

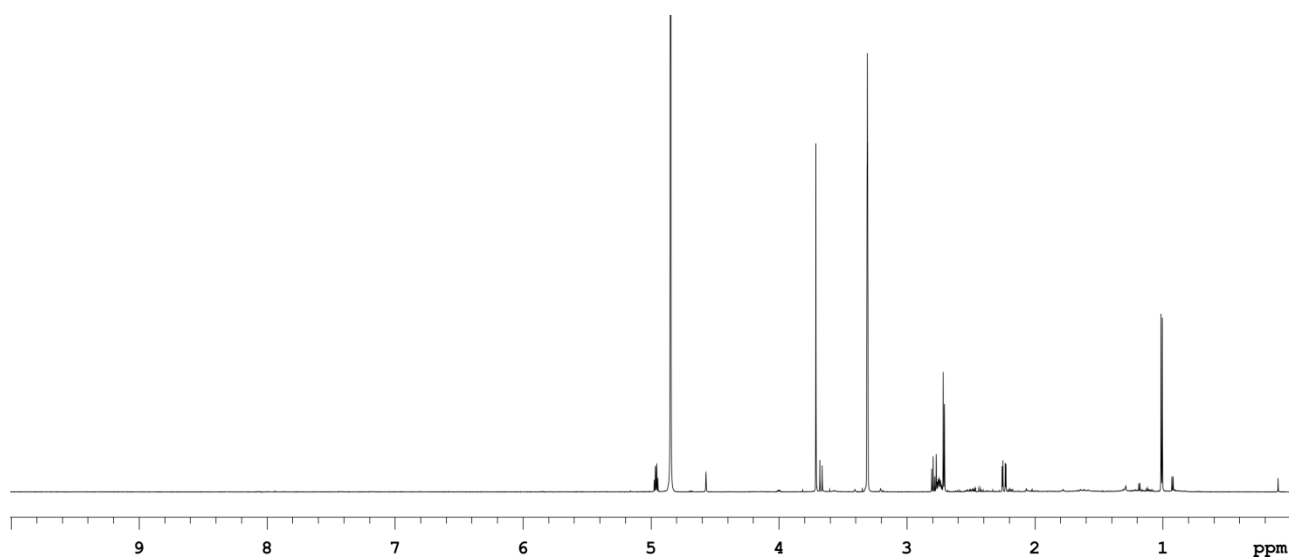
# Supplementary Materials: Plakofuranolactone as a Quorum Quenching Agent from the Indonesian Sponge *Plakortis cf. lita*

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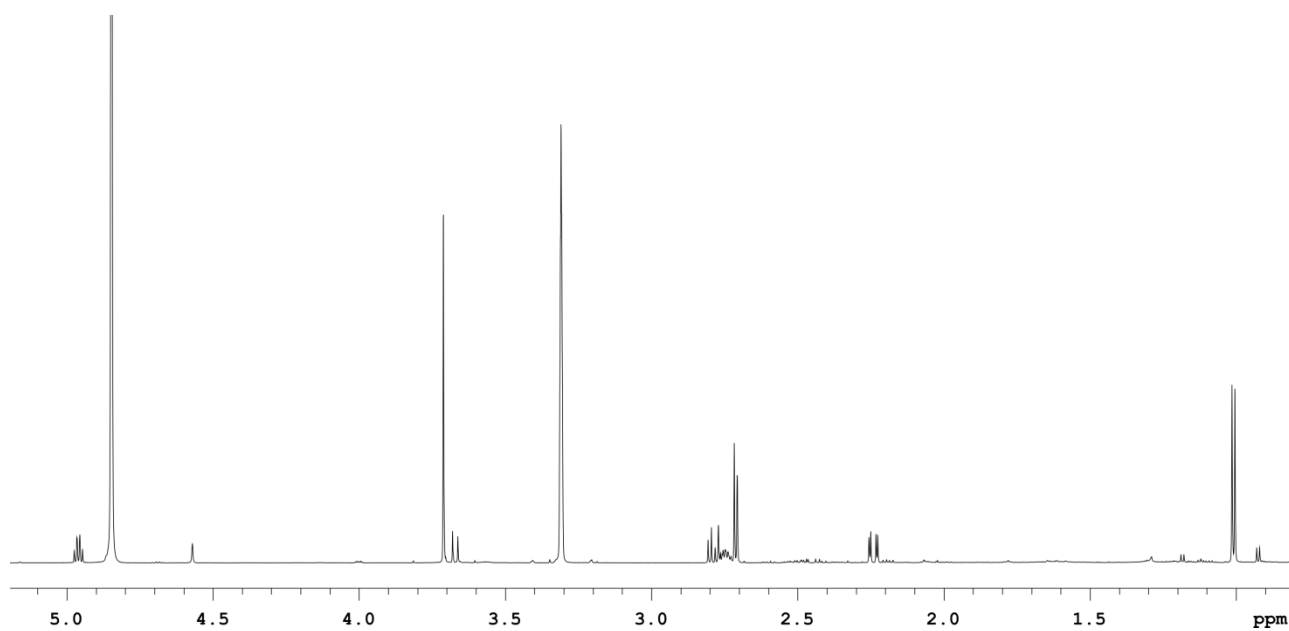
**Table S1.** Calculated relative energies ( $\Delta E$ ), relative free energies ( $\Delta G$ ), and optical rotations of the conformers of **1** at the CAM-B3LYP/AUG-cc-pVDZ level.

