

Supplementary Information

New 24-membered macrolactines from an Arctic bacteria *Bacillus amyloliquefaciens* SCSIO 41392 and their anti-pathogenicity evaluation

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Table S1. The tested *P. aeruginosa* strains used in this study.

Physicochemical data of known compounds **4–5**.

The 16S gene sequence data of *Bacillus amyloliquefaciens* SCSIO 41392

CTGTTACGACTTCACCCAATCATCTGTCCCACCTCGGCGGCTGGCTCCAT
AAAGGTTACCTCACCGACTTCGGGTGTTACAAACTCTCGTGGTGTGACGGG
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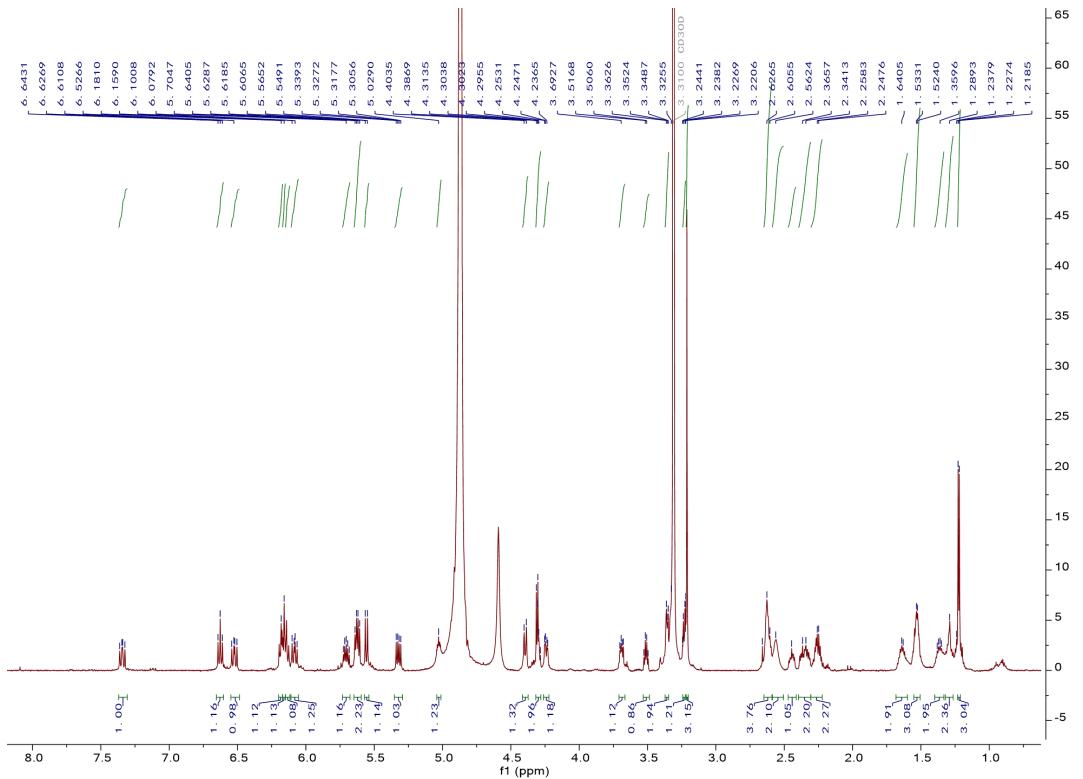


Figure S1. ¹H NMR spectrum of compound **1** (CD₃OD, 700MHz).

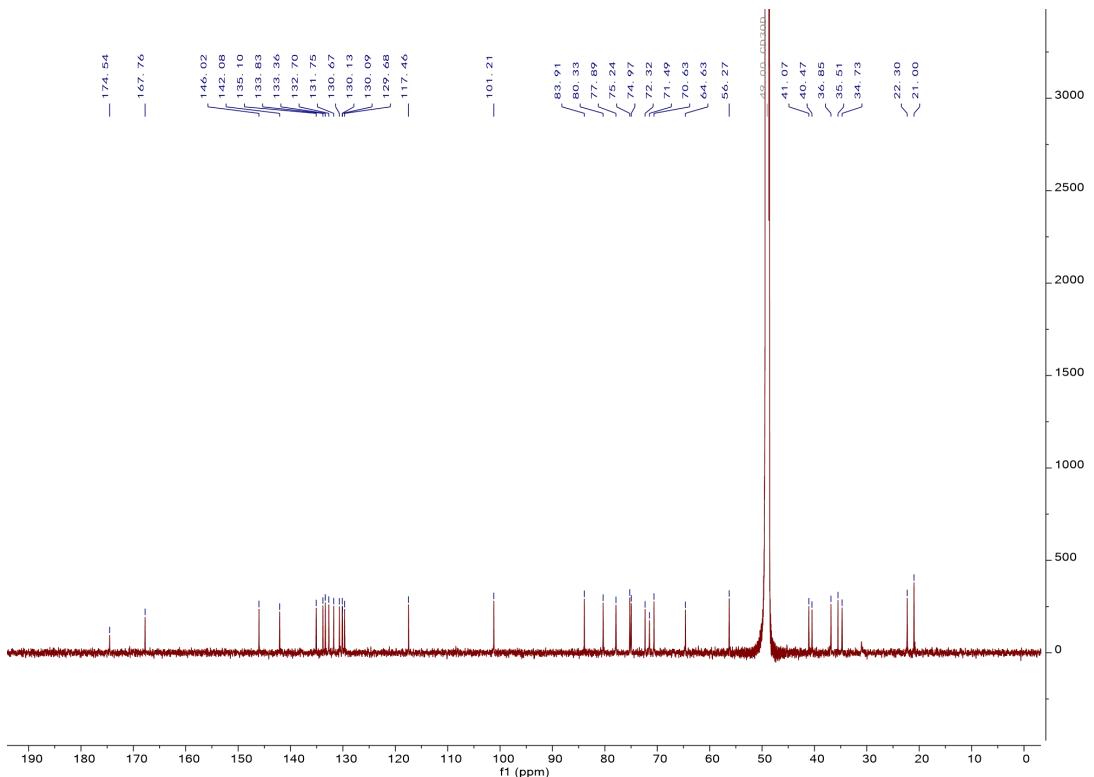


Figure S2. ¹³C NMR spectrum of compound **1** (CD₃OD, 175MHz).

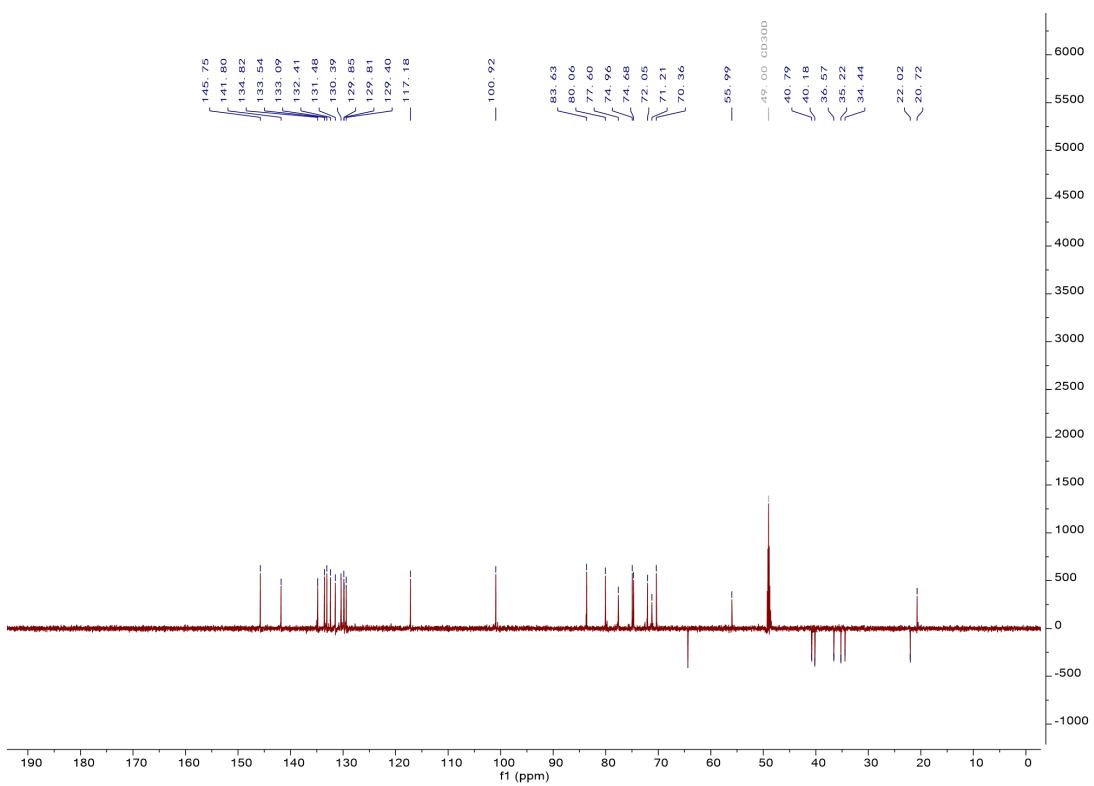


Figure S3. ^{13}C -DEPT135 NMR spectrum of compound **1** (CD_3OD , 175MHz).

