

Supporting Information

New Fusarin Derivatives from the Marine Algicolous Fungus *Penicillium steckii* SCSIO41040

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The ITS gene sequence data of *Penicillium* sp. SCSIO 41040

GATATGCTTAAGTTCAGCGGGTATCCCTACCTGATCCGAGGTCAACCTGAGAAAAAATA
AAAGGTTGGGGGTTCGGCTGGCGCCGGCCGGGCCTACAAGAGCGGGTGACGAAGCCCC
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ACTTCAGACAGCGTTCAGAGGGGGGCTTCGGCGGGCGCGGGCCCCGGGGGCGGATGCC
CCCCGGCGGCCTGGCGGCGGGCCCCGCCGAAGCAACACAGGTTCGTGCAACACGGGTG
GGAGGTTGGACCCAGAGGGCCCTCACTCGGTAATGATCCTTCCGCAG

The NMR spectra were uploaded to the Harvard Dataverse (<https://doi.org/10.7910/DVN/PXCKSJ>).

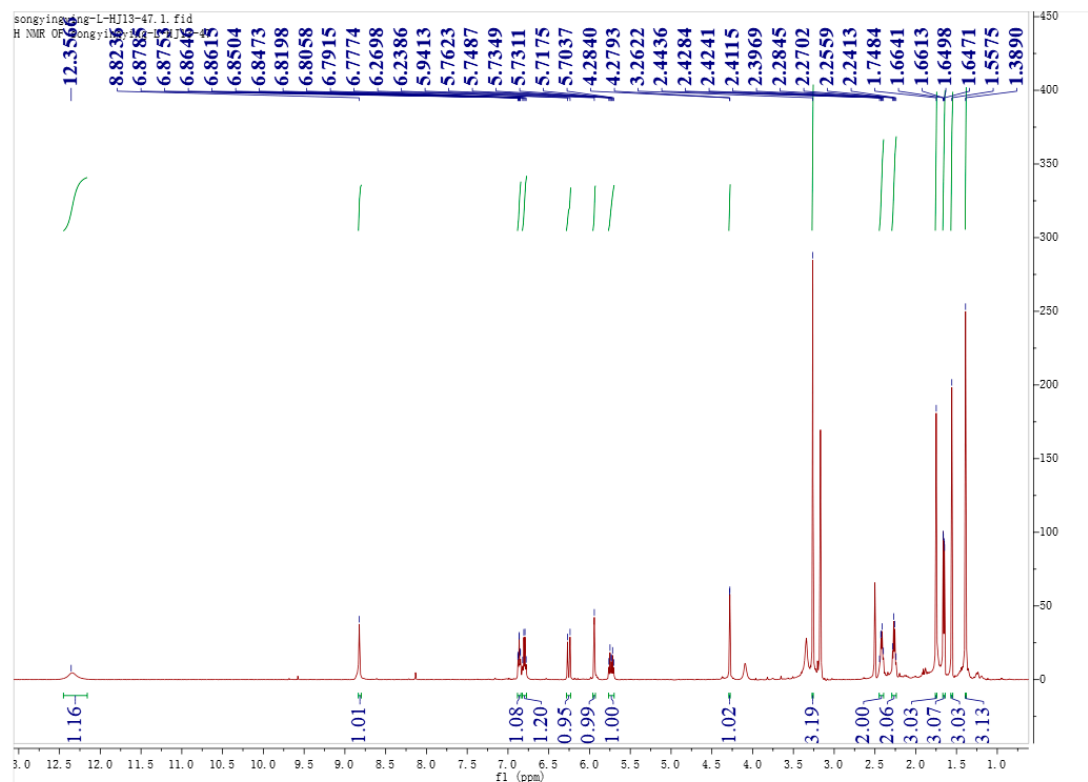


Figure S1 ^1H NMR spectrum of compound **1** in $\text{DMSO}-d_6$

