Aspersymmetide A, a New Centrosymmetric Cyclohexapeptide from the Marine-derived Fungus *Aspergillus versicolor*

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Supplementary Information

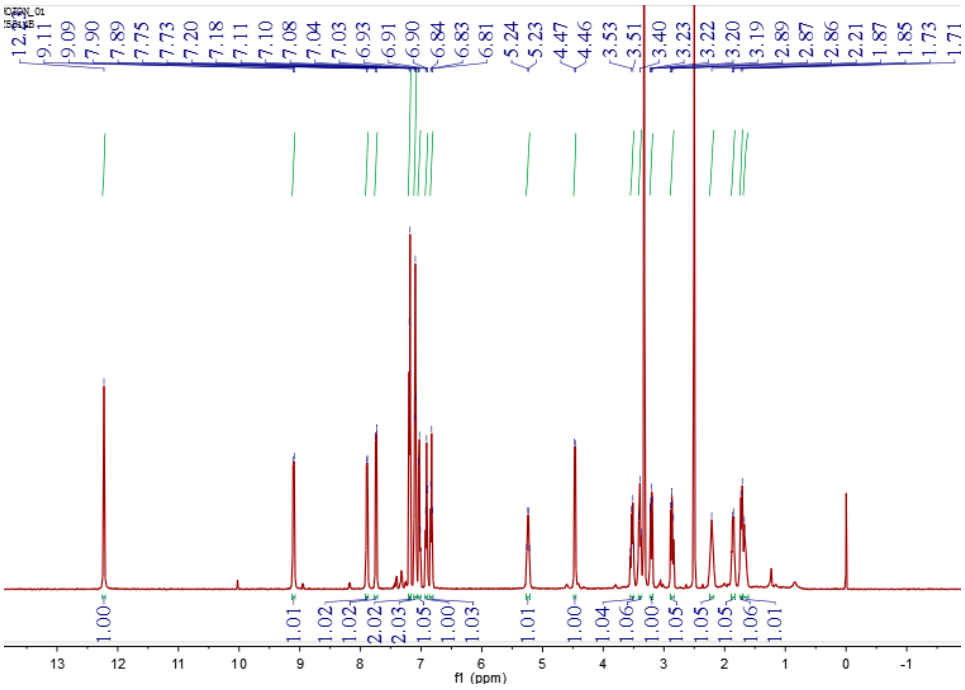

Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**.

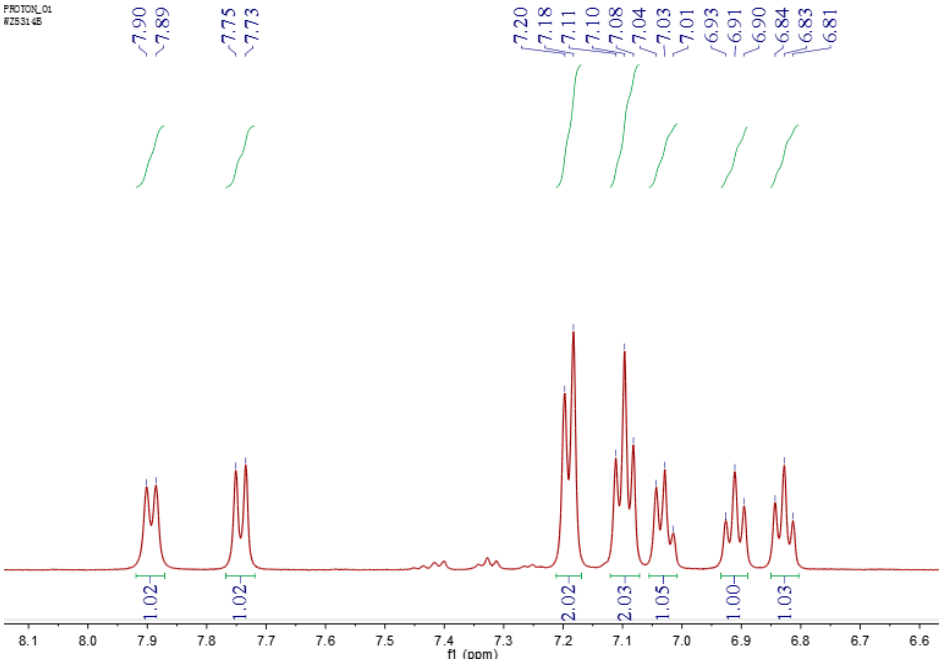

Figure S2. Partial ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**.

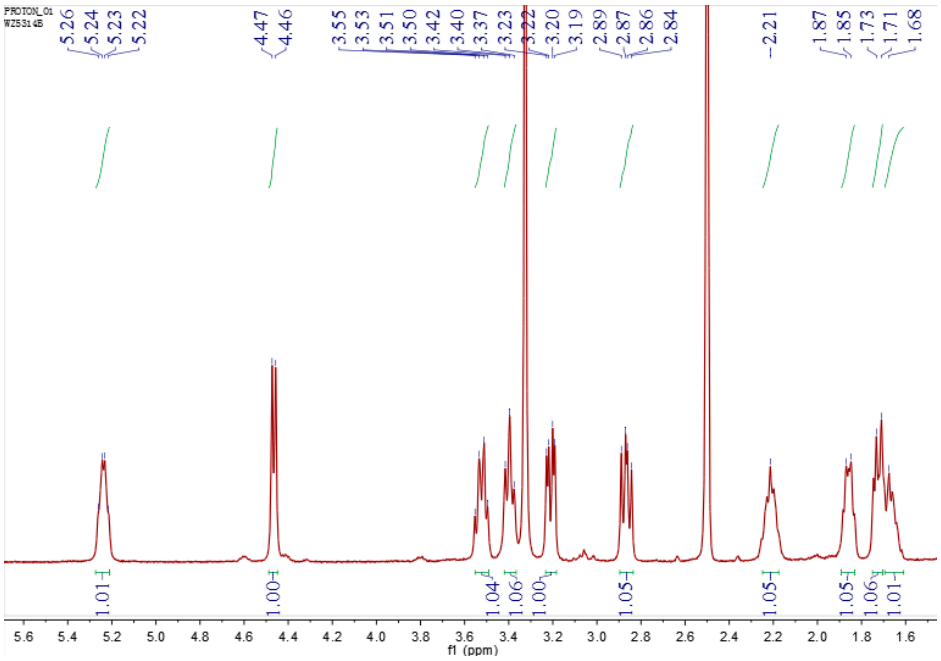

Figure S3. Partial ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**.

