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Supplementary Materials

(±)-Cryptamides A–D, Four Pairs of Novel Dopamine Enantiomer Trimers from the Periostracum Cicadae

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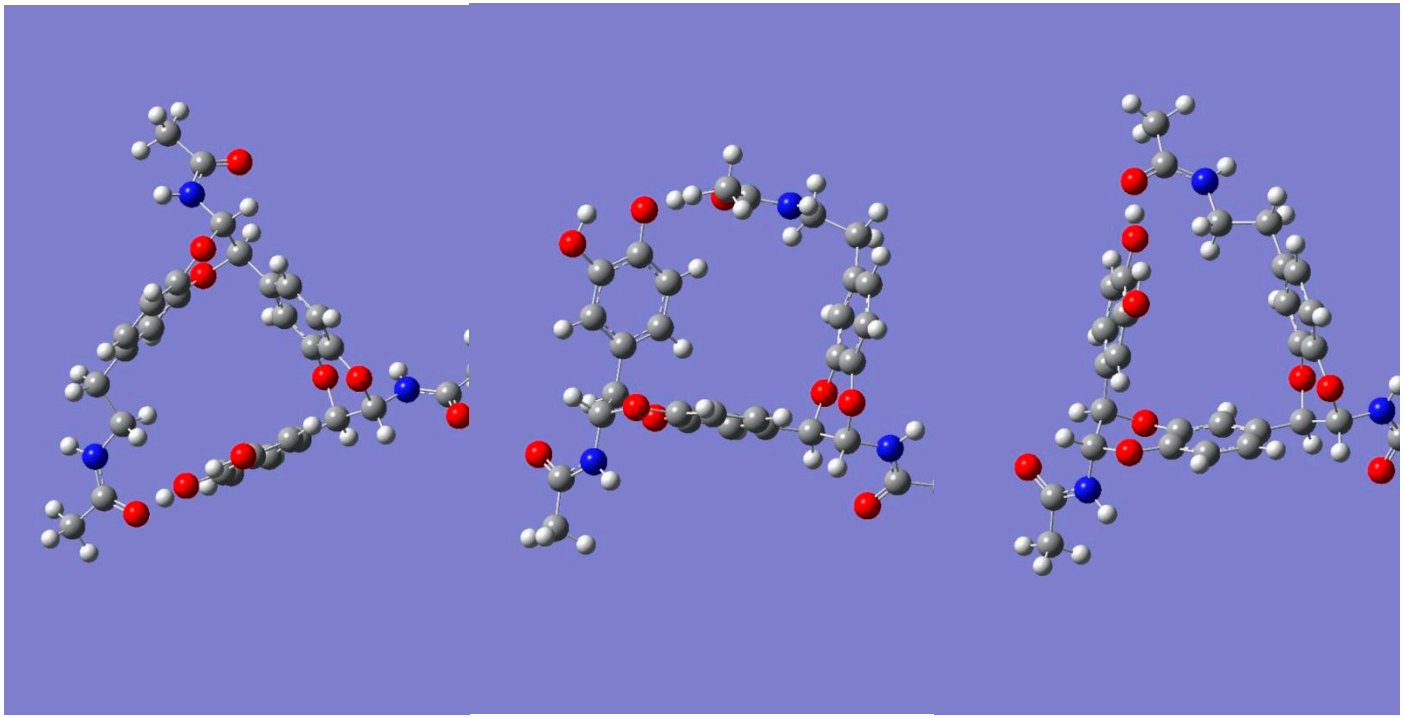
Computational Analysis

Table S1. Energy analysis for **1**.

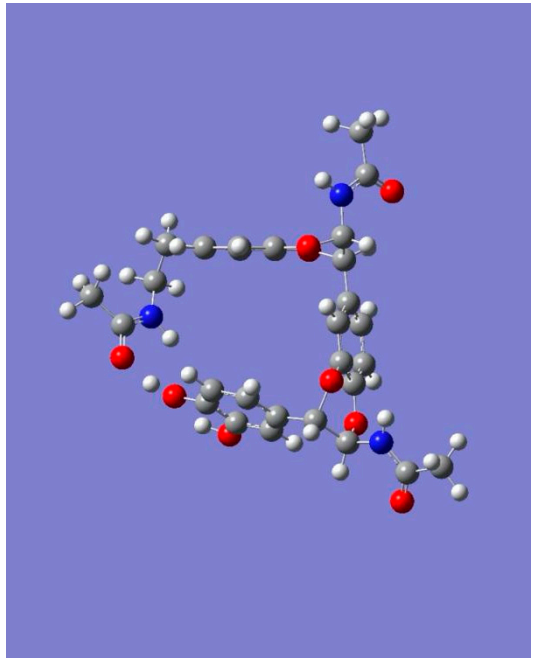
Conformer	Gibbs free energy (298.15 K)		
	G (Hartree)	ΔE (kcal/mol)	Population (%)
1a	-2003.2431	0.0000	99.04
1b	-2003.2383	3.0160	0.61
1c	-2003.2378	3.3405	0.35



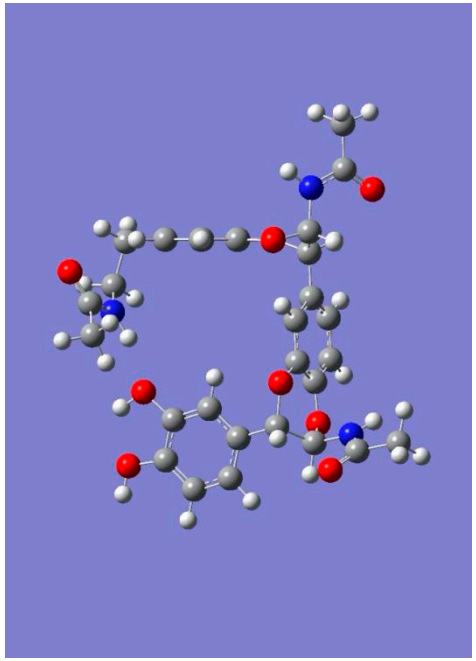
1a **1b** **1c**

Table S2. Energy analysis for **2**.

Conformer	Gibbs free energy (298.15 K)		
	G (Hartree)	ΔE (kcal/mol)	Population (%)
2a	-2003.2384	0.0000	100
2b	-2003.2278	6.6484	0



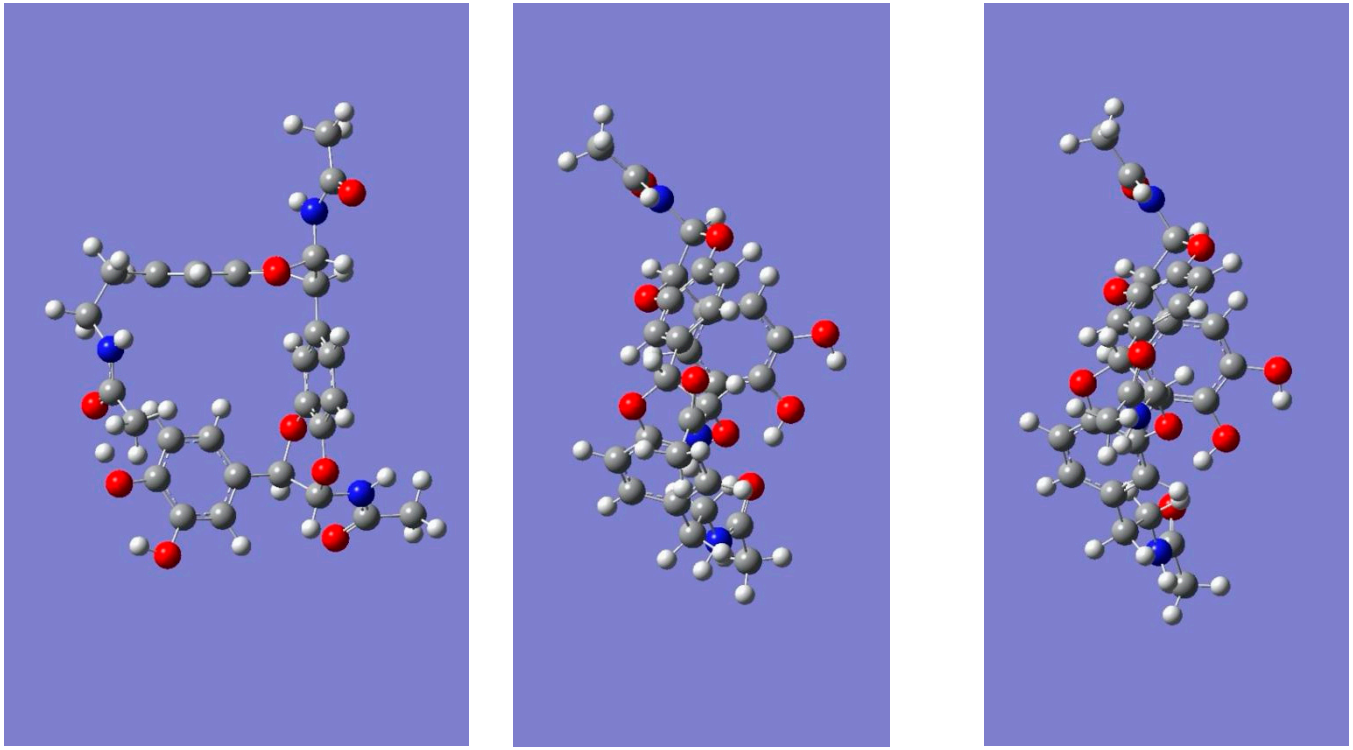
2a



2b

Table S3. Energy analysis for **3**.

Conformer	Gibbs free energy (298.15 K)		
	G (Hartree)	ΔE (kcal/mol)	Population (%)
3a	-2003.2445	0.0000	99.92
3b	-2003.2364	5.0774	0.02
3c	-2003.2376	4.3398	0.07



3a **3b** **3c**

Table S4. Energy analysis for **4**.

Conformer	Gibbs free energy (298.15 K)		
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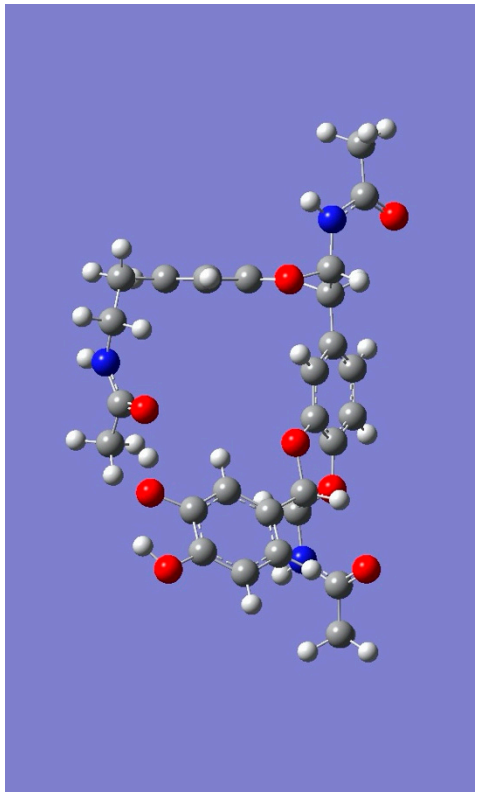
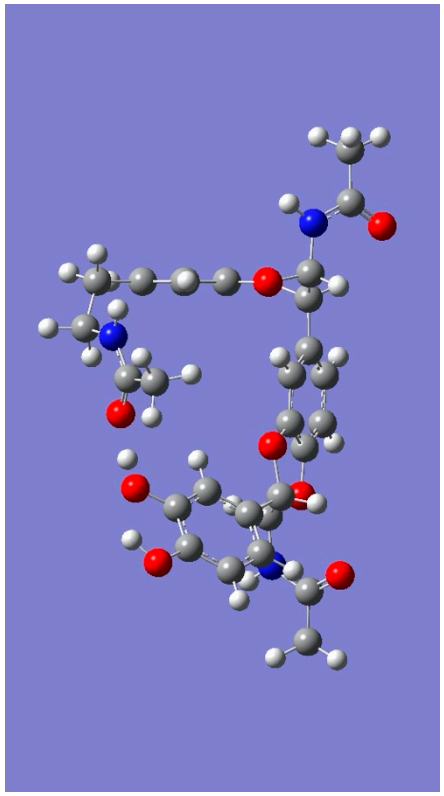
4a	-2003.2441	0.1745	42.68
4b	-2003.2444	0.0000	57.32



