SUPPORTING INFORMATION

Thioester-containing benzoate derivatives with α-glucosidase inhibitory activity from the deep-sea-derived fungus *Talaromyces indigoticus* FS688

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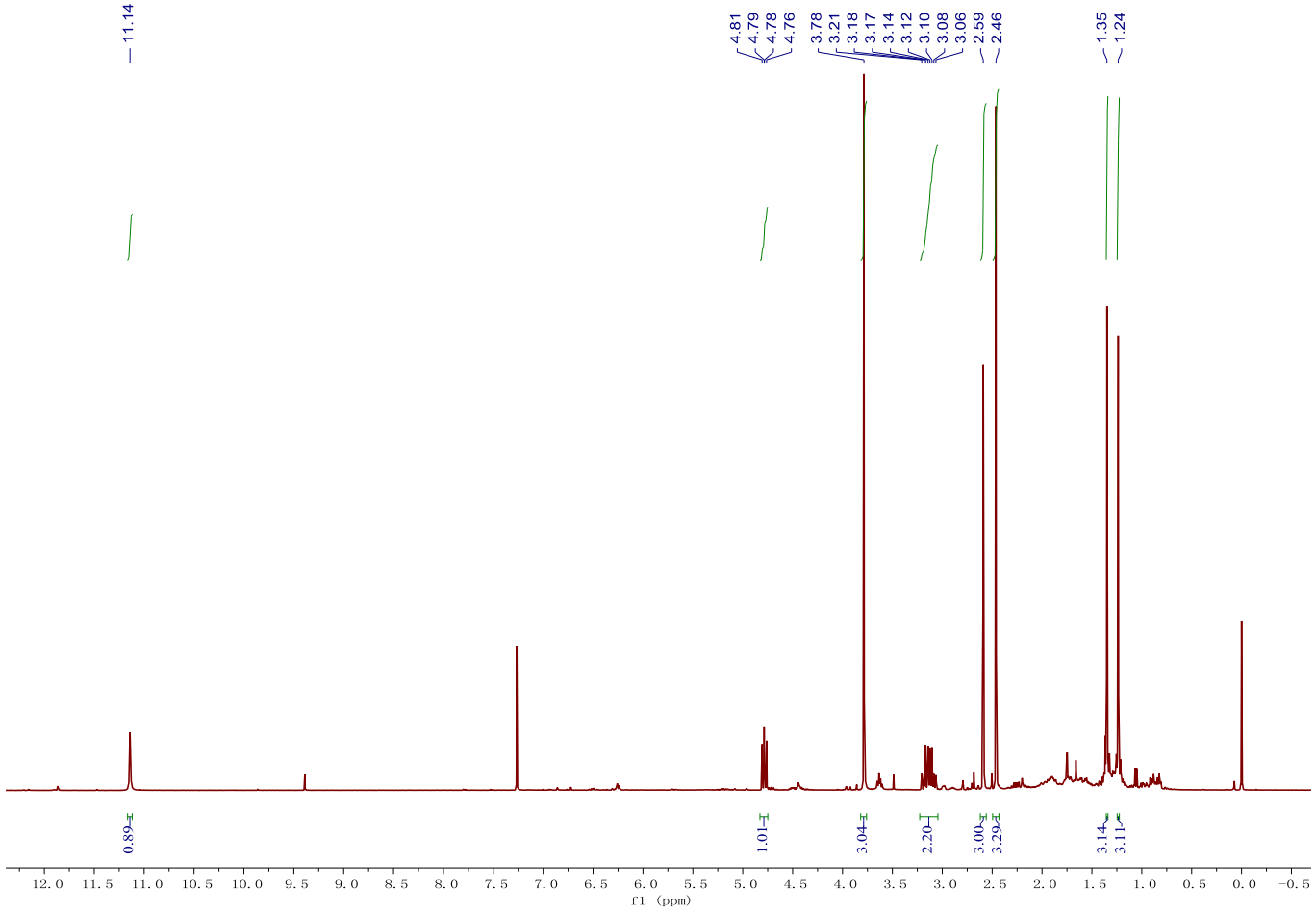


Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$.

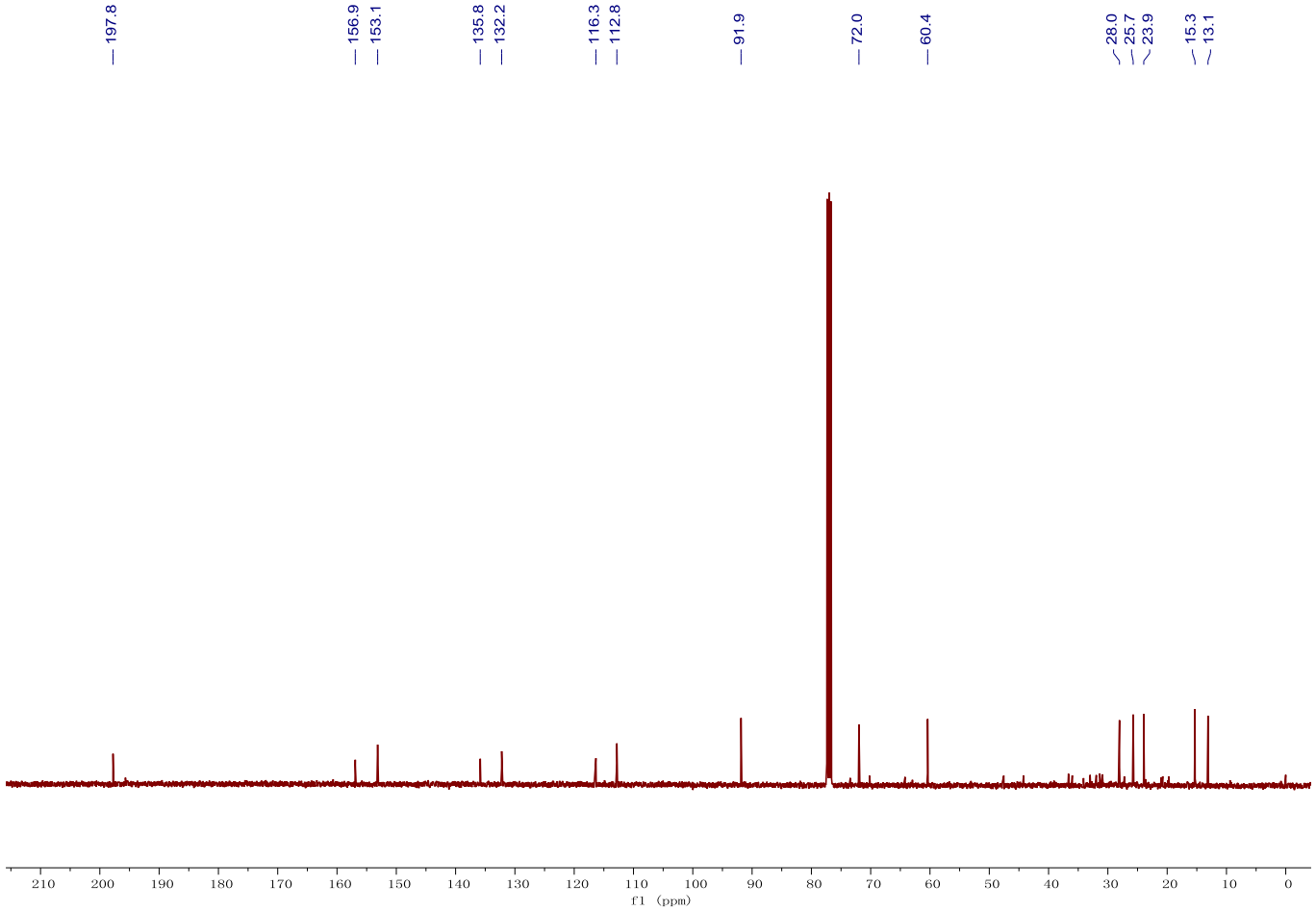
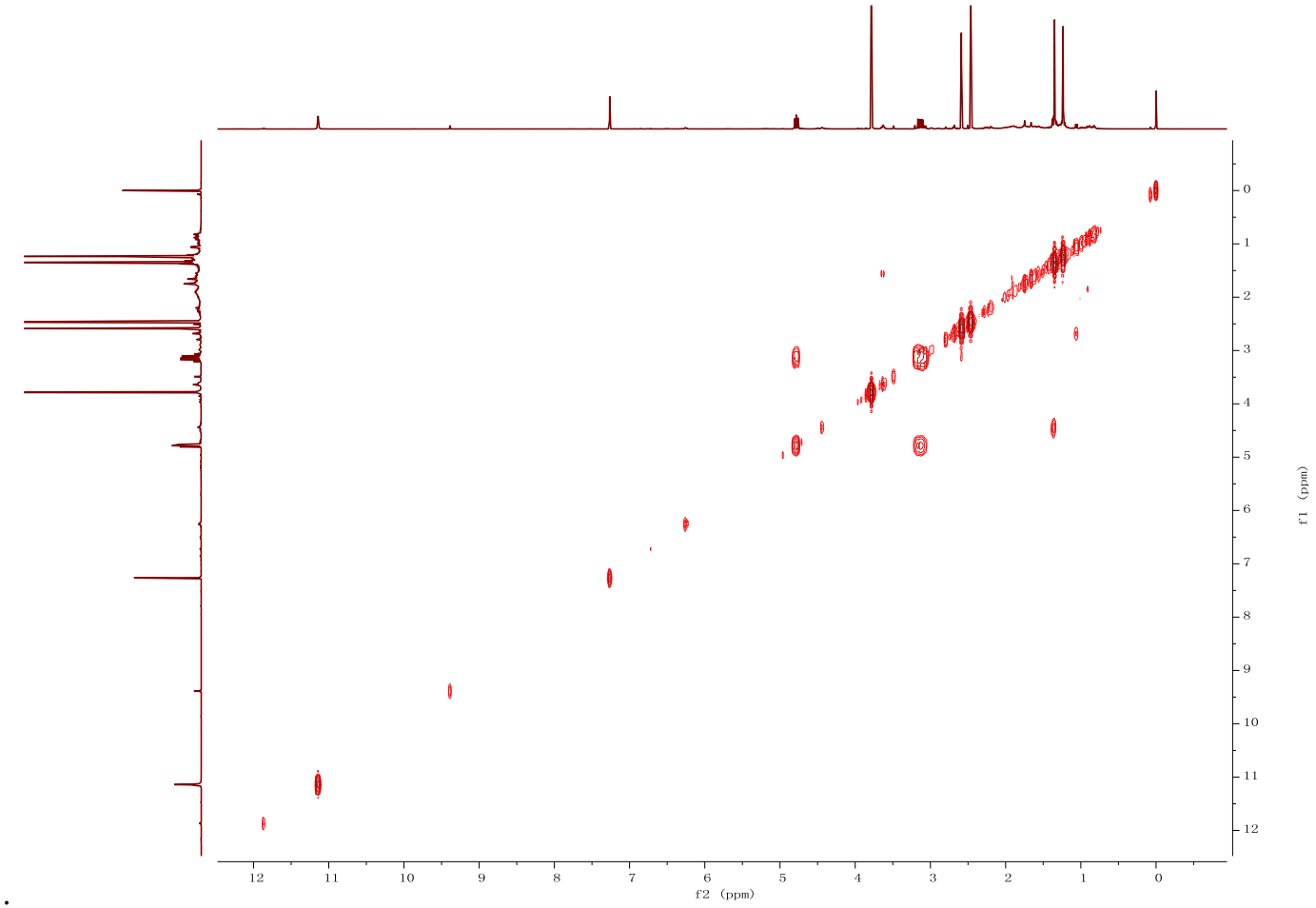


Figure S3. ^{1}H, ^{1}H-COSY spectrum of **1** in $CDCl_3$.



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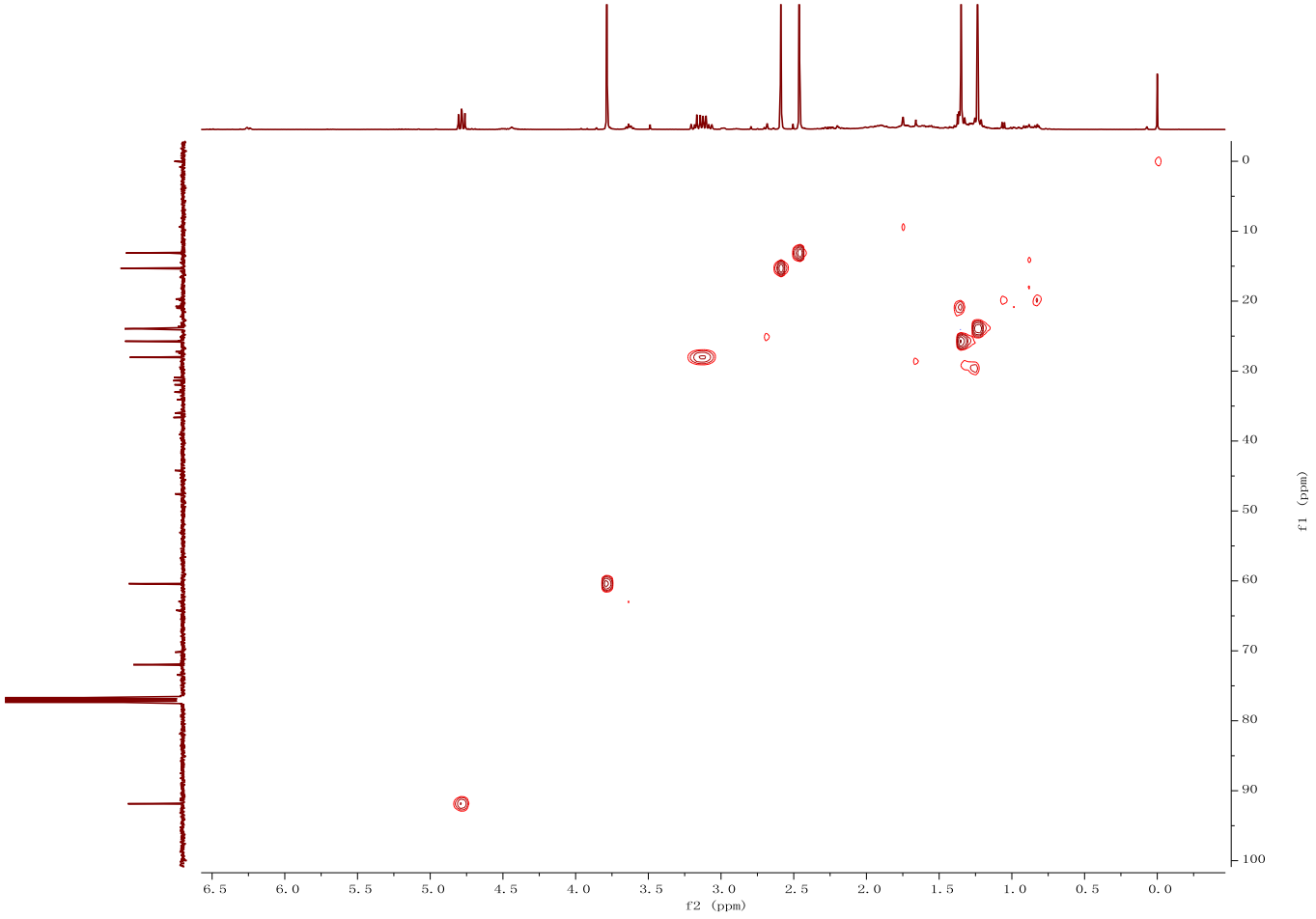


Figure S5. HMBC spectrum of **1** in $CDCl_3$.

