

Supplementary Materials

Genome Mining of Marine-derived *Streptomyces* sp. SCSIO 40010 Leads to New Polycyclic Tetramate Macrolactams

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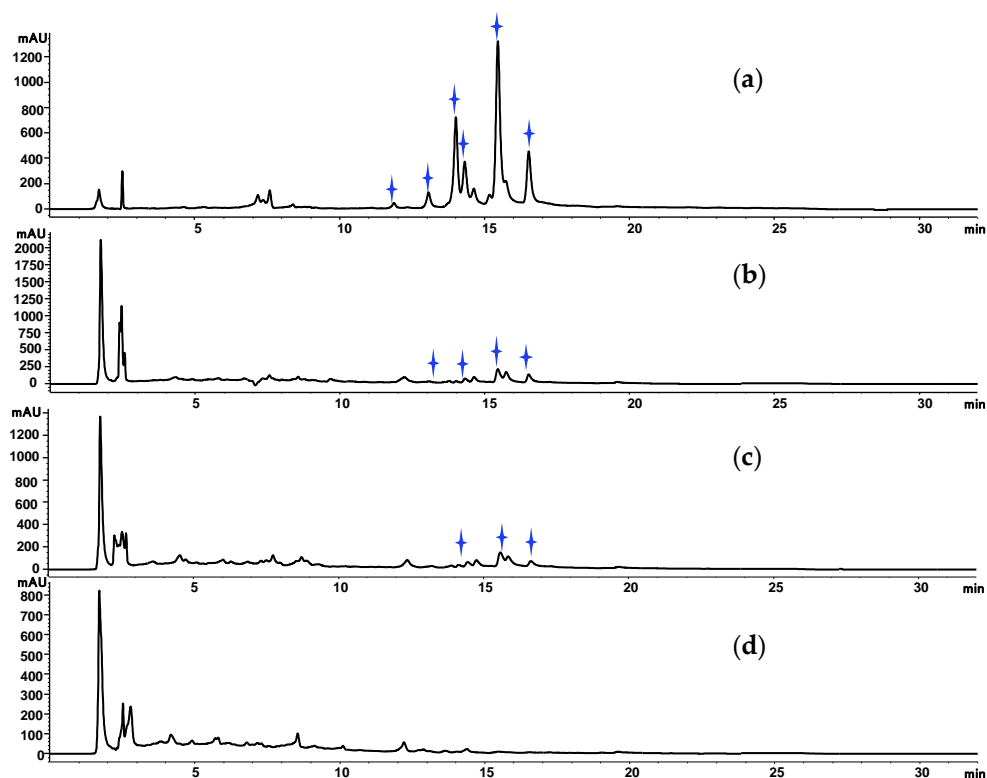
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Content

Figure S1. HPLC analysis of metabolite profiles of <i>Streptomyces</i> sp. SCSIO 40010 cultured in different media.....	S4
Figure S2. HRESIMS (a) and IR(b) of compound 1	S5
Figure S3. ¹ H NMR spectrum of compound 1 in DMSO- <i>d</i> ₆	S6
Figure S4. The ¹³ C NMR and DEPT 135 spectra of compound 1 in DMSO- <i>d</i> ₆	S7
Figure S5. The HSQC spectrum of compound 1 in DMSO- <i>d</i> ₆	S8
Figure S6. The HMBC spectrum of compound 1 in DMSO- <i>d</i> ₆	S9
Figure S7. The ¹ H- ¹ H COSY spectrum of compound 1 in DMSO- <i>d</i> ₆	S10
Figure S8. The NOESY spectrum of compound 1 in DMSO- <i>d</i> ₆	S11
Figure S9. The key NOESY spectrum of compound 1 in DMSO- <i>d</i> ₆	S12
Figure S10. Comparison of ECD spectra of compound 1-6 and the known compounds.....	S13
Figure S11. HRESIMS (a) and IR(b) of compound 2	S14
Figure S12. ¹ H NMR spectrum of compound 2 in DMSO- <i>d</i> ₆	S15
Figure S13. The ¹³ C NMR and DEPT 135 spectra of compound 2 in DMSO- <i>d</i> ₆	S16
Figure S14. The HSQC spectrum of compound 2 in DMSO- <i>d</i> ₆	S17
Figure S15. The HMBC spectrum of compound 2 in DMSO- <i>d</i> ₆	S18
Figure S16. The ¹ H- ¹ H COSY spectrum of compound 2 in DMSO- <i>d</i> ₆	S19
Figure S17. The NOESY spectrum of compound 2 in DMSO- <i>d</i> ₆	S20
Figure S18. The key NOESY spectrum of compound 2 in DMSO- <i>d</i> ₆	S21
Figure S19. HRESIMS (a) and IR(b) of compound 3	S22
Figure S20. ¹ H NMR spectrum of compound 3 in DMSO- <i>d</i> ₆	S23
Figure S21. The ¹³ C NMR and DEPT 135 spectra of compound 3 in DMSO- <i>d</i> ₆	S24
Figure S22. The HSQC spectrum of compound 3 in DMSO- <i>d</i> ₆	S25
Figure S23. The HMBC spectrum of compound 3 in DMSO- <i>d</i> ₆	S26
Figure S24. The ¹ H- ¹ H COSY spectrum of compound 3 in DMSO- <i>d</i> ₆	S27
Figure S25. The NOESY spectrum of compound 3 in DMSO- <i>d</i> ₆	S28
Figure S26. The key NOESY spectrum of compound 3 in DMSO- <i>d</i> ₆	S29
Figure S27. HRESIMS (a) and IR(b) of compound 4	S30
Figure S28. ¹ H NMR spectrum of compound 4 in DMSO- <i>d</i> ₆	S31
Figure S29. The ¹³ C NMR and DEPT 135 spectra of compound 4 in DMSO- <i>d</i> ₆	S32
Figure S30. The HSQC spectrum of compound 4 in DMSO- <i>d</i> ₆	S33
Figure S31. The HMBC spectrum of compound 4 in DMSO- <i>d</i> ₆	S34

Figure S32. The ^1H - ^1H HCOSY spectrum of compound 4 in $\text{DMSO-}d_6$	S35
Figure S33. The NOESY spectrum of compound 4 in $\text{DMSO-}d_6$	S36
Figure S34. The key NOESY spectrum of compound 4 in $\text{DMSO-}d_6$	S37
Figure S35. HRESIMS (a) and IR(b) of compound 5	S38
Figure S36. ^1H NMR spectrum of compound 5 in $\text{DMSO-}d_6$	S39
Figure S37. The ^{13}C NMR and DEPT 135 spectra of compound 5 in $\text{DMSO-}d_6$	S40
Figure S38. The HSQC spectrum of compound 5 in $\text{DMSO-}d_6$	S41
Figure S39. The HMBC spectrum of compound 5 in $\text{DMSO-}d_6$	S42
Figure S40. The ^1H - ^1H HCOSY spectrum of compound 5 in $\text{DMSO-}d_6$	S43
Figure S41. The NOESY spectrum of compound 5 in $\text{DMSO-}d_6$	S44
Figure S42. The key NOESY spectrum of compound 5 in $\text{DMSO-}d_6$	S45
Figure S43. HRESIMS (a) and IR(b) of compound 6	S46
Figure S44. ^1H NMR spectrum of compound 6 in $\text{DMSO-}d_6$	S47
Figure S45. The ^{13}C NMR and DEPT 135 spectra of compound 6 in $\text{DMSO-}d_6$	S48
Figure S46. The HSQC spectrum of compound 6 in $\text{DMSO-}d_6$	S49
Figure S47. The HMBC spectrum of compound 6 in $\text{DMSO-}d_6$	S50
Figure S48. The ^1H - ^1H HCOSY spectrum of compound 6 in $\text{DMSO-}d_6$	S51
Figure S49. The NOESY spectrum of compound 6 in $\text{DMSO-}d_6$	S52
Figure S50. The key NOESY spectrum of compound 6 in $\text{DMSO-}d_6$	S53

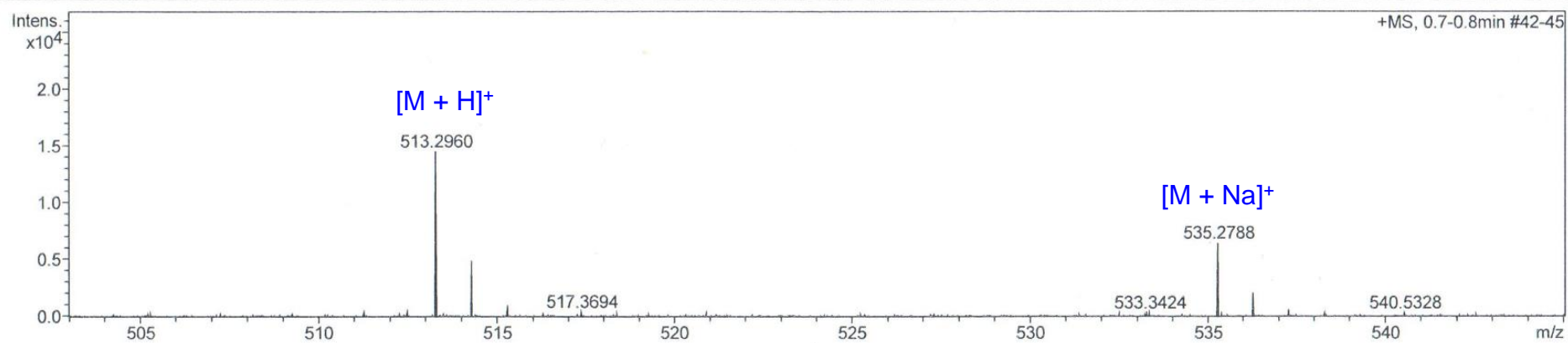
Figure S1. HPLC analysis of metabolite profiles of *Streptomyces* sp. SCSIO 40010 cultured in different media.



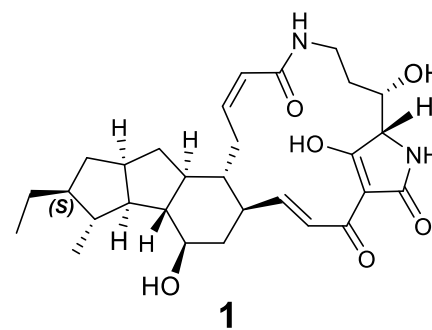
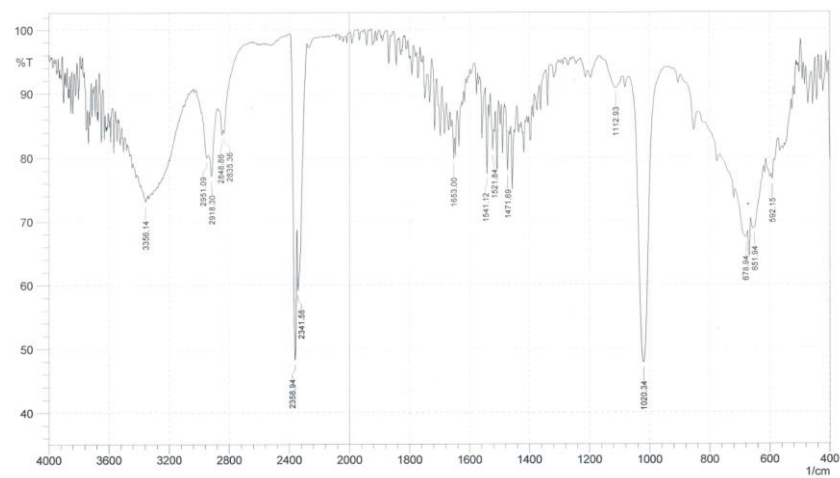
Note: blue star-PTM analogue. (a) modified-A1BFe+C (soluble starch 1.0%, yeast extract 0.4%, tryptone 0.2%, CaCO_3 0.2%, sea salts 3%, pH 7.2–7.4); (b) AM6 medium (soluble starch 2.0%, glucose 1.0%, tryptone 0.5%, yeast extract 0.5%, CaCO_3 0.2%, sea salts 3%, pH 7.2–7.4); (c) AM6-4 (glycerol 0.1%, bacterial peptone 0.5%, glycine 0.01%, alanine 0.01%, CaCO_3 0.5%, sea salts 3%, pH 7.2–7.4). (d) Modified-ISP3 (oat meal 1.5%, FeSO_4 0.0001%, MnCl_2 0.0001%, ZnSO_4 0.0001%, sea salts 3%, pH 7.2–7.4).

Figure S2. HRESIMS (a) and IR(b) of compound 1.

(a) HRESIMS



(b) IR



Chemical Formula: C₂₉H₄₀N₂O₆
calculated for [M+H]⁺: 513.2965
calculated for [M+Na]⁺: 535.2784

Figure S3. ^1H NMR spectrum of compound **1** in $\text{DMSO-}d_6$.

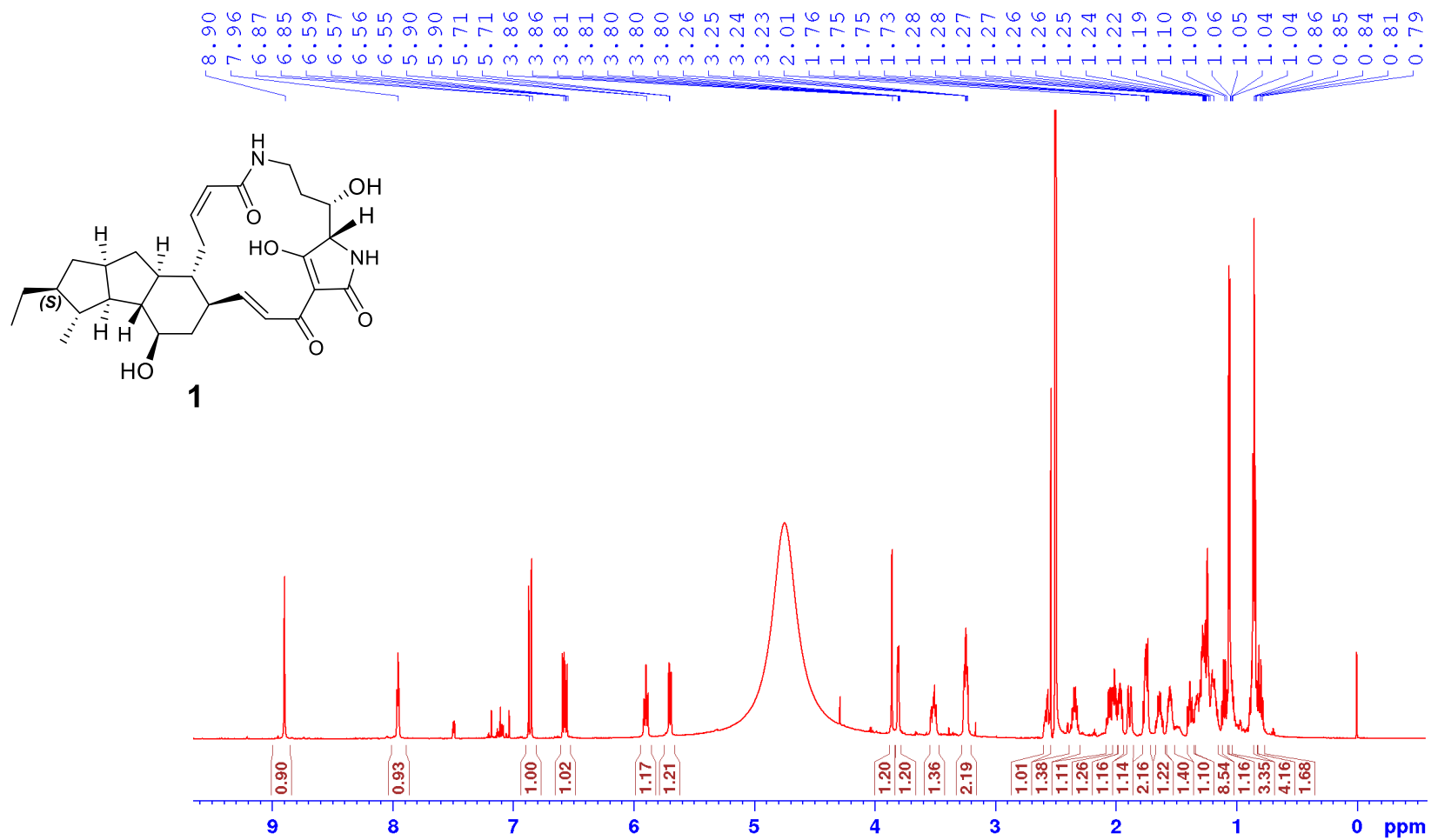


Figure S4. The ^{13}C NMR and DEPT 135 spectra of compound **1** in $\text{DMSO-}d_6$.

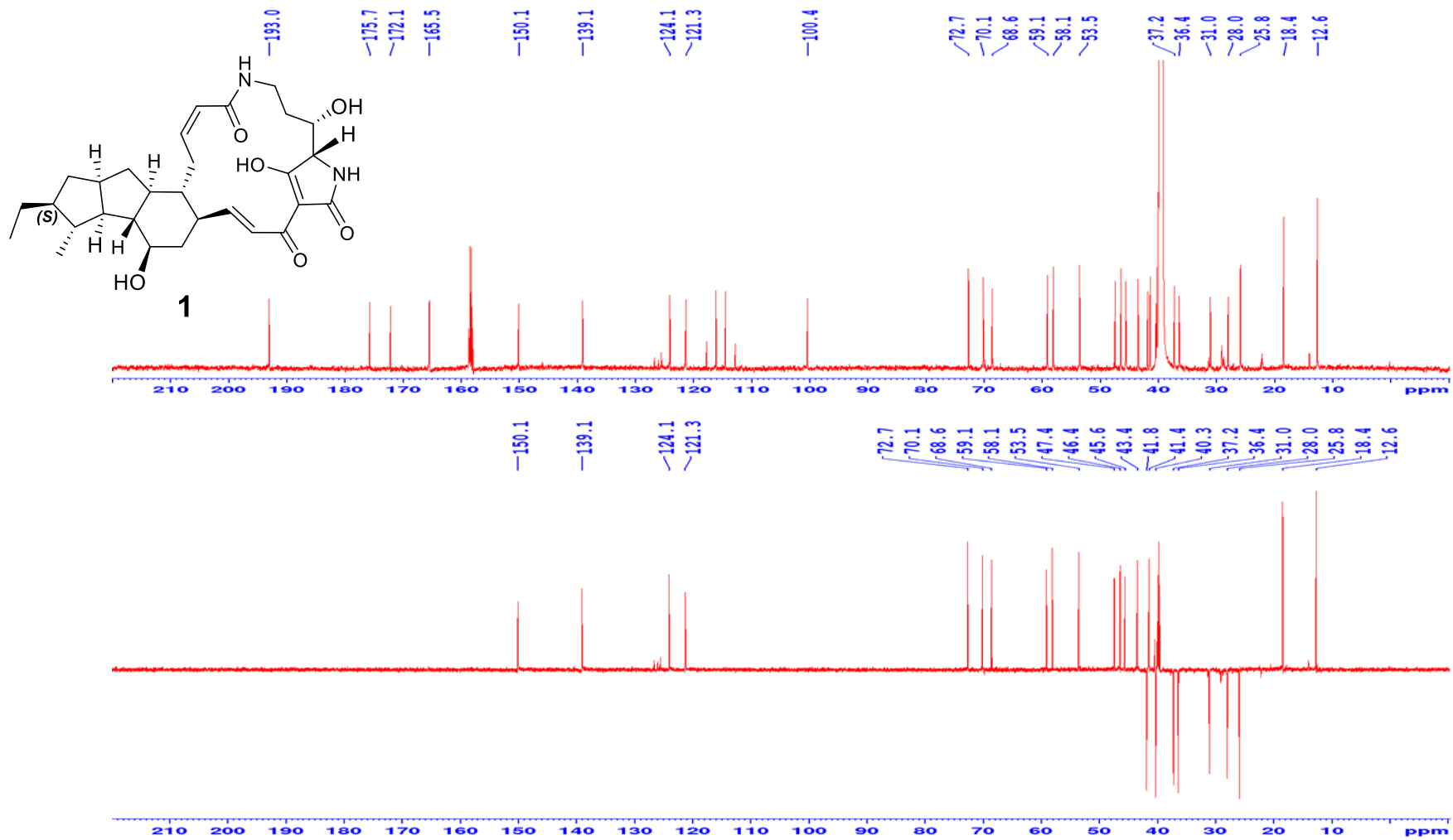


Figure S5. The HSQC spectrum of compound **1** in DMSO-*d*₆.

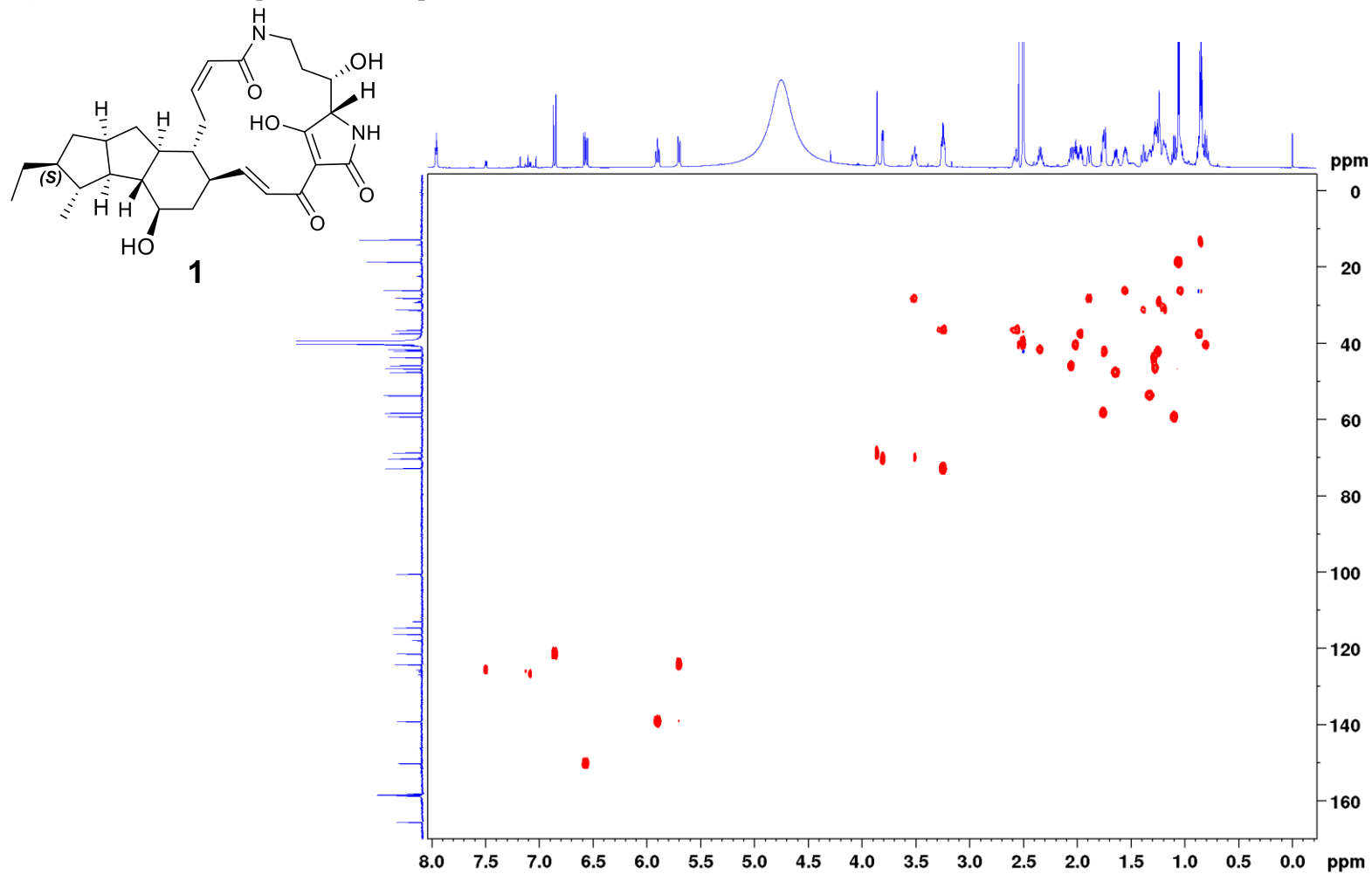


Figure S6. The HMBC spectrum of compound **1** in DMSO-*d*₆.

