Supporting Information

Mechanistic Insight into Catalytic Aerobic Chemoselective α-Oxidation of Acylpyrazoles

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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 oxygen 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 40–50 μm) 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

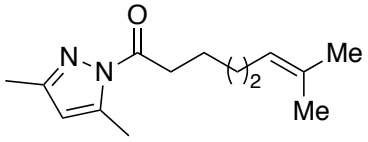
relative to NMR solvent ($CDCl_3$: 77.0 ppm) as an internal reference. NMR data are reported as follows: chemical shifts, multiplicity (s: singlet, d: doublet, dd: doublet of doublets, dt: doublet of triplets, t: triplet, q: quartet, quin: quintet, m: multiplet, br: broad signal), coupling constant (Hz), and integration. Infrared (IR) spectra were recorded on with Shimadzu FTIR-8400. High-resolution mass spectroscopy (HRMS) was obtained with Waters ACQUITY UPLCR–LCT-Premier™ XE system and Bruker MicrOTOF II.

3. Materials

DMF was dried over MS4A. 3,5-dimethylpyrazole and commercially available carboxylic acids were purchased from TCI and used as received. CuCl was purified[1] and stored in glove box. THF was purchased from Wako Pure Chemical Industries, Ltd. (Deoxidized, Stabilizer Free) and stored in glove box. Molecular Sieves 4A was purchased from Nacalai Tesque, Inc. Zinc dust was purchased from Aldrich. TEMPO was purchased from Carbosynth Limited. Acylpyrazoles were prepared according to the previous report.[2,3]

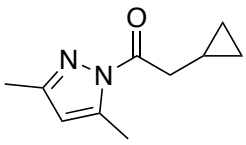
4. Substrate Syntheses and Characterization

General procedure for the synthesis acylpyrazole (EDC/HOBt method)[2,3]: The round bottom flask equipped with a magnetic stirring bar and 3-way glass stopcock was evacuated and filled with argon (three cycles). To the solution of carboxylic acid (1.0 equiv.) in dry DMF (1.0 M) was added EDC·HCl (1.2 equiv.), HOBt·H_2O (1.2 equiv.), 3,5-dimethylpyrazole (1.1 equiv.) and *N*-methylmorpholine (2.0 equiv.) at 0 °C. After stirring for 24 h at room temperature, it was quenched by 0.1 M HCl or 10% citric acid aq. The resultant mixture was extracted with EtOAc, and combined organic layer was washed with sat. $NaHCO_3$ solution and brine. The resulting organic layer was dried over Na_2SO_4 and filtered. After removal of solvent under reduced pressure, the crude mixture was purified by silica gel column chromatography to afford the desired acylpyrazole **1**.



1-(3,5-dimethyl-1H-pyrazol-1-yl)-7-methyloct-6-en-1-one (5) (colorless oil); ^{1}H-NMR (500 MHz, $CDCl_3$) (ppm) δ 5.94 (s, 1H, *pyrazole*), 5.12 (t, *J* = 7.0 Hz, 1H, CH_2CHC), 3.10 (t, *J* = 7.5 Hz, 2H, $COCH_2$), 2.53 (s, 3H, $ArCH_3$), 2.24 (s, 3H, $ArCH_3$), 2.03 (q, *J* = 7.5 Hz, 2H, CH_2CHC), 1.74 (quin, *J* = 7.5 Hz, 2H, CH_2), 1.68 (s, 3H, $CHCCH_3$), 1.61 (s, 3H, $CHCCH_3$), 1.44 (quin, *J* = 7.5 Hz, 2H, CH_2);

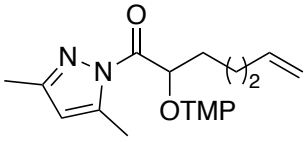
^{13}C-NMR (125 MHz, $CDCl_3$) δ 174.2, 151.7, 144.0, 131.6, 124.3, 110.9, 35.1, 29.3, 27.8, 25.7, 24.0, 17.7, 14.6, 13.8; IR (thin film, NaCl) 2928, 2858, 1728, 1581, 1442, 1411, 1381, 1346, 1327, 1249, 960, 802, 740 cm^{-1}; HRMS (ESI, H) m/z calc'd for $C_{14}H_{23}N_2O$ $(M + H)^+$ 235.1805, found 235.1809.



2-cyclopropyl-1-(3,5-dimethyl-1H-pyrazol-1-yl)ethan-1-one (8) (colorless oil); ^{1}H-NMR (500 MHz, $CDCl_3$) (ppm) δ 5.95 (s, 1H, *pyrazole*), 3.01 (d, *J* = 7.0 Hz, 2H, COC*H*$_2$), 2.56 (s, 3H, ArC*H*$_3$), 2.23 (s, 3H, ArC*H*$_3$), 1.23-1.13 (m, 1H, CH_2C*H*), 0.61-0.57 (m, 2H, *cyclopropyl*), 0.26-0.22 (m, 2H, *cyclopropyl*); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 173.8, 151.9, 144.1, 111.0, 40.4, 14.6, 13.8, 6.5, 4.3; IR (thin film, NaCl) 3005, 2928, 1732, 1581, 1377, 1346, 1303, 1242, 1022, 960, 806, 736 cm^{-1}; HRMS (ESI, H) m/z calc'd for $C_{10}H_{15}N_2O$ $(M + H)^+$ 179.1179, found 179.1180.

5. General Procedure and Characterization of Products

General procedure for catalytic α-oxidation of acylpyrazoles: CuCl (1.0 mg, 0.010 mmol) and dried MS 4A (50 mg) were added to a 4 ml vial under inert atmosphere. To the vial was added the addition of TEMPO **2** (0.031 g, 0.20 mmol) followed by acylpyrazole **1** (0.30 mmol) and dry THF (0.20 ml) via syringe with stainless-steel needle. After filling the vial with oxygen, the resulting orange suspension was stirred at 40 °C for 24 h and diluted with EtOAc. The diluted solution was filtered through silica gel short pad column and washed with EtOAc (ca. 30 ml). After evaporation of the solvent under reduced pressure, the crude mixture was purified by silica gel column chromatography to give the desired product **3**.

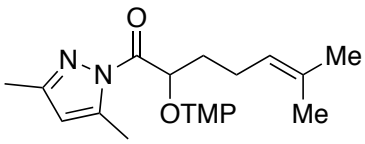


Reaction conditions

Acylpyrazole (0.30 mmol), TEMPO (0.20 mmol), THF (0.20 ml), CuCl (0.010 mmol), 40 °C, 48 h

1-(3,5-dimethyl-1H-pyrazol-1-yl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)hept-6-en-1-one (6) (orange oil, 6% Et_2O/*n*-hexane, 83% yield); ^{1}H-NMR (500 MHz, $CDCl_3$) (ppm) δ 5.95 (s, 1H,

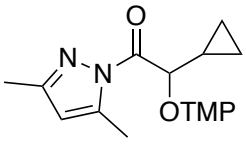
pyrazole), 5.78-5.70 (m, 2H, COC*H*, CH_2CHCH_2), 4.98-4.89 (m, 2H, CH_2CHCH_2), 2.54 (s, 3H, $ArCH_3$), 2.22 (s, 3H, $ArCH_3$), 2.08-1.99 (m, 3H, $COCHCH_2$, CH_2CHCH_2), 1.92-1.85 (m, 1H, $COCHCH_2$), 1.57-0.83 (m, 20H, CH_2, OTMP, overlapped with H_2O); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 174.4, 151.7, 143.9, 138.5, 114.6, 111.2, 82.7, 59.8, 59.5, 40.3 (overlapped), 33.9, 33.8, 33.1, 32.0, 23.1, 20.3, 20.1, 17.1, 14.5, 13.9; IR (thin film, NaCl) 2970, 2931, 2870, 1732, 1585, 1458, 1442, 1381, 1361, 1307, 1242, 1134, 987, 956, 910, 802 cm^{-1}; HRMS (ESI, H) m/z calc'd for $C_{21}H_{36}N_3O_2$ $(M + H)^+$ 362.2802, found 362.2801.



