

Supplementary data

Brominated Depsidones with Antibacterial Effects from a Deep-Sea-Derived Fungus *Spiromastix* sp.

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Table S1. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 1

No.	δ_{H}	δ_{C}	COSY	HMBC
1		111.1, qC		
2		161.7, qC		
3	6.80, s	105.3, CH		C-1, C-2, C-4, C-5
4		159.7, qC		
5		113.6, qC		
6		146.9, qC		
7		162.9, qC		
8	2.81, t (7.9)	36.0, CH ₂	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.54, m	23.0, CH ₂	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.89, t (7.3)	14.3, CH ₃	H ₂ -9	C-8, C-9
1'		141.3, C		
2'		144.6, C		
3'	6.50, d (2.7)	105.5, CH	H-5'	C-1', C-2', C-4', C-5'
4'		155.2, C		
5'	6.47, d (2.7)	113.2, CH	H-3'	C-1', C-3', C-4', C-7'
6'		135.8, C		
7'	2.65, t (7.8)	31.4, CH ₂	H ₂ -8'	C-1', C-5', C-6', C-8', C-9'
8'	1.57, m	23.7, CH ₂	H ₂ -7', H ₃ -9'	C-6', C-7', C-9'
9'	0.97, t (7.3)	14.4, CH ₃	H ₂ -8'	C-7', C-8'

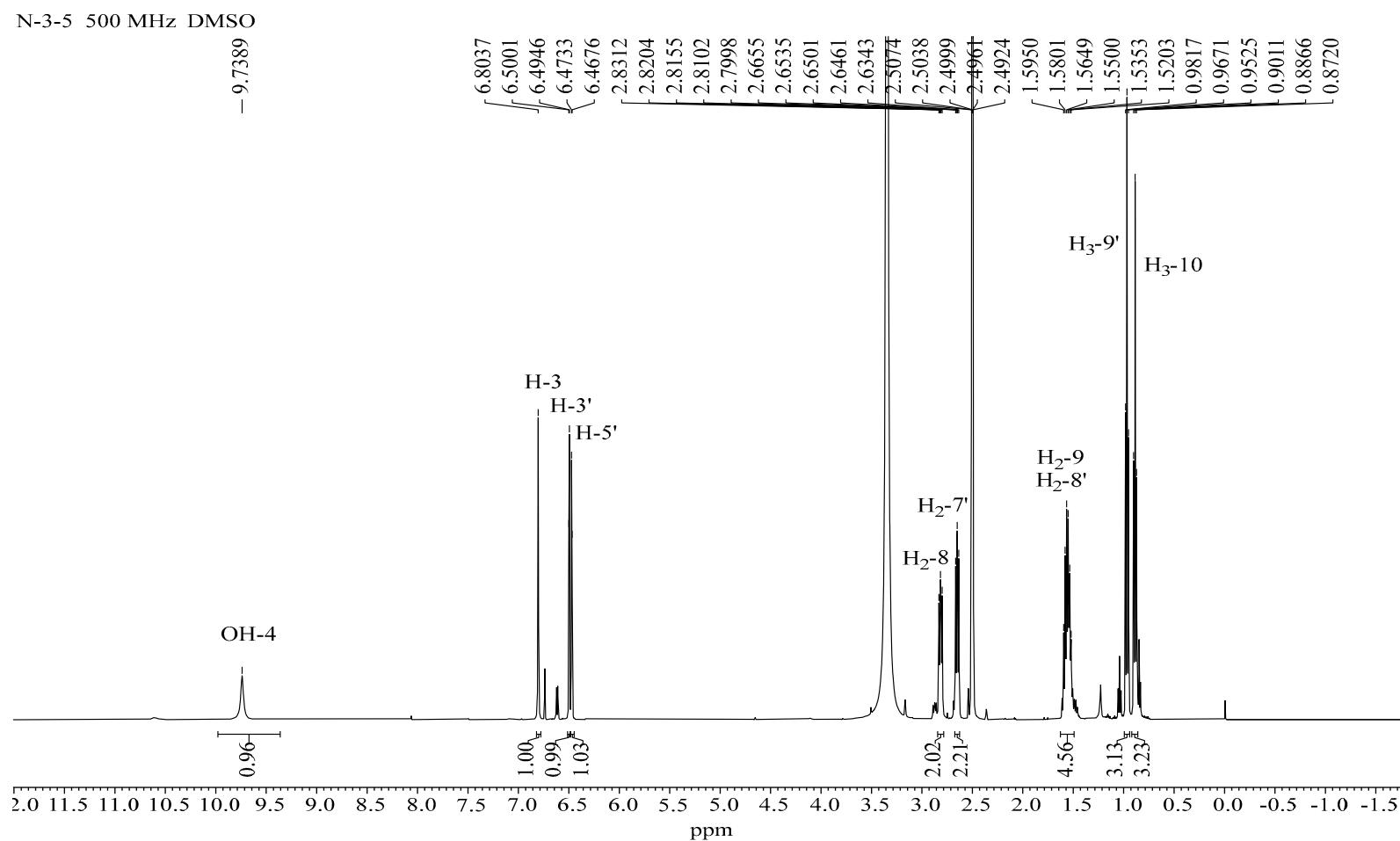


Figure S1. ^1H -NMR spectrum of **1** in $\text{DMSO}-d_6$ (500 MHz)

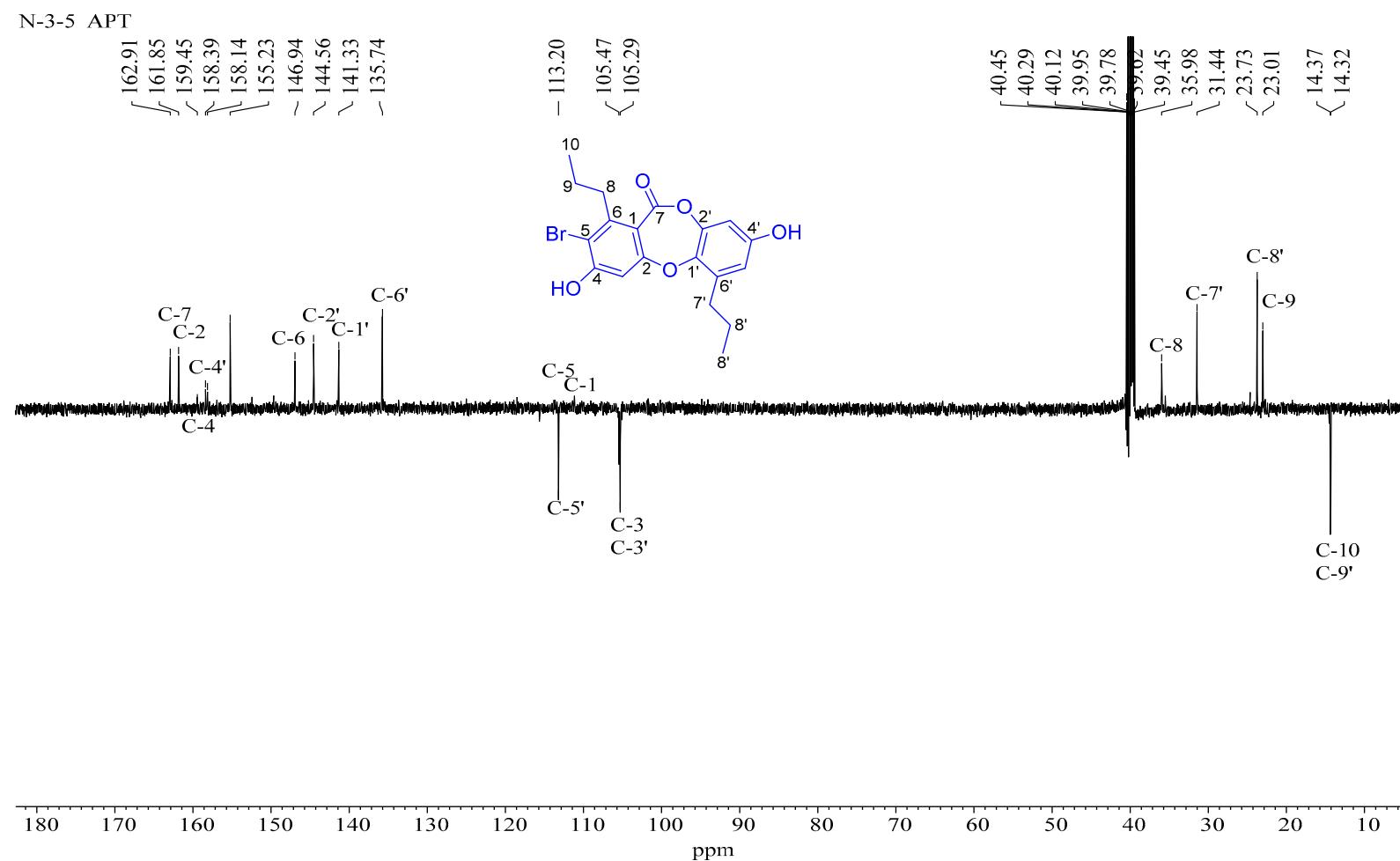


Figure S2. APT spectrum of **1** in $\text{DMSO}-d_6$ (125 MHz)

N-3-5 HSQC

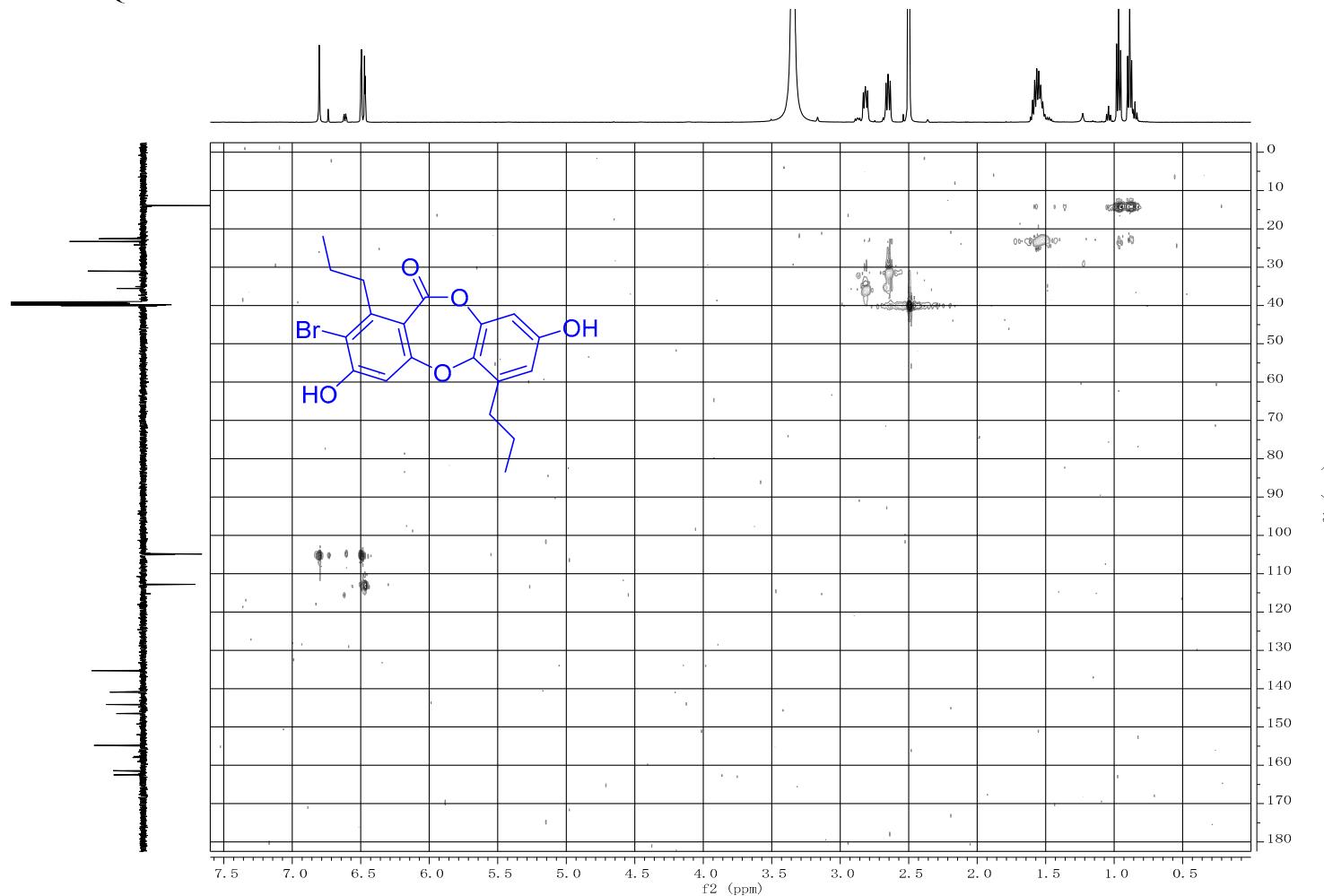


Figure S3. HSQC spectrum of **1** in $\text{DMSO}-d_6$

N-3-5 COSY

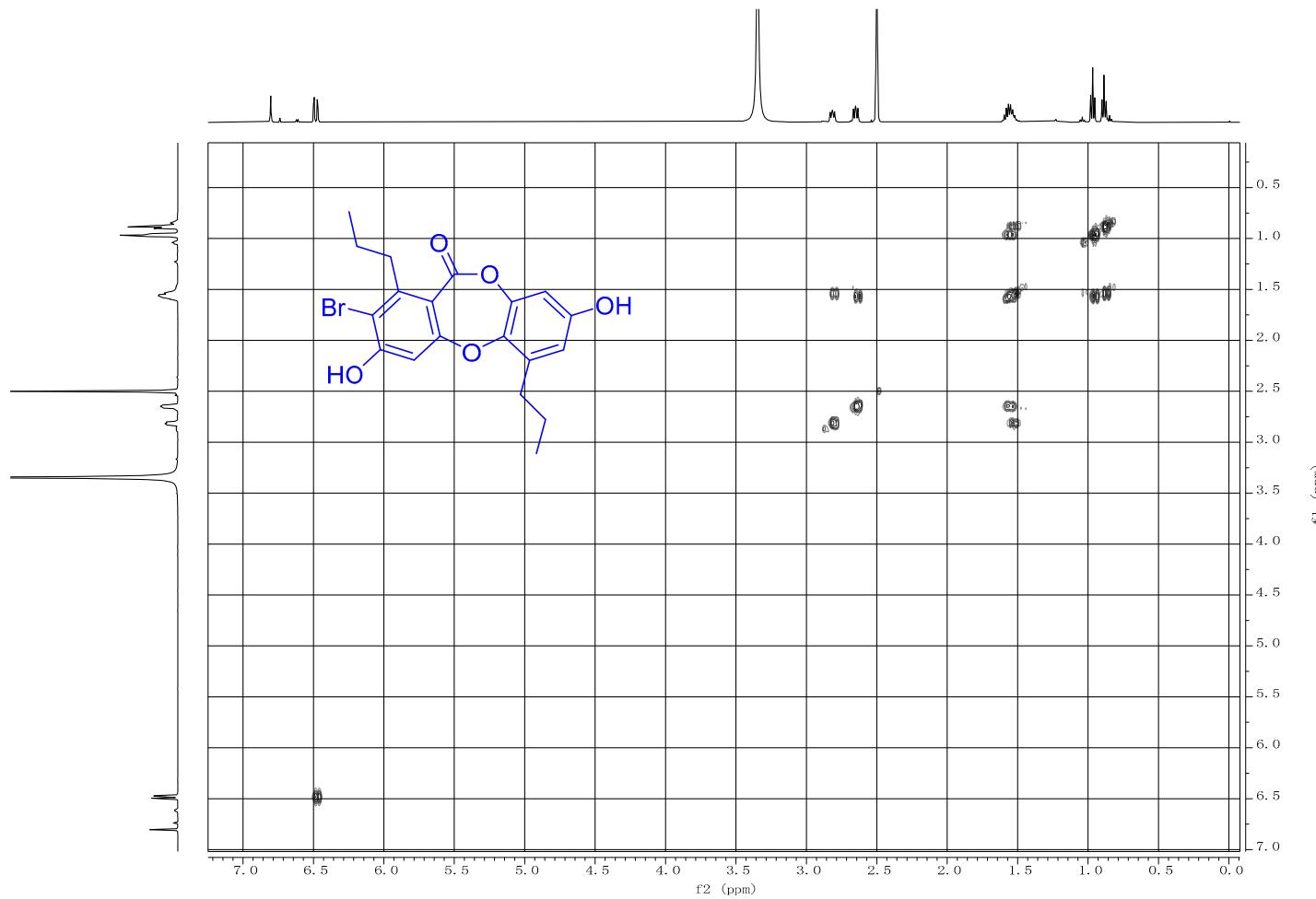


Figure S4. ^1H - ^1H COSY spectrum of **1** in $\text{DMSO}-d_6$

N-3-5 HMBC

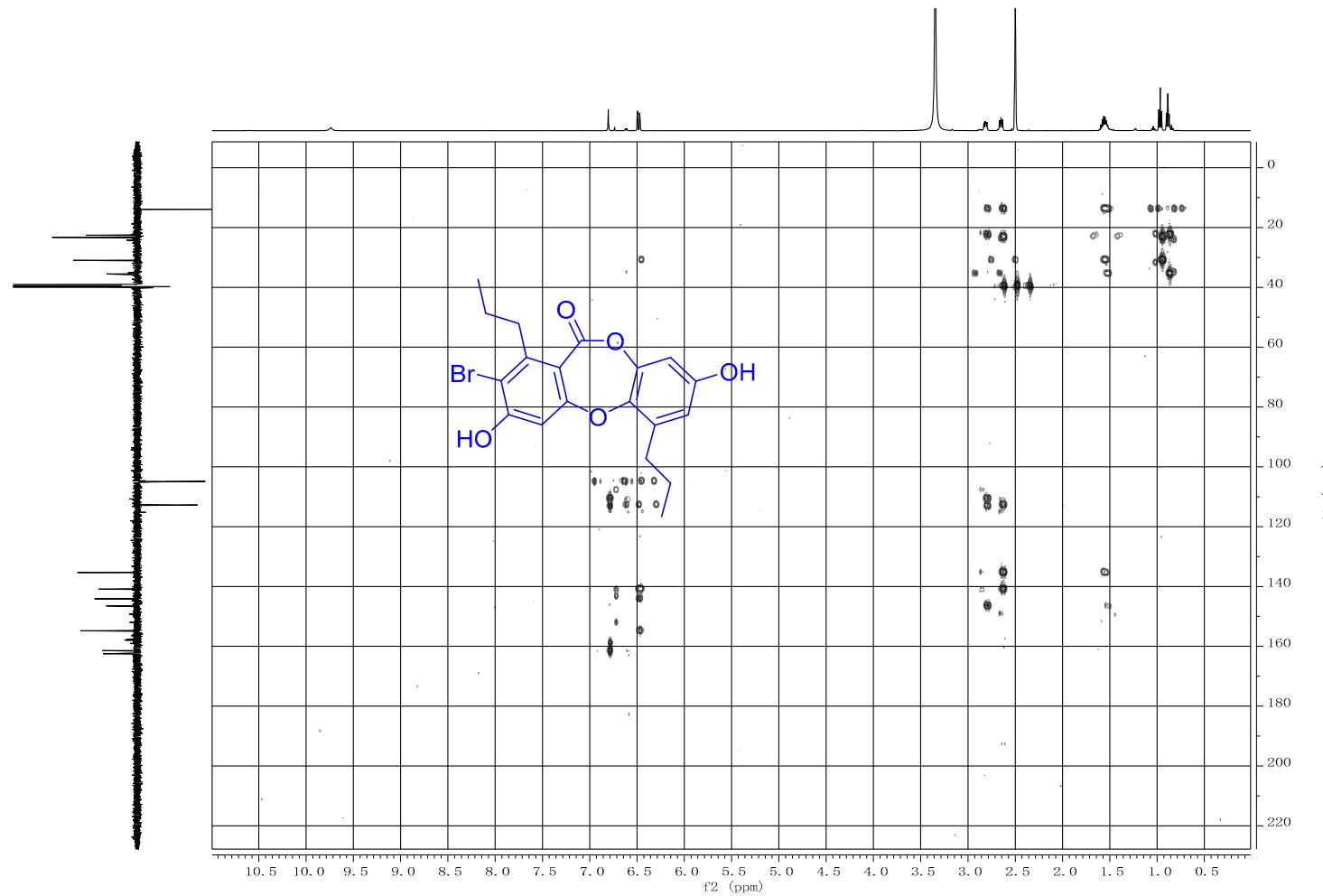


Figure S5. HMBC spectrum of **1** in $\text{DMSO}-d_6$

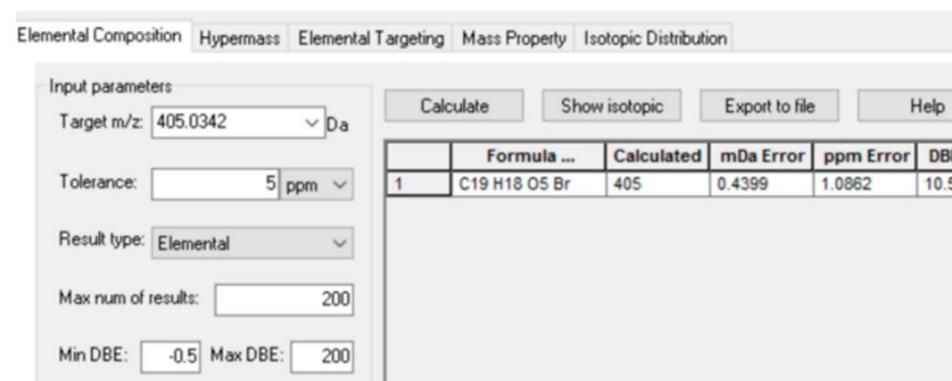
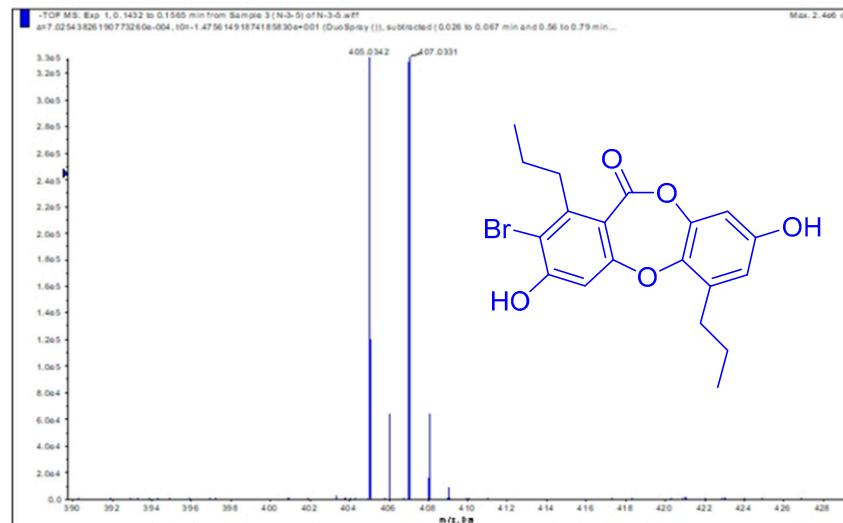


