

ESI for

## **Concise synthesis of polyselenide: An efficient catalyst for oxidative cracking reaction of alkenes allowing the utilization of O<sub>2</sub> as partial oxidant under mild conditions**

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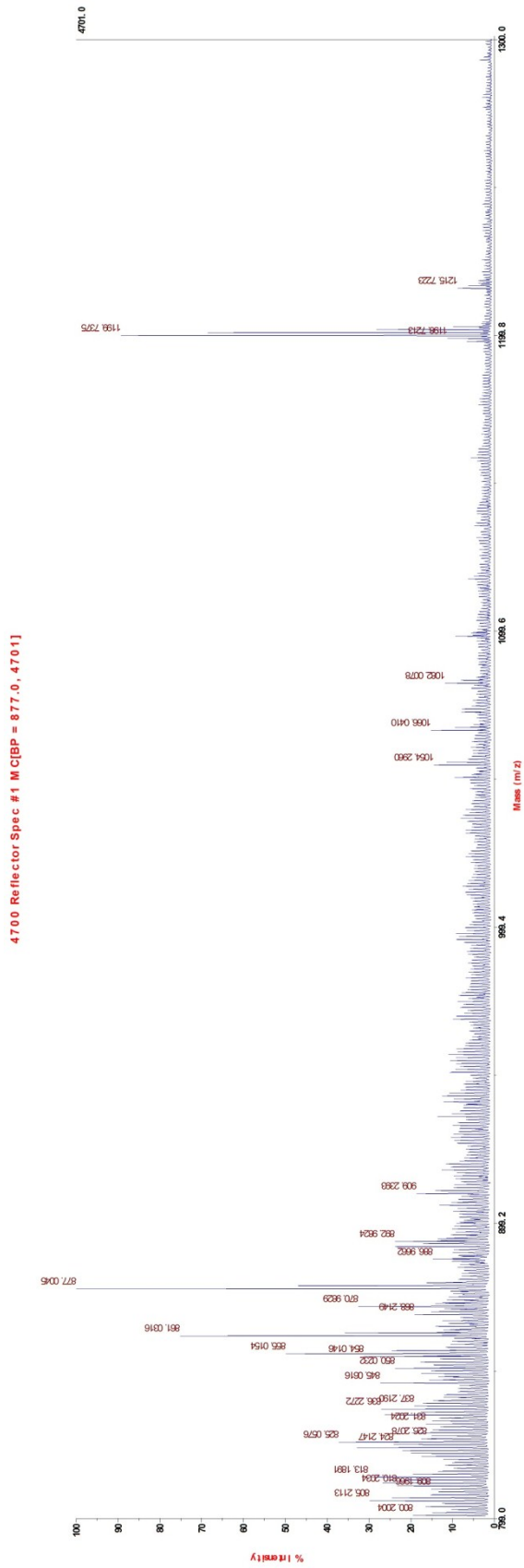
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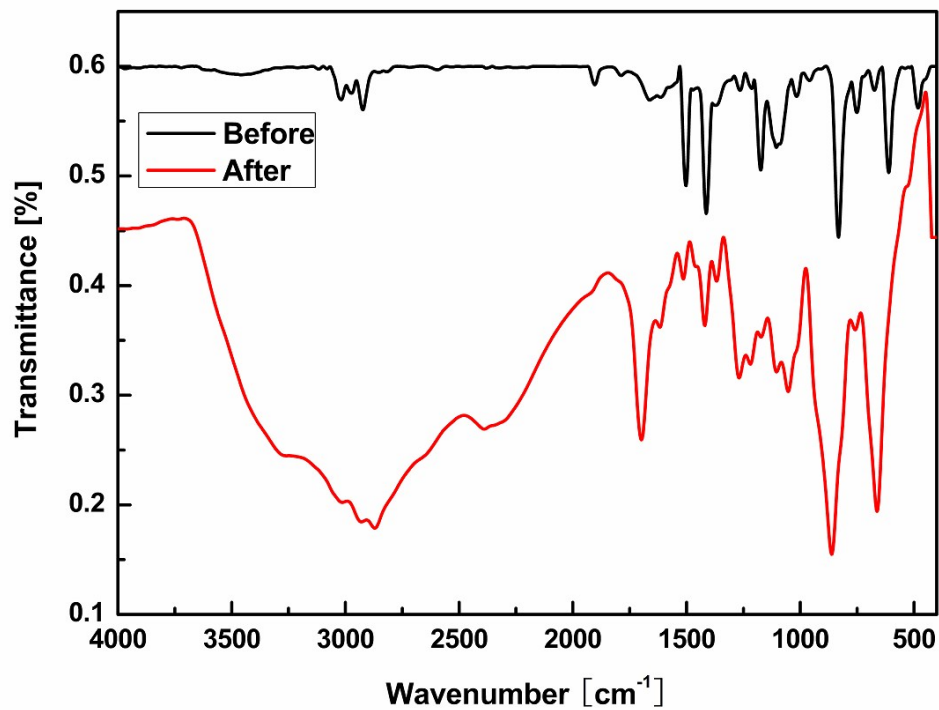
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# TOF-MS spectrum of the material (2i)



## IR spectra of 2i before and after reaction



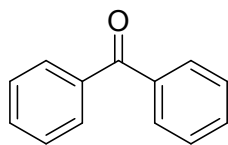
## Recycle and reuse of the catalyst

**Table S1** Recycle and reuse of the catalyst<sup>a</sup>

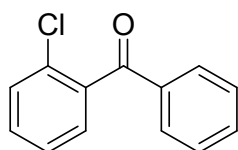
Entry	Cycle NO.	C <sup>b</sup>	S <sup>b</sup>	Y <sup>b</sup>
1	1	75	100	75
2	2	76	96	73
3	3	76	98	74
4	4	75	97	73
5	5	76	97	74
6	6	74	96	71

<sup>a</sup> 1 mmol of **3a**, 1.5 mmol of H<sub>2</sub>O<sub>2</sub> (30 w/w%), 50 mg of polyselenide **2i** and 2 mL of EtOH were used. <sup>b</sup> Abbreviations: C = Conversion ratio of **3a**/%; S = Selectivity of **4a**/%; Y = Isolated yield of **4a**/%.

