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Supporting Information

for

Four bioactive new steroids from the soft coral *Lobophytum pauciflorum* collected in South China Sea

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Crystal data and structure refinement for compounds 1–3 and NMR, MS, and IR spectra of compounds 1–4

Content

Table S1. Crystal data and structure refinement for compound **1**.

Identification code	cu_0717_4_0m
Empirical formula	$C_{60}H_{102}O_7$
Formula weight	935.41
Temperature/K	150.0
Crystal system	triclinic
Space group	P1
a/Å	7.5758(4)
b/Å	19.0127(11)
c/Å	20.3233(11)
α/°	69.925(3)
β/°	89.856(3)
γ/°	79.736(3)
Volume/Å^3	2700.0(3)
Z	2
ρ_{calc}g/cm^3	1.151
μ/mm^{-1}	0.562
F(000)	1036.0
Crystal size/mm^3	0.11 × 0.1 × 0.09
Radiation	Cu Kα (λ = 1.54178)
Index ranges	$-8 \le h \le 8$, $-22 \le k \le 22$, $-24 \le l \le 23$
Reflections collected	32954
Independent reflections	12597 [R_{int} = 0.0693, R_{sigma} = 0.0843]
Data/restraints/parameters	12597/15/1287
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0659, wR_2 = 0.1674
Final R indexes [all data]	R_1 = 0.0747, wR_2 = 0.1788
Largest diff. peak/hole / e Å^{-3}	0.23/-0.20
Flack parameter	0.0(2)

Crystallographic data of **1** have been deposited in the Cambridge Crystallographic Data Center (Deposition number: CCDC 2133384). The data can be obtained free of charge via www.ccdc.cam.ac.uk/products/csd/request.

Table S2. Crystal data and structure refinement for compound **2**.

Empirical formula	$C_{30}H_{52}O_5$
Formula weight	492.72
Temperature/K	293
Crystal system	monoclinic
Space group	P21
a/Å	8.8931(14)
b/Å	10.1189(16)
c/Å	16.102(2)
α/°	90
β/°	96.085(13)
γ/°	90
Volume/Å^3	1440.8(4)
Z	2
ρ_{calc}g/cm^3	1.136
μ/mm^{-1}	0.590
F(000)	544
Crystal size/mm^3	0.12 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -19 ≤ l ≤ 19
Reflections collected	4834
Independent reflections	3381 [R_{int} = 0.0424, R_{sigma} = 0.0812]
Data/restraints/parameters	3381/1/329
Goodness-of-fit on F^2	0.974
Final R indexes [I>=2σ (I)]	R_1 = 0.0532, wR_2 = 0.0957
Final R indexes [all data]	R_1 = 0.096, wR_2 = 0.1190
Largest diff. peak/hole / e Å^{-3}	0.16/-0.134
Flack parameter	0.3(4)

Crystallographic data of **2** have been deposited in the Cambridge Crystallographic Data Center (Deposition number: CCDC 2133391). The data can be obtained free of charge via www.ccdc.cam.ac.uk/products/csd/request.

Table S3. Crystal data and structure refinement for compound **3**.

Empirical formula	$C_{28}H_{48}O_4$
Formula weight	448.66
Temperature/K	150.0
Crystal system	orthorhombic
Space group	$P2_12_12$
a/Å	10.3615(3)
b/Å	33.2315(8)
c/Å	7.4685(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2571.61(12)
Z	4
ρ_{calc}g/cm^3	1.159
μ/mm^{-1}	0.586
F(000)	992.0
Crystal size/mm^3	0.12 × 0.1 × 0.09
Radiation	Cu Kα (λ = 1.54178)
Index ranges	$-12 \leq h \leq 12$, $-39 \leq k \leq 39$, $-8 \leq l \leq 8$
Reflections collected	23207
Independent reflections	4477 [R_{int} = 0.0407, R_{sigma} = 0.0259]
Data/restraints/parameters	4477/0/295
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.0600, wR_2 = 0.1521
Final R indexes [all data]	R_1 = 0.0646, wR_2 = 0.1583
Largest diff. peak/hole / e Å^{-3}	0.27/-0.18
Flack parameter	-0.11(9)

Crystallographic data of **3** have been deposited in the Cambridge Crystallographic Data Center (Deposition number: CCDC 2133404). The data can be obtained free of charge via www.ccdc.cam.ac.uk/products/csd/request.

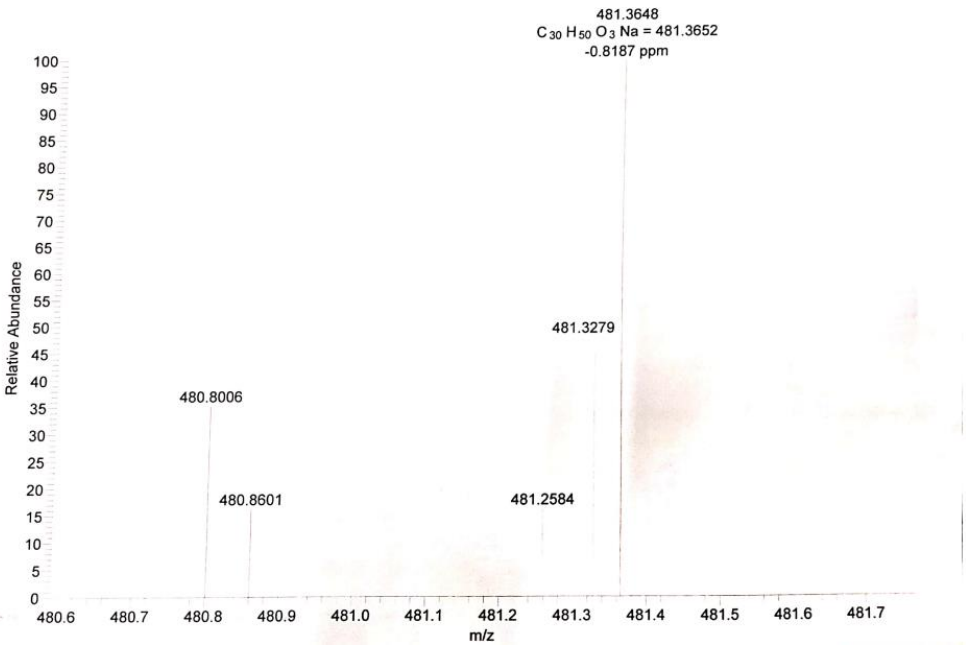

Fig.S1. HRESIMS spectrum of compound **1**.