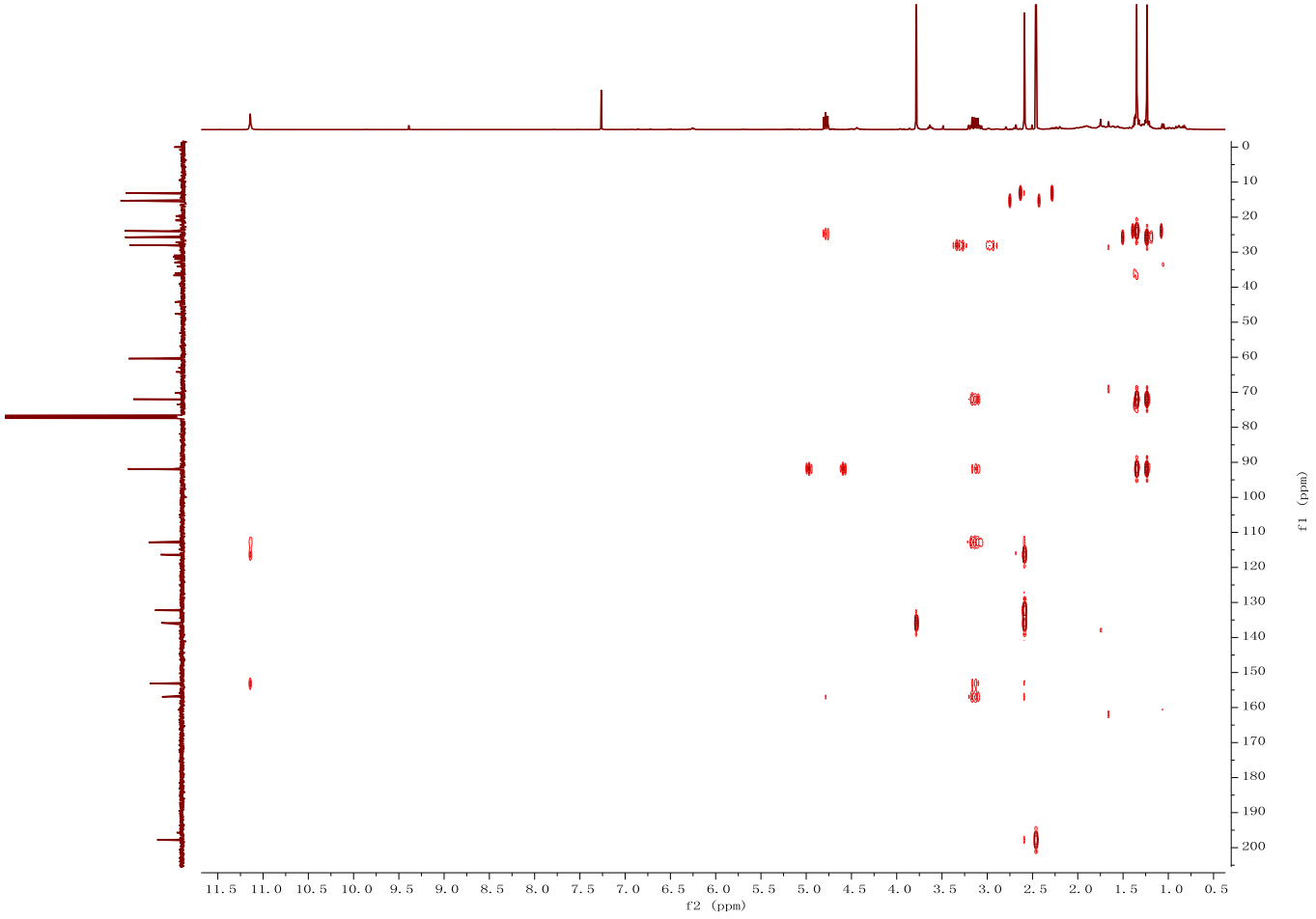


Figure S6. ^{1}H-NMR spectrum of **2** in MeOD.

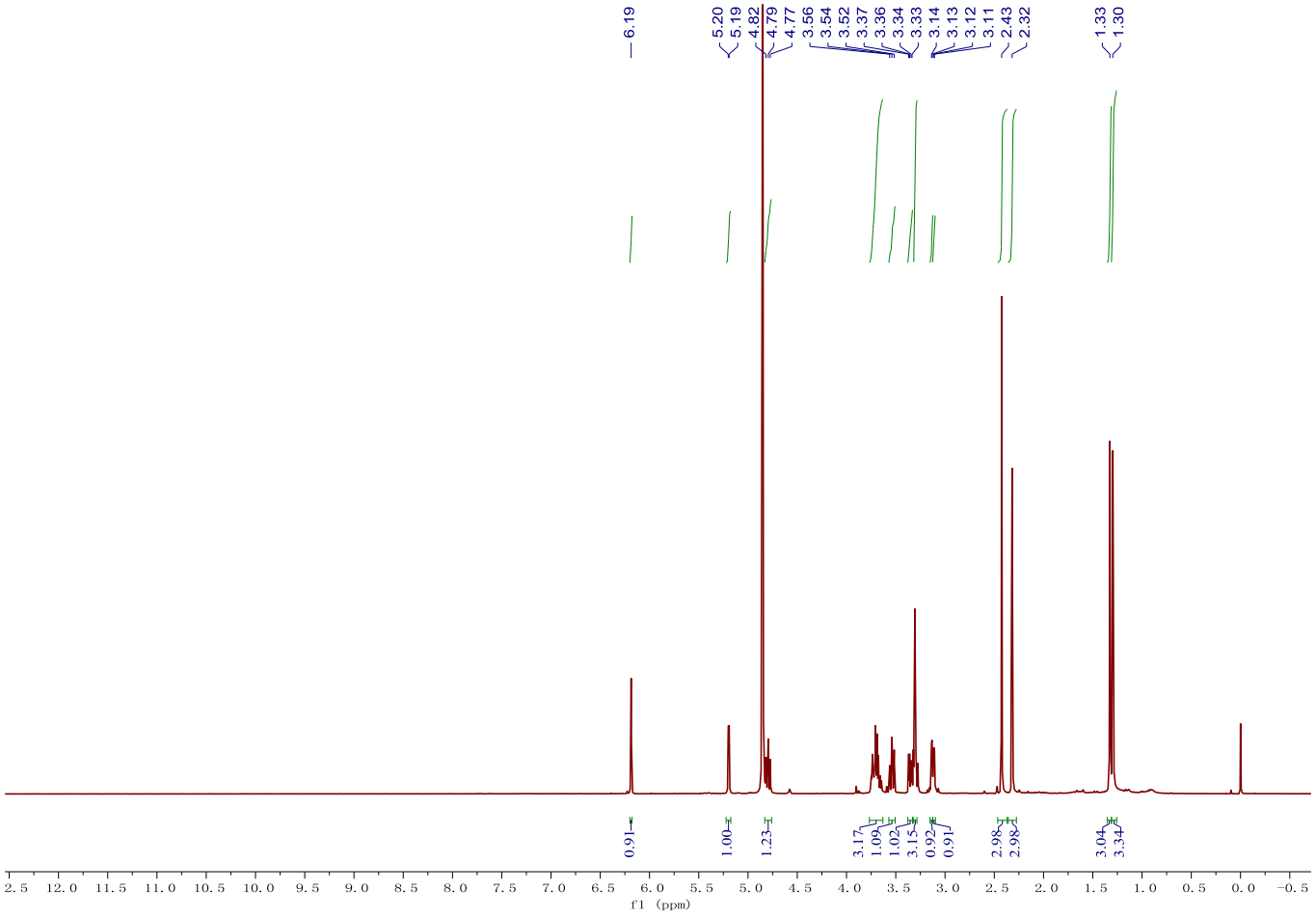
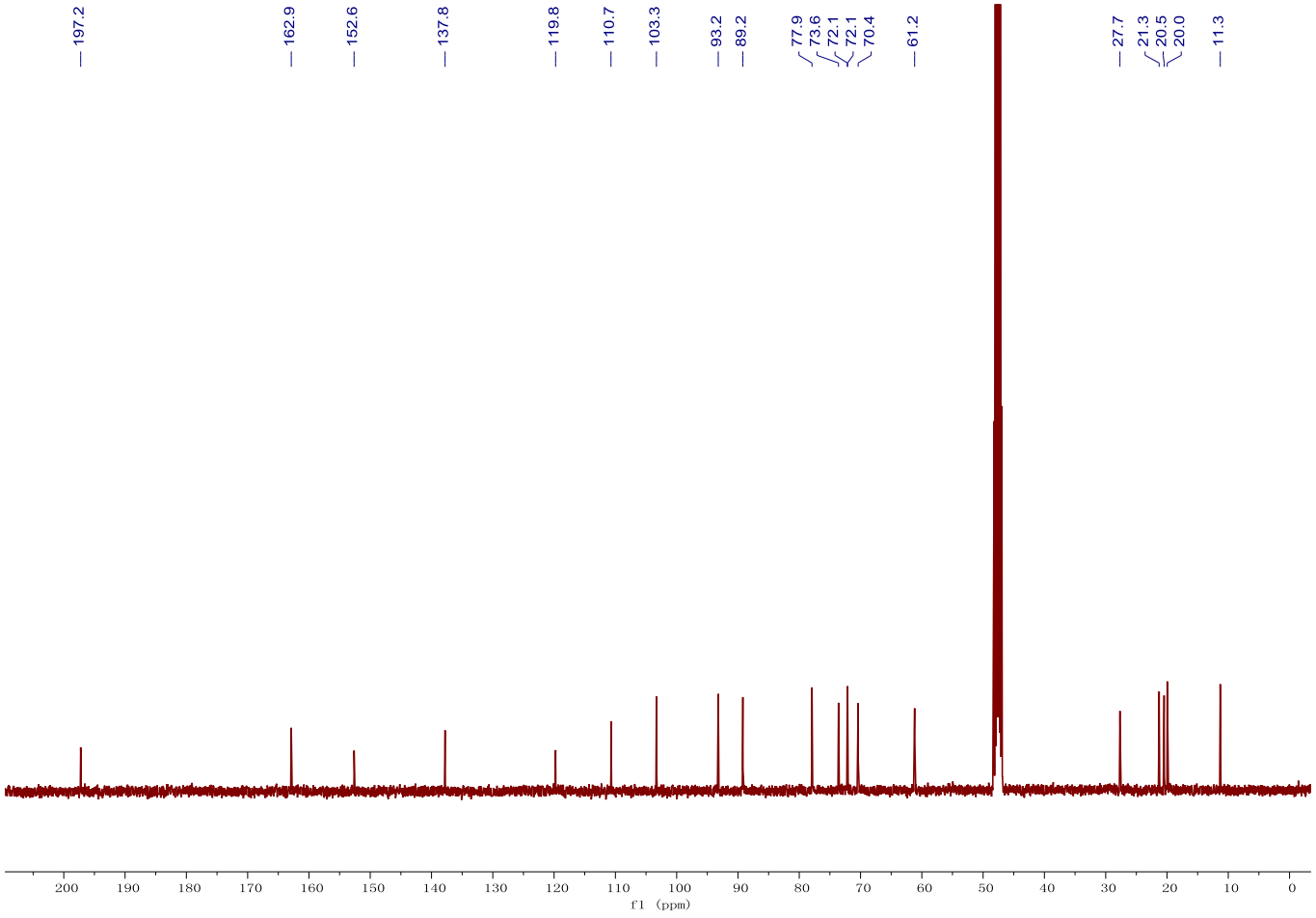


Figure S7. ^{13}C-NMR spectrum of **2** in MeOD.



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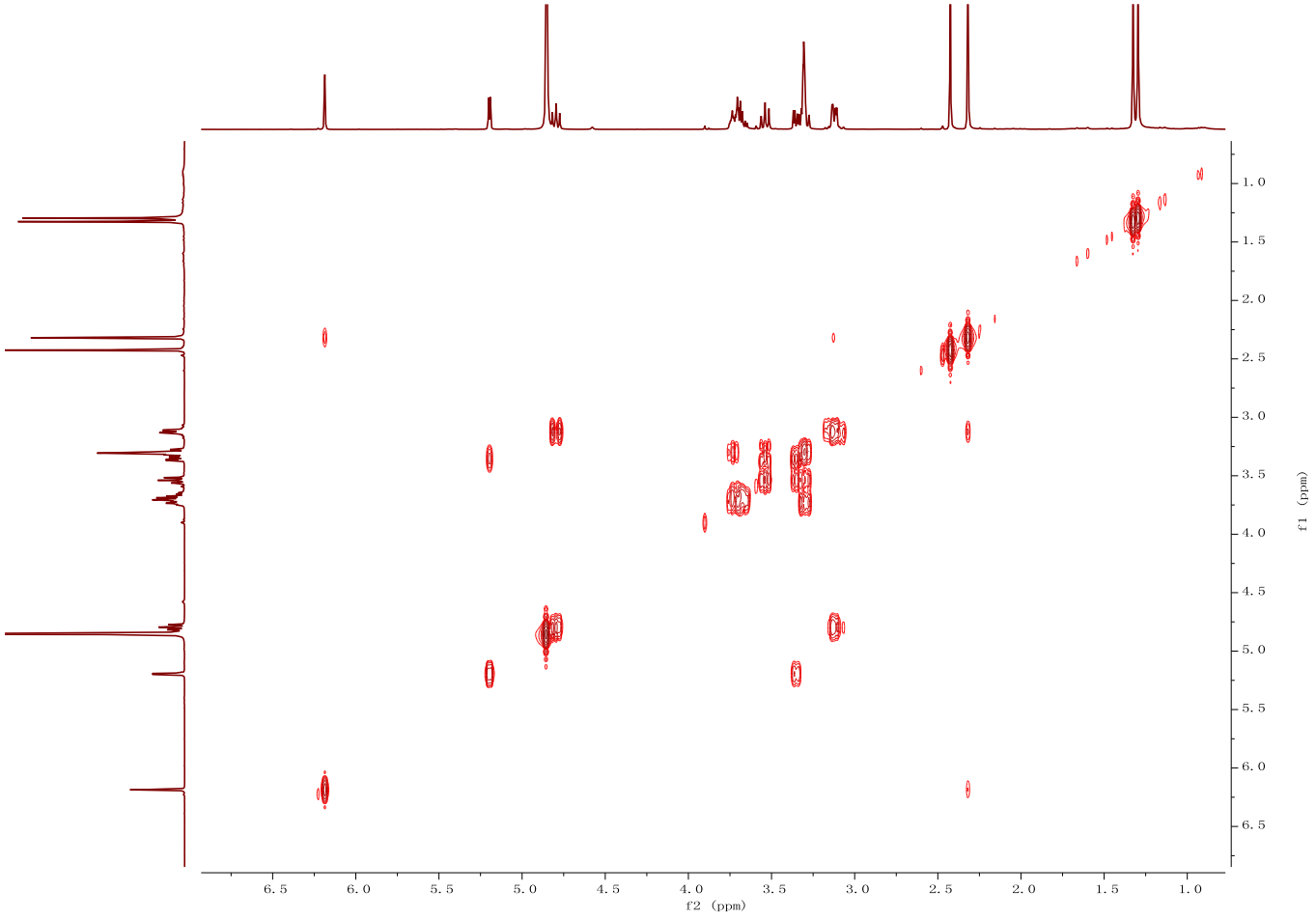


Figure S9. HSQC spectrum of **2** in MeOD.

