

Supporting Information

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A New Acetylenic Compound and Other Bioactive Metabolites from a Shark Gill-derived *Penicillium* Strain

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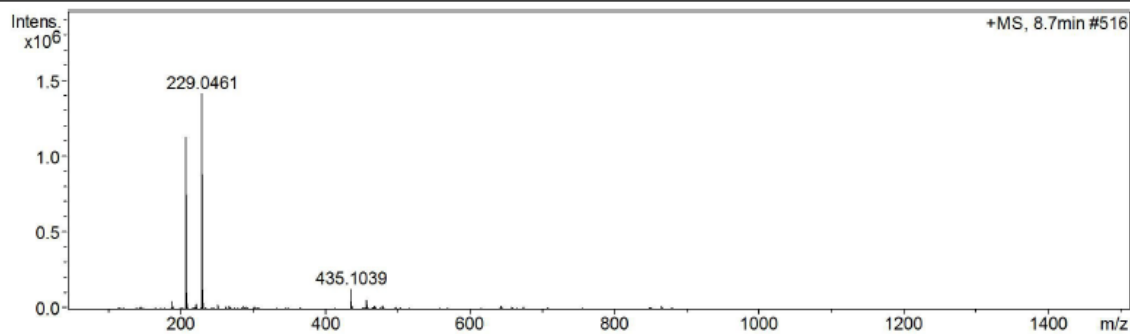
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Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name C:\Users\ADMINI~1\AppData\Local\Temp\Rar\$DR00.751\PC-6_RC3_01_114.d
Method hplc_ms_martina.m
Sample Name PC-6
Comment
Acquisition Date 2013/1/24 12:19:37
Operator Lui
Instrument / Ser# maXis 4G 21253

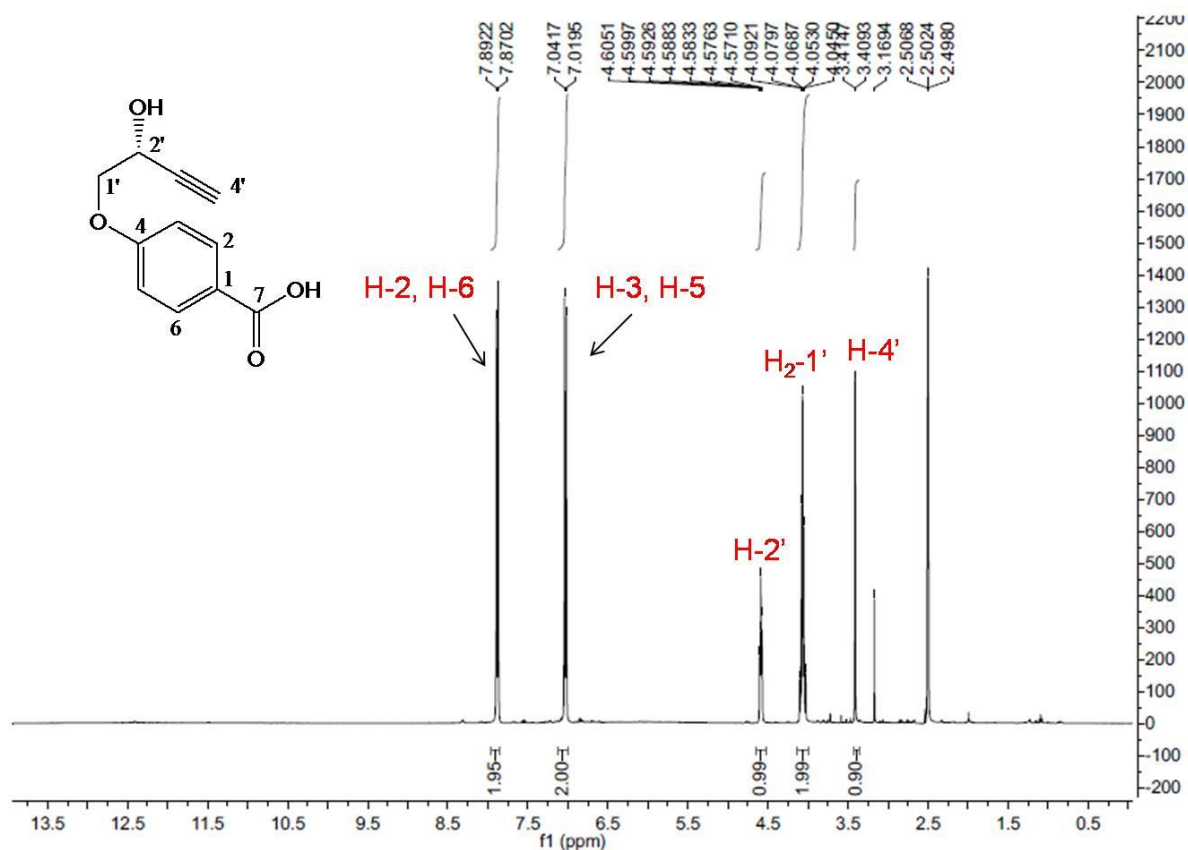
Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 1.2 Bar
Focus Not active Set Capillary 3200 V Set Dry Heater 180 °C
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 6.0 l/min
Scan End 1000 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Waste



