Supporting information

NHPI and Ferric Nitrate: A Mild and Selective System for Aerobic Oxidation of Benzylic Methylenes

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Experiment of ^{18}O isotopic labeling with $^{18}O_2$ for the oxidation of diphenylmethane: After a 15 mL test tube containing diphenylmethane (1 mmol), $Fe(NO_3)_3 \cdot 9H_2O$ (8 mol%) and NHPI (10 mol%) was evacuated several times, $^{18}O_2$ was added by syringe. Then 1.5 mL of degassed acetonitrile was added to the above mixture and the solution was stirred for 40 h at 25 °C. After the reaction was quenched by $Na_2S_2O_3$ solution, the product was analyzed by GC-MS.

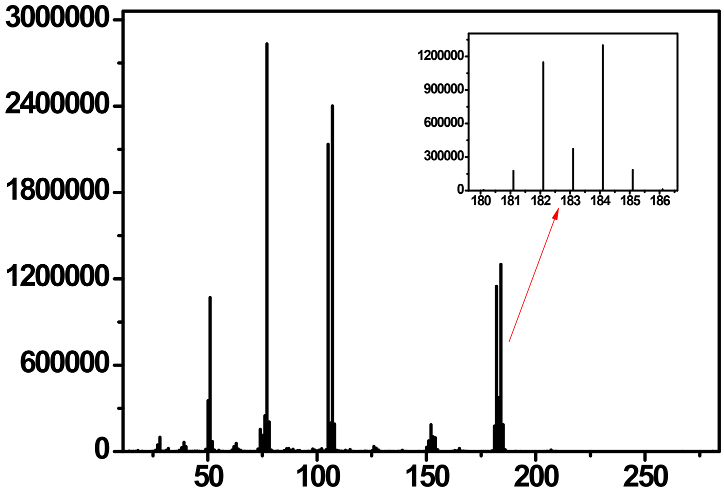
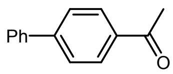
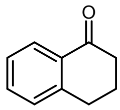


Figure S1. MS of ^{18}O isotopic labeling with $^{18}O_2$ for the oxidation of diphenylmethane.

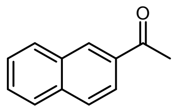
2. Characterization of the products



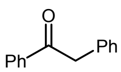
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.93 (m, 2H), 7.67-7.59 (m, 2H), 7.59-7.53 (m, 2H), 7.45-7.37 (m, 2H), 7.37-7.30 (m, 1H), 2.57 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 145.8, 134.0, 135.9, 129.0, 128.9, 128.3, 127.3, 127.2, 26.7. GC-MS (EI) m/z: 196.1.



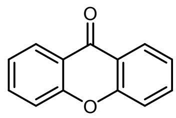
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J = 7.8, 0.8 Hz, 1H), 7.39 (td, J = 7.5, 1.3 Hz, 1H), 7.28-7.13 (m, 2H), 2.90 (t, J = 6.1 Hz, 2H), 2.64-2.51 (m, 2H), 2.14-2.01 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.4, 143.5, 132.4, 131.6, 127.8, 126.1, 125.6, 38.2, 28.7, 22.3. GC-MS (EI) m/z: 146.1.



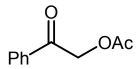
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.04 (dd, J = 8.6, 1.7 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.94-7.86 (m, 2H), 7.59 (dtd, J = 14.8, 6.9, 1.3 Hz, 2H), 2.74 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.1, 135.6, 134.5, 132.5, 130.2, 129.6, 128.5, 128.4, 127.8, 126.8, 123.9, 26.7. GC-MS (EI) m/z: 170.1.



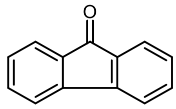
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.88 (m, 2H), 7.54-7.34 (m, 3H), 7.33-7.10 (m, 5H), 4.21 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.6, 136.6, 134.6, 133.2, 129.5, 128.7, 128.67, 128.64, 127.0, 45.5. GC-MS (EI) m/z: 196.1.



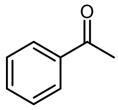
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (dd, J = 8.0, 1.5 Hz, 2H), 7.63 (ddd, J = 8.7, 7.1, 1.7 Hz, 2H), 7.40 (dd, J = 8.5, 0.6 Hz, 2H), 7.29 (ddd, J = 8.1, 7.2, 1.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.2, 155.1, 133.8, 125.7, 122.9, 120.8, 116.9. GC-MS (EI) m/z: 196.1.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.4 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 2H), 5.28 (s, 2H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.1, 169.4, 133.2, 132.9, 127.9, 126.7, 65.0, 19.6. GC-MS (EI) m/z: 178.1.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.4 Hz, 2H), 7.53-7.41 (m, 4H), 7.32-7.23 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 144.4, 134.7, 134.1, 129.1, 124.3, 120.3. GC-MS (EI) m/z: 180.1.



