Supporting Information:

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Experimental Methods

General Experimental Procedures. Optical rotation was obtained from a Rudolph Autopol VI (Hackettstown, NJ, USA) polarimeter with a path length of 10 mm. Electronic circular dichroism (ECD) was measured on a Chirascan (Applied Photophysics, Surrey, UK) spectrophotometer. Nuclear magnetic resonance (NMR) spectra were recorded on an Agilent 600 MHz NMR (Agilent, Santa Clara, CA, USA) spectrometer with a cold probe. Vacuum liquid chromatography (VLC) was performed using either LiChroprep® RP-18 (40-63 μm) (Merck Millipore, Billerica, MA, USA) or Sep-Pak® Vac 35cc (10g) C18 cartridge (Waters, Milford, MA, USA). High performance liquid chromatography (HPLC) purification was accomplished on an Agilent Prepstar HPLC system, when needed, with an Agilent Polaris C18-A 5 μm (21.2 × 250 mm), Phenomenex Luna C18(2) or C8(2) (100Å) 10 μm (10.0 × 250 mm) (Phenomenex, Torrance, CA, USA), and an Agilent Phenyl-Hexyl 5 μm (9.4 × 250 mm) columns. Analytical HPLC-mass (MS) was acquired by using an Agilent 1260 Infinity Quaternary LC system consisting of an autosampler, a quaternary solvent delivery system, thermostatted column compartment, and a photo diode array (PDA) detector coupled to an Agilent 6120 Quadrupole low-resolution (LR) electrospray ionization (ESI) mass spectrometer. High-resolution mass spectra (HRMS) were obtained from an Agilent iFunnel 6550 QTOF (quadrupole time of flight) MS instrument fitted with an ESI source coupled to an Agilent 1290 Infinity HPLC system. Agilent Software packages, including OpenLAB CDS ChemStation (Version C.01.04), MassHunter Workstation Data Acquisition (Version B.05.01), and MassHunter Qualitative Analysis (Version B.05.00), were used for the analyses of UV-HPLC-MS spectra.

LC-HRMS Metabolite Profiles from *P. luminescens* in Response to Redox Stress. A frozen stock of *Photorhabdus luminescens* TT01 was thawed, streaked, grown, and when needed, the strain was cultivated on lysogeny broth (LB) agar plates in a 30 °C stationary incubator. Three single colonies for biological triplicates were inoculated into 5 ml LB liquid medium in 3×14 ml polypropylene round-bottom culture tubes and incubated with 250 rpm at 30 °C for 18 h. Methyl viologen dichloride hydrate (MilliporeSigma, Burlington, MA, USA) was prepared and supplemented into fresh LB medium in two subinhibitory concentrations of 12.5 and 6.25 μM, which was followed by sterile filtration through 0.2 μm diameter filters. 2 μl overnight *P. luminescens* cultures were then dispensed into the paraquat-conditioned LB medium in the three

biological replicates. A cell-free control was prepared in fresh LB medium supplemented with tapinarof (100 μM) in the presence of methyl viologen dichloride hydrate with two different concentrations as described above. *P. luminescens* under the subinhibitory paraquat-induced redox stress was incubated in a shaker with 250 rpm at 30 °C, and the OD_{600} was measured at the 48 h post-stressed condition. The cultures (5 ml) were centrifuged at 2,000 × *g* for 20 min at 4 °C and the supernatants were extracted with ethyl acetate (6 ml). The ethyl acetate-soluble layers were dried under reduced pressure on a HT-4X evaporation system (Genevac Inc., Gardiner, NY). Dried crude materials were redissolved in 100 μl methanol, and 2 μl was injected for the high-resolution ESI-QTOF-MS analysis [column; Phenomenex Kinetex C_{18} (100 Å) 5 μm (4.6 × 250 mm), flow rate; 0.7 ml min^{-1}, mobile phase; a H_2O/ACN gradient containing 0.1% formic acid (v/v): 0–30 min, 10–100% ACN; hold for 5 min, 100% ACN; 2min, 100–10% ACN; 5 min post-time, 10% ACN]. Metabolic profiles were achieved by the comparison of UV and LC-HRMS traces of the non-stressed group versus the stressed group, which was followed by extracted ion counts (EIC) corresponding to the observed *m/z* of the compounds of interest.

Cultivation, Extraction, and Isolation. 5 ml *P. luminescens* culture was prepared, and 5 μl of overnight culture was dispensed into 12 × 5 ml fresh LB medium and further incubated in 250 rpm at 30 °C. 12 × 4 l Erlenmeyer flasks each containing 1 l LB medium were prepared for the larger-scale cultivation. Each 5 ml culture was transferred into the corresponding 1 l LB medium and grown for 4 days. Dark brownish *P. luminescens* culture broth was centrifuged with 14,000 × *g* for 30 min and the supernatant was subsequently extracted by ethyl acetate (2×12 l), and evaporated *in vacuo*. A sticky crude extract (approx. 800 mg from 12 l culture broth) was powdered with adsorbent SiO_2 (Celite®110, Millipore Sigma, St. Louis, MO, USA), and the sample was loaded and fractionated by solid phase extraction (SPE) on a vacuum manifold equipped with Sep-Pak® Vac 35cc (10g) C18 cartridge with a step gradient elution (40%, 60%, 80% and 100 % aqueous MeOH). The desired 80% MeOH fraction was separated by a reversed-phase Agilent HPLC system with an Agilent Polaris C18 column (20 × 250 mm, 8 ml min^{-1}, 50-100% aqueous ACN in 0.01% TFA for 60 min, 1 min fraction). Compounds **4** and **5** were collected in fractions 36 and 38, and further isolated by Phenomenex C18 column (10 × 250 mm, 4 ml min^{-1}, 50-100% aqueous ACN in 0.01% TFA for 30 min), eluting the impure **4** and **5** at t_R = 16.3 and 17.4 min, respectively. Compounds **4** (0.2 mg) and **5** (0.1 mg) were purified by Phenyl-Hexyl column (10 × 250 mm, 4 ml min^{-1}, 60-100% aqueous ACN in 0.01% TFA for 30 min) at t_R = 11.2

and 13.6 min. Of note, this entire process was repeated 10 times, resulting in a yield of ~ 1 mg of natural **4** and **5** from a total of ~ 100 l *P. luminescens* cultivation.

NMR Studies. ^{1}H and ^{13}C chemical shifts given in ppm (δ) and coupling constants (J) in Hz were referenced to the residual peaks of MeOH-d_4 (δ_H 3.29 and δ_C 47.6). NMR spectra were analyzed using MestReNova software (Version 10.0.1). LR-HSQMBC was performed utilizing the t1 increments (indirect dimension) of 640, to evolve long-range heteronuclear correlations with the $^{n}J_{CH}$ value being optimized to 2 Hz (transfer delay of 250 ms).[1] The 1,1-ADEQUATE was initially implemented with 2 s relaxation time, 128 t1 increments, 160 scans, and $^{1}J_{CC}$ 50 Hz. The homonuclear coupling constant ($^{1}J_{CC}$) was adjusted to 10 Hz to specifically develop two-bond correlations for the detection of the core cyclopropyl motif comprising carbocyclinone-534 (**4**). The practical amount required for this experiment was ~7 mg in our laboratory setting. The 1D NOESY for PANIC analysis was conducted using the double-pulse field gradient spin-echo NOE (DPFGSENOE) excitation sculpted selective sequence incorporated with a zero-quantum filter component (500 ms mixing time, 2 s relaxation time, 64 scans). The resonance for proton at 6.8 ppm was selectively irradiated using 1D NOESY pulse and the corresponding integration was normalized into -1000 as an arbitrary number. The generated NOE intensity for proton at 7.0 ppm was then integrated with reference to -1000. The normalized integration value ($NOE_{reference}$) and the interproton distance of proton at 6.8 ppm with proton 7.0 ppm being 2.5 Å ($r_{reference}$), were used to solve an equation below to calibrate an interproton distance between protons at 3.9 and 4.4 ppm ($r_{unknown}$). The $NOE_{unknown}$ value was acquired by NOE-integration of proton at 3.9 ppm upon selective irradiation of proton at 4.4 ppm and normalization of the NOE integration value (-1000).[2]

Equation: $NOE_{unknown}/NOE_{reference} = (r_{reference})^6/(r_{unknown})^6$

X-ray Crystal Structure Analysis. Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å) for the structure of carbocyclinone-534 (**4**). The diffraction images were processed and scaled using Rigaku Oxford Diffraction software. The structure was solved with SHELXT and was refined against F2 on all data by full-matrix least squares with SHELXL.[3] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they

are linked (1.5 times for methyl groups). A summary of the general crystallographic information is reported in Table S3. The hydrogen positions associated with oxygen atoms O1, O4, O7, and O10 were found in the difference map and freely refined (see Table S4). One isopropyl group with atoms (C66, C67, C68) showed signs of a positional disordered. The second position was identified with atoms of the same number with the addition of a "B" suffix. When the occupancies of these "B" atoms were freely refined, the site occupancy split between the major and minor components converged to values of 0.839(4)/0.161(4) respectively. The chemically identical C-C bond distances were restrained to be similar. Two of the four acetonitriles were disordered over two positions. In a similar fashion to the isopropyl, the chemically identical C-C and C-N bond distances were restrained to be similar. The site occupancies were freely refined to values of 0.862(3)/0.138(3), with the minor site having atoms labels with the suffix "B". The methyl carbon atom, C74, was shared between the major and minor sites. The atom was split, then constrained to have identical x, y, z parameters for the major and minor site. Due to the small amount of electron density, the thermal parameters of atoms with “B” labels were constrained to be identical to their chemically identical component. All of the hydrogen atoms associated with disordered atoms were generated geometrically to correspond to the disordered atoms on which they ride. The full numbering scheme of carbocyclinone-534 (**4**) can be found in the full details of the X-ray structure determination (CIF), which is included as Supplementary Materials. CCDC number 1871126 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center.

Computational ECD Calculation. The initial conformers for ECD calculation were found at the MMFF94 force field and optimized at the B3LYP/6-31+G(d,p) using the polarizable continuum model (PCM) mode with a dielectric constant representing MeOH,[4] and excited state calculations were performed at the identical theory level and basis set. The generated excitation energies were weighted based upon the Boltzmann population from the calculated Gibbs free energy of each conformer (see Table S5) and fitted with a Gaussian function to visualize the ECD spectrum, utilizing SpecDis.[5]

Cloning and Expression of Plu1886. The gene encoding Plu1886 was PCR amplified from *P. luminescens* genomic DNA using the primers noted in Table S7. Following PCR purification, the gene was digested with NdeI/HindIII restriction enzymes and ligated into plasmid

pET28a. The ligation reaction was transformed into *E. coli* DH10b, purified, and sequence validated. Purified plasmid encoding Plu1886 with an N-terminal His_6 tag was transformed into BL21(DE3) cells for expression. An overnight culture (5 ml) in LB supplemented with kanamycin (50 μg ml^{-1}) was subcultured into 1 l of terrific broth (TB) and grown at 37 °C until the OD_{600} reached ~0.5. Protein expression was then induced with 1 mM IPTG and cells were grown overnight at 25 °C. Cells were harvested by centrifugation at 5000 rpm for 30 min and resuspended in lysis buffer (50 mM NaH_2PO_4, 300 mM NaCl, 10 mM imidazole, 1 mg ml^{-1} lysozyme, pH 8.0). Following incubation on ice for 30 min, cells were lysed via sonication (10 seconds on, 10 seconds off, 2 min total). The lysate was cleared by centrifugation at 30,000 × *g* for 30 min. The supernatant was then incubated with 500 μl Ni-NTA resin with agitation at 4°C for 1 h. The resin was then washed with 1 × 5 ml lysis buffer followed by 2 × 5 ml wash buffer (100 mM Tris, 300 mM NaCl, 50 mM imidazole, 10% glycerol, pH 8.0), and the protein was eluted with 4 × 500 μl elution buffer (100 mM Tris, 300 mM NaCl, 250 mM imidazole, 10% glycerol, pH 8.0). Fractions were run on SDS-PAGE (Figure S23) to confirm the presence, size and purity of Plu1886 and were then combined and concentrated, diluted with 50 mM Tris buffer (pH 7.4) and concentrated again.

Enzymatic Assays. For the plant stilbene substrates, resveratrol and piceatannol were purchased from Tokyo Chemical Industry and VWR International, respectively. Pinosylvin and chiricanine A were synthesized as previously described.[6] Small scale (100 μl) enzymatic assays were prepared with 10 μM enzyme and 1 mM stilbene substrate in 100 mM sodium phosphate buffer (pH 7.4). Metal ions ($NiCl_2$, $CaCl_2$, $FeSO_4$, $CuSO_4$, $ZnSO_4$, $CoCl_2$, $MgSO_4$, $MnCl_2$) were supplemented at 1 mM. Reactions were incubated at 37 °C overnight (Figure 3b, c, e; 4b) or 2 h (Figure 3f; 4c), lyophilized, and extracted with MeOH. Following incubation, all reactions were lyophilized and extracted with MeOH. Enzymatic products were analyzed by single quadrupole LC/MS (Agilent 6120) or high-resolution LC-ESI-QTOF-MS using a Phenomenex Kinetix C18 (100 Å) 5 μm (4.6 × 250 mm) column with the following H_2O-ACN gradient containing 0.1% formic acid at a flow rate of 0.7 ml min^{-1}: 0-30 min 10-100% ACN, 30-35 min 100% ACN, 35-37 min 10% ACN; or 0-20 min 10-100% ACN, 20-21 min 10% ACN.

Construction of *plu1886* Deletion Mutant. Allelic-exchange was used to remove gene *plu1886* in this study as previously described.[7] All primers used are included in Table S7.

AhR and Nrf2 Assay. Hct116 cells were cultured at 37 °C with 5% CO_2 in DMEM/F12 medium supplemented with 5% heat-inactivated FBS and 25 mM HEPES. Cells were seeded into 24-well tissue culture plates and grown to 60% confluence. Compounds, diluted in DMSO were then added, ensuring a constant 0.5% DMSO v/v vehicle concentration. Cells were incubated with compounds for 24 hours. Total RNA was then collected with the Qiagen RNeasy Plus Mini Kit. qRT-PCR was performed using the NEB Luna One-Step RT-qPCR kit (E3005) following the standard manufacturer's protocol. Relative transcript levels of *cyp1a1* and *nqo1* were quantified using the ddCq method, using glyceraldehyde-3-phosphate dehydrogenase (GAPDH) as the reference gene. Melt curve analysis was used to monitor qPCR amplification.

Disk Diffusion Test. Growth inhibitory properties of compounds against *Mycobacterium smegmatis* was performed by the disk diffusion method. *Mycobacterium smegmatis* was grown on an LB agar plate at 37 °C for 72 h. A single colony was inoculated into 5 ml of Middlebrook 7H9 liquid medium and incubated for 48 h. The overnight culture was diluted to OD_{600} = 0.1 with sterilized medium and a sterile cotton swab was soaked in the diluted culture and streaked on an LB agar plate. Compounds (10 µl of each sample with a concentration of 100 µg/disk) were added to sterile paper disks (7 mm) and allowed to air dry. DMSO (Santa Cruz Biotechnology, Dallas, TX, USA) was used as a vehicle negative control. Paper disks soaked with samples were placed and incubated at 37 °C for 48 h, and the zones of inhibition were then imaged.

Growth Inhibition Assays. Compounds were prepared in DMSO to a concentration of 10 mM. DMSO was used as a vehicle negative control, and vancomycin (MRSA) and ampicillin (VRE) were also prepared as positive controls for minimum inhibitory concentration (MIC) tests. We purchased a MRSA strain from ATCC (ATCC®BAA-1717™) and a VRE clinical isolate was obtained from Professor Martin Kriegel at Yale School of Medicine. Compounds were tested for antimicrobial activity against MRSA and VRE at 100, 50, 25, 12.5, 6.25, 3.13, 1.56, 0.78, and 0.39 µM. MRSA was grown in tryptic soy broth and VRE was grown in brain heart infusion medium. Overnight cultures of bacteria were diluted to OD_{600} = 0.1 and 50 µl of cell culture broth was added to each well. Media (50 µl) containing compound at the appropriate concentration was then added to the cell cultures and the plates were sealed and incubated at 37 °C overnight. Plates were then read for OD_{600} using a PerkinElmer Envision 2100 multimode plate reader (PerkinElmer, Waltham, MA, USA). The data was fit to a Gompertz model[8] and MICs were determined as the compound

concentration that completely inhibited cell growth during the incubation period. All samples were tested in triplicate.

Antioxidant Activity Assay. Antioxidant activity assay of compounds was evaluated through the DPPH free radical scavenging assay in a 96-well plate. 2,2-diphenyl-1-picrylhydrazyl (DPPH) was purchased (MilliporeSigma, Burlington, MA, USA) and used without further manipulation. Desired compounds and L-ascorbic acid (MilliporeSigma, Burlington, MA, USA) as a positive control were dissolved in DMSO with a concentration of 10 mM. A two-fold serial dilution was initiated in fresh DMSO to eight different concentrations. 10 μl of the serial dilution of the compound was then dispensed to the 96-well plate. 90 μl of freshly prepared 0.2 mM DPPH in methanol was subsequently added to the experimental wells, while 100 μl of MeOH containing DMSO was added to the blank controls. The reactions were stored in the dark for 30 minutes and then measured at 517 nm using a PerkinElmer Envision 2100 multimode plate reader. The IC_{50} (the concentration required to scavenge 50% of radicals) values of tested compounds were calculated using the GraphPad Prism 7 software.

BioMAP® Phenotypic Profiling Assay. BioMAP Diversity PLUS assay was performed by Eurofins DiscoverX. Human primary cells in BioMAP systems were used at early passage (passage 4 or earlier) to minimize adaptation to cell culture conditions and preserve physiological signaling responses. All cells were from a pool of multiple human donors (n = 2 – 6), commercially purchased and handled according to the recommendations of the manufacturers. Human blood derived CD14+ monocytes are differentiated into macrophages *in vitro* before being added to the lMphg system. Abbreviations are used as follows: Human umbilical vein endothelial cells (HUVEC), Peripheral blood mononuclear cells (PBMC), Human neonatal dermal fibroblasts (HDFn), B cell receptor (BCR), T cell receptor (TCR) and Toll-like receptor (TLR). Cell types and stimuli used in each system are as follows: 3C system [HUVEC +(IL-1β, TNFα and IFNγ)], 4H system [HUVEC +(IL-4 and histamine)], LPS system [PBMC and HUVEC + LPS (TLR4 ligand)], SAg system [PBMC and HUVEC + TCR ligands (1×)], BT system [CD19+ B cells and PBMC + (α-IgM and TCR ligands (0.001×))], BF4T system [bronchial epithelial cells and HDFn + (TNFα and IL-4)], BE3C system [bronchial epithelial cells + (IL-1β, TNFα and IFNγ)], CASM3C system [coronary artery smooth muscle cells + (IL-1β, TNFα and IFNγ)], HDF3CGF system [HDFn + (IL-1β, TNFα, IFNγ, EGF, bFGF and PDGF-BB)], KF3CT system [keratinocytes

and HDFn + (IL-1β, TNFα and IFNγ)], MyoF system [differentiated lung myofibroblasts + (TNFα and TGFβ)] and lMphg system [HUVEC and M1 macrophages + Zymosan (TLR2 ligand)]. Systems are derived from either single cell types or co-culture systems. Adherent cell types were cultured in 96 or 384-well plates until confluence, followed by the addition of PBMC (SAg and LPS systems). The BT system consists of CD19+ B cells co-cultured with PBMC and stimulated with a BCR activator and low levels of TCR stimulation. Metabolite **4** was prepared in DMSO (final concentration ≤ 0.1%) and added at a final concentration of 29 μM, 1 h before stimulation and remained in culture for 24 h or as otherwise indicated (48-hrs: MyoF system; 72 h: BT system (soluble readouts); 168 h: BT system (secreted IgG)). Each plate contained drug controls, negative controls (*e.g.*, non-stimulated conditions) and vehicle controls (*e.g.*, 0.1% DMSO) appropriate for each system. Direct ELISA was used to measure biomarker levels of cell-associated and cell membrane targets. Soluble factors from supernatants were quantified using either HTRF® detection, bead-based multiplex immunoassay or capture ELISA. Overt adverse effects of test agents on cell proliferation and viability (cytotoxicity) were detected by sulforhodamine B (SRB) staining, for adherent cells, and alamarBlue® reduction for cells in suspension. For proliferation assays, individual cell types were cultured at subconfluence and measured at time points optimized for each system (48 h: 3C and CASM3C systems; 72 h: BT and HDF3CGF systems; 96 h: SAg system). Cytotoxicity for adherent cells was measured by SRB (24 h: 3C, 4H, LPS, SAg, BF4T, BE3C, CASM3C, HDF3CGF, KF3CT, lMphg systems; 48 h: MyoF system), and by alamarBlue staining for cells in suspension (24 h: SAg system; 42 h: BT system) at the time points indicated.