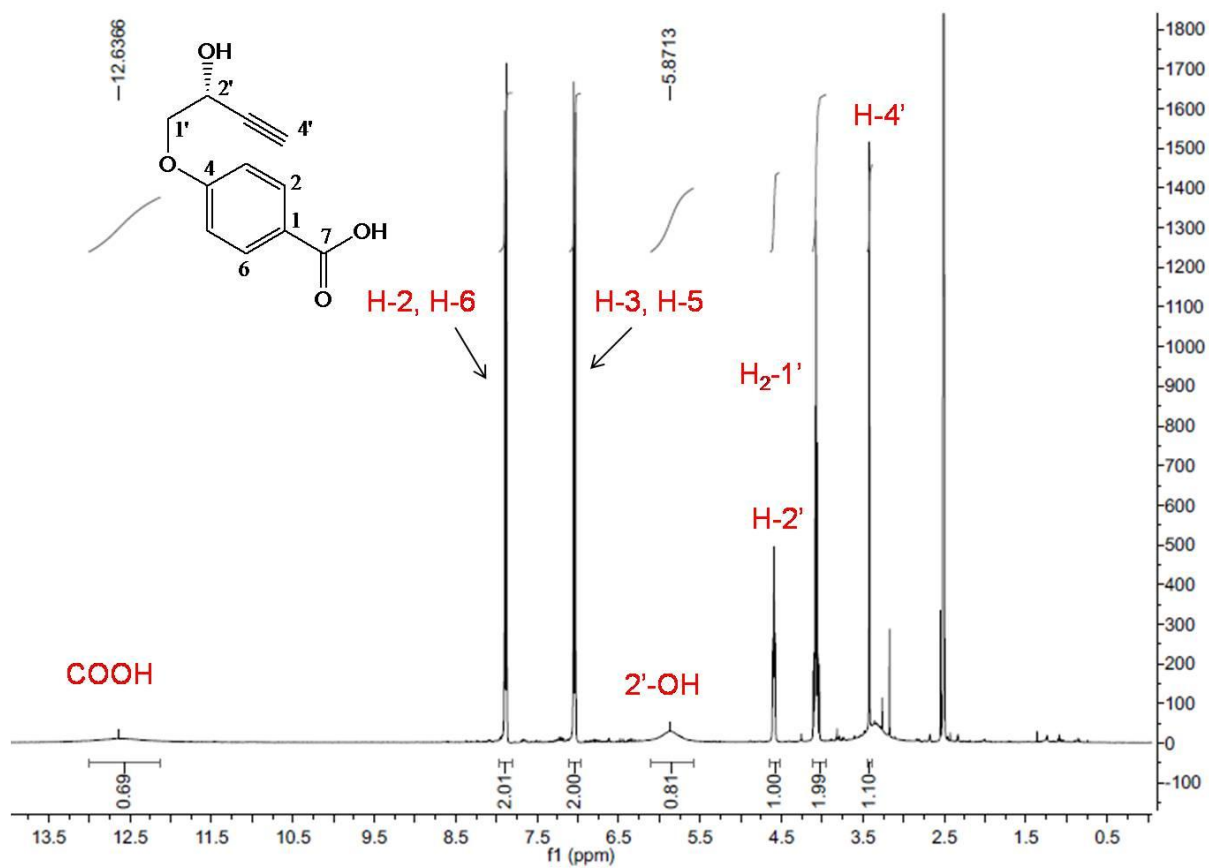
| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | ej%Conf | N-Rule |
|-----------|---|--------------------|--------|----------|-----------|-----------|--------|-----|---------|--------|
| 229.0461 | 1 | C 11 H 10 Na O 4 | 100.00 | 229.0471 | 1.0 | 4.4 | 15.4 | 6.5 | even | ok |
| | 2 | C 7 H 6 N 6 Na O 2 | 81.42 | 229.0444 | -1.7 | -7.3 | 3.9 | 7.5 | even | ok |

