

Supporting Information

Non-Metal Lewis Acid-catalyzed Cross-Claisen Condensation for β -Keto

Esters

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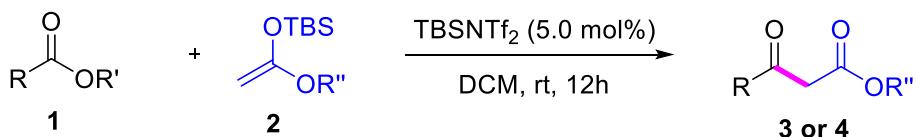
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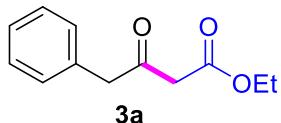
I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. Anhydrous dichloromethane was purified by the Innovative® solvent purification system. ¹H, and ¹³C NMR spectra were collected on a Bruker AV 300 MHz or 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (¹H NMR: CDCl₃ at 7.26 ppm; ¹³C NMR: CDCl₃ at 77.0 ppm). HRMS spectra were performed on a Waters mass spectrometer. IR spectra were recorded on Bruker TENSOR 27 spectrometer and reported in terms of frequency of absorption (cm⁻¹).

II. General Procedure A for β -Keto Esters.



At room temperature, to a mixture of the esters **1** (0.6 mmol) and SKAs **2** (2.0 equiv, 1.2 mmol) was added a solution of TBSNTf₂ in DCM (0.03 mmol, 2.0 mL, 0.015 M).^[1] The mixture was kept stirring at room temperature for 12 h. The reaction mixture was diluted with dichloromethane (30 mL) and then sequentially washed with an aqueous solution of HCl (10 mL, 1%) and brine (10 mL), dried over anhydrous Na₂SO₄, and concentrated in vacuo. The residue was purified by silica gel column chromatography to afford the desired β -keto esters **3-4**.



Ethyl 3-oxo-4-phenylbutanoate (3a) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 78% yield (96.8 mg).

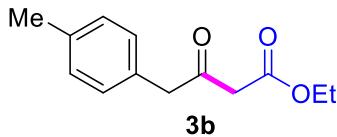
¹H NMR (300 MHz, CDCl₃) δ 7.38-7.28 (m, 3H), 7.25-7.18 (m, 2H), 4.17 (q, J = 7.2 Hz, 2H), 3.83 (s, 2H), 3.45 (s, 2H), 1.26 (t, J = 6.9 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 200.5, 167.1, 133.2, 129.5, 128.8, 127.3, 61.4, 50.0, 48.3, 14.0 ppm.

HRMS (CI⁺) Calcd for C₁₂H₁₅O₃ [M+H]⁺: 207.1017, Found: 207.1021.

IR (thin film) 2981, 1738, 1713, 1649, 1496, 1454, 1312, 1232, 1029 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[2]



Ethyl 3-oxo-4-(p-tolyl)butanoate (3b) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 79% yield (104.8 mg).

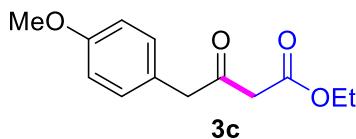
¹H NMR (400 MHz, CDCl₃) δ 7.15 (dd, *J*₁ = 8.0, *J*₂ = 2.4 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.78 (s, 2H), 3.43 (s, 2H), 2.33 (s, 3H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 200.8, 167.1, 137.0, 130.1, 129.5, 129.4, 61.4, 49.7, 48.1, 21.1, 14.0 ppm.

HRMS (CI⁺) Calcd for C₁₃H₁₇O₃ [M+H]⁺: 221.1172, Found: 221.1178.

IR (thin film) 2980, 1740, 1714, 1650, 1514, 1410, 1312, 1229, 1062 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[2]



Ethyl 4-(4-methoxyphenyl)-3-oxobutanoate (3c) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 3:1) in 74% yield (104.4 mg).

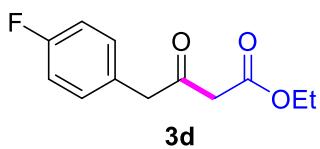
¹H NMR (300 MHz, CDCl₃) δ 7.19-7.08 (m, 2H), 6.92-6.82 (m, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.79 (s, 3H), 3.76 (s, 2H), 3.43 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 200.9, 167.2, 158.8, 130.6, 125.1, 114.2, 61.4, 55.2, 49.1, 48.1, 14.0 ppm.

HRMS (CI⁺) Calcd for C₁₃H₁₇O₄ [M+H]⁺: 237.1121, Found: 237.1127.

IR (thin film) 2980, 1715, 1610, 1510, 1464, 1301, 1245, 1029 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[3]



Ethyl 4-(4-fluorophenyl)-3-oxobutanoate (3d) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 70% yield (94.2 mg).

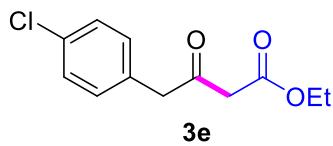
¹H NMR (300 MHz, CDCl₃) δ 7.25-7.12 (m, 2H), 7.08-6.96 (m, 2H), 4.18 (q, *J* = 6.9 Hz, 2H), 3.81 (s, 2H), 3.46 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 200.3, 167.0, 160.1 (d, *J* = 244.5 Hz), 131.1(d, *J* = 7.5 Hz), 128.8(d, *J* = 3.0 Hz), 115.7(d, *J* = 21.8 Hz), 60.5, 48.9, 48.3, 14.0 ppm.

HRMS (CI⁺) Calcd for C₁₂H₁₄FO₃ [M+H]⁺: 225.0921, Found: 225.0927.

IR (thin film) 2984, 1739, 1714, 1602, 1508, 1314, 1220, 1157, 1028 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[2]



Ethyl 4-(4-chlorophenyl)-3-oxobutanoate (3e) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 76% yield (109.5 mg).

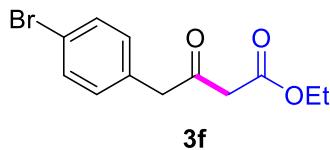
¹H NMR (300 MHz, CDCl₃) δ 7.34-7.27 (m, 2H), 7.21-7.10 (m, 2H), 4.18 (q, *J* = 6.9 Hz, 2H), 3.82 (s, 2H), 3.46 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 199.9, 167.0, 131.6, 130.9, 128.9, 128.7, 61.5, 49.0, 48.4, 14.1 ppm.

HRMS (CI⁺) Calcd for C₁₂H₁₄ClO₃ [M+H]⁺: 241.0626, Found: 241.0631.

IR (thin film) 2982, 1735, 1715, 1491, 1407, 1312, 1090, 1028, 1016 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[4]



Ethyl 4-(4-bromophenyl)-3-oxobutanoate (3f) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 80% yield (136.3 mg).

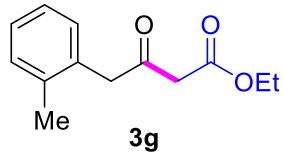
¹H NMR (300 MHz, CDCl₃) δ 7.50-7.41 (m, 2H), 7.15-7.04 (m, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.70 (s, 2H), 3.46 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 199.8, 167.0, 132.1, 131.9, 131.3, 121.4, 61.5, 49.1, 48.4, 14.0 ppm.

HRMS (CI⁺) Calcd for C₁₂H₁₄BrO₃ [M+H]⁺: 285.0121, Found: 285.0126.

IR (thin film) 2981, 1740, 1713, 1488, 1406, 1314, 1259, 1070, 1028 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[5]



Ethyl 3-oxo-4-(o-tolyl)butanoate (3g) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 61% yield (80.6 mg).

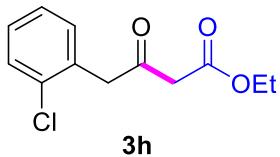
¹H NMR (300 MHz, CDCl₃) δ 7.22-7.19 (m, 2H), 7.19-7.10 (m, 2H), 4.17 (q, *J* = 6.6 Hz, 2H), 3.85 (s, 2H), 3.43 (s, 2H), 2.25 (s, 3H), 1.26 (t, *J* = 6.9 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 200.4, 167.1, 137.1, 132.1, 130.6, 130.5, 127.7, 126.3, 61.4, 48.3, 48.2, 19.6, 14.1 ppm.

HRMS (CI⁺) Calcd for C₁₃H₁₇O₃ [M+H]⁺: 221.1172, Found: 221.1178.

IR (thin film) 2979, 1739, 1715, 1652, 1462, 1410, 1314, 1225, 1029 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[3]



Ethyl 4-(2-chlorophenyl)-3-oxobutanoate (3h) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 59% yield (84.7 mg).

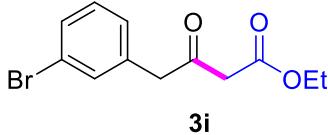
¹H NMR (400 MHz, CDCl₃) δ 7.43-7.36 (m, 2H), 7.26-7.21 (m, 2H), 4.19 (q, *J* = 6.8 Hz, 2H), 3.98 (s, 2H), 3.51 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 199.2, 167.0, 134.4, 131.9, 131.8, 129.6, 129.0, 127.1, 61.5, 48.7, 47.6, 14.1 ppm.

HRMS (CI⁺) Calcd for C₁₂H₁₄ClO₃ [M+H]⁺: 241.0626, Found: 241.0631.

IR (thin film) 2984, 1740, 1716, 1649, 1474, 1444, 1409, 1313, 1275, 1260, 1193, 1028 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[6]



Ethyl 4-(3-bromophenyl)-3-oxobutanoate (3i) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 44% yield (74.5 mg).

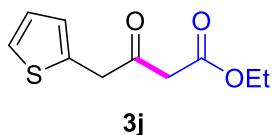
¹H NMR (300 MHz, CDCl₃) δ 7.46-7.34 (m, 2H), 7.25-7.17 (m, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.81 (s, 2H), 3.47 (s, 2H), 1.27 (t, *J* = 6.9 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 199.6, 166.9, 135.3, 132.6, 130.5, 130.3, 128.2, 122.7, 61.6, 49.2, 48.5, 14.1 ppm.

HRMS (Cl⁺) Calcd for C₁₂H₁₄BrO₃ [M+H]⁺: 285.0121, Found: 285.0128.

IR (thin film) 2980, 1738, 1715, 1625, 1568, 1474, 1409, 1314, 1232, 1196, 1028 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[7]



Ethyl 3-oxo-4-(thiophen-2-yl)butanoate (3j) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 68% yield (86.1 mg).

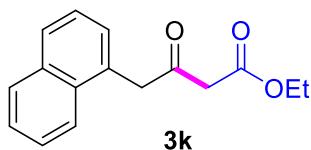
¹H NMR (300 MHz, CDCl₃) δ 7.2-7.23 (m, 1H), 7.02-6.96 (m, 1H), 6.94-6.89 (m, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 4.04 (s, 2H), 3.50 (s, 2H), 1.27 (t, *J* = 6.9 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 199.2, 167.0, 134.1, 127.4, 127.2, 125.5, 61.5, 47.9, 43.6, 14.1 ppm.

HRMS (Cl⁺) Calcd for C₁₀H₁₃O₃S [M+H]⁺: 213.0580, Found: 213.0585.

IR (thin film) 2982, 1716, 1651, 1408, 1444, 1367, 1315, 1205, 1156, 1026 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[3]



Ethyl 4-(naphthalen-1-yl)-3-oxobutanoate (3k) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 59% yield (90.7 mg).

¹H NMR (300 MHz, CDCl₃) δ 7.93-7.78 (m, 3H), 7.58-7.49 (m, 2H), 7.49-7.36 (m, 2H), 4.27 (s, 2H), 4.14 (q, *J* = 7.2 Hz, 2H), 3.42 (s, 2H), 1.23 (t, *J* = 7.2 Hz, 3H)

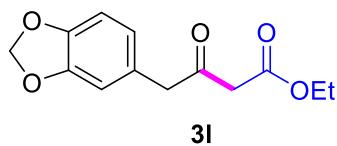
ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 200.9, 167.1, 133.8, 132.1, 129.9, 128.8, 128.5, 128.4, 126.7, 126.0, 125.5, 123.7, 61.4, 48.2, 47.8, 14.0 ppm.

HRMS (Cl^+) Calcd for $\text{C}_{16}\text{H}_{17}\text{O}_3$ [$\text{M}+\text{H}]^+$: 257.1172, Found: 257.1178.

IR (thin film) 2980, 1737, 1713, 1596, 1398, 1366, 1313, 1222, 1192, 1027 cm^{-1} .

The characteristic data of NMR matched with the reported literature.^[8]



Ethyl 4-(benzo[d][1,3]dioxol-5-yl)-3-oxobutanoate (3l) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 93% yield (139.8 mg).

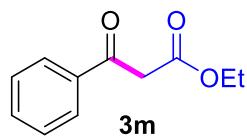
^1H NMR (400 MHz, CDCl_3) δ 6.77 (d, J = 7.6 Hz, 1H), 6.70-6.62 (m, 2H), 5.94 (s, 2H), 4.17 (q, J = 7.2 Hz, 2H), 3.73 (s, 2H), 3.44 (s, 2H), 1.26 (t, J = 6.8 Hz, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 200.7, 167.1, 147.9, 146.9, 126.7, 122.7, 109.8, 108.5, 101.1, 61.4, 49.6, 48.1, 14.0 ppm.

HRMS (Cl^+) Calcd for $\text{C}_{13}\text{H}_{15}\text{O}_5$ [$\text{M}+\text{H}]^+$: 251.0914, Found: 251.0919.

IR (thin film) 2979, 1720, 1503, 1488, 1443, 1244, 1187, 1148, 1032 cm^{-1} .

The characteristic data of NMR matched with the reported literature.^[9]



Ethyl 3-oxo-3-phenylpropanoate (3m) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 50% yield (58.1 mg).

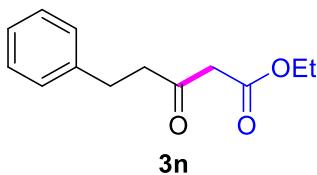
¹H NMR (300 MHz, CDCl₃) δ 7.97-7.91 (m, 2H), 7.64-7.56 (m, 1H), 7.52-7.37 (m, 2H), 4.21 (q, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 1.25 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 192.5, 167.5, 133.7, 128.8, 128.5, 126.0, 61.5, 46.0, 14.0 ppm.

HRMS (CI⁺) Calcd for C₁₁H₁₃O₃ [M+H]⁺: 193.0859, Found: 193.0865.

IR (thin film) 2981, 1736, 1684, 1622, 1449, 1263, 1324, 1196, 1144, 1034, 1022 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[10]



Ethyl 3-oxo-5-phenylpentanoate (3n) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 79% yield (105.4 mg).

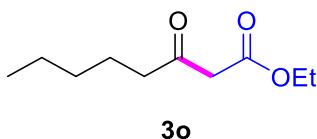
¹H NMR (400 MHz, CDCl₃) δ 7.32-7.26 (m, 2H), 7.23-7.15 (m, 3H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.42 (s, 2H), 2.97-2.83 (m, 4H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 201.9, 167.1, 140.5, 128.5, 128.3, 126.2, 61.4, 49.4, 44.5, 29.4, 14.1 ppm.

HRMS (CI⁺) Calcd for C₁₃H₁₇O₃ [M+H]⁺: 221.1172, Found: 221.1178.

IR (thin film) 2979, 1738, 1712, 1454, 1366, 1275, 1260, 1029 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[11]



Ethyl 3-oxooctanoate (3o) was prepared according to the General Procedure A

as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 78% yield (71.1 mg).

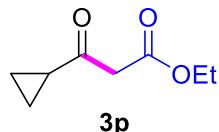
¹H NMR (300 MHz, CDCl₃) δ 4.18 (q, *J* = 7.2 Hz, 2H), 3.42 (s, 2H), 2.52 (t, *J* = 7.5 Hz, 2H), 1.68-1.52 (m, 2H), 1.31-1.23 (m, 7H), 0.88 (t, *J* = 6.6 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 203.0, 167.3, 61.3, 49.3, 43.0, 31.1, 23.1, 22.4, 14.1, 13.8 ppm.

HRMS (CI⁺) Calcd for C₁₀H₁₉O₃ [M+H]⁺: 187.1329, Found: 187.1334.

IR (thin film) 2958, 1740, 1715, 1464, 1367, 1275, 1260, 1150, 1029 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[12]



Ethyl 3-cyclopropyl-3-oxopropanoate (3p) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 58% yield (54.1 mg).

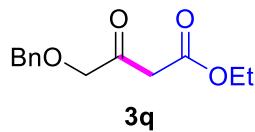
¹H NMR (300 MHz, CDCl₃) δ 4.18 (q, *J* = 7.2 Hz, 2H), 3.54 (s, 2H), 2.07-1.96 (s, 1H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.14-1.05 (m, 2H), 0.98-0.89 (m, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 202.8, 167.2, 61.2, 49.9, 20.7, 14.0, 11.6 ppm.

HRMS (CI⁺) Calcd for C₈H₁₃O₃ [M+H]⁺: 157.0859, Found: 157.0865.

IR (thin film) 2984, 1736, 1698, 1622, 1383, 1310, 1260, 1144, 1022 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[13]



Ethyl 4-(benzyloxy)-3-oxobutanoate (3q) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 78% yield (71.1 mg).

ether/EtOAc = 4:1) in 89% yield (126.7 mg).

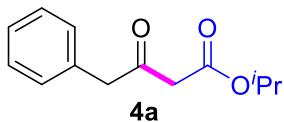
¹H NMR (300 MHz, CDCl₃) δ 7.40-7.27 (m, 5H), 4.58 (s, 2H), 4.24-4.11 (m, 4H), 3.53 (s, 2H), 1.24 (t, *J* = 6.9 Hz, 7H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 201.6, 166.9, 136.8, 128.4, 128.0, 127.8, 74.7, 73.4, 61.3, 46.0, 13.9 ppm.

HRMS (CI⁺) Calcd for C₁₃H₁₇O₄ [M+H]⁺: 237.1121, Found: 237.1127.

IR (thin film) 2984, 1719, 1454, 1367, 1317, 1228, 1096, 1028 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[14]



Isopropyl 3-oxo-4-phenylbutanoate (4a) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc = 4:1) in 76% yield (103.2 mg).

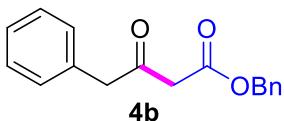
¹H NMR (300 MHz, CDCl₃) δ 7.39-7.27 (m, 3H), 7.24-7.16 (m, 2H), 5.11-4.96 (m, 1H), 3.83 (s, 2H), 3.42 (s, 2H), 1.24 (d, *J* = 6.3 Hz, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 200.6, 166.6, 133.2, 129.6, 128.8, 127.3, 69.1, 50.0, 48.6, 21.7 ppm.

HRMS (CI⁺) Calcd for C₁₃H₁₇O₃ [M+H]⁺: 221.1172, Found: 221.1178.

IR (thin film) 2980, 1738, 1714, 1641, 1467, 1311, 1239, 1103 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[15]



Benzyl 3-oxo-4-phenylbutanoate (4b) was prepared according to the General Procedure A as a yellow oil (chromatography eluent: petroleum ether/EtOAc

= 4:1) in 46% yield (73.7 mg).

¹H NMR (300 MHz, CDCl₃) δ 7.37-7.27 (m, 8H), 7.20-7.12 (m, 2H), 5.15 (s, 2H), 3.81 (s, 2H), 3.52 (s, 2H) ppm.

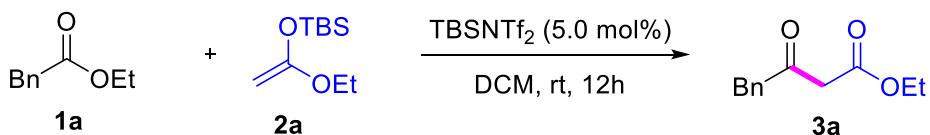
¹³C NMR (75 MHz, CDCl₃) δ 200.3, 166.9, 135.1, 133.0, 129.5, 128.8, 128.6, 128.5, 128.4, 127.4, 67.2, 50.0, 48.2 ppm.

HRMS (CI⁺) Calcd for C₁₇H₁₇O₃ [M+H]⁺: 269.1172, Found: 269.1178.

IR (thin film) 2980, 1740, 1714, 1622, 1454, 1314, 1266, 1190, 1028 cm⁻¹.

The characteristic data of NMR matched with the reported literature.^[15]

III. Large-Scale Reaction Procedure.



At room temperature, to a mixture of the ethyl 2-phenylacetate **1a** (987 mg, 6.0 mmol) and SKAs **2a** (2.42 g, 12.0 mmol) was added a solution of TBSNTf₂ in DCM (0.3 mmol, 20.0 mL, 0.015 M). The mixture was kept stirring at room temperature for 12 h. The reaction mixture was diluted with dichloromethane (100 mL) and then sequentially washed with an aqueous solution of HCl (50 mL, 1%) and brine (50 mL), dried over anhydrous Na₂SO₄, and concentrated in vacuo. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 4:1 to 3:1) to afford the desired ethyl 3-oxo-4-phenylbutanoate **3a** (1.05 g, 85%).

