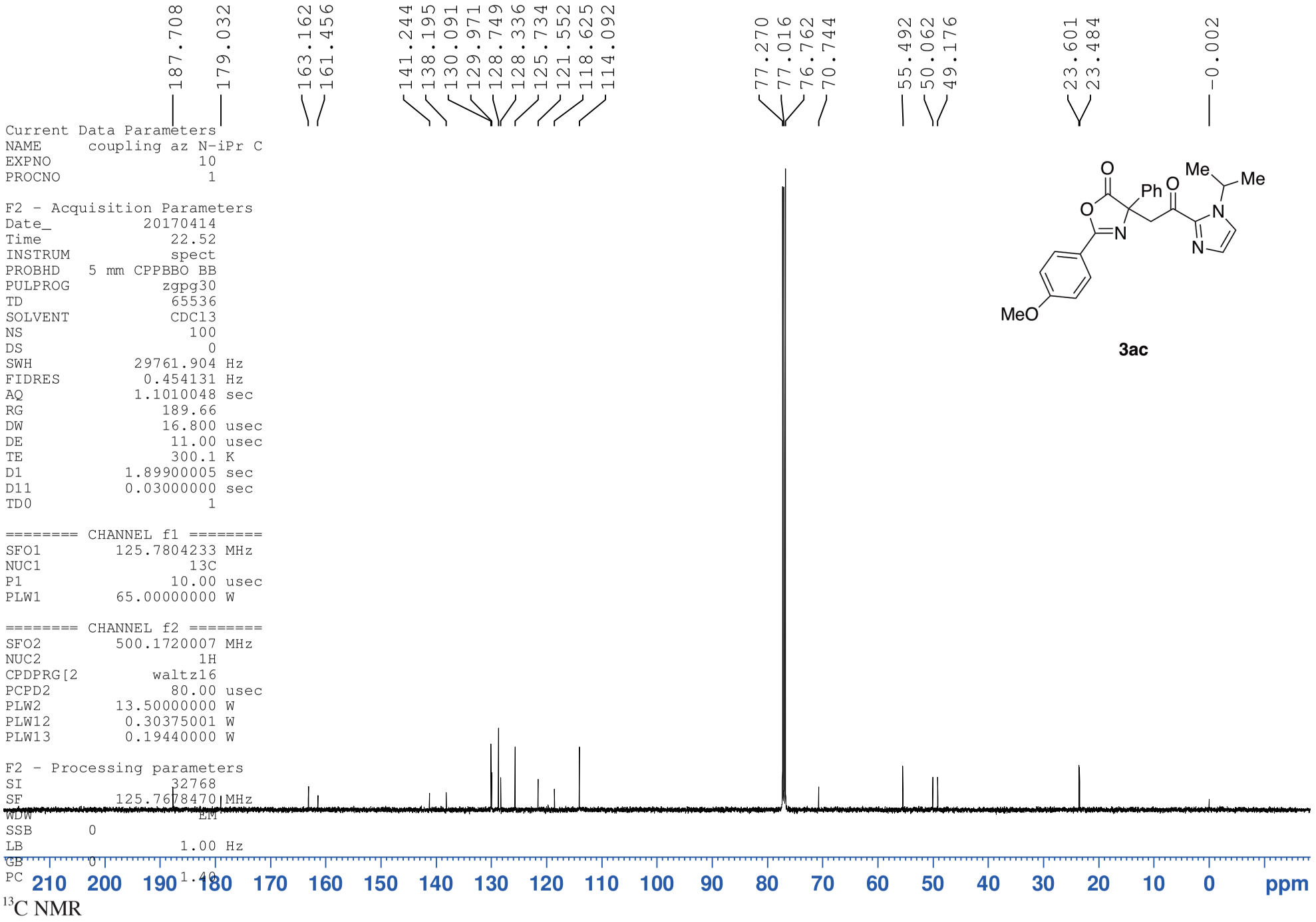
^{1}H NMR


193.045
179.728
163.103
160.585
141.606
138.225
130.093
129.255
128.497
128.323
126.988
126.421
119.036
114.121
77.271
77.017
76.763
73.951
55.519
52.582
36.232
13.698
-0.000
Current Data Parameters
NAME coupling a-=Me N-Me
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170406
Time 22.46
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Me
N
MeO
3ab
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

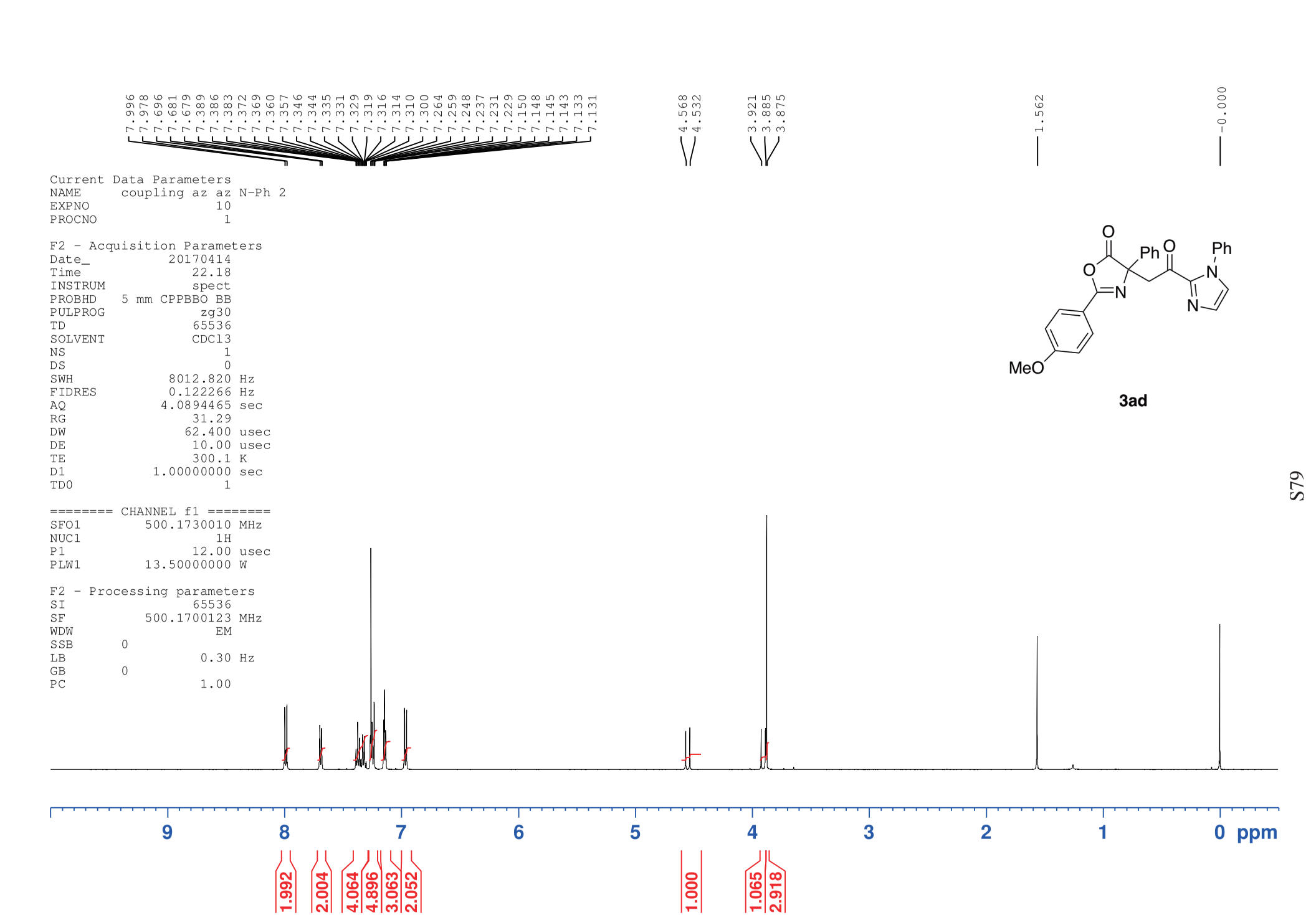
^{13}C NMR


8.062
8.044
7.709
7.694
7.692
7.384
7.370
7.355
7.325
7.311
7.296
7.260
7.233
7.130
6.991
6.973
5.450
5.437
5.424
5.410
5.397
5.384
5.371
4.537
4.500
3.962
3.925
3.877
1.549
1.379
1.366
1.318
1.305
0.000
Current Data Parameters
NAME coupling az N-iPr 2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.06
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
Me
O
N
N
N
MeO
3ac
9
8
7
6
5
4
3
2
1
0 ppm
1.993
2.022
2.023
1.046
1.001
1.004
2.010
1.006
1.000
1.024
3.060
3.107
3.136

^{1}H NMR


187.708
179.032
163.162
161.456
141.244
138.195
130.091
129.971
128.749
128.336
125.734
121.552
118.625
114.092
77.270
77.016
76.762
70.744
55.492
50.062
49.176
23.601
23.484
-0.002
Current Data Parameters
NAME coupling az N-iPr C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.52
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
Me
O
N
N
N
MeO
3ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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7.978
7.696
7.681
7.679
7.389
7.386
7.383
7.372
7.369
7.360
7.357
7.346
7.344
7.335
7.331
7.329
7.319
7.316
7.314
7.310
7.300
7.264
7.259
7.248
7.237
7.231
7.229
7.150
7.148
7.145
7.143
7.133
7.131
4.568
4.532
3.921
3.885
3.875
1.562
-0.000
Current Data Parameters
NAME coupling az az N-Ph 2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.18
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Ph
O
N
N
N
MeO
3ad
9
8
7
6
5
4
3
2
1
0 ppm
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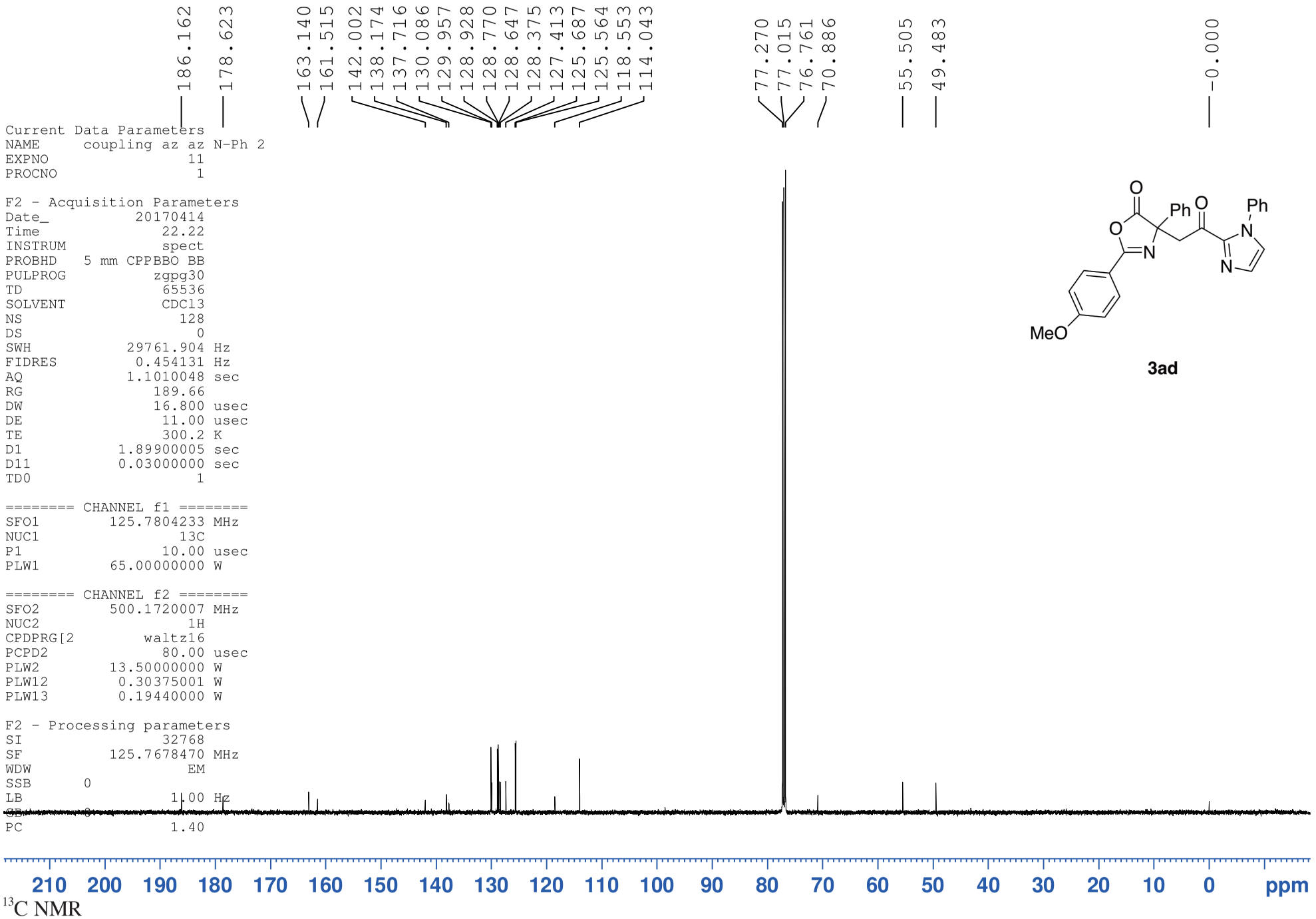
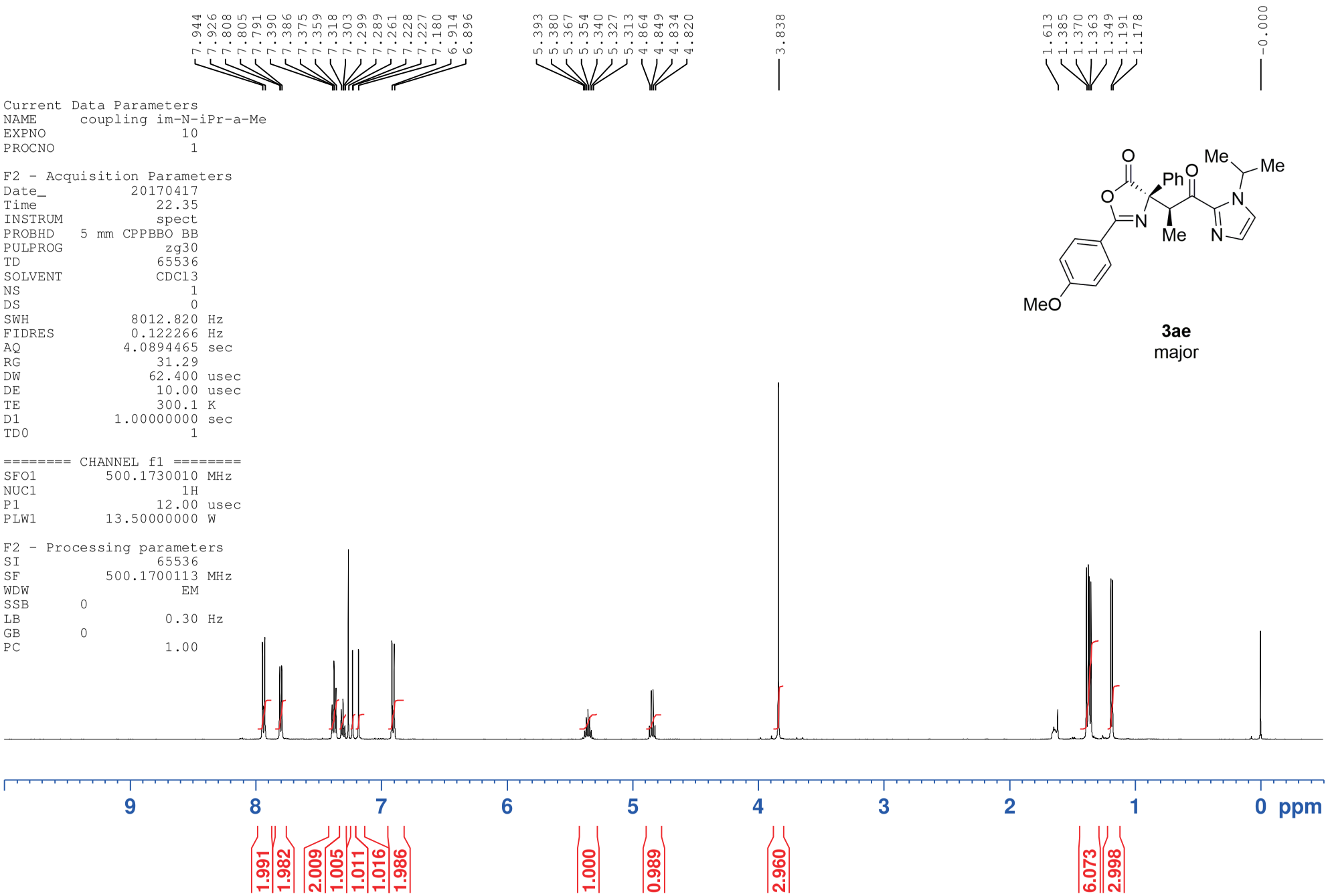
2.004
4.064
4.896
3.063
2.052
1.000
1.065
2.918

^{1}H NMR

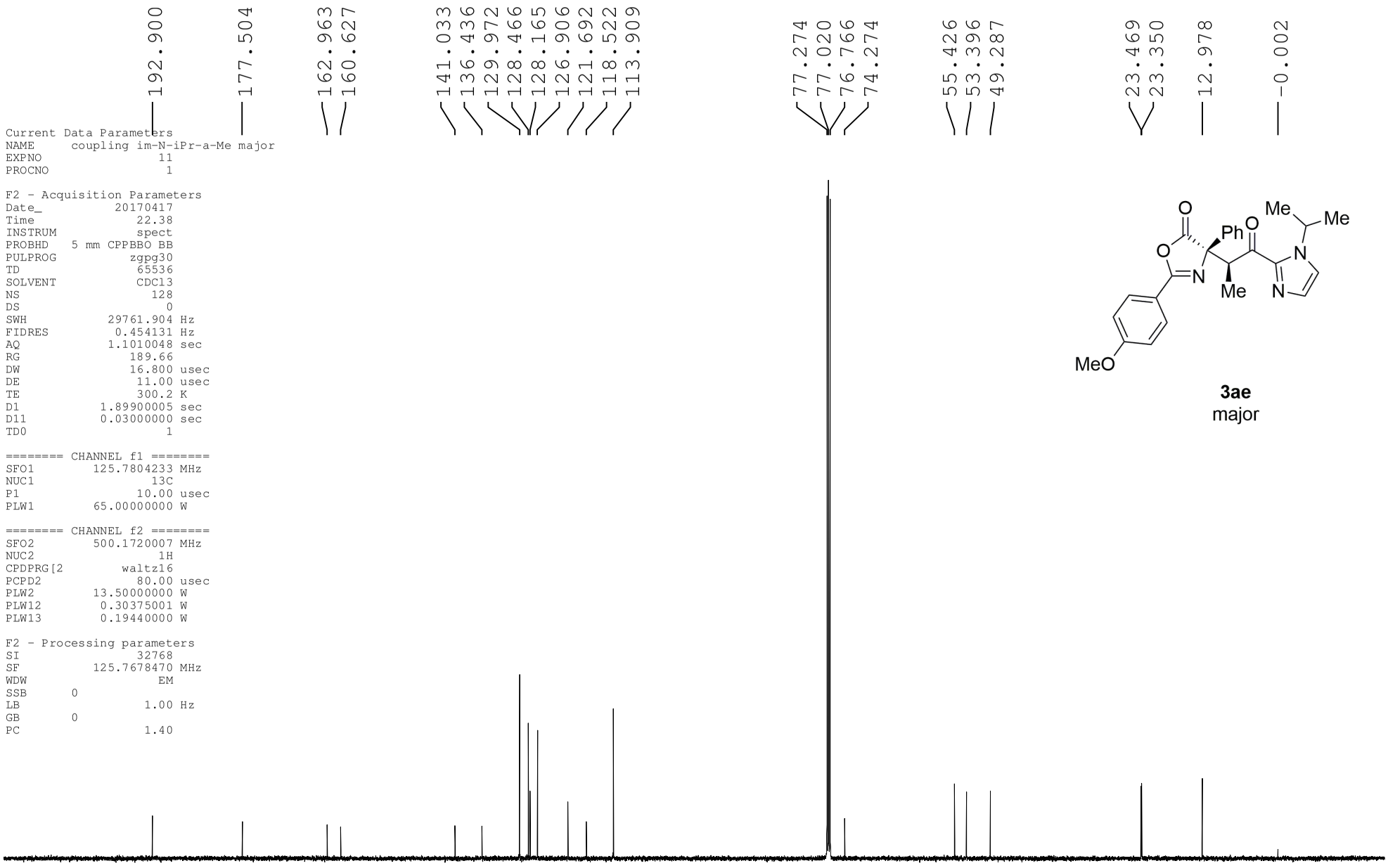

186.162
178.623
163.140
161.515
142.002
138.174
137.716
130.086
129.957
128.928
128.770
128.647
128.375
127.413
125.687
125.564
118.553
114.043
77.270
77.015
76.761
70.886
55.505
49.483
-0.000
Current Data Parameters
NAME coupling az az N-Ph 2
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.22
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Ph
O
N
N
N
MeO
3ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR

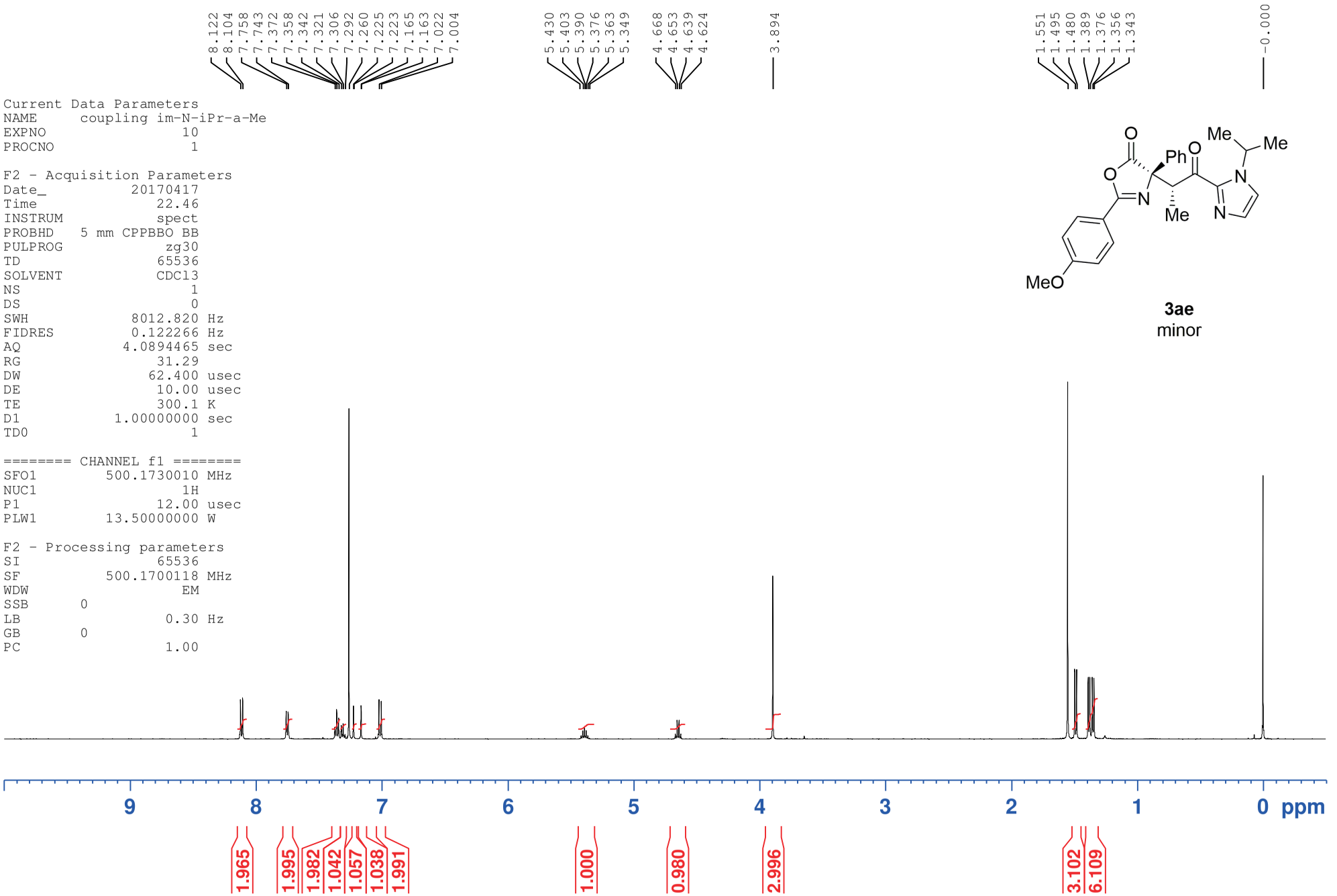


3ae
major

^{1}H NMR


192.900
177.504
162.963
160.627
141.033
136.436
129.972
128.466
128.165
126.906
121.692
118.522
113.909
77.274
77.020
76.766
74.274
55.426
53.396
49.287
23.469
23.350
12.978
-0.002
Current Data Parameters
NAME coupling im-N-iPr-a-Me major
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 22.38
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
Me
O
N
N
Me
N
MeO
3ae
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

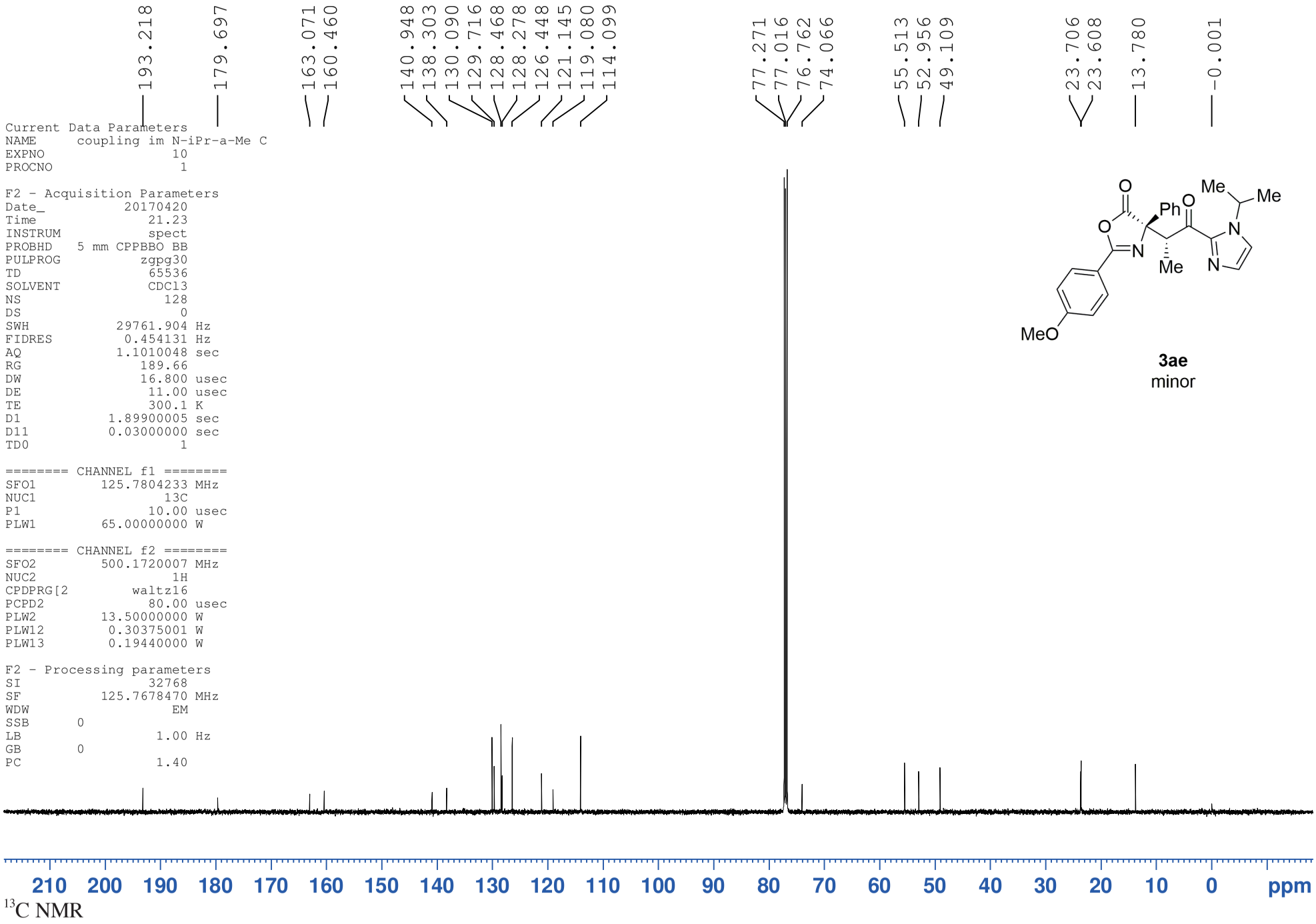
^{13}C NMR



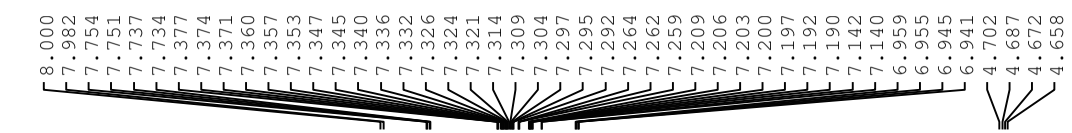
3ae
minor

S83

^{1}H NMR


193.218
179.697
163.071
160.460
140.948
138.303
130.090
129.716
128.468
128.278
126.448
121.145
119.080
114.099
77.271
77.016
76.762
74.066
55.513
52.956
49.109
23.706
23.608
13.780
-0.001
Current Data Parameters
NAME coupling im N-iPr-a-Me C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170420
Time 21.23
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
Me
N
N
Me
N
MeO
3ae
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR

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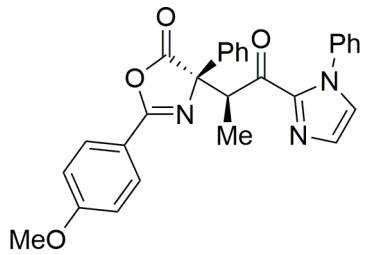
Current Data Parameters
NAME      acylimidazole N-Ph Me
EXPNO                   10
PROCNO                   1

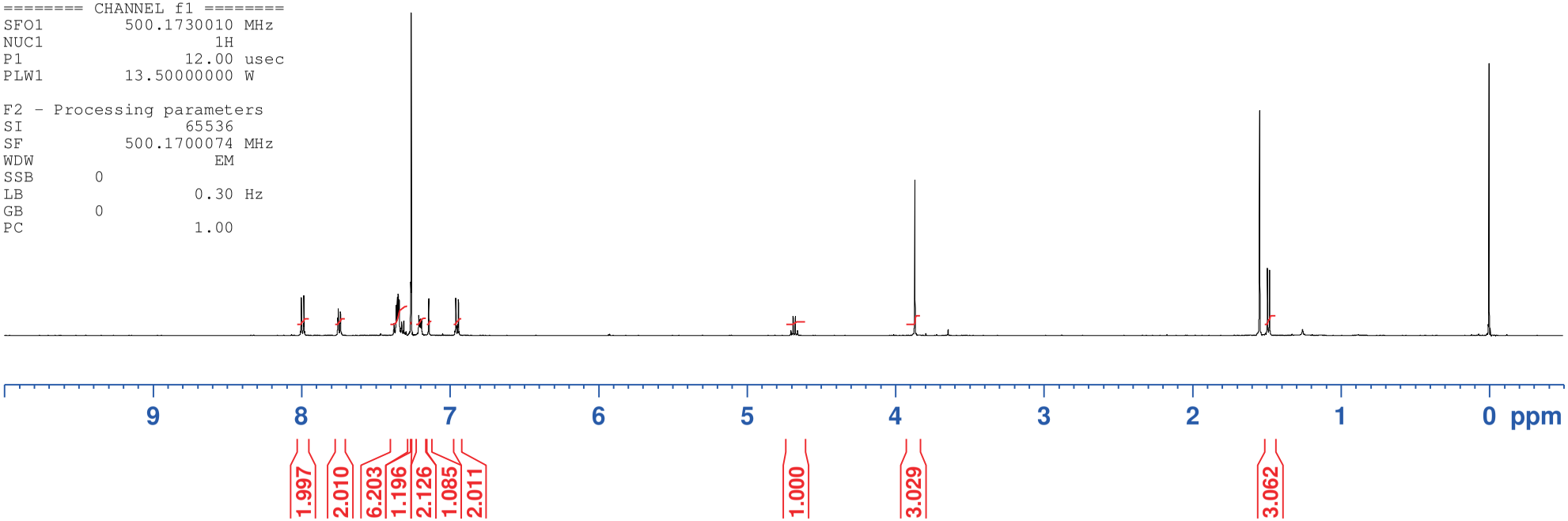
F2 - Acquisition Parameters
Date_           20161114
Time               13.11
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     1
DS                     0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  31.29
DW                 62.400 usec
DE                 10.00 usec
TE                 300.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1730010 MHz
NUC1                1H
P1                 12.00 usec
PLW1         13.50000000 W

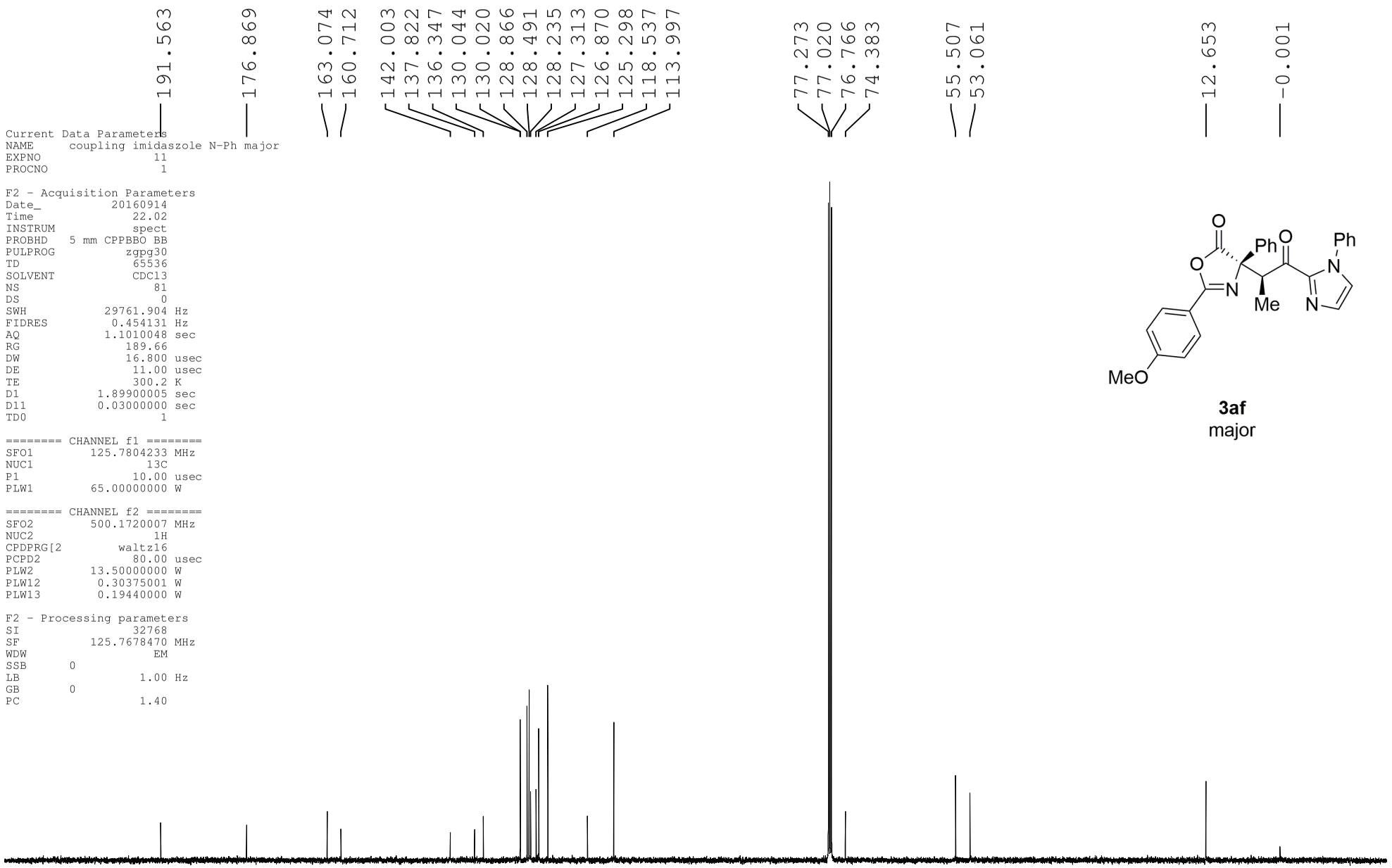
F2 - Processing parameters
SI                 65536
SF           500.1700074 MHz
WDW                  EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

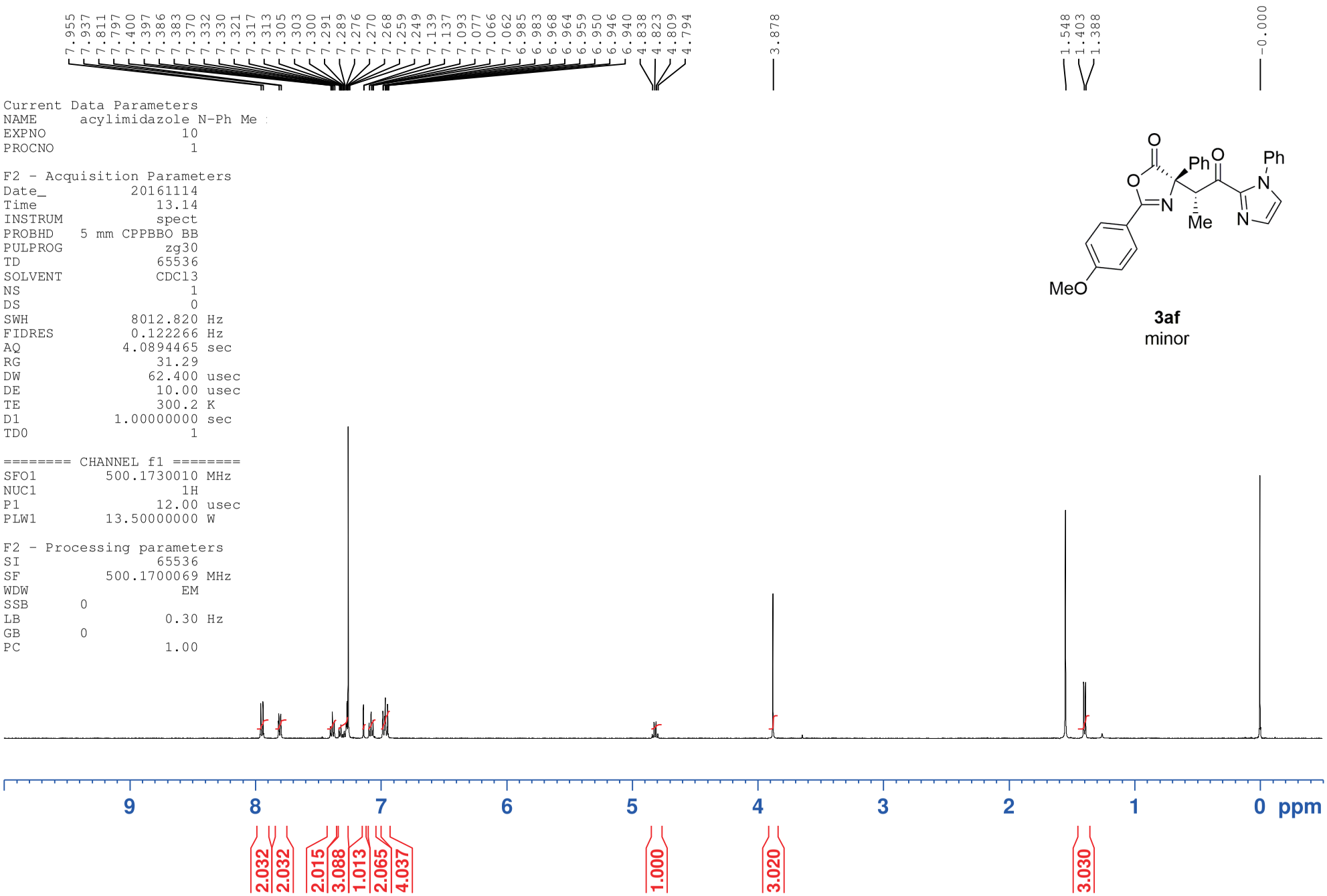


3af
major

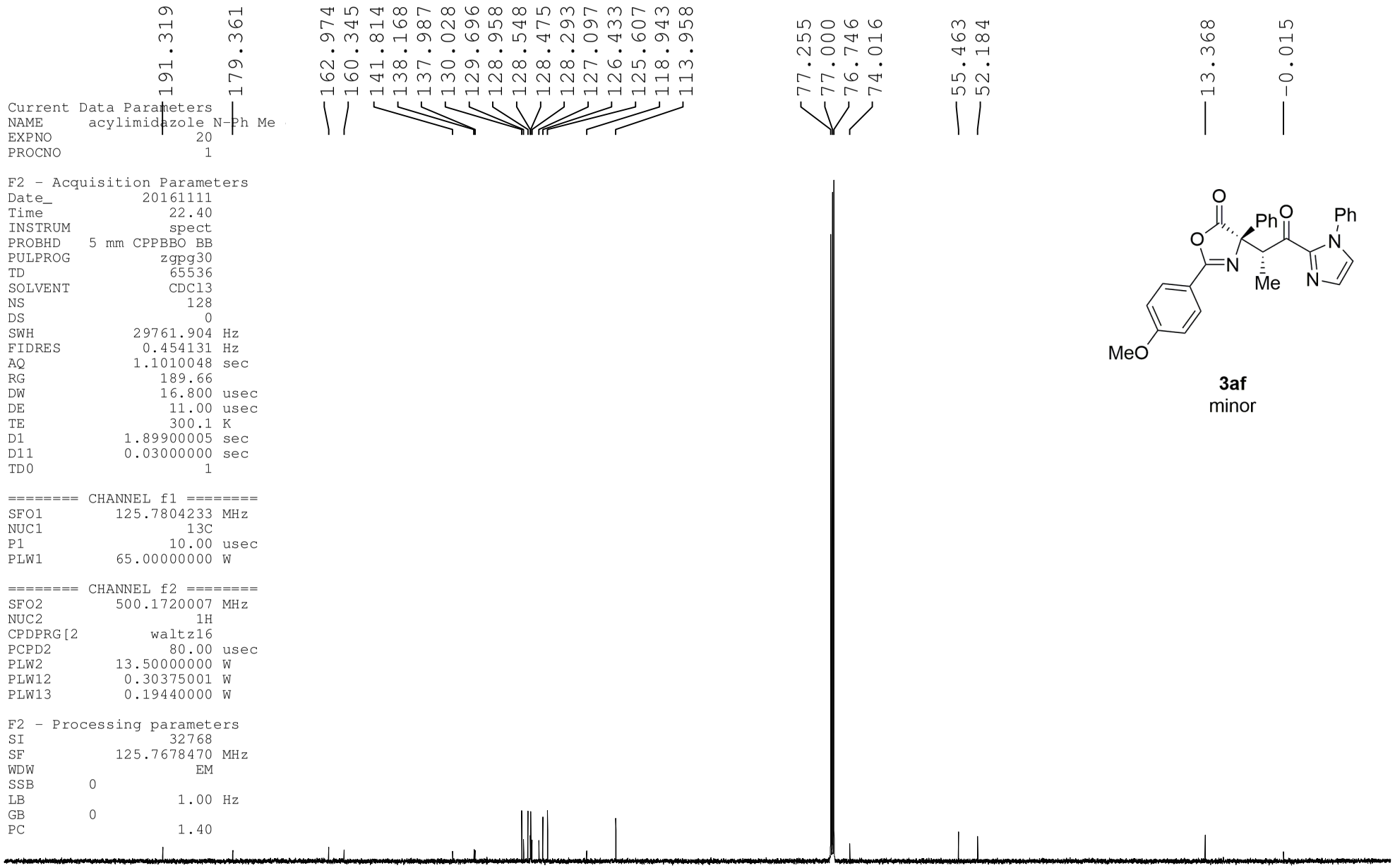


^{1}H NMR

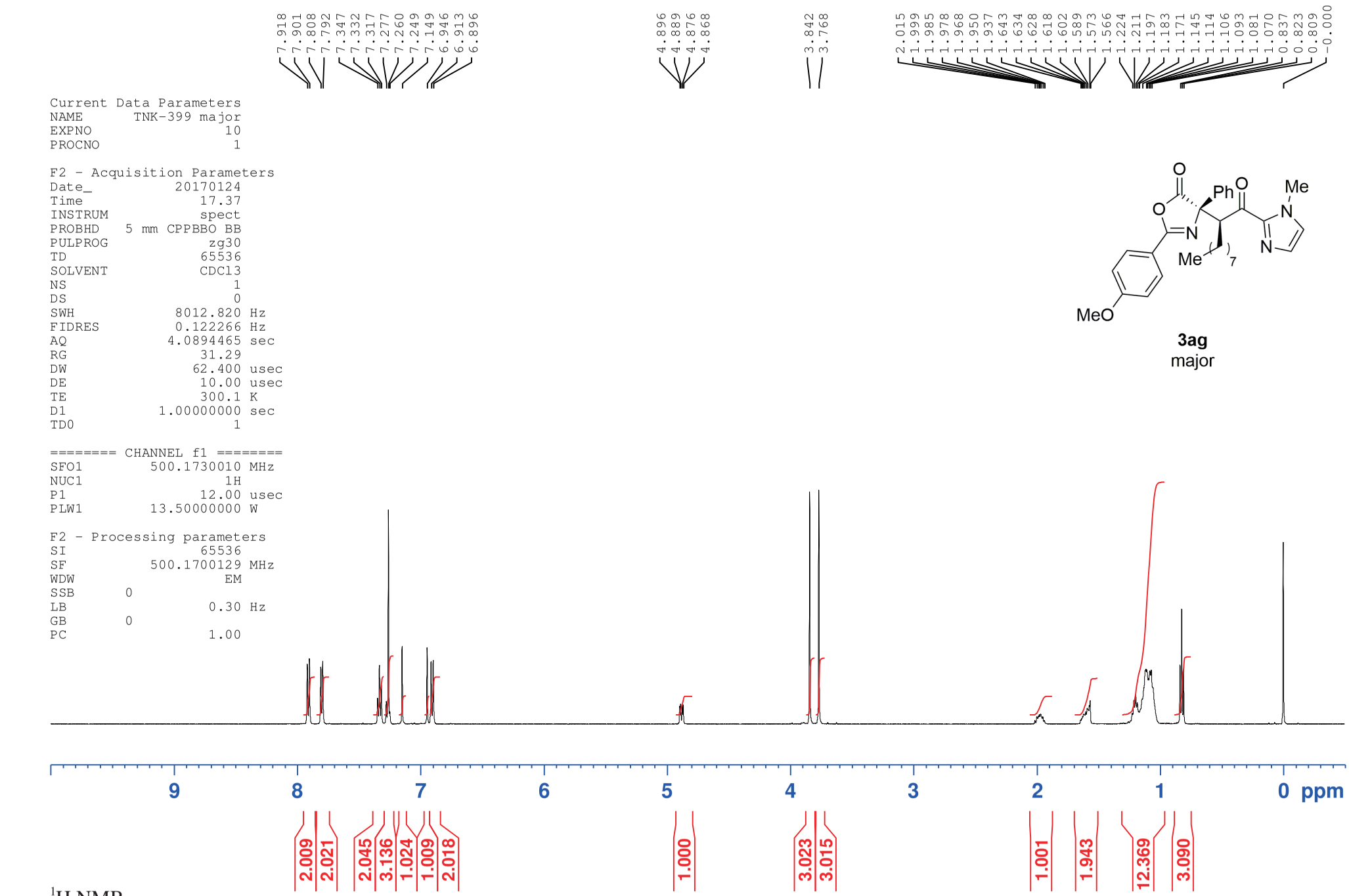

191.563
176.869
163.074
160.712
142.003
137.822
136.347
130.044
130.020
128.866
128.491
128.235
127.313
126.870
125.298
118.537
113.997
77.273
77.020
76.766
74.383
55.507
53.061
12.653
-0.001
Current Data Parameters
NAME coupling imidaszole N-Ph major
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160914
Time 22.02
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 81
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Ph
N
N
Me
N
MeO
3af
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
1H NMR


