**Electronic supplementary information**

# Co-catalyzed decarbonylative alkylative esterification of styrenes with aliphatic aldehydes and hypervalent iodine(III) reagents

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## I. General information

Unless otherwise noted, all commercially available compounds were used as purchased without further purification. Dry solvents (toluene, ethyl acetate, dichloromethane, acetonitrile, chlorobenzene, fluorobenzene, trifluoromethyl benzene) were used as commercially available. Thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm) or Sorbent Silica Gel 60 F254 plates. The developed chromatography was analyzed by UV lamp (254 nm). High-resolution mass spectra (HRMS) were obtained from a JEOL JMS-700 instrument (ESI) or Thermo Scientific LTQ Orbitrap XL (ESI). Melting points are uncorrected. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance 400 spectrometer at ambient temperature. Chemical shifts for $^{1}H$ NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard (chloroform: $\delta$ 7.26 ppm). Chemical shifts for $^{13}C$ NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard ($CDCl_3$: $\delta$ 77.16 ppm). Data are reported as following: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, m = multiplet, br = broad signal), coupling constant (Hz), and integration.

## II. General experimental procedure

A general experimental procedure for the synthesis of **acetates (3a-3m, 4b-4m)** is described as following:

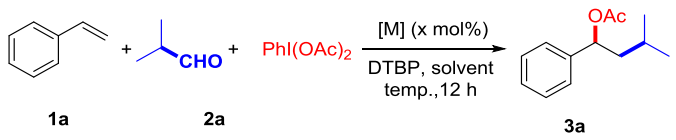
An oven-dried reaction vessel was successively charged with $Co(OAc)_2{\cdot}4H_2O$ (0.01 mmol, 5 mol%), iodobenzene diacetate (0.4 mmol, 2.0 equiv), styrene (**1a**, 0.2 mmol, 1.0 equiv), isobutyraldehyde (**2a**, 0.6 mmol, 3 equiv), trifluoromethyl benzene (1.0 mL) and di-*tert*-butyl

peroxide (DTBP, 0.24 mmol, 1.2 equiv). The vessel was sealed and stirred at 120 °C (oil bath temperature) for 12 h. Afterwards the resulting mixture was cooled to room temperature, the solvent was removed in vacuum. The residue was purified by column chromatography on silica gel with a mixture of dichloromethane/petroleum ether as eluent to give products **3a**.

A general experimental procedure for the synthesis of **benzoates** (**6a-6f**) is described as following:

An oven-dried reaction vessel was successively charged with $Co(OAc)_2{\cdot}4H_2O$ (0.01 mmol, 5 mol%), iodobenzene diacetate (0.3 mmol, 1.5 equiv), PhCOOH (0.64 mmol, 3.2 equiv), $Na_2CO_3$ (0.32 mmol, 1.6 equiv), styrene (**1a**, 0.2 mmol, 1.0 equiv), isobutyraldehyde (**2a**, 0.6 mmol, 3 equiv), trifluoromethyl benzene (1.2 mL) and di-*tert*-butyl peroxide (DTBP, 0.4 mmol, 2 equiv). The vessel was sealed and stirred at 120 °C (oil bath temperature) for 12 h. Afterwards the resulting mixture was cooled to room temperature, the solvent was removed in vacuum. The residue was purified by column chromatography on silica gel with a mixture of dichloromethane/petroleum ether as eluent to give products **6a**.

## III. Condition optimization




**1a** **2a** **3a**

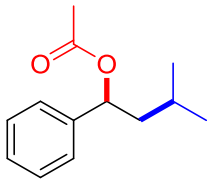
| entry | Cat. (mol%) | Sol. (1 mL) | [O] (3 equiv) | Temp. (℃) | Yield [%] |
|---|---|---|---|---|---|
| 1 | -- | $CH_3CN$ | DTBP | 120 | 0 |
| 2 | $FeCl_3$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 3 | $Fe(acac)_3$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 4 | $Fe(OAc)_2$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 5 | $CuCl_2$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 6 | $Cu(OAc)_2$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 7 | $Cu(acac)_2$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 8 | $MnCl_2$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 9 | $NiCl_2$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 10 | $CoCl_2$(5) | $CH_3CN$ | DTBP | 120 | 25 |
| 11 | $Co_2(CO)_8$(5) | $CH_3CN$ | DTBP | 120 | 15 |
| 12 | $Co(OAc)_2$(5) | $CH_3CN$ | DTBP | 120 | 34 |
| 13 | $CoSO_4$(5) | $CH_3CN$ | DTBP | 120 | 0 |
| 14 | $Co(acac)_2$(5) | $CH_3CN$ | DTBP | 120 | 22 |
| 15 | $Co(acac)_3$(5) | $CH_3CN$ | DTBP | 120 | 19 |
| 16 | $Co(OAc)_2{\cdot}4H_2O$(5) | $CH_3CN$ | DTBP | 120 | 43 |
| 17 | $Co(OAc)_2{\cdot}4H_2O$(7.5) | $PhCF_3$ | DTBP | 120 | 51 |
| 18 | $Co(OAc)_2{\cdot}4H_2O$(5) | $PhCF_3$ | DTBP | 120 | 75 |
| 19 | $Co(OAc)_2{\cdot}4H_2O$(2.5) | $PhCF_3$ | DTBP | 120 | 66 |
| 20 | $Co(OAc)_2{\cdot}4H_2O$(5) | PhCl | DTBP | 120 | 53 |
| 21 | $Co(OAc)_2{\cdot}4H_2O$(5) | $PhCH_3$ | DTBP | 120 | 0 |

| | | | | | |
|---|---|---|---|---|---|
| 22 | $Co(OAc)_2·4H_2O$(5) | DMF | DTBP | 120 | 0 |
| 23 | $Co(OAc)_2·4H_2O$(5) | DMSO | DTBP | 120 | 0 |
| 24 | $Co(OAc)_2·4H_2O$(5) | DCM | DTBP | 120 | 0 |
| 25 | $Co(OAc)_2·4H_2O$(5) | EA | DTBP | 120 | 0 |
| 26 | $Co(OAc)_2·4H_2O$(5) | PhF | DTBP | 120 | 68 |
| 27 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP | 120 | 75 |
| 28 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | TBHP in decane | 120 | 0 |
| 29 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | $H_2O_2$ | 120 | 0 |
| 30 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP(1) | 120 | 84 |
| 31 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP(1.2) | 120 | 90 |
| 32 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP(1.5) | 120 | 86 |
| 33 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP(1.2) | 110 | 81 |
| 34 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP(1.2) | 120 | 90 |
| 35 | $Co(OAc)_2·4H_2O$(5) | $PhCF_3$ | DTBP(1.2) | 130 | 50 |

Reaction conditions: **1a** (0.2 mmol, 1.0 equiv), **2a** (0.6 mmol, 3.0 equiv), $PhI(OAc)_2$ (0.4 mmol, 2.0 equiv), DTBP (0.6 mmol, 3.0 equiv), Cat. (0.01 mmol, x mol%), solvent (1.0 mL), stirred at y °C for 12 h under air.

## IV Spectra data of products 3a-3m, 4b-4m, 6a-6f

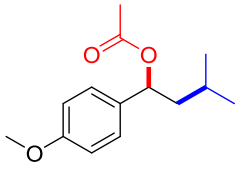
### (3a) 3-methyl-1-phenylbutyl acetate[1]



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (37.1 mg, 90%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.33 – 7.26 (m, 5H), 5.83 – 5.80 (m, 1H), 2.05 (d, $J$ = 1.6 Hz, 3H), 1.85 (dd, $J$ = 9.2, 16.4 Hz, 1H), 1.62 – 1.57 (m, 2H), 0.94 (t, $J$ = 13.2 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.48, 141.23, 128.54, 127.93, 126.63, 74.66, 45.54, 24.83, 22.88, 22.48, 21.40. IR ($cm^{-1}$): 2958, 2871, 2837, 1736, 1073, 699.

### (3b) 1-(4-methoxyphenyl)-3-methylbutyl acetate

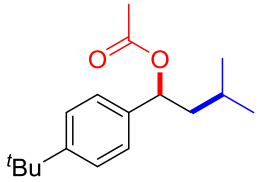


The title compound was prepared according to the general procedure described above by the reaction between 4-methoxylstyrene (**1b**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (27.4 mg, 58%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.28 (d, $J$ = 8.8 Hz, 2H), 6.87 (d, $J$ = 8.4 Hz, 2H), 5.79 (dd, $J$ = 8.4, 6.0 Hz, 1H), 3.79 (s, 3H), 2.03 (s, 3H), 1.88 – 1.81 (m, 1H), 1.62 – 1.50 (m, 2H), 0.92 (dd, $J$ = 10.8,

6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.58, 159.34, 133.24, 128.16, 113.91, 74.41, 55.38, 45.21, 24.86, 22.77, 22.60, 21.49. IR ($cm^{-1}$): 2958, 2871, 2837, 1736, 1073, 699. HRMS: calcd. for $C_{14}H_{20}O_3Na^+$ $[M+Na]^+$: 259.1305; Found: 259.1293.

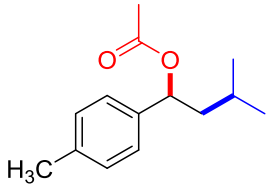
**(3c) 1-(4-(tert-butyl)phenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-*tert*-butylstyrene (**1c**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (47.3 mg, 83%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.36 – 7.34 (m, 2H), 7.27 – 7.25 (m, 2H), 5.83 – 5.80 (m, 1H), 2.04 (s, 3H), 1.88 – 1.83 (m, 1H), 1.61 – 1.56 (m, 2H), 1.31 (s, 9H), 0.96 – 0.92 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.58, 150.84, 138.15, 126.42, 125.45, 74.51, 45.49, 34.66, 31.57, 31.47, 24.88, 22.92, 22.52, 21.48. IR ($cm^{-1}$): 2959, 2870, 1736, 1192, 833. HRMS: calcd. for $C_{17}H_{26}O_2Na^+$ $[M+Na]^+$: 285.1825; Found: 285.1818.

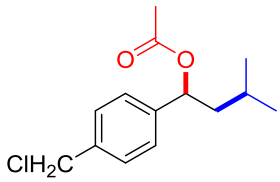
**(3d) 3-methyl-1-(p-tolyl)butyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-methylstyrene (**1d**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (34.3 mg, 78%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.23 (t, $J$ = 4.4 Hz, 2H), 7.14 (d, $J$ = 7.6 Hz, 2H), 5.80 – 5.77 (m, 1H), 2.33 (s, 3H), 2.03 (s, 3H), 1.88 – 1.82 (m, 1H), 1.61 – 1.51 (m, 2H), 0.93 (dd, $J$ = 10.4, 6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.49, 138.19, 137.66, 129.21, 126.67, 74.58, 45.38, 24.83, 22.81, 22.53, 21.42, 21.24. IR ($cm^{-1}$): 2957, 2870, 1736, 1240, 812. HRMS: calcd. for $C_{14}H_{20}O_2Na^+$ $[M+Na]^+$: 243.1356; Found: 243.1348.

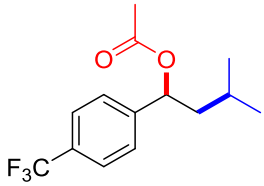
**(3e) 1-(4-(chloromethyl)phenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-chloromethylstyrene (**1e**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (47.6 mg, 86%).

$^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.37 – 7.32 (m, 4H), 5.82 – 5.79 (m, 1H), 4.57 (s, 2H), 2.05 (s, 3H), 1.89 – 1.80 (m, 1H), 1.59 – 1.53 (m, 2H), 0.95 – 0.92 (dd, $J$ = 9.2, 6.4Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.47, 141.59, 137.12, 128.84, 127.05, 74.30, 46.04, 45.49, 24.83, 22.88, 22.47, 21.39. IR ($cm^{-1}$): 2958, 2870, 1735, 1236, 826. HRMS: calcd. for $C_{14}H_{19}ClO_2Na^+$ $[M+Na]^+$: 277.0966; Found: 277.0951.

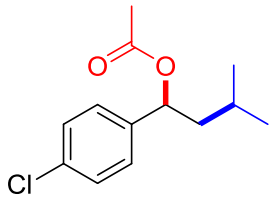
**(3f) 3-methyl-1-(4-(trifluoromethyl)phenyl)butyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-trifluoromethylstyrene (**1f**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (33.8 mg, 57%).

$^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.60 (d, $J$ = 8.4 Hz, 2H), 7.44 (d, $J$ = 8 Hz, 2H), 5.85 – 5.81 (m, 1H), 2.07 (s, 3H), 1.89 – 1.83 (m, 1H), 1.59 – 1.52 (m, 2H), 0.97 – 0.93 (t, $J$ = 7 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.45, 145.36, 130.12 (q, $J$ = 32.1 Hz), 127.06, 125.61 (q, $J$ = 2.7 Hz), 124.18 (d, $J$ = 270.6 Hz), 74.03, 45.55, 24.82, 22.91, 22.38, 21.30. IR ($cm^{-1}$): 2959, 2870, 1741, 1125, 825. HRMS: calcd. for $C_{14}H_{17}F_3O_2Na^+$ $[M+Na]^+$: 297.1073; Found: 297.1074.

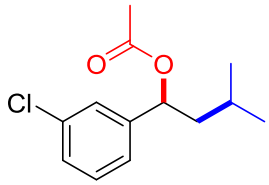
**(3g) 1-(4-chlorophenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-chlorostyrene (**1g**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (45.2 mg, 86%).

$^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.32 – 7.30 (m, 2H), 7.28 (d, $J$ = 6.4 Hz, 2H), 5.78 – 5.75 (m, 1H), 2.05 (s, 3H), 1.87 – 1.80 (m, 1H), 1.57 – 1.51 (m, 2H), 0.93 (dd, $J$ = 9.2, 6.4 Hz, 6H). $^{13}$C NMR (400 MHz, $CDCl_3$) $\delta$ 170.43, 139.79, 133.71, 128.77, 128.10, 73.99, 45.40, 24.82, 22.85, 22.47, 21.37. IR ($cm^{-1}$): 2959, 2870, 2097, 1736, 699. HRMS: calcd. For $C_{13}H_{17}ClO_2Na^+$ $[M+Na]^+$: 263.0809; Found: 263.0795.

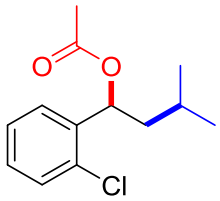
**(3h) 1-(3-chlorophenyl)-3-methylbutyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between 3-chlorostyrene (**1h**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (42.1 mg, 80%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.32 (s, 1H), 7.26 – 7.25(m, 2H), 7.21 – 7.19 (m, 1H), 5.78 – 5.74 (m, 1H), 2.07 (s, 3H), 1.86 – 1.80 (m, 1H), 1.59 – 1.52 (m, 2H), 0.96 – 0.92 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.38, 143.42, 134.48, 129.86, 128.10, 126.69, 124.85, 73.93, 45.53, 24.81, 22.92, 22.39, 21.33. IR (cm$^{-1}$): 2959, 2871, 1736, 1158, 867. HRMS: calcd. For $C_{13}H_{17}ClO_2Na^+$ $[M+Na]^+$: 263.0809; Found: 263.0809.

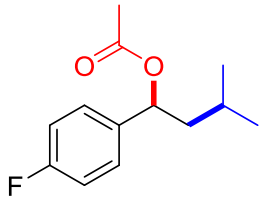
**(3i) 1-(2-chlorophenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 2-chlorostyrene (**1i**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (38.9 mg, 74%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.37 (dd, J = 8, 2 Hz, 1H), 7.33 (dd, J = 8, 1.2 Hz, 1H), 7.25 – 7.19 (m, 2H), 6.21 (dd, J = 9.2, 3.6 Hz, 1H), 2.10 (s, 3H), 1.80 – 1.69 (m, 2H), 1.58 – 1.54 (m, 1H), 0.97 (dd, J = 17.2, 6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.20, 139.65, 132.14, 129.71, 128.73, 127.17, 126.81, 71.37, 44.86, 25.11, 23.43, 21.89, 21.25. IR (cm$^{-1}$): 2958, 2870, 1736, 1123, 785. HRMS: calcd. For $C_{13}H_{17}ClO_2Na^+$ $[M+Na]^+$: 263.0809; Found: 263.0795.

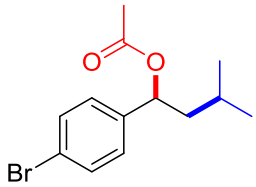
**(3j) 1-(4-fluorophenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-fluorostyrene (**1j**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (39.0 mg, 79%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.33 – 7.29 (m, 2H), 7.04 – 7.00 (m, 2H), 5.80 – 5.77 (m, 1H), 2.04 (s, 3H), 1.86 – 1.80 (m, 1H), 1.57 – 1.51 (m, 2H), 0.95 – 0.91 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.49, 162.42 (d, $J$ = 244.6 Hz ), 137.04 (d, $J$ = 3.2 Hz ), 128.47 (d, $J$ = 8.1 Hz ), 115.45 (d, $J$ = 21.3 Hz ), 74.02, 45.44, 24.83, 22.83, 22.50, 21.41. IR (cm$^{-1}$): 2959, 2871, 1740, 1158, 837. HRMS: calcd. For $C_{13}H_{17}FO_2Na^+$ $[M+Na]^+$: 247.1105; Found: 247.1091.

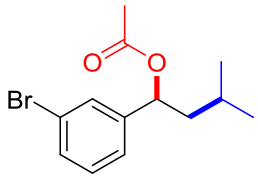
**(3k) 1-(4-bromophenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 4-boromostyrene (**1k**) with iodobenzene diacetate and isobutyraldehyde (2**a**), and purified by flash column chromatography as colorless oil (45.4 mg, 74%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.46 (d, $J$ = 8.4 Hz, 2H), 7.21 (d, $J$ = 8.4 Hz, 2H), 5.77 - 5.73 (m, 1H), 2.05 (s, 3H), 1.88 – 1.78 (m, 1H), 1.59 – 1.50 (m, 2H), 0.93 (dd, $J$ = 2, 6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.40, 140.30, 131.71, 128.41, 121.82, 74.01, 45.35, 24.79, 22.84, 22.45, 21.34. IR (cm$^{-1}$): 2958, 2870, 1736, 1299, 817. HRMS: calcd. For $C_{13}H_{17}BrO_2Na^+$ $[M+Na]^+$: 307.0304; Found: 307.0296.

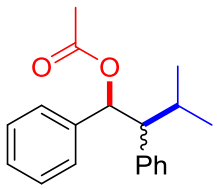
**(3l) 1-(3-bromophenyl)-3-methylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between 3-boromostyrene (**1l**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (47.9 mg, 78%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.47 (t, $J$ = 1.8 Hz, 1H), 7.42 – 7.39 (m, 1H), 7.25 – 7.18 (m, 2H), 5.76 – 5.73 (m, 1H), 2.07 (s, 3H), 1.87 – 1.80 (m, 1H), 1.58 – 1.50 (m, 2H), 0.94 (dd, $J$ = 4.8, 6.8 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.37, 143.67, 131.04, 130.16, 129.59, 125.33, 122.68, 73.86, 45.54, 24.81, 22.92, 22.38, 21.34. IR (cm$^{-1}$): 2958, 2870, 1739, 782. HRMS: calcd. For $C_{13}H_{17}BrO_2Na^+$ $[M+Na]^+$: 307.0304; Found: 307.0296.

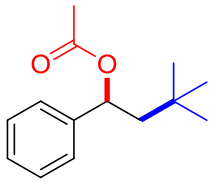
**(3m) 3-methyl-1,2-diphenylbutyl acetate**




The title compound was prepared according to the general procedure described above by the reaction between trans-1,2-diphenylethene (**1m**) with iodobenzene diacetate and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (32.9 mg, 54%, d.r. = 1.7 : 1).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.24 – 7.07 (m, 9H), 6.93 – 6.91 (m, 1H), 6.25 (dd, $J$ = 17.6, 7.6 Hz, 1H), 3.10 – 2.78 (m, 1H), 2.80 (t, $J$ = 7.2 Hz, 0.37×1H), 2.28 – 2.20 (m, 0.6×1H), 2.08 (s, 1.88×1H), 1.90 (s,, 1.12×1H), 1.88 – 1.83 (m, 0.37×1H), 0.87 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.33, 170.24, 140.08, 139.42, 138.85, 137.93, 130.31, 129.84, 128.24, 127.86, 127.78, 127.66, 127.64, 127.56, 126.93, 126.44, 76.53, 76.18, 58.36, 57.01, 28.74, 28.44, 21.88, 21.86, 21.44, 21.10, 19.29, 18.44. IR (cm$^{-1}$): 2960, 2930, 2873, 1739, 1234, 761. HRMS: calcd. For $C_{19}H_{22}O_2Na^+$ $[M+Na]^+$: 305.1512; Found: 305.1503.

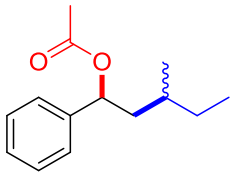
**(4b) 3,3-dimethyl-1-phenylbutyl acetate**[2]



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and pivaldehyde (**2b**), and purified by flash column chromatography as colorless oil (37.8 mg, 86%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.33 – 7.24 (m, 5H), 5.88 – 5.85 (m, 1H), 2.03 (s, 3H), 1.99 – 1.93 (m, 1H), 1.63 – 1.61 (m, 1H), 0.95 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.42, 142.56, 128.58, 127.80, 126.45, 74.11, 50.05, 30.60, 30.02, 21.60. IR ($cm^{-1}$): 3030, 2955, 2870, 1739, 1239, 699.

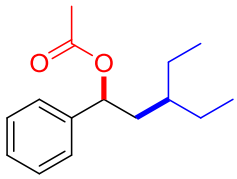
**(4c) 3-methyl-1-phenylpentyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 2-methylbutanal (**2c**), and purified by flash column chromatography as colorless oil (36.5 mg, 75%, d.r. = 1.2 : 1).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 – 7.27 (m, 5H), 5.86 – 5.80 (m, 1H), 2.05 (d, $J$ = 6.4 Hz, 3H), 1.76 (t, $J$ = 7.0 Hz, 1H), 1.50 – 1.12 (m, 4H), 0.93 – 0.81 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.56, 170.50, 141.59, 141.03, 128.56, 128.01, 127.89, 126.84, 126.52, 74.89, 74.36, 43.72, 43.08, 31.05, 29.78, 29.33, 21.48, 21.42, 19.36, 19.05, 11.26, 11.10. IR ($cm^{-1}$): 2964, 2930, 2875, 1739, 1236, 698. HRMS: calcd. For $C_{14}H_{20}O_2Na^+$ $[M+Na]^+$: 243.1356; Found: 243.1348.

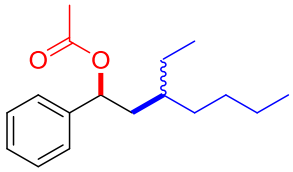
**(4d) 3-ethyl-1-phenylpentyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 2-ethylbutanal (**2d**), and purified by flash column chromatography as colorless oil (41.6 mg, 81%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 – 7.25 (m, 5H), 5.81 (dd, J = 8.8, 6.0 Hz, 1H), 2.05 (s, 3H), 1.91 – 1.84 (m, 1H), 1.65 (dd, $J$ = 13.2, 6.0 Hz, 1H), 1.40 – 1.28 (m, 4H), 1.22 (dd, $J$ = 12.4, 6.0 Hz, 1H), 0.83 (dt, $J$ = 19.2, 7.2 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.53, 141.36, 128.54, 127.93, 126.66, 74.70, 39.98, 36.79, 25.48, 25.15, 21.42, 10.67, 10.51. IR ($cm^{-1}$): 2963, 2932, 2875, 1736, 1236, 699. HRMS: calcd. For $C_{15}H_{22}O_2Na^+$ $[M+Na]^+$: 257.1512; Found: 257.1509.

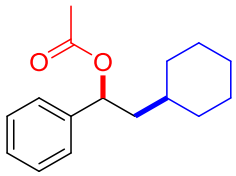
**(4e) 3-ethyl-1-phenylheptyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 2-ethylhexanal (**2e**), and purified by flash column chromatography as colorless oil (47.9 mg, 84%, d.r. = 1.2 : 1).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.33 – 7.25 (m, 5H), 5.81 (t, $J$ = 7.0 Hz, 1H), 2.05 (s, 3H), 1.89 – 1.85 (m, 1H), 1.65 (d, $J$ = 8.8 Hz, 1H), 1.35 – 1.21 (m, 9H), 0.89 – 0.79 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.52, 141.40, 141.34, 128.53, 127.92, 126.68, 126.64, 74.77, 74.72, 40.45, 40.40, 35.38, 32.87, 32.59, 28.72, 28.58, 26.03, 25.66, 23.16, 23.10, 21.42, 14.25, 14.22, 10.62, 10.47. IR ($cm^{-1}$): 2963, 2932, 2875, 1739, 1235, 699. HRMS: calcd. For $C_{17}H_{26}O_2Na^+$ $[M+Na]^+$: 285.1825; Found: 285.1822.

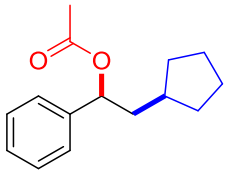
**(4f) 2-cyclohexyl-1-phenylethyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and cyclohexanecarboxaldehyde (**2f**), and purified by flash column chromatography as colorless oil (43.0 mg, 80%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.33 – 7.26 (m, 5H), 5.84 (dd, $J$ = 8.8, 6.0 Hz, 1H), 2.05 (s, 3H), 1.88 – 1.81 (m, 1H), 1.76 – 1.61 (m, 6H), 1.29 – 1.14 (m, 4H), 1.01 – 0.90 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.52, 141.37, 128.54, 127.90, 126.63, 74.11, 44.20, 34.19, 33.60, 33.09, 26.58, 26.27, 26.18, 21.45. IR ($cm^{-1}$): 3064, 2923, 2851, 1736, 1237, 699. HRMS: calcd. For $C_{16}H_{22}O_2Na^+$ $[M+Na]^+$: 269.1512; Found: 269.1503.

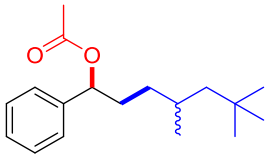
**(4g) 2-cyclopentyl-1-phenylethyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and cyclopentanecarbaldehyde (**2g**), and purified by flash column chromatography as colorless oil (37.6 mg, 81%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 – 7.28 (m, 5H), 5.78 – 5.74 (m, 1H), 2.06 (s, 3H), 1.99 – 1.92 (m, 1H), 1.81 – 1.67 (m, 4H), 1.59 – 1.41 (m, 4H), 1.20 – 1.08 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.52, 141.37, 128.54, 127.90, 126.63, 74.11, 44.20, 34.19, 33.60, 33.09, 26.58, 26.27, 26.18, 21.45. IR ($cm^{-1}$): 3064, 2950, 2867, 1736, 1237, 699. HRMS: calcd. For $C_{15}H_{20}O_2Na^+$ $[M+Na]^+$: 255.1356; Found: 255.1370.

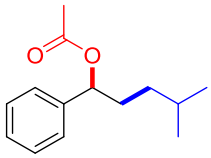
**(4h) 4,6,6-trimethyl-1-phenylheptyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 3,5,5-trimethylhexanal (**2h**), and purified by flash column chromatography as colorless oil (40.9 mg, 78%, d.r. = 1.2 : 1).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 –7.28 (m, 5H), 5.72 – 5.64 (m, 1H), 2.06 (s, 3H), 1.92 – 1.73 (m, 2H), 1.49 – 1.42 (m, 1H), 1.23 – 1.14 (m, 2H), 1.10 – 1.01 (m, 2H), 0.90 – 0.85 (m, 12H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.56, 141.06, 140.94, 128.53, 127.96, 126.73, 126.67, 126.65, 76.62, 76.48, 51.15, 50.69, 38.33, 35.12 (d, $J$ = 5.4 Hz ), 34.07, 31.31, 31.16, 30.13, 29.19, 29.11, 27.73, 25.62, 24.22, 22.64, 22.61, 21.43. IR (cm$^{-1}$): 3064, 2950, 2867, 1736, 1236, 699. HRMS: calcd. For $C_{18}H_{28}O_2Na^+$ $[M+Na]^+$: 299.1982; Found: 299.1987.

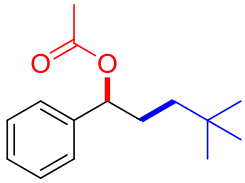
**(4i) 5-methyl-1-phenylhexyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 4-methylpentanal (**2i**), and purified by flash column chromatography as colorless oil (33.7 mg, 72%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 – 7.28 (m, 5H), 5.70 (dd, $J$ = 7.2, 6.4 Hz, 1H), 2.07 (s, 3H), 1.95 – 1.85 (m, 1H), 1.81 – 1.72 (m, 1H), 1.57 – 1.49 (m, 1H), 1.26 – 1.19 (m, 1H), 1.13 – 1.06 (m, 1H), 0.86 (dd, $J$ = 6.4, 2.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.56, 141.01, 128.54, 127.95, 126.68, 76.56, 34.66, 34.35, 27.98, 22.63, 22.60, 21.44. IR (cm$^{-1}$): 3064, 2956, 2870, 1736, 1237, 700. HRMS: calcd. For $C_{14}H_{20}O_2Na^+$ $[M+Na]^+$: 243.1356; Found: 243.1366.

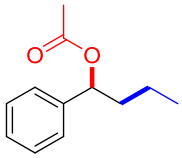
**(4j) 4,4-dimethyl-1-phenylpentyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 3,3-dimethylbutanal (**2j**), and purified by flash column chromatography as colorless oil (29.6 mg, 63%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.35 – 7.27 (m, 5H), 5.69 – 5.65 (m, 1H), 2.07 (s, 3H), 1.92 – 1.83 (m, 1H), 1.79 – 1.71 (m, 1H), 1.26 – 1.21 (m, 1H), 1.10 – 0.94 (m, 1H), 0.85 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.57, 141.00, 128.55, 127.97, 126.72, 76.99, 39.63, 31.68, 30.19, 29.39, 21.45. IR (cm-$^{1}$): 3064, 2956, 2870, 1736, 1236, 699. HRMS: calcd. For $C_{15}H_{22}O_2Na^+$ $[M+Na]^+$: 257.1512; Found: 257.1499.

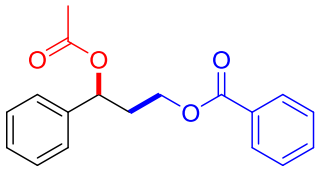
**(4k) 1-phenylbutyl acetate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and propionaldehyde (**2k**), and purified by flash column chromatography as colorless oil (20.7 mg, 54%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 – 7.27 (m, 5H), 5.76 – 5.72 (m, 1H), 2.06 (s, 3H), 1.93 – 1.86 (m, 1H), 1.77 – 1.71 (m, 1H), 1.40 – 1.32 (m, 1H), 1.29 – 1.23 (m, 1H), 0.91 (t, $J$ = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.56, 141.00, 128.52, 127.93, 126.65, 76.05, 38.56, 21.42, 18.92, 13.92. IR (cm-$^1$): 3064, 2956, 2870, 1736, 1236, 699. HRMS: calcd. For $C_{12}H_{16}O_2Na^+$ $[M+Na]^+$: 215.1043; Found: 215.1050.

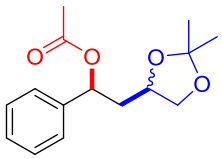
**(4l) 3-acetoxy-3-phenylpropyl benzoate**



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and 2-oxopropyl benzoate **(2l)**, and purified by flash column chromatography as colorless oil (32.2 mg, 54%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.02 – 7.98 (m, 2H), 7.56 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.37 – 7.28 (m, 5H), 5.97 (dd, J = 8.0, 6.0 Hz, 1H), 4.42 – 4.28 (m, 2H), 2.45 – 2.36 (m, 1H), 2.30 – 2.22 (m, 1H), 2.07 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.31, 166.57, 139.99, 133.30, 133.16, 130.14, 129.84, 129.72, 128.78, 128.51, 128.32, 126.55, 73.23, 61.36, 35.49, 21.33. IR (cm$^{-1}$): 3063, 2962, 2933, 1720, 1275, 700. HRMS: calcd. For $C_{18}H_{18}O_4Na^+$ $[M+Na]^+$: 321.1097; Found: 321.1083.

**(4m) 2-(2,2-dimethyl-1,3-dioxolan-4-yl)-1-phenylethyl acetate**

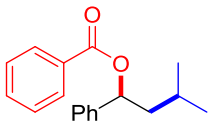


The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with iodobenzene diacetate and (R)-2,2-dimethyl-1,3-dioxolane-4-carbaldehyde (**2m**), and purified by flash column chromatography as colorless oil (33.8 mg, 64%, d.r. = 1.5 : 1).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.35 – 7.29 (m, 5H), 5.89 – 5.85 (m, 1H), 4.18 – 4.12 (m, 1H), 4.05 – 4.01 (m, 1H), 3.59 – 3.52 (m, 1H), 2.08 (s, 3H), 1.42 – 1.34 (m, 6H), 1.30 (s, 1H). 1.26 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 170.18, 140.64, 128.72, 128.20, 126.69, 126.31, 108.93, 73.39,

73.06, 69.60, 41.08, 40.32, 27.13, 25.86, 21.34. IR ($cm^{-1}$): 2959, 2870, 2097, 1245, 699. HRMS: calcd. For $C_{15}H_{20}O_4Na^+$ $[M+Na]^+$:301.1410; Found: 301.1420.

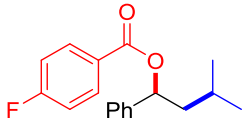
**(6a) 3-methyl-1-phenylbutyl benzoate**




The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with benzoic acid (**5a**) and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (43.4 mg, 81%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.07 (d, $J$ = 8.0 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.45 – 7.41 (m, 4H), 7.34 (t, $J$ = 7.6 Hz, 2H), 7.27 (t, $J$ = 7.4 Hz, 1H), 6.07 (dd, $J$ = 8.8, 4.8 Hz, 1H), 2.05 – 1.99 (m, 1H), 1.74 – 1.66 (m, 2H), 0.97 (dd, $J$ = 8.4, 6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 165.93, 141.32, 132.96, 130.62, 129.71, 128.57, 128.42, 127.94, 126.52, 75.29, 45.82, 24.95, 23.01, 22.47. IR ($cm^{-1}$): 3089, 3064, 2957, 2870, 1716, 1271, 712. HRMS: calcd. For $C_{18}H_{20}O_2Na^+$ $[M+Na]^+$: 291.1356; Found: 291.1360.

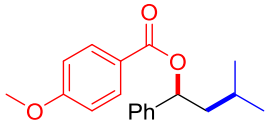
**(6b) 3-methyl-1-phenylbutyl 4-fluorobenzoate**




The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with 4-fluorobenzoic acid (**5b**) and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (42.3 mg, 74%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.08 (dd, $J$ = 8.8, 5.6 Hz, 2H), 7.41 (d, $J$ = 7.6 Hz, 2H), 7.34 (t, $J$ = 7.4 Hz, 2H), 7.30 – 7.26 (m, 1H), 7.10 (t, $J$ = 8.6 Hz, 2H), 6.05 (dd, $J$ = 8.4, 4.8 Hz, 1H), 2.06 – 2.00 (m, 1H), 1.75 – 1.63 (m, 2H), 0.98 (dd, $J$ = 9.2, 6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 167.13, 165.04, 164.61, 141.18, 132.33, 132.23, 128.65, 128.07, 126.57, 115.71, 115.49, 75.55, 45.76, 24.98, 23.00, 22.51. IR ($cm^{-1}$): 2958, 2871, 2837, 1736, 1073, 699. HRMS: calcd. For $C_{18}H_{19}FO_2Na^+$ $[M+Na]^+$: 309.1261; Found: 309.1257.

**(6c) 4-methoxybenzoic acid**

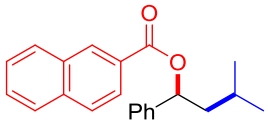



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with 4-methoxybenzoic acid (**5c**) and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (50.1 mg, 84%).

$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.03 (d, $J$ = 8.8 Hz, 2H), 7.41 (d, $J$ = 7.2 Hz, 2H), 7.34 (t, $J$ = 7.4 Hz, 2H), 7.29 – 7.25 (m, 1H), 6.92 (d, $J$ = 9.2 Hz, 2H), 6.03 (dd, $J$ = 8.8, 5.2 Hz, 1H), 3.85 (s, 3H), 2.06 – 1.97 (m, 1H), 1.74 – 1.64 (m, 2H), 0.97 (dd, $J$ = 8.0, 6.4 Hz, 6H).$^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$

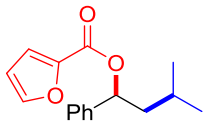
165.76, 163.44, 141.58, 131.77, 128.57, 127.87, 126.51, 123.05, 113.70, 77.48, 77.16, 76.84, 74.95, 55.54, 45.91, 24.97, 23.06, 22.51. IR ($cm^{-1}$): 3018, 2871, 2834, 1746, 1073, 699. HRMS: calcd. For $C_{19}H_{22}O_3Na^+$ $[M+Na]^+$: 321.1461; Found: 321.1476.

