DDQ-promoted Direct C5-alkylation of Oxazole with Alkylboronic Acids via Palladium-catalyzed C-H Bond Activation

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Supporting Information

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General Remarks

All commercially available compounds were purchased from Sigma-Aldrich, Alfa-Aesar, Acros, J&K Chemicals, Adamas and Aladdin Chemicals. Palladium(II) diacetate were purchased from Acros (99.9% purity, CAS No. 3375-31-3). Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. Oxazole-4-carboxylic derivatives **1a-1p** were prepared from corresponding nitriles by our previous reported methods[1]. 2,4-Diphenyloxazole **1q** was prepared using the method in literature.[2] Products were purified by flash chromatography on silica gel using petroleum ether and ethyl acetate as the effluent. Melting point (m.p.) was measured on a microscopic melting point apparatus. ^{1}H-NMR spectra were recorded on Bruker AVANCE III-400 spectrometers. Chemical shifts (in ppm) were referenced with TMS in $CDCl_3$ (0 ppm). ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.00 ppm). High resolution mass spectra were obtained from an Agilent QTOF 6520 mass spectrometer with electron spray ionization (ESI) as the ion source.

References

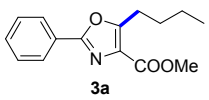
[1] For the preparation of various oxazole-4-carboxylic derivative substrates, see: (a) Huang, Y.; Gan, H.; Li, S.; Xu, J.; Wu, X.; Yao, H. *Tetrahedron Lett.* **2010**, *51*, 1751. (b) Huang, Y.; Ni, L.; Gan, H.; He, Y.; Xu, J.; Wu, X.; Yao, H. *Tetrahedron* **2011**, *67*, 2066. (c) Wang, Y.; Li, Z.; Huang, Y.; Tang, C.; Wu, X.; Xu, J.; Yao, H. *Tetrahedron* **2011**, *67*, 7406.

[2] For the preparation of various 2,4-diphenyloxazole, see: (a) Liu, L.; Feng, S.; Li, C. *ACS Sustainable Chem. Eng.* **2016**, *4*, 6754.

Experimental Procedure and Characterization Data

Typical Procedure: To a reaction tube charged with $Pd(OAc)_2$ (6.7 mg, 0.03 mmol, 10 mol%), AgOAc (200 mg, 1.2 mmol, 4 eq), DDQ (34 mg, 0.15 mmol, 0.5 eq), alkylboronic acid **2** (1.2 mmol, 4 eq) was added a solution of oxazole **1** (0.3 mmol, 1 equiv) in ethylbenzene (1 mL) and acetic acid (1 mL). The reaction mixture was then stirred at 120 °C for 24 hours. After cooling to room temperature, the mixture was diluted with ethyl acetate, washed with saturated sodium bicarbonate, water and brine, dried over anhydrous sodium sulfate, and concentrated *in vacuo* to give dark residue, which was purified by flash chromatography (using petroleum ether and ethyl acetate as the effluent) on silica gel to afford the C5-alkylated oxazole **3a** – **3y**.

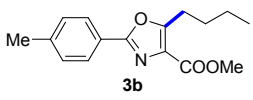
Methyl 5-*n*-Butyl-2-phenyloxazole-4-carboxylate (3a):



3a

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 80% of **3a** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.46-7.44 (m, 3H), 3.95 (s, 3H), 3.12 (t, 2H, *J* = 7.6 Hz), 1.75 (p, 2H, *J* = 7.6 Hz), 1.43 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 160.3, 159.6, 130.7, 128.7, 128.0, 126.6, 126.5, 51.9, 29.8, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{17}NO_3+H]^+$ 260.1287, found 260.1282.

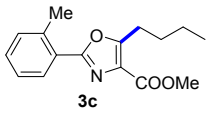
Methyl 5-*n*-Butyl-2-(4-methylphenyl)oxazole-4-carboxylate (3b):



3b

The reaction of 0.3 mmol of methyl 2-(4-methylphenyl)oxazole-4-carboxylate (**1b**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 81% of **3b** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1 to 15:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 63-65 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 7.96 (d, 2H, *J* = 8.4 Hz), 7.26 (d, 2H, *J* = 8.4 Hz), 3.94 (s, 3H), 3.11 (t, 2H, *J* = 7.2 Hz), 2.40 (s, 3H), 1.74 (p, 2H, *J* = 7.2 Hz), 1.43 (h, 2H, *J* = 7.2 Hz), 0.96 (t, 3H, *J* = 7.2 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 160.0, 159.8, 141.0, 129.3, 127.9, 126.5, 123.9, 51.8, 29.8, 25.7, 22.2, 21.4, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{19}NO_3+H]^+$ 274.1443, found 274.1439.

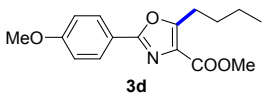
Methyl 5-*n*-Butyl-2-(2-methylphenyl)oxazole-4-carboxylate (3c):



3c

The reaction of 0.3 mmol of methyl 2-(2-methylphenyl)oxazole-4-carboxylate (**1c**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 75% of **3c** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1 to 15:1, *v*/*v*) as the effluent. Colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.00-7.97 (m, 1H), 7.37-7.33 (m, 1H), 7.29-7.27 (m, 2H), 3.94 (s, 3H), 3.13 (t, 2H, *J* = 7.2 Hz), 2.67 (s, 3H), 1.75 (p, 2H, *J* = 7.2 Hz), 1.43 (h, 2H, *J* = 7.2 Hz), 0.96 (t, 3H, *J* = 7.2 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.9, 160.1, 160.0, 137.4, 131.5, 130.3, 129.2, 127.8, 125.9, 125.8, 51.8, 29.8, 25.6, 22.2, 21.7, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{19}NO_3+Na]^+$ 296.1263, found 296.1265.

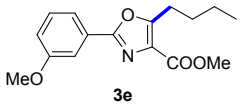
Methyl 5-*n*-Butyl-2-(4-methoxylphenyl)oxazole-4-carboxylate (3d):



3d

The reaction of 0.3 mmol of methyl 2-(4-methoxylphenyl)oxazole-4-carboxylate (**1d**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 71% of **3c** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1 to 15:1, *v*/*v*) as the effluent. Light yellow solid, m.p. 66-68 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.01 (d, 2H, *J* = 8.4 Hz), 6.96 (d, 2H, *J* = 8.4 Hz), 3.94 (s, 3H), 3.85 (s, 3H), 3.10 (t, 2H, *J* = 7.2 Hz), 1.73 (p, 2H, *J* = 7.2 Hz), 1.43 (h, 2H, *J* = 7.2 Hz), 0.96 (t, 3H, *J* = 7.2 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.9, 161.6, 159.8, 159.7, 128.2, 127.8, 119.3, 114.0, 55.3, 51.8, 29.8, 25.6, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{19}NO_4+H]^+$ 290.1392, found 290.1385.

Methyl 5-*n*-Butyl-2-(3-methoxylphenyl)oxazole-4-carboxylate (3e):

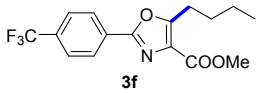


3e

The reaction of 0.3 mmol of methyl 2-(3-methoxylphenyl)oxazole-4-carboxylate (**1e**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 74% of **3d** after flash chromatography on silica gel using petroleum ether and ethyl acetate (12:1 to 10:1, *v*/*v*) as the effluent. Light yellow solid, m.p. 53-55 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 7.66-7.60 (m, 2H), 7.36 (t, 1H, *J* = 8.0 Hz), 7.02-7.00 (m, 1H), 3.95 (s, 3H), 3.88 (s, 3H), 3.12 (t, 2H, *J* = 7.6 Hz), 1.75 (p, 2H, *J* = 7.6 Hz), 1.43 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.7, 160.4, 159.8, 159.5, 129.7, 128.0, 127.7, 119.0, 117.3, 111.0, 55.4, 51.9, 29.8, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{19}NO_4+H]^+$

290.1392, found 290.1383.

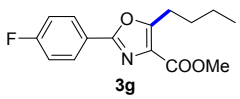
Methyl 5-*n*-Butyl-2-(4-trifluoromethylphenyl)oxazole-4-carboxylate (3f):



3f

The reaction of 0.3 mmol of methyl 2-(4-trifluoromethylphenyl)oxazole-4-carboxylate (**1f**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 60% of **3e** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 57-59 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.19 (d, 2H, *J* = 8.0 Hz), 7.72 (d, 2H, *J* = 8.0 Hz), 3.96 (s, 3H), 3.14 (t, 2H, *J* = 7.6 Hz), 1.76 (p, 2H, *J* = 7.6 Hz), 1.44 (h, 2H, *J* = 7.6 Hz), 0.98 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.5, 161.1, 158.2, 132.3 (q, *J* = 32.6 Hz), 129.7, 128.5, 126.8, 125.8 (d, *J* = 11.1 Hz), 125.7 (d, *J* = 3.7 Hz), 52.1, 29.8, 25.8, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{16}F_3NO_3+H]^+$ 328.1161, found 328.1155.

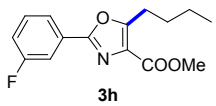
Methyl 5-*n*-Butyl-2-(4-fluorophenyl)oxazole-4-carboxylate (3g):



3g

The reaction of 0.3 mmol of methyl 2-(4-fluorophenyl)oxazole-4-carboxylate (**1g**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 75% of **3f** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 41-42 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.08-8.05 (m, 2H), 7.17-7.12 (m, 2H), 3.95 (s, 3H), 3.11 (t, 2H, *J* = 7.6 Hz), 1.74 (p, 2H, *J* = 7.6 Hz), 1.43 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 164.2 (d, *J* = 250.3 Hz), 162.7, 160.4, 158.8, 128.7 (d, *J* = 8.6 Hz), 128.1, 122.9 (d, *J* = 3.1 Hz), 115.9 (d. *J* = 22.2 Hz), 115.8, 51.9, 29.8, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{16}FNO_3+H]^+$ 278.1193, found 278.1189.

Methyl 5-*n*-Butyl-2-(3-fluorophenyl)oxazole-4-carboxylate (3h):

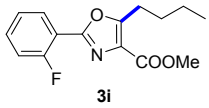


3h

The reaction of 0.3 mmol of methyl 2-(3-fluorophenyl)oxazole-4-carboxylate (**1h**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 68% of **3g** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 54-56 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 7.87 (t, 1H, *J* = 8.0 Hz), 7.79-7.75 (m, 1H), 7.46-7.40 (m, 1H), 7.19-7.14 (m, 1H), 3.95 (s, 3H), 3.12 (t, 2H, *J* = 7.6 Hz), 1.75 (p,

2H, *J* = 7.6 Hz), 1.44 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8 (d, *J* = 245.3 Hz), 162.6, 160.7, 158.4 (d, *J* = 3.6 Hz) , 130.4 (d, *J* = 8.1 Hz), 128.5 (d, *J* = 8.6 Hz), 128.2, 122.2 (d, *J* = 3.0 Hz), 117.7 (d, *J* = 21.2 Hz), 113.5 (d, *J* = 24.0 Hz), 52.0, 29.8, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{16}FNO_3+H]^+$ 278.1193, found 278.1188.

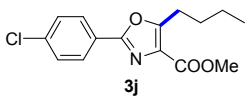
Methyl 5-*n*-Butyl-2-(2-fluorophenyl)oxazole-4-carboxylate (3i):



3i

The reaction of 0.3 mmol of methyl 2-(2-fluorophenyl)oxazole-4-carboxylate (**1i**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 72% of **3h** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 36-37 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.08 (t, 1H, *J* = 7.6 Hz), 7.48-7.42 (m, 1H), 7.26-7.17 (m, 2H), 3.95 (s, 3H), 3.14 (t, 2H, *J* = 7.6 Hz), 1.75 (p, 2H, *J* = 7.6 Hz), 1.43 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.7, 160.7 (d, *J* = 1.3 Hz), 160.0 (d, *J* = 255.8 Hz), 156.2 (d, *J* = 4.3 Hz), 132.4 (d, *J* = 8.5 Hz), 129.8 (d, *J* = 1.3 Hz), 128.0, 124.2 (d, *J* = 3.7 Hz), 116.7 (d, *J* = 21.1 Hz), 114.9 (d, *J* = 11.0 Hz), 51.9, 29.7, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{16}FNO_3+H]^+$ 278.1193, found 278.1186.

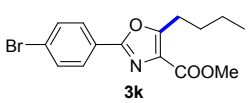
Methyl 5-*n*-Butyl-2-(4-chlorophenyl)oxazole-4-carboxylate (3j):



3j

The reaction of 0.3 mmol of methyl 2-(4-chlorophenyl)oxazole-4-carboxylate (**1j**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 69% of **3i** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Light yellow solid, m.p. 71-73 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.01 (d, 2H, *J* = 8.8 Hz), 7.43 (d, 2H, *J* = 8.8 Hz), 3.95 (s, 3H), 3.11 (t, 2H, *J* = 7.6 Hz), 1.74 (p, 2H, *J* = 7.6 Hz), 1.43 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.6, 160.5, 158.7, 136.9, 129.0, 128.2, 127.8, 125.1, 52.0, 29.8, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{16}ClNO_3+H]^+$ 294.0891, found 294.0887.

Methyl 5-*n*-Butyl-2-(4-bromophenyl)oxazole-4-carboxylate (3k):

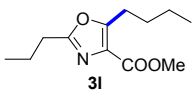


3k

The reaction of 0.3 mmol of methyl 2-(4-bromophenyl)oxazole-4-

carboxylate (**1k**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 62% of **3j** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Light yellow solid, m.p. 62-63 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 7.94 (d, 2H, *J* = 8.4 Hz), 7.59 (d, 2H, *J* = 8.4 Hz), 3.95 (s, 3H), 3.11 (t, 2H, *J* = 7.6 Hz), 1.74 (p, 2H, *J* = 7.6 Hz), 1.43 (h, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.6, 160.6, 158.7, 132.0, 128.2, 127.9 125.5, 125.3, 52.0, 29.8, 25.7, 22.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{16}BrNO_3+H]^+$ 338.0392, found 338.0385.

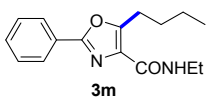
Methyl 5-*n*-Butyl-2-*n*-propyloxazole-4-carboxylate (3l):



3l

The reaction of 0.3 mmol of methyl 2-*n*-propyloxazole-4-carboxylate (**1l**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 65% of **3l** after flash chromatography on silica gel using petroleum ether and ethyl acetate (50:1, *v*/*v*) as the effluent. Colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 3.89 (s, 3H), 3.01 (t, 2H, *J* = 7.6 Hz), 2.72 (t, 2H, *J* = 7.6 Hz), 1.79 (q, 2H, *J* = 7.6 Hz), 1.66 (p, 2H, *J* = 7.6 Hz), 1.37 (h, 2H, *J* = 7.6 Hz), 0.98 (t, 3H, *J* = 7.6 Hz), 0.94 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.9, 160.0, 143.6, 126.6, 51.7, 29.8, 29.7, 25.5, 22.1, 20.4, 13.6, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{12}H_{19}NO_3+Na]^+$ 248.1263, found 248.1263.

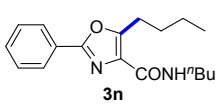
***N*-Ethyl 5-*n*-Butyl-2-phenyloxazole-4-formamide (3m):**



3m

The reaction of 0.3 mmol of *N*-ethyl 2-phenyloxazole-4-formamide (**1m**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 70% of **3m** after flash chromatography on silica gel using petroleum ether and ethyl acetate (12:1, *v*/*v*) as the effluent. Yellow solid, m.p. 55-57 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.02-7.99 (m, 2H), 7.47-7.44 (m, 3H), 7.09 (s, 1H), 3.50-3.44 (m, 2H), 3.16 (t, 2H, *J* = 7.6 Hz), 1.74 (p, 2H, *J* = 7.6 Hz), 1.44 (h, 2H, *J* = 7.6 Hz), 1.26 (t, 3H, *J* = 7.2 Hz), 0.96 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 161.8, 158.4, 156.7, 130.4, 129.9, 128.7, 126.9, 126.2, 33.7, 30.0, 25.5, 22.3, 14.9, 13.7 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{20}N_2O_2+H]^+$ 273.1603, found 273.1598.

***N*-n-Butyl 5-*n*-Butyl-2-phenyloxazole-4-formamide (3n):**

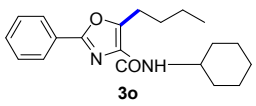


3n

The reaction of 0.3 mmol of *N*-n-butyl 2-phenyloxazole-4-formamide (**1n**)

and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 69% of **3n** after flash chromatography on silica gel using petroleum ether and ethyl acetate (10:1, *v*/*v*) as the effluent. Light yellow oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.02-7.99 (m, 2H), 7.46-7.44 (m, 3H), 7.13-7.11 (m, 1H), 3.42 (q, 2H, *J* = 7.2 Hz), 3.16 (t, 2H, *J* = 7.6 Hz), 1.74 (p, 2H, *J* = 7.6 Hz), 1.61 (p, 2H, *J* = 7.2 Hz), 1.46-1.40 (m, 4H), 0.98-0.94 (m, 6H) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 161.9, 158.4, 156.7, 130.4, 130.0, 128.7, 126.9, 126.2, 38.6, 31.8, 30.0, 25.5, 22.3, 20.1, 13.7, 13.7 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{18}H_{24}N_2O_2+H]^+$ 301.1916, found 301.1909.

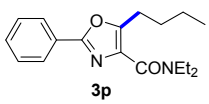
***N*-Cyclohexyl 5-*n*-Butyl-2-phenyloxazole-4-formamide (3o):**



3o

The reaction of 0.3 mmol of *N*-cyclohexyl 2-phenyloxazole-4-formamide (**1o**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 63% of **3o** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Light yellow oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.02-8.00 (m, 2H), 7.47-7.45 (m, 3H), 7.00-6.98 (m, 1H), 3.97-3.90 (m, 1H), 3.16 (t, 2H, *J* = 7.6 Hz), 2.04-2.00 (m, 2H), 1.79-1.64 (m, 4H), 1.46-1.20 (m, 8H), 0.96 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 161.0, 158.3, 156.7, 130.4, 130.0, 128.7, 126.9, 126.2, 47.7, 33.2, 30.0, 25.5, 25.5, 24.9, 22.3, 13.7 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{20}H_{26}N_2O_2+H]^+$ 327.2073, found 327.2066.

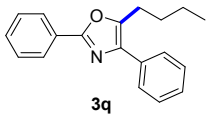
***N*,*N*-Diethyl 5-*n*-Butyl-2-phenyloxazole-4-formamide (3p):**



3p

The reaction of 0.3 mmol of *N*,*N*-diethyl 2-phenyloxazole-4-formamide (**1p**) and 1.2 mmol of *n*-butylboronic acid (**2a**) afforded 45% of **3p** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Light yellow oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.01-7.99 (m, 2H), 7.47-7.43 (m, 3H), 3.74 (q, 2H, *J* = 6.8 Hz), 3.52 (q, 2H, *J* = 6.8 Hz), 3.01 (t, 2H, *J* = 7.6 Hz), 1.73 (p, 2H, *J* = 7.6 Hz), 1.42 (h, 2H, *J* = 7.6 Hz), 1.32-1.23 (m, 6H), 0.95 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 163.0, 157.8, 157.1, 131.7, 130.1, 128.7, 127.4, 126.1, 43.1, 40.6, 30.1, 25.7, 22.3, 14.6, 13.7, 12.9 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{18}H_{24}N_2O_2+H]^+$ 301.1916, found 301.1910.

***N*,*N*-Diethyl 5-*n*-Butyl-2,4-diphenyloxazole (3q):**

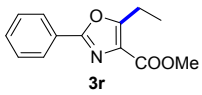


3q

The reaction of 0.3 mmol of *N*,*N*-diethyl 2,4-diphenyloxazole (**1q**) and 1.2

mmol of *n*-butylboronic acid (**2a**) afforded 78% of **3q** after flash chromatography on silica gel using petroleum ether and ethyl acetate (50:1, *v*/*v*) as the effluent. Light yellow oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.10-8.07 (m, 2H), 7.73-7.71 (m, 2H) 7.47-7.40 (m, 6H), 2.94 (t, 2H, *J* = 7.6 Hz), 1.78 (p, 2H, *J* = 7.6 Hz), 1.46 (h, 2H, *J* = 7.6 Hz), 0.96 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 159.4, 148.2, 135.8, 132.5, 129.9, 128.6, 128.6, 127.7, 127.3, 127.0, 126.1, 30.4, 25.7, 22.4, 13.8 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{19}H_{19}NO+H]^+$ 278.1545, found 278.1543.

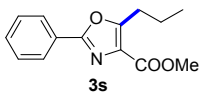
Methyl 5-Ethyl-2-phenyloxazole-4-carboxylate (3r):



3r

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of ethylboronic acid (**2b**) afforded 70% of **3r** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 72-73 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.47-7.44 (m, 3H), 3.95 (s, 3H), 3.15 (q, 2H, *J* = 7.6 Hz), 1.35 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 161.2, 159.6, 130.7, 128.7, 127.6, 126.6, 126.5, 51.9, 19.7, 12.1 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{13}H_{13}NO_3+H]^+$ 232.0974, found 232.0965.

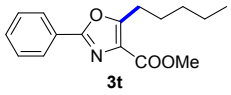
Methyl 5-*n*-Propyl-2-phenyloxazole-4-carboxylate (3s):



3s

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of *n*-propylboronic acid (**2c**) afforded 73% of **3s** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.46-7.45 (m, 3H), 3.95 (s, 3H), 3.10 (t, 2H, *J* = 7.6 Hz), 1.80 (h, 2H, *J* = 7.6 Hz), 1.03 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 160.1, 159.6, 130.7, 128.7, 128.2, 126.6, 126.5, 51.9, 27.8, 21.2, 13.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{14}H_{15}NO_3+H]^+$ 246.1130, found 246.1125.

Methyl 5-*n*-Pentyl-2-phenyloxazole-4-carboxylate (3t):

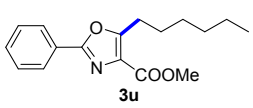


3t

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of *n*-pentylboronic acid (**2d**) afforded 77% of **3t** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent.

Colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.47-7.44 (m, 3H), 3.95 (s, 3H), 3.11 (t, 2H, *J* = 7.6 Hz), 1.76 (p, 2H, *J* = 7.6 Hz), 1.40-1.37 (m, 4H), 0.91 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 160.4, 159.6, 130.7, 128.7, 128.0, 126.6, 126.5, 51.9, 31.2, 27.4, 25.9, 22.2, 13.8 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{16}H_{19}NO_3+H]^+$ 274.1443, found 274.1437.

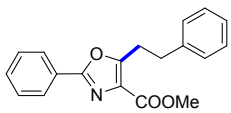
Methyl 5-*n*-Hexyl-2-phenyloxazole-4-carboxylate (3u):



3u

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of *n*-hexylboronic acid (**2e**) afforded 68% of **3u** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.47-7.45 (m, 3H), 3.95 (s, 3H), 3.11 (t, 2H, *J* = 7.6 Hz), 1.76 (p, 2H, *J* = 7.6 Hz), 1.42-1.31 (m, 6H), 0.89 (t, 3H, *J* = 7.6 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 160.4, 159.6, 130.7, 128.7, 128.0, 126.6, 126.5, 51.9, 31.3, 28.7, 27.7, 26.0, 22.4, 14.0 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{17}H_{21}NO_3+H]^+$ 288.1600, found 288.1593.

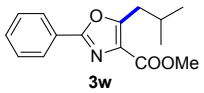
Methyl 5-(2-Phenylethyl)-2-phenyloxazole-4-carboxylate (3v):



3v

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of 2-phenylethylboronic acid (**2f**) afforded 72% of **3v** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1, *v*/*v*) as the effluent. Light yellow solid, m.p. 65-67 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.05-8.03 (m, 2H), 7.46-7.44 (m, 3H), 7.31-7.21 (m, 5H), 3.92 (s, 3H), 3.43 (t, 2H, *J* = 8.0 Hz), 3.07 (t, 2H, *J* = 8.0 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.6, 159.8, 159.0, 140.0, 130.8, 128.7, 128.5, 128.3, 126.6, 126.5, 126.4, 52.0, 34.0, 28.0 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{19}H_{17}NO_3+H]^+$ 308.1281, found 308.1278.

Methyl 5-(2-Methylpropyl)-2-phenyloxazole-4-carboxylate (3w):

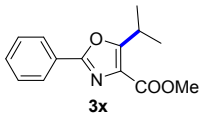


3w

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of 2-methylpropylboronic acid (**2g**) afforded 64% of **3w** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1, *v*/*v*) as the effluent.

Light yellow solid, m.p. 38-39 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.48-7.44 (m, 3H), 3.95 (s, 3H), 3.01 (d, 2H, *J* = 6.8 Hz), 2.21-2.11 (m, 1H), 1.01 (t, 6H, *J* = 6.8 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 162.8, 159.7, 159.5, 130.7, 128.8, 128.7, 126.6, 126.5, 51.9, 34.6, 28.1, 22.3 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{15}H_{17}NO_3+H]^+$ 260.1287, found 260.1283.

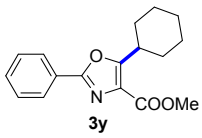
Methyl 5-*i*-Propyl-2-phenyloxazole-4-carboxylate (3x):



3x

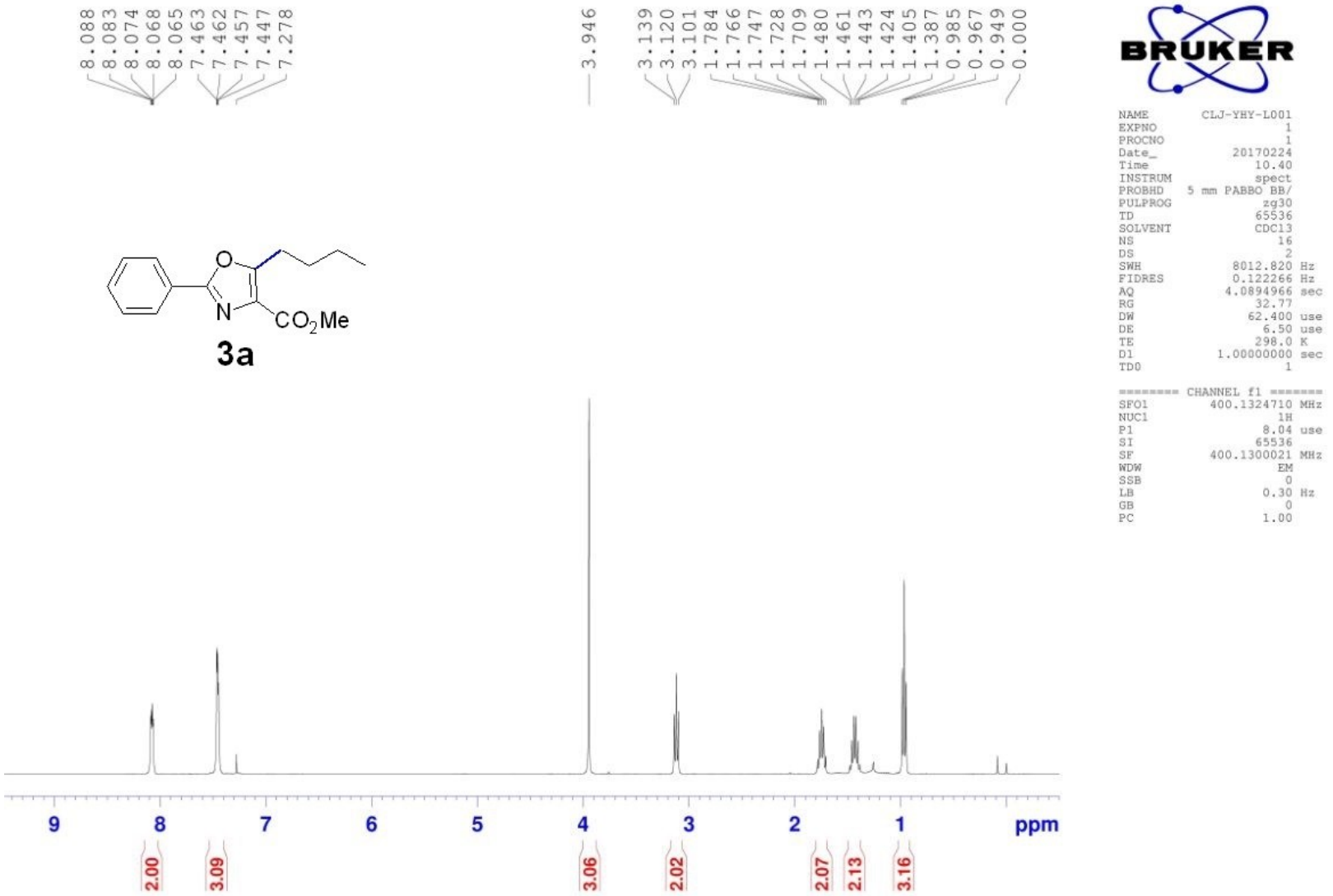
The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of *i*-propylboronic acid (**2h**) afforded 83% of **3x** after flash chromatography on silica gel using petroleum ether and ethyl acetate (20:1, *v*/*v*) as the effluent. Offwhite solid, m.p. 48-50 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.07 (m, 2H), 7.48-7.44 (m, 3H), 3.95 (s, 3H), 3.86 (sept, 1H, *J* = 7.2 Hz), 1.37 (d, 6H, *J* = 7.2 Hz) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 164.3, 162.7, 159.3, 130.6, 128.6, 126.6, 126.5, 126.5, 51.9, 26.1, 20.6 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{14}H_{15}NO_3+H]^+$ 246.1130, found 246.1125.

