Supplementary Material

Catalyst-free rapid conversion of arylboronic acids to phenols under green condition

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Experimental part

Reactions were carried out using commercial available reagents in over-dried apparatus. H_2O_2 and ethanol was commercially available and used directly. All the products are known compounds and reported by previous work.

General procedure for the oxidation using H_2O_2

A 25 ml flask was charged with phenylboronic acid (1 mmol). Then 1.6 mL H_2O_2 was added under stirring. The reaction was stirred for 1 min, then quenched by water (10 ml). The aqueous layer was extracted with 20 mL ethyl acetate for three times. The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The pure product was obtained without flash column chromatography and the purity was determine by TLC (thin layer chromatography).

General procedure for the oxidation using H_2O_2

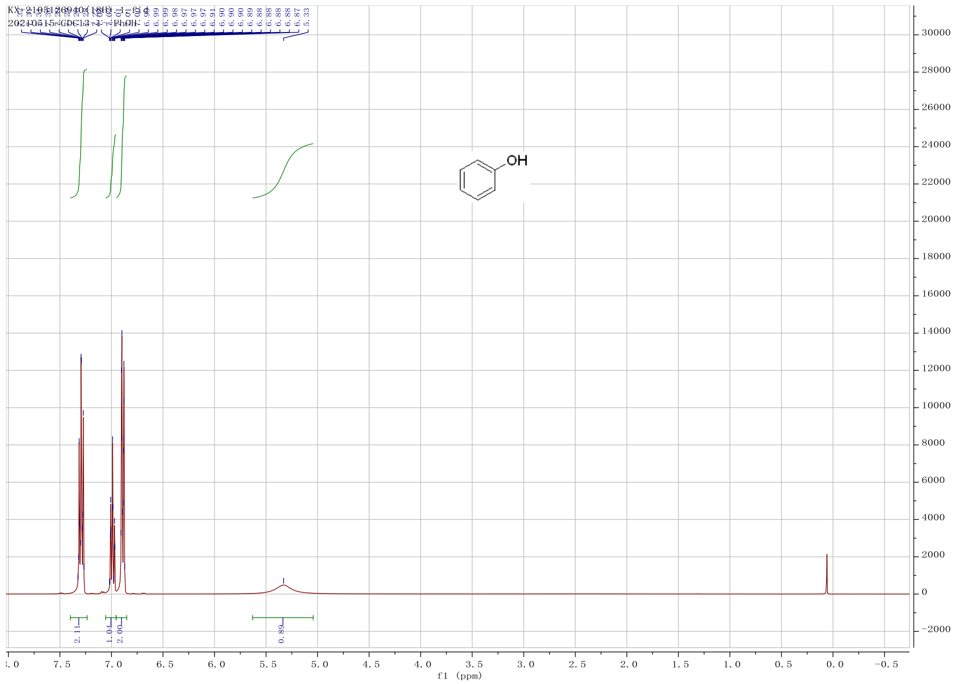
A 25 ml flask was charged with phenylboronic acid (1 mmol). Then 1.6 mL H_2O_2 and 1 mL EtOH were added under stirring. The reaction was stirred for 1 min, then quenched by water (10 ml). The aqueous layer was extracted with 20 mL ethyl acetate for three times. The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The pure product was obtained without flash column chromatography and the purity was determine by TLC.

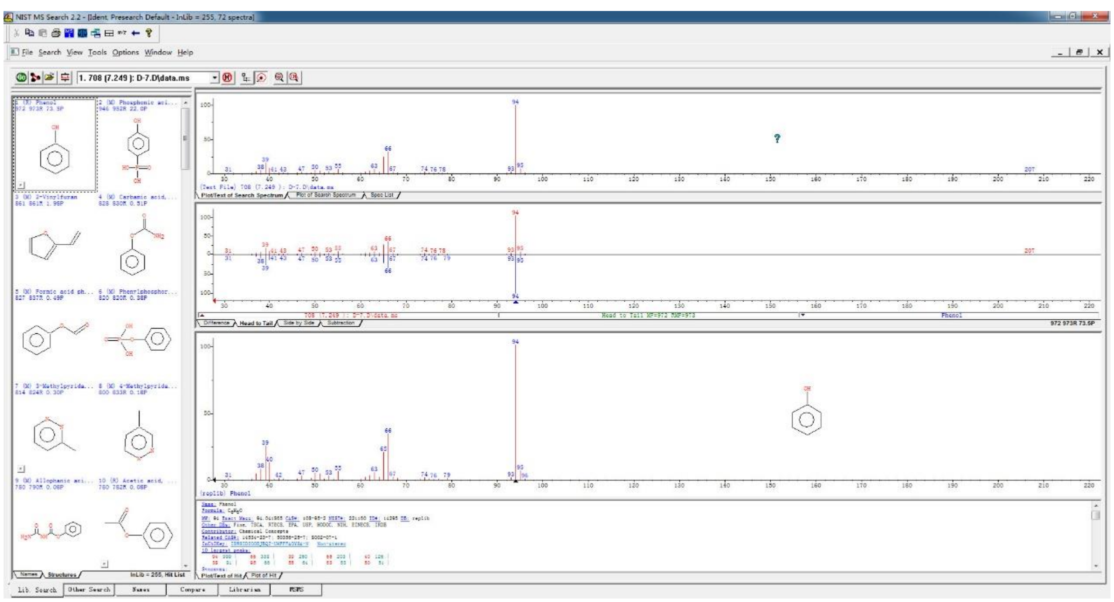
Characterization of the obtained oxidative product

All the products were known compounds. ^{1}H NMR data and GC-MS spectra of the products were in agreement with the experimental values from NIST.

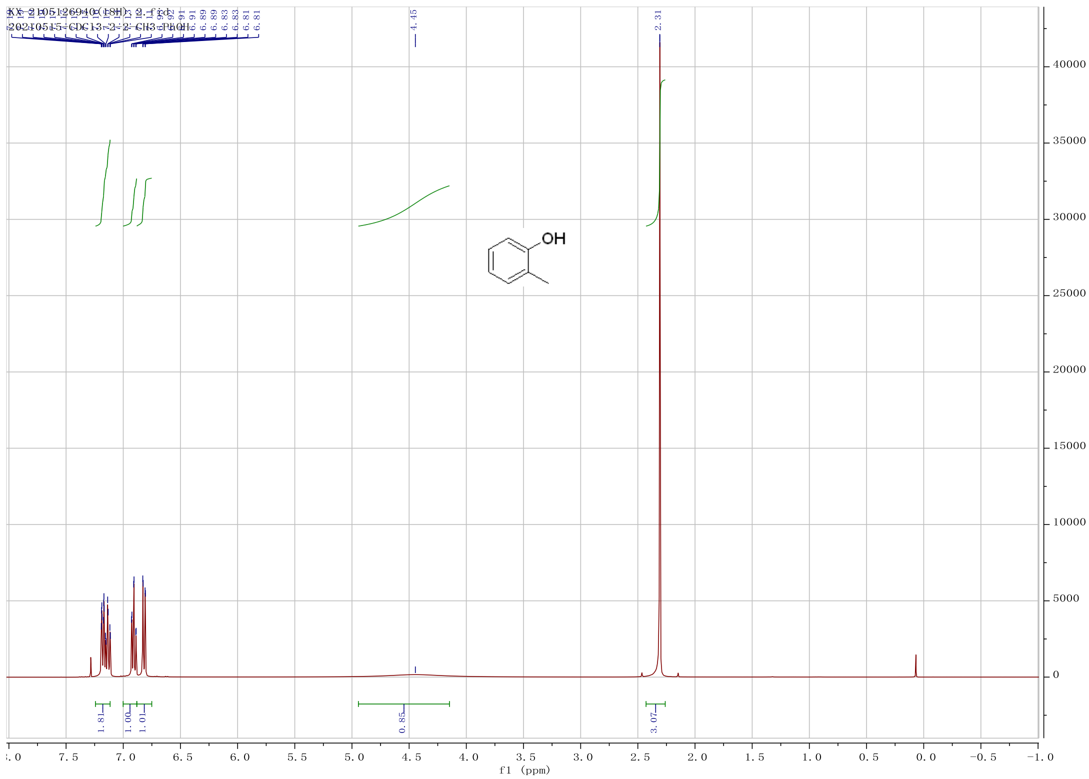
https://webbook.nist.gov/chemistry/

2a, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.24 (m, 2H), 6.99 (tt, *J* = 7.3, 1.1 Hz, 1H), 6.95 – 6.85 (m, 2H), 5.33 (s, 1H). calcd for C6H6O 94.0419, found 94.0.