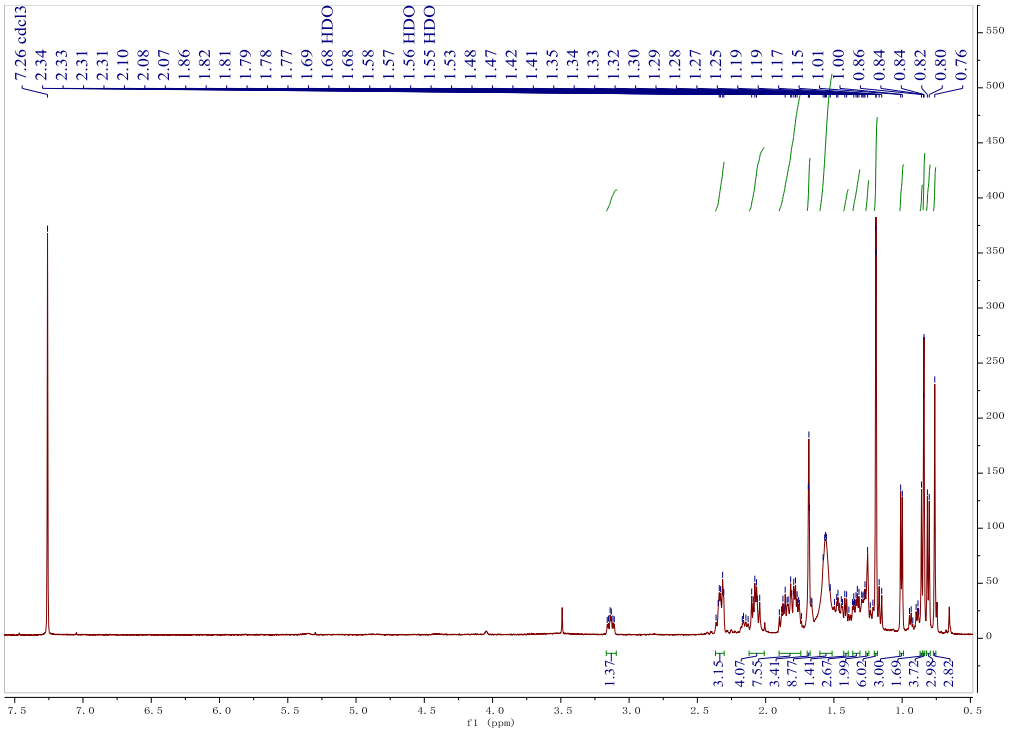

Fig.S2. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

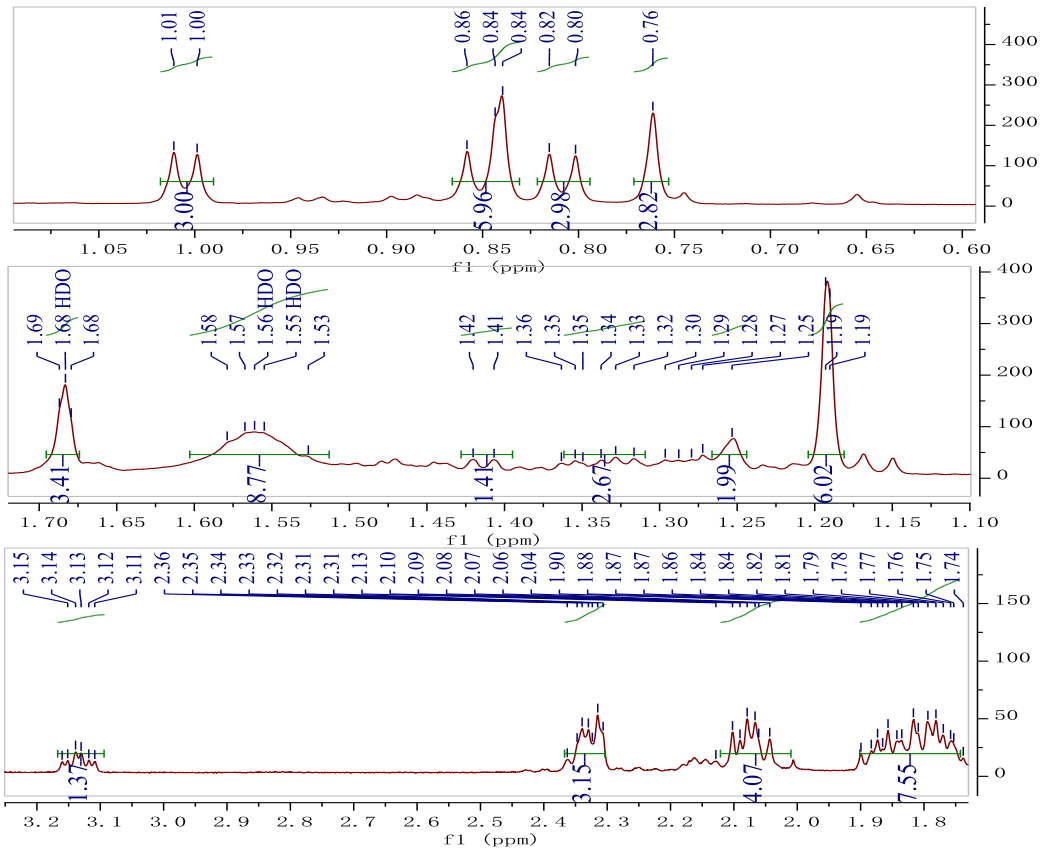

Fig.S3. The amplificatory ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

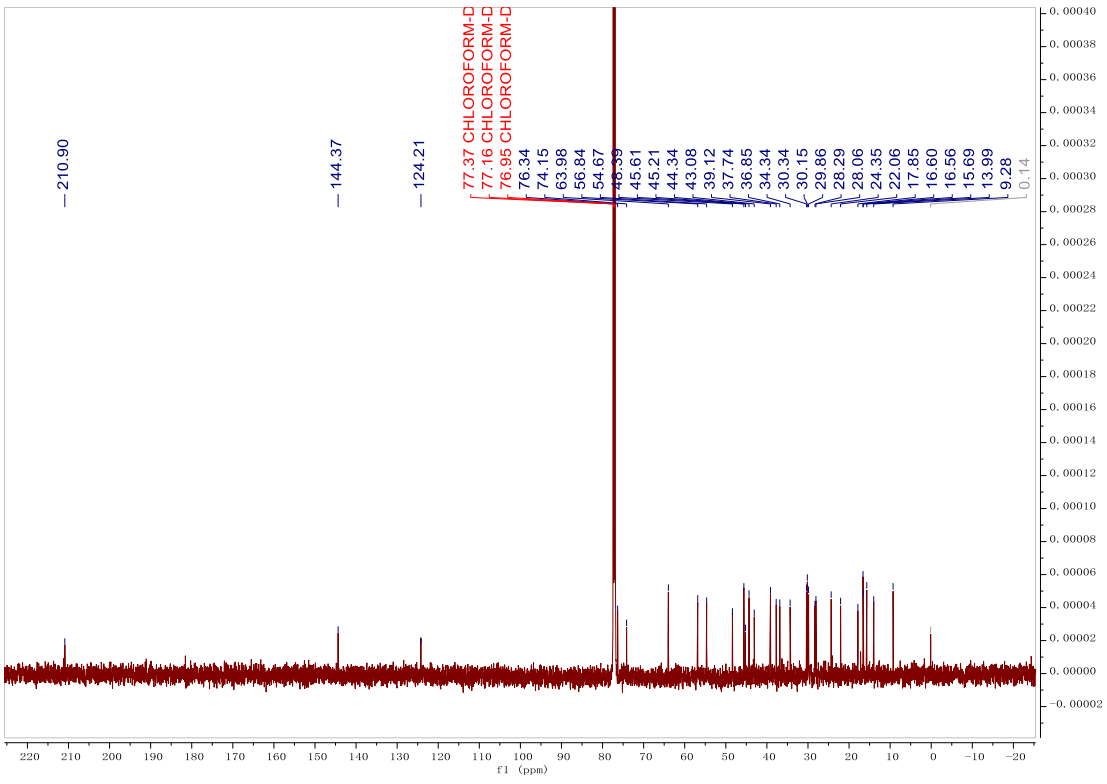

Fig.S4. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

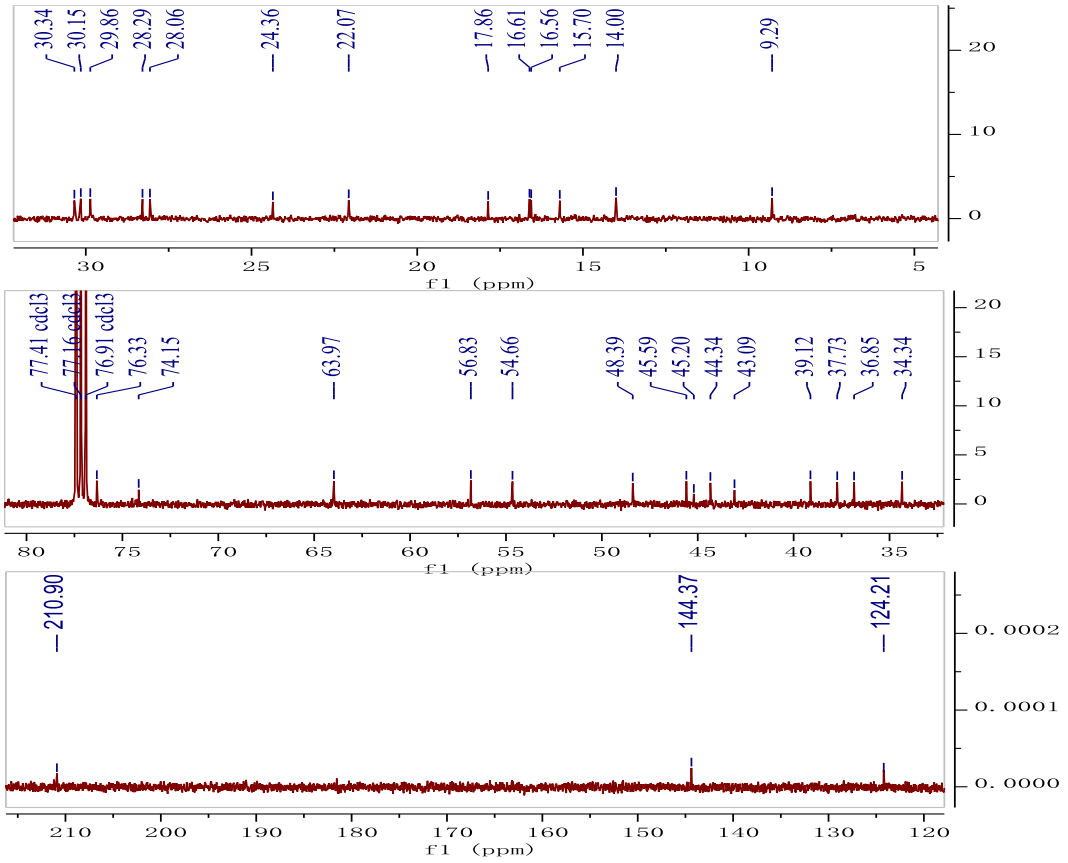

Fig.S5. The amplificatory ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

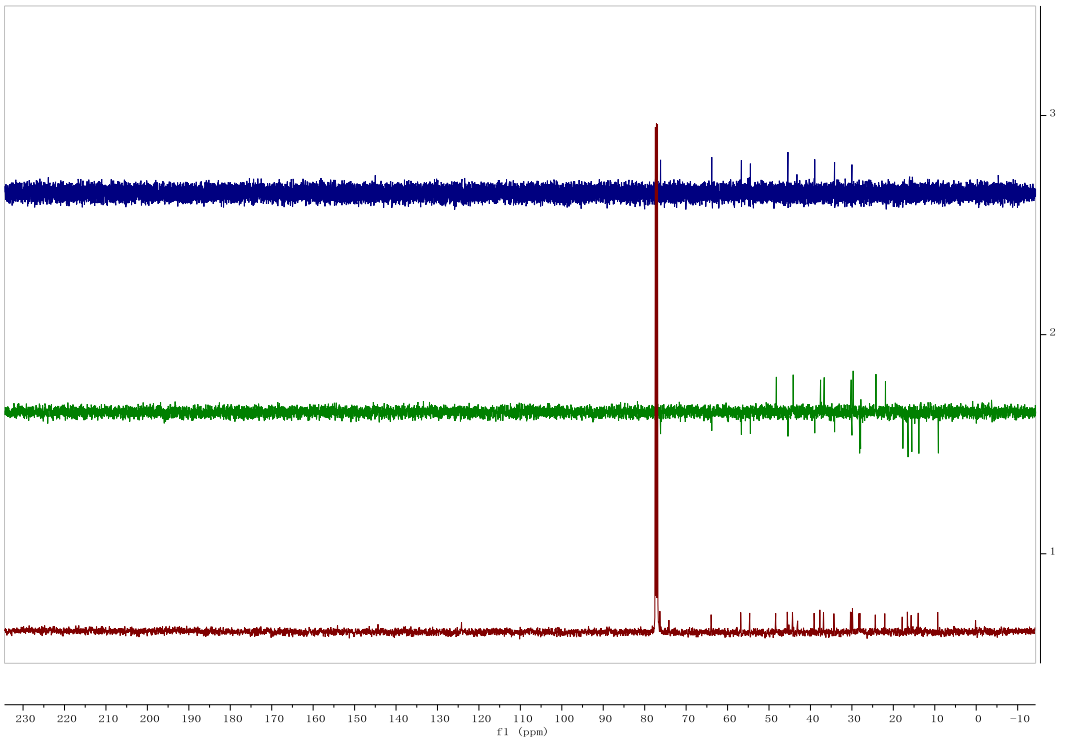

Fig.S6. DEPT spectrum of compound **1** in $CDCl_3$.

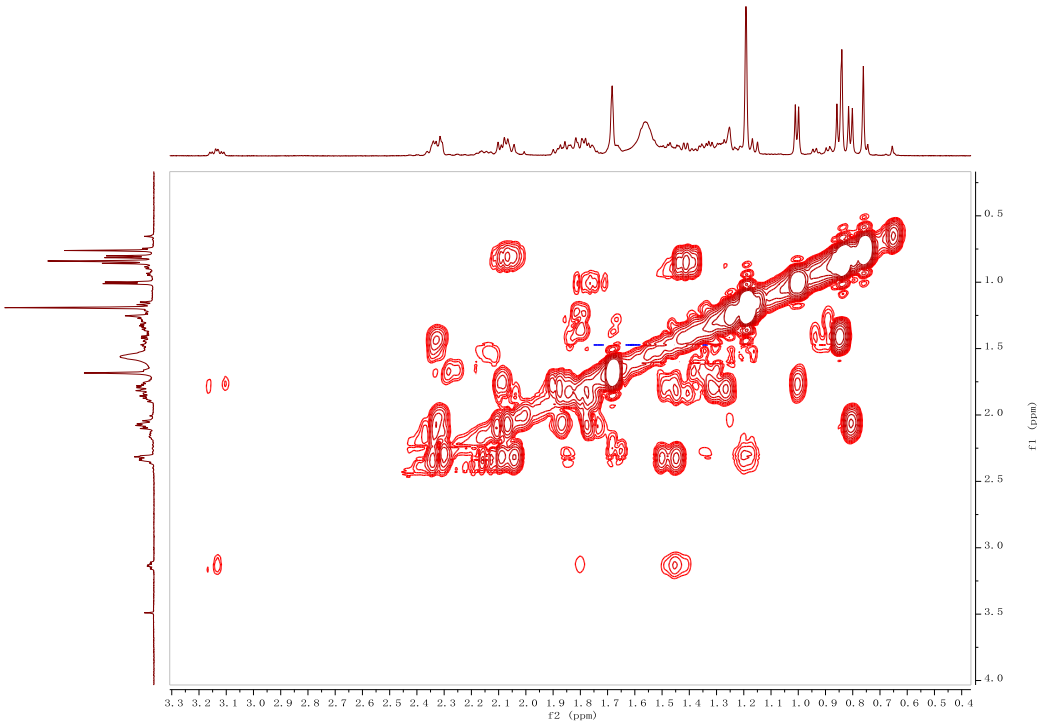

Fig.S7. $^{1}H,^{1}H$-COSY spectrum of compound **1** in $CDCl_3$.

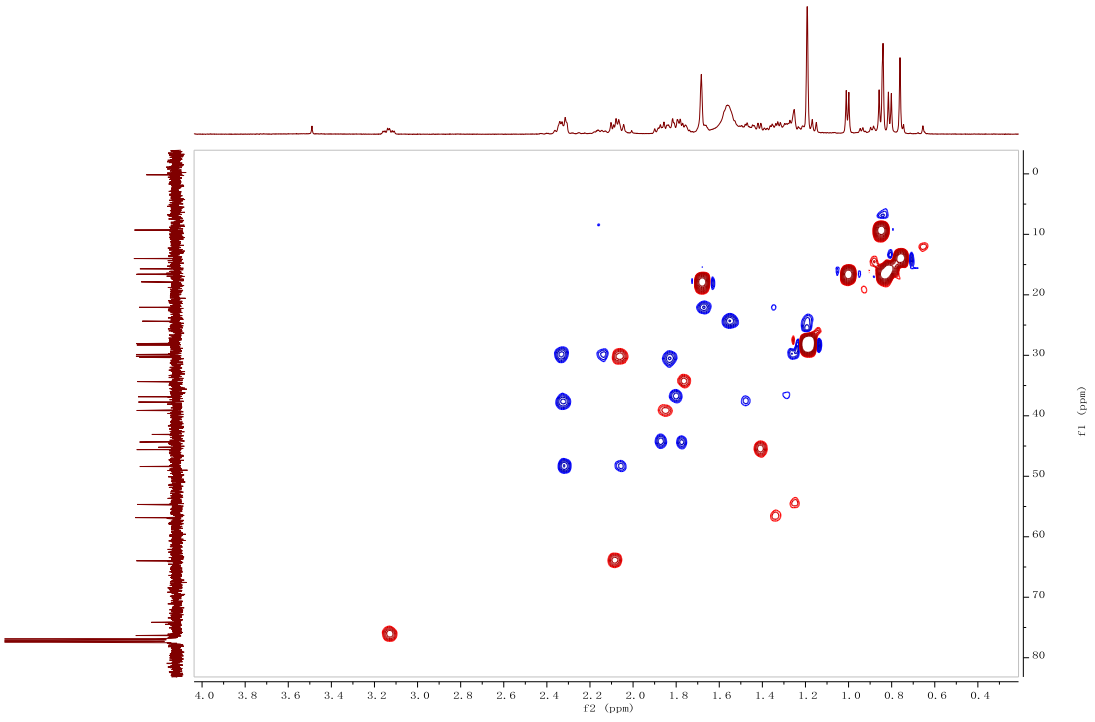

Fig.S8. HSQC spectrum of compound **1** in $CDCl_3$.

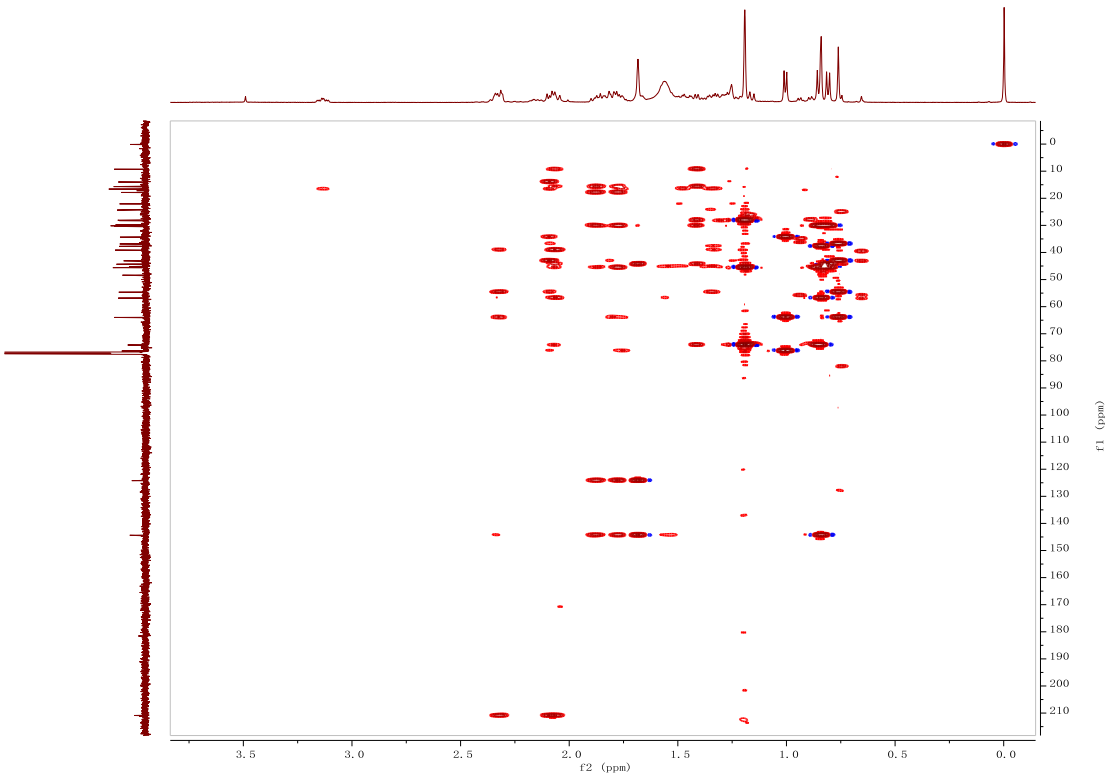

Fig.S9. HMBC spectrum of compound **1** in $CDCl_3$.

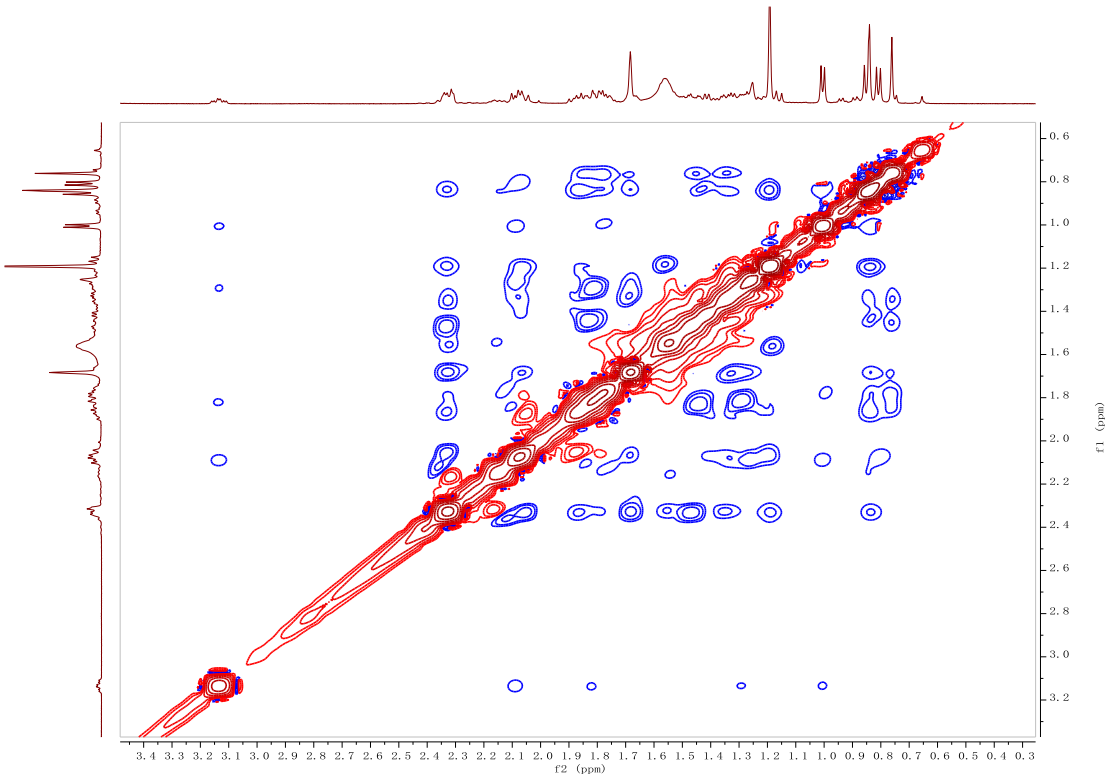

Fig.S10. NOESY spectrum of compound **1** in $CDCl_3$.