Conformer	$\Delta E$ (kcal/mol)	$\Delta G$ (kcal/mol)	Boltzmann factor <sup>a</sup>	$[\alpha]$
1	0.00	0.00	1.00	-120.1
2	0.35	0.37	0.54	-130.5
3	0.45	0.49	0.43	+5.4
4	0.61	0.48	0.45	-82.9
5	0.73	0.83	0.25	-84.4
6	1.02	1.19	0.13	+52.5
7	1.22	1.15	0.14	-55.9
8	1.65	2.06	0.03	-11.6
9	1.89	2.27	0.02	-66.8
10	3.03	3.58	0.00	+65.8
11	3.72	4.08	0.00	+59.6
12	3.91	4.49	0.00	-32.7
weighted mean				-82.8
experimental value				-84.0

<sup>a</sup> At T = 298 K, calculated on  $\Delta G$ .



**Figure S1.**  $^1\text{H}$ -NMR spectrum of plakofuranolactone (**1**) (700 MHz,  $\text{CD}_3\text{OD}$ ).



**Figure S2.** Expansion of the  $^1\text{H}$ -NMR spectrum of plakofuranolactone (**1**) (700 MHz,  $\text{CD}_3\text{OD}$ ).

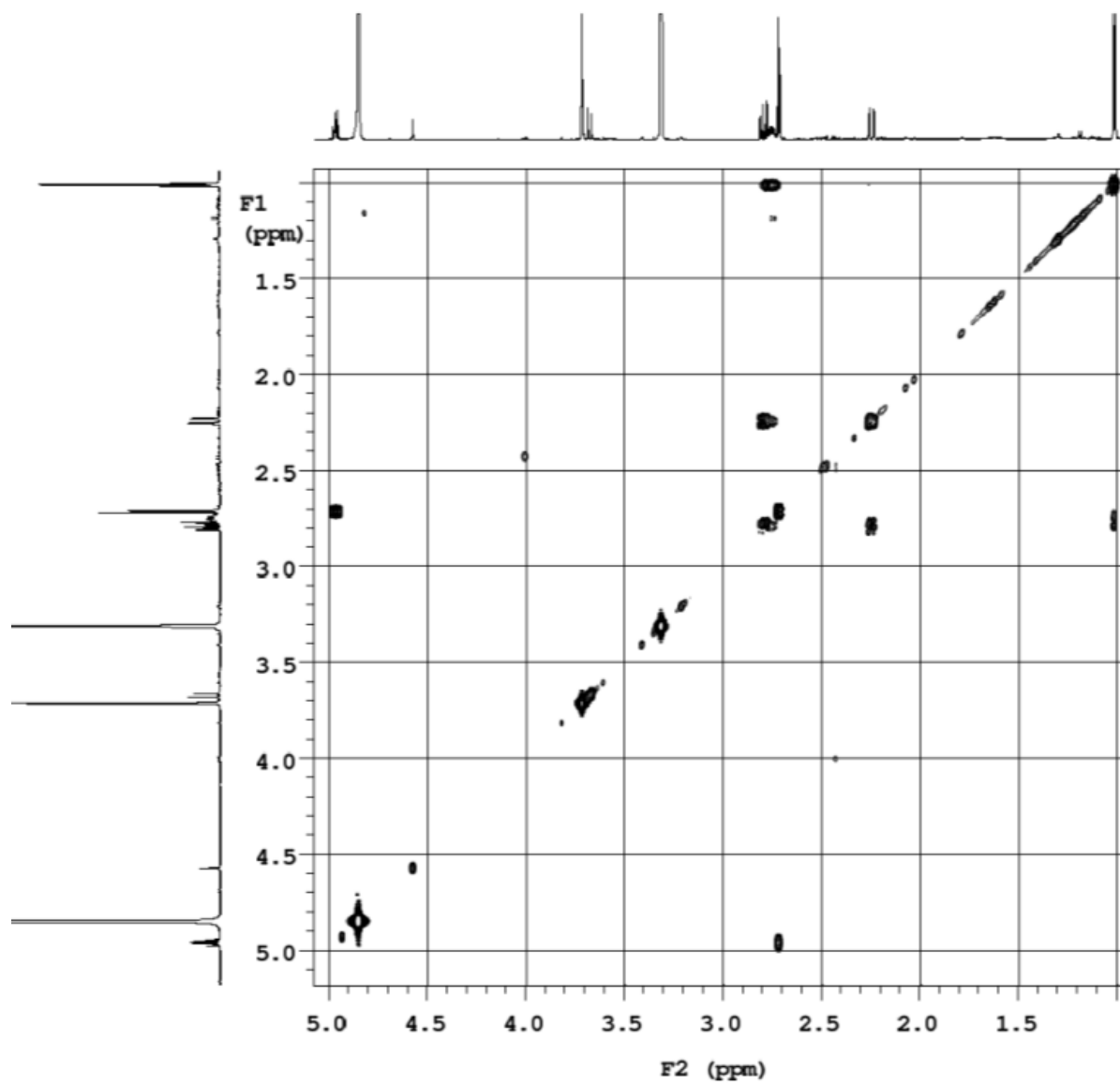


Figure S3. COSY spectrum of plakofuranolactone (1) (700 MHz, CD<sub>3</sub>OD).