S1: HRESI-MS spectrum of compound 1

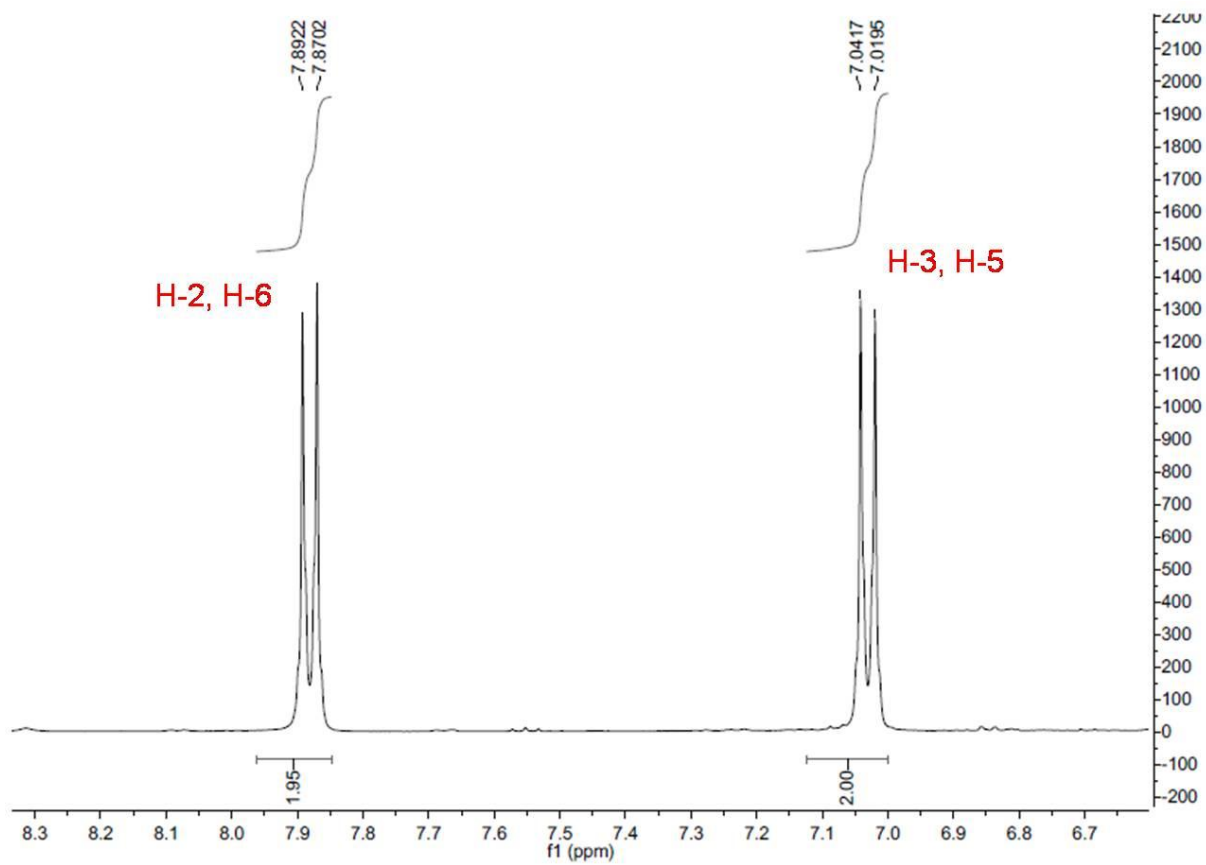


S2: ¹H NMR spectra of compound **1** (400 MHz, DMSO-d₆, tested for the first time)

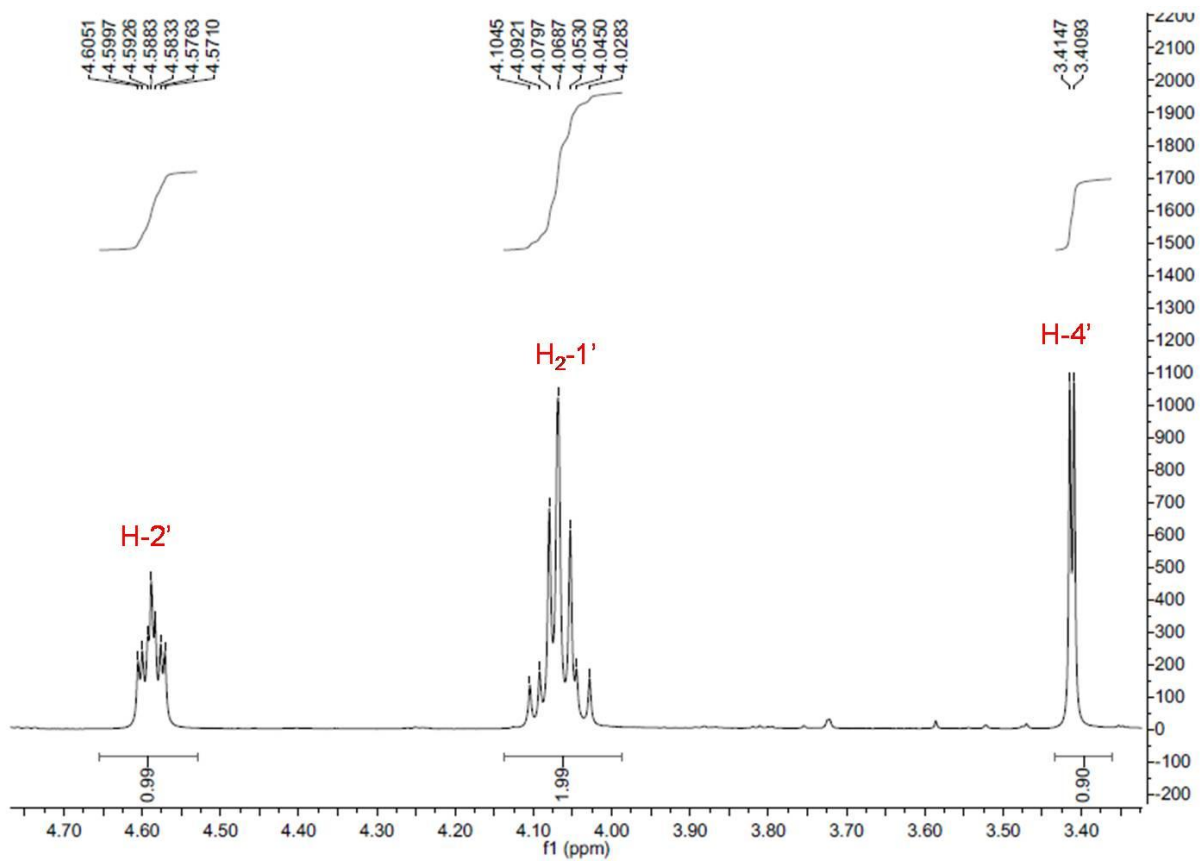
(-)-WA (**1**): Amorphous powder. ¹H-NMR (DMSO-d₆, 400 MHz), δ : 3.41 (1H, d, $J = 2.2$ Hz, H-4'), 4.07 (2H, m, H₂-1'), 4.59 (1H, m, H-2'), 5.87 (1H, brs, 2'-OH), 7.03 (2H, d, $J = 8.9$ Hz, H-3 and H-5), 7.88 (2H, d, $J = 8.9$ Hz, H-2 and H-6), 12.64 (1H, brs, COOH). ¹³C-NMR (DMSO-d₆, 100 MHz), δ : 59.4 (C-2'), 71.4 (C-1'), 75.7 (C-4'), 83.5 (C-3'), 114.4 (C-3 and C-5), 123.6 (C-1), 131.3 (C-2 and C-6), 161.7 (C-4), 167.1 (C-7). HR-ESI-MS m/z 229.0461 ([M+Na]⁺, C₁₁H₁₀NaO₄⁺; calcd. 229.0471).