**(6d) 3-methyl-1-phenylbutyl 2-naphthoate**



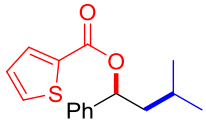

The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with 2-naphthoic acid (**5d**) and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (50 mg, 79%).
$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.63 (s, 1H), 8.09 (dd, $J$ = 8.4, 1.2 Hz, 1H), 7.96 (d, $J$ = 8.0 Hz, 1H), 7.87 (d, $J$ = 8.4 Hz, 2H), 7.60 – 7.52 (m, 2H), 7.47 (d, $J$ = 7.2 Hz, 2H), 7.36 (t, $J$ = 7.4 Hz, 2H), 7.29 (d, $J$ = 7.2 Hz, 1H), 6.13 (dd, $J$ = 8.8, 4.8 Hz, 1H), 2.13 – 2.06 (m, 1H), 1.80 – 1.71 (m, 2H), 1.01 (dd, $J$ = 9.6, 6.4 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 166.18, 141.40, 135.67, 132.65, 131.17, 129.49, 128.65, 128.33, 128.25, 128.01, 127.89, 126.74, 126.64, 125.46, 75.51, 45.89, 25.05, 23.07, 22.57. IR ($cm^{-1}$): 2958, 2871, 2837, 1736, 1073, 699. HRMS: calcd. For $C_{22}H_{22}O_2Na^+$ $[M+Na]^+$: 341.1512; Found: 341.1517.

**(6e) 3-methyl-1-phenylbutyl furan-2-carboxylate**




The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with furan-2-carboxylic acid (**5e**) and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (30 mg, 58%).
$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.57 (s, 1H), 7.41 (d, $J$ = 7.2 Hz, 2H), 7.34 (t, $J$ = 7.0 Hz, 2H), 7.29 (d, $J$ = 6.4 Hz, 1H), 7.20 (s, 1H), 6.50 (s, 1H), 6.06 – 6.03 (m, 1H), 2.01 (t, $J$ = 8.0 Hz, 1H), 1.73 – 1.64 (m, 2H), 0.97 (t, $J$ = 5.6 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.26, 146.39, 145.10, 140.92, 128.63, 128.11, 126.71, 117.99, 111.89, 75.32, 45.62, 24.93, 23.00, 22.49. IR ($cm^{-1}$): 2958, 2871, 2837, 1736, 1073, 699. HRMS: calcd. For $C_{16}H_{18}O_3Na^+$ $[M+Na]^+$: 281.1148; Found: 281.1151.

**(6f) 3-methyl-1-phenylbutyl thiophene-2-carboxylate**




The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with thiophene-2-carboxylic acid (**5f**) and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (35.1 mg, 64%).

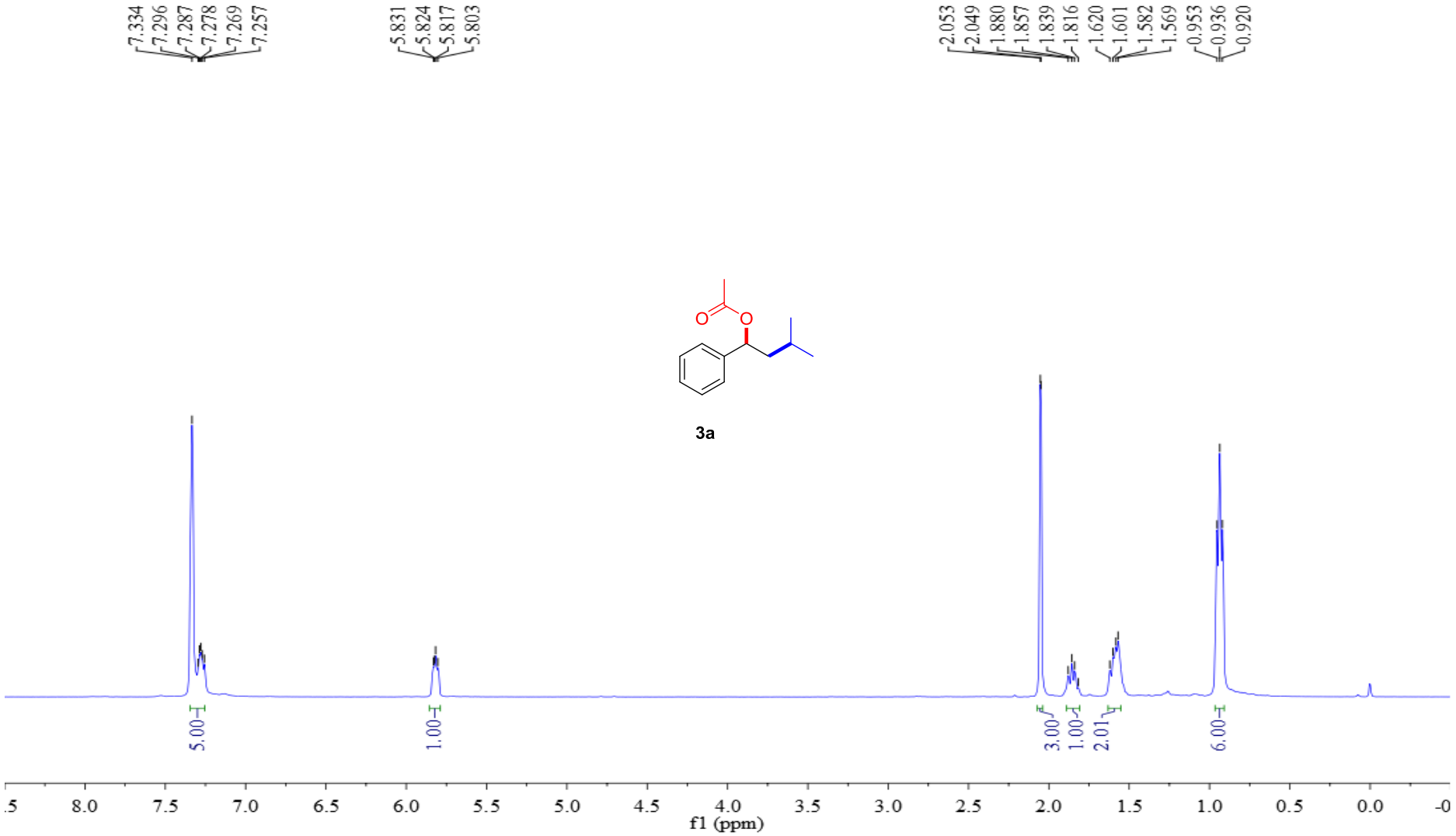
$^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.81 (d, $J$ = 3.2 Hz, 1H), 7.55 (d, $J$ = 4.8 Hz, 1H), 7.41 (d, $J$ = 7.6 Hz, 2H), 7.34 (t, $J$ = 7.4 Hz, 2H), 7.29 (d, $J$ = 7.2 Hz, 1H), 7.09 (t, $J$ = 4.4 Hz, 1H), 6.01 (dd, $J$ = 8.8, 4.8 Hz, 1H), 2.03 – 1.99 (m, 1H), 1.70 – 1.67 (m, 2H), 0.98 (t, $J$ = 6.2 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.71, 141.15, 134.32, 133.51, 132.42, 128.63, 128.04, 127.86, 126.58, 75.64, 45.80, 24.99, 23.05, 22.52. IR ($cm^{-1}$): 2958, 2871, 2837, 1736, 1073, 699. HRMS: calcd. For $C_{16}H_{18}O_2SNa^+$ $[M+Na]^+$: 297.0920; Found: 297.0936.

## V. References

[1]D. Basavaiah & S. Bhaskar Raju, *Synthetic Communications*, 1991**, 21**, 1859.

[2]D. V. Banthorpe, E. D. Hughes and Christopher Ingold Sir, *J. Chem. Soc.*, 1960, 4054.

## VI. Copies of $^{1}$H and $^{13}$C NMR spectra of products 3a-3m, 4b-4m, 6a-6f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7.278
7.269
7.257
5.831
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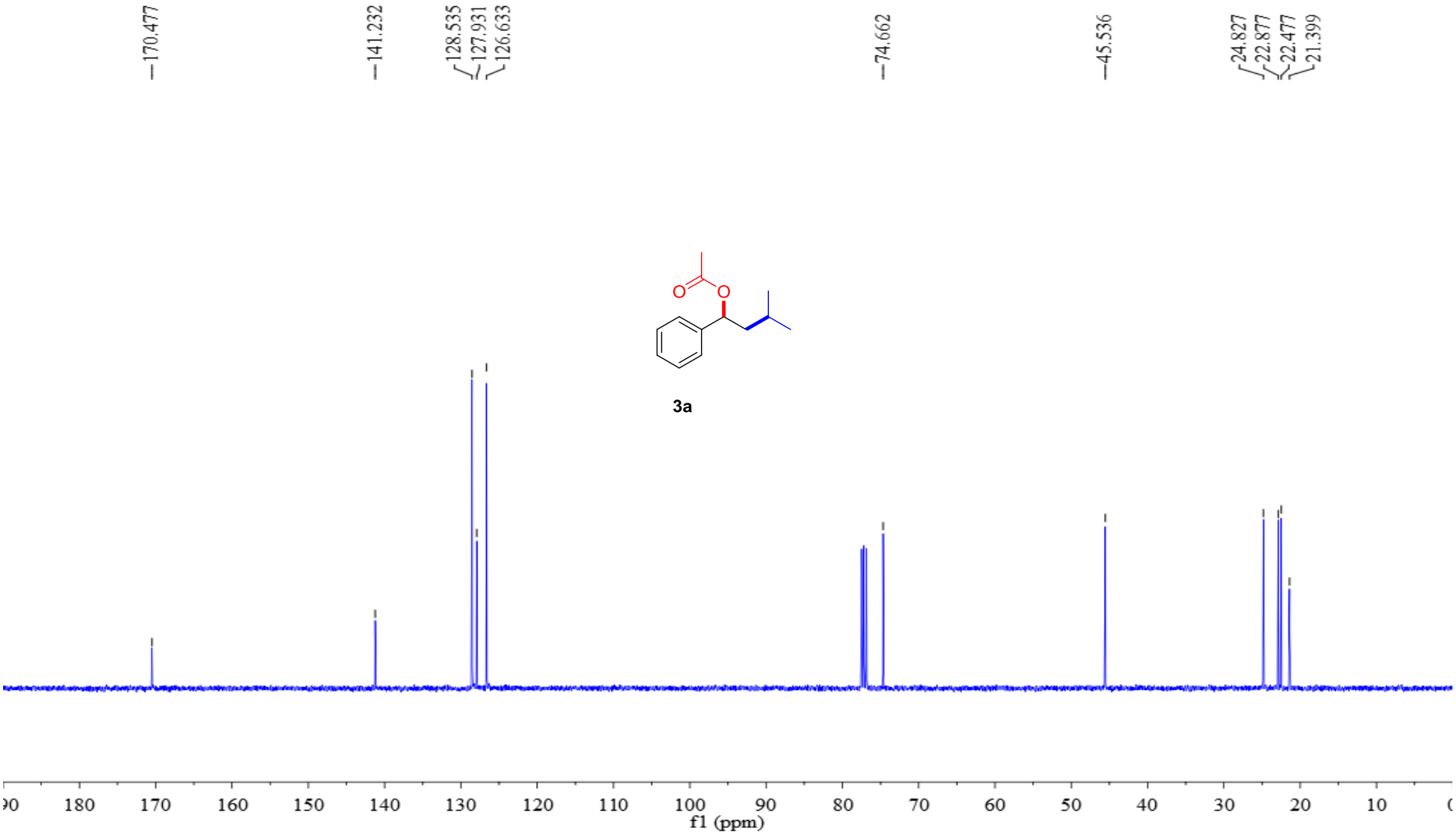
5.803
2.053
2.049
1.880
1.857
1.839
1.816
1.620
1.601
1.582
1.569
0.953
0.936
0.920
O
O
3a
5.00
1.00
3.00
1.00
2.01
6.00
f1 (ppm)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141.232
128.535
127.931
126.633
74.662
45.536
24.827
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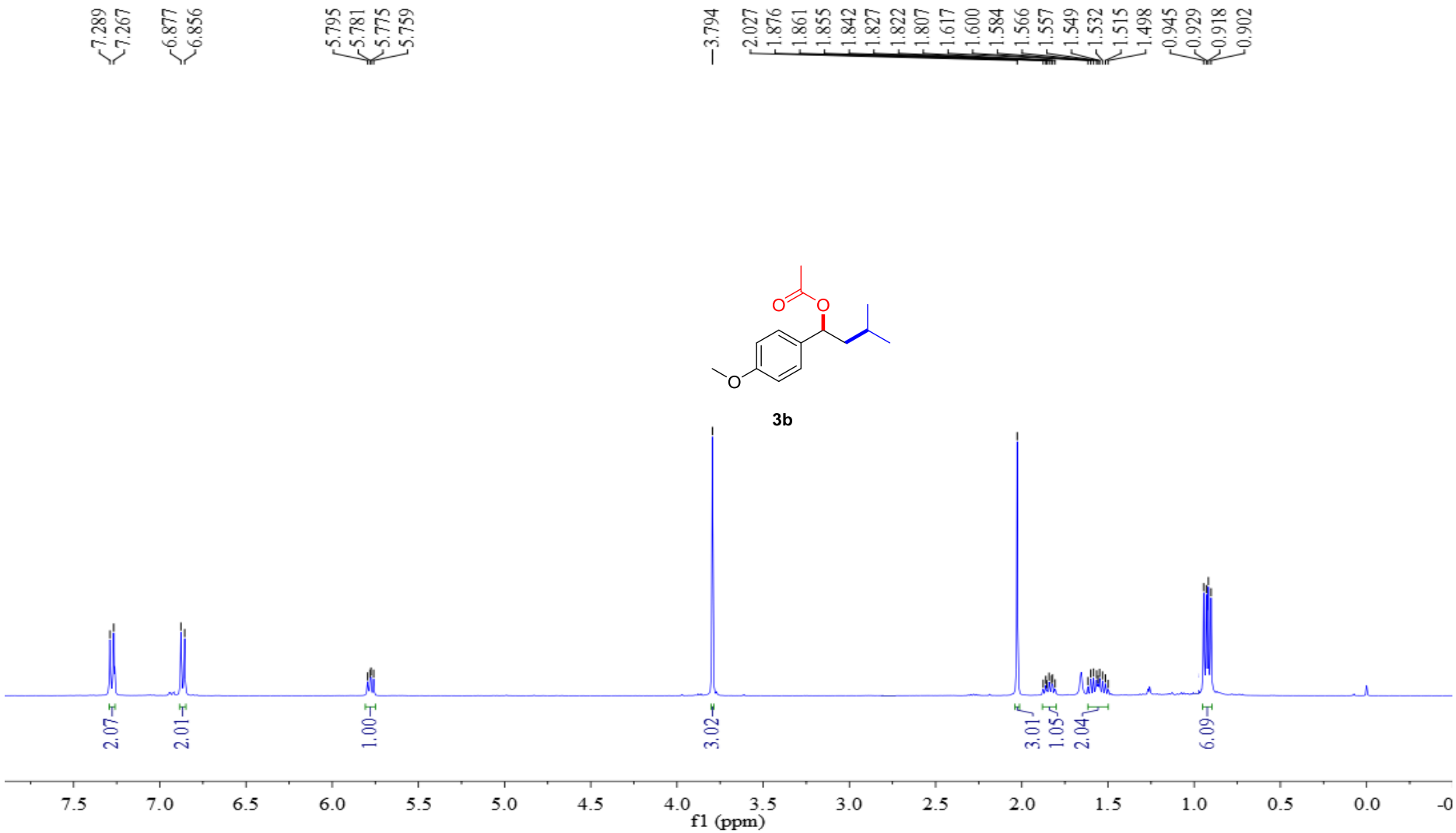
22.477
21.399
O
O
3a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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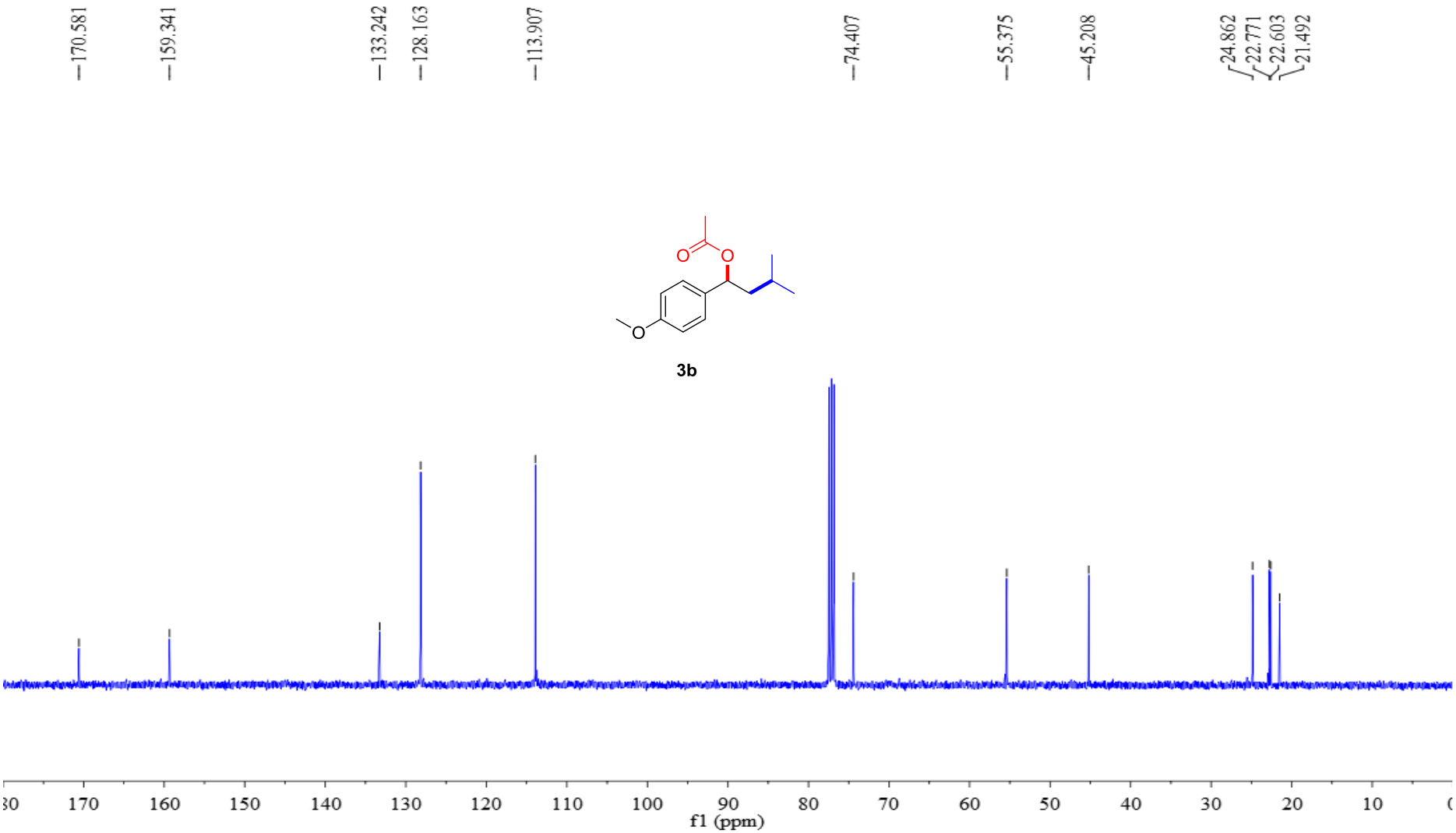
7.267
6.877
6.856
5.795
5.781
5.775
5.759
3.794
2.027
1.876
1.861
1.855
1.842
1.827
1.822
1.807
1.617
1.600
1.584
1.566
1.557
1.549
1.532
1.515
1.498
0.945
0.929
0.918
0.902
O
O
O
3b
2.07
2.01
1.00
3.02
3.01
1.05
2.04
6.09
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)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133.242
128.163
113.907
74.407
55.375
45.208
24.862
22.771
22.603
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O
O
O
3b
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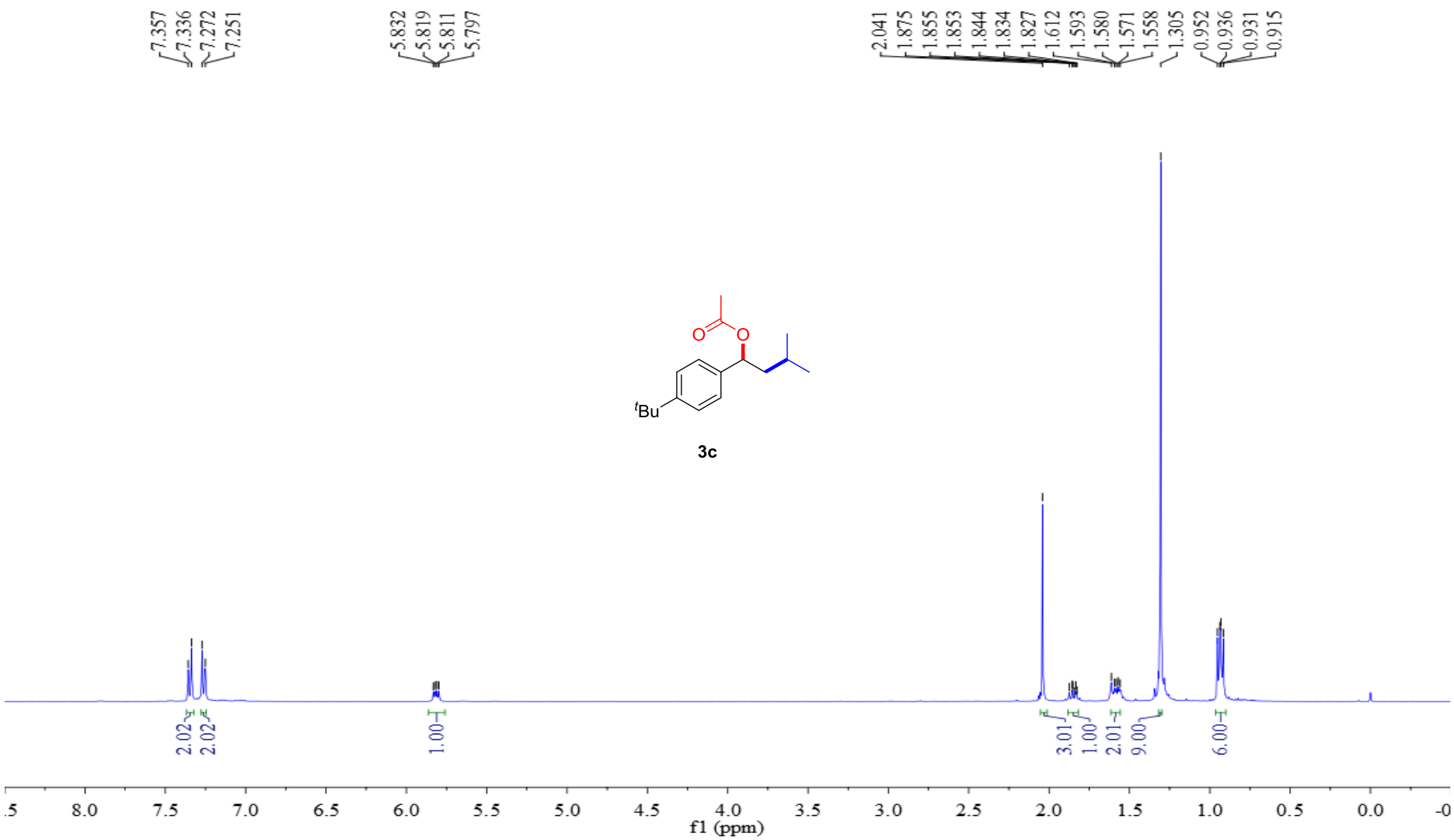
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.251
5.832
5.819
5.811
5.797
2.041
1.875
1.855
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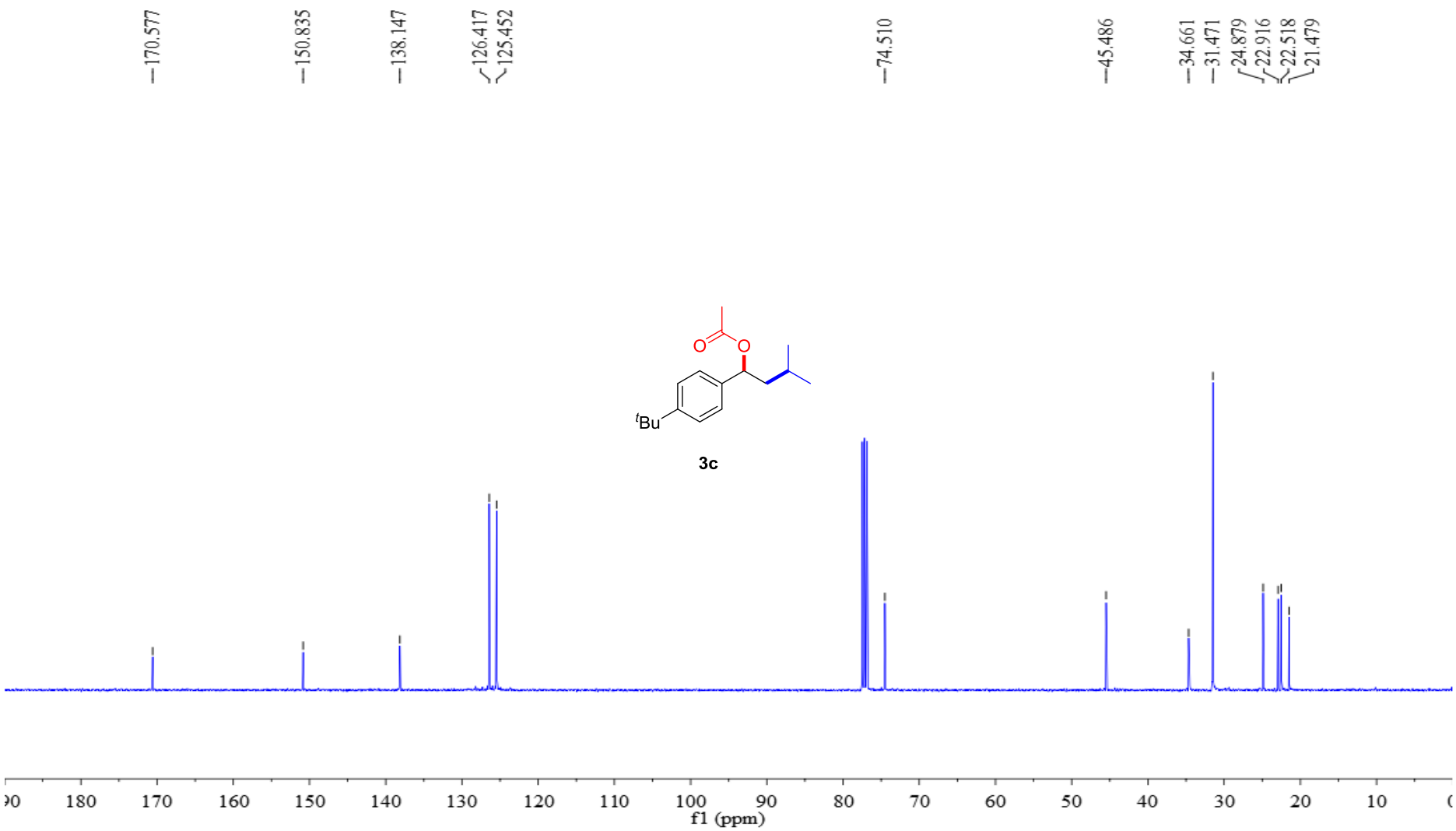
1.844
1.834
1.827
1.612
1.593
1.580
1.571
1.558
1.305
0.952
0.936
0.931
0.915
O
O
tBu
3c
2.02
2.02
1.00
3.01
1.00
2.01
9.00
6.00
f1 (ppm)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125.452
74.510
45.486
34.661
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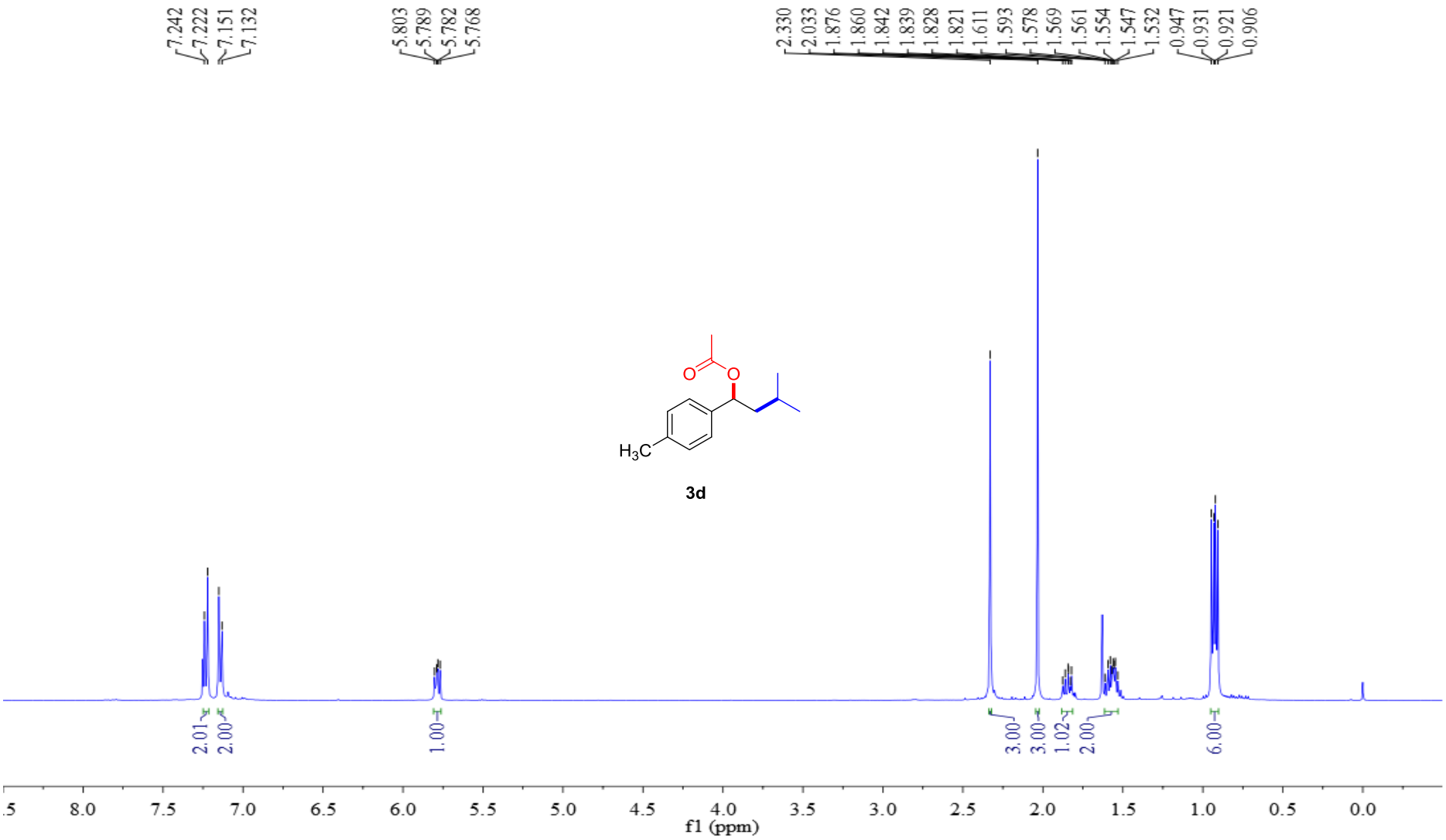
22.916
22.518
21.479
O
O
tBu
3c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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5.768
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2.033
1.876
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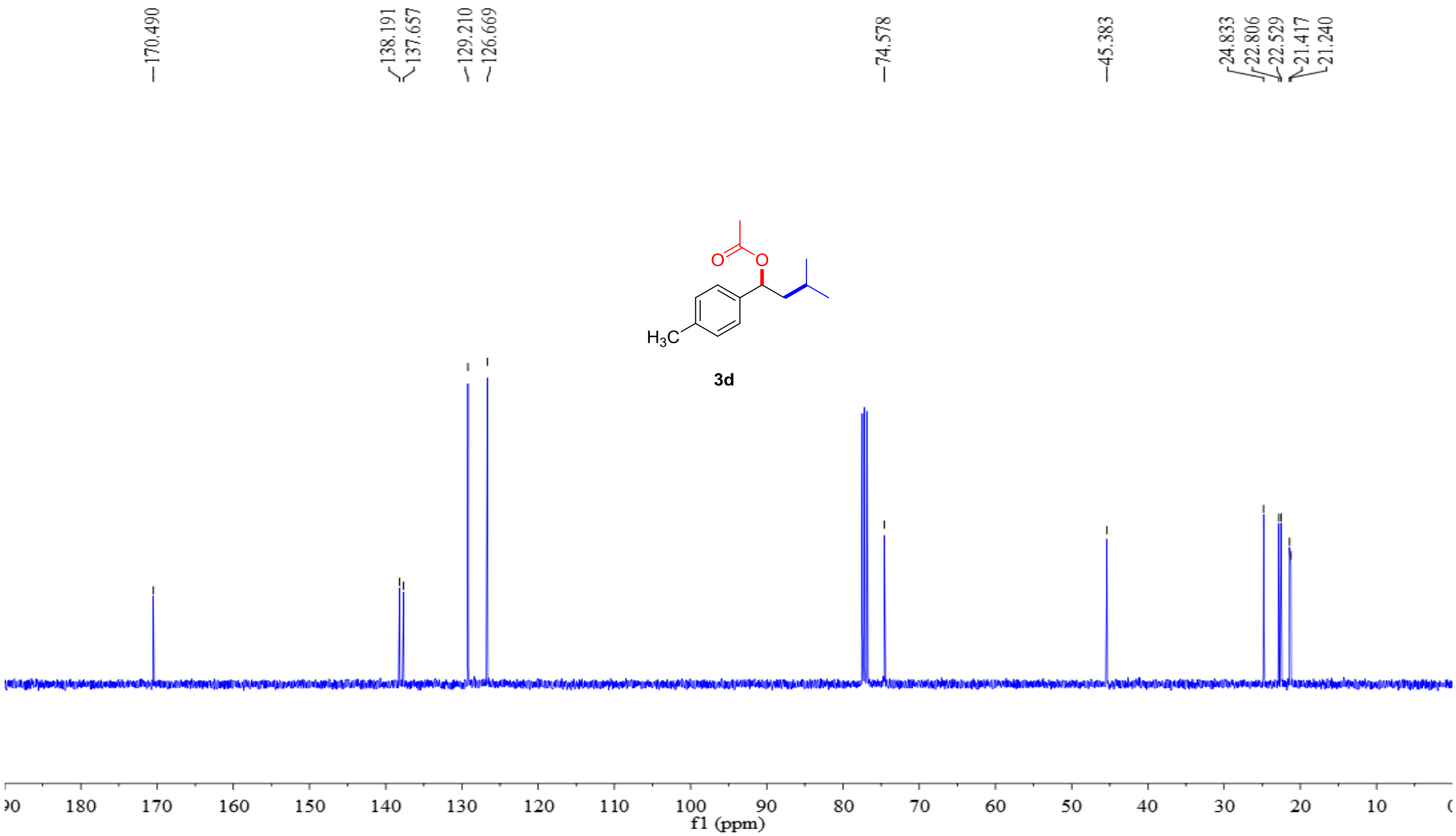
1.839
1.828
1.821
1.611
1.593
1.578
1.569
1.561
1.554
1.547
1.532
0.947
0.931
0.921
0.906
O
O
H3C
2.01
2.00
1.00
3.00
3.00
1.02
2.00
6.00
f1 (ppm)

