Supporting Information

Tundrenone: An Atypical Secondary Metabolite from Bacteria with Highly Restricted Primary Metabolism

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Experimental Procedures

General procedures

Optical rotation data was measured on a JASCO P-2000 polarimeter, circular dichroism spectra on a JASCO J-815 spectropolarimeter, and UV spectra on an Amersham Biosciences Ultrospec 5300-pro UV/Visible spectrophotometer. NMR data were acquired for a ~3 mg sample of **1** dissolved in 35 µL DMSO-d_6 on either a 500 MHz Varian VNMRS (Varian NMR System), 500 MHz spectrometer equipped with an inverse cold probe (500 and 125 MHz for ^{1}H and ^{13}C NMR, respectively), Bruker AVANCE II 600 MHz spectrometer equipped with a ^{1}H{^{13}C/^{15}N} cryoprobe, or Bruker AVANCE 500 MHz spectrometer equipped with a broadband cryoprobe with DMSO as an internal standard (δ_C 39.52, δ_H 2.50). Routine LR-LCMS data were obtained using an Agilent 1200 series HPLC system equipped with a photo-diode array detector and a 6130-quadrupole mass spectrometer. HPLC purifications were carried out using Agilent 1100 or 1200 series HPLC systems equipped with a photo-diode array detector, or a Varian ProStar 210 with UV detector. All solvents were of HPLC quality.

High Resolution LC-MS/MS

LC-MS/MS experiments were performed on a Vanquish ultra-high performance liquid chromatography (UHPLC) system coupled to a Q-Exactive mass spectrometer (Thermo Fisher Scientific, Bremen, Germany). A C18 core-shell column (Kinetex, 50 x 2 mm, 1.8 µm particle size, 100 A pore size, Phenomenex, Torrance, USA) was used for reversed phase separation. A flowrate of 0.5 mL/min was used. Solvent A: Water + 0.1 % formic acid, Solvent B: Acetonitrile + 0.1 % formic acid. Gradient: 0-0.5 min, 5% B. 0.5-4 min, 5-50% B. 4-5 min, 50-99% B. 5-7 min, 99% B. 7-9 min, 5% B. For MS and MS/MS measurements the electrospray ionization (ESI) parameters were set to 35 L/min sheath gas flow, 10 L/min auxiliary gas flow, 2 L/min sweep gas flow and 400 °C auxiliary gas temperature. The spray voltage was set to 3.5 kV, the inlet capillary was set to 250 °C and a 50 V S-lens radio frequency (RF) level was applied. MS/MS spectra were recorded in data dependent acquisition (DDA) mode. For MS1 survey scans (300-2000 *m*/*z*) and up to 5 MS/MS scans of the most abundant ions per duty cycle resolution (R) was set to 140,000 with 1 micro-scan in positive mode. For MS1 scans, internal

was calibration was used. The maximum ion injection time was set to 100 ms and a MS/MS precursor selection window was set to 1 *m*/*z*. Normalized collision energy was set to 30 % with *z* = 1 as default charge state. MS/MS experiments were automatically triggered at the apex of a peak within 2 to 15 s from their first occurrence. A dynamic exclusion was set to 5 s. Ion species with unassigned charge states as well as isotope peaks were excluded.

MS/MS dataset deposition

To facilitate future compound dereplication, MS/MS spectra were annotated and included in the Global Natural Product Social Molecular Networking database (GNPS)[1] under MassIVE ID MSV000081637 (https://massive.ucsd.edu/).

Source of microbial strains

M. tundripaludum 21/22 was originally isolated from lake sediment from Lake Washington (Seattle, WA, USA).[2] The acyl-homoserine lactone mutant Δ*mbaI* was constructed previously.[3]

Strain growth and genetic manipulation

M. tundripaludum 21/22 was cultured in an atmosphere of 25% methane in air. Plates were incubated at room temperature in sealed jars (Oxoid Limited, Hampshire, United Kingdom), while liquid cultures were grown at 18ºC in 250-ml glass serum bottles (Kimble Chase, Vineland, NJ, USA) or 18- by 150-mm tubes (Bellco Glass, Vineland, NJ, USA) sealed with rubber stoppers and aluminum seals (Wheaton, Millville, NJ, USA) shaken at 200 rpm. Cultures were grown in nitrate mineral salts (NMS) medium[4] containing 0.2 g/L $MgSO_4 \cdot 7H_2O$, 0.2 g/L $CaCl_2 \cdot 6H_2O$, 1 g/L KNO_3, and 30 µM $LaCl_3$ as well as 1X trace elements. 500X trace elements contains 1.0 g/L Na_2-EDTA, 2.0 g/L $FeSO_4 \cdot 7H_2O$, 0.8 g/L $ZnSO_4 \cdot 7H_2O$, 0.03 g/L $MnCl_2 \cdot 4H_2O$, 0.03 g/L H_3BO_3, 0.2 g/L $CoCl_2 \cdot 6H_2O$, 0.6 g/L $CuCl_2 \cdot 2H_2O$, 0.02 g/L $NiCl_2 \cdot 6H_2O$, and 0.05 g/L $Na_2MoO_4 \cdot 2H_2O$. A final concentration of 5.8 mM phosphate buffer, pH 6.8 was added immediately before use.

Knock out plasmids for the predicted acyl-CoA ligase gene *tunJ* as well as the predicted anthranilate synthase genes *tunN* and *tunO* were constructed via Gibson assembly using the pCM433kanT backbone and introduced via conjugation using *E. coli* donor strain S17-1 as previously described.[3,5] Primers used for plasmid construction are listed in Table S2. Successful integrants (single crossovers) were selected on NMS plates containing kanamycin (50 µg/mL). Subsequent sucrose counterselection was performed as previously described.[5] *tunN* and *tunO* deletion strains could not be constructed despite multiple attempts.

*Extraction and purification of tundrenone (**1**)*

Routinely a total of 2.2 liters of phosphate buffered NMS medium was divided into seven one-liter bottles (Kimble Chase, Vineland, NJ, USA) with gas tight caps with butyl septa (Wheaton, Millville, NJ, USA) and each inoculated with exponentially growing *M. tundripaludum* to an OD of 0.02. These cultures were grown at 20ºC to stationary phase (approximately 48 hours). The culture was centrifuged (5000 rpm for 20 minutes) and the supernatant was extracted twice with an equal volume of ethyl acetate containing 0.01% (v/v) acetic acid. This extract was then dried *in vacuo*, and dissolved in 500 µL of MeOH. This was diluted to 25% MeOH in water and loaded onto a preequilibrated Discovery C_{18} solid phase extraction column (3 mL, 500 mg) (Supelco, Bellefonte, PA, USA), which was washed and eluted with 6 mL of 25%, 50%, 75%, and 100% MeOH in water. The molecule was found in the 75% MeOH fraction by LCMS. This fraction was subsequently dried and resuspended in 200 µL of 50% MeOH in water and separated using a Nucleosil C_{18} column (5 µm, 250 mm x 4.6 mm) (Supelco, Bellefonte, PA) at 0.75 mL/min using an isocratic run of 55% MeOH in water for 25 minutes. This process was repeated to get the quantities used in these studies.

Tundrenone (1): pale yellow oil; $[\alpha]^{22}_{D}$ -66.4 (*c* 0.27, MeOH); UV (MeOH) λ_{max} (log ε) 207.0 (3.62), 223.0 (3.42), 297.0 (3.84) nm; NMR (500 MHz, CD_3OD) and ^{13}C NMR (125 MHz, CD_3OD) see table S1; HRESIMS $[M+H]^+$ 421.1857 *m/z* (calcd for $C_{22}H_{29}O_8$ 421.1857, 0 ppm).

LC-MS analysis of mutant strains

Concentrated extracts of supernatant from wildtype or mutant stationary phase cultures containing the equivalent of 1 mL of supernatant were analyzed by LC-MS using a Linear Trap Quadrupole Orbitrap Xcalibur 2.0 DS (Thermo Fisher Scientific) connected to an ACQUITY UPLC system (Waters). Samples were separated using an ACQUITY UPLC HSS T3 column (1.8 µM, 2.1 mm x 100 mm; Waters) using a flow rate of 0.2 mL/min. Solvent A: Water containing 0.1 % formic acid. Solvent B: Acetonitrile containing 0.1% formic acid. Gradient: 0-1 min, 5% B. 1-8 min, 5- 95% B. 8-8.1 min, 95% B. 8.1-12 min, 5% B.

Quantification of tundrenone and the acyl-homoserine lactone 3-OH-C_{10}-HSL

The supernatant of centrifuged 50 mL stationary phase *M. tundripaludum* cultures was extracted twice with an equal volume of ethyl acetate containing 0.01% (v/v) acetic acid. For tundrenone quantification, the extract was then dried *in vacuo* and dissolved in 250 µL of MeOH. This was diluted to 25% MeOH in water and loaded onto a preequilibrated Discovery C_{18} solid phase extraction column (1 mL, 100 mg) (Supelco, Bellefonte, PA, USA), which was washed and eluted with 2 mL of 25%, 50%, and 75% MeOH in water. The 75% MeOH fraction, where tundrenone is the only UV-active compound as assessed by routine HPLC, was then dried under an N_2 (g) and resuspended in 500 µL MeOH. The UV/vis spectrum was then recorded for dilutions of this semi-purified extract using a DU 640B spectrophotometer (Beckman, Brea, CA, USA), and the quantity of tundrenone was calculated using its extinction coefficient at 297 nm.

3-OH-C_{10}-HSL was quantified using an *E. coli* reporter strain containing plasmids pAWP112 and pAWP113 as previously described.[2] Dilutions of extracts were dried under an N_2 stream and resuspended in 500 µL of an overnight culture of the reporter strain subdiluted to an OD of 0.1 in LB containing kanamycin (50 µg/mL) and chloramphenicol (35 µg/mL). Cultures were shaken at 37C for 4 hours and then pelleted and resuspended in 500 µL of 50 mM Tris pH 7.5. 100 µL was measured for GFP fluorescence (485 nm excitation, 510 nm emission) in a 96-well plate (Nunc black optical bottom) by plate reader (Tecan Infinite F500) and compared to a standard curve of commercially available 3-OH-C_{10}-HSL (Cayman Chemical, Ann Arbor, MI, USA).

Computational procedures

Conformational searches for **i**–**iv** were performed in *Schrödinger Release 2016-1* using *MacroModel*.[6] Conformational searches were performed using the mixed torsional / low-mode sampling algorithm with extended torsion sampling and the OPLS3[7] molecular mechanics force field for gas-phase minimization and energy calculation. The default energy window (5 kcal/mol) was used for the search with the default root mean square deviation (RMSD) cutoff of 0.5 Å to eliminate redundant conformers. The $^{3}J_{HH}$ coupling constants were calculated using the ^{1}H NMR coupling measurement tool within *Maestro* (version 10.5.014) in *Schrödinger Release 2016-1*.

All subsequent quantum-chemical DFT calculations were performed in *Gaussian 09, Revision D.01*.[8] For calculation of the ^{13}C NMR chemical shifts, all generated conformers for **i** and **iii** were subjected to gas-phase geometry optimization calculations at the B3LYP/6-31+G(d,p) level of theory.[9] Frequency calculations were performed at the same level of theory to ensure that all structures are minima on the potential energy hypersurface (i.e., no first or higher order saddle points). Structurally redundant conformers or those that have a *G* greater than 2.5 kcal/mol of the global minimum structure were rejected from further analysis. The global minimum structure and conformers with a *G* value within 2.5 kcal/mol of the global minimum were subjected to NMR calculations using a procedure by Tantillo and co-workers.[10] NMR properties were calculated using the gauge-independent atomic orbital (GIAO)[11] method at the mPW1PW91/6-311+G(2d,p) level of theory.[12] The self-consistent reaction field (SCRF) was invoked for solvation with the default integral equation formalism polarizable continuum model (IEFPCM)[13] and using DMSO as the solvent. The calculated isotropic chemical shifts were scaled according to the procedure by Tantillo and co-workers using scaling factors reported by Pierens (^{1}H: slope = -1.0580, intercept = 31.7217 | ^{13}C: slope = -1.0496, intercept = 186.2534).[10,14] Finally, the scaled chemical shifts for conformers of **i** and **iii** were subjected to Boltzmann weighting at a temperature of 298.15 K using the calculated ΔG values to afford the final calculated ^{13}C chemical shifts. The corrected mean absolute deviation (CMAD) between theoretical and experimental values were calculated for **i** (^{13}C: 1.6 ppm, ^{1}H: 0.20 ppm) and **iii** (^{13}C: 5.3 ppm, ^{1}H: 0.24 ppm)

For calculation of the optical rotation of **i**, a procedure from Fuchter that we have used previously was employed.[15,16] The conformers for **i** optimized at the gas-phase B3LYP/6-

31+G(d,p) level of theory were reoptimized using a triple-ζ basis set at the wB97XD/6-311++G(d,p) level of theory[17] with SCRF invocation using the conductor-like polarizable continuum model (CPCM)[18] and MeOH as the solvent. Frequency calculations were performed to ensure the structures represent minima. Optical rotation calculations were performed at the same level of theory using the "polar=OptRot" directive and the sodium D-line wavelength (589.3 nm) was inputted using the "CPHF=RdFreq" directive. The optical rotation value for each conformer was subjected to Boltzmann weighting as stated above to afford the final optical rotation value.