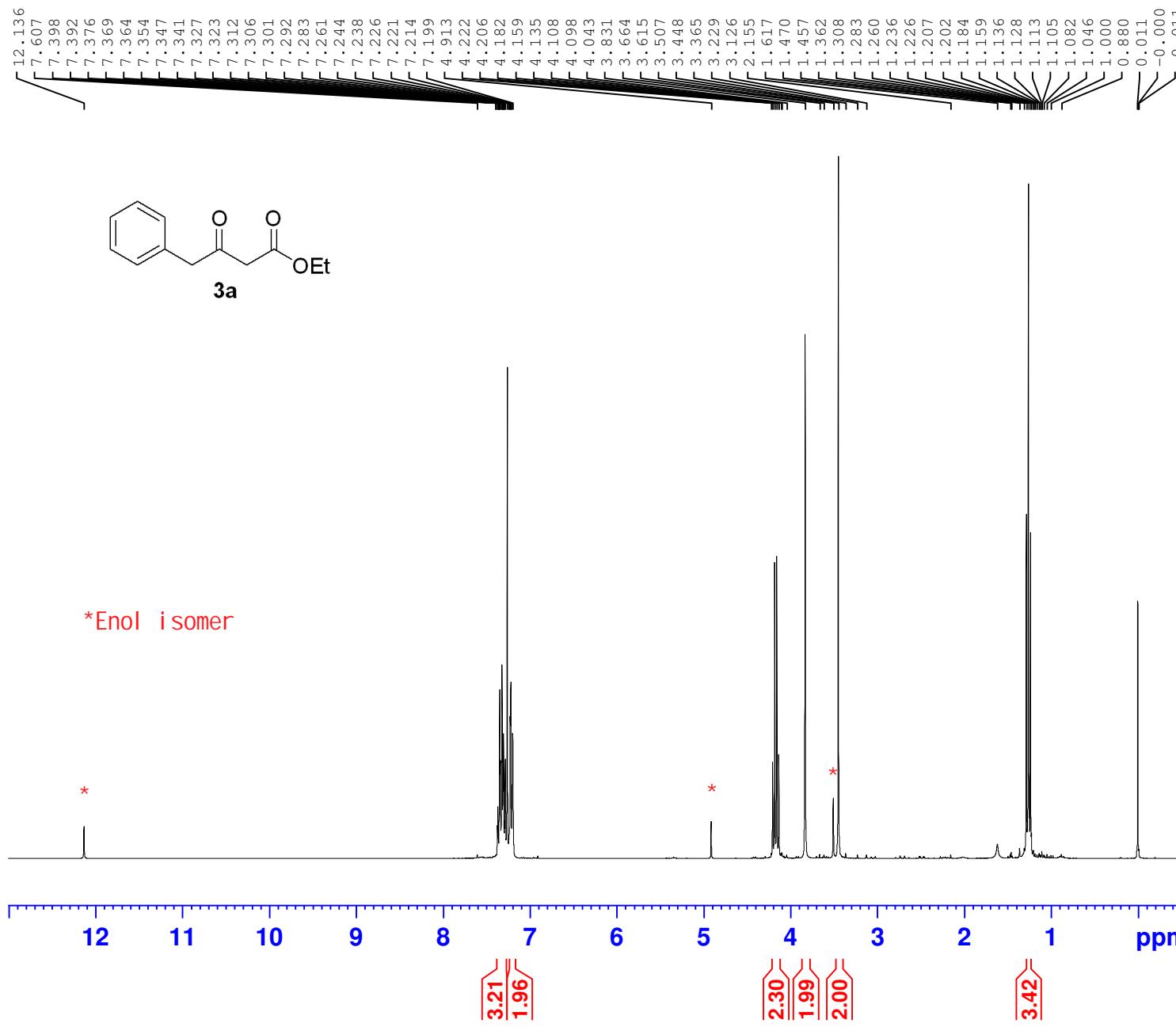
Reference

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3sjwei 1760 zty-5-7a 1h cdcl3



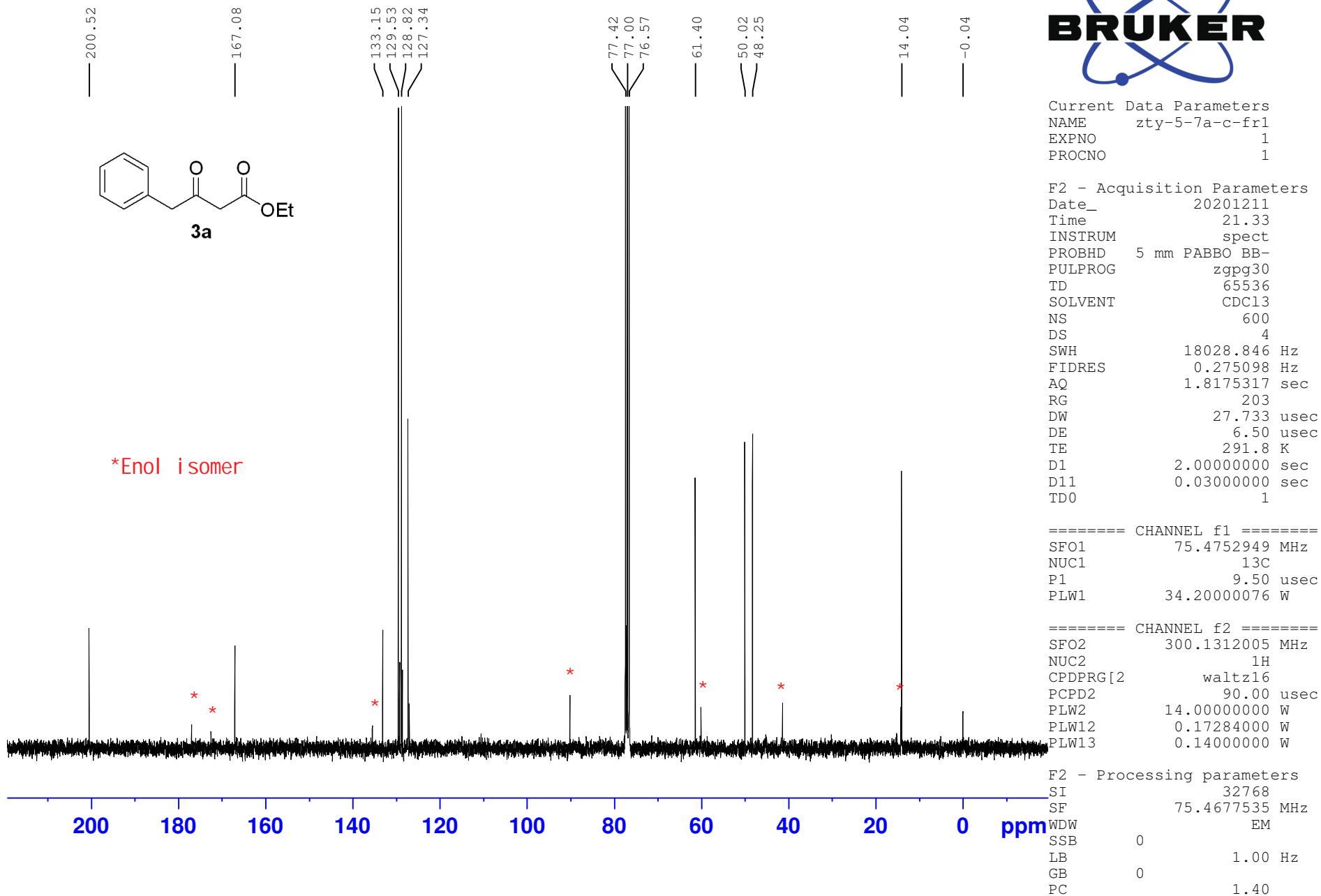
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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 304.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
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PLW1 14.00000000 W

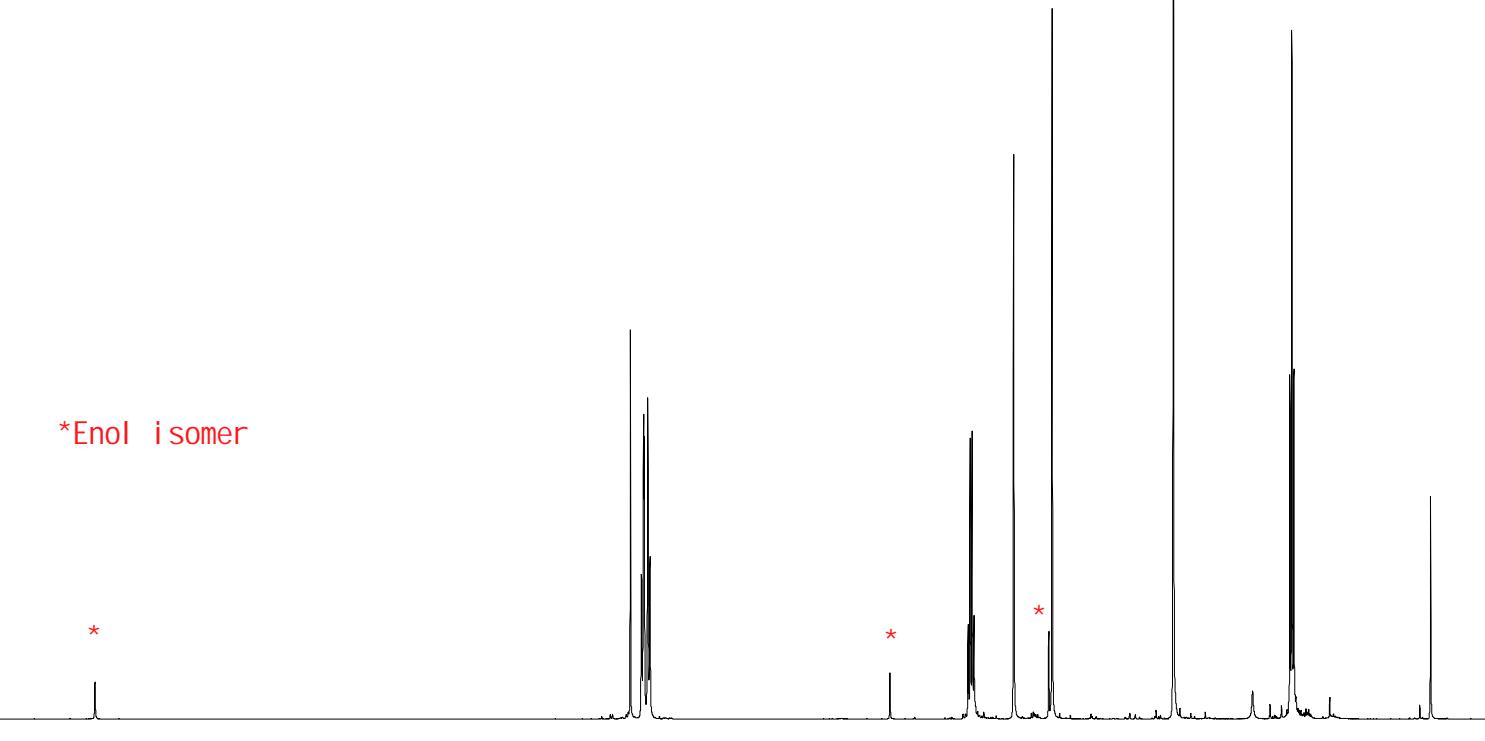
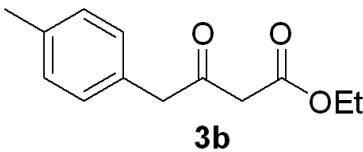
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3sjwei 2150 zty-5-7a 13c cdcl3



4sunjianwei4/155 zty-5-10b

— 12.116



Current Data Parameters
NAME zty-5-10b-h-fr
EXPNO 1
PROCNO 1

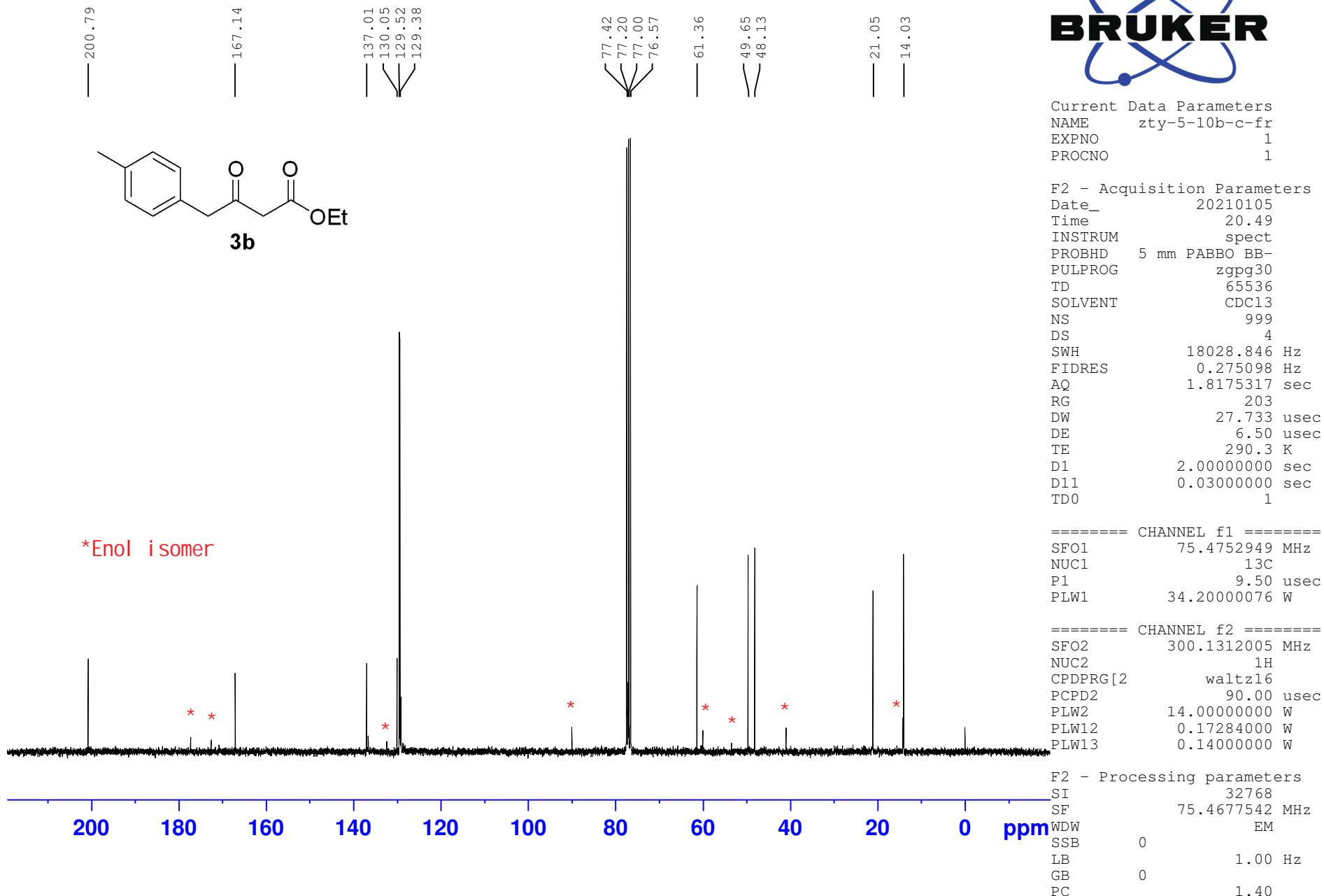
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FIDRES 0.125483 Hz
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RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 294.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======

NUC1 1H
P1 14.40 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900159 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2399 zty-5-10b 13c cdcl3



Current Data Parameters
NAME zty-5-10b-c-fr
EXPNO 1
PROCNO 1

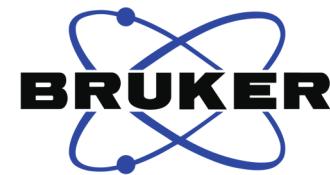
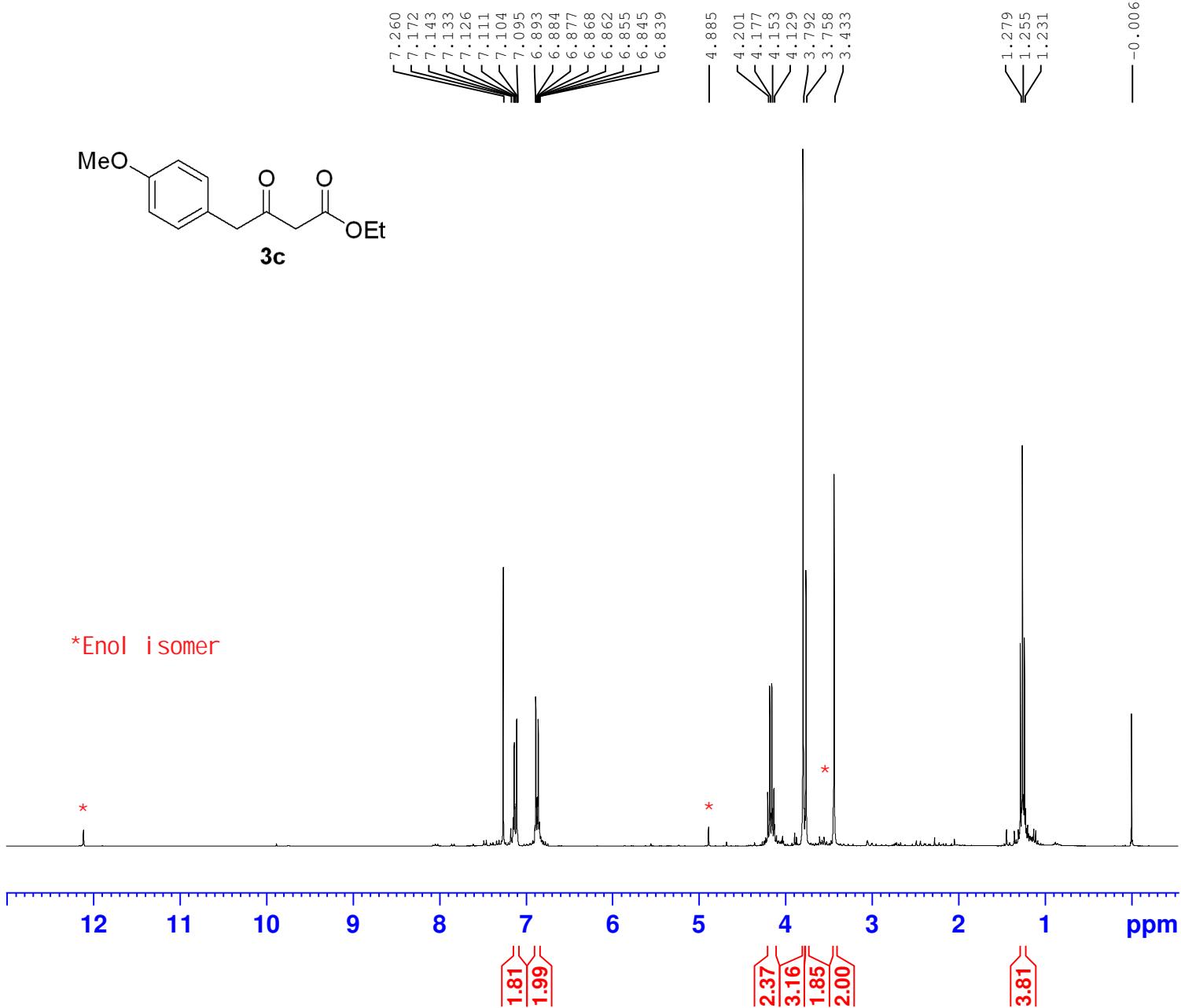
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TD 65536
SOLVENT CDCl3
NS 999
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2145 zty-5-10f 1h cdcl3