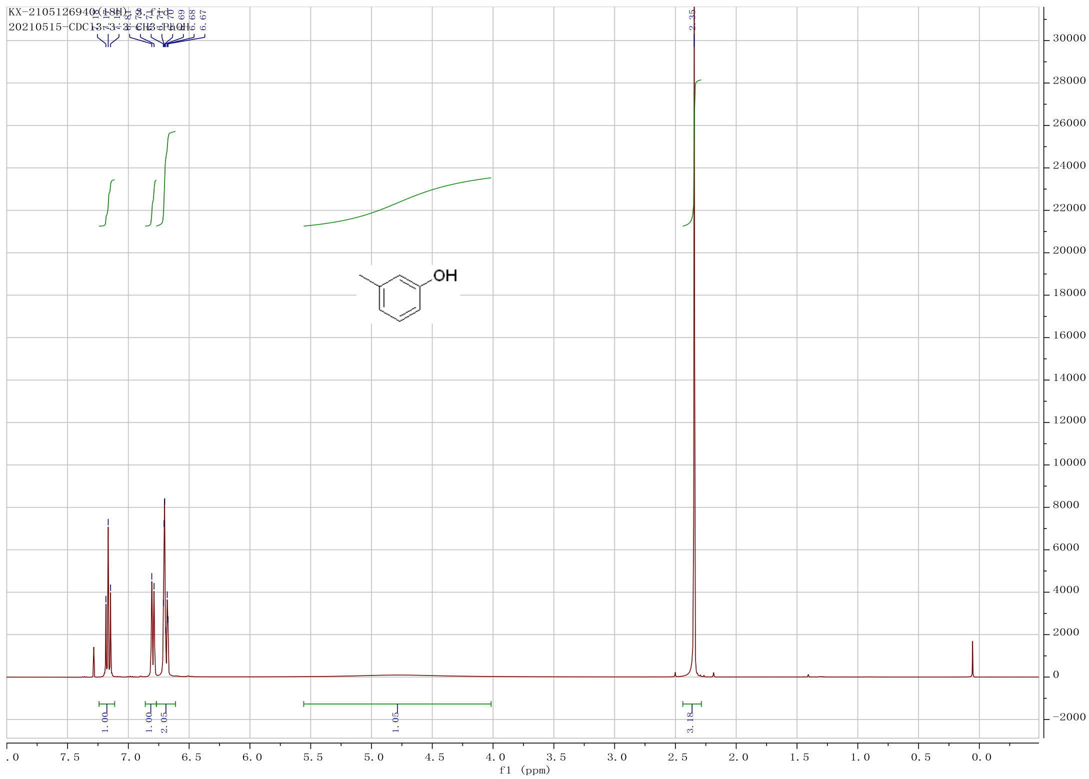


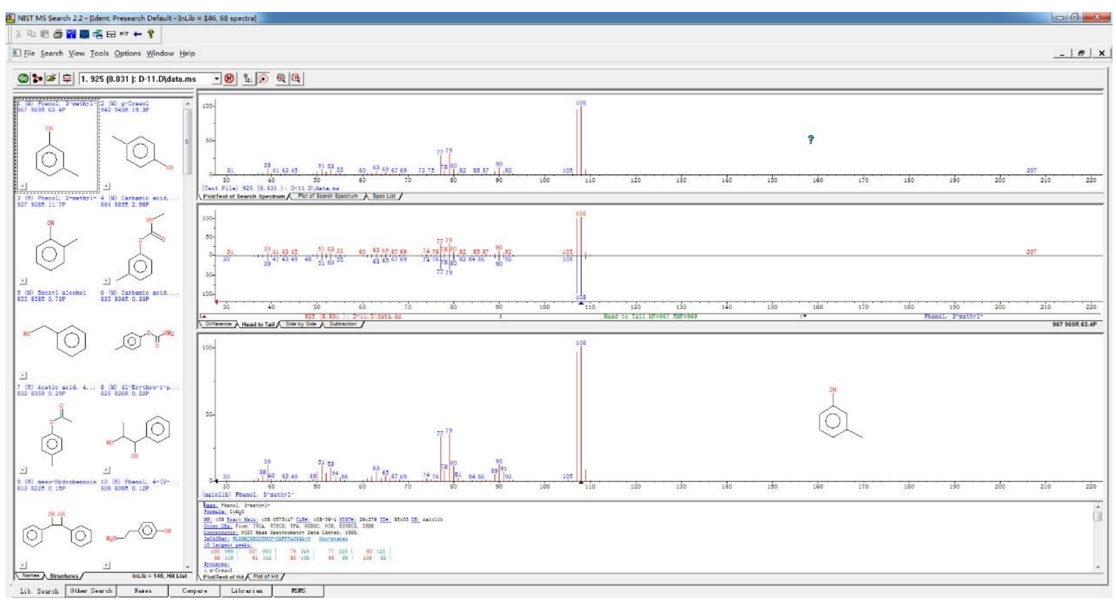


2b, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.24 – 7.11 (m, 2H), 6.91 (td, *J* = 7.4, 1.2 Hz, 1H), 6.82 (dd, *J* = 8.0, 1.2 Hz, 1H), 4.45 (s, 1H), 2.31 (s, 3H). calcd for C_7H_8O 108.0575, found 108.0.

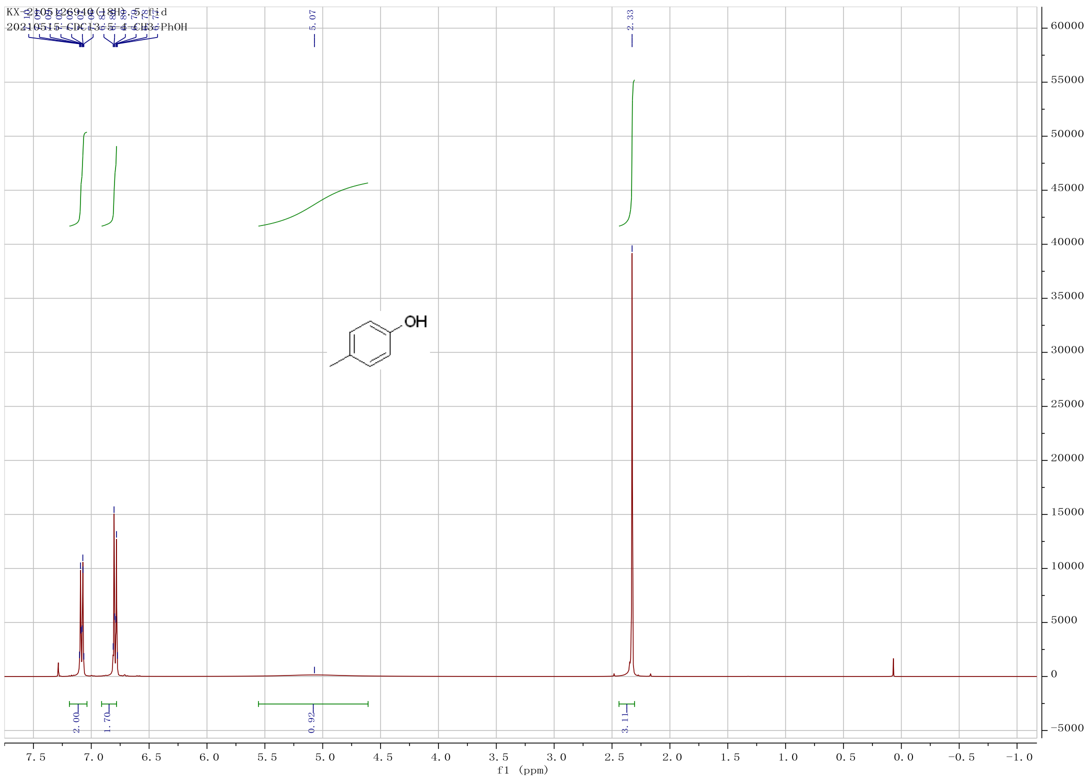


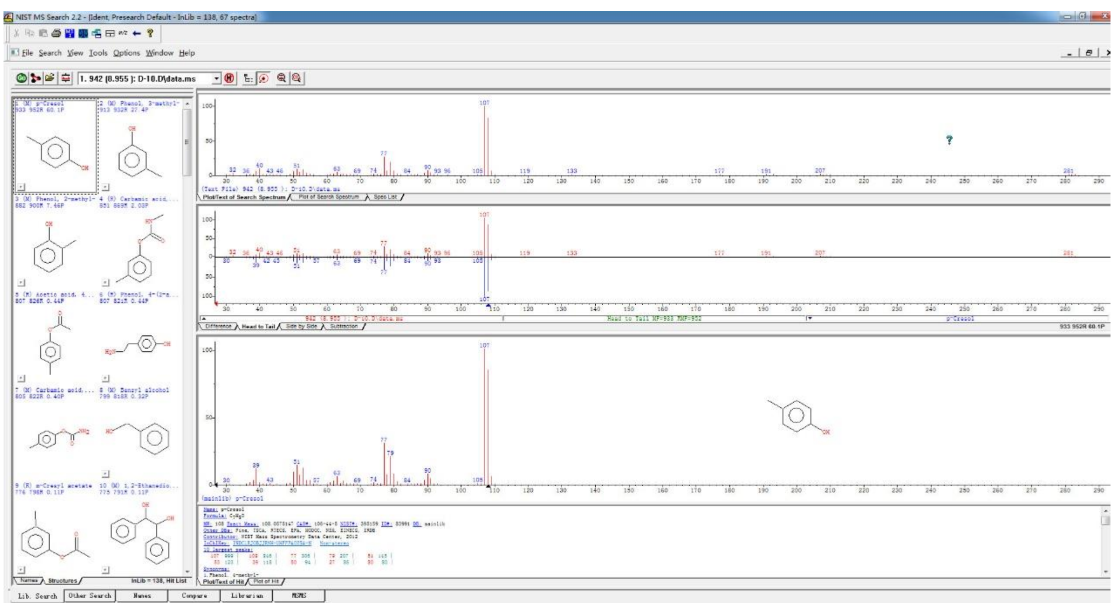
2c, colorless oil, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.17 (t, *J* = 7.7 Hz, 1H), 6.80 (d, *J* = 7.5 Hz, 1H), 6.77 – 6.61 (m, 2H), 4.77 (s, 1H), 2.35 (s, 3H). calcd for C_7H_8O 108.0575, found 108.0.



