Supporting Information

^{n}Bu$_4$NBr-Catalyzed Esterification of Methoxyarenes with Acyl Bromide

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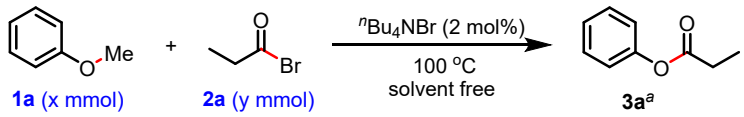
1. General Information

Unless stated otherwise, all reactions were conducted under N_2 atmosphere. All solvents were received from commercial sources without further purification. Melting points were measured on X-4B microscope melting point apparatus and uncorrected. Thin-layer chromatography (TLC) was performed by UV absorbance (254 nm). 200–300 mesh silica gel was used for column chromatography separation. NMR spectra were recorded on Bruker AV 400 spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR), 376 MHz (^{19}F NMR) . Proton and carbon chemical shifts are reported relative to the solvent used as an internal reference ($CDCl_3$: δ_H = 7.26 ppm; δ_C = 77.16 ppm). All coupling constants (J values) were reported in Hertz (Hz). Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), triplet of doublets (td), quartet (q), and multiplet (m). High resolution mass spectra (HRMS) were recorded on an Agilent 6520 Q-TOF LC/MS with Electron Spray Ionization (ESI) resource. Optical rotations were determined by a Rudolph Autopol VI polarimeter. Single crystal X-ray diffraction data were collected on Rigaku Saturn70 diffractometer.

2. Optimization of Reaction Conditions

Table S1. Effect of substrates (1a/2) loading in the reaction of 1a and 2a

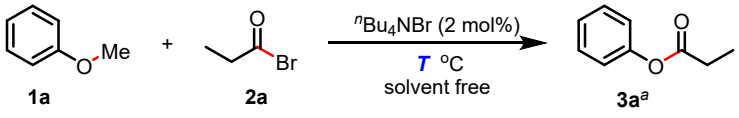


1a (x mmol) + **2a** (y mmol) → **3a**[a]

entry	**1a** (x mmol)	**2a** (y mmol)	yield (%)[b]
1	1	1	72
2	1	1.2	93
3	1	1.5	93

[a]Reaction conditions: N_2, 100 °C, 10 h. [b]Isolated yield.

Table S2. Effect of reaction temperature in the reaction

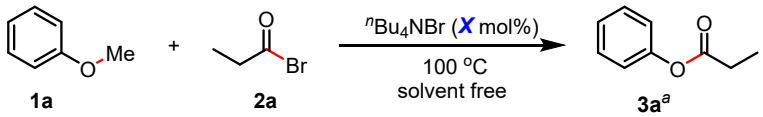


1a + **2a** → **3a**[a]

entry	***T*** **(°C)**	yield (%)[b]
1	80	69
2	90	81
3	100	93
4	110	93

[a]Reaction conditions: N_2, 100 °C, 10 h. [b]Isolated yield.

Table S3. Catalyst Loading Effects



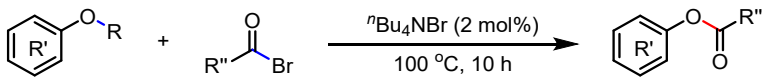
1a **2a** **3a**[a]

entry	X	yield (%)[b]
1	1	70
2	2	93
3	5	93
4	10	93

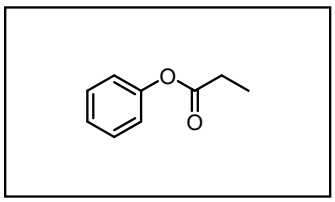
[a]Reaction conditions: N_2, 100 °C, 10 h. [b]Isolated yield.

3. General Procedure for the Preparation of 3/4

To a 15 mL oven dried tube in glove box were added ^{n}Bu$_4$NBr (6.4 mg, 0.02 mmol, 2 mol%), substate **1** (1 mmol) and substate **2** (1.2 mmol). The tube was capped, taken outside the glove box, and stirred at 100 °C for 10 h. Then the mixture was cooled to r.t., quenched with aq. $NaHCO_3$ solution (sat.). The aqueous phase was then extracted with DCM (3 × 5 mL) and the combined organic phases were dried over anhydrous Na_2SO_4. The filtration was concentrated in *vacuo* to afford the crude product, which was further purified by flash column chromatography on silica gel (EtOAc/hexanes).

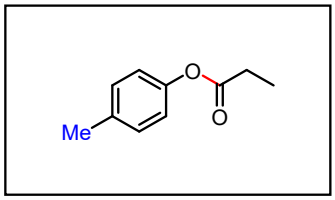


1 **2**



Phenyl propionate (3a) [1]

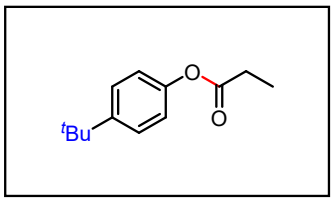
Reaction of **1a** (108 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3a** (oil, 139.5 mg, 93% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (t, J = 7.7 Hz, 2H), 7.24 – 7.16 (m, 1H), 7.07 (d, J = 7.9 Hz, 2H), 2.57 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.5 Hz, 3H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.0, 150.9, 129.4, 125.8, 121.6, 27.8, 9.1.



***p*-Tolyl propionate (3b)** [2]

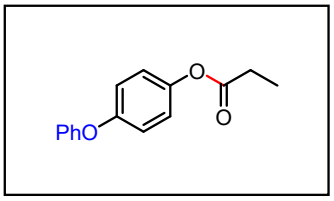
Reaction of 1b (122 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3b** (oil, 137.8 mg, 84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.13 (d, J = 8.3 Hz, 2H), 6.94 (d, J =

8.4 Hz, 2H), 2.53 (d, J = 7.6 Hz, 2H), 2.30 (s, 3H), 1.23 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.1, 148.6, 135.2, 129.9, 121.2, 27. 7, 20.8, 9.1.



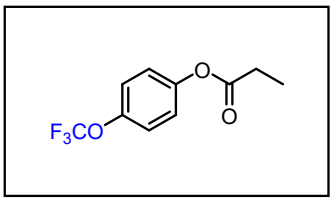
4-(*tert*-Butyl)phenyl propionate (3c) [3]

Reaction of **1c** (164.1 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3c** (oil, 185.5 mg, 90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.3 Hz, 2H), 6.99 (d, J = 8.4 Hz, 2H), 2.52 (q, J = 7.7 Hz, 2H), 1.29 (s, 9H), 1.21 (t, J = 7.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.9, 148.4, 148.3, 126.2, 120.8, 34.3, 31.3, 27.6, 9.0.



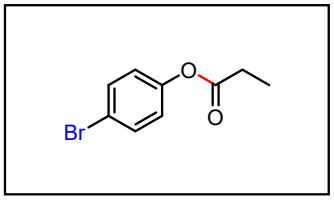
4-Phenoxyphenyl propionate (3d) [4]

Reaction of **1d** (200.1 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3o** (white solid, 210.6 mg, 87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (t, J = 8.0 Hz, 2H), 7.18 – 7.12 (m, 1H), 7.13 – 6.95 (m, 6H), 2.63 (q, J = 7.6 Hz, 2H), 1.31 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.2, 157.3, 154.7, 146.3, 129.9, 123.4, 122.8, 119.7, 118.9, 27.8, 9.2.



4-(Trifluoromethoxy)phenyl propionate (3e)

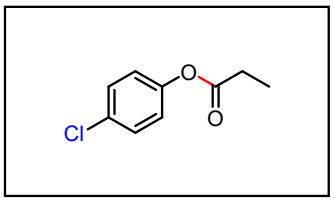
Reaction of **1e** (192 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3e** (oil, 142.8 mg, 61% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (d, J = 8.6 Hz, 2H), 7.08 (d, J = 8.6 Hz, 2H), 2.56 (q, J = 7.5 Hz, 2H), 1.24 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.7, 149.2, 146.5, 123.0, 122.1, 118.0 (q, J = 255 Hz), 27.6, 8.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.2. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{10}H_{10}F_3O_3$ 235.0577; Found 235.0560.



4-Bromophenyl propionate (3f)

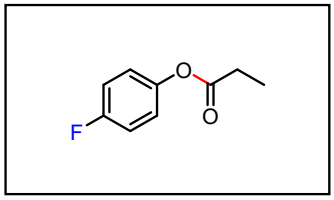
Reaction of **1f** (186 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3f** (oil, 196.1 mg, 86% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, J = 8.3 Hz, 2H), 6.96 (d, J = 8.4 Hz, 2H), 2.56 (q, J = 7.6 Hz, 2H), 1.23 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz,

$CDCl_3$) δ 172.6, 149.8, 132.4, 123.4, 123.4, 118.8, 27.7, 9.0. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_9H_{10}BrO_2$ 228.9859; Found 228.9861.



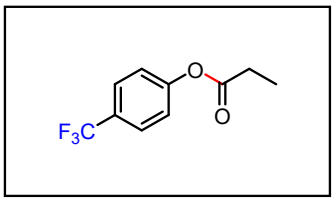
4-Chlorophenyl propionate (3g) [5]

Reaction of **1g** (142 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3g** (oil, 161.9 mg, 88% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.8 Hz, 2H), 2.57 (q, J = 7.5 Hz, 2H), 1.24 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.7, 149.3, 131.1, 129.5, 123.0, 27.7, 9.0.



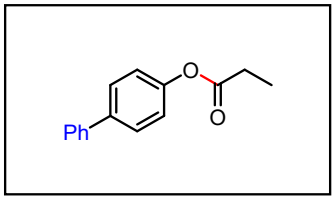
4-Fluorophenyl propionate (3h) [6]

Reaction of **1h** (126.1 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3f** (oil, 137.8 mg, 82% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.01 (d, J = 6.3 Hz, 4H), 2.62 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.8, 160.1 (q, J = 242.2 Hz), 146.6 (q, J = 2.8 Hz), 122.9 (q, J = 8.4 Hz), 115.9 (q, J = 23.3 Hz), 27.5, 8.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -117.4.



4-(Trifluoromethyl)phenyl propionate (3i)

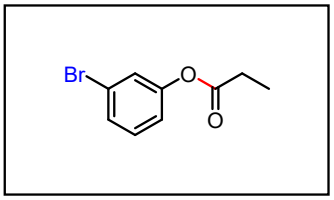
Reaction of **1i** (176 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3h** (oil, 115.6 mg, 53% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.7 Hz, 2H), 7.19 (d, J = 8.7 Hz, 2H), 2.59 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.5, 153.4 (q, J = 1.1 Hz), 128.0 (q, J = 32.6 Hz), 126.8 (q, J = 3.8 Hz), 124.0 (q, J = 270.2 Hz), 122.2, 27.7, 8.8. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.37. **HRMS (ESI)** *m/z:* $[M+H]^+$ Calcd. for $C_{10}H_{10}F_3O_2$ 219.0628; Found 219.0630.



[1,1'-Biphenyl]-4-yl propionate (3j)

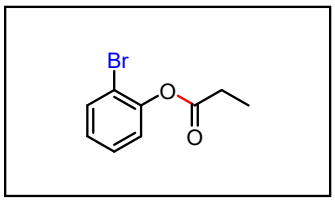
Reaction of **1j** (184.1 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3e** (white solid, 210 mg, 93% yield). m.p. 91–92 °C**. ^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 – 7.52 (m, 4H), 7.43 (t, J = 7.5 Hz, 2H), 7.35 (d, J = 7.3 Hz, 1H), 7.19 – 7.11 (m, 2H), 2.62

(q, J = 7.6 Hz, 2H), 1.29 (t, J = 7.5 Hz, 3H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.2, 150.3, 140.5, 139.0, 128.9, 128.3, 127.4, 127.2, 122.0, 27.9, 9.2. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{15}H_{15}O_2$ 227.1067; Found 227.1068.



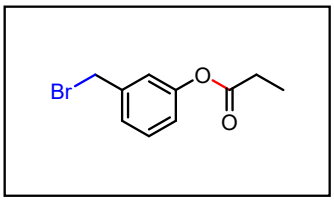
3-Bromophenyl propionate (3k) [7]

Reaction of **1k** (186 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3k** (oil, 196.1 mg, 86% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.1 Hz, 1H), 7.28 (s, 1H), 7.22 (t, J = 8.1 Hz, 1H), 7.03 (d, J = 8.1 Hz, 1H), 2.56 (q, J = 7.5 Hz, 2H), 1.24 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.5, 151.3, 130.5, 128.9, 125.1, 122.4, 120.5, 27.7, 9.0. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_9H_{10}BrO_2$ 228.9859; Found 228.9861.



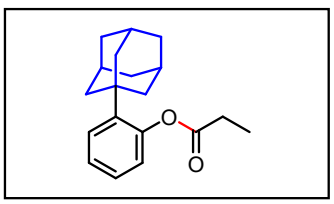
2-Bromophenyl propionate (3l)

Reaction of **1l** (186 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3l** (oil, 191.5 mg, 84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.1 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.16 – 7.04 (m, 2H), 2.64 (q, J = 7.5 Hz, 2H), 1.29 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.0, 148.3, 133.3, 128.5, 127.3, 123.8, 116.3, 27.6, 9.1. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_9H_{10}BrO_2$ 228.9859; Found 228.9861.



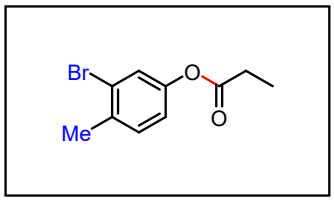
3-(Bromomethyl)phenyl propionate (3m)

Reaction of **1m** (200 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3m** (oil, 200.8 mg, 83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26 (t, J = 7.9 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 7.10 (s, 1H), 6.99 (d, J = 8.2 Hz, 1H), 4.38 (s, 2H), 2.51 (q, J = 7.5 Hz, 2H), 1.19 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.4, 150.6, 139.0, 129.5, 126.1, 121.4, 32.5, 27.4, 8.8. **HRMS (ESI)** *m/z:* $[M+H]^+$ Calcd. for $C_{10}H_{12}BrO_2$ 243.0016; Found 243.0016.



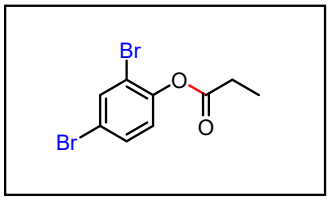
2-((3*r*,5*r*,7*r*)-Adamantan-1-yl)phenyl propionate (3n)

Reaction of **1n** (242.2 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3n** (white solid, 252.9 mg, 89% yield). m.p. 93–94 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) 7.44 (d, J = 2.4 Hz, 1H), 7.31 (dd, J = 8.5, 2.4 Hz, 1H), 6.85 (d, J = 8.6 Hz, 1H), 2.64 (q, J = 7.6 Hz, 2H), 2.12 – 2.05 (m, 3H), 1.97 (d, J = 2.9 Hz, 6H), 1.75 (q, J = 12.5 Hz, 6H), 1.31 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.8, 148.6, 143.5, 130.7, 129.7, 126.0, 119.3, 41.0, 37.1, 36.9, 28.9, 28.5, 9.1. **HRMS (ESI)** *m/z:* $[M+H]^+$ Calcd. for $C_9H_{25}O_2$ 285.1850; Found 285.1848.



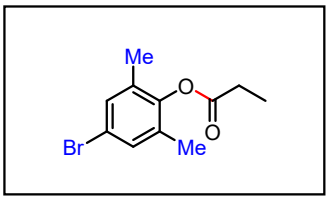
3-Bromo-4-methylphenyl propionate (3o)

Reaction of **1o** (200 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3o** (oil, 193.6 mg, 80% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (s, 1H), 7.24 (d, J = 8.3 Hz, 1H), 6.99 (d, J = 8.3 Hz, 1H), 2.59 (q, J = 7.6 Hz, 2H), 2.40 (s, 3H), 1.28 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.6, 148.9, 135.2, 130.9, 125.4, 124.4, 120.5, 27.6, 22.2, 9.0. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{10}H_{12}BrO_2$ 243.0016; Found 243.0014.



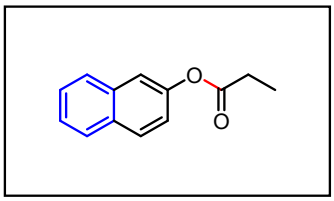
2,4-Dibromophenyl propionate (3p)

Reaction of **1p** (265.9 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3p** (oil, 258.6 mg, 84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.44 (d, J = 8.6 Hz, 1H), 7.01 (d, J = 8.6 Hz, 1H), 2.65 (q, J = 7.5 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.5, 147.5, 135.5, 131.4, 125.0, 119.2, 117.2, 27.4, 9.0. **HRMS (ESI)** *m/z:* $[M+H]^+$ Calcd. for $C_9H_9Br_2O_2$ 308.8944; Found 308.8945.



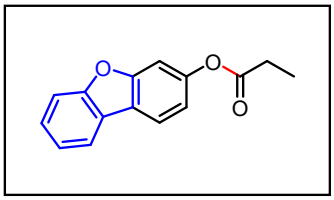
4-Bromo-2,6-dimethylphenyl propionate (3q)

Reaction of **1q** (214 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3q** (oil, 212.5 mg, 83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.19 (s, 2H), 2.62 (q, J = 7.6, Hz, 2H), 2.11 (s, 3H), 2.10 (s, 3H), 1.30 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.0, 147.4, 132.5, 131.3, 118.7, 27.4, 16.2, 9.4. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{11}H_{14}BrO_2$ 257.0172; Found 257.0167.



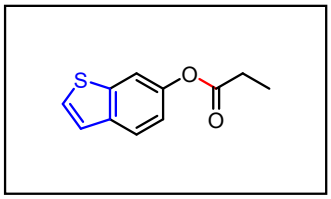
Naphthalen-2-yl propionate (3r) [8]

Reaction of **1r** (158.1 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3r** (white solid, 182 mg, 91% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 – 7.76 (m, 3H), 7.54 (d, J = 2.3 Hz, 1H), 7.46 – 7.42 (m, 2H), 7.21 (dd, J = 8.8, 2.3 Hz, 1H), 2.62 (q, J = 7.5 Hz, 2H), 1.28 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.2, 148.5, 133.9, 131.5, 129.45, 127.8, 127.7, 126.6, 125.7, 121.3, 118.6, 27.9, 9.2. **HRMS (ESI)** *m/z:* $[M+H]^+$ Calcd. for $C_{13}H_{13}O_2$ 201.0911; Found 201.0912.



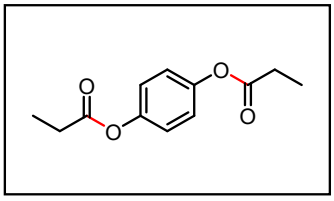
Dibenzo[*b*,*d*]furan-3-yl propionate (3s)

Reaction of **1s** (198 mg, 0.2 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3s** (white solid, 213.7 mg, 89% yield). m.p. 82–83 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.7 Hz, 1H), 7.64 (d, J = 2.4 Hz, 1H), 7.51 (dd, J = 8.6, 6.9 Hz, 2H), 7.41 (t, J = 7.7 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.12 (dd, J = 8.8, 2.5 Hz, 1H), 2.61 (q, J = 7.6 Hz, 2H), 1.28 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.5, 157.0, 153.6, 146.3, 127.6, 125.0, 124.0, 122.8, 120.9, 120.7, 113.6, 112.1, 111.8, 27.8, 9.2. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{15}H_{13}O_3$ 241.0860; Found 241.0861.



Benzo[*b*]thiophen-6-yl propionate (3t)

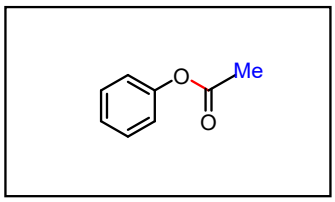
Reaction of **1t** (164 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **3t** (white solid, 164.8 mg, 80% yield). m.p. 70–71 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, J = 8.6 Hz, 1H), 7.49 (s, 1H), 7.42 (d, J = 5.4 Hz, 1H), 7.23 (d, J = 5.4 Hz, 1H), 7.03 (d, J = 8.7 Hz, 1H), 2.57 (q, J = 7.5 Hz, 2H), 1.24 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.4, 148.2, 140.4, 137.1, 128.2, 123.8, 123.2, 118.8, 116.0, 27.9, 9.2. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{11}H_{11}O_2S$ 207.0475; Found 207.0478.



1,4-Phenylene dipropionate (3u)

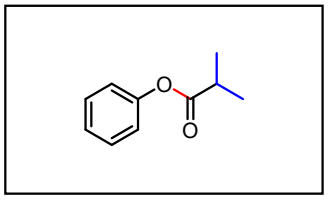
Reaction of **1u** (138.1 mg, 1 mmol) and **2a** (326.4 mg, 2.4 mmol), product **3u** (white

solid, 195.4 mg, 88% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.08 (s, 4H), 2.56 (d, J = 7.5 Hz, 4H), 1.25 (t, J = 7.6 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.9, 148.1, 122.4, 27.7, 9.1. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{12}H_{15}O_4$ 223.0965; Found 223.0965.



Phenyl acetate (4a) [9]

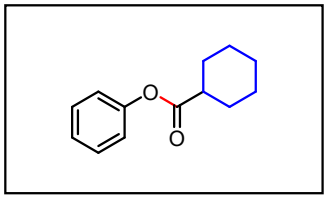
Reaction of **1a** (108 mg, 1 mmol) and **2b** (146.3 mg, 1.2 mmol), product **4a** (oil, 129.2 mg, 95% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (*t*, J = 7.7 Hz, 2H), 7.25 – 7.19 (*t*, J = 7.7 Hz, 1H), 7.08 (d, J = 7.8 Hz, 2H), 2.29 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.6, 150.8, 129.6, 129.5, 125.9, 121.7, 21.2.



Phenyl isobutyrate(4b) [10]

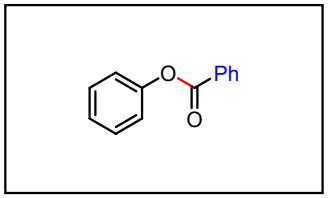
Reaction of **1a** (108 mg, 1 mmol) and **2c** (180 mg, 1.2 mmol), product **4b** (oil, 151.1 mg, 92% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (t, J = 7.7 Hz, 2H), 7.22 (d, J = 7.2 Hz, 1H), 7.16 – 7.01 (m, 2H), 2.83 (hept, J = 7.0 Hz, 1H), 1.32 (d, J = 7.1 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 151.0, 129.5, 125.8, 121.6, 34.3, 19.1.



Phenyl cyclohexanecarboxylate (4c) [11]

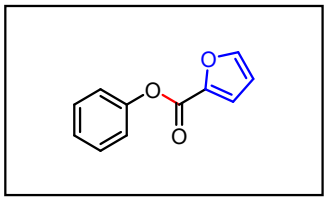
Reaction of **1a** (108 mg, 1 mmol) and **2d** (228 mg, 1.2 mmol), product **4c** (oil, 181.7 mg, 92% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 (t, J = 7.7 Hz, 2H), 7.36 (t, J = 7.5 Hz, 1H), 7.23 (d, J = 8.0 Hz, 2H), 2.75 – 2.65 (m, 1H), 2.23 (d, J = 13.2 Hz, 2H), 2.01 – 1.98 (m, 2H), 1.88 – 1.72 (m, 3H), 1.56 – 1.39 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.4, 150.9, 129.3, 125.5, 121.5, 43.1, 28.9, 25.7, 25.3.



Phenyl benzoate (4d) [11]

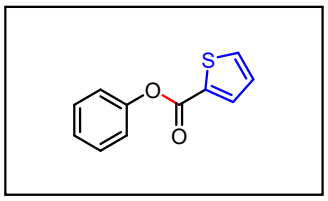
Reaction of **1a** (108 mg, 1 mmol) and **2e** (220.7 mg, 1.2 mmol), product **4d** (white solid, 178.2 mg, 90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25 – 8.11 (m, 2H), 7.68 – 7.59

(m, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.43 (t, J = 7.9 Hz, 2H), 7.31 – 7.14 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.3, 151.1, 133.7, 130.3, 129.7, 129.6, 128.7, 126.0, 121.9.



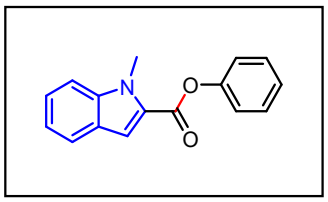
Phenyl furan-2-carboxylate (4e) [11]

Reaction of **1a** (108 mg, 1 mmol) and **2f** (208.7 mg, 1.2 mmol), product **4e** (white solid, 146.6 mg, 78% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.44 – 7.32 (m, 3H), 7.25 – 7.13 (m, 3H), 6.53 – 6.52 (m, 1H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.9, 150.1, 147.2, 143.9, 129.5, 126.0, 121.6, 119.4, 112.2.



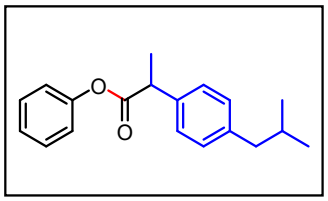
Phenyl thiophene-2-carboxylate (4f) [11]

Reaction of **1a** (108 mg, 1 mmol) and **2g** (227.9 mg, 1.2 mmol), product **4f** (white solid, 163.2 mg, 80% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07-8.05 (m, 1H), 7.71 – 7.63 (m, 1H), 7.50 (t, J = 7.9 Hz, 2H), 7.38 – 7.29 (m, 3H), 7.19 (t, J = 4.3 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) 160.4, 150.4, 134.5, 133.5, 132.6, 129.3, 127.9, 125.8, 121.5.



Phenyl 1-methyl-1H-indole-2-carboxylate(4g) [12]

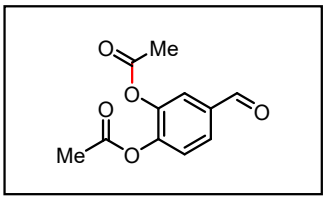
Reaction of **1a** (108 mg, 1 mmol) and **2h** (284.4 mg, 1.2 mmol), product **4g** (white solid, 165.7 mg, 66% yield). m.p. 101–102 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 – 7.62 (m, 1H), 7.47 (d, J = 4.0 Hz, 1H), 7.39 – 7.31 (m, 4H), 7.22 – 7.08 (m, 4H), 4.03 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.8, 150.7, 140.3, 129.7, 126.9, 126.1, 125.7, 123.0, 122.0, 121.0, 111.8, 110.5, 31.8.



Phenyl 2-(4-isobutylphenyl)propanoate (4h)

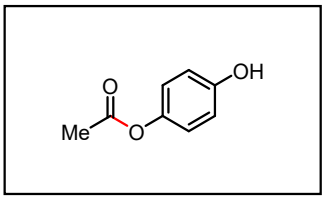
Reaction of **1a** (108 mg, 1 mmol) and **2i** (321.7mg, 1.2 mmol), product **4h** (oil, 214.4 mg, 76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 4H), 7.18 – 7.09 (m, 3H), 6.98 (d, J = 7.9 Hz, 2H), 3.92 (d, J = 7.1 Hz, 1H), 2.46 (d, J = 7.2 Hz, 2H), 1.92 – 1.79 (m, 1H), 1.59 (d, J = 7.2 Hz, 3H), 0.91 (s, 3H), 0.90 (s, 3H). **^{13}C NMR** (100 MHz,

$CDCl_3$) δ 173.3, 151.0, 140.9, 137.4, 129.6, 129.4, 127.4, 125.8, 121.5, 45.4, 30.3, 22.5, 22.5, 18.7. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{19}H_{23}O_2$ 283.1693; Found 283.1693.



