Supporting Information

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A New Isobenzofuranone Derivative from Arctic Fungus *Gyoerffyella* sp. CPCC 401434

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Table of Contents	Page

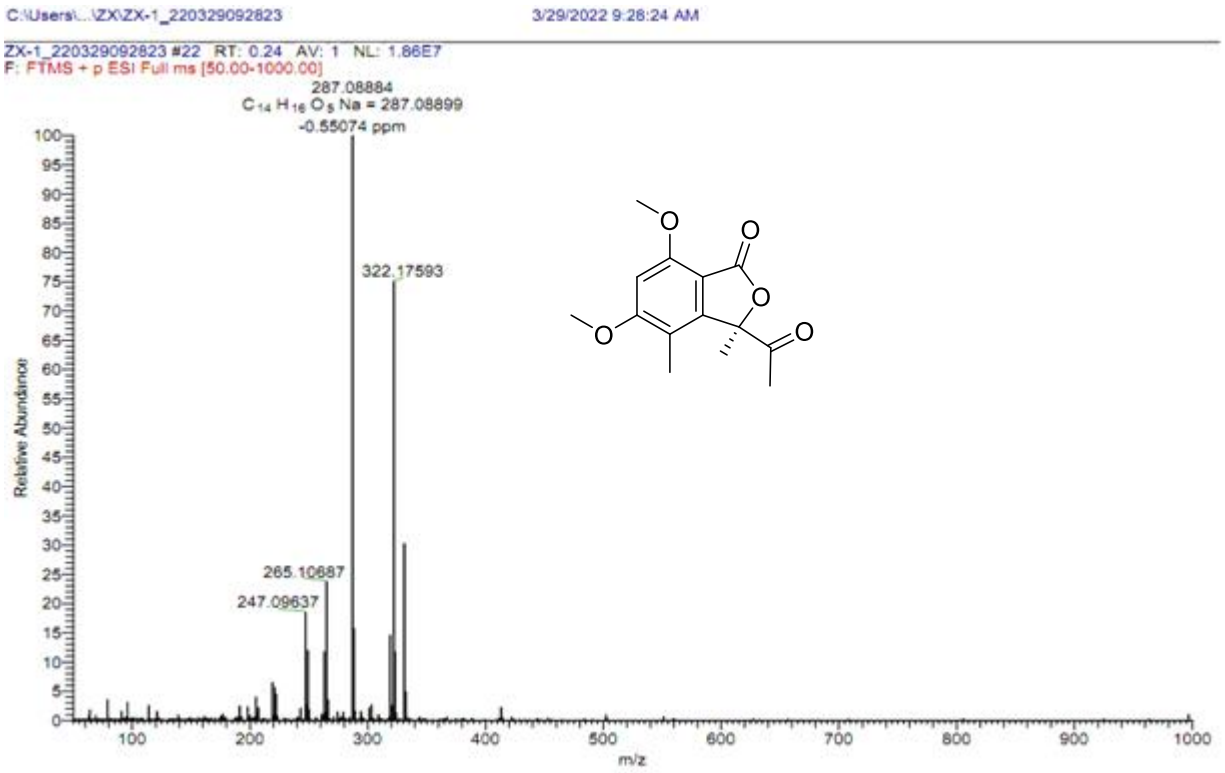

Figure S1: HR-ESI-MS spectrum of **1**

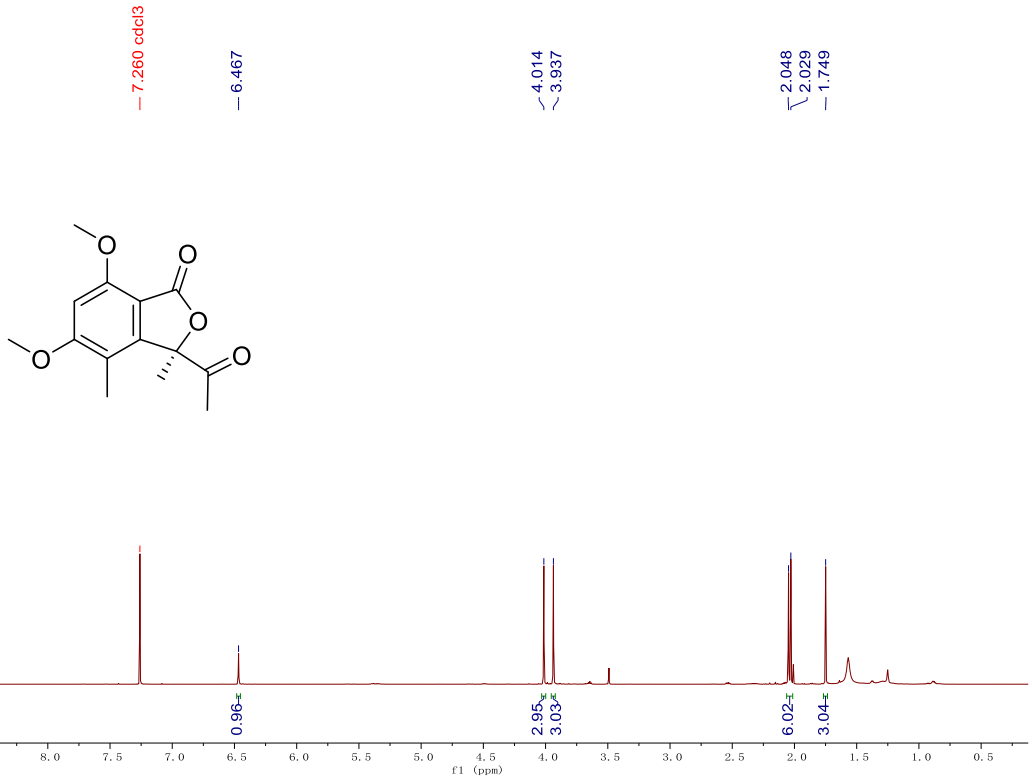

Figure S2: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1**

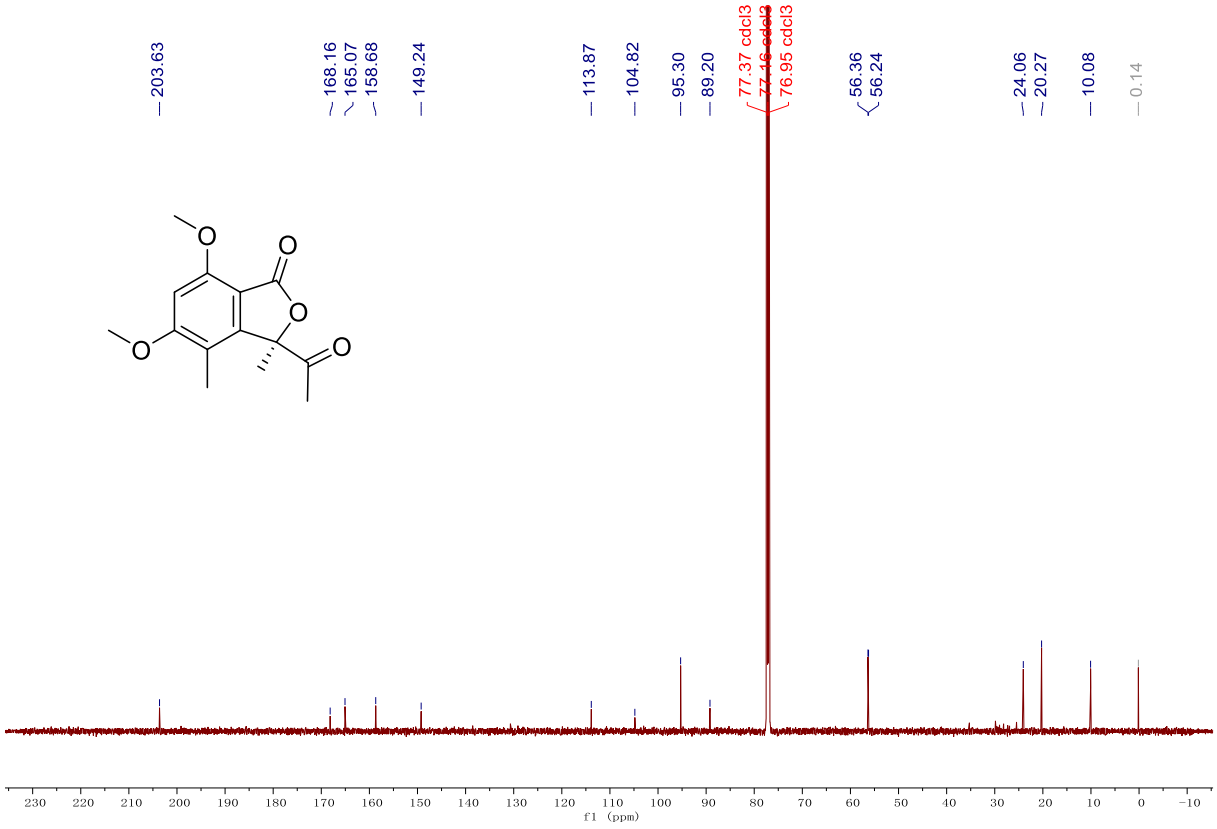

Figure S3: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1**

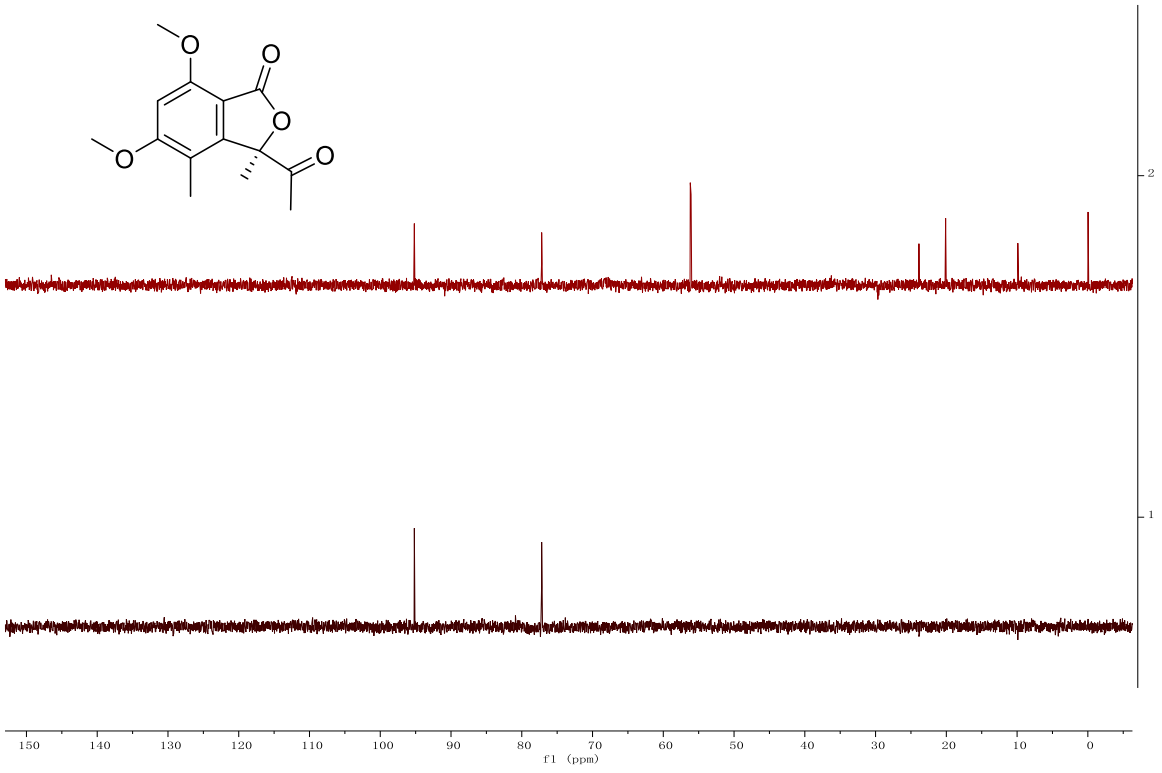

Figure S4: DEPT spectrum of **1**

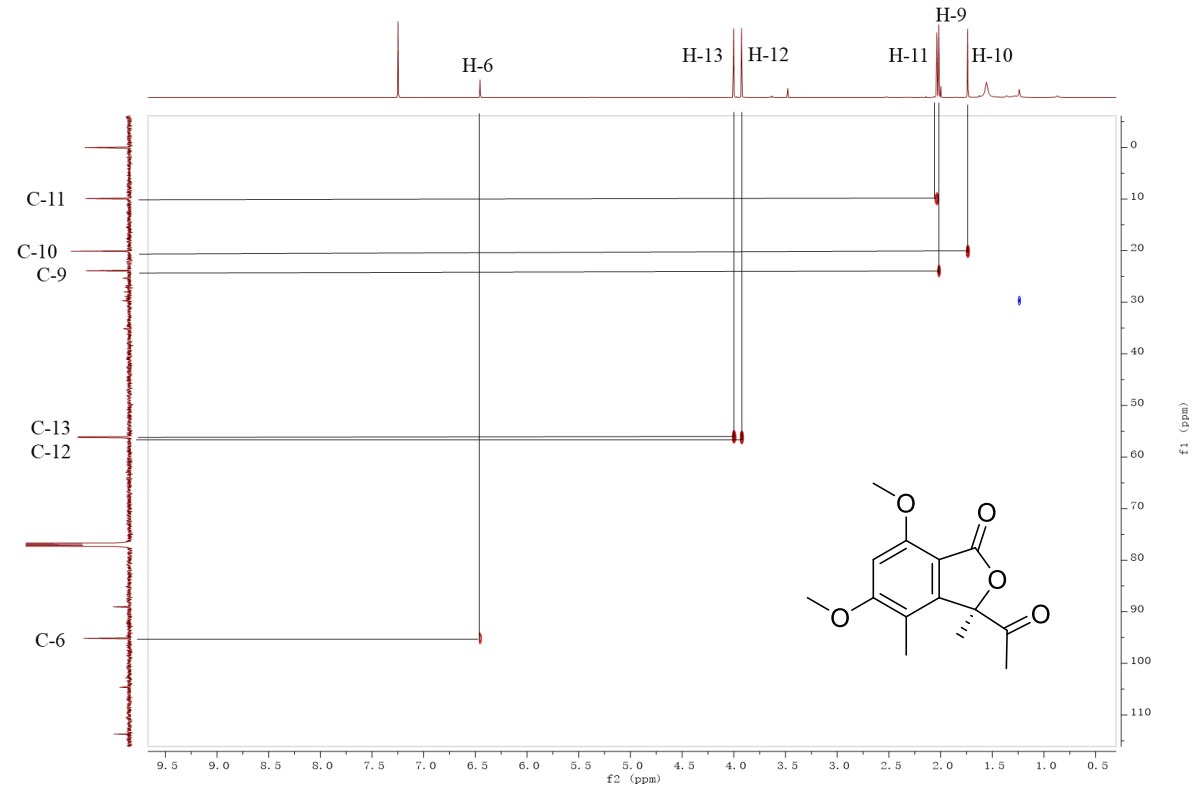

Figure S5: HSQC spectrum of **1**

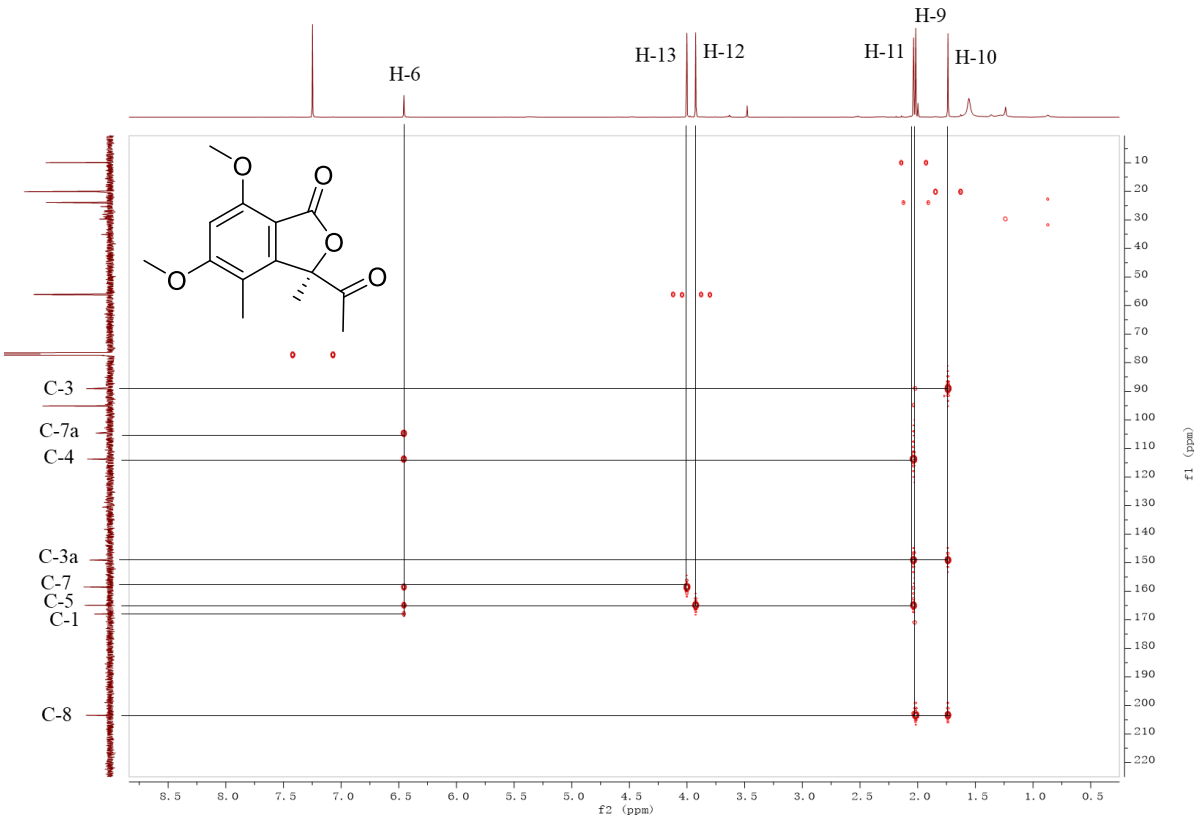

Figure S6: HMBC spectrum of **1**

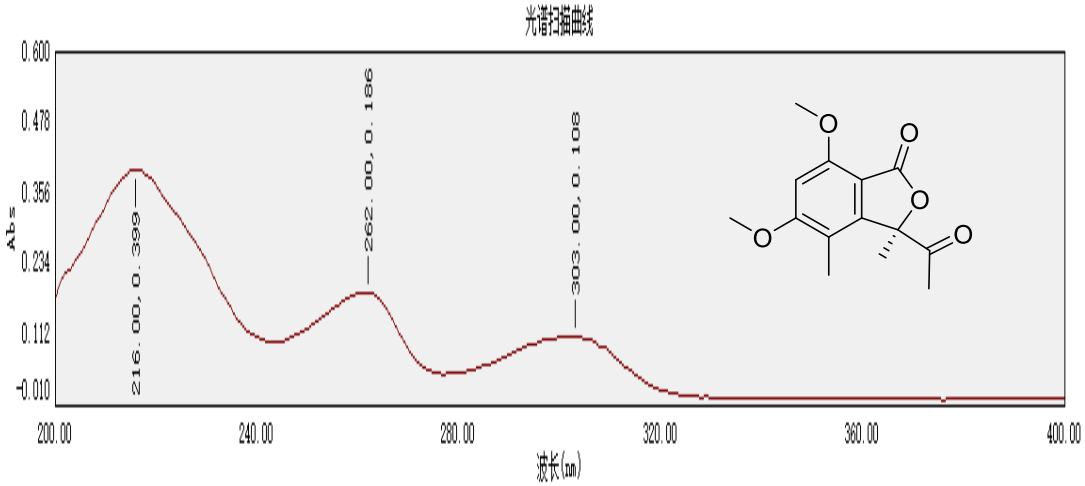

Figure S7: UV spectrum of **1**