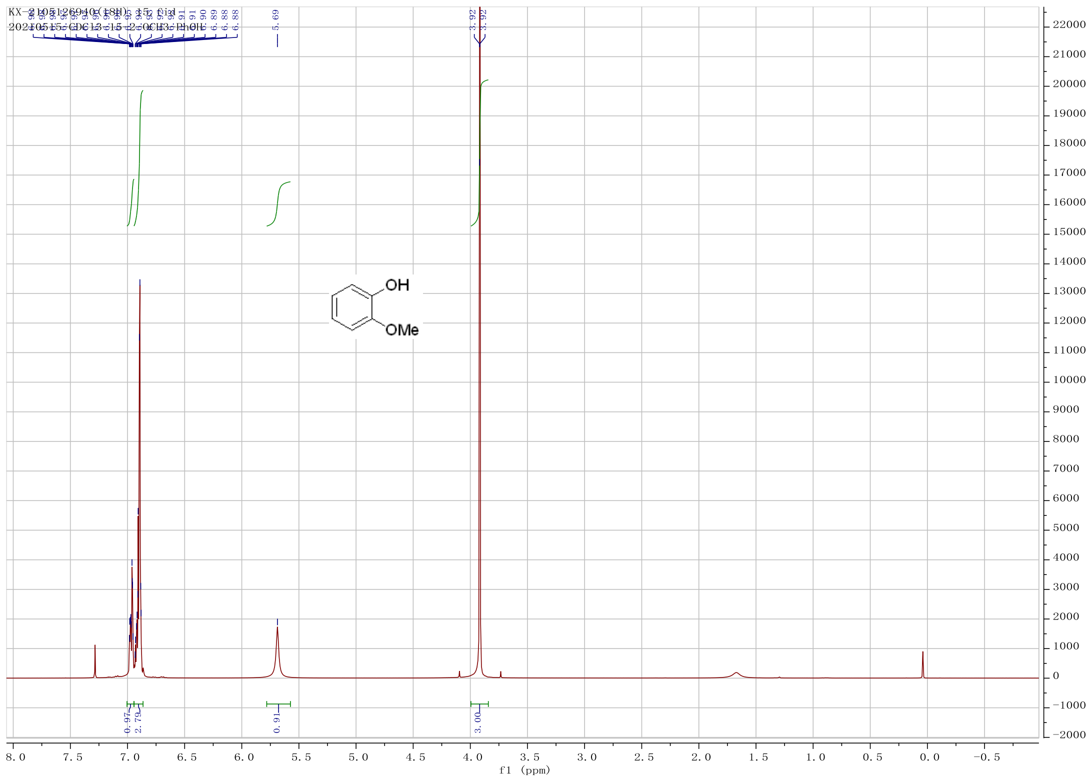


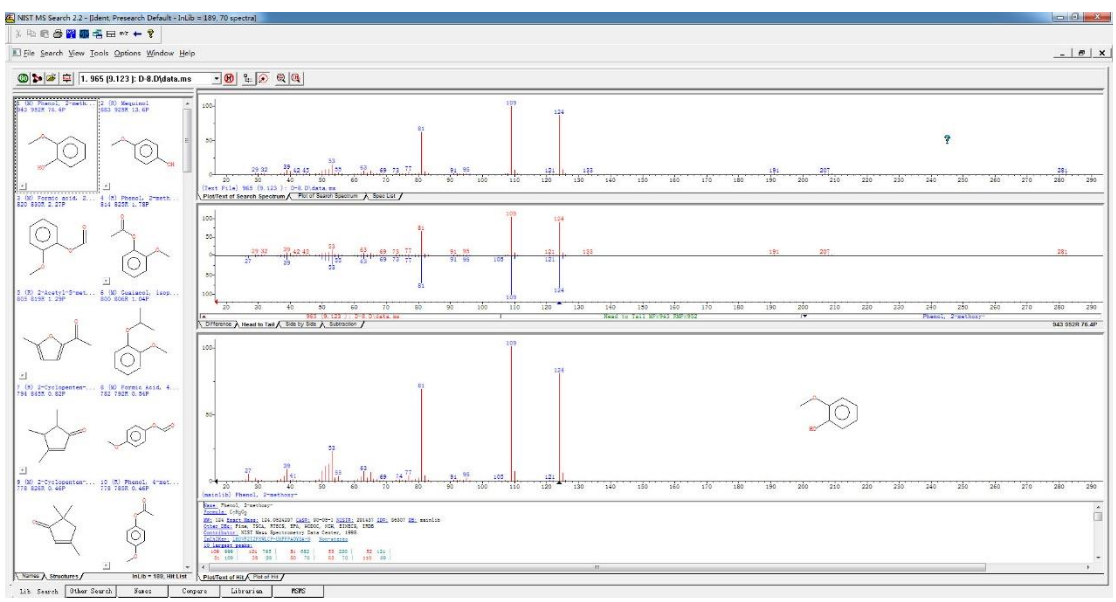
2d, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 – 7.04 (m, 2H), 6.91 – 6.78 (m, 2H), 5.07 (s, 1H), 2.33 (s, 3H). calcd for C_7H_8O 108.0575, found 108.0.



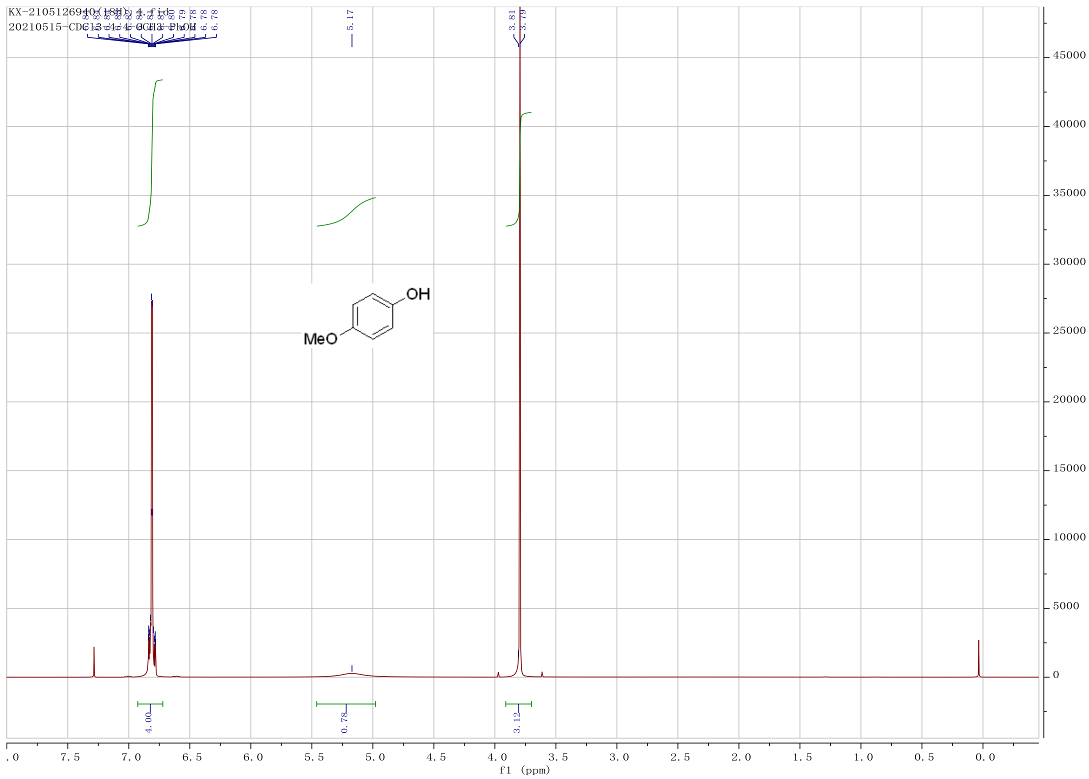


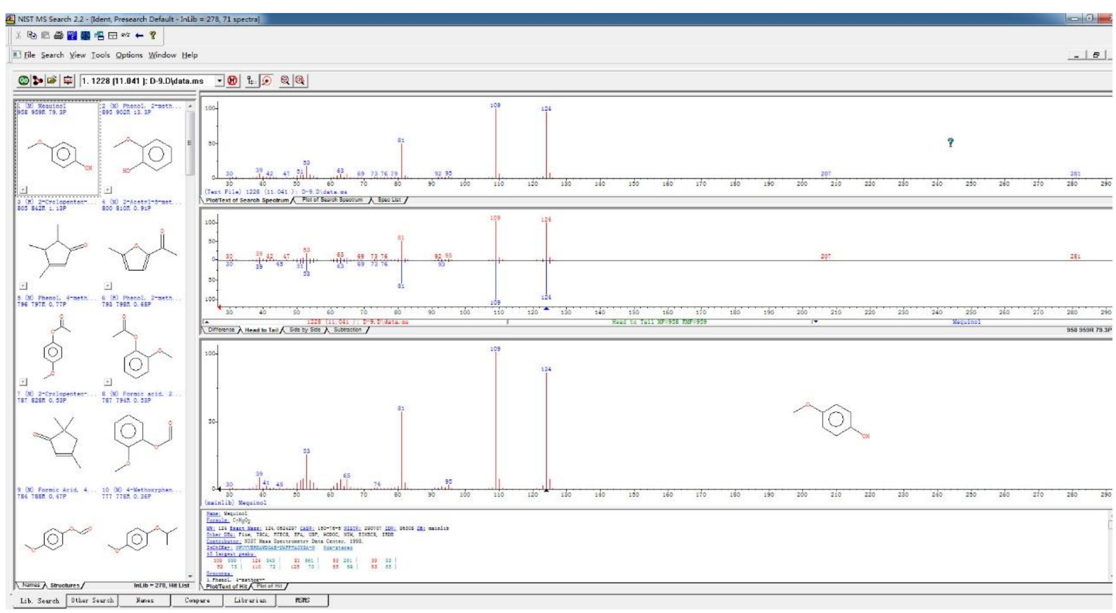
2e, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.00 – 6.94 (m, 1H), 6.94 – 6.86 (m, 3H), 5.69 (s, 1H), 3.92 (d, *J* = 1.0 Hz, 3H). calcd for $C_7H_8O_2$ 124.0524, found 124.0.