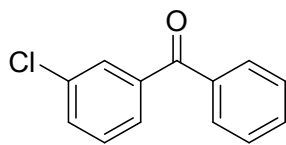
## Characterization of the Products



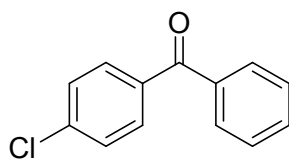
**Diphenyl-methanone (4a):** Solid; m. p. 47.1-48.6 °C (*lit.* 47-51 °C); IR (KBr): 1662, 1595, 1577, 1448, 1326, 1281, 1176, 1160, 1074, 999, 974, 941, 919, 809, 763, 700, 638 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ 7.81-7.79 (m, 4H), 7.60-7.56 (m, 2H), 7.49-7.45 (m, 4H); Known compound.<sup>1</sup>



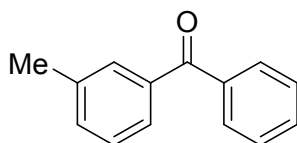
**(2-Chlorophenyl)phenyl-methanone (4b):** Solid; m. p. 44.2-47.4 °C (*lit.* 44-47 °C); IR (KBr): 1664, 1597, 1580, 1451, 1320, 1297, 1253, 1154, 1056, 936, 927, 802, 766, 744, 693, 636 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS, ppm): δ 7.81 (d, *J* = 7.9 Hz, 2H), 7.61-7.58 (m, 1H), 7.48-7.36 (m, 6H); Known compound.<sup>2</sup>



**(3-Chlorophenyl)(phenyl)methanone (4c):** Solid; m. p. 85.3-87.2 °C (*lit.* 85-87 °C); IR (KBr): 1653, 1568, 1423, 1314, 1279, 1076, 961, 897, 765, 718, 697, 682 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS, ppm): δ 7.78 (d, *J* = 8.2 Hz, 3H), 7.66 (d, *J* = 7.5 Hz, 1H), 7.63-7.59 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.51-7.47 (m, 2H), 7.44-7.40 (m, 1H); Known compound.<sup>2</sup>

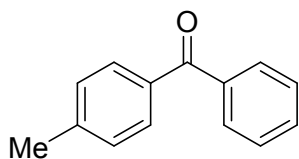


**4-Chlorobenzophenone (4d):** Solid; m. p. 93.6-95.4 °C (*lit.* 93-96 °C); IR (KBr): 1662, 1597, 1586, 1483, 1319, 1301, 1286, 1147, 1091, 976, 940, 846, 729, 696, 665, 476 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS, ppm): δ 7.78-7.73 (m, 4H), 7.62-7.57 (m, 1H), 7.50-7.44 (m, 4H); Known compound.<sup>2</sup>

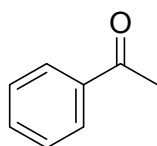


**3-Methylbenzophenone (4f):** Oil; IR (KBr): 1661, 1603, 1598, 1443, 1319, 1311, 1282, 1212, 1176, 964, 957, 779, 725, 706, 696, 643 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>,

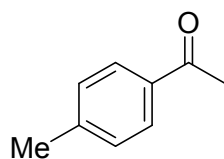
TMS, ppm):  $\delta$  7.81-7.78 (m, 2H), 7.63-7.61 (m, 1H), 7.58 -7.54 (m, 2H), 7.48 -7.43 (m, 2H), 7.39-7.32 (m, 2H), 2.40 (s, 3H); Known compound.<sup>2</sup>



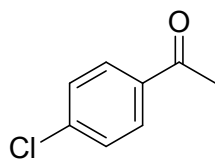
**4-Methylbenzophenone (4g):** Solid; m. p. 56.3-56.8 °C (*lit.* 56.5-57 °C); IR (KBr): 2963, 2925, 2856, 1655, 1606, 1461, 1447, 1317, 1304, 1281, 1178, 936, 922, 841, 733, 699  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , TMS, ppm):  $\delta$  7.79-7.76 (m, 2H), 7.73-7.70 (m, 2H), 7.59-7.54 (m, 1H), 7.49-7.44 (m, 2H), 7.28-7.24 (m, 2H), 2.43 (s, 3H); Known compound.<sup>2</sup>



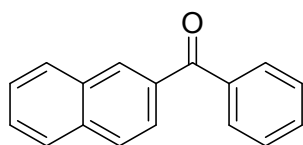
**Acetophenone (4h):** Oil; IR (film): 1685, 1597, 1449, 1383, 1303, 1245, 1176, 1094, 1050, 954, 759, 690  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400MHz,  $\text{CDCl}_3$ , TMS, ppm):  $\delta$  7.97 -7.94 (m, 2H), 7.58-7.53 (m, 1H), 7.48-7.43 (m, 2H), 2.60 (s, 3H); Known compound.<sup>1</sup>



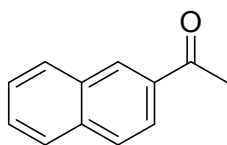
**4'-Methylacetophenone (4i):** Oil; IR (film): 1681, 1606, 1573, 1429, 1406  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400MHz,  $\text{CDCl}_3$ , TMS, ppm):  $\delta$  7.83 (d,  $J = 7.3$  Hz, 2H), 7.23 (d,  $J = 7.5$  Hz, 2H), 2.55 (s, 3H), 2.38 (s, 3H); Known compound.<sup>1</sup>



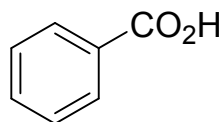
**4'-Chloroacetophenone (4j):** Oil; IR (film): 1686, 1589, 1487, 1462, 1396, 1357, 1260, 1174, 1094, 1013, 957, 821, 761, 622  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400MHz,  $\text{CDCl}_3$ , TMS, ppm):  $\delta$  7.89-7.86 (m, 2H), 7.43-7.40 (m, 2H), 2.57 (s, 3H); Known compound.<sup>1</sup>



**2-Naphthyl phenyl ketone (4k):** Solid; m. p. 76.3-81.8 °C (*lit.* 76-82 °C); IR (film): 2925, 2855, 1658, 1465, 1447, 1378, 754, 717, 698, 485 cm<sup>-1</sup>; <sup>1</sup>H NMR (400MHz, CDCl<sub>3</sub>, TMS, ppm): δ 8.27 (s, 1H), 7.95-7.85 (m, 6H), 7.65-7.50 (m, 5H); Known compound.<sup>2</sup>



**2-Acetonaphthone (4l):** Solid; m. p. 52.3-56.6 °C (*lit.* 52-56 °C); IR (film): 1677, 1625, 1468, 1433, 1366, 1282, 1270, 1194, 1128, 870, 834, 823, 756, 486 cm<sup>-1</sup>; <sup>1</sup>H NMR (400MHz, CDCl<sub>3</sub>, TMS, ppm): δ 8.46 (s, 1H), 8.03 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.90-7.86 (m, 2H), 7.62-7.53 (m, 2H), 2.72 (s, 3H); Known compound.<sup>2</sup>