DSS-induced colitis model. C57BL/6 mice were used in this study. 8-10-week-old mice were administered 2.5% DSS (MP Bio) for 5 days and returned to regular drinking water and monitored daily. Tested compounds were orally administrated by 5 or 10 mg per kilogram body weight daily from day-1 to day 7. Weight loss was measured daily. On day 8, endoscopy was performed and clinical scores were used as a metric of colitis severity. The colon lengths were measured on day 8. All experiments were performed using cohoused mice littermates. All mouse studies were performed in compliance with Yale Institutional Animal Care and Use Committee protocols. No formal blinding or randomization was conducted; however, control and treated groups were chosen arbitrarily for each experiment. Mice weights and colon length were measured in a blinded manner.

Supplemental Figures

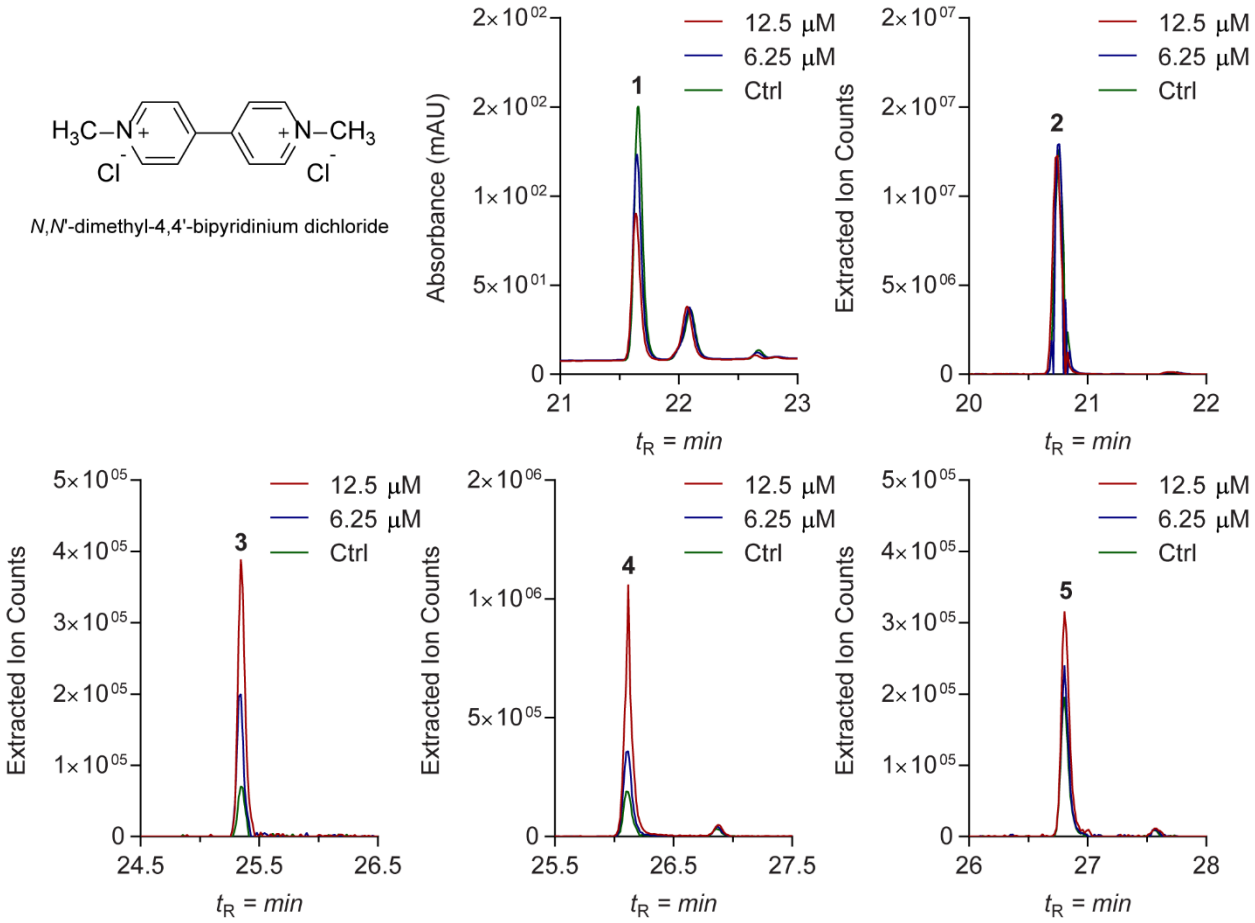

Figure S1. Comparative UV-LC-HRMS profiles for five metabolites **1**-**5** from *P. luminescens* in response to sublethal paraquat-induced redox stress. UV traces of **1** measured at 254 nm and extracted ion counts (EICs) representing the calculated mass of the positively charged metabolites **2**-**5** are shown in the same scale of y axis. Structure of paraquat is shown at the top left, and numbers of compounds are noted in bold. Samples prepared in biological triplicates were analyzed using a reversed-phase C_{18} HPLC analytical column (Phenomenex Kinetex C_{18} (100 Å) 5 µm (4.6 × 250 mm) with a linear gradient from 10 to 100% aqueous ACN in 0.1% formic acid over 30 min with a flow rate of 0.7 ml min^{-1}.

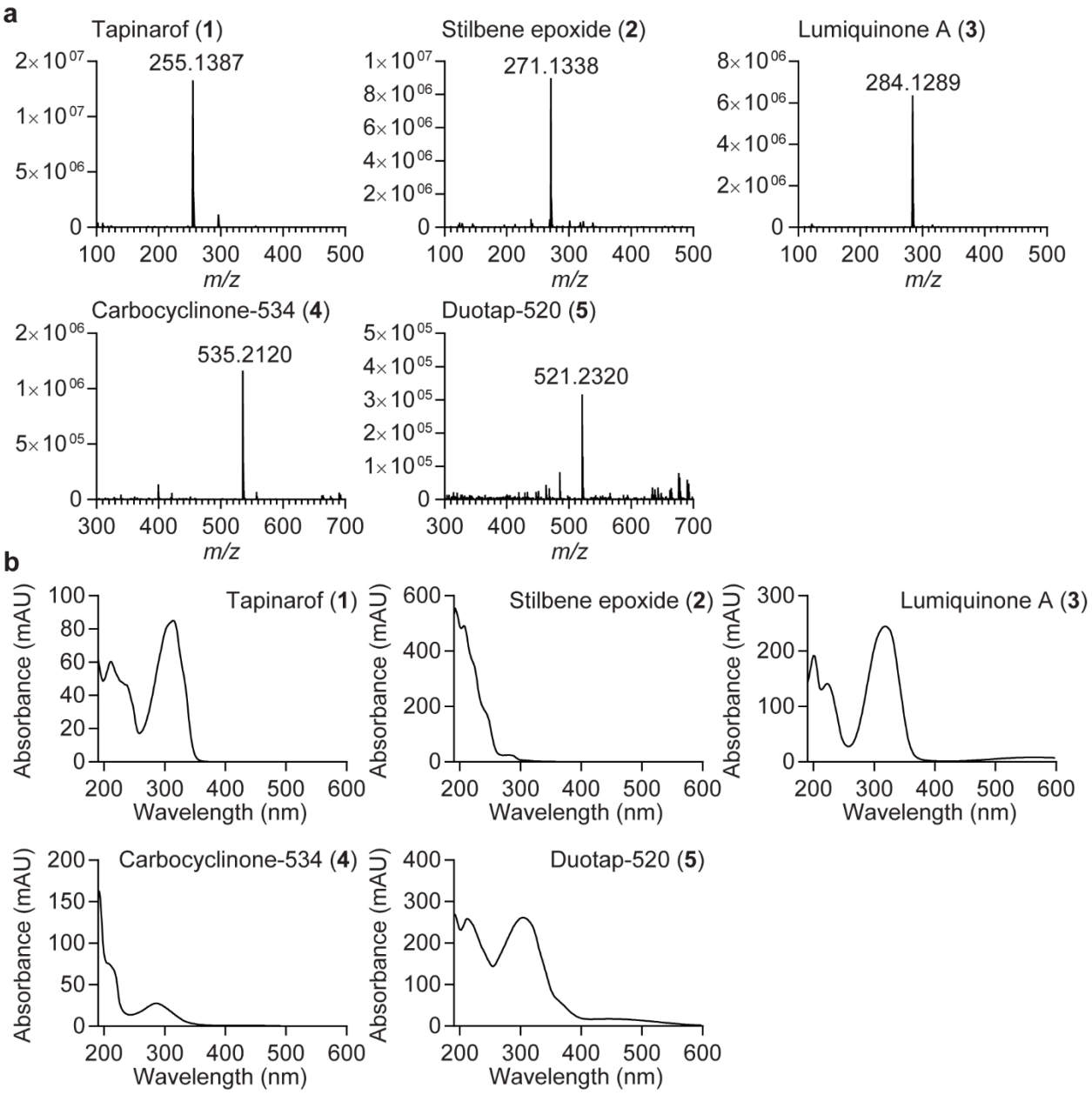

Figure S2. HR-ESI-QTOF-MS (**a**) and UV-visible (**b**) spectra of metabolites **1-5**.

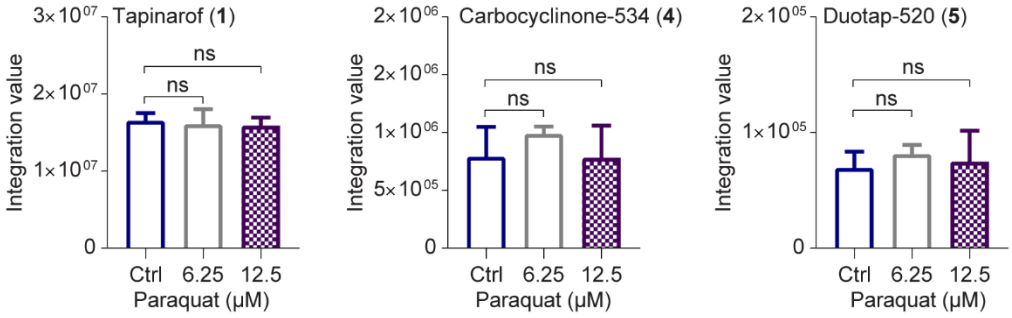

Figure S3. Responses of **1**, **4**, and **5** in the cell-free LB medium supplemented with paraquat. No significant conversion was observed in these control experiments.

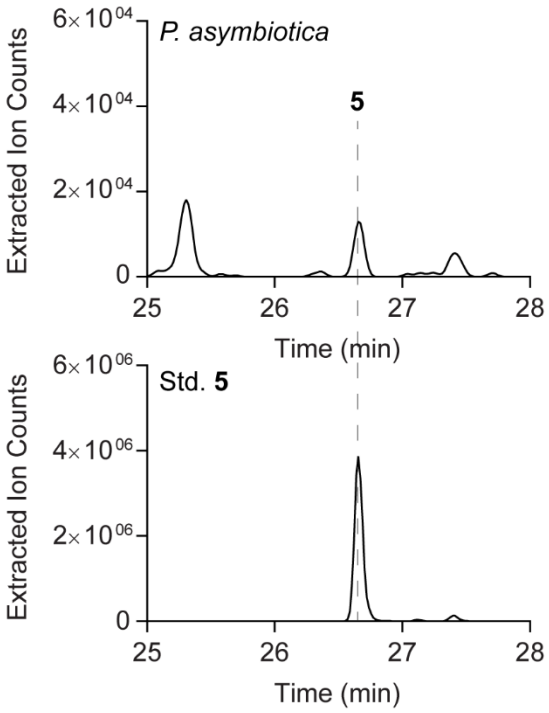

Figure S4. Detection of duotap-520 (**5**) from the 1-liter culture of *P. asymbiotica.*