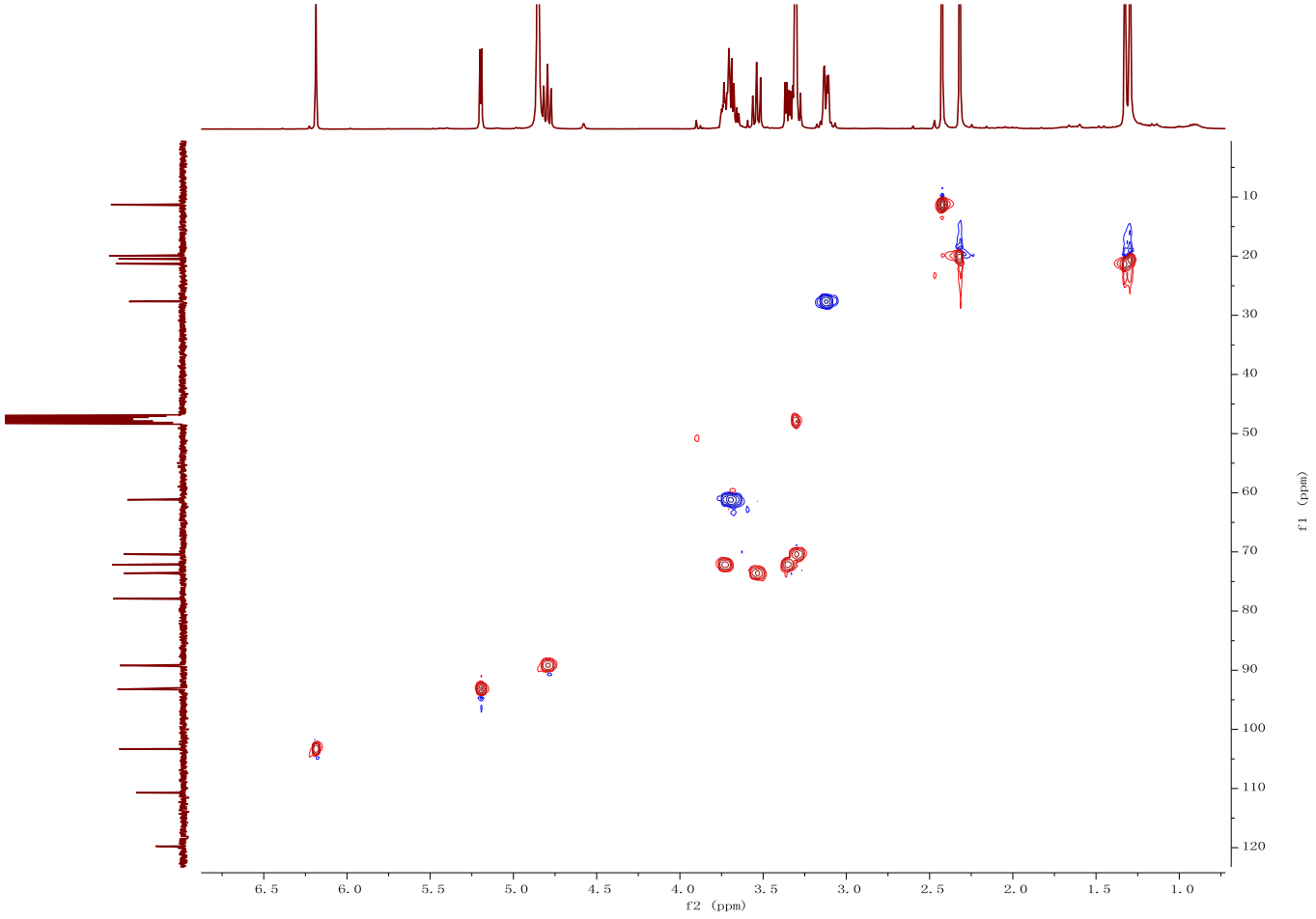


Figure S10. HMBC spectrum of **2** in MeOD.

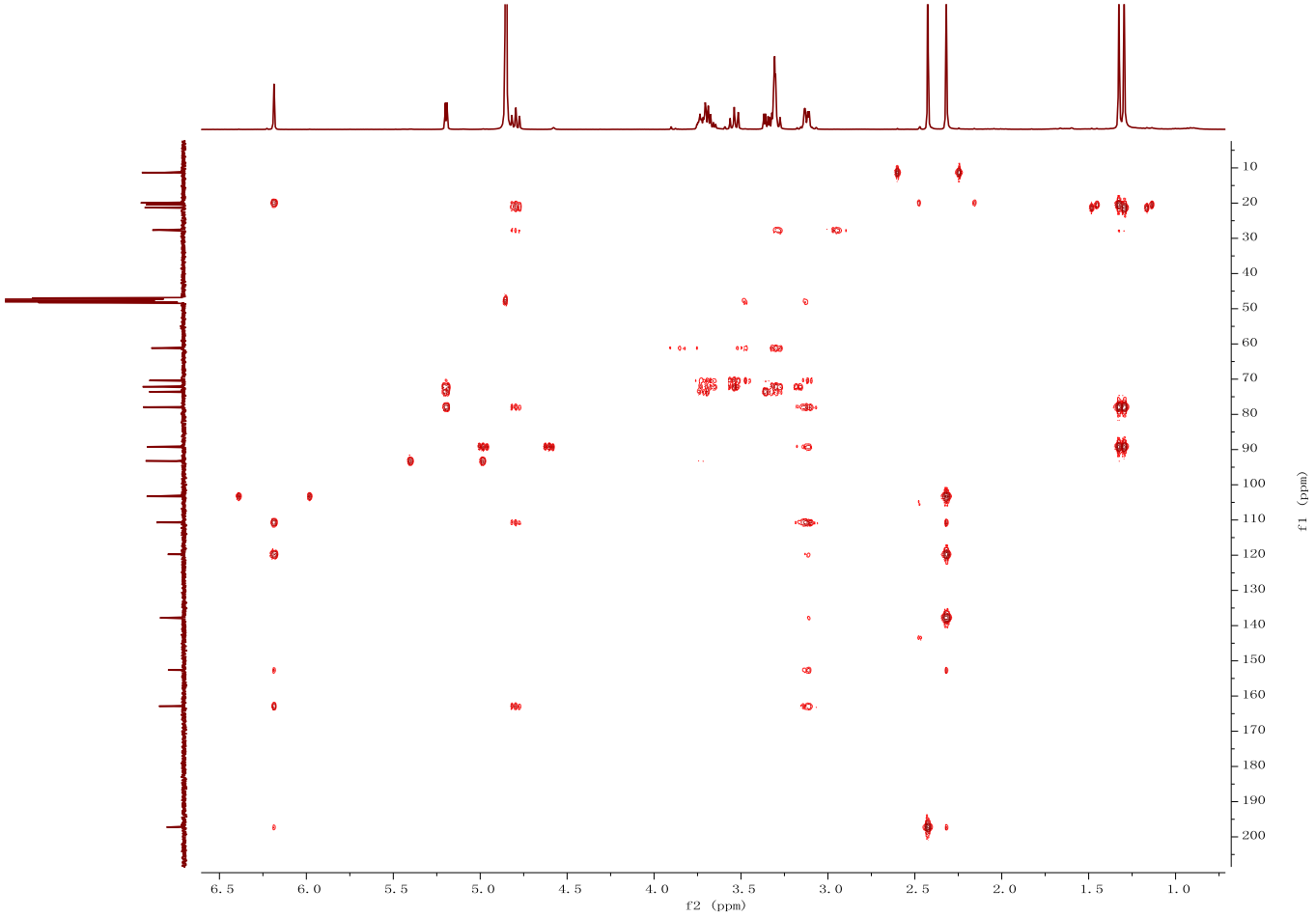


Figure S11. ^{1}H NMR spectrum of **3** in $CDCl_3$.

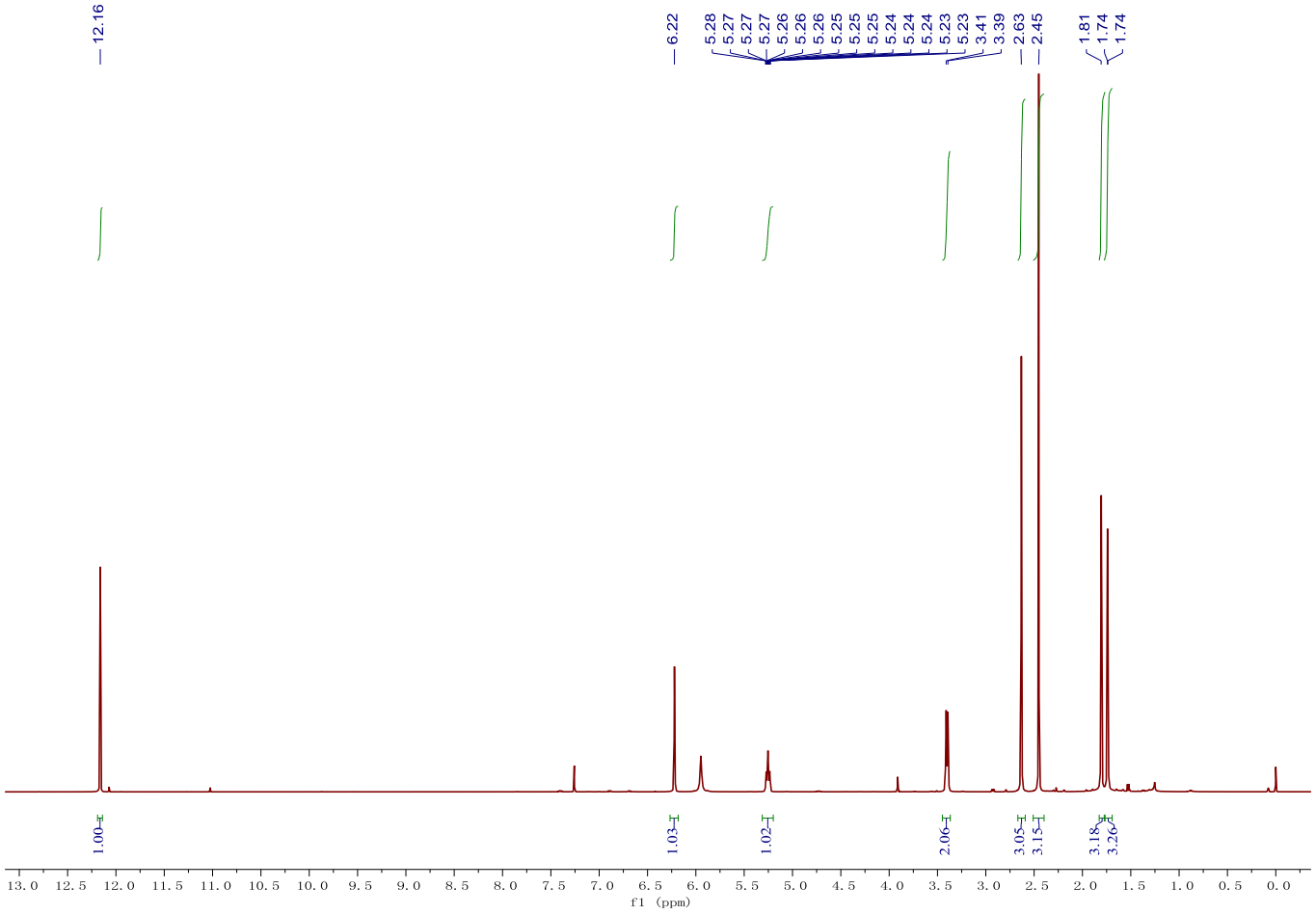
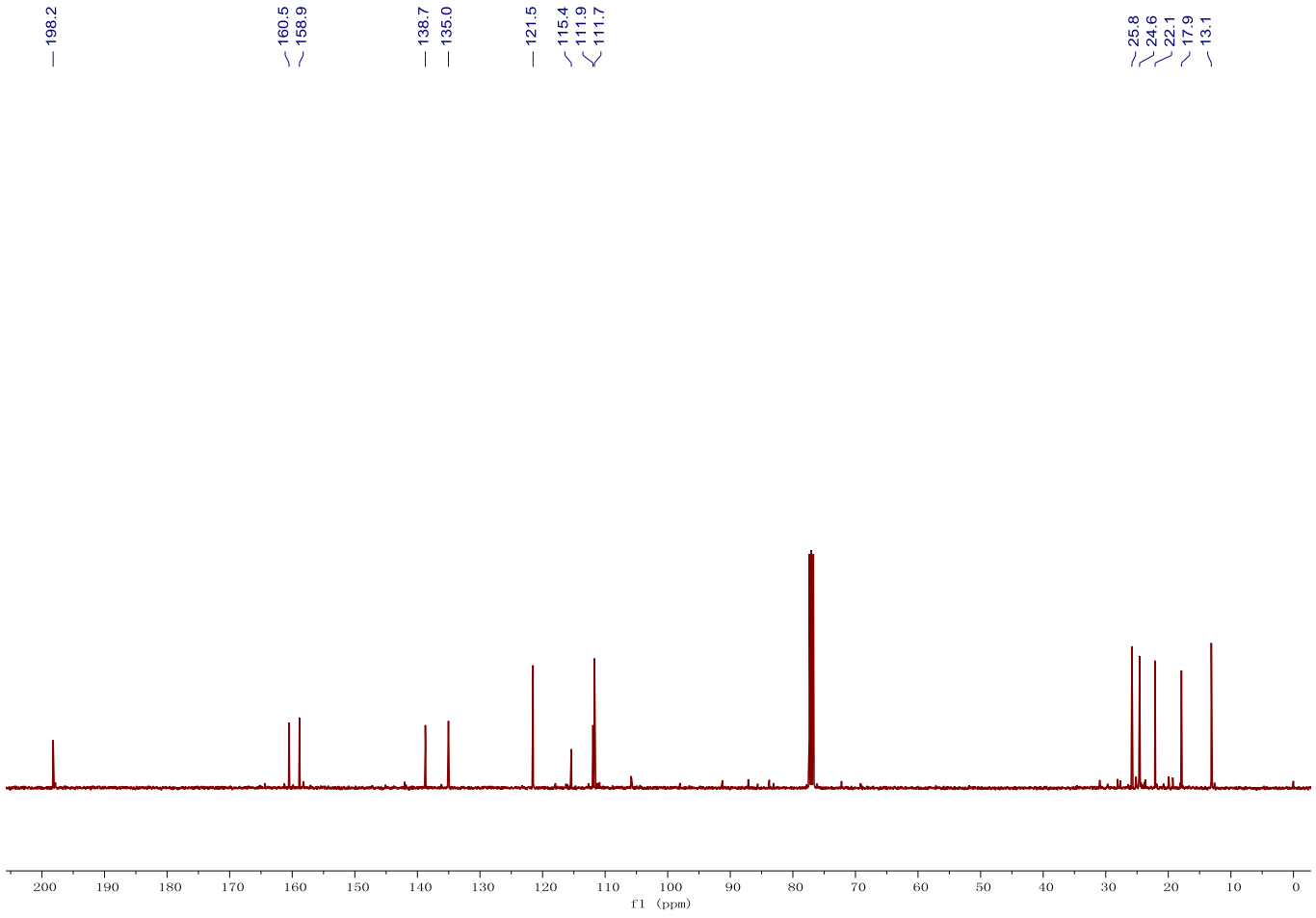


Figure S12. ^{13}C NMR spectrum of **3** in $CDCl_3$.



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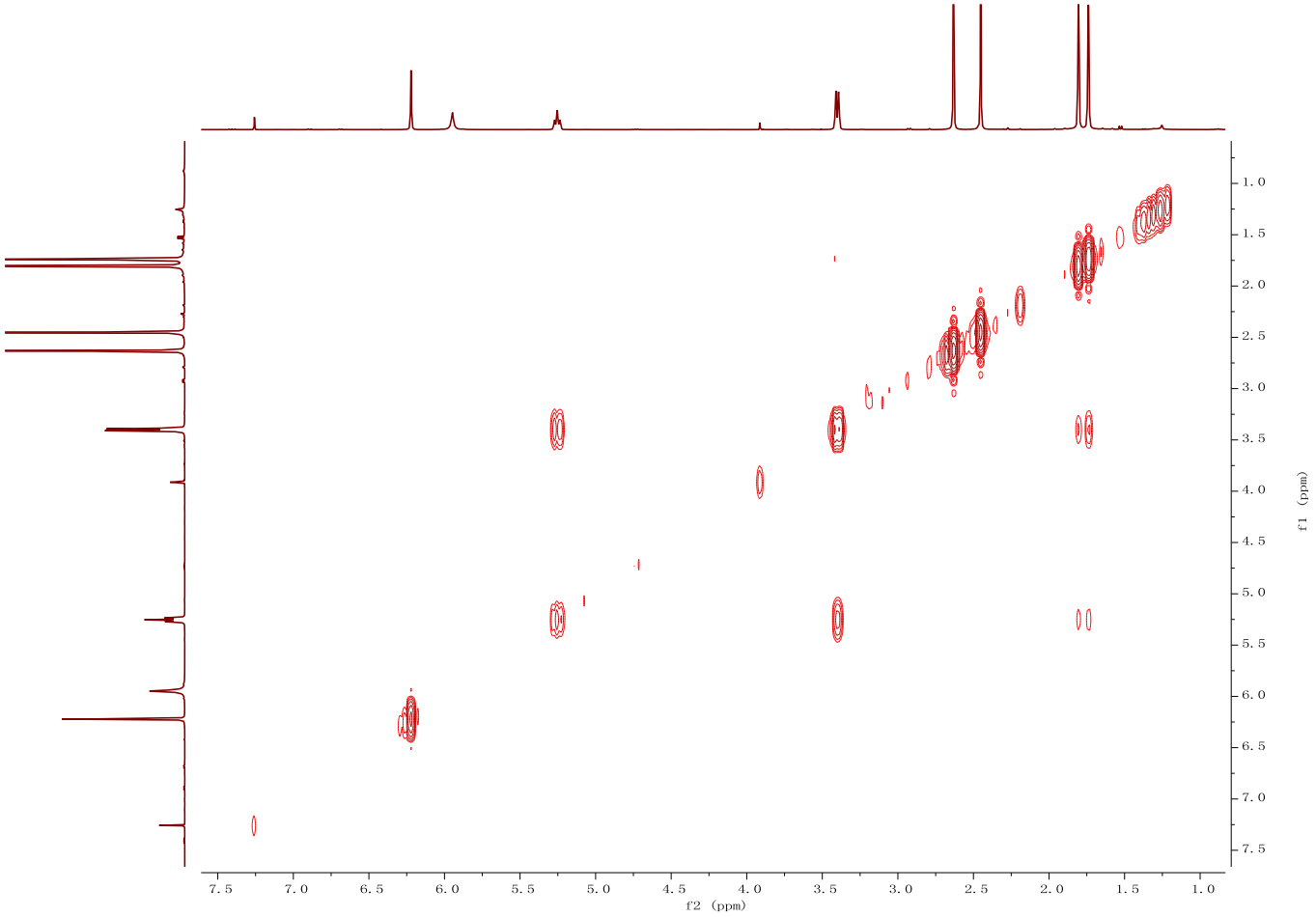


Figure S14. HSQC spectrum of **3** in $CDCl_3$.