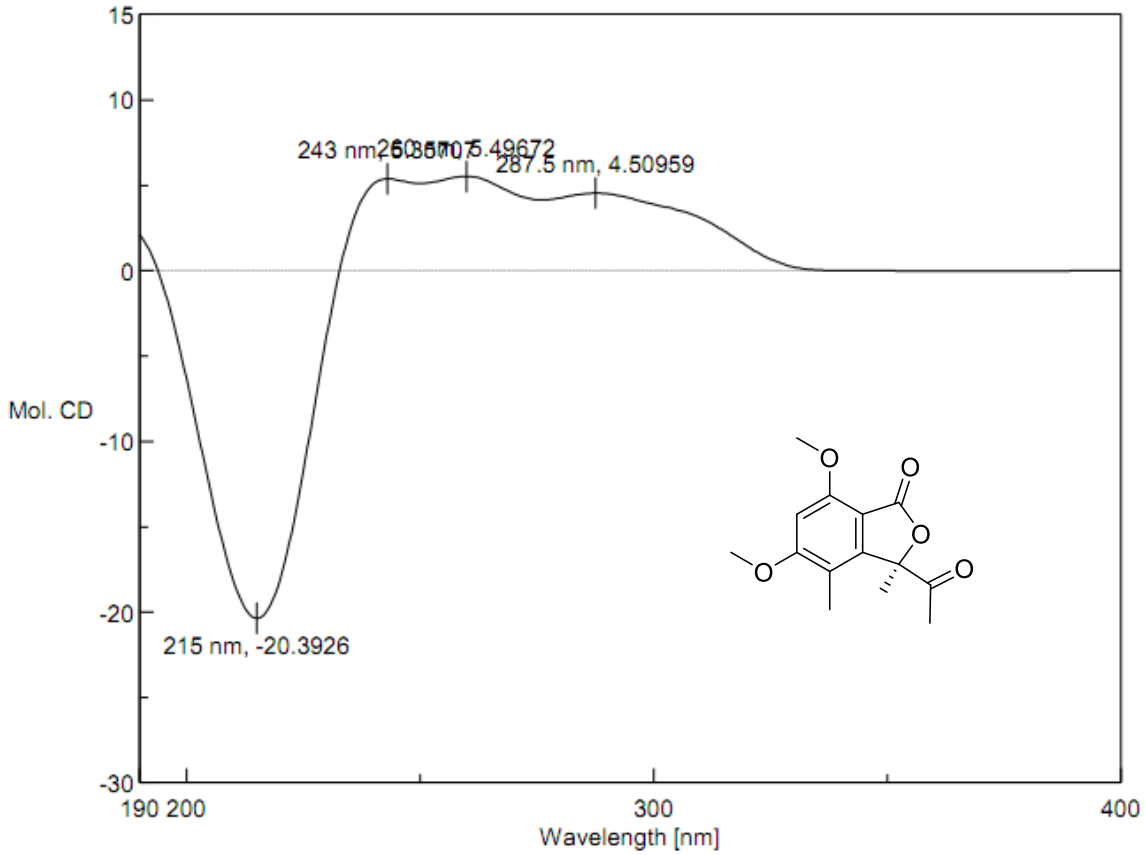

Figure S8: ECD spectrum of **1**

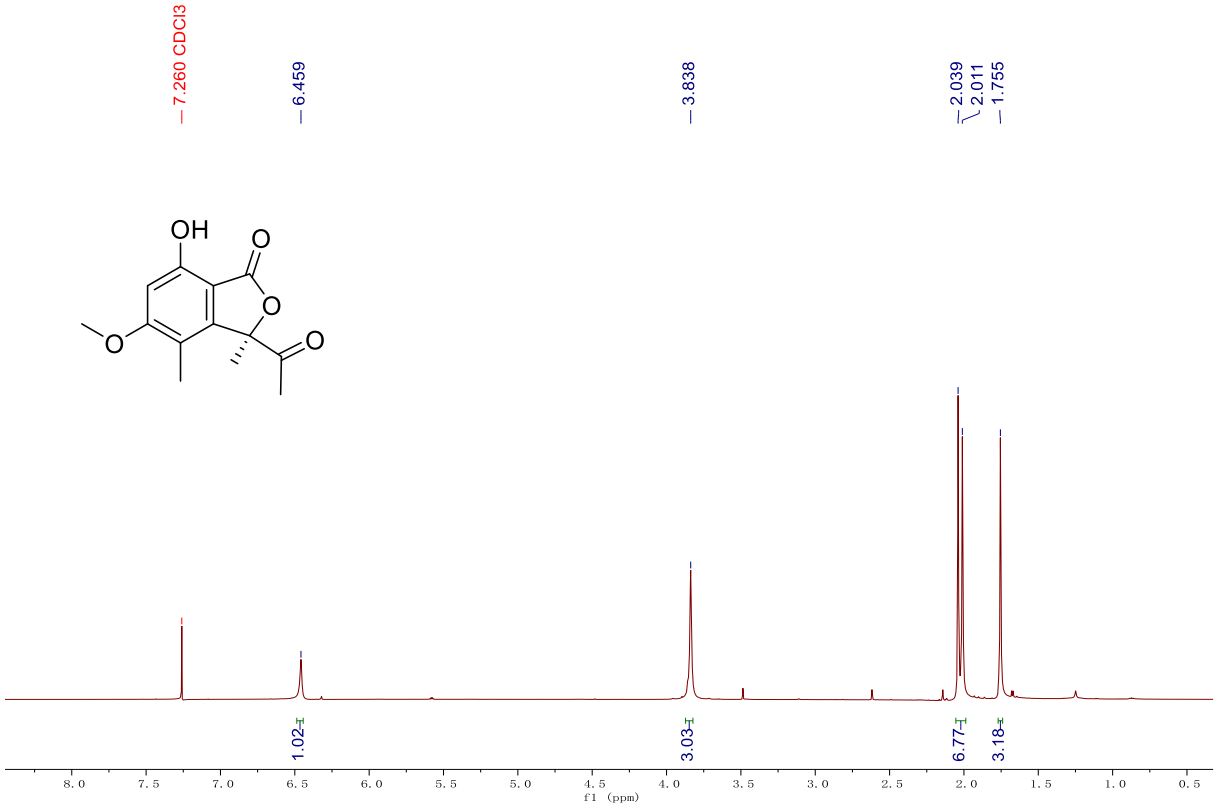

Figure S9: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **2**

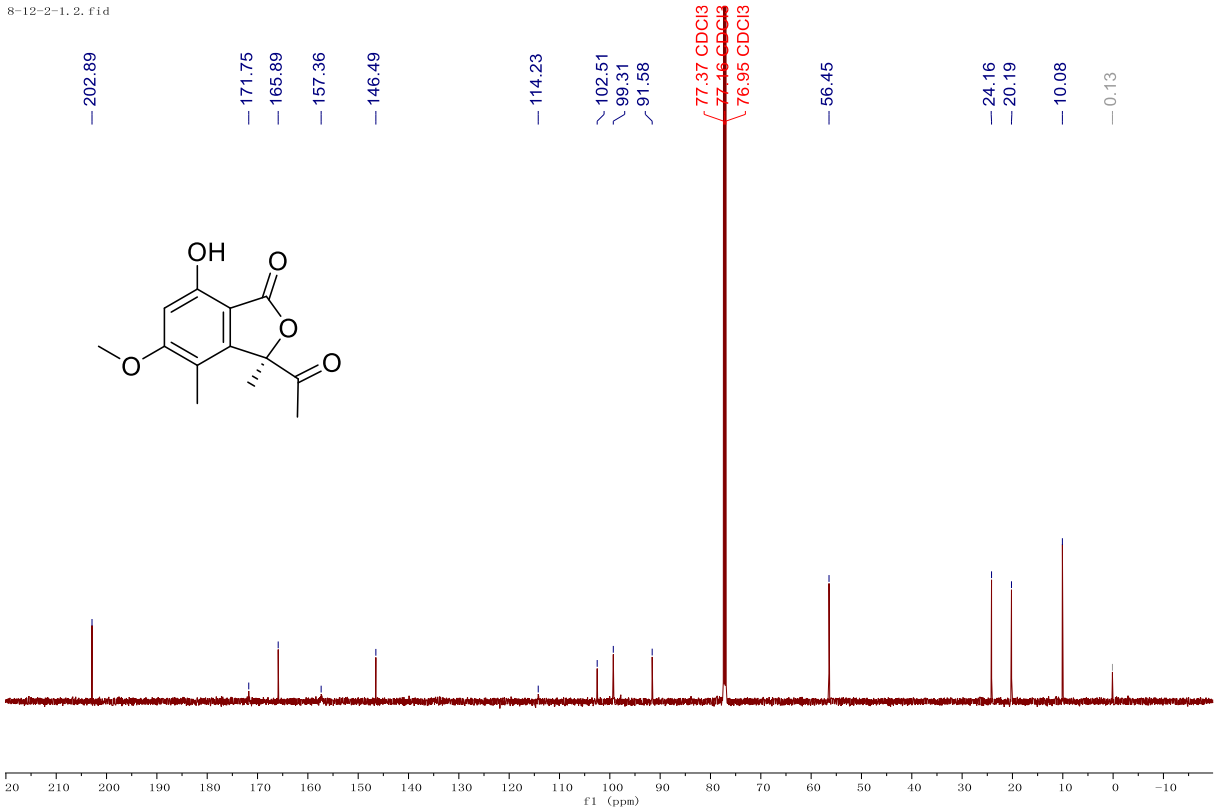

Figure S10: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **2**

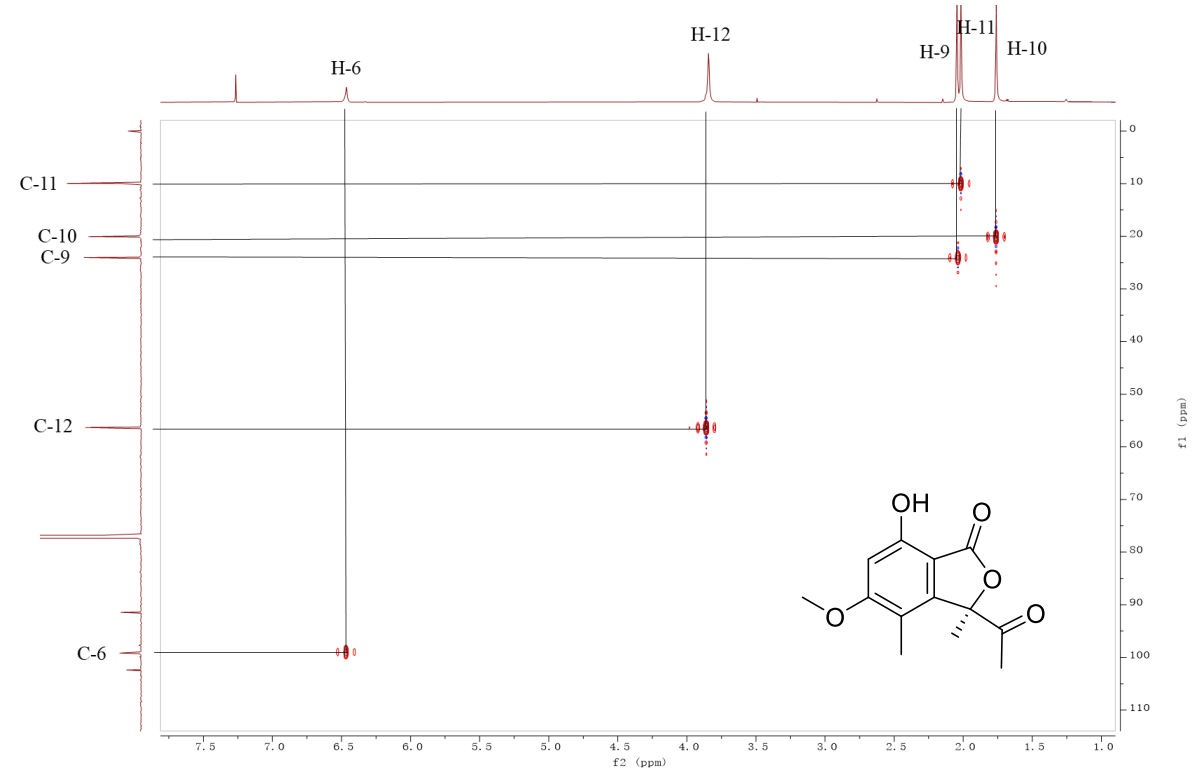

Figure S11: HSQC spectrum of **2**

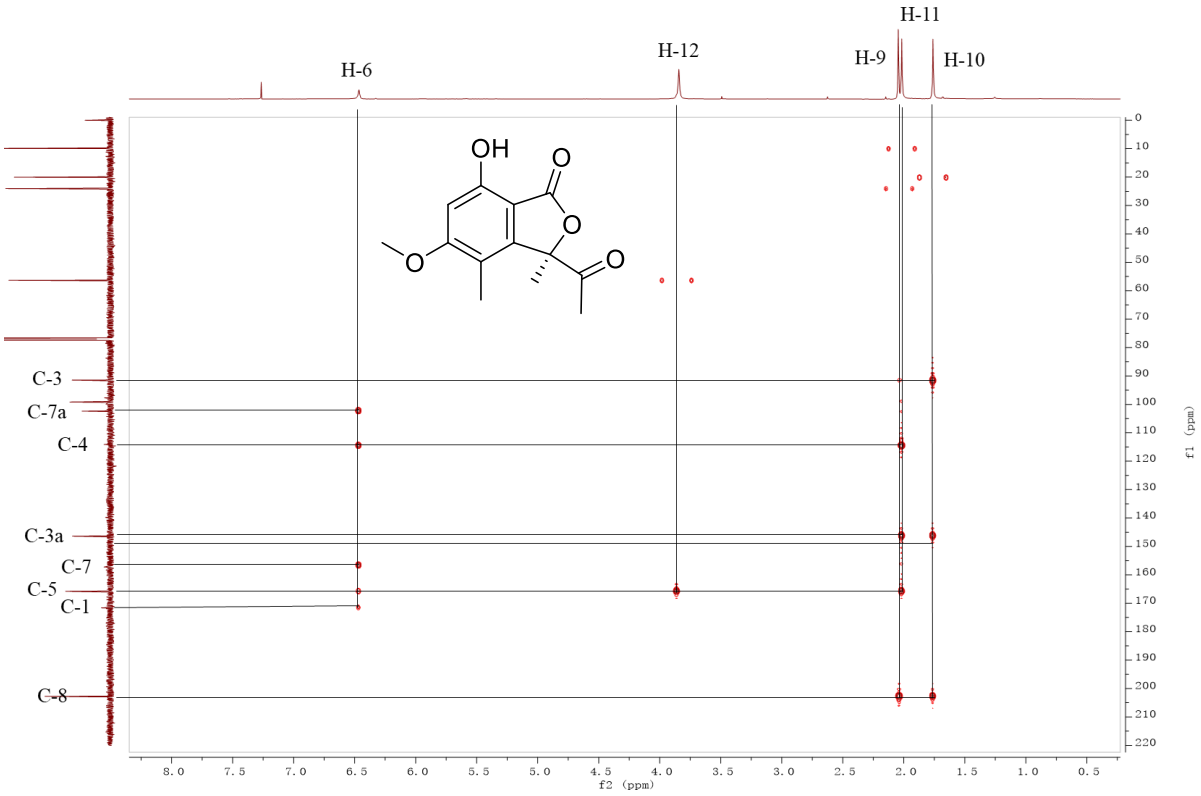

Figure S12: HMBC spectrum of **2**

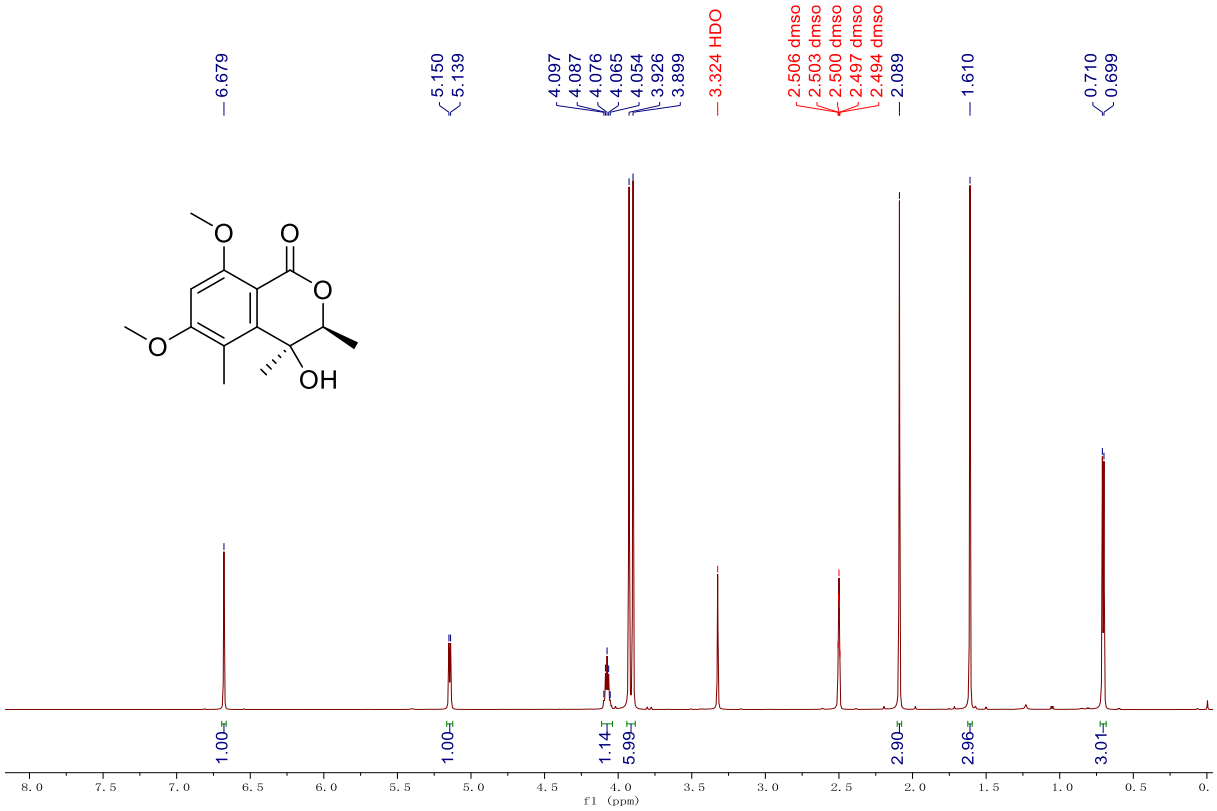

Figure S13: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **3**

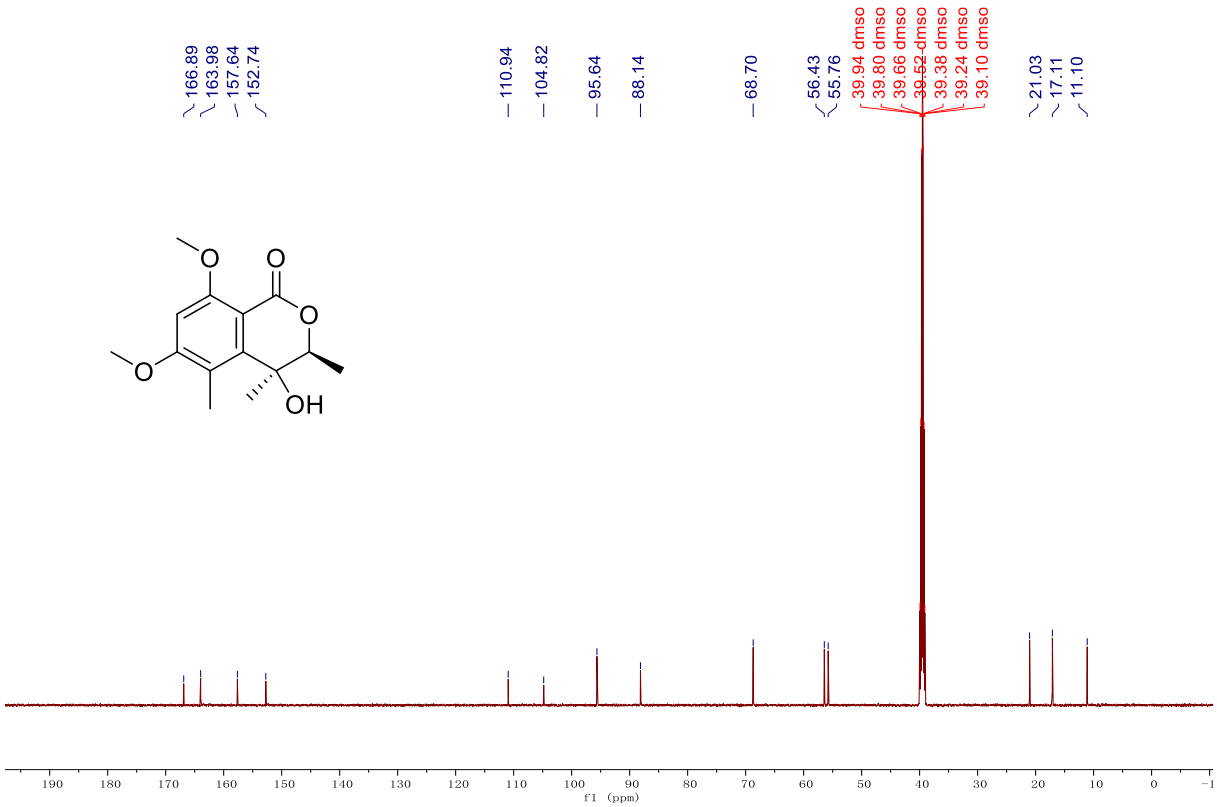

Figure S14: ^{13}C-NMR (600 MHz, DMSO-d_6) spectrum of **3**

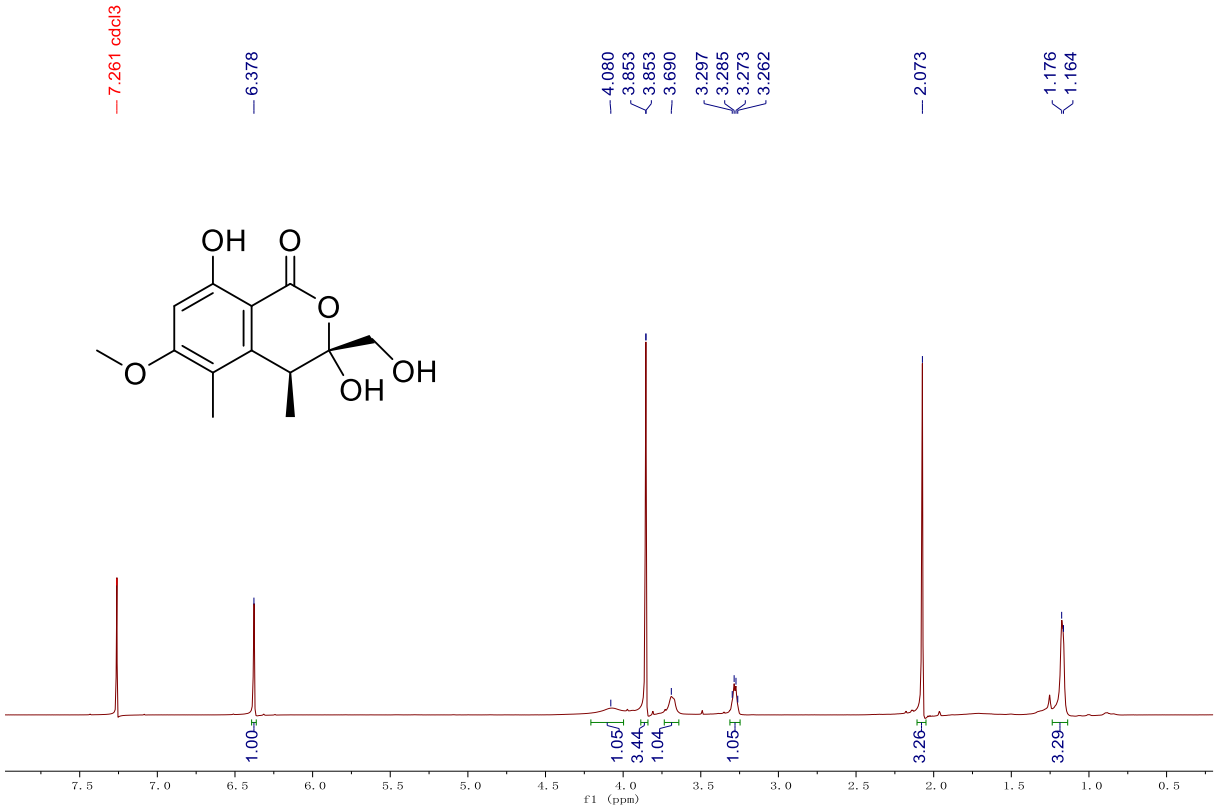

Figure S15: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **4**

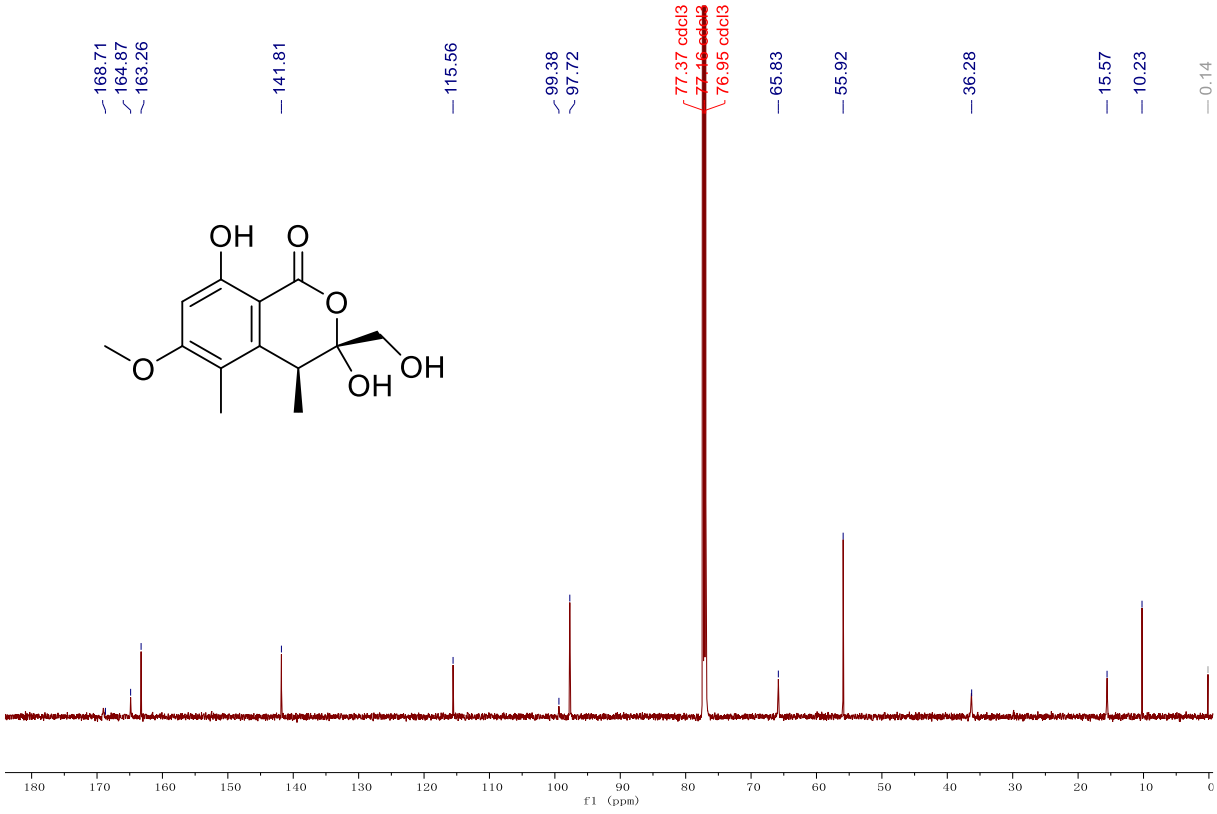