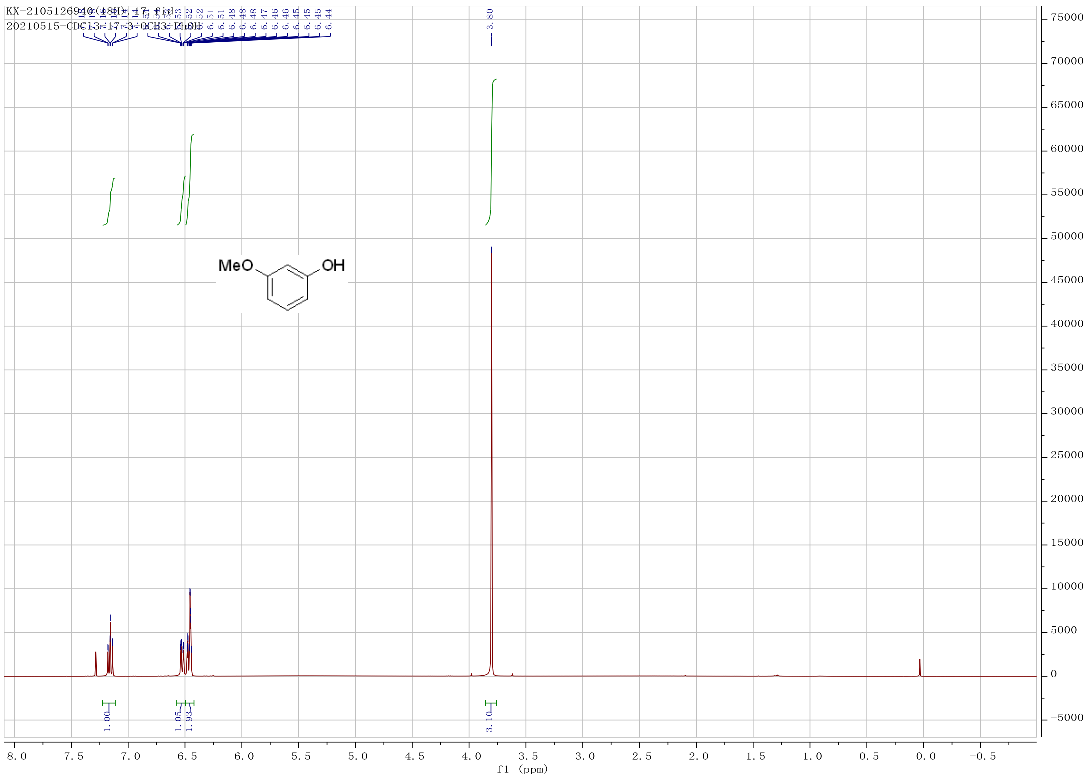


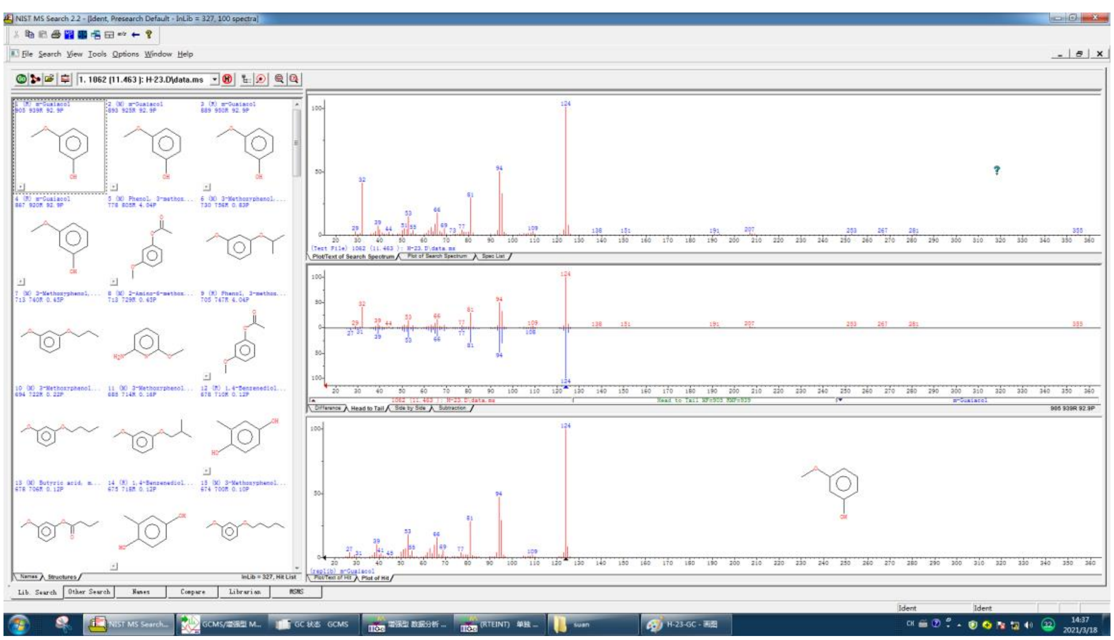
2f, white solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.93 – 6.72 (m, 4H), 5.17 (s, 1H), 3.79 (s, 3H). calcd for $C_7H_8O_2$ 124.0524, found 124.0.



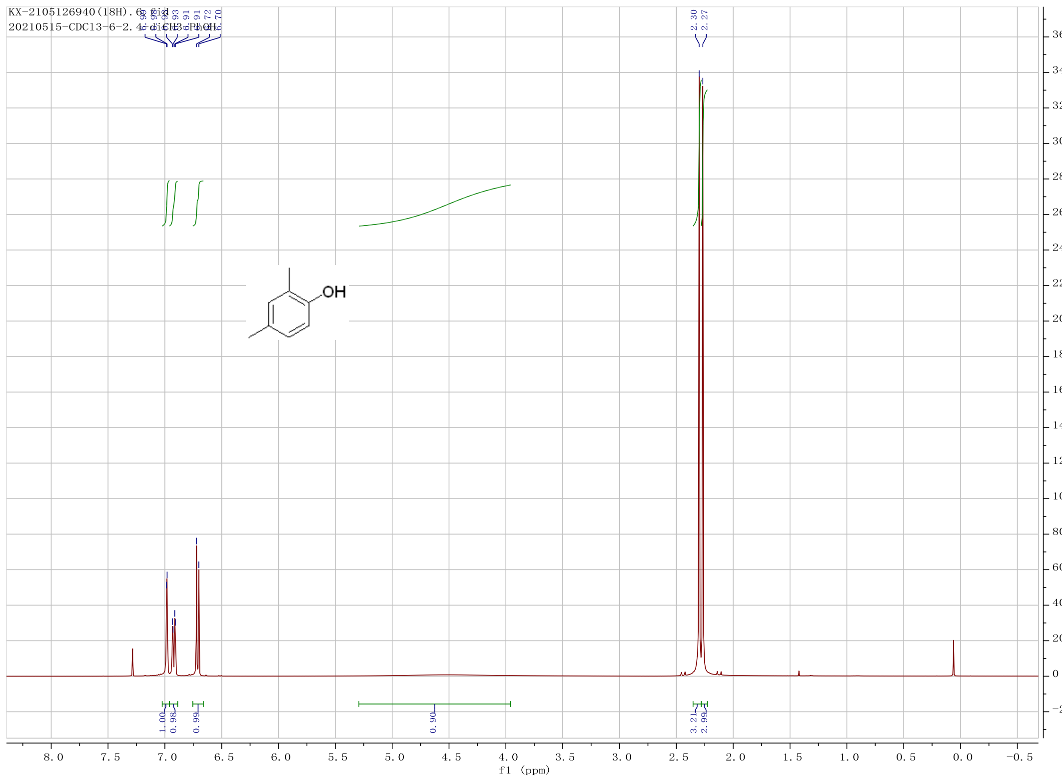


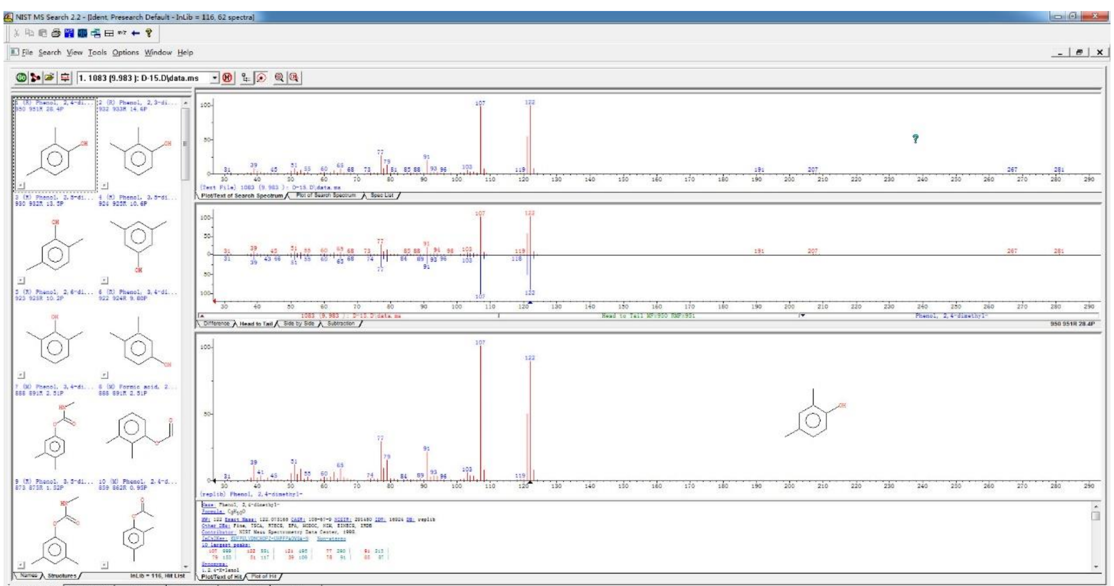
2g, white solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.22 – 7.11 (m, 1H), 6.52 (ddd, *J* = 8.3, 2.3, 1.0 Hz, 1H), 6.49 – 6.42 (m, 2H), 3.80 (s, 3H).
calcd for $C_7H_8O_2$ 124.0524, found 124.0.