All quantum-chemical calculations were performed on the Odyssey cluster maintained by FAS Research Computing at Harvard University. Each calculation utilized a maximum of 64 processing cores and 64 GB of RAM.

Cartesian coordinates for relevant structures / conformers are given through a two-part numbering system (e.g., **1-2**). The first number refers to compound number, and the second refers to the conformer number as obtained after a conformer search in *Schrödinger Release 2016-1*. Some conformers are not listed (e.g., **1-3**) because it is either redundant or has a *G* that is greater than 2.5 kcal/mol of the global minimum.

Additional Experimental Tables and Figures

Table S1. NMR assignments for tundrenone (**1**) in d_6-DMSO

Position	δ_C [c]	δ_H (*J* in Hz)[a]	COSY[a]	HMBC[a]	ROESY[b]
1	31.0	3.15 (ddd; *6.6, 3.5, 3.3*)	2a, 2b, 9	4, 5, 9	2a, 9
2a	33.7	2.41 (dd; *18.0, 6.5*)	1, 2b	1, 3, 4, 5	1, 2b
2b		2.13 (dd; *17.9, 3.5*)	1, 2a	1, 3, 9	2a
3	200.9				
4	147.5				
5	134.6				
6	121.7	6.79 (d: *9.9*)	7	1, 4	7
7	130.0	5.91 (dd; *9.8, 5.2*)	6, 8	5, 8, 9	6, 8
8	62.1	4.10 (dd; *5.1, 1.9*)	7	1, 6, 7, 9	7, 22b
9	76.2	4.16 (bs)	1	1, 5, 7, 8	1, 22b
10	149.3				
11	161.5				
12	63.4	4.53 (m)		11, 13, 14, 21	
13	141.2				
14	77.8	4.53 (m)		12, 13, 15, 21	
15	209.9				
16	36.3	2.48 (t; *7.4*)	17	15, 17, 18	
17	22.3	1.42 (m)	16, 18	15, 16, 18, 19	
18	30.5	1.17 (m)	17	16, 19, 20	
19	21.7	1.23 (m)	20	17, 18, 20	
20	13.6	0.84 (t; *7.4*)	19	18, 19	
21a	115.0	5.33 (bs)	21b	12, 13, 14	21b
21b		5.19 (bs)	21a	12, 13, 14	21a
22a	96.9	5.29 (d; *2.7*)	22b	10, 11	22b
22b		5.03 (d; *2.7*)	22a	10, 11	8, 9, 22a

[a] 600 MHz for ^{1}H NMR, dqfCOSY, gHSQC, and HMBC
[b] 500 MHz for ROESY
[c] 125 MHz for ^{13}C NMR

Figure S1. ^{1}H NMR spectrum of tundrenone (**1**) in d_6-DMSO (600 MHz)

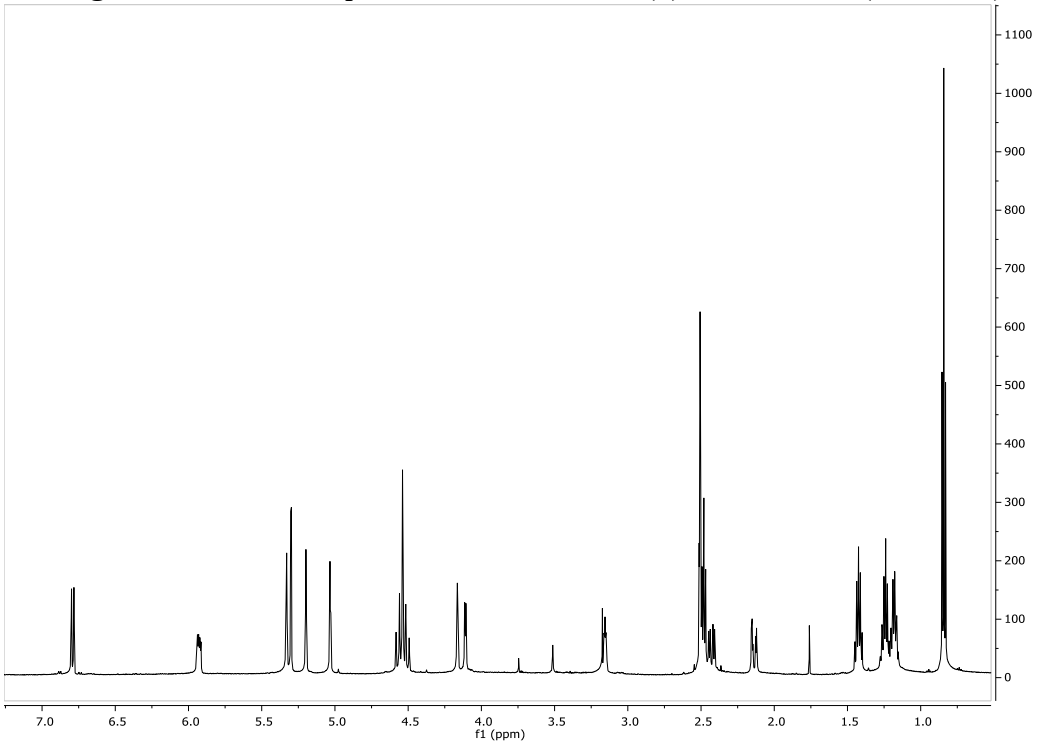

Figure S2. ^{13}C NMR spectrum of tundrenone (**1**) in d_6-DMSO (125 MHz)

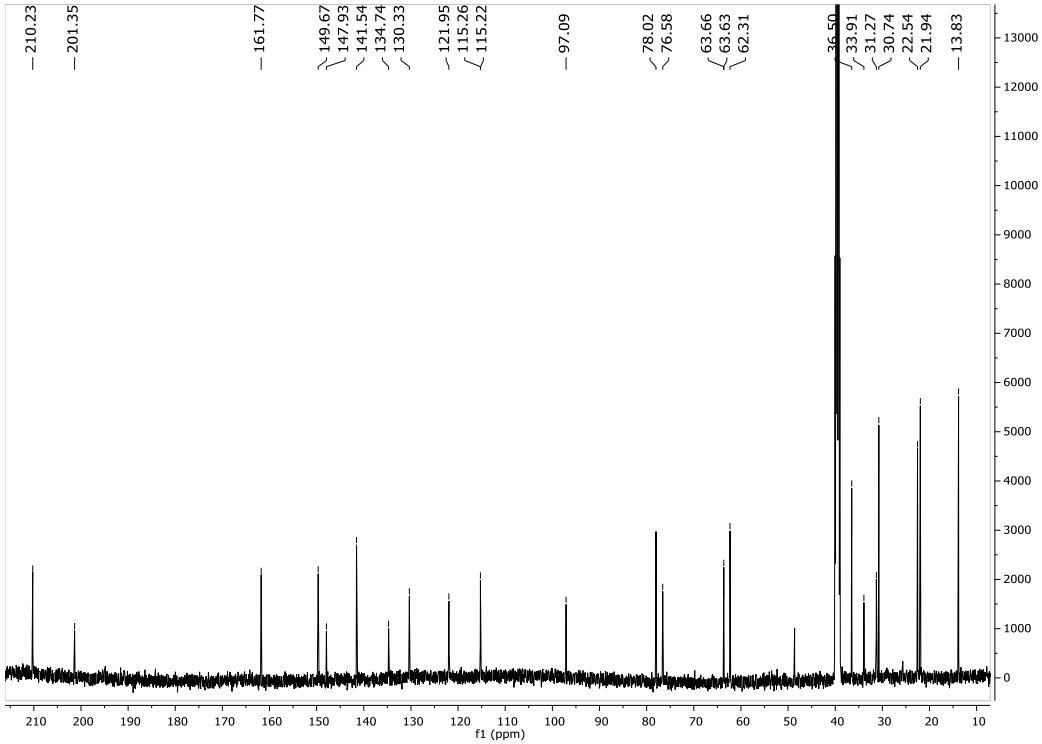

Figure S3. gHSQC spectrum of tundrenone (**1**) in d_6-DMSO (^{1}H – 600 MHz)

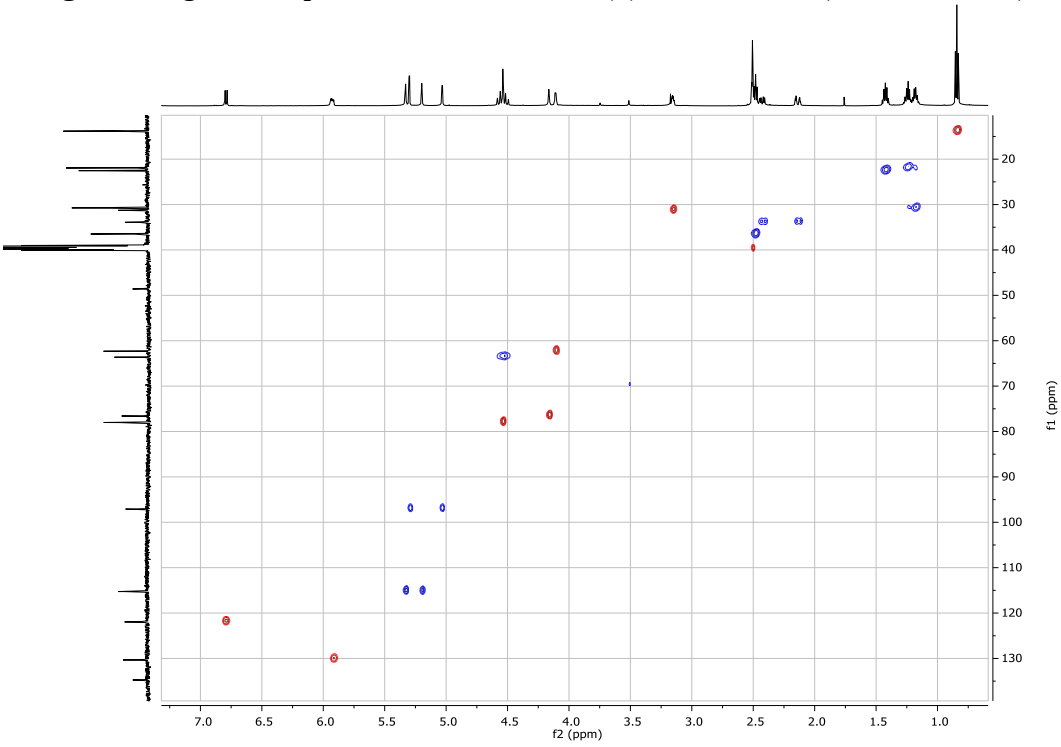

Figure S4. dqfCOSY spectrum of tundrenone (**1**) in d_6-DMSO (600 MHz)

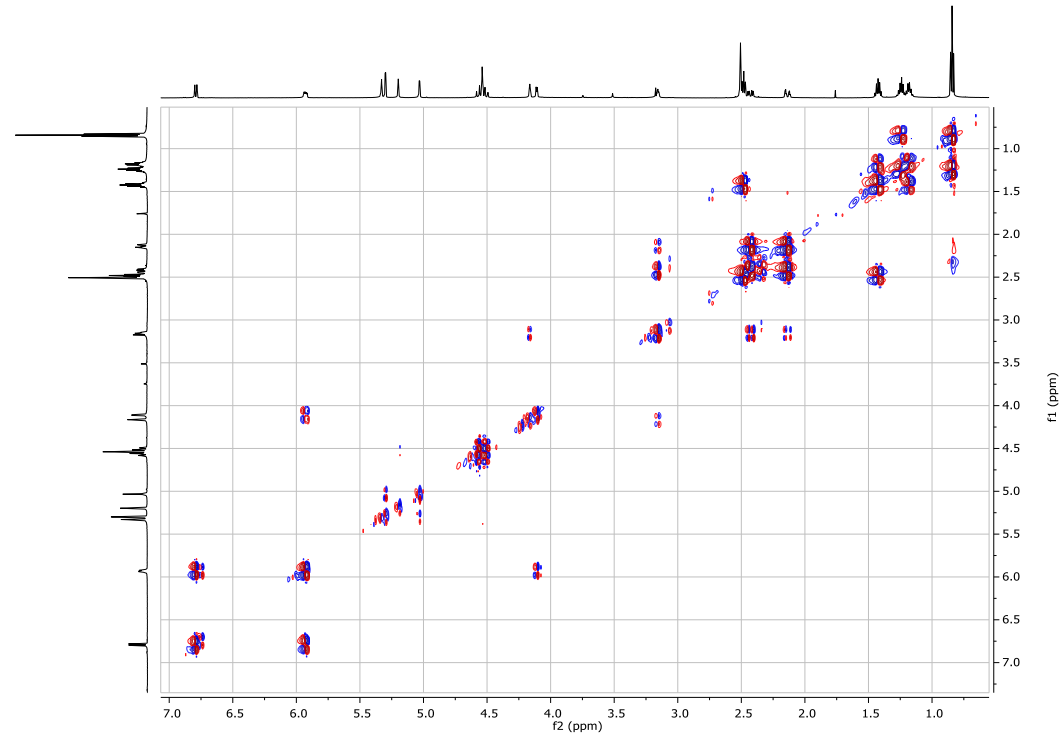

Figure S5. gHMBCAD spectrum of tundrenone (**1**) in d_6-DMSO (^{1}H – 600 MHz)