Reaction conditions

Acylpyrazole (0.30 mmol), TEMPO (0.20 mmol), THF (0.20 ml), CuCl (0.010 mmol), 40 °C, 48 h

1-(3,5-dimethyl-1H-pyrazol-1-yl)-7-methyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)oct-6-en-1-one (7) (colorless oil, 9% Et_2O/*n*-hexane, 60% yield); ^{1}H-NMR (500 MHz, $CDCl_3$) (ppm) δ 5.94 (s, 1H, *pyrazole*), 5.70 (dd, *J* = 8.5, 3.0 Hz, 1H, COC*H*), 5.05 (t, *J* = 7.0 Hz, 1H, CH_2CHC), 2.54 (s, 3H, $ArCH_3$), 2.22 (s, 3H, $ArCH_3$), 2.09-2.02 (m, 1H, CH_2), 1.95-1.93 (m, 2H, CH_2), 1.89-1.79 (m, 1H, CH_2), 1.64 (s, 3H, $CHCCH_3$), 1.56-0.92 (m, 23H, OTMP, $CHCCH_3$, CH_2, overlapped with H_2O); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 174.5, 151.7, 143.9, 131.6, 124.4, 111.1, 82.8, 59.8, 59.5, 40.3 (overlapped), 33.9, 33.1, 32.0, 28.0, 25.7, 23.9, 20.2, 20.1, 17.8, 17.2, 14.5, 13.9; IR (thin film, NaCl) 2966, 2928, 2870, 1735, 1585, 1454, 1381, 1350, 1307, 1242, 1134, 956, 802 cm^{-1}; HRMS (ESI, H) m/z calc'd for $C_{23}H_{40}N_3O_2$ $(M + H)^+$ 390.3115, found 390.3105.



Reaction conditions

Acylpyrazole (0.30 mmol), TEMPO (0.20 mmol), THF (0.20 ml), CuCl (0.010 mmol), 40 °C, 48 h

2-cyclopropyl-1-(3,5-dimethyl-1H-pyrazol-1-yl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethan-1-one (9) (white solid, 2% to 6% Et_2O/*n*-hexane, 68% yield); ^{1}H-NMR (500 MHz, $CDCl_3$) (ppm) δ 5.94 (s, 1H, *pyrazole*), 5.56 (d, *J* = 8.5 Hz, 1H, COC*H*), 2.55 (s, 3H, $ArCH_3$), 2.21 (s, 3H, $ArCH_3$), 1.58-1.13 (m, 16H, OTMP/COCHC*H*, overlapped with H_2O), 0.91 (s, 3H, OTMP), 0.71-0.66 (m, 1H,

cyclopropyl), 0.57-0.52 (m, 1H, *cyclopropyl*), 0.46-0.34 (m, 2H, *cyclopropyl*); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 172.3, 150.5, 142.9, 110.1, 84.2, 59.1, 58.5, 39.2 (overlapped), 33.0, 32.2, 19.2, 19.0, 16.1, 13.4, 13.3, 12.7, 5.7; IR (KBr) 3001, 2970, 2931, 2870, 2360, 1724, 1585, 1381, 1346, 1292, 1234, 1134, 1041, 960, 840, 752 cm^{-1}; HRMS (ESI, H) m/z calc'd for $C_{19}H_{32}N_3O_2$ $(M + H)^+$ 334.2489, found 334.2486.

6. Procedure for Mechanistic Studies

CuCl was premixed under O_2 atmosphere: CuCl (9.9 mg, 0.10 mmol) was added to a 4 ml vial under inert atmosphere. To the vial was added dry THF (0.20 ml) via syringe with stainless-steel needle. After filling the vial with oxygen, the mixture was stirred at 40 °C for 24 h. After evaporation of the solvent under reduced pressure and sufficient vacuum drying, **1a** (0.068 g, 0.30 mmol), **2** (0.031 g, 0.20 mmol), and dry THF (0.20 ml) were added to the vial in glove box. The mixture was stirred at 40 °C for 24 h under inert atmosphere and diluted with EtOAc. The diluted solution was filtered through silica gel short pad column and washed with EtOAc (ca. 30 ml). After evaporation of the solvent under reduced pressure, yield was determined by ^{1}H-NMR analysis using 2-methoxynaphthalene as an internal standard.

CuCl and 1a were premixed under O_2 atmosphere: CuCl (9.9 mg, 0.10 mmol) and **1a** (0.068 g, 0.30 mmol) were added to a 4 ml vial under inert atmosphere. To the vial was added dry THF (0.20 ml) via syringe with stainless-steel needle. After filling the vial with oxygen, the mixture was stirred at 40 °C for 24 h. After evaporation of the solvent under reduced pressure and sufficient vacuum drying, **2** (0.031 g, 0.20 mmol) and dry THF (0.20 ml) were added to the vial in glove box. The mixture was stirred at 40 °C for 24 h under inert atmosphere and diluted with EtOAc. The diluted solution was filtered through silica gel short pad column and washed with EtOAc (ca. 30 ml). After evaporation of the solvent under reduced pressure, yield was determined by ^{1}H-NMR analysis using 2-methoxynaphthalene as an internal standard.

CuCl and 2 were premixed under O_2 atmosphere: CuCl (9.9 mg, 0.10 mmol) and **2** (0.031 g, 0.20 mmol) were added to a 4 ml vial under inert atmosphere. To the vial was added dry THF (0.20 ml) via syringe with stainless-steel needle. After filling the vial with oxygen, the mixture was stirred at 40 °C for 24 h. After evaporation of the solvent under reduced pressure and sufficient vacuum drying, **1a** (0.068 g, 0.30 mmol), **2** (0.031 g, 0.20 mmol), and dry THF (0.20 ml) were added to the vial in glove box. The mixture was stirred at 40 °C for 24 h under inert atmosphere and diluted with EtOAc. The diluted solution was filtered through silica gel short pad column and washed with EtOAc (ca. 30 ml). After evaporation of the solvent under

reduced pressure, yield was determined by ^{1}H-NMR analysis using 2-methoxynaphthalene as an internal standard.

7. Kinetic Isotope Effect Experiments

CuCl (1.0 mg, 0.010 mmol) and dried MS 4A (50 mg) were added to a 4 ml vial under inert atmosphere. To the vial was added the addition of TEMPO **2** (0.031 g, 0.20 mmol) followed by acylpyrazole **1a** (0.30 mmol) or **1a(*d*^{2})**, 2-methoxynaphthalene and dry THF (0.20 ml) via syringe with stainless-steel needle. After filling the vial with oxygen, the resulting orange suspension was stirred at 40 °C. At the specified period, an aliquot of reaction mixture was extracted via a syringe filled by EtOAc with a stainless-steel needle from the test tube and diluted with EtOAc. The diluted solution was filtered through silica gel short pad column and washed with EtOAc. After evaporation of the solvent under reduced pressure, the crude mixture was analyzed by ^{1}H NMR to determine the chemical yield. The results were summarized in the Figure S1.