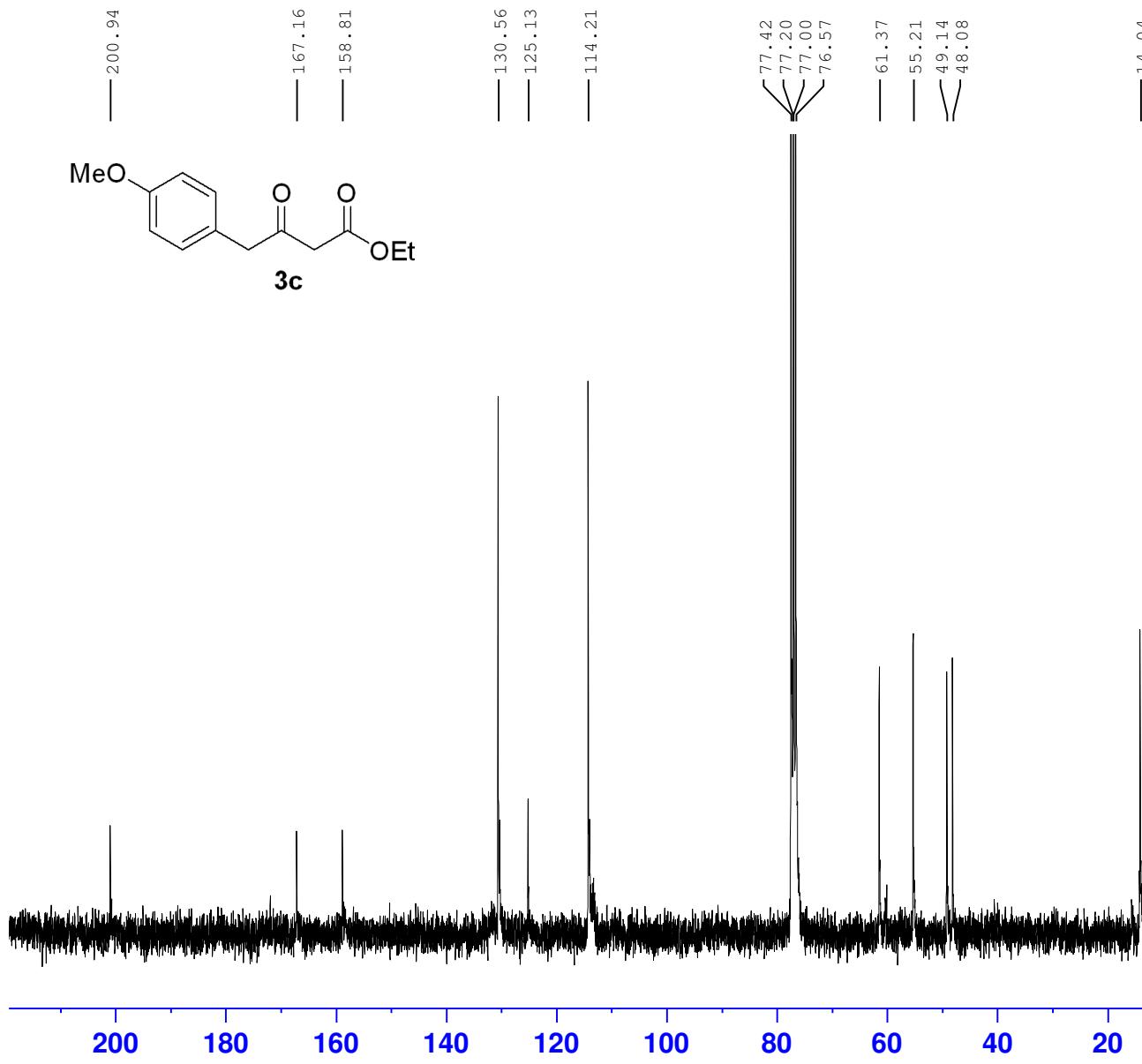
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EXPNO 1
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 291.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2401 zty-5-10f 13c cdcl3



Current Data Parameters
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PROCNO 1

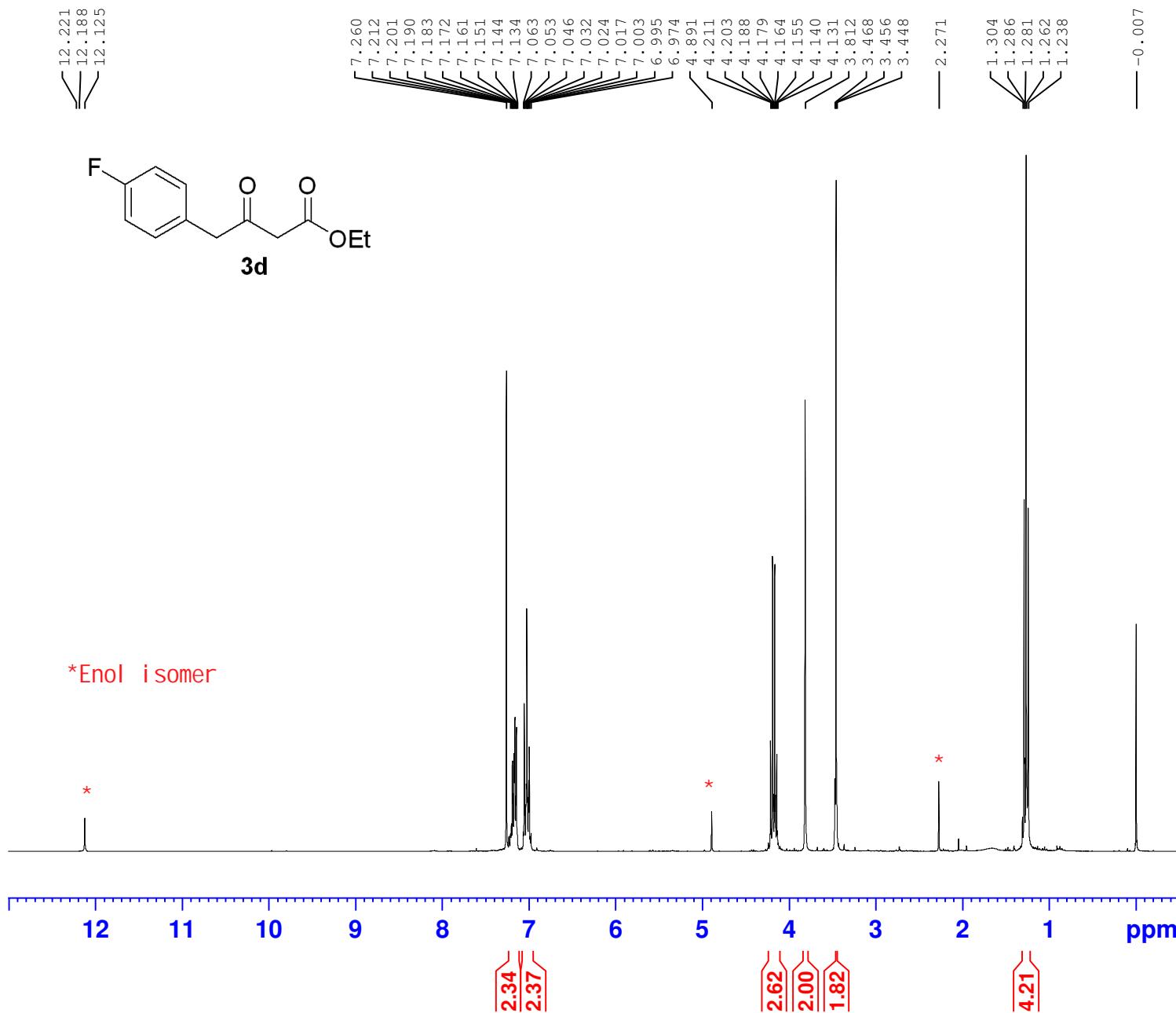
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677541 MHz
WDW
SSB 0 EM
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2144 zty-5-10e 1h cdcl3



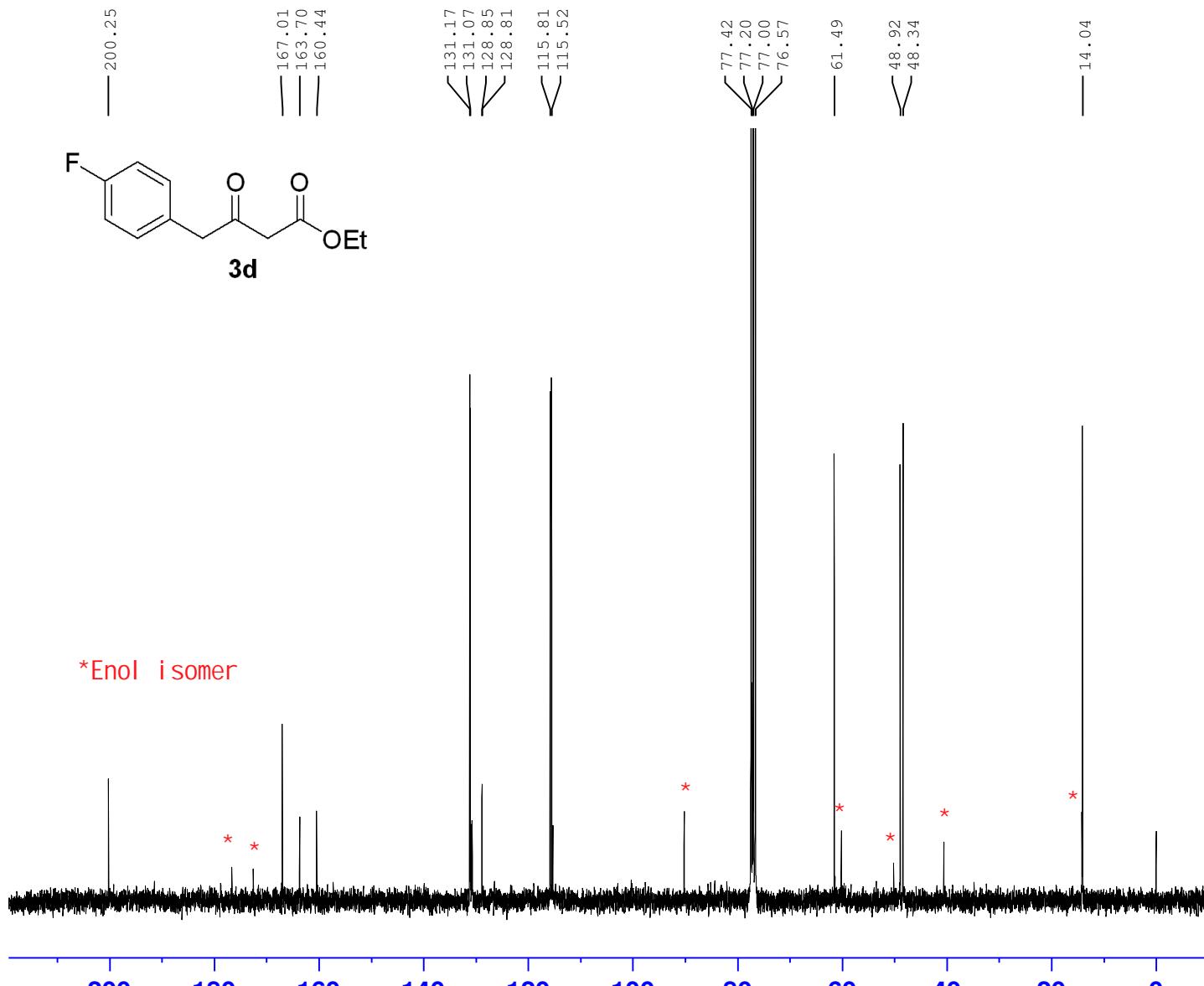
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EXPNO 1
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 291.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2393 zty-5-10e 13c cdcl3



Current Data Parameters
NAME ZTY-5-10e-c-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210105
Time 12.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

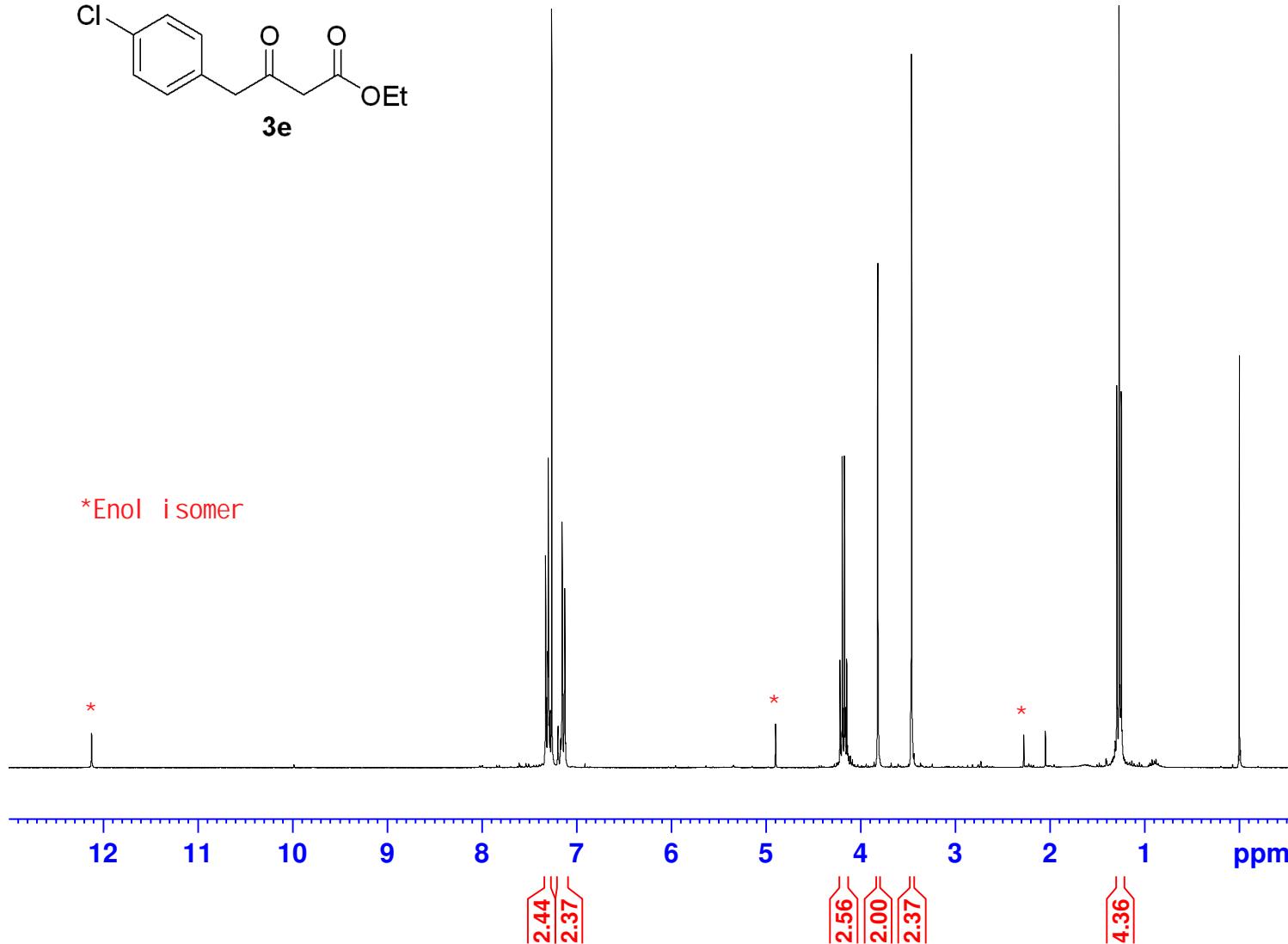
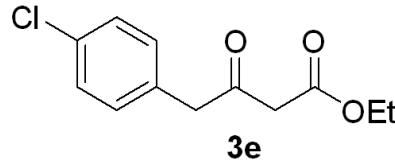
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SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
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NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677533 MHz
WDW
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2510 zty-5-10c-h-fr 1h cdcl3

— 12.122



Current Data Parameters
NAME zty-5-10c-h-fr
EXPNO 1
PROCNO 1

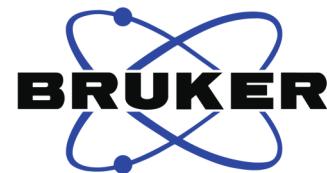
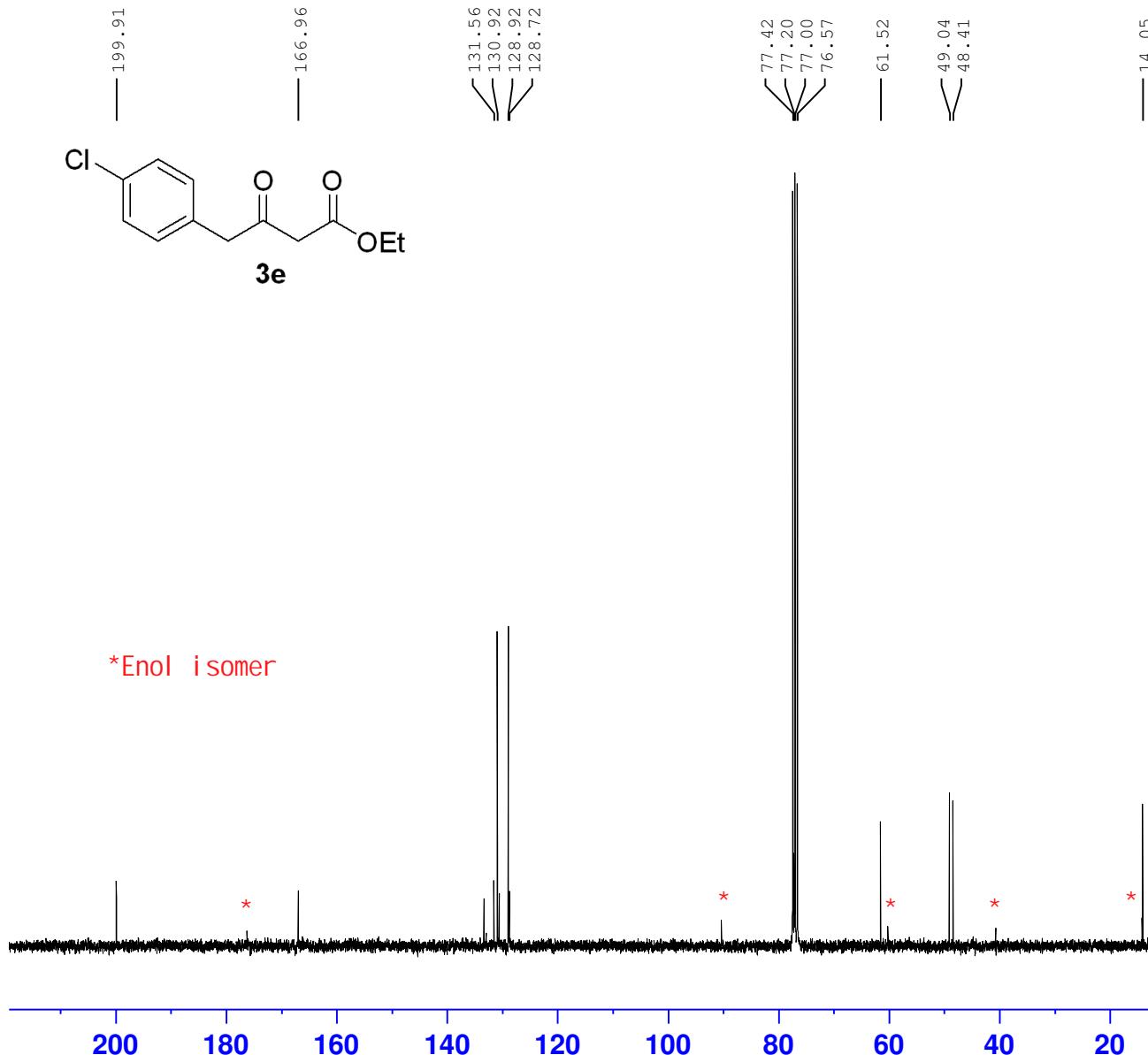
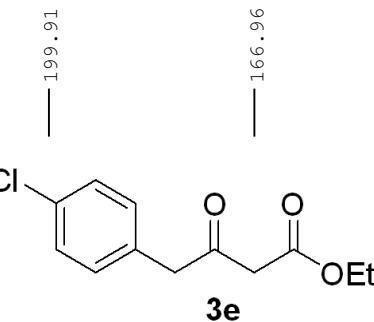
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SOLVENT CDCl3
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DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 291.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======

SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2525 zty-5-10c-c-fr 13c cdcl3



Current Data Parameters
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PROCNO 1