Figure S6. HRESIMS spectrum of **1**

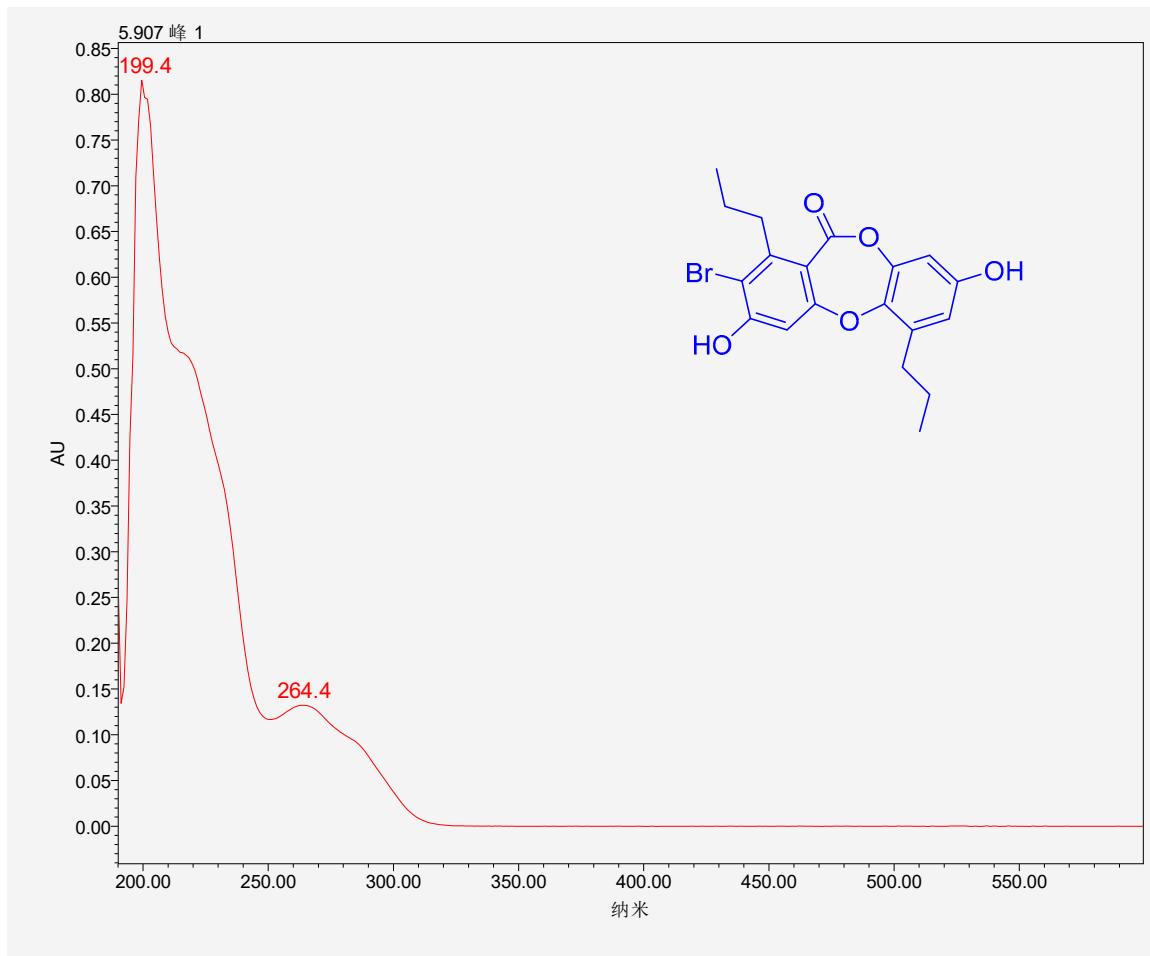


Figure S7. UV spectrum of **1**

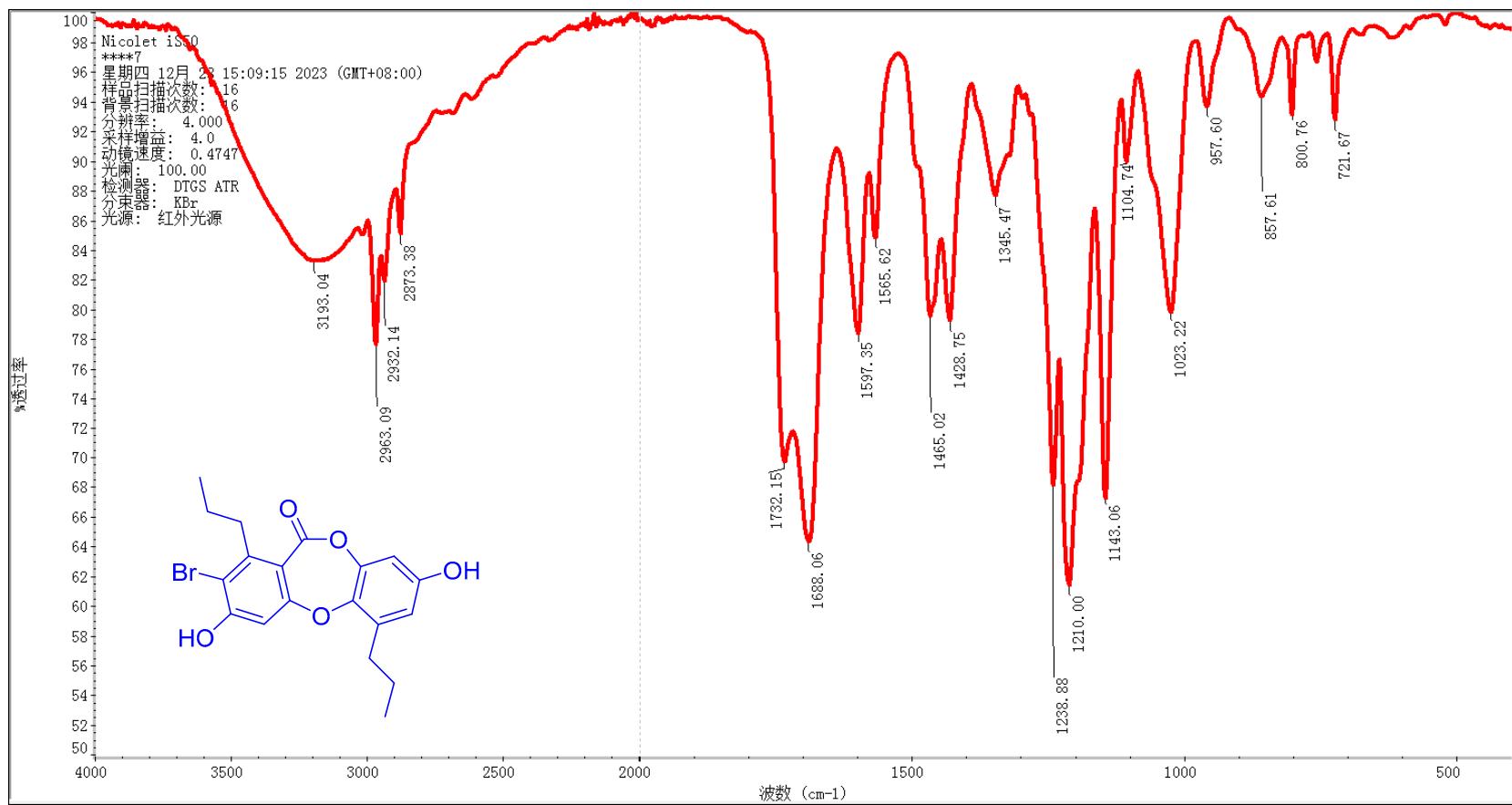


Figure S8. IR spectrum of 1

Table S2. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 2

No.	δ_{H}	δ_{C}	COSY	HMBC
1		112.5, C		
2		160.4, C		
3		98.9, C		
4		159.6, C		
5	6.79, s	115.1, CH		C-1, C-3, C-4, C-8
6		148.5, C		
7		162.1, C		
8	2.66, t (7.8)	35.7, CH_2		C-1, C-5, C-6, C-9, C-10
9	1.49, m	24.5, CH_2		C-6, C-8, C-10
10	0.86, t (7.3)	14.3, CH_3		C-8, C-9
1'		142.0, C		
2'		143.4, C		
3'	6.77, s	105.6, CH		C-1', C-2', C-4', C-5'
4'		152.9, C		
5'		108.8, C		
6'		136.0, C		
7'	3.13, t (8.0)	33.0, CH_2		C-1', C-5', C-6', C-8', C-9'
8'	1.48, m	23.1, CH_2		C-6', C-7', C-9'
9'	1.00, t (7.3)	14.4, CH_3		C-7', C-8'

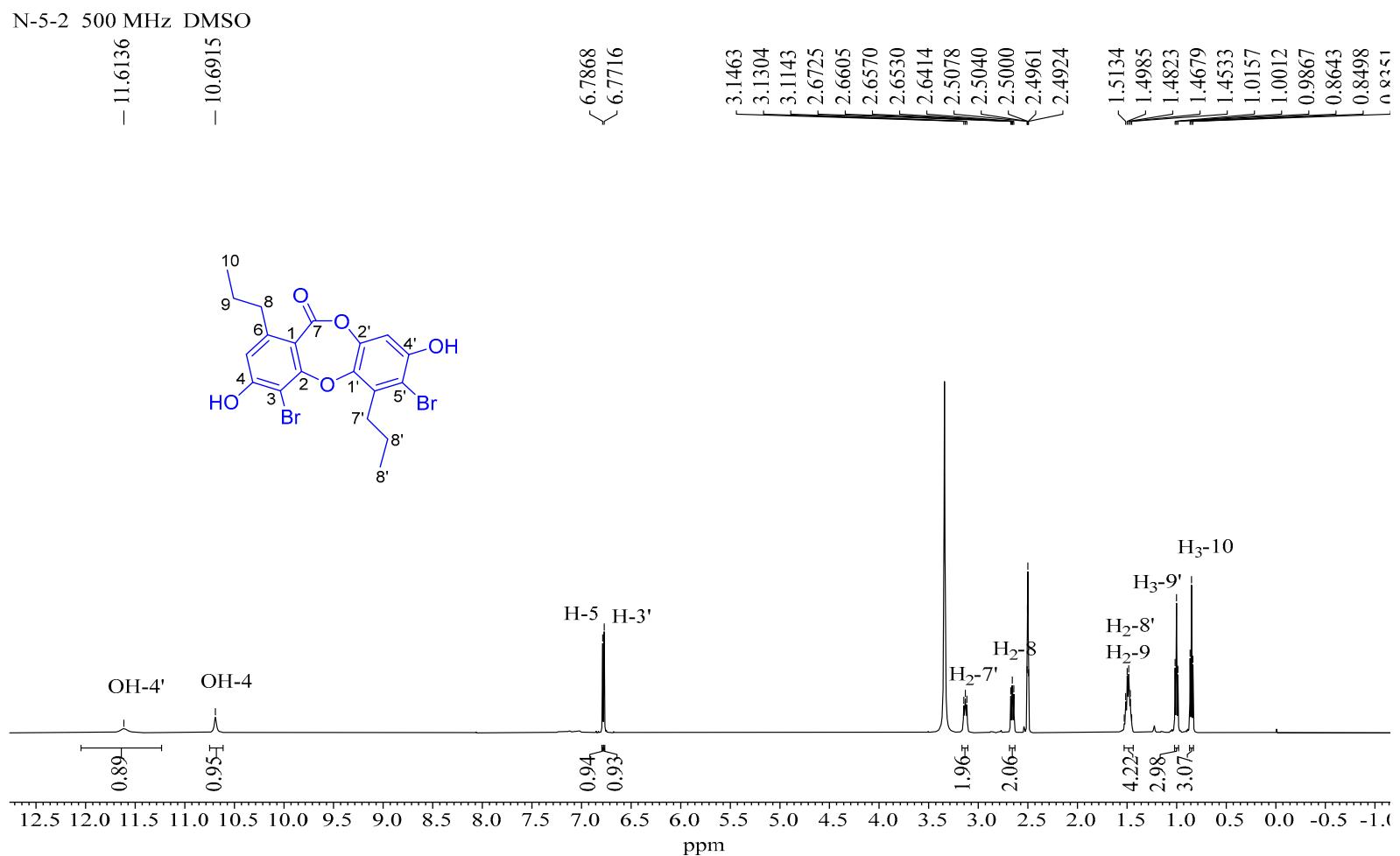


Figure S9. ^1H -NMR spectrum of **2** in $\text{DMSO}-d_6$ (500 MHz)

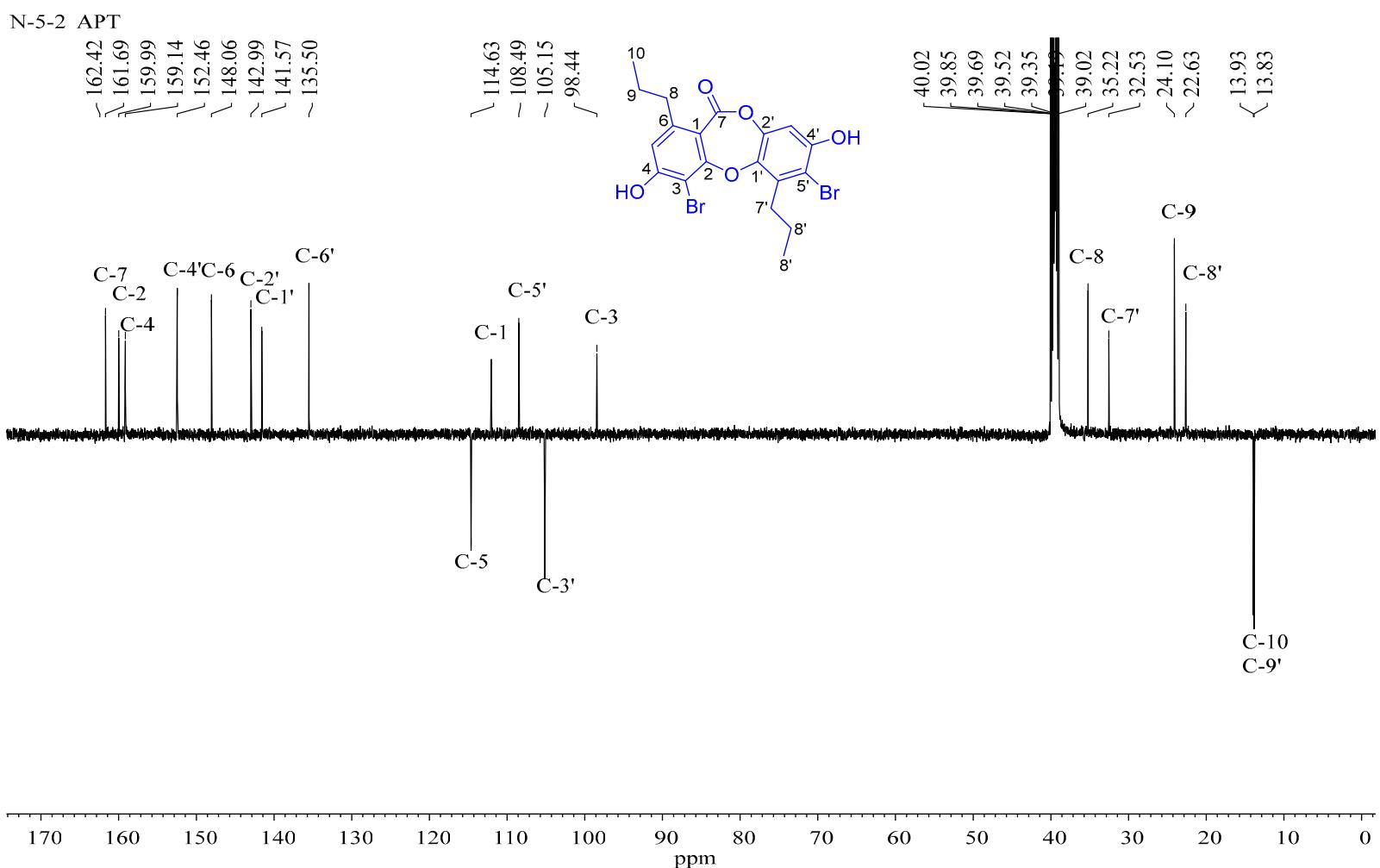


Figure S10. APT spectrum of **2** in DMSO-*d*₆ (125 MHz)

