Supporting Material

Two new phenylpropanoids from the leaves of *Rauvolfia vomitoria*

ZHANG Fuxin[#], MIAO Rongkun[#], YANG Kailing, YANG Tao, ZHOU Ruixi, ZHAN Guanqun[*], GUO Zengjun[*]

School of Pharmacy, Health Science Center, Xi'an Jiaotong University, Xi'an 710061, China

List of Supporting Information

[#]These authors contributed equally to this work.
[[*]Corresponding author] E-mail: zhanguanqun@mail.xjtu.edu.cn (ZHAN Guanqun); guozj@mail.xjtu.edu.cn (GUO Zengjun).

Known compounds information

Compound **3**: white amorphous powder; ESI-MS *m/z* 253.1 $[M+H]^+$; ^{1}H-NMR ($CDCl_3$, 600 MHz): δ_H 7.61 (1H, d, *J* = 15.9 Hz, H-7), 6.75 (2H, s, H-2, H-6), 6.35 (1H, d, *J* = 15.9 Hz, H-8), 3.89 (6H, s, 3, 5-OCH_3), 3.88, (3H, s, 4-OCH_3), 3.81 (3H, s, 9-OCH_3). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ_C 167.4 (C-9), 153.4 (C-3, C-5), 144.9 (C-7), 140.1 (C-4), 129.9 (C-1), 117.0 (C-8), 105.2 (C-2, C-6), 60.9 (4-OCH_3), 56.2 (3,5-OCH_3), 51.7 (9-OCH_3). Comparing these NMR data with refs. [1], compound **3** was identified as methyl *trans*-3,4,5-trimethoxycinnamate.

Compound **4**: white amorphous powder; ESI-MS *m/z* 253.1 $[M+H]^+$; ^{1}H-NMR ($CDCl_3$, 600 MHz): δ_H 7.06 (2H, s, H-2, H-6), 6.82 (1H, d, *J* = 12.9 Hz, H-7), 5.90 (1H, d, *J* = 12.9 Hz, H-8), 3.88 (9H, s, 3, 4, 5-OCH_3), 3.74 (3H, s, 9-OCH_3). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ_C 166.7 (C-9), 152.7 (C-3, C-5), 143.3 (C-7), 139.2 (C-4), 130.0 (C-1), 118.3 (C-8), 107.9 (C-2, C-6), 60.9 (4-OCH_3), 56.2 (3,5-OCH_3), 51.5 (9-OCH_3). Comparing these NMR data with ref. [1], compound **4** was identified as methyl *cis*-3,4,5-trimethoxycinnamate.

Compound **5**: white amorphous powder; ESI-MS *m/z* 227.1 $[M+H]^+$; ^{1}H-NMR ($CDCl_3$, 600 MHz): δ_H 7.30 (2H, s, H-2, H-6), 3.91 (12H, s, 3, 4, 5, 7-OCH_3). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ_C 166.7 (C-7), 152.9 (C-3, 5), 142.1 (C-4), 125.1 (C-1), 106.8 (C-2, 6), 60.9 (4-OCH_3), 56.2 (3, 5-OCH_3), 52.2 (7-OCH_3). Comparing these NMR data with ref. [2], compound **5** was identified as 3,4,5-trimethoxybenzoic acid methyl ester.

[1] Guido S, Luciano DS, Maria RDG. A new gas chromatographic method for the estimation of reserpine and rescinnamine. J Chromatogr A, 1976, 116: 263-270.

[2] Terazzi E, Guenee LL, Morgantini PY *et al*. Tuning the polarization along linear polyaromatic strands for rationally inducing mesomorphism in lanthanide nitrate complexes. *Chem-Eur J,* 2007, **13**: 1674-1691.