4a



4b

NMR spectra of compounds **1–4**

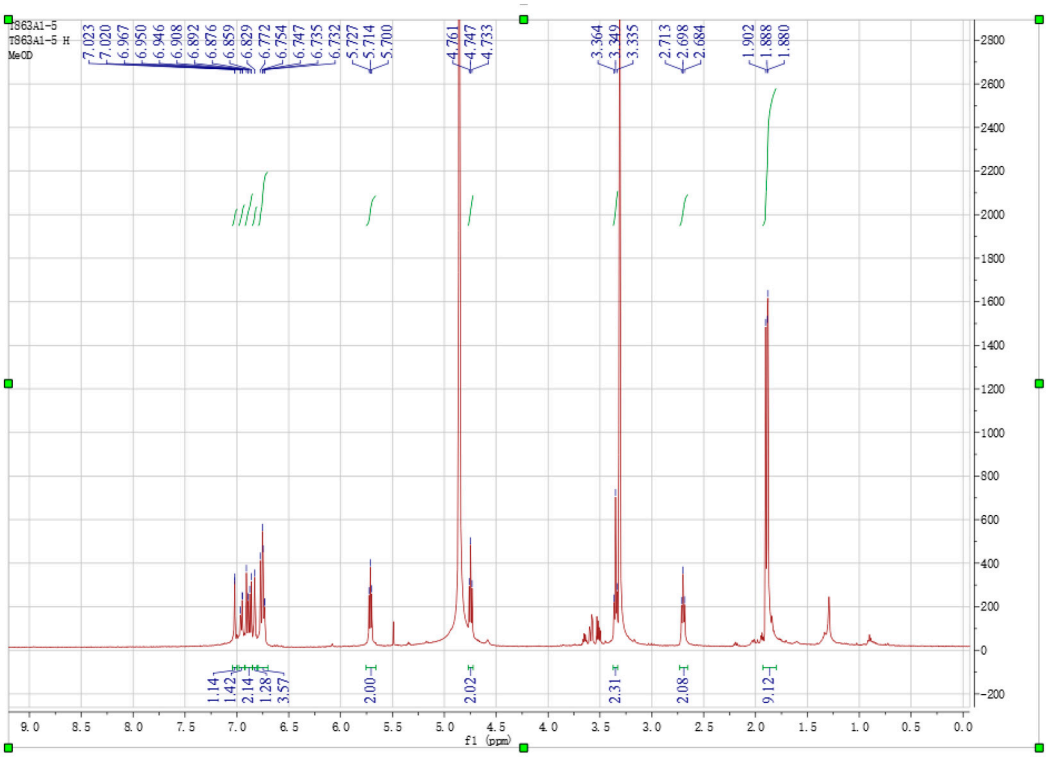


Figure S1. [1]H-NMR spectrum of **1** in methanol-d_4.

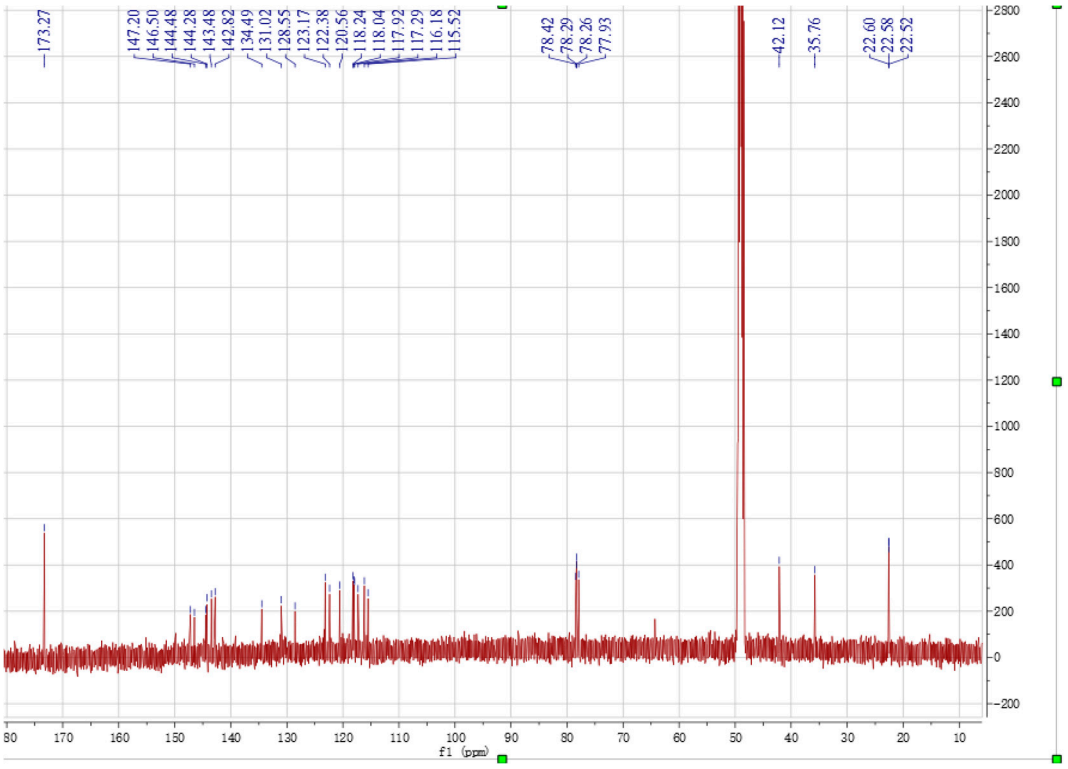


Figure S2. [13]C-NMR spectrum of **1** in methanol-d_4.

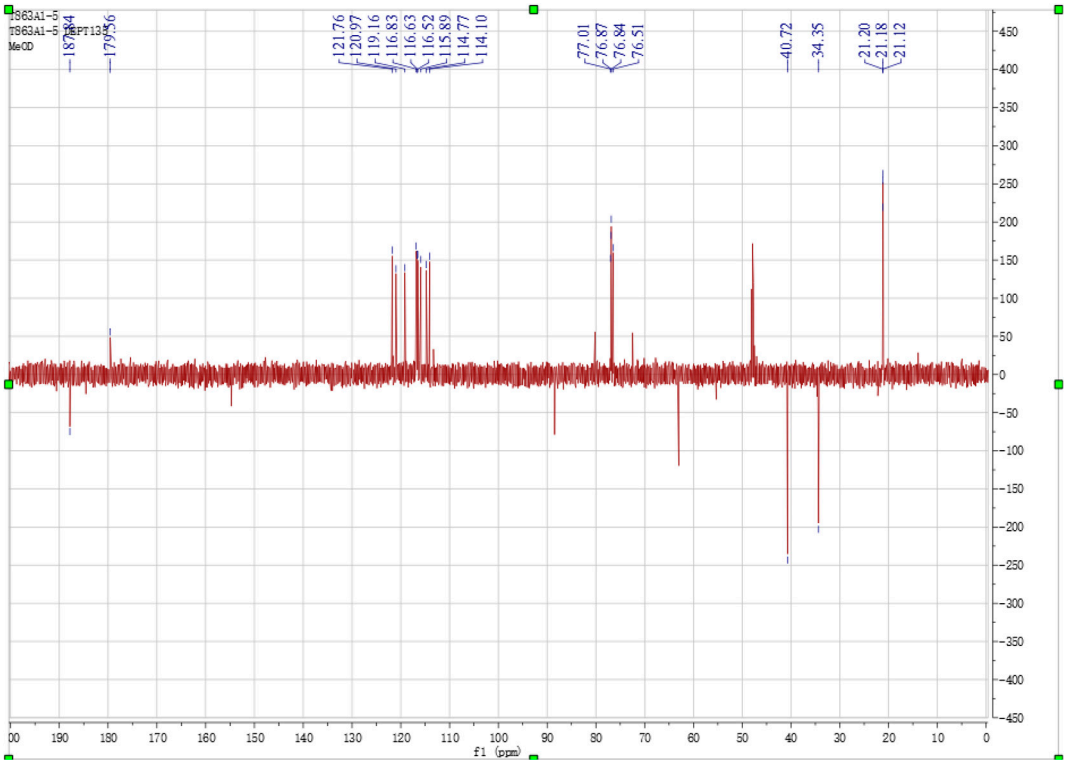


Figure S3. DEPT spectrum of **1** in methanol-d_4.

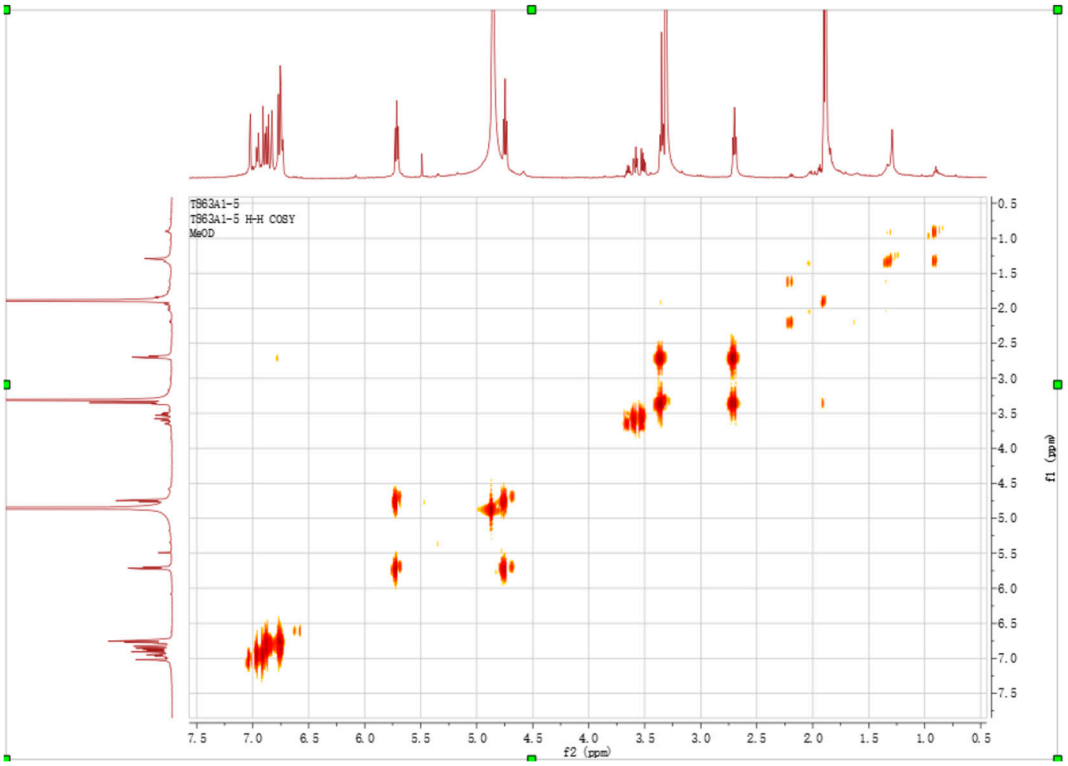


Figure S4. ^{1}H-^{1}H-COSY spectrum of **1** in methanol-d_4.

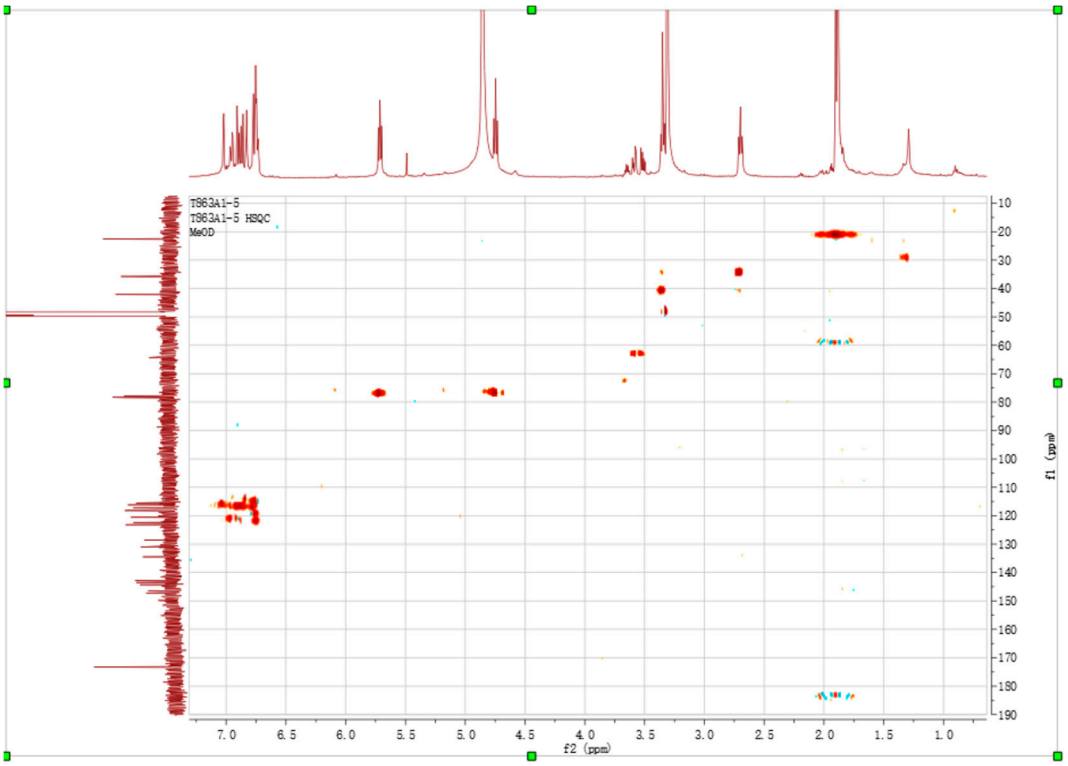


Figure S5. HSQC spectrum of **1** in methanol-d_4.