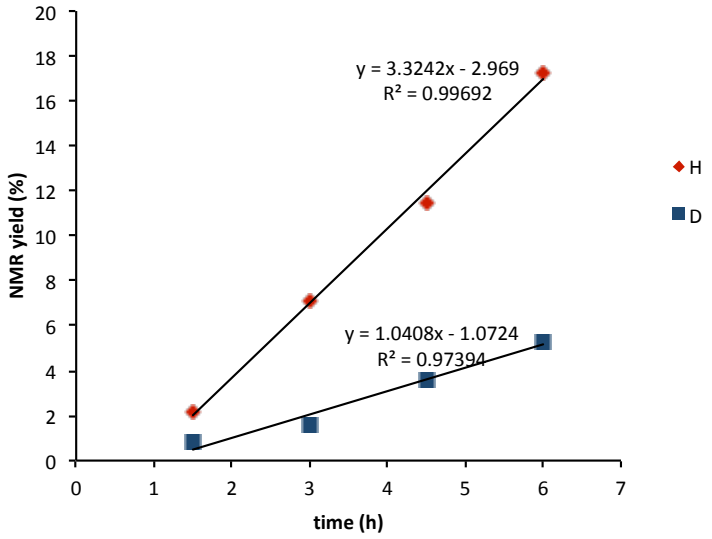
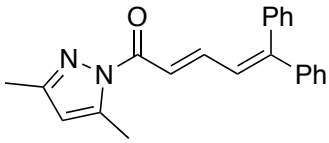
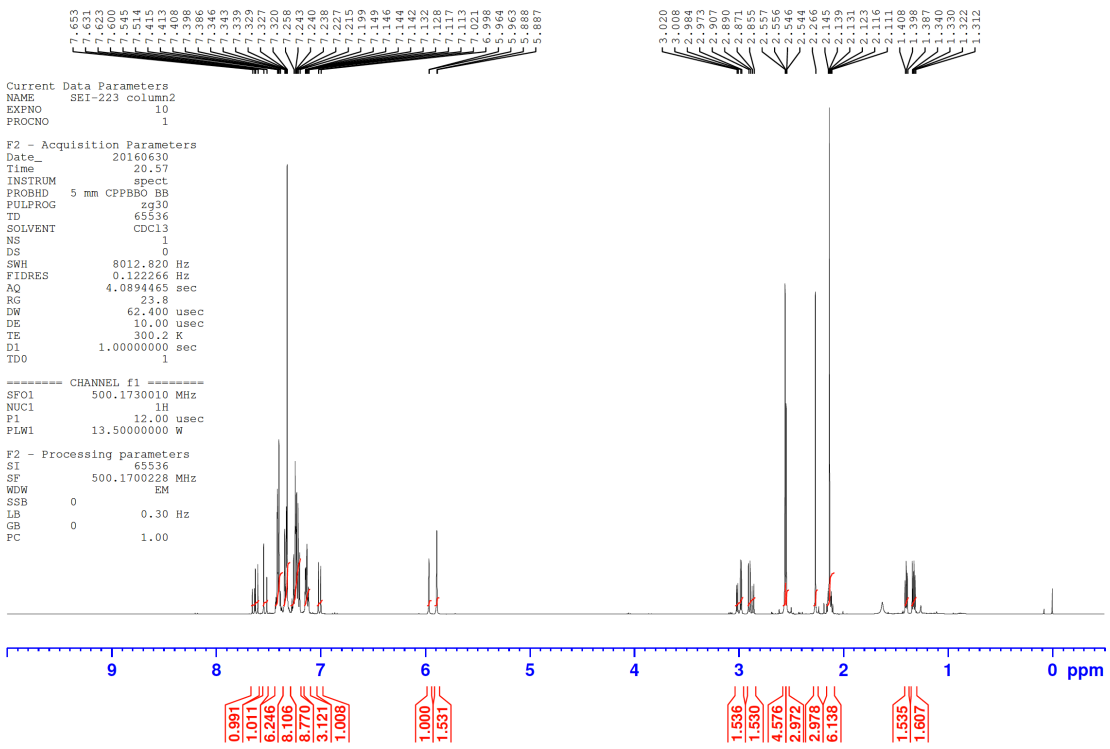


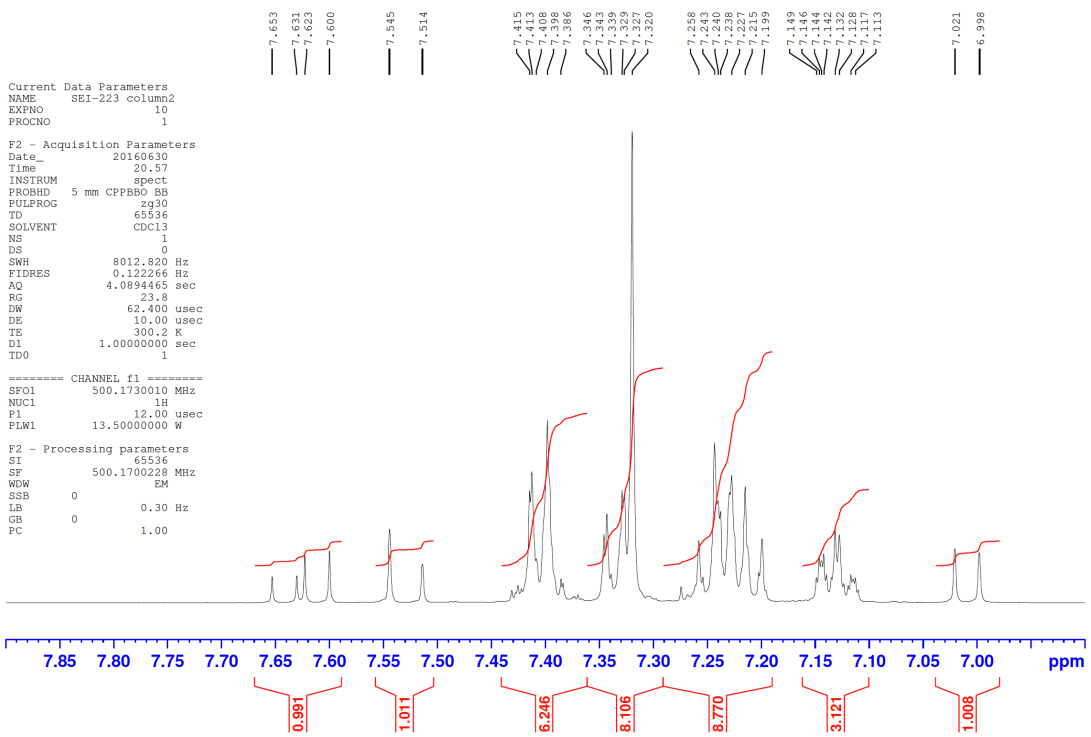
Figure S1. Kinetic Isotope Effect Experiments using **1a**/**1a(*d*^{2})**