7.955
7.937
7.811
7.797
7.400
7.397
7.386
7.383
7.370
7.332
7.330
7.321
7.317
7.313
7.305
7.303
7.300
7.291
7.289
7.276
7.270
7.268
7.259
7.249
7.139
7.137
7.093
7.077
7.066
7.062
6.985
6.983
6.968
6.964
6.959
6.950
6.946
6.940
4.838
4.823
4.809
4.794
3.878
1.548
1.403
1.388
0.000
Current Data Parameters
NAME acylimidazole N-Ph Me
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161114
Time 13.14
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Ph
O
N
N
Me
N
MeO
3af
minor
9
8
7
6
5
4
3
2
1
0 ppm
2.032
2.032
2.015
3.088
1.013
2.065
4.037
1.000
3.020
3.030

^{1}H NMR


191.319
179.361
162.974
160.345
141.814
138.168
137.987
130.028
129.696
128.958
128.548
128.475
128.293
127.097
126.433
125.607
118.943
113.958
77.255
77.000
76.746
74.016
55.463
52.184
13.368
-0.015
Current Data Parameters
NAME acylimidazole N-Ph Me
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161111
Time 22.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Ph
N
N
Me
N
MeO
3af
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR


7.918
7.901
7.808
7.792
7.347
7.332
7.317
7.277
7.260
7.249
7.149
6.946
6.913
6.896
4.896
4.889
4.876
4.868
3.842
3.768
2.015
1.999
1.985
1.978
1.968
1.950
1.937
1.643
1.634
1.628
1.618
1.602
1.589
1.573
1.566
1.224
1.211
1.197
1.183
1.171
1.145
1.114
1.106
1.093
1.081
1.070
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0.823
0.809
0.000
Current Data Parameters
NAME TNK-399 major
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170124
Time 17.37
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
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NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
O
N
N
Me
7
MeO
3ag
major
9
8
7
6
5
4
3
2
1
0 ppm
2.009
2.021
2.045
3.136
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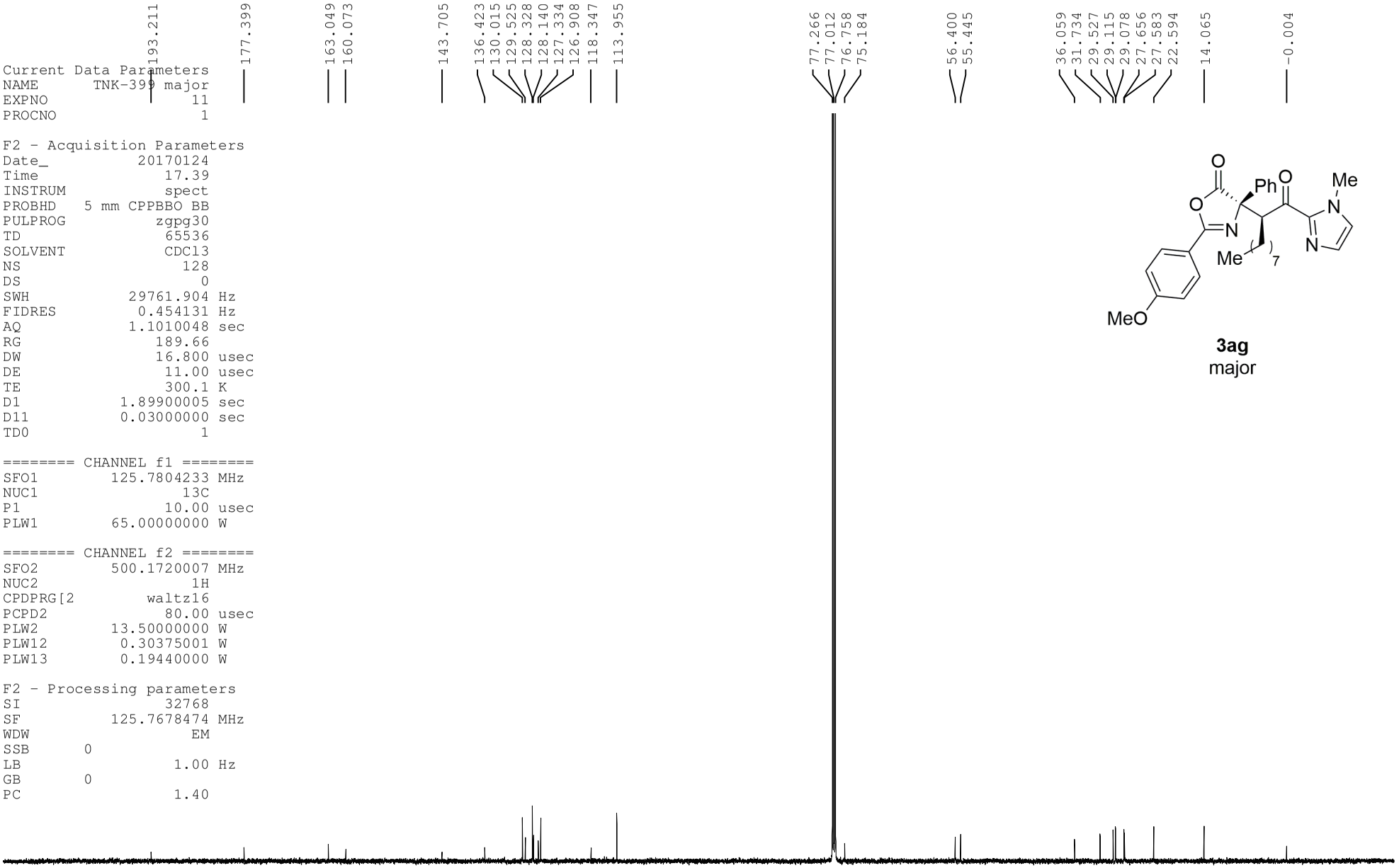
2.018
1.000
3.023
3.015
1.001
1.943
12.369
3.090

^{1}H NMR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143.705
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127.334
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113.955
77.266
77.012
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75.184
56.400
55.445
36.059
31.734
29.527
29.115
29.078
27.656
27.583
22.594
14.065
-0.004
Current Data Parameters
NAME TNK-399 major
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170124
Time 17.39
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678474 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
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Me
7
MeO
3ag
major
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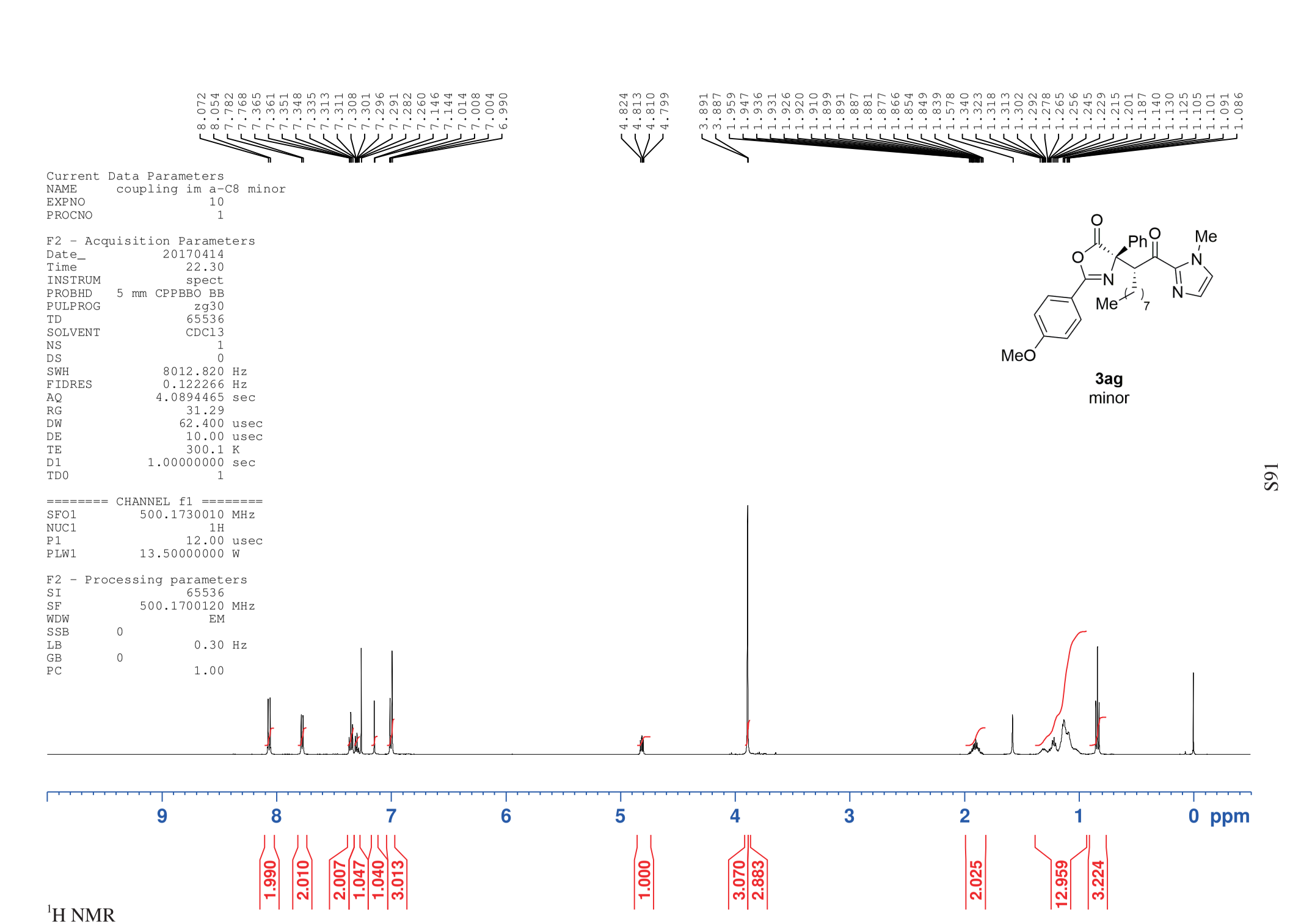
^{13}C NMR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7.365
7.361
7.351
7.348
7.335
7.313
7.311
7.308
7.301
7.296
7.291
7.282
7.260
7.146
7.144
7.014
7.008
7.004
6.990
4.824
4.813
4.810
4.799
3.891
3.887
1.959
1.947
1.936
1.931
1.926
1.920
1.910
1.899
1.891
1.887
1.881
1.877
1.866
1.854
1.849
1.839
1.578
1.340
1.323
1.318
1.313
1.302
1.292
1.278
1.265
1.256
1.245
1.229
1.215
1.201
1.187
1.140
1.130
1.125
1.105
1.101
1.091
1.086
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NAME coupling im a-C8 minor
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.30
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
N
Me
7
MeO
3ag
minor
9
8
7
6
5
4
3
2
1
0 ppm
1.990
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1.040
3.013
1.000
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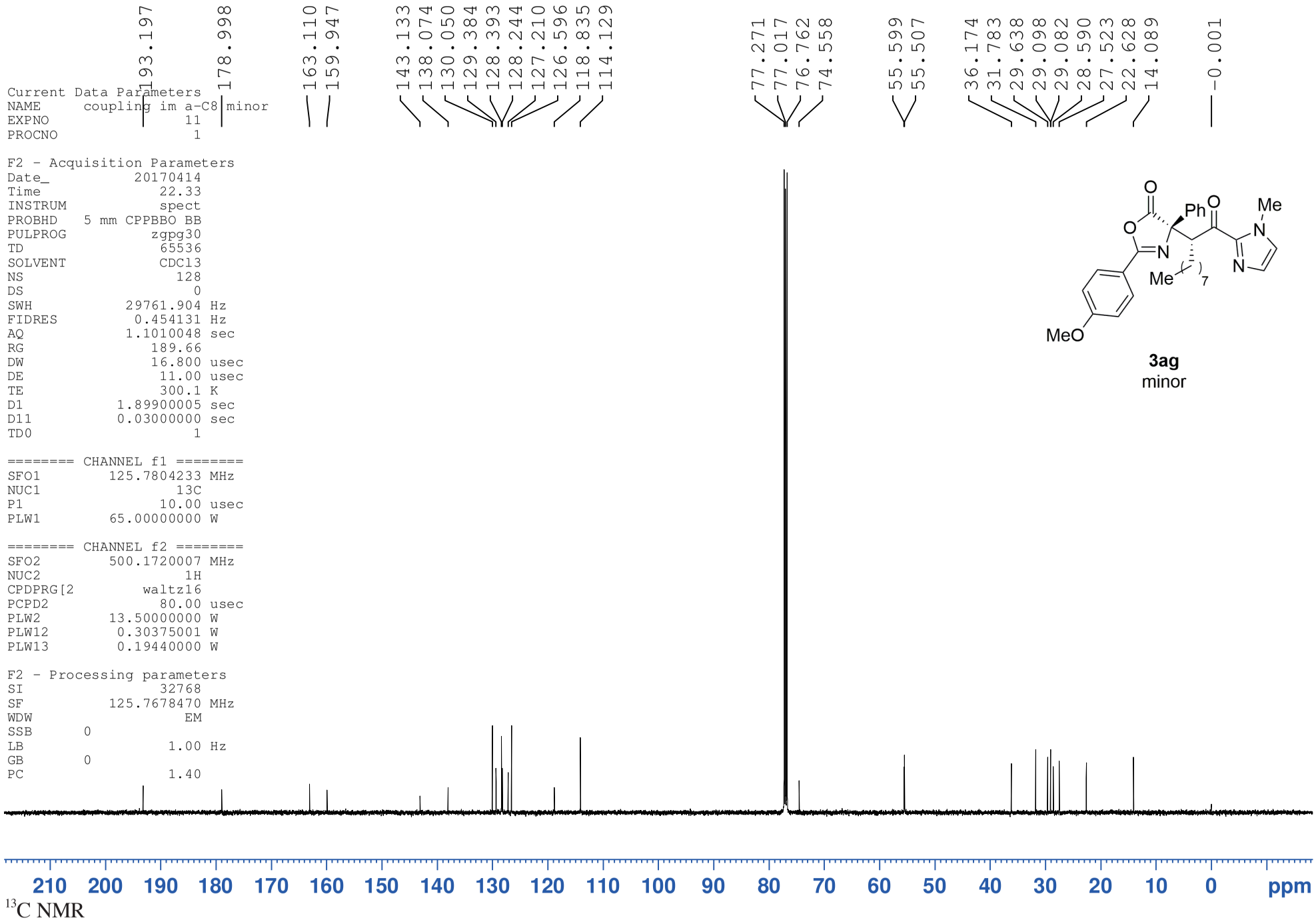
2.025
12.959
3.224

^{1}H NMR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138.074
130.050
129.384
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128.244
127.210
126.596
118.835
114.129
77.271
77.017
76.762
74.558
55.599
55.507
36.174
31.783
29.638
29.098
29.082
28.590
27.523
22.628
14.089
-0.001
Current Data Parameters
NAME coupling im a-C8 minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.33
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Me
7
N
MeO
3ag
minor
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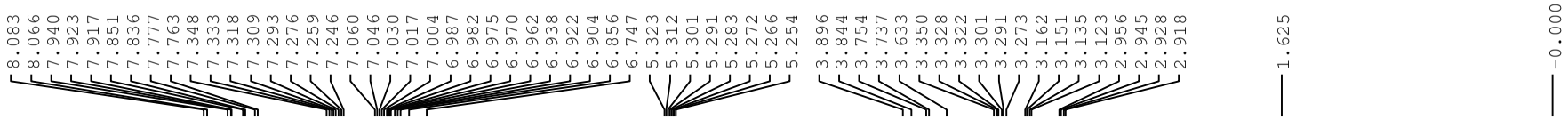
^{13}C NMR

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Current Data Parameters
NAME      couplng azlactone b-Ph
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_            20170207
Time                16.52
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      1
DS                      0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  31.29
DW                 62.400 usec
DE                 10.00 usec
TE                 300.1 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         500.1730010 MHz
NUC1                1H
P1                 12.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                  65536
SF           500.1700114 MHz
WDW                 EM
SSB       0
LB                  0.30 Hz
GB        0
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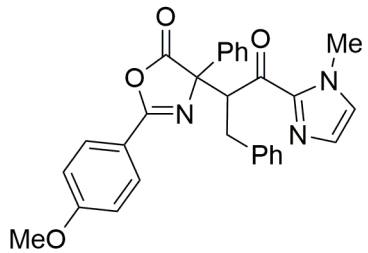
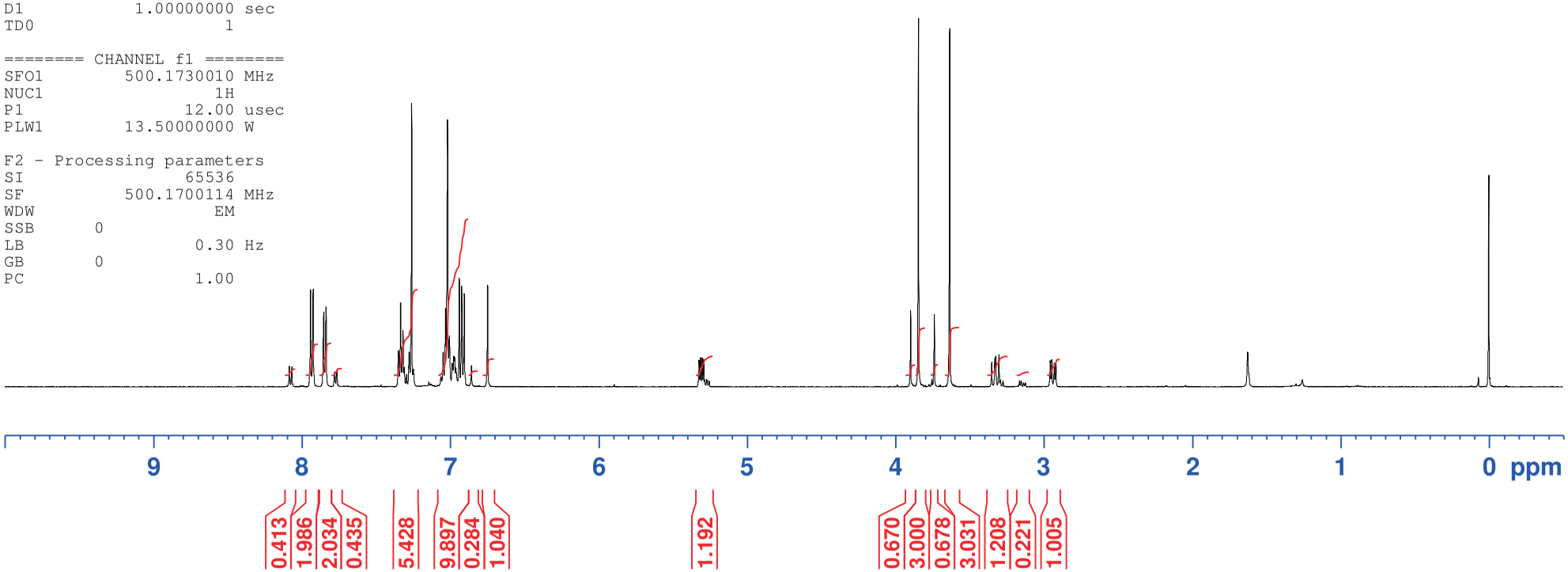
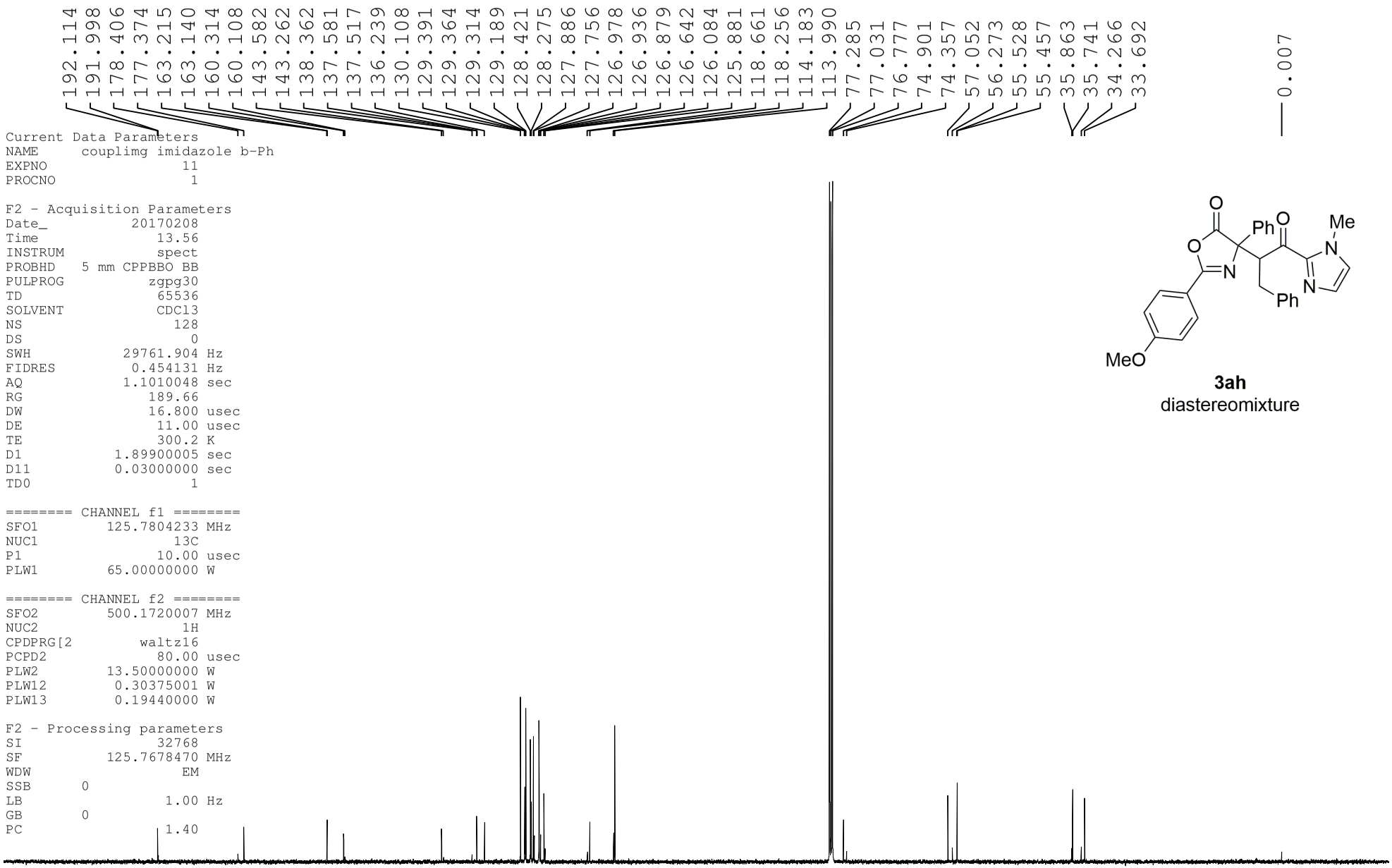


3ah
diastereomixture



^{1}H NMR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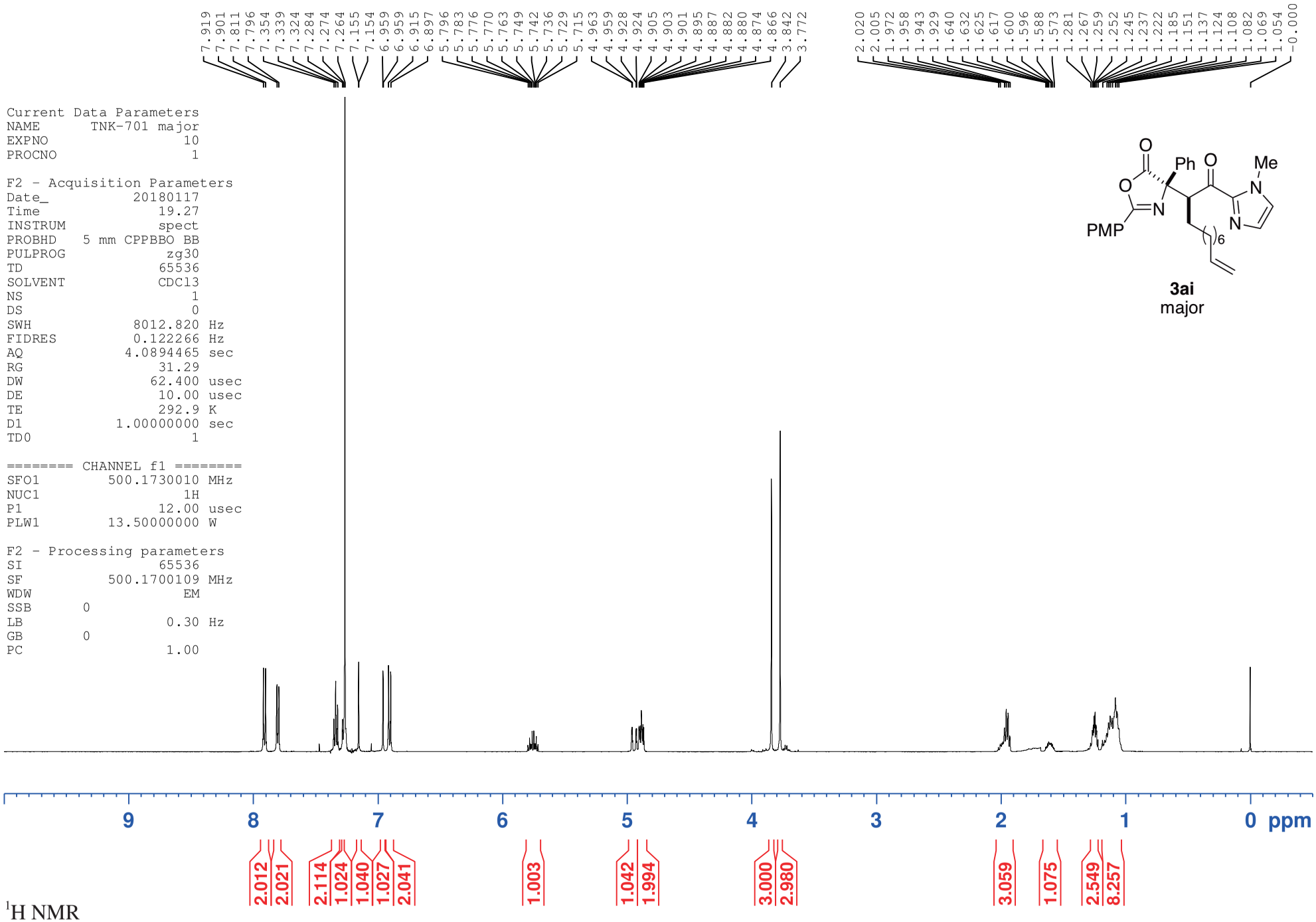
177.374
163.215
163.140
160.314
160.108
143.582
143.262
138.362
137.581
137.517
136.239
130.108
129.391
129.364
129.314
129.189
128.421
128.275
127.886
127.756
126.978
126.936
126.879
126.642
126.084
125.881
118.661
118.256
114.183
113.990
77.285
77.031
76.777
74.901
74.357
57.052
56.273
55.528
55.457
35.863
35.741
34.266
33.692
0.007
Current Data Parameters
NAME couplimg imidazole b-Ph
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170208
Time 13.56
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Ph
MeO
3ah
diastereomixture
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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7.264
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7.154
6.959
6.959
6.915
6.897
5.796
5.783
5.776
5.770
5.763
5.749
5.742
5.736
5.729
5.715
4.963
4.959
4.928
4.924
4.905
4.903
4.901
4.895
4.887
4.882
4.880
4.874
4.866
3.842
3.772
2.020
2.005
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1.958
1.943
1.929
1.640
1.632
1.625
1.617
1.600
1.596
1.588
1.573
1.281
1.267
1.259
1.252
1.245
1.237
1.222
1.185
1.151
1.137
1.124
1.108
1.082
1.069
1.054
-0.000
Current Data Parameters
NAME TNK-701 major
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180117
Time 19.27
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
PMP
N
6
3ai
major
9
8
7
6
5
4
3
2
1
0 ppm
2.012
2.021
2.114
1.024
1.040
1.027
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1.042
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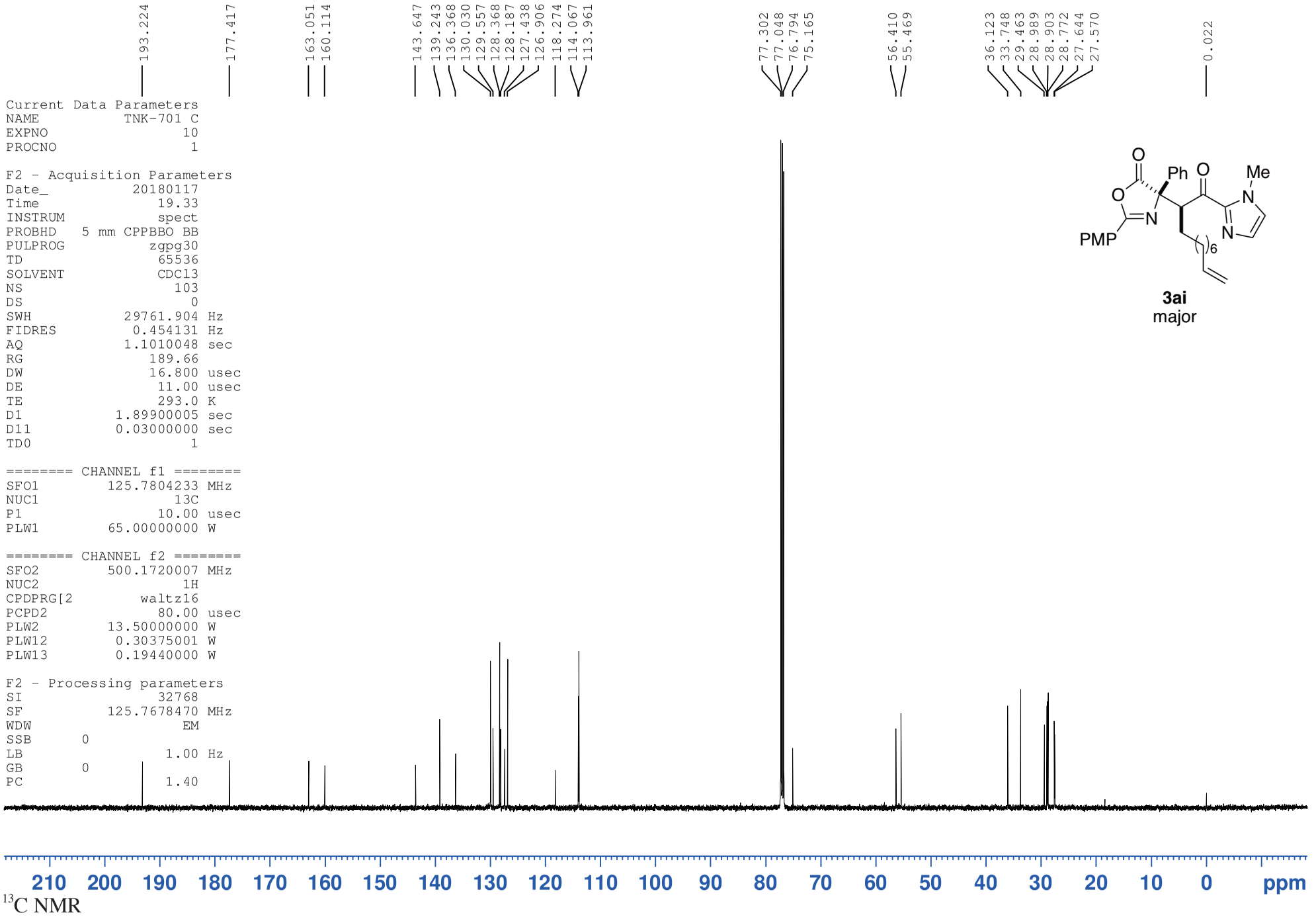
8.257

^{1}H NMR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128.368
128.187
127.438
126.906
118.274
114.067
113.961
77.302
77.048
76.794
75.165
56.410
55.469
36.123
33.748
29.463
28.989
28.903
28.772
27.644
27.570
0.022
Current Data Parameters
NAME TNK-701 C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180117
Time 19.33
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 103
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 293.0 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
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major
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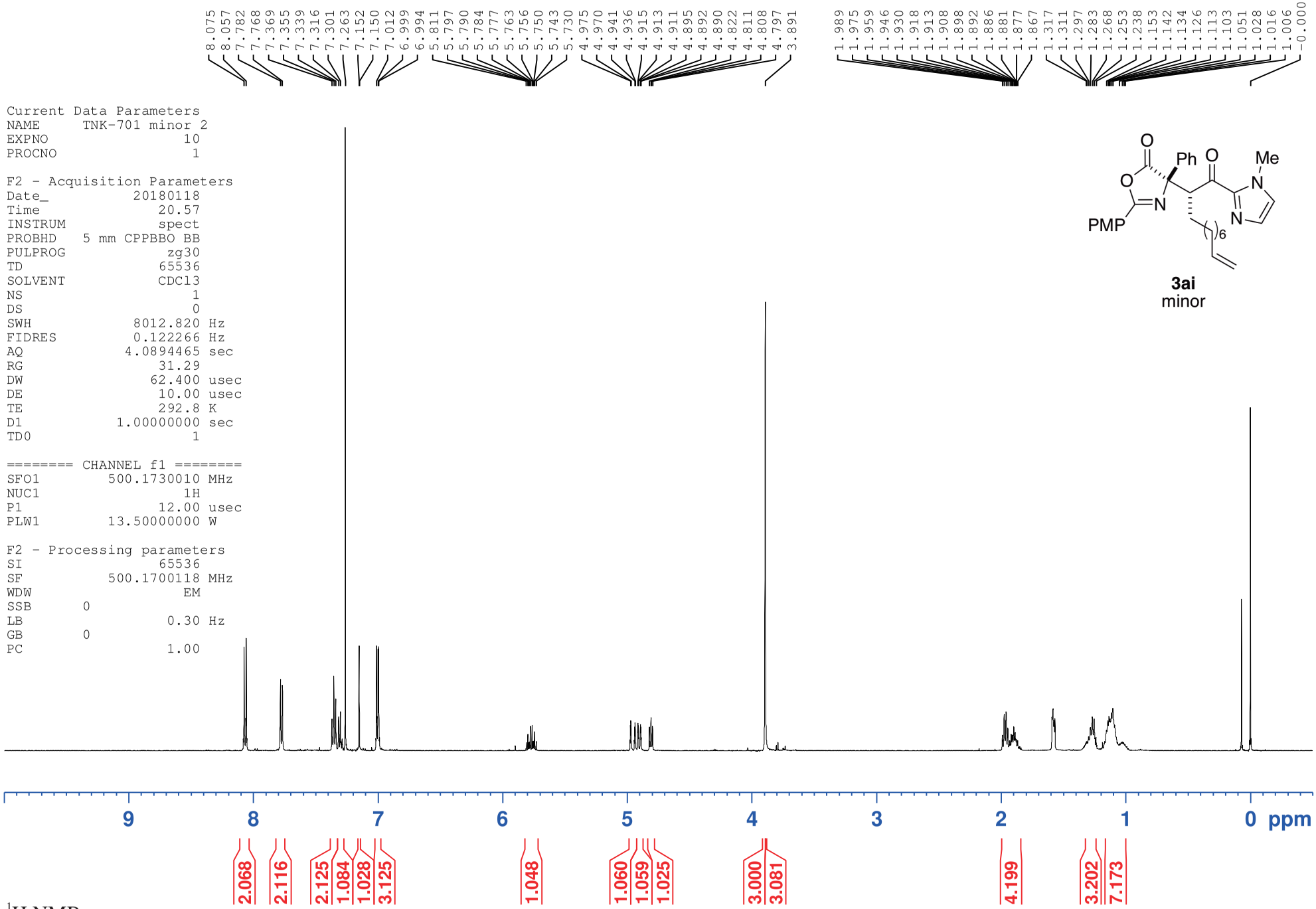
^{13}C NMR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7.768
7.369
7.355
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7.263
7.152
7.150
7.012
6.999
6.994
5.811
5.797
5.790
5.784
5.777
5.763
5.756
5.750
5.743
5.730
4.975
4.970
4.941
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4.915
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4.911
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4.822
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1.892
1.886
1.881
1.877
1.867
1.317
1.311
1.297
1.283
1.268
1.253
1.238
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1.142
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1.126
1.113
1.103
1.051
1.028
1.016
1.006
0.000
Current Data Parameters
NAME TNK-701 minor 2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180118
Time 20.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
PMP
N
6
3ai
minor
9
8
7
6
5
4
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2
1
0 ppm
2.068
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2.125
1.084
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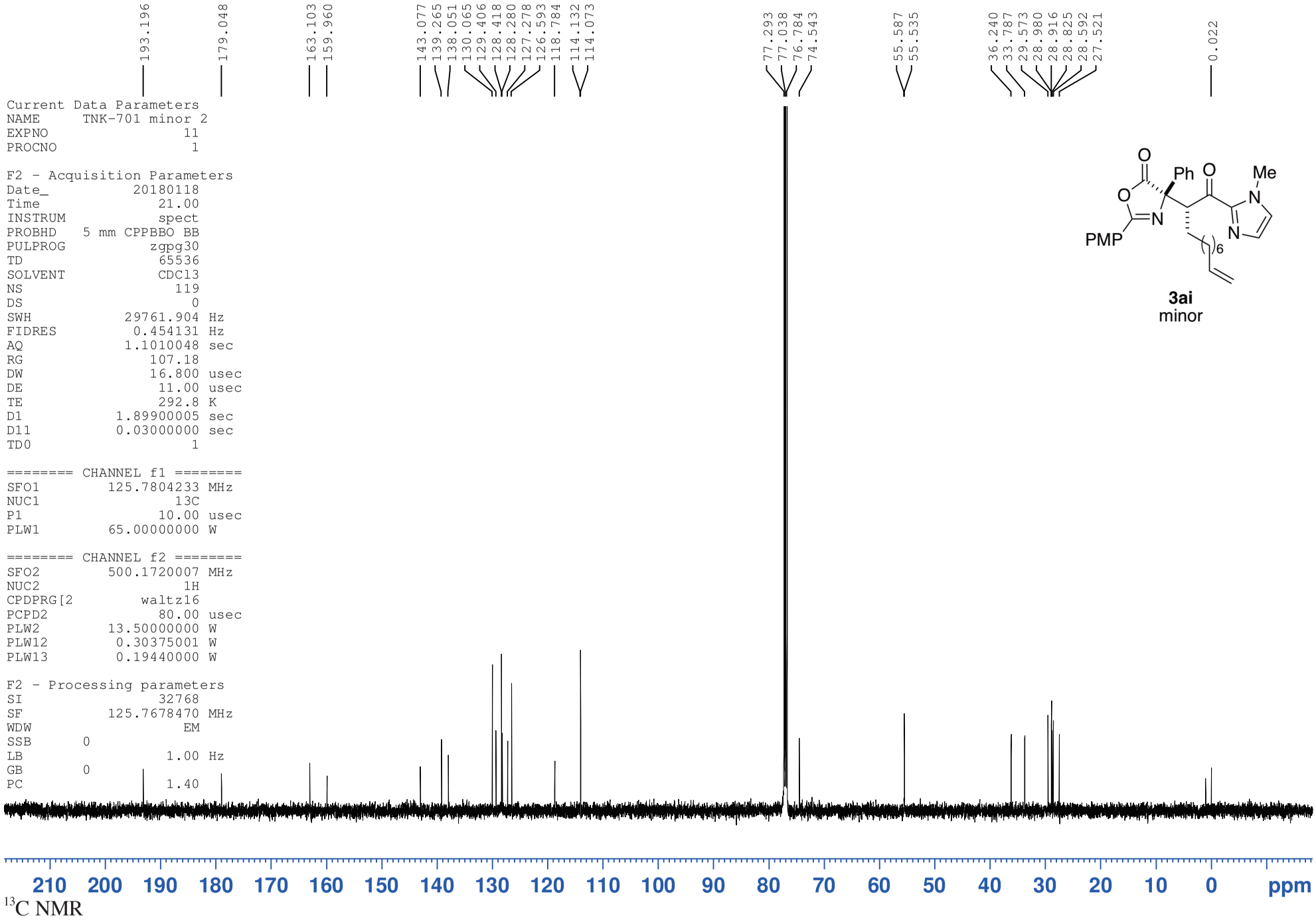
7.173

^{1}H NMR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118.784
114.132
114.073
77.293
77.038
76.784
74.543
55.587
55.535
36.240
33.787
29.573
28.980
28.916
28.825
28.592
27.521
0.022
Current Data Parameters
NAME TNK-701 minor 2
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180118
Time 21.00
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 119
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 292.8 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
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PMP
N
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minor
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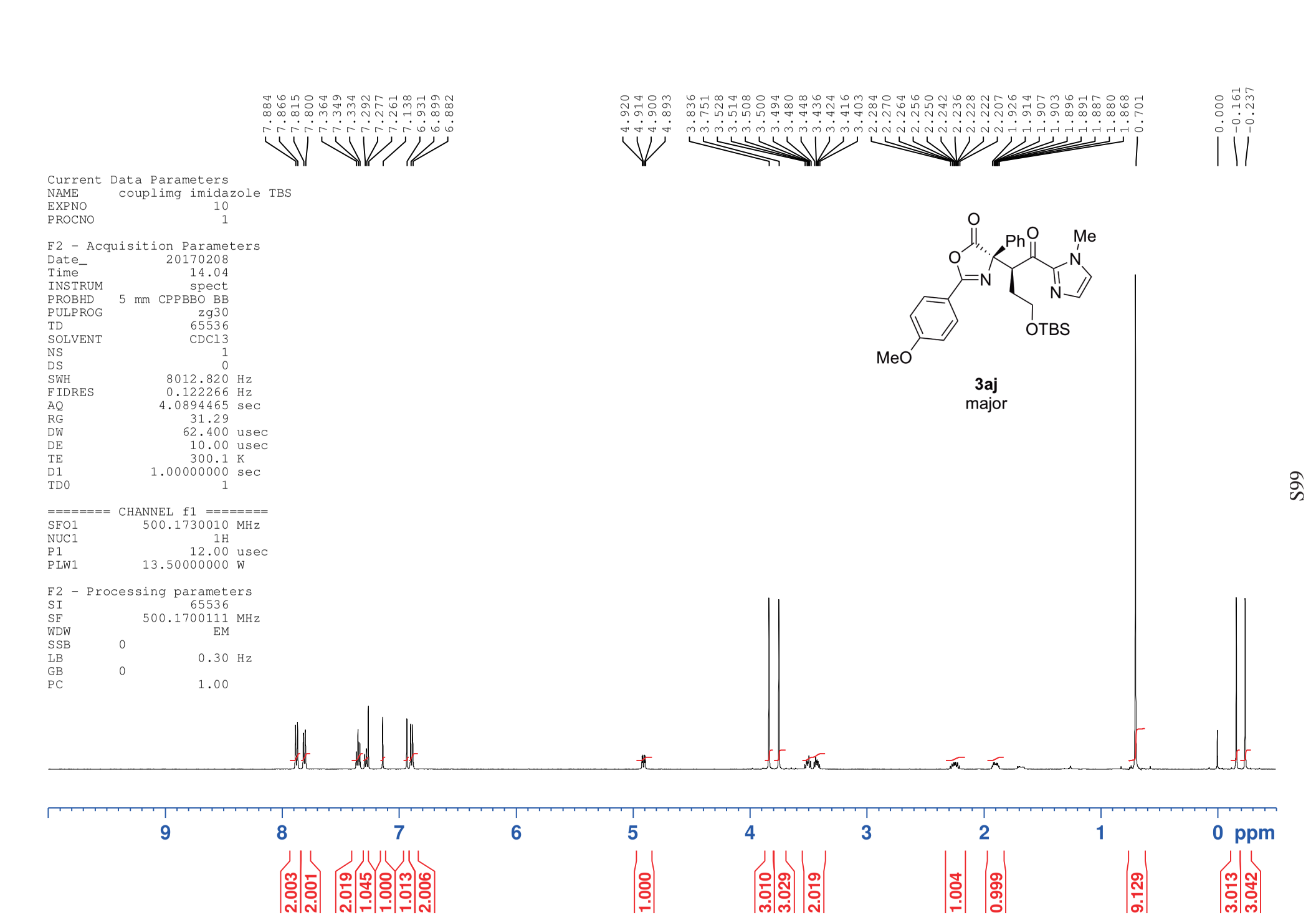
^{13}C NMR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6.899
6.882
4.920
4.914
4.900
4.893
3.836
3.751
3.528
3.514
3.508
3.500
3.494
3.480
3.448
3.436
3.424
3.416
3.403
2.284
2.270
2.264
2.256
2.250
2.242
2.236
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2.207
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1.914
1.907
1.903
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1.887
1.880
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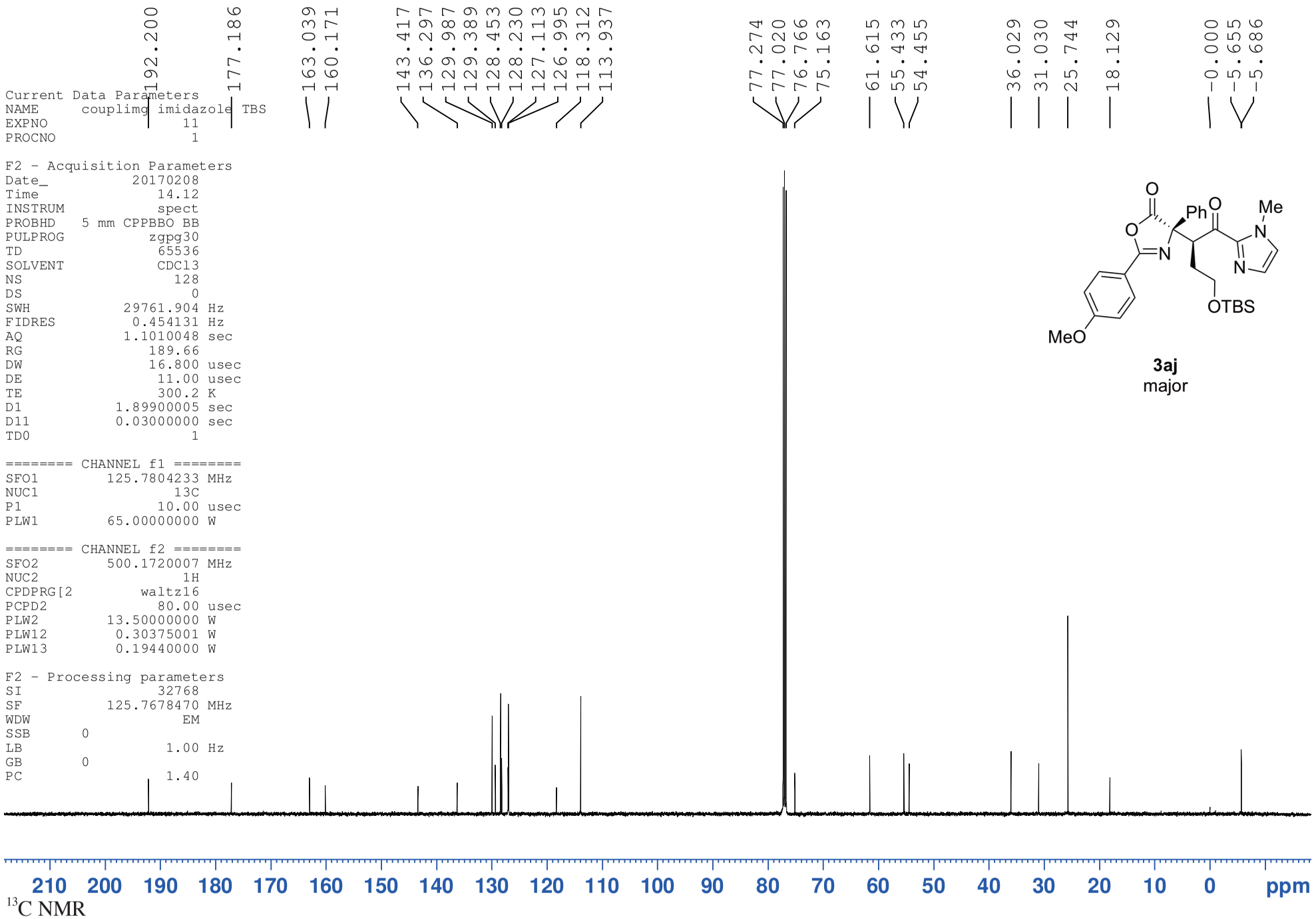
-0.161
-0.237
Current Data Parameters
NAME couplimg imidazole TBS
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170208
Time 14.04
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
N
OTBS
MeO
3aj
major
9
8
7
6
5
4
3
2
1
0
ppm
2.003
2.001
2.019
1.045
1.000
1.013
2.006
1.000
3.010
3.029
2.019
1.004
0.999
9.129
3.013
3.042