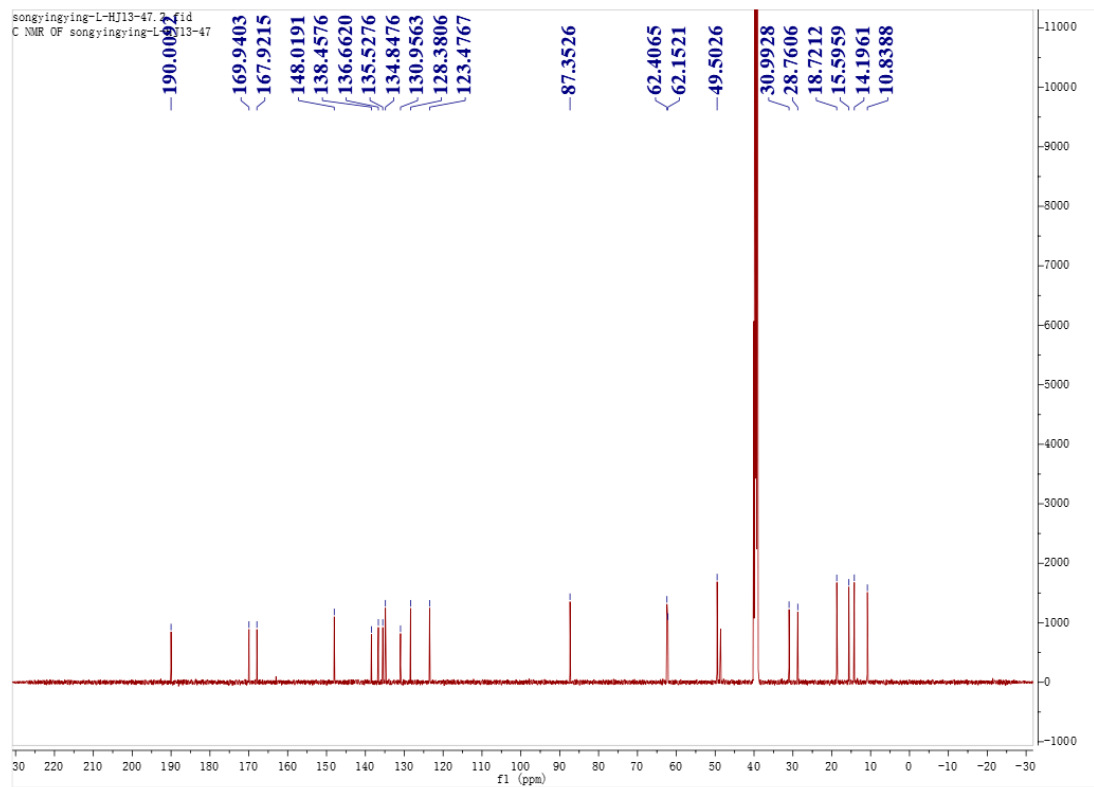


Figure S2 ^{13}C NMR spectrum of compound **1** in $\text{DMSO}-d_6$

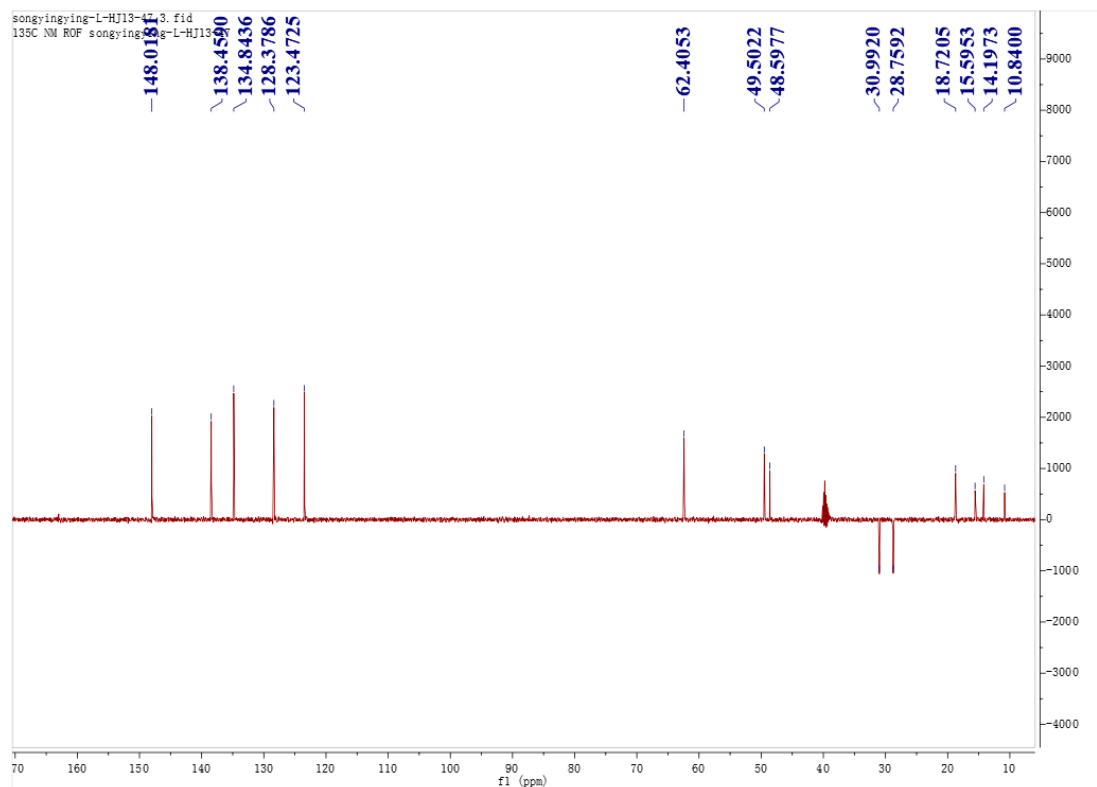


Figure S3 DEPT135 spectrum of compound **1** in DMSO- d_6

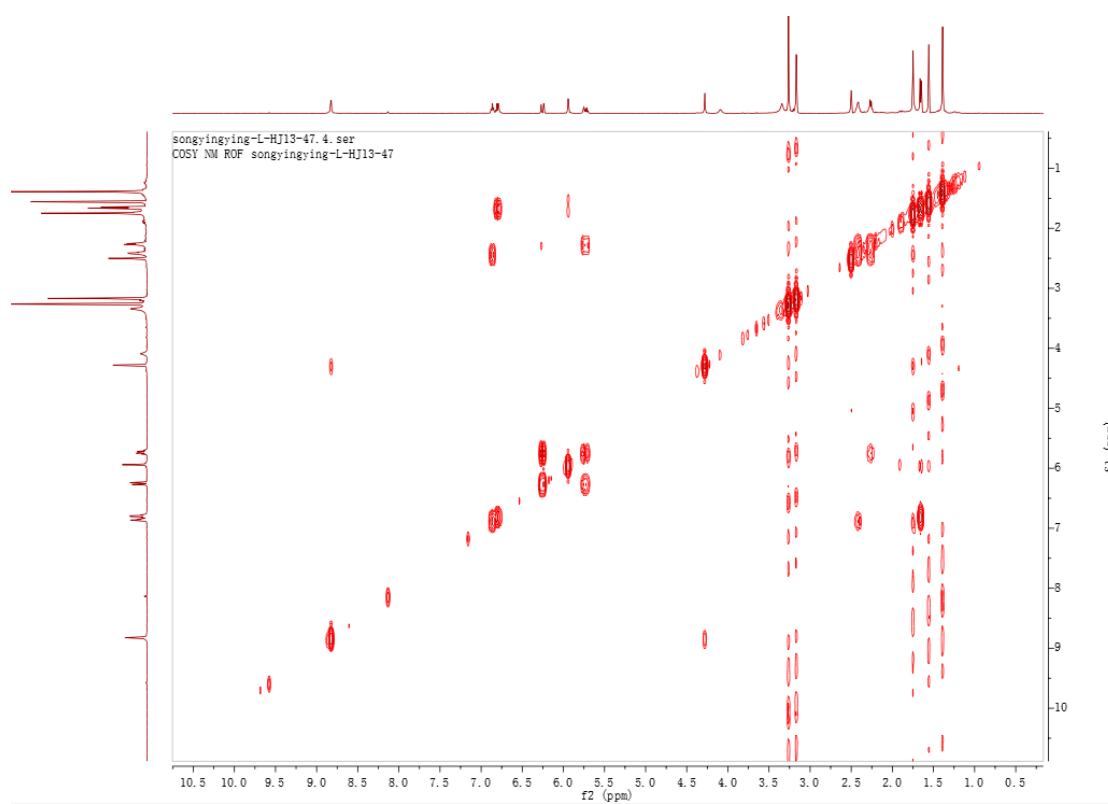


Figure S4 ^1H - ^1H COSY spectrum of compound **1** in DMSO- d_6

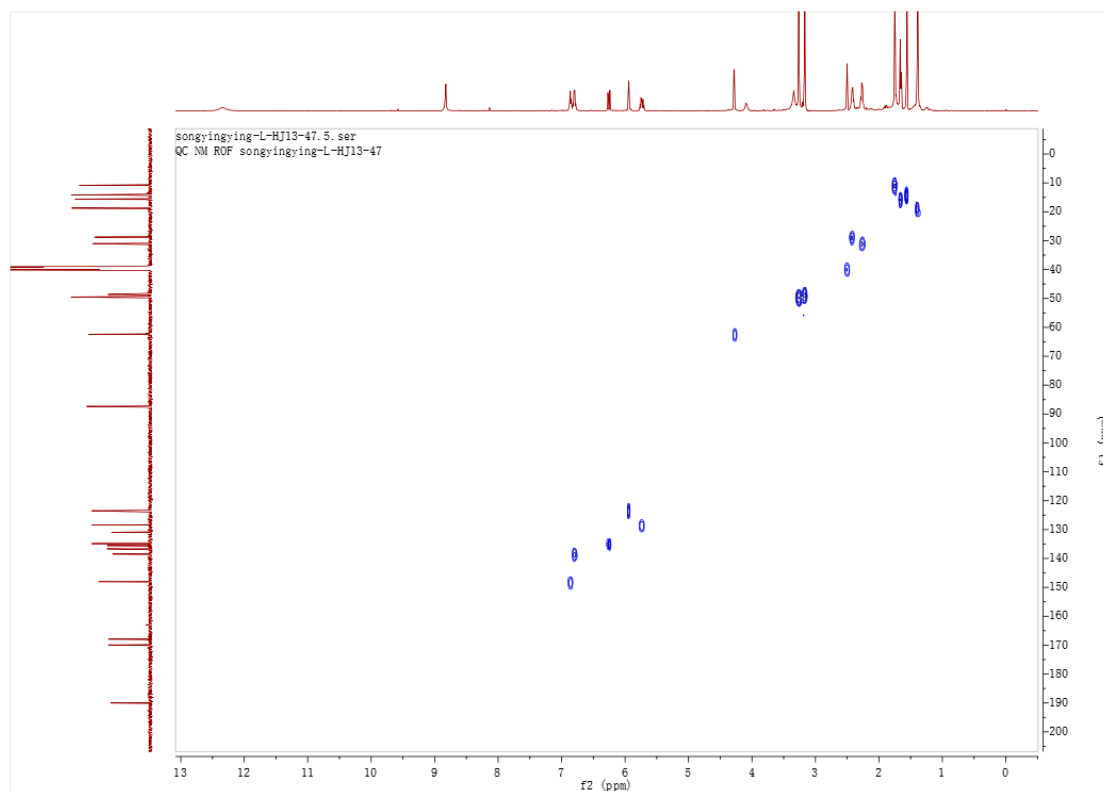


Figure S5 HSQC spectrum of compound **1** in DMSO- d_6

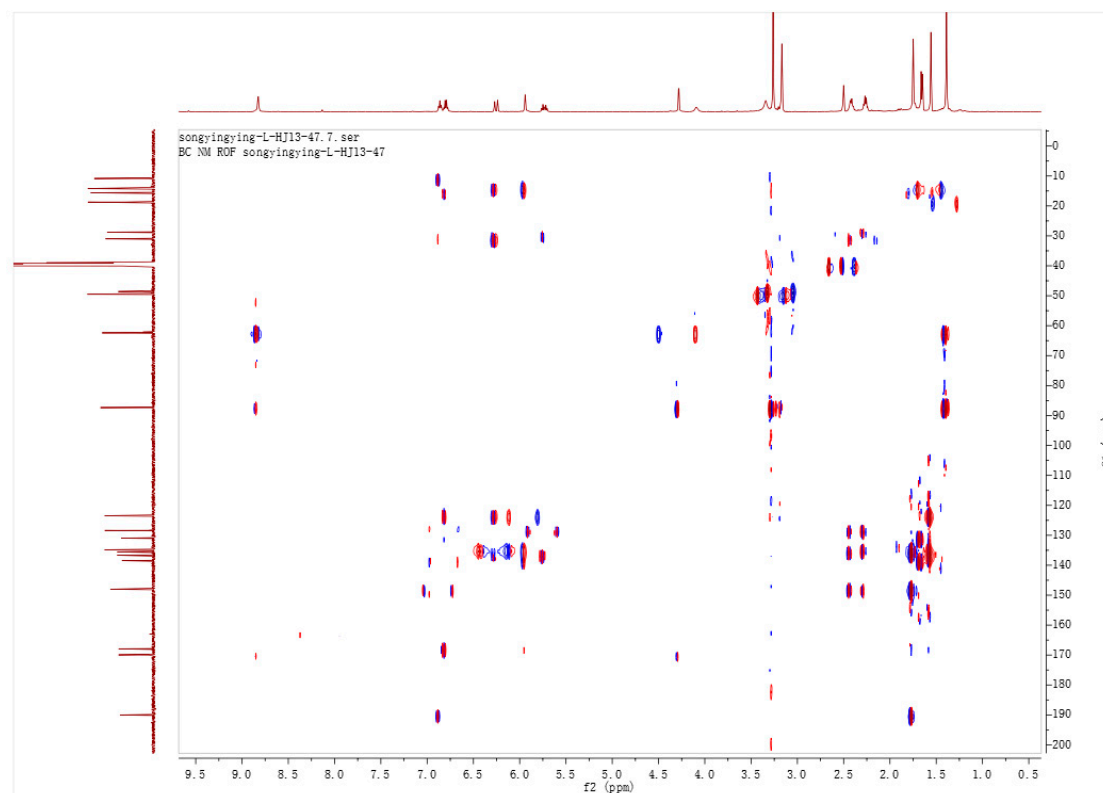


Figure S6 HMBC spectrum of compound **1** in DMSO- d_6

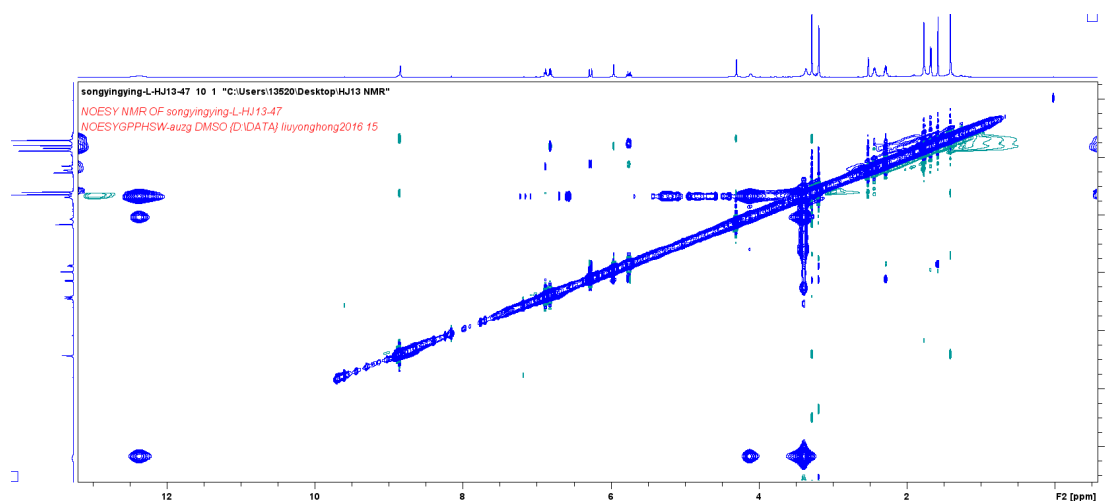


Figure S7 NOESY spectrum of compound **1** in DMSO- d_6

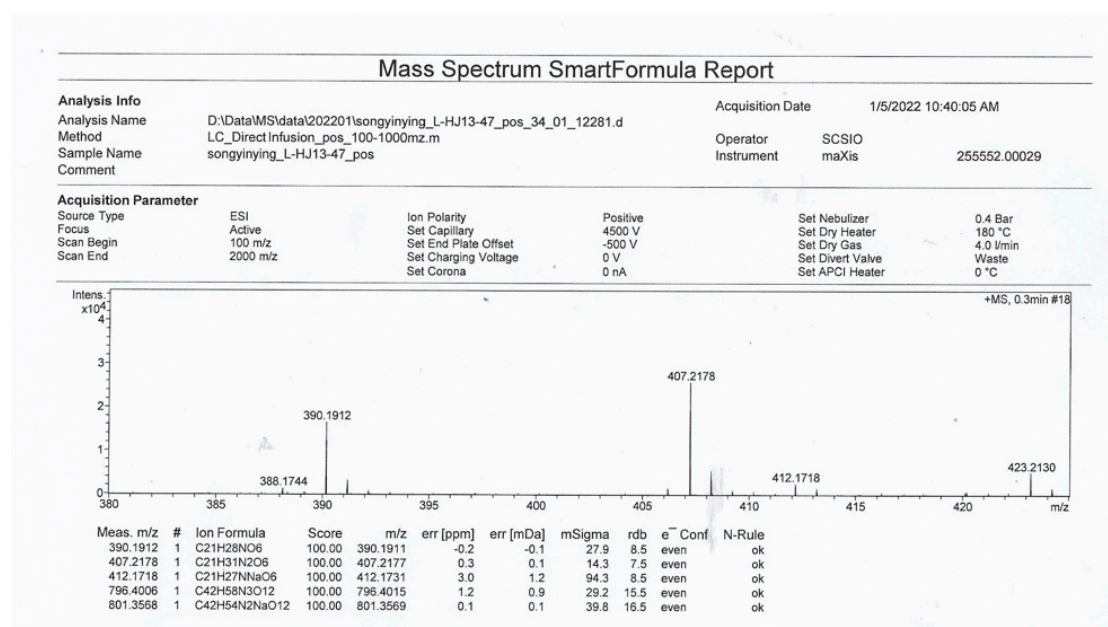


Figure S8 HRESIMS spectrum of compound **1**

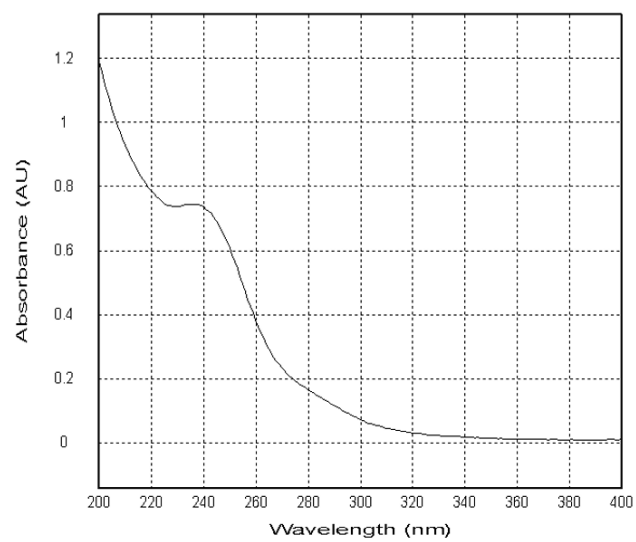


