Supplementary Materials: Cytotoxic 1,3-Thiazole and 1,2,4-Thiadiazole Alkaloids from *Penicillium oxalicum*: Structural Elucidation and Total Synthesis

Zheng Yang, Nianyu Huang, Bang Xu, Wenfeng Huang, Tianpeng Xie, Fan Cheng and Kun Zou

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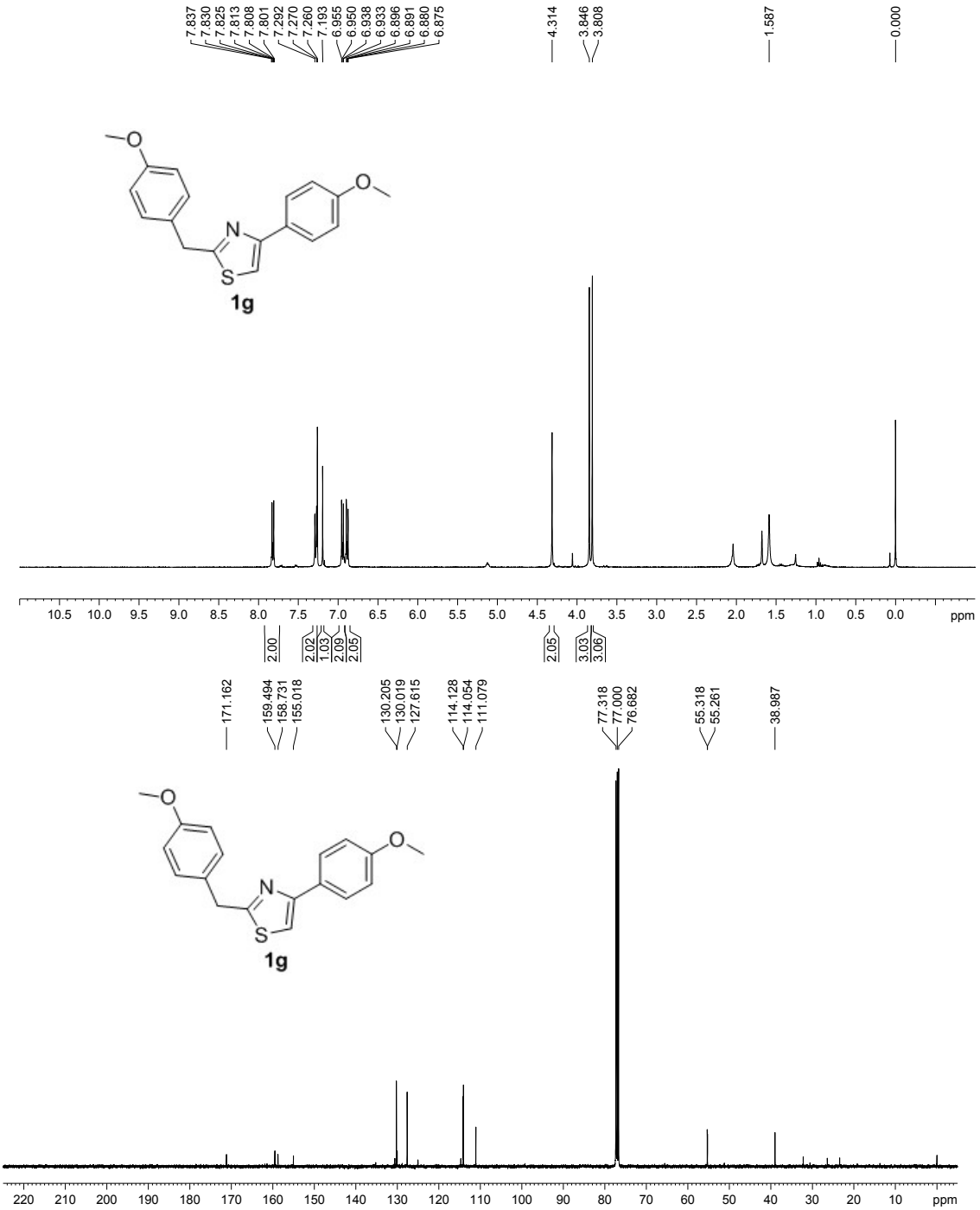


Figure S1. ^{1}H-NMR and ^{13}C-NMR of compound **1g**.