Methyl 5-Cyclohexyl-2-phenyloxazole-4-carboxylate (3y):



3y

The reaction of 0.3 mmol of methyl 2-phenyloxazole-4-carboxylate (**1a**) and 1.2 mmol of cyclohexylboronic acid (**2i**) afforded 40% of **3y** after flash chromatography on silica gel using petroleum ether and ethyl acetate (15:1, *v*/*v*) as the effluent. Light yellow solid, m.p. 107-108 °C. **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ = 8.09-8.06 (m, 2H), 7.46-7.45 (m, 3H), 3.95 (s, 3H), 3.57-3.49 (m, 1H), 1.96-1.61 (m, 6H), 1.50-1.20 (m, 4H) ppm; **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 164.0, 162.9, 159.3, 130.7, 128.7, 126.7, 126.7, 126.5, 51.9, 35.6, 30.8, 25.9, 25.7 ppm; **HRMS** *m/z* (ESI) calcd for $[C_{17}H_{19}NO_3+H]^+$ 286.1443, found 286.1438.


8.088
8.083
8.074
8.068
8.065
7.463
7.462
7.457
7.447
7.278
3.946
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3.120
3.101
1.784
1.766
1.747
1.728
1.709
1.480
1.461
1.443
1.424
1.405
1.387
0.985
0.967
0.949
0.000
BRUKER
NAME CLJ-YHY-L001
EXPNO 1
PROCNO 1
Date_ 20170224
Time 10.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 32.77
DW 62.400 use
DE 6.50 use
TE 298.0 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
P1 8.04 use
SI 65536
SF 400.1300021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
N
CO2Me
3a
9
8
7
6
5
4
3
2
1
ppm
2.00
3.09
3.06
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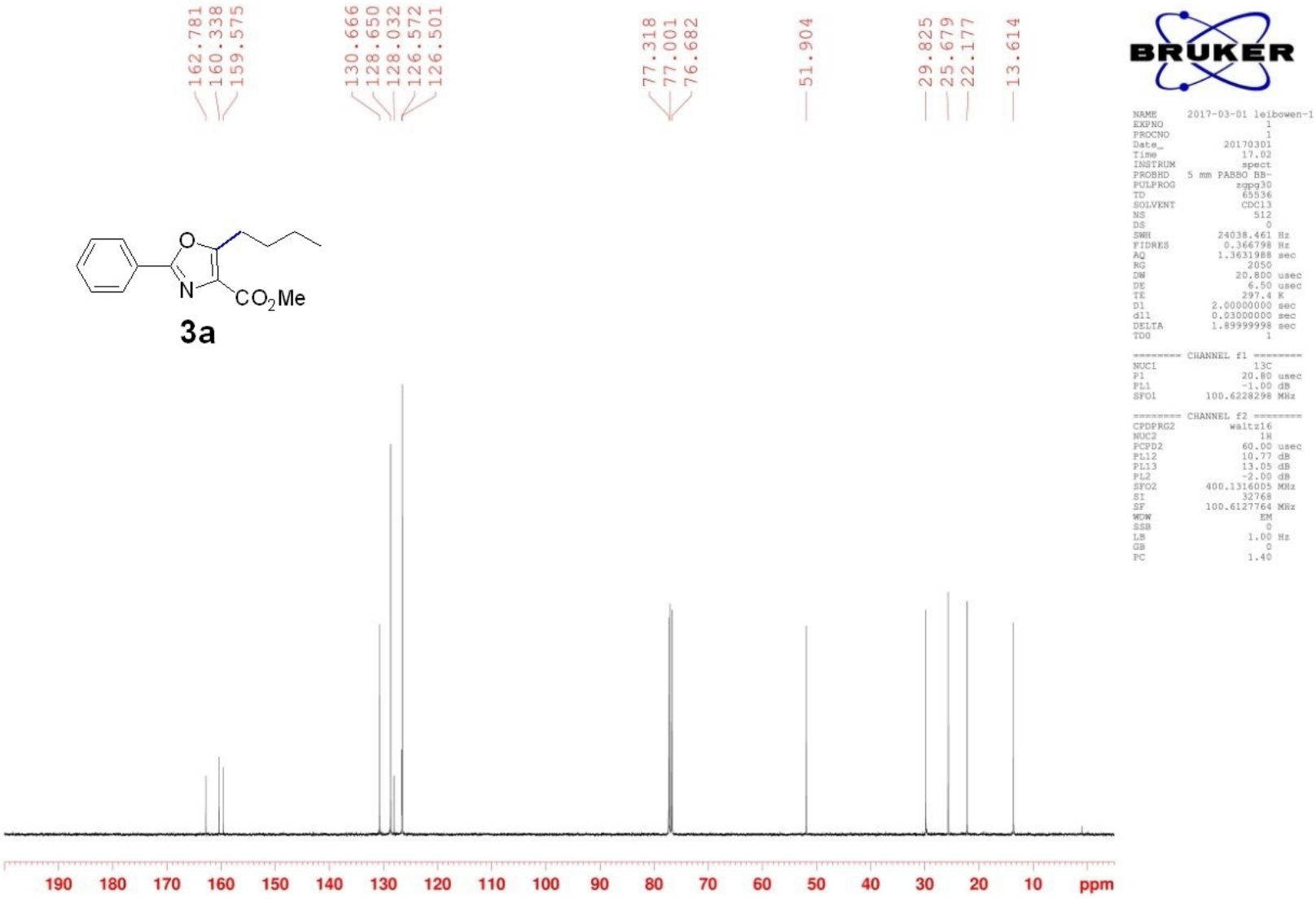
2.07
2.13
3.16



BRUKER

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PROCNO                        1
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TD                       65536
SOLVENT                  CDCl3
NS                         512
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FIDRES              0.366798 Hz
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RG                        2050
DW                      20.800 usec
DE                       6.50 usec
TE                      297.4 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                       20.80 usec
PL1                      -1.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    60.00 usec
PL12                     10.77 dB
PL13                     13.05 dB
PL2                      -2.00 dB
SFO2               400.1316005 MHz
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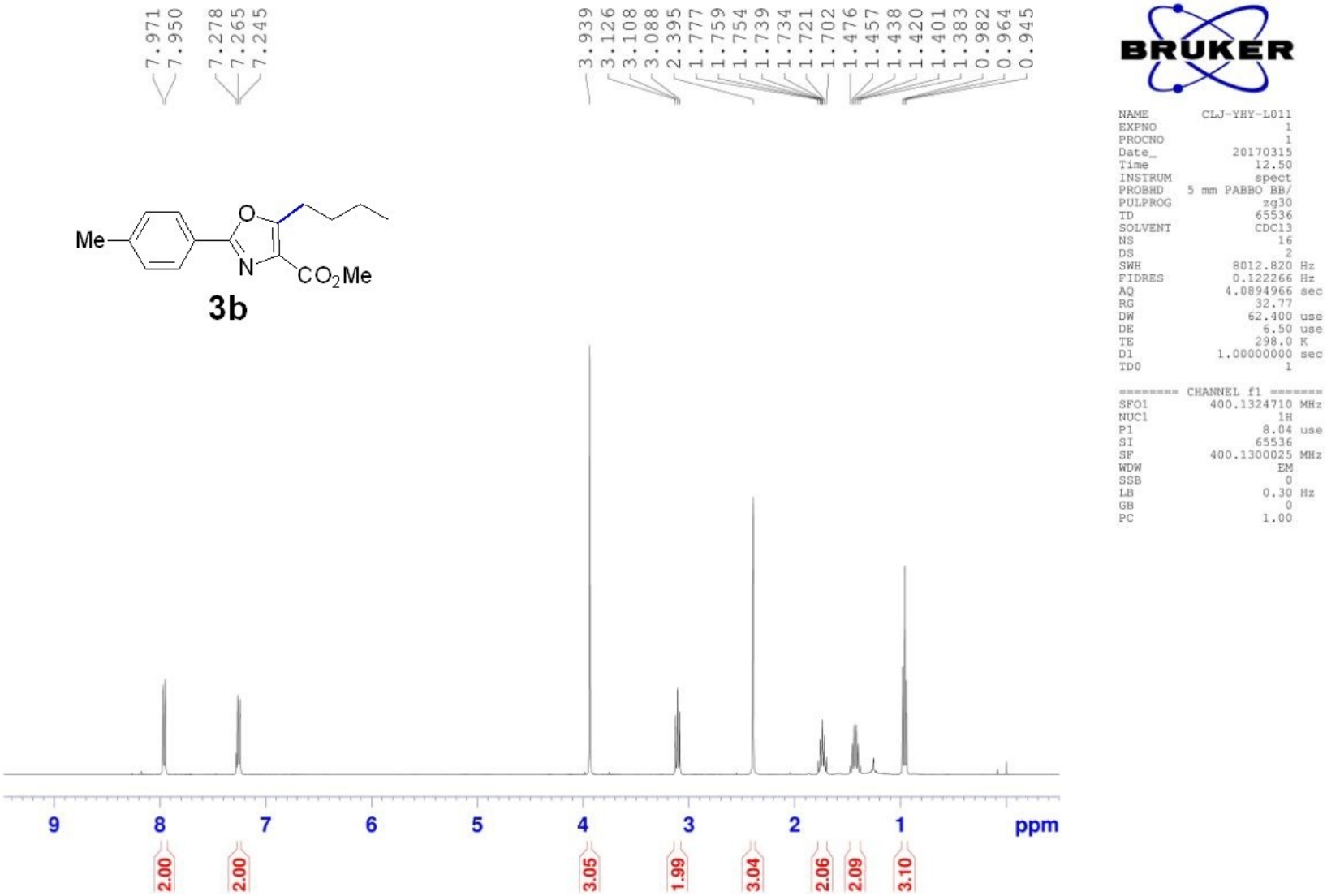


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TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 =======
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NUC1                       1H
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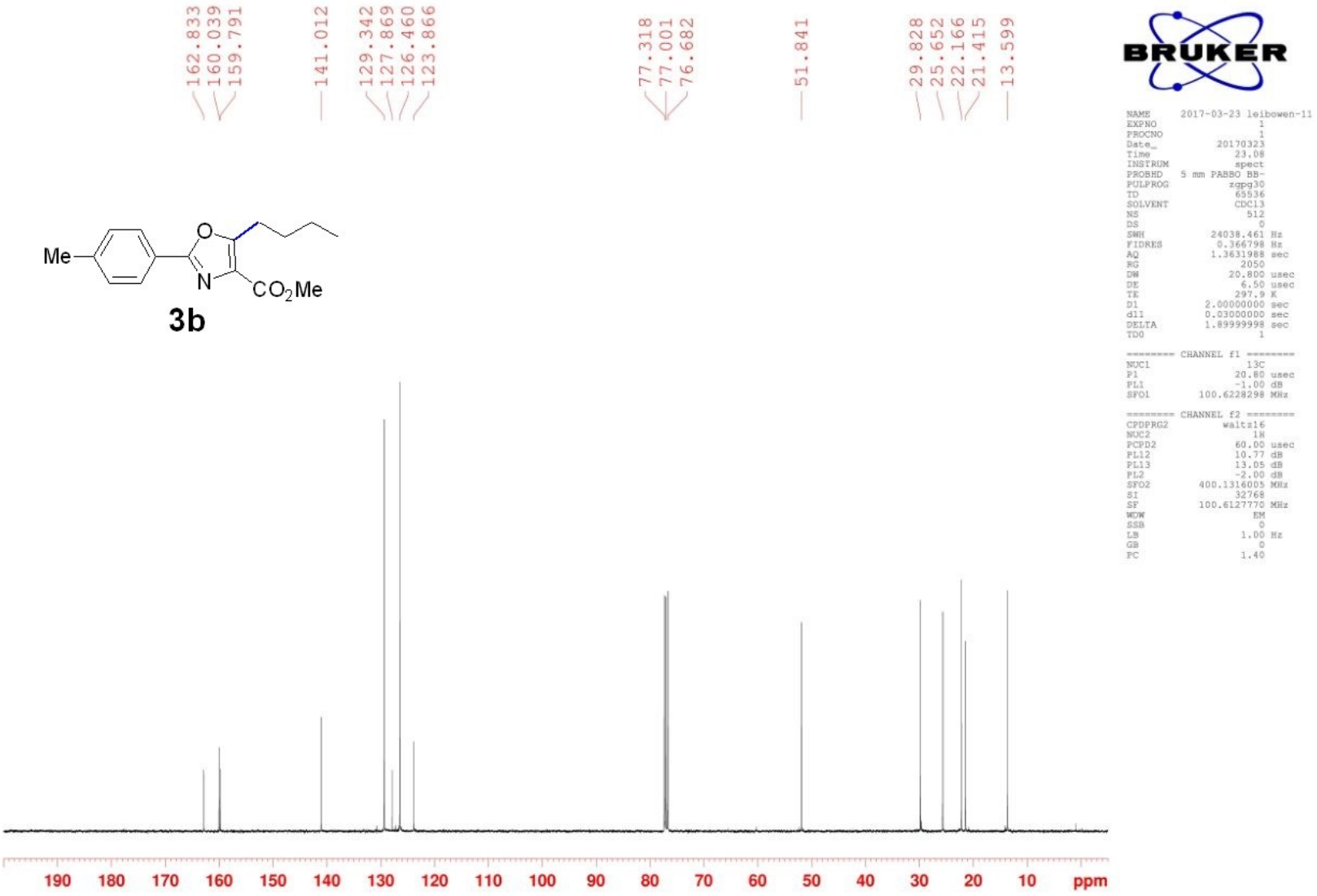


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PROCNO                   1
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DS                       0
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    2050
DW                 20.800 usec
DE                  6.50 usec
TE                 297.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
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P1                   20.80 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 10.77 dB
PL13                 13.05 dB
PL2                  -2.00 dB
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SF             100.6127770 MHz
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SSB                      0
LB                    1.00 Hz
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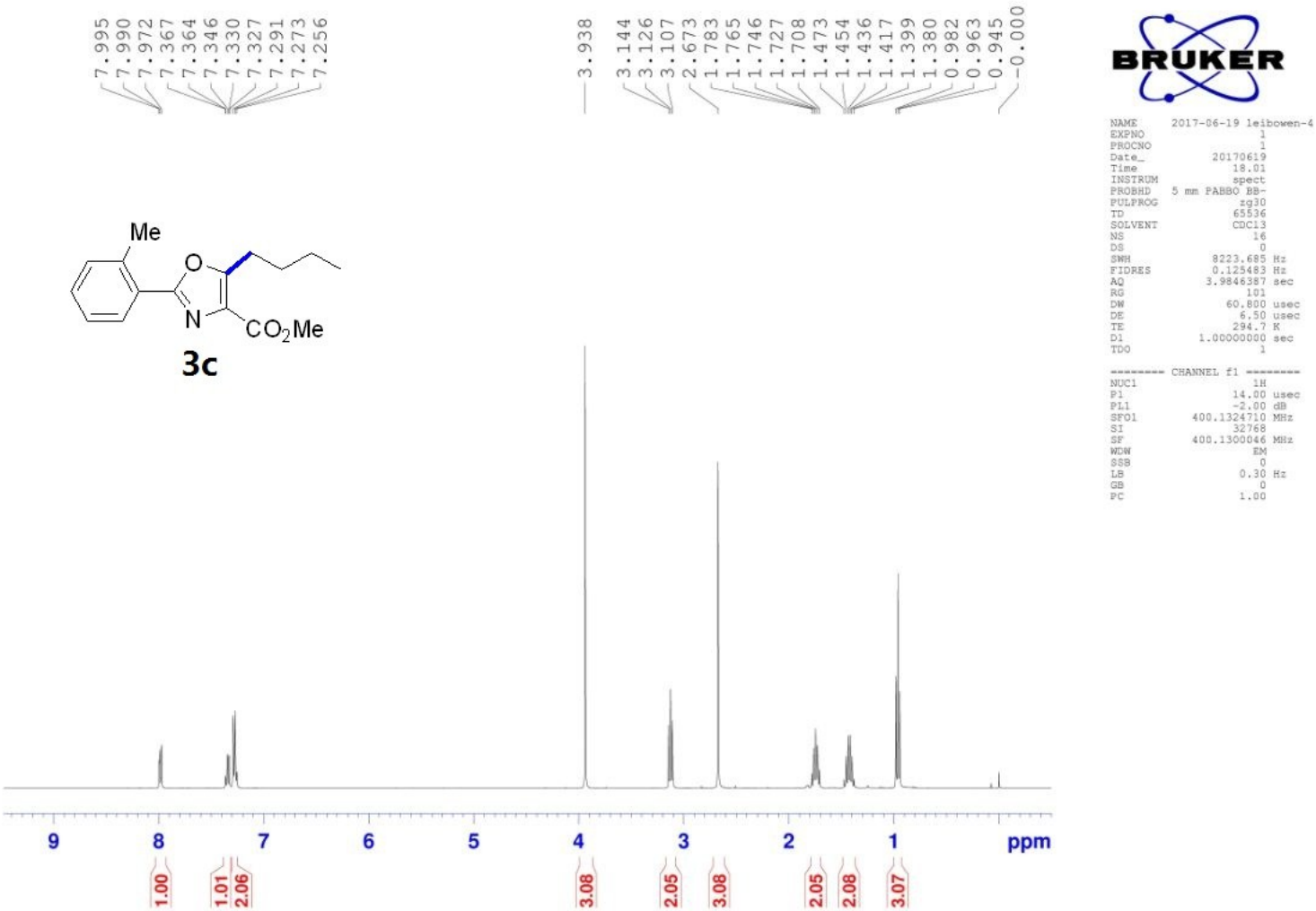


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PROCNO                   1
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DE                  6.50 usec
TE                 294.7 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
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P1                  14.00 usec
PL1                 -2.00 dB
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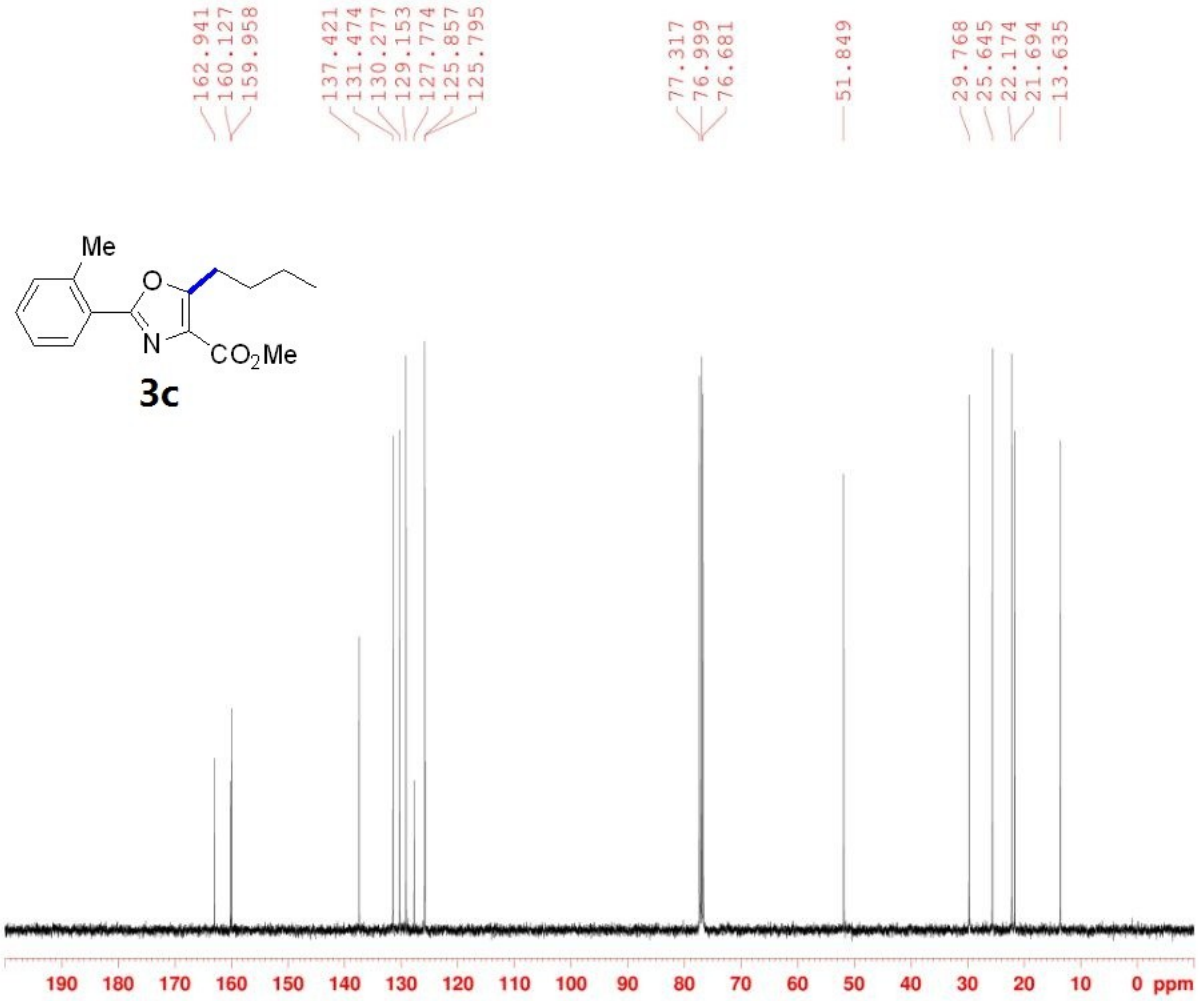
SI                  32768
SF           400.1300046 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