Figure S9 UV spectrum of **1**

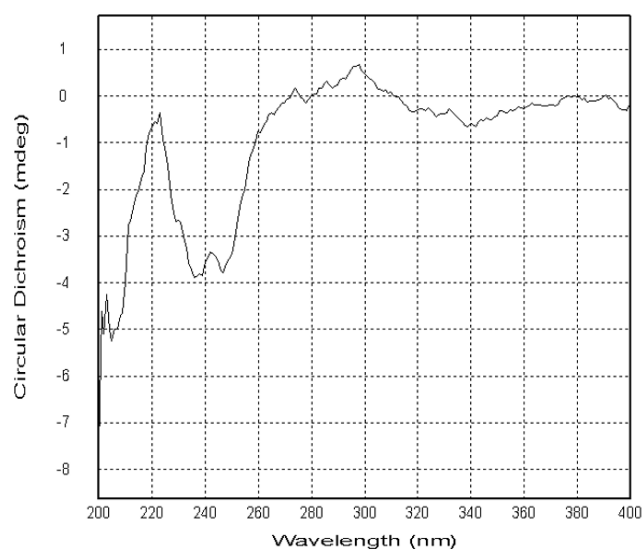


Figure S10 CD spectrum of **1**

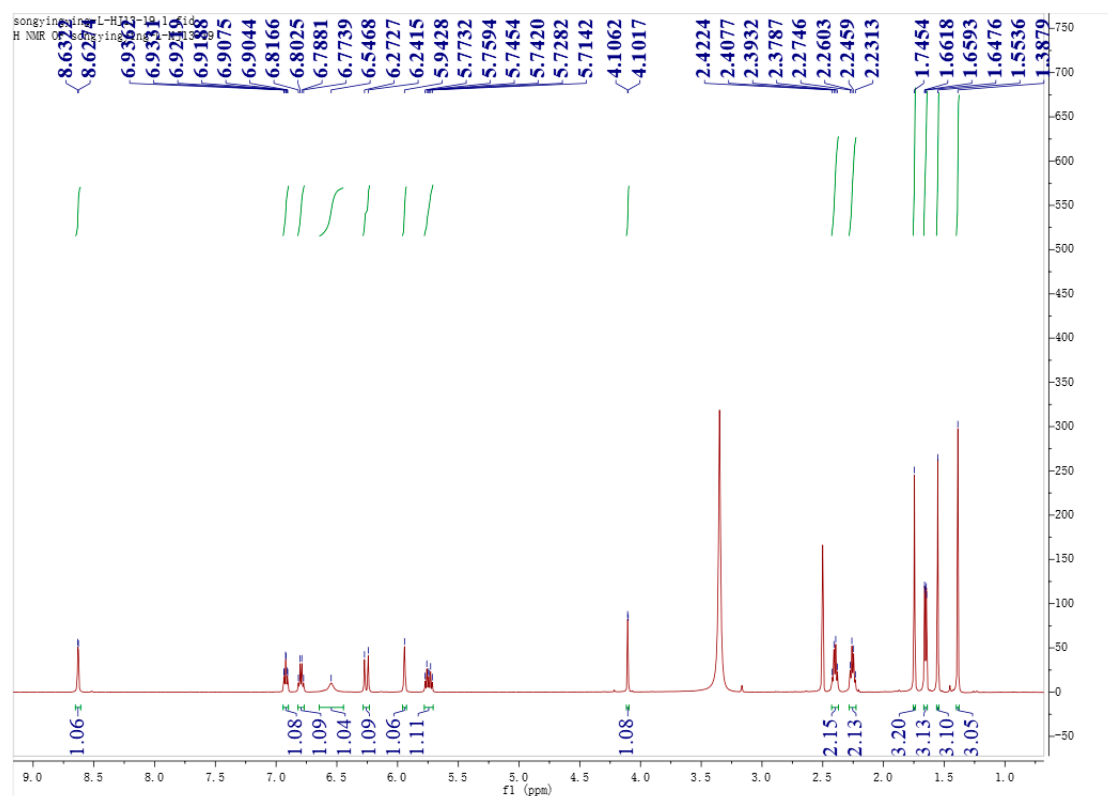


Figure S11 ^1H NMR spectrum of compound **2** in $\text{DMSO-}d_6$

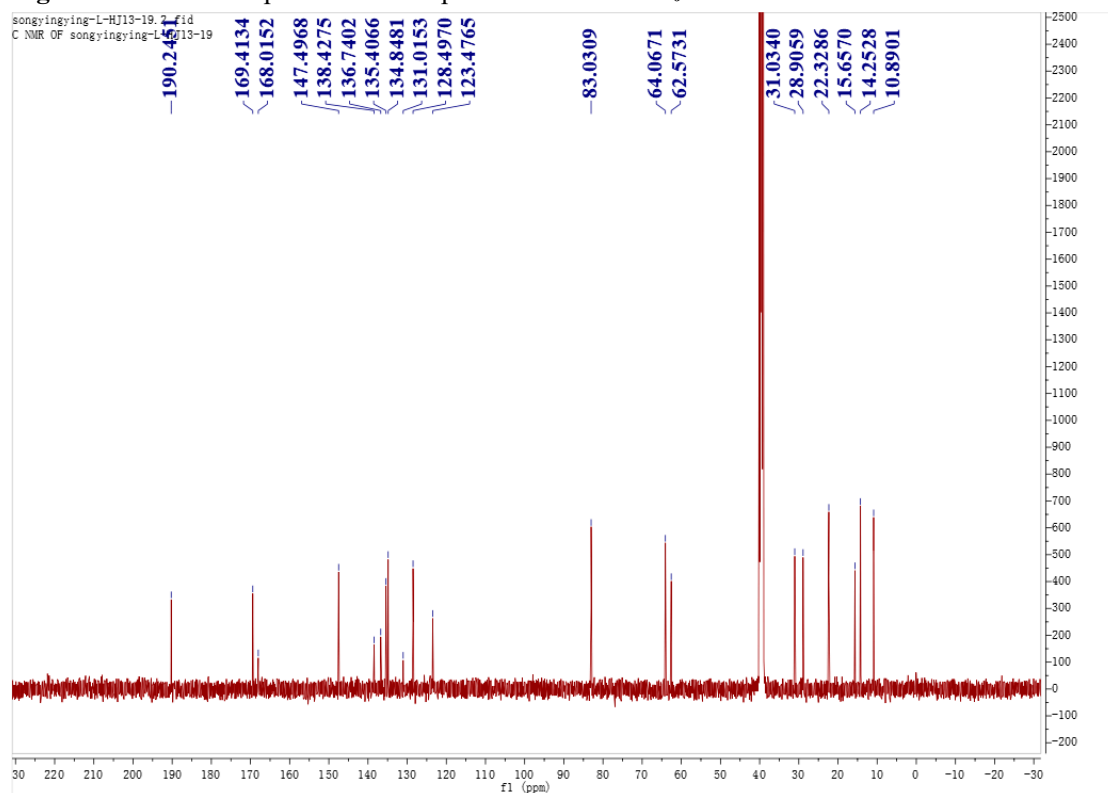


Figure S12 ^{13}C NMR spectrum of compound **2** in $\text{DMSO-}d_6$

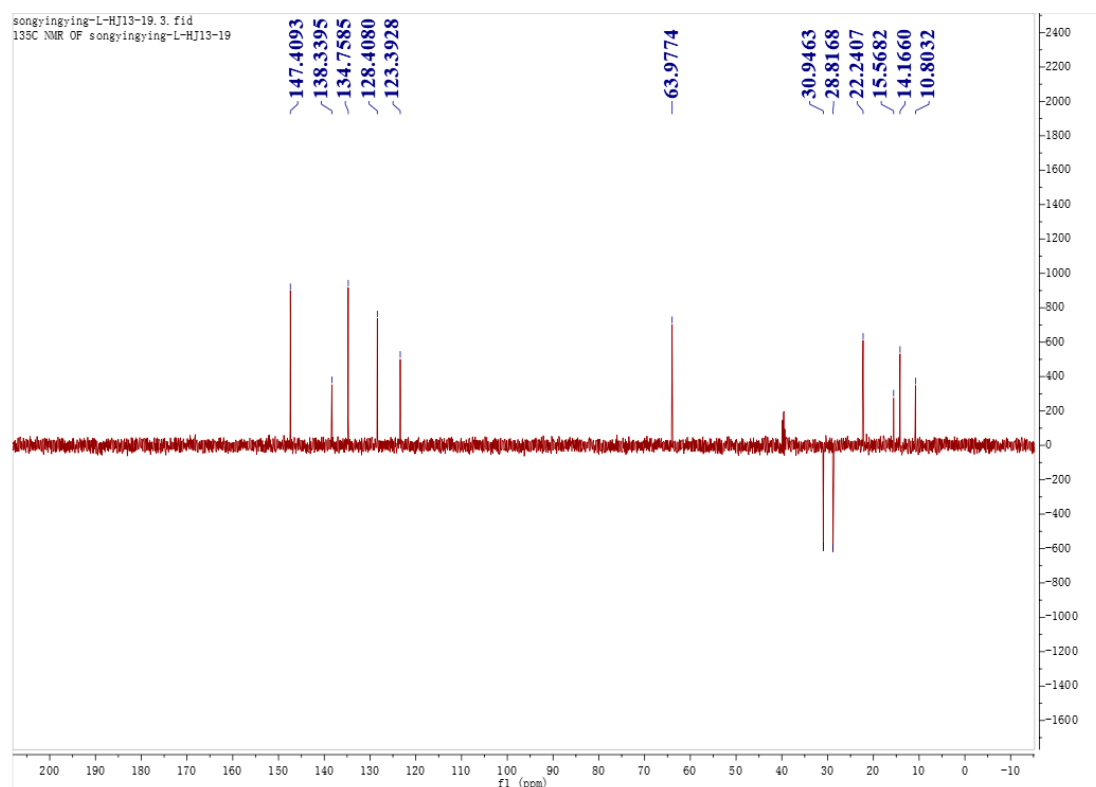


Figure S13 DEPT135 spectrum of compound **2** in DMSO- d_6

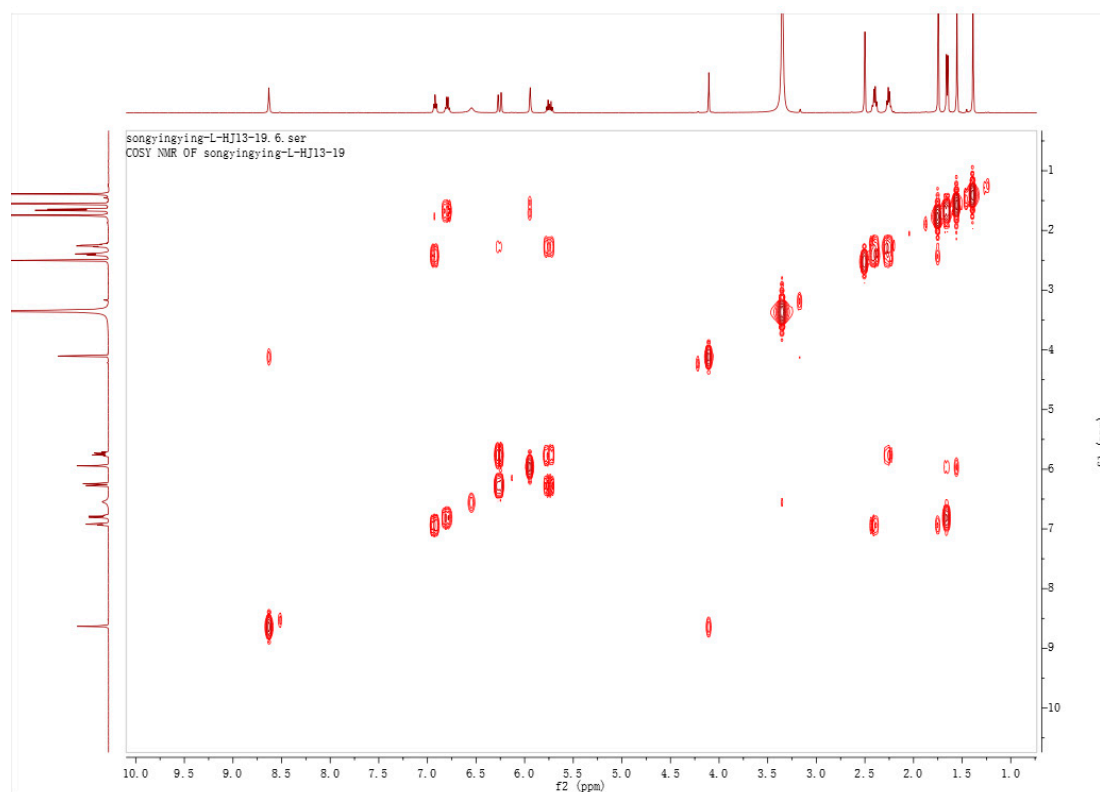


Figure S14 ^1H - ^1H COSY spectrum of compound **2** in DMSO- d_6

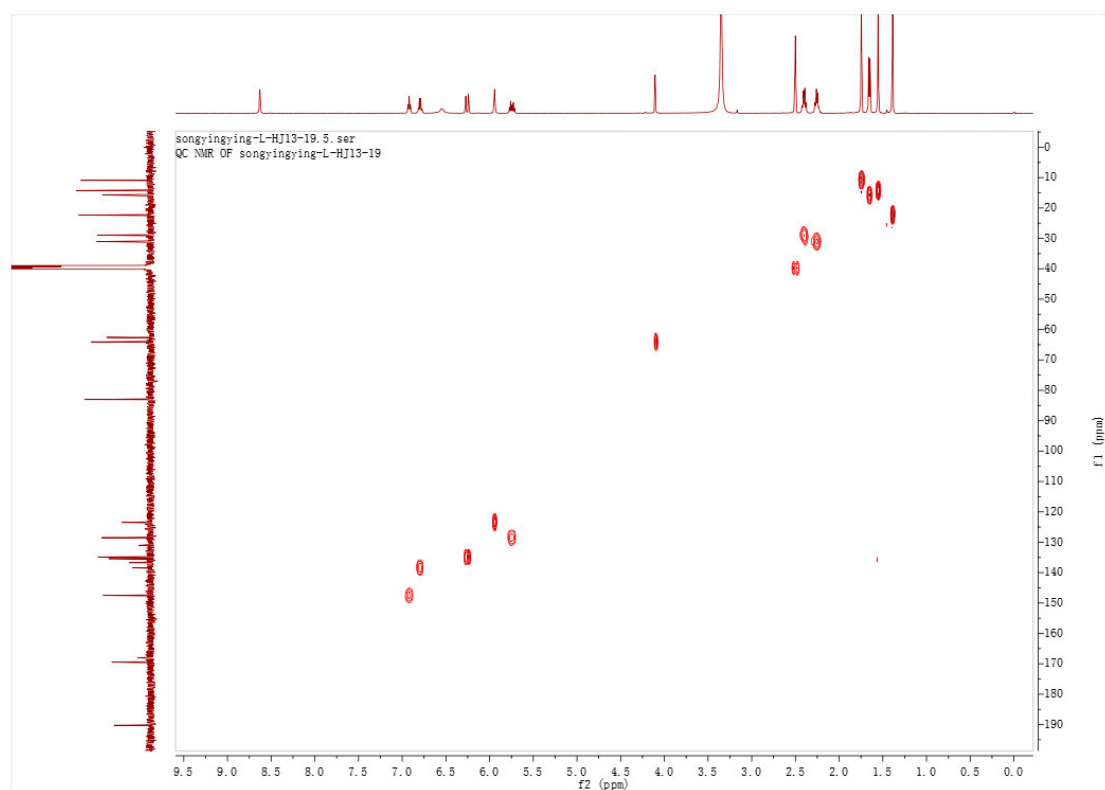


Figure S15 HSQC spectrum of compound **2** in DMSO- d_6

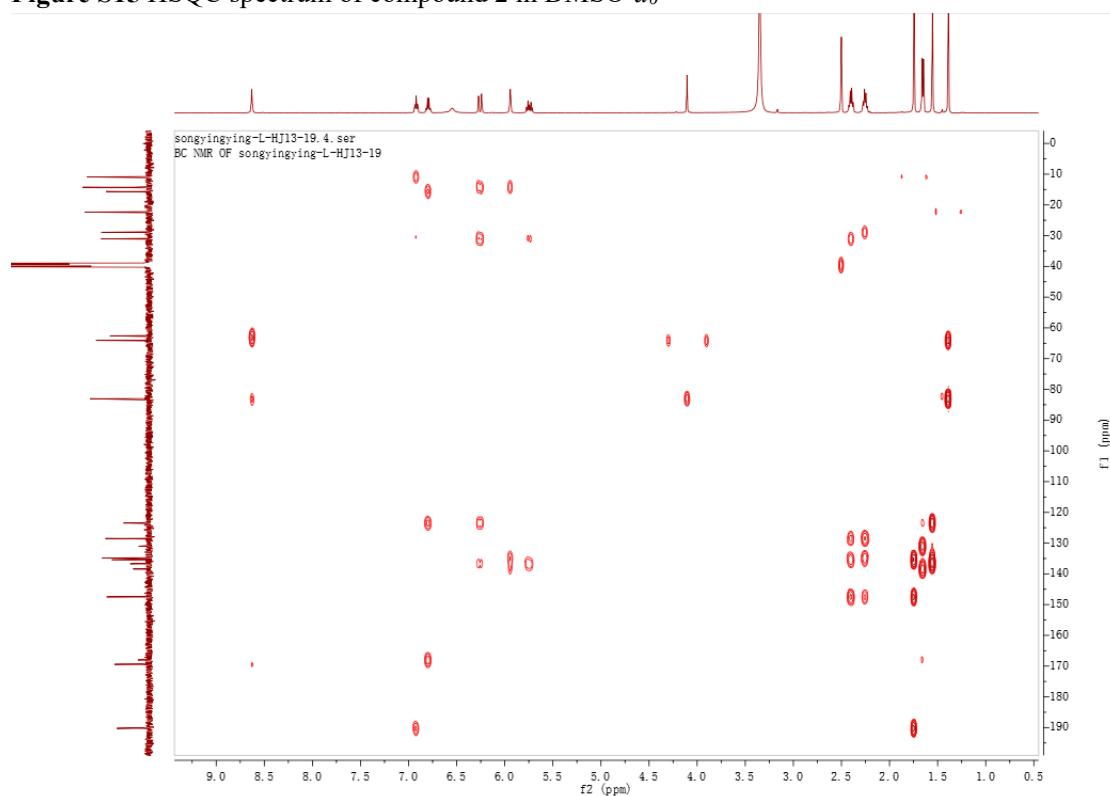


Figure S16 HMBC spectrum of compound **2** in DMSO- d_6

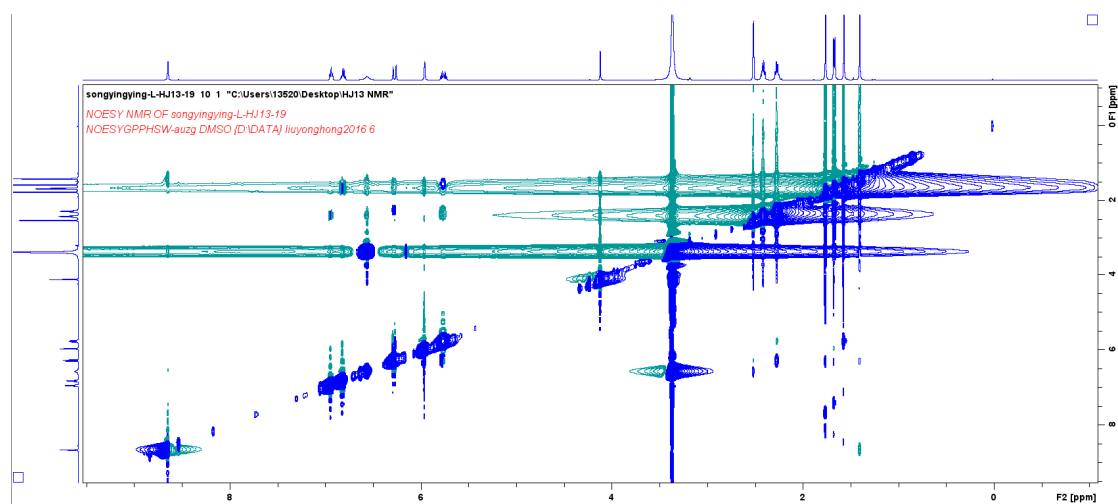