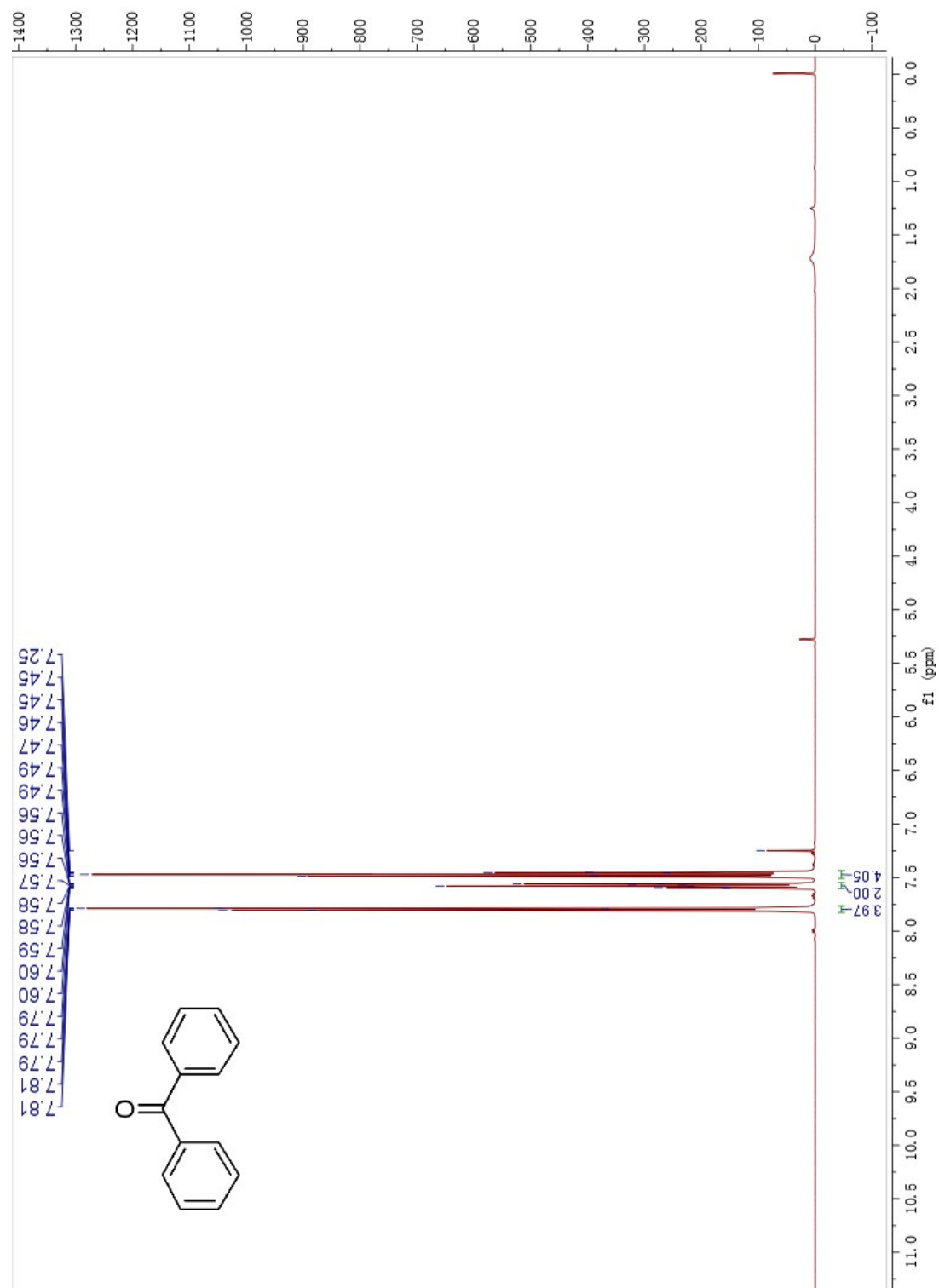
**Benzoic acid (5a):** Solid; m. p. 121.3-122.6 °C (*lit.* 122.13 °C); IR (KBr): 1689, 1464, 1426, 1327, 1294, 943, 936, 708 cm<sup>-1</sup>; <sup>1</sup>H NMR (400MHz, CDCl<sub>3</sub>, TMS): δ 8.14 – 8.12 (m, 2H), 7.65 – 7.60 (m, 1H), 7.51 – 7.47 (m, 2H) ; Known compound.<sup>2</sup>

## References

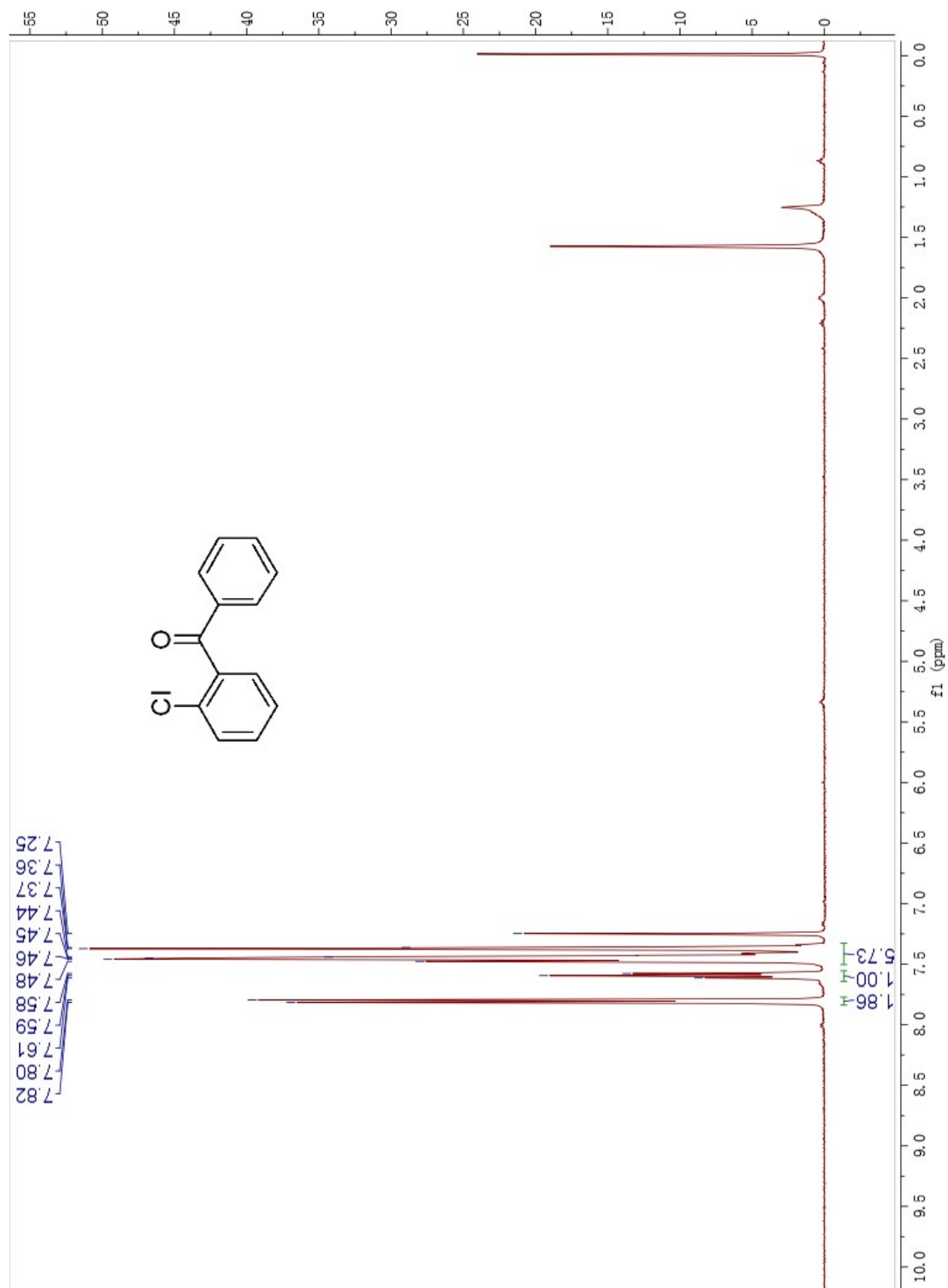
1. T.-T. Wang, X.-B. Jing, C. Chen and L. Yu, *J. Org. Chem.*, 2017, **82**, 9342
2. Spectral Database for Organic Compounds, SDBS.  
[http://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct\\_frame\\_top.cgi](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi).