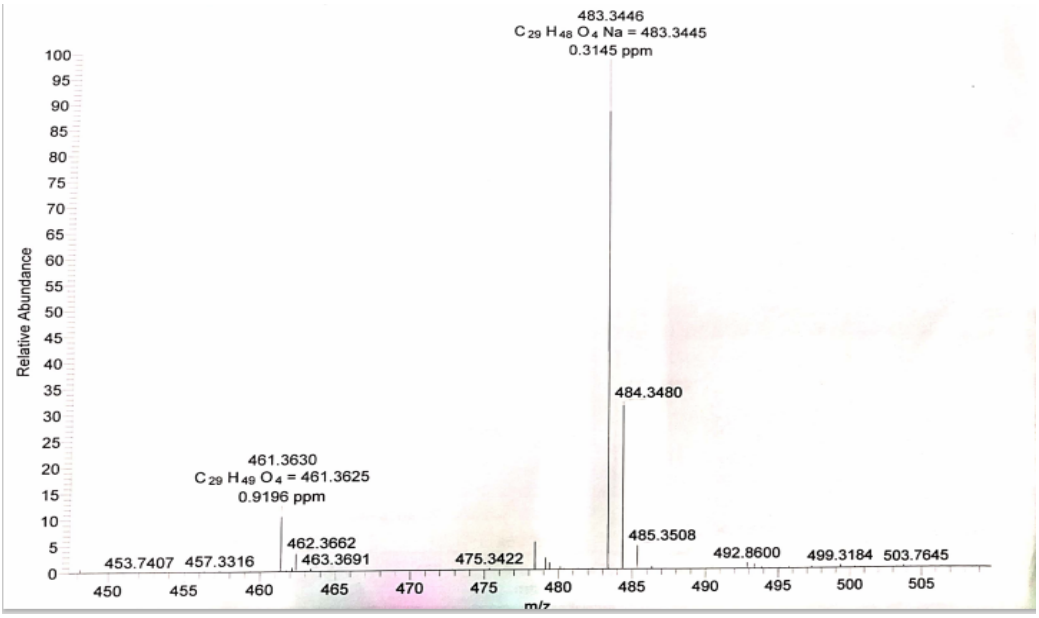

Fig.S11. HRESIMS spectrum of compound **2**.

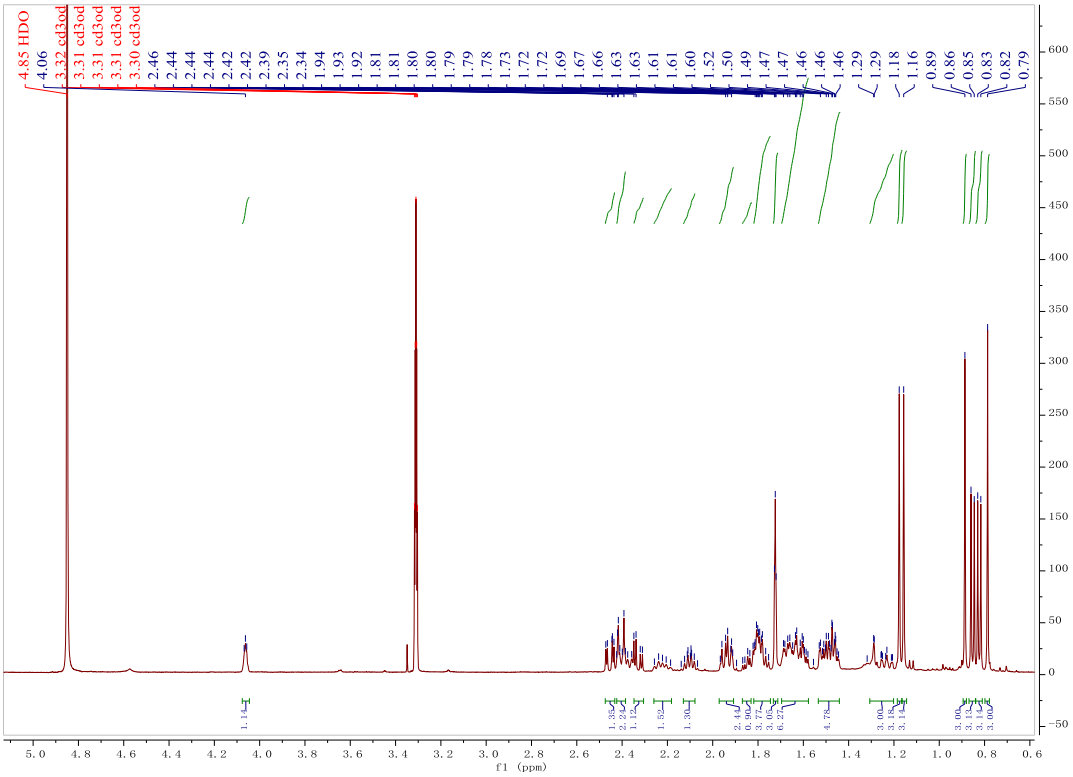

Fig.S12. ^{1}H NMR spectrum of compound **2** in CD_3OD.

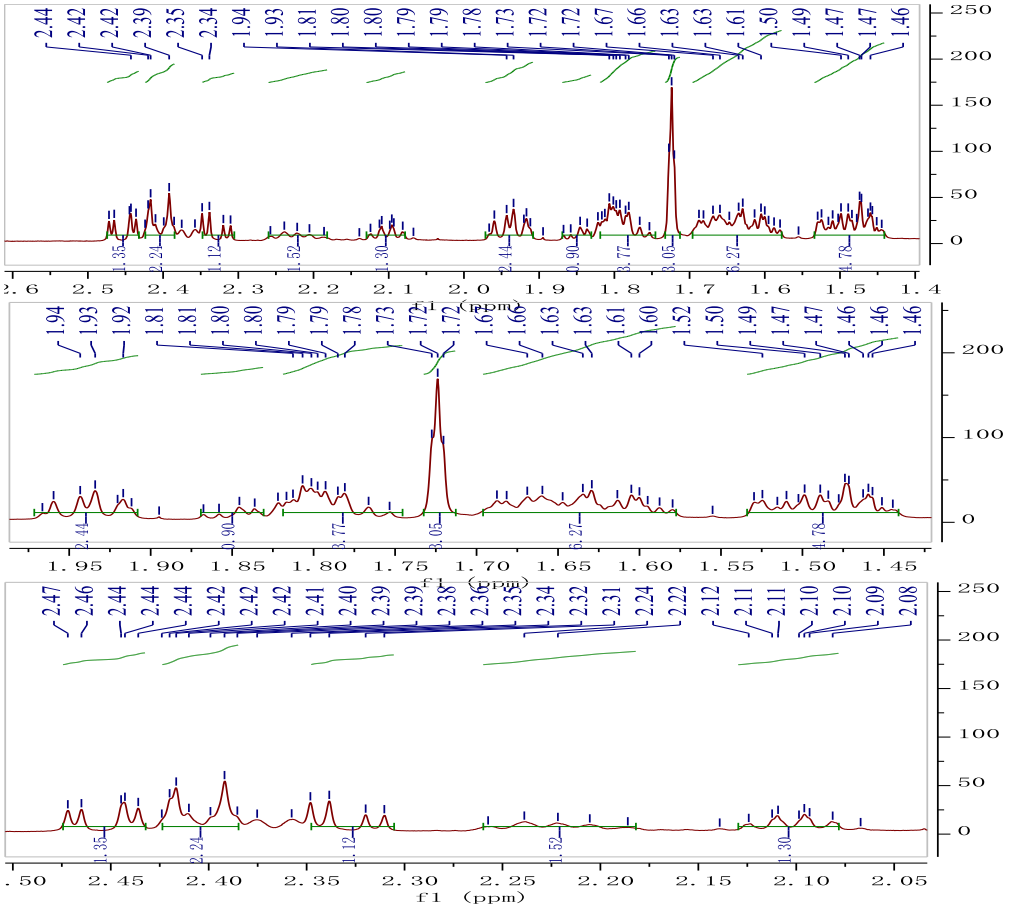

Fig.S13. The amplificatory ^{1}H NMR spectrum of compound **2** in CD_3OD.

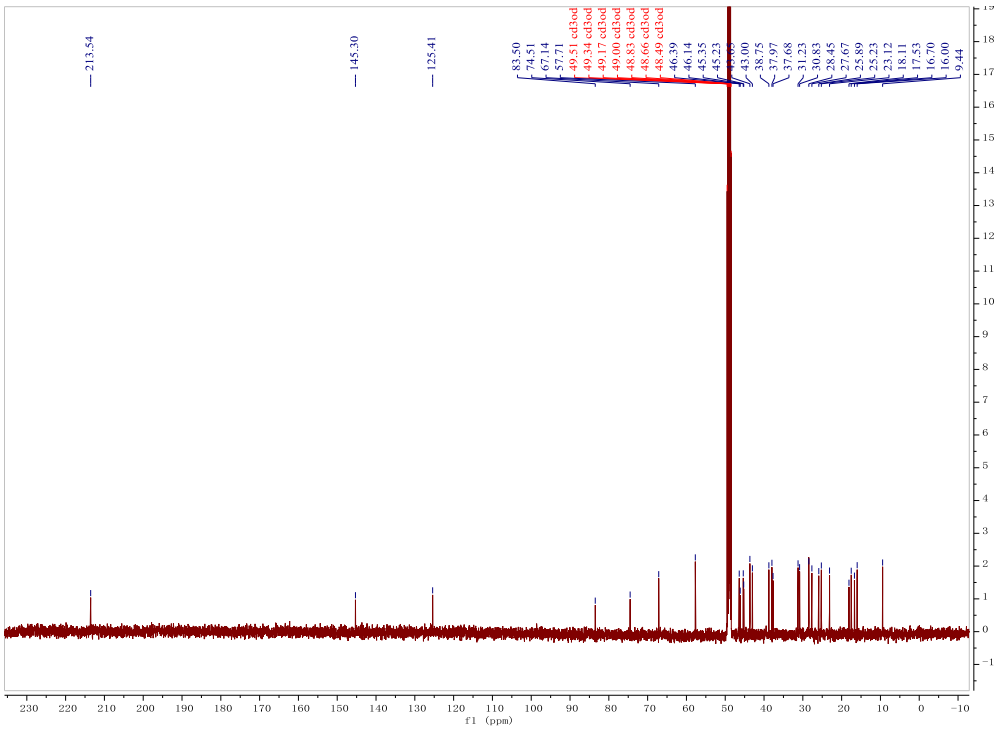

Fig.S14. ^{13}C NMR spectrum of compound **2** in CD_3OD.

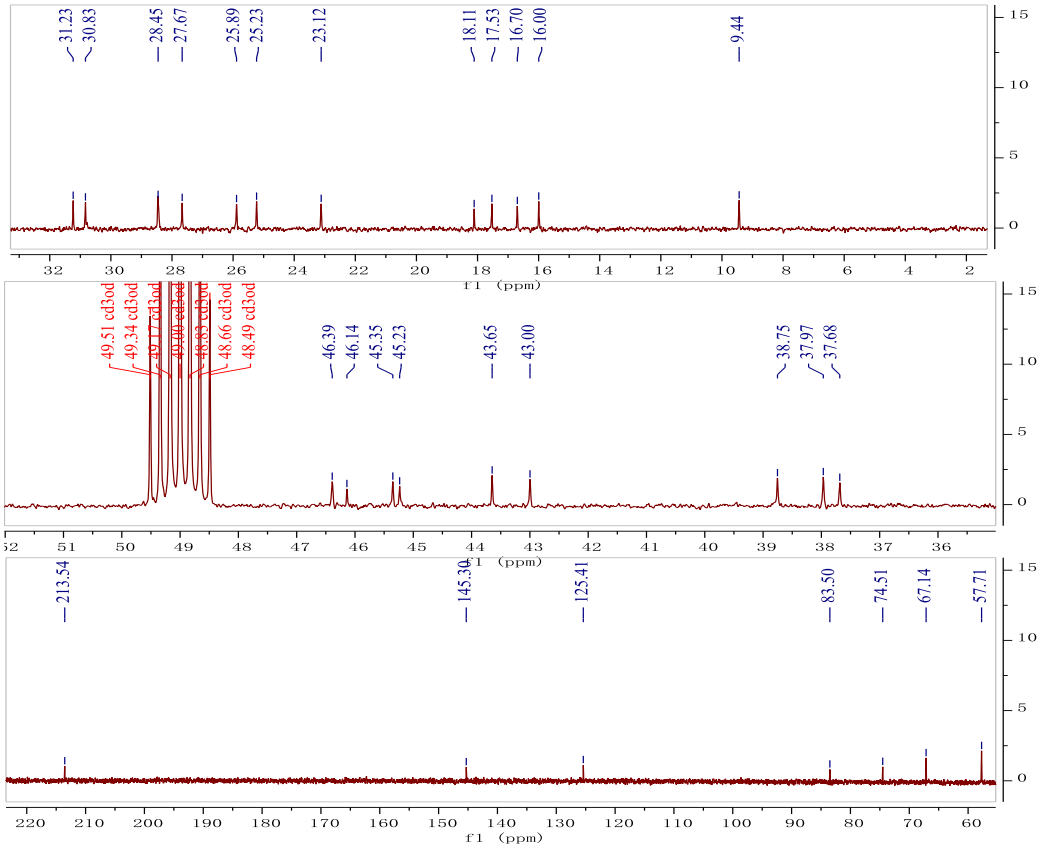

Fig.S15. The amplificatory ^{13}C NMR spectrum of compound **2** in CD_3OD.

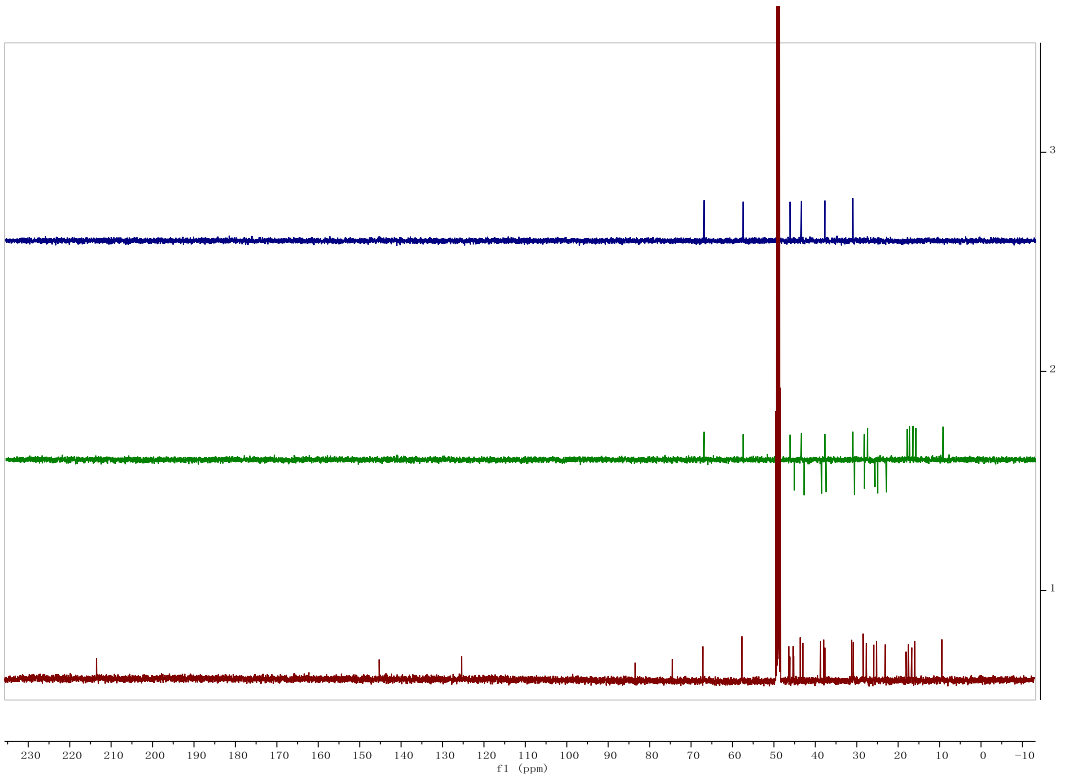

Fig.S16. DEPT spectrum of compound **2** in CD_3OD.