Figure S6. ROESY spectrum of tundrenone (**1**) in d_6-DMSO (500 MHz)

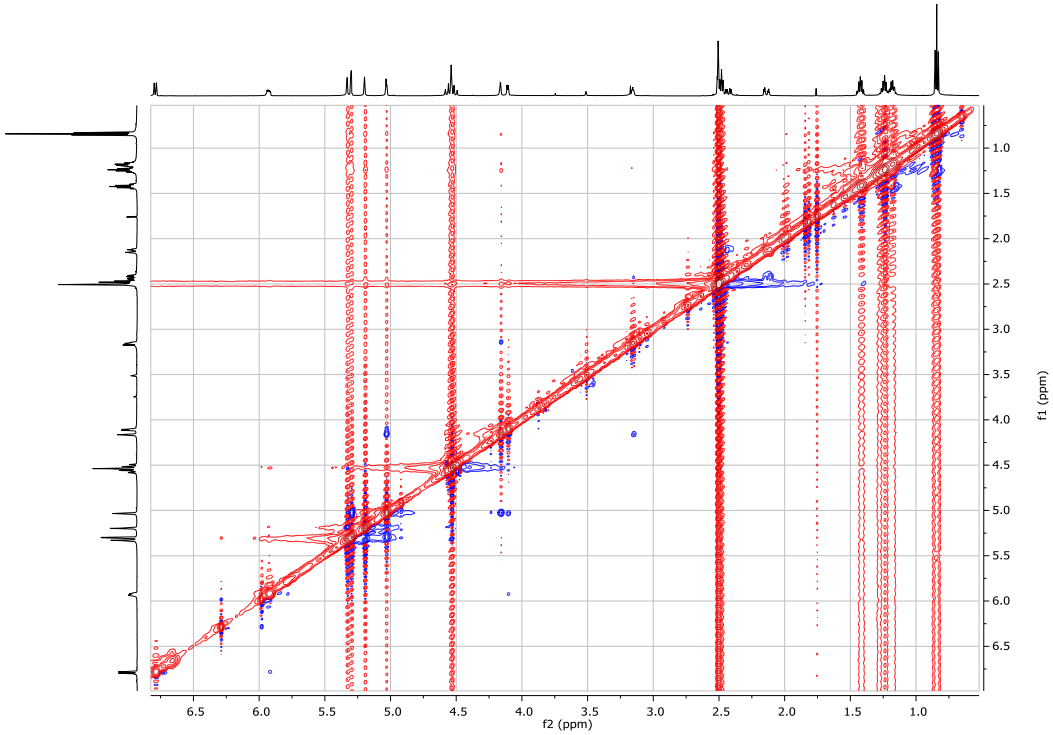

Figure S7. High resolution MS1 and MS2 spectra of tundrenone (**1**). MS1 (A, inset) and subsequent MS/MS scans of tundrenone $[M+H]^+$ (B) and $[M+Na]^+$ (C) ions are shown. The MS1 scan resulted in exact masses of *m/z* 421.1857 ($[M+H]^+$) and *m/z* 443.1681 ($[M+Na]^+$). These masses corresponded to calculated masses for tundrenone ions (421.1857 for $C_{22}H_{29}O_8$ and 443.1676 for $C_{22}H_{28}O_8Na$) with 0.00 and 1.13 ppm mass error, respectively. MS/MS fragment spectra of $[M+H]^+$ shows the dehydrated lipid tail (*m/z* 169.1221), while fragmentation of $[M+Na]^+$ shows the bicyclic ring with attached dehydro-serine hydroxy acid (*m/z* 275.0521) as well as the dehydro-serine hydroxy acid with attached lipid tail (*m/z* 279.1200).

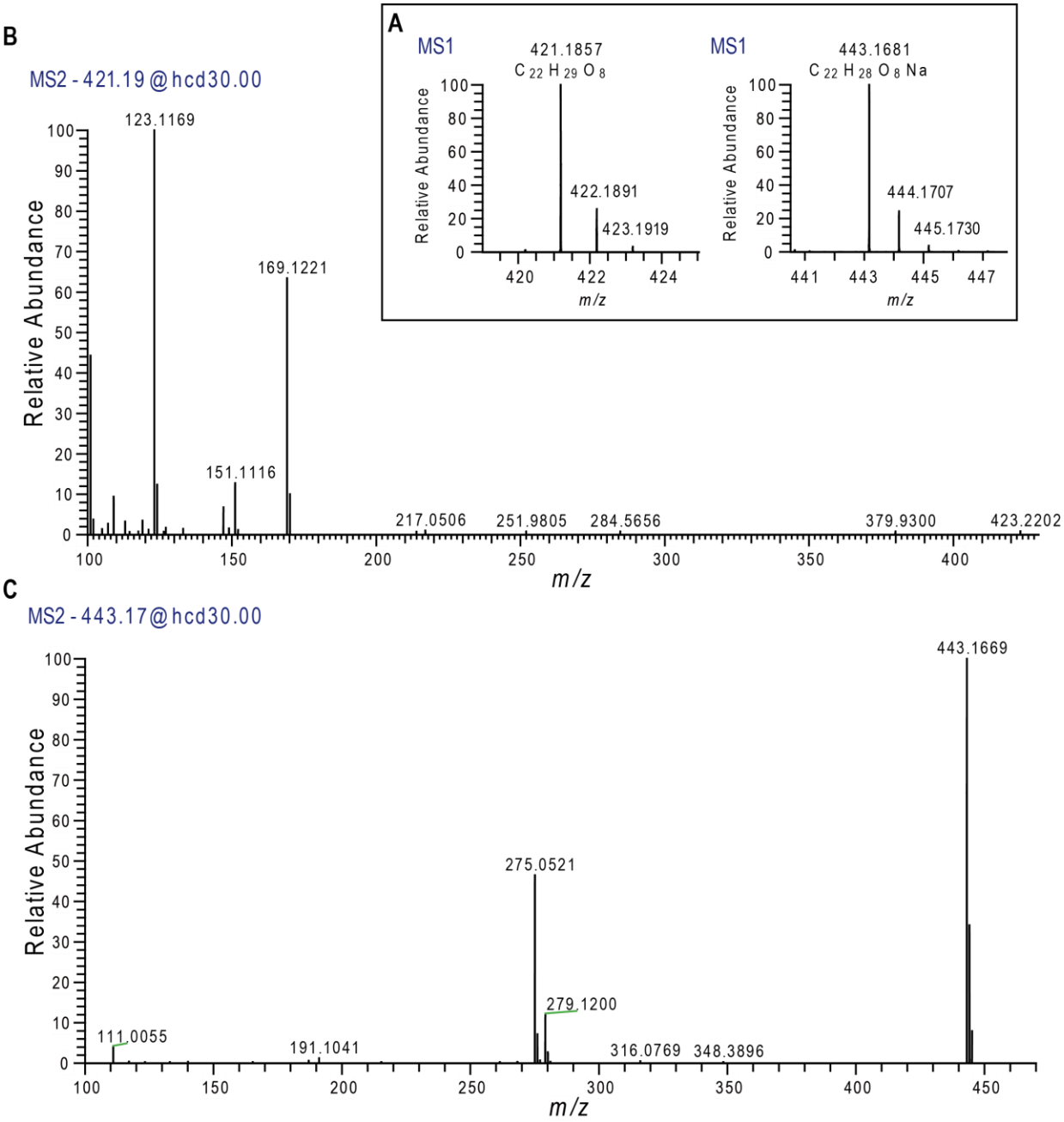

Figure S8. CD spectrum of tundrenone (**1**) – 1.27 mg/mL in MeOH

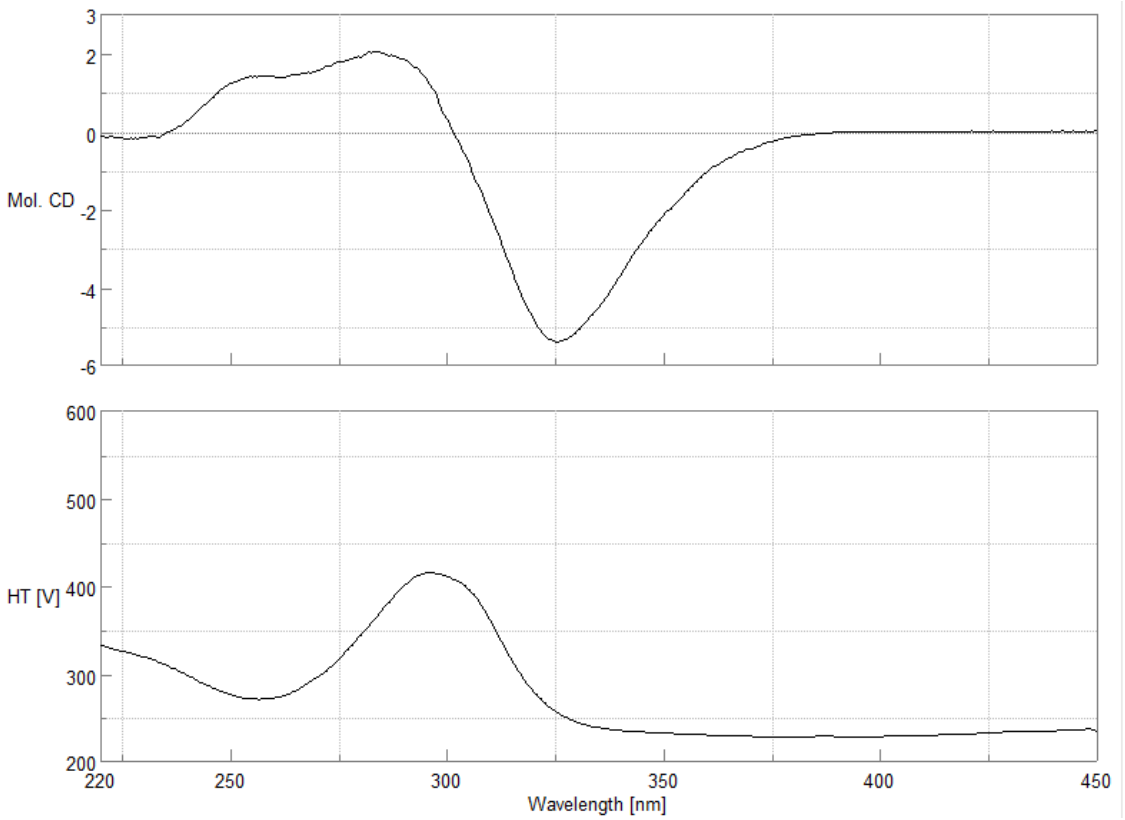

Figure S9. Acyl-CoA ligase mutant (Δ*tunJ*) produces the quorum sensing signal 3-OH-C_{10}-HSL.

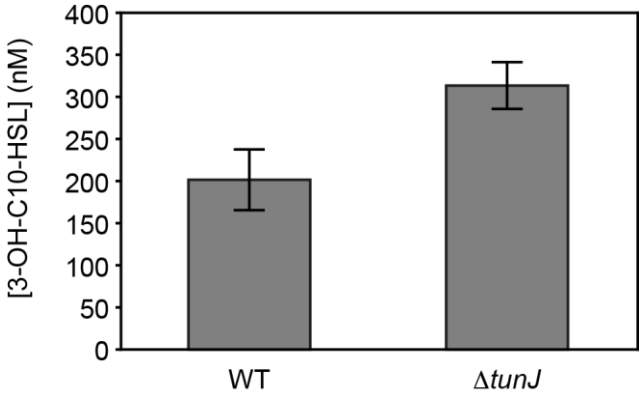

Figure S10. Extracted ion chromatogram of the bicyclic ring.
Bicyclic ring (*m/z* 253.06-253.08) from supernatant extracts of wild type (WT) and the acyl-CoA ligase mutant (Δ*tunJ*) *M. tundripaludum* strains.