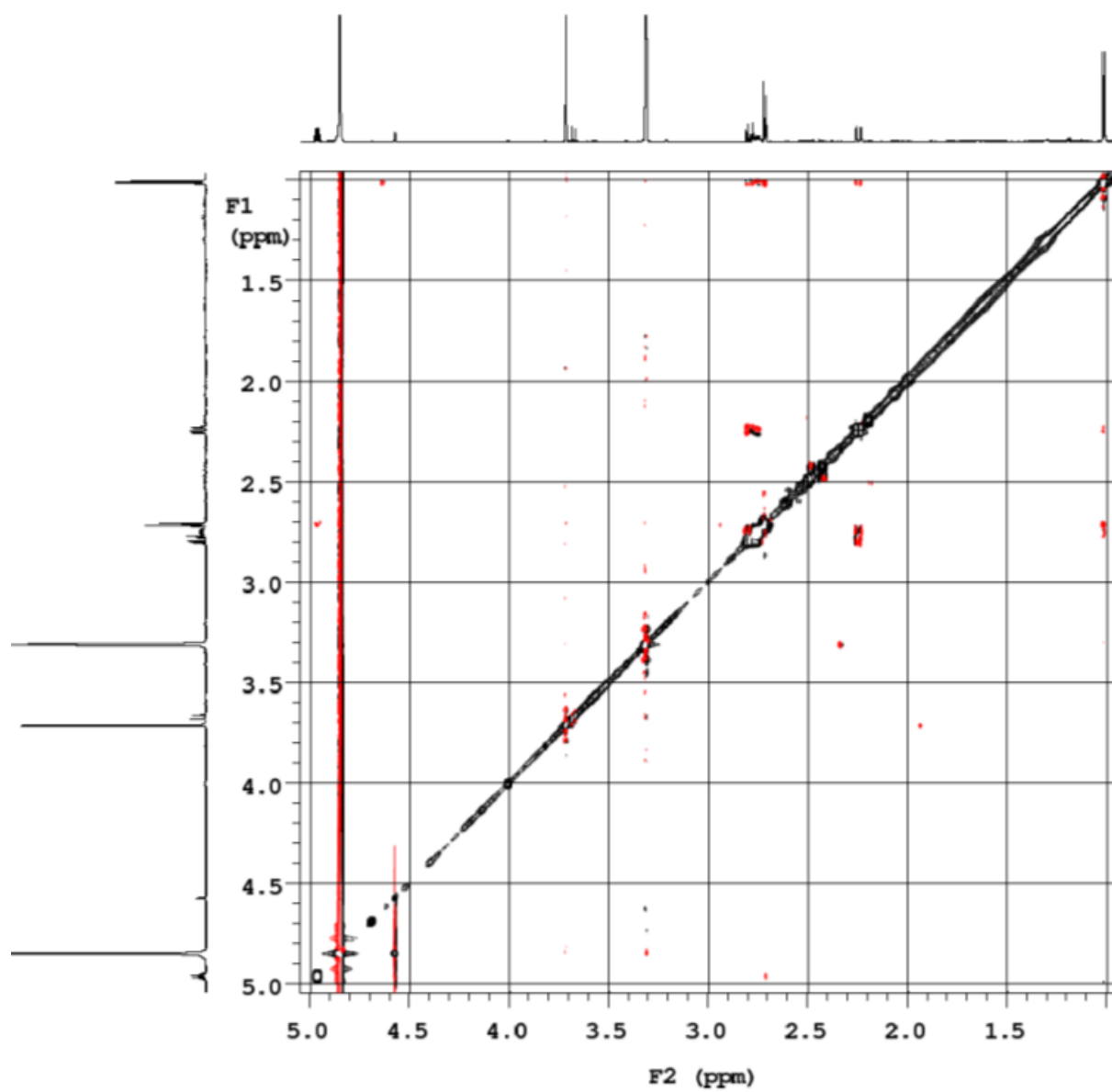


Figure S4. NOESY spectrum of plakofuranolactone (1) (700 MHz, CD<sub>3</sub>OD).