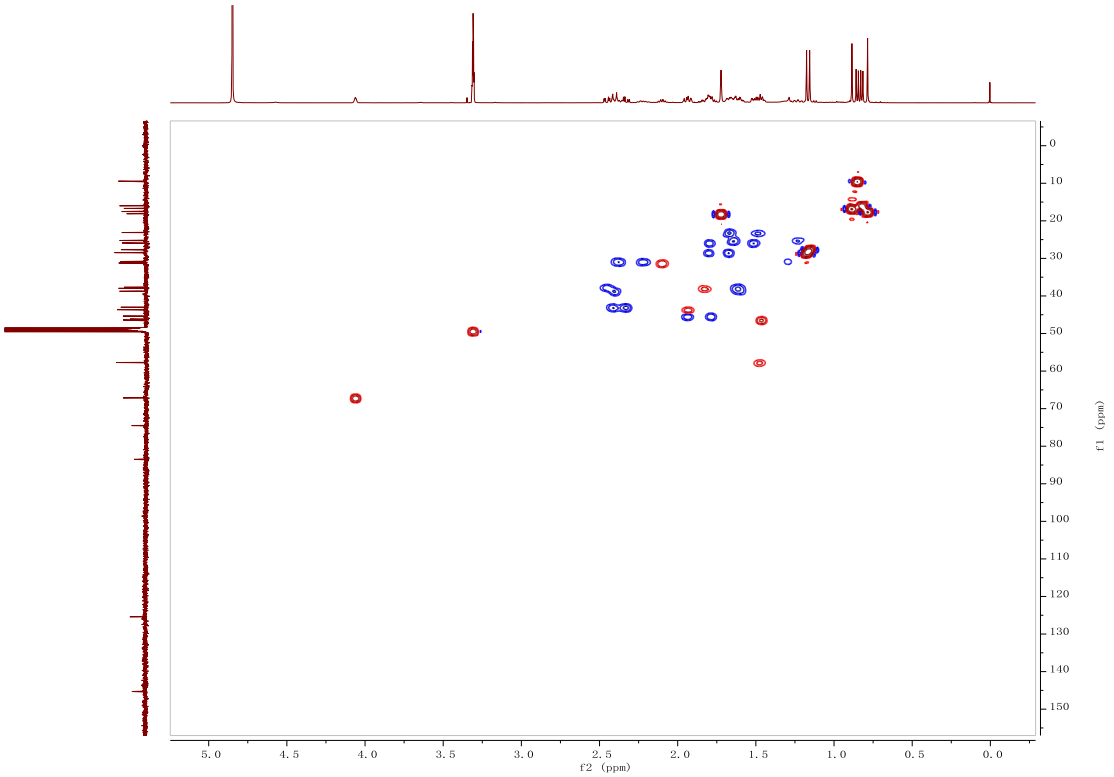

Fig.S17. HSQC spectrum of compound **2** in CD_3OD.

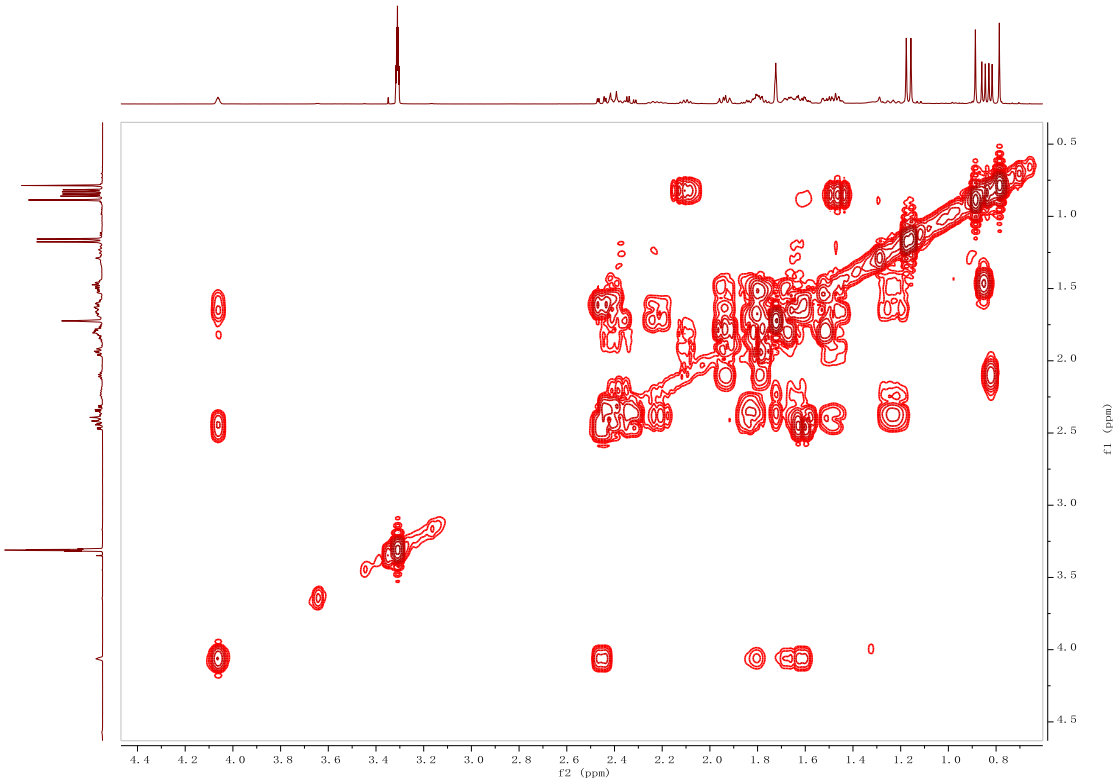

Fig.S18. $^1H,^1H$ COSY spectrum of compound **2** in CD_3OD.

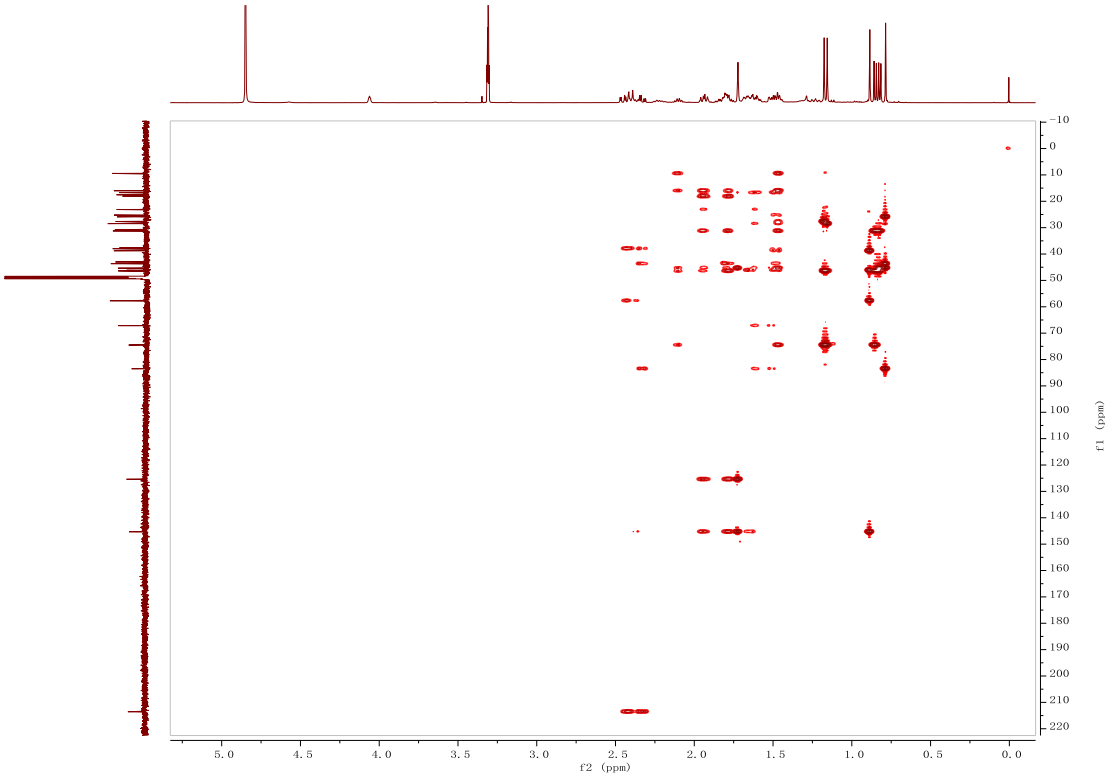

Fig.S19. HMBC spectrum of compound **2** in CD_3OD.

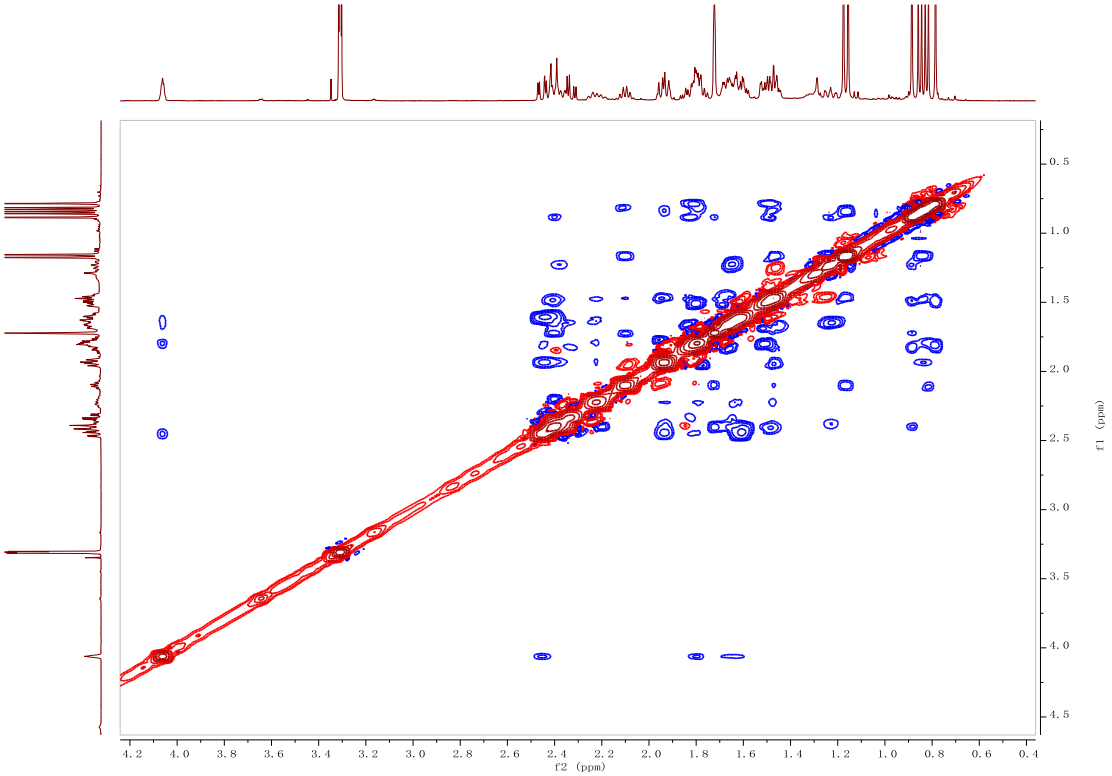

Fig.S20. NOESY spectrum of compound **2** in CD_3OD.