**3d**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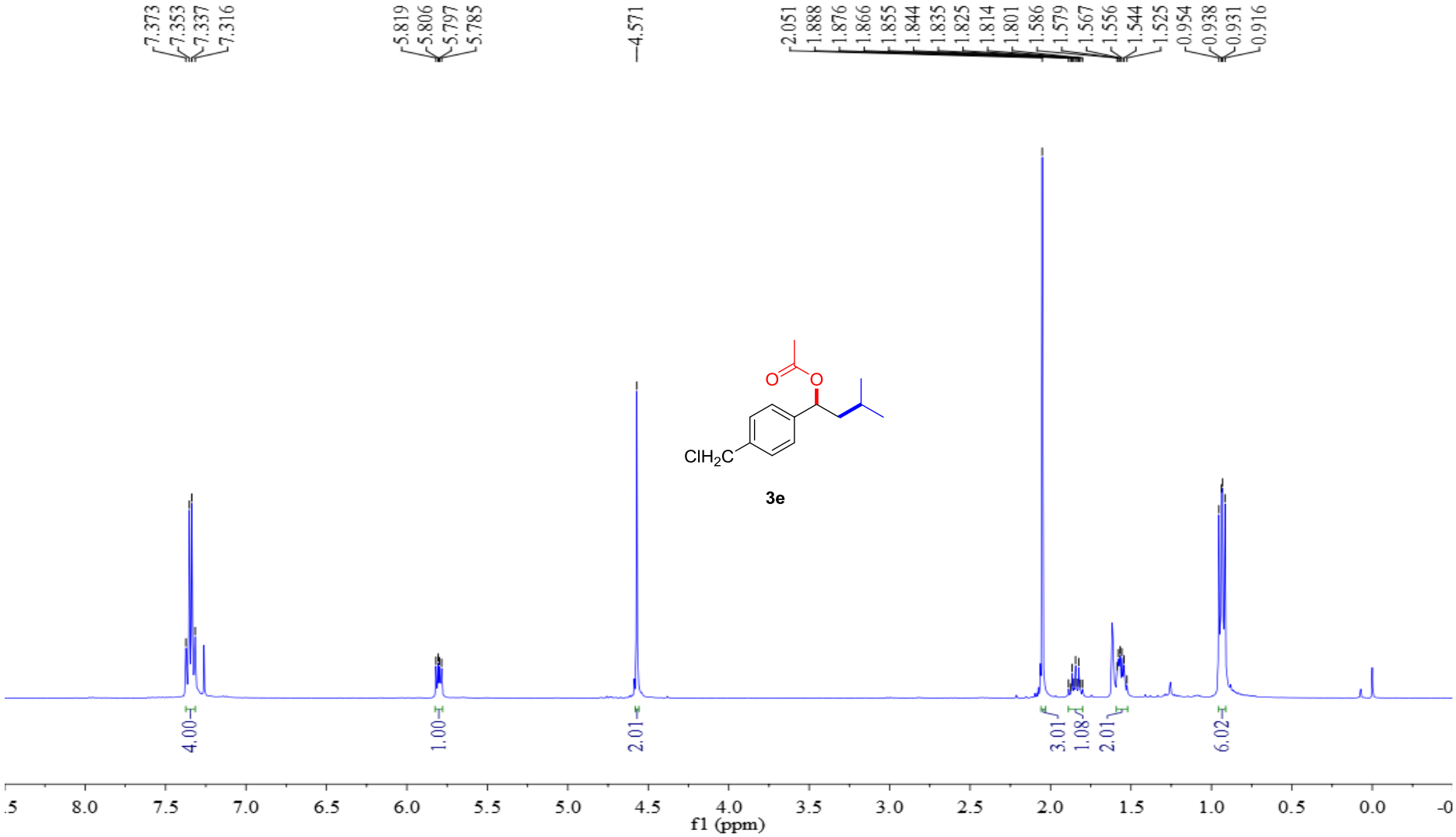
74.578
45.383
24.833
22.806
22.529
21.417
21.240
O
O
H3C
3d
f1 (ppm)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7.353
7.337
7.316
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5.806
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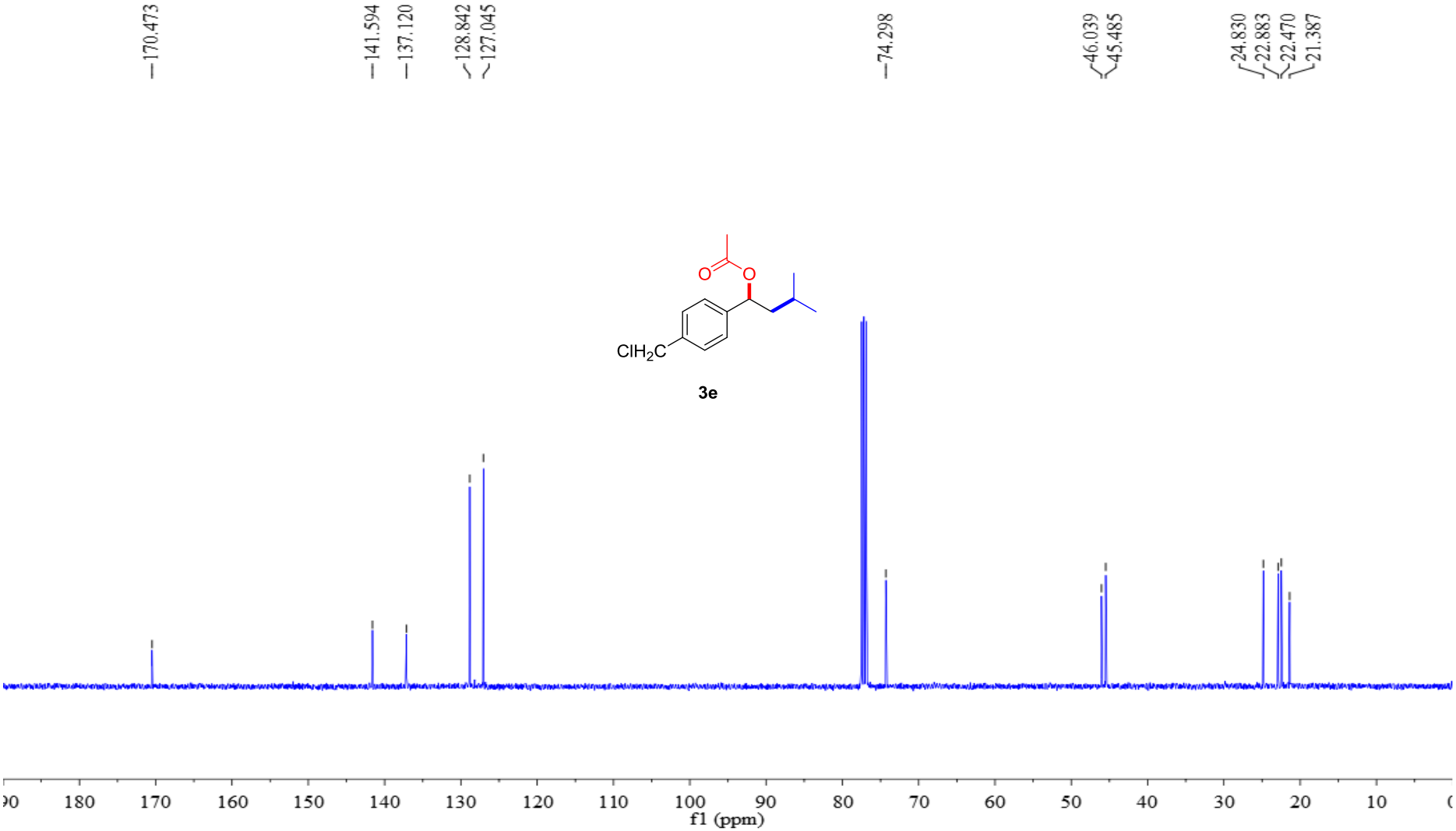
5.785
4.571
2.051
1.888
1.876
1.866
1.855
1.844
1.835
1.825
1.814
1.801
1.586
1.579
1.567
1.556
1.544
1.525
0.954
0.938
0.931
0.916
O
O
ClH2C
3e
4.00
1.00
2.01
3.01
1.08
2.01
6.02
f1 (ppm)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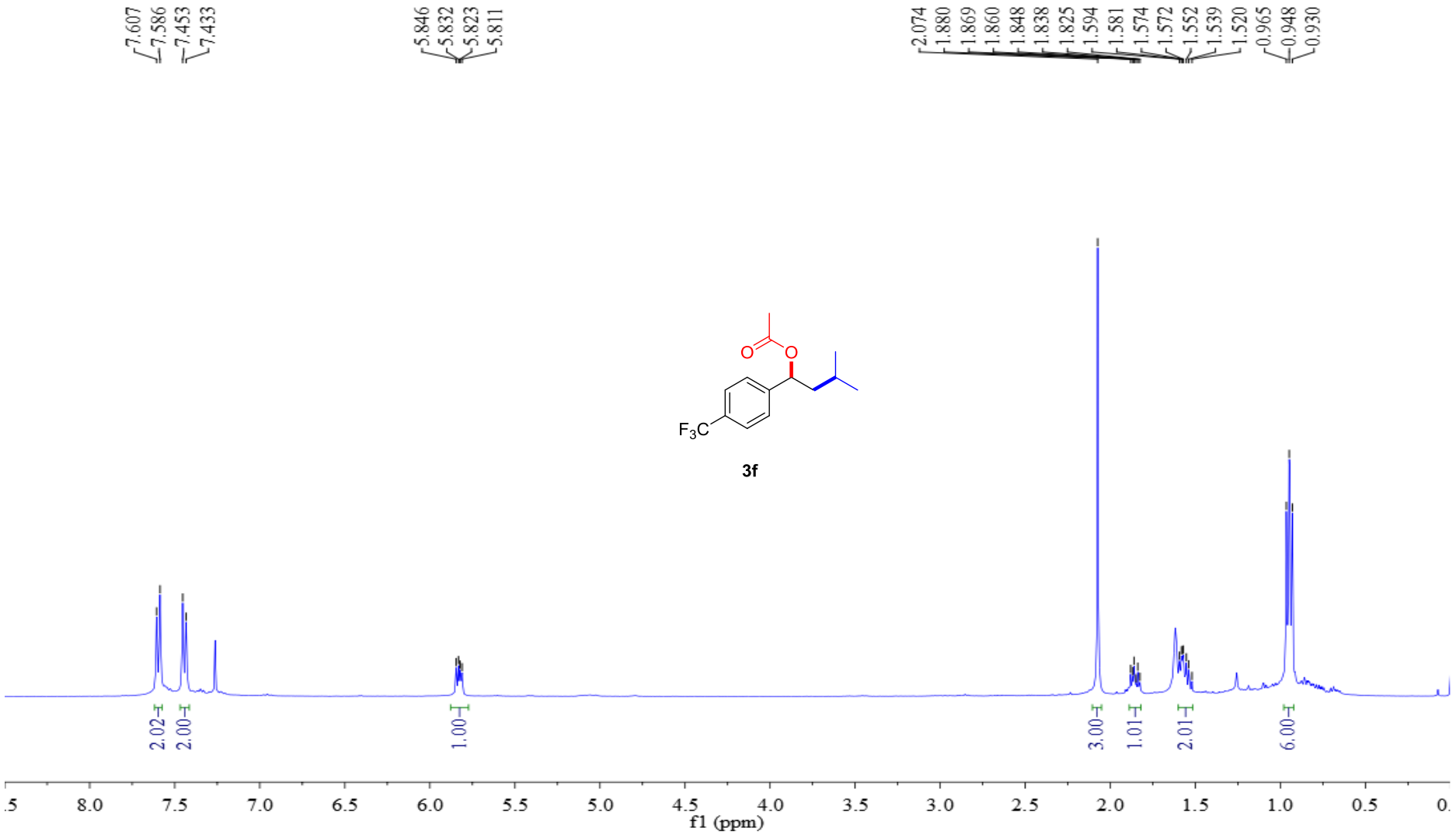
O
ClH2C
3e
f1 (ppm)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5.832
5.823
5.811
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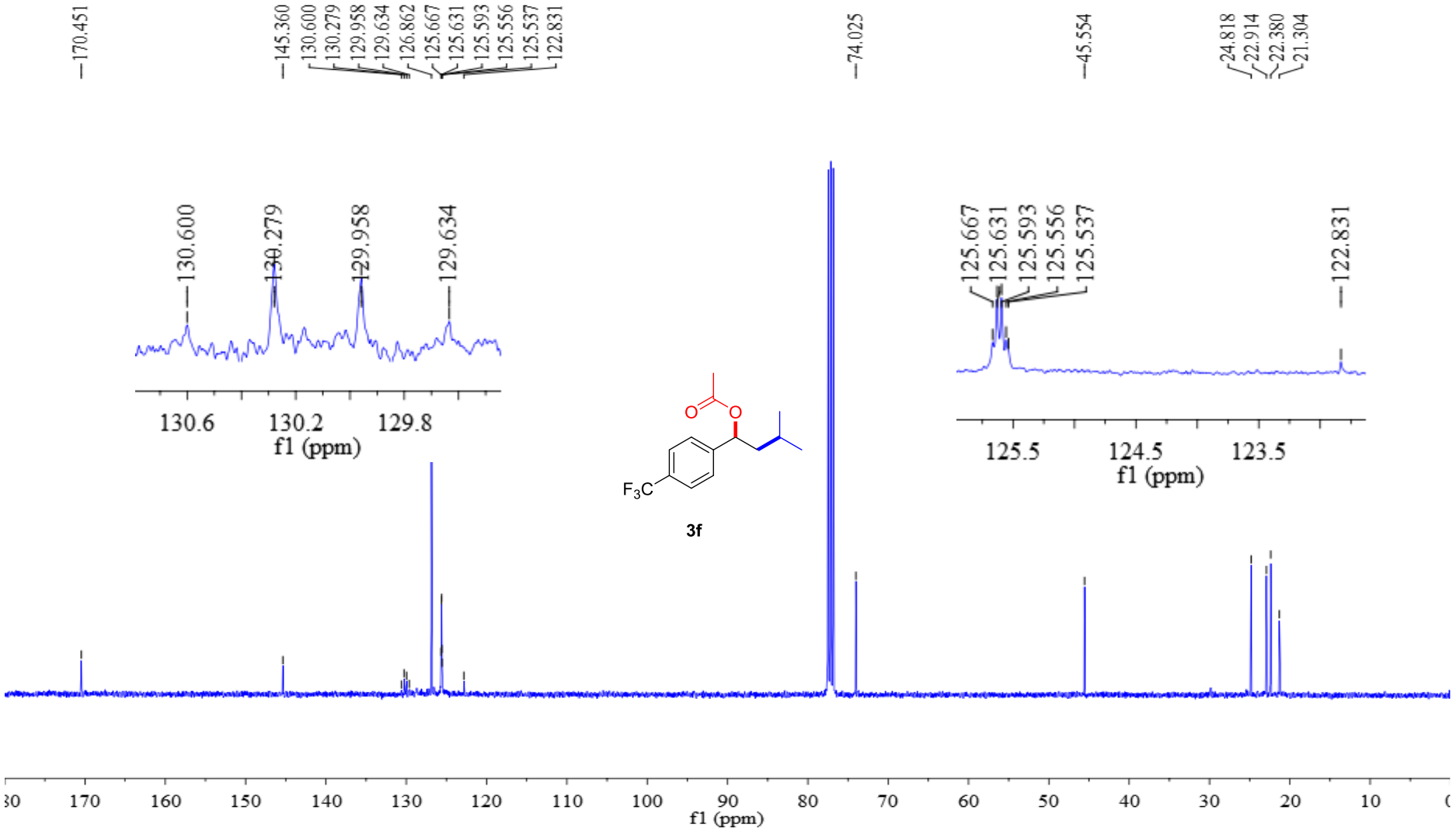
1.860
1.848
1.838
1.825
1.594
1.581
1.574
1.572
1.552
1.539
1.520
0.965
0.948
0.930
O
O
F3C
2.02
2.00
1.00
3.00
1.01
2.01
6.00
f1 (ppm)

**3f**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122.831
74.025
45.554
24.818
22.914
22.380
21.304
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f1 (ppm)
125.5
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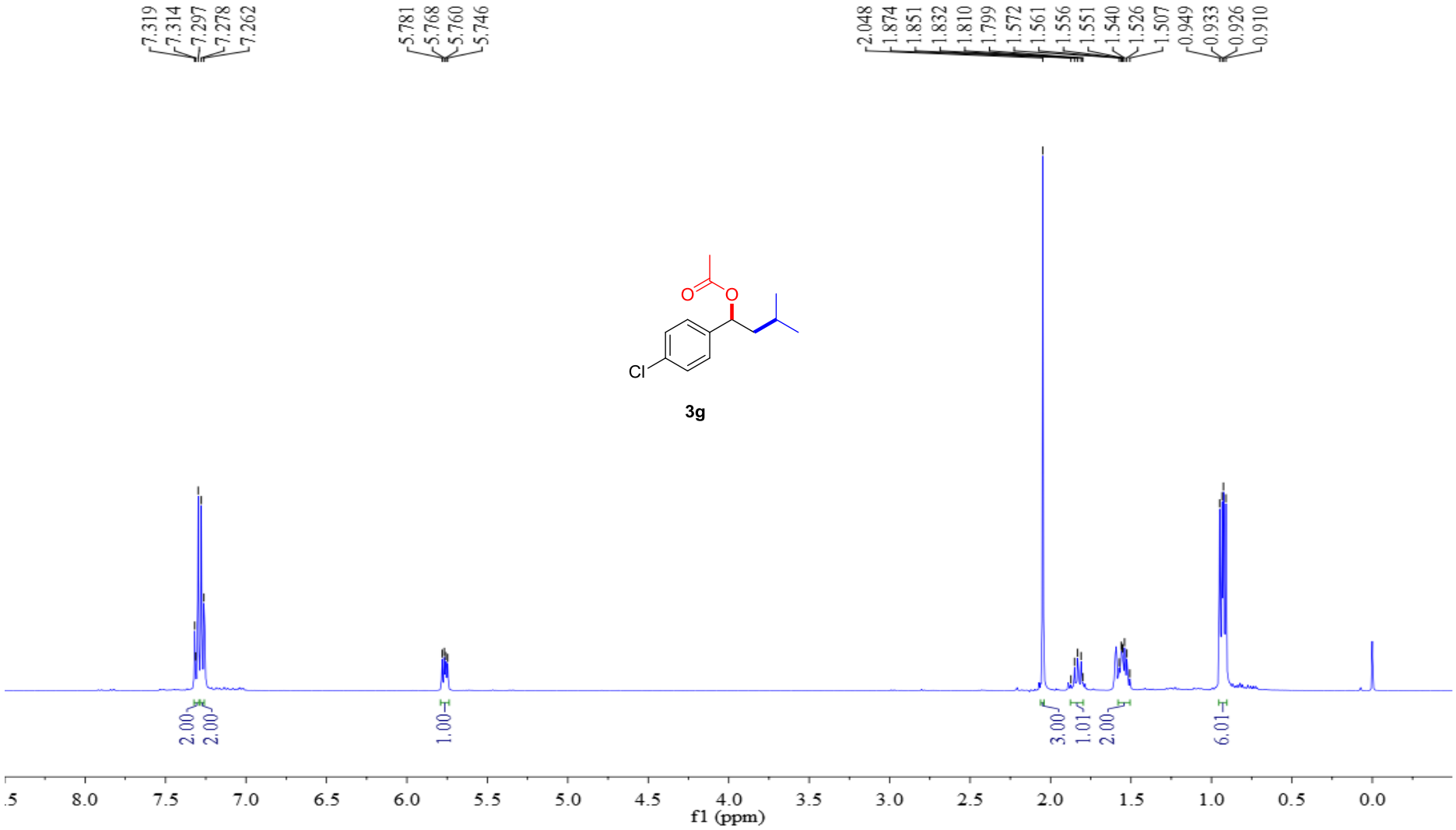
123.5
f1 (ppm)
F3C
3f
f1 (ppm)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5.760
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2.048
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1.810
1.799
1.572
1.561
1.556
1.551
1.540
1.526
1.507
0.949
0.933
0.926
0.910
O
O
Cl
2.00
2.00
1.00
3.00
1.01
2.00
6.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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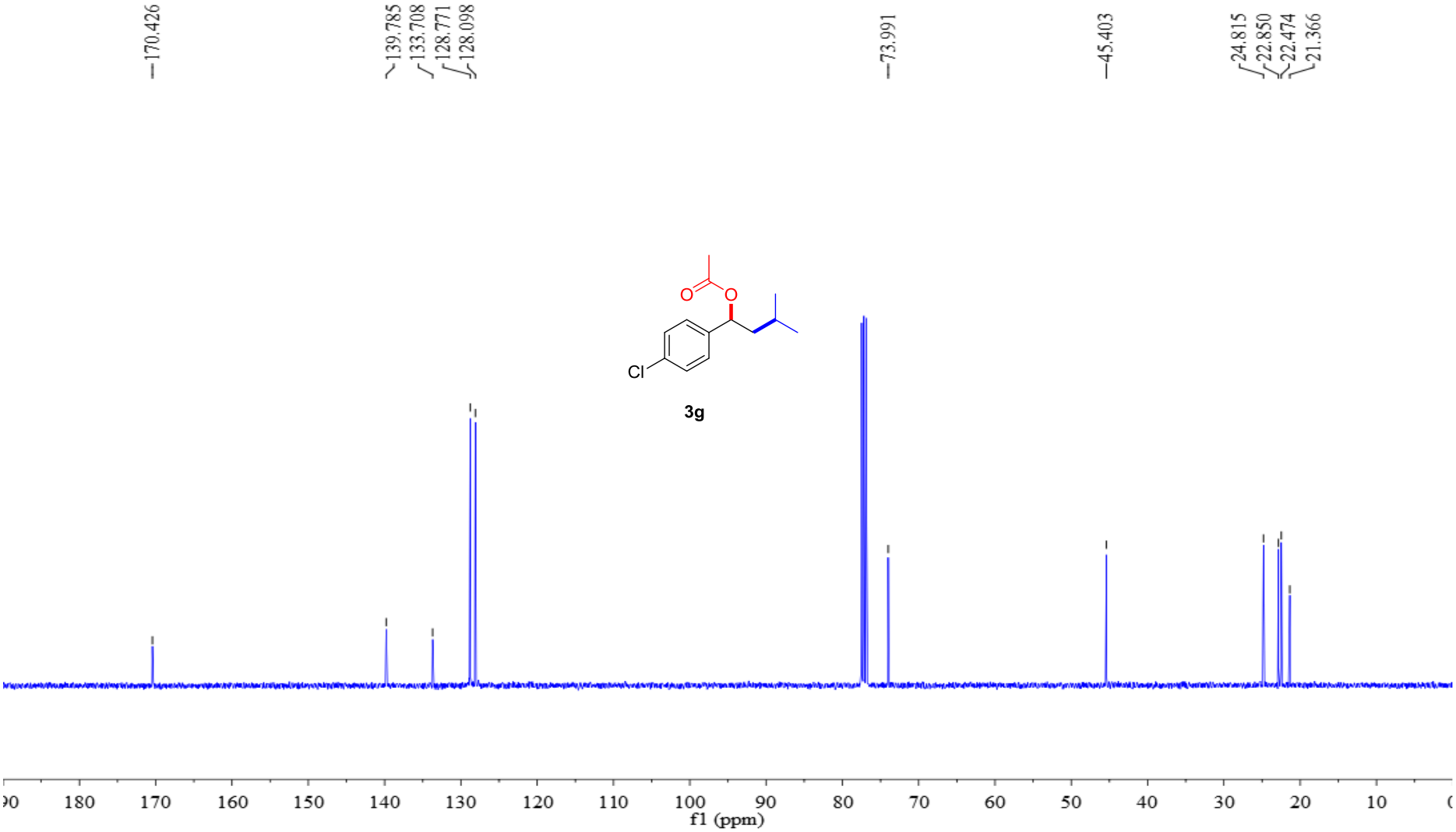
0.5
0.0
f1 (ppm)