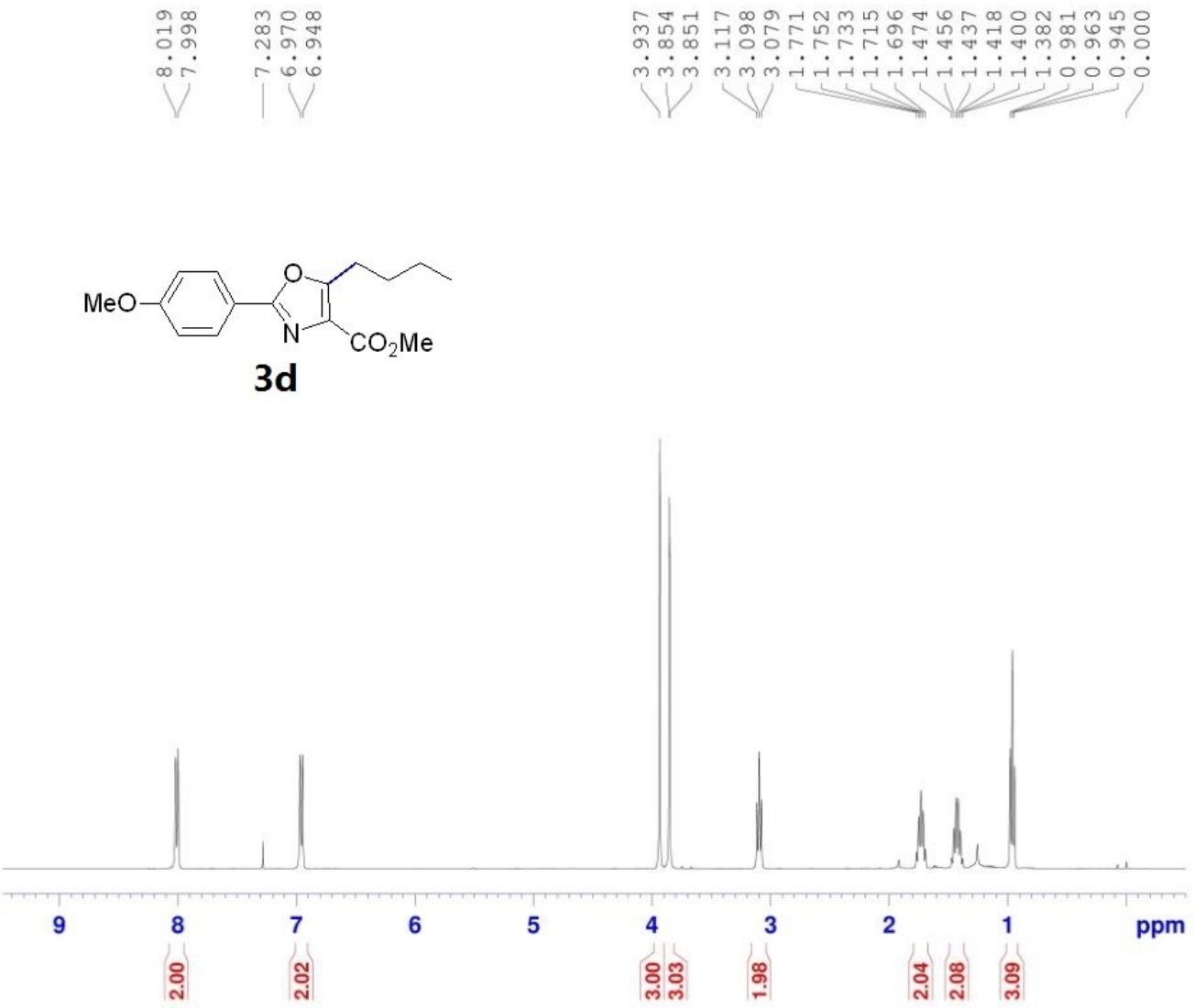


BRUKER

```
NAME          2017-06-19 leibowen-43
EXPNO                    2
PROCNO                   1
Date_             20170619
Time                 18.18
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        0
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     2050
DW                  20.800 usec
DE                   6.50 usec
TE                   296.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1

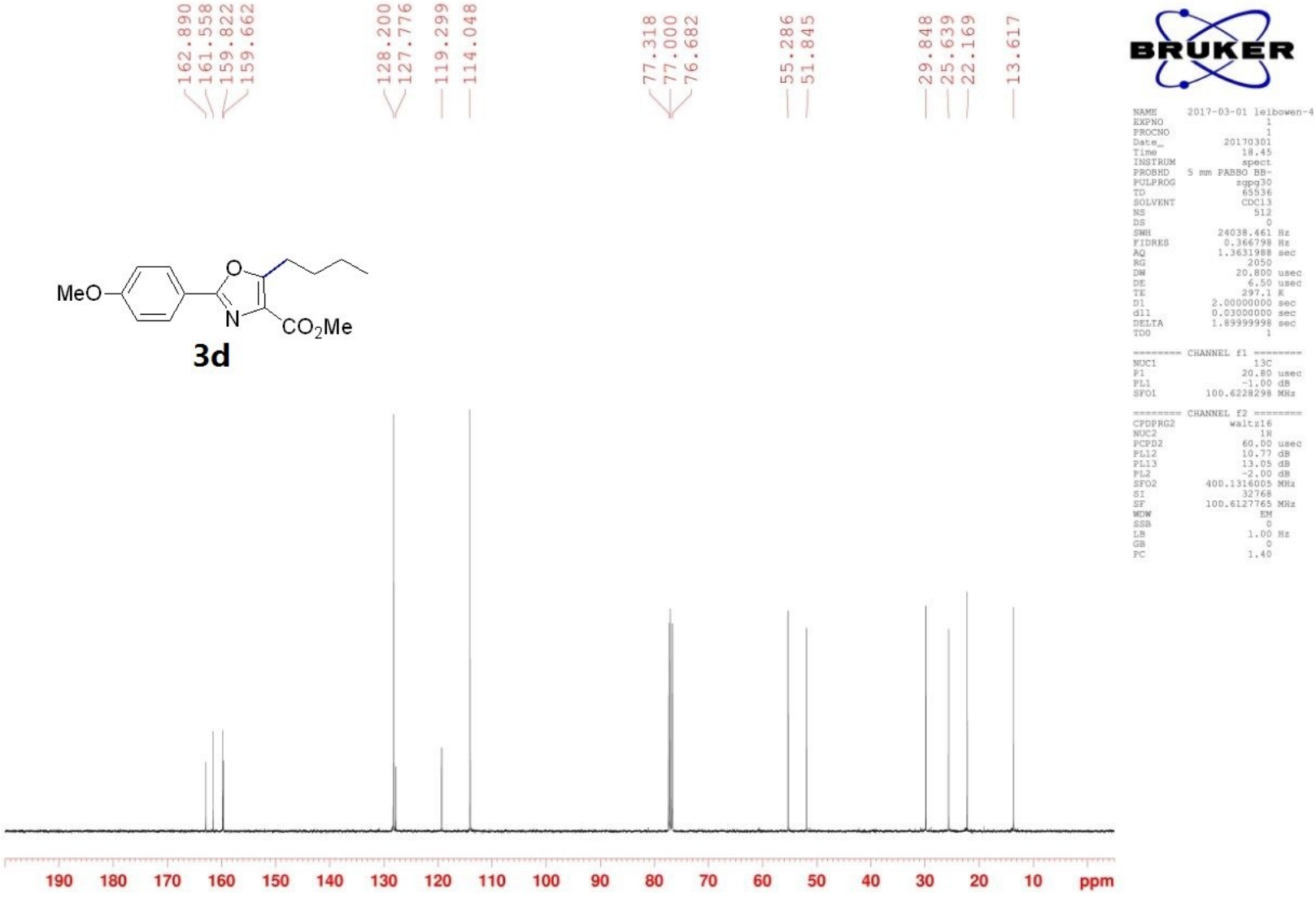
======== CHANNEL f1 ========
NUC1                    13C
P1                   20.80 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 10.77 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2           400.1316005 MHz
SI                     32768
SF             100.6127760 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



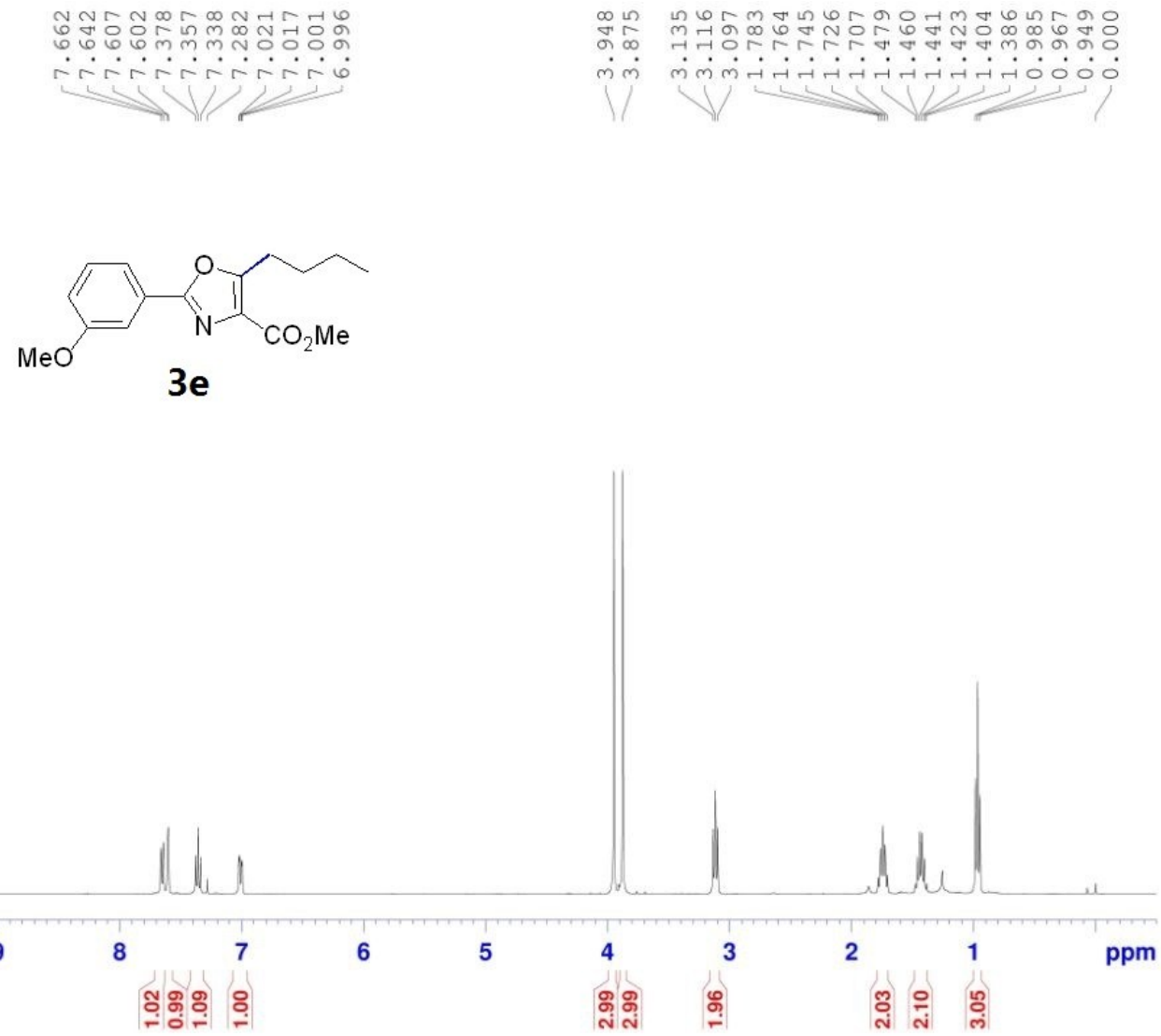
BRUKER

NAME	CLJ-YHY-L004
EXPNO	1
PROCNO	1
Date_	20170224
Time	10.52
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300004 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



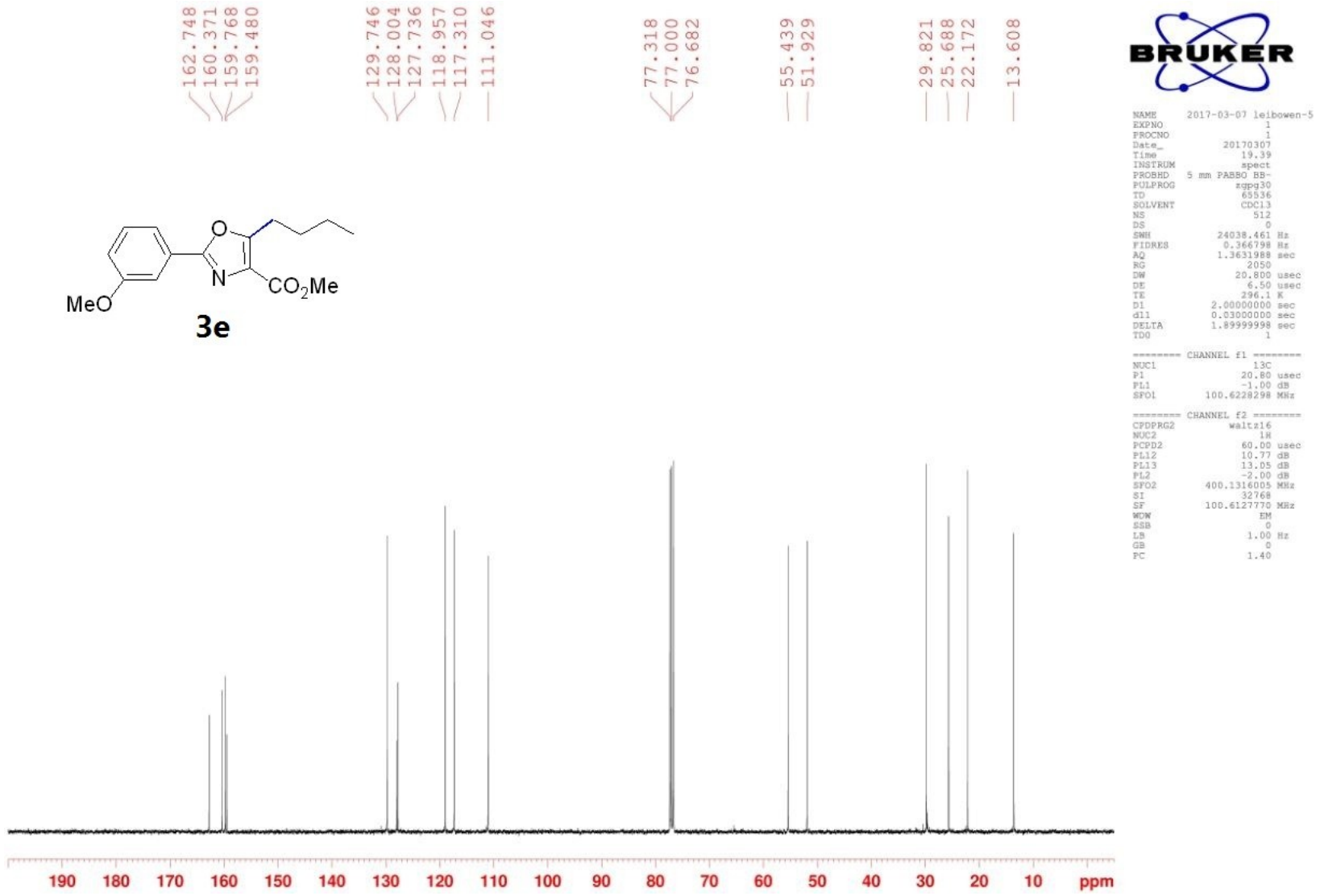
BRUKER

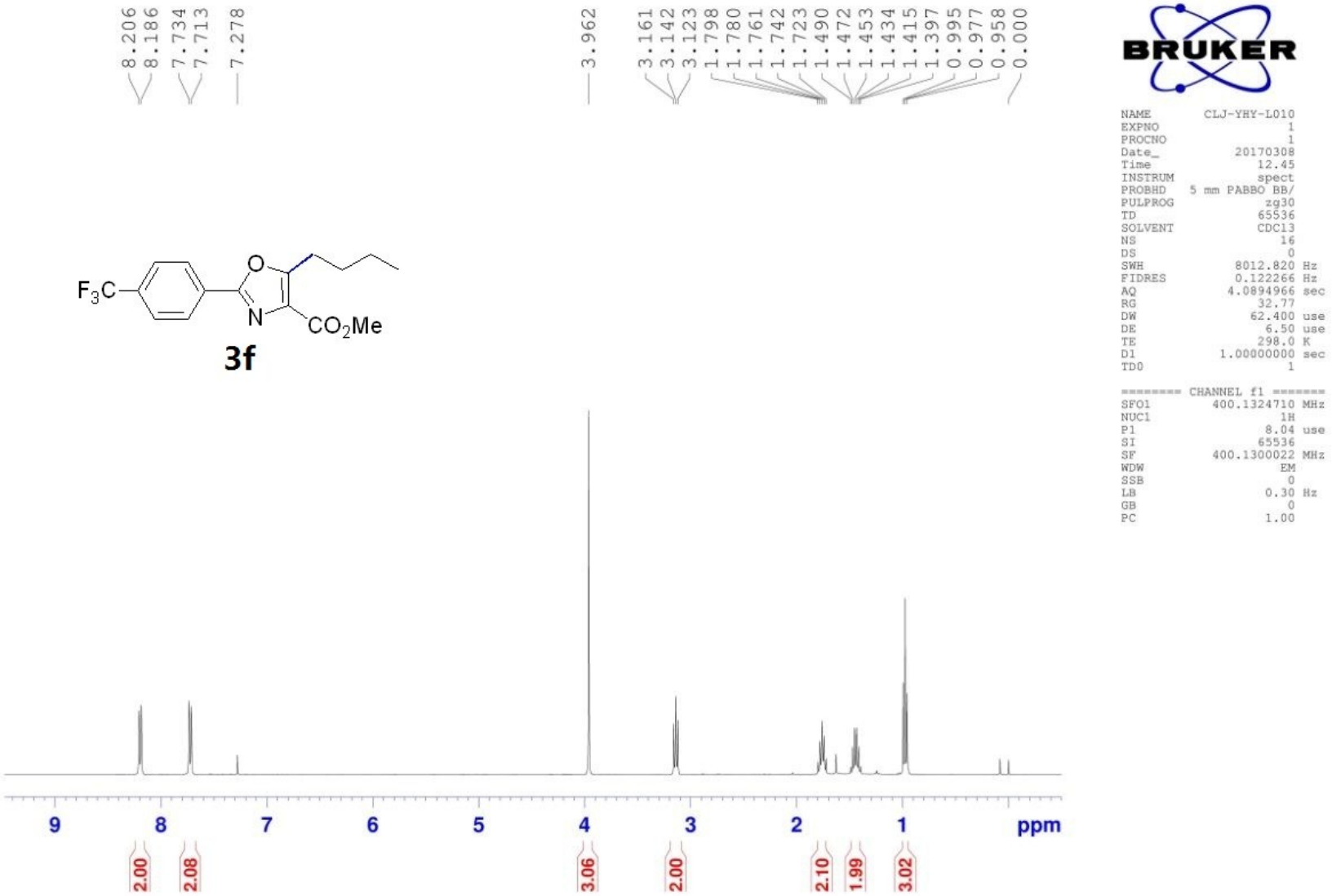
NAME	2017-03-01 leibowen-4
EXPNO	1
PROCNO	1
Date_	20170301
Time	18.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127765 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

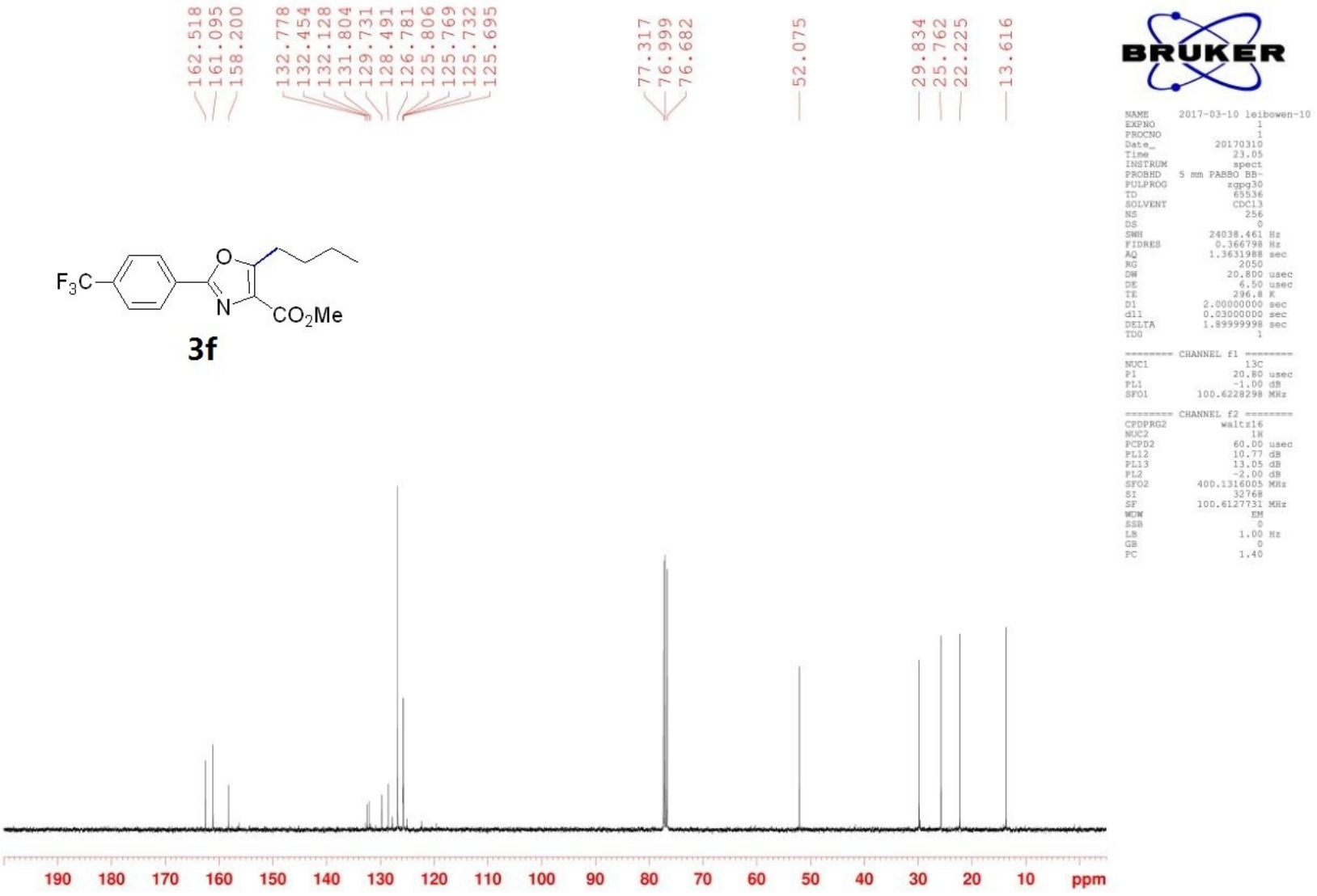


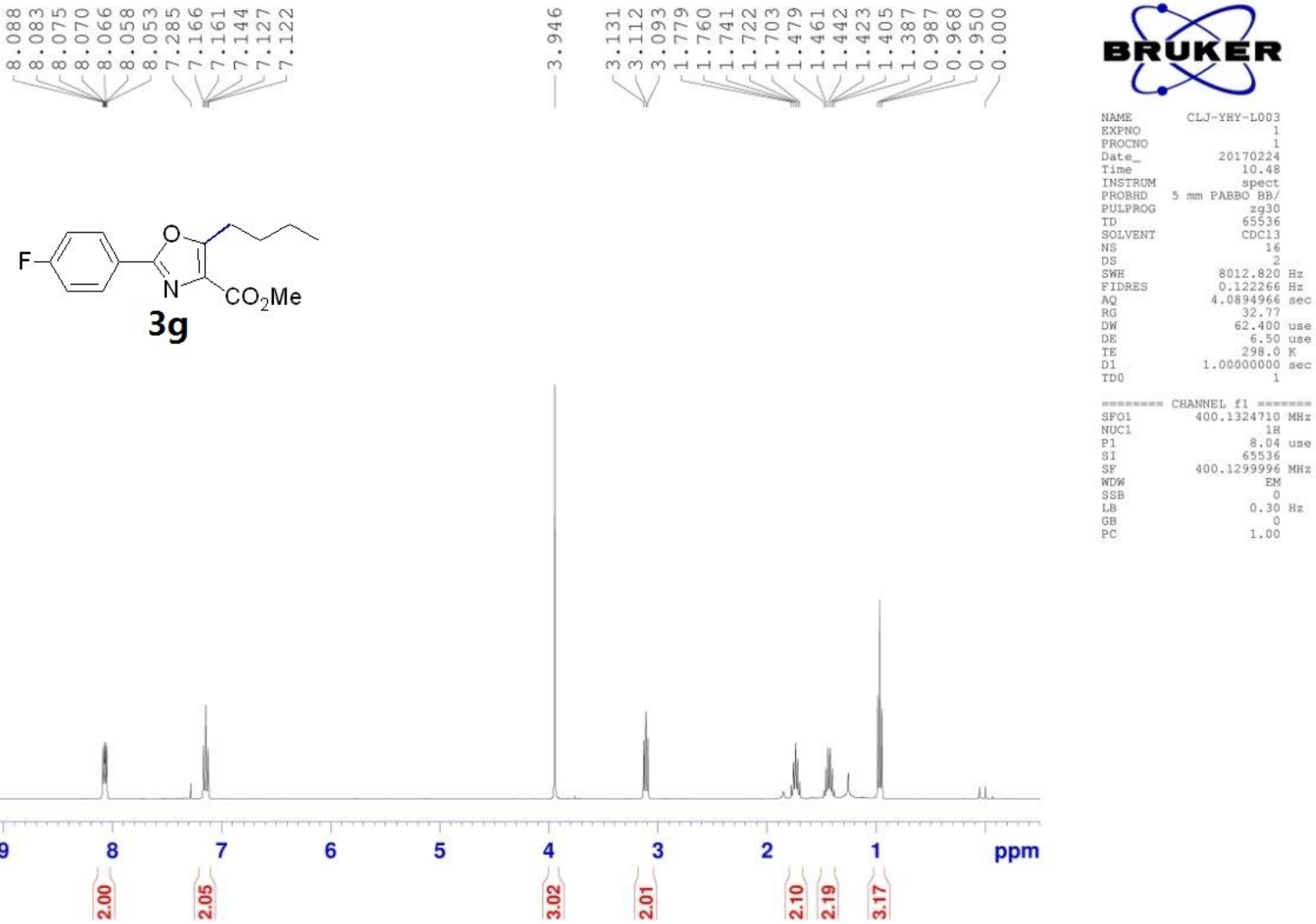
BRUKER

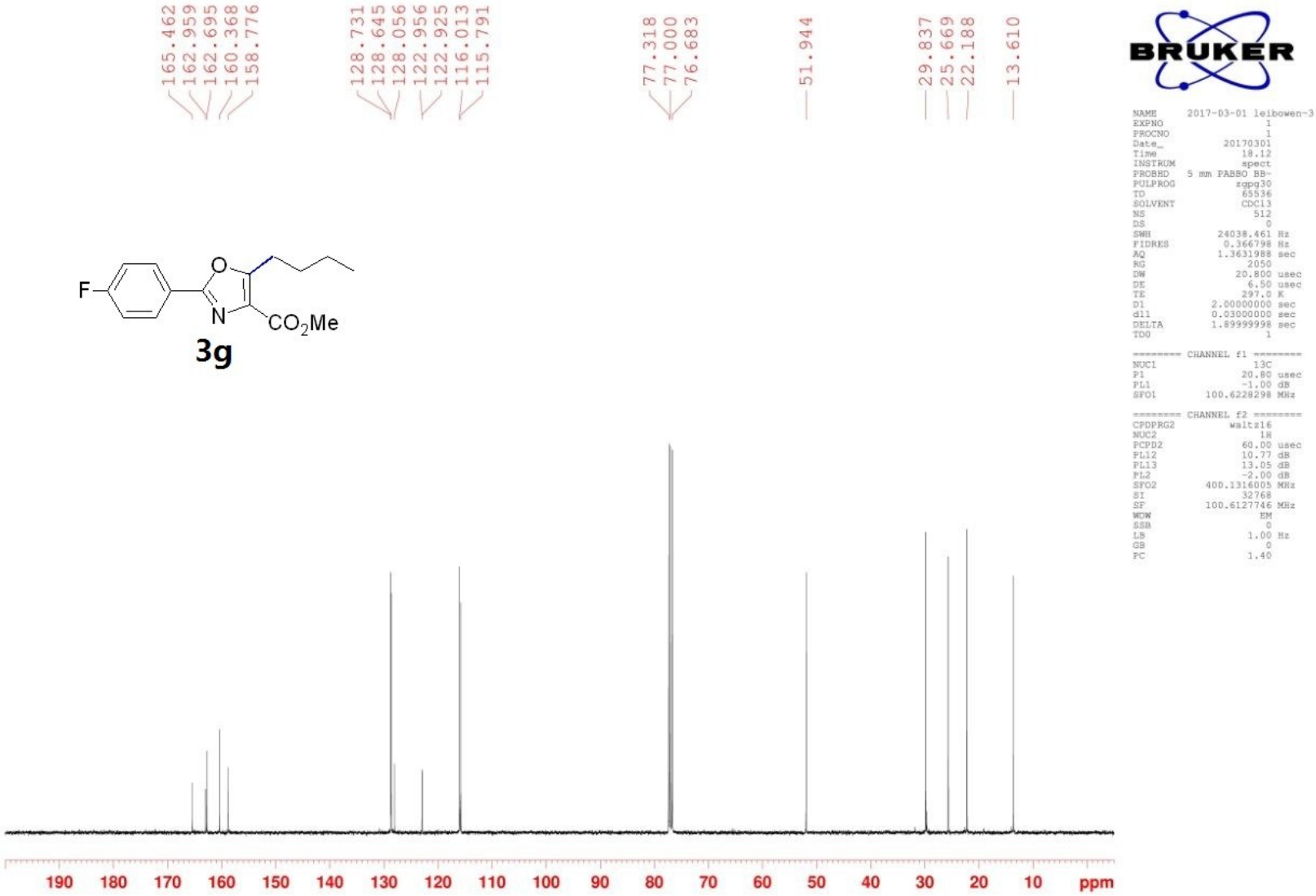
NAME	CLJ-YHY-L005
EXPNO	1
PROCNO	1
Date_	20170302
Time	9.24
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300004 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00


162.748
160.371
159.768
159.480
129.746
128.004
127.736
118.957
117.310
111.046
77.318
77.000
76.682
55.439
51.929
29.821
25.688
22.172
13.608
BRUKER
NAME 2017-03-07 leibowen-5
EXPNO 1
PROCNO 1
Date_ 20170307
Time 19.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 20.80 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 10.77 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127770 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
N
O
CO2Me
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.206
8.186
7.734
7.713
7.278
3.962
3.161
3.142
3.123
1.798
1.780
1.761
1.742
1.723
1.490
1.472
1.453
1.434
1.415
1.397
0.995
0.977
0.958
0.000
BRUKER
NAME CLJ-YHY-L010
EXPNO 1
PROCNO 1
Date_ 20170308
Time 12.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 32.77
DW 62.400 use
DE 6.50 use
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 400.1324710 MHz
NUC1 1H
P1 8.04 use
SI 65536
SF 400.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F3C
O
N
CO2Me
3f
9
8
7
6
5
4
3
2
1
ppm
2.00
2.08
3.06
2.00
2.10
1.99
3.02


162.518
161.095
158.200
132.778
132.454
132.128
131.804
129.731
128.491
126.781
125.806
125.769
125.732
125.695
77.317
76.999
76.682
52.075
29.834
25.762
22.225
13.616
BRUKER
NAME 2017-03-10 leibowen-10
EXPNO 1
PROCNO 1
Date_ 20170310
Time 23.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 20.80 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 10.77 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
F3C
O
N
CO2Me
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.088
8.083
8.075
8.070
8.066
8.058
8.053
7.285
7.166
7.161
7.144
7.127
7.122
3.946
3.131
3.112
3.093
1.779
1.760
1.741
1.722
1.703
1.479
1.461
1.442
1.423
1.405
1.387
0.987
0.968
0.950
0.000
F
O
N
CO2Me
3g
BRUKER
NAME CLJ-YHY-L003
EXPNO 1
PROCNO 1
Date_ 20170224
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 32.77
DW 62.400 use
DE 6.50 use
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 400.1324710 MHz
NUC1 1H
P1 8.04 use
SI 65536
SF 400.1299996 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.00
2.05
3.02
2.01
2.10
2.19
3.17

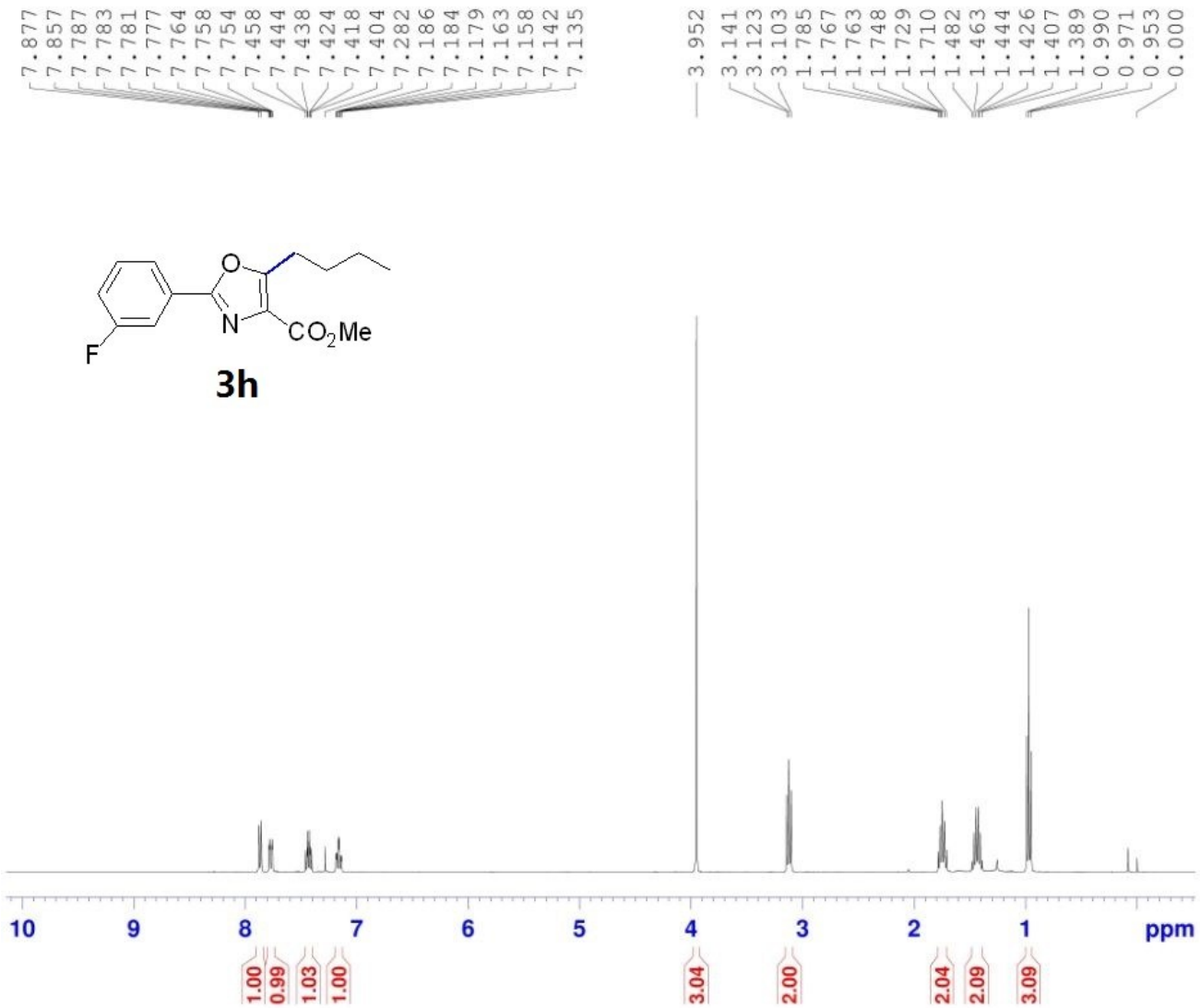


BRUKER