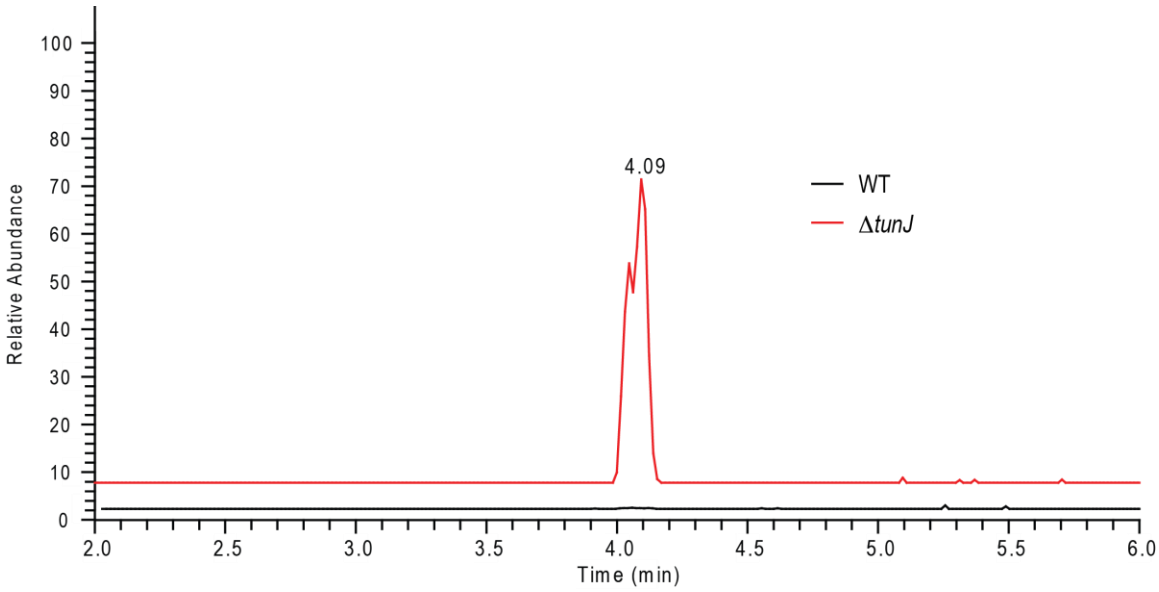

Figure S11. Extracted ion chromatogram of an ion corresponding to the modified lipid tail. (A) Extracted ion chromatogram of the dehydrated lipid tail (*m/z* 169.11-169.13) from supernatant extracts of wild type (WT) and the acyl-CoA ligase mutant (Δ*tunJ*) *M. tundripaludum* strains. (B) Extracted ion chromatogram of tundrenone (*m/z* 421.18-421.19) from the supernatant extracts of the WT and Δ*tunJ* strains. Panel B shows that the ions correlating to the dehydrated lipid tail in the WT strain are the result of in-source fragmentation of complete tundrenone.

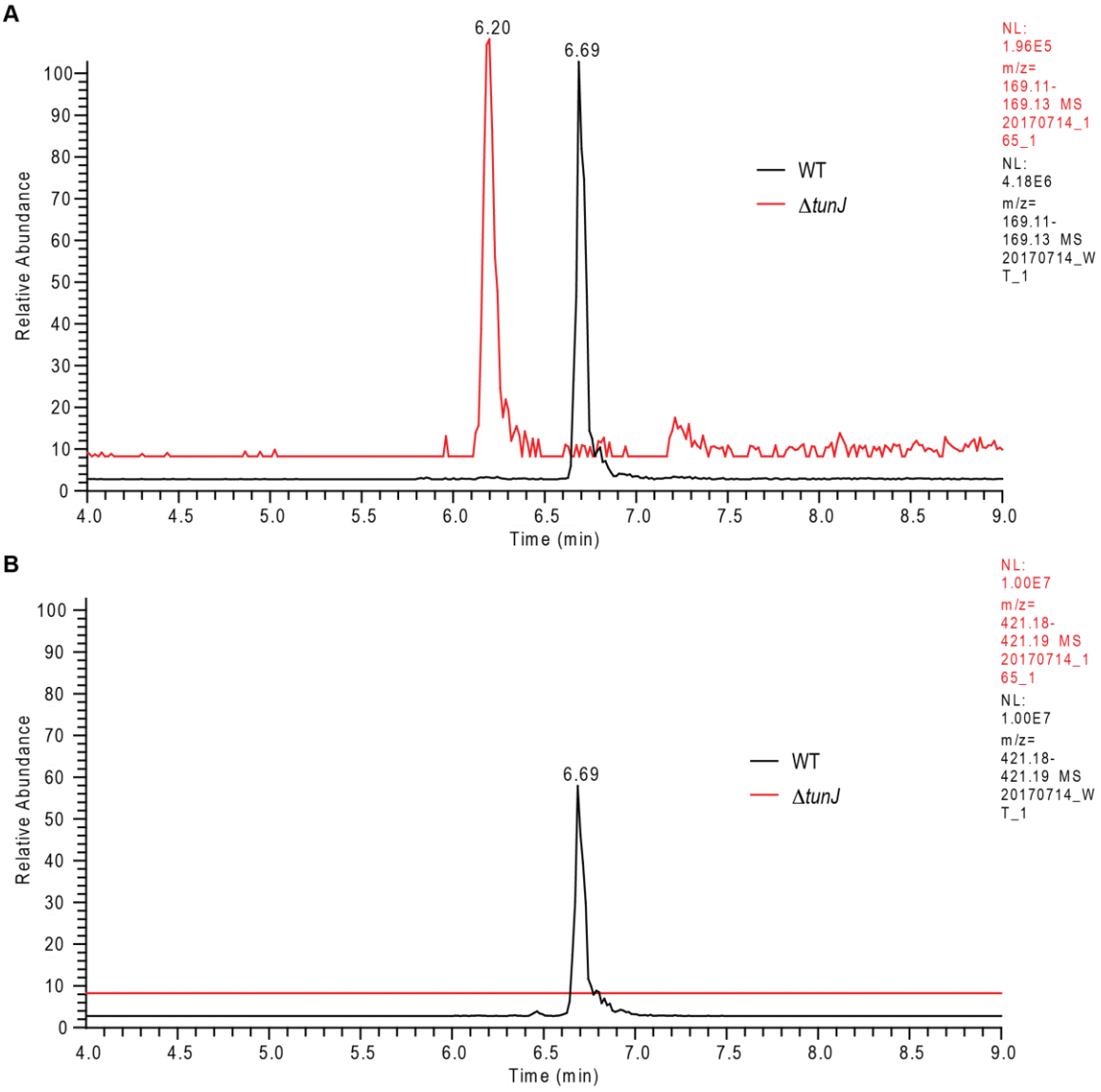

Table S2. Primers used in this study.
Homology regions used for Gibson Assembly are underlined.

Primer Name	Sequence (5' to 3')	Description
AP186_pCM433kanT_fwd1	ATGTGCAGGTTGTCGGTGTC	For amplifying the backbone of pCM433kanT [ref 3].
AP187_pCM433kanT_rev1	TGGTAACTGTCAGACCAAGTTTACTC	
AP634_165U_fwd1	ATATGAGTAAACTTGGTCTGACAGTTACCAACTGTAACAGCTTGCGAATG	For amplifying flanks to knock out the annotated acyl-CoA ligase gene *tunJ* (T451DRAFT_0812)
AP635_165U_rev1	ATAAAGTTTTTCTAACATAATATATGTCTTTAAATTTTAACGG	
AP636_165D_fwd1	AAGACATATATTATGTTAGAAAAACTTTATGCCTAAC	
AP637_165D_rev1	CGTGCATCACGACACCGACAACCTGCACATTTTCCTTGCATCAGACTCTC	
AP705_183U_fwd1	ATATGAGTAAACTTGGTCTGACAGTTACCACCTTGTTTGGCTTACAGTTGG	For amplifying flanks to knock out the annotated anthranilate synthase component I gene *tunN* (T451DRAFT_0816)
AP706_183U_rev1	TTCCTTTTCAAAGCTCATGTACTAGTATTGTAGTACGCG	
AP707_183D_fwd1	CAATACTAGTACATGAGCTTTGAAAAGGAACAATAA	
AP708_183D_rev1	CGTGCATCACGACACCGACAACCTGCACATCGCATCTTGAGAAGGAGTCAC	
AP710_184U_fwd1	ATATGAGTAAACTTGGTCTGACAGTTACCATTTGGAGAAACCGAATGCAC	For amplifying flanks to knock out the annotated anthranilate synthase component II gene *tunO* (T451DRAFT_0817)
AP711_184U_rev1	AAGAAAGTTTGCTAACATGATTATTGTTCCTTTTCAA	
AP712_184D_fwd1	GGAACAATAATCATGTTAGCAAACTTTCTTCTATAAAAC	
AP713_184D_rev1	CGTGCATCACGACACCGACAACCTGCACATAGTATTTGTGGCGCGATTTG	

Computational Data

Table S3. Atom numbers equivalences from manuscript to supporting information

Carbon number		**Proton number**	
Manuscript	SI – computational data	Manuscript	SI – computational data
1	1	1	19
2	9	2a/b	26/27
3	10	6	20
4	11	7	21
5	2	8	22
6	3	9	23
7	4	22a/b	29/30
8	5	C11-OH	28
9	6	C5-OH	24
10	15	C6-OH	23
11	16	C16-OH	25
22	17		

Figure S12. Atom numbering for computational data

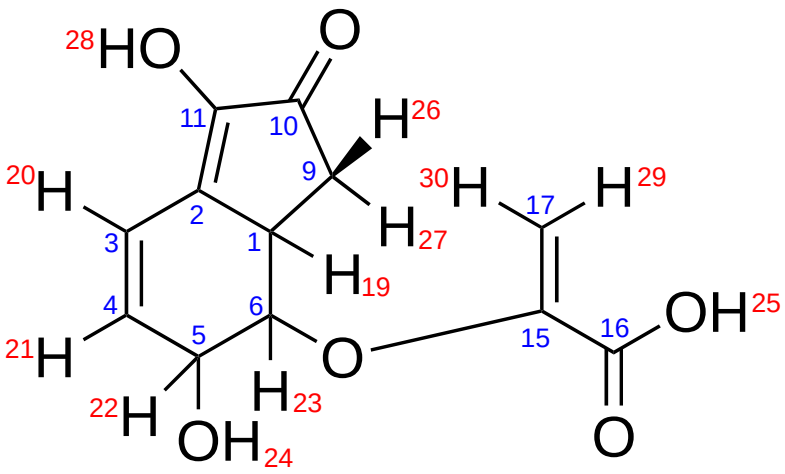

Table S4. Coordinates of lowest energy structure of **i** (gas phase, molecular mechanics)

C	-1.97590000	0.90720000	1.19160000
C	-2.84000000	2.15140000	1.17690000
C	-3.50680000	2.55860000	2.39710000
C	-3.58650000	1.73510000	3.46180000
C	-3.05020000	0.30120000	3.46660000
C	-2.69740000	-0.19530000	2.01640000
O	-1.94260000	0.21810000	4.34070000
O	-5.97880000	-0.72550000	-0.04850000
C	-1.70580000	0.63980000	-0.29410000
C	-2.09730000	1.92700000	-1.00440000
C	-2.84400000	2.72750000	-0.03630000
O	-1.89190000	2.24690000	-2.17450000
O	-3.42970000	3.87400000	-0.48130000
O	-3.87520000	-0.52890000	1.26170000
C	-4.53820000	-1.70530000	1.50400000
C	-5.75630000	-1.83110000	0.71050000
C	-4.17010000	-2.68310000	2.36570000
O	-6.50870000	-2.80260000	0.71580000
H	-1.03420000	1.13290000	1.69940000
H	-3.95790000	3.54000000	2.47120000
H	-4.09330000	2.10120000	4.34260000
H	-3.82240000	-0.34840000	3.88130000
H	-2.04260000	-1.06820000	2.04860000
H	-2.21110000	0.52460000	5.21090000
H	-5.24100000	-0.14740000	0.16520000
H	-0.66400000	0.39340000	-0.49680000
H	-2.32640000	-0.16710000	-0.68300000
H	-3.21580000	3.97210000	-1.41720000
H	-4.76930000	-3.57790000	2.48140000
H	-3.27950000	-2.62960000	2.97180000

Table S5. Coordinates of lowest energy structure of **ii** (gas phase, molecular mechanics)

C	-2.43010000	0.80060000	0.36590000
C	-1.74750000	1.75130000	-0.59560000
C	-0.88860000	1.21520000	-1.63210000
C	-0.87780000	-0.10070000	-1.92270000
C	-1.75100000	-1.13310000	-1.21110000
C	-2.92480000	-0.43580000	-0.43200000
O	-2.19810000	-2.07680000	-2.16430000
O	-4.24680000	-2.61760000	2.53970000
C	-3.48750000	1.68480000	1.03640000
C	-3.03990000	3.11190000	0.75870000
C	-2.04860000	3.02960000	-0.31110000
O	-3.44870000	4.15520000	1.26660000
O	-1.61190000	4.19690000	-0.86030000
O	-3.49520000	-1.27870000	0.58120000
C	-4.48520000	-2.17580000	0.26160000
C	-4.89520000	-2.98610000	1.40440000
C	-5.07140000	-2.35240000	-0.94650000
O	-5.71730000	-3.89780000	1.36760000
H	-1.70400000	0.46600000	1.11130000
H	-0.24920000	1.87190000	-2.20880000
H	-0.20790000	-0.44790000	-2.69700000
H	-1.11650000	-1.66670000	-0.50060000
H	-3.69280000	-0.08080000	-1.12250000
H	-2.64930000	-2.79190000	-1.70420000
H	-3.68370000	-1.89480000	2.25230000
H	-3.57140000	1.50980000	2.10840000
H	-4.47300000	1.54550000	0.59240000
H	-2.04770000	4.92360000	-0.39910000
H	-5.84960000	-3.09370000	-1.08420000
H	-4.81160000	-1.78040000	-1.82390000