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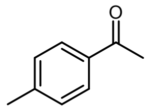

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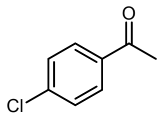

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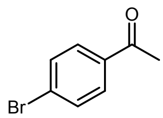

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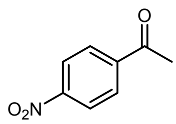

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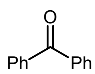

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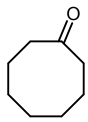
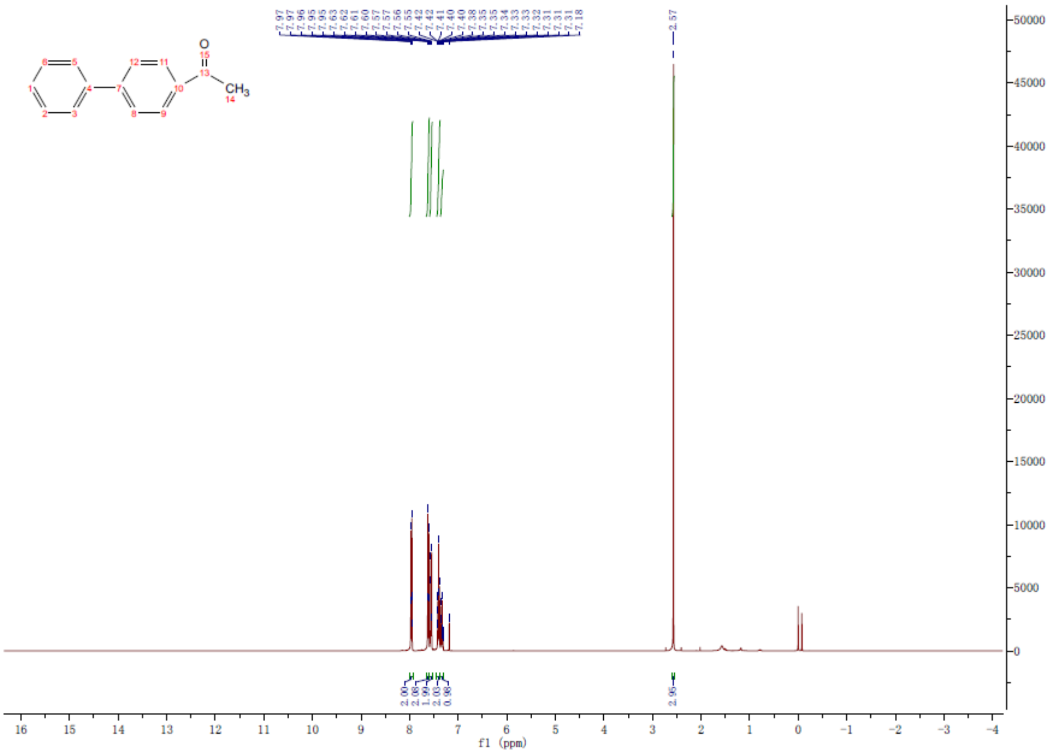
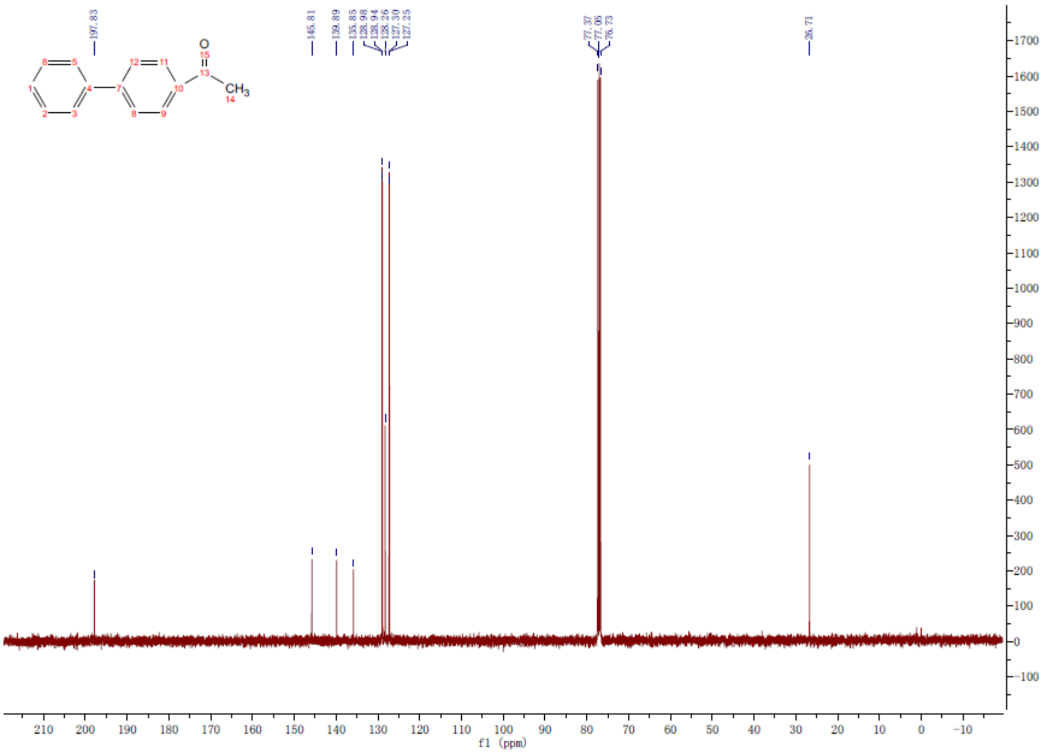
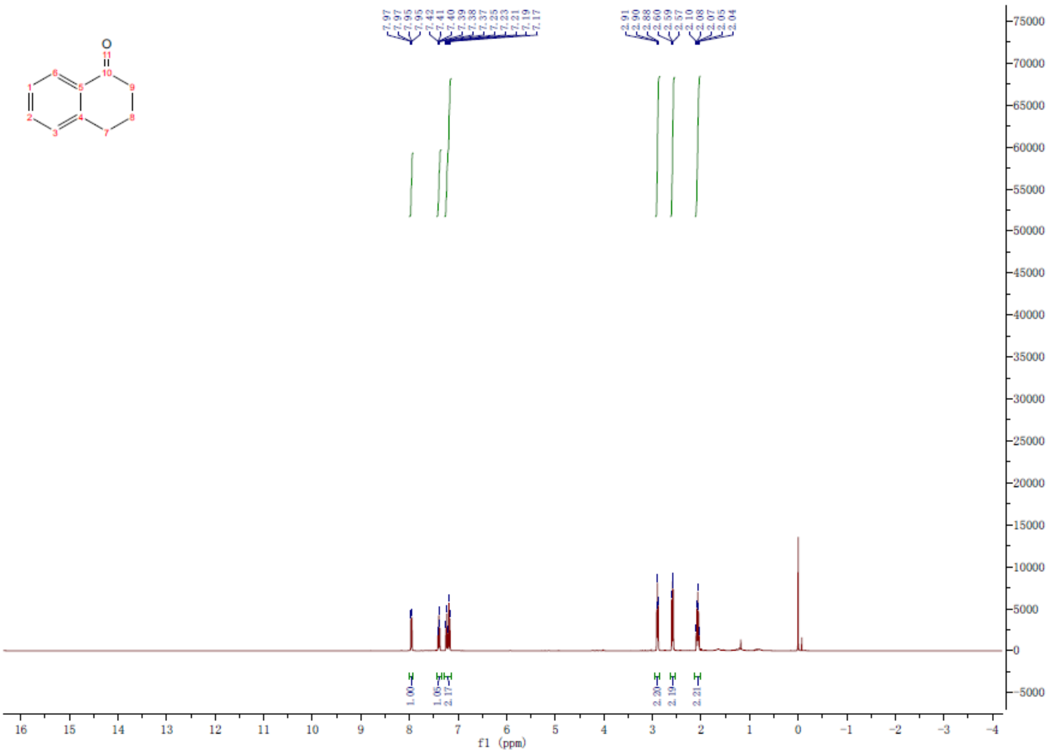