Figure S16: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **4**

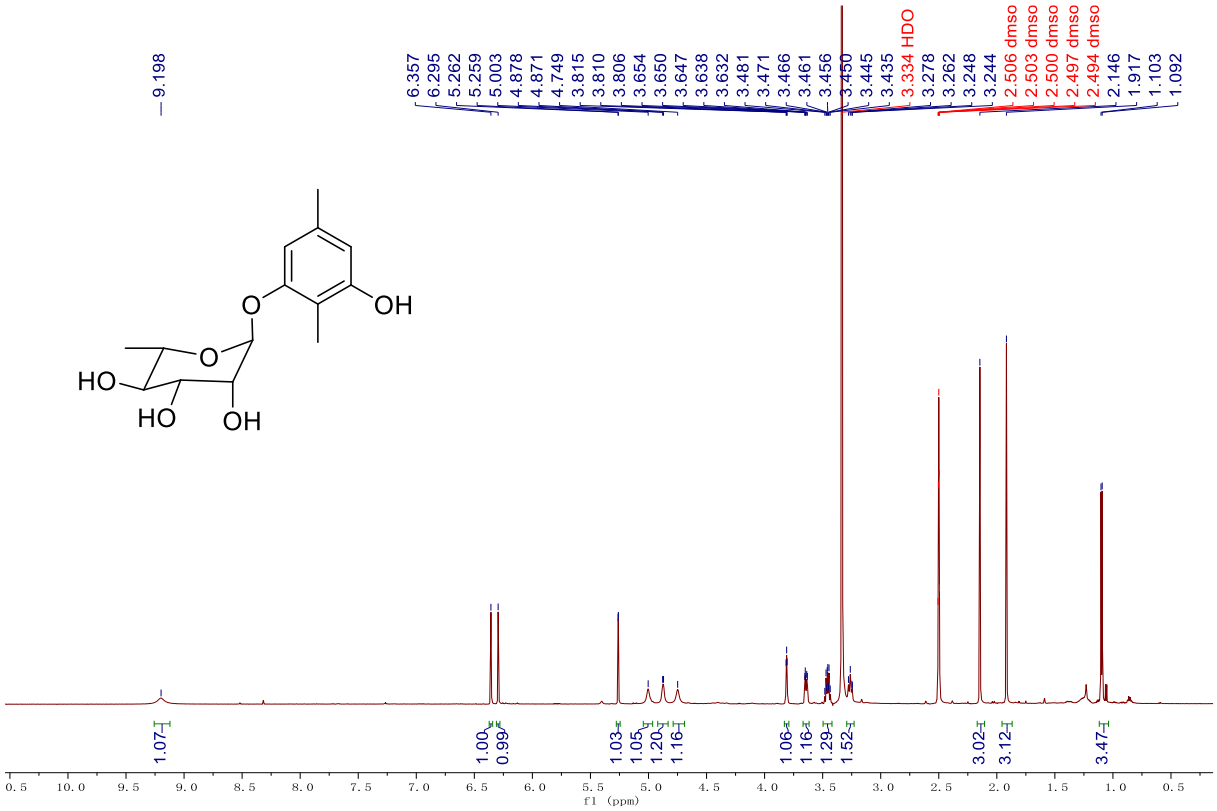

Figure S17: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **5**

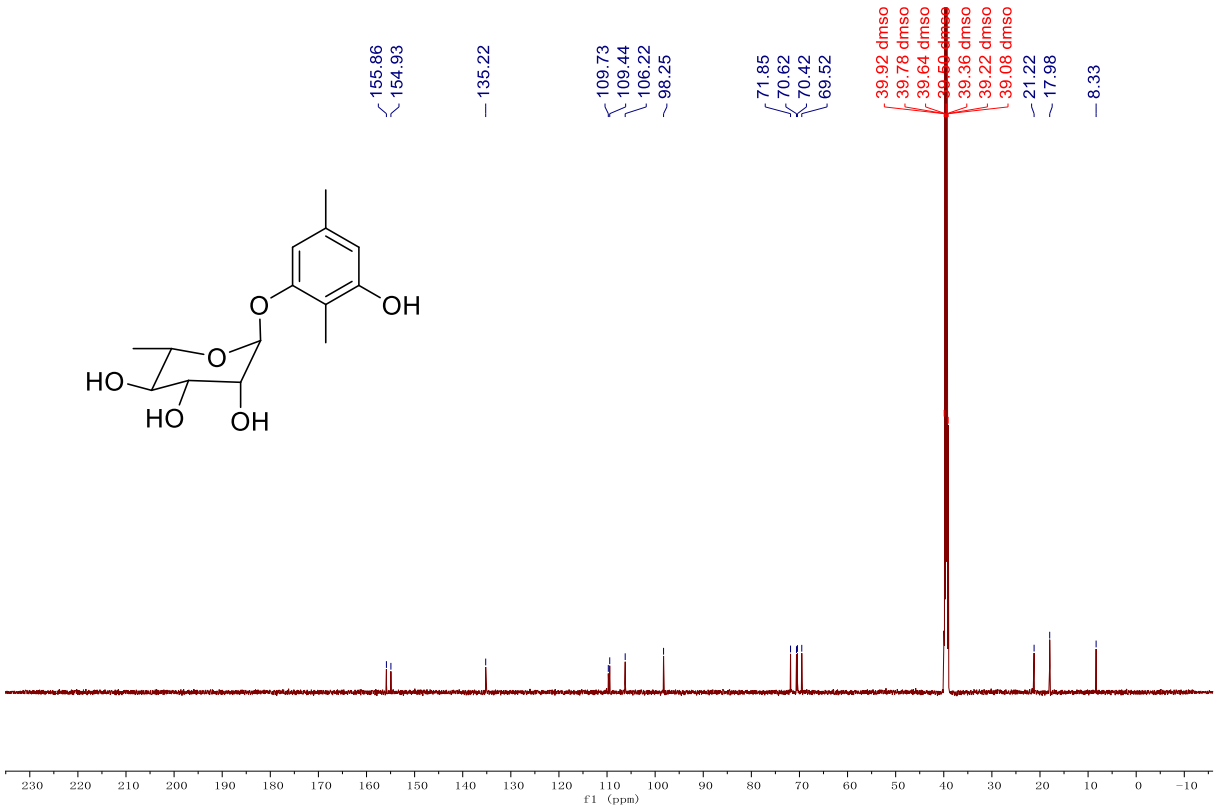

Figure S18: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of **5**

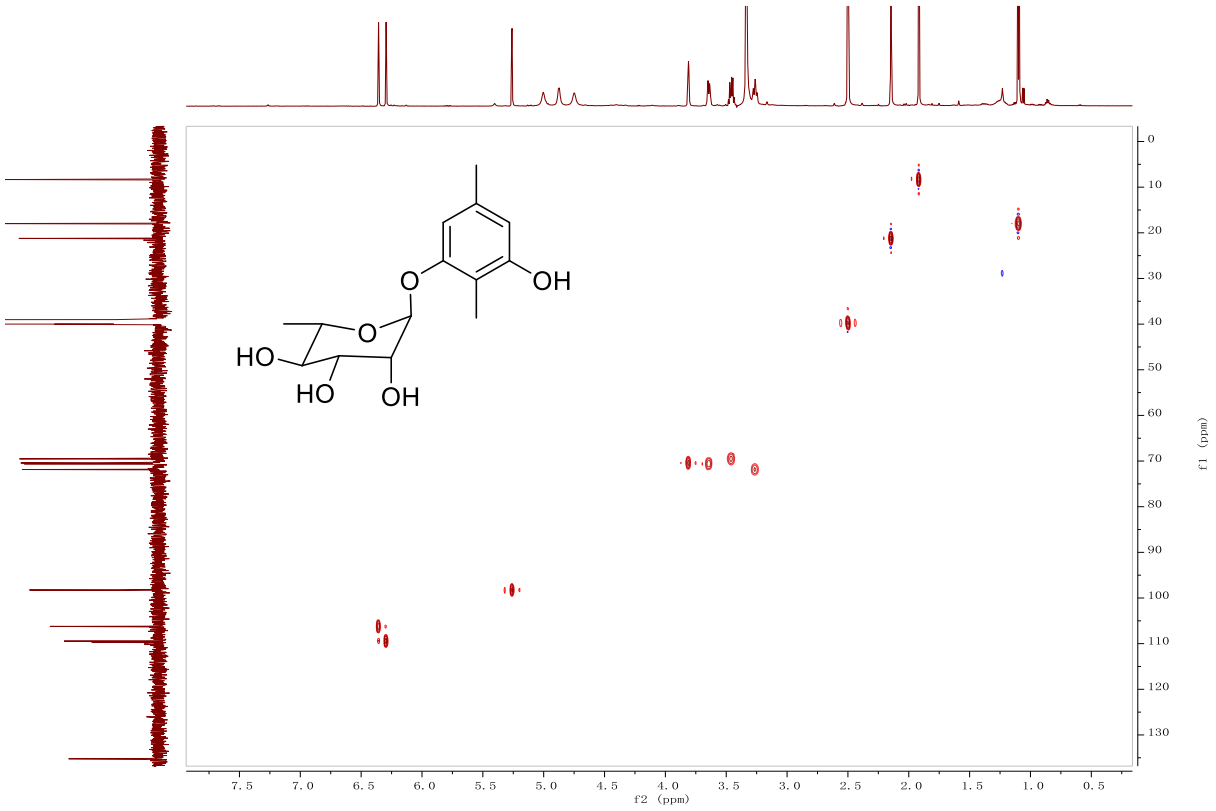

Figure S19: HSQC spectrum of **5**

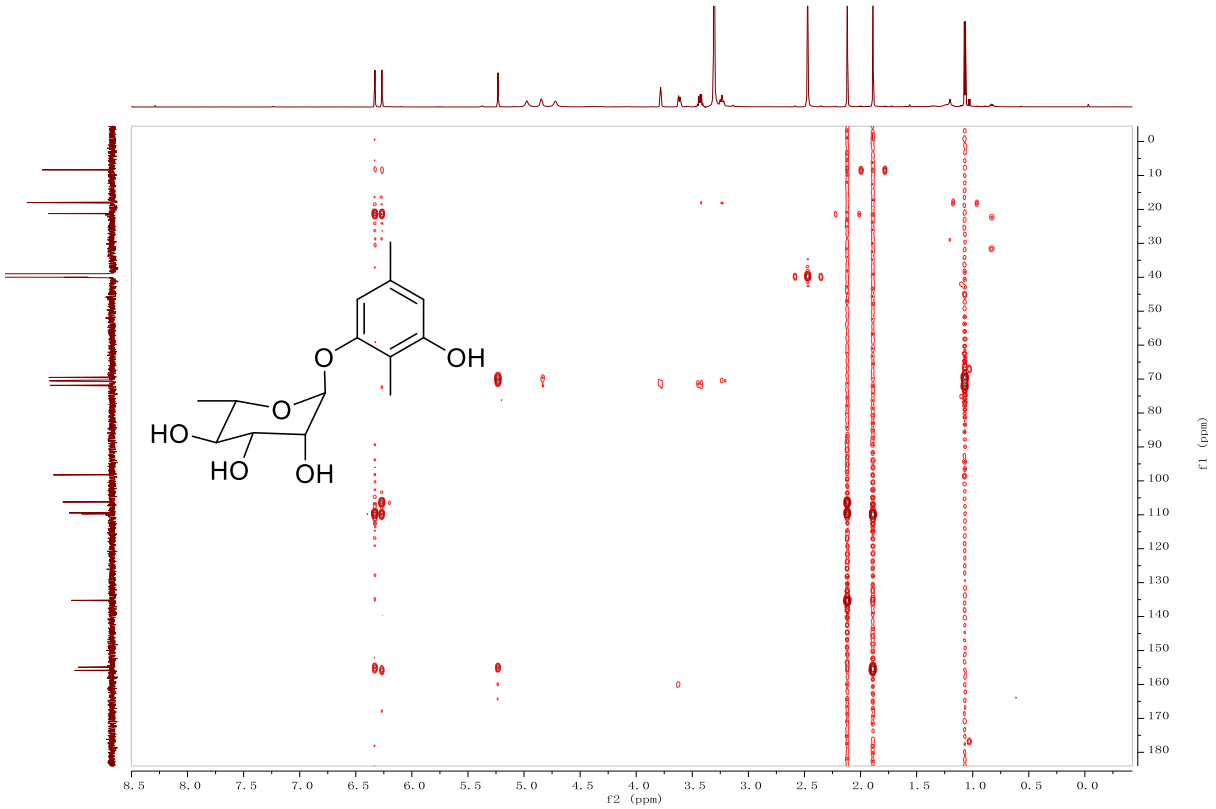

Figure S20: HMBC spectrum of **5**

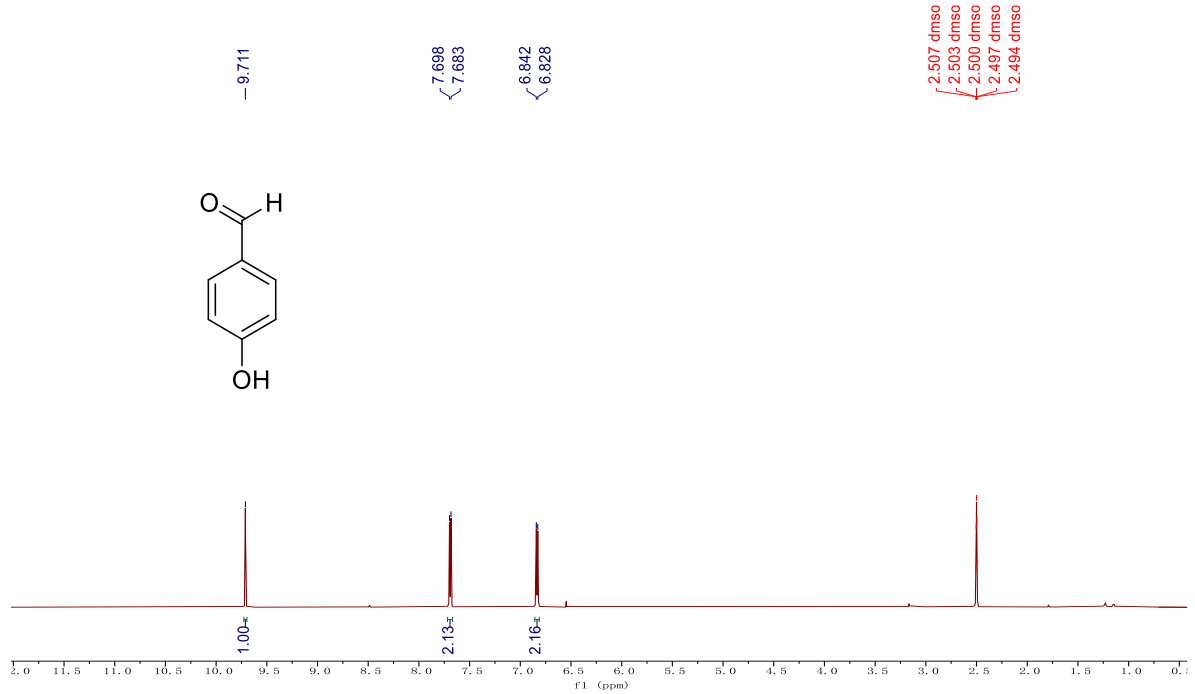

Figure S21: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **6**

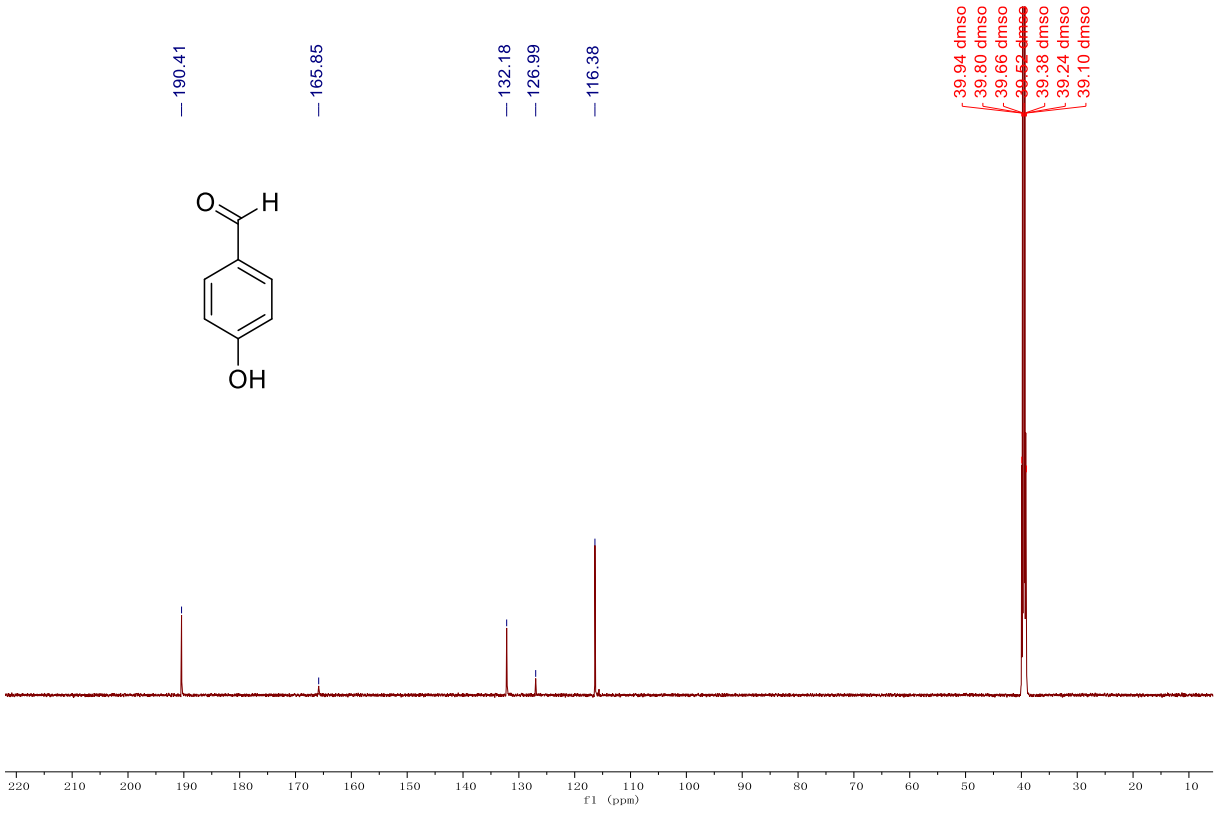

Figure S22: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of **6**

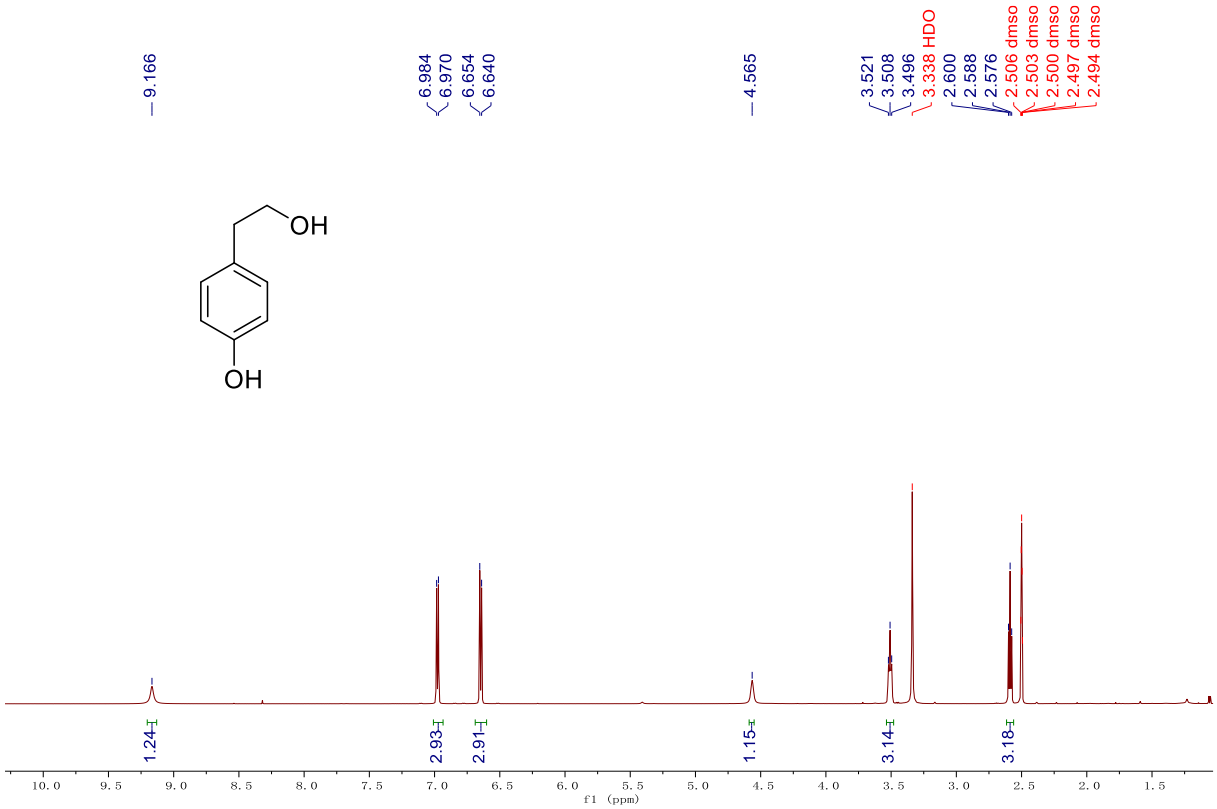

Figure S23: ^{1}H-NMR (600 MHz, DMSO-d_6 spectrum of **7**

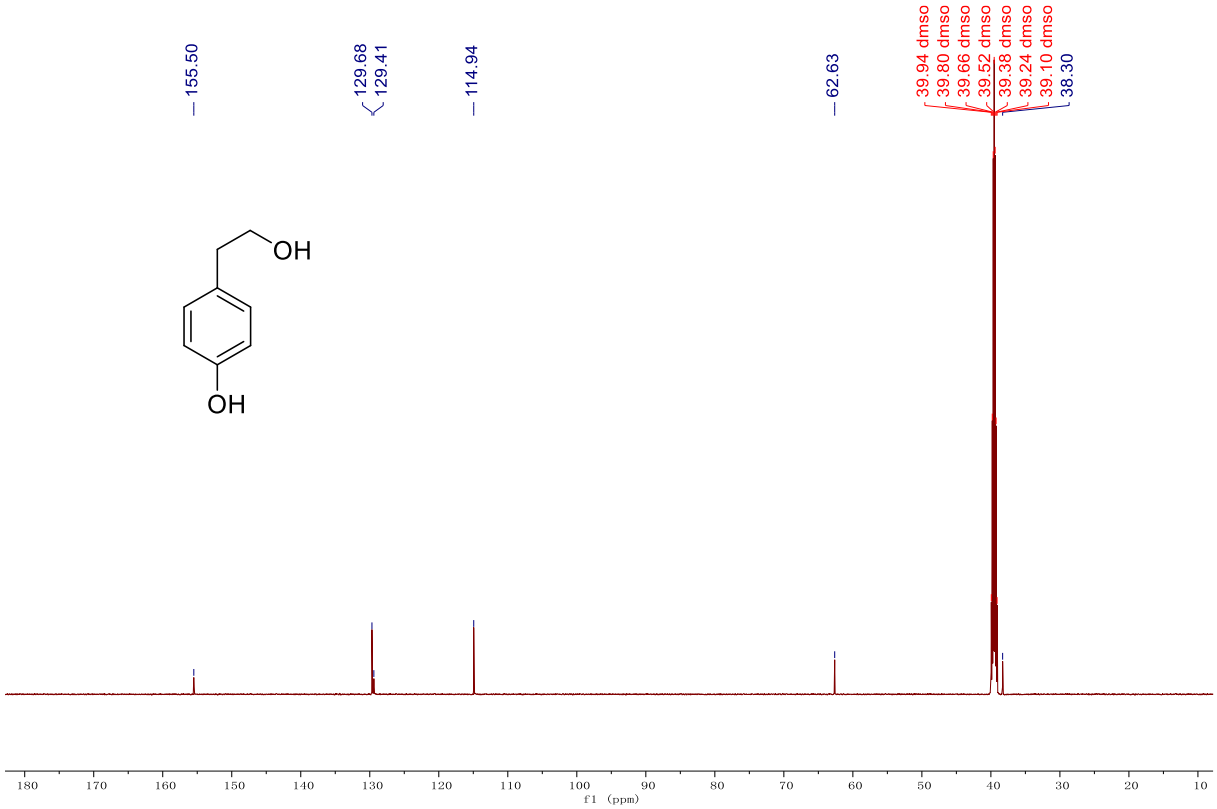