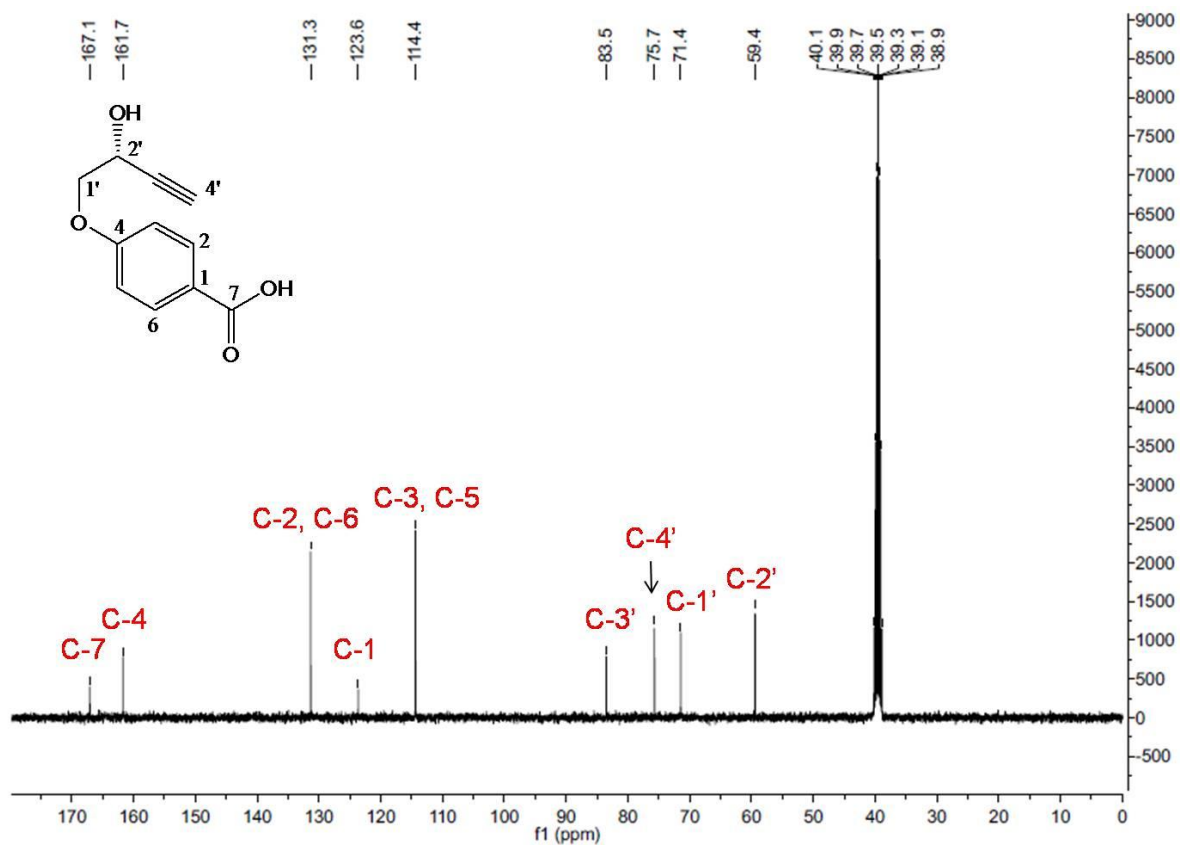
S3: ^1H NMR spectra of compound **1** (400 MHz, DMSO-d_6 , tested for the second time; showing the signals of the active protons)