# <sup>1</sup>H NMR Spectra of the Products

**4a**, <sup>1</sup>H NMR, CDCl<sub>3</sub>, 400 MHz

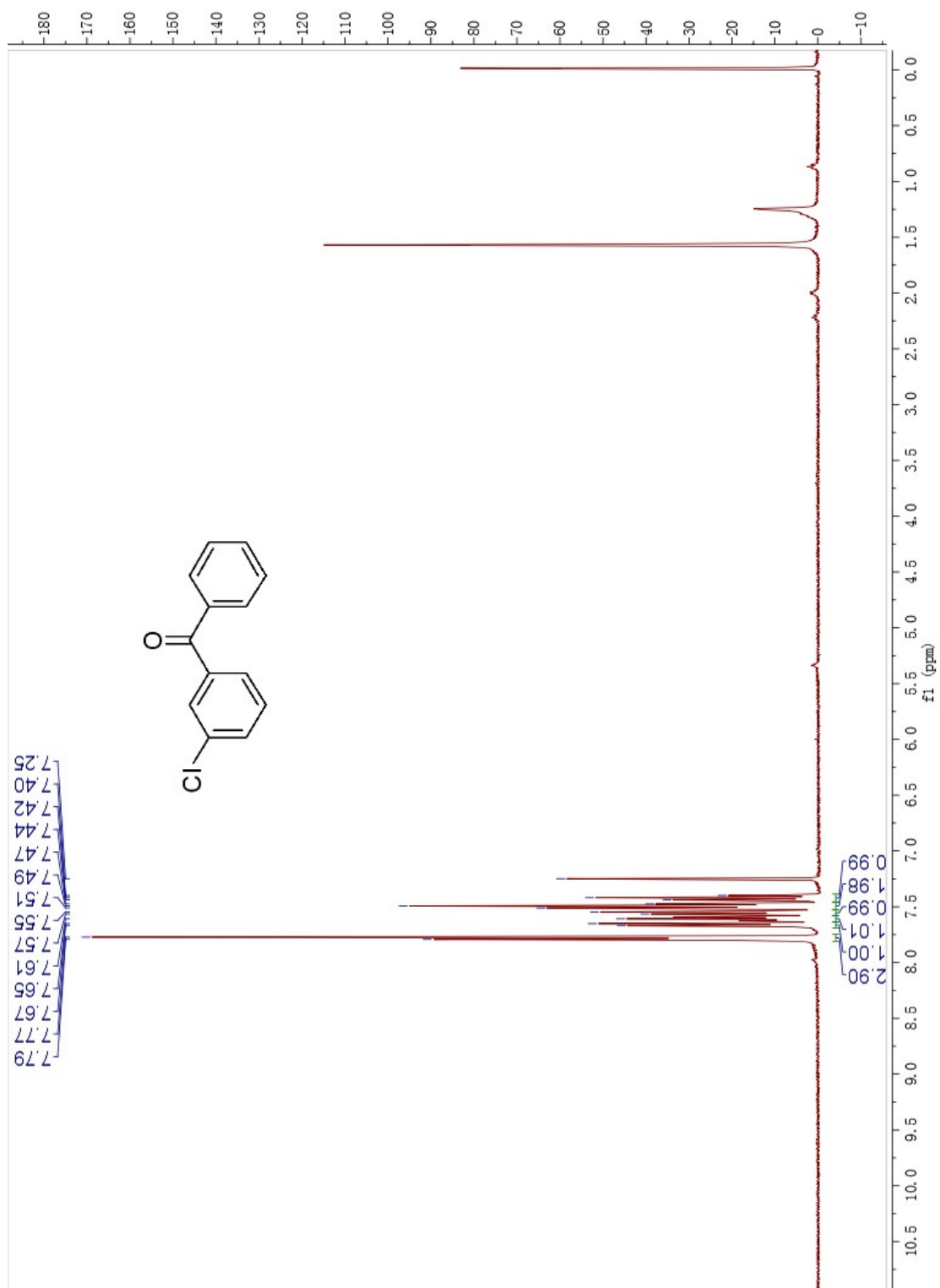


**4b**,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz

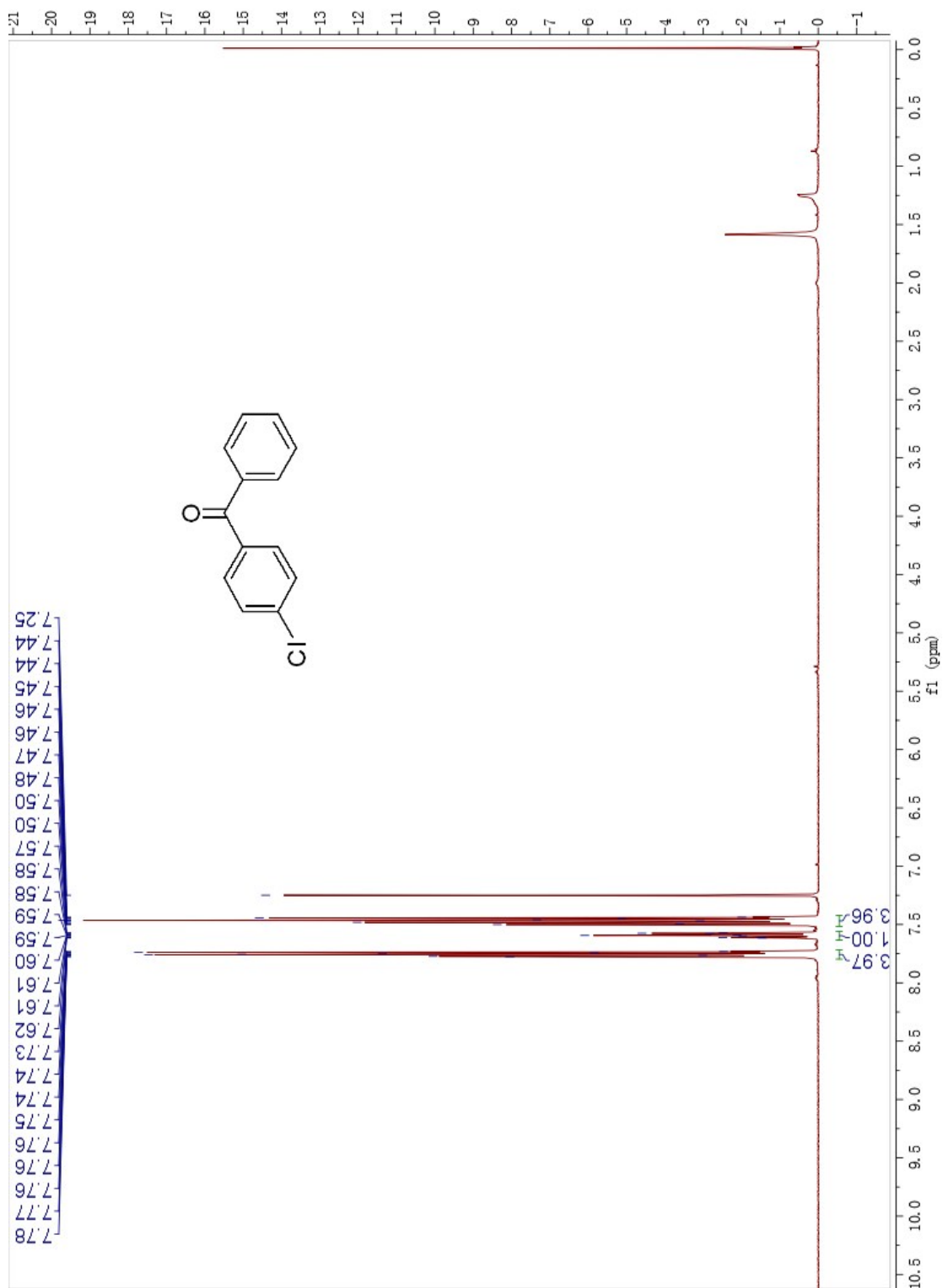