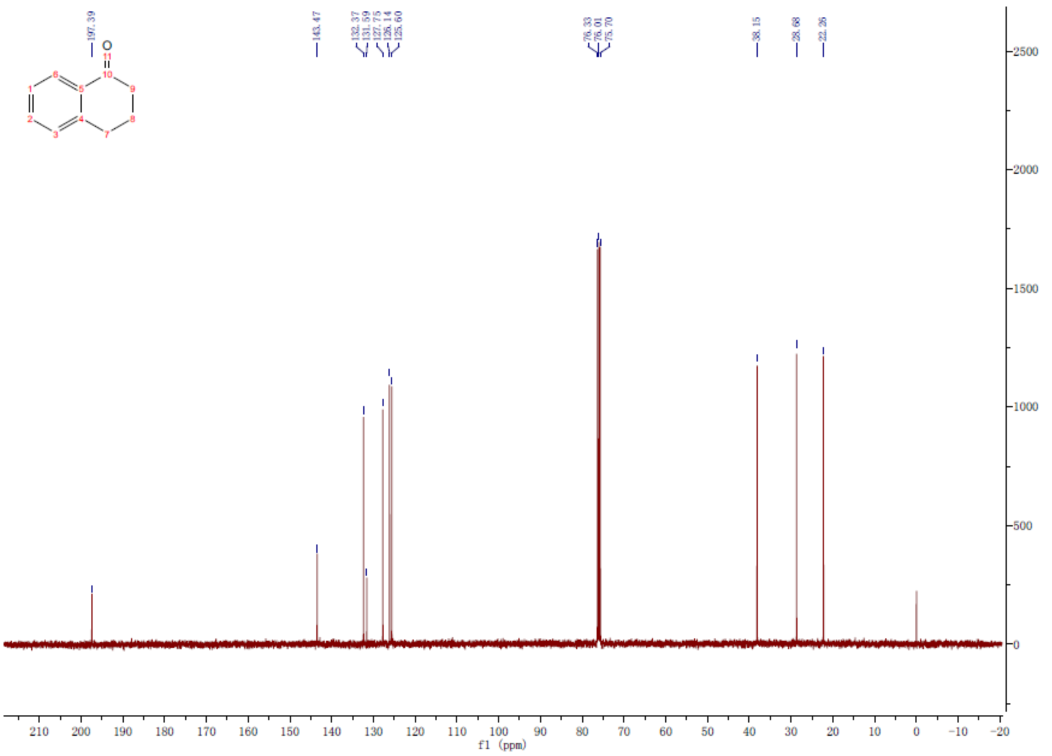
GC-MS (EI) m/z: 126.1.