8. Radical Clock Experiments



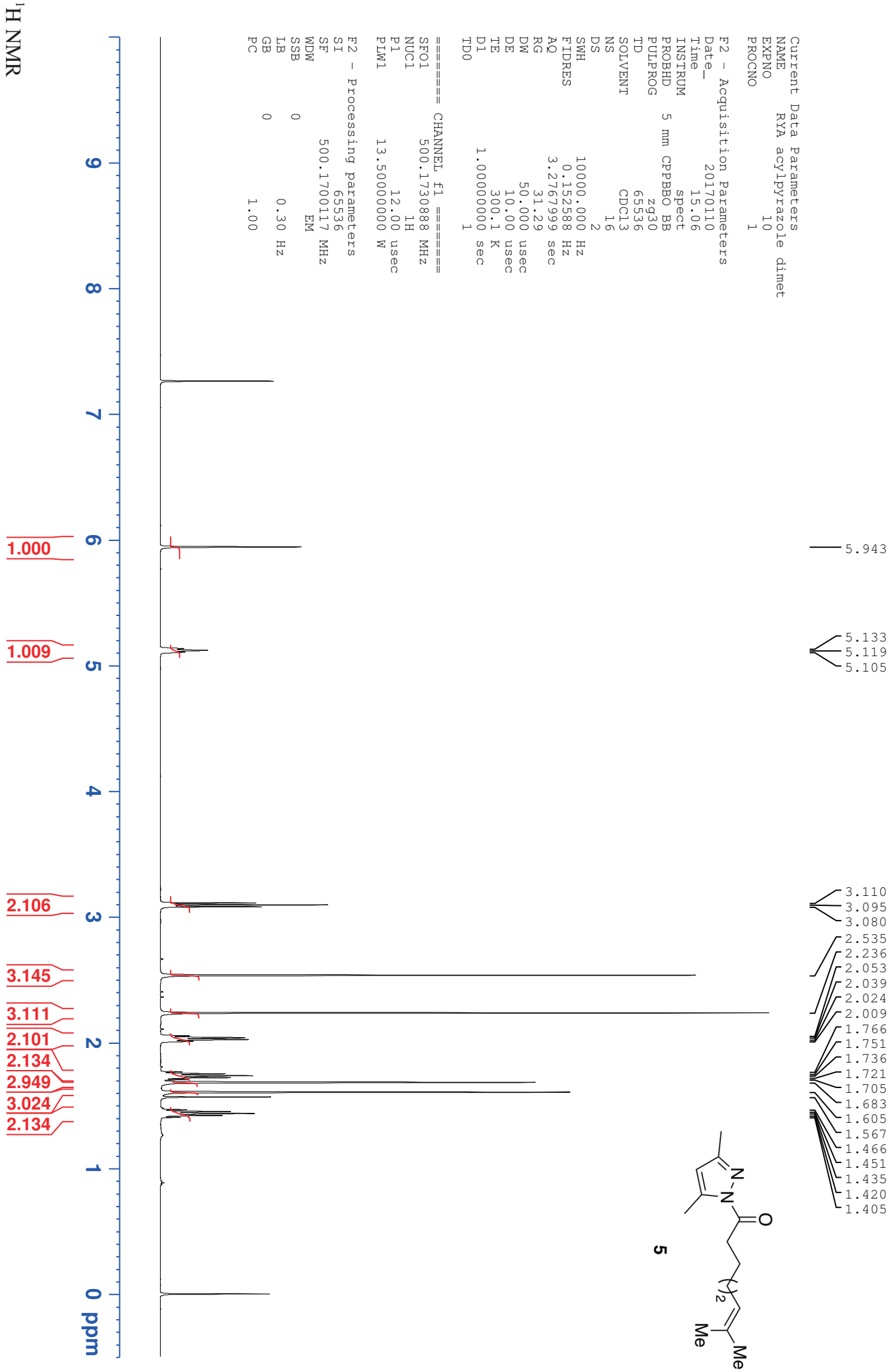
(*E*)-1-(3,5-dimethyl-1H-pyrazol-1-yl)-5,5-diphenylpenta-2,4-dien-1-one (12); Pure compound **12** could not be isolated. Compound **12** was confirmed using ^{1}H-NMR and HRMS. ^{1}H-NMR (500 MHz, $CDCl_3$) (ppm) δ 7.63 (dd, *J* = 15.5, 11.5 Hz, 1H, C*H*), 7.53 (d, *J* = 15.5 Hz, 1H, C*H*), 7.01 (d, *J* = 11.5 Hz, 1H, C*H*), 5.96 (s, 1H, *pyrazole*), 2.55 (s, 3H, ArCH_3), 2.27 (s, 3H, ArCH_3);
HRMS (ESI, H) m/z calc'd for $C_{22}H_{21}N_2O$ $(M + H)^+$ 329.1648, found 329.1648.