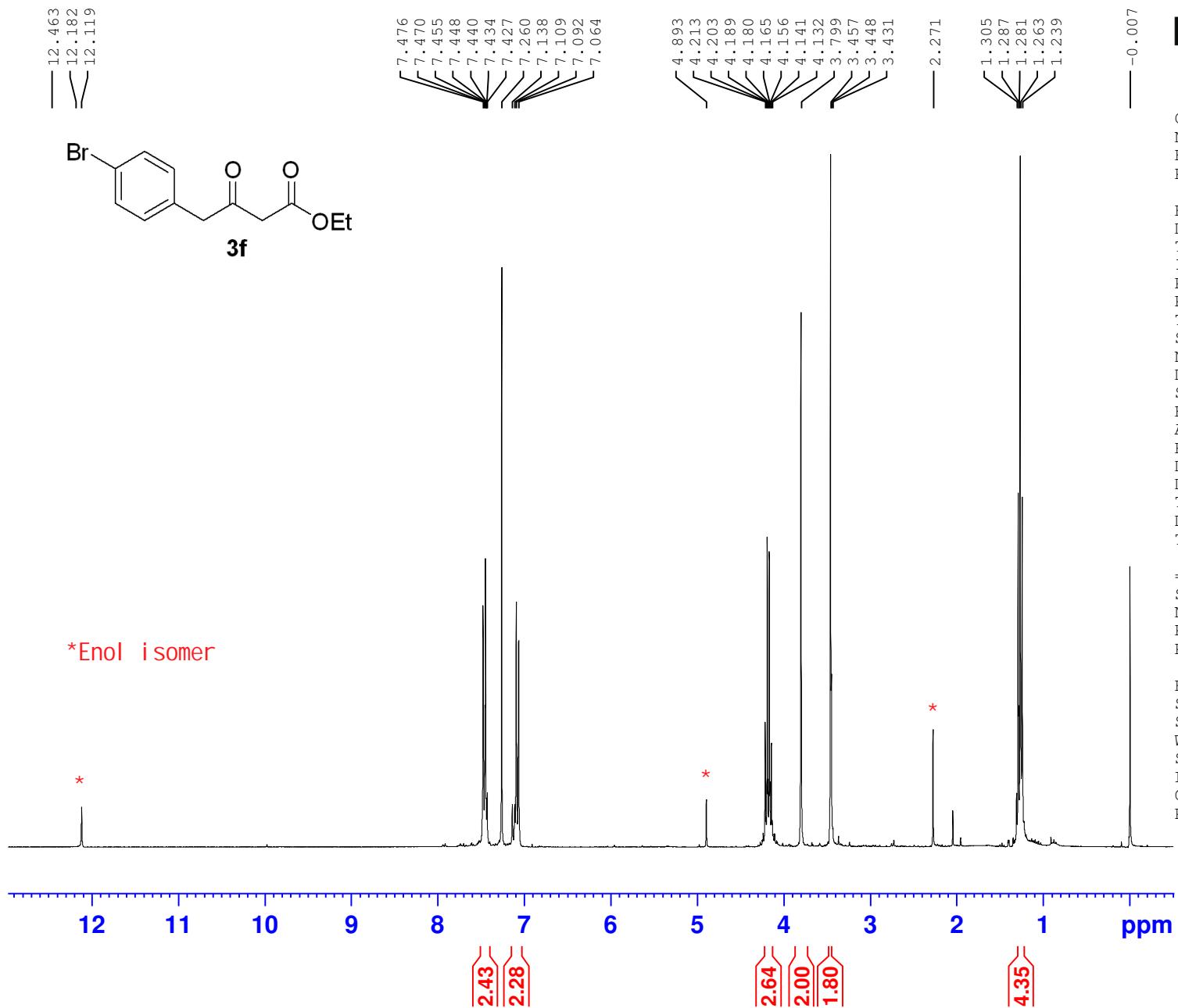
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DS 4
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FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 292.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
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WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2143 zty-5-10d 1h cdcl3



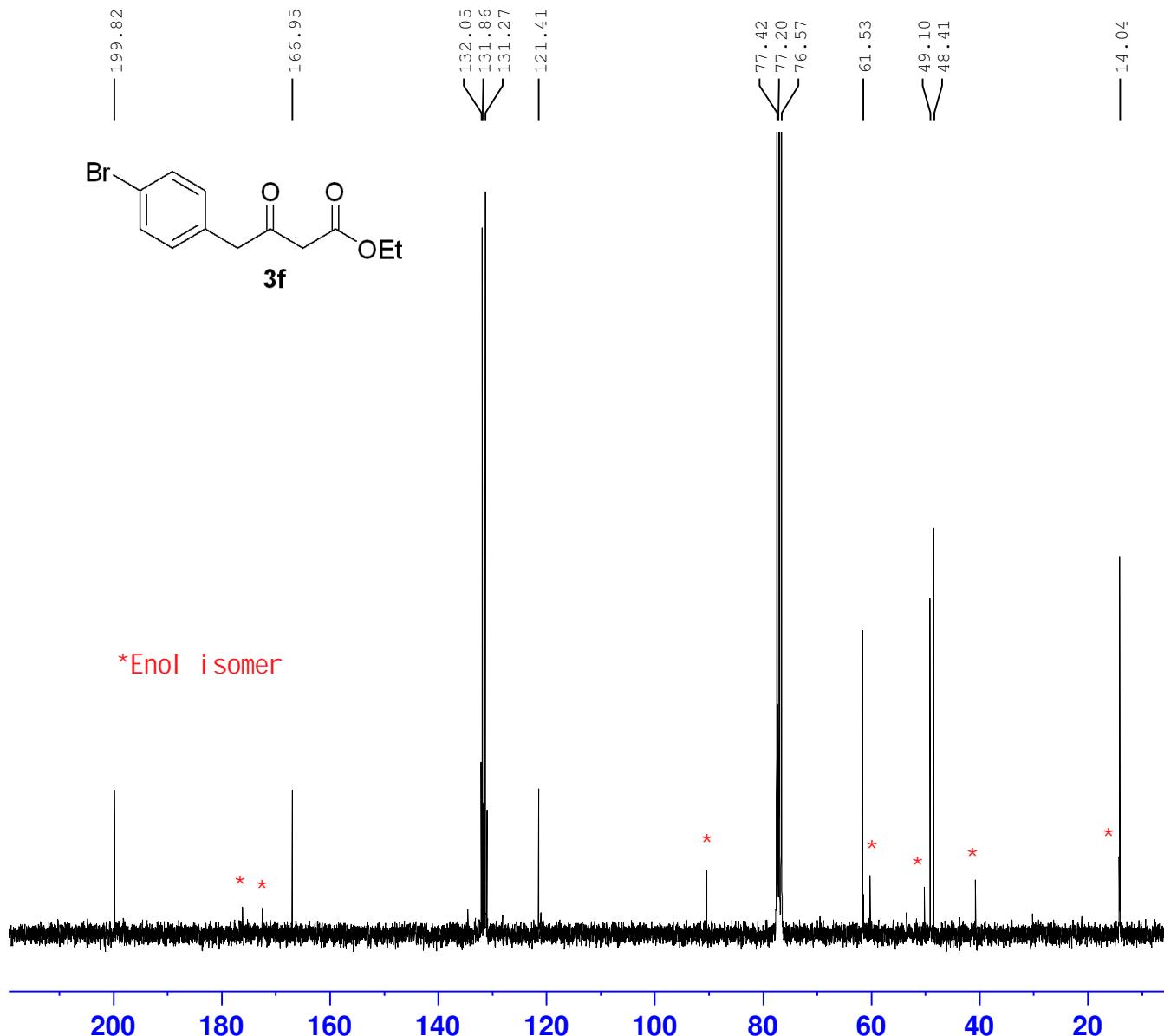
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EXPNO 1
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 291.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2398 zty-5-10d 13c cdcl3



Current Data Parameters
NAME zty-5-10d-c-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210105
Time 19.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

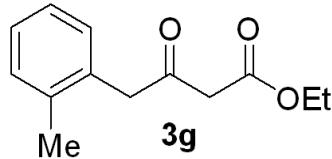
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NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
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NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677536 MHz
WDW
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2156 zty-5-10h 1h cdcl3

— 12.189



3g

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7.172
7.167
7.146
7.140
7.127
7.123
7.113

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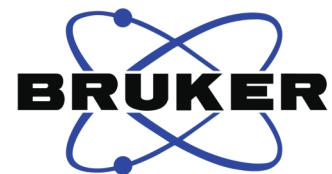
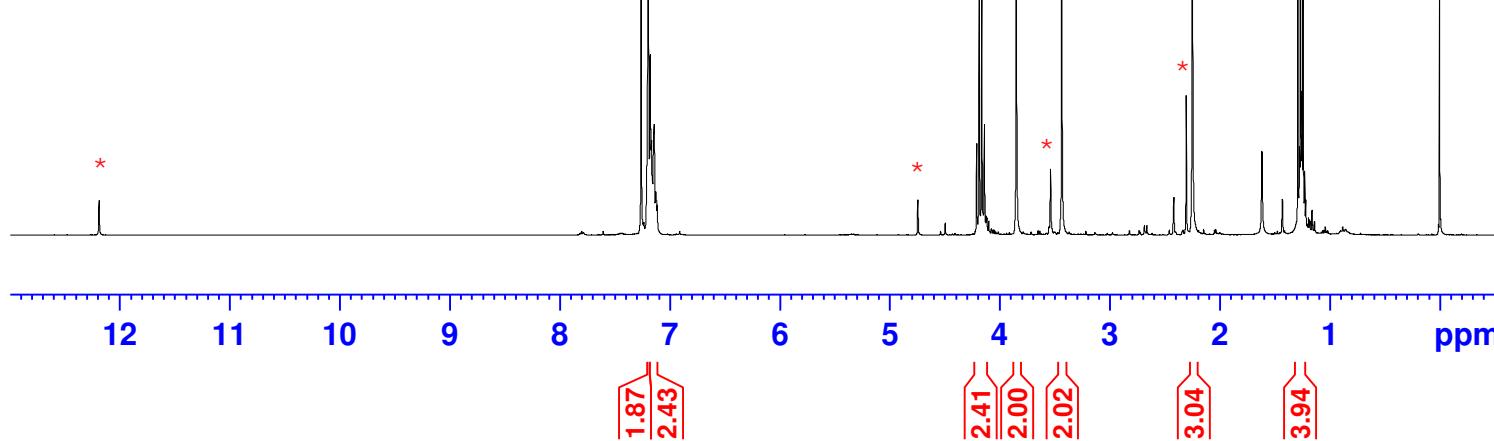
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SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 290.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======

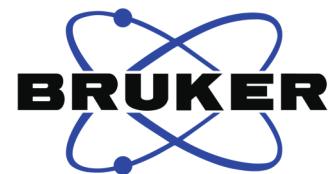
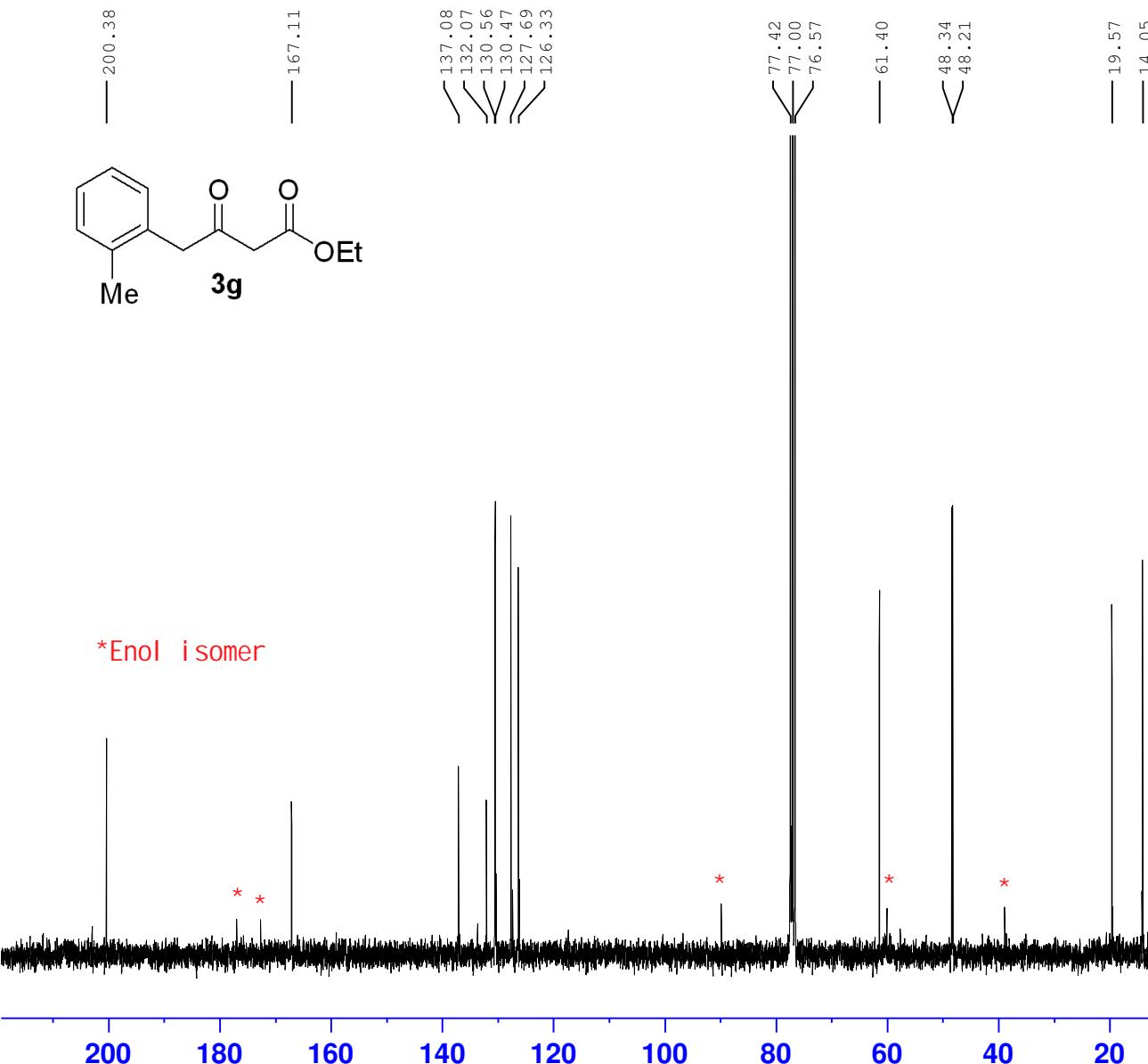
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NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

*Enol isomer



3sjwei 2835 zty-5-10h 13c cdcl3



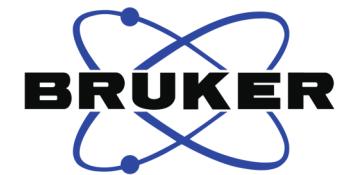
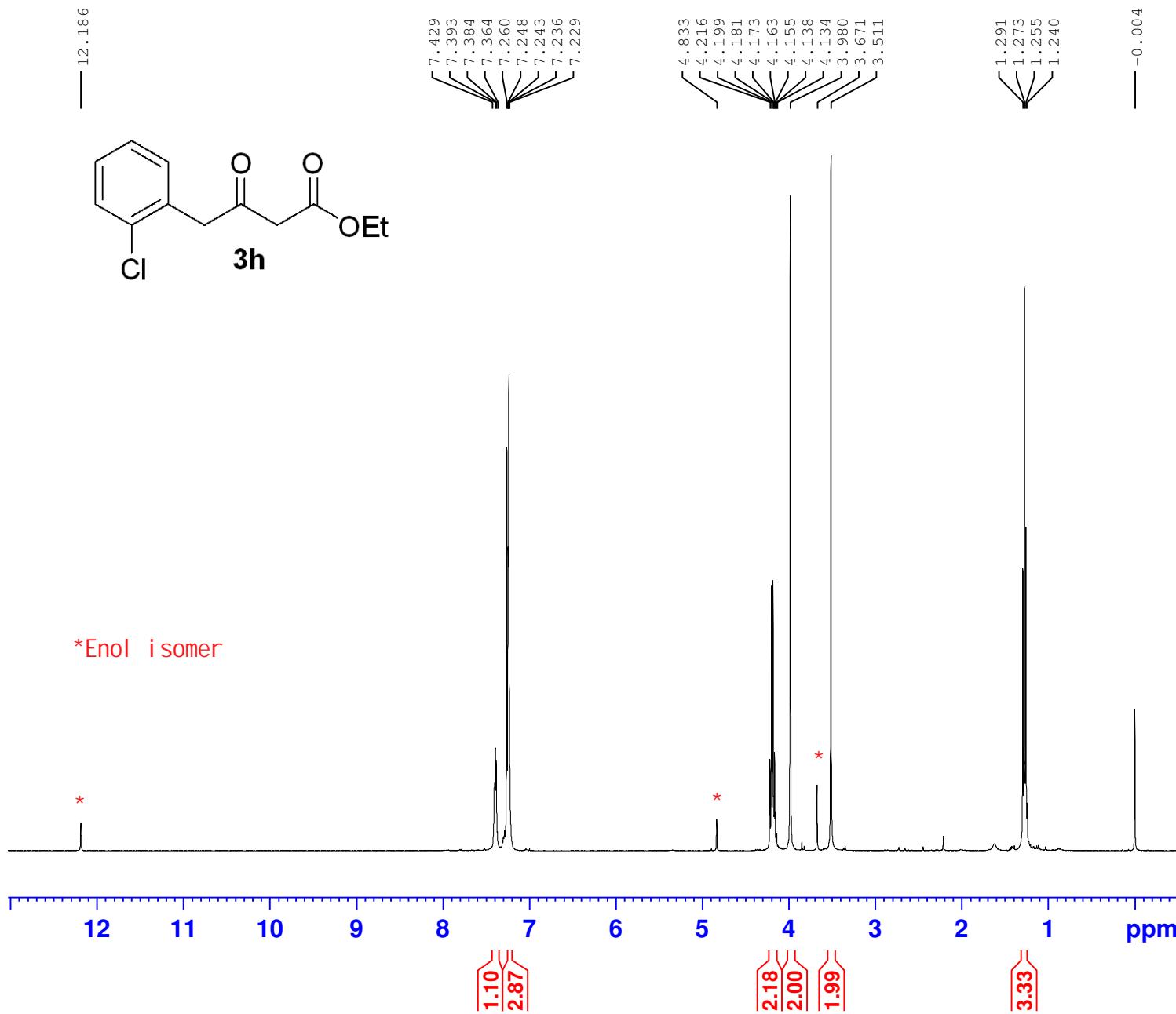
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
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WDW
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



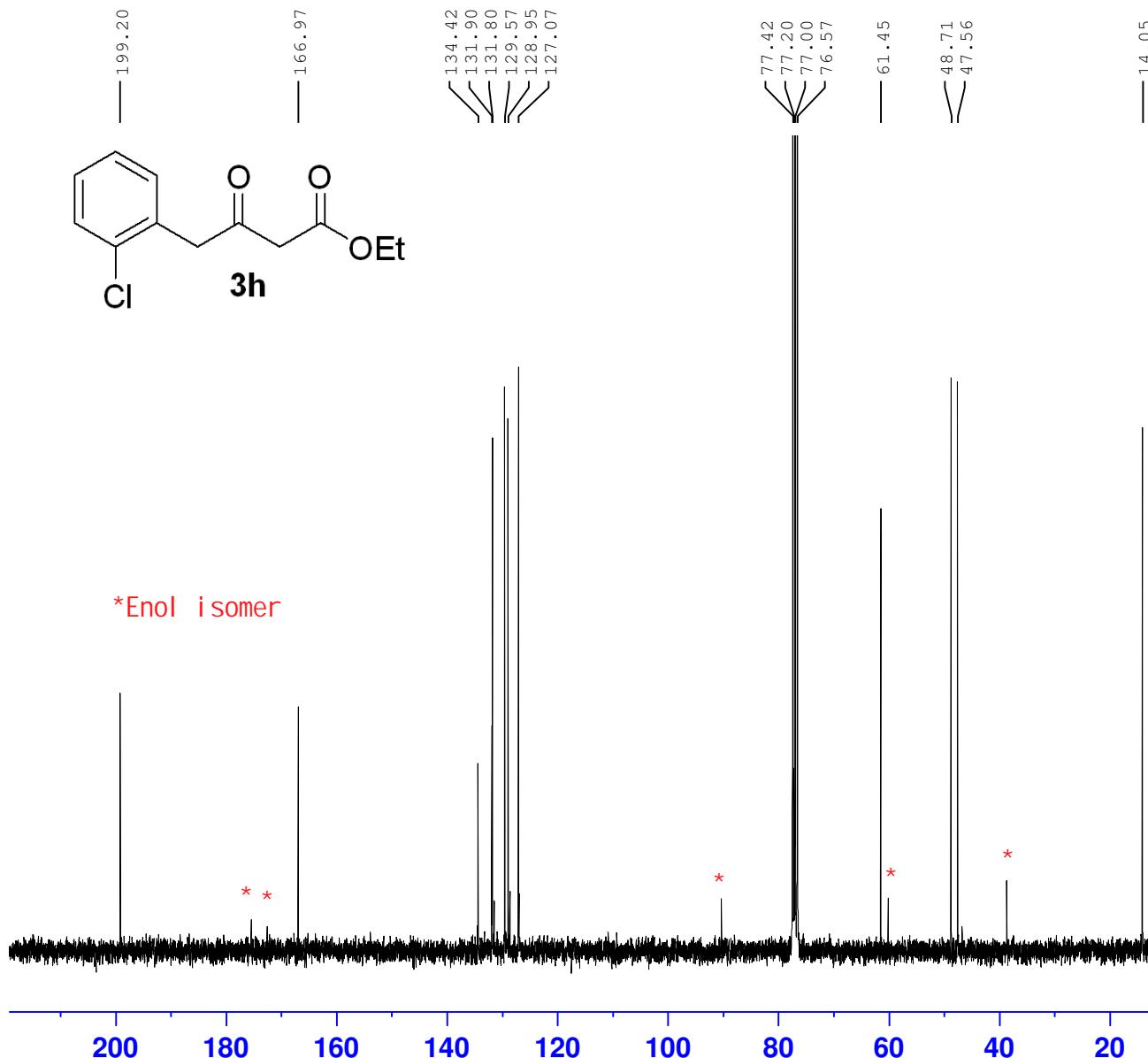
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 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 6
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 100.49
 DW 60.800 usec
 DE 6.50 usec
 TE 292.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.40 usec
 PLW1 14.00000000 W
 SFO1 400.1924713 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1900153 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

