SUPPLEMENTARY MATERIALS

Cytotoxic Indole-Diterpenoids from a *Sphagneticola trilobata* Derived Fungus *Aspergillus* sp. PQJ-1

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Abstract: Two new indole diterpene derivatives 5*S*-hydroxy-*β*-aflatrem (**1**), 14*R*-hydroxy-*β*-aflatrem (**2**), along with one known analogue 14-(*N,N*-dimethl-*L*-valyloxy)paspalinine (**3**), were isolated from the fermentation broth of the fungus *Aspergillus* sp. PQJ-1 derived from *Sphagneticola trilobata*. The structures of the new compounds were elucidated from spectroscopic data and ECD spectroscopic analyses. All the compounds (**1**-**3**) were evaluated for their cytotoxicity against A549, Hela, Hep G2, and MCF-7 cell lines. Compounds **1** and **2** exhibited selective inhibition against Hela cells. Further studies showed that compound **1** significantly induced apoptosis, and suppressed migration and invasion in Hela cells. Moreover, **1** could up-regulate pro-apoptotic genes BAX, Caspase-3, and down-regulate anti-apoptotic genes Bcl-xL, XIXP.

Keywords: *Sphagneticola trilobata*; *Aspergillus* sp. PQJ-1; secondary metabolites; cytotoxic activity