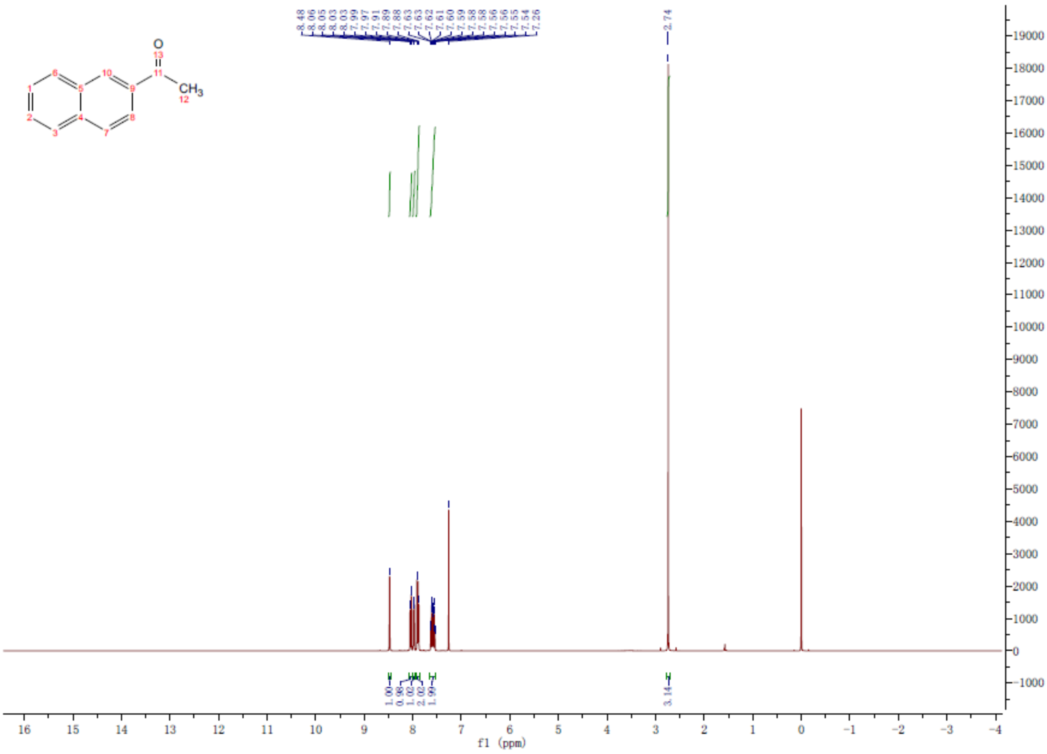
3. ¹H and ¹³C NMR spectra of the products







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7.58
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1.02
1.02
2.02
1.99
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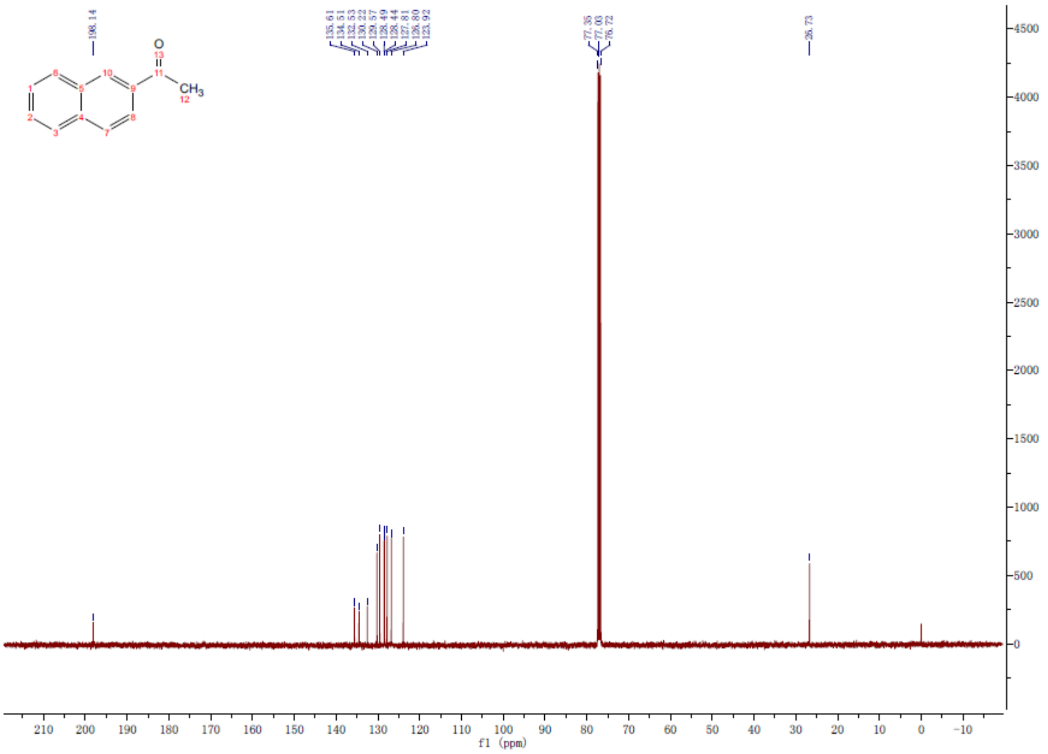
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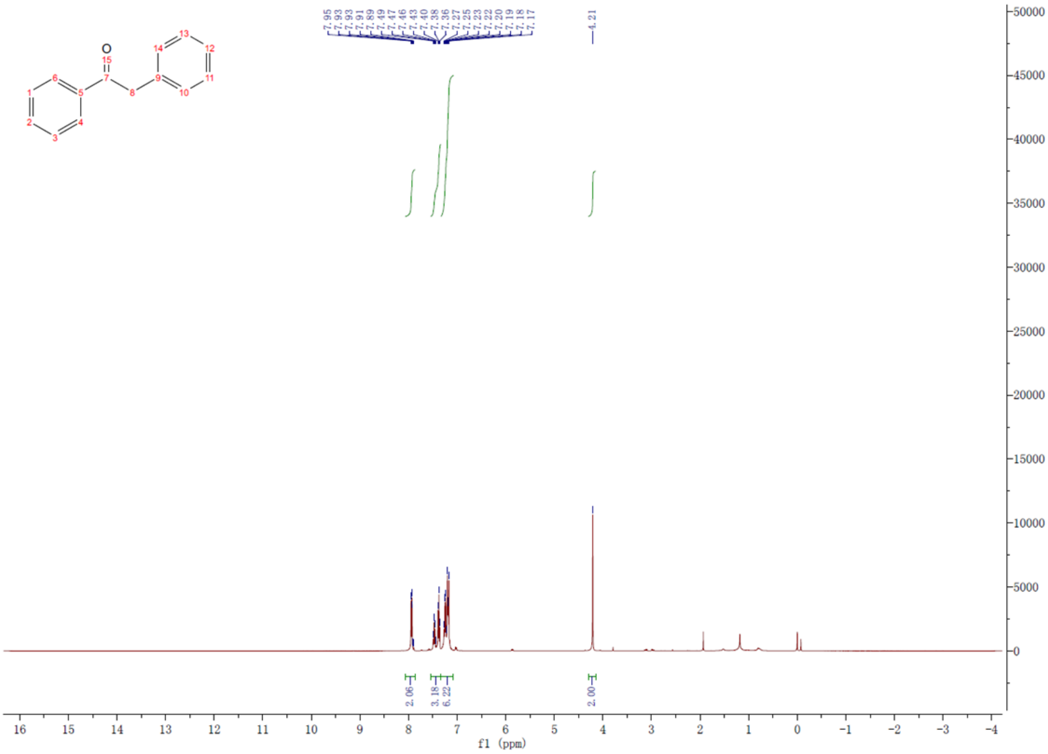

