Supporting Information

Unprecedented *nor-seco*-polycyclic polyprenylated acylphloroglucinols counteract myocardial cell injury *via* activation of the Akt/mTOR signaling pathway

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Contents

Experimental section

General experimental procedures

Optical rotations and UV spectra were recorded on a PerkinElmer 341 polarimeter (PerkinElmer Inc., Fremont, California, USA) and a Lambda 35 instrument (PerkinElmer Inc., Fremont, California, USA), respectively. IR spectra were obtained using a Bruker Vertex 70 FT-IR spectrophotometer (Bruker, Karlsruhe, Germany). Experimental ECD data were collected on a JASCO J-810 spectrometer (JASCO, Tokyo, Japan). The NMR spectra were recorded on a Bruker AM-600 spectrometer with TMS as the internal standard. All chemical shifts (δ) were expressed in ppm relative to the solvent signal (chloroform-*d*: δ_H 7.26, δ_C 77.16). HRESIMS data were recorded in the positive-ion mode on a Bruker micrOTOF-Q II spectrometer (Bruker, Karlsruhe, Germany). Column chromatography (CC) was performed with silica gel (200–300 mesh, Qingdao Marine Chemical, Inc., Qingdao, China), Sephadex LH-20 (40–70 μm, Amersham Pharmacia Biotech AB, Uppsala, Sweden), and octadecylsilyl (ODS, 50 μm, YMC Co. Ltd., Japan). Preparative HPLC was a performed on Sanotac instrument China (Shanghai Sanotac Scientifc Instruments Co.,Ltd, Shang-Hai, China) with a UV detector and a YMC C18 column (250 × 20 mm, 5 μm, YMC, Kyoto, Japan). Semi-preparative HPLC separations were conducted on an Agilent 1100 liquid chromatograph with a reversed-phase (RP) C_{18} column (5 μm, 10 × 250 mm, Welch Materials, Inc.). Thin-layer chromatography (TLC) was carried out with silica gel 60 F_{254} (Yantai Chemical Industry Research Institute). Fractions were monitored by TLC, and spots were visualized by heating silica gel plates sprayed with 10% H_2SO_4 in EtOH.

Plant material

The aerial parts of *Hypericum monogynum* L. were collected from Shennongjia Forestry, Hubei Province, People's Republic of China, in September 30, 2022. The plant was identified by Professor Jingming Jia of Shenyang Pharmaceutical University. A voucher specimen (No. HB20220930) has been deposited in the herbarium of School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology.

Exaction and isolation

The air-dried aerial parts of *H. monogynum* (20 kg) were percolated with 95% EtOH three times at room temperature. The combined EtOH extract was concentrated under vacuum (water-bath temperature for evaporation was maintained below 50 °C) to yield a residue (1320 g). Then, the resulting residue was suspended in H_2O and extracted three times with petroleum ether to afford a crude extract.

The petroleum ether extract (310 g) was subjected to silica gel CC, eluted with petroleum ether/acetate extract (10:1, 5:1, 3:1, 2:1, 1:1, and 1:2, v/v) to afford six main fractions (A–F). Fr. E (29 g) was chromatographed on an MCI gel column (6 × 80 cm) and eluted with CH_3OH/H_2O (30:70, 40:60, 50:50, 60:40, 70:30, 80:20, and 90:10, v/v) to get seven subfractions (Fr. E1 –Fr. E7). Fraction E6 (5.5 g) was further purified on Sephadex LH-20 eluted with CH_3OH to give six subfractions (Fr. E6-1–Fr. E6-6). Fr. E6-4 (1.2 g) was separated by MPLC over octadecylsilane (ODS), eluted with a step gradient of CH_3OH/H_2O (60:40–90:10, v/v, flow rate: 25 mL/min) to give six subfractions (Fr. E6-4A–Fr. E6-4F), and Fr. E6-4D (224 mg) purified by preparative HPLC (CH_3CN/H_2O, 60/40, v/v, flow rate: 8 mL/min) to yield **1** (8.7 mg, t_R 18.6 min), **2** (11.2 mg, t_R 21.4 min), and **3** (4.6 mg, t_R 22.6 min) and Fr. E6-3D4. Fr. E6-4D4 (7.1 mg) was purified by Semi-preparative HPLC (CH_3OH /H_2O, 80/20, v/v, flow rate: 3 mL/min) to yield **4** (2.3 mg, t_R 26.4 min) and **5** (2.5 mg, t_R 18.1 min). Fr. E6-4E (72 mg) was purified by preparative HPLC (CH_3CN/H_2O, 60/40, v/v, flow rate: 8 mL/min) to yield **6** (34.2 mg, t_R 21.8 min) and Fr. E6-4E2. Fr. E6-4E2 (26.7 mg) was purified by preparative HPLC (CH_3OH /H_2O, 80/20, v/v, flow rate: 8 mL/min) to yield **7** (17.5 mg, t_R 38.4 min)

Physical data of 1–5

Hypermonol A (**1**): colorless needle crystals, mp 171–172 °C; $[\alpha]_D^{25}$: +25.8 (MeOH, *c* 0.1); UV (MeOH) λ_{max} (log ε): 201 (4.22), 211 (3.93), 240 (4.46) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 201 (+13.18), 254 (–0.94), 324 (+1.41) nm; IR (KBr) ν_{max}: 3443, 2921, 2851, 1767, 1706, 1645, 1467, 1384, 1132, 915 cm^{-1}; For ^1H and ^{13}C NMR data, see Table 1; HRESIMS *m*/*z* 455.2421 ($[M + Na]^+$, calcd for $C_{25}H_{36}O_6Na^+$, 455.2410).

Hypermonol B (**2**): colorless needle crystals, mp 163–164 °C; $[\alpha]_D^{25}$: –64.6 (MeOH, *c* 0.1); UV (MeOH) λ_{max} (log ε): 201 (4.24) nm, 211 (4.03) nm, 240 (4.42) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 207 (–14.08) nm, 233 (+6.72) nm, 329 (–2.67) nm; IR (KBr) ν_{max}: 3363, 2961, 2921, 2872, 1767, 1704, 1635, 1468, 1383, 1112, 914 cm^{-1}; For ^1H and ^{13}C NMR data, see Table 1; HRESIMS *m*/*z* 455.2401 ($[M + Na]^+$, calcd for $C_{25}H_{36}O_6Na^+$, 455.2410).

Hypermonol C (**3**): white solids; $[\alpha]_D^{25}$: +10.4 (MeOH, *c* 0.1); UV (MeOH) λ_{max} (log ε): 201 (4.34), 211 (4.17), 240 (4.64) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 200 (–11.2), 230 (+9.16), 326 (–3.43) nm; IR (KBr) ν_{max}: 3364, 2920, 2850, 1768, 1707, 1645, 1468 cm^{-1}; For ^1H and ^{13}C NMR data, see Table 2; HRESIMS *m*/*z* 469.2554 ($[M + Na]^+$, calcd for $C_{26}H_{38}O_6Na^+$, 469.2566).

Hypermonol D (**4**): white solids; $[\alpha]_D^{25}$: +5.4 (MeOH, *c* 0.1); UV (MeOH) λ_{max} (log ε): 201 (4.29), 211 (4.06), 240 (4.30) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 200 (–10.7), 231 (+7.53), 326 (–2.16) nm; IR (KBr) ν_{max}: 3445, 2968, 2933, 2875, 1764, 1737, 1698, 1460, 1381, 1109, 913 cm^{-1}; For ^1H and ^{13}C NMR data, see Table 2; HRESIMS *m*/*z* 469.2554 ($[M + Na]^+$, calcd for $C_{26}H_{38}O_6Na^+$, 469.2566).

Hypermonol E (**5**): white solids; $[\alpha]_D^{25}$: +18.8 (MeOH, *c* 0.1); UV (MeOH) λ_{max} (log ε): 201 (4.21), 211 (3.88), 240 (4.13) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 201 (+12.52), 246 (–0.23), 325 (+1.80) nm; IR (KBr) ν_{max}: 3423, 2924, 2874, 1743, 1665, 1458,1148, 1066 cm^{-1}; For ^1H and ^{13}C NMR data, see Table 2; HRESIMS *m*/*z* 469.2554 ($[M + Na]^+$, calcd for $C_{26}H_{38}O_6Na^+$, 469.2566).

Single-crystal X-ray diffraction analysis

Crystal data for compound **1** (CCDC No. 2348446): M = $C_{25}H_{36}O_6$, M = 432.54, a = 8.53350(10) Å, b = 15.00880(10) Å, c = 19.05170(10) Å, α = 90°, β = 90°, γ = 90°, V = 2440.10(4) $Å^3$, T = 293(2) K, space group $P2_12_12_1$, Z = 4, μ(Cu Kα) = 0.671 mm^{-1}, 13567 reflections measured, 4783 independent reflections (R_{int} = 0.0244). The final R_1 values were 0.0295 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.077. ($I > 2\sigma(I)$). The final R_1 values were 0.0301 (all data). The final $wR(F^2)$ values were 0.0775 (all data). The goodness of fit on F^2 was 1.046. Flack parameter = 0.01(4).

Crystal data for compound **2** (CCDC No. 2348447): $C_{25}H_{36}O_6 \bullet H_2O$, M = 450.55, a = 17.7841(6) Å, b = 40.4402(11) Å, c = 6.9564(2) Å, α = 90°, β = 90°, γ = 90°, V = 5003.0(3) $Å^3$, T = 150.(2) K, space group $P2_12_12$, Z = 8, μ(Cu Kα) = 0.704 mm^{-1}, 35897 reflections measured, 9144 independent reflections (R_{int} = 0.1679). The final R_1 values were 0.0679 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1719 ($I > 2\sigma(I)$). The final R_1 values were 0.0966 (all data). The final $wR(F^2)$ values were 0.1940 (all data). The goodness of fit on F^2 was 0.992. Flack parameter = 0.3(2).

Cytotoxicity assay

The cytotoxicity of the title compounds was tested through MTT analysis on H9C2 cells. Cells were seeded in 96-well plates at a density of 1 x 10^4 cells/well. At the end of 24 h, the cells were treated with test compounds and incubated at 37 °C for 24 h. MTT (Sigma) was added to each well with a final concentration of 0.5 mg/ml and incubated for 4 h. Then, the medium was decanted, and 150 μL of DMSO was added to each well. The absorbance was obtained by a microplate reader (B20-TEKELX800UV, USA) at 570 nm, and all

measurements were conducted three times under the same condition. Quercetin (50 μM) served as a positive control.

Assay for testing the protective effects against myocardial cell injury induced by H_2O_2

H9C2 cells (the Cell Bank of the Chinese Academy of Sciences Shanghai, China) were seeded into 96-well flat microtiter plates at a density of 1×10^4 per well and allowed 24 h to adhere before drugs were introduced. After incubation with different concentrations of compounds **1**–**5** for 12 h, the cells were treated with 600 μM H_2O_2 for 4 h. The cells in the control groups were treated with the same volume of phosphate-buffered saline (PBS). Cell viability was evaluated by 3-(4,5-dimethylthiazol-2-yl)-25-diphenyltetrazo-lium bromide (MTT) assay, which is based on the reduction of MTT by the mitochondrial dehydrogenase of intact cells to a purple formazan product. Absorbance was read on an ELISA plate reader at 540 nm as a measure of quantity of formazan, the percentage cell viability was calculated as a ratio of optical density (OD) value of sample to the OD value of control. All experiments were done for three times, and quercetin (50 μM) served as a positive control.

Western blotting

H9C2 cells were washed with ice-cold PBS, pelleted by cell scraper and lysed in 100 μL lysis buffer containing 1 μL phosphatase inhibitor, 0.1 μL protease inhibitor and 0.5 μL PMSF. The extracted proteins were quantified with the bicinchoninic acid Protein assay kit (Thermo Fisher Scientific, Inc.). A total of 20 μg protein extracts per lane were separated by 6-15% SDS-PAGE. The proteins were transferred onto polyvinylidene difluoride membranes or nitrocellulose filter membrane. The membranes were blocked with 5% BSA (Gibco; Thermo Fisher Scientific, Inc.) at room temperature for 2 h and incubated overnight at 4°C with primary antibodies against rabbit anti-Akt (1:1,000; cat. no. 9272), rabbit anti-phosphory-lated (p)-Akt (p-Akt; 1:1000; cat. no.4060), rabbit anti-mTOR (1:1000; cat.no.2983), rabbit anti-p-mTOR (p-mTOR;1:1000; cat. no. 5536), and rabbit anti-GAPDH (1:1000; cat. no. 5174; all from Cell Signaling Technology, Inc.). The membranes were subsequently washed for 2 h with TBST (10 mM Tris, pH 7.5, 150 mM NaCl, and 0.05% Tween-20), and incubated with horseradish peroxidase-conjugated goat anti-rabbit secondary antibody (1:500; cat. no.sc-2004; Santa Cruz Biotechnology, Inc.) for 1 h at room temperature. The antigen-antibody complexes on the membranes were detected using the SuperSignal™ West Femto Maximum Sensitivity substrate (Thermo Fisher Scientific, Inc.) and quantified on the ChemiDoc™ XRSImaging system (Bio-Rad Laboratories, Inc.).

Prediction of potential targets

The targets of **1** were obtained from SwissTargetPrediction (http://swisstargetprediction.ch), PharmMapper (http://www.lilab-ecust.cn/pharmmapper), Targetnet (http://targetnet.scbdd.com), STITC (http://stitch.embl.de), and SEA (https://sea.bkslab.org) databases. The potential targets of myocardial ischemia were screened from DisGeNET (https://www.disgenet.org), OMIM (https://omim.org) and Genecards (https://www.genecards.org) online databases. To investigate interactions between compounds and their target proteins, target genes for **1**, used inmyocardial ischemiatreatment, were obtained through the intersection and then uploaded to the String database (https://string-db.org), with "Homo sapiens" specified as the species, to construct a protein-protein interaction (PPI) network. Cytoscape 3.9.1

Structure-based virtual screening (SBVS) was performed on the basis of their 3D structures and the 3568 pharmacophores in ePharmaLib. Finally, 432 PDB protein hits (96 unique proteins) were retrieved for **1**. The top-ten human protein hits were show in Table S7.

Molecular docking

The protein hits, given by literature analysis above, were used as receptors for molecular docking. All the 3D structures of these targets were downloaded from the PDB database (PDB web site: https: //www. rcsb.org). Molecular docking studies were carried out using Maestro from Schrödinger. Protein Preparation wizard was used to refine the raw PDB structure and the corrections were carried out. **1** was prepared and optimized potential for liquid simulations (OPLS 2005) force field using LigPrep. Grid box was prepared for protein-ligand binding. Ligand docking was performed in extra precision mode. XP visualizer analyzes the specific ligand-protein interactions and the docking score. The best scoring conformation was utilized to demonstrate the bond formed between the ligand and the binding pocket of receptors based on the Protein-Ligand Interaction Profiler (PLIP) and further visualized using PyMOL 2.5.

NMR calculation details for 3 and 4

Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 5.0 kcal/mol.[1] The results showed nine lowest energy conformers. Subsequently, the conformers were re-optimized at the B3LYP-D3(BJ)/6-31G* level in PCM chloroform by the GAUSSIAN09 program.[2] All conformers used for property calculations in this work were characterized to be stable point on potential energy surface (PES) with no imaginary frequencies. NMR shielding constants were computed using the GIAO method at the mPW1PW91/6-311+G(d,p)//ωB97XD/6-31G(d) level in PCM chloroform by the GAUSSIAN09 program.[2] Gibbs free energies for conformers were determined by using thermal correction at B3LYP-D3(BJ)/6-31G* level and electronic energies evaluated at the wB97M-V/def2-TZVP level in PCM chloroform using ORCA[3][4] Boltzmann weights were computed using relative gibbs free energies.[5] The unscaled chemical shifts (δ_u) were computed using TMS (Tetramethylsilane) as a reference standard according to $\delta_u = \delta_0 - \delta_x$, where δ_x is the Boltzmann averaged shielding tensor (over all significantly populated conformations) and δ_0 is the shielding tensor of the TMS computed at the same level of theory employed for δ_x. The scaled chemical shifts (δ_s) were calculated as $\delta_s = (\delta_u - b)/m$, where m and b are the slope and intercept, respectively, deduced from a linear regression calculation on a plot of δ_u against δ_{exp}. The DP4+ calculations were run by the Excel spreadsheet available for free at sarotti-nmr.weebly.com or as part of the Supporting Information of the original paper.[5]

[1] Sybyl Software, version X 2.0; Tripos Associates Inc.: St. Louis, MO, 2013.

[2] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, ?. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[3] Neese, F. (2012) The ORCA program system, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2, 73–78

[4] Neese, F. (2017) Software update: the ORCA program system, version 4.0, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 8, e1327.

[5] Nicolás Grimblat, María M. Zanardi, and Ariel M. Sarotti J. Org. Chem. 2015, 80, 12526–12534.

ECD calculation details for 2

Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 5 kcal/mol.[1] The results showed nine lowest energy conformers. Subsequently, geometry optimizations and frequency analyses were implemented at the B3LYP-D3(BJ)/6-31G* level in CPCM methanol using ORCA5.0.3[2] All conformers used for property calculations in this work were characterized to be stable point on potential energy surface (PES) with no imaginary frequencies. The excitation energies, oscillator strengths, and rotational strengths (velocity) of the first 60 excited states were calculated using the TD-DFT methodology at the PBE0/def2-TZVP level in CPCM methanol using ORCA5.0.3.[2] The ECD spectra were simulated by the overlapping Gaussian function (half the bandwidth at 1/e peak height, sigma = 0.30 for all).[3] Gibbs free energies for conformers were determined by using thermal correction at B3LYP-D3(BJ)/6-31G* level and electronic energies evaluated at the wB97M-V/def2-TZVP level in CPCM methanol using ORCA5.0.3[2] To get the final spectra, the simulated spectra of the conformers were averaged according to the boltzmann distribution theory and their relative Gibbs free energy (ΔG). By comparing the experiment spectra with the calculated model molecules, the absolute configuration of the only chiral center was determined to be 4*S*,6*R*,8*S*,9*R*,12*R*,13*S*,23*R*.

[1] Sybyl Software, version X 2.0; Tripos Associates Inc.: St. Louis, MO, 2013.

[2] Neese, F. (2012) The ORCA program system, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2, 73-78.

[3] Stephens, P. J.; Harada, N. ECD cotton effect approximated by the Gaussian curve and other methods. Chirality2010, 22, 229–233.

Table S1. Top-ten ranking human protein hits of **1** and docking score

	PDBID	docking score
AKT	6hhi	-10.5
EGFR	2xkn	-8.4
HSP90AB1	5ucj	-8.1
mTOR	4j6t	-9.1
GSK3B	5f95	-8.3
SRC	1skj	-6.2
MDM2	4jrg	-7.6
PIK3CA	7r9v	-8.4
MAPK1	2ojj	-9.0
HSP90AA1	5h22	-8.3

Figure S1. Comparison of the NMR spectroscopic data between **1** and **2** and between **3** and **4**.

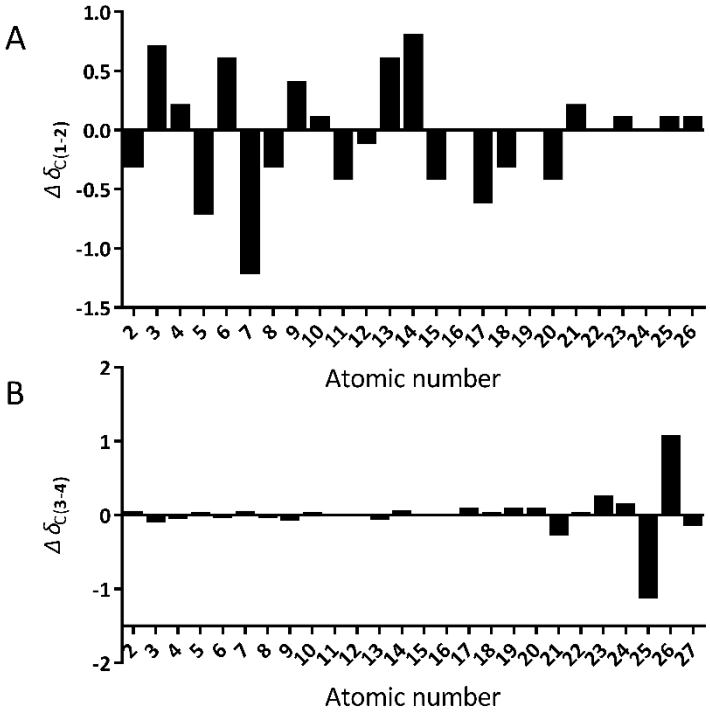

Figure S2. R^2 analysis of ^{13}C NMR chemical shifts of **3** and **4** based on the calculated and experimental values.

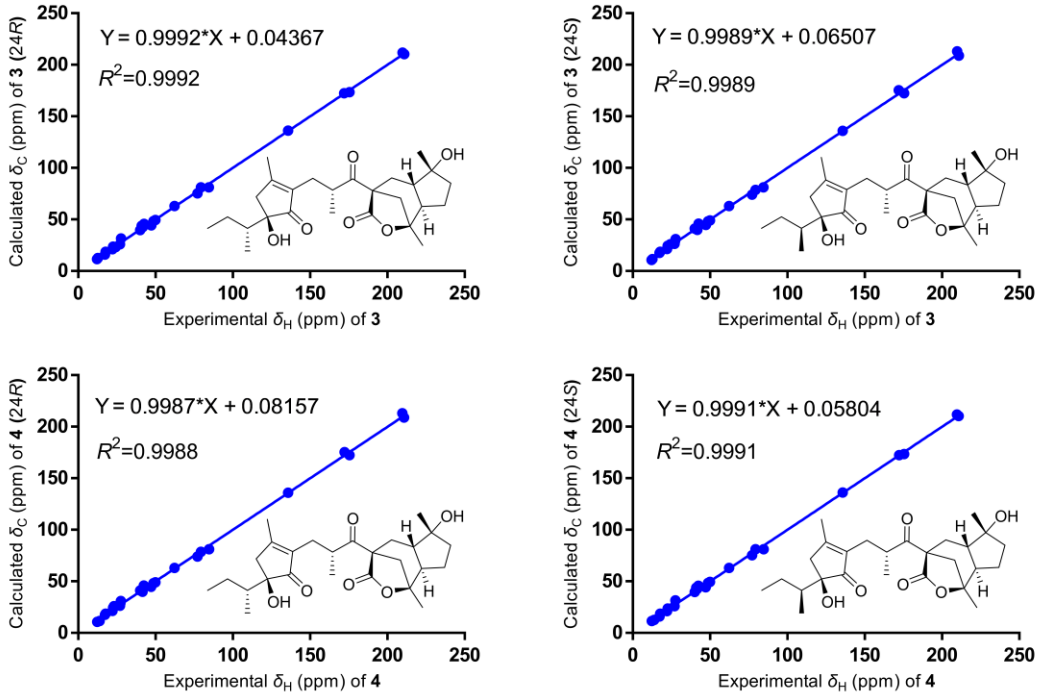

Figure S3. 2D and 3D ligand interactions of **1** with 4j6t-mTOR and 6hhi-AKT.

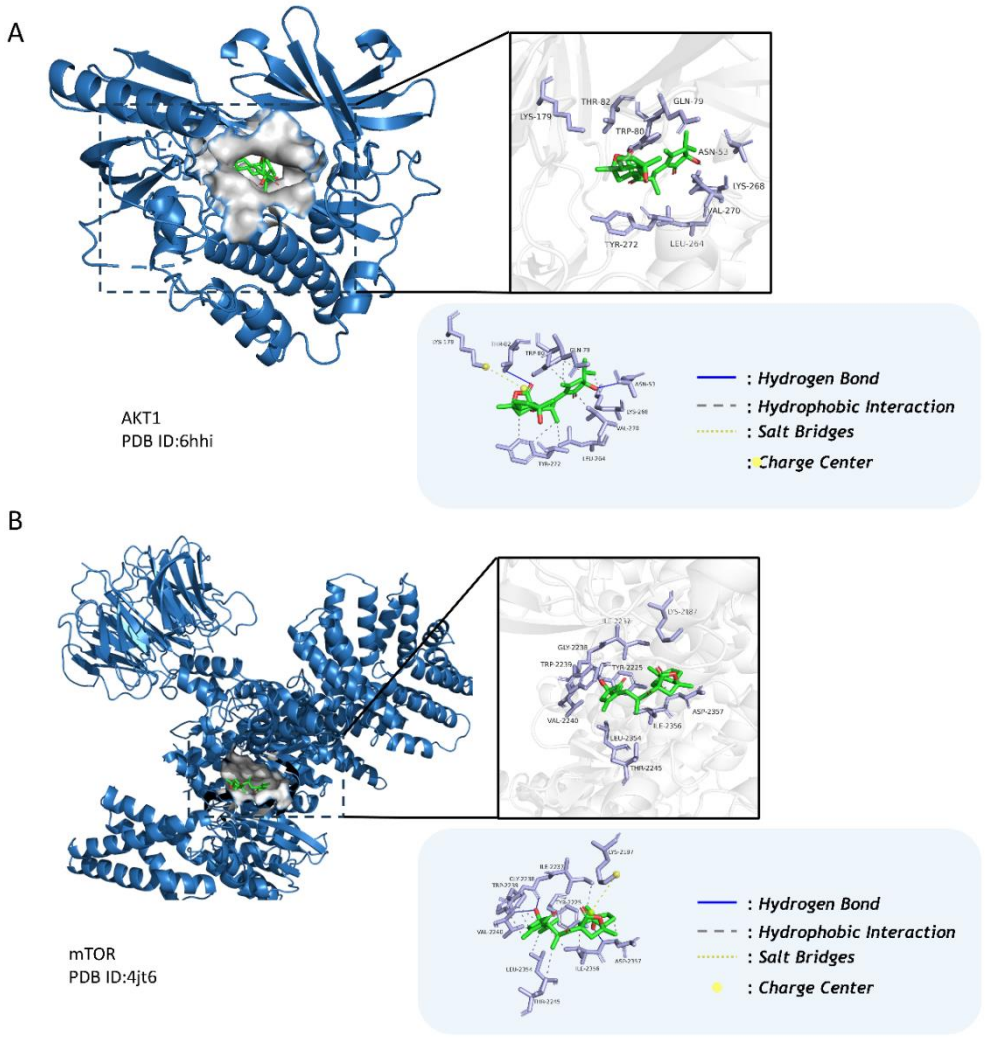

Figure S4. 2D ligand interactions of **1** with top-ten ranking human protein hits.

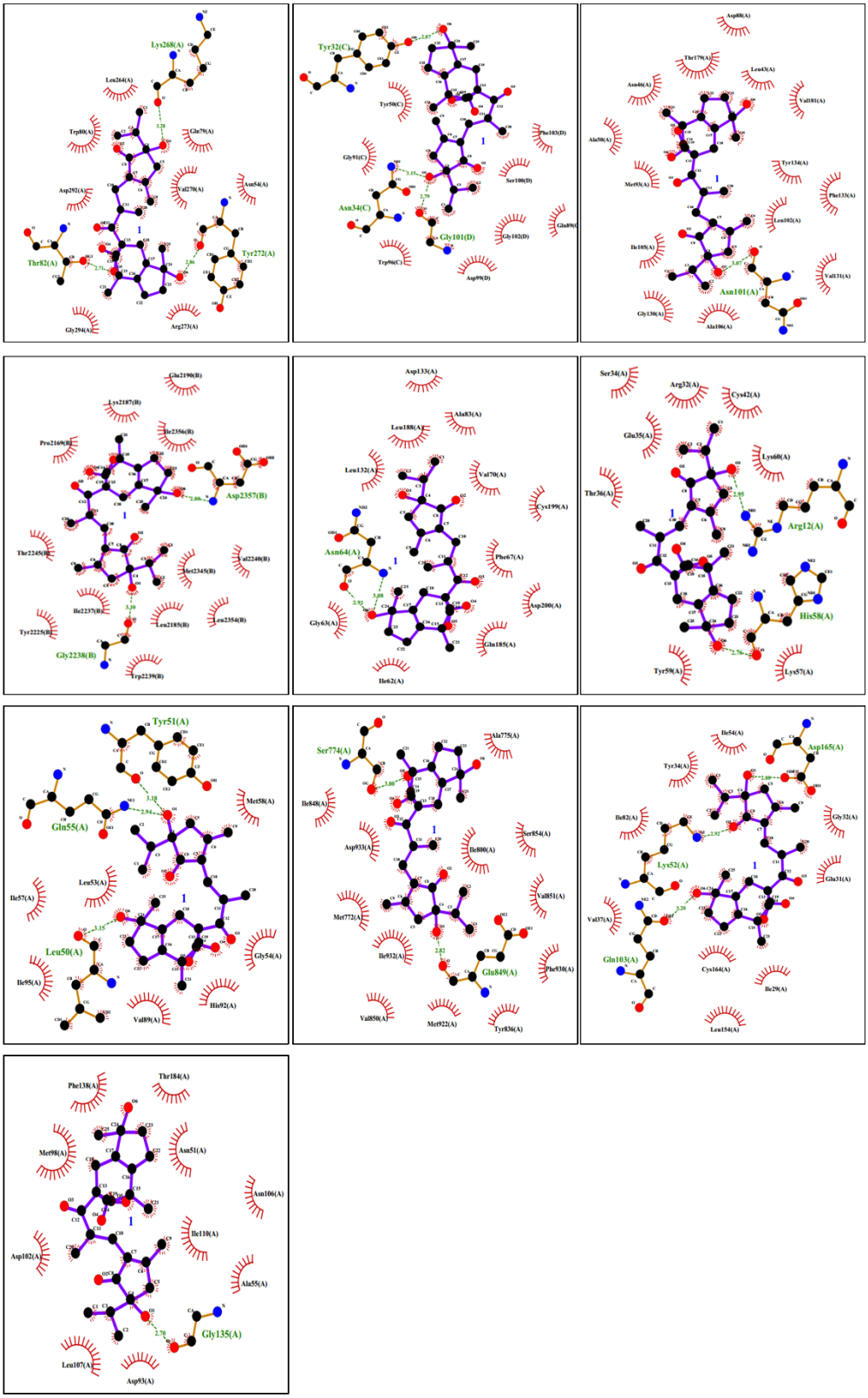

Figure S5. The raw images for all Western blot.