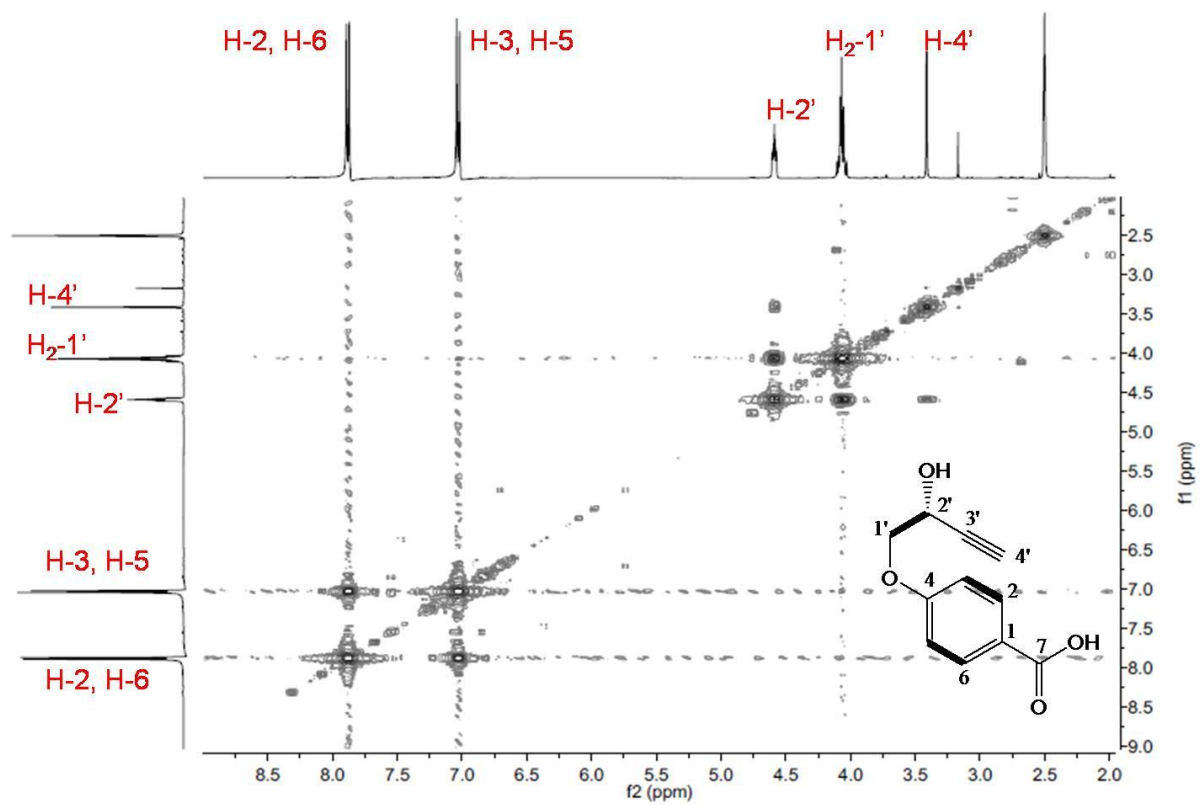
S4: Expansion of the $^1\text{H-NMR}$ Spectrum of Compound **1** (From 6.60 to 8.30 ppm)



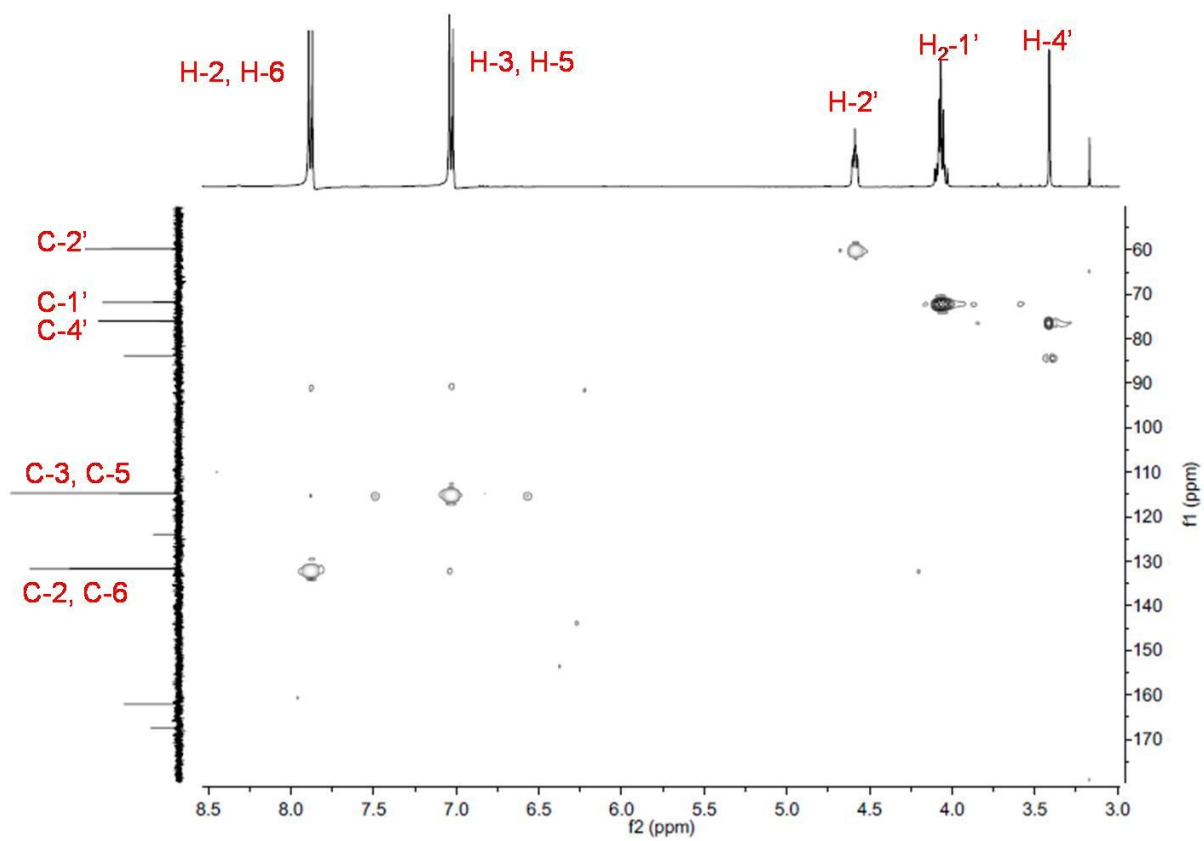
S5: Expansion of the ¹H-NMR Spectrum of Compound **1** (From 3.35 to 4.75 ppm)