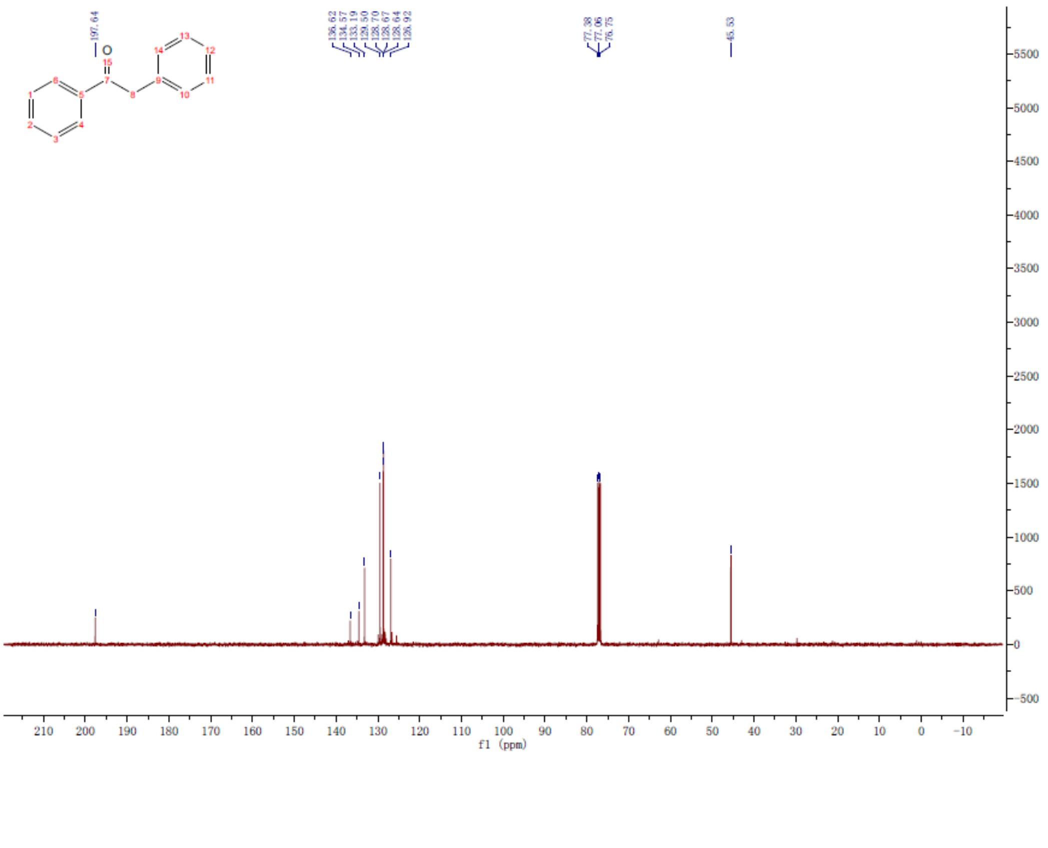

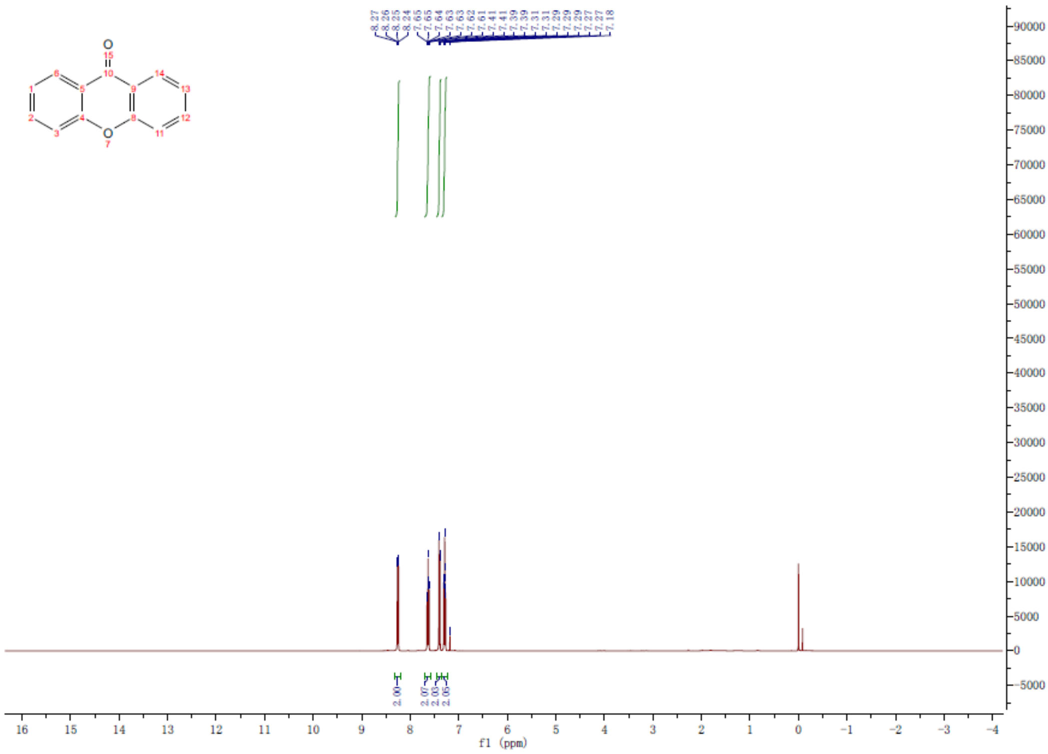
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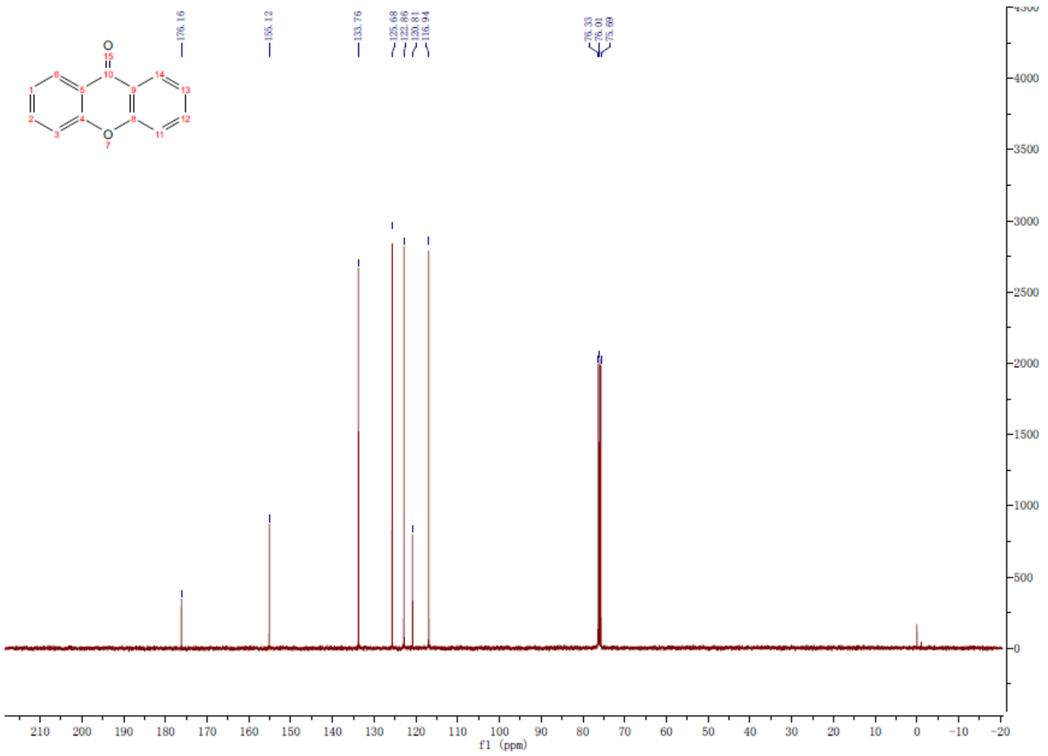
2.06