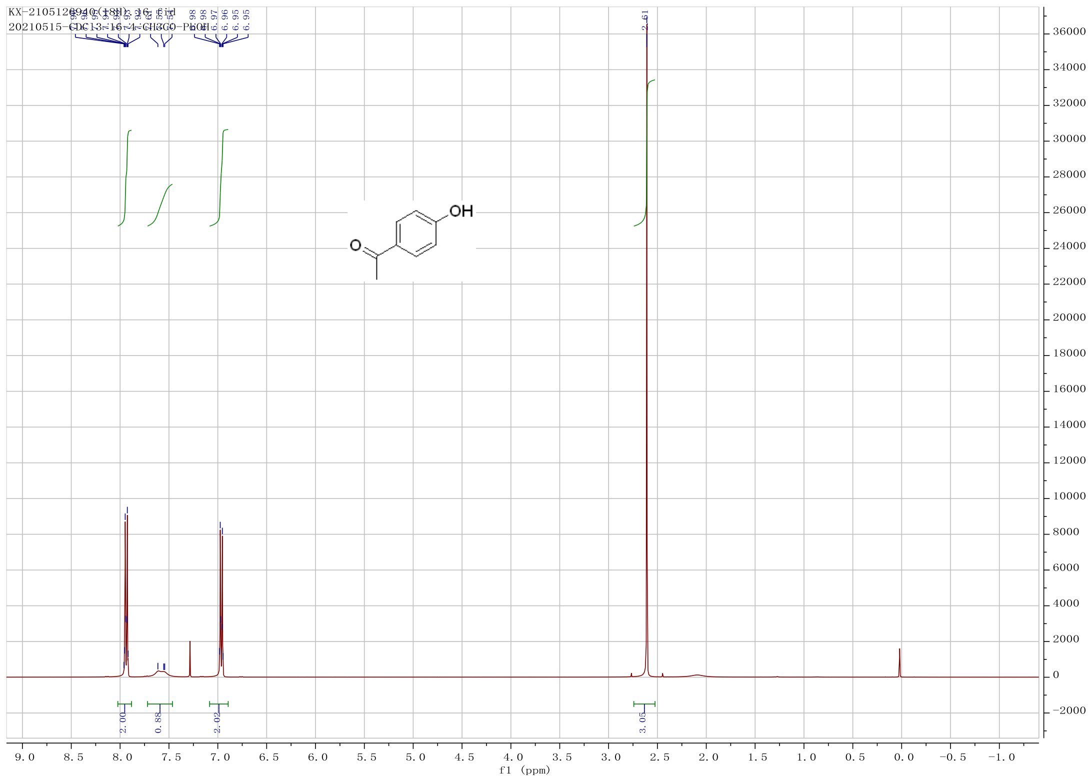


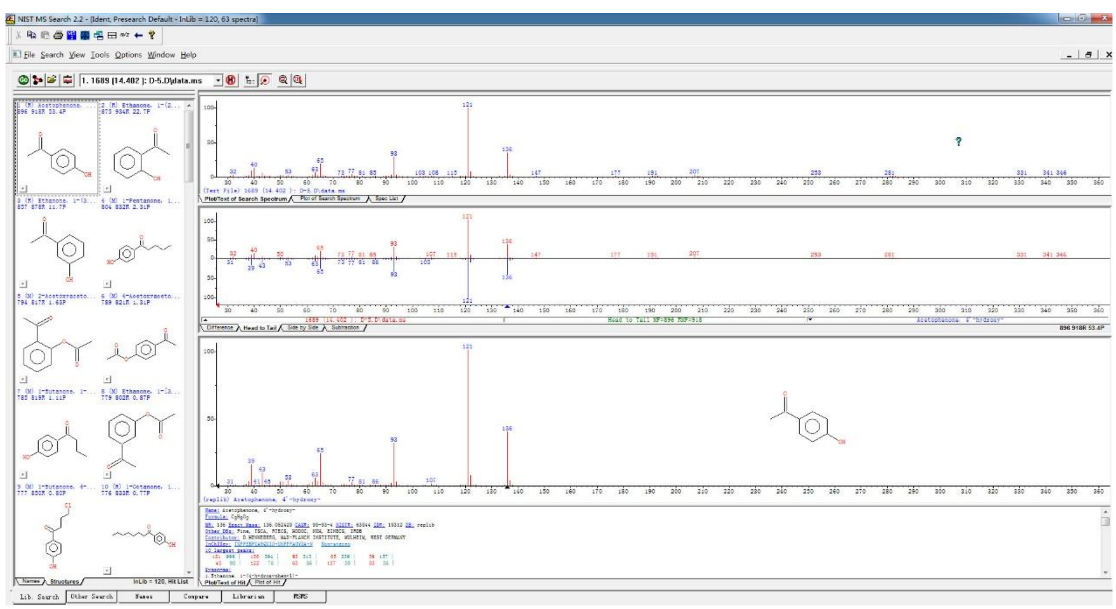
2h, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.98 (d, *J* = 2.2 Hz, 1H), 6.92 (dd, *J* = 8.1, 2.2 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 4.51 (s, 1H), 2.30 (s, 3H), 2.27 (s, 3H). calcd for $C_8H_{10}O$ 122.0732, found 122.0.



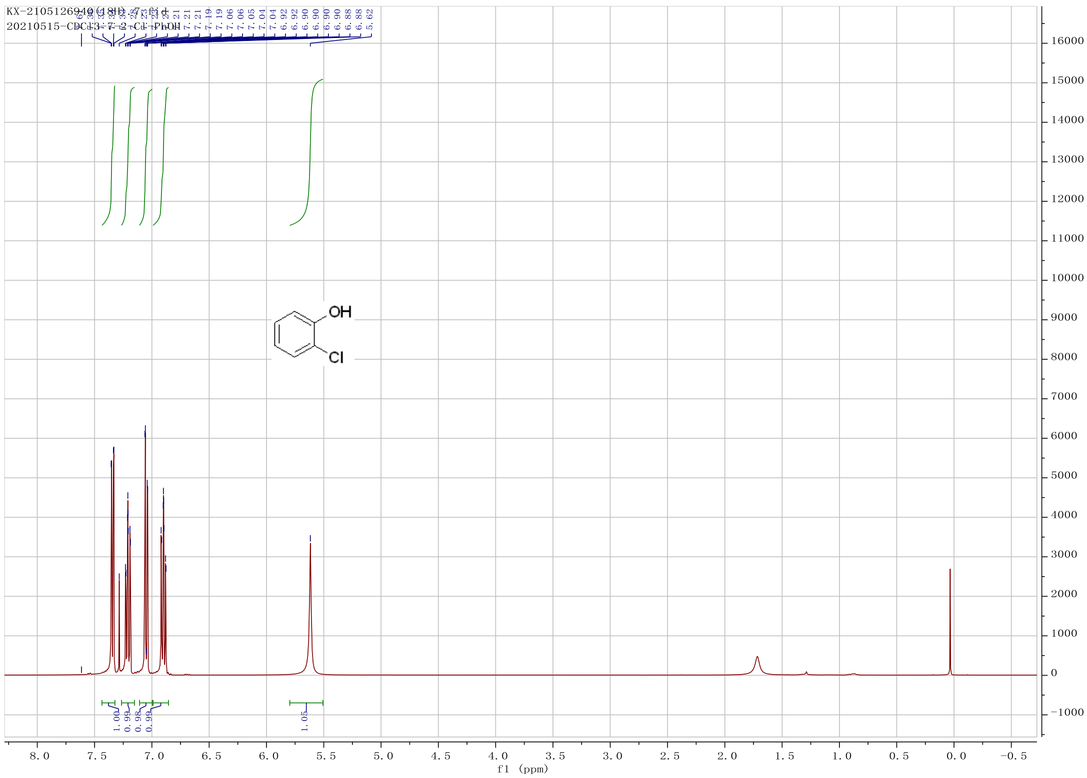


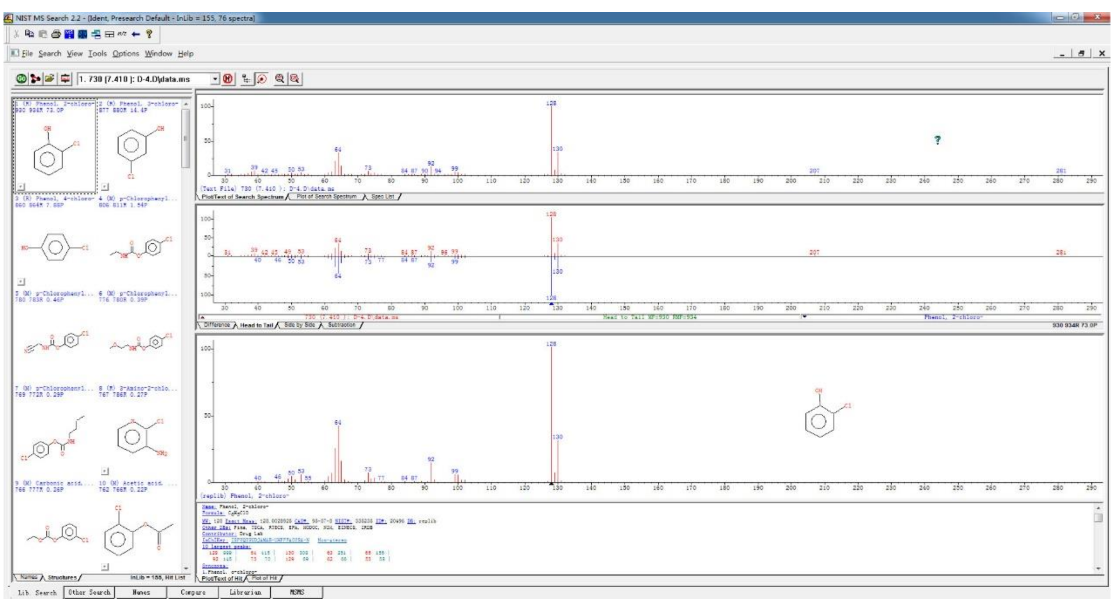
2i, white solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.88 (m, 2H), 7.58 (d, *J* = 24.0 Hz, 1H), 7.08 – 6.89 (m, 2H), 2.61 (s, 3H). calcd for $C_8H_8O_2$ 136.0524, found 136.0.