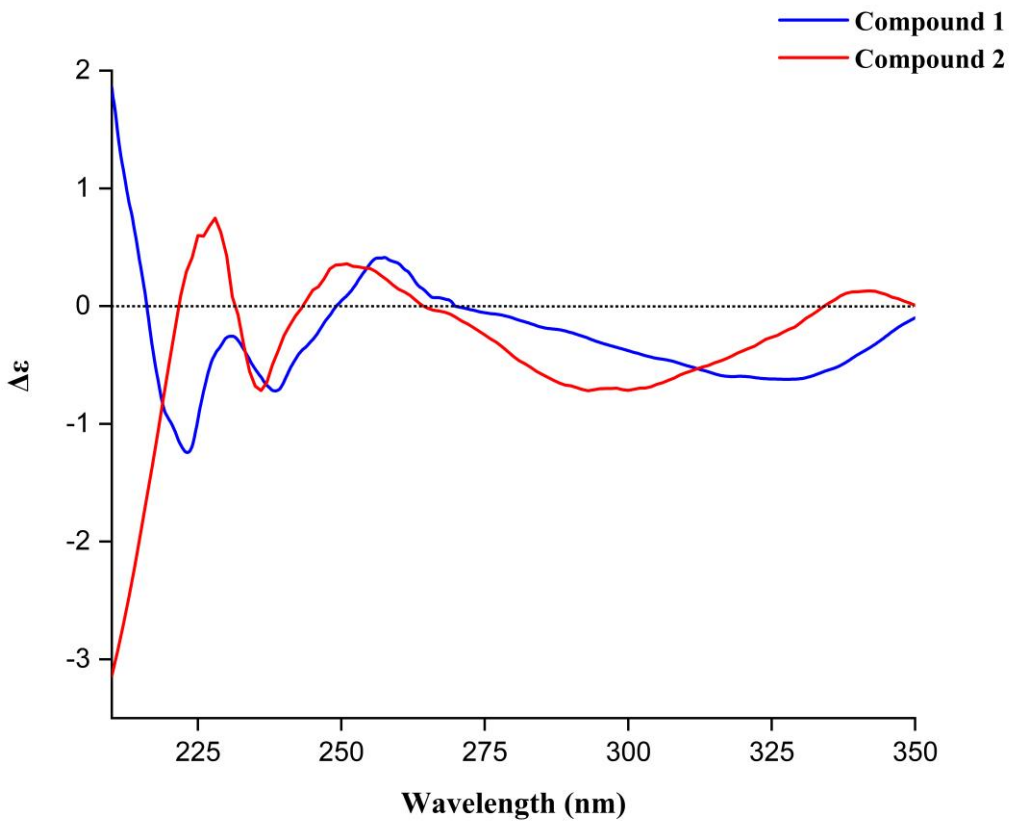

Figure S1. CD spectrum of **1** and **2**

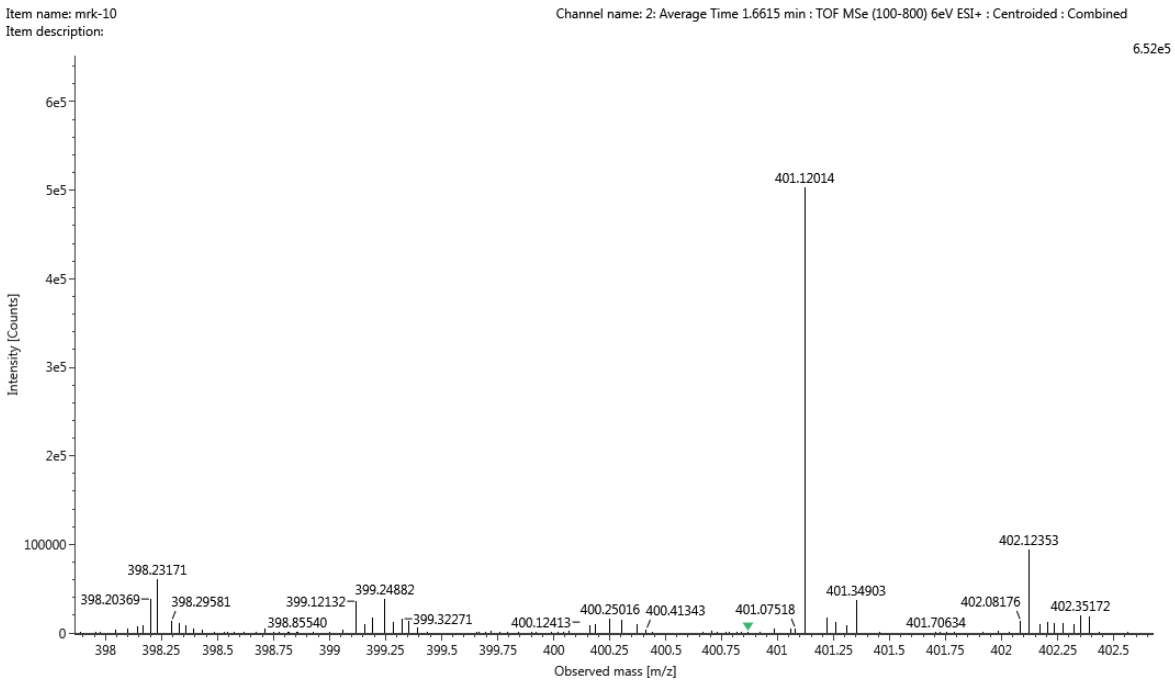

Figure S2. (+)-HR-ESI-MS spectrum of **1**

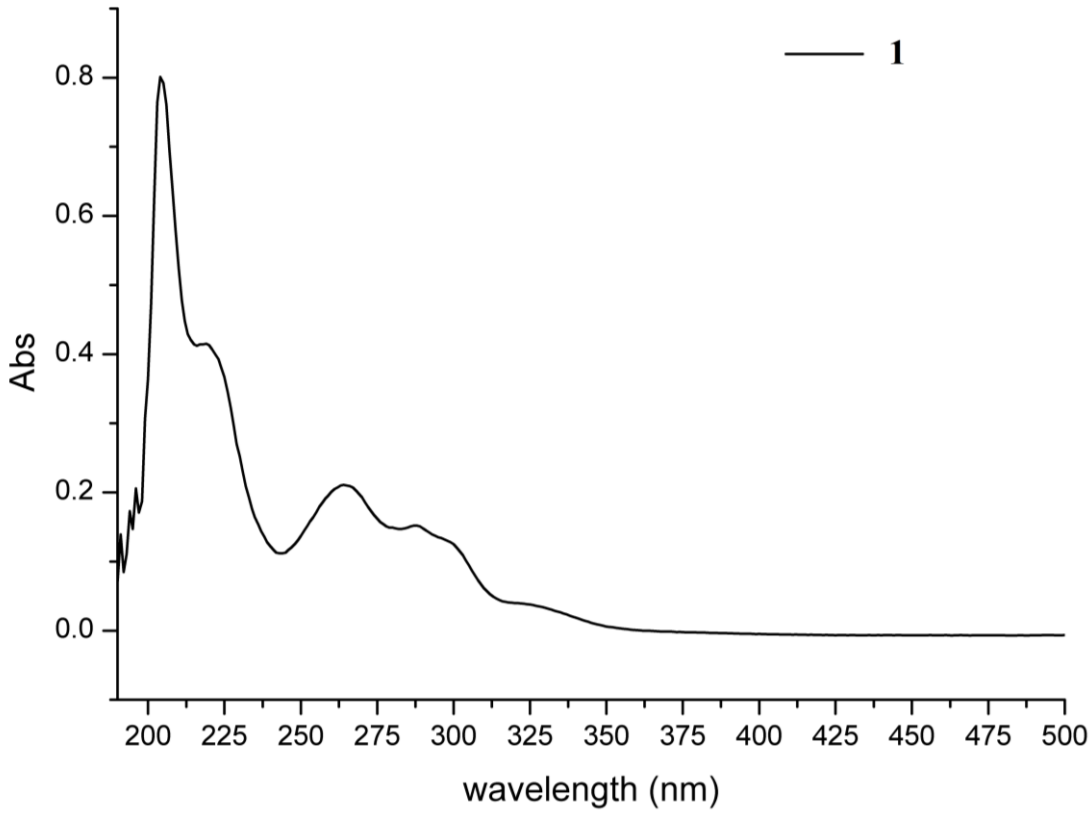

Figure S3. UV spectrum of **1** in MeOH