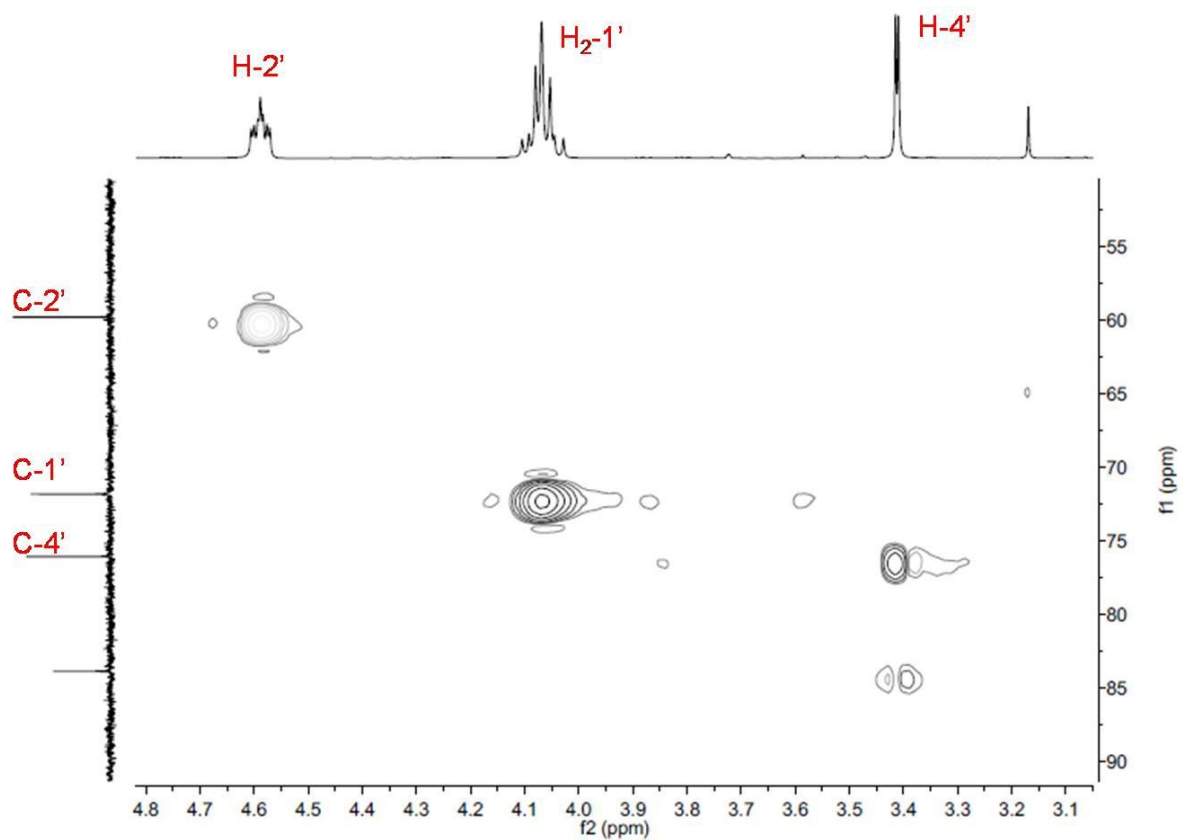
S6: ^{13}C NMR spectra of compound 1 (100 MHz, DMSO- d_6)