Figure S24: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of **7**

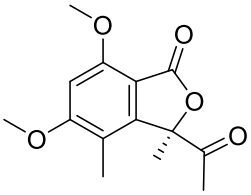

Figure S25: The Scifinder similarity report for new compound **1**

Spectroscopic Data of the Compounds 2-7

*(R)-3-acetyl-7-hydroxy-5-methoxyl-3H-isobenzofuran-l-one (**2**):* $[\alpha]^{25}_{D}$ +127.2 (*c* 0.08, MeOH); ESIMS *m/z* 251 $[M+H]^+$; CD (MeOH) λ_{max} ($\Delta\varepsilon$): 215 (–17.5), 241 (+4.8), 286 (+5.0) nm; ^{1}H and ^{13}C NMR data, see Table 1.

*Banksialactone D (**3**):* ESIMS *m/z* 267 $[M+H]^+$; ^{1}H NMR (600 MHz, DMSO-d_6) δ_H: 6.68 (1H, s, H-7), 5.14 (1H, d, *J* = 6.6 Hz, 4-OH), 4.08 (1H, m, H-3), 3.93 (3H, s, H-12), 3.90 (3H, s, H-13), 2.09 (3H, s, H-11), 1.61 (3H, s, H-10), 0.70 (3H, d, *J* = 6.6 Hz, H-9); ^{13}C NMR (150 MHz, DMSO-d_6) δ_C: 166.9 (C-1), 164.0 (C-6), 157.6 (C-8), 152.7 (C-4a), 