9. References

1. Armarego, W. L. F.; Chai, C. L. L. (2009) P*URIFICATION OF LABORATORY CHEMICALS (SIXTH EDITION)*: BUTTERWORTH HEINEMANN.
2. Tokumasu, K.; Yazaki, R.; Ohshima, T. *J. Am. Chem. Soc.* **2016**, *138*, 2664.
3. Taninokuchi, S.; Yazaki, R.; Ohshima, T. *Org. Lett.* **2017**, *19*, 3187.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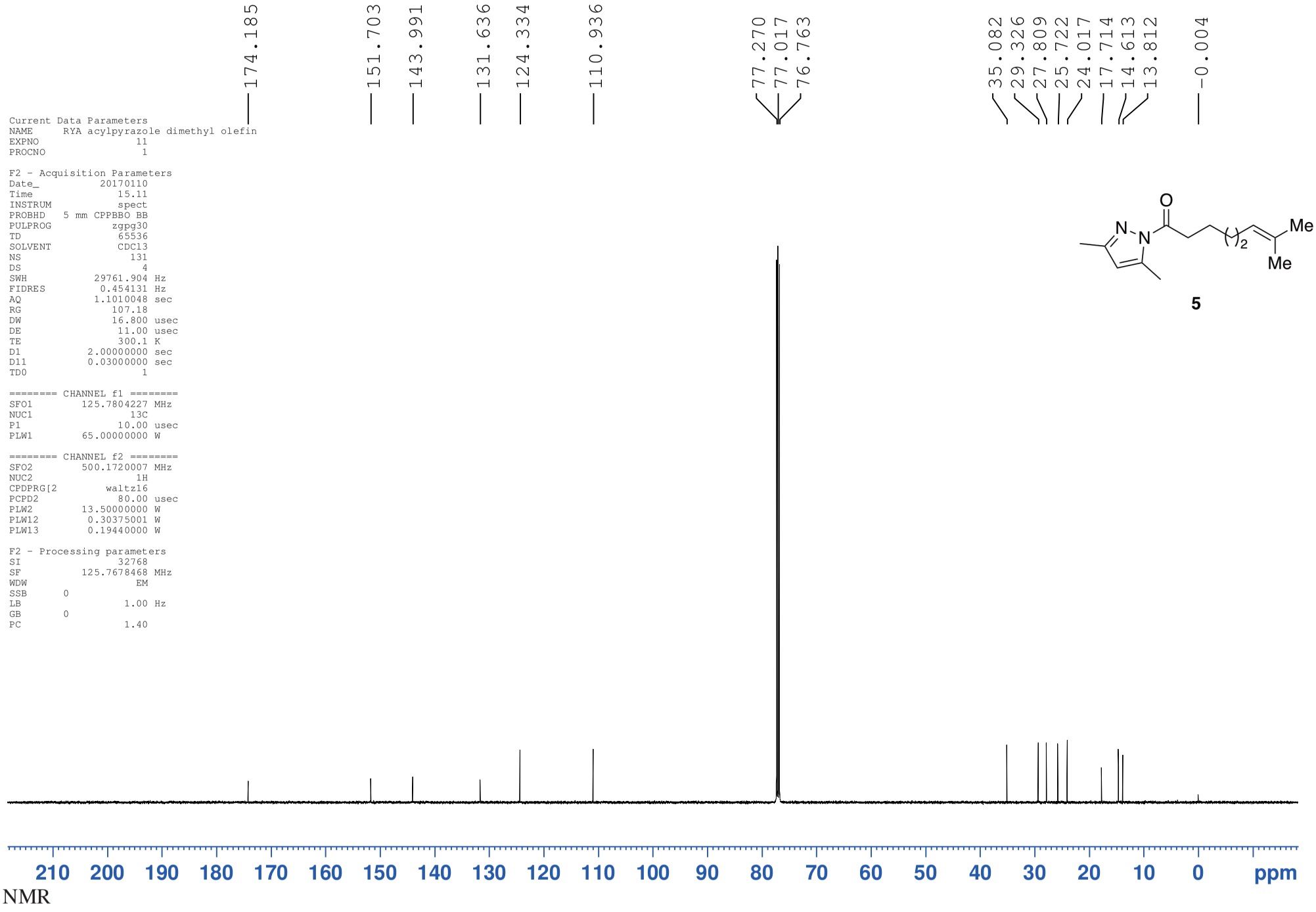
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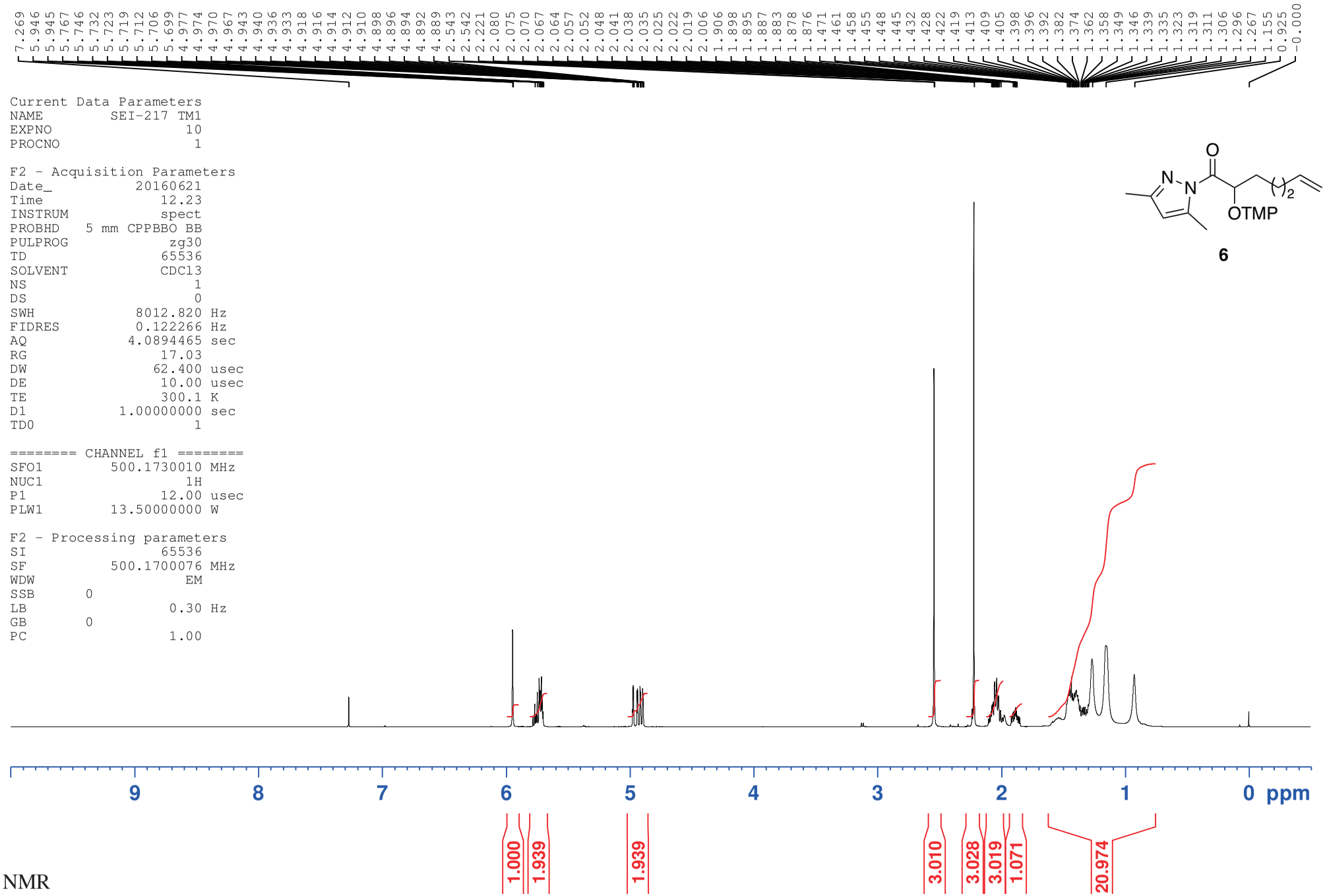