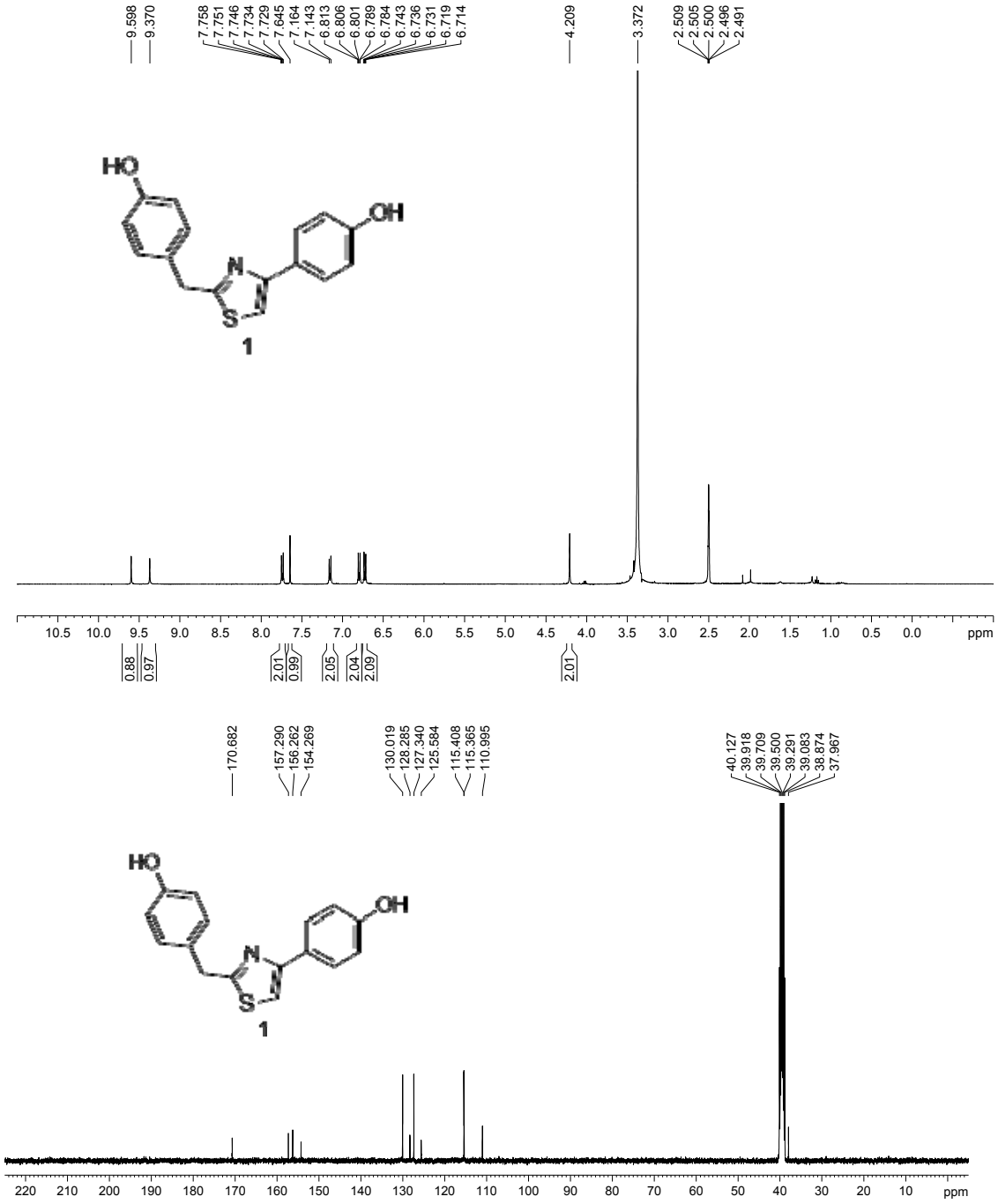


Figure S2. ^{1}H-NMR and ^{13}C-NMR of compound **1**.

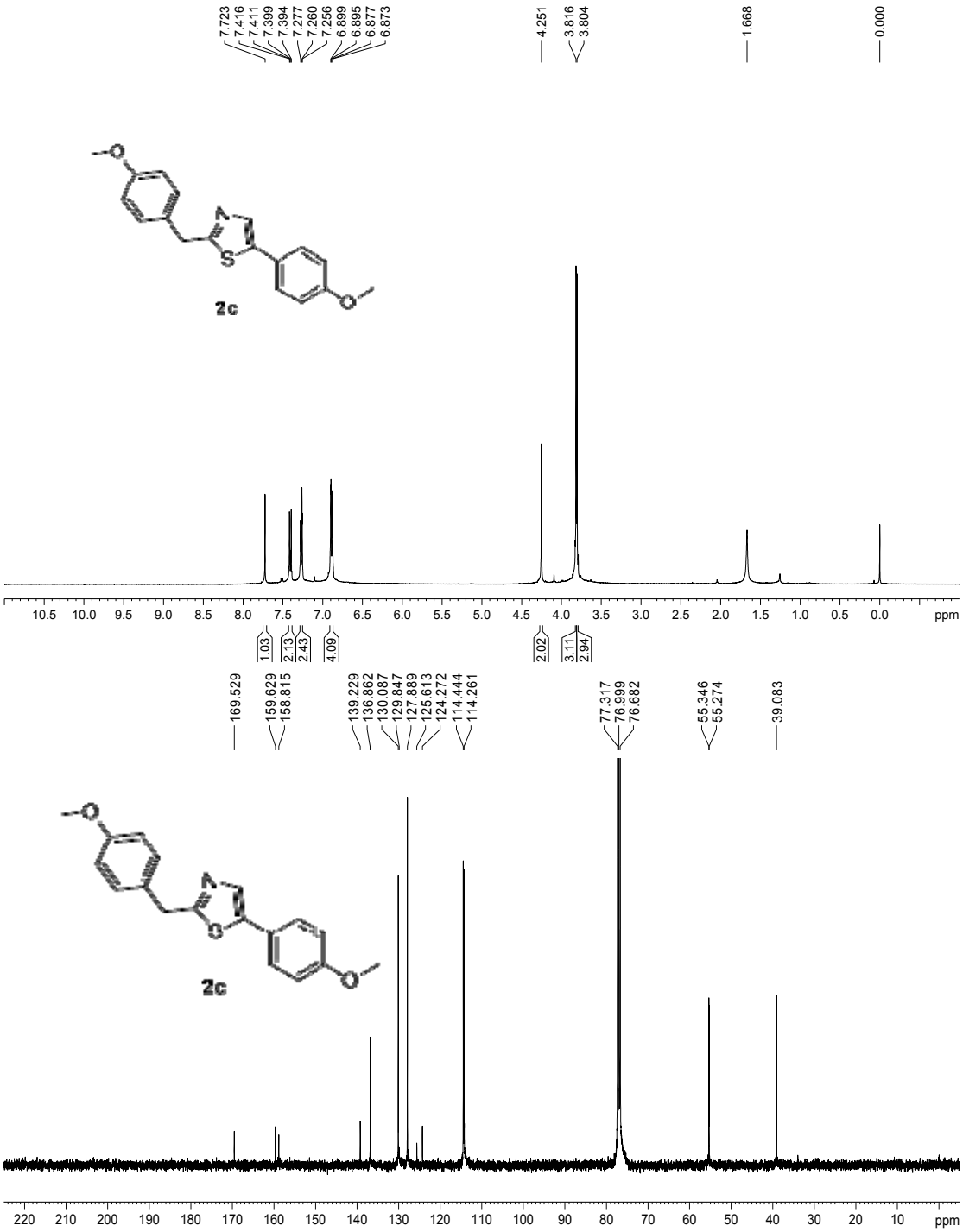


Figure S3. ^{1}H-NMR and ^{13}C-NMR of compound **2c**.