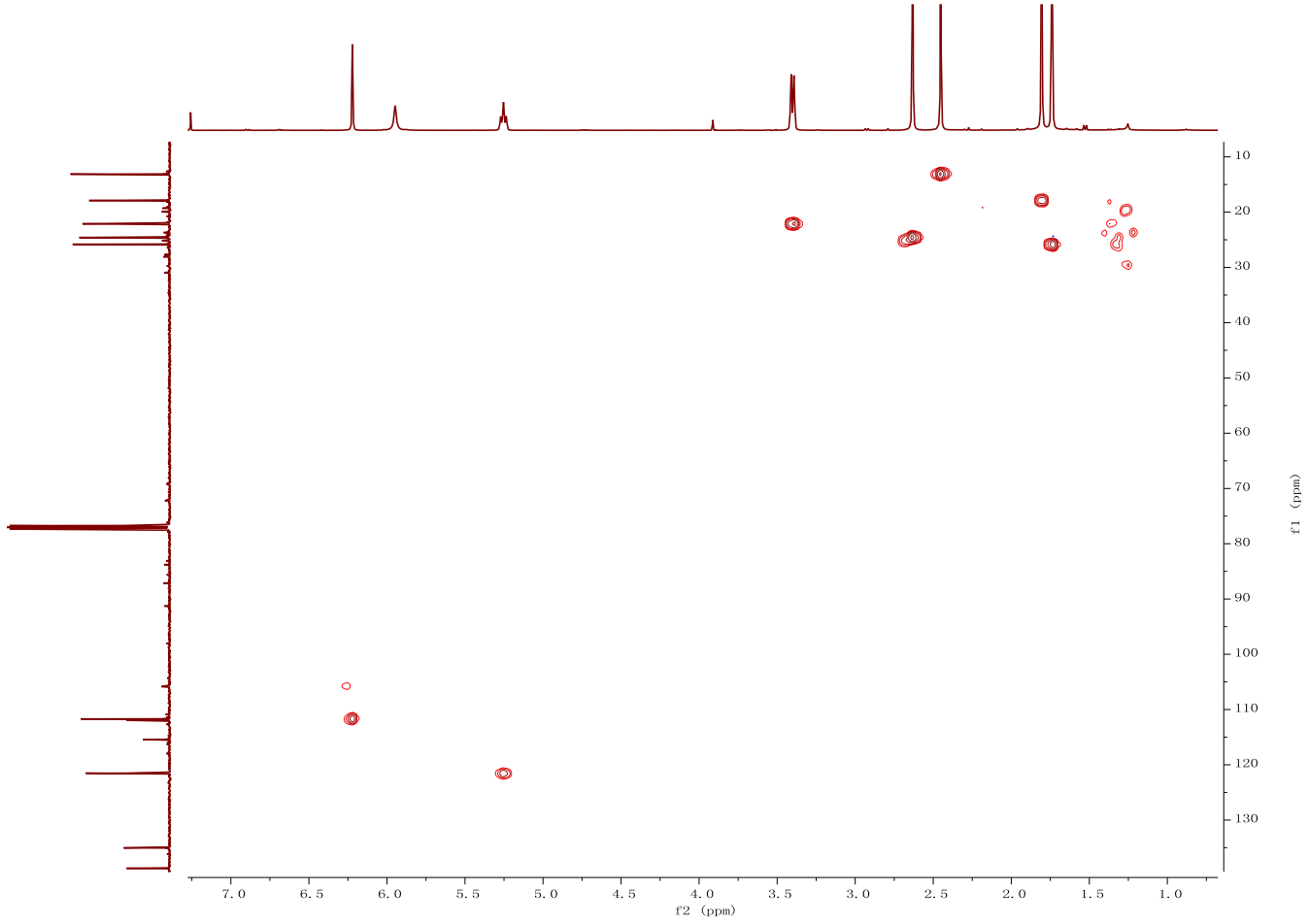


Figure S15. HMBC spectrum of **3** in $CDCl_3$.

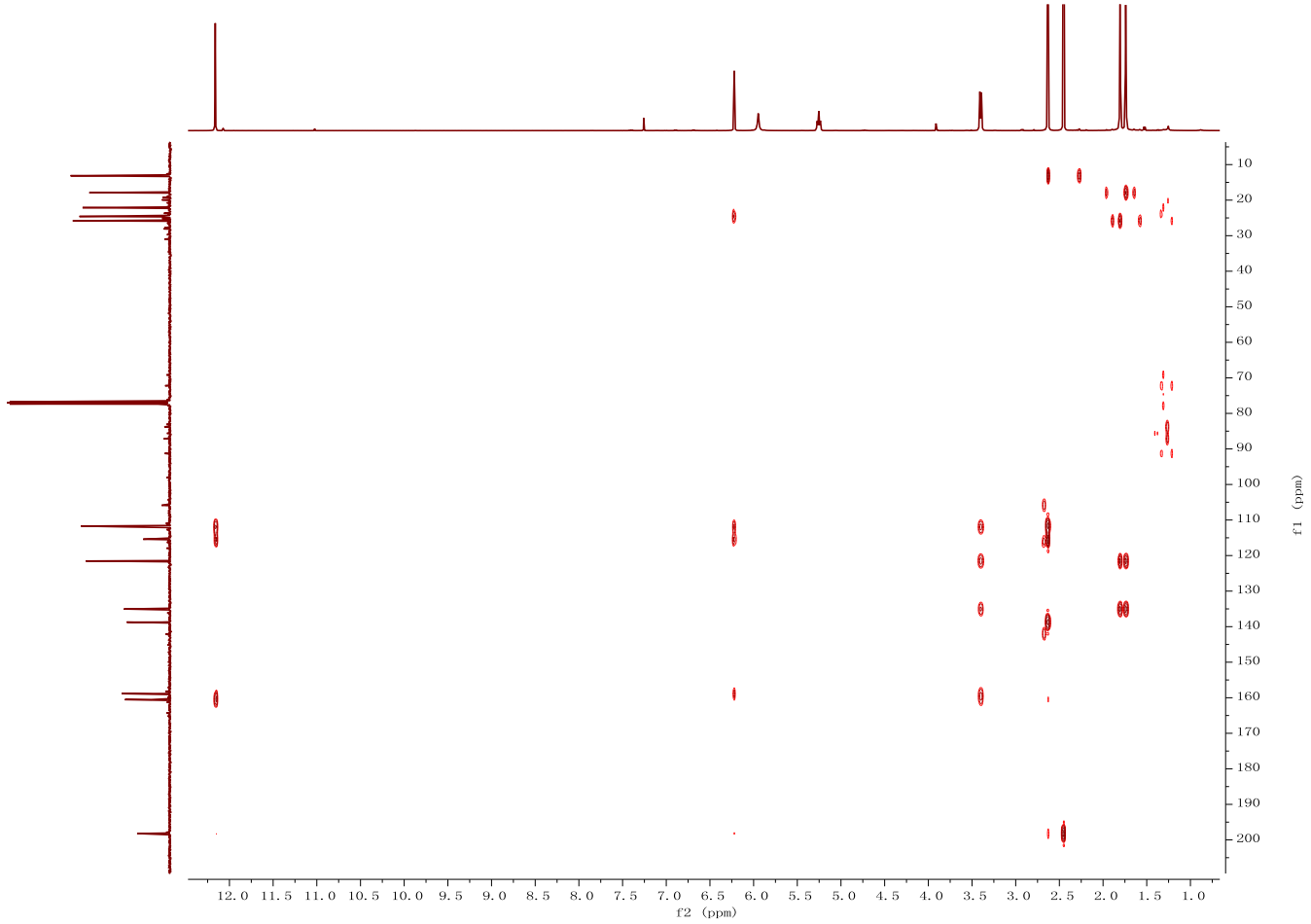


Figure S16. ^{1}H NMR spectrum of **4** in MeOD.

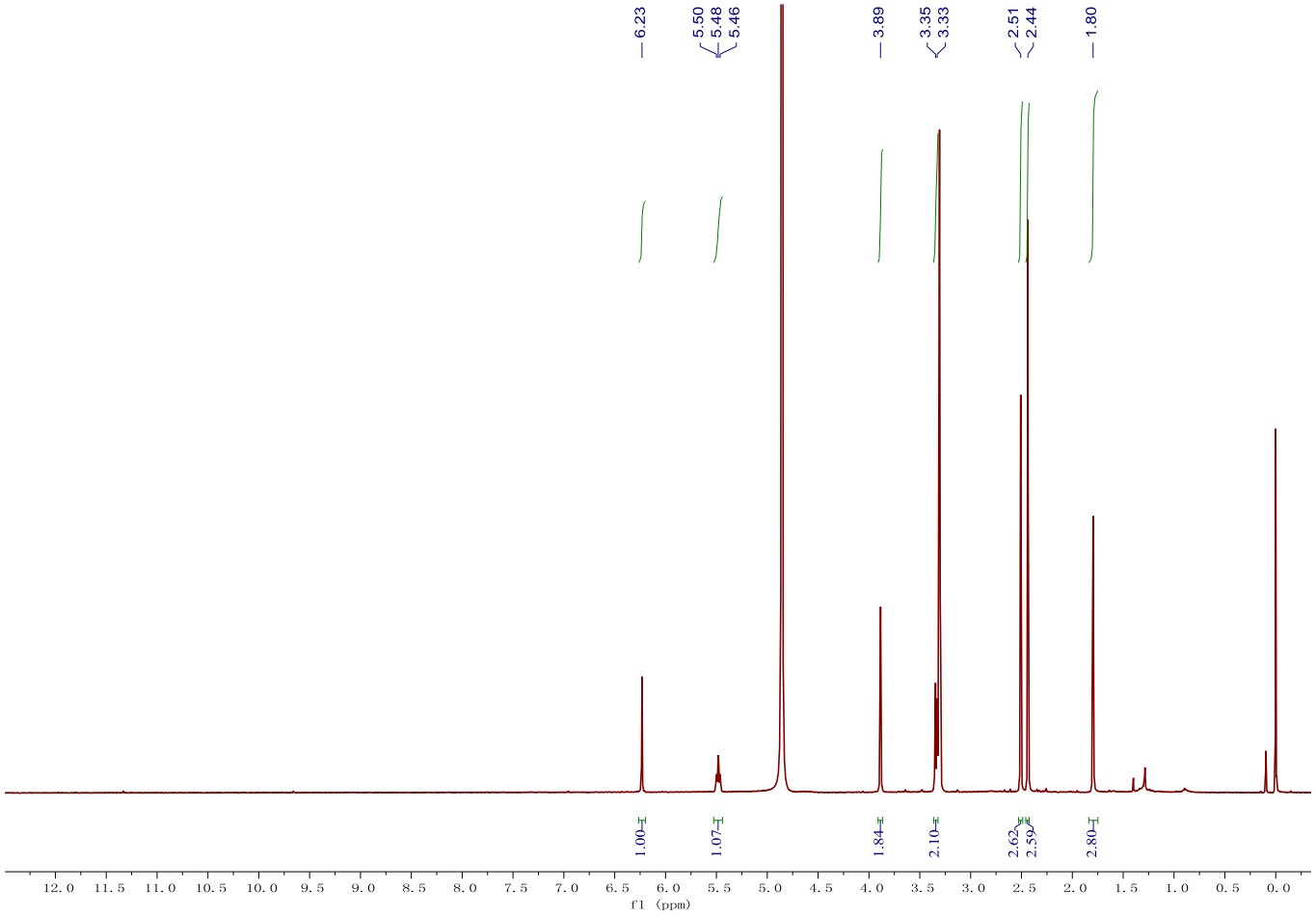
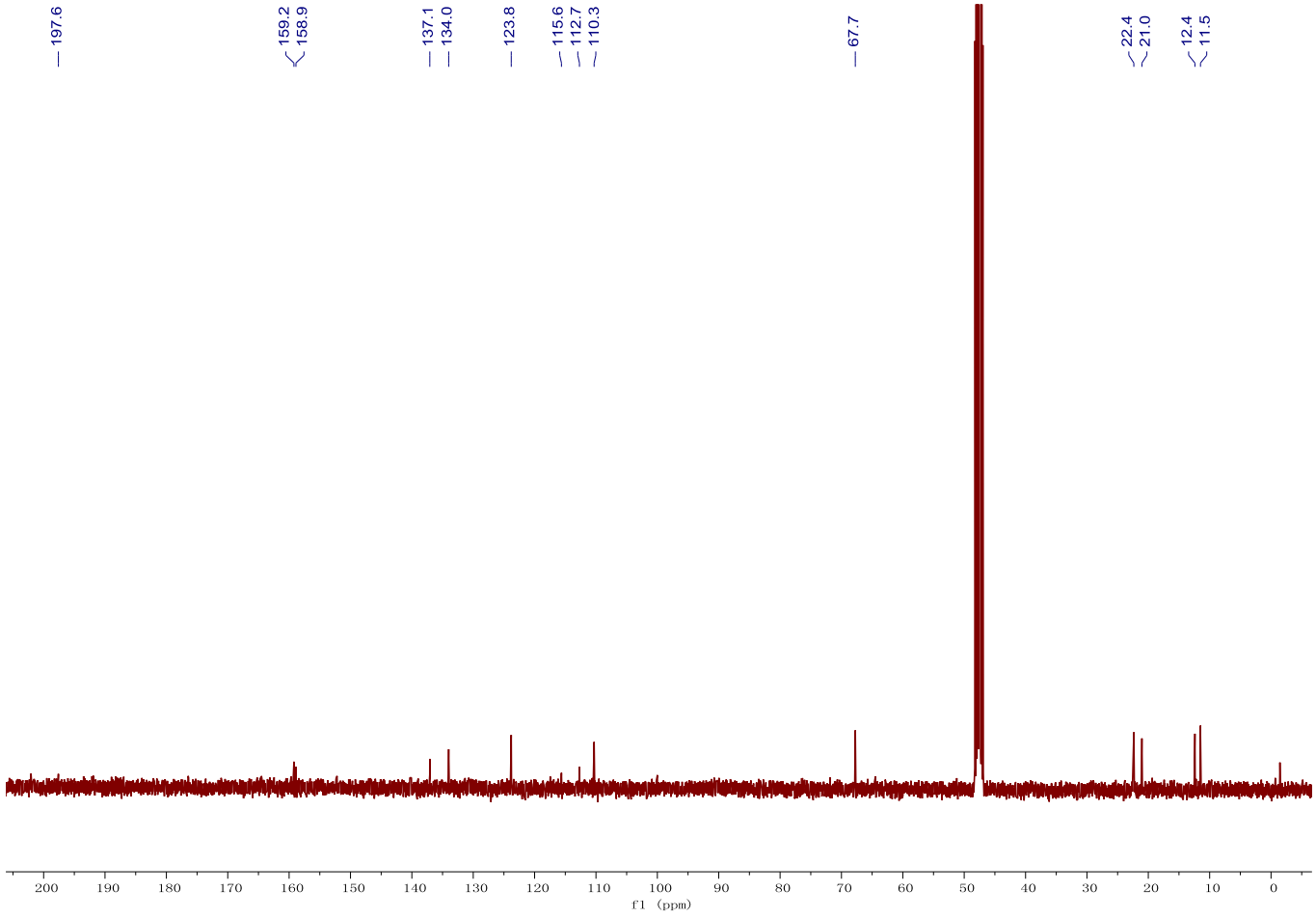


Figure S17. ^{13}C NMR spectrum of **4** in MeOD.