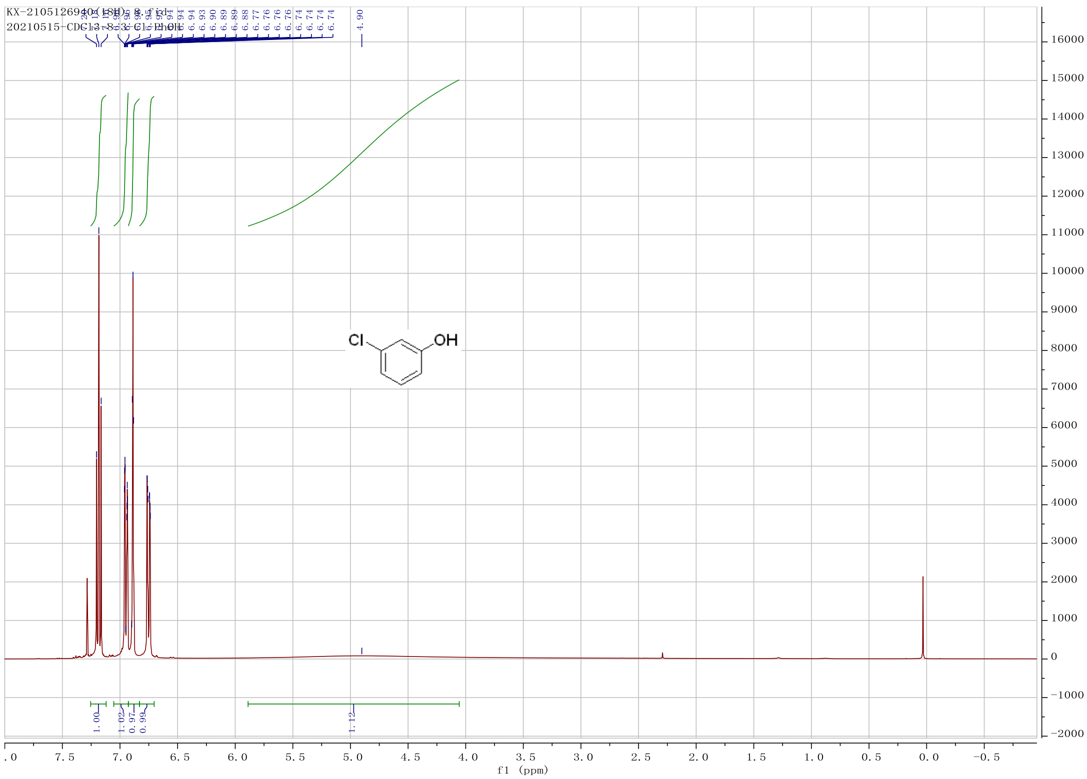


2j, colorless oil, [1]H NMR (400 MHz, Chloroform-*d*) δ 7.34 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.21 (ddd, *J* = 8.1, 7.4, 1.6 Hz, 1H), 7.05 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.90 (ddd, *J* = 7.9, 7.3, 1.6 Hz, 1H), 5.62 (s, 1H). calcd for C_6H_5ClO 128.0029, found 128.0.

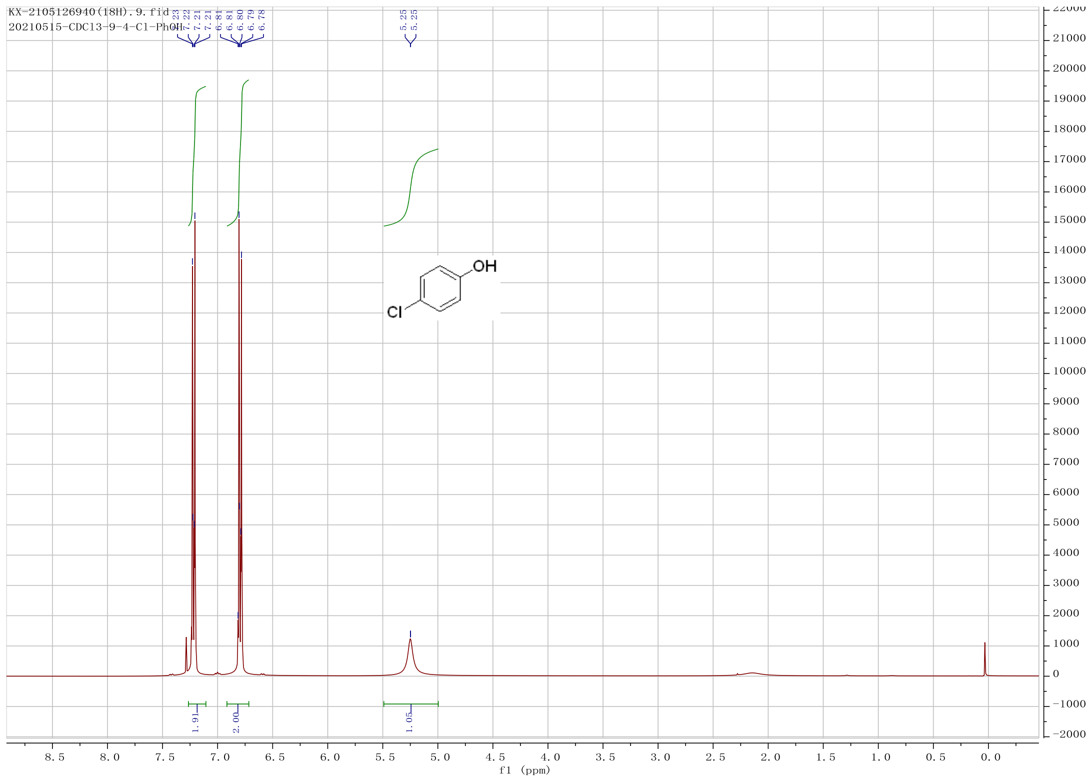


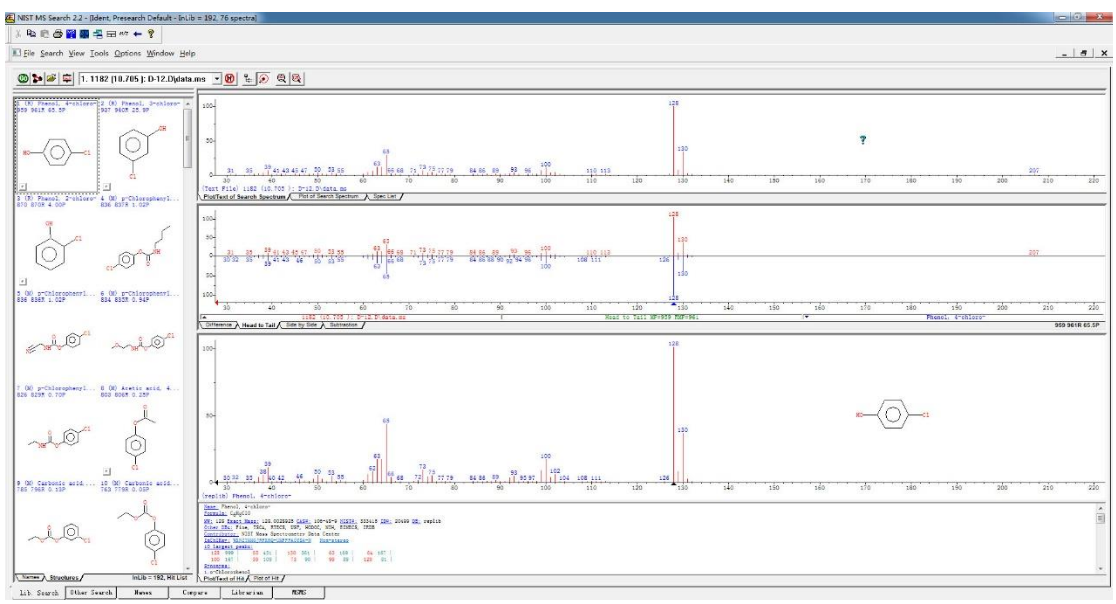


2k, white solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.18 (t, *J* = 8.1 Hz, 1H), 6.95 (ddd, *J* = 8.0, 1.9, 0.9 Hz, 1H), 6.89 (t, *J* = 2.2 Hz, 1H), 6.75 (ddd, *J* = 8.2, 2.5, 0.9 Hz, 1H), 4.90 (s, 1H). calcd for C_6H_5ClO 128.0029, found 128.0.

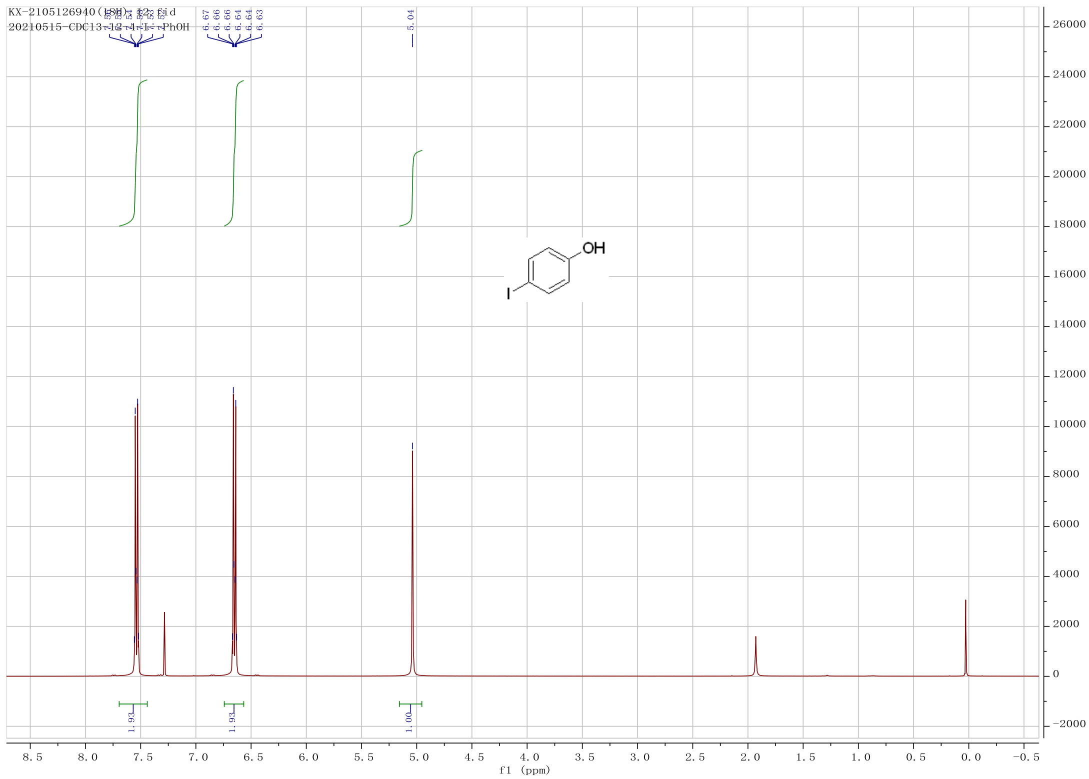


2l, white solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.11 (m, 2H), 6.92 – 6.72 (m, 2H), 5.49 – 5.00 (m, 1H). calcd for C_6H_5ClO 128.0029, found 128.0.