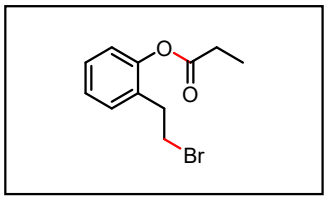
4-formyl-1,2-phenylene diacetate (7) [13]

Reaction of Vanillin acetate (194 mg, 1 mmol) and Acetyl bromide (146.3 mg, 1.2 mmol), product 7 (oil, 110 mg, 50% yield).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.95 (s, 1H), 7.79 (d, J = 8.3 Hz, 1H), 7.74 (s, 1H), 7.39 (d, J = 8.2 Hz, 1H), 2.32 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 190.2, 168.0, 167.8, 147.1, 142.9, 134.8, 128.3, 124.4, 124.3, 20.7, 20.6.



4-hydroxyphenyl acetate (8) [13]

Reaction of monobenzone (200 mg, 1 mmol) and Acetyl bromide (146.3 mg, 1.2 mmol), product 7 (solid, 110 mg, 70% yield).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 6.88 (d, J = 8.9 Hz, 2H), 6.72 (d, J = 8.9 Hz, 2H), 6.32 (s, 1H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ171.0, 153.8, 143.9, 122.4, 116.3, 116.2, 21.2.



2-(2-Bromoethyl)phenyl propionate (9)

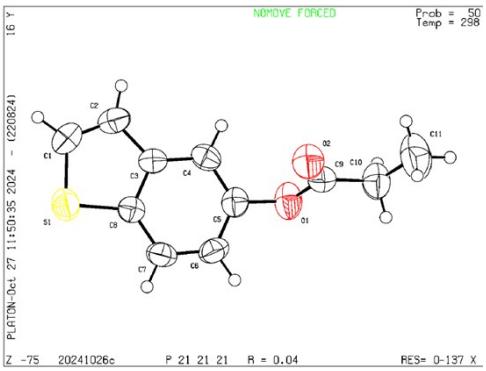
Reaction of **6** (121.1 mg, 1 mmol) and **2a** (163.2 mg, 1.2 mmol), product **7** (oil, 179.2 mg, 70% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 2H), 7.23 (d, J = 8.0 Hz, 1H), 7.12 (d, J = 8.0 Hz, 1H), 3.60 – 3.50 (t, J = 7.8 Hz, 2H), 3.12 (t, J = 7.8 Hz, 2H), 2.66 (q, J = 7.6, 2H), 1.34 (t, J = 7.6, Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.6, 149.0, 130.6, 130.5, 128.1, 126.0, 122.5, 34.0, 31.0, 27.6, 9.2. **HRMS (ESI)** *m/z*: $[M+H]^+$ Calcd. for $C_{11}H_{14}BrO_2$ 257.0172; Found 257.0170.

4. Crystal Structure Information of 3t

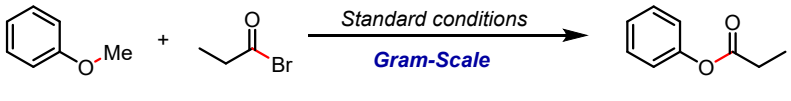
CCDC 2394783, Compound Name: Benzo[*b*]thiophen-6-yl propionate (**3t**), Formula: $C_{11}H_{10}O_2S$

General procedure for crystal culture of 3t: To a test tube (15 mL) with added 3t (100 mg), dichloromethane (1.5 mL) was added slowly to make it dissolve completely. After

it dissolved, petroleum ether (10.0 mL) was added slowly. Then, the test tube was sealed with a rubber stopper, and connected to air with a syringe needle. Finally, the tube was put in a dry and ventilated place to make the organic solvent to volatilize slowly. After a few days, the crystal of 3y was obtained. The X-ray crystal structure of 3t was shown below.



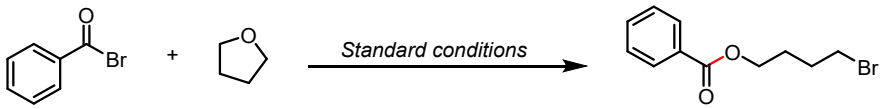
5. Gram-Scale Reaction



1a 10.0 mmol **2a** **3a** **1.32 g, 88%**

To a 35 mL oven dried tube in glove box were added $^{n}Bu_4NBr$ (64 mg, 0.2 mmol, 2 mol%), anisole **1** (10 mmol) and propionyl bromide **2** (12 mmol). The tube was capped, taken outside the glove box, and stirred at 100 °C for 10 h. Then the mixture was cooled to r.t., quenched with aq. $NaHCO_3$ solution (sat.). The aqueous phase was then extracted with DCM (3 × 5 mL) and the combined organic phases were dried over anhydrous Na_2SO_4. The filtration was concentrated in *vacuo* to afford the crude product, which was further purified by flash column chromatography on silica gel (EtOAc/hexanes = 100:1, V/V) to give product **3a** (1.32 g 88%).

6. Reaction of dialkyl ethers



To a 35 mL oven dried tube in glove box were added $^{n}Bu_4NBr$ (64 mg, 0.2 mmol, 2 mol%), tetrahydrofuran (1 mmol) and benzoyl bromide **2** (1.2 mmol). The tube was capped, taken outside the glove box, and stirred at 100 °C for 10 h. Then the mixture was cooled to r.t., quenched with aq. $NaHCO_3$ solution (sat.). The aqueous phase was then extracted with DCM (3 × 5 mL) and the combined organic phases were dried over anhydrous Na_2SO_4. The filtration was concentrated in *vacuo* to afford the crude

product, which was further purified by flash column chromatography on silica gel (EtOAc/hexanes = 50:1, V/V) to give product **3a** (204.8 mg 80%).[14]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.90 (m, 2H), 7.46 – 7.41 (m, 1H), 7.32 (t, J = 7.7 Hz, 2H), 4.23 (t, J = 6.2 Hz, 2H), 3.35 (t, J = 6.5 Hz, 2H), 1.94 – 1.86 (m, 2H), 1.85 – 1.77 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.4, 132.9, 130.1, 129.5, 128.3, 63.9, 33.1, 29.3, 27.3.

7. References

[1] Ai, H.-J.; Wang, H.; Li, C.-L.; Wu, X.-F. *ACS Catal*. **2020**, *10*, 5147−5152.

[2] Zhong, Z. L.; Snowden, T. S.; Best, M. D.; Anslyn, E. V. *J. Am. Chem. Soc.* **2004**, *126*, 3488−3495.

[3] Toriumi, N.; Inoue, T.; Iwasawa, N. Shining *J. Am. Chem. Soc*. **2022**, *144*,19592−19602.

[4] Lucena, V.; Szajnman, S. H.; Rodriguez, J. N.; Bonesi, S. M. *European Journal of Organic Chemistry*. **2024**, *27*, e202400201.

[5] Narv´aez, E.-G.; Bonilla, P. -M. Bonilla.; Zurita, D.-A.; Alcívar, C.-D.; Heredia-Moya, J.; Ulic, S.E.; Langer, P. *J. Fluor. Chem*. 242 (2021), 109717

[6] Schimler, S. D.; Sanford, M. S. *Synlett* **2016**, *27*, 2279−2284.

[7] Simonetti, S. O.; Larghi, E. L.; Bracca, A. B. J.; Kaufman, T. S. *Org. Biomol. Chem*. **2012**, *10*, 4124− 4134.

[8] Alden-Danforth, E.; Scerba, M. T.; Lectka, T. *Org. Lett*. **2008**, *10*, 4951-4953.

[9] Zhang, Z.; Zhao, Z.; Liu, M.; Liu, H.; Li, Q.; Xiang, J.; Wu, T.; Han, B. *Green Chem.* **2022**, *24*, 9763−9771.

[10] Hayashi, H.; Yasukochi, S.;Sakamoto, T.; Hatano, M.; Ishihara, K. *J.Org.Chem*. **2021**, *86*, 5197− 5212.

[11] Y.; Liu, X.; Cao, H.; Bie, F.; Han, Y.; Yan, P.; Szostak, R.; Szostak, M.; Liu, C. *Org. Biomol. Chem.* **2021**, *19*, 2991−2996.

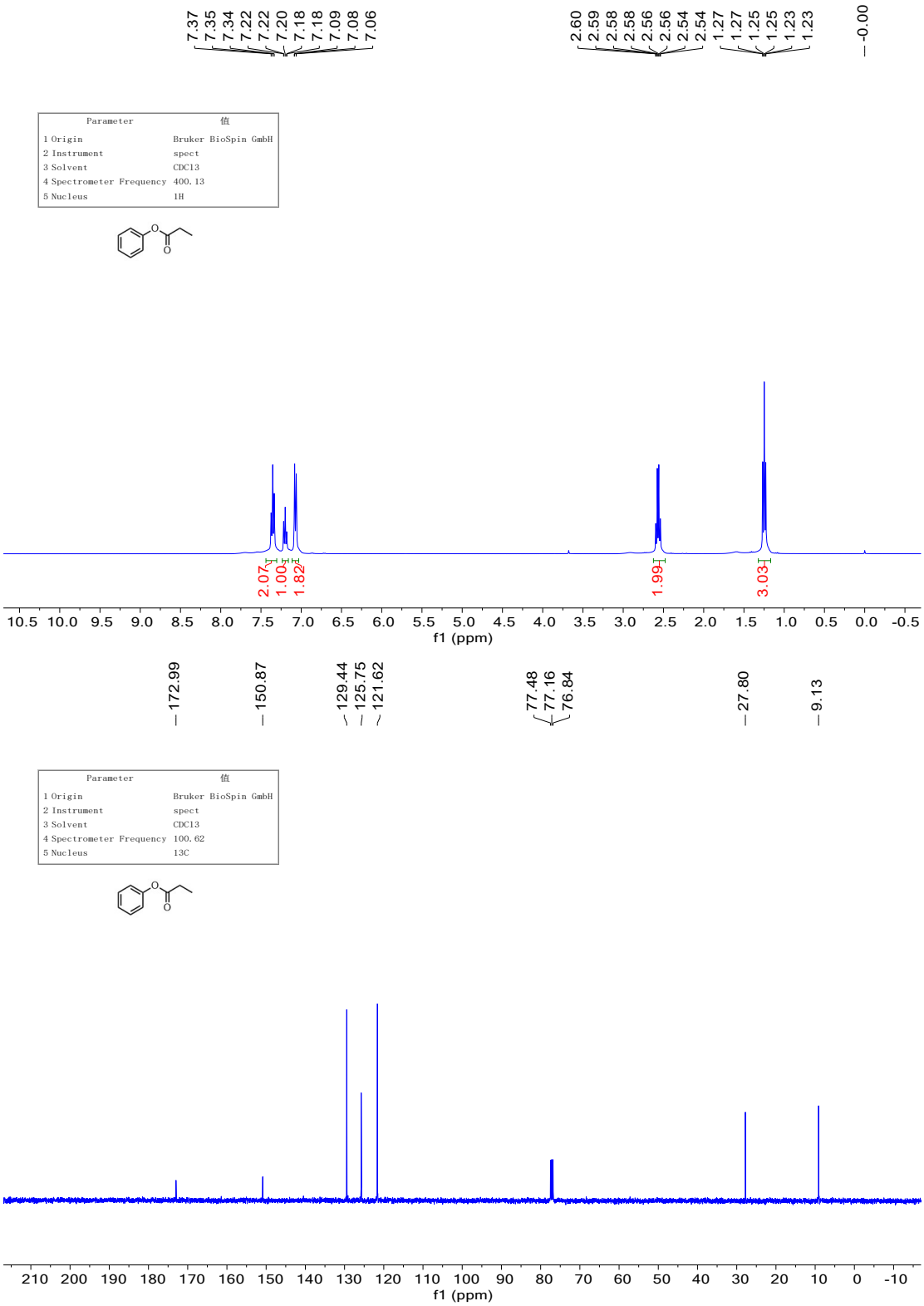
[12] Hoang, K. L. M.; Leow, M. L.; Liu, X.-W. *Org. Chem. Front*. **2015**, 2, 502−505.

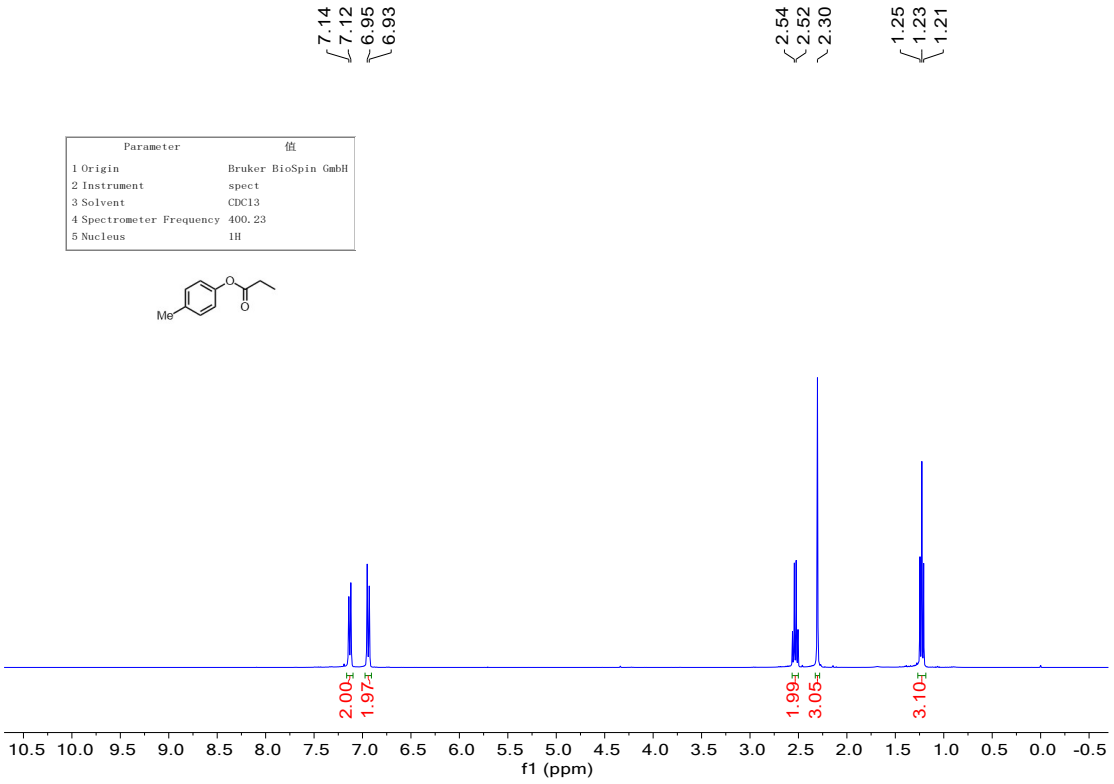
[13] Fymeaux, R.; Menozzi-Smarrito, C.; Stalmach, A.; Munari, C.; Kraehenbuel, K.; Steiling, H.; Crozier, A.; Williamson, G.; Barron, D. *Org. Biomol. Chem*. **2010**, *8*, 5199−5211.

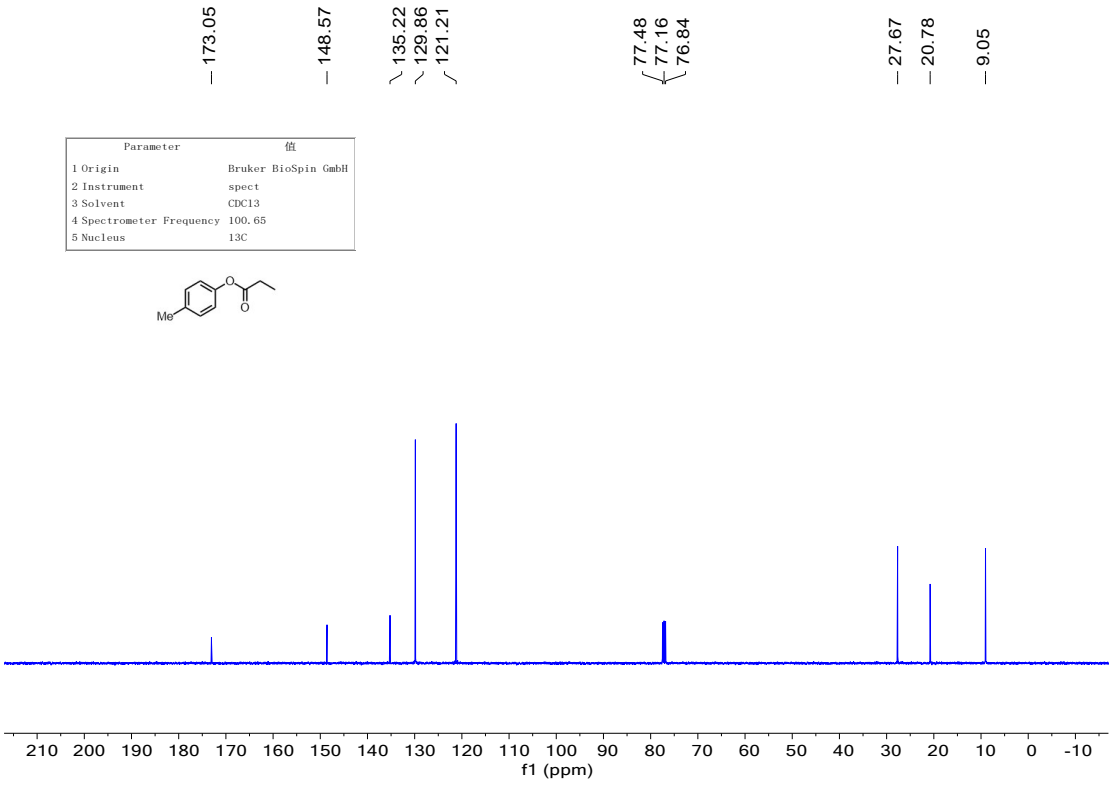
[14] Jha, Dhiraj K.; et al. Visible Light-Assisted Ring-Opening of Cyclic Ethers with Carboxylic Acids Mediated by Triphenylphosphine and N-Halosuccinimides. *Org. Lett*. **2024**, *26*, 172-177

[15] Panchgalle, S. P.; Kalkote, U. R.; Niphadkar, P. S.; Joshi, P. N.; Chavan, S. P.; Chaphekar, G. M. *Green Chem*. **2004**, *6*, 308-309.

8. NMR Spectra




7.14
7.12
6.95
6.93
2.54
2.52
2.30
1.25
1.23
1.21
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.23
5 Nucleus 1H
Me
O
O
2.00
1.97
1.99
3.05
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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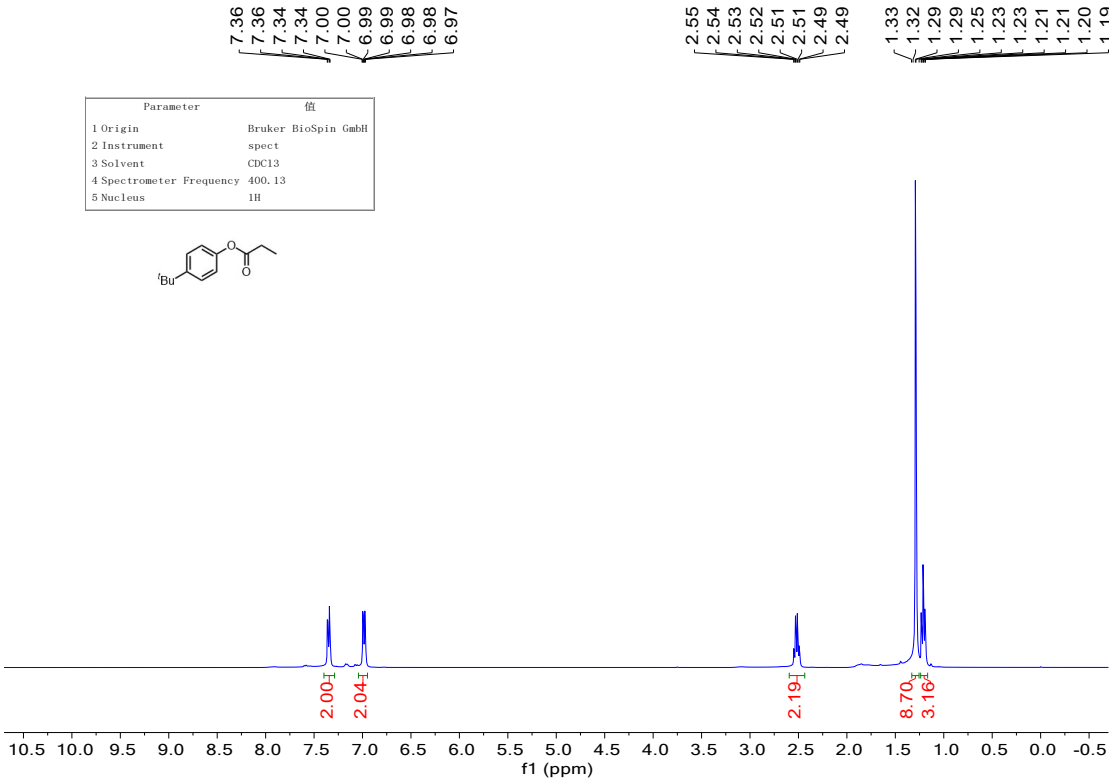
148.57
135.22
129.86
121.21
77.48
77.16
76.84
27.67
20.78
9.05
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.65
5 Nucleus 13C
Me
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.36
7.36
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7.34
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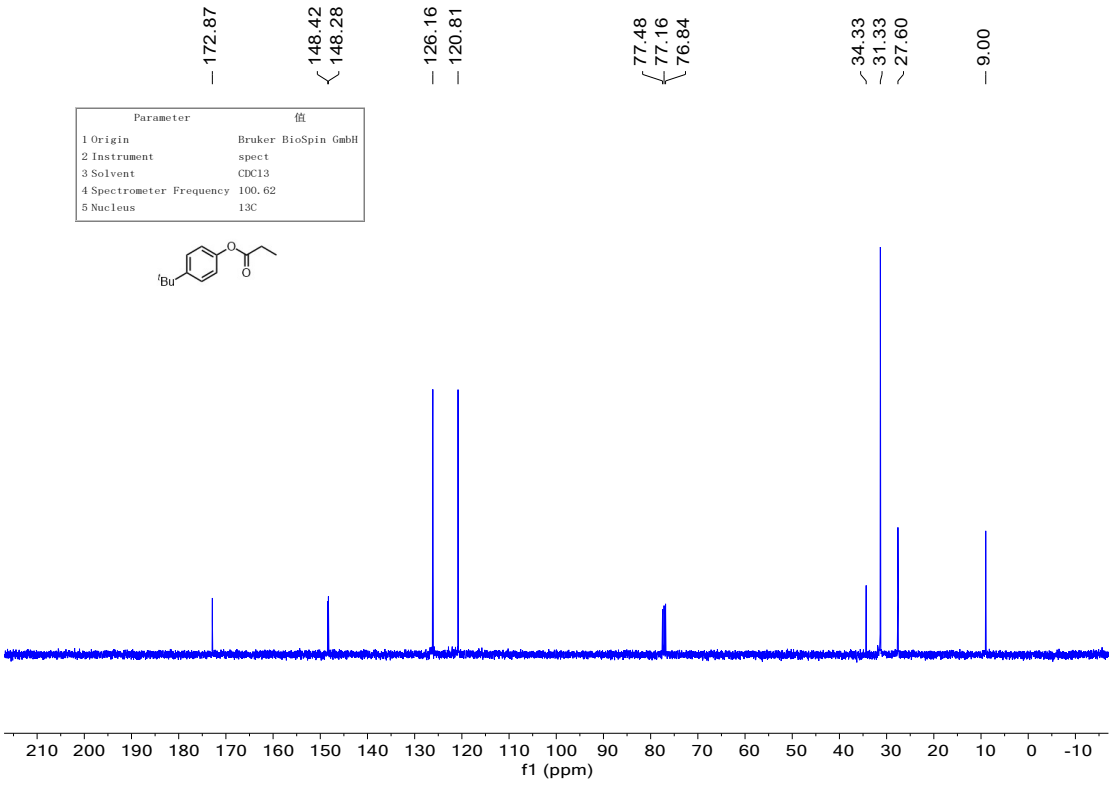
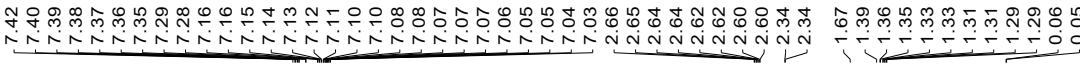
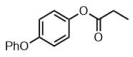
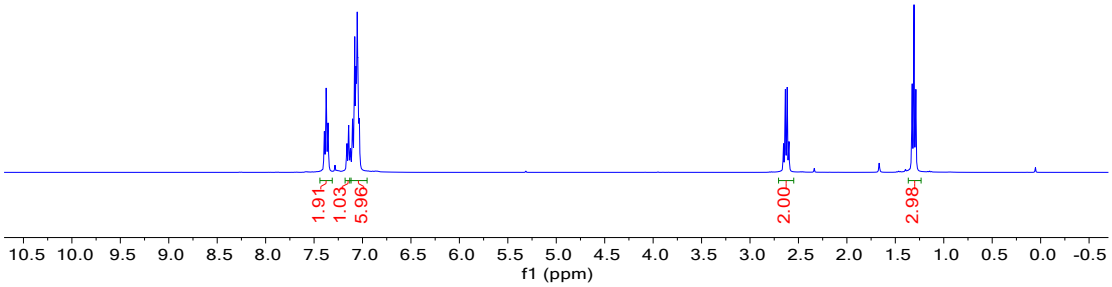
7.00
6.99
6.99
6.98
6.98
6.97
2.55
2.54
2.53
2.52
2.51
2.51
2.49
2.49
1.33
1.32
1.29
1.29
1.25
1.23
1.23
1.21
1.21
1.20
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
tBu
O
O
2.00
2.04
2.19
8.70
3.16
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

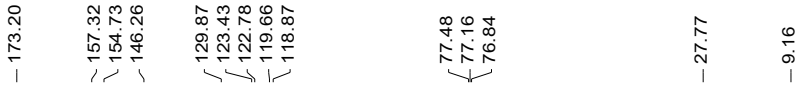

172.87
148.42
148.28
126.16
120.81
77.48
77.16
76.84
34.33
31.33
27.60
9.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
tBu
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



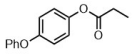
Parameter	值
1 Origin	Bruker BioSpin GmbH
2 Instrument	spect
3 Solvent	CDCl3
4 Spectrometer Frequency	400.13
5 Nucleus	1H