^{1}H NMR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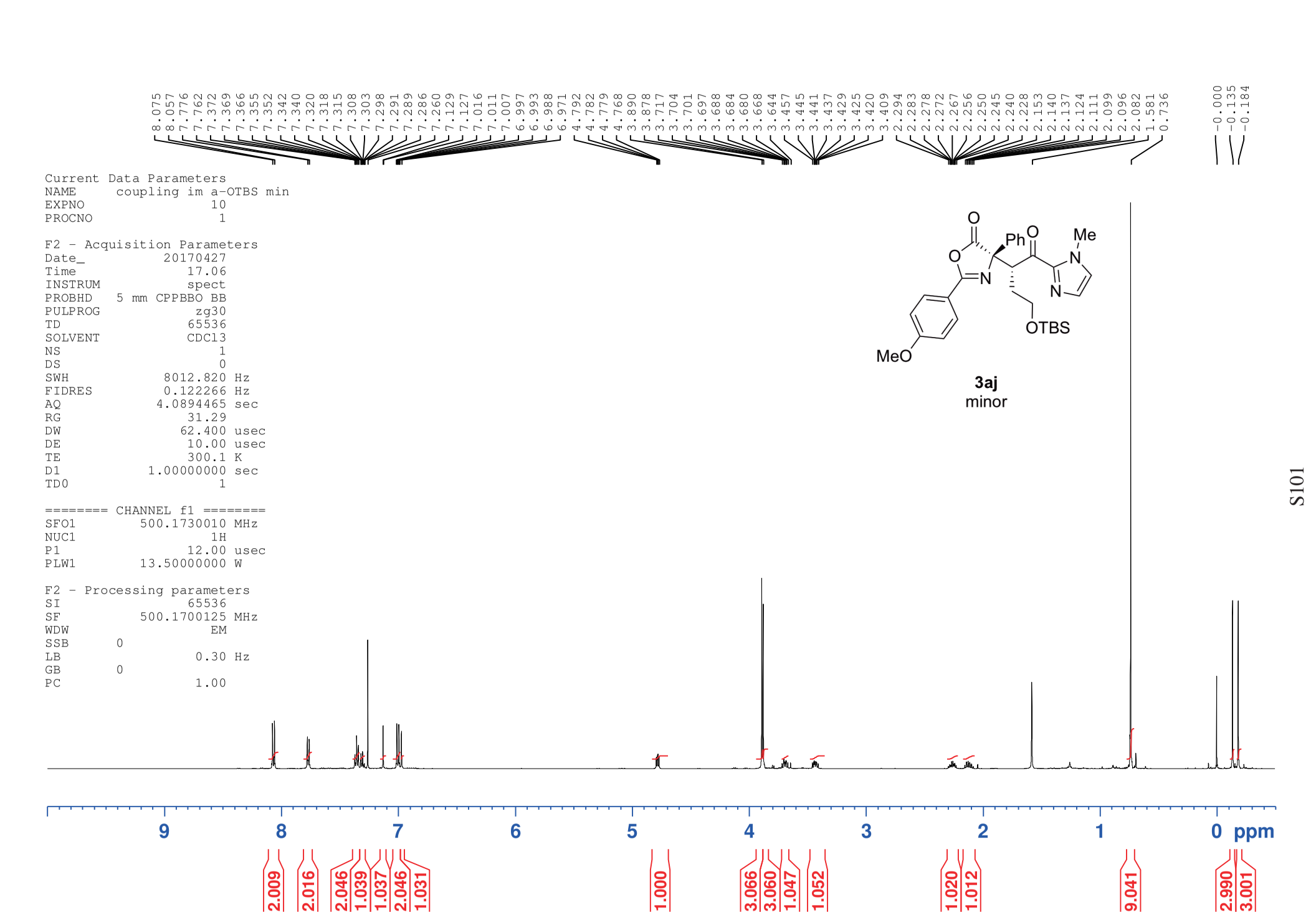
163.039
160.171
143.417
136.297
129.987
129.389
128.453
128.230
127.113
126.995
118.312
113.937
77.274
77.020
76.766
75.163
61.615
55.433
54.455
36.029
31.030
25.744
18.129
-0.000
-5.655
-5.686
Current Data Parameters
NAME coupling imidazole TBS
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170208
Time 14.12
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
N
N
N
OTBS
MeO
3aj
major
S100
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
13C NMR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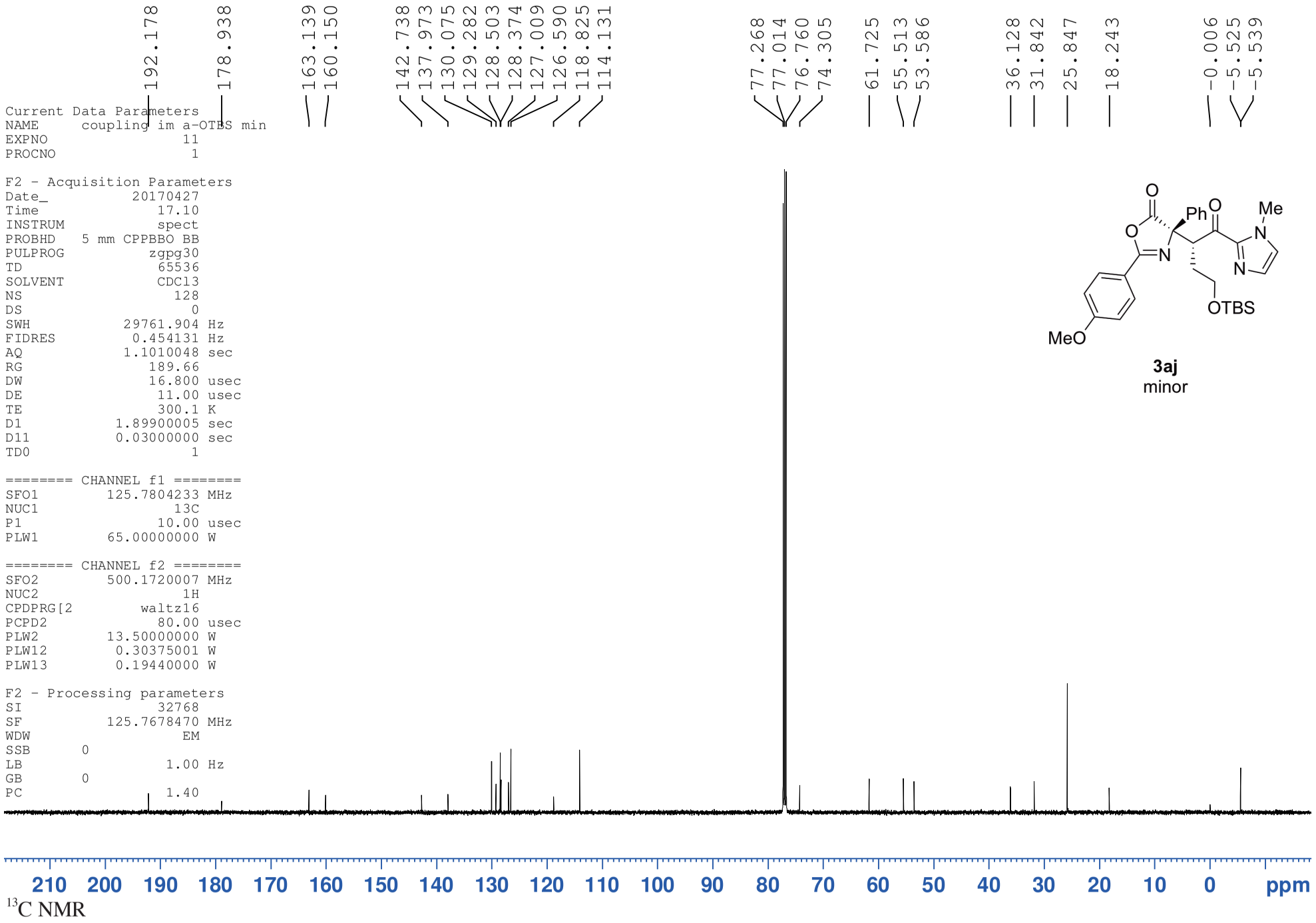
8.057
7.776
7.762
7.372
7.369
7.366
7.355
7.352
7.342
7.340
7.320
7.318
7.315
7.308
7.303
7.298
7.291
7.289
7.286
7.260
7.129
7.127
7.016
7.011
7.007
6.997
6.993
6.988
6.971
4.792
4.782
4.779
4.768
3.890
3.878
3.717
3.704
3.701
3.697
3.688
3.684
3.680
3.668
3.644
3.457
3.445
3.441
3.437
3.429
3.425
3.420
3.409
2.294
2.283
2.278
2.272
2.267
2.256
2.250
2.245
2.240
2.228
2.153
2.140
2.137
2.124
2.111
2.099
2.096
2.082
1.581
0.736
-0.000
-0.135
-0.184
Current Data Parameters
NAME coupling im a-OTBS min
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170427
Time 17.06
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
N
OTBS
MeO
3aj
minor
9
8
7
6
5
4
3
2
1
0 ppm
2.009
2.016
2.046
1.039
1.037
2.046
1.031
1.000
3.066
3.060
1.047
1.052
1.020
1.012
9.041
2.990
3.001

^{1}H NMR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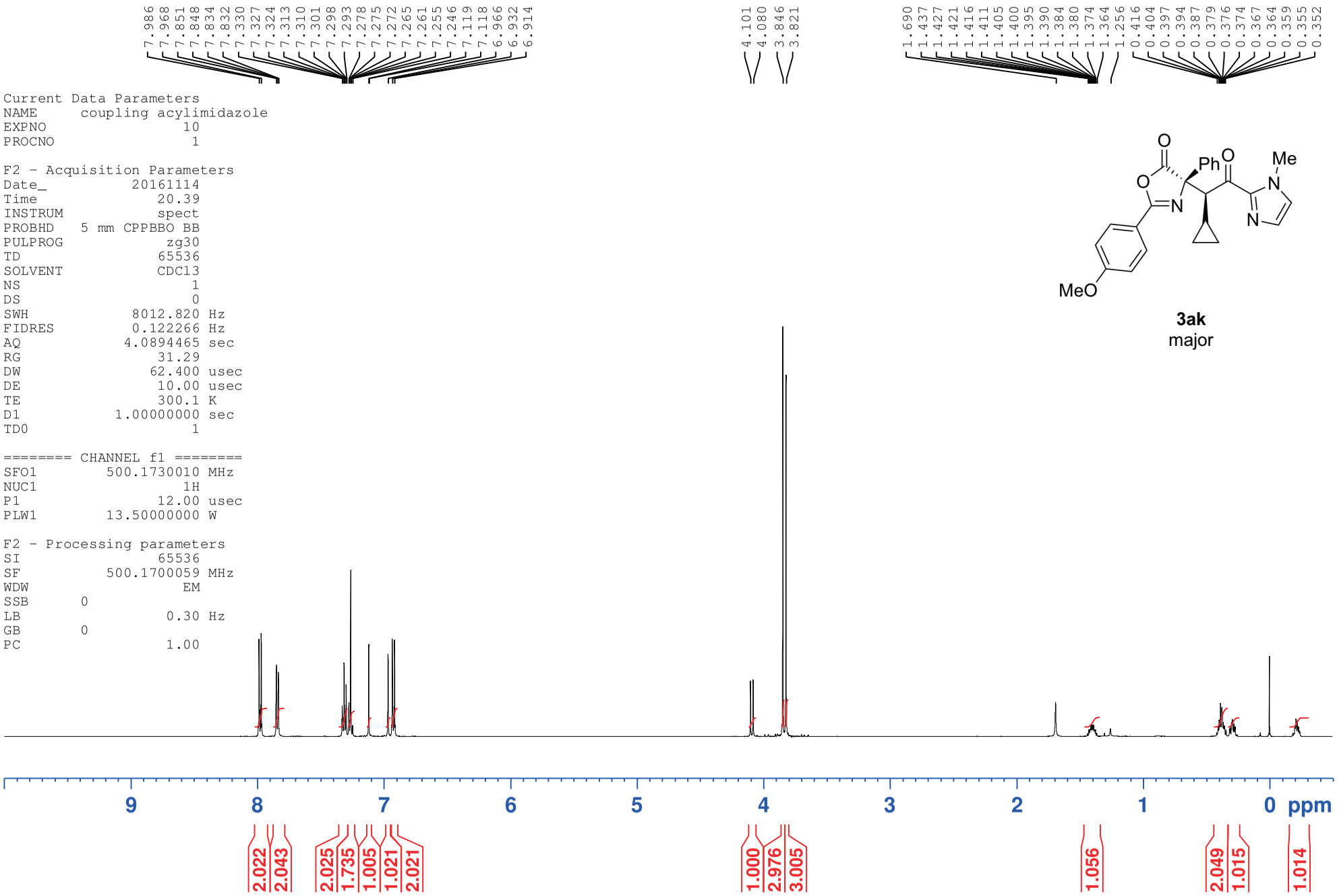
178.938
163.139
160.150
142.738
137.973
130.075
129.282
128.503
128.374
127.009
126.590
118.825
114.131
77.268
77.014
76.760
74.305
61.725
55.513
53.586
36.128
31.842
25.847
18.243
-0.006
-5.525
-5.539
Current Data Parameters
NAME coupling im a-OTBS min
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170427
Time 17.10
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
N
OTBS
MeO
3aj
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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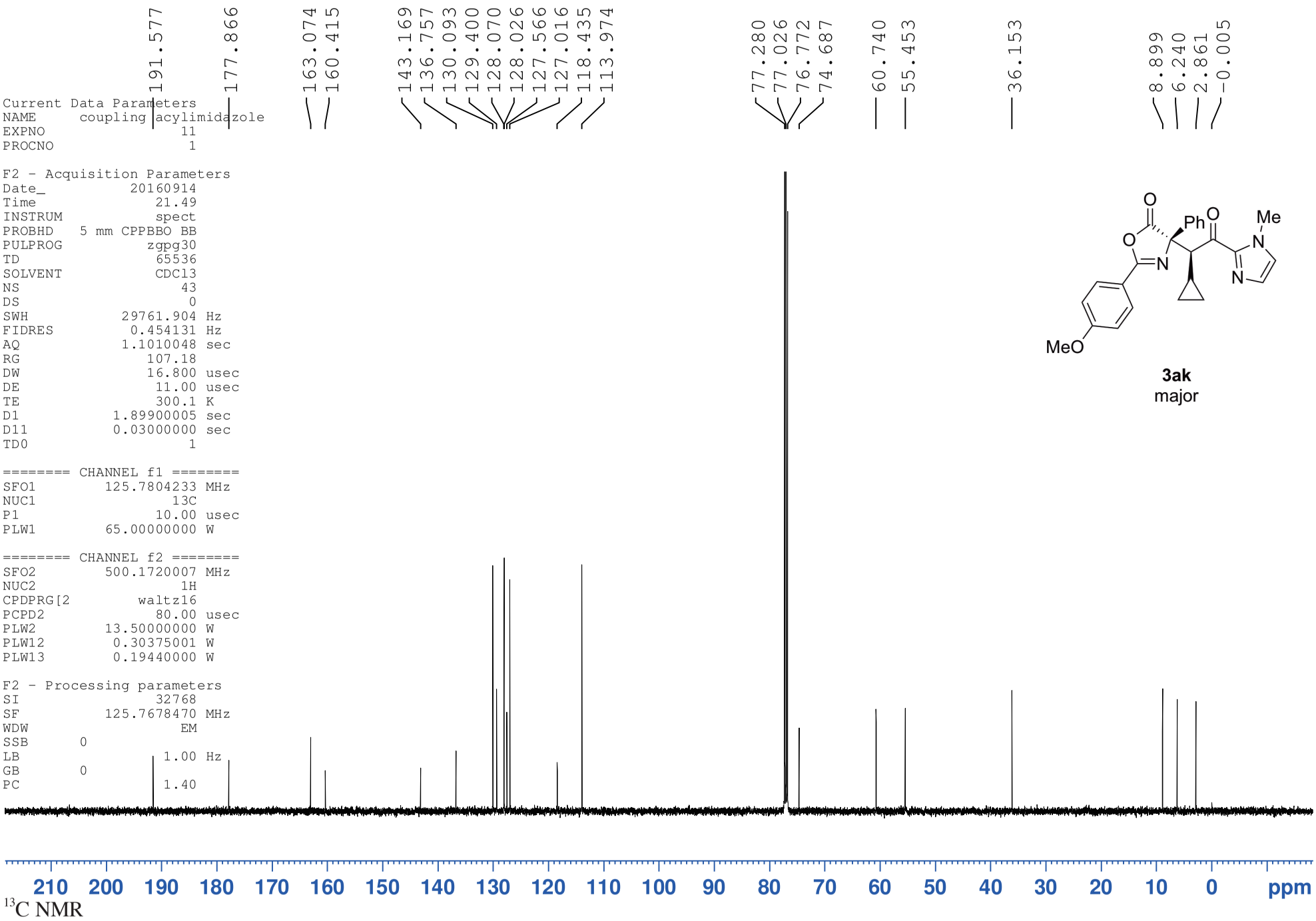
7.851
7.848
7.834
7.832
7.330
7.327
7.324
7.313
7.310
7.301
7.298
7.293
7.278
7.275
7.272
7.265
7.261
7.255
7.246
7.119
7.118
6.966
6.932
6.914
4.101
4.080
3.846
3.821
1.690
1.437
1.427
1.421
1.416
1.411
1.405
1.400
1.395
1.390
1.384
1.380
1.374
1.364
1.256
0.416
0.404
0.397
0.394
0.387
0.379
0.376
0.374
0.367
0.364
0.359
0.355
0.352
Current Data Parameters
NAME coupling acylimidazole
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161114
Time 20.39
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
N
MeO
3ak
major
9
8
7
6
5
4
3
2
1
0 ppm
2.022
2.043
2.025
1.735
1.005
1.021
2.021
1.000
2.976
3.005
1.056
2.049
1.015
1.014

^{1}H NMR


191.577
177.866
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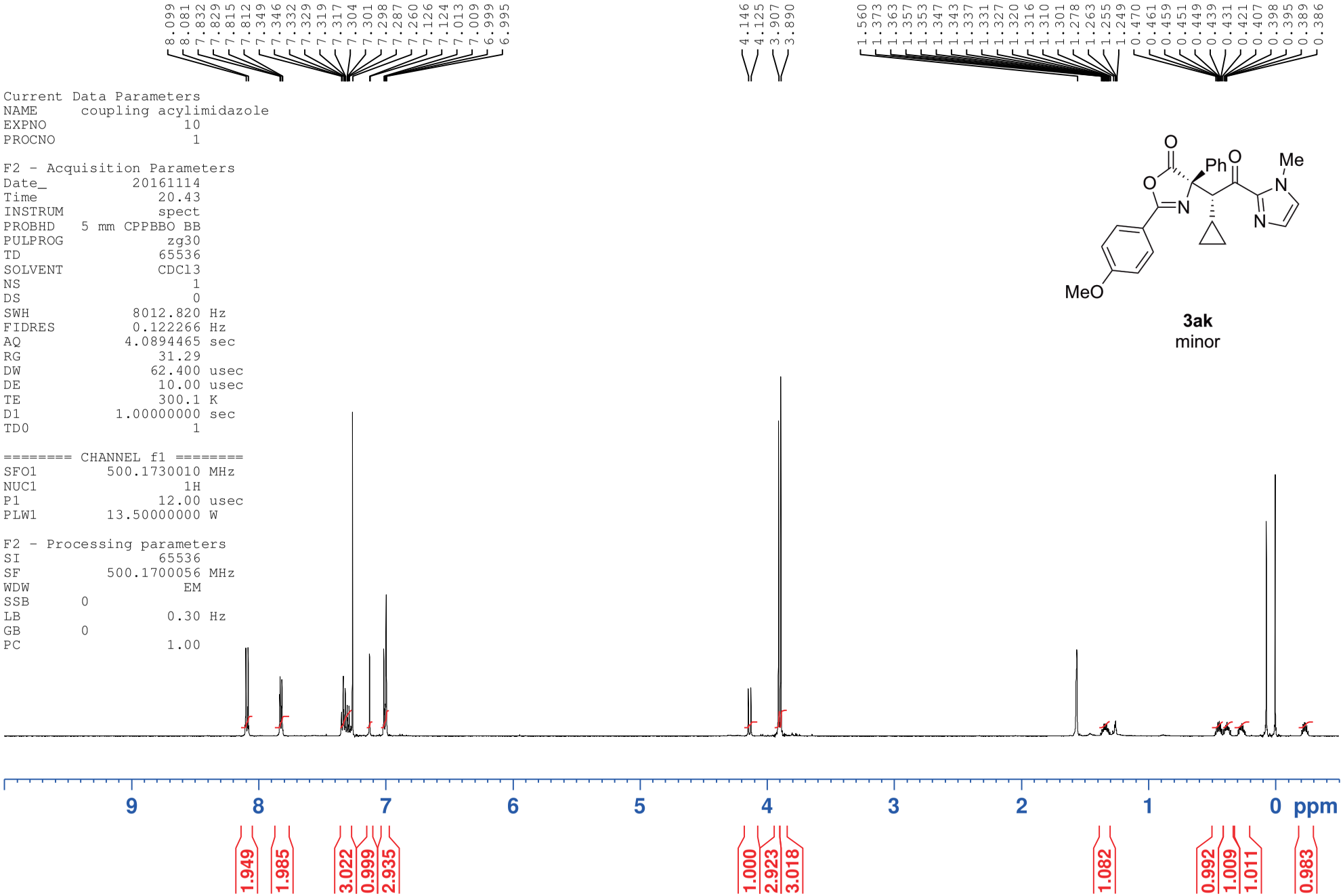
160.415
143.169
136.757
130.093
129.400
128.070
128.026
127.566
127.016
118.435
113.974
77.280
77.026
76.772
74.687
60.740
55.453
36.153
8.899
6.240
2.861
-0.005
Current Data Parameters
NAME coupling acylimidazole
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160914
Time 21.49
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 43
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
N
MeO
3ak
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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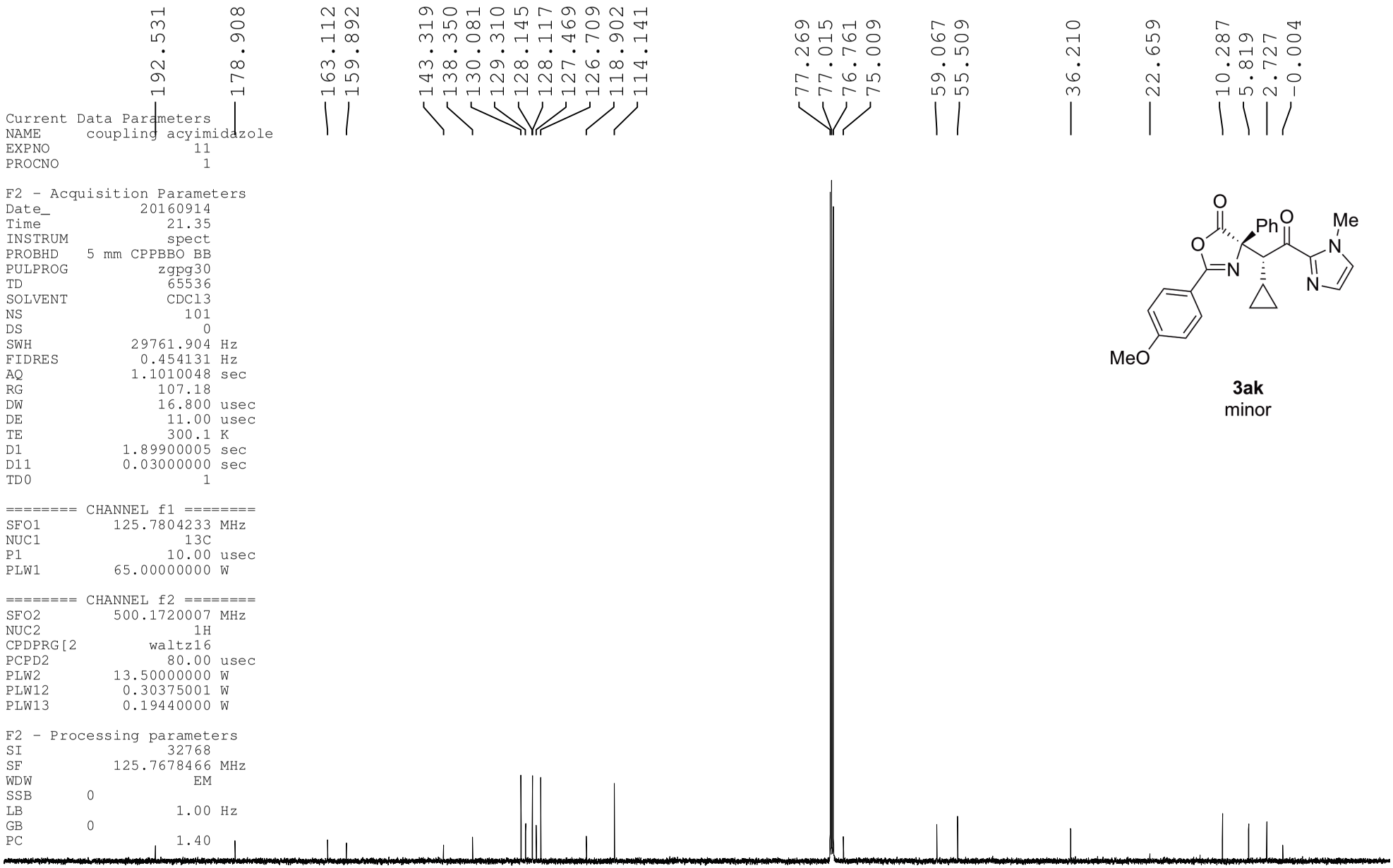
7.832
7.829
7.815
7.812
7.349
7.346
7.332
7.329
7.319
7.317
7.304
7.301
7.298
7.287
7.260
7.126
7.124
7.013
7.009
6.995
4.146
4.125
3.907
3.890
1.560
1.373
1.363
1.357
1.353
1.347
1.343
1.337
1.331
1.327
1.320
1.316
1.310
1.301
1.278
1.263
1.255
1.249
0.470
0.461
0.459
0.451
0.449
0.439
0.431
0.421
0.407
0.398
0.395
0.389
0.386
Current Data Parameters
NAME coupling acylimidazole
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161114
Time 20.43
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
N
MeO
3ak
minor
9
8
7
6
5
4
3
2
1
0
ppm
1.949
1.985
3.022
0.999
2.935
1.000
2.923
3.018
1.082
0.992
1.009
1.011
0.983

^{1}H NMR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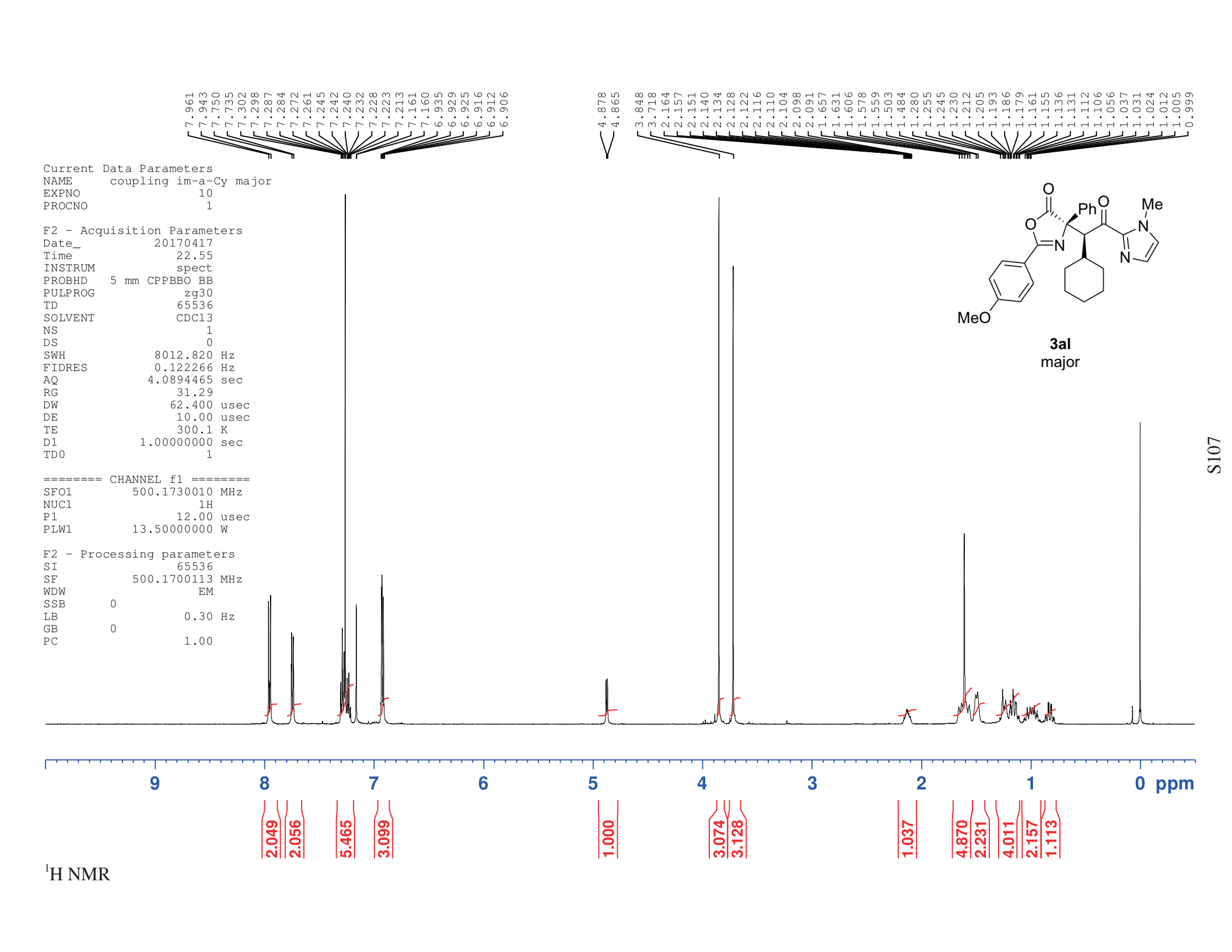
178.908
163.112
159.892
143.319
138.350
130.081
129.310
128.145
128.117
127.469
126.709
118.902
114.141
77.269
77.015
76.761
75.009
59.067
55.509
36.210
22.659
10.287
5.819
2.727
-0.004
Current Data Parameters
NAME coupling acyimidazole
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160914
Time 21.35
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678466 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
N
MeO
3ak
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR


7.961
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7.750
7.735
7.302
7.298
7.287
7.284
7.272
7.261
7.245
7.242
7.240
7.232
7.228
7.223
7.213
7.161
7.160
6.935
6.929
6.925
6.916
6.912
6.906
4.878
4.865
3.848
3.718
2.164
2.157
2.151
2.140
2.134
2.128
2.122
2.116
2.110
2.104
2.098
2.091
1.657
1.631
1.606
1.578
1.559
1.503
1.484
1.280
1.255
1.245
1.230
1.212
1.205
1.193
1.186
1.179
1.161
1.155
1.136
1.131
1.112
1.106
1.056
1.037
1.031
1.024
1.012
1.005
0.999
Current Data Parameters
NAME coupling im-a-Cy major
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 22.55
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
O
N
N
MeO
3al
major
9
8
7
6
5
4
3
2
1
0 ppm
2.049
2.056
5.465
3.099
1.000
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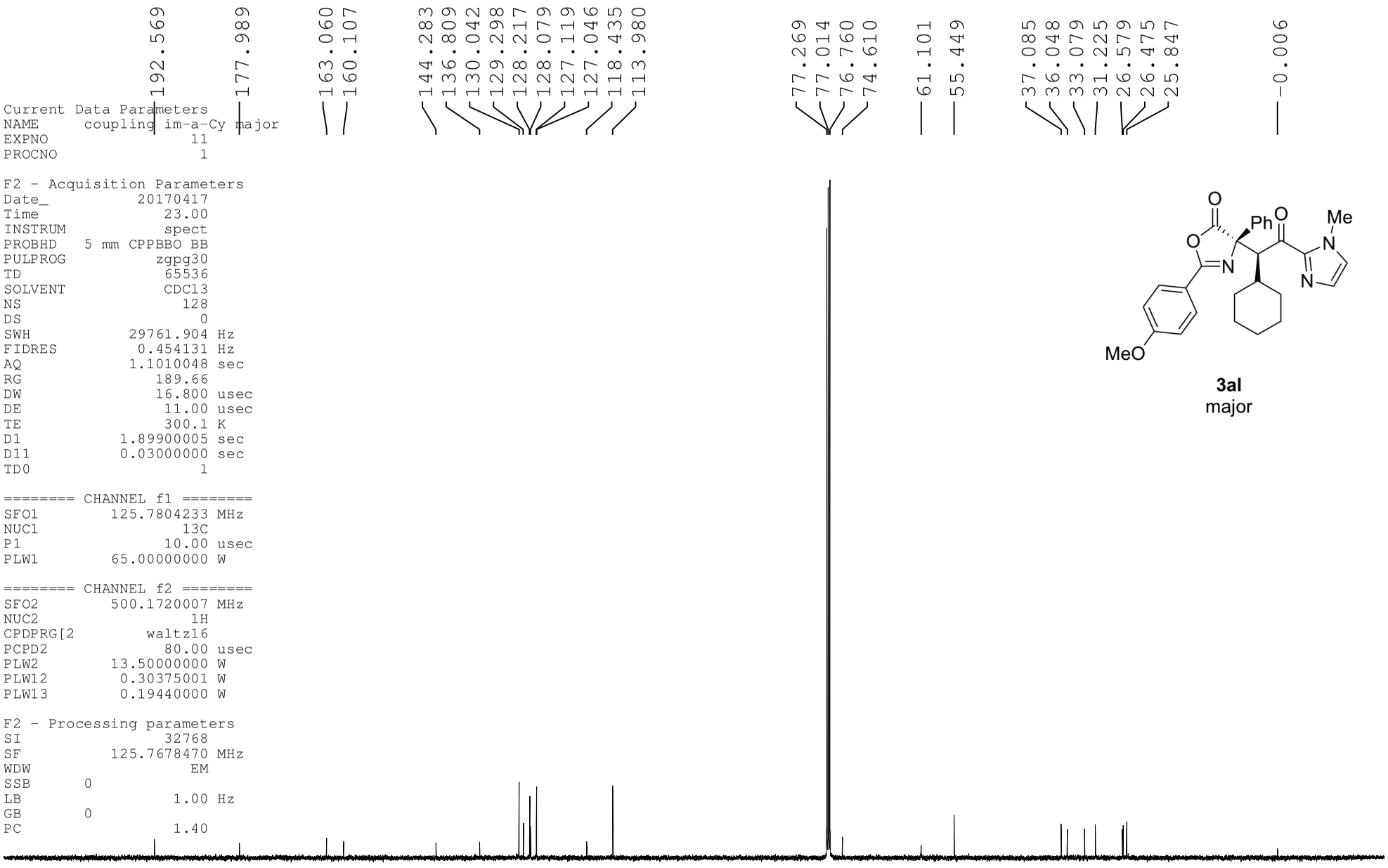
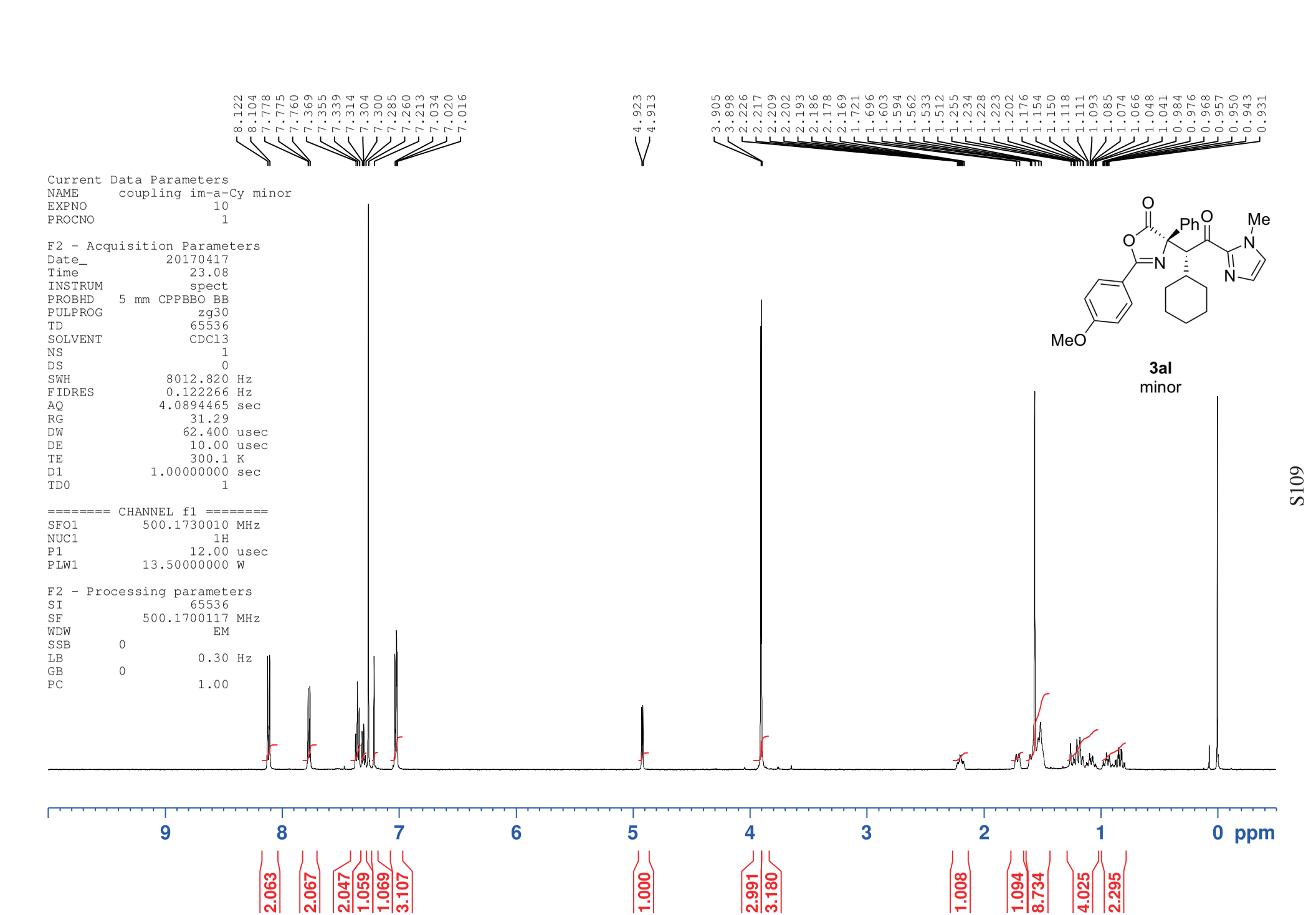
1.037
4.870
2.231
4.011
2.157
1.113

^{1}H NMR


192.569
177.989
163.060
160.107
144.283
136.809
130.042
129.298
128.217
128.079
127.119
127.046
118.435
113.980
77.269
77.014
76.760
74.610
61.101
55.449
37.085
36.048
33.079
31.225
26.579
26.475
25.847
-0.006
Current Data Parameters
NAME coupling im-a-Cy major
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 23.00
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
N
N
N
MeO
3al
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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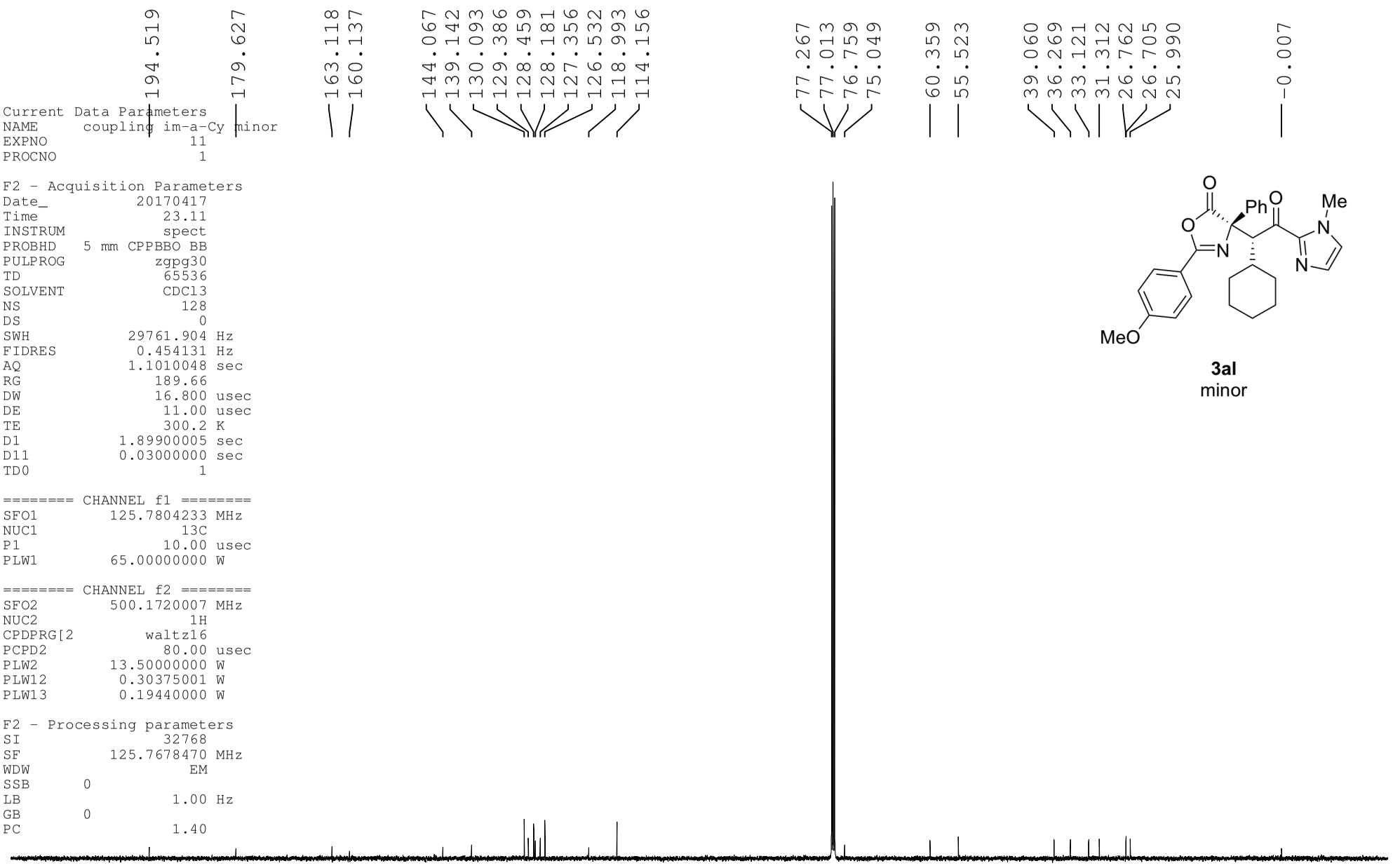
7.775
7.760
7.369
7.355
7.339
7.314
7.304
7.300
7.285
7.260
7.213
7.034
7.020
7.016
4.923
4.913
3.905
3.898
2.226
2.217
2.209
2.202
2.193
2.186
2.178
2.169
1.721
1.696
1.603
1.594
1.562
1.533
1.512
1.255
1.234
1.228
1.223
1.202
1.176
1.154
1.150
1.118
1.111
1.093
1.085
1.074
1.066
1.048
1.041
0.984
0.976
0.968
0.957
0.950
0.943
0.931
Current Data Parameters
NAME coupling im-a-Cy minor
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 23.08
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
N
MeO
3al
minor
9
8
7
6
5
4
3
2
1
0 ppm
2.063
2.067
2.047
1.059
1.069
3.107
1.000
2.991
3.180
1.008
1.094
8.734
4.025
2.295