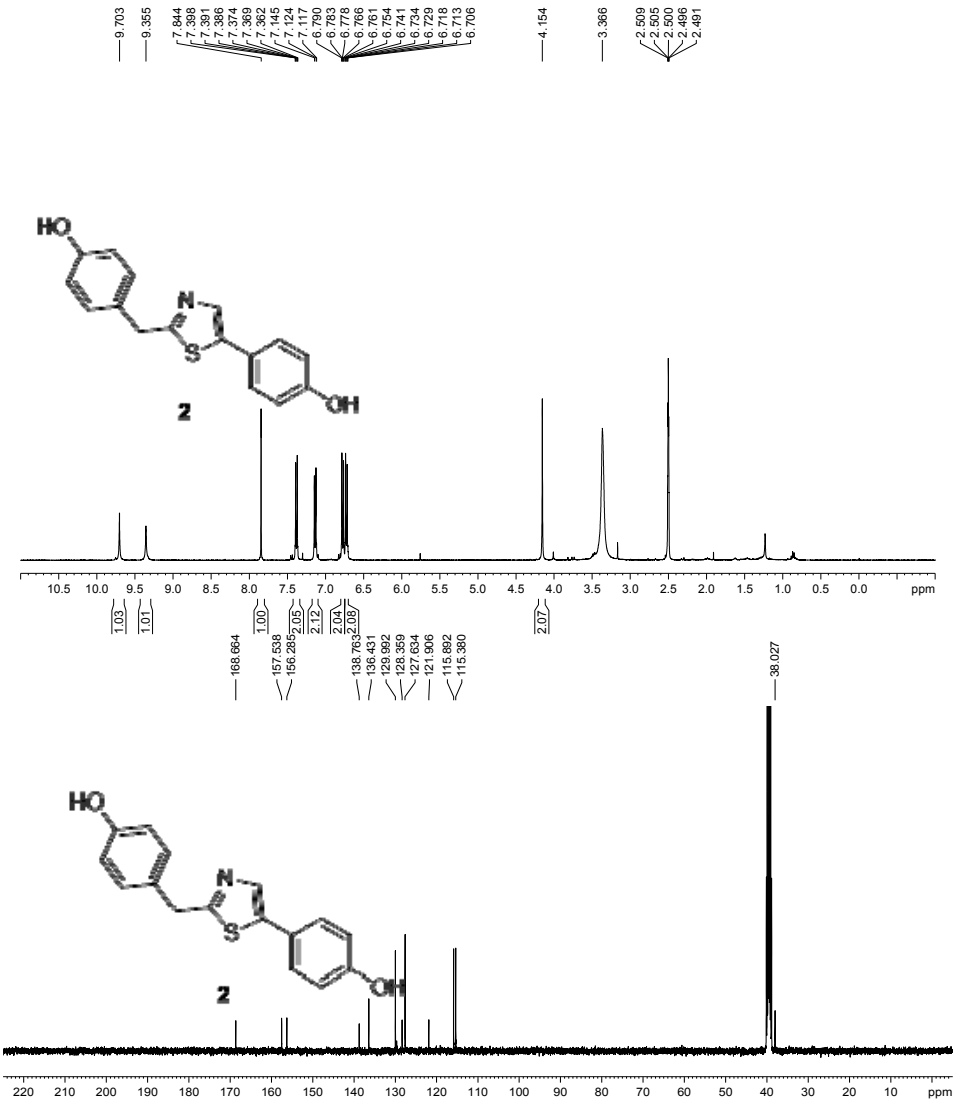


Figure S4. ^{1}H-NMR and ^{13}C-NMR of compound **2**.

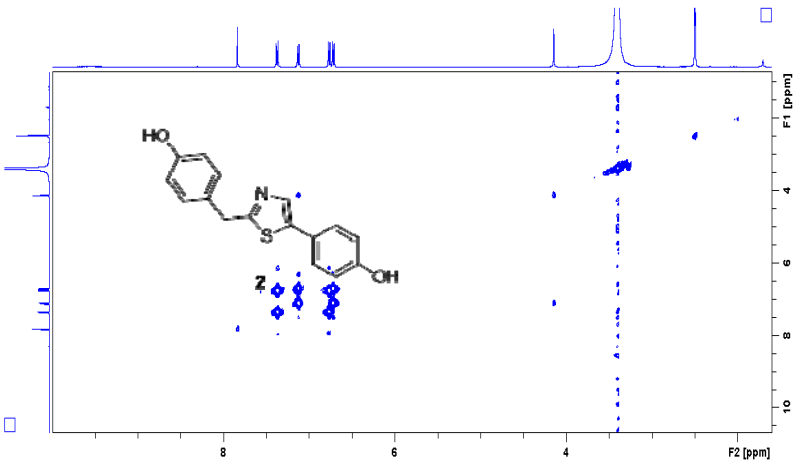


Figure S5. ^{1}H-^{1}H COSY of compound **2**.

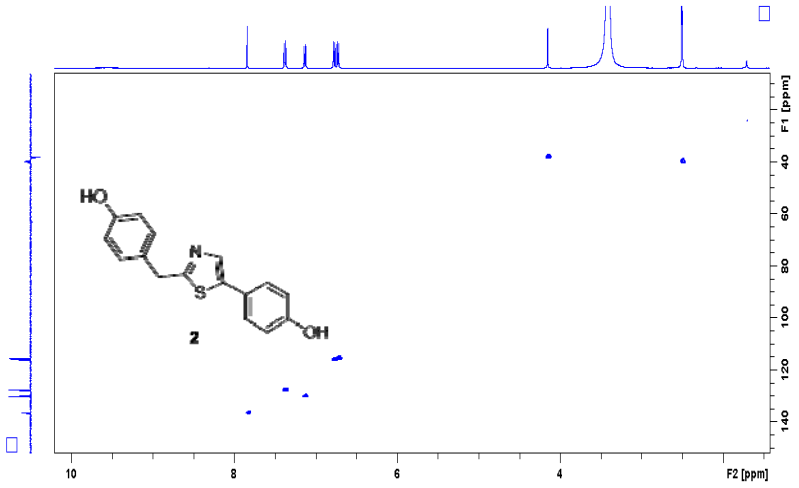


Figure S6. HSQC of compound **2**.

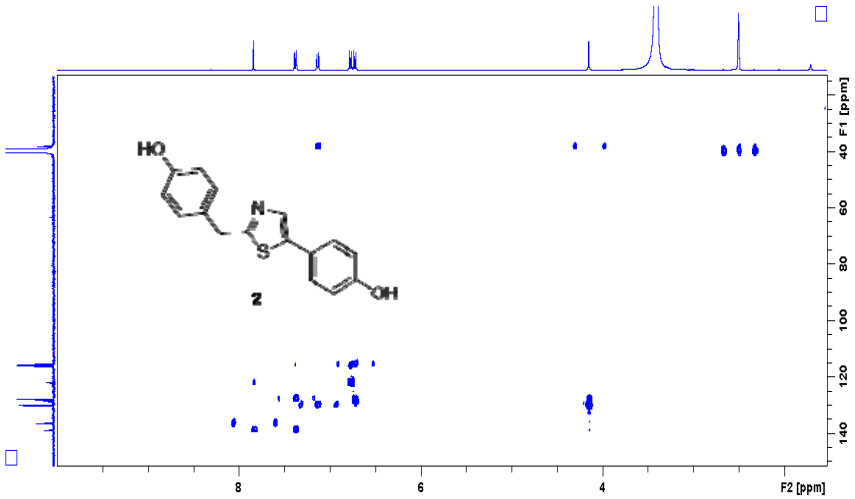


Figure S7. HMBC of compound **2**.

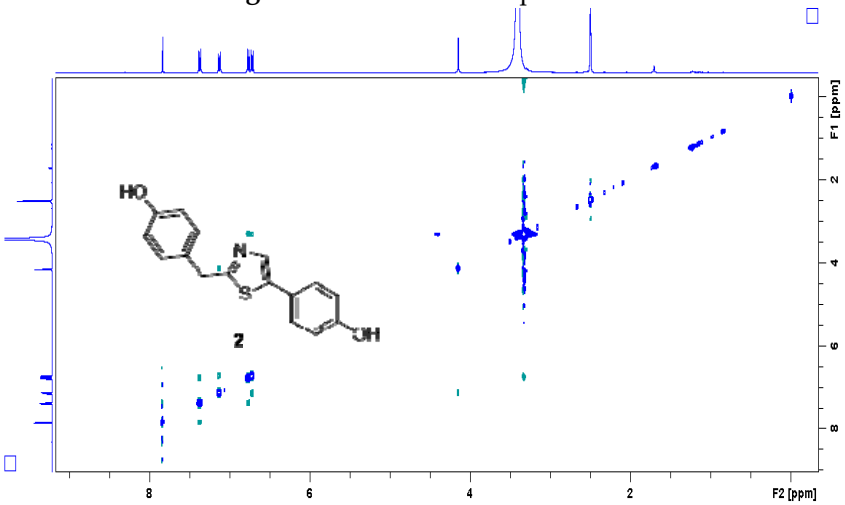


Figure S8. NOESY of compound **2**.