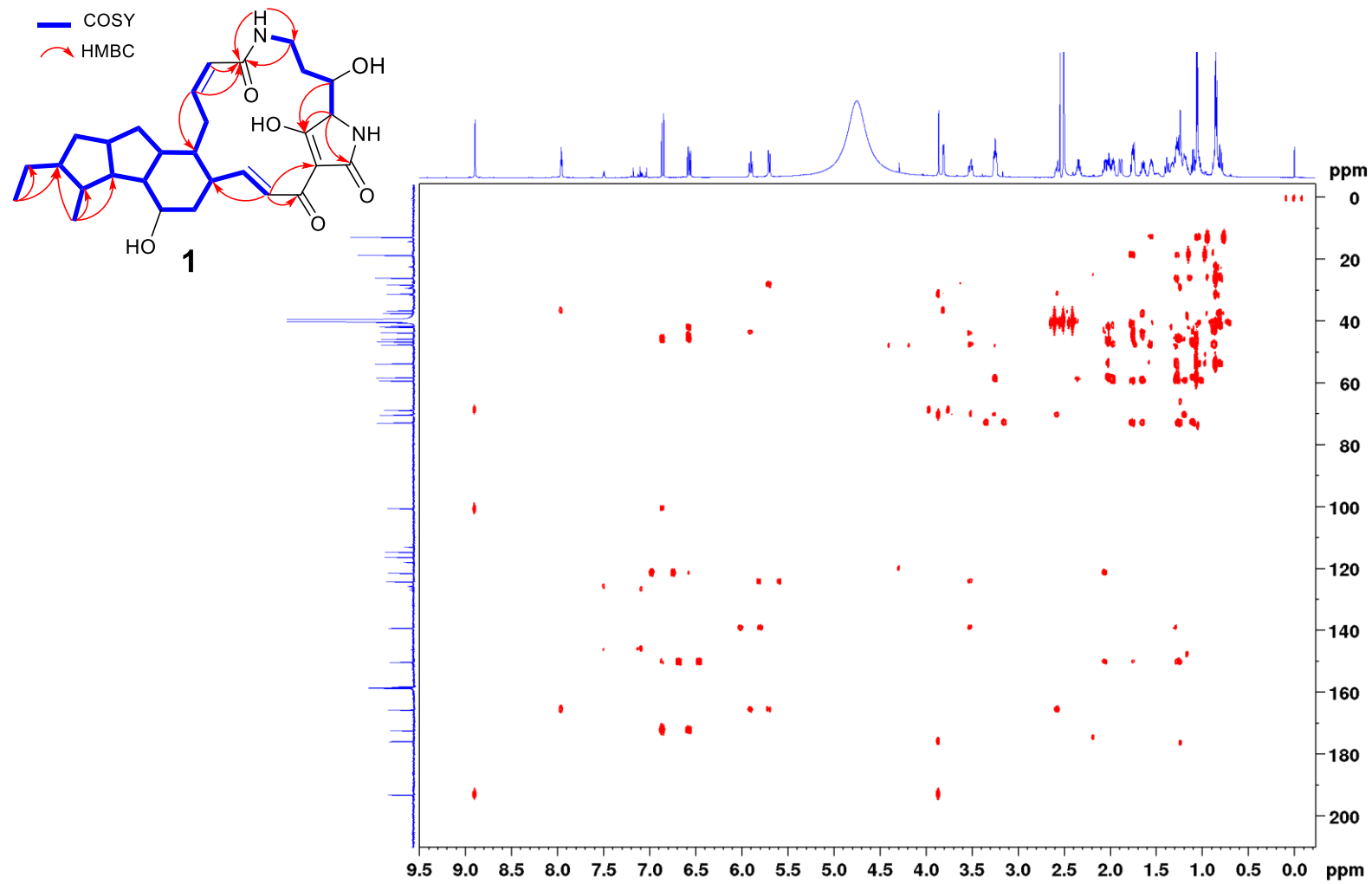


Figure S7. The ^1H - ^1H COSY spectrum of compound **1** in $\text{DMSO-}d_6$.

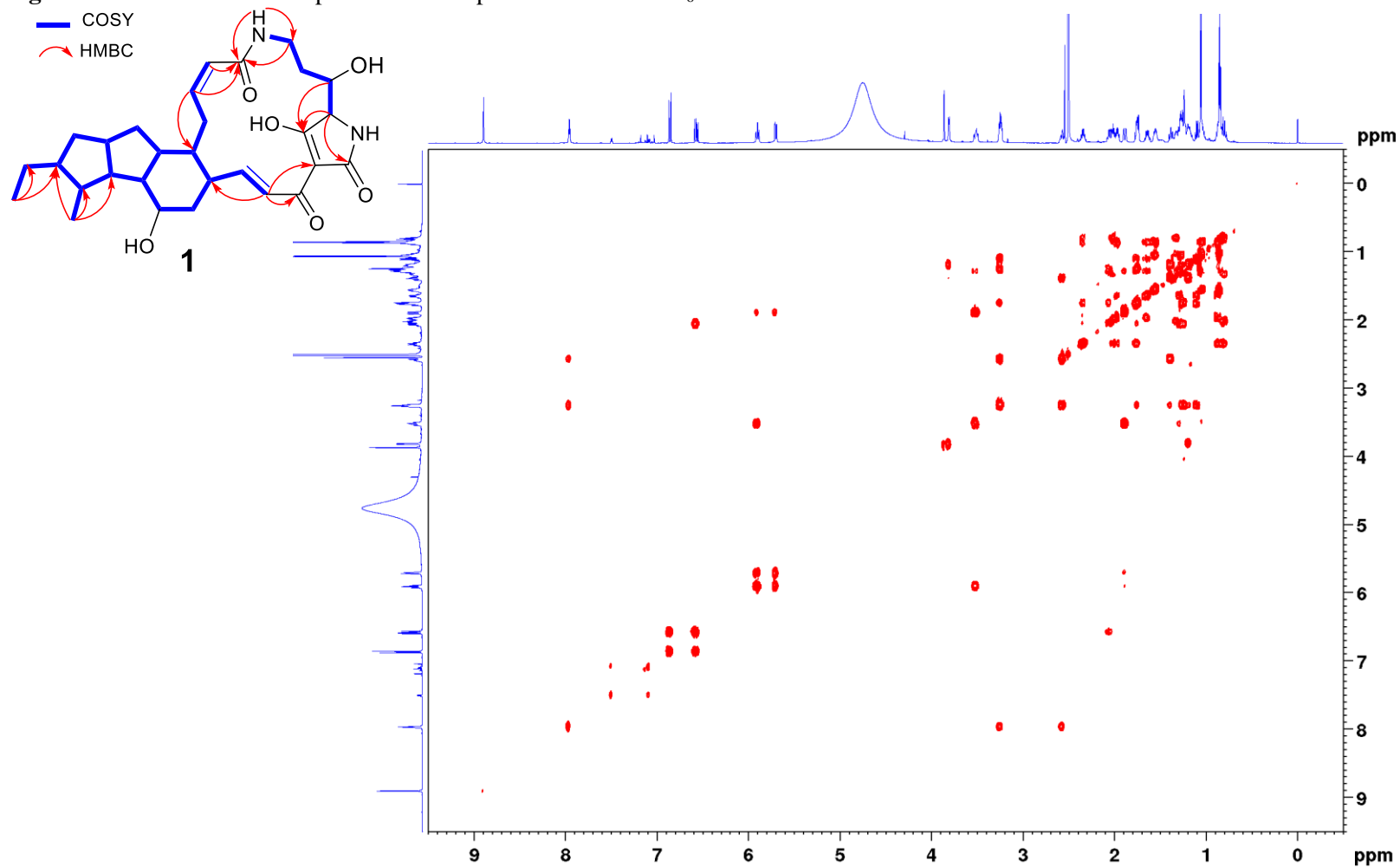


Figure S9. The key NOESY spectrum of compound **1** in DMSO- d_6 .

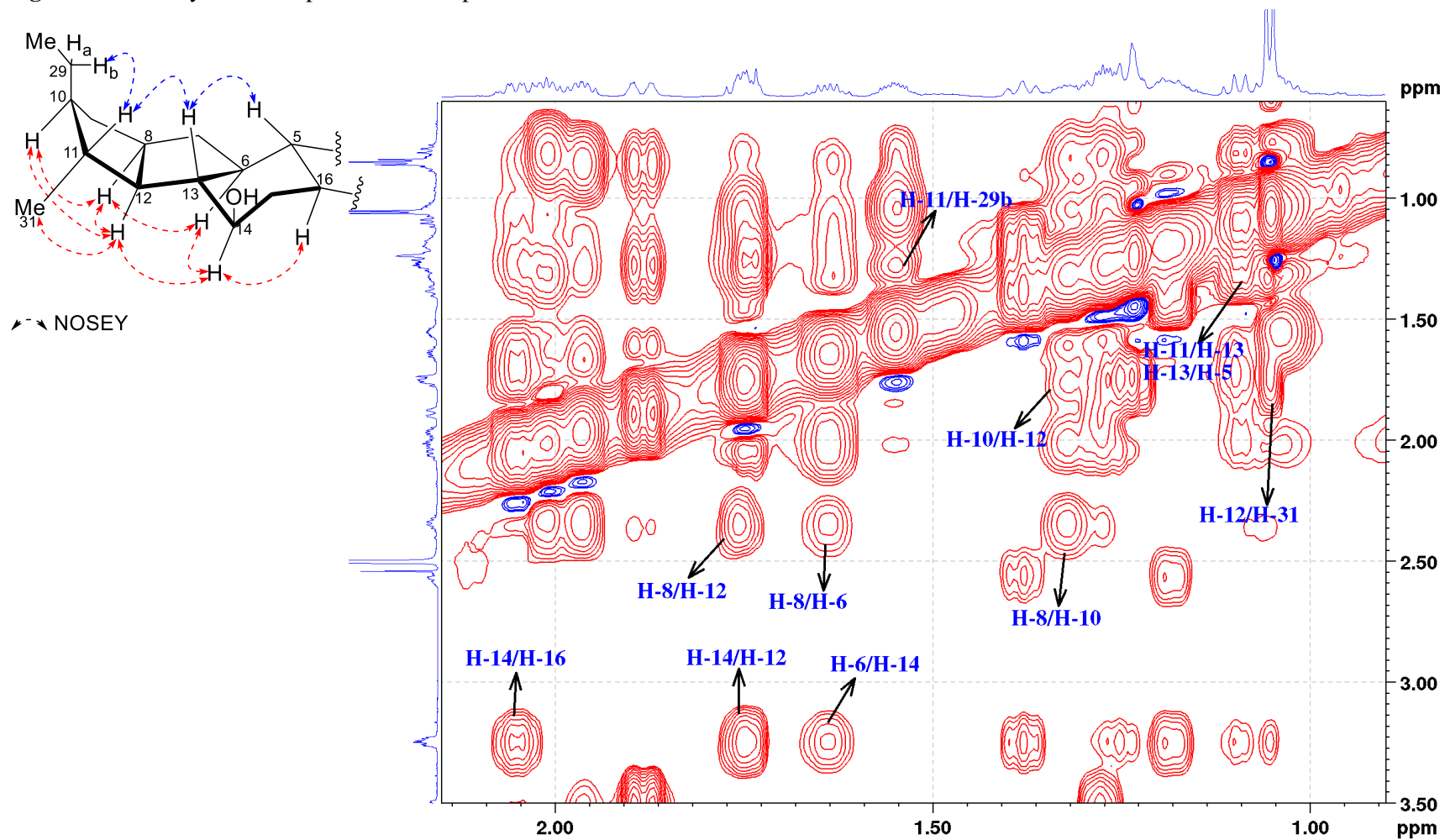
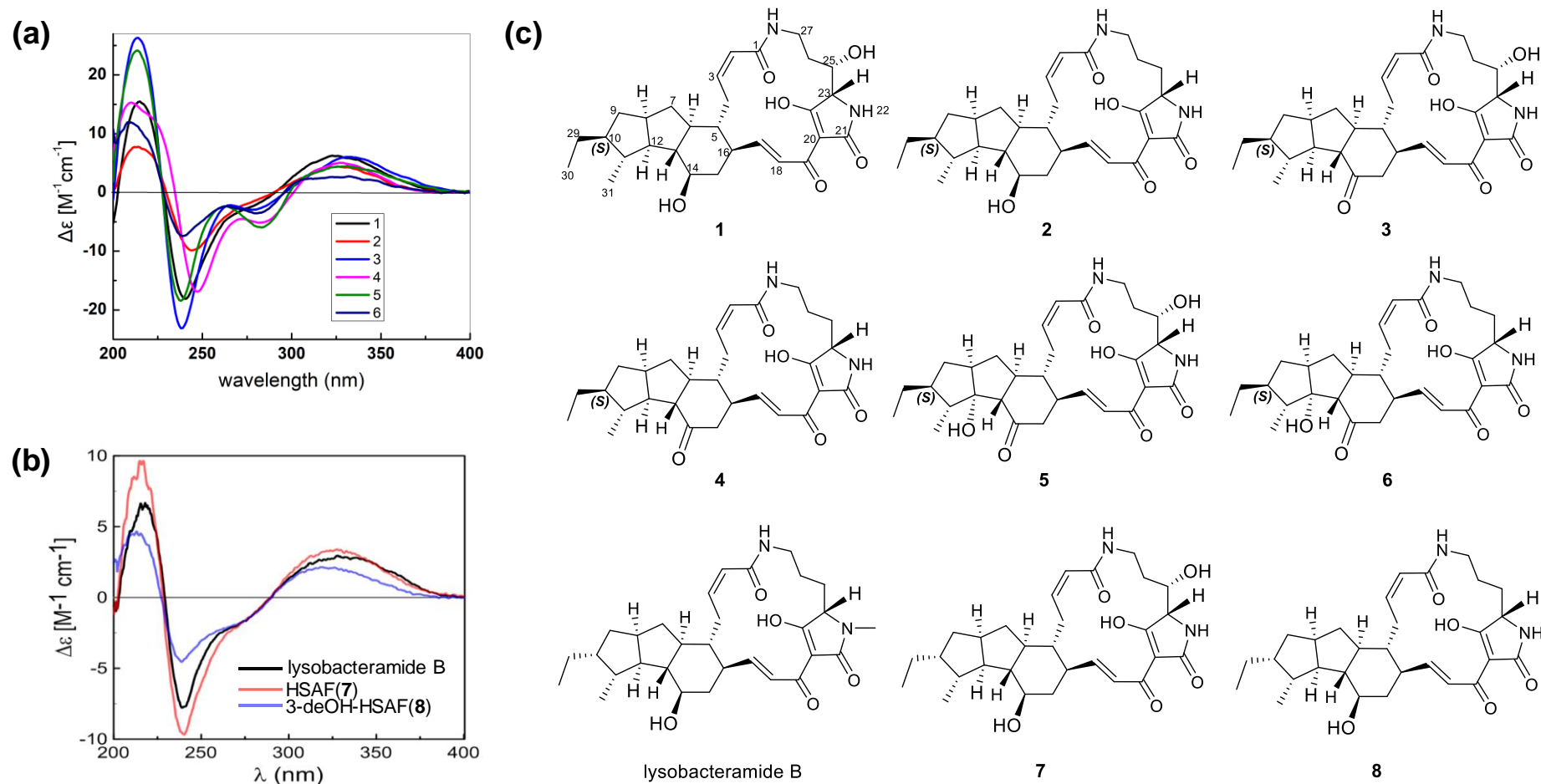


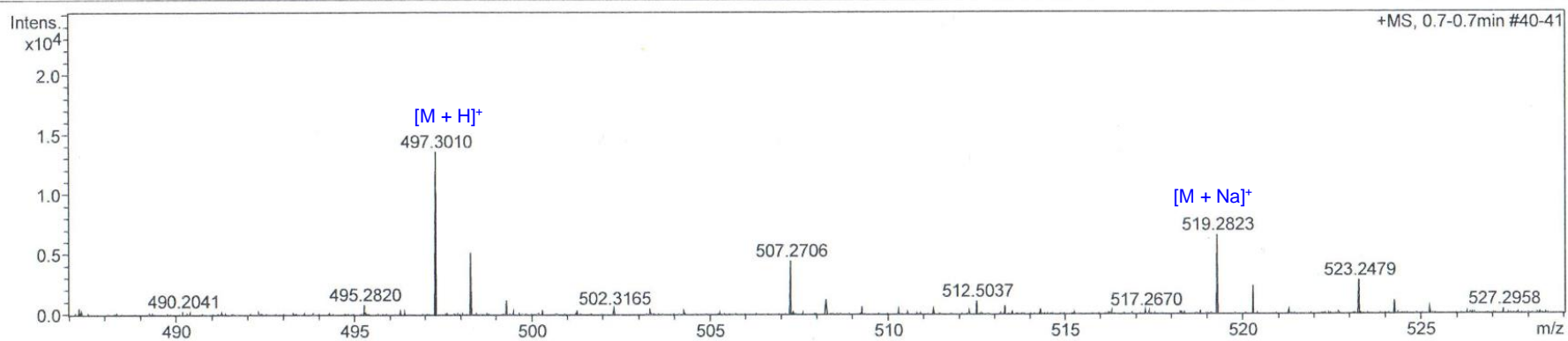
Figure S10. Comparison of ECD spectra of compound 1-6 and the known compounds.



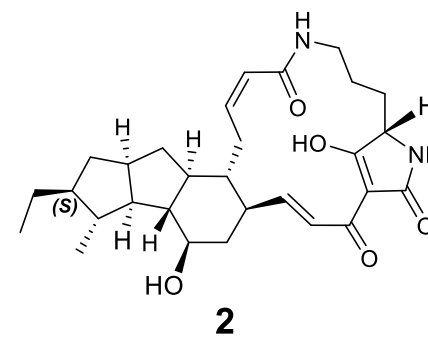
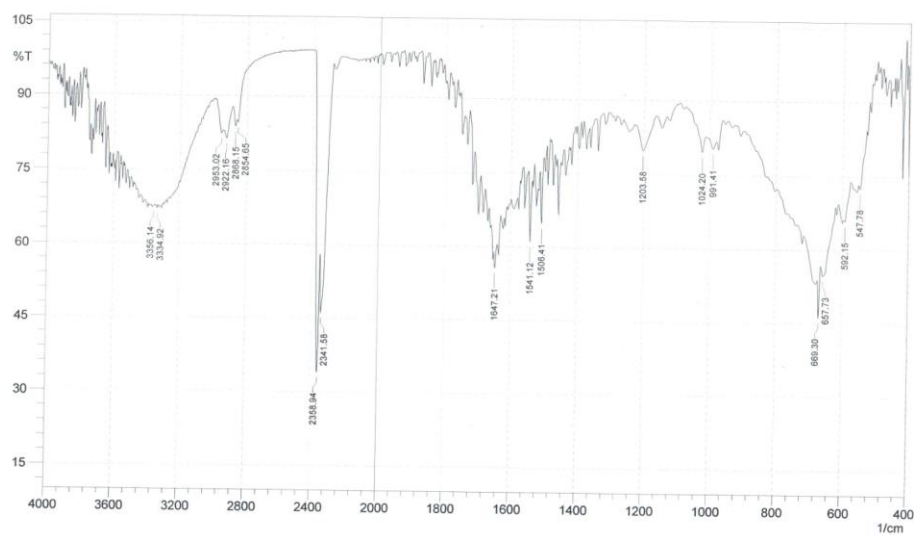
Note: (a) ECD spectra measured for compound 1-6; (b) ECD spectra of lysobacteramide B, HSAF and 3-deOH-HSAF from reference; (c) Chemical structures.

Figure S11. HRESIMS (a) and IR(b) of compound **2**.

(a) HRESIMS



(b) IR



Chemical Formula: C₂₉H₄₀N₂O₅

calculated for [M+H]⁺: 497.3015

calculated for [M+Na]⁺: 519.2835

Figure S12. The ^1H NMR spectrum of compound **2** in $\text{DMSO-}d_6$.

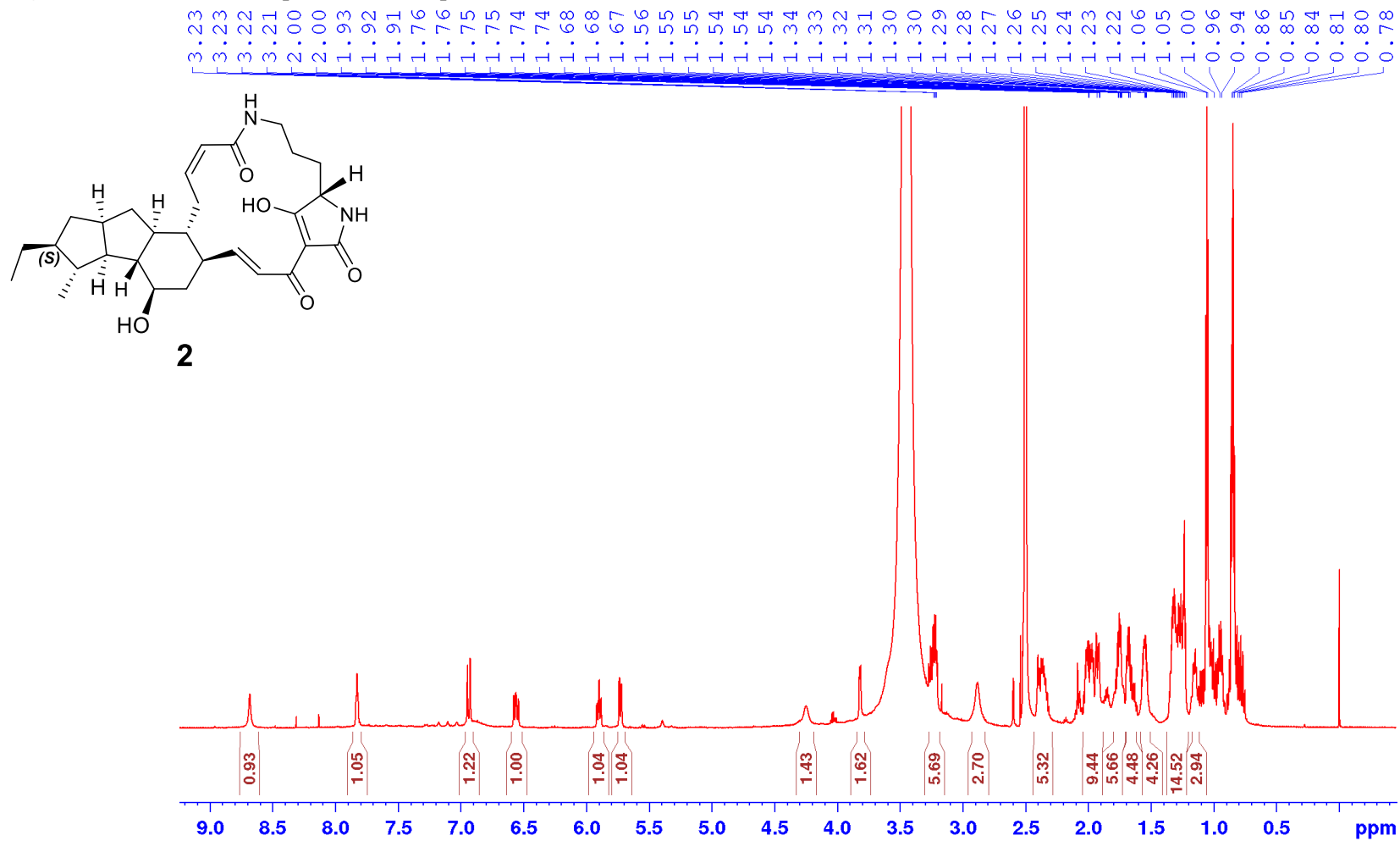


Figure S13. The ^{13}C NMR and DEPT 135 spectra of compound **2** in $\text{DMSO-}d_6$.