```
NAME          2017-03-01 leibowen-3
EXPNO                    1
PROCNO                   1
Date_             20170301
Time                 18.12
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     512
DS                       0
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    2050
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

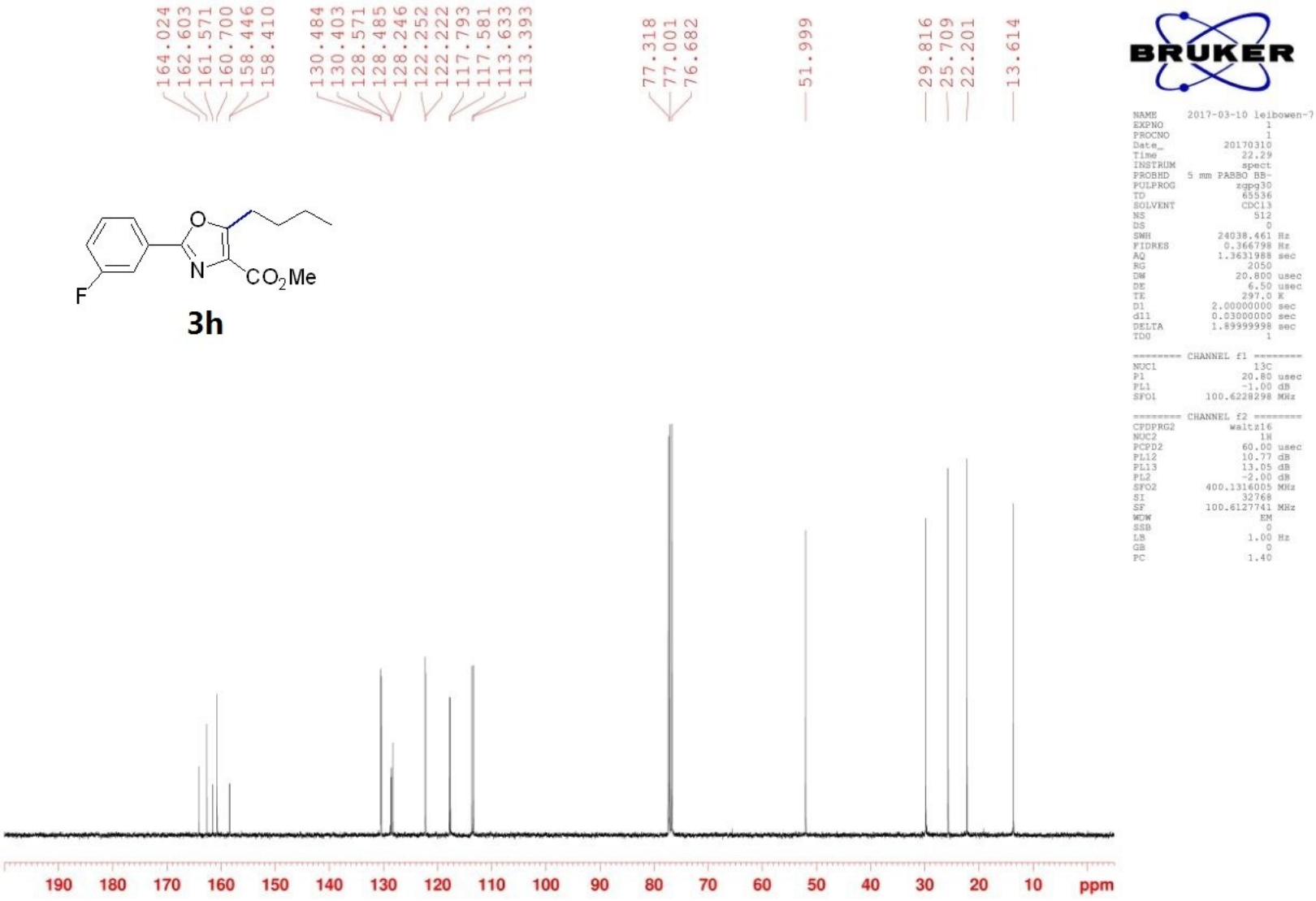
======== CHANNEL f1 ========
NUC1                   13C
P1                20.80 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

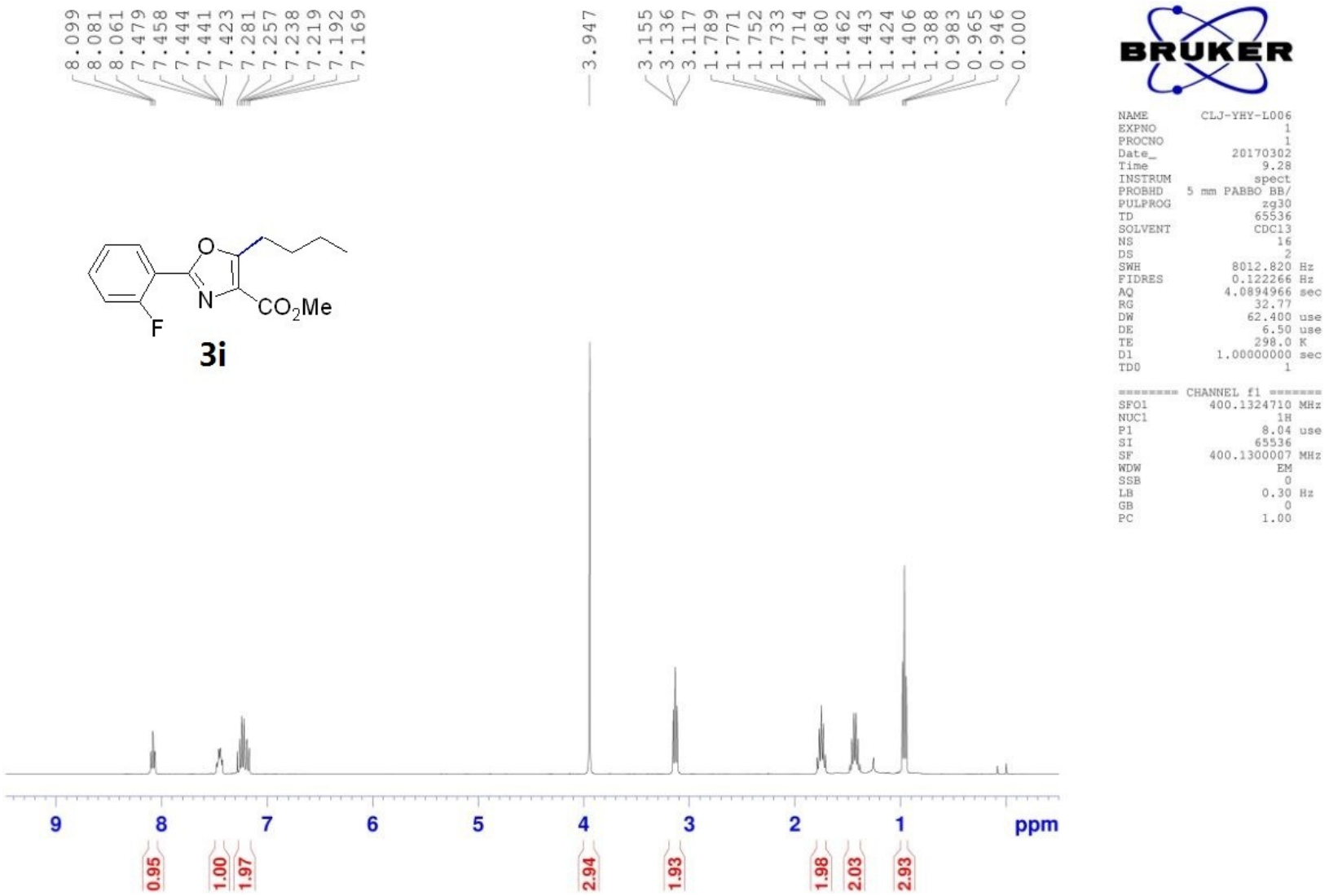
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2             60.00 usec
PL12              10.77 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127746 MHz
WDW                     EM
SSB                      0
LB                1.00 Hz
GB                       0
PC                    1.40
```




```
NAME          CLJ-YHY-L007
EXPNO                    1
PROCNO                   1
Date_             20170308
Time                 12.33
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                    32.77
DW                   62.400 use
DE                    6.50 use
TE                   298.0 K
D1               1.00000000 sec
TD0                      1

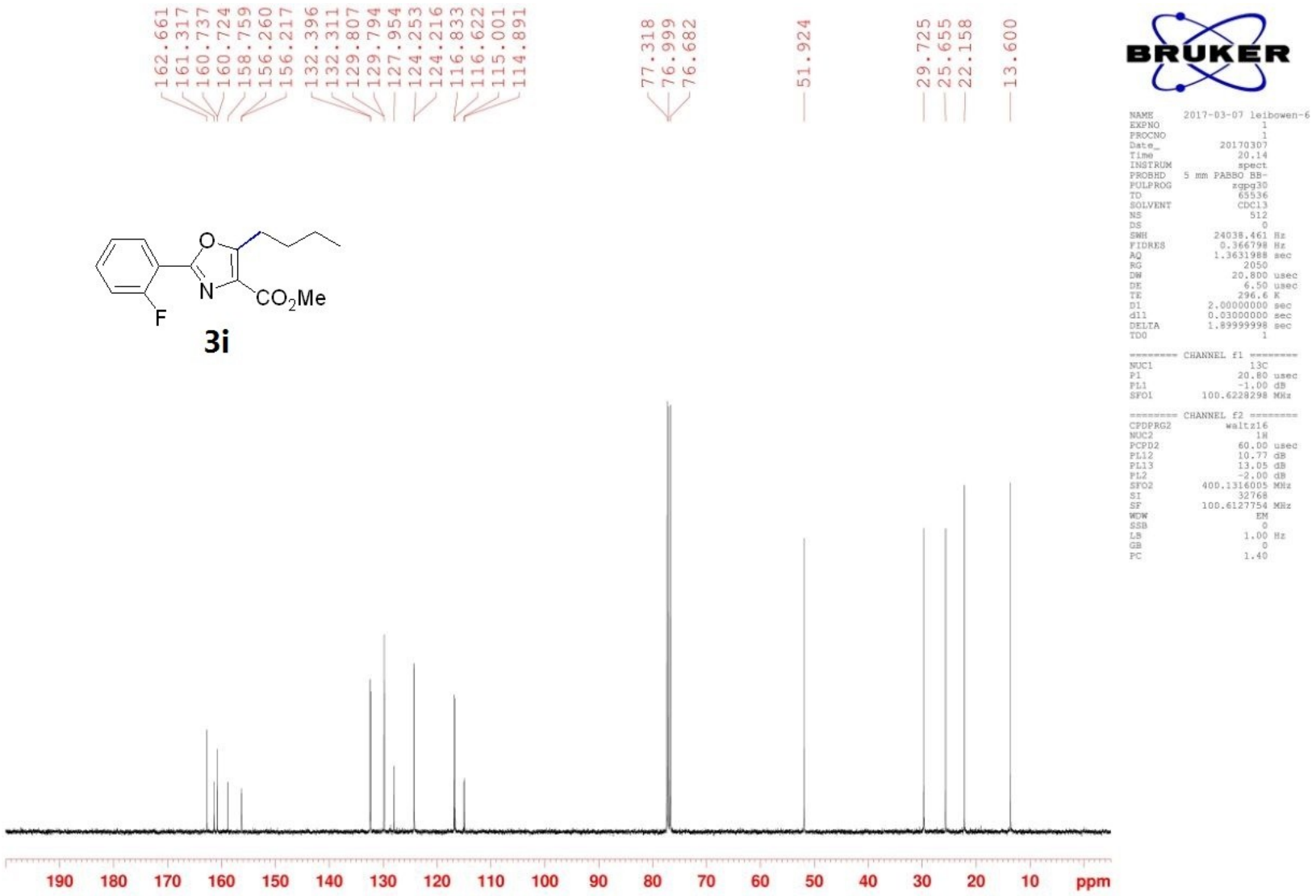
======== CHANNEL f1 =======
SFO1         400.1324710 MHz
NUC1                   1H
P1                   8.04 use
SI                  65536
SF           400.1300004 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

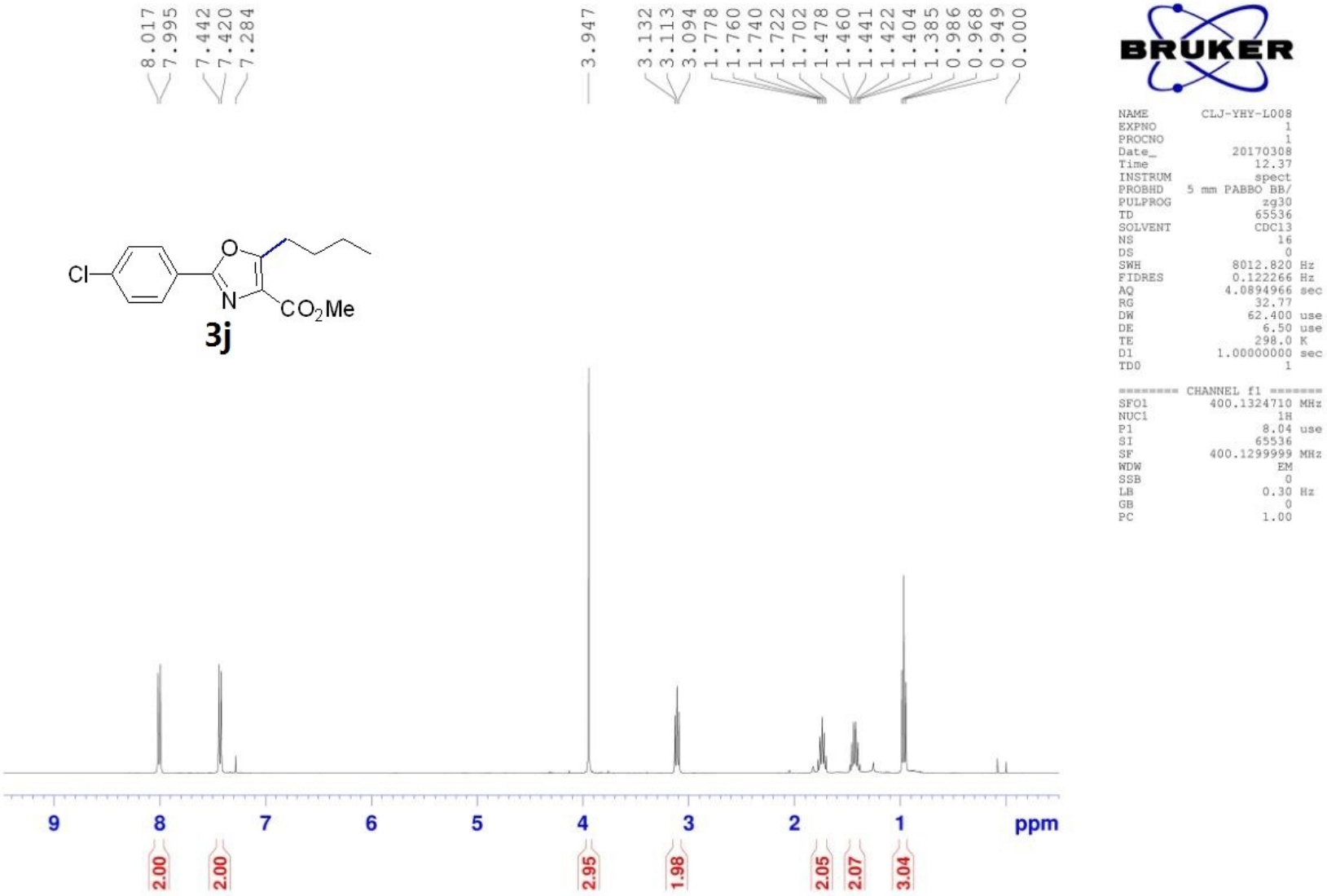

164.024
162.603
161.571
160.700
158.446
158.410
130.484
130.403
128.571
128.485
128.246
122.252
122.222
117.793
117.581
113.633
113.393
77.318
77.001
76.682
51.999
29.816
25.709
22.201
13.614
BRUKER
NAME 2017-03-10 leibowen-7
EXPNO 1
PROCNO 1
Date_ 20170310
Time 22.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 20.80 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 10.77 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127741 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
CO2Me
F
3h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



BRUKER

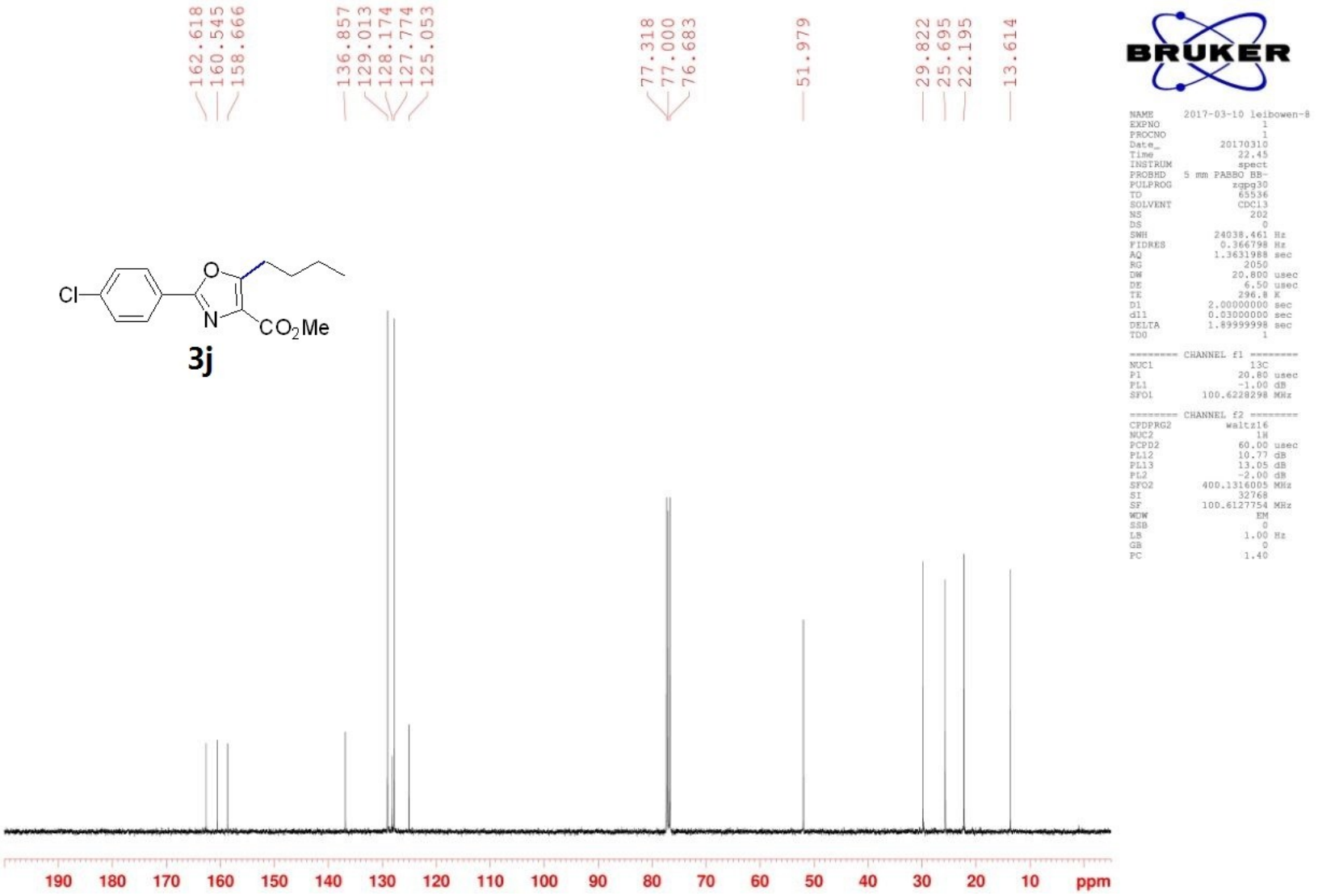
NAME	CLJ-YHY-L006
EXPNO	1
PROCNO	1
Date_	20170302
Time	9.28
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 =======
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300007 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00


162.661
161.317
160.737
160.724
158.759
156.260
156.217
132.396
132.311
129.807
129.794
127.954
124.253
124.216
116.833
116.622
115.001
114.891
77.318
76.999
76.682
51.924
29.725
25.655
22.158
13.600
BRUKER
NAME 2017-03-07 leibowen-6
EXPNO 1
PROCNO 1
Date_ 20170307
Time 20.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 20.80 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 10.77 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
CO2Me
F
3i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



BRUKER

NAME	CLJ-YHY-L008
EXPNO	1
PROCNO	1
Date_	20170308
Time	12.37
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1299999 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

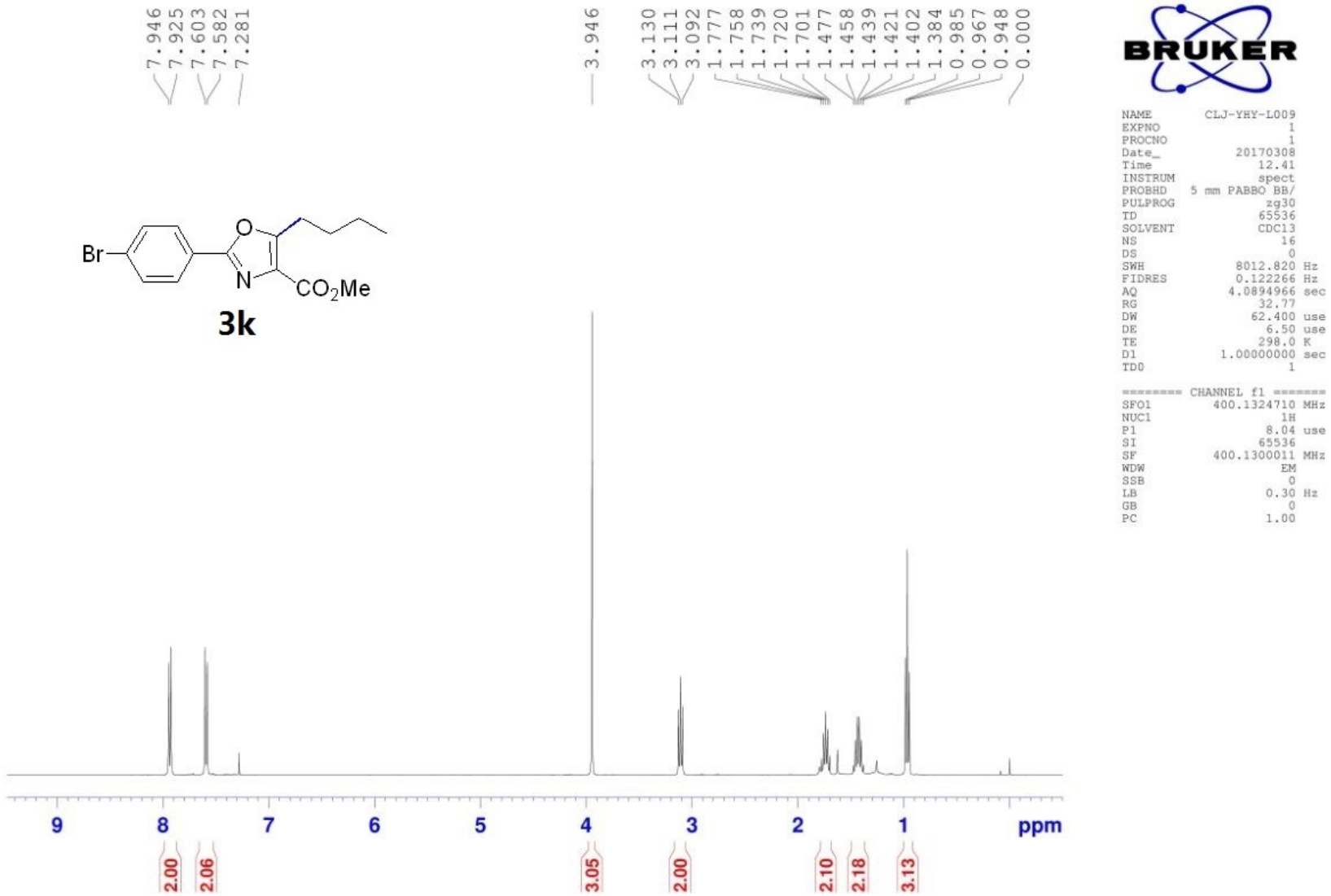


BRUKER

```
NAME          2017-03-10 leibowen-8
EXPNO                    1
PROCNO                   1
Date_             20170310
Time                 22.45
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     202
DS                       0
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    2050
DW                20.800 usec
DE                 6.50 usec
TE                296.8 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

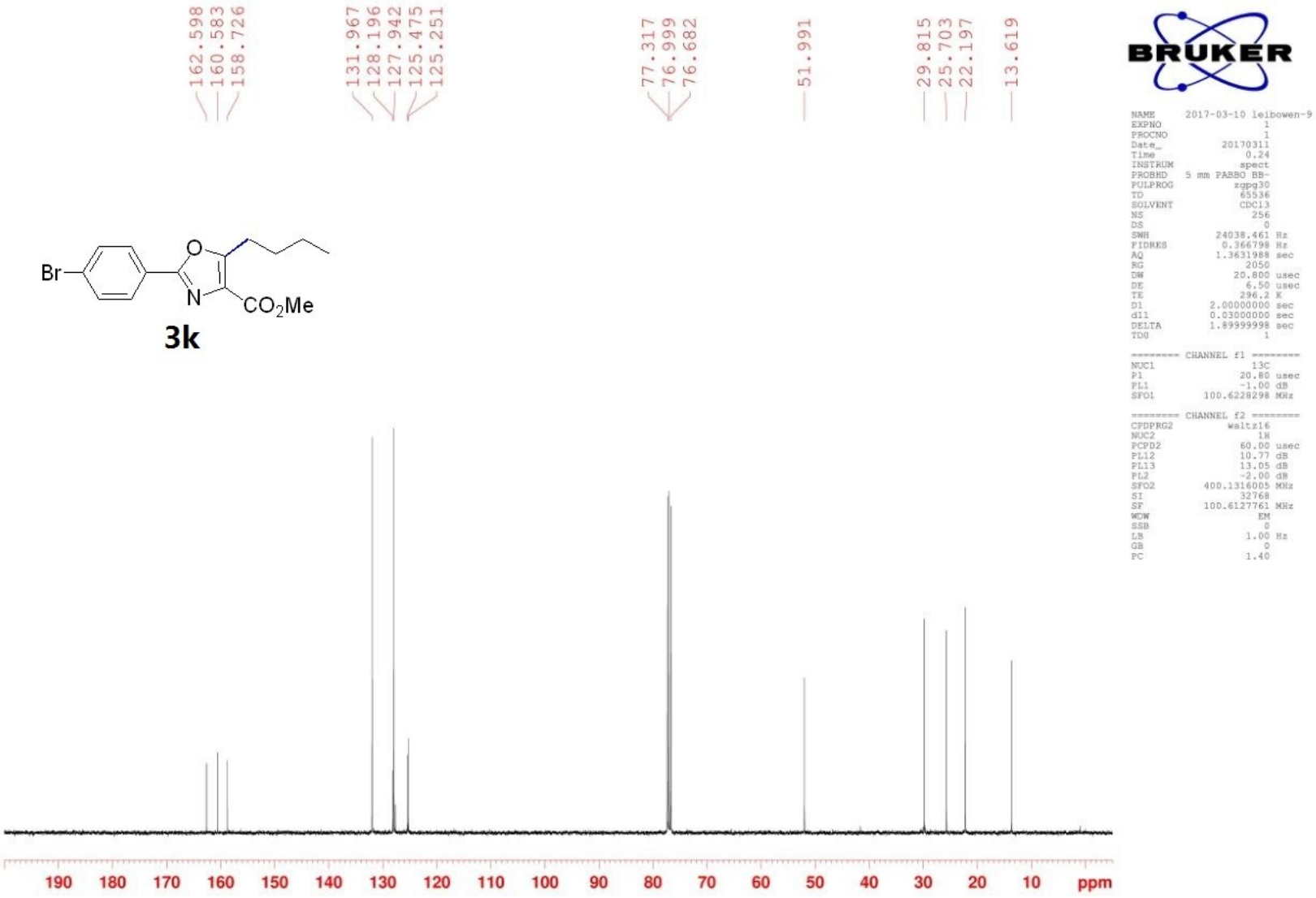
======== CHANNEL f1 ========
NUC1                   13C
P1                20.80 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2             60.00 usec
PL12              10.77 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127754 MHz
WDW                    EM
SSB                     0
LB                1.00 Hz
GB                      0
PC                1.40
```