**3g**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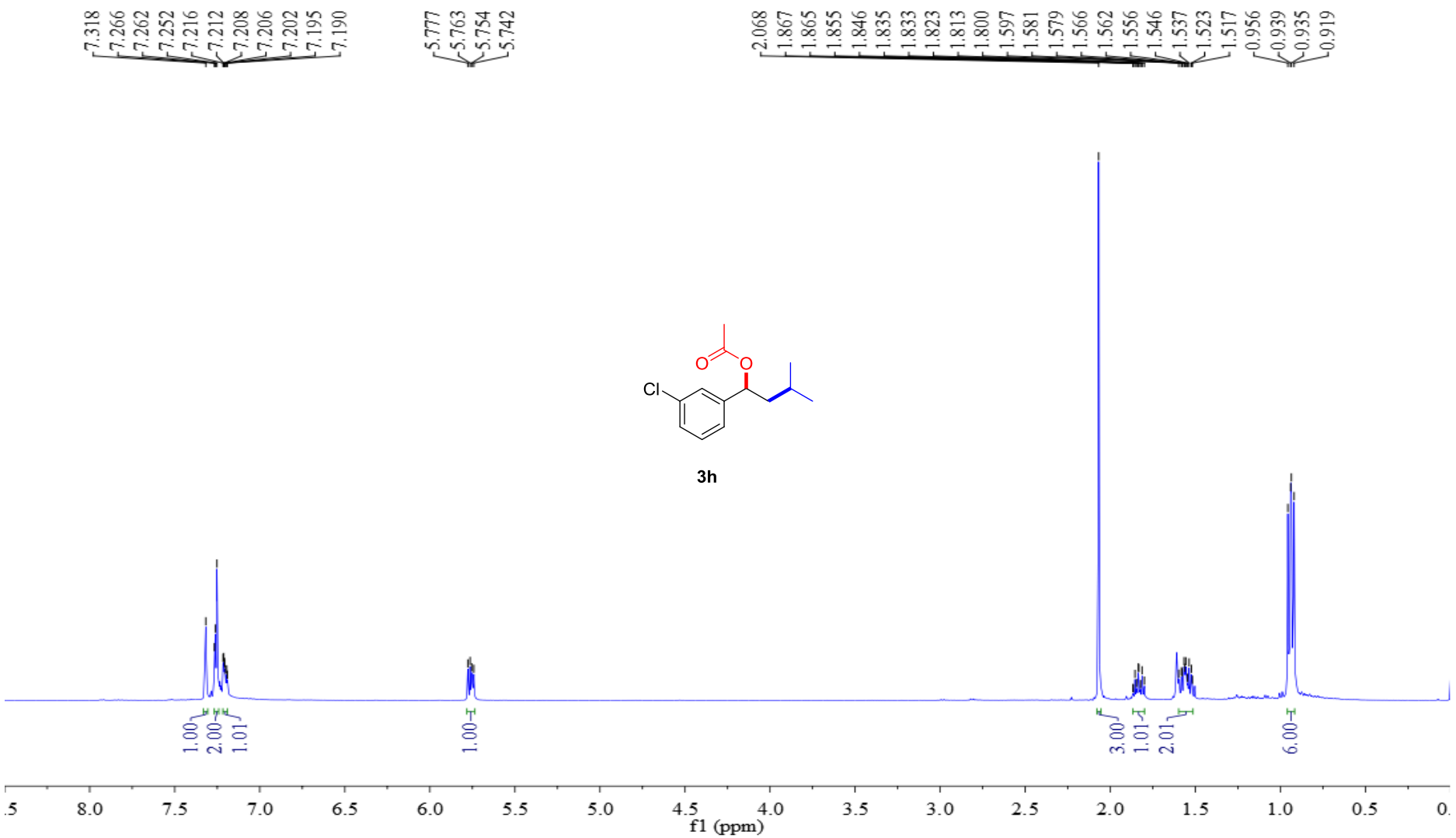
O
O
Cl
3g
f1 (ppm)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5.754
5.742
2.068
1.867
1.865
1.855
1.846
1.835
1.833
1.823
1.813
1.800
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1.581
1.579
1.566
1.562
1.556
1.546
1.537
1.523
1.517
0.956
0.939
0.935
0.919
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O
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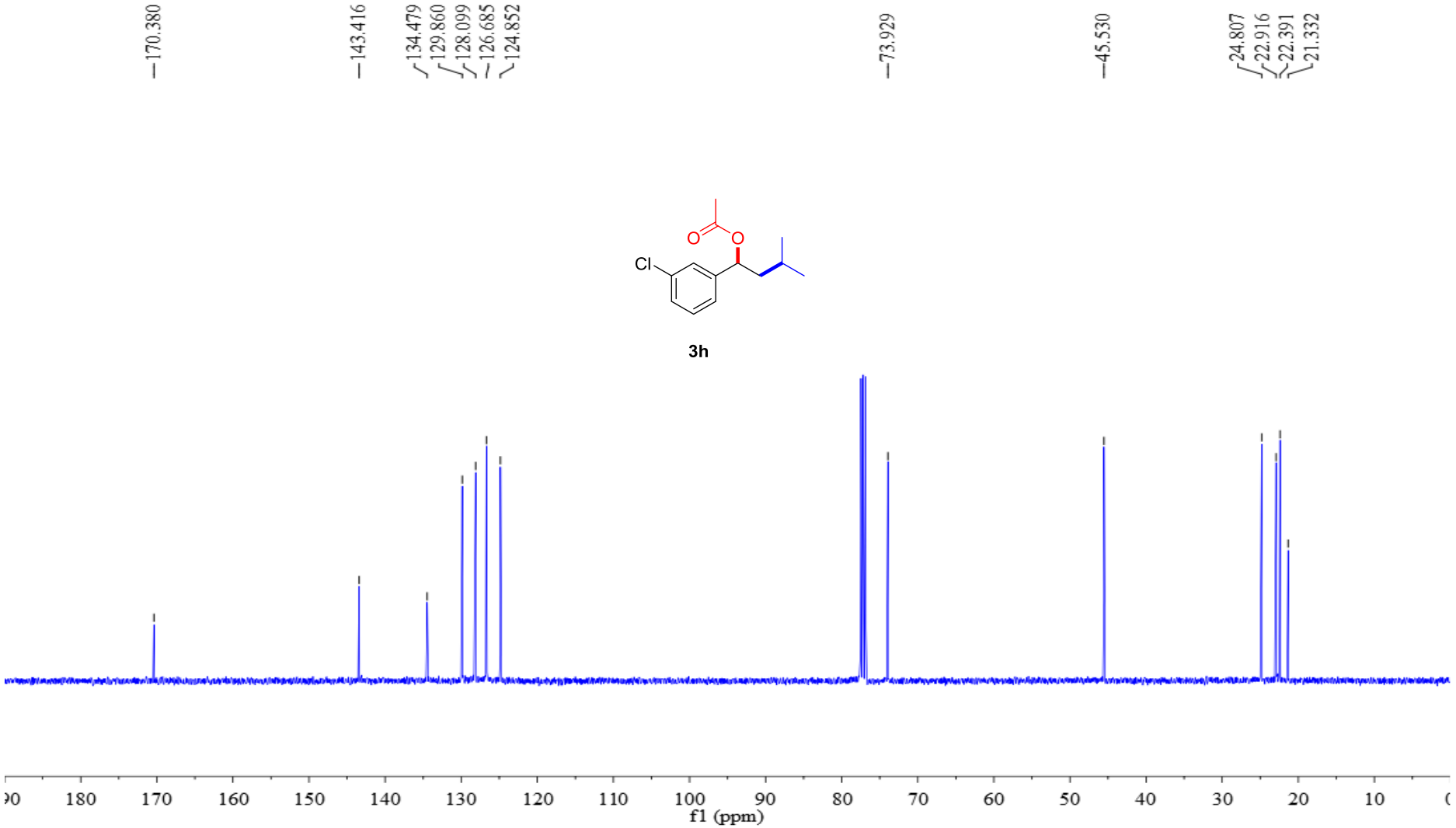
f1 (ppm)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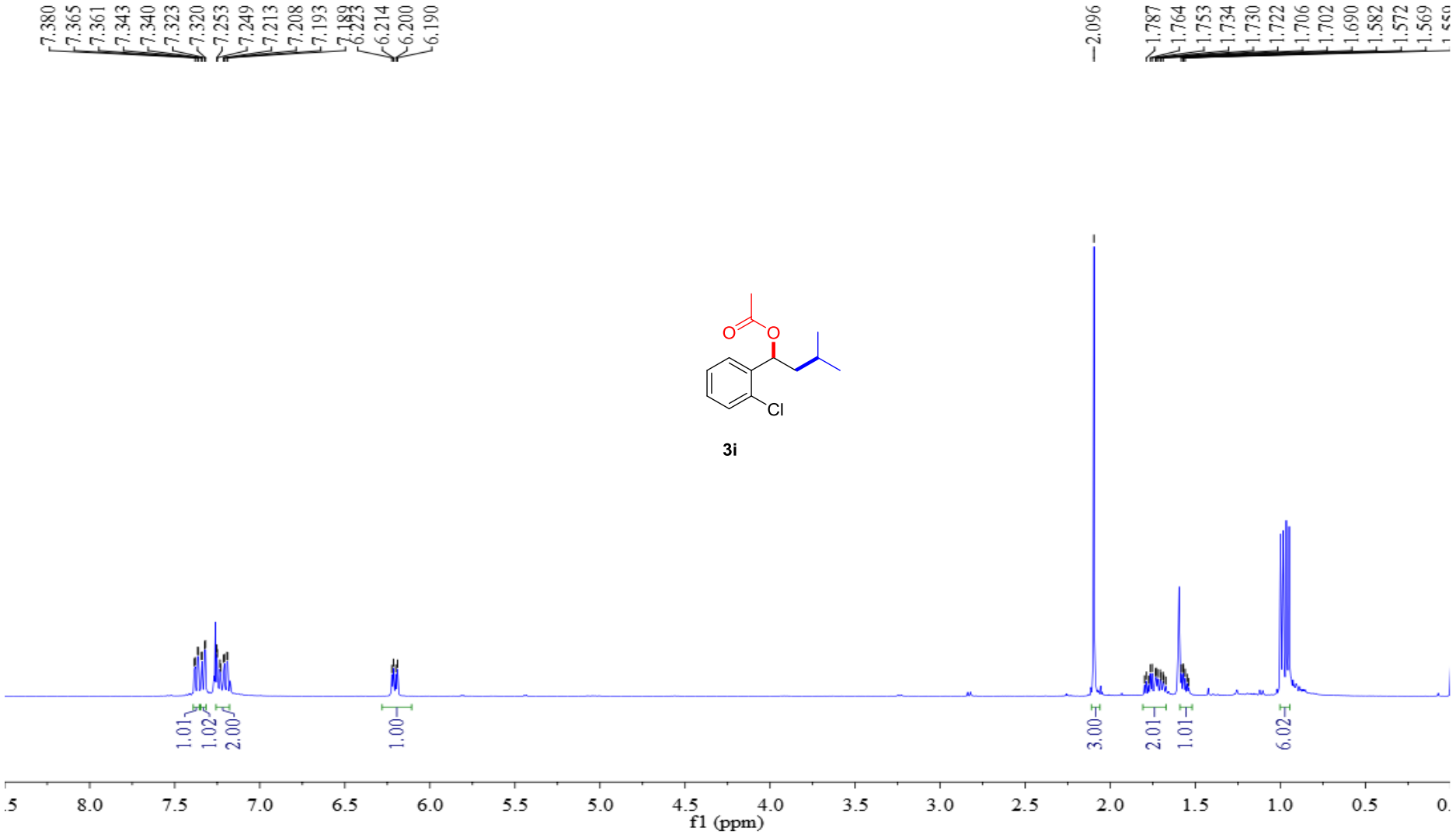
O
Cl
3h
f1 (ppm)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6.190
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1.730
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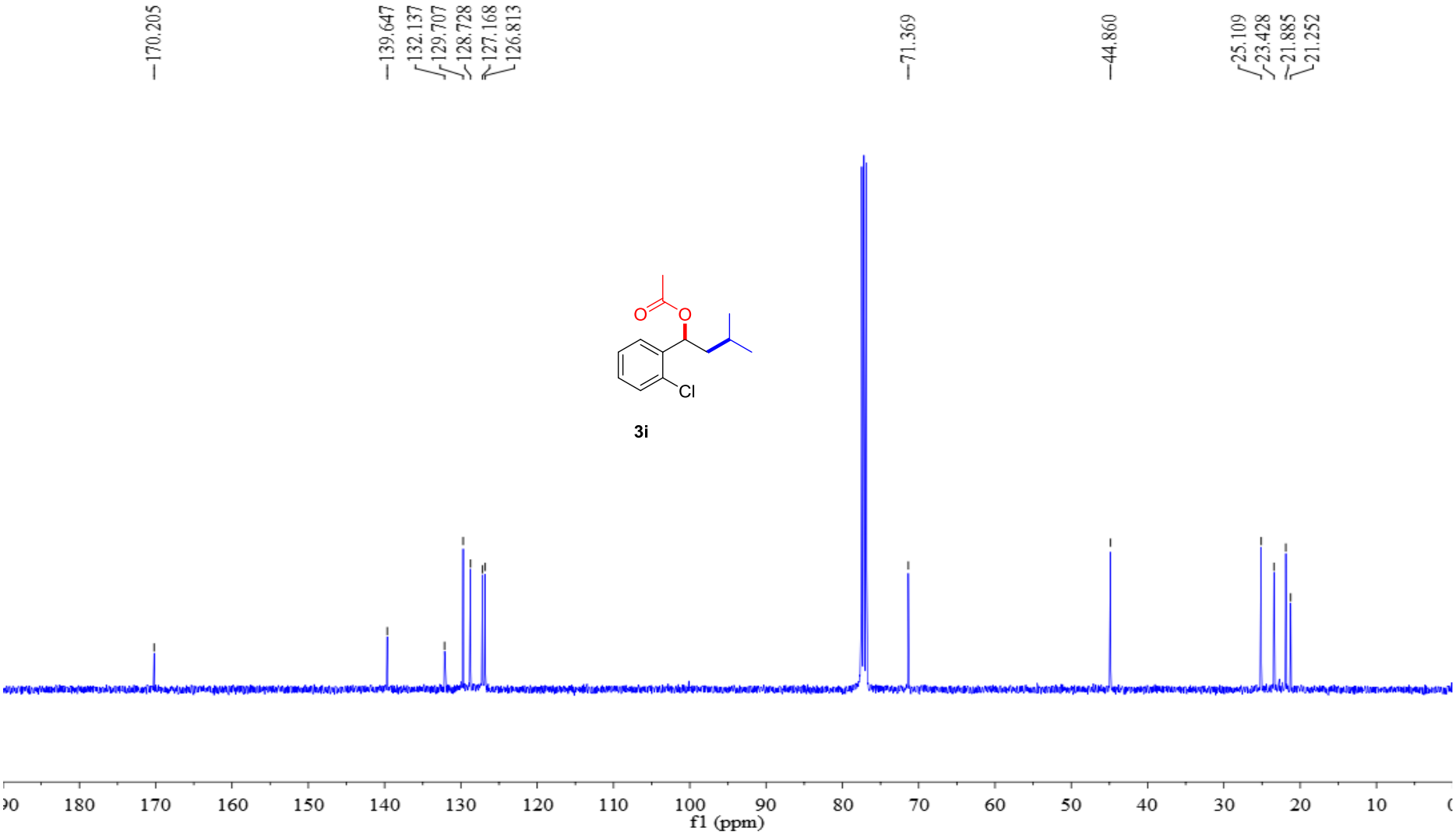
**3i**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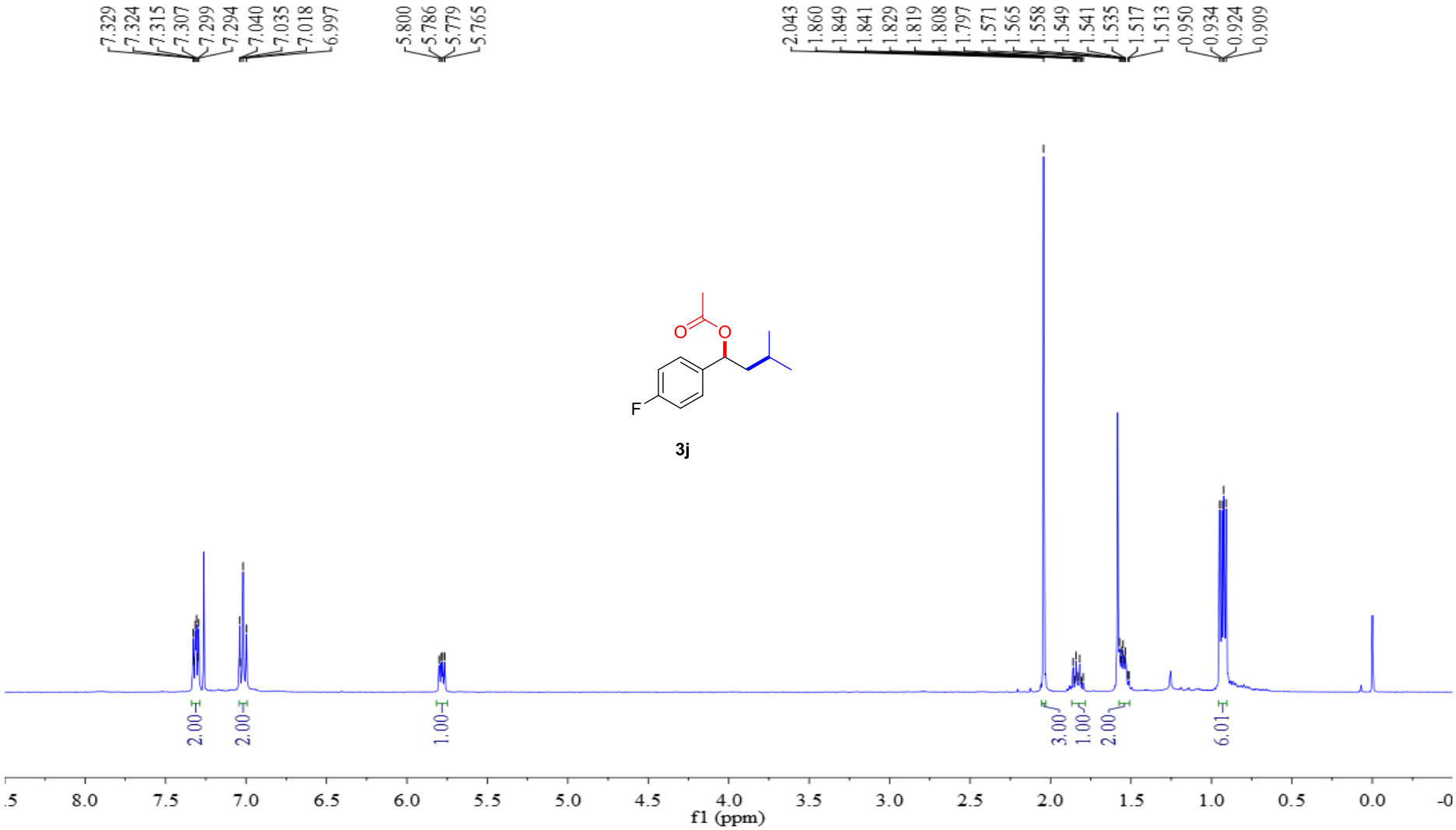
Cl
3i
f1 (ppm)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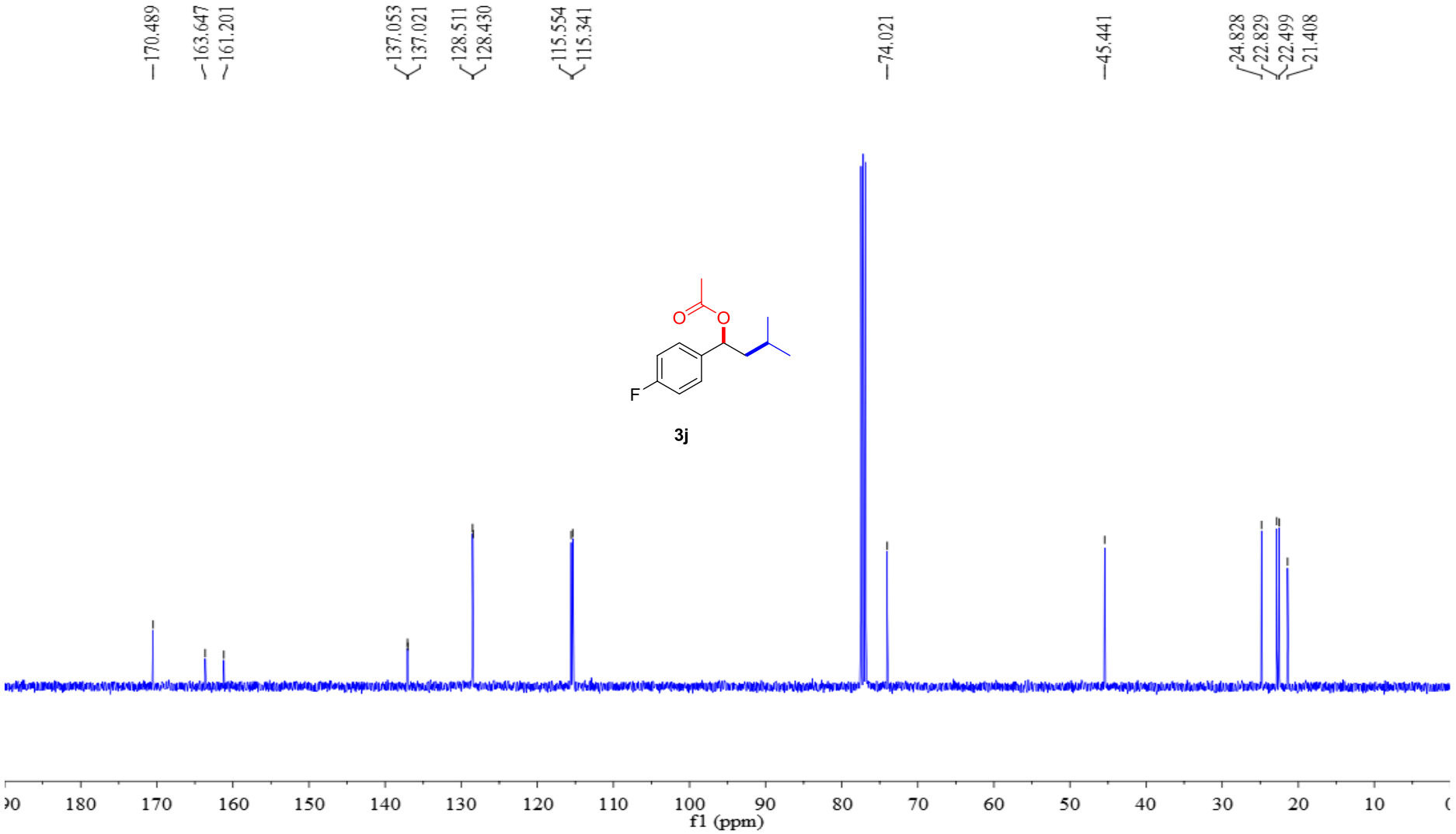
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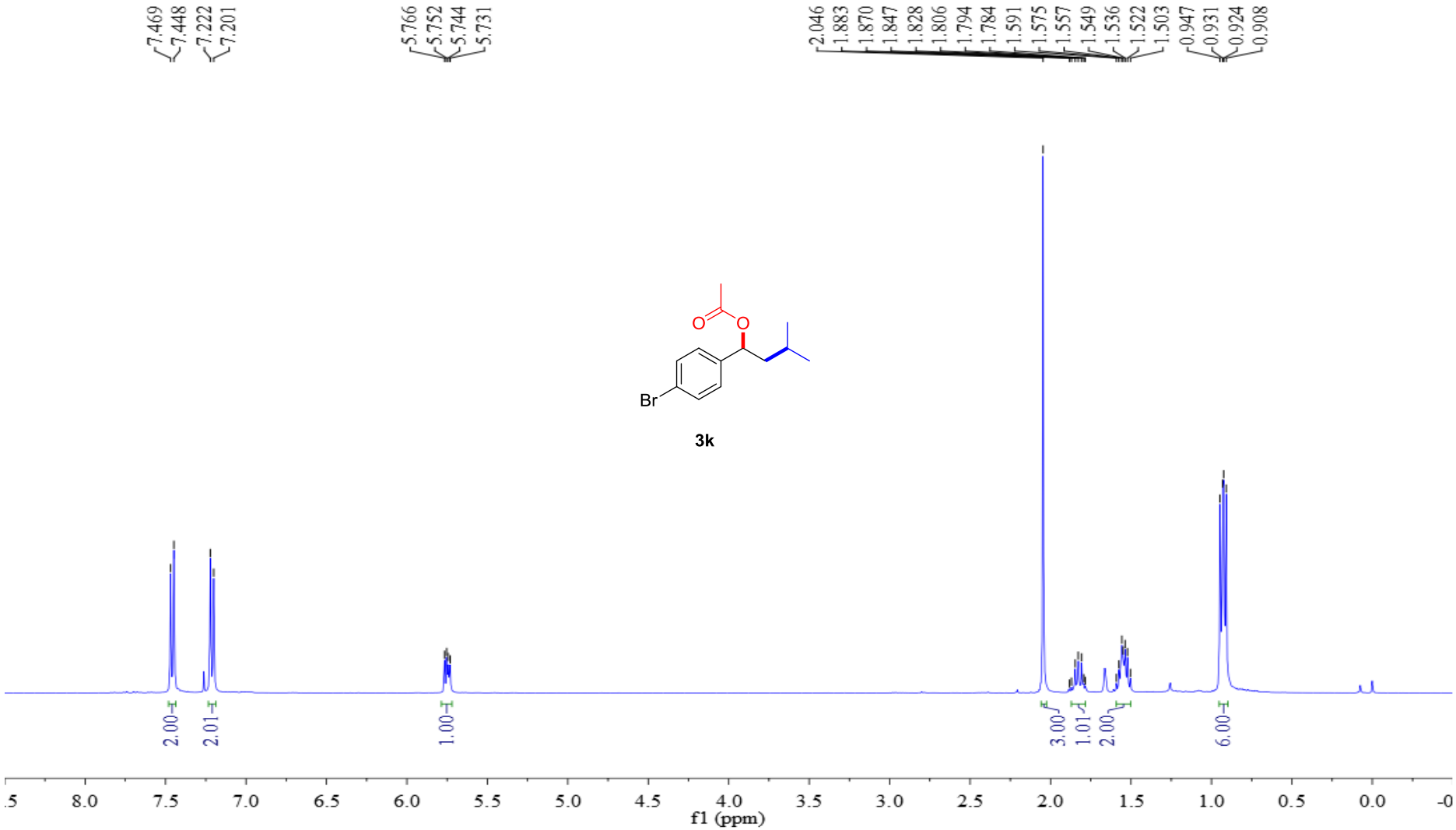
60
50
40
30
20
10
f1 (ppm)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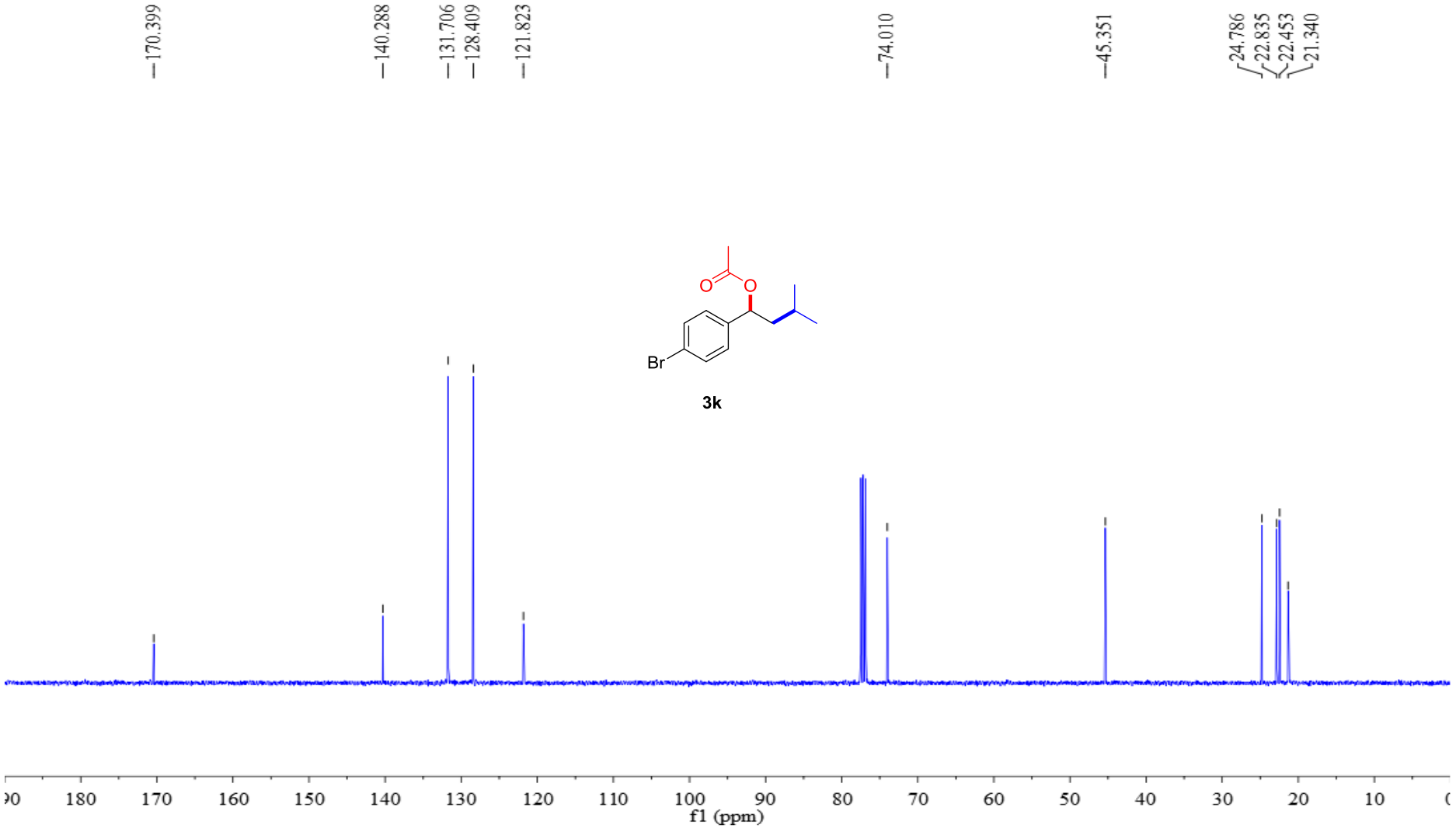
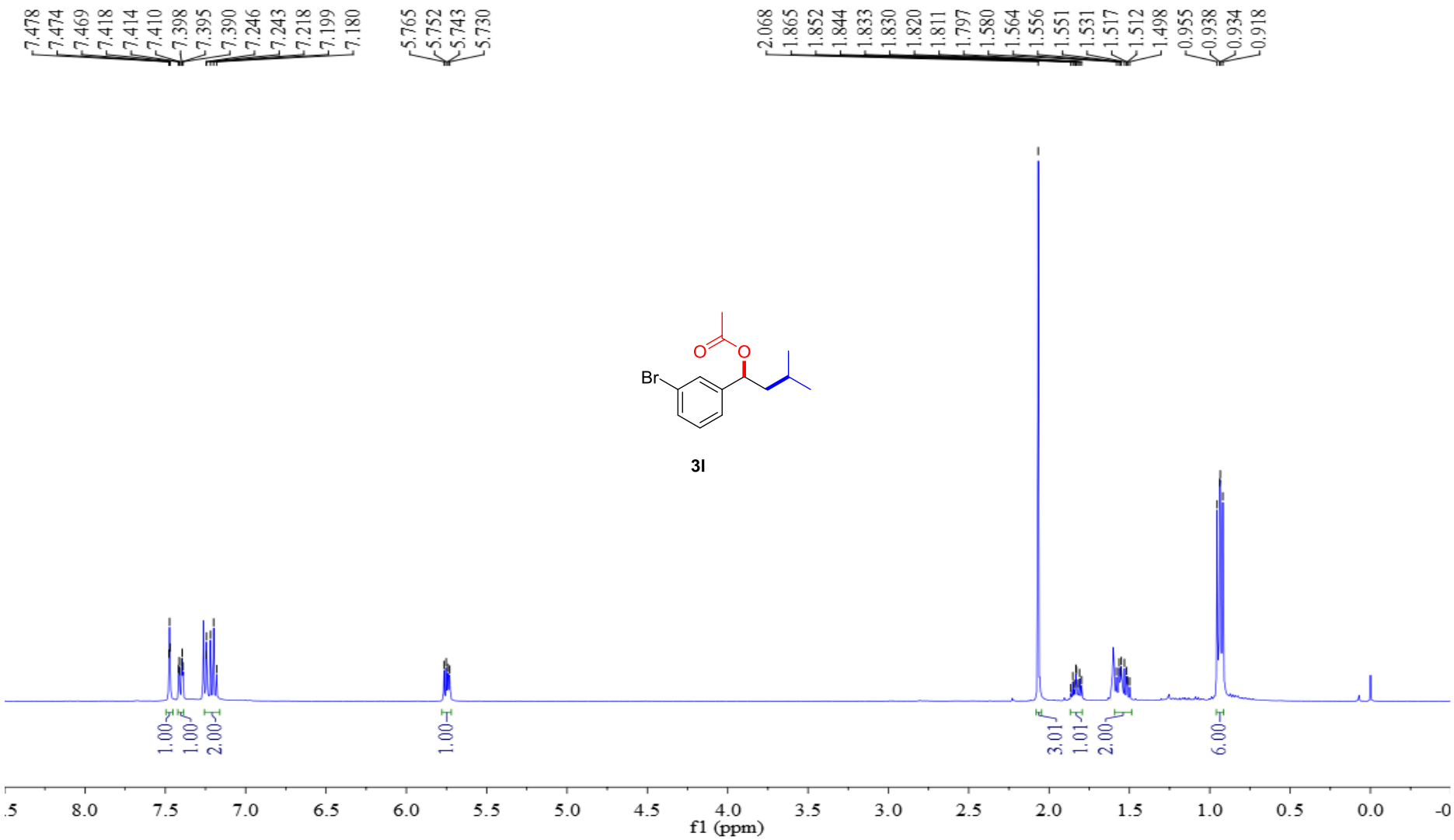
7.448
7.222
7.201
5.766
5.752
5.744
5.731
2.046
1.883
1.870
1.847
1.828
1.806
1.794
1.784
1.591
1.575
1.557
1.549
1.536
1.522
1.503
0.947
0.931
0.924
0.908
O
O
Br
3k
2.00
2.01
1.00
3.00
1.01
2.00
6.00
f1 (ppm)


170.399
140.288
131.706
128.409
121.823
74.010
45.351
24.786
22.835
22.453
21.340
O
O
Br
3k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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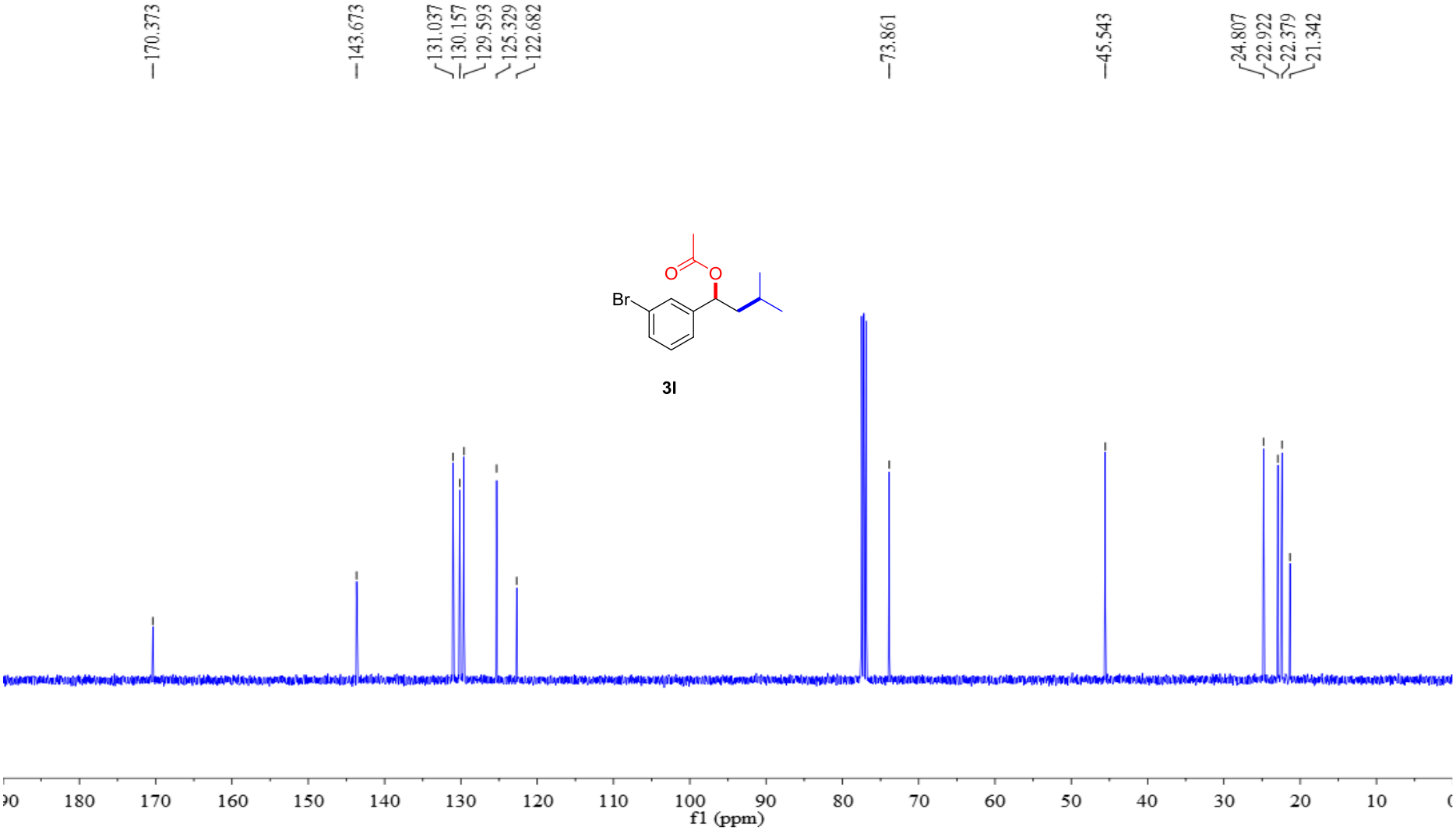
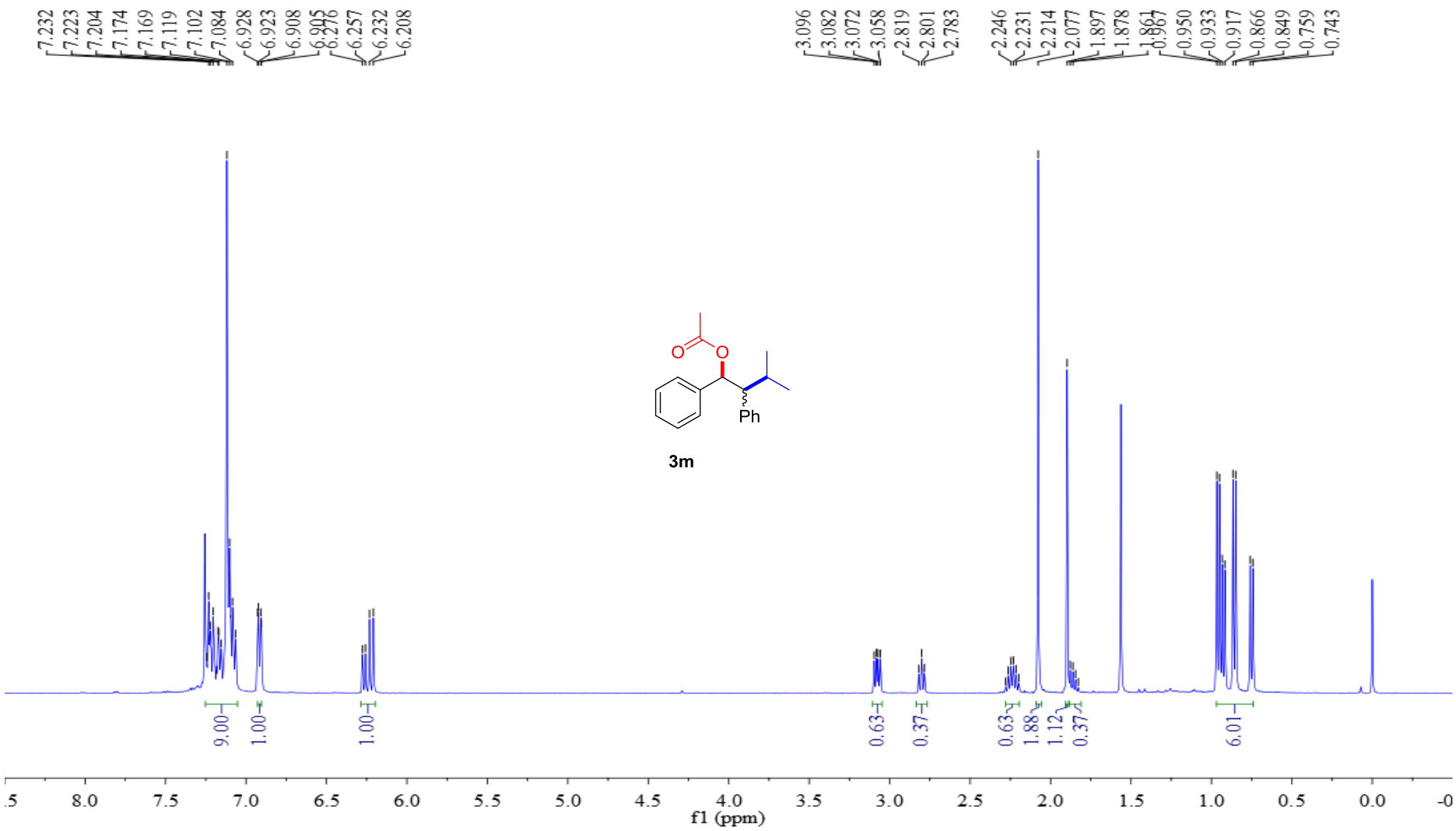
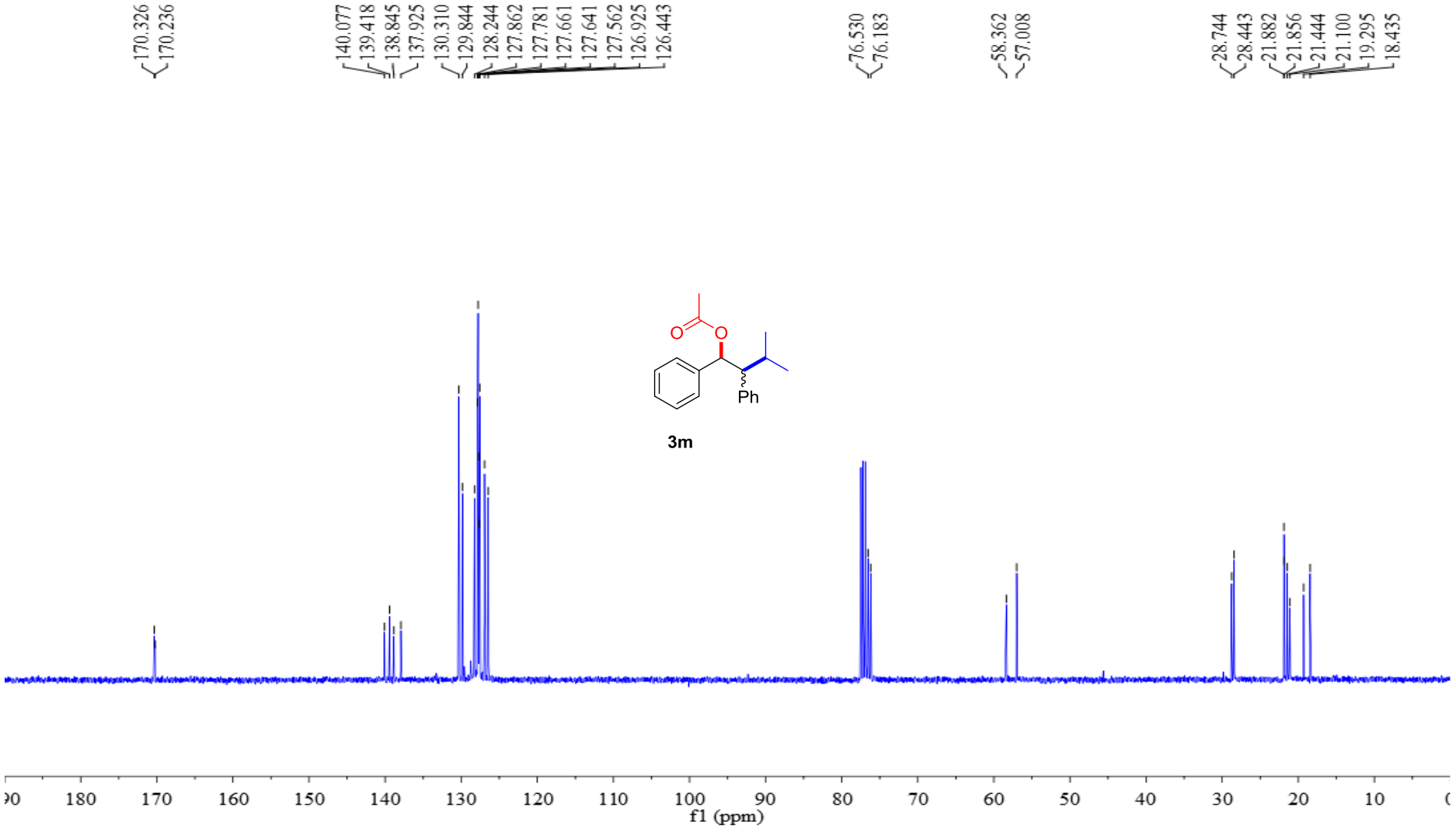
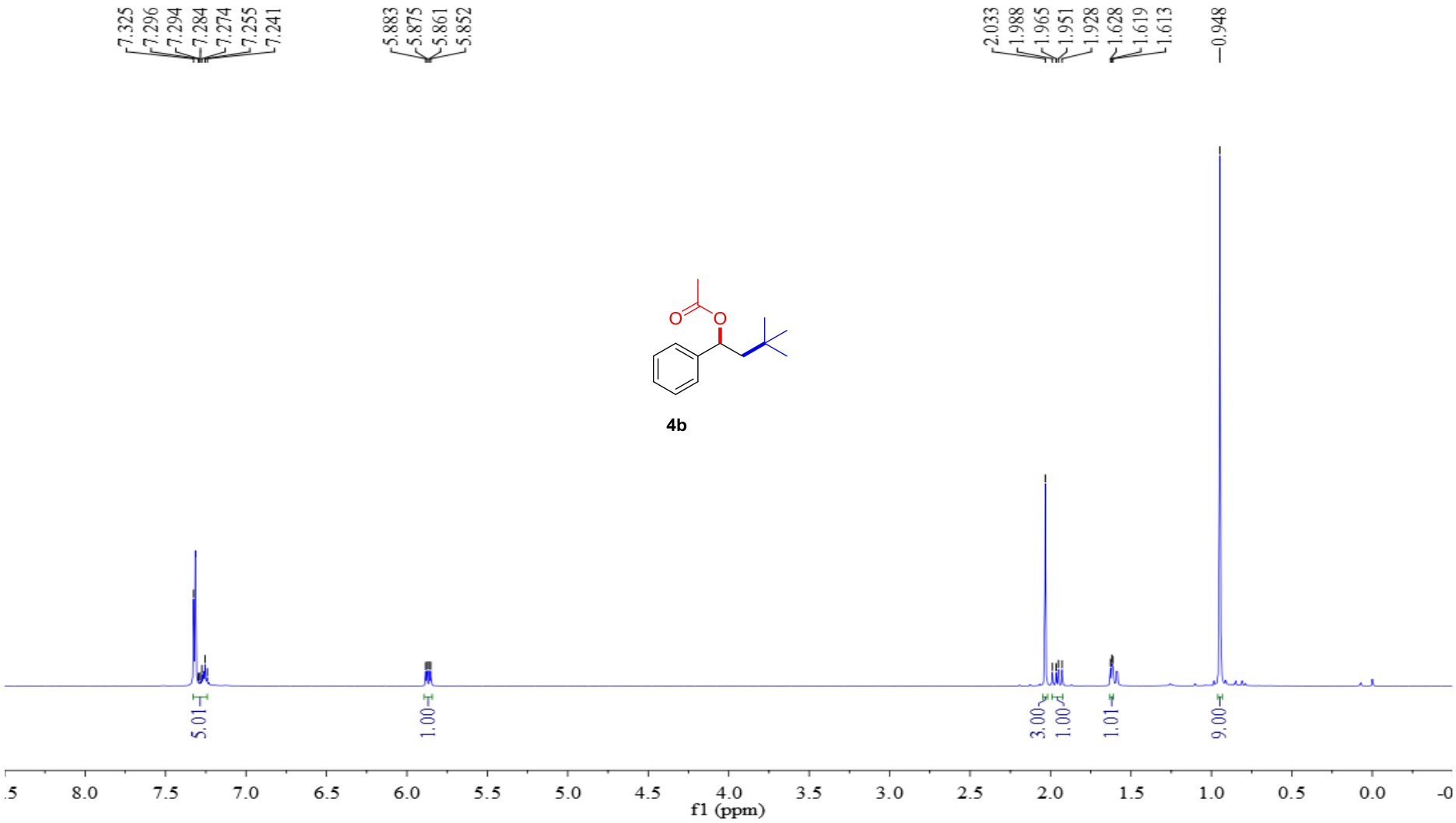
7.474
7.469
7.418
7.414
7.410
7.398
7.395
7.390
7.246
7.243
7.218
7.199
7.180
5.765
5.752
5.743
5.730
2.068
1.865
1.852
1.844
1.833
1.830
1.820
1.811
1.797
1.580
1.564
1.556
1.551
1.531
1.517
1.512
1.498
0.955
0.938
0.934
0.918
Br
O
O
1.00
1.00
2.00
1.00
3.01
1.01
2.00
6.00
f1 (ppm)