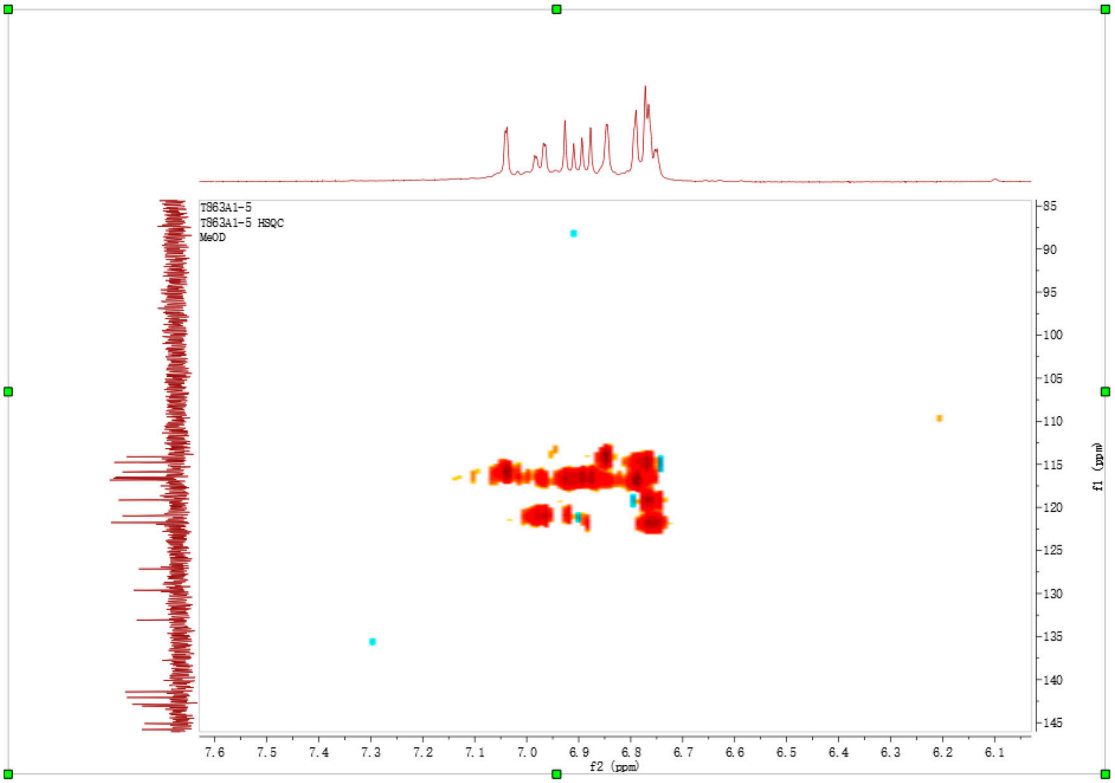


Figure S6. zoomed aromatic region of HSQC spectra of **1**.

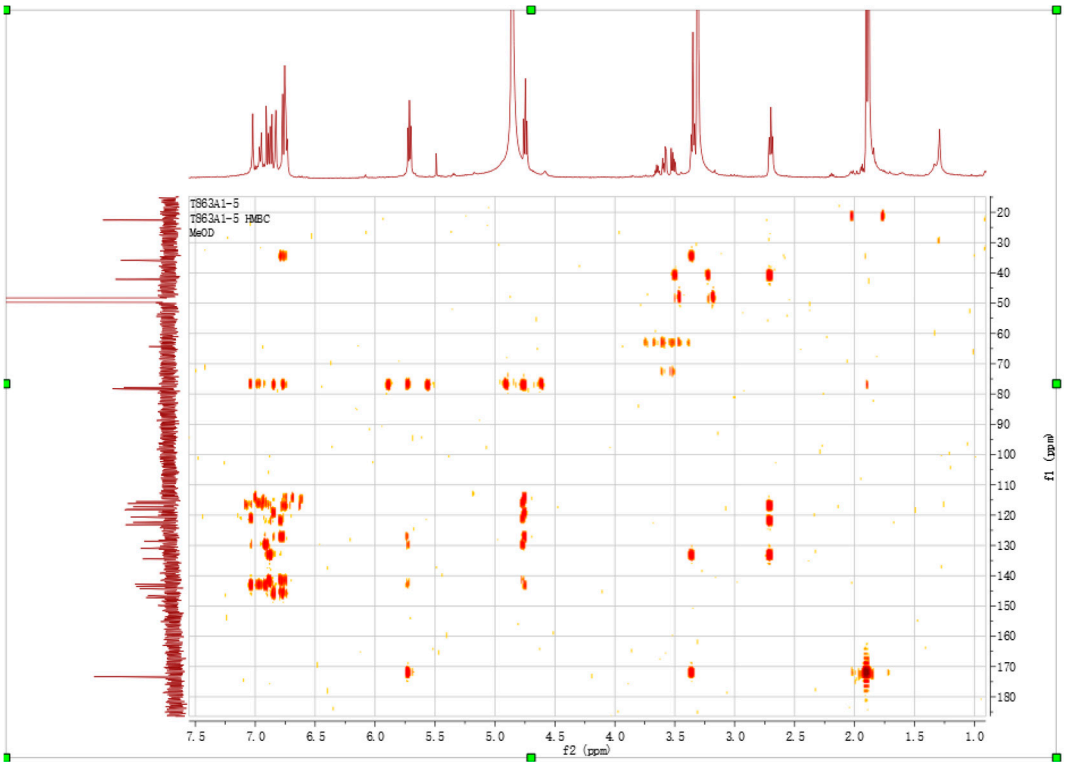


Figure S7. HMBC spectrum of **1** in methanol-d_4.

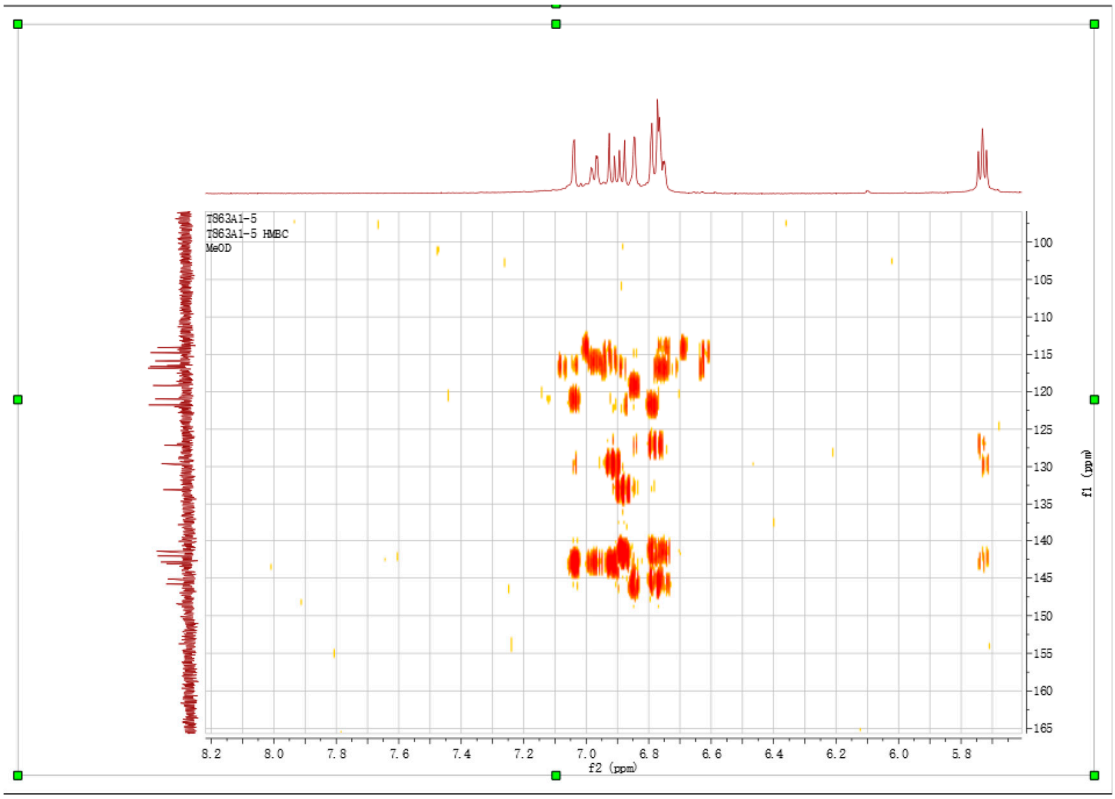


Figure S8. zoomed aromatic region of HMBC spectra of **1**.

Figure S9. [1]H-NMR spectrum of **2** in methanol-d_4.

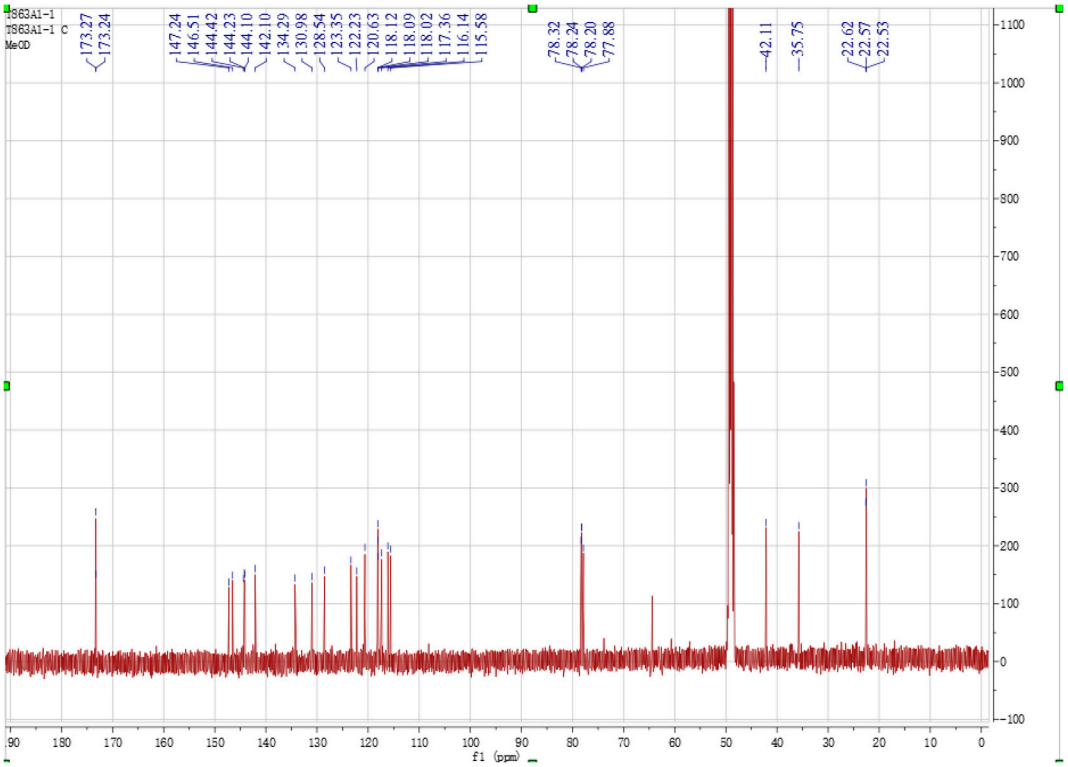


Figure S10. [13]C-NMR spectrum of **2** in methanol-d_4.

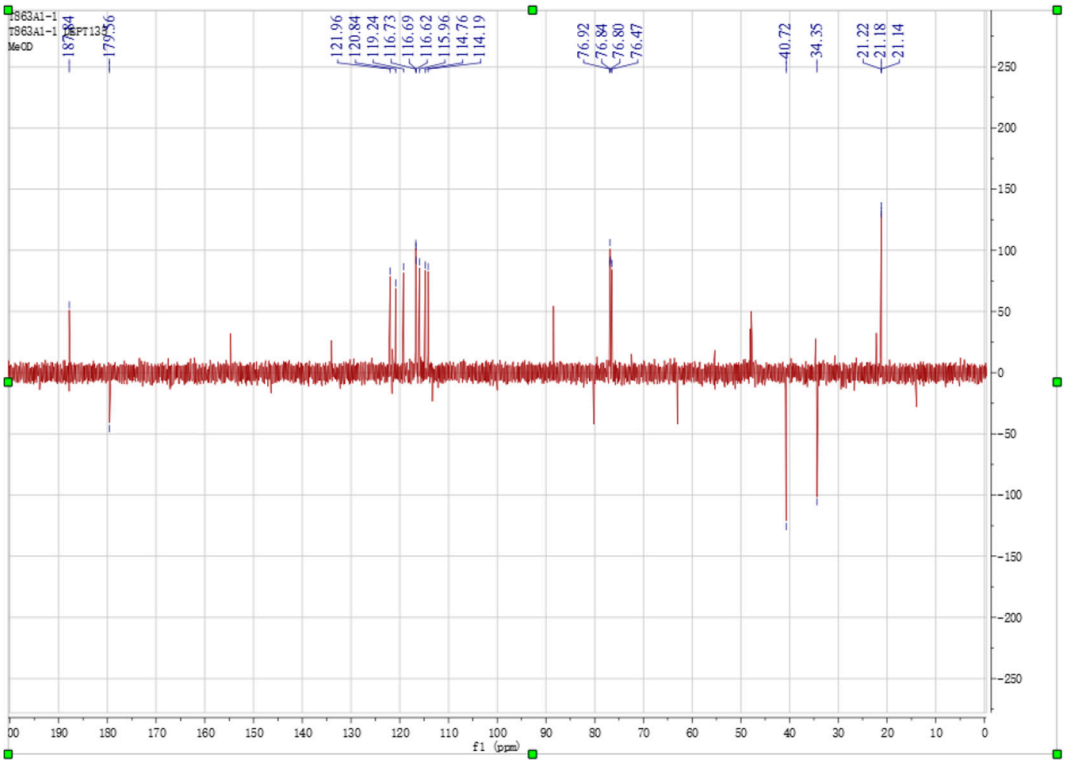


Figure S11. DEPT spectrum of **2** in methanol-d_4.