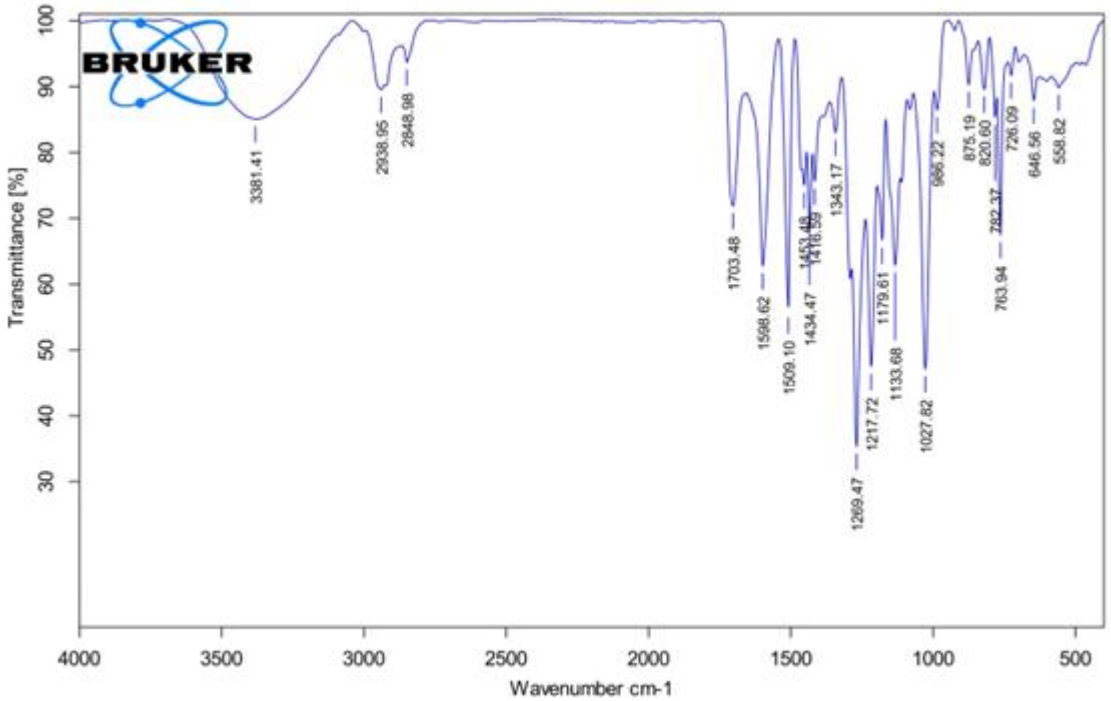

Figure S4. IR spectrum of **1**

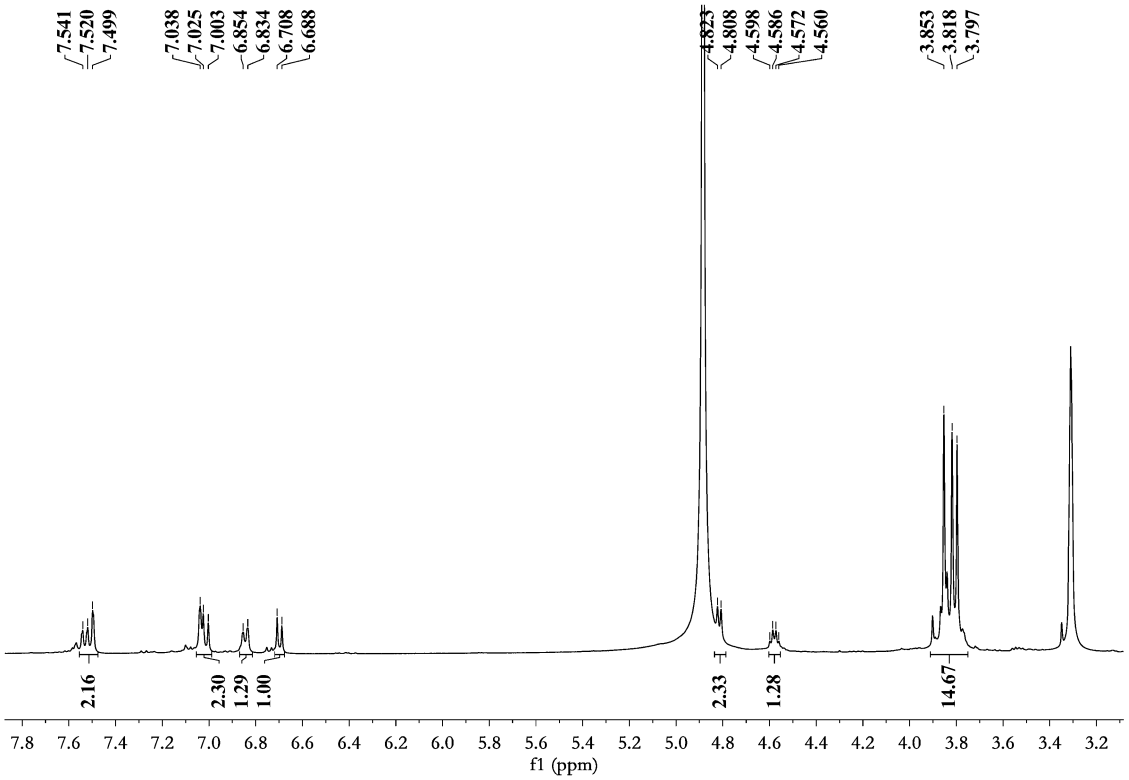

Figure S5. ^{1}H NMR (600 MHz) spectrum of **1** in CD_3OD

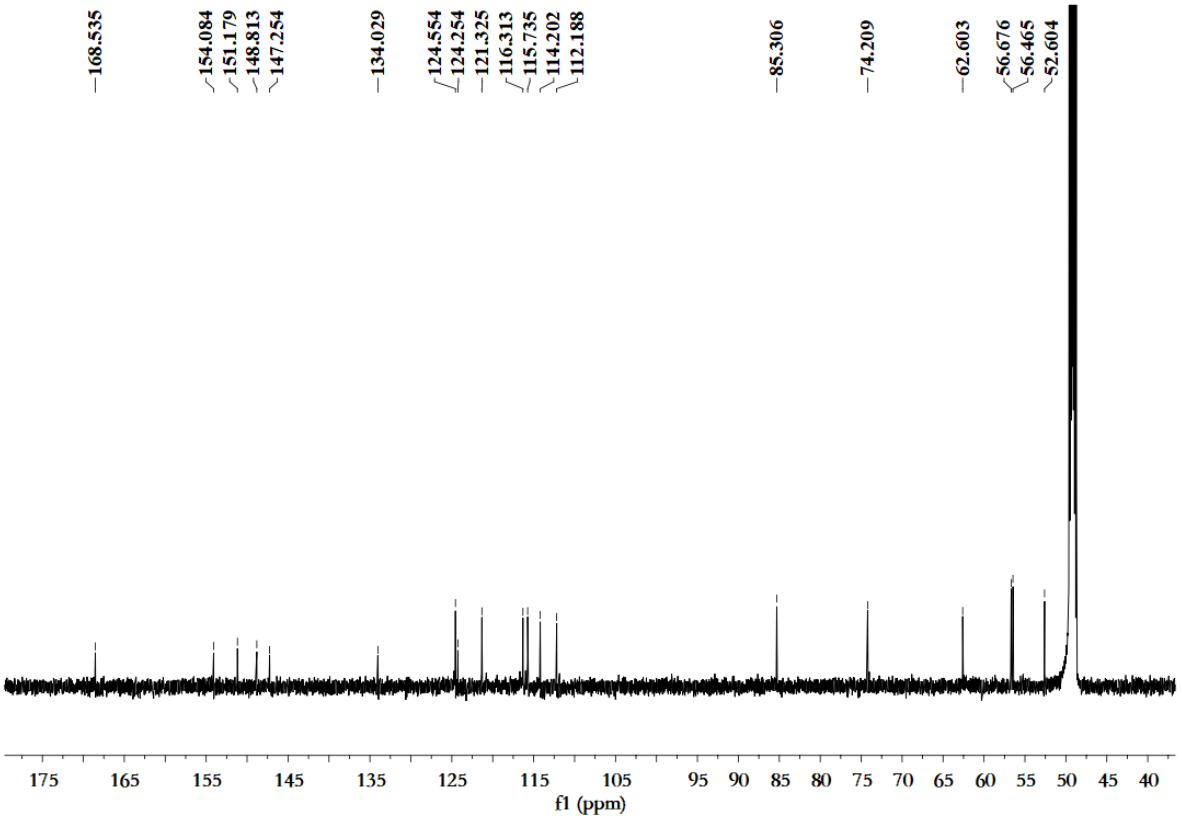

Figure S6. ^{13}C NMR (150 MHz) spectrum of **1** in CD_3OD