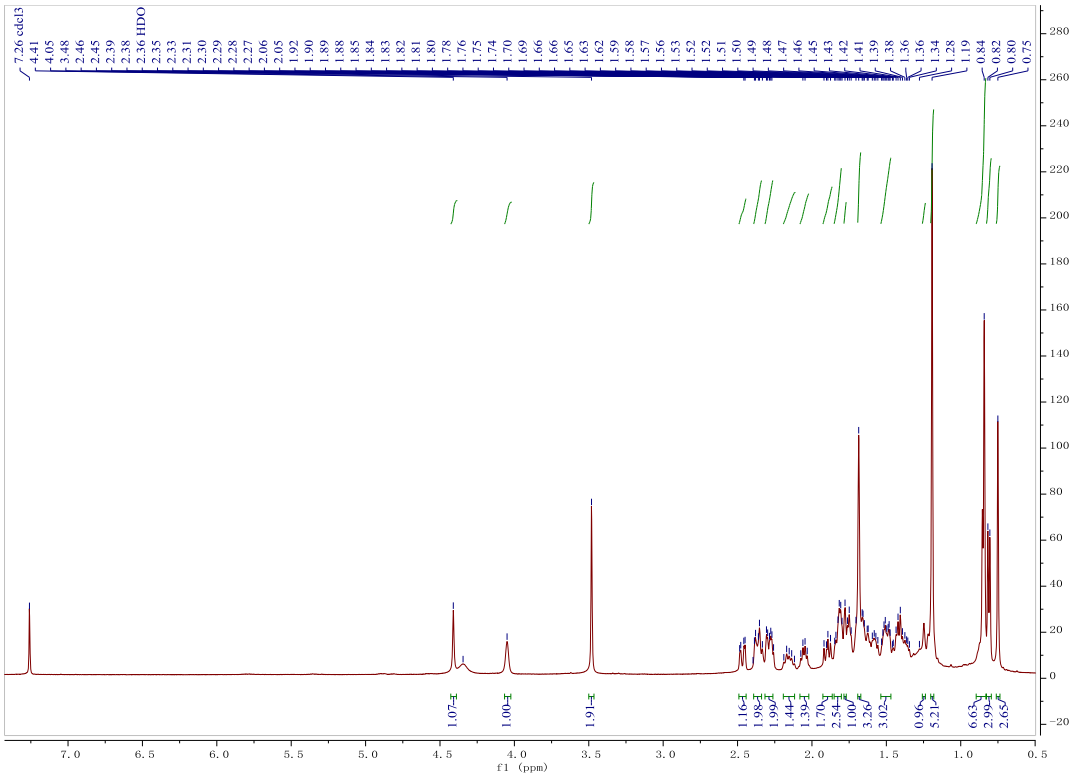

Fig.S21. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

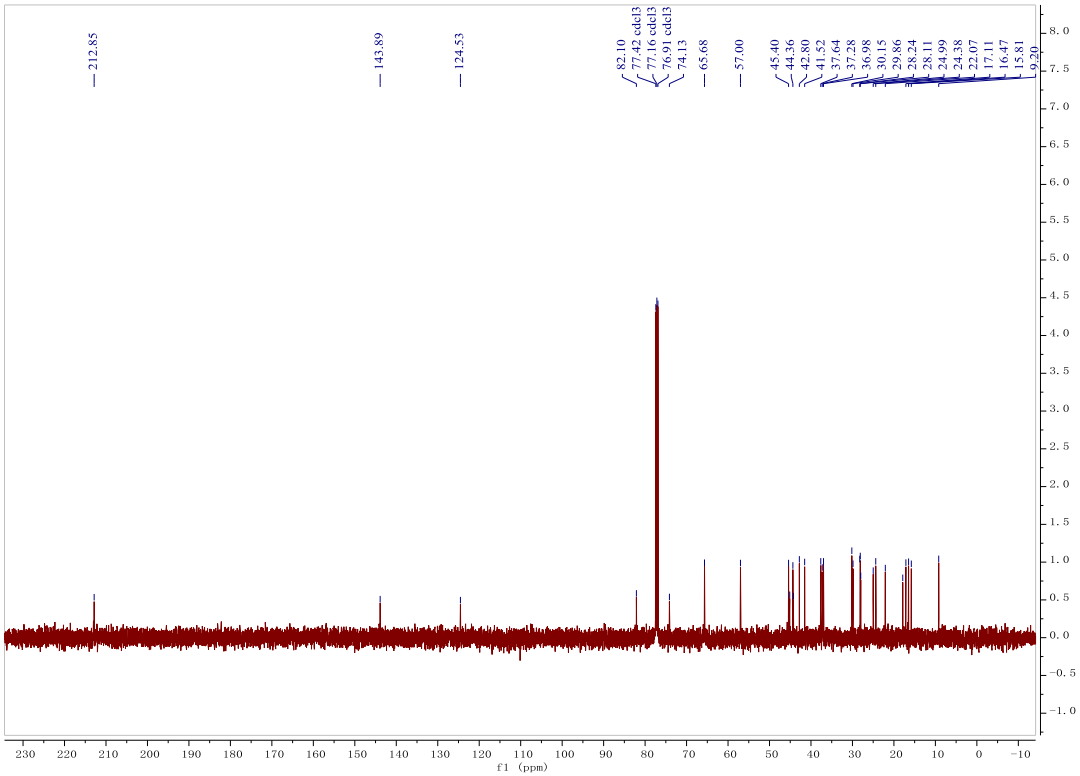

Fig.S22. ^{13}C NMR spectrum of compound **2** in $CDCl_3$

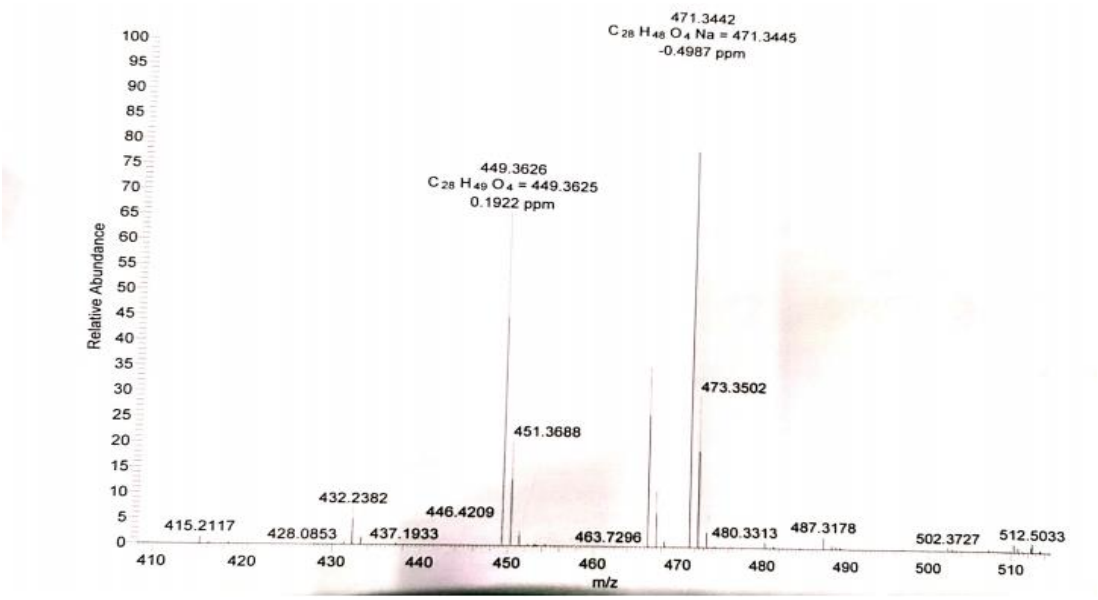

Fig.S23. HRESIMS spectrum of compound **3**.

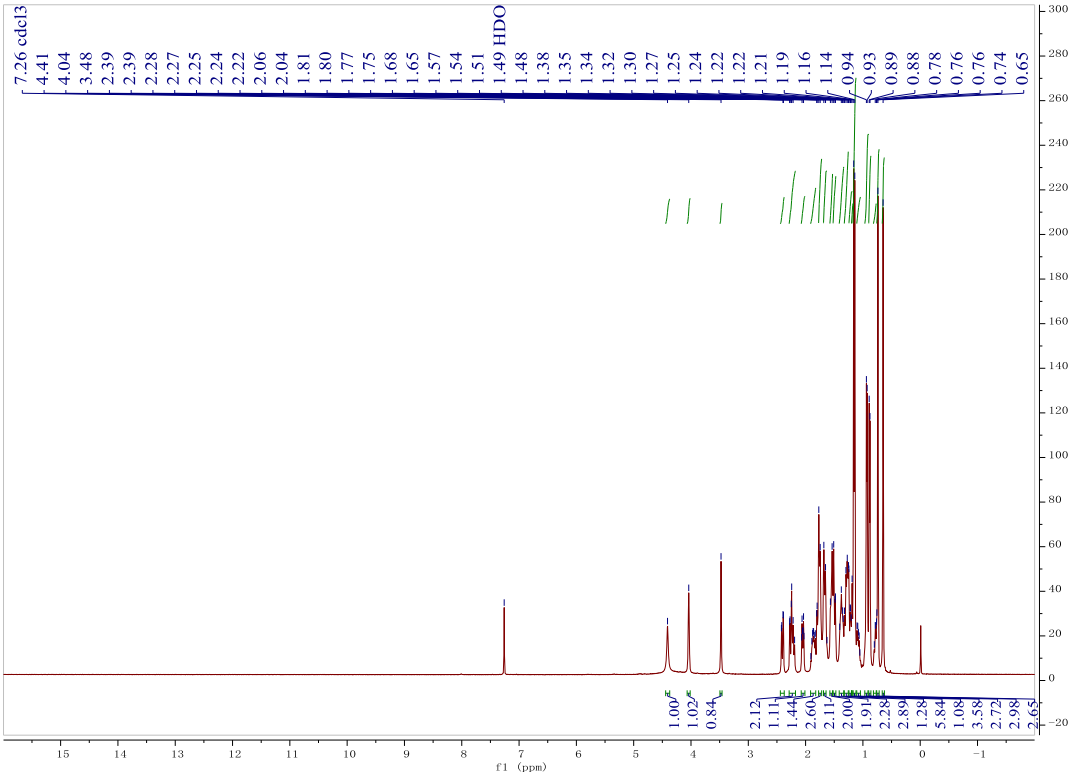

Fig.S24. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

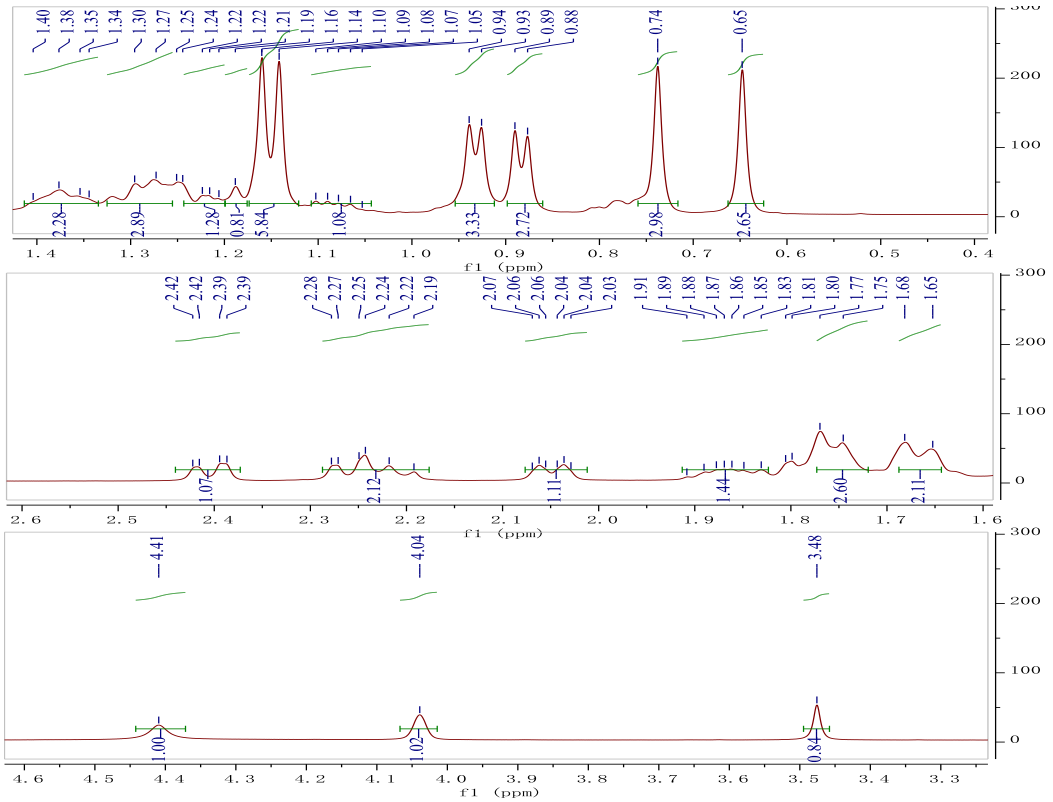

Fig.S25. The amplificatory ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

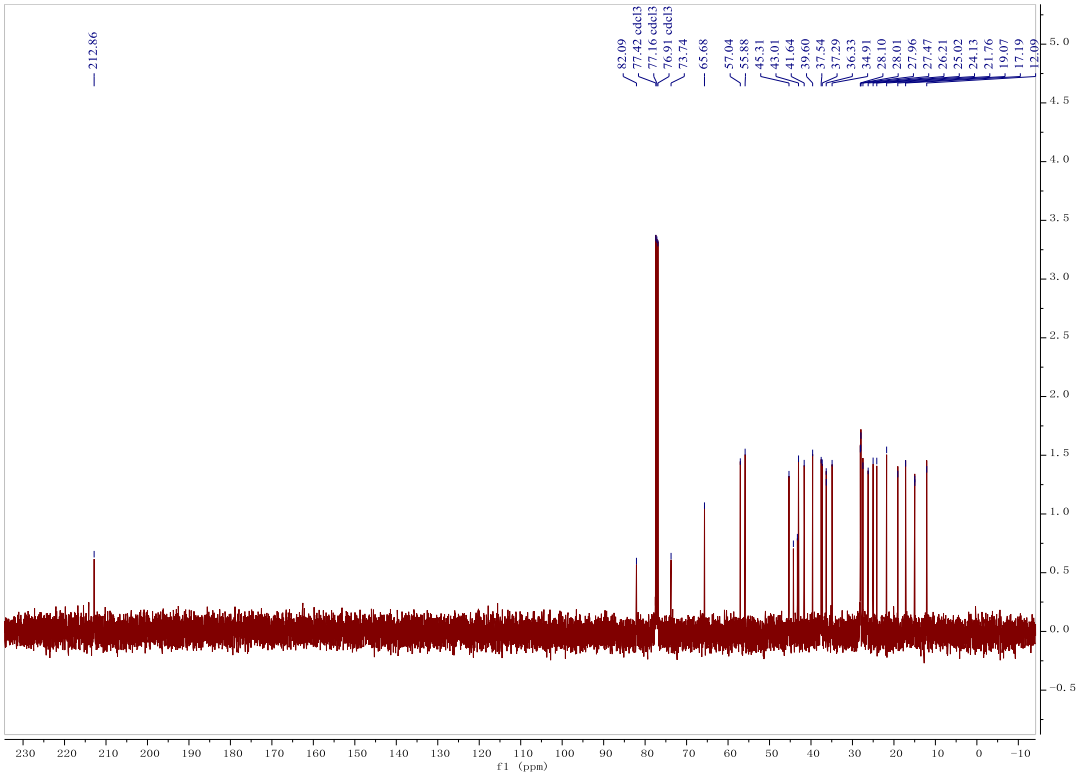

Fig.S26. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

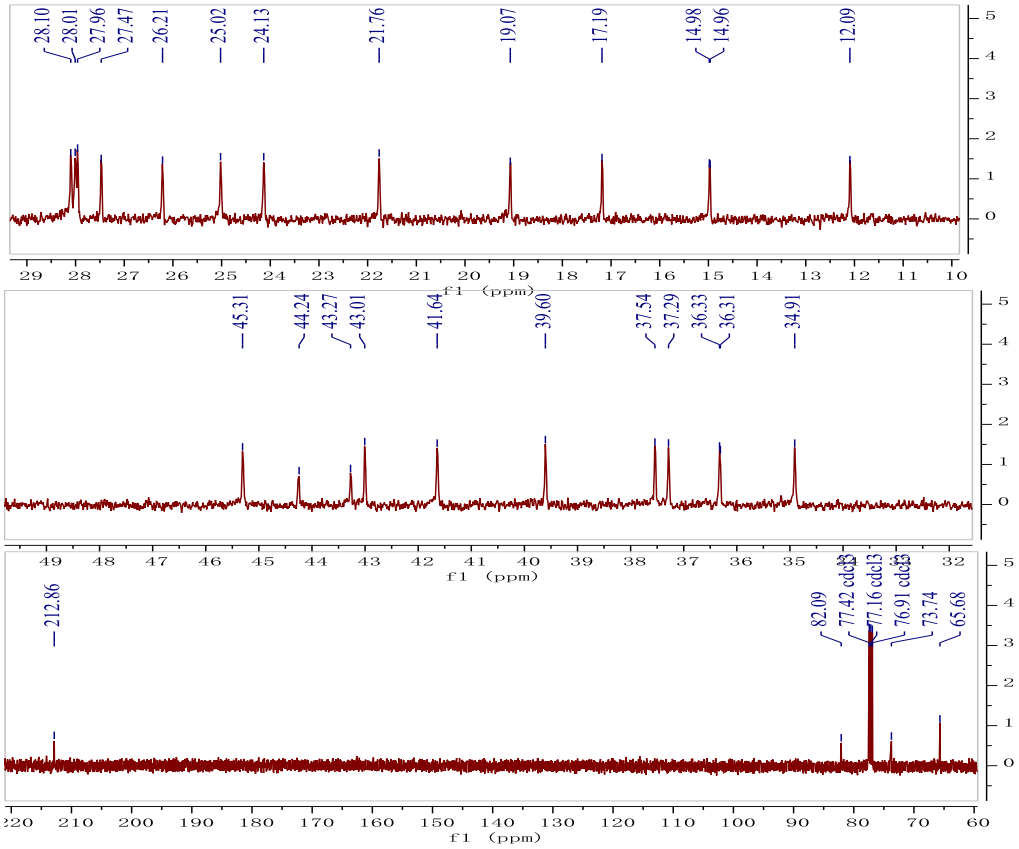

Fig.S27. The amplificatory ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

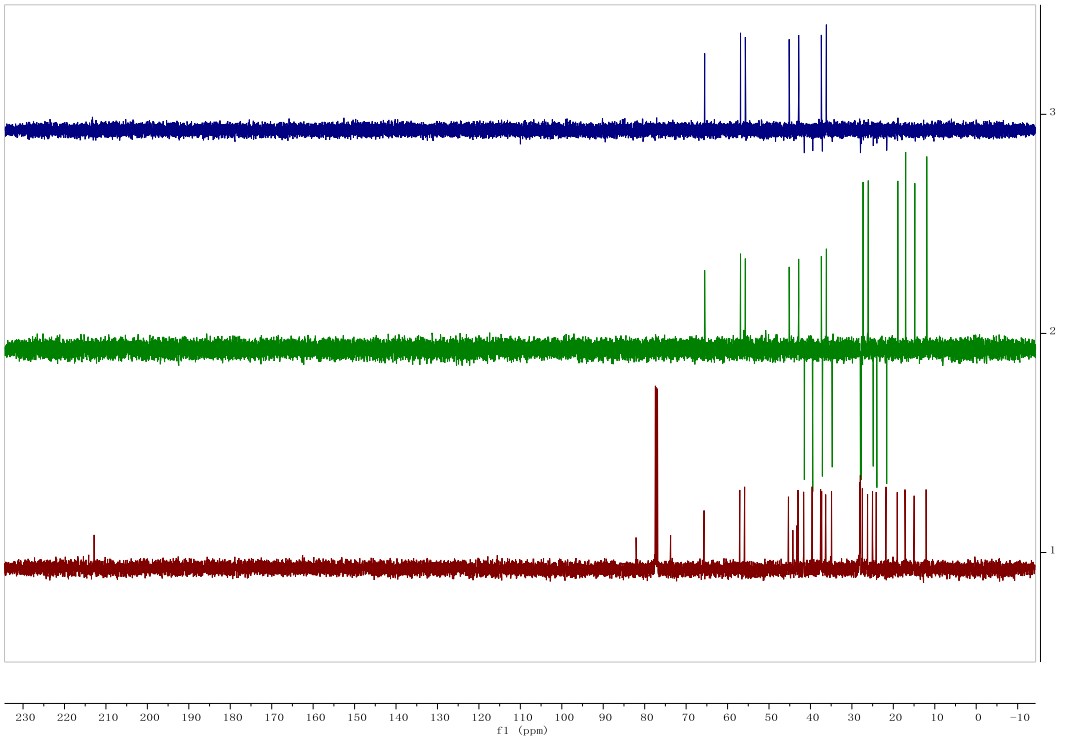

Fig.S28. DEPT spectrum of compound **3** in $CDCl_3$.