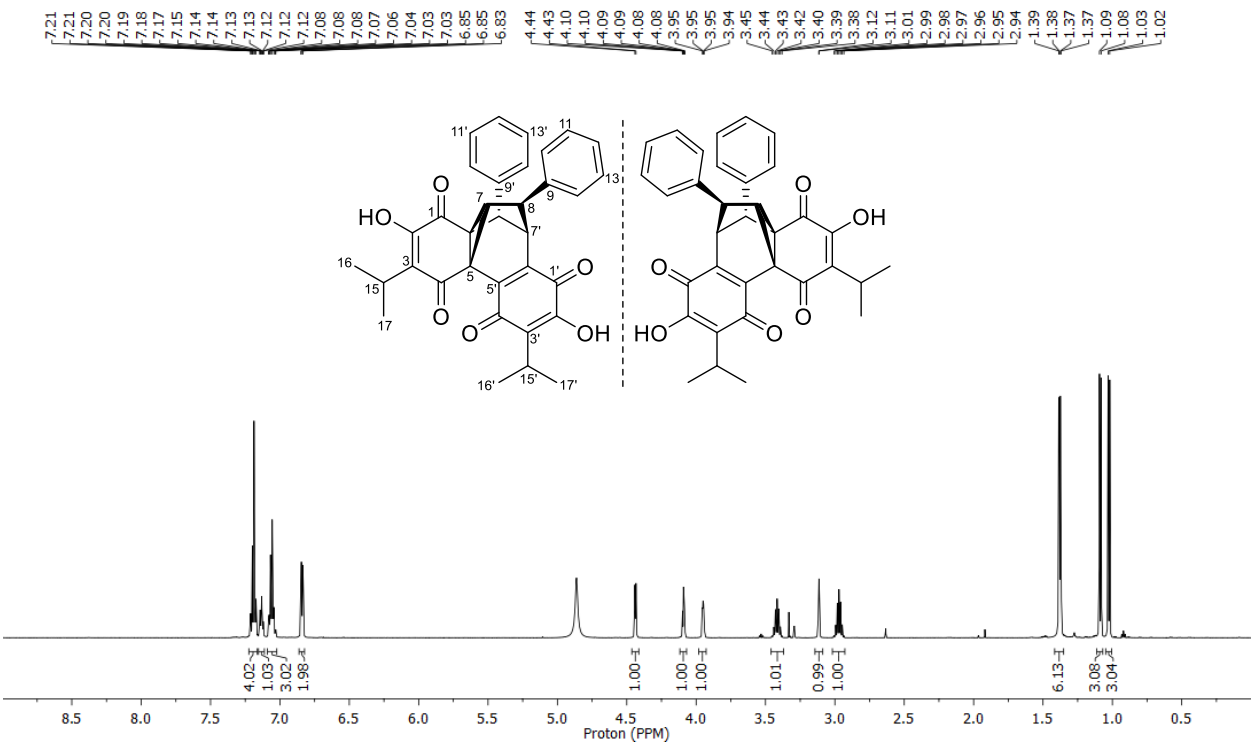

Figure S5. ^{1}H NMR spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

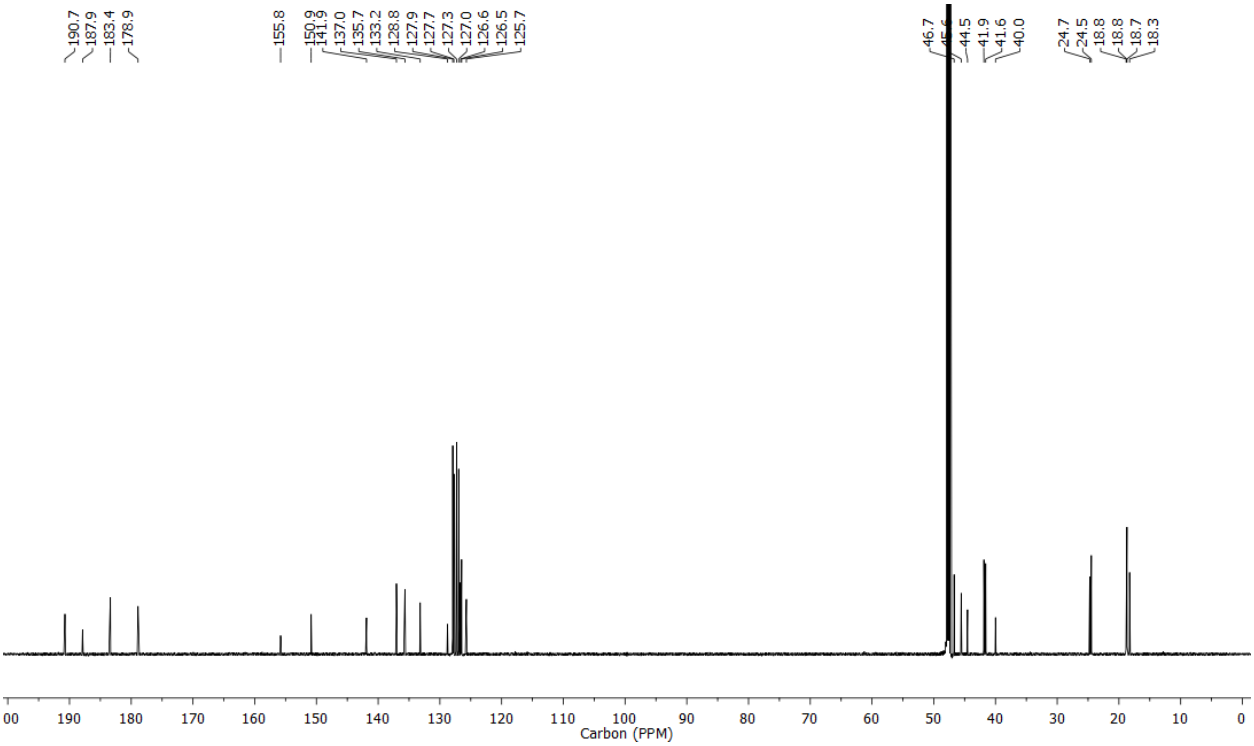

Figure S6. ^{13}C NMR spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

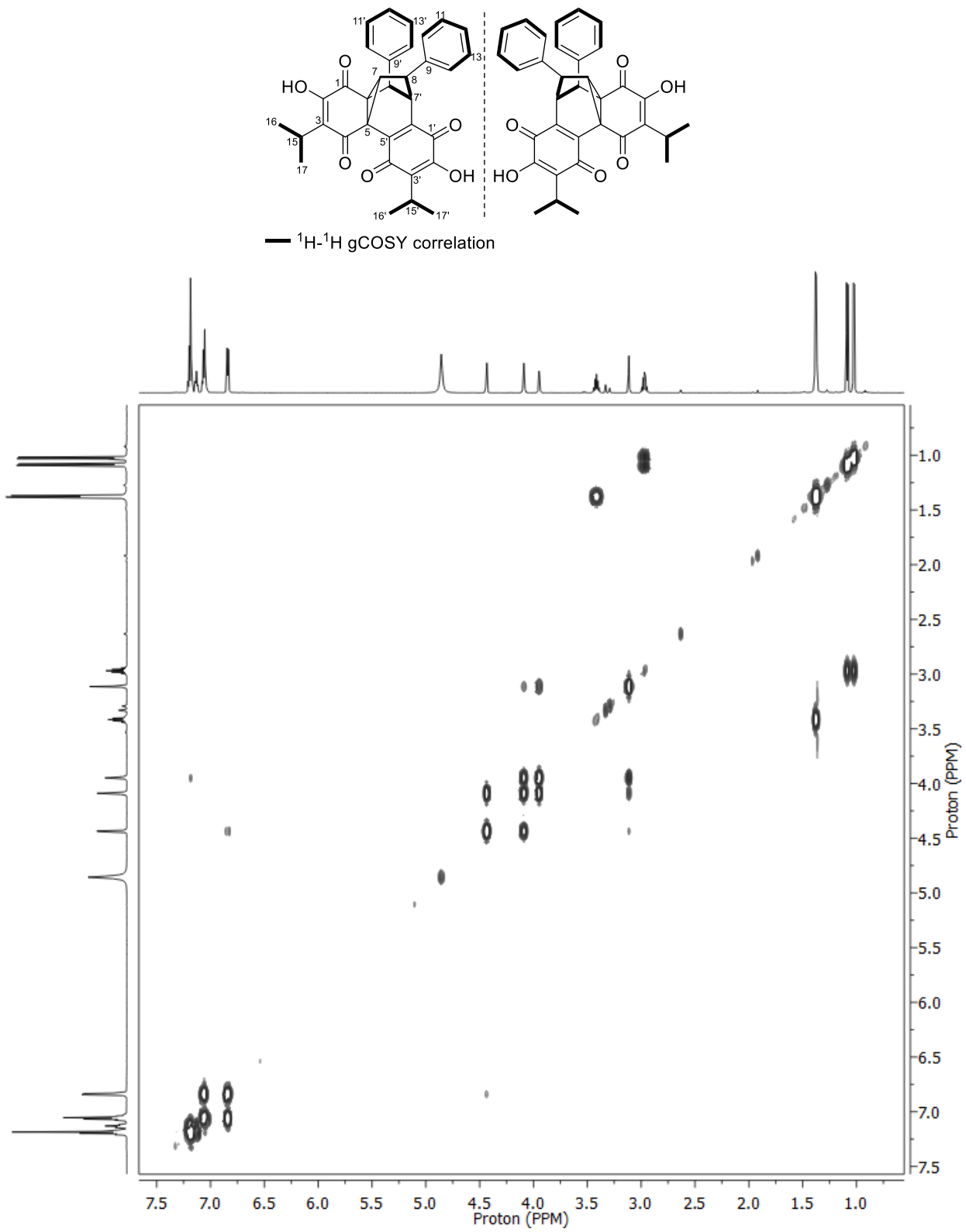

Figure S7. gCOSY NMR spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

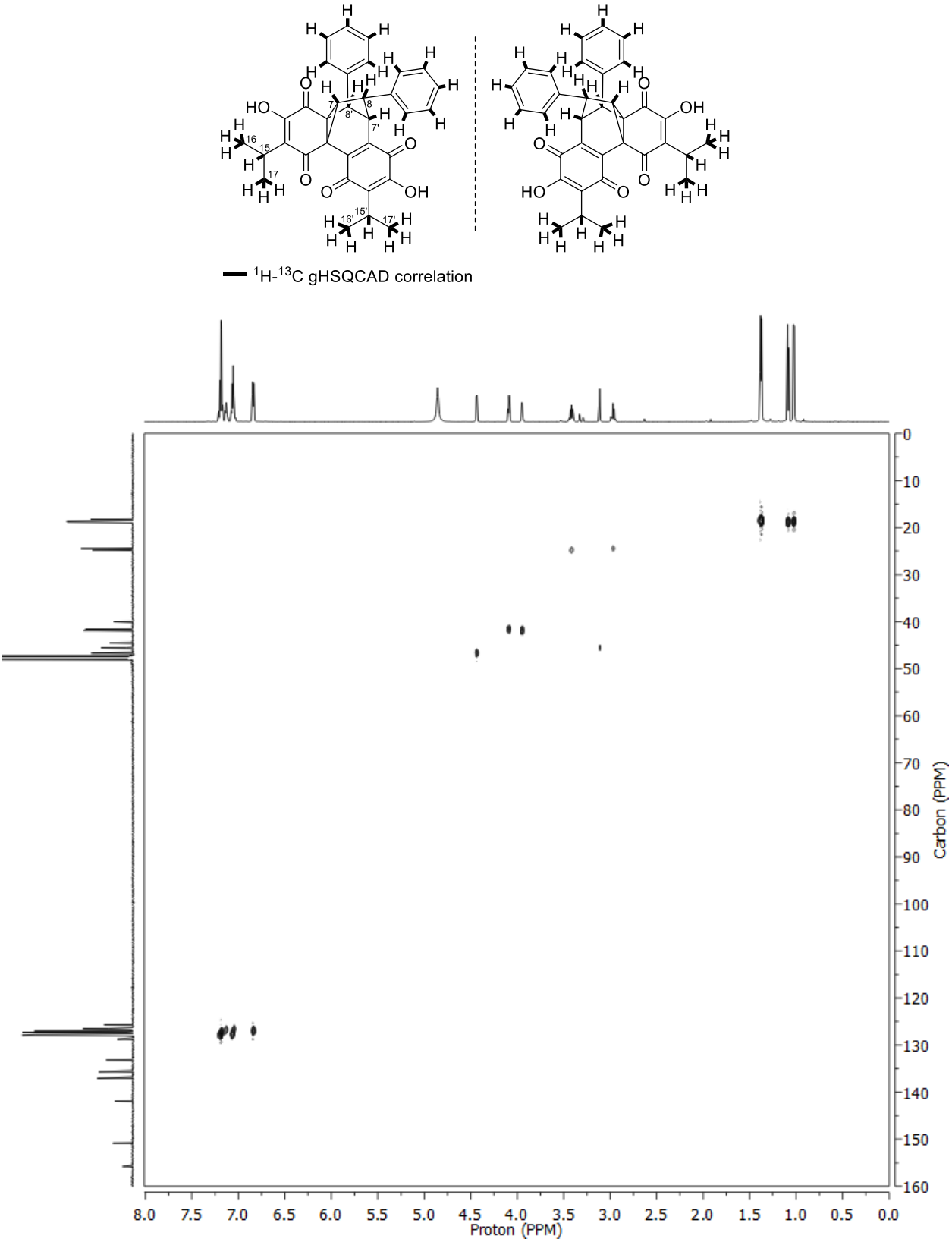

Figure S8. gHSQCAD NMR spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

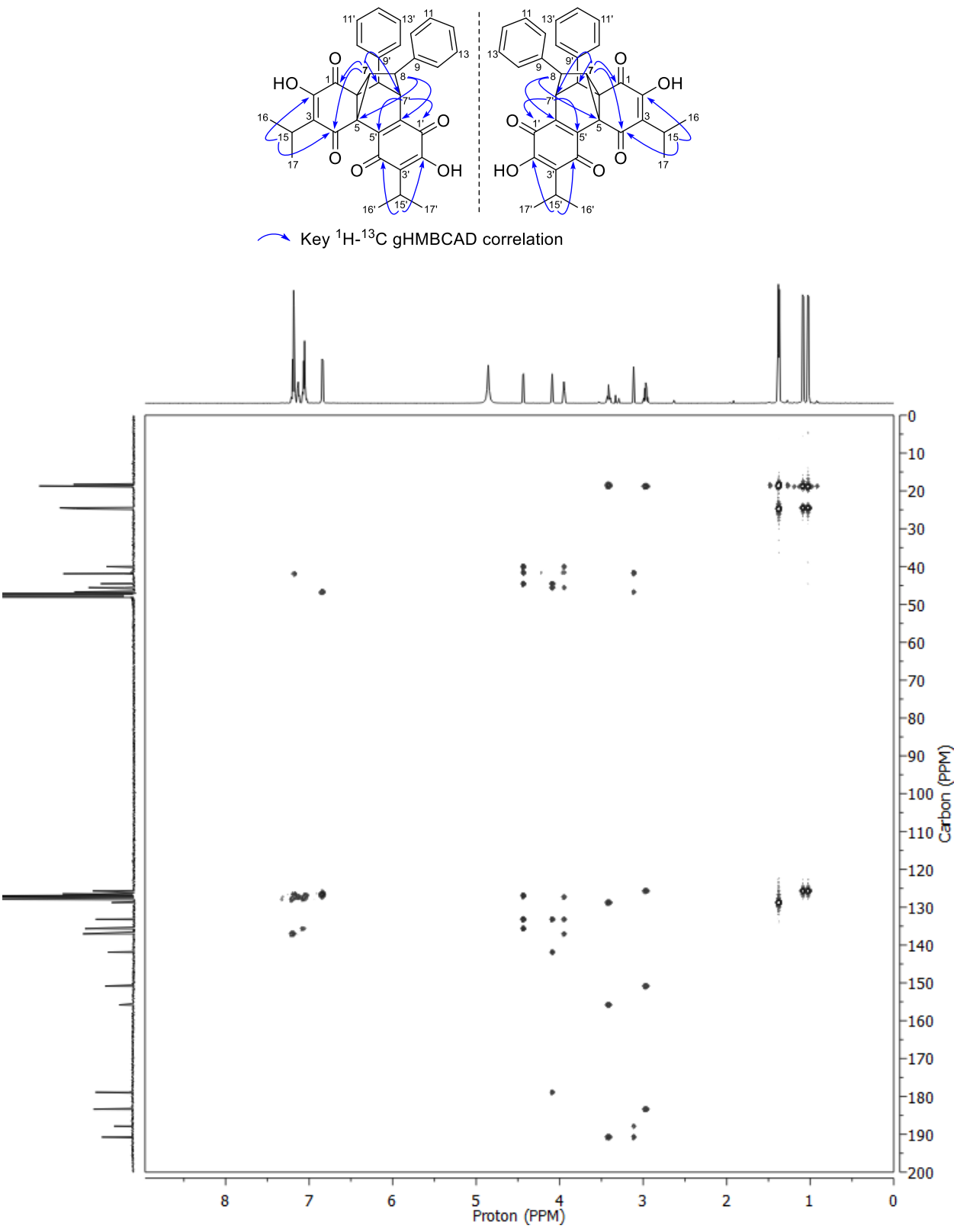

Figure S9. gHMBCAD NMR spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

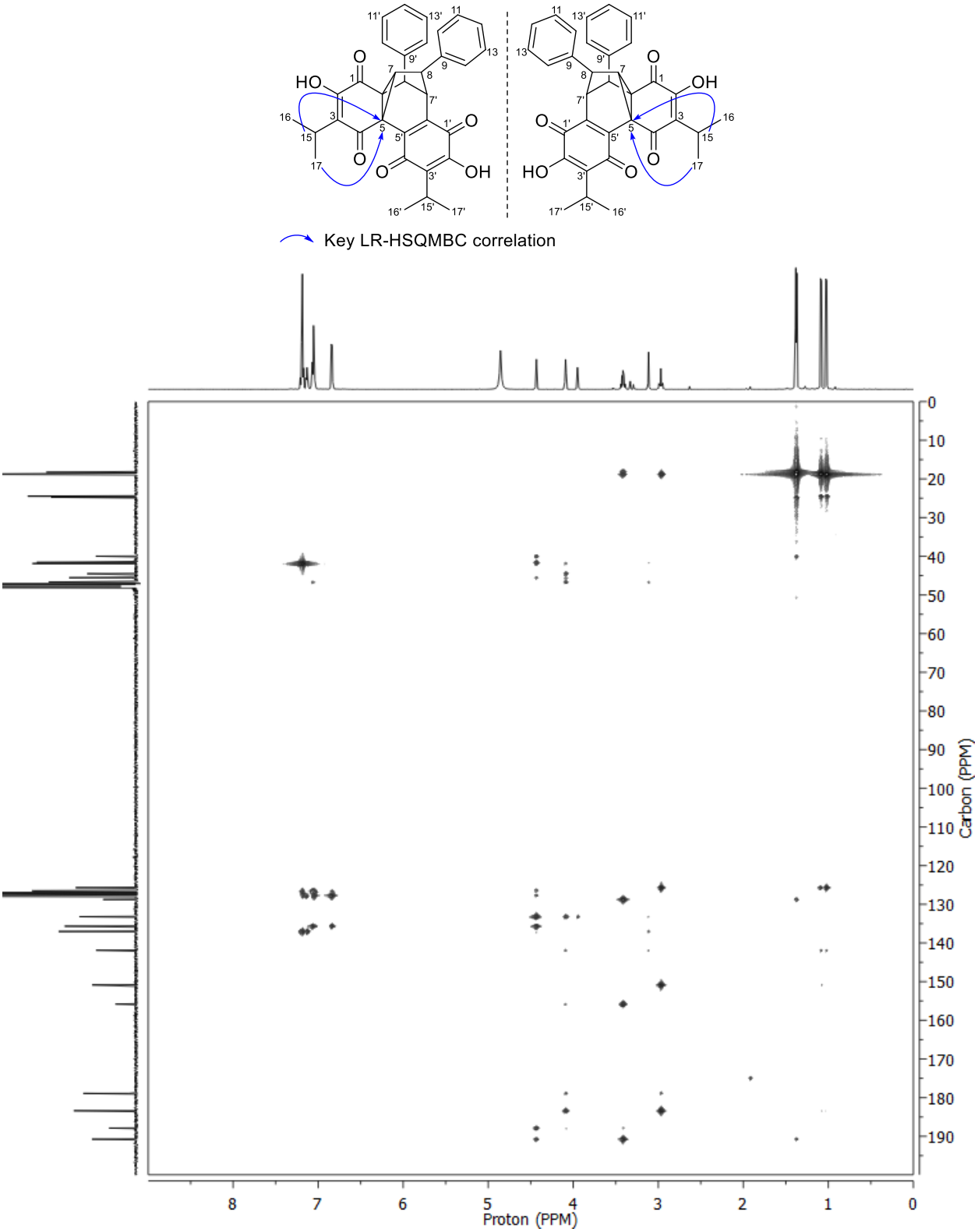

Figure S10. LR-HSQMBC NMR ($^{n}J_{CH}$ = 2 Hz, ni = 640) spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

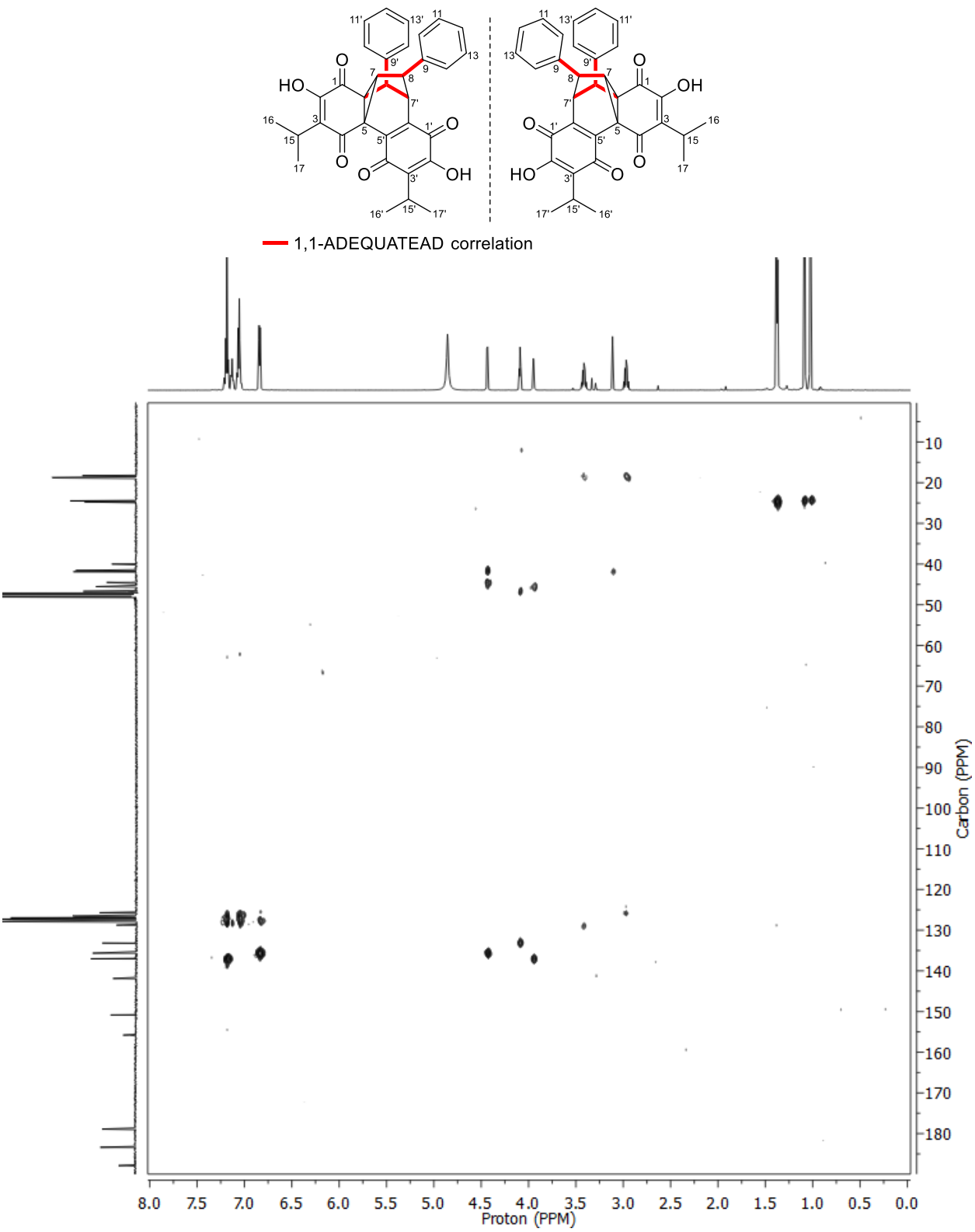

Figure S11. 1,1-ADEQUATEAD NMR ($^{1}J_{CC}$ = 50 Hz) spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