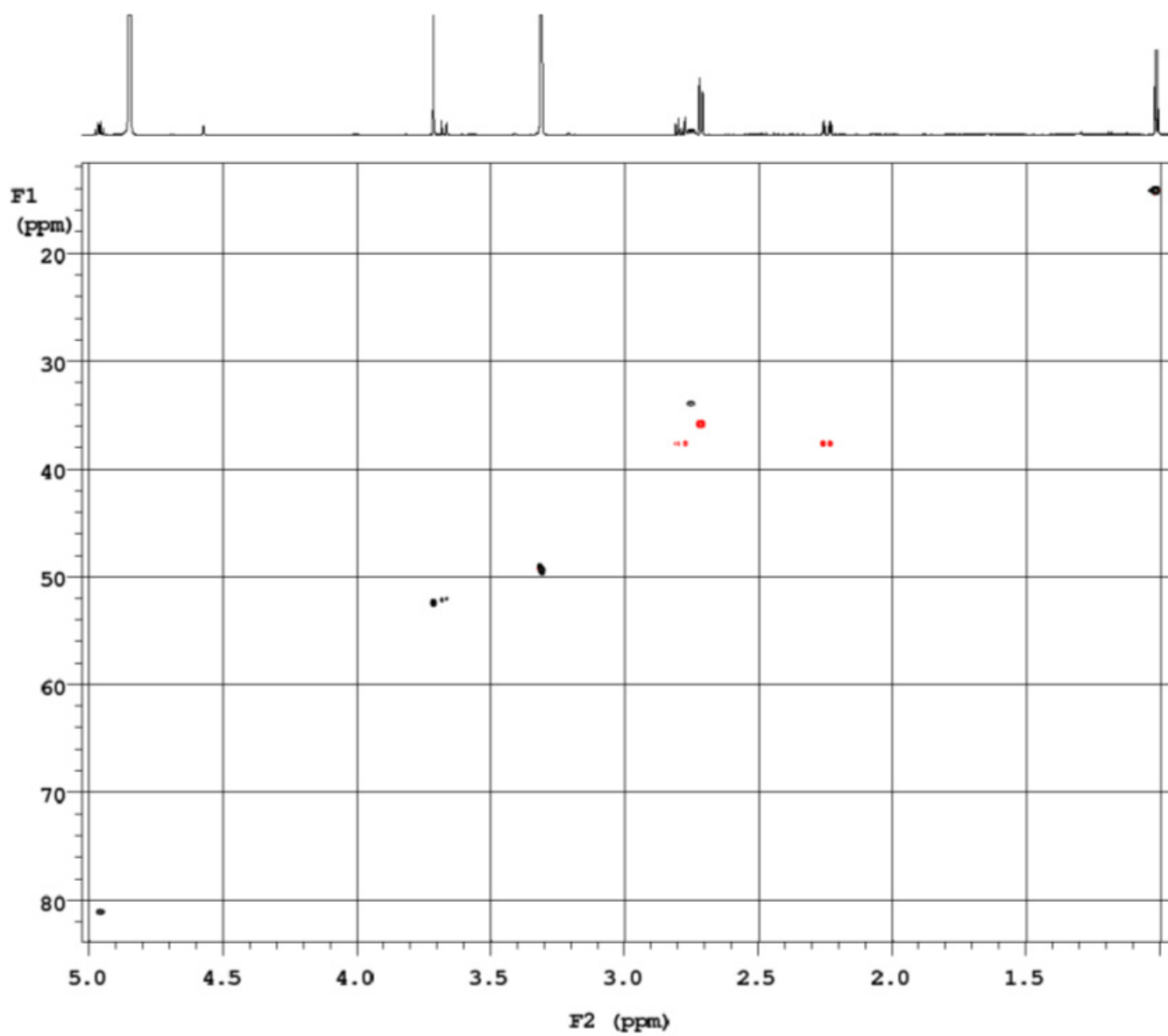


Figure S5. HSQC spectrum of plakofuranolactone (1) (700 MHz, CD<sub>3</sub>OD).

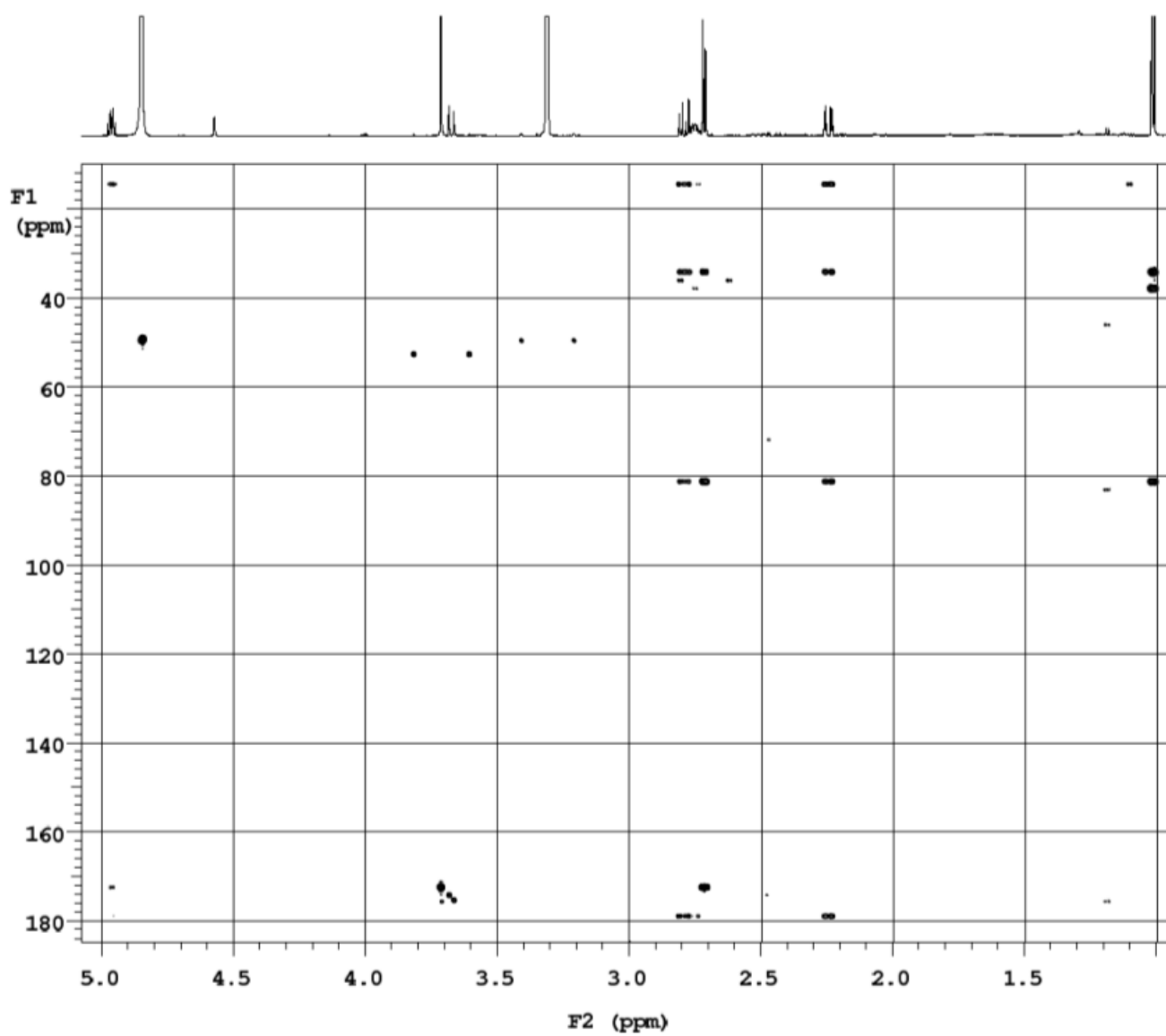
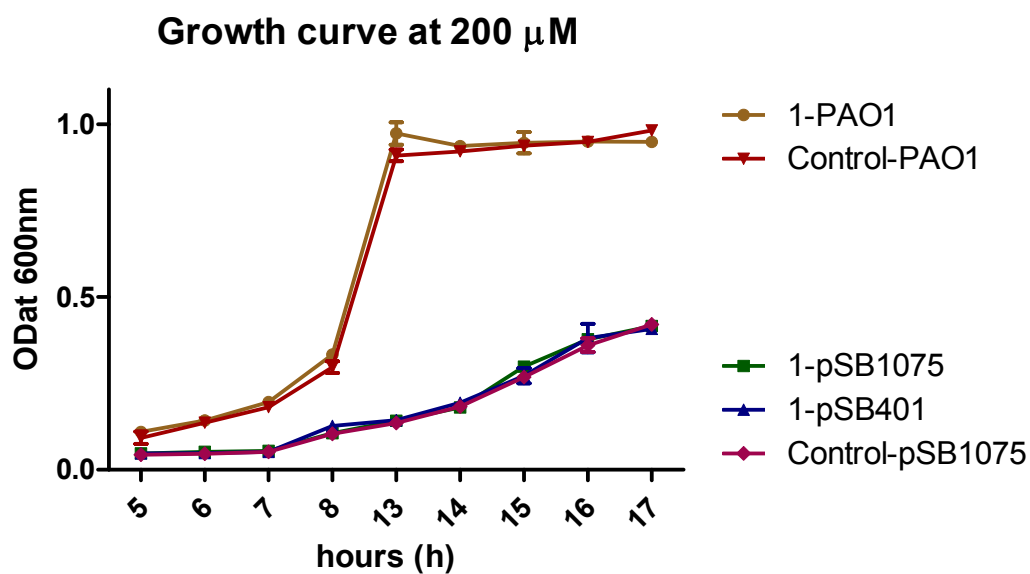
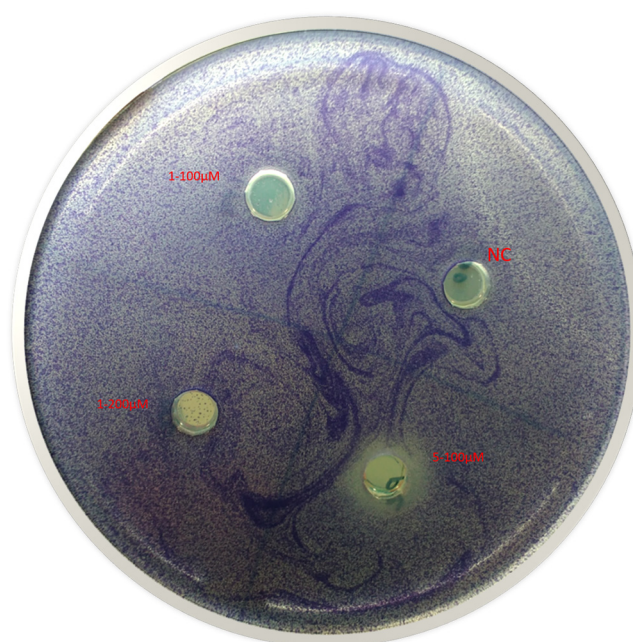


Figure S6. HMBC spectrum of plakofuranolactone (1) (700 MHz, CD<sub>3</sub>OD).



**Figure S7.** Growth curve inhibition profile of plakofuranolactone (**1**) at 200  $\mu$ M against *Pseudomonas aeruginosa* PAO1, *E.coli* pSB401 and *E.coli* pSB1075. The control represents the growth of the tested organism grown in the presence of the solvent used for dilutions (methanol).



**Figure S8.** Overlaid well diffusion assay of plakofuranolactone (**1**) and penicillic acid (PA, **5**) on the QS dependent CviI/CviR-based reporter *Chromobacterium violaceum* strain CV026 induced by 3-oxo-C6-HSL (final concentration of 1  $\mu$ M). The solvent used for dilution was used as a negative control (NC). A white halo around the well, representing the inhibition of violacein production, interpreted as QQ activity, can only be observed in the treatment PA, **5**.