Figure S17 NOESY spectrum of compound **2** in DMSO-*d*₆

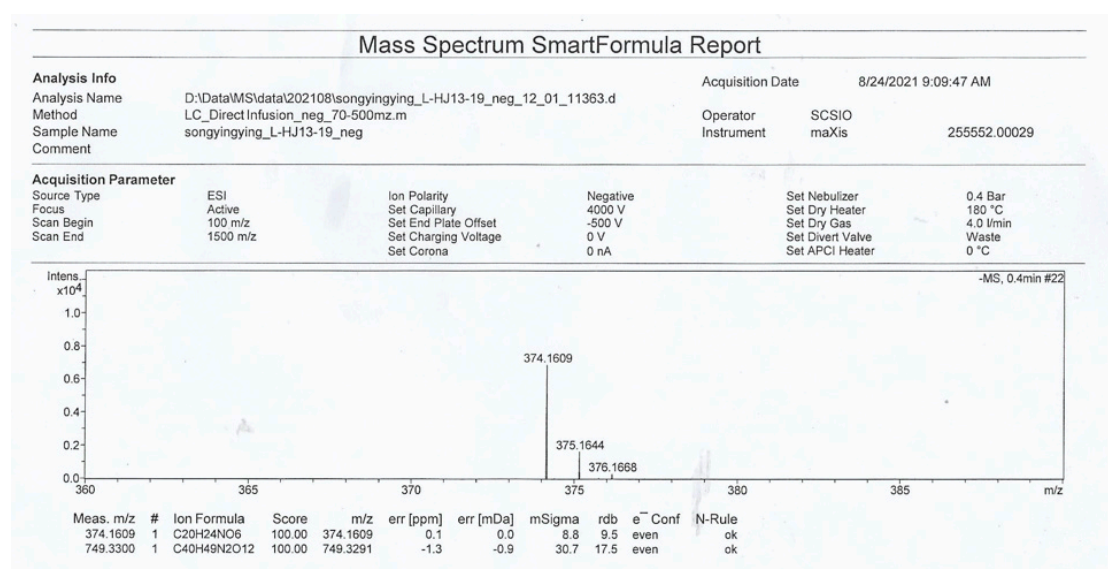


Figure S18 HRESIMS spectrum of compound **2**

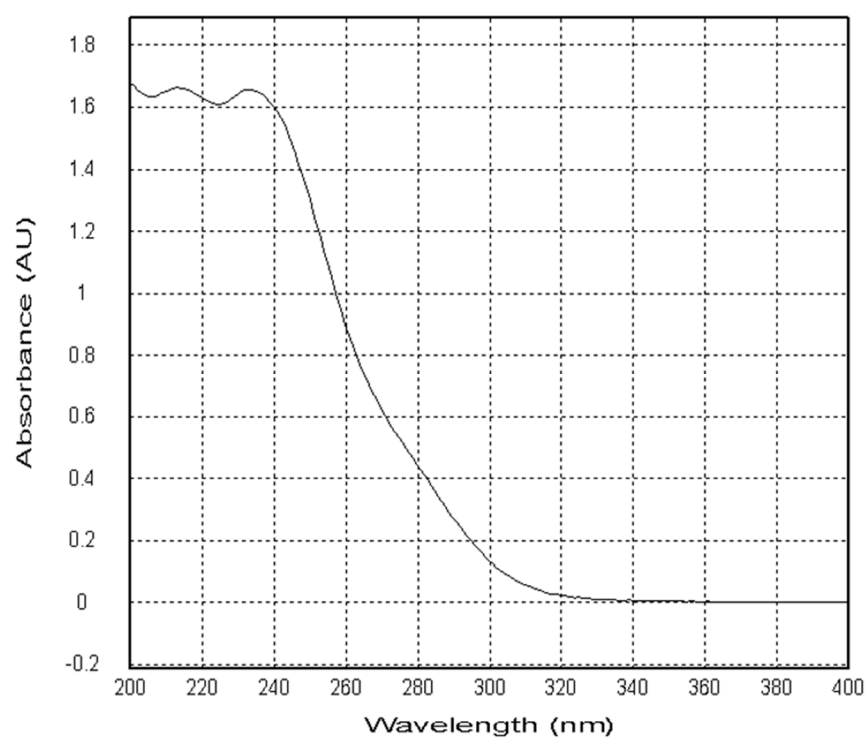


Figure S19 UV spectrum of **2**

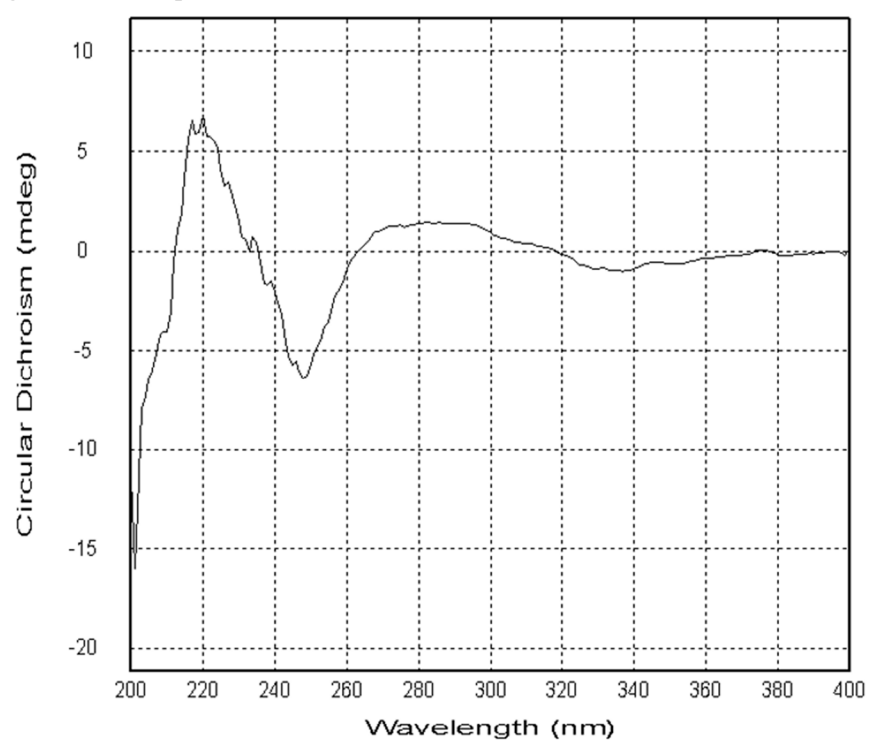


Figure S20 CD spectrum of **2**

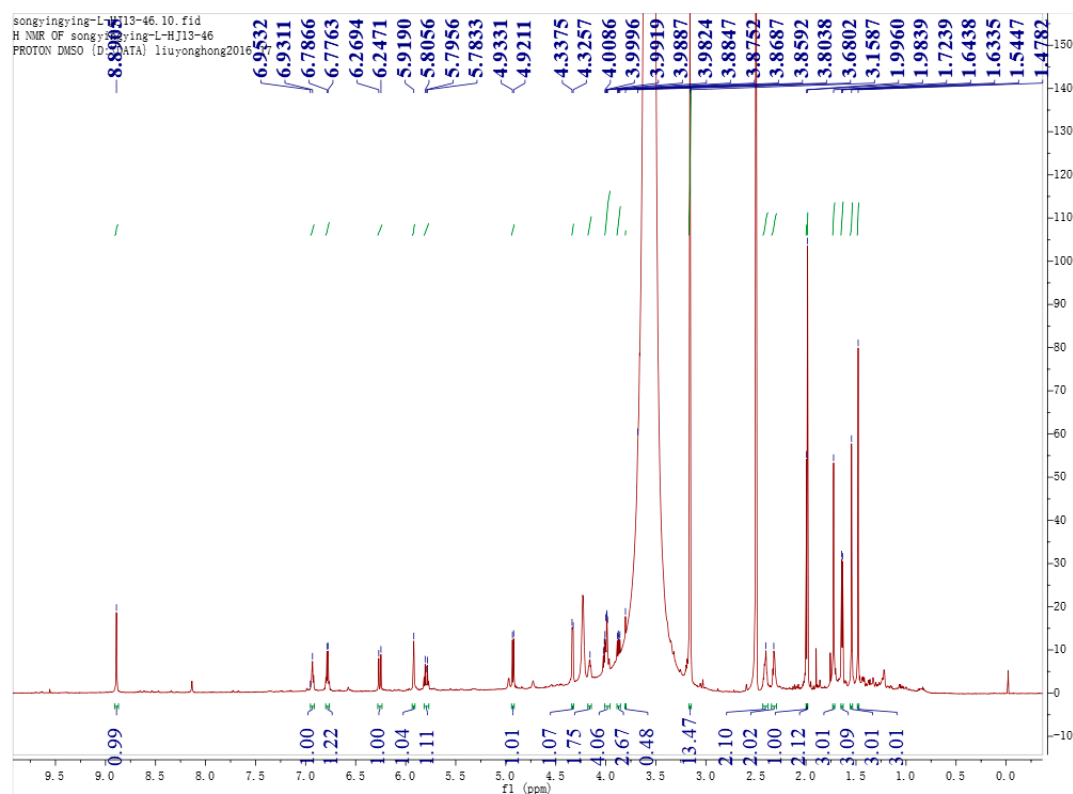


Figure S21 ^1H NMR spectrum of compound **3** in $\text{DMSO-}d_6$

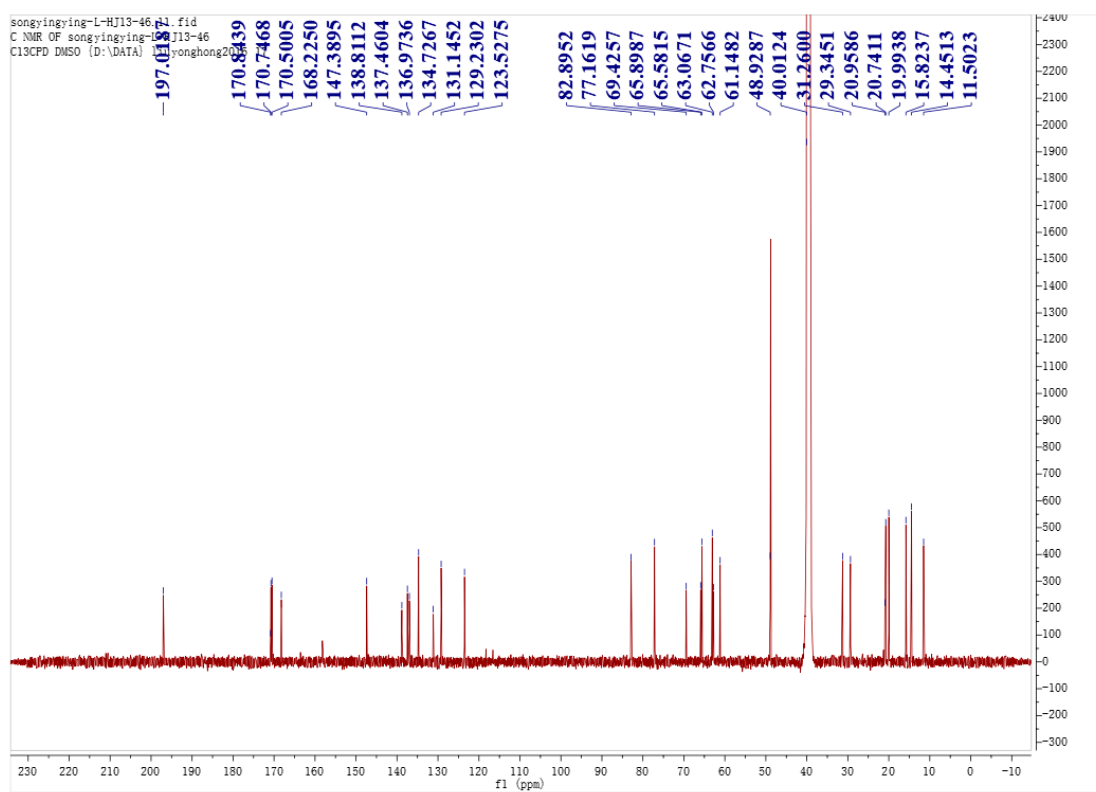


Figure S22 ^{13}C NMR spectrum of compound **3** in $\text{DMSO-}d_6$

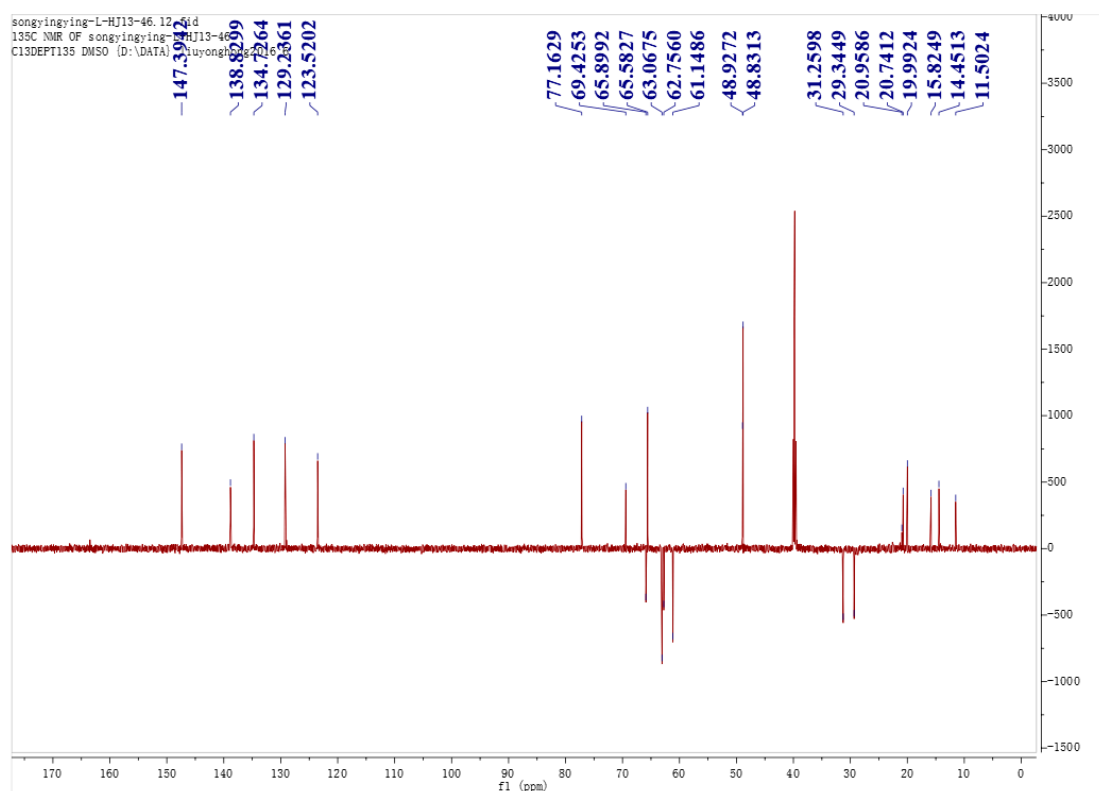


Figure S23 DEPT135 spectrum of compound **3** in DMSO- d_6

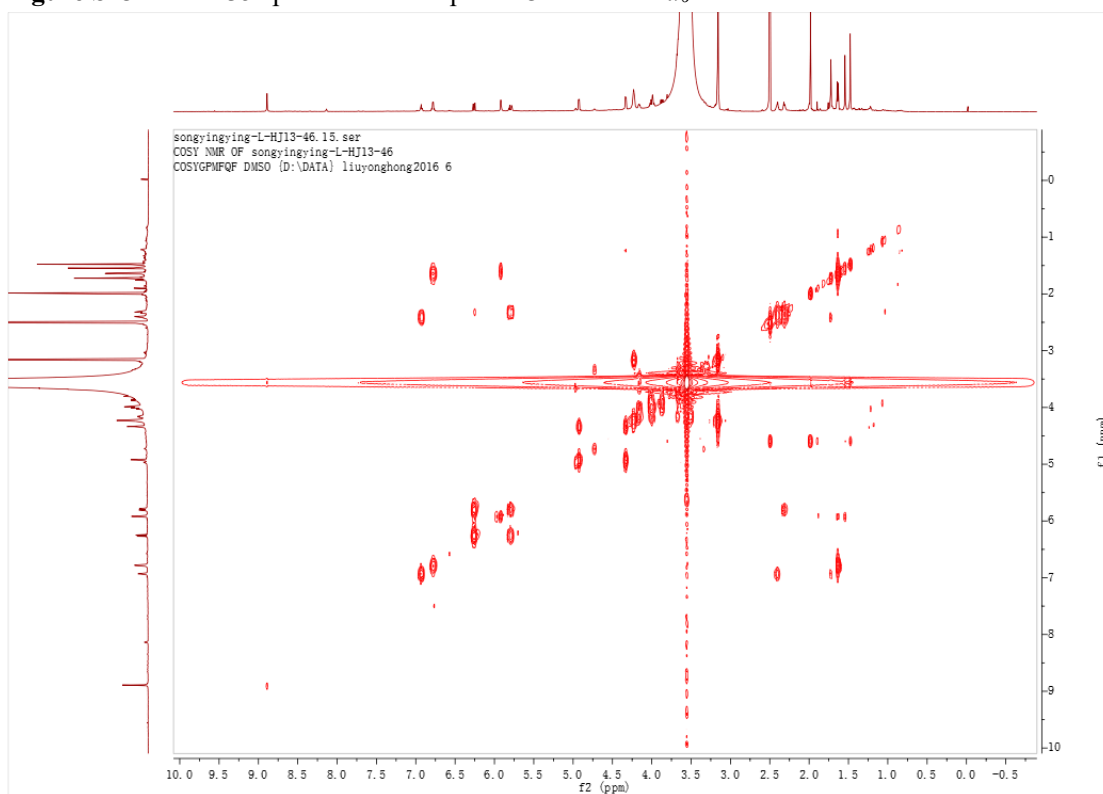


Figure S24 ^1H - ^1H COSY spectrum of compound **3** in DMSO- d_6