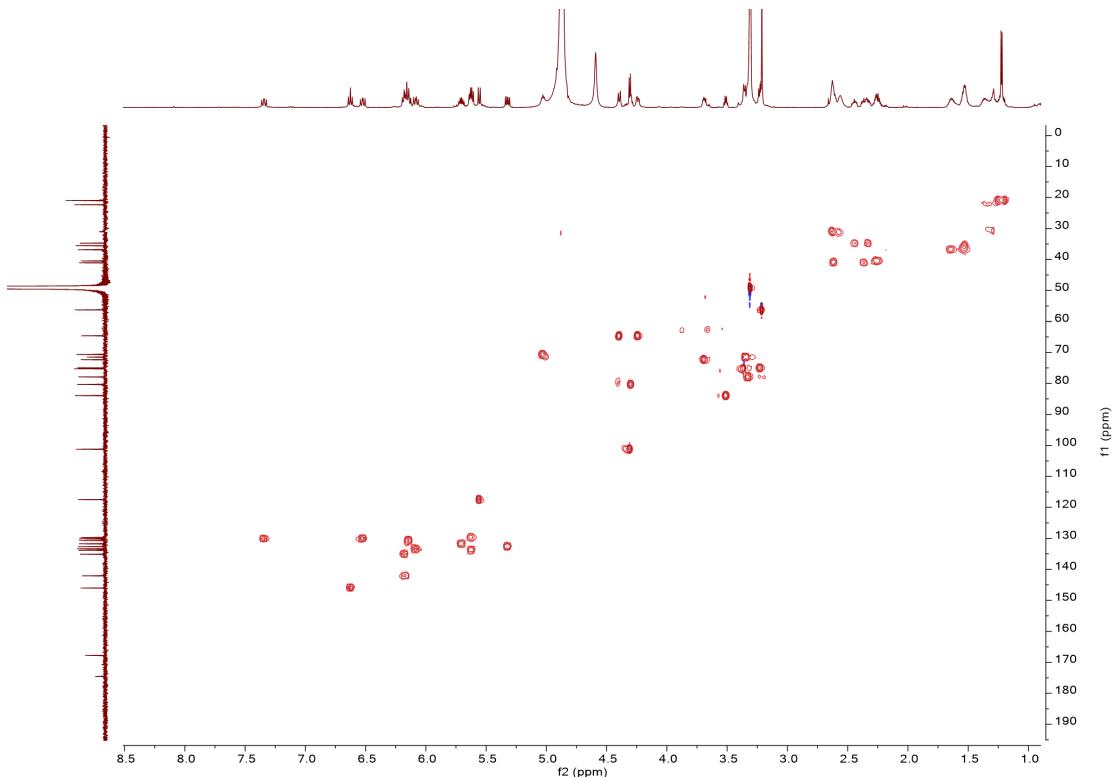


Figure S4. HSQC spectrum of compound **1** (CD_3OD).

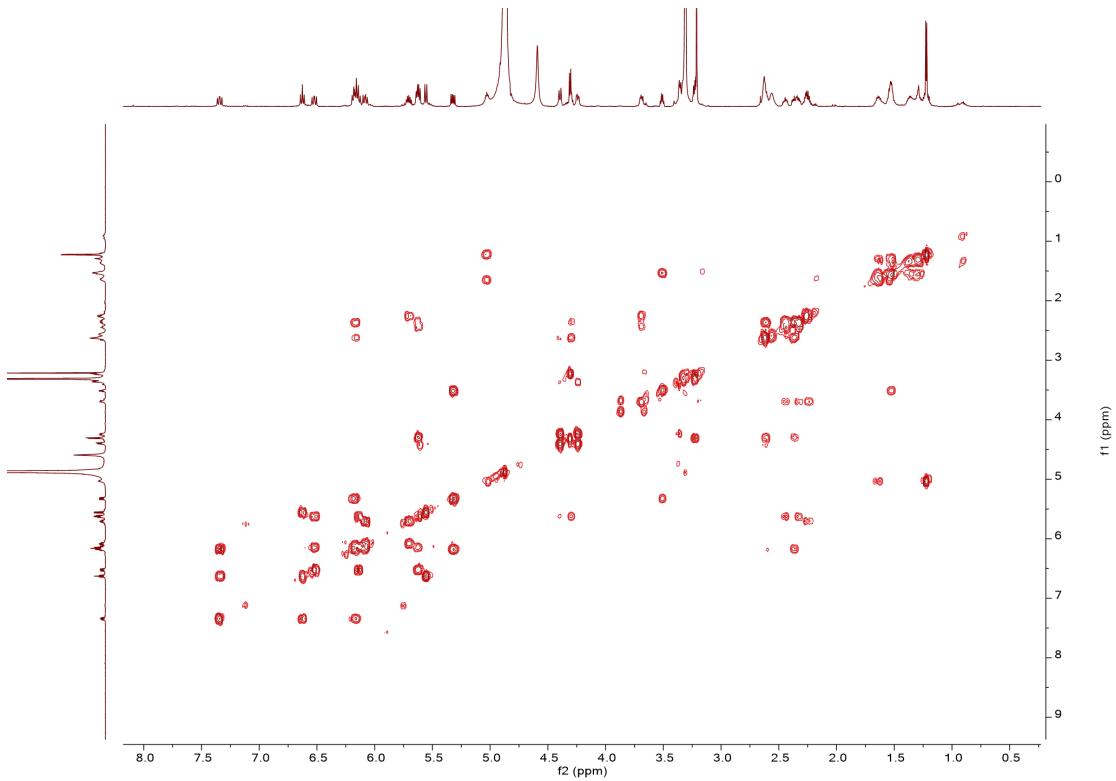


Figure S5. ^1H - ^1H COSY spectrum of compound **1** (CD_3OD).

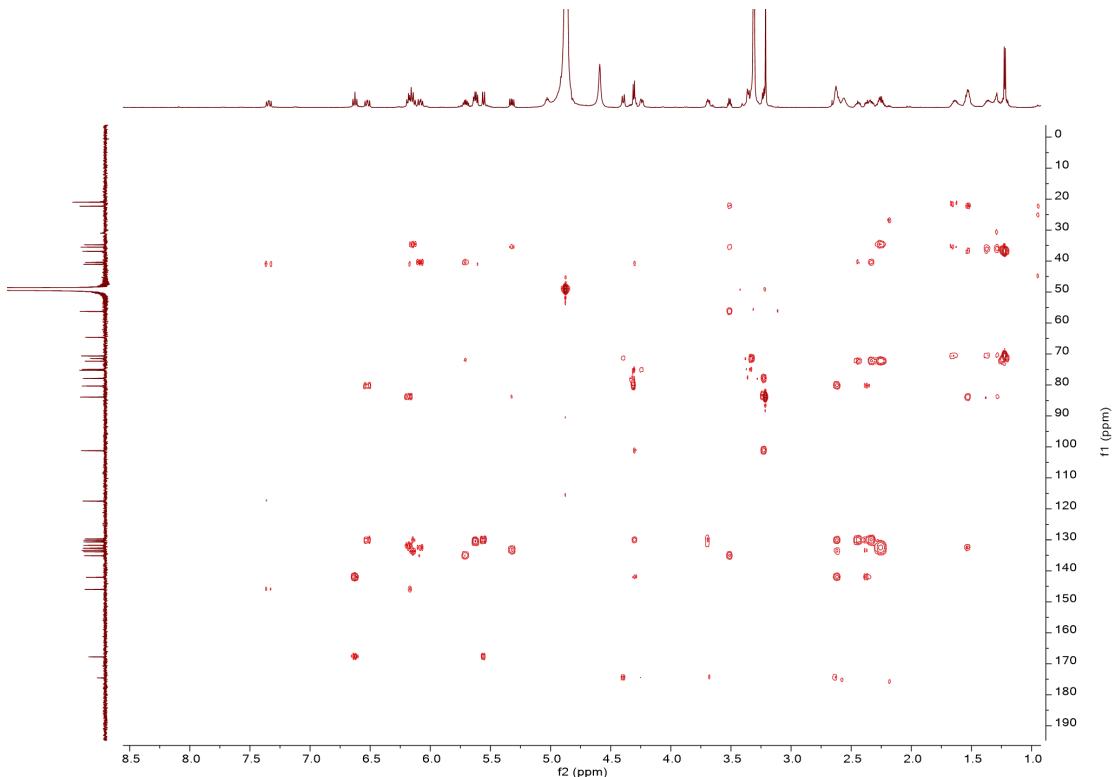


Figure S6. HMBC spectrum of compound **1** (CD_3OD).

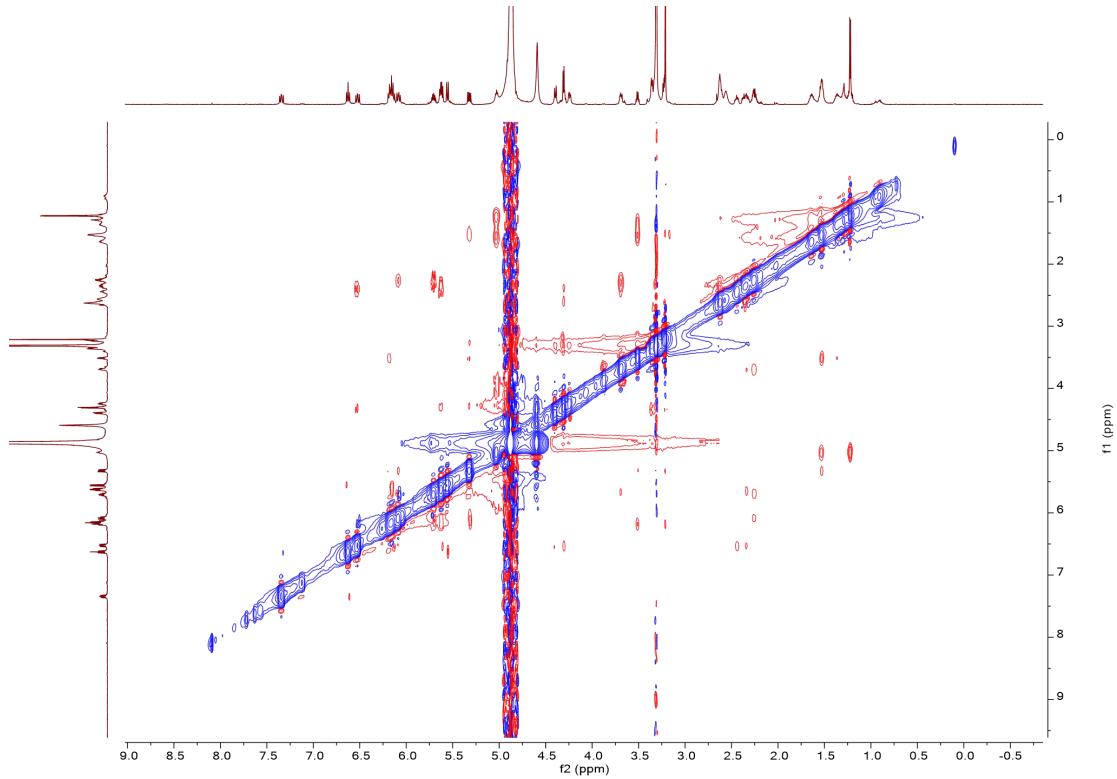


Figure S7. NOESY spectrum of compound **1** (CD_3OD).