**3l**


170.373
143.673
131.037
130.157
129.593
125.329
122.682
73.861
45.543
24.807
22.922
22.379
21.342
Br
O
O
3l
f1 (ppm)


7.232
7.223
7.204
7.174
7.169
7.119
7.102
7.084
6.928
6.923
6.908
6.905
6.276
6.257
6.232
6.208
3.096
3.082
3.072
3.058
2.819
2.801
2.783
2.246
2.231
2.214
2.077
1.897
1.878
1.861
0.967
0.950
0.933
0.917
0.866
0.849
0.759
0.743
O
O
Ph
3m
9.00
1.00
1.00
0.63
0.37
0.63
1.88
1.12
0.37
6.01
f1 (ppm)


170.326
170.236
140.077
139.418
138.845
137.925
130.310
129.844
128.244
127.862
127.781
127.661
127.641
127.562
126.925
126.443
76.530
76.183
58.362
57.008
28.744
28.443
21.882
21.856
21.444
21.100
19.295
18.435
O
O
Ph
3m
f1 (ppm)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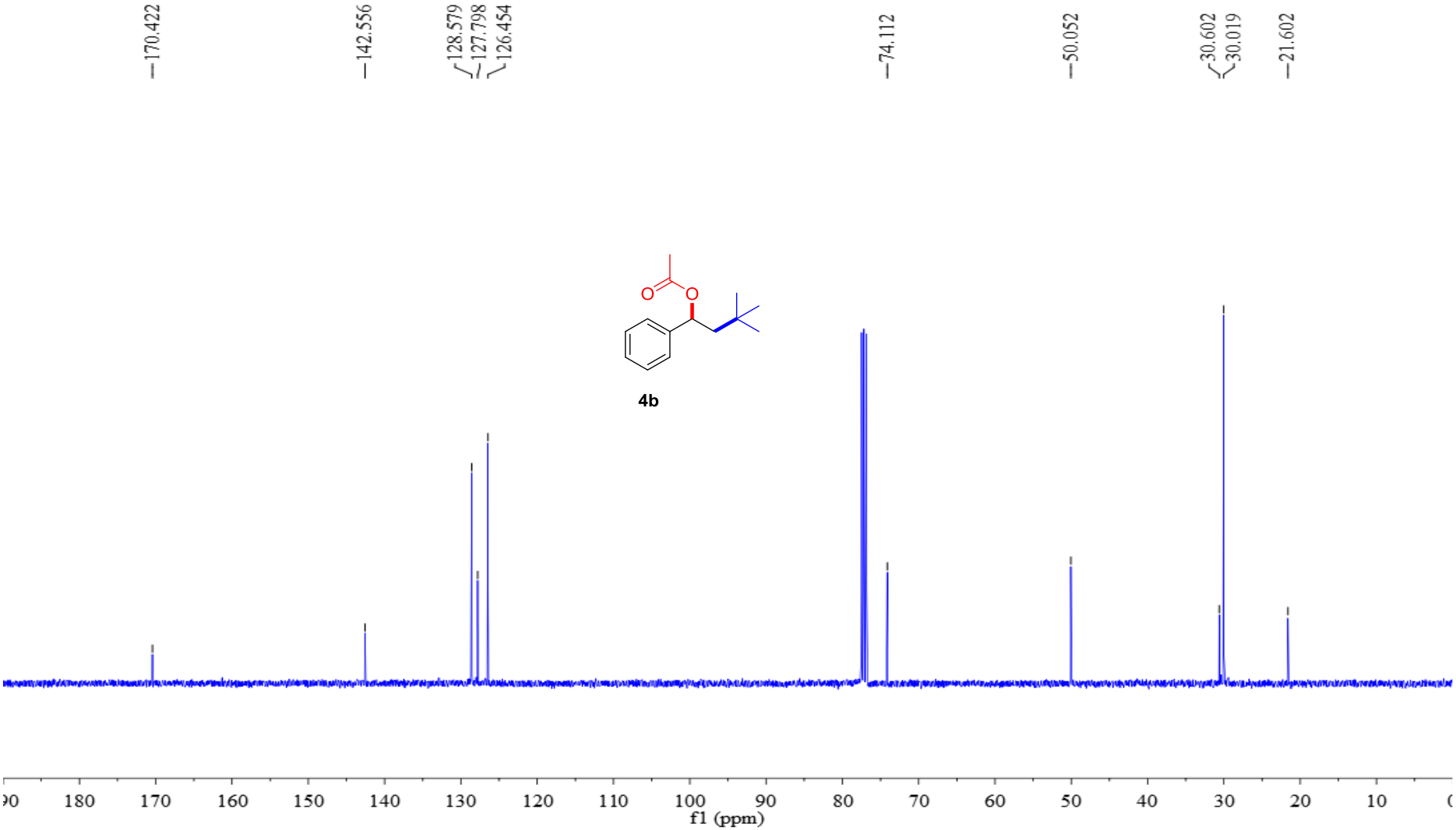
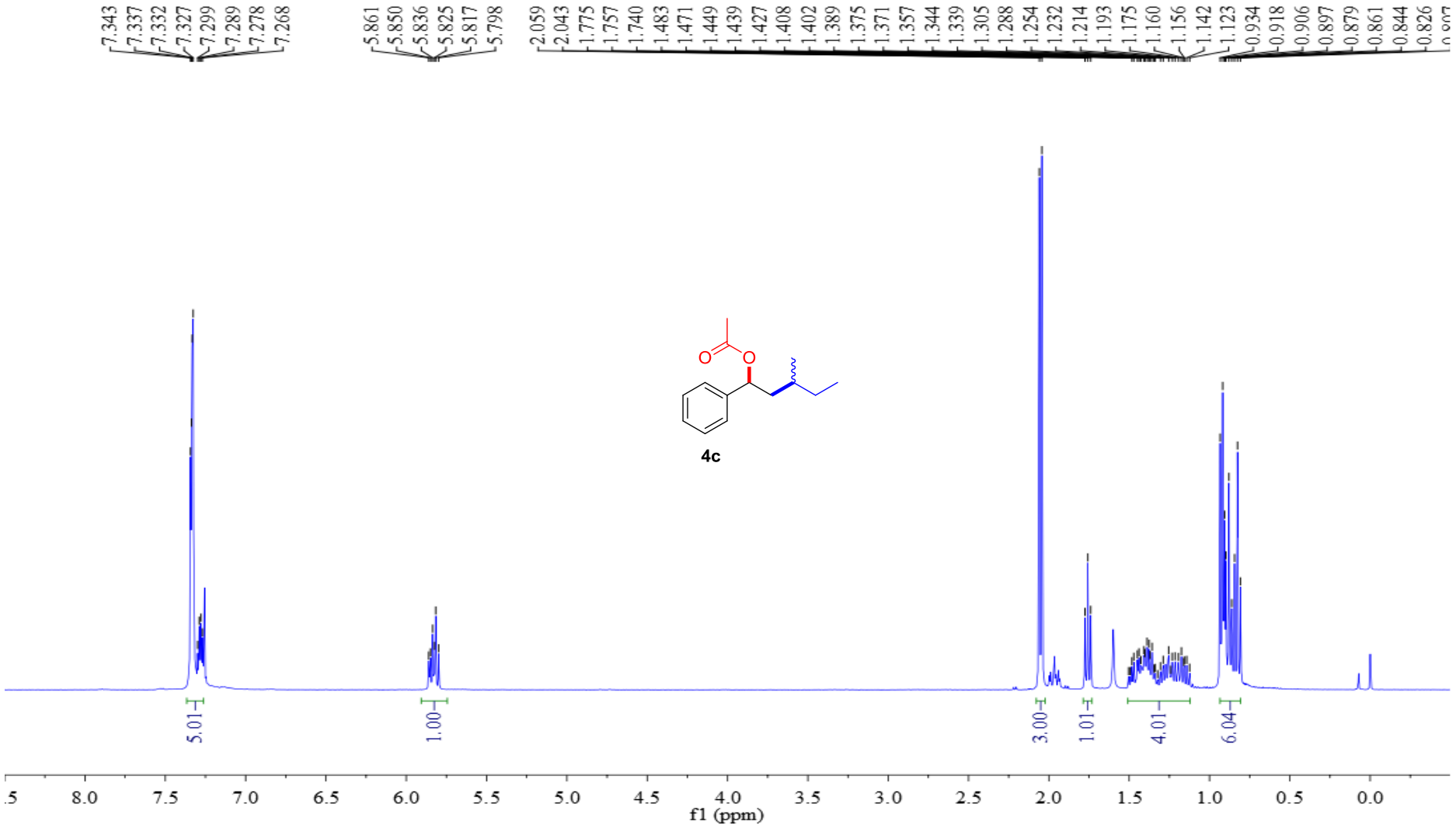
7.296
7.294
7.284
7.274
7.255
7.241
5.883
5.875
5.861
5.852
2.033
1.988
1.965
1.951
1.928
1.628
1.619
1.613
0.948
O
O
5.01
1.00
3.00
1.00
1.01
9.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

**4b**


170.422
142.556
128.579
127.798
126.454
74.112
50.052
30.602
30.019
21.602
O
O
4b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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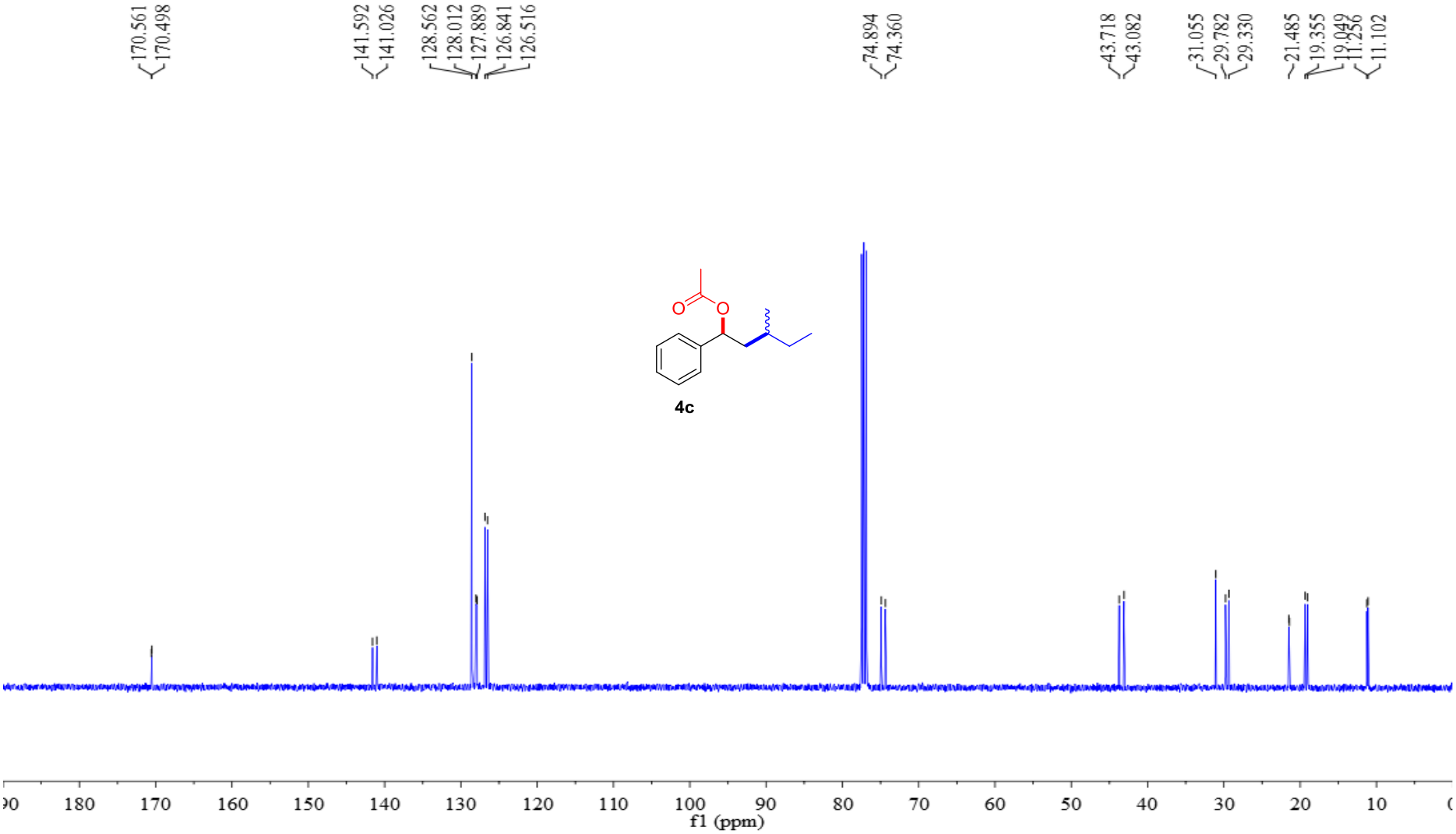
7.337
7.332
7.327
7.299
7.289
7.278
7.268
5.861
5.850
5.836
5.825
5.817
5.798
2.059
2.043
1.775
1.757
1.740
1.483
1.471
1.449
1.439
1.427
1.408
1.402
1.389
1.375
1.371
1.357
1.344
1.339
1.305
1.288
1.254
1.232
1.214
1.193
1.175
1.160
1.156
1.142
1.123
0.934
0.918
0.906
0.897
0.879
0.861
0.844
0.826
O
O
4c
5.01
1.00
3.00
1.01
4.01
6.04
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
f1 (ppm)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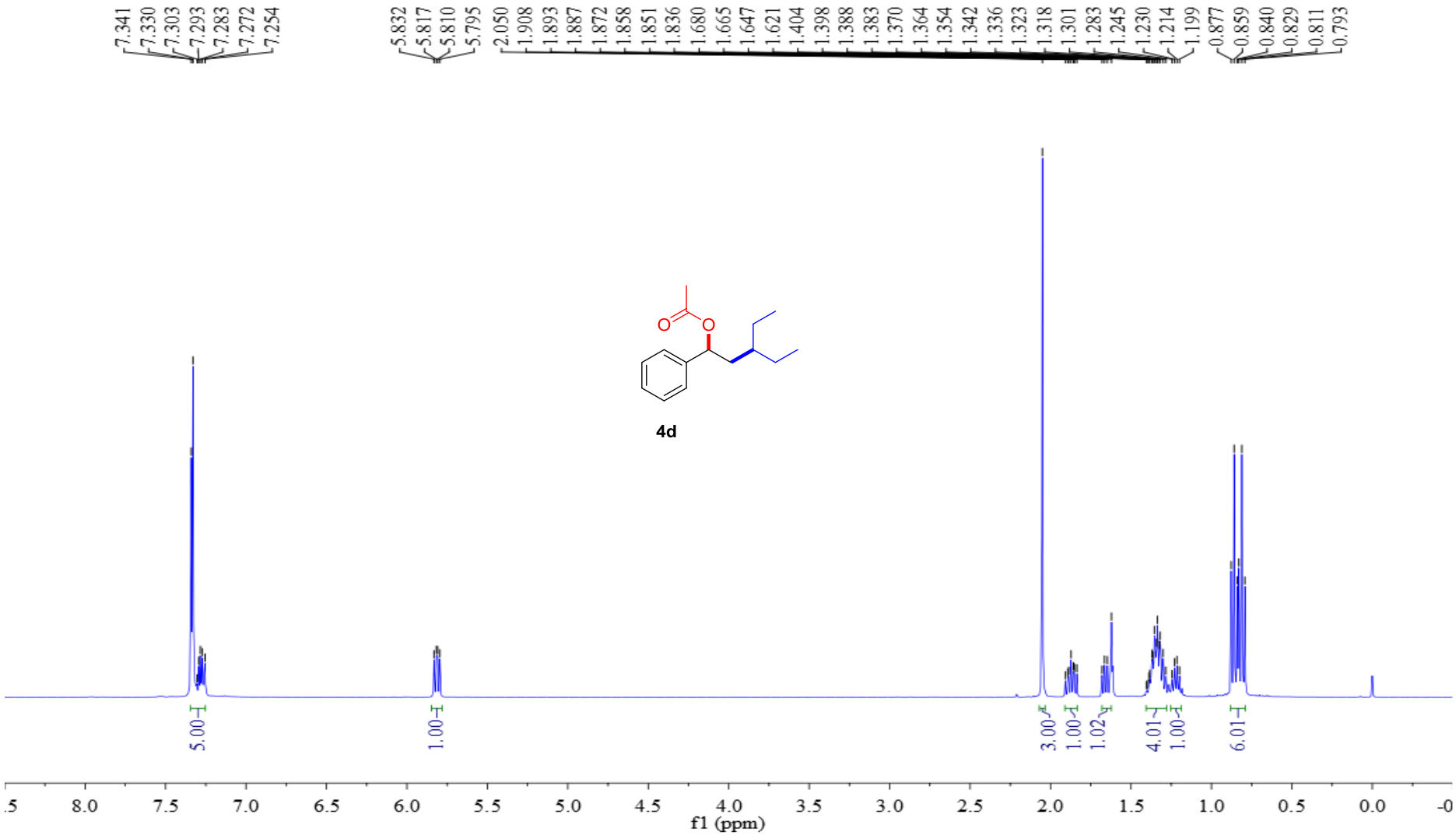
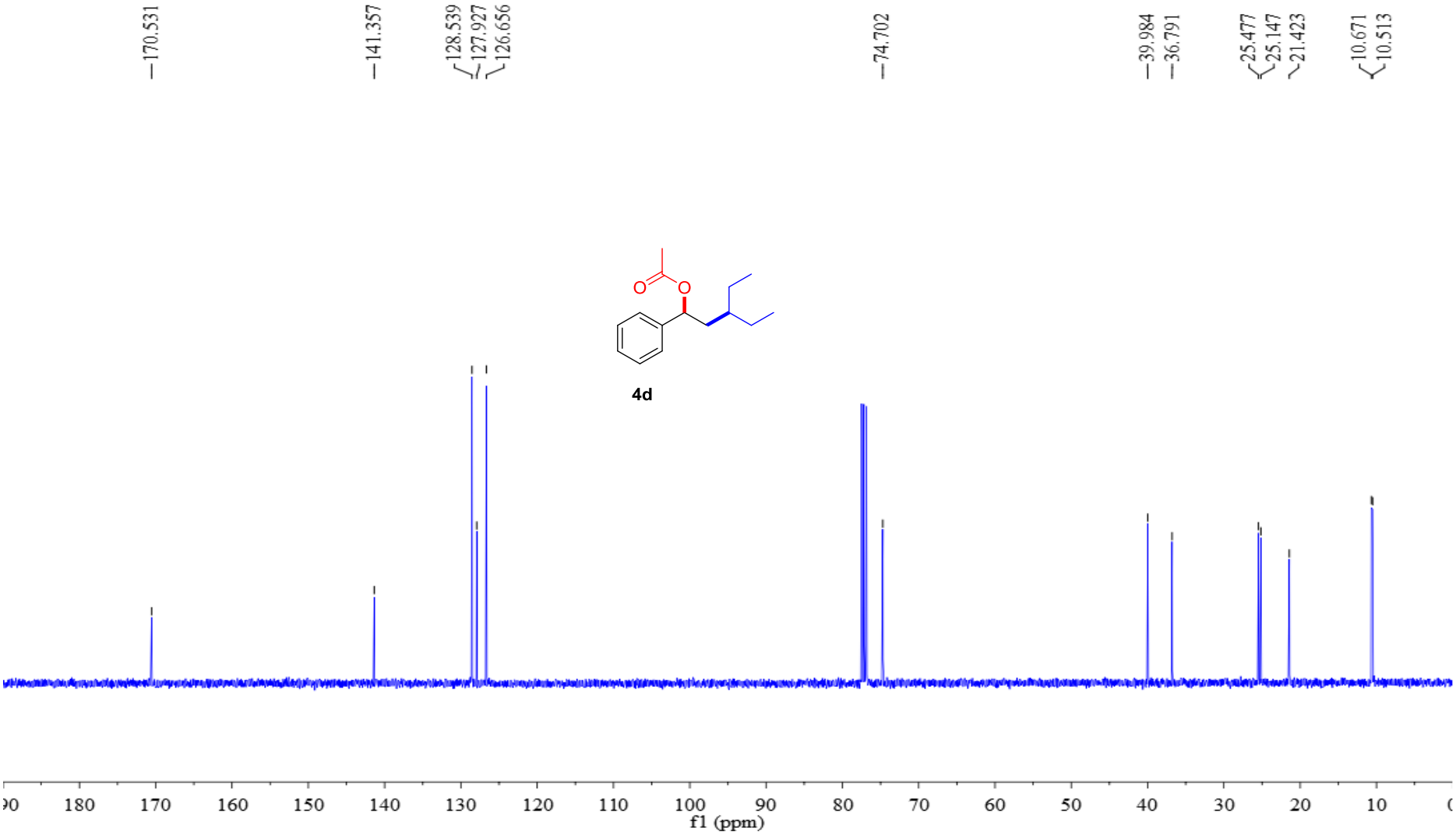
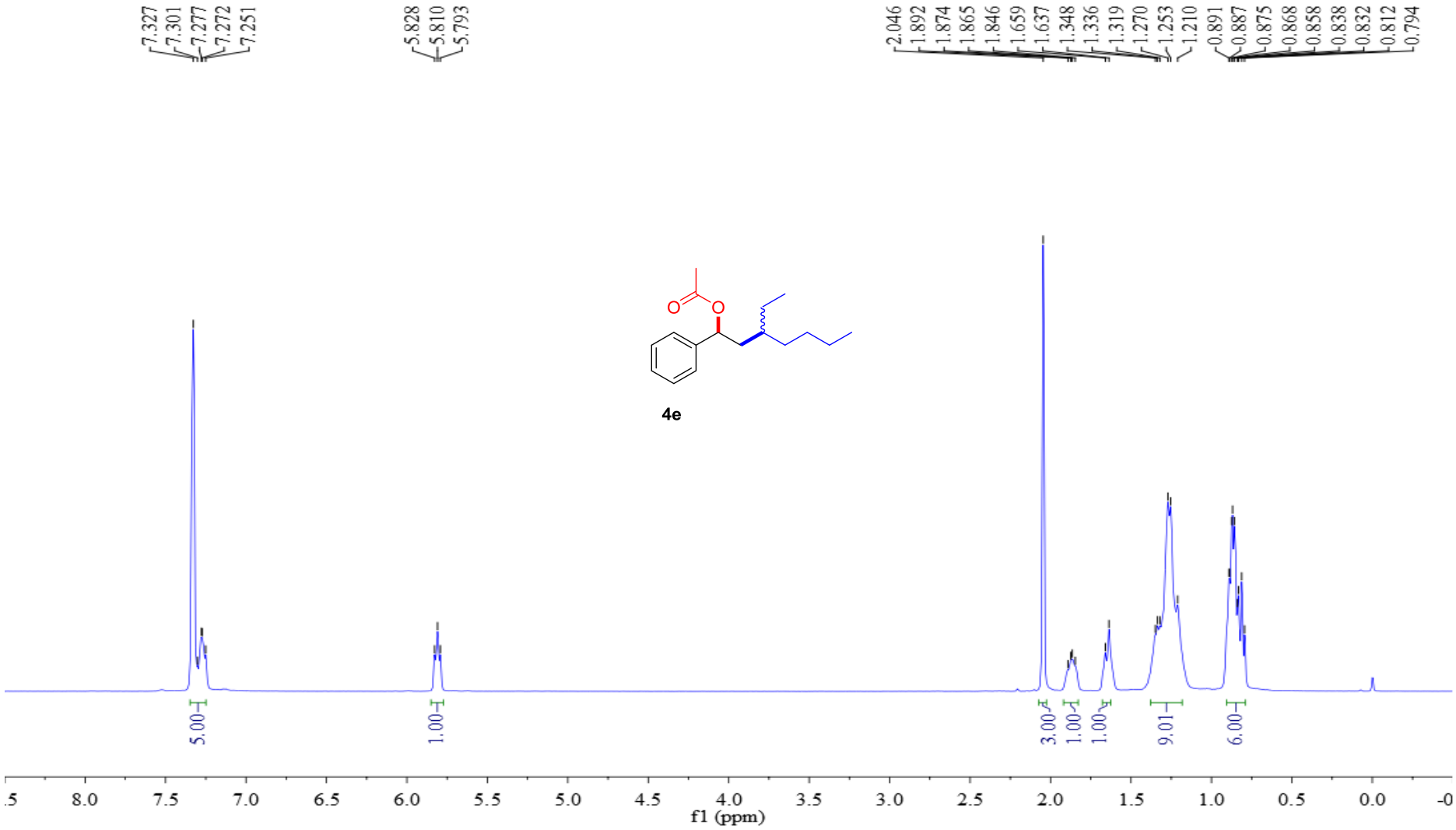
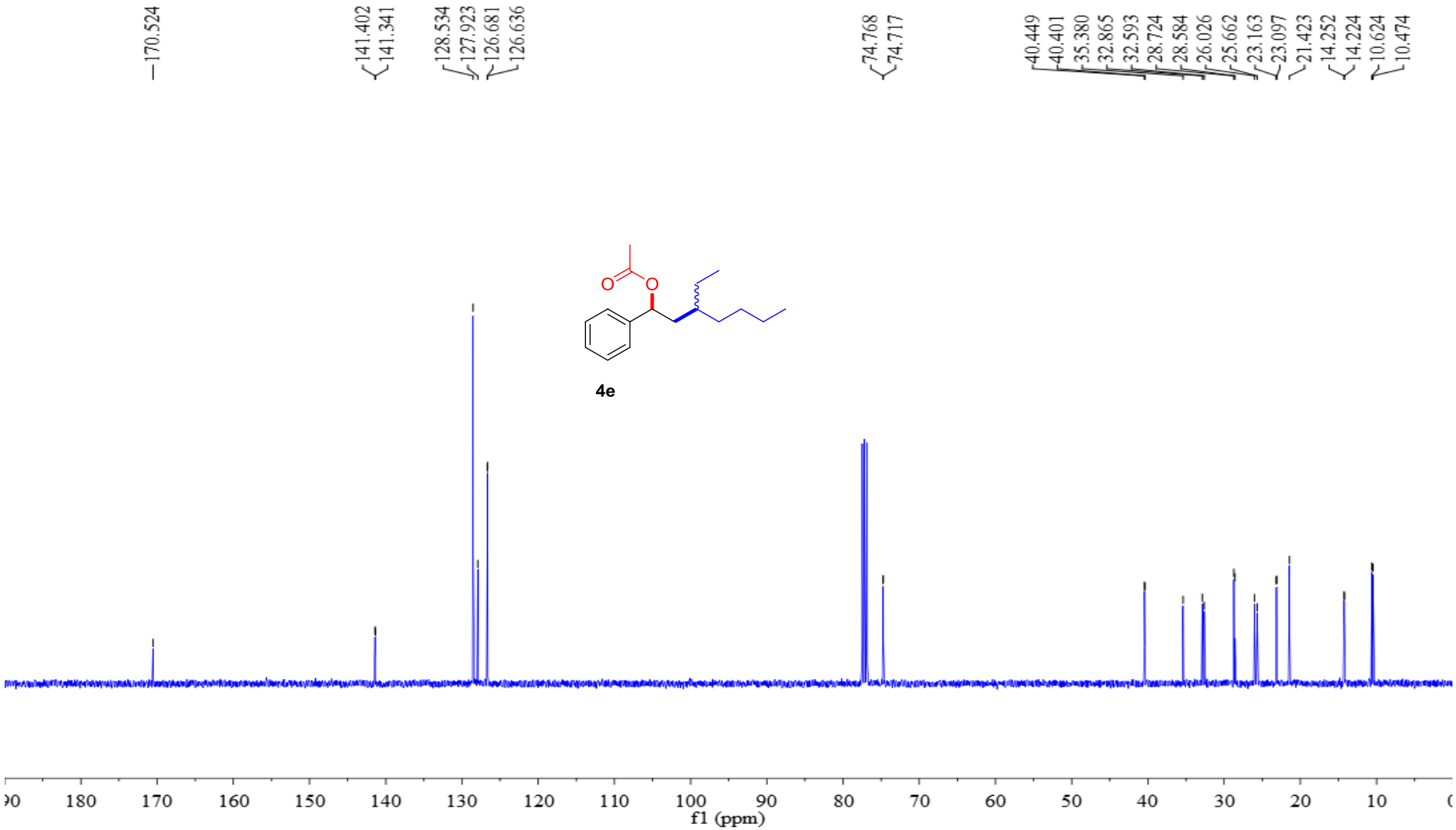
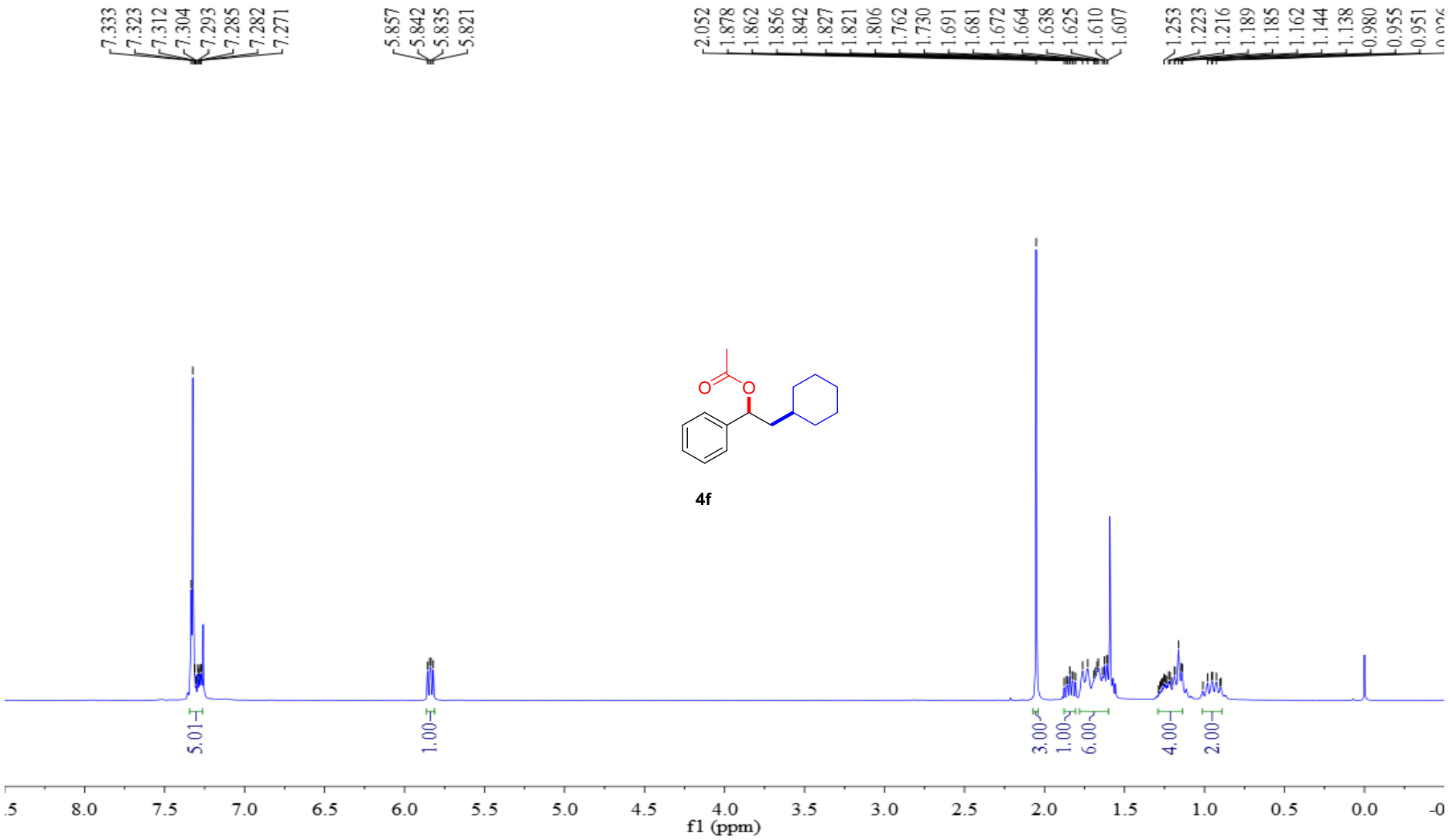
170.498
141.592
141.026
128.562
128.012
127.889
126.841
126.516
74.894
74.360
43.718
43.082
31.055
29.782
29.330
21.485
19.355
19.049
11.256
11.102
4c
f1 (ppm)


7.341
7.330
7.303
7.293
7.283
7.272
7.254
5.832
5.817
5.810
5.795
2.050
1.908
1.893
1.887
1.872
1.858
1.851
1.836
1.680
1.665
1.647
1.621
1.404
1.398
1.388
1.383
1.370
1.364
1.354
1.342
1.336
1.323
1.318
1.301
1.283
1.245
1.230
1.214
1.199
0.877
0.859
0.840
0.829
0.811
0.793
O
O
4d
5.00
1.00
3.00
1.00
1.02
4.01
1.00
6.01
f1 (ppm)

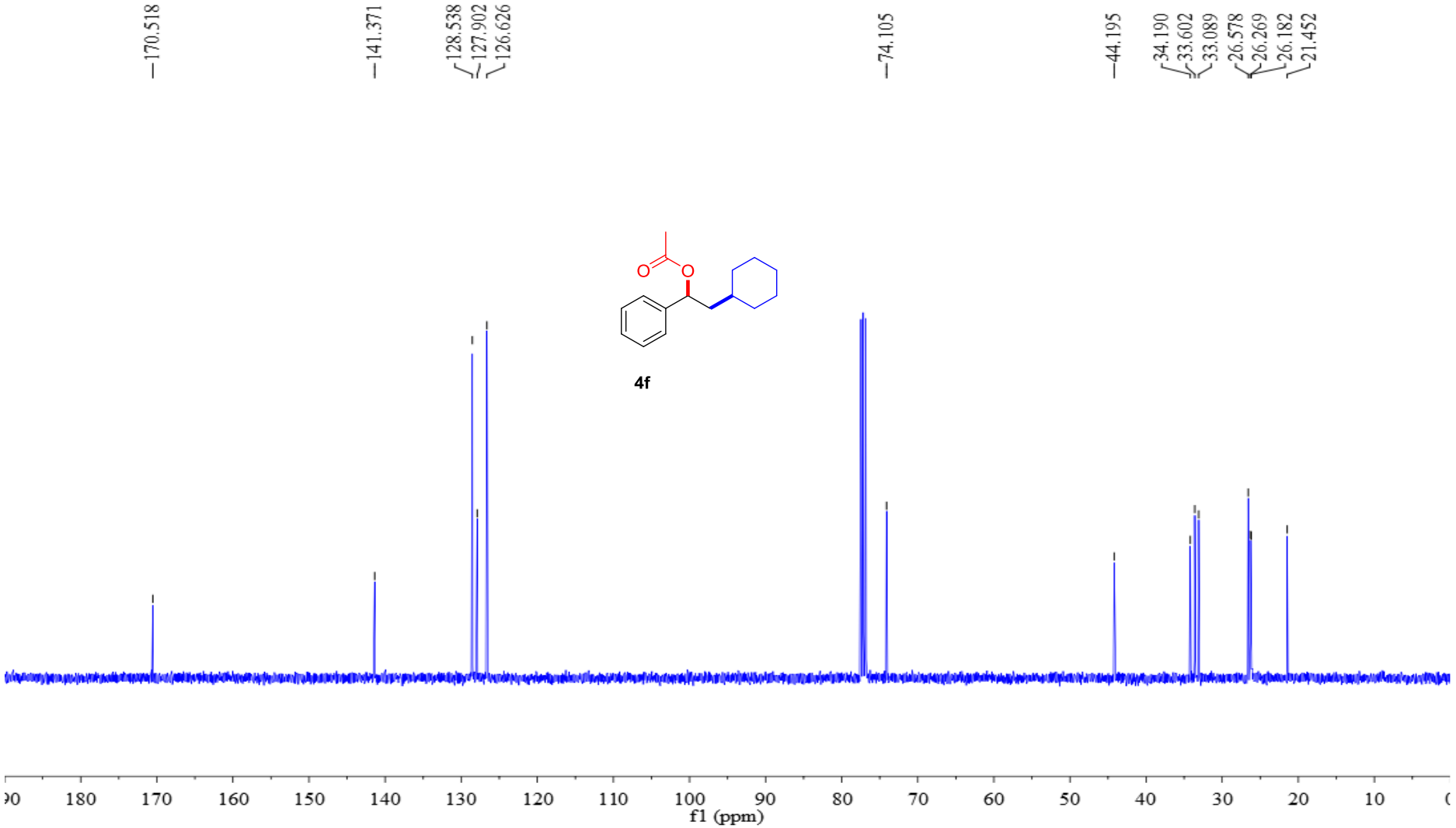

170.531
141.357
128.539
127.927
126.656
74.702
39.984
36.791
25.477
25.147
21.423
10.671
10.513
O
O
4d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