Table S6. Coordinates of lowest energy structure of **iii** (gas phase, molecular mechanics)

C	-2.00230000	-4.42730000	2.97220000
C	-0.72160000	-3.72410000	3.38400000
C	-0.73780000	-2.28900000	3.59640000
C	-1.79310000	-1.53690000	3.22310000
C	-3.04390000	-2.11940000	2.56510000
C	-2.75700000	-3.53560000	1.94280000
O	-3.57280000	-1.18630000	1.64920000
O	-0.04290000	-3.44520000	-0.88300000
C	-1.51660000	-5.80910000	2.51790000
C	-0.10980000	-5.93680000	3.08360000
C	0.29540000	-4.59460000	3.49620000
O	0.60090000	-6.93880000	3.14550000
O	1.58760000	-4.41580000	3.88820000
O	-1.85790000	-3.47560000	0.81890000
C	-2.33520000	-3.29140000	-0.45330000
C	-1.27010000	-3.30080000	-1.45120000
C	-3.62550000	-3.11460000	-0.82310000
O	-1.43560000	-3.18570000	-2.66300000
H	-2.64210000	-4.54770000	3.85020000
H	0.11020000	-1.79260000	4.05160000
H	-1.76650000	-0.47640000	3.43160000
H	-3.80200000	-2.22570000	3.34340000
H	-3.68050000	-4.04900000	1.67140000
H	-2.94590000	-1.09370000	0.92480000
H	-0.21500000	-3.50000000	0.06070000
H	-2.14750000	-6.62170000	2.87690000
H	-1.45340000	-5.88420000	1.43240000
H	2.03320000	-5.27080000	3.84500000
H	-3.89460000	-2.98220000	-1.86390000
H	-4.44300000	-3.09120000	-0.11960000

Table S7. Coordinates of lowest energy structure of **iv** (gas phase, molecular mechanics)

C	-2.93630000	1.11990000	0.12870000
C	-1.94630000	1.72360000	-0.84730000
C	-0.87310000	0.89810000	-1.36580000
C	-0.87830000	-0.44070000	-1.20490000
C	-2.00990000	-1.20830000	-0.52120000
C	-3.28880000	-0.30420000	-0.37300000
O	-1.53080000	-1.69190000	0.71870000
O	-5.75140000	-1.50990000	2.42980000
C	-4.06130000	2.16010000	0.17530000
C	-3.45760000	3.42340000	-0.41960000
C	-2.22150000	3.01720000	-1.08340000
O	-3.91600000	4.56510000	-0.41550000
O	-1.56920000	3.95000000	-1.83140000
O	-4.24560000	-0.81110000	0.57020000
C	-5.03860000	-1.88040000	0.23640000
C	-5.89250000	-2.31000000	1.33990000
C	-5.08330000	-2.51890000	-0.95720000
O	-6.64920000	-3.27710000	1.31390000
H	-2.46270000	1.02860000	1.11020000
H	-0.03900000	1.34840000	-1.88910000
H	-0.03910000	-1.00390000	-1.58700000
H	-2.25400000	-2.07890000	-1.13090000
H	-3.77960000	-0.18810000	-1.34240000
H	-2.21760000	-2.22810000	1.12510000
H	-5.11110000	-0.84760000	2.15950000
H	-4.42170000	2.34890000	1.18600000
H	-4.91200000	1.86630000	-0.43920000
H	-2.05600000	4.78000000	-1.76110000
H	-5.74970000	-3.35890000	-1.11320000
H	-4.47920000	-2.23720000	-1.80410000

Table S8. Coordinates of **i-1** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.049283	0.665094	-0.895989
2	6	0	-1.713754	0.497611	0.458288
3	6	0	-1.351349	1.393775	1.529385
4	6	0	-0.278147	2.204066	1.402635
5	6	0	0.620320	2.218988	0.186219
6	6	0	0.436237	0.984910	-0.724890
7	8	0	0.375743	3.352346	-0.668026
8	8	0	1.916931	-2.220471	1.159948
9	6	0	-1.431761	-0.599882	-1.696462
10	6	0	-2.518658	-1.253875	-0.854282
11	6	0	-2.581733	-0.544964	0.437481
12	8	0	-3.225548	-2.215963	-1.124505
13	8	0	-3.404861	-0.974280	1.410487
14	8	0	1.075725	-0.157780	-0.129531
15	6	0	2.426827	-0.352284	-0.282918
16	6	0	2.880062	-1.591349	0.455074
17	6	0	3.295007	0.398932	-0.970310
18	8	0	4.017595	-1.997872	0.427825
19	1	0	-1.471996	1.555006	-1.381283
20	1	0	-1.934093	1.383055	2.446428
21	1	0	-0.002323	2.869000	2.218819
22	1	0	1.665870	2.243149	0.522858
23	1	0	0.893330	1.191162	-1.697760
24	1	0	0.234686	4.139125	-0.124574
25	1	0	1.079480	-1.734510	1.059466
26	1	0	-1.791252	-0.395002	-2.708869
27	1	0	-0.590074	-1.297529	-1.778334
28	1	0	-3.880253	-1.749822	1.058756
29	1	0	4.328525	0.078260	-0.993764
30	1	0	3.020817	1.304142	-1.496697

Rotational constants (GHZ): 0.5433184 0.3252699 0.2539359

T = 298.15 K

Zero-point correction=	0.229519 (Hartree/Particle)
Thermal correction to Energy=	0.245932
Thermal correction to Enthalpy=	0.246876
Thermal correction to Gibbs Free Energy=	0.184476
Sum of electronic and zero-point Energies=	-915.629306
Sum of electronic and thermal Energies=	-915.612892
Sum of electronic and thermal Enthalpies=	-915.611948
Sum of electronic and thermal Free Energies=	-915.674349

Table S9. NMR isotropic and chemical shifts for **i-1** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.131	3.393856
H20	24.3809	6.938374
H21	25.2019	6.162382
H22	27.057	4.408979
H23	27.1161	4.353119
H24	30.5767	1.082231
H25	23.3382	7.923913
H26	29.058	2.517675
H27	29.2549	2.331569
H28	26.1444	5.27155
H29	25.7999	5.597164
H30	26.5161	4.920227
C1	149.3812	35.12976
C2	45.3155	134.2777
C3	56.2659	123.8448
C4	46.9157	132.7531
C5	120.5618	62.58727
C6	109.4415	73.18207
C9	149.8856	34.6492
C10	-23.2669	199.6192
C11	33.9737	145.0836
C15	30.829	148.0796
C16	17.538	160.7426
C17	85.6081	95.8892

Table S10. Coordinates of **i-2** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.056984	0.701282	-0.889471
2	6	0	-1.695850	0.501509	0.472725
3	6	0	-1.311921	1.375899	1.554733
4	6	0	-0.239380	2.185064	1.427819
5	6	0	0.649588	2.210882	0.207984
6	6	0	0.434450	0.994743	-0.730581
7	8	0	0.380475	3.429776	-0.506445
8	8	0	1.875418	-2.203457	1.196240
9	6	0	-1.467510	-0.535878	-1.718858
10	6	0	-2.539513	-1.207592	-0.870564
11	6	0	-2.570127	-0.535376	0.440241
12	8	0	-3.256749	-2.158377	-1.154409
13	8	0	-3.374866	-0.987236	1.419518
14	8	0	1.056721	-0.173877	-0.159988
15	6	0	2.400472	-0.395821	-0.317268
16	6	0	2.840620	-1.616988	0.460488
17	6	0	3.277969	0.311070	-1.039653
18	8	0	3.971095	-2.042593	0.434130
19	1	0	-1.477822	1.610902	-1.339336
20	1	0	-1.889811	1.362116	2.474586
21	1	0	0.034084	2.865393	2.229308
22	1	0	1.695441	2.201685	0.542098
23	1	0	0.885290	1.200521	-1.707521
24	1	0	1.189398	3.737638	-0.936990
25	1	0	1.044161	-1.708170	1.088239
26	1	0	-1.850766	-0.297192	-2.715119
27	1	0	-0.633923	-1.237068	-1.842770
28	1	0	-3.864668	-1.748066	1.056129
29	1	0	4.305431	-0.028452	-1.058650
30	1	0	3.015552	1.194034	-1.607900
Rotational constants (GHZ):			0.5393656	0.3265453	0.2556700

T = 298.15 K

Zero-point correction=	0.229486 (Hartree/Particle)
Thermal correction to Energy=	0.245858
Thermal correction to Enthalpy=	0.246802
Thermal correction to Gibbs Free Energy=	0.184456
Sum of electronic and zero-point Energies=	-915.627908
Sum of electronic and thermal Energies=	-915.611536
Sum of electronic and thermal Enthalpies=	-915.610592
Sum of electronic and thermal Free Energies=	-915.672938

Table S11. NMR isotropic and chemical shifts for **i-2** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.1961	3.332325
H20	24.4391	6.883365
H21	25.2071	6.157467
H22	27.0492	4.416352
H23	27.1182	4.351134
H24	29.9163	1.706427
H25	23.3419	7.920416
H26	29.0659	2.510208
H27	29.2928	2.295747
H28	26.1807	5.23724
H29	25.7996	5.597448
H30	26.5931	4.847448
C1	149.6385	34.88462
C2	45.0884	134.4941
C3	57.43	122.7357
C4	46.5046	133.1448
C5	120.5654	62.58384
C6	107.8272	74.72008
C9	149.7783	34.75143
C10	-23.2318	199.5857
C11	34.129	144.9356
C15	31.0193	147.8983
C16	17.5494	160.7317
C17	86.1741	95.34994

Table S12. Coordinates of **i-4** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.054147	0.623325	-0.905391
2	6	0	-1.758607	0.493305	0.432281
3	6	0	-1.453463	1.436812	1.478922
4	6	0	-0.394304	2.265643	1.357490
5	6	0	0.546752	2.254045	0.175259
6	6	0	0.418336	0.990943	-0.707528
7	8	0	0.323472	3.363880	-0.718171
8	8	0	1.938872	-2.281800	0.972429
9	6	0	-1.371817	-0.688231	-1.657637
10	6	0	-2.470556	-1.333557	-0.826229
11	6	0	-2.598550	-0.571206	0.427810
12	8	0	-3.141849	-2.327308	-1.077180
13	8	0	-3.443952	-0.983005	1.390942
14	8	0	1.068637	-0.121565	-0.079682
15	6	0	2.413794	-0.274774	-0.217897
16	6	0	2.920622	-1.534018	0.426214
17	6	0	3.281010	0.535720	-0.845280
18	8	0	4.090990	-1.858535	0.454901
19	1	0	-1.488577	1.476812	-1.443320
20	1	0	-2.065572	1.445532	2.376662
21	1	0	-0.158999	2.964723	2.157960
22	1	0	1.577229	2.305110	0.552491
23	1	0	0.887007	1.194996	-1.676717
24	1	0	0.082208	4.144754	-0.202304
25	1	0	2.370783	-3.064304	1.355261
26	1	0	-1.694643	-0.544487	-2.692784
27	1	0	-0.508413	-1.363452	-1.663754
28	1	0	-3.879230	-1.788841	1.056105
29	1	0	4.322879	0.244955	-0.871199
30	1	0	2.991545	1.462827	-1.322388

Rotational constants (GHZ): 0.5404650 0.3265140 0.2495813

T = 298.15 K

Zero-point correction=	0.229576 (Hartree/Particle)
Thermal correction to Energy=	0.246009
Thermal correction to Enthalpy=	0.246954
Thermal correction to Gibbs Free Energy=	0.184403
Sum of electronic and zero-point Energies=	-915.629869
Sum of electronic and thermal Energies=	-915.613435
Sum of electronic and thermal Enthalpies=	-915.612491
Sum of electronic and thermal Free Energies=	-915.675042

Table S13. NMR isotropic and scaled chemical shifts for **i-4** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.1787	3.348771
H20	24.3861	6.933459
H21	25.2065	6.158034
H22	27.0017	4.461248
H23	27.2499	4.226654
H24	30.6732	0.991021
H25	25.3638	6.009357
H26	29.0795	2.497353
H27	29.1869	2.395841
H28	26.1984	5.22051
H29	25.7843	5.611909
H30	26.5745	4.865028
C1	149.2252	35.27839
C2	44.9662	134.6105
C3	56.4193	123.6986
C4	47.1117	132.5664
C5	120.5901	62.56031
C6	109.6152	73.01658
C9	149.7429	34.78516
C10	-23.7276	200.0581
C11	34.3618	144.7138
C15	29.5208	149.326
C16	15.3411	162.8357
C17	83.8135	97.59899