Contents

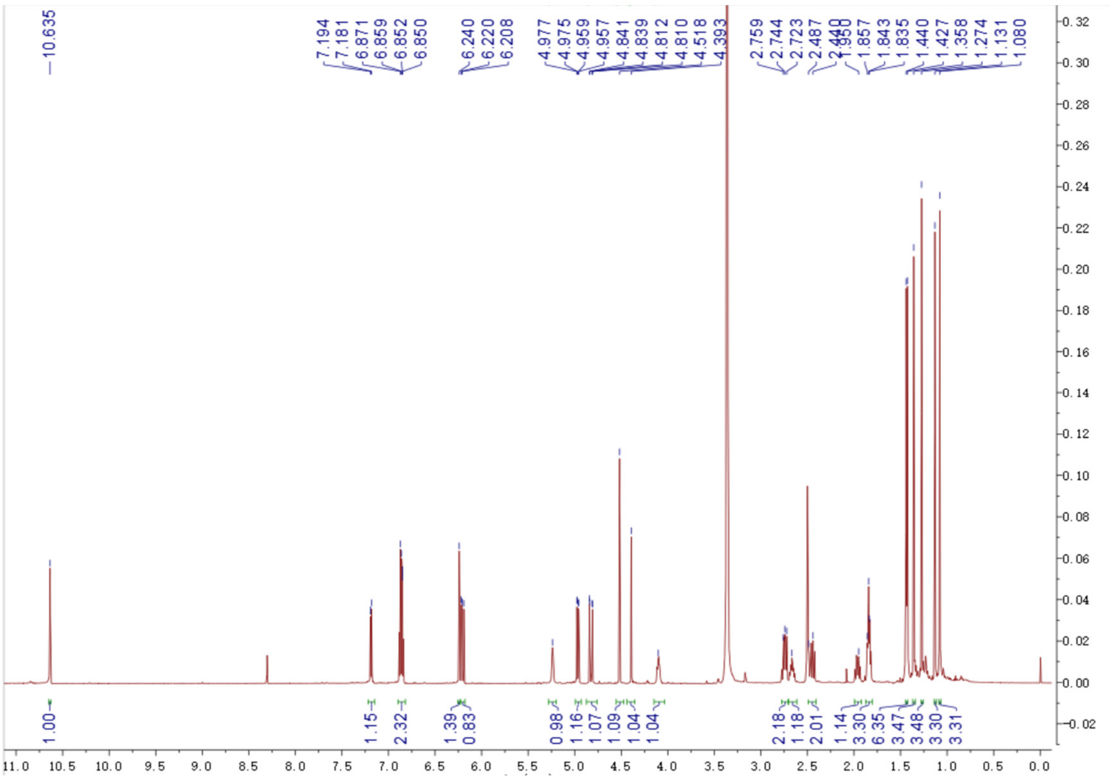

Figure S1. ^{1}H NMR spectrum of **1** in DMSO-d_6

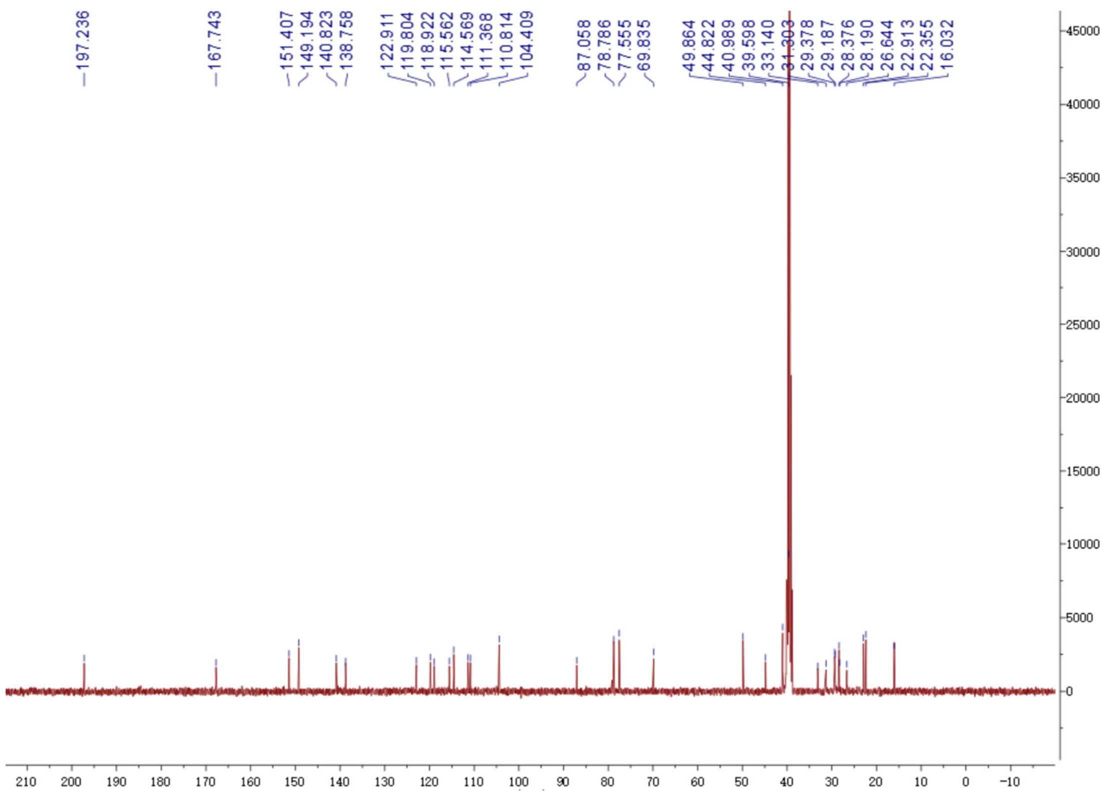

Figure S2. ^{13}C NMR spectrum of **1** in DMSO-d_6