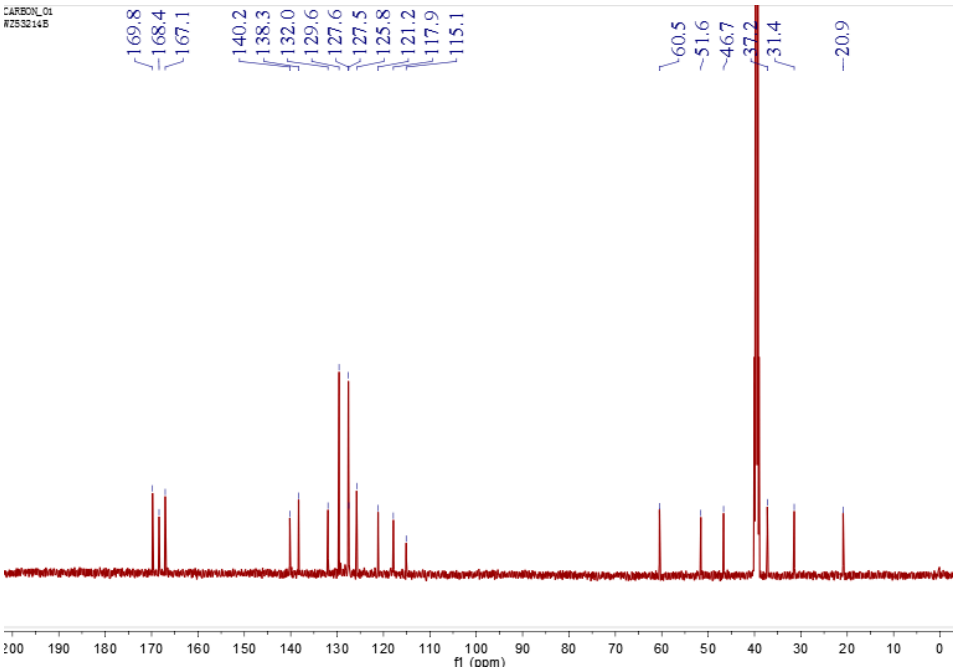

Figure S4. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **1**.

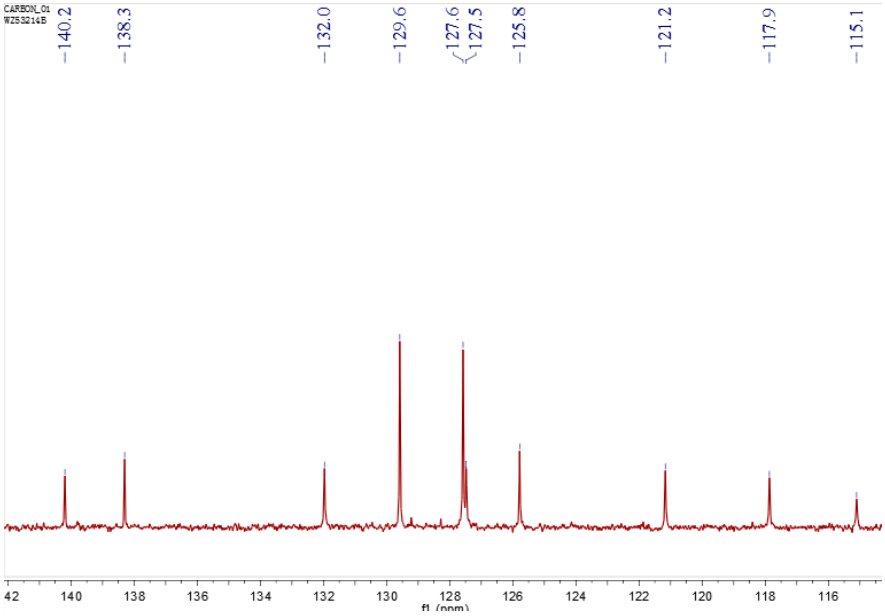

Figure S5. Partial ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **1**.