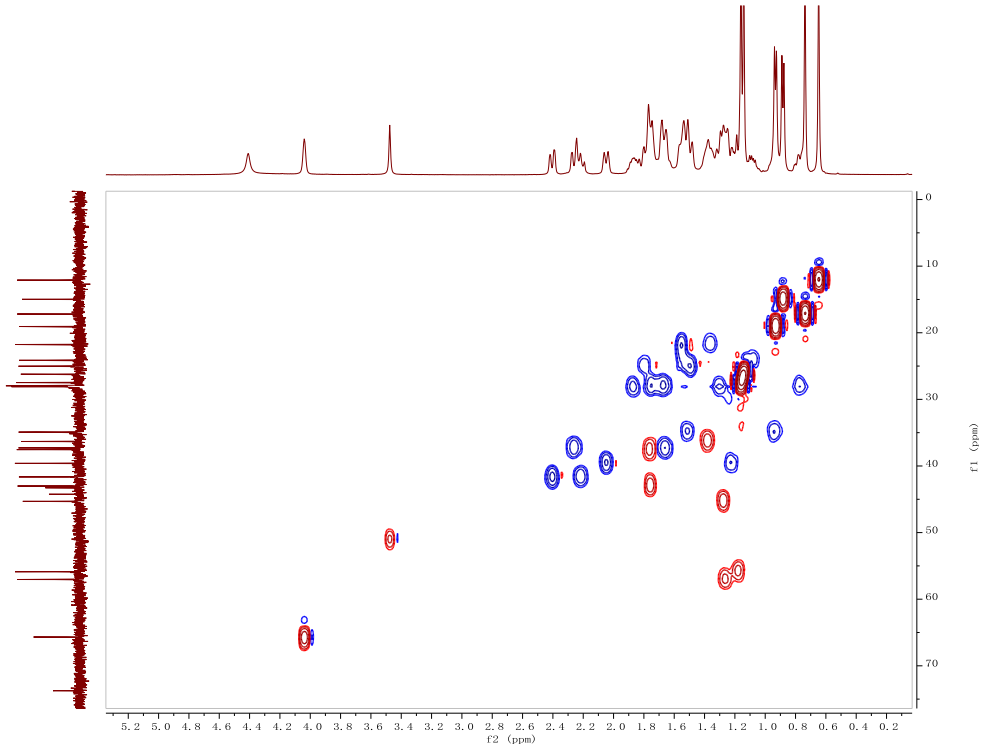

Fig.S29. HSQC spectrum of compound **3** in $CDCl_3$.

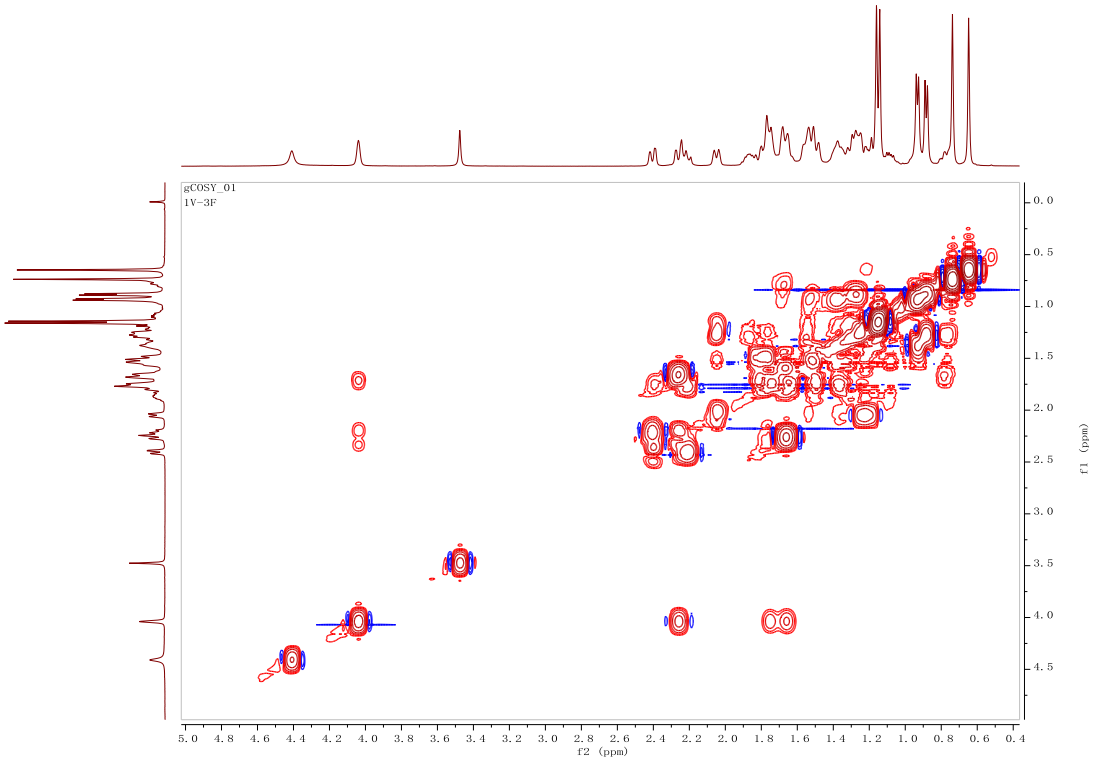

Fig.S30. $^1H,^1H$-COSY spectrum of compound **3** in $CDCl_3$.

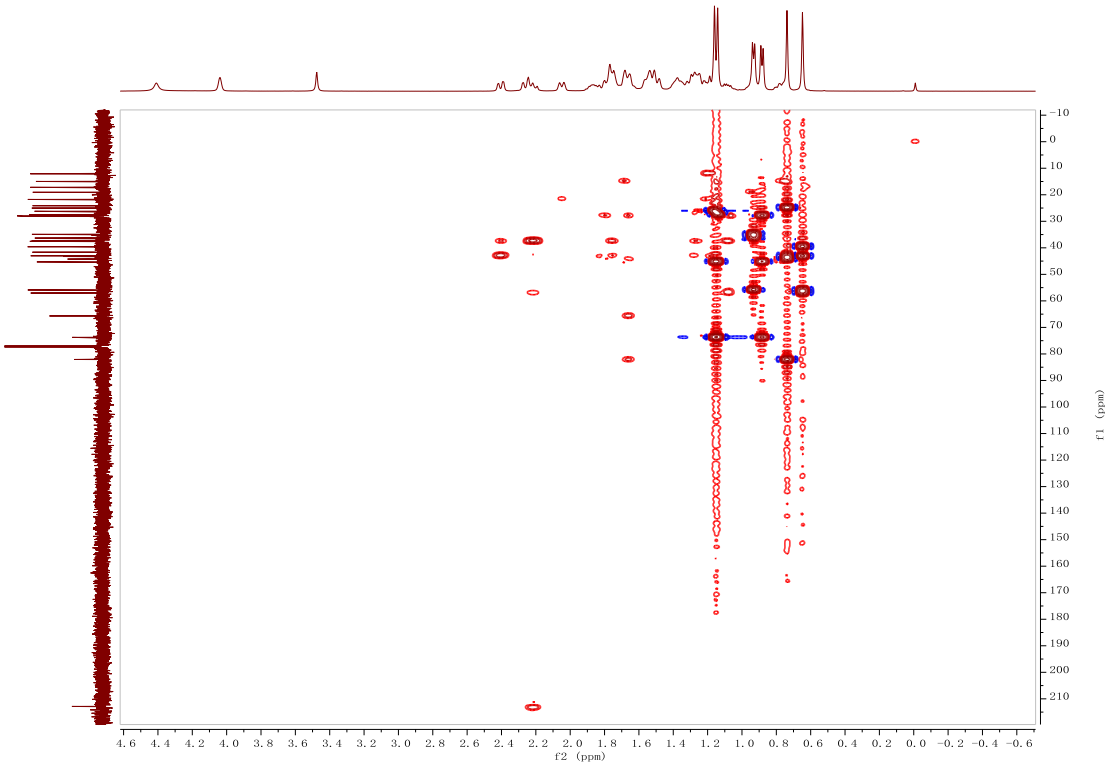

Fig.S31. HMBC spectrum of compound **3** in $CDCl_3$.

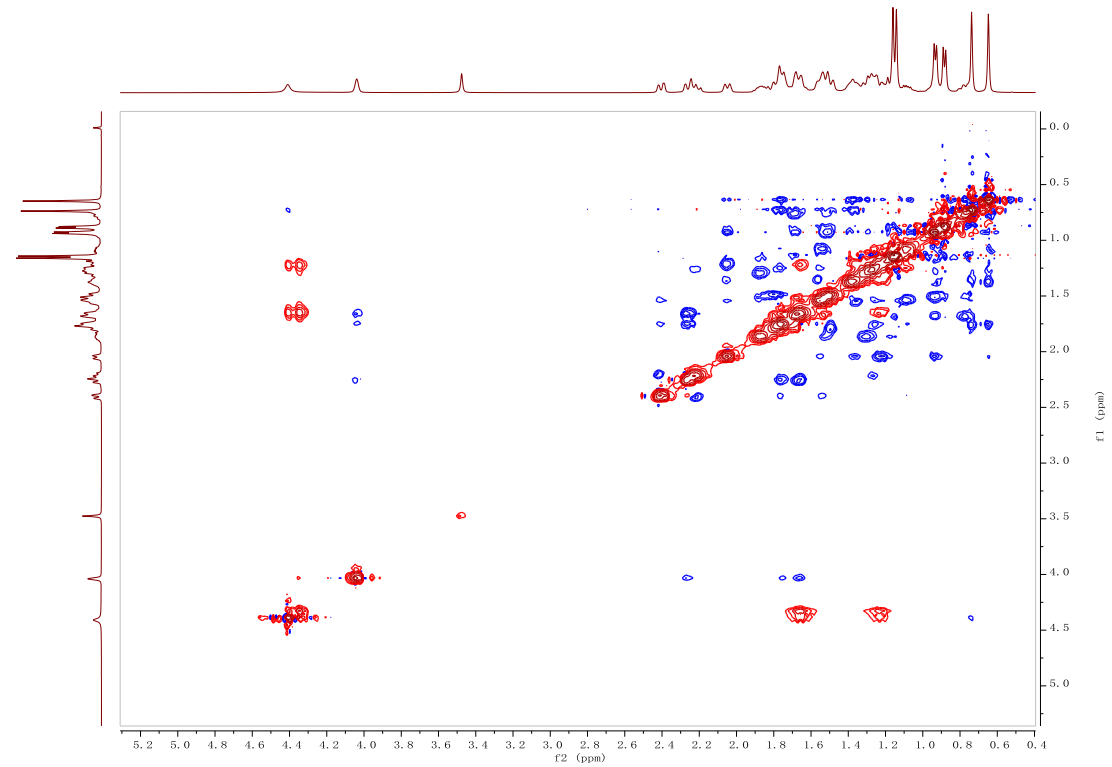

Fig.S32. NOESY spectrum of compound **3** in $CDCl_3$.

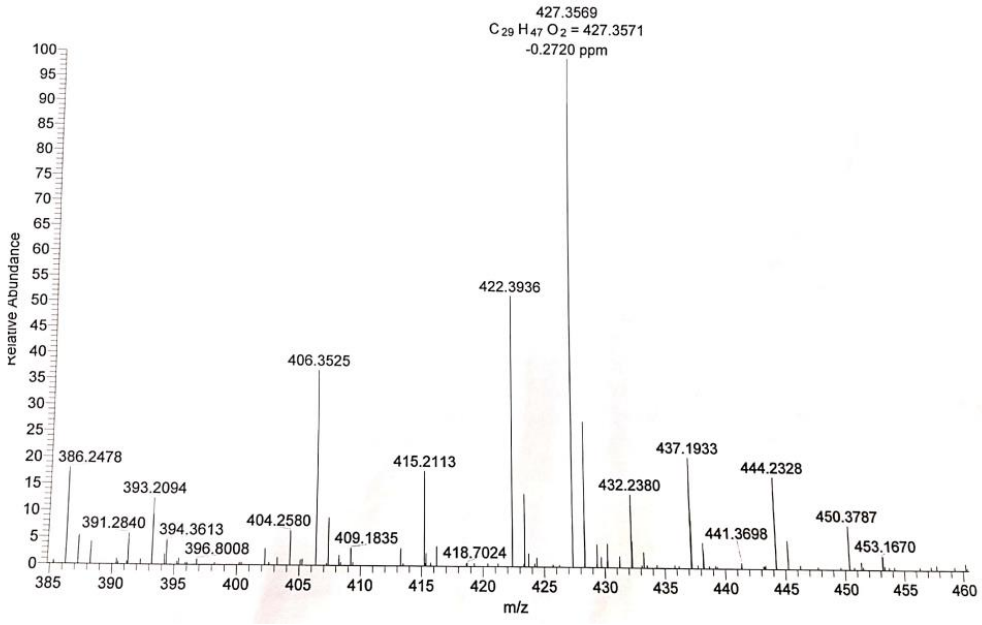

Fig.S33. HRESIMS spectrum of compound **4**.