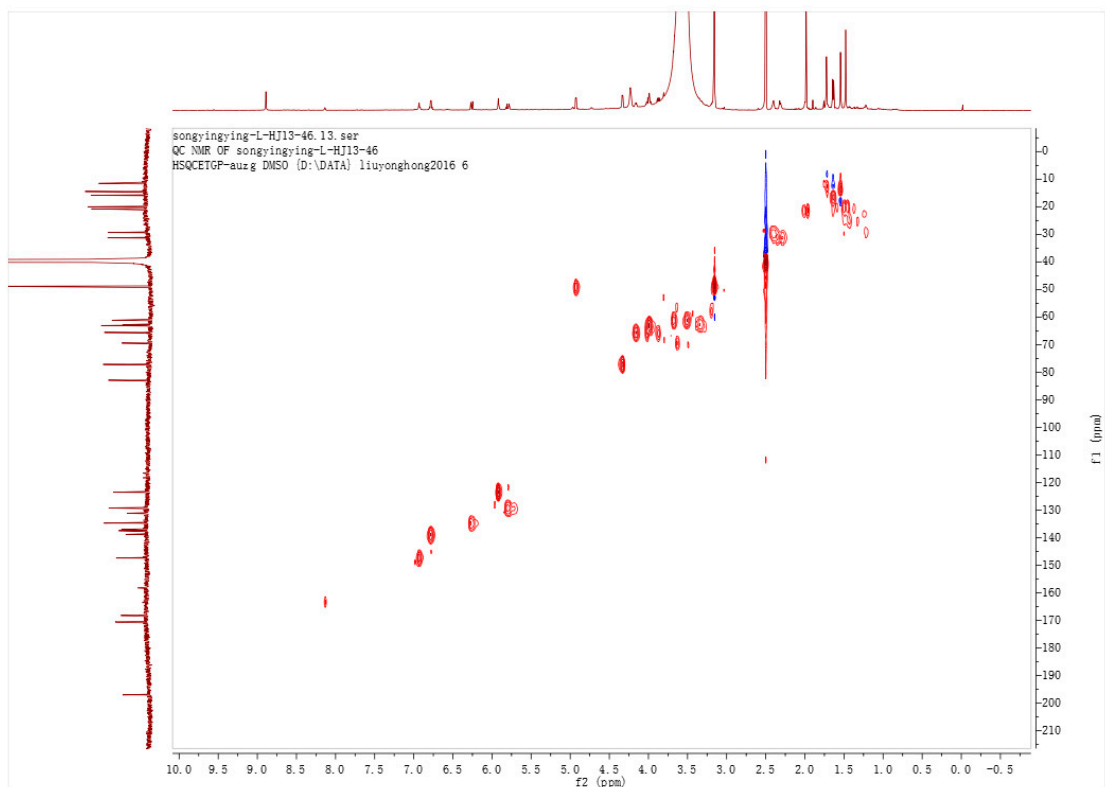


Figure S25 HSQC spectrum of compound **3** in DMSO-*d*₆

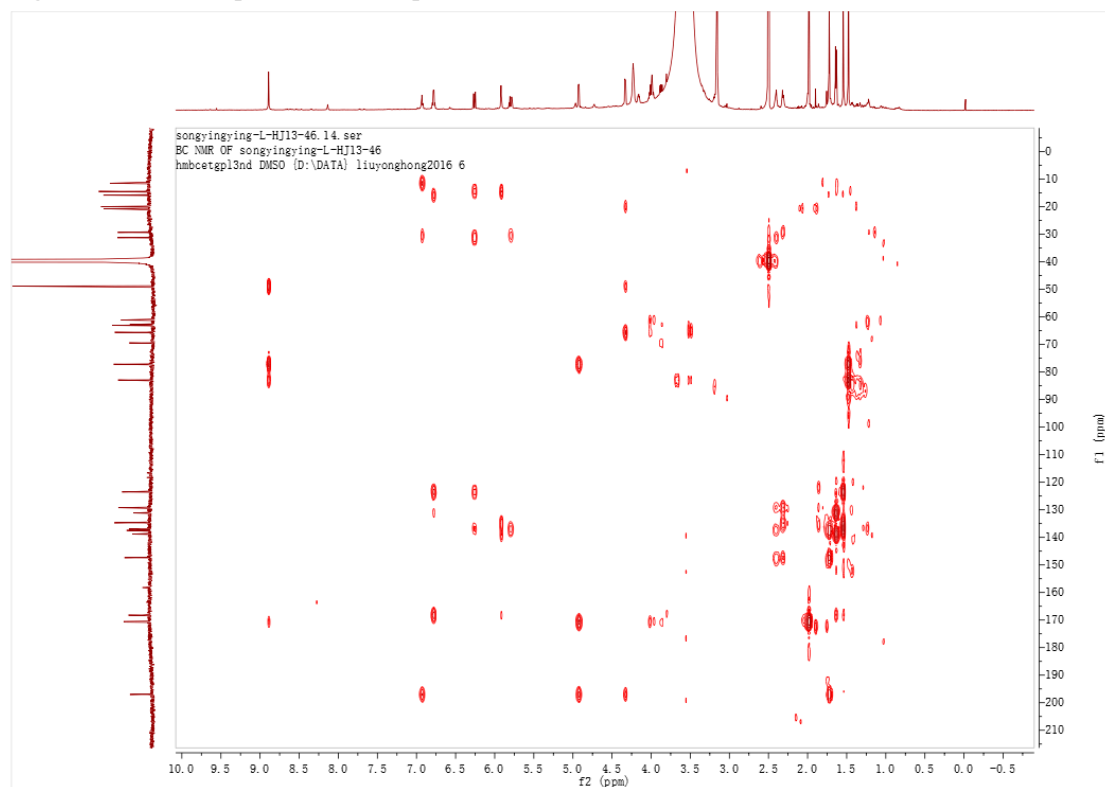


Figure S26 HMBC spectrum of compound **3** in DMSO-*d*₆

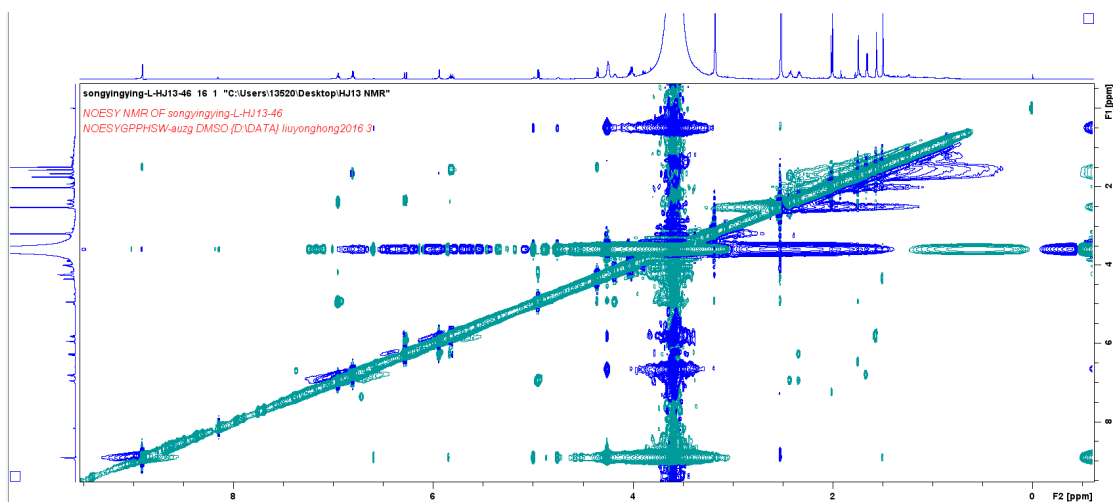


Figure S27 NOESY spectrum of compound **3** in DMSO- d_6

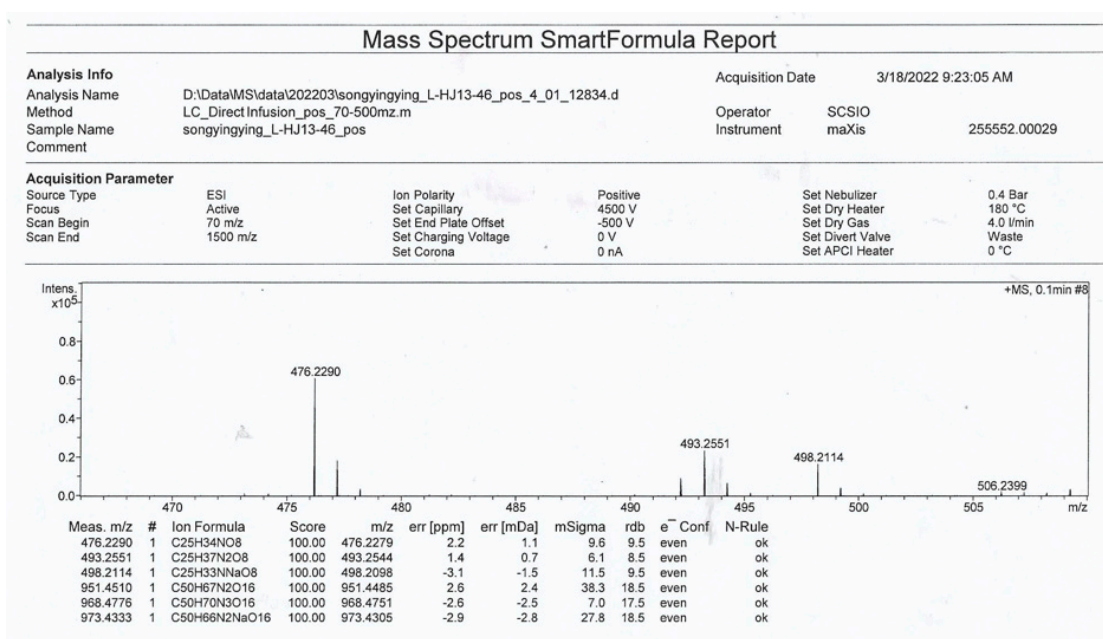


Figure S28 HRESIMS spectrum of compound **3**

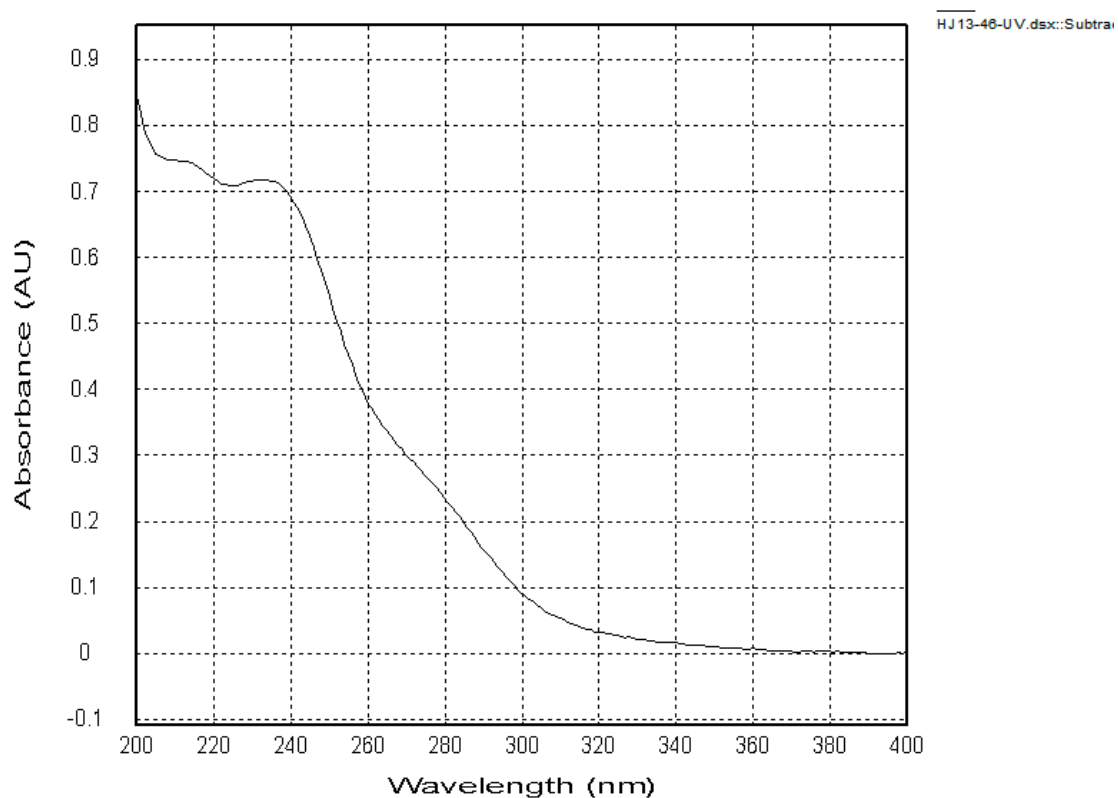


Figure S29 UV spectrum of **3**

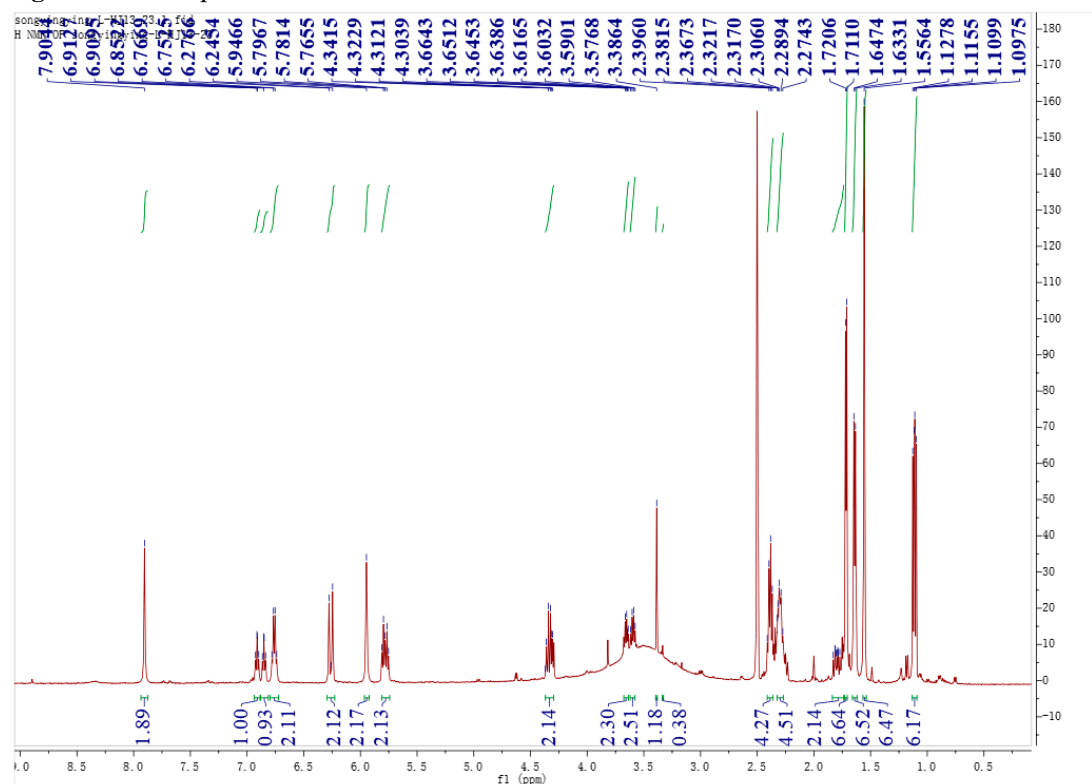


Figure S30 ^1H NMR spectrum of compound **4** in $\text{DMSO}-d_6$

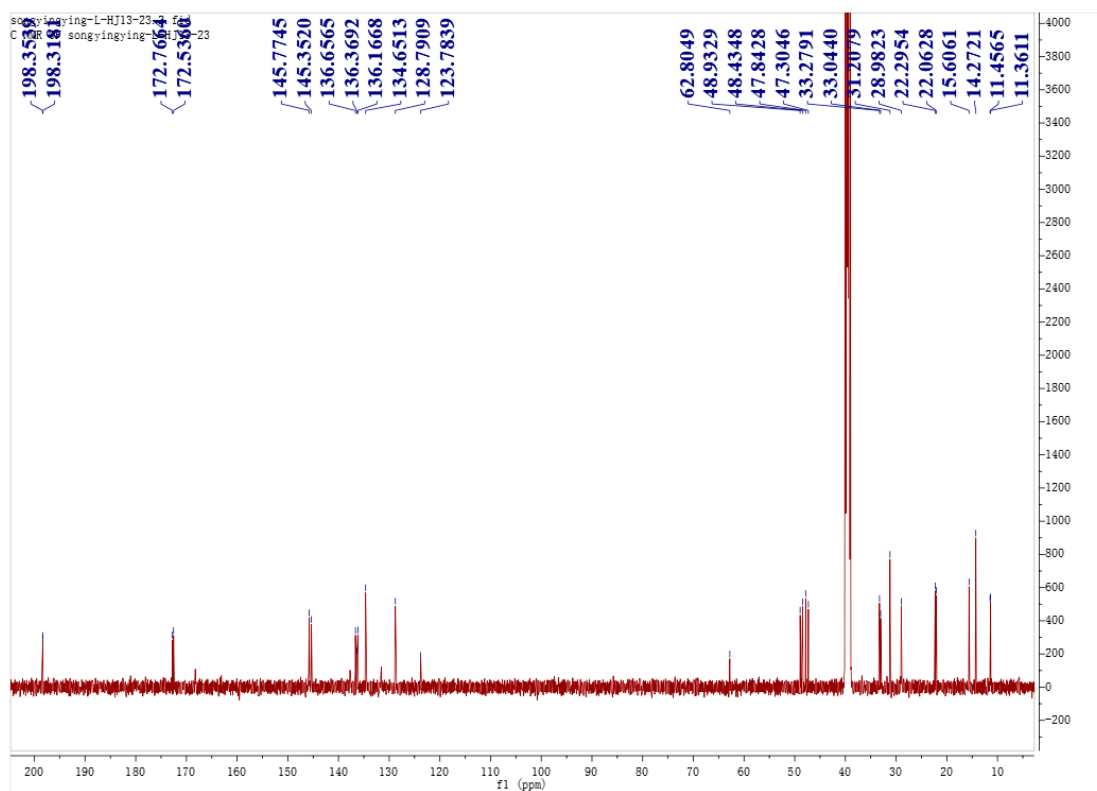


Figure S31 ^{13}C NMR spectrum of compound **4** in $\text{DMSO}-d_6$

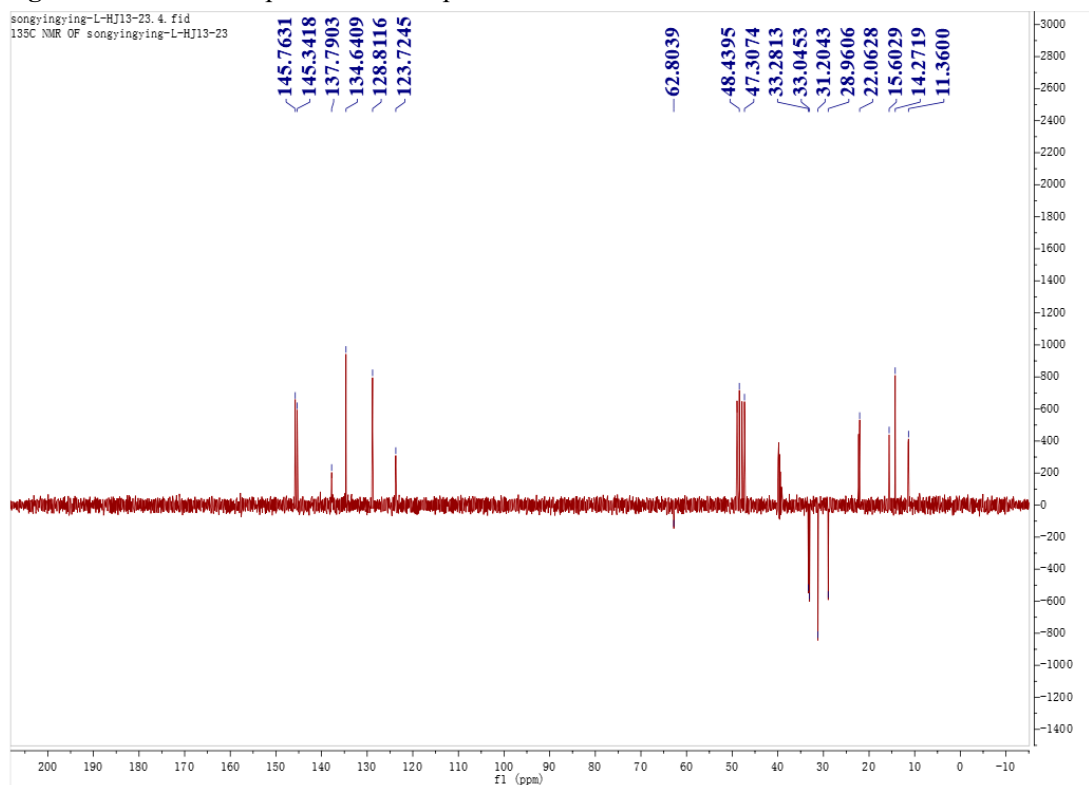


Figure S32 DEPT135 spectrum of compound **4** in $\text{DMSO}-d_6$