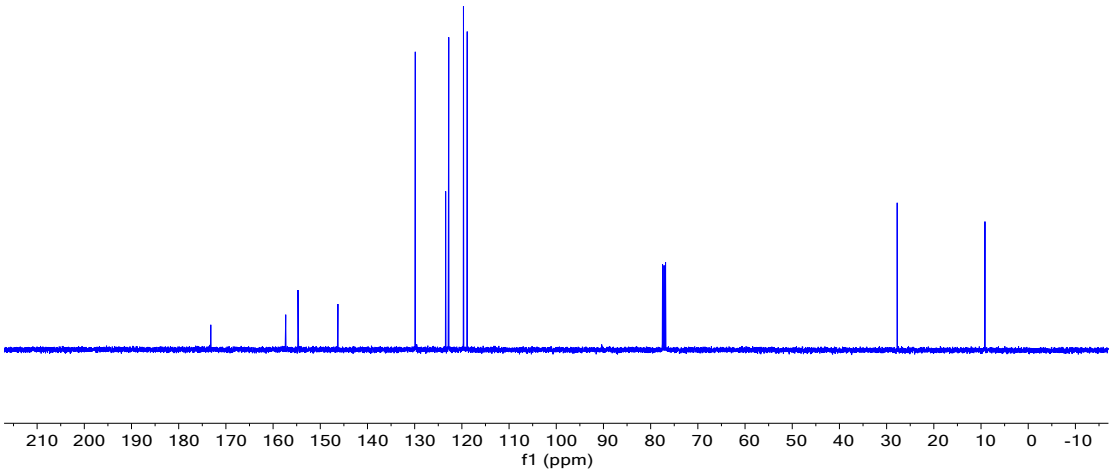


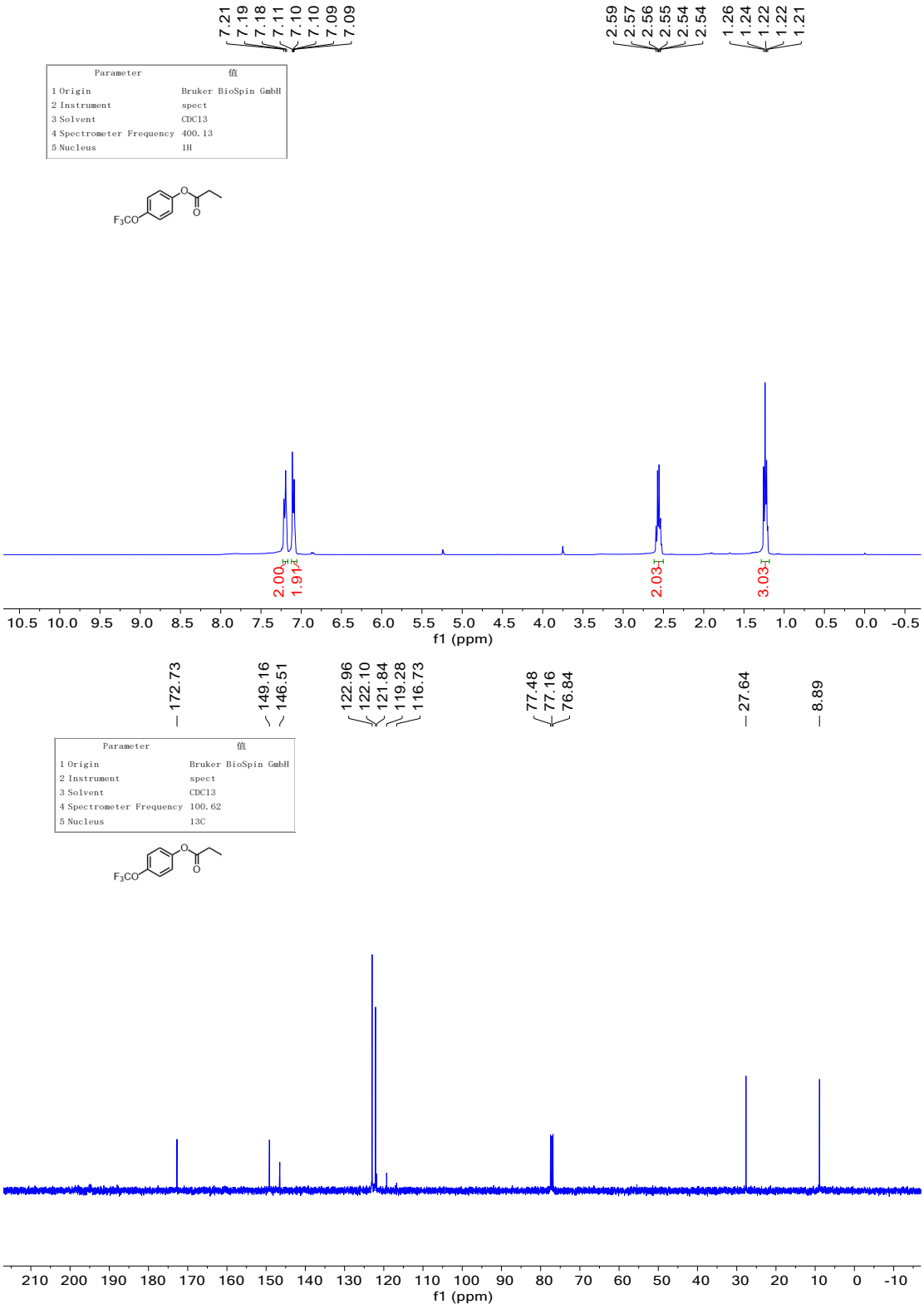


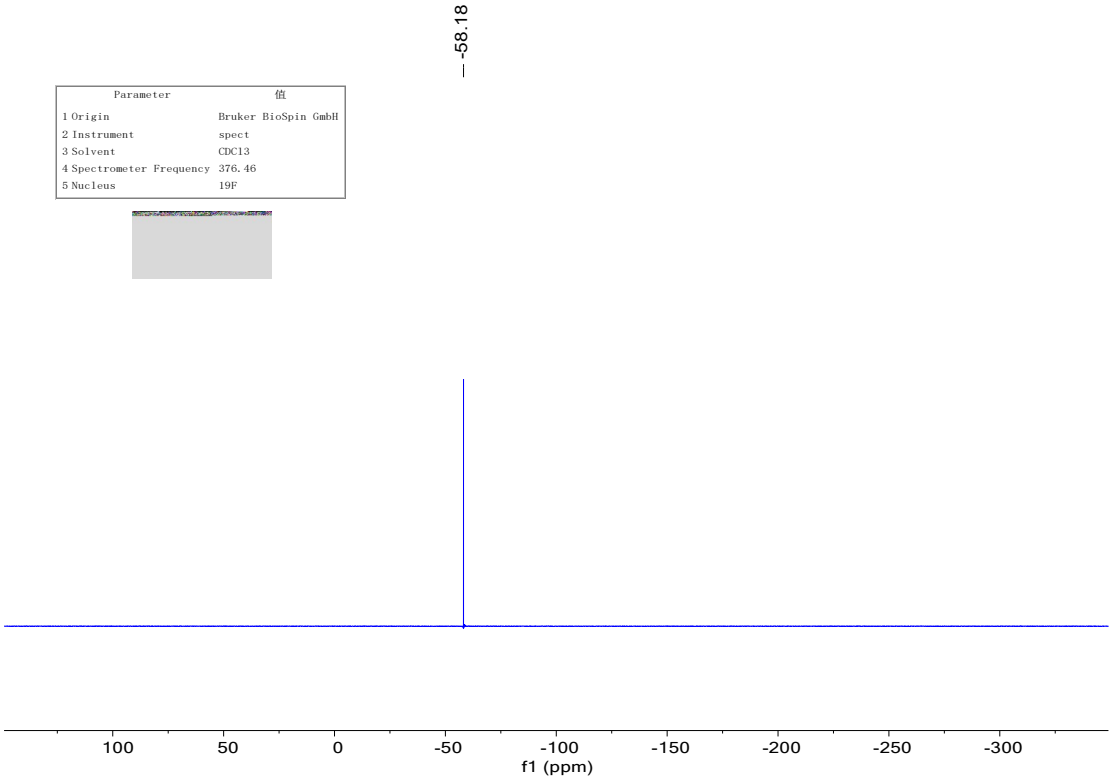


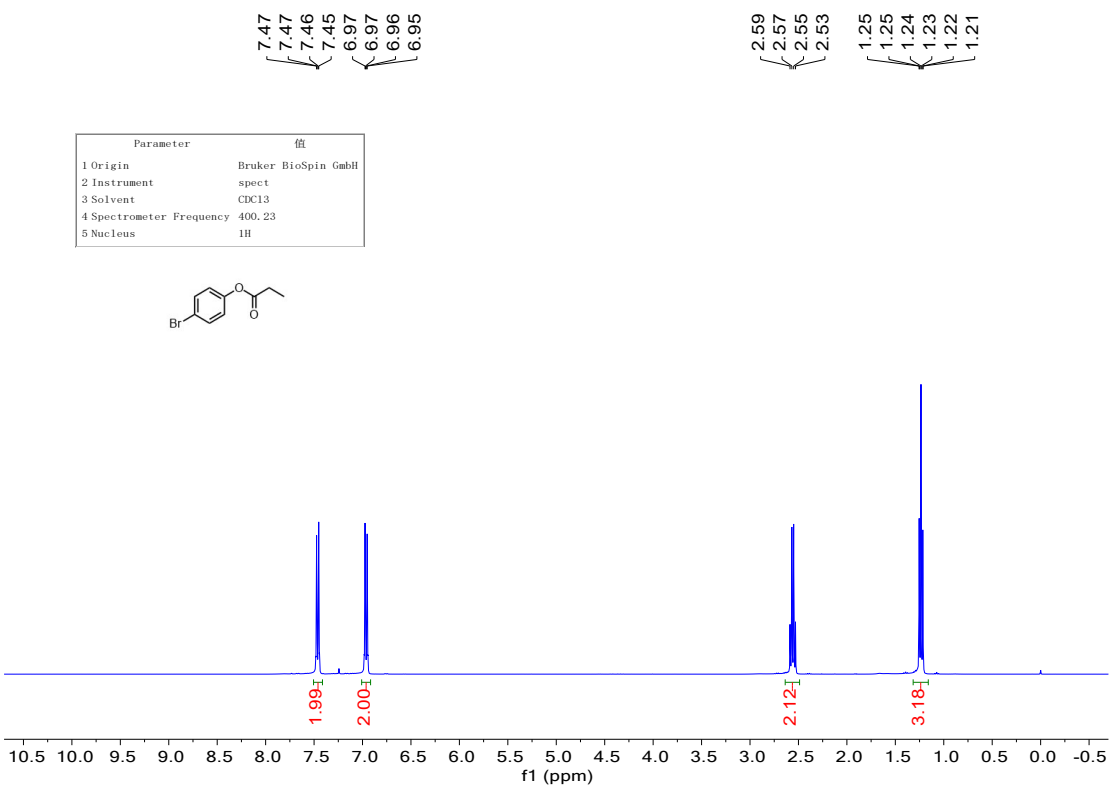
Parameter	值
1 Origin	Bruker BioSpin GmbH
2 Instrument	spect
3 Solvent	CDCl3
4 Spectrometer Frequency	100.62
5 Nucleus	13C

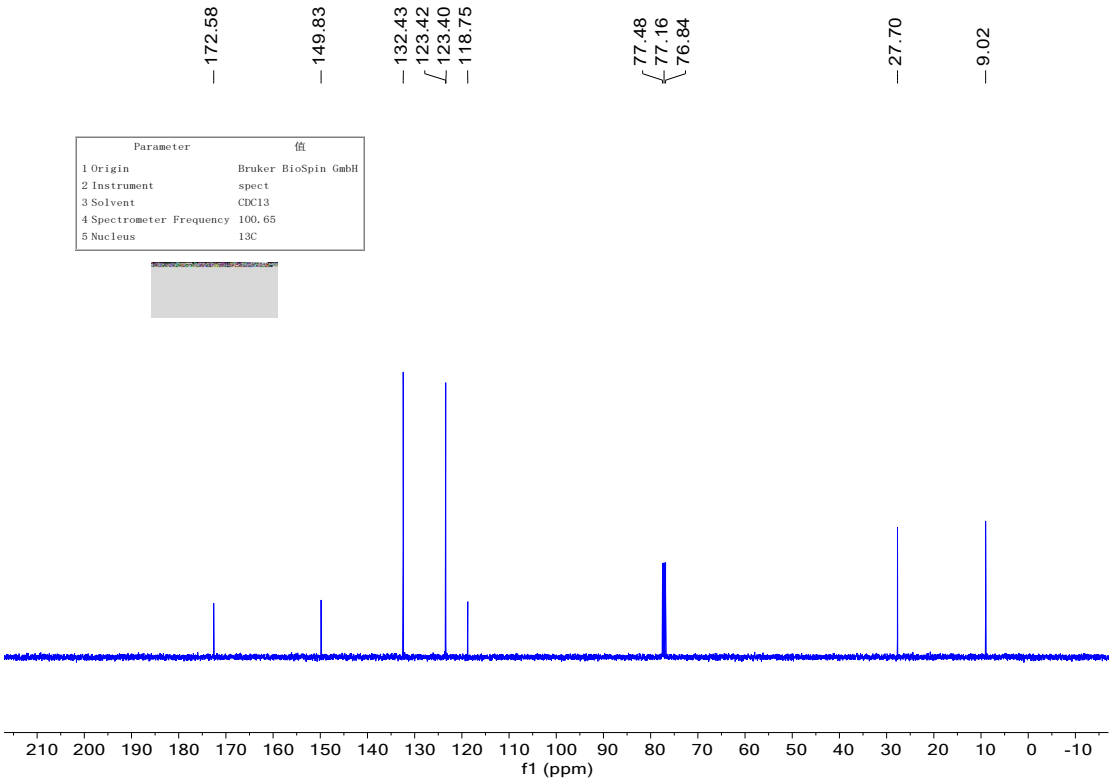





7.21
7.19
7.18
7.11
7.10
7.10
7.09
7.09
2.59
2.57
2.56
2.55
2.54
2.54
1.26
1.24
1.22
1.22
1.21
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
F3CO
O
2.00
1.91
2.03
3.03
f1 (ppm)
172.73
149.16
146.51
122.96
122.10
121.84
119.28
116.73
77.48
77.16
76.84
27.64
8.89
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
F3CO
O
f1 (ppm)


-58.18
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 376.46
5 Nucleus 19F
100 50 0 -50 -100 -150 -200 -250 -300
f1 (ppm)


7.47 7.47 7.46 7.45 6.97 6.97 6.96 6.95
2.59 2.57 2.55 2.53
1.25 1.25 1.24 1.23 1.22 1.21
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.23
5 Nucleus 1H
Br
O
O
1.99
2.00
2.12
3.18
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


172.58
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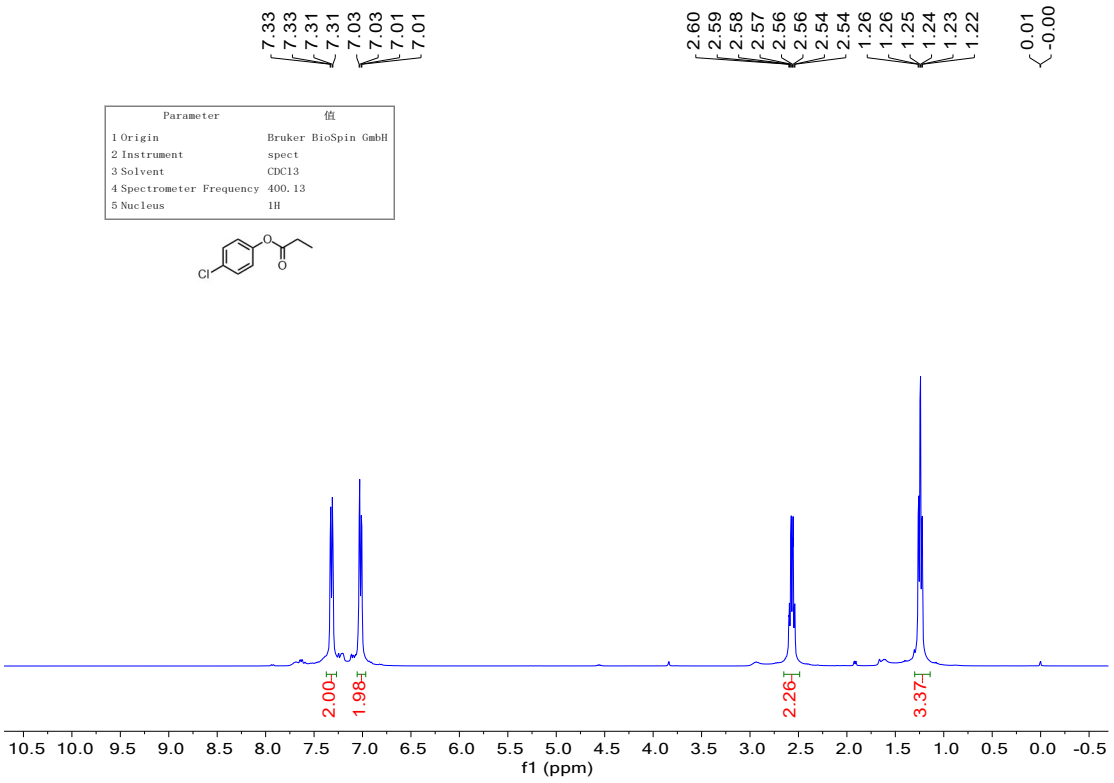
132.43
123.42
123.40
118.75
77.48
77.16
76.84
27.70
9.02
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.65
5 Nucleus 13C
f1 (ppm)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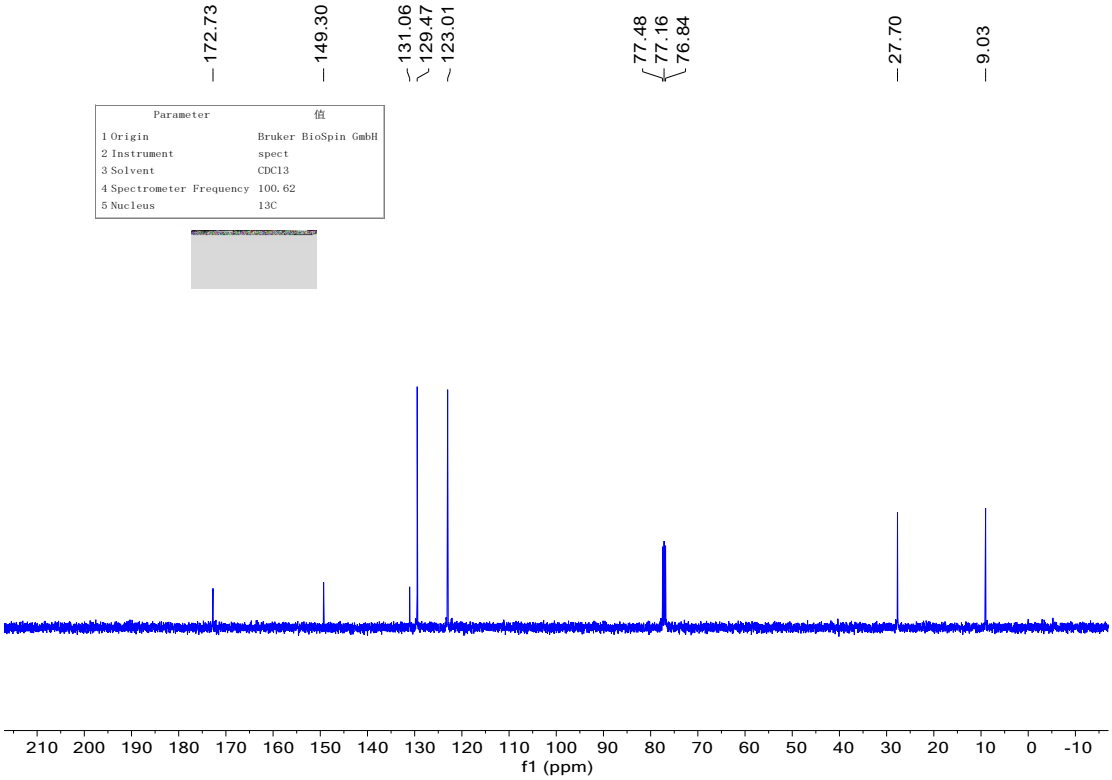
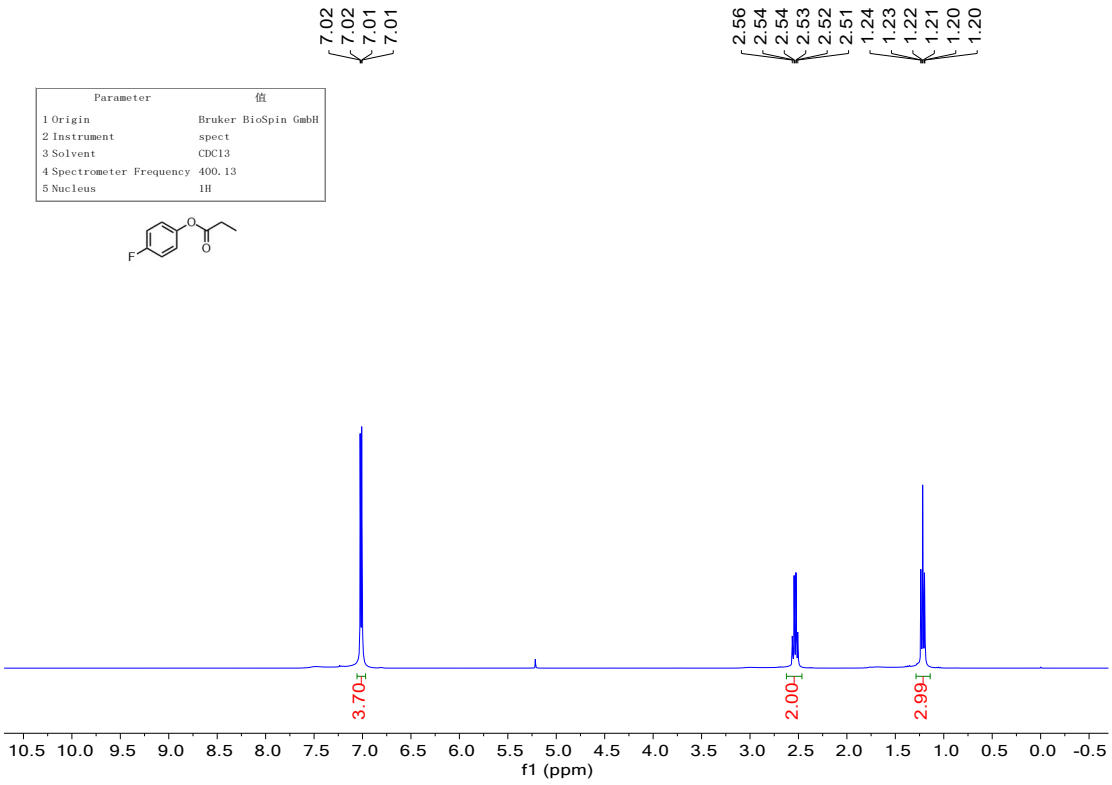
7.33
7.31
7.31
7.03
7.03
7.01
7.01
2.60
2.59
2.58
2.57
2.56
2.56
2.54
2.54
1.26
1.26
1.25
1.24
1.23
1.22
0.01
-0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Cl
O
O
2.00
1.98
2.26
3.37
f1 (ppm)