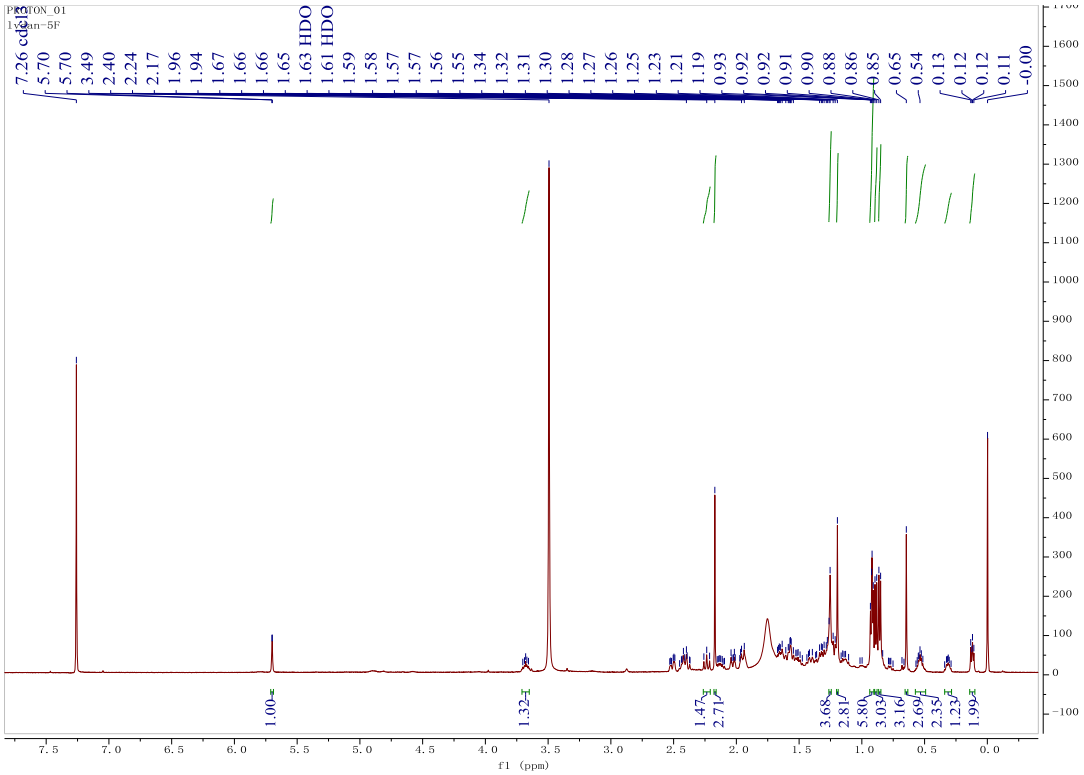

Fig.S34. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

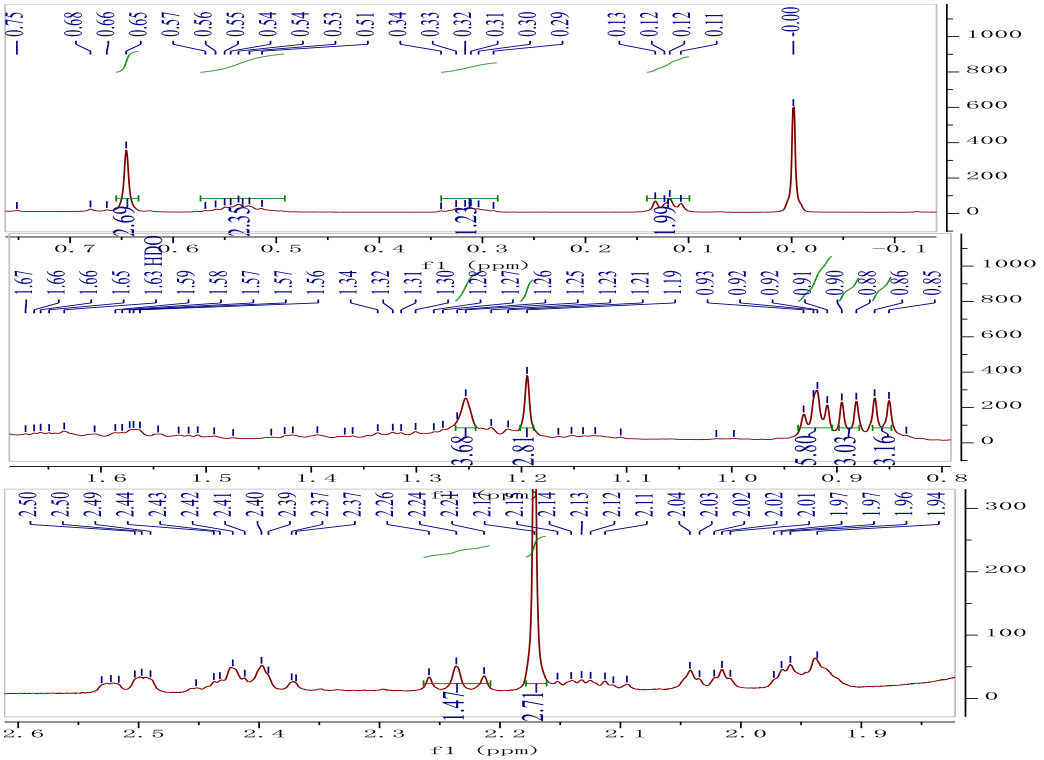

Fig.S35. The amplificatory ^{1}H NMR spectrum of compound **4** in $CDCl_3$

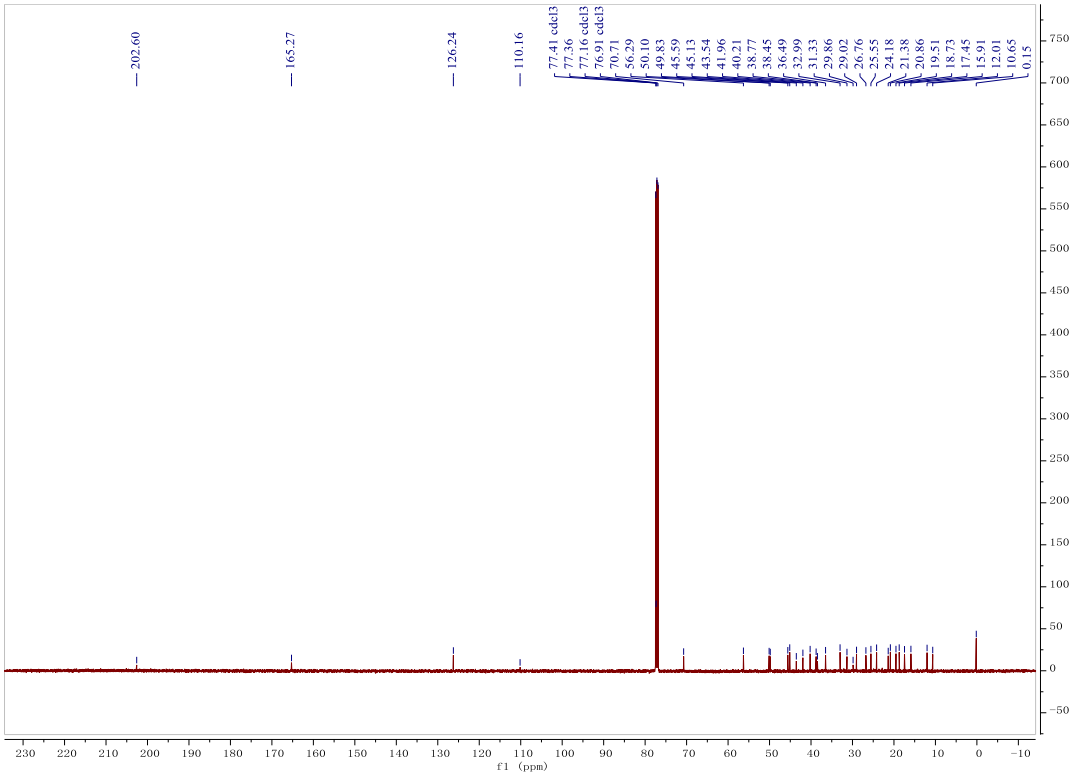

Fig.S36. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

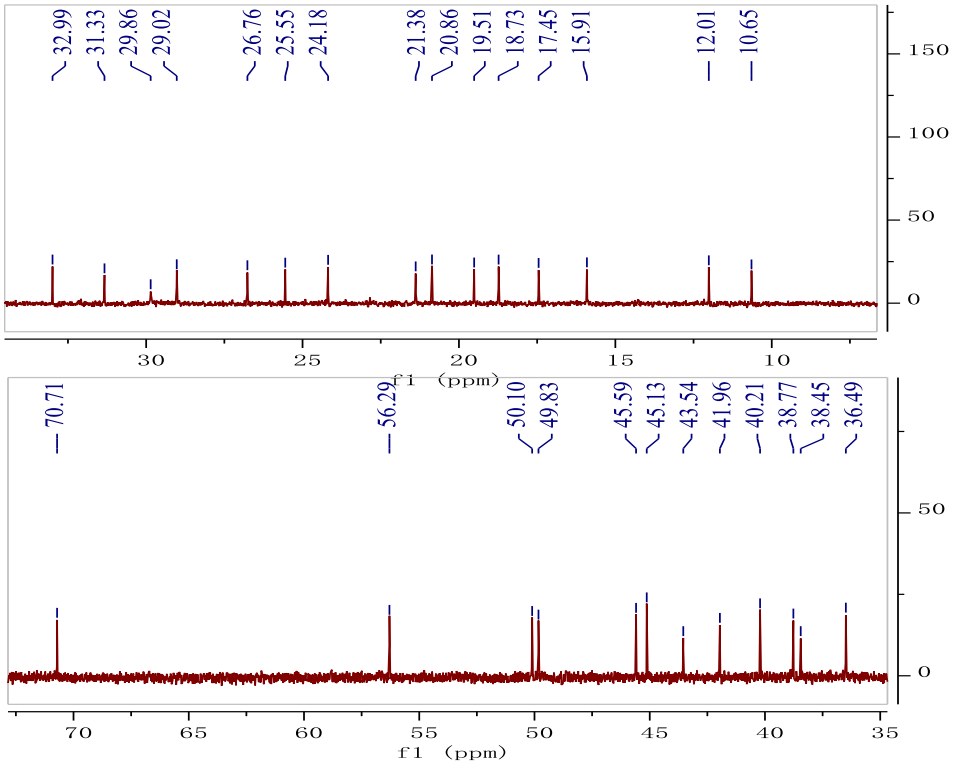

Fig.S37. The amplificatory ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

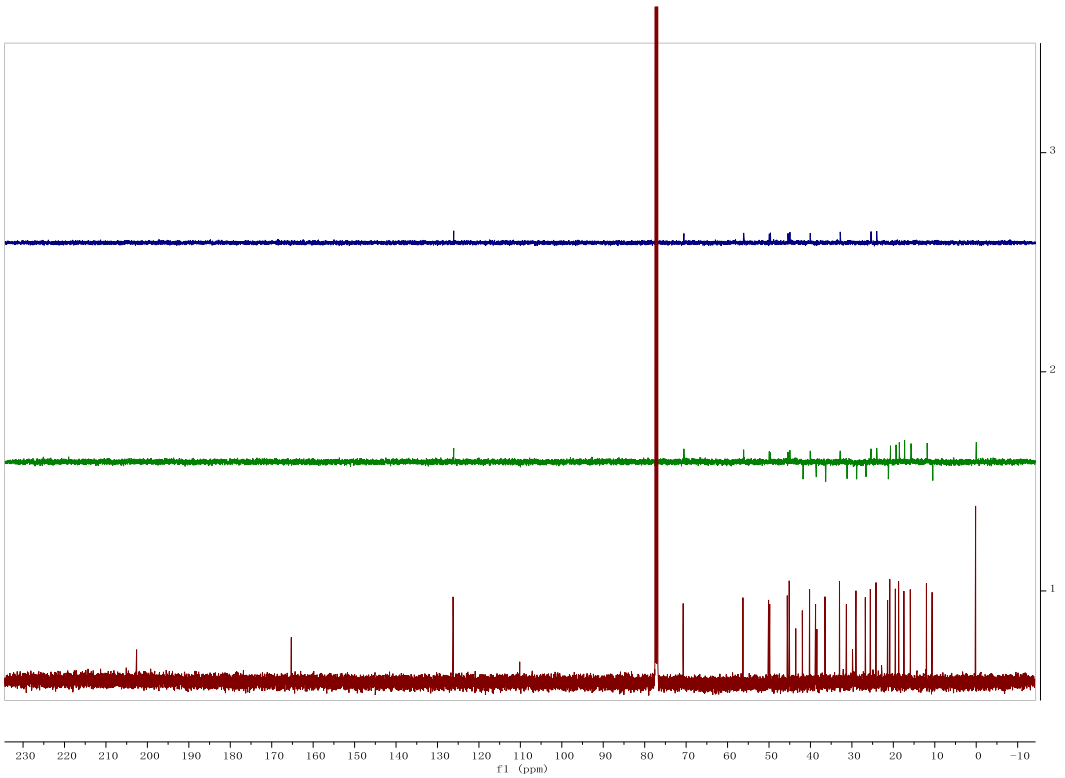

Fig.S38. DEPT spectrum of compound **4** in $CDCl_3$.

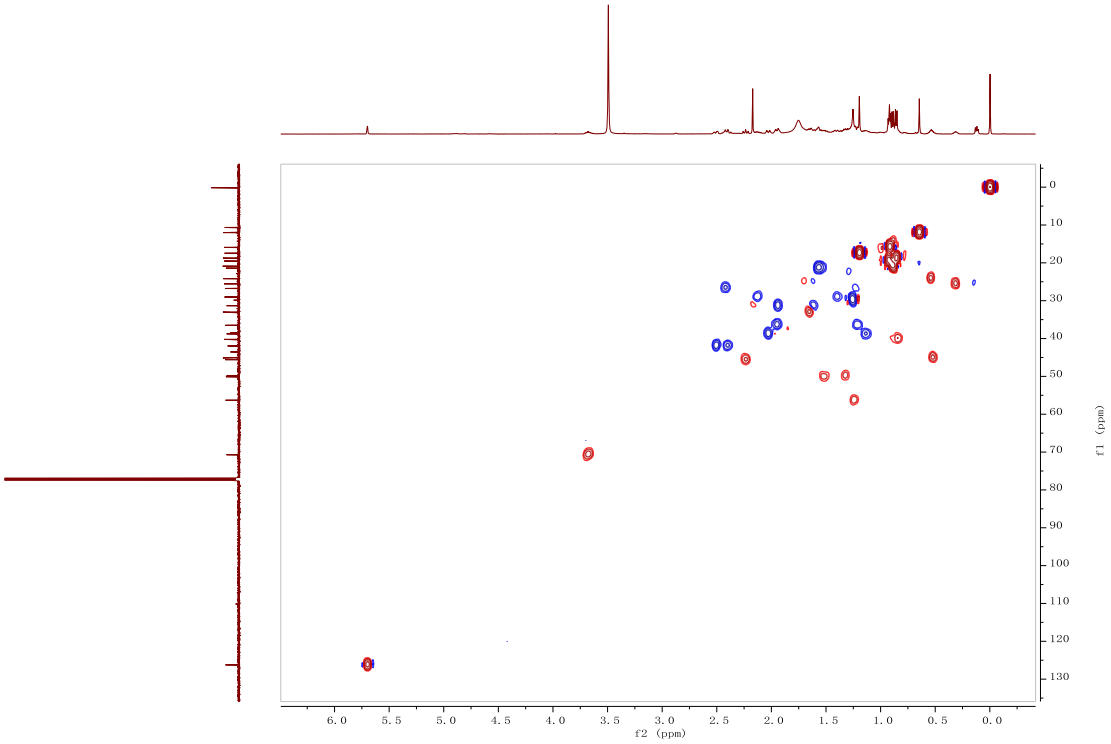

Fig.S39. HSQC spectrum of compound **4** in $CDCl_3$.