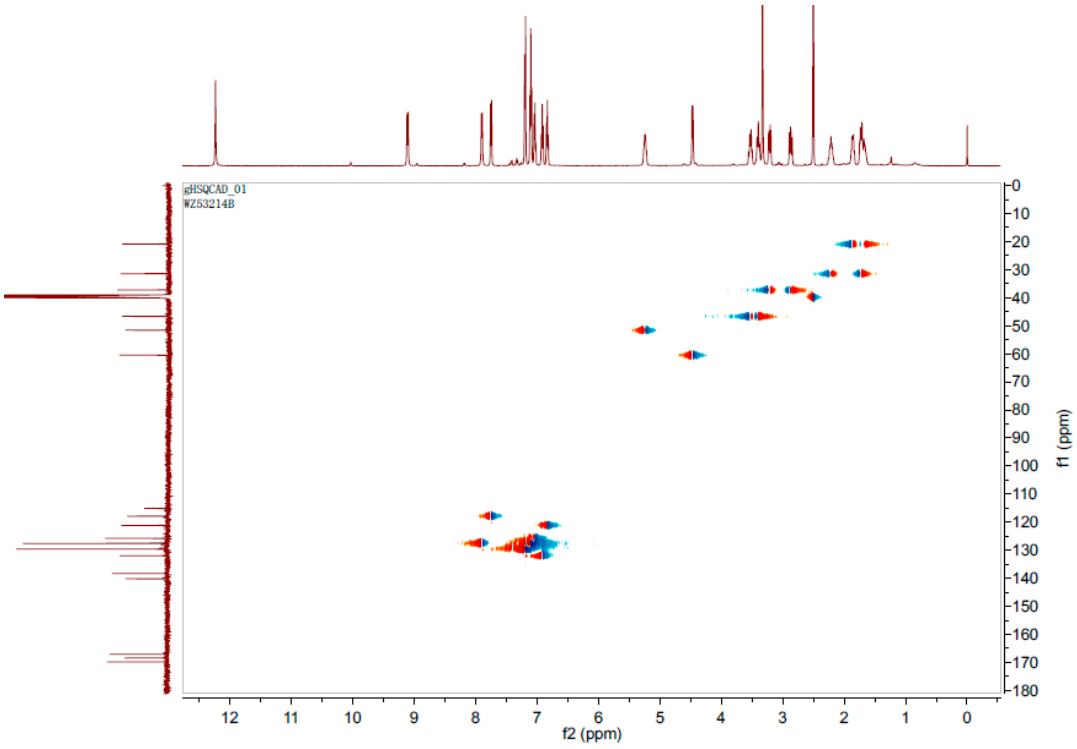

Figure S6. HMQC (DMSO-d_6) spectrum of compound **1**.

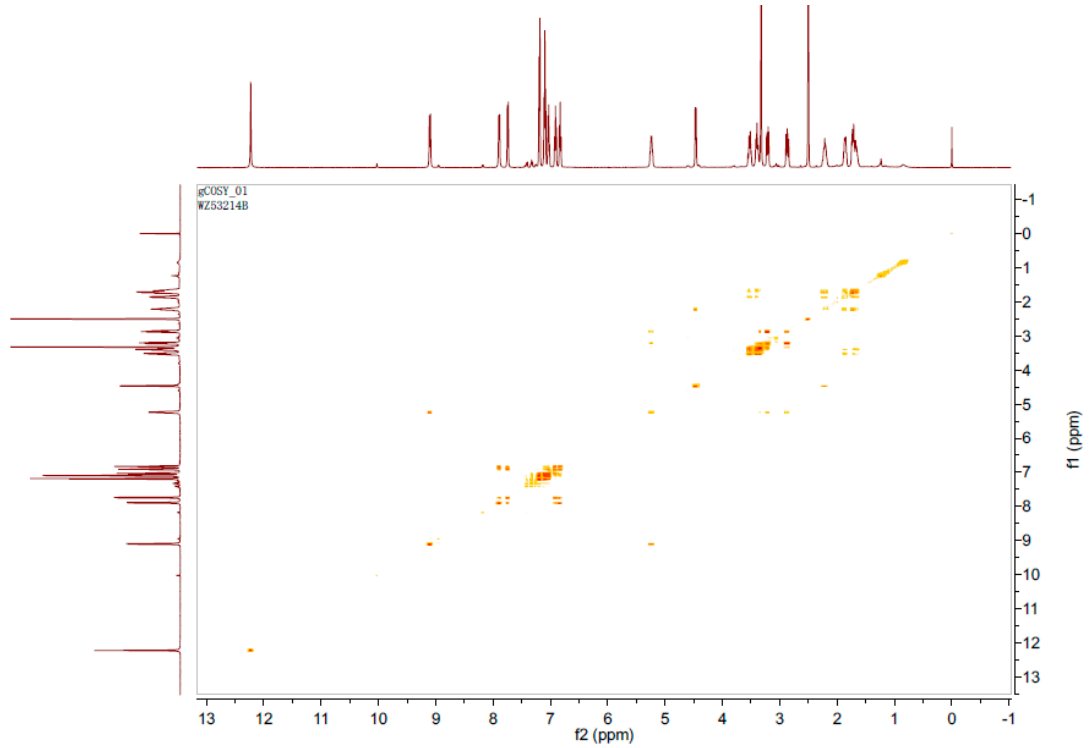

Figure S7. ^{1}H–^{1}H COSY (DMSO-d_6) spectrum of compound **1**.

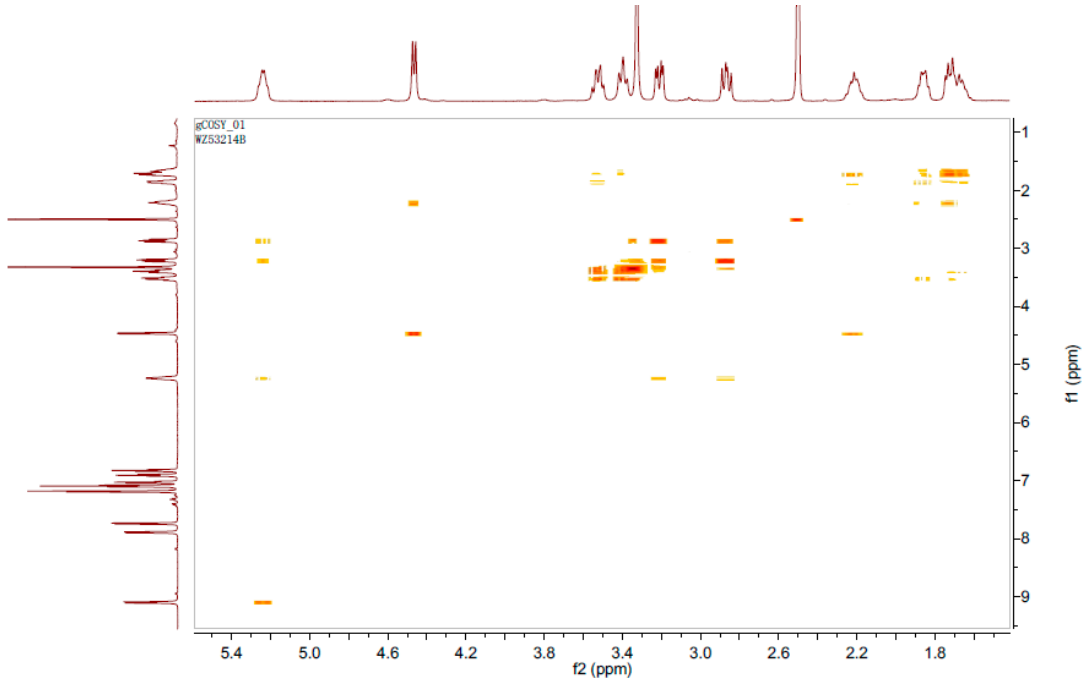

Figure S8. Partial ^{1}H–^{1}H COSY (DMSO-d_6) spectrum of compound **1**.