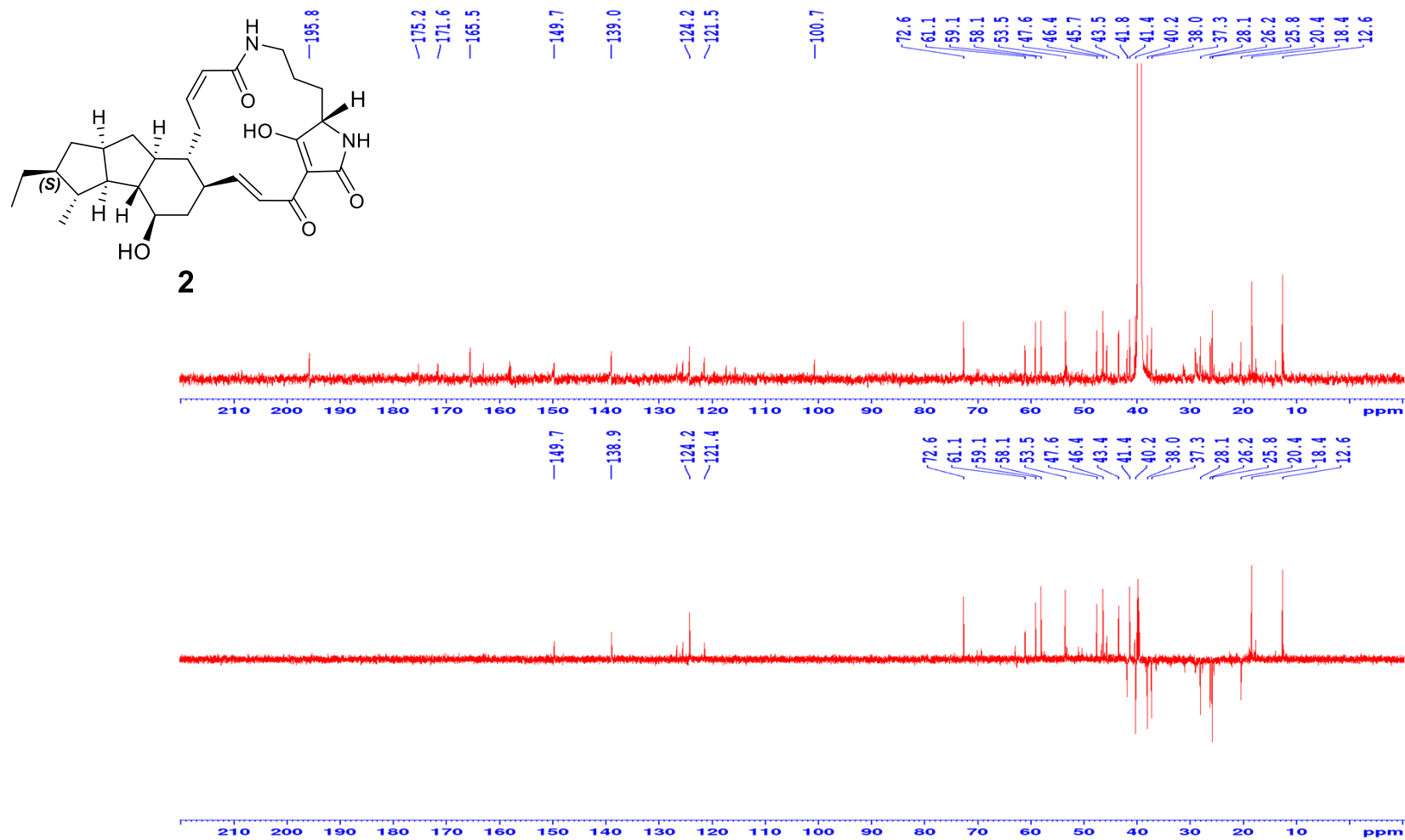


Figure S14. The HSQC spectrum of compound **2** in DMSO- d_6 .

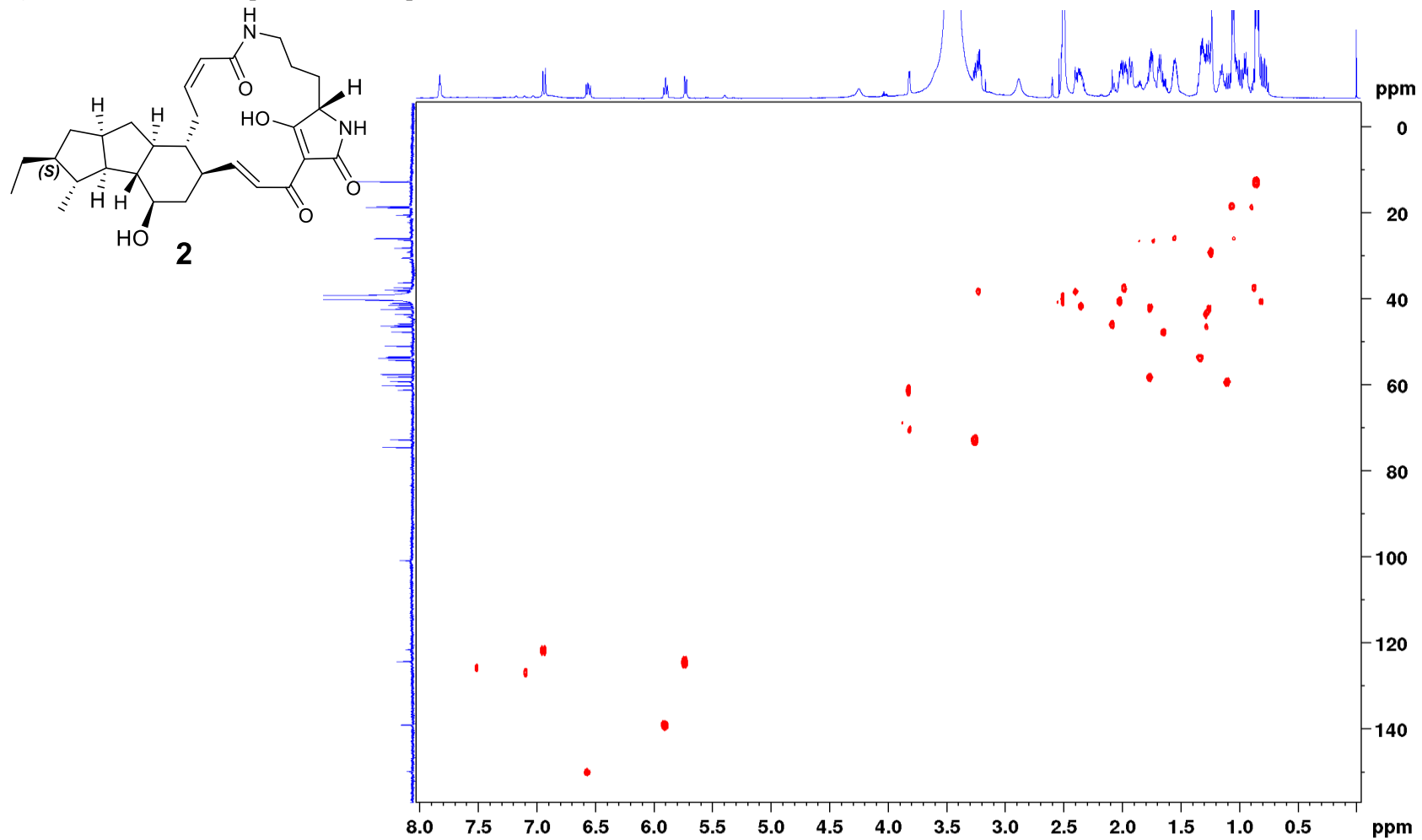


Figure S15. The HMBC spectrum of compound **2** in DMSO-*d*₆.

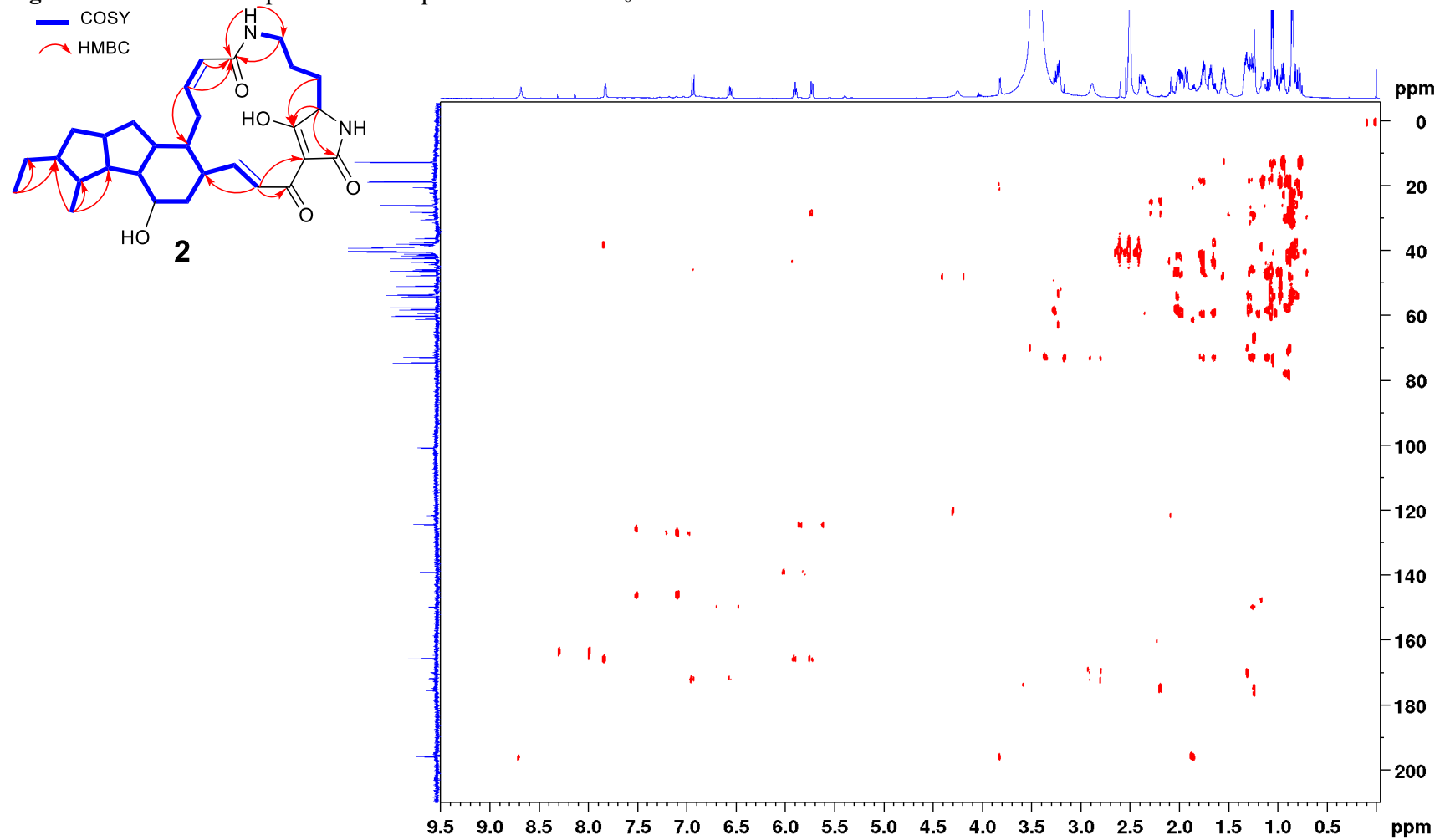


Figure S16. The ^1H - ^1H HCOSY spectrum of compound **2** in $\text{DMSO-}d_6$.

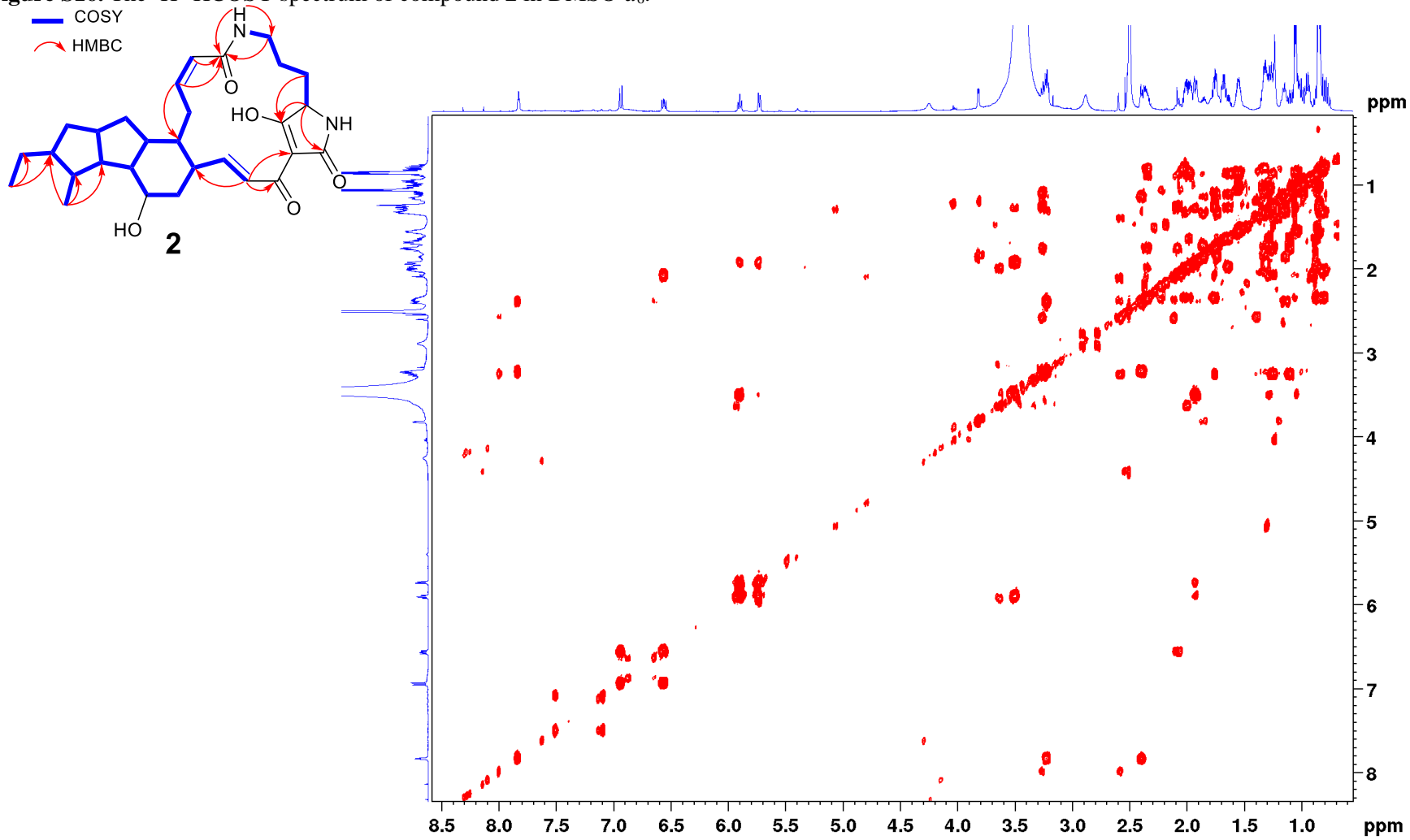


Figure S17. The NOESY spectrum of compound 2 in DMSO- d_6 .

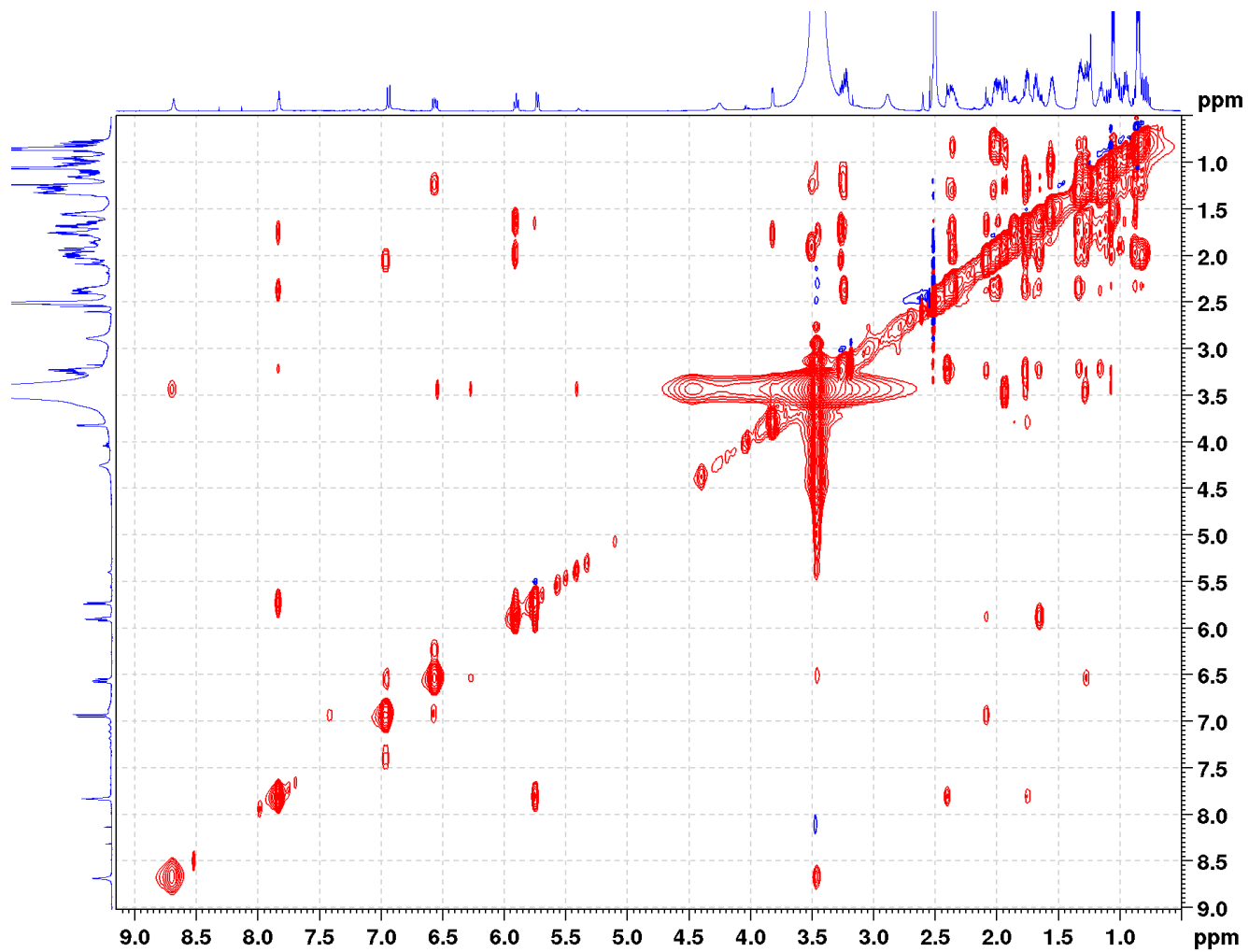


Figure S18. The key NOESY spectrum of compound **2** in DMSO-*d*₆.

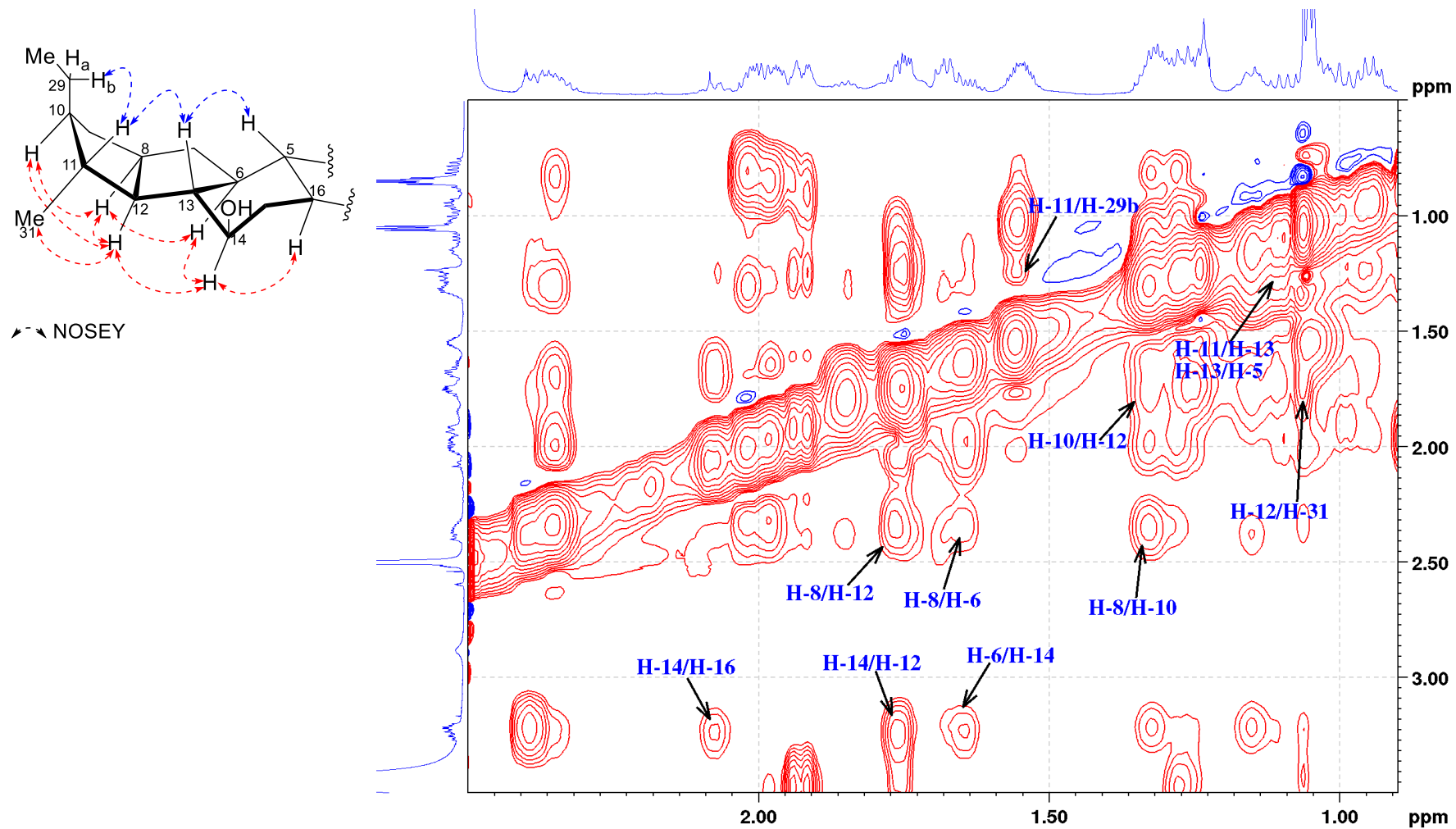
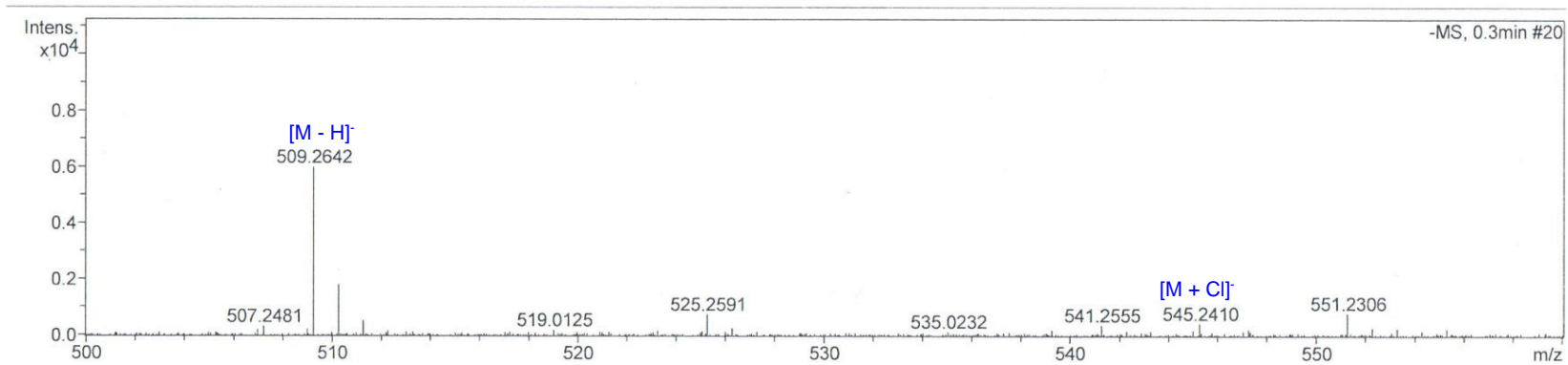
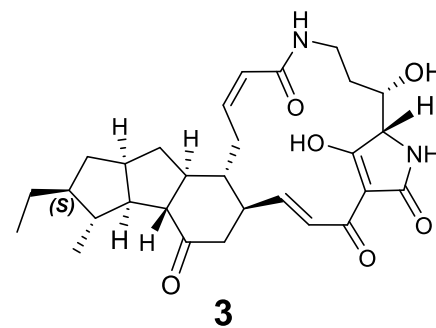
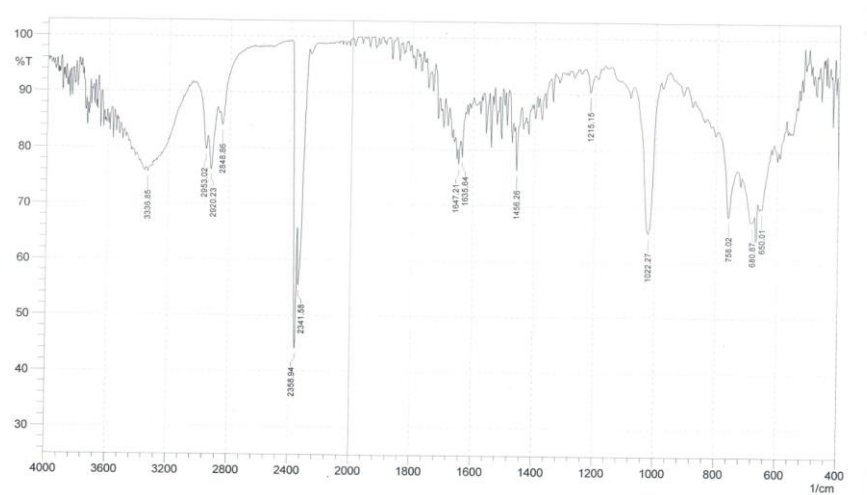


Figure S19. HRESIMS (a) and IR (b) of compound **3**.