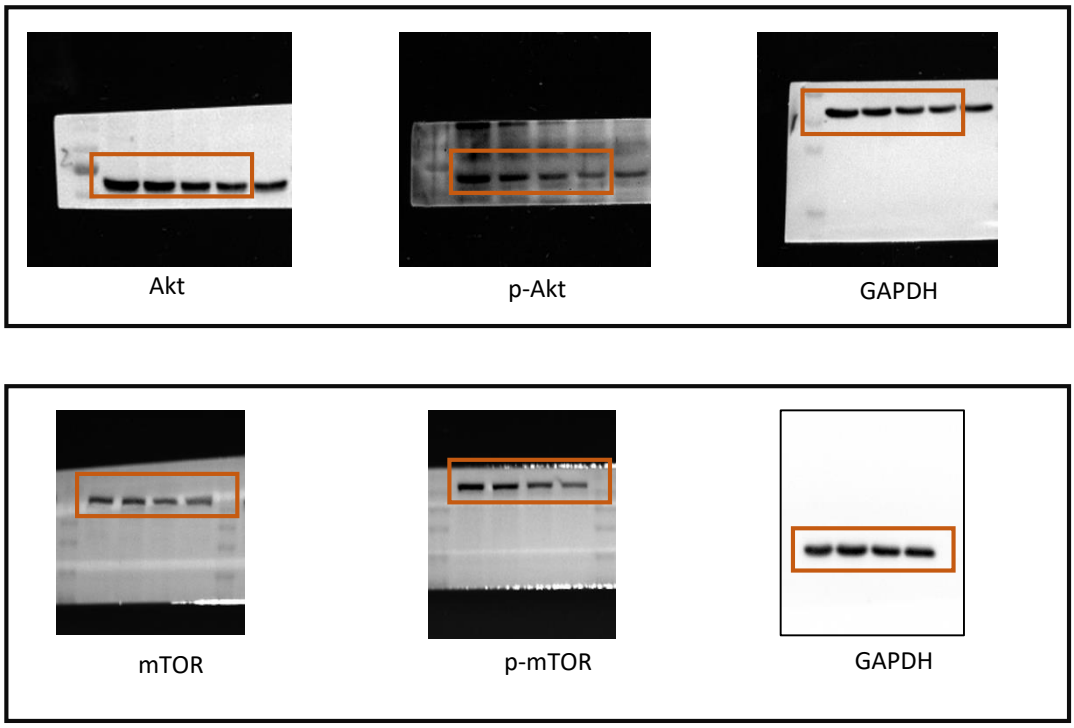

Figure S6. ^{1}H NMR spectrum of compound **1** (recorded in chloroform-*d*)

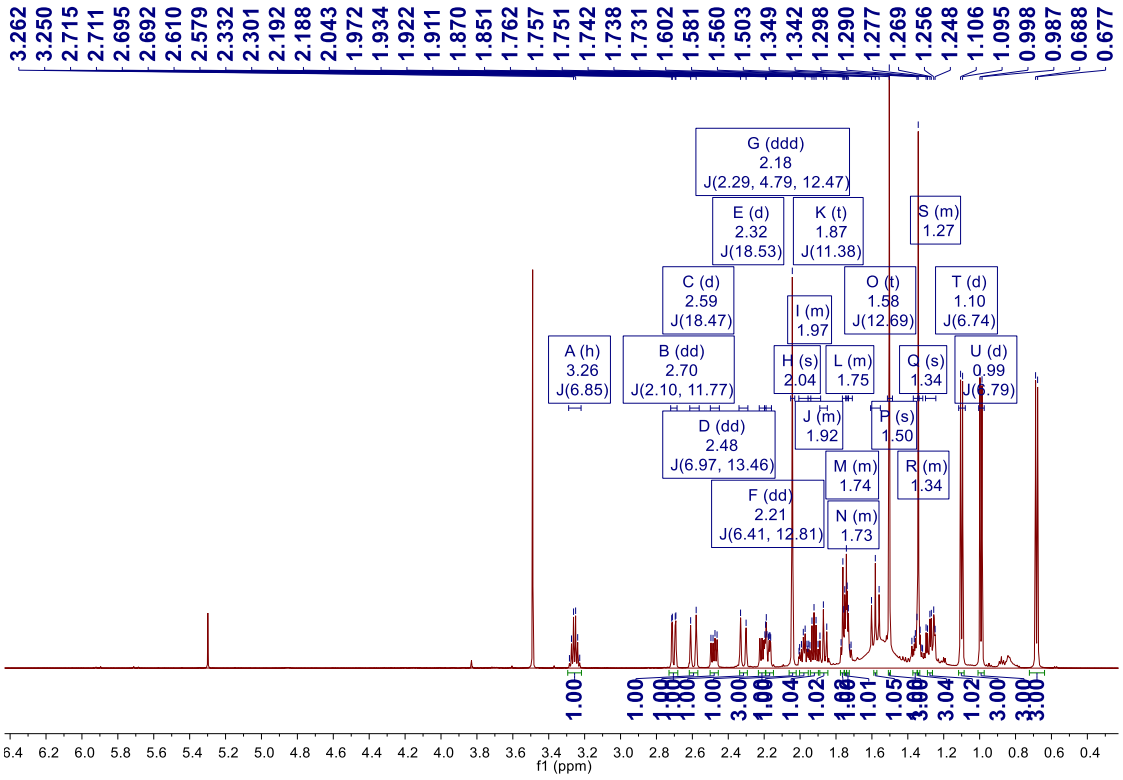

Figure S7. ^{13}C NMR spectrum of compound **1** (recorded in chloroform-*d*)

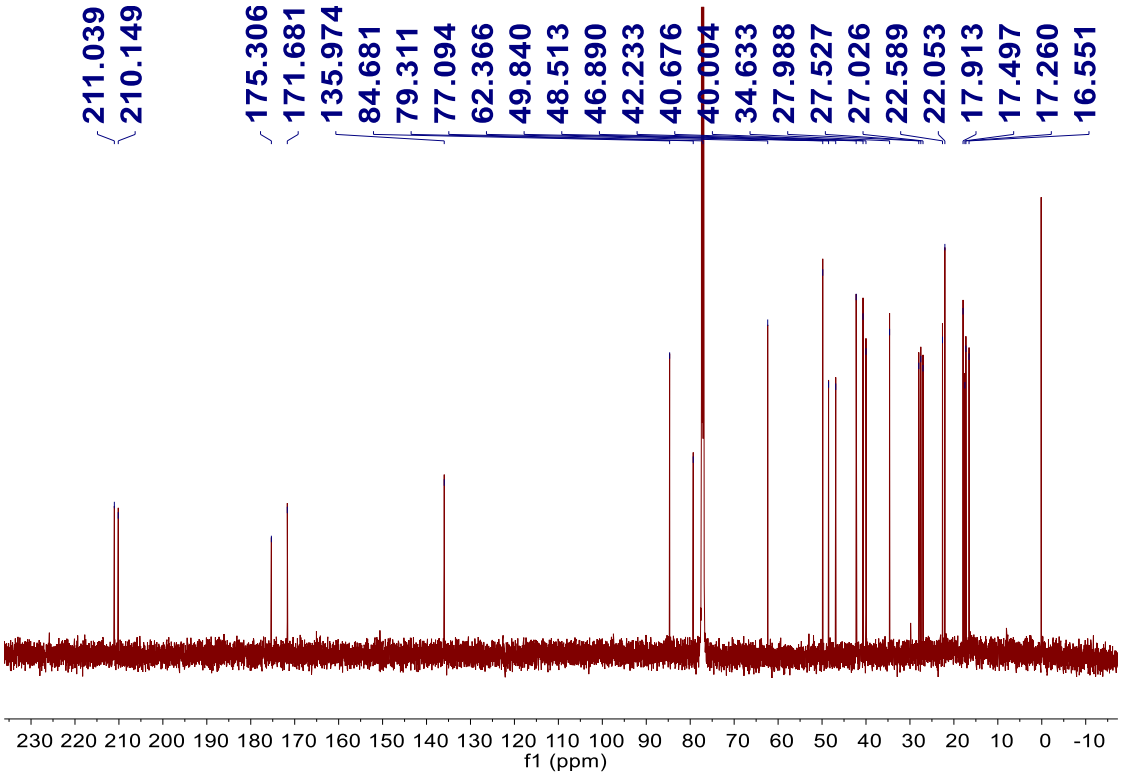

Figure S8. DEPT spectrum of compound **1** (recorded in chloroform-*d*)

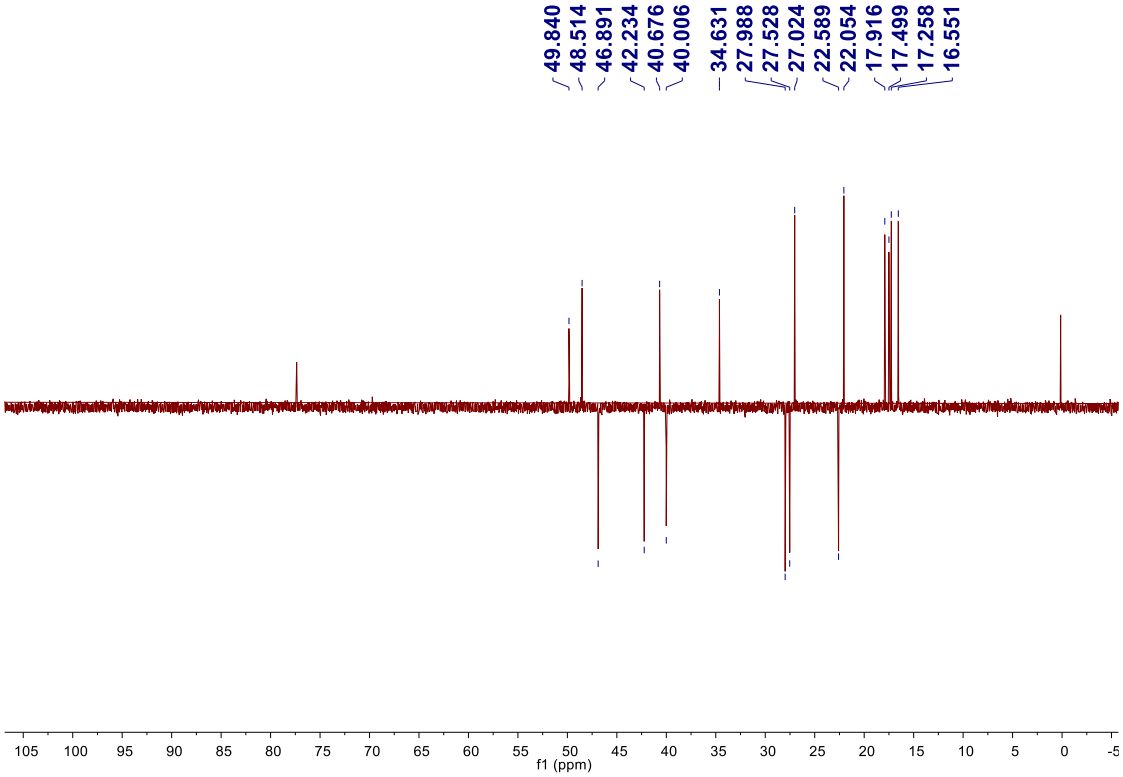

Figure S9. HSQC spectrum of compound **1** (recorded in chloroform-*d*)

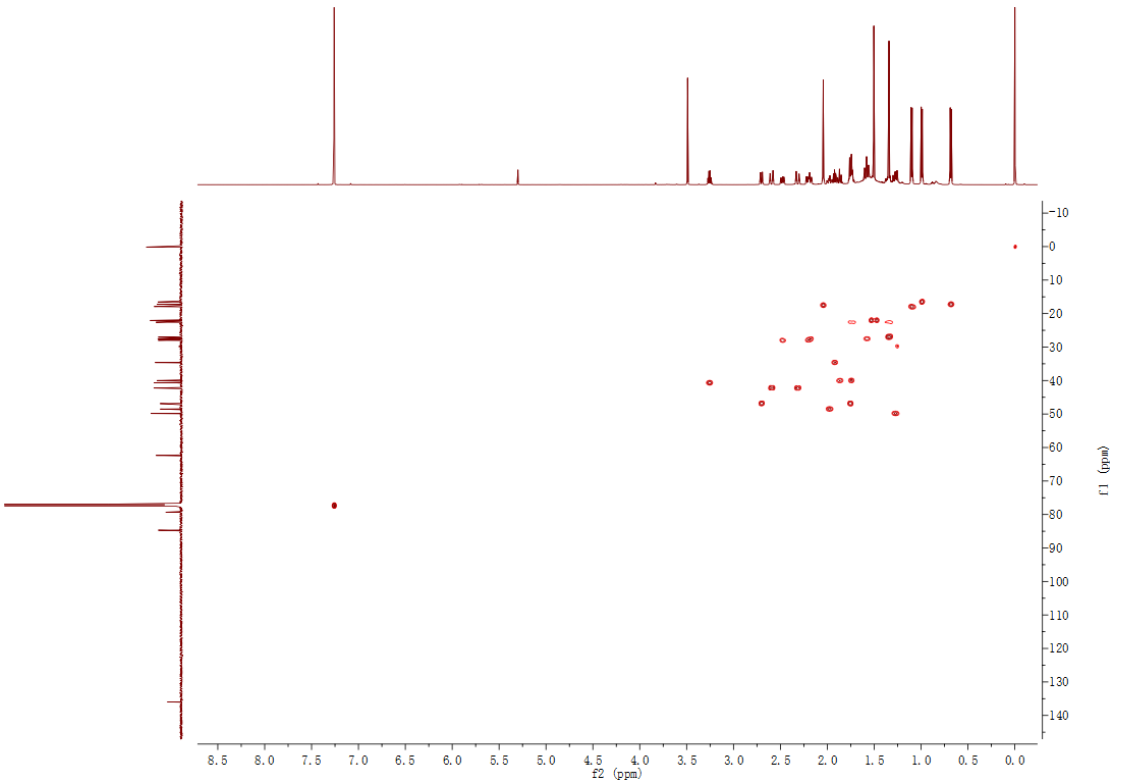

Figure S10. HMBC spectrum of compound **1** (recorded in chloroform-*d*)

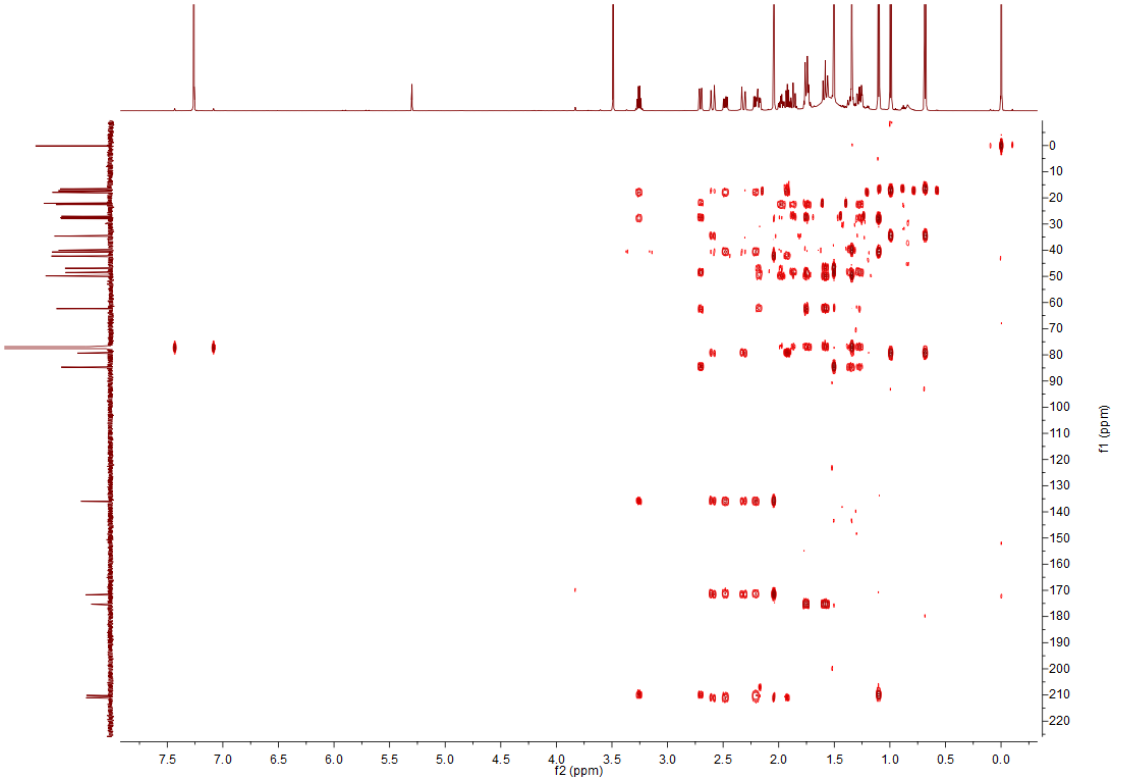

Figure S11. $^{1}H-^{1}H$ COSY spectrum of compound **1** (recorded in chloroform-*d*)

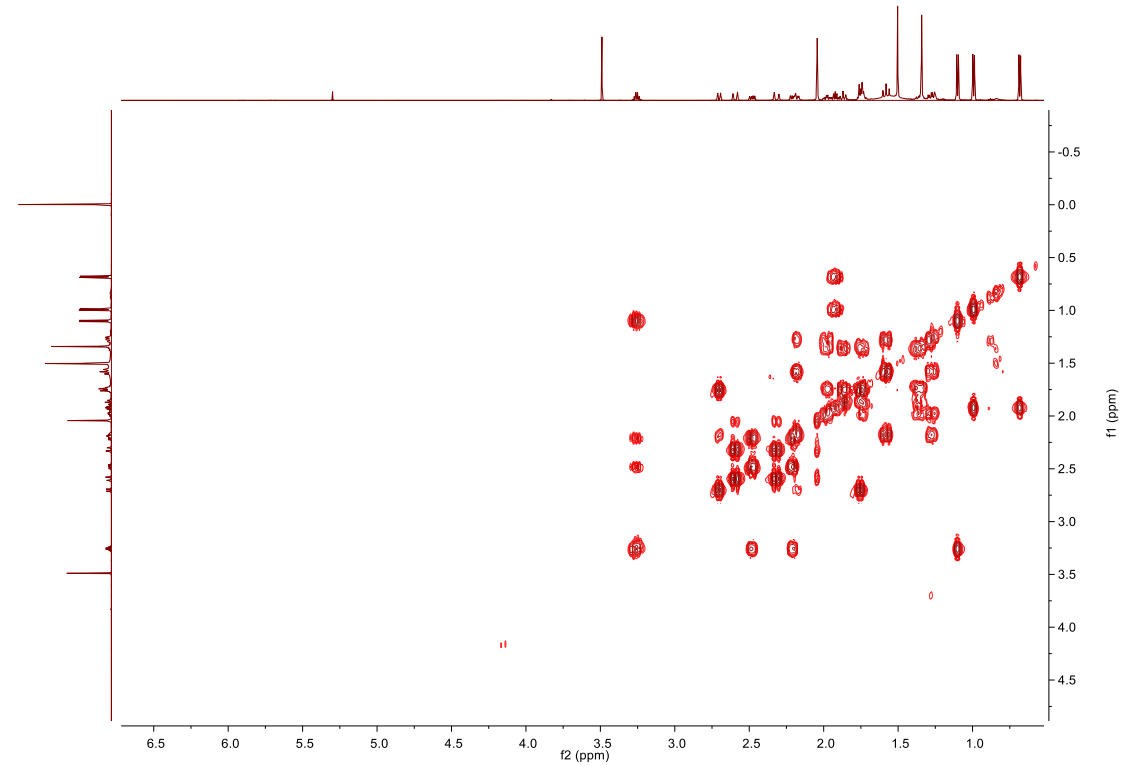

Figure S12. ROESY spectrum of compound **1** (recorded in chloroform-*d*)

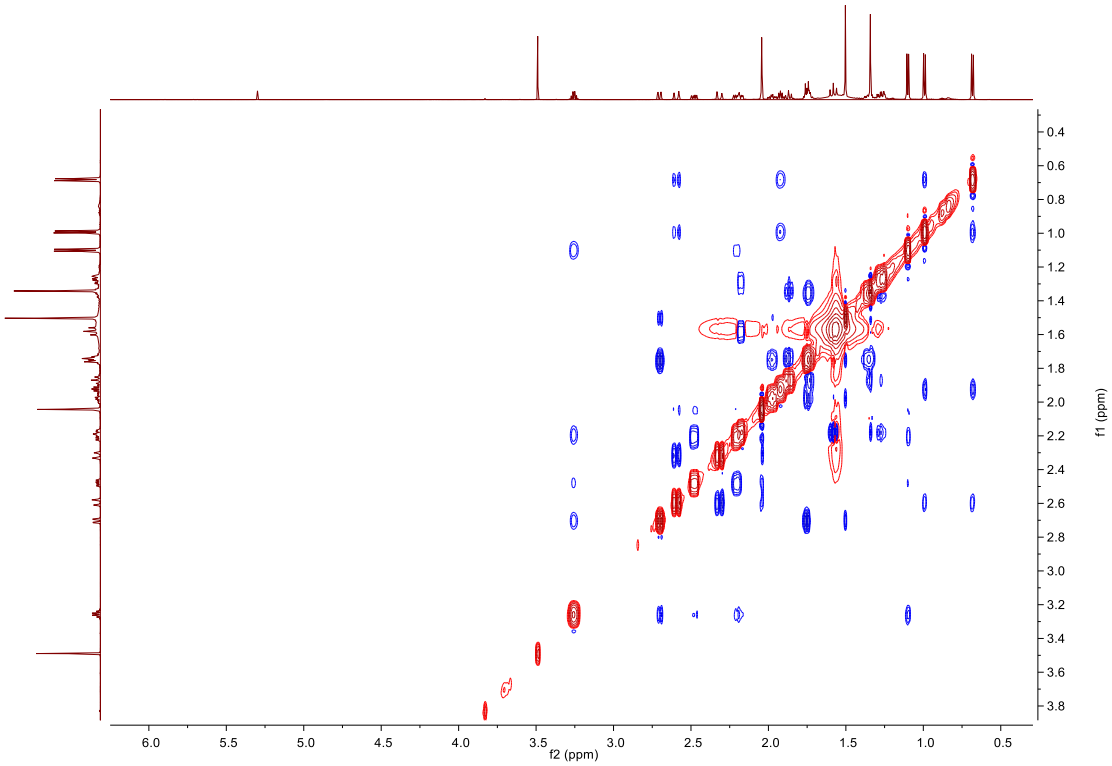

Figure S13. HRESIMS spectrum of compound **1**

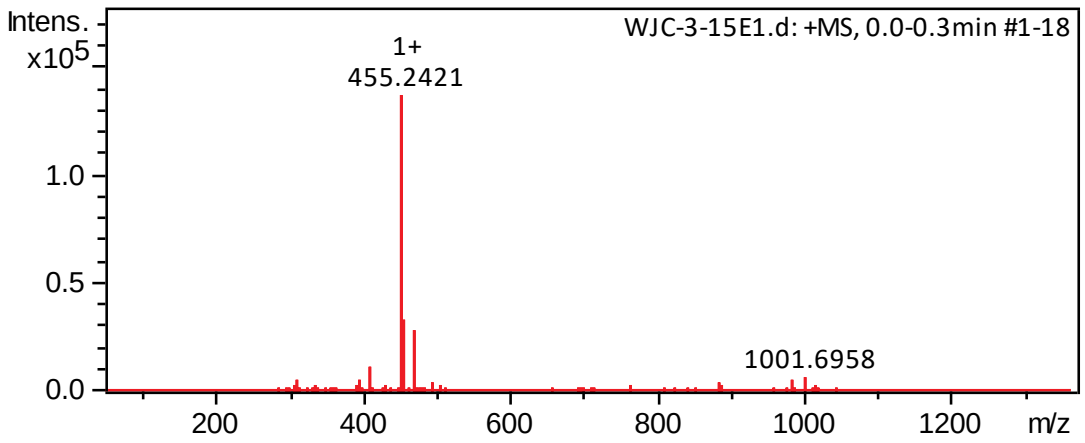

Figure S14. IR spectrum of compound **1**

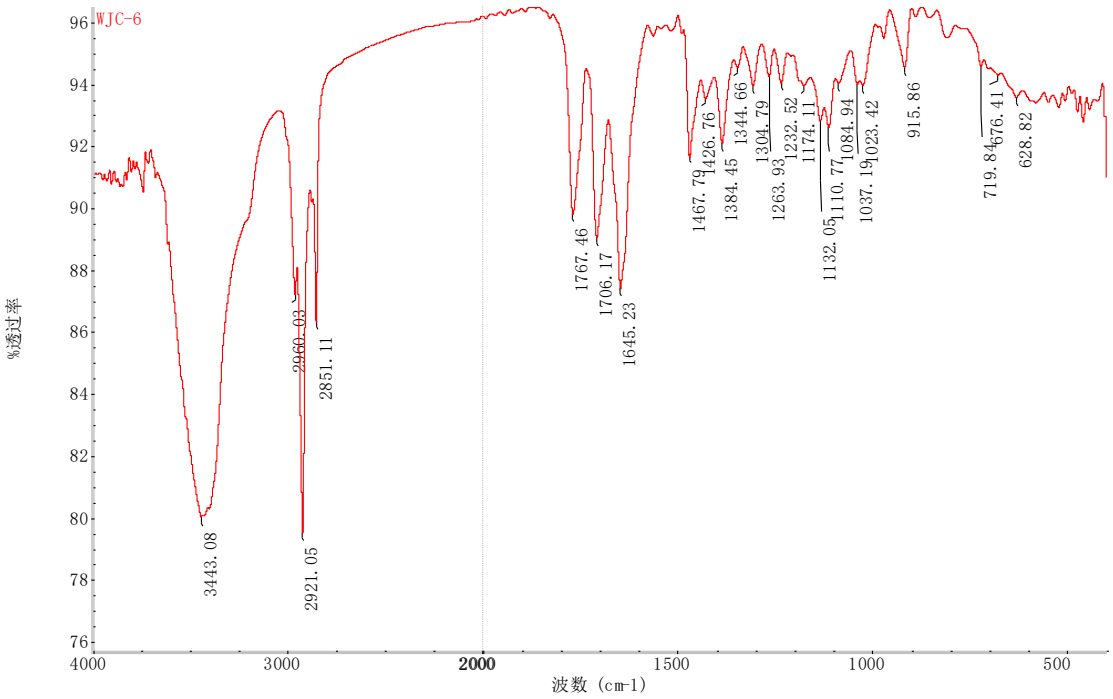

Figure S15. UV spectrum of compound **1**

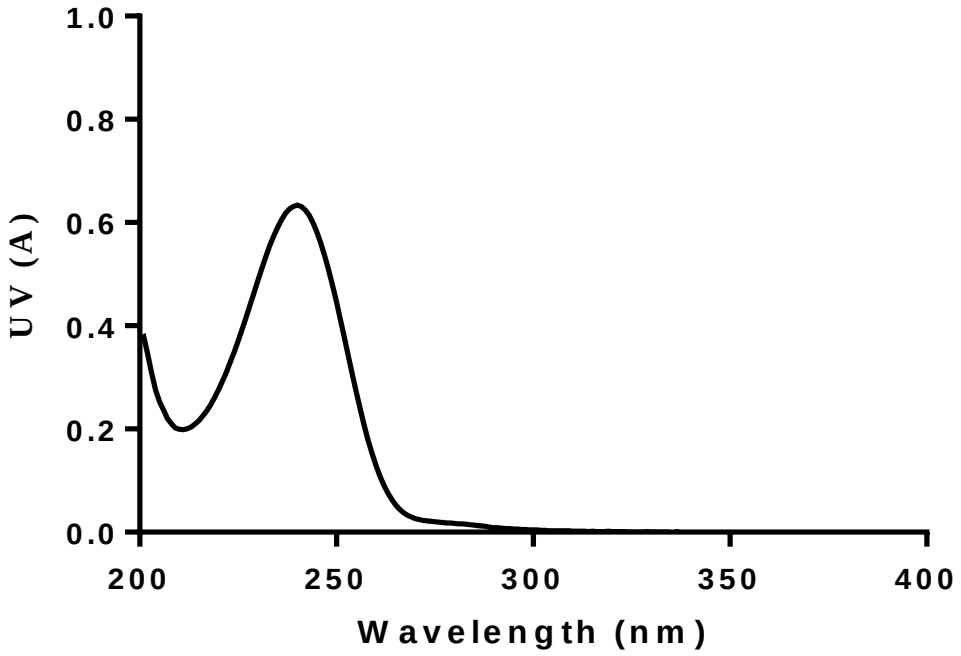

Figure S16. CD spectrum of **1** in methanol

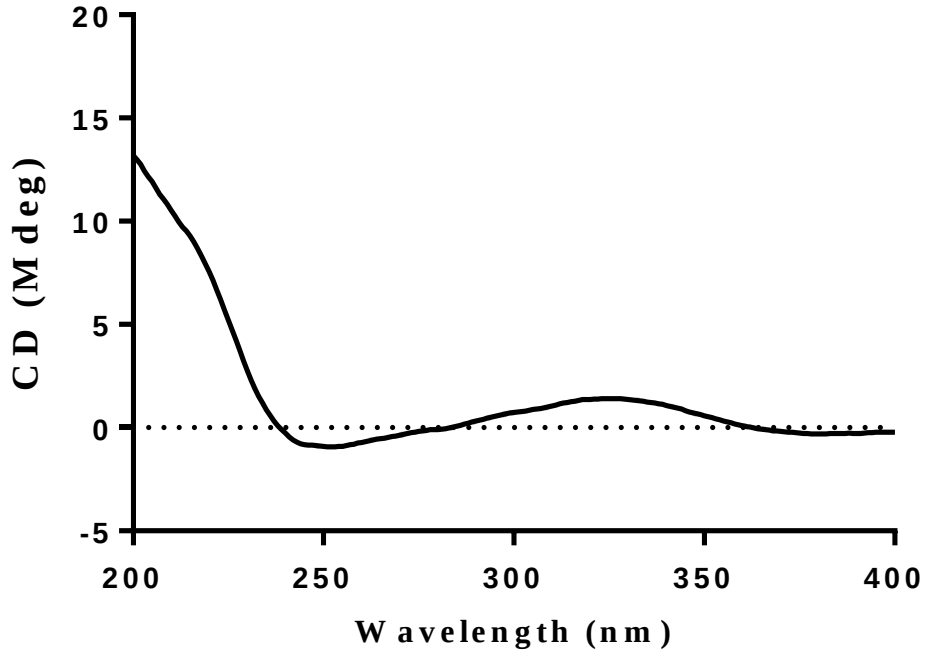

Figure S17. ^{1}H NMR spectrum of compound **2** (recorded in chloroform-*d*)

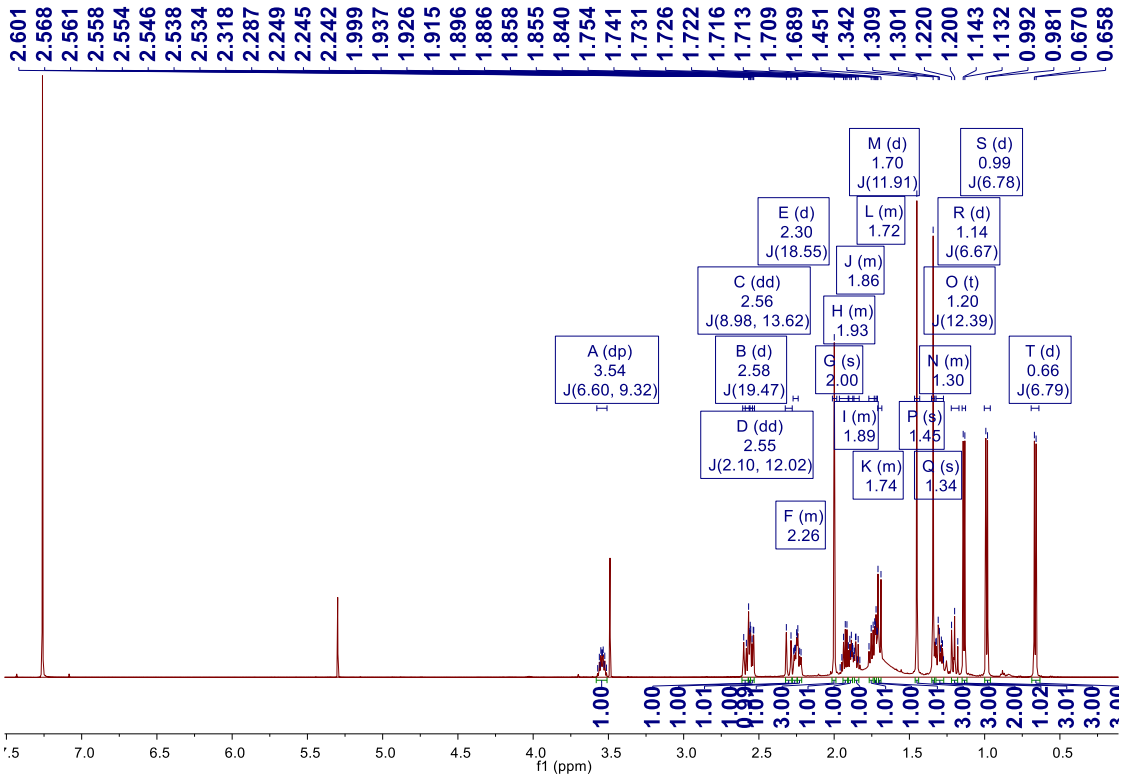

Figure S18. ^{13}C NMR spectrum of compound **2** (recorded in chloroform-*d*)

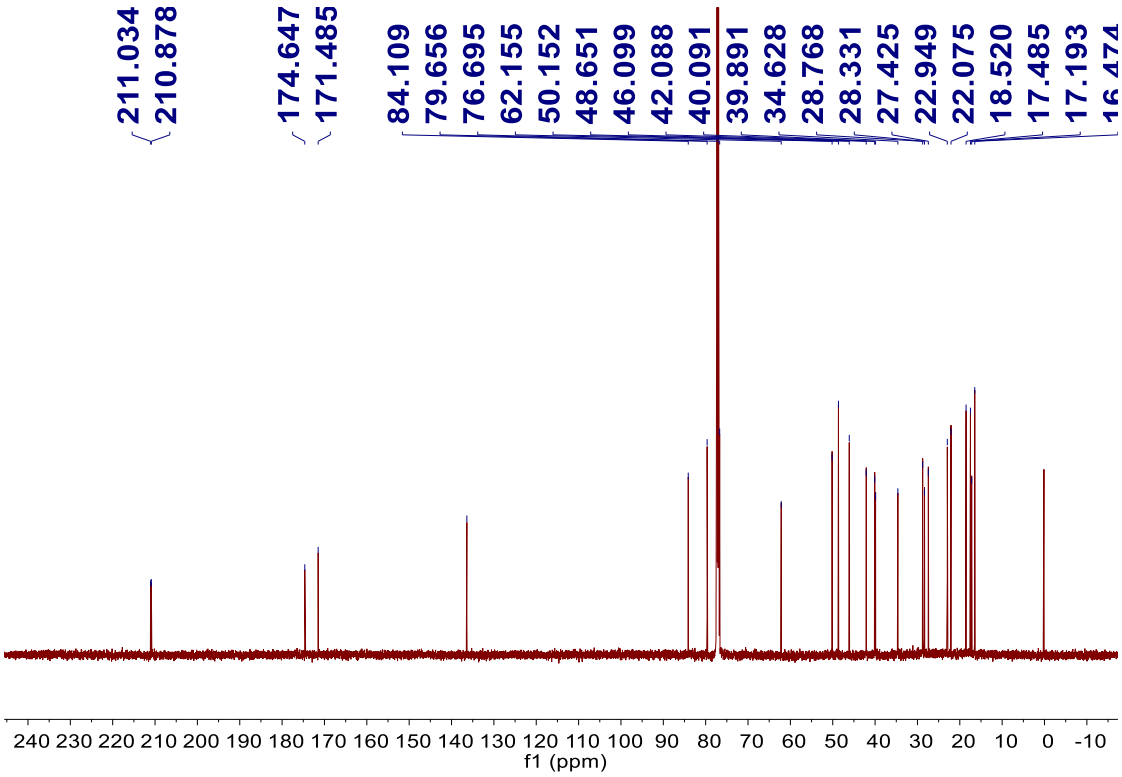

Figure S19. DEPT spectrum of compound **2** (recorded in chloroform-*d*)

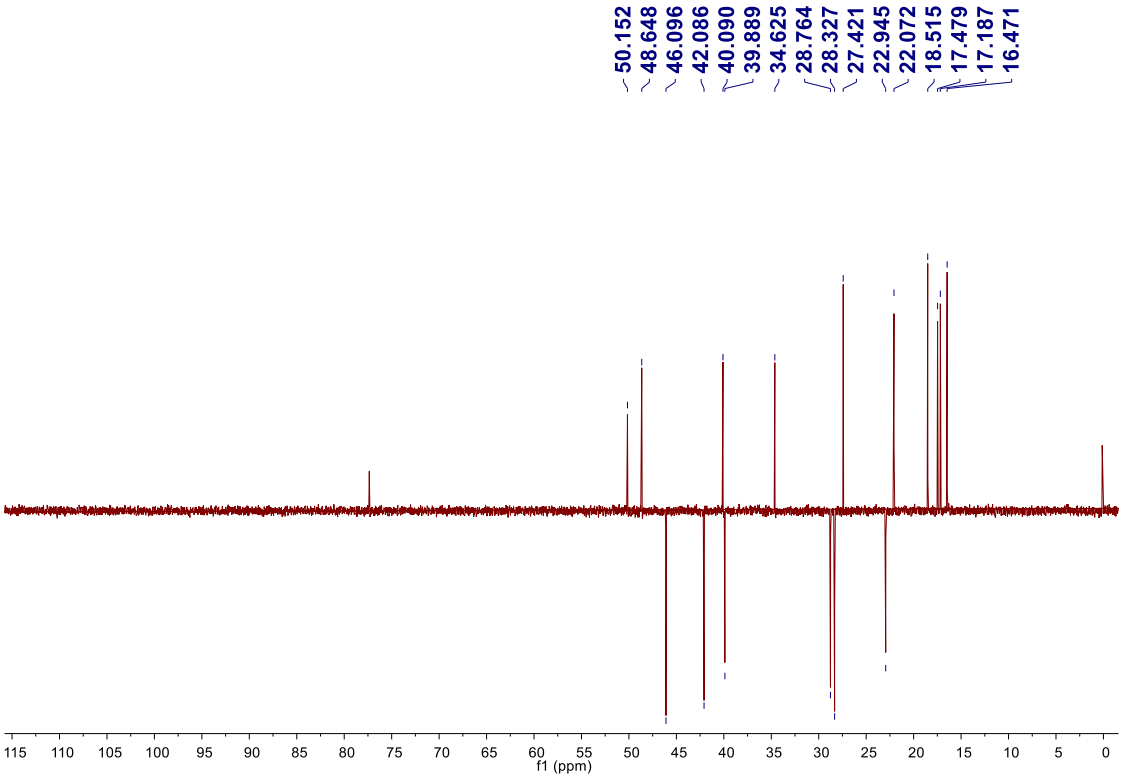

Figure S20. HSQC spectrum of compound **2** (recorded in chloroform-*d*)