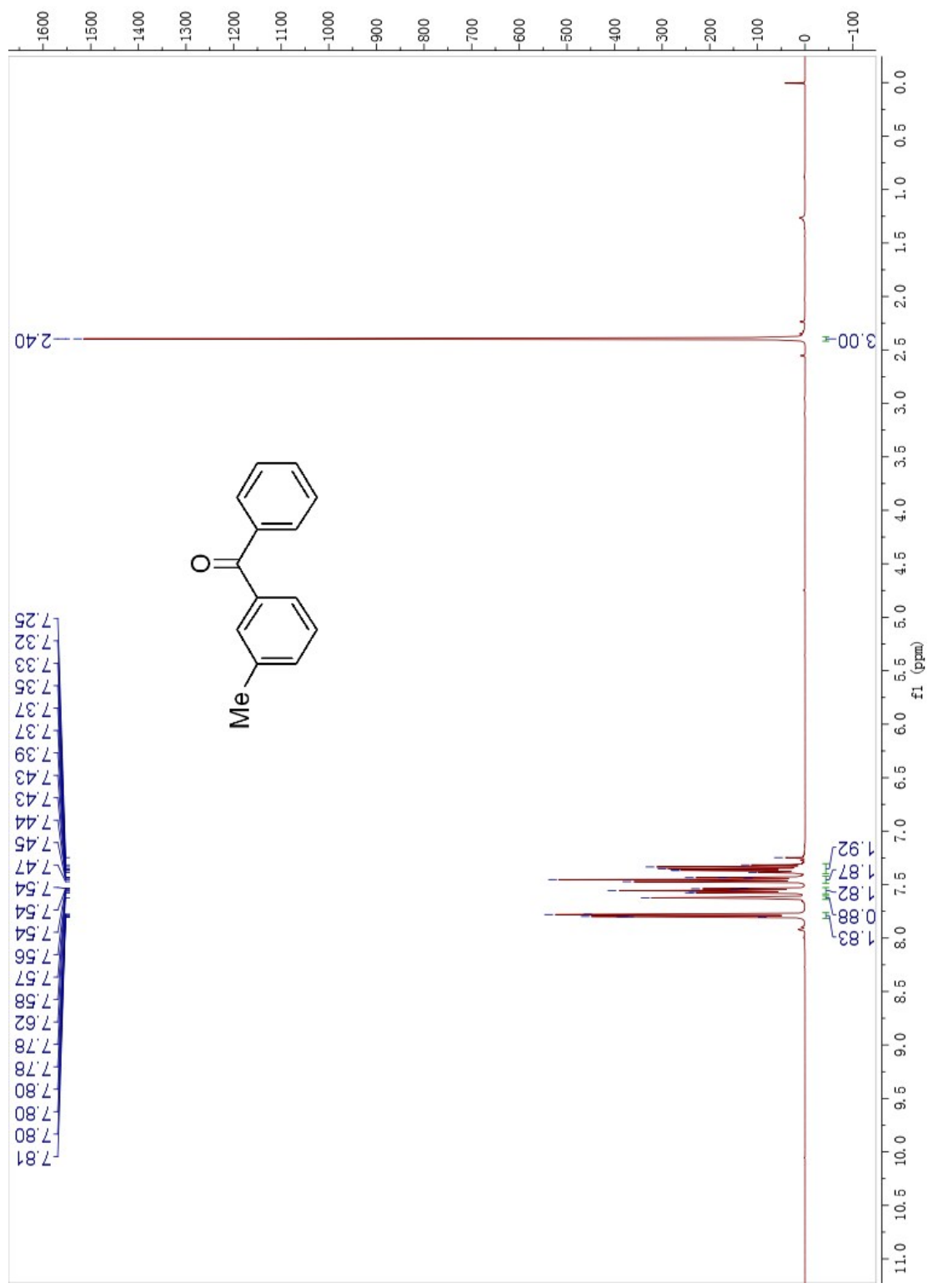
4c,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz



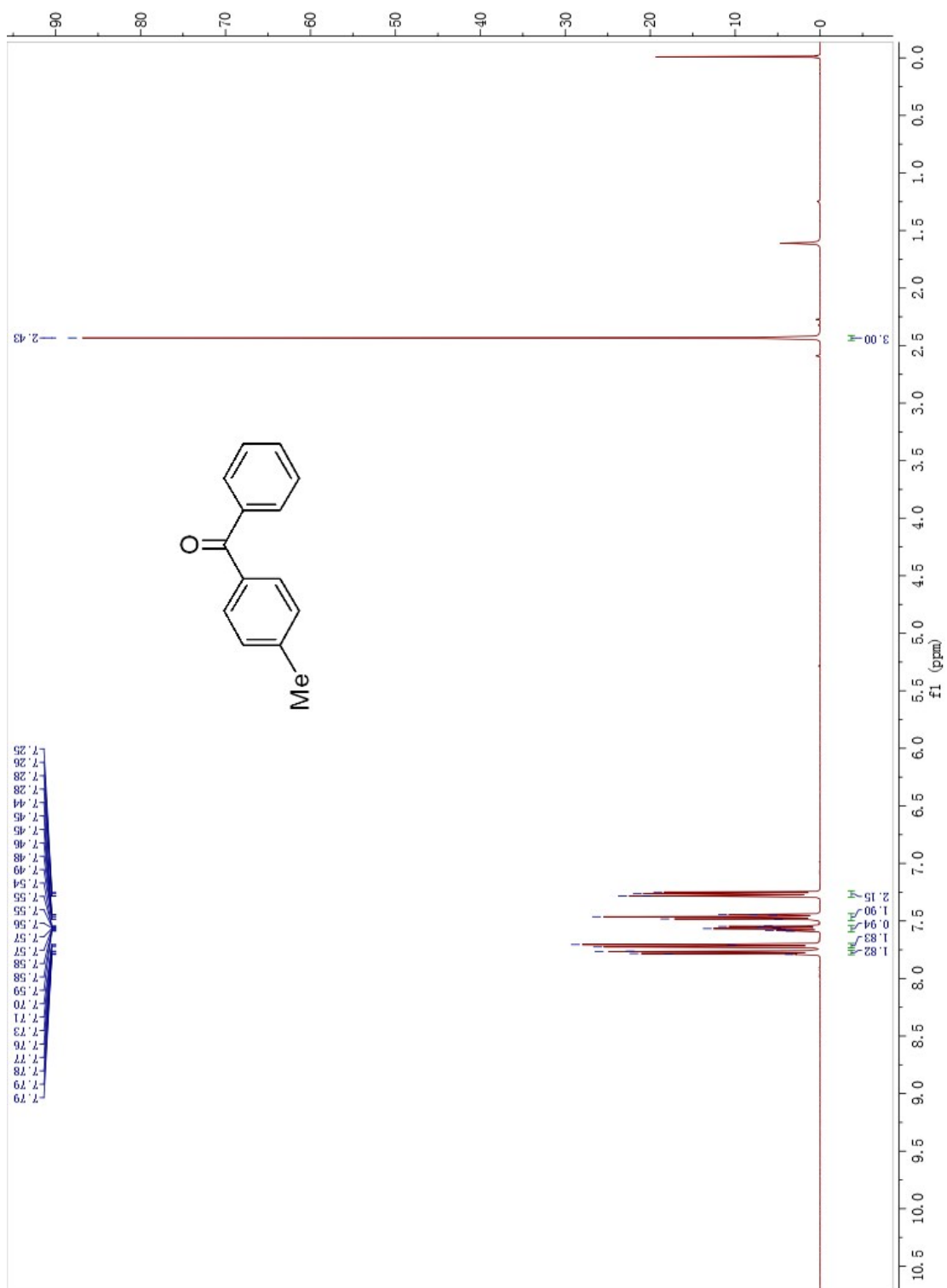
4d, <sup>1</sup>H NMR, CDCl<sub>3</sub>, 400 MHz