Table S14. Coordinates of **i-5** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.083390	0.578592	-0.904447
2	6	0	-1.794287	0.461975	0.431087
3	6	0	-1.510232	1.427593	1.462959
4	6	0	-0.465723	2.273693	1.332660
5	6	0	0.479936	2.260302	0.154642
6	6	0	0.380476	0.980146	-0.707632
7	8	0	0.241747	3.352426	-0.757369
8	8	0	4.193496	-1.676862	0.414870
9	6	0	-1.371523	-0.754107	-1.630977
10	6	0	-2.475602	-1.393651	-0.802265
11	6	0	-2.620771	-0.612970	0.439227
12	8	0	-3.139706	-2.393526	-1.046383
13	8	0	-3.470016	-1.016652	1.401635
14	8	0	1.051422	-0.107644	-0.061009
15	6	0	2.395770	-0.243013	-0.199796
16	6	0	2.847801	-1.508019	0.471055
17	6	0	3.245885	0.578967	-0.838029
18	8	0	2.110008	-2.305119	1.006543
19	1	0	-1.531578	1.411792	-1.462731
20	1	0	-2.125510	1.439044	2.358486
21	1	0	-0.245427	2.988494	2.123421
22	1	0	1.507366	2.337988	0.535626
23	1	0	0.846605	1.179174	-1.679231
24	1	0	-0.061936	4.122481	-0.258630
25	1	0	4.384084	-2.519376	0.859441
26	1	0	-1.677006	-0.640254	-2.675004
27	1	0	-0.499971	-1.418396	-1.602515
28	1	0	-3.887817	-1.837485	1.081358
29	1	0	4.295132	0.322336	-0.878157
30	1	0	2.930408	1.496164	-1.319261

Rotational constants (GHZ): 0.5447354 0.3197985 0.2457186

T = 298.15 K

Zero-point correction= 0.229427 (Hartree/Particle)
Thermal correction to Energy= 0.245936
Thermal correction to Enthalpy= 0.246880
Thermal correction to Gibbs Free Energy= 0.184025
Sum of electronic and zero-point Energies= -915.629179
Sum of electronic and thermal Energies= -915.612669
Sum of electronic and thermal Enthalpies= -915.611725
Sum of electronic and thermal Free Energies= -915.674581

Table S15. NMR isotropic and chemical shifts for **i-5** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.1901	3.337996
H20	24.3981	6.922117
H21	25.2212	6.14414
H22	27.024	4.44017
H23	27.2796	4.198582
H24	30.7068	0.959263
H25	25.5213	5.860491
H26	29.1038	2.474386
H27	29.2176	2.366824
H28	26.2089	5.210586
H29	25.8012	5.595936
H30	26.4024	5.027694
C1	149.2698	35.2359
C2	45.3095	134.2834
C3	56.3059	123.8067
C4	47.4131	132.2792
C5	120.57	62.57946
C6	110.0483	72.60394
C9	149.6753	34.84956
C10	-23.7486	200.0781
C11	34.3778	144.6986
C15	31.0443	147.8745
C16	16.4665	161.7634
C17	83.6891	97.71751

Table S16. Coordinates of **i-6** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.060479	0.658203	-0.900843
2	6	0	-1.740891	0.498734	0.445948
3	6	0	-1.417633	1.424805	1.503148
4	6	0	-0.361523	2.255193	1.380759
5	6	0	0.571516	2.253576	0.195312
6	6	0	0.417774	1.002653	-0.711618
7	8	0	0.310863	3.447945	-0.565260
8	8	0	1.886966	-2.283410	0.995934
9	6	0	-1.402474	-0.629746	-1.682494
10	6	0	-2.487214	-1.291486	-0.844289
11	6	0	-2.585838	-0.561580	0.429610
12	8	0	-3.166828	-2.276268	-1.109470
13	8	0	-3.414436	-0.993683	1.399689
14	8	0	1.053024	-0.132394	-0.102190
15	6	0	2.392003	-0.312983	-0.241793
16	6	0	2.879071	-1.568804	0.427817
17	6	0	3.275472	0.463640	-0.889724
18	8	0	4.043503	-1.913406	0.454820
19	1	0	-1.495160	1.531346	-1.406691
20	1	0	-2.026088	1.431188	2.403145
21	1	0	-0.132070	2.972625	2.163638
22	1	0	1.602832	2.276034	0.571629
23	1	0	0.883091	1.202486	-1.684674
24	1	0	1.120810	3.727023	-1.013379
25	1	0	2.303732	-3.066365	1.394493
26	1	0	-1.748708	-0.454552	-2.705252
27	1	0	-0.544346	-1.310054	-1.728045
28	1	0	-3.863006	-1.786574	1.052372
29	1	0	4.311276	0.152220	-0.911803
30	1	0	3.004191	1.381119	-1.394613

Rotational constants (GHZ): 0.5354445 0.3285674 0.2509782

T = 298.15 K

Zero-point correction= 0.229535 (Hartree/Particle)
Thermal correction to Energy= 0.245929
Thermal correction to Enthalpy= 0.246873
Thermal correction to Gibbs Free Energy= 0.184374
Sum of electronic and zero-point Energies= -915.628250
Sum of electronic and thermal Energies= -915.611855
Sum of electronic and thermal Enthalpies= -915.610911
Sum of electronic and thermal Free Energies= -915.673410

Table S17. NMR isotropic and chemical shifts for **i-6** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.2327	3.297732
H20	24.4441	6.878639
H21	25.2016	6.162665
H22	26.985	4.477032
H23	27.272	4.205766
H24	29.978	1.64811
H25	25.3768	5.99707
H26	29.0876	2.489698
H27	29.2403	2.345369
H28	26.2487	5.172968
H29	25.7895	5.606994
H30	26.717	4.73034
C1	149.3831	35.12795
C2	44.696	134.8679
C3	57.6424	122.5333
C4	46.5443	133.107
C5	120.5542	62.59451
C6	107.8875	74.66263
C9	149.6771	34.84785
C10	-23.6632	199.9968
C11	34.6238	144.4642
C15	29.7796	149.0795
C16	15.4193	162.7611
C17	84.6654	96.78735

Table S18. Coordinates of **iii-2** (gas phase, B3LYP/6-31+G(d,p)) (redundant to **iii-1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.991098	0.633211	-1.093300
2	6	0	-1.752305	0.745258	0.217268
3	6	0	-1.469572	1.857724	1.093472
4	6	0	-0.403313	2.650819	0.853648
5	6	0	0.564717	2.438783	-0.292563
6	6	0	0.479612	1.011696	-0.884504
7	8	0	1.897012	2.773969	0.078403
8	8	0	1.426383	-2.057188	1.448791
9	6	0	-1.308629	-0.780569	-1.628531
10	6	0	-2.447297	-1.265661	-0.739022
11	6	0	-2.604748	-0.300872	0.362346
12	8	0	-3.120789	-2.282119	-0.845525
13	8	0	-3.487480	-0.531208	1.351949
14	8	0	1.063581	0.072739	0.044662
15	6	0	2.281590	-0.521727	-0.208277
16	6	0	2.459367	-1.767313	0.630272
17	6	0	3.238853	-0.107210	-1.044819
18	8	0	3.449560	-2.458201	0.584628
19	1	0	-1.391856	1.383689	-1.791280
20	1	0	-2.109647	2.030020	1.954125
21	1	0	-0.179641	3.495063	1.500940
22	1	0	0.324961	3.141895	-1.102147
23	1	0	1.034215	0.965354	-1.825469
24	1	0	2.162573	2.202403	0.813832
25	1	0	0.735073	-1.380136	1.339455
26	1	0	-1.598584	-0.800739	-2.682918
27	1	0	-0.460274	-1.464525	-1.508564
28	1	0	-3.928844	-1.376614	1.148807
29	1	0	4.132850	-0.712257	-1.126484
30	1	0	3.169992	0.807092	-1.619502

Rotational constants (GHZ): 0.5469815 0.3502153 0.2616061

T = 298.15 K

Zero-point correction=	0.229760 (Hartree/Particle)
Thermal correction to Energy=	0.245890
Thermal correction to Enthalpy=	0.246834
Thermal correction to Gibbs Free Energy=	0.185046
Sum of electronic and zero-point Energies=	-915.628520
Sum of electronic and thermal Energies=	-915.612390
Sum of electronic and thermal Enthalpies=	-915.611446
Sum of electronic and thermal Free Energies=	-915.673234

Table S19. NMR isotropic and chemical shifts for **iii-2** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.3282	3.207467
H20	24.4843	6.840643
H21	25.267	6.100851
H22	26.7676	4.682514
H23	26.8893	4.567486
H24	30.2599	1.381664
H25	23.1653	8.087335
H26	29.1304	2.449244
H27	29.4768	2.121834
H28	26.2342	5.186673
H29	25.6883	5.702647
H30	26.1722	5.245274
C1	144.3109	39.96046
C2	44.1972	135.3432
C3	58.4499	121.764
C4	39.6529	139.6727
C5	111.1162	71.58651
C6	103.1684	79.15873
C9	148.993	35.49962
C10	-22.3767	198.7711
C11	34.5947	144.4919
C15	26.9843	151.7427
C16	17.6582	160.628
C17	81.8543	99.46561

Table S20. Coordinates of **iii-3** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.983740	0.605962	1.096134
2	6	0	1.790465	0.745746	-0.183446
3	6	0	1.564298	1.892085	-1.030097
4	6	0	0.506104	2.698678	-0.803219
5	6	0	-0.509428	2.469120	0.296204
6	6	0	-0.473216	1.026335	0.859440
7	8	0	-1.820900	2.831665	-0.127976
8	8	0	-1.353063	-2.209880	-1.146380
9	6	0	1.243028	-0.837800	1.580099
10	6	0	2.389803	-1.323189	0.703619
11	6	0	2.616672	-0.317640	-0.344429
12	8	0	3.020431	-2.371288	0.780810
13	8	0	3.522895	-0.537621	-1.317096
14	8	0	-1.051014	0.111474	-0.089913
15	6	0	-2.284989	-0.430858	0.134018
16	6	0	-2.478573	-1.750363	-0.558163
17	6	0	-3.285931	0.083818	0.863553
18	8	0	-3.531990	-2.354584	-0.586704
19	1	0	1.382156	1.316844	1.836093
20	1	0	2.237960	2.077546	-1.861891
21	1	0	0.322311	3.567334	-1.430612
22	1	0	-0.298274	3.151186	1.131414
23	1	0	-1.047247	0.982057	1.790639
24	1	0	-2.053568	2.276628	-0.887120
25	1	0	-1.585493	-3.059376	-1.558650
26	1	0	1.498421	-0.913122	2.641062
27	1	0	0.379279	-1.485897	1.395241
28	1	0	3.922500	-1.408229	-1.136203
29	1	0	-4.202566	-0.484991	0.950864
30	1	0	-3.218194	1.050540	1.344968

Rotational constants (GHZ): 0.5451864 0.3563558 0.2570285

T = 298.15 K

Zero-point correction=	0.229795 (Hartree/Particle)
Thermal correction to Energy=	0.245945
Thermal correction to Enthalpy=	0.246889
Thermal correction to Gibbs Free Energy=	0.184982
Sum of electronic and zero-point Energies=	-915.629483
Sum of electronic and thermal Energies=	-915.613334
Sum of electronic and thermal Enthalpies=	-915.612390
Sum of electronic and thermal Free Energies=	-915.674296

Table S21. NMR isotropic and chemical shifts for **iii-3** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.3743	3.163894
H20	24.527	6.800284
H21	25.3067	6.063327
H22	26.7816	4.669282
H23	27.0224	4.441682
H24	30.2819	1.36087
H25	25.3634	6.009735
H26	29.1427	2.437618
H27	29.3303	2.260302
H28	26.2827	5.140832
H29	25.6118	5.774953
H30	26.0266	5.382892
C1	143.903	40.34909
C2	43.2616	136.2346
C3	58.6505	121.5729
C4	39.7047	139.6234
C5	110.9713	71.72456
C6	101.7533	80.50696
C9	148.817	35.6673
C10	-22.8358	199.2085
C11	35.1665	143.9471
C15	25.1908	153.4514
C16	15.2816	162.8923
C17	77.6713	103.4509

Table S22. Coordinates of **iii-4** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.003098	0.530428	1.082111
2	6	0	1.836685	0.693668	-0.177827
3	6	0	1.661765	1.876063	-0.985541
4	6	0	0.631834	2.713785	-0.742438
5	6	0	-0.403388	2.485180	0.337972
6	6	0	-0.431775	1.022961	0.849946
7	8	0	-1.696158	2.912432	-0.086950
8	8	0	-3.692410	-2.139612	-0.611029
9	6	0	1.198377	-0.943446	1.502044
10	6	0	2.372002	-1.415494	0.654769
11	6	0	2.641022	-0.383030	-0.358240
12	8	0	2.994486	-2.468118	0.726656
13	8	0	3.567403	-0.589048	-1.314163
14	8	0	-1.045790	0.168987	-0.132747
15	6	0	-2.289689	-0.346744	0.082214
16	6	0	-2.411063	-1.697329	-0.561695
17	6	0	-3.293106	0.219794	0.770219
18	8	0	-1.477680	-2.341604	-0.988922
19	1	0	1.420221	1.189130	1.859549
20	1	0	2.352611	2.065814	-1.802175
21	1	0	0.489341	3.610732	-1.340087
22	1	0	-0.176965	3.128907	1.199149
23	1	0	-1.015616	0.972200	1.775110
24	1	0	-1.931836	2.402916	-0.876594
25	1	0	-3.664748	-3.026620	-1.006904
26	1	0	1.394065	-1.085081	2.568680
27	1	0	0.330178	-1.553478	1.228074
28	1	0	3.938734	-1.476804	-1.157826
29	1	0	-4.230296	-0.309913	0.874244
30	1	0	-3.199069	1.202888	1.214827