172.73
149.30
131.06
129.47
123.01
77.48
77.16
76.84
27.70
9.03
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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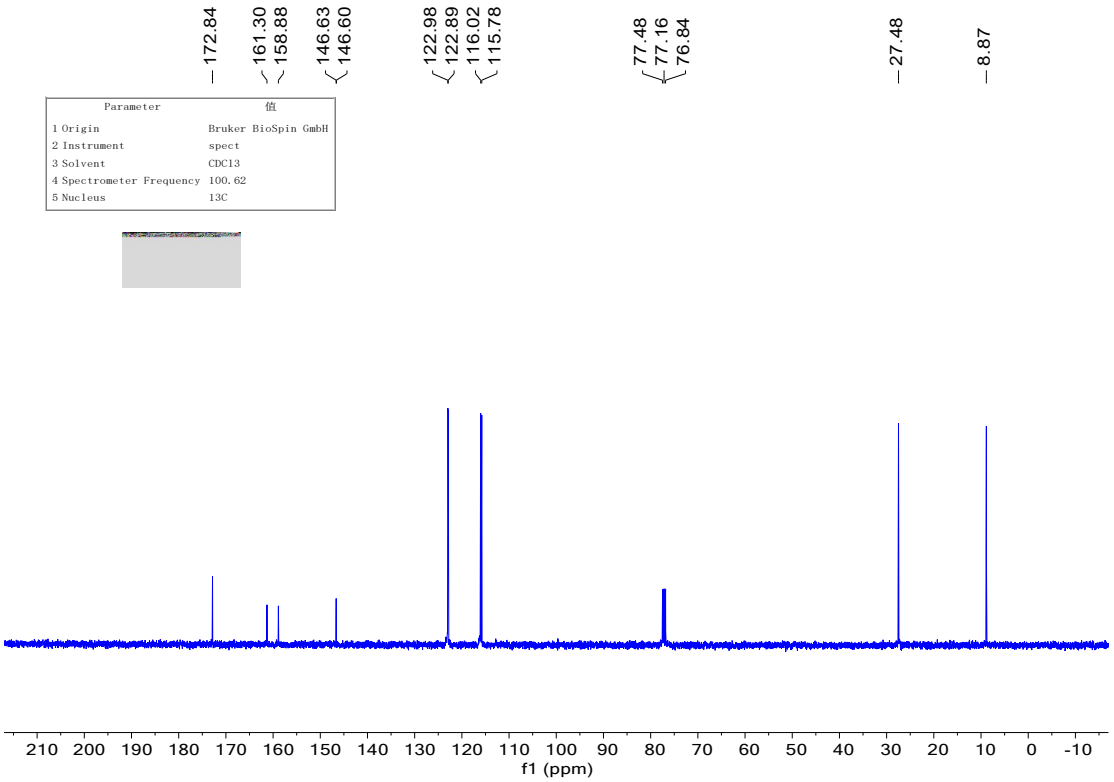
7.02
7.01
7.01
2.56
2.54
2.54
2.53
2.52
2.51
1.24
1.23
1.22
1.21
1.20
1.20
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
F
O
O
3.70
2.00
2.99
f1 (ppm)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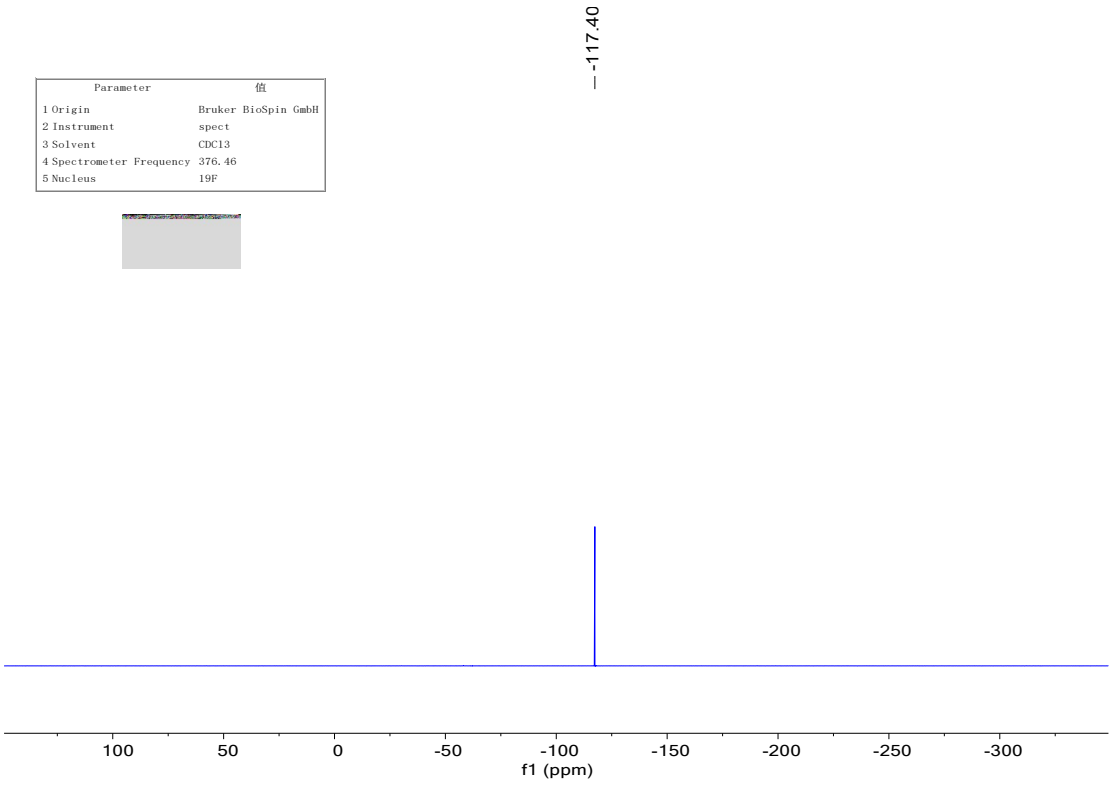
161.30
158.88
146.63
146.60
122.98
122.89
116.02
115.78
77.48
77.16
76.84
27.48
8.87
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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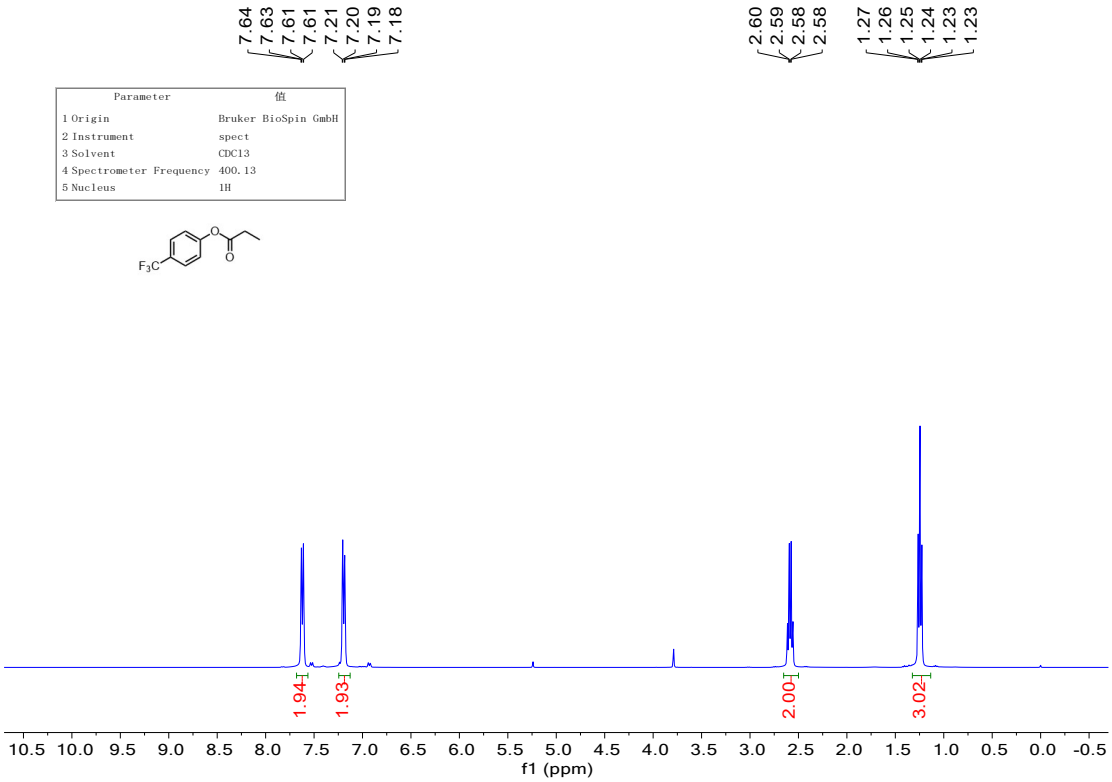
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 376.46
5 Nucleus 19F
100 50 0 -50 -100 -150 -200 -250 -300
f1 (ppm)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7.61
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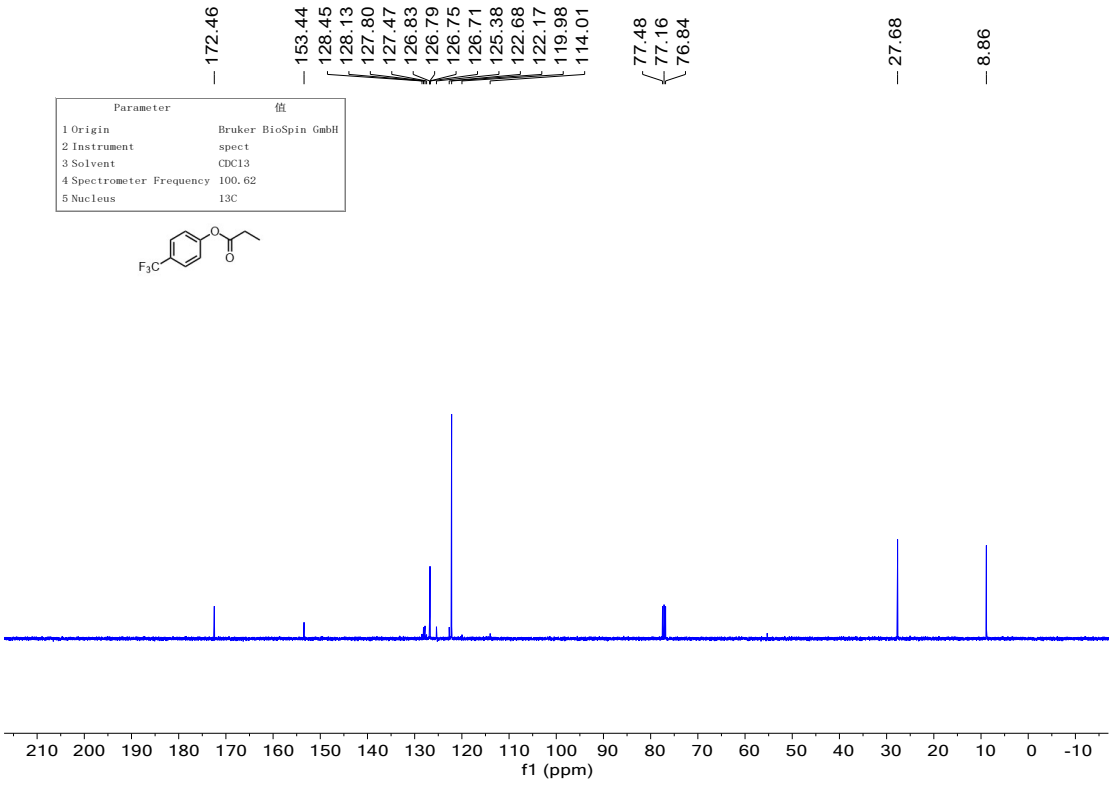
7.18
2.60
2.59
2.58
2.58
1.27
1.26
1.25
1.24
1.23
1.23
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
F3C
O
O
1.94
1.93
2.00
3.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.71
125.38
122.68
122.17
119.98
114.01
77.48
77.16
76.84
27.68
8.86
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
F3C
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Parameter	值
1 Origin	Bruker BioSpin GmbH
2 Instrument	spect
3 Solvent	CDCl3
4 Spectrometer Frequency	376.46
5 Nucleus	19F

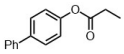
7.59 7.59 7.58 7.57 7.57 7.56 7.55 7.55 7.45 7.45 7.43 7.43 7.41 7.36 7.34 7.25 7.17 7.16 7.15 7.15

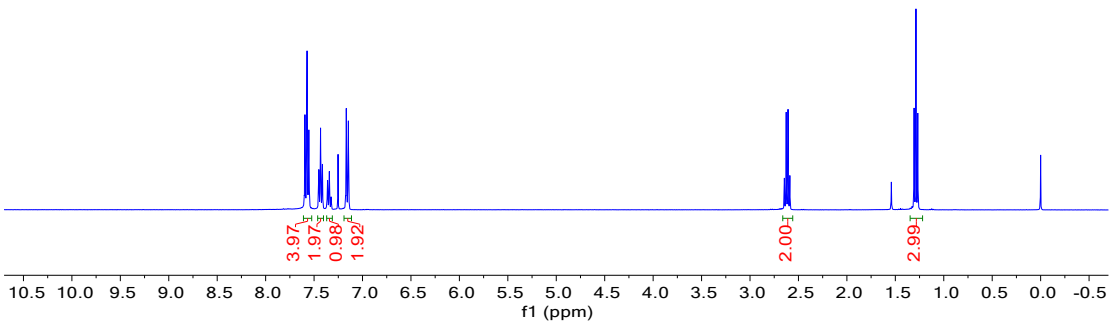
2.65 2.63 2.61 2.59

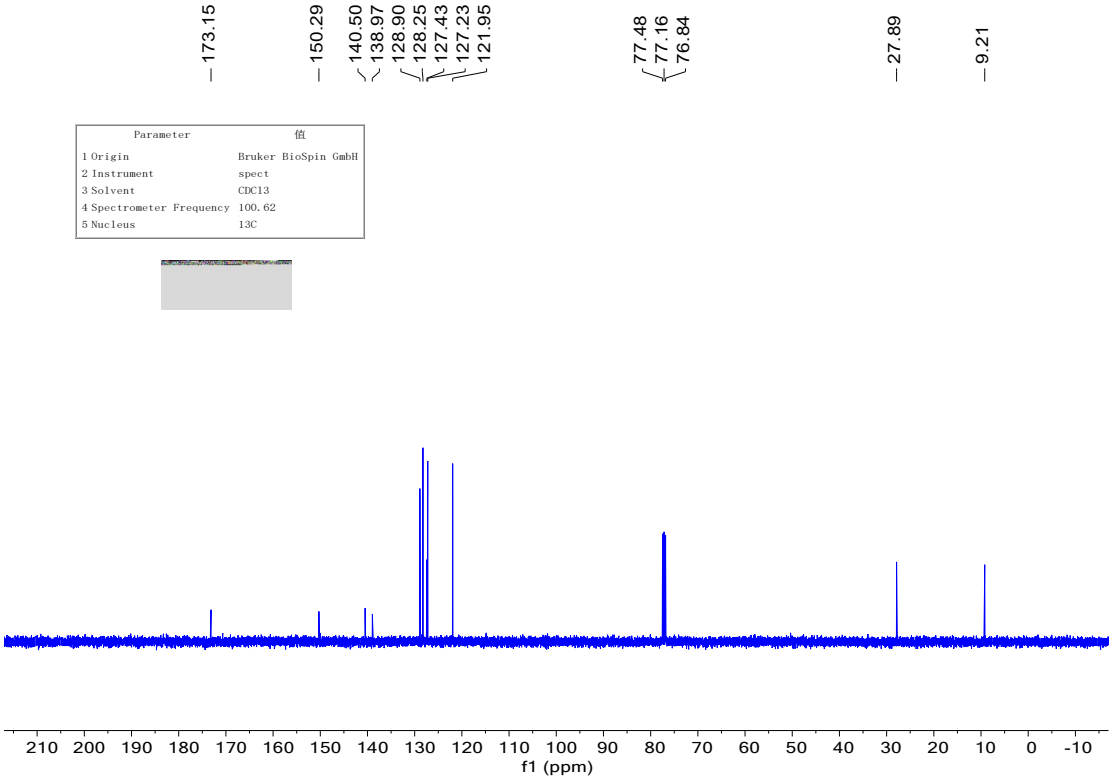
1.31 1.29 1.27

0.00

Parameter	值
1 Origin	Bruker BioSpin GmbH
2 Instrument	spect
3 Solvent	CDCl3
4 Spectrometer Frequency	400.23
5 Nucleus	1H