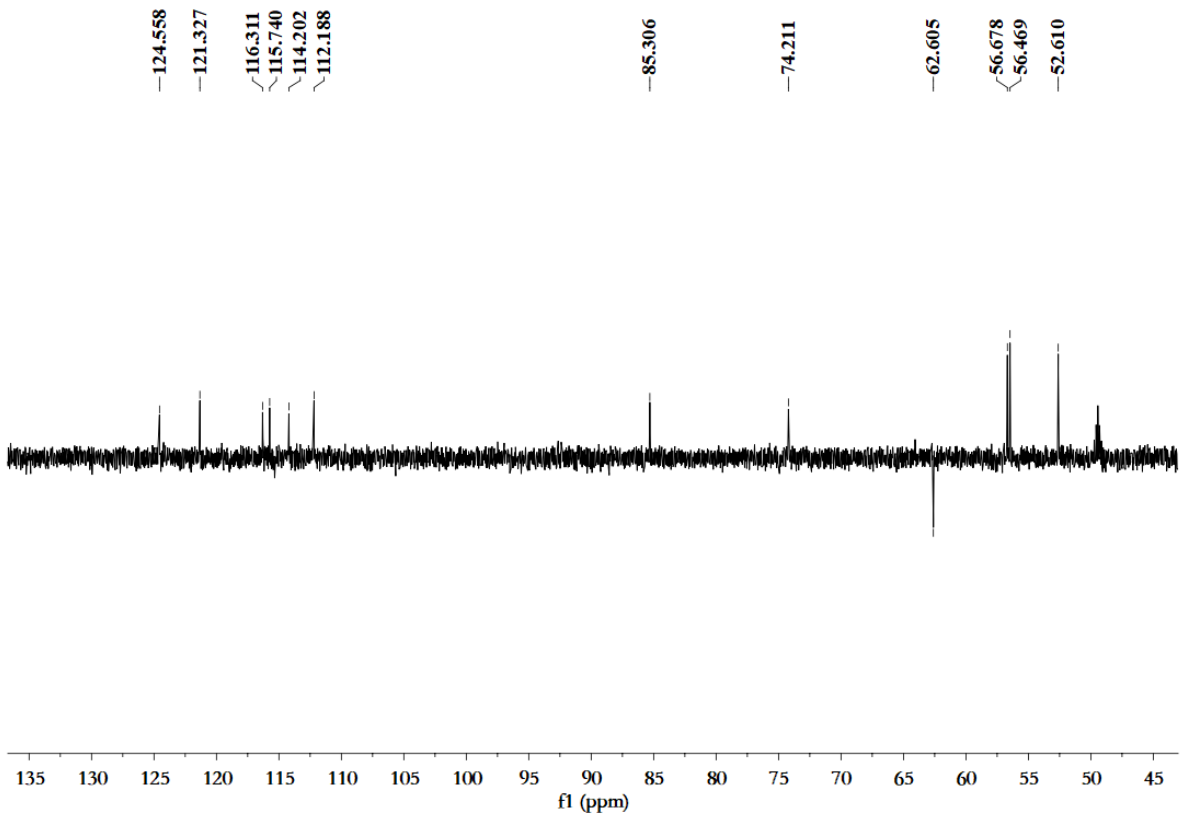

Figure S7. DEPT 135 spectrum of **1** in CD_3OD

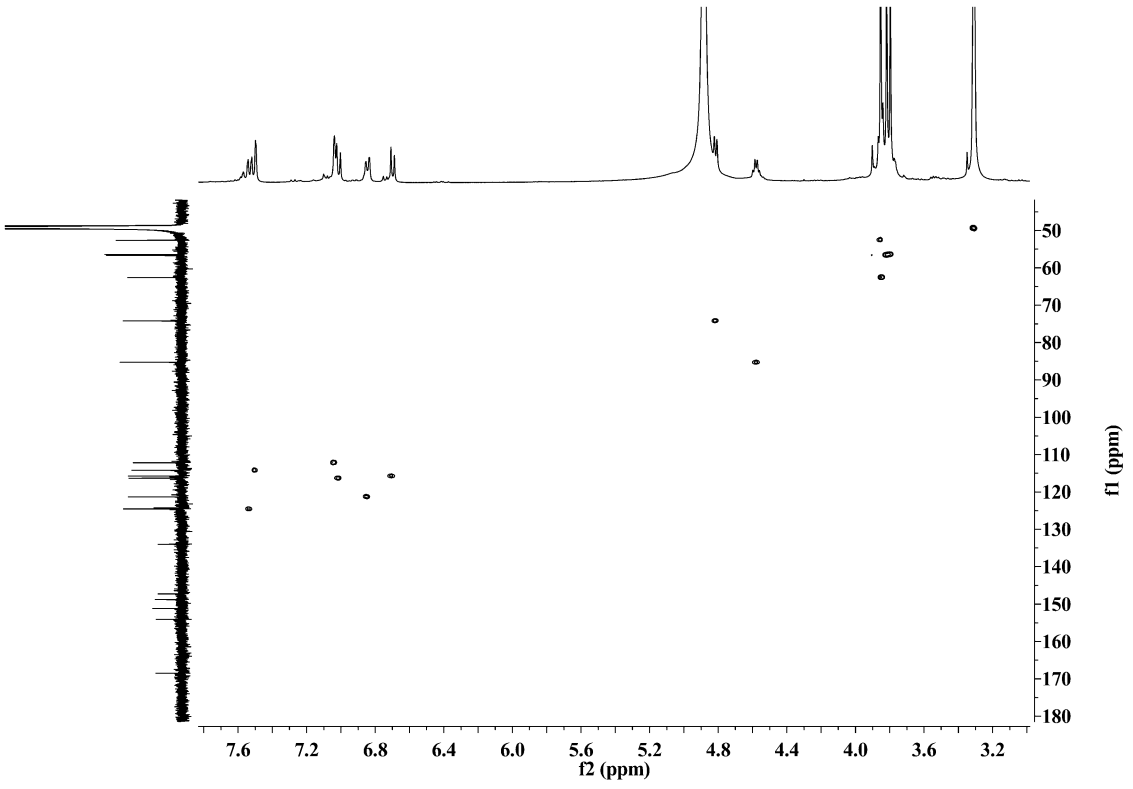

Figure S8. HSQC spectrum of **1** in CD_3OD

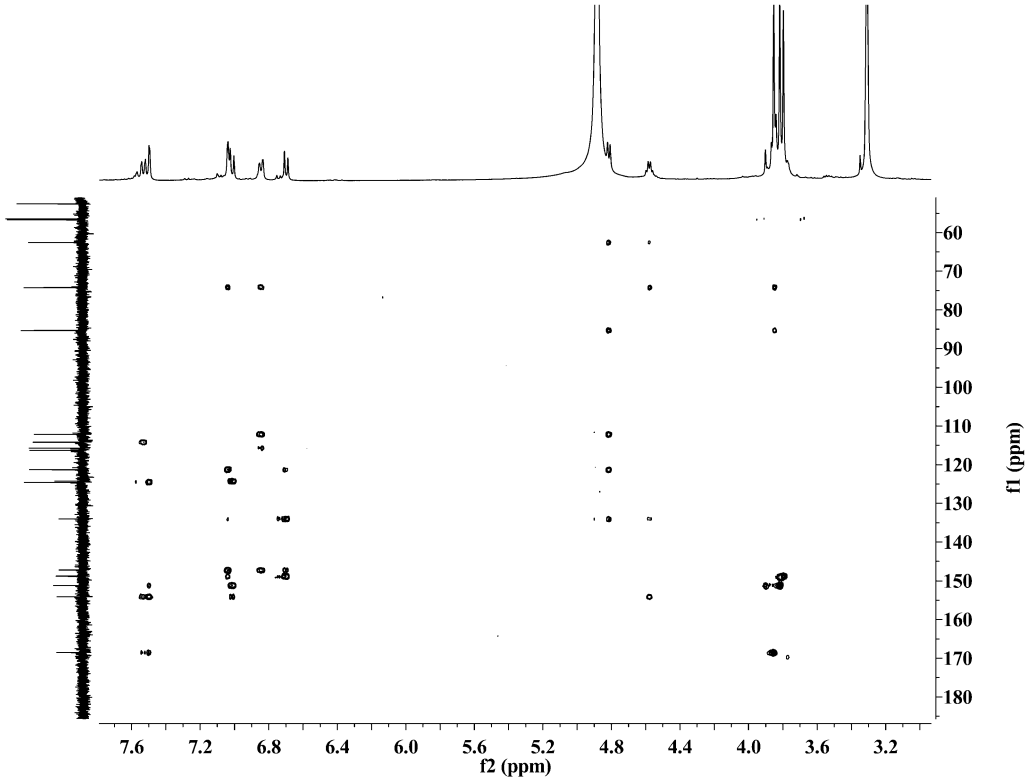

Figure S9. HMBC spectrum of **1** in CD_3OD