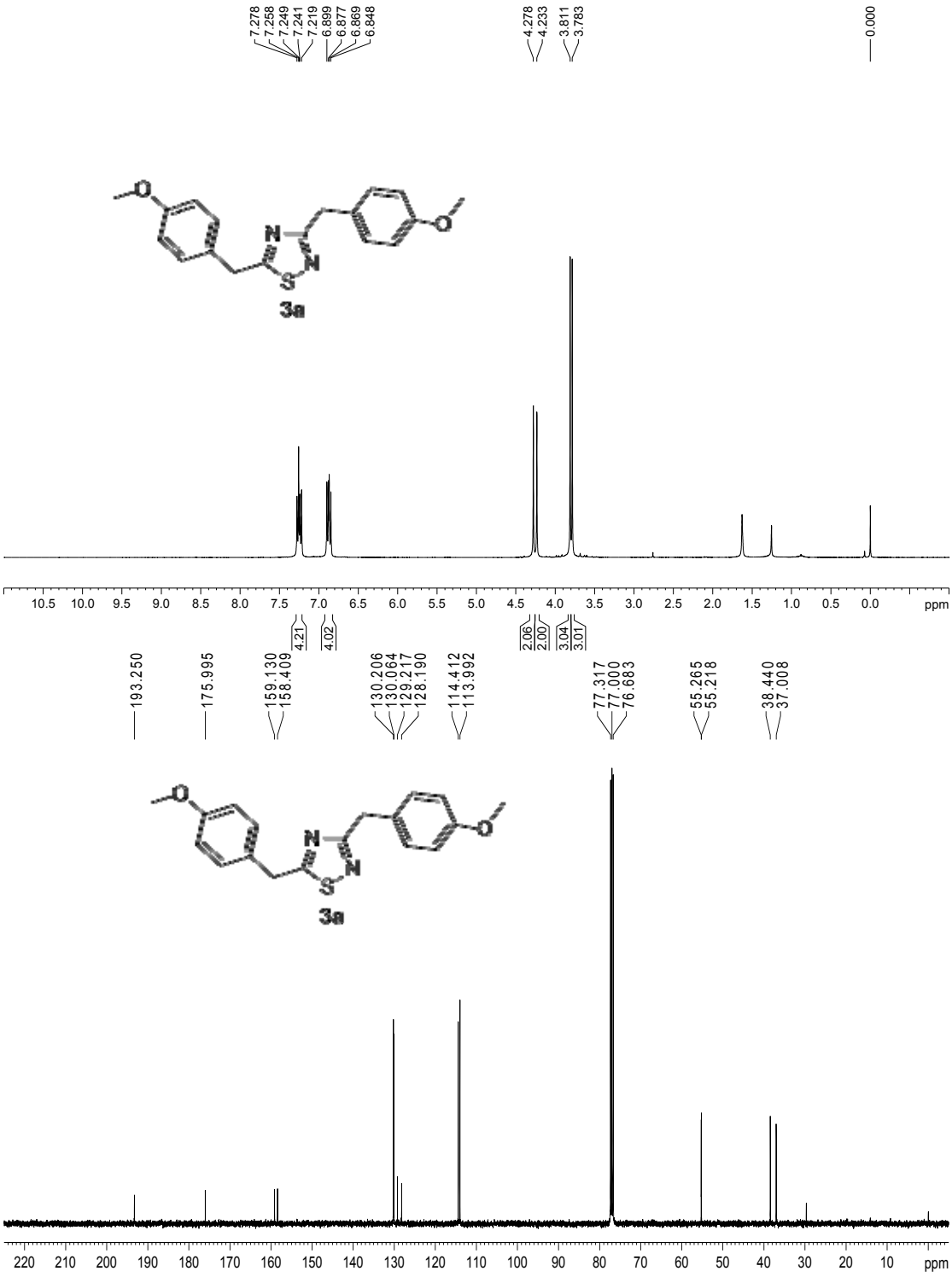


Figure S9. ^{1}H-NMR and ^{13}C-NMR of compound **3a**.

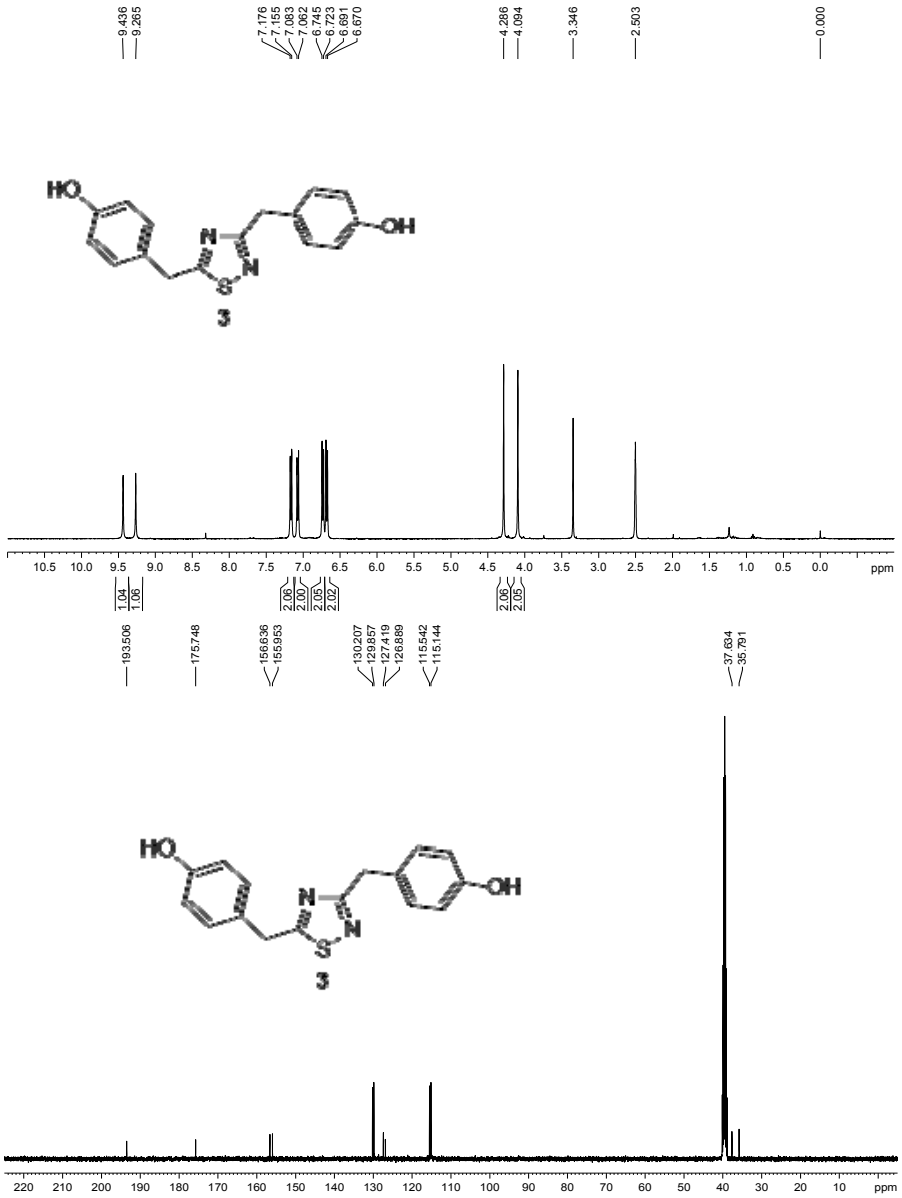


Figure S10. ^{1}H-NMR and ^{13}C-NMR of compound **3**.