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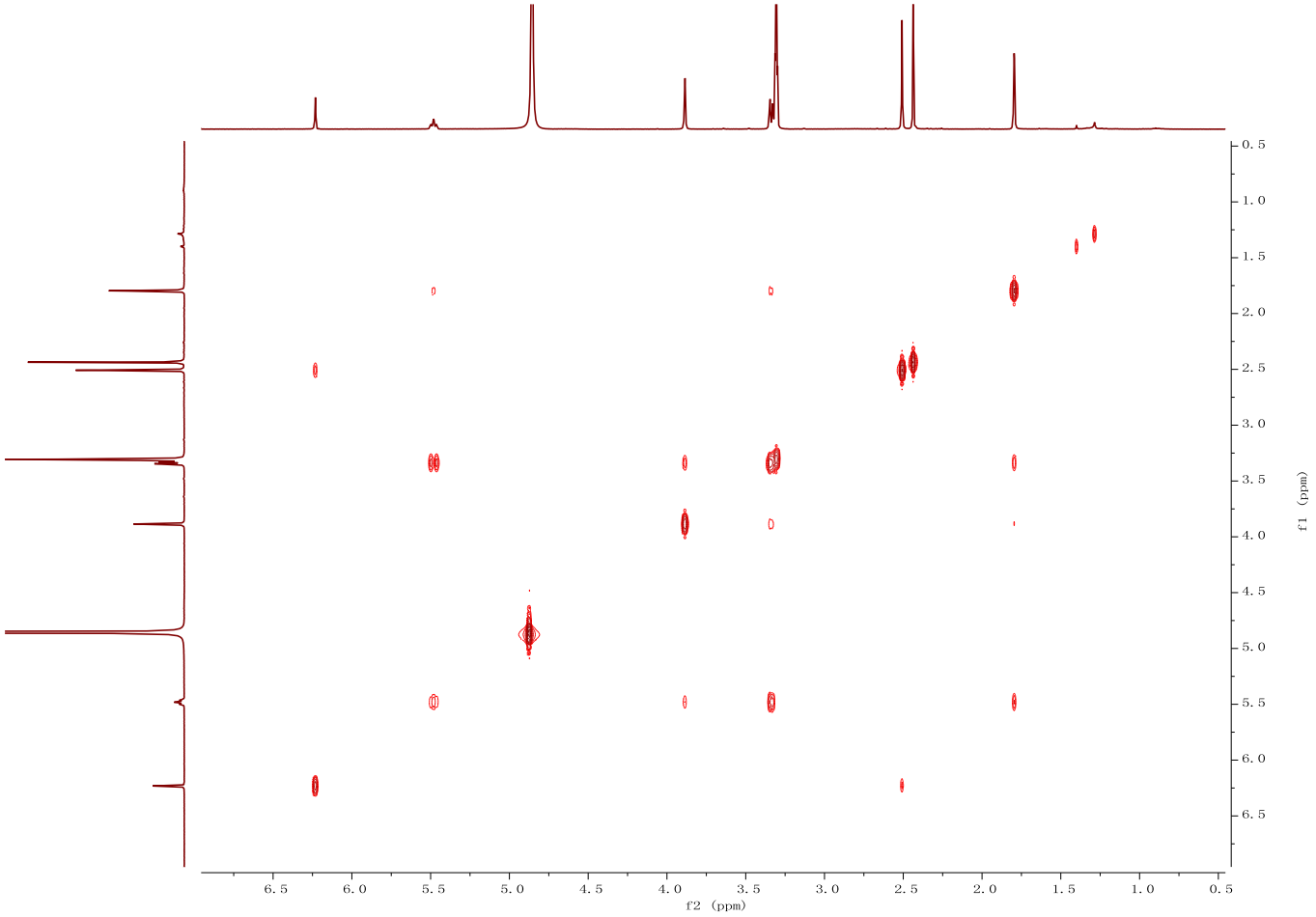
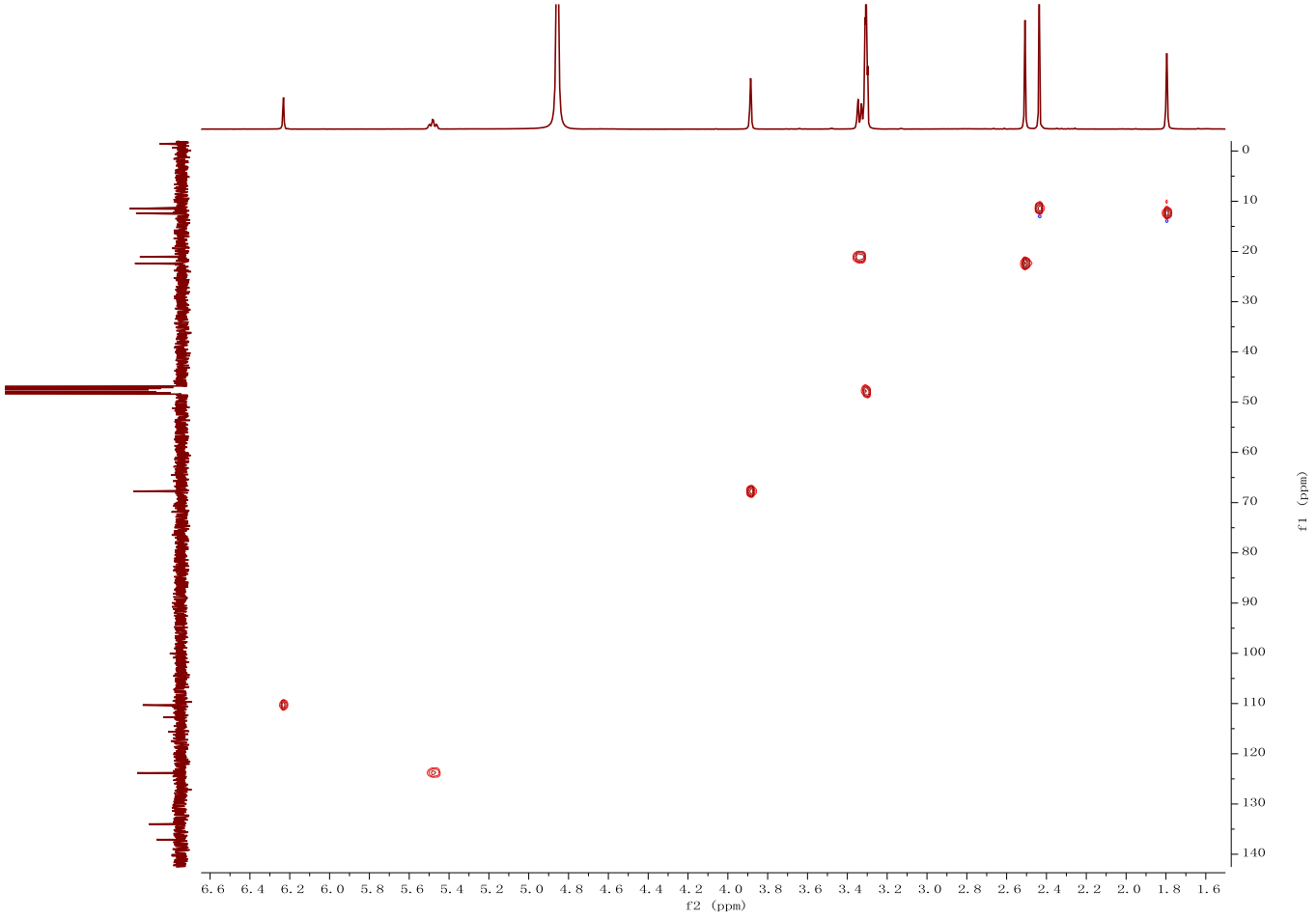


Figure S19. HSQC spectrum of **4** in MeOD.



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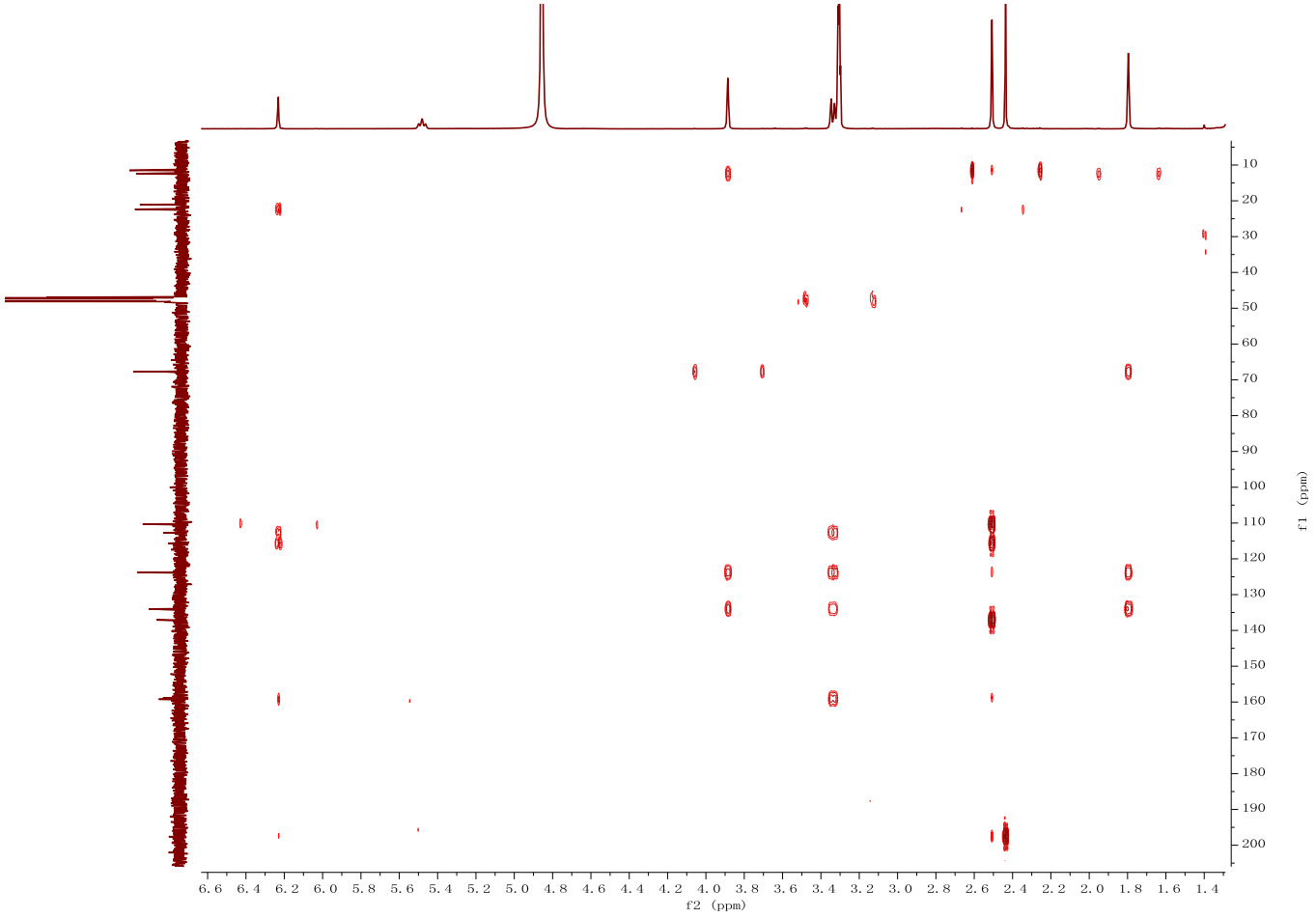

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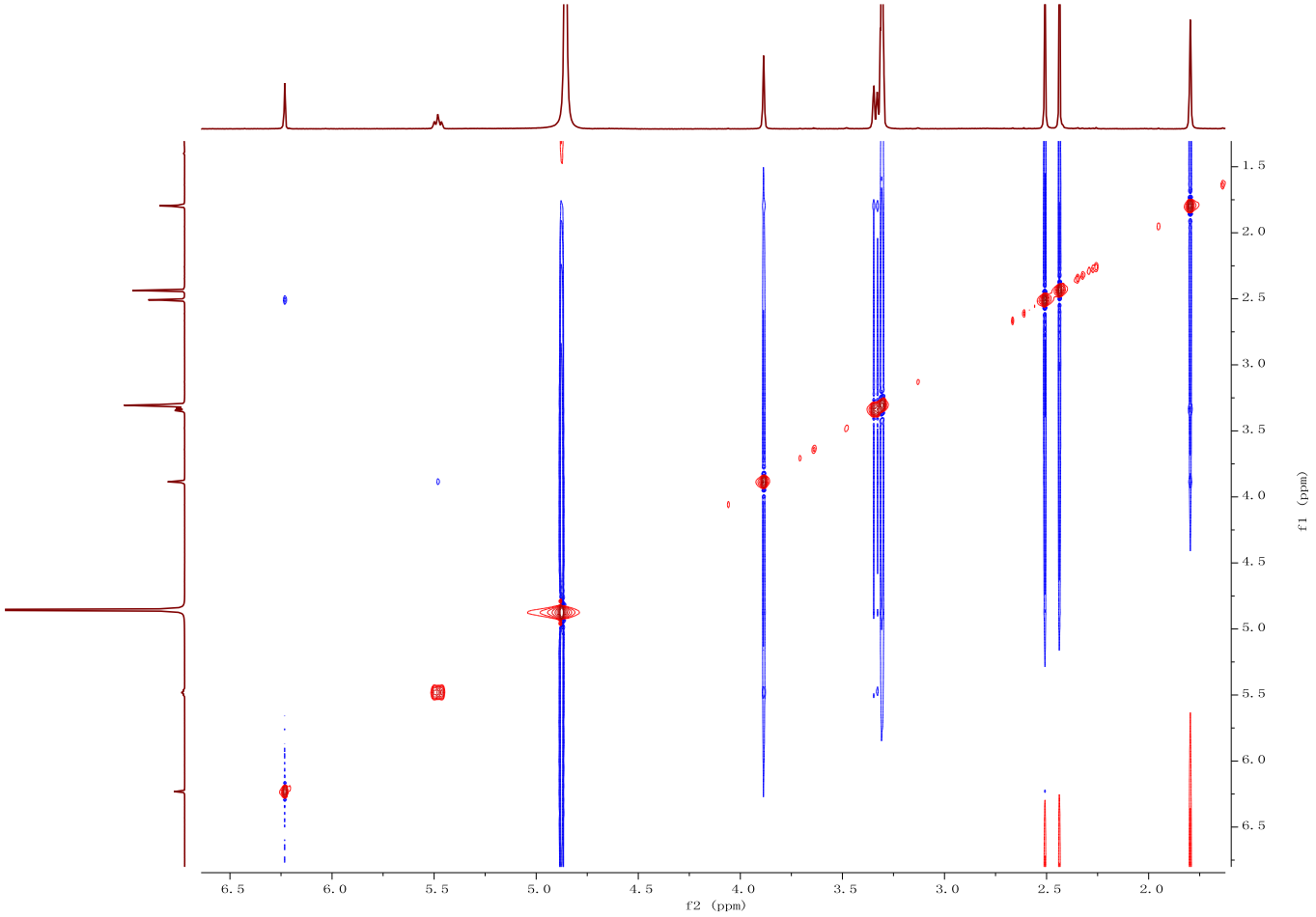


Figure S22. ^{1}H NMR spectrum of **5** in MeOD.