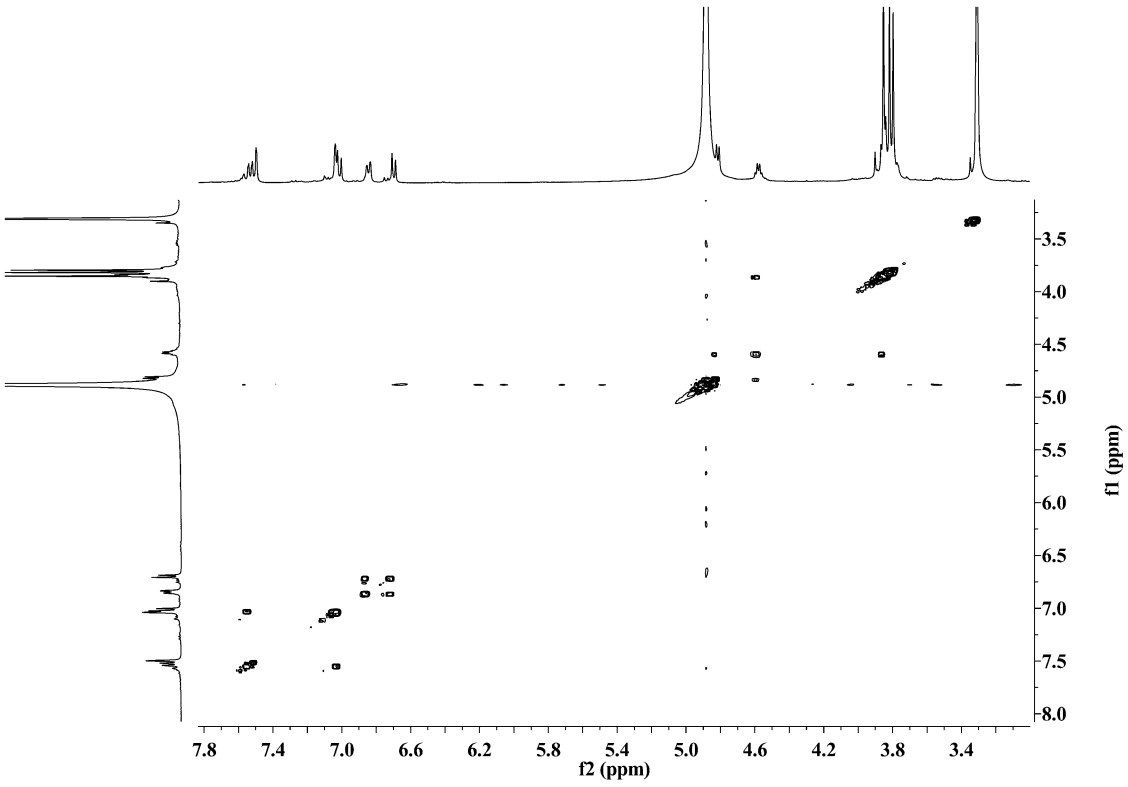

Figure S10. ^1H–^1H COSY spectrum of **1** in CD_3OD

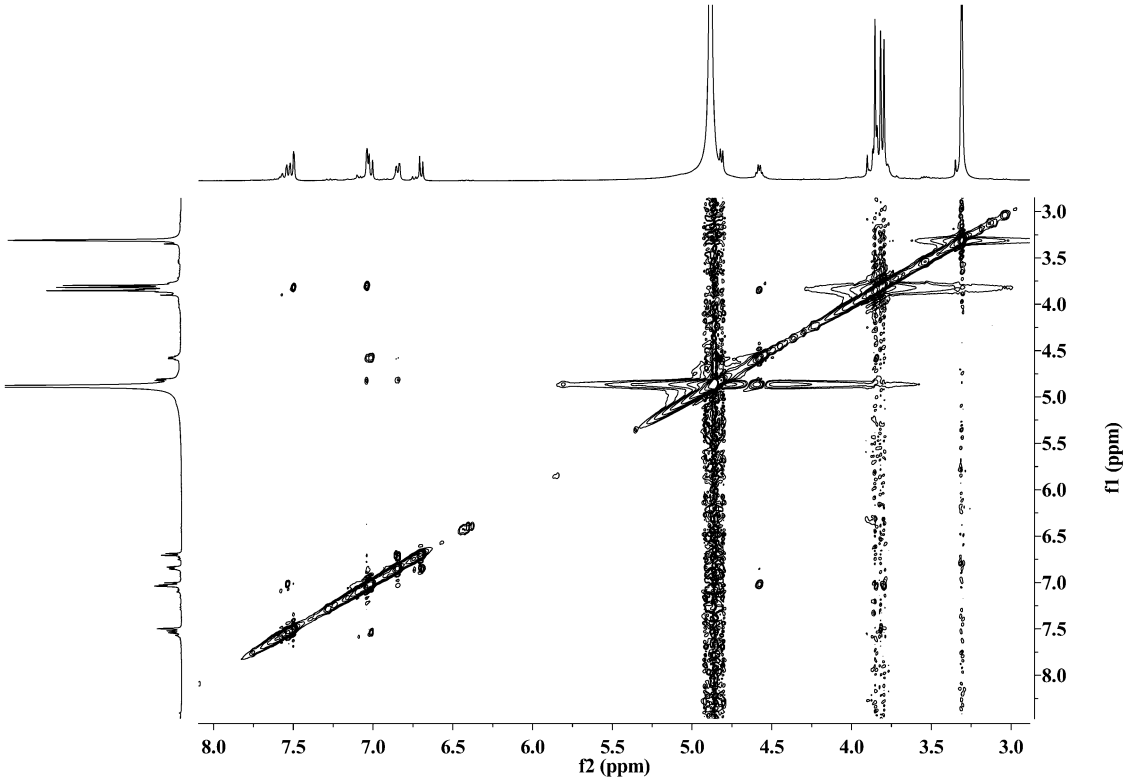

Figure S11. NOESY spectrum of **1** in CD_3OD

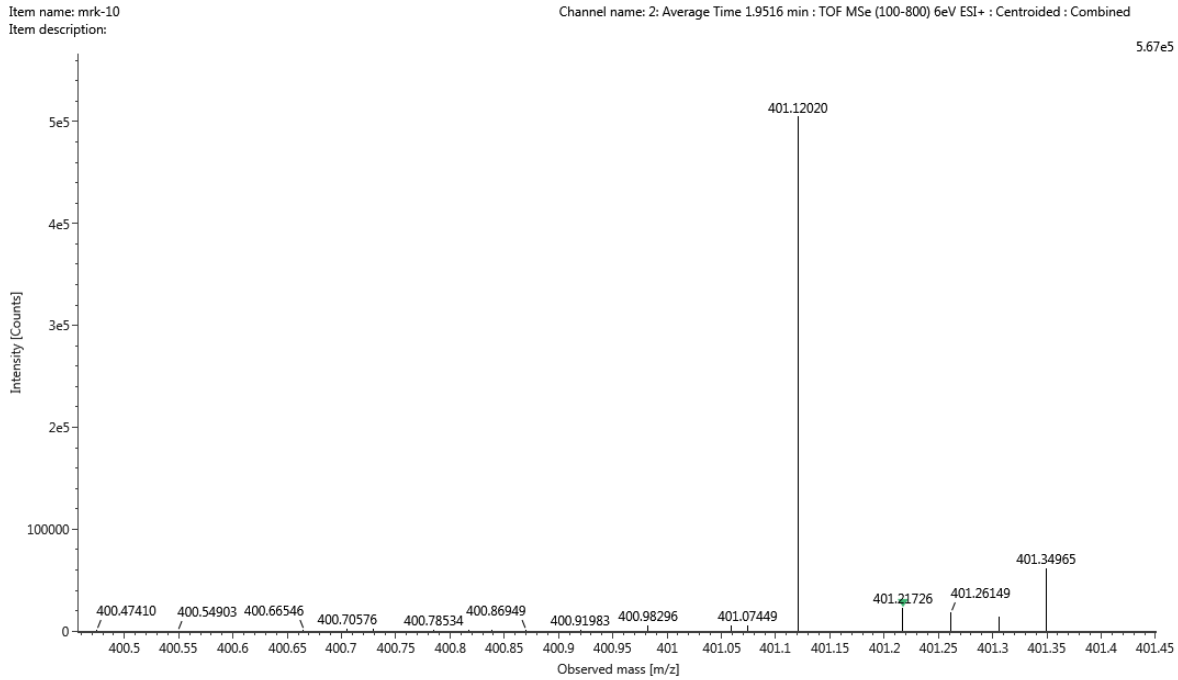

Figure S12. (+)-HR-ESI-MS spectrum of **2**