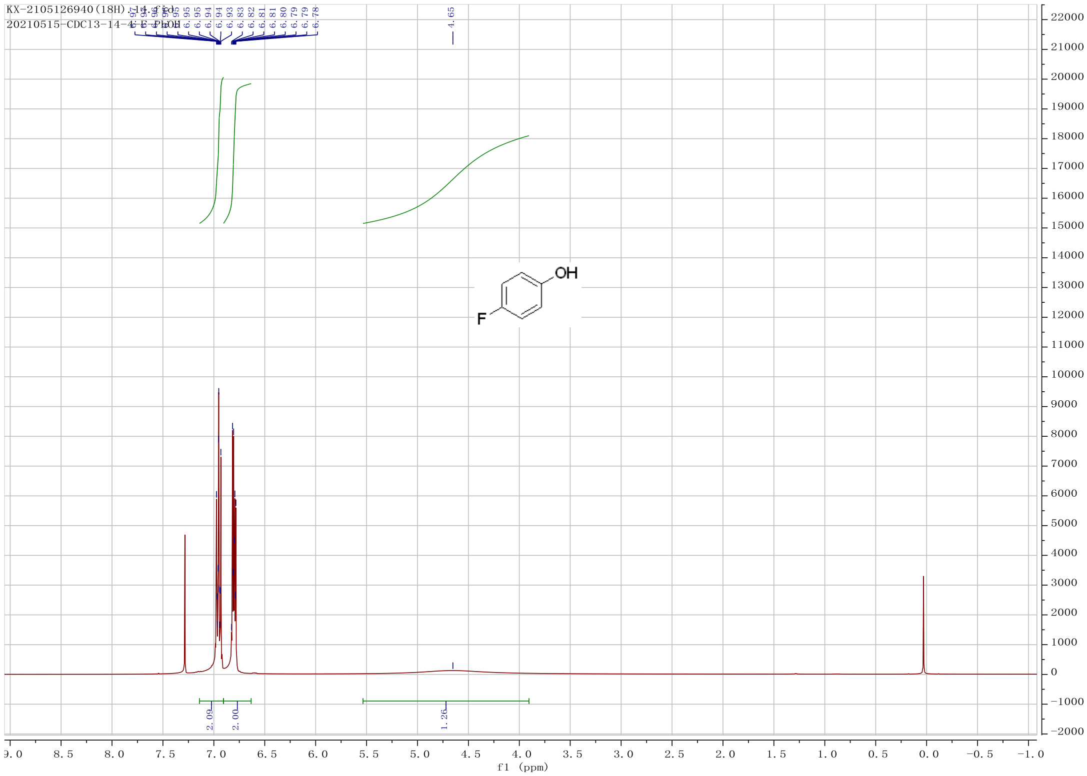


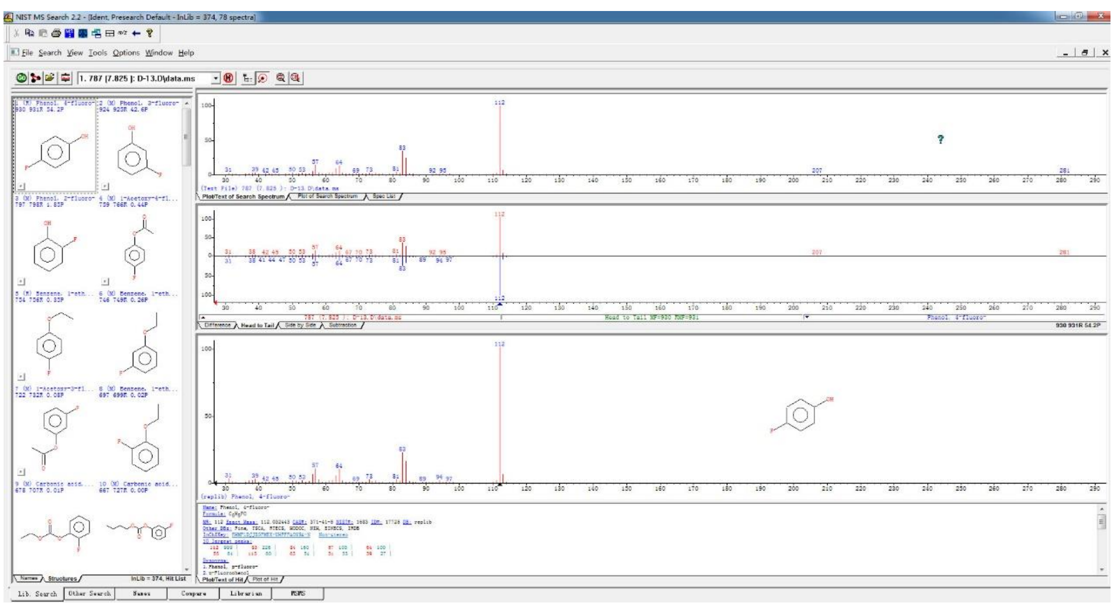


2m, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.44 (m, 2H), 6.74 – 6.57 (m, 2H), 5.04 (s, 1H). calcd for C_6H_5IO 219.9385, found 219.9.

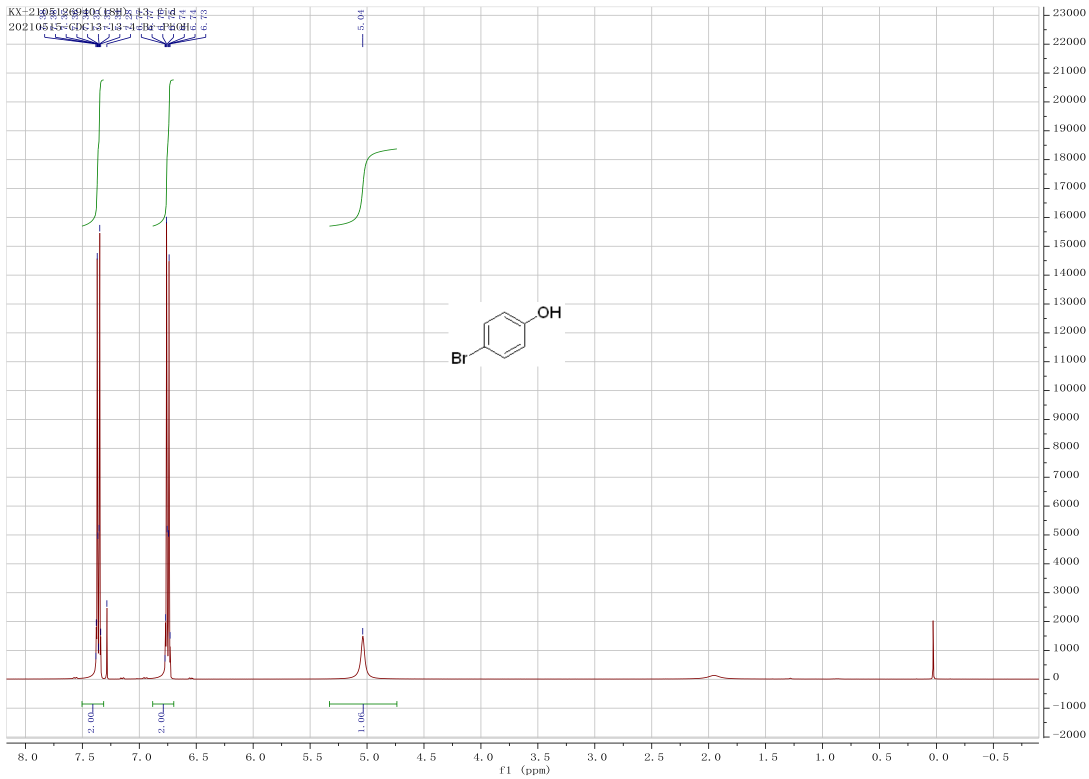


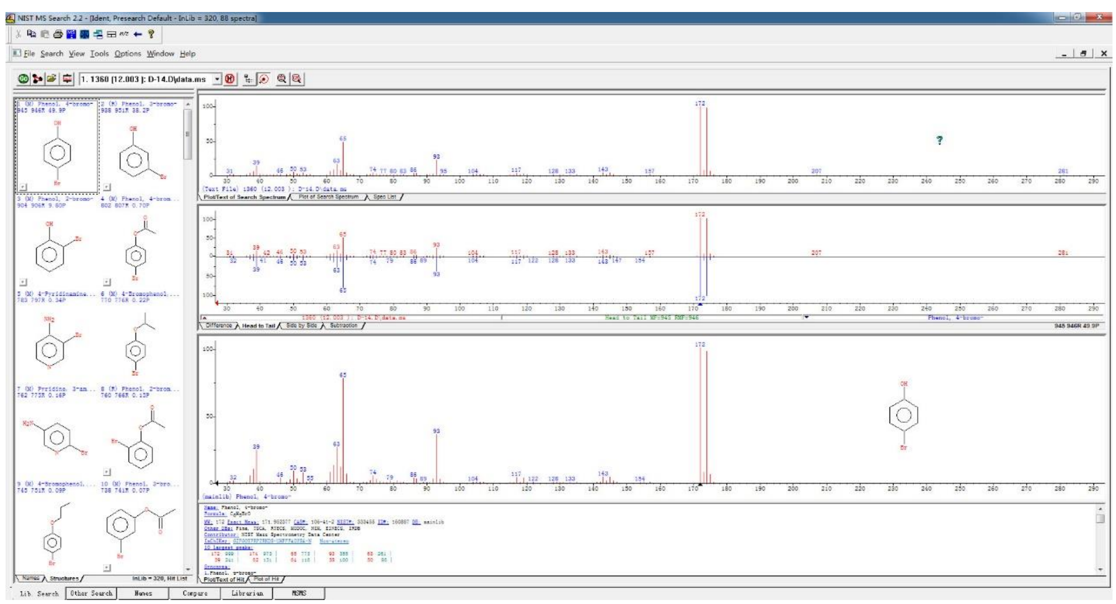
2n, colorless solid, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.14 – 6.90 (m, 2H), 6.90 – 6.63 (m, 2H), 4.65 (s, 1H). calcd for C_6H_5FO 112.0324, found 112.0.