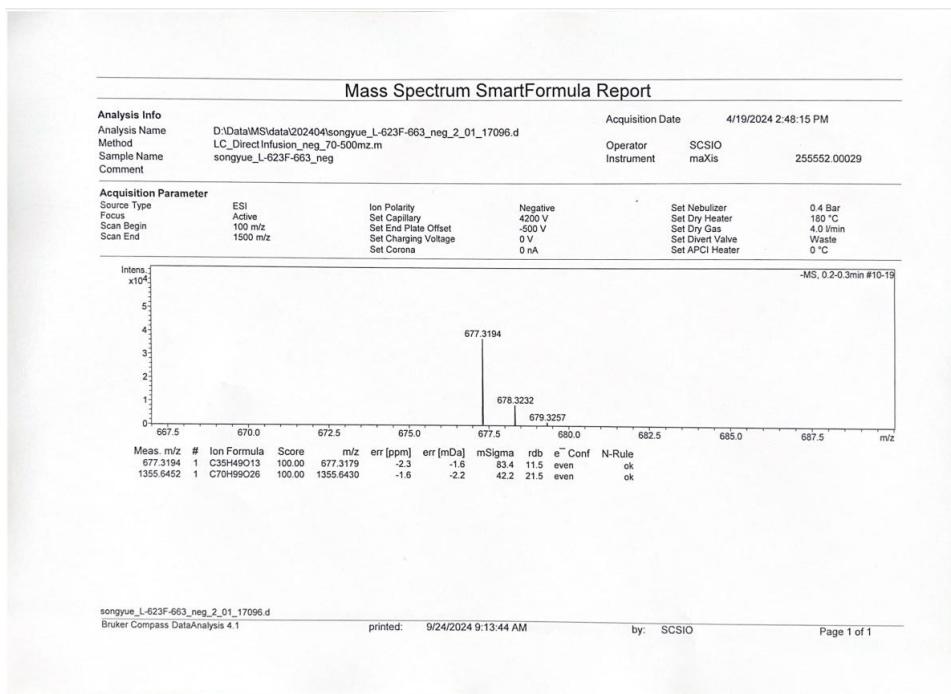


Figure S8. HR-ESI-MS spectrum of compound **1**.

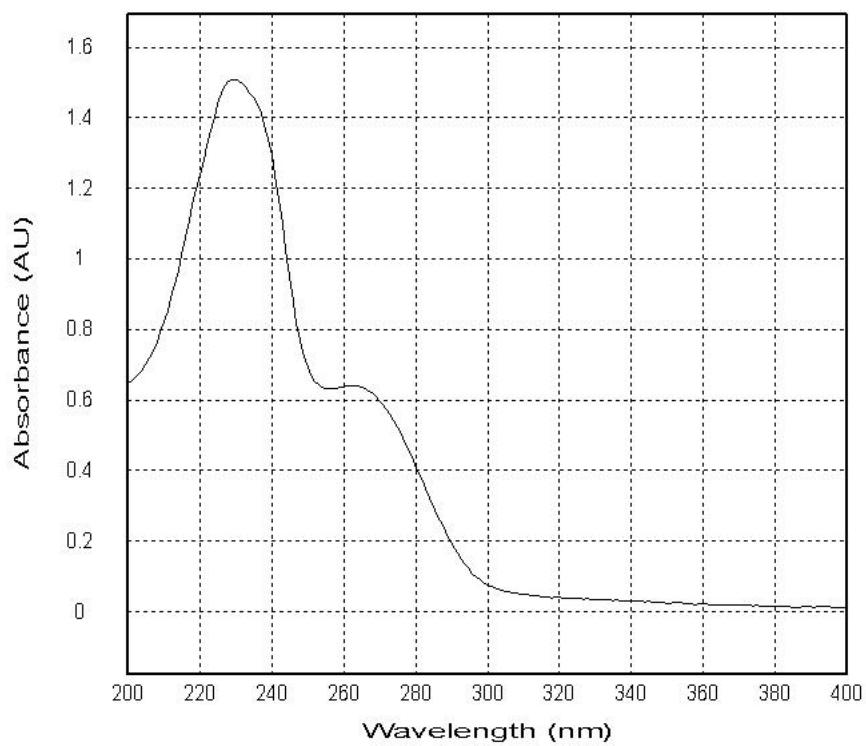


Figure S9. UV spectrum of compound 1.

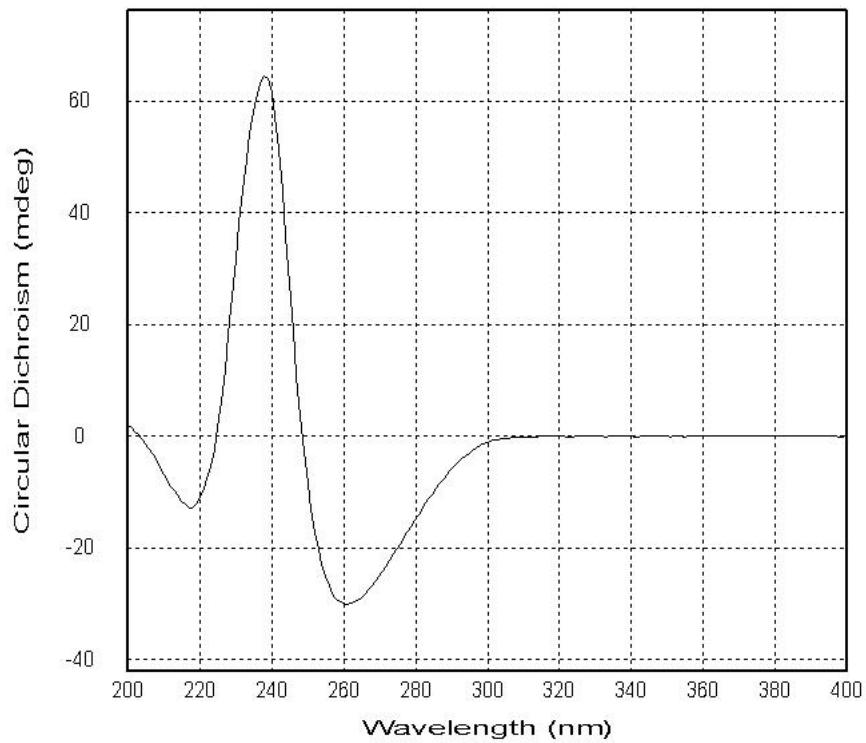


Figure S10. CD spectrum of compound 1.

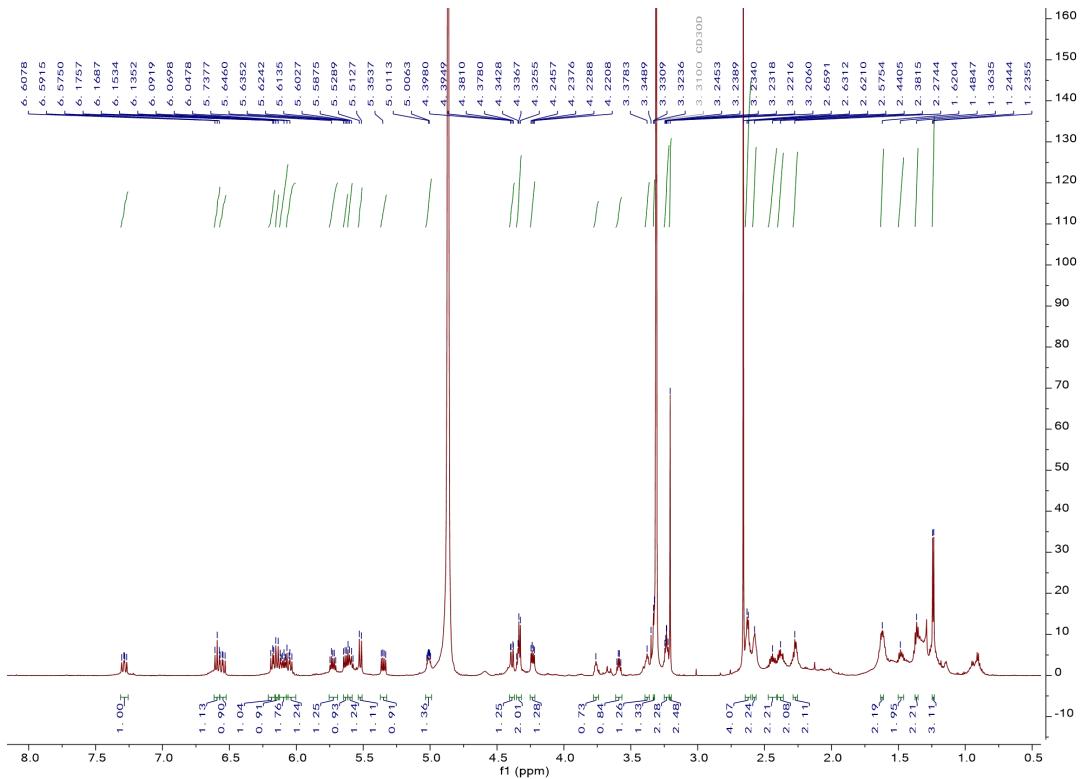


Figure S11. ^1H NMR spectrum of compound 2 (CD_3OD , 700MHz).