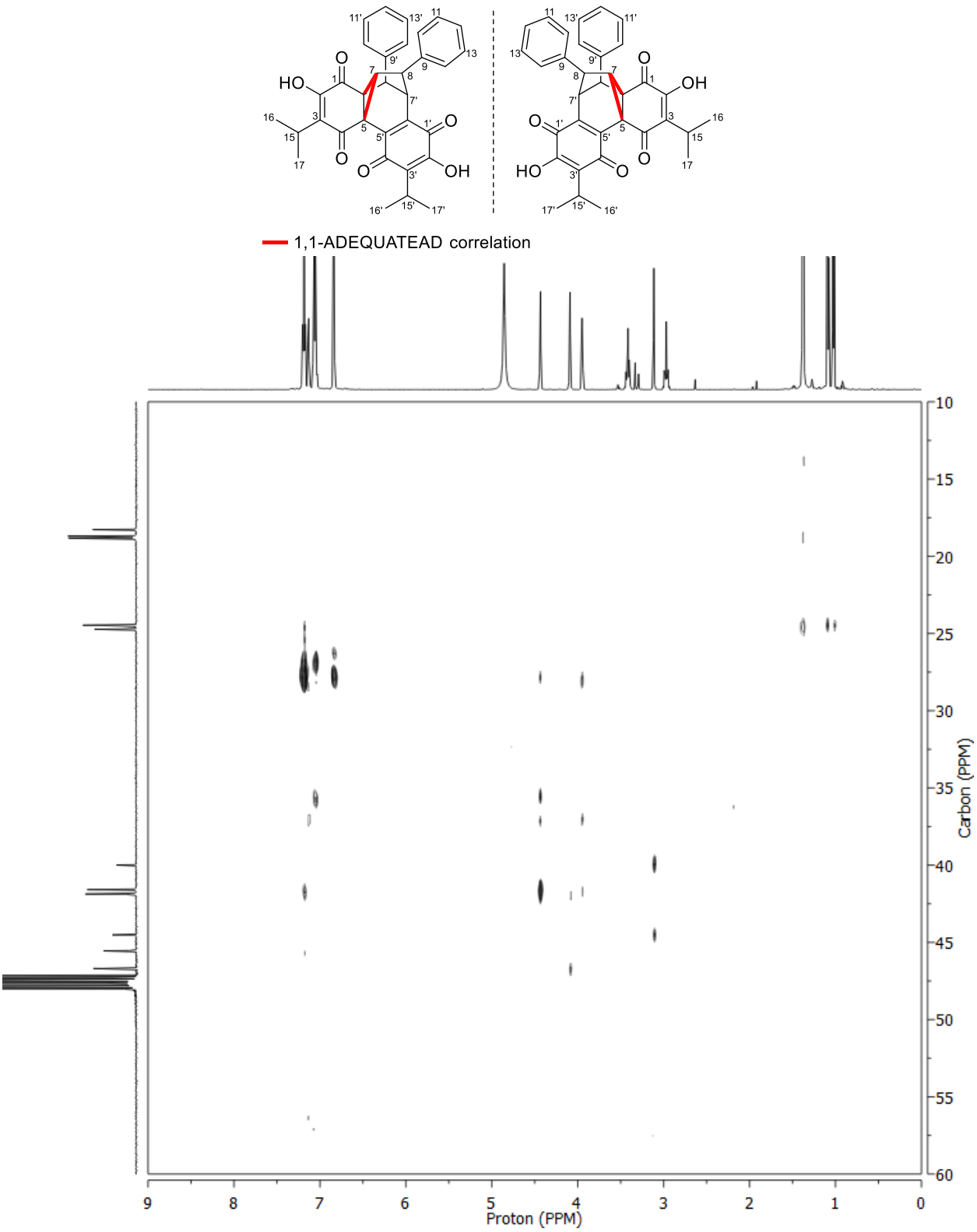

Figure S12. 1,1-ADEQUATEAD NMR ($^{1}J_{CC}$ = 10 Hz) spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

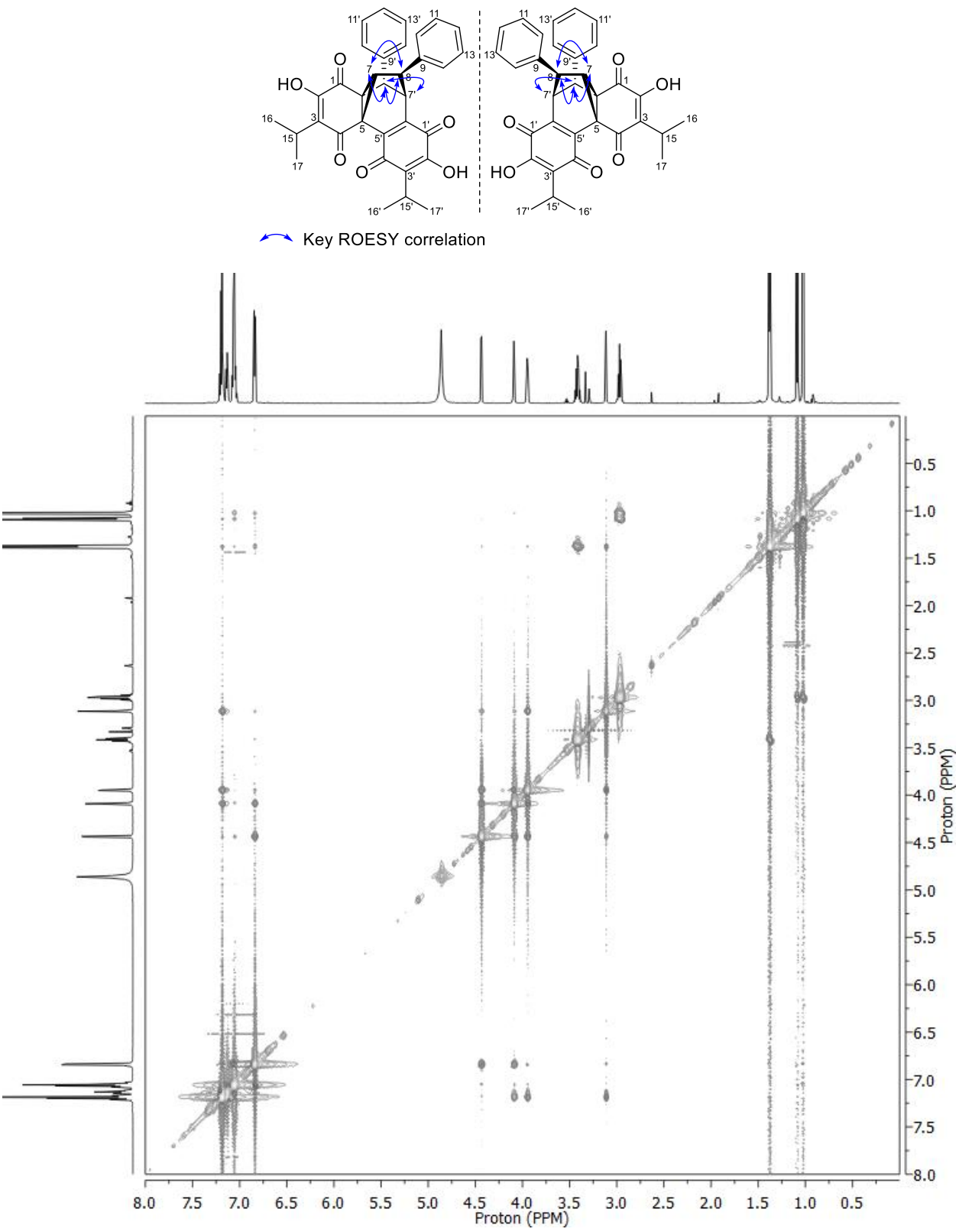

Figure S13. ROESYAD NMR spectrum of carbocyclinone-534 (**4**) in methanol-d_4.

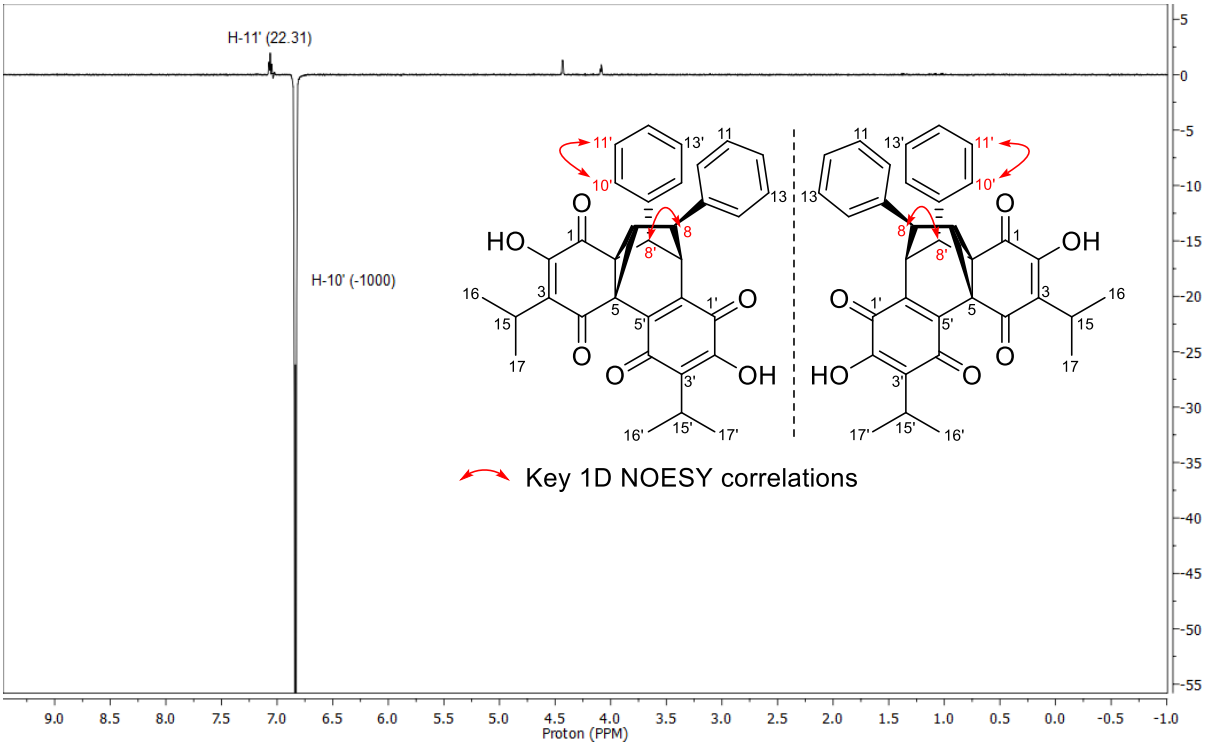

Figure S14. 1D NOESY NMR spectrum with irradiation of H-10′ in methanol-d_4.

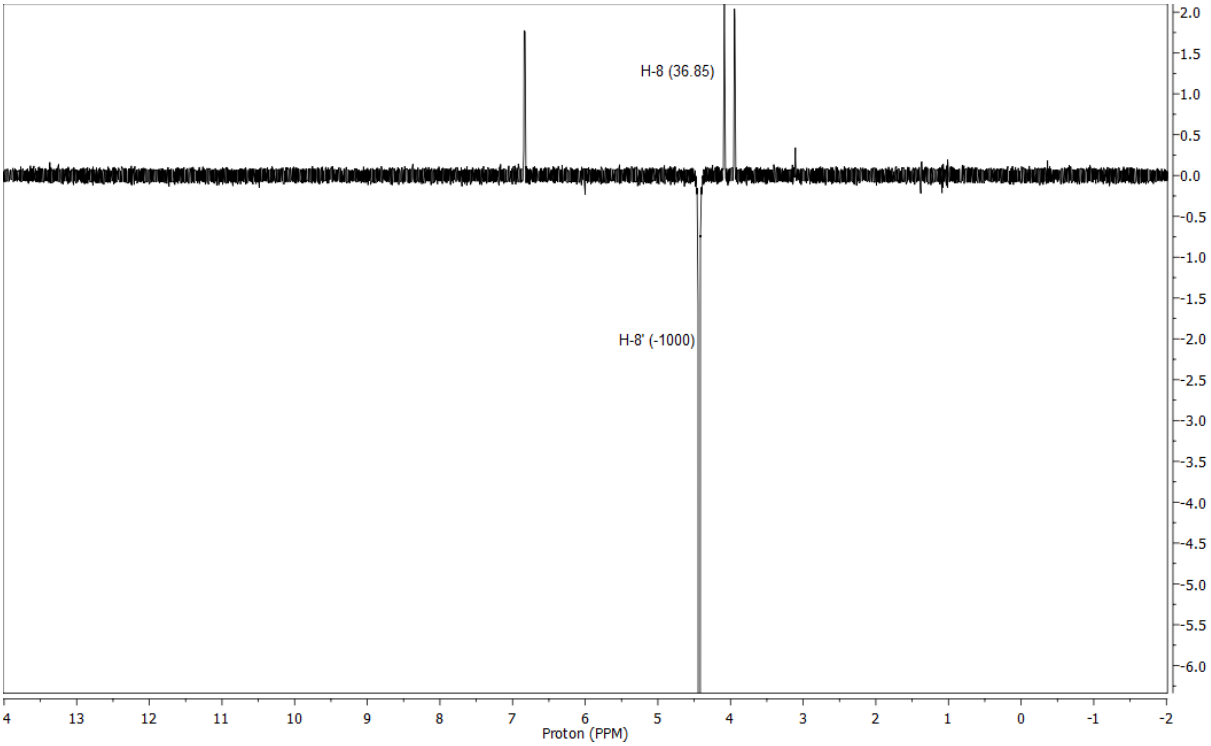

Figure S15. 1D NOESY NMR spectrum with irradiation of H-8′ in methanol-d_4.

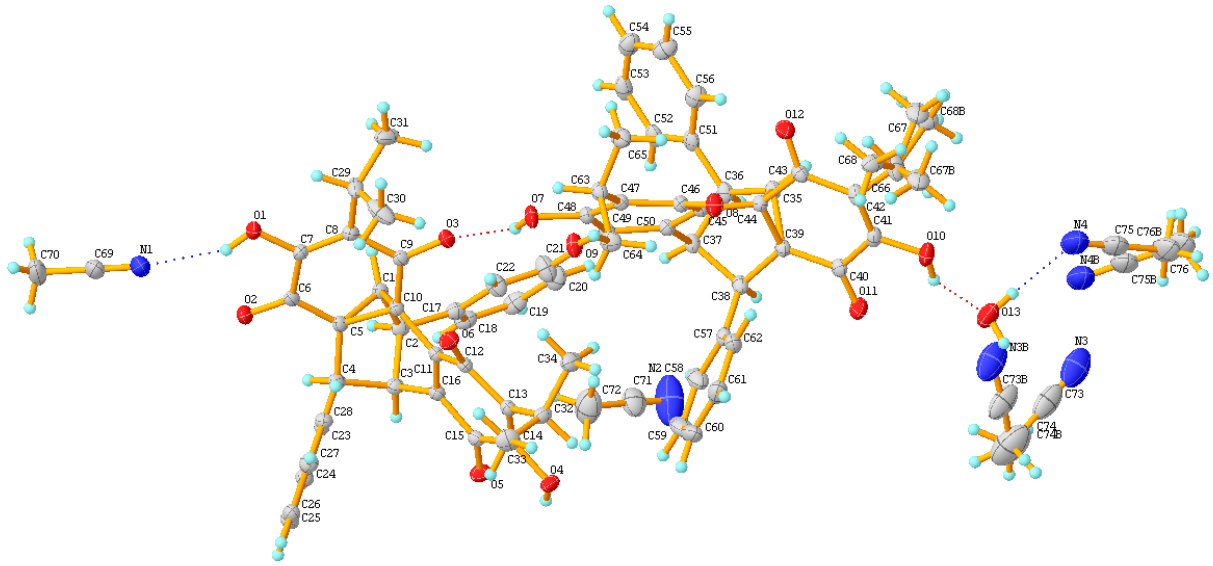

Figure S16. The complete numbering scheme of carbocyclinone-534 (**4**) with 50% thermal ellipsoid probability levels. The hydrogen atoms are shown as circles for clarity.

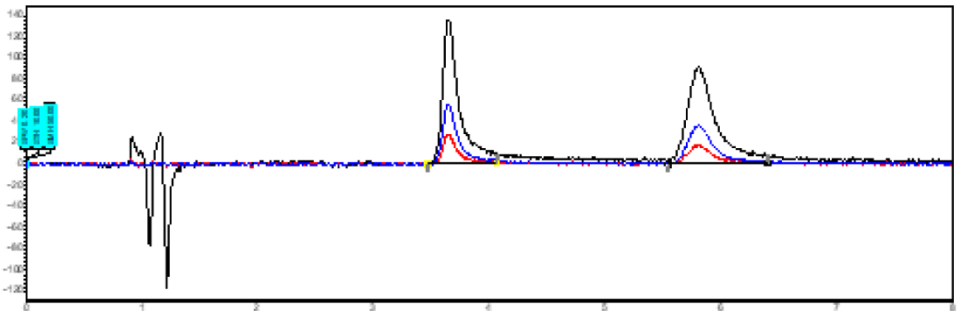

Figure S17. HPLC separation trace of a racemic carbocyclinone-534 (**4**). The racemic mixture **4** was separated on an AD-H column (2 × 25 cm; eluted with 30% isopropanol/CO_2 in 0.1% DEA; 60 ml min^{-1}) to obtain (+)-**4** (3.0 mg, t_R = 3.48 min) and (−)-**4** (1.0 mg, t_R = 5.45 min). Analytical method is as follows: Column; AD-H (0.46 × 25 cm; eluted with 30% isopropanol/CO_2 in 0.1% DEA; 3 ml min^{-1}). Image was provided from Lotus Separations, LLC.

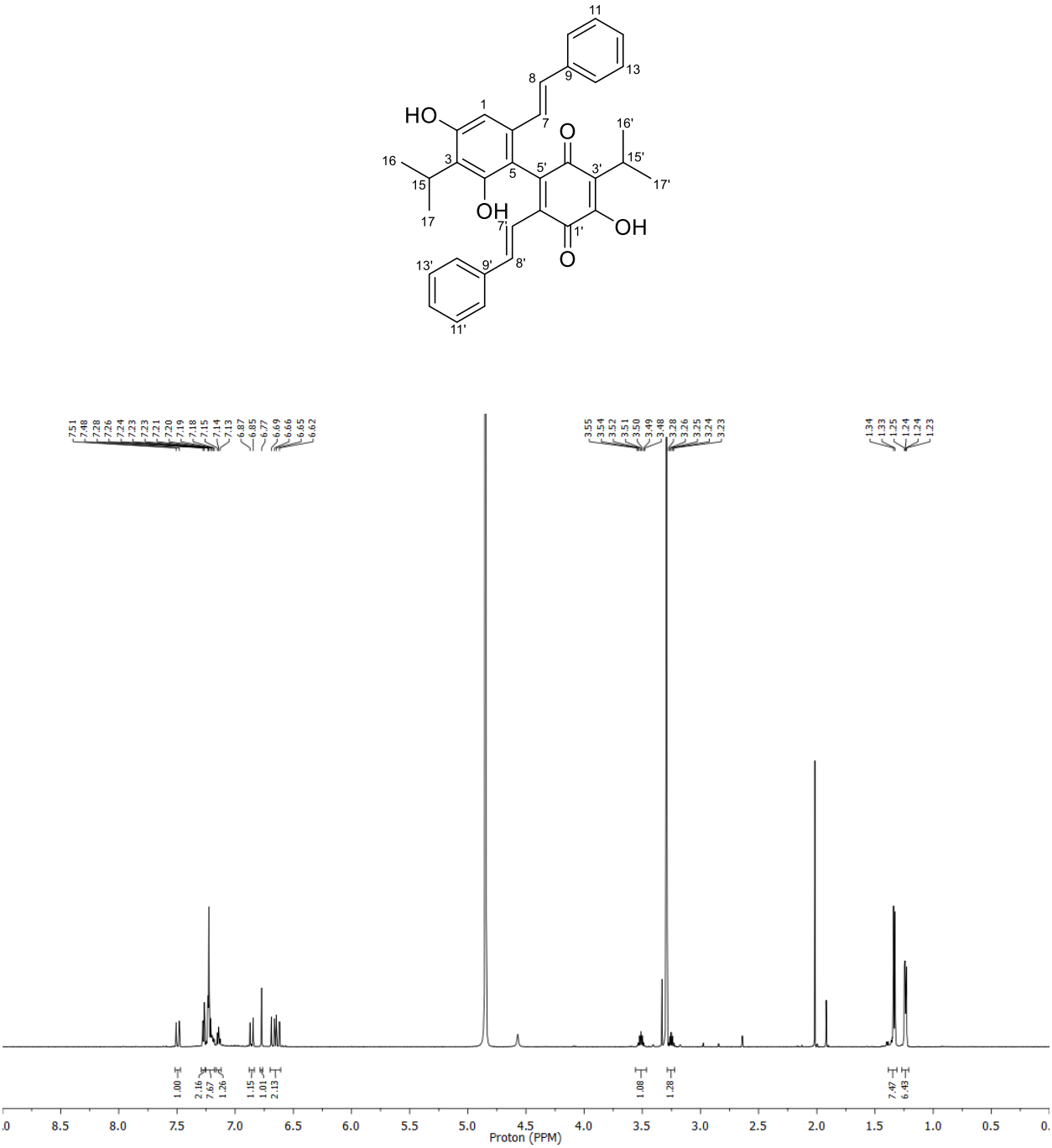

Figure S18. ^{1}H NMR spectrum of duotap-520 (**5**) in methanol-d_4.