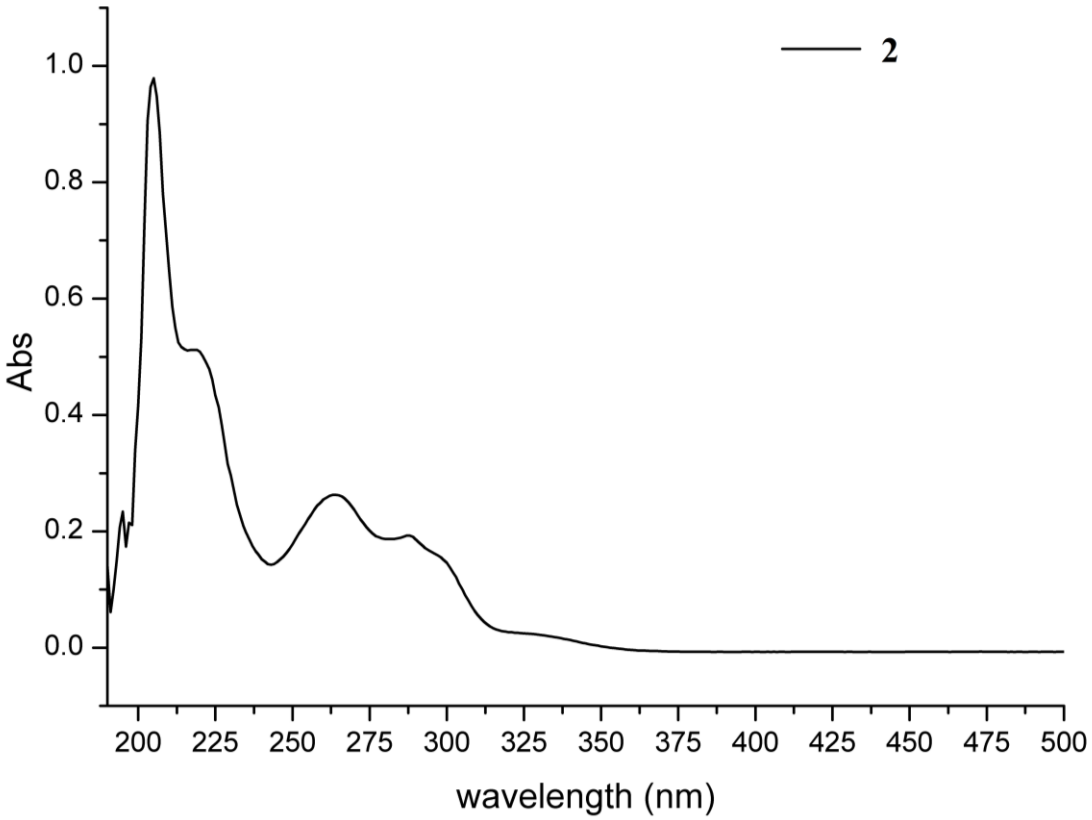

Figure S13. UV spectrum of **2** in MeOH

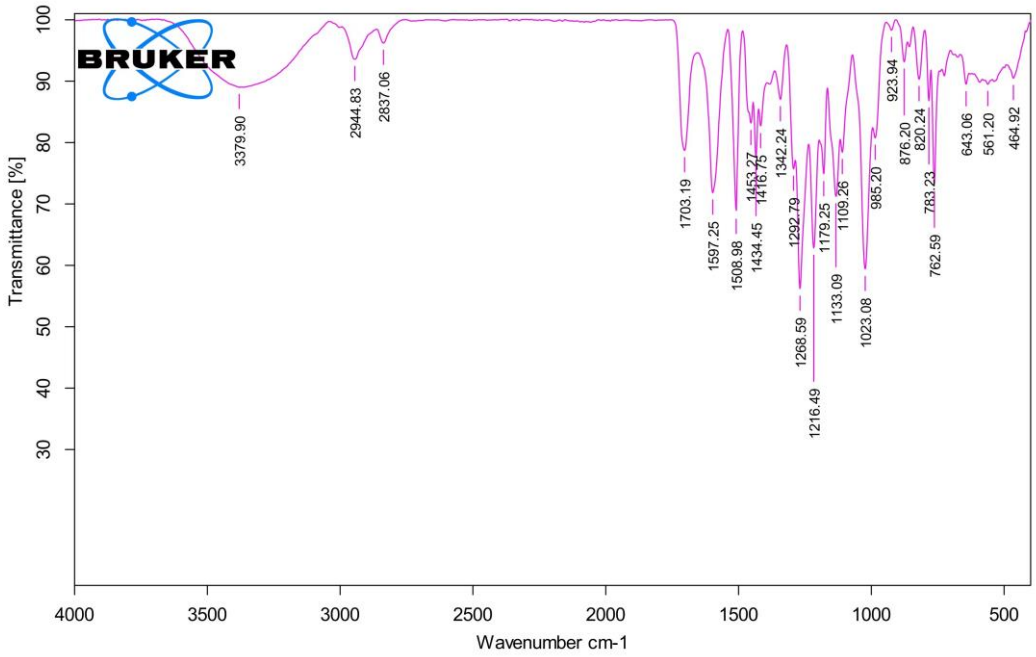

Figure S14. IR spectrum of **2**

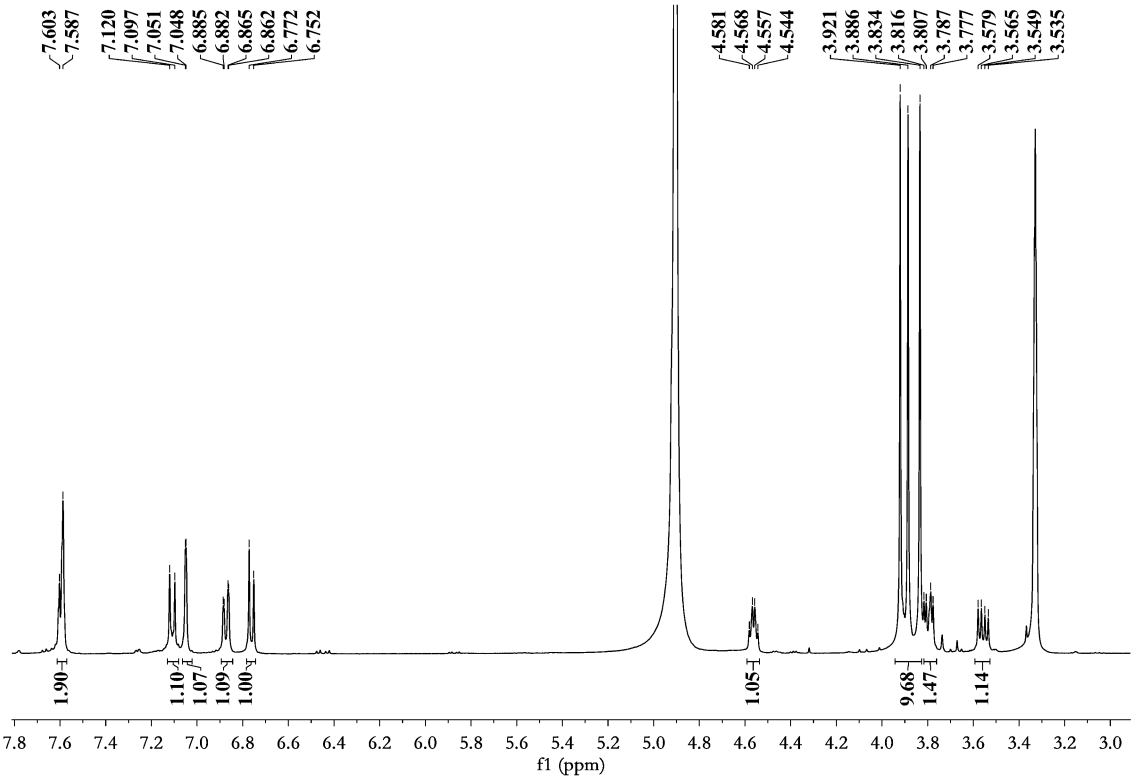

Figure S15. ^{1}H NMR (600 MHz) spectrum of **2** in CD_3OD