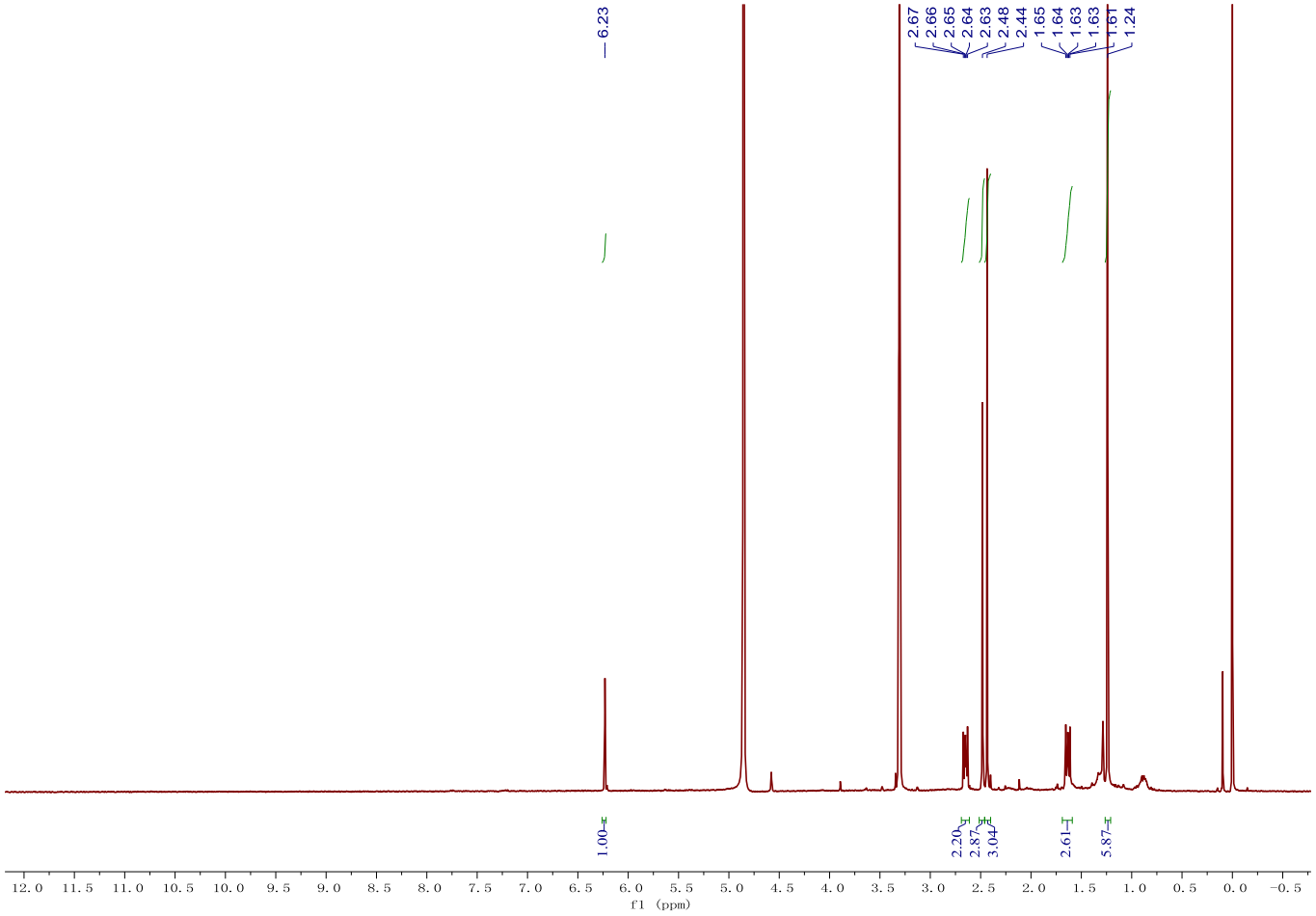


Figure S23. ^{13}C NMR spectrum of **5** in MeOD.

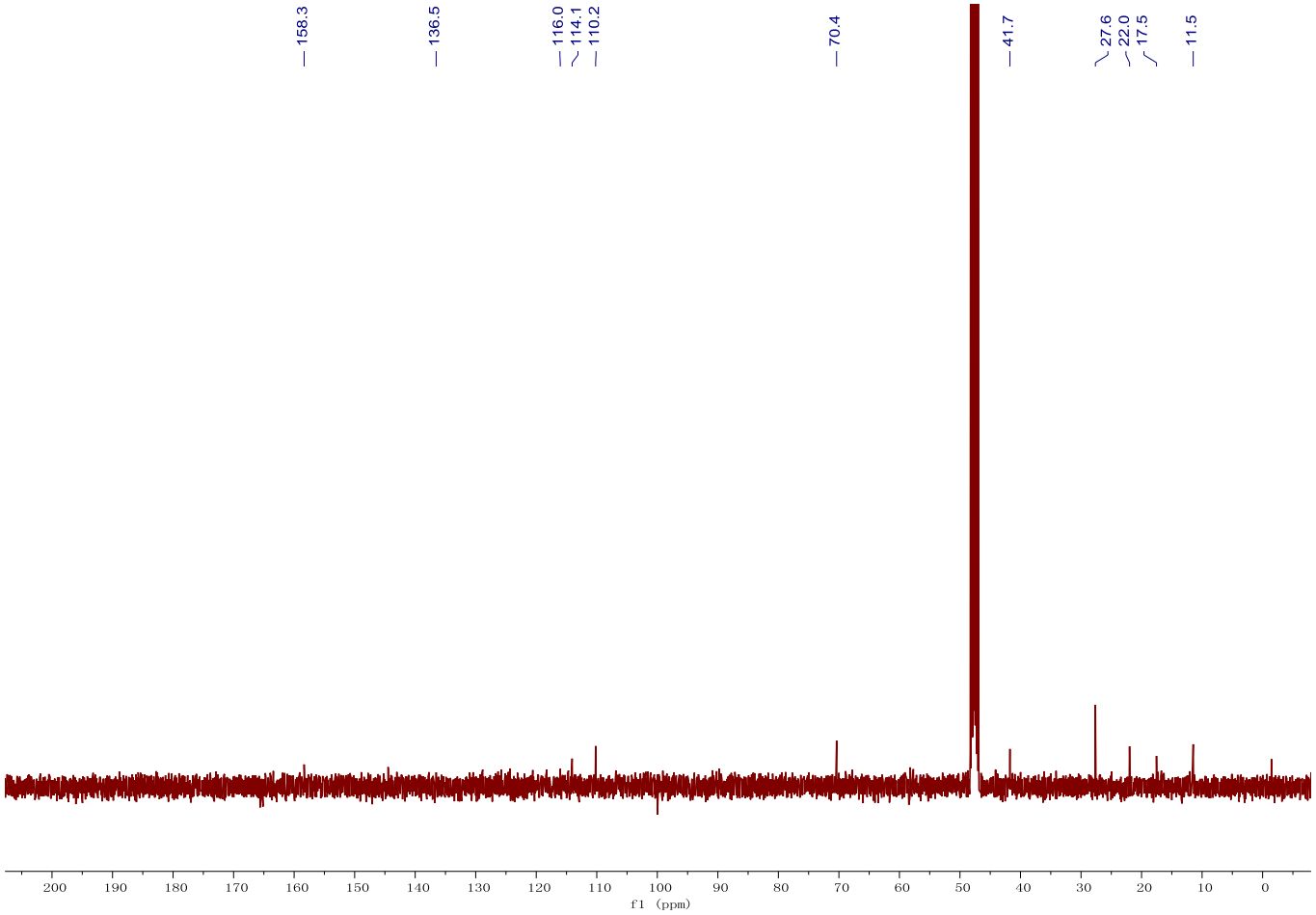


Figure S24. ^{1}H, ^{1}H-COSY spectrum of **5** in MeOD.

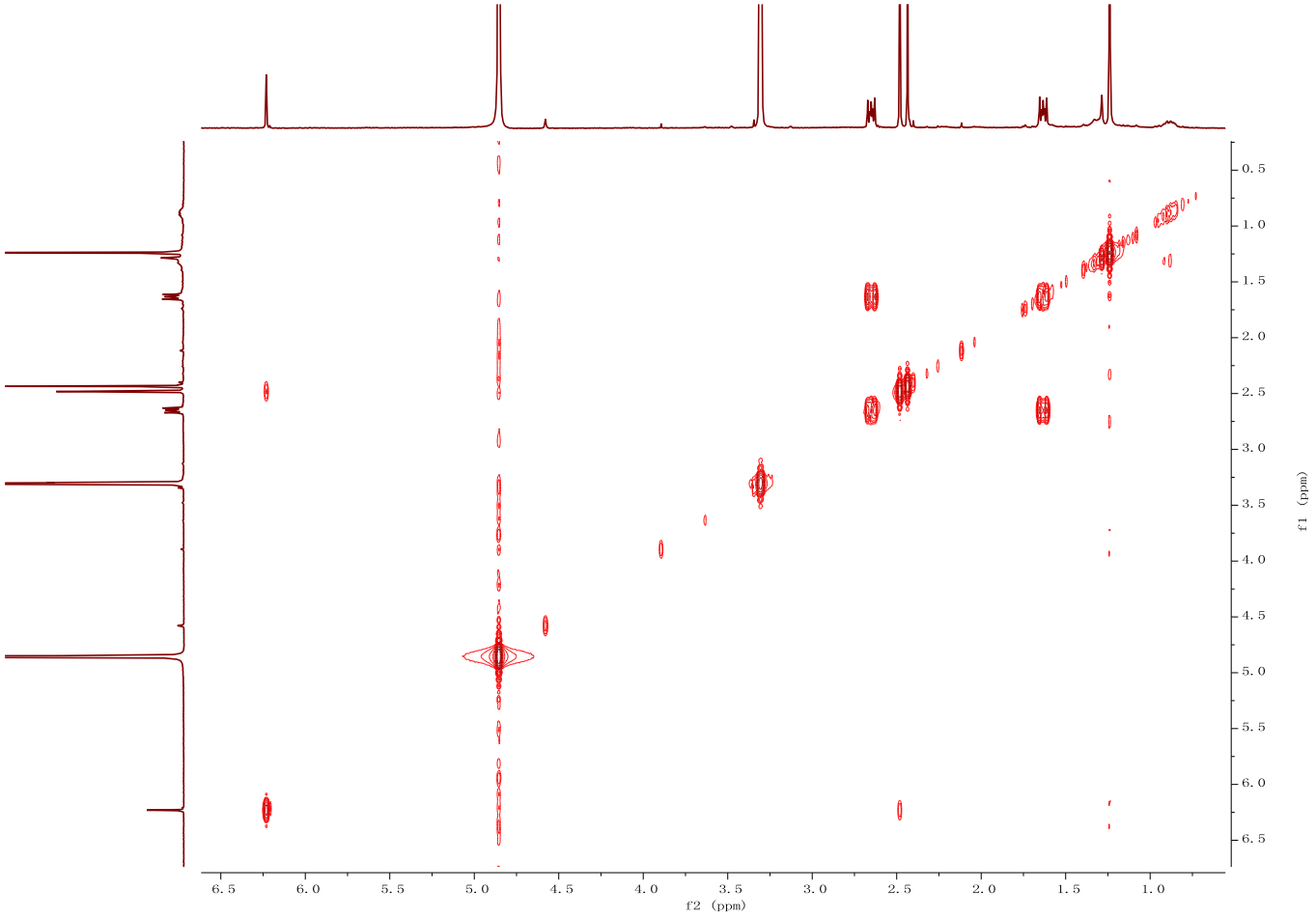


Figure S25. HSQC spectrum of **5** in MeOD.

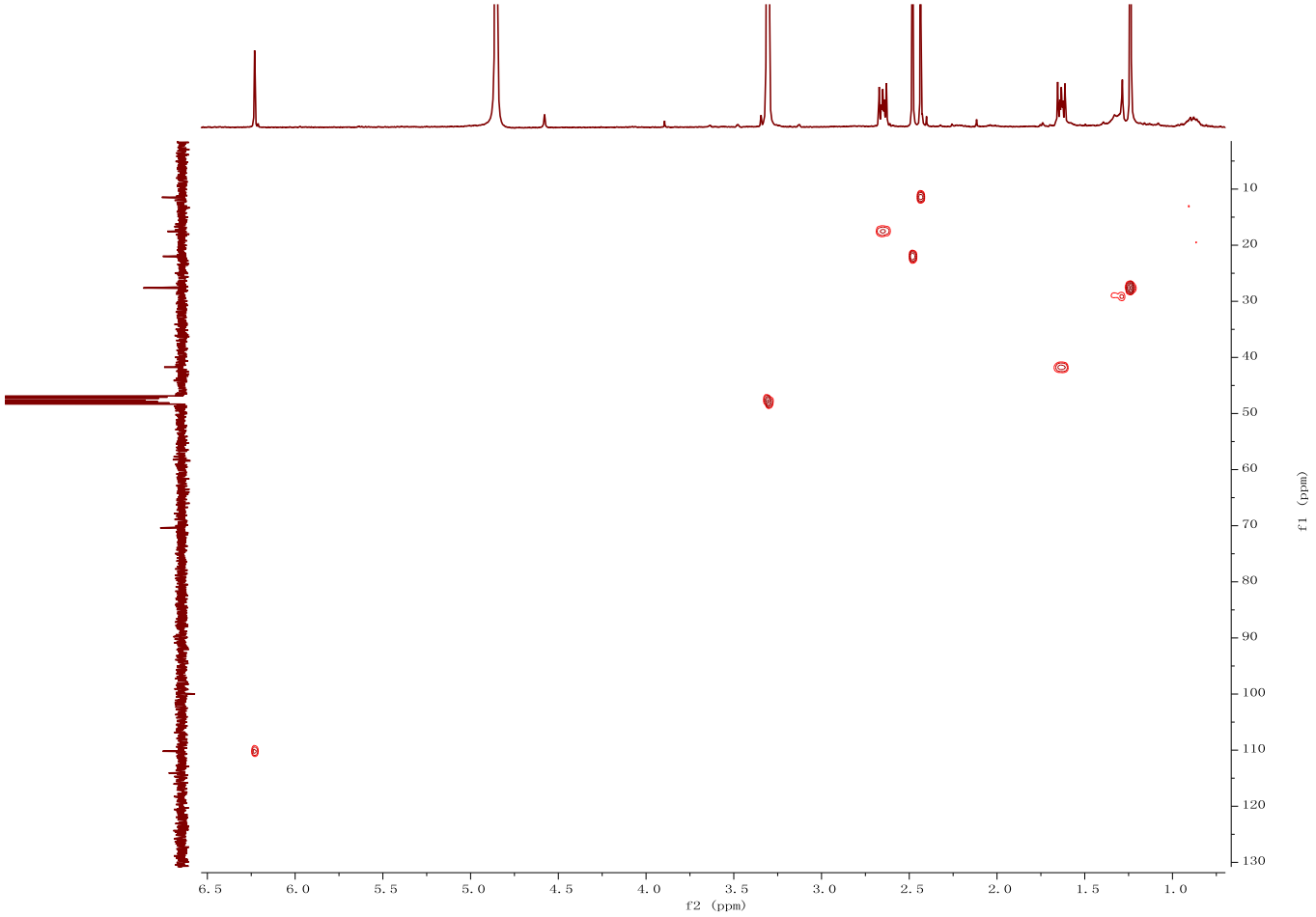


Figure S26. HMBC spectrum of **5** in MeOD.