N-5-2 HSQC

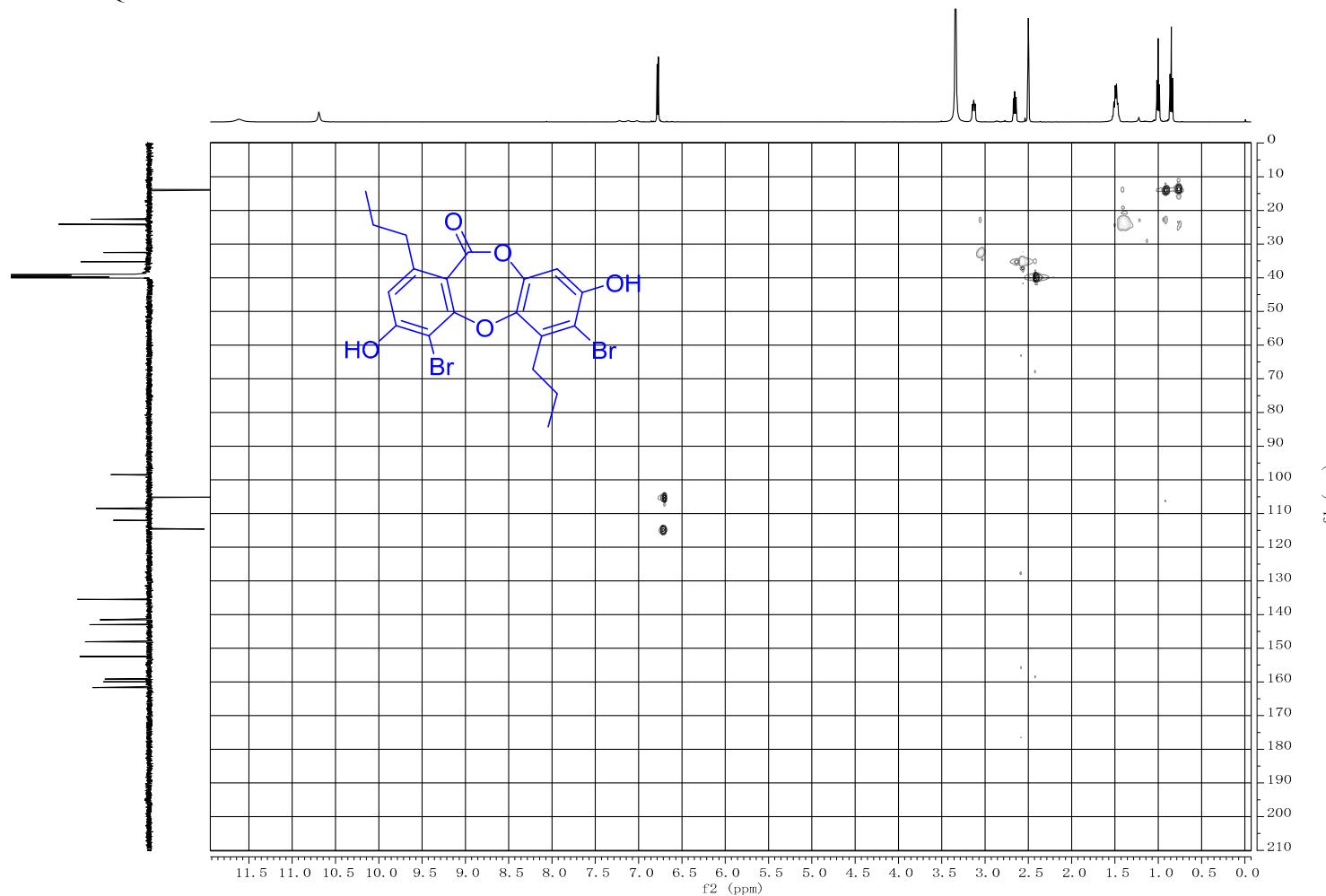


Figure S11. HSQC spectrum of **2** in $\text{DMSO}-d_6$

N-5-2 COSY

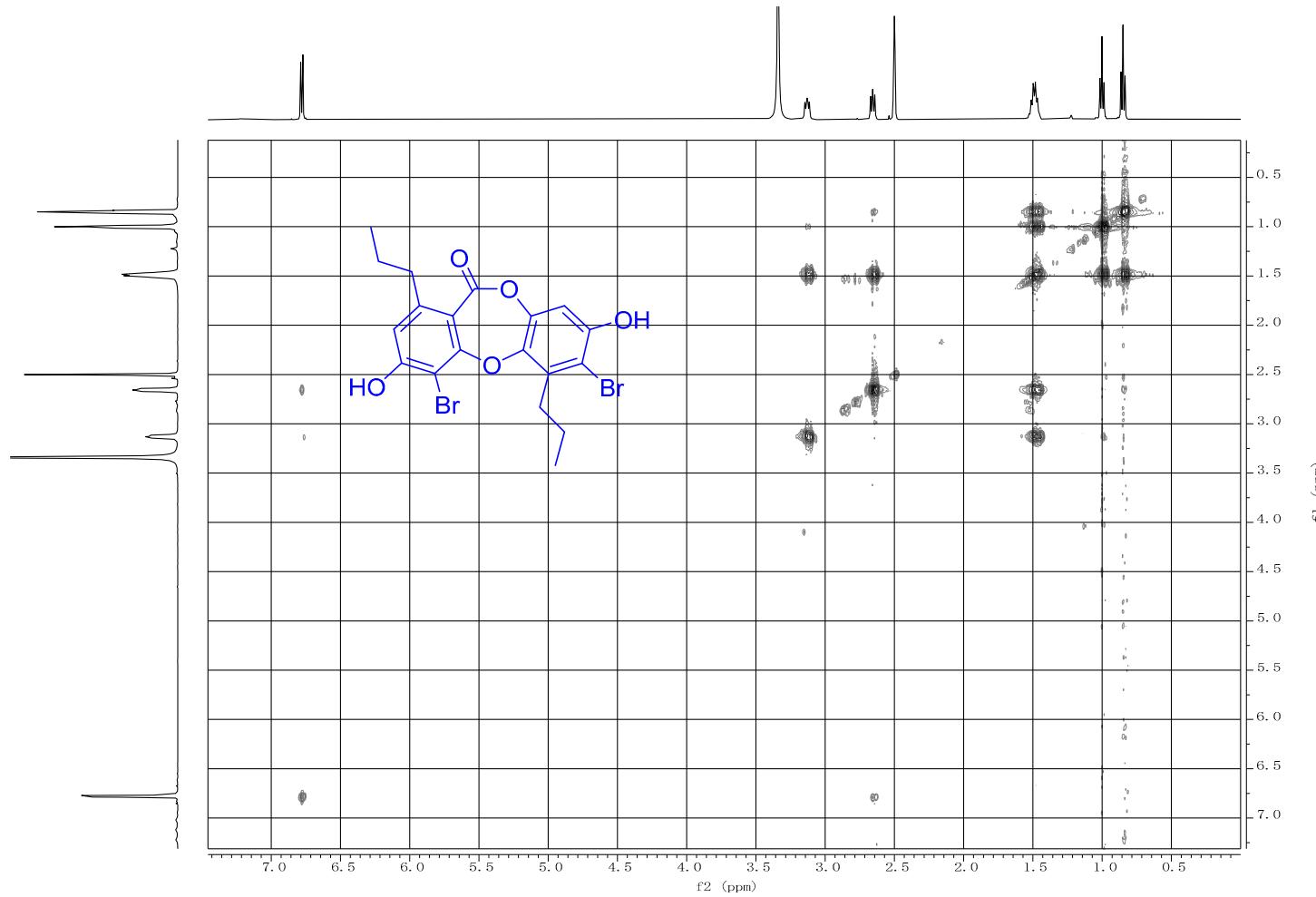


Figure S12. ^1H - ^1H COSY spectrum of **2** in $\text{DMSO}-d_6$

N-5-2 HMBC

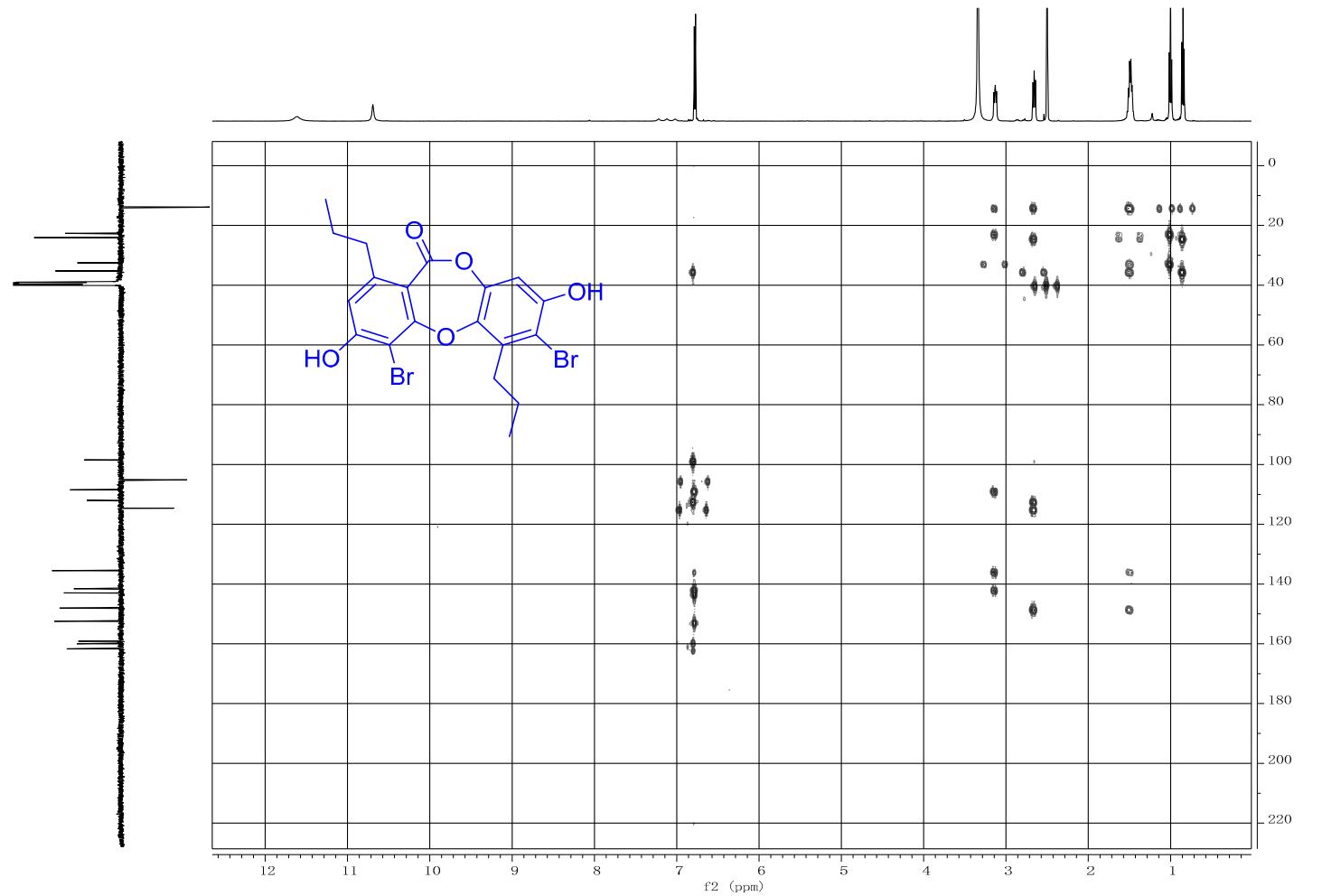


Figure S13. HMBC spectrum of **2** in $\text{DMSO}-d_6$

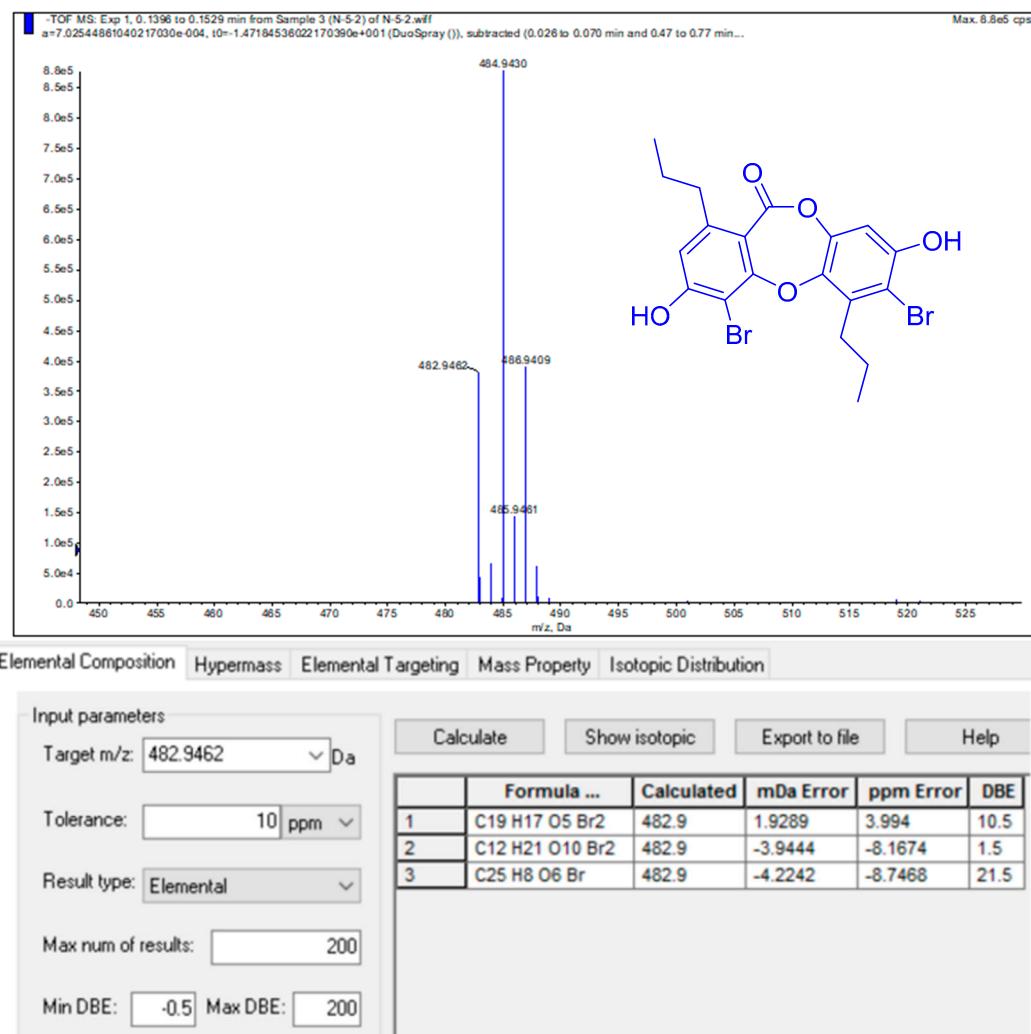


Figure S14. HRESIMS spectrum of **2**

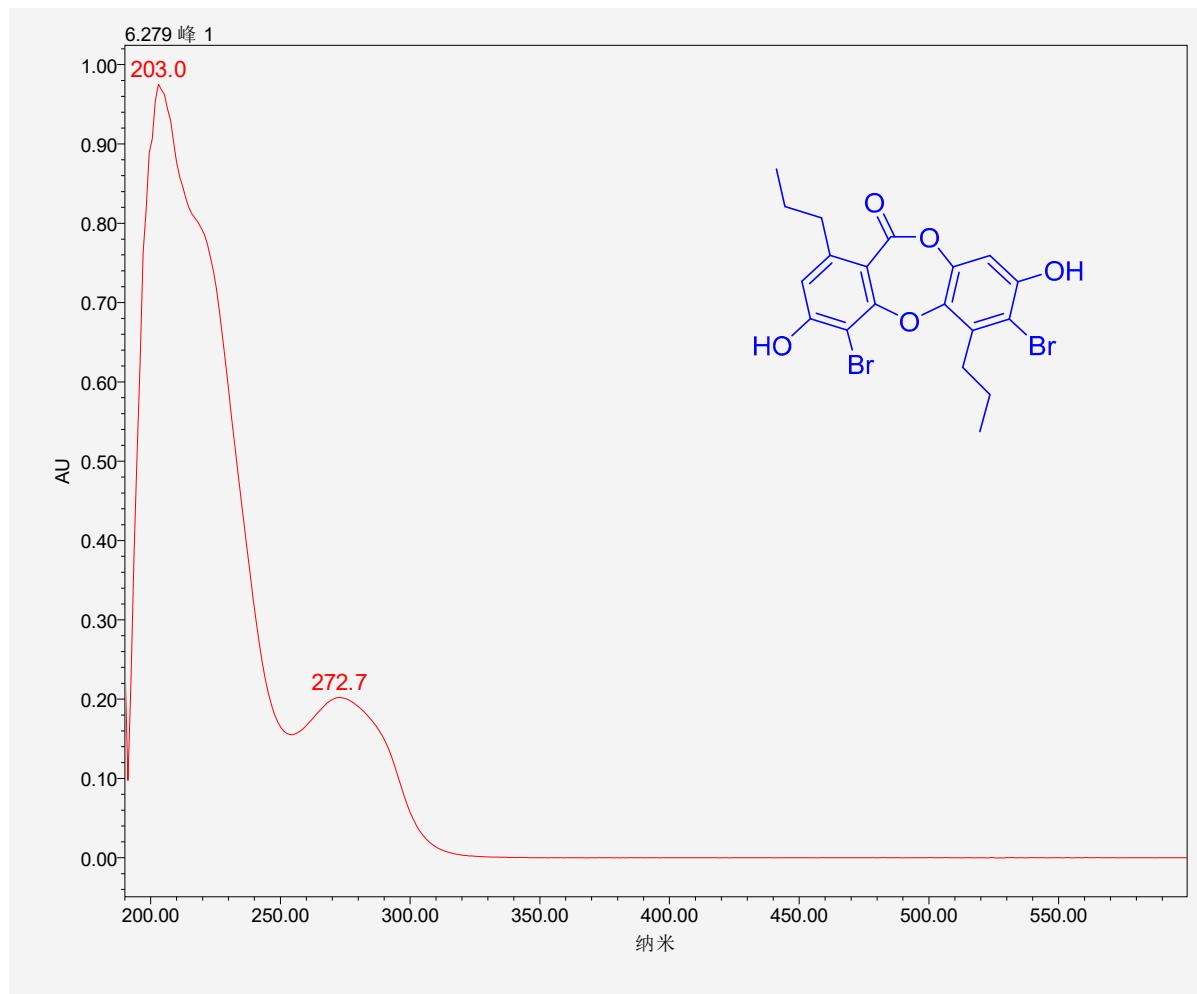


Figure S15. UV spectrum of **2**

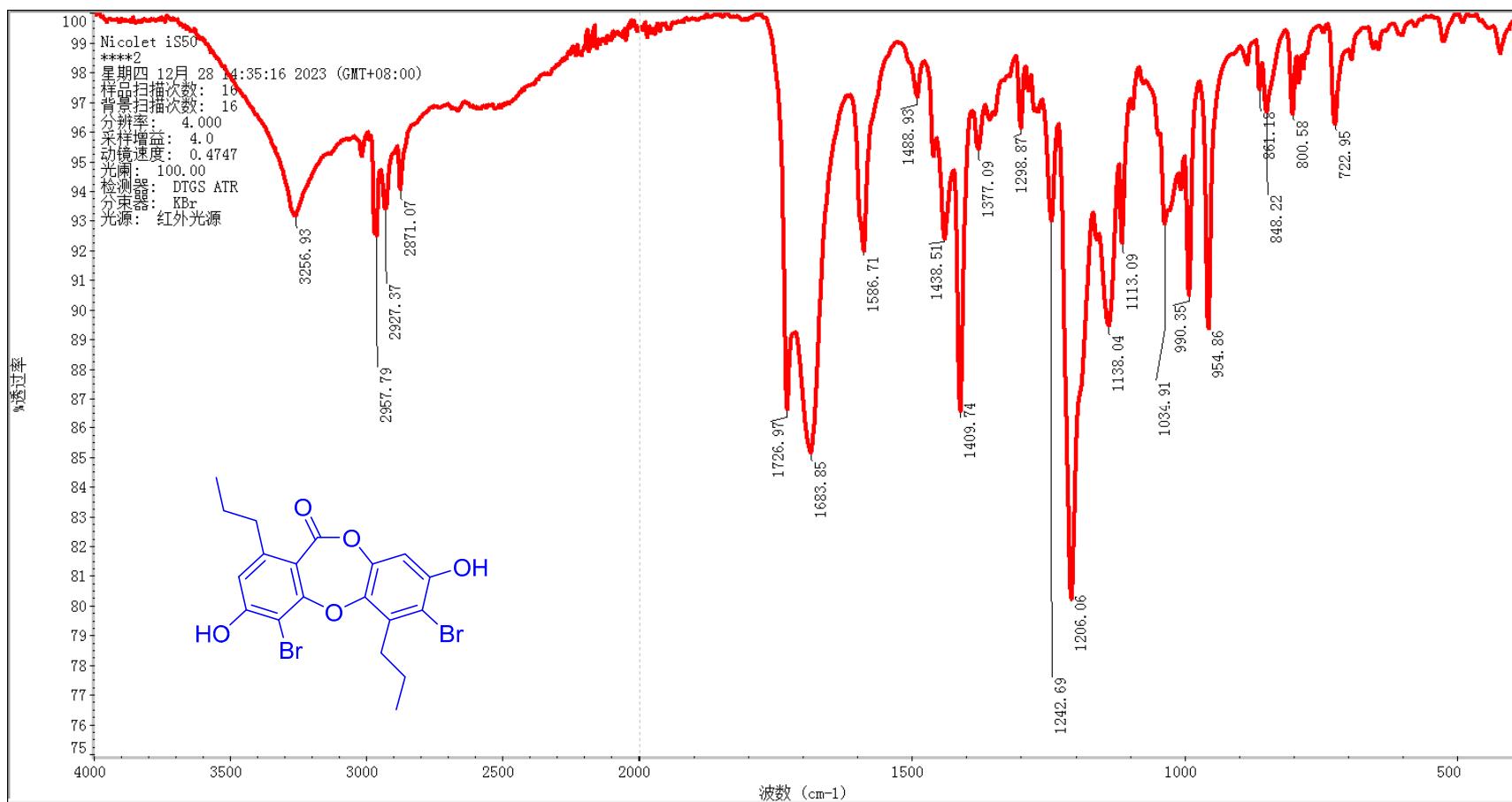


Figure S16. IR spectrum of 2

Table S3. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 3

No.	δ_{H}	δ_{C}	COSY	HMBC
1		112.3, C		
2		160.6, C		
3		99.0, C		
4		159.7, C		
5	6.80, s	115.3, C		C-1, C-3, C-4, C-8
6		148.1, C		
7		161.8, C		
8	2.70, t (7.6)	35.5, CH ₂		C-1, C-5, C-6, C-9, C-10
9	1.49, m	24.6, CH ₂		C-6, C-8, C-10
10	0.83, t (7.2)	14.1, CH ₃		C-8, C-9
1'		142.7, C		
2'		142.9, C		
3'		99.5, C		
4'		153.0, C		
5'	6.69, s	113.3, CH		C-1', C-4', C-5', C-7'
6'		134.8, C		
7'	2.90, t (7.8)	32.7, CH ₂		C-1', C-5', C-6', C-8', C-9'
8'	1.47, m	24.2, CH ₂		C-6', C-7', C-9'
9'	0.95, t (7.2)	14.1, CH ₃		C-7', C-8'

I-8-2 500 MHz DMSO

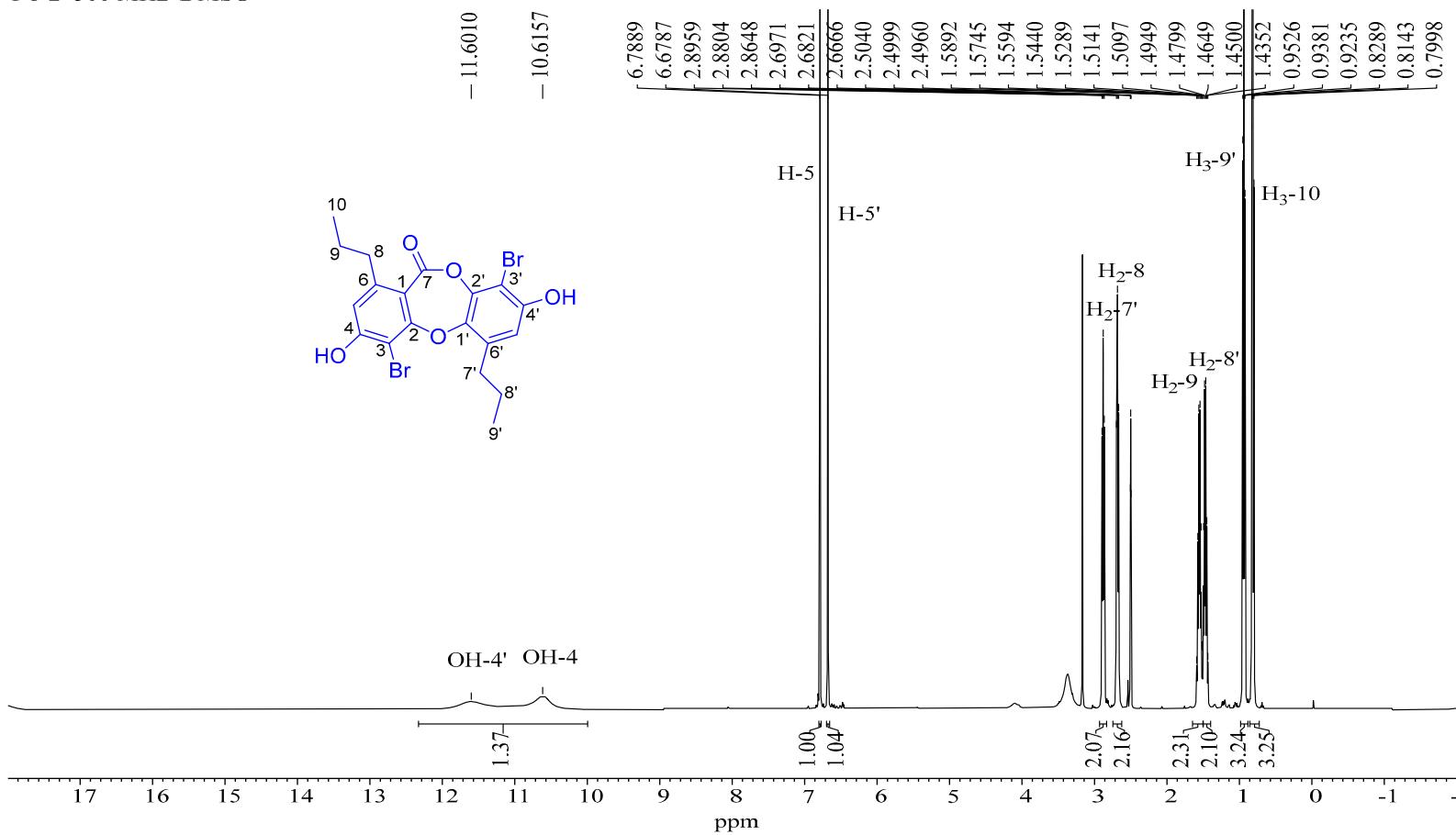


Figure S17. ^1H -NMR spectrum of **3** in $\text{DMSO}-d_6$ (500 MHz)

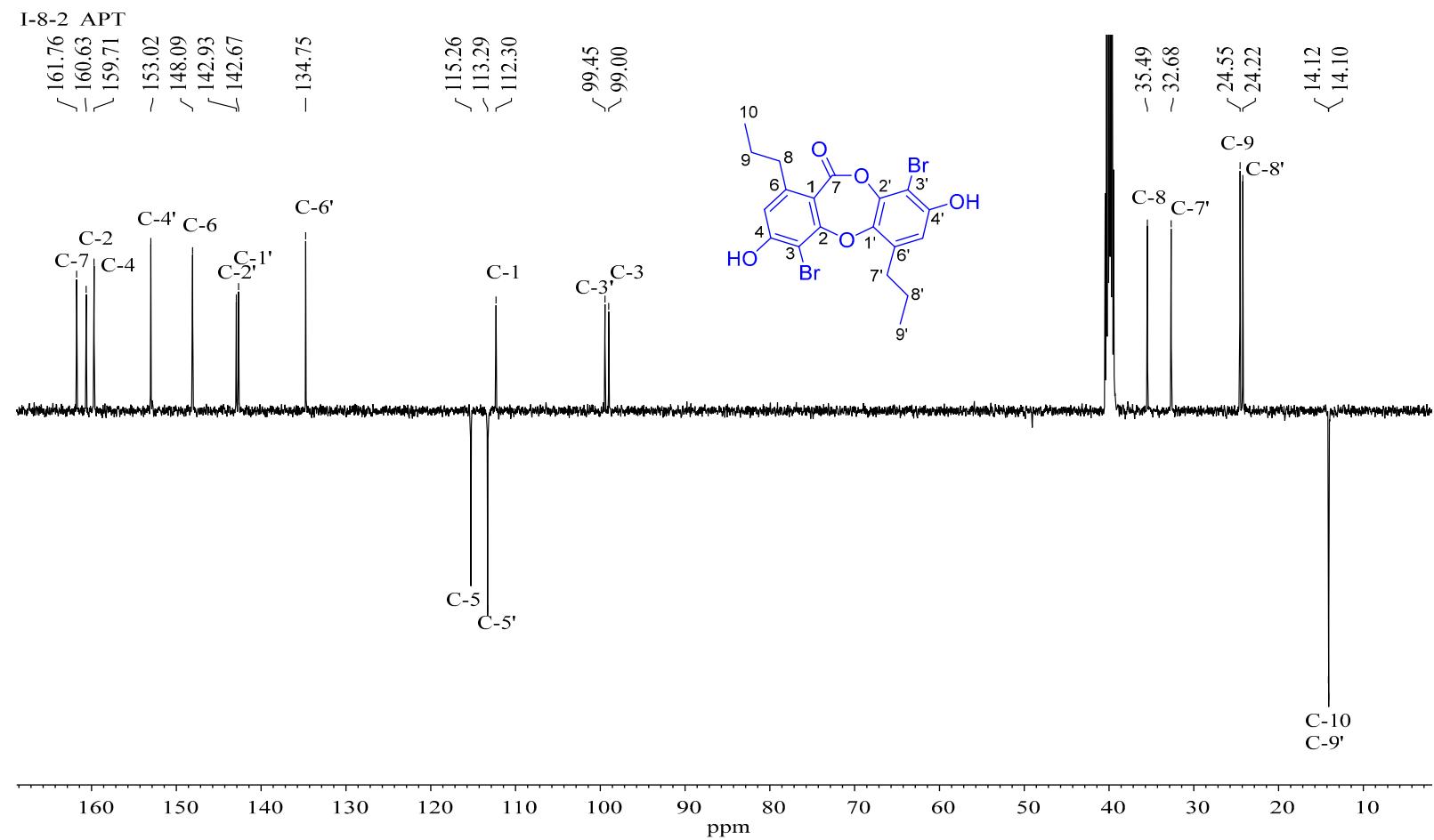


Figure S18. APT spectrum of **3** in $\text{DMSO}-d_6$ (125 MHz)