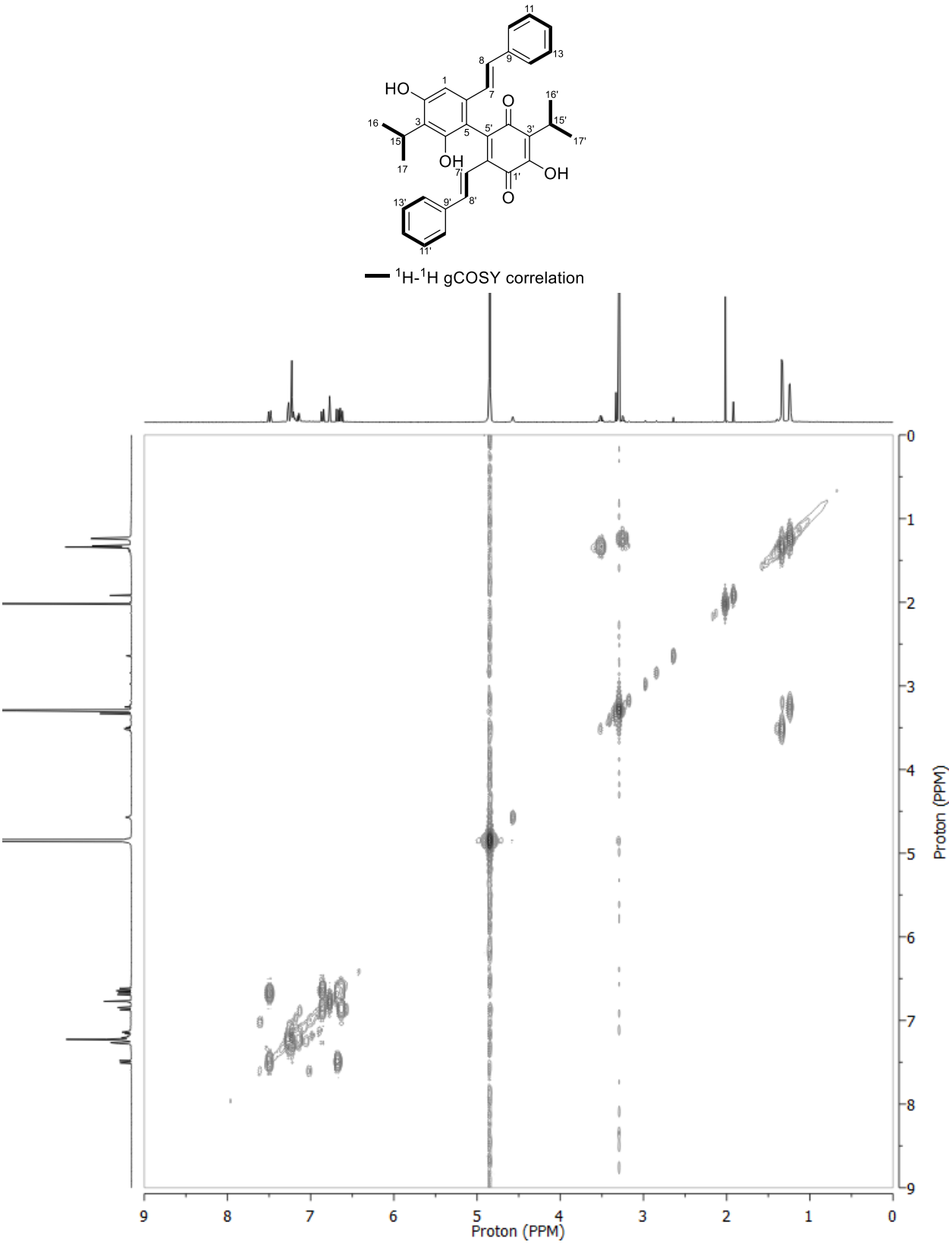

Figure S19. gCOSY NMR spectrum of duotap-520 (**5**) in methanol-d_4.

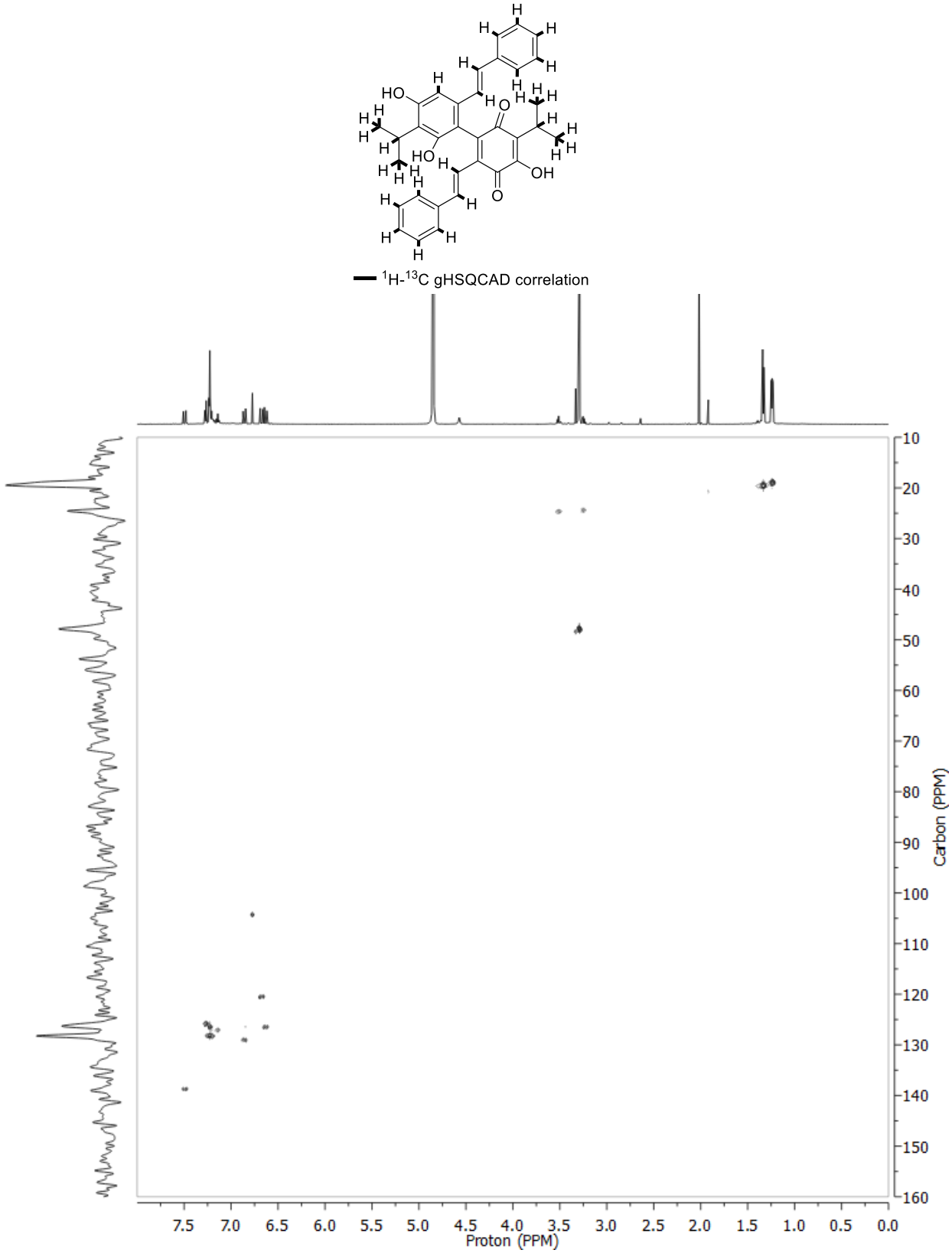

Figure S20. gHSQCAD NMR spectrum of duotap-520 (**5**) in methanol-d_4.

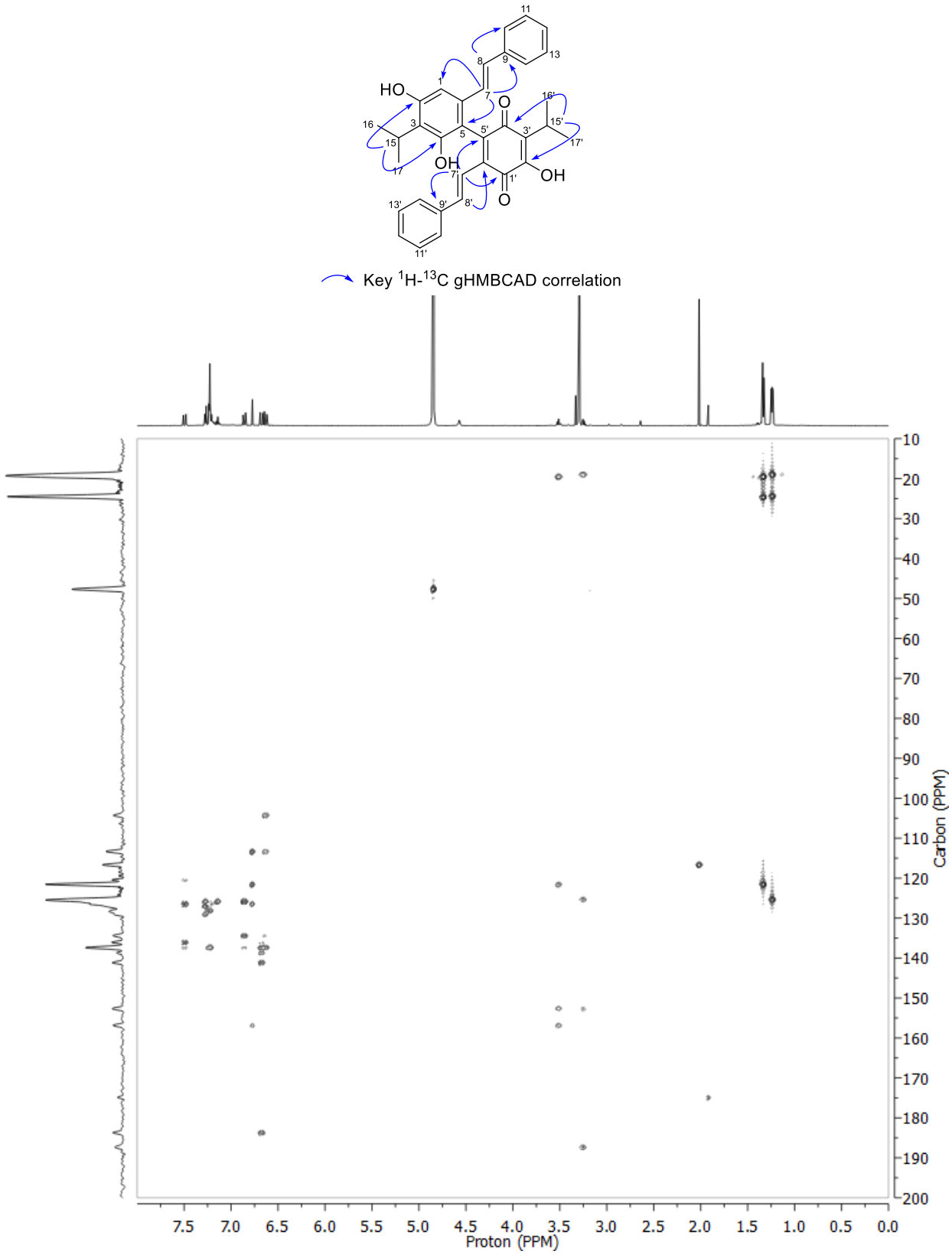

Figure S21. gHMBCAD NMR spectrum of duotap-520 (**5**) in methanol-d_4.

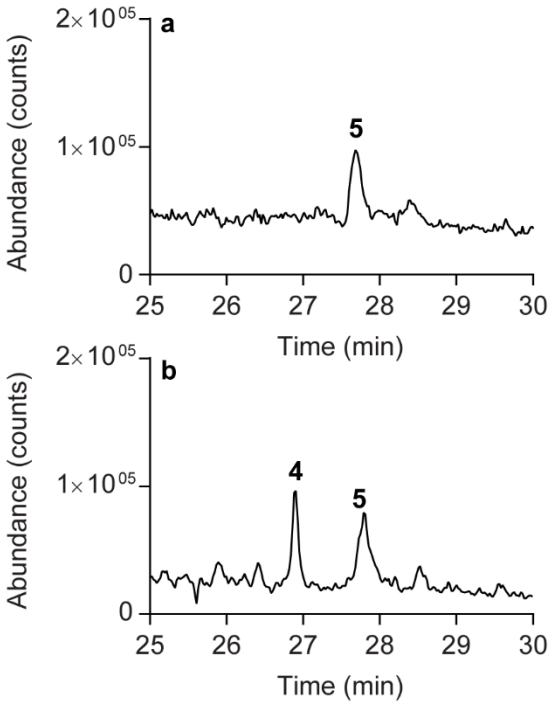

Figure S22. Slow conversion of duotap-520 (**5**) to carbocyclinone-534 (**4**). **a**. TIC chromatogram of duotap-520 (**5**). **b**. TIC chromatogram of duotap-520 (**5**) incubated for overnight at 37 °C in buffer.

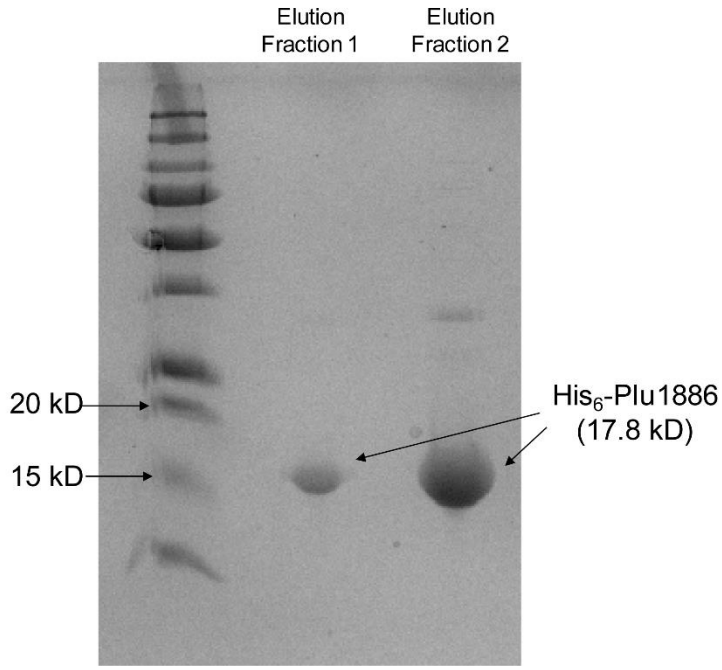

Figure S23. SDS-PAGE gel of elution fractions from the purification of His_6-Plu1886.

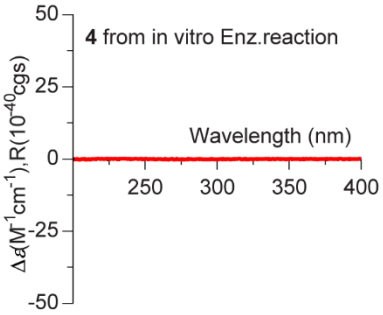

Figure S24. ECD spectrum of **4** isolated from *in vitro* reconstitution of Plu1886.

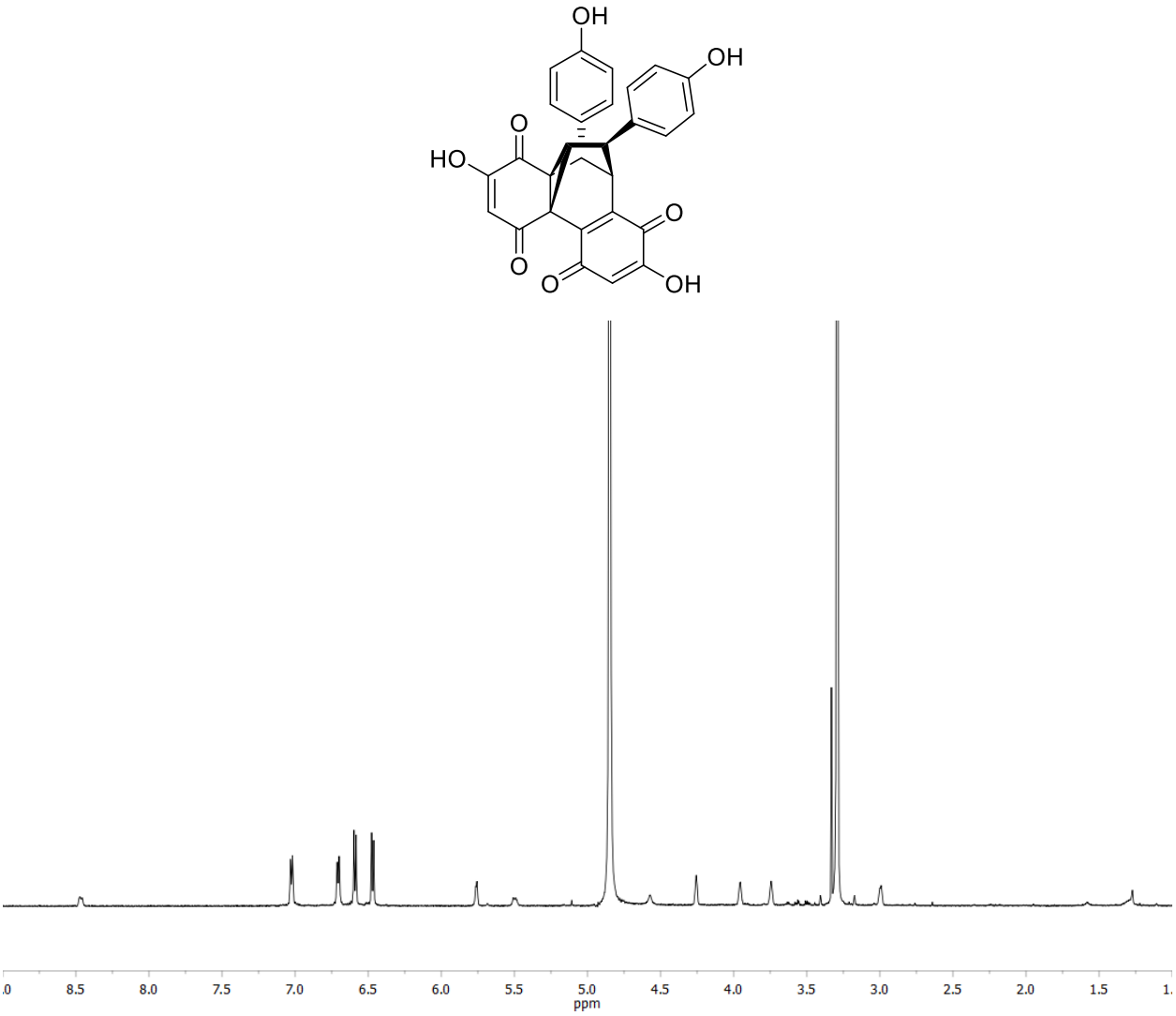

Figure S25. ^{1}H NMR spectrum of carbocyclinone-482 in methanol-d_4.