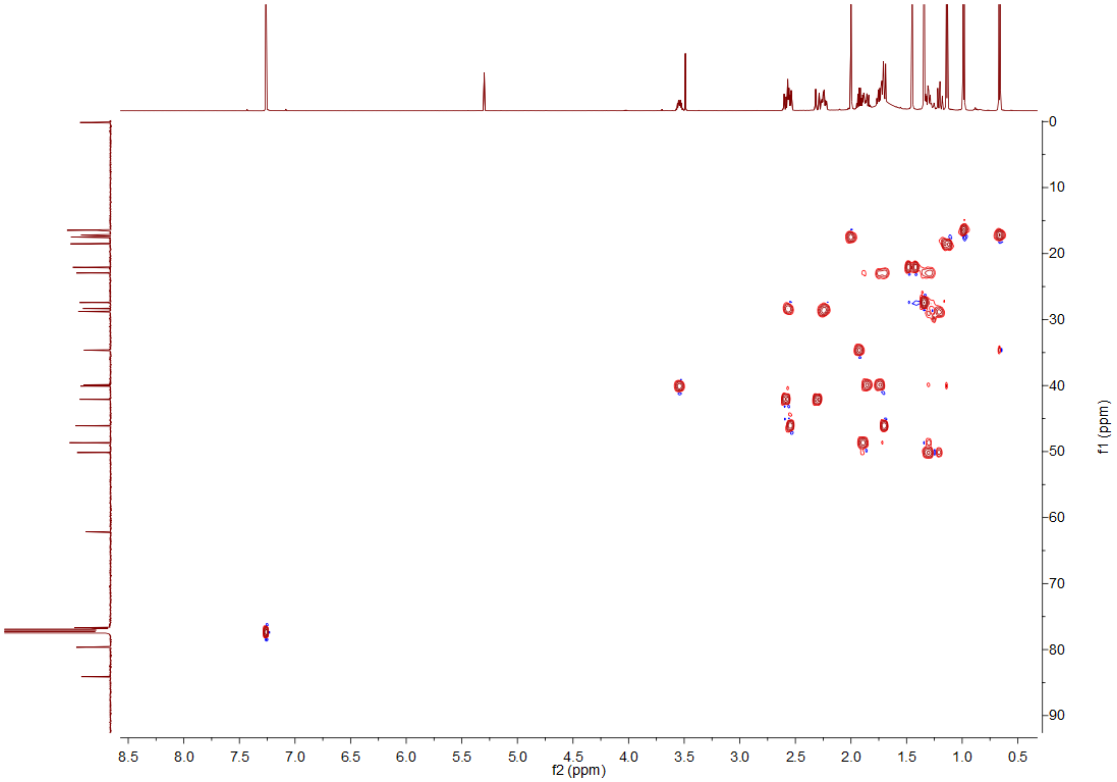

Figure S21. HMBC spectrum of compound **2** (recorded in chloroform-*d*)

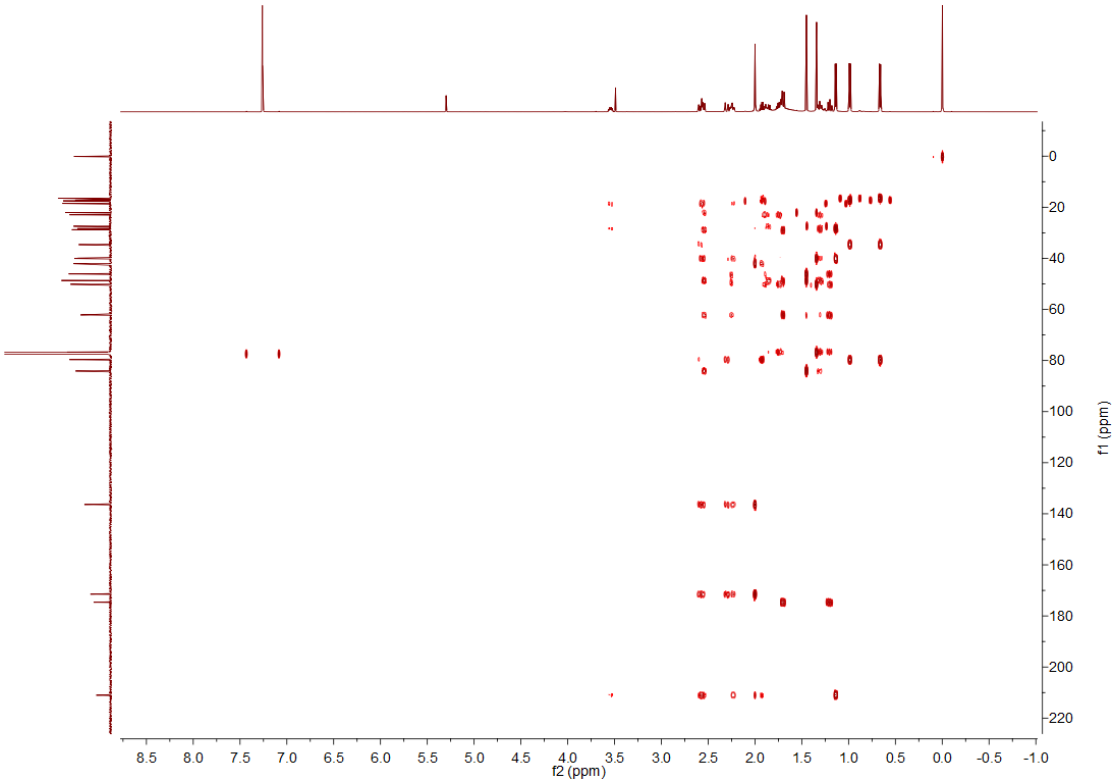

Figure S22. $^{1}H-^{1}H$ COSY spectrum of compound **2** (recorded in chloroform-*d*)

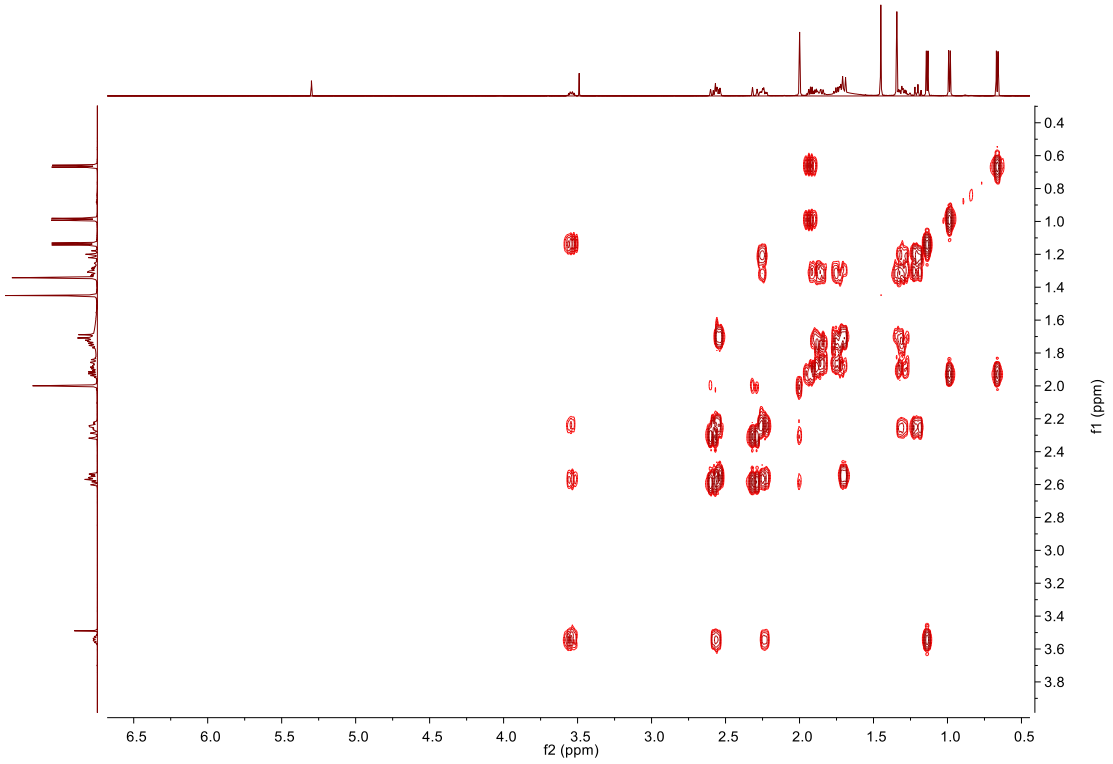

Figure S23. ROESY spectrum of compound **2** (recorded in chloroform-*d*)

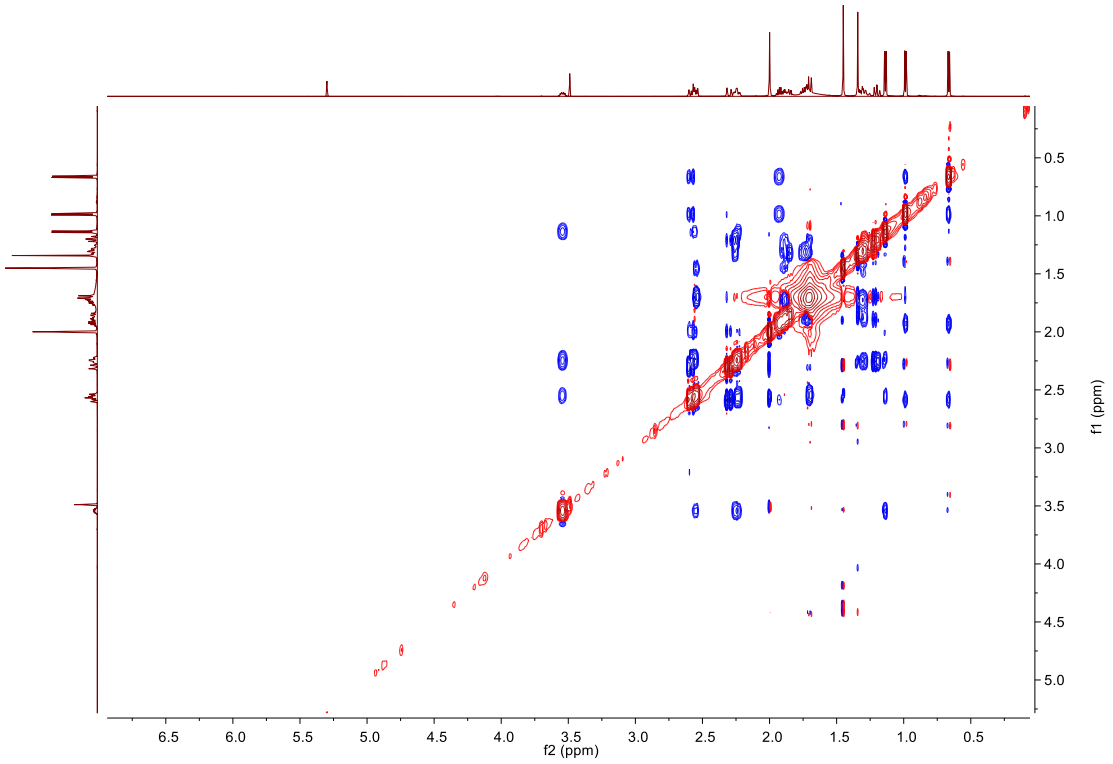

Figure S24. HRESIMS spectrum of compound **2**

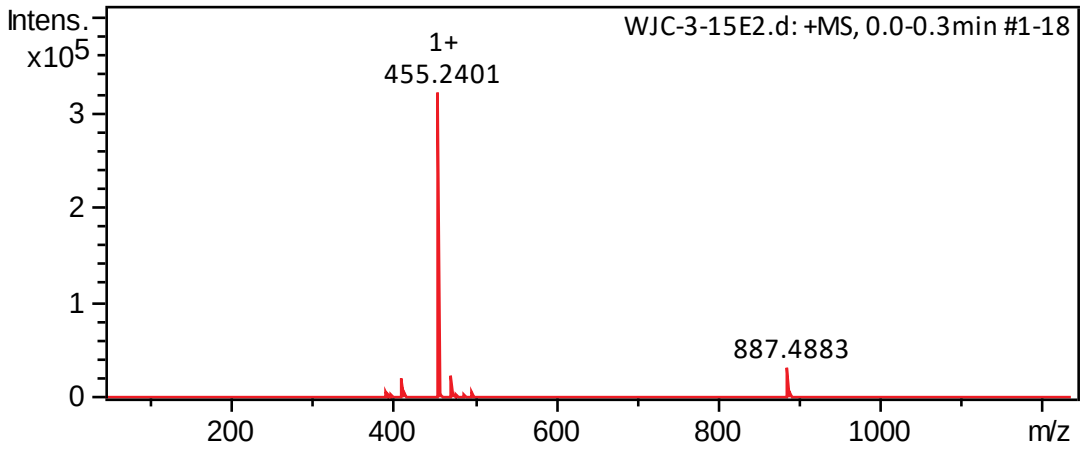

Figure S25. IR spectrum of compound **2**

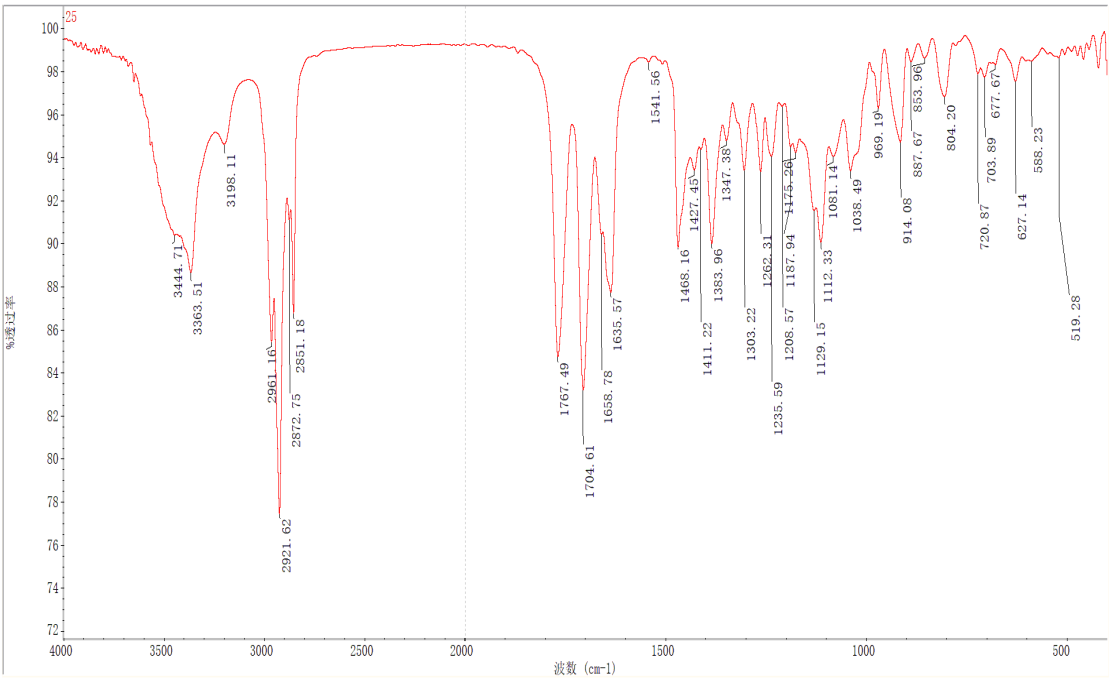

Figure S26. UV spectrum of compound **2**

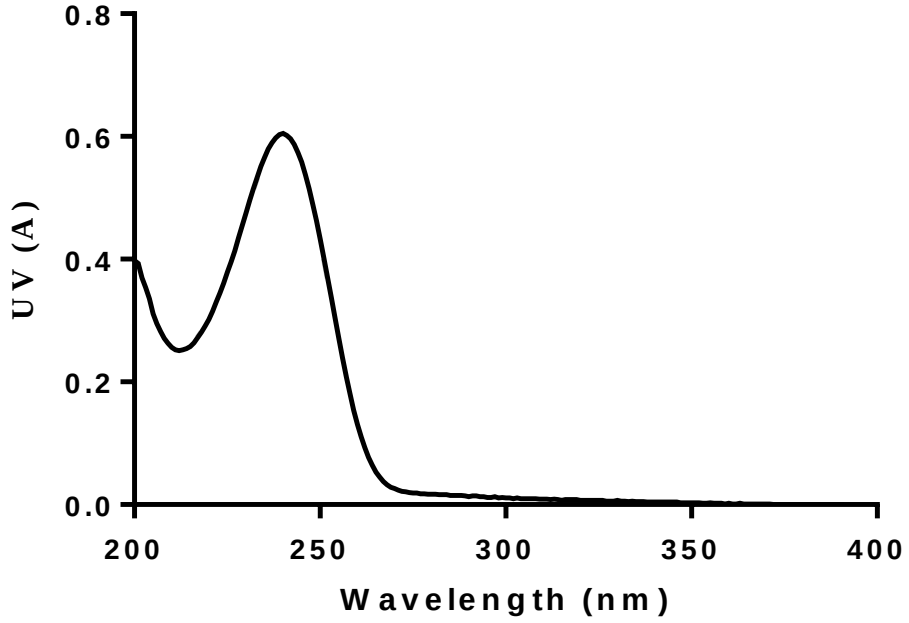

Figure S27. CD spectrum of **2** in methanol

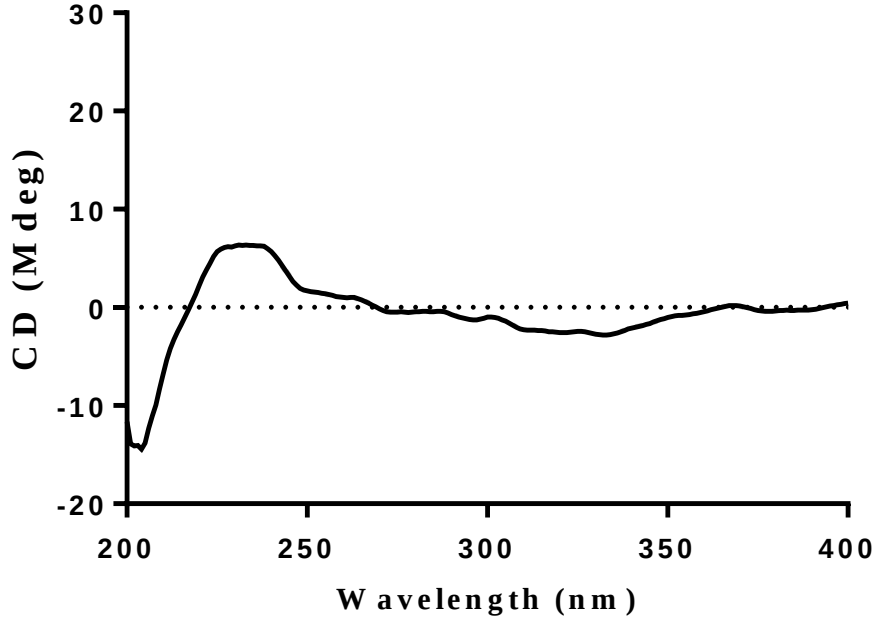

Figure S28. ^{1}H NMR spectrum of compound **3** (recorded in chloroform-*d*)

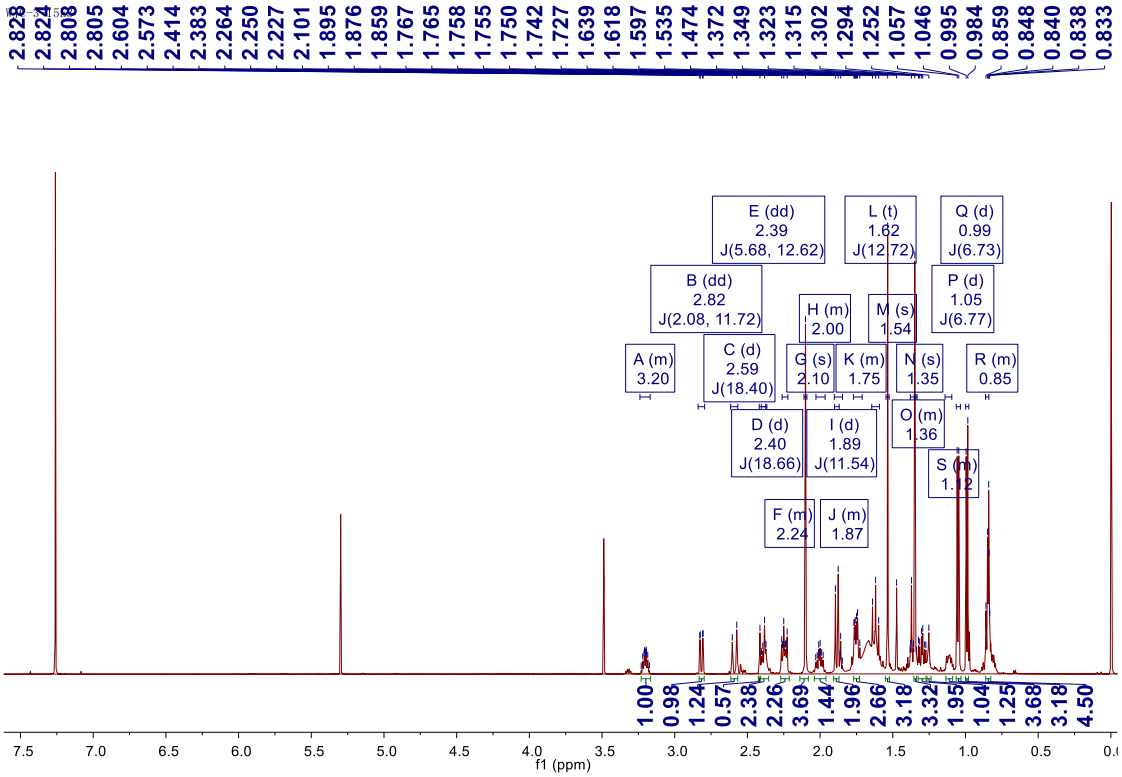

Figure S29. ^{13}C NMR spectrum of compound **3** (recorded in chloroform-*d*)

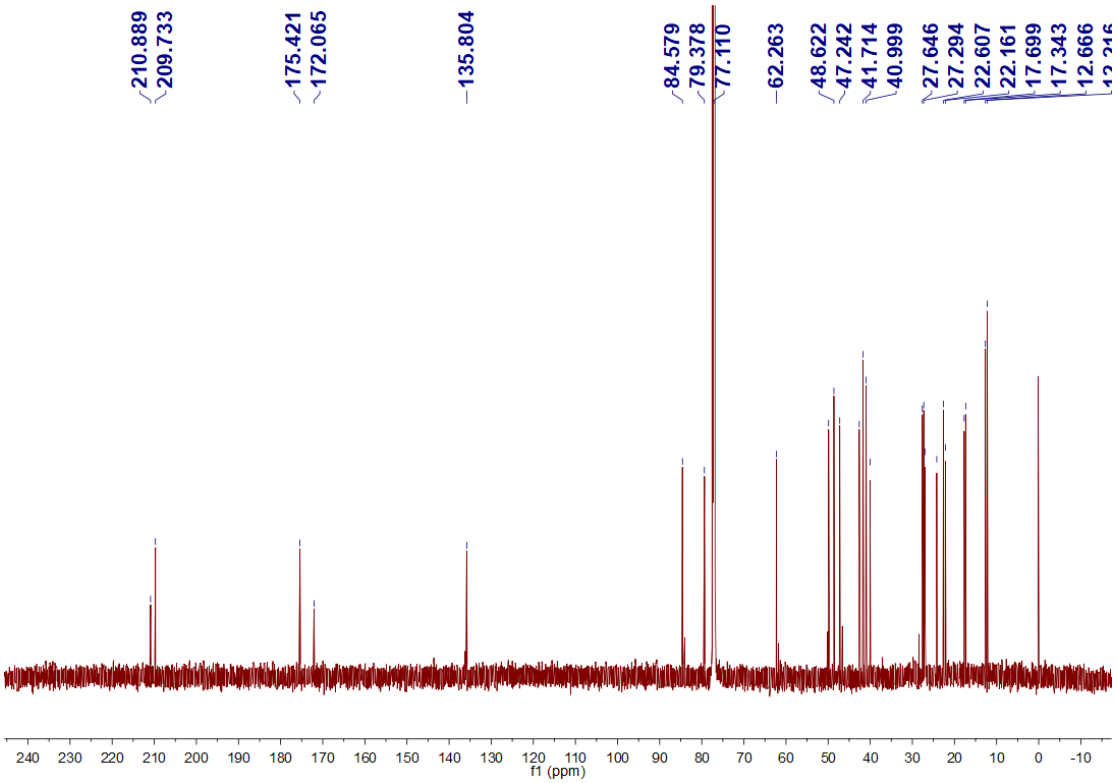

Figure S30. DEPT spectrum of compound **3** (recorded in chloroform-*d*)

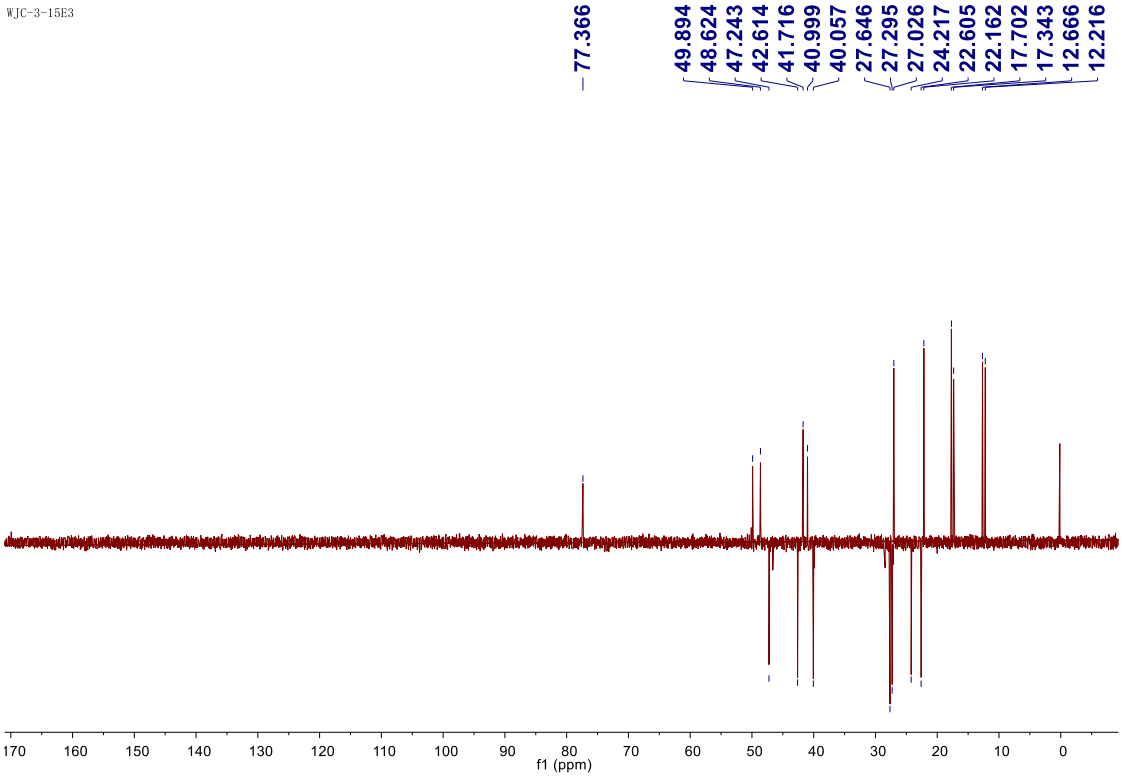

Figure S31. HSQC spectrum of compound **3** (recorded in chloroform-*d*)

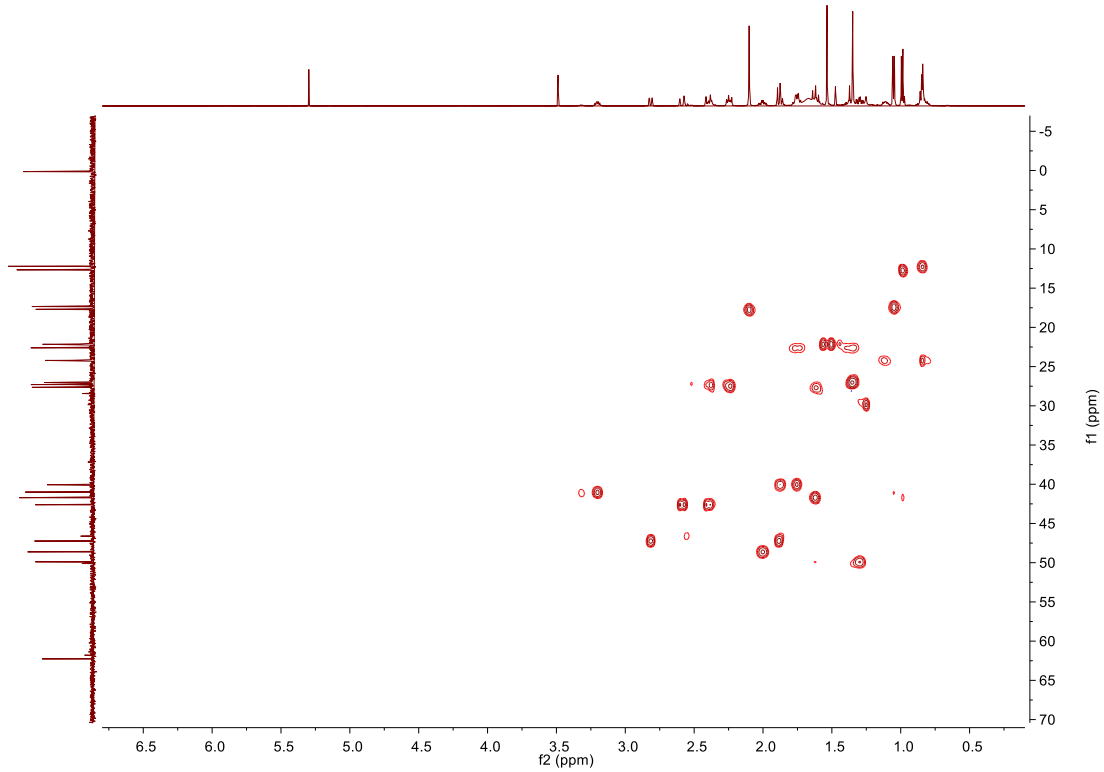

Figure S32. HMBC spectrum of compound **3** (recorded in chloroform-*d*)

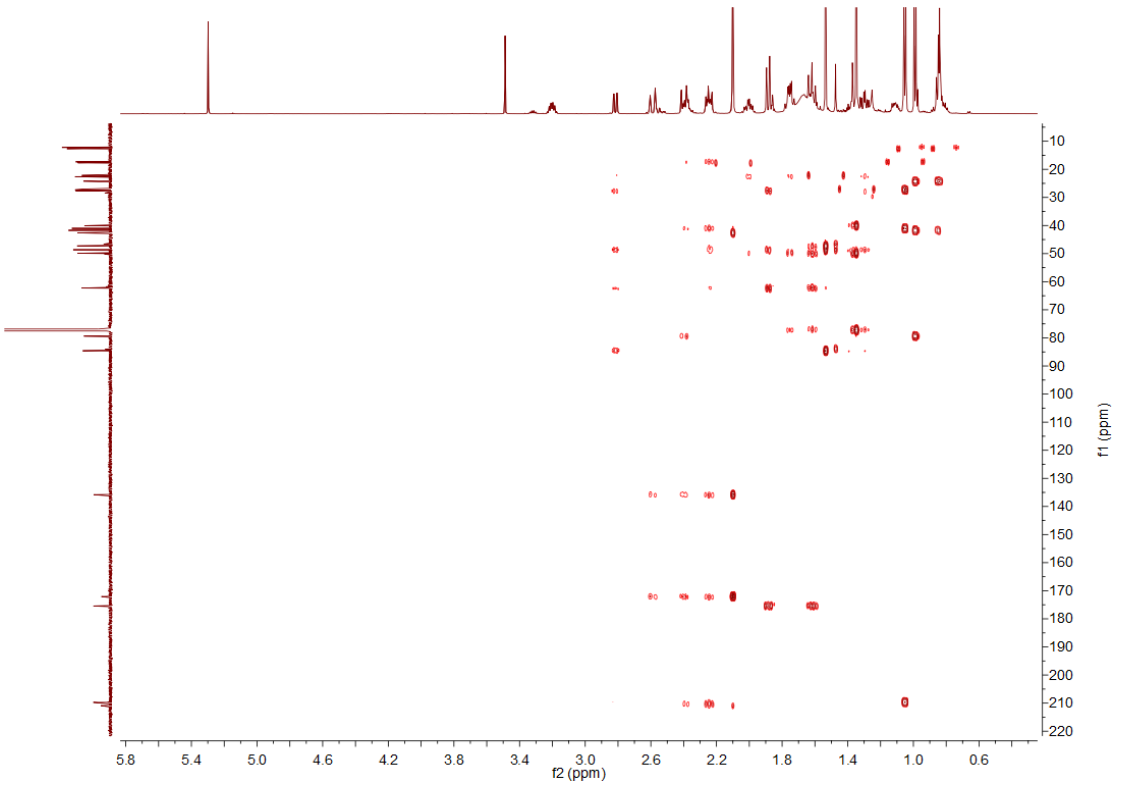

Figure S33. $^{1}H-^{1}H$ COSY spectrum of compound **3** (recorded in chloroform-*d*)