I-8-2 HSQC

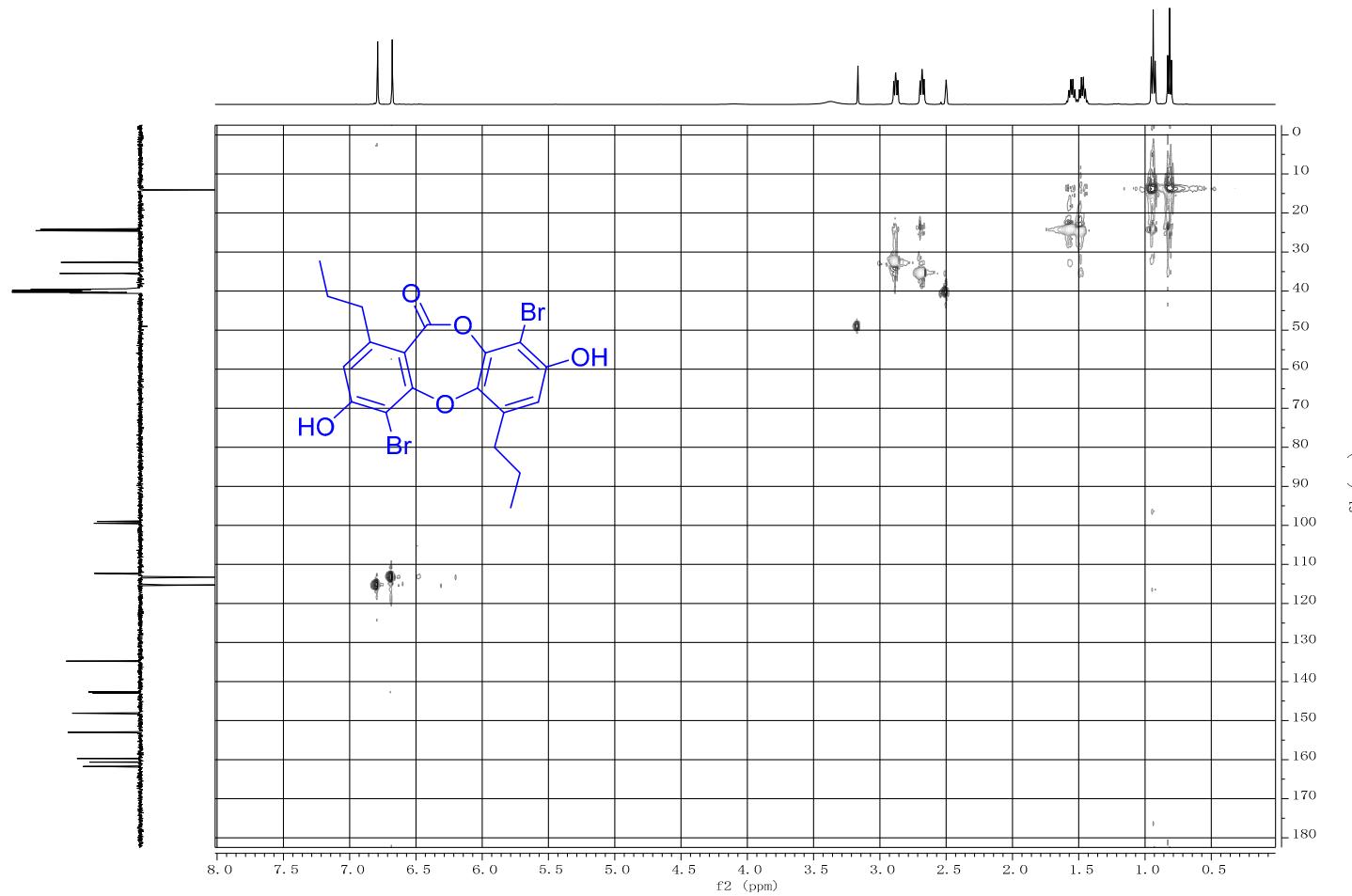


Figure S19. HSQC spectrum of **3** in $\text{DMSO}-d_6$

I-8-2 COSY

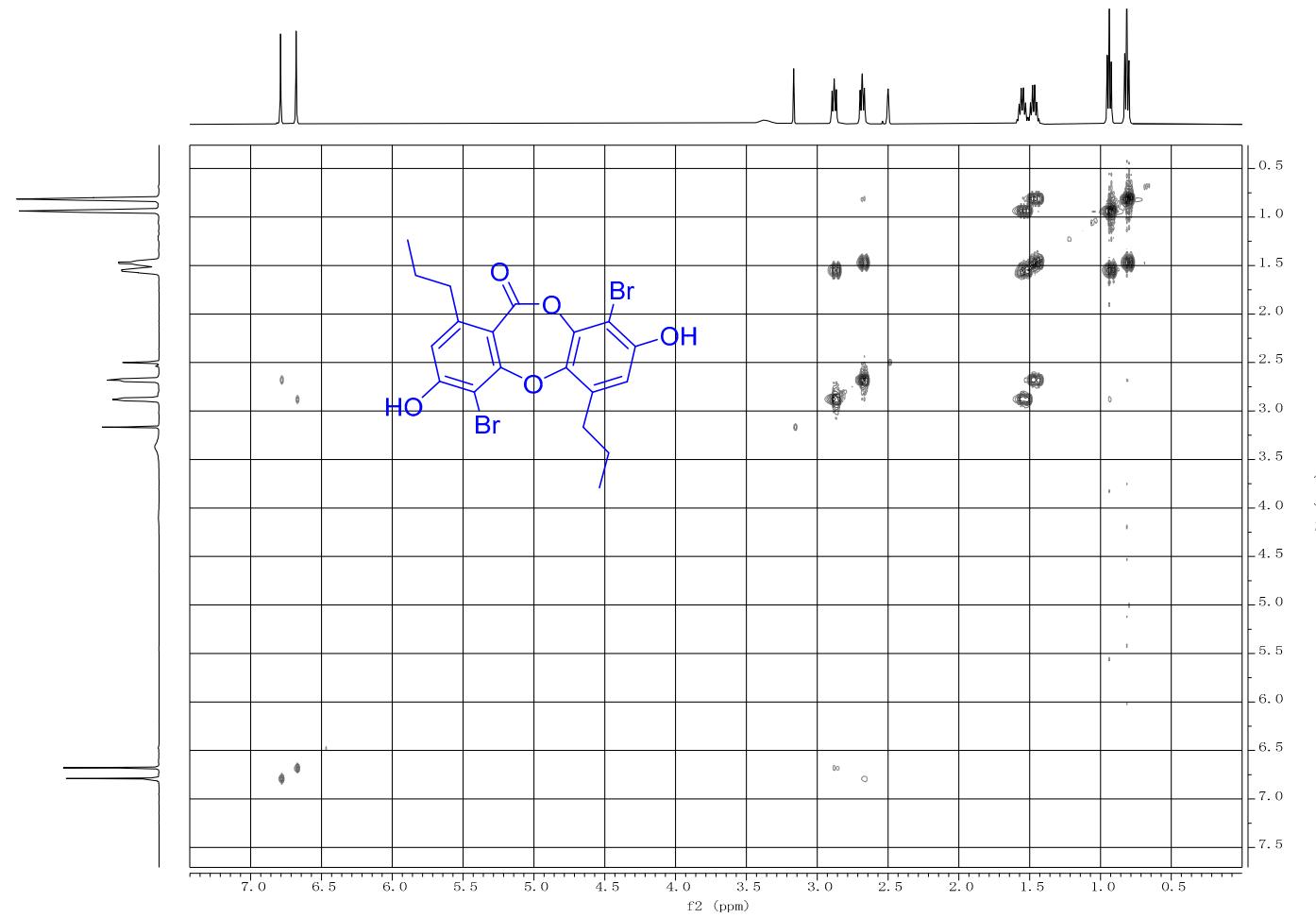


Figure S20. ^1H - ^1H COSY spectrum of **3** in $\text{DMSO}-d_6$

I-8-2 HMBC

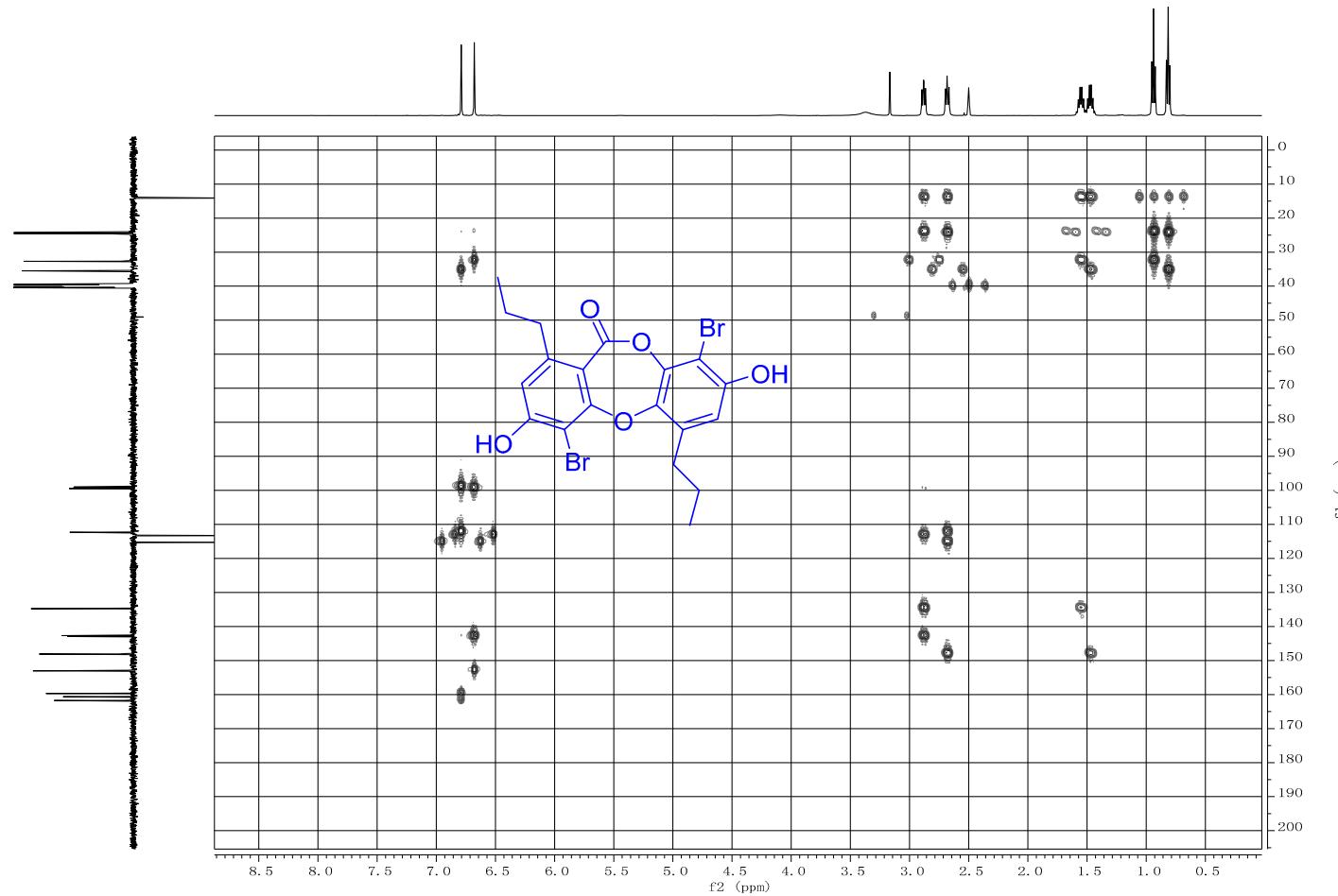


Figure S21. HMBC spectrum of **3** in $\text{DMSO}-d_6$

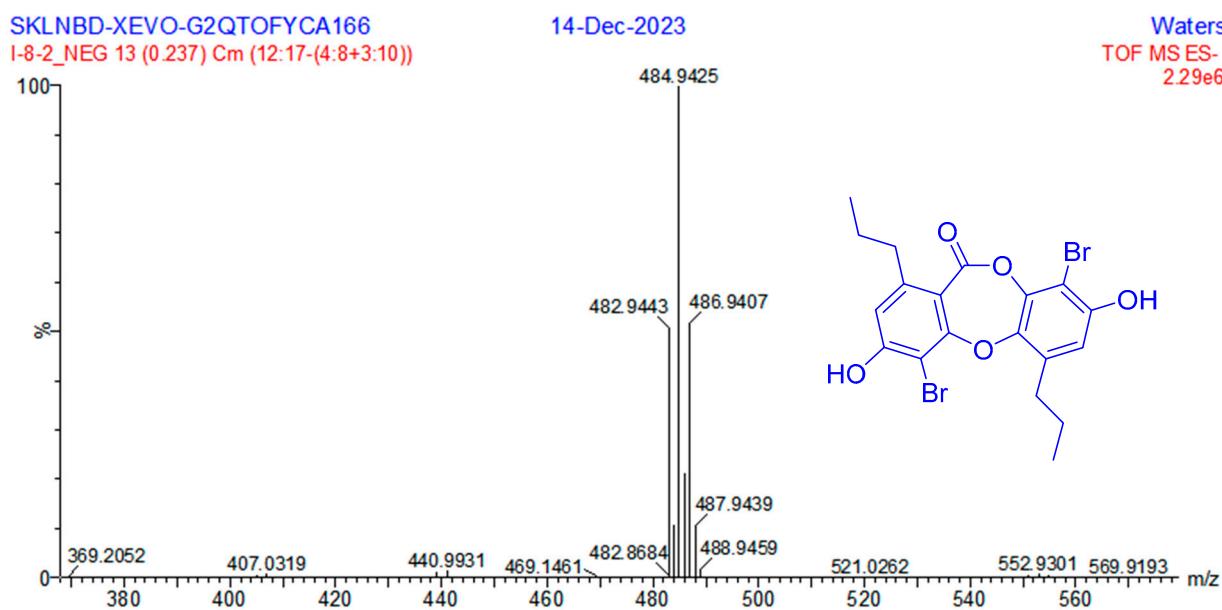


Figure S22. HRESIMS spectrum of 3

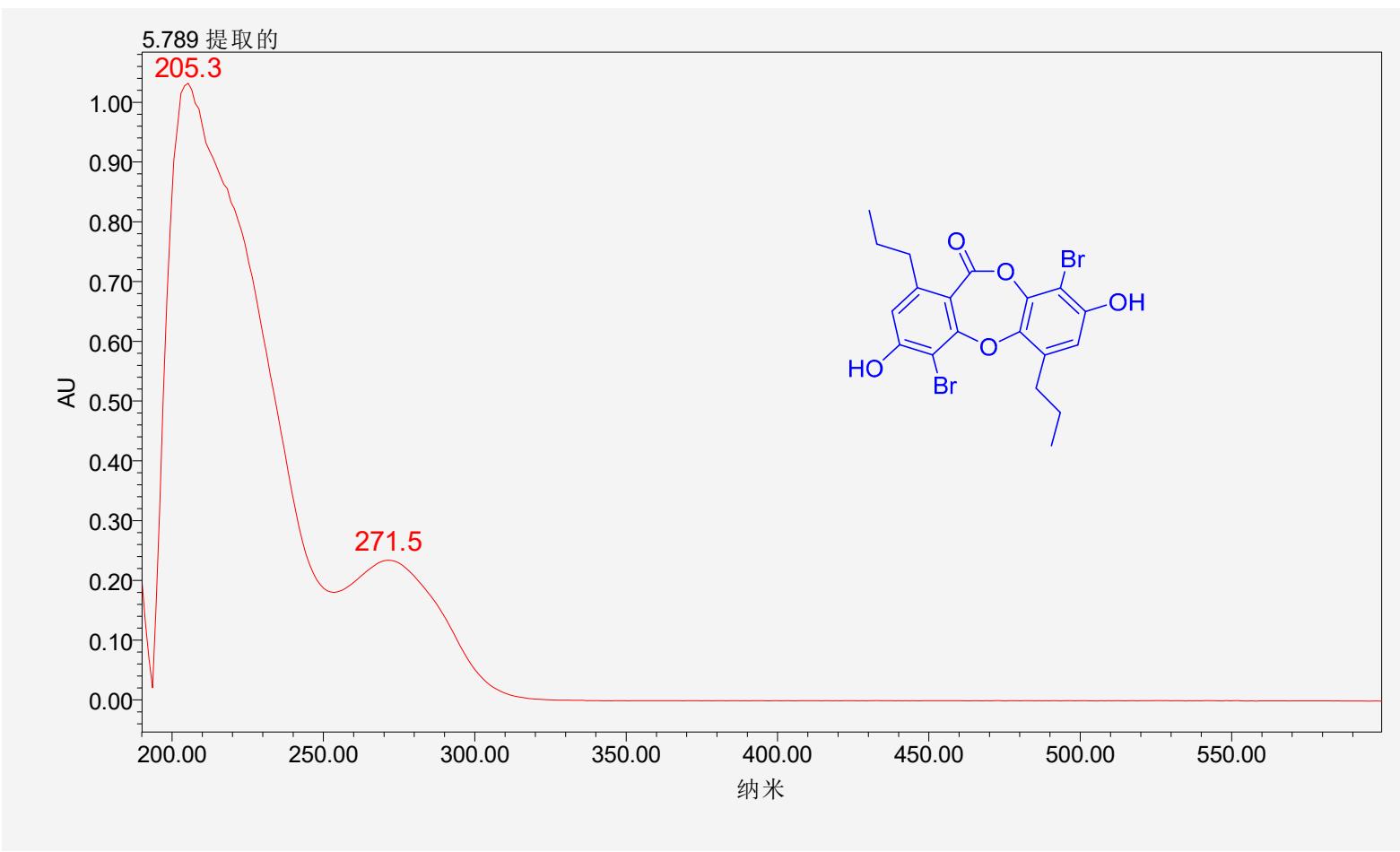


Figure S23. UV spectrum of **3**

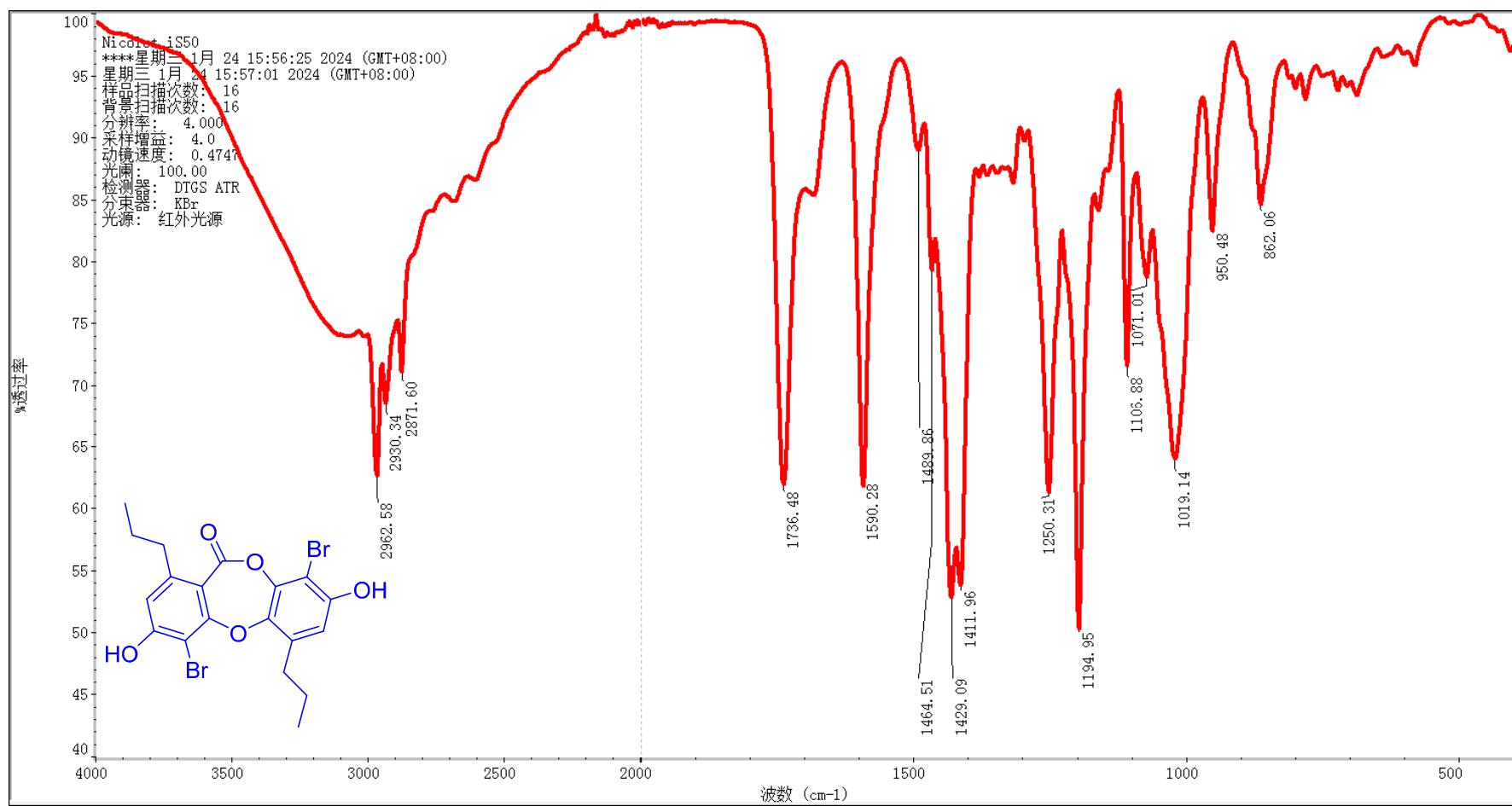


Figure S24. IR spectrum of 3

Table S4. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 4

No.	δ_{H}	δ_{C}	COSY	HMBC
1		112.9, C		
2		161.7, C		
3	6.71, s	105.2, CH		C-1, C-2 C-4, C-5
4		161.7, C		
5		110.3, C		
6		146.9, C		
7		161.9, C		
8	2.86, t (7.7)	35.7, CH_2	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.54, m	22.9, CH_2	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.86, t (7.3)	14.2, CH_3	H ₂ -9	C-8, C-9
1'		142.0, C		
2'		142.1, C		
3'		102.2, C		
4'		151.0, C		
5'		111.1, C		
6'		134.0, C		
7'	2.81, t (8.1)	32.6, CH_2	H ₂ -8'	C-1', C-5', C-6', C-8', C-9'
8'	1.51, m	22.5, CH_2	H ₂ -7', H ₃ -9'	C-6', C-7', C-9'
9'	0.98, t (7.3)	14.9, CH_3	H ₂ -8'	C-7', C-8'