BRUKER

NAME	CLJ-YHY-L009
EXPNO	1
PROCNO	1
Date_	20170308
Time	12.41
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300011 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

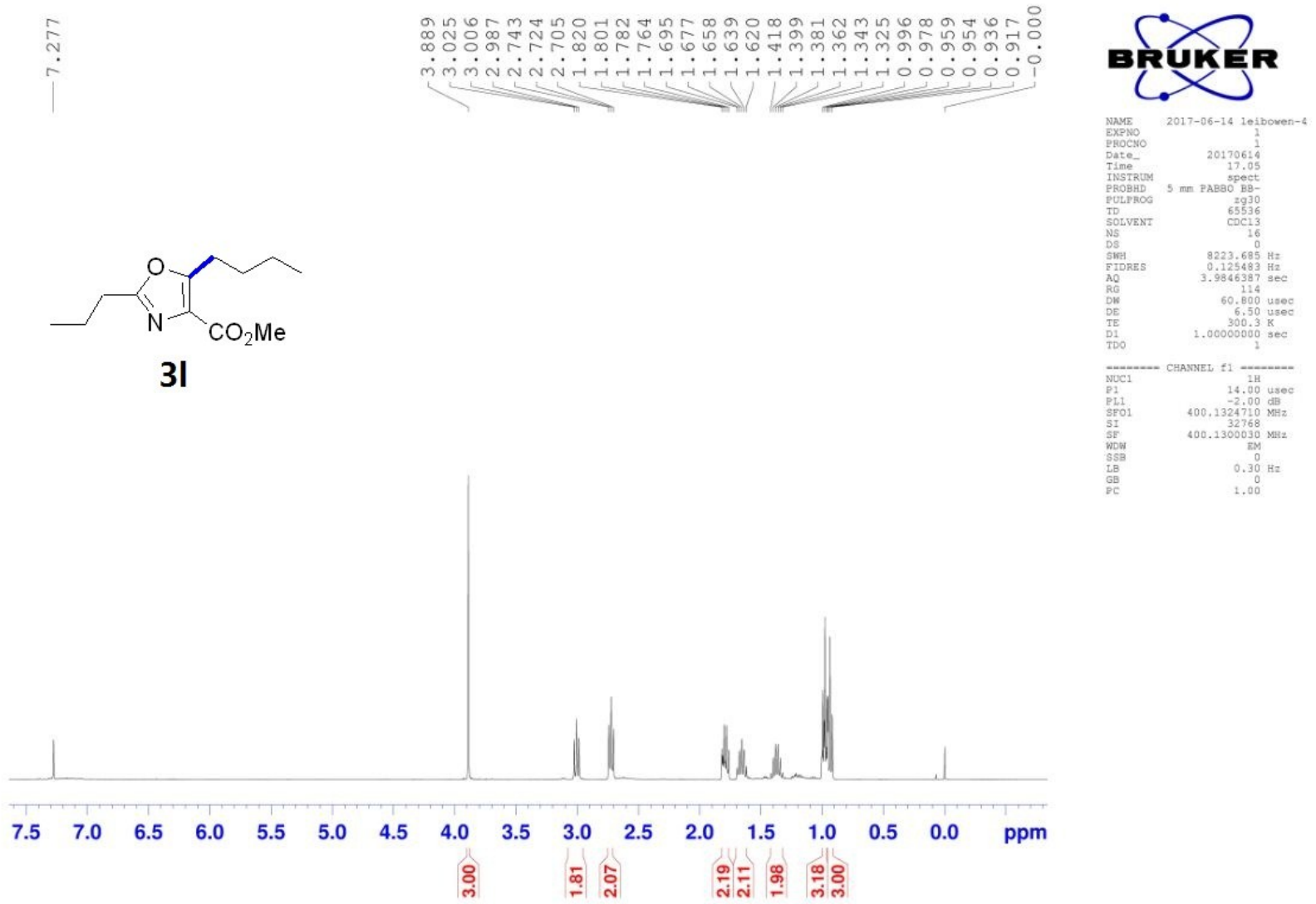


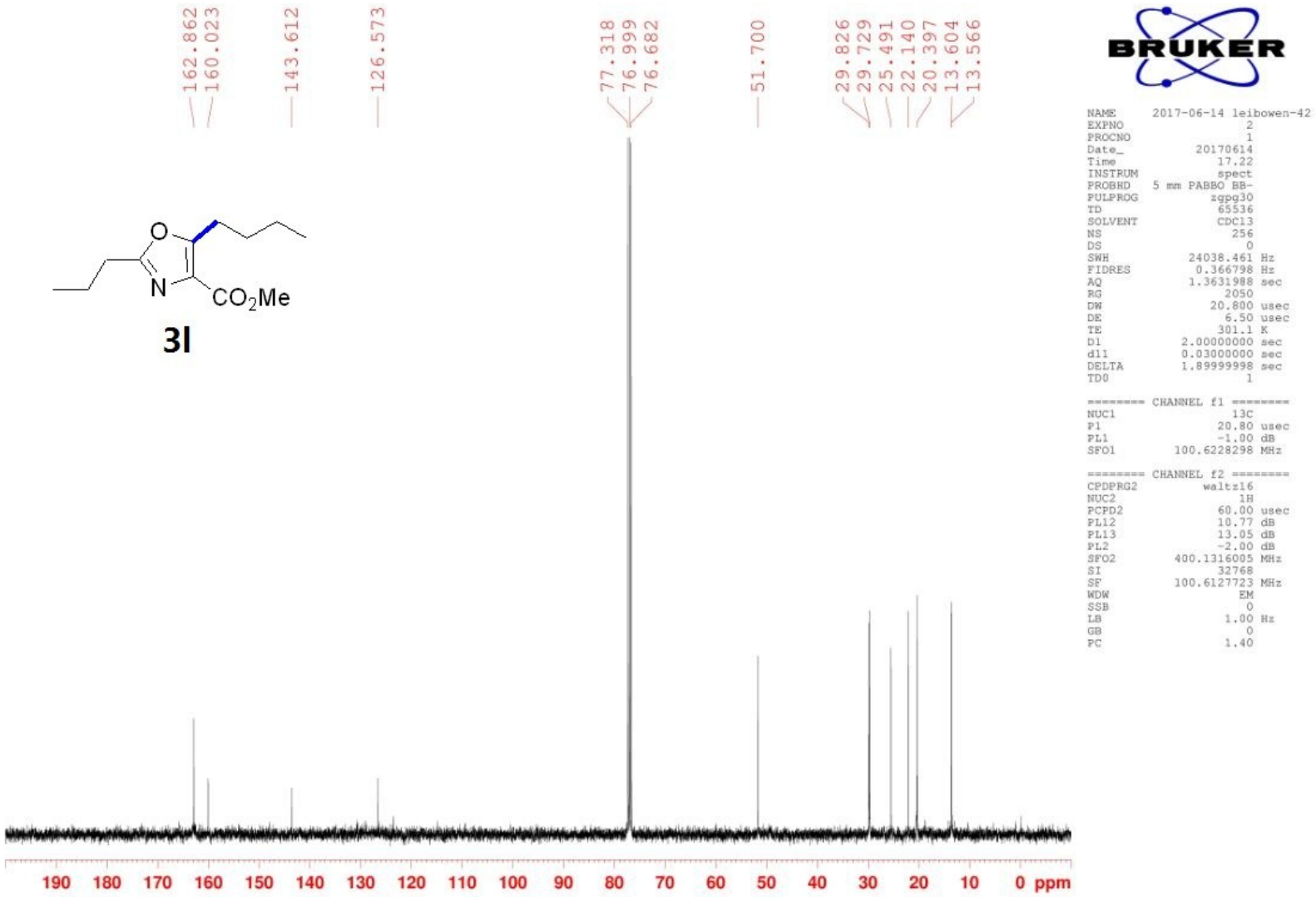
BRUKER

```
NAME          2017-03-10 leibowen-9
EXPNO                    1
PROCNO                   1
Date_             20170311
Time                 0.24
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  2050
DW               20.800 usec
DE                6.50 usec
TE                296.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                20.80 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             60.00 usec
PL12              10.77 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127761 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

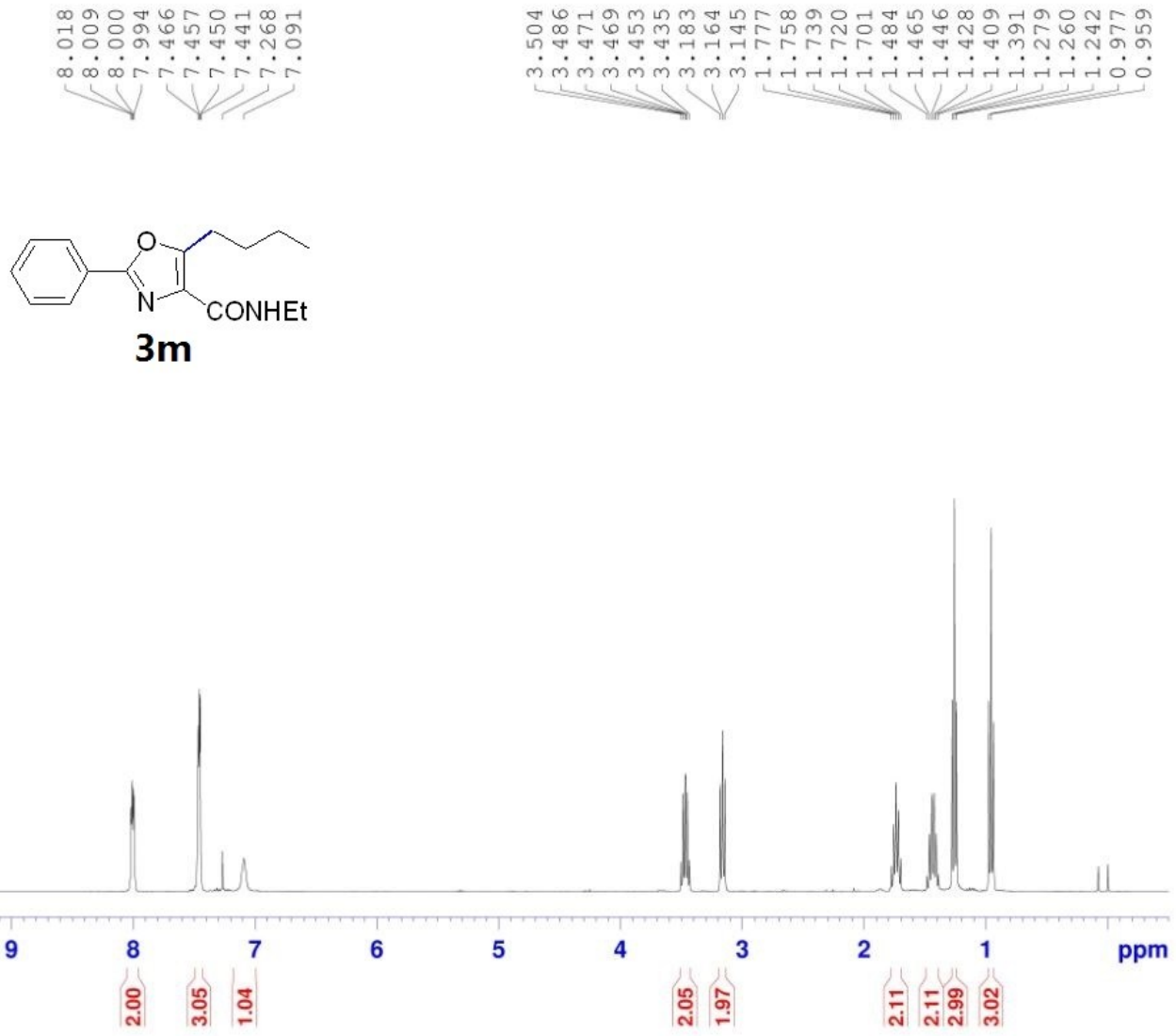

7.277
3.889
3.025
3.006
2.987
2.743
2.724
2.705
1.820
1.801
1.782
1.764
1.695
1.677
1.658
1.639
1.620
1.418
1.399
1.381
1.362
1.343
1.325
0.996
0.978
0.959
0.954
0.936
0.917
0.000
O
N
CO2Me
3l
BRUKER
NAME 2017-06-14 leibowen-4
EXPNO 1
PROCNO 1
Date_ 20170614
Time 17.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
TDO 1
-------- CHANNEL f1 --------
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
SI 32768
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
3.00
1.81
2.07
2.19
2.11
1.98
3.18
3.00

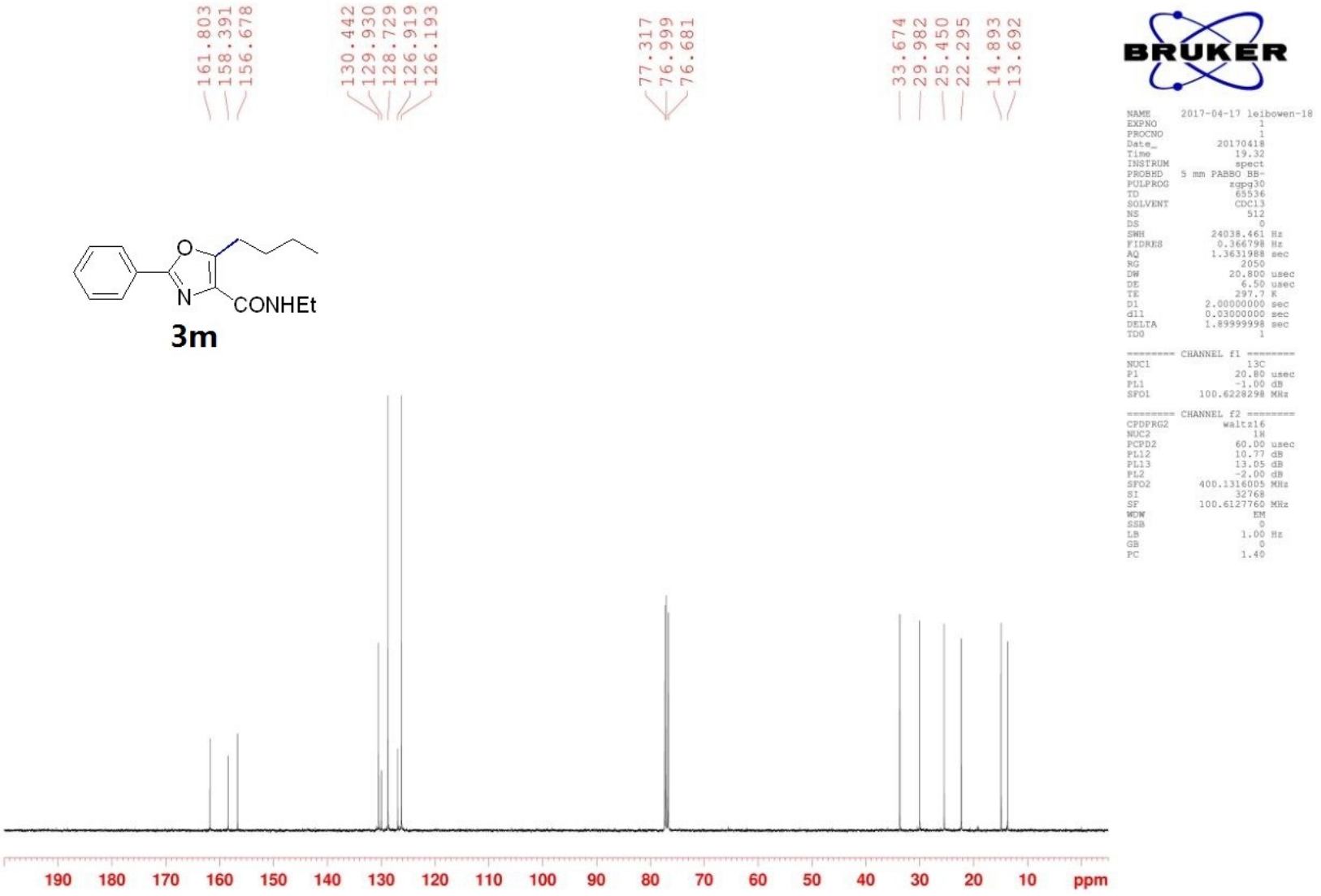



```
NAME          2017-06-14 leibowen-42
EXPNO                            2
PROCNO                           1
Date_                     20170614
Time                         17.22
INSTRUM                      spect
PROBHD       5 mm PABBO BB-
PULPROG                   zgpg30
TD                            65536
SOLVENT                     CDCl3
NS                              256
DS                                0
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631988 sec
RG                             2050
DW                       20.800 usec
DE                        6.50 usec
TE                         301.1 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                           13C
P1                       20.80 usec
PL1                       -1.00 dB
SFO1                 100.6228298 MHz

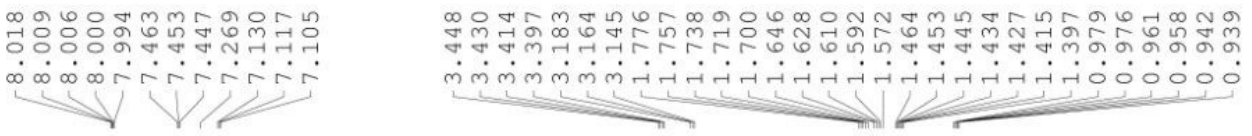
======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                    60.00 usec
PL12                      10.77 dB
PL13                      13.05 dB
PL2                       -2.00 dB
SFO2                400.1316005 MHz
SI                            32768
SF                  100.6127723 MHz
WDW                            EM
SSB                               0
LB                        1.00 Hz
GB                                0
PC                             1.40
```

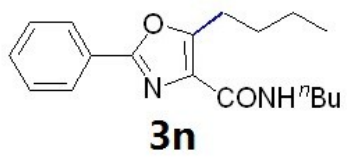

8.018
8.009
8.000
7.994
7.466
7.457
7.450
7.441
7.268
7.091
3.504
3.486
3.471
3.469
3.453
3.435
3.183
3.164
3.145
1.777
1.758
1.739
1.720
1.701
1.484
1.465
1.446
1.428
1.409
1.391
1.279
1.260
1.242
0.977
0.959
O
N
CONHEt
3m
BRUKER
NAME CLJ-YHY-L018
EXPNO 1
PROCNO 1
Date_ 20170406
Time 17.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 32.77
DW 62.400 use
DE 6.50 use
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 400.1324710 MHz
NUC1 1H
P1 8.04 use
SI 65536
SF 400.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.00
3.05
1.04
2.05
1.97
2.11
2.11
2.99
3.02



BRUKER

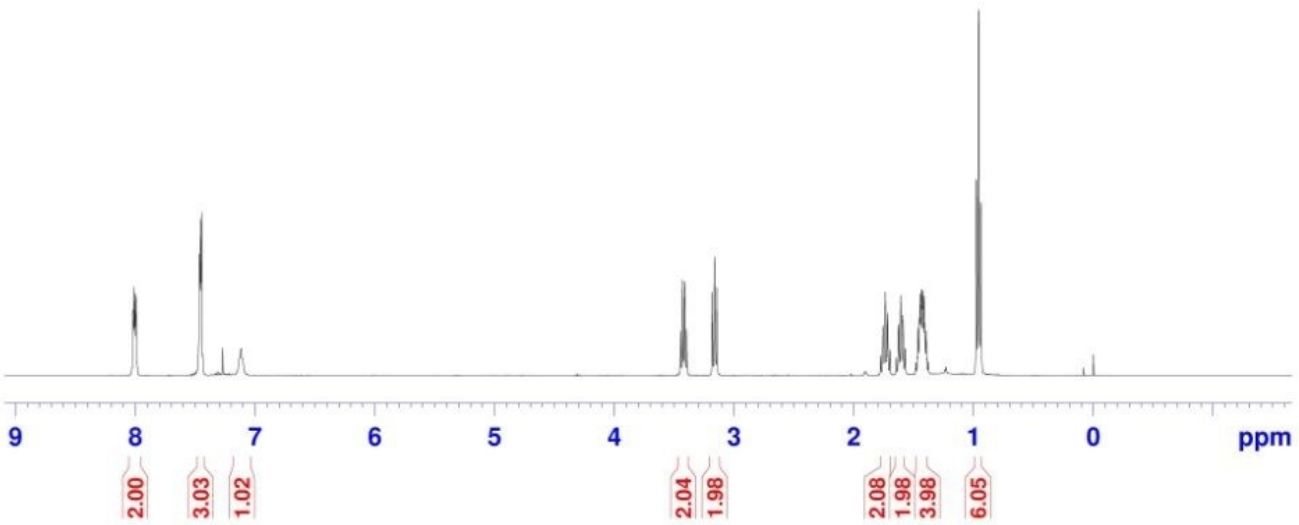
NAME	2017-04-17 leibowen-18
EXPNO	1
PROCNO	1
Date_	20170418
Time	19.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127760 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

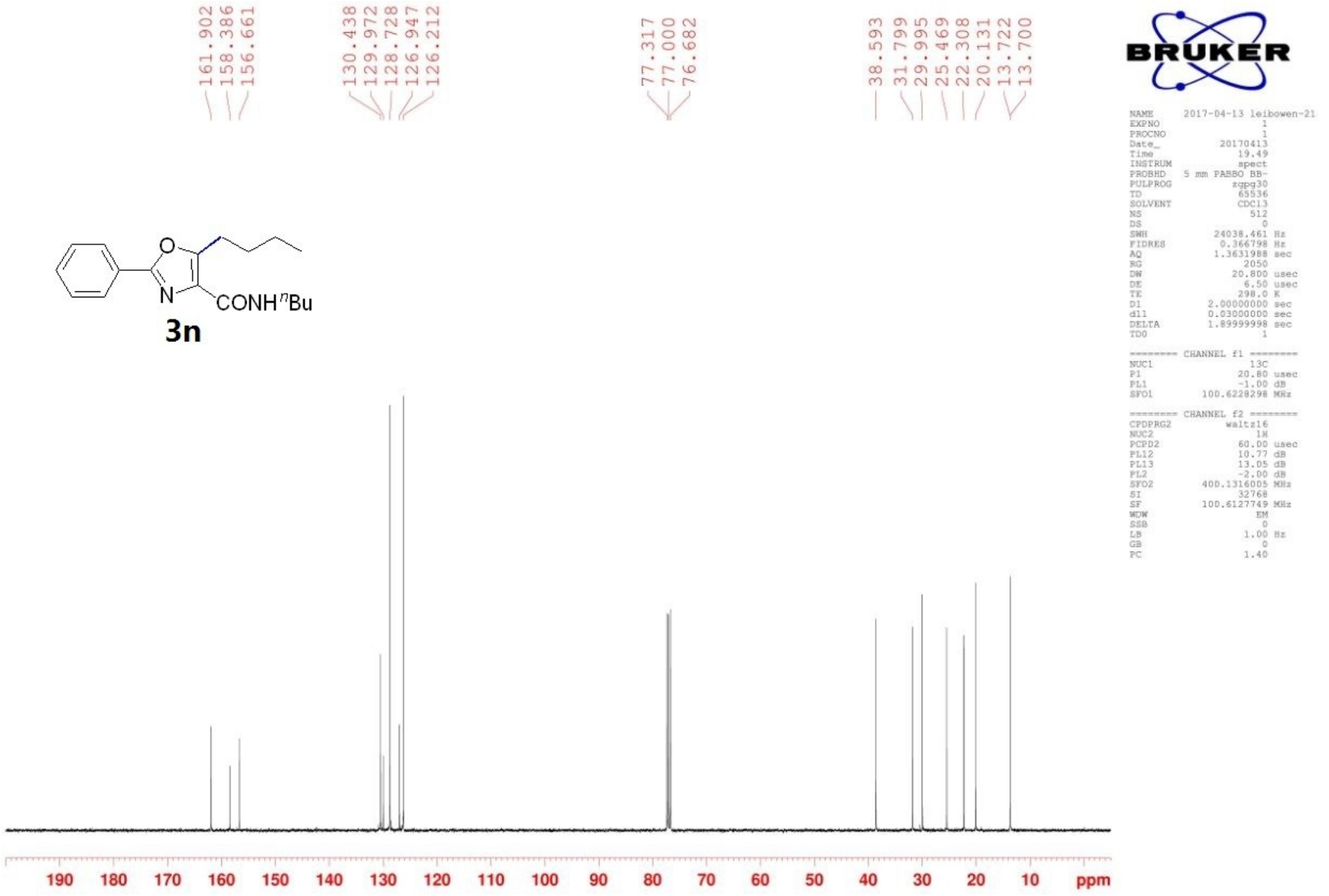




3n

NAME	CLJ-YHY-L021
EXPNO	1
PROCNO	1
Date_	20170411
Time	16.46
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300057 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



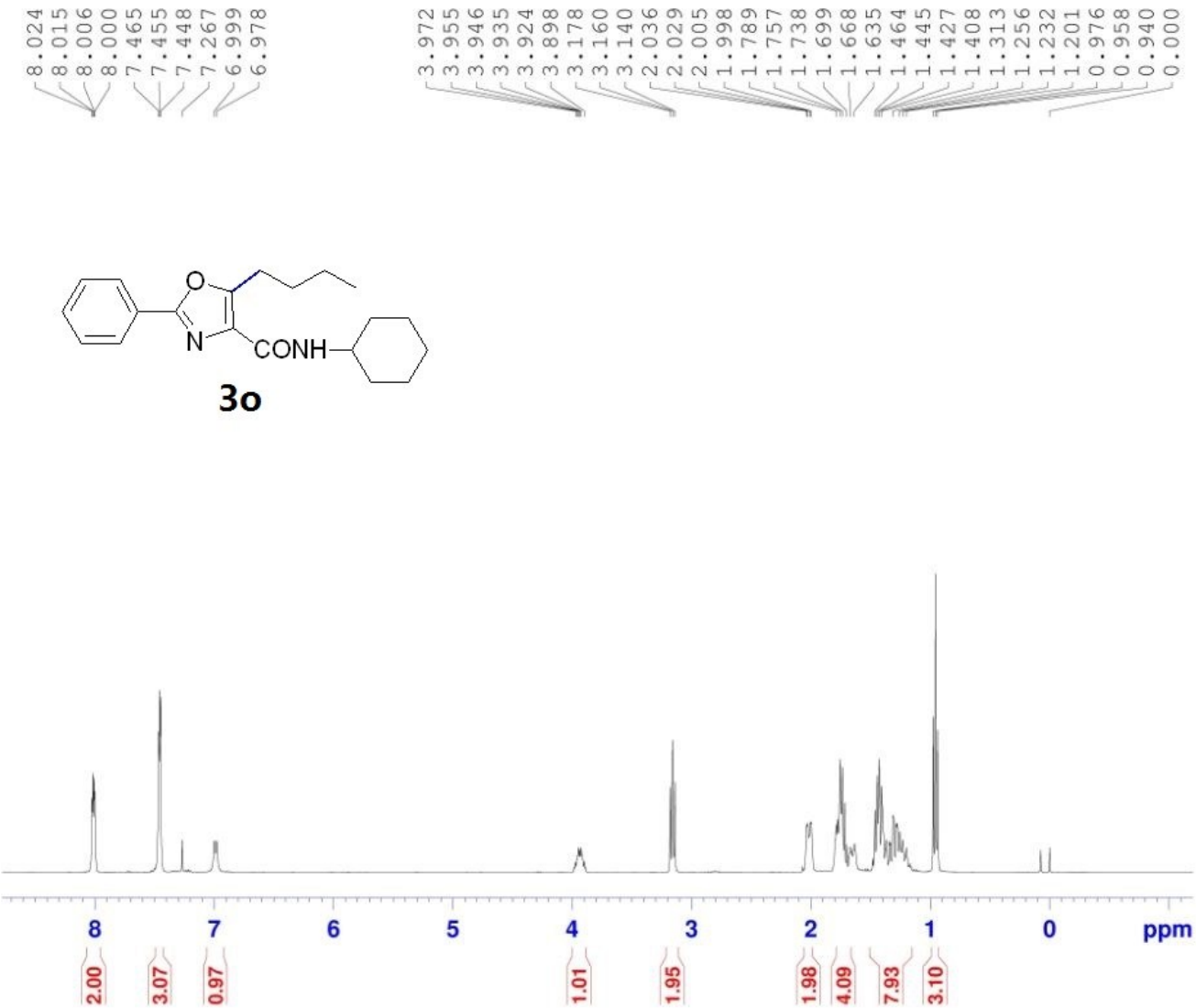


BRUKER