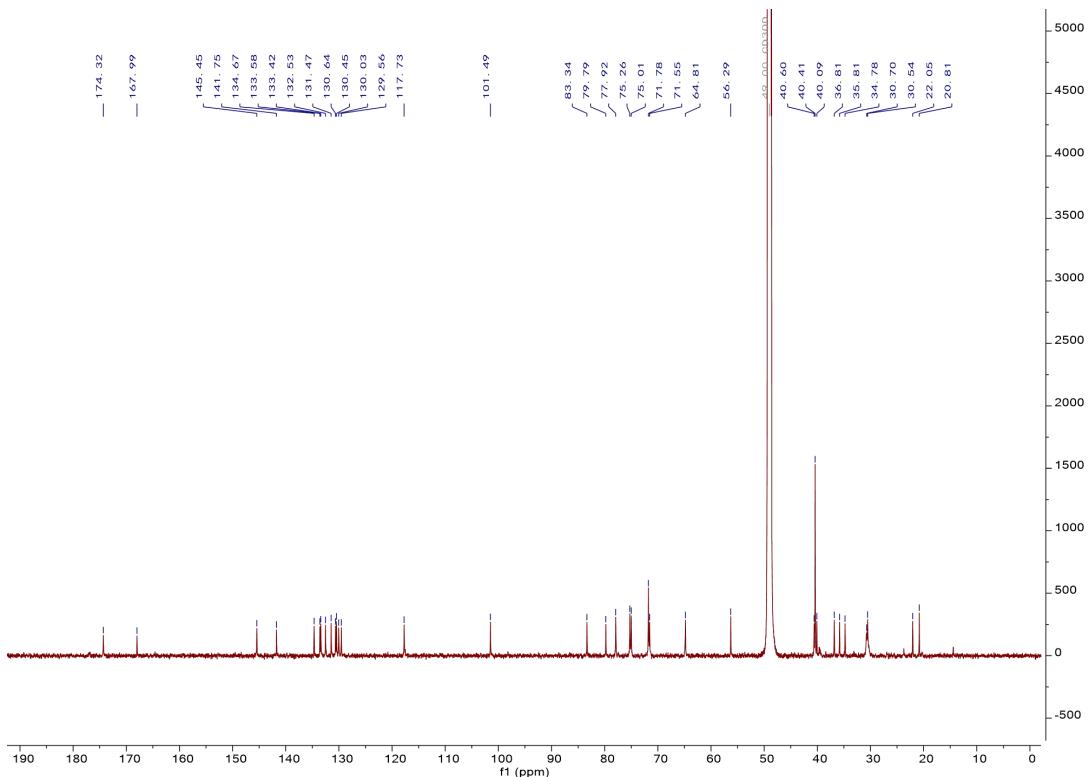


Figure S12. ^{13}C NMR spectrum of compound 2 (CD_3OD , 175MHz).

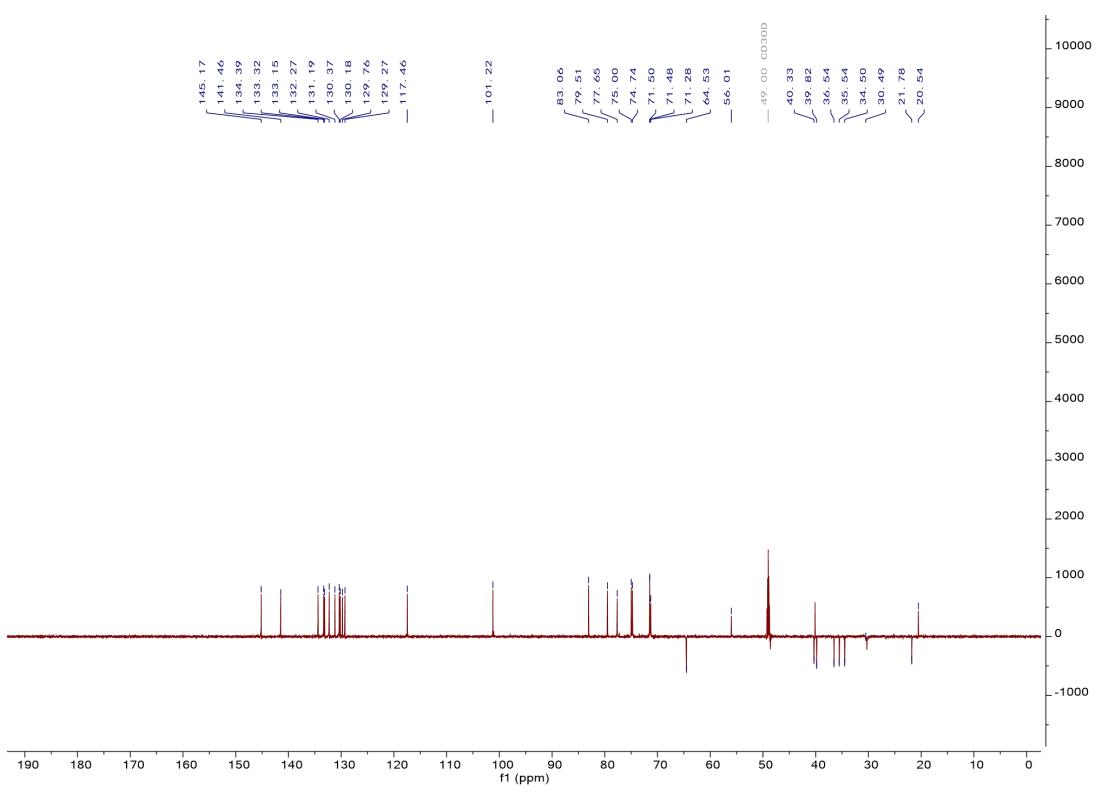


Figure S13. ^{13}C -DEPT135 NMR spectrum of compound 2 (CD_3OD , 175MHz).

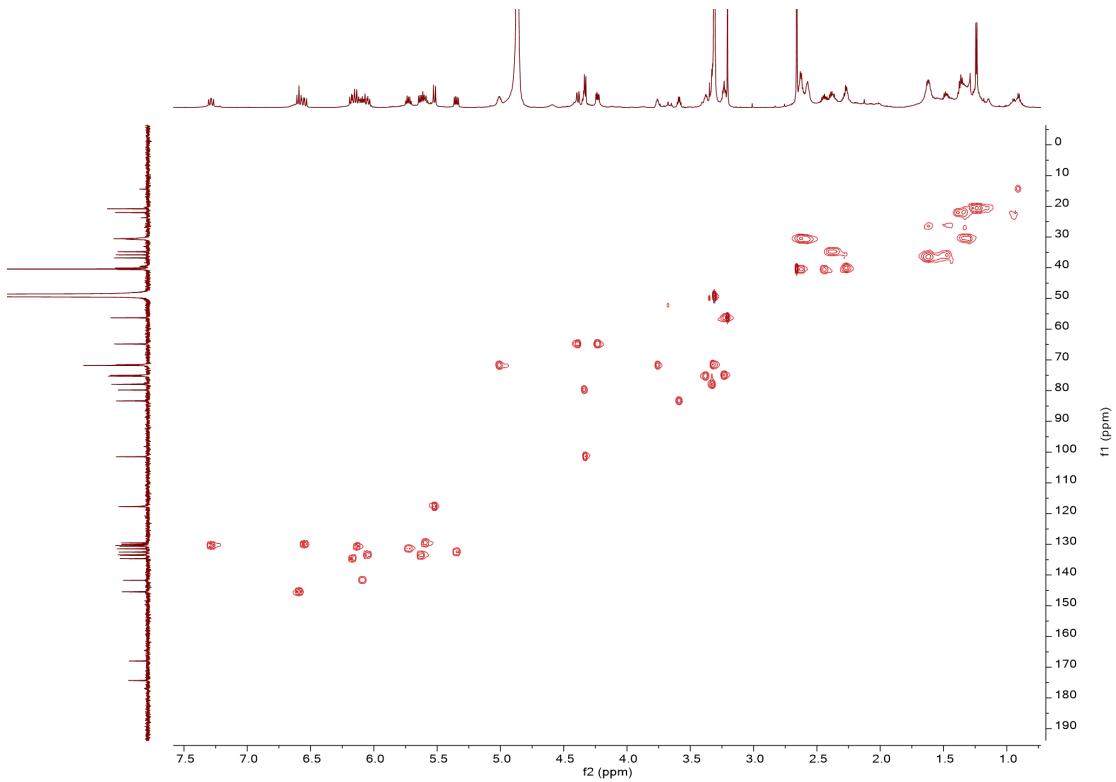


Figure S14. HSQC spectrum of compound 2 (CD_3OD).

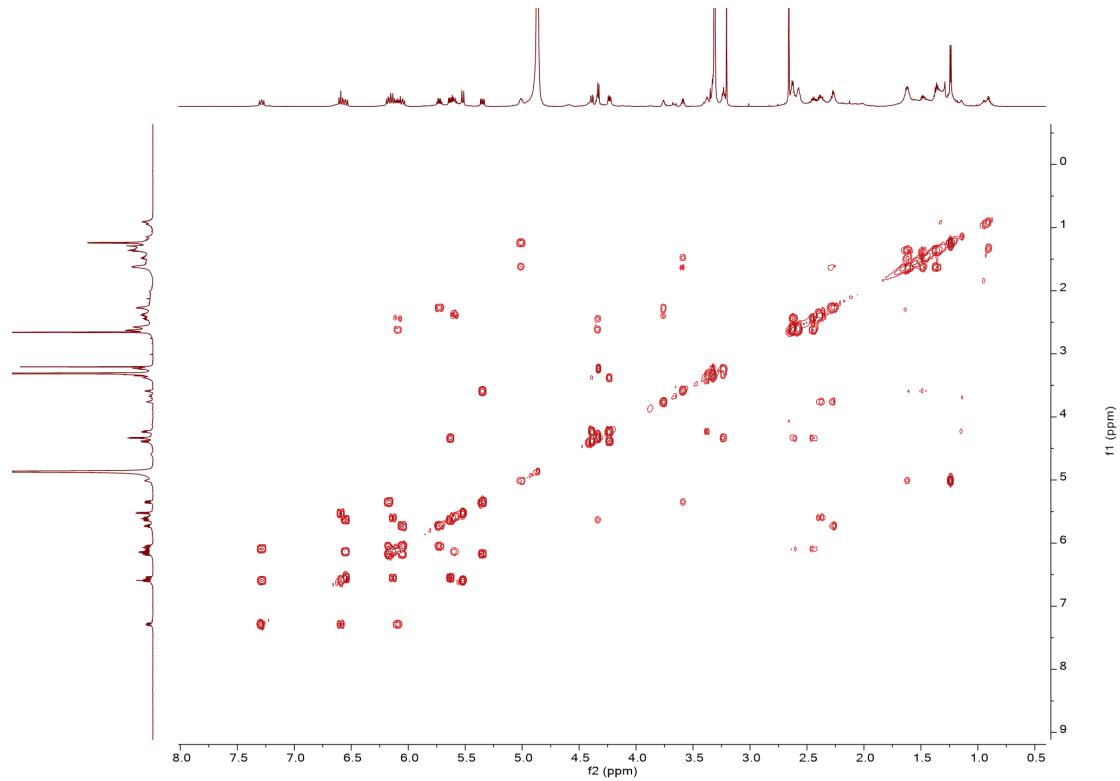


Figure S15. ^1H - ^1H COSY spectrum of compound **2** (CD_3OD).