N-6-5-Y 500 MHz DMSO

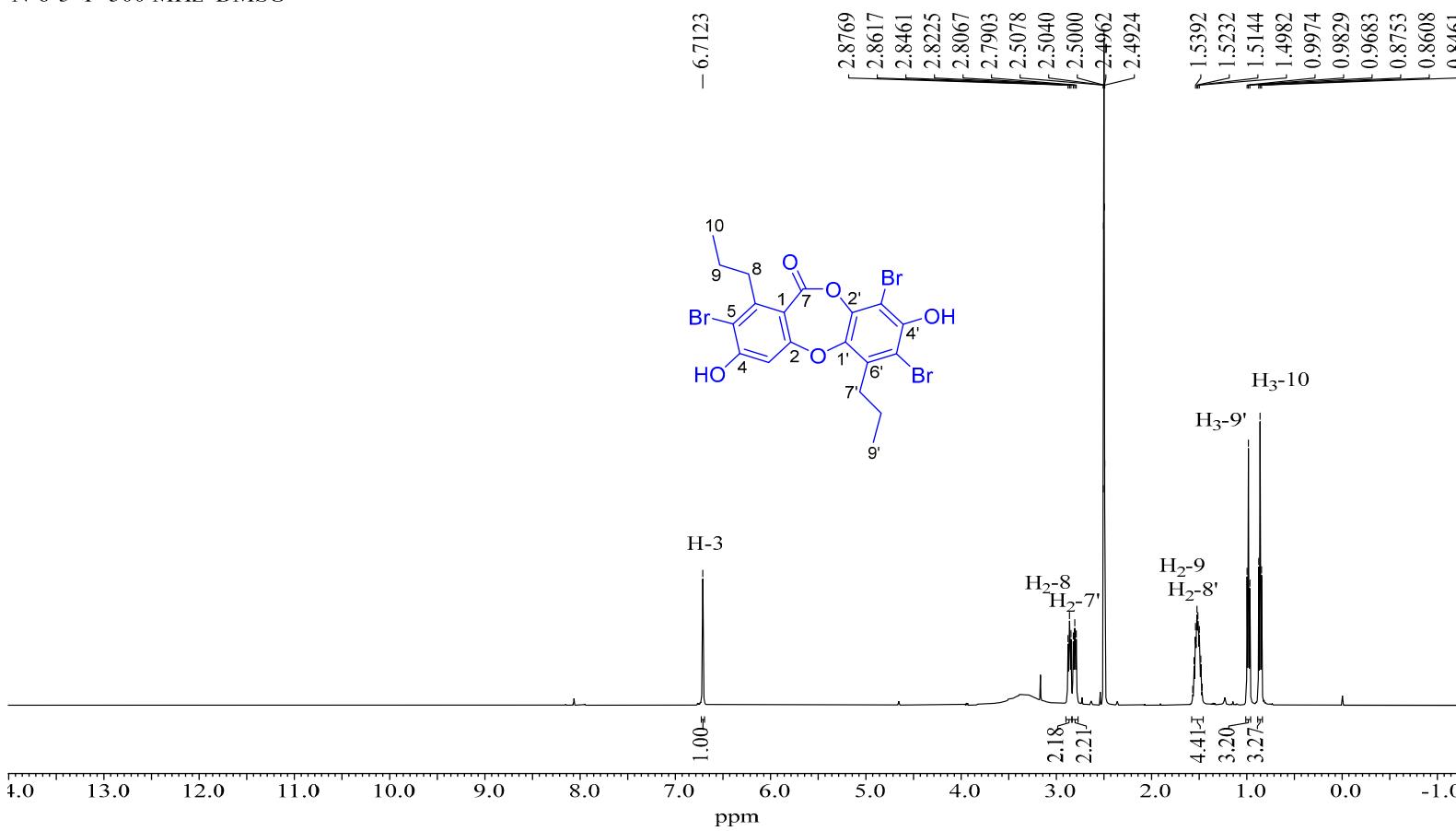


Figure S25. ^1H -NMR spectrum of **4** in $\text{DMSO}-d_6$ (500 MHz)

N-6-5-Y APT

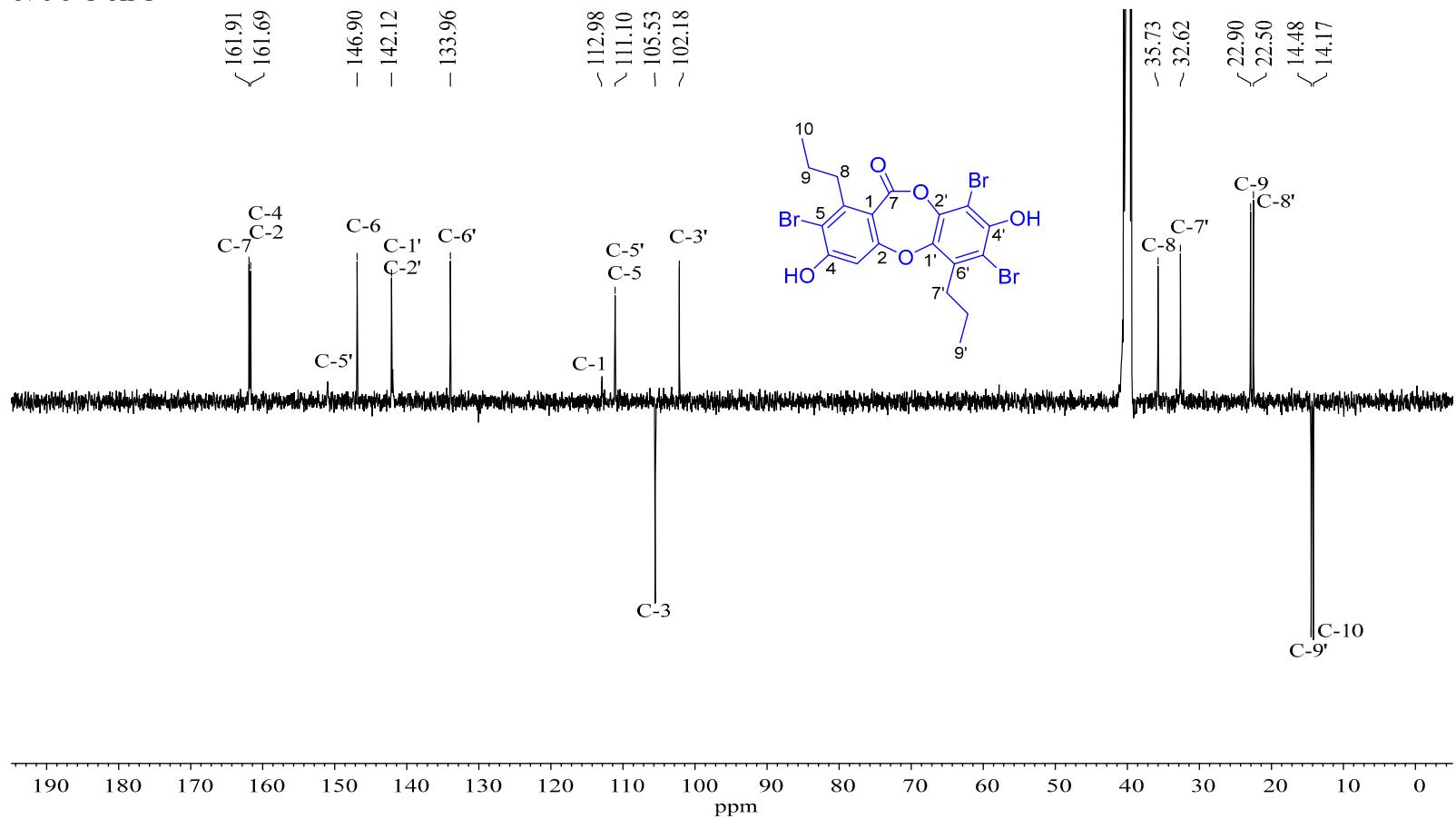


Figure S26. APT spectrum of **4** in DMSO-*d*6 (125 MHz)

N-6-5-Y HSQC

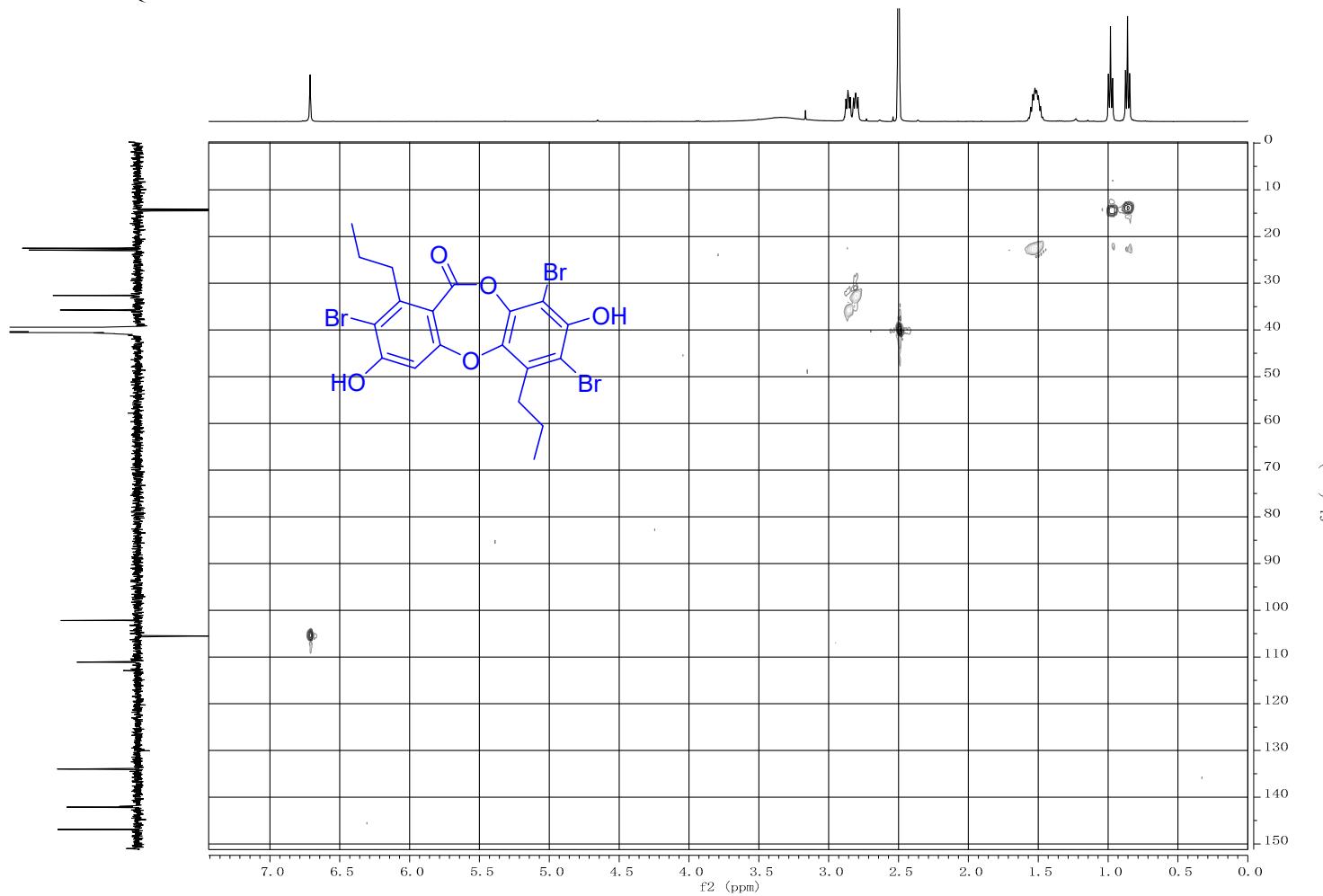


Figure S27. HSQC spectrum of **4** in $\text{DMSO}-d_6$

N-6-5-Y COSY

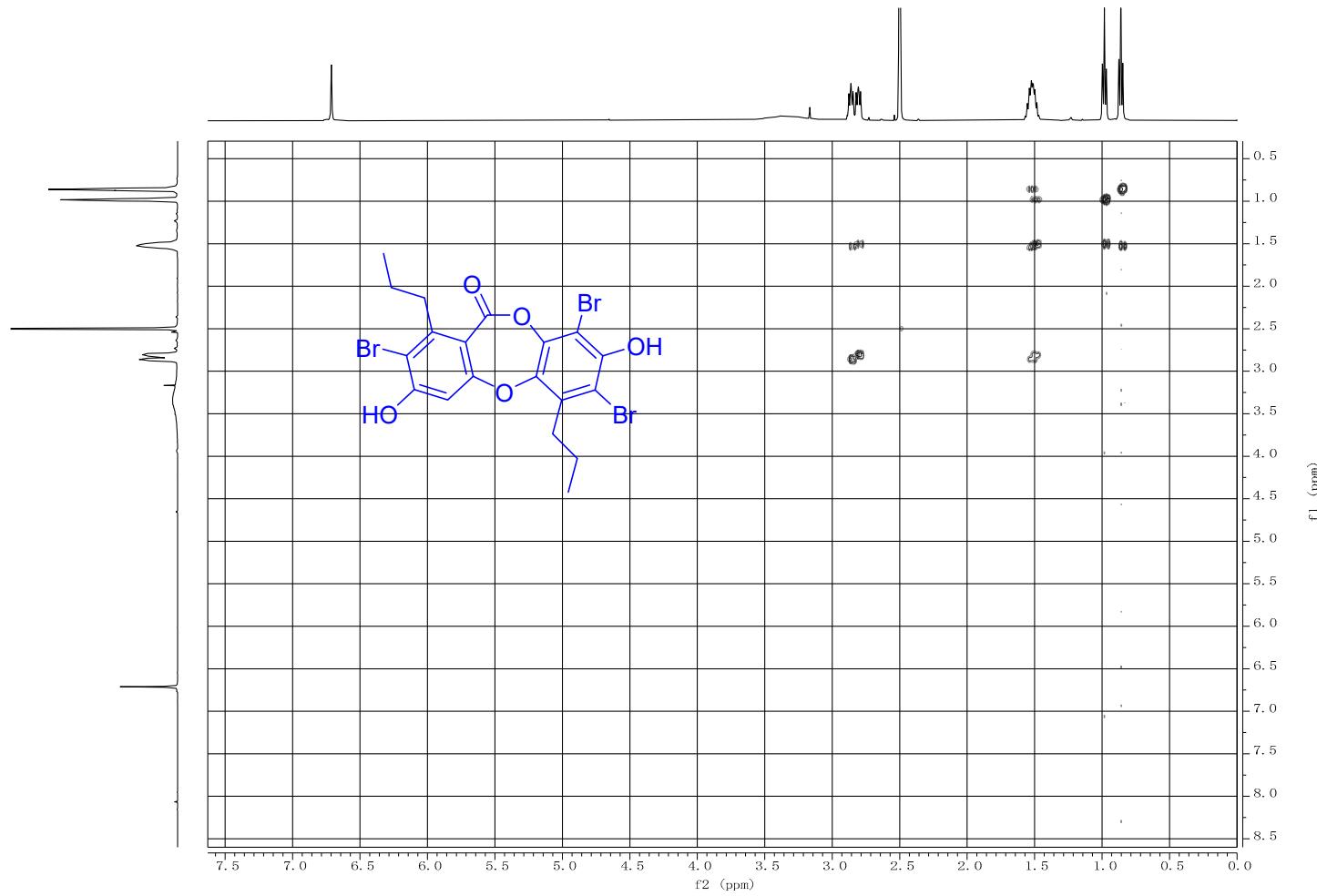


Figure S28. ^1H - ^1H COSY spectrum of **4** in $\text{DMSO}-d_6$

N-6-5-Y HMBC

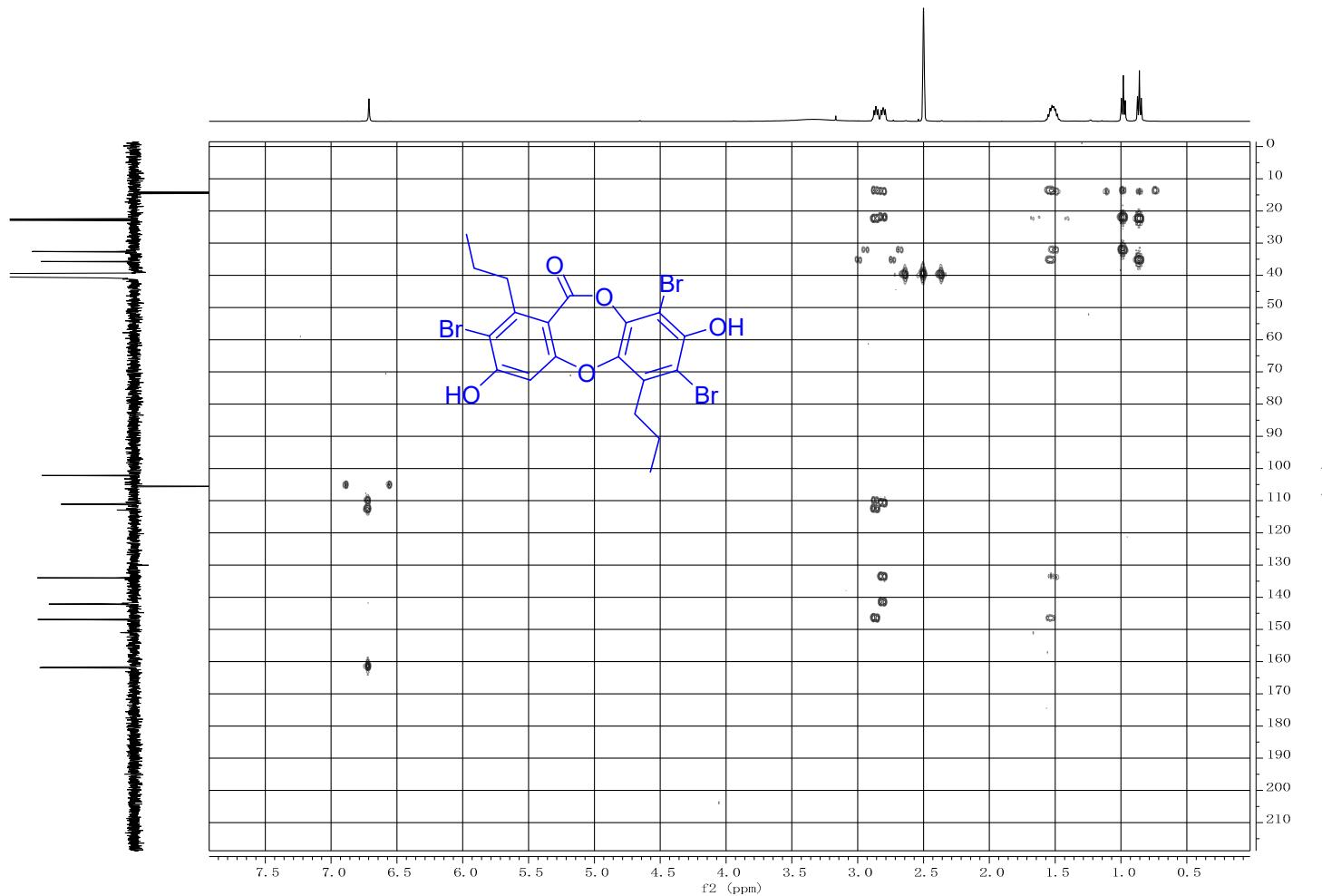
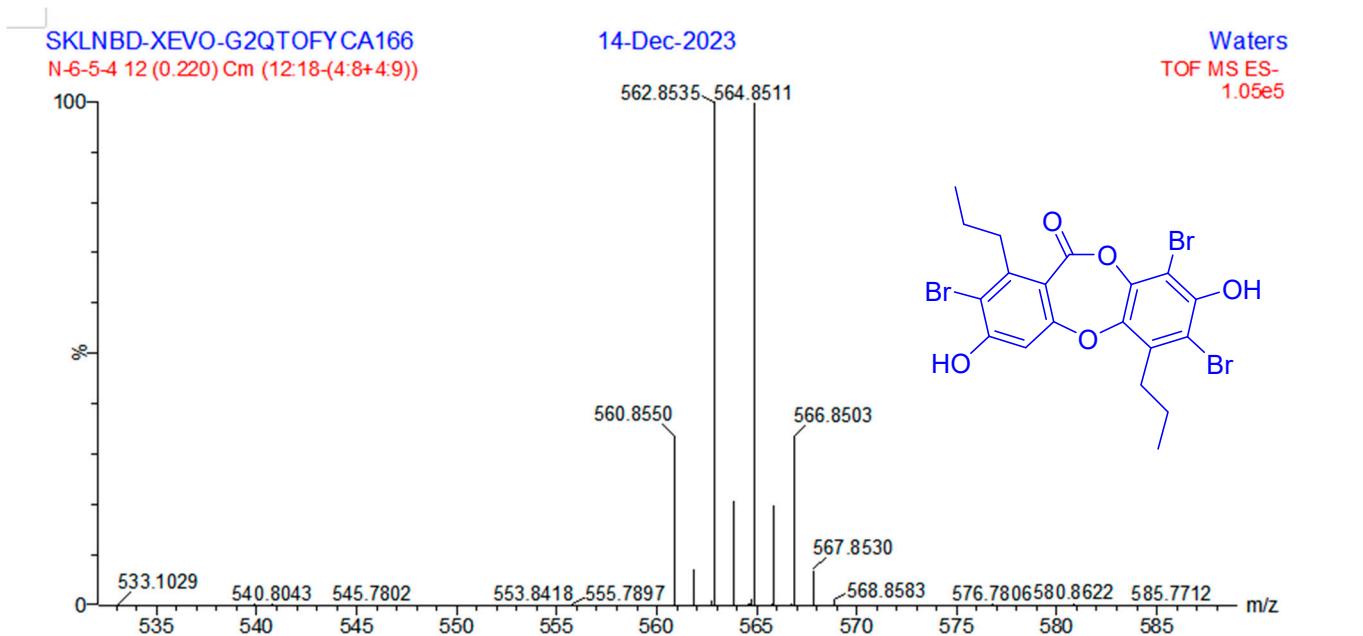


Figure S29. HMBC spectrum of **4** in $\text{DMSO}-d_6$



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
560.8550	560.8551	-0.1	-0.2	30.5	253.8	14.560	0.00	C ₃₂ H ₃ O Br ₂
	560.8548	0.2	0.4	10.5	239.2	0.000	100.00	C ₁₉ H ₁₆ O ₅ Br ₃
	560.8574	-2.4	-4.3	-0.5	254.7	15.479	0.00	C ₇ H ₁₅ O ₁₉ Br ₂
	560.8577	-2.7	-4.8	19.5	258.7	19.441	0.00	C ₂₀ H ₂ O ₁₅ Br