f1 (ppm)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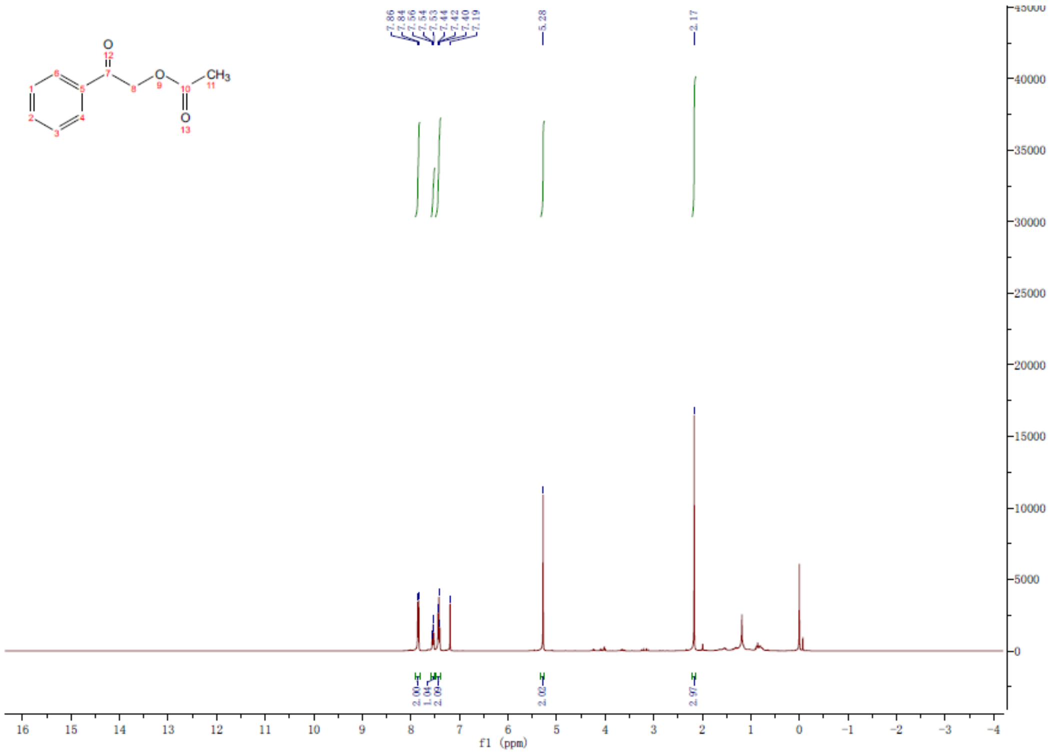
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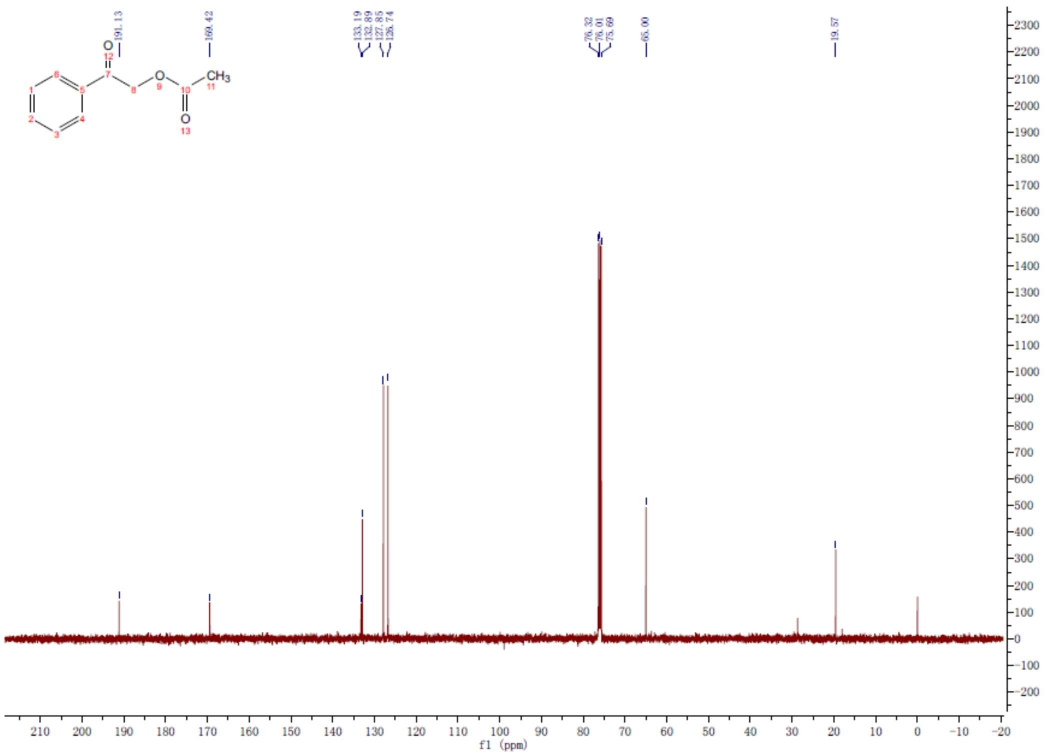
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