(a) HRESIMS



(b) IR



Chemical Formula: $C_{29}H_{38}N_2O_6$
calculated for [M-H]⁻: 509.2652
calculated for [M+Cl]⁻: 545.2418

Figure S20. The ^1H NMR spectrum of compound **3** in $\text{DMSO-}d_6$.

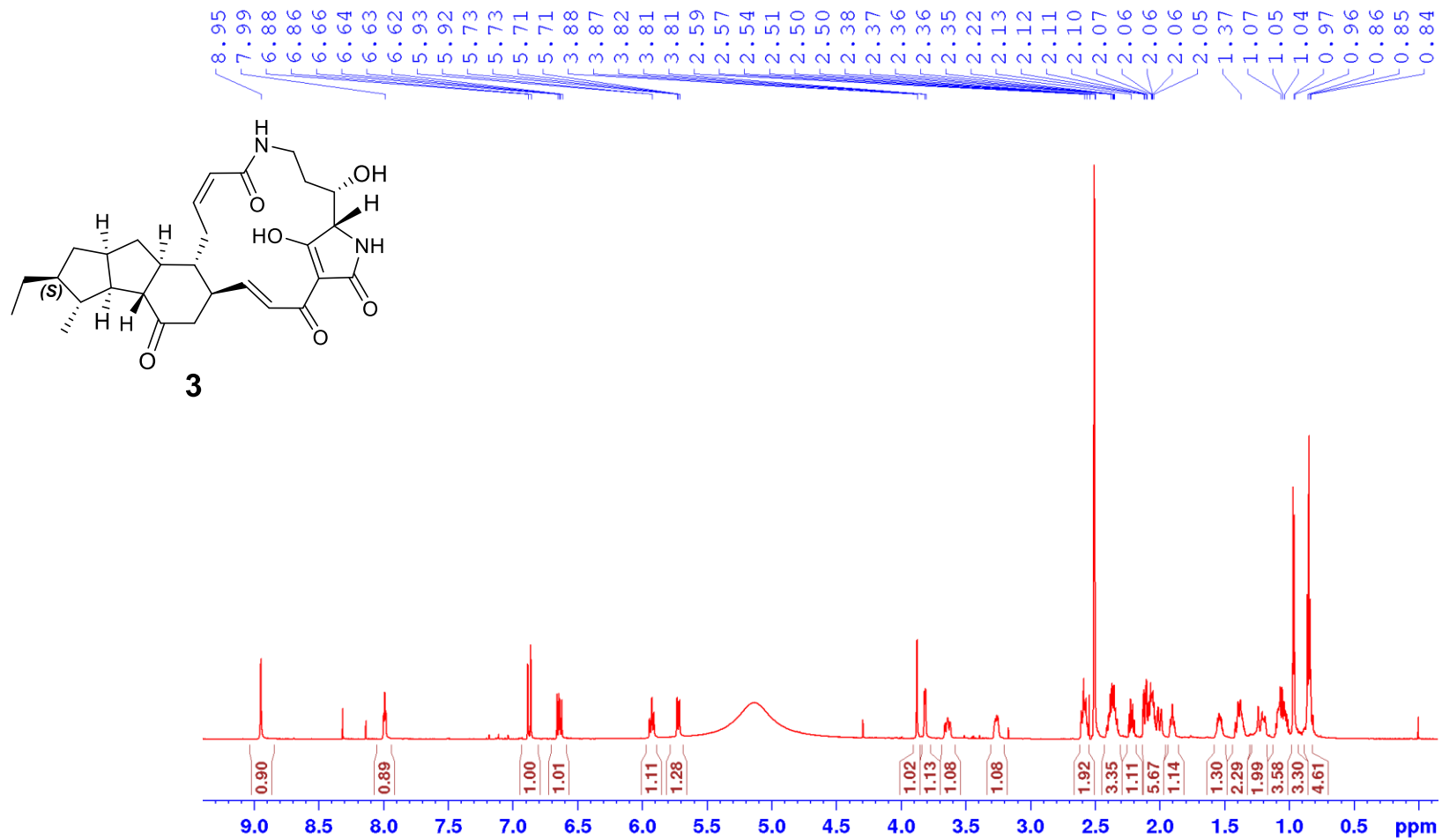


Figure S21. The ^{13}C NMR and DEPT 135 spectra of compound **3** in $\text{DMSO-}d_6$.

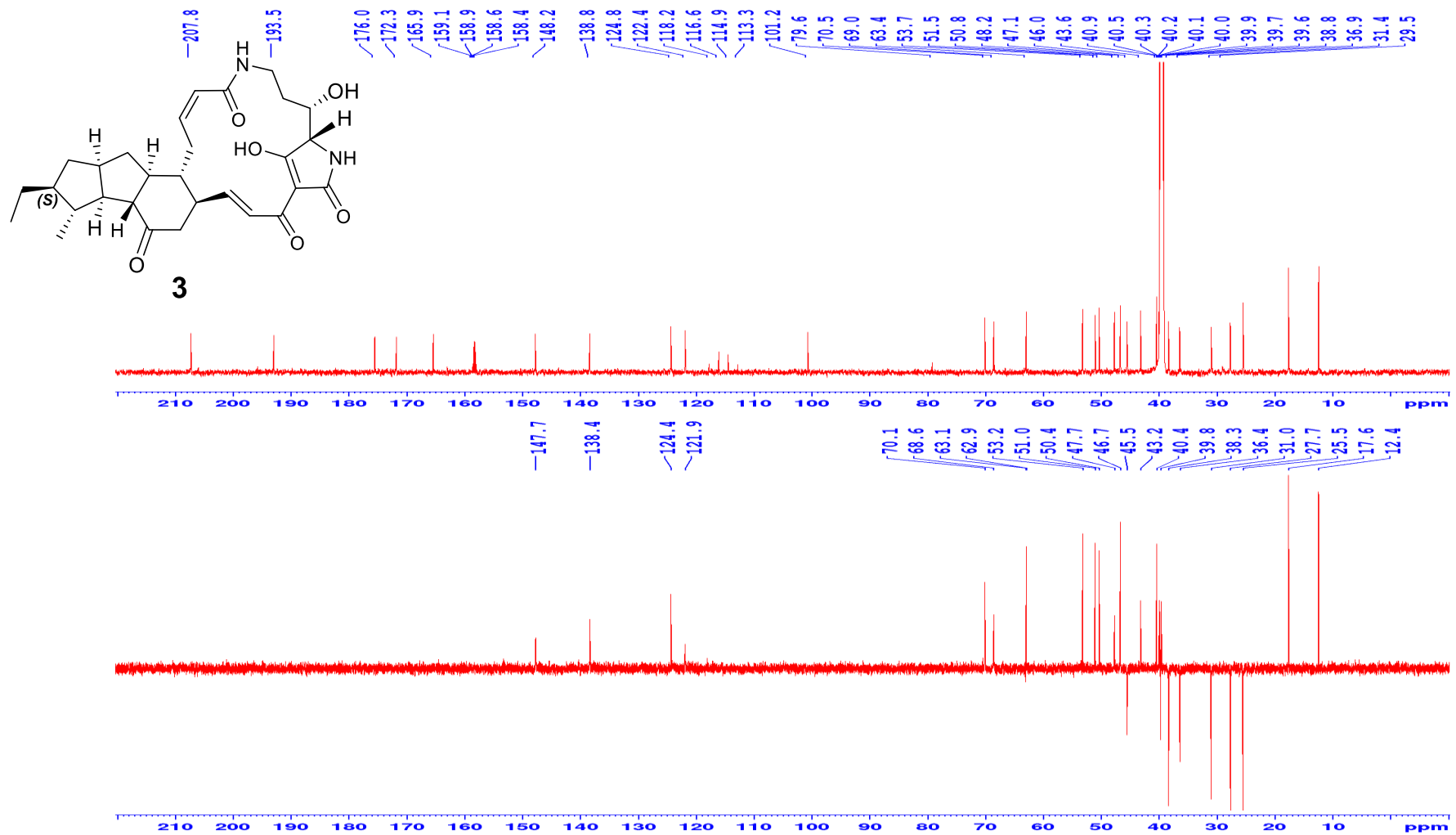


Figure S22. The HSQC spectrum of compound **3** in DMSO- d_6 .

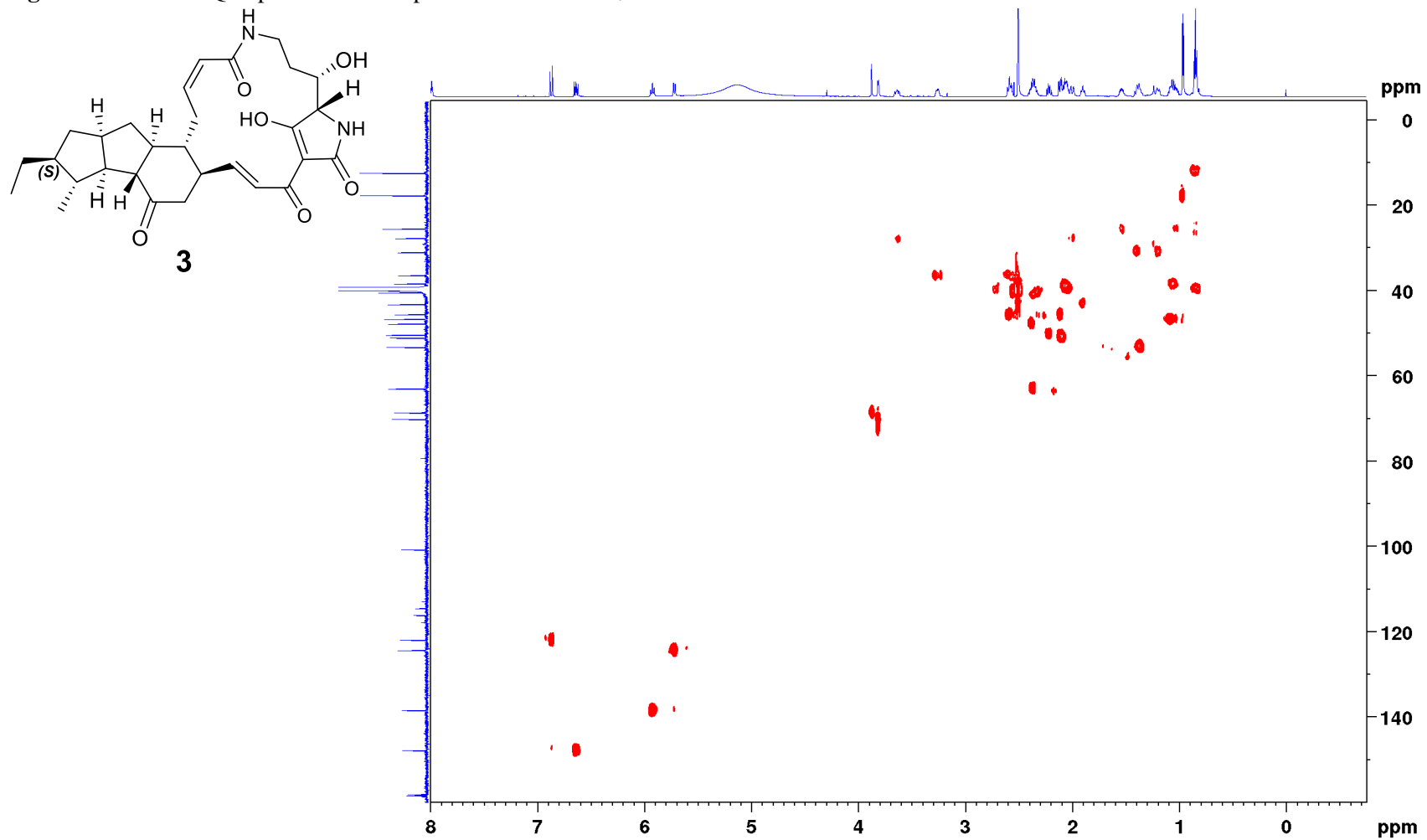


Figure S23. The HMBC spectrum of compound **3** in DMSO-*d*₆.

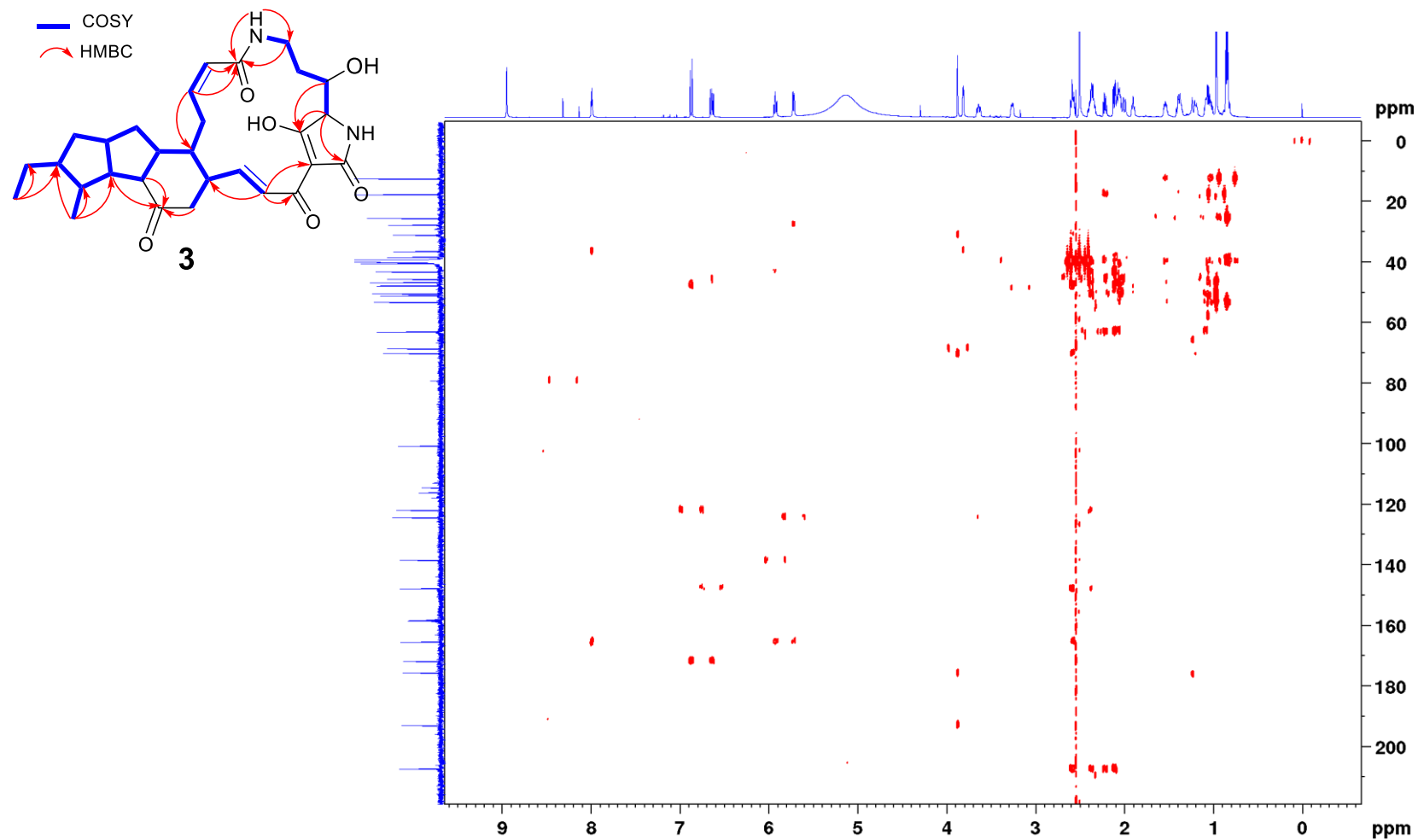


Figure S24. The ^1H - ^1H COSY spectrum of compound **3** in $\text{DMSO-}d_6$.

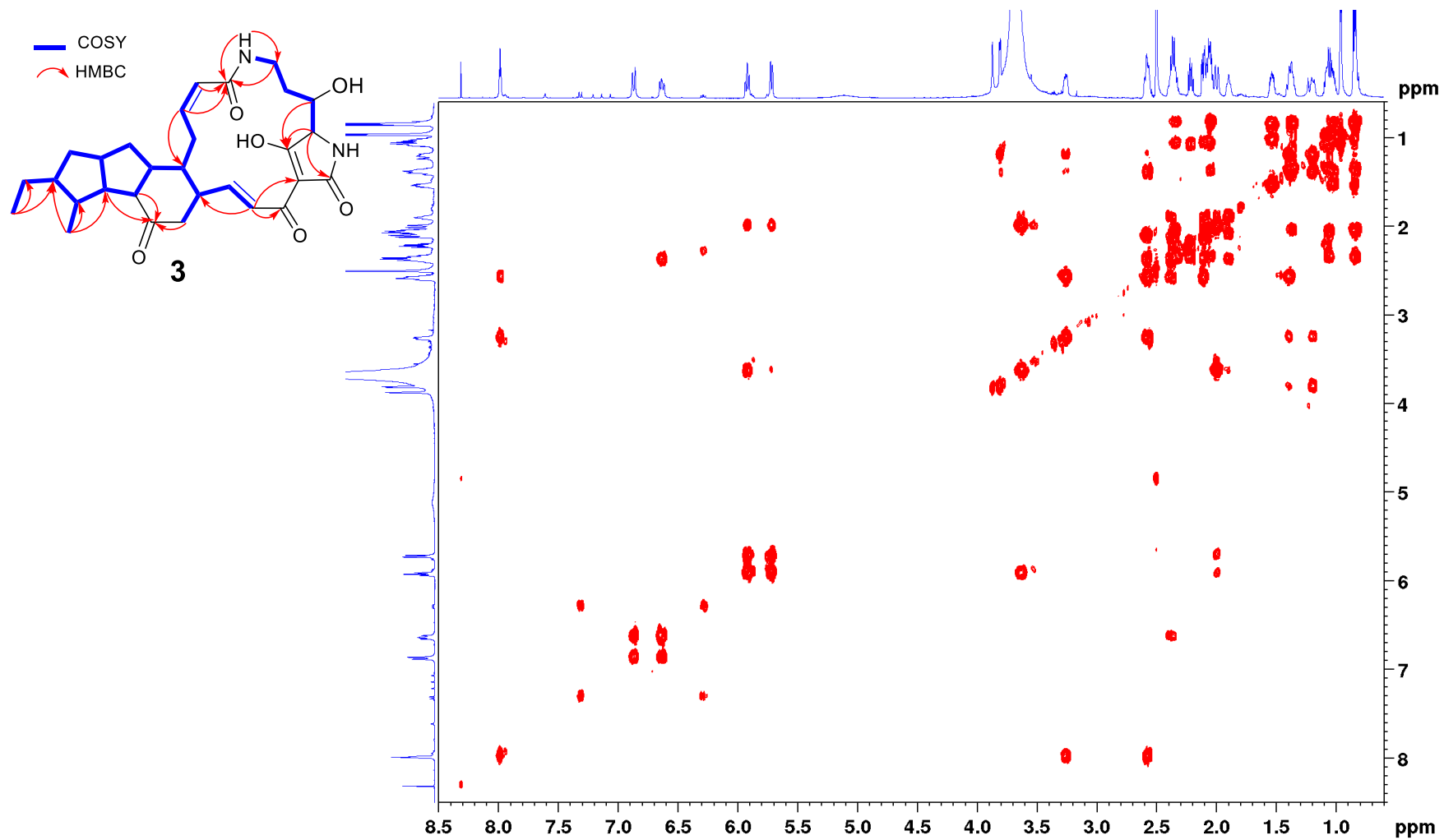


Figure S25. The NOESY spectrum of compound **3** in DMSO-*d*₆.