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128.25
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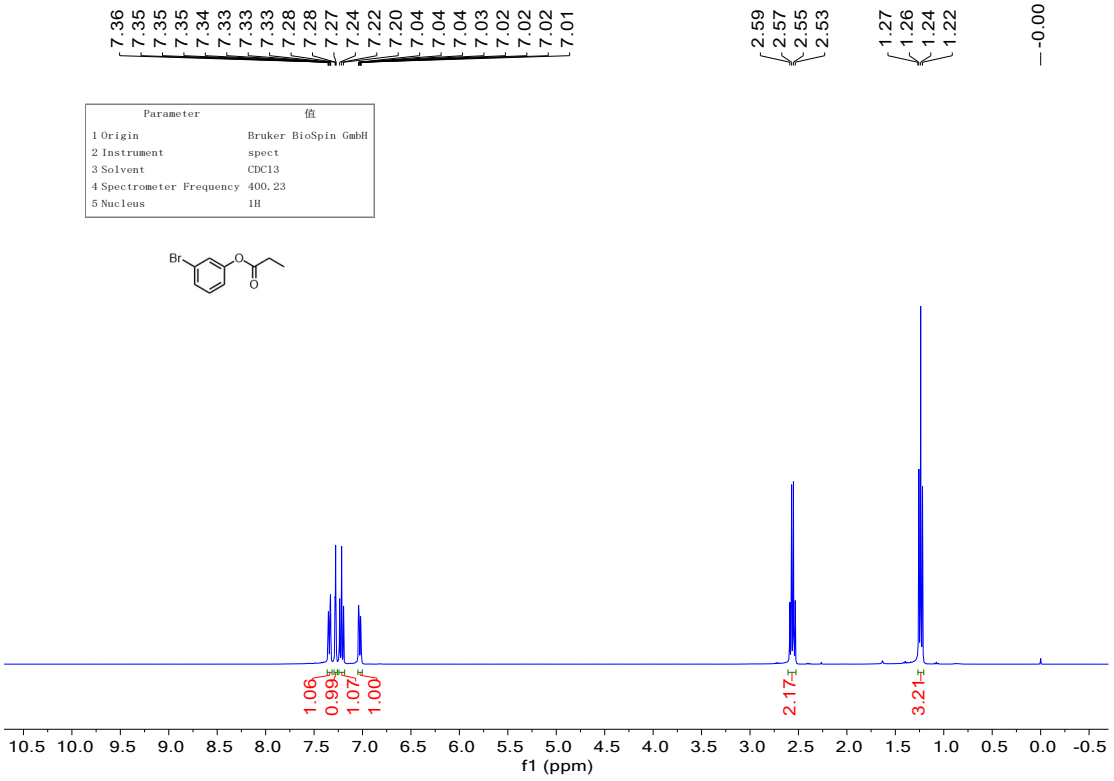
127.23
121.95
77.48
77.16
76.84
27.89
9.21
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.33
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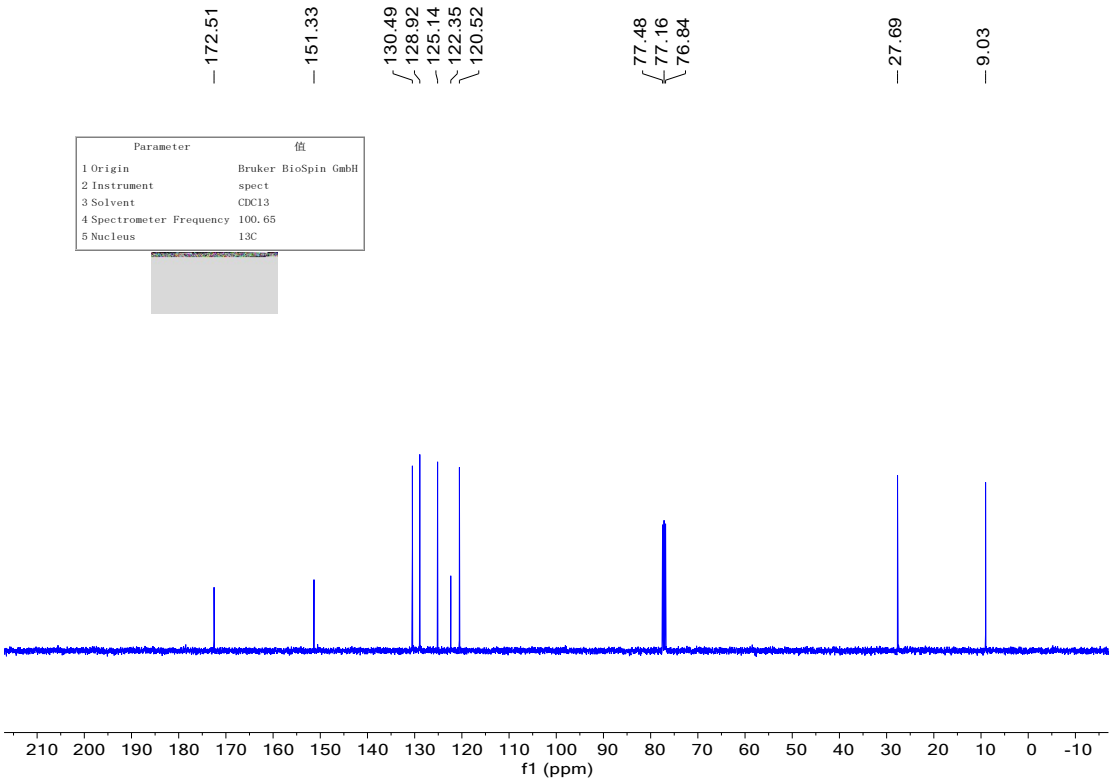
7.28
7.27
7.24
7.22
7.20
7.04
7.04
7.04
7.03
7.02
7.02
7.02
7.01
2.59
2.57
2.55
2.53
1.27
1.26
1.24
1.22
-0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.23
5 Nucleus 1H
Br
O
O
1.06
0.99
1.07
1.00
2.17
3.21
f1 (ppm)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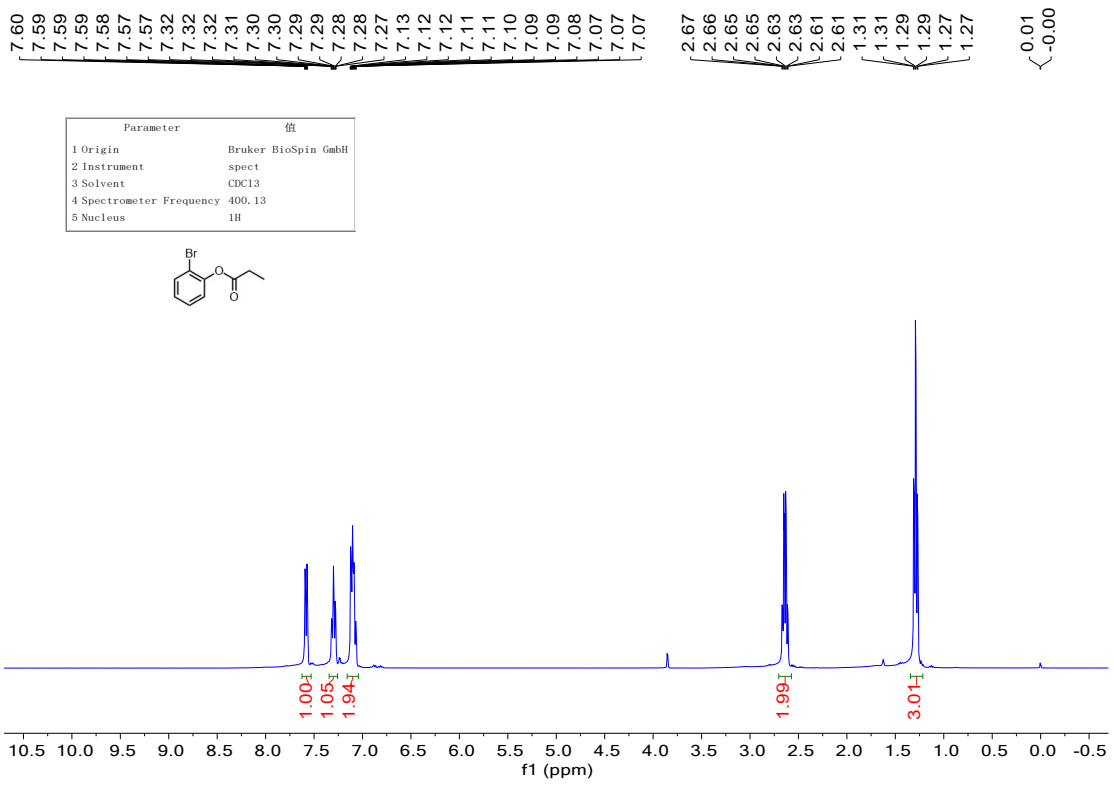
122.35
120.52
77.48
77.16
76.84
27.69
9.03
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.65
5 Nucleus 13C
f1 (ppm)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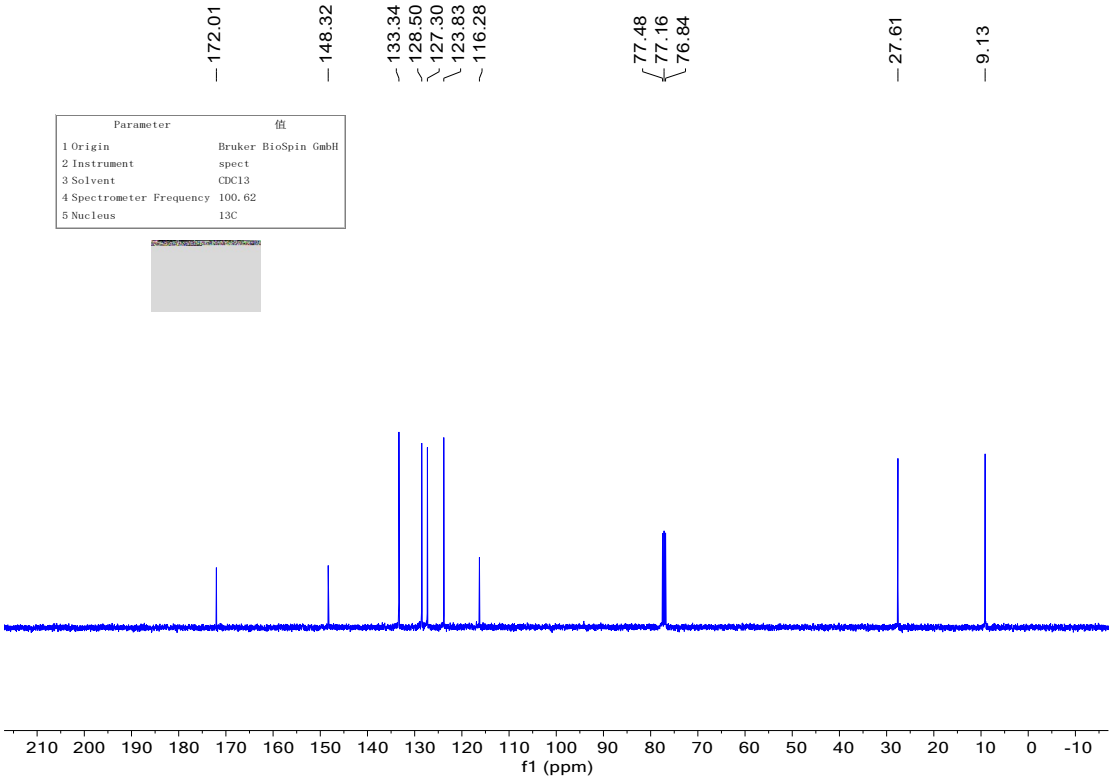
2.67 2.66 2.65 2.65 2.63 2.63 2.61 2.61
1.31 1.31 1.29 1.29 1.27 1.27
0.01 -0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Br
O
O
1.00 1.05 1.94 1.99 3.01
f1 (ppm)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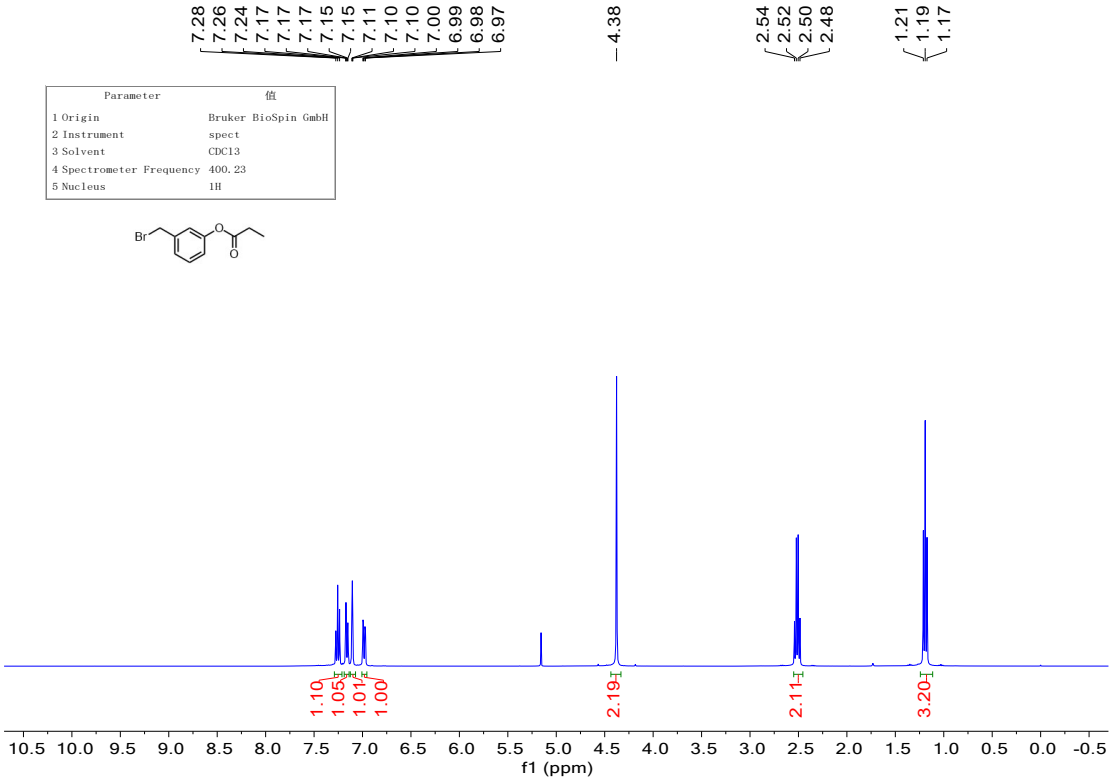
127.30
123.83
116.28
77.48
77.16
76.84
27.61
9.13
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.26
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7.17
7.17
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7.15
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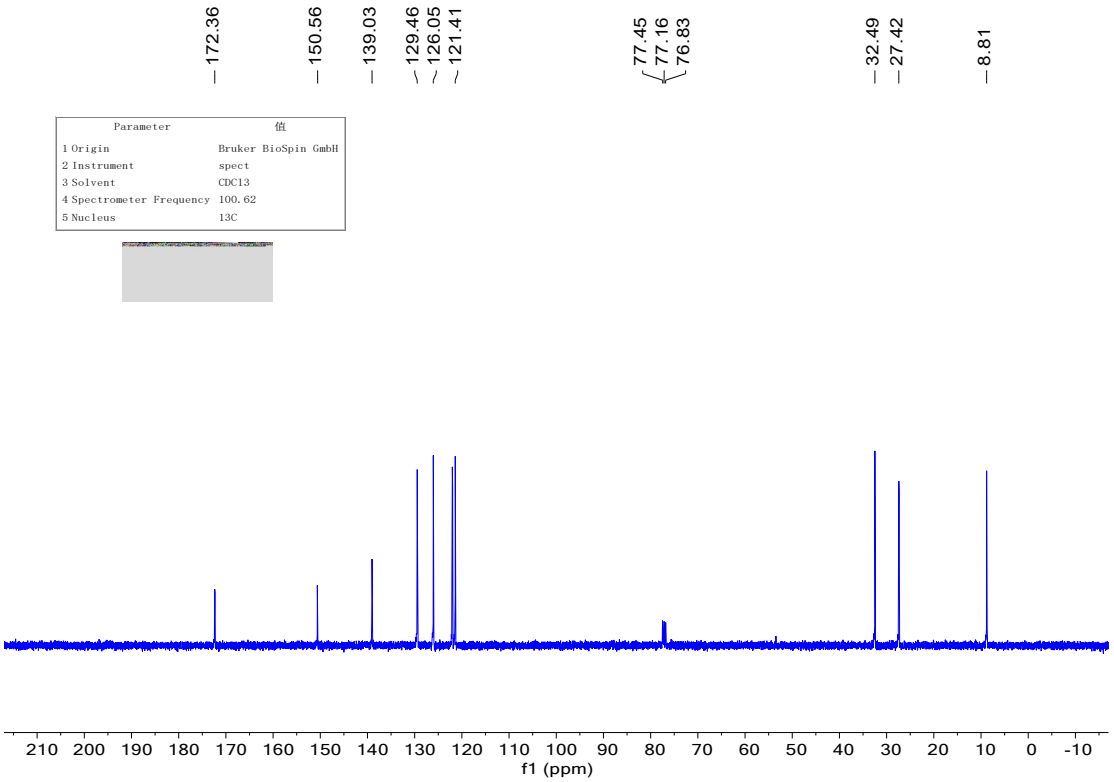
7.10
7.10
7.00
6.99
6.98
6.97
4.38
2.54
2.52
2.50
2.48
1.21
1.19
1.17
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.23
5 Nucleus 1H
Br
O
O
1.10
1.05
1.01
1.00
2.19
2.11
3.20
f1 (ppm)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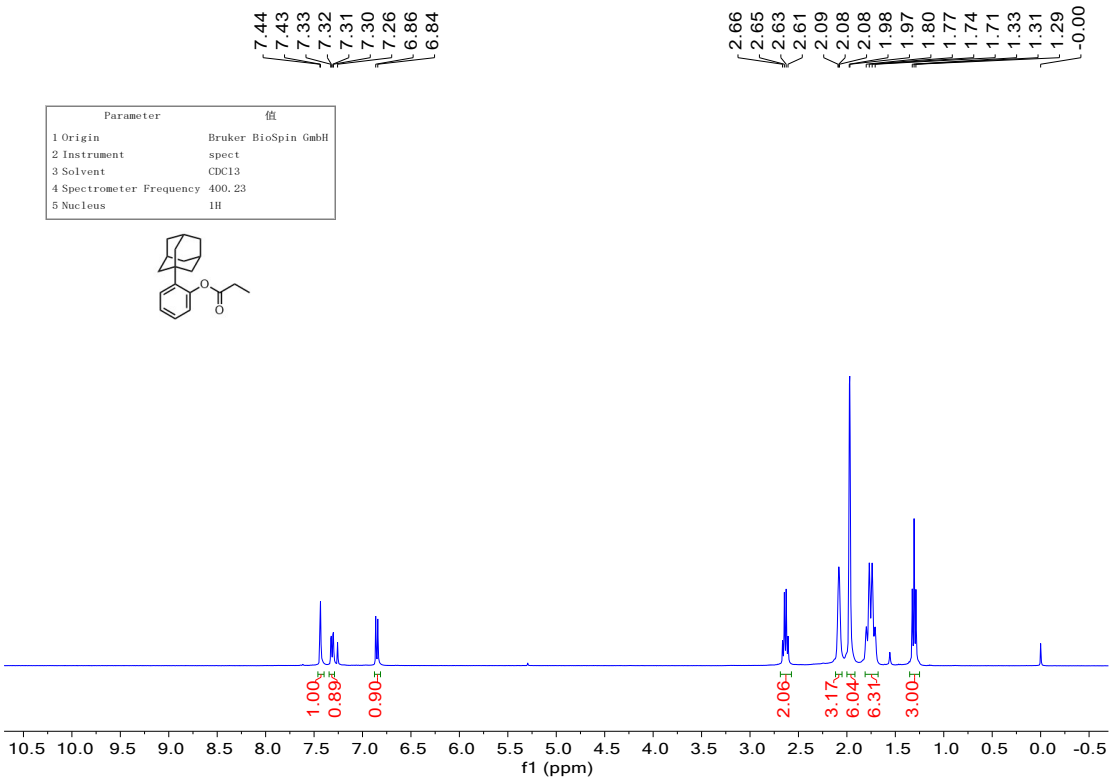
126.05
121.41
77.45
77.16
76.83
32.49
27.42
8.81
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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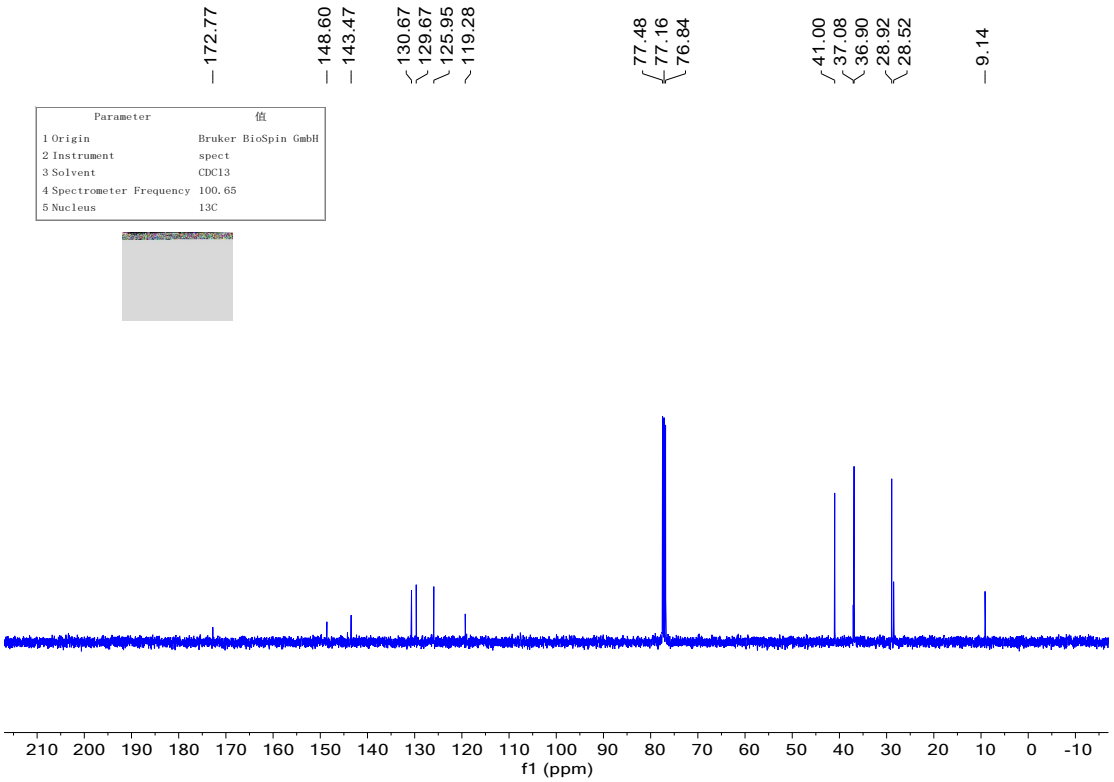
2.65
2.63
2.61
2.09
2.08
2.08
1.98
1.97
1.80
1.77
1.74
1.71
1.33
1.31
1.29
-0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.23
5 Nucleus 1H
O
O
1.00
0.89
0.90
2.06
3.17
6.04
6.31
3.00
f1 (ppm)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77.48
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76.84
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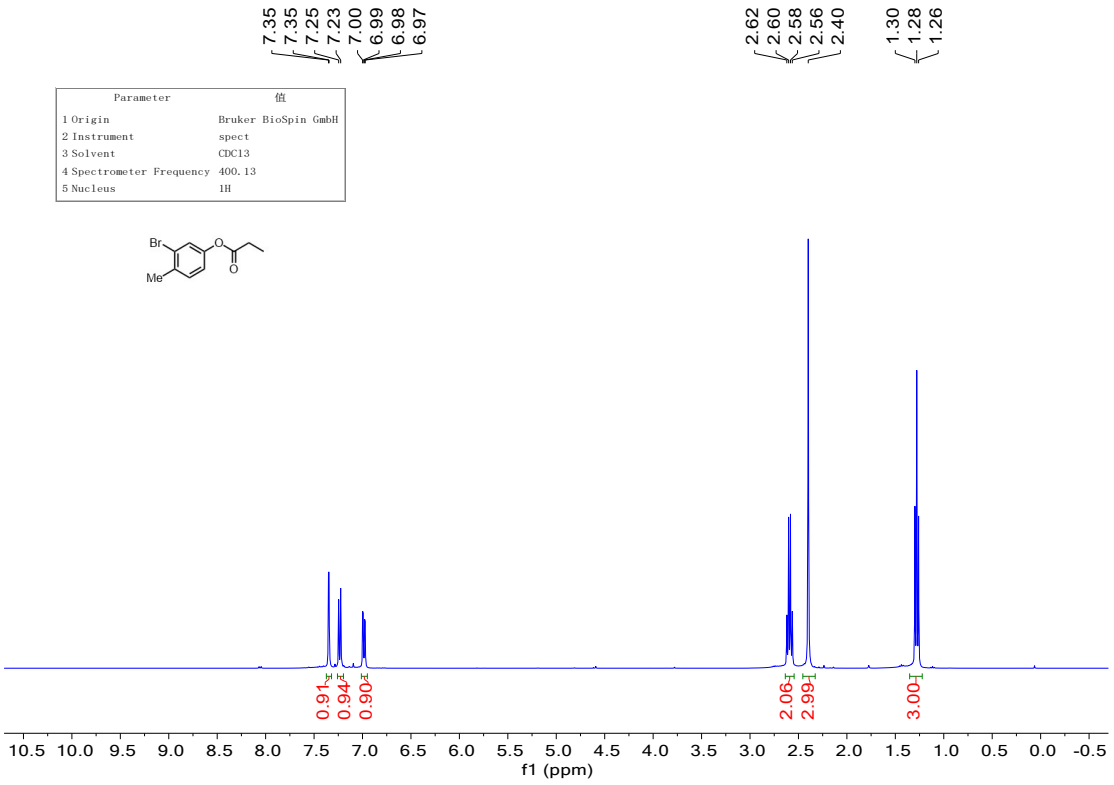
37.08
36.90
28.92
28.52
9.14
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.65
5 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.97
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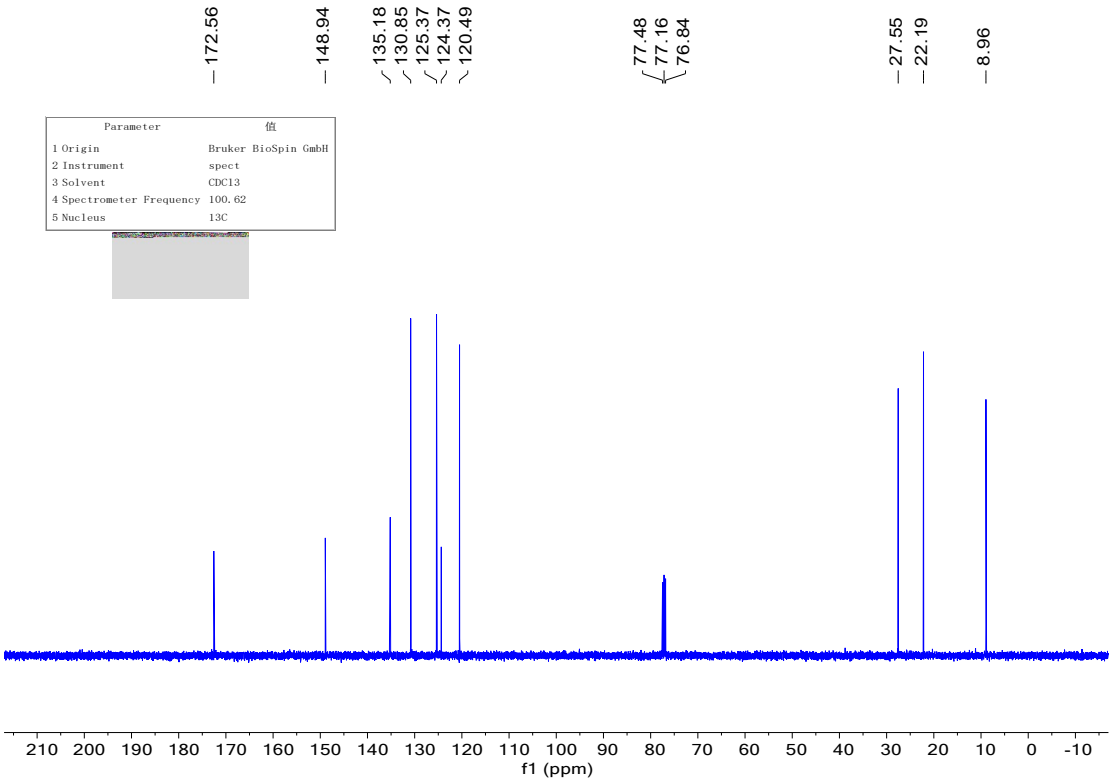
2.40
1.30
1.28
1.26
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Br
O
O
Me
0.91
0.94
0.90
2.06
2.99
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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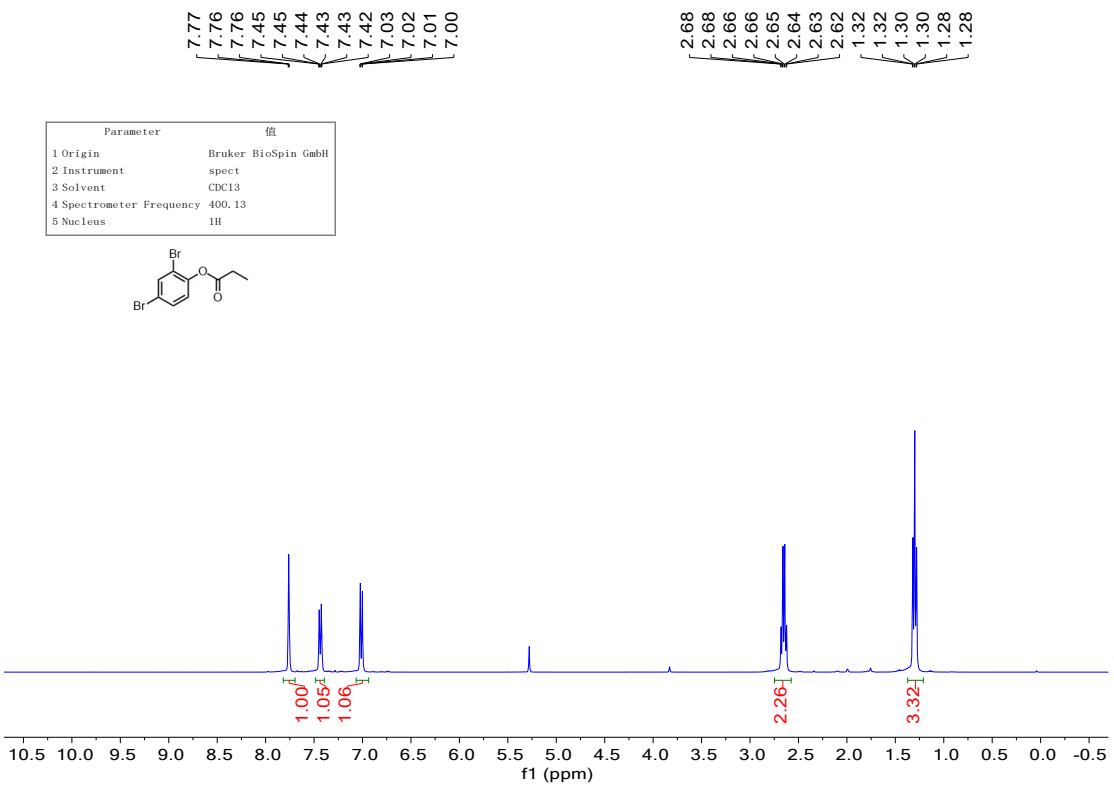
76.84
27.55
22.19
8.96
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.43
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7.02
7.01
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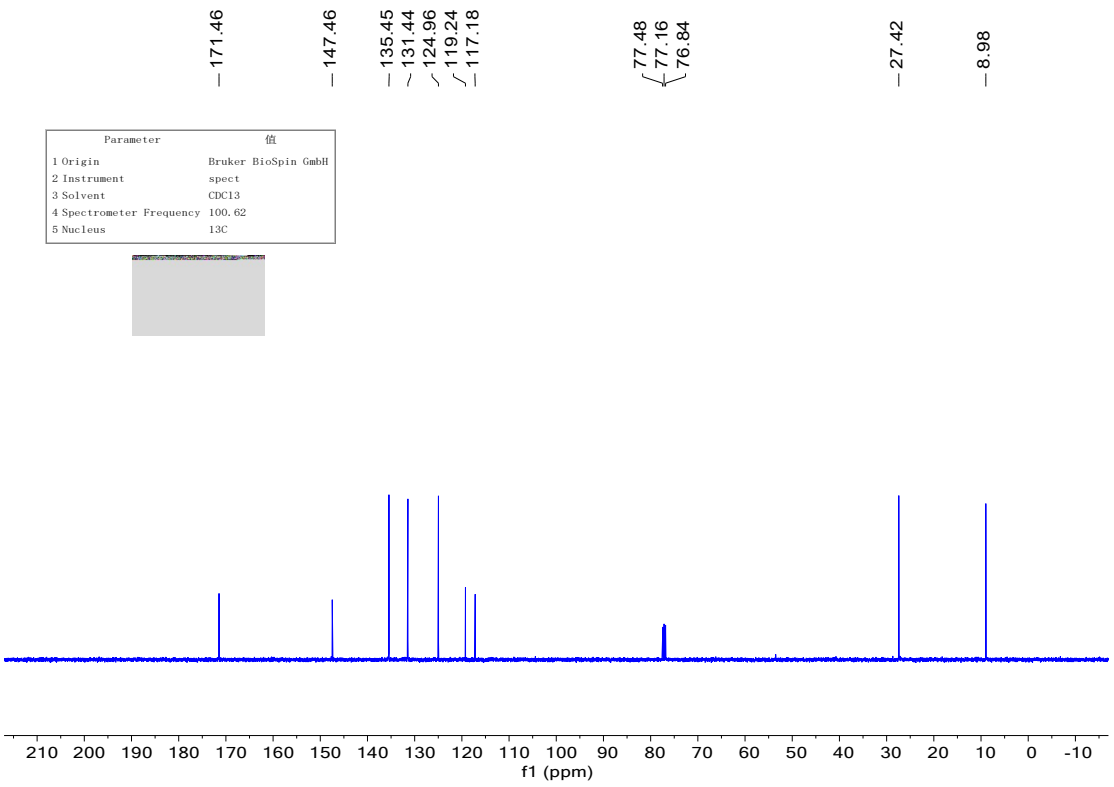
2.68
2.66
2.66
2.65
2.64
2.63
2.62
1.32
1.32
1.30
1.30
1.28
1.28
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Br
Br
O
O
1.00
1.05
1.06
2.26
3.32
f1 (ppm)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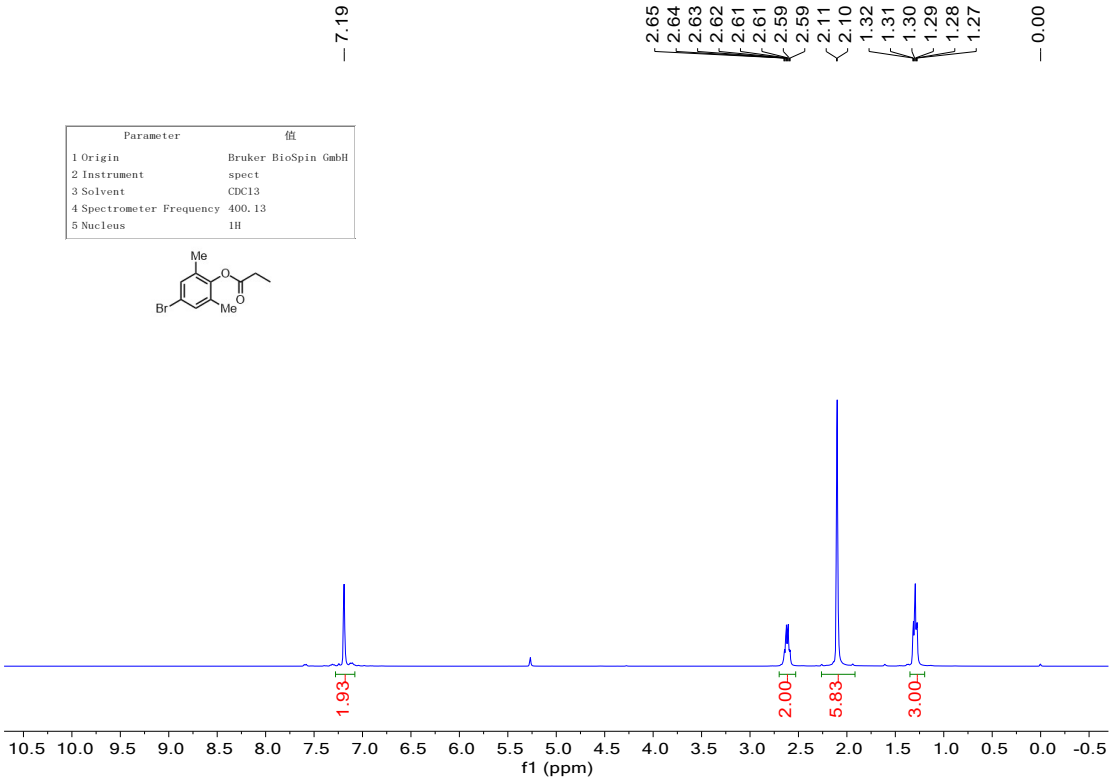
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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2.11
2.10
1.32
1.31
1.30
1.29
1.28
1.27
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Me
O
O
Br
Me
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2.00
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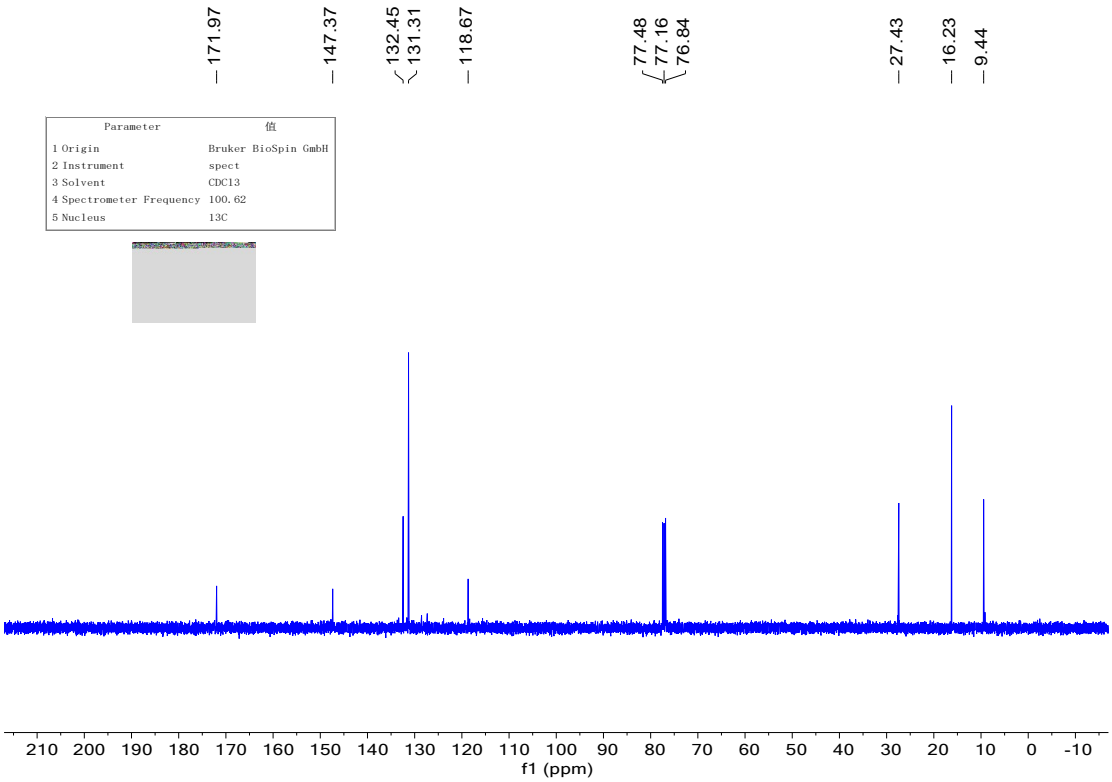
3.00
f1 (ppm)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76.84
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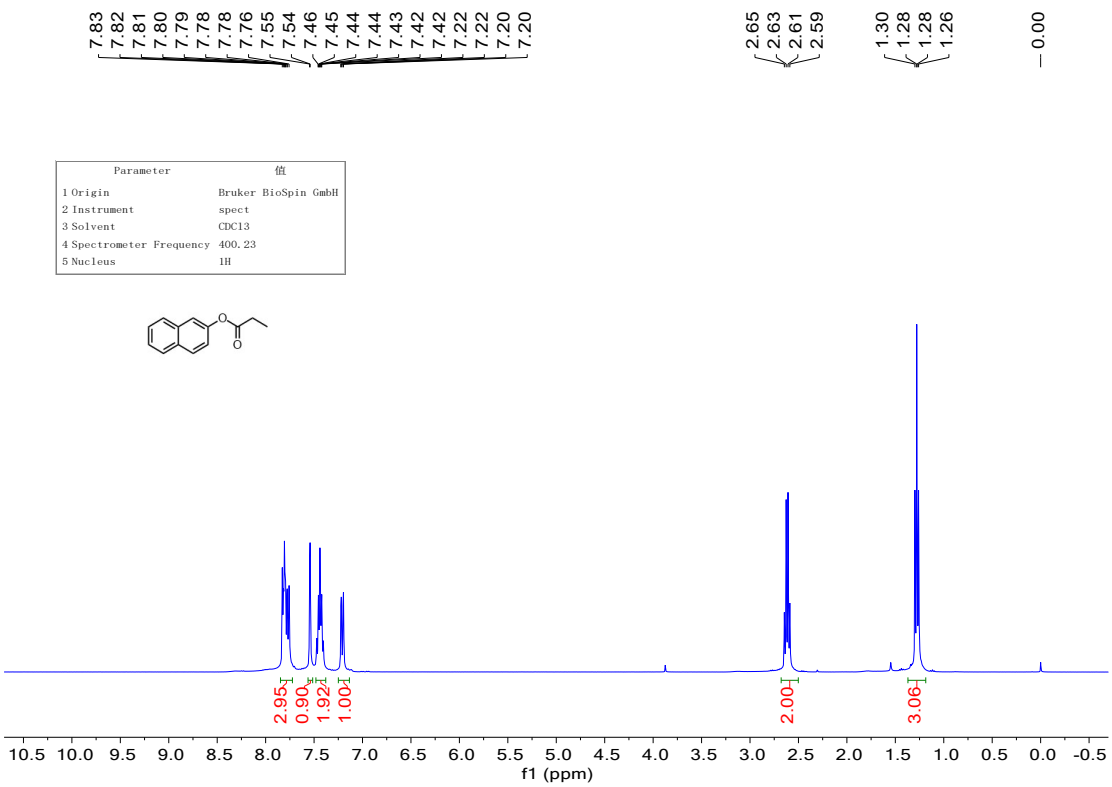
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.76
7.55
7.54
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.22
7.22
7.20
7.20
2.65
2.63
2.61
2.59
1.30
1.28
1.28
1.26
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
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O
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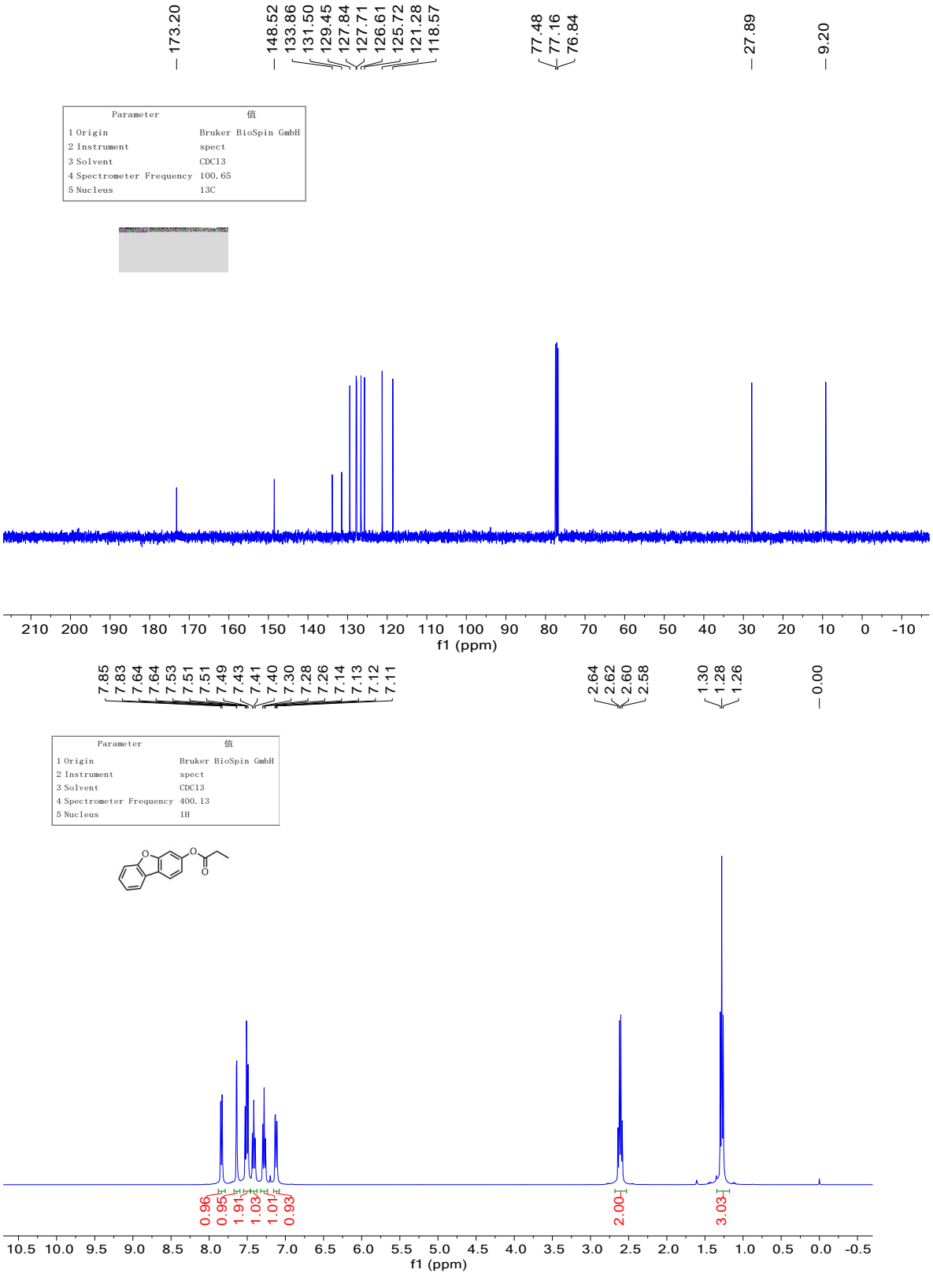
1.00
2.00
3.06
f1 (ppm)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126.61
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121.28
118.57
77.48
77.16
76.84
27.89
9.20
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.65
5 Nucleus 13C
f1 (ppm)
7.85
7.83
7.64
7.64
7.53
7.51
7.51
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7.30