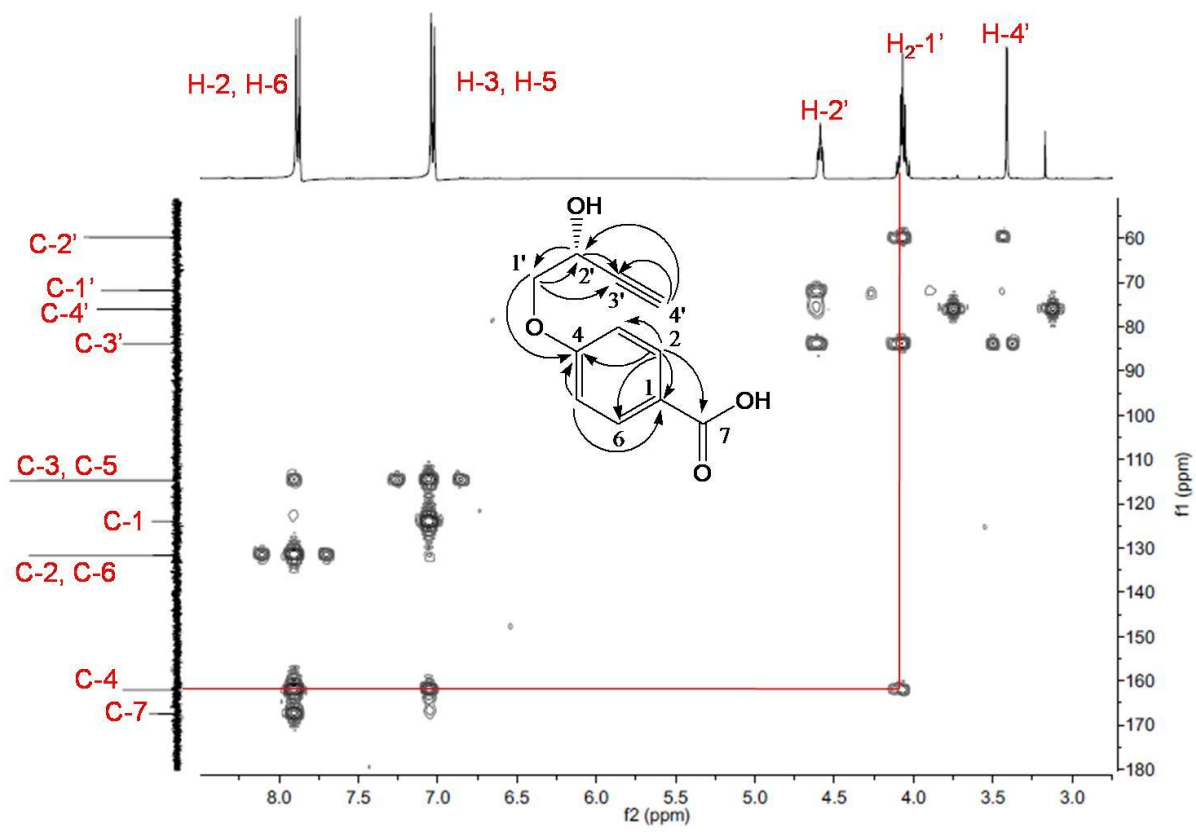
S7: COSY (400 MHz) Spectrum of Compound 1



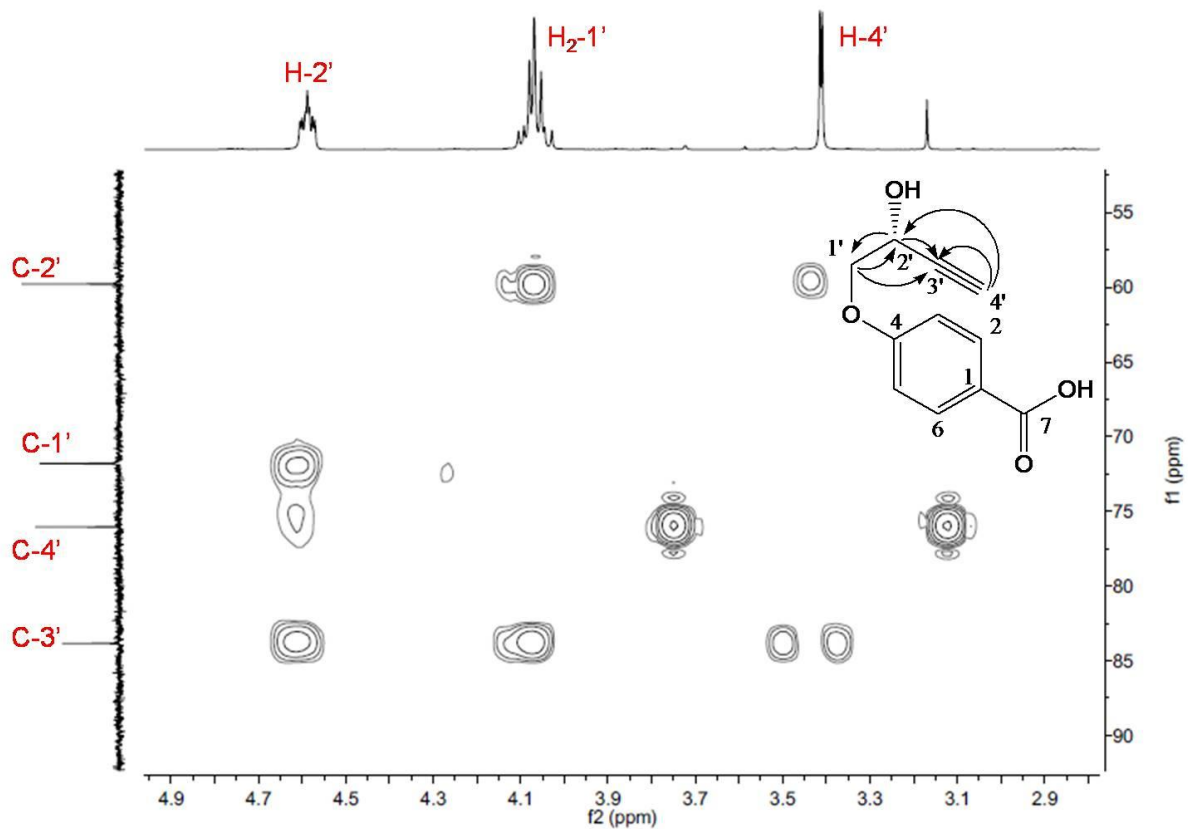
S8: HSQC (400 MHz) Spectrum of Compound 1