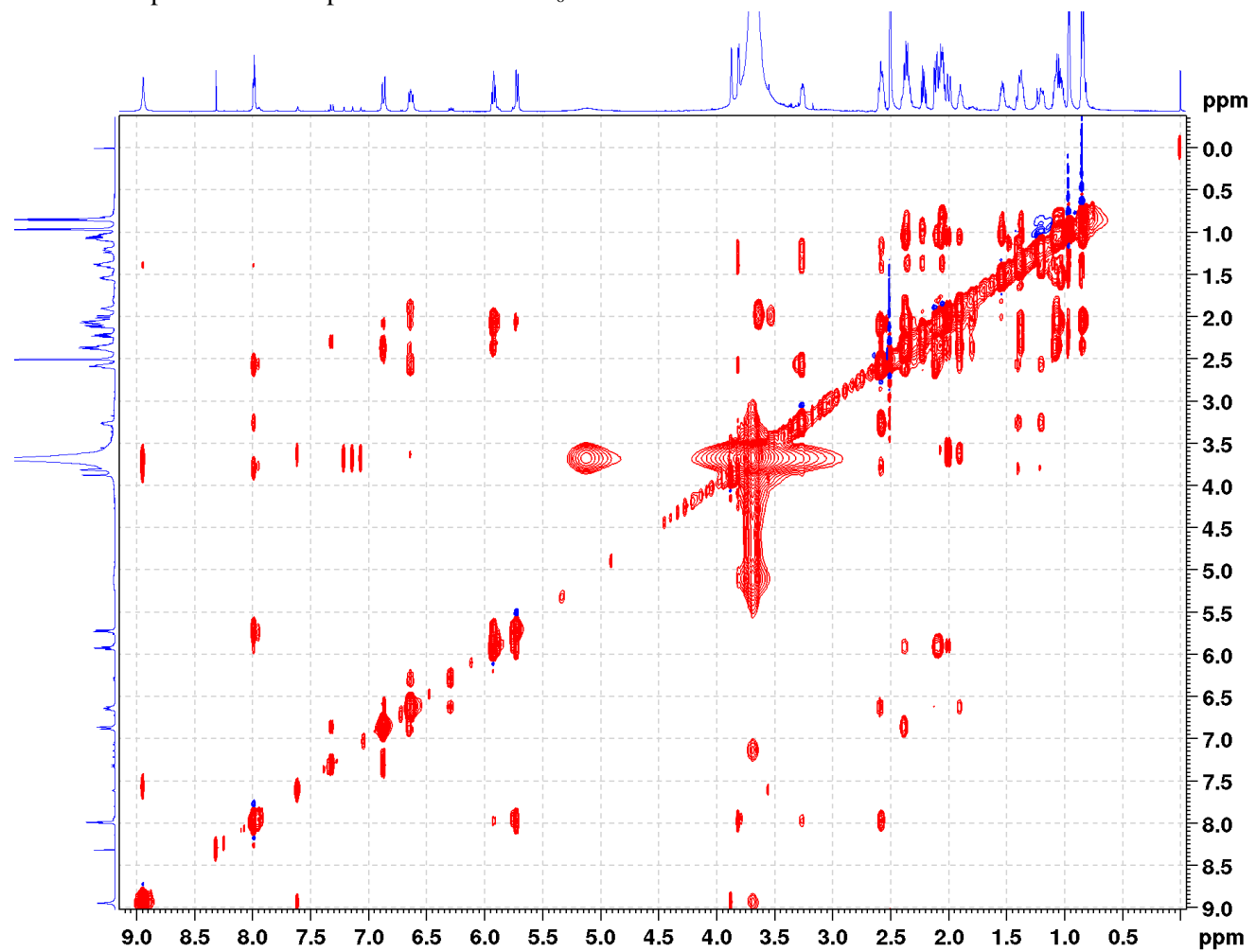


Figure S26. The key NOESY spectrum of compound **3** in DMSO-*d*₆.

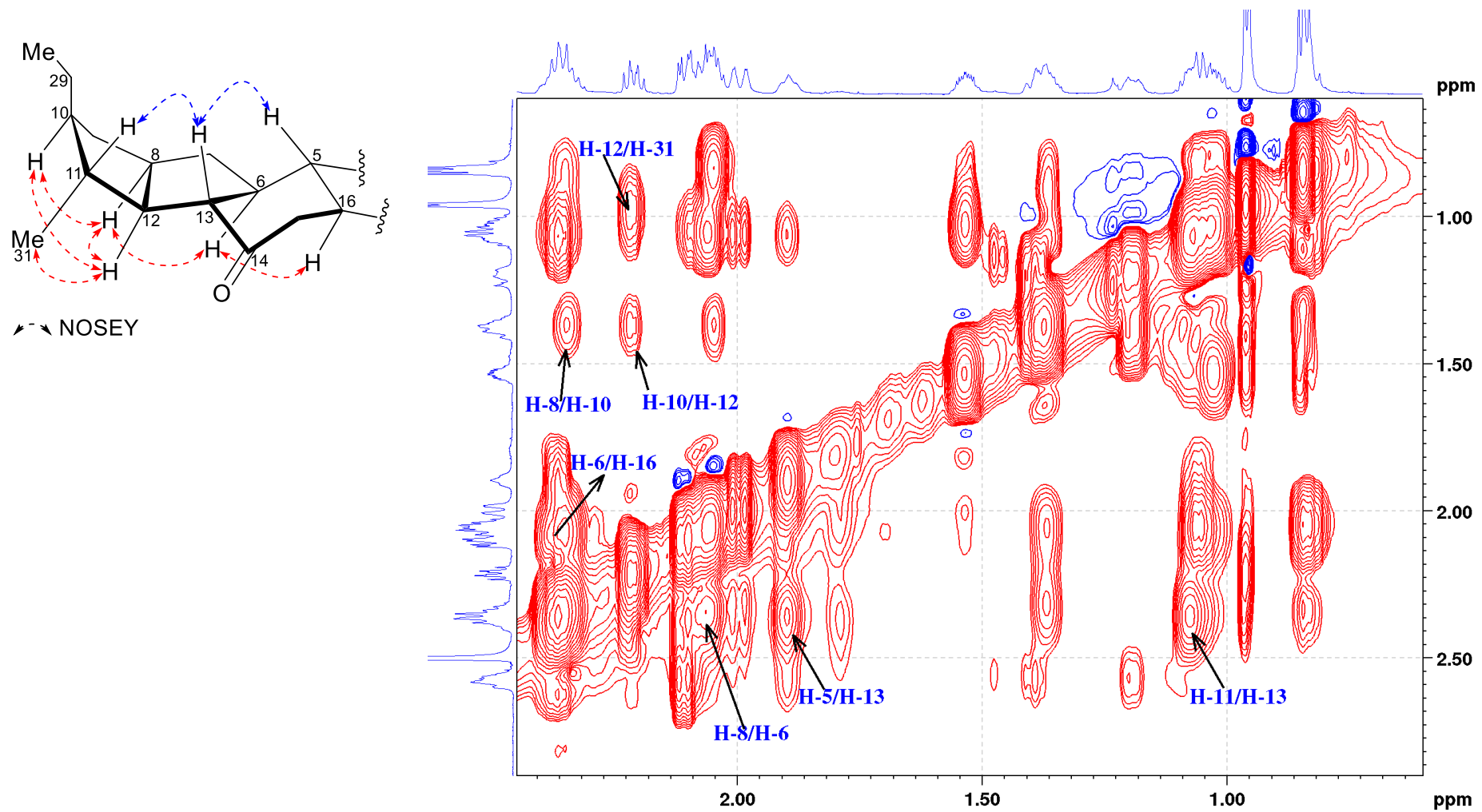
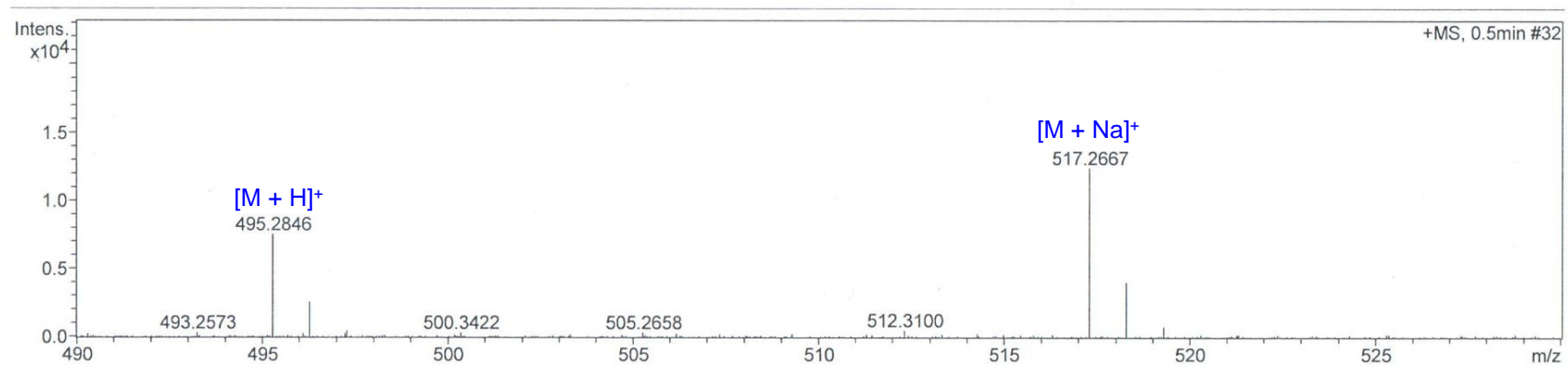
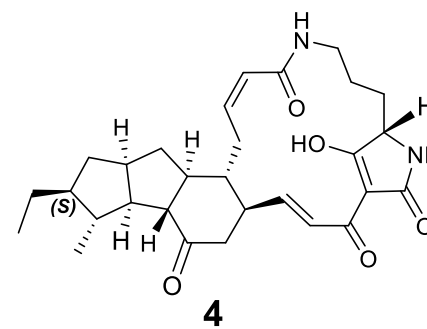
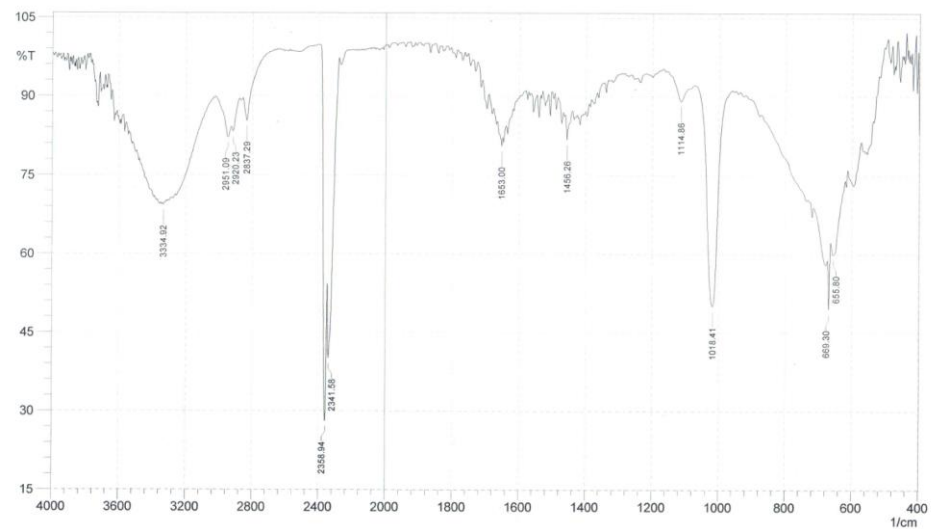


Figure S27. HRESIMS (a) and IR (b) of compound 4.

(a) HRESIMS



(b) IR



Chemical Formula: $C_{29}H_{38}N_2O_5$
calculated for $[M+H]^+$: 495.2859
calculated for $[M+H]^+$: 517.2678

Figure S28. The ^1H NMR spectrum of compound **4** in $\text{DMSO-}d_6$.

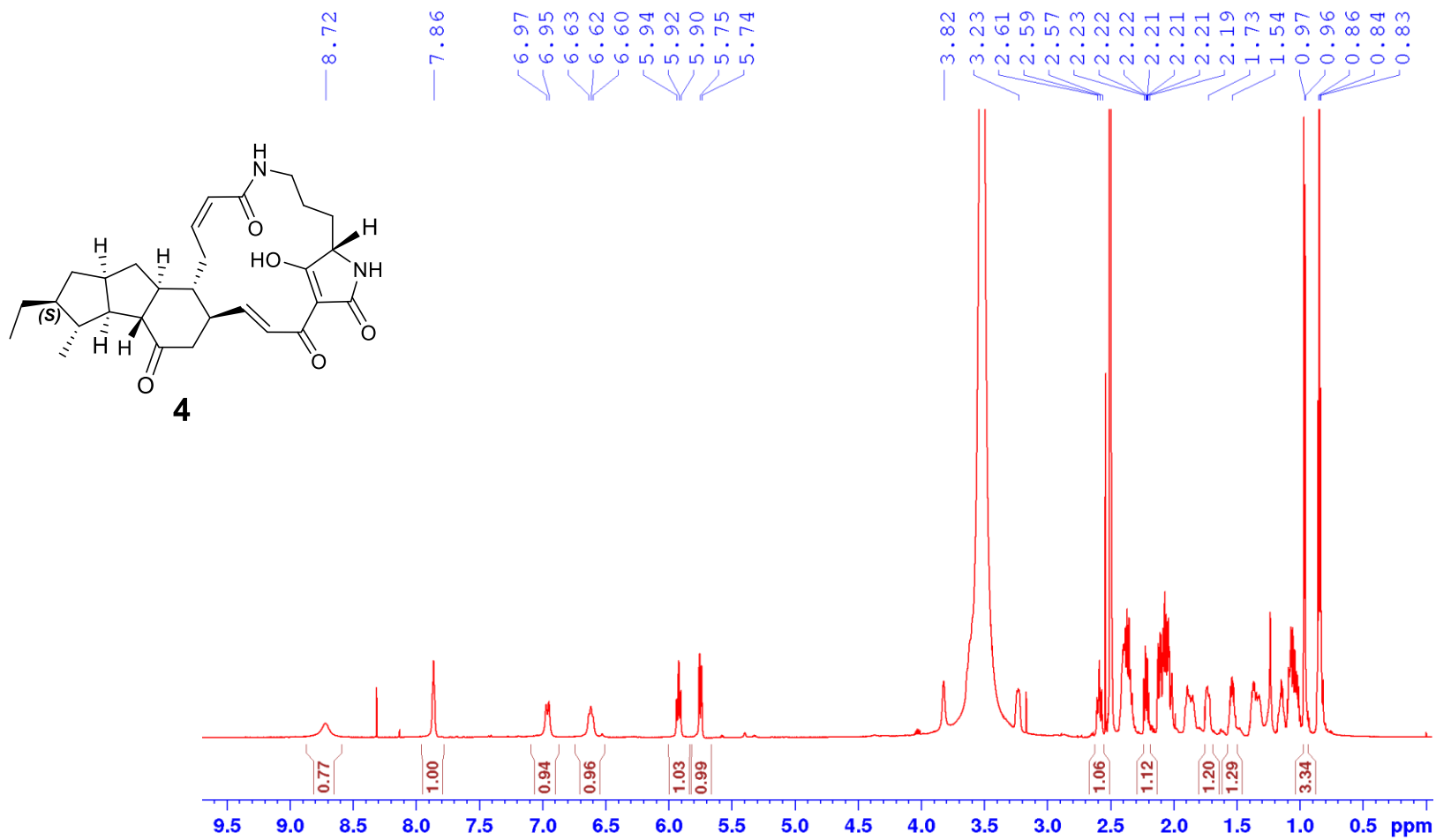


Figure S29. The ^{13}C NMR and DEPT 135 spectra of compound **4** in $\text{DMSO-}d_6$.

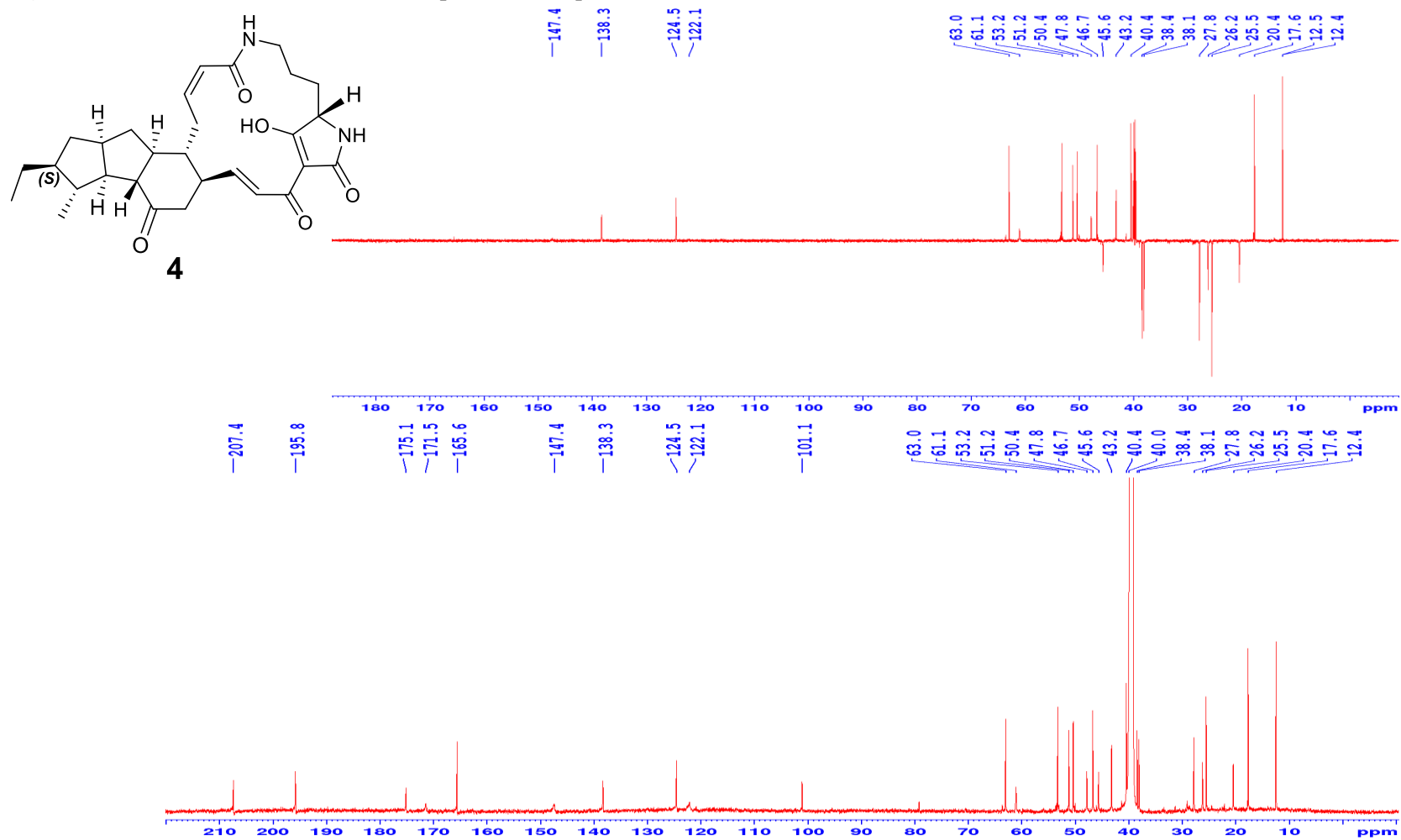


Figure S30. The HSQC spectrum of compound **4** in DMSO- d_6 .

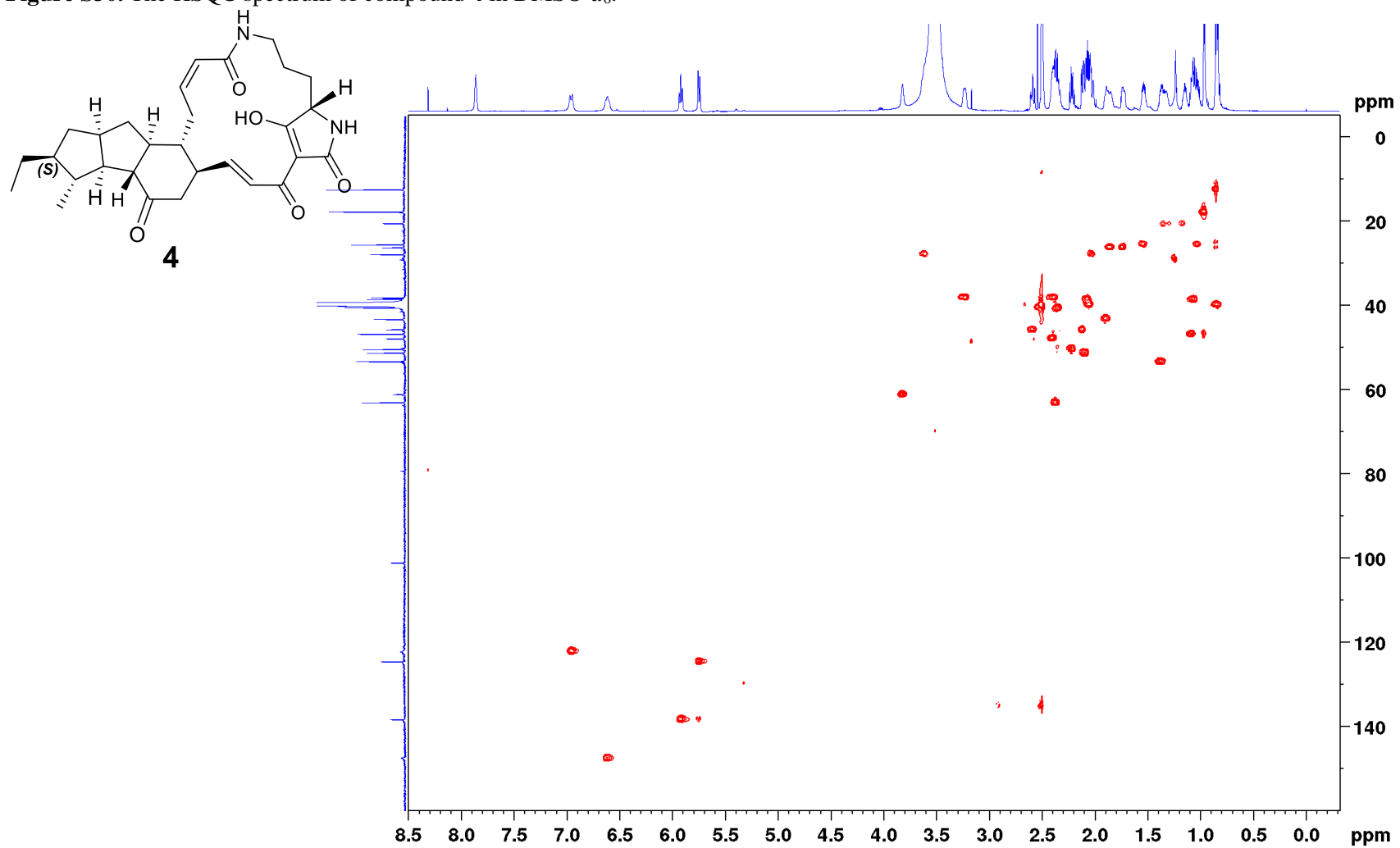


Figure S31. The HMBC spectrum of compound **4** in DMSO-*d*₆.

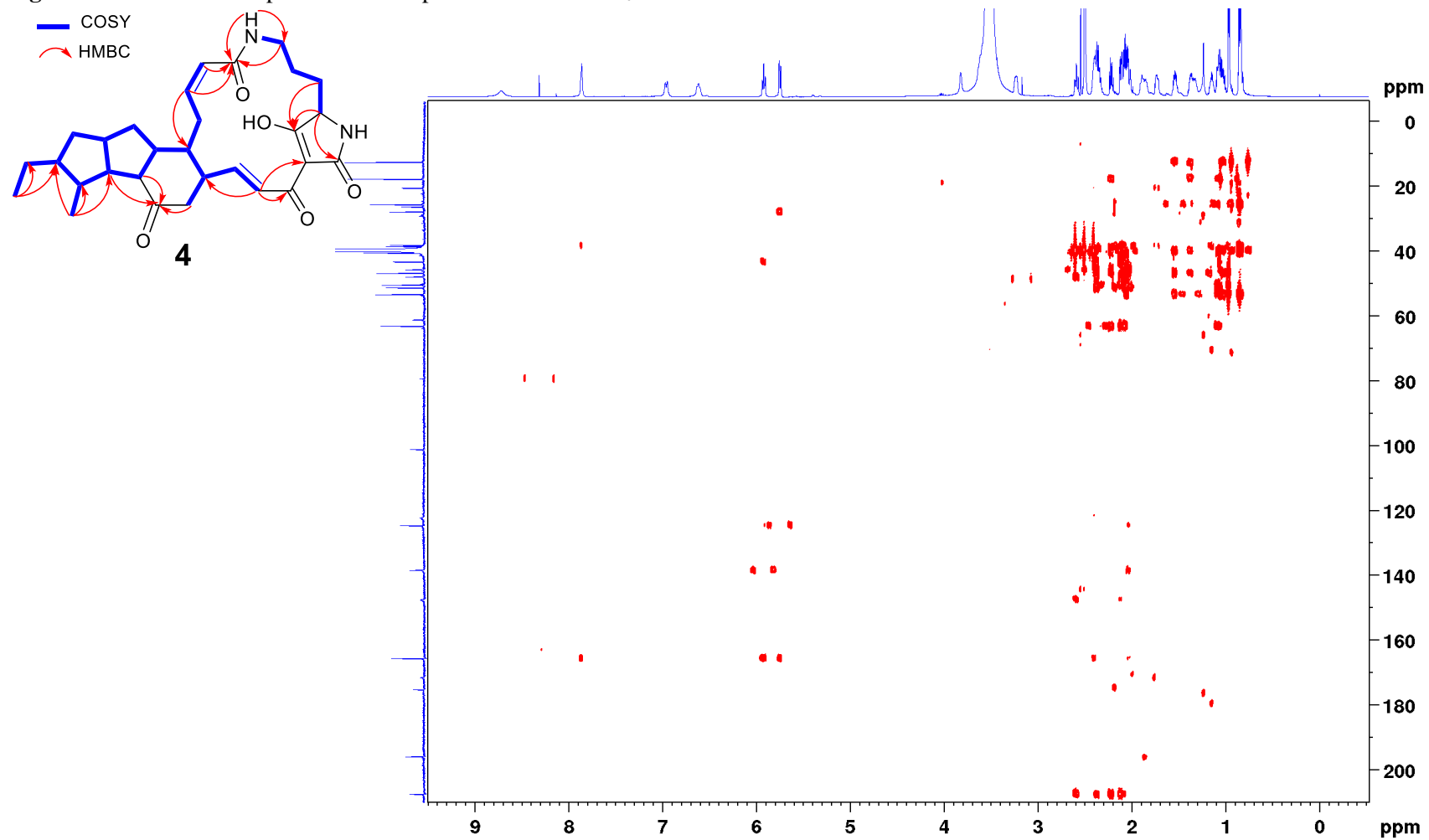


Figure S32. The ^1H - ^1H COSY spectrum of compound **4** in $\text{DMSO-}d_6$.