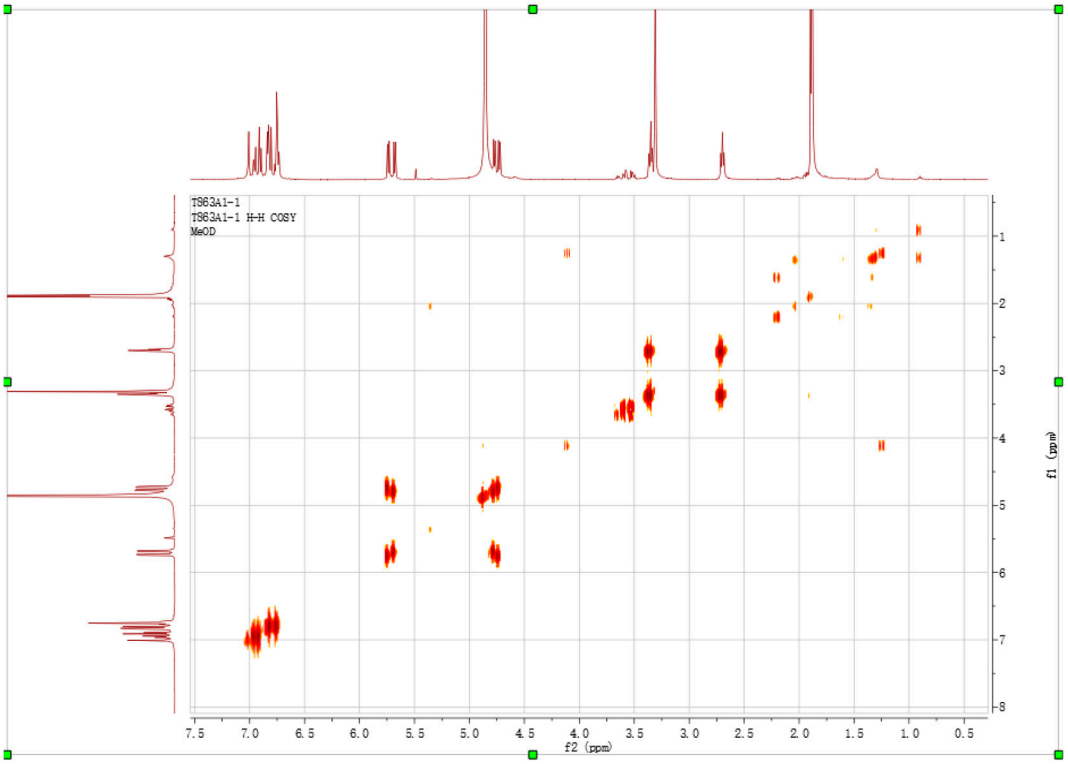


Figure S12. ^{1}H-^{1}H-COSY spectrum of **2** in methanol-d_4.

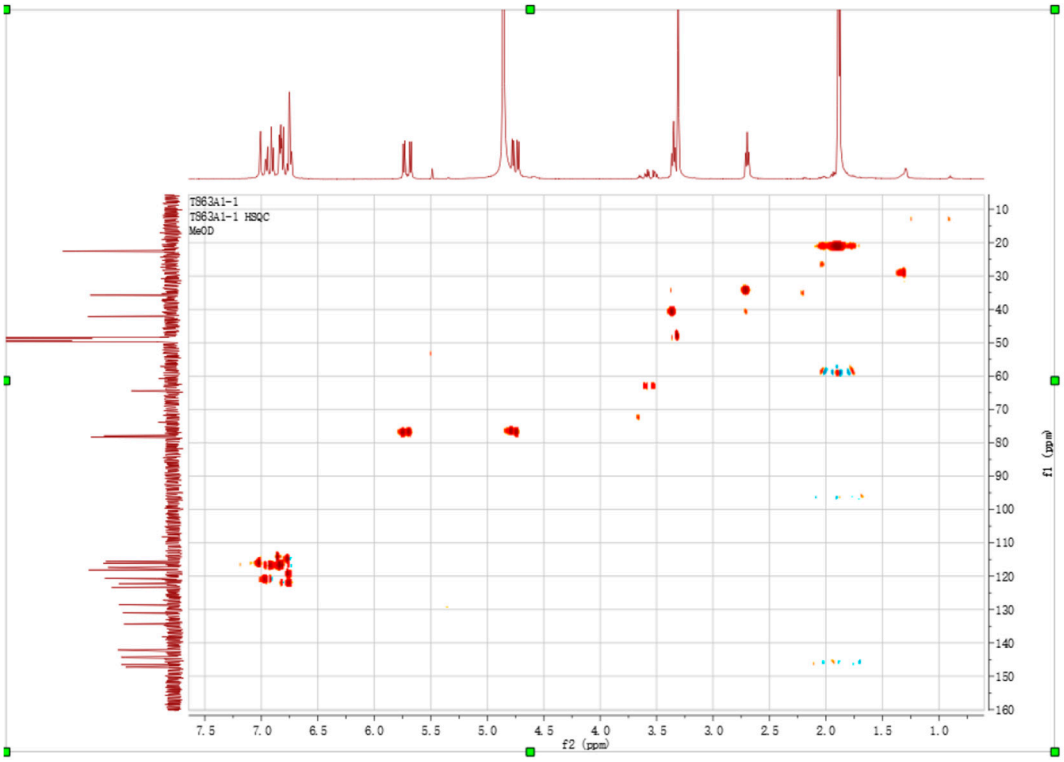


Figure S13. HSQC spectrum of **2** in methanol-d_4.

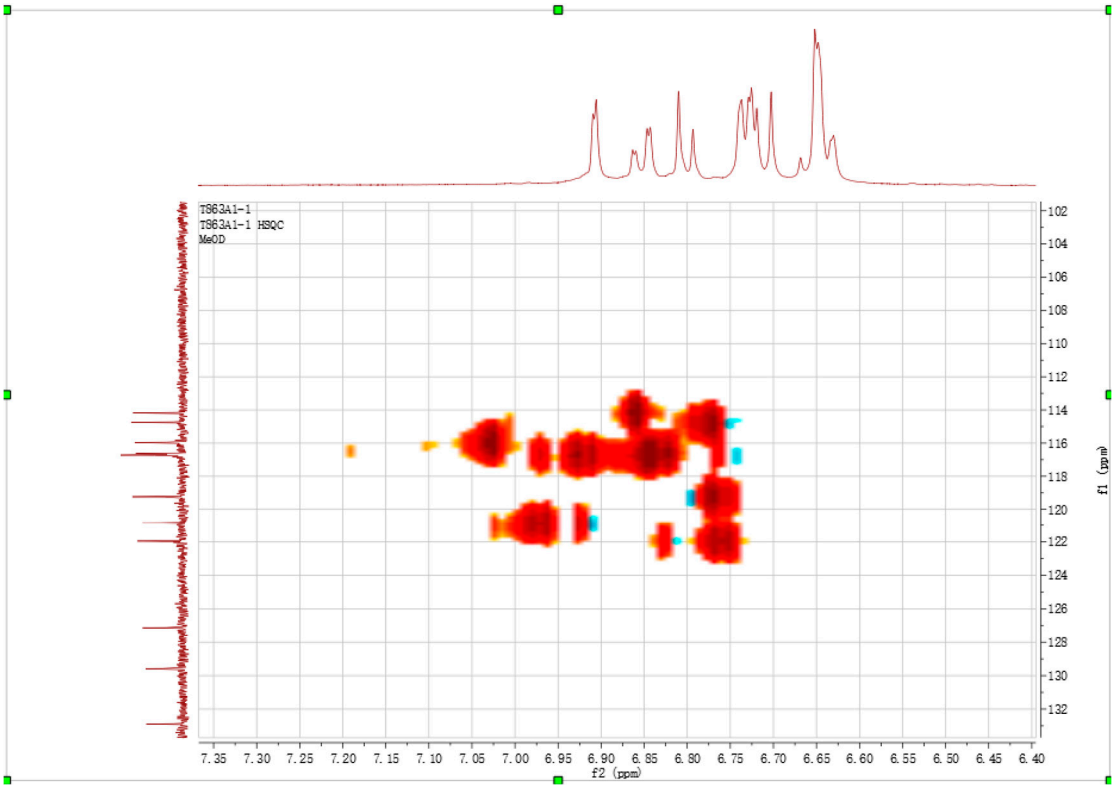


Figure S14. zoomed aromatic region of HSQC spectra of **2**.

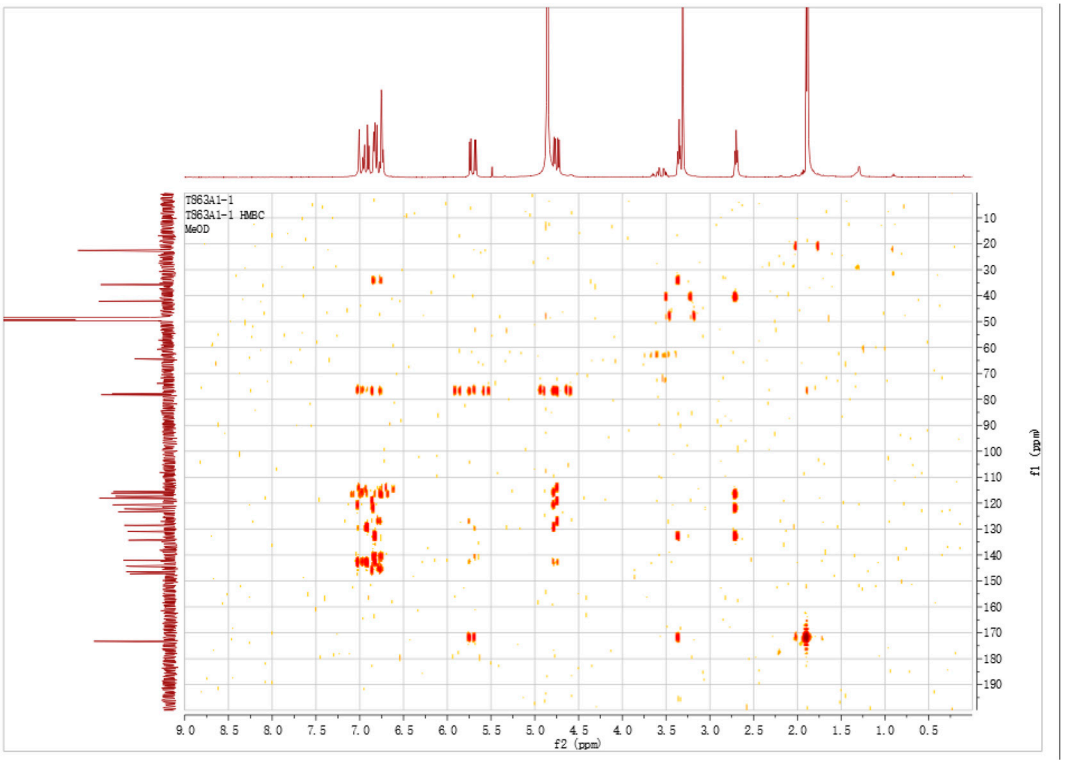


Figure S15. HMBC spectrum of **2** in methanol-d_4.