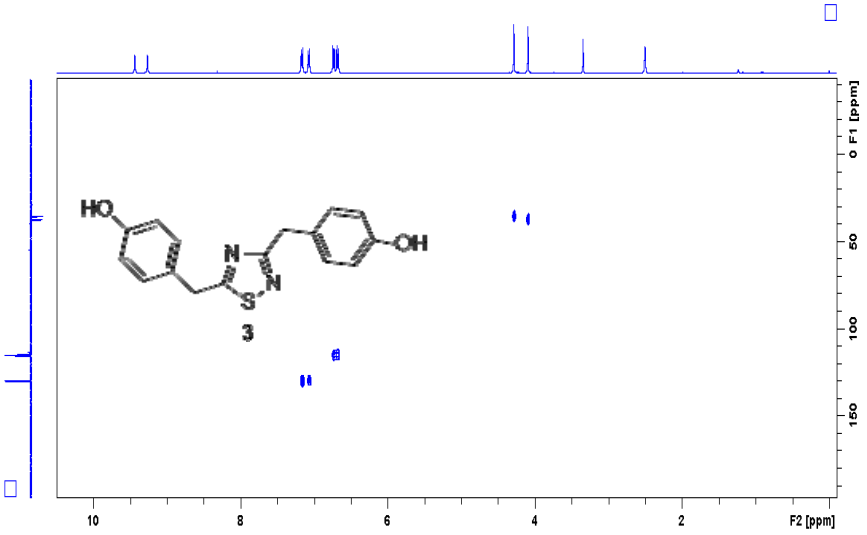


Figure S11. HSQC of compound **3**.

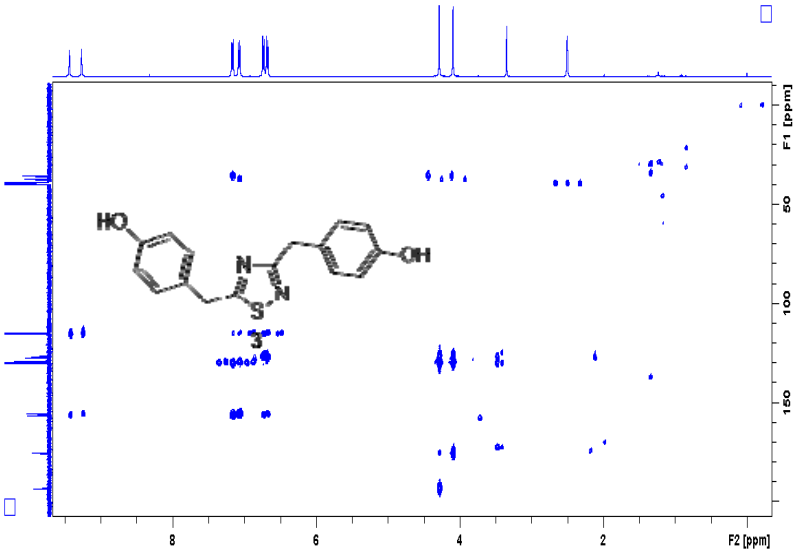


Figure S12. HMBC of compound **3**.

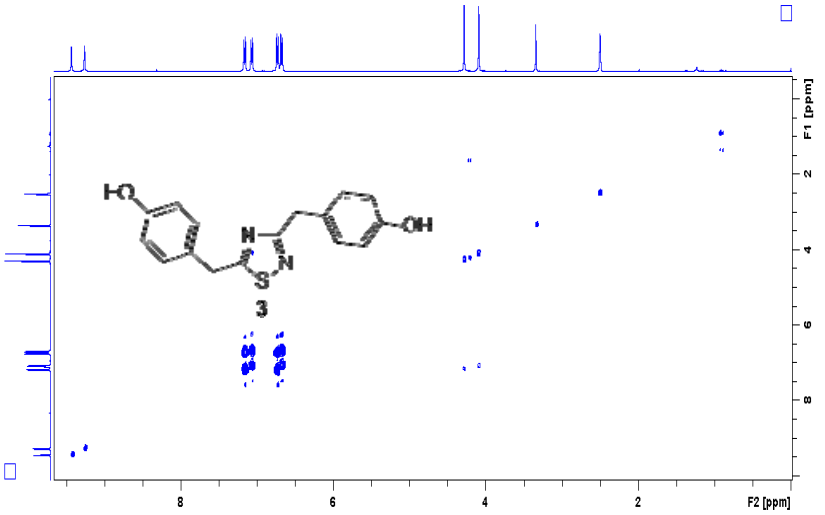


Figure S13. ^{1}H-^{1}H COSY of compound 3.

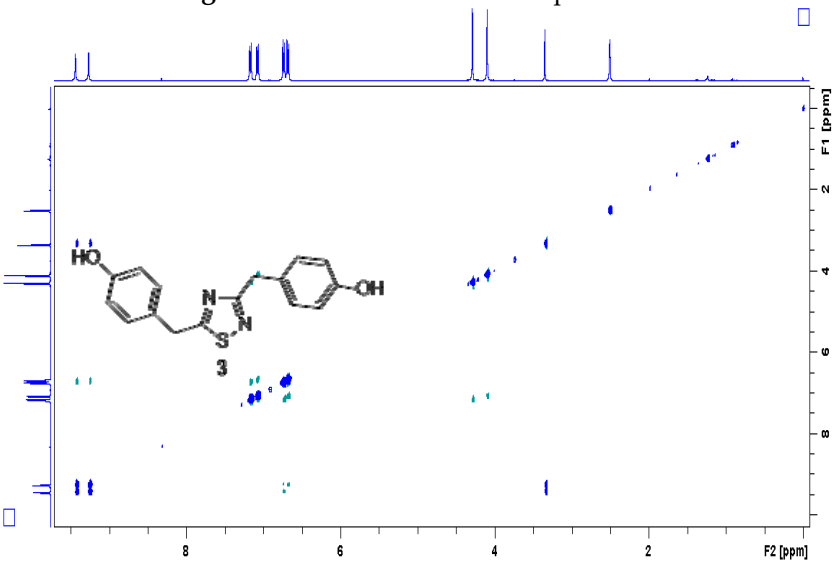


Figure S14. NOESY of compound **3**.