^{13}C NMR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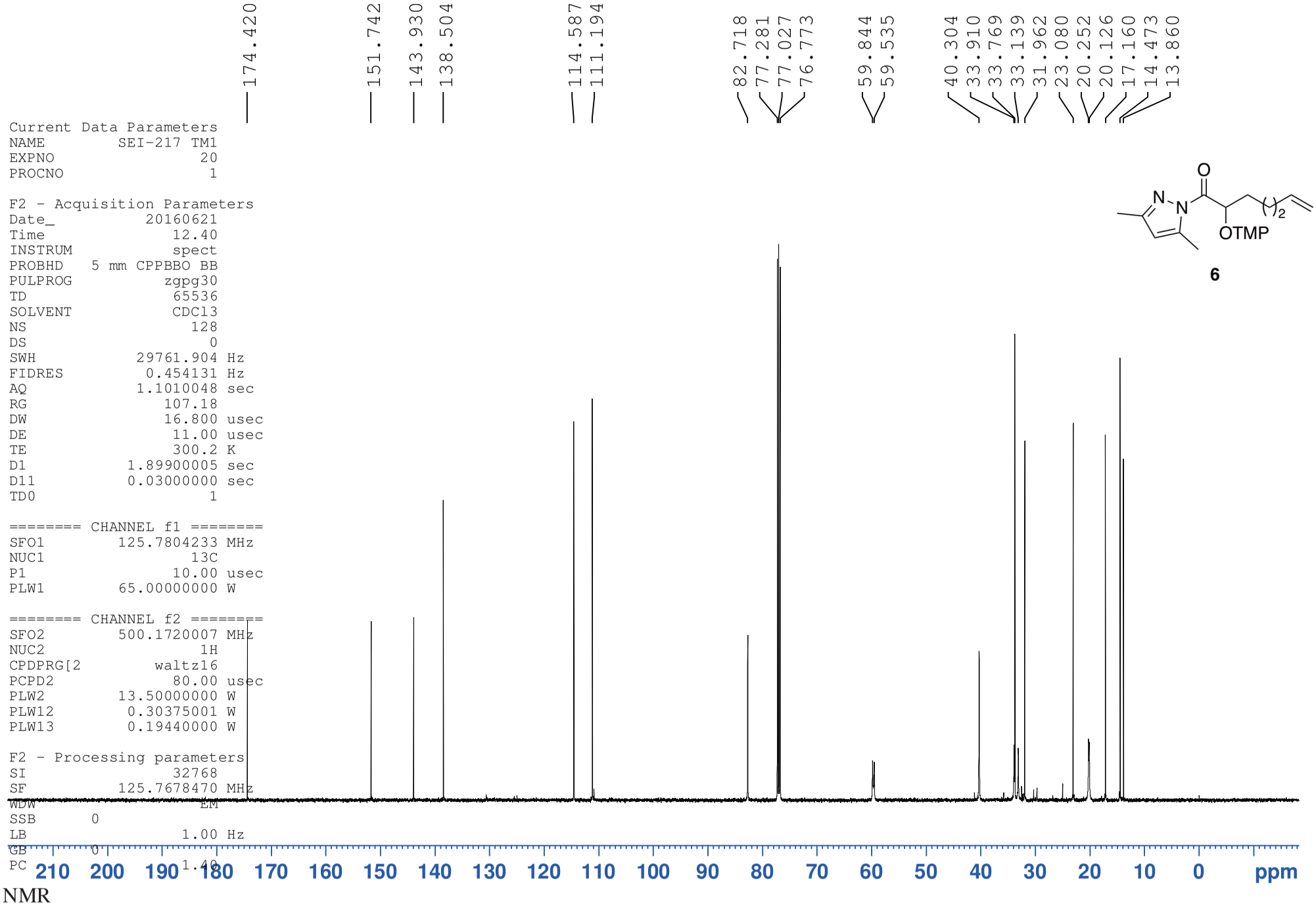
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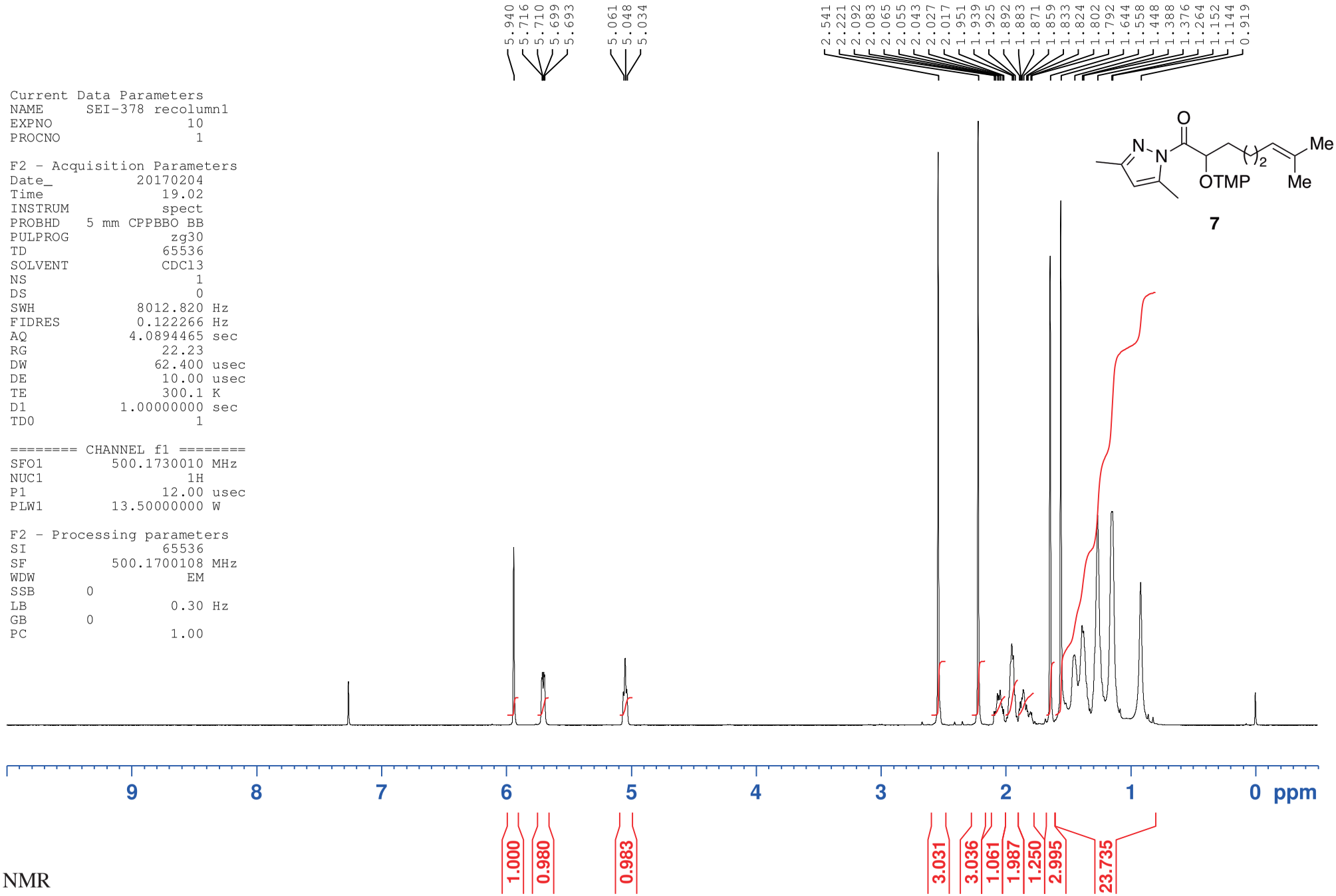
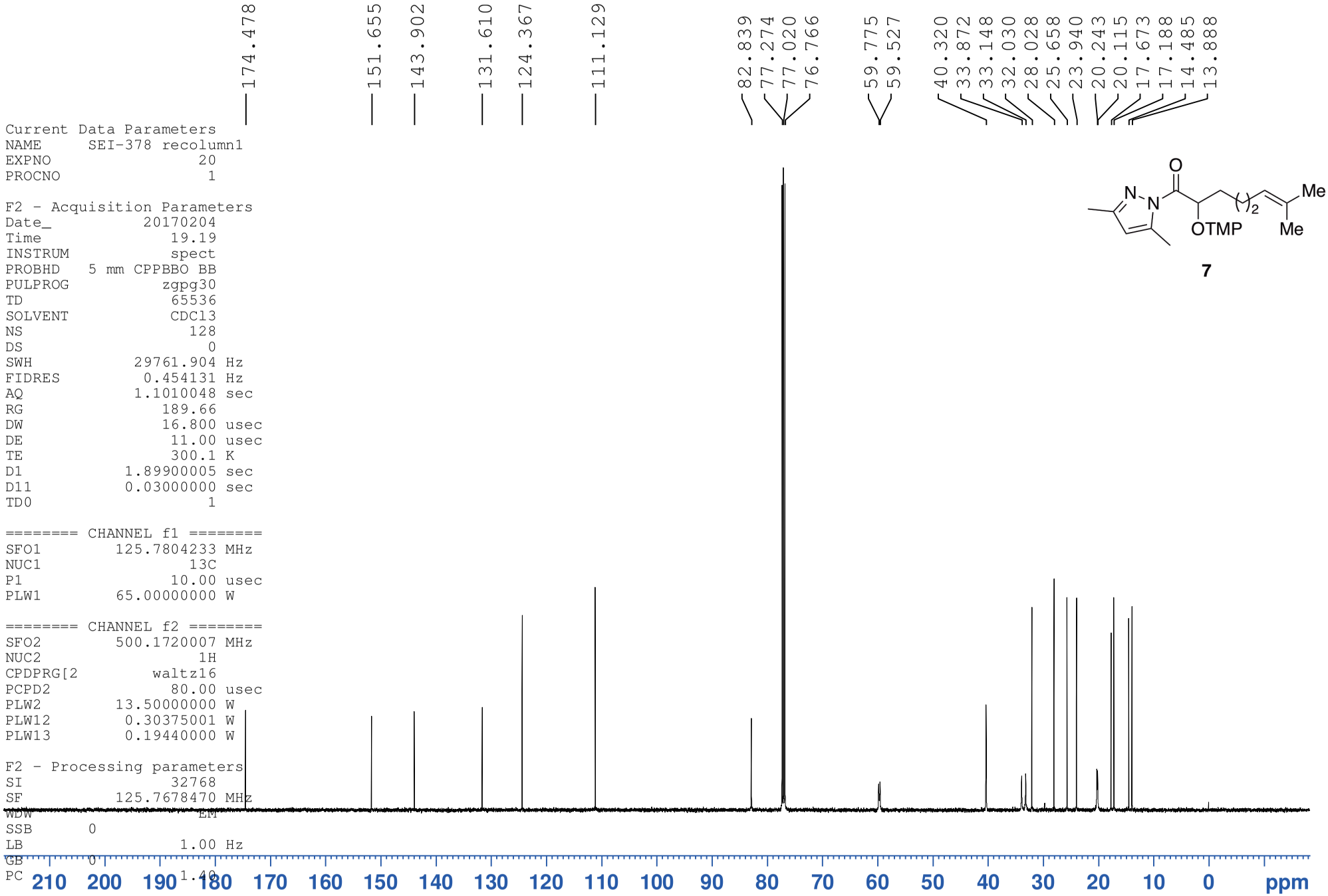
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160621
Time 12.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.18
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== 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
O
N
N
OTMP
2
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