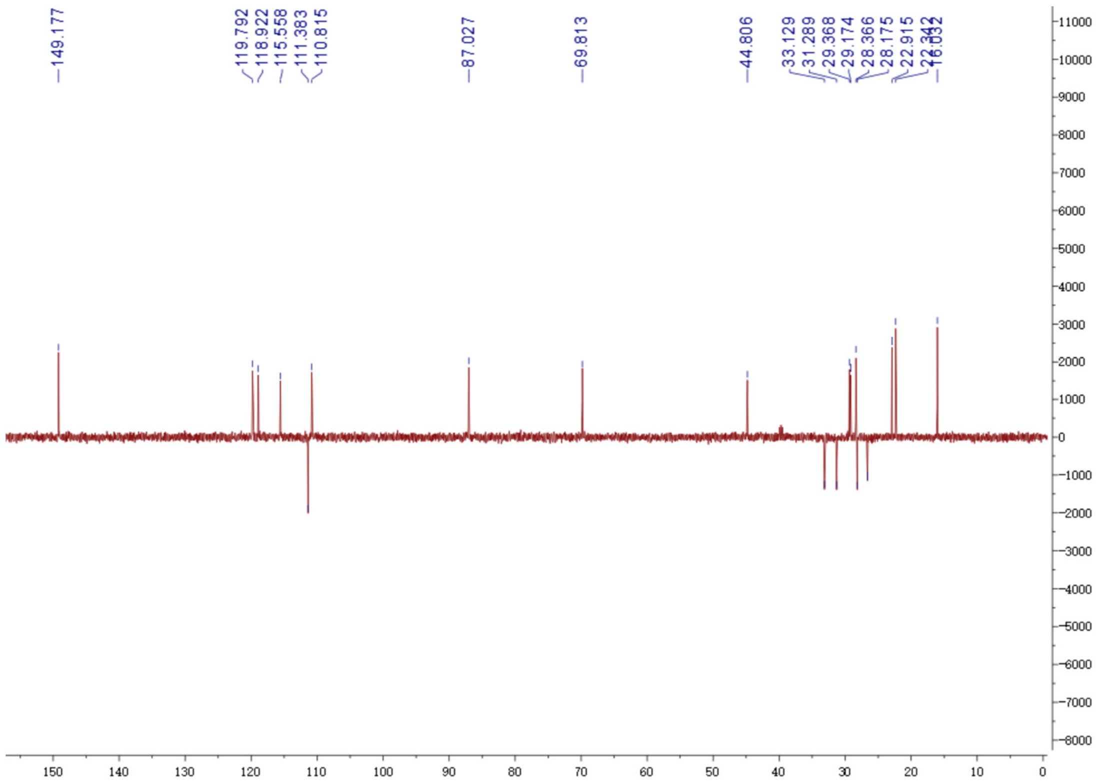

Figure S3. 135-DEPT spectrum of **1** in DMSO-d_6

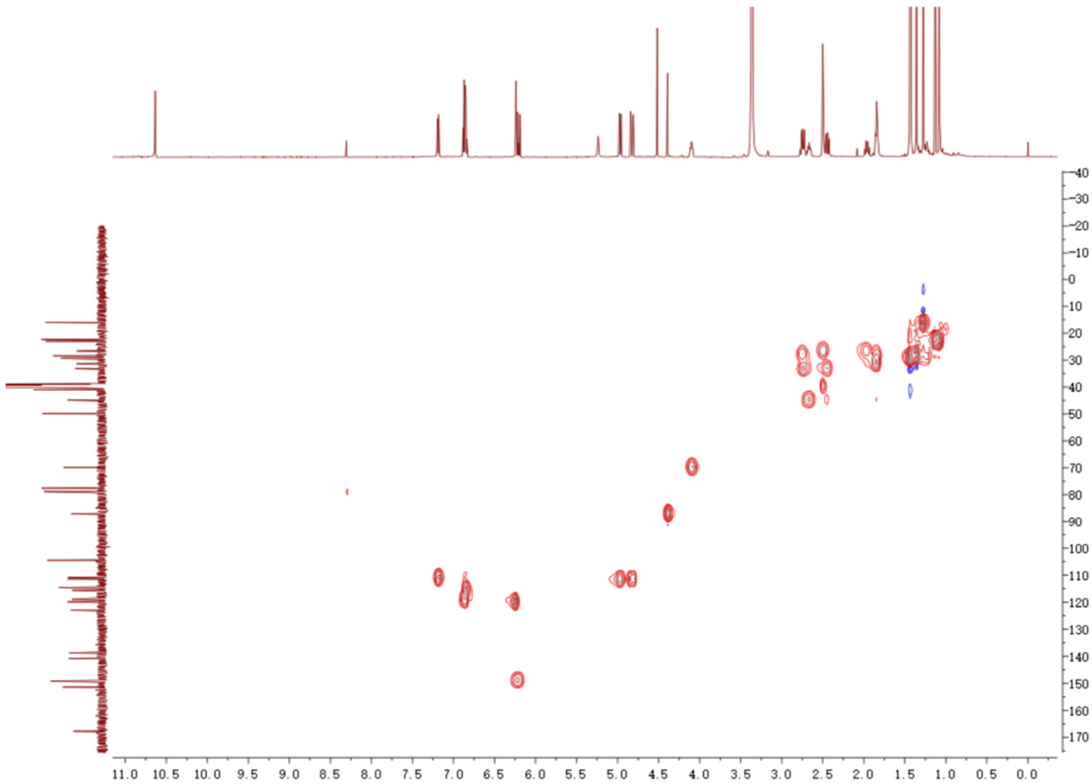

Figure S4. HSQC spectrum of **1** in DMSO-d_6

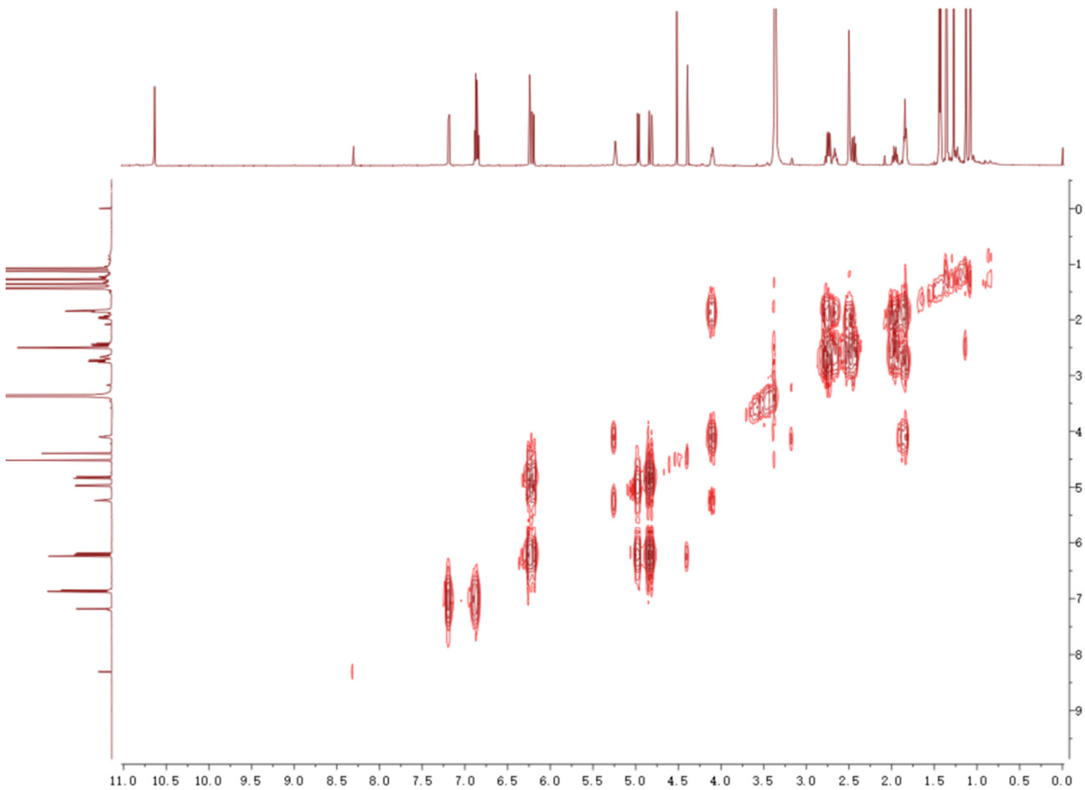