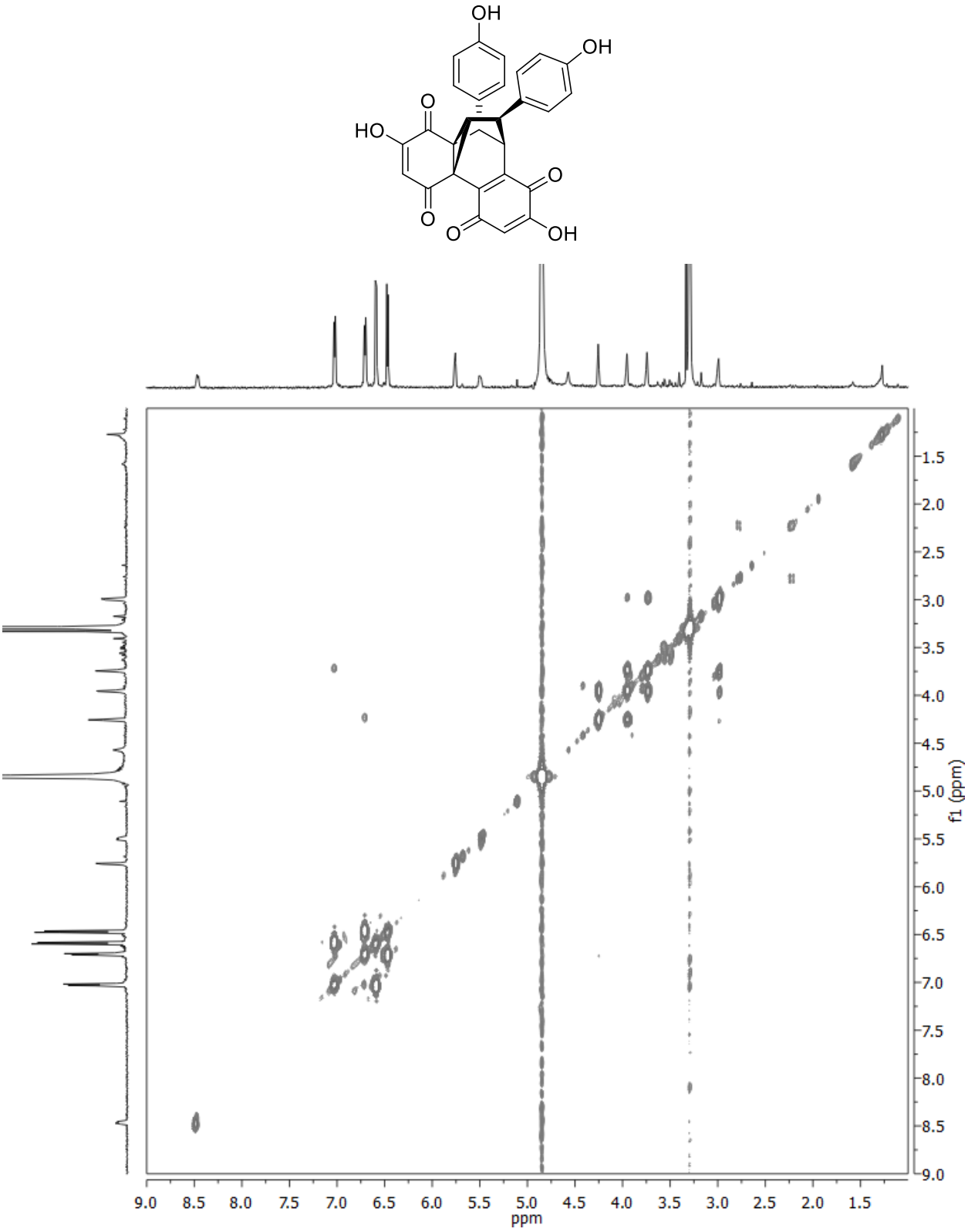

Figure S26. gCOSY NMR spectrum of carbocyclinone-482 in methanol-d_4.

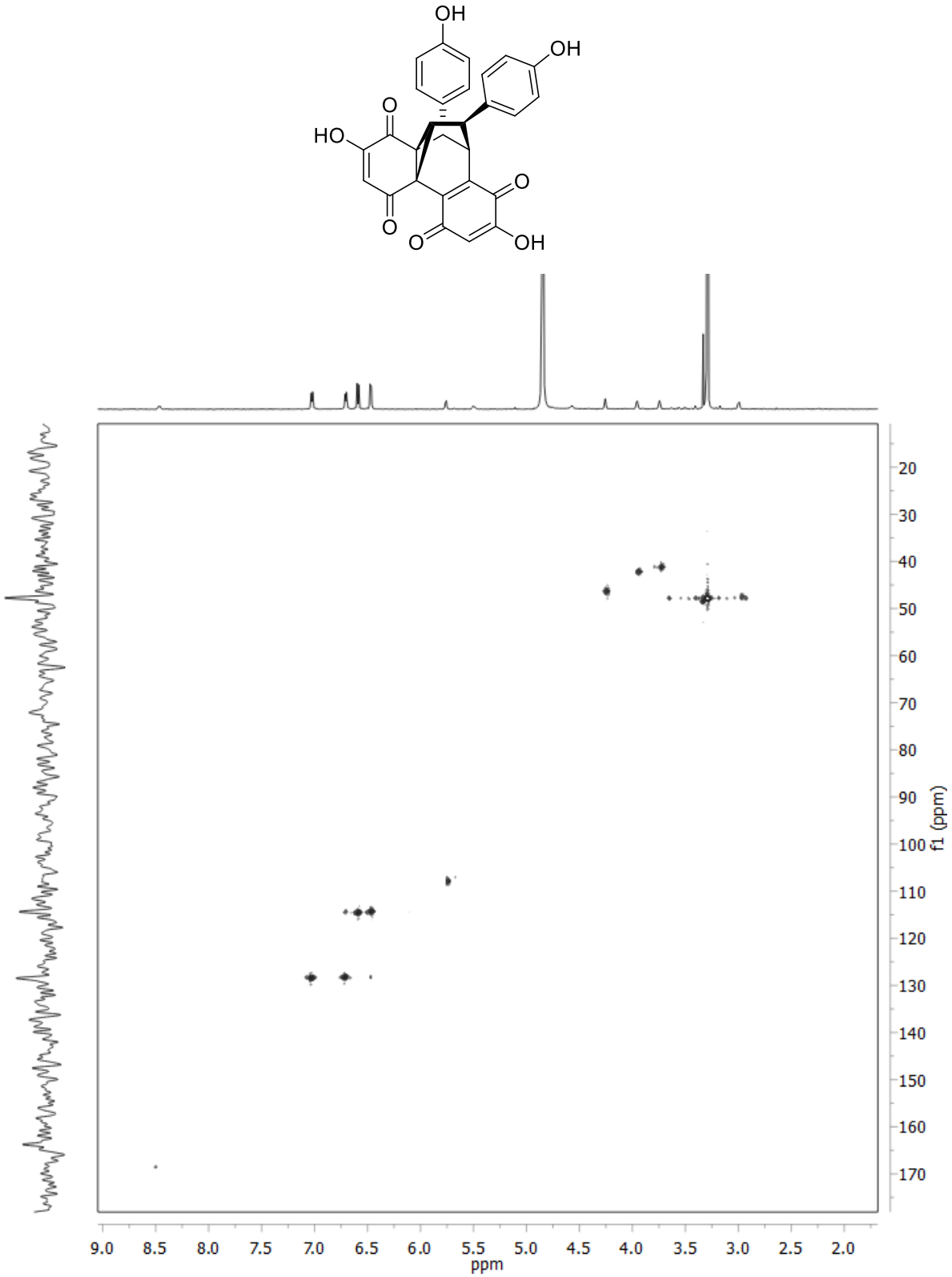

Figure S27. gHSQCAD NMR spectrum of carbocyclinone-482 in methanol-d_4.

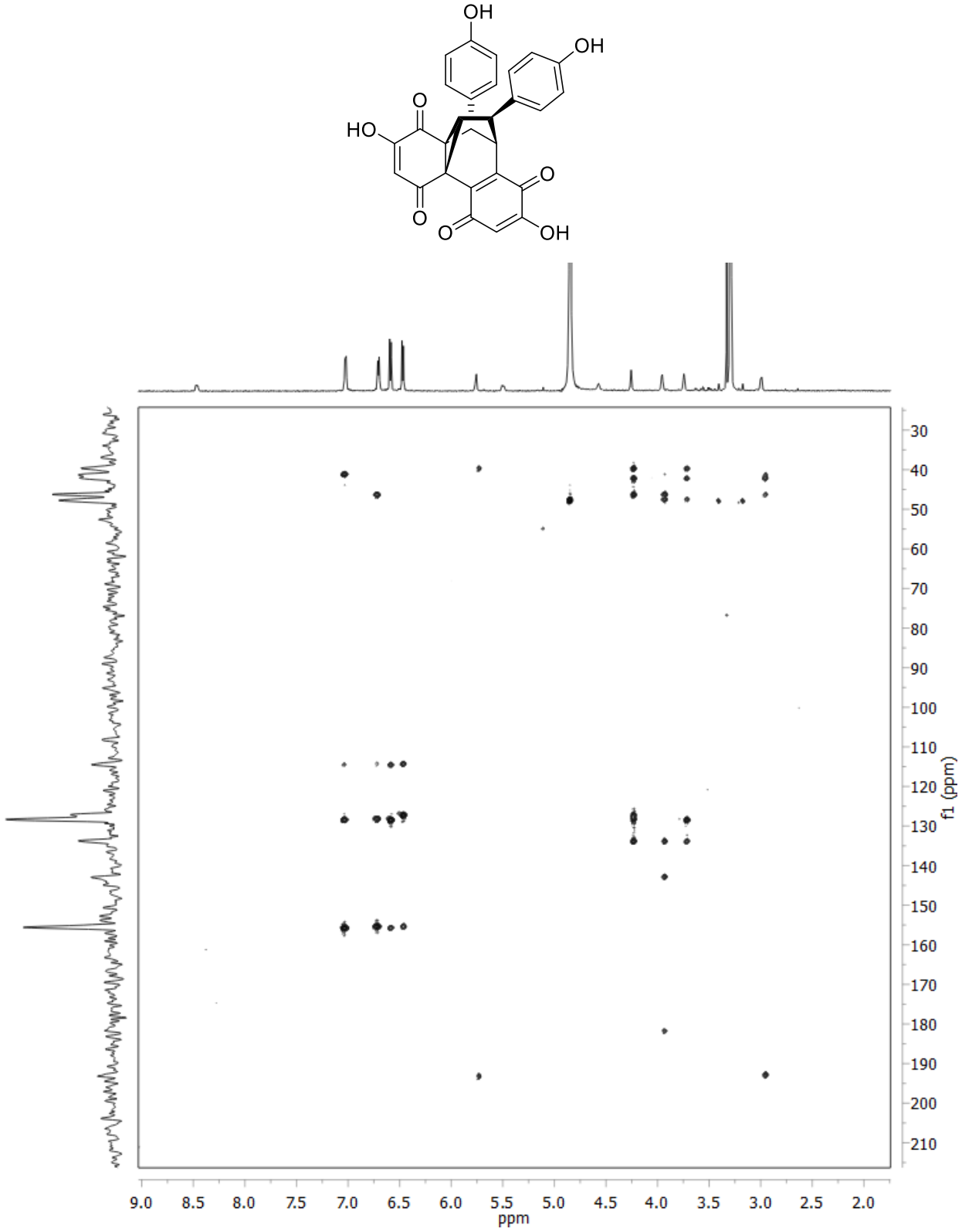

Figure S28. gHMBCAD NMR spectrum of carbocyclinone-482 in methanol-d_4.

Figure S29. ^{1}H NMR spectrum of duotap-436 in methanol-d_4.

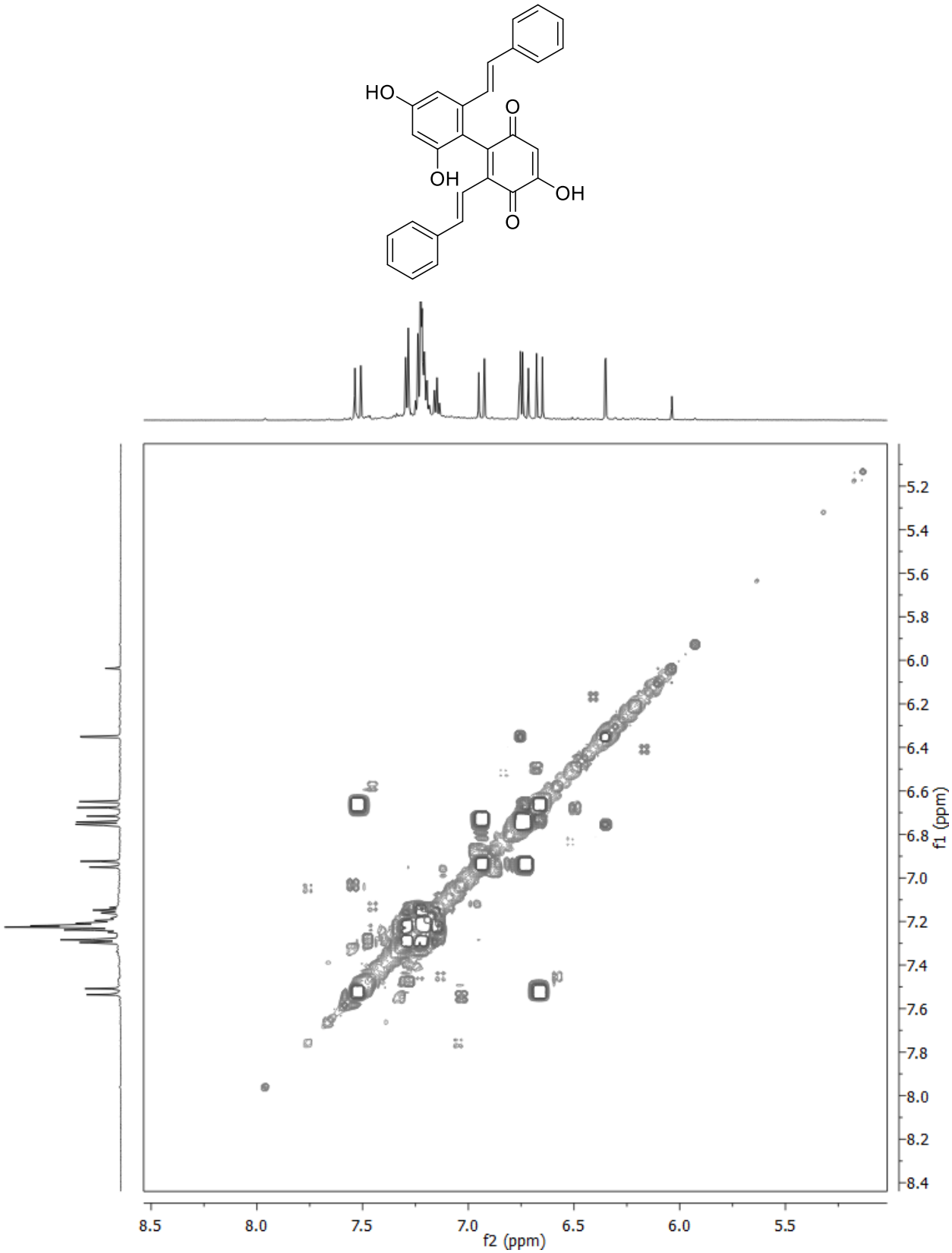

Figure S30. gCOSYAD NMR spectrum of duotap-436 in methanol-d_4.

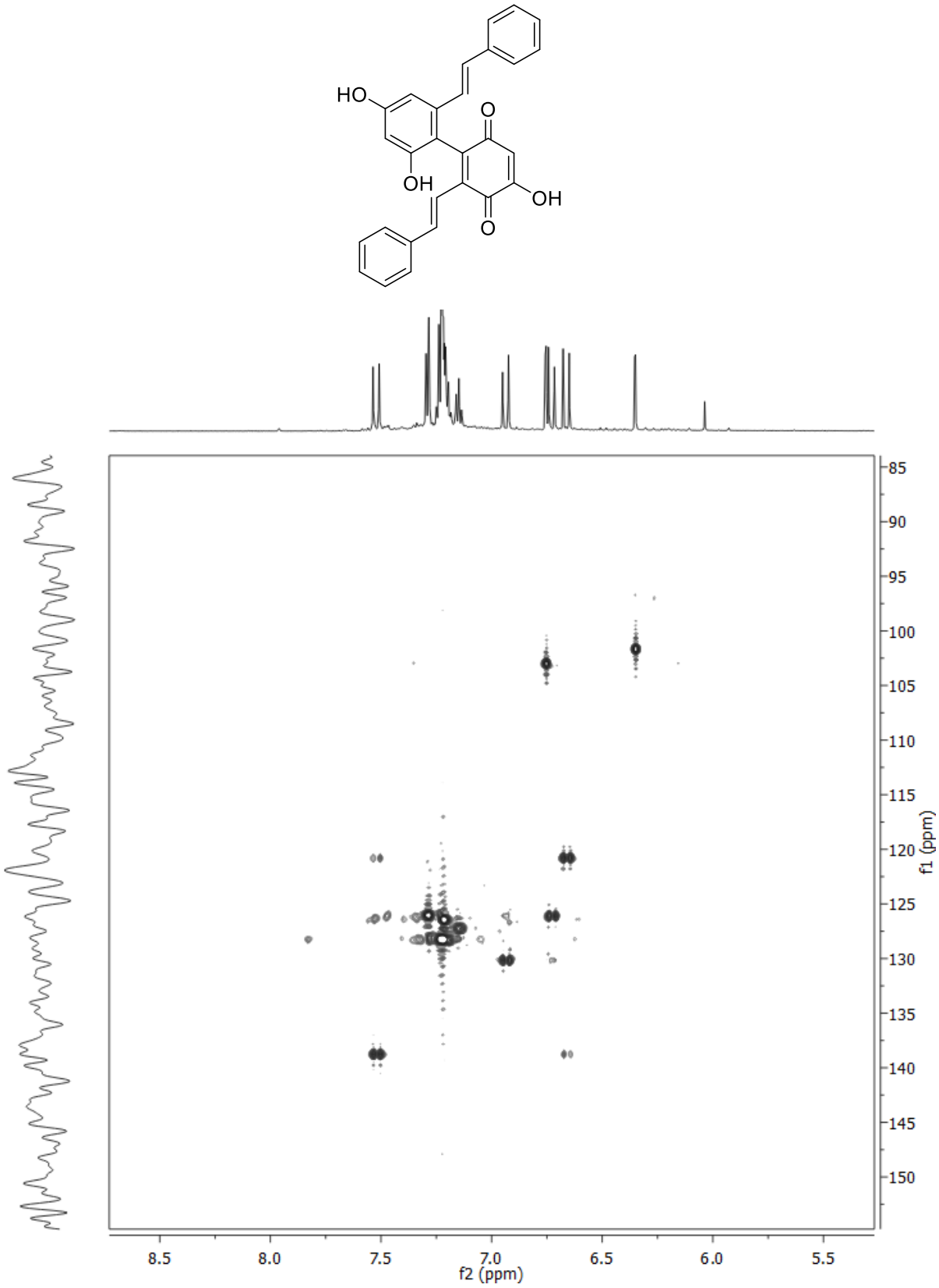

Figure S31. gHSQCAD NMR spectrum of duotap-436 in methanol-d_4.