3sjwei 2504 zty-5-10i-c-fr 13c cdcl3



Current Data Parameters
NAME zty-5-10i-c-fr
EXPNO 1
PROCNO 1

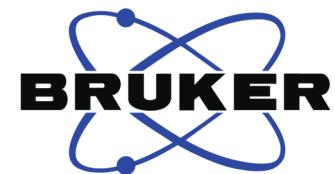
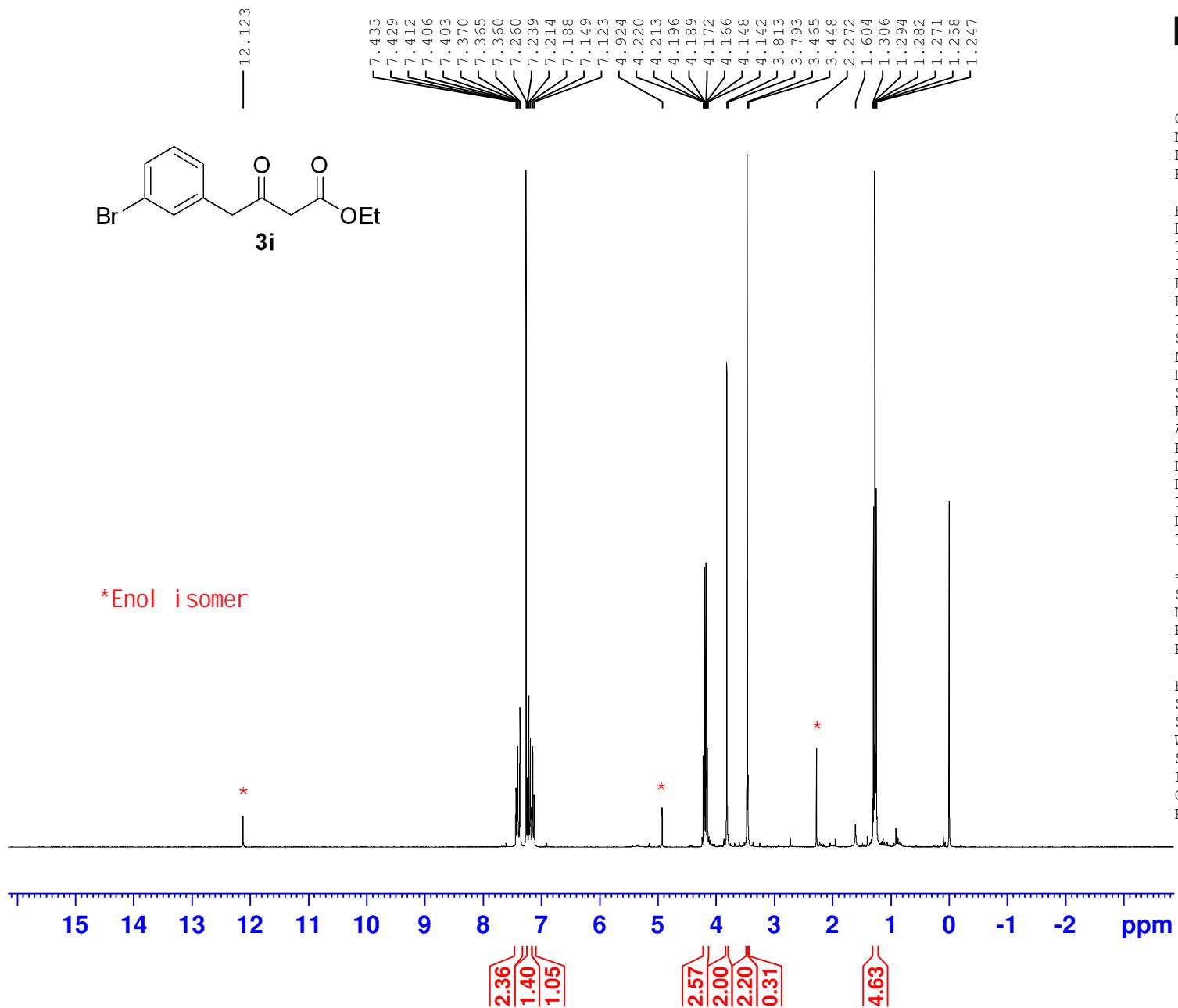
F2 - Acquisition Parameters
Date_ 20210114
Time 10.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 291.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677539 MHz
WDW
SSB 0 EM
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2565 zty-5-30-h 1h cdcl₃



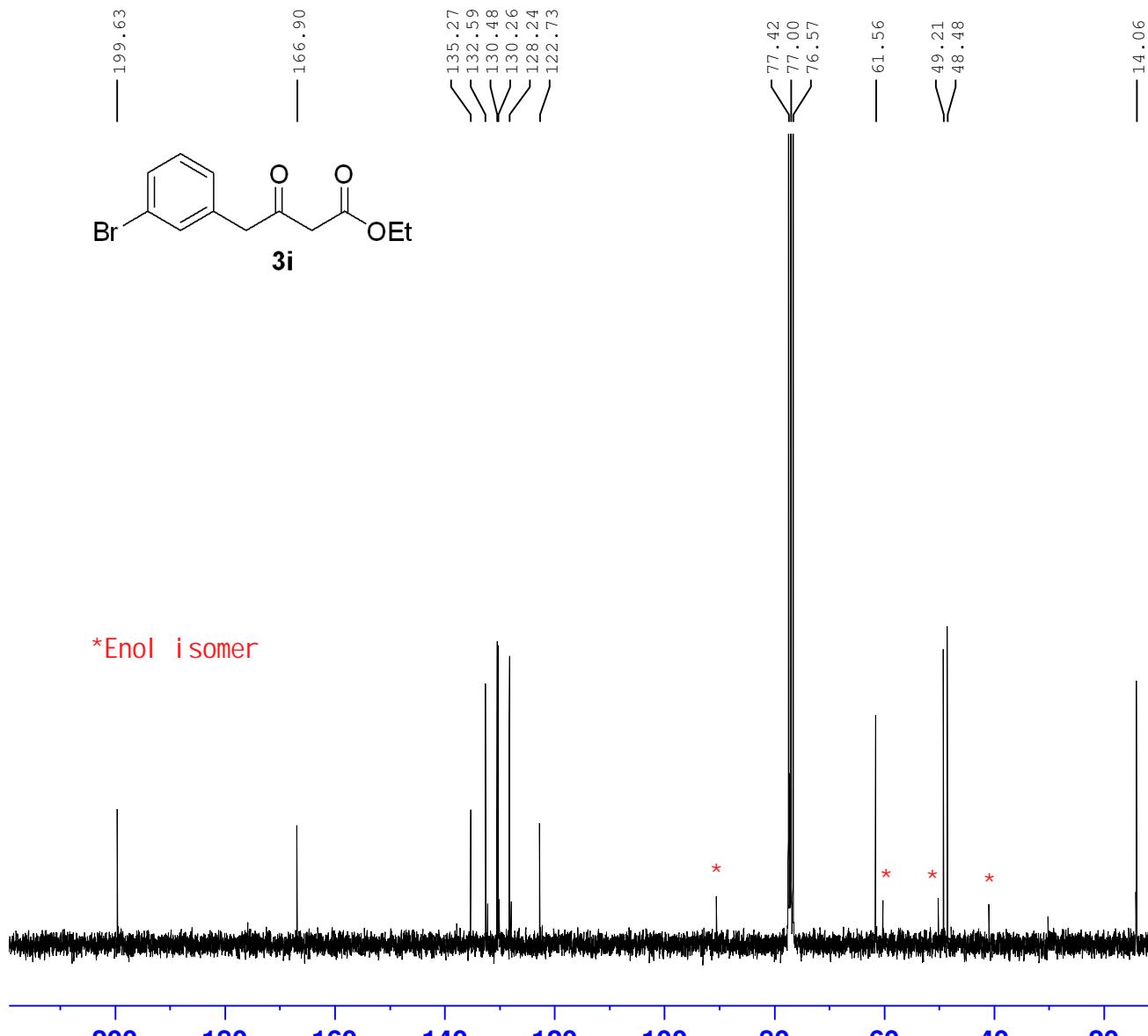
Current Data Parameters
NAME ZTY-5-30-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210119
Time 19.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 290.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2566 zty-5-30-c 13c cdc13



*Enol isomer



Current Data Parameters
NAME ZTY-5-30-c-fr
EXPNO 1
PROCNO 1

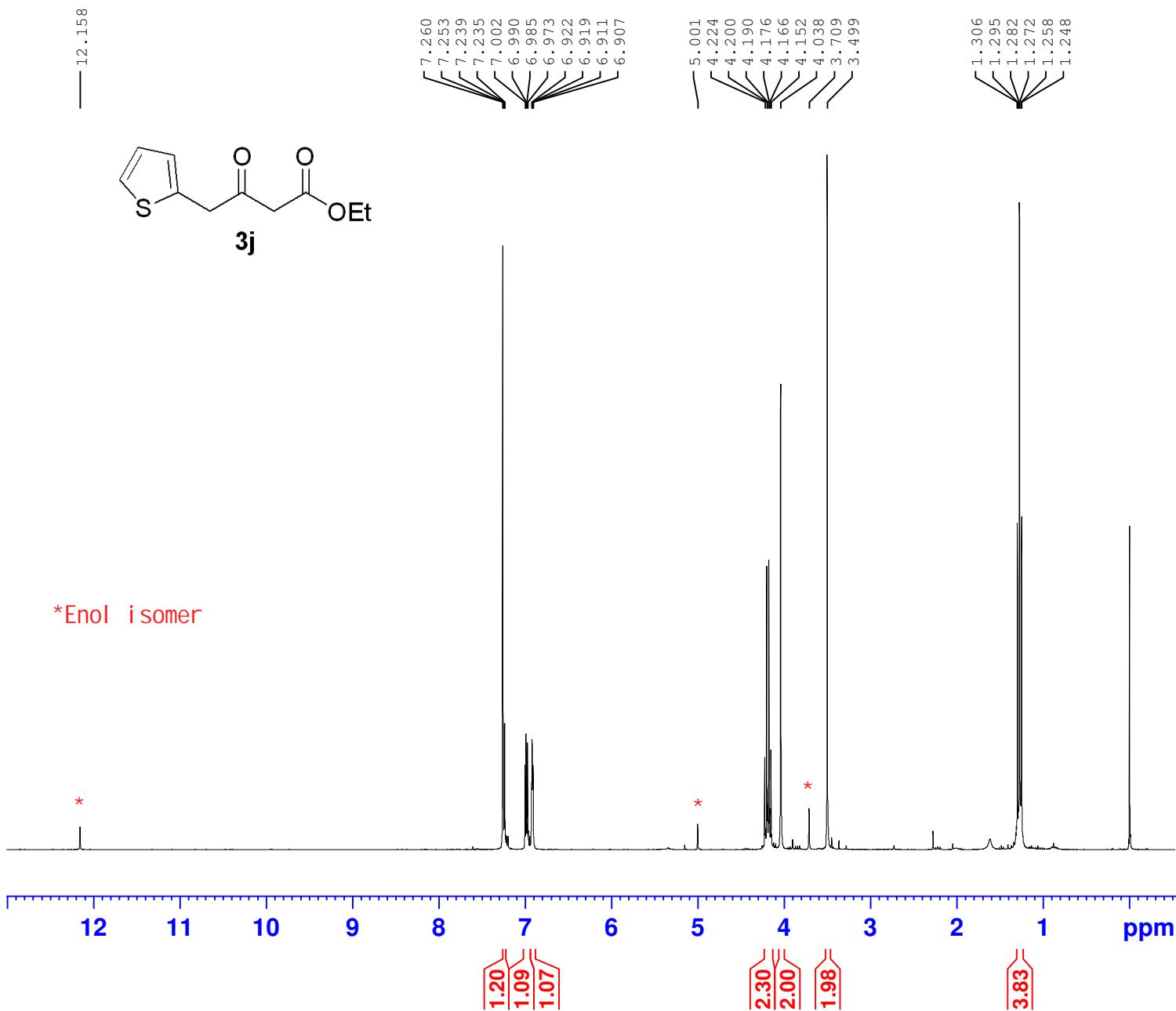
F2 - Acquisition Parameters
Date_ 20210119
Time 19.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 291.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677527 MHz
WDW
SSB 0 EM
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2511 zty-5-23-h 1h cdcl3



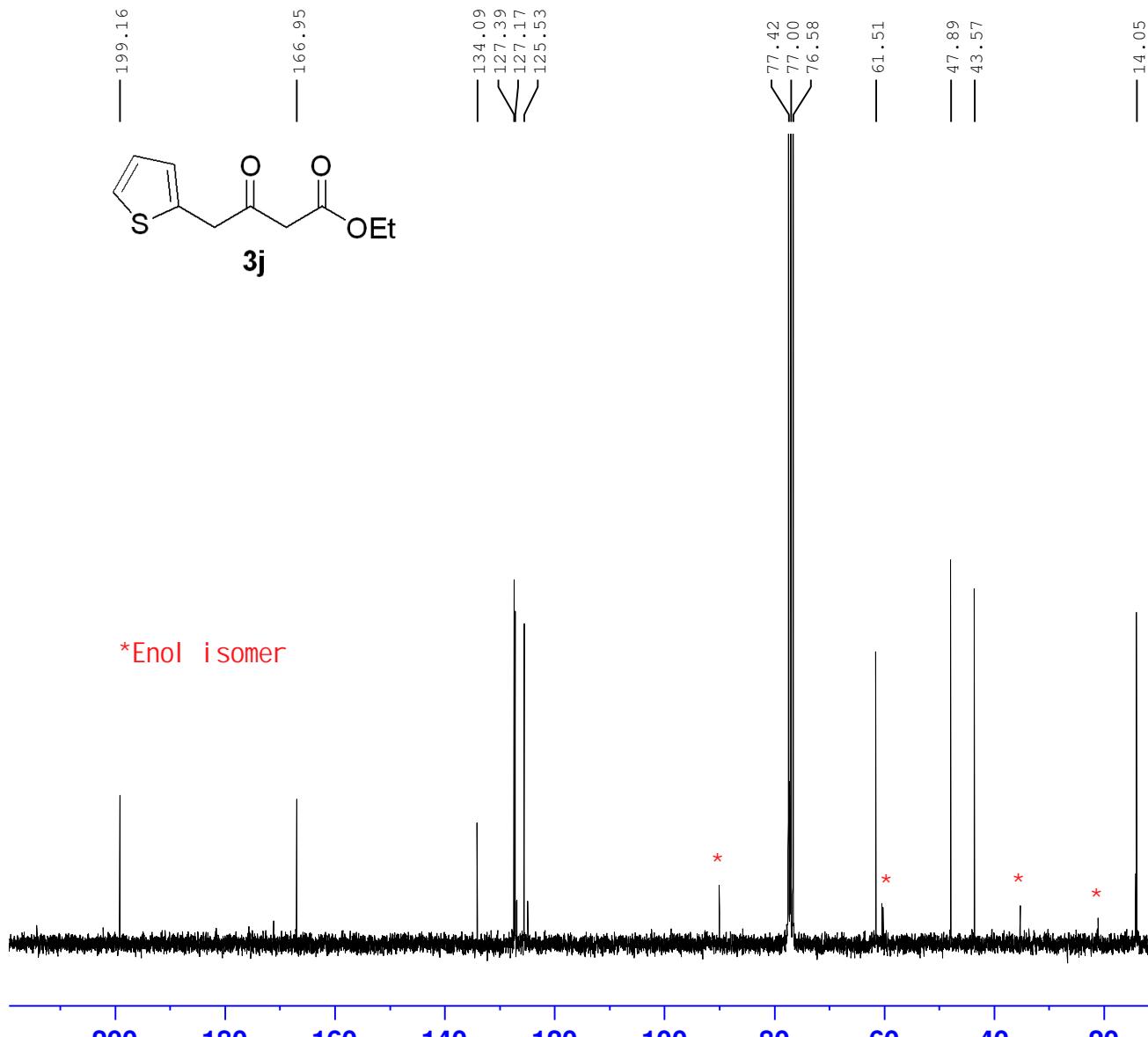
Current Data Parameters
NAME ZTY-5-23-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210115
Time 12.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2640 zty-5-23-c 13c cdcl3



Current Data Parameters
NAME ZTY-5-23-c-fr
EXPNO 1
PROCNO 1

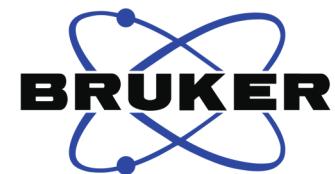
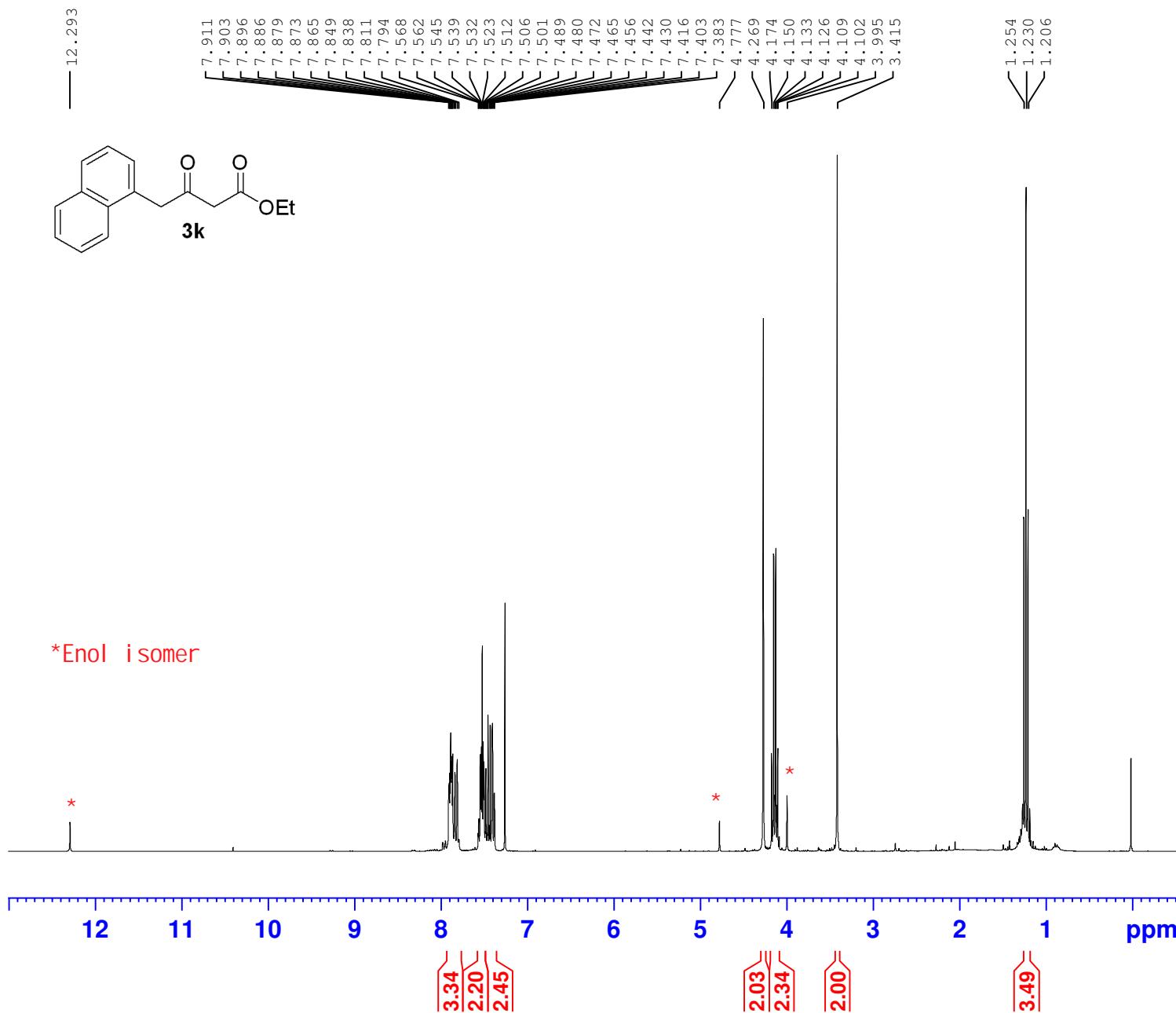
F2 - Acquisition Parameters
Date_ 20210123
Time 18.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 292.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677530 MHz
WDW
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2833 zty-5-10j 1h cdcl3