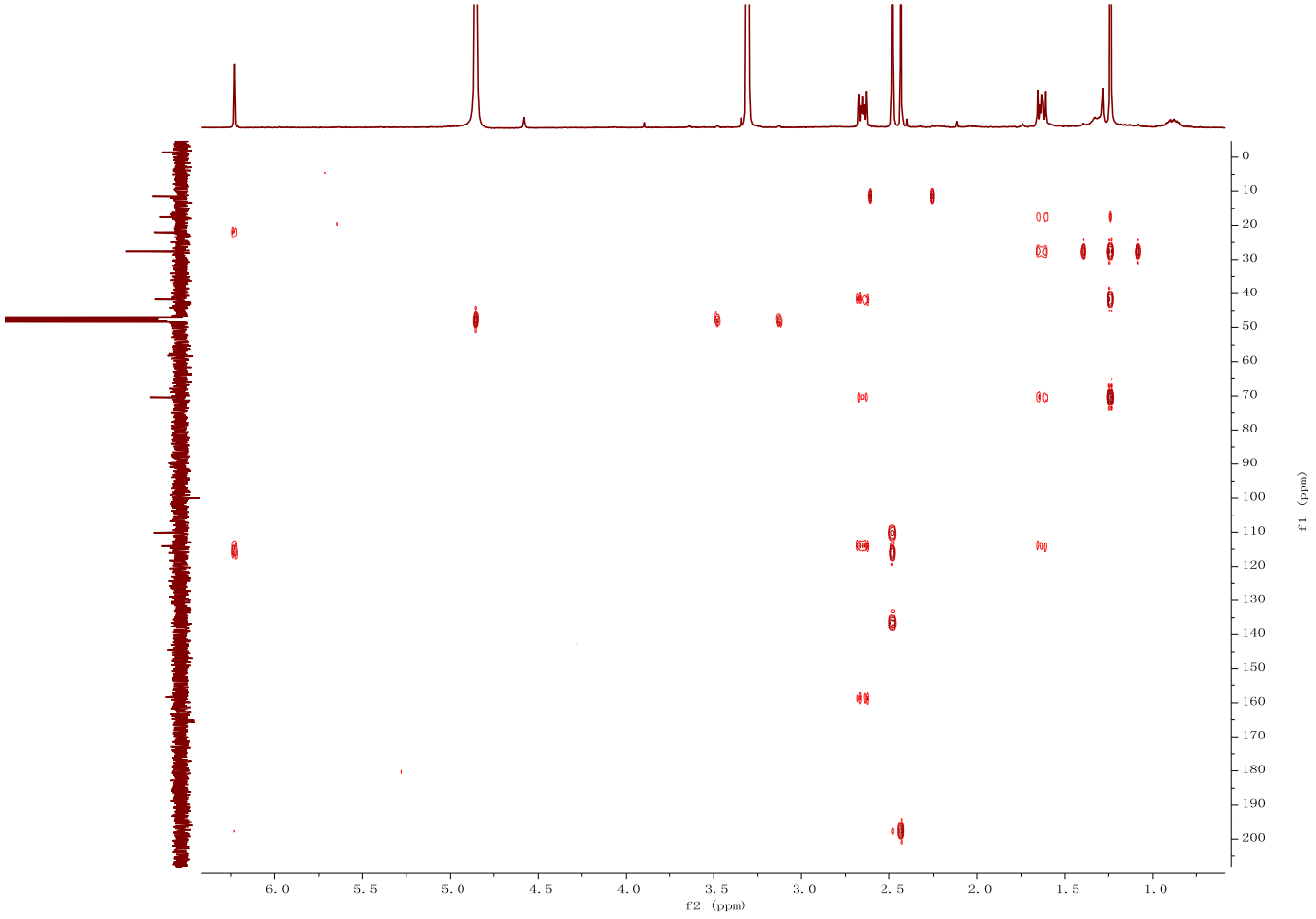


Figure S27. ^{1}H NMR spectrum of **6** in $CDCl_3$.

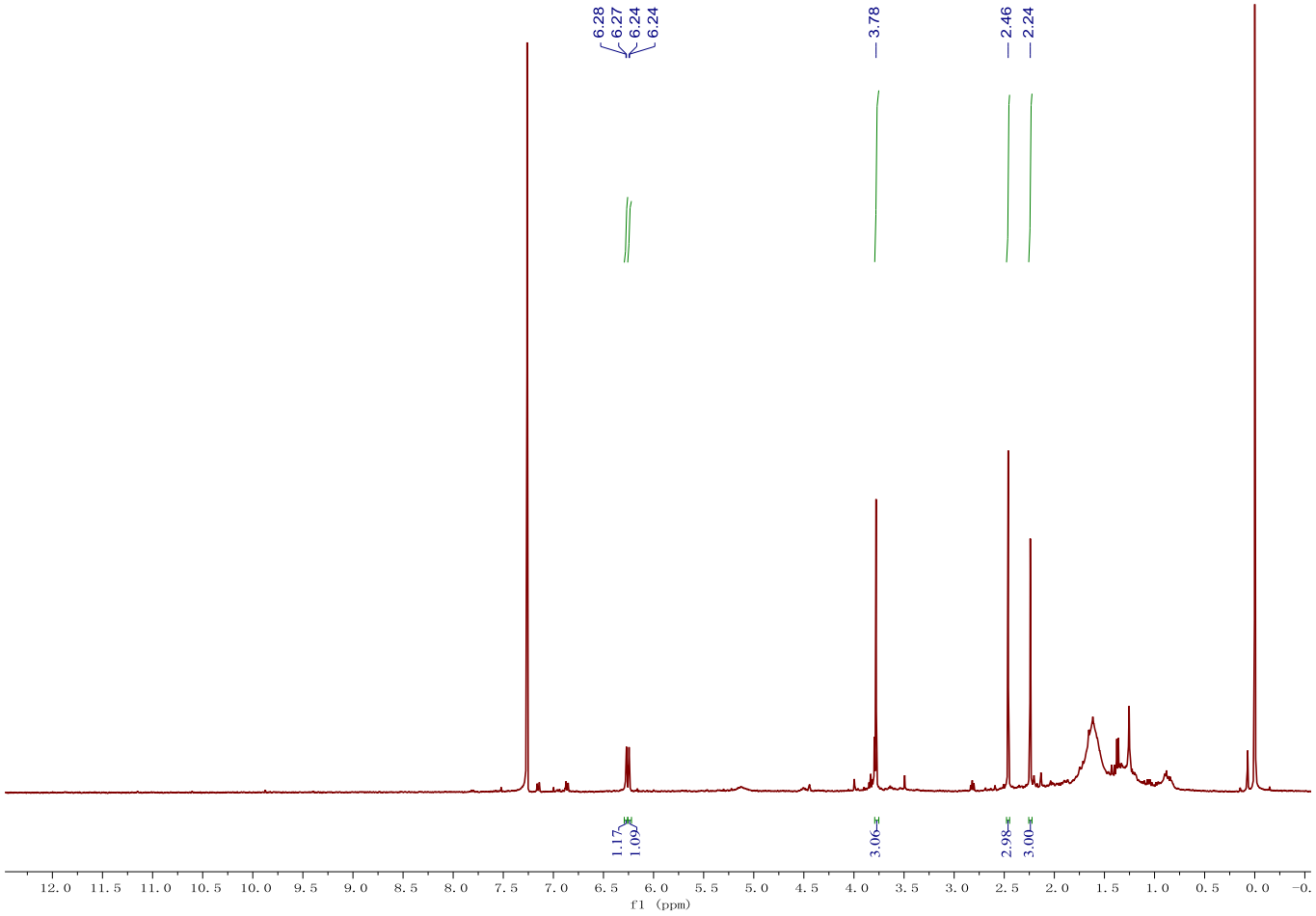


Figure S28. ^{13}C NMR spectrum of **6** in $CDCl_3$.

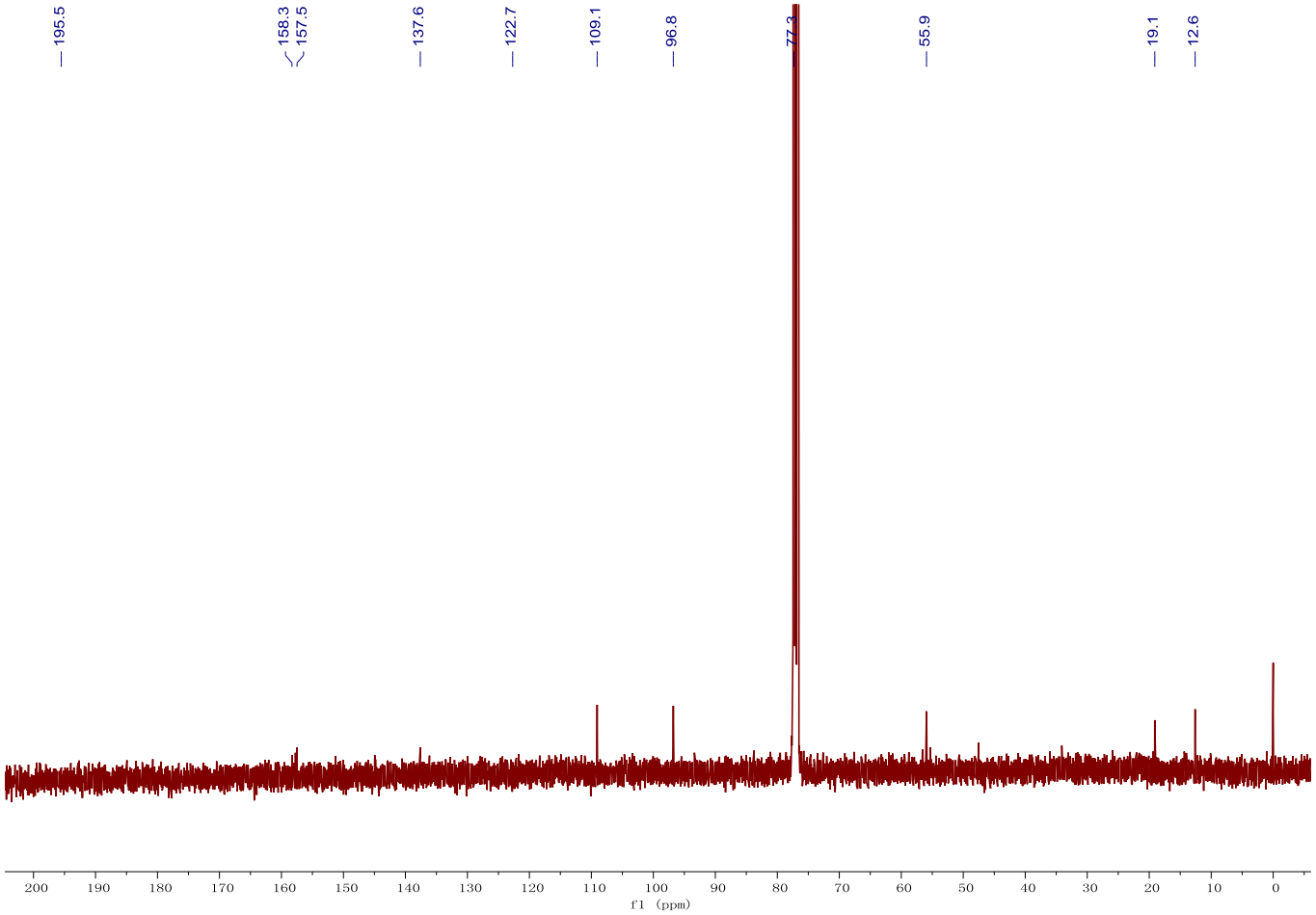


Figure S29. ^{1}H, ^{1}H-COSY spectrum of **6** in $CDCl_3$.

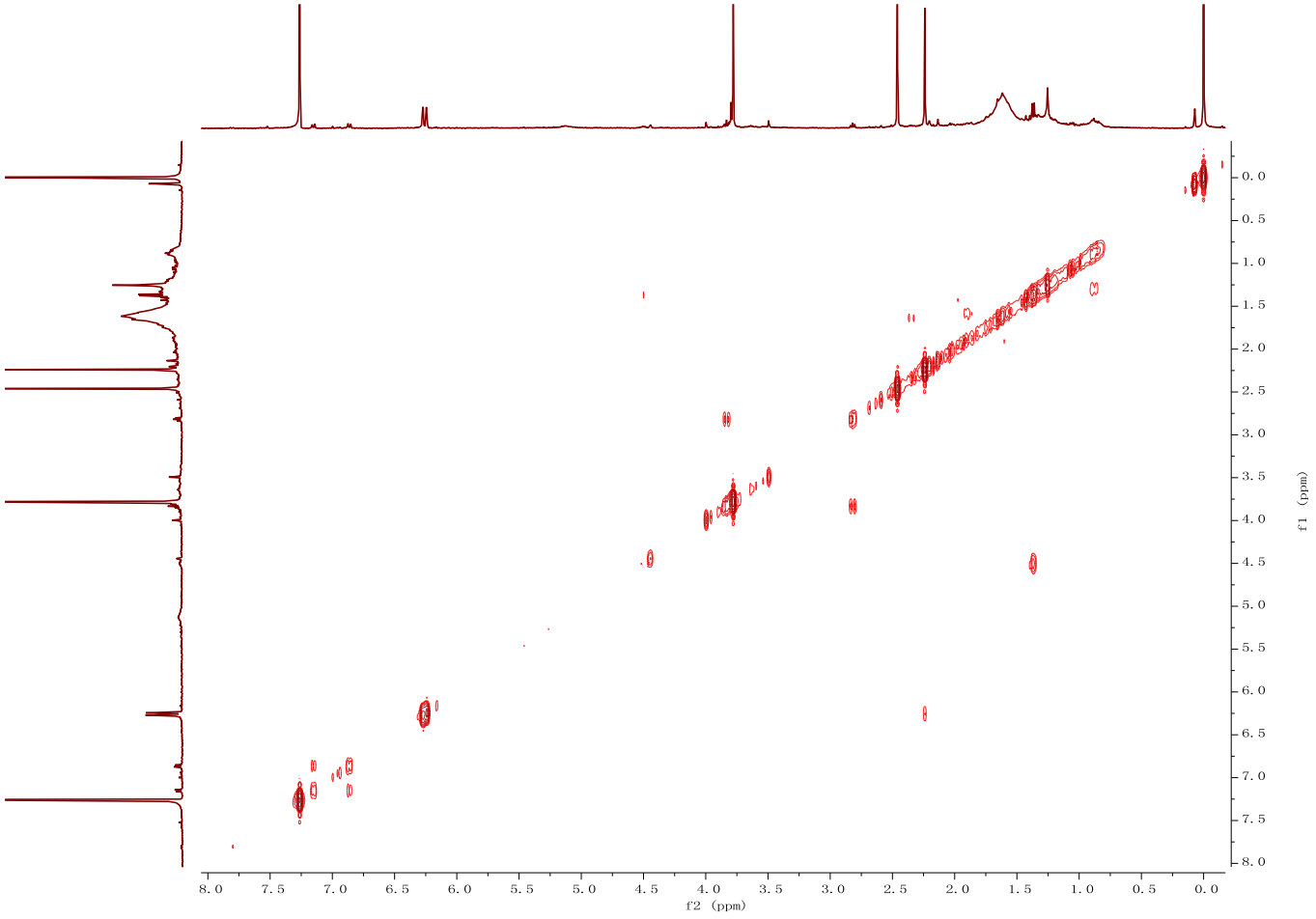


Figure S30. HSQC spectrum of **6** in $CDCl_3$.

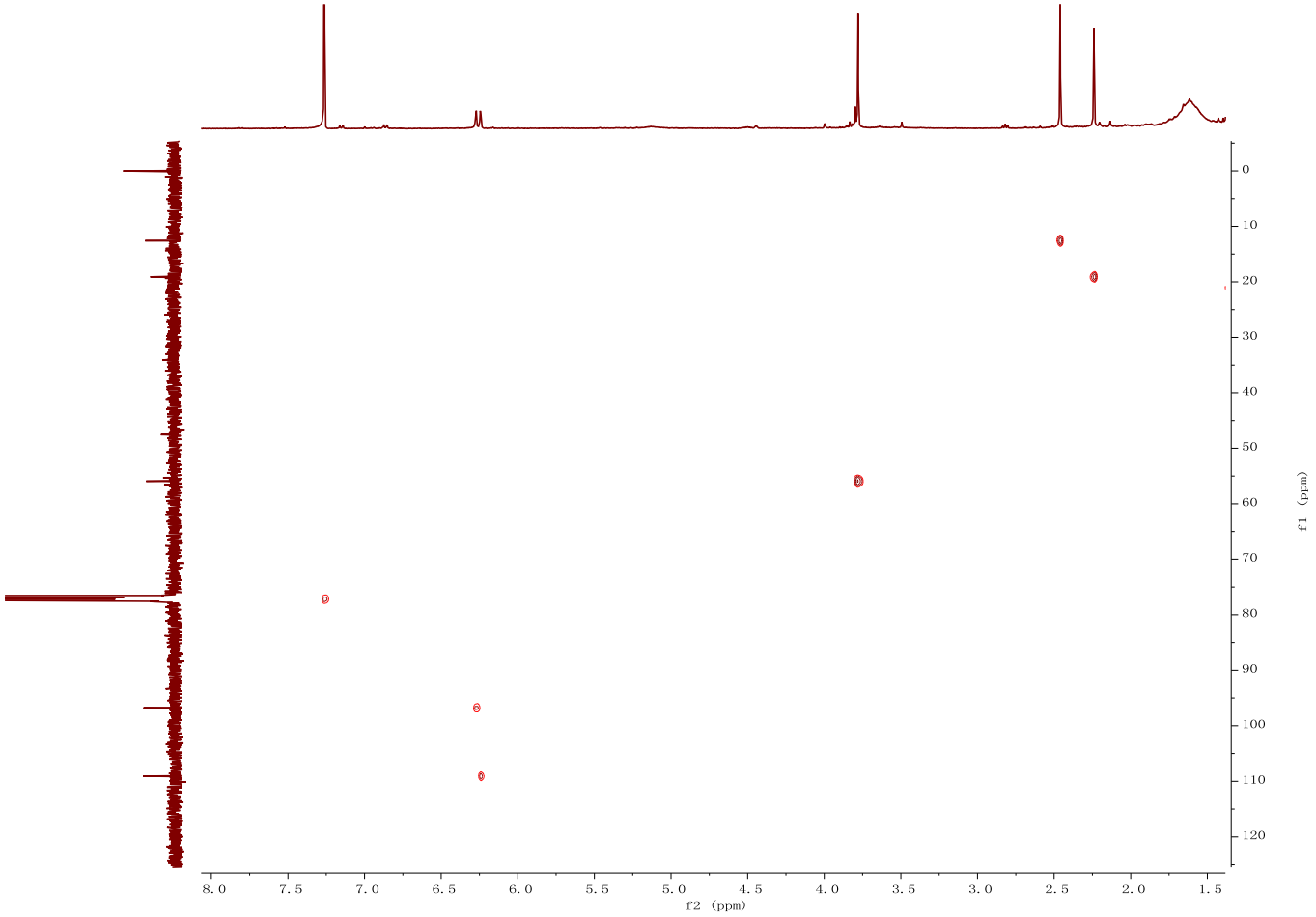


Figure S31. HMBC spectrum of **6** in $CDCl_3$.