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7.26
7.14
7.13
7.12
7.11
2.64
2.62
2.60
2.58
1.30
1.28
1.26
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
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0.95
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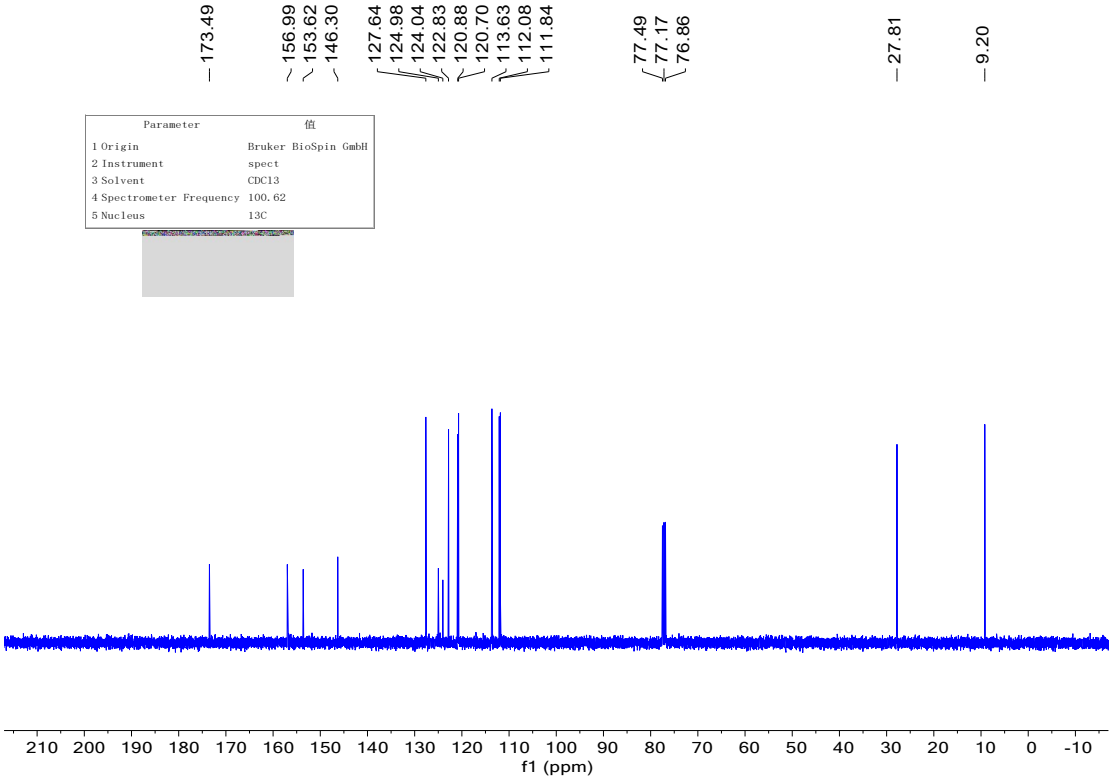
1.03
1.01
0.93
2.00
3.03
f1 (ppm)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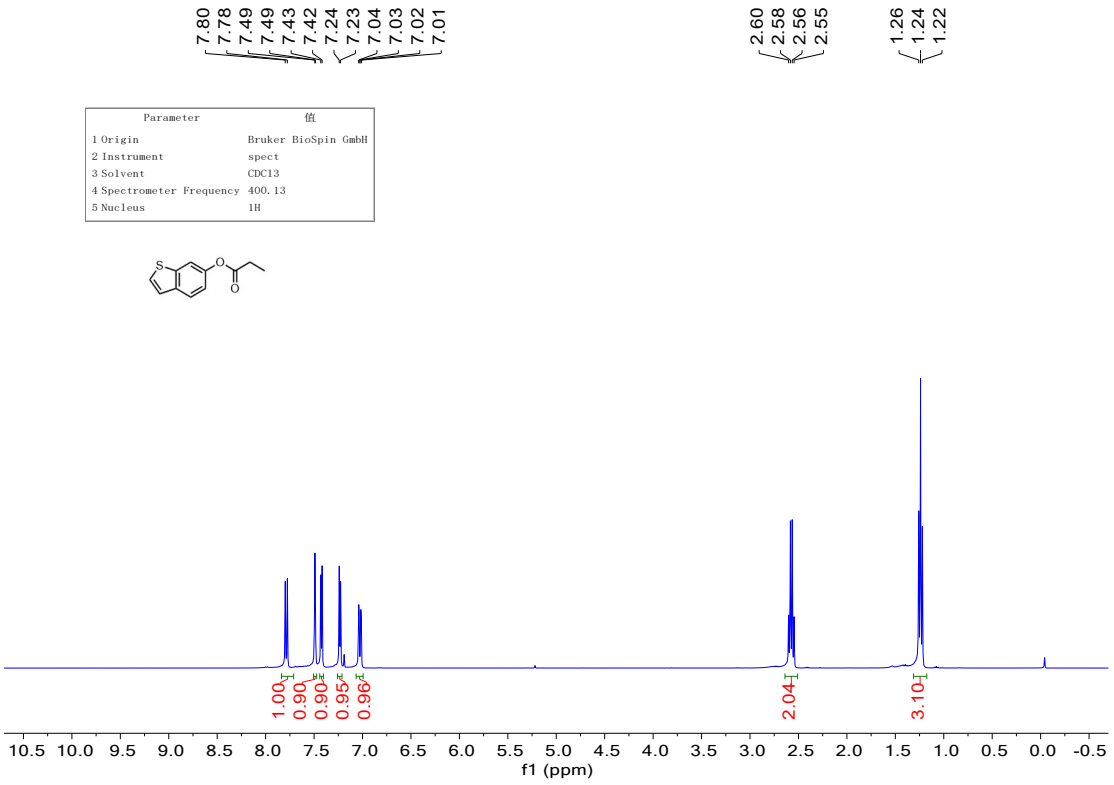
120.70
113.63
112.08
111.84
77.49
77.17
76.86
27.81
9.20
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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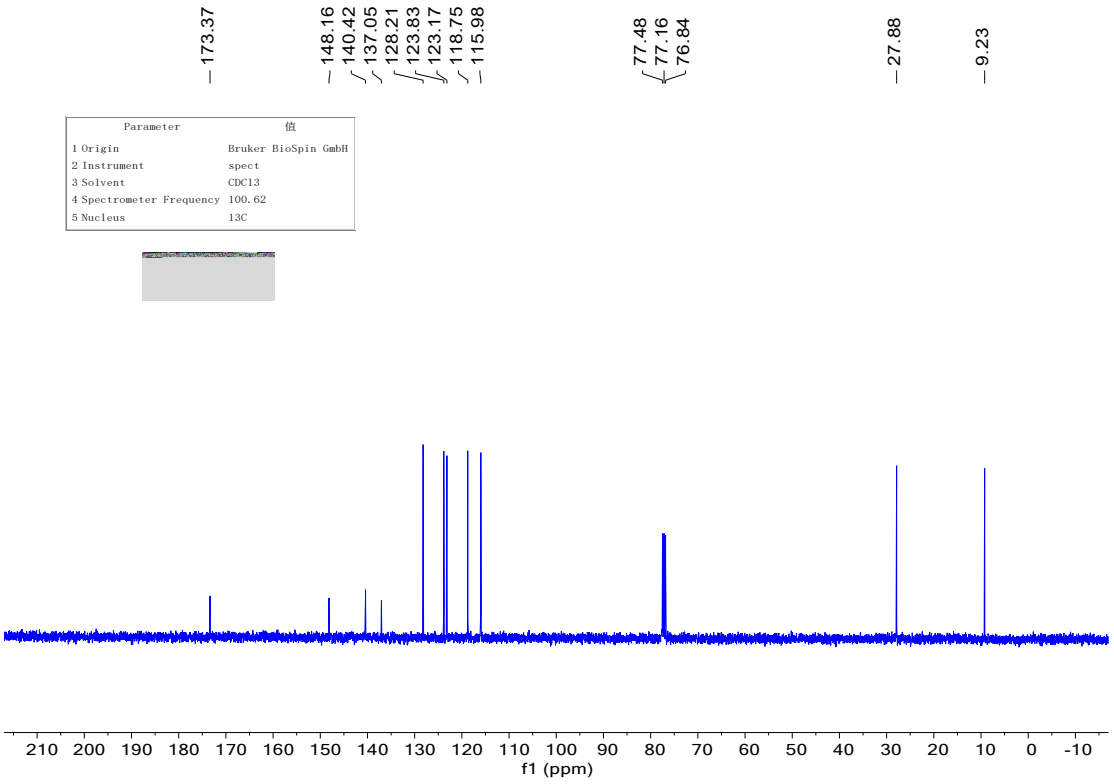
7.03
7.02
7.01
2.60
2.58
2.56
2.55
1.26
1.24
1.22
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
S
O
O
1.00
0.90
0.90
0.95
0.96
2.04
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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123.17
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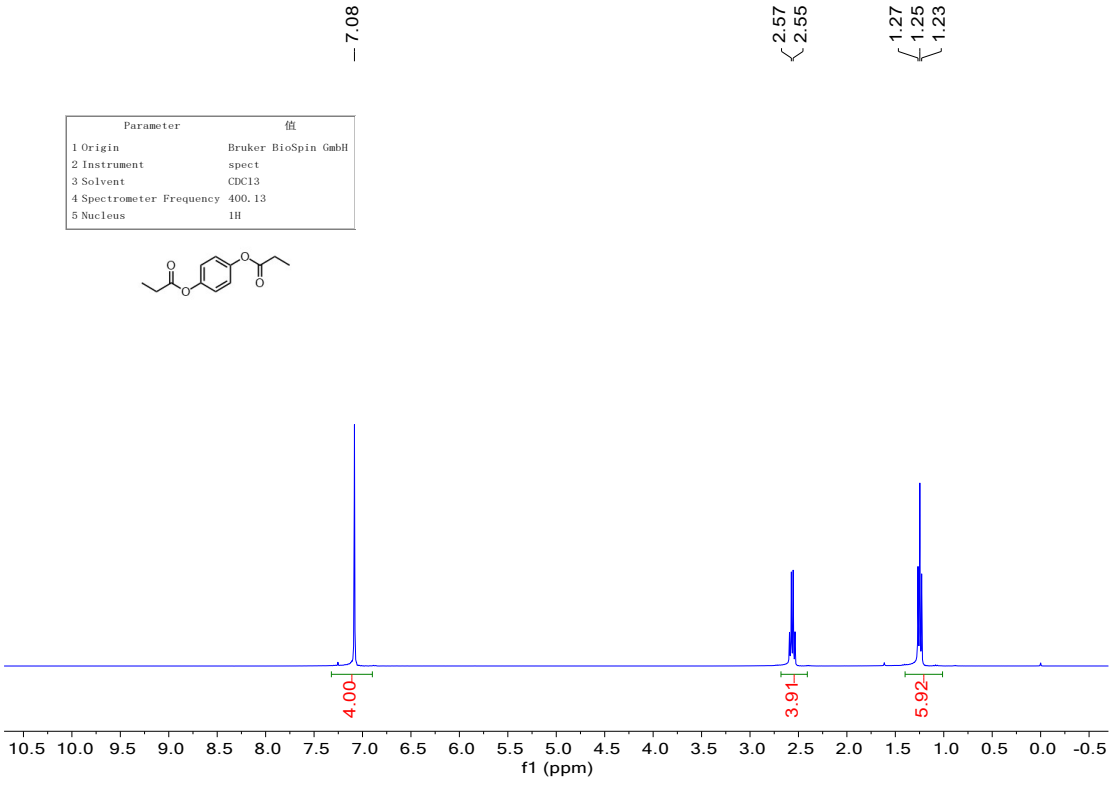
77.48
77.16
76.84
27.88
9.23
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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1.23
Parameter 值
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2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
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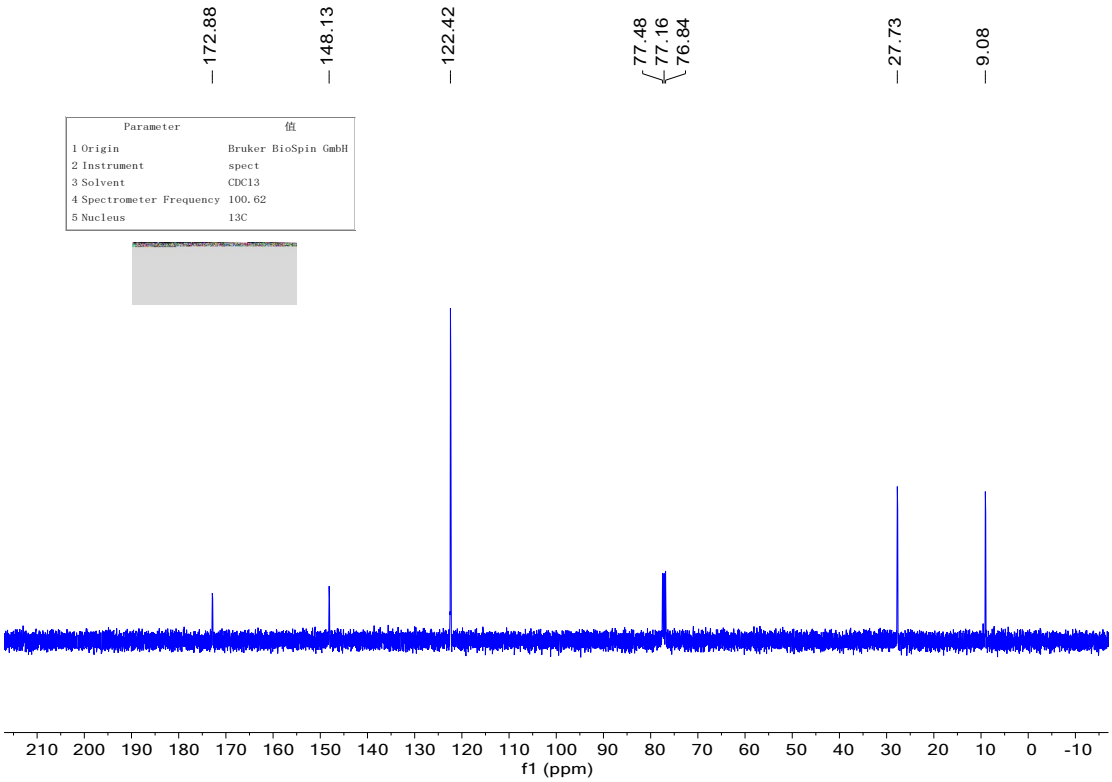
5.92
f1 (ppm)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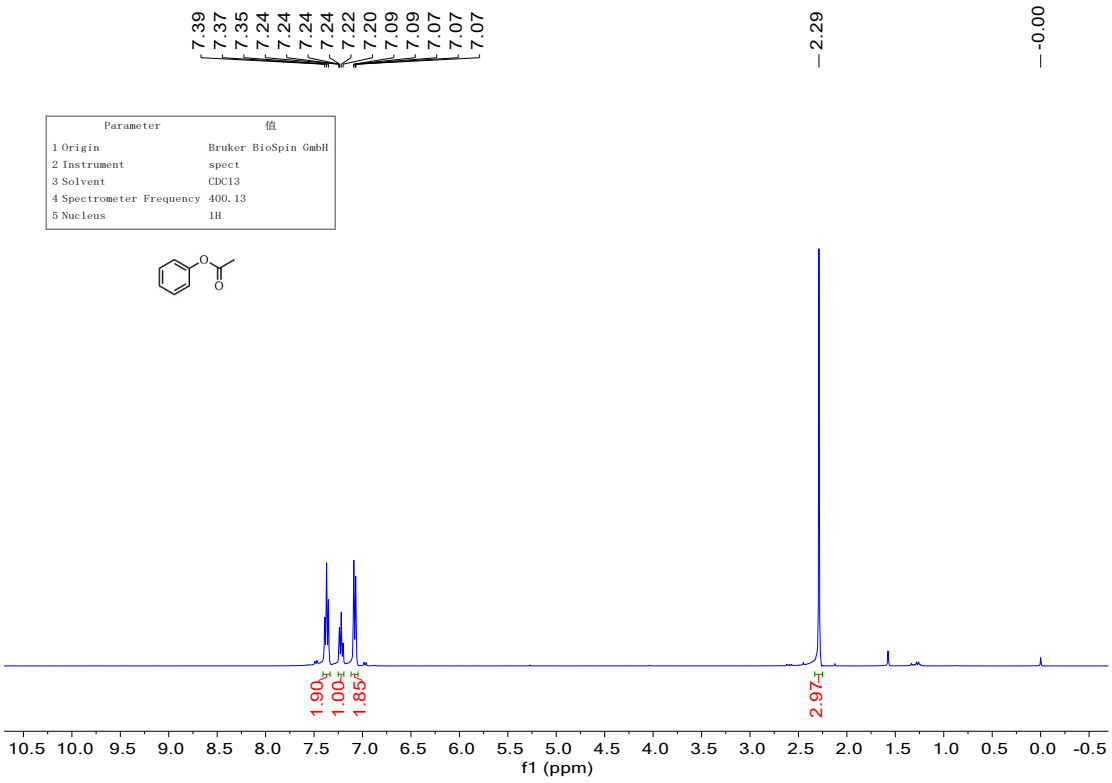
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.09
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7.07
7.07
2.29
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
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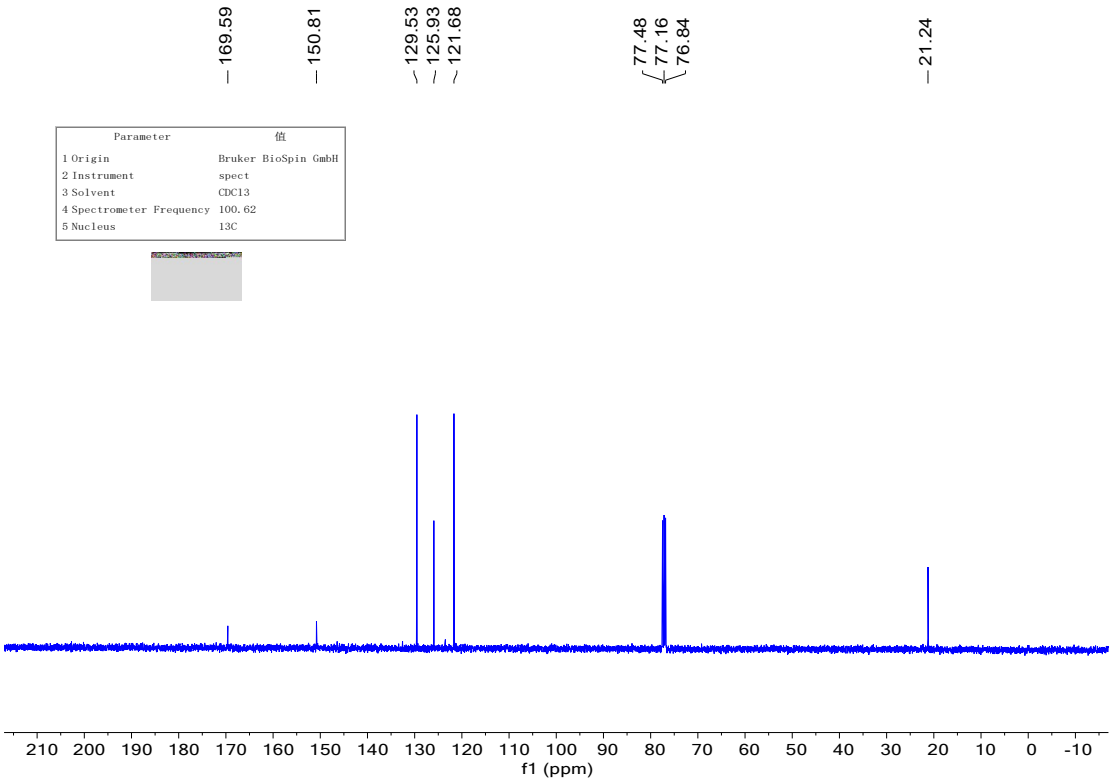
1.00
1.85
2.97
f1 (ppm)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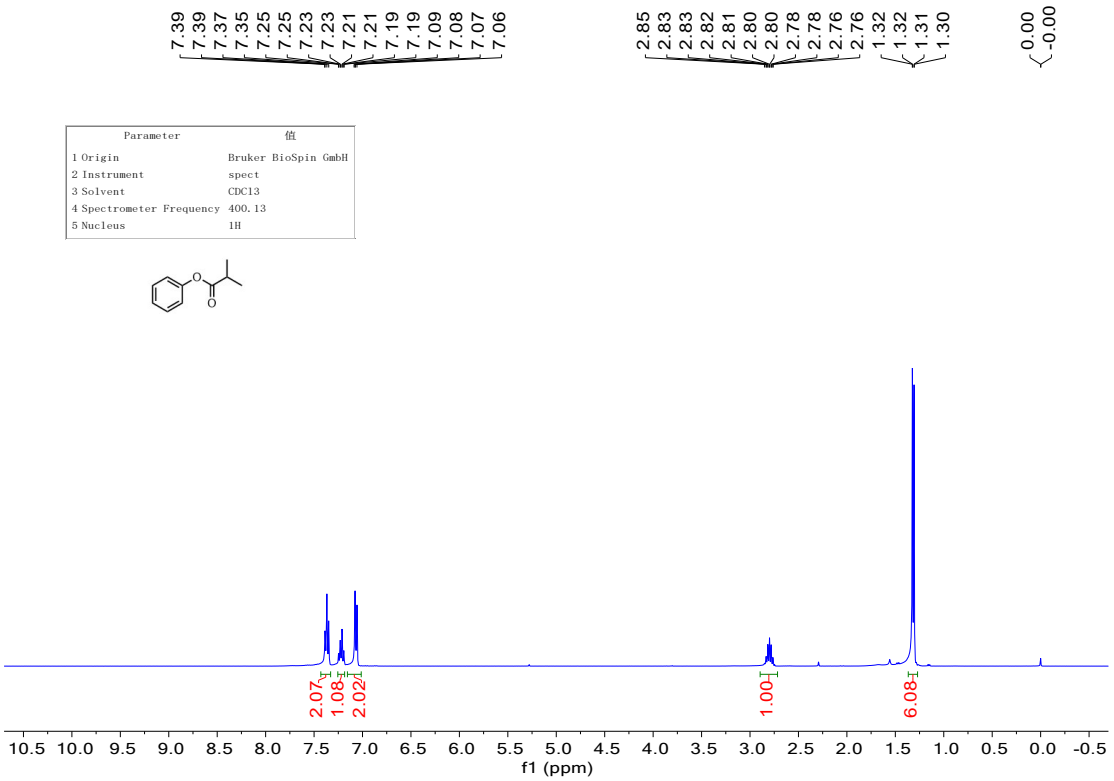
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.19
7.19
7.09
7.08
7.07
7.06
2.85
2.83
2.83
2.82
2.81
2.80
2.80
2.78
2.78
2.76
2.76
1.32
1.32
1.31
1.30
0.00
-0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
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O
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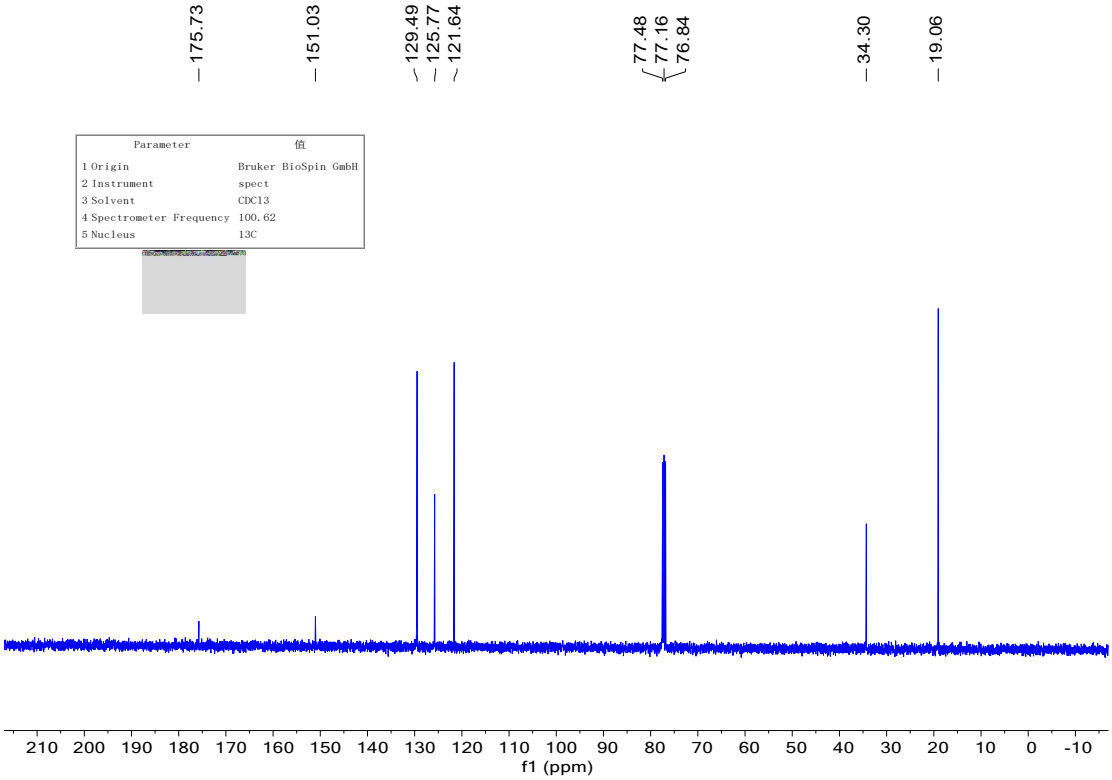
1.08
2.02
1.00
6.08
f1 (ppm)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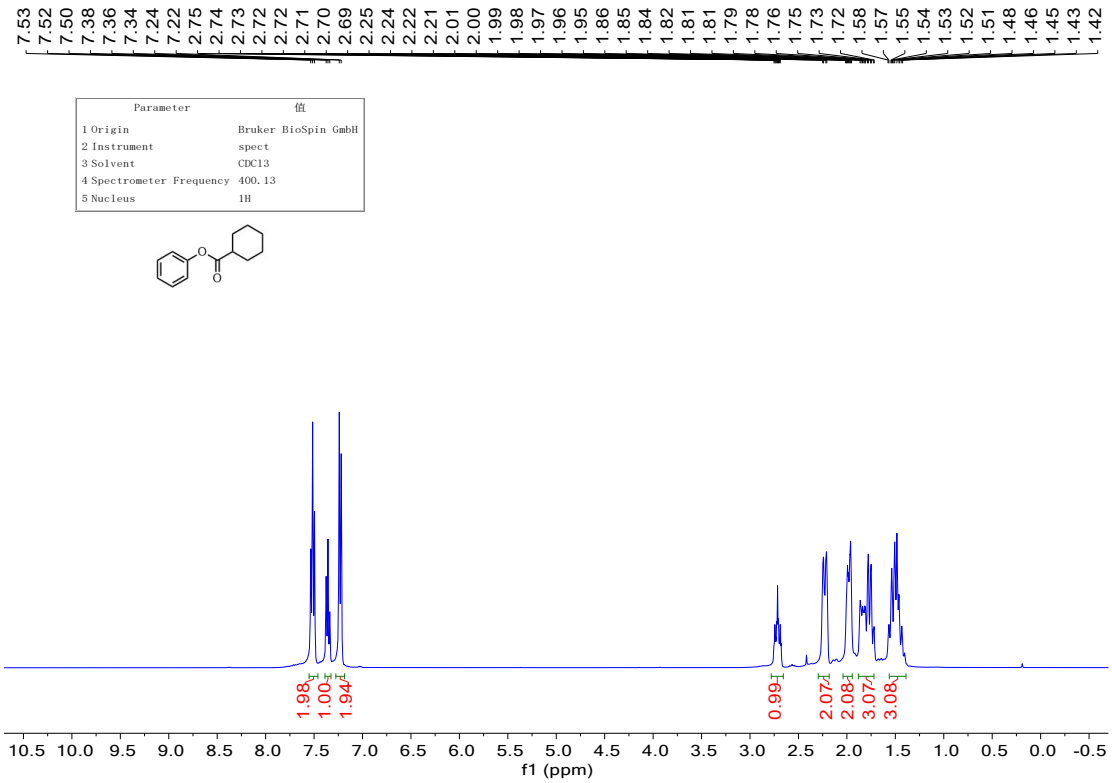
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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Parameter 值
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2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
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2.08
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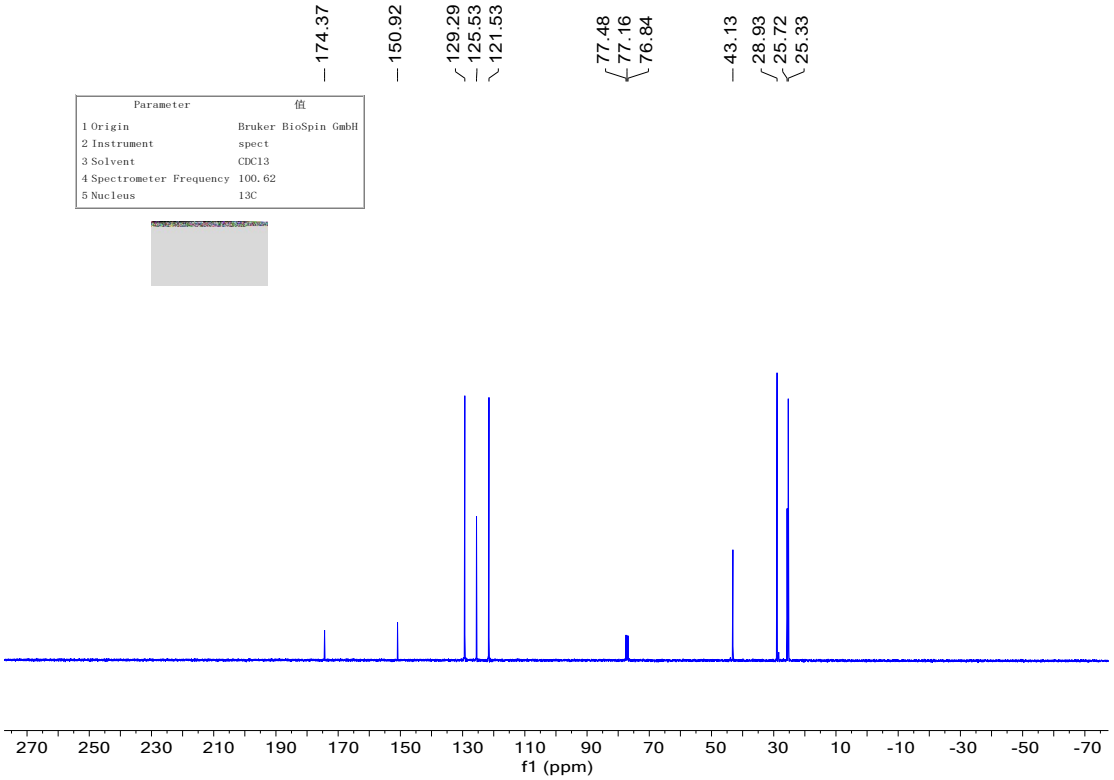
3.08
f1 (ppm)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28.93
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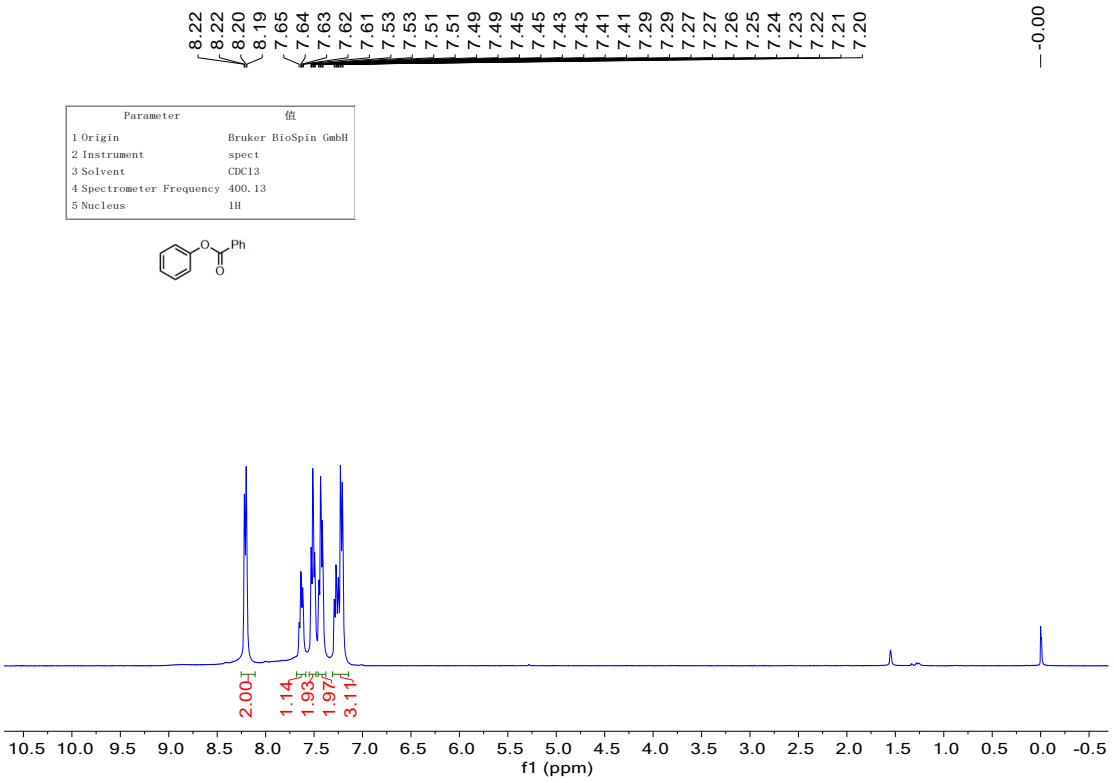
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.24
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7.22
7.21
7.20
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
O
Ph
O
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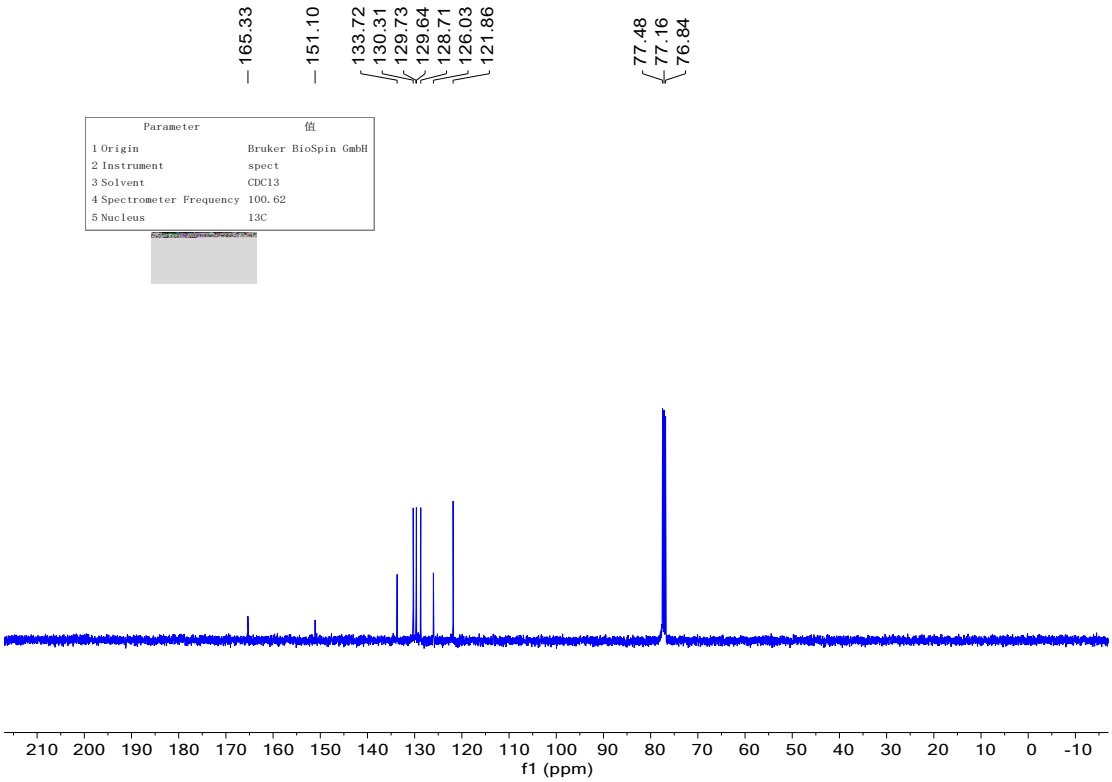
1.93
1.97
3.11
f1 (ppm)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77.48
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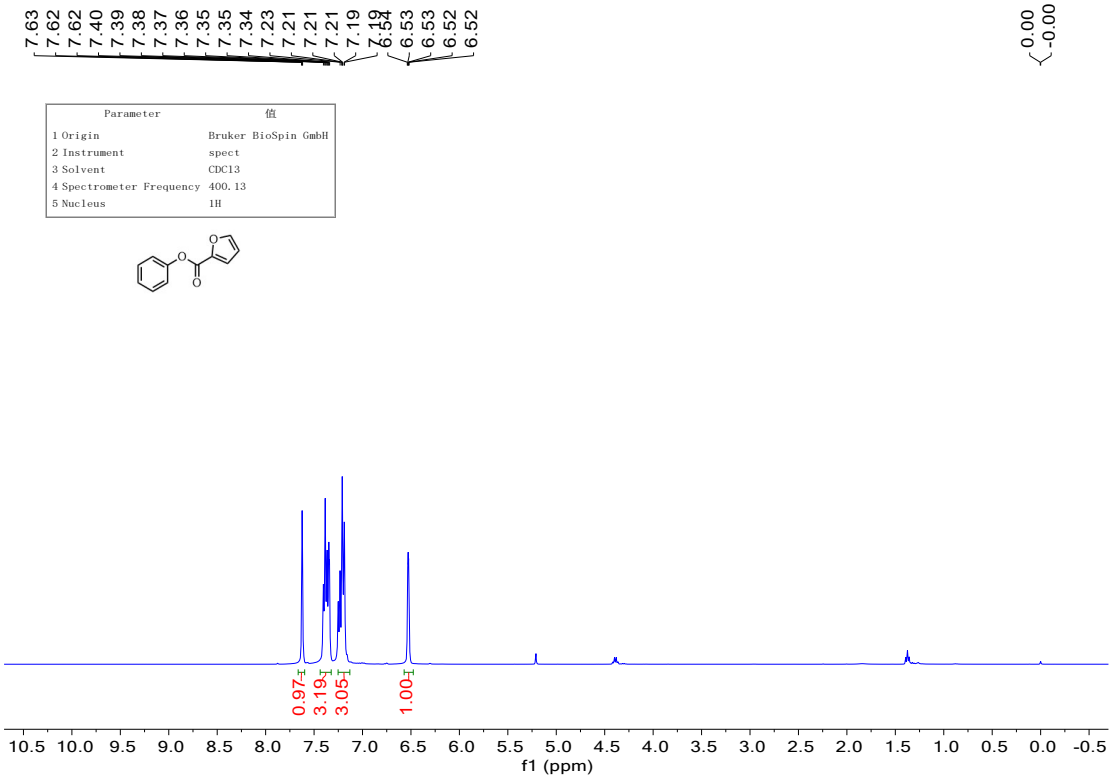
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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7.21
7.19
7.19
6.54
6.53
6.53
6.52
6.52
0.00
-0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
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O
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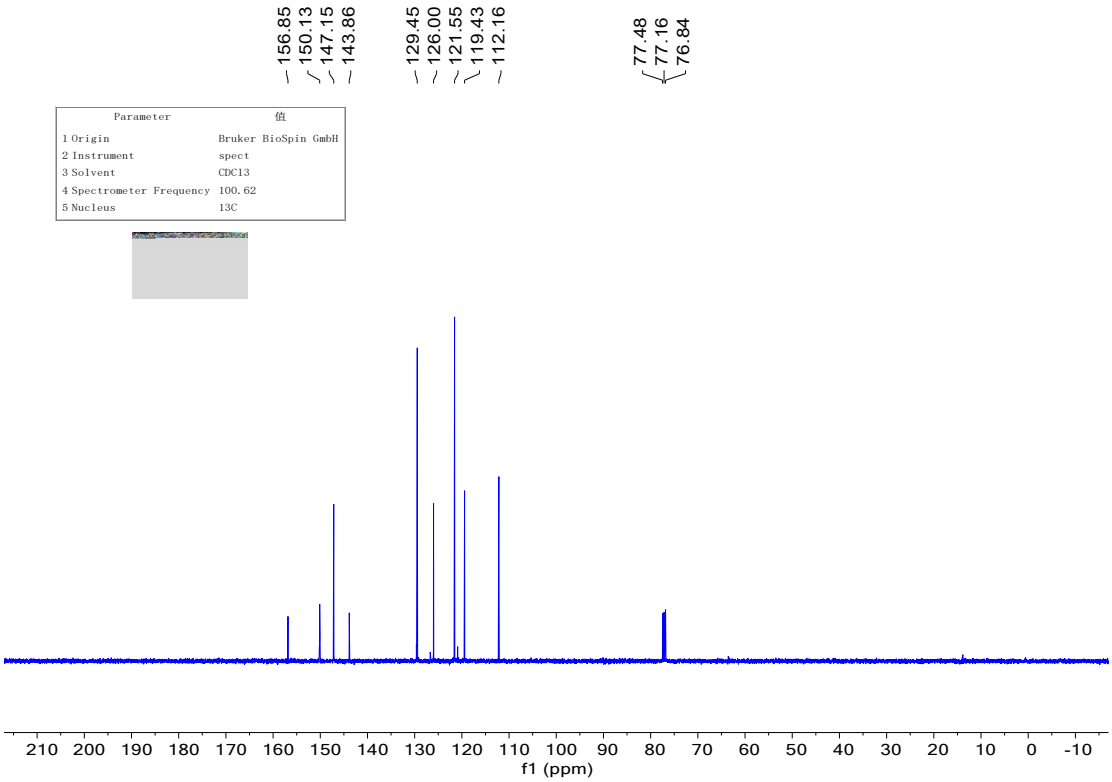
f1 (ppm)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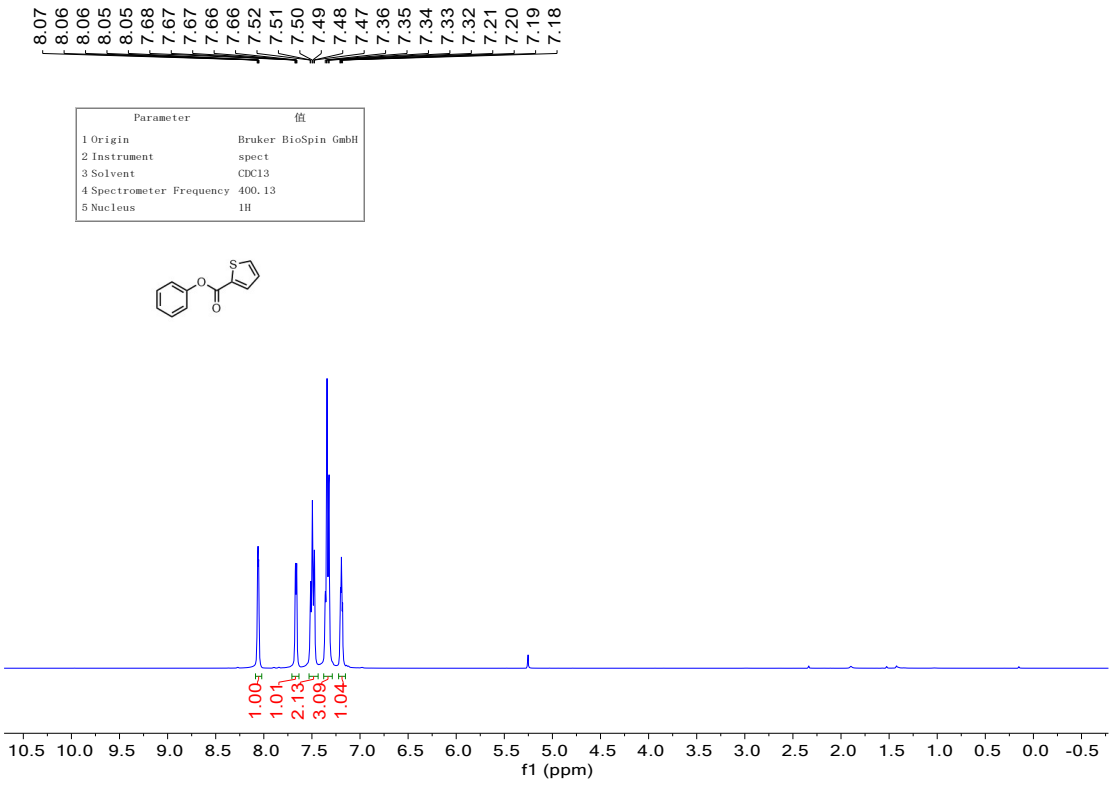
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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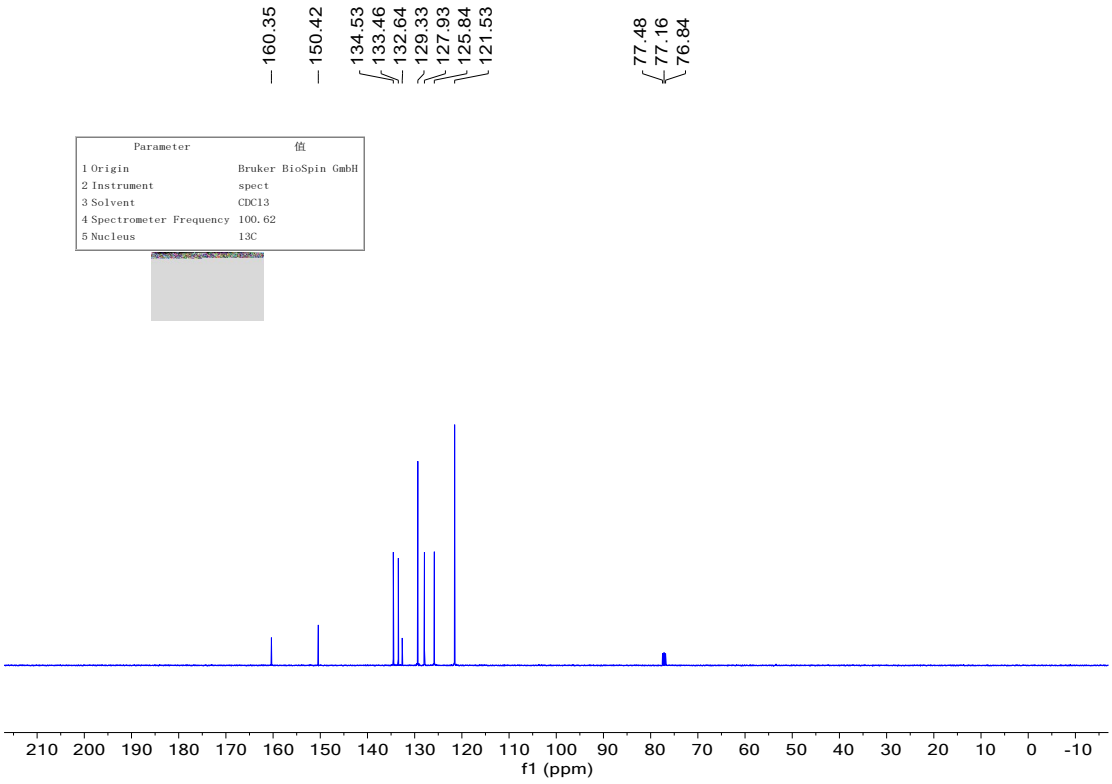
7.32
7.21
7.20
7.19
7.18
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
S
O
O
1.00
1.01
2.13
3.09
1.04
f1 (ppm)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77.48
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Parameter 值
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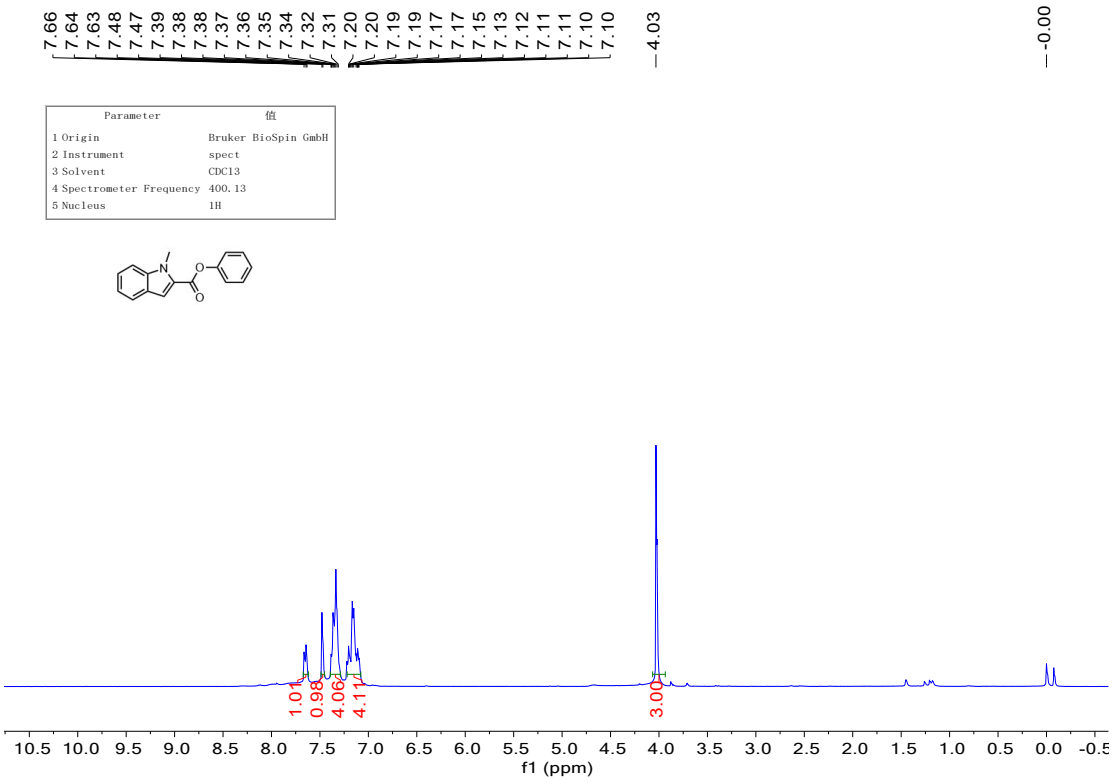
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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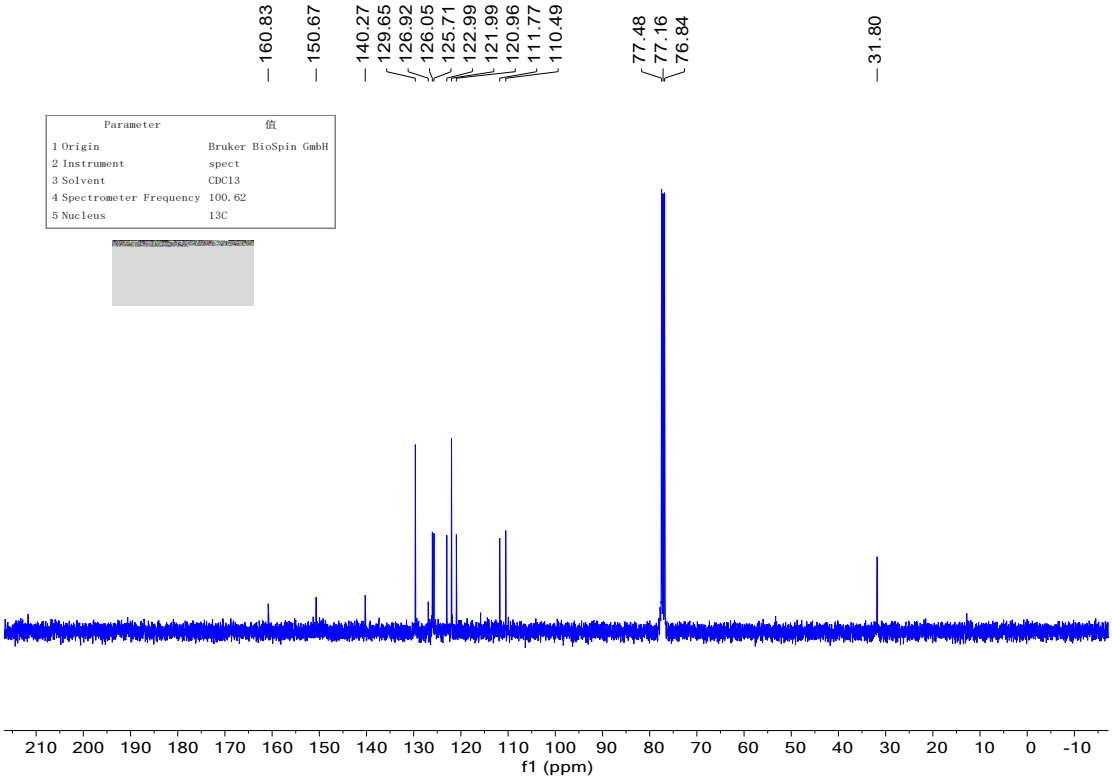
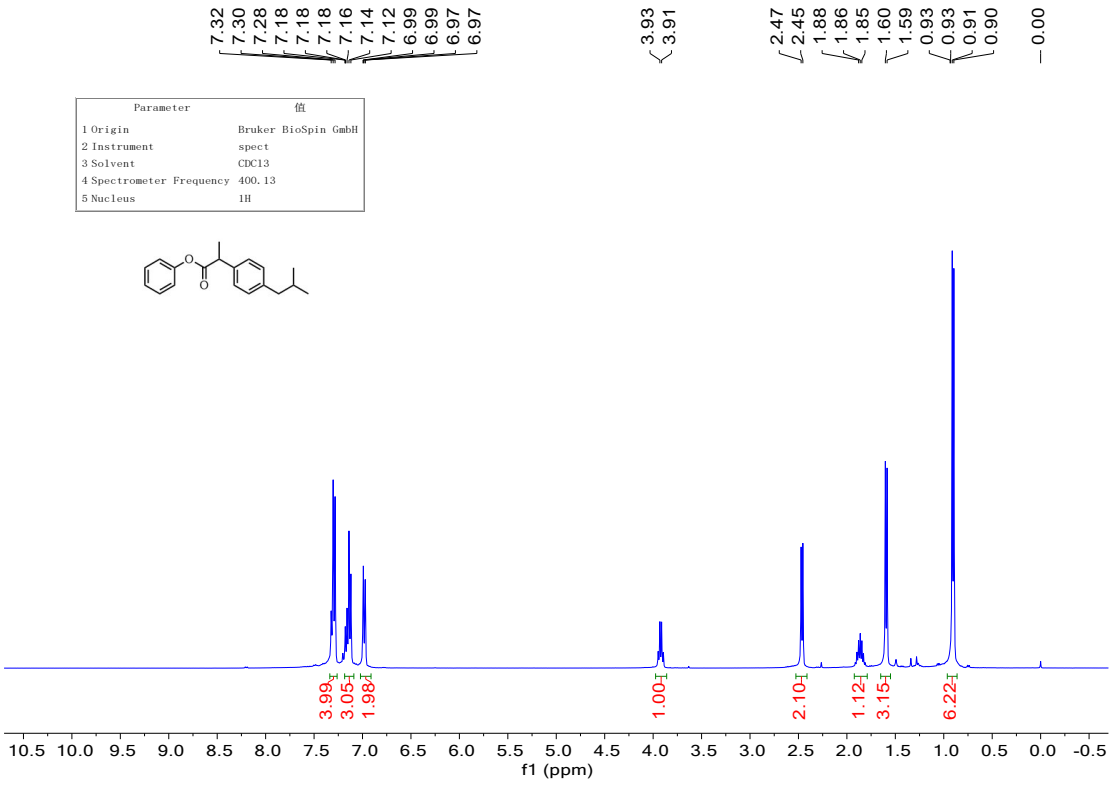
7.15
7.13
7.12
7.11
7.11
7.10
7.10
4.03
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
1.01
0.98
4.06
4.11
3.00
f1 (ppm)