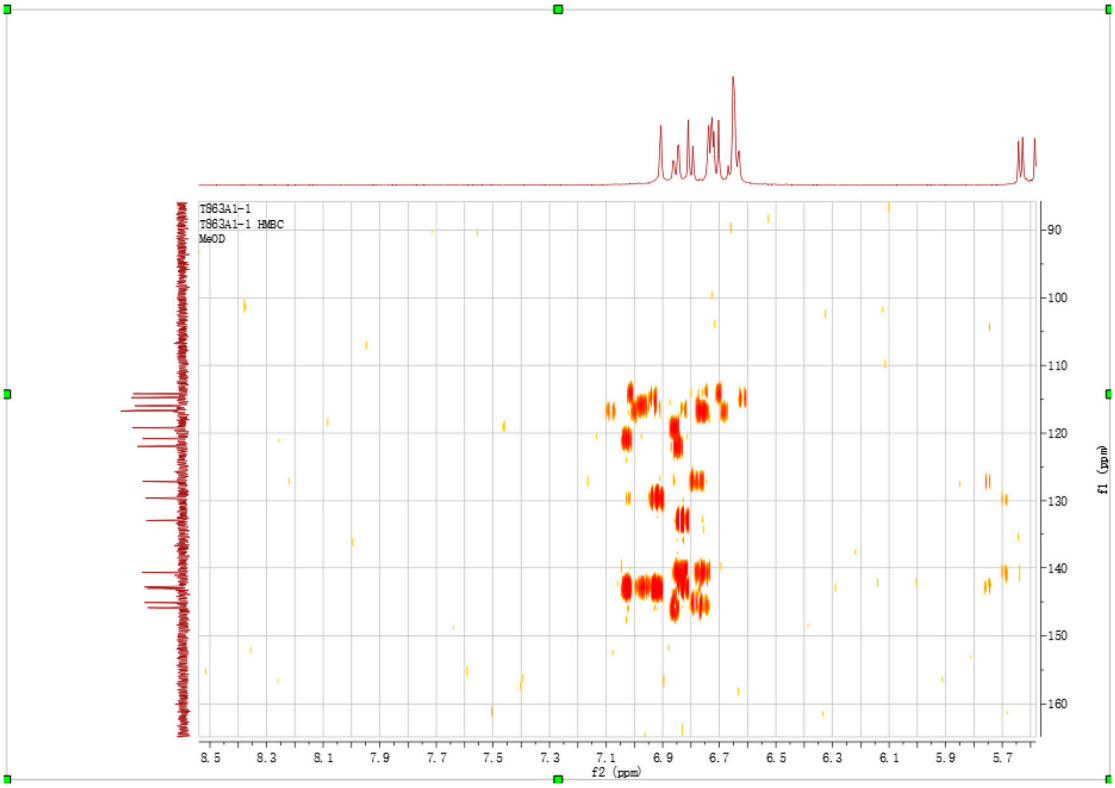


Figure S16. zoomed aromatic region of HMBC spectra of **2**.

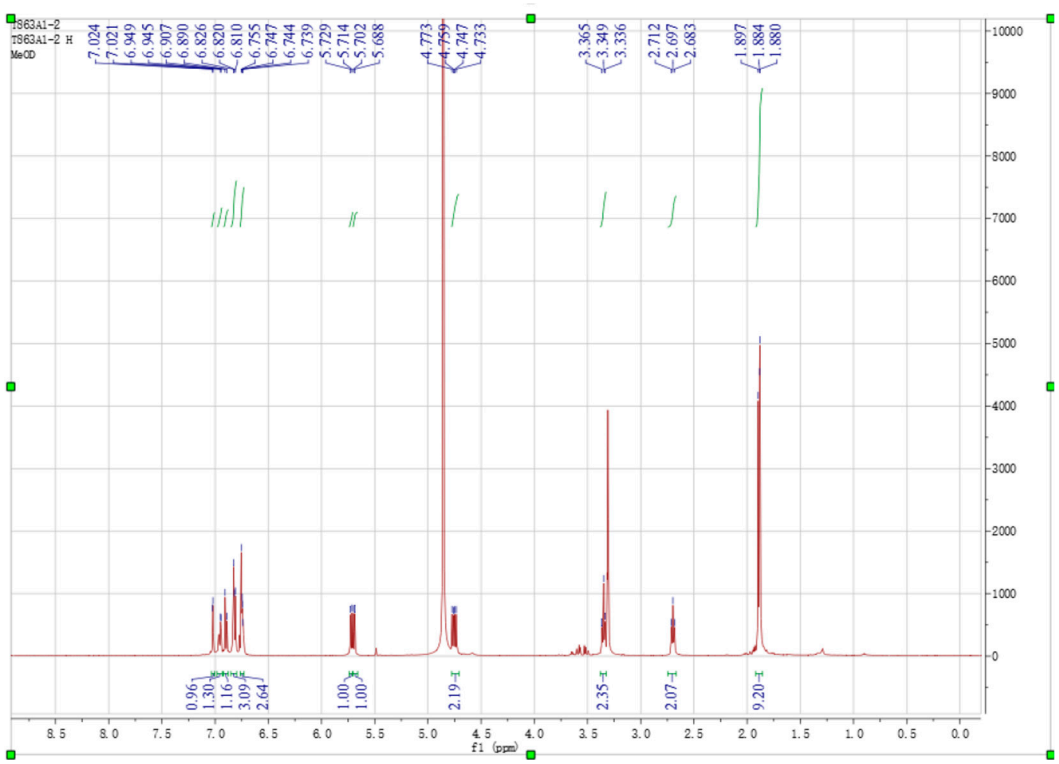


Figure S17. [1]H-NMR spectrum of **3** in methanol-d_4.

Figure S18. [13]C-NMR spectrum of **3** in methanol-d_4.

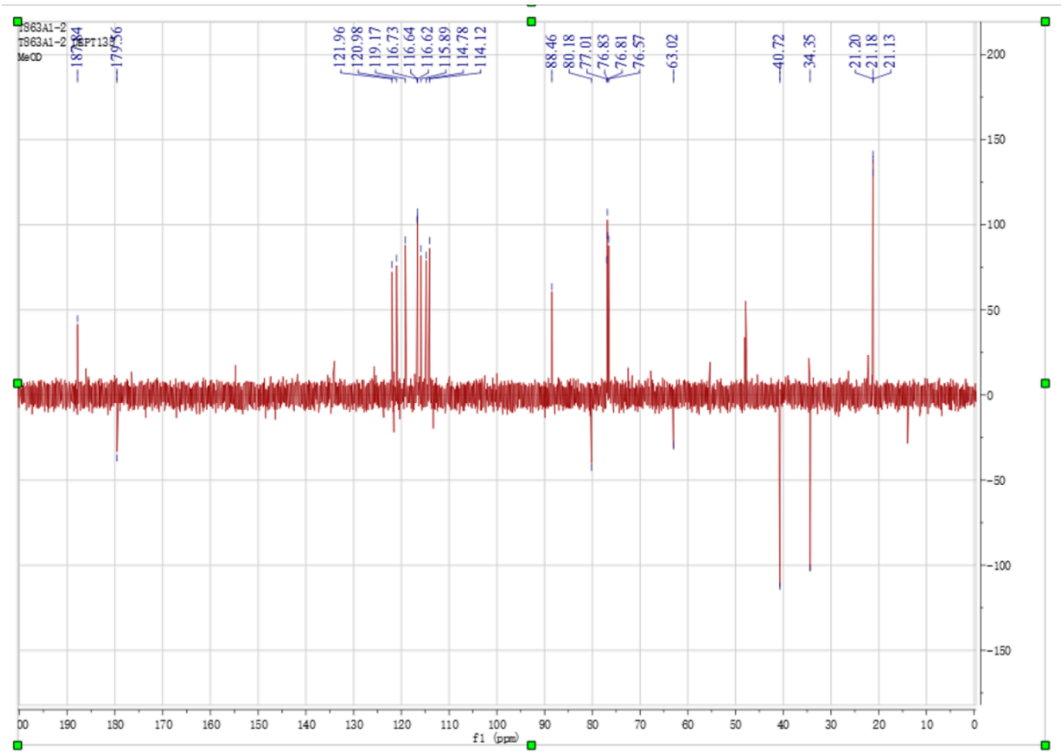


Figure S19. DEPT spectrum of **3** in methanol-d_4.

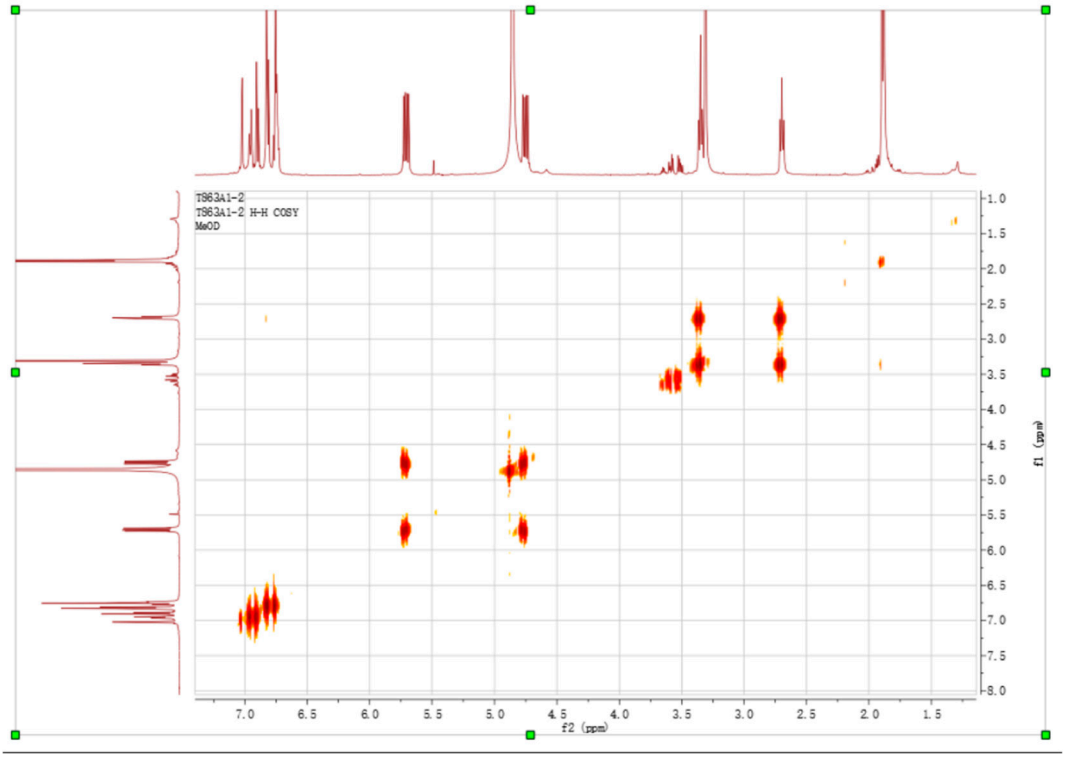


Figure S20. ^{1}H-^{1}H COSY spectrum of **3** in methanol-d_4.

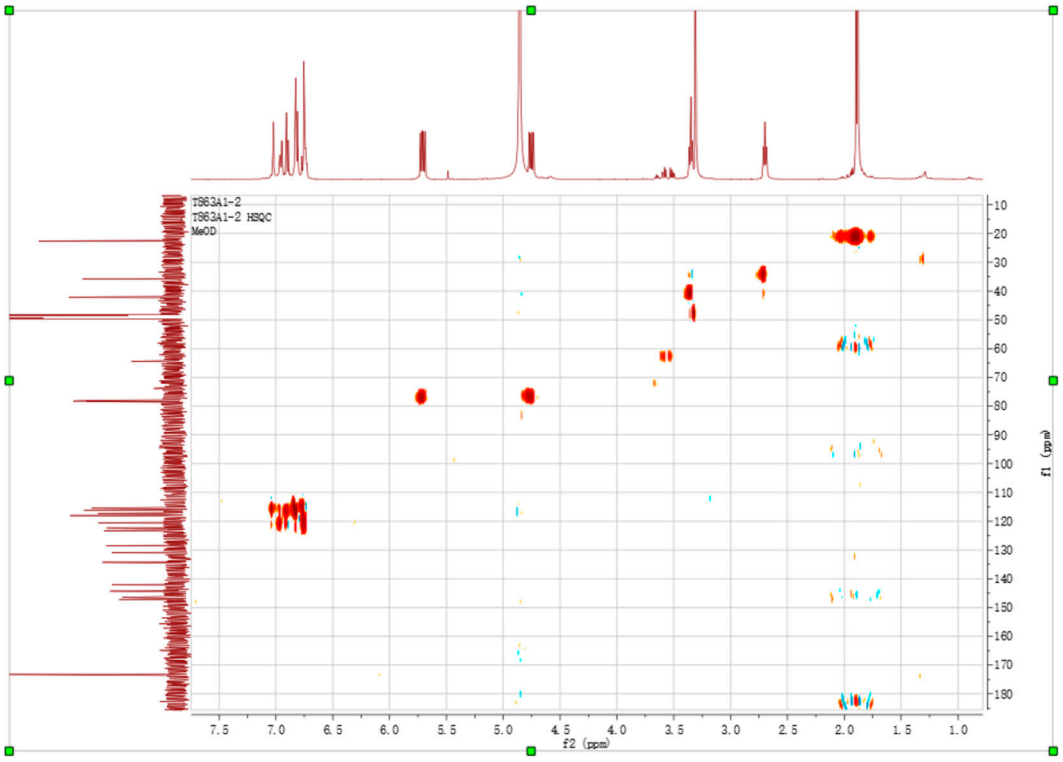


Figure S21. HSQC spectrum of **3** in methanol-d_4.