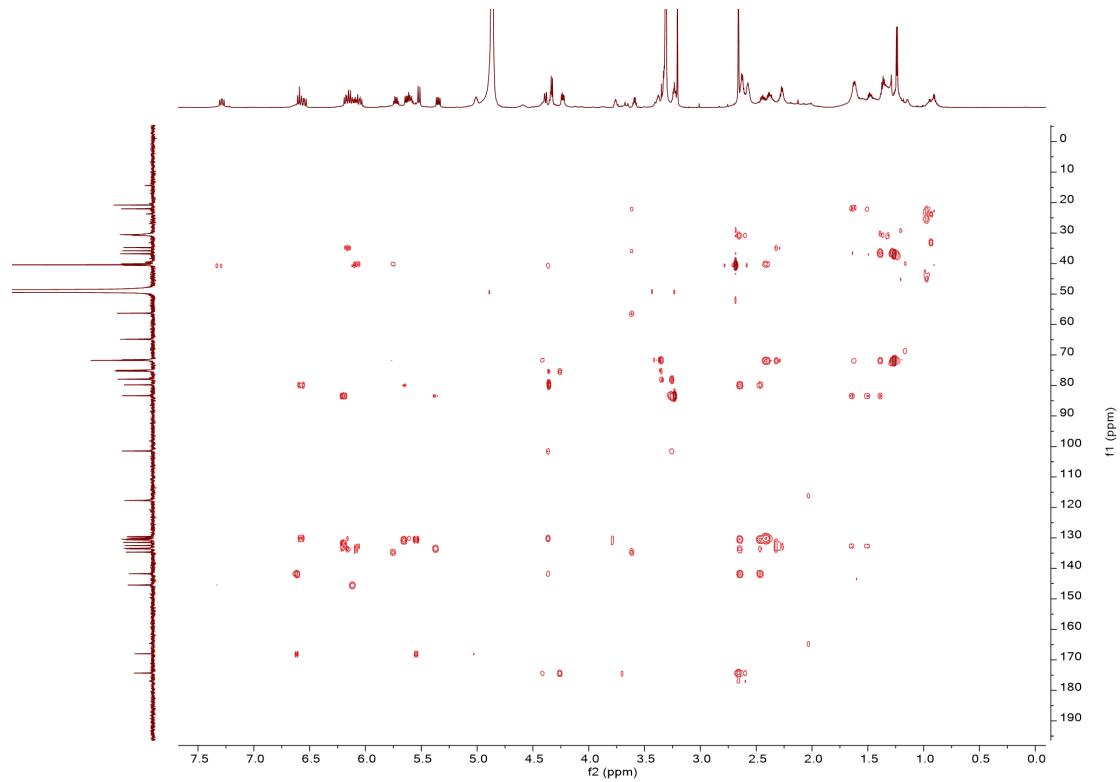


Figure S16. HMBC spectrum of compound **2** (CD_3OD).

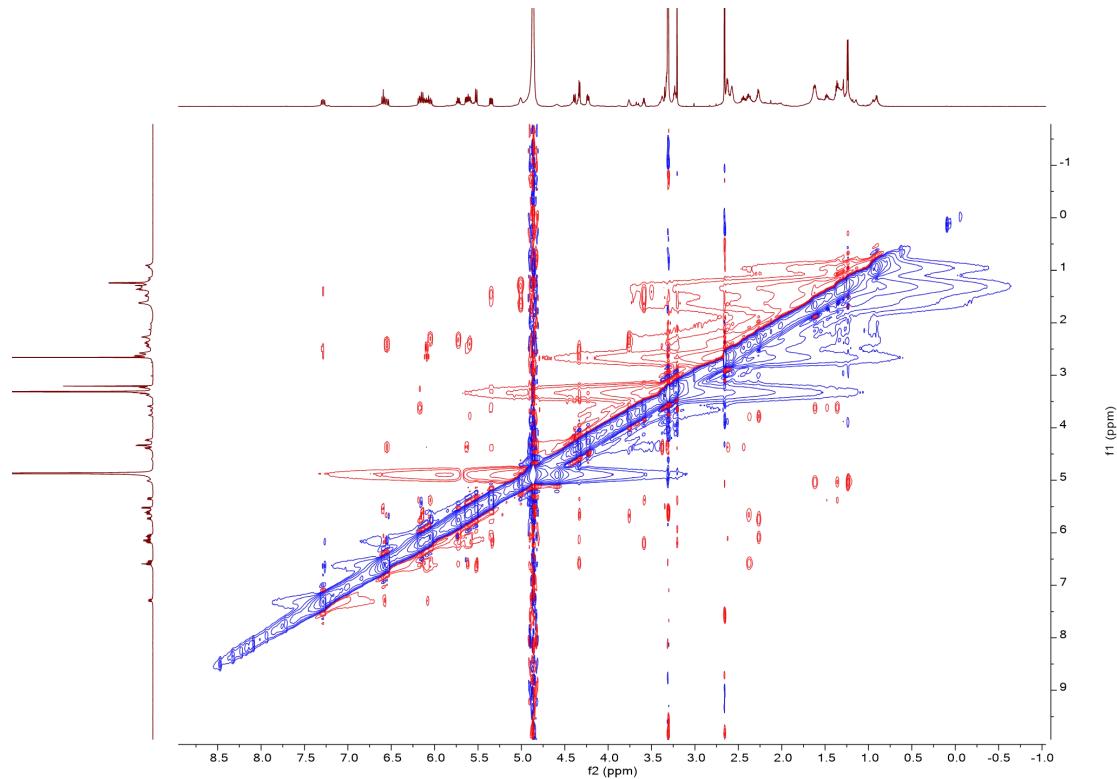
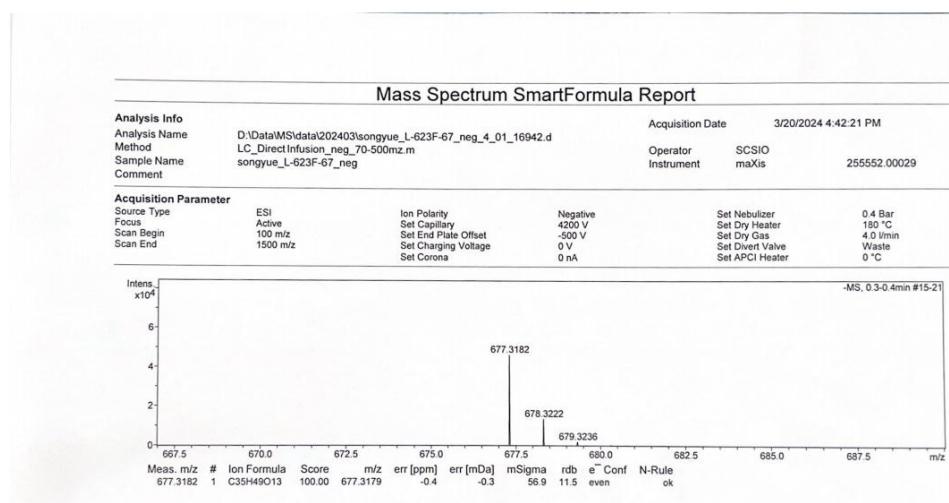


Figure S17. NOESY spectrum of compound 2 (CD_3OD).



songyue_L-623F-67_neg_4_01_16942.d
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Figure S18. HR-ESI-MS spectrum of compound 2.

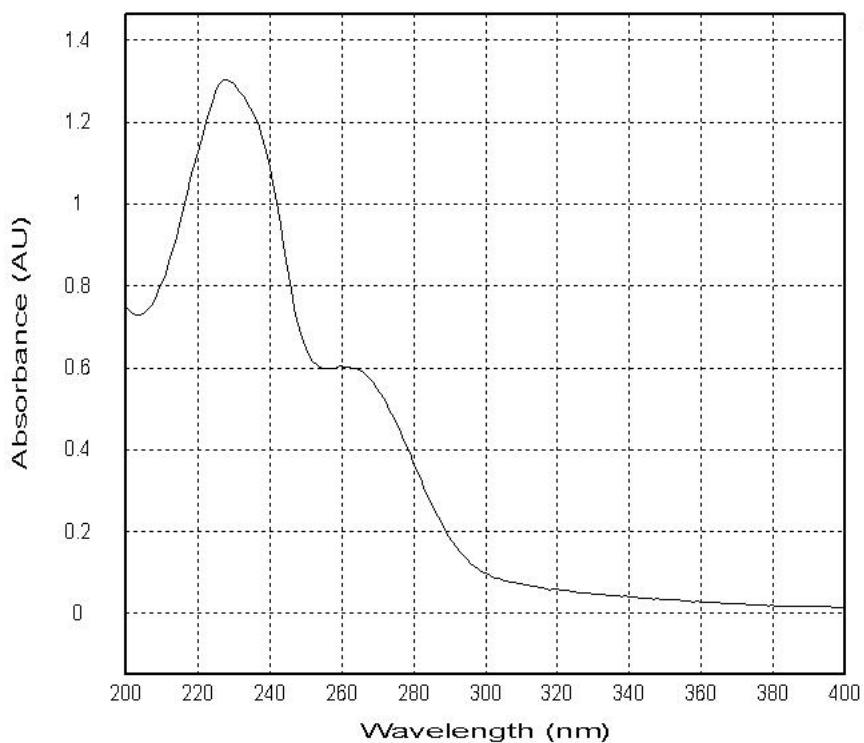


Figure S19. UV spectrum of compound 2.