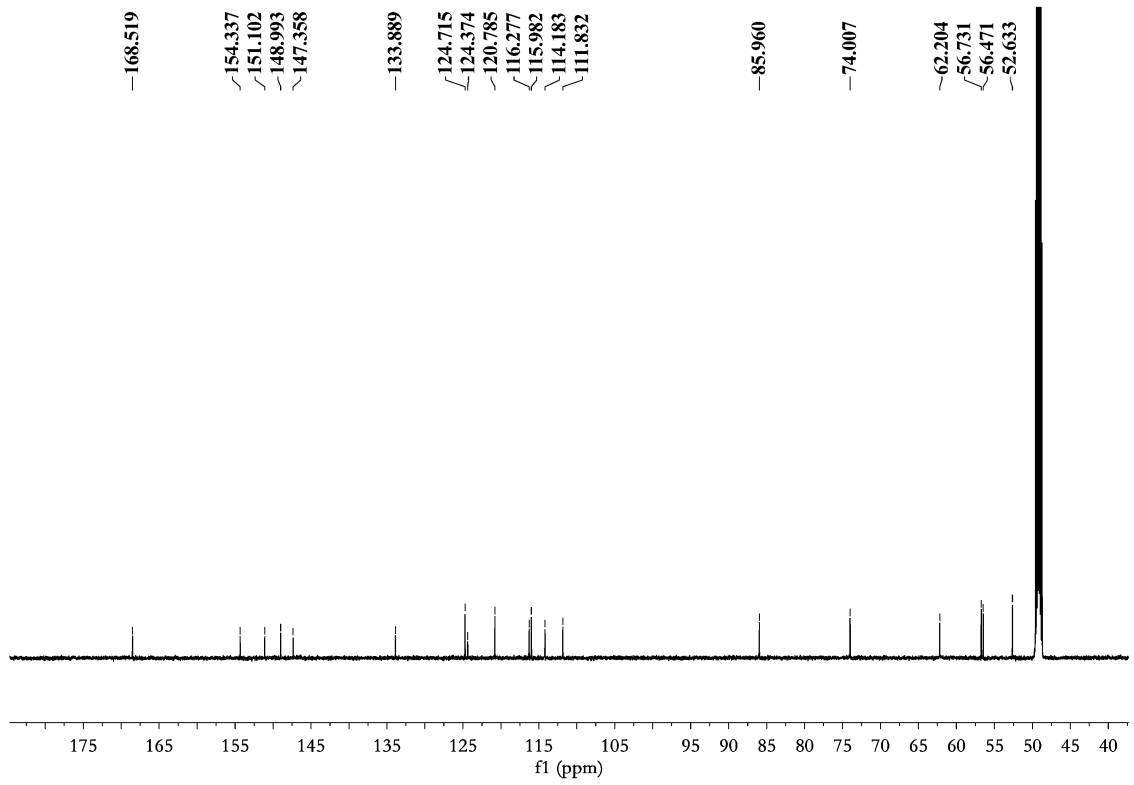

Figure S16. ^{13}C NMR (150 MHz) spectrum of **2** in CD_3OD

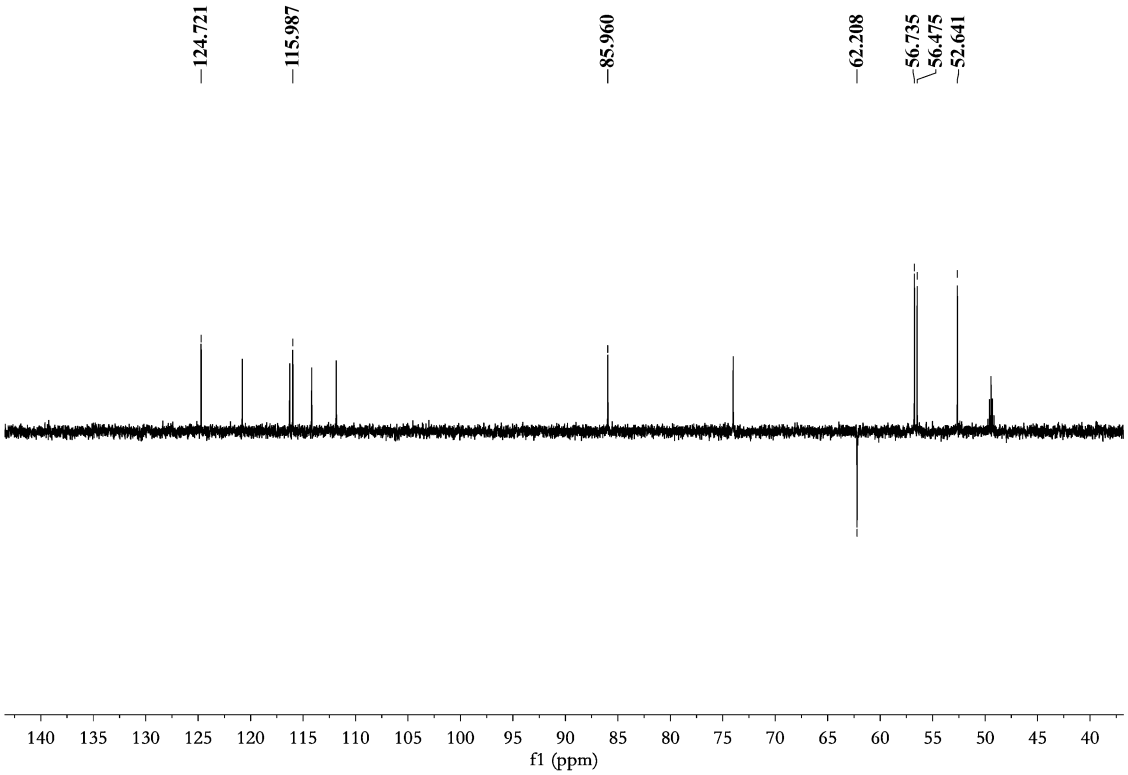

Figure S17. DEPT 135 spectrum of **2** in CD_3OD

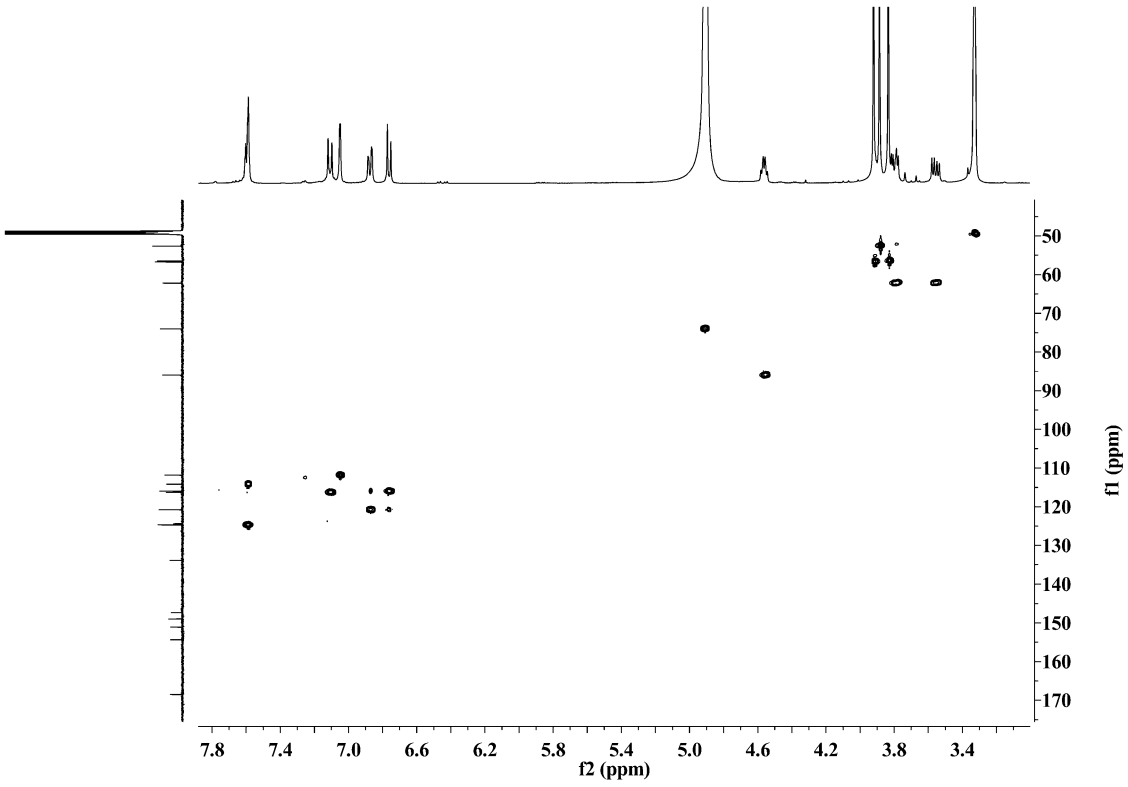

Figure S18. HSQC spectrum of **2** in CD_3OD