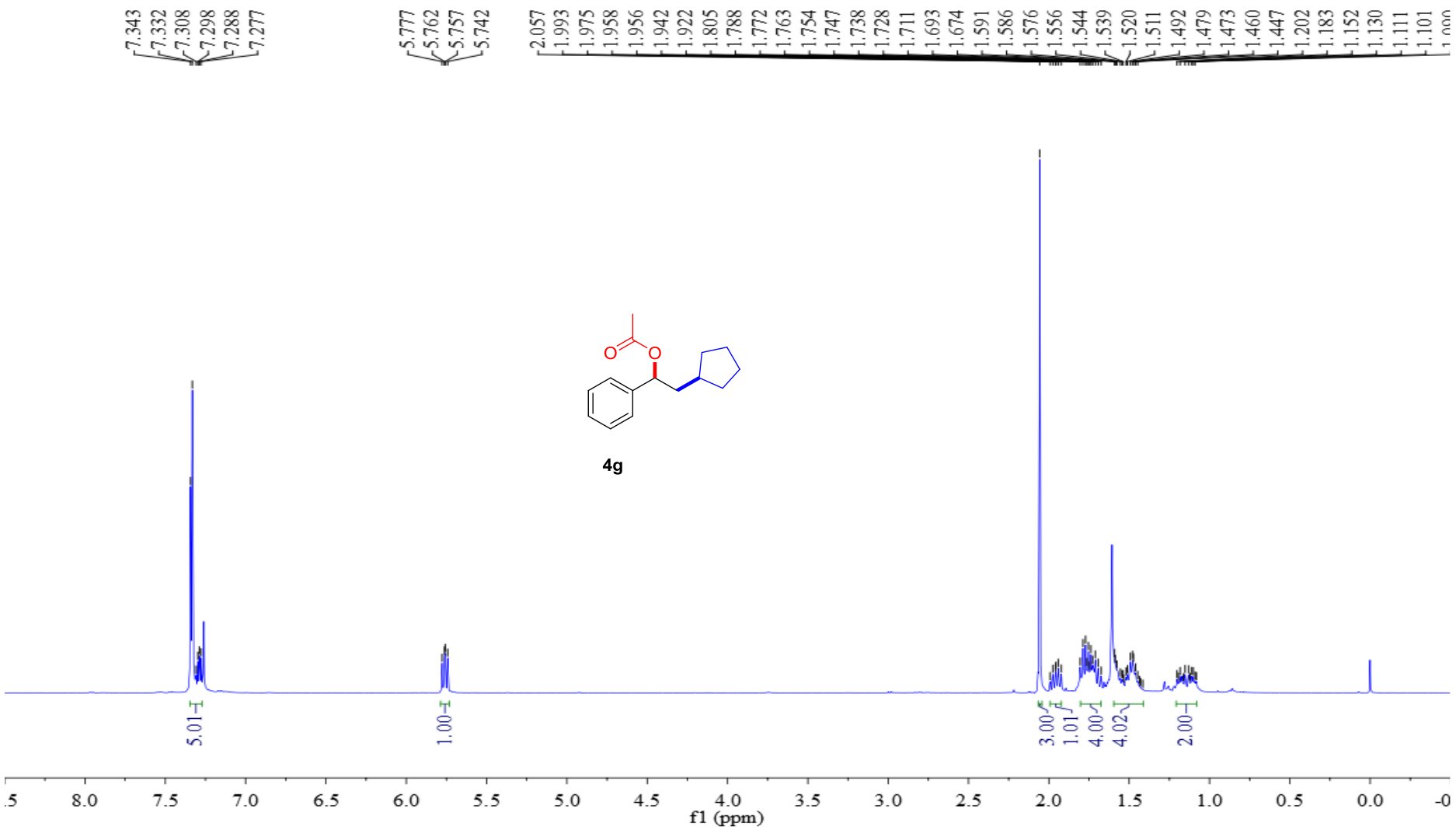

7.327
7.301
7.277
7.272
7.251
5.828
5.810
5.793
2.046
1.892
1.874
1.865
1.846
1.659
1.637
1.348
1.336
1.319
1.270
1.253
1.210
0.891
0.887
0.875
0.868
0.858
0.838
0.832
0.812
0.794
O
O
4e
5.00
1.00
3.00
1.00
1.00
9.01
6.00
f1 (ppm)

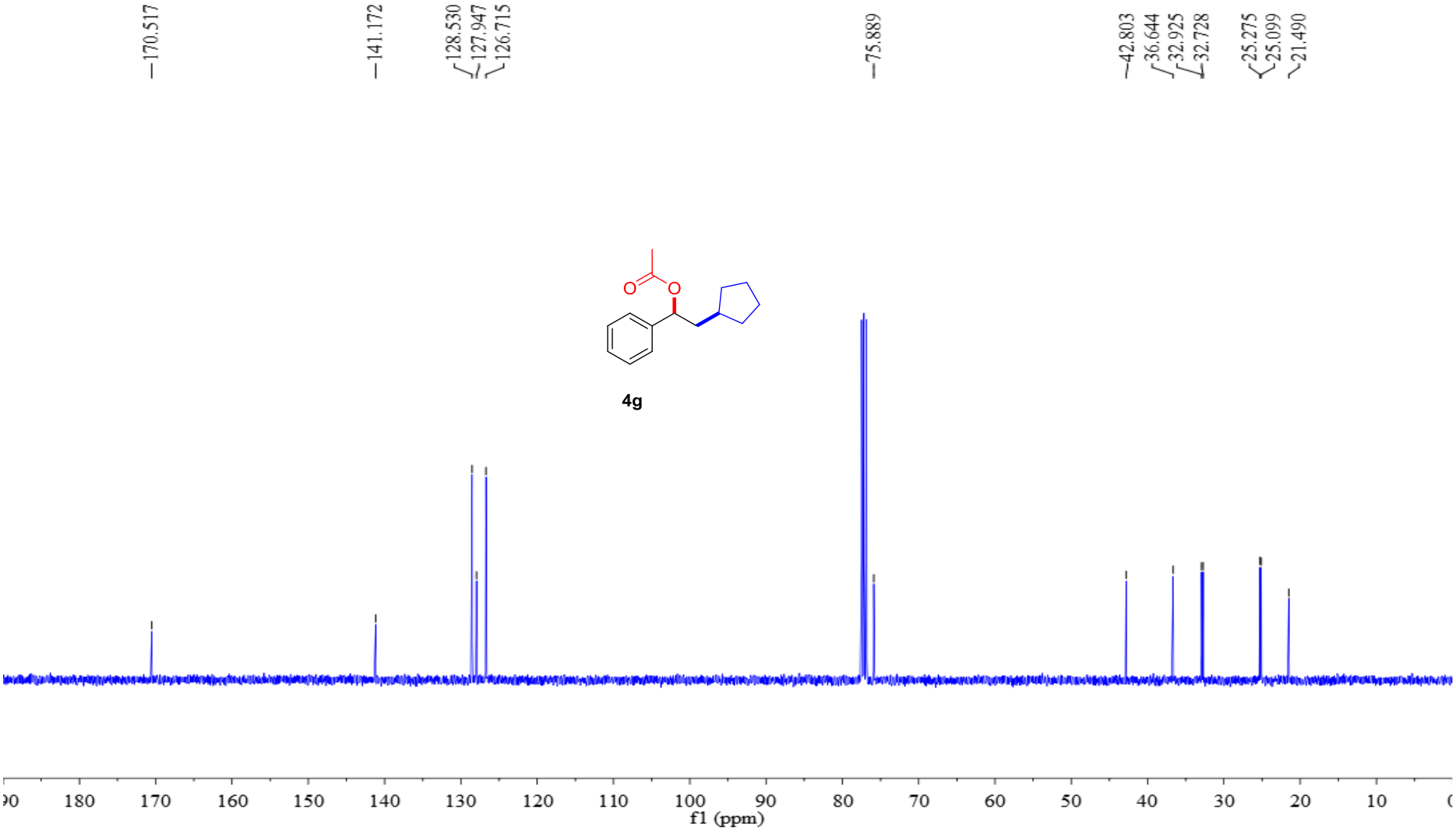

170.524
141.402
141.341
128.534
127.923
126.681
126.636
74.768
74.717
40.449
40.401
35.380
32.865
32.593
28.724
28.584
26.026
25.662
23.163
23.097
21.423
14.252
14.224
10.624
10.474
4e
f1 (ppm)

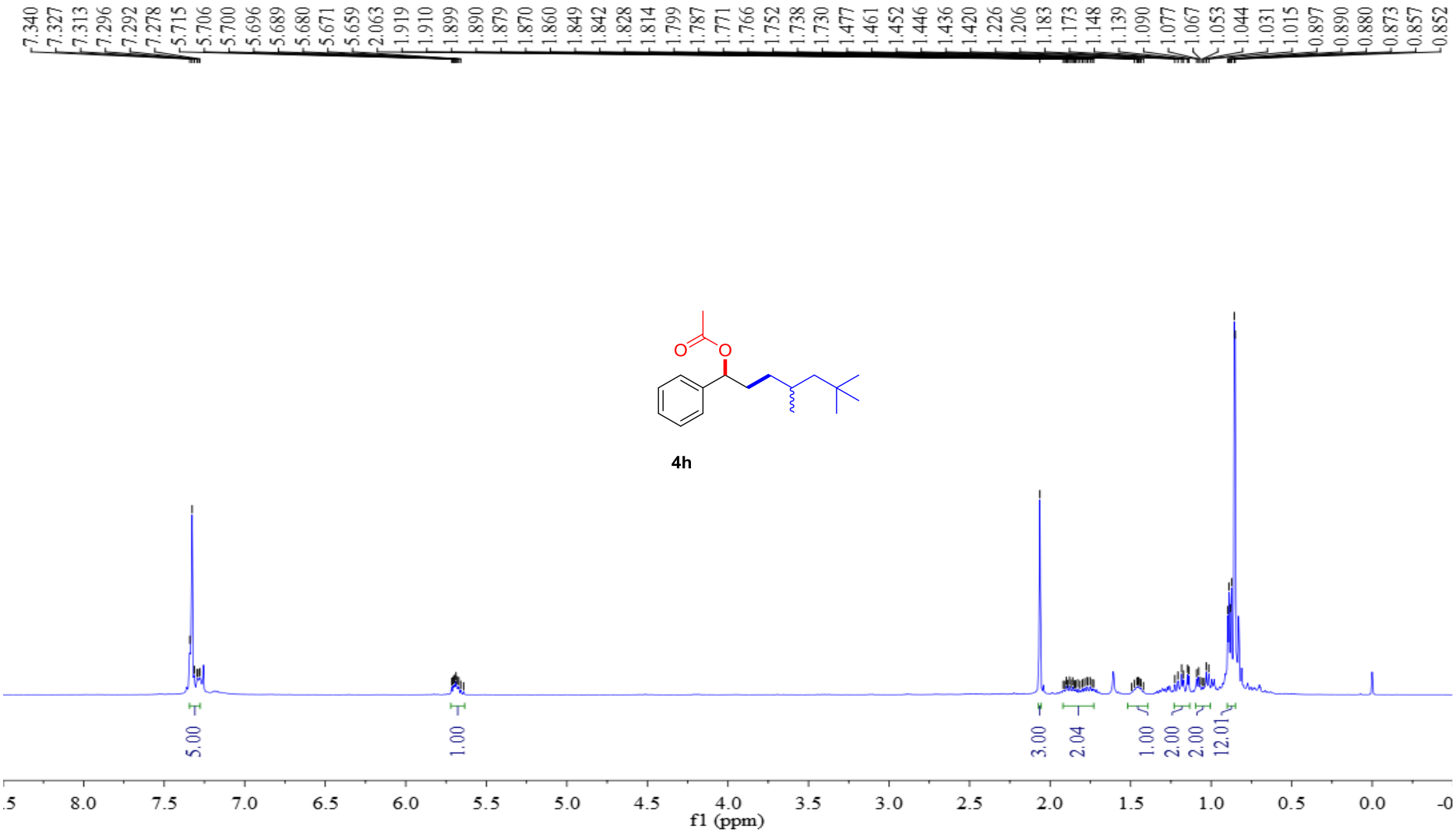

7.333
7.323
7.312
7.304
7.293
7.285
7.282
7.271
5.857
5.842
5.835
5.821
2.052
1.878
1.862
1.856
1.842
1.827
1.821
1.806
1.762
1.730
1.691
1.681
1.672
1.664
1.638
1.625
1.610
1.607
1.253
1.223
1.216
1.189
1.185
1.162
1.144
1.138
0.980
0.955
0.951
5.01
1.00
3.00
1.00
6.00
4.00
2.00
f1 (ppm)

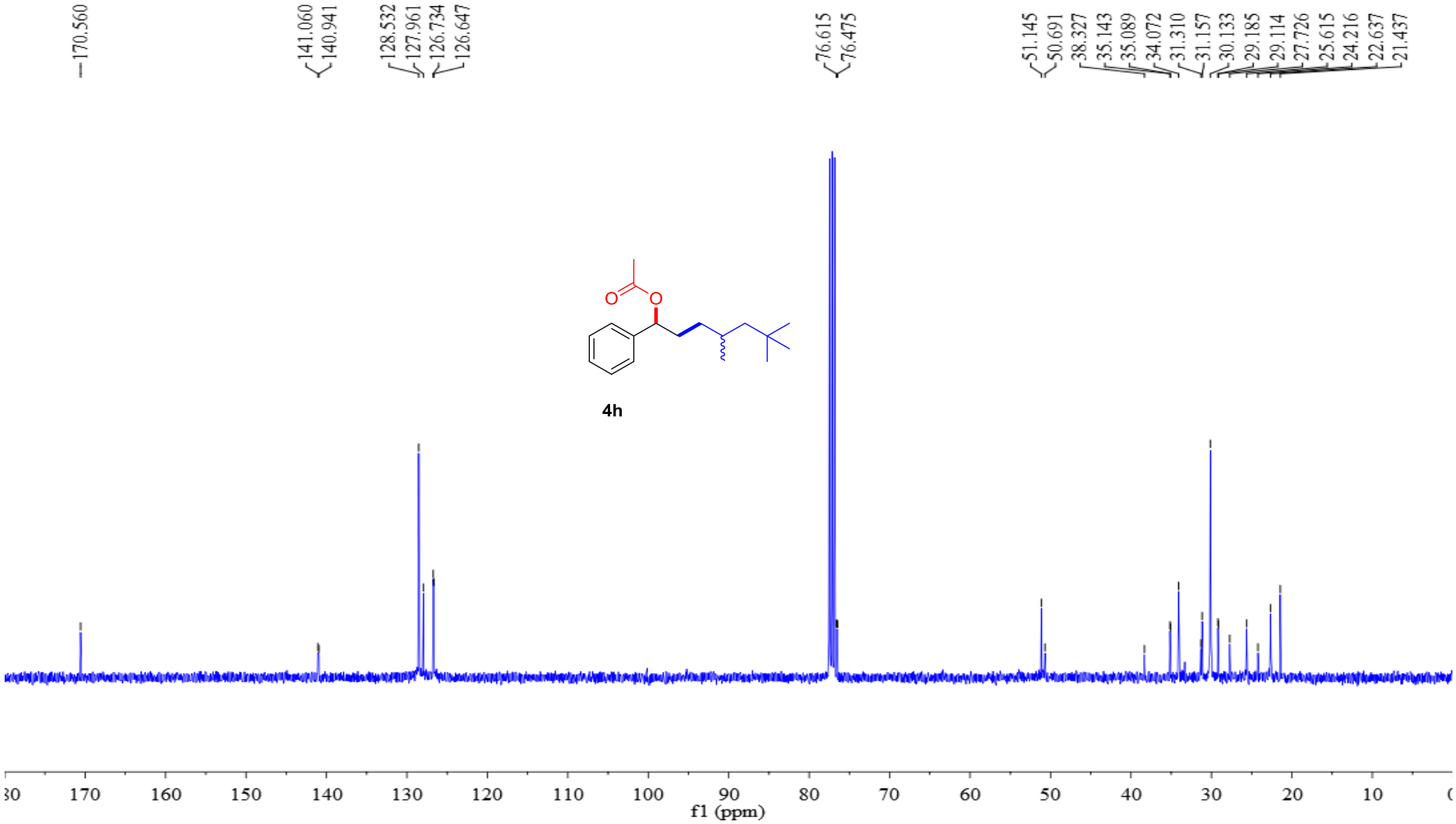
**4f**


170.518
141.371
128.538
127.902
126.626
74.105
44.195
34.190
33.602
33.089
26.578
26.269
26.182
21.452
O
O
4f
f1 (ppm)


7.343
7.332
7.308
7.298
7.288
7.277
5.777
5.762
5.757
5.742
2.057
1.993
1.975
1.958
1.956
1.942
1.922
1.805
1.788
1.772
1.763
1.754
1.747
1.738
1.728
1.711
1.693
1.674
1.591
1.586
1.576
1.556
1.544
1.539
1.520
1.511
1.492
1.479
1.473
1.460
1.447
1.202
1.183
1.152
1.130
1.111
1.101
O
O
4g
5.01
1.00
3.00
1.01
4.00
4.02
2.00
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
f1 (ppm)


170.517
141.172
128.530
127.947
126.715
75.889
42.803
36.644
32.925
32.728
25.275
25.099
21.490
4g
f1 (ppm)


7.340
7.327
7.313
7.296
7.292
7.278
5.715
5.706
5.700
5.696
5.689
5.680
5.671
5.659
2.063
1.919
1.910
1.899
1.890
1.879
1.870
1.860
1.849
1.842
1.828
1.814
1.799
1.787
1.771
1.766
1.752
1.738
1.730
1.477
1.461
1.452
1.446
1.436
1.420
1.226
1.206
1.183
1.173
1.148
1.139
1.090
1.077
1.067
1.053
1.044
1.031
1.015
0.897
0.890
0.880
0.873
0.857
0.852
O
O
4h
5.00
1.00
3.00
2.04
1.00
2.00
2.00
12.01
f1 (ppm)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141.060
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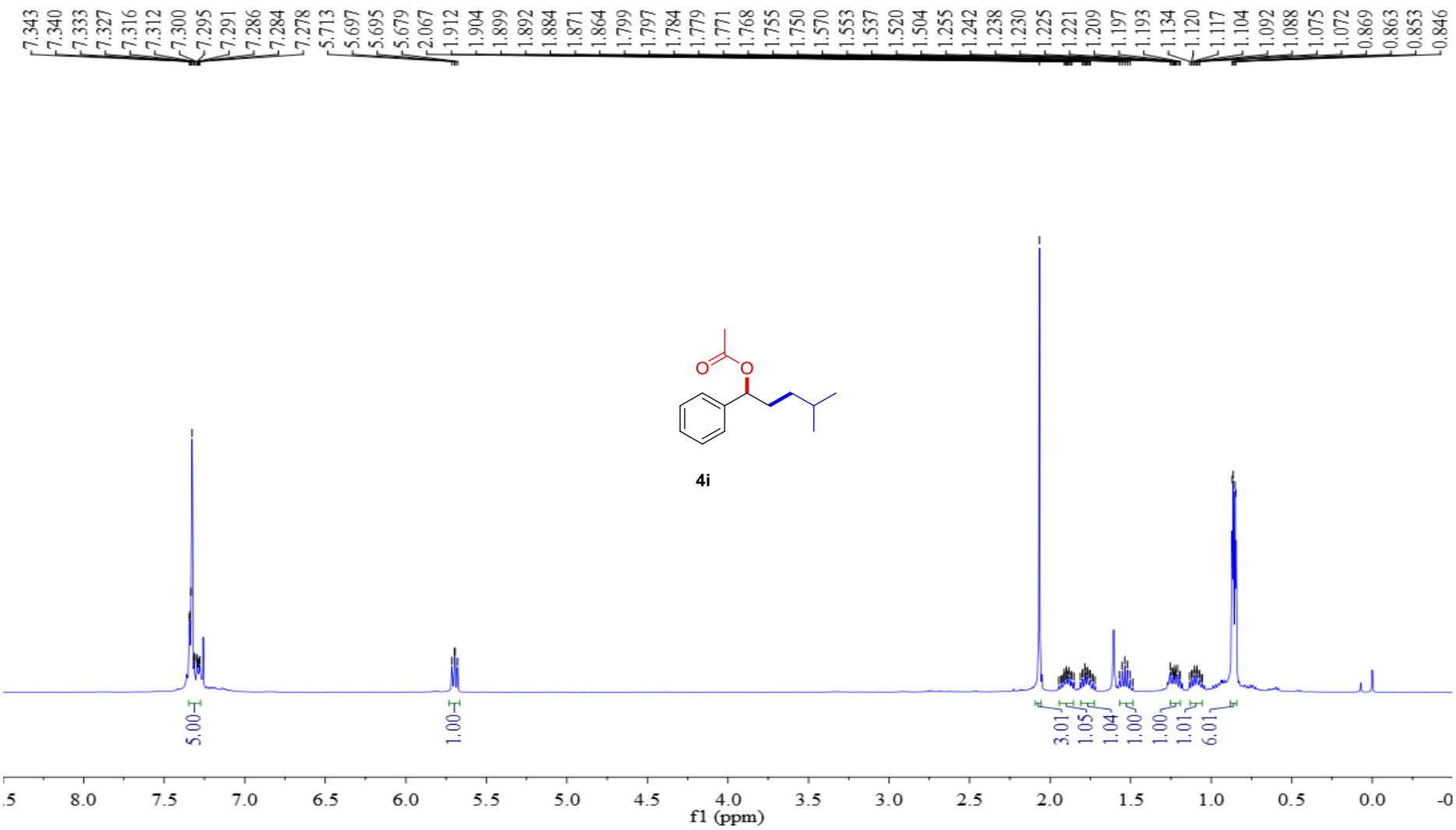
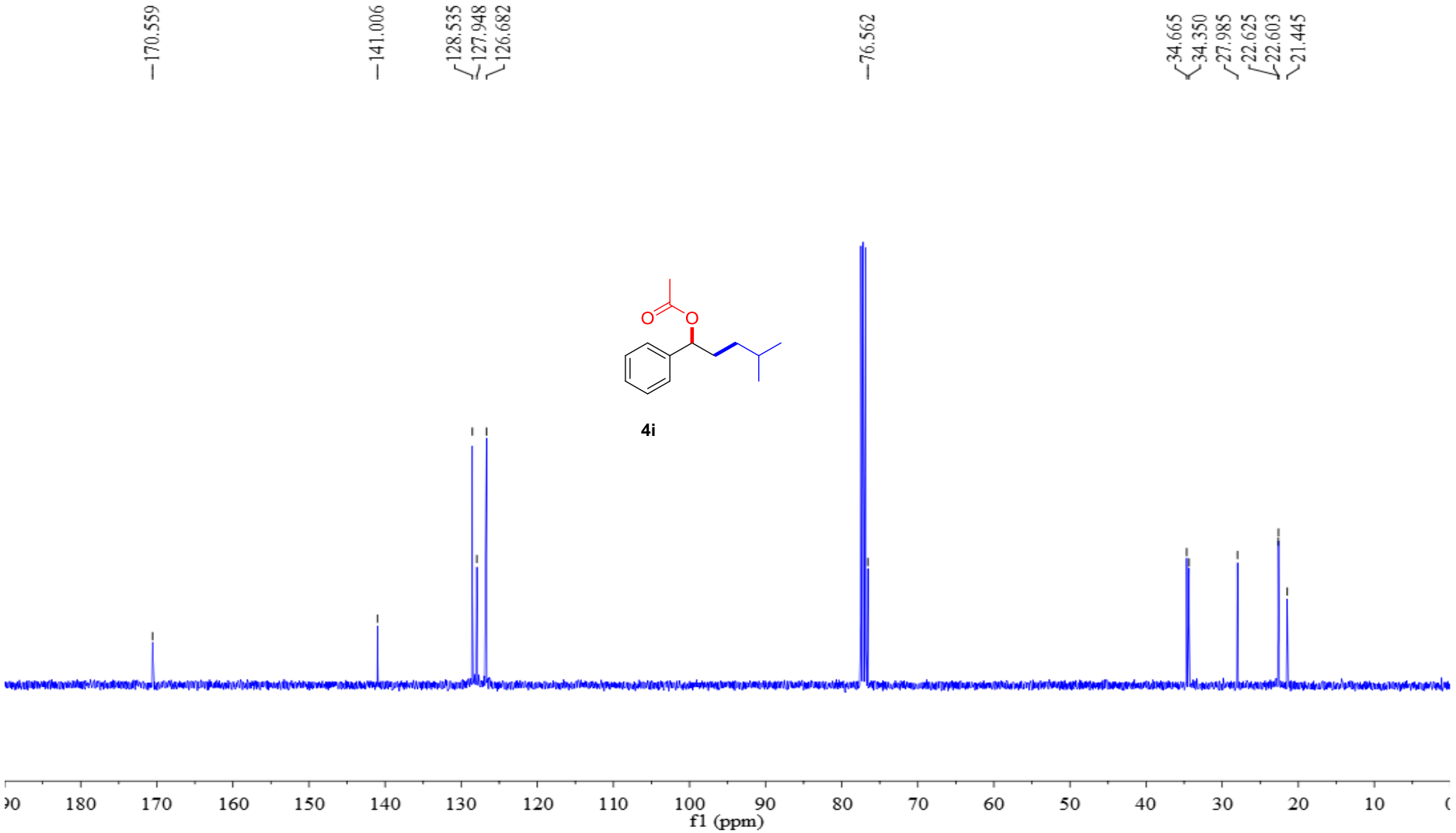
128.532
127.961
126.734
126.647
76.615
76.475
51.145
50.691
38.327
35.143
35.089
34.072
31.310
31.157
30.133
29.185
29.114
27.726
25.615
24.216
22.637
21.437
O
O
4h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.343
7.340
7.333
7.327
7.316
7.312
7.300
7.295
7.291
7.286
7.284
7.278
5.713
5.697
5.695
5.679
2.067
1.912
1.904
1.899
1.892
1.884
1.871
1.864
1.799
1.797
1.784
1.779
1.771
1.768
1.755
1.750
1.570
1.553
1.537
1.520
1.504
1.255
1.242
1.238
1.230
1.225
1.221
1.209
1.197
1.193
1.134
1.120
1.117
1.104
1.092
1.088
1.075
1.072
0.869
0.863
0.853
0.846
O
O
4i
5.00
1.00
3.01
1.05
1.04
1.00
1.00
1.01
6.01
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
f1 (ppm)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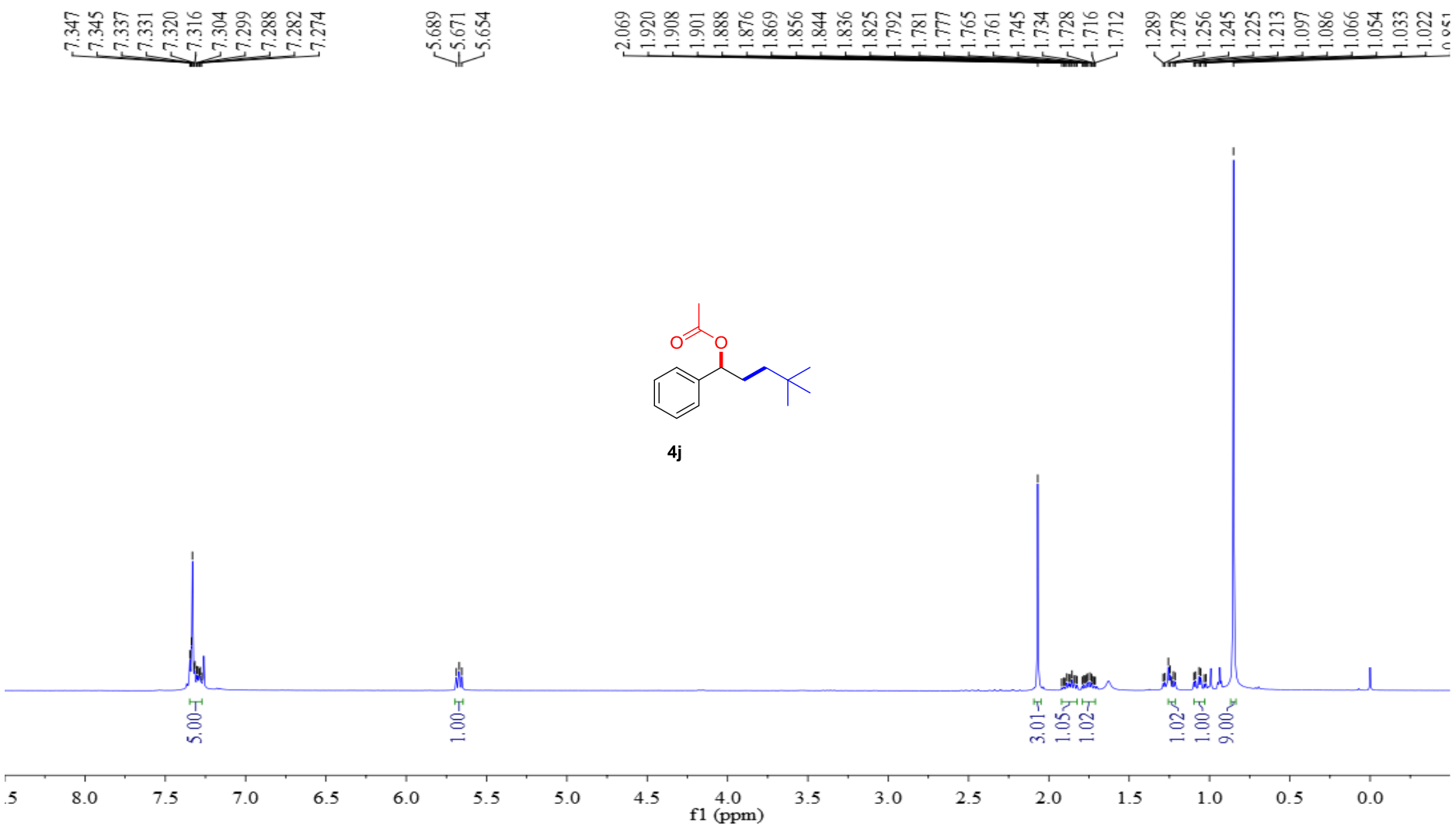
76.562
34.665
34.350
27.985
22.625
22.603
21.445
O
O
4i
f1 (ppm)