^{1}H NMR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179.627
163.118
160.137
144.067
139.142
130.093
129.386
128.459
128.181
127.356
126.532
118.993
114.156
77.267
77.013
76.759
75.049
60.359
55.523
39.060
36.269
33.121
31.312
26.762
26.705
25.990
-0.007
Current Data Parameters
NAME coupling im-a-Cy minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 23.11
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
N
N
N
MeO
3al
minor
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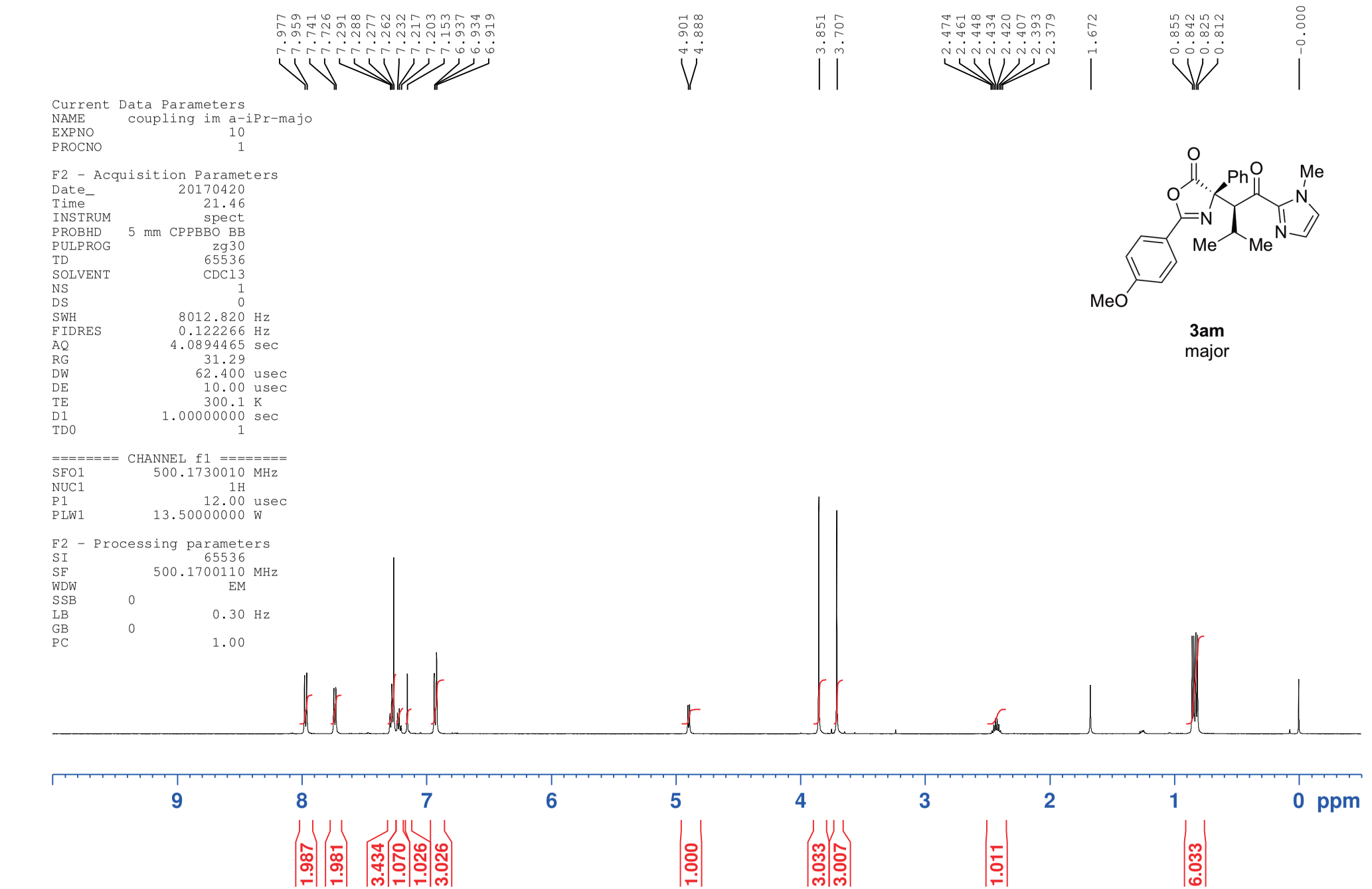
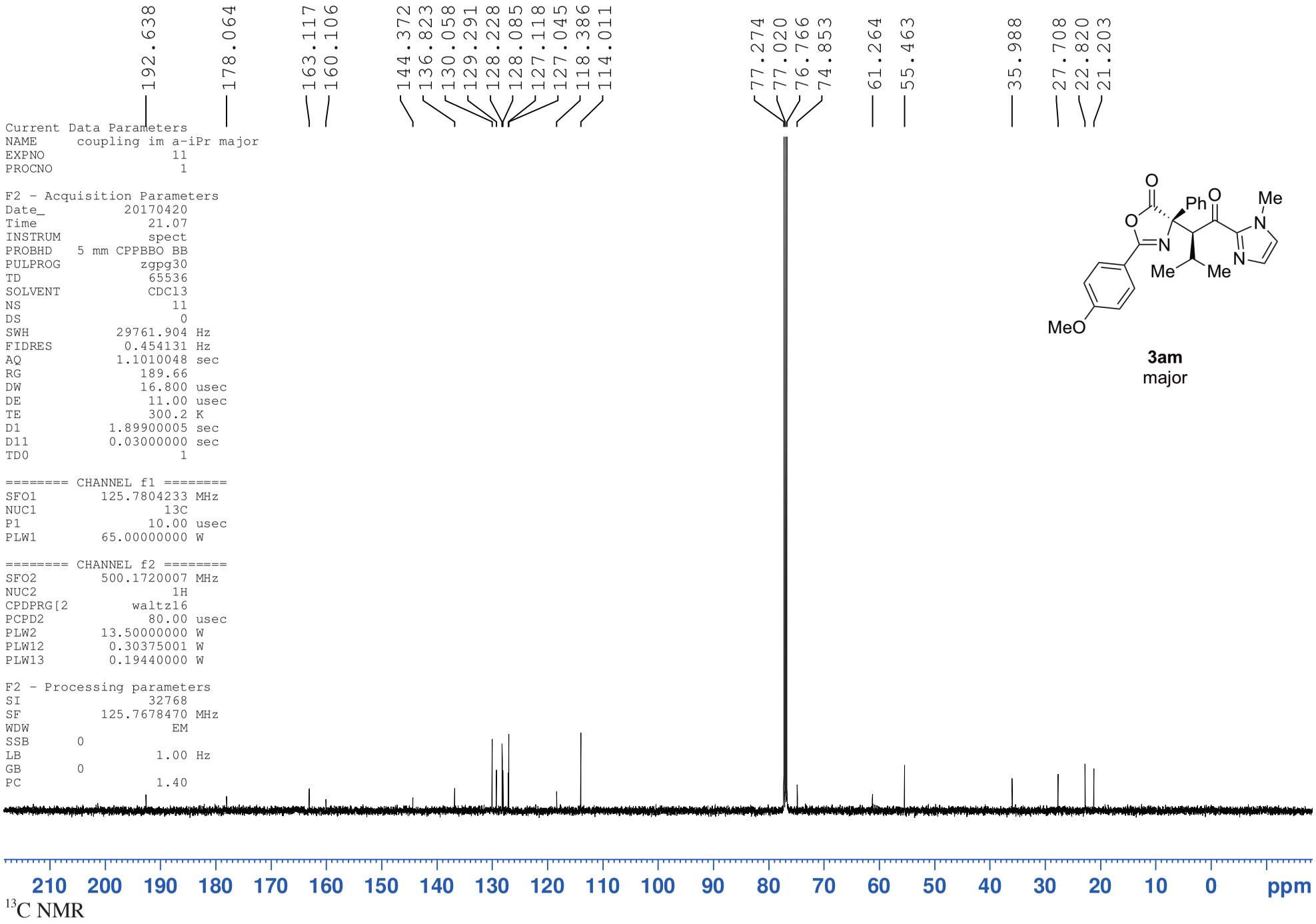
^{13}C NMR



3am
major

^{1}H NMR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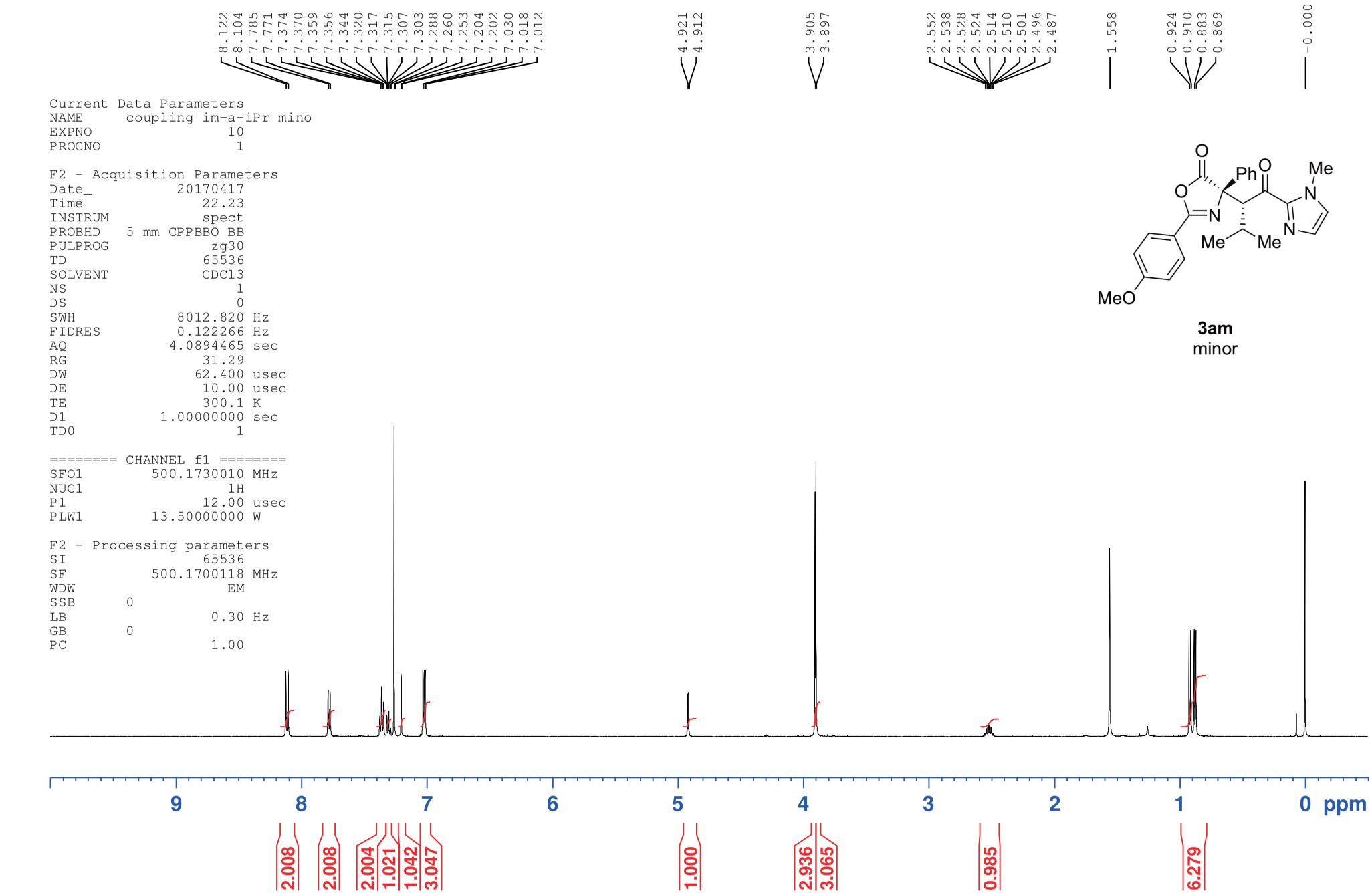
163.117
160.106
144.372
136.823
130.058
129.291
128.228
128.085
127.118
127.045
118.386
114.011
77.274
77.020
76.766
74.853
61.264
55.463
35.988
27.708
22.820
21.203
Current Data Parameters
NAME coupling im a-iPr major
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170420
Time 21.07
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Me
Me
MeO
3am
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
13C NMR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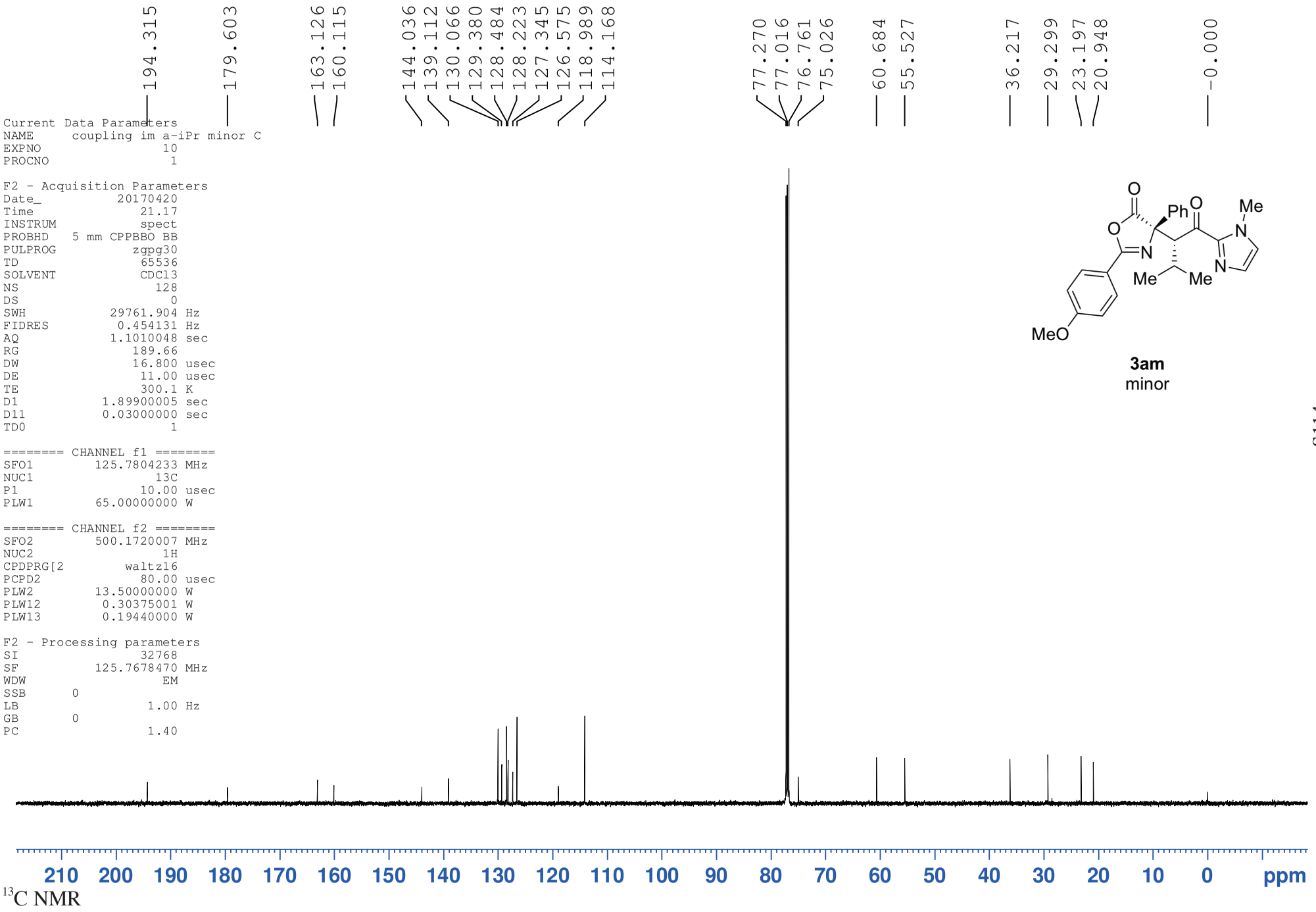
8.104
7.785
7.771
7.374
7.370
7.359
7.356
7.344
7.320
7.317
7.315
7.307
7.303
7.288
7.260
7.253
7.204
7.202
7.030
7.018
7.012
4.921
4.912
3.905
3.897
2.552
2.538
2.528
2.524
2.514
2.510
2.501
2.496
2.487
1.558
0.924
0.910
0.883
0.869
-0.000
Current Data Parameters
NAME coupling im-a-iPr mino
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 22.23
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
Me
Me
N
MeO
3am
minor
9
8
7
6
5
4
3
2
1
0 ppm
2.008
2.008
2.004
1.021
1.042
3.047
1.000
2.936
3.065
0.985
6.279

^{1}H NMR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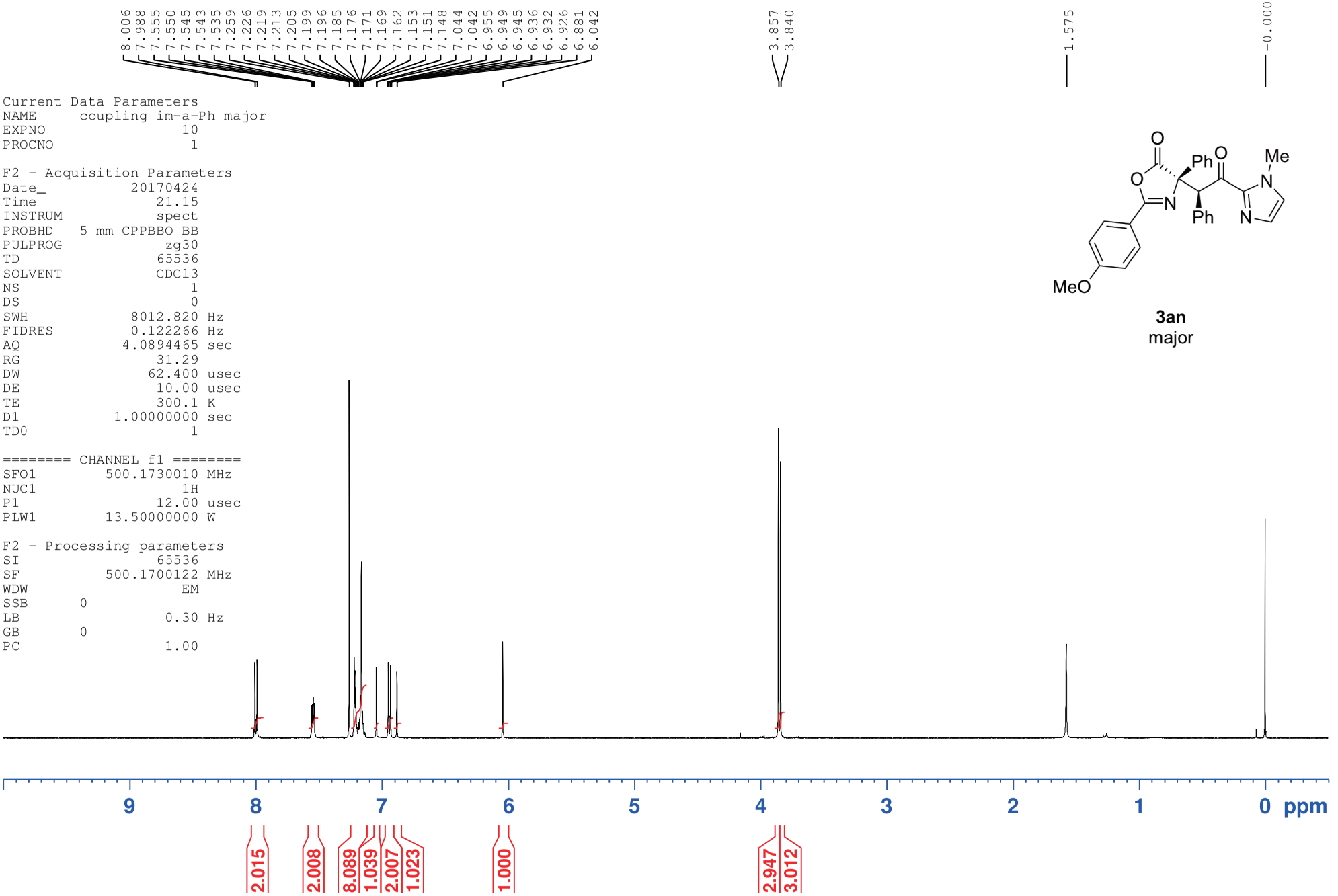
163.126
160.115
144.036
139.112
130.066
129.380
128.484
128.223
127.345
126.575
118.989
114.168
77.270
77.016
76.761
75.026
60.684
55.527
36.217
29.299
23.197
20.948
-0.000
Current Data Parameters
NAME coupling im a-iPr minor C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170420
Time 21.17
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Me
Me
MeO
3am
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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7.543
7.535
7.259
7.226
7.219
7.213
7.205
7.199
7.196
7.185
7.176
7.171
7.169
7.162
7.153
7.151
7.148
7.044
7.042
6.955
6.949
6.945
6.936
6.932
6.926
6.881
6.042
3.857
3.840
1.575
-0.000
Current Data Parameters
NAME coupling im-a-Ph major
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170424
Time 21.15
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
Ph
N
MeO
3an
major
9
8
7
6
5
4
3
2
1
0 ppm
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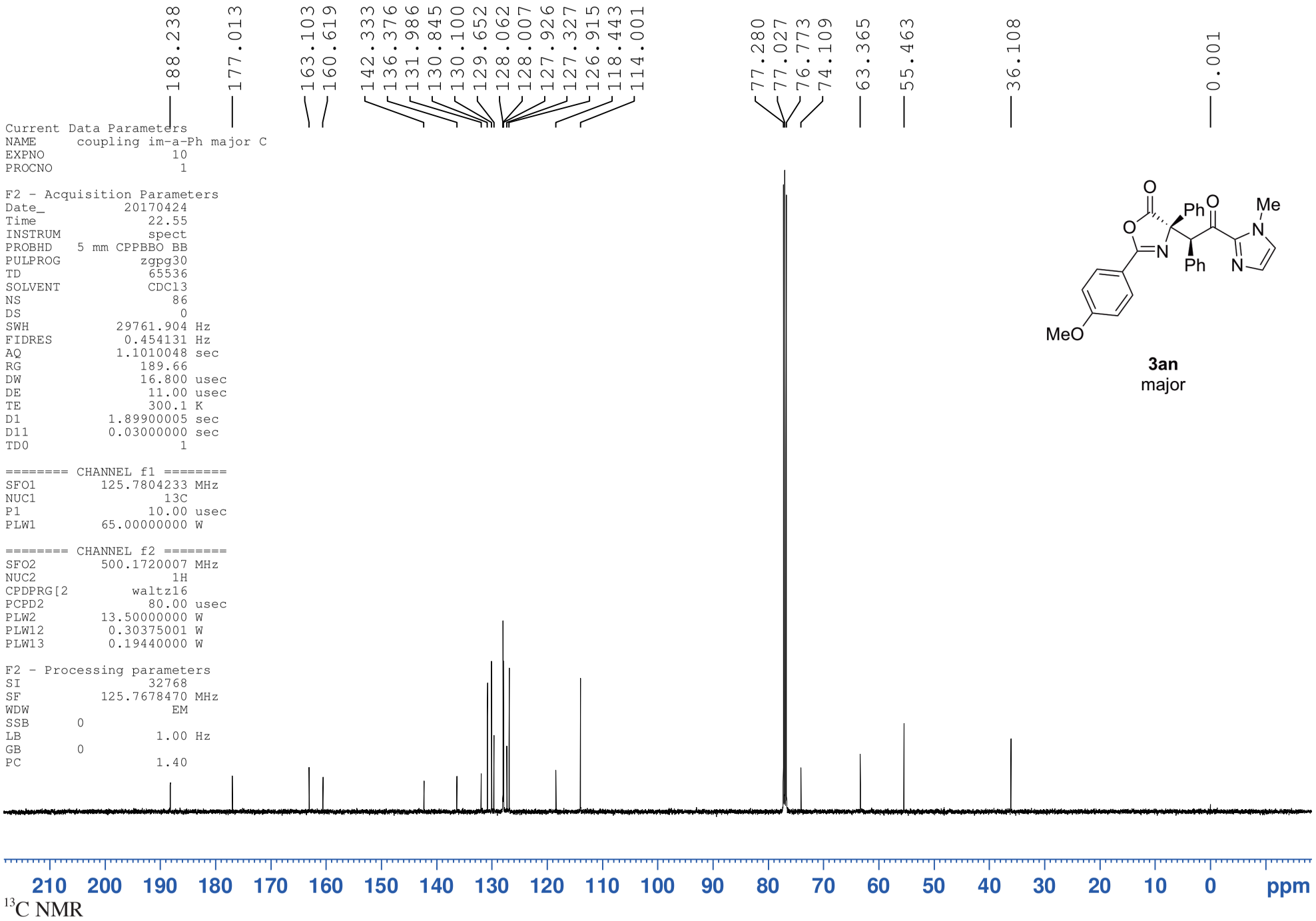
2.008
8.089
1.039
2.007
1.023
1.000
2.947
3.012

^{1}H NMR


188.238
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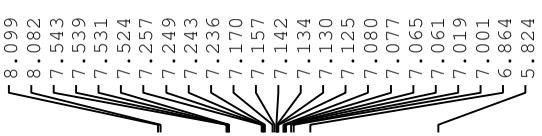
160.619
142.333
136.376
131.986
130.845
130.100
129.652
128.062
128.007
127.926
127.327
126.915
118.443
114.001
77.280
77.027
76.773
74.109
63.365
55.463
36.108
0.001
Current Data Parameters
NAME coupling im-a-Ph major C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170424
Time 22.55
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 86
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Ph
N
MeO
3an
major
S116
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR