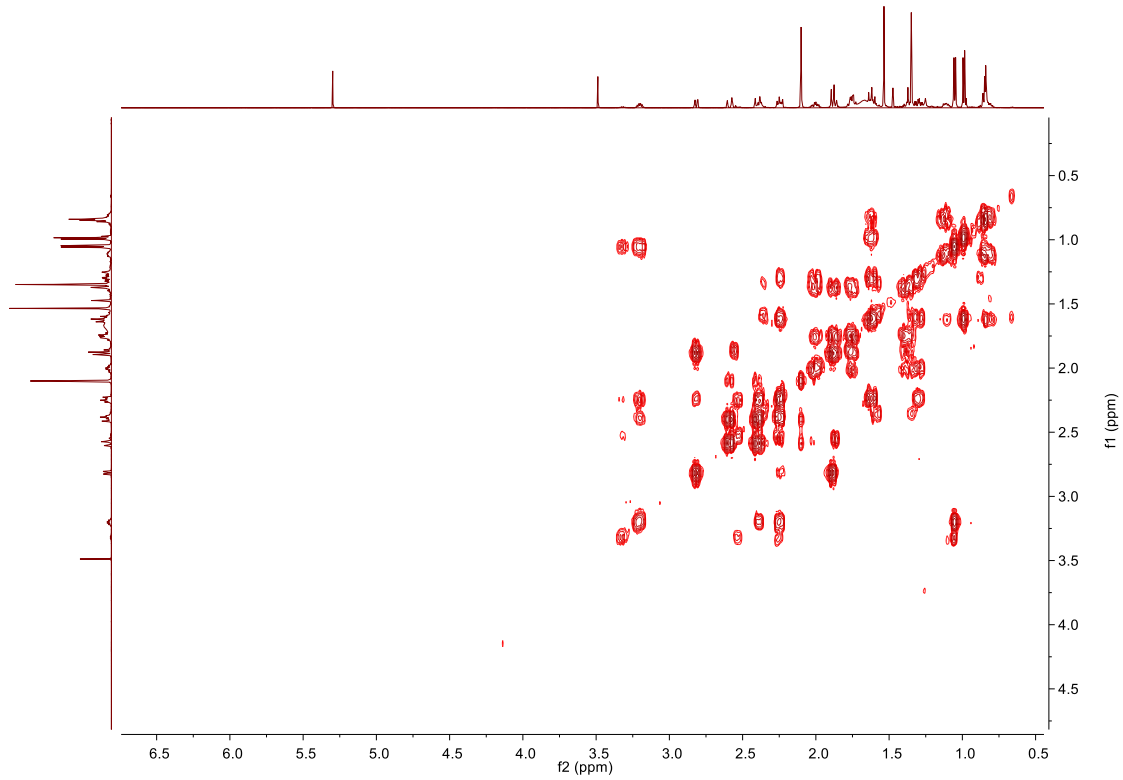

Figure S34. ROESY spectrum of compound **3** (recorded in chloroform-*d*)

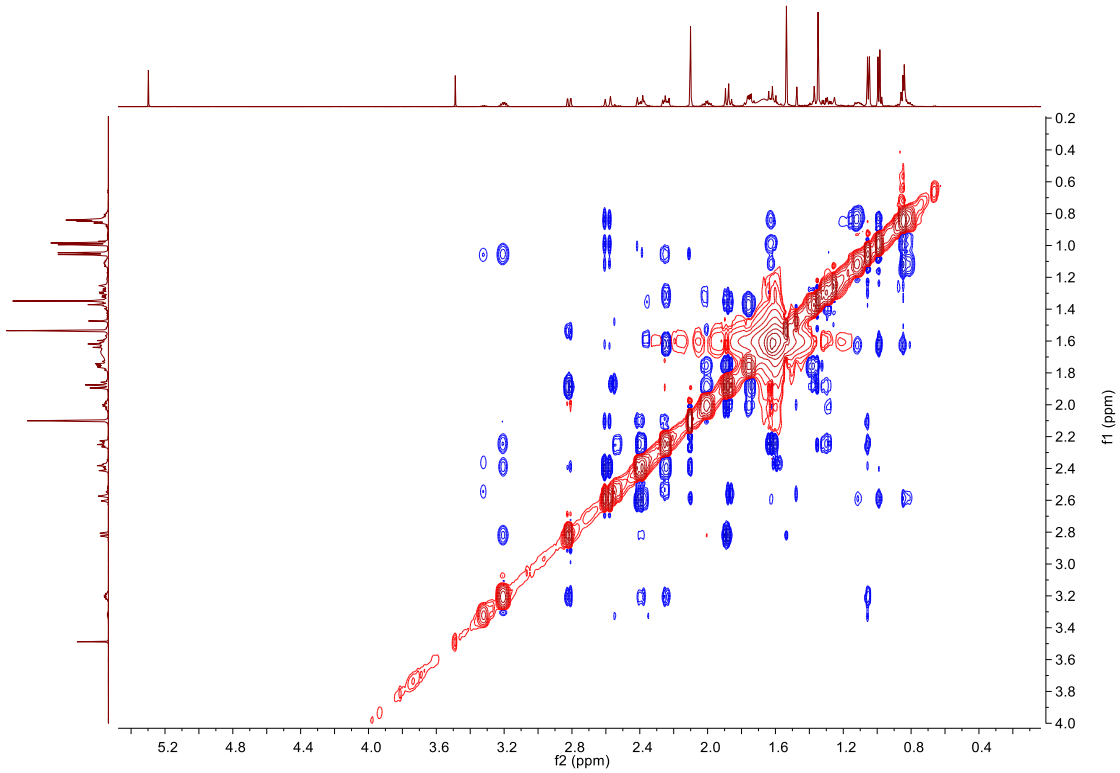

Figure S35. HRESIMS spectrum of compound **3**

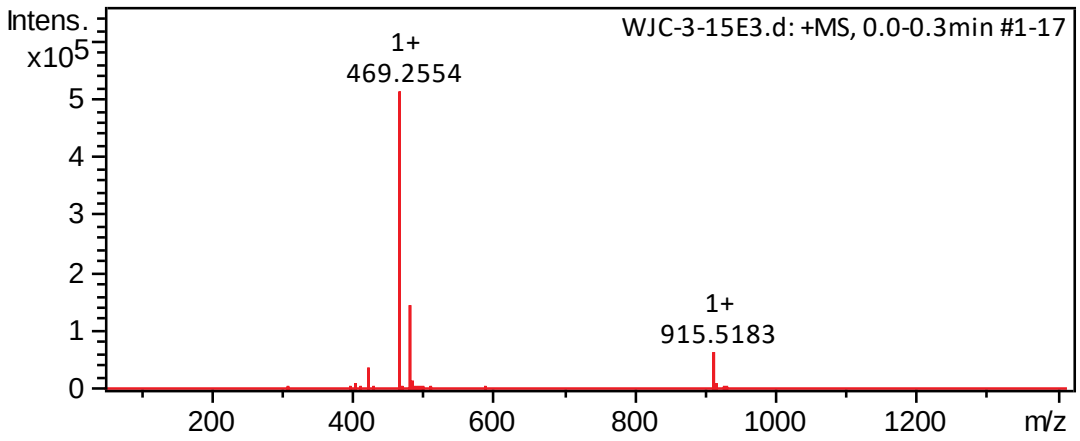

Figure S36. IR spectrum of compound **3**

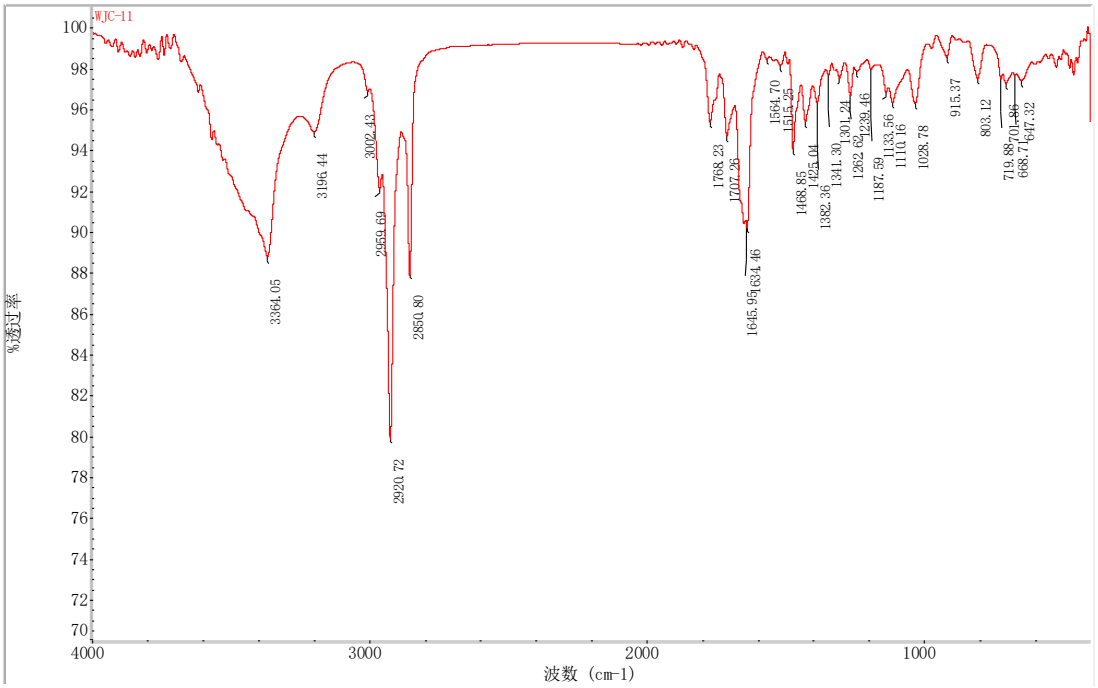

Figure S37. UV spectrum of compound **3**

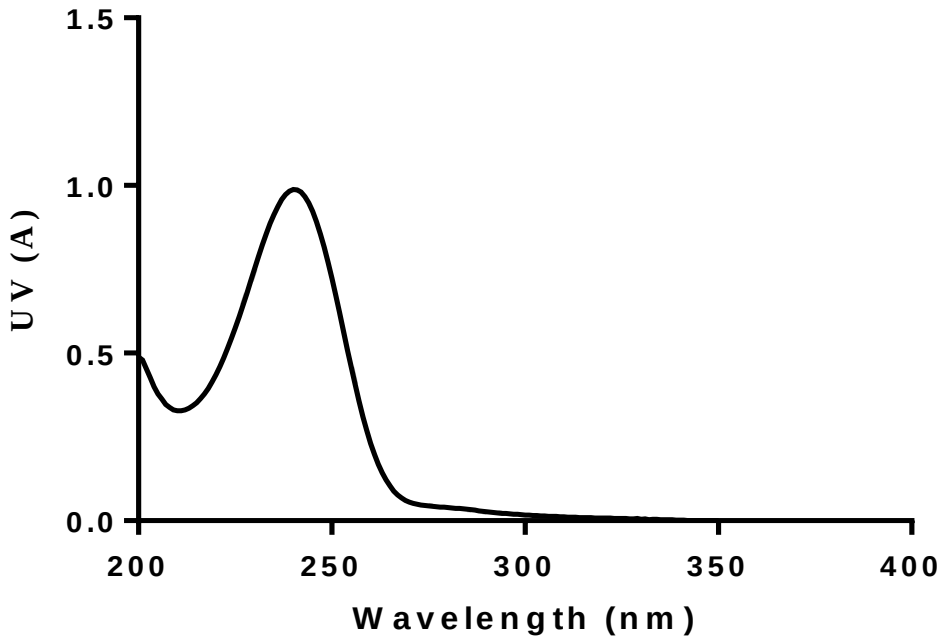

Figure S38. CD spectrum of **3** in methanol

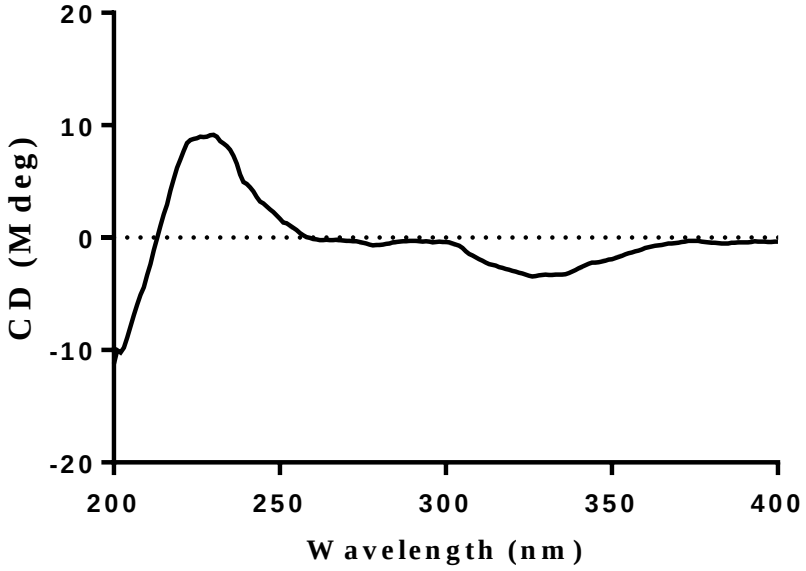

Figure S39. ^{1}H NMR spectrum of compound **4** (recorded in chloroform-*d*)

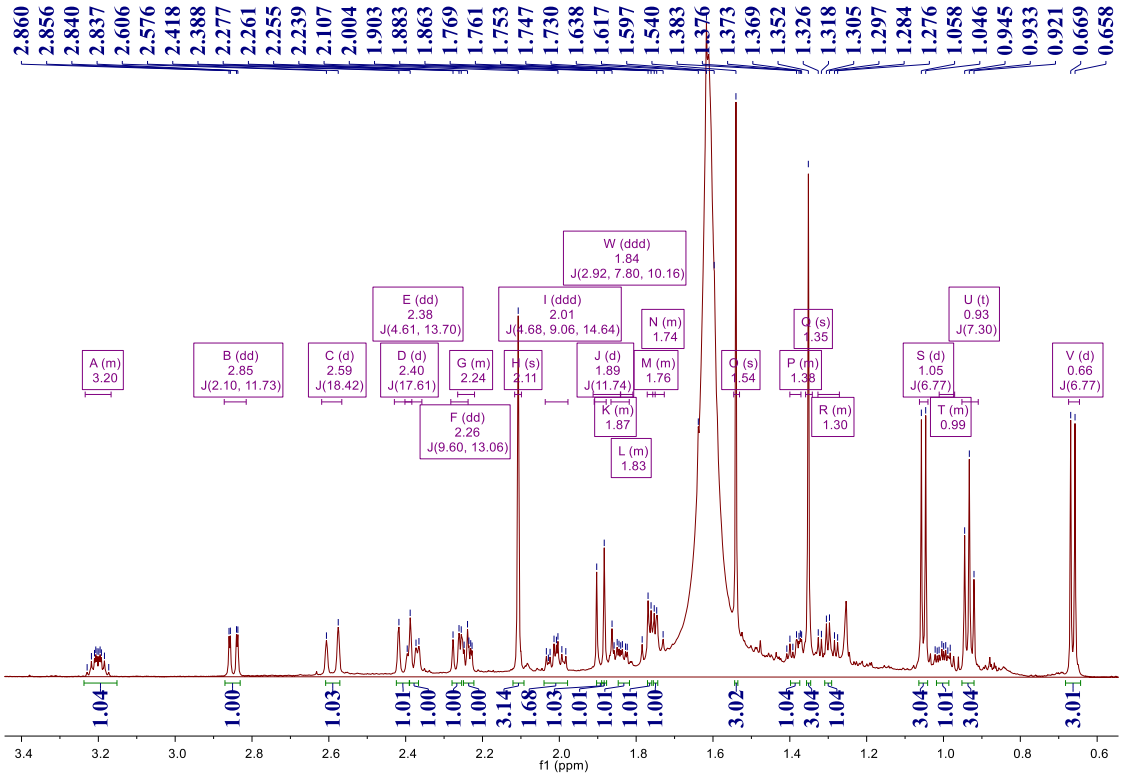

Figure S40. ^{13}C NMR spectrum of compound **4** (recorded in chloroform-*d*)

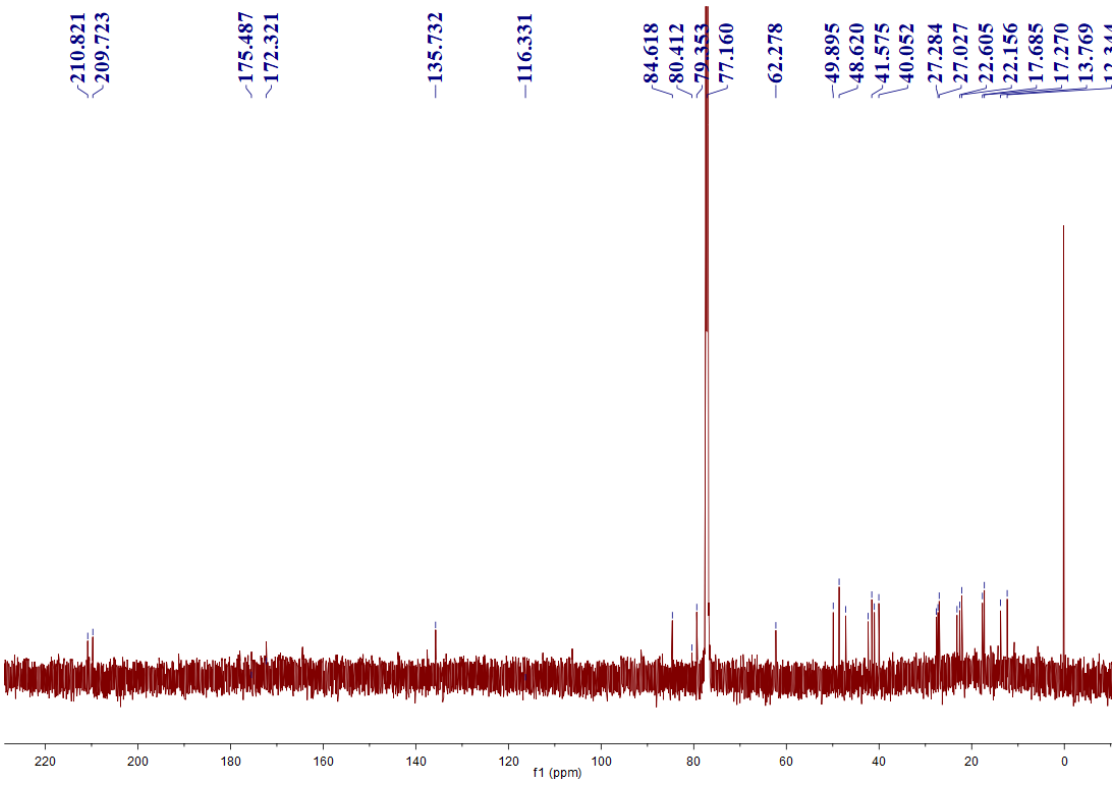

Figure S41. DEPT spectrum of compound **4** (recorded in chloroform-*d*)

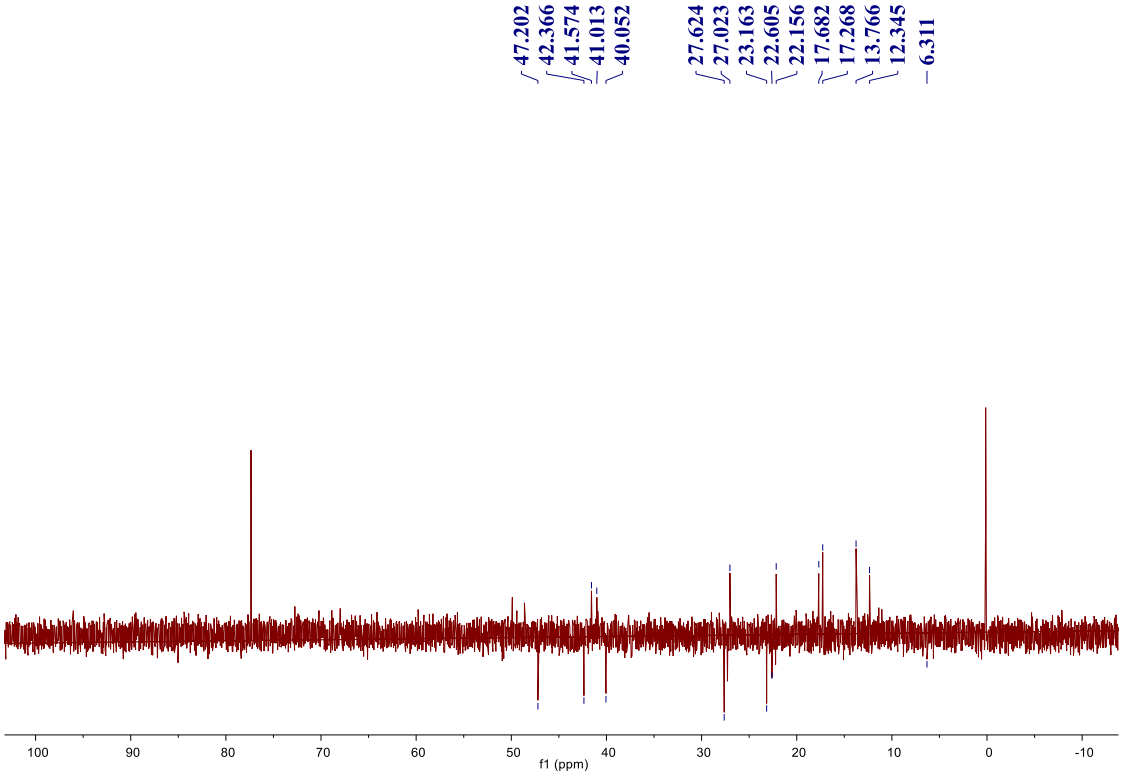

Figure S42. HSQC spectrum of compound **4** (recorded in chloroform-*d*)

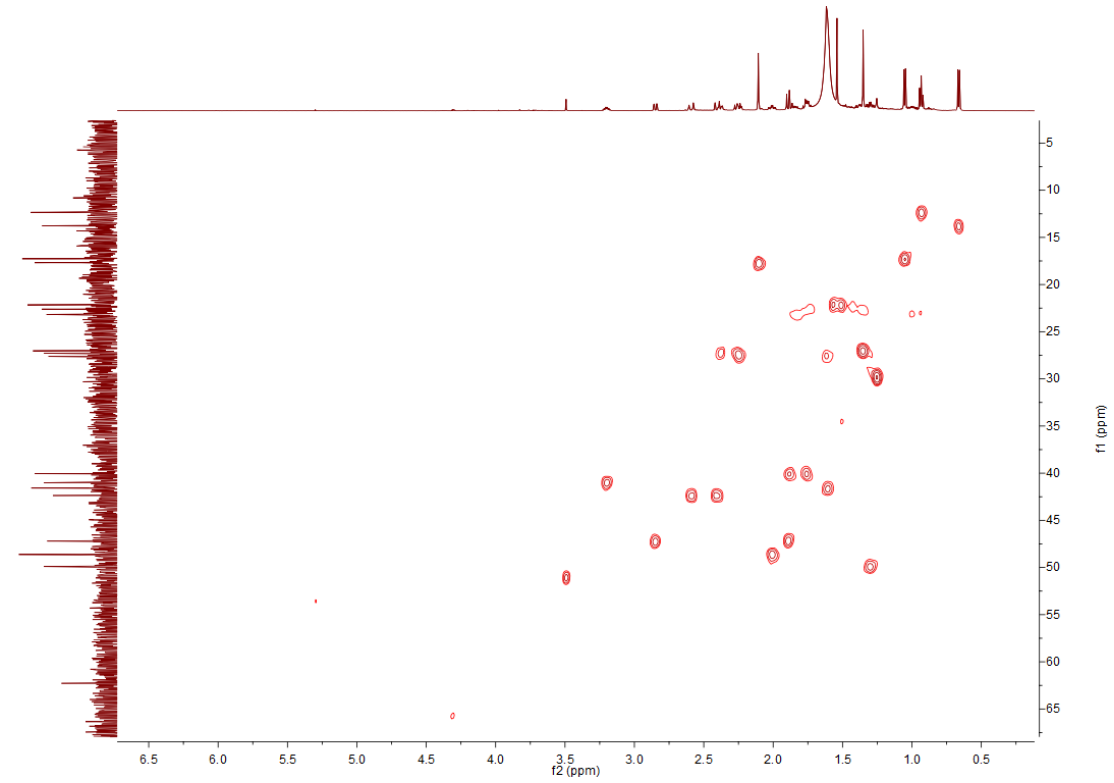

Figure S43. HMBC spectrum of compound **4** (recorded in chloroform-*d*)

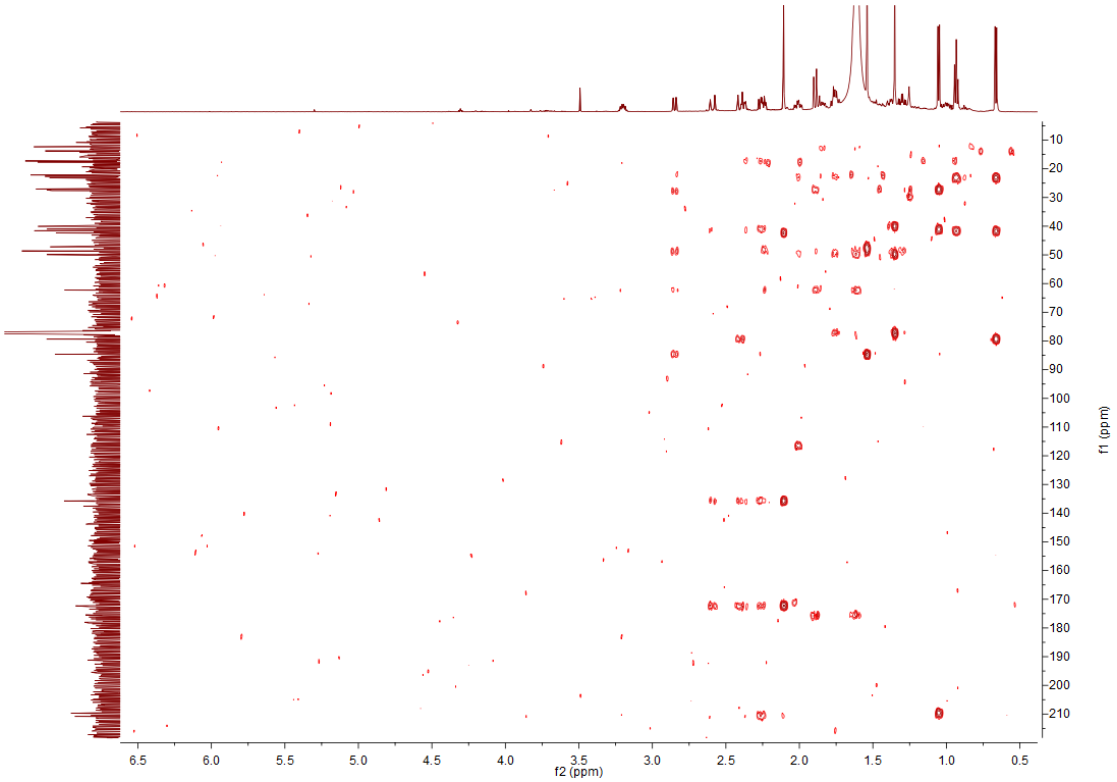

Figure S44. $^{1}H-^{1}H$ COSY spectrum of compound **4** (recorded in chloroform-*d*)

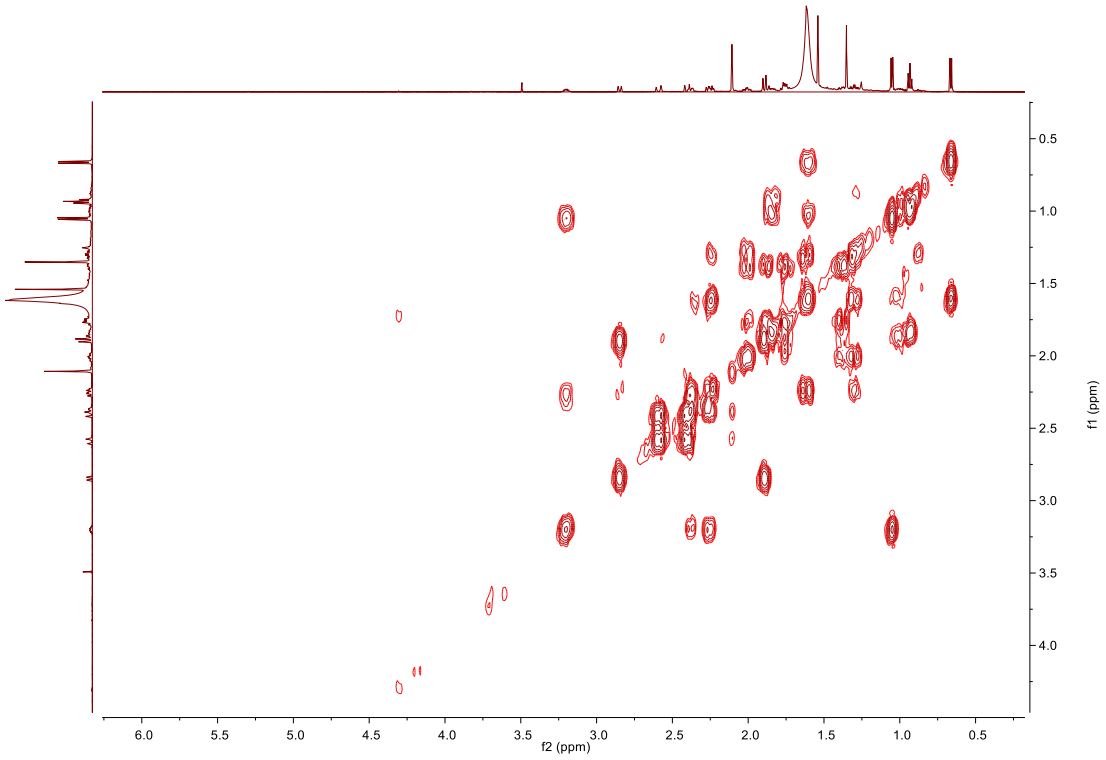

Figure S45. ROESY NMR spectrum of compound **4** (recorded in chloroform-*d*)