```
NAME          2017-04-13 leibowen-21
EXPNO                              1
PROCNO                             1
Date_                       20170413
Time                           19.49
INSTRUM                        spect
PROBHD     5 mm PABBO BB-
PULPROG                     zgpg30
TD                              65536
SOLVENT                         CDCl3
NS                                512
DS                                  0
SWH                       24038.461 Hz
FIDRES                        0.366798 Hz
AQ                         1.3631988 sec
RG                               2050
DW                             20.800 usec
DE                              6.50 usec
TE                            298.0 K
D1                        2.00000000 sec
d11                       0.03000000 sec
DELTA                     1.89999998 sec
TD0                                1

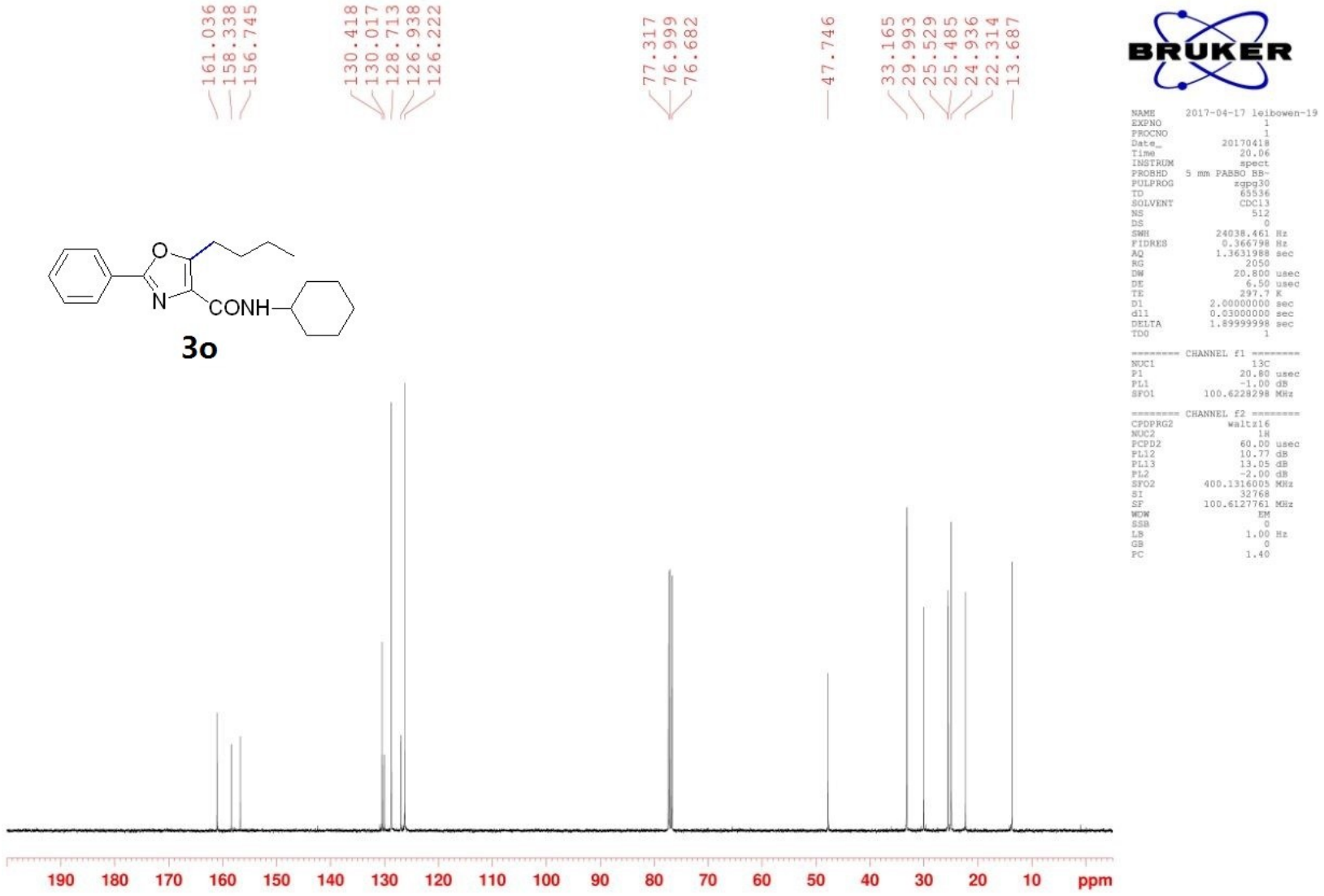
======== CHANNEL f1 ========
NUC1                             13C
P1                             20.80 usec
PL1                            -1.00 dB
SFO1                    100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                     waltz16
NUC2                             1H
PCPD2                          60.00 usec
PL12                           10.77 dB
PL13                           13.05 dB
PL2                            -2.00 dB
SFO2                    400.1316005 MHz
SI                               32768
SF                      100.6127749 MHz
WDW                                EM
SSB                                0
LB                             1.00 Hz
GB                                 0
PC                              1.40
```



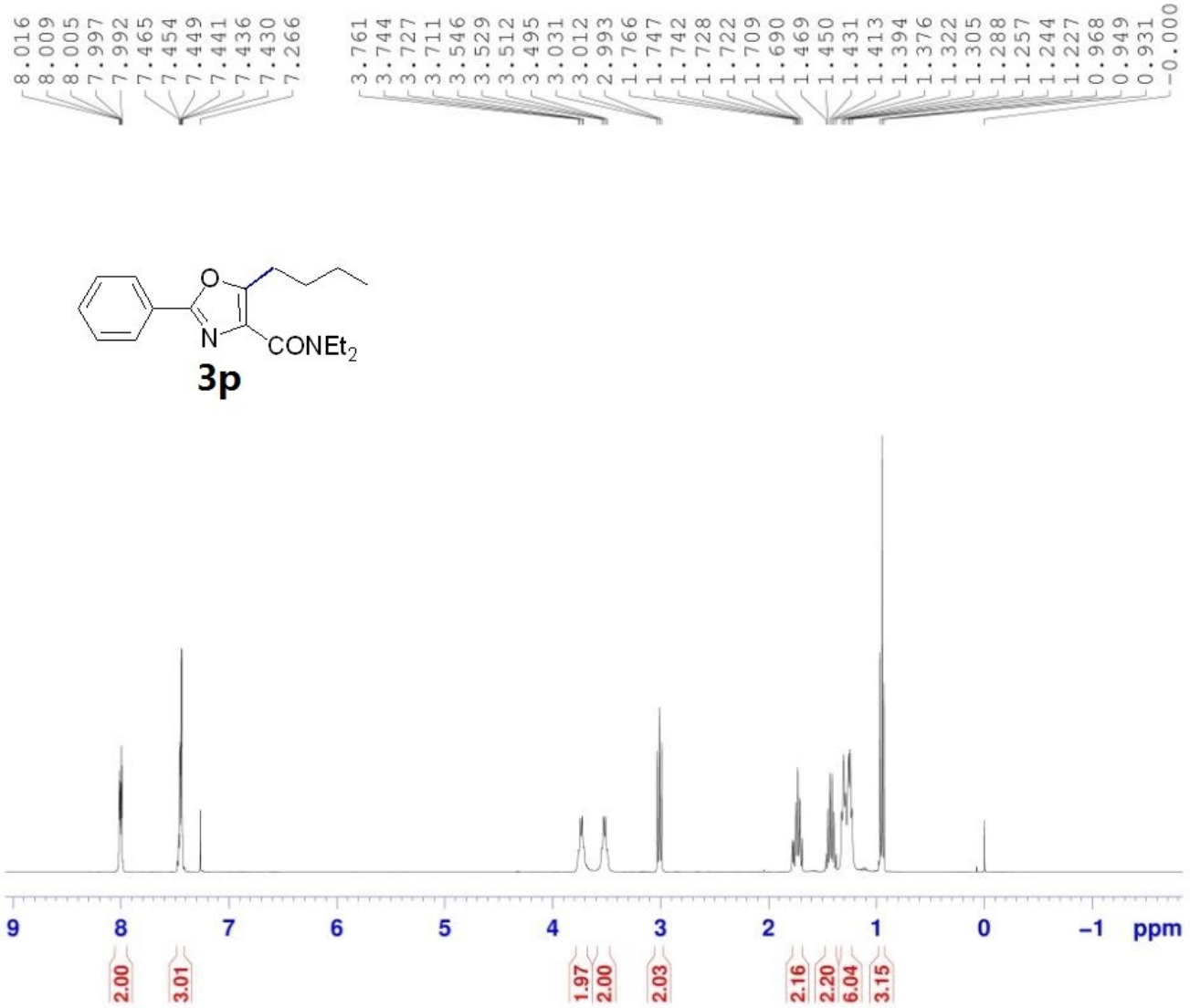
BRUKER

NAME	CLJ-YHY-L019
EXPNO	1
PROCNO	1
Date_	20170406
Time	18.03
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300067 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



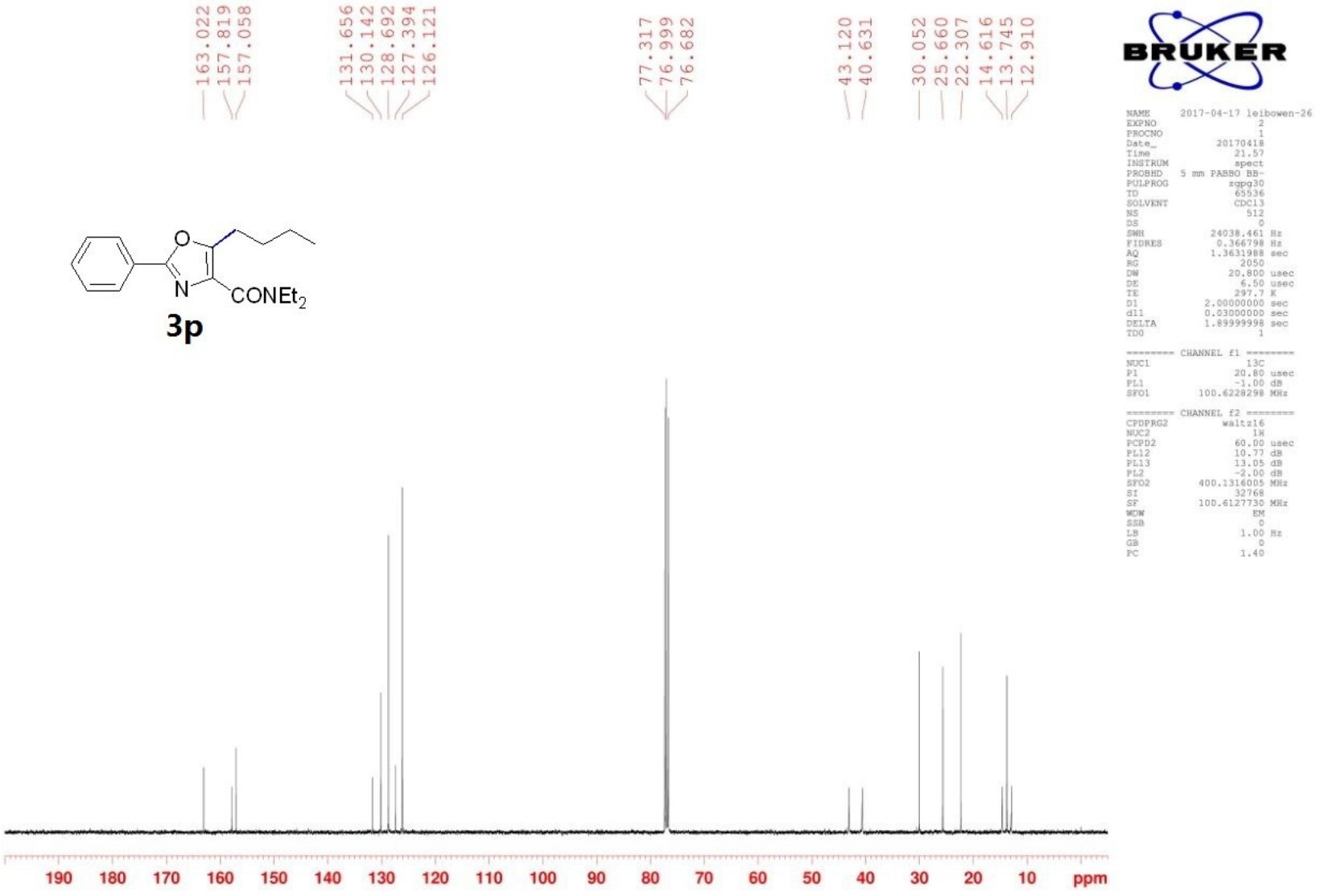
BRUKER

NAME	2017-04-17 leibowen-19
EXPNO	1
PROCNO	1
Date_	20170418
Time	20.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127761 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



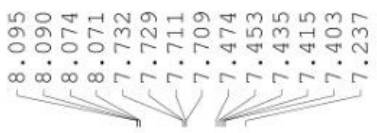
BRUKER

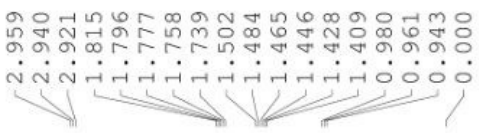
NAME	2017-04-17 leibowen-2
EXPNO	1
PROCNO	1
Date_	20170418
Time	21.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
--------	CHANNEL f1 --------
NUC1	1H
P1	14.00 usec
PL1	-2.00 dB
SFO1	400.1324710 MHz
SI	32768
SF	400.1300070 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

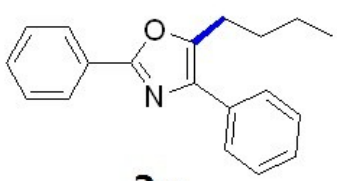


BRUKER

NAME	2017-04-17 leibowen-26
EXPNO	2
PROCNO	1
Date_	20170418
Time	21.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127730 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



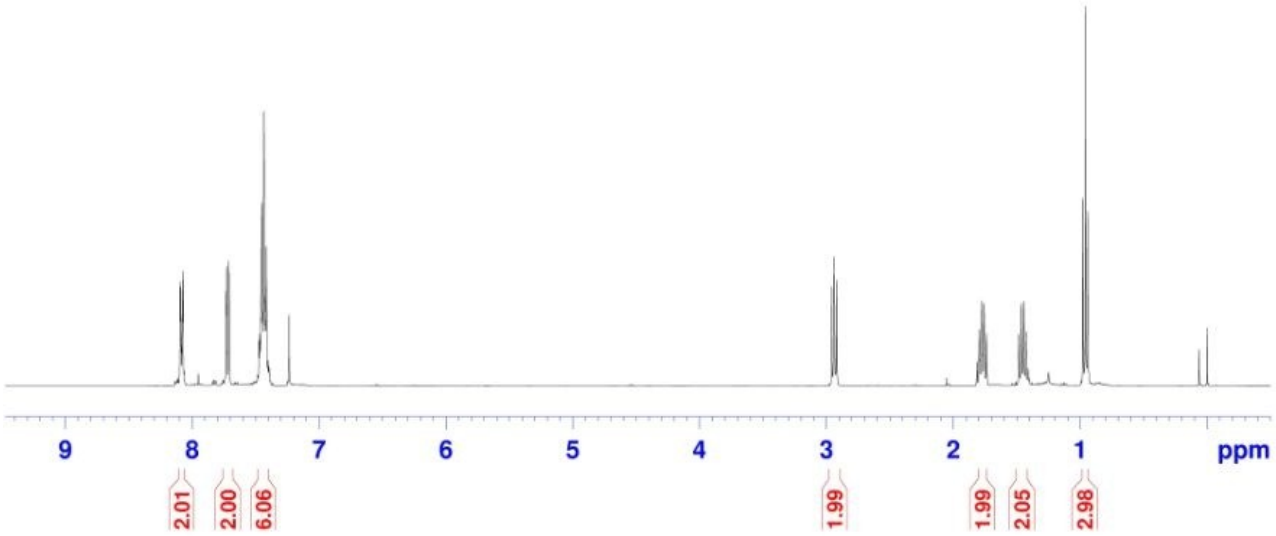


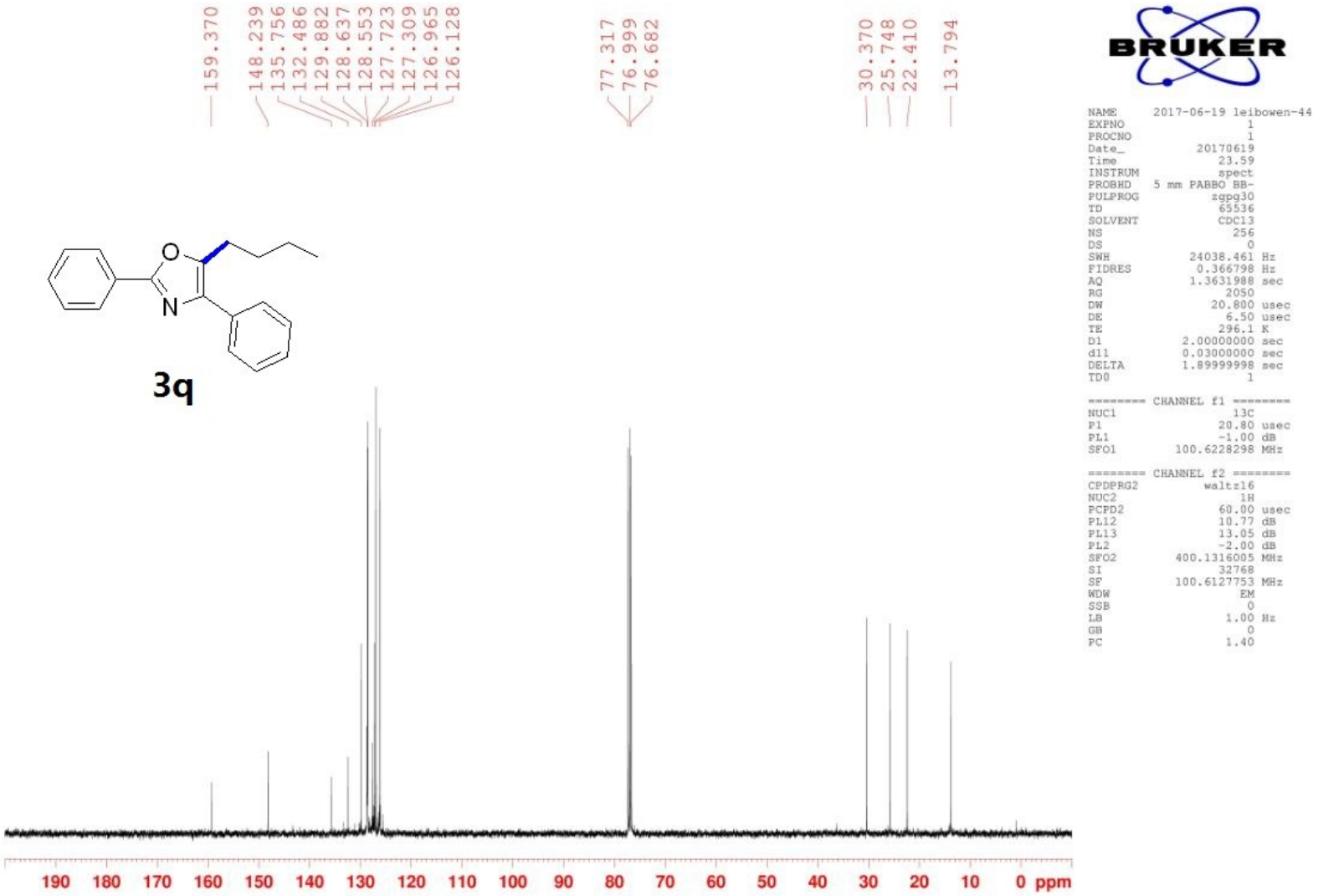


3q


```
NAME            CLJ-YHY-L044
EXPNO                      1
PROCNO                     1
Date_               20170616
Time                   16.31
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894966 sec
RG                     32.77
DW                     62.400 use
DE                      6.50 use
TE                     300.0 K
D1                1.00000000 sec
TD0                        1

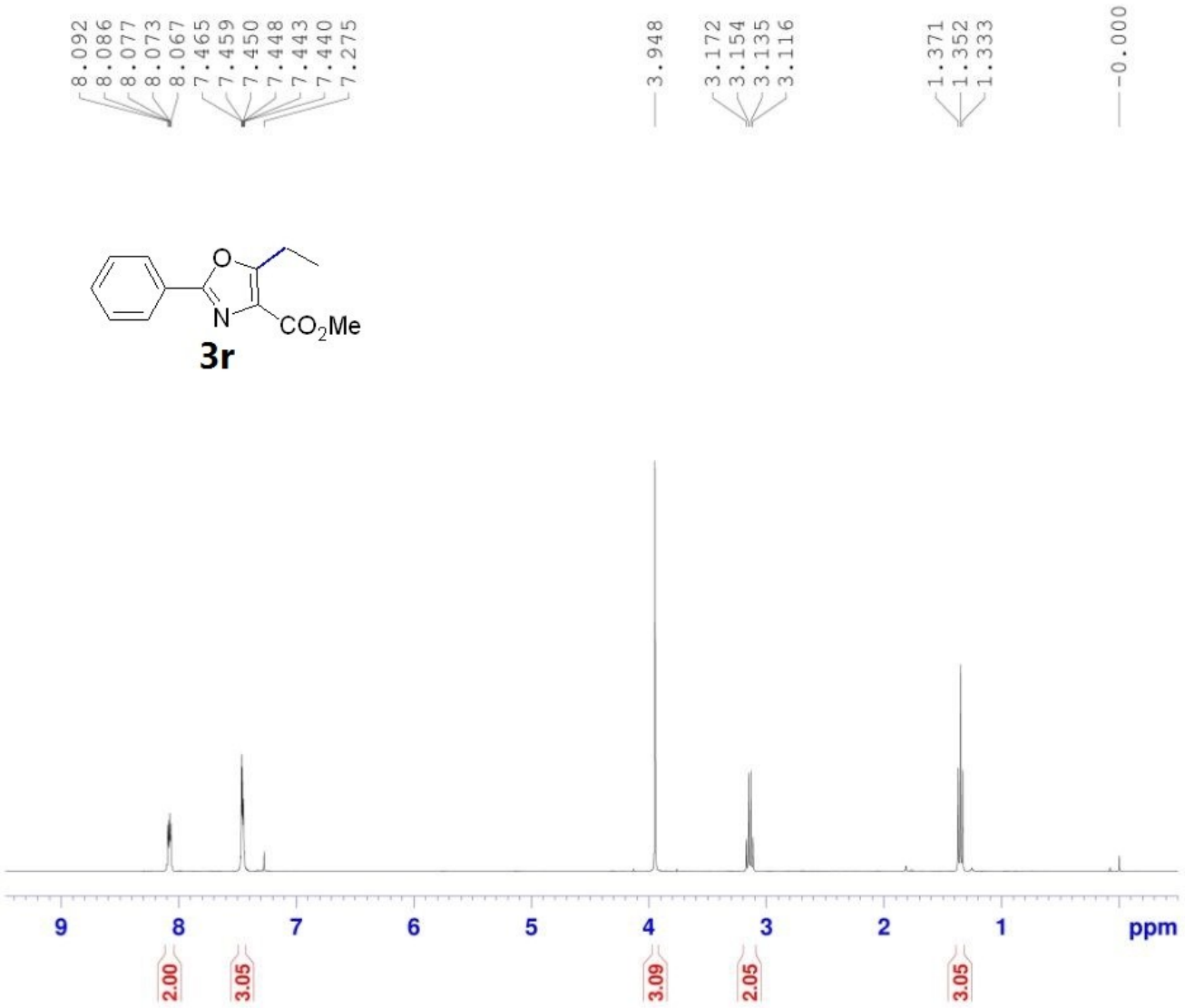
======== CHANNEL f1 =======
SFO1           400.1324710 MHz
NUC1                     1H
P1                     8.04 use
SI                    65536
SF             400.1300186 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```





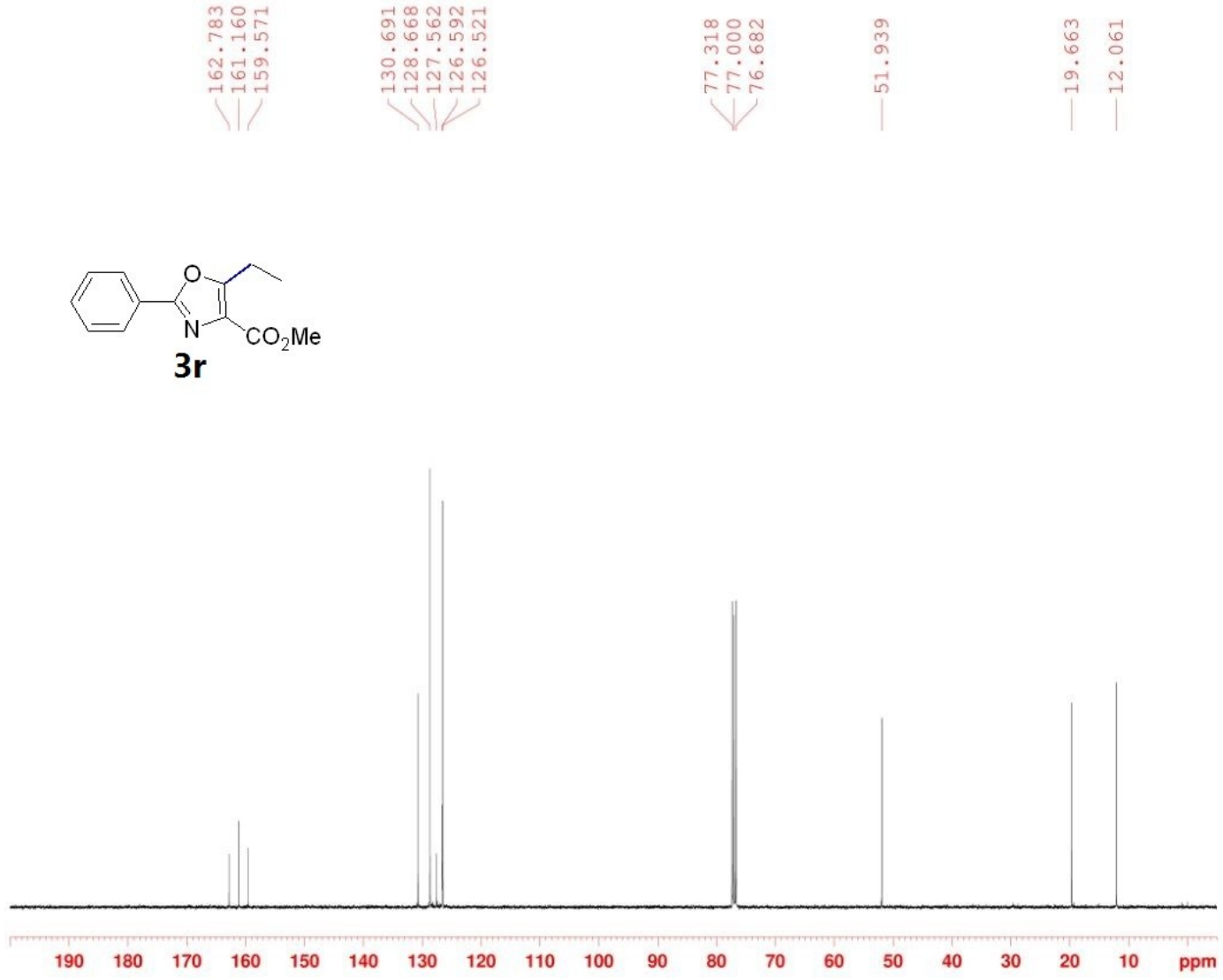
BRUKER

NAME	2017-06-19 leibowen-44
EXPNO	1
PROCNO	1
Date_	20170619
Time	23.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127753 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	CLJ-YHY-L016
EXPNO	1
PROCNO	1
Date_	20170320
Time	12.05
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300036 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