Figure S5. ^{1}H-^{1}H COSY spectrum of **1** in DMSO-d_6

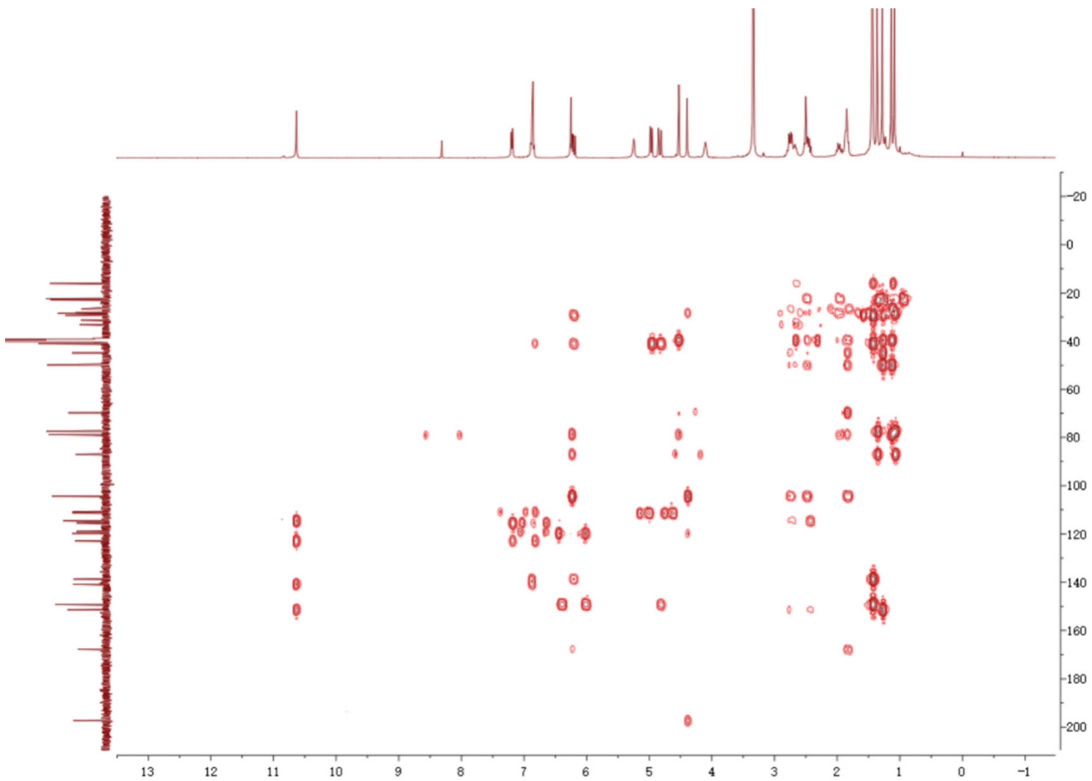

Figure S6. HMBC spectrum of **1** in DMSO-d_6

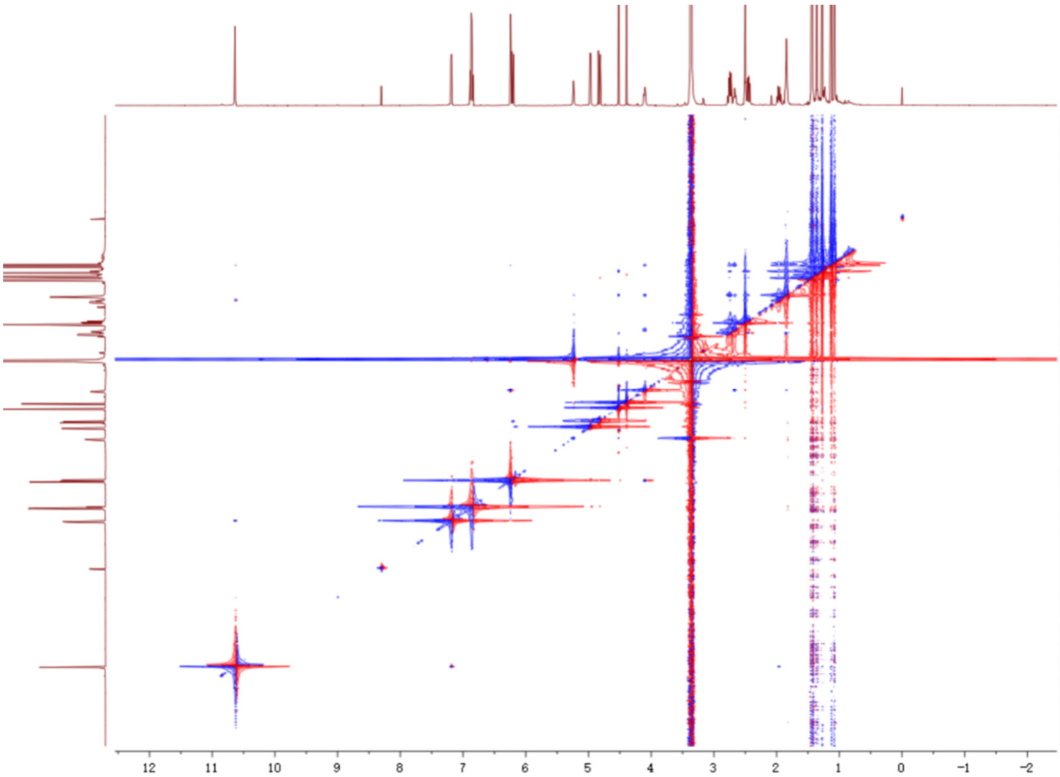