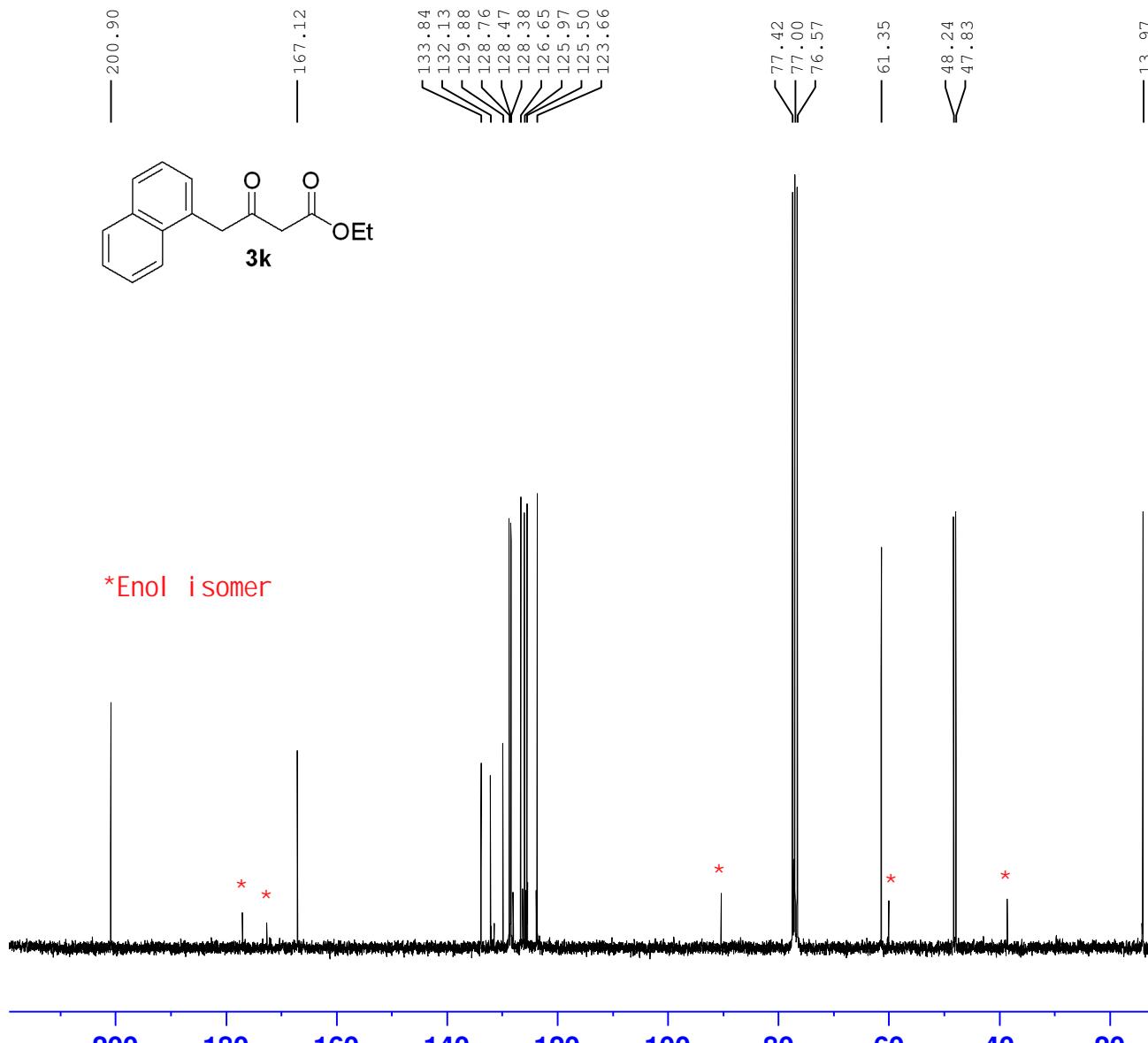
Current Data Parameters
NAME ZTY-5-10j-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210401
Time 1.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 90.5
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2834 zty-5-10j 13c cdcl3



Current Data Parameters
NAME ZTY-5-10j-c-fr
EXPNO 1
PROCNO 1

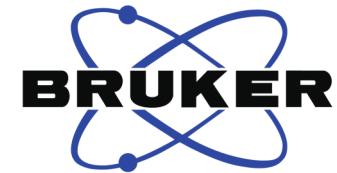
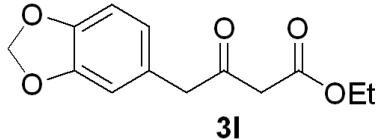
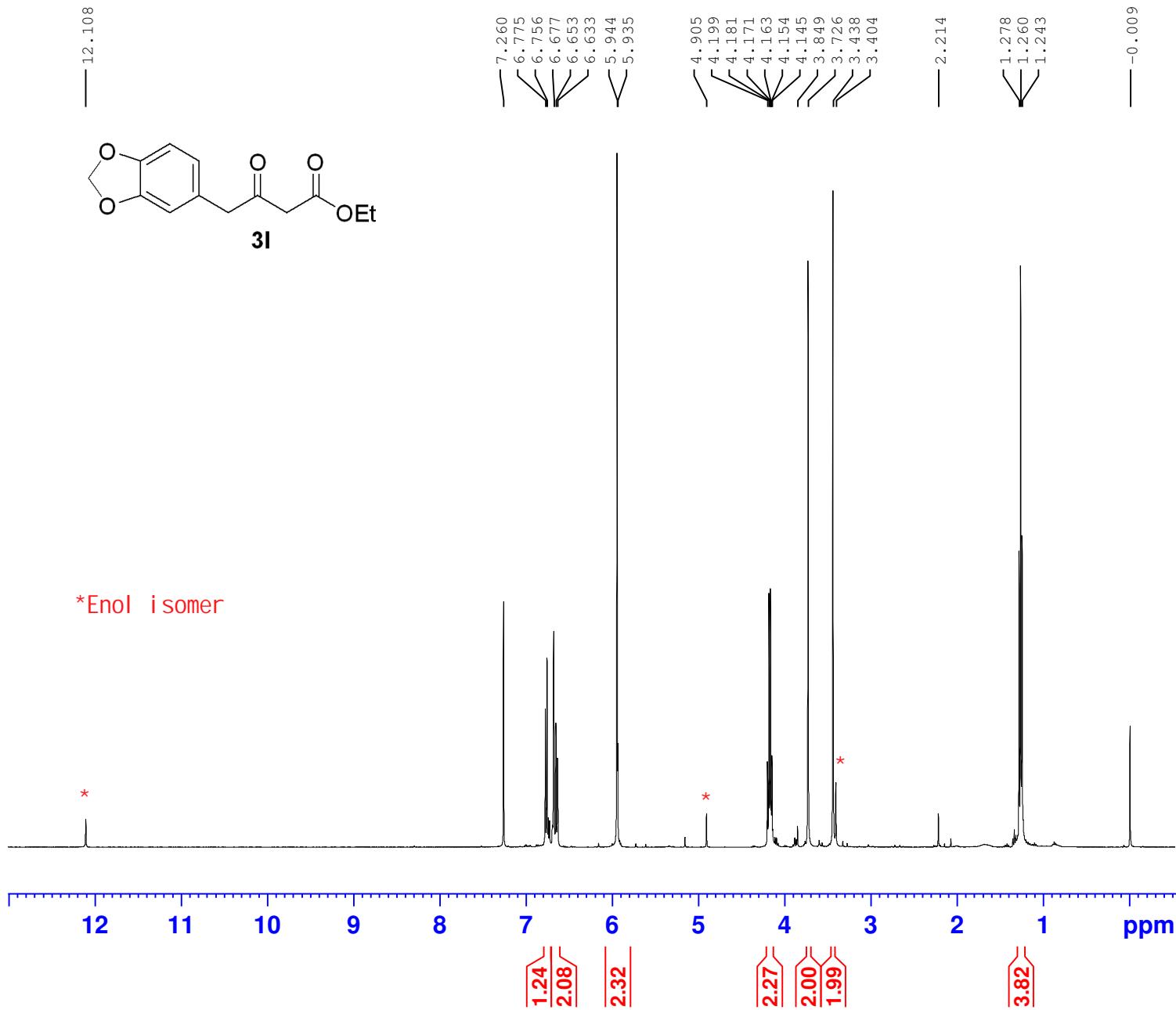
F2 - Acquisition Parameters
Date_ 20210401
Time 2.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677552 MHz
WDW
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4sunjianwei5/136 zty-5-20b-h



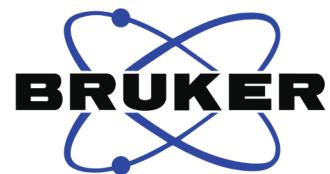
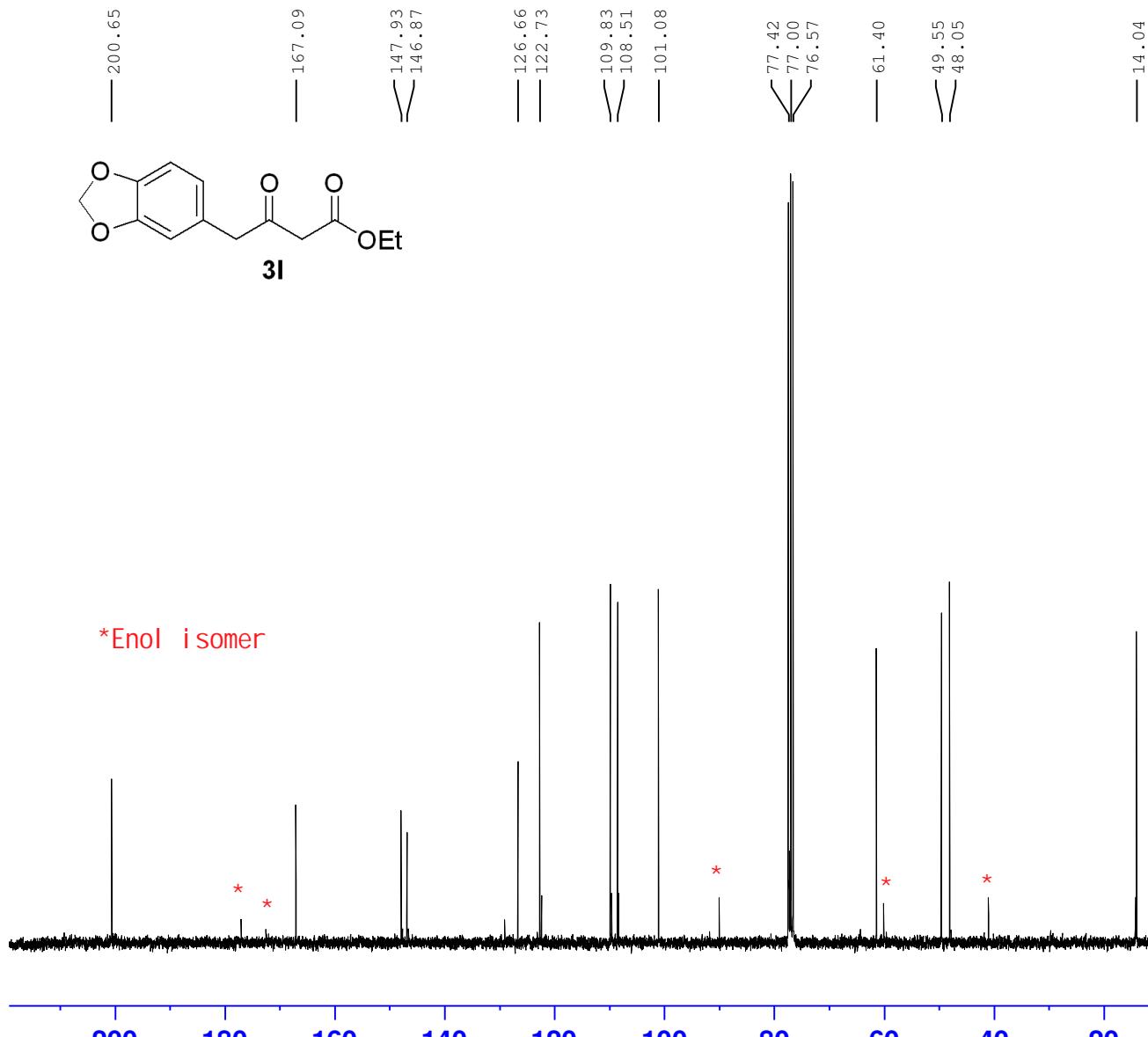
Current Data Parameters
NAME ZTY-5-20b-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210113
Time 14.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900154 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2506 zty-5-20b-c-fr 13c cdcl3



Current Data Parameters
NAME ZTY-5-20b-c-fr
EXPNO 1
PROCNO 1

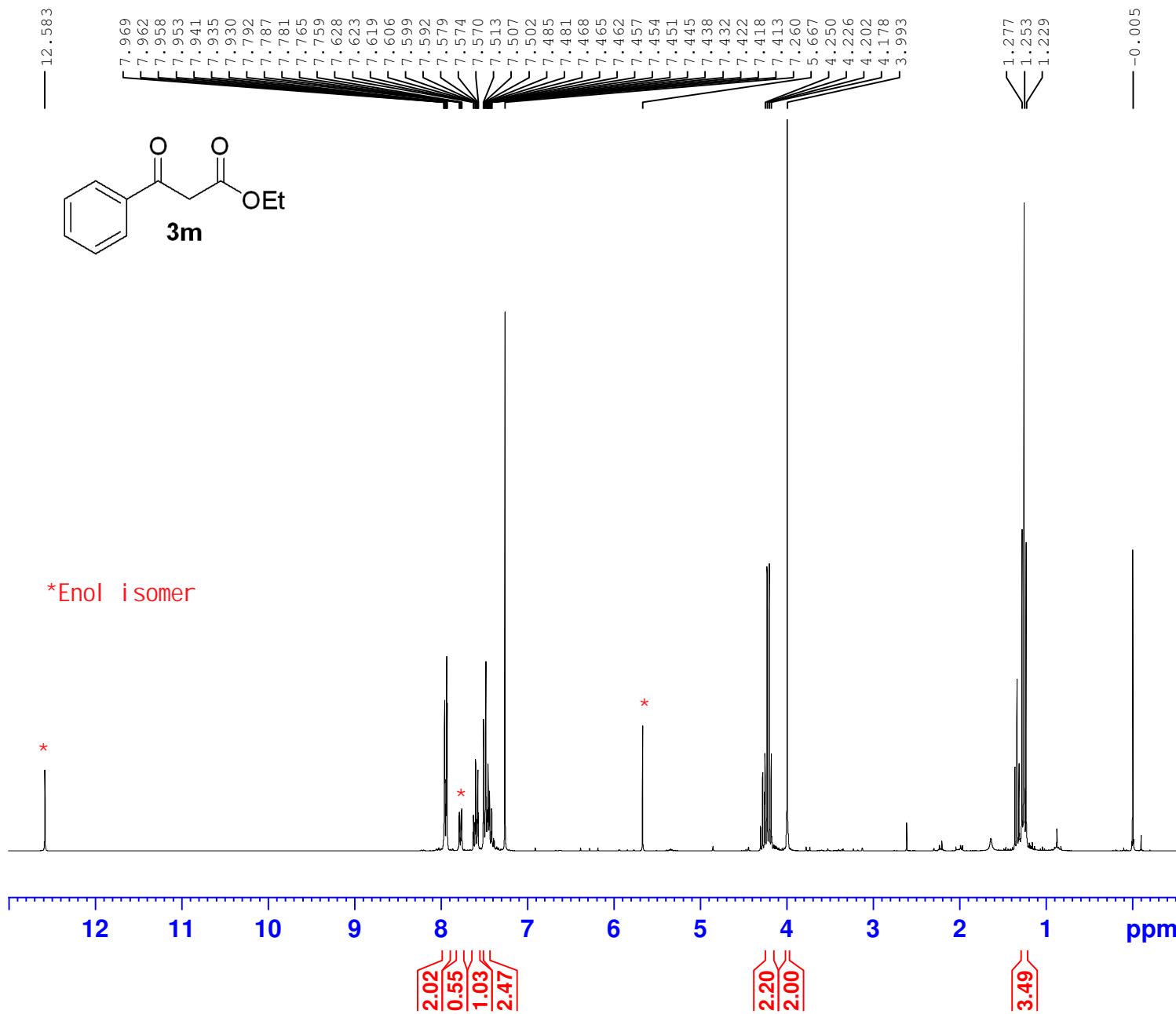
F2 - Acquisition Parameters
Date_ 20210114
Time 11.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 291.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677541 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 1762 zty-5-8a 1h cdcl3



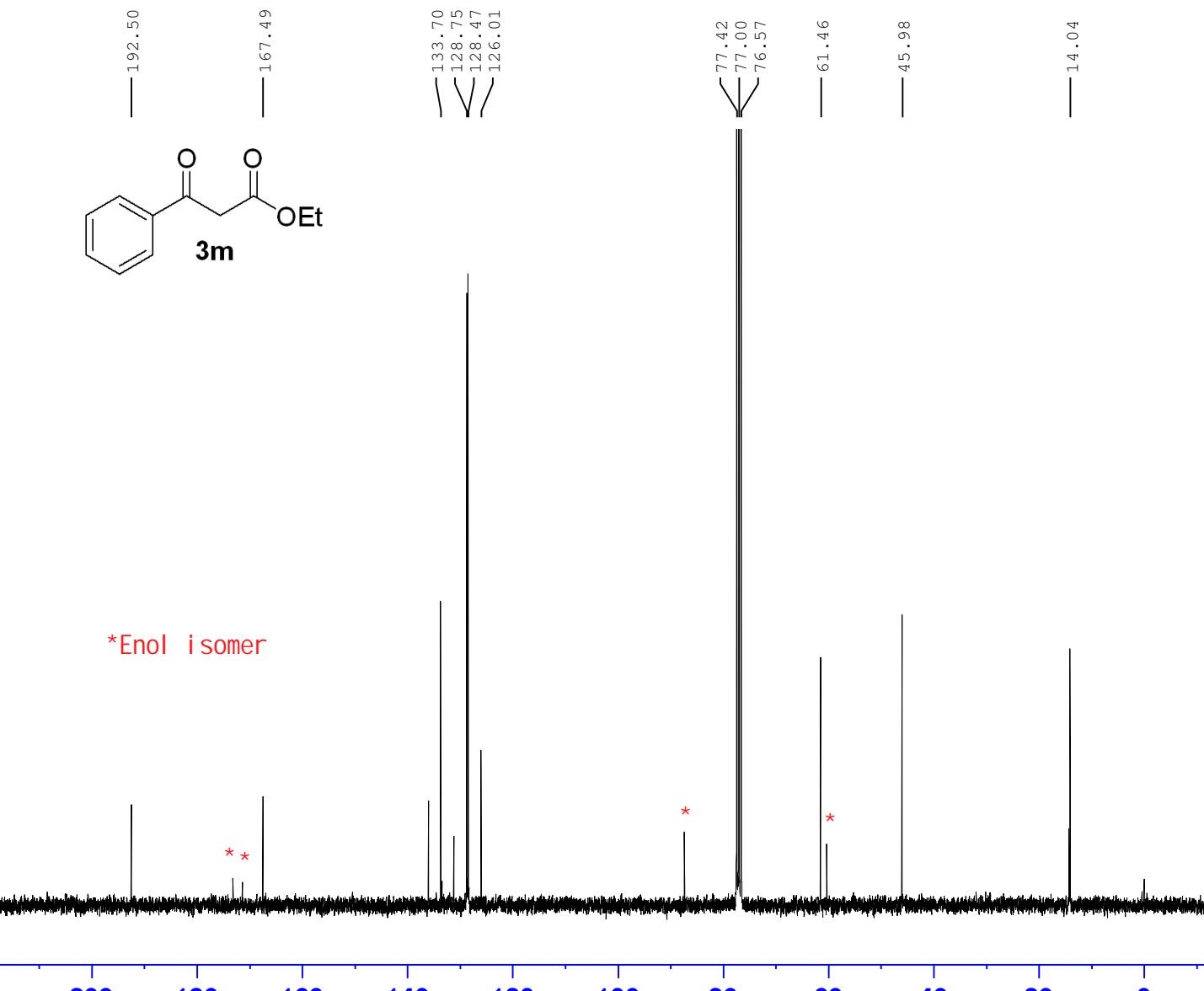
Current Data Parameters
NAME ZTY-5-8a-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201110
Time 20.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 304.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2836 zty-5-8a 13c cdcl3