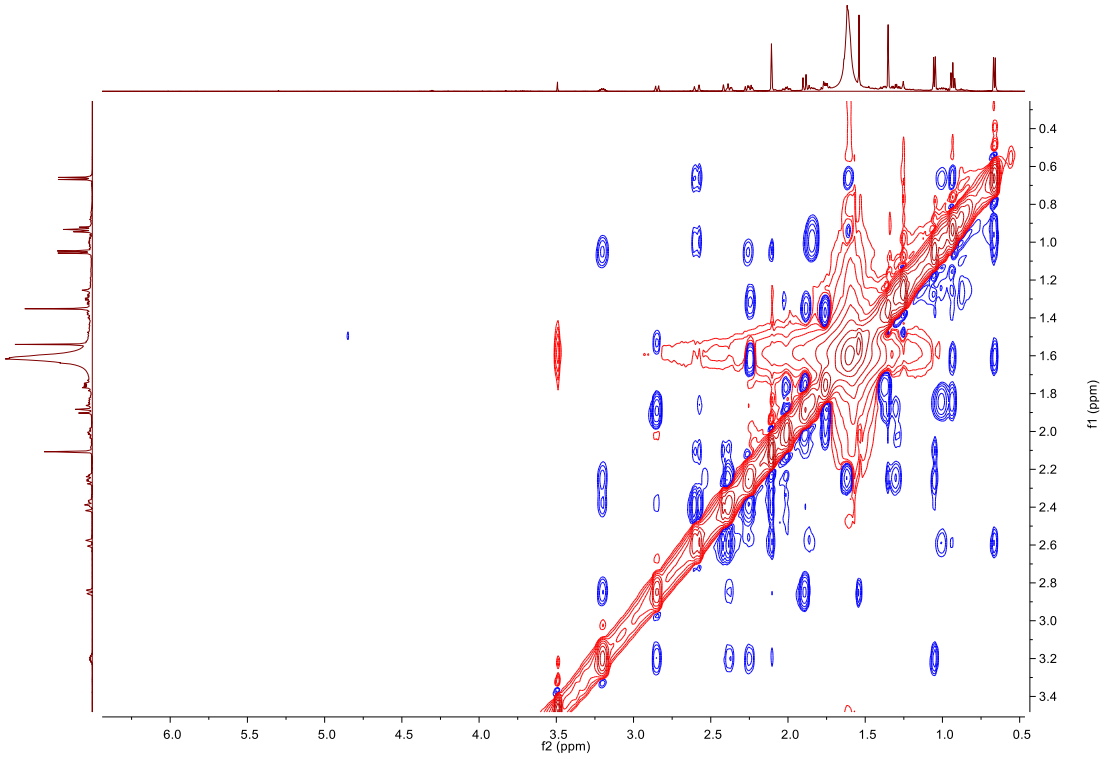

Figure S46. HRESIMS spectrum of compound **4**

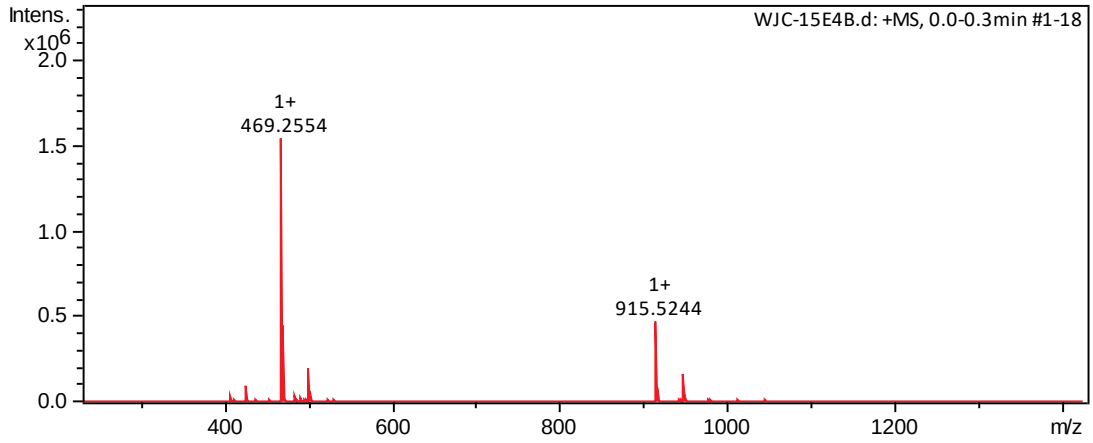

Figure S47. IR spectrum of compound **4**

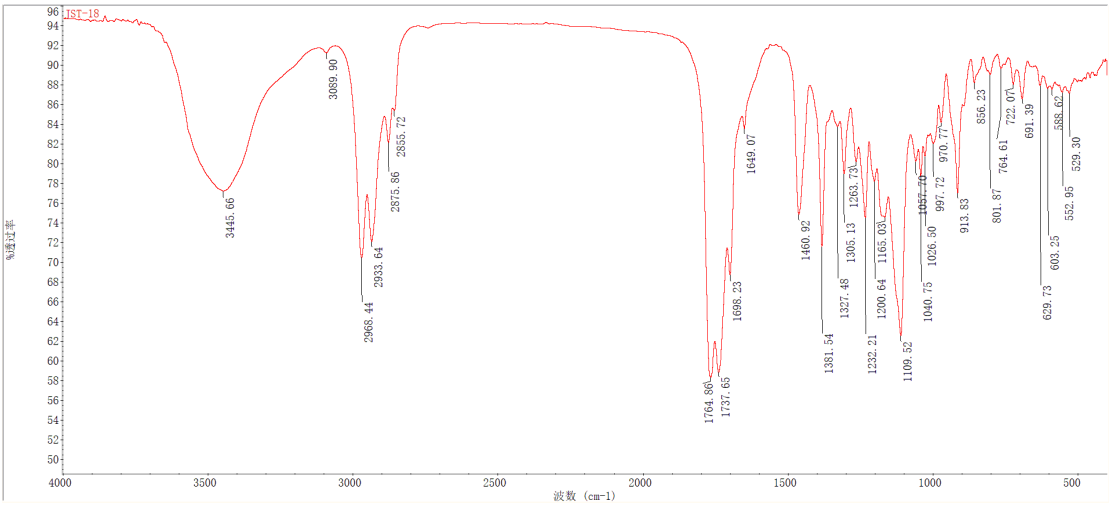

Figure S48. UV spectrum of compound **4**

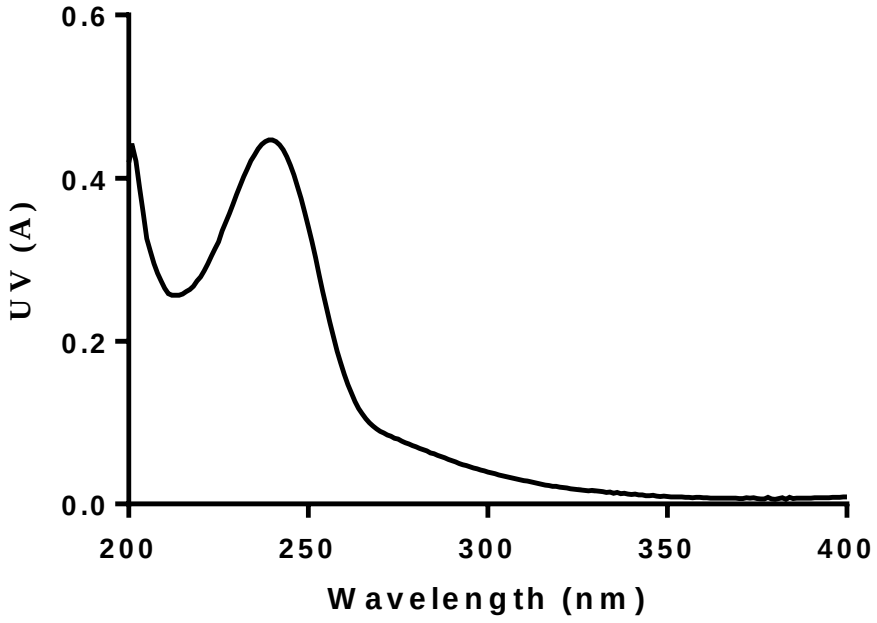

Figure S49. CD spectrum of **4** in methanol

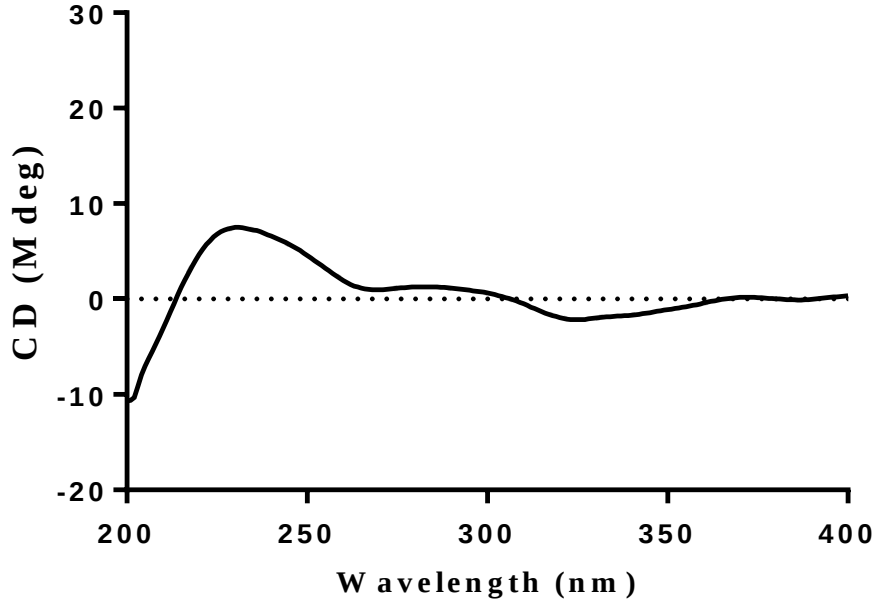

Figure S50. ^{1}H NMR spectrum of compound **5** (recorded in chloroform-*d*)

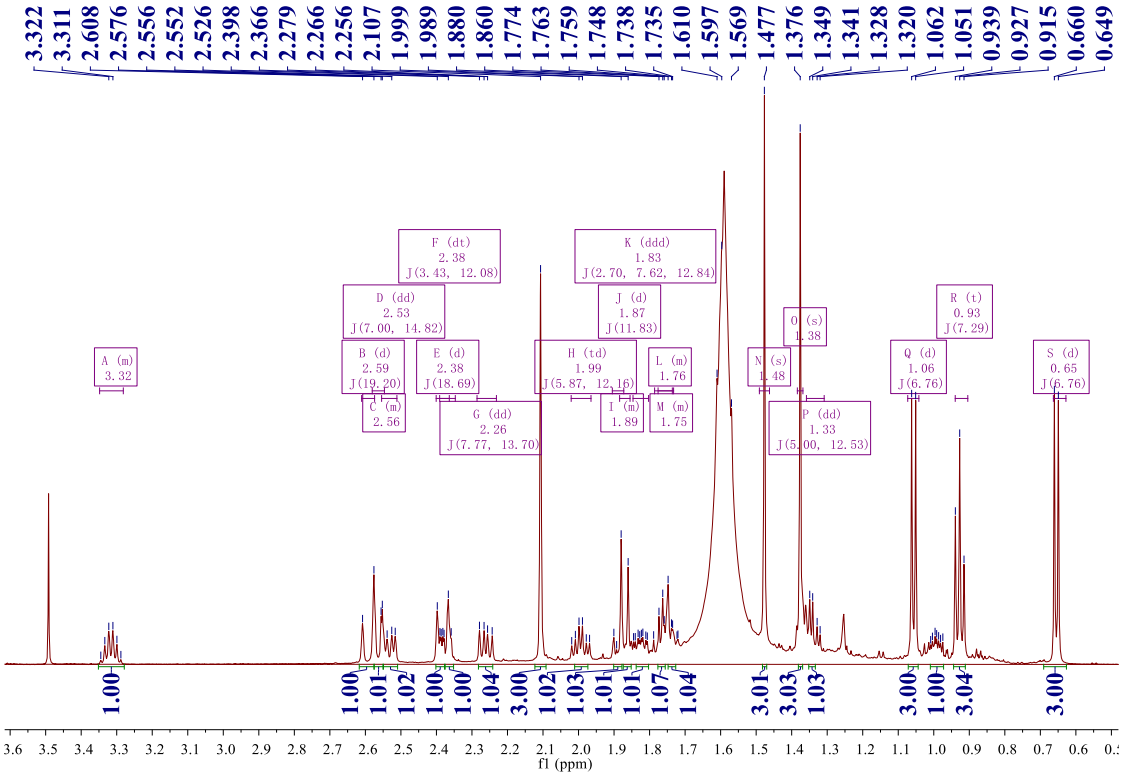

Figure S54. ^{13}C NMR spectrum of compound **5** (recorded in chloroform-*d*)

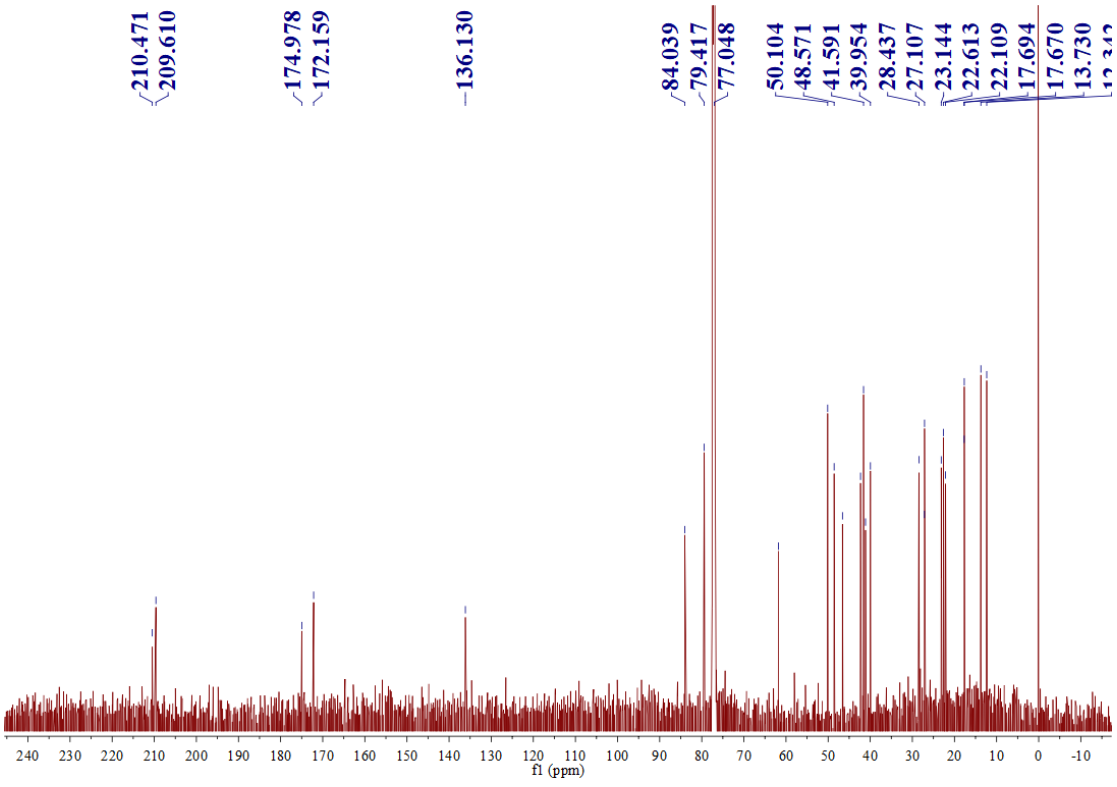

Figure S52. DEPT spectrum of compound **5** (recorded in chloroform-*d*)

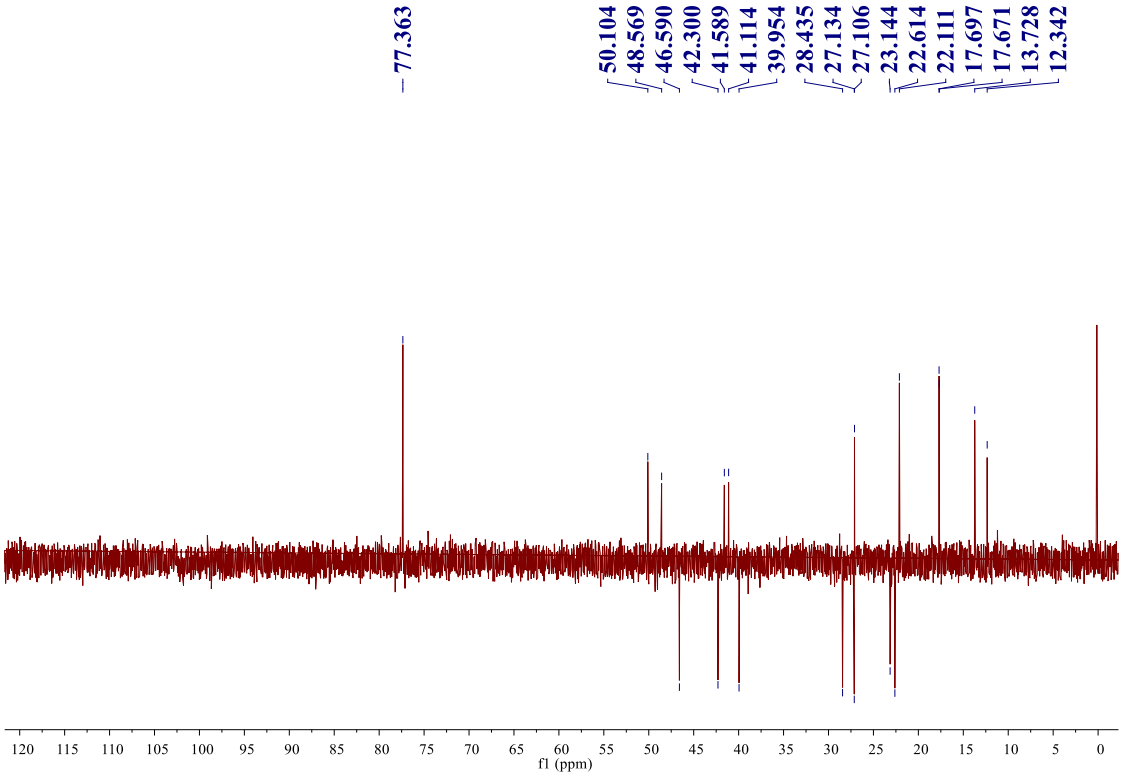

Figure S53. HSQC spectrum of compound **5** (recorded in chloroform-*d*)

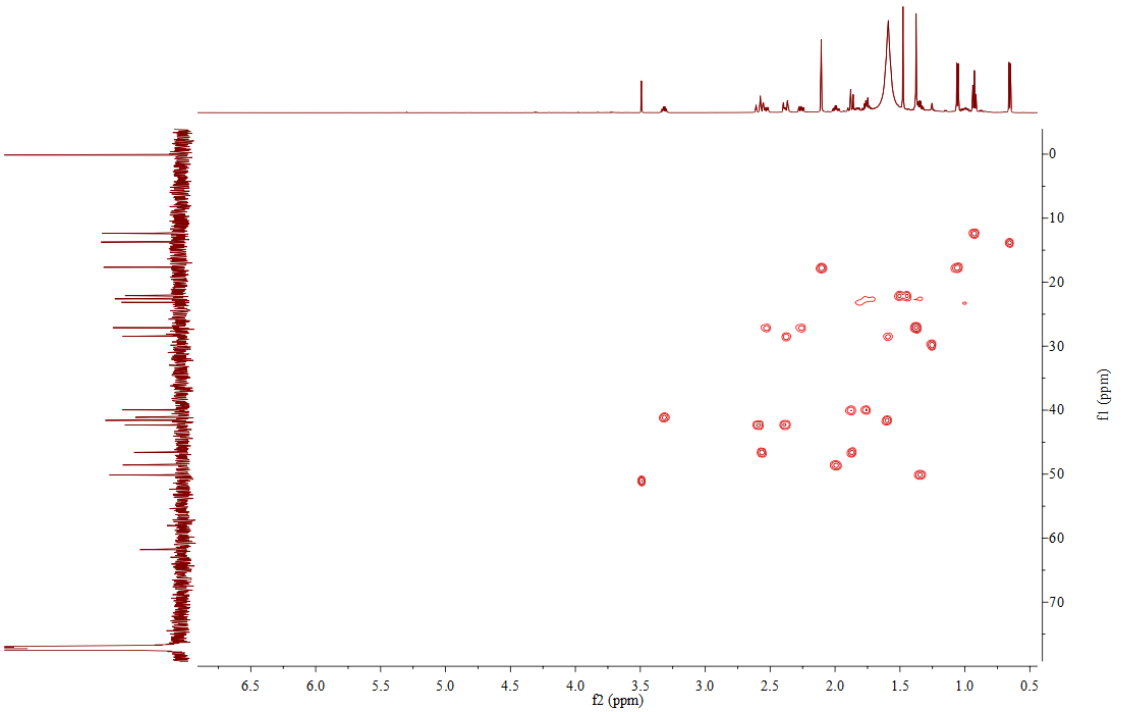

Figure S54. HMBC spectrum of compound **5** (recorded in chloroform-*d*)

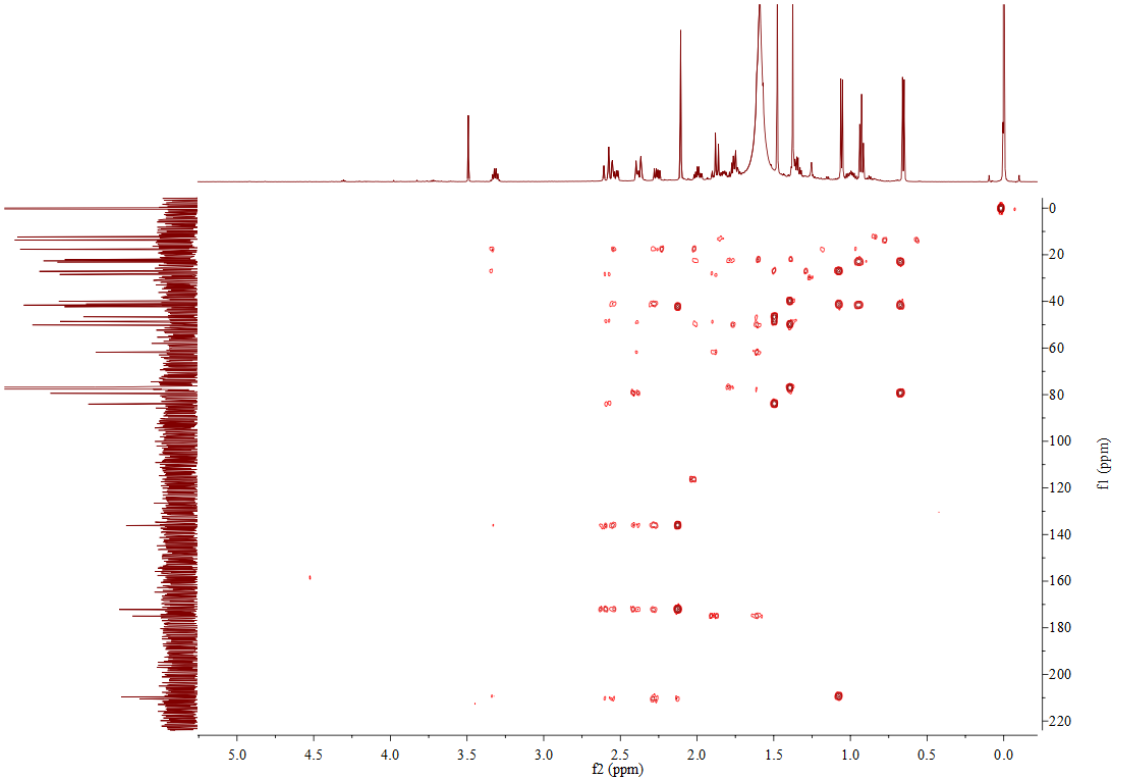

Figure S55. $^{1}H-^{1}H$ COSY spectrum of compound **5** (recorded in chloroform-*d*)

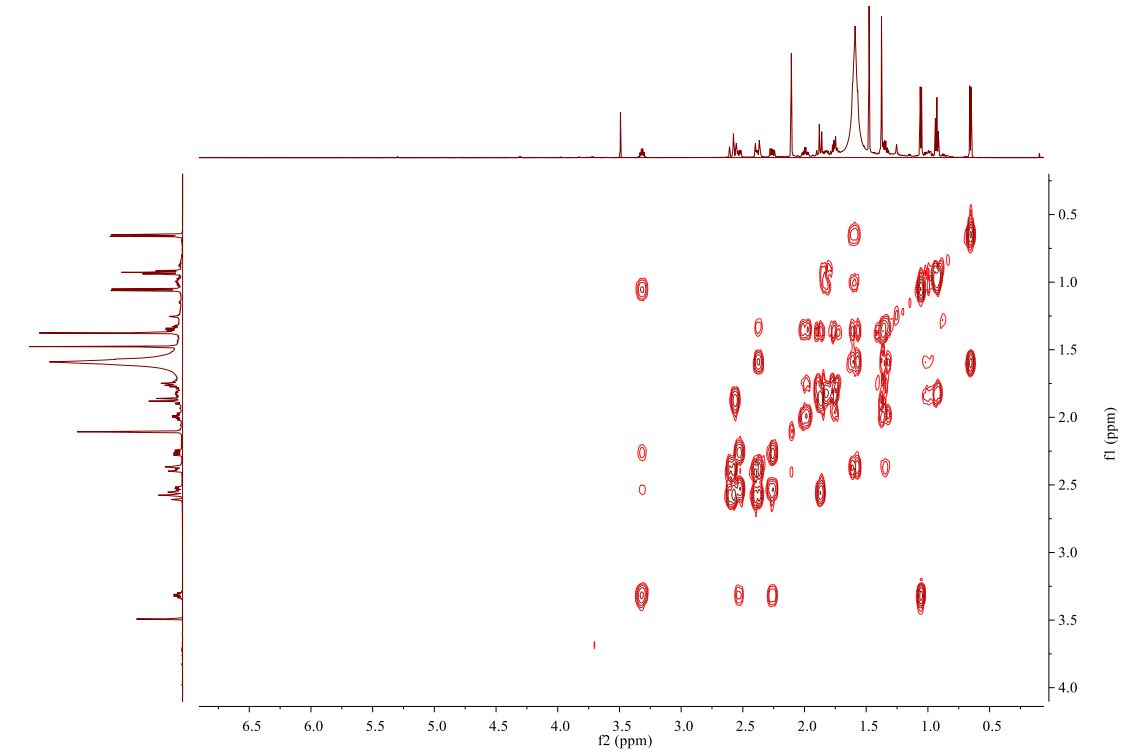

Figure S56. ROESY spectrum of compound **5** (recorded in chloroform-*d*)

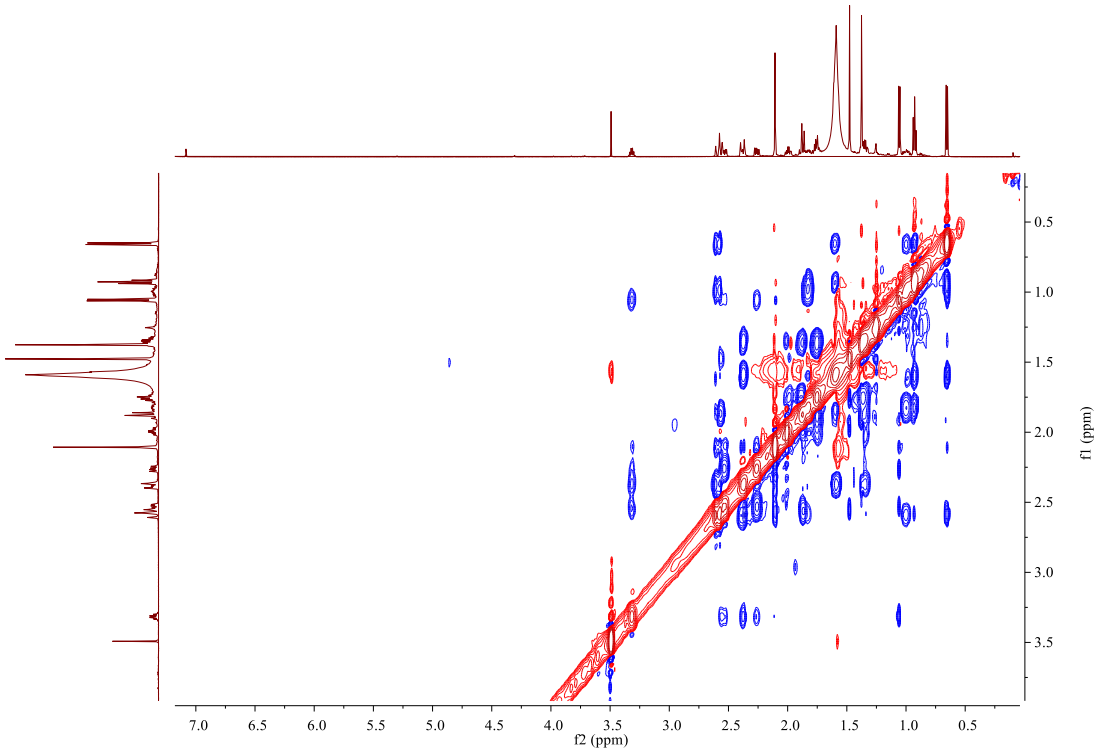

Figure S57. HRESIMS spectrum of compound **5**

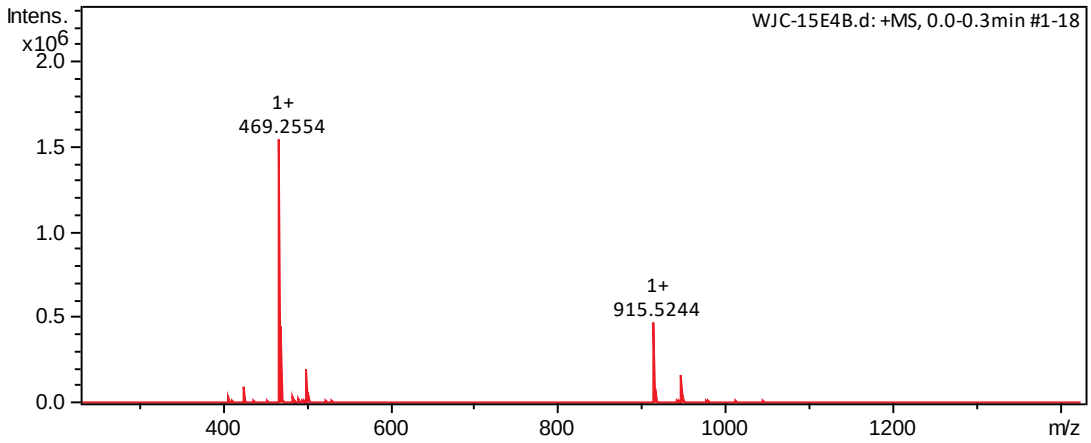

Figure S58. IR spectrum of compound **5**

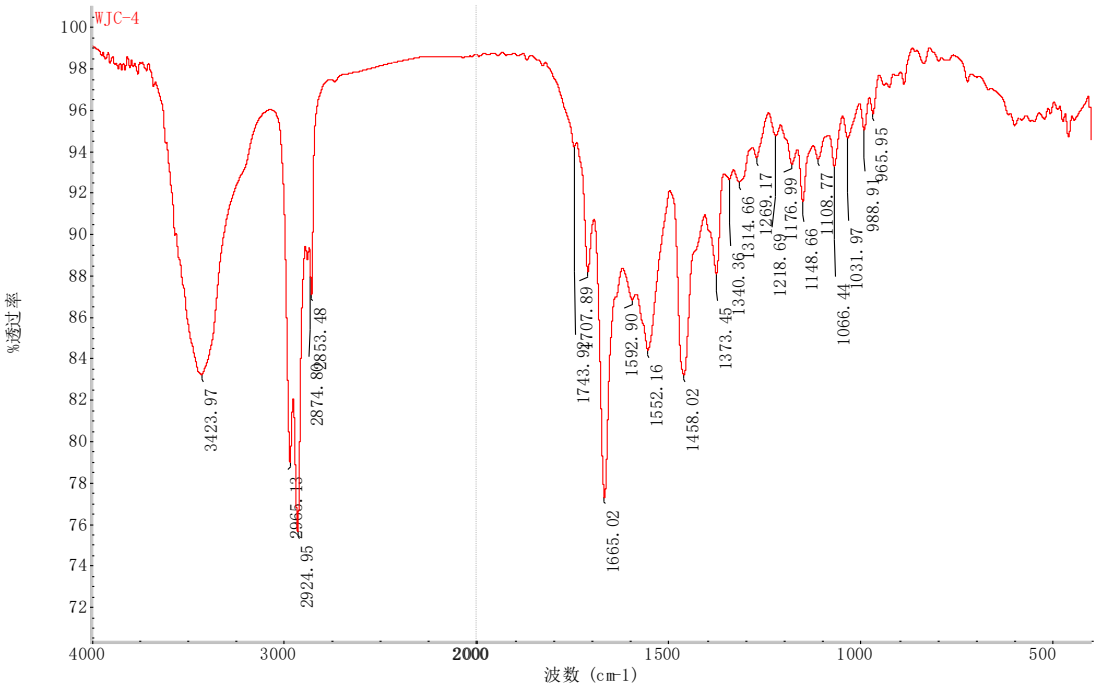

Figure S59. UV spectrum of compound **5**

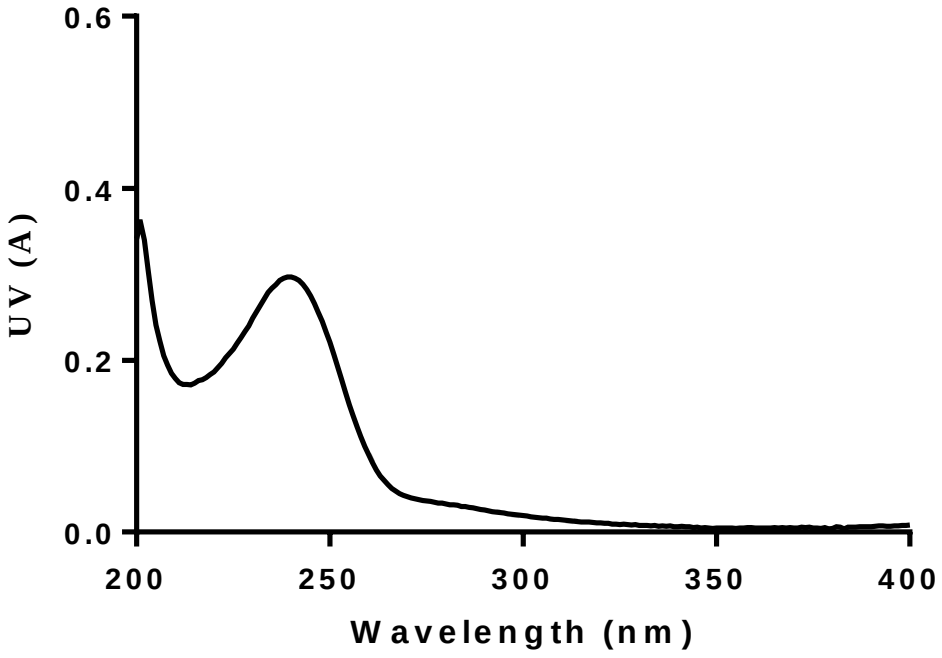

Figure S60. CD spectrum of **5** in methanol

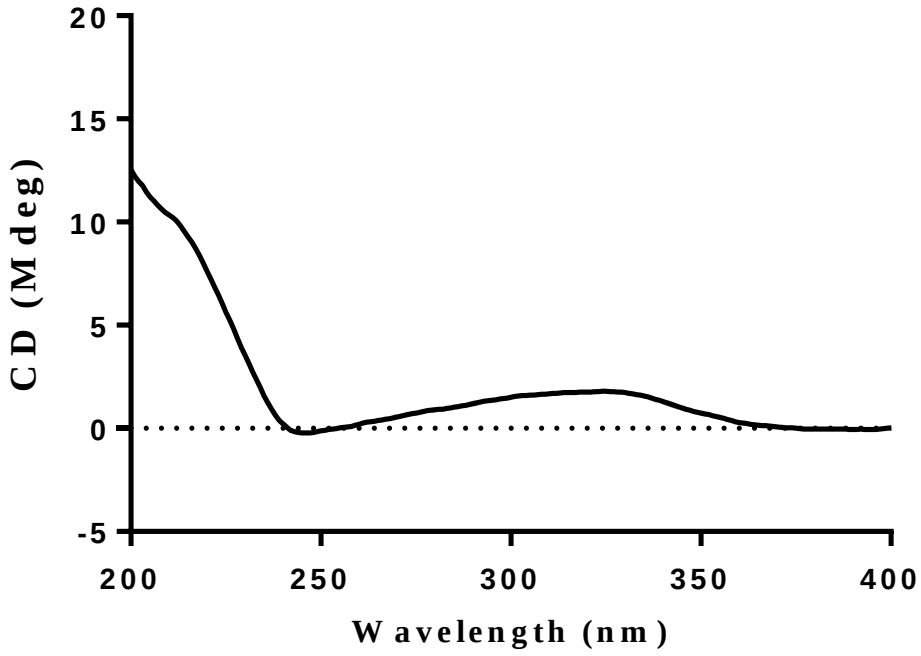

Table S2. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **3**.

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
3-1_en_	0.00672	0.04	-1464.507517
3-2_en_	0.00065	23.7	-1464.513591
3-3_en_	0.00192	6.2	-1464.512325
3-4_en_	0.00669	0.04	-1464.507553
3-5_en_	0.00334	1.37	-1464.510897
3-6_en_	0.00197	5.84	-1464.512268
3-7_en_	0.00321	1.58	-1464.511032
3-8_en_	0.00115	14.02	-1464.513095
3-9_en_	0.0	47.21	-1464.514241

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S3. Cartesian coordinates for the low-energy reoptimized random research conformers of **3** at B3LYP-D3(BJ)/6-31G* level of theory in chloroform.