Figure S7. NOESY spectrum of **1** in DMSO-d_6

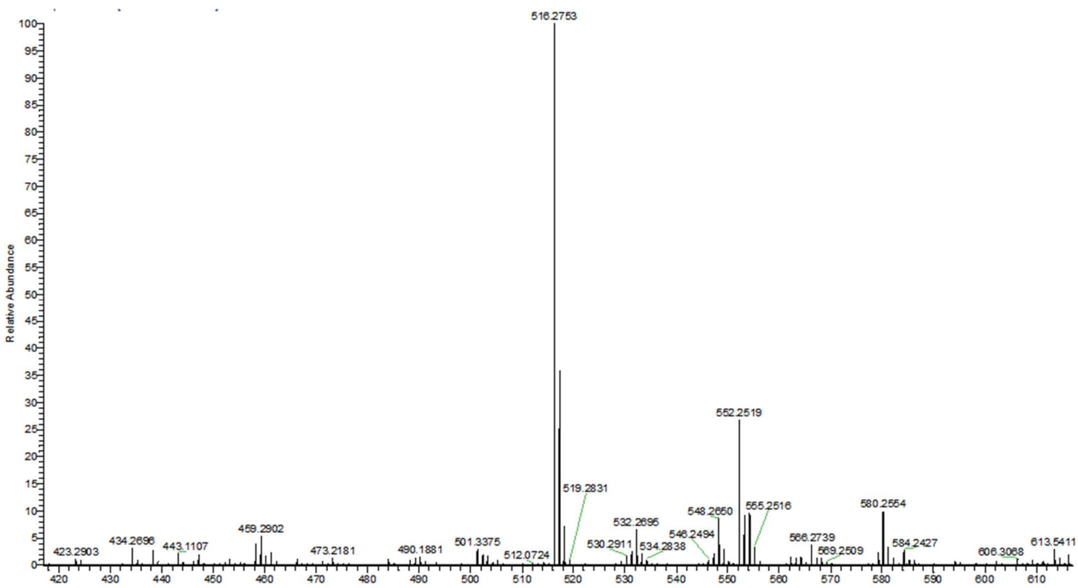

Figure S8. HRESIMS spectrum of **1**

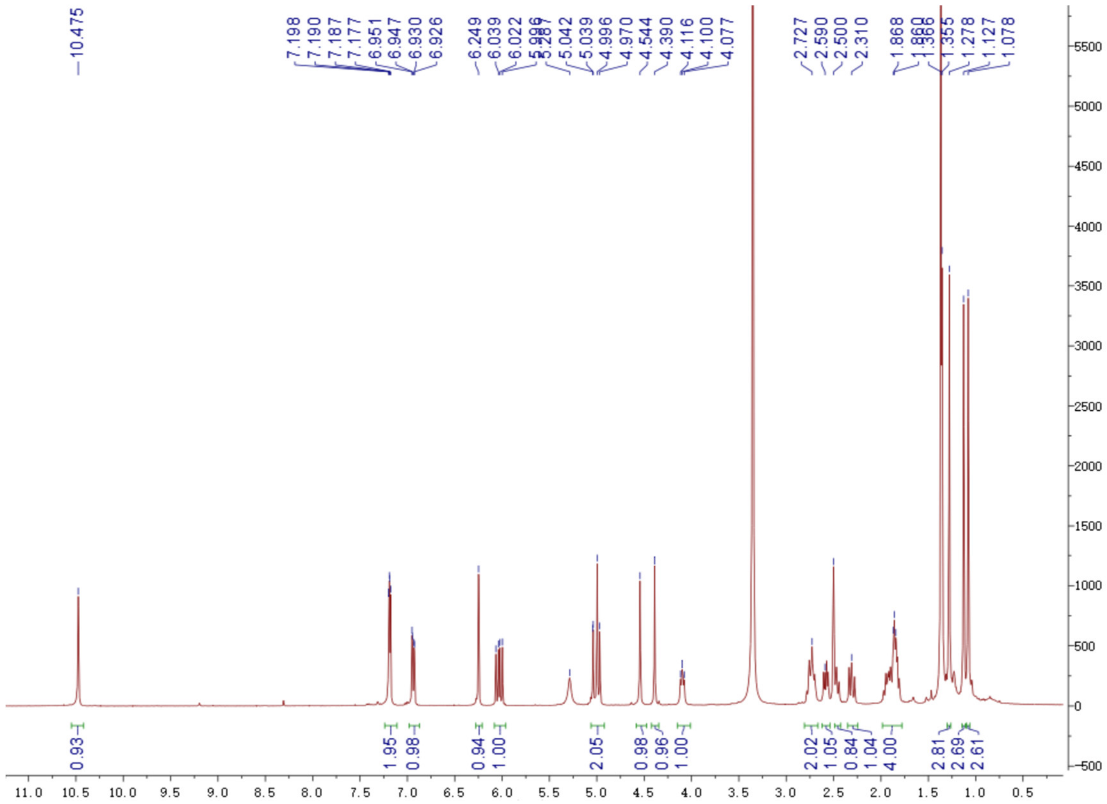

Figure S9. ^{1}H NMR spectrum of **2** in DMSO-d_6