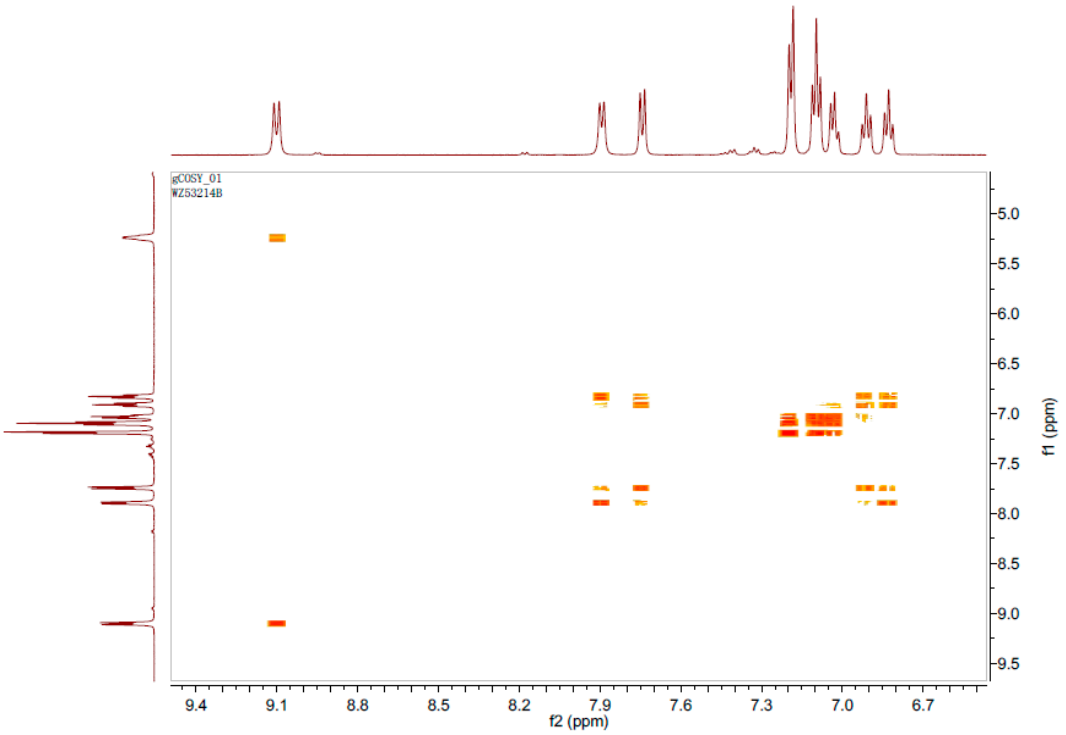

Figure S9. Partial ^{1}H–^{1}H COSY (DMSO-d_6) spectrum of compound **1**.

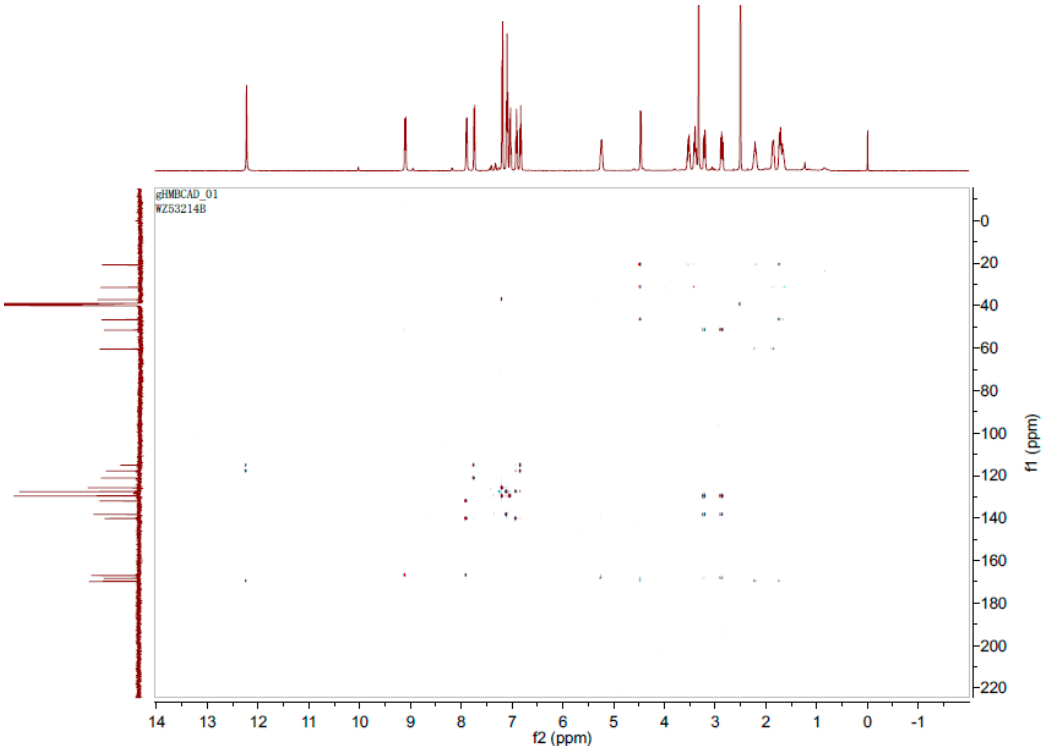

Figure S10. HMBC (DMSO-d_6) spectrum of compound **1**.