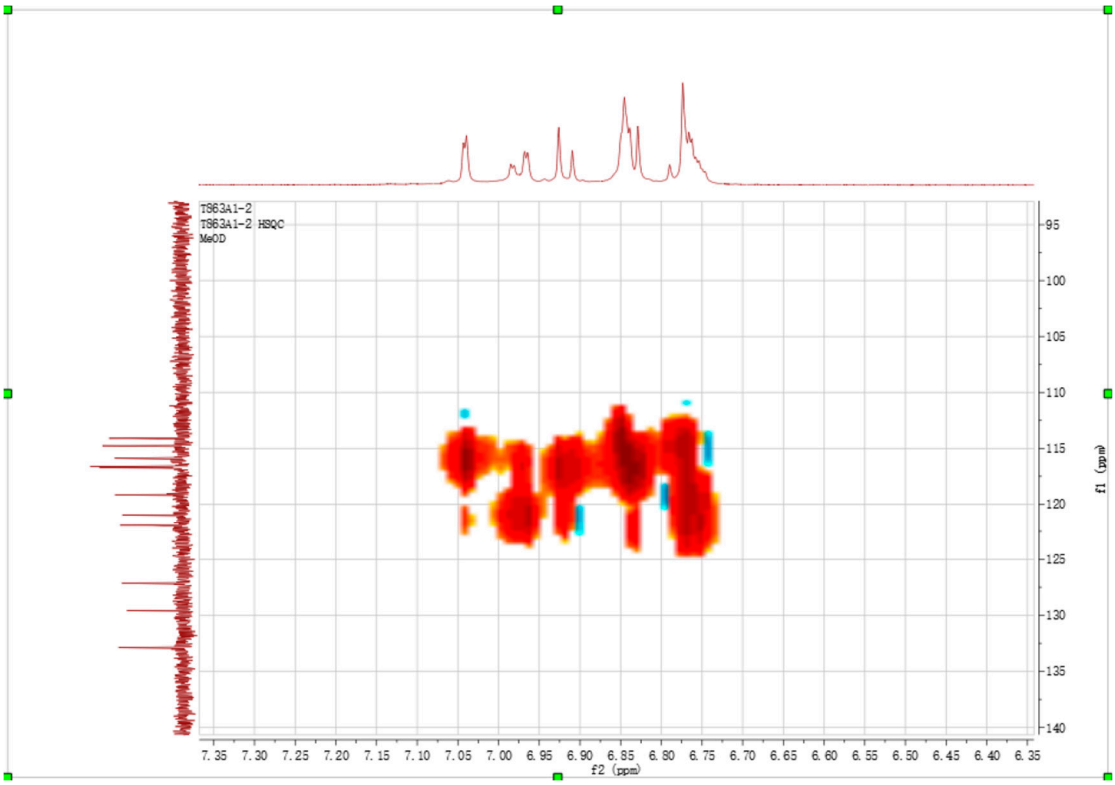


Figure S22. zoomed aromatic region of HSQC spectra of **3**.

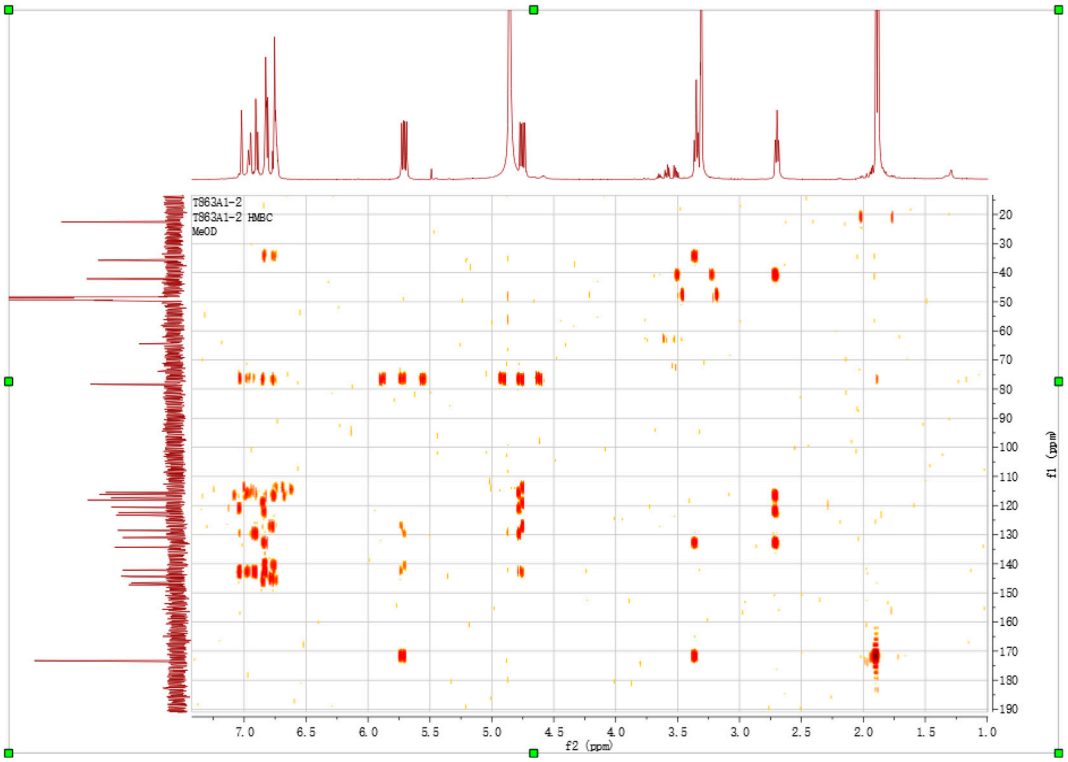


Figure S23. HMBC spectrum of **3** in methanol-d_4.

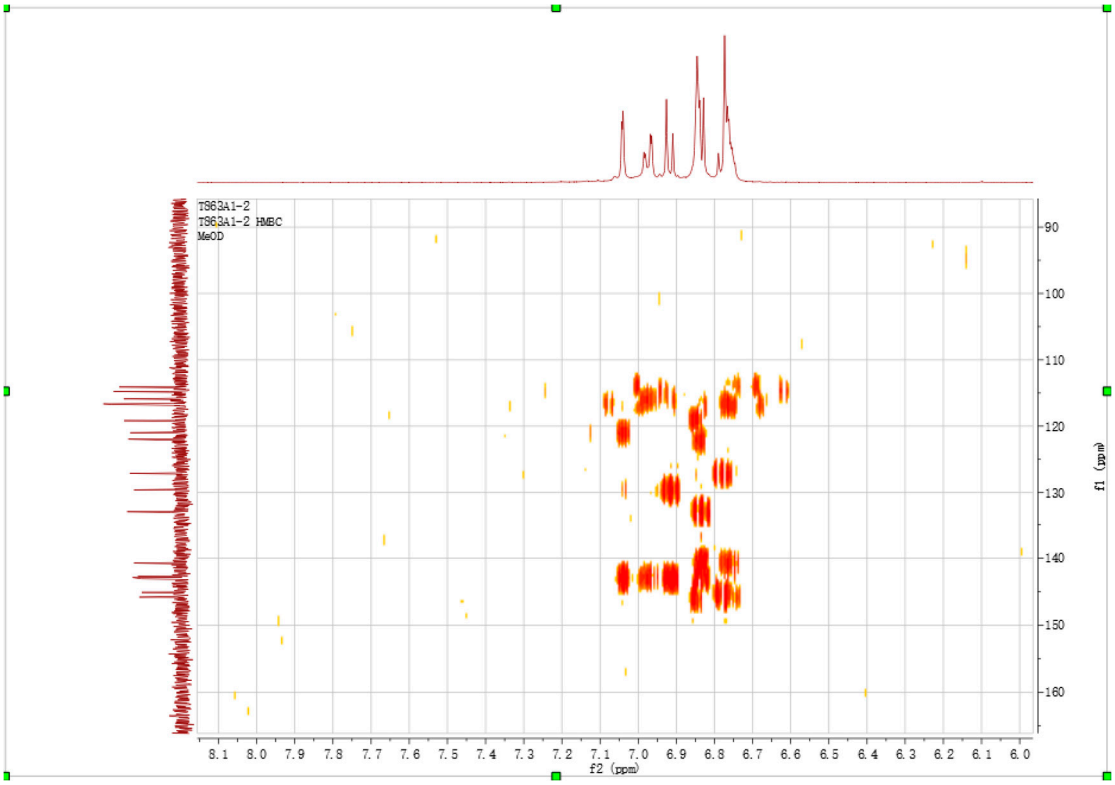


Figure S24. zoomed aromatic region of HMBC spectra of **3**.

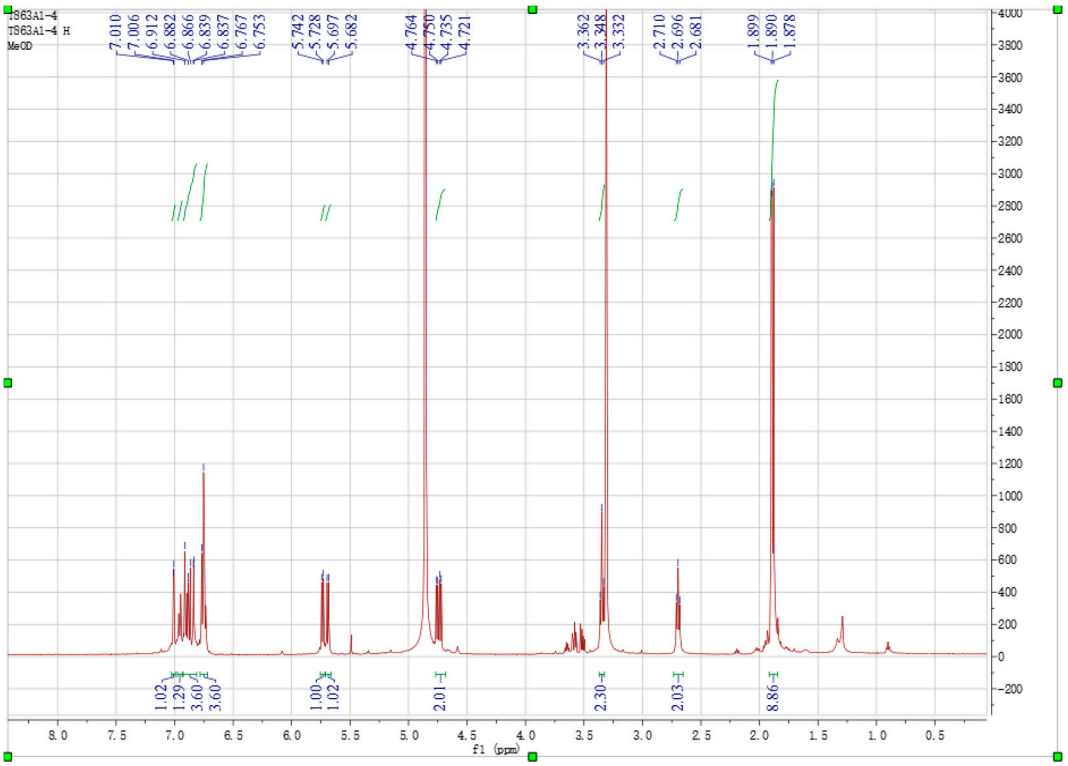


Figure S25. [1]H-NMR spectrum of **4** in methanol-d_4.

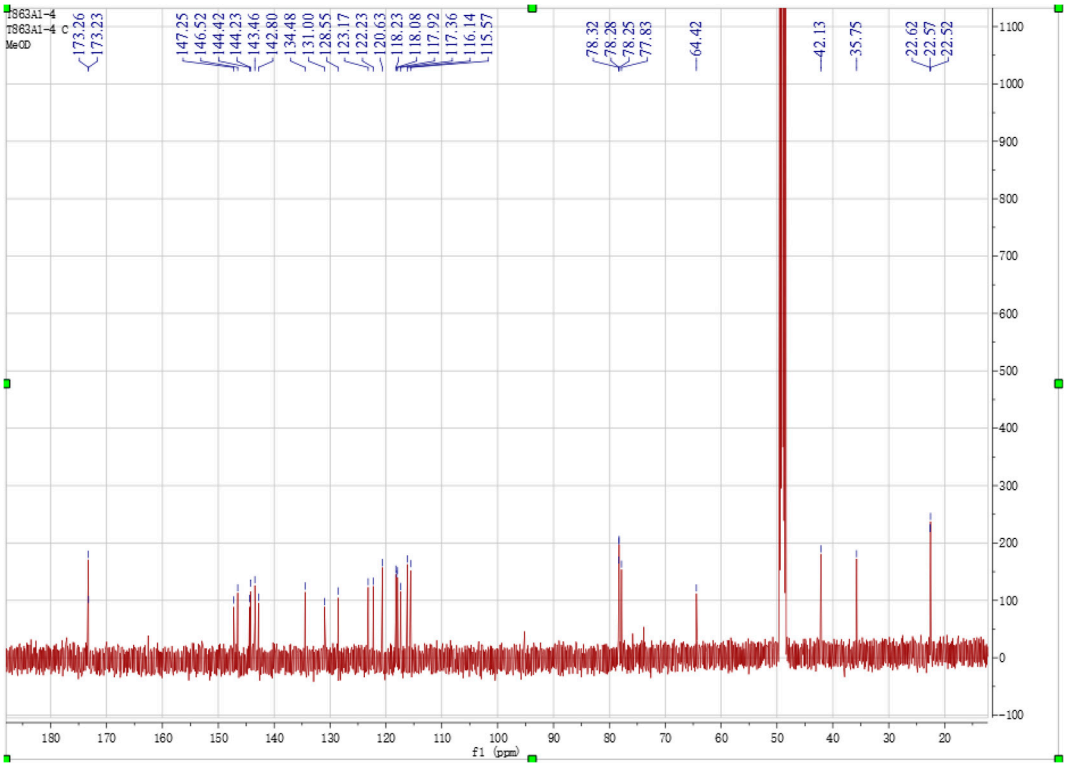


Figure S26. [13]C-NMR spectrum of **4** in methanol-d_4.