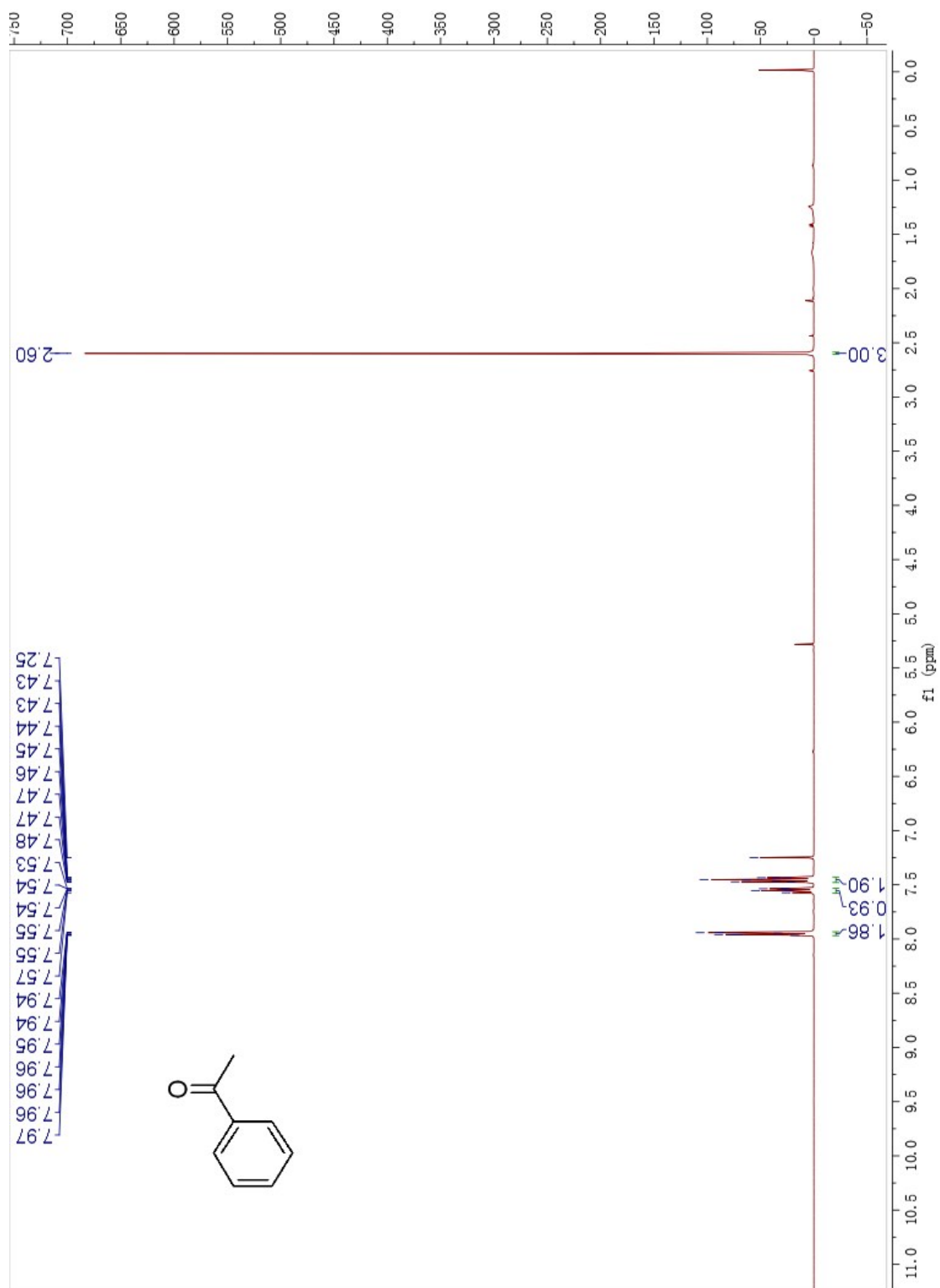
4f, <sup>1</sup>H NMR, CDCl<sub>3</sub>, 400 MHz