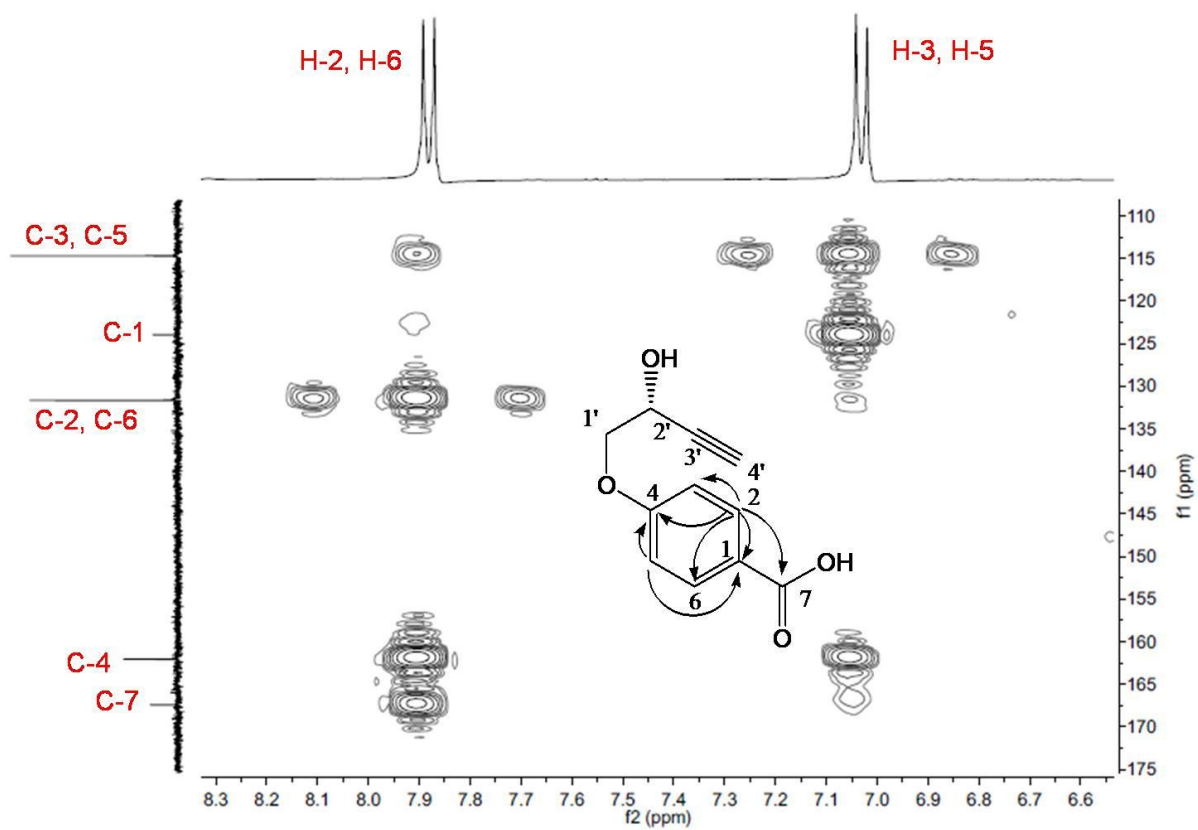
S9: Expansion of the HSQC (400 MHz) Spectrum of Compound **1** (From 50 to 90 ppm)



S10: HMBC (400 MHz) Spectrum of Compound 1



S11: Expansion of the HMBC (400 MHz) Spectrum of Compound **1** (From 52.5 to 90 ppm)



S12: Expansion of the HMBC (400 MHz) Spectrum of Compound **1** (From 110 to 175 ppm)