Figure S30. HRESIMS spectrum of 4

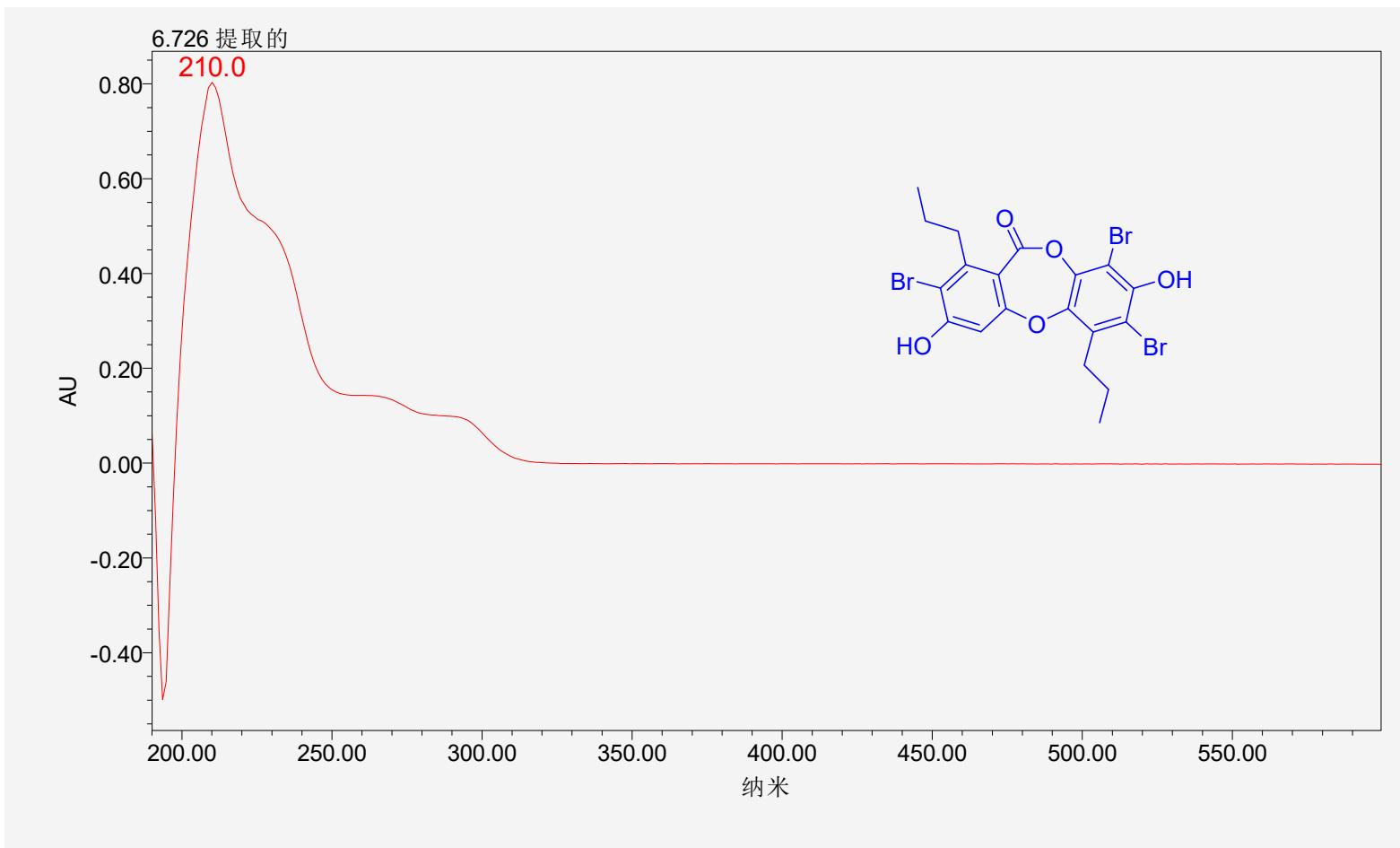


Figure S31. UV spectrum of 4

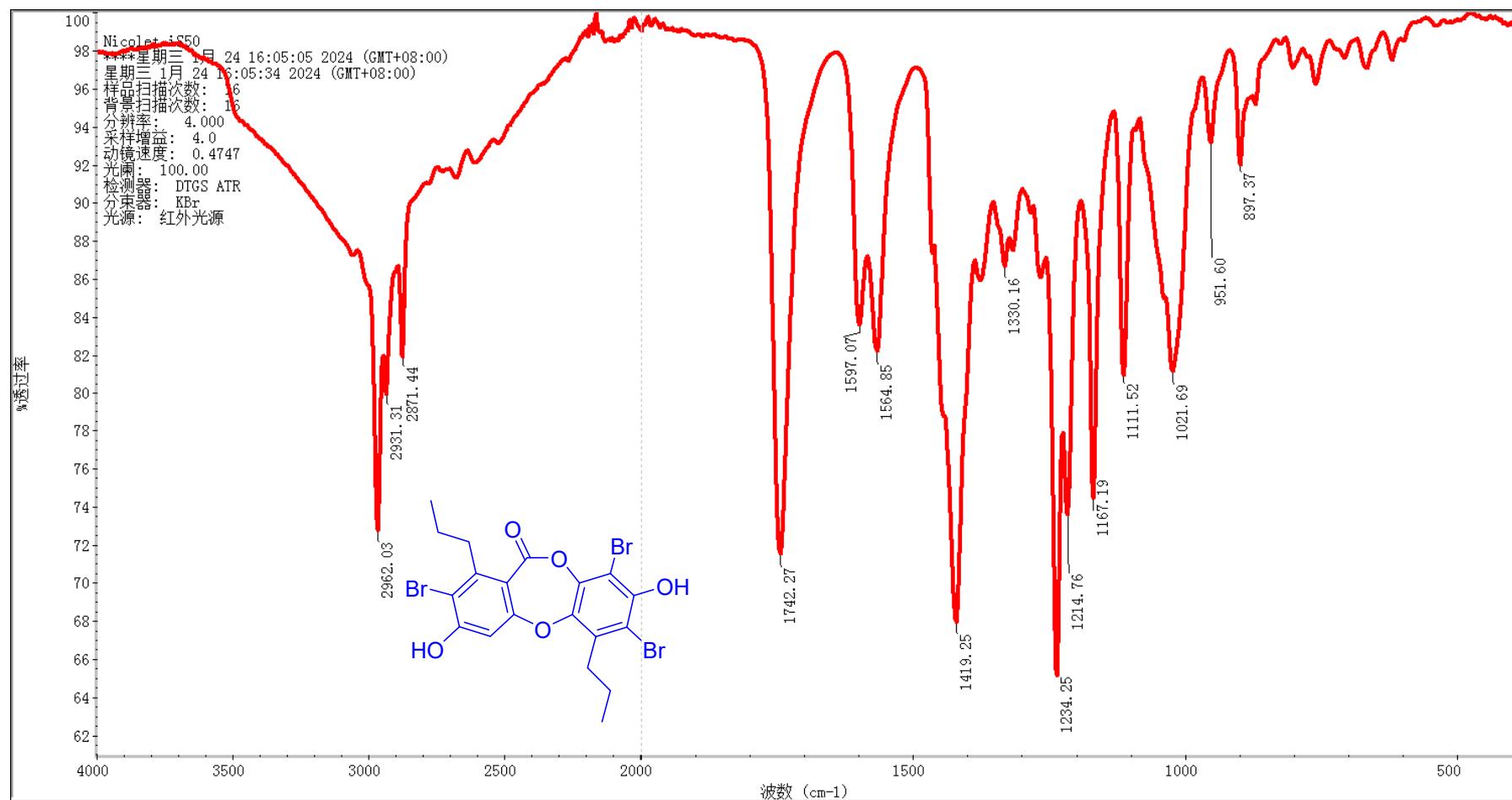


Figure S32. IR spectrum of 4

Table S5. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 5

No.	δ_{H}	δ_{C}	COSY	HMBC
1		113.6, C		
2		159.3, C		
3		101.3, C		
4		159.3, C		
5		112.8, C		
6		145.8, C		
7		162.0, C		
8	3.11, t (8.0)	36.9, CH_2		C-1, C-5, C-6, C-9, C-10
9	1.59, m	22.9, CH_2		C-6, C-8, C-10
10	0.88, t (7.3)	14.3, CH_3		C-8, C-9
1'		142.0, C		
2'		143.4, C		
3'	6.80, s	105.6, C		C-1, C-2, C-4, C-5
4'		153.0, C		
5'		108.9, C		
6'		135.9, C		
7'	2.76, t (7.8)	33.0, CH_2		C-1', C-5', C-6', C-8', C-9'
8'	1.48, m	23.1, CH_2		C-6', C-7', C-9'
9'	1.01, t (7.3)	14.4, CH_3		C-7', C-8'

N-6-6 500 MHz DMSO

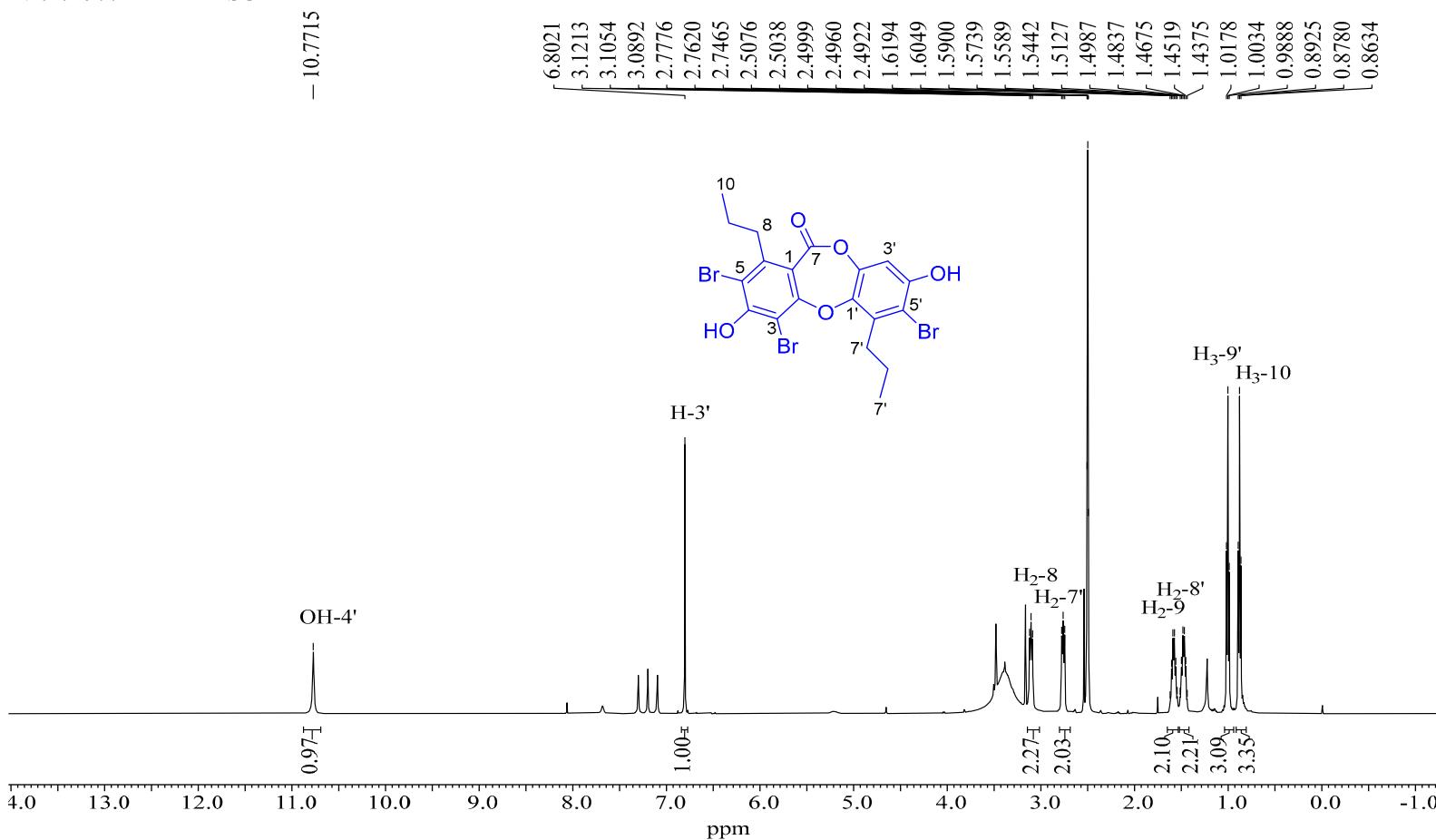


Figure S33. ^1H -NMR spectrum of **5** in $\text{DMSO}-d_6$ (500 MHz)

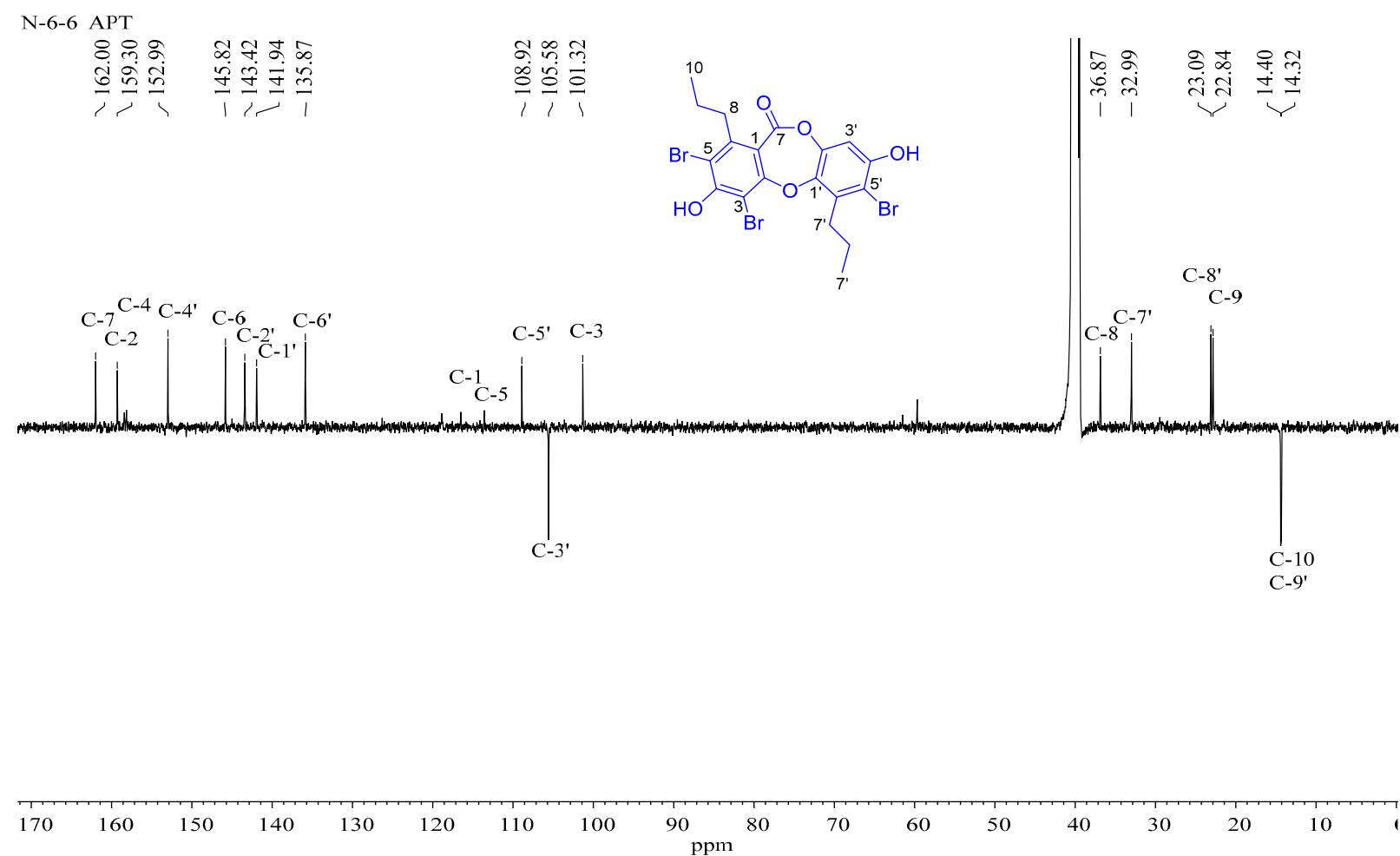


Figure S34. APT spectrum of **5** in $\text{DMSO}-d_6$ (125 MHz)