3-1_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	2.889858	0.289122	-0.580012
1	6	C	0.490693	-1.286606	-1.23694
2	6	C	1.388535	-3.765933	-2.470462
3	8	O	1.593703	-3.402098	-4.992628
4	6	C	0.968739	-0.779353	-5.642769
5	6	C	3.346372	0.848401	-5.34822
6	6	C	4.679167	0.298294	-2.836561
7	6	C	-0.857605	-0.048528	-3.502561
8	6	C	5.54155	0.693409	-7.224661
9	6	C	7.77297	1.911606	-5.74915
10	6	C	6.94278	2.12872	-2.935139
11	6	C	-1.150452	-1.650614	1.111999
12	6	C	-2.981593	-3.875549	1.309984
13	8	O	-0.859882	-0.240597	2.901585
14	6	C	-0.167389	-0.767926	-8.266873
15	8	O	1.920734	-5.723137	-1.453313
16	1	H	5.508406	-1.610433	-2.993071
17	6	C	9.033592	1.507394	-1.052306
18	8	O	6.116245	4.678743	-2.587655
19	1	H	2.702862	2.828373	-5.282803
20	6	C	-4.702304	-3.541068	3.624841
21	6	C	-4.437938	-4.662126	-1.070322
22	6	C	-6.469183	-1.300707	3.614502
23	6	C	-8.434173	-0.921097	5.229478
24	6	C	-9.814715	1.53058	4.741516
25	6	C	-8.029373	3.003881	2.977933
26	6	C	-6.430594	0.859193	1.858613
27	6	C	-9.281568	-2.638496	7.295499
28	8	O	-5.481509	1.023093	-0.23986
29	6	C	-6.333555	4.854739	4.544556
30	8	O	-9.325319	4.263768	1.022259
31	6	C	-3.802666	5.583406	3.290876
32	6	C	-7.876781	7.186216	5.294734
33	6	C	-3.940007	6.943007	0.741118
34	1	H	3.793715	-0.50943	1.112277
35	1	H	2.257232	2.210581	-0.099761
36	1	H	-2.735405	-0.856801	-3.819167

37	1	H	-1.077857	1.999869	-3.275659
38	1	H	5.946099	-1.301467	-7.661719
39	1	H	5.15333	1.665916	-9.019189
40	1	H	8.205249	3.824362	-6.431154
41	1	H	9.507009	0.779823	-5.919157
42	1	H	-1.677928	-5.452043	1.744868
43	1	H	1.192437	-1.486536	-9.66391
44	1	H	-1.873064	-1.954708	-8.331077
45	1	H	-0.688019	1.175131	-8.796492
46	1	H	8.349239	1.701753	0.907718
47	1	H	9.709925	-0.445103	-1.291554
48	1	H	10.63875	2.806106	-1.304013
49	1	H	5.62731	4.87962	-0.839163
50	1	H	-5.802589	-5.292068	3.869187
51	1	H	-3.491316	-3.364901	5.3078
52	1	H	-3.184228	-5.074886	-2.670865
53	1	H	-5.785787	-3.195463	-1.646144
54	1	H	-5.492872	-6.411221	-0.676166
55	1	H	-11.611393	1.179815	3.7452
56	1	H	-10.276172	2.524929	6.510772
57	1	H	-11.307584	-3.087546	7.091304
58	1	H	-8.208295	-4.412389	7.369589
59	1	H	-9.081324	-1.678834	9.138261
60	1	H	-5.825298	3.816569	6.281441
61	1	H	-8.306328	4.026522	-0.485305
62	1	H	-2.802623	6.811536	4.650131
63	1	H	-2.616643	3.885407	3.100567
64	1	H	-6.72083	8.485753	6.437414
65	1	H	-9.555398	6.679837	6.414846
66	1	H	-8.546807	8.198574	3.611085
67	1	H	-5.177243	8.61471	0.800472
68	1	H	-2.044838	7.59385	0.172852
69	1	H	-4.623564	5.679514	-0.759222

3-2_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	1.490204	0.227054	-0.027526
1	6	C	1.590495	2.309207	-2.124549
2	6	C	0.170287	1.292069	-4.468718
3	8	O	1.830635	0.040334	-5.940621
4	6	C	4.345964	0.020626	-4.761913
5	6	C	4.482337	-2.210081	-2.910393
6	6	C	2.126634	-2.308362	-1.225232
7	6	C	4.27297	2.464988	-3.192547
8	6	C	4.648586	-4.946547	-3.843185
9	6	C	3.762258	-6.523564	-1.520195
10	6	C	2.636104	-4.618281	0.441409
11	6	C	0.520521	4.7957	-1.134586
12	6	C	-2.258634	4.803344	-0.380572
13	8	O	1.843722	6.651037	-0.916297
14	6	C	6.294935	-0.051346	-6.852047
15	8	O	-2.036071	1.474216	-4.987056
16	1	H	0.52535	-2.862636	-2.443332
17	6	C	0.303984	-5.595373	1.823332
18	8	O	4.521107	-3.855631	2.21785
19	1	H	6.115974	-1.849629	-1.671474
20	6	C	-2.566542	5.162901	2.522744
21	6	C	-3.686265	6.822211	-1.880198
22	6	C	-4.935667	3.862888	3.343424
23	6	C	-7.329245	4.716744	3.6886
24	6	C	-9.145092	2.585856	4.297911
25	6	C	-7.662491	0.160727	3.640078
26	6	C	-4.939171	1.120226	3.802118
27	6	C	-8.23929	7.378472	3.545271
28	8	O	-3.137984	-0.230276	4.302772
29	6	C	-8.215686	-0.730633	0.868939
30	8	O	-8.052051	-1.817547	5.375925
31	6	C	-6.35945	-2.79389	-0.013746
32	6	C	-10.95299	-1.65112	0.655093
33	6	C	-6.35158	-3.238195	-2.869287
34	1	H	-0.366071	0.163614	0.888981
35	1	H	2.886324	0.704677	1.435956
36	1	H	4.484088	4.141583	-4.402825
37	1	H	5.734958	2.527006	-1.723853
38	1	H	3.348103	-5.216094	-5.44585
39	1	H	6.552755	-5.473749	-4.485674

40	1	H	5.341678	-7.544891	-0.633707
41	1	H	2.344976	-7.941447	-2.070487
42	1	H	-3.052546	2.958051	-0.890606
43	1	H	6.101197	1.603715	-8.094788
44	1	H	8.20509	-0.045814	-6.028093
45	1	H	6.081965	-1.76941	-8.001154
46	1	H	-1.193102	-6.124411	0.47986
47	1	H	0.770144	-7.291081	2.945289
48	1	H	-0.45292	-4.142707	3.102733
49	1	H	4.829695	-5.252286	3.351215
50	1	H	-0.9711	4.283829	3.528368
51	1	H	-2.547906	7.186991	2.992454
52	1	H	-5.685282	6.869205	-1.308919
53	1	H	-3.617044	6.402807	-3.913945
54	1	H	-2.847119	8.696207	-1.549851
55	1	H	-9.607576	2.556034	6.329827
56	1	H	-10.937674	2.797069	3.266438
57	1	H	-9.669561	7.568469	2.038026
58	1	H	-9.187638	7.92229	5.321355
59	1	H	-6.708077	8.727009	3.167869
60	1	H	-7.950881	0.937132	-0.359898
61	1	H	-6.407998	-2.600267	5.613082
62	1	H	-4.427281	-2.302841	0.564815
63	1	H	-6.814539	-4.563999	0.992456
64	1	H	-11.284331	-3.17922	2.025492
65	1	H	-11.347181	-2.37826	-1.250972
66	1	H	-12.330788	-0.141416	1.034259
67	1	H	-5.739837	-1.53162	-3.892073
68	1	H	-5.020004	-4.759909	-3.367735
69	1	H	-8.220873	-3.797882	-3.592816

3-3_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	2.618385	-0.923202	-0.300467
1	6	C	0.665493	0.209711	-2.197357
2	6	C	0.879793	-1.317014	-4.684724
3	8	O	2.64355	-0.206328	-6.166682
4	6	C	3.744054	1.985801	-4.88379
5	6	C	5.92755	1.075515	-3.197664
6	6	C	5.146349	-1.242486	-1.643611
7	6	C	1.579548	2.791124	-3.124355
8	6	C	8.45561	0.2074	-4.305815
9	6	C	9.668359	-1.337867	-2.116834
10	6	C	7.549349	-1.847122	-0.115677
11	6	C	-2.063309	0.20769	-1.24379
12	6	C	-3.143423	-2.237724	-0.1823
13	8	O	-3.310254	2.13034	-1.354022
14	6	C	4.491869	3.89546	-6.875643
15	8	O	-0.24055	-3.194793	-5.27847
16	1	H	4.947608	-2.810903	-3.003852
17	6	C	7.588787	-4.511615	0.959542
18	8	O	7.777771	-0.20751	2.015442
19	1	H	6.295627	2.66039	-1.884245
20	6	C	-3.135881	-2.121837	2.763517
21	6	C	-5.773256	-2.721896	-1.28662
22	6	C	-4.716556	-0.035842	3.823906
23	6	C	-4.042892	2.324365	4.55851
24	6	C	-6.280873	3.838177	5.490479
25	6	C	-8.603037	2.32063	4.592178
26	6	C	-7.447852	-0.321758	4.253578
27	6	C	-1.473466	3.475445	4.493724
28	8	O	-8.658754	-2.271026	4.436686
29	6	C	-9.589482	3.332306	1.995024
30	8	O	-10.560964	2.225675	6.393265
31	6	C	-11.59426	1.570166	0.832137
32	6	C	-10.654675	6.008295	2.309974
33	6	C	-12.107004	2.079992	-1.965322
34	1	H	1.957634	-2.750197	0.431956
35	1	H	2.830244	0.371227	1.313967
36	1	H	0.068584	3.749581	-4.17723
37	1	H	2.201934	4.044247	-1.590848
38	1	H	8.096305	-1.010461	-5.954407
39	1	H	9.658119	1.77856	-4.940385

40	1	H	11.217951	-0.306091	-1.189376
41	1	H	10.476371	-3.122282	-2.810245
42	1	H	-1.895348	-3.799713	-0.744137
43	1	H	2.833272	4.474515	-7.985883
44	1	H	5.304127	5.581244	-5.966664
45	1	H	5.908437	3.101496	-8.171978
46	1	H	6.071202	-4.74591	2.362307
47	1	H	7.329372	-5.922327	-0.54491
48	1	H	9.399631	-4.871358	1.915912
49	1	H	8.045251	1.496918	1.423583
50	1	H	-3.897654	-3.93301	3.451977
51	1	H	-1.178415	-1.977329	3.447607
52	1	H	-5.631142	-3.044954	-3.334675
53	1	H	-7.022918	-1.097126	-0.972964
54	1	H	-6.641792	-4.389338	-0.403401
55	1	H	-6.300426	3.924236	7.57312
56	1	H	-6.216563	5.795734	4.795703
57	1	H	-1.442043	5.003844	3.074716
58	1	H	-0.994823	4.338766	6.328975
59	1	H	0.007403	2.109146	3.996266
60	1	H	-7.944143	3.388174	0.71196
61	1	H	-11.201582	0.504959	6.327367
62	1	H	-11.009473	-0.412145	1.045456
63	1	H	-13.358699	1.756906	1.928169
64	1	H	-9.204928	7.383568	2.881869
65	1	H	-12.143669	6.003244	3.761695
66	1	H	-11.475818	6.696884	0.529457
67	1	H	-12.826636	4.003578	-2.300649
68	1	H	-10.368409	1.858483	-3.092932
69	1	H	-13.519635	0.750107	-2.719126

3-4_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	2.683929	-0.972336	-0.654026
1	6	C	0.868966	0.242959	-2.6362
2	6	C	1.067731	-1.344419	-5.086568
3	8	O	2.942626	-0.377166	-6.527276
4	6	C	4.144094	1.767626	-5.242229
5	6	C	6.206112	0.760571	-3.46762
6	6	C	5.228089	-1.47966	-1.910098
7	6	C	1.97593	2.743299	-3.576892
8	6	C	8.708619	-0.277329	-4.486187
9	6	C	9.724405	-1.928146	-2.272519
10	6	C	7.535013	-2.178715	-0.305442
11	6	C	-1.882638	0.433435	-1.765461
12	6	C	-3.155957	-1.920477	-0.710237
13	8	O	-2.997703	2.431491	-1.934832
14	6	C	5.078794	3.580598	-7.245799
15	8	O	-0.147882	-3.163096	-5.682143
16	1	H	4.976644	-3.071504	-3.233931
17	6	C	7.372587	-4.77995	0.922936
18	8	O	7.72615	-0.269197	1.595232
19	1	H	6.639968	2.300383	-2.135592
20	6	C	-3.208255	-1.792446	2.233377
21	6	C	-5.787161	-2.22596	-1.873356
22	6	C	-4.706965	0.360172	3.285418
23	6	C	-3.937086	2.705489	3.956903
24	6	C	-6.088156	4.300178	4.932626
25	6	C	-8.516987	2.777827	4.32573
26	6	C	-7.445711	0.112757	3.761765
27	6	C	-1.336563	3.778778	3.80392
28	8	O	-8.6634	-1.828256	3.717753
29	6	C	-9.829774	3.843512	1.907905
30	8	O	-10.175688	2.58475	6.404454
31	6	C	-11.749496	2.043808	0.648271
32	6	C	-11.020959	6.438748	2.433012
33	6	C	-13.979512	1.181571	2.274133
34	1	H	1.8808	-2.738594	0.086009
35	1	H	2.926824	0.343071	0.937167
36	1	H	0.563464	3.770042	-4.700386
37	1	H	2.624912	3.984344	-2.045485
38	1	H	8.346615	-1.454229	-6.164277
39	1	H	10.042227	1.214732	-5.042966

40	1	H	11.36826	-1.05296	-1.346144
41	1	H	10.328573	-3.800218	-2.944957
42	1	H	-2.00767	-3.569895	-1.234196
43	1	H	6.475521	2.661093	-8.479191
44	1	H	3.498453	4.247573	-8.419406
45	1	H	5.979574	5.223862	-6.342713
46	1	H	5.803888	-4.838239	2.28713
47	1	H	7.072548	-6.269771	-0.497204
48	1	H	9.132828	-5.225366	1.947869
49	1	H	9.207127	-0.61586	2.604216
50	1	H	-4.076985	-3.561619	2.902956
51	1	H	-1.261066	-1.744347	2.960398
52	1	H	-6.812961	-3.785966	-0.964541
53	1	H	-5.619969	-2.616947	-3.90788
54	1	H	-6.900345	-0.491376	-1.635767
55	1	H	-5.94389	4.539259	6.998603
56	1	H	-6.048269	6.205287	4.092081
57	1	H	-0.800368	4.685296	5.602536
58	1	H	0.093979	2.353461	3.328241
59	1	H	-1.279607	5.254869	2.332396
60	1	H	-8.289146	4.132182	0.531377
61	1	H	-11.339664	3.98658	6.350371
62	1	H	-12.460299	3.017321	-1.056036
63	1	H	-10.748313	0.358325	-0.039101
64	1	H	-11.792543	7.239938	0.675686
65	1	H	-9.650587	7.80227	3.1982
66	1	H	-12.615294	6.324246	3.771557
67	1	H	-15.271114	-0.001416	1.148852
68	1	H	-13.314072	0.066014	3.890707
69	1	H	-15.097599	2.78597	2.994909

3-5_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	2.575946	-1.172589	-0.671181
1	6	C	0.843194	0.208456	-2.618383
2	6	C	0.99871	-1.286031	-5.130802
3	8	O	2.935837	-0.354215	-6.504451
4	6	C	4.217755	1.683116	-5.12146
5	6	C	6.207676	0.514792	-3.364717
6	6	C	5.120573	-1.738314	-1.904301
7	6	C	2.075462	2.690649	-3.442505
8	6	C	8.678313	-0.58866	-4.383365
9	6	C	9.63151	-2.260289	-2.163551
10	6	C	7.389309	-2.585042	-0.284026
11	6	C	-1.902099	0.495065	-1.757247
12	6	C	-3.312693	-1.844465	-0.852242
13	8	O	-2.90277	2.5585	-1.807241
14	6	C	5.256195	3.526807	-7.043904
15	8	O	-0.299124	-3.015664	-5.812763
16	1	H	4.818795	-3.269537	-3.288179
17	6	C	7.135903	-5.253409	0.771347
18	8	O	7.814882	-0.829849	1.728501
19	1	H	6.692794	1.980663	-1.966269
20	6	C	-3.410596	-1.870258	2.091056
21	6	C	-5.940707	-1.945046	-2.056584
22	6	C	-4.824755	0.293825	3.232629
23	6	C	-3.957919	2.555969	4.068081
24	6	C	-6.042403	4.186393	5.13486
25	6	C	-8.511426	2.840309	4.37389
26	6	C	-7.561602	0.172158	3.710928
27	6	C	-1.305674	3.501959	4.026553
28	8	O	-8.901878	-1.698829	3.723987
29	6	C	-9.712531	4.143185	2.01147
30	8	O	-10.224819	2.703644	6.41644
31	6	C	-11.629033	2.516807	0.532035
32	6	C	-10.86338	6.688816	2.778764
33	6	C	-13.96014	1.578022	1.965176
34	1	H	1.677954	-2.927013	-0.01512
35	1	H	2.830948	0.082979	0.970747
36	1	H	0.725331	3.828418	-4.534904
37	1	H	2.763671	3.836723	-1.855342
38	1	H	8.284051	-1.749001	-6.066448
39	1	H	10.058947	0.863834	-4.930152

40	1	H	11.191684	-1.360849	-1.130521
41	1	H	10.307272	-4.107101	-2.8334
42	1	H	-2.246315	-3.522186	-1.453204
43	1	H	6.621275	2.590661	-8.299723
44	1	H	3.72063	4.312055	-8.203794
45	1	H	6.223357	5.090064	-6.070367
46	1	H	5.517027	-5.385418	2.080583
47	1	H	6.827335	-6.639141	-0.748331
48	1	H	8.853881	-5.784312	1.8168
49	1	H	6.604022	-1.176484	3.050091
50	1	H	-4.367908	-3.630455	2.656593
51	1	H	-1.476976	-1.953565	2.851832
52	1	H	-5.771538	-2.241593	-4.106498
53	1	H	-6.960372	-0.165434	-1.74184
54	1	H	-7.0608	-3.49333	-1.242339
55	1	H	-5.923956	4.259492	7.214691
56	1	H	-5.898236	6.143986	4.444304
57	1	H	-0.761357	4.272434	5.884605
58	1	H	0.060188	2.036685	3.484731
59	1	H	-1.147609	5.057939	2.647575
60	1	H	-8.12949	4.502033	0.698928
61	1	H	-11.089808	1.096694	6.249962
62	1	H	-12.251924	3.669984	-1.091317
63	1	H	-10.65265	0.87576	-0.292234
64	1	H	-12.346914	6.426643	4.207513
65	1	H	-11.693122	7.640972	1.12502
66	1	H	-9.442631	7.969272	3.595273
67	1	H	-14.931195	3.109222	2.984152
68	1	H	-15.329881	0.741138	0.639455
69	1	H	-13.455255	0.092027	3.326009

3-6_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	3.370624	-1.396929	-0.058965
1	6	C	1.793952	1.00789	-0.719479
2	6	C	-0.058413	0.251536	-2.836328
3	8	O	1.078406	0.648198	-5.091256
4	6	C	3.67277	1.558402	-4.729934
5	6	C	5.428334	-0.72063	-4.370792
6	6	C	4.313979	-2.620869	-2.489516
7	6	C	3.470892	2.897781	-2.163423
8	6	C	6.151716	-2.439451	-6.581884
9	6	C	7.13664	-4.868244	-5.251652
10	6	C	6.368489	-4.685942	-2.417514
11	6	C	0.711289	2.153424	1.716964
12	6	C	-2.067624	2.834134	1.839241
13	8	O	2.142778	2.499154	3.472509
14	6	C	4.335816	3.236132	-6.94821
15	8	O	-2.138283	-0.643317	-2.661117
16	1	H	2.673896	-3.509863	-3.424092
17	6	C	5.475962	-7.181823	-1.28876
18	8	O	8.554469	-3.801499	-1.099601
19	1	H	7.188443	0.016411	-3.534622
20	6	C	-2.931826	3.383297	4.564024
21	6	C	-2.665228	5.043587	0.045243
22	6	C	-5.747486	3.252447	4.699332
23	6	C	-7.533692	5.085659	4.814306
24	6	C	-10.183227	4.000416	4.794542
25	6	C	-9.829059	1.226767	3.9665
26	6	C	-7.044201	0.787991	4.651376
27	6	C	-7.127999	7.869987	4.965616
28	8	O	-6.154652	-1.278422	5.13439
29	6	C	-10.182774	0.897384	1.048645
30	8	O	-11.383836	-0.465195	5.310516
31	6	C	-9.463405	-1.781597	0.154327
32	6	C	-12.908552	1.511763	0.284112
33	6	C	-8.87147	-1.938331	-2.670591
34	1	H	2.18583	-2.711963	1.035611
35	1	H	4.933089	-0.776095	1.163833
36	1	H	2.512723	4.732385	-2.37179
37	1	H	5.304709	3.208863	-1.247636
38	1	H	4.461818	-2.854717	-7.724632
39	1	H	7.571646	-1.594549	-7.840987

40	1	H	9.205682	-5.016327	-5.336805
41	1	H	6.350395	-6.584204	-6.119645
42	1	H	-3.086892	1.162876	1.129044
43	1	H	3.024803	4.845024	-7.070256
44	1	H	6.270707	3.965861	-6.724703
45	1	H	4.238432	2.172035	-8.729856
46	1	H	6.990371	-8.603512	-1.397517
47	1	H	4.955965	-6.947374	0.71702
48	1	H	3.805195	-7.909259	-2.291208
49	1	H	8.164453	-3.762319	0.684436
50	1	H	-2.133712	1.932126	5.820565
51	1	H	-2.189932	5.217495	5.201324
52	1	H	-2.216168	4.610245	-1.935295
53	1	H	-1.6174	6.755028	0.602119
54	1	H	-4.69684	5.475673	0.124288
55	1	H	-11.008737	4.023095	6.708289
56	1	H	-11.449952	5.105227	3.57167
57	1	H	-5.117801	8.383285	5.022956
58	1	H	-8.002819	8.814681	3.323325
59	1	H	-8.06316	8.655741	6.656062
60	1	H	-8.888114	2.255012	0.127796
61	1	H	-10.355489	-1.960664	5.591429
62	1	H	-7.811271	-2.472273	1.207564
63	1	H	-11.029824	-3.070931	0.638225
64	1	H	-13.394852	3.513901	0.561763
65	1	H	-14.221537	0.364932	1.4186
66	1	H	-13.227954	1.075407	-1.722883
67	1	H	-8.562105	-3.912489	-3.25292
68	1	H	-10.417947	-1.181992	-3.84259
69	1	H	-7.132549	-0.890435	-3.129449

3-7_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	2.447321	-1.154486	-0.595226
1	6	C	0.578088	0.007606	-2.558253
2	6	C	0.7293	-1.625683	-4.981816
3	8	O	2.558942	-0.672147	-6.48684
4	6	C	3.776404	1.504813	-5.271525
5	6	C	5.886973	0.54575	-3.528014
6	6	C	4.964105	-1.668915	-1.901959
7	6	C	1.641745	2.49745	-3.573566
8	6	C	8.370697	-0.496519	-4.586025
9	6	C	9.457807	-2.080074	-2.357908
10	6	C	7.31386	-2.318061	-0.338777
11	6	C	-2.149268	0.193703	-1.620741
12	6	C	-3.384177	-2.156658	-0.510233
13	8	O	-3.277873	2.184947	-1.775111
14	6	C	4.651102	3.284715	-7.330898
15	8	O	-0.486708	-3.464709	-5.510923
16	1	H	4.693314	-3.289456	-3.186556
17	6	C	7.204242	-4.899629	0.936291
18	8	O	7.527441	-0.375094	1.525026
19	1	H	6.342664	2.115092	-2.238086
20	6	C	-3.411724	-1.968458	2.428281
21	6	C	-6.023179	-2.51185	-1.638782
22	6	C	-4.911821	0.196148	3.453091
23	6	C	-4.132118	2.538173	4.142794
24	6	C	-6.270901	4.135365	5.153171
25	6	C	-8.688095	2.65304	4.482972
26	6	C	-7.634231	-0.009558	3.977511
27	6	C	-1.525035	3.592811	3.994365
28	8	O	-8.897364	-1.927691	4.134545
29	6	C	-9.931158	3.768042	2.047834
30	8	O	-10.402321	2.567844	6.526401
31	6	C	-11.784772	1.989057	0.66736
32	6	C	-11.177265	6.310793	2.661454
33	6	C	-14.096167	1.06916	2.1436
34	1	H	1.67446	-2.91095	0.199104
35	1	H	2.715746	0.194824	0.963243
36	1	H	0.195164	3.492294	-4.682237
37	1	H	2.316891	3.772156	-2.081792
38	1	H	7.9748	-1.718803	-6.223588
39	1	H	9.6759	0.991423	-5.216274

40	1	H	11.103407	-1.154163	-1.485721
41	1	H	10.082186	-3.956439	-2.999025
42	1	H	-2.223261	-3.803535	-1.012765
43	1	H	6.021221	2.348845	-8.58163
44	1	H	3.038945	3.922827	-8.476931
45	1	H	5.566016	4.948295	-6.481004
46	1	H	5.663048	-4.951733	2.331721
47	1	H	6.893641	-6.416676	-0.452334
48	1	H	8.988875	-5.308079	1.933942
49	1	H	9.033018	-0.690481	2.507557
50	1	H	-4.254652	-3.731362	3.14703
51	1	H	-1.457539	-1.888943	3.13367
52	1	H	-5.874909	-2.940387	-3.666942
53	1	H	-7.149154	-0.78321	-1.421459
54	1	H	-7.023495	-4.067059	-0.692233
55	1	H	-6.136869	4.310666	7.226
56	1	H	-6.215859	6.062238	4.37055
57	1	H	-0.985971	4.501093	5.79056
58	1	H	-0.10205	2.159012	3.519746
59	1	H	-1.462138	5.066508	2.52027
60	1	H	-8.360311	4.103448	0.715177
61	1	H	-11.171237	0.904619	6.471671
62	1	H	-12.431913	3.015042	-1.030181
63	1	H	-10.751676	0.330681	-0.044768
64	1	H	-12.644752	6.081289	4.112303
65	1	H	-12.048775	7.124989	0.956279
66	1	H	-9.804991	7.694067	3.38819
67	1	H	-15.427294	0.106758	0.864204
68	1	H	-13.559175	-0.310567	3.600609
69	1	H	-15.124457	2.629621	3.056411

3-8_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	2.384058	-1.119226	-0.480241
1	6	C	0.455322	0.040408	-2.386661
2	6	C	0.507896	-1.616768	-4.798368
3	8	O	2.288683	-0.690623	-6.377019
4	6	C	3.565585	1.487112	-5.226248
5	6	C	5.729842	0.527714	-3.550463
6	6	C	4.850215	-1.662526	-1.868868
7	6	C	1.501394	2.512392	-3.462205
8	6	C	8.166844	-0.544299	-4.684991
9	6	C	9.321138	-2.11225	-2.479069
10	6	C	7.249572	-2.30879	-0.3816
11	6	C	-2.233856	0.258672	-1.351713
12	6	C	-3.444576	-2.068242	-0.167914
13	8	O	-3.349495	2.259147	-1.485328
14	6	C	4.38132	3.241975	-7.33091
15	8	O	-0.737539	-3.453101	-5.26452
16	1	H	4.525171	-3.295698	-3.124735
17	6	C	7.167821	-4.872477	0.931305
18	8	O	7.542659	-0.342874	1.446918
19	1	H	6.243781	2.106638	-2.294583
20	6	C	-3.330172	-1.8543	2.770042
21	6	C	-6.138293	-2.40288	-1.170019
22	6	C	-4.746138	0.3561	3.810941
23	6	C	-3.905461	2.68724	4.461701
24	6	C	-6.014839	4.360341	5.420446
25	6	C	-8.454923	2.968858	4.637883
26	6	C	-7.475037	0.252217	4.329149
27	6	C	-1.27404	3.674108	4.289924
28	8	O	-8.795744	-1.613955	4.600818
29	6	C	-9.470552	3.977565	2.051909
30	8	O	-10.352076	3.036463	6.504823
31	6	C	-11.622982	2.316254	1.010993
32	6	C	-10.353645	6.722744	2.333823
33	6	C	-12.224949	2.799564	-1.773123
34	1	H	1.626684	-2.864354	0.352951
35	1	H	2.714243	0.239998	1.057322
36	1	H	0.0241	3.510328	-4.526632
37	1	H	2.239955	3.793261	-2.00632
38	1	H	7.70536	-1.78058	-6.294586
39	1	H	9.458917	0.927978	-5.376126

40	1	H	11.00505	-1.191271	-1.67771
41	1	H	9.905212	-4.001429	-3.120502
42	1	H	-2.328027	-3.7323	-0.713041
43	1	H	2.735247	3.886179	-8.424146
44	1	H	5.340991	4.903485	-6.527528
45	1	H	5.697659	2.283596	-8.621709
46	1	H	5.675675	-4.895518	2.379876
47	1	H	6.79952	-6.405776	-0.424937
48	1	H	8.983299	-5.279625	1.872198
49	1	H	9.080583	-0.655404	2.378997
50	1	H	-4.173375	-3.592569	3.5464
51	1	H	-1.345606	-1.80365	3.385314
52	1	H	-6.087691	-2.833555	-3.202565
53	1	H	-7.249854	-0.672424	-0.903118
54	1	H	-7.101393	-3.953273	-0.178445
55	1	H	-5.959813	4.499486	7.499689
56	1	H	-5.851189	6.292457	4.672599
57	1	H	0.10759	2.200946	3.813393
58	1	H	-1.18679	5.139458	2.807999
59	1	H	-0.696425	4.57942	6.075694
60	1	H	-7.873737	3.896919	0.709717
61	1	H	-11.094787	1.356002	6.504862
62	1	H	-11.145369	0.307598	1.244259
63	1	H	-13.324692	2.628894	2.17539
64	1	H	-11.782074	6.846592	3.840311
65	1	H	-11.199943	7.418422	0.568021
66	1	H	-8.799317	8.016759	2.812901
67	1	H	-12.837724	4.757332	-2.122595
68	1	H	-10.554676	2.445557	-2.968075
69	1	H	-13.749169	1.546056	-2.434891

3-9_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	1.458402	0.061866	0.010297
1	6	C	1.734121	2.362542	-1.821661
2	6	C	0.343601	1.688619	-4.304272
3	8	O	1.991141	0.531558	-5.863837
4	6	C	4.46226	0.245184	-4.62275
5	6	C	4.425619	-2.181964	-3.028188
6	6	C	2.006249	-2.353704	-1.450077
7	6	C	4.452079	2.502485	-2.793883
8	6	C	4.51472	-4.804302	-4.243163
9	6	C	3.585722	-6.572141	-2.087706
10	6	C	2.326418	-4.876371	-0.034811
11	6	C	0.73768	4.785292	-0.619716
12	6	C	-2.018431	4.782397	0.211164
13	8	O	2.096867	6.599467	-0.300718
14	6	C	6.475404	0.30917	-6.650725
15	8	O	-1.834847	2.04488	-4.846271
16	1	H	0.42719	-2.66221	-2.778435
17	6	C	-0.147531	-5.927876	1.006443
18	8	O	4.132014	-4.612547	1.95896
19	1	H	6.02101	-2.037183	-1.694557
20	6	C	-2.191393	4.799778	3.148006
21	6	C	-3.434327	7.002185	-0.979584
22	6	C	-4.627267	3.604888	3.925643
23	6	C	-6.914574	4.606351	4.511413
24	6	C	-8.888487	2.574633	4.933635
25	6	C	-7.667763	0.149884	3.864644
26	6	C	-4.863135	0.835794	4.013281
27	6	C	-7.577811	7.332025	4.762275
28	8	O	-3.170747	-0.719963	4.220987
29	6	C	-8.39063	-0.278027	1.023741
30	8	O	-8.189532	-2.01324	5.320625
31	6	C	-6.827128	-2.412113	-0.199718
32	6	C	-11.222994	-0.830399	0.783148
33	6	C	-6.778492	-2.315216	-3.087908
34	1	H	-0.424686	-0.005918	0.867955
35	1	H	2.838089	0.313997	1.549256
36	1	H	4.772549	4.289869	-3.804405
37	1	H	5.872802	2.337602	-1.291909
38	1	H	3.2087	-4.86587	-5.863959
39	1	H	6.402462	-5.324463	-4.938247

40	1	H	5.161505	-7.579584	-1.186199
41	1	H	2.251597	-8.000737	-2.791906
42	1	H	-2.887137	3.029284	-0.476233
43	1	H	8.353591	0.117505	-5.777522
44	1	H	6.218828	-1.249703	-8.000524
45	1	H	6.405526	2.105635	-7.693902
46	1	H	-1.546673	-6.191762	-0.510308
47	1	H	0.185117	-7.764732	1.924868
48	1	H	-0.979058	-4.627882	2.406057
49	1	H	3.301088	-3.776134	3.354468
50	1	H	-0.639758	3.675085	3.959104
51	1	H	-1.972984	6.74321	3.849922
52	1	H	-5.407774	7.036983	-0.324882
53	1	H	-3.451992	6.820305	-3.049177
54	1	H	-2.523225	8.800995	-0.471033
55	1	H	-9.251555	2.296418	6.966801
56	1	H	-10.702244	3.078368	4.052774
57	1	H	-8.381879	7.717184	6.647484
58	1	H	-5.94762	8.580731	4.464882
59	1	H	-9.056565	7.840984	3.381511
60	1	H	-7.951435	1.498911	0.018285
61	1	H	-6.639481	-2.996284	5.334893
62	1	H	-4.866634	-2.347132	0.480044
63	1	H	-7.587972	-4.241794	0.450957
64	1	H	-12.404693	0.793692	1.319148
65	1	H	-11.728426	-2.430675	2.010956
66	1	H	-11.714391	-1.326325	-1.174383
67	1	H	-5.721351	-3.933872	-3.861676
68	1	H	-8.688497	-2.379414	-3.913706
69	1	H	-5.837739	-0.587114	-3.768562

Table S4. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **4**.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
4-1_en	0.00075	28.66	-1464.51661
4-2_en	0.00336	1.81	-1464.514001
4-3_en	0.01316	0.0	-1464.504196
4-4_en	0.00629	0.08	-1464.511074
4-5_en	0.0	63.45	-1464.51736
4-6_en	0.00494	0.34	-1464.512423
4-7_en	0.00411	0.82	-1464.513253
4-8_en	0.00309	2.42	-1464.514275
4-9_en	0.00308	2.43	-1464.514279

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S5. Cartesian coordinates for the low-energy reoptimized random research conformers of **4** at B3LYP-D3(BJ)/6-31G* level of theory in chloroform.