Rotational constants (GHZ): 0.5471475 0.3524533 0.2510411

T = 298.15 K

Zero-point correction=	0.229637 (Hartree/Particle)
Thermal correction to Energy=	0.245872
Thermal correction to Enthalpy=	0.246816
Thermal correction to Gibbs Free Energy=	0.184236
Sum of electronic and zero-point Energies=	-915.628939
Sum of electronic and thermal Energies=	-915.612705
Sum of electronic and thermal Enthalpies=	-915.611761
Sum of electronic and thermal Free Energies=	-915.674340

Table S23. NMR isotropic and chemical shifts for **iii-4** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.3923	3.146881
H20	24.5545	6.774291
H21	25.3294	6.041871
H22	26.7933	4.658223
H23	27.1145	4.354631
H24	30.2635	1.378261
H25	25.4984	5.882136
H26	29.2007	2.382798
H27	29.233	2.352268
H28	26.2742	5.148866
H29	25.6456	5.743006
H30	25.7435	5.650473
C1	143.6425	40.59728
C2	43.6744	135.8413
C3	58.6325	121.59
C4	39.986	139.3554
C5	111.1223	71.5807
C6	100.55	81.65339
C9	148.6383	35.83756
C10	-23.0727	199.4342
C11	35.1724	143.9415
C15	26.3809	152.3175
C16	15.8986	162.3045
C17	76.1433	104.9067

Table S24. Coordinates of **iii-6** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.208269	0.175730	-1.111922
2	6	0	-1.854839	0.799849	0.114905
3	6	0	-1.378119	2.075783	0.589893
4	6	0	-0.242145	2.601317	0.084727
5	6	0	0.605006	1.928045	-0.975496
6	6	0	0.305128	0.412217	-1.106713
7	8	0	1.987064	2.163814	-0.770131
8	8	0	4.000997	-1.644544	0.996569
9	6	0	-1.718778	-1.282021	-1.131286
10	6	0	-2.855129	-1.291008	-0.115974
11	6	0	-2.822443	-0.014858	0.607064
12	8	0	-3.650589	-2.191725	0.128626
13	8	0	-3.662266	0.210083	1.638598
14	8	0	0.897500	-0.253890	0.029913
15	6	0	1.984803	-1.057103	-0.131069
16	6	0	3.094283	-0.665874	0.797888
17	6	0	2.103047	-2.067133	-1.004029
18	8	0	3.187752	0.432588	1.314034
19	1	0	-1.584376	0.702349	-2.002342
20	1	0	-1.925666	2.583224	1.378973
21	1	0	0.137067	3.555424	0.441941
22	1	0	0.381960	2.387094	-1.949743
23	1	0	0.774313	0.031482	-2.019850
24	1	0	2.254736	1.756869	0.075106
25	1	0	4.700987	-1.276043	1.561837
26	1	0	-2.059935	-1.626156	-2.111988
27	1	0	-0.951519	-1.979681	-0.776355
28	1	0	-4.211613	-0.589262	1.732982
29	1	0	3.013673	-2.650351	-1.037285
30	1	0	1.311432	-2.315214	-1.702079

Rotational constants (GHZ): 0.6677333 0.2917002 0.2441766

T = 298.15 K

Zero-point correction=	0.230147 (Hartree/Particle)
Thermal correction to Energy=	0.246015
Thermal correction to Enthalpy=	0.246959
Thermal correction to Gibbs Free Energy=	0.186320
Sum of electronic and zero-point Energies=	-915.631273
Sum of electronic and thermal Energies=	-915.615405
Sum of electronic and thermal Enthalpies=	-915.614461
Sum of electronic and thermal Free Energies=	-915.675100

Table S25. NMR isotropic and chemical shifts for **iii-6** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.316	3.218998
H20	24.5495	6.779017
H21	25.2293	6.136484
H22	27.0599	4.406238
H23	27.2526	4.224102
H24	27.7114	3.790454
H25	25.2274	6.13828
H26	28.9542	2.615784
H27	29.2048	2.378922
H28	26.3206	5.105009
H29	25.4755	5.903781
H30	25.9752	5.431474
C1	144.0949	40.16625
C2	42.4347	137.0224
C3	59.5965	120.6716
C4	37.4882	141.7351
C5	111.8583	70.87948
C6	94.6197	87.30345
C9	147.4434	36.97599
C10	-22.357	198.7523
C11	35.8627	143.2838
C15	24.8086	153.8155
C16	12.1107	165.9134
C17	69.96	110.7978

Table S26. Coordinates of **iii-7** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.174615	0.200544	-1.113405
2	6	0	-1.840939	0.784033	0.122822
3	6	0	-1.416714	2.073792	0.610073
4	6	0	-0.304541	2.651657	0.109799
5	6	0	0.573432	2.022462	-0.951230
6	6	0	0.328437	0.499042	-1.115881
7	8	0	1.947854	2.291711	-0.712492
8	8	0	3.052205	0.242737	1.480268
9	6	0	-1.627735	-1.276829	-1.146913
10	6	0	-2.763947	-1.339297	-0.133794
11	6	0	-2.776065	-0.071787	0.607102
12	8	0	-3.528295	-2.269057	0.097970
13	8	0	-3.621693	0.108986	1.641560
14	8	0	0.974992	-0.149332	-0.001317
15	6	0	1.984225	-1.041345	-0.210784
16	6	0	3.088542	-0.932346	0.799545
17	6	0	2.075145	-1.954690	-1.187393
18	8	0	3.944454	-1.770353	0.984646
19	1	0	-1.577512	0.720930	-1.996029
20	1	0	-1.986753	2.552213	1.401415
21	1	0	0.031334	3.619855	0.472464
22	1	0	0.359231	2.496347	-1.919373
23	1	0	0.803305	0.162795	-2.042647
24	1	0	2.203072	1.835894	0.106855
25	1	0	3.810385	0.235799	2.089152
26	1	0	-1.953627	-1.624968	-2.131340
27	1	0	-0.835952	-1.949175	-0.797545
28	1	0	-4.142947	-0.710243	1.725518
29	1	0	2.943477	-2.599896	-1.219422
30	1	0	1.318504	-2.068504	-1.953773

Rotational constants (GHZ): 0.6338013 0.3002116 0.2487605

T = 298.15 K

Zero-point correction=	0.230009 (Hartree/Particle)
Thermal correction to Energy=	0.246011
Thermal correction to Enthalpy=	0.246955
Thermal correction to Gibbs Free Energy=	0.185596
Sum of electronic and zero-point Energies=	-915.629864
Sum of electronic and thermal Energies=	-915.613862
Sum of electronic and thermal Enthalpies=	-915.612918
Sum of electronic and thermal Free Energies=	-915.674277

Table S27. NMR isotropic and chemical shifts for **iii-7** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.2622	3.269849
H20	24.5189	6.80794
H21	25.2423	6.124197
H22	27.0135	4.450095
H23	27.1074	4.361342
H24	28.8625	2.702457
H25	25.1915	6.172212
H26	28.9484	2.621267
H27	29.2749	2.312665
H28	26.2956	5.128639
H29	25.6221	5.765217
H30	26.3391	5.087524
C1	144.1502	40.11357
C2	43.1124	136.3767
C3	59.1485	121.0984
C4	38.511	140.7607
C5	112.5683	70.20303
C6	97.9169	84.16206
C9	147.348	37.06688
C10	-22.2907	198.6891
C11	35.5611	143.5712
C15	24.2775	154.3216
C16	15.0074	163.1536
C17	75.6209	105.4044

Table S28. Coordinates of **iii-10** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.148888	0.345123	-1.133562
2	6	0	-1.793517	0.752820	0.181842
3	6	0	-1.356140	1.963029	0.836318
4	6	0	-0.256773	2.612756	0.400079
5	6	0	0.561440	2.155156	-0.783497
6	6	0	0.352959	0.652284	-1.101802
7	8	0	1.923388	2.458361	-0.496142
8	8	0	2.551241	-0.376373	1.968109
9	6	0	-1.582332	-1.121006	-1.355078
10	6	0	-2.687748	-1.338452	-0.328867
11	6	0	-2.702384	-0.175668	0.572615
12	8	0	-3.429553	-2.303880	-0.199434
13	8	0	-3.519737	-0.148316	1.641761
14	8	0	0.980850	-0.123196	-0.068731
15	6	0	2.071123	-0.914061	-0.334213
16	6	0	2.924489	-1.106088	0.901568
17	6	0	2.395951	-1.500441	-1.492005
18	8	0	3.871784	-1.856880	0.935528
19	1	0	-1.567722	0.972665	-1.934777
20	1	0	-1.900458	2.318274	1.706421
21	1	0	0.101085	3.510242	0.896341
22	1	0	0.236846	2.718815	-1.675659
23	1	0	0.820554	0.419088	-2.063202
24	1	0	2.454399	2.384043	-1.300483
25	1	0	1.791903	0.180982	1.718272
26	1	0	-1.936073	-1.334978	-2.367708
27	1	0	-0.768739	-1.820763	-1.130445
28	1	0	-4.023245	-0.983045	1.636695
29	1	0	3.294054	-2.103913	-1.519558
30	1	0	1.804541	-1.411851	-2.395007

Rotational constants (GHZ): 0.5990472 0.3083052 0.2610168

T = 298.15 K

Zero-point correction=	0.229290 (Hartree/Particle)
Thermal correction to Energy=	0.245638
Thermal correction to Enthalpy=	0.246582
Thermal correction to Gibbs Free Energy=	0.182825
Sum of electronic and zero-point Energies=	-915.625504
Sum of electronic and thermal Energies=	-915.609157
Sum of electronic and thermal Enthalpies=	-915.608212
Sum of electronic and thermal Free Energies=	-915.671969

Table S29. NMR isotropic and chemical shifts for **iii-10** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.2587	3.273157
H20	24.4849	6.840076
H21	25.2418	6.124669
H22	26.5447	4.893195
H23	26.9619	4.498866
H24	30.5065	1.148582
H25	22.9137	8.325142
H26	29.0451	2.529868
H27	29.3808	2.212571
H28	26.291	5.132987
H29	25.7428	5.651134
H30	26.467	4.966635
C1	145.2812	39.03601
C2	43.8303	135.6927
C3	58.7898	121.4402
C4	41.6336	137.7856
C5	111.7493	70.98333
C6	103.0207	79.29945
C9	148.1021	36.34842
C10	-22.3469	198.7427
C11	35.0439	144.0639
C15	26.0929	152.5919
C16	17.2843	160.9843
C17	83.0224	98.35271

Table S30. Coordinates of **iii-11** (gas phase, B3LYP/6-31+G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.968917	0.040773	-1.084847
2	6	0	-1.905142	0.716279	-0.095179
3	6	0	-1.678149	2.099566	0.251438
4	6	0	-0.533032	2.709408	-0.123105
5	6	0	0.566077	2.015675	-0.899363
6	6	0	0.475831	0.473631	-0.818057
7	8	0	1.859966	2.488232	-0.530157
8	8	0	4.134525	-1.370069	0.248820
9	6	0	-1.298843	-1.465588	-0.993225
10	6	0	-2.567507	-1.517491	-0.155836
11	6	0	-2.829137	-0.165265	0.360952
12	8	0	-3.271883	-2.484760	0.112996
13	8	0	-3.855718	0.052894	1.207399
14	8	0	0.815580	0.028333	0.517649
15	6	0	2.095973	-0.305312	0.852538
16	6	0	2.820043	-1.260820	-0.048744
17	6	0	2.600991	0.066522	2.039081
18	8	0	2.296009	-1.895355	-0.943809
19	1	0	-1.208105	0.407431	-2.094190
20	1	0	-2.424555	2.627806	0.838151
21	1	0	-0.346969	3.750666	0.128823
22	1	0	0.479163	2.285588	-1.961453
23	1	0	1.161218	0.027367	-1.539753
24	1	0	2.001401	2.302223	0.408831
25	1	0	4.504995	-2.038997	-0.351559
26	1	0	-1.450353	-1.943562	-1.965428
27	1	0	-0.505875	-2.018380	-0.478424
28	1	0	-4.300417	-0.806100	1.331181
29	1	0	3.575348	-0.279356	2.355825
30	1	0	2.017199	0.686853	2.710891

Rotational constants (GHZ): 0.6426682 0.3137088 0.2488655

T = 298.15 K

Zero-point correction= 0.229540 (Hartree/Particle)
Thermal correction to Energy= 0.245746
Thermal correction to Enthalpy= 0.246690
Thermal correction to Gibbs Free Energy= 0.184631
Sum of electronic and zero-point Energies= -915.628960
Sum of electronic and thermal Energies= -915.612755
Sum of electronic and thermal Enthalpies= -915.611811
Sum of electronic and thermal Free Energies= -915.673869

Table S31. NMR isotropic and chemical shifts for **iii-11** (in ppm) (SCRF-mPW1PW91/6-311+G(2d,p)//B3LYP/6-31+G(d,p), SCRF = IEFPCM, solvent = DMSO)