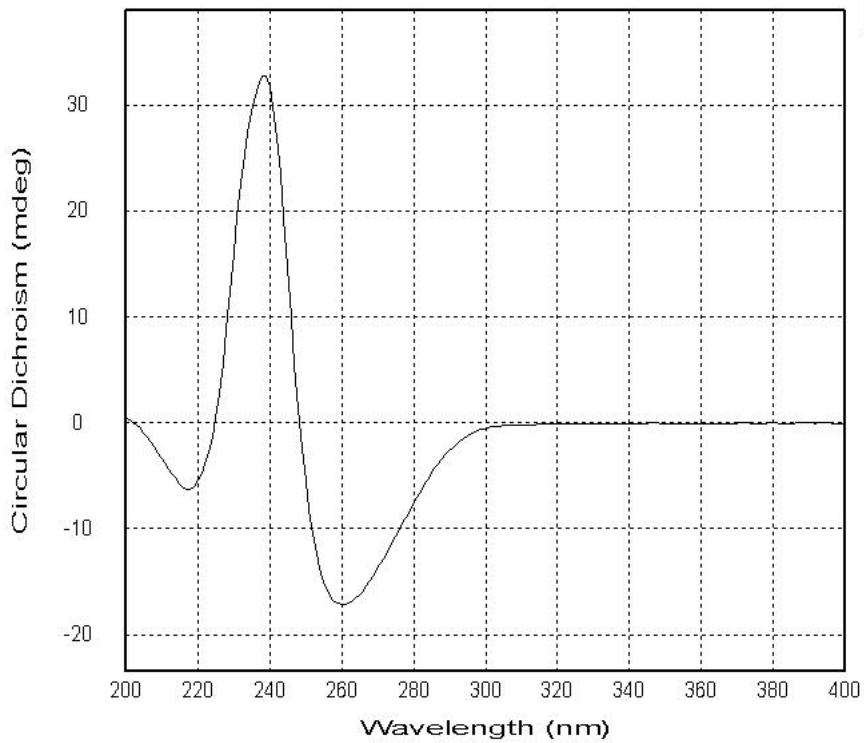


Figure S20. CD spectrum of compound 2.

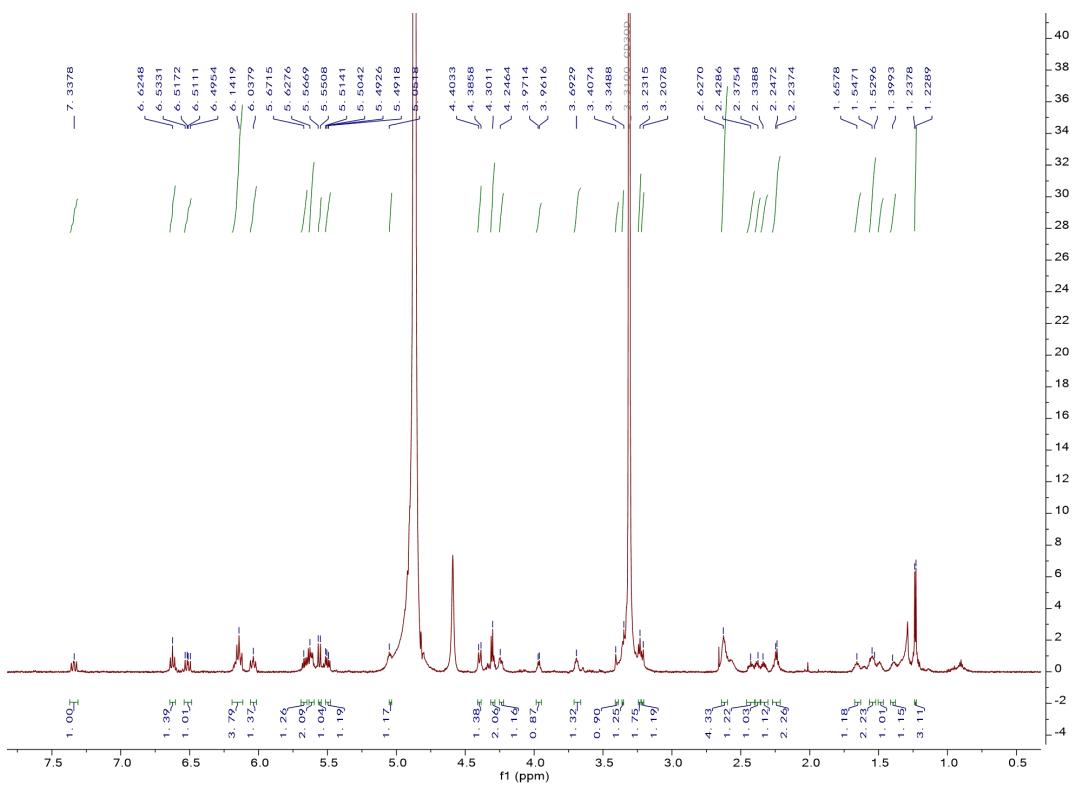


Figure S21. ^1H NMR spectrum of compound 3 (CD₃OD, 700MHz).

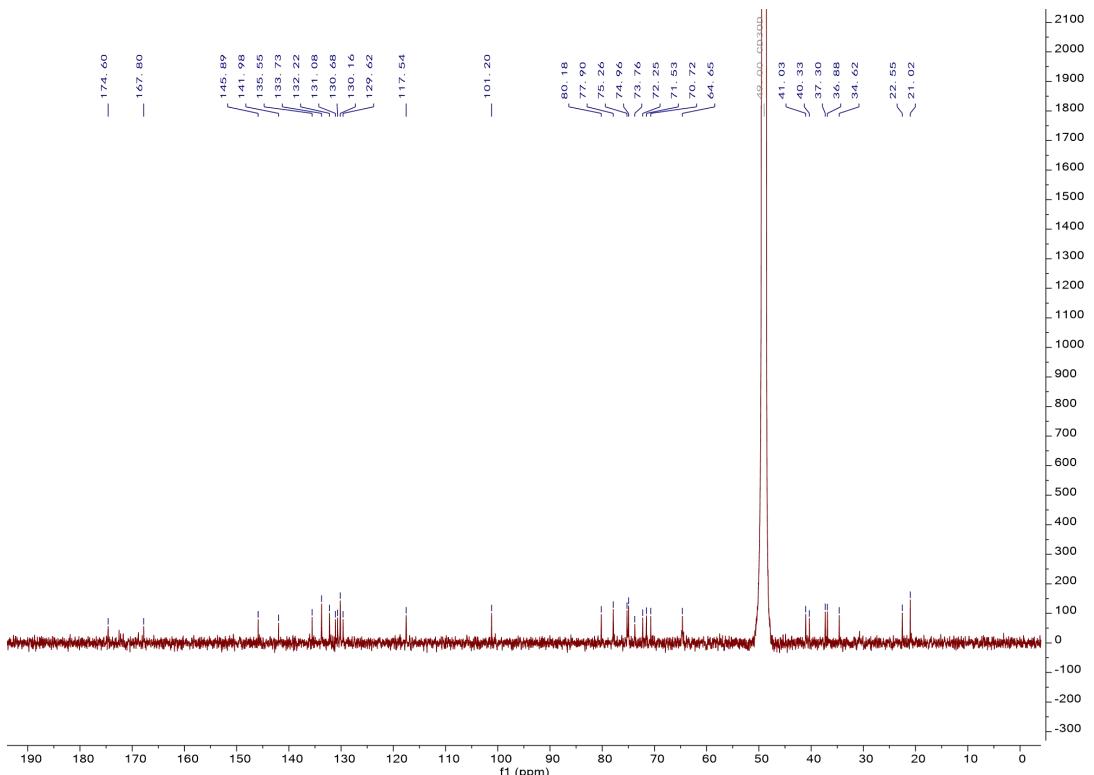


Figure S22. ^{13}C NMR spectrum of compound 3 (CD₃OD, 175MHz).

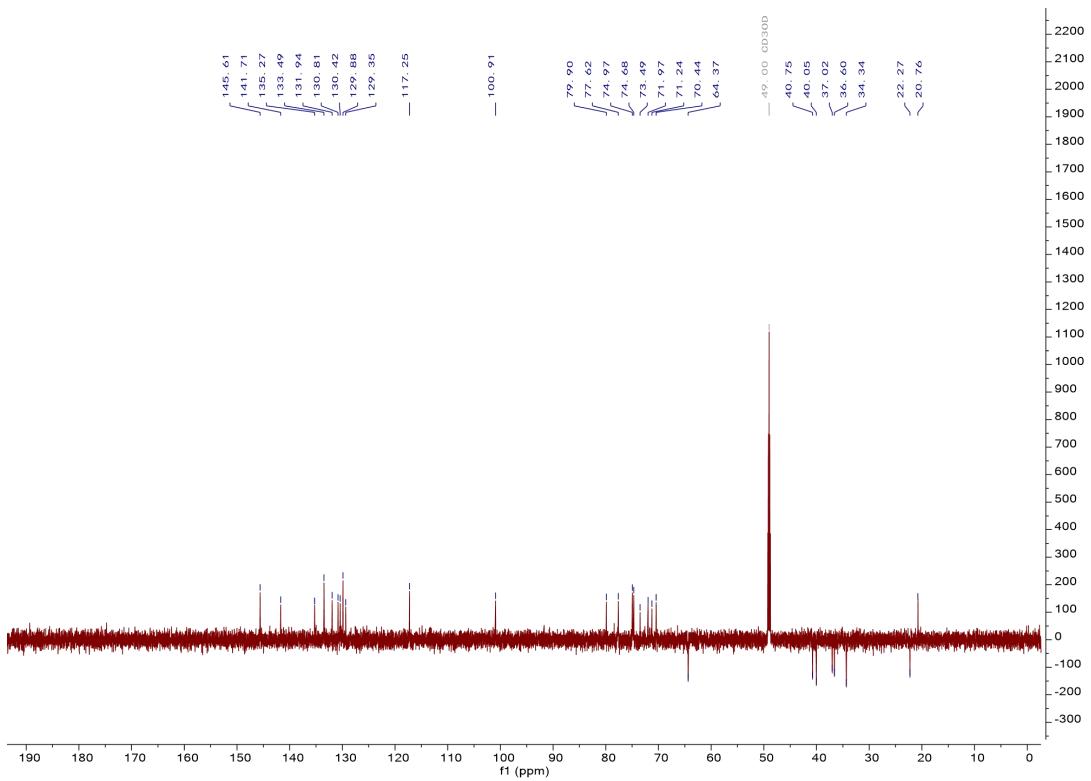


Figure S23. ^{13}C -DEPT135 NMR spectrum of compound **3** (CD_3OD , 175MHz).