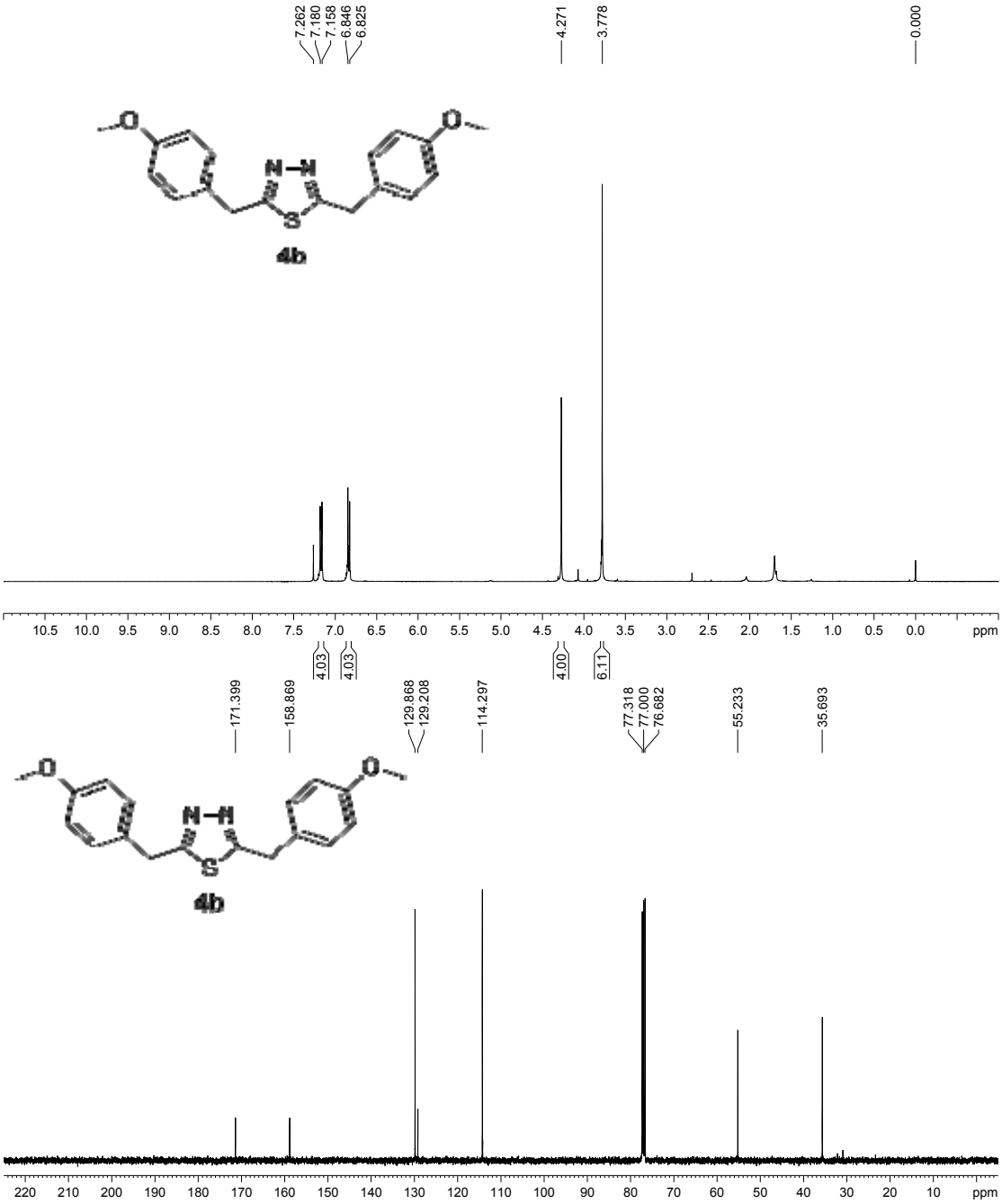


Figure S15. ^{1}H-NMR and ^{13}C-NMR of compound **4b**.

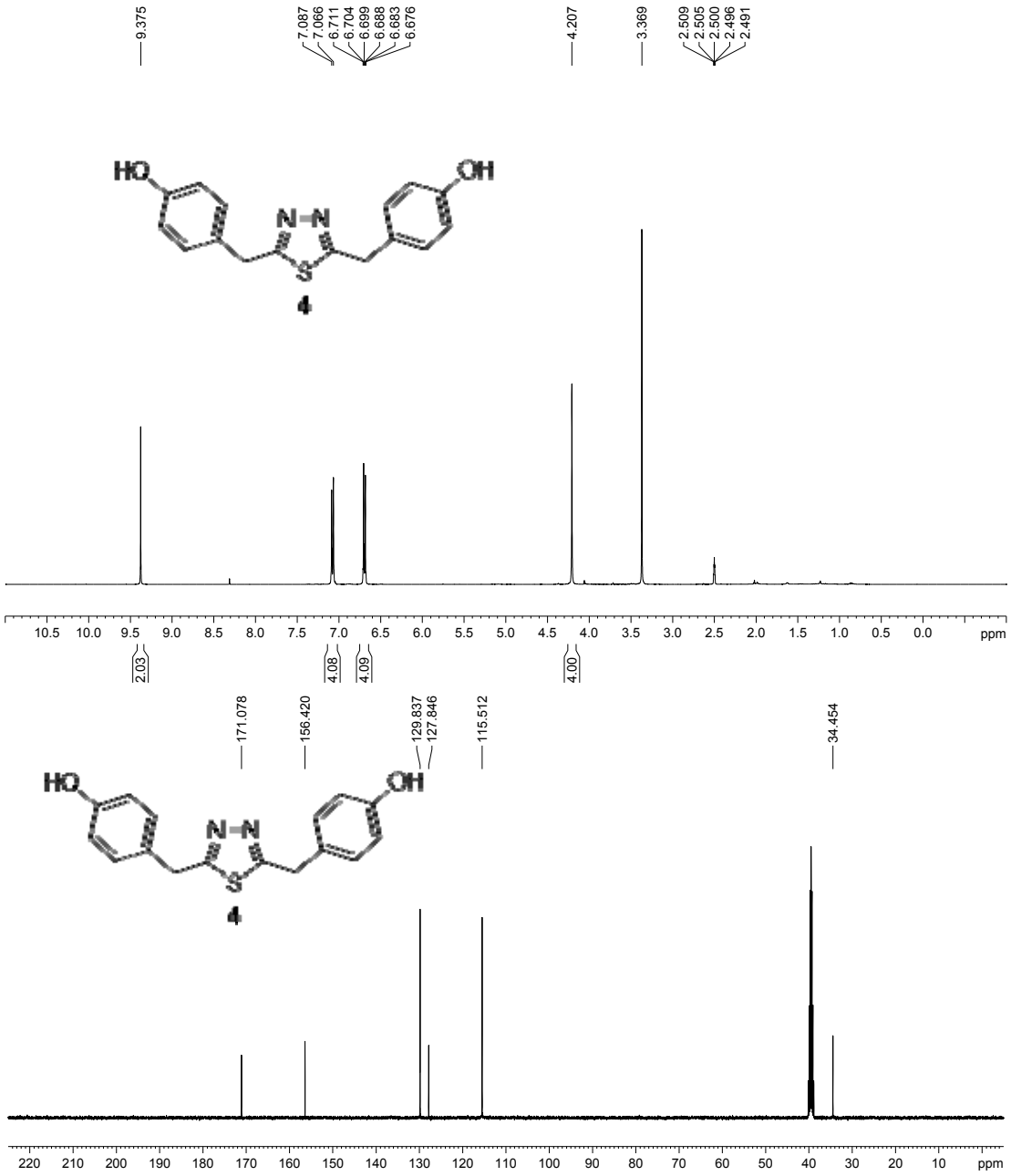


Figure S16. ^{1}H-NMR and ^{13}C-NMR of compound **4**.