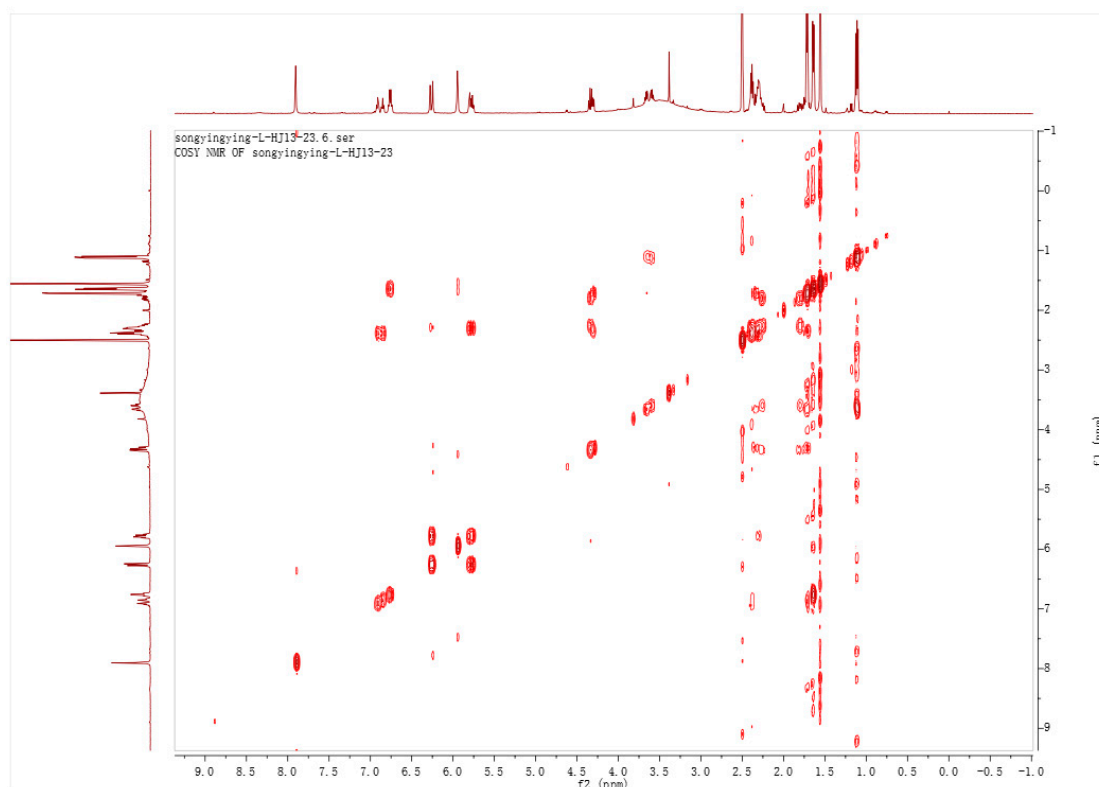


Figure S33 ^1H - ^1H COSY spectrum of compound **4** in $\text{DMSO-}d_6$

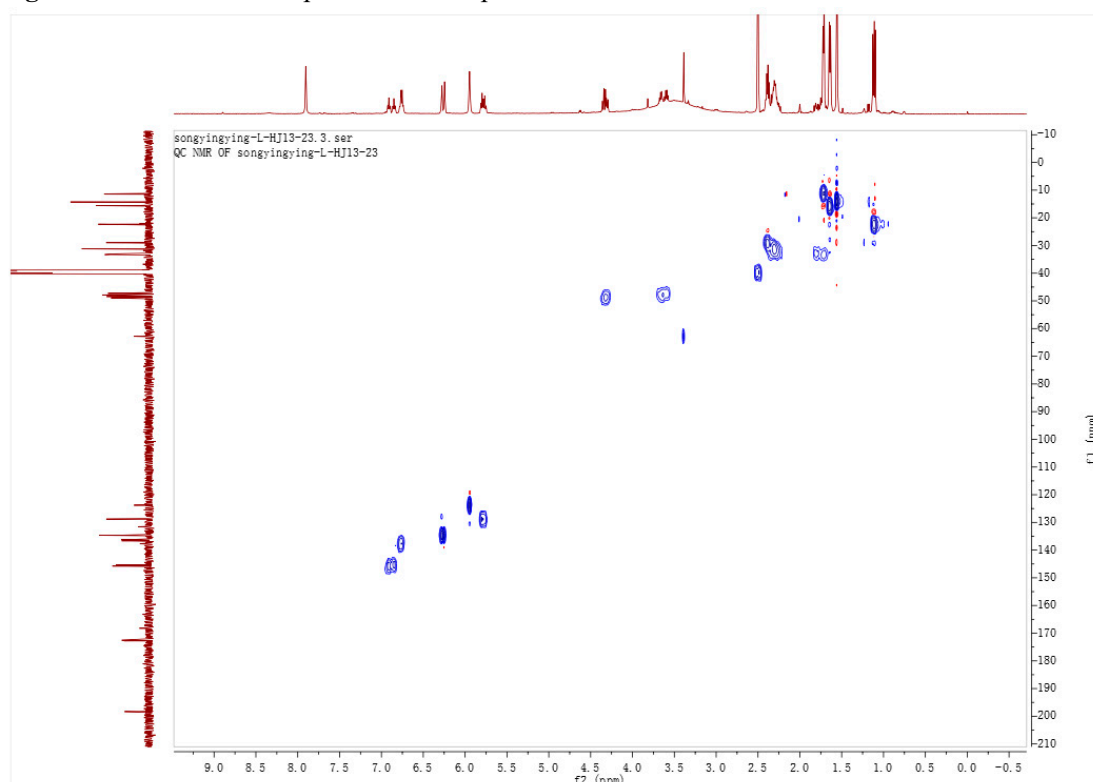


Figure S34 HSQC spectrum of compound **4** in $\text{DMSO-}d_6$

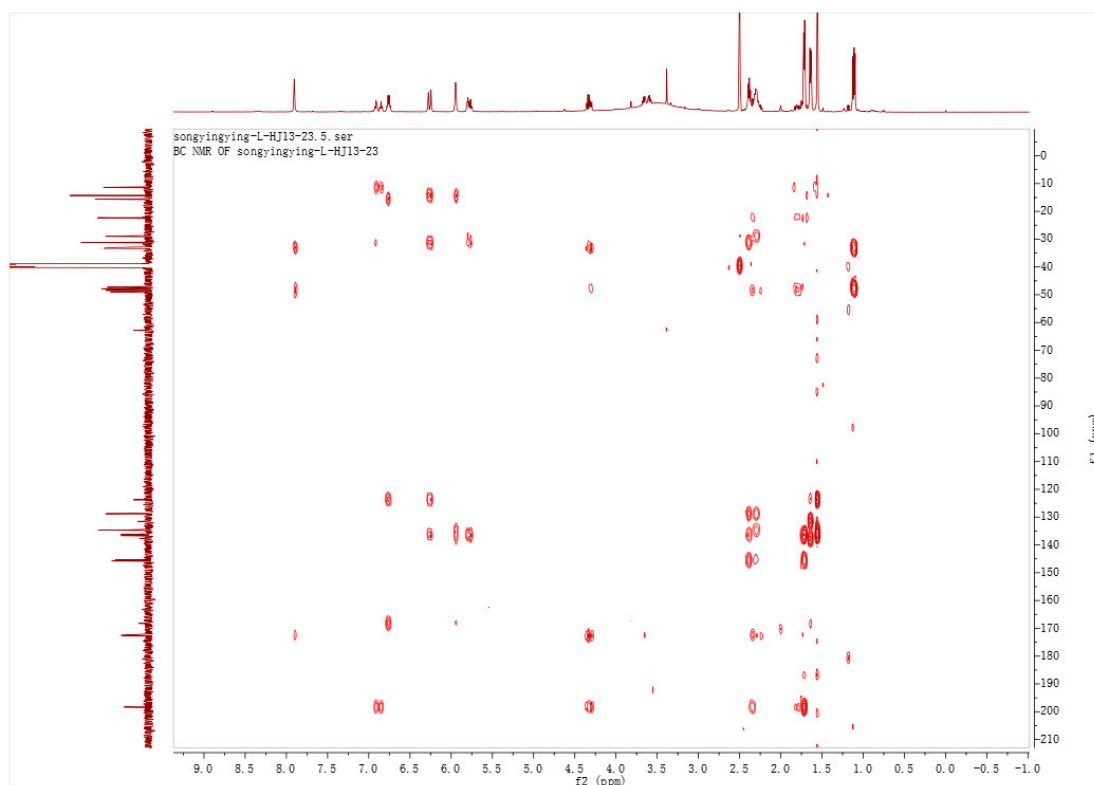


Figure S35 HMBC spectrum of compound **4** in DMSO- d_6

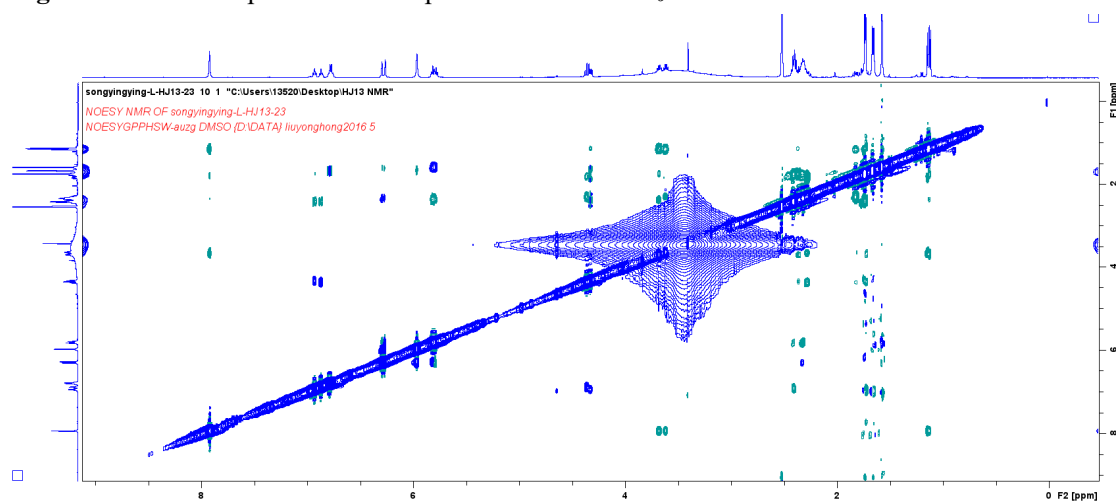


Figure S36 NOESY spectrum of compound **4** in DMSO- d_6

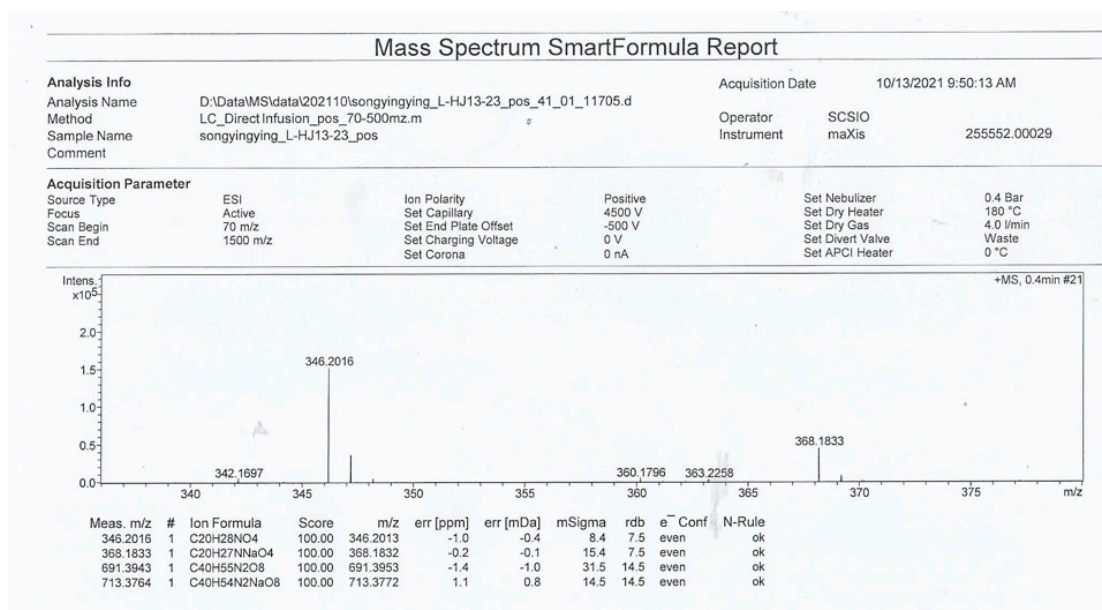


Figure S37 HRESIMS spectrum of compound **4**

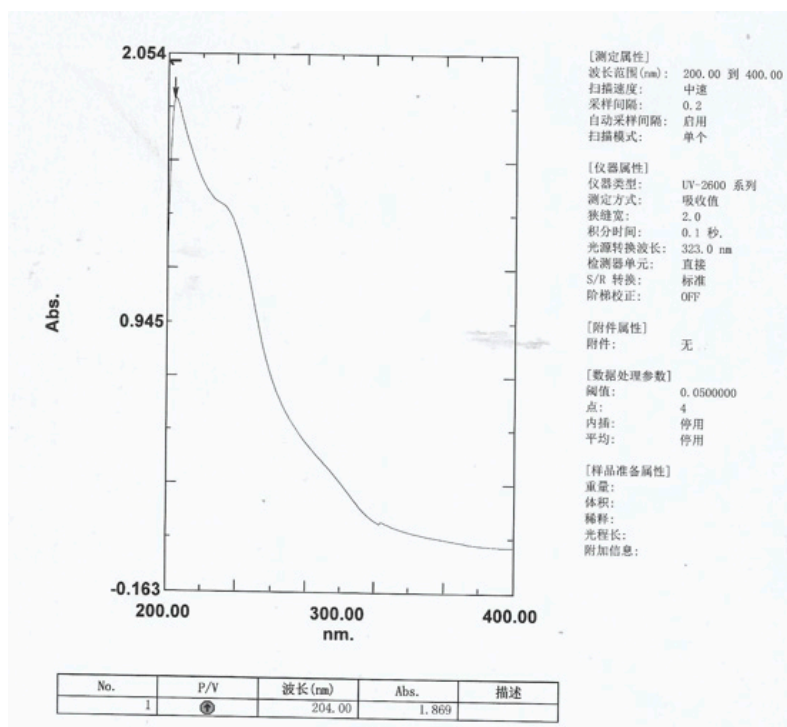


Figure S38 UV spectrum of **4**

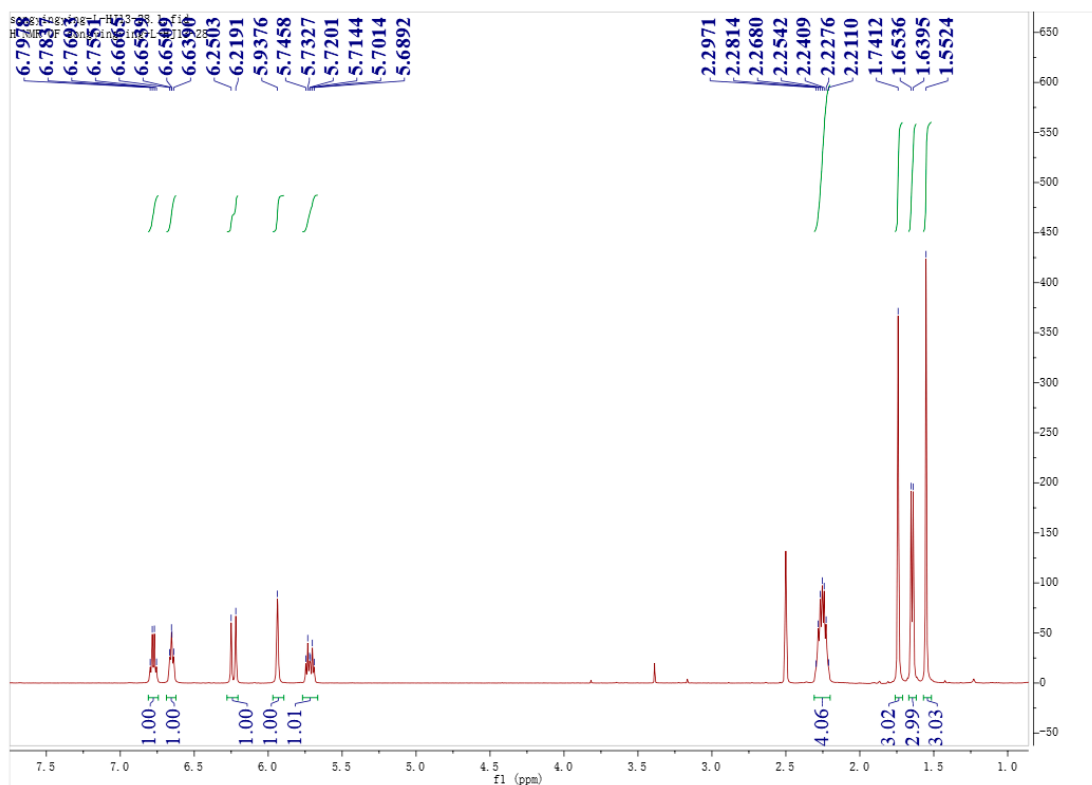


Figure S39 ¹H NMR spectrum of compound **5** in DMSO-*d*₆

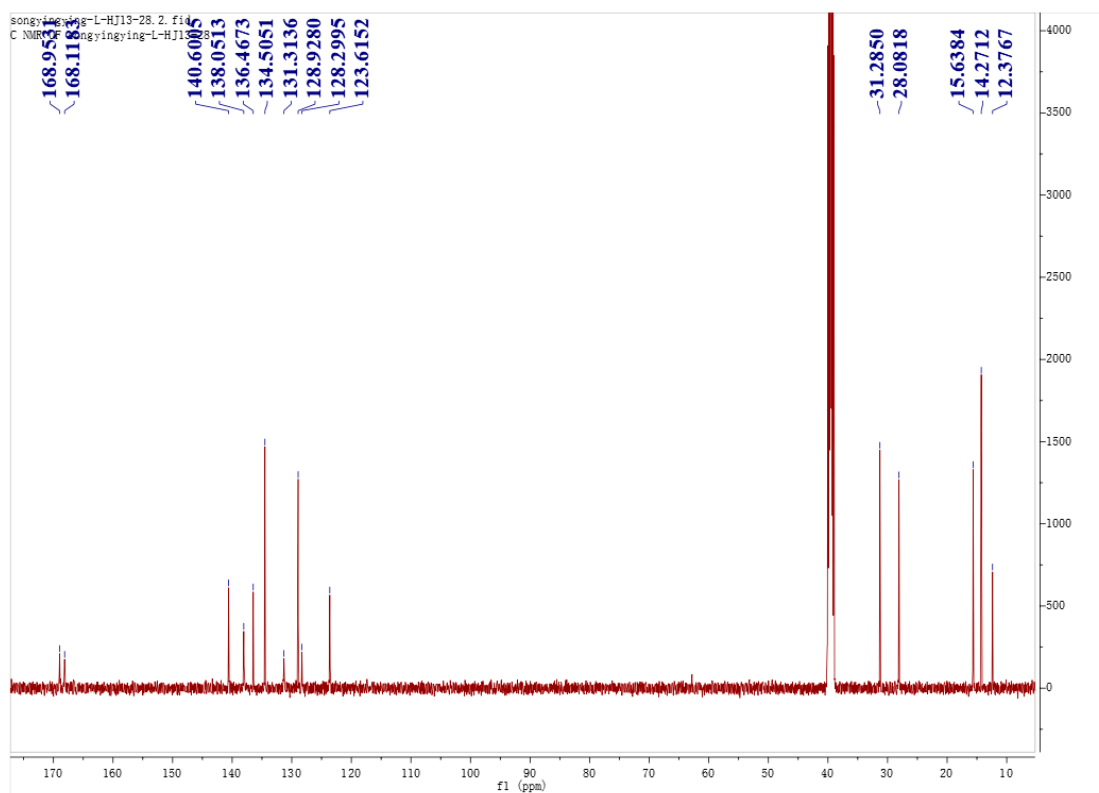