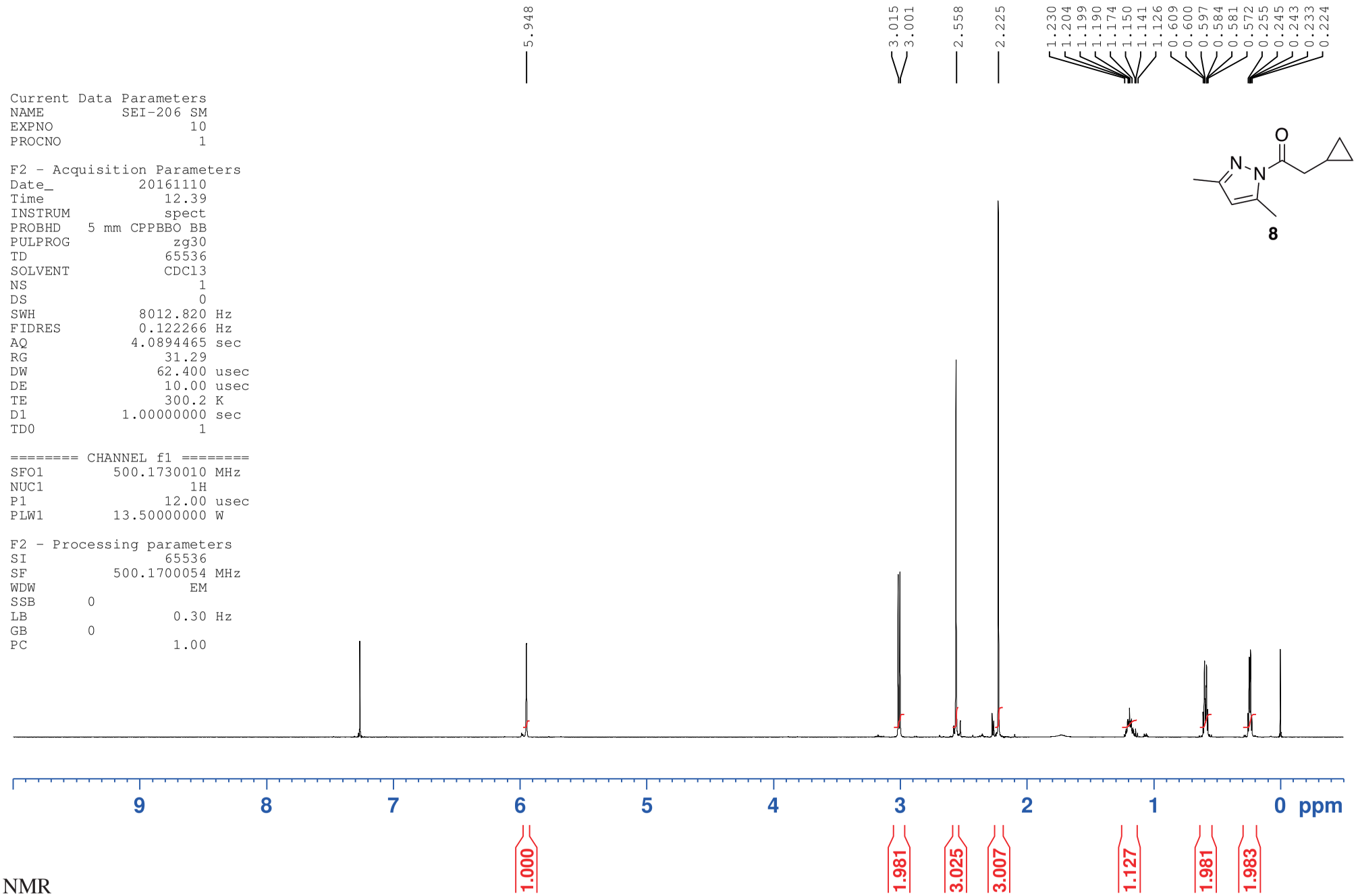
^{13}C NMR


5.940
5.716
5.710
5.699
5.693
5.061
5.048
5.034
2.541
2.221
2.092
2.083
2.065
2.055
2.043
2.027
2.017
1.951
1.939
1.925
1.892
1.883
1.871
1.859
1.833
1.824
1.802
1.792
1.644
1.558
1.448
1.388
1.376
1.264
1.152
1.144
0.919
Current Data Parameters
NAME SEI-378 recolumn1
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170204
Time 19.02
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 22.23
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 500.1700108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
N
N
Me
OTMP
Me
7
9
8
7
6
5
4
3
2
1
0 ppm
1.000
0.980
0.983
3.031
3.036
1.061
1.987
1.250
2.995
23.735

^{1}H NMR

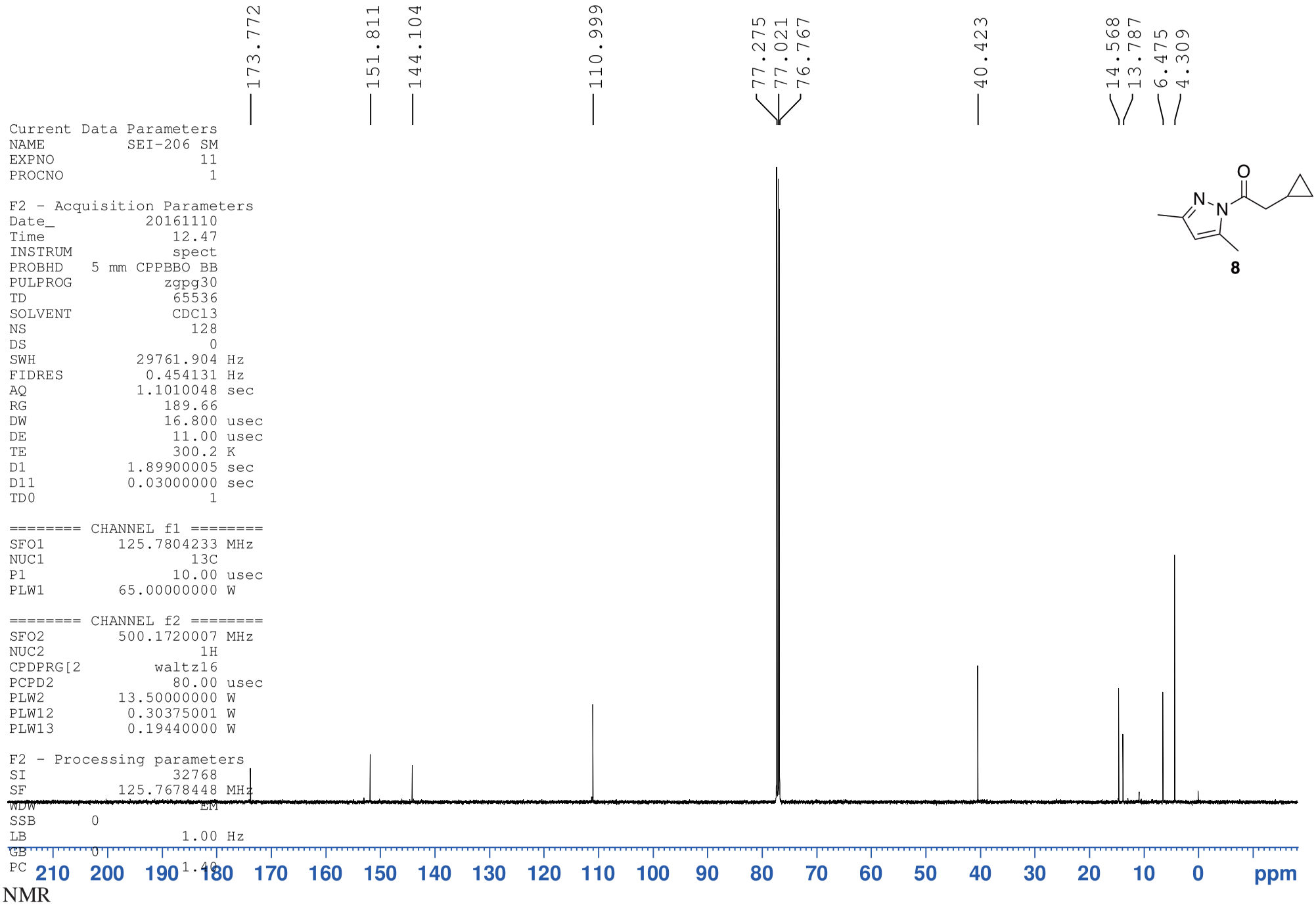

174.478
151.655
143.902
131.610
124.367
111.129
82.839
77.274
77.020
76.766
59.775
59.527
40.320
33.872
33.148
32.030
28.028
25.658
23.940
20.243
20.115
17.673
17.188
14.485
13.888
Current Data Parameters
NAME SEI-378 recolumn1
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170204
Time 19.19
INSTRUM 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
N
N
Me
OTMP
Me
7
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