2. HPLC and ^{13}C-NMR Comparing Analysis

2.1. HPLC Comparing Analysis for Compound **2**

Mobile phase: CH_3CN-H_2O with a linear gradient of CH_3CN from 10% to 65% in 30 min. The flow rate of 1.0 mL/min with UV detection at 224 nm using Venusil XBP C_{18} column (5 μm, 100 Å, 4.6 × 250 mm i.d), 30 °C.

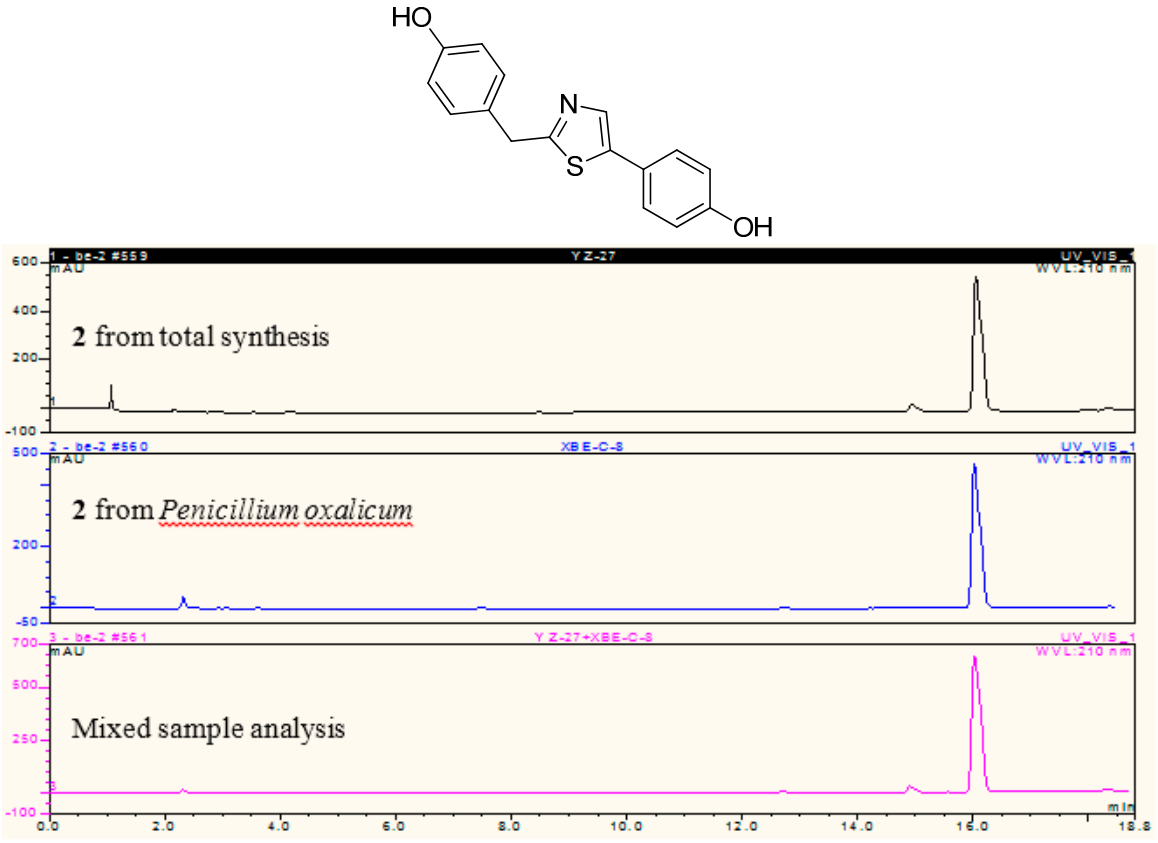


Figure S17. HPLC comparing analysis for compound **2**.

2.2. ^{13}C-NMR Comparing Analysis for Compound **1** *and* **2**

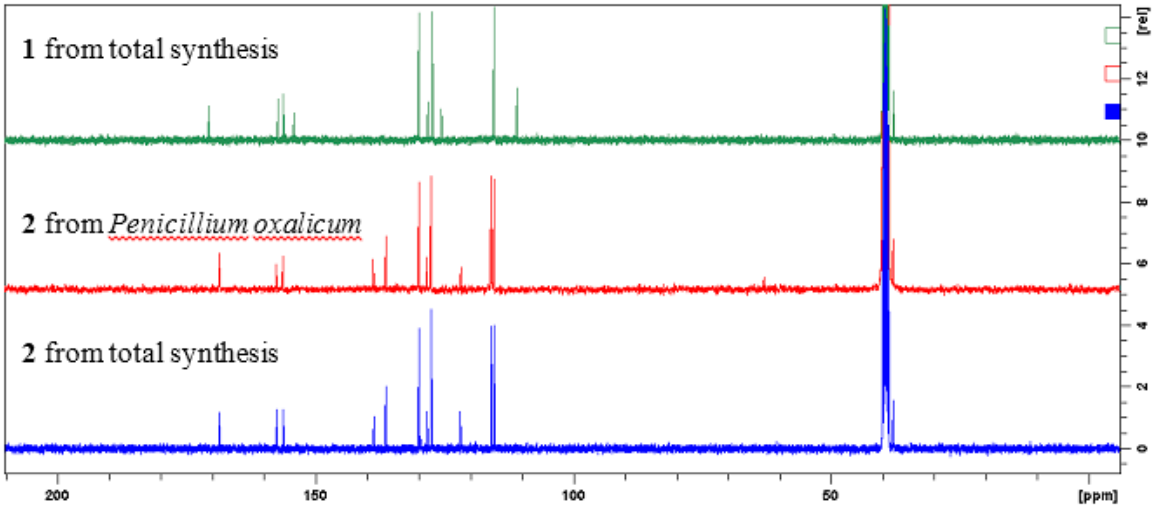


Figure S18. ^{13}C-NMR comparing analysis for compound **1** and **2**.

2.3. HPLC Comparing Analysis for Compound **3**

Mobile phase: MeCN-H_2O with a linear gradient of MeCN from 10% to 100% in 30 min. The flow rate of 1.0 mL/min with UV detection at 224 nm using Venusil XBP C_{18} column (5 μm, 100 Å, 4.6 × 250 mm i.d), 30 °C.