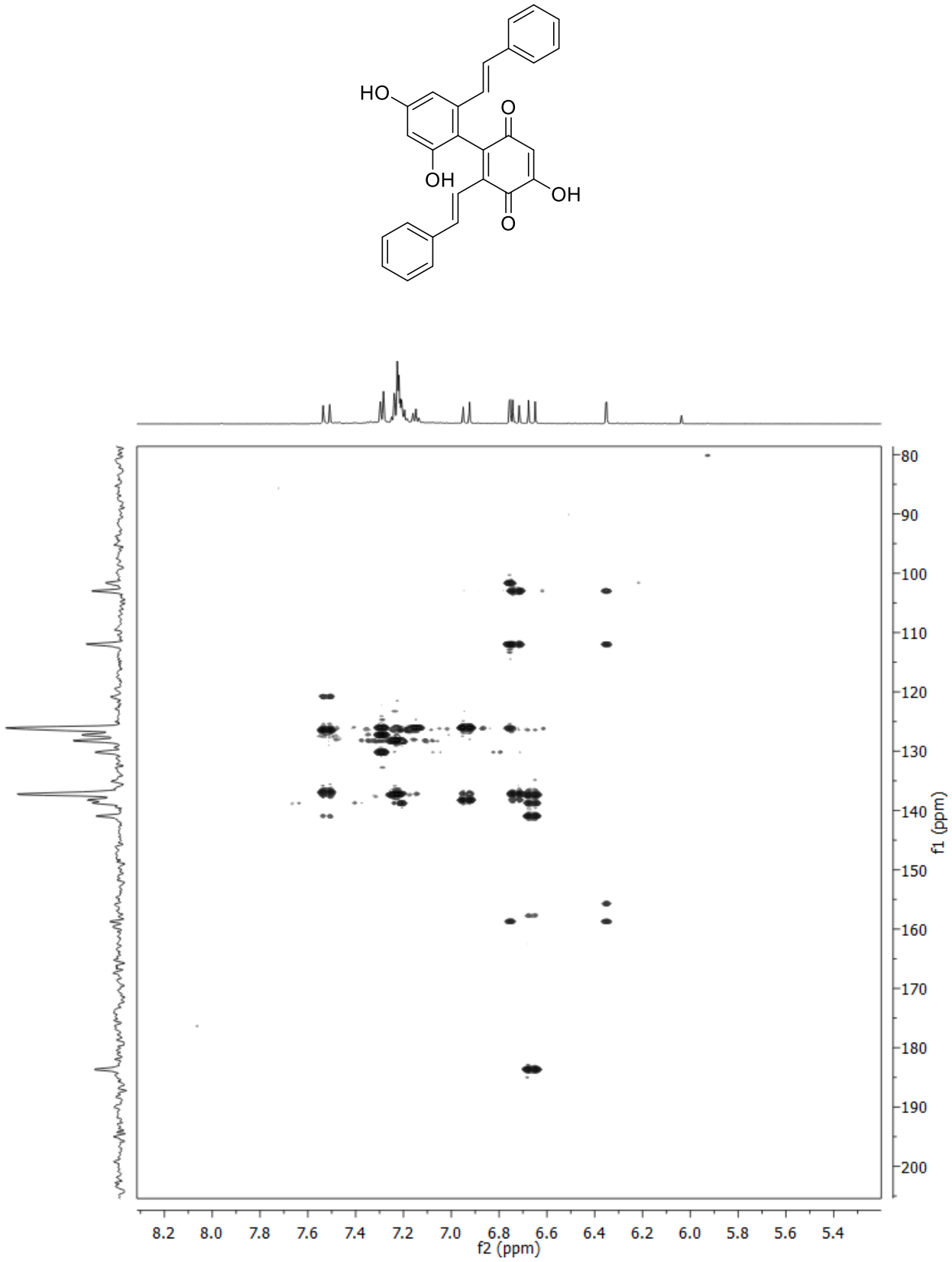

Figure S32. gHMBCAD NMR spectrum of duotap-436 in methanol-d_4.

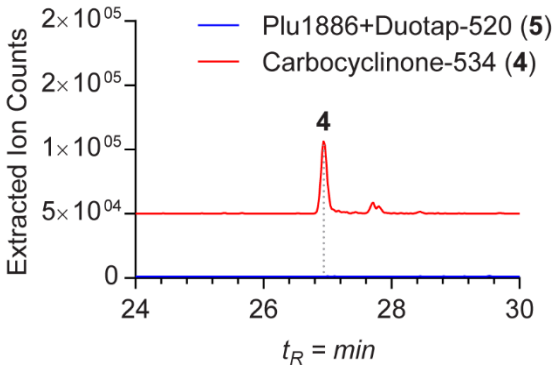

Figure S33. A representative trial of *in vitro* production of carbocyclinone-534 (**4**) from the supplementation of duotap-520 (**5**) in the presence of Plu1886 at 37 °C for overnight. Red line indicates the EIC data of pure compound carbocyclinone-534 (**4**) and blue line indicates the EIC data of in vitro reaction of duotap-520 in the presence of Plu1886.

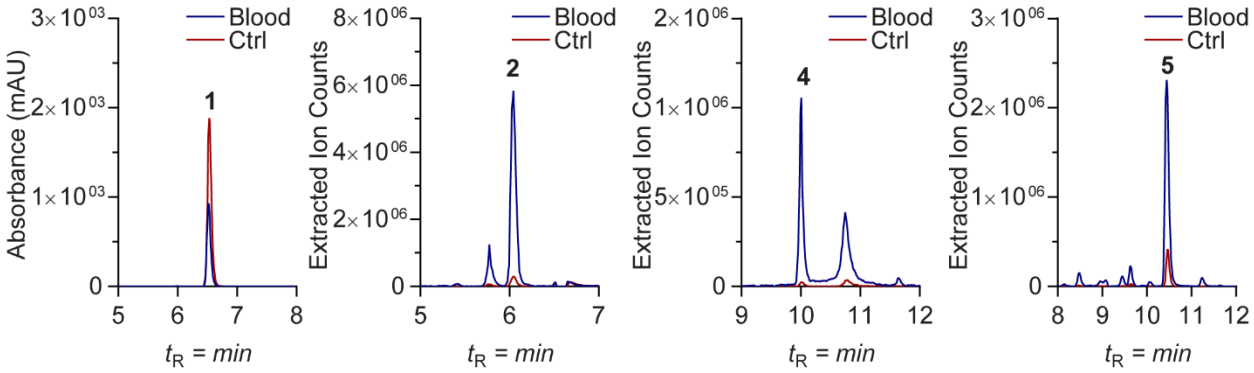

Figure S34. Extracted ion chromatograms for compounds **1**, **2**, **4**, and **5** following incubation of **1** on blood agar plates versus water agar plate controls. The molecules could be formed spontaneously over long incubation periods, and blood accelerated the transformations relative to controls. Samples (100 mg ml^{-1}) in triplicate were spread on the agar plate and aerobically incubated at 37 °C for 4 h. Whole agar plates were extracted with MeOH and analyzed using a reversed-phase C_{18} HPLC analytical column (Phenomenex Kinetex C_{18} (100 Å) 5 µm (4.6 × 250 mm) with a linear gradient from 50 to 100% aqueous ACN in 0.1% formic acid over 15 min with a flow rate of 0.7 ml min^{-1}.

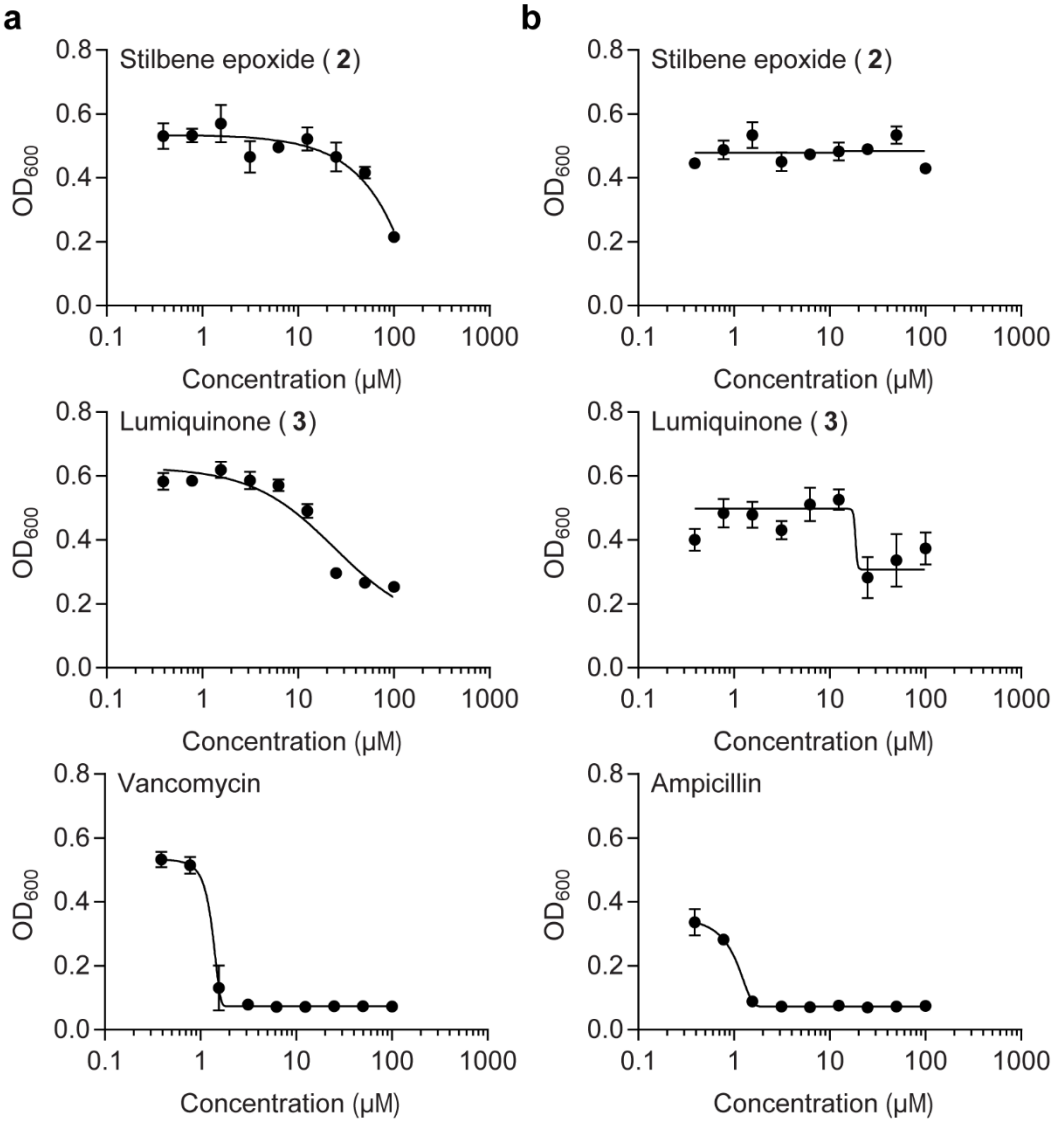

Figure S35. Growth inhibitory effects of stilbene epoxide (**2**) and lumiquinone (**3**) against methicillin-resistant *Staphylococcus aureus* (MRSA, **a**) and vancomycin-resistant *Enterococcus faecalis* (VRE, **b**). Vancomycin and ampicillin were used for positive antibiotic controls. Triplicate data is presented with error bars representing the standard deviation.

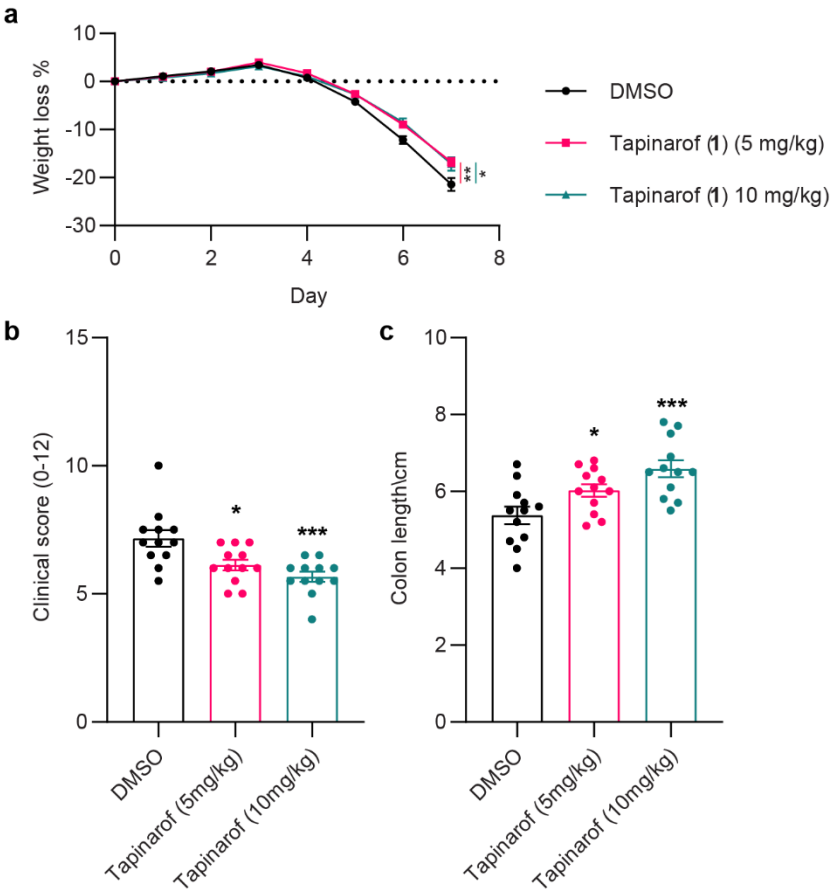

Figure S36. In vivo study of tapinarof (**1**) with two different concentrations in a colitis mouse model. **a**, Body weight loss (%). **b** and **c**, Endoscopy clinical score (**b**) and colon length (**c**). Statistical significance (two-tailed t-test) compared to control (DMSO): *P<0.05; **P<0.01; and ***P<0.001.

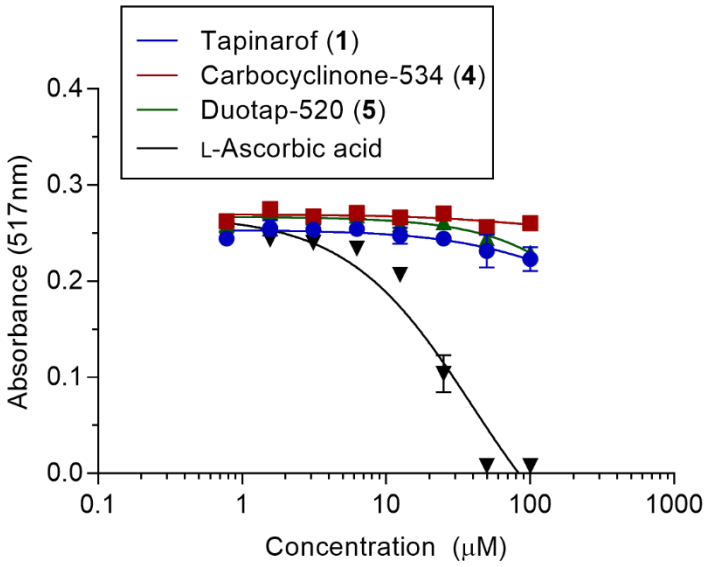

Figure S37. DPPH radical scavenging assay data of tapinarof (**1**), carbocyclinone-534 (**4**), and duotap-520 (**5**). Triplicate data is presented with error bars representing the standard deviation.

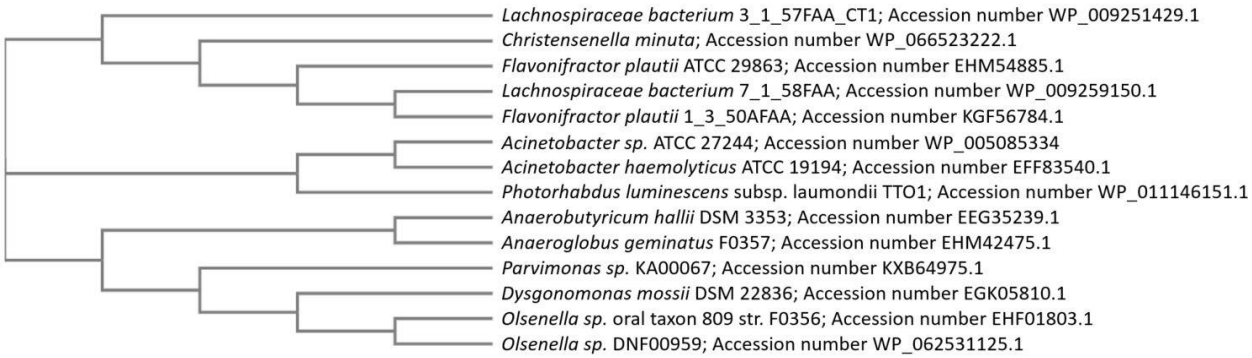

Figure S38. Phylogenetic tree showing relationship between Plu1886 from *Photorhabdus luminescens* and homologous cupin domain-containing proteins from the human microbiome. Protein sequences were obtained using NCBI BLAST for sequences similar to Plu1886, and results were limited to data from the human microbiome project.[9] The phylogenetic tree was prepared using Clustal Omega at EMBL-EBI.[10]

Supplemental Tables

Table S1. NMR data of carbocyclinone-534 (**4**) in methanol-d_4.

No	δ_C	type	δ_H	Multiplet (*J*)	HMBC	1,1-ADEQUATE
1	187.9	C				
2	155.8	C				
3	128.8	C				
4	190.7	C				
5	40.0	C				
6	44.5	C				
7	45.6	CH	3.12	brs	1, 4, 7′, 8′	5[a], 6[a], 8
8	41.9	CH	3.95	dd (4.7, 2.3)	5, 7, 9, 10, 14, 6′, 7′	7, 9, 7′[a],
9	137.0	C				
10	127.3	CH	7.22-7.16		8, 12	9, 11
11	127.9	CH	7.22-7.16		9, 13	10, 12
12	126.6	CH	7.15-7.11		10, 14	11, 13
13	127.9	CH	7.22-7.16		9, 11	12, 14
14	127.3	CH	7.22-7.16		8, 12	9, 13
15	24.7	CH	3.42	h (7.0)	2, 3, 4, 16, 17	3, 16, 17
16	18.8	CH_3	1.38	d (7.0)	3, 15, 17	15
17	18.3	CH_3	1.38	d (7.0)	3, 15, 16	15
1′	178.9	C				
2′	150.9	C				
3′	125.7	C				
4′	183.4	C				
5′	141.9	C				
6′	133.2	C				
7′	41.6	CH	4.09	dt (4.8, 1.0)	6, 7, 1′, 5′, 6′	6′, 8′
8′	46.7	CH	4.44	d (4.5)	5, 6, 6′, 7′, 9′, 10′, 14′	6, 7′, 9′
9′	135.7	C				
10′	127.0	CH	6.86-6.81		8′, 12′	9′, 11′
11′	127.7	CH	7.09-7.03		9′, 13′	10′, 12′
12′	126.5	CH	7.09-7.03		10′, 14′	11′, 13′
13′	127.7	CH	7.09-7.03		9′, 11′	12′, 14′
14′	127.0	CH	6.86-6.81		8′, 12′	9′, 13′
15′	24.5	CH	2.97	h (7.0)	2′, 3′, 4′, 16′, 17′	3′, 16′, 17′
16′	18.8	CH_3	1.09	d (7.0)	3′, 15′, 17′	15′
17′	18.7	CH_3	1.02	d (7.0)	3′, 15′, 16′	15′

[a]ADEQUATE observed in 10 Hz

Table S2. NMR data of duotap-520 (**5**) in methanol-d_4.