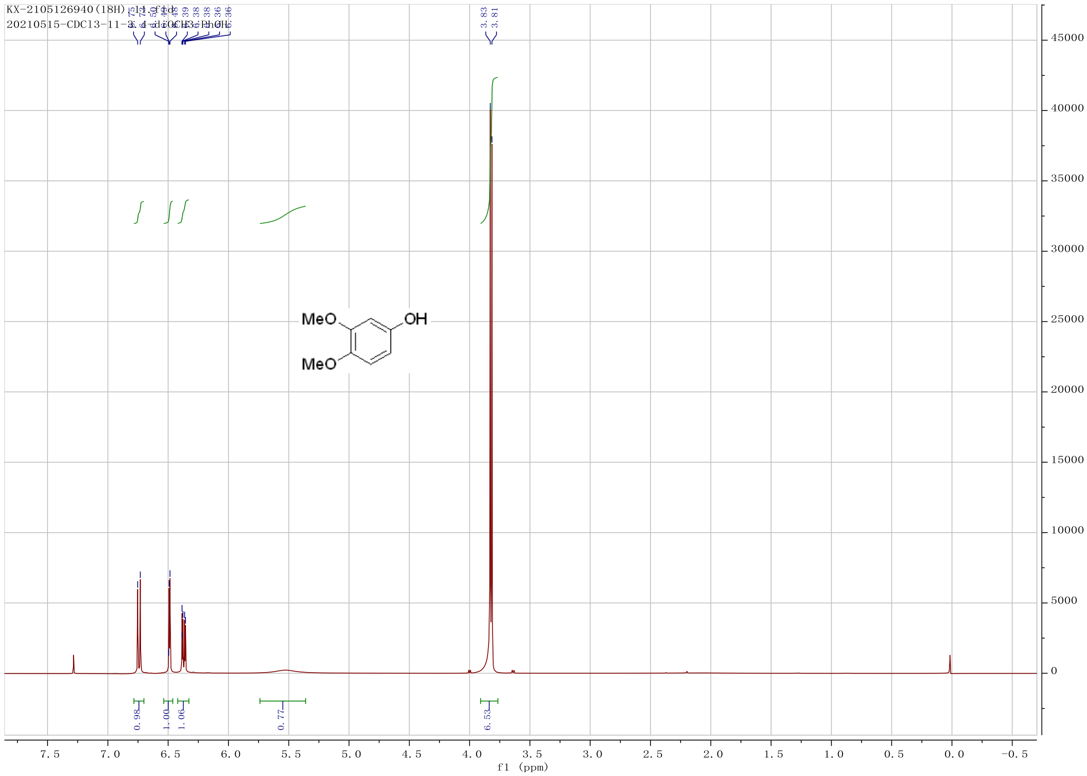


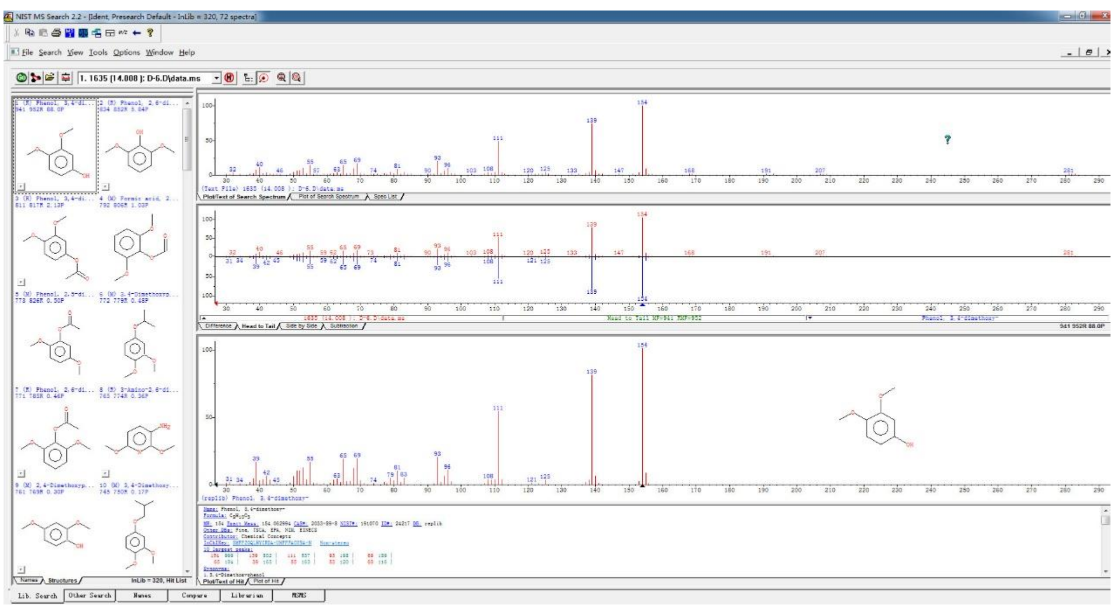
2o, colorless solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.31 (m, 2H), 6.88 – 6.70 (m, 2H), 5.04 (s, 1H). calcd for C_6H_5BrO 171.9524, found 171.9.



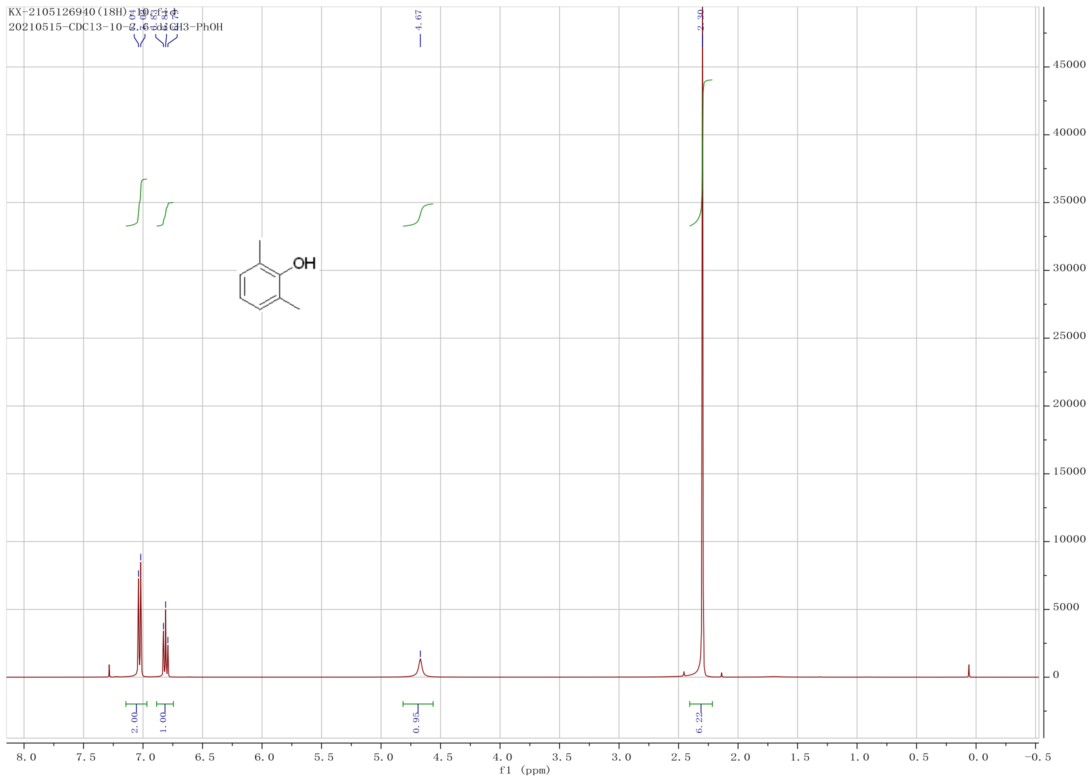


2p, white solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.74 (d, *J* = 8.6 Hz, 1H), 6.49 (d, *J* = 2.8 Hz, 1H), 6.37 (dd, *J* = 8.6, 2.8 Hz, 1H), 5.53 (s, 1H), 3.82 (d, *J* = 5.5 Hz, 7H). calcd for $C_8H_{10}O_3$ 154.0630, found 154.0.





2q, yellow solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.03 (d, *J* = 7.5 Hz, 2H), 6.81 (t, *J* = 7.5 Hz, 1H), 4.67 (s, 1H), 2.30 (s, 6H). calcd for C_8H_{10} 122.0732, found 122.0.



2r, yellow solid, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.23 (m, 2H), 6.90 – 6.71 (m, 2H), 4.77 (s, 1H), 1.32 (s, 9H). calcd for C_8H_{10} 150.1045, found 150.05.