Atom	Isotropic	Scaled
H19	28.471	3.072495
H20	24.5698	6.75983
H21	25.1375	6.223251
H22	26.9666	4.494423
H23	26.4892	4.945652
H24	30.3682	1.279301
H25	25.3637	6.009452
H26	29.1233	2.455955
H27	28.9341	2.634783
H28	26.2621	5.160302
H29	25.7444	5.649622
H30	25.9636	5.442439
C1	144.7054	39.5846
C2	42.7462	136.7256
C3	59.1073	121.1377
C4	39.9418	139.3975
C5	108.9093	73.68912
C6	105.7612	76.68845
C9	148.8386	35.64672
C10	-23.2692	199.6214
C11	34.7359	144.3574
C15	27.7042	151.0568
C16	16.1796	162.0368
C17	70.2163	110.5536

Table S32. Coordinates of **i-1** (wB97XD/6-311++G(d,p), SCRF = CPCM, solvent = MeOH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.032106	0.722883	-0.913466
2	6	0	-1.675367	0.525392	0.436641
3	6	0	-1.330545	1.433213	1.510277
4	6	0	-0.270981	2.241793	1.386353
5	6	0	0.634305	2.256590	0.176433
6	6	0	0.446323	1.029104	-0.728047
7	8	0	0.396800	3.388236	-0.655456
8	8	0	1.679899	-2.290653	1.013804
9	6	0	-1.386786	-0.535265	-1.716338
10	6	0	-2.407704	-1.247185	-0.858705
11	6	0	-2.480735	-0.550572	0.435263
12	8	0	-3.055765	-2.240962	-1.125049
13	8	0	-3.251199	-1.015213	1.429484
14	8	0	1.032725	-0.116375	-0.111788
15	6	0	2.360200	-0.362339	-0.231122
16	6	0	2.706058	-1.664480	0.439797
17	6	0	3.287382	0.375479	-0.834066
18	8	0	3.817290	-2.125940	0.469633
19	1	0	-1.467475	1.610449	-1.383559
20	1	0	-1.923191	1.429821	2.418601
21	1	0	-0.010596	2.925932	2.188254
22	1	0	1.673952	2.269556	0.524868
23	1	0	0.925269	1.210772	-1.693543
24	1	0	0.492489	4.186309	-0.130402
25	1	0	0.874172	-1.767532	0.881003
26	1	0	-1.788377	-0.328038	-2.708880
27	1	0	-0.522602	-1.195654	-1.834519
28	1	0	-3.691471	-1.814228	1.110461
29	1	0	4.304693	0.010440	-0.843174
30	1	0	3.074879	1.321745	-1.312259

Rotational constants (GHZ): 0.5306313 0.3515647 0.2641050

T = 298.15 K

Zero-point correction= 0.232023 (Hartree/Particle)
Thermal correction to Energy= 0.248310
Thermal correction to Enthalpy= 0.249255
Thermal correction to Gibbs Free Energy= 0.187142
Sum of electronic and zero-point Energies= -915.568029
Sum of electronic and thermal Energies= -915.551742
Sum of electronic and thermal Enthalpies= -915.550798
Sum of electronic and thermal Free Energies= -915.612910

w= 0.077318 a.u., Optical Rotation Beta= 1.5676 au.
Molar Mass = 252.2232 grams/mole, [Alpha] (5893.0 A) = 240.23 deg.

Table S33. Coordinates of **i-2** (wB97XD/6-311++G(d,p), SCRF = CPCM, solvent = MeOH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.031508	0.740290	-0.910156
2	6	0	-1.665347	0.524920	0.441955
3	6	0	-1.313614	1.418615	1.525371
4	6	0	-0.259000	2.233395	1.404985
5	6	0	0.635450	2.267258	0.192213
6	6	0	0.447457	1.042222	-0.725970
7	8	0	0.348343	3.464450	-0.521248
8	8	0	1.648161	-2.288723	1.016450
9	6	0	-1.391733	-0.507489	-1.726744
10	6	0	-2.406389	-1.230714	-0.871279
11	6	0	-2.470480	-0.551046	0.431970
12	8	0	-3.055563	-2.221581	-1.145800
13	8	0	-3.232932	-1.029679	1.425924
14	8	0	1.029337	-0.111321	-0.116361
15	6	0	2.352595	-0.374751	-0.238244
16	6	0	2.681845	-1.678879	0.438592
17	6	0	3.290718	0.343803	-0.847548
18	8	0	3.786839	-2.154919	0.469312
19	1	0	-1.468802	1.634308	-1.366155
20	1	0	-1.899962	1.402336	2.437556
21	1	0	0.002768	2.915449	2.206761
22	1	0	1.675159	2.281014	0.538707
23	1	0	0.925692	1.221638	-1.693064
24	1	0	1.106986	3.697335	-1.062111
25	1	0	0.849384	-1.755260	0.882459
26	1	0	-1.800284	-0.287799	-2.713777
27	1	0	-0.528192	-1.166049	-1.859203
28	1	0	-3.674419	-1.825158	1.099878
29	1	0	4.301433	-0.039249	-0.854710
30	1	0	3.096782	1.289865	-1.333422

Rotational constants (GHZ): 0.5269371 0.3536563 0.2648355

T = 298.15 K

Zero-point correction= 0.232110 (Hartree/Particle)
Thermal correction to Energy= 0.248362
Thermal correction to Enthalpy= 0.249306
Thermal correction to Gibbs Free Energy= 0.187079
Sum of electronic and zero-point Energies= -915.568358
Sum of electronic and thermal Energies= -915.552106
Sum of electronic and thermal Enthalpies= -915.551162
Sum of electronic and thermal Free Energies= -915.613389

w= 0.077318 a.u., Optical Rotation Beta= 1.1445 au.
Molar Mass = 252.2232 grams/mole, [Alpha] (5893.0 A) = 175.39 deg.

Table S34. Coordinates of **i-4** (wB97XD/6-311++G(d,p), SCRF = CPCM, solvent = MeOH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.058749	0.676770	-0.910153
2	6	0	-1.724673	0.497066	0.430759
3	6	0	-1.414715	1.431957	1.491169
4	6	0	-0.366508	2.255281	1.368455
5	6	0	0.561376	2.260121	0.176153
6	6	0	0.411999	1.014697	-0.712810
7	8	0	0.326428	3.377705	-0.677102
8	8	0	1.824730	-2.273501	0.959177
9	6	0	-1.380390	-0.602850	-1.692462
10	6	0	-2.412948	-1.306998	-0.843135
11	6	0	-2.519446	-0.586503	0.434321
12	8	0	-3.046973	-2.312141	-1.103598
13	8	0	-3.306156	-1.040244	1.422116
14	8	0	1.021314	-0.109731	-0.087050
15	6	0	2.352423	-0.290951	-0.212794
16	6	0	2.817275	-1.573319	0.412737
17	6	0	3.239603	0.505841	-0.809242
18	8	0	3.968184	-1.936458	0.421278
19	1	0	-1.503590	1.546006	-1.405680
20	1	0	-2.024363	1.438575	2.388219
21	1	0	-0.133091	2.961447	2.159714
22	1	0	1.592462	2.294798	0.547174
23	1	0	0.886530	1.205434	-1.679469
24	1	0	0.394108	4.183532	-0.159634
25	1	0	2.202204	-3.078495	1.337444
26	1	0	-1.759265	-0.423766	-2.699402
27	1	0	-0.505292	-1.254673	-1.770929
28	1	0	-3.732993	-1.848337	1.107957
29	1	0	4.274318	0.195355	-0.832933
30	1	0	2.977270	1.448408	-1.269020

Rotational constants (GHZ): 0.5350182 0.3425626 0.2582968

T = 298.15 K

Zero-point correction= 0.231908 (Hartree/Particle)
Thermal correction to Energy= 0.248264
Thermal correction to Enthalpy= 0.249208
Thermal correction to Gibbs Free Energy= 0.186632
Sum of electronic and zero-point Energies= -915.565458
Sum of electronic and thermal Energies= -915.549102
Sum of electronic and thermal Enthalpies= -915.548158
Sum of electronic and thermal Free Energies= -915.610733

w= 0.077318 a.u., Optical Rotation Beta= 1.3605 au.
Molar Mass = 252.2232 grams/mole, [Alpha] (5893.0 A) = 208.49 deg.

Table S35. Coordinates of **i-5** (wB97XD/6-311++G(d,p), SCRF = CPCM, solvent = MeOH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.097959	0.642596	-0.908929
2	6	0	-1.759277	0.460974	0.433942
3	6	0	-1.464678	1.408992	1.487023
4	6	0	-0.431322	2.249788	1.356782
5	6	0	0.494891	2.262435	0.163197
6	6	0	0.367076	1.007767	-0.716388
7	8	0	0.238934	3.369585	-0.697587
8	8	0	4.064025	-1.762876	0.355770
9	6	0	-1.398872	-0.647546	-1.682013
10	6	0	-2.418550	-1.363120	-0.826714
11	6	0	-2.535704	-0.635774	0.445979
12	8	0	-3.036301	-2.380201	-1.079839
13	8	0	-3.313822	-1.095645	1.437709
14	8	0	0.997376	-0.099984	-0.083860
15	6	0	2.331254	-0.258615	-0.208222
16	6	0	2.753344	-1.531920	0.462013
17	6	0	3.198725	0.549377	-0.819658
18	8	0	1.995574	-2.271731	1.036486
19	1	0	-1.558291	1.500617	-1.409882
20	1	0	-2.073185	1.411412	2.384874
21	1	0	-0.209633	2.965797	2.142559
22	1	0	1.525653	2.318408	0.532673
23	1	0	0.834868	1.200970	-1.685849
24	1	0	0.292176	4.179950	-0.185543
25	1	0	4.260911	-2.593573	0.806851
26	1	0	-1.781997	-0.481497	-2.689592
27	1	0	-0.512947	-1.284974	-1.757364
28	1	0	-3.726843	-1.913295	1.129885
29	1	0	4.242652	0.275291	-0.849049
30	1	0	2.906786	1.477991	-1.291047

Rotational constants (GHZ): 0.5386593 0.3355570 0.2551986

T = 298.15 K

Zero-point correction= 0.231944 (Hartree/Particle)
Thermal correction to Energy= 0.248300
Thermal correction to Enthalpy= 0.249245
Thermal correction to Gibbs Free Energy= 0.186563
Sum of electronic and zero-point Energies= -915.565433
Sum of electronic and thermal Energies= -915.549078
Sum of electronic and thermal Enthalpies= -915.548133
Sum of electronic and thermal Free Energies= -915.610815

w= 0.077318 a.u., Optical Rotation Beta= 1.1359 au.
Molar Mass = 252.2232 grams/mole, [Alpha] (5893.0 A) = 174.07 deg.

Table S36. Coordinates of **i-6** (wB97XD/6-311++G(d,p), SCRF = CPCM, solvent = MeOH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.060166	0.699577	-0.905534
2	6	0	-1.709366	0.493842	0.440225
3	6	0	-1.385296	1.406296	1.516206
4	6	0	-0.343752	2.237797	1.396554
5	6	0	0.561001	2.274764	0.191606
6	6	0	0.411756	1.032965	-0.712871
7	8	0	0.252400	3.458596	-0.537422
8	8	0	1.786968	-2.271439	0.956576
9	6	0	-1.389263	-0.566218	-1.706985
10	6	0	-2.410332	-1.287623	-0.858312
11	6	0	-2.502386	-0.590913	0.433132
12	8	0	-3.045048	-2.289596	-1.129340
13	8	0	-3.274278	-1.065787	1.422961
14	8	0	1.016542	-0.100391	-0.095127
15	6	0	2.343738	-0.301080	-0.223562
16	6	0	2.789765	-1.588042	0.407799
17	6	0	3.244254	0.475629	-0.826184
18	8	0	3.935188	-1.968020	0.417978
19	1	0	-1.509903	1.577717	-1.380467
20	1	0	-1.981169	1.390999	2.422297
21	1	0	-0.102960	2.934287	2.192629
22	1	0	1.596286	2.318691	0.548500
23	1	0	0.884677	1.222260	-1.681577
24	1	0	1.006876	3.698526	-1.080913
25	1	0	2.152662	-3.080452	1.337844
26	1	0	-1.780002	-0.370353	-2.706249
27	1	0	-0.513858	-1.214809	-1.806769
28	1	0	-3.701890	-1.869904	1.099839
29	1	0	4.272881	0.145389	-0.847905
30	1	0	3.002502	1.418786	-1.294688

Rotational constants (GHZ): 0.5307394 0.3453603 0.2596353

T = 298.15 K

Zero-point correction= 0.232050 (Hartree/Particle)
Thermal correction to Energy= 0.248329
Thermal correction to Enthalpy= 0.249273
Thermal correction to Gibbs Free Energy= 0.186855
Sum of electronic and zero-point Energies= -915.565648
Sum of electronic and thermal Energies= -915.549369
Sum of electronic and thermal Enthalpies= -915.548425
Sum of electronic and thermal Free Energies= -915.610843

w= 0.077318 a.u., Optical Rotation Beta= 0.9360 au.
Molar Mass = 252.2232 grams/mole, [Alpha] (5893.0 A) = 143.43 deg.

References

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