160.83
150.67
140.27
129.65
126.92
126.05
125.71
122.99
121.99
120.96
111.77
110.49
77.48
77.16
76.84
31.80
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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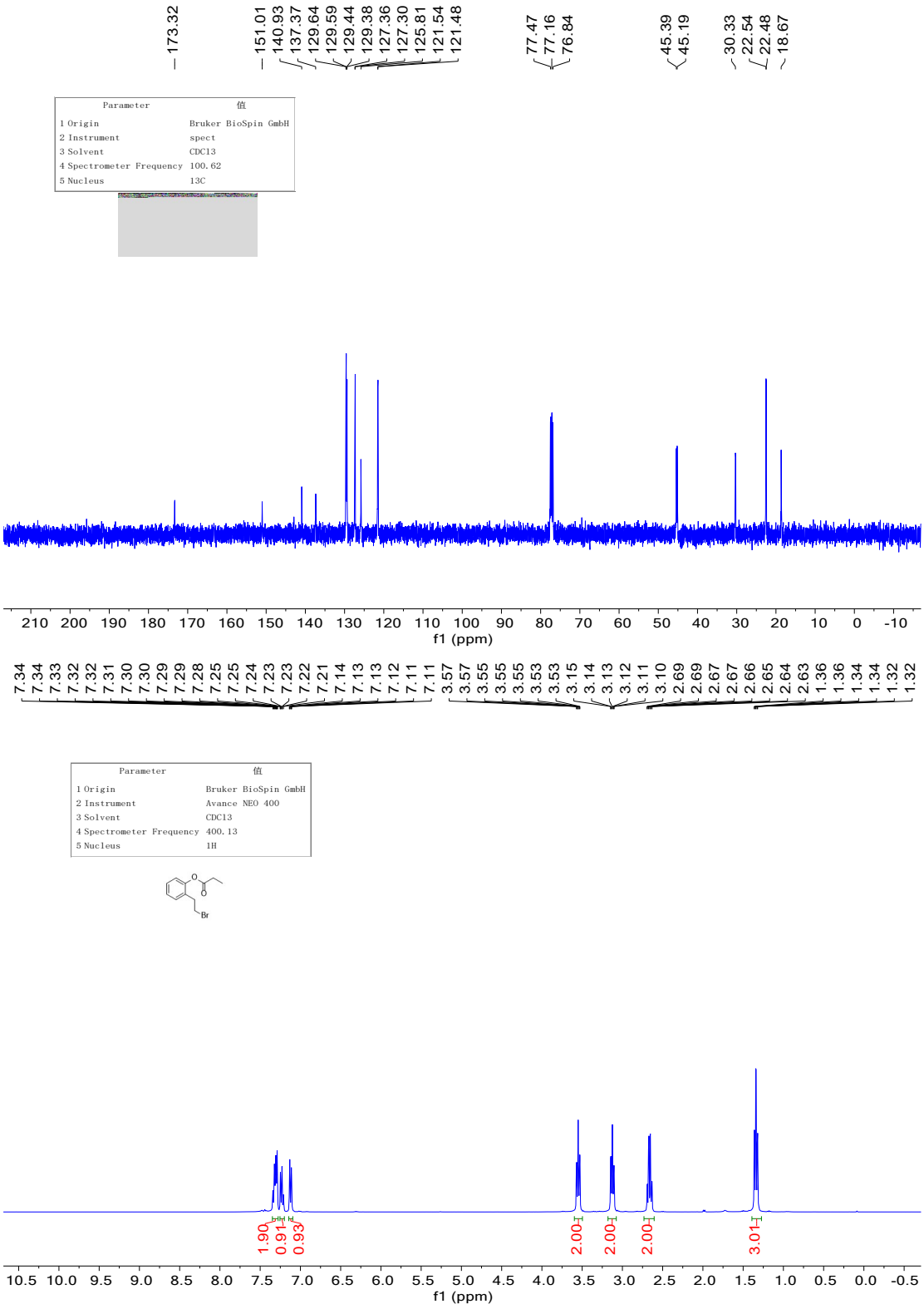
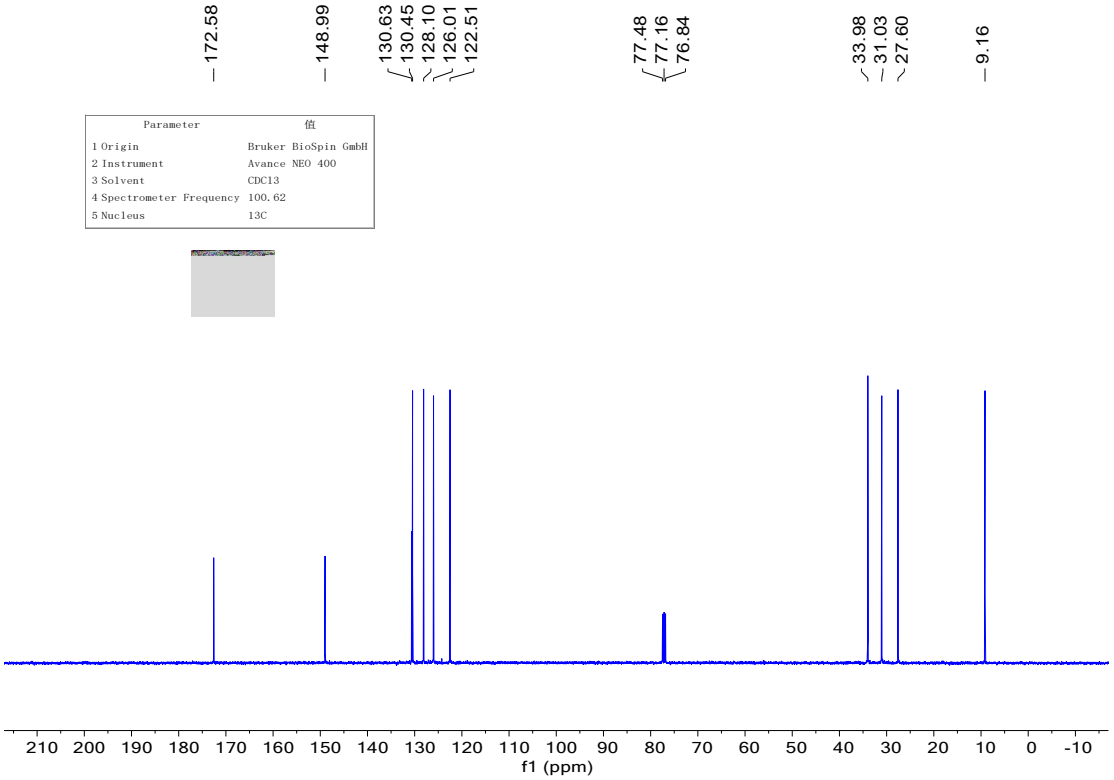
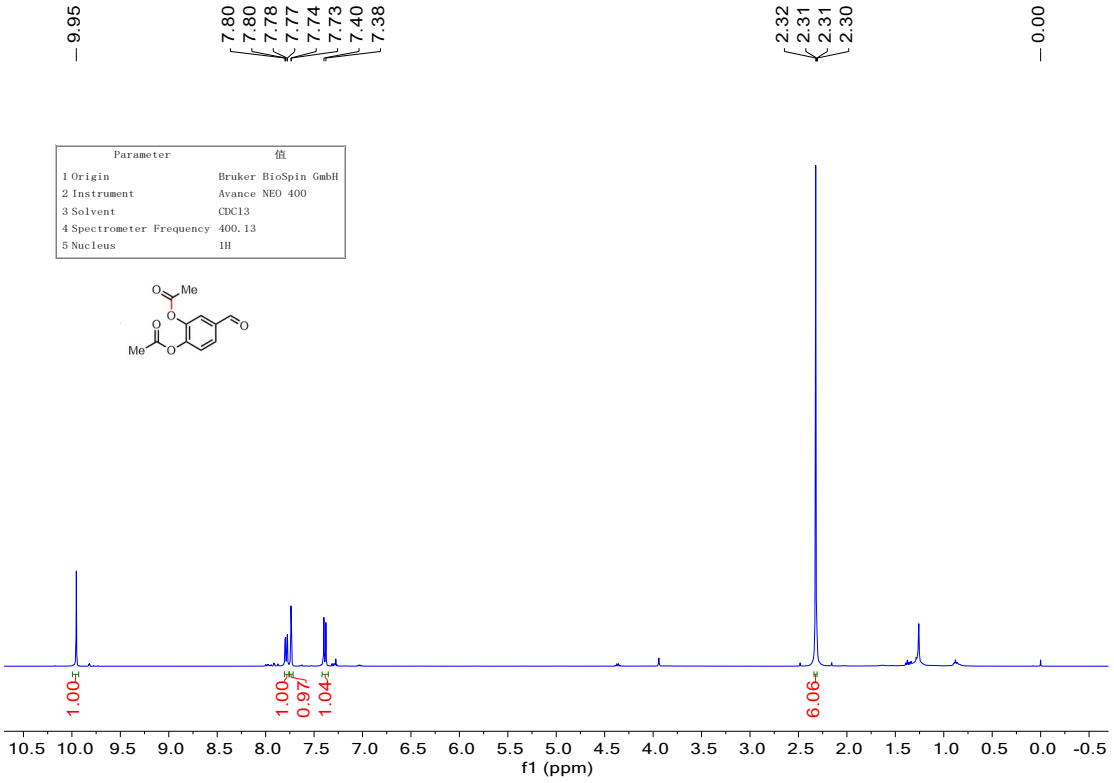
7.30
7.28
7.18
7.18
7.18
7.16
7.14
7.12
6.99
6.99
6.97
6.97
3.93
3.91
2.47
2.45
1.88
1.86
1.85
1.60
1.59
0.93
0.93
0.91
0.90
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
O
O
3.99
3.05
1.98
1.00
2.10
1.12
3.15
6.22
f1 (ppm)