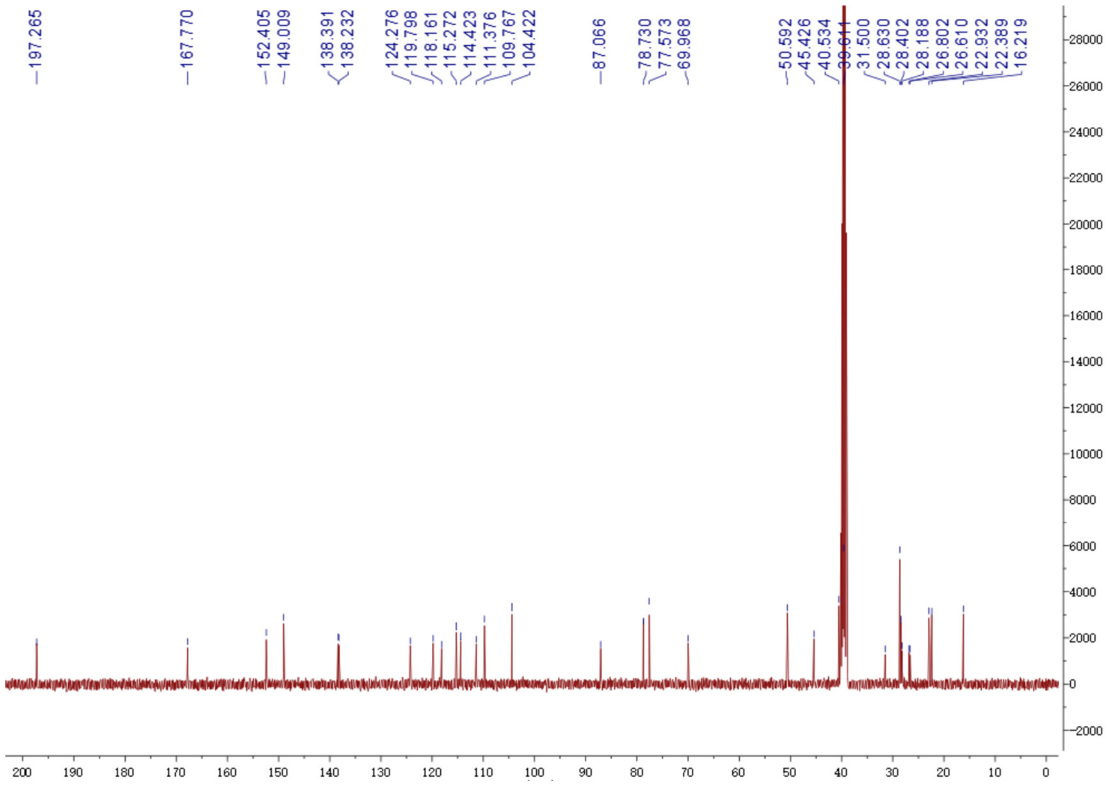

Figure S10. ^{13}C NMR spectrum of **2** in DMSO-d_6

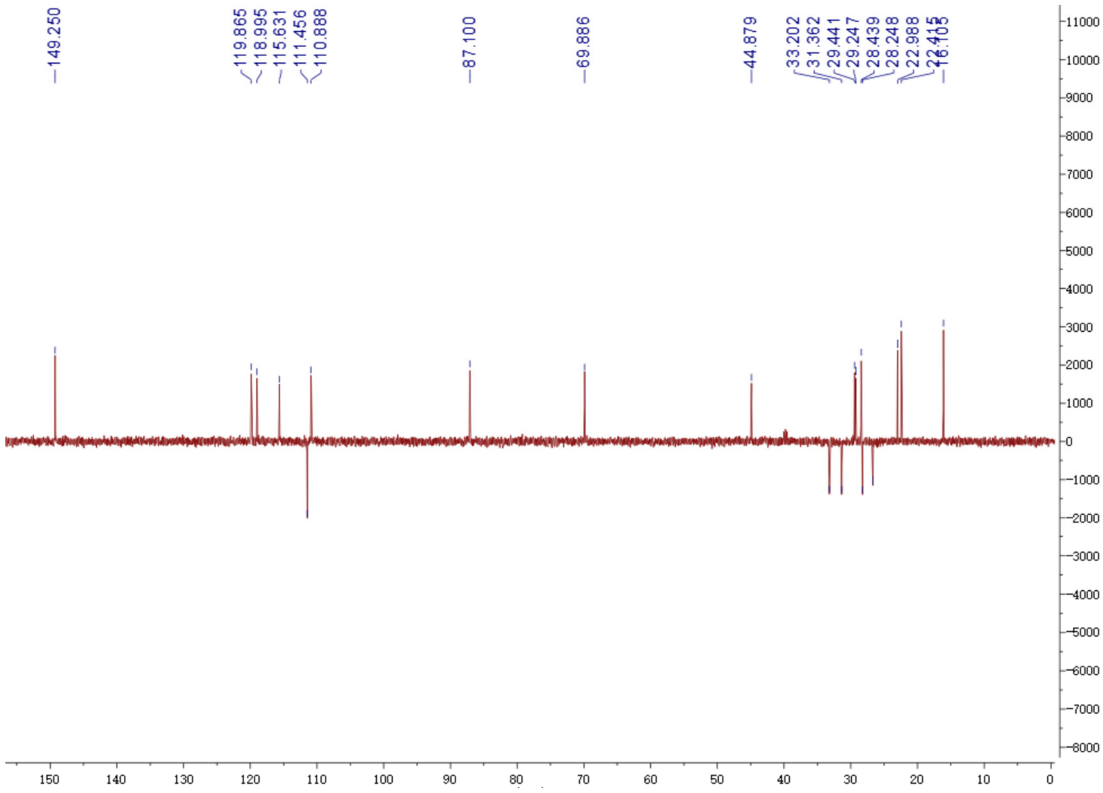

Figure S11. 135-DEPT spectrum of **2** in DMSO-d_6

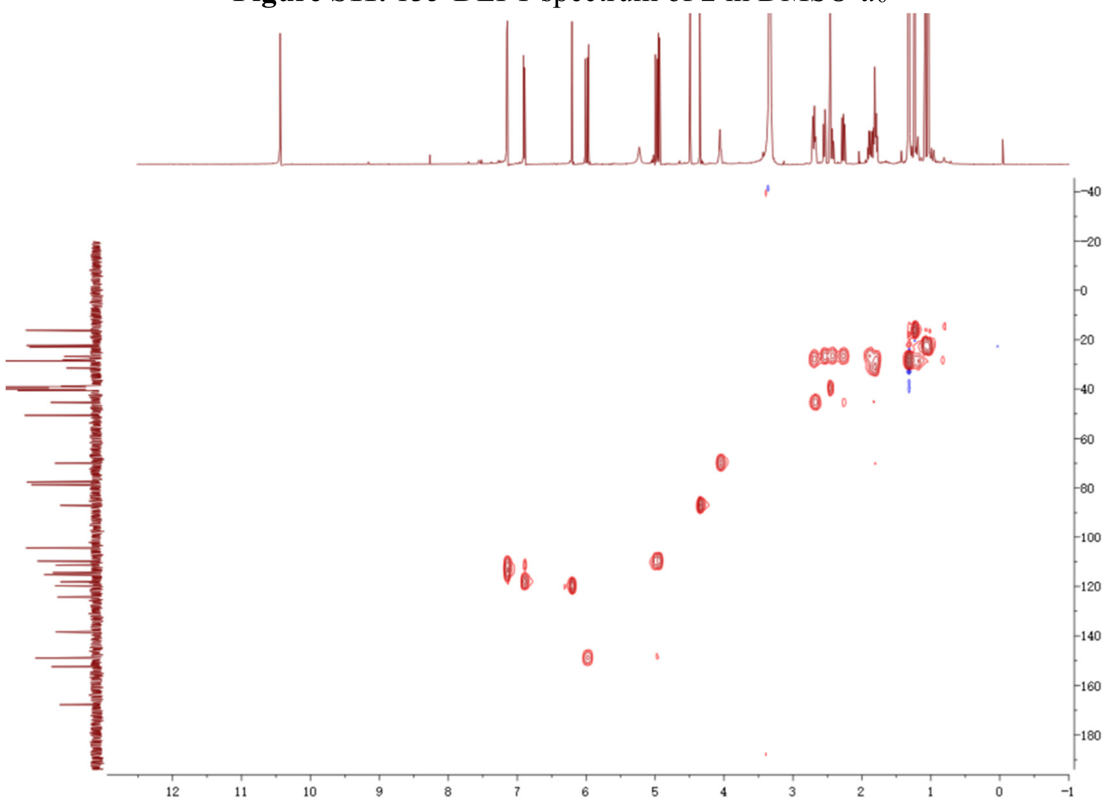