110.9 (C-5), 104.8 (C-8a), 95.6 (C-7), 88.1 (C-4), 68.7 (C-3), 56.4 (C-12), 55.7 (C-13), 21.0 (C-10), 17.1 (C-9), 11.1 (C-11).

*(3R,4S)-3,8-dihydroxy-3-hydroxymethyl-6-methoxy-4,5-dimethyl-isochroman-1-one (**4**):* ESIMS *m/z* 269 $[M+H]^+$; ^{1}H NMR(600 MHz, $CDCl_3$) δ_H: 11.24 (1H, s, 8-OH), 6.38 (1H, s, H-7), 4.08 (1H, br s, Ha-9), 3.85 (3H, s, H-12), 3.69 (1H, m, Hb-9), 3.28 (1H, q, *J* = 6.6 Hz, H-4), 2.07 (3H, s, H-11), 1.17 (3H, d, *J* = 6.6 Hz, H-10); ^{13}C NMR (150 MHz, $CDCl_3$) δ_H: 168.7 (C-1), 164.9 (C-6), 163.3 (C-8), 141.8 (C-4a), 115.6 (C-5), 99.4 (C-8a), 97.7 (C-7), 65.8 (C-9), 55.9 (C-12), 36.3 (C-4), 15.6 (C-10), 10.2 (C-11).

*1-O-[α-L-rhamnopyranosyl]-2,5-dimethyl-3-phenol (**5**):* $[\alpha]^{25}_{D}$ -123.3 (*c* 0.01, MeOH); ESIMS *m/z* 283 $[M-H]^-$; ^{1}H NMR (600 MHz, DMSO-d_6) δ_H: 6.36 (1H, s, H-6), 