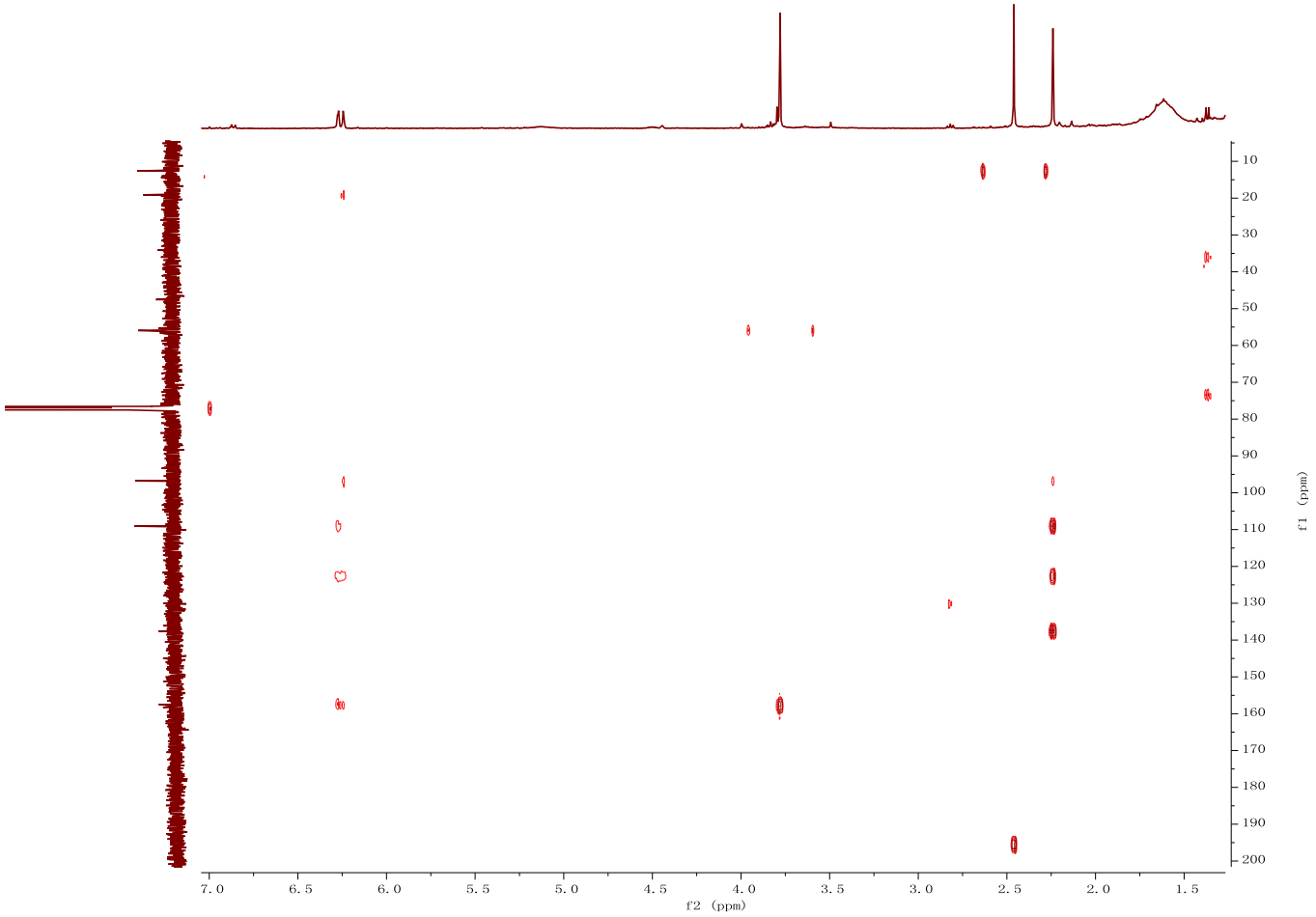
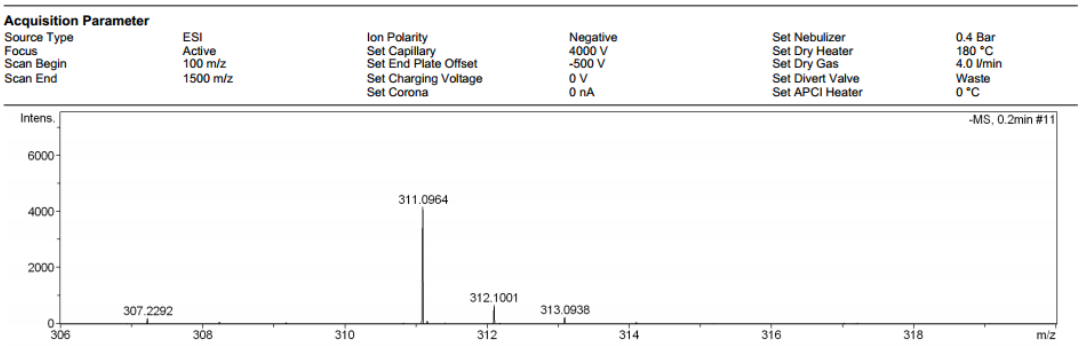


Figure S32. HRESI TOF MS spectrum of **1**.

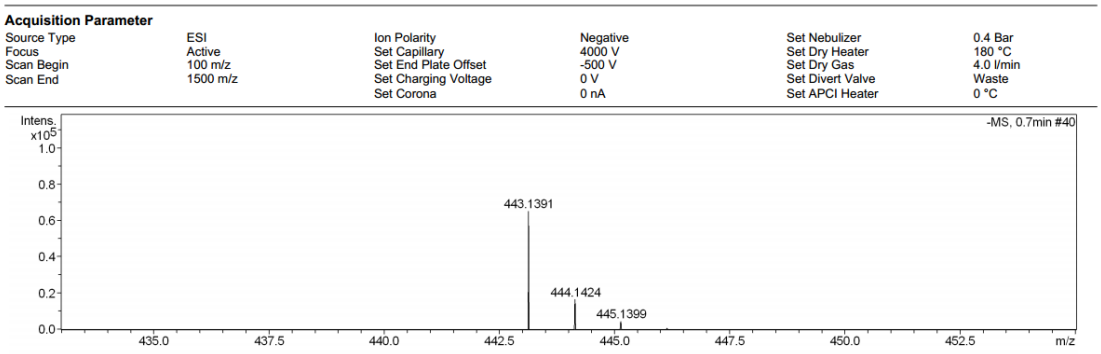


SPECTRUM - simulation :				
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
311.0964	311.0959	1.6	6.5	C15 H19 O5 S

Limits:

1) Charge: −1
2) Nitrogen-role: Do not use
3) Mass tolerance: 5 ppm
4) Element in use: ^{12}C(0~30), ^{1}H(0~60), ^{16}O(0~10), ^{32}S(0~10)

Figure S33. HRESI TOF MS spectrum of **2**.



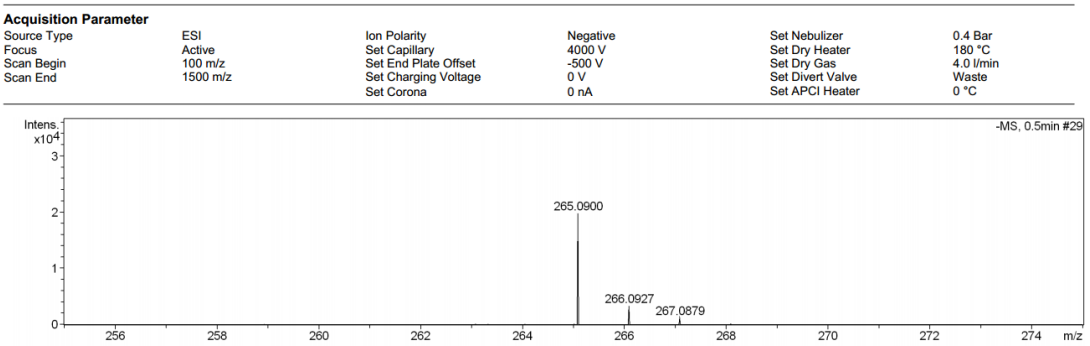
SPECTRUM
- simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
443.1391	443.1381	-2.2	7.5	C20 H27 O9 S

Limits:

1) Charge: −1
2) Nitrogen-role: Do not use
3) Mass tolerance: 5 ppm
4) ^{12}C(0~30), ^{1}H(0~60), ^{16}O(0~10), ^{32}S(0~10)

Figure S34. HRESI TOF MS spectrum of **3**.

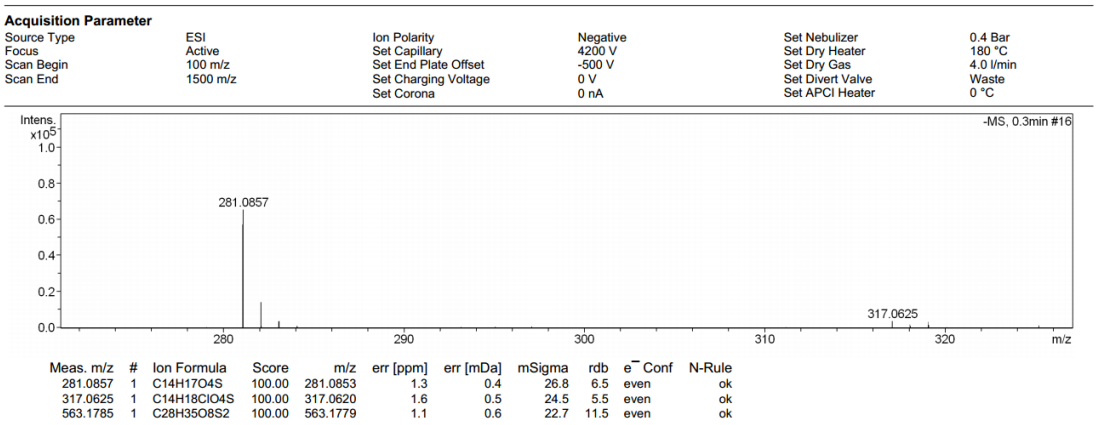


SPECTRUM - simulation :				
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
265.0900	265.0904	-1.6	6.5	C14 H17 O3 S

Limits:

1) Charge: −1
2) Nitrogen-role: Do not use
3) Mass tolerance: 5 ppm
4) Element in use: ^{12}C(0~30), ^{1}H(0~60), ^{16}O(0~10), ^{32}S(0~10)

Figure S35. HRESI TOF MS spectrum of **4**.



SPECTRUM

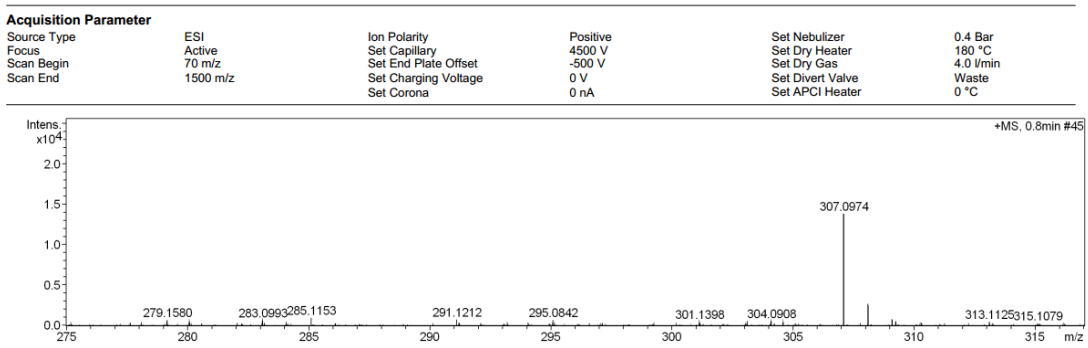
- simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
281.0857	281.0583	1.3	6.5	C14 H17 O4 S

Limits:

1) Charge: −1
2) Nitrogen-role: Do not use
3) Mass tolerance: 5 ppm
4) Element in use: ^{12}C(0~30), ^{1}H(0~60), ^{16}O(0~10), ^{32}S(0~10)

Figure S36. HRESI TOF MS spectrum of **5**.

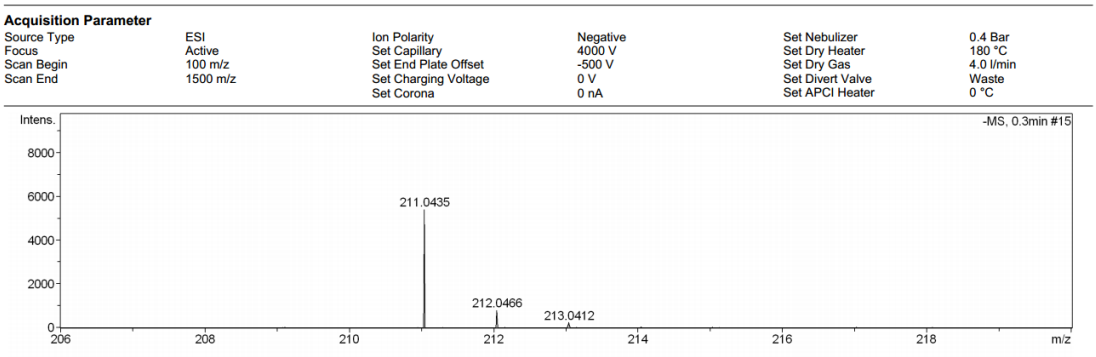


SPECTRUM - simulation :				
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
307.0974	307.0975	-0.7	4.5	C14 H20 O4 S Na

Limits:

(1) Charge: +1
(2) Nitrogen-Rule: Do not use
(3) Mass tolerance: 5.00 ppm
(4) Elements in use: ^{12}C(0~30), ^{1}H(0~60), ^{16}O(0~10), ^{32}S(0~10)

Figure S37. HRESI TOF MS spectrum of **6**.



SPECTRUM - simulation :				
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
211.0435	211.0434	0.1	5.5	C10 H11 O3 S

Limits:

(1) Charge: −1
(2) Nitrogen-Rule: Do not use
(3) Mass tolerance: 5.00 ppm
(4) Elements in use: ^{12}C(0~30), ^{1}H(0~60), ^{16}O(0~10), ^{32}S(0~10)

Figure S38. The observed key NOE correlation between H-10 and H_2-12 in **4**.

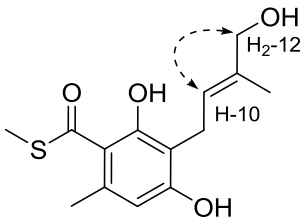
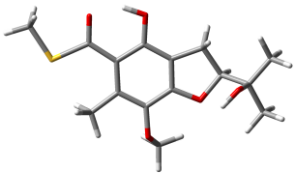
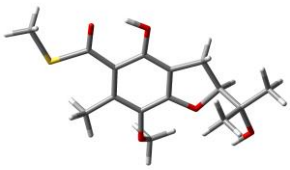


Table S1. Energy analysis for the Conformers of 10*R*-**1**.

compounds	Conformation	G (Hartree)	G (Kcal/mol)	ΔG (Kcal/mol)	Boltzmann Dist (%)
10*R*-**1**	10*R*-**1-1**	-1357.94367667	-852113.5951	0	64.00%
	10*R*-**1-2**	-1357.94275144	-852113.0146	0.58	36.00%



10*R*-**1-1**



10*R*-**1-2**