Current Data Parameters
NAME ZTY-5-8a-c-fr
EXPNO 1
PROCNO 1

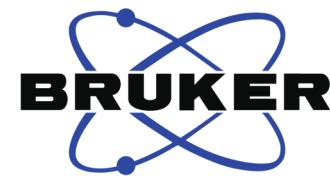
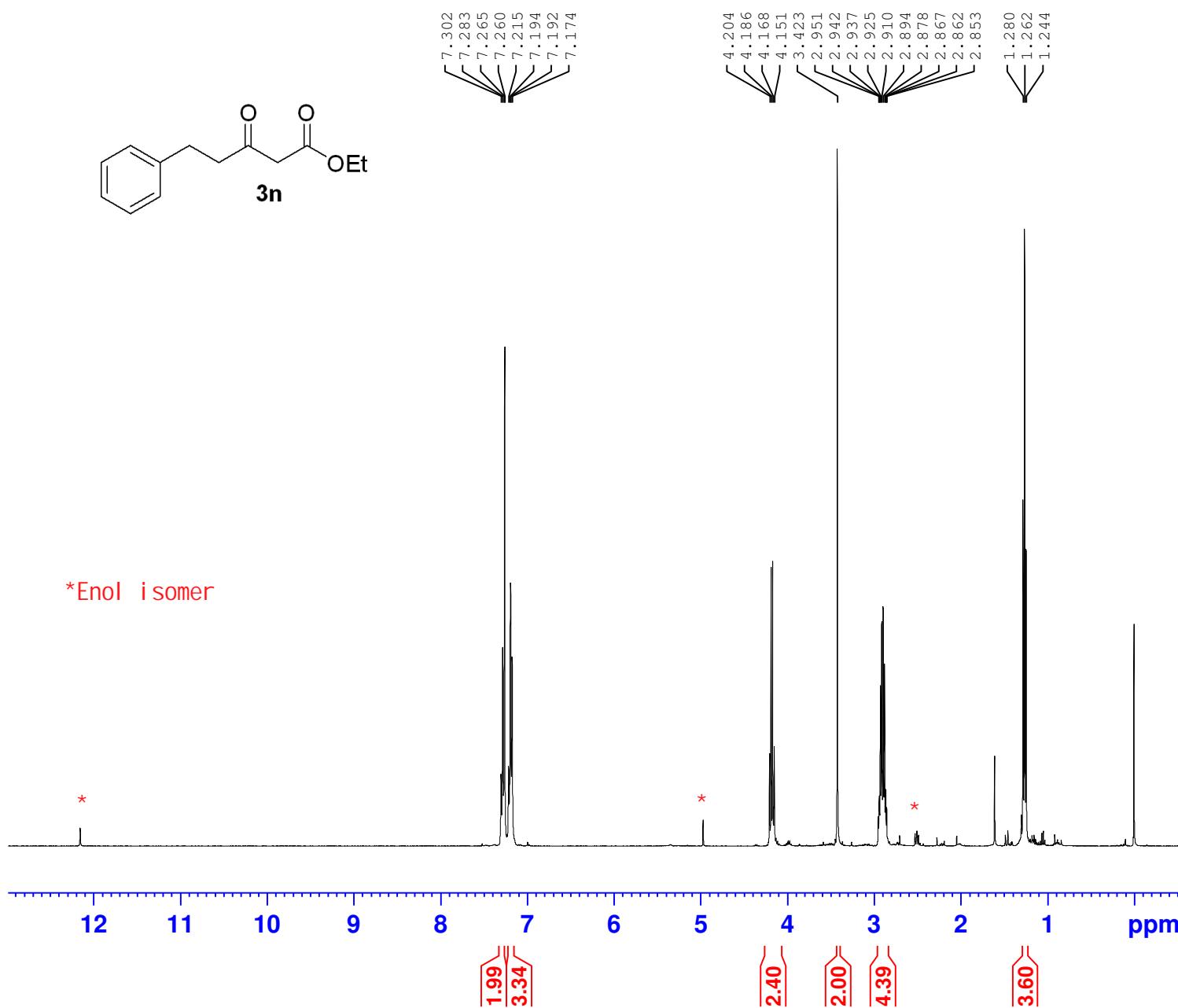
F2 - Acquisition Parameters
Date_ 20210401
Time 4.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677519 MHz
WDW
SSB 0 EM
LB 1.00 Hz
GB 0
PC 1.40

4sunjianwei5/23 zty-5-14-1



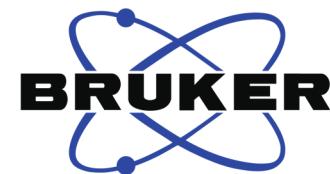
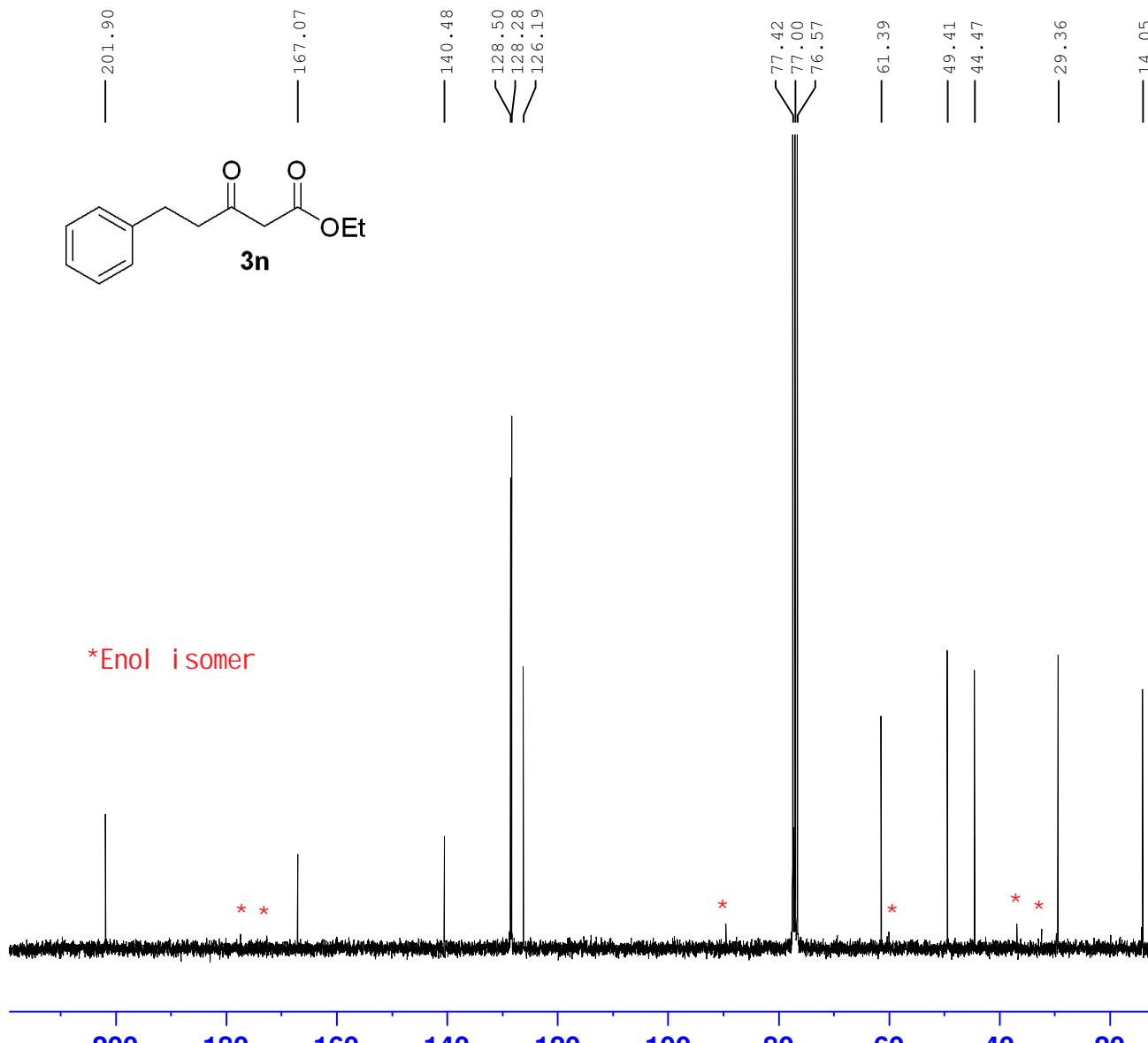
Current Data Parameters
NAME ZTY-5-14a-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201210
Time 14.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 294.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900154 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2394 zty-5-14a-1 13c cdcl3



Current Data Parameters
NAME ZTY-5-14a-c-fr
EXPNO 1
PROCNO 1

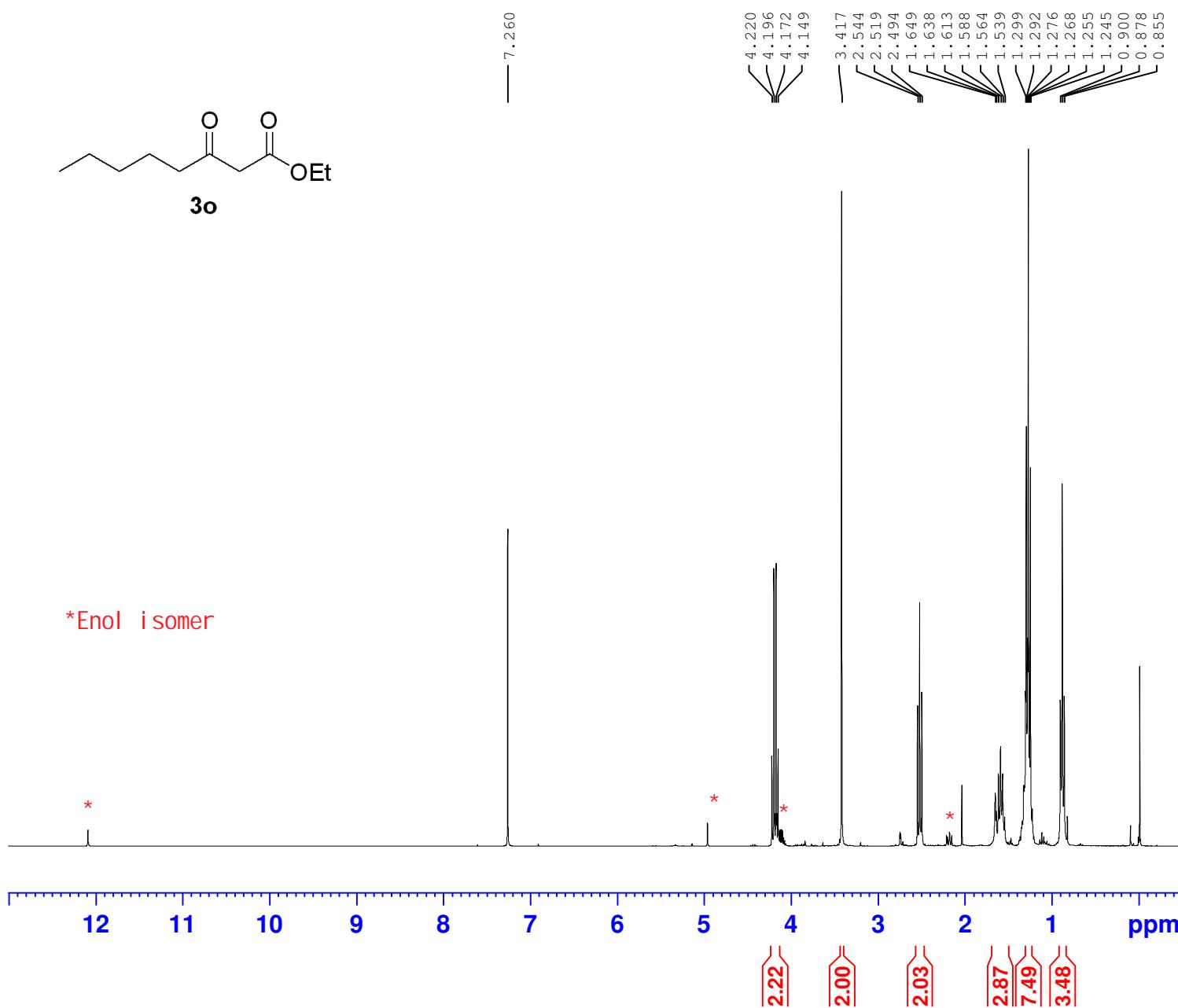
F2 - Acquisition Parameters
Date_ 20210105
Time 13.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677535 MHz
WDW
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 2773 zty-5-13c 1h cdcl3



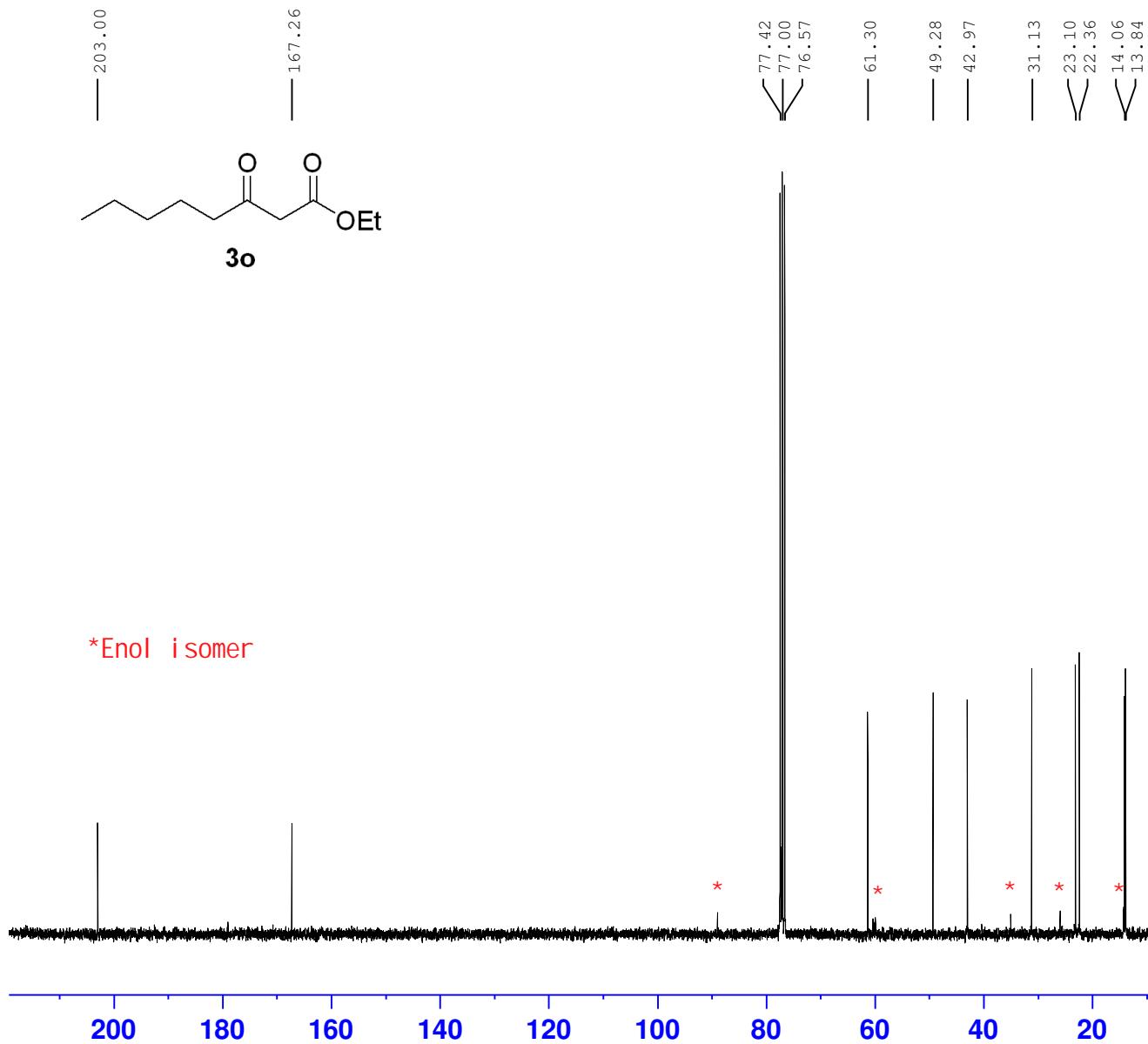
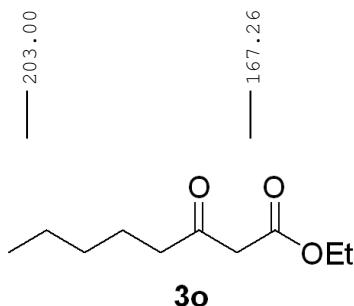
Current Data Parameters
NAME ZTY-5-13c-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210330
Time 1.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2774 zty-5-13c 13c cdcl3



Current Data Parameters
NAME ZTY-5-13c-c-fr
EXPNO 1
PROCNO 1

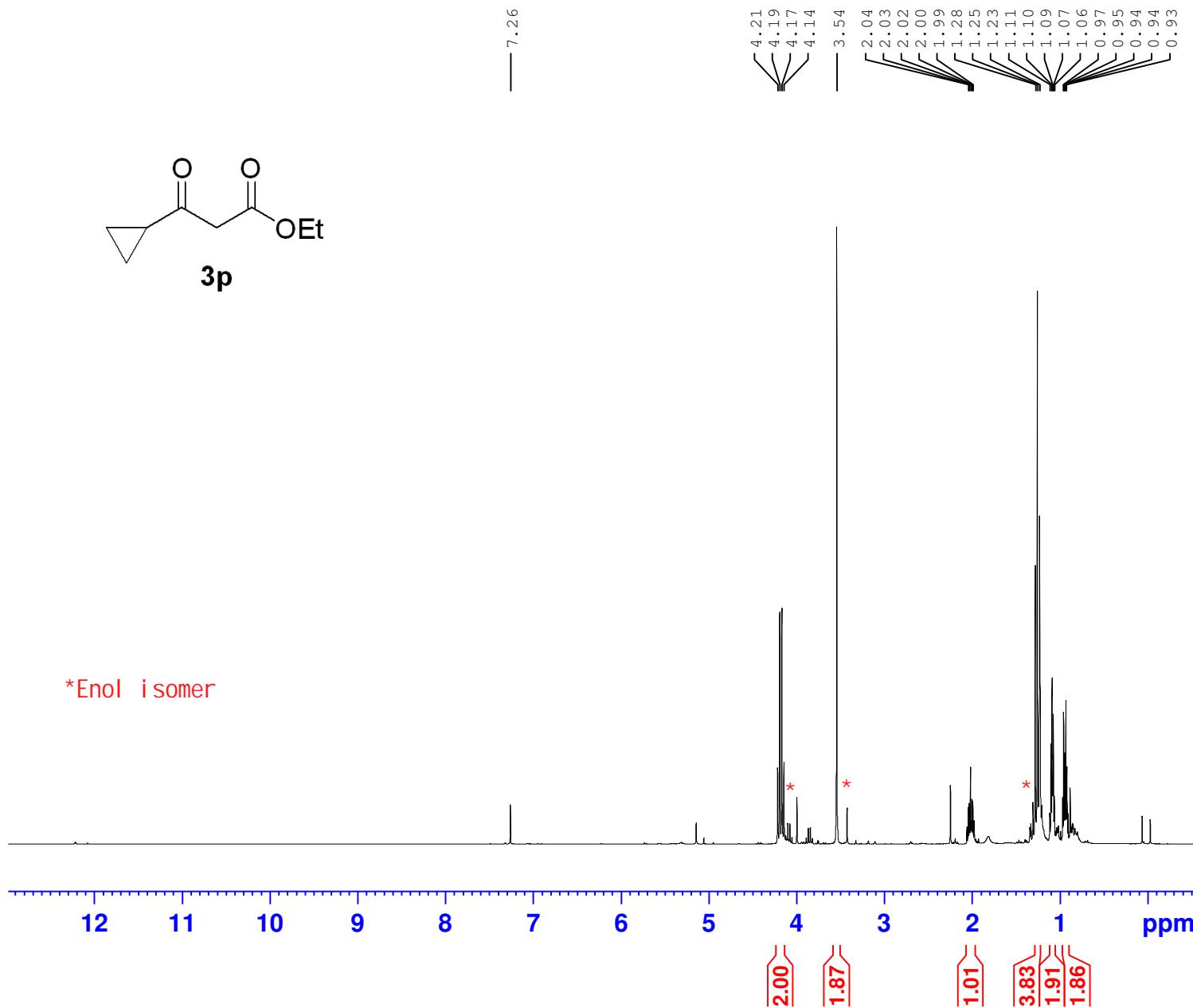
F2 - Acquisition Parameters
Date_ 20210330
Time 2.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5437 yzk-3-6-fr 1h cdcl3