N-6-6 HSQC

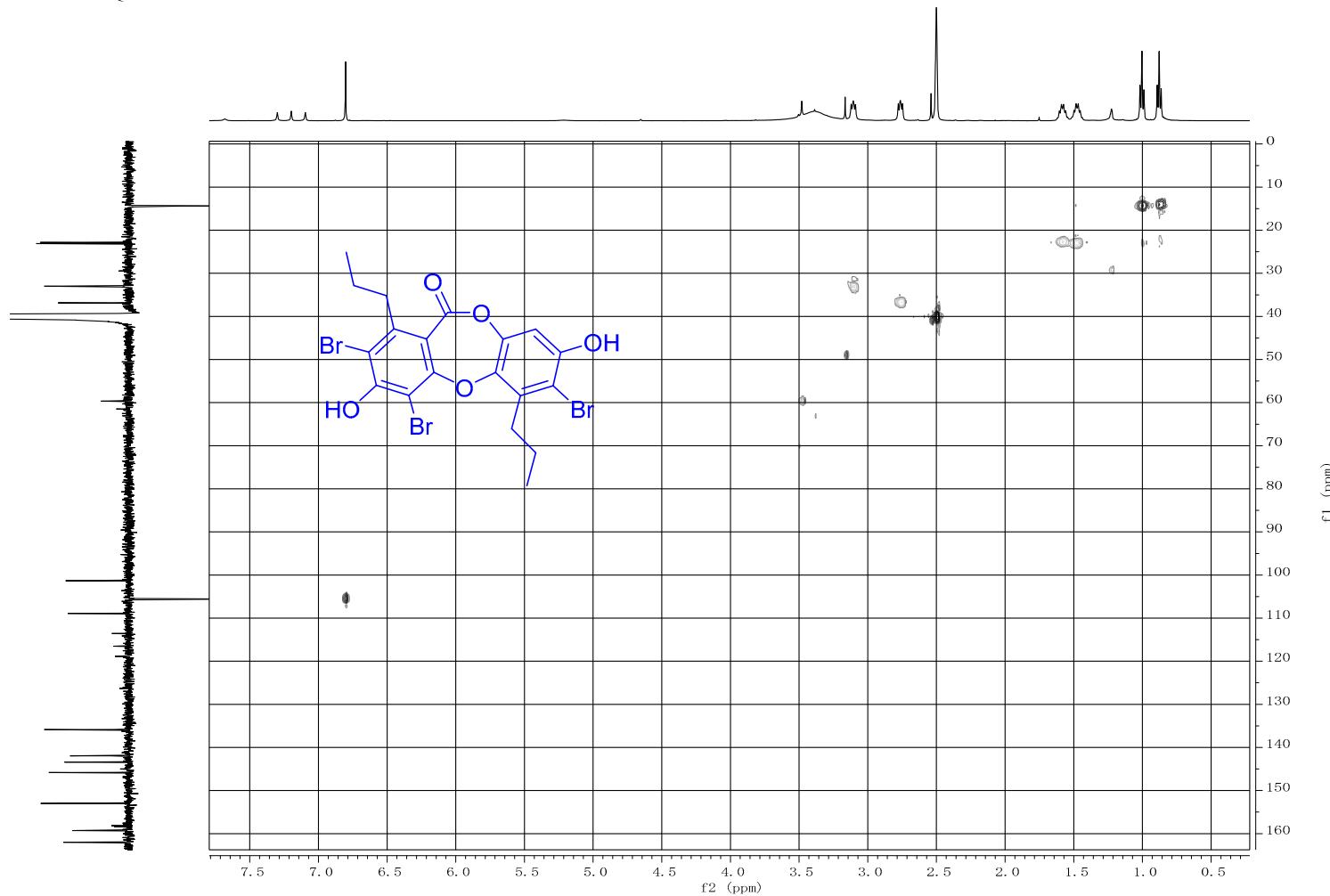


Figure S35. HSQC spectrum of **5** in $\text{DMSO}-d_6$

N-6-6 COSY

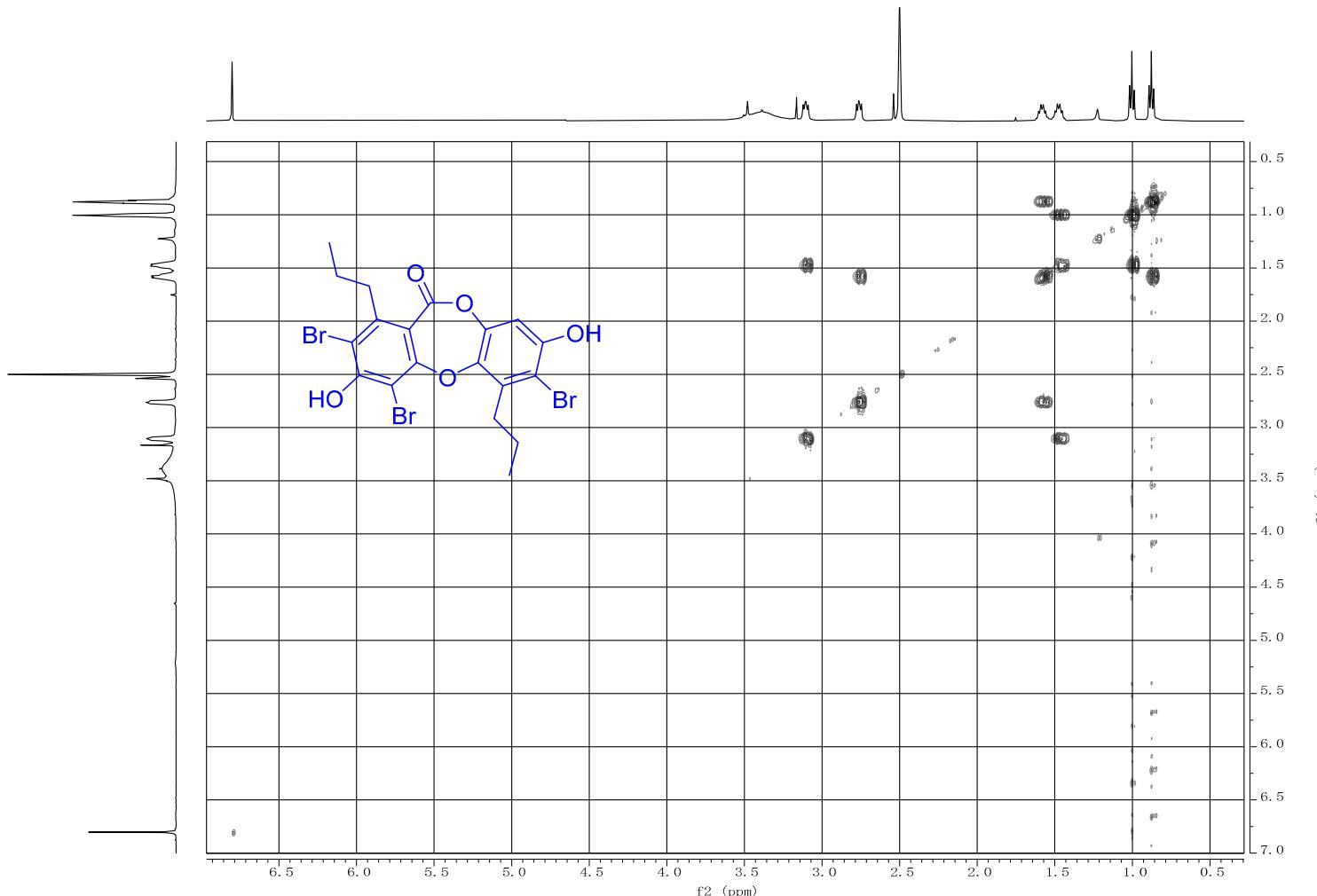


Figure S36. ^1H - ^1H COSY spectrum of **5** in $\text{DMSO}-d_6$

N-6-6 HMBC

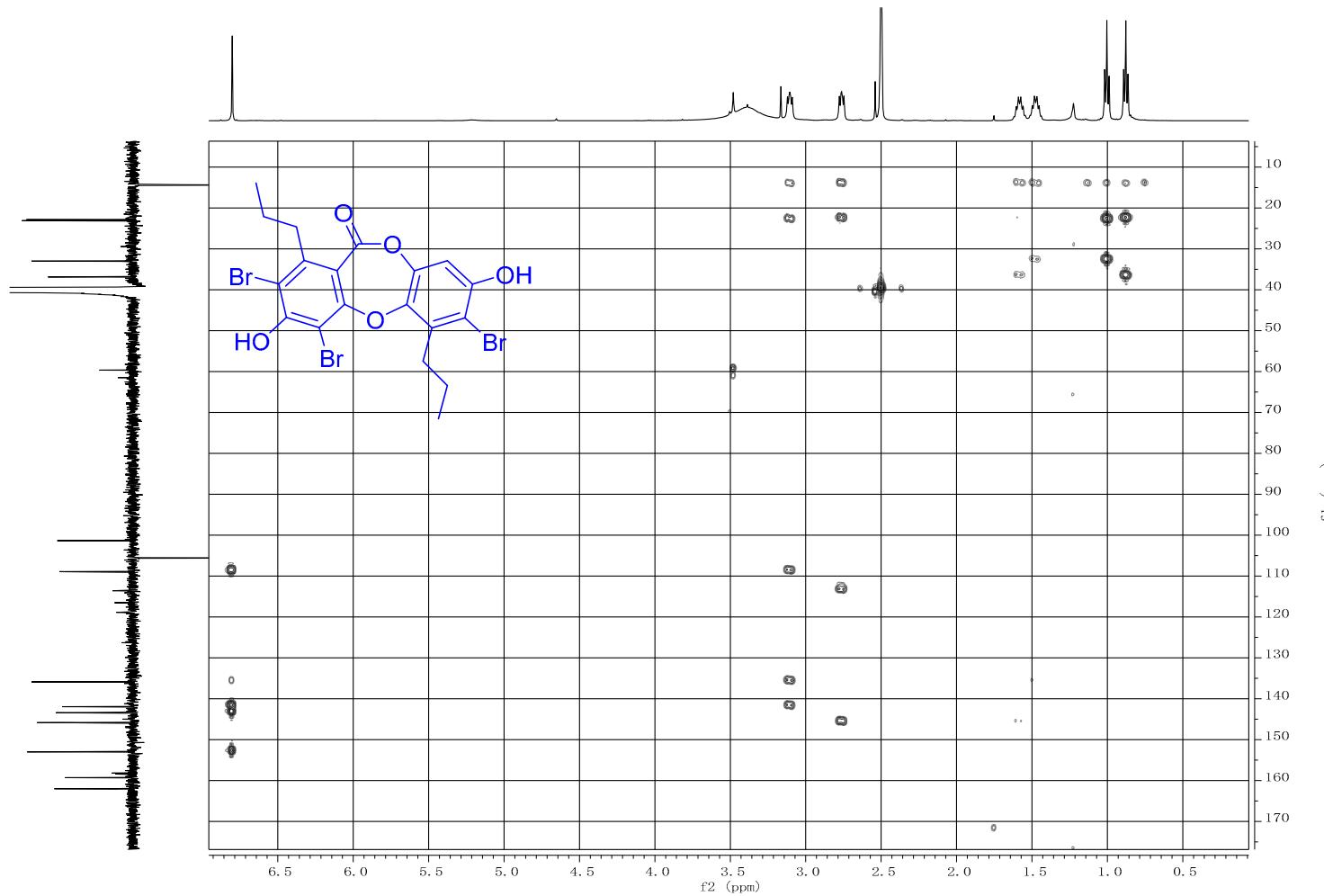
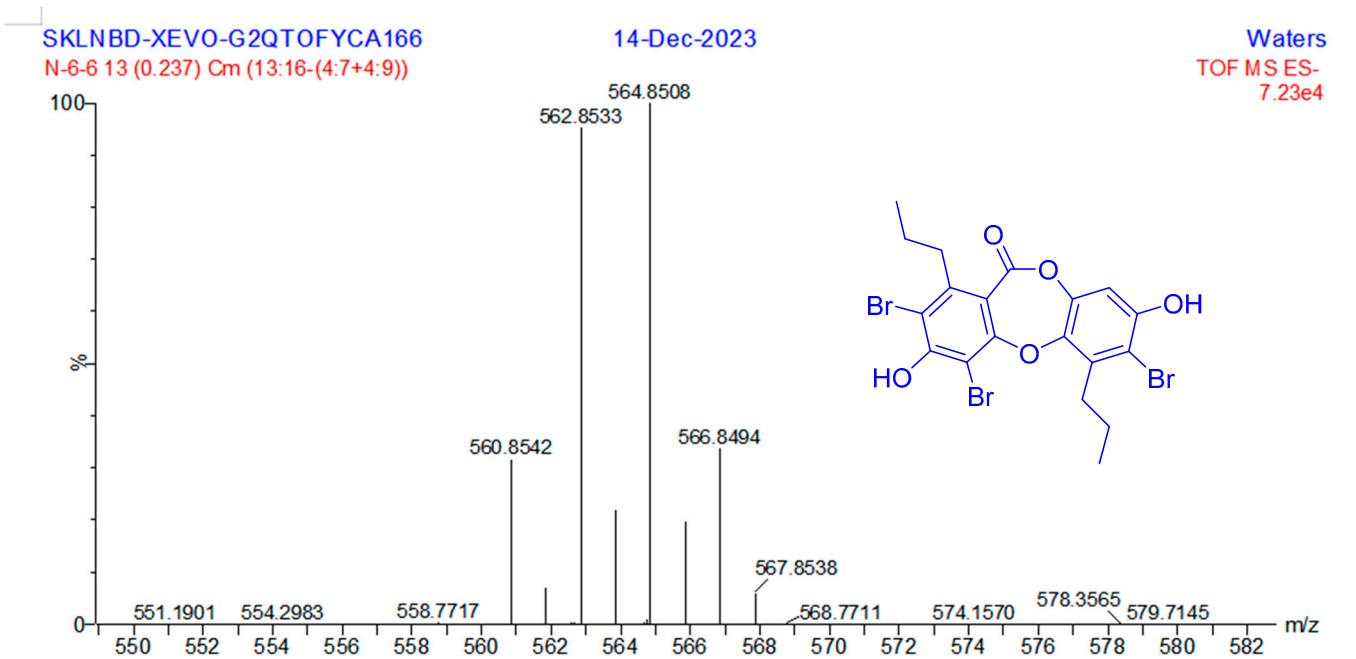


Figure S37. HMBC spectrum of **5** in $\text{DMSO}-d_6$



Mass	<u>Calc.</u> Mass	mDa	PPM	DBE	i-FIT	Norm	<u>Conf(%)</u>	Formula
560.8542	560.8548	-0.6	-1.1	10.5	216.0	0.000	100.00	C ₁₉ H ₁₆ O ₅ Br ₃
	560.8551	-0.9	-1.6	30.5	229.1	13.105	0.00	C ₃₂ H ₃ OBr ₂
	560.8516	2.6	4.6	8.5	229.9	13.979	0.00	C ₁₄ H ₁₁ O ₁₄ Br ₂

Figure S38. HRESIMS spectrum of 5

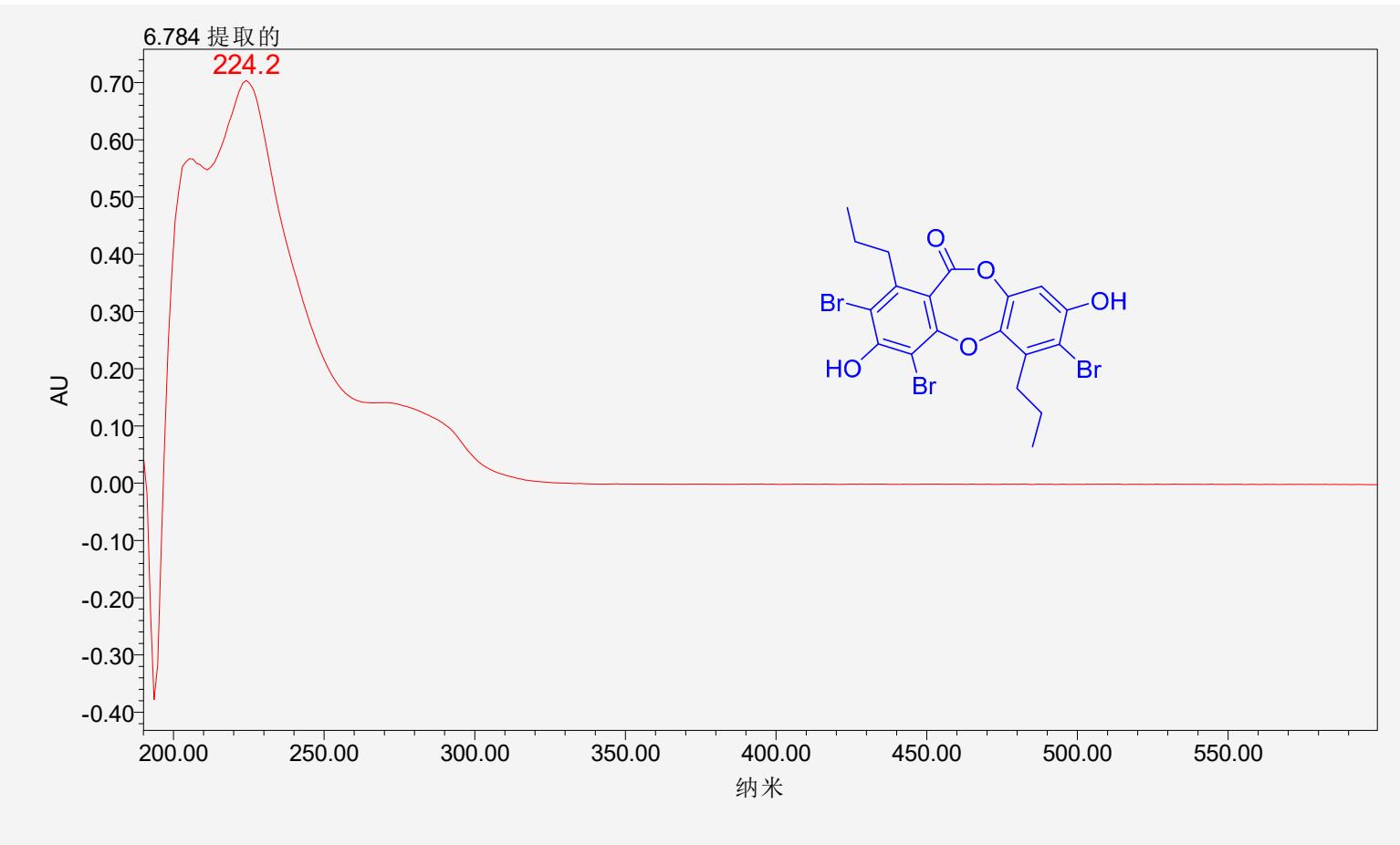


Figure S39. UV spectrum of **5**

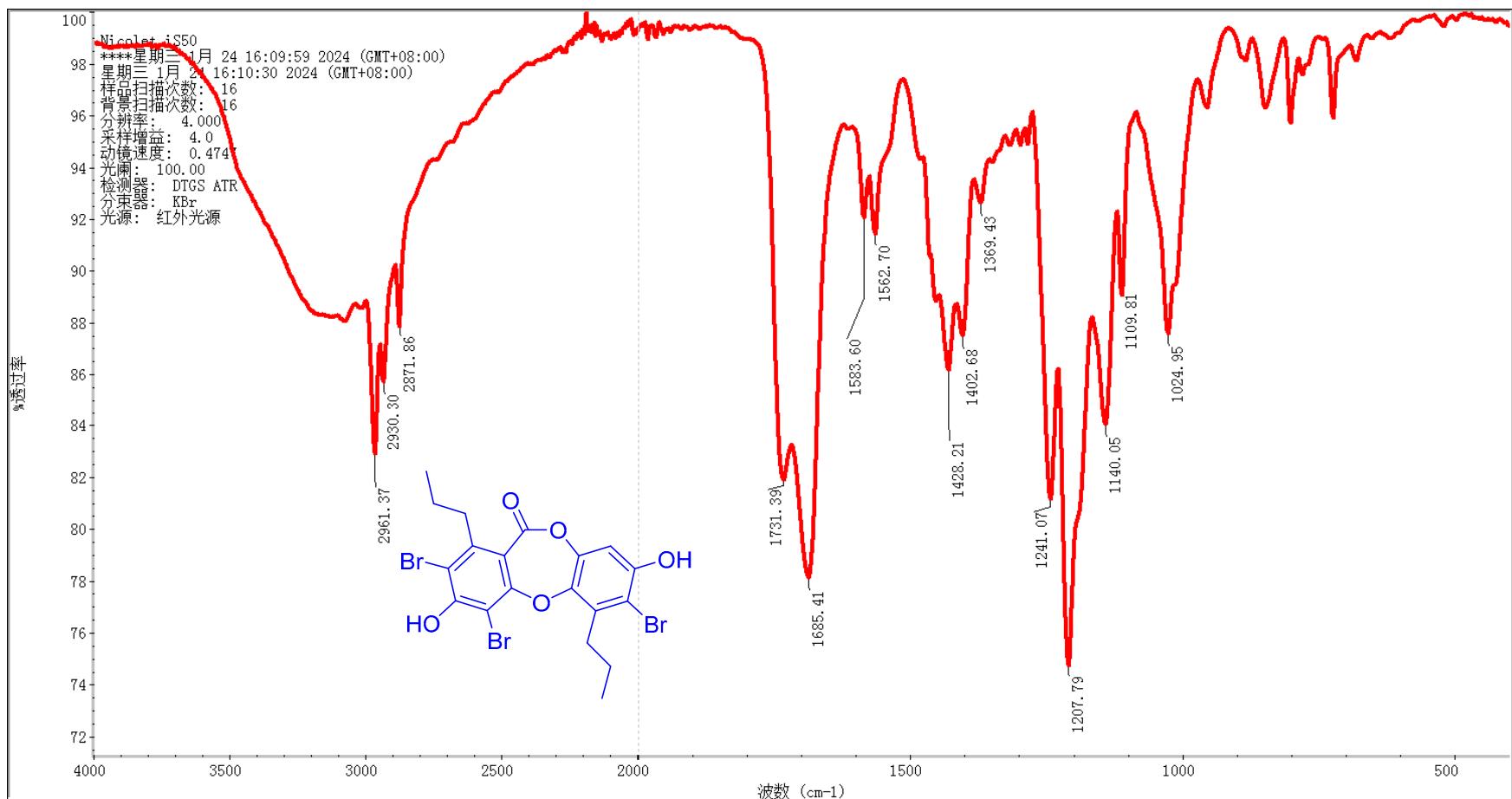


Figure S40. IR spectrum of 5

Table S6. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 6

No.	δ_{H}	δ_{C}	COSY	HMBC
1		113.2, C		
2		159.2, C		
3		101.3, C		
4		159.2, C		
5		114.1, C		
6		146.1, C		
7		161.7, C		
8	2.78, t (7.9)	27.1, CH_2		C-1, C-5, C-6, C-9, C-10
9	1.47, m	23.1, CH_2		C-6, C-8, C-10
10	0.90, t (7.3)	14.4, CH_3		C-8, C-9
1'		143.0, C		
2'		143.7, C		
3'	7.12, s	103.5, CH		C-1, C-2, C-4, C-5
4'		154.4, C		
5'		110.0, C		
6'		136.1, C		
7'	3.14, t (7.5)	33.0, CH_2		C-1', C-5', C-6', C-8', C-9'
8'	1.61, m	22.9, CH_2		C-6', C-7', C-9'
9'	1.01, t (7.3)	14.4, CH_3		C-7', C-8'
MeO	3.84, s	57.6, CH_3		C-4'

Fr.C-1 400 MHz DMSO

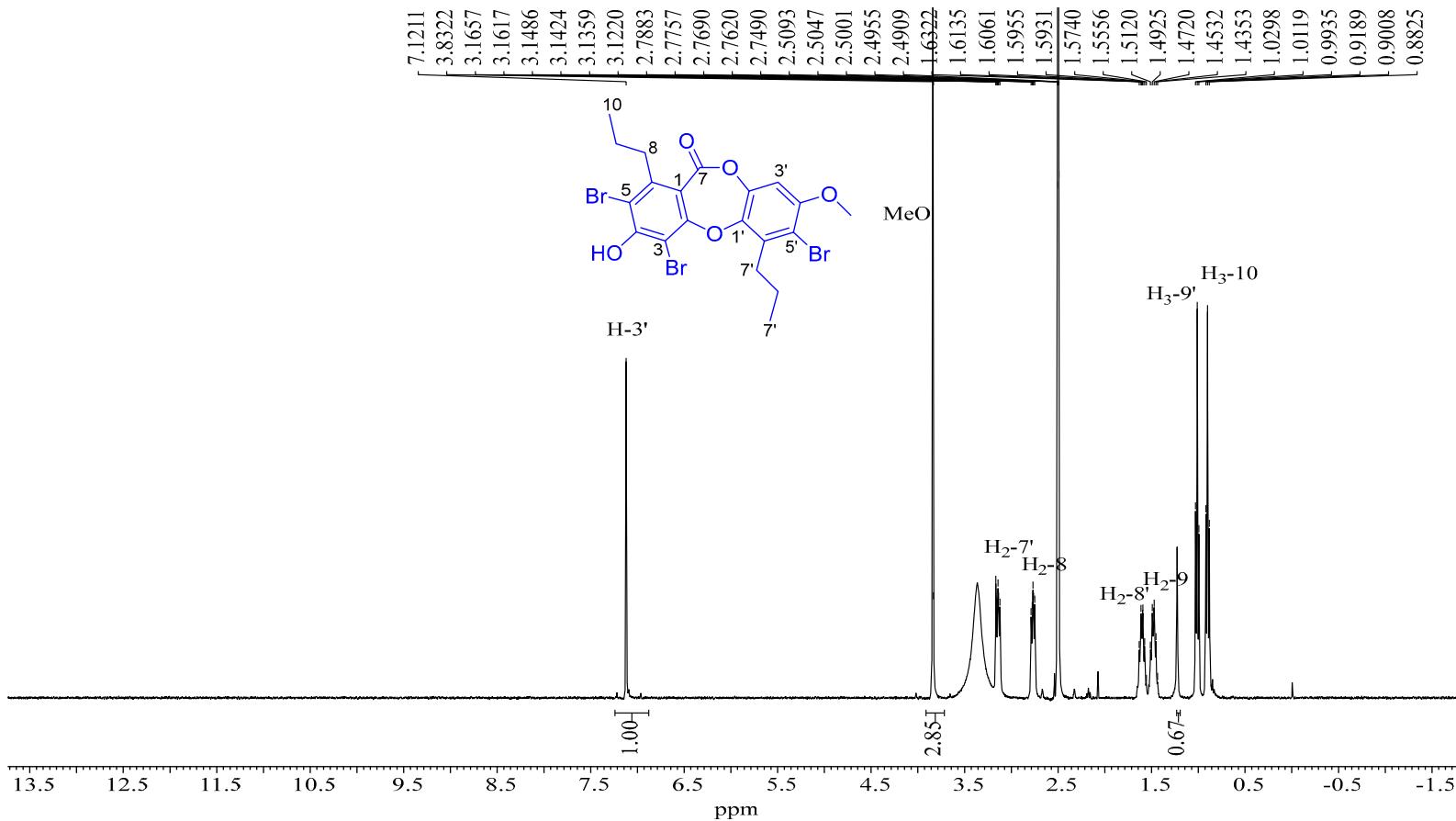


Figure S41. ^1H -NMR spectrum of **6** in $\text{DMSO}-d_6$ (400 MHz)

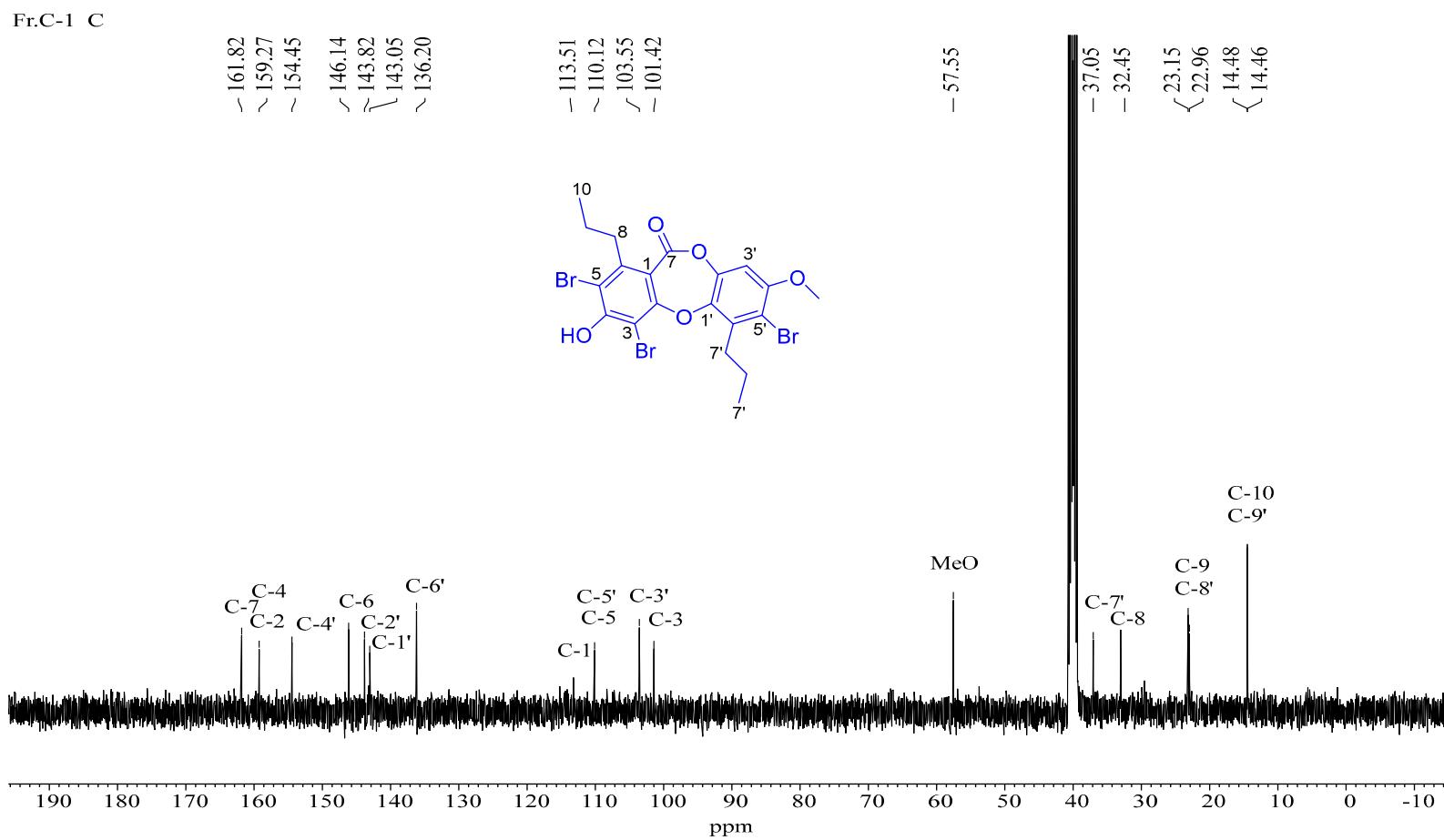


Figure S42. ^{13}C -NMR spectrum of **6** in $\text{DMSO}-d_6$ (100 MHz)