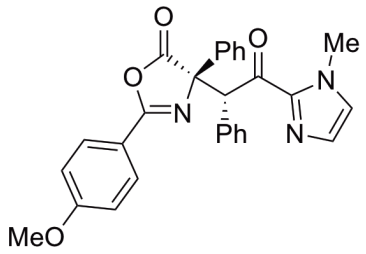



```
Current Data Parameters
NAME      coupling imi-a-Ph mino
EXPNO                  10
PROCNO                  1

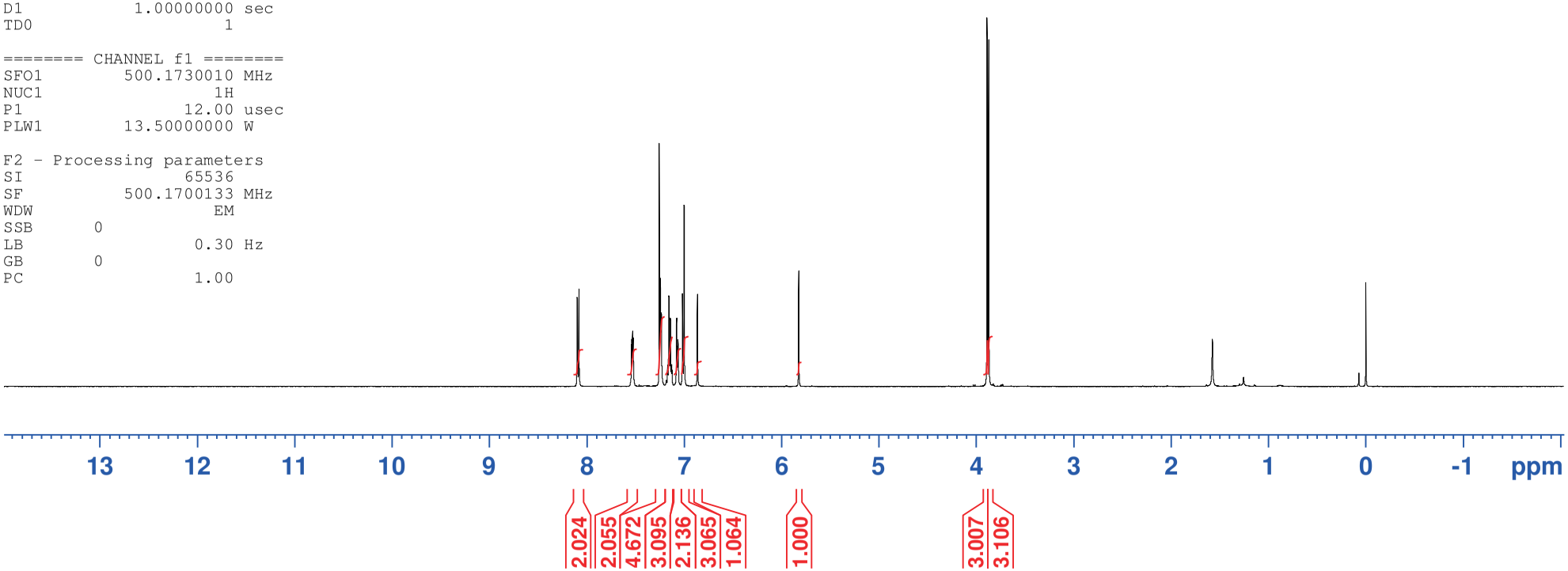
F2 - Acquisition Parameters
Date_           20170424
Time               21.26
INSTRUM            spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     1
DS                     0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                 31.29
DW                62.400 usec
DE                10.00 usec
TE                300.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1730010 MHz
NUC1                1H
P1                12.00 usec
PLW1         13.50000000 W

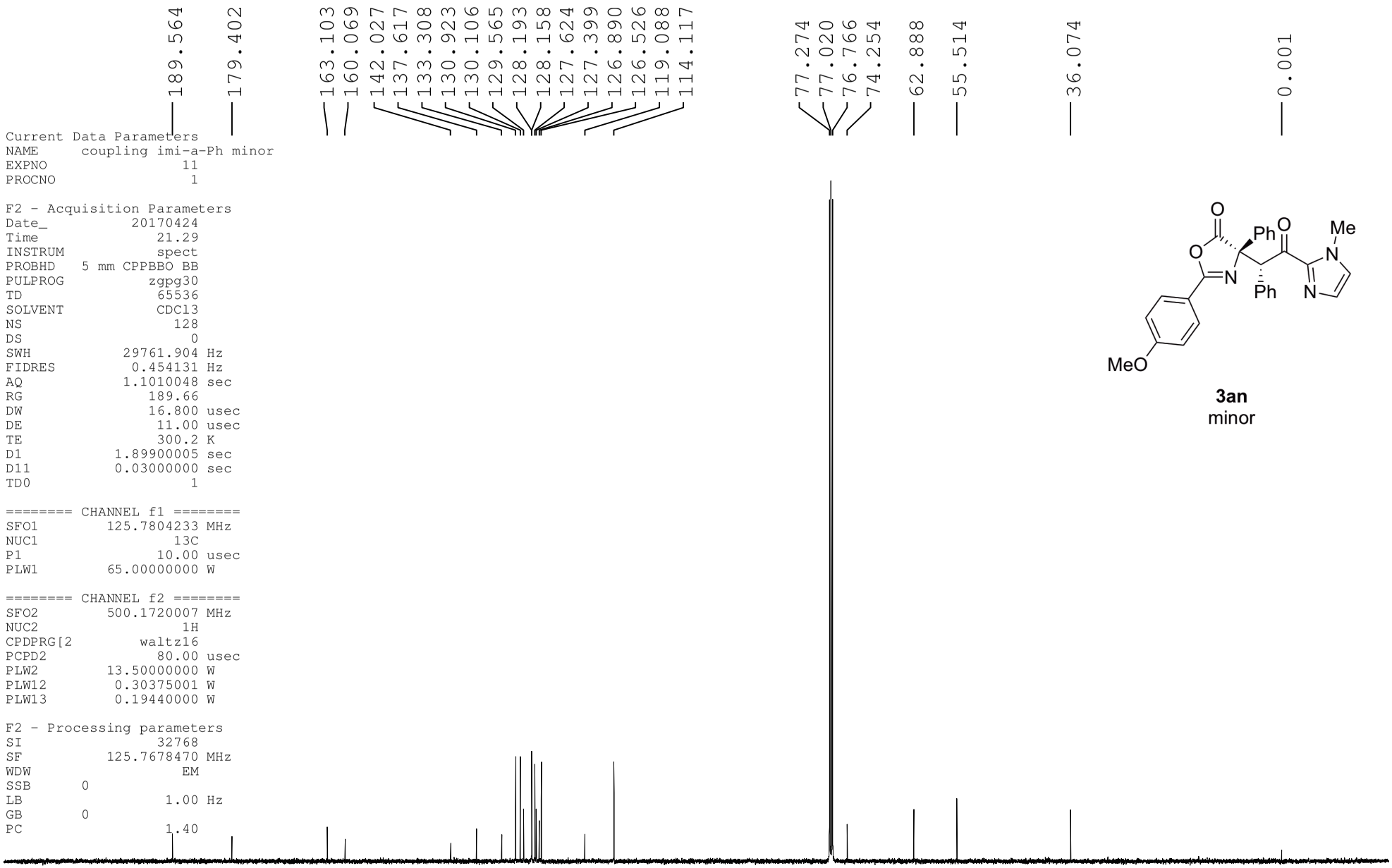
F2 - Processing parameters
SI                 65536
SF           500.1700133 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



3an
minor



^{1}H NMR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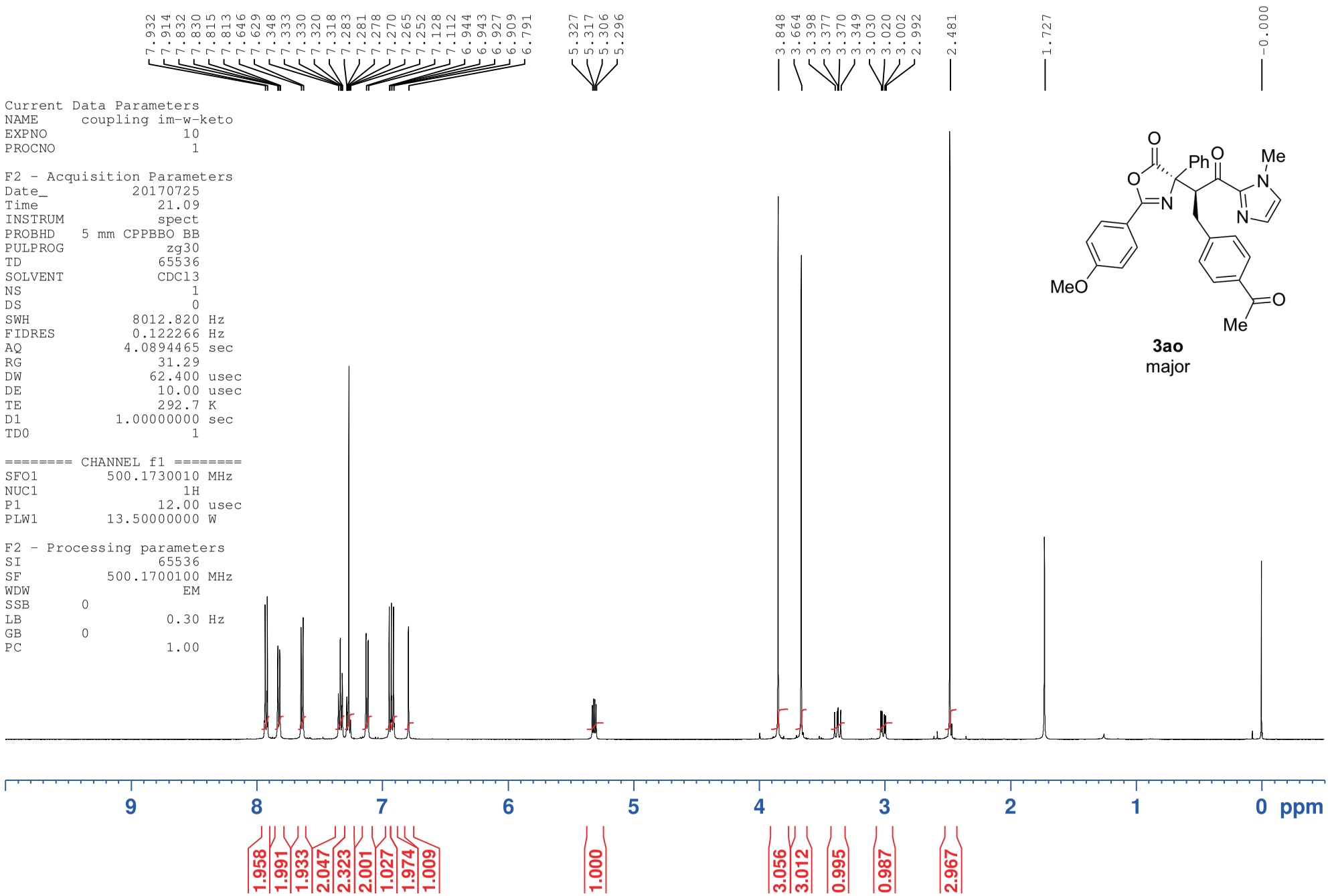
163.103
160.069
142.027
137.617
133.308
130.923
130.106
129.565
128.193
128.158
127.624
127.399
126.890
126.526
119.088
114.117
77.274
77.020
76.766
74.254
62.888
55.514
36.074
0.001
Current Data Parameters
NAME coupling imi-a-Ph minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170424
Time 21.29
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Ph
N
MeO
3an
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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7.830
7.815
7.813
7.646
7.629
7.348
7.333
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7.320
7.318
7.283
7.281
7.278
7.270
7.265
7.252
7.128
7.112
6.944
6.943
6.927
6.909
6.791
5.327
5.317
5.306
5.296
3.848
3.664
3.398
3.377
3.370
3.349
3.030
3.020
3.002
2.992
2.481
1.727
-0.000
Current Data Parameters
NAME coupling im-w-keto
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 21.09
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
N
MeO
O
Me
3ao
major
9
8
7
6
5
4
3
2
1
0 ppm
1.958
1.991
1.933
2.047
2.323
2.001
1.027
1.974
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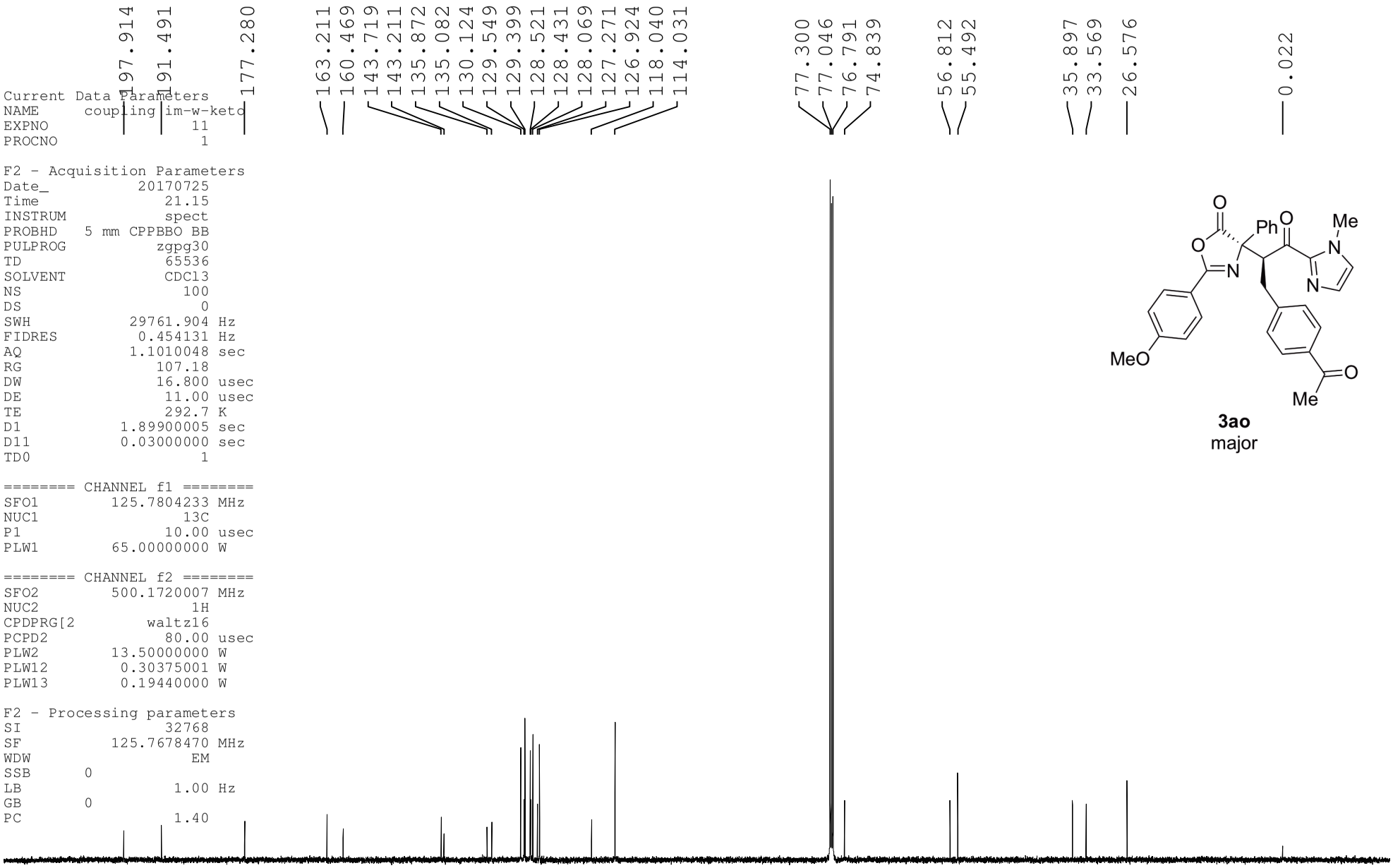
1.000
3.056
3.012
0.995
0.987
2.967

^{1}H NMR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177.280
163.211
160.469
143.719
143.211
135.872
135.082
130.124
129.549
129.399
128.521
128.431
128.069
127.271
126.924
118.040
114.031
77.300
77.046
76.791
74.839
56.812
55.492
35.897
33.569
26.576
0.022
Current Data Parameters
NAME coupling im-w-keto
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 21.15
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 292.7 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
N
N
N
MeO
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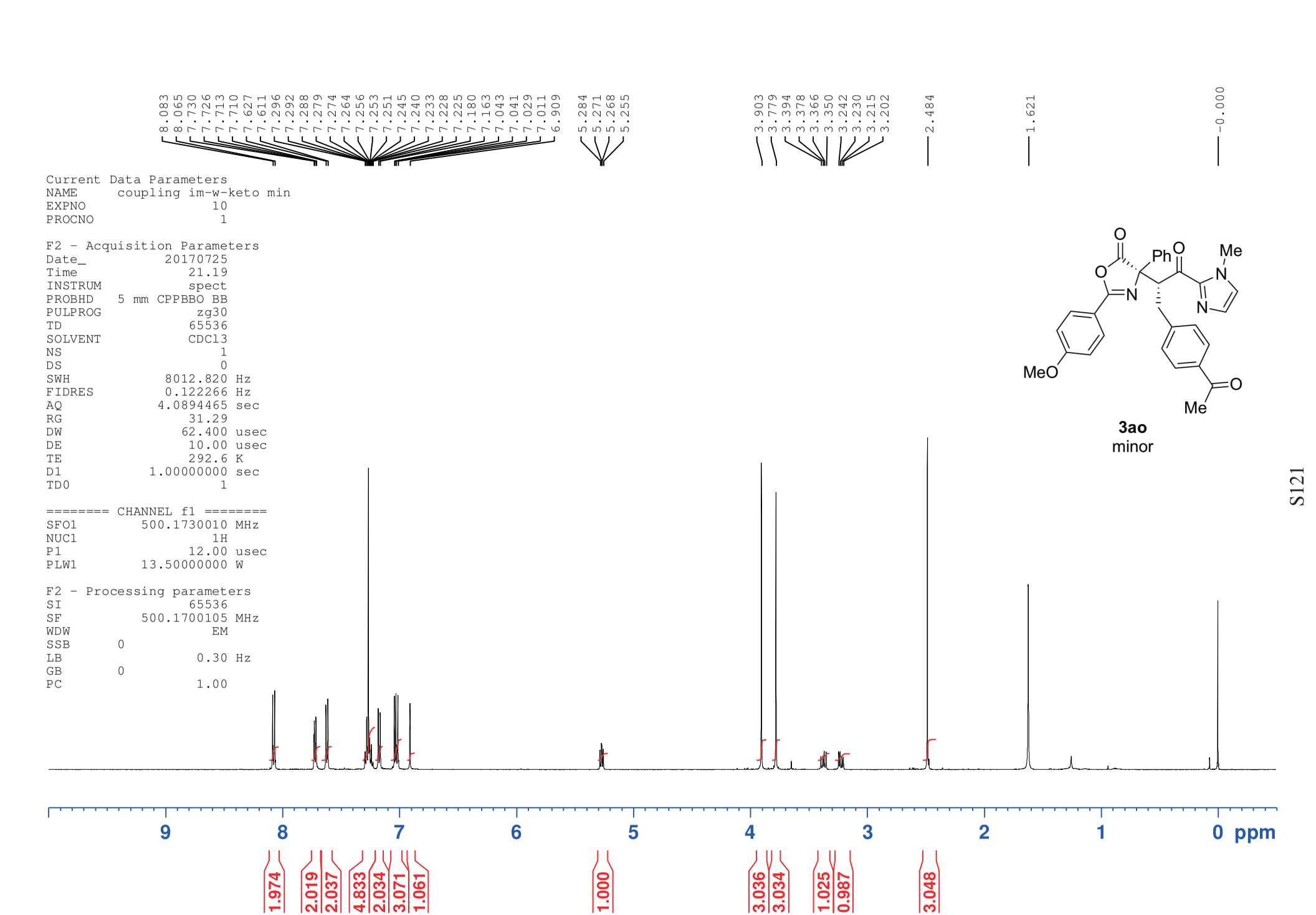
Me
3ao
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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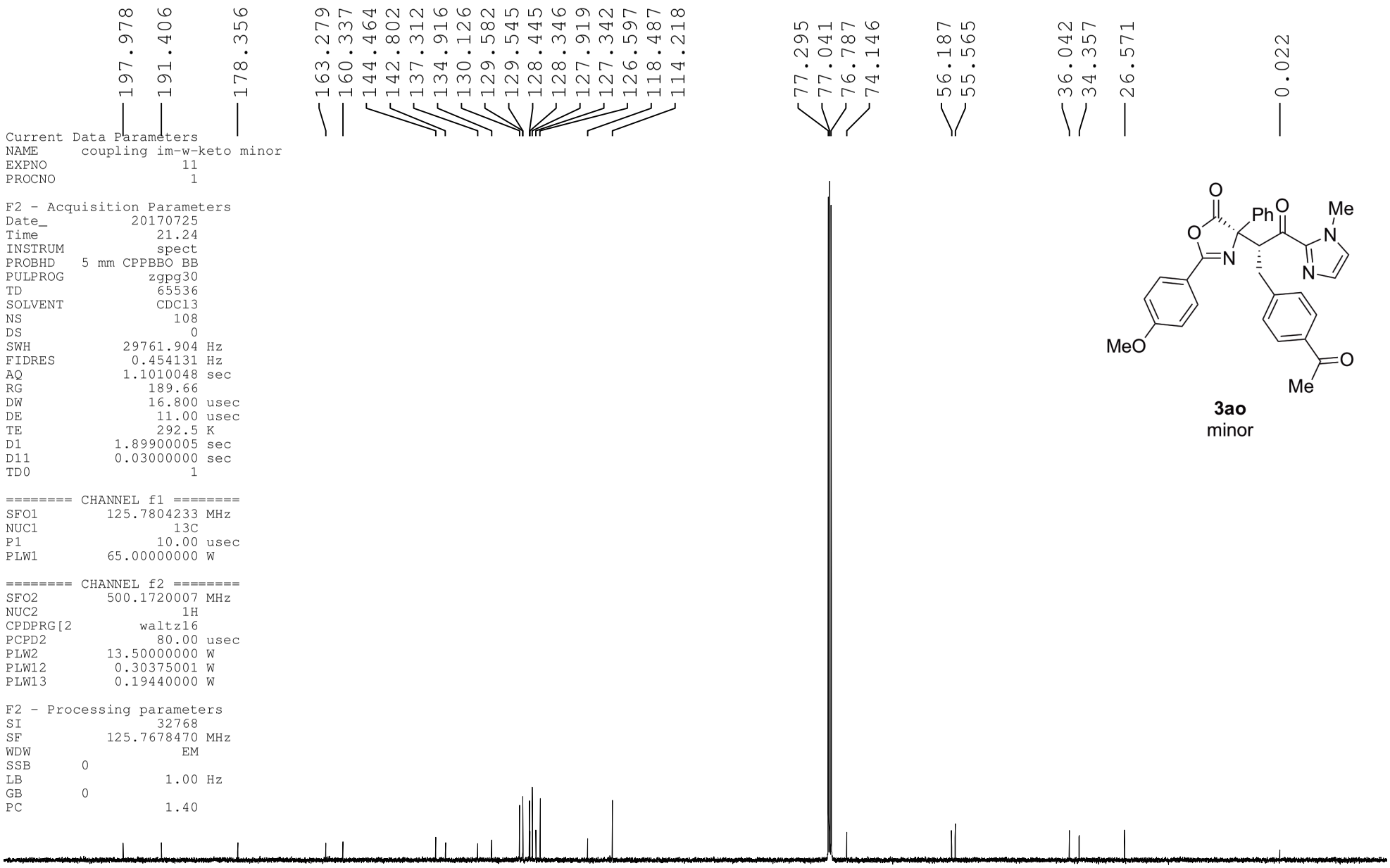
7.726
7.713
7.710
7.627
7.611
7.296
7.292
7.288
7.279
7.274
7.264
7.256
7.253
7.251
7.245
7.240
7.233
7.228
7.225
7.180
7.163
7.043
7.041
7.029
7.011
6.909
5.284
5.271
5.268
5.255
3.903
3.779
3.394
3.378
3.366
3.350
3.242
3.230
3.215
3.202
2.484
1.621
-0.000
Current Data Parameters
NAME coupling im-w-keto min
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 21.19
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
N
MeO
O
Me
3ao
minor
9
8
7
6
5
4
3
2
1
0 ppm
1.974
2.019
2.037
4.833
2.034
3.071
1.061
1.000
3.036
3.034
1.025
0.987
3.048

^{1}H NMR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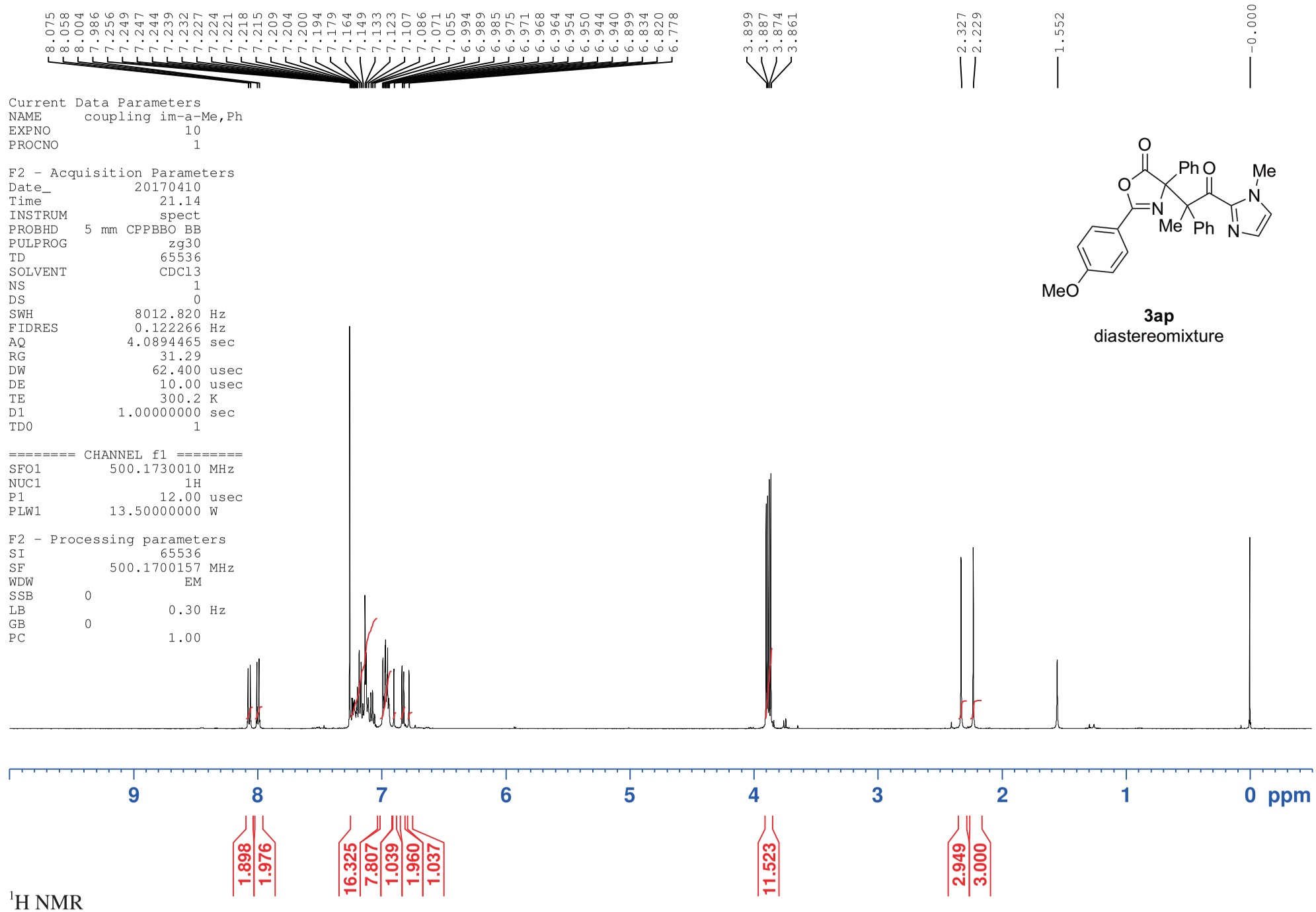
128.445
128.346
127.919
127.342
126.597
118.487
114.218
77.295
77.041
76.787
74.146
56.187
55.565
36.042
34.357
26.571
0.022
Current Data Parameters
NAME coupling im-w-keto minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 21.24
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 108
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.5 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
MeO
O
Me
3ao
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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8.058
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7.986
7.256
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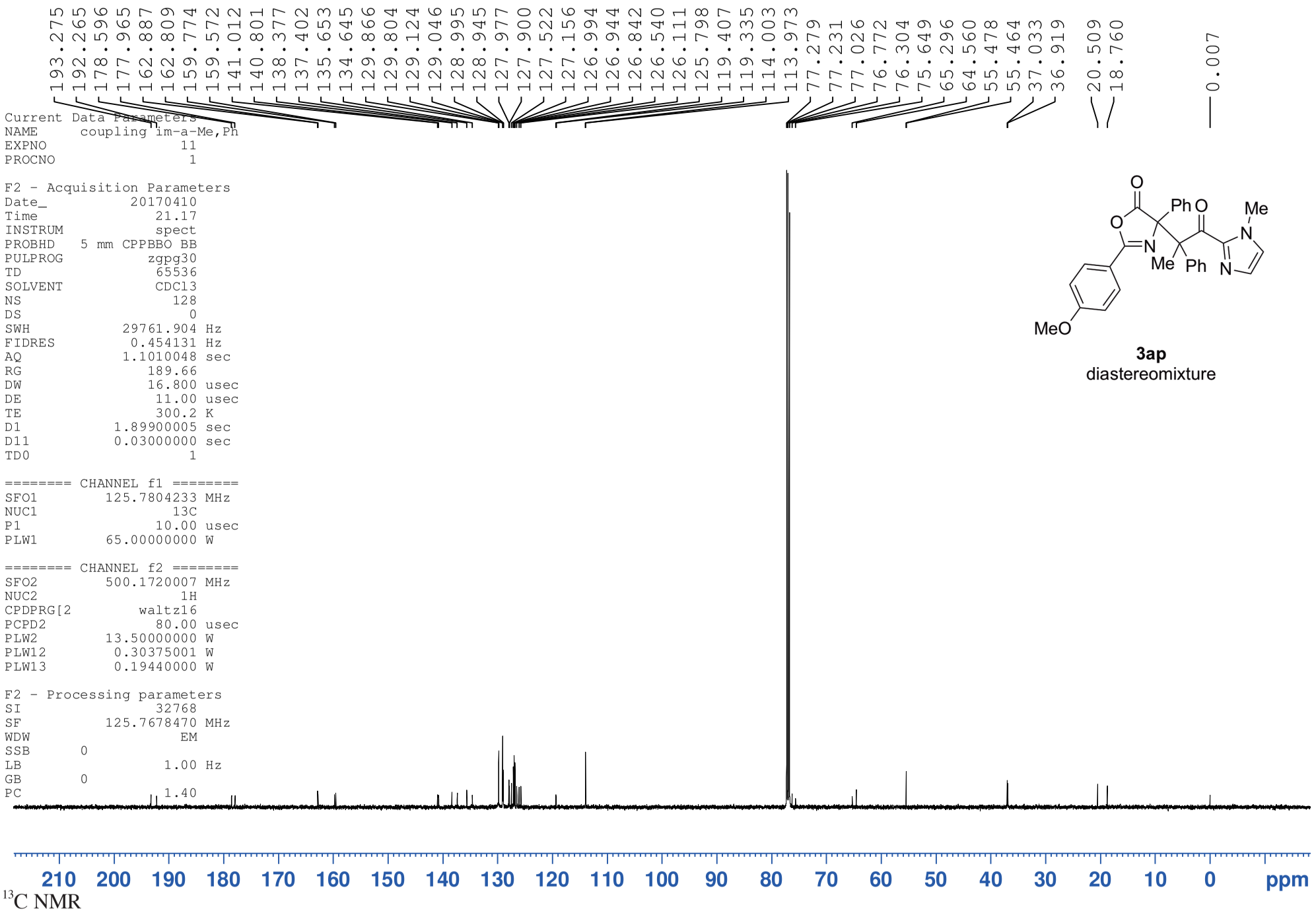
7.247
7.244
7.239
7.232
7.227
7.224
7.221
7.218
7.215
7.209
7.204
7.200
7.194
7.179
7.164
7.149
7.133
7.123
7.107
7.086
7.071
7.055
6.994
6.989
6.985
6.975
6.971
6.968
6.964
6.954
6.950
6.944
6.940
6.899
6.834
6.820
6.778
3.899
3.887
3.874
3.861
2.327
2.229
1.552
-0.000
Current Data Parameters
NAME coupling im-a-Me,Ph
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170410
Time 21.14
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700157 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph O
Me
O
N
N
Me
Ph
N
MeO
3ap
diastereomixture
9
8
7
6
5
4
3
2
1
0 ppm
1.898
1.976
16.325
7.807
1.039
1.960
1.037
11.523
2.949
3.000
1H NMR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192.265
178.596
177.965
162.887
162.809
159.774
159.572
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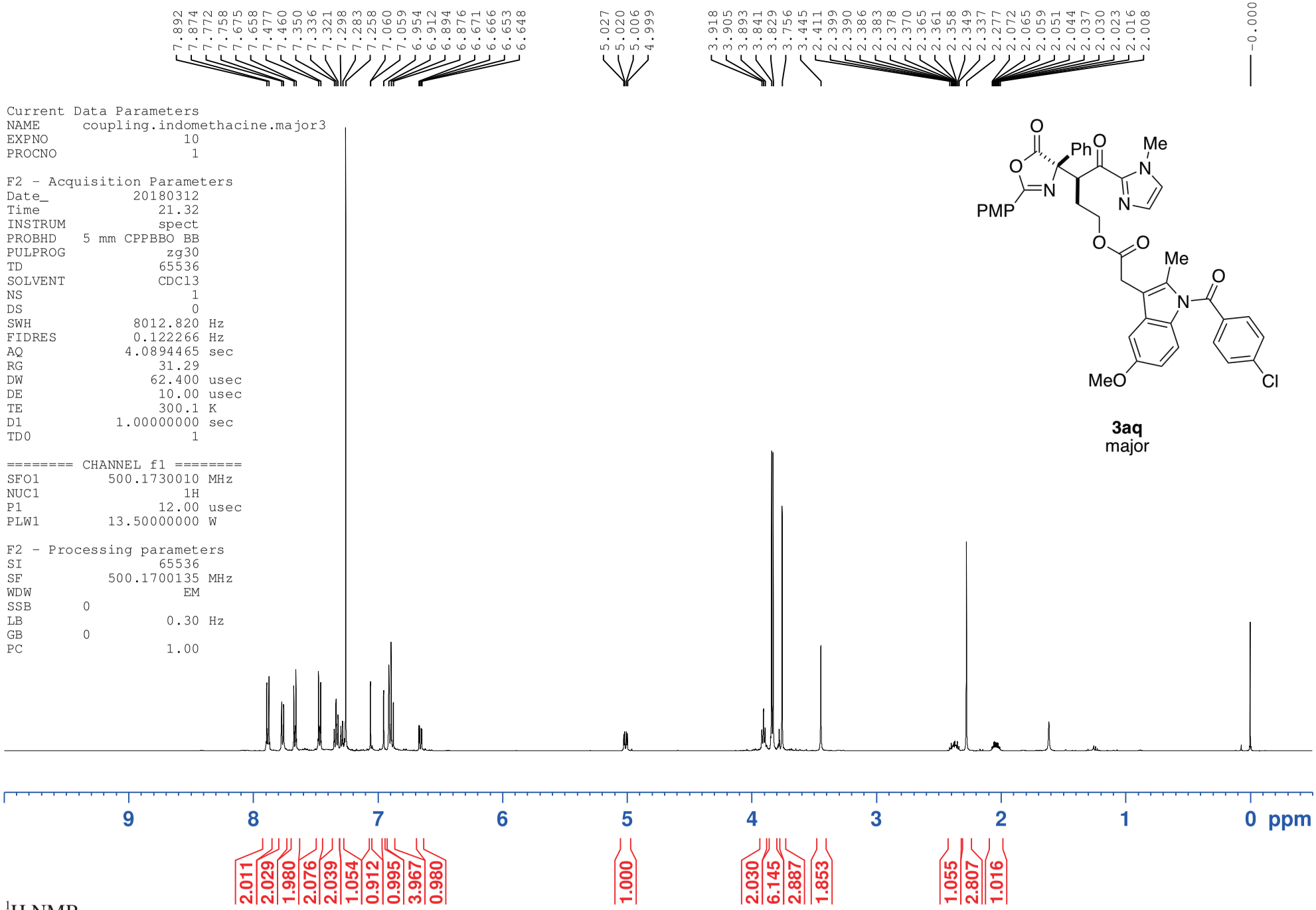
140.801
138.377
137.402
135.653
134.645
129.866
129.804
129.124
129.046
128.995
128.945
127.977
127.900
127.522
127.156
126.994
126.944
126.842
126.540
126.111
125.798
119.407
119.335
114.003
113.973
77.279
77.231
77.026
76.772
76.304
75.649
65.296
64.560
55.478
55.464
37.033
36.919
20.509
18.760
0.007
Current Data Parameters
NAME coupling im-a-Me,Ph
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170410
Time 21.17
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
Me
Ph
N
MeO
3ap
diastereomixture
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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7.874
7.772
7.758
7.675
7.658
7.477
7.460
7.350
7.336
7.321
7.298
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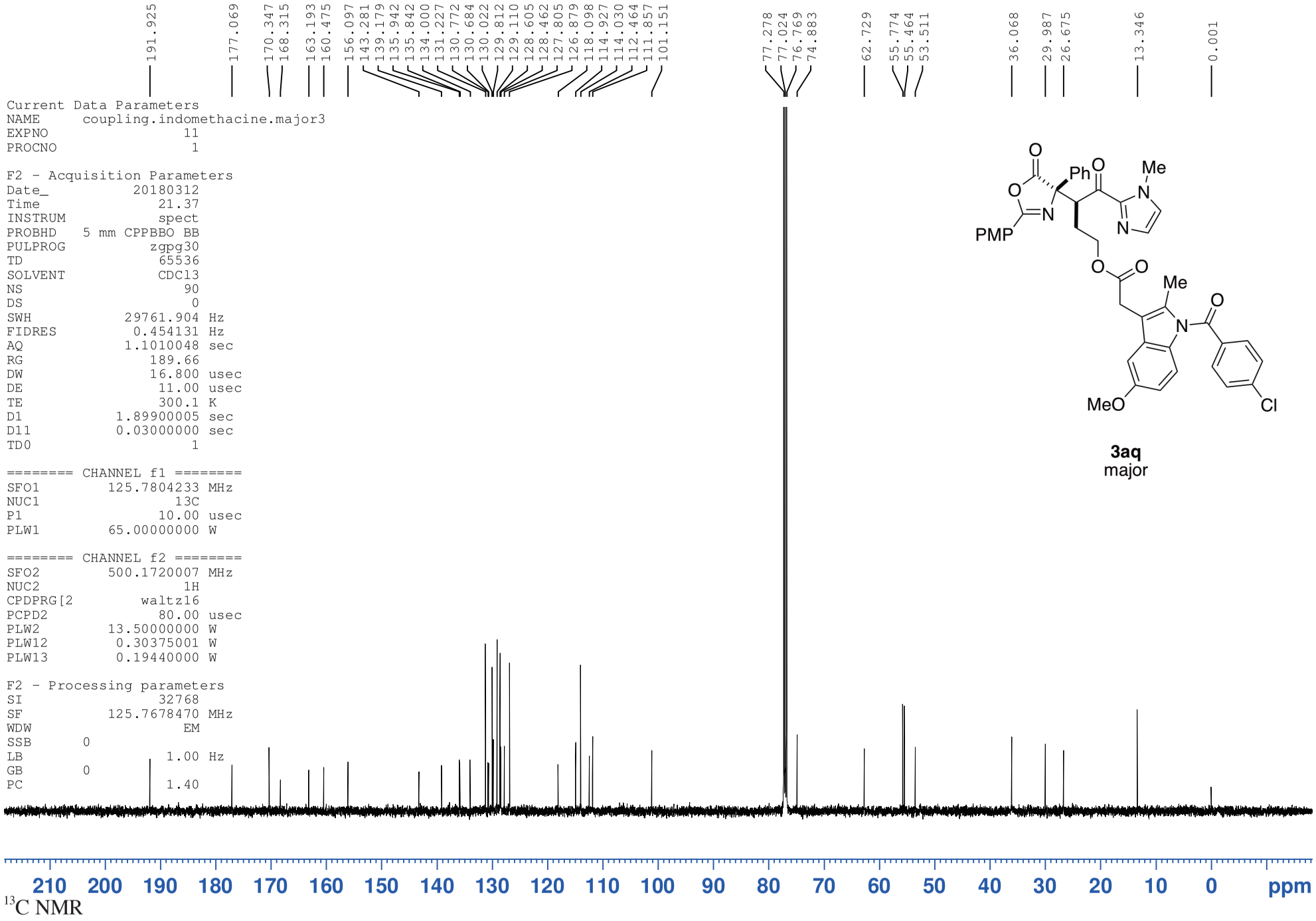
7.258
7.060
7.059
6.954
6.912
6.894
6.876
6.671
6.666
6.653
6.648
5.027
5.020
5.006
4.999
3.918
3.905
3.893
3.841
3.829
3.756
3.445
2.411
2.399
2.390
2.386
2.383
2.378
2.370
2.365
2.361
2.358
2.349
2.337
2.277
2.072
2.065
2.059
2.051
2.044
2.037
2.030
2.023
2.016
2.008
-0.000
Current Data Parameters
NAME coupling.indomethacine.major3
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180312
Time 21.32
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
PMP
O
O
Me
N
O
MeO
Cl
3aq
major
9
8
7
6
5
4
3
2
1
0 ppm
2.011
2.029
1.980
2.076
2.039
1.054
0.912
0.995
3.967
0.980
1.000
2.030
6.145
2.887
1.853
1.055
2.807
1.016

^{1}H NMR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156.097
143.281
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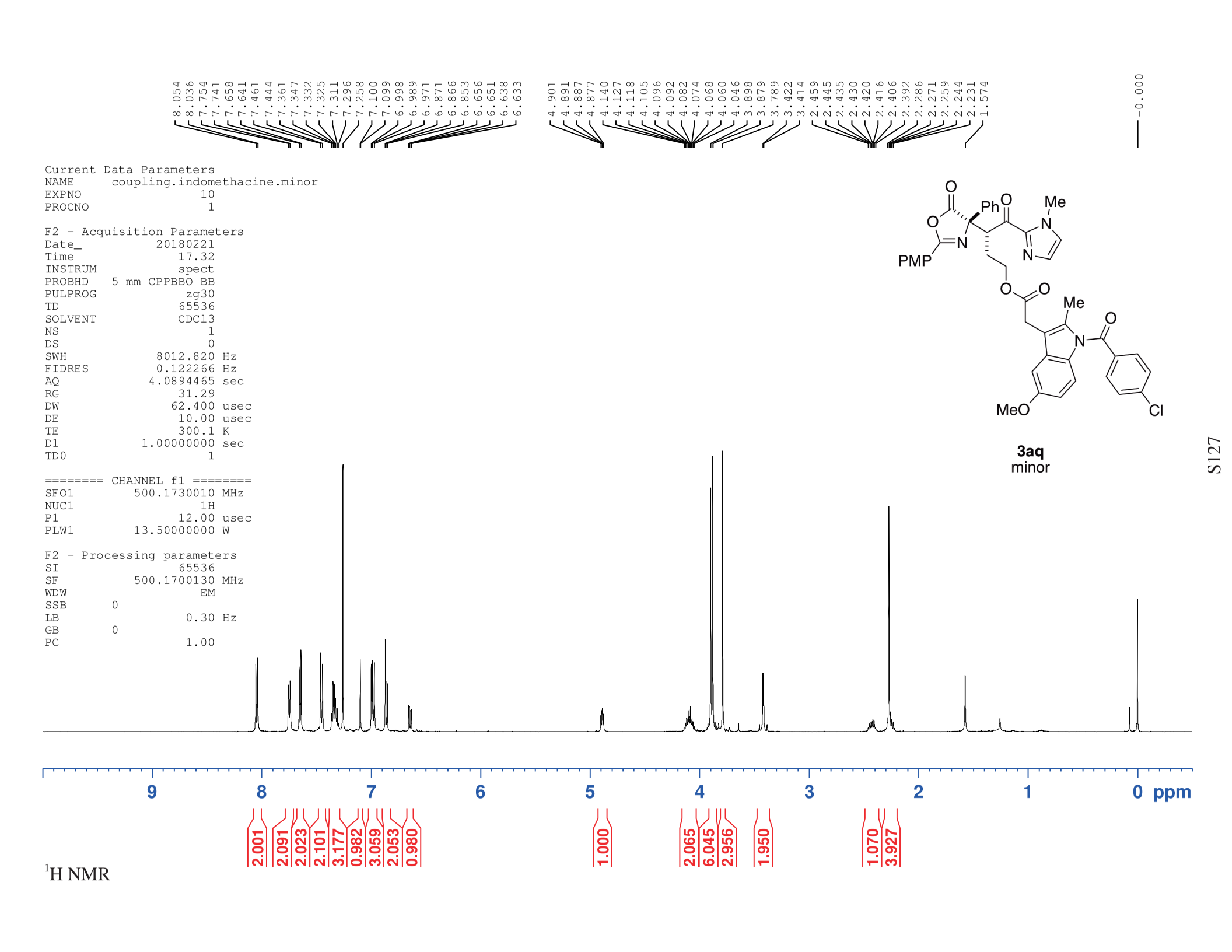
135.942
135.842
134.000
131.227
130.772
130.684
130.022
129.812
129.110
128.605
128.462
127.805
126.879
118.098
114.927
114.030
112.464
111.857
101.151
77.278
77.024
76.769
74.883
62.729
55.774
55.464
53.511
36.068
29.987
26.675
13.346
0.001
Current Data Parameters
NAME coupling.indomethacine.major3
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180312
Time 21.37
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 90
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
Ph
O
Me
N
PMP
N
N
O
O
Me
O
N
MeO
Cl
3aq
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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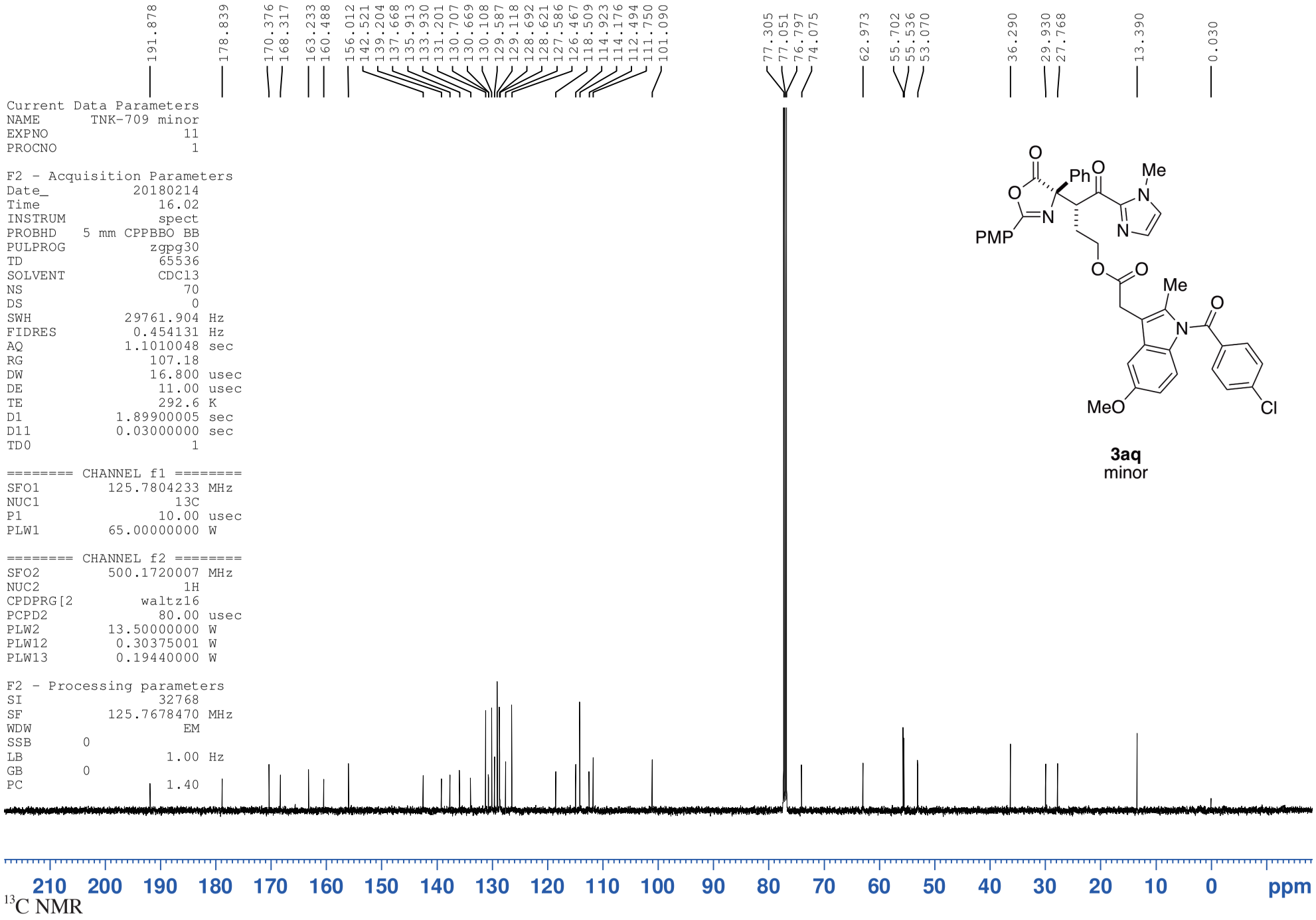
7.741
7.658
7.641
7.461
7.444
7.361
7.347
7.332
7.325
7.311
7.296
7.258
7.100
7.099
6.998
6.989
6.971
6.871
6.866
6.853
6.656
6.651
6.638
6.633
4.901
4.891
4.887
4.877
4.140
4.127
4.118
4.105
4.096
4.092
4.082
4.074
4.068
4.060
4.046
3.898
3.879
3.789
3.422
3.414
2.459
2.445
2.435
2.430
2.420
2.416
2.406
2.392
2.286
2.271
2.259
2.244
2.231
1.574
0.000
Current Data Parameters
NAME coupling.indomethacine.minor
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180221
Time 17.32
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
O
N
N
PMP
O
O
Me
N
O
MeO
Cl
3aq
minor
9
8
7
6
5
4
3
2
1
0 ppm
2.001
2.091
2.023
2.101
3.177
0.982
3.059
2.053
0.980
1.000
2.065
6.045
2.956
1.950
1.070
3.927
1H NMR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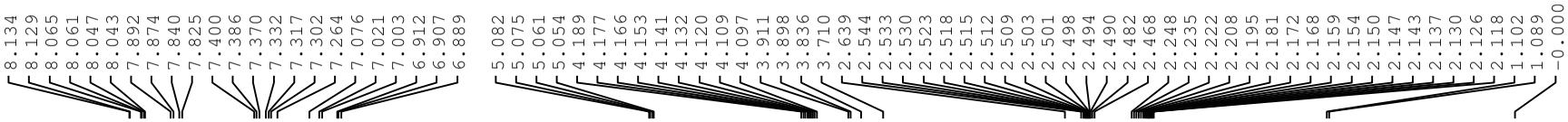
168.317
163.233
160.488
156.012
142.521
139.204
137.668
135.913
133.930
131.201
130.707
130.669
130.108
129.587
129.118
128.692
128.621
127.586
126.467
118.509
114.923
114.176
112.494
111.750
101.090
77.305
77.051
76.797
74.075
62.973
55.702
55.536
53.070
36.290
29.930
27.768
13.390
0.030
Current Data Parameters
NAME TNK-709 minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180214
Time 16.02
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 70
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 292.6 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
PMP
N
N
O
O
Me
O
N
MeO
Cl
3aq
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
13C NMR




```
Current Data Parameters
NAME      TNK-710 TM major
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180309
Time               17.00
INSTRUM            spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.29
DW                62.400 usec
DE                10.00 usec
TE                300.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1730010 MHz
NUC1                1H
P1                 12.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 65536
SF           500.1700107 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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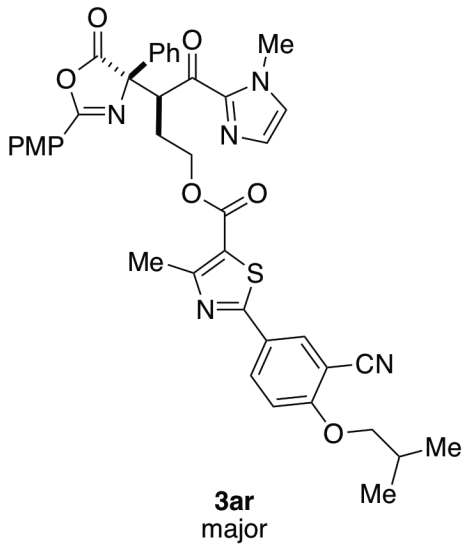
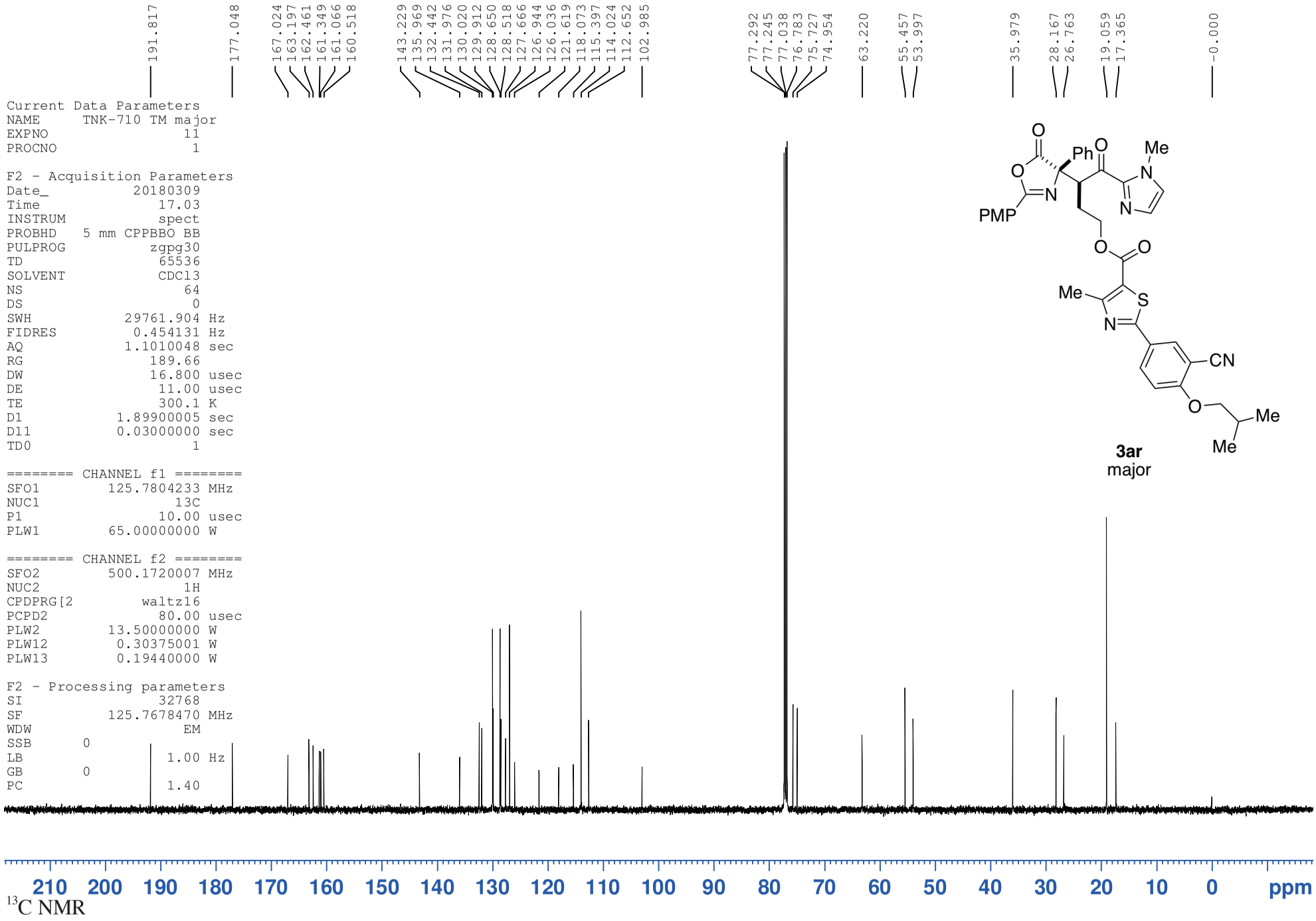


3ar
major

^{1}H NMR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161.349
161.066
160.518
143.229
135.969
132.442
131.976
130.020
129.912
128.650
128.518
127.666
126.944
126.036
121.619
118.073
115.397
114.024
112.652
102.985
77.292
77.245
77.038
76.783
75.727
74.954
63.220
55.457
53.997
35.979
28.167
26.763
19.059
17.365
-0.000
Current Data Parameters
NAME TNK-710 TM major
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180309
Time 17.03
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
PMP
N
O
O
Me
S
N
CN
O
Me
Me
3ar
major
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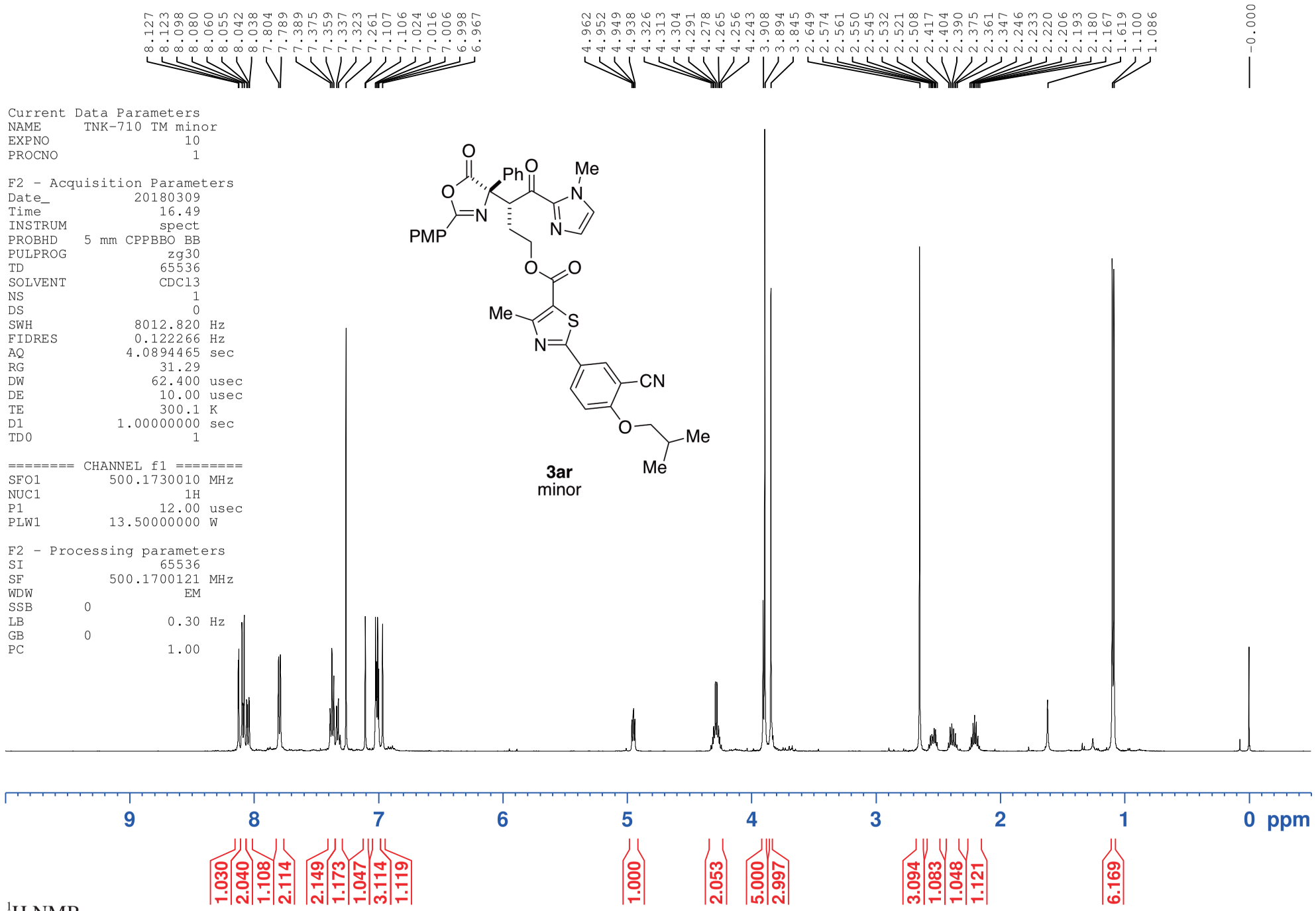
^{13}C NMR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8.055
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8.038
7.804
7.789
7.389
7.375
7.359
7.337
7.323
7.261
7.107
7.106
7.024
7.016
7.006
6.998
6.967
4.962
4.952
4.949
4.938
4.326
4.313
4.304
4.291
4.278
4.265
4.256
4.243
3.908
3.894
3.845
2.649
2.574
2.561
2.550
2.545
2.532
2.521
2.508
2.417
2.404
2.390
2.375
2.361
2.347
2.246
2.233
2.220
2.206
2.193
2.180
2.167
1.619
1.100
1.086
-0.000
Current Data Parameters
NAME TNK-710 TM minor
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180309
Time 16.49
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
N
PMP
N
O
O
Me
S
N
CN
O
Me
Me
3ar
minor
9
8
7
6
5
4
3
2
1
0 ppm
1.030
2.040
1.108
2.114
2.149
1.173
1.047
3.114
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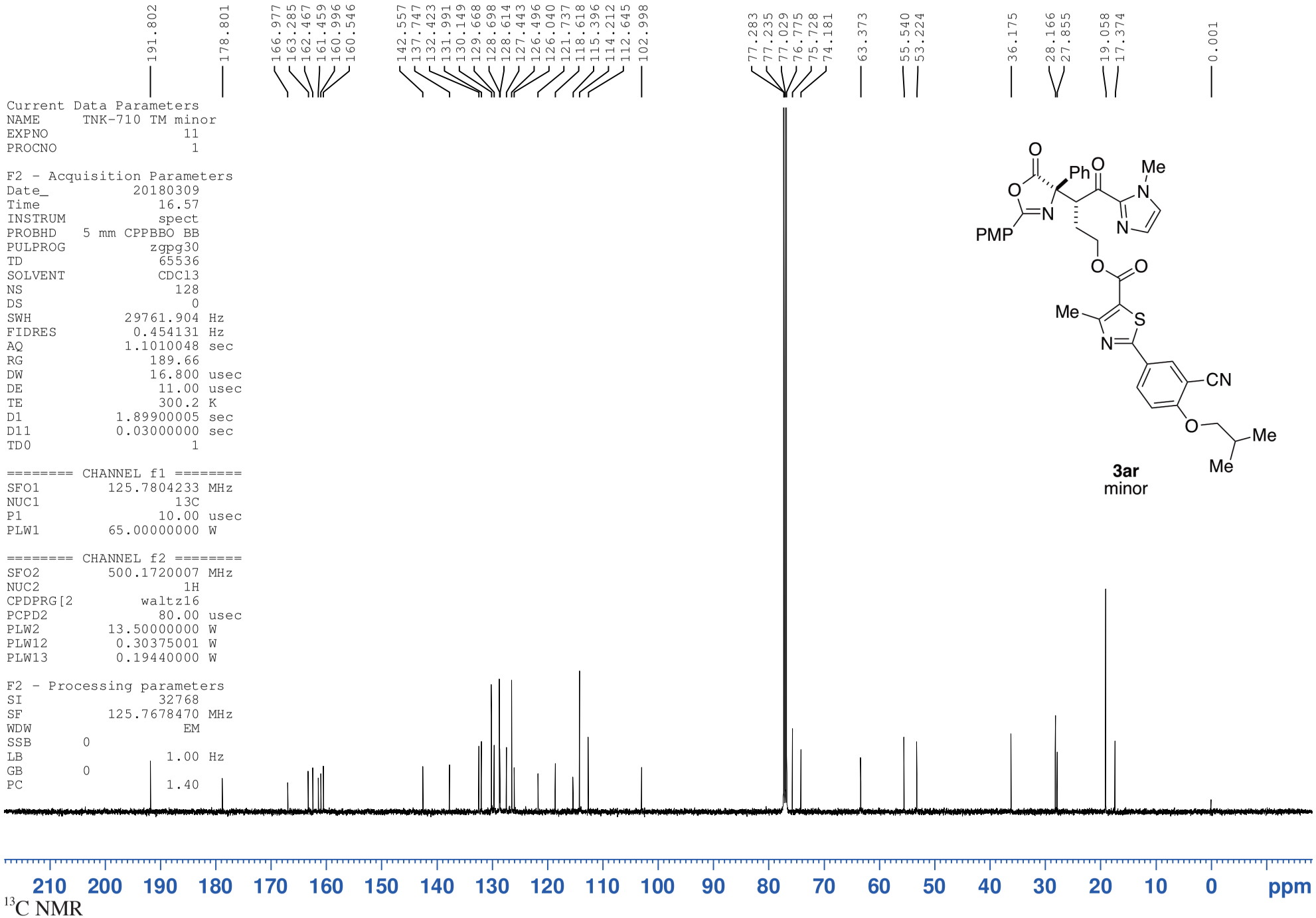
1.048
1.121
6.169