No	δ_C	type	δ_H	Multiplet (*J*)	COSY	HMBC
1	104.3	CH	6.77	S		
2	152.6	C				
3	121.6	C				
4	156.9	C				
5	113.4	C				
6	134.5	C				
7	126.4	CH	6.63	d (16.1)	8	1, 5, 6, 9
8	129.0	CH	6.86	d (16.1)	7	6, 9, 10, 14
9	137.4	C				
10	125.8	CH	7.27	d (7.6)		8, 12, 14
11	128.2	CH	7.24-7.17	m		9, 13
12	127.1	CH	7.14	t (7.2)		10, 14
13	128.2	CH	7.24-7.17			9, 11
14	125.8	CH	7.27	d (7.6)		8, 10, 12
15	24.6	CH	3.51	h (7.0)	16, 17	2, 3, 4, 16, 17
16	19.5	CH_3	1.33	d (7.0)	15	3, 15, 17
17	19.5	CH_3	1.33	d (7.0)	15	3, 15, 16
1′	183.8	C				
2′	152.7	C				
3′	125.4	C				
4′	187.3	C				
5′	141.1	C				
6′	136.1	C				
7′	120.5	CH	6.68	d (16.5)	8′	1′, 5′, 6′, 8′, 9′
8′	138.7	CH	7.49	d (16.5)	7′	6′, 7′, 9′, 10′, 14′
9′	137.4	C				
10′	126.5	CH	7.24-7.17			
11′	128.2[a]	CH	7.24-7.17			
12′	126.5[a]	CH	7.24-7.17			
13′	128.2[a]	CH	7.24-7.17			
14′	126.5	CH	7.24-7.17			
15′	24.4	CH	3.25	m	16′, 17′	2′, 3′, 4′, 16′, 17′
16′	19.0	CH_3	1.25-1.23		15′	3′, 15′, 17′
17′	19.0	CH_3	1.25-1.23		15′	3′, 15′, 16′

[a]not assignable

Table S3. Crystal data and structure refinement for carbocyclinone-534 (**4**).

Identification code	007b-18001	
Empirical formula	C_{38} H_{37} N_2 $O_{6.50}$	
Formula weight	625.69	
Temperature	93(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.1644(4) Å	a= 74.489(3)°.
	b = 13.2656(5) Å	b= 86.231(2)°.
	c = 21.5604(5) Å	g = 82.205(3)°.
Volume	3319.88(19) $Å^3$	
Z	4	
Density (calculated)	1.252 Mg/m^3	
Absorption coefficient	0.694 mm^{-1}	
F(000)	1324	
Crystal size	0.150 × 0.080 × 0.020 mm^3	
Crystal color and habit	Colorless Plate	
Diffractometer	Rigaku Saturn 944+ CCD	
Theta range for data collection	2.128 to 66.595°.	
Index ranges	-13<=h<=14, -15<=k<=15, -25<=l<=25	
Reflections collected	119266	
Independent reflections	11536 [R(int) = 0.0624]	
Observed reflections (I > 2sigma(I))	9605	
Completeness to theta = 66.595°	98.4%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.88108	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	11536 / 18 / 896	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1035	
R indices (all data)	R1 = 0.0528, wR2 = 0.1101	
Largest diff. peak and hole	0.303 and -0.399 e.$Å^{-3}$	

Table S4. Hydrogen bonds for carbocyclinone-534 (**4**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)	0.85(3)	2.13(2)	2.6282(17)	116.7(19)
O(1)-H(1)...N(1)	0.85(3)	2.14(2)	2.882(2)	145(2)
O(4)-H(4)...O(5)	0.89(3)	2.14(3)	2.6668(16)	118(2)
O(4)-H(4)...O(12)#1	0.89(3)	2.12(3)	2.8509(17)	139(2)
O(7)-H(7)...O(3)	0.87(3)	1.96(3)	2.7384(16)	148(2)
O(7)-H(7)...O(9)	0.87(3)	2.22(2)	2.6818(17)	113(2)
O(10)-H(10)...O(11)	0.90(4)	2.16(3)	2.6301(18)	111(3)
O(10)-H(10)...O(13)	0.90(4)	1.96(4)	2.767(2)	148(3)
O(13)-H(13A)...N(4)	0.85	2.14	2.990(3)	176.8
O(13)-H(13B)...O(8)#2	0.85	2.09	2.9213(18)	167

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x,-y+2,-z+1

Table S5. Gibbs free energies (kcal/mol) and Boltzmann populations (%) of conformers.

Conformer	Gibbs free energies	Boltzmann populations
Carbo_A_1	-1764.630692	**10.7**
Carbo_A_2	-1764.631346	**21.5**
Carbo_A_3	-1764.630942	**14.0**
Carbo_A_4	-1764.63192	**39.8**
Carbo_A_5	-1764.630942	**14.0**

Table S6. Coordinates for conformers of carbocyclinone-534 (**4**).

	Carbocyclinone A-1			Carbocyclinone A-2			Carbocyclinone A-3		
O	3.12526	1.23134	-2.5458	3.19186	0.56347	-2.59596	3.46488	1.2226	-2.16322
C	2.67207	0.49572	-1.66722	2.67611	0.02054	-1.61737	2.92365	0.51333	-1.3132
C	3.64574	-0.14006	-0.72551	3.59144	-0.48182	-0.54456	3.7836	-0.03208	-0.2167
O	4.92536	0.14249	-1.02839	4.89002	-0.3087	-0.84332	5.08179	0.28749	-0.36298
C	3.31616	-0.94668	0.32666	3.19022	-1.0768	0.61726	3.34324	-0.79477	0.82785
C	4.40155	-1.58918	1.17715	4.15807	-1.61561	1.65759	4.32545	-1.34228	1.85242
C	4.4943	-3.11157	0.93298	5.02355	-0.50009	2.28046	4.52152	-2.86686	1.6994
C	4.25767	-1.25864	2.67645	5.02098	-2.77306	1.11298	3.95624	-0.95718	3.29923
C	1.2348	0.2185	-1.50793	1.22052	-0.14406	-1.46012	1.48826	0.1857	-1.32986
C	0.69392	-1.20235	-1.6189	0.59037	-1.52814	-1.35625	1.01458	-1.25917	-1.43302
C	-0.65932	-1.13732	-2.30089	-0.74507	-1.49175	-2.07624	-0.2384	-1.28316	-2.2882
C	-1.62817	-2.27333	-2.03219	-1.79109	-2.50413	-1.64881	-1.19353	-2.44386	-2.08288
C	-2.70788	-2.46039	-2.91163	-1.72715	-3.19062	-0.42718	-2.14012	-2.72438	-3.08251
C	-3.63572	-3.48226	-2.70221	-2.72351	-4.10669	-0.07099	-3.04928	-3.77371	-2.93607
C	-3.49441	-4.34433	-1.60885	-3.79858	-4.34902	-0.92937	-3.02161	-4.56992	-1.78549
C	-2.4193	-4.17425	-0.73327	-3.8692	-3.67365	-2.15309	-2.07874	-4.30626	-0.78904
C	-1.49311	-3.1458	-0.94226	-2.87176	-2.76363	-2.50846	-1.17151	-3.2506	-0.9356
C	0.81999	-0.55093	-0.23294	0.73259	-0.66834	-0.09098	0.93341	-0.53547	-0.07997
C	-0.42781	-0.07097	0.41219	-0.49241	-0.01488	0.43345	-0.40382	-0.07324	0.36847
C	-0.51941	0.2152	1.88688	-0.58962	0.50976	1.84027	-0.70325	0.27942	1.79798
C	-1.84674	0.47525	2.48731	-1.90743	0.9427	2.35524	-2.10688	0.51891	2.20717
C	-2.02414	0.54922	3.99485	-2.10795	1.26094	3.82751	-2.41443	0.65289	3.68869
C	-1.40657	1.8341	4.58903	-1.41682	2.5801	4.23674	-3.4416	-0.39643	4.1618
C	-1.51115	-0.71339	4.71516	-1.69585	0.09412	4.74675	-2.84983	2.08429	4.0657
C	-2.86705	0.7431	1.63142	-2.89259	1.13322	1.43942	-3.0151	0.69627	1.21273
O	-4.10487	1.07221	2.04795	-4.11363	1.59928	1.76453	-4.3089	0.98989	1.43942
C	-2.70921	0.7403	0.14178	-2.70942	0.88235	-0.02648	-2.65691	0.62588	-0.2407
O	-3.68151	1.06645	-0.54493	-3.64577	1.15505	-0.78279	-3.53933	0.87682	-1.06631
O	0.51922	0.3135	2.54027	0.44223	0.64687	2.4977	0.23199	0.44723	2.58133
C	-1.42614	0.31491	-0.41902	-1.44819	0.29189	-0.47626	-1.29651	0.22745	-0.60516
C	-1.13616	0.29668	-1.88856	-1.13337	0.01663	-1.91463	-0.81307	0.1485	-2.02051
C	0.17725	1.13229	-2.13125	0.23563	0.71981	-2.25171	0.49202	1.02492	-2.1334
C	0.12903	2.58218	-1.68473	0.27159	2.22254	-2.04232	0.33278	2.49026	-1.77183
C	0.72475	3.04268	-0.50241	0.87296	2.82973	-0.93118	0.73445	3.02773	-0.54077
C	0.63842	4.38988	-0.13412	0.86125	4.22087	-0.78105	0.54653	4.38476	-0.2559
C	-0.04888	5.29847	-0.94239	0.24541	5.02783	-1.74054	-0.04959	5.22648	-1.19786
C	-0.64493	4.85156	-2.12684	-0.35347	4.43392	-2.85707	-0.45019	4.70311	-2.43215
C	-0.55207	3.50756	-2.49332	-0.33561	3.04577	-3.0054	-0.25622	3.34961	-2.71456
C	1.89282	-1.24104	0.58778	1.74496	-1.26636	0.86306	1.90988	-1.13891	0.91149
O	1.54339	-2.10592	1.38942	1.33192	-1.97756	1.77842	1.4868	-1.97927	1.70374

H	1.36219	-2.03226	-1.82548	1.20623	-2.42062	-1.40703	1.73139	-2.07109	-1.50502
H	-0.47136	-1.09984	-3.38158	-0.53845	-1.64458	-3.1433	0.08777	-1.29286	-3.33607
H	-1.97818	0.65467	-2.47955	-1.93971	0.32506	-2.57866	-1.58061	0.44324	-2.73483
H	0.35113	1.11868	-3.21376	0.42727	0.52151	-3.31278	0.80778	0.96849	-3.18182
H	4.90233	0.73779	-1.8069	4.91779	0.13558	-1.71705	5.14336	0.84024	-1.1702
H	5.34676	-1.15336	0.84189	3.53084	-2.02587	2.45352	5.28738	-0.87186	1.63073
H	3.58839	-3.62189	1.26868	5.70468	-0.05928	1.54749	3.60035	-3.40905	1.92635
H	5.34708	-3.51924	1.48681	5.62348	-0.91684	3.09662	5.30153	-3.20598	2.38985
H	4.64518	-3.33273	-0.12896	4.39985	0.29872	2.69512	4.83611	-3.12493	0.68267
H	4.22018	-0.17654	2.84085	4.39496	-3.57913	0.71605	3.83804	0.12667	3.40252
H	3.35496	-1.704	3.10064	5.69382	-2.43685	0.31912	3.02826	-1.43758	3.61721
H	5.1244	-1.65126	3.21914	5.63043	-3.18794	1.92319	4.75838	-1.27364	3.97471
H	-2.82051	-1.80138	-3.7692	-0.89868	-3.01956	0.25304	-2.16253	-2.117	-3.98414
H	-4.46352	-3.60899	-3.39396	-2.65474	-4.6306	0.87809	-3.77306	-3.97341	-3.721
H	-4.21207	-5.14298	-1.44572	-4.57077	-5.06061	-0.65208	-3.72421	-5.39012	-1.67095
H	-2.2963	-4.84141	0.11508	-4.69639	-3.85933	-2.83215	-2.04428	-4.92167	0.1054
H	-0.66286	-3.03316	-0.25198	-2.93068	-2.24973	-3.46494	-0.44528	-3.0649	-0.15024
H	-3.10404	0.60335	4.16545	-3.18491	1.40896	3.95588	-1.47307	0.45191	4.20844
H	-1.64032	1.89534	5.65769	-1.75043	3.41204	3.60765	-3.57232	-0.32076	5.24677
H	-0.31979	1.839	4.47299	-1.66709	2.82024	5.27608	-4.4166	-0.24467	3.69002
H	-1.81106	2.72797	4.10273	-0.32995	2.49823	4.15405	-3.10367	-1.41251	3.93266
H	-1.97526	-1.61817	4.30816	-1.96742	0.32873	5.78158	-2.09214	2.81746	3.77033
H	-0.42618	-0.81278	4.62602	-2.20905	-0.83182	4.46579	-3.79479	2.35407	3.58514
H	-1.76275	-0.65628	5.77967	-0.61805	-0.08464	4.70941	-2.9859	2.15632	5.15037
H	-4.63527	1.24876	1.24463	-4.61789	1.67829	0.92953	-4.72908	1.10801	0.56303
H	1.26864	2.35832	0.14112	1.363	2.22635	-0.17344	1.20449	2.39725	0.20748
H	1.11184	4.72533	0.78406	1.33604	4.66961	0.08666	0.86901	4.78006	0.70302
H	-0.11425	6.34431	-0.65726	0.23724	6.10752	-1.62422	-0.19447	6.2798	-0.97678
H	-1.17563	5.54934	-2.76811	-0.82847	5.05059	-3.6146	-0.90745	5.34866	-3.17641
H	-1.0103	3.17231	-3.42068	-0.79552	2.5944	-3.88128	-0.56221	2.95455	-3.68034

	Carbocyclinone A-4			Carbocyclinone A-5		
O	-3.44453	-0.72622	-2.27092	3.46502	1.2231	-2.16287
C	-2.87951	-0.17481	-1.32488	2.92373	0.51394	-1.31283
C	-3.7227	0.22261	-0.15341	3.78367	-0.0318	-0.21648
O	-5.02832	-0.03317	-0.34061	5.08189	0.28767	-0.3627
C	-3.25732	0.8058	0.99039	3.34324	-0.79463	0.82793
C	-4.16145	1.24428	2.13054	4.32544	-1.34231	1.85244
C	-4.90129	0.05663	2.78111	4.52212	-2.86673	1.69856
C	-5.1366	2.36234	1.70553	3.95583	-0.95817	3.29938
C	-1.43385	0.10528	-1.30001	1.48838	0.18614	-1.32967
C	-0.91325	1.53296	-1.18375	1.01476	-1.25872	-1.43317

C	0.34113	1.64756	-2.02883	-0.23813	-1.28261	-2.28847
C	1.33426	2.72978	-1.64935	-1.19322	-2.44339	-2.08345
C	1.33319	3.35287	-0.39259	-1.17144	-3.25015	-0.93619
C	2.27482	4.34191	-0.08619	-2.07864	-4.30588	-0.7899
C	3.23229	4.72134	-1.02992	-3.02124	-4.56957	-1.78659
C	3.23957	4.10897	-2.28838	-3.04868	-3.77333	-2.93716
C	2.29606	3.12618	-2.59374	-2.13955	-2.72393	-3.08333
C	-0.8551	0.60906	0.042	0.93343	-0.53527	-0.07997
C	0.46488	0.03839	0.40944	-0.40385	-0.07322	0.36843
C	0.74618	-0.54378	1.76583	-0.70348	0.27882	1.79805
C	2.1369	-0.9059	2.12541	-2.10716	0.51816	2.20714
C	2.43295	-1.28546	3.56604	-2.41488	0.65164	3.68867
C	3.50886	-0.37588	4.19404	-3.44213	-0.39778	4.16135
C	2.79397	-2.77824	3.71325	-2.85024	2.08294	4.06608
C	3.03919	-0.96252	1.11158	-3.01525	0.69588	1.21266
O	4.31798	-1.3455	1.28304	-4.30905	0.98958	1.43928
C	2.69026	-0.64354	-0.31057	-2.65691	0.62593	-0.24077
O	3.56553	-0.79248	-1.16777	-3.53931	0.87691	-1.06639
O	-0.19676	-0.79071	2.51851	0.23165	0.44599	2.58167
C	1.34709	-0.14065	-0.60306	-1.29648	0.22762	-0.60521
C	0.86808	0.17296	-1.98731	-0.81291	0.14898	-2.02055
C	-0.46542	-0.63142	-2.22878	0.49215	1.02548	-2.13314
C	-0.35603	-2.13984	-2.10143	0.33279	2.49074	-1.77126
C	-0.79005	-2.84888	-0.97278	-0.25651	3.3502	-2.71371
C	-0.65147	-4.23952	-0.90303	-0.45061	4.70361	-2.43101
C	-0.07316	-4.94361	-1.96175	-0.04986	5.2268	-1.19669
C	0.35999	-4.24759	-3.09576	0.54654	4.38498	-0.255
C	0.21547	-2.86053	-3.16348	0.7346	3.02802	-0.54018
C	-1.81057	1.08322	1.11666	1.90987	-1.13887	0.91141
O	-1.36122	1.7761	2.02905	1.48683	-1.97952	1.70336
H	-1.60331	2.36859	-1.12684	1.73161	-2.0706	-1.5052
H	0.01734	1.82983	-3.06164	0.08813	-1.2921	-3.33632
H	1.62614	-0.03238	-2.74182	-1.58041	0.44382	-2.73488
H	-0.77832	-0.40043	-3.25379	0.80807	0.96928	-3.18153
H	-5.10598	-0.45171	-1.22404	5.14353	0.84062	-1.16978
H	-3.49352	1.66706	2.8857	5.28724	-0.87143	1.63118
H	-5.61696	-0.40045	2.09252	3.60103	-3.40938	1.92472
H	-5.45099	0.40798	3.66097	5.30191	-3.20605	2.38917
H	-4.19739	-0.71521	3.10933	4.83729	-3.12404	0.68181
H	-4.5966	3.21924	1.28922	3.83685	0.12555	3.40319
H	-5.85341	2.01098	0.95803	3.02817	-1.43936	3.61707
H	-5.69827	2.71035	2.57924	4.75814	-1.27437	3.97477
H	0.59594	3.07602	0.35459	-0.4454	-3.06444	-0.15067

H	2.25546	4.81506	0.89143	-2.04434	-4.92132	0.10452
H	3.96206	5.48935	-0.79101	-3.72382	-5.38982	-1.67224
H	3.97481	4.40012	-3.03302	-3.77224	-3.97305	-3.72227
H	2.30368	2.66253	-3.57735	-2.16178	-2.1165	-3.98493
H	1.50065	-1.12163	4.11446	-1.47357	0.45043	4.20845
H	3.62325	-0.62004	5.25576	-3.57282	-0.32256	5.24636
H	4.4797	-0.50782	3.70803	-4.41714	-0.24574	3.68966
H	3.22749	0.67969	4.11838	-3.1043	-1.41379	3.93178
H	2.00292	-3.41721	3.30727	-2.09243	2.81614	3.77112
H	3.72799	-3.01722	3.19615	-3.79507	2.35297	3.5854
H	2.91862	-3.02593	4.77313	-2.98656	2.15464	5.15074
H	4.7351	-1.33862	0.39728	-4.72912	1.108	0.56288
H	-1.2479	-2.32611	-0.13897	-0.56261	2.95529	-3.67952
H	-0.99902	-4.76861	-0.02044	-0.9081	5.34925	-3.17506
H	0.03304	-6.02304	-1.90808	-0.19484	6.28005	-0.97534
H	0.80433	-4.78418	-3.92906	0.86914	4.78013	0.70394
H	0.54739	-2.3302	-4.05284	1.20488	2.39747	0.20786

Table S7. Oligonucleotide primers used for cloning of Plu1886.

Primer Name	Sequence
1886-F	5'-GAATTCCATATGGAATTTATTAAAAATAGATTTTGTCACTGGAACGG-3'
1886-R	5'-GAATTCAAGCTTTTAAACCTTTAATTCCTCTGGCGTTCCC-3'
1886Up-F (Del1886F (SphI))	gatagcta-gcatgc-ATTTCTGCGGAACAAATCAGTTACCTTG
1886Dwn-R (Del1886R (SphI))	gatagcta-gcatgc-ACAAAAGTTGACTTCAAGAATAATATCGAATGAAGG
1886Dwn-F (DwnF)	AATAAAATTTTATTTGTAGAGATAAAAGGAAGGTAAT-CTTGGGATAAATTAAATATGTGCTAGTGCTTGATGG
1886Up-R (UpR)	CACTAGCACATATTTAATTTATCCCAAG - ATTACCTTCCTTTTATCTCTACAAATAAAATTTTATTTTAAAGTGACTATC

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