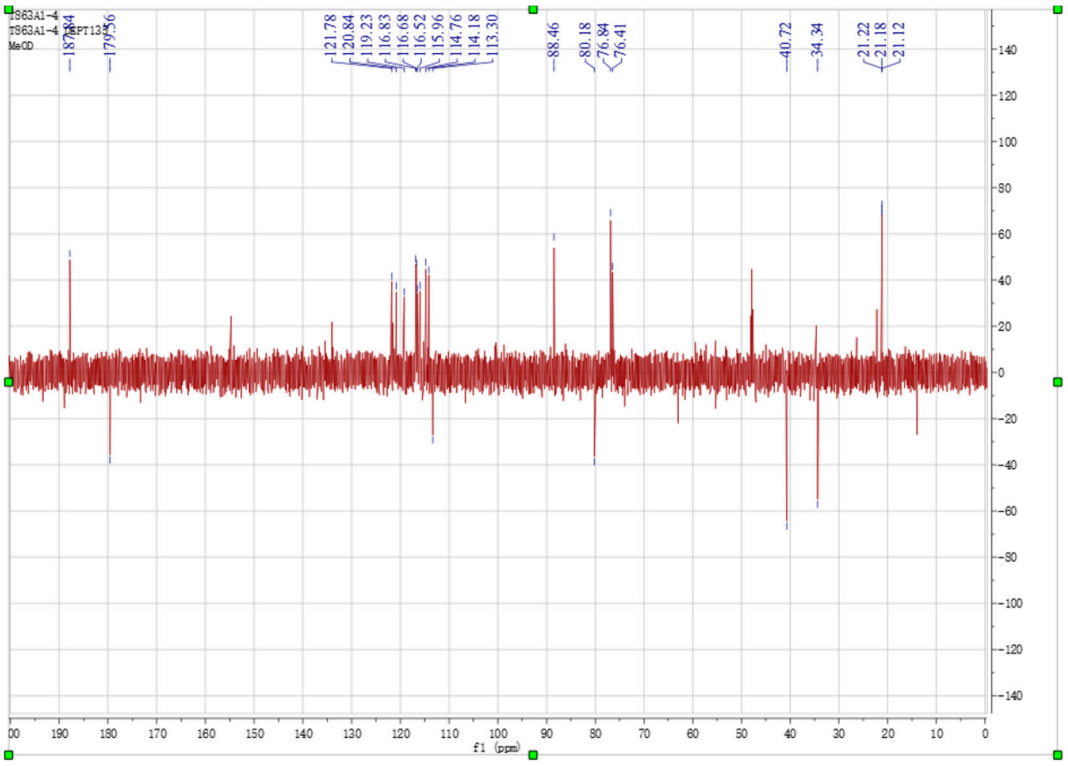


Figure S27. DEPT spectrum of **4** in methanol-d_4.

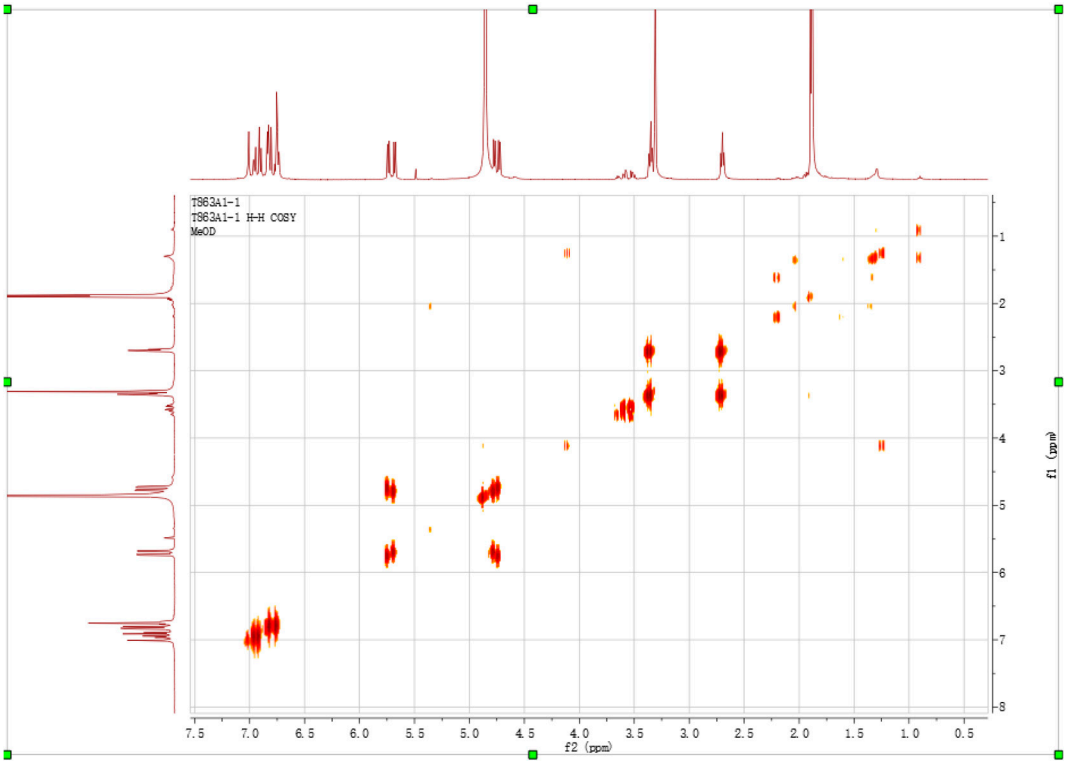


Figure S28. ^{1}H-^{1}H-COSY spectrum of **4** in methanol-d_4.

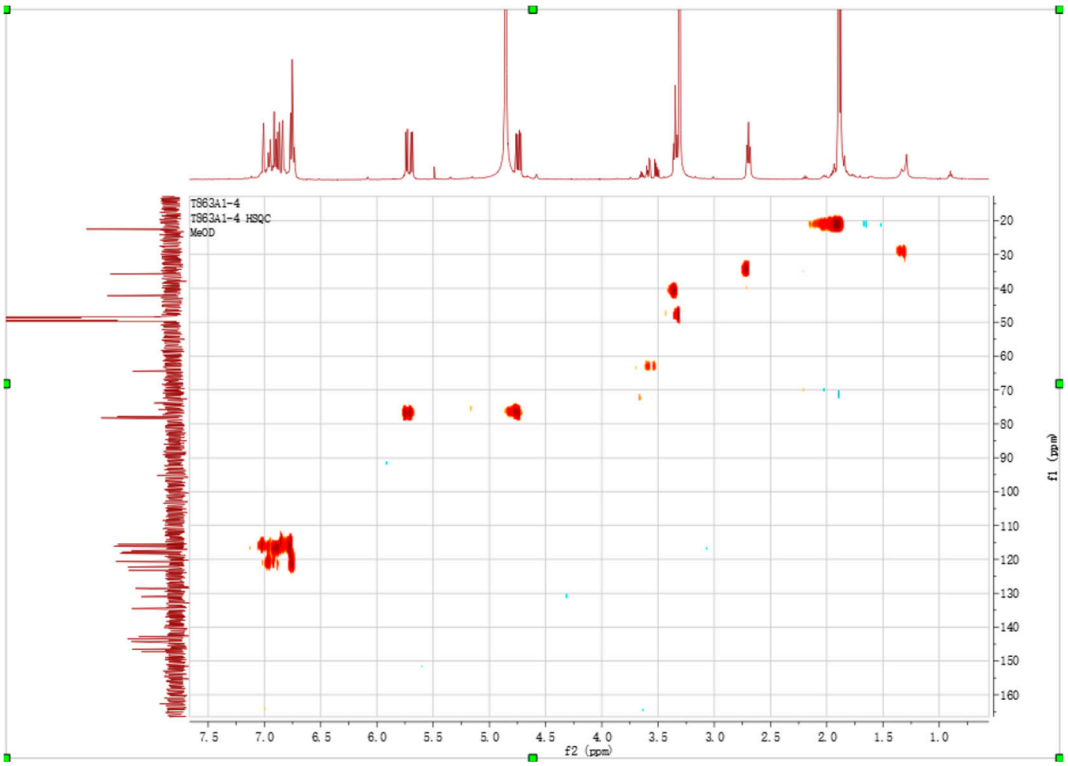


Figure S29. HSQC spectrum of **4** in methanol-d_4.

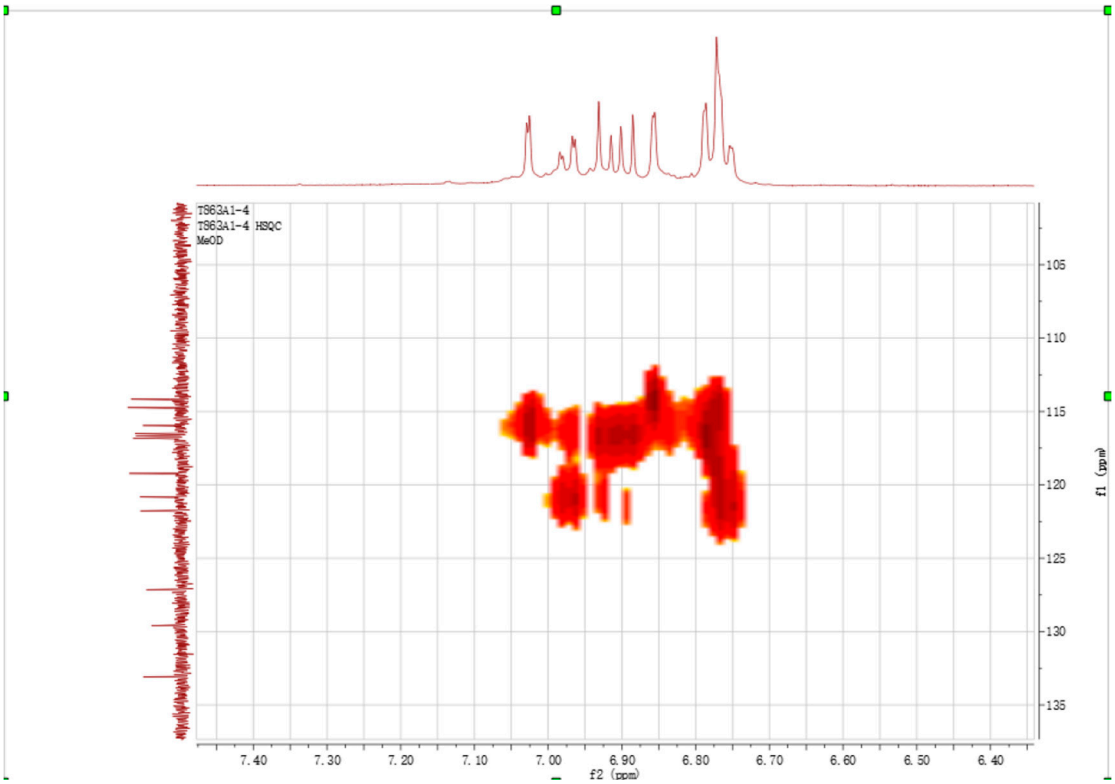


Figure S30. zoomed aromatic region of HSQC spectra of **4**.