173.32
151.01
140.93
137.37
129.64
129.59
129.44
129.38
127.36
127.30
125.81
121.54
121.48
77.47
77.16
76.84
45.39
45.19
30.33
22.54
22.48
18.67
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument spect
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
7.34 7.34 7.33 7.32 7.32 7.31 7.30 7.30 7.29 7.29 7.28 7.25 7.25 7.24 7.23 7.23 7.22 7.21 7.14 7.13 7.13 7.12 7.11 7.11
3.57 3.57 3.55 3.55 3.53 3.53 3.15 3.14 3.13 3.12 3.11 3.10 2.69 2.69 2.67 2.67 2.66 2.65 2.64 2.63 1.36 1.36 1.34 1.34 1.32 1.32
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Br
1.90
0.91
0.93
2.00
2.00
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


172.58
148.99
130.63
130.45
128.10
126.01
122.51
77.48
77.16
76.84
33.98
31.03
27.60
9.16
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)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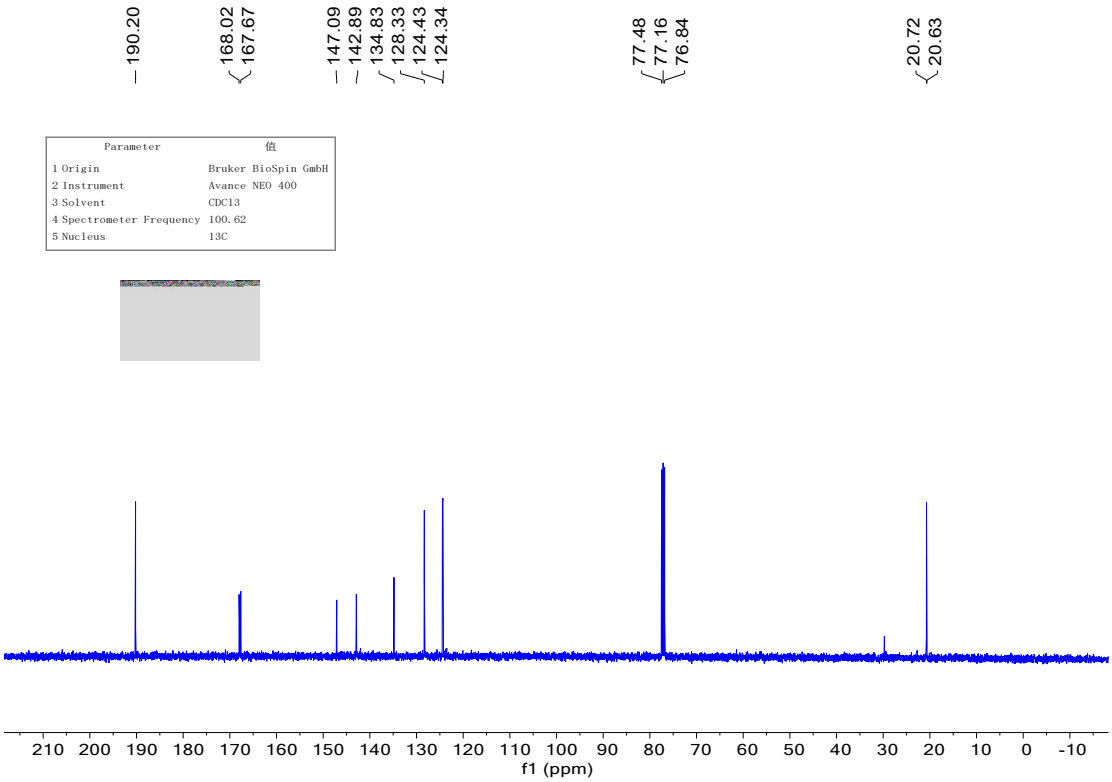
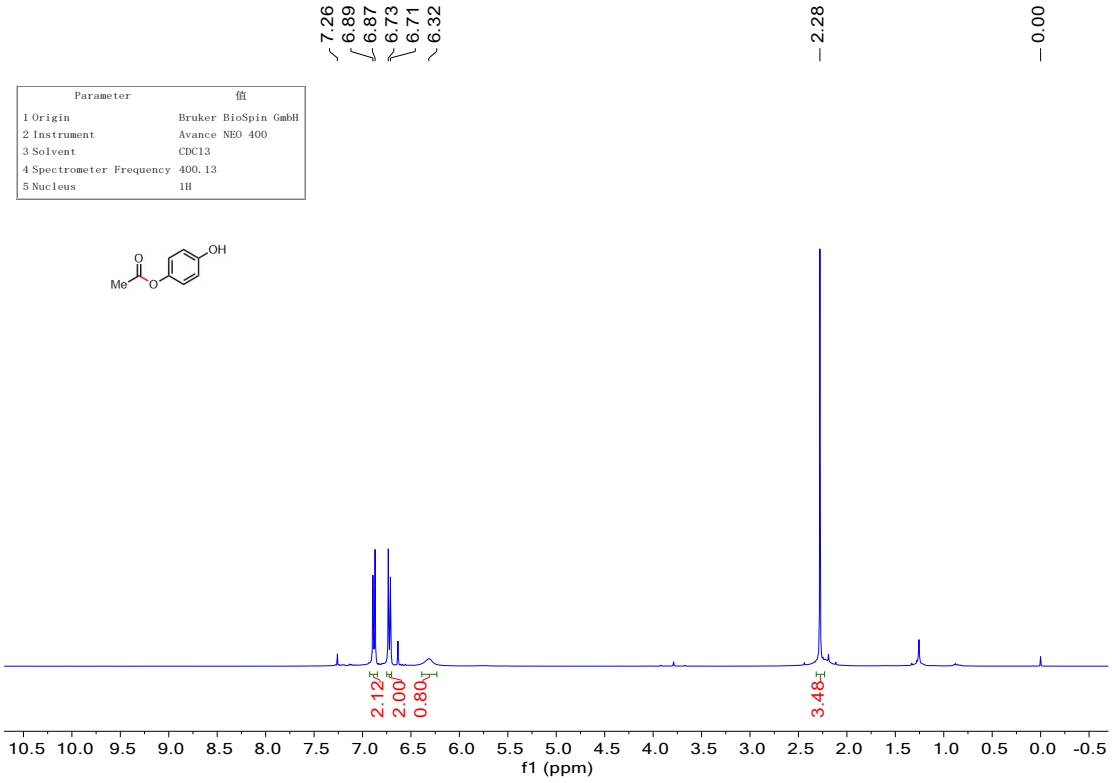
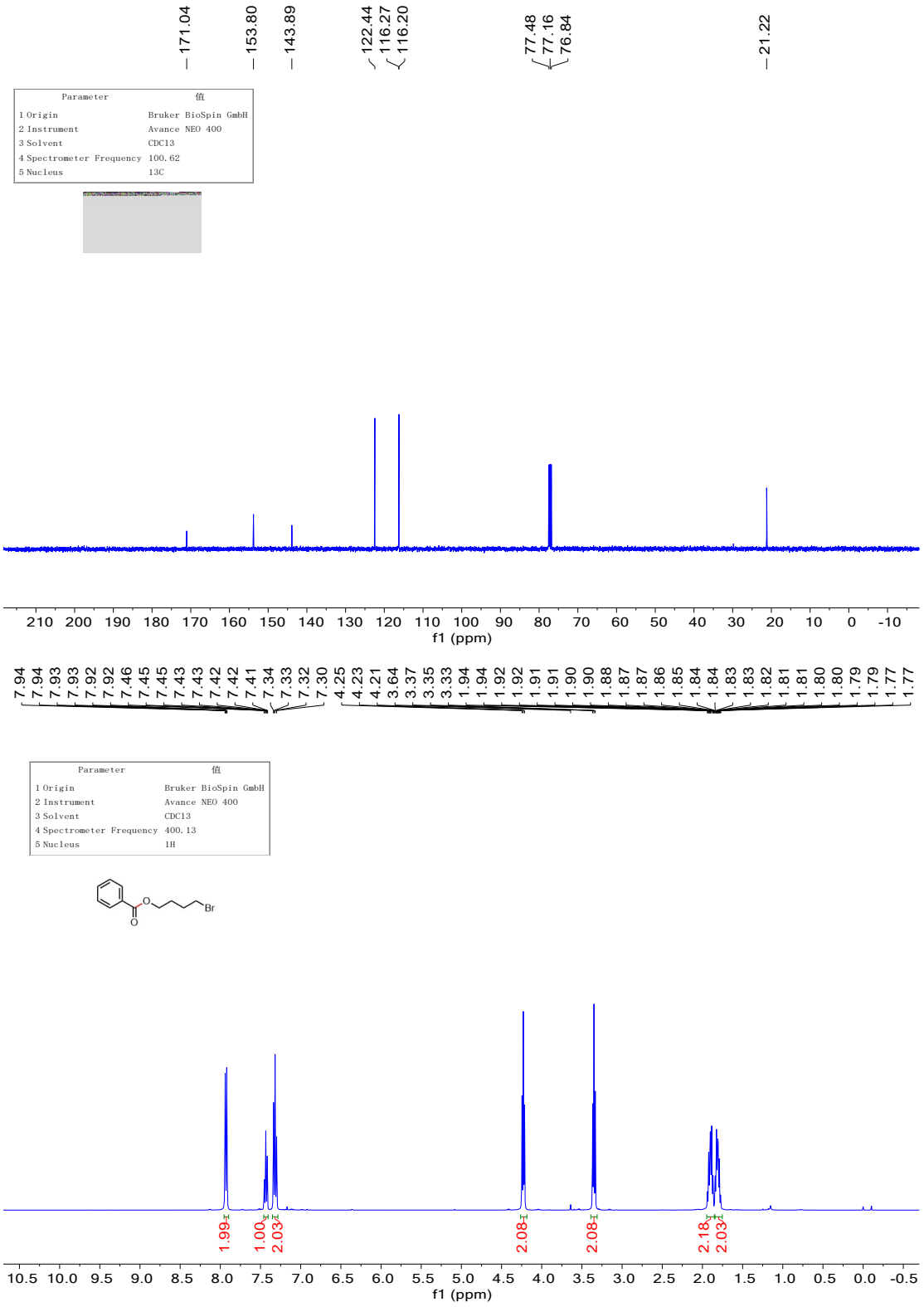
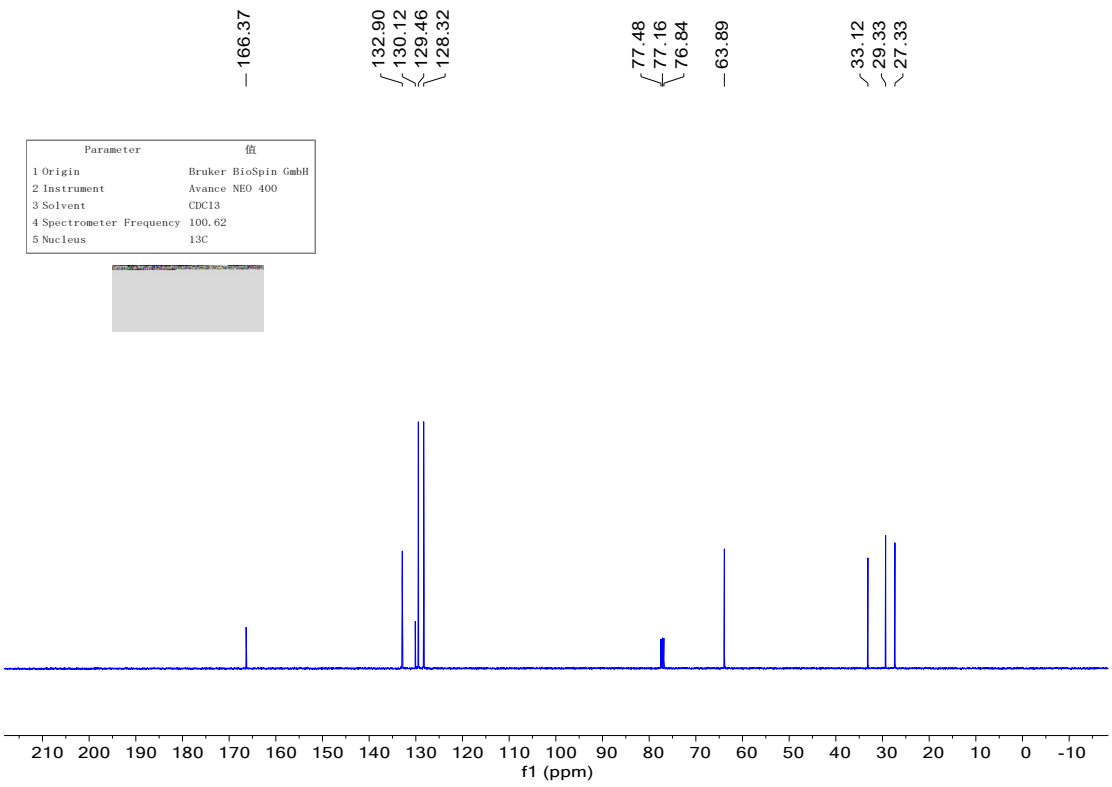
7.80
7.80
7.78
7.77
7.74
7.73
7.40
7.38
2.32
2.31
2.31
2.30
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
Me
Me
1.00
1.00
0.97
1.04
6.06
f1 (ppm)


190.20
168.02
167.67
147.09
142.89
134.83
128.33
124.43
124.34
77.48
77.16
76.84
20.72
20.63
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)


7.26
6.89
6.87
6.73
6.71
6.32
2.28
0.00
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
OH
O
Me
O
2.12
2.00
0.80
3.48
f1 (ppm)


171.04
153.80
143.89
122.44
116.27
116.20
77.48
77.16
76.84
21.22
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
f1 (ppm)
7.94 7.94 7.93 7.93 7.92 7.92 7.46 7.45 7.45 7.43 7.43 7.42 7.42 7.41 7.34 7.33 7.32 7.30 4.25 4.23 4.21 3.64 3.37 3.35 3.33 1.94 1.94 1.92 1.92 1.91 1.91 1.90 1.90 1.88 1.87 1.87 1.86 1.85 1.84 1.84 1.83 1.83 1.82 1.81 1.81 1.80 1.80 1.79 1.79 1.77 1.77
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 400.13
5 Nucleus 1H
O
O
Br
1.99
1.00
2.03
2.08
2.08
2.18
2.03
f1 (ppm)


166.37
132.90
130.12
129.46
128.32
77.48
77.16
76.84
63.89
33.12
29.33
27.33
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Instrument Avance NEO 400
3 Solvent CDCl3
4 Spectrometer Frequency 100.62
5 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)