4-1_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	0.670741	-0.736834	0.598083
1	6	C	1.638194	1.137547	-1.470303
2	6	C	0.814483	0.103142	-4.076643
3	8	O	2.638661	-1.460776	-4.938372
4	6	C	4.700002	-1.654439	-3.08829
5	6	C	4.03291	-3.716074	-1.156914
6	6	C	1.304887	-3.418195	-0.227762
7	6	C	4.507935	0.906682	-1.730917
8	6	C	4.114373	-6.525859	-1.847538
9	6	C	2.424353	-7.790928	0.204113
10	6	C	1.021274	-5.615344	1.633941
11	6	C	0.676992	3.81937	-1.040629
12	6	C	-2.173298	4.178108	-0.829749
13	8	O	2.12861	5.577684	-0.825558
14	6	C	7.129073	-2.112649	-4.524614
15	8	O	-1.102931	0.516746	-5.219542
16	1	H	0.061707	-3.903208	-1.831545
17	6	C	-1.714684	-6.224156	2.304146
18	8	O	2.387179	-4.900453	3.852078
19	1	H	5.282262	-3.413902	0.480844
20	6	C	-2.844398	4.687673	1.980551
21	6	C	-3.064875	6.307154	-2.566019
22	6	C	-5.591831	4.253525	2.458144
23	6	C	-7.517516	5.913656	2.800558
24	6	C	-10.014578	4.595372	3.23241
25	6	C	-9.507715	1.788872	2.660629
26	6	C	-6.605368	1.67228	2.625386
27	6	C	-7.363998	8.725143	2.813057
28	8	O	-5.414853	-0.297337	2.795109
29	6	C	-10.626847	0.964772	0.055484
30	8	O	-10.439065	0.246469	4.633943
31	6	C	-10.340058	-1.895946	-0.372212
32	6	C	-9.569893	2.49897	-2.161755
33	6	C	-11.707544	-2.879856	-2.718785
34	1	H	-1.368928	-0.535674	0.913007
35	1	H	1.634827	-0.293572	2.386235
36	1	H	5.257699	2.443995	-2.910735

37	1	H	5.497535	0.933292	0.09155
38	1	H	3.292814	-6.803402	-3.740038
39	1	H	6.040891	-7.303215	-1.881975
40	1	H	3.558423	-8.871434	1.572017
41	1	H	1.067842	-9.114952	-0.649726
42	1	H	-3.091609	2.412415	-1.412804
43	1	H	7.031488	-3.891049	-5.595018
44	1	H	7.497221	-0.559285	-5.855946
45	1	H	8.719593	-2.236771	-3.18953
46	1	H	-2.803527	-6.732952	0.606056
47	1	H	-1.808056	-7.840297	3.619867
48	1	H	-2.636115	-4.588561	3.196699
49	1	H	2.216627	-6.242344	5.077059
50	1	H	-1.776082	3.380987	3.199098
51	1	H	-2.250437	6.614706	2.48342
52	1	H	-5.095656	6.663022	-2.29683
53	1	H	-2.760019	5.791502	-4.555936
54	1	H	-2.014631	8.056136	-2.164308
55	1	H	-10.598437	4.772587	5.224814
56	1	H	-11.536444	5.423665	2.075934
57	1	H	-8.090633	9.489561	4.612302
58	1	H	-5.432124	9.422111	2.520528
59	1	H	-8.579699	9.51203	1.311243
60	1	H	-12.671789	1.365242	0.220821
61	1	H	-9.321031	-1.203334	4.723976
62	1	H	-8.317105	-2.384173	-0.474371
63	1	H	-11.10044	-2.87035	1.300976
64	1	H	-7.575505	2.029988	-2.533575
65	1	H	-10.629729	2.098394	-3.902577
66	1	H	-9.686893	4.54874	-1.837662
67	1	H	-13.720526	-2.337063	-2.703622
68	1	H	-10.872654	-2.152671	-4.480105
69	1	H	-11.619016	-4.957182	-2.808066

4-2_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-2.076762	0.491874	-2.146714
1	6	C	-0.111019	1.817221	-0.39033
2	6	C	2.06585	2.704097	-2.124206
3	8	O	3.783211	0.823597	-2.284722
4	6	C	2.956329	-1.384485	-0.815449
5	6	C	1.223375	-3.022543	-2.464895
6	6	C	-0.723085	-1.392308	-3.857422
7	6	C	1.282448	-0.154188	1.204955
8	6	C	2.249052	-4.662469	-4.612872
9	6	C	-0.145141	-5.237486	-6.216653
10	6	C	-2.250008	-3.368569	-5.354023
11	6	C	-1.260549	3.946296	1.202626
12	6	C	-2.720256	6.083427	-0.073044
13	8	O	-1.017778	3.909363	3.48053
14	6	C	5.289874	-2.718338	0.156798
15	8	O	2.258001	4.662818	-3.252102
16	1	H	0.325389	-0.299842	-5.291878
17	6	C	-3.779327	-2.258102	-7.528481
18	8	O	-3.88335	-4.761905	-3.705093
19	1	H	0.188003	-4.265193	-1.152833
20	6	C	-5.321126	6.417751	1.227176
21	6	C	-1.174448	8.535905	0.085583
22	6	C	-6.725545	3.994865	1.656595
23	6	C	-8.003524	2.499091	0.015873
24	6	C	-9.14556	0.207416	1.296285
25	6	C	-7.934825	0.161077	3.949267
26	6	C	-7.038203	2.912423	4.211613
27	6	C	-8.418162	2.956449	-2.734283
28	8	O	-6.835442	3.978971	6.232129
29	6	C	-5.626946	-1.667427	4.034487
30	8	O	-9.667141	-0.402399	5.887476
31	6	C	-6.492555	-4.442782	3.889841
32	6	C	-3.95656	-1.208014	6.352439
33	6	C	-4.421242	-6.243769	2.982278
34	1	H	-3.093308	1.90263	-3.277114
35	1	H	-3.461582	-0.480034	-0.942969
36	1	H	2.419861	0.78763	2.663773
37	1	H	0.016345	-1.502948	2.140837
38	1	H	3.638393	-3.577473	-5.720592
39	1	H	3.188412	-6.390092	-3.943897

40	1	H	-0.846038	-7.165688	-5.899332
41	1	H	0.230887	-5.036807	-8.249897
42	1	H	-2.994535	5.616109	-2.078449
43	1	H	4.732507	-4.368314	1.294269
44	1	H	6.477037	-3.375921	-1.416677
45	1	H	6.417188	-1.440844	1.346962
46	1	H	-4.742788	-3.770502	-8.581488
47	1	H	-5.233431	-0.940871	-6.820025
48	1	H	-2.563108	-1.200371	-8.842161
49	1	H	-5.297963	-3.698344	-3.255936
50	1	H	-5.022188	7.289416	3.091368
51	1	H	-6.445746	7.753012	0.09165
52	1	H	-2.266277	10.117235	-0.713187
53	1	H	0.599503	8.357579	-0.975159
54	1	H	-0.744195	8.974327	2.072623
55	1	H	-11.209094	0.420151	1.49583
56	1	H	-8.823895	-1.528851	0.190157
57	1	H	-7.464739	4.670515	-3.412417
58	1	H	-7.737968	1.337141	-3.859174
59	1	H	-10.456612	3.125783	-3.141604
60	1	H	-4.499279	-1.250794	2.33351
61	1	H	-9.277981	0.770661	7.247778
62	1	H	-7.196543	-5.007197	5.766045
63	1	H	-8.131034	-4.616895	2.614542
64	1	H	-3.020311	0.642337	6.294721
65	1	H	-5.096151	-1.315377	8.090093
66	1	H	-2.472715	-2.658901	6.488755
67	1	H	-2.712339	-6.118061	4.165665
68	1	H	-5.065207	-8.222128	3.042253
69	1	H	-3.870504	-5.828851	1.01671

4-3_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-1.355967	0.243165	-1.83226
1	6	C	0.832534	2.03013	-1.051945
2	6	C	3.065658	1.489686	-2.833798
3	8	O	4.394834	-0.472164	-1.857836
4	6	C	3.292984	-1.306265	0.555283
5	6	C	1.196938	-3.269298	0.055604
6	6	C	-0.417533	-2.432887	-2.184002
7	6	C	1.969833	1.124532	1.449911
8	6	C	1.661604	-6.044528	-0.587888
9	6	C	-1.03046	-6.900611	-1.362389
10	6	C	-2.388316	-4.56132	-2.540219
11	6	C	-0.003917	4.793895	-1.058234
12	6	C	-1.661284	5.699465	-3.243018
13	8	O	0.603094	6.200821	0.645902
14	6	C	5.42096	-2.246419	2.215532
15	8	O	3.580159	2.497787	-4.798277
16	1	H	0.811642	-2.510469	-3.864555
17	6	C	-3.110152	-4.935409	-5.307142
18	8	O	-4.656161	-4.074059	-1.119113
19	1	H	-0.003998	-3.23733	1.762038
20	6	C	-4.497235	6.020639	-2.419664
21	6	C	-0.612654	8.179271	-4.301202
22	6	C	-5.440629	4.547473	-0.175443
23	6	C	-5.388064	5.273798	2.288555
24	6	C	-6.598339	3.361432	4.012885
25	6	C	-7.135265	1.021214	2.377408
26	6	C	-6.637413	2.040516	-0.352574
27	6	C	-4.332472	7.651709	3.354713
28	8	O	-7.020227	0.848449	-2.297286
29	6	C	-9.828452	-0.068017	2.741309
30	8	O	-5.192936	-0.756597	2.951744
31	6	C	-10.466634	-0.635788	5.535487
32	6	C	-10.392332	-2.359123	1.054527
33	6	C	-9.052223	-2.838933	6.765568
34	1	H	-2.335731	0.922001	-3.521974
35	1	H	-2.673216	0.263928	-0.251078
36	1	H	3.342028	2.51352	2.159003
37	1	H	0.539413	0.783887	2.913613
38	1	H	2.988693	-6.201041	-2.186516
39	1	H	2.422899	-7.168552	0.986109

40	1	H	-2.112031	-7.452805	0.3243
41	1	H	-1.021275	-8.527832	-2.654437
42	1	H	-1.567704	4.273888	-4.743336
43	1	H	6.815674	-0.741257	2.547442
44	1	H	4.657076	-2.86471	4.049245
45	1	H	6.385273	-3.860436	1.329609
46	1	H	-4.517551	-6.456697	-5.483595
47	1	H	-3.930764	-3.190113	-6.097987
48	1	H	-1.445693	-5.433665	-6.449654
49	1	H	-5.656444	-2.819715	-2.030425
50	1	H	-4.802728	8.040847	-2.032418
51	1	H	-5.681052	5.534363	-4.059102
52	1	H	-1.839775	8.899237	-5.819706
53	1	H	1.291248	7.886901	-5.082904
54	1	H	-0.494008	9.613128	-2.800004
55	1	H	-5.360464	2.866859	5.610216
56	1	H	-8.335358	4.178838	4.824555
57	1	H	-2.585622	7.21796	4.406347
58	1	H	-3.832135	9.039519	1.898957
59	1	H	-5.670334	8.501793	4.708141
60	1	H	-11.115321	1.469872	2.149453
61	1	H	-5.145937	-2.124978	1.702223
62	1	H	-10.174304	1.081477	6.677912
63	1	H	-12.51701	-1.014215	5.623562
64	1	H	-9.010714	-3.88859	1.326768
65	1	H	-12.269657	-3.130606	1.517017
66	1	H	-10.376297	-1.847061	-0.953576
67	1	H	-9.375772	-4.622606	5.743367
68	1	H	-7.004683	-2.504592	6.794362
69	1	H	-9.708913	-3.118796	8.721611

4-4_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	0.415991	-0.544607	0.687453
1	6	C	1.393478	1.377043	-1.33266
2	6	C	0.680465	0.345784	-3.972922
3	8	O	2.574711	-1.153598	-4.794402
4	6	C	4.577336	-1.318143	-2.878448
5	6	C	3.896559	-3.421587	-0.996248
6	6	C	1.13384	-3.198261	-0.154121
7	6	C	4.275509	1.223397	-1.501907
8	6	C	4.063487	-6.218943	-1.723098
9	6	C	2.334452	-7.551507	0.252402
10	6	C	0.831979	-5.429331	1.662952
11	6	C	0.337328	4.021254	-0.892259
12	6	C	-2.531083	4.294058	-0.835077
13	8	O	1.722997	5.813165	-0.555138
14	6	C	7.063814	-1.698771	-4.237325
15	8	O	-1.213056	0.712694	-5.171828
16	1	H	-0.044932	-3.684926	-1.805628
17	6	C	-1.912997	-6.10411	2.223361
18	8	O	2.103736	-4.721996	3.939225
19	1	H	5.085321	-3.114745	0.685479
20	6	C	-3.398535	4.747384	1.932172
21	6	C	-3.380172	6.411699	-2.607228
22	6	C	-6.139496	4.136754	2.227893
23	6	C	-8.190625	5.669247	2.329756
24	6	C	-10.612353	4.18526	2.61675
25	6	C	-9.871472	1.397458	2.131249
26	6	C	-6.966947	1.477328	2.362163
27	6	C	-8.236827	8.483141	2.220716
28	8	O	-5.61434	-0.370601	2.557104
29	6	C	-10.620473	0.467967	-0.567772
30	8	O	-10.831112	-0.225753	4.019782
31	6	C	-9.606169	-2.173593	-1.283416
32	6	C	-9.883201	2.324335	-2.671014
33	6	C	-10.264193	-4.39709	0.436498
34	1	H	-1.633833	-0.39551	0.953366
35	1	H	1.322827	-0.100946	2.505072
36	1	H	5.025628	2.790555	-2.64212
37	1	H	5.205744	1.254056	0.351483
38	1	H	3.310815	-6.484717	-3.645729
39	1	H	6.007084	-6.953345	-1.70473

40	1	H	3.446278	-8.622679	1.645291
41	1	H	1.039912	-8.894892	-0.66533
42	1	H	-3.356364	2.508747	-1.491419
43	1	H	7.047579	-3.465447	-5.331428
44	1	H	7.437693	-0.119848	-5.536759
45	1	H	8.611065	-1.800528	-2.850491
46	1	H	-2.925438	-6.618089	0.480063
47	1	H	-2.020249	-7.738088	3.516108
48	1	H	-2.907919	-4.500866	3.094652
49	1	H	1.856707	-6.055629	5.160042
50	1	H	-2.330497	3.498421	3.209056
51	1	H	-2.959024	6.703664	2.479178
52	1	H	-5.435166	6.698337	-2.470398
53	1	H	-2.928894	5.928811	-4.577602
54	1	H	-2.419346	8.190808	-2.121729
55	1	H	-11.313513	4.329863	4.57389
56	1	H	-12.126557	4.897445	1.375829
57	1	H	-9.34132	9.116748	0.567738
58	1	H	-9.19736	9.265183	3.898802
59	1	H	-6.339478	9.312128	2.089433
60	1	H	-12.715358	0.365239	-0.512344
61	1	H	-12.448077	-0.862743	3.465433
62	1	H	-10.326629	-2.566706	-3.20091
63	1	H	-7.535916	-2.057824	-1.47183
64	1	H	-10.681076	1.688865	-4.482694
65	1	H	-10.567499	4.255768	-2.334165
66	1	H	-7.819198	2.409775	-2.909432
67	1	H	-9.641003	-6.181226	-0.437735
68	1	H	-9.344721	-4.217095	2.285086
69	1	H	-12.323541	-4.557451	0.739253

4-5_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-1.014256	-0.101346	-0.937963
1	6	C	1.050556	1.993502	-1.116427
2	6	C	2.5272	1.530751	-3.588475
3	8	O	4.436237	-0.090912	-3.086886
4	6	C	4.424177	-0.819956	-0.404416
5	6	C	2.638217	-3.078813	-0.030678
6	6	C	0.15769	-2.672005	-1.455532
7	6	C	3.143437	1.482779	0.813468
8	6	C	3.324408	-5.766329	-0.835274
9	6	C	0.734431	-7.14068	-0.713587
10	6	C	-1.37546	-5.07457	-0.8282
11	6	C	-0.06963	4.644552	-0.936948
12	6	C	-2.209484	5.408146	-2.715328
13	8	O	0.707262	6.113427	0.645388
14	6	C	7.131043	-1.294863	0.382143
15	8	O	2.109552	2.367044	-5.655082
16	1	H	0.603648	-2.784378	-3.489662
17	6	C	-3.408705	-5.627374	-2.80302
18	8	O	-2.455691	-4.887725	1.627891
19	1	H	2.183527	-3.131615	2.00399
20	6	C	-4.551374	6.163645	-1.127584
21	6	C	-1.327704	7.603677	-4.389165
22	6	C	-5.468871	4.090941	0.573265
23	6	C	-4.966468	3.660907	3.055552
24	6	C	-6.036898	1.169928	3.964517
25	6	C	-7.746387	0.239026	1.81023
26	6	C	-6.896898	1.92653	-0.41568
27	6	C	-3.460705	5.256633	4.817885
28	8	O	-7.274593	1.376377	-2.620606
29	6	C	-10.616811	0.629446	2.342452
30	8	O	-7.197349	-2.318859	1.164457
31	6	C	-11.525444	-0.468767	4.889206
32	6	C	-12.252113	-0.329834	0.148072
33	6	C	-11.088028	-3.293895	5.318968
34	1	H	-2.552771	0.275195	-2.273114
35	1	H	-1.796733	-0.067662	0.981996
36	1	H	4.434677	3.106112	0.918857
37	1	H	2.425176	1.091017	2.719987
38	1	H	4.069774	-5.745771	-2.77996
39	1	H	4.753957	-6.659991	0.380175

40	1	H	0.501664	-8.145354	1.088418
41	1	H	0.52523	-8.535473	-2.239861
42	1	H	-2.713708	3.808028	-3.933597
43	1	H	8.286513	0.409224	0.096674
44	1	H	7.196768	-1.818069	2.394619
45	1	H	7.957139	-2.847306	-0.724613
46	1	H	-4.518994	-7.29822	-2.251294
47	1	H	-4.700141	-4.007332	-3.010067
48	1	H	-2.561889	-5.981745	-4.668864
49	1	H	-4.076528	-4.017553	1.511566
50	1	H	-4.079843	7.857215	-0.018943
51	1	H	-6.071965	6.675247	-2.453502
52	1	H	-0.705855	9.203384	-3.21414
53	1	H	-2.883359	8.242014	-5.613983
54	1	H	0.250183	7.002421	-5.598128
55	1	H	-4.495169	-0.200932	4.271344
56	1	H	-7.005202	1.37979	5.789751
57	1	H	-1.817529	4.179028	5.516252
58	1	H	-2.742232	6.983948	3.92888
59	1	H	-4.601586	5.747042	6.49408
60	1	H	-10.876611	2.698103	2.465373
61	1	H	-7.715889	-2.526588	-0.585227
62	1	H	-10.663441	0.598253	6.457182
63	1	H	-13.567468	-0.063674	5.023334
64	1	H	-12.135402	-2.399163	-0.031011
65	1	H	-14.247642	0.148507	0.487007
66	1	H	-11.686106	0.496689	-1.669579
67	1	H	-11.957941	-4.449846	3.824395
68	1	H	-9.066879	-3.771083	5.355748
69	1	H	-11.925169	-3.884202	7.131079

4-6_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-0.591466	-0.368488	-0.448962
1	6	C	1.331821	1.740343	-1.214638
2	6	C	2.135973	1.222032	-3.96587
3	8	O	4.142673	-0.370778	-3.921855
4	6	C	4.834319	-1.002085	-1.315691
5	6	C	3.255106	-3.277445	-0.442199
6	6	C	0.467911	-2.944917	-1.157393
7	6	C	3.853469	1.311386	0.135481
8	6	C	3.76803	-5.970445	-1.358335
9	6	C	1.299178	-7.393781	-0.639232
10	6	C	-0.779523	-5.354343	-0.094406
11	6	C	0.194313	4.342714	-0.730091
12	6	C	-2.075308	5.21499	-2.275739
13	8	O	1.072589	5.662127	0.929559
14	6	C	7.662368	-1.416399	-1.231851
15	8	O	1.207201	1.977464	-5.889741
16	1	H	0.375129	-3.131163	-3.231933
17	6	C	-3.329012	-5.960267	-1.269036
18	8	O	-1.249777	-5.097589	2.557319
19	1	H	3.410339	-3.270846	1.643649
20	6	C	-4.24649	5.977263	-0.475139
21	6	C	-1.258543	7.44193	-3.947155
22	6	C	-5.353939	3.769762	0.909356
23	6	C	-4.855348	2.838383	3.249611
24	6	C	-6.237176	0.380959	3.748714
25	6	C	-8.215657	0.200485	1.620943
26	6	C	-7.082823	2.005687	-0.359003
27	6	C	-3.109669	3.900847	5.188042
28	8	O	-7.505935	1.820019	-2.616243
29	6	C	-10.871592	1.196023	2.450393
30	8	O	-8.37546	-2.243115	0.550443
31	6	C	-11.935478	-0.103323	4.836332
32	6	C	-12.762836	1.082009	0.258282
33	6	C	-12.280597	-2.970743	4.70904
34	1	H	-2.418804	-0.050573	-1.377671
35	1	H	-0.894268	-0.257598	1.602389
36	1	H	5.101949	2.951374	-0.128168
37	1	H	3.651366	0.977445	2.172376
38	1	H	4.036858	-5.954913	-3.422146
39	1	H	5.462884	-6.824633	-0.511952

40	1	H	1.540625	-8.555217	1.069702
41	1	H	0.694827	-8.683065	-2.152133
42	1	H	-2.717527	3.674558	-3.506648
43	1	H	8.667479	0.294112	-1.851262
44	1	H	8.255302	-1.86905	0.710336
45	1	H	8.214535	-2.990486	-2.470953
46	1	H	-4.025024	-7.784717	-0.552677
47	1	H	-4.731285	-4.514489	-0.762896
48	1	H	-3.172166	-6.072961	-3.339353
49	1	H	0.34737	-4.946154	3.426249
50	1	H	-3.543965	7.416059	0.84996
51	1	H	-5.740363	6.852974	-1.630121
52	1	H	-2.878962	8.129804	-5.054838
53	1	H	0.224513	6.854535	-5.277104
54	1	H	-0.539376	9.004272	-2.776938
55	1	H	-4.916684	-1.228486	3.596405
56	1	H	-7.029938	0.324391	5.667799
57	1	H	-2.102617	5.587883	4.528218
58	1	H	-4.167679	4.356617	6.927868
59	1	H	-1.689614	2.472765	5.730208
60	1	H	-10.59383	3.20455	2.949359
61	1	H	-8.633243	-1.973451	-1.249686
62	1	H	-10.737041	0.366422	6.474673
63	1	H	-13.776522	0.791581	5.241859
64	1	H	-13.119333	-0.883705	-0.31624
65	1	H	-14.581985	1.912043	0.833459
66	1	H	-12.082057	2.109408	-1.412807
67	1	H	-13.115715	-3.676035	6.481334
68	1	H	-13.549712	-3.525385	3.156852
69	1	H	-10.47753	-3.952176	4.396884

4-7_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-0.159778	-1.660696	-1.02248
1	6	C	1.472313	0.766027	-1.323936
2	6	C	2.182709	1.000919	-4.156336
3	8	O	4.360169	-0.273147	-4.562484
4	6	C	5.250718	-1.445873	-2.216966
5	6	C	3.968641	-4.028063	-1.911721
6	6	C	1.121101	-3.834019	-2.418871
7	6	C	4.115984	0.317328	-0.212208
8	6	C	4.705944	-6.29278	-3.557473
9	6	C	2.384107	-8.087774	-3.342943
10	6	C	0.233449	-6.560187	-2.012573
11	6	C	0.287826	3.238821	-0.343379
12	6	C	-2.559533	3.399699	0.013814
13	8	O	1.645832	5.027067	0.106384
14	6	C	8.107544	-1.537067	-2.3016
15	8	O	1.029386	2.037412	-5.809095
16	1	H	0.900794	-3.488001	-4.464344
17	6	C	-2.39731	-7.108948	-3.051344
18	8	O	0.275578	-6.970449	0.655006
19	1	H	4.211569	-4.572565	0.08244
20	6	C	-3.234729	5.459147	1.956511
21	6	C	-3.83266	3.871568	-2.557821
22	6	C	-5.955809	5.337631	2.703703
23	6	C	-7.889709	6.954436	2.229894
24	6	C	-10.328627	6.120702	3.462781
25	6	C	-9.803407	3.453297	4.493438
26	6	C	-6.907833	3.241364	4.262613
27	6	C	-7.795141	9.336858	0.7311
28	8	O	-5.670464	1.60563	5.312662
29	6	C	-11.163693	1.362667	2.921461
30	8	O	-10.484798	3.30219	7.076246
31	6	C	-10.892074	-1.255633	4.154784
32	6	C	-10.33237	1.343266	0.148465
33	6	C	-12.472053	-3.323354	2.90043
34	1	H	-2.065637	-1.355857	-1.788888
35	1	H	-0.348417	-2.110263	0.999102
36	1	H	5.14599	2.117678	-0.126061
37	1	H	4.072237	-0.536444	1.679315
38	1	H	4.967192	-5.671276	-5.526686
39	1	H	6.472723	-7.198837	-2.946985

40	1	H	2.814958	-9.776312	-2.207362
41	1	H	1.769957	-8.752308	-5.214892
42	1	H	-3.217208	1.576337	0.766142
43	1	H	8.762907	-2.673701	-3.913032
44	1	H	8.894154	0.378514	-2.480343
45	1	H	8.835425	-2.397212	-0.552968
46	1	H	-2.521328	-6.659662	-5.078783
47	1	H	-2.879904	-9.124246	-2.817998
48	1	H	-3.822714	-5.987136	-2.03349
49	1	H	-0.240192	-8.691518	0.975986
50	1	H	-2.078951	5.15701	3.661269
51	1	H	-2.715902	7.322423	1.201552
52	1	H	-3.195831	5.689231	-3.344073
53	1	H	-5.8963	3.935538	-2.326967
54	1	H	-3.352379	2.413952	-3.953787
55	1	H	-10.795506	7.372241	5.062142
56	1	H	-11.934993	6.207073	2.138467
57	1	H	-8.48235	10.945438	1.866387
58	1	H	-5.887573	9.772484	0.041312
59	1	H	-9.070783	9.195141	-0.914361
60	1	H	-13.188427	1.877307	2.99877
61	1	H	-9.328104	2.102896	7.840525
62	1	H	-8.882599	-1.805542	4.177097
63	1	H	-11.478694	-1.084455	6.142706
64	1	H	-11.537867	0.081347	-0.978661
65	1	H	-10.435052	3.226483	-0.726225
66	1	H	-8.371672	0.667249	-0.044973
67	1	H	-14.482327	-2.780718	2.795512
68	1	H	-11.835088	-3.740357	0.963611
69	1	H	-12.358594	-5.098453	3.980964

4-8_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-0.853559	-1.333422	-0.977239
1	6	C	0.336396	1.361438	-0.794319
2	6	C	0.107936	2.553586	-3.434947
3	8	O	2.203701	1.97622	-4.778244
4	6	C	3.888518	0.344189	-3.296958
5	6	C	3.045927	-2.410684	-3.618813
6	6	C	0.171514	-2.663853	-3.316417
7	6	C	3.230861	1.124442	-0.579791
8	6	C	3.509331	-3.857165	-6.081731
9	6	C	1.590781	-6.082532	-5.937991
10	6	C	-0.23339	-5.508752	-3.684361
11	6	C	-0.807059	2.793251	1.450084
12	6	C	-1.590874	5.545413	1.163634
13	8	O	-0.98194	1.688327	3.449571
14	6	C	6.575833	0.874618	-4.117109
15	8	O	-1.634173	3.706394	-4.332656
16	1	H	-0.688858	-1.77273	-4.994942
17	6	C	-2.968586	-6.253057	-4.18804
18	8	O	0.641007	-6.68585	-1.418747
19	1	H	3.930013	-3.480338	-2.067334
20	6	C	-3.546626	6.278535	3.181437
21	6	C	0.768858	7.243296	1.245491
22	6	C	-5.855477	4.639713	3.071678
23	6	C	-7.578138	4.397447	1.187058
24	6	C	-9.637877	2.522215	1.843438
25	6	C	-8.61176	1.110147	4.175629
26	6	C	-6.630777	2.98999	5.170363
27	6	C	-7.575935	5.748396	-1.290861
28	8	O	-6.016043	3.101715	7.381048
29	6	C	-7.348453	-1.426424	3.358109
30	8	O	-10.438944	0.694841	6.06887
31	6	C	-9.406901	-3.384204	2.723703
32	6	C	-5.501607	-2.439114	5.342851
33	6	C	-8.467321	-5.572798	1.091788
34	1	H	-2.92481	-1.161377	-1.064301
35	1	H	-0.38114	-2.368042	0.757358
36	1	H	4.102012	2.954242	-0.11513
37	1	H	3.811869	-0.269458	0.840168
38	1	H	3.081656	-2.627871	-7.706102
39	1	H	5.471457	-4.508501	-6.286178

40	1	H	2.54291	-7.897714	-5.586992
41	1	H	0.531287	-6.281785	-7.715608
42	1	H	-2.4413	5.742381	-0.7172
43	1	H	7.891778	-0.310657	-3.026092
44	1	H	6.826797	0.447055	-6.134693
45	1	H	7.059269	2.8719	-3.801825
46	1	H	-3.120518	-8.297118	-4.571633
47	1	H	-4.146724	-5.823645	-2.531904
48	1	H	-3.73912	-5.242881	-5.835257
49	1	H	0.41666	-8.4891	-1.590171
50	1	H	-2.720635	6.111387	5.081782
51	1	H	-4.048651	8.281825	2.893895
52	1	H	1.797692	7.001204	3.038631
53	1	H	0.209079	9.240349	1.086973
54	1	H	2.073433	6.839452	-0.323101
55	1	H	-11.393935	3.519535	2.360525
56	1	H	-10.090087	1.282821	0.23249
57	1	H	-6.578062	4.608256	-2.727631
58	1	H	-9.512556	6.070292	-1.980087
59	1	H	-6.592157	7.576633	-1.185368
60	1	H	-6.270833	-1.016551	1.617229
61	1	H	-9.581886	1.072607	7.650872
62	1	H	-10.207646	-4.091747	4.50975
63	1	H	-10.99139	-2.453678	1.741817
64	1	H	-3.836793	-1.21871	5.544414
65	1	H	-6.436801	-2.581469	7.196691
66	1	H	-4.830072	-4.338328	4.824649
67	1	H	-6.852911	-6.560529	1.958727
68	1	H	-9.966117	-6.983423	0.779606
69	1	H	-7.849815	-4.894742	-0.779296

4-9_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	-1.229311	-0.239418	-1.207842
1	6	C	0.816457	1.844357	-1.572353
2	6	C	2.419682	1.114947	-3.891889
3	8	O	4.31718	-0.411476	-3.102093
4	6	C	4.165708	-0.818934	-0.360614
5	6	C	2.394841	-3.067979	0.160359
6	6	C	-0.016557	-2.827367	-1.415225
7	6	C	2.803886	1.596869	0.512041
8	6	C	3.178529	-5.797281	-0.400627
9	6	C	0.610514	-7.231808	-0.551644
10	6	C	-1.525416	-5.197186	-0.727743
11	6	C	-0.418946	4.444225	-1.780522
12	6	C	-2.485358	4.803202	-3.761835
13	8	O	0.191957	6.142639	-0.367263
14	6	C	6.82867	-1.154857	0.625215
15	8	O	2.110113	1.674239	-6.068296
16	1	H	0.5399	-3.121967	-3.403707
17	6	C	-3.631445	-5.81675	-2.591724
18	8	O	-2.613152	-4.757051	1.728225
19	1	H	1.855182	-2.940902	2.168582
20	6	C	-5.01364	5.632587	-2.515831
21	6	C	-1.615665	6.768314	-5.708929
22	6	C	-5.701408	4.3976	-0.055467
23	6	C	-5.560378	5.41058	2.300101
24	6	C	-6.566366	3.649557	4.299938
25	6	C	-7.01538	1.107589	2.963351
26	6	C	-6.697413	1.803849	0.121816
27	6	C	-4.572113	7.944351	3.020694
28	8	O	-7.113067	0.377586	-1.641772
29	6	C	-9.606157	-0.114262	3.558641
30	8	O	-4.965331	-0.446895	3.733035
31	6	C	-9.741124	-2.884935	2.686252
32	6	C	-11.788977	1.46045	2.482295
33	6	C	-12.128219	-4.271777	3.535833
34	1	H	-2.750283	-0.043383	-2.594088
35	1	H	-2.042678	0.03461	0.677282
36	1	H	4.087579	3.230753	0.493905
37	1	H	1.975829	1.42841	2.406444
38	1	H	4.16082	-5.87655	-2.2339
39	1	H	4.452889	-6.600696	1.030035

40	1	H	0.295051	-8.403724	1.138168
41	1	H	0.549267	-8.507432	-2.191708
42	1	H	-2.779246	3.008151	-4.754022
43	1	H	7.734768	-2.813997	-0.237845
44	1	H	7.979947	0.522476	0.199644
45	1	H	6.785215	-1.427504	2.687143
46	1	H	-2.880893	-6.06067	-4.515993
47	1	H	-4.597542	-7.585019	-2.056322
48	1	H	-5.037471	-4.284164	-2.61124
49	1	H	-3.367723	-6.315845	2.308882
50	1	H	-4.956387	7.691553	-2.241223
51	1	H	-6.525365	5.24367	-3.894734
52	1	H	-3.133805	7.138365	-7.083799
53	1	H	0.048855	6.079771	-6.741512
54	1	H	-1.134002	8.555946	-4.75969
55	1	H	-5.204836	3.383092	5.850293
56	1	H	-8.300241	4.445199	5.141707
57	1	H	-2.979385	7.709864	4.345494
58	1	H	-3.877397	9.029914	1.39892
59	1	H	-6.031663	9.042159	4.029132
60	1	H	-9.749193	-0.111897	5.645075
61	1	H	-4.732751	-1.919094	2.64934
62	1	H	-9.566733	-2.949378	0.613199
63	1	H	-8.087414	-3.890591	3.45214
64	1	H	-13.619293	0.81968	3.228091
65	1	H	-11.609302	3.477736	2.959693
66	1	H	-11.85837	1.304	0.408317
67	1	H	-13.846185	-3.483819	2.665789
68	1	H	-12.045724	-6.28567	3.014905
69	1	H	-12.369218	-4.166658	5.60442