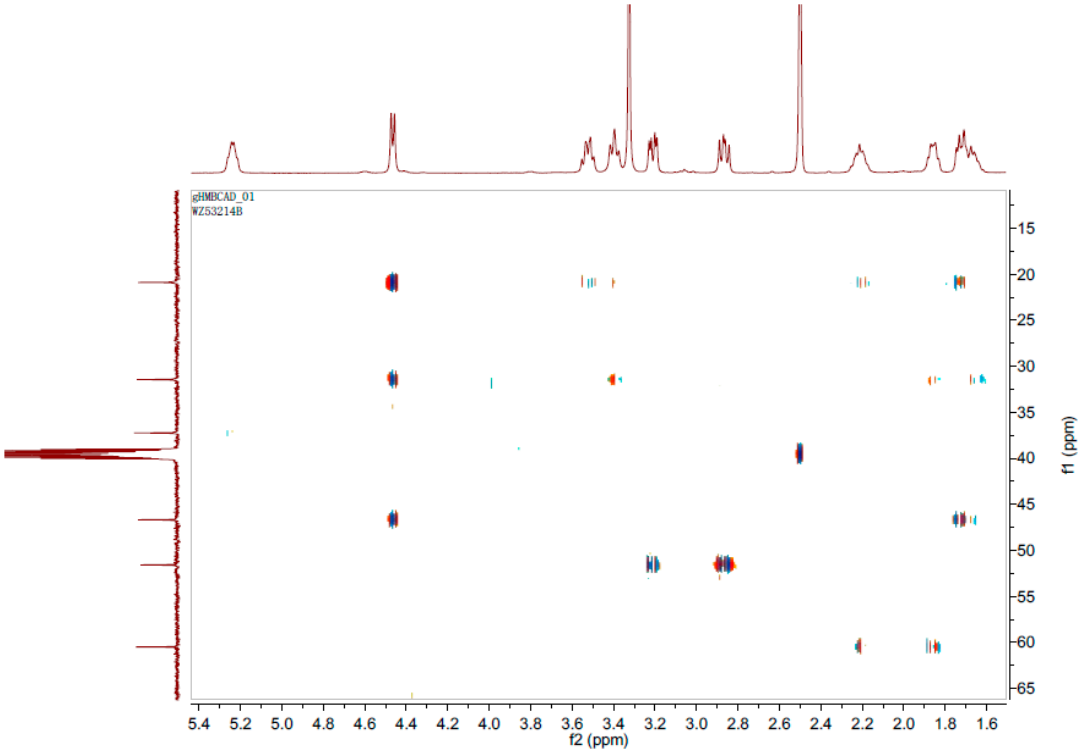

Figure S11. Partial HMBC (DMSO-d_6) spectrum of compound **1**.

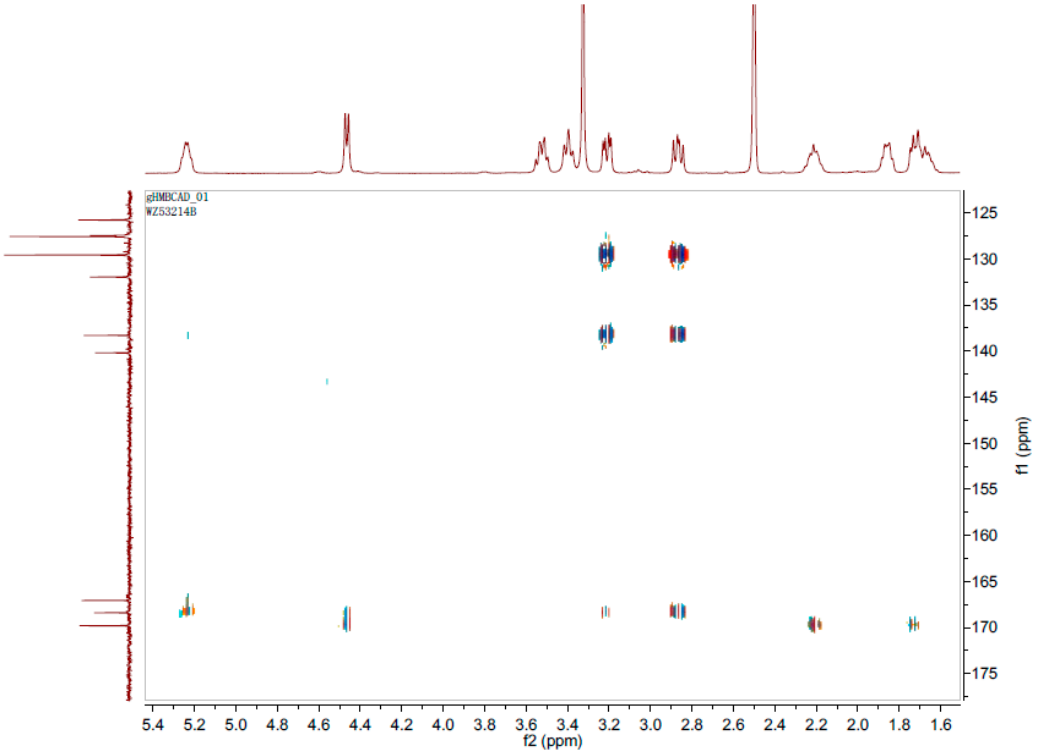

Figure S12. Partial HMBC (DMSO-d_6) spectrum of compound **1**.