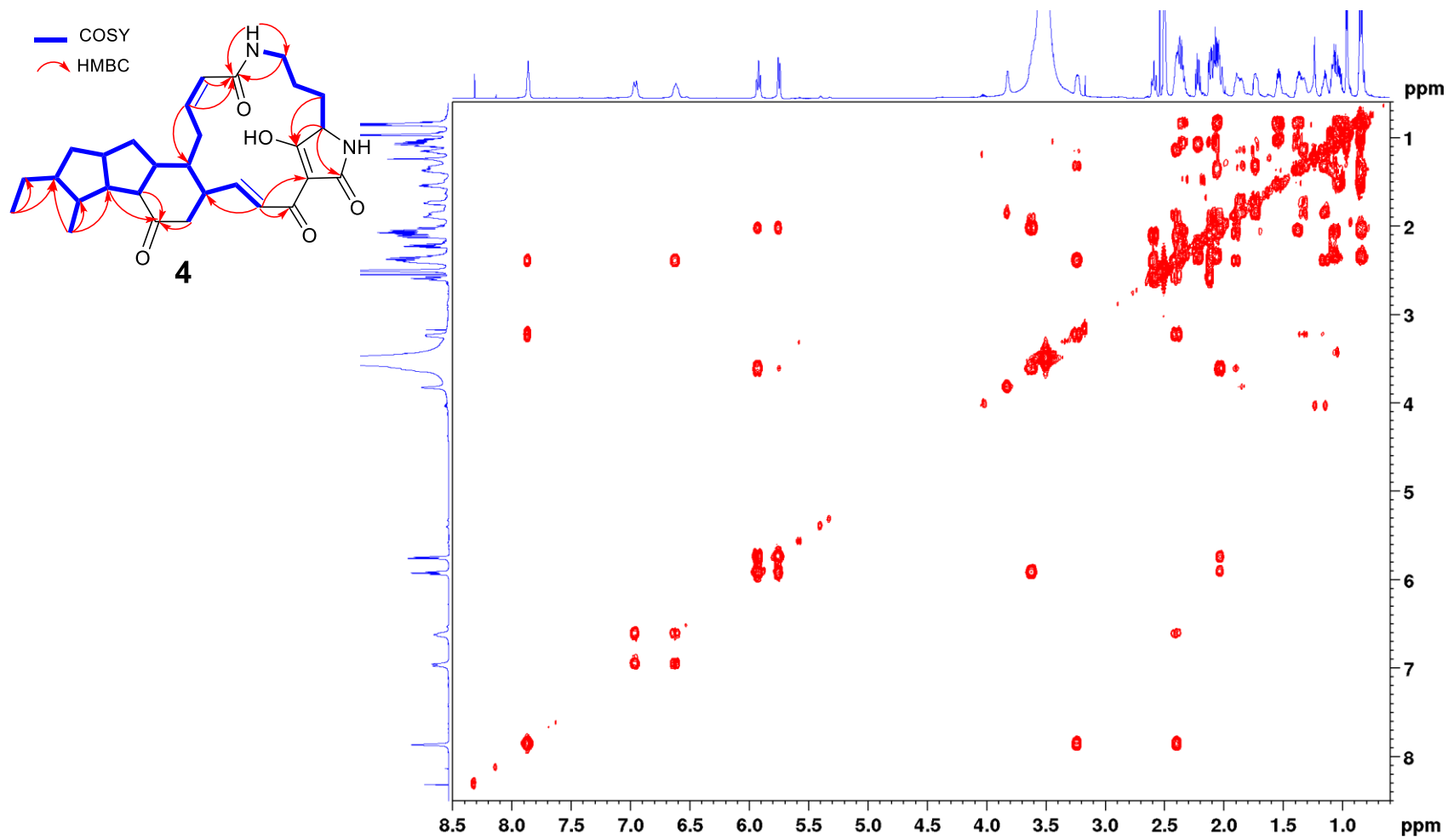


Figure S33. The NOESY spectrum of compound 4 in DMSO-*d*₆.

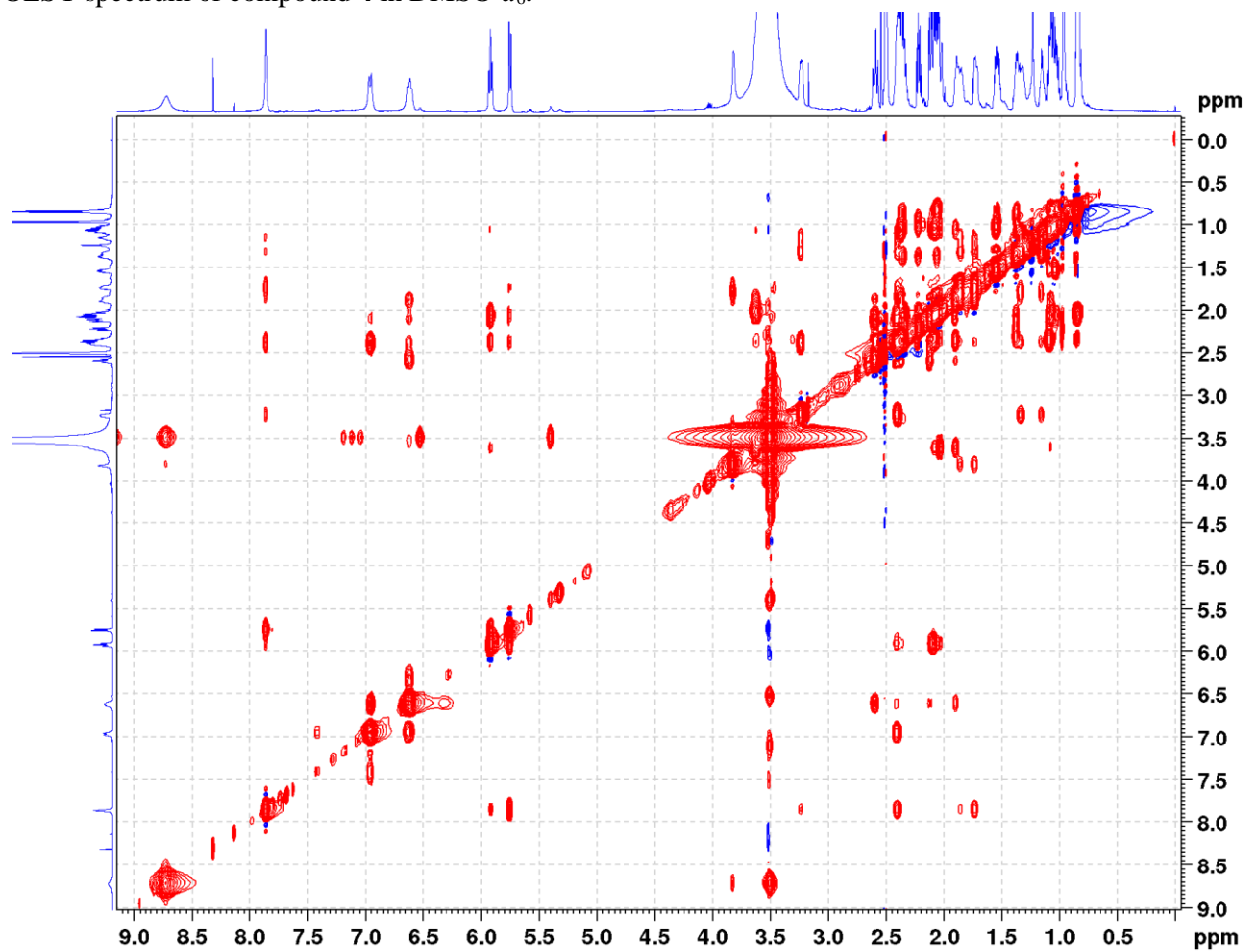


Figure S34. The key NOESY spectrum of compound 4 in DMSO-*d*₆.

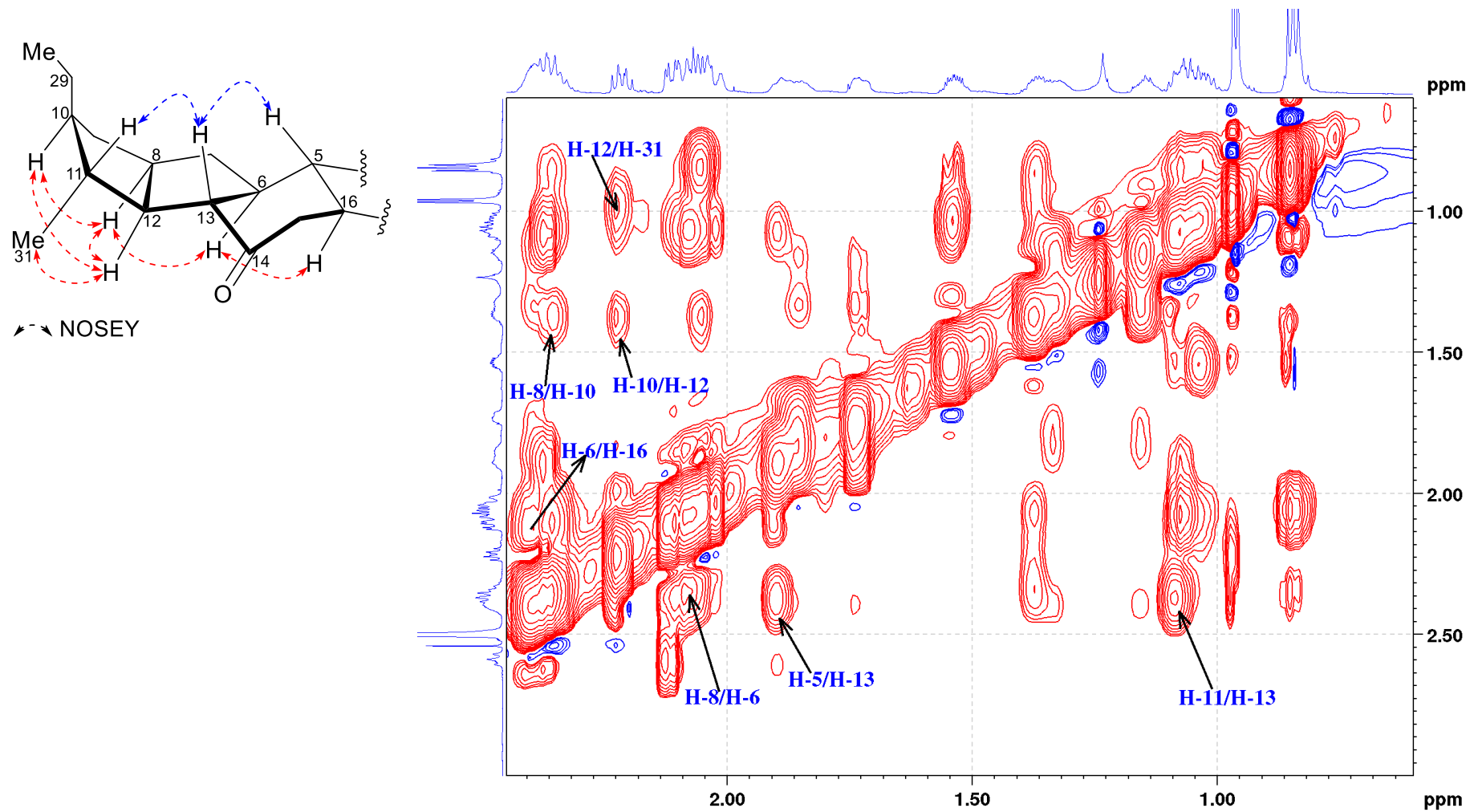
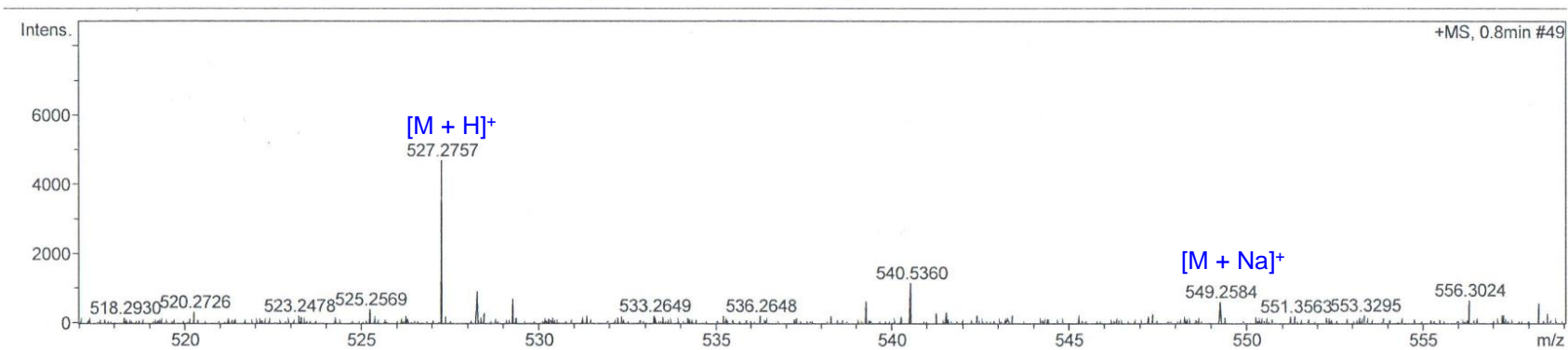
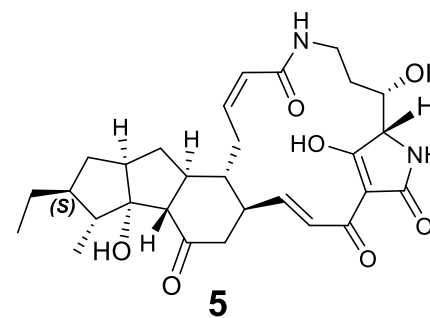
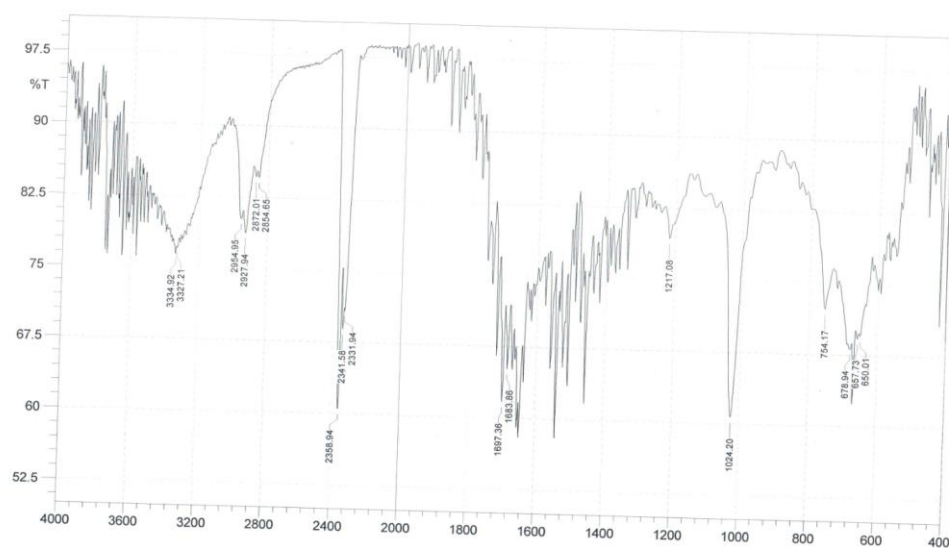


Figure S35. HRESIMS (a) and IR (b) of compound **5**.

(a) HR-ESI-MS



(b) IR



Chemical Formula: C₂₉H₃₈N₂O₇

calculated for [M+H]⁺: 527.2757

calculated for [M+H]⁺: 549.2577

Figure S36. The ^1H NMR spectrum of compound **5** in $\text{DMSO-}d_6$.

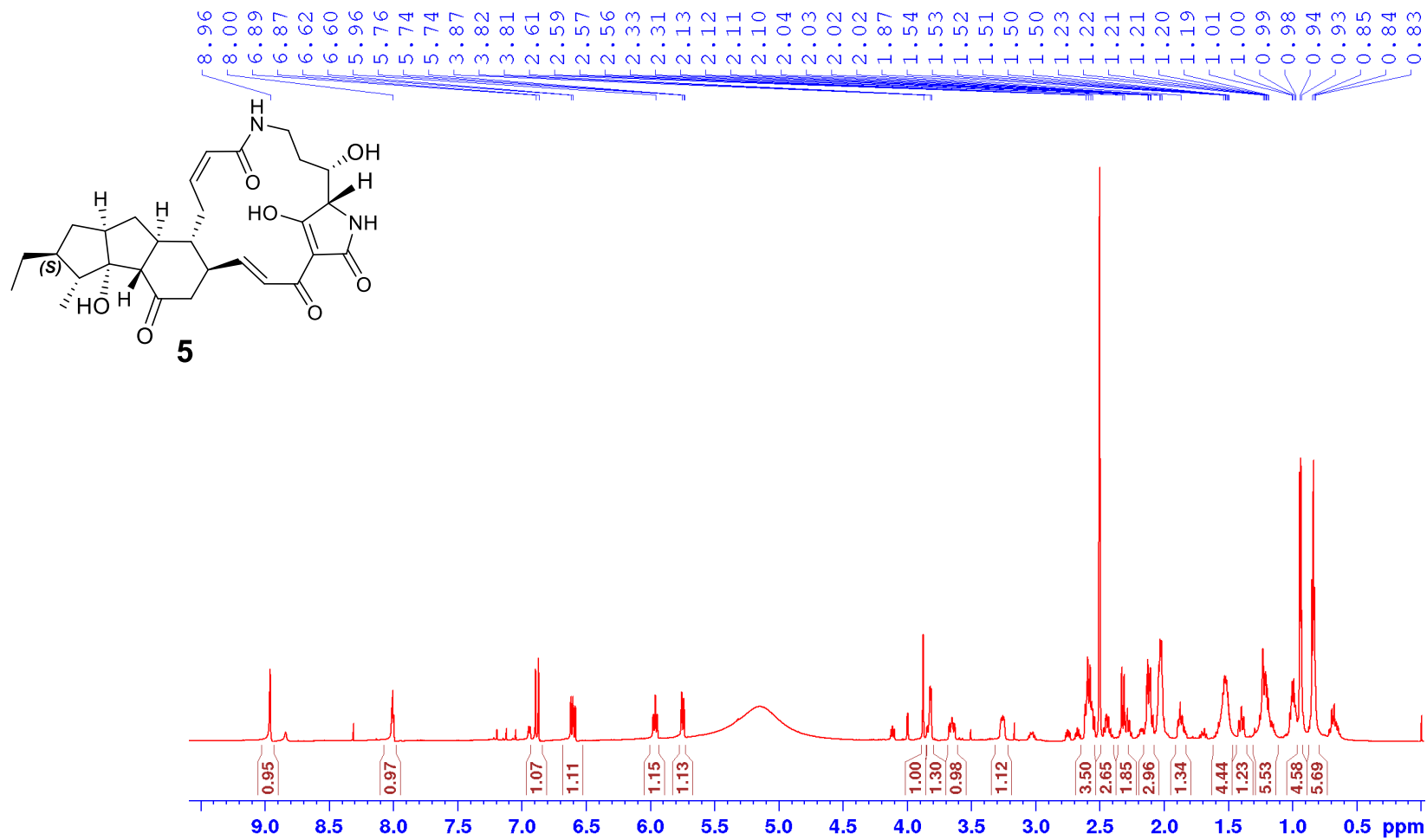


Figure S37. The ^{13}C NMR and DEPT 135 spectra of compound **5** in $\text{DMSO-}d_6$.

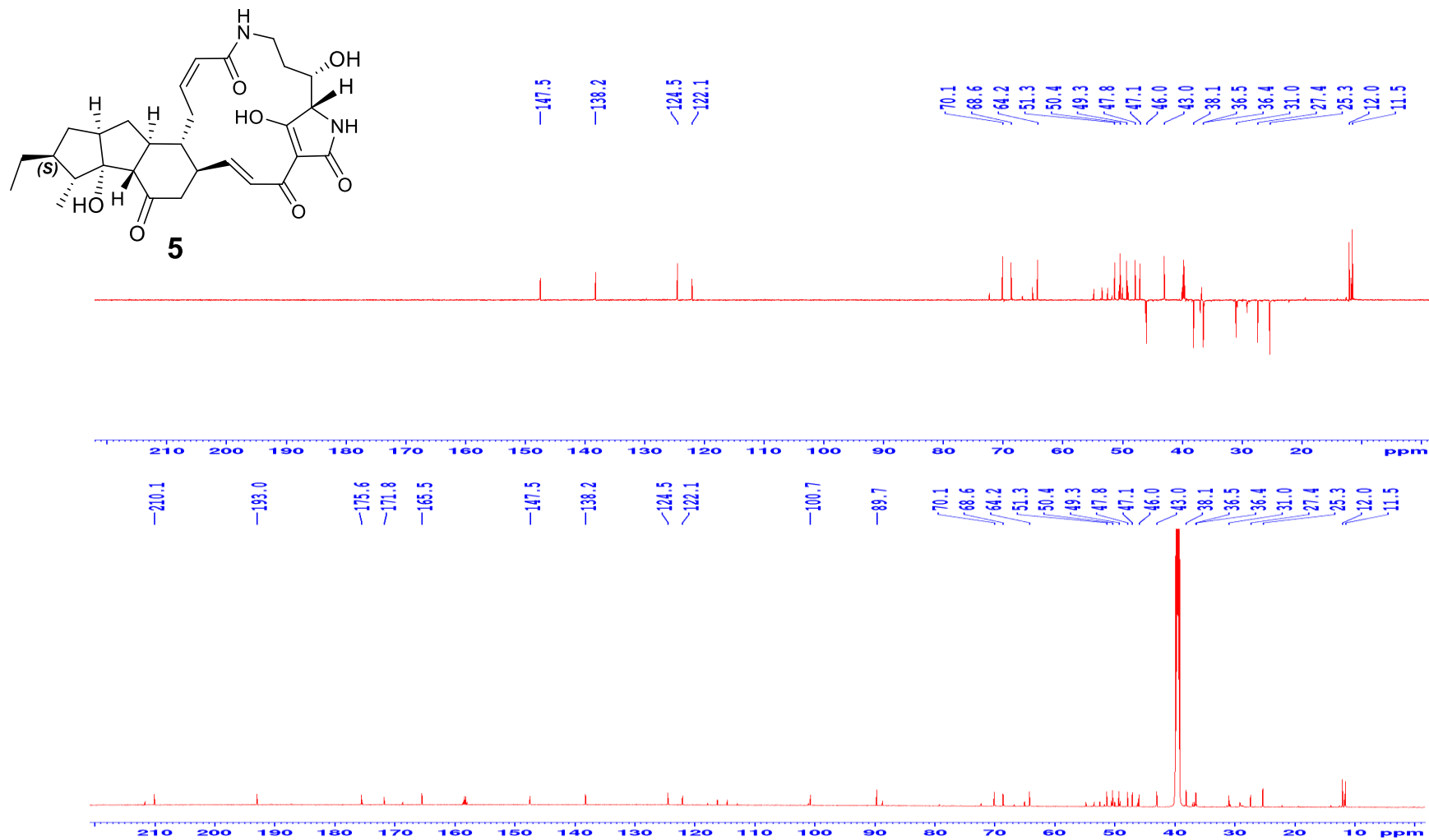


Figure S38. The HSQC spectrum of compound **5** in DMSO-*d*₆.