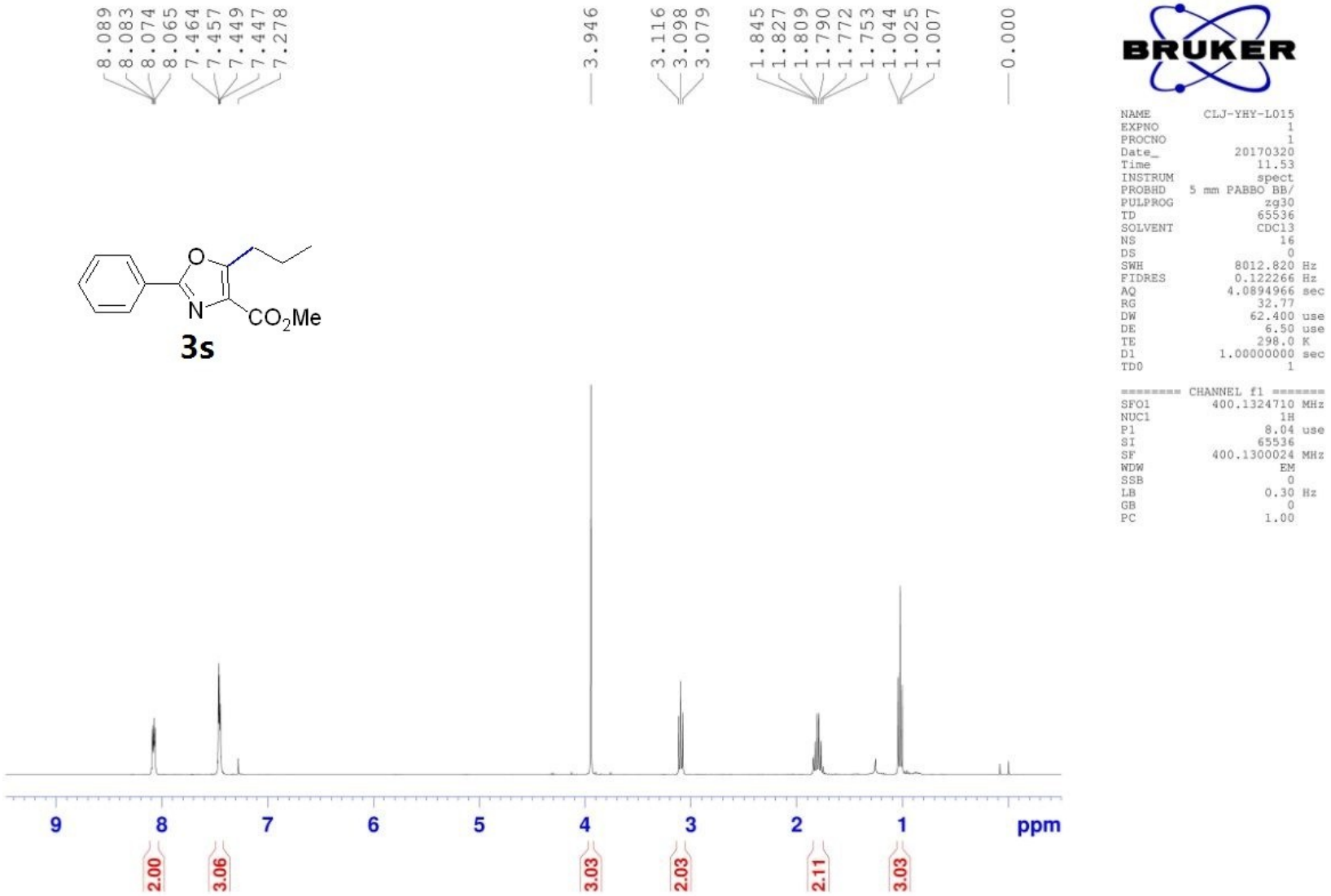


BRUKER

```
NAME          2017-03-23 leibowen-16
EXPNO                    1
PROCNO                   1
Date_             20170324
Time                  1.27
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     0
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

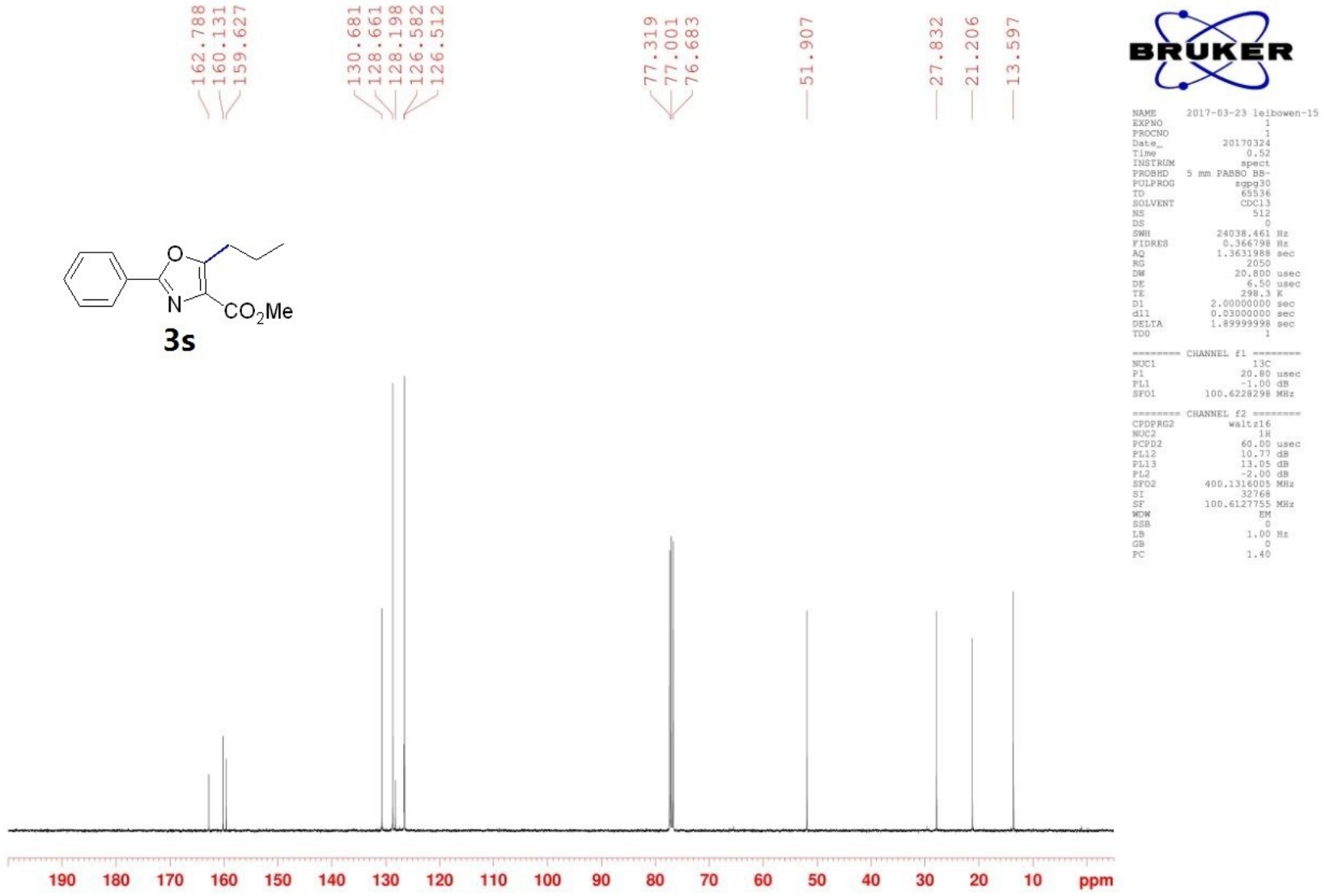
======== CHANNEL f1 ========
NUC1                13C
P1                20.80 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             60.00 usec
PL12              10.77 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127747 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```



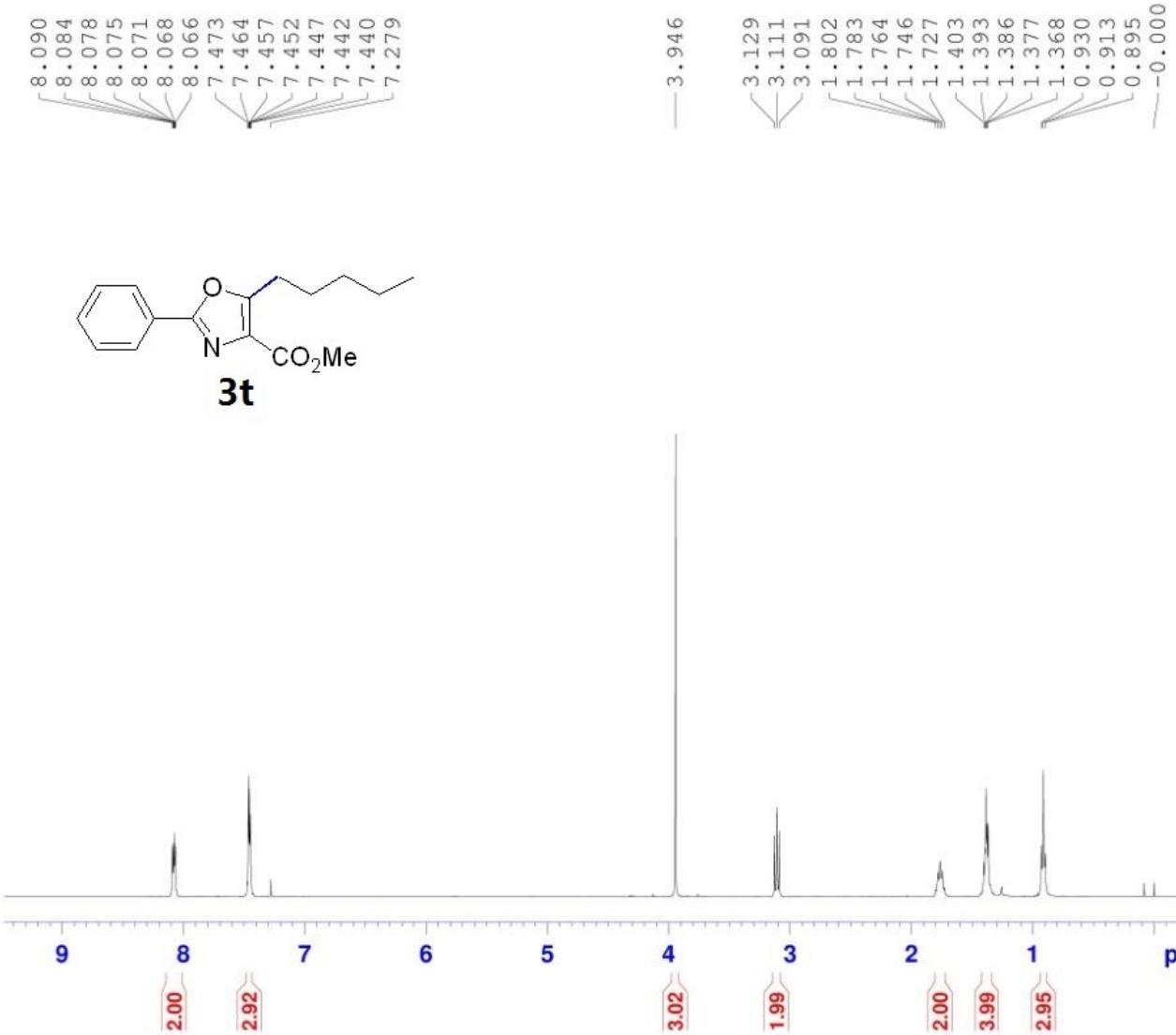
BRUKER

NAME	CLJ-YHY-L015
EXPNO	1
PROCNO	1
Date_	20170320
Time	11.53
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 =======
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300024 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



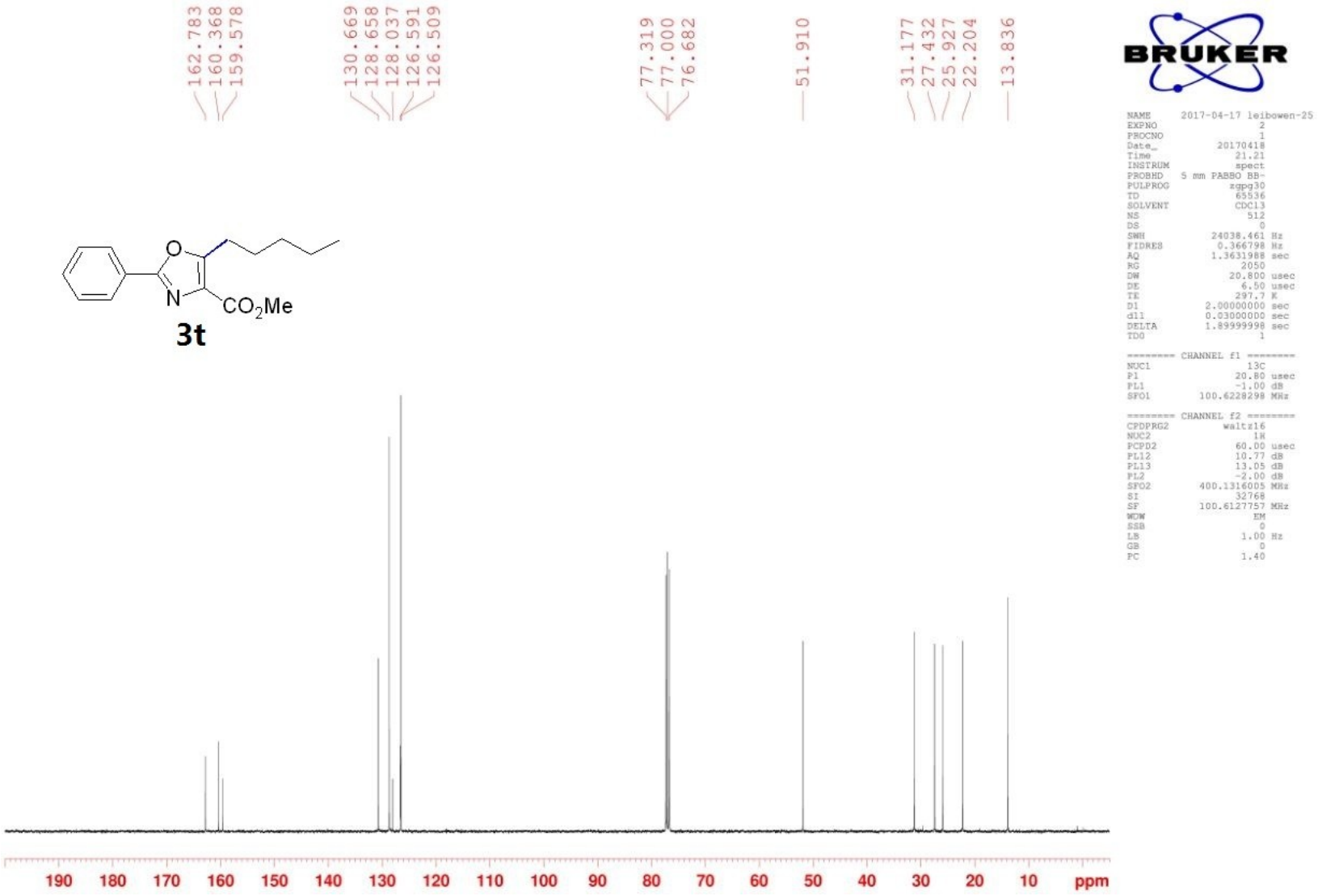
BRUKER

NAME	2017-03-23 leibowen-15
EXPNO	1
PROCNO	1
Date_	20170324
Time	0.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



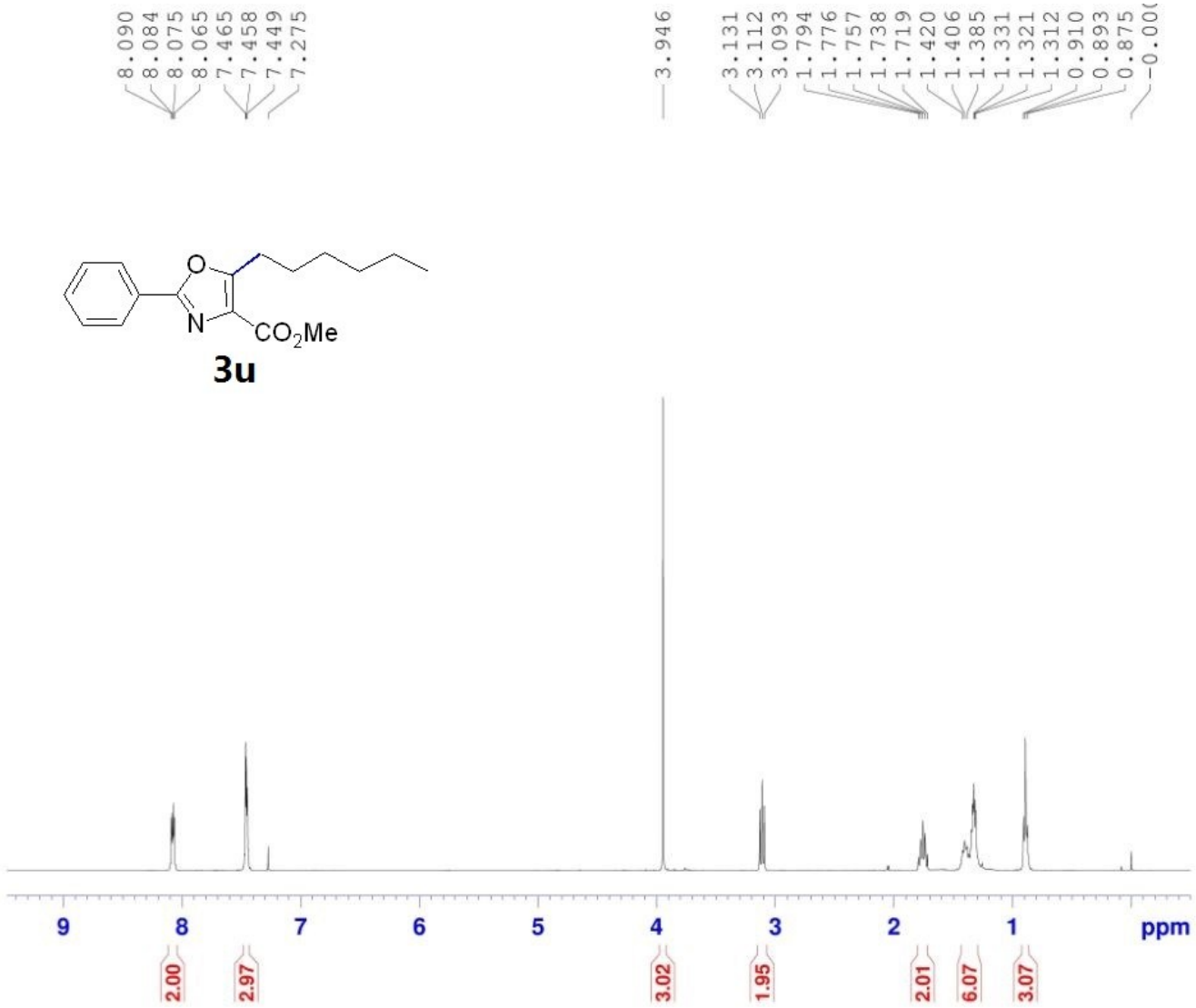
BRUKER

NAME	2017-04-17 leibowen-2
EXPNO	1
PROCNO	1
Date_	20170418
Time	20.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	64
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	-2.00 dB
SFO1	400.1324710 MHz
SI	32768
SF	400.1300019 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



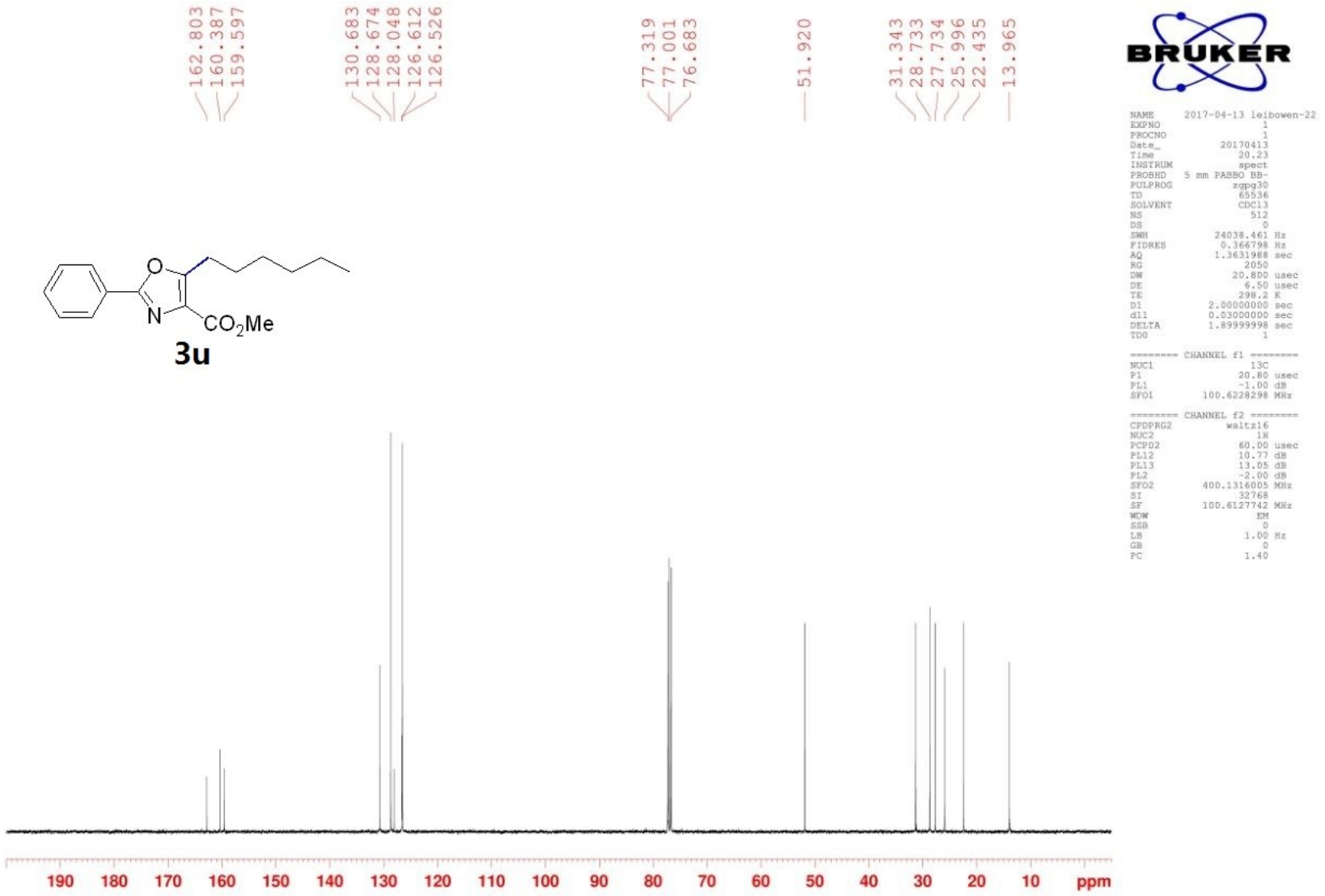
BRUKER

NAME	2017-04-17 leibowen-25
EXPNO	2
PROCNO	1
Date_	20170418
Time	21.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127757 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	CLJ-YHY-L022
EXPNO	1
PROCNO	1
Date_	20170411
Time	16.50
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300035 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

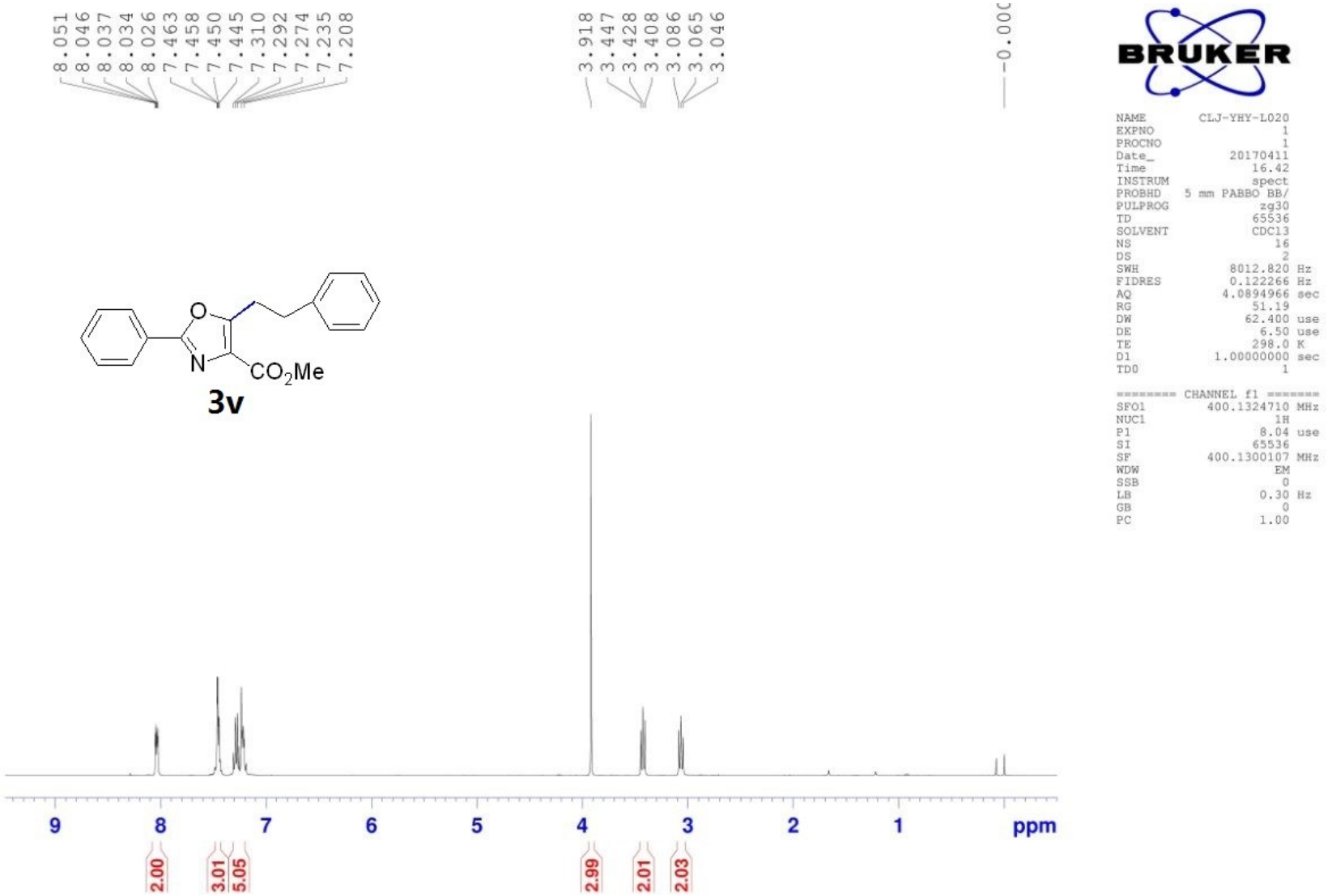


BRUKER