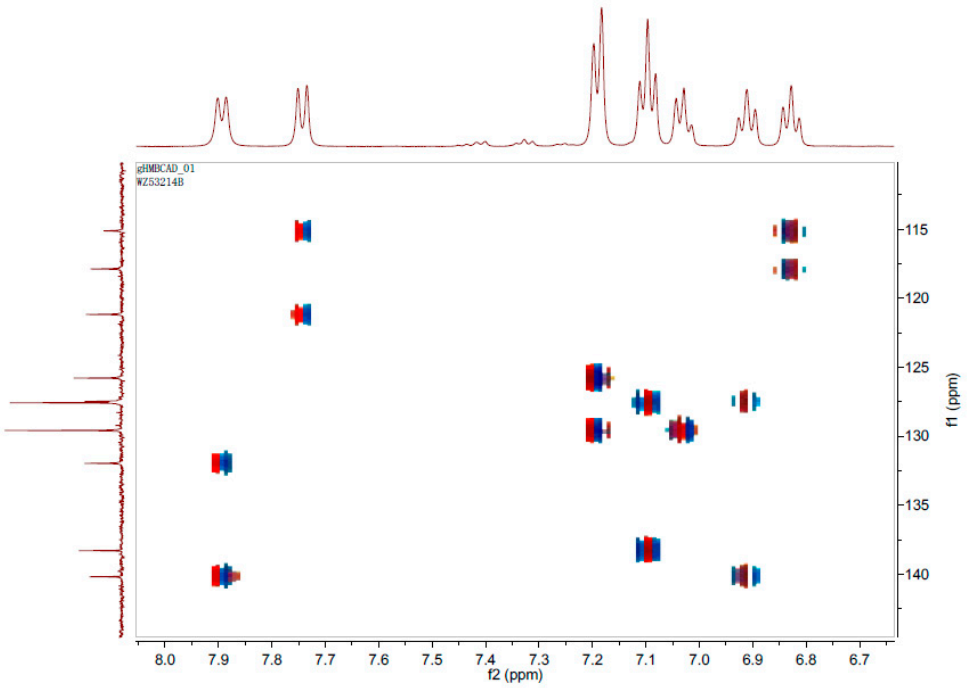

Figure S13. Partial HMBC (DMSO-d_6) spectrum of compound **1**.