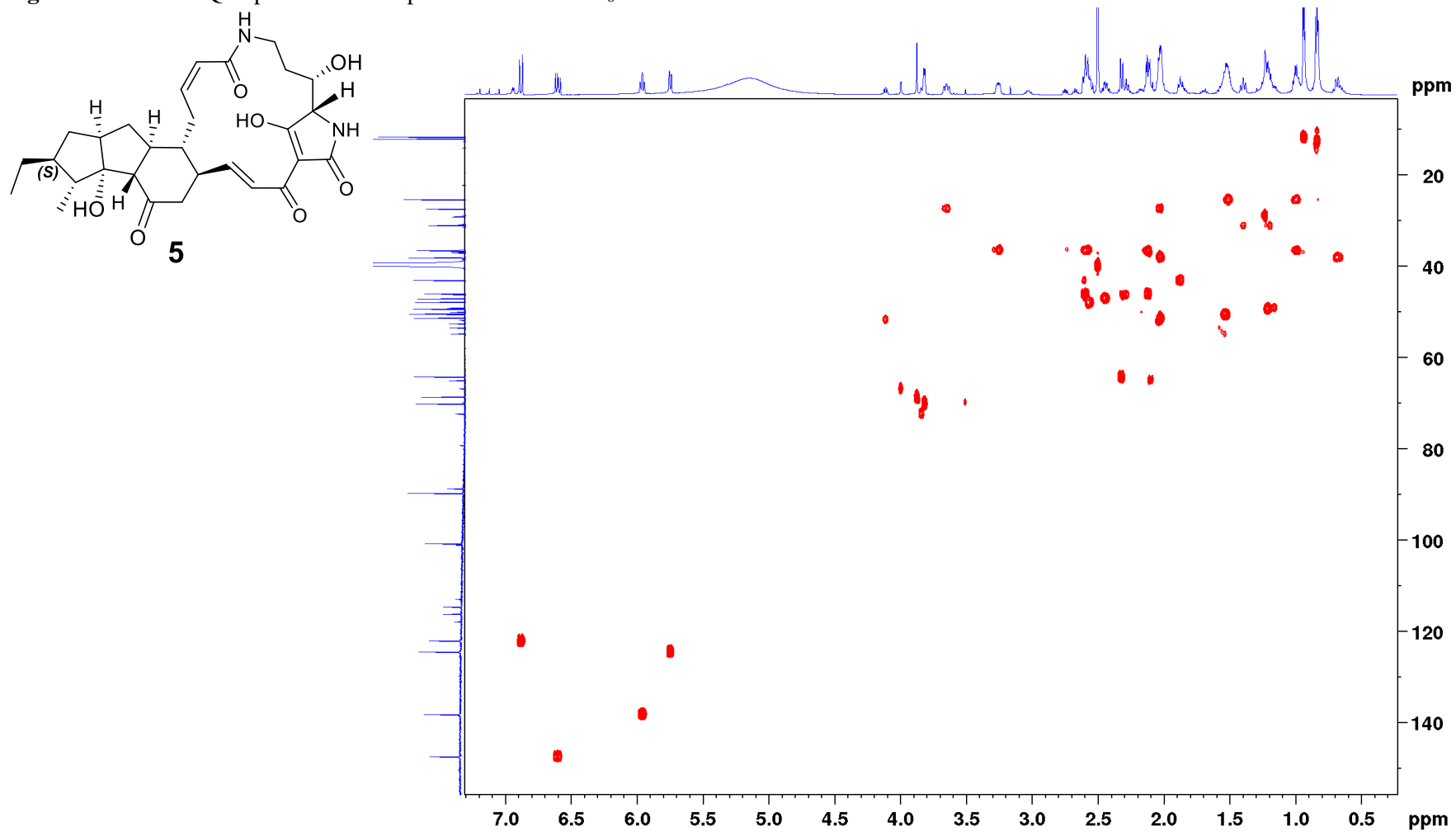


Figure S39. The HMBC spectrum of compound **5** in DMSO-*d*₆.

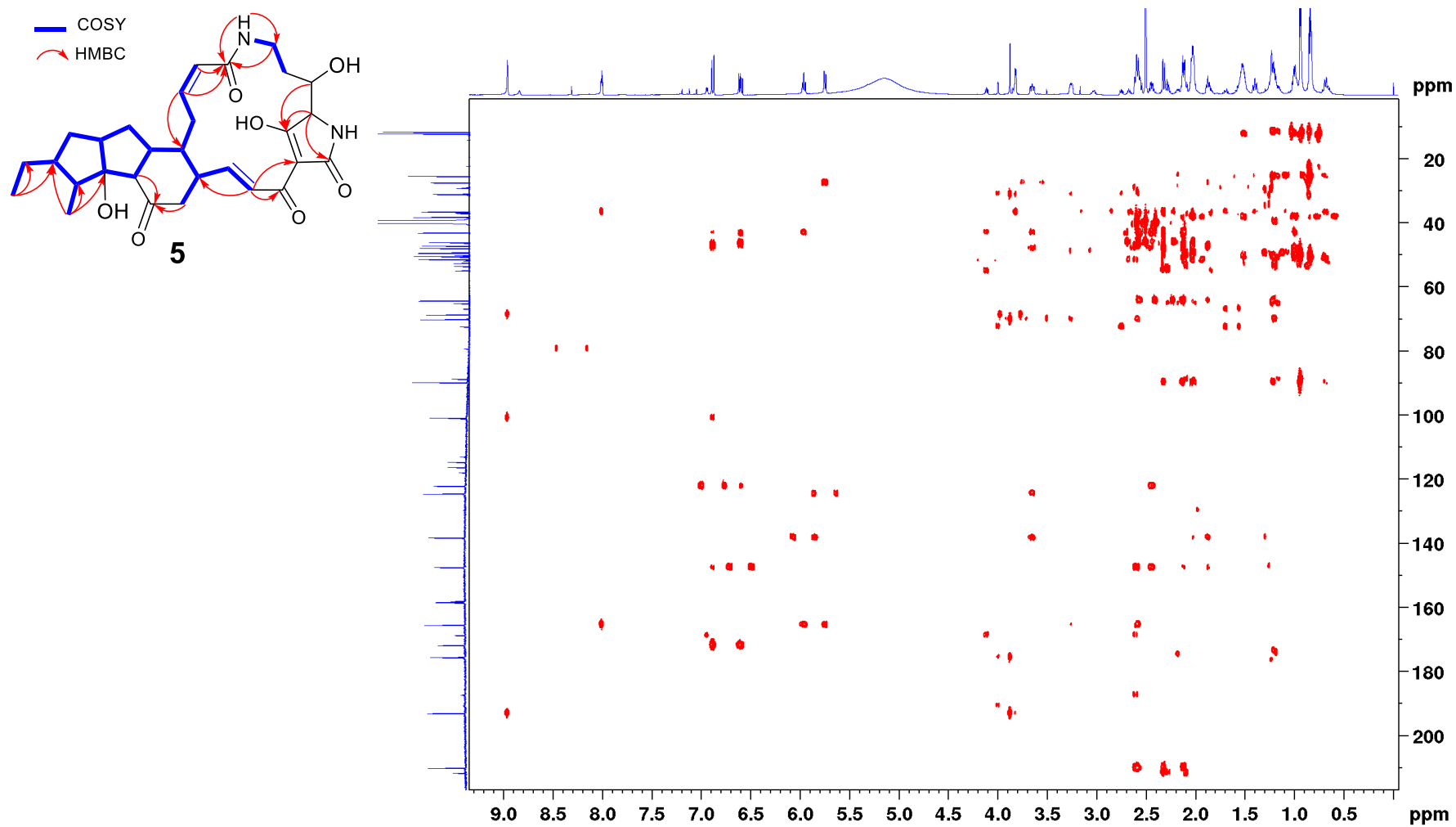


Figure S40. The ^1H - ^1H COSY spectrum of compound **5** in $\text{DMSO-}d_6$.

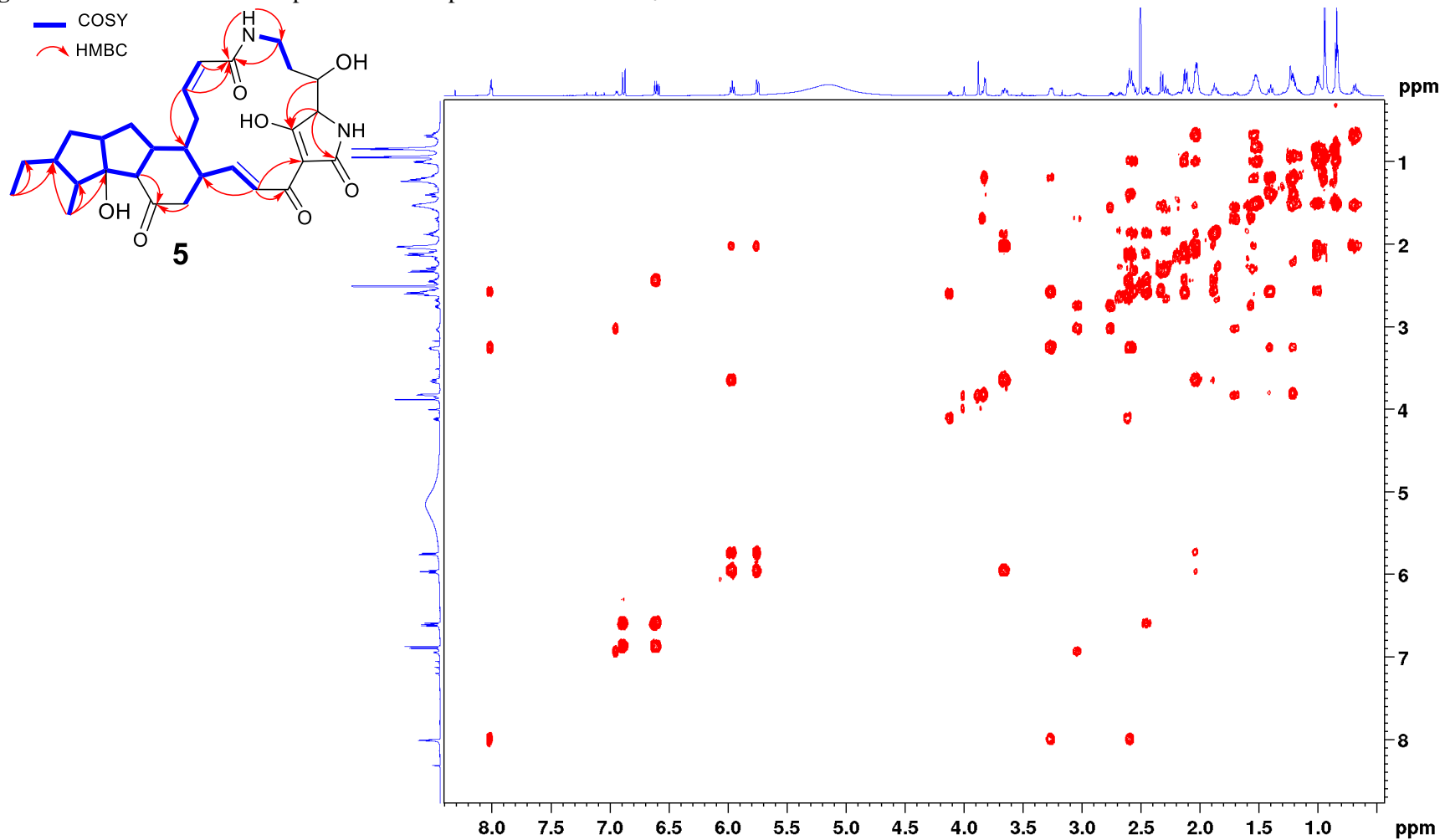


Figure S41. The NOESY spectrum of compound **5** in DMSO- d_6 .

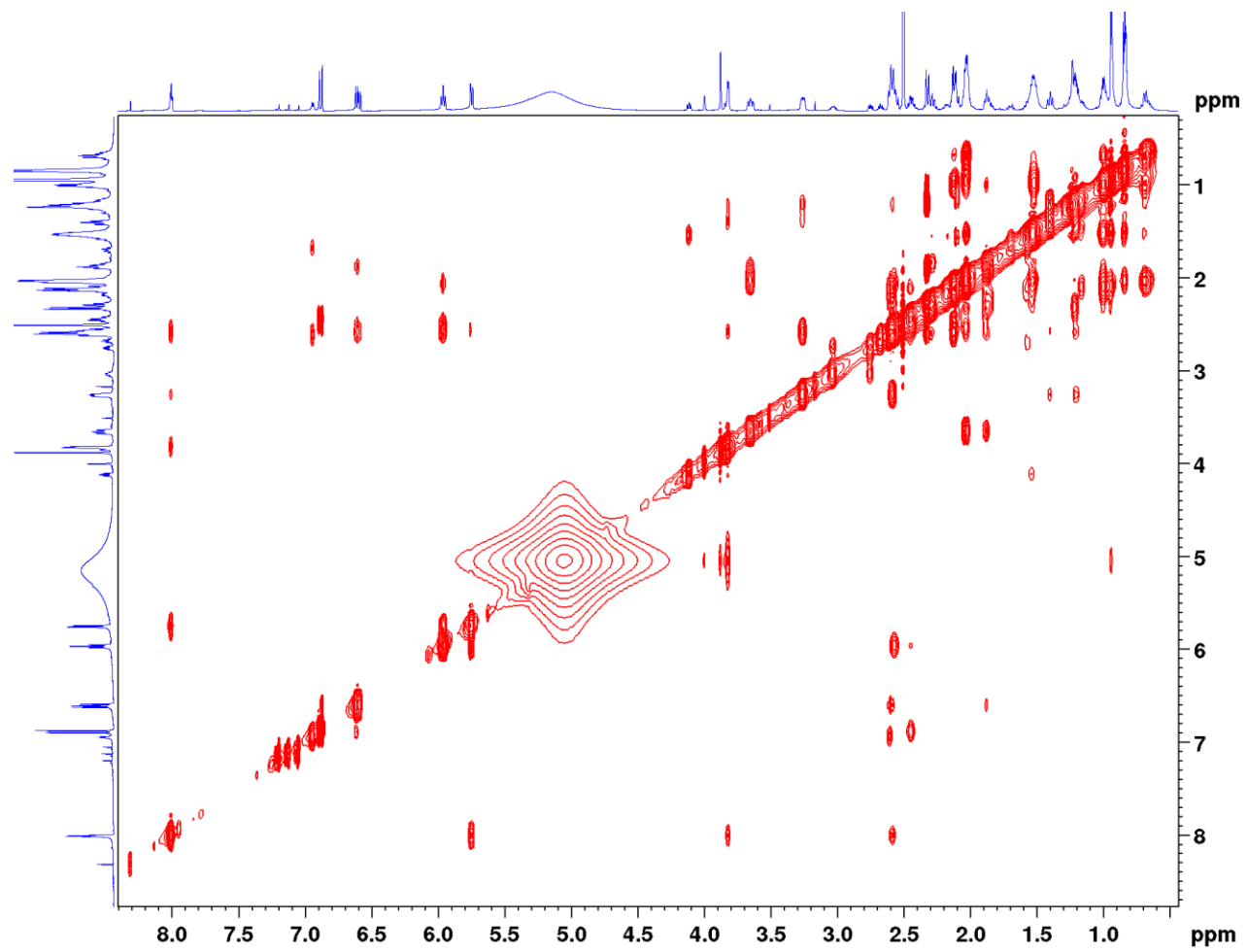


Figure S42. The key NOESY spectrum of compound **5** in DMSO-*d*₆.

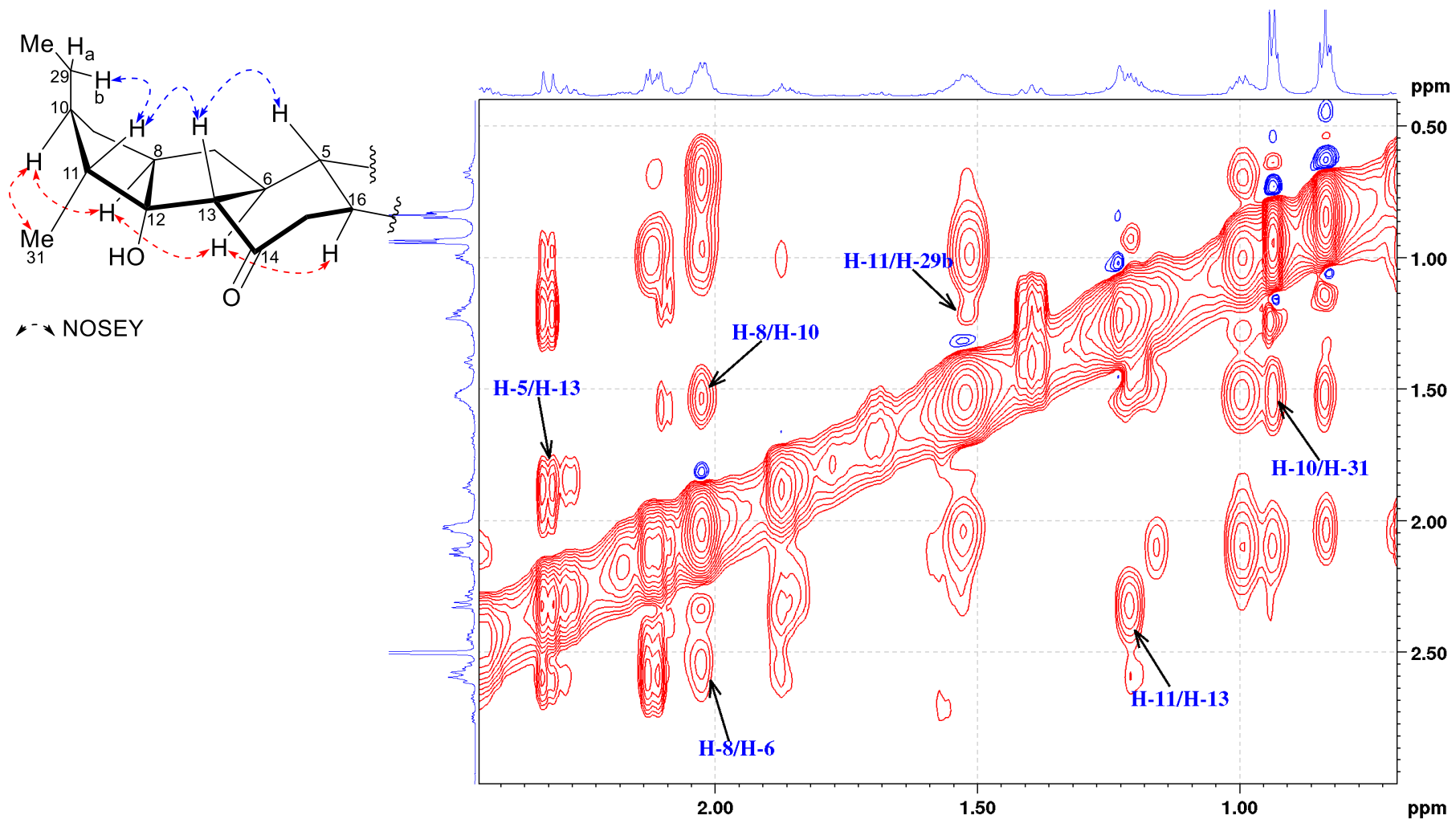
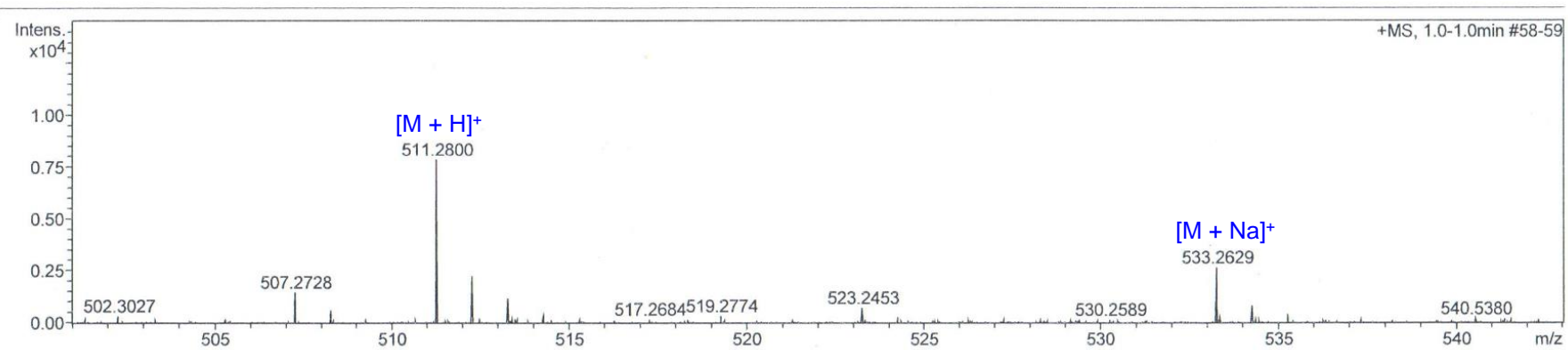
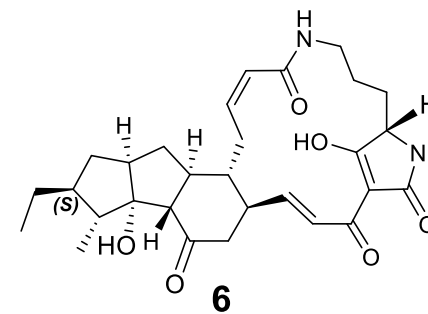
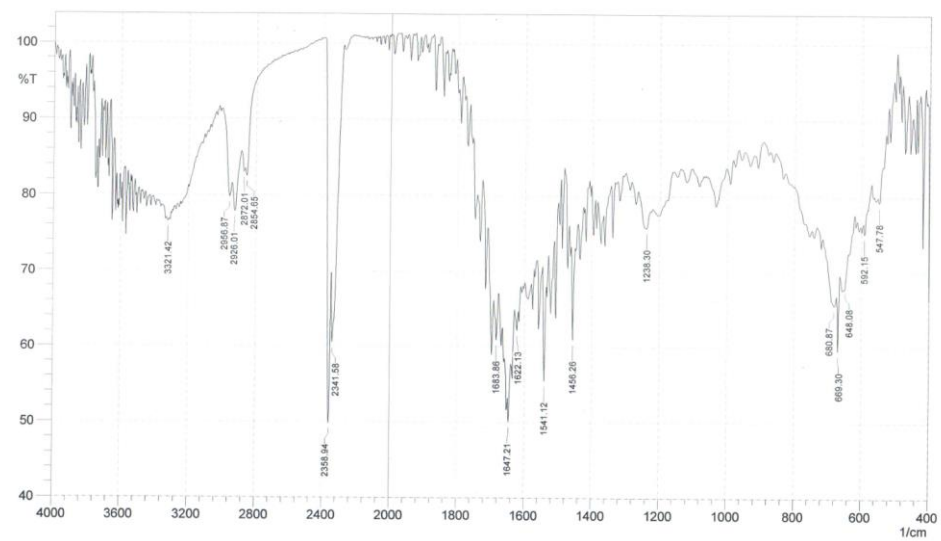


Figure S43. HRESIMS (a) and IR (b) of compound **6**.