6.30 (1H, s, H-4), 5.23 (1H, d, *J* = 1.8 Hz, H-1′), 3.81 (1H, m, H-2′), 3.65 (1H, m, H-3′), 3.46 (1H, m, H-5′), 3.26 (1H, m, H-4′), 2.15 (3H, s, H-8), 1.92 (3H, s, H-7), 1.10 (3H, d, *J* = 6.6 Hz, H-6′),; ^{13}C NMR (150 MHz, DMSO-d_6) δ_C: 155.9 (C-3), 154.9 (C-1), 135.2 (C-5), 109.7 (C-2), 109.4 (C-4), 106.2 (C-6), 98.3 (C-1′), 71.9 (C-4′), 70.6 (C-3′), 70.4 (C-2′), 69.5 (C-5′), 21.2 (C-8), 18.0 (C-6′), 8.3 (C-7).

p-hydroxybenzaldehyde (**6**): ESIMS *m/z* 123 $[M+H]^+$; ^{1}H NMR (600 MHz, DMSO-d_6) δ_H: 9.71 (1H, s, H-7), 7.69 (2H, d, *J* = 8.4 Hz, H-3, H-5), 6.84 (2H, d, *J* = 8.4 Hz, H-2, H-6); ^{13}C NMR (150 MHz, DMSO-d_6) δ_C: 190.4 (C-7), 165.9 (C-4), 132.2 (C-2, C-6), 127.0 (C-1), 116.4 (C-3, C-5).