Figure S40 ¹³C NMR spectrum of compound **5** in DMSO-*d*₆

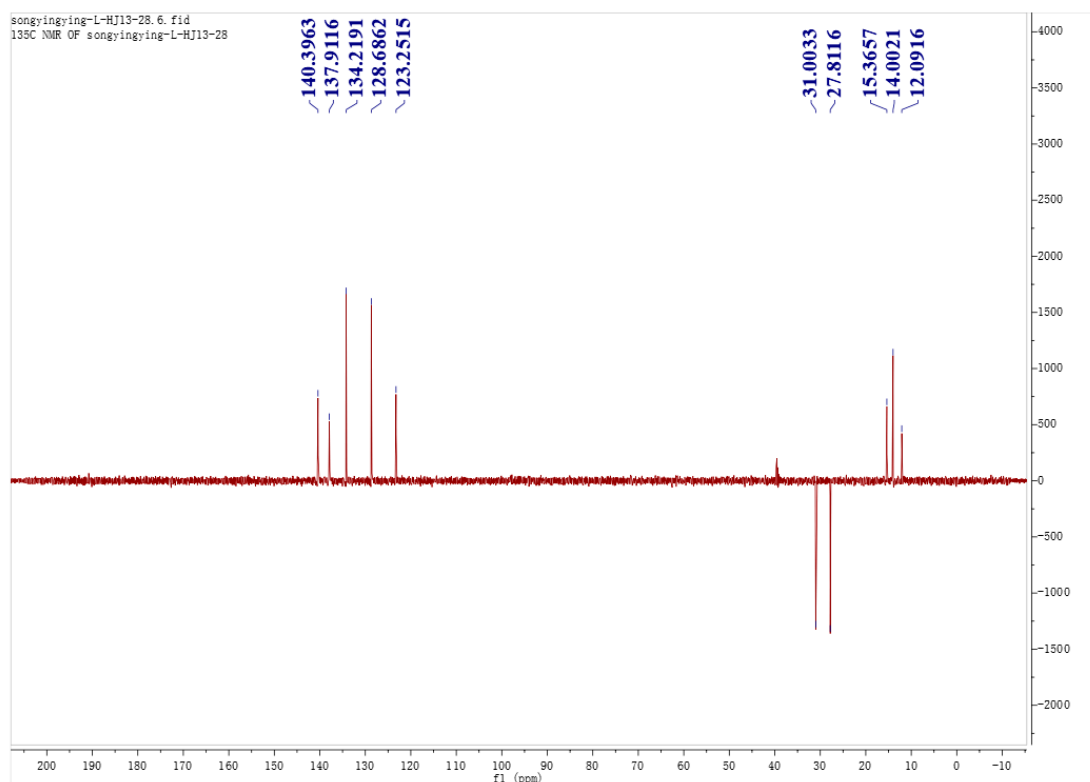


Figure S41 DEPT135 spectrum of compound **5** in DMSO- d_6

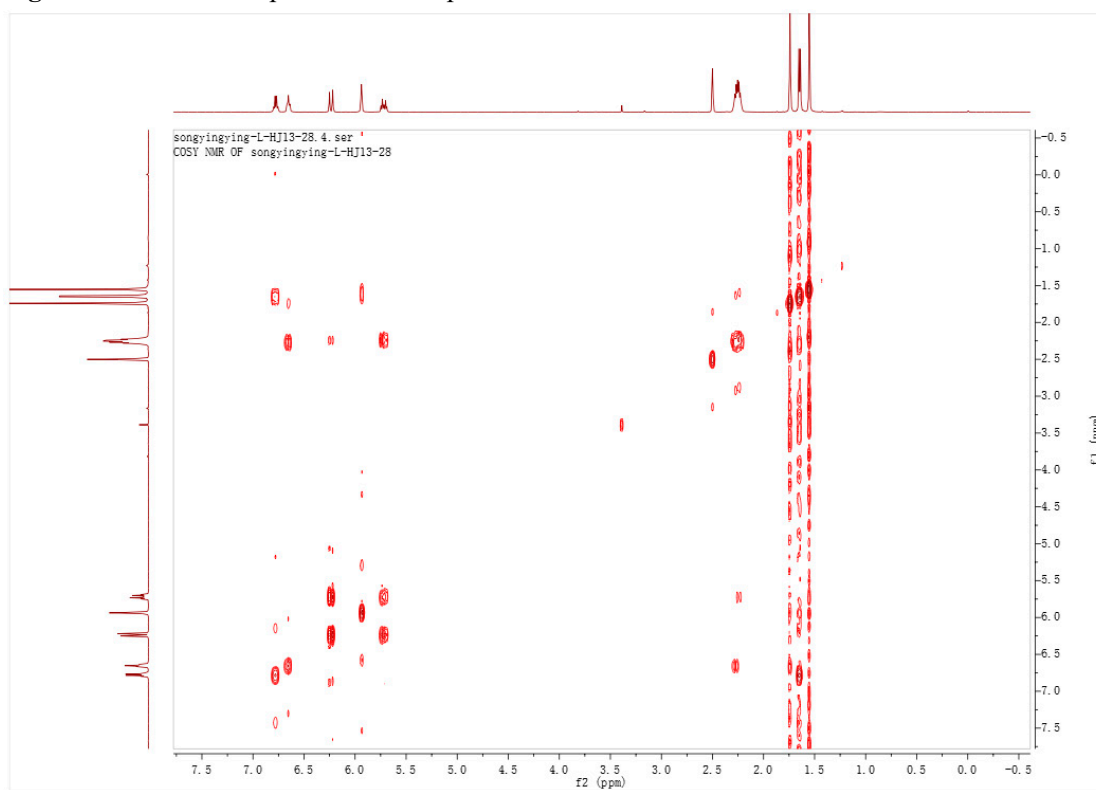


Figure S42 ^1H - ^1H COSY spectrum of compound **5** in DMSO- d_6

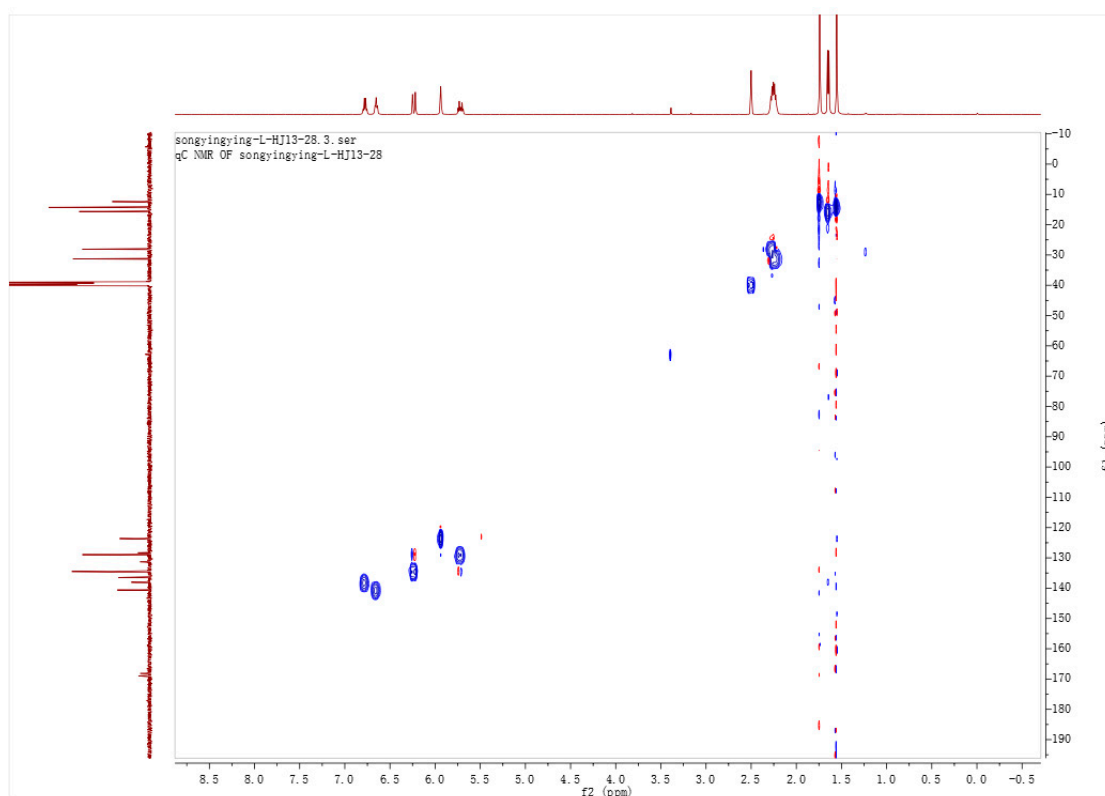


Figure S43 HSQC spectrum of compound **5** in DMSO- d_6

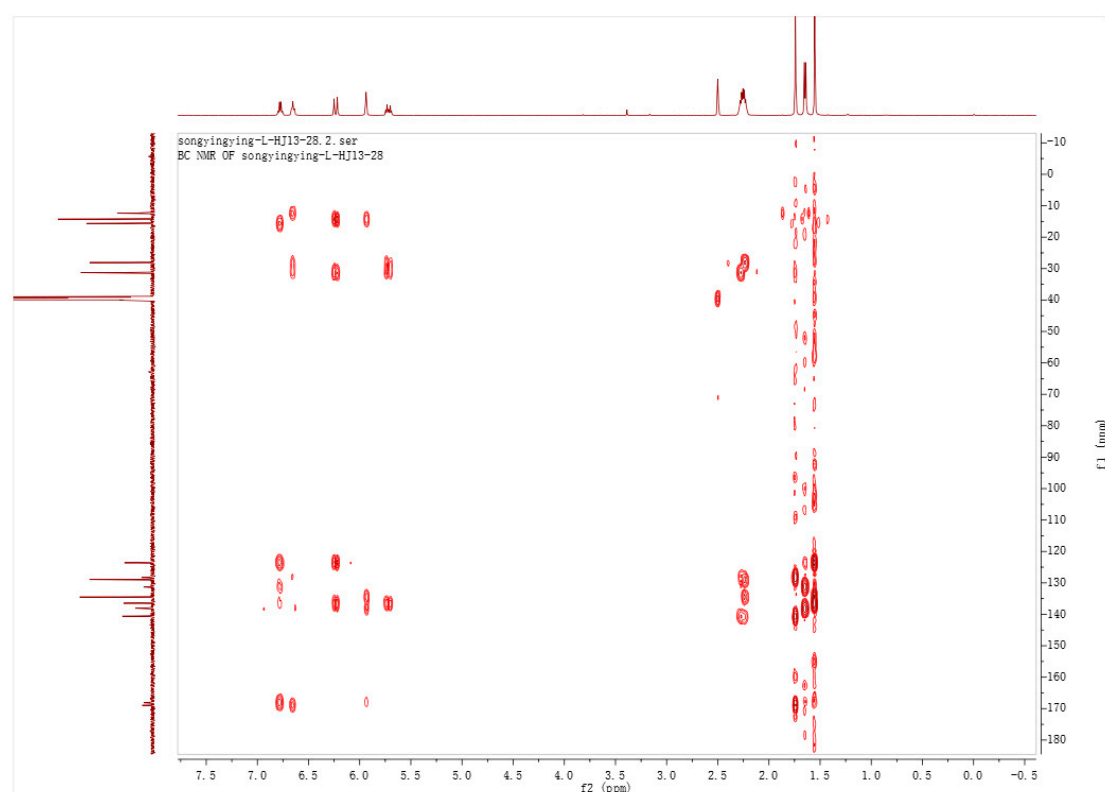


Figure S44 HMBC spectrum of compound **5** in DMSO- d_6

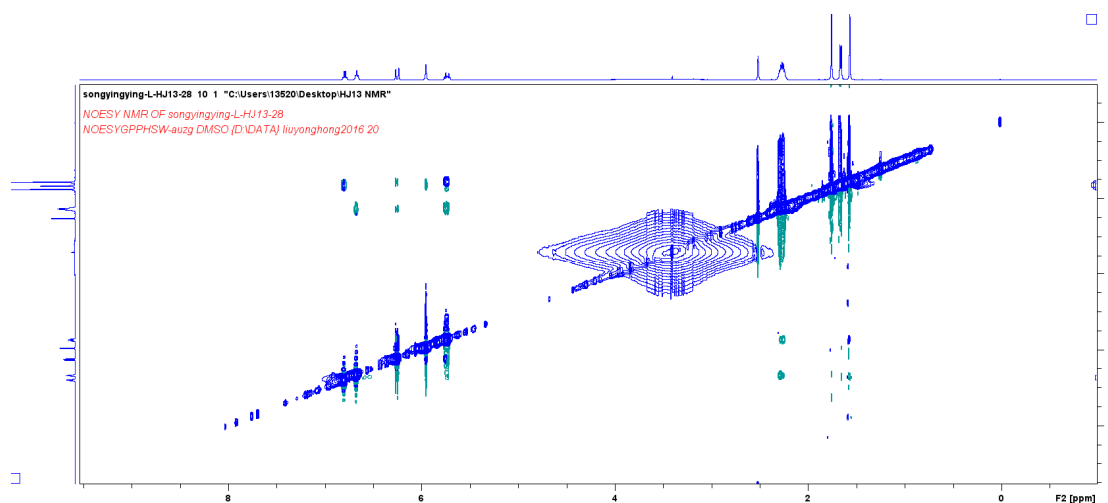


Figure S45 NOESY spectrum of compound **5** in DMSO- d_6

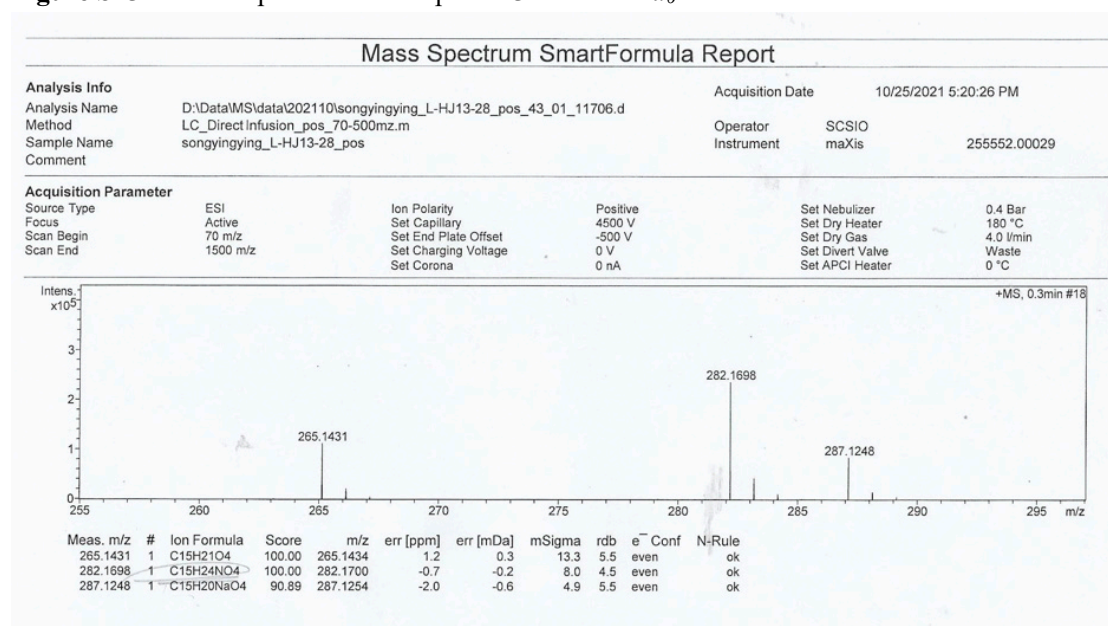


Figure S46 HRESIMS spectrum of compound **5**

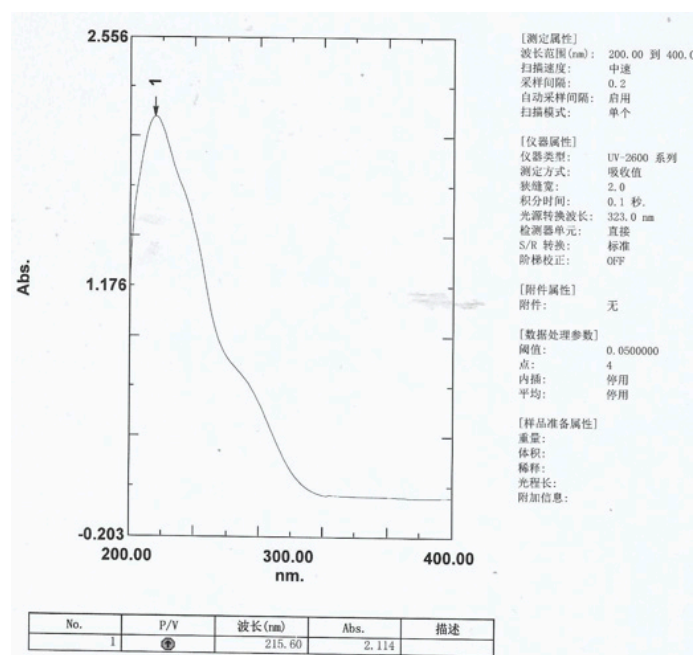
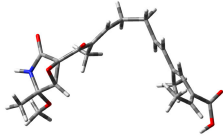