(a) HR-ESI-MS



(b) IR



Chemical Formula: $C_{29}H_{38}N_2O_6$
 caculated for $[M+H]^+$: 511.2808
 caculated for $[M+Na]^+$: 533.2628

Figure S44. The 1H NMR spectrum of compound **6** in $DMSO-d_6$.

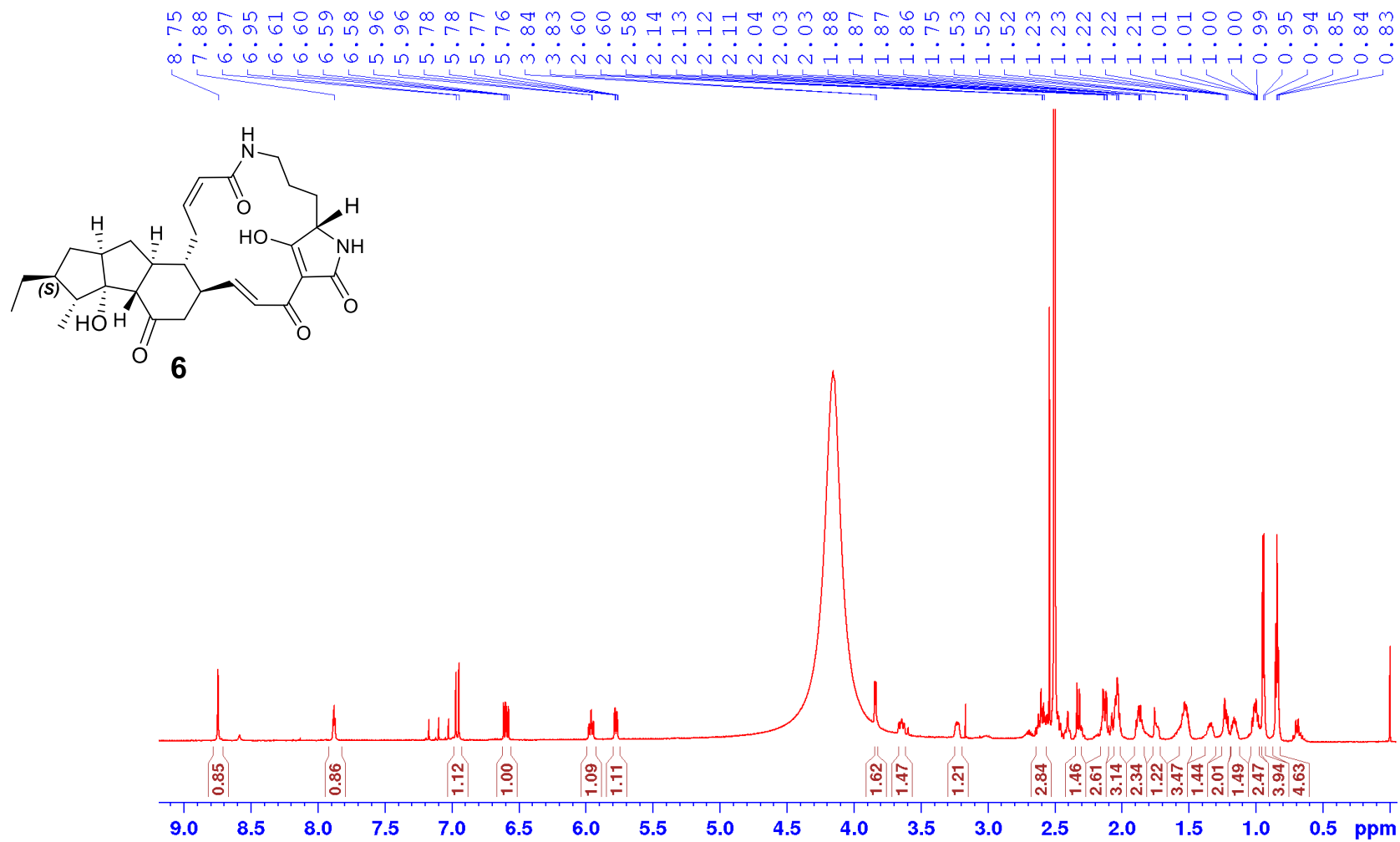
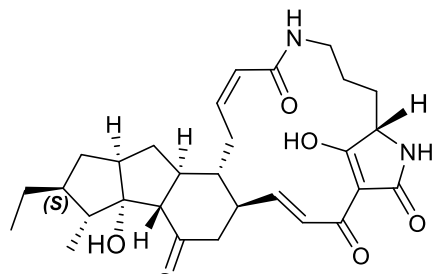


Figure S45. The ^{13}C NMR and DEPT 135 spectra of compound **6** in $\text{DMSO-}d_6$.



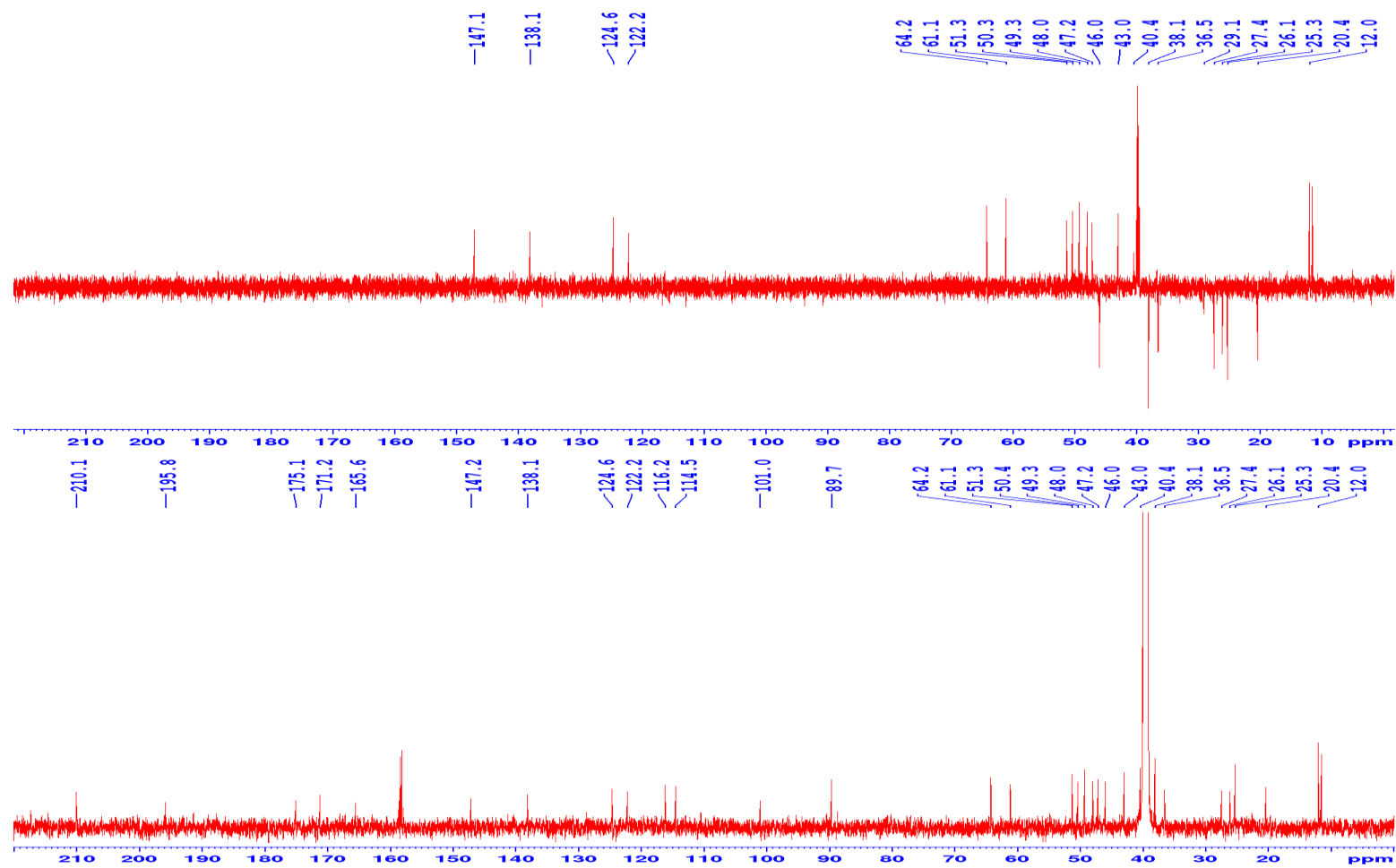


Figure S46. The HSQC spectrum of compound **6** in DMSO- d_6 .

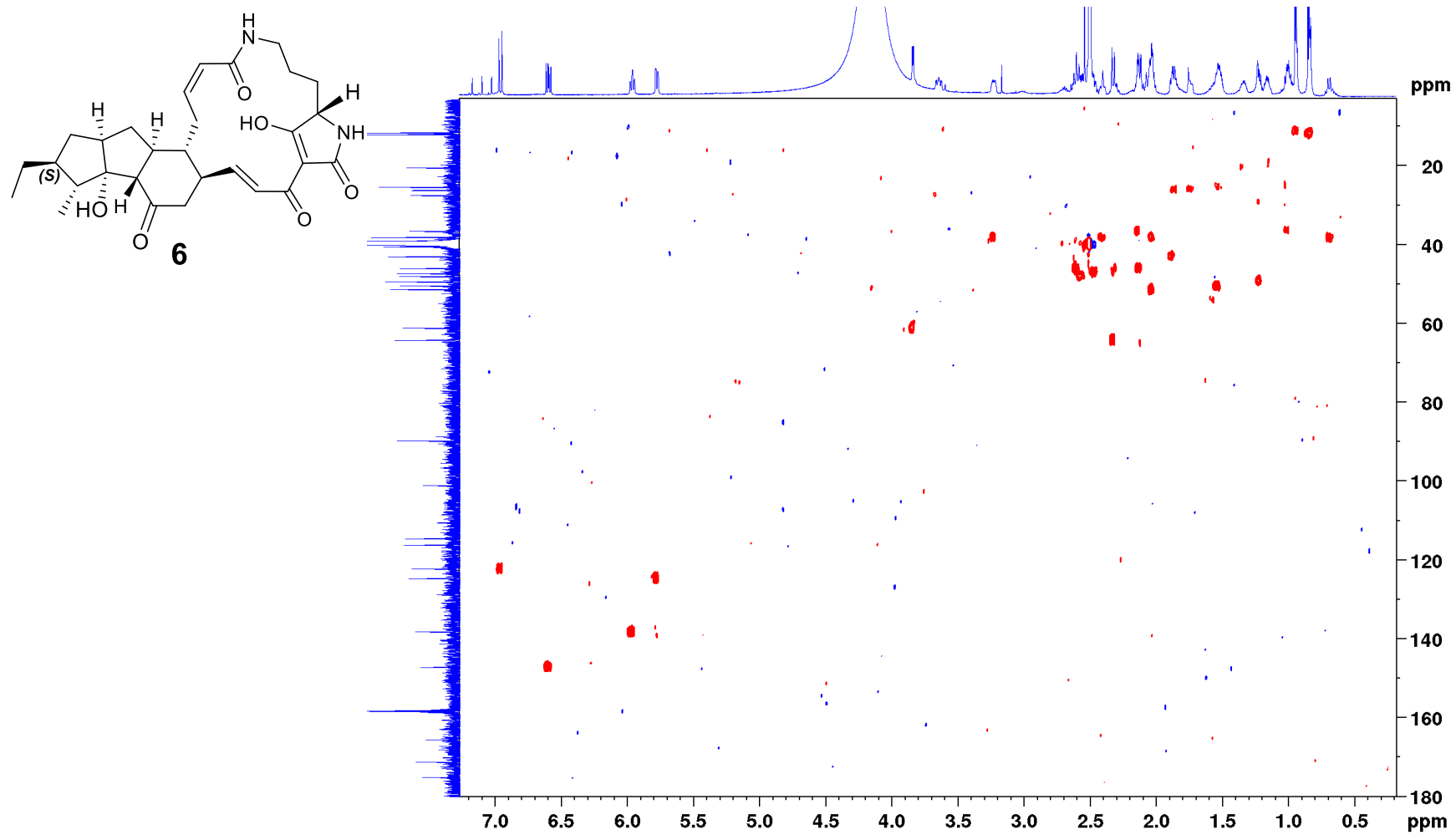


Figure S47. The HMBC spectrum of compound **6** in DMSO-*d*₆.

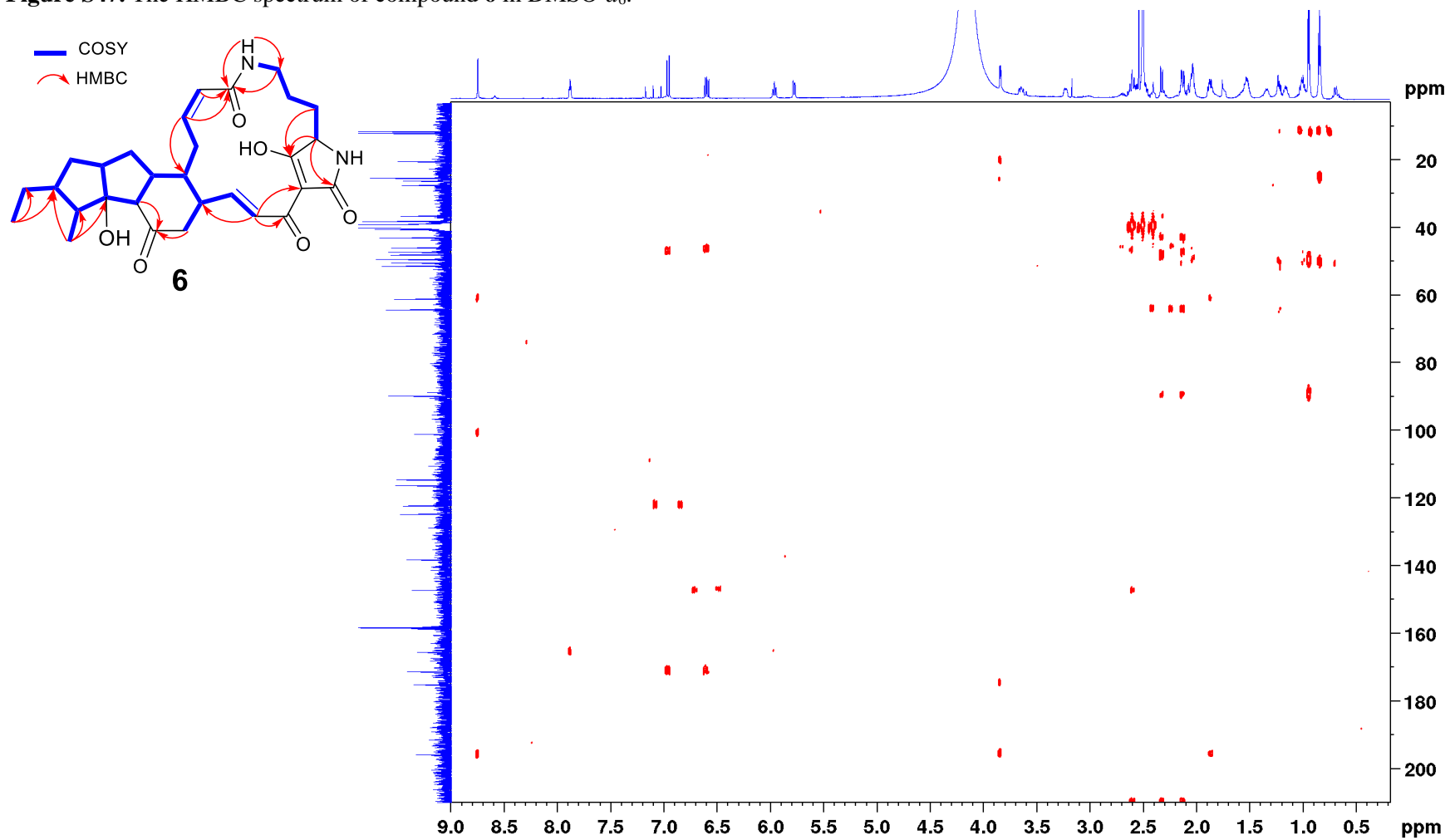


Figure S48. The ^1H - ^1H COSY spectrum of compound **6** in $\text{DMSO-}d_6$

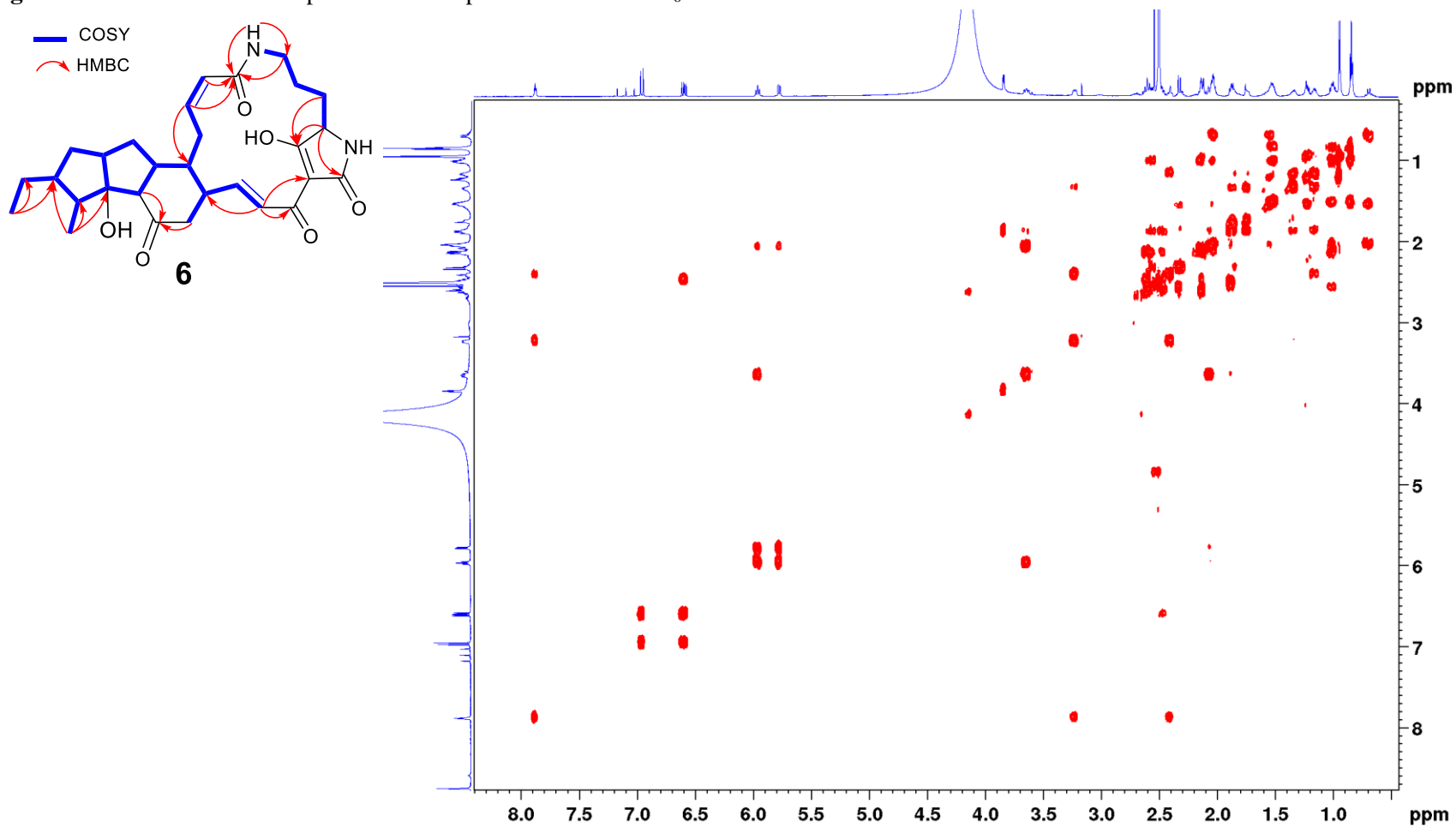


Figure S49. The NOESY spectrum of compound **6** in DMSO-*d*₆.

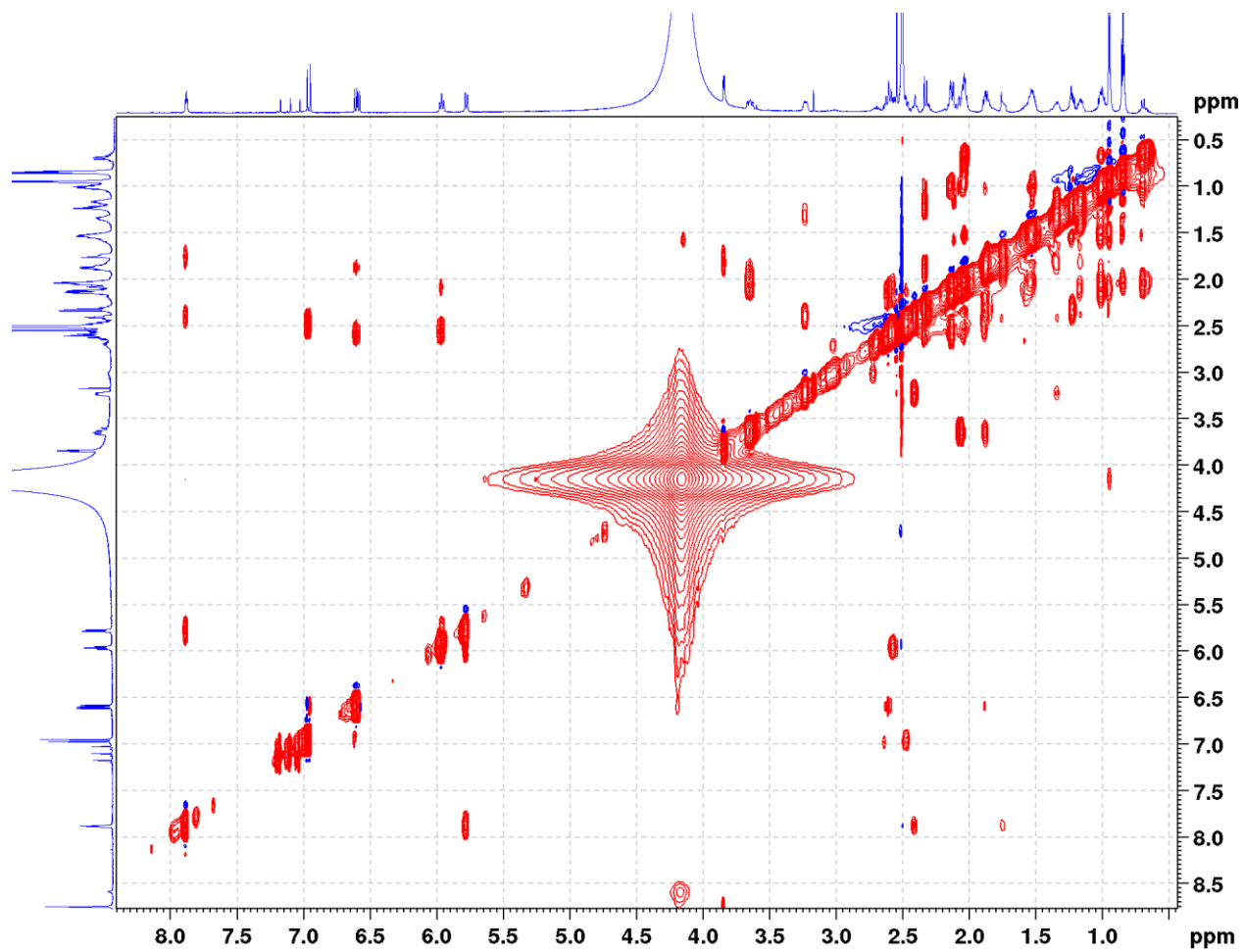


Figure S50. The key NOESY spectrum of compound **6** in DMSO-*d*₆.