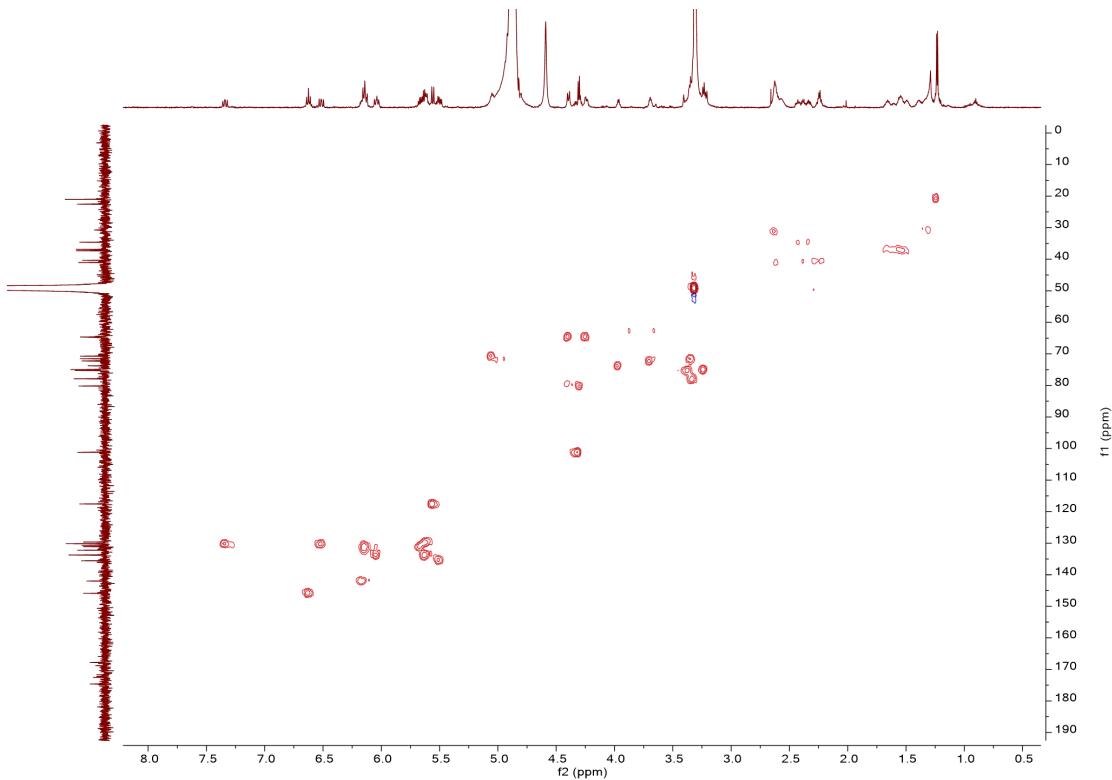


Figure S24. HMQC spectrum of compound **3** (CD_3OD).

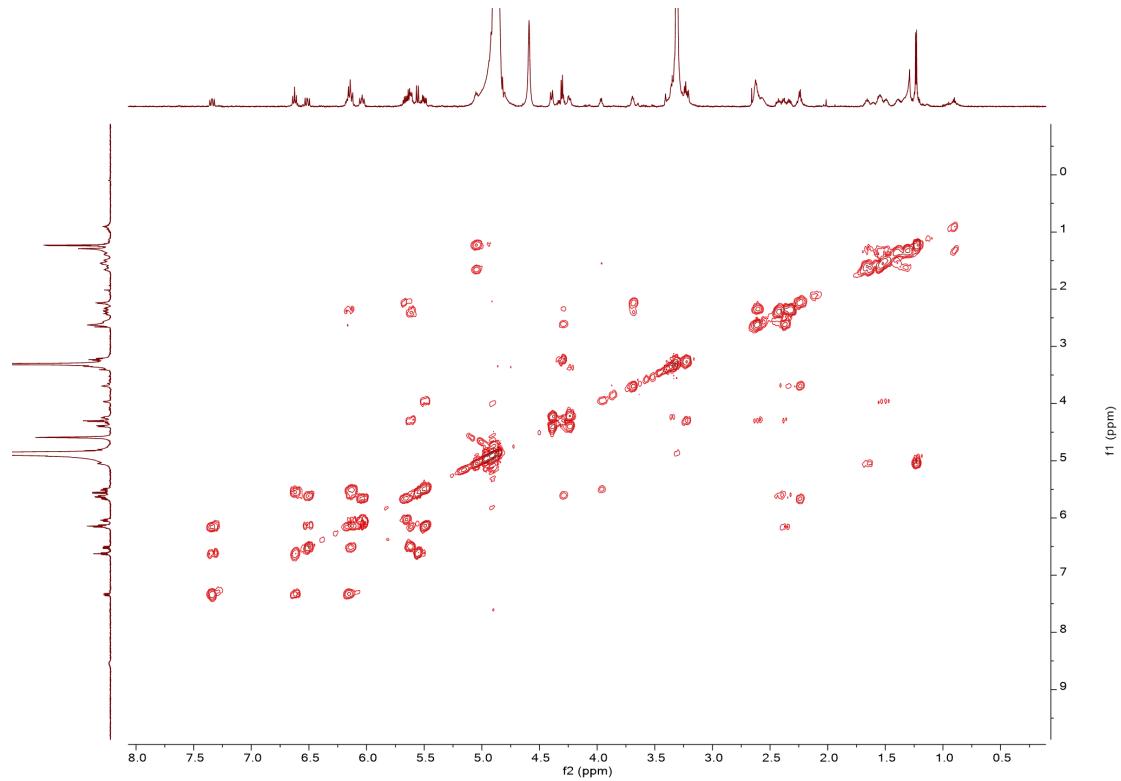


Figure S25. ^1H - ^1H COSY spectrum of compound **3** (CD_3OD).

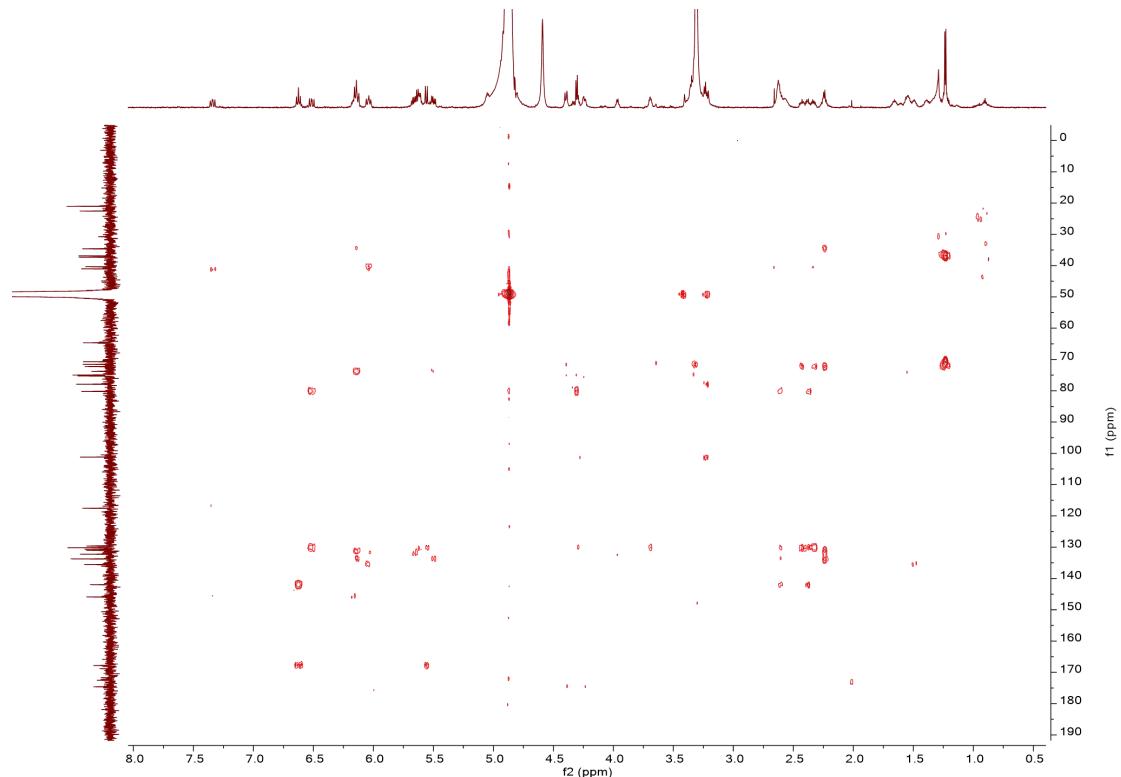


Figure S26. HMBC spectrum of compound **3** (CD_3OD).