Figure S12. HSQC spectrum of **2** in DMSO-d_6

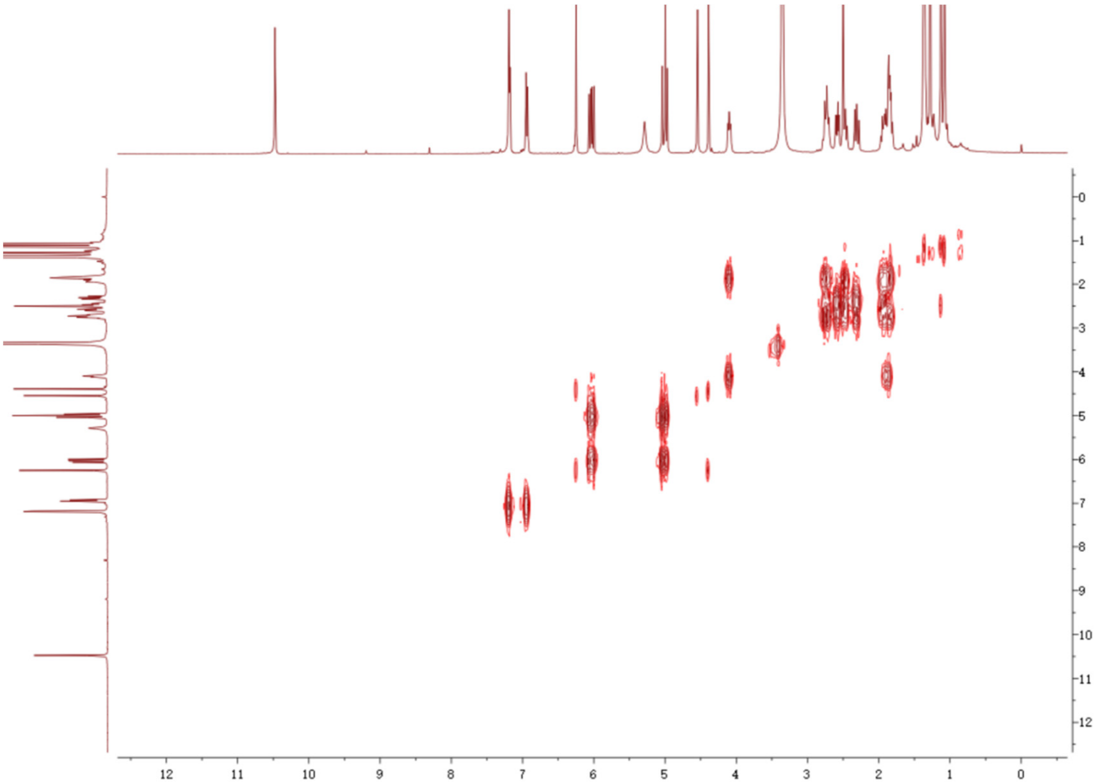

Figure S13. ^{1}H-^{1}H COSY spectrum of **2** in DMSO-*d*6

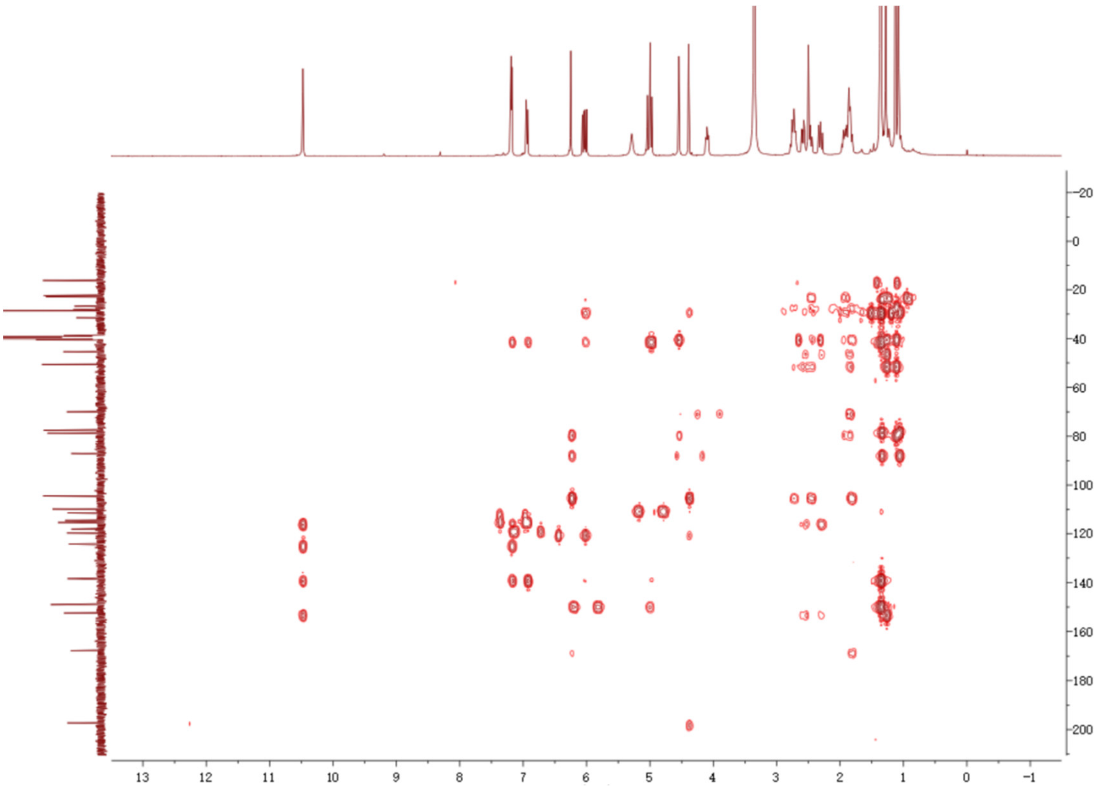