^{1}H NMR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166.977
163.285
162.467
161.459
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160.546
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137.747
132.423
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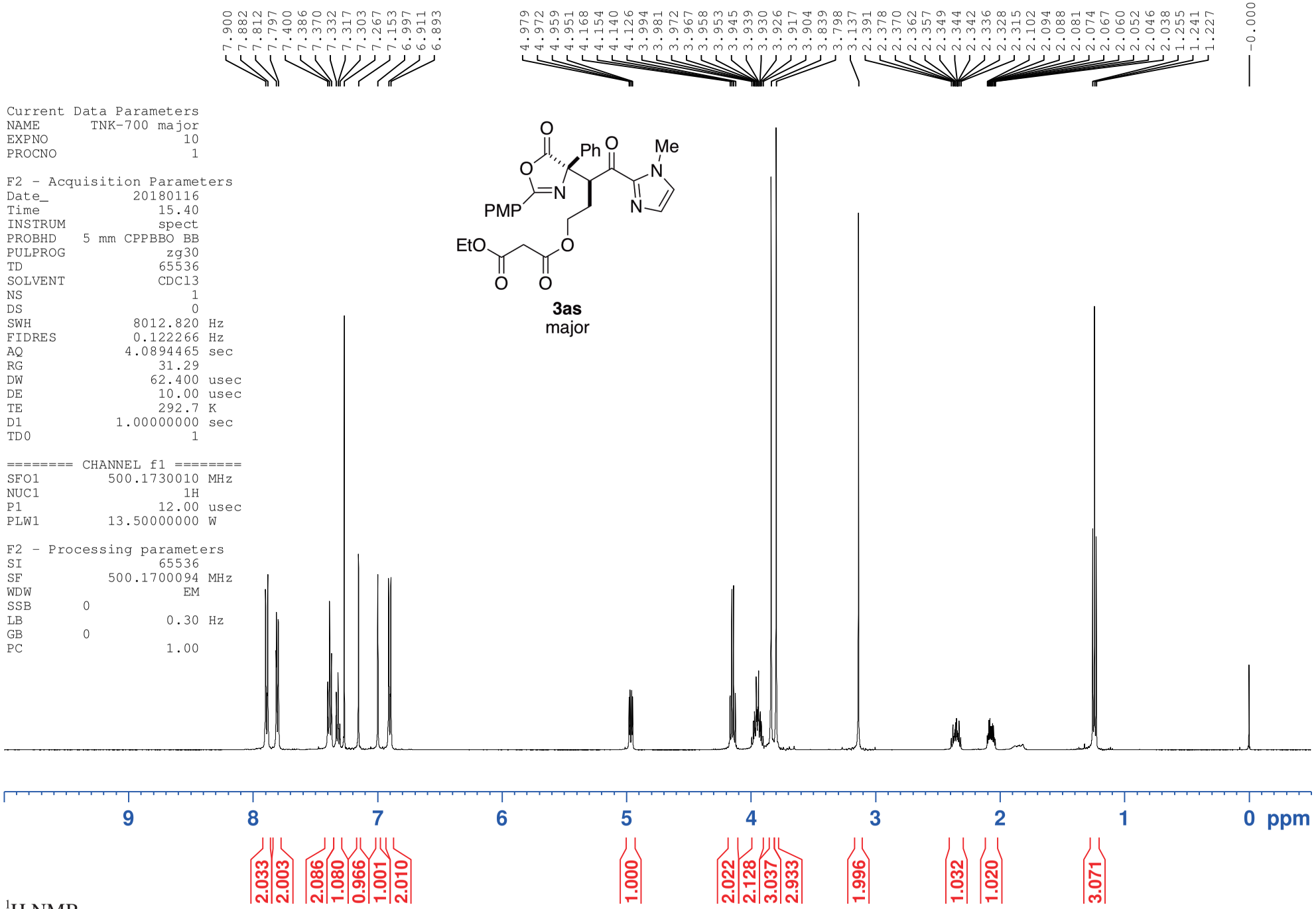
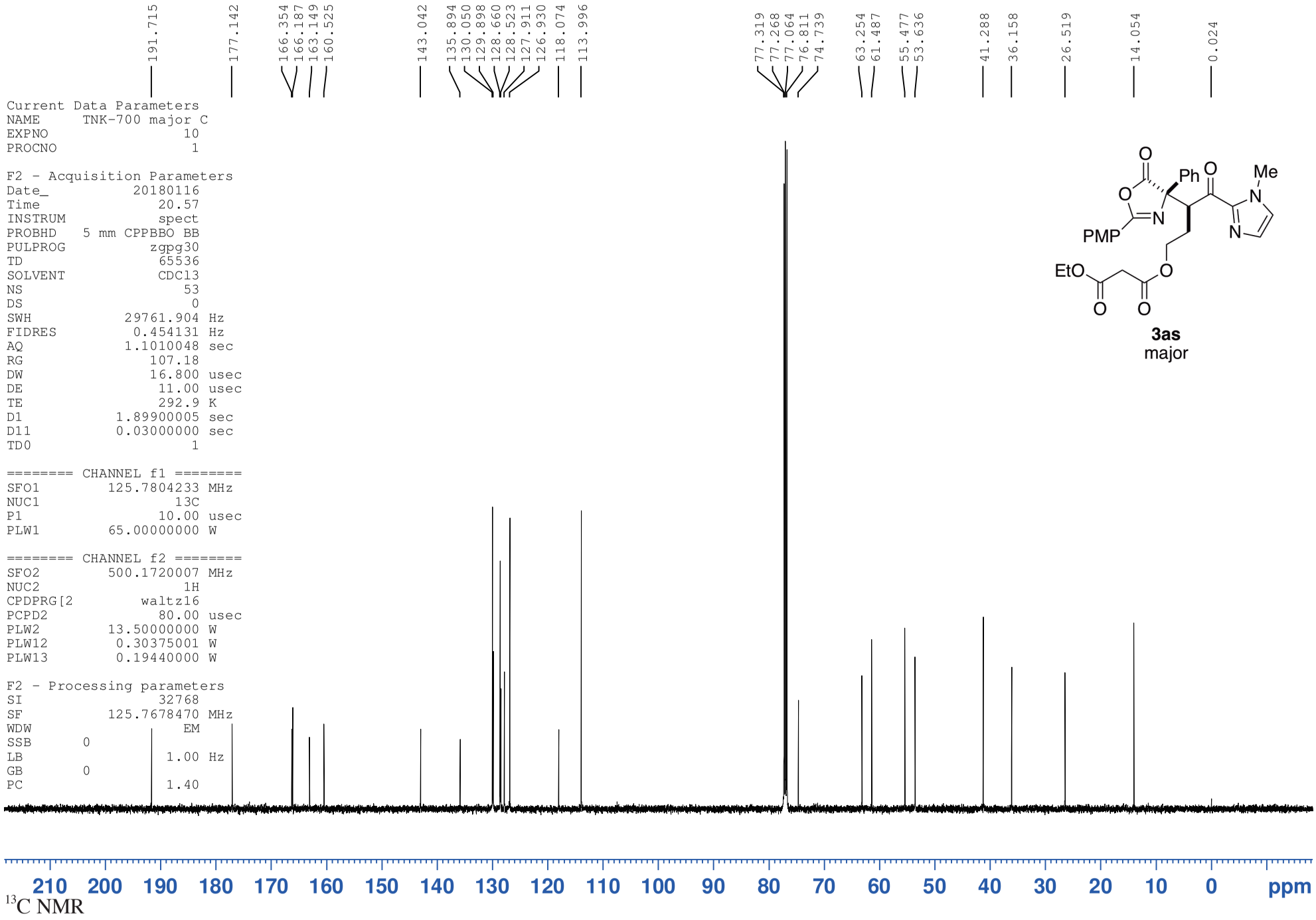
130.149
129.668
128.698
128.614
127.443
126.496
126.040
121.737
118.618
115.396
114.212
112.645
102.998
77.283
77.235
77.029
76.775
75.728
74.181
63.373
55.540
53.224
36.175
28.166
27.855
19.058
17.374
0.001
Current Data Parameters
NAME TNK-710 TM minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180309
Time 16.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
PMP
Ph
Me
Me
Me
CN
Me
Me
3ar
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

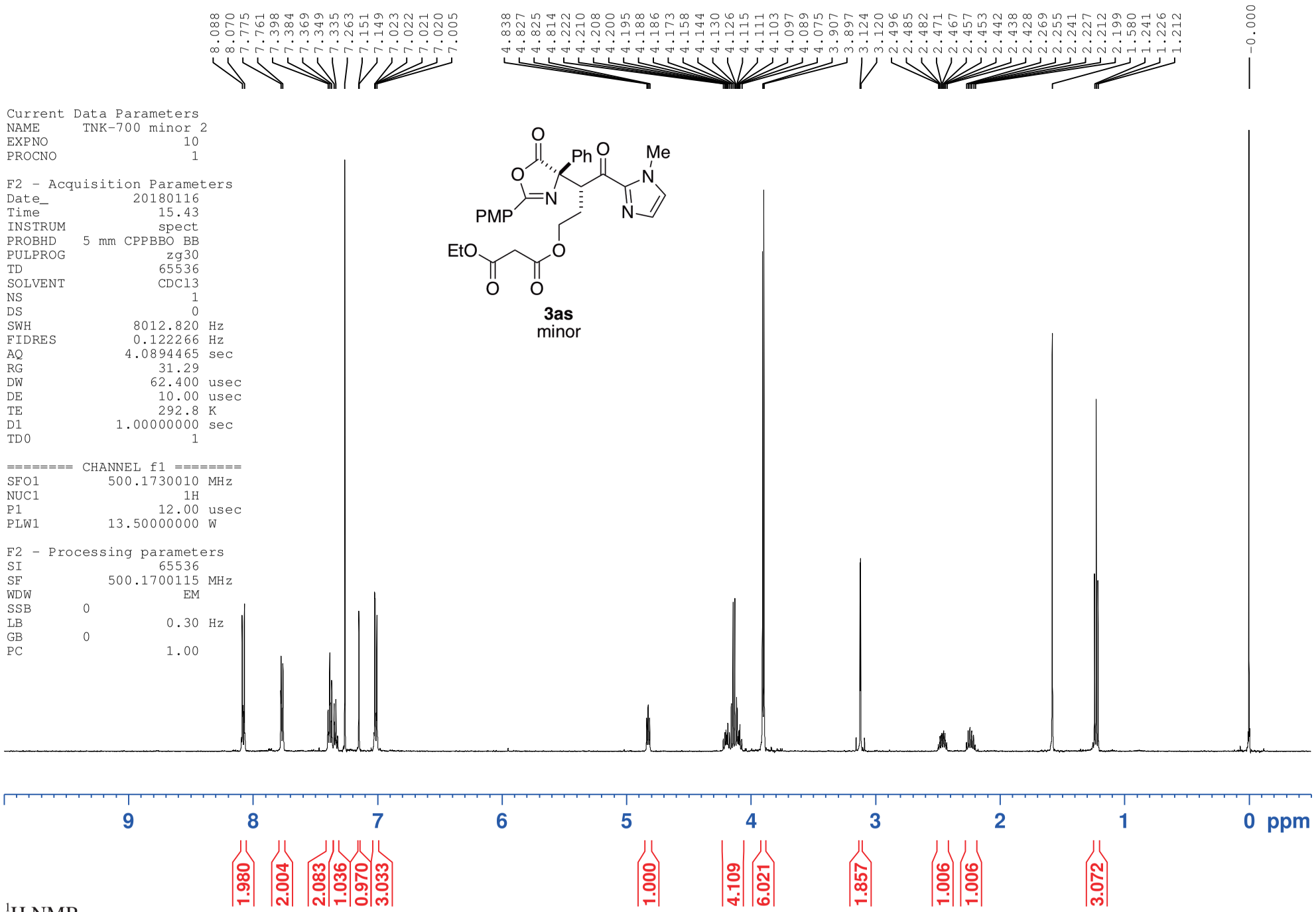
^{13}C NMR


7.900
7.882
7.812
7.797
7.400
7.386
7.370
7.332
7.317
7.303
7.267
7.153
6.997
6.911
6.893
4.979
4.972
4.959
4.951
4.168
4.154
4.140
4.126
3.994
3.981
3.972
3.967
3.958
3.953
3.945
3.939
3.930
3.926
3.917
3.904
3.839
3.798
3.137
2.391
2.378
2.370
2.362
2.357
2.349
2.344
2.342
2.336
2.328
2.315
2.102
2.094
2.088
2.081
2.074
2.067
2.060
2.052
2.046
2.038
1.255
1.241
1.227
0.000
Current Data Parameters
NAME TNK-700 major
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180116
Time 15.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
N
N
PMP
EtO
O
O
O
3as
major
9
8
7
6
5
4
3
2
1
0 ppm
2.033
2.003
2.086
1.080
0.966
1.001
2.010
1.000
2.022
2.128
3.037
2.933
1.996
1.032
1.020
3.071

^{1}H NMR


191.715
177.142
166.354
166.187
163.149
160.525
143.042
135.894
130.050
129.898
128.660
128.523
127.911
126.930
118.074
113.996
77.319
77.268
77.064
76.811
74.739
63.254
61.487
55.477
53.636
41.288
36.158
26.519
14.054
0.024
Current Data Parameters
NAME TNK-700 major C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180116
Time 20.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 53
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 292.9 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
PMP
N
EtO
O
O
O
3as
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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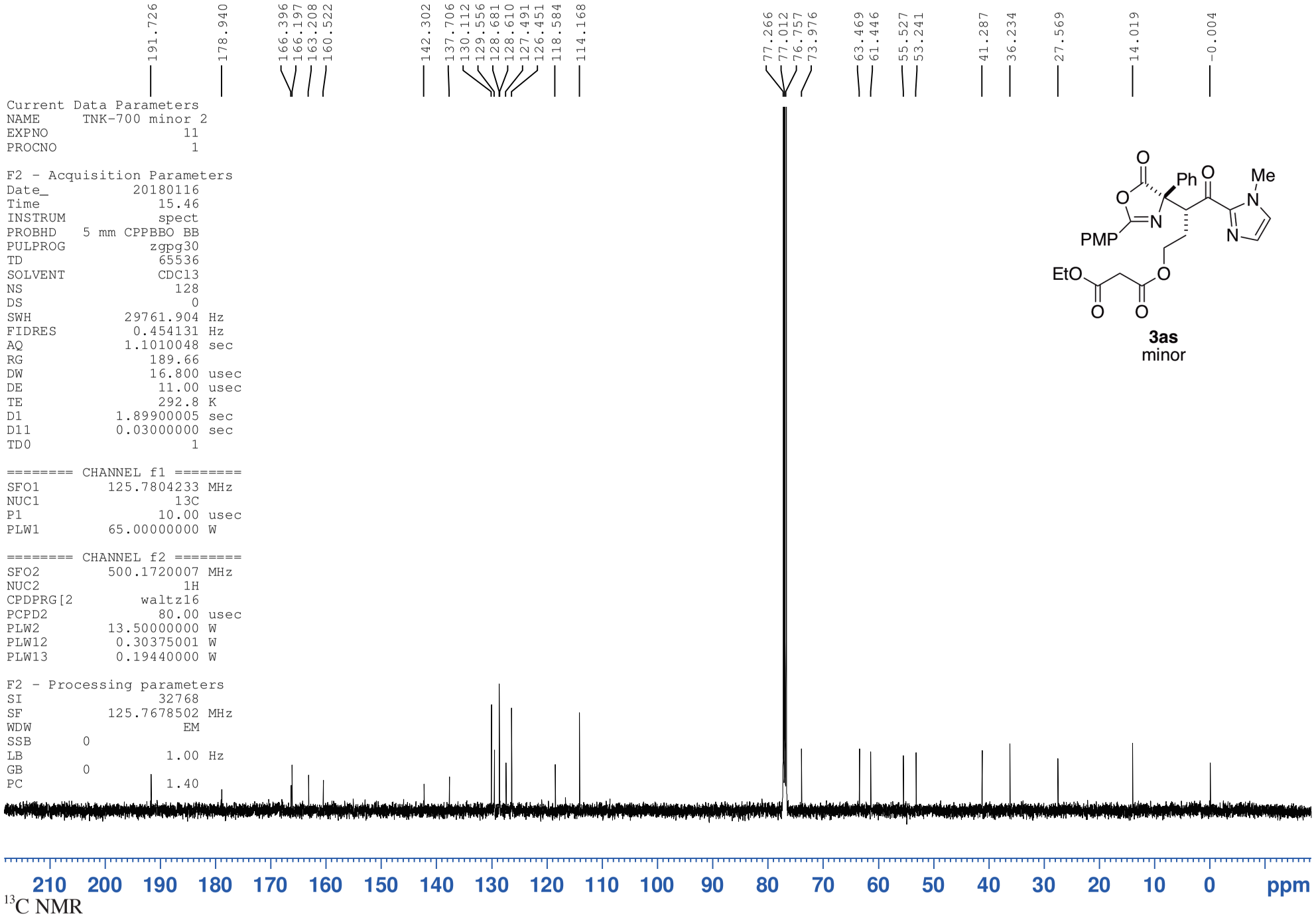
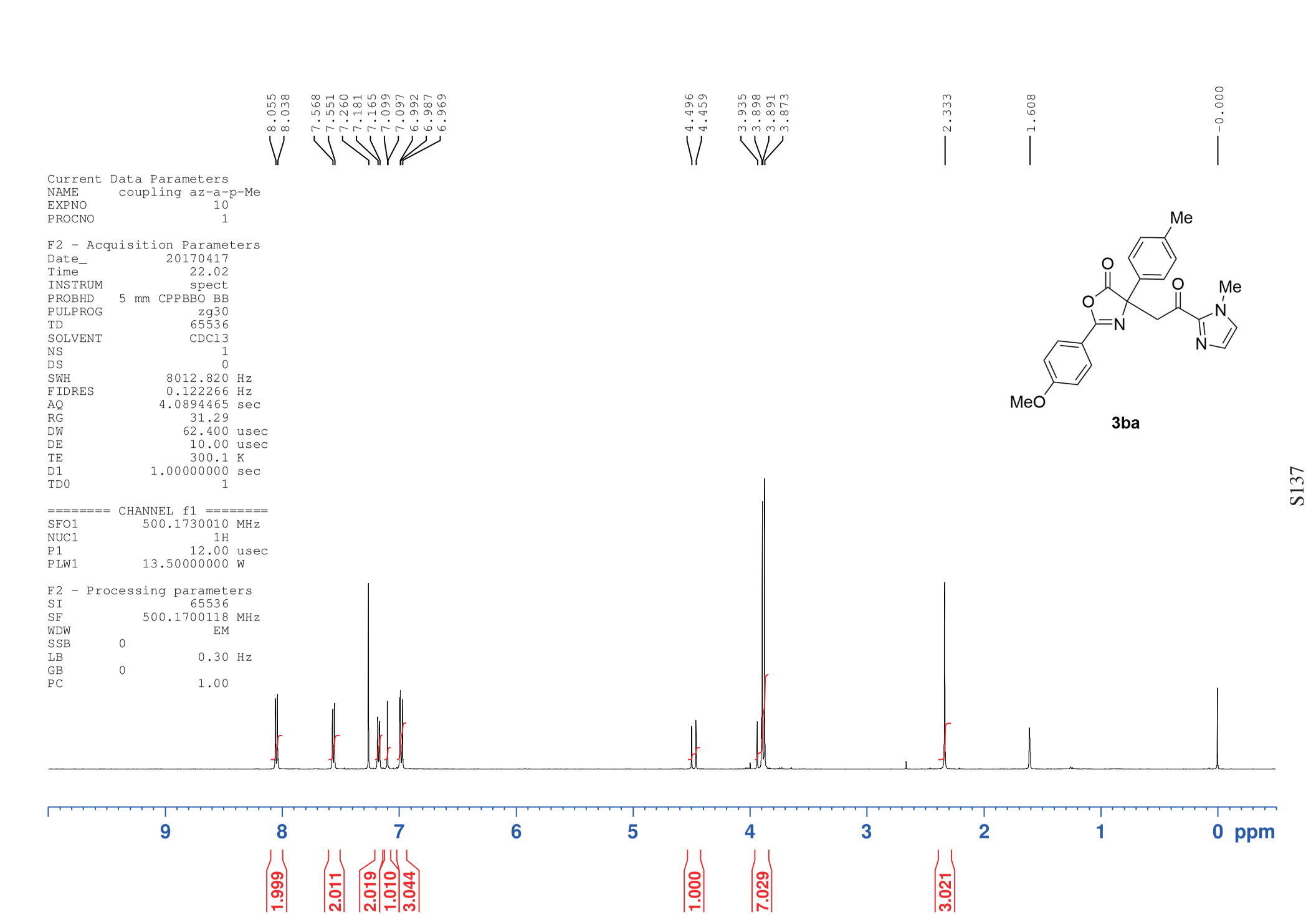
8.070
7.775
7.761
7.398
7.384
7.369
7.349
7.335
7.263
7.151
7.149
7.023
7.022
7.021
7.020
7.005
4.838
4.827
4.825
4.814
4.222
4.210
4.208
4.200
4.195
4.188
4.186
4.173
4.158
4.144
4.130
4.126
4.115
4.111
4.103
4.097
4.089
4.075
3.907
3.897
3.124
3.120
2.496
2.485
2.482
2.471
2.467
2.457
2.453
2.442
2.438
2.428
2.269
2.255
2.241
2.227
2.212
2.199
1.580
1.241
1.226
1.212
0.000
Current Data Parameters
NAME TNK-700 minor 2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180116
Time 15.43
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
Ph
O
Me
N
O
N
N
PMP
EtO
O
O
O
3as
minor
9
8
7
6
5
4
3
2
1
0 ppm
1.980
2.004
2.083
1.036
0.970
3.033
1.000
4.109
6.021
1.857
1.006
1.006
3.072

^{1}H NMR


191.726
178.940
166.396
166.197
163.208
160.522
142.302
137.706
130.112
129.556
128.681
128.610
127.491
126.451
118.584
114.168
77.266
77.012
76.757
73.976
63.469
61.446
55.527
53.241
41.287
36.234
27.569
14.019
-0.004
Current Data Parameters
NAME TNK-700 minor 2
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180116
Time 15.46
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.8 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678502 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
N
PMP
N
EtO
O
O
O
3as
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

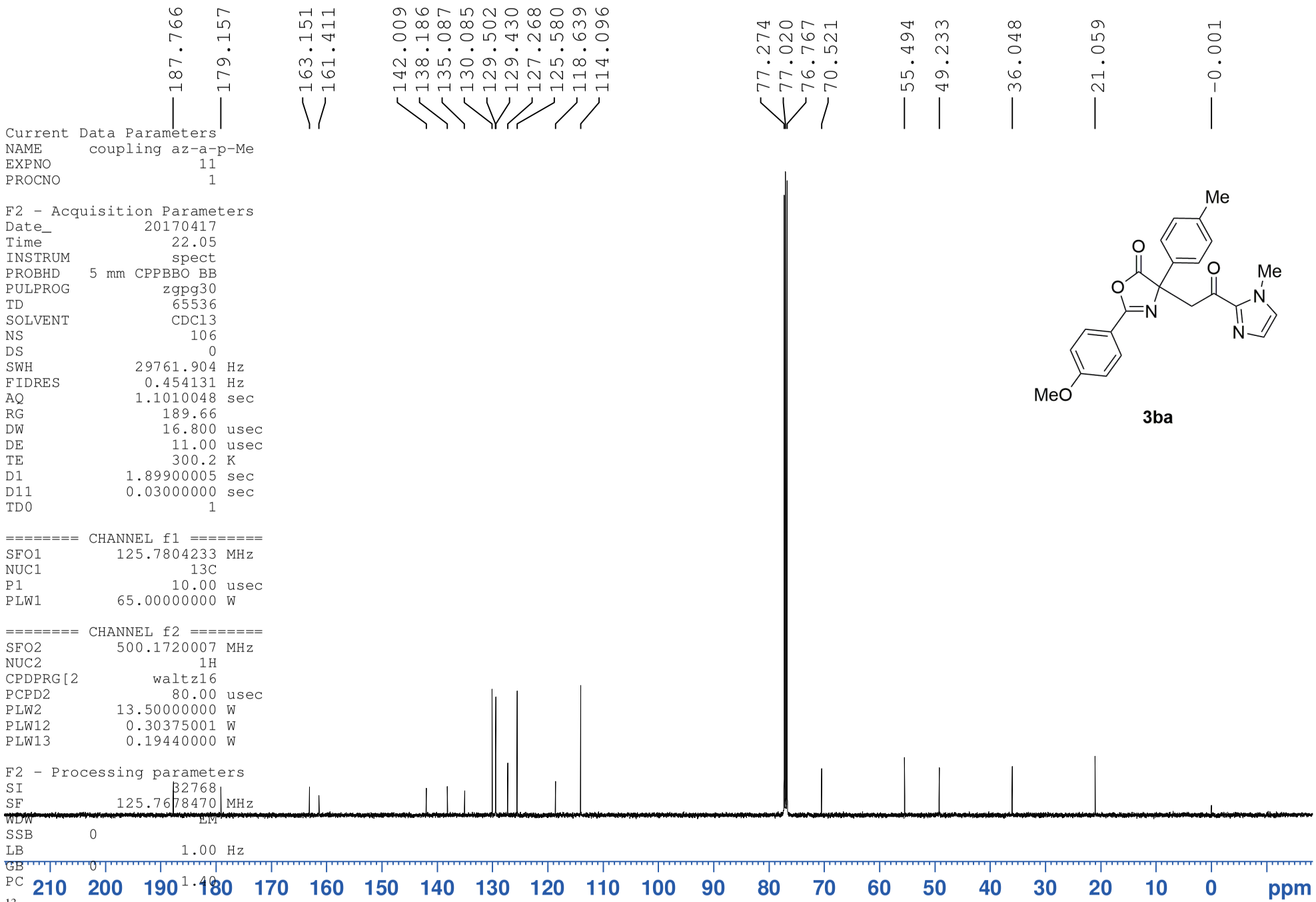
^{13}C NMR



3ba

S137

^{1}H NMR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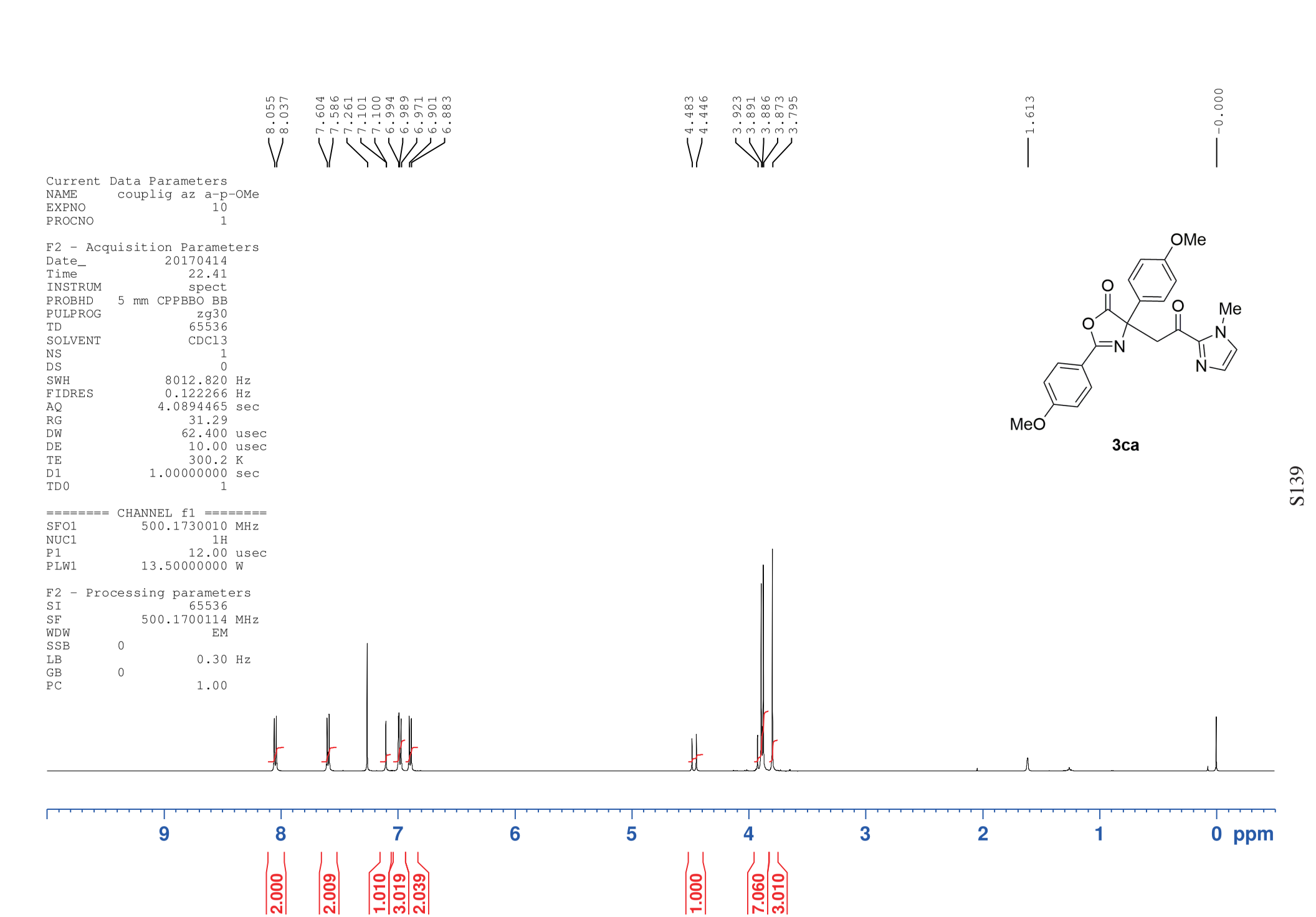
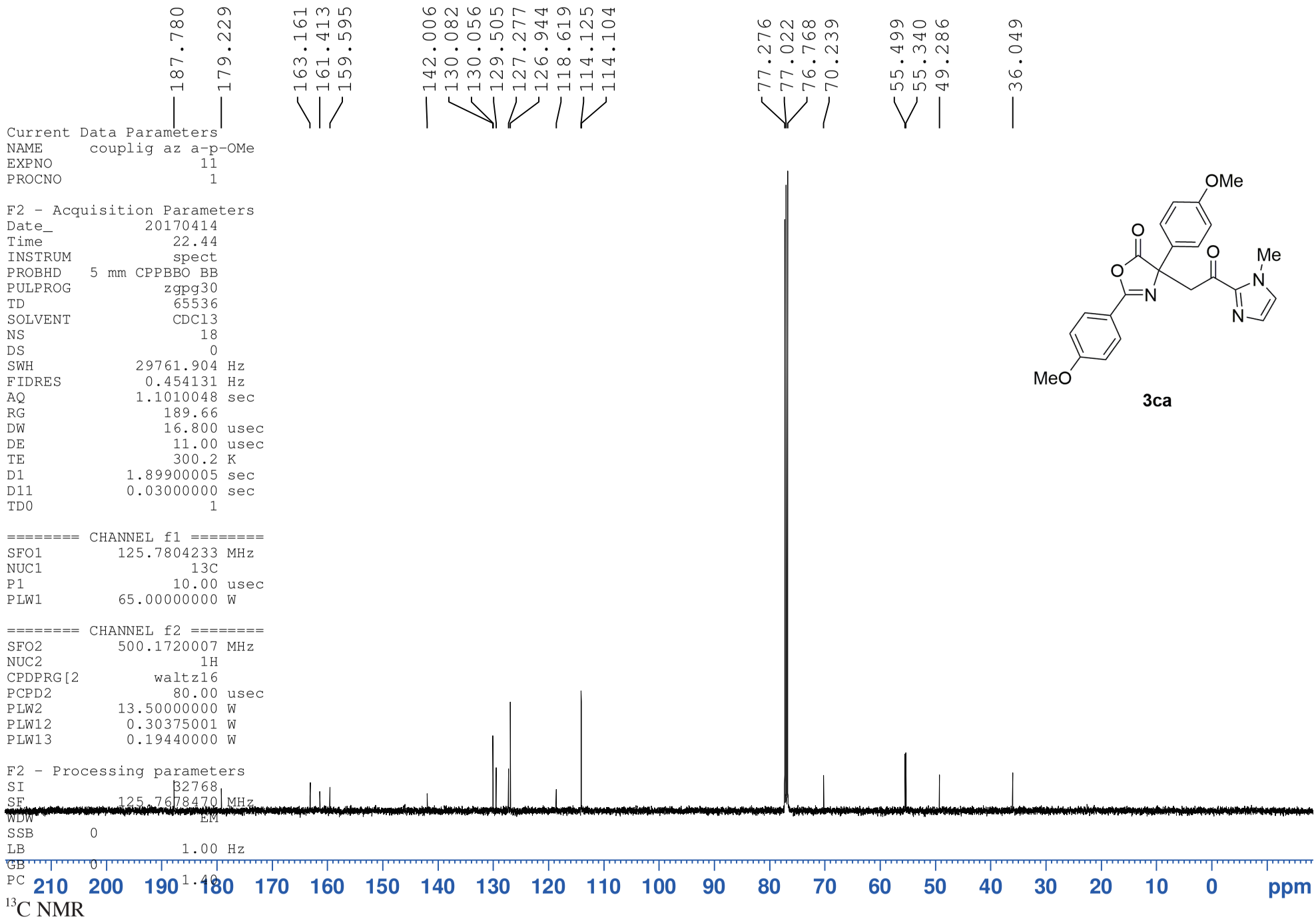
179.157
163.151
161.411
142.009
138.186
135.087
130.085
129.502
129.430
127.268
125.580
118.639
114.096
77.274
77.020
76.767
70.521
55.494
49.233
36.048
21.059
-0.001
Current Data Parameters
NAME coupling az-a-p-Me
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170417
Time 22.05
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 106
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
O
O
Me
O
N
N
N
MeO
3ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR


8.055
8.037
7.604
7.586
7.261
7.101
7.100
6.994
6.989
6.971
6.901
6.883
4.483
4.446
3.923
3.891
3.886
3.873
3.795
1.613
-0.000
Current Data Parameters
NAME couplig az a-p-OMe
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.41
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
O
O
O
N
Me
N
N
MeO
3ca
9
8
7
6
5
4
3
2
1
0 ppm
2.000
2.009
1.010
3.019
2.039
1.000
7.060
3.010

^{1}H NMR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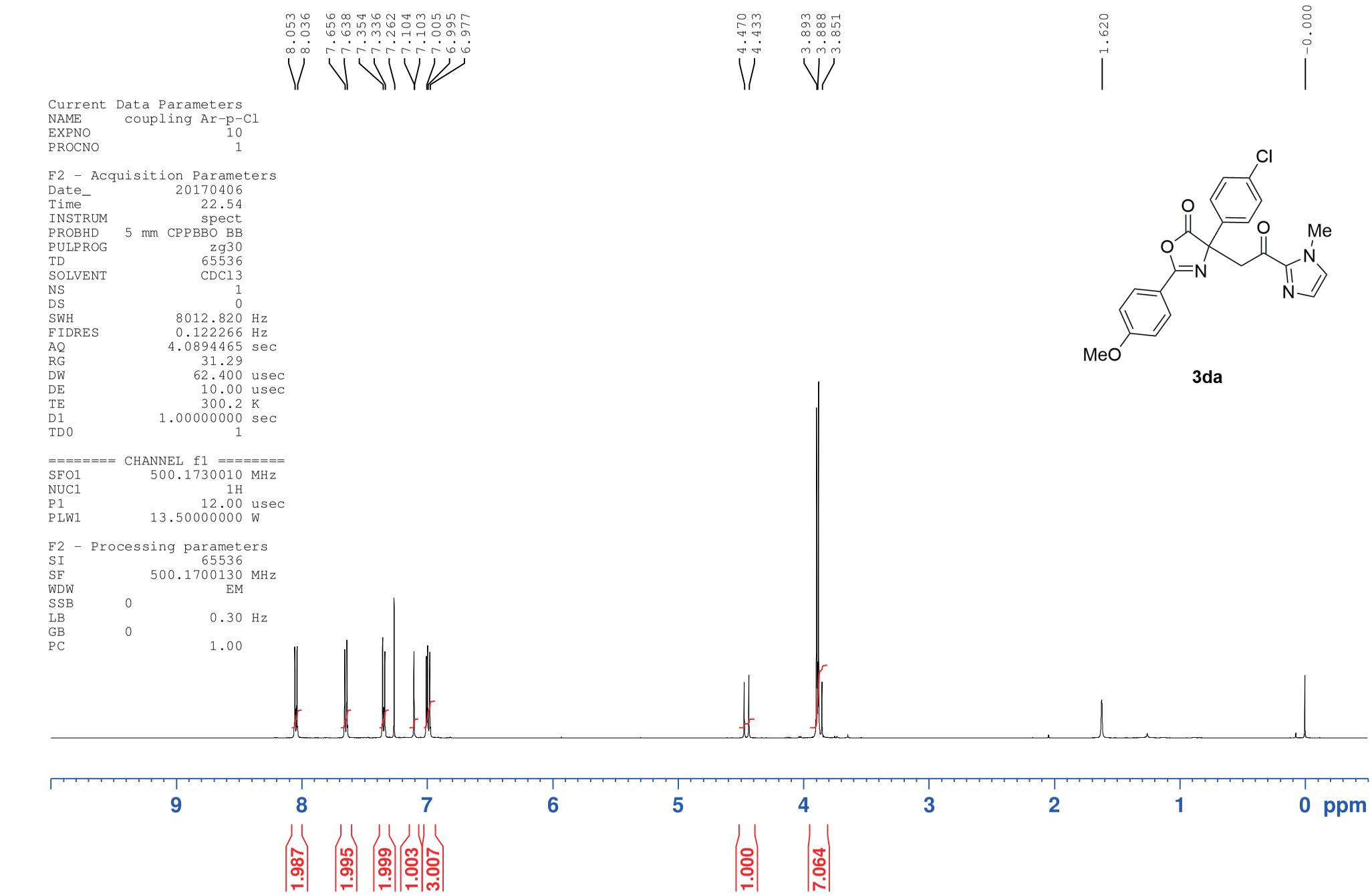
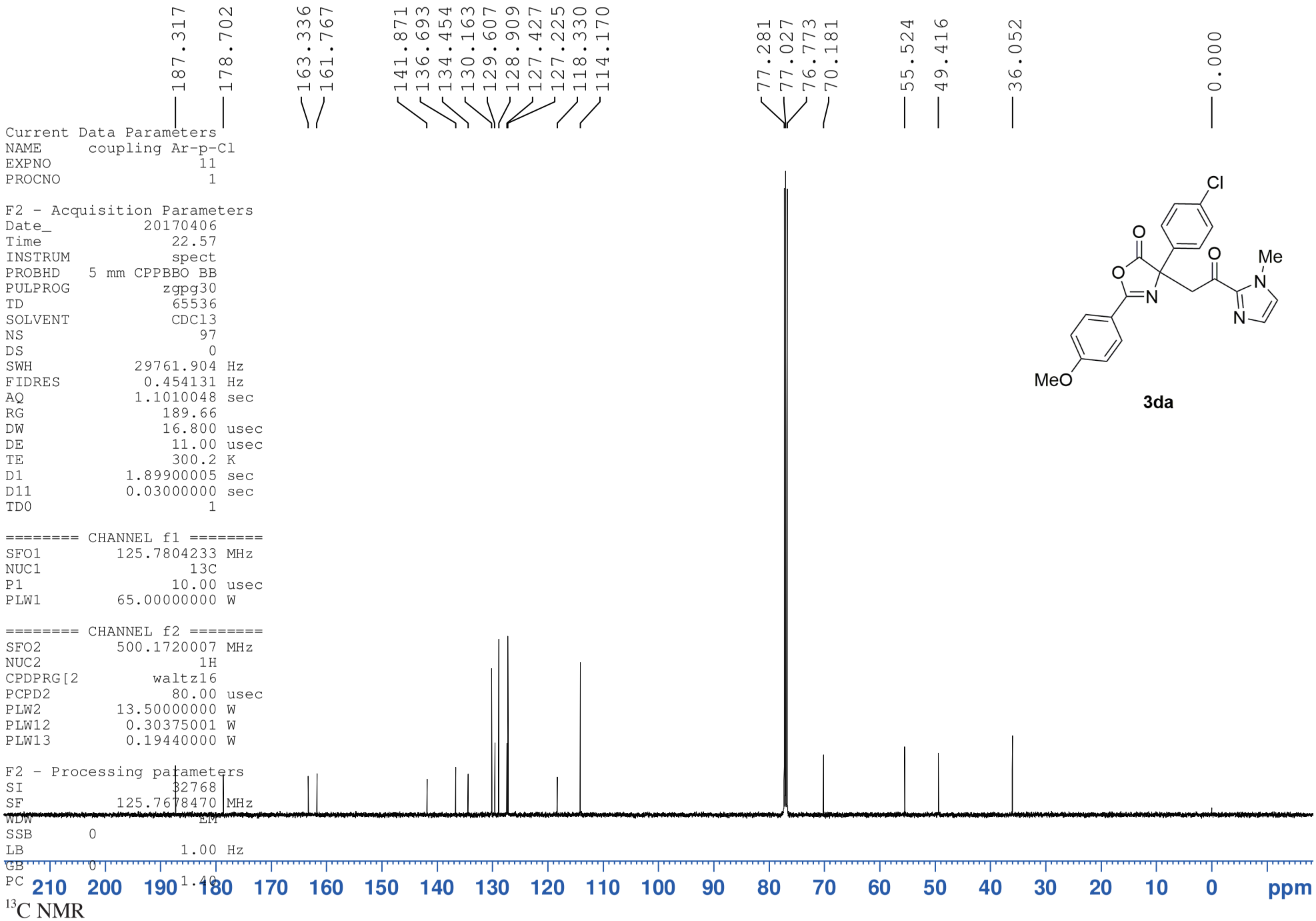
161.413
159.595
142.006
130.082
130.056
129.505
127.277
126.944
118.619
114.125
114.104
77.276
77.022
76.768
70.239
55.499
55.340
49.286
36.049
Current Data Parameters
NAME couplig az a-p-OMe
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170414
Time 22.44
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 18
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OMe
MeO
O
O
O
N
N
Me
3ca
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR


8.053
8.036
7.656
7.638
7.354
7.336
7.262
7.104
7.103
7.005
6.995
6.977
4.470
4.433
3.893
3.888
3.851
1.620
-0.000
Current Data Parameters
NAME coupling Ar-p-Cl
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170406
Time 22.54
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
O
O
O
N
N
Me
N
MeO
3da
9
8
7
6
5
4
3
2
1
0 ppm
1.987
1.995
1.999
1.003
3.007
1.000
7.064

^{1}H NMR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141.871
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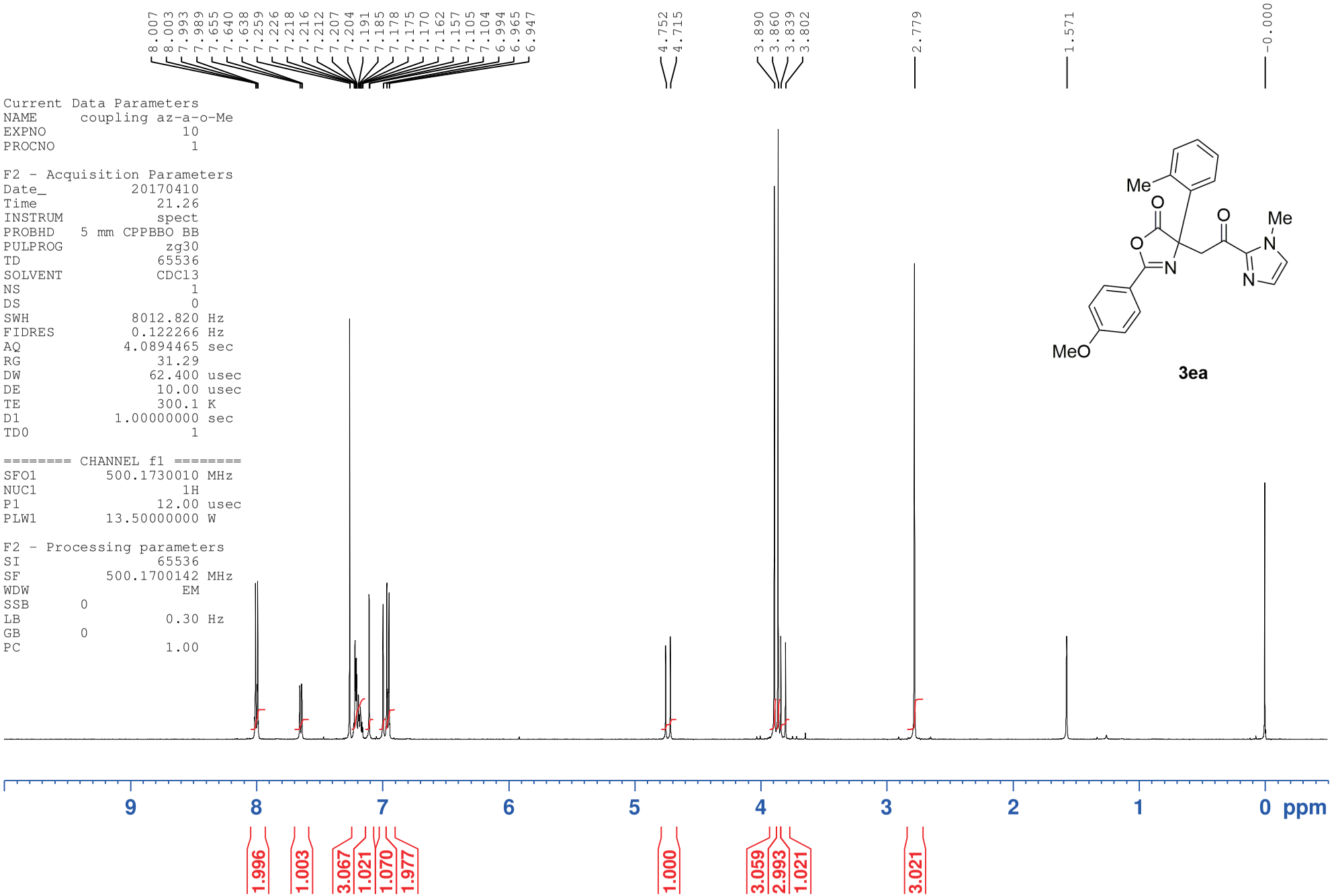
130.163
129.607
128.909
127.427
127.225
118.330
114.170
77.281
77.027
76.773
70.181
55.524
49.416
36.052
0.000
Current Data Parameters
NAME coupling Ar-p-Cl
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170406
Time 22.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 97
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
O
O
O
N
Me
N
N
MeO
3da
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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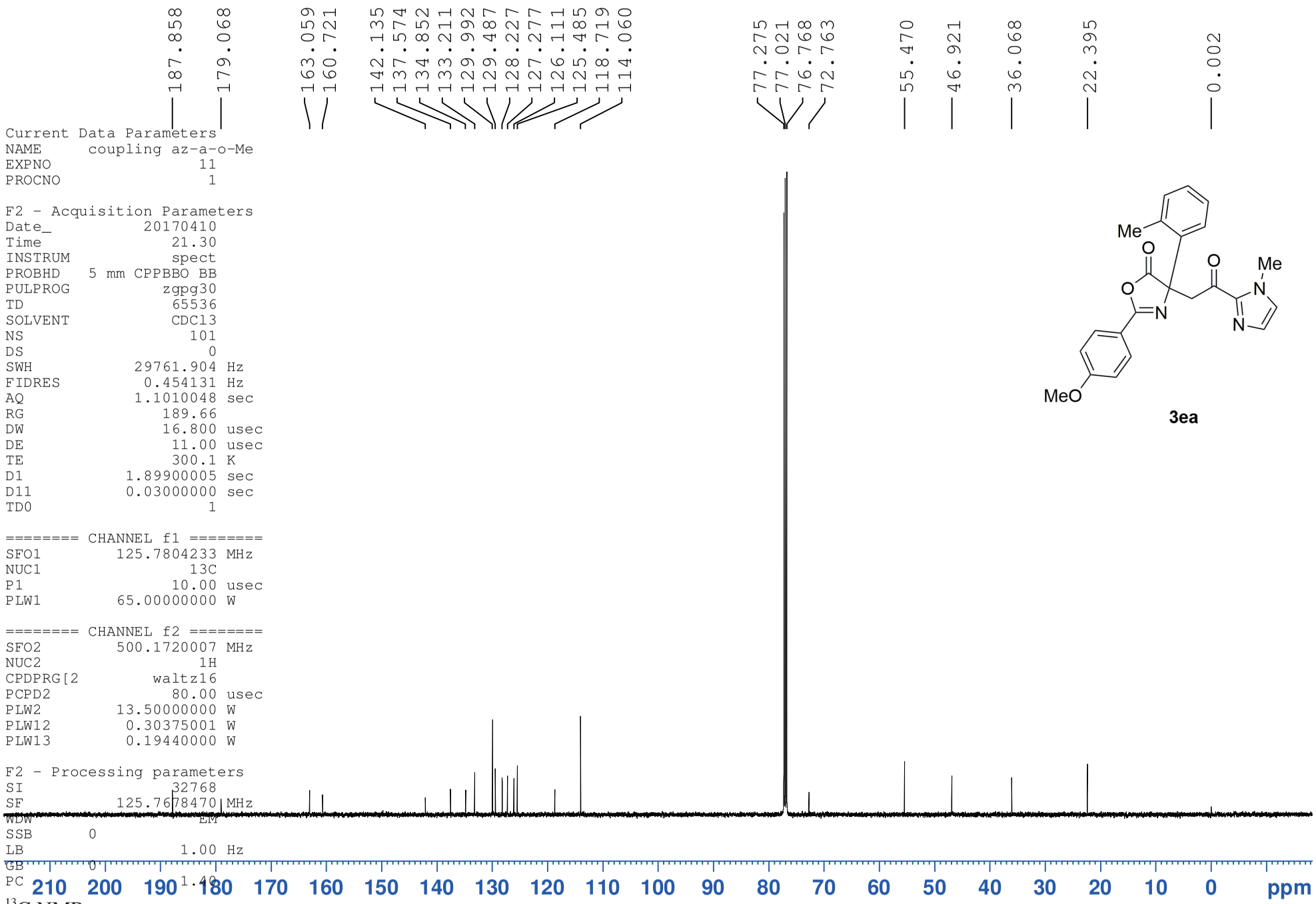
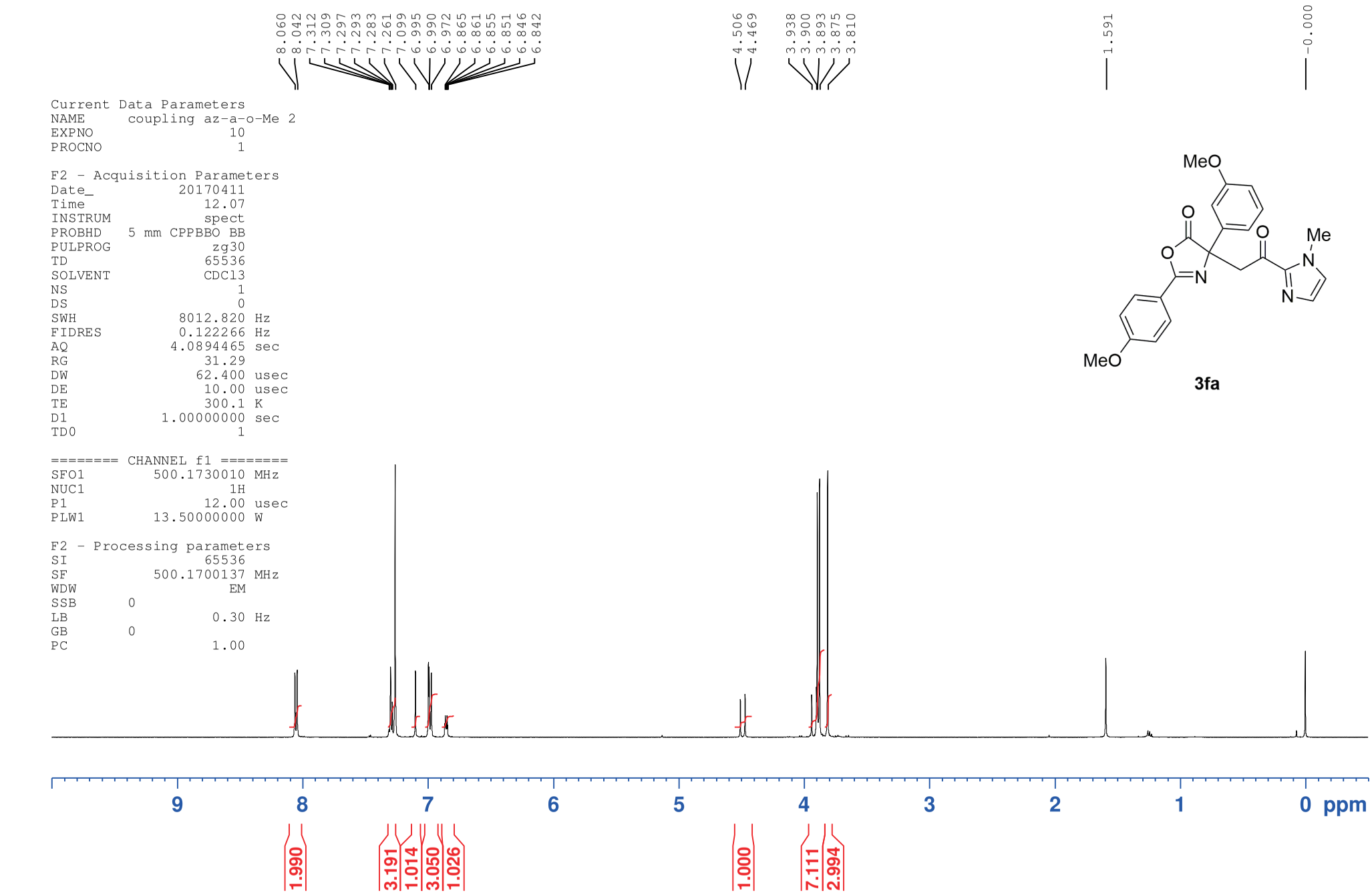
8.003
7.993
7.989
7.655
7.640
7.638
7.259
7.226
7.218
7.216
7.212
7.207
7.204
7.191
7.185
7.178
7.175
7.170
7.162
7.157
7.105
7.104
6.994
6.965
6.947
4.752
4.715
3.890
3.860
3.839
3.802
2.779
1.571
-0.000
Current Data Parameters
NAME coupling az-a-o-Me
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170410
Time 21.26
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
O
O
O
N
Me
N
N
MeO
3ea
9
8
7
6
5
4
3
2
1
0 ppm
1.996
1.003
3.067
1.021
1.070
1.977
1.000
3.059
2.993
1.021
3.021