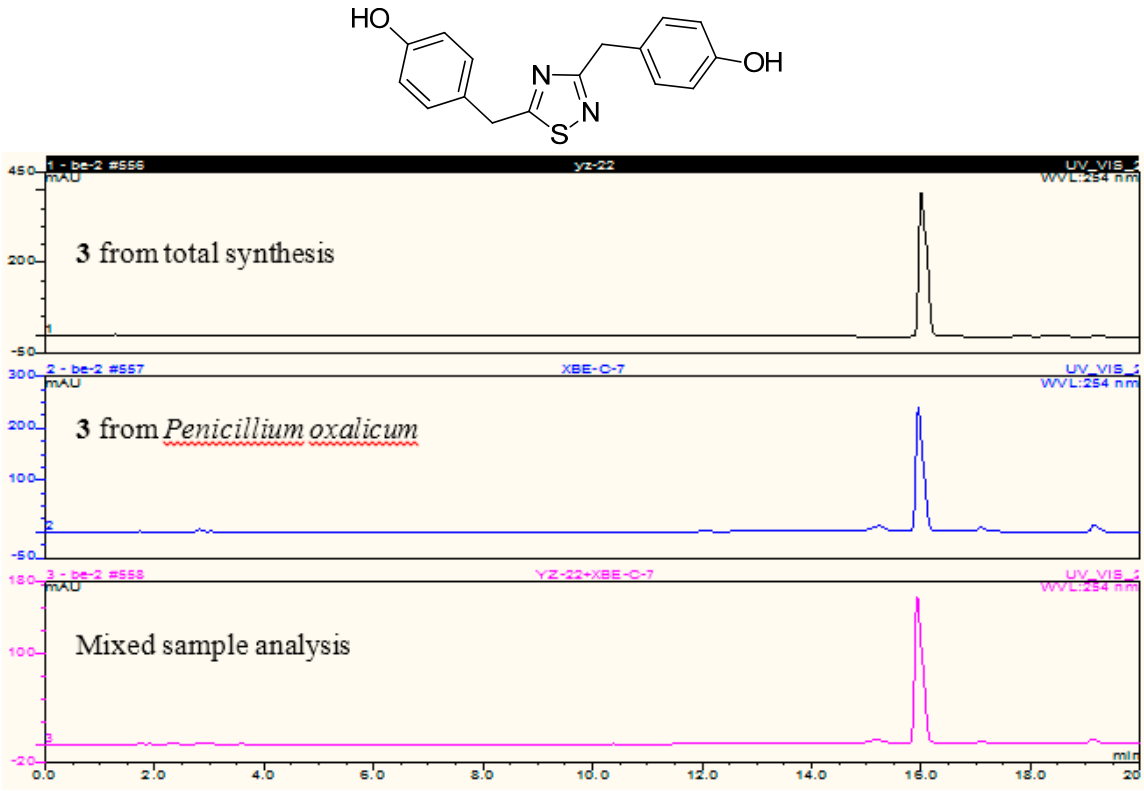


Figure S19. HPLC comparing analysis for compound **3**.

2.4. ^{13}C-NMR Comparing Analysis for Compound **3** and **4**

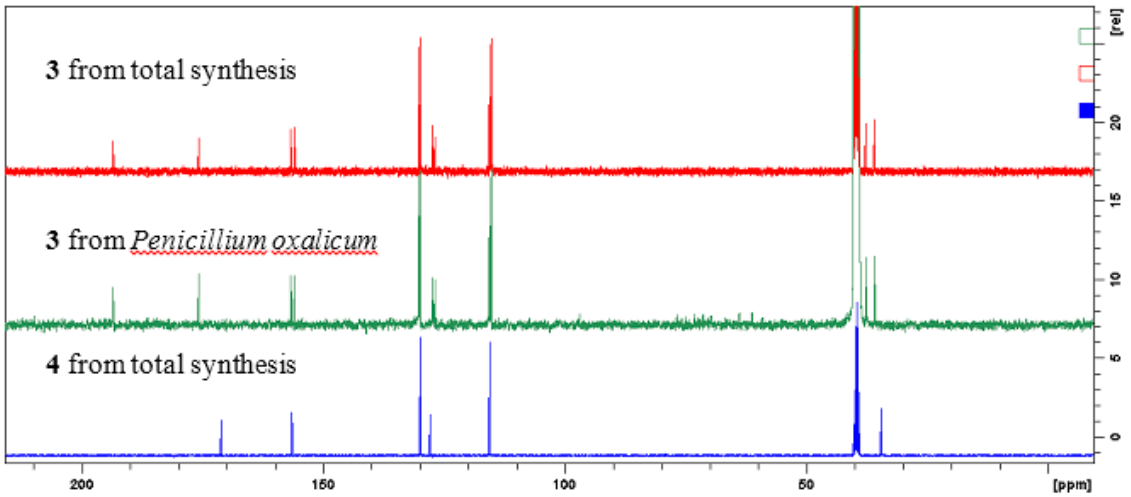
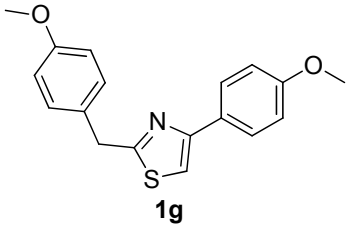


Figure S20. ^{13}C-NMR comparing analysis for compound **3** and **4**.

3. The Crystal Structure of 1g with Numbered Atoms



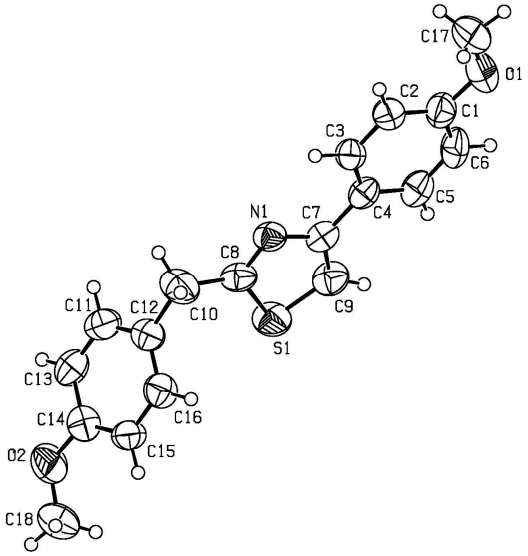
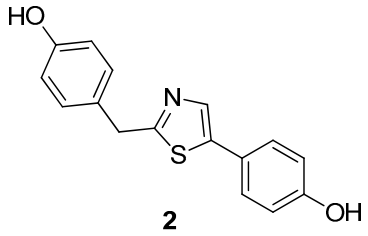


Figure S21. The crystal structure of compound **1g** with numbered atoms.

4. The Crystal Structure of 2 with Numbered Atoms



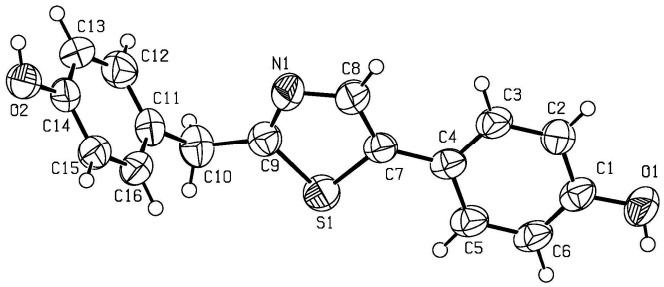


Figure S22. The crystal structure of compound **2** with numbered atoms.