Figure S14. HMBC spectrum of **2** in DMSO-*d*6

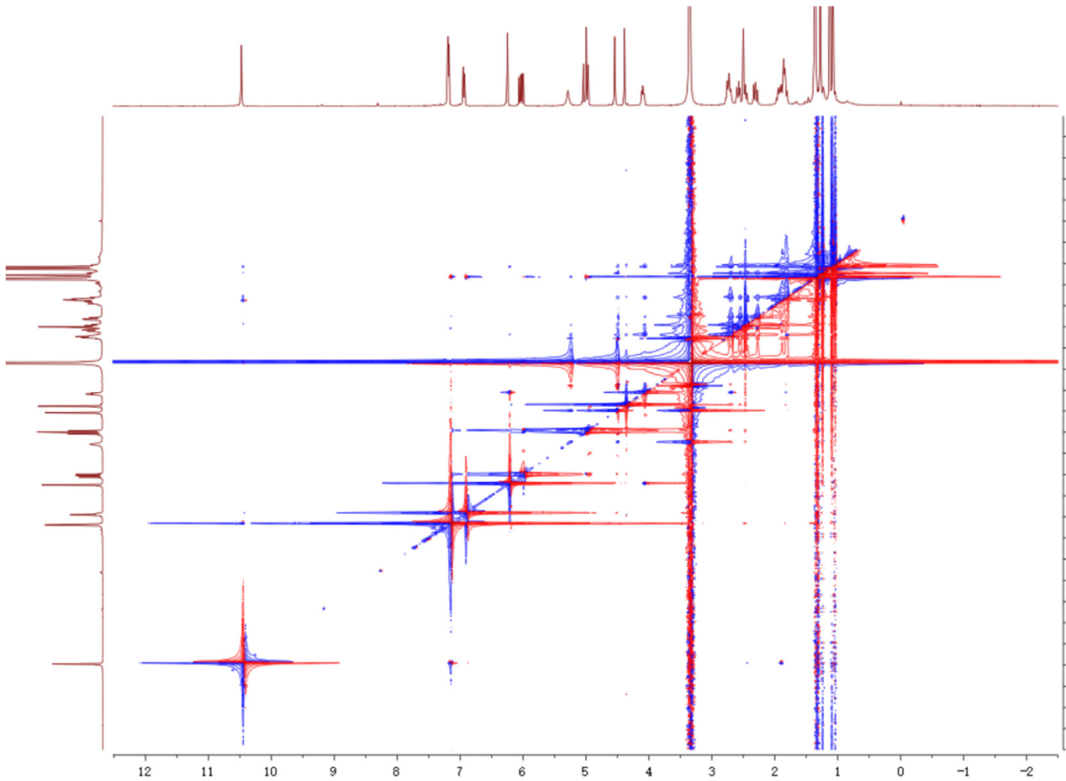

Figure S15. NOESY spectrum of **2** in DMSO-d_6

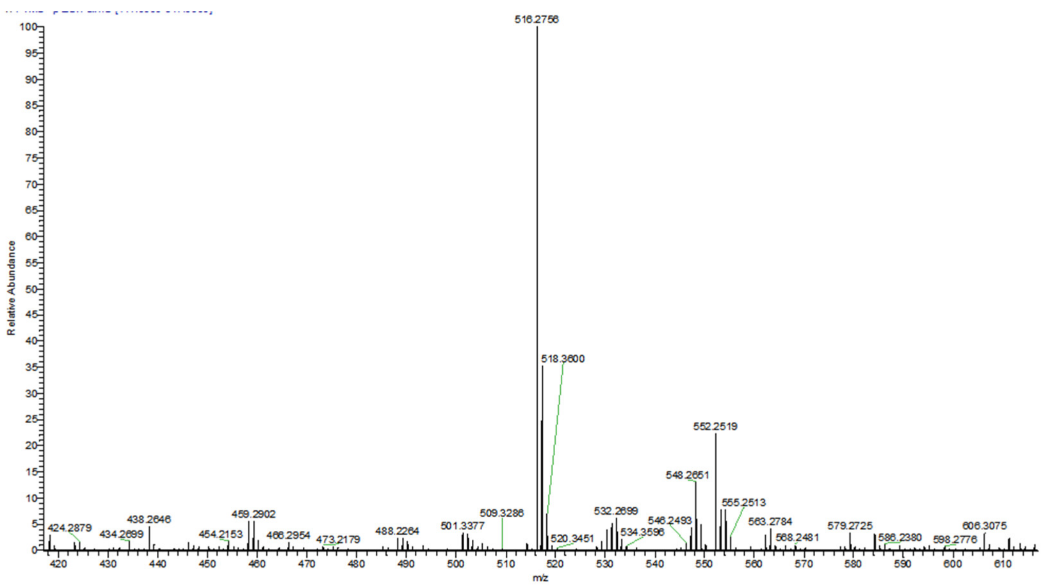

Figure S16. HRESIMS spectrum of **2**