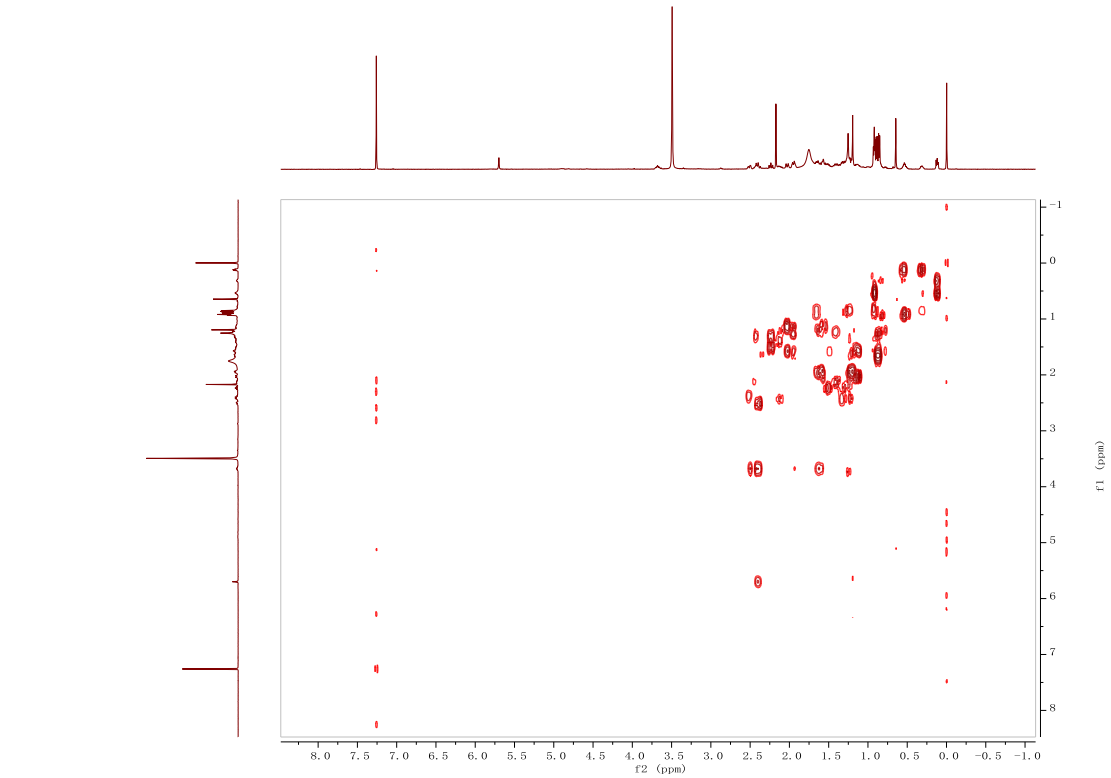

Fig. S40. $^{1}H,^{1}H$-COSY spectrum of compound **4** in $CDCl_3$.

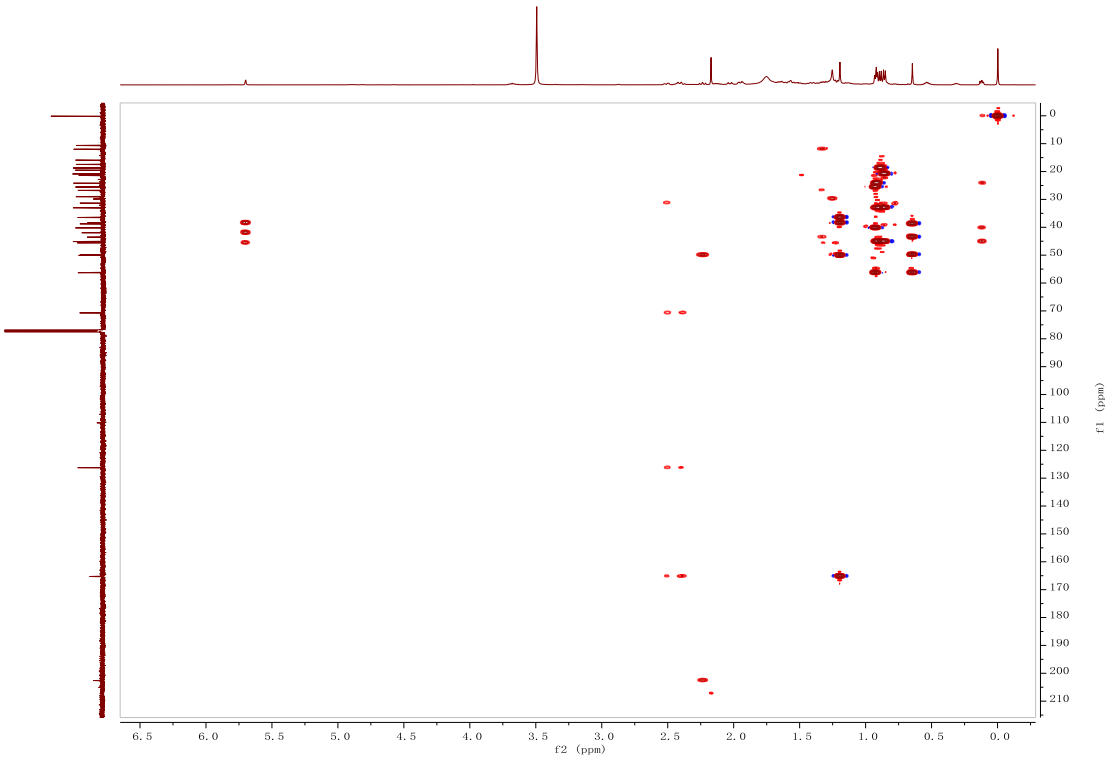

Fig. S41. HMBC spectrum of compound **4** in $CDCl_3$.

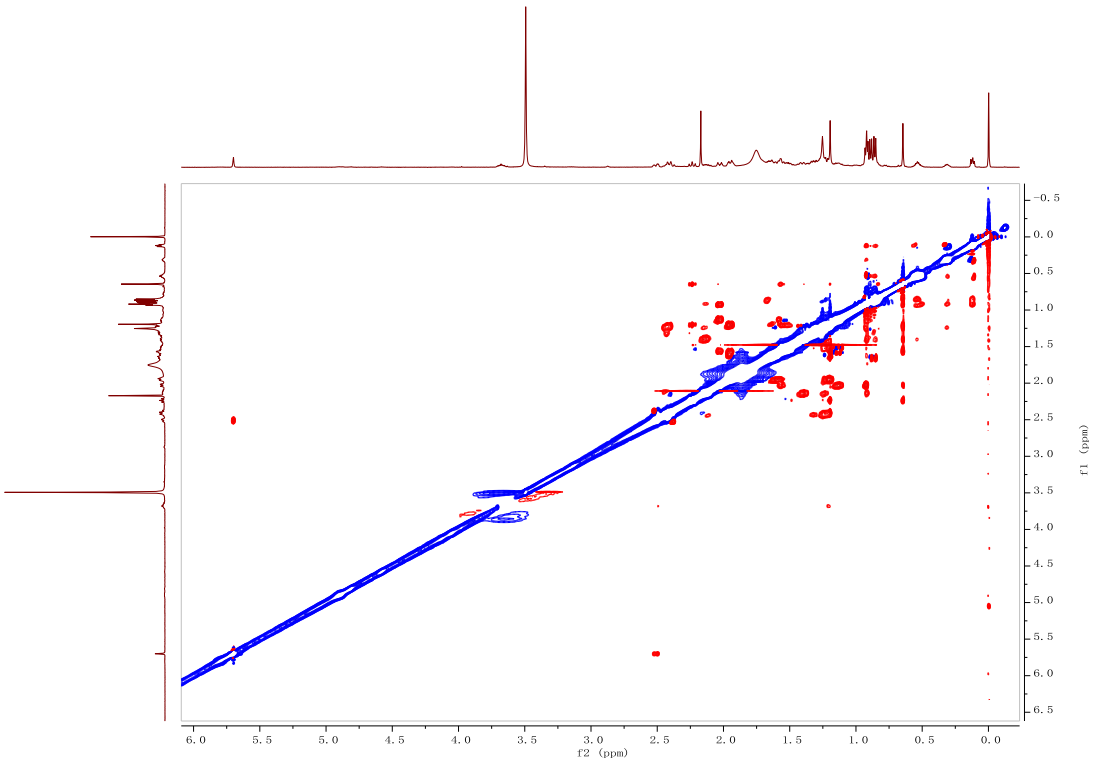

Fig. S42. NOESY spectrum of compound **4** in $CDCl_3$.

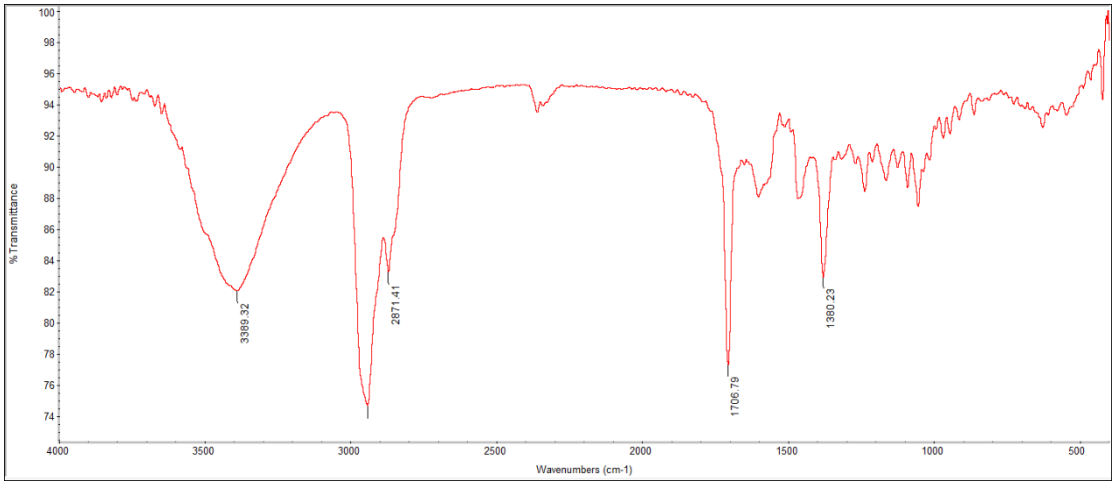

Fig. S43. IR (KBr disc) spectrum of compound **1**.

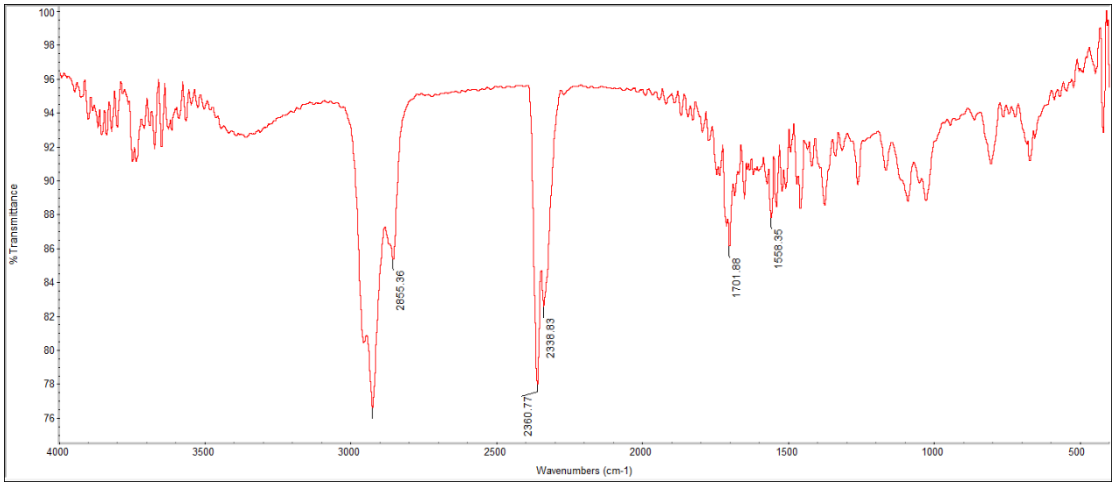

Fig. S44. IR (KBr disc) spectrum of compound **2**.

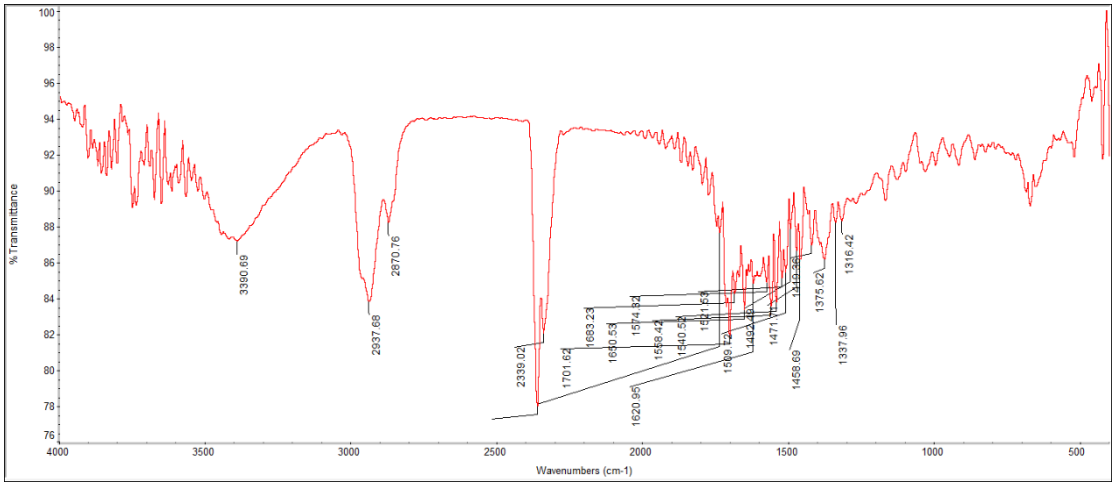

Fig. S45. IR (KBr disc) spectrum of compound **3**.

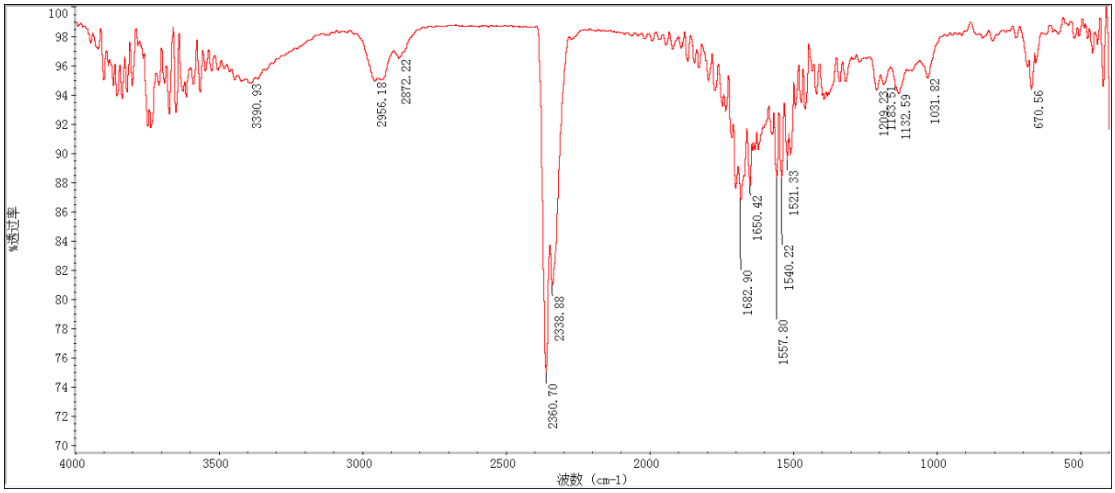

Fig. S46. IR (KBr disc) spectrum of compound **4**.