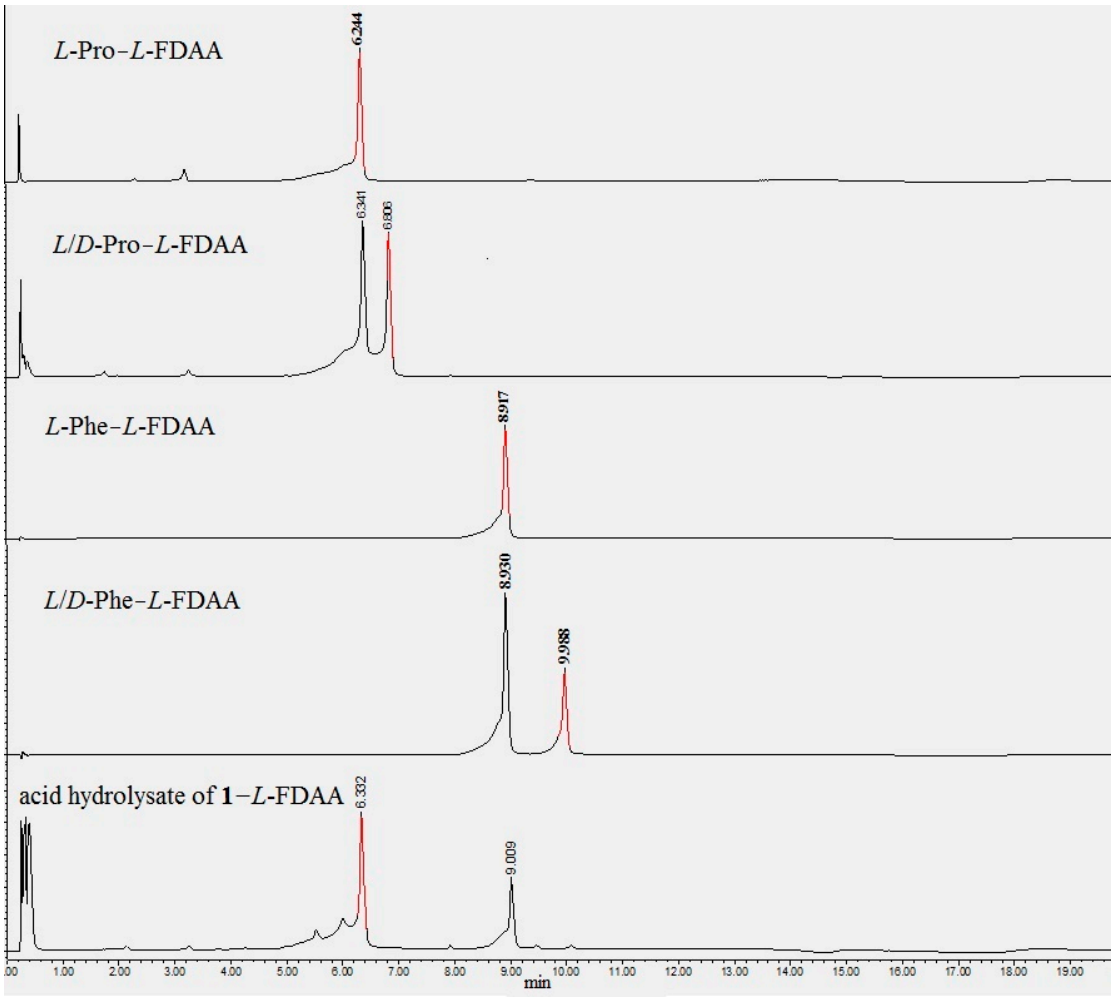

Figure S14. Marfey's analysis of the amino acids in **1** on UPLC-MS

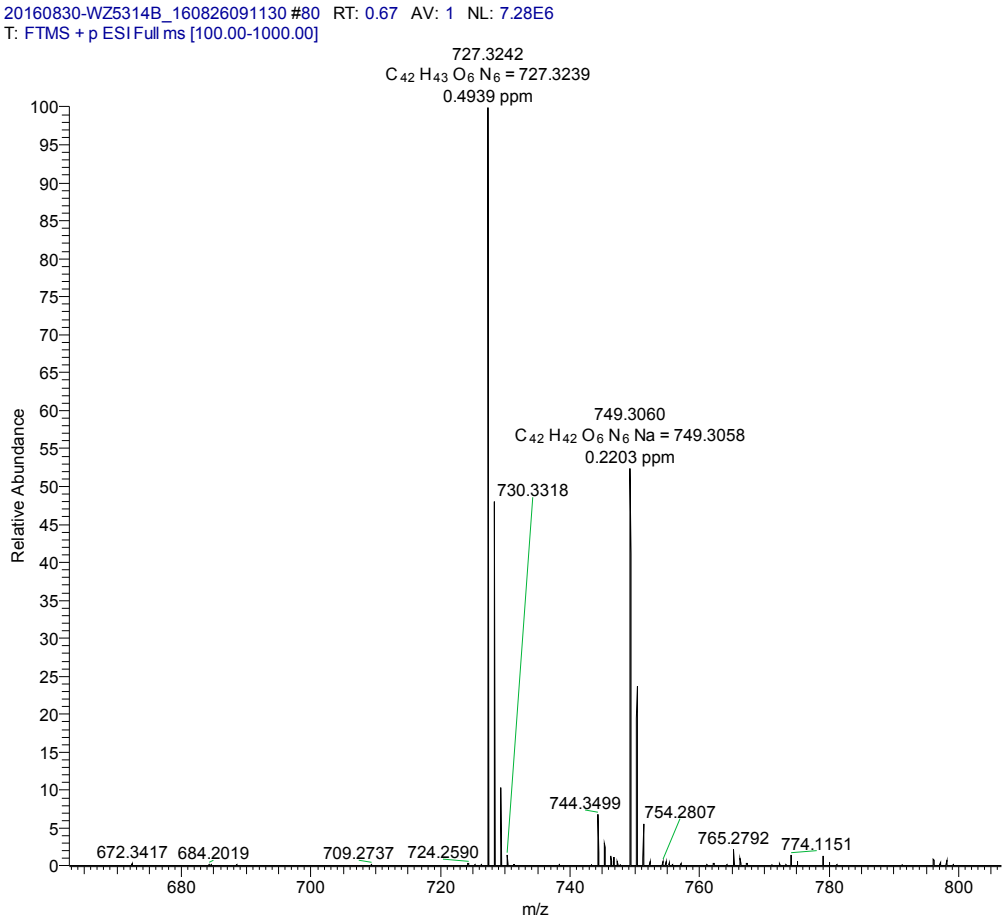

Figure S15. HRESIMS spectrum of compound **1**.

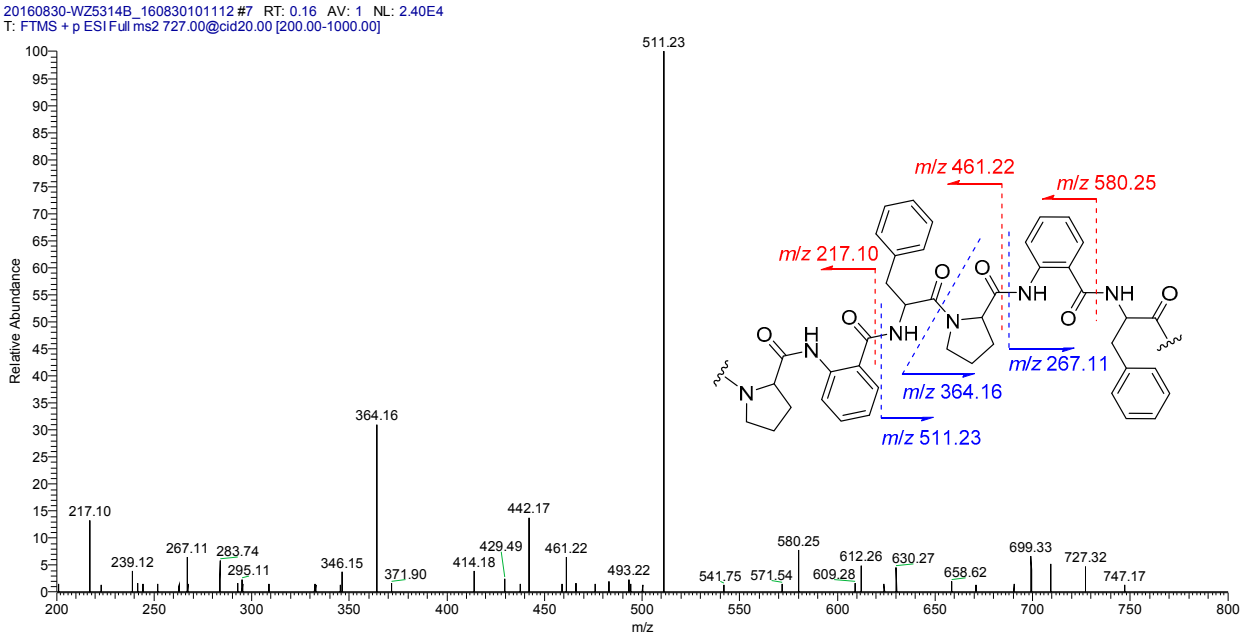

Figure S16. ESI MS^2 spectrum of compound **1**.