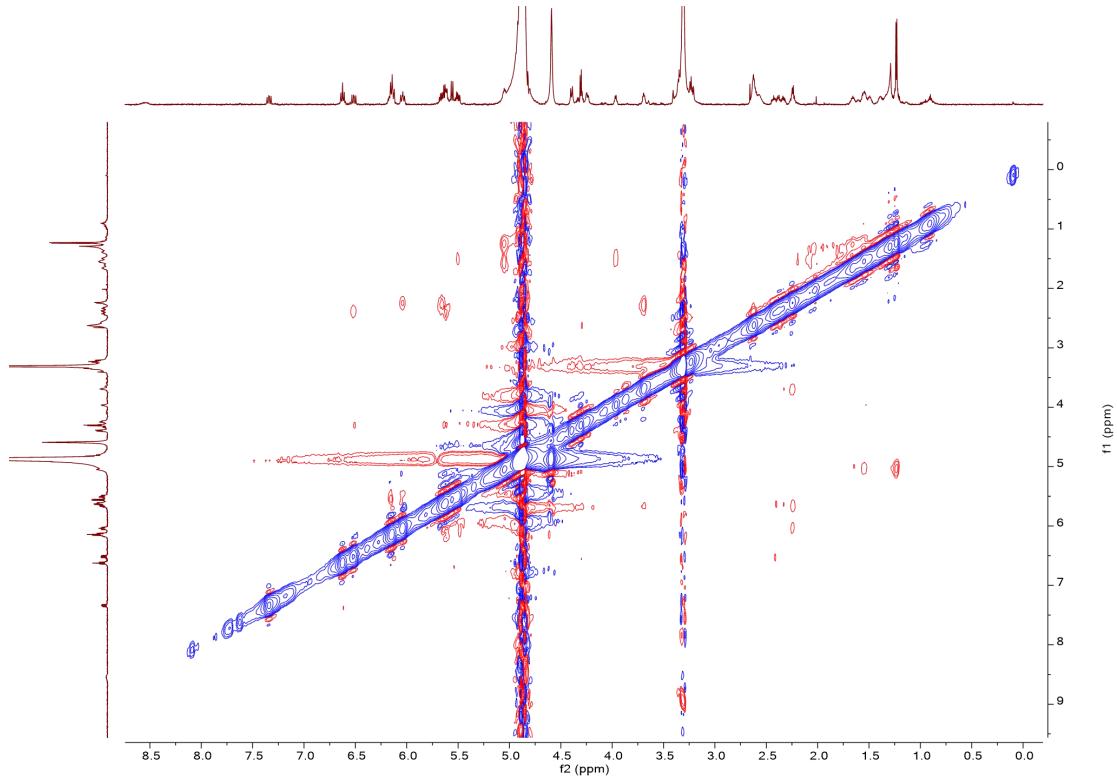


Figure S27. NOESY spectrum of compound 3 (CD_3OD).

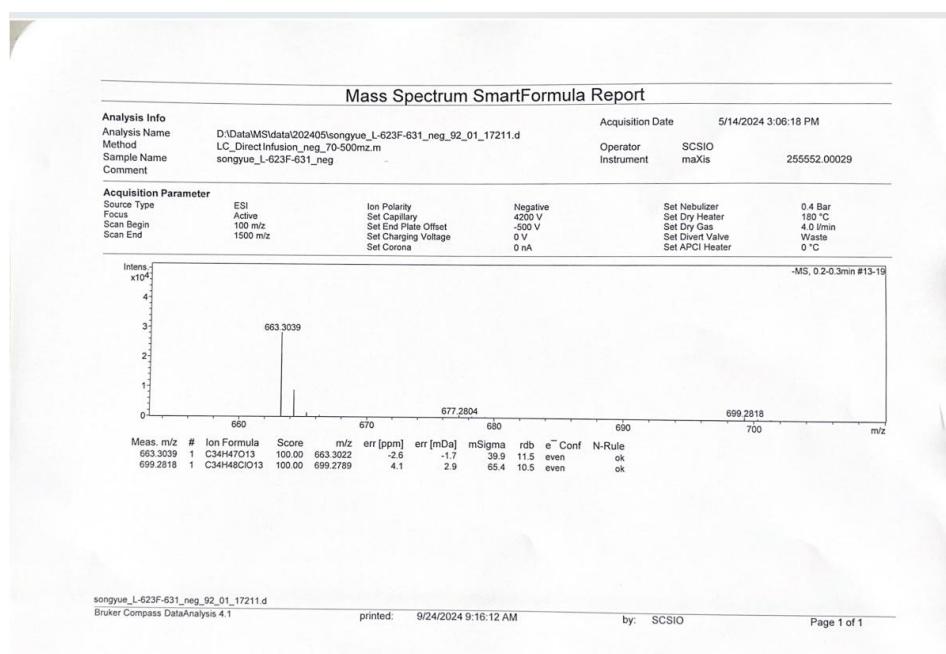


Figure S28. HR-ESI-MS spectrum of compound 3.

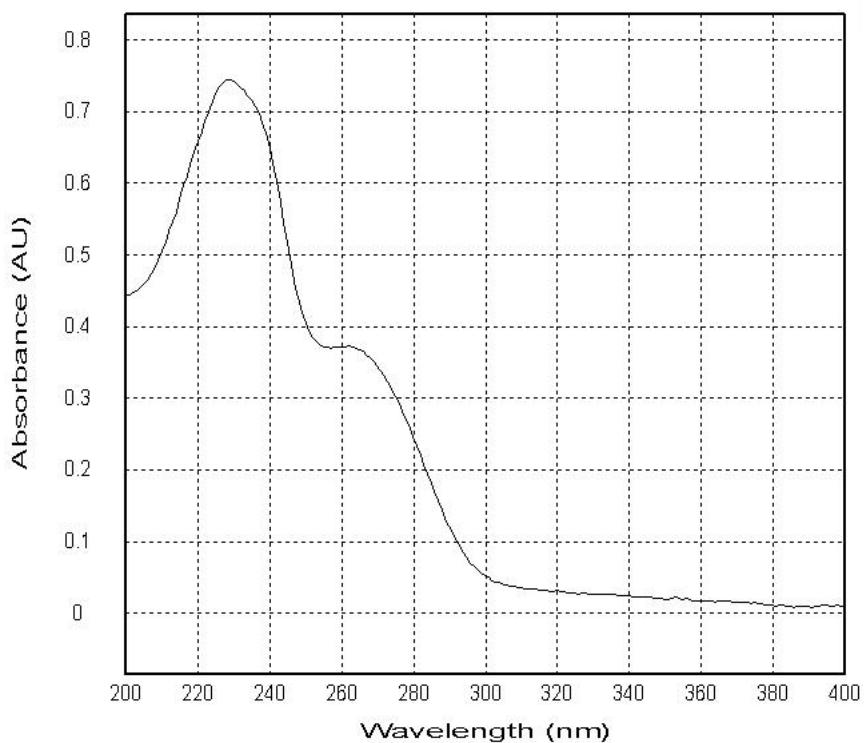


Figure S29. UV spectrum of compound 3.

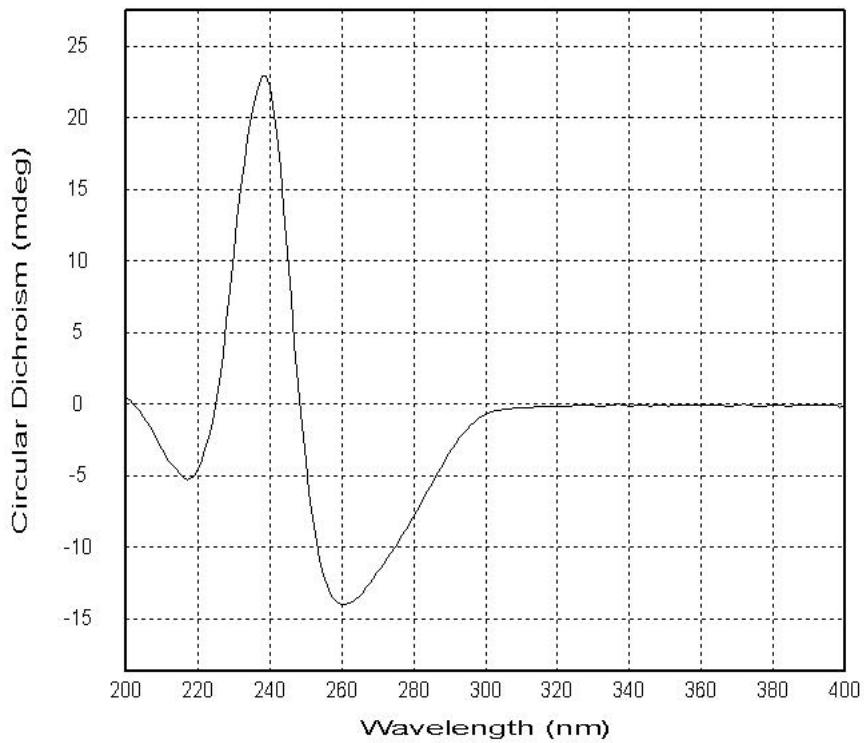


Figure S30. CD spectrum of compound 3.

Strains	relevant genotype and/or characteristics
PAO1	ATCC <i>Pseudomonas aeruginosa</i>
PAO1- <i>pqsA-gfp</i>	PAO1 containing <i>pqsA-gfp</i> (ASV) translational reporter fusion
PAO1Δ <i>lasI</i> Δ <i>rhlI</i>	PAO1 <i>lasI</i> and <i>rhlI</i> mutant

Table S1. The tested *P. aeruginosa* strains used in this study.

Physicochemical data of known compounds **4–5**.

Stellarine A (4): Green powder, ¹H NMR (700 MHz, DMSO-*d*₆) δ_H 12.20 (s, 1H, 9-NH), 9.14 (s, 1H, H-4), 8.44 (d, *J* = 7.6 Hz, 1H, H-5), 8.25 (s, 1H, 11-NH₂), 7.84 (d, *J* = 7.9 Hz, 1H, H-8), 7.63 (t, *J* = 7.4 Hz, 1H, H-7), 7.35 (t, *J* = 7.3 Hz, 1H, H-6), 2.85 (s, 3H, H-13). ¹³C NMR (176 MHz, DMSO-*d*₆) δ_C 201.2(C-12), 166.7(C-10), 142.3(C-13), 134.99(C-1), 134.93(C-9a), 131.5(C-4a), 129.3(C-7), 122.2(C-5), 120.9(C-6, 4b), 113.4(C-8), 25.8(C-15).

9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid (5): Yellow powder, ¹H NMR (700 MHz, DMSO-*d*₆) δ_H 11.64 (s, 1H, 9-NH), 8.82 (s, 1H, H-4), 8.39 (s, 1H, H-5), 7.83 (s, 1H, H-8), 7.63 (s, 1H, H-7), 7.44 (s, 1H, H-3'), 7.33 (s, 1H, H-6), 6.61 (s, 1H, H-4'), 4.68 (s, 2H, H-6'). ¹³C NMR (176 MHz, DMSO-*d*₆) δ_C 167.4(C-10), 157.2(C-5'), 151.1(C-2'), 141.5(C-8a), 139.1(C-3), 132.1(C-1), 131.7(C-9a), 129.95(C-4a), 128.8(C-7), 121.98(C-5), 121.0(C-4b), 120.5(C-6), 115.5(C-4), 112.9(C-8), 110.98(C-3'), 109.2(C-4'), 55.94(C-6').