^{1}H NMR


187.858
179.068
163.059
160.721
142.135
137.574
134.852
133.211
129.992
129.487
128.227
127.277
126.111
125.485
118.719
114.060
77.275
77.021
76.768
72.763
55.470
46.921
36.068
22.395
0.002
Current Data Parameters
NAME coupling az-a-o-Me
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170410
Time 21.30
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
O
O
Me
O
N
N
N
MeO
3ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

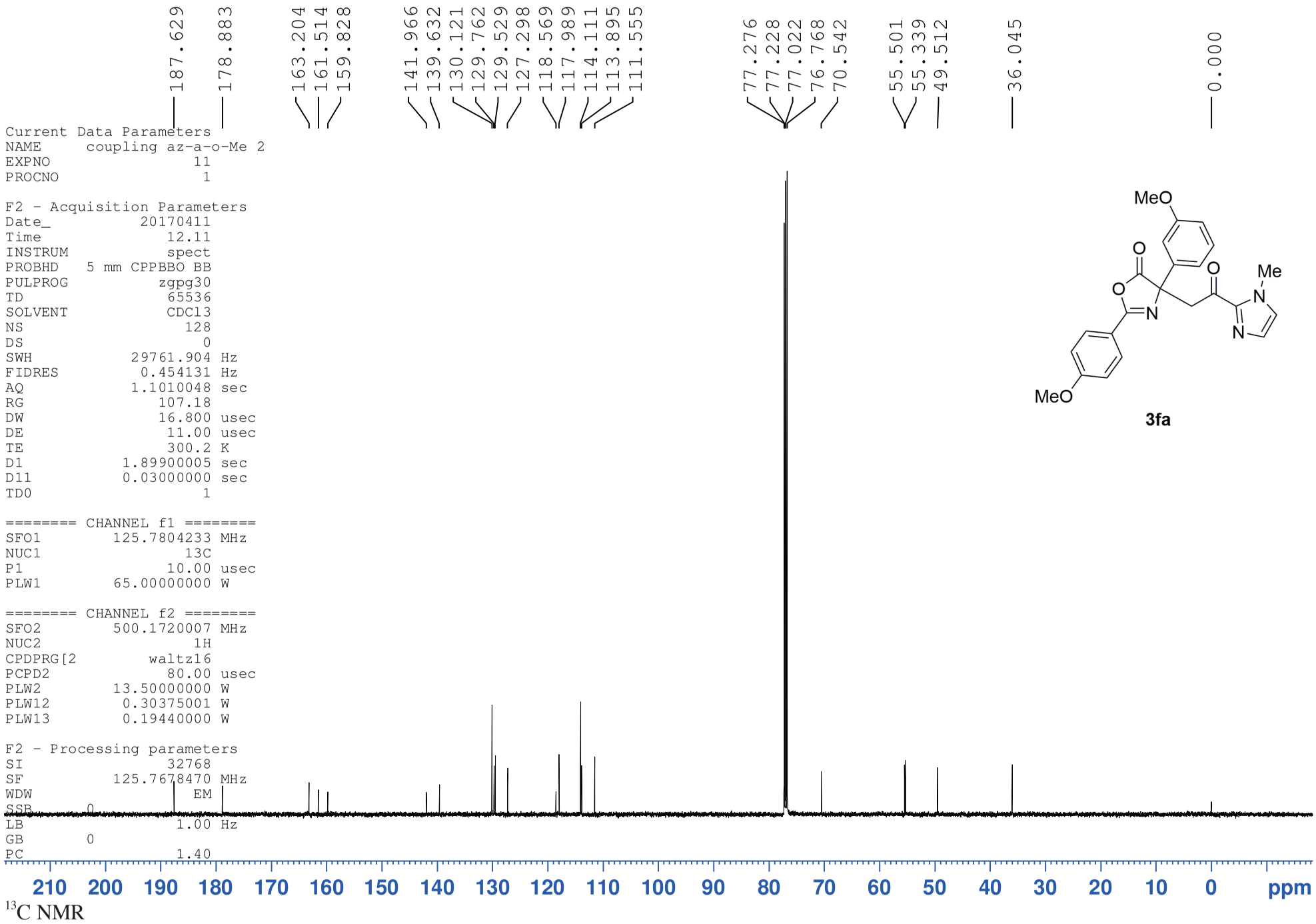
^{13}C NMR



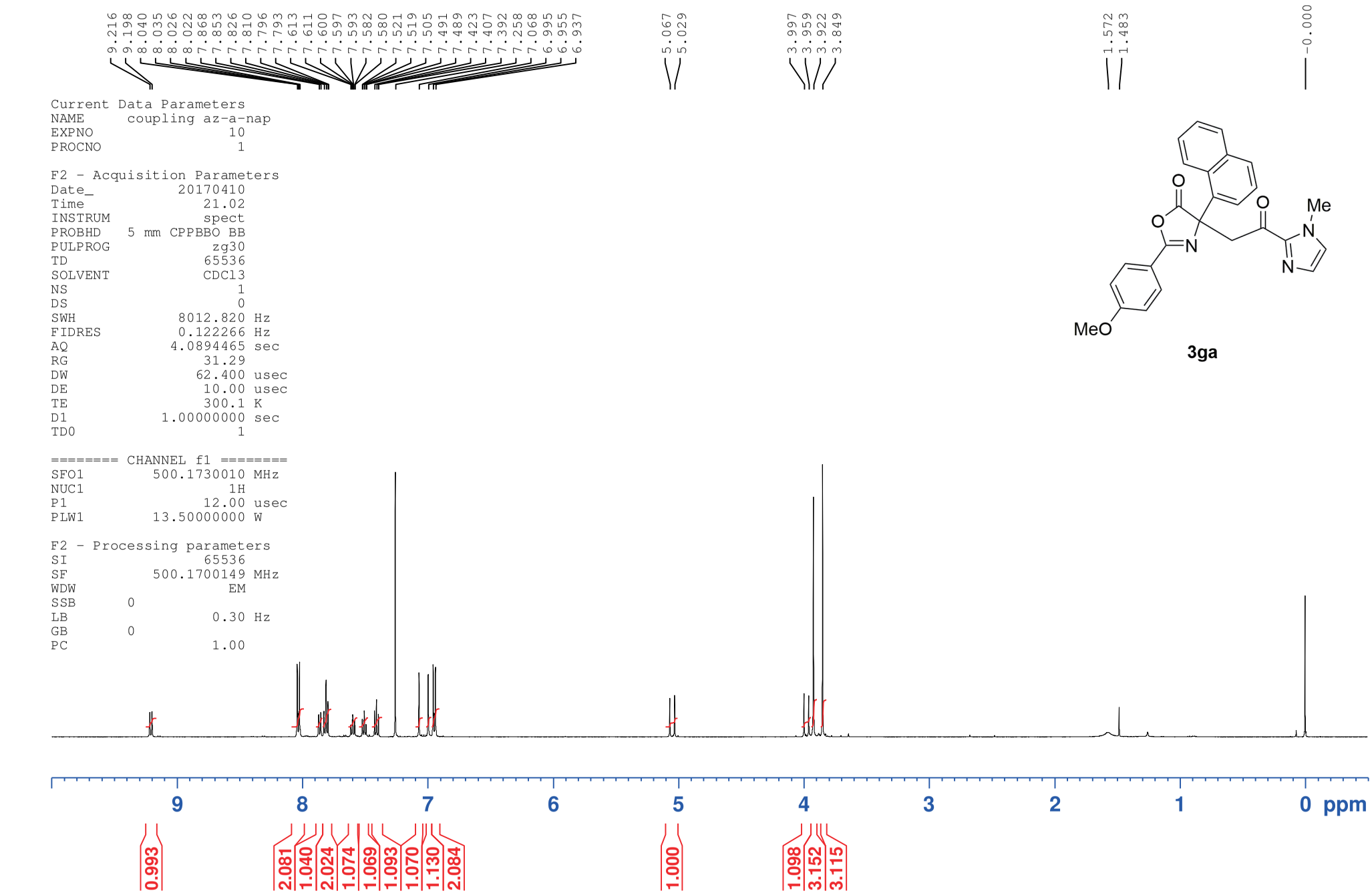
3fa

S145

^{1}H NMR


187.629
178.883
163.204
161.514
159.828
141.966
139.632
130.121
129.762
129.529
127.298
118.569
117.989
114.111
113.895
111.555
77.276
77.228
77.022
76.768
70.542
55.501
55.339
49.512
36.045
0.000
Current Data Parameters
NAME coupling az-a-o-Me 2
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170411
Time 12.11
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
O
O
O
N
N
Me
N
MeO
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR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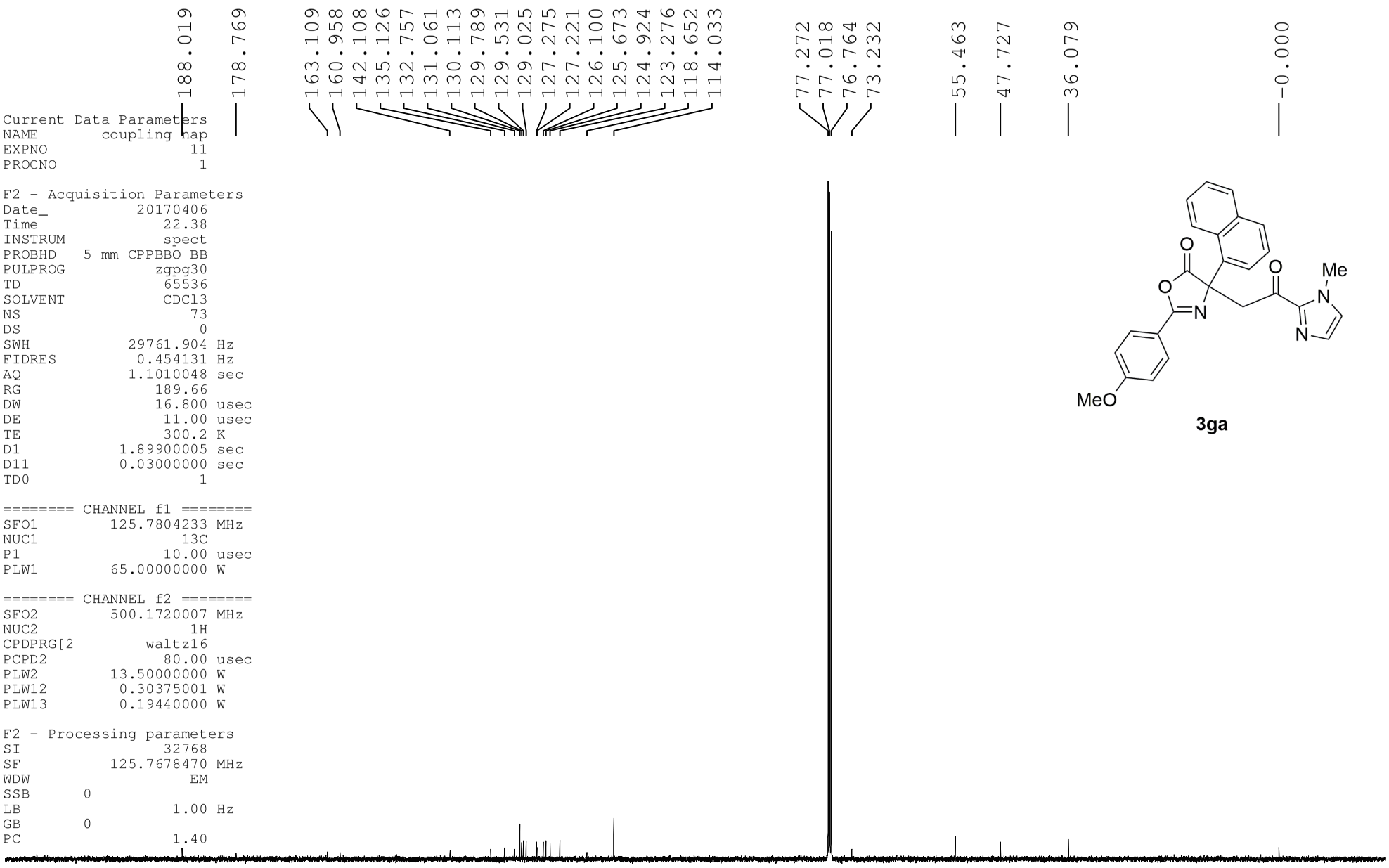
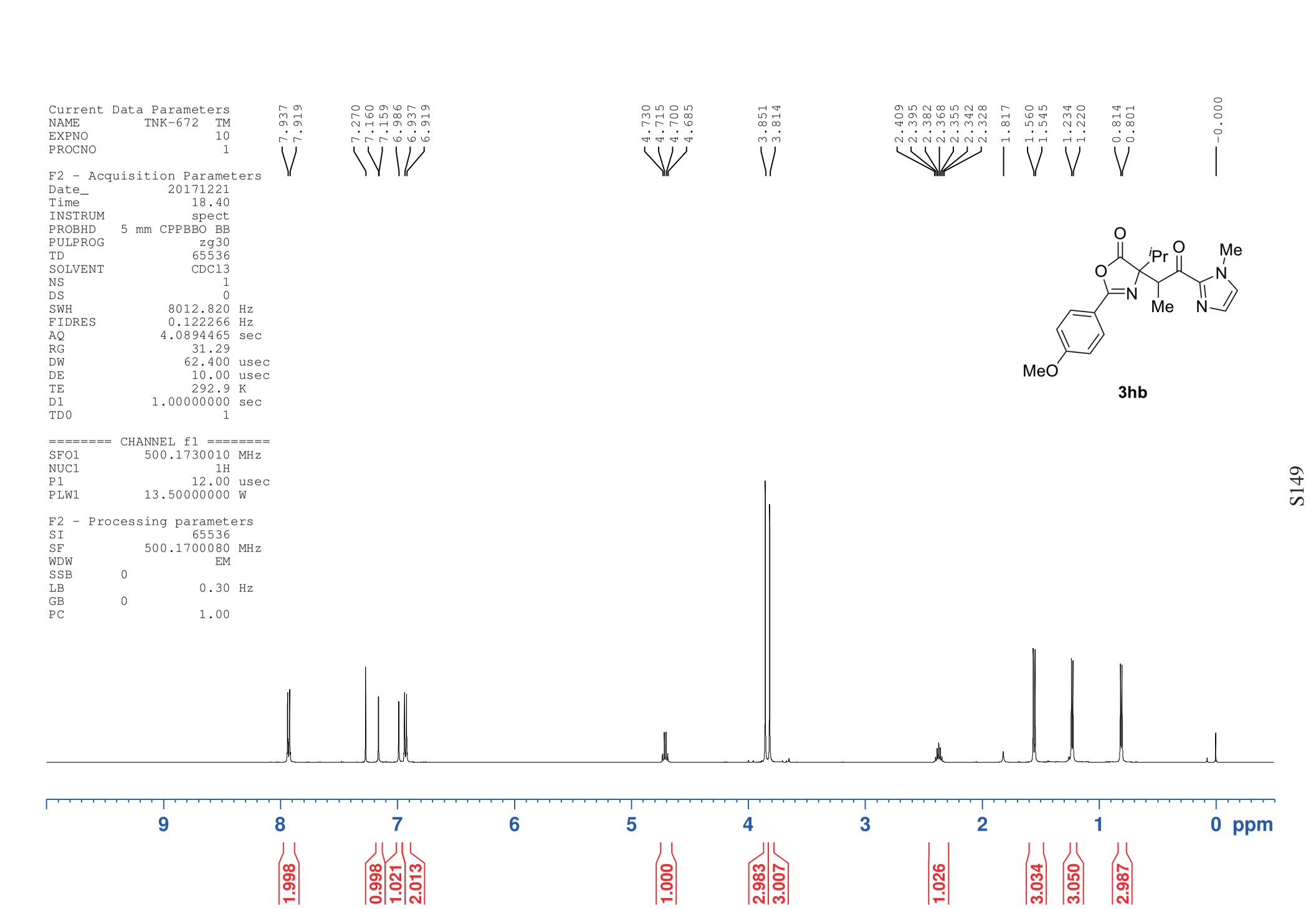
9.198
8.040
8.035
8.026
8.022
7.868
7.853
7.826
7.810
7.796
7.793
7.613
7.611
7.600
7.597
7.593
7.582
7.580
7.521
7.519
7.505
7.491
7.489
7.423
7.407
7.392
7.258
7.068
6.995
6.955
6.937
5.067
5.029
3.997
3.959
3.922
3.849
1.572
1.483
-0.000
Current Data Parameters
NAME coupling az-a-nap
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170410
Time 21.02
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700149 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
O
Me
N
N
MeO
9
8
7
6
5
4
3
2
1
0 ppm
0.993
2.081
1.040
2.024
1.074
1.069
1.093
1.070
1.130
2.084
1.000
1.098
3.152
3.115

3ga

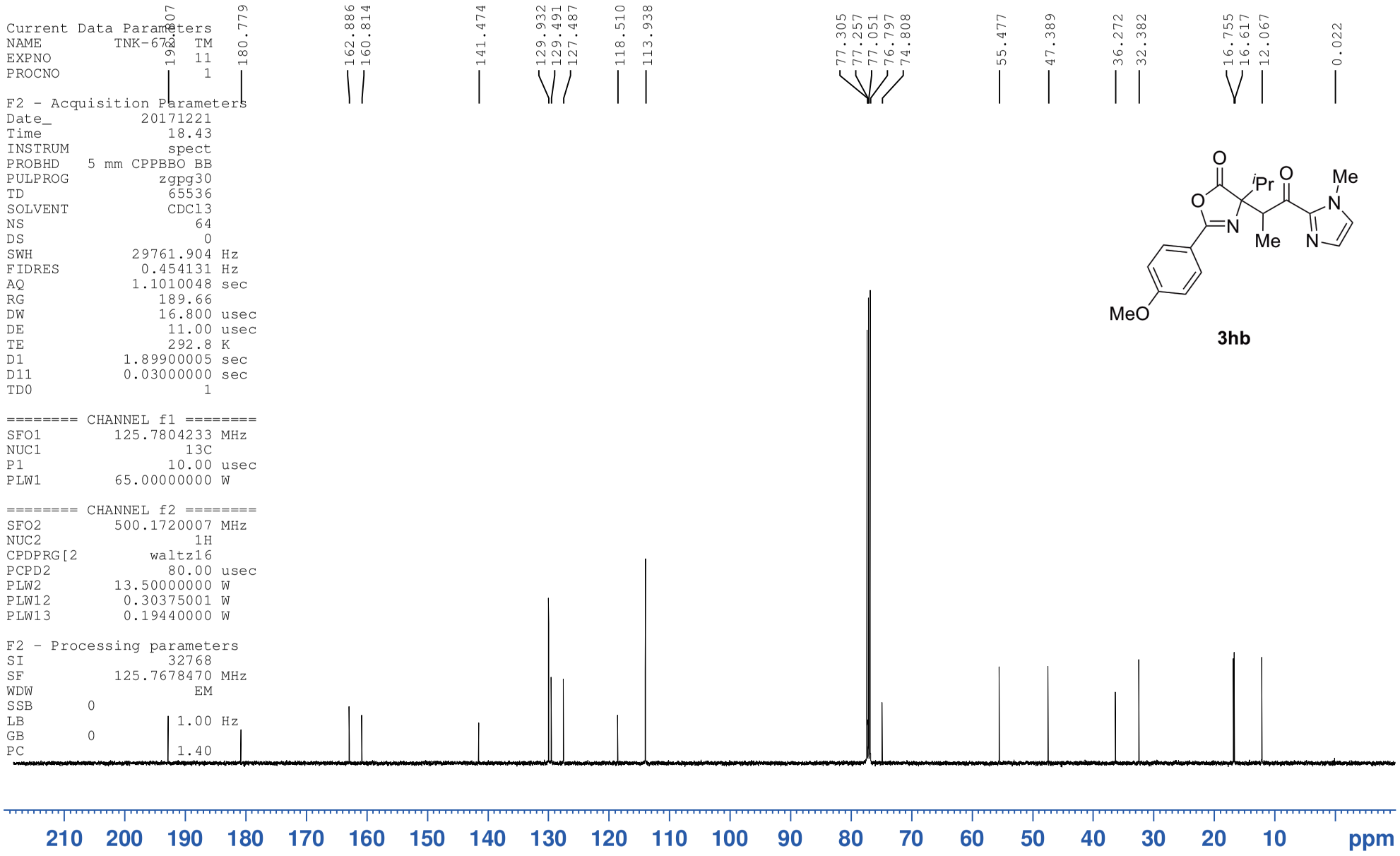
^{1}H NMR


188.019
178.769
163.109
160.958
142.108
135.126
132.757
131.061
130.113
129.789
129.531
129.025
127.275
127.221
126.100
125.673
124.924
123.276
118.652
114.033
77.272
77.018
76.764
73.232
55.463
47.727
36.079
0.000
Current Data Parameters
NAME coupling nap
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170406
Time 22.38
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 73
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
N
O
Me
N
N
MeO
3ga
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

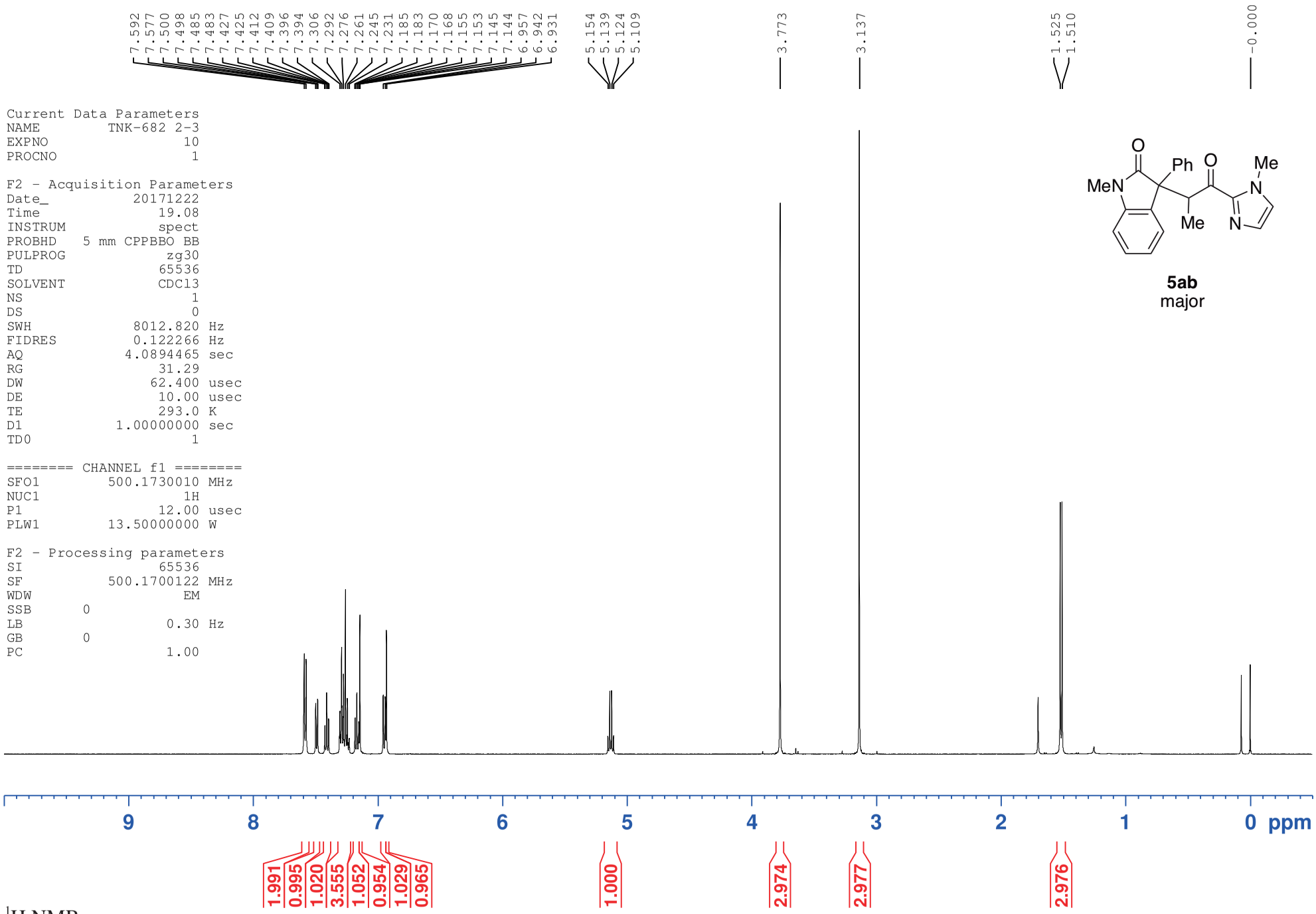
^{13}C NMR


Current Data Parameters
NAME TNK-672 TM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time 18.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.937
7.919
7.270
7.160
7.159
6.986
6.937
6.919
4.730
4.715
4.700
4.685
3.851
3.814
2.409
2.395
2.382
2.368
2.355
2.342
2.328
1.817
1.560
1.545
1.234
1.220
0.814
0.801
-0.000
O
O
iPr
O
Me
N
N
Me
N
MeO
3hb
9
8
7
6
5
4
3
2
1
0 ppm
1.998
0.998
1.021
2.013
1.000
2.983
3.007
1.026
3.034
3.050
2.987

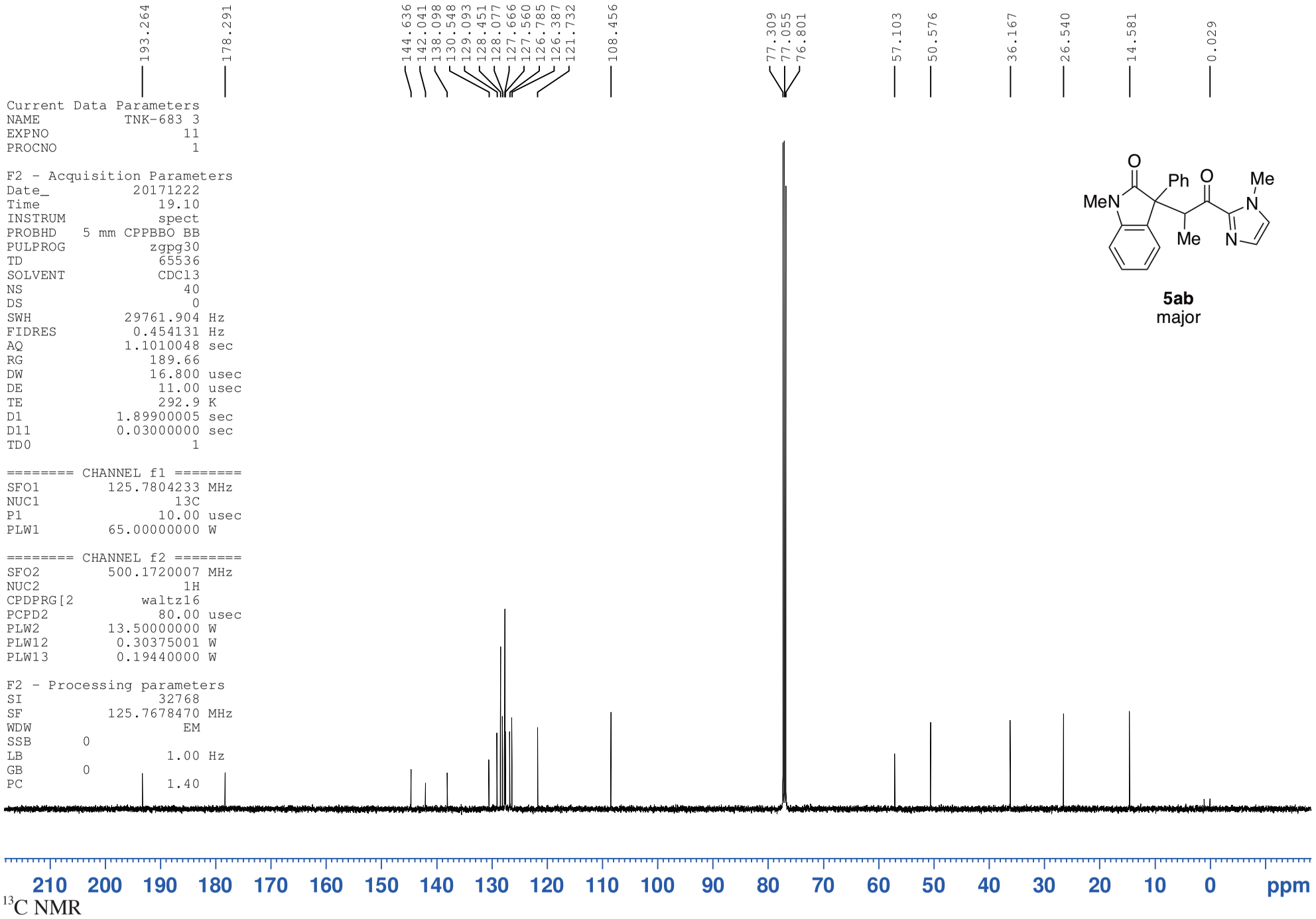
^{1}H NMR


Current Data Parameters
NAME TNK-67-2 TM
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time 18.43
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.8 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
192.007
180.779
162.886
160.814
141.474
129.932
129.491
127.487
118.510
113.938
77.305
77.257
77.051
76.797
74.808
55.477
47.389
36.272
32.382
16.755
16.617
12.067
0.022
O
O
O
iPr
Me
N
N
Me
MeO
3hb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

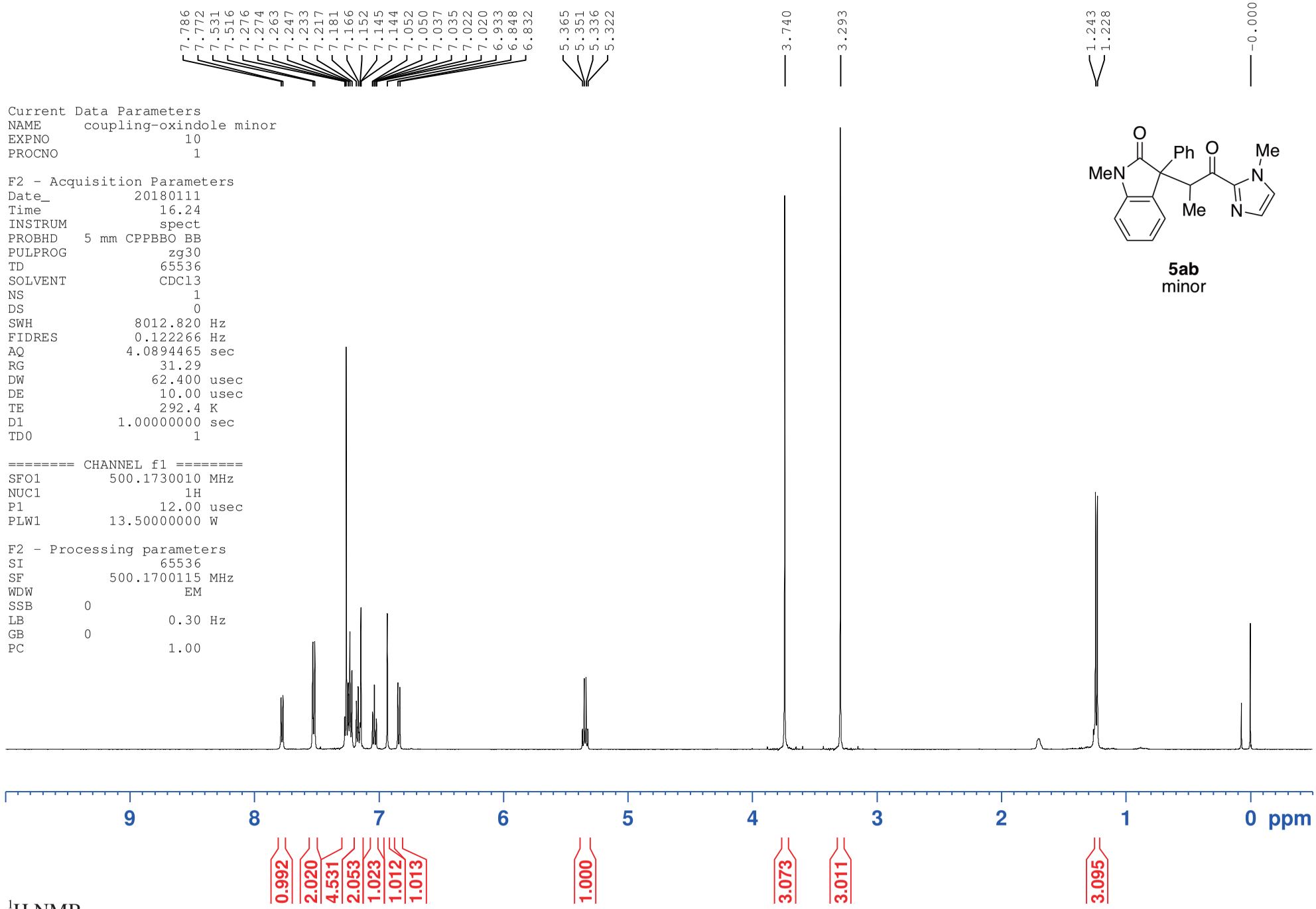
^{13}C NMR


7.592
7.577
7.500
7.498
7.485
7.483
7.427
7.425
7.412
7.409
7.396
7.394
7.306
7.292
7.276
7.261
7.245
7.231
7.185
7.183
7.170
7.168
7.155
7.153
7.145
7.144
6.957
6.942
6.931
5.154
5.139
5.124
5.109
3.773
3.137
1.525
1.510
0.000
Current Data Parameters
NAME TNK-682 2-3
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171222
Time 19.08
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
MeN
N
Me
N
5ab
major
9
8
7
6
5
4
3
2
1
0 ppm
1.991
0.995
1.020
3.555
1.052
0.954
1.029
0.965
1.000
2.974
2.977
2.976

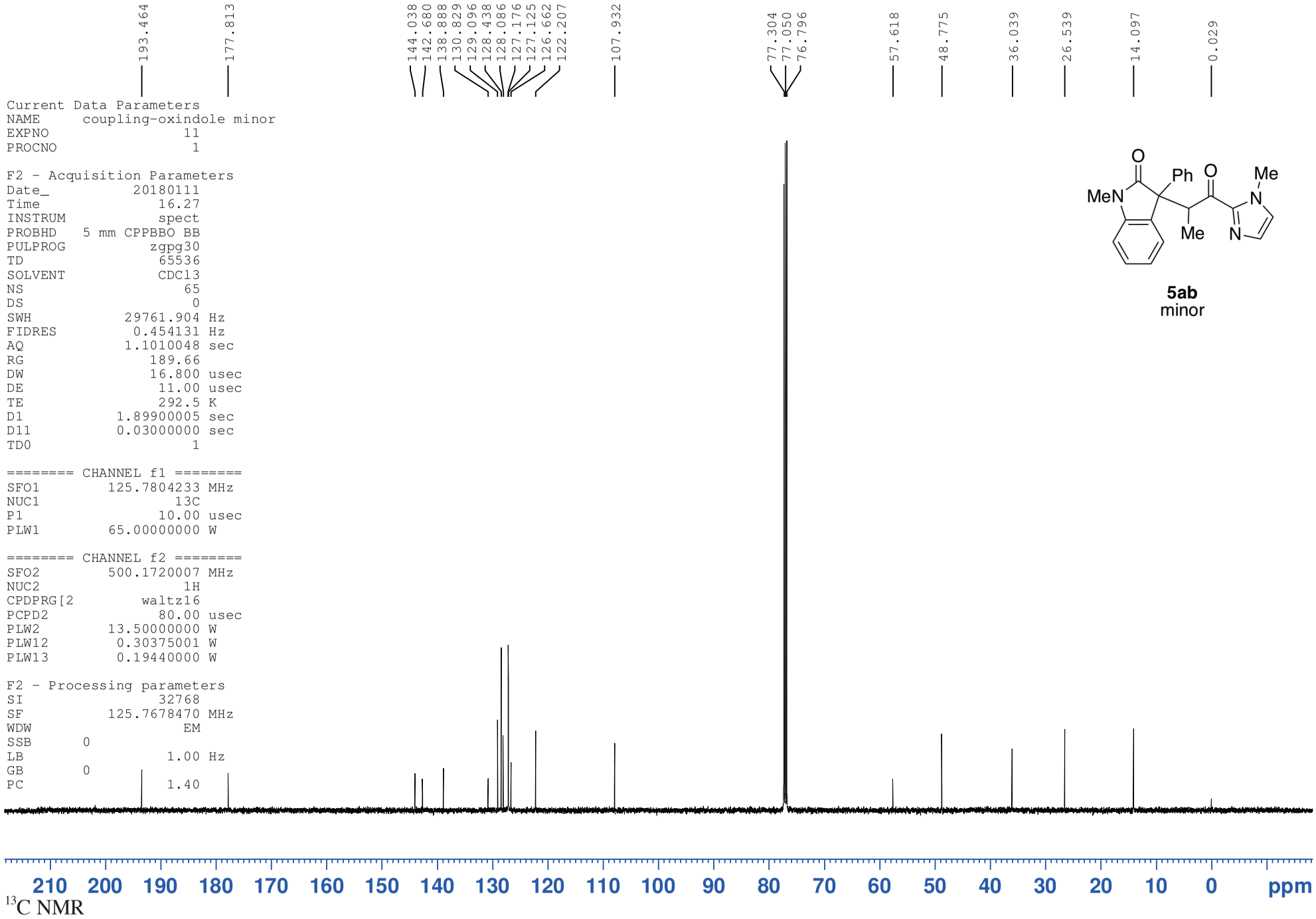
^{1}H NMR


193.264
178.291
144.636
142.041
138.098
130.548
129.093
128.451
128.077
127.666
127.560
126.785
126.387
121.732
108.456
77.309
77.055
76.801
57.103
50.576
36.167
26.540
14.581
0.029
Current Data Parameters
NAME TNK-683 3
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171222
Time 19.10
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.9 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
MeN
N
Me
N
5ab
major
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

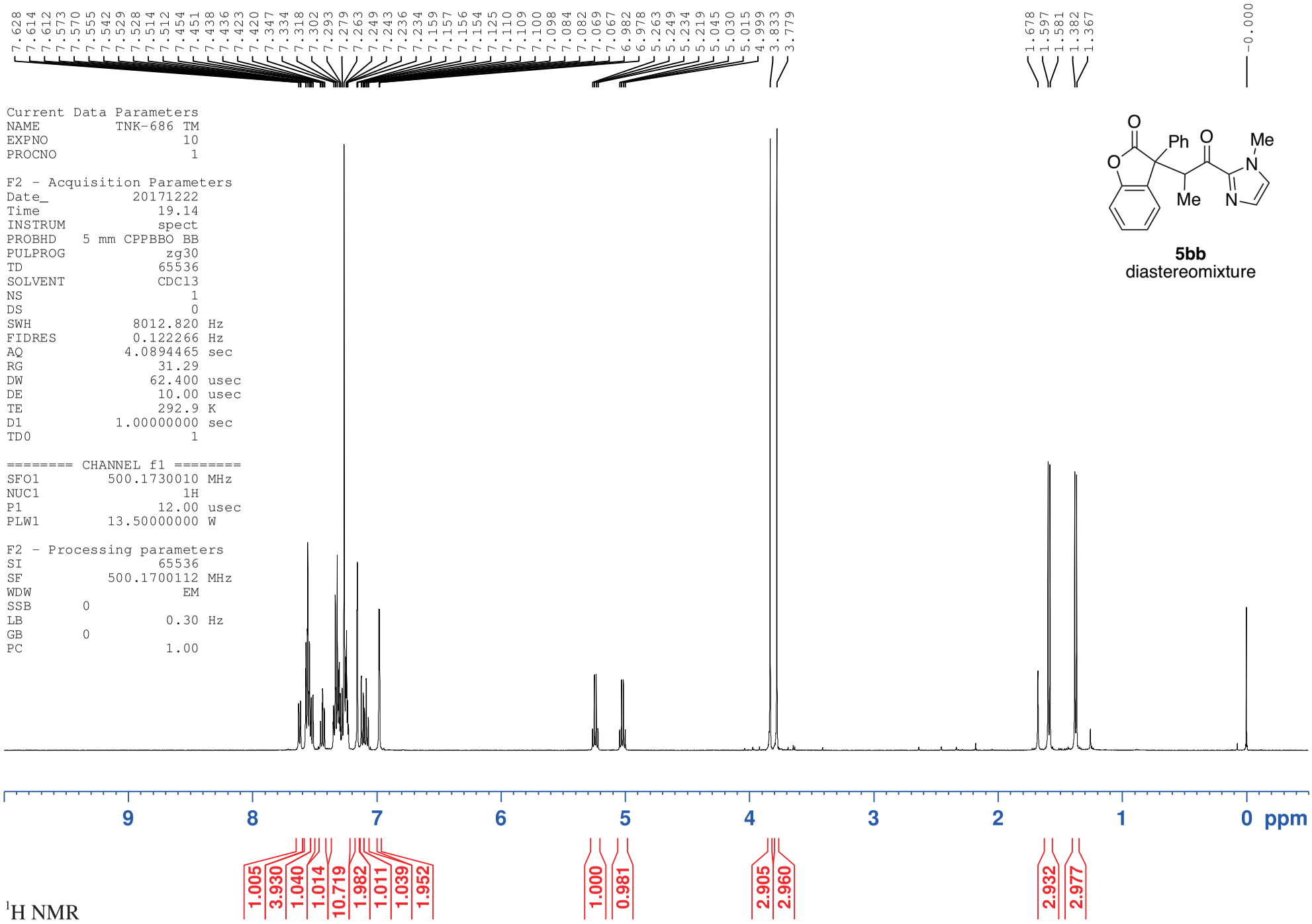
^{13}C NMR


7.786
7.772
7.531
7.516
7.276
7.274
7.263
7.247
7.233
7.217
7.181
7.166
7.152
7.145
7.144
7.052
7.050
7.037
7.035
7.022
7.020
6.933
6.848
6.832
5.365
5.351
5.336
5.322
3.740
3.293
1.243
1.228
0.000
Current Data Parameters
NAME coupling-oxindole minor
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180111
Time 16.24
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
MeN
N
Me
N
5ab
minor
9
8
7
6
5
4
3
2
1
0 ppm
0.992
2.020
4.531
2.053
1.023
1.012
1.013
1.000
3.073
3.011
3.095