7.347
7.345
7.337
7.331
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7.299
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7.282
7.274
5.689
5.671
5.654
2.069
1.920
1.908
1.901
1.888
1.876
1.869
1.856
1.844
1.836
1.825
1.792
1.781
1.777
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1.761
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1.716
1.712
1.289
1.278
1.256
1.245
1.225
1.213
1.097
1.086
1.066
1.054
1.033
1.022
O
O
4j
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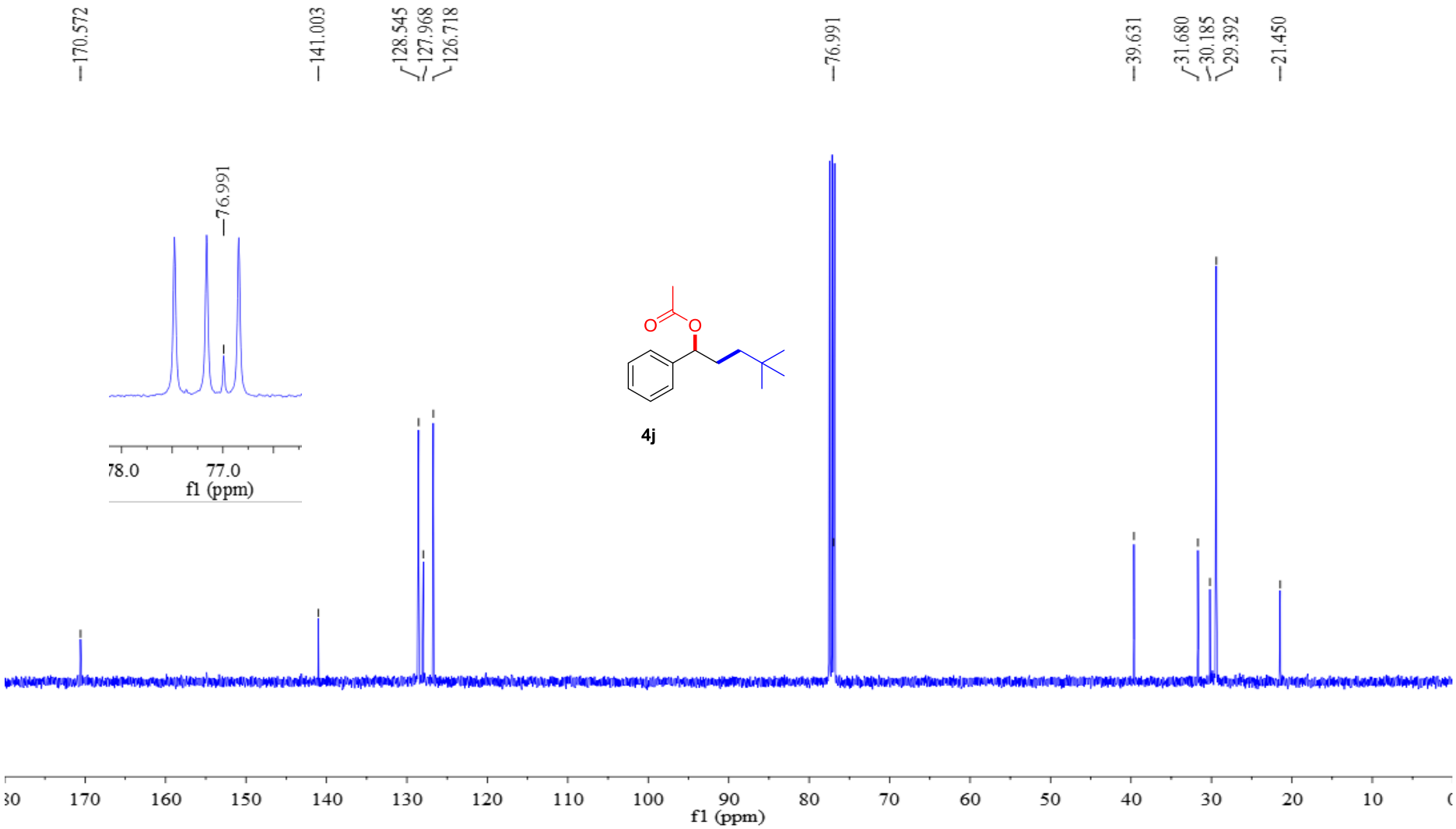
1.00
3.01
1.05
1.02
1.02
1.00
9.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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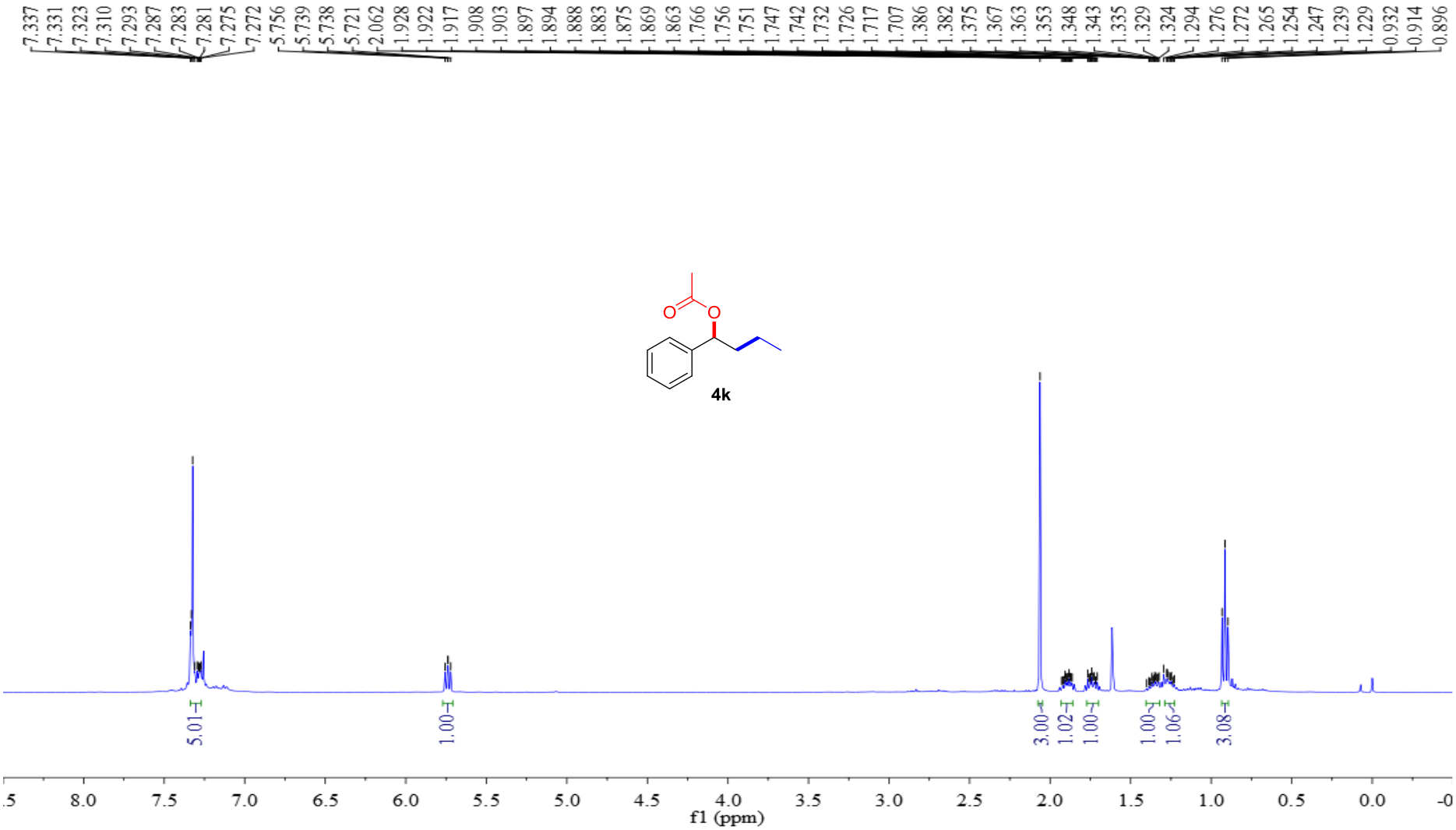
141.003
128.545
127.968
126.718
76.991
39.631
31.680
30.185
29.392
21.450
76.991
78.0
77.0
f1 (ppm)
O
O
4j
30
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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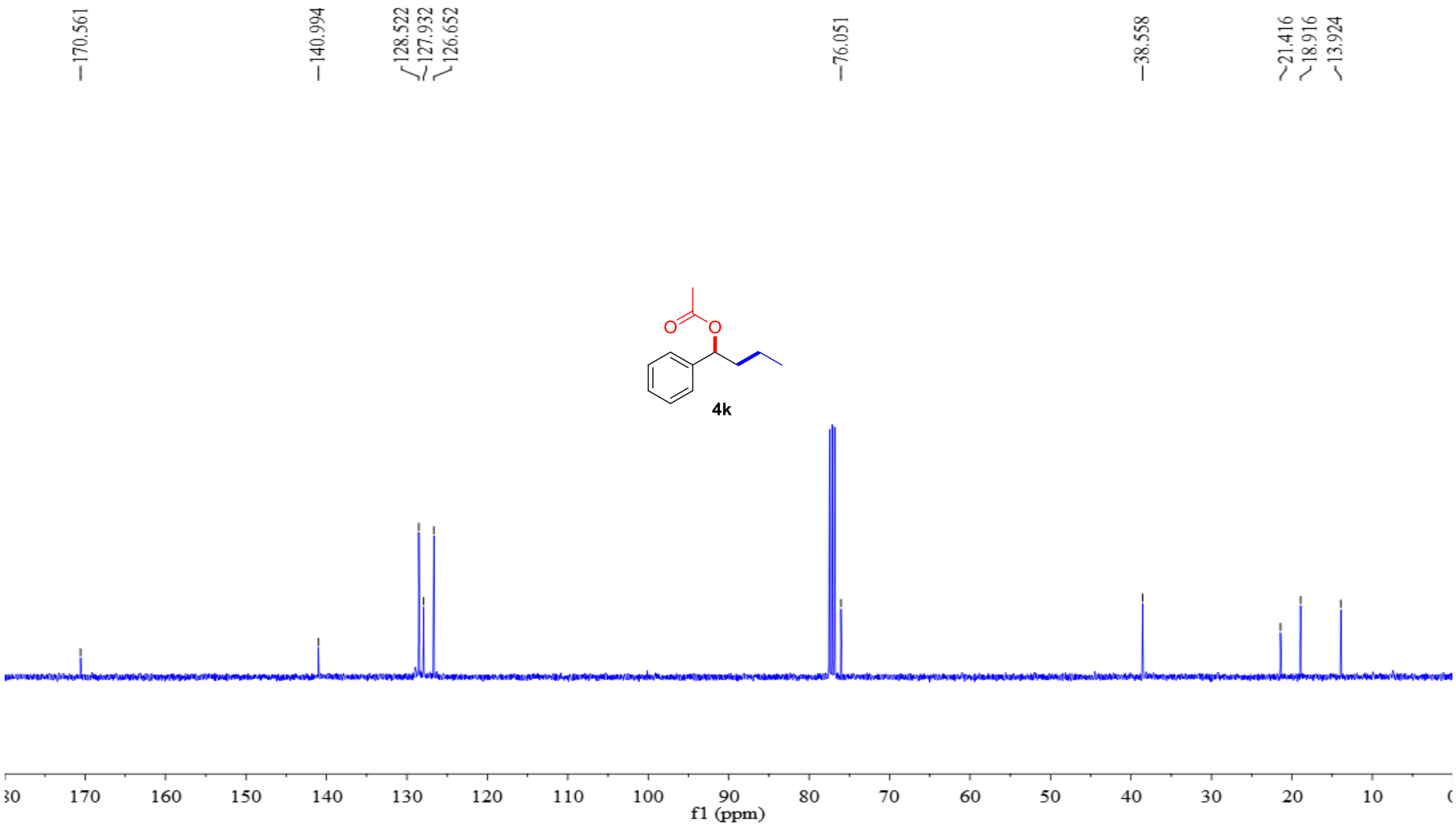
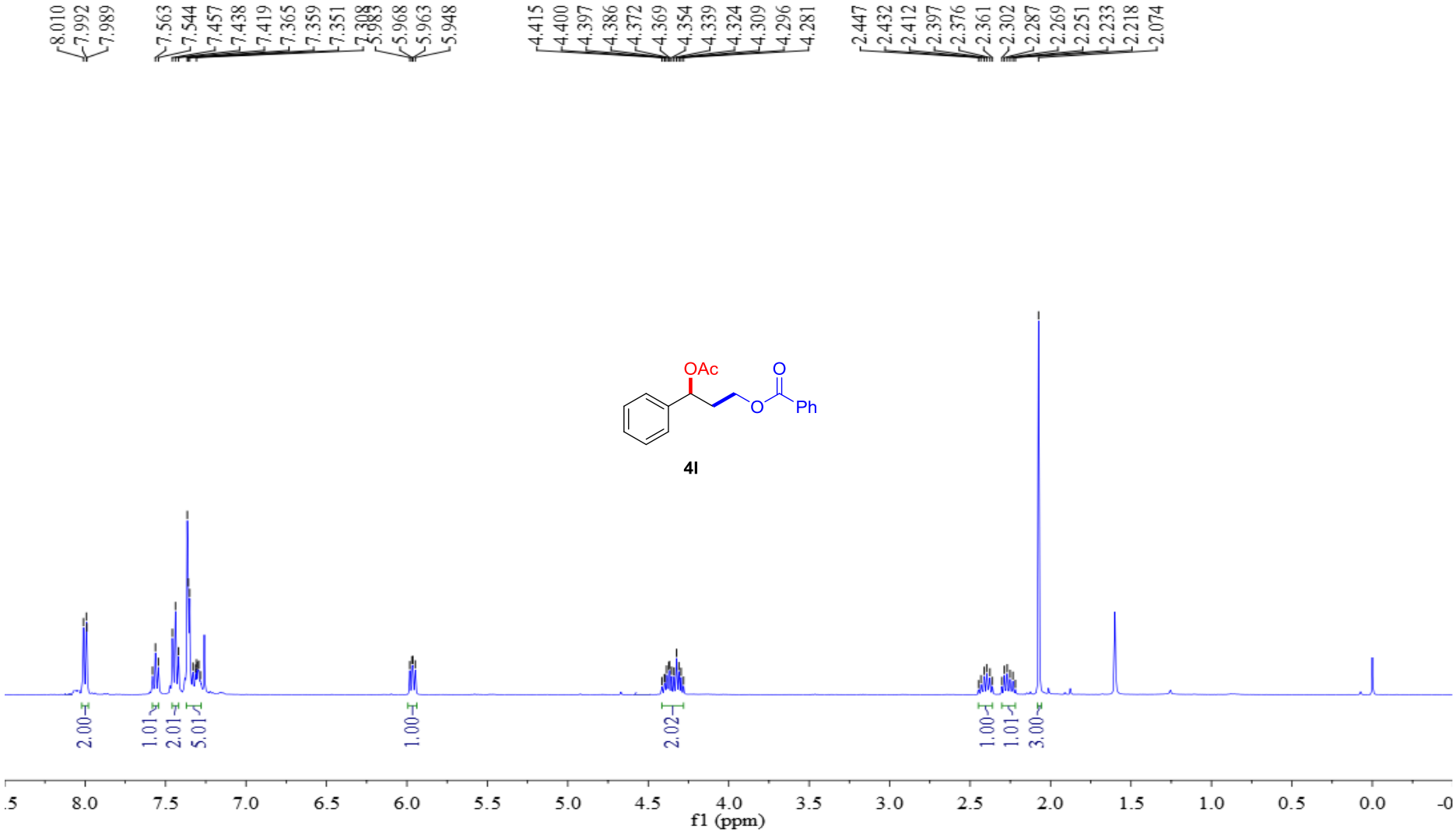
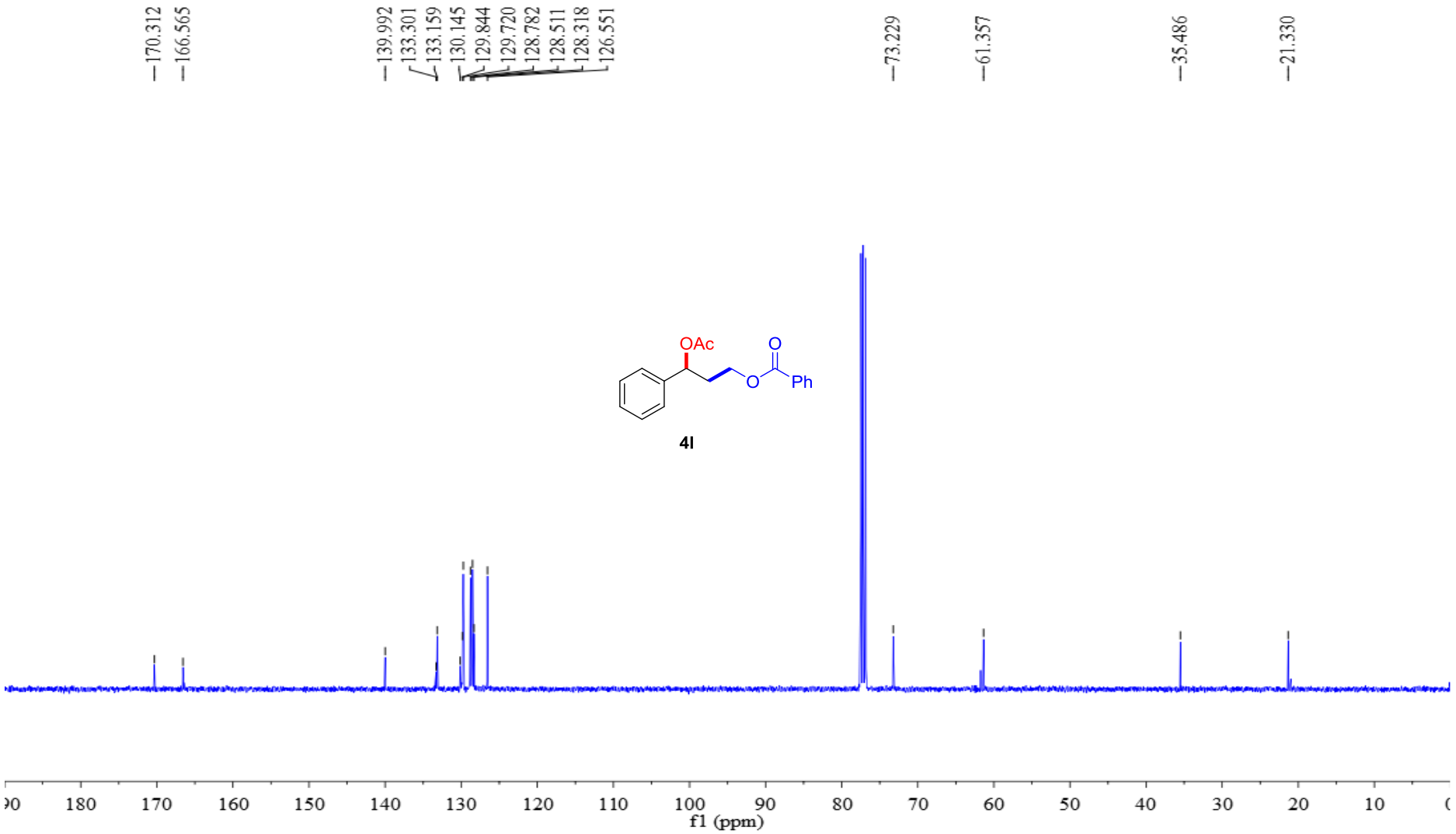
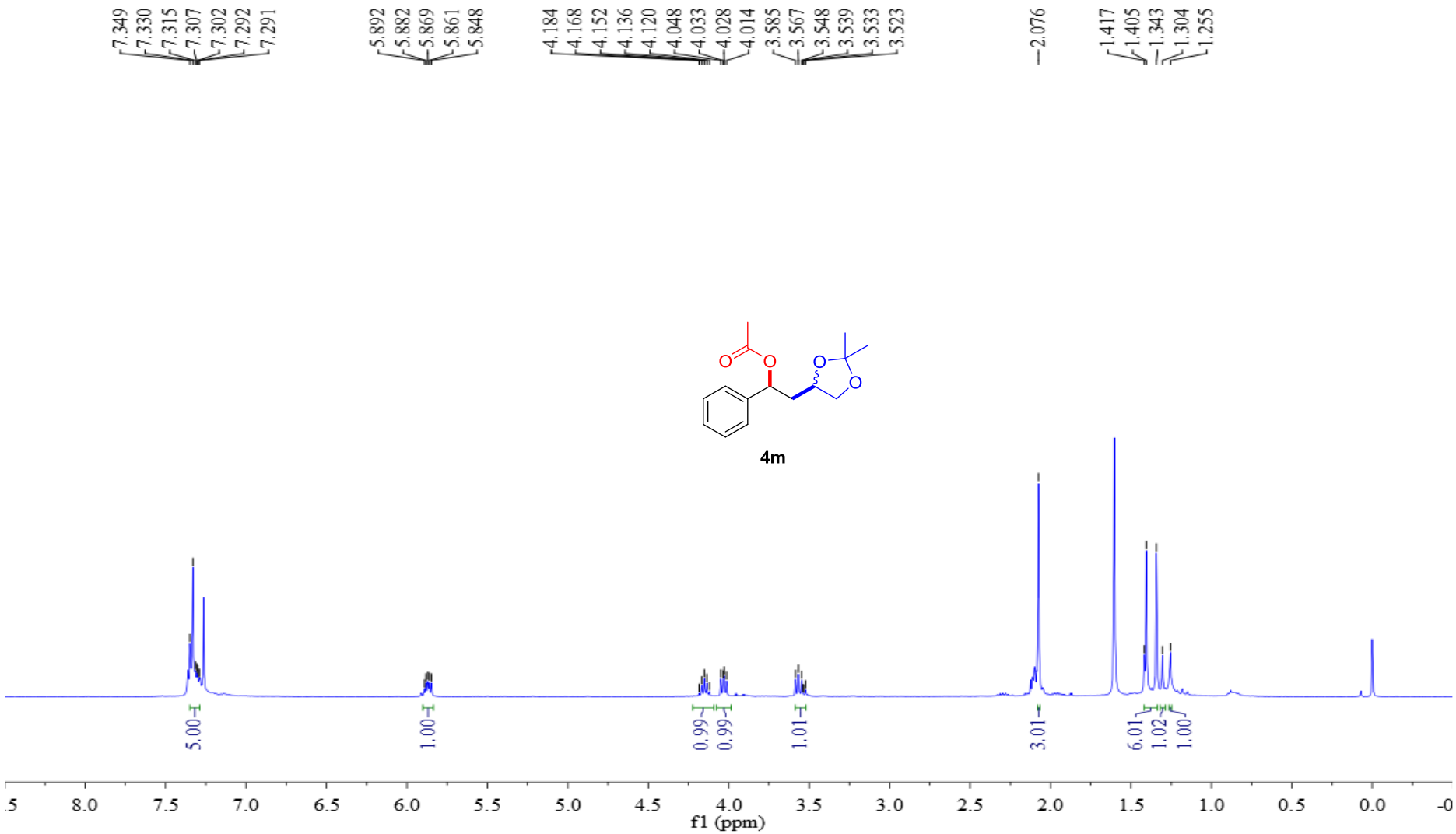
7.331
7.323
7.310
7.293
7.287
7.283
7.281
7.275
7.272
5.756
5.739
5.738
5.721
2.062
1.928
1.922
1.917
1.908
1.903
1.897
1.894
1.888
1.883
1.875
1.869
1.863
1.766
1.756
1.751
1.747
1.742
1.732
1.726
1.717
1.707
1.386
1.382
1.375
1.367
1.363
1.353
1.348
1.343
1.335
1.329
1.324
1.294
1.276
1.272
1.265
1.254
1.247
1.239
1.229
0.932
0.914
0.896
O
O
4k
5.01
1.00
3.00
1.02
1.00
1.00
1.06
3.08
f1 (ppm)

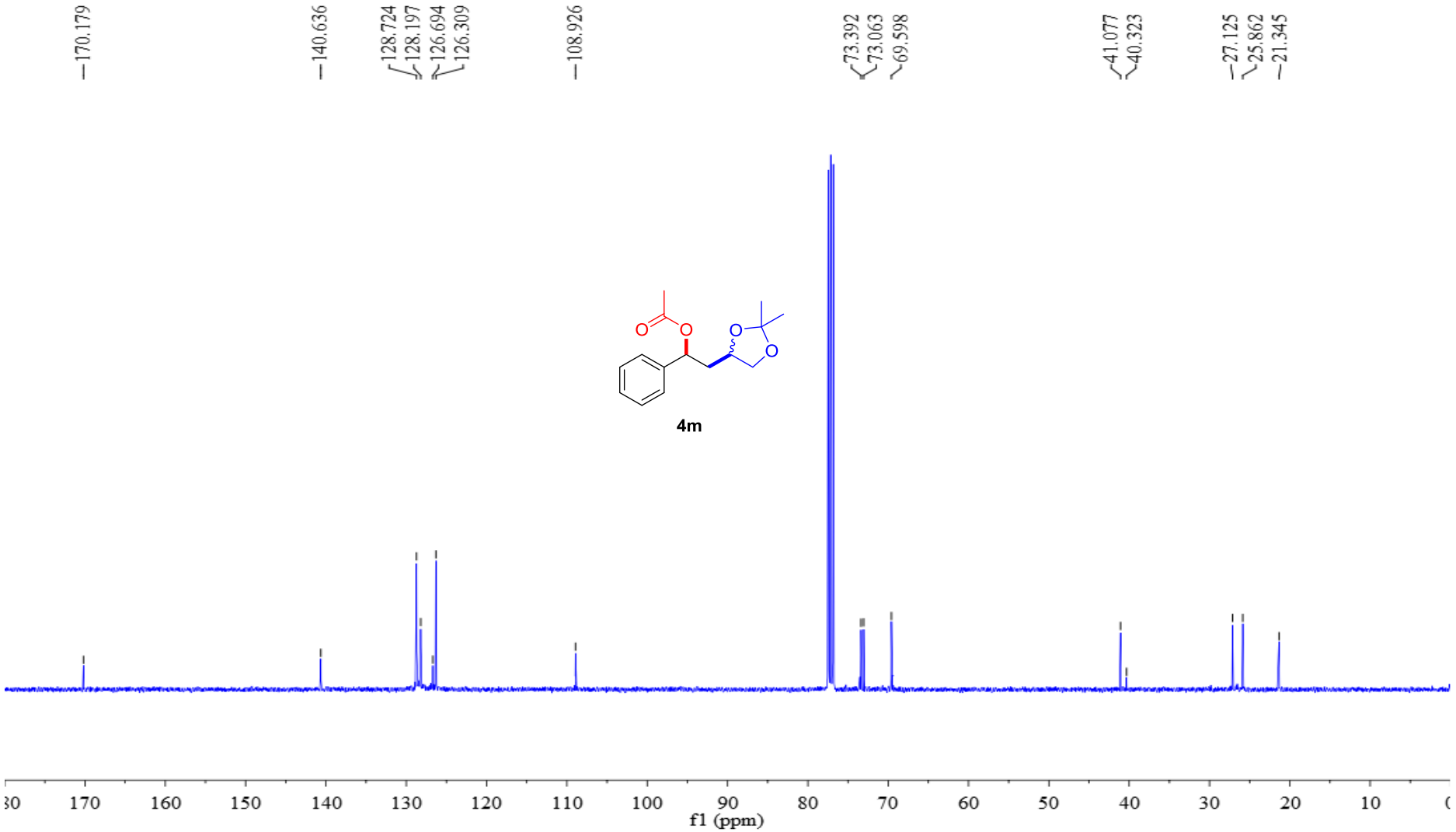

170.561
140.994
128.522
127.932
126.652
76.051
38.558
21.416
18.916
13.924
4k
f1 (ppm)

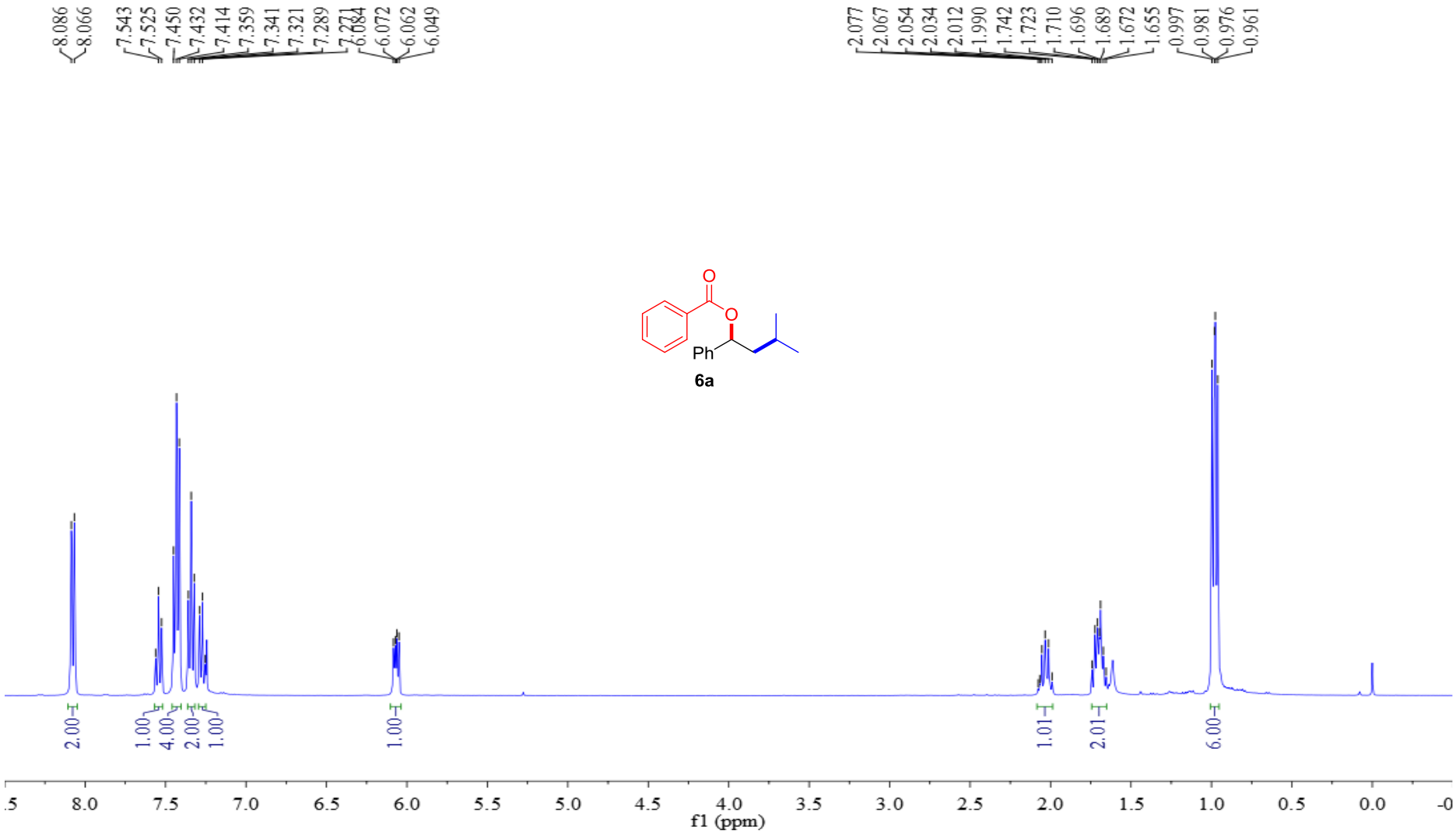

8.010
7.992
7.989
7.563
7.544
7.457
7.438
7.419
7.365
7.359
7.351
7.308
5.983
5.968
5.963
5.948
4.415
4.400
4.397
4.386
4.372
4.369
4.354
4.339
4.324
4.309
4.296
4.281
2.447
2.432
2.412
2.397
2.376
2.361
2.302
2.287
2.269
2.251
2.233
2.218
2.074
OAc
O
O
Ph
2.00
1.01
2.01
5.01
1.00
2.02
1.00
1.01
3.00
f1 (ppm)

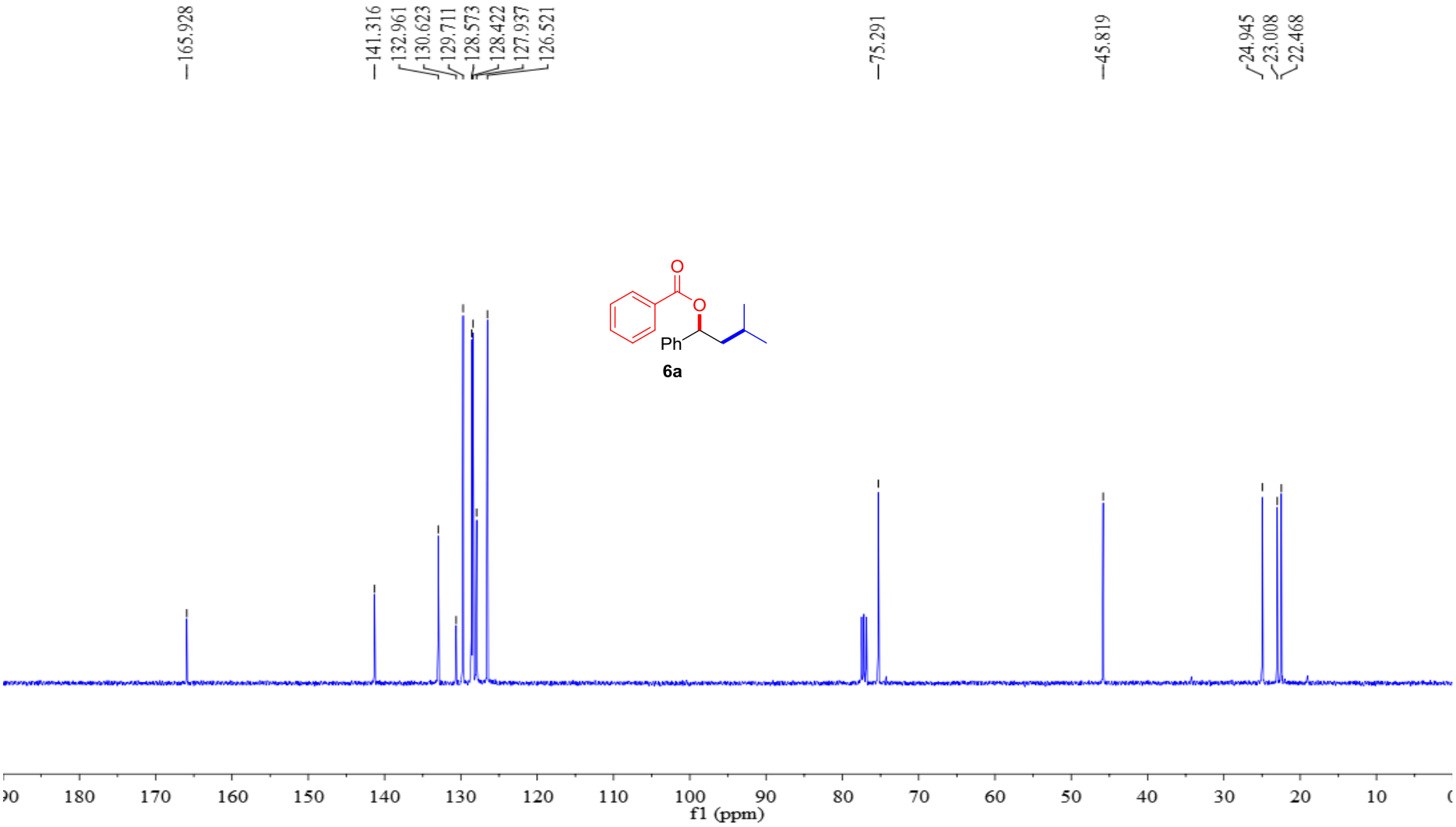
**4l**

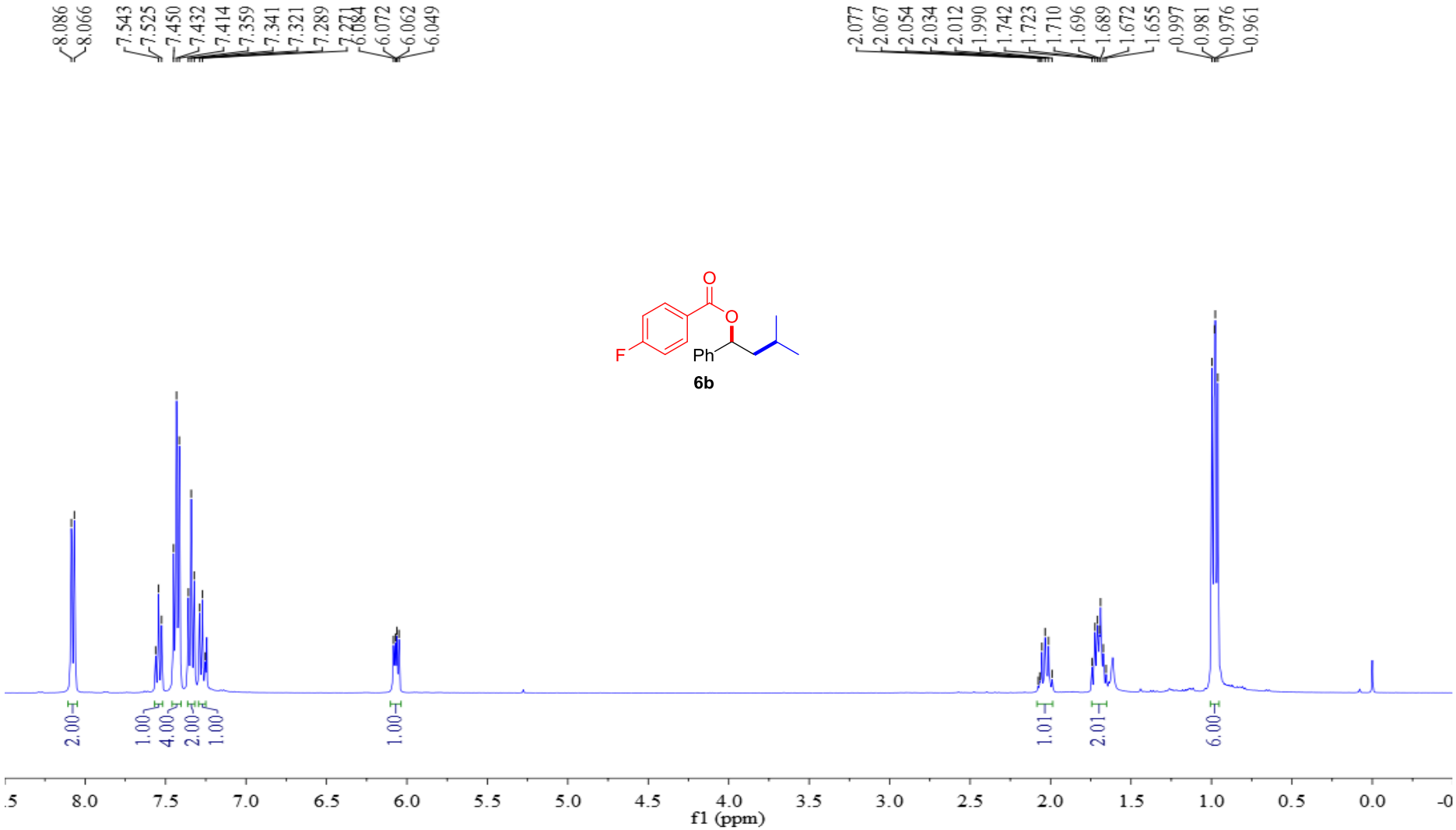

170.312
166.565
139.992
133.301
133.159
130.145
129.844
129.720
128.782
128.511
128.318
126.551
73.229
61.357
35.486
21.330
OAc
O
O
Ph
4l
f1 (ppm)