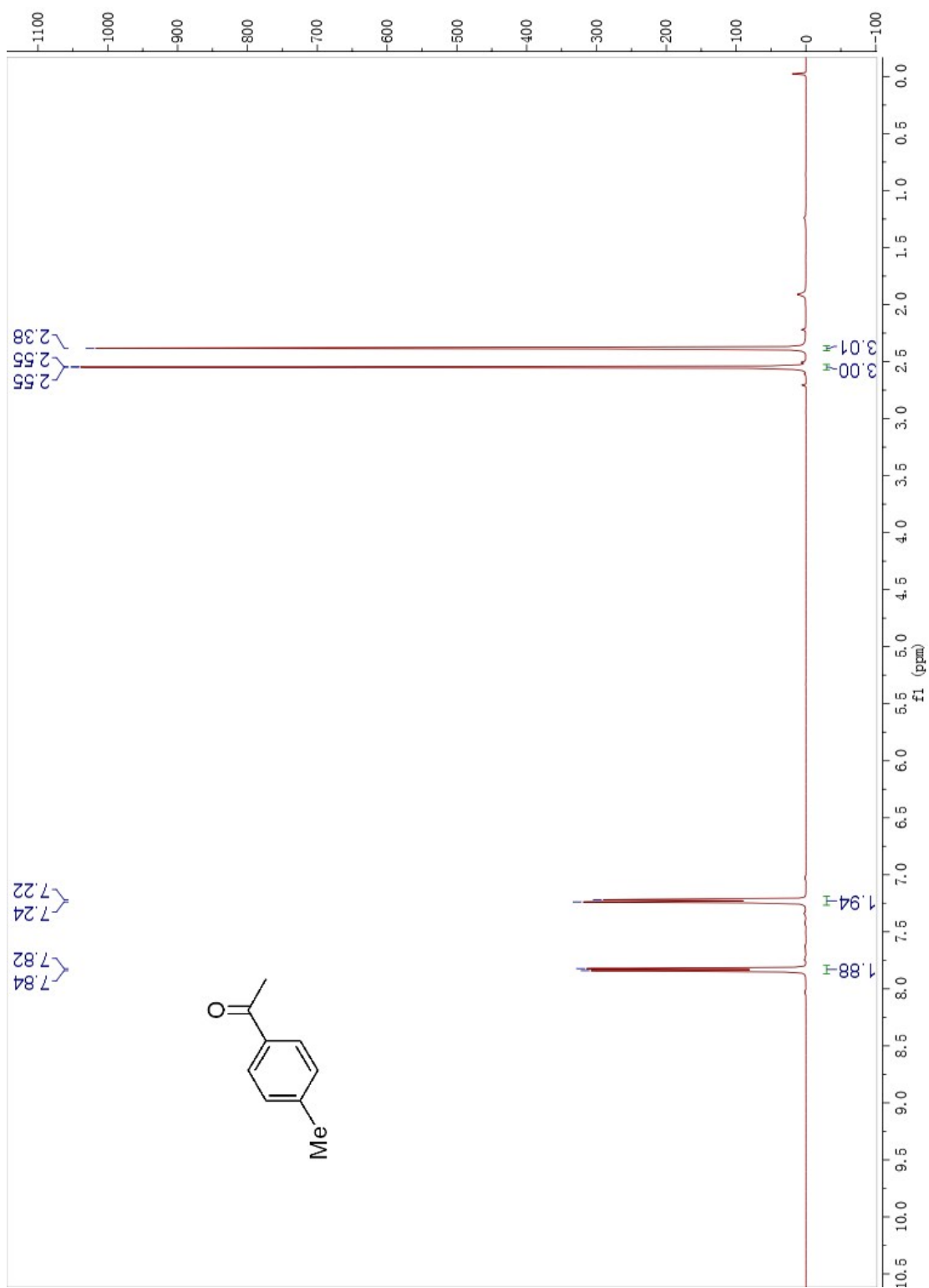
4g,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz



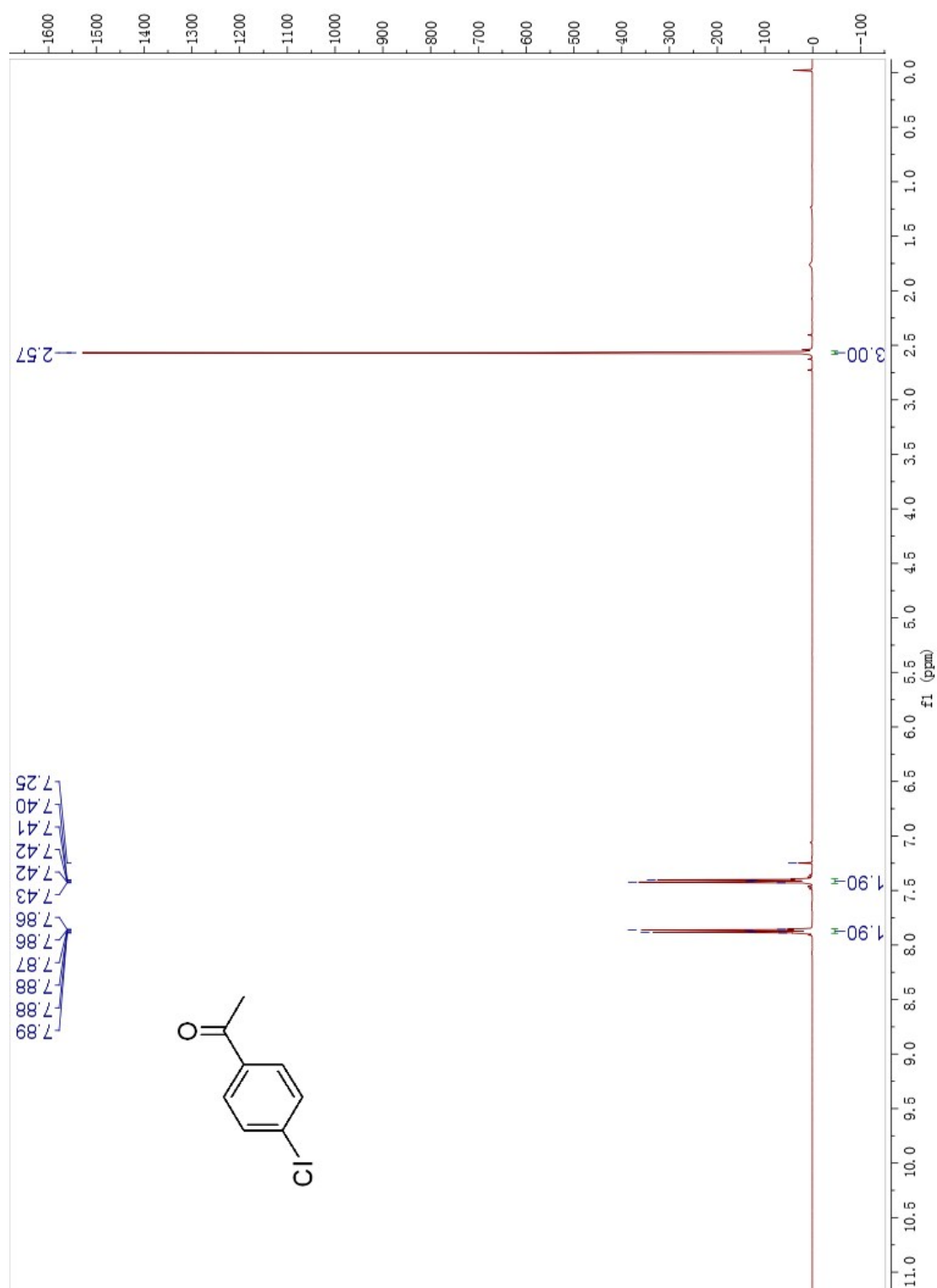
**4h**,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz



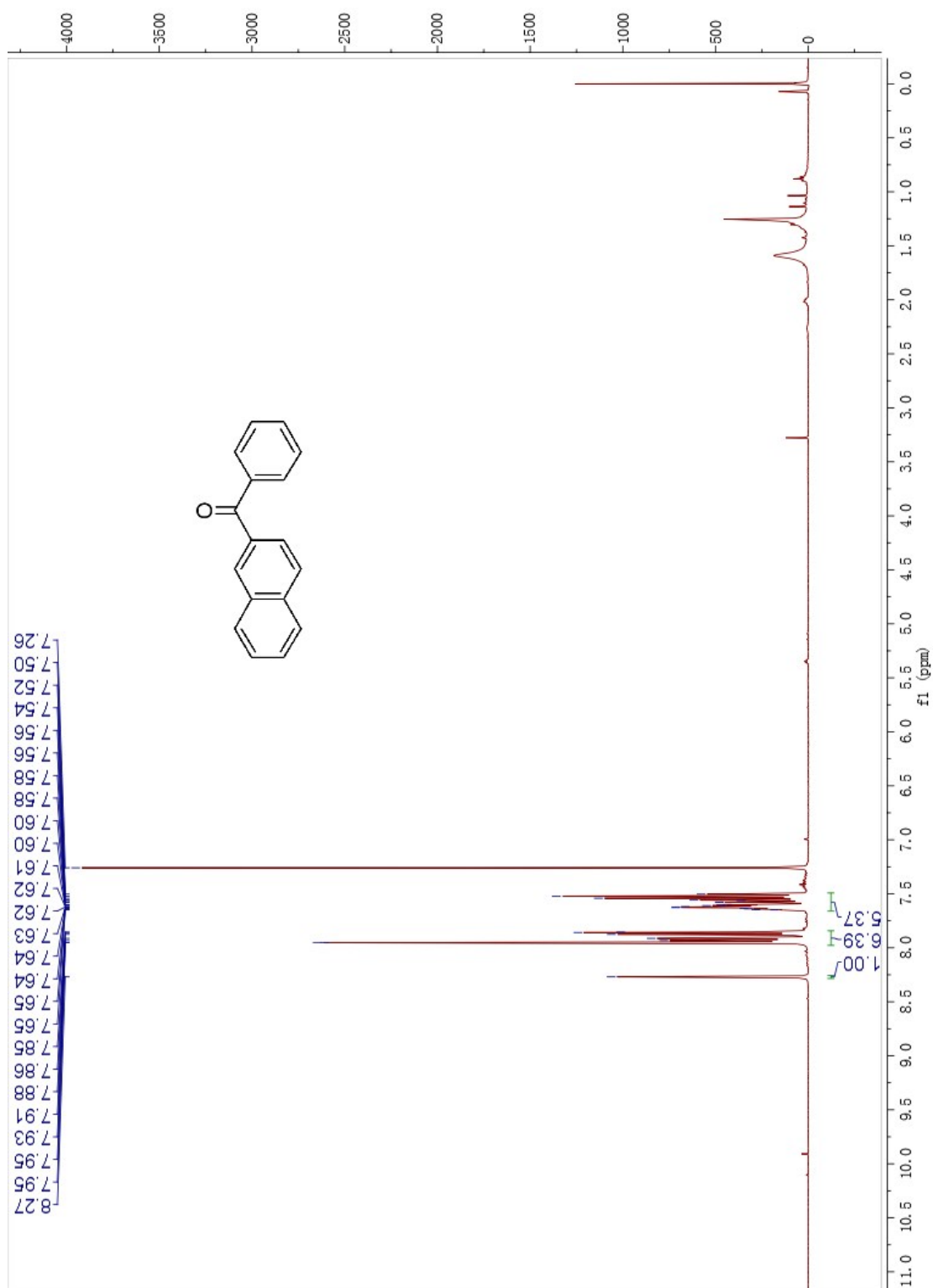
4i,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz



4j,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz

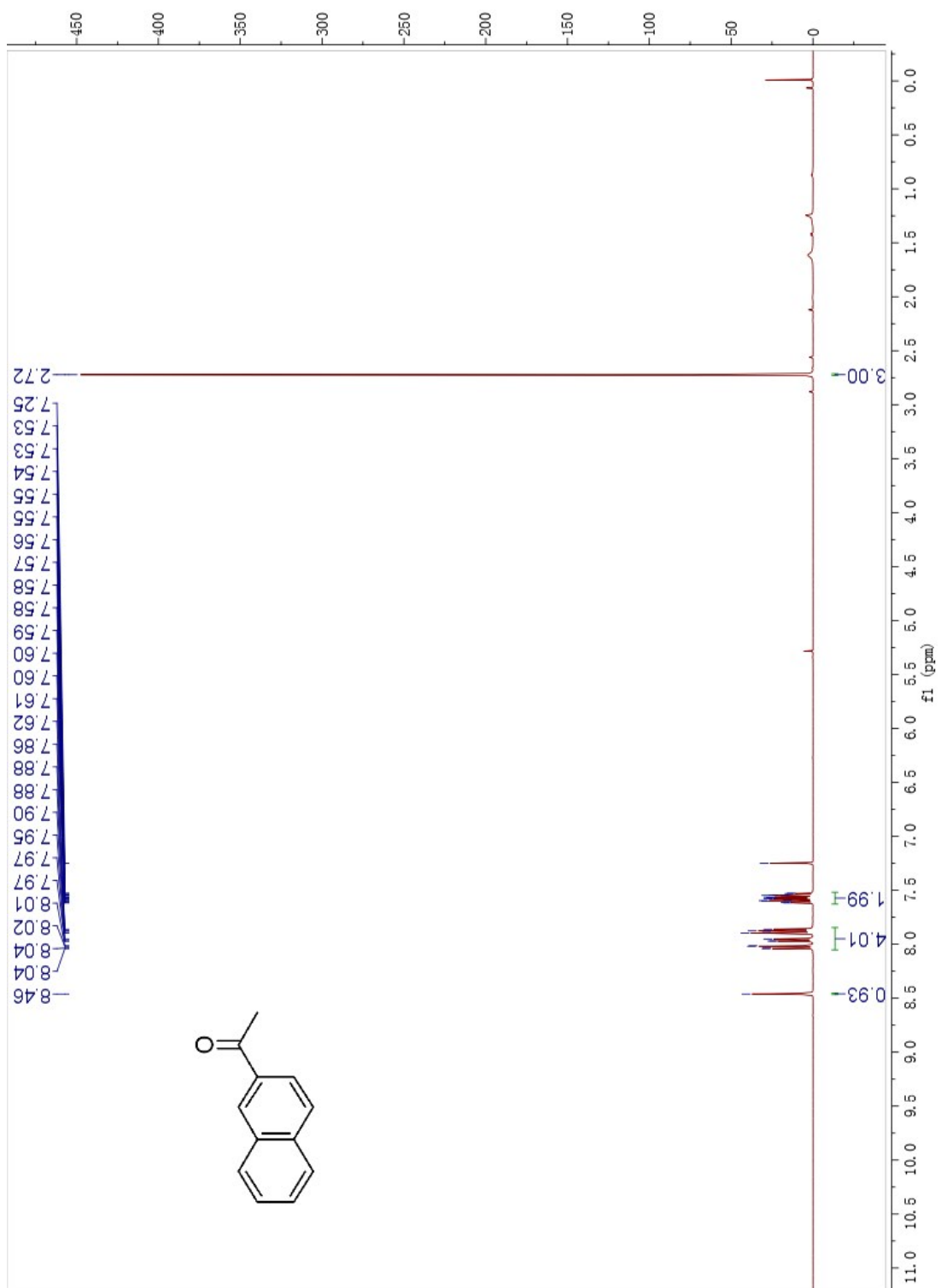


4k,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz





4l,  $^1\text{H}$  NMR,  $\text{CDCl}_3$ , 400 MHz



5a, <sup>1</sup>H NMR, CDCl<sub>3</sub>, 400 MHz