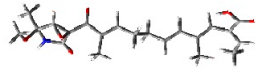
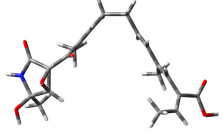


Figure S47 UV spectrum of **5**

Table S1 Energies of **1** and **2** at MMFF94 force field

Conformer	Energy (kcal/mol)	ΔE (kcal/mol)	Population (%)
13 <i>R</i> , 14 <i>R</i> , 15 <i>R</i> -1	22.42	0.00	100.00
13 <i>S</i> , 14 <i>R</i> , 15 <i>R</i> -1	30.13	0.00	100.00
13 <i>R</i> , 14 <i>R</i> , 15 <i>R</i> -2	32.42	0.00	100.00

Table S2 Energies of **1** and **2** at B97-3c level in methanol

Conformer	Configuration	E (Hartree)	Energy (kcal/mol)	ΔE (kcal/mol)	Population (%)
13 <i>R</i> , 14 <i>R</i> , 15 <i>R</i> -1		-2529	-1392032.79	0.00	100.00
13 <i>S</i> , 14 <i>R</i> , 15 <i>R</i> -1		-2390	-1499748.9	0.00	100.00
13 <i>R</i> , 14 <i>R</i> , 15 <i>R</i> -2		-2379	-1485709.29	0.00	100.00