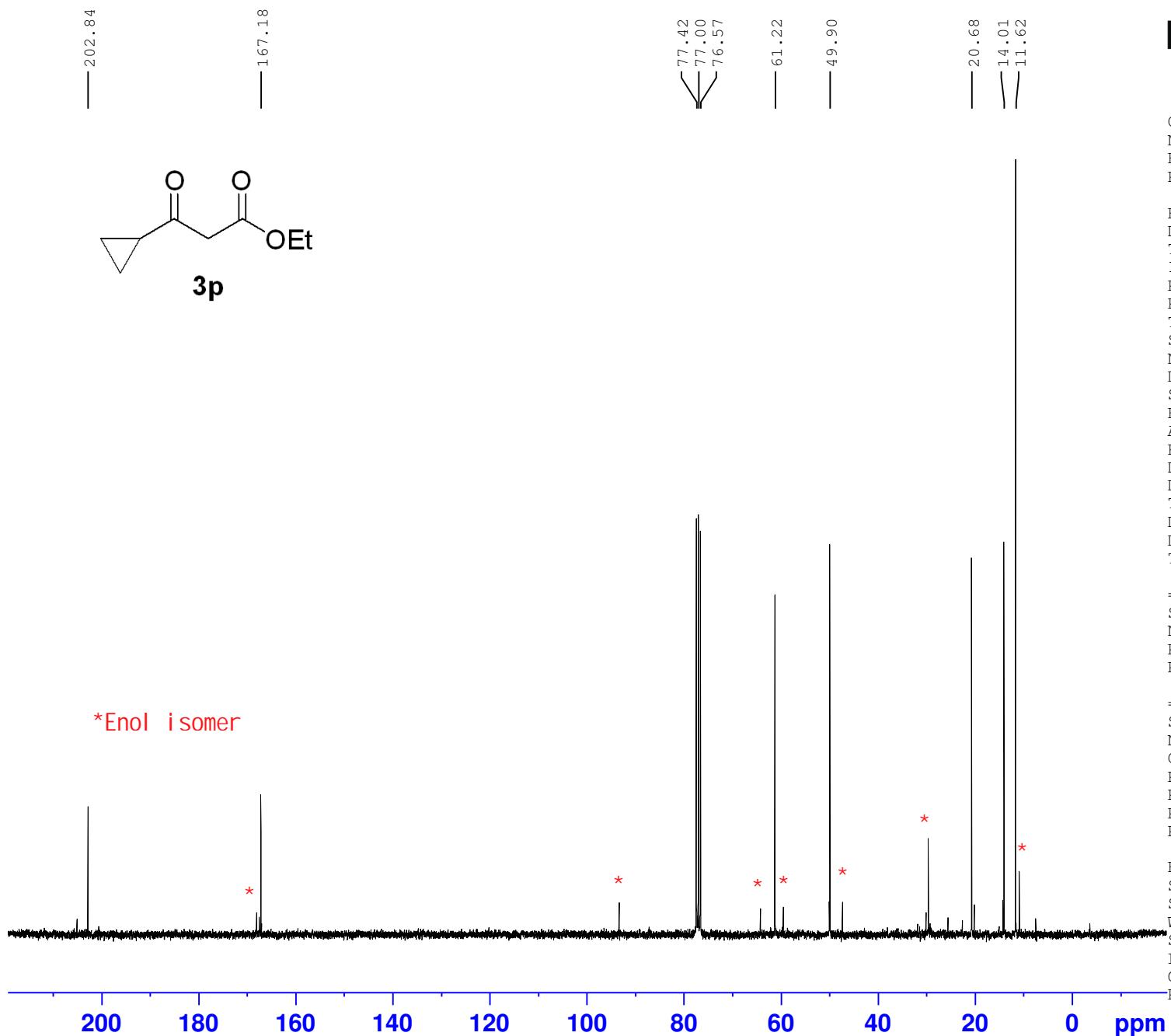
Current Data Parameters
NAME 5437a
EXPNO 5437
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210927
Time 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 71.8
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 5451 yzk-3-6-fr 13c cdcl3



Current Data Parameters
NAME 5451a
EXPNO 5451
PROCNO 1

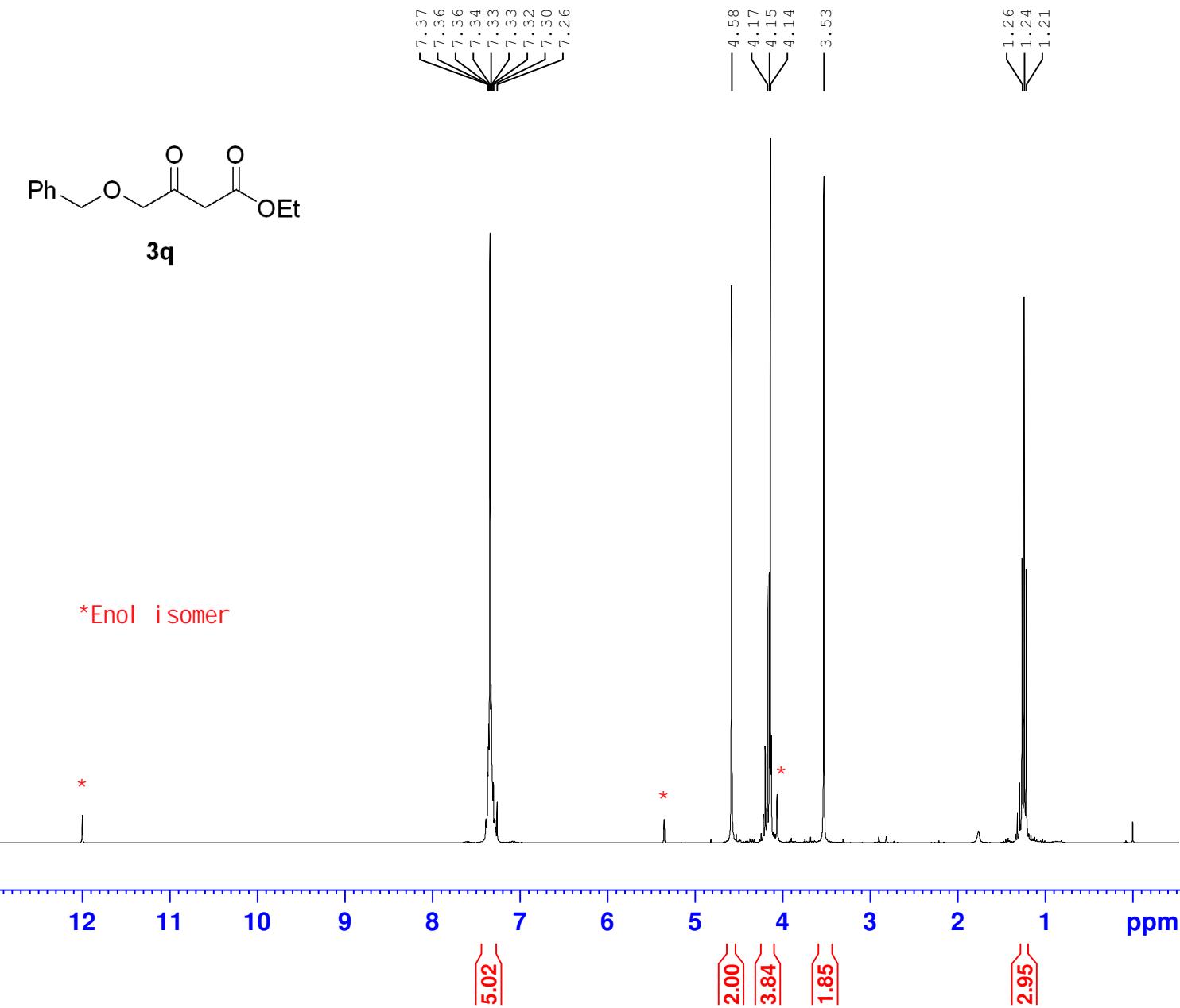
F2 - Acquisition Parameters
Date_ 20210928
Time 10.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 ^{13}C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677544 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5436 yzk-3-5-fr 1h cdcl3



Current Data Parameters
NAME 5436a
EXPNO 5436
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210927
Time 9.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 64
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

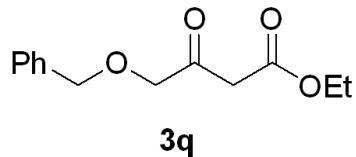
F2 - Processing parameters
SI 65536
SF 300.1300067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 5452 yzk-3-5-fr 13c cdcl3

— 201.63

— 166.90

— 136.82
— 128.44
— 128.00
— 127.75



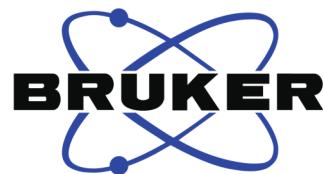
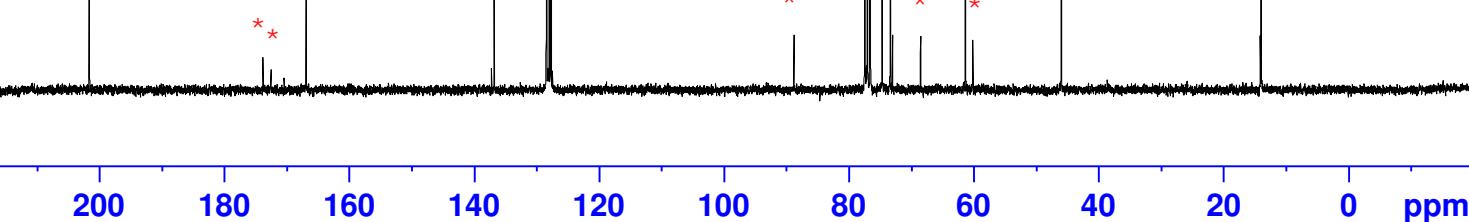
*Enol isomer

— 77.42
— 77.00
— 76.57
— 74.68
— 73.36

— 61.30

— 45.95

— 13.94



Current Data Parameters
NAME 5452a
EXPNO 5452
PROCNO 1

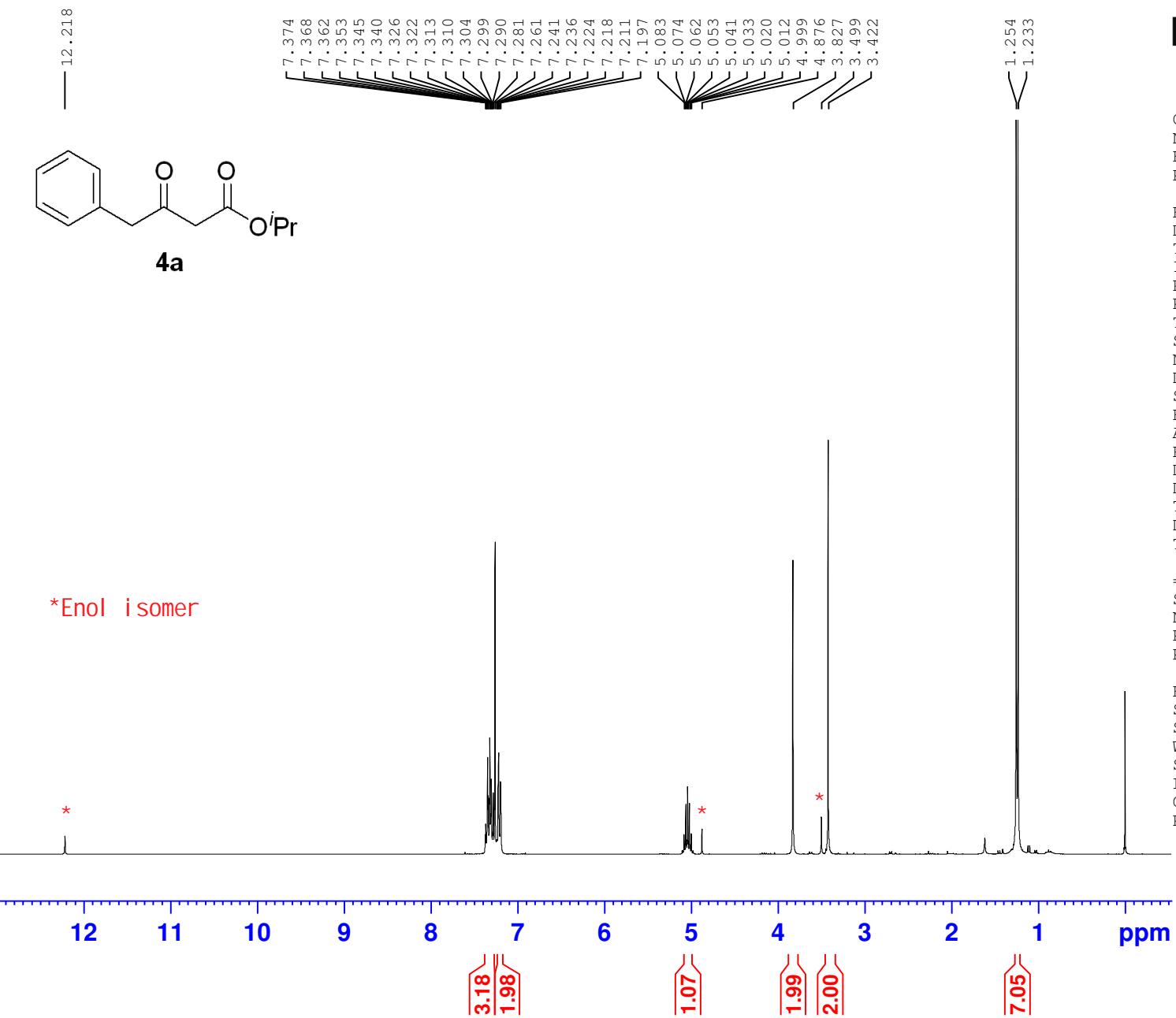
F2 - Acquisition Parameters
Date_ 20210928
Time 11.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677580 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 1761 zty-5-7b 1h cdcl3



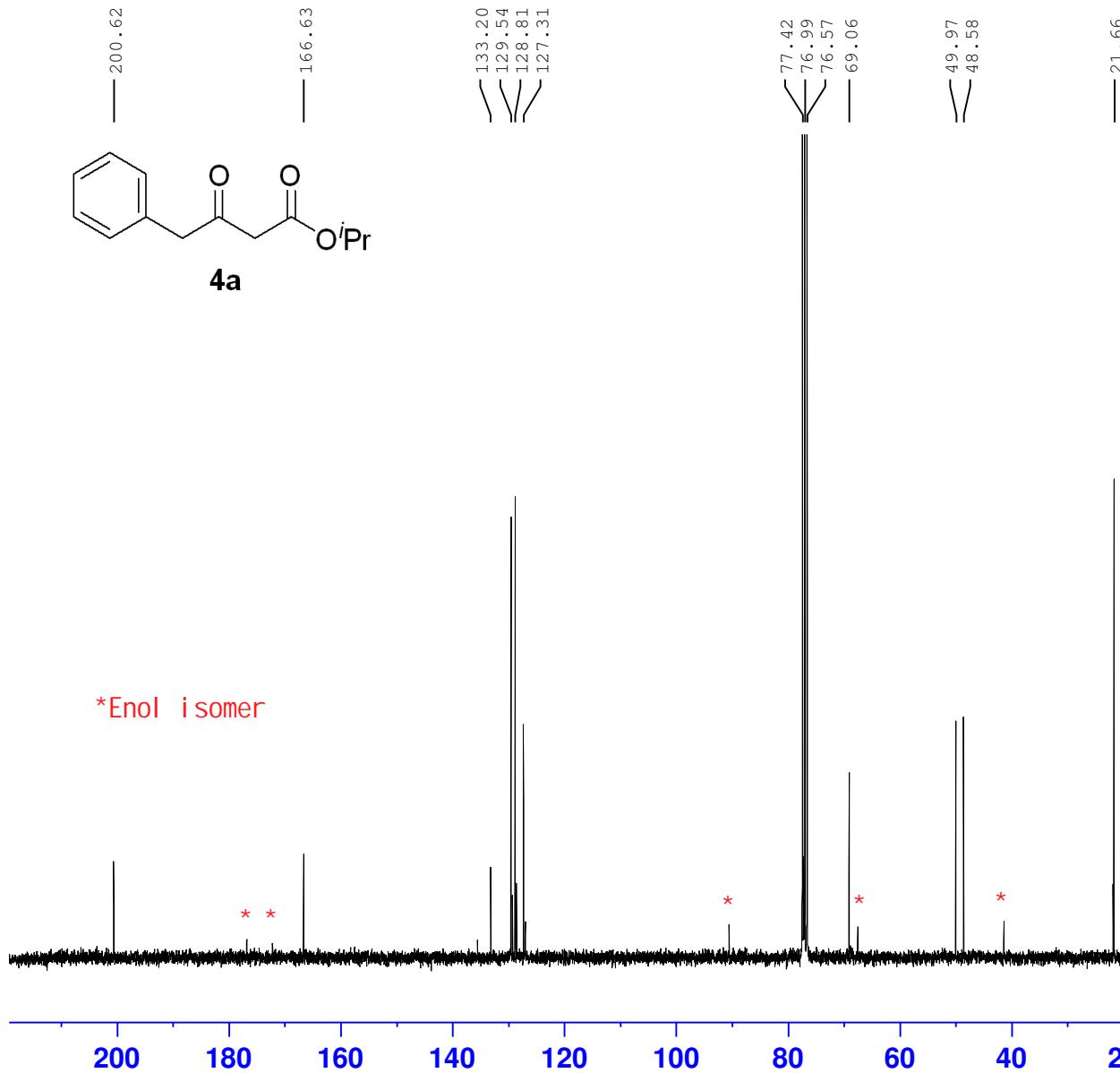
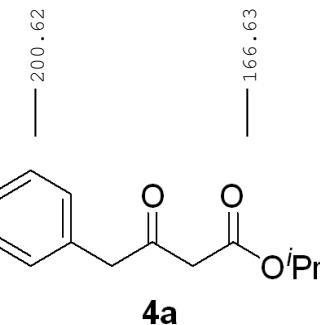
Current Data Parameters
NAME ZTY-5-7b-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201110
Time 20.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 304.5 K
D1 1.00000000 sec
TD0 1

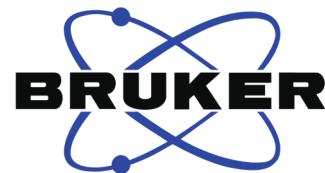
===== CHANNEL f1 ======
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2395 zty-5-7b 13c cdcl3



*Enol isomer



Current Data Parameters
NAME ZTY-5-7b-c-fr
EXPNO 1
PROCNO 1

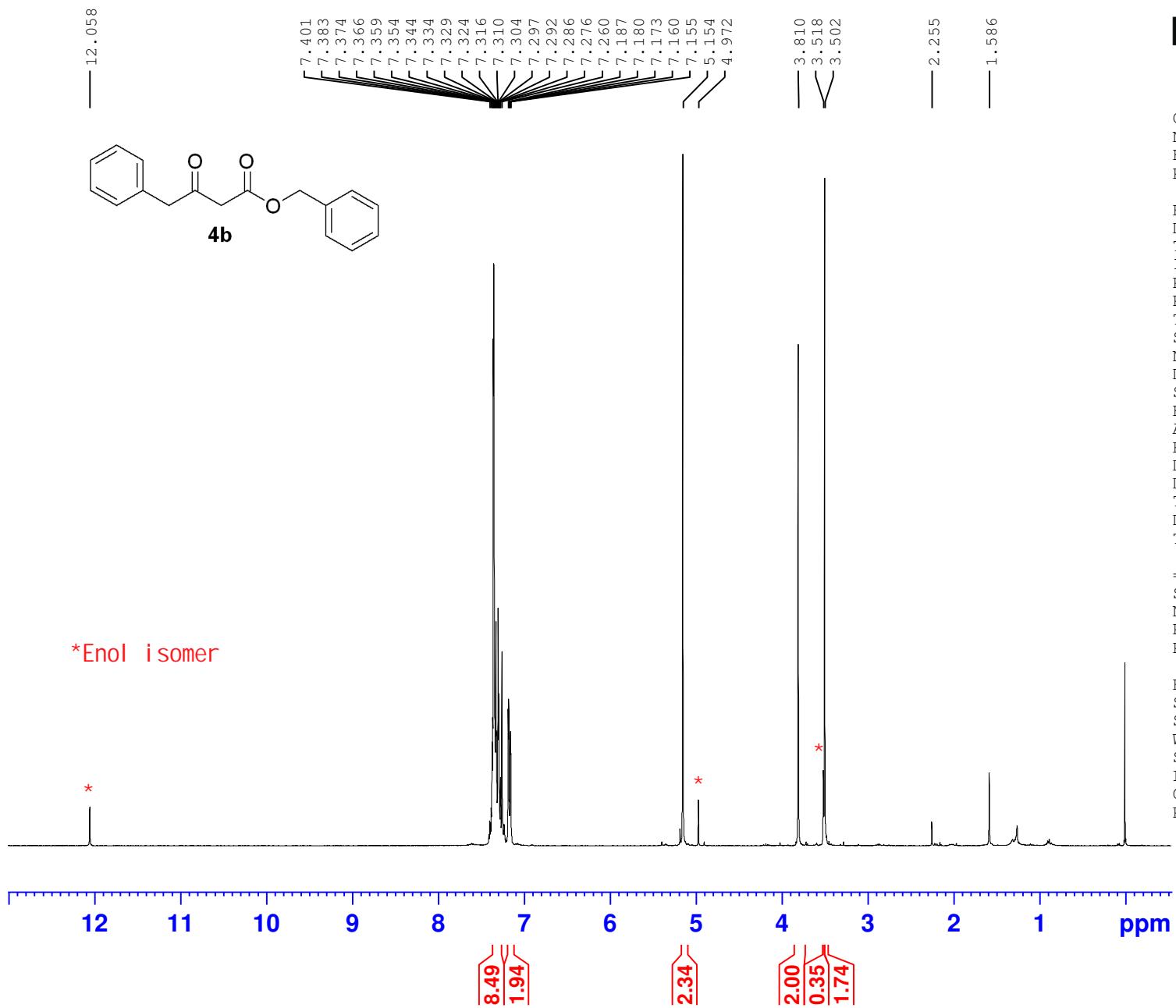
F2 - Acquisition Parameters
Date_ 20210105
Time 13.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 ======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677536 MHz
WDW
SSB 0 EM
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 1463 zty-5-6b 1h cdcl3



Current Data Parameters
NAME ZTY-5-6b-h-fr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201024
Time 18.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE 293.4 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 2396 zty-5-6b 13c cdcl3