*2-(4-hydroxyphenyl) ethanol (**7**):* ESIMS *m/z* 139 $[M+H]^+$; ^{1}H NMR(600 MHz, DMSO-d_6) δ_H: 9.17 (1H, s, 4′-OH), 6.98 (2H, d, *J* = 8.4 Hz, H-2′, H-6′), 6.65 (2H, d, *J* = 8.4 Hz, H-3′, H-5′), 4.57 (1H, br s, 1-OH), 3.51 (2H, t, *J* = 7.2 Hz, H-1), 2.59 (2H, t, *J* = 7.2 Hz, H-2); ^{13}C NMR (150 MHz, DMSO-d_6) δ_C: 155.5 (C-4′), 129.7 (C-1′), 129.4 (C-2′, C-6′), 114.9 (C-3′, C-5′), 62.6 (C-1), 38.3 (C-2).

Cytotoxic Activity Assays

MTT assay was used to measure the cytotoxicities of compounds. Five human cancer cell lines (HeLa, HCT116, HepG2, A549, and H460) were obtained from ATCC. Cells (5×10^3 cells/well) were

added to 96-well culture dishes and grown for 24 h followed by the addition of fresh medium (100mL) and the test compound. After an additional 48 h, the media was removed and fresh media with MTT solution was added. The cells were incubated for 1 h and then the optical density at 450 nm was determined. Compounds **1**–**7** were tested for five cancer cell lines at three concentrations (50, 5, 0.5 μM). Each concentration of the compounds was tested in three parallels. IC_{50} values for each cell line were determined with Sigmaplot software.

Antibacterial Activity Assays

The minimal inhibitory concentrations (MICs) of the isolated compounds were determined by the broth microdilution method in 96-well plates according to Clinical and Laboratory Standards Institute. All the test strains used in this study were standard strains obtained from American Type Culture Collection (ATCC), and levofloxacin was used as positive control. The final concentrations of compounds ranged from 0.5 to 64 μg/mL. Culture plates were incubated at 37 ^{o}C for 18 h. The MICs were defined as the lowest concentration that prevented visible growth of the bacteria.