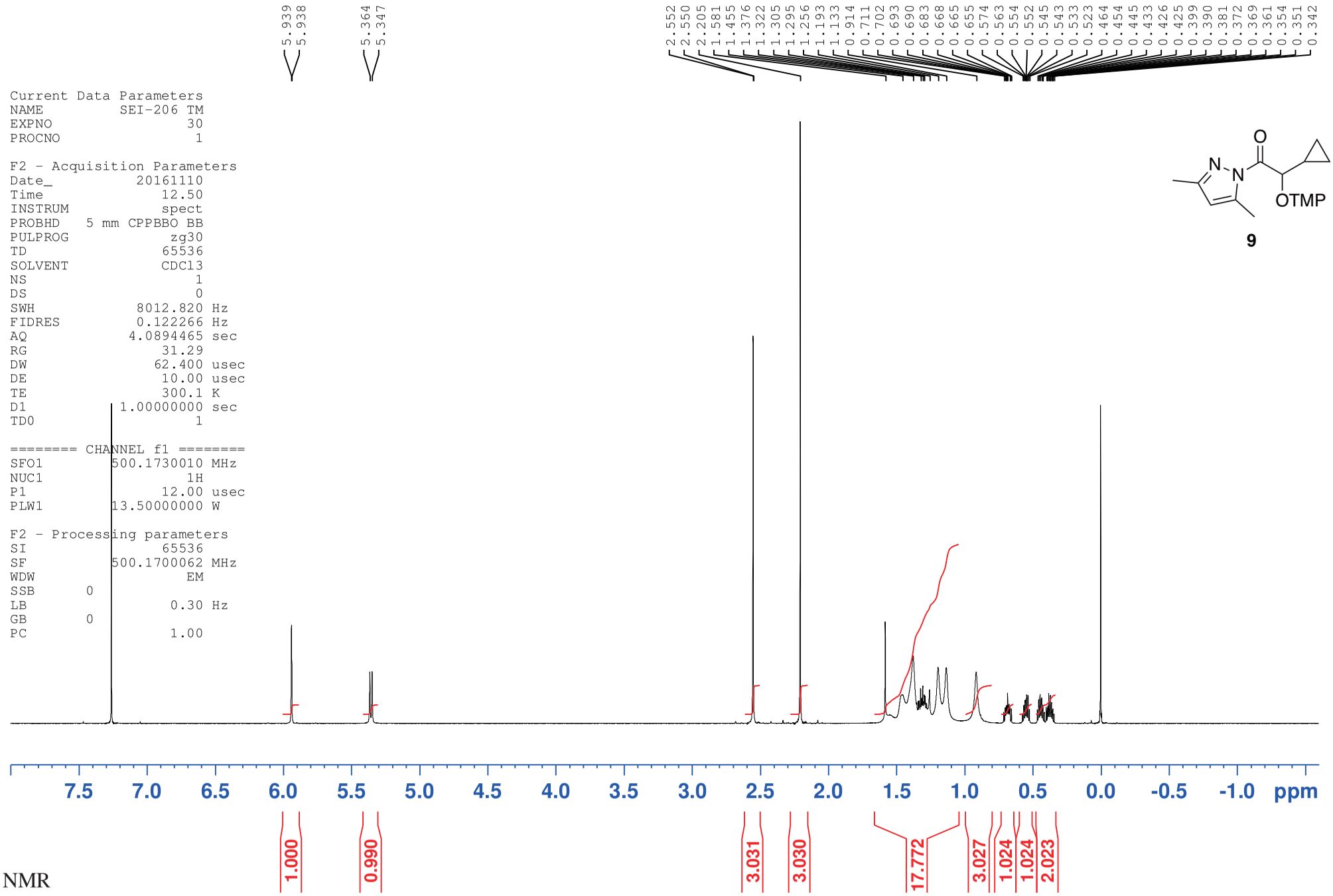

5.948
3.015
3.001
2.558
2.225
1.230
1.204
1.199
1.190
1.174
1.150
1.141
1.126
0.609
0.600
0.597
0.584
0.581
0.572
0.255
0.245
0.243
0.233
0.224
Current Data Parameters
NAME SEI-206 SM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161110
Time 12.39
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
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 300.2 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 500.1700054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
N
N
8
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.981
3.025
3.007
1.127
1.981
1.983

S15

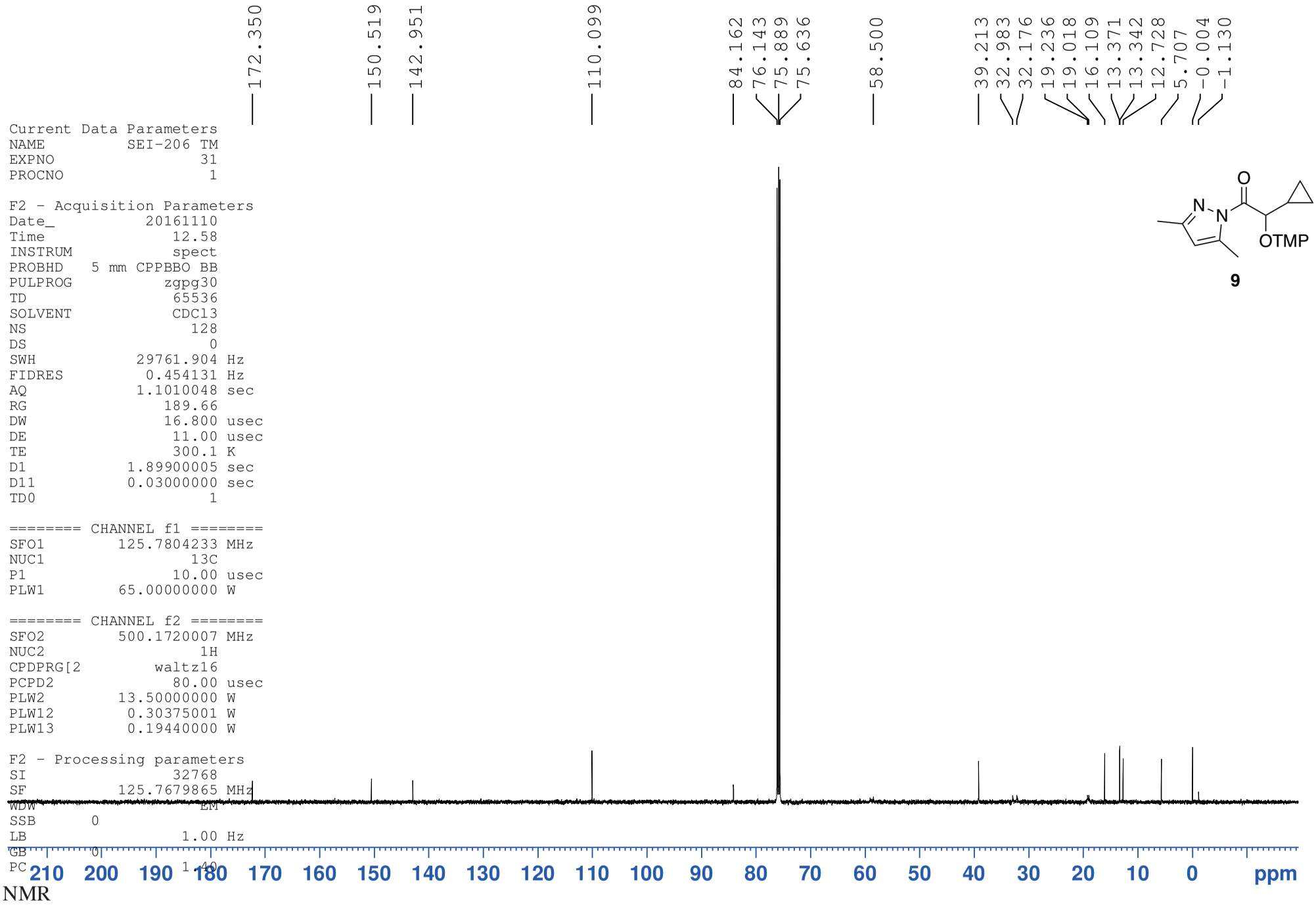
^{1}H NMR


173.772
151.811
144.104
110.999
77.275
77.021
76.767
40.423
14.568
13.787
6.475
4.309
Current Data Parameters
NAME SEI-206 SM
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161110
Time 12.47
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 125.7678448 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
N
8
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


5.939
5.938
5.364
5.347
2.552
2.550
2.205
1.581
1.455
1.376
1.322
1.305
1.295
1.256
1.193
1.133
0.914
0.711
0.702
0.693
0.690
0.683
0.668
0.665
0.655
0.574
0.563
0.554
0.552
0.545
0.543
0.533
0.523
0.464
0.454
0.445
0.433
0.426
0.425
0.399
0.390
0.381
0.372
0.369
0.361
0.354
0.351
0.342
Current Data Parameters
NAME SEI-206 TM
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161110
Time 12.50
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 500.1700062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
N
N
OTMP
9
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
ppm
1.000
0.990
3.031
3.030
17.772
3.027
1.024
1.024
2.023

^{1}H NMR


172.350
150.519
142.951
110.099
84.162
76.143
75.889
75.636
58.500
39.213
32.983
32.176
19.236
19.018
16.109
13.371
13.342
12.728
5.707
-0.004
-1.130
Current Data Parameters
NAME SEI-206 TM
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161110
Time 12.58
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 125.7679865 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
N
OTMP
9
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