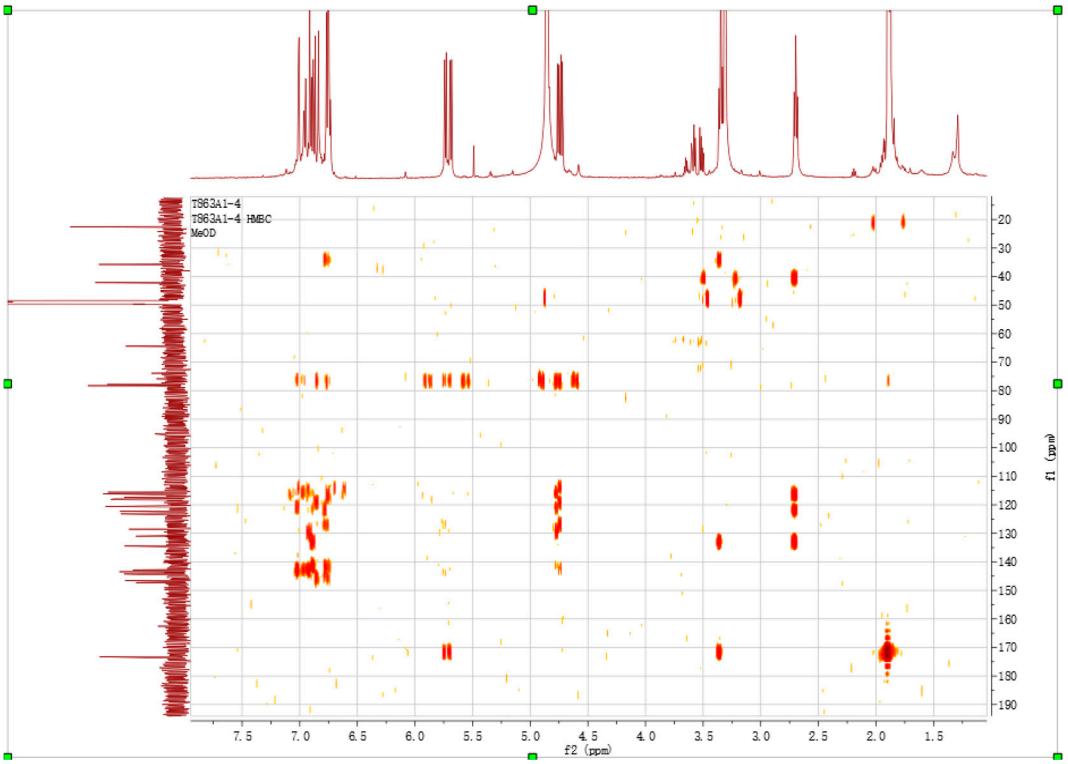


Figure S31. HMBC spectrum of **4** in methanol-d_4.

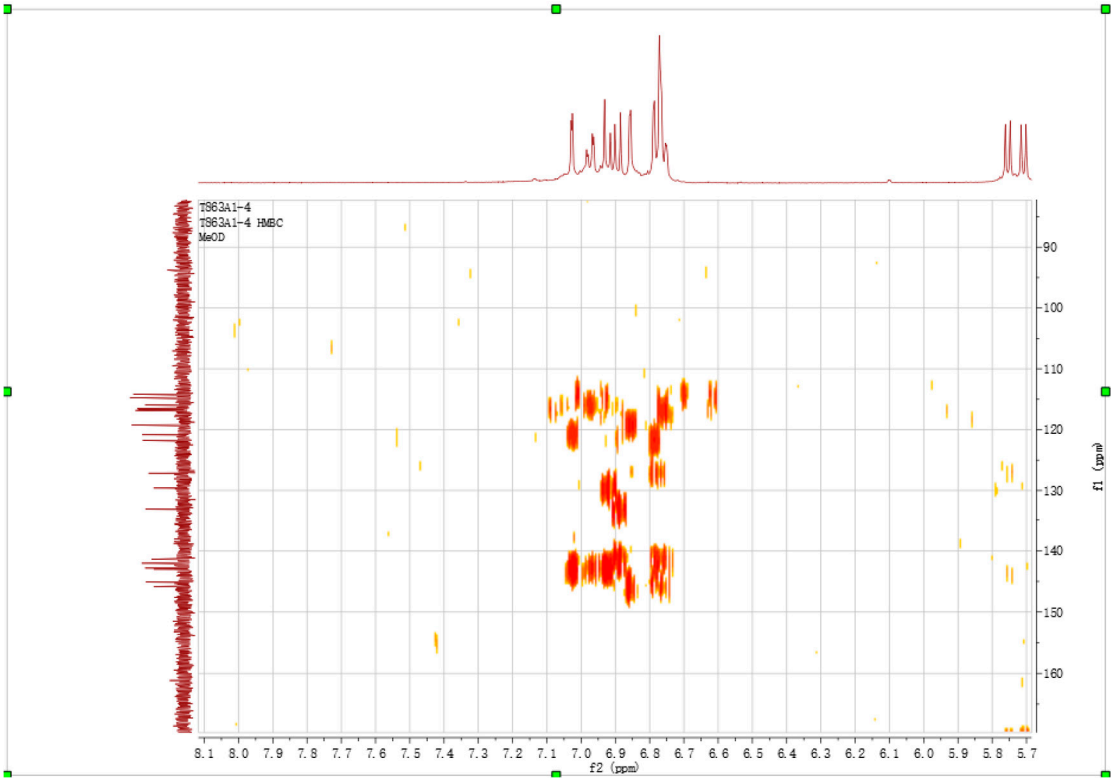


Figure S32. zoomed aromatic region of HMBC spectra of **4**.

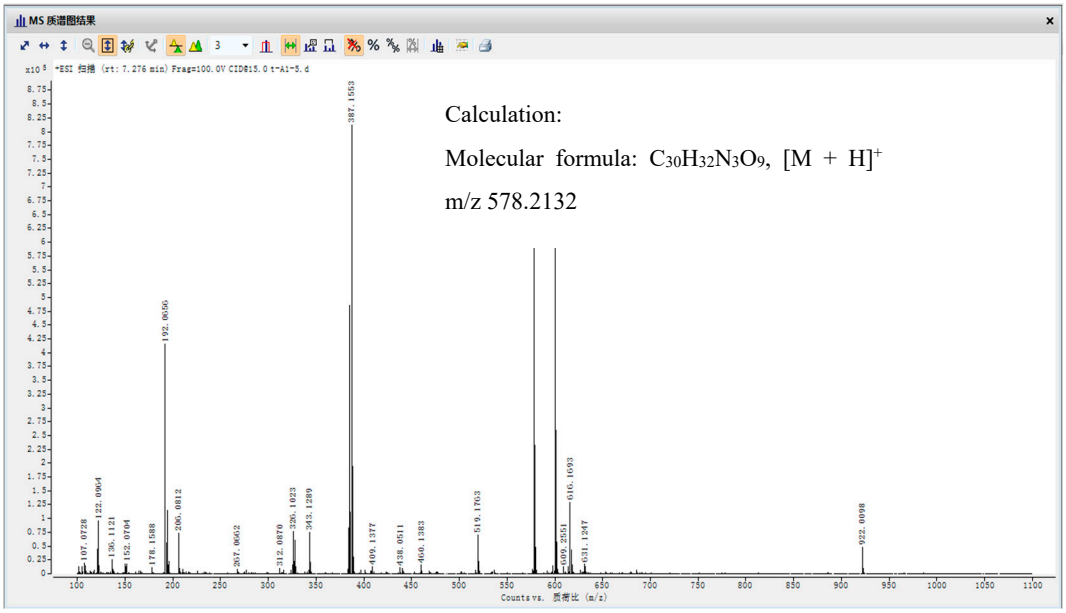


Figure S33. HR-ESI-MS of **1**.

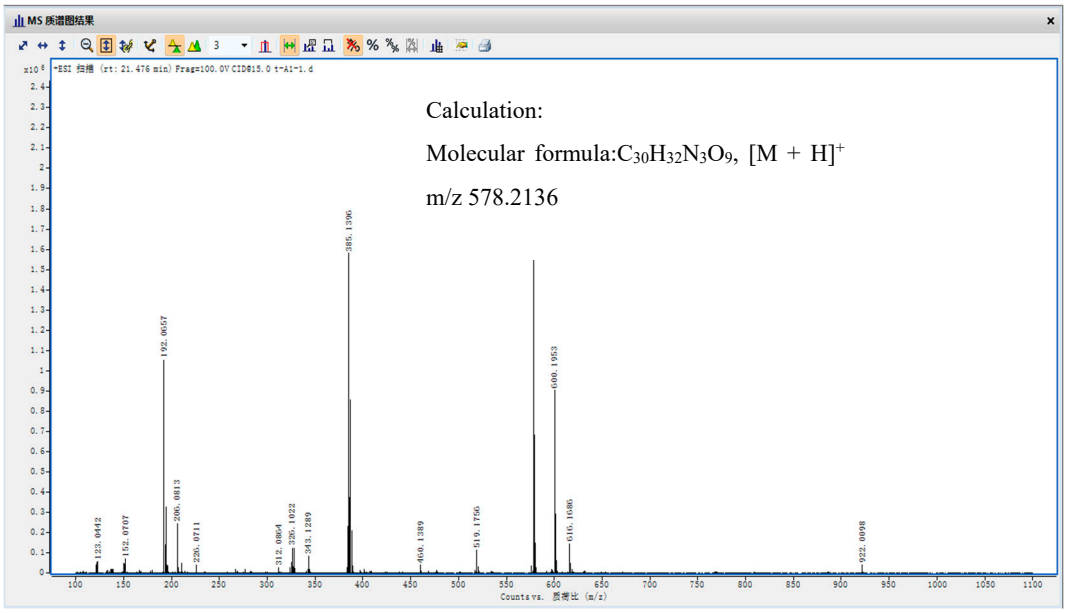


Figure S34. HR-ESI-MS of **2**.

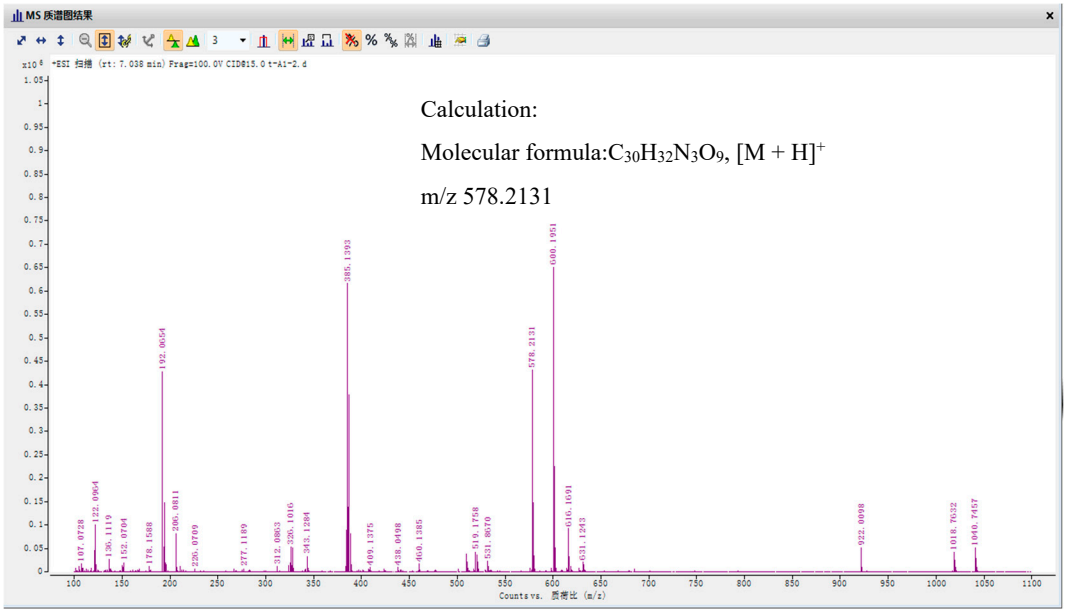


Figure S35. HR-ESI-MS of **3**.

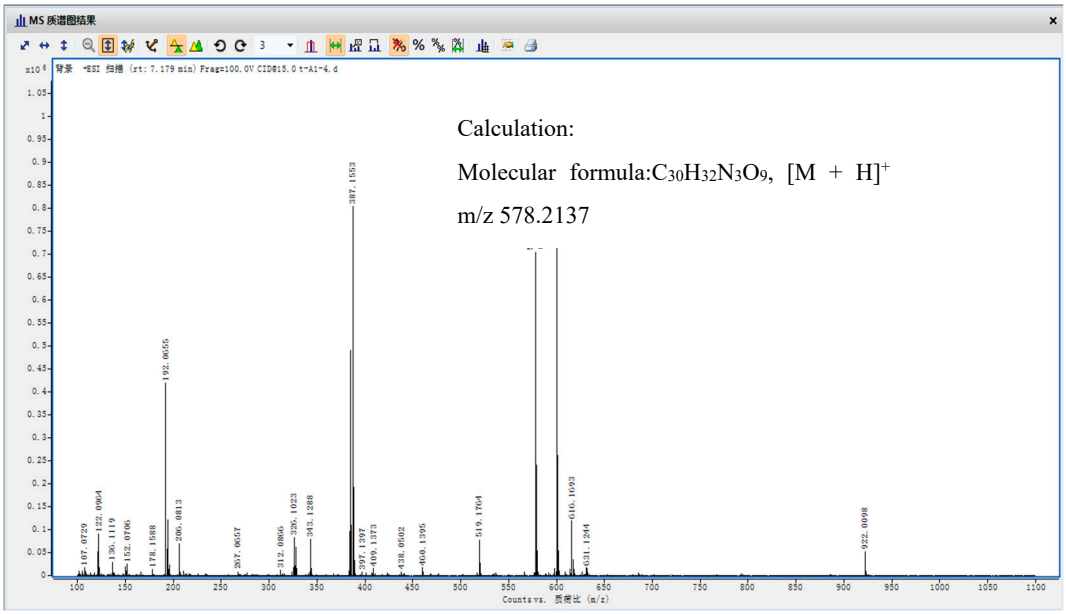


Figure S36. HR-ESI-MS of **4**.