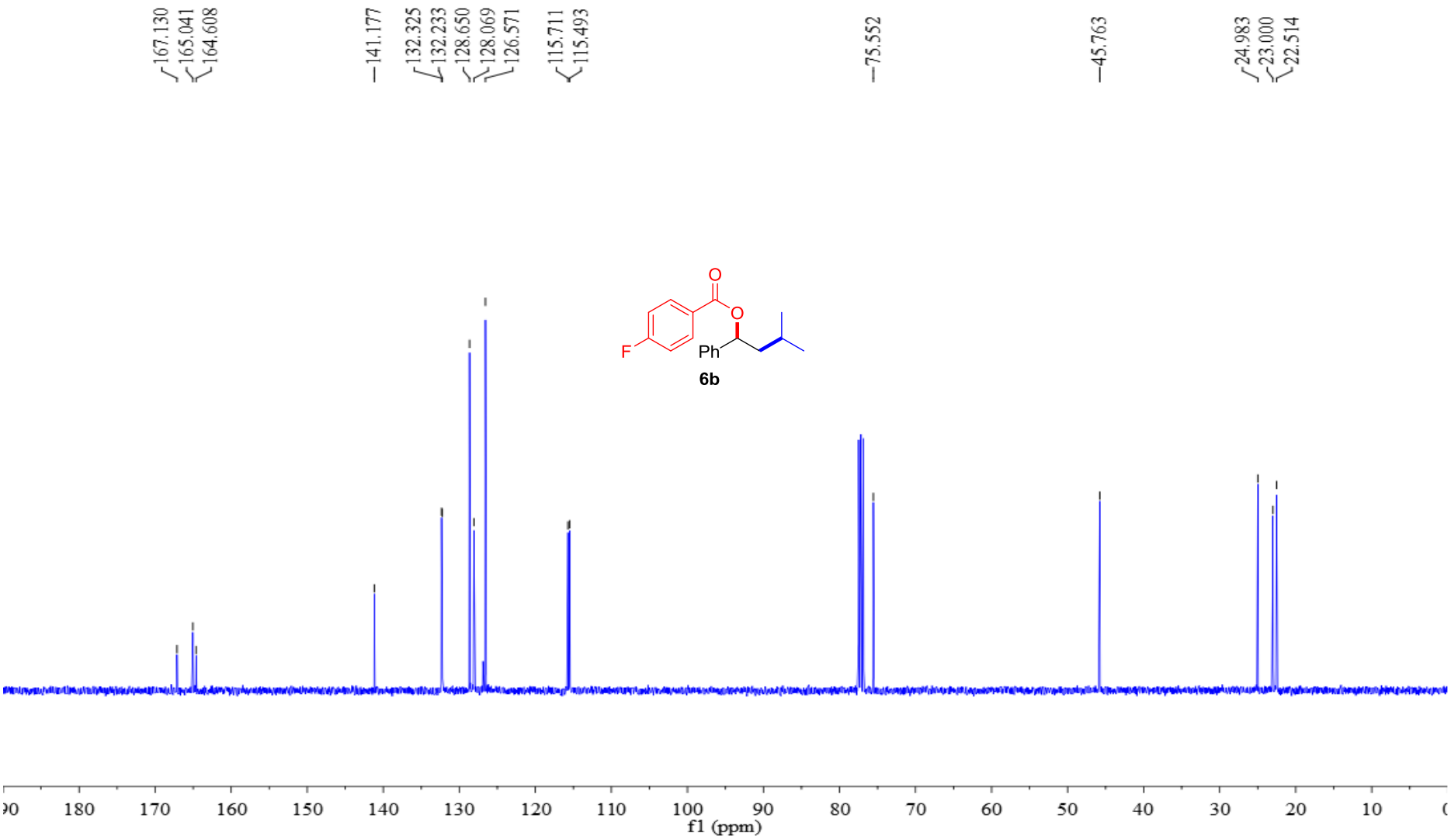

7.349
7.330
7.315
7.307
7.302
7.292
7.291
5.892
5.882
5.869
5.861
5.848
4.184
4.168
4.152
4.136
4.120
4.048
4.033
4.028
4.014
3.585
3.567
3.548
3.539
3.533
3.523
2.076
1.417
1.405
1.343
1.304
1.255
4m
5.00
1.00
0.99
0.99
1.01
3.01
6.01
1.02
1.00
f1 (ppm)

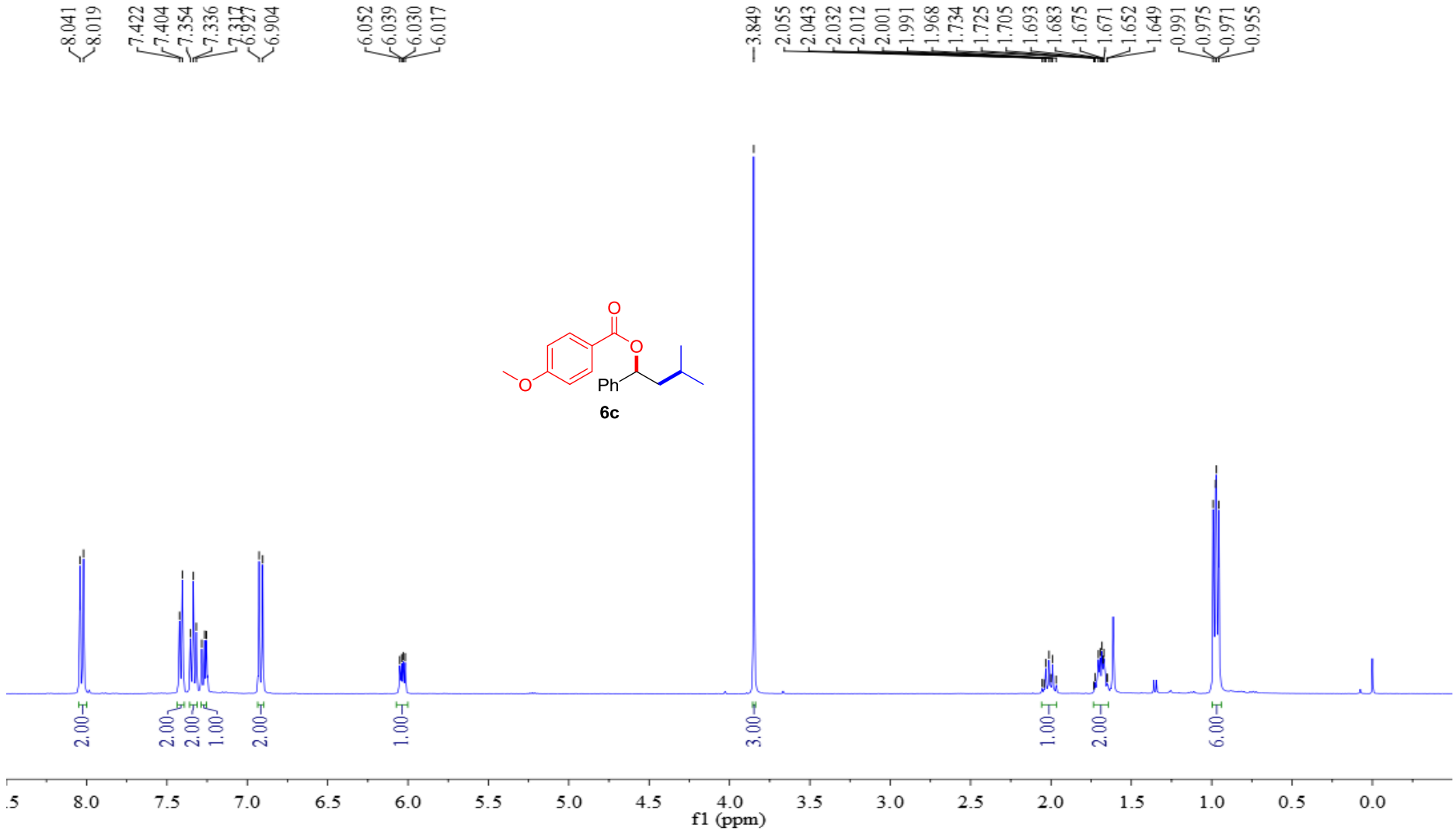

170.179
140.636
128.724
128.197
126.694
126.309
108.926
73.392
73.063
69.598
41.077
40.323
27.125
25.862
21.345
4m
f1 (ppm)

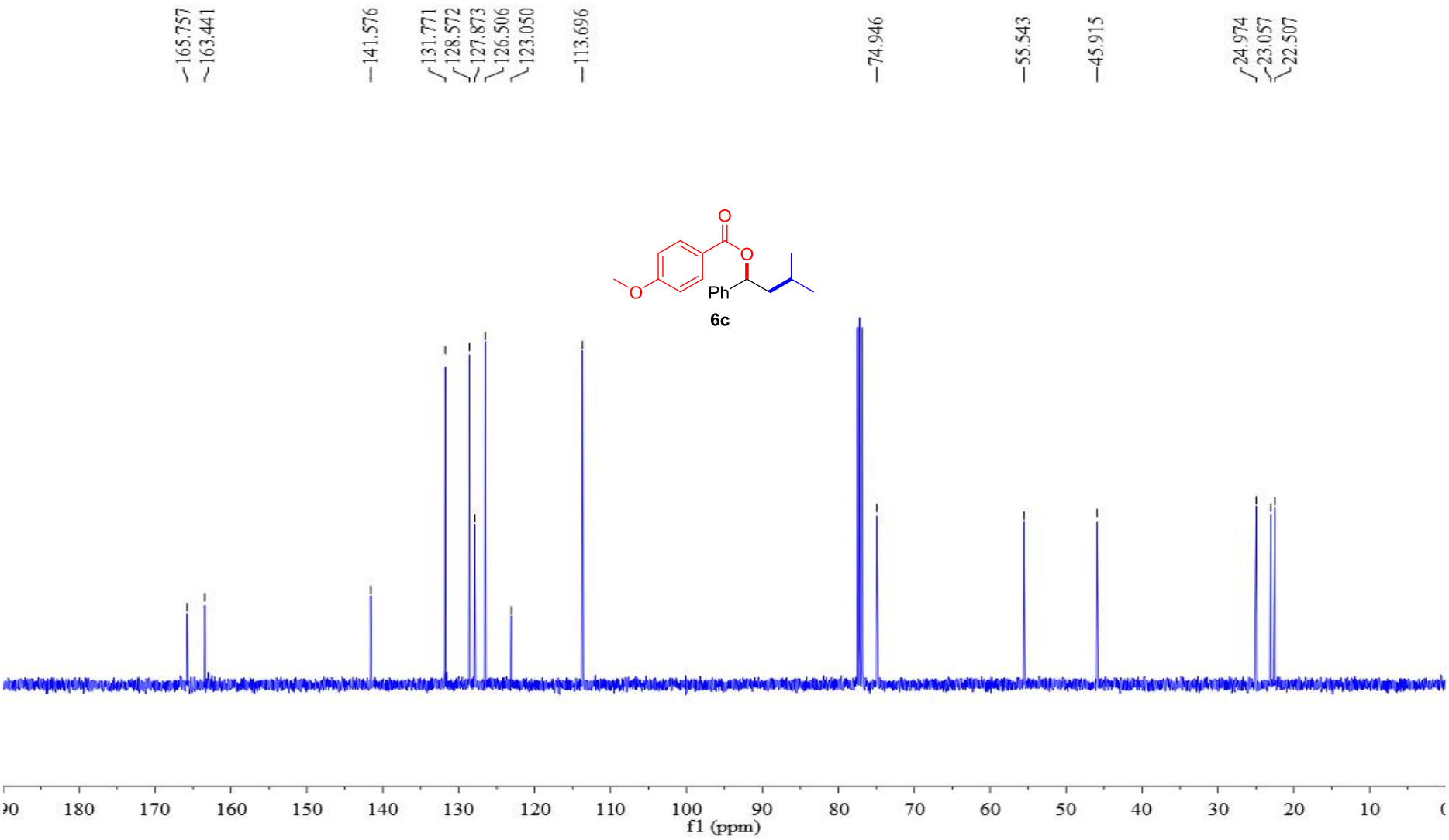

8.086
8.066
7.543
7.525
7.450
7.432
7.414
7.359
7.341
7.321
7.289
7.271
6.084
6.072
6.062
6.049
2.077
2.067
2.054
2.034
2.012
1.990
1.742
1.723
1.710
1.696
1.689
1.672
1.655
0.997
0.981
0.976
0.961
O
O
Ph
6a
2.00
1.00
4.00
2.00
1.00
1.00
1.01
2.01
6.00
f1 (ppm)


165.928
141.316
132.961
130.623
129.711
128.573
128.422
127.937
126.521
75.291
45.819
24.945
23.008
22.468
O
O
Ph
6a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.086
8.066
7.543
7.525
7.450
7.432
7.414
7.359
7.341
7.321
7.289
7.271
6.084
6.072
6.062
6.049
2.077
2.067
2.054
2.034
2.012
1.990
1.742
1.723
1.710
1.696
1.689
1.672
1.655
0.997
0.981
0.976
0.961
O
O
F
Ph
6b
2.00
1.00
4.00
2.00
1.00
1.00
1.01
2.01
6.00
f1 (ppm)


167.130
165.041
164.608
141.177
132.325
132.233
128.650
128.069
126.571
115.711
115.493
75.552
45.763
24.983
23.000
22.514
O
O
F
Ph
6b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.041
8.019
7.422
7.404
7.354
7.336
7.317
6.927
6.904
6.052
6.039
6.030
6.017
3.849
2.055
2.043
2.032
2.012
2.001
1.991
1.968
1.734
1.725
1.705
1.693
1.683
1.675
1.671
1.652
1.649
0.991
0.975
0.971
0.955
O
O
O
Ph
6c
2.00
2.00
2.00
1.00
2.00
1.00
3.00
1.00
2.00
6.00
f1 (ppm)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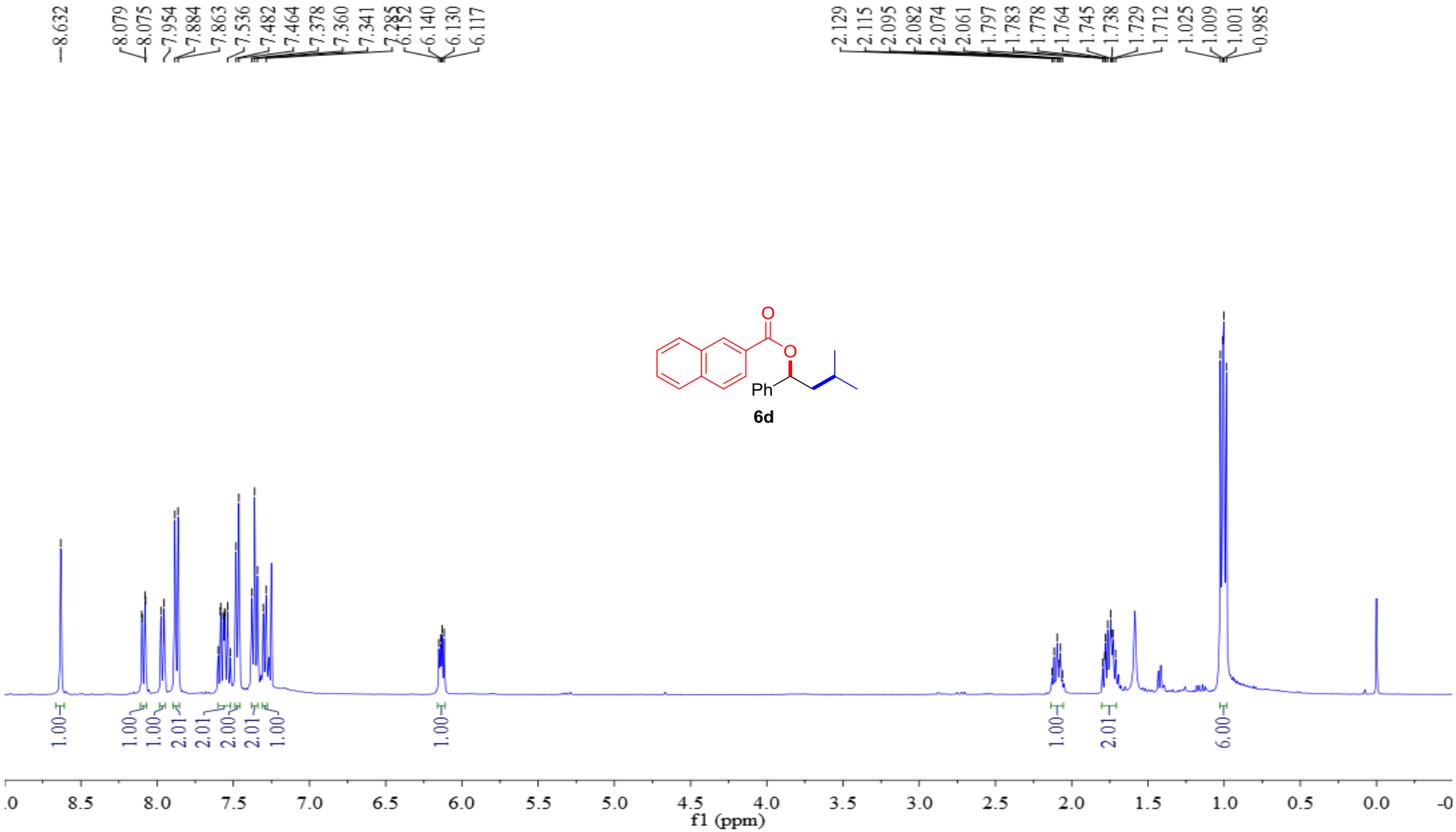
163.441
141.576
131.771
128.572
127.873
126.506
123.050
113.696
74.946
55.543
45.915
24.974
23.057
22.507
O
O
O
Ph
6c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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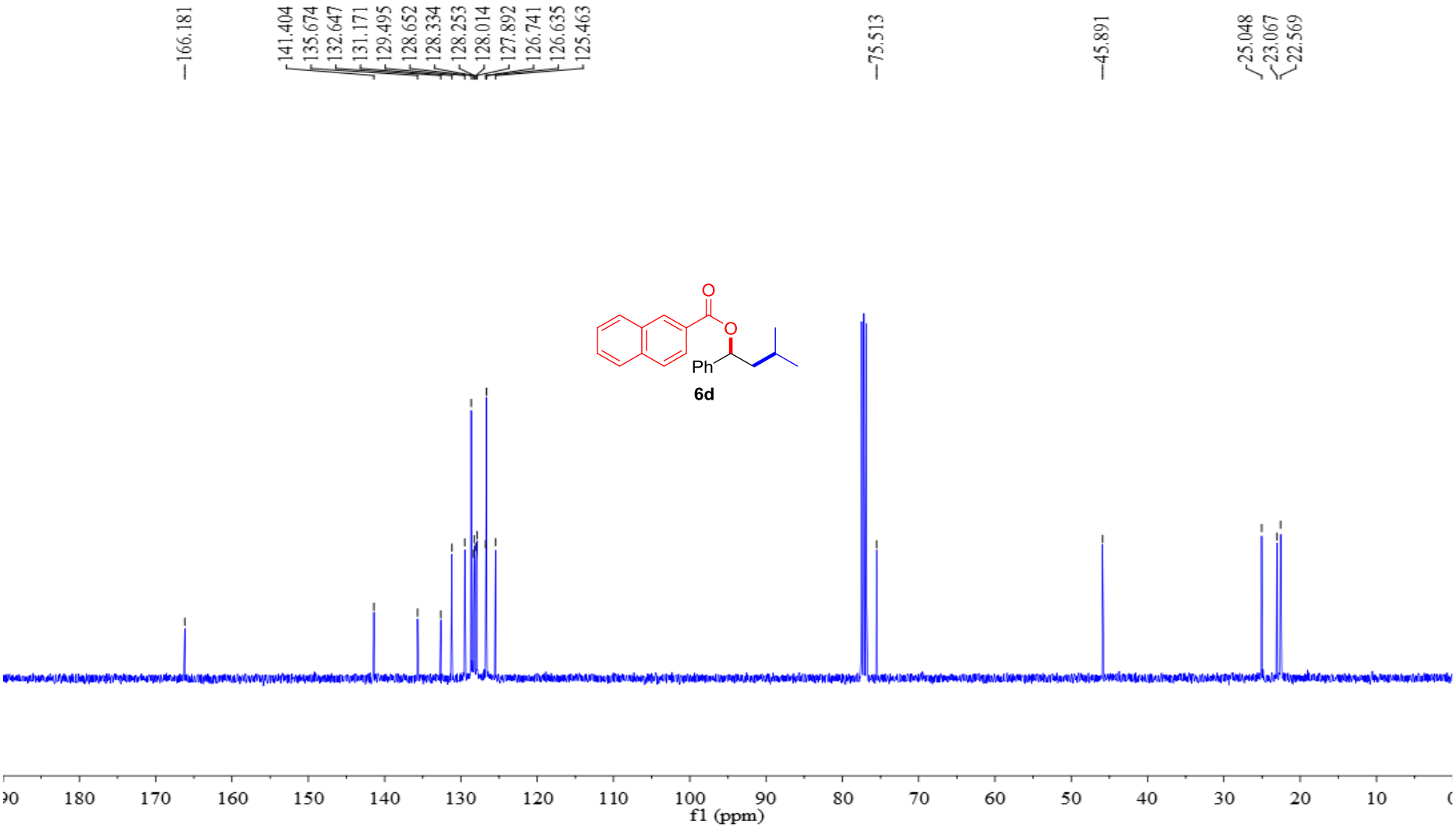
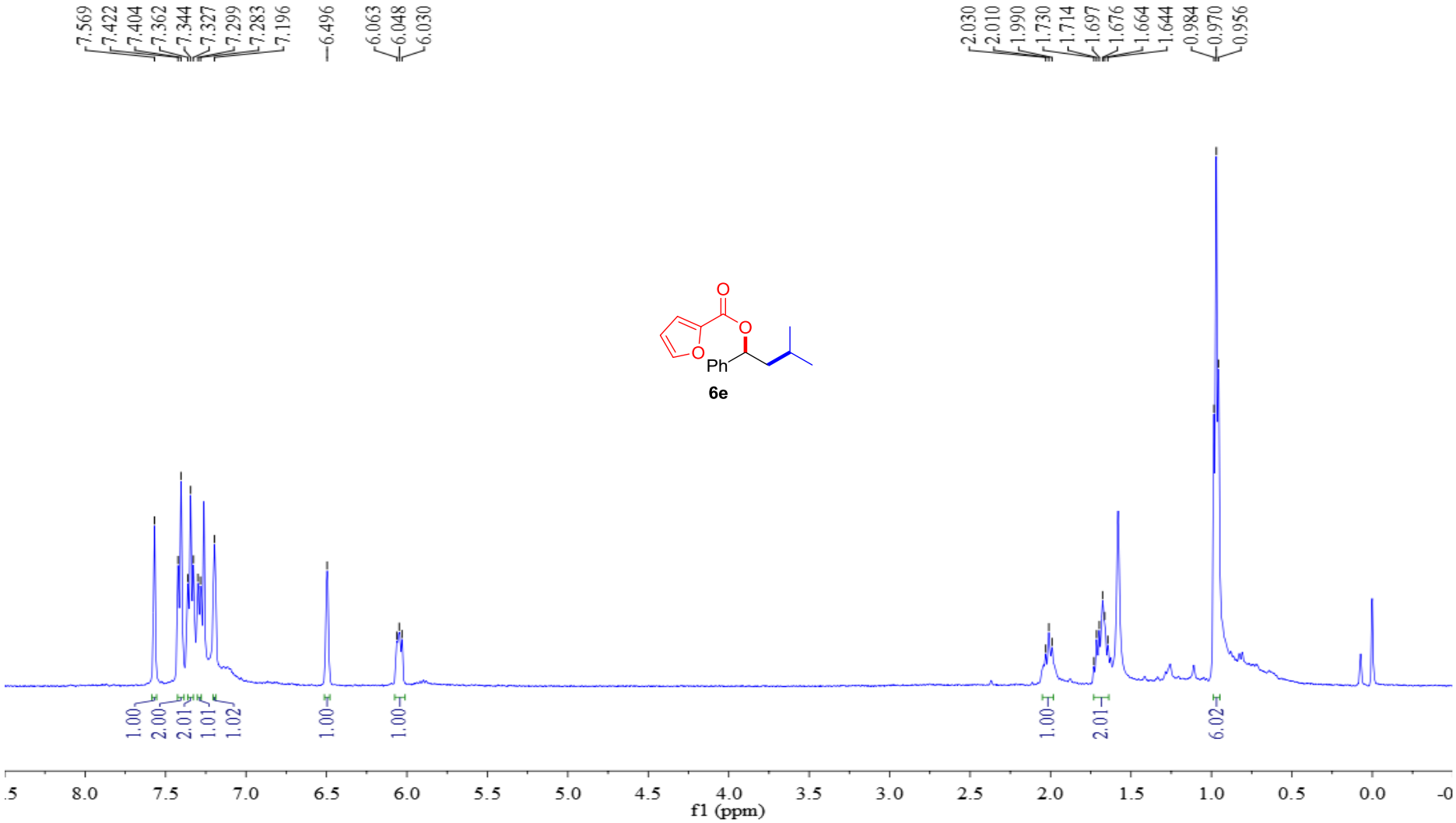
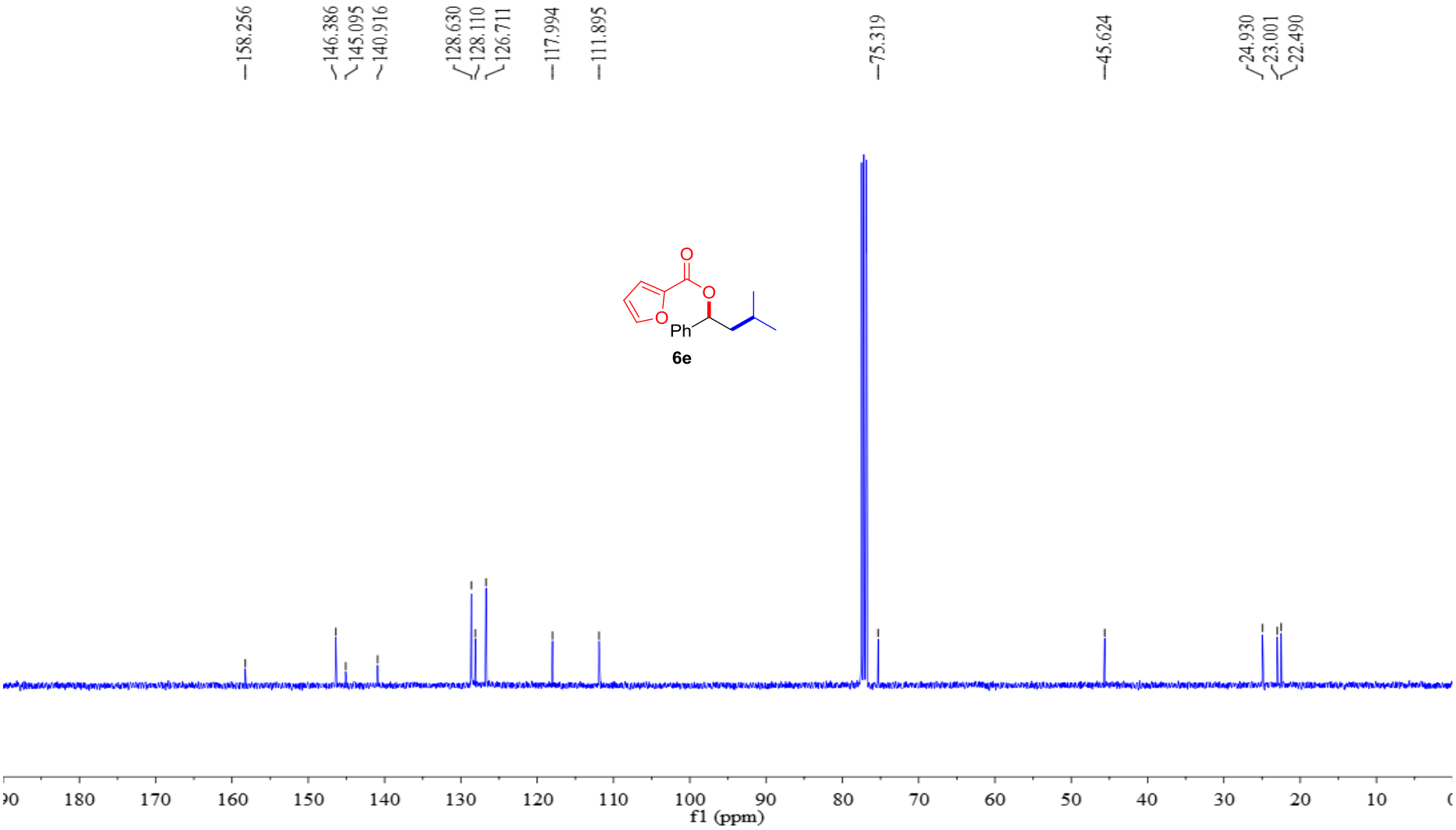
8.079
8.075
7.954
7.884
7.863
7.536
7.482
7.464
7.378
7.360
7.341
7.285
7.152
6.140
6.130
6.117
2.129
2.115
2.095
2.082
2.074
2.061
1.797
1.783
1.778
1.764
1.745
1.738
1.729
1.712
1.025
1.009
1.001
0.985
O
O
Ph
6d
1.00
1.00
1.00
2.01
2.01
2.00
2.01
1.00
1.00
1.00
2.01
6.00
f1 (ppm)


166.181
141.404
135.674
132.647
131.171
129.495
128.652
128.334
128.253
128.014
127.892
126.741
126.635
125.463
75.513
45.891
25.048
23.067
22.569
O
O
Ph
6d
f1 (ppm)


7.569
7.422
7.404
7.362
7.344
7.327
7.299
7.283
7.196
6.496
6.063
6.048
6.030
2.030
2.010
1.990
1.730
1.714
1.697
1.676
1.664
1.644
0.984
0.970
0.956
O
O
O
Ph
6e
1.00
2.00
2.01
1.01
1.02
1.00
1.00
1.00
2.01
6.02
f1 (ppm)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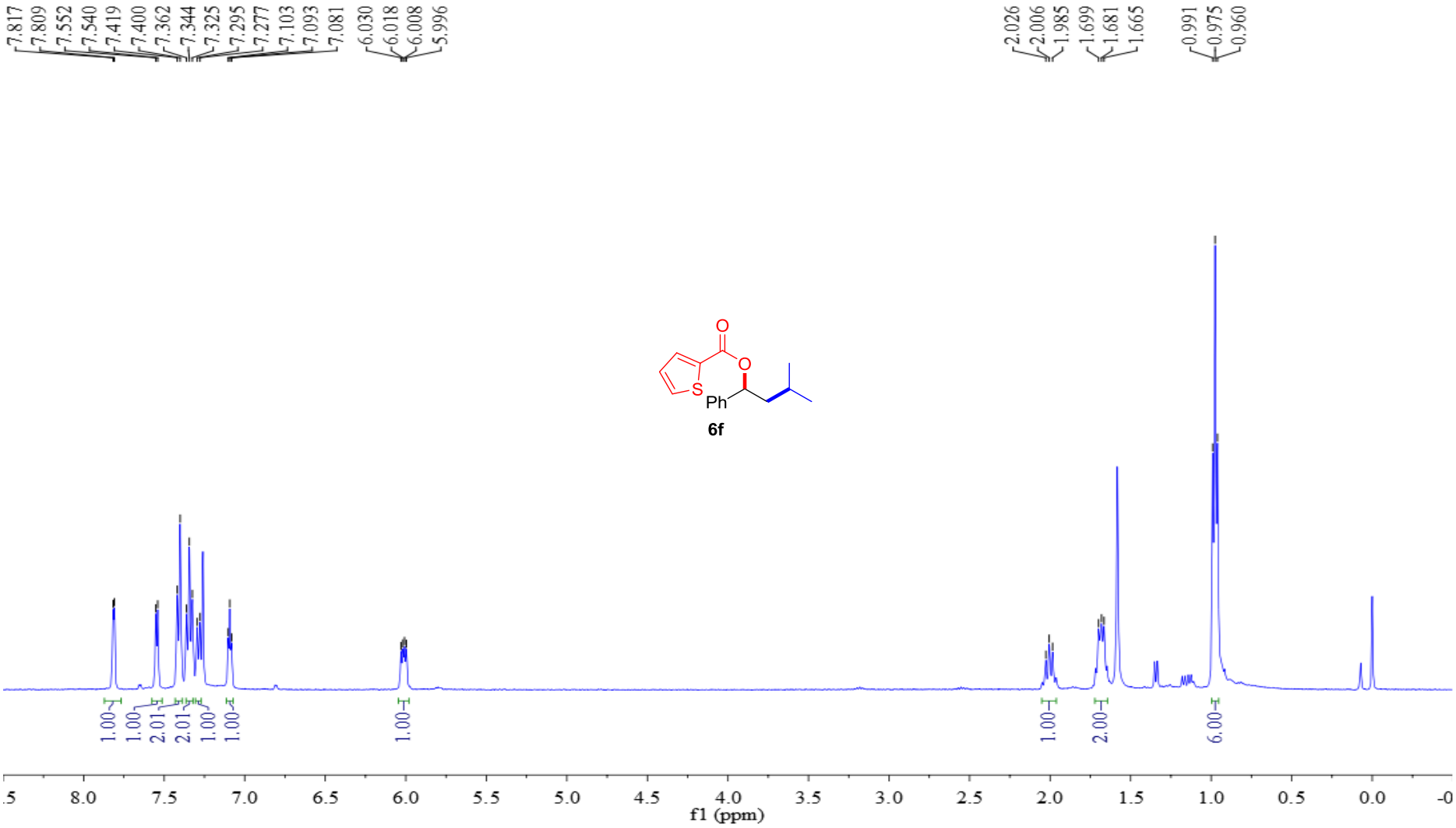
146.386
145.095
140.916
128.630
128.110
126.711
117.994
111.895
75.319
45.624
24.930
23.001
22.490
O
O
O
Ph
6e
f1 (ppm)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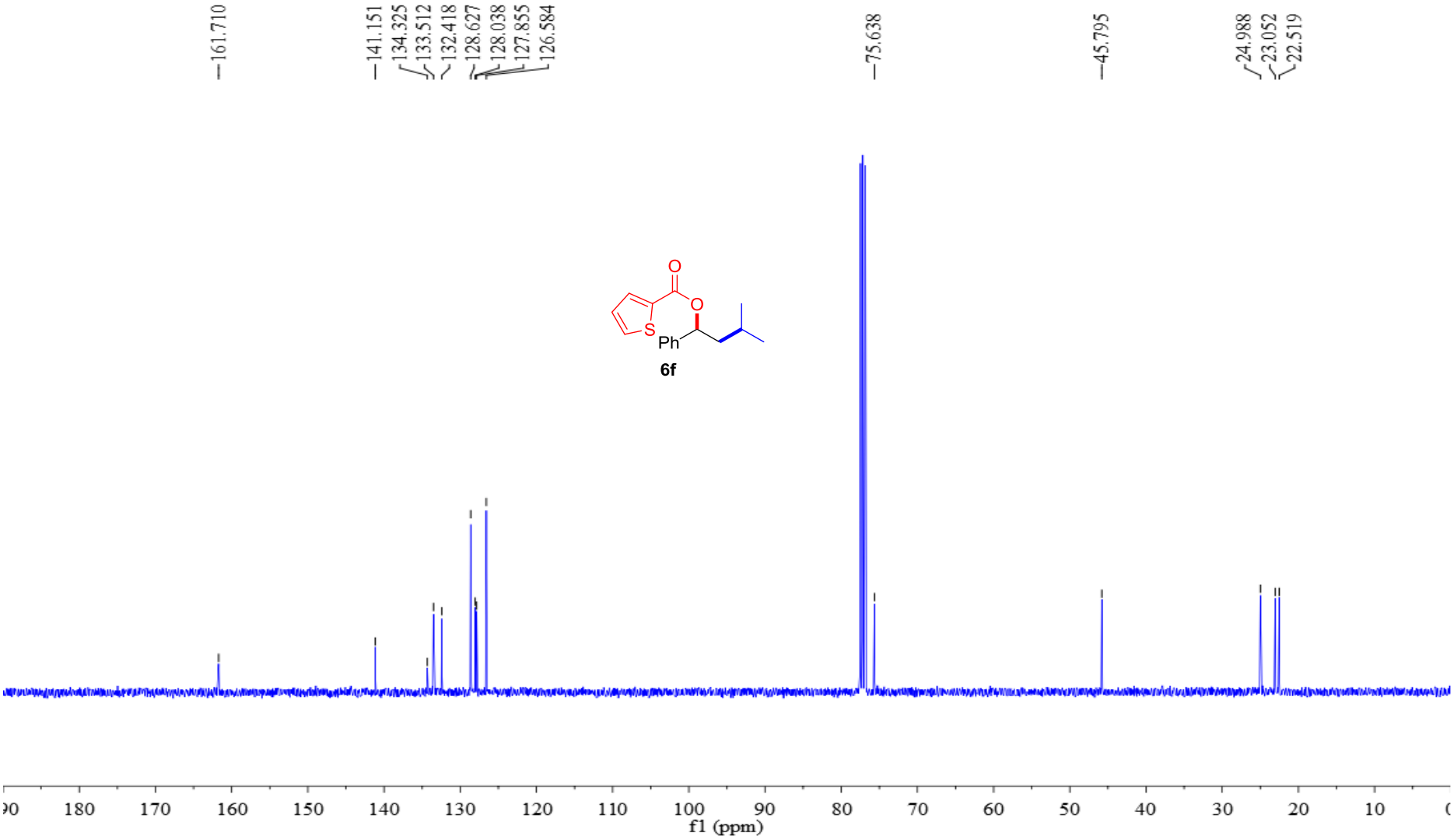
7.809
7.552
7.540
7.419
7.400
7.362
7.344
7.325
7.295
7.277
7.103
7.093
7.081
6.030
6.018
6.008
5.996
2.026
2.006
1.985
1.699
1.681
1.665
0.991
0.975
0.960
O
O
S
Ph
6f
1.00
1.00
2.01
2.01
1.00
1.00
1.00
1.00
2.00
6.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.710
141.151
134.325
133.512
132.418
128.627
128.038
127.855
126.584
75.638
45.795
24.988
23.052
22.519
O
O
S
Ph
6f
f1 (ppm)