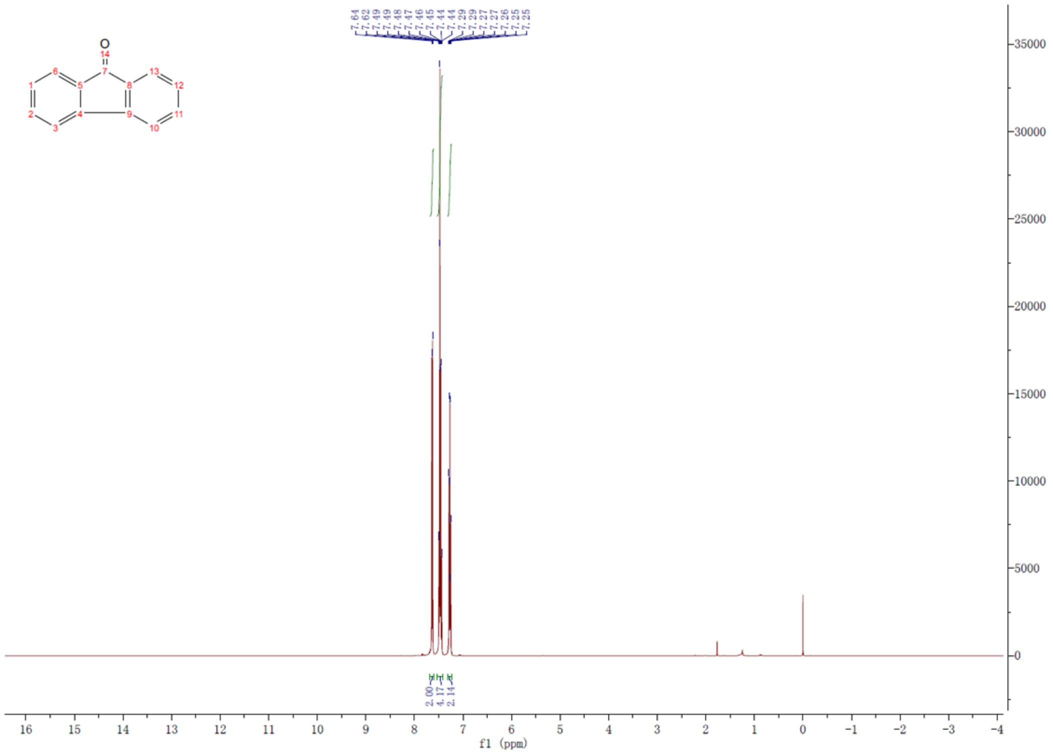
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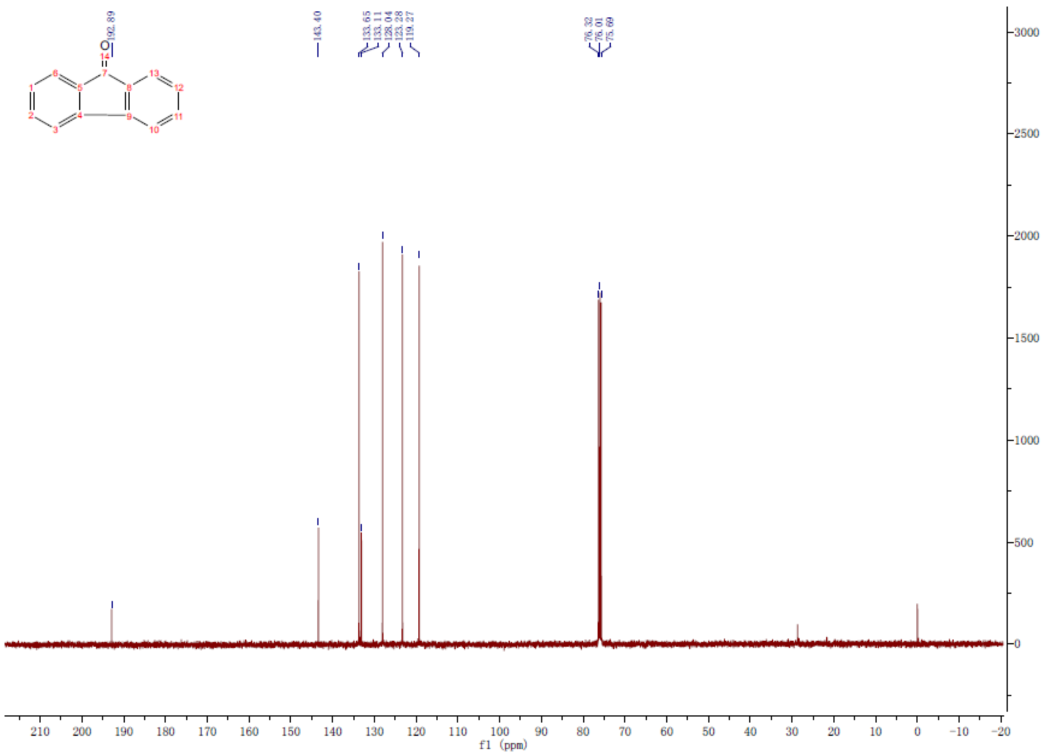
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f1 (ppm)