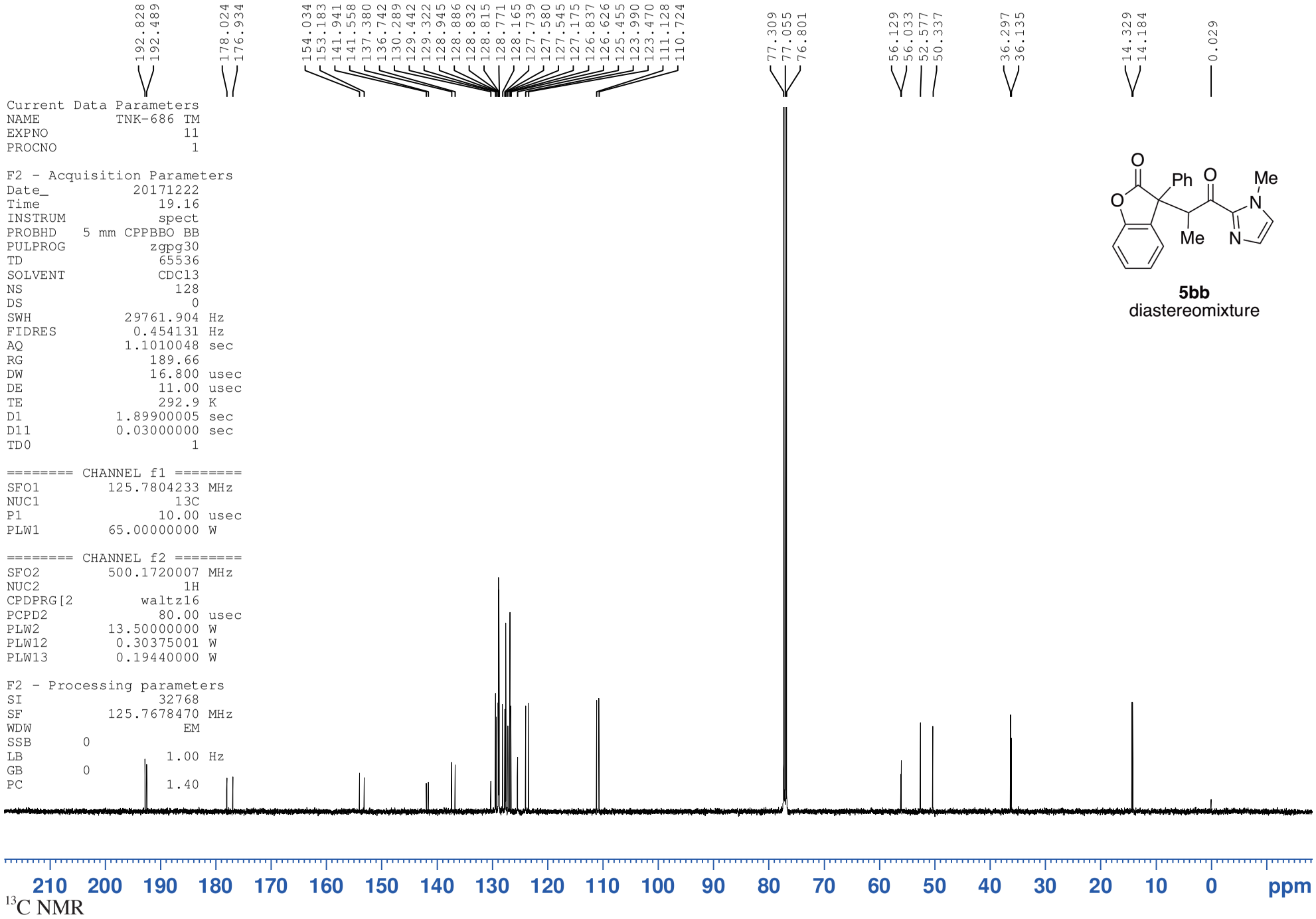
^{1}H NMR


193.464
177.813
144.038
142.680
138.888
130.829
129.096
128.438
128.086
127.176
127.125
126.662
122.207
107.932
77.304
77.050
76.796
57.618
48.775
36.039
26.539
14.097
0.029
Current Data Parameters
NAME coupling-oxindole minor
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180111
Time 16.27
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 65
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.5 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
MeN
N
Me
N
5ab
minor
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

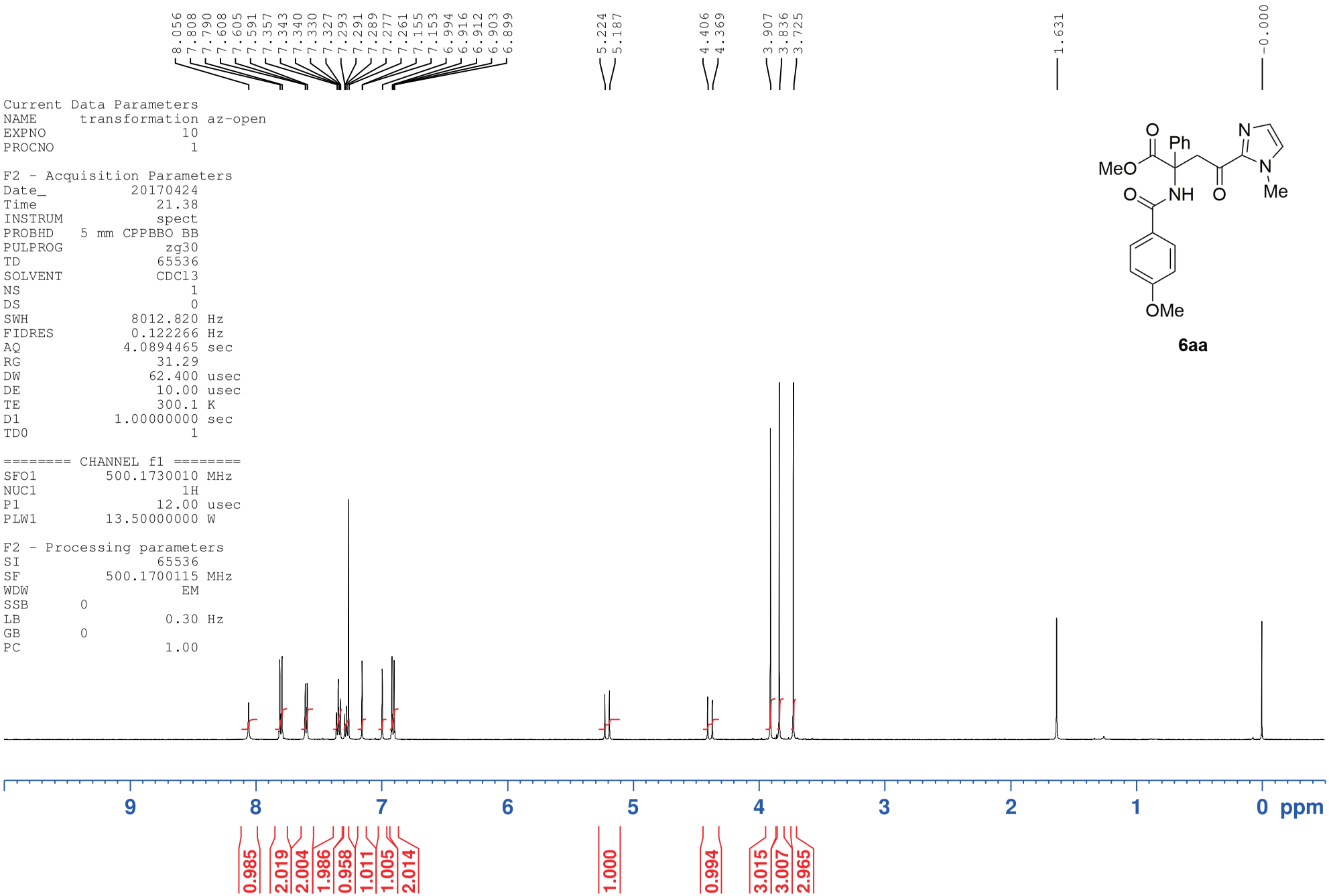
^{13}C NMR


7.628 7.614 7.612 7.573 7.570 7.555 7.542 7.529 7.528 7.514 7.512 7.454 7.451 7.438 7.436 7.423 7.420 7.347 7.334 7.318 7.302 7.293 7.279 7.263 7.249 7.243 7.236 7.234 7.159 7.157 7.156 7.154 7.125 7.110 7.109 7.100 7.098 7.084 7.082 7.069 7.067 6.982 6.978 5.263 5.249 5.234 5.219 5.045 5.030 5.015 4.999 3.833 3.779
1.678 1.597 1.581 1.382 1.367
-0.000
Current Data Parameters
NAME TNK-686 TM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171222
Time 19.14
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
O
Me
O
N
Me
N
5bb
diastereomixture
9 8 7 6 5 4 3 2 1 0 ppm
1.005 3.930 1.040 1.014 10.719 1.982 1.011 1.039 1.952
1.000 0.981
2.905 2.960
2.932 2.977

^{1}H NMR


192.828
192.489
178.024
176.934
154.034
153.183
141.941
141.558
137.380
136.742
130.289
129.442
129.322
128.945
128.886
128.832
128.815
128.771
128.165
127.739
127.580
127.545
127.175
126.837
126.626
125.455
123.990
123.470
111.128
110.724
77.309
77.055
76.801
56.129
56.033
52.577
50.337
36.297
36.135
14.329
14.184
0.029
Current Data Parameters
NAME TNK-686 TM
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171222
Time 19.16
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.9 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
O
Me
O
N
Me
N
5bb
diastereomixture
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

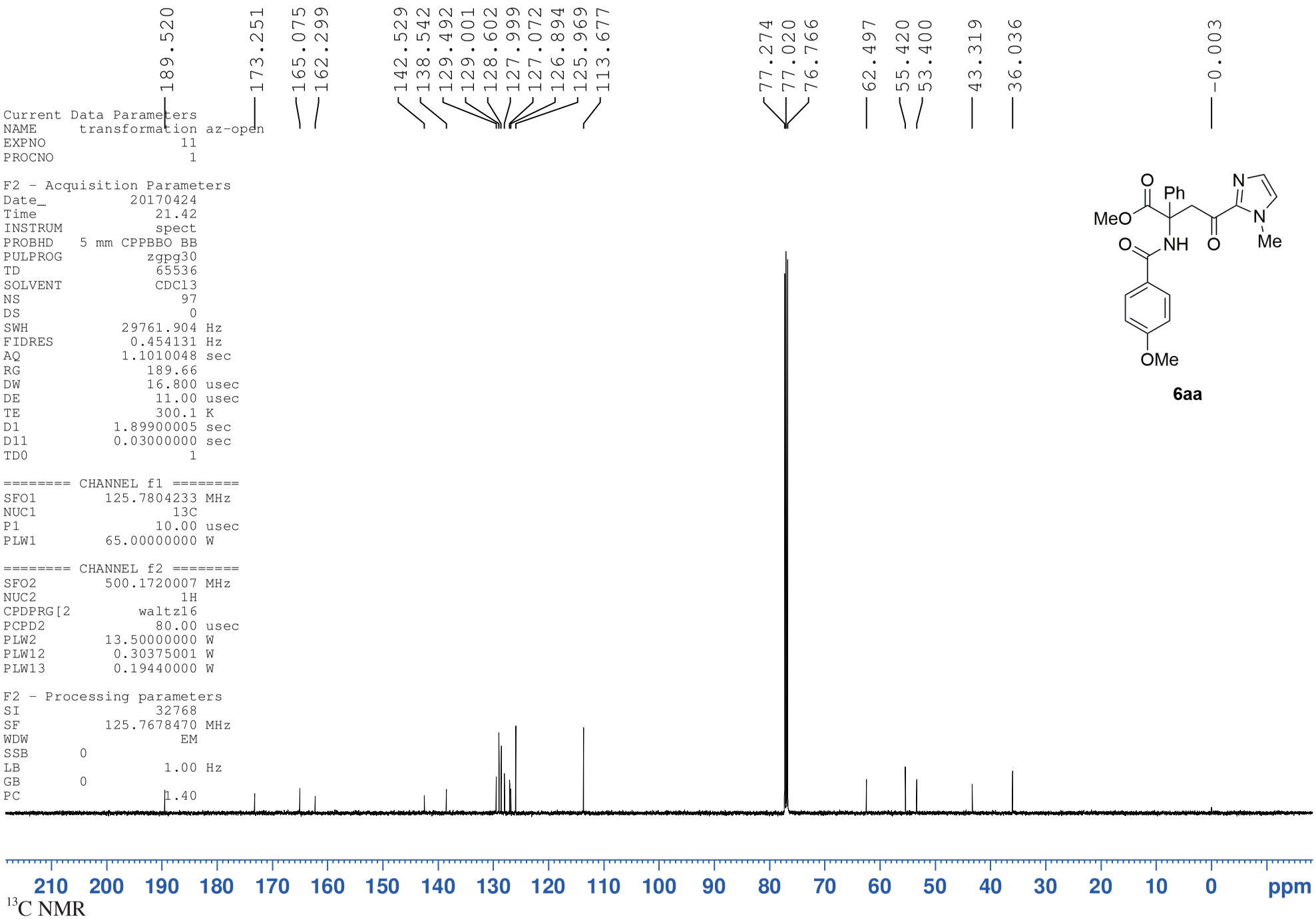
^{13}C NMR



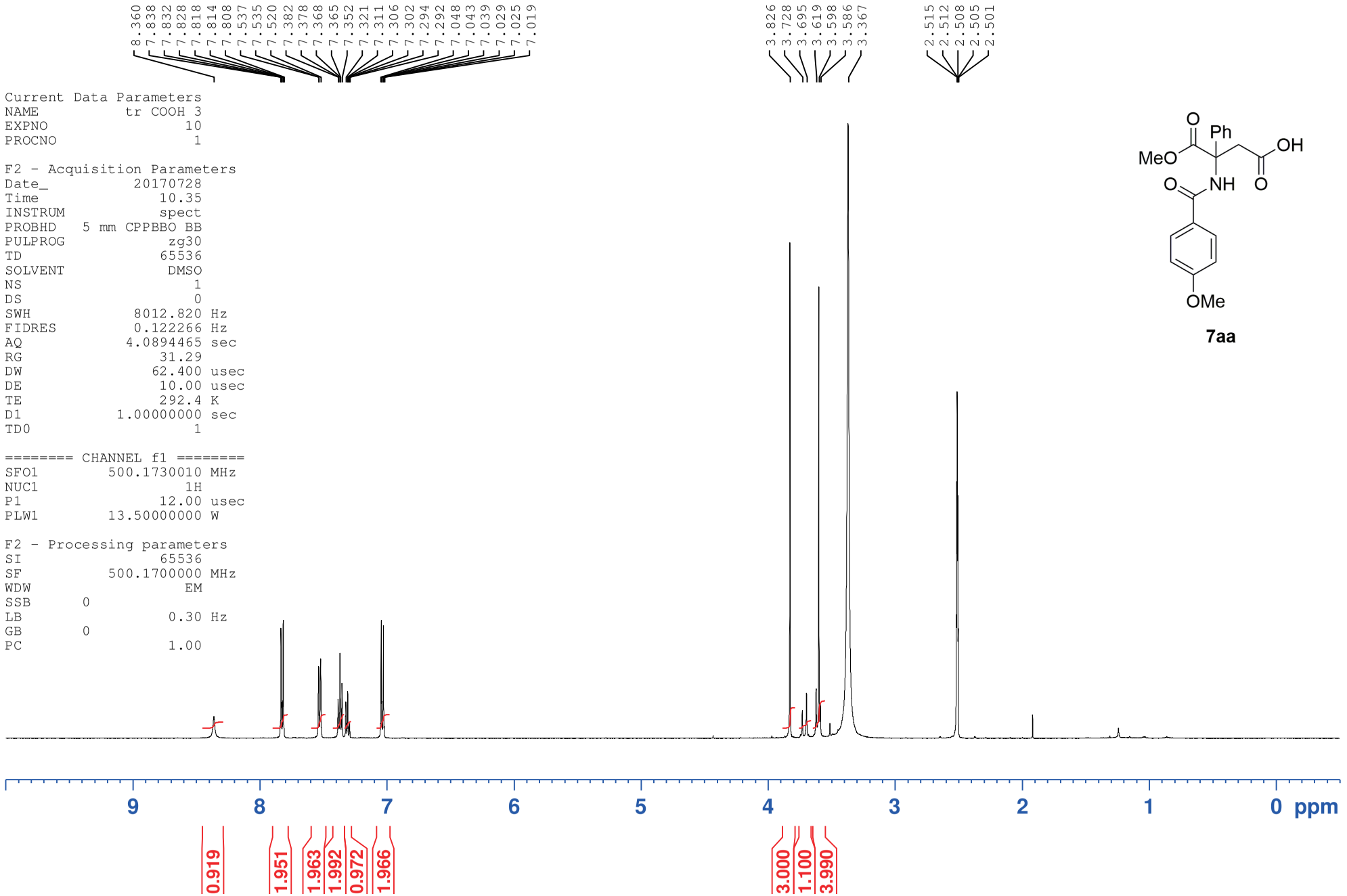
6aa

S157

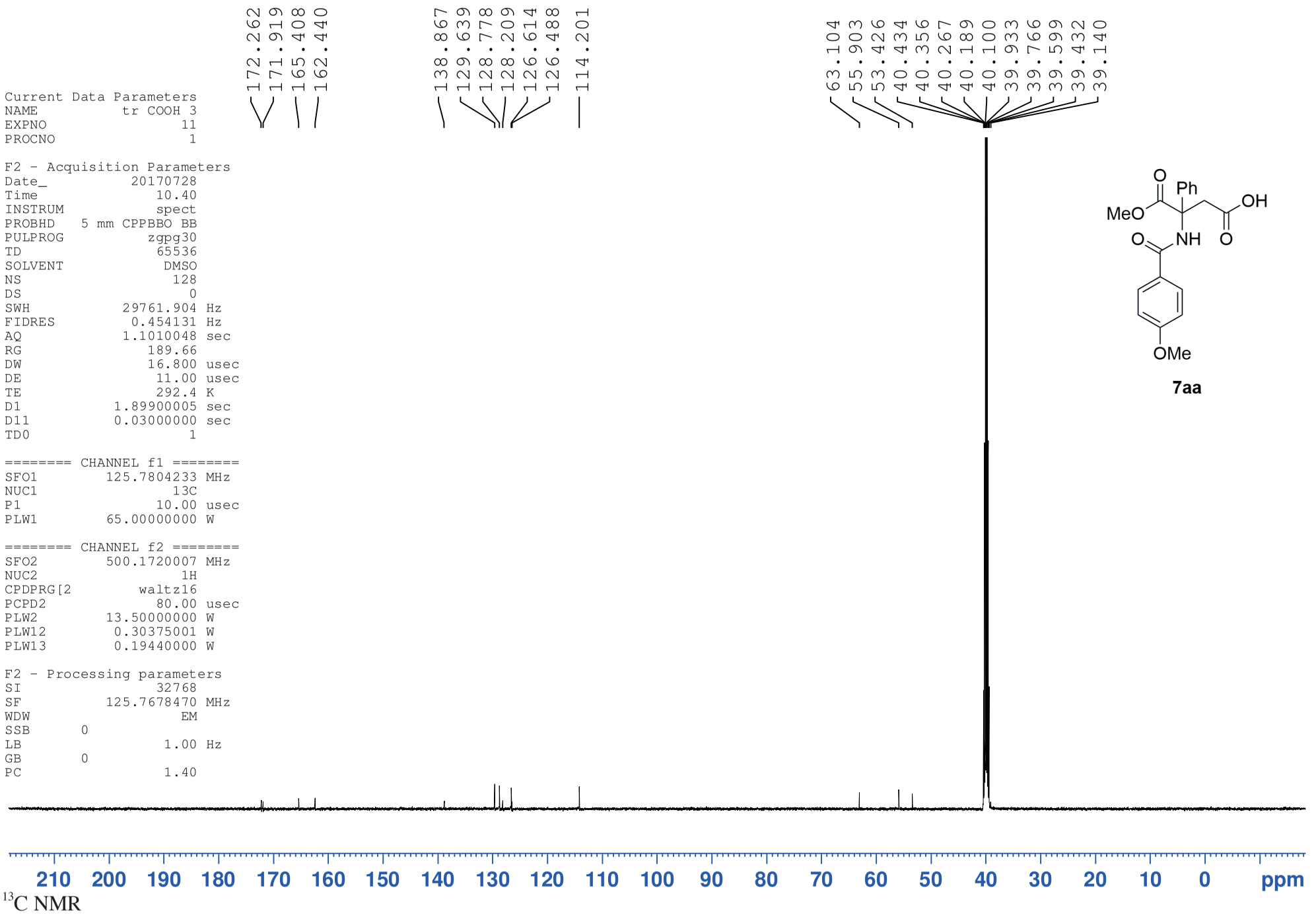
^{1}H NMR


189.520
173.251
165.075
162.299
142.529
138.542
129.492
129.001
128.602
127.999
127.072
126.894
125.969
113.677
77.274
77.020
76.766
62.497
55.420
53.400
43.319
36.036
-0.003
Current Data Parameters
NAME transformation az-open
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170424
Time 21.42
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 97
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
O
Ph
N
O
NH
O
N
Me
OMe
6aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

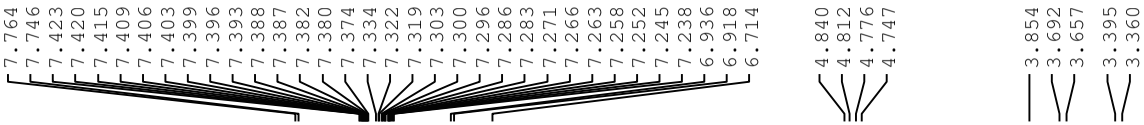
^{13}C NMR


8.360
7.838
7.832
7.828
7.818
7.814
7.808
7.537
7.535
7.520
7.382
7.378
7.368
7.365
7.352
7.321
7.311
7.306
7.302
7.294
7.292
7.048
7.043
7.039
7.029
7.025
7.019
3.826
3.728
3.695
3.619
3.598
3.586
3.367
2.515
2.512
2.508
2.505
2.501
Current Data Parameters
NAME tr COOH 3
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170728
Time 10.35
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
MeO
OH
NH
O
O
OMe
7aa
9
8
7
6
5
4
3
2
1
0 ppm
0.919
1.951
1.963
1.992
0.972
1.966
3.000
1.100
3.990

^{1}H NMR


172.262
171.919
165.408
162.440
138.867
129.639
128.778
128.209
126.614
126.488
114.201
63.104
55.903
53.426
40.434
40.356
40.267
40.189
40.100
39.933
39.766
39.599
39.432
39.140
Current Data Parameters
NAME tr COOH 3
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170728
Time 10.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 292.4 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
MeO
OH
O
NH
O
OMe
7aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR

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Current Data Parameters
NAME          tr amide 2
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170728
Time               10.46
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.29
DW                62.400 usec
DE                10.00 usec
TE                292.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1730010 MHz
NUC1                   1H
P1                 12.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 65536
SF           500.1700110 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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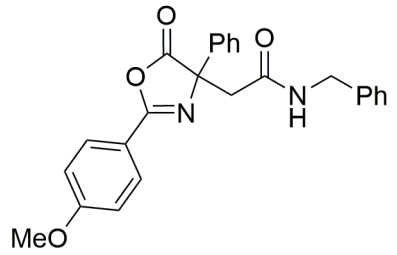
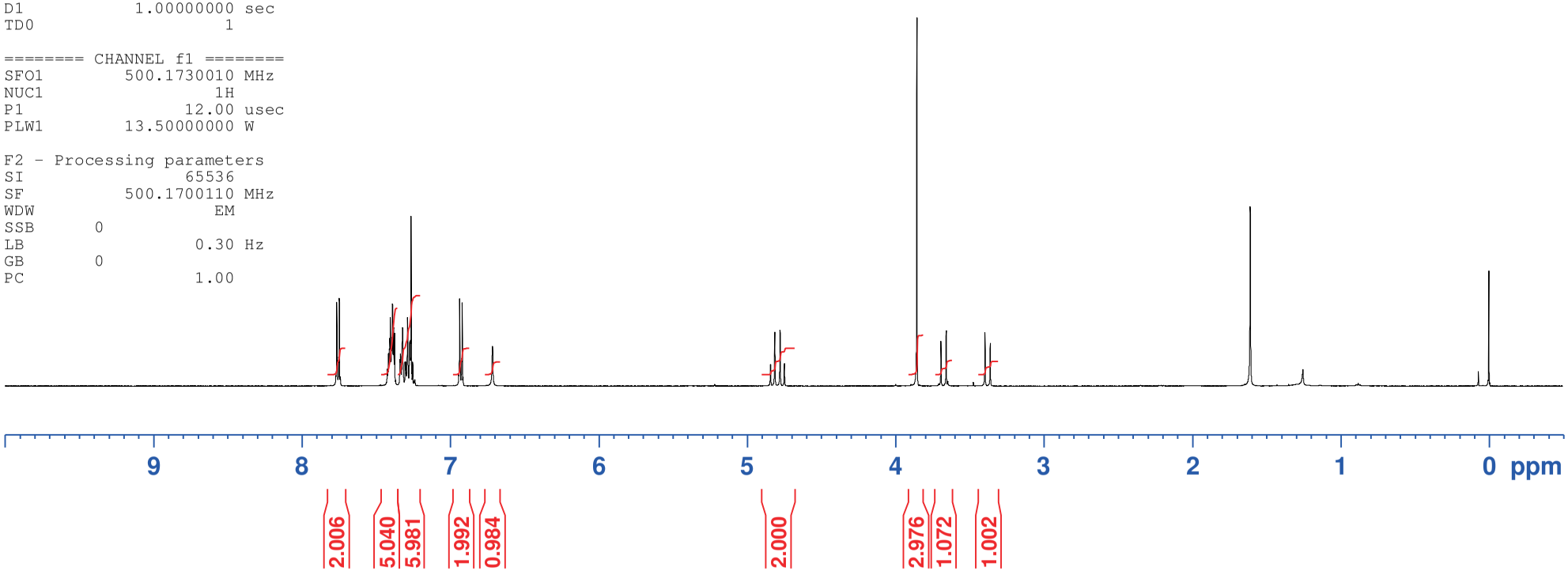
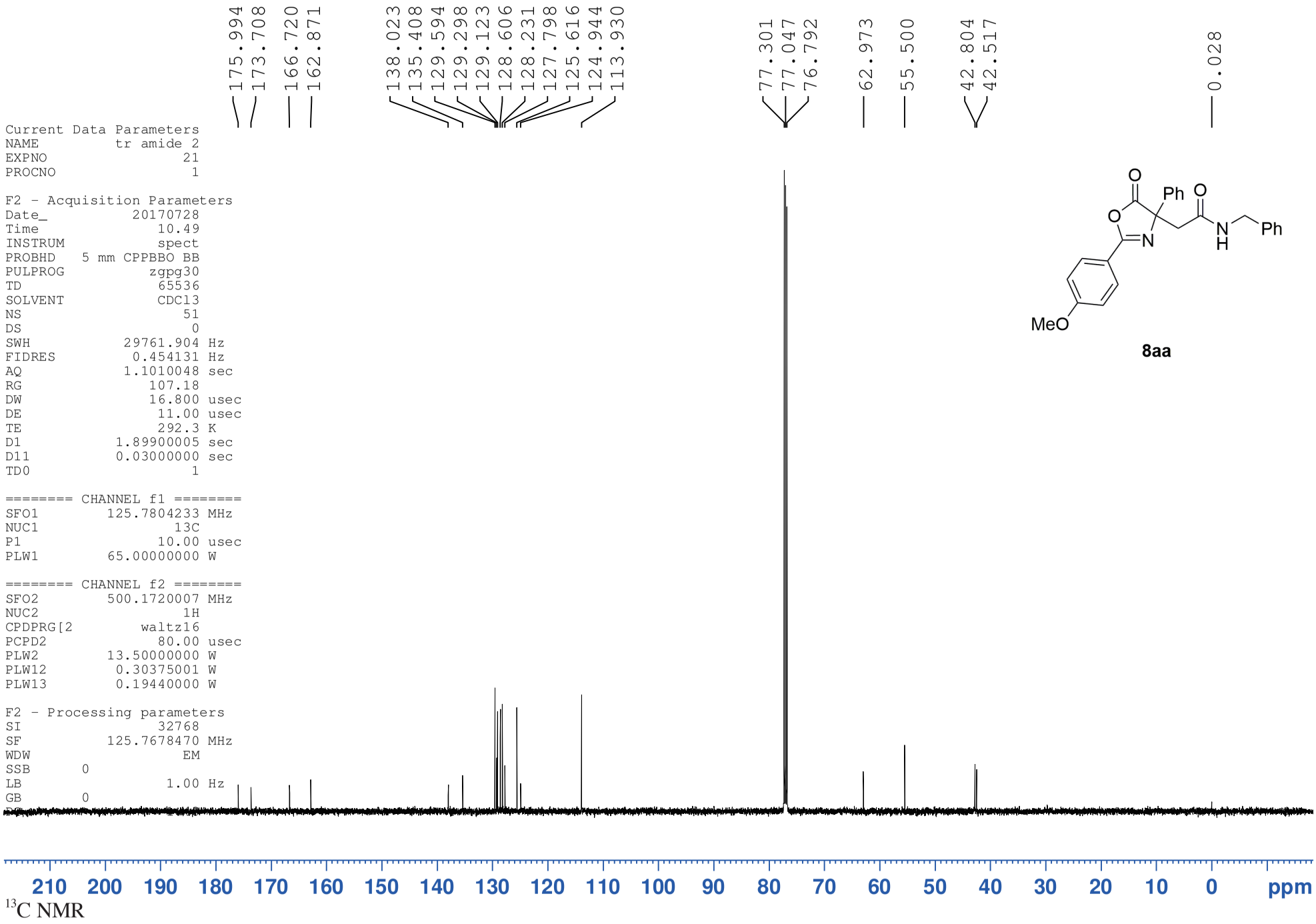


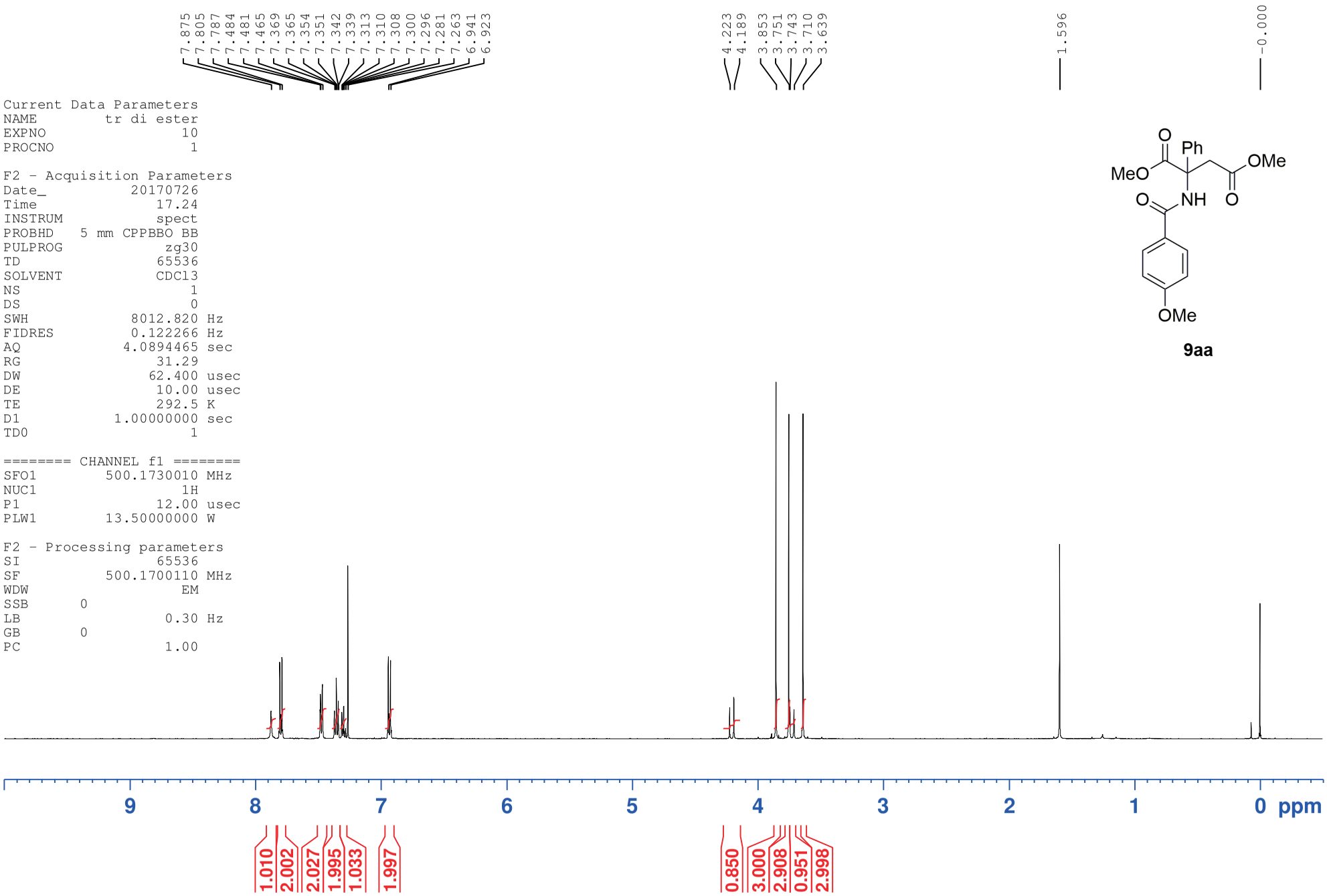
8aa



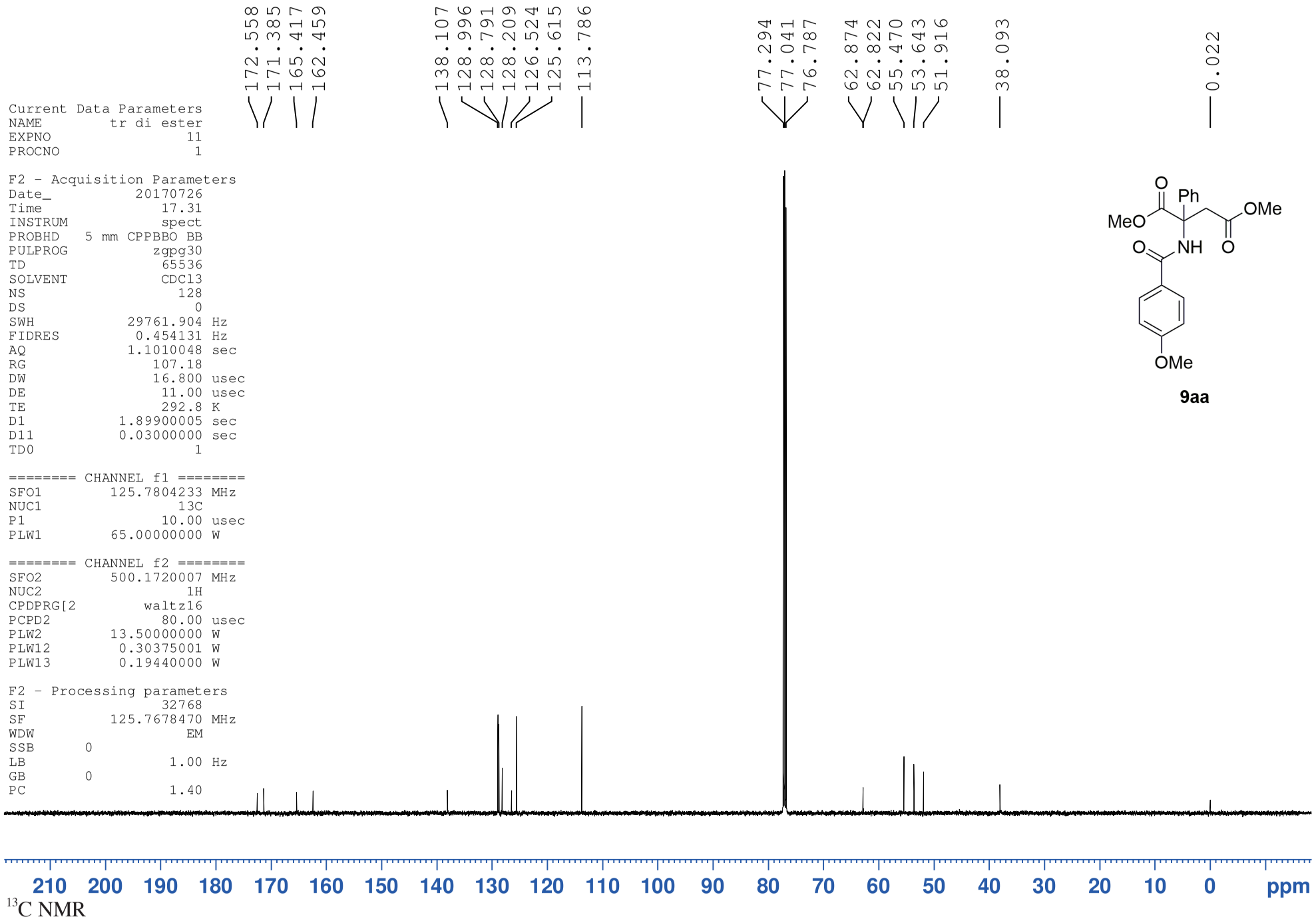
^{1}H NMR


175.994
173.708
166.720
162.871
138.023
135.408
129.594
129.298
129.123
128.606
128.231
127.798
125.616
124.944
113.930
77.301
77.047
76.792
62.973
55.500
42.804
42.517
0.028
Current Data Parameters
NAME tr amide 2
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170728
Time 10.49
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 51
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 292.3 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
O
Ph
O
O
N
N
H
Ph
MeO
8aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

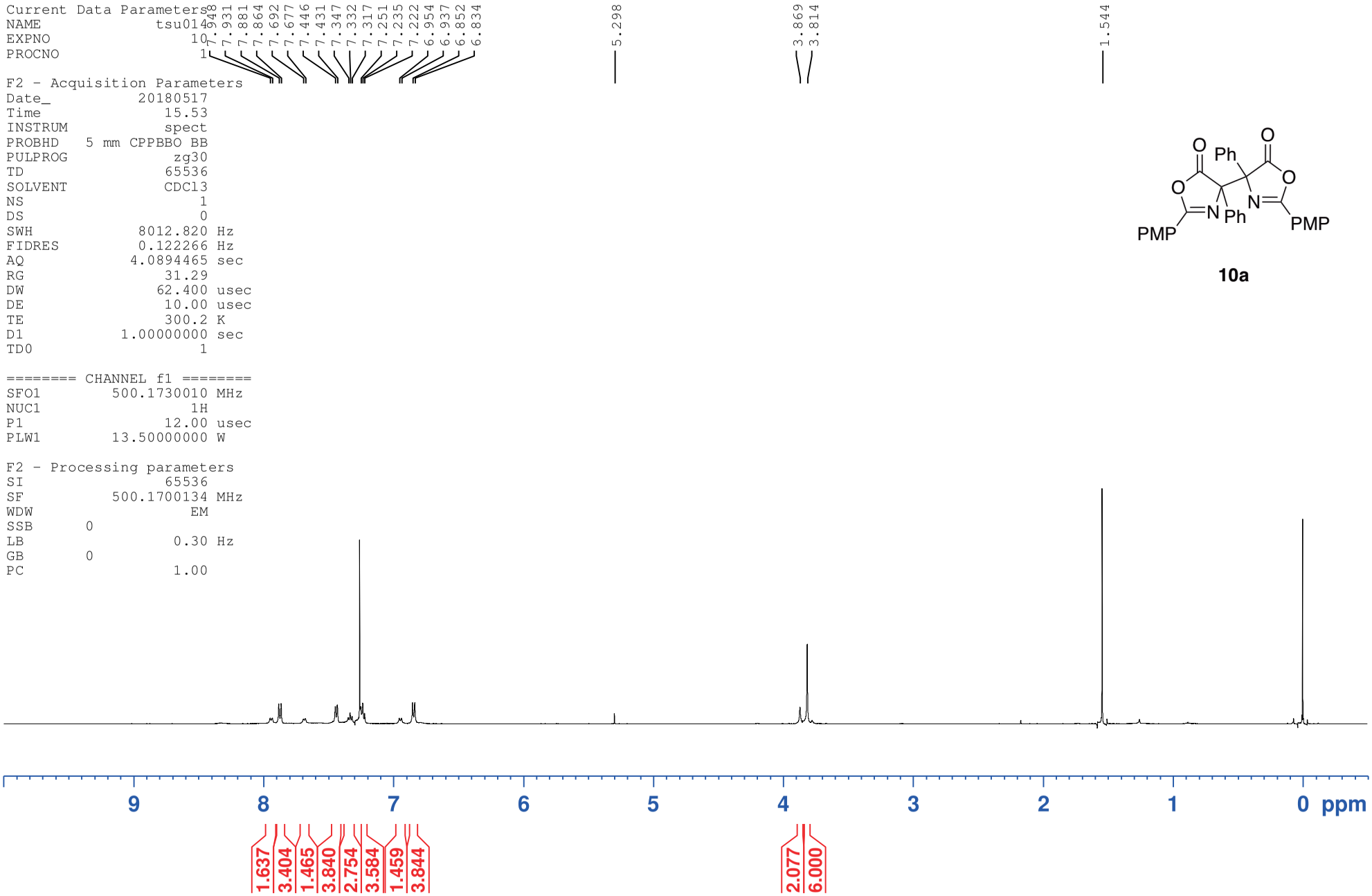
^{13}C NMR


7.875
7.805
7.787
7.484
7.481
7.465
7.369
7.365
7.354
7.351
7.342
7.339
7.313
7.310
7.308
7.300
7.296
7.281
7.263
6.941
6.923
4.223
4.189
3.853
3.751
3.743
3.710
3.639
1.596
-0.000
Current Data Parameters
NAME tr di ester
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170726
Time 17.24
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Ph
MeO
OMe
O
NH
O
OMe
9aa
9
8
7
6
5
4
3
2
1
0 ppm
1.010
2.002
2.027
1.995
1.033
1.997
0.850
3.000
2.908
0.951
2.998

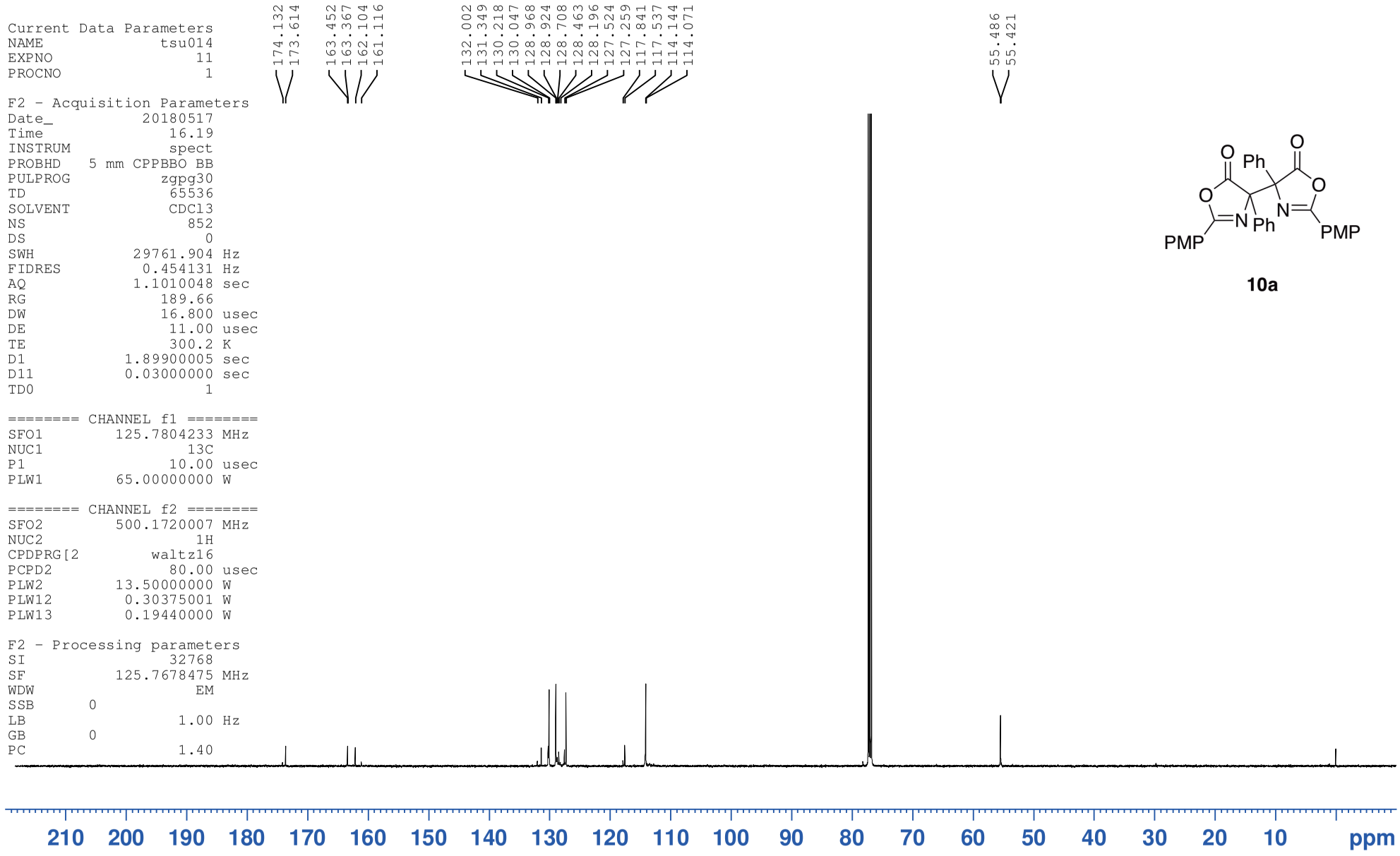
^{1}H NMR


172.558
171.385
165.417
162.459
138.107
128.996
128.791
128.209
126.524
125.615
113.786
77.294
77.041
76.787
62.874
62.822
55.470
53.643
51.916
38.093
0.022
Current Data Parameters
NAME tr di ester
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170726
Time 17.31
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 292.8 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
Ph
MeO
OMe
O
NH
O
OMe
9aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR


Current Data Parameters
NAME tsu014
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180517
Time 15.53
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.29
DW 62.400 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730010 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.948
7.931
7.881
7.864
7.692
7.677
7.446
7.431
7.347
7.332
7.317
7.251
7.235
7.222
6.954
6.937
6.852
6.834
5.298
3.869
3.814
1.544
O
Ph
O
O
N
Ph
N
O
PMP
PMP
10a
9
8
7
6
5
4
3
2
1
0 ppm
1.637
3.404
1.465
3.840
2.754
3.584
1.459
3.844
2.077
6.000

^{1}H NMR


Current Data Parameters
NAME tsu014
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180517
Time 16.19
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 852
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7678475 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
174.132
173.614
163.452
163.367
162.104
161.116
132.002
131.349
130.218
130.047
128.968
128.924
128.708
128.463
128.196
127.524
127.259
117.841
117.537
114.144
114.071
55.486
55.421
Ph
Ph
PMP
PMP
10a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{13}C NMR