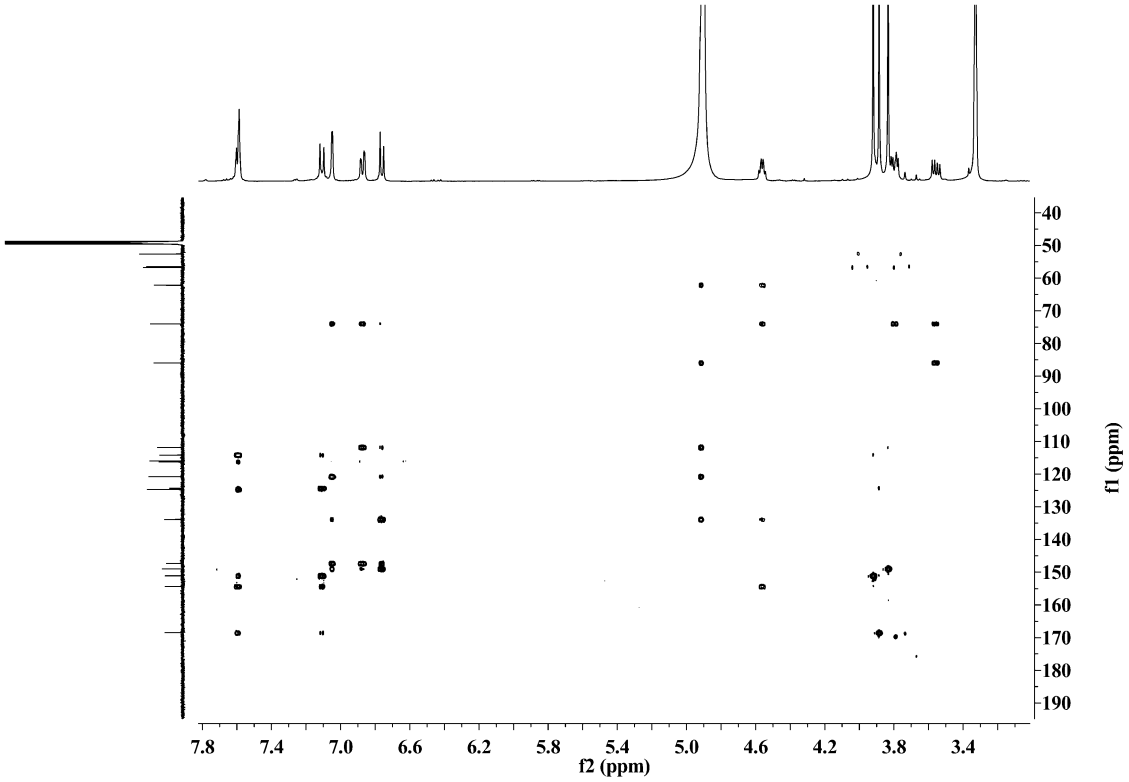

Figure S19. HMBC spectrum of **2** in CD_3OD

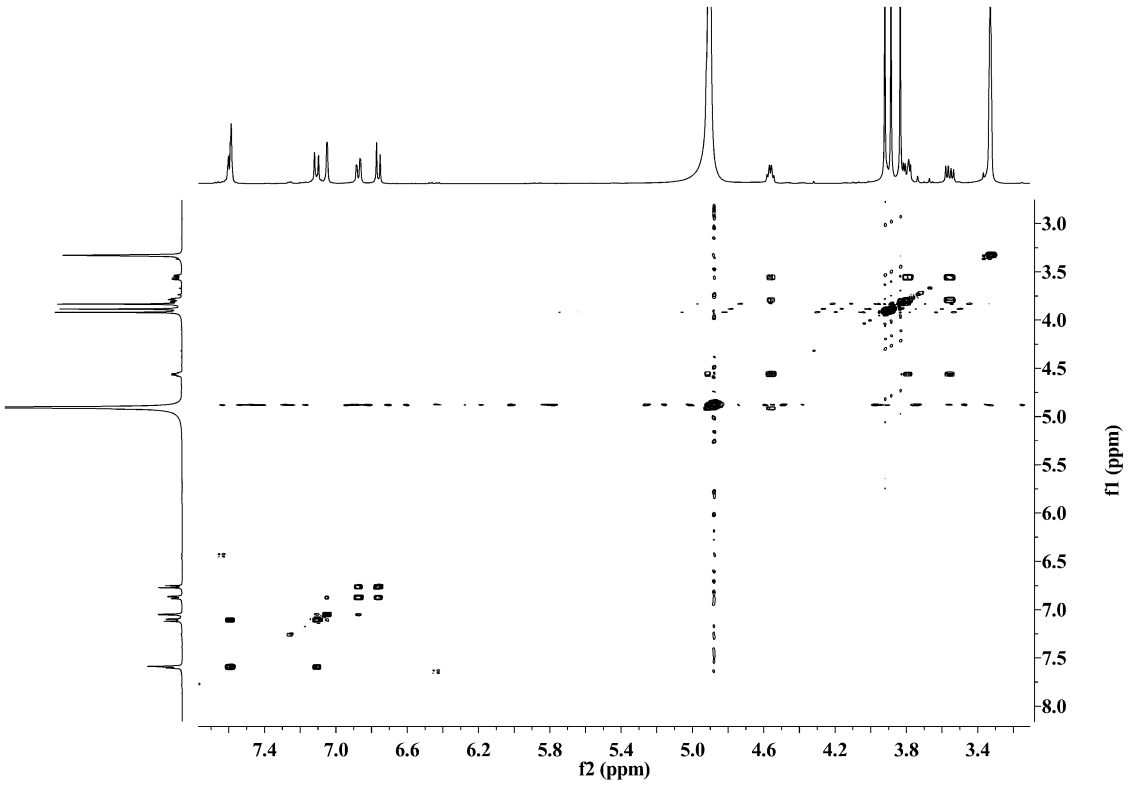

Figure S20. $^{1}H–^{1}H$ COSY spectrum of **2** in CD_3OD

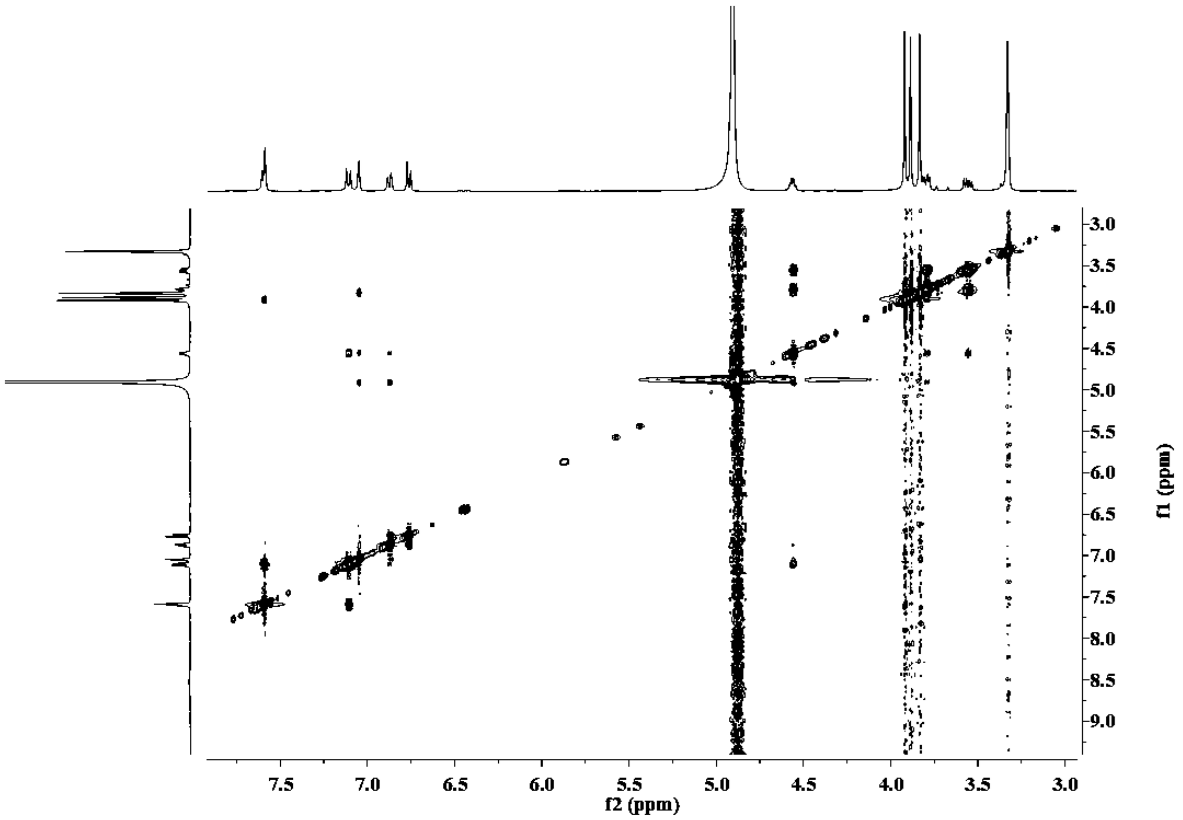

Figure S21. NOESY spectrum of **2** in CD_3OD