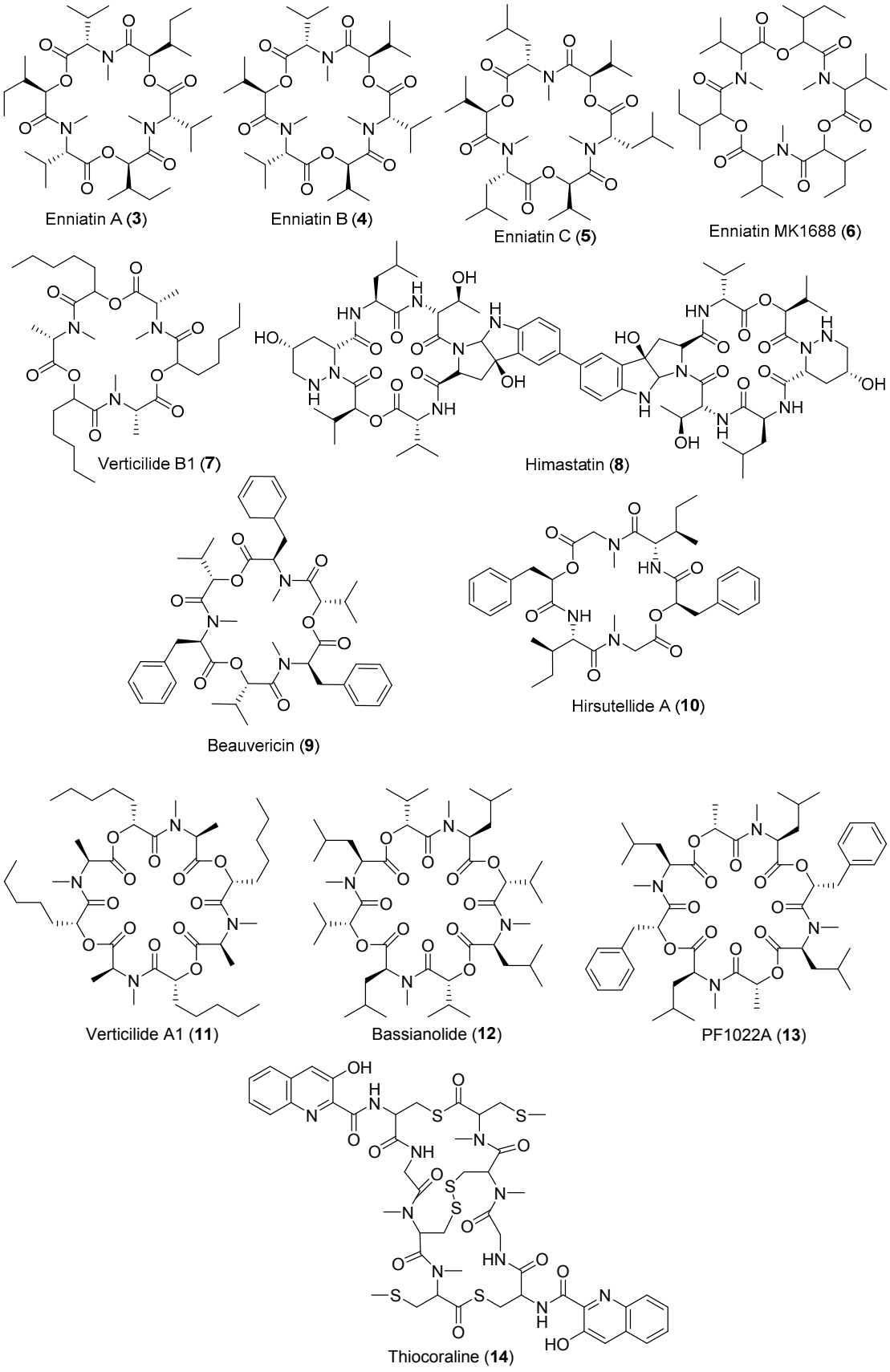

Figure S17. The reported centrosymmetric cyclopeptides **3**–**14** from nature.

Asperphenamate (2): white powder; ^{1}H NMR (500 MHz, $CDCl_3$, *J* in Hz) δ_H 7.70 (2H, d, *J* = 7.5 Hz), 7.66 (2H, d, *J* = 7.5 Hz), 7.50 (1H, d, *J* = 7.4 Hz), 7.43 (1H, d, *J* = 7.4 Hz), 7.39 (2H, d, *J* = 7.7 Hz), 7.35−7.25 (6H, overlapped), 7.25−7.15 (6H, overlapped), 6.66 (1H, d, *J* = 8.4 Hz, NH), 6.57 (1H, d, *J* = 6.4 Hz, NH), 4.92 (1H, q, *J* = 6.4 Hz, H-2'), 4.62 (1H, dddd, *J* = 8.4, 6.4, 4.2, 3.1 Hz, H-2), 4.54 (1H, dd, *J* = 11.3, 3.1 Hz, Ha-1), 4.04 (1H, dd, *J* = 11.3, 4.2 Hz, Hb-1), 3.29 (1H, dd, *J* = 13.9, 6.4 Hz, Ha-3'), 3.21 (1H, dd, *J* = 13.9, 7.0 Hz, Hb-3'), 3.00 (1H, dd, *J* = 13.6, 6.4 Hz, Ha-3), 2.89 (1H, dd, *J* = 13.6, 8.4 Hz, Hb-3); ^{13}C NMR (125 MHz, $CDCl_3$) δ_C 172.0 (C, C-1'), 167.6 (C, C-10), 167.3 (C, C-10'), 137.3 (C, C-4), 135.9 (C, C-4'), 134.4 (C, C-11), 133.5 (C, C-11'), 132.2 (CH, C-14), 131.5 (CH, C-14'), 129.4 (CH, C-5/9), 129.3 (CH, C-5'/9'), 129.0 (CH, C-13/15), 128.8 (CH, C-6'/8'), 128.8 (CH, C-6/8), 128.6 (CH, C-13'/15'), 127.5 (CH, C-7'), 127.3 (CH, C-12'/16'), 127.2 (CH, C-12/16), 127.0(CH, C-7), 65.6 (CH_2, C-1), 54.6 (CH, C-2'), 50.4 (CH, C-2), 37.7 (CH_2, C-3'), 37.4 (CH_2, C-3). ESI MS *m*/*z* 507 $[M + H]^+$, 529 $[M + Na]^+$.