```
NAME          2017-04-13 leibowen-22
EXPNO                  1
PROCNO                 1
Date_           20170413
Time               20.23
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               298.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

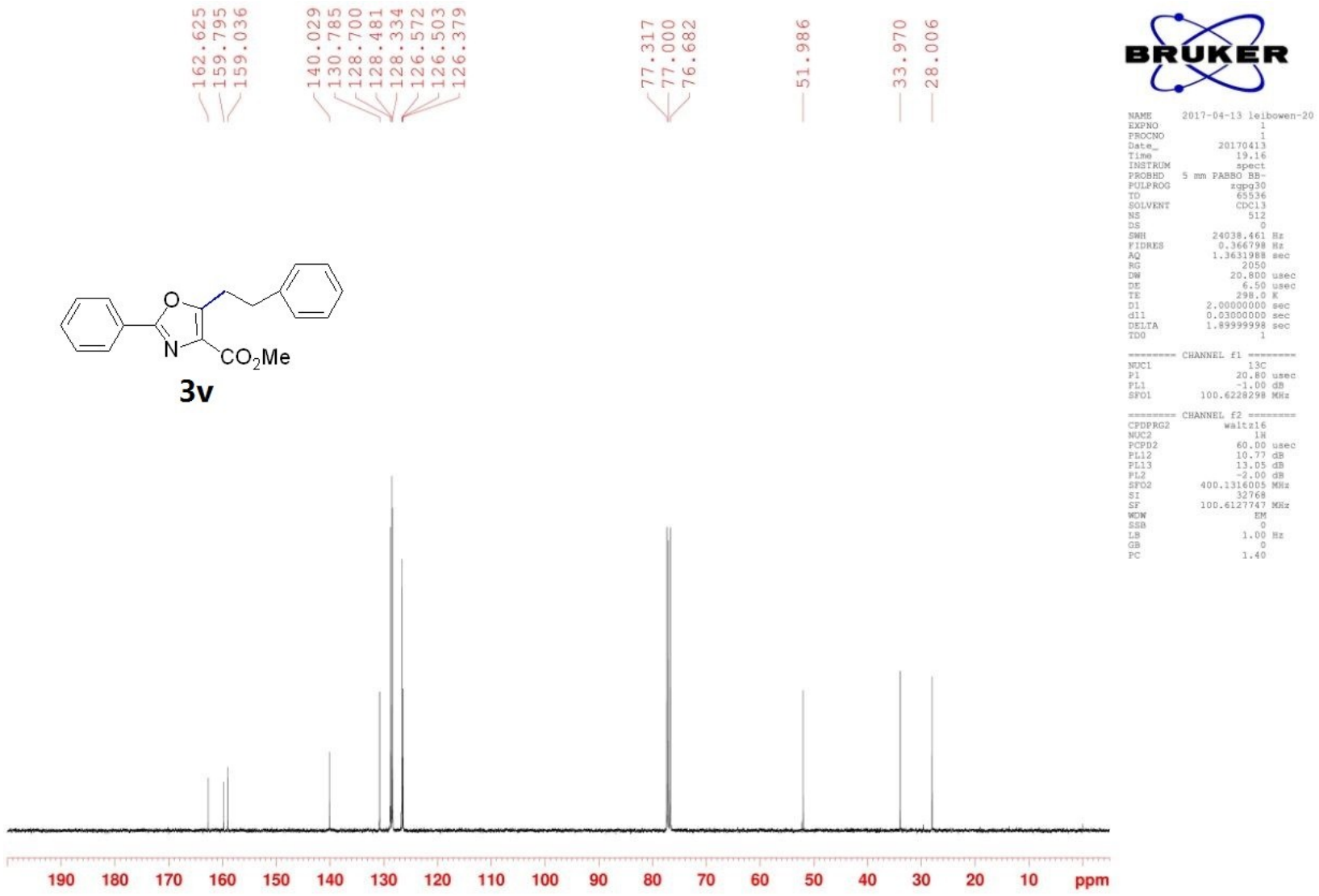
======== CHANNEL f1 ========
NUC1                13C
P1                20.80 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             60.00 usec
PL12              10.77 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127742 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



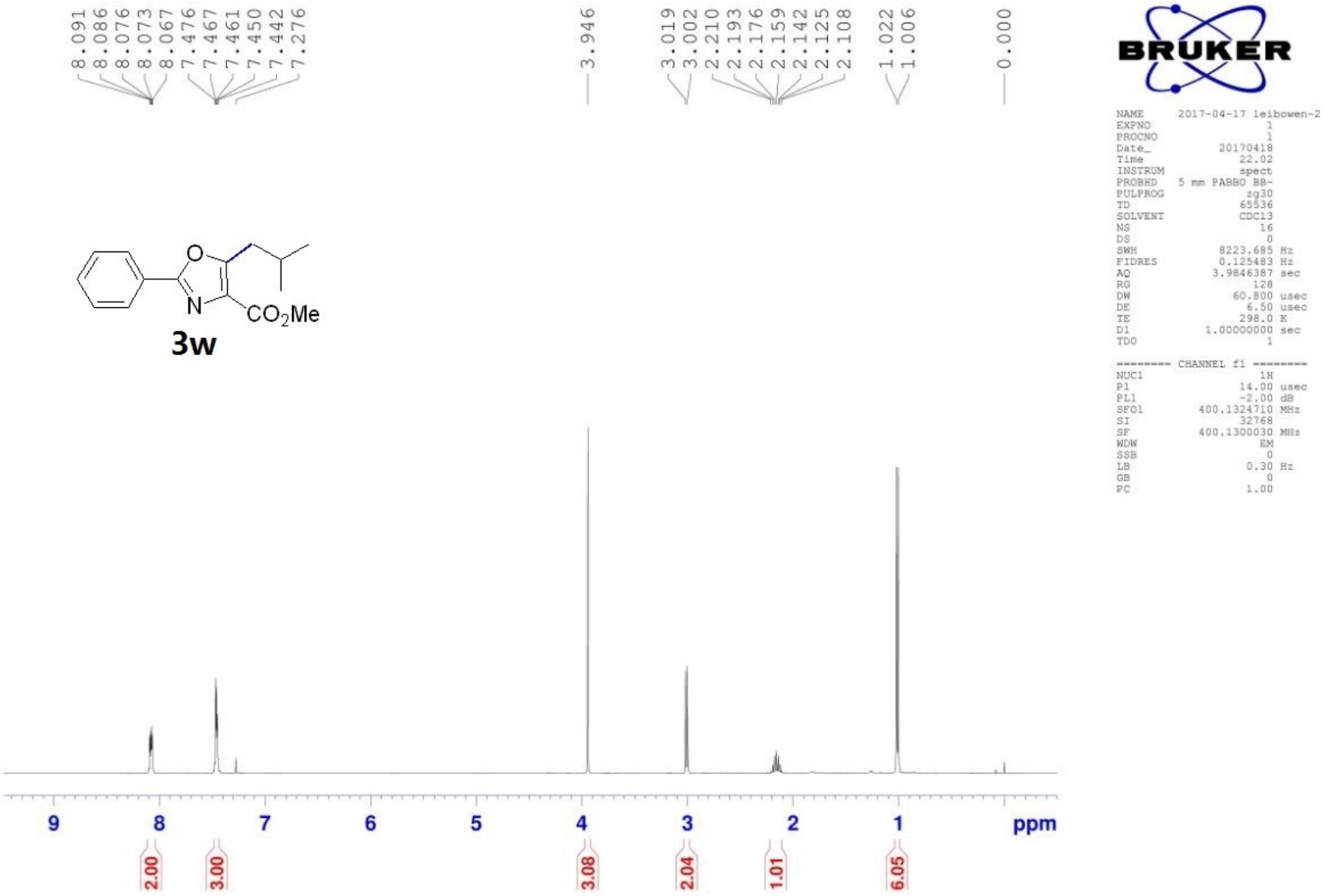
BRUKER

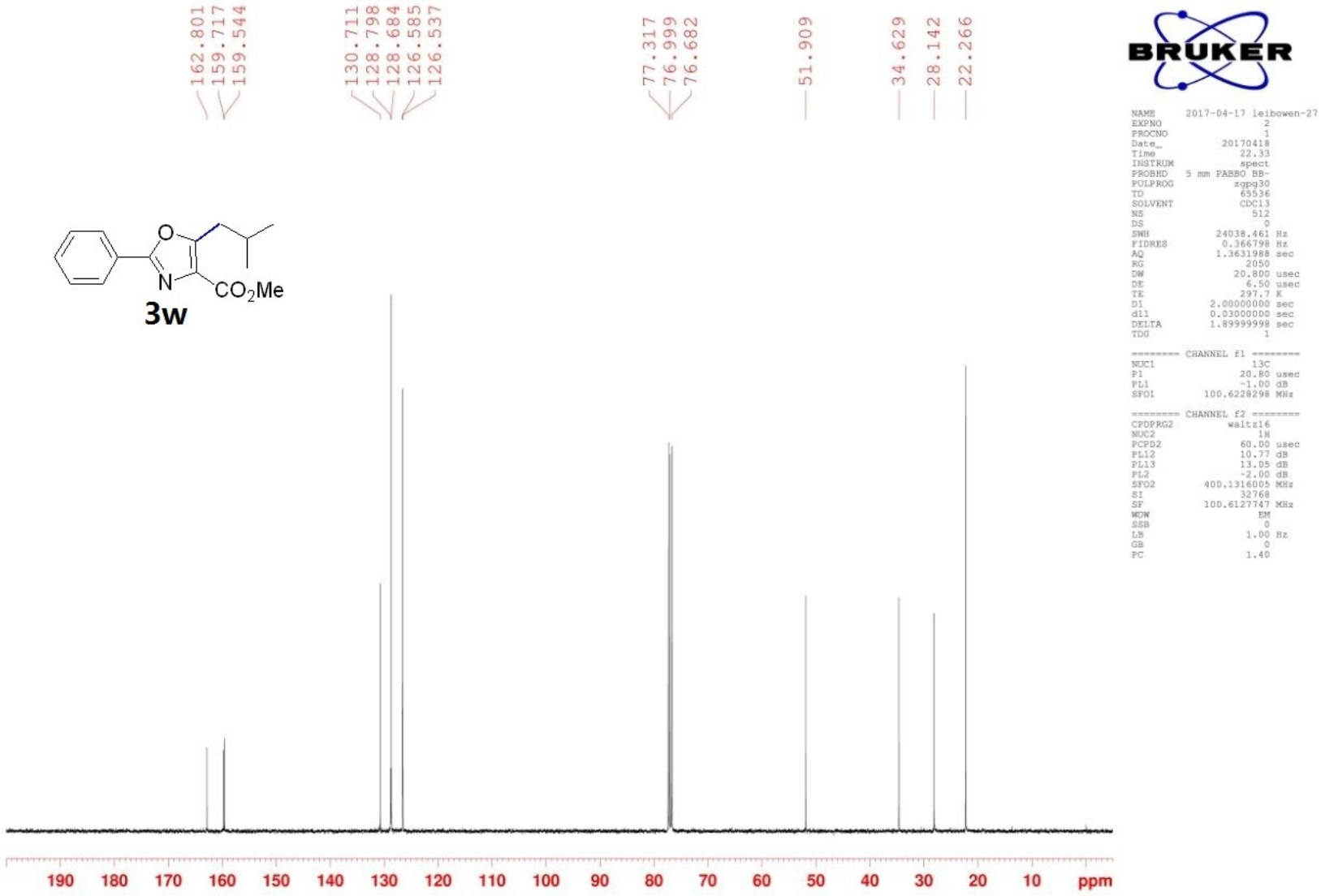
NAME	CLJ-YHY-L020
EXPNO	1
PROCNO	1
Date_	20170411
Time	16.42
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	51.19
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300107 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

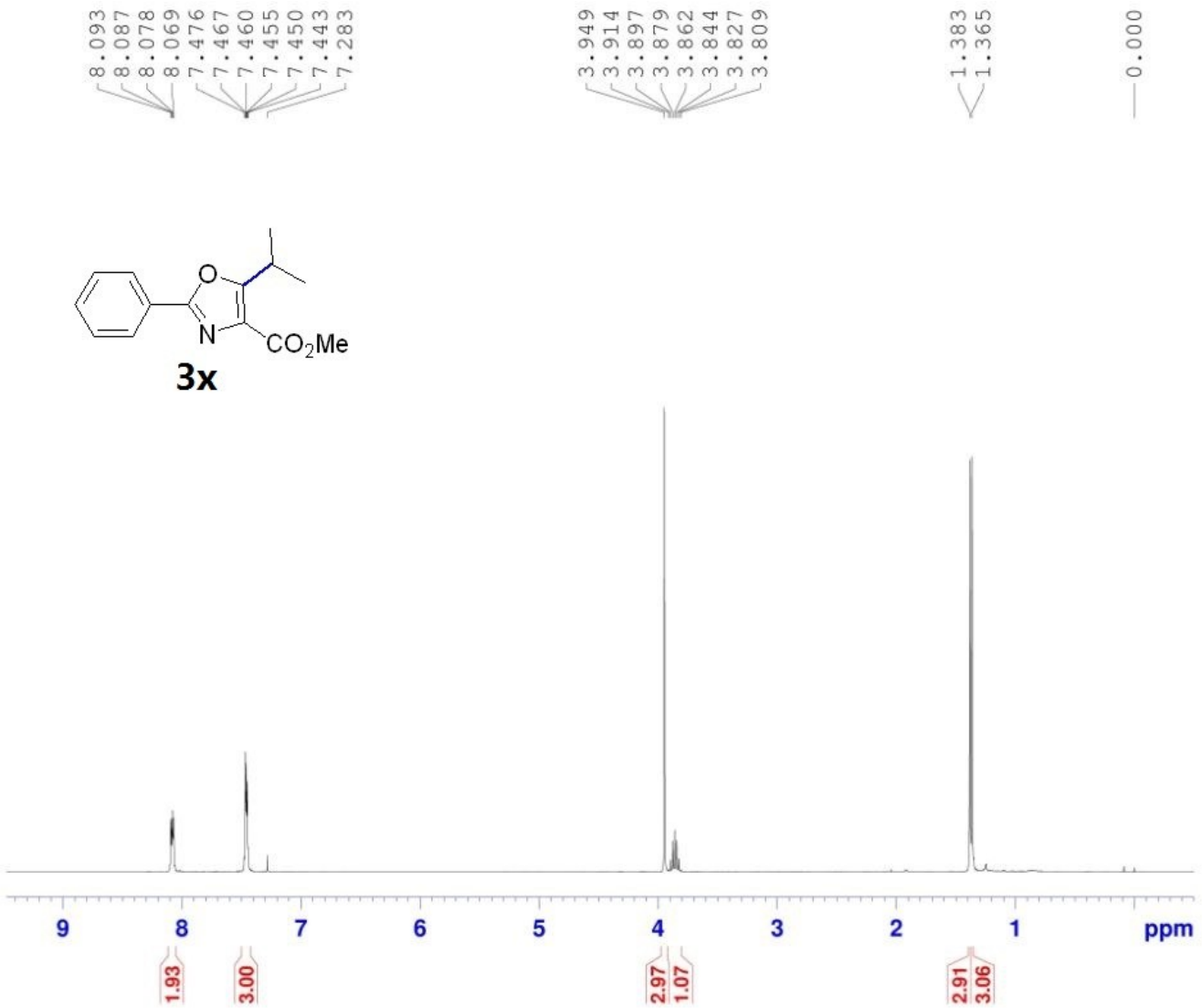
NAME	2017-04-13 leibowen-20
EXPNO	1
PROCNO	1
Date_	20170413
Time	19.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127747 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


8.091
8.086
8.076
8.073
8.067
7.476
7.467
7.461
7.450
7.442
7.276
3.946
3.019
3.002
2.210
2.193
2.176
2.159
2.142
2.125
2.108
1.022
1.006
0.000
BRUKER
NAME 2017-04-17 leibowen-2
EXPNO 1
PROCNO 1
Date_ 20170418
Time 22.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
SI 32768
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
N
CO2Me
3w
9
8
7
6
5
4
3
2
1
ppm
2.00
3.00
3.08
2.04
1.01
6.05



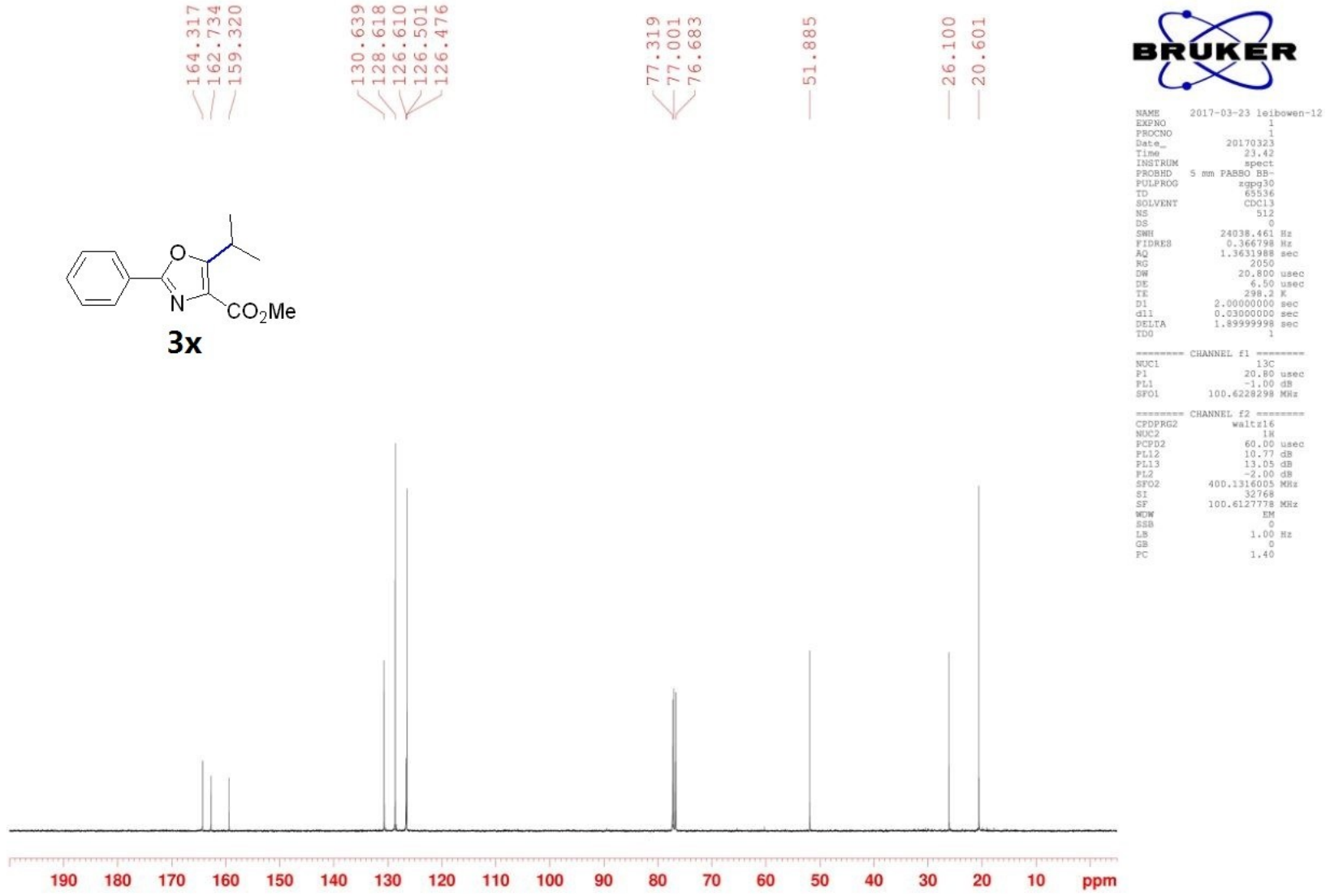
BRUKER

NAME	2017-04-17 leibowen-27
EXPNO	2
PROCNO	1
Date_	20170418
Time	22.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	20.80 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL12	10.77 dB
PL13	13.05 dB
PL2	-2.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127747 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

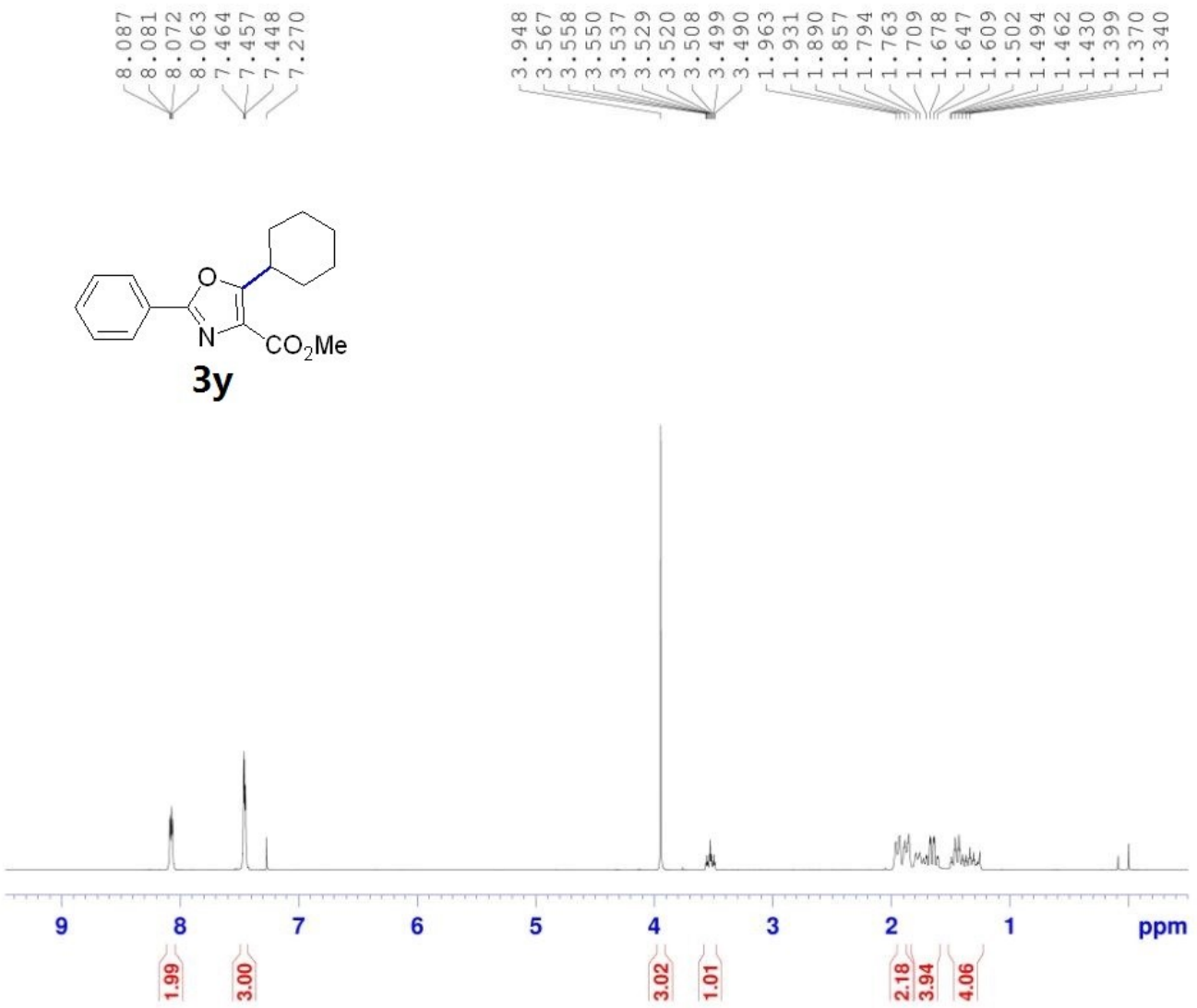
NAME	CLJ-YHY-L012
EXPNO	1
PROCNO	1
Date_	20170315
Time	12.54
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 =======
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300004 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME          2017-03-23 leibowen-12
EXPNO                  1
PROCNO                 1
Date_           20170323
Time               23.42
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    0
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               298.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

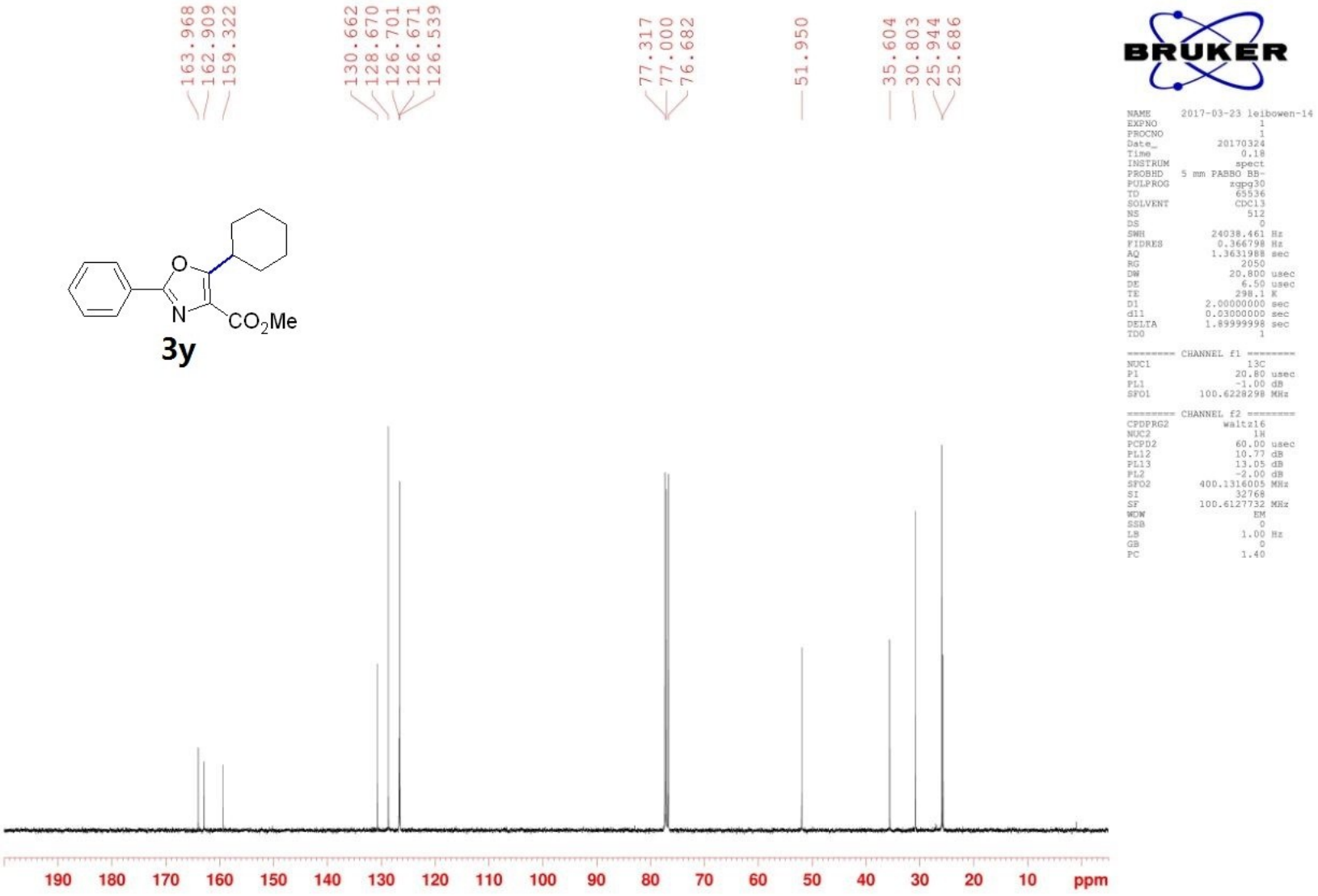
======== CHANNEL f1 ========
NUC1                13C
P1                20.80 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             60.00 usec
PL12              10.77 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127778 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



BRUKER

NAME	CLJ-YHY-L014
EXPNO	1
PROCNO	1
Date_	20170320
Time	11.49
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	32.77
DW	62.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	8.04 use
SI	65536
SF	400.1300056 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME          2017-03-23 leibowen-14
EXPNO                    1
PROCNO                   1
Date_             20170324
Time                 0.18
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     512
DS                       0
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    2050
DW                 20.800 usec
DE                  6.50 usec
TE                 298.1 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   20.80 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 10.77 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127732 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```