Table S6. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
2-1_en	0.0	27.27	-1538.588163
2-2_en	0.00287	1.31	-1538.585295
2-3_en	0.00289	1.28	-1538.585274
2-4_en	0.00053	15.51	-1538.58763
2-5_en	3e-05	26.27	-1538.588128
2-6_en	0.00107	8.77	-1538.587091
2-7_en	0.00274	1.5	-1538.585425
2-8_en	0.00089	10.65	-1538.587275
2-9_en	0.00122	7.45	-1538.586938

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S7. G Cartesian coordinates for the low-energy reoptimized random reseach conformers of **2** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

2-1_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	4.785339	1.48788	0.32564
1	6	C	3.013605	-0.279552	-1.207737
2	6	C	3.589032	-3.015959	-0.386767
3	8	O	5.433507	-3.957414	-1.873632
4	6	C	6.304754	-2.031559	-3.667689
5	6	C	8.315119	-0.3895	-2.377435
6	6	C	7.463866	0.428239	0.269007
7	6	C	3.917865	-0.396706	-3.972949
8	6	C	10.980581	-1.387096	-1.859532
9	6	C	12.006698	0.45983	0.18476
10	6	C	9.723118	2.033281	1.165483
11	6	C	0.235425	0.479791	-0.912927
12	6	C	-1.805567	-1.206119	-2.063279
13	8	O	-0.30195	2.417266	0.179511
14	6	C	7.190813	-3.365149	-6.036682
15	8	O	2.682533	-4.177301	1.343109
16	1	H	7.491699	-1.277162	1.471956
17	6	C	9.763258	2.502703	4.007343
18	8	O	9.799428	4.38522	-0.162977
19	1	H	8.494364	1.33844	-3.527091
20	6	C	-3.097757	-2.839071	0.018302
21	6	C	-3.715831	0.420882	-3.510913
22	6	C	-4.640493	-1.367699	1.874701
23	6	C	-3.977937	-0.414063	4.165433
24	6	C	-6.189602	0.793451	5.511555
25	6	C	-8.221363	1.075157	3.44826
26	6	C	-7.321861	-0.858336	1.451989
27	6	C	-1.443346	-0.500314	5.380634
28	8	O	-8.762103	-1.817491	-0.069099
29	6	C	-8.006801	3.774188	2.279362
30	8	O	-10.695318	0.512907	4.211638
31	6	C	-10.426008	5.009825	1.335051
32	8	O	-5.962125	4.789507	2.143609
33	6	C	-10.092039	7.867096	1.110872
34	6	C	-11.196754	3.807794	-1.204031
35	1	H	4.063072	1.663993	2.265167

36	1	H	4.693464	3.37595	-0.542761
37	1	H	2.534883	-1.363287	-5.187118
38	1	H	4.321012	1.473256	-4.775599
39	1	H	10.867881	-3.32712	-1.11267
40	1	H	12.177747	-1.43521	-3.556771
41	1	H	13.404134	1.783964	-0.592129
42	1	H	12.915274	-0.566023	1.746092
43	1	H	-0.902782	-2.55507	-3.3673
44	1	H	5.655156	-4.498244	-6.860871
45	1	H	7.814274	-1.962227	-7.439789
46	1	H	8.788138	-4.624862	-5.616861
47	1	H	11.477628	3.551873	4.542244
48	1	H	8.108749	3.62743	4.595718
49	1	H	9.717421	0.714256	5.068092
50	1	H	8.472207	5.452715	0.496872
51	1	H	-4.379417	-4.15466	-0.961812
52	1	H	-1.656248	-3.969081	0.988795
53	1	H	-4.450803	1.915775	-2.269749
54	1	H	-5.308125	-0.733536	-4.179887
55	1	H	-2.825519	1.344904	-5.149617
56	1	H	-6.922753	-0.477379	6.991546
57	1	H	-5.654585	2.592163	6.403296
58	1	H	-0.656272	1.431151	5.396204
59	1	H	-1.595287	-1.116048	7.365636
60	1	H	-0.109926	-1.736592	4.380603
61	1	H	-11.386752	-0.586644	2.910225
62	1	H	-11.904756	4.554362	2.726349
63	1	H	-8.566945	8.323712	-0.226302
64	1	H	-11.851557	8.751049	0.438672
65	1	H	-9.588816	8.719787	2.939765
66	1	H	-12.983294	4.642784	-1.867699
67	1	H	-11.442962	1.752009	-1.06184
68	1	H	-9.741501	4.169822	-2.649167

2-2_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	5.351697	-1.175817	1.063781
1	6	C	3.565299	1.11551	0.554766
2	6	C	2.199519	0.582795	-1.962106
3	8	O	3.607113	1.539978	-3.871041
4	6	C	5.95246	2.646115	-2.891943
5	6	C	7.939114	0.552172	-2.622969
6	6	C	6.826661	-1.791531	-1.332337
7	6	C	5.160084	3.427212	-0.210623
8	6	C	9.236034	-0.61033	-4.932879
9	6	C	10.31925	-3.140915	-3.899826
10	6	C	9.120139	-3.586356	-1.251945
11	6	C	1.947505	1.634102	2.907494
12	6	C	-0.861018	2.091799	2.601546
13	8	O	2.992202	1.687645	4.947376
14	6	C	6.713528	4.790422	-4.62358
15	8	O	0.276058	-0.567682	-2.32447
16	1	H	5.495906	-2.656511	-2.686661
17	6	C	8.440233	-6.336156	-0.728046
18	8	O	10.934178	-2.720867	0.55372
19	1	H	9.421329	1.301094	-1.366079
20	6	C	-2.243692	2.037564	5.161577
21	6	C	-1.365791	4.554928	1.136215
22	6	C	-5.028489	1.882684	4.723128
23	6	C	-6.899584	3.603871	5.068471
24	6	C	-9.449549	2.5927	4.246969
25	6	C	-8.750796	0.354084	2.517232
26	6	C	-6.146918	-0.385795	3.590719
27	6	C	-6.660408	6.212158	6.092692
28	8	O	-5.337791	-2.537589	3.515092
29	6	C	-8.319242	1.40762	-0.213118
30	8	O	-10.397319	-1.706371	2.534373
31	6	C	-8.764458	-0.373395	-2.417669
32	8	O	-7.61888	3.571054	-0.493268
33	6	C	-9.076691	1.101382	-4.878673
34	6	C	-6.562119	-2.280569	-2.576964
35	1	H	4.217691	-2.803807	1.691784
36	1	H	6.599457	-0.626036	2.632507
37	1	H	3.995719	5.149008	-0.266461
38	1	H	6.766365	3.748564	1.060113
39	1	H	7.823753	-0.964923	-6.420631

40	1	H	10.70923	0.611472	-5.740809
41	1	H	12.38021	-3.0683	-3.660403
42	1	H	9.890291	-4.725774	-5.172784
43	1	H	-1.551641	0.514135	1.430053
44	1	H	8.462537	5.670141	-3.921299
45	1	H	7.05862	4.093575	-6.550174
46	1	H	5.222478	6.236727	-4.702408
47	1	H	10.141948	-7.528651	-0.818386
48	1	H	7.607208	-6.54638	1.171804
49	1	H	7.053679	-7.047695	-2.105611
50	1	H	10.265467	-3.037171	2.223819
51	1	H	-1.620824	0.359309	6.221186
52	1	H	-1.722682	3.695719	6.300307
53	1	H	-3.408059	4.805154	0.852509
54	1	H	-0.496337	4.542261	-0.749967
55	1	H	-0.632891	6.199579	2.184006
56	1	H	-10.527518	1.858896	5.87149
57	1	H	-10.592966	4.04745	3.302745
58	1	H	-7.218241	7.579127	4.61871
59	1	H	-7.958037	6.504524	7.698057
60	1	H	-4.728172	6.656348	6.705051
61	1	H	-9.347468	-3.185721	2.847009
62	1	H	-10.499591	-1.436303	-1.979609
63	1	H	-7.354842	2.184553	-5.307479
64	1	H	-9.442978	-0.204534	-6.455724
65	1	H	-10.654454	2.451784	-4.766083
66	1	H	-6.873042	-3.557603	-4.189705
67	1	H	-6.394335	-3.433825	-0.860346
68	1	H	-4.74397	-1.309835	-2.868755

2-3_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	5.346245	-1.321152	0.995389
1	6	C	3.555596	0.987929	0.597135
2	6	C	2.132768	0.533439	-1.90335
3	8	O	3.496224	1.550493	-3.813448
4	6	C	5.865972	2.621762	-2.85427
5	6	C	7.853399	0.517379	-2.694926
6	6	C	6.765837	-1.863689	-1.451537
7	6	C	5.138578	3.319097	-0.131745
8	6	C	9.09696	-0.575284	-5.066736
9	6	C	10.207601	-3.131014	-4.130717
10	6	C	9.056781	-3.663263	-1.476747
11	6	C	1.989809	1.439246	2.998549
12	6	C	-0.822581	1.91547	2.765272
13	8	O	3.077164	1.425146	5.016754
14	6	C	6.590948	4.819281	-4.534263
15	8	O	0.201915	-0.607512	-2.256437
16	1	H	5.404044	-2.685932	-2.801721
17	6	C	8.381296	-6.428846	-1.035604
18	8	O	10.905885	-2.862898	0.322864
19	1	H	9.36514	1.22562	-1.449426
20	6	C	-2.151627	1.791758	5.35131
21	6	C	-1.35047	4.419029	1.378718
22	6	C	-4.944393	1.642533	4.965154
23	6	C	-6.808484	3.354749	5.384901
24	6	C	-9.373386	2.362924	4.587405
25	6	C	-8.707341	0.164951	2.79388
26	6	C	-6.084239	-0.599804	3.801708
27	6	C	-6.549457	5.939295	6.463437
28	8	O	-5.276983	-2.749054	3.660846
29	6	C	-8.326665	1.282407	0.081034
30	8	O	-10.354202	-1.895154	2.792613
31	6	C	-8.819791	-0.444947	-2.155645
32	8	O	-7.62842	3.45093	-0.161512
33	6	C	-9.162885	1.086865	-4.577214
34	6	C	-6.635181	-2.364156	-2.395717
35	1	H	4.222034	-2.965783	1.59687
36	1	H	6.630461	-0.823463	2.551893
37	1	H	3.980174	5.045473	-0.103254
38	1	H	6.77614	3.593477	1.10961
39	1	H	7.65081	-0.890949	-6.53066

40	1	H	10.54918	0.671613	-5.874331
41	1	H	12.271796	-3.054238	-3.92253
42	1	H	9.766095	-4.678369	-5.44484
43	1	H	-1.542343	0.372768	1.564914
44	1	H	8.357863	5.673527	-3.8456
45	1	H	6.888271	4.185223	-6.490298
46	1	H	5.100934	6.268764	-4.529988
47	1	H	10.077613	-7.620003	-1.208113
48	1	H	7.591898	-6.706945	0.874175
49	1	H	6.962275	-7.08813	-2.406019
50	1	H	10.269455	-3.238089	1.993351
51	1	H	-1.502438	0.088842	6.353808
52	1	H	-1.61142	3.422303	6.520577
53	1	H	-0.522126	4.454796	-0.525381
54	1	H	-0.590365	6.032835	2.454529
55	1	H	-3.397644	4.680698	1.145505
56	1	H	-10.422677	1.592649	6.213859
57	1	H	-10.532487	3.839515	3.69788
58	1	H	-7.821742	6.197585	8.09461
59	1	H	-4.60729	6.367181	7.055624
60	1	H	-7.12723	7.339363	5.028754
61	1	H	-9.299455	-3.381602	3.049826
62	1	H	-10.555054	-1.505552	-1.711452
63	1	H	-7.440967	2.168476	-5.009598
64	1	H	-9.562896	-0.181153	-6.176809
65	1	H	-10.729611	2.444229	-4.408903
66	1	H	-6.987468	-3.605566	-4.027535
67	1	H	-6.443409	-3.552611	-0.706072
68	1	H	-4.816163	-1.399942	-2.703497

2-4_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	4.455616	-0.923486	0.780233
1	6	C	2.815566	-0.819311	-1.66909
2	6	C	3.297179	-3.296101	-3.144879
3	8	O	5.288656	-2.929719	-4.708825
4	6	C	6.28646	-0.363631	-4.42414
5	6	C	8.193206	-0.342916	-2.233448
6	6	C	7.133819	-1.721077	0.085034
7	6	C	3.941089	1.090801	-3.52665
8	6	C	10.816138	-1.542466	-2.470473
9	6	C	11.668318	-1.887713	0.325205
10	6	C	9.286245	-1.470504	2.02896
11	6	C	0.002805	-0.399232	-1.146199
12	6	C	-1.365468	-2.22904	0.605661
13	8	O	-1.077039	1.375949	-2.111223
14	6	C	7.36145	0.453452	-6.94431
15	8	O	2.201811	-5.2731	-2.979356
16	1	H	7.078771	-3.743542	-0.421323
17	6	C	9.081304	-3.318781	4.219159
18	8	O	9.287607	0.981601	3.15569
19	1	H	8.438402	1.676701	-1.750626
20	6	C	-1.642178	-1.039133	3.282673
21	6	C	-3.91499	-2.969374	-0.548222
22	6	C	-3.453457	1.127315	3.432142
23	6	C	-3.038508	3.653133	3.223762
24	6	C	-5.414412	5.184023	3.658168
25	6	C	-7.547367	3.231783	3.522646
26	6	C	-6.136519	0.7236	3.977753
27	6	C	-0.603895	4.945618	2.663754
28	8	O	-7.20552	-1.162458	4.751948
29	6	C	-8.625269	3.075937	0.79013
30	8	O	-9.495987	3.529011	5.299227
31	6	C	-11.107819	1.65249	0.474128
32	8	O	-7.512229	4.026524	-0.964322
33	6	C	-13.300478	3.556953	0.661413
34	6	C	-11.131768	0.213508	-2.033328
35	1	H	3.64416	-2.260463	2.146524
36	1	H	4.472786	0.959586	1.666659
37	1	H	2.617326	1.434637	-5.088965
38	1	H	4.399664	2.916244	-2.65293
39	1	H	10.64134	-3.387049	-3.417854

40	1	H	12.147342	-0.395007	-3.578706
41	1	H	13.126189	-0.512477	0.880833
42	1	H	12.480018	-3.774912	0.637313
43	1	H	-0.194881	-3.932501	0.804982
44	1	H	8.911668	-0.799664	-7.531108
45	1	H	5.888479	0.411857	-8.409756
46	1	H	8.101559	2.392595	-6.801473
47	1	H	10.728794	-3.131566	5.473756
48	1	H	7.377621	-2.914281	5.341354
49	1	H	8.97706	-5.27749	3.531269
50	1	H	9.671872	2.219304	1.872221
51	1	H	-2.349249	-2.535164	4.545885
52	1	H	0.223724	-0.471032	4.001013
53	1	H	-5.002766	-1.271071	-1.047019
54	1	H	-5.024745	-4.107743	0.788992
55	1	H	-3.61802	-4.077203	-2.281712
56	1	H	-5.397475	6.028304	5.562918
57	1	H	-5.611533	6.705515	2.258419
58	1	H	1.026867	3.667464	2.784076
59	1	H	-0.677805	5.699373	0.721716
60	1	H	-0.301462	6.555759	3.95009
61	1	H	-9.799197	1.857021	6.001906
62	1	H	-11.271035	0.306411	2.053278
63	1	H	-13.165463	4.964294	-0.866773
64	1	H	-15.123868	2.571165	0.47357
65	1	H	-13.266024	4.548476	2.485137
66	1	H	-12.949439	-0.764999	-2.29126
67	1	H	-9.613024	-1.206372	-2.099485
68	1	H	-10.845388	1.522145	-3.622544

2-5_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	3.420284	-0.182939	1.145045
1	6	C	3.682765	2.173189	-0.623562
2	6	C	2.800467	1.368717	-3.290387
3	8	O	4.814985	0.467452	-4.569499
4	6	C	7.078966	0.503092	-2.961593
5	6	C	7.141622	-1.93343	-1.386109
6	6	C	4.554184	-2.463083	-0.19546
7	6	C	6.475714	2.693442	-1.154297
8	6	C	7.767415	-4.494651	-2.579849
9	6	C	6.699823	-6.434773	-0.641345
10	6	C	5.010189	-4.922946	1.258711
11	6	C	2.216399	4.434002	0.400277
12	6	C	-0.614686	4.092397	0.774376
13	8	O	3.285338	6.386106	0.939403
14	6	C	9.350801	0.885852	-4.65459
15	8	O	0.708428	1.431474	-4.172508
16	1	H	3.268341	-2.987921	-1.752165
17	6	C	2.588274	-6.290019	2.014588
18	8	O	6.421817	-4.242363	3.458179
19	1	H	8.486494	-1.593968	0.167148
20	6	C	-1.202195	3.87532	3.642118
21	6	C	-2.090636	6.235729	-0.483391
22	6	C	-3.762572	2.736415	3.974939
23	6	C	-6.012598	3.792456	4.626566
24	6	C	-8.149865	1.888328	4.550984
25	6	C	-7.059069	-0.251005	2.926278
26	6	C	-4.207695	0.08201	3.323924
27	6	C	-6.507485	6.474653	5.308561
28	8	O	-2.716419	-1.662225	3.080701
29	6	C	-7.467765	0.379703	0.067584
30	8	O	-7.846054	-2.705878	3.500038
31	6	C	-7.03944	-1.765658	-1.794517
32	8	O	-8.045947	2.494549	-0.579474
33	6	C	-9.594651	-3.066298	-2.297863
34	6	C	-5.815487	-0.774296	-4.221569
35	1	H	1.433932	-0.545405	1.622975
36	1	H	4.451861	0.204034	2.908294
37	1	H	6.702925	4.531176	-2.097462
38	1	H	7.651329	2.686866	0.554244
39	1	H	6.780323	-4.670074	-4.404174

40	1	H	9.797045	-4.758361	-2.937299
41	1	H	8.223036	-7.374495	0.417952
42	1	H	5.604454	-7.925775	-1.589775
43	1	H	-1.159574	2.308839	-0.131561
44	1	H	11.081905	0.945631	-3.502697
45	1	H	9.52566	-0.668868	-6.022197
46	1	H	9.186591	2.673132	-5.702953
47	1	H	3.026772	-8.06841	3.012272
48	1	H	1.432308	-5.098549	3.265638
49	1	H	1.446223	-6.767971	0.343114
50	1	H	6.739939	-5.761335	4.418474
51	1	H	0.198134	2.636875	4.558144
52	1	H	-1.042822	5.745962	4.531788
53	1	H	-1.507181	8.074905	0.292785
54	1	H	-4.132849	5.976064	-0.19294
55	1	H	-1.742731	6.241999	-2.532389
56	1	H	-8.562655	1.144644	6.452274
57	1	H	-9.887324	2.712392	3.767492
58	1	H	-7.500761	6.604438	7.13667
59	1	H	-4.774874	7.612277	5.400379
60	1	H	-7.774258	7.317569	3.881577
61	1	H	-6.316099	-3.722339	3.592713
62	1	H	-5.776723	-3.147335	-0.883837
63	1	H	-9.336024	-4.659672	-3.610985
64	1	H	-10.424577	-3.787016	-0.535596
65	1	H	-10.928376	-1.723744	-3.165039
66	1	H	-3.928036	0.027553	-3.875486
67	1	H	-6.997901	0.710855	-5.068381
68	1	H	-5.609076	-2.31947	-5.599437

2-6_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	5.299215	-1.348471	1.261728
1	6	C	3.619731	1.00267	0.662517
2	6	C	2.242748	0.434911	-1.838748
3	8	O	3.69467	1.263405	-3.773412
4	6	C	6.083327	2.301091	-2.822291
5	6	C	7.973057	0.130197	-2.466832
6	6	C	6.749702	-2.115066	-1.104925
7	6	C	5.313955	3.213547	-0.177154
8	6	C	9.229467	-1.168075	-4.726571
9	6	C	10.188499	-3.710004	-3.602085
10	6	C	8.955395	-4.010958	-0.949639
11	6	C	2.034846	1.669222	2.998172
12	6	C	-0.783644	2.078538	2.722204
13	8	O	3.119874	1.870775	5.007613
14	6	C	6.9475	4.34254	-4.627578
15	8	O	0.278963	-0.656355	-2.168517
16	1	H	5.384229	-2.963512	-2.434839
17	6	C	8.140491	-6.705845	-0.339045
18	8	O	10.796949	-3.172181	0.840443
19	1	H	9.480932	0.855311	-1.226719
20	6	C	-2.109636	2.115048	5.312805
21	6	C	-1.329298	4.481738	1.173889
22	6	C	-4.905108	1.976019	4.948434
23	6	C	-6.732673	3.759285	5.210379
24	6	C	-9.320182	2.767362	4.487036
25	6	C	-8.713169	0.37835	2.960554
26	6	C	-6.083644	-0.337325	3.975715
27	6	C	-6.411883	6.424551	6.050183
28	8	O	-5.28403	-2.492883	3.910566
29	6	C	-8.226937	1.091166	0.143096
30	8	O	-10.404192	-1.638826	3.192786
31	6	C	-8.295318	-1.057829	-1.76034
32	8	O	-7.758099	3.255627	-0.438047
33	6	C	-11.013207	-1.302351	-2.775288
34	6	C	-6.373134	-0.616679	-3.875101
35	1	H	4.091374	-2.900266	1.943215
36	1	H	6.5679	-0.796602	2.812965
37	1	H	4.22005	4.978387	-0.303145
38	1	H	6.925109	3.516978	1.091423
39	1	H	7.813282	-1.506638	-6.21431

40	1	H	10.763156	-0.042053	-5.560422
41	1	H	12.2493	-3.724682	-3.351684
42	1	H	9.693898	-5.314632	-4.825381
43	1	H	-1.482926	0.453843	1.622942
44	1	H	8.729042	5.171364	-3.945545
45	1	H	7.273352	3.557437	-6.523149
46	1	H	5.522386	5.848921	-4.773655
47	1	H	9.784956	-7.978987	-0.361085
48	1	H	7.272962	-6.806891	1.554259
49	1	H	6.739711	-7.401302	-1.710345
50	1	H	10.105049	-3.403892	2.514926
51	1	H	-1.478463	0.462969	6.407876
52	1	H	-1.54275	3.800941	6.386585
53	1	H	-0.624318	6.172128	2.166282
54	1	H	-3.375203	4.689574	0.878927
55	1	H	-0.458082	4.419838	-0.710394
56	1	H	-10.416863	2.22687	6.173402
57	1	H	-10.407163	4.174916	3.413585
58	1	H	-4.467079	6.851378	6.634135
59	1	H	-6.927628	7.703729	4.484932
60	1	H	-7.700545	6.866889	7.62801
61	1	H	-9.370239	-3.125449	3.520647
62	1	H	-7.825621	-2.808942	-0.73741
63	1	H	-11.575142	0.442583	-3.762263
64	1	H	-11.125133	-2.875229	-4.132948
65	1	H	-12.356563	-1.661454	-1.233192
66	1	H	-4.421626	-0.574065	-3.158784
67	1	H	-6.748007	1.193095	-4.827651
68	1	H	-6.502913	-2.141696	-5.284637

2-7_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	5.231713	-1.233141	1.090411
1	6	C	3.674858	1.137866	0.268239
2	6	C	2.166889	0.376344	-2.10392
3	8	O	3.592721	0.880739	-4.168863
4	6	C	6.073258	1.865286	-3.422387
5	6	C	7.841997	-0.367178	-2.877195
6	6	C	6.53082	-2.355608	-1.22026
7	6	C	5.467685	3.120206	-0.878104
8	6	C	8.915411	-1.996606	-5.015548
9	6	C	9.706636	-4.483127	-3.656285
10	6	C	8.600068	-4.360626	-0.918892
11	6	C	2.230522	2.170232	2.562628
12	6	C	-0.594182	2.574946	2.377573
13	8	O	3.426293	2.659237	4.455577
14	6	C	6.980879	3.630038	-5.481575
15	8	O	0.130421	-0.617786	-2.253553
16	1	H	5.069941	-3.255664	-2.406333
17	6	C	7.653288	-6.898273	0.062774
18	8	O	10.407987	-3.321849	0.795415
19	1	H	9.438145	0.397985	-1.782403
20	6	C	-1.816525	2.867855	5.002603
21	6	C	-1.166062	4.846279	0.647817
22	6	C	-4.621047	2.669852	4.750231
23	6	C	-6.469891	4.441148	4.912445
24	6	C	-9.060633	3.334577	4.398131
25	6	C	-8.455933	0.841623	3.015375
26	6	C	-5.795189	0.26159	4.045448
27	6	C	-6.171741	7.17832	5.485479
28	8	O	-4.986351	-1.881811	4.254791
29	6	C	-8.18279	1.441907	0.131568
30	8	O	-10.093095	-1.180063	3.456023
31	6	C	-8.760479	-0.662925	-1.730656
32	8	O	-7.501041	3.525947	-0.531088
33	6	C	-9.229883	0.4079	-4.369303
34	6	C	-6.566885	-2.586549	-1.720495
35	1	H	3.95825	-2.618446	1.979669
36	1	H	6.610237	-0.622925	2.515958
37	1	H	4.480601	4.927518	-1.174878
38	1	H	7.142398	3.458873	0.295109
39	1	H	7.427144	-2.376649	-6.420243

40	1	H	10.500639	-1.093418	-6.009268
41	1	H	11.774045	-4.676096	-3.539171
42	1	H	8.991762	-6.153731	-4.666235
43	1	H	-1.363446	0.876186	1.455493
44	1	H	8.842598	4.405965	-4.973128
45	1	H	7.162099	2.622149	-7.289467
46	1	H	5.647451	5.204273	-5.736735
47	1	H	9.203488	-8.292274	0.116484
48	1	H	6.904905	-6.69535	1.992451
49	1	H	6.152314	-7.668444	-1.15381
50	1	H	11.754169	-4.535977	1.007778
51	1	H	-1.131534	1.337582	6.234469
52	1	H	-1.226745	4.657614	5.876687
53	1	H	-0.414208	6.603452	1.476312
54	1	H	-3.218165	5.047855	0.395985
55	1	H	-0.346331	4.616746	-1.247403
56	1	H	-10.051889	2.882735	6.173805
57	1	H	-10.251523	4.629186	3.292765
58	1	H	-7.410114	7.752393	7.061222
59	1	H	-4.214875	7.687659	5.951579
60	1	H	-6.76557	8.290715	3.823282
61	1	H	-9.018544	-2.600417	3.92081
62	1	H	-10.462091	-1.628761	-1.021251
63	1	H	-9.694727	-1.125794	-5.695537
64	1	H	-10.799187	1.772971	-4.371013
65	1	H	-7.54037	1.396021	-5.070074
66	1	H	-6.28267	-3.442291	0.148114
67	1	H	-4.776464	-1.687594	-2.285281
68	1	H	-6.978985	-4.109401	-3.077175

2-8_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	4.543602	-0.938582	0.847767
1	6	C	2.939544	-0.784977	-1.622118
2	6	C	3.435481	-3.239262	-3.137583
3	8	O	5.439115	-2.850568	-4.669878
4	6	C	6.453941	-0.292172	-4.311804
5	6	C	8.324023	-0.329923	-2.096317
6	6	C	7.227326	-1.751692	0.177051
7	6	C	4.100972	1.154528	-3.425569
8	6	C	10.937657	-1.544756	-2.335534
9	6	C	11.75694	-1.944946	0.458561
10	6	C	9.373151	-1.539988	2.134508
11	6	C	0.116149	-0.377632	-1.145803
12	6	C	-1.276909	-2.217055	0.576101
13	8	O	-0.957352	1.388801	-2.134714
14	6	C	7.568135	0.570234	-6.799123
15	8	O	2.327776	-5.213935	-3.012886
16	1	H	7.15086	-3.769177	-0.347759
17	6	C	9.146644	-3.406079	4.316876
18	8	O	9.531191	0.984937	3.089863
19	1	H	8.592563	1.652897	-1.515529
20	6	C	-1.612005	-1.042219	3.255275
21	6	C	-3.796798	-2.966856	-0.63554
22	6	C	-3.392934	1.151785	3.373446
23	6	C	-2.933534	3.657596	3.113181
24	6	C	-5.299338	5.230509	3.402489
25	6	C	-7.473944	3.31438	3.446965
26	6	C	-6.105845	0.745625	3.841471
27	6	C	-0.467189	4.911079	2.593492
28	8	O	-7.156894	-1.214911	4.382836
29	6	C	-8.77278	3.080226	0.830646
30	8	O	-9.261772	3.625191	5.399877
31	6	C	-11.199101	1.527103	0.754202
32	8	O	-7.866013	4.053885	-1.029439
33	6	C	-13.472136	3.338716	0.691781
34	6	C	-11.170147	-0.229268	-1.545162
35	1	H	3.689779	-2.277342	2.187652
36	1	H	4.547928	0.949063	1.73027
37	1	H	2.801209	1.531328	-5.000384
38	1	H	4.558266	2.960234	-2.511524
39	1	H	10.770928	-3.36881	-3.325034

40	1	H	12.286745	-0.37504	-3.397026
41	1	H	13.190078	-0.566564	1.055228
42	1	H	12.550498	-3.841935	0.754908
43	1	H	-0.102817	-3.916579	0.791082
44	1	H	9.119058	-0.679544	-7.390689
45	1	H	6.116236	0.57151	-8.286363
46	1	H	8.320139	2.499659	-6.60068
47	1	H	10.785759	-3.240512	5.586631
48	1	H	7.425438	-3.032511	5.434765
49	1	H	9.033189	-5.365021	3.627885
50	1	H	8.20441	1.209281	4.323797
51	1	H	-2.376082	-2.538735	4.4834
52	1	H	0.243362	-0.506987	4.026386
53	1	H	-4.890103	-1.273406	-1.137299
54	1	H	-4.92388	-4.124112	0.669013
55	1	H	-3.45299	-4.052279	-2.374535
56	1	H	-5.254746	6.272	5.208102
57	1	H	-5.475868	6.599777	1.847167
58	1	H	-0.464739	5.636063	0.639836
59	1	H	-0.178455	6.53661	3.864794
60	1	H	1.142135	3.614151	2.783753
61	1	H	-10.115976	5.217803	5.142545
62	1	H	-11.283202	0.406888	2.501056
63	1	H	-13.377173	4.581334	-0.97558
64	1	H	-15.249459	2.260683	0.601856
65	1	H	-13.549546	4.531918	2.394978
66	1	H	-12.946041	-1.307591	-1.655858
67	1	H	-9.598281	-1.58539	-1.425033
68	1	H	-10.942289	0.86556	-3.297907

2-9_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	C	4.4885	-0.926494	0.788876
1	6	C	2.872039	-0.759055	-1.672203
2	6	C	3.377078	-3.192152	-3.214987
3	8	O	5.374497	-2.77376	-4.752419
4	6	C	6.367615	-0.211504	-4.376794
5	6	C	8.250738	-0.250927	-2.171666
6	6	C	7.171586	-1.711566	0.088533
7	6	C	4.009007	1.208176	-3.46185
8	6	C	10.874808	-1.441474	-2.436032
9	6	C	11.693746	-1.927016	0.347943
10	6	C	9.30432	-1.512312	2.036719
11	6	C	0.049626	-0.374747	-1.175818
12	6	C	-1.318798	-2.236229	0.542041
13	8	O	-1.043148	1.39185	-2.143931
14	6	C	7.460801	0.684841	-6.861984
15	8	O	2.288633	-5.178585	-3.108362
16	1	H	7.119037	-3.721922	-0.463843
17	6	C	9.08305	-3.380577	4.218629
18	8	O	9.217922	1.017443	2.978575
19	1	H	8.498543	1.728526	-1.575489
20	6	C	-1.630125	-1.091341	3.237162
21	6	C	-3.847836	-2.984246	-0.651061
22	6	C	-3.414211	1.097716	3.394835
23	6	C	-2.960097	3.606963	3.155991
24	6	C	-5.325134	5.173741	3.48215
25	6	C	-7.496634	3.254969	3.535518
26	6	C	-6.12106	0.683362	3.885949
27	6	C	-0.499784	4.869699	2.631619
28	8	O	-7.16541	-1.283685	4.418091
29	6	C	-8.835492	3.048226	0.938111
30	8	O	-9.258625	3.544805	5.516458
31	6	C	-11.254624	1.482535	0.880289
32	8	O	-7.966834	4.052251	-0.924312
33	6	C	-13.537851	3.28162	0.863872
34	6	C	-11.244803	-0.253661	-1.434977
35	1	H	3.660126	-2.296407	2.112194
36	1	H	4.505023	0.936308	1.712941
37	1	H	2.698031	1.5927	-5.025697
38	1	H	4.458337	3.005994	-2.528971
39	1	H	10.724559	-3.238926	-3.474804

40	1	H	12.218282	-0.234437	-3.462465
41	1	H	13.183377	-0.60774	0.953346
42	1	H	12.445592	-3.850085	0.589084
43	1	H	-0.135039	-3.932512	0.728098
44	1	H	9.021115	-0.543814	-7.473592
45	1	H	6.000976	0.684593	-8.34148
46	1	H	8.193416	2.620404	-6.650012
47	1	H	10.724515	-3.22737	5.495343
48	1	H	7.368802	-2.99091	5.330071
49	1	H	8.996927	-5.341887	3.531238
50	1	H	10.589423	1.230729	4.163843
51	1	H	-2.381237	-2.602934	4.454815
52	1	H	0.23105	-0.561024	3.996263
53	1	H	-4.95415	-1.290521	-1.122499
54	1	H	-4.955946	-4.160825	0.65263
55	1	H	-3.518335	-4.048909	-2.405773
56	1	H	-5.262383	6.203131	5.29419
57	1	H	-5.520517	6.553538	1.938273
58	1	H	1.112754	3.572614	2.783714
59	1	H	-0.519017	5.632729	0.692448
60	1	H	-0.199544	6.471792	3.930041
61	1	H	-10.114169	5.141009	5.287508
62	1	H	-11.309257	0.345523	2.617312
63	1	H	-13.471058	4.539358	-0.793571
64	1	H	-15.310359	2.194431	0.787943
65	1	H	-13.598158	4.459192	2.578663
66	1	H	-13.016499	-1.340187	-1.534096
67	1	H	-9.664545	-1.602302	-1.344742
68	1	H	-11.043176	0.858093	-3.180343