Fr.C-1 HSQC

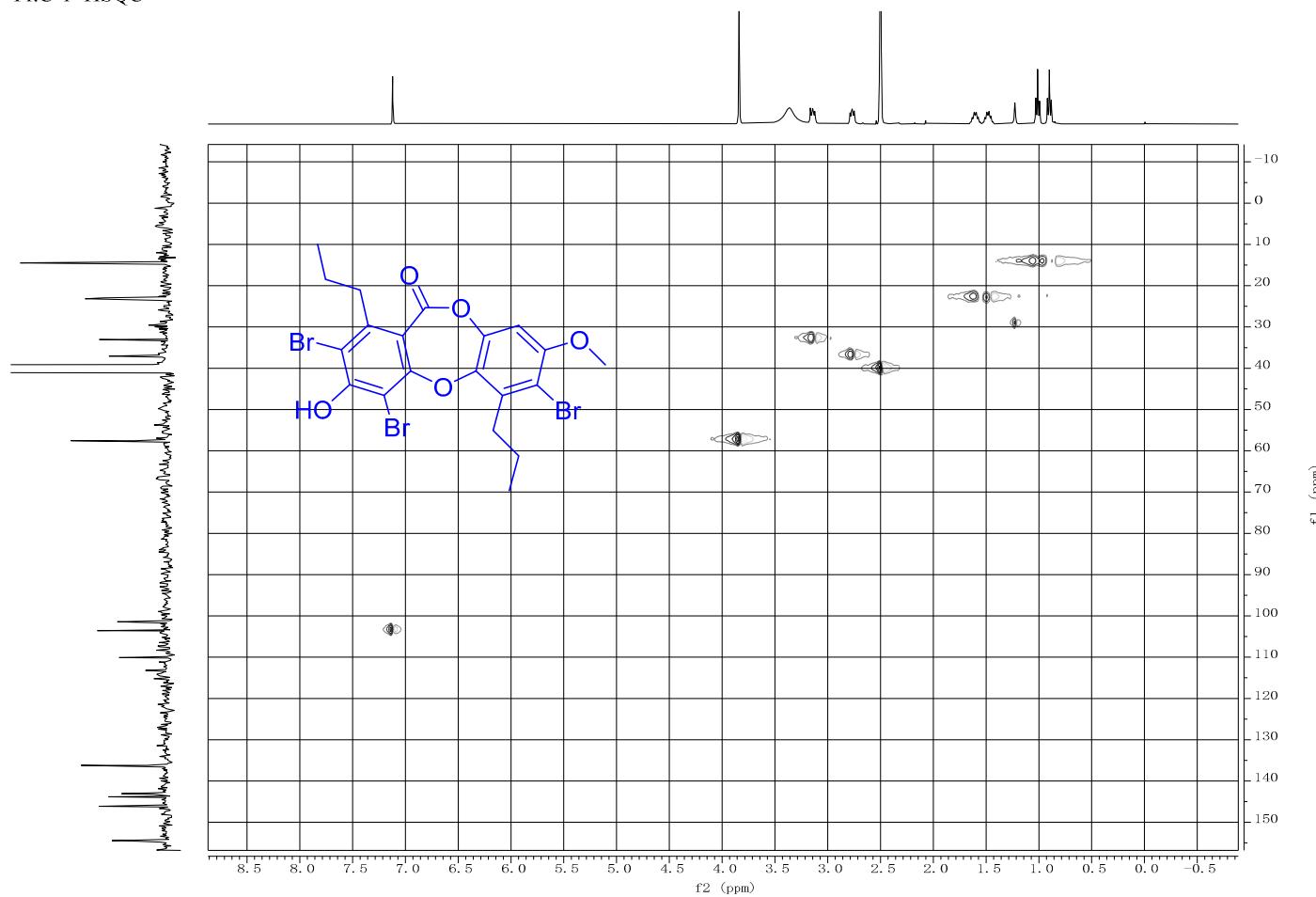


Figure S43. HSQC spectrum of **6** in DMSO-*d*6

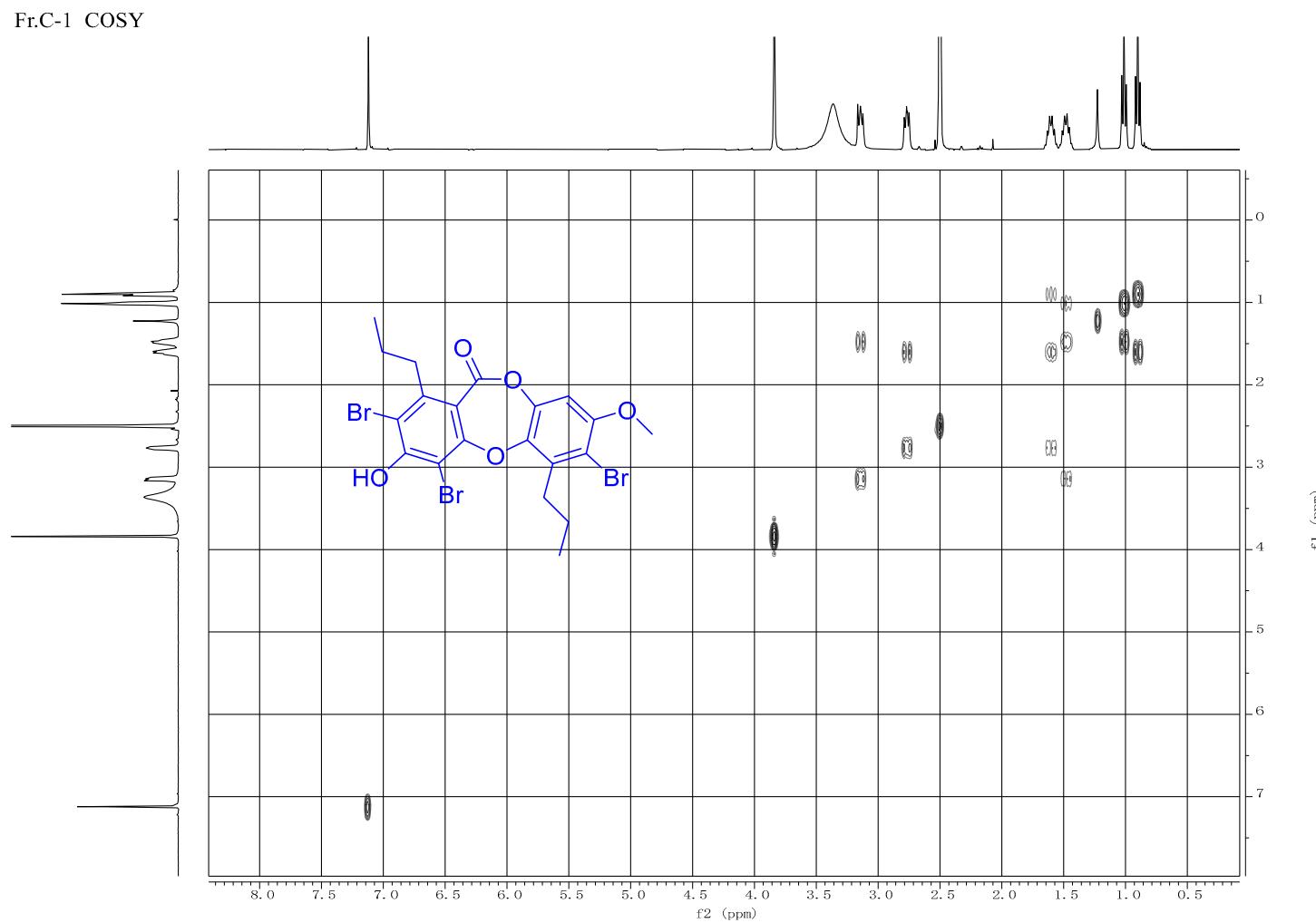


Figure S44. ^1H - ^1H COSY spectrum of **6** in $\text{DMSO}-d_6$

Fr.C-1 HMBC

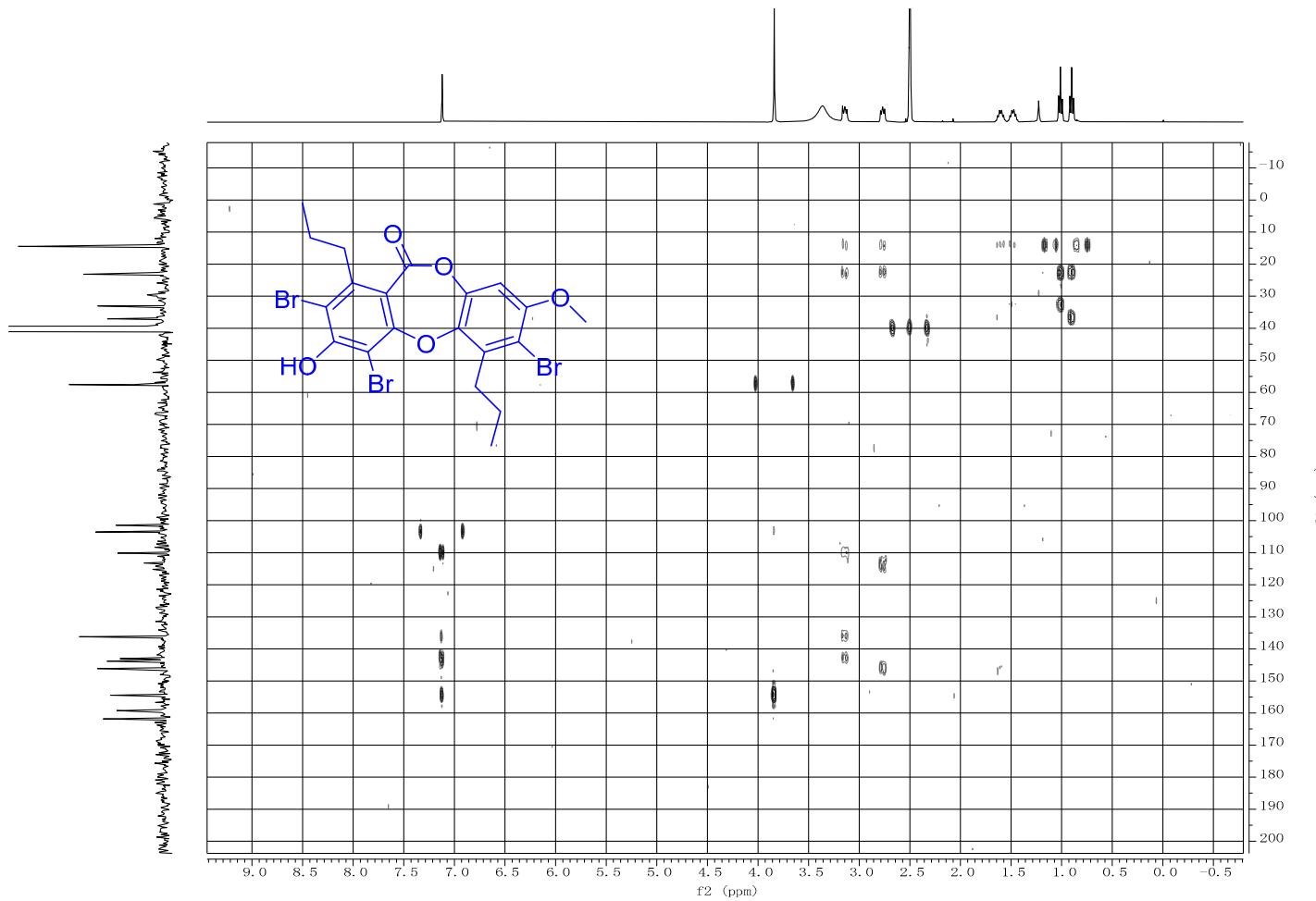


Figure S45. HMBC spectrum of **6** in $\text{DMSO}-d_6$

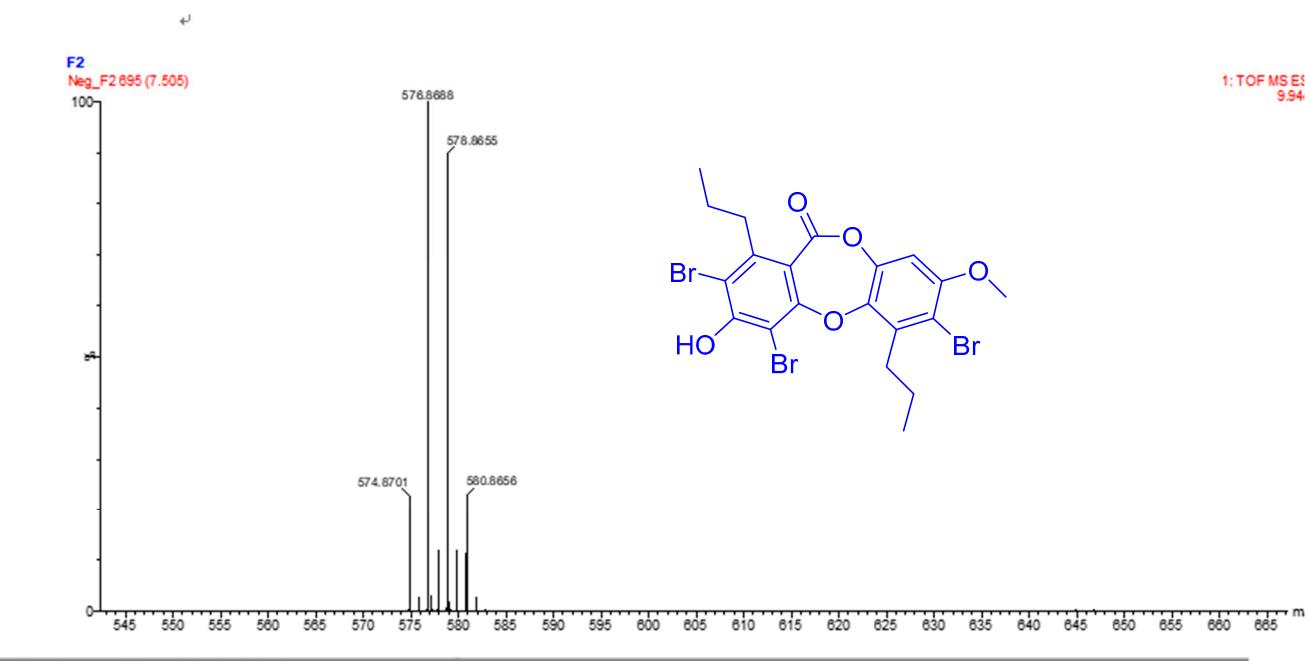


Figure S46. HRESIMS spectrum of **6**

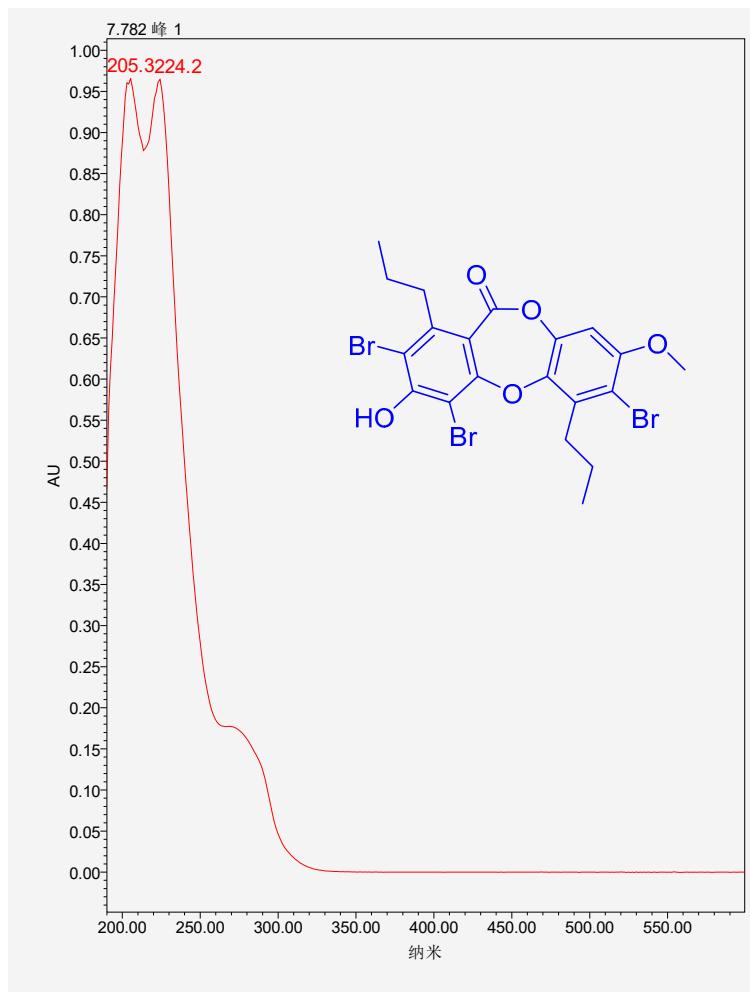


Figure S47. UV spectrum of **6**

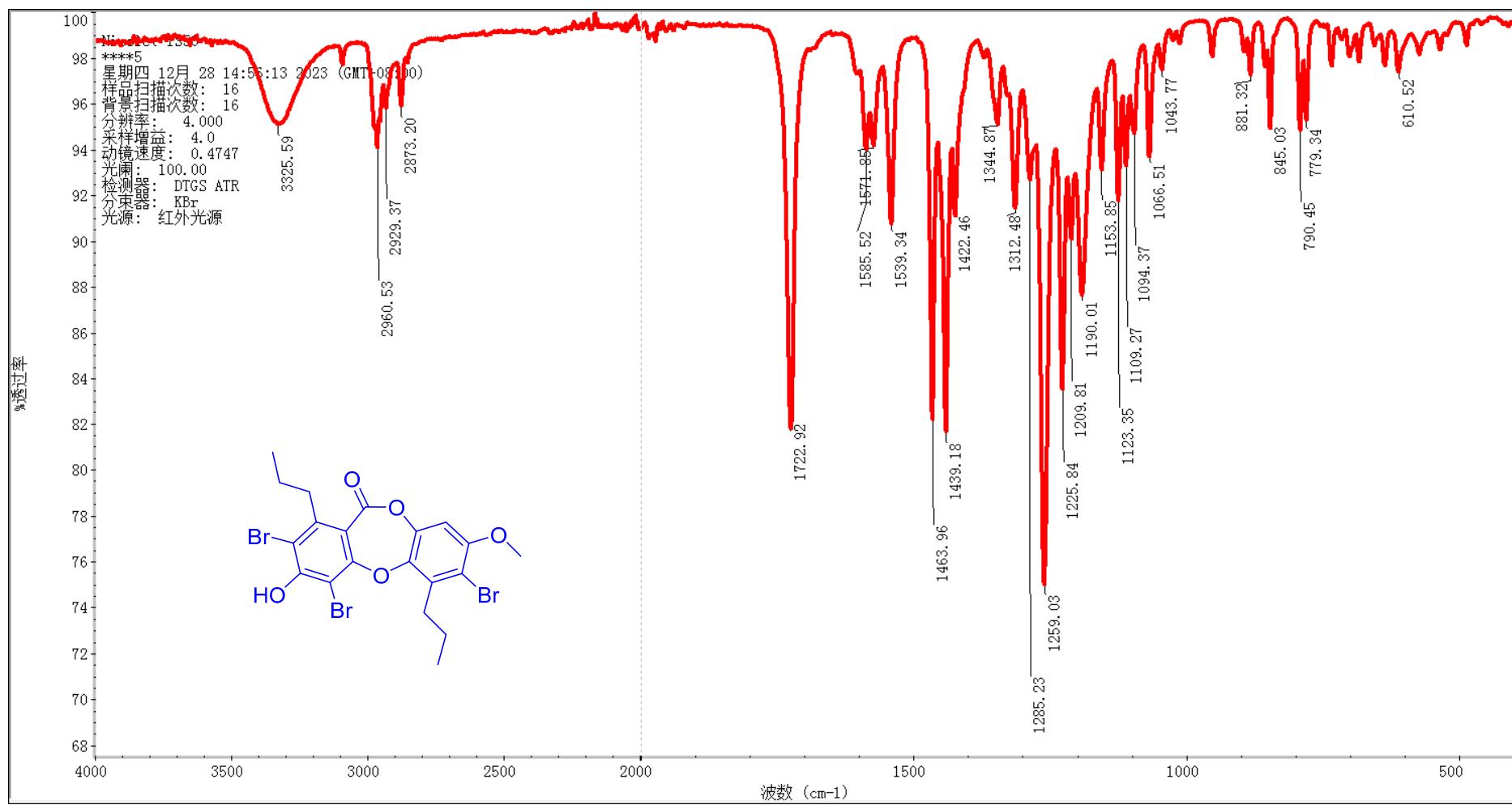


Figure S48. IR spectrum of 6

Table S7. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 7

No.	δ_{H}	δ_{C}	COSY	HMBC
1		111.5, C		
2		160.2, C		
3		99.2, C		
4		160.0, C		
5	6.84, s	115.6, C		C-1, C-3, C-4, C-8
6		148.8, C		
7		160.7, C		
8	2.68, t (7.7)	35.7, CH_2	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.48, m	24.5, CH_2	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.83, t (7.3)	14.2, CH_3	H ₂ -9	C-8, C-9
1'		146.7, C		
2'		142.2, C		
3'		108.3, C		
4'		152.8, C		
5'		117.2, C		
6'		135.5, C		
7'	3.16, t (8.0)	33.2, CH_2	H ₂ -8'	C-1', C-5', C-6', C-8', C-9'
8'	1.50, m	22.8, CH_2	H ₂ -7', H ₃ -9'	C-6', C-7', C-9'
9'	1.00, t (7.2)	14.3, CH_3	H ₂ -8'	C-7', C-8'
MeO	3.78, s	60.9, CH_3		C-4'

M-16-1 500 MHz DMSO

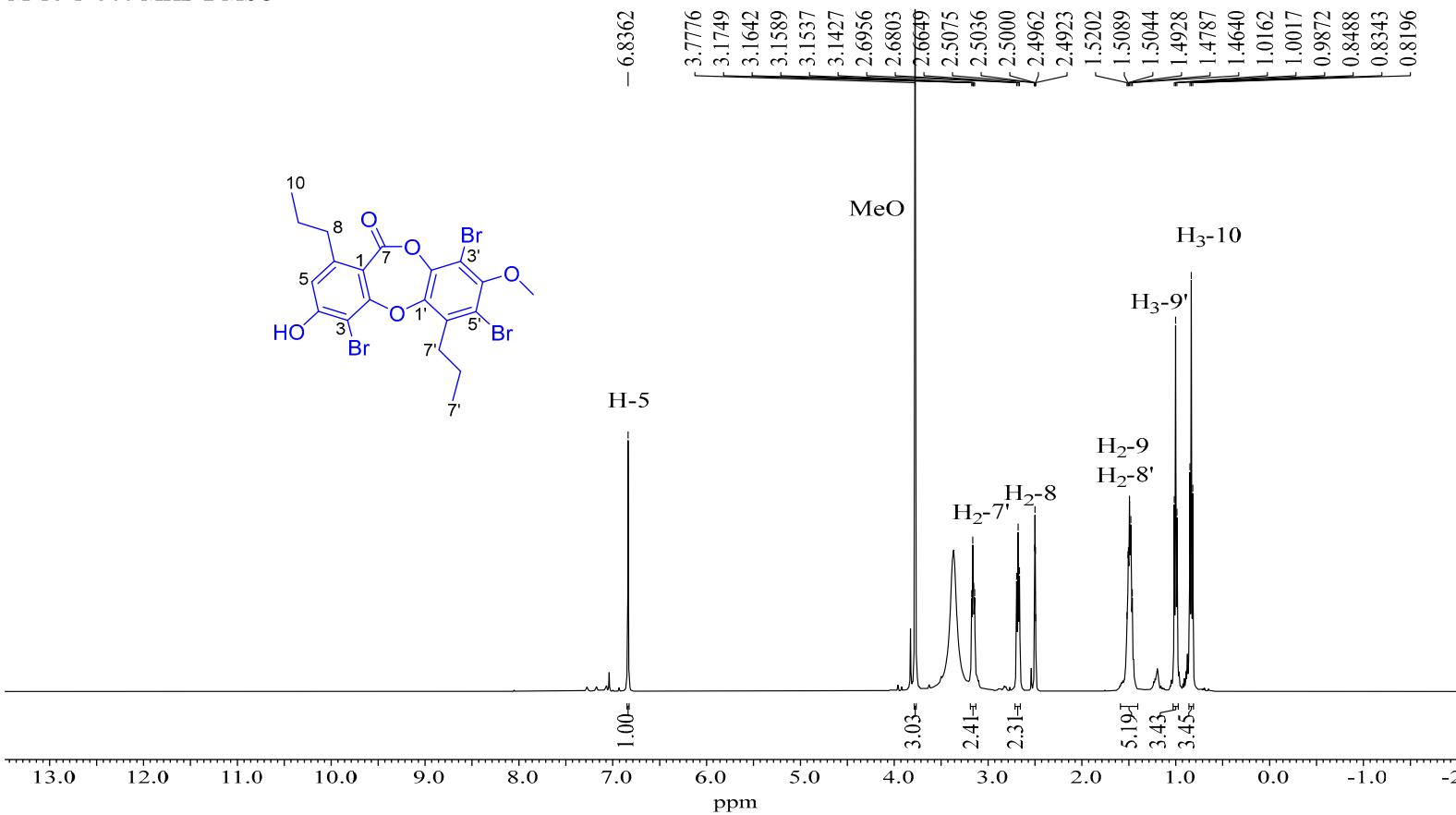


Figure S49. ^1H -NMR spectrum of 7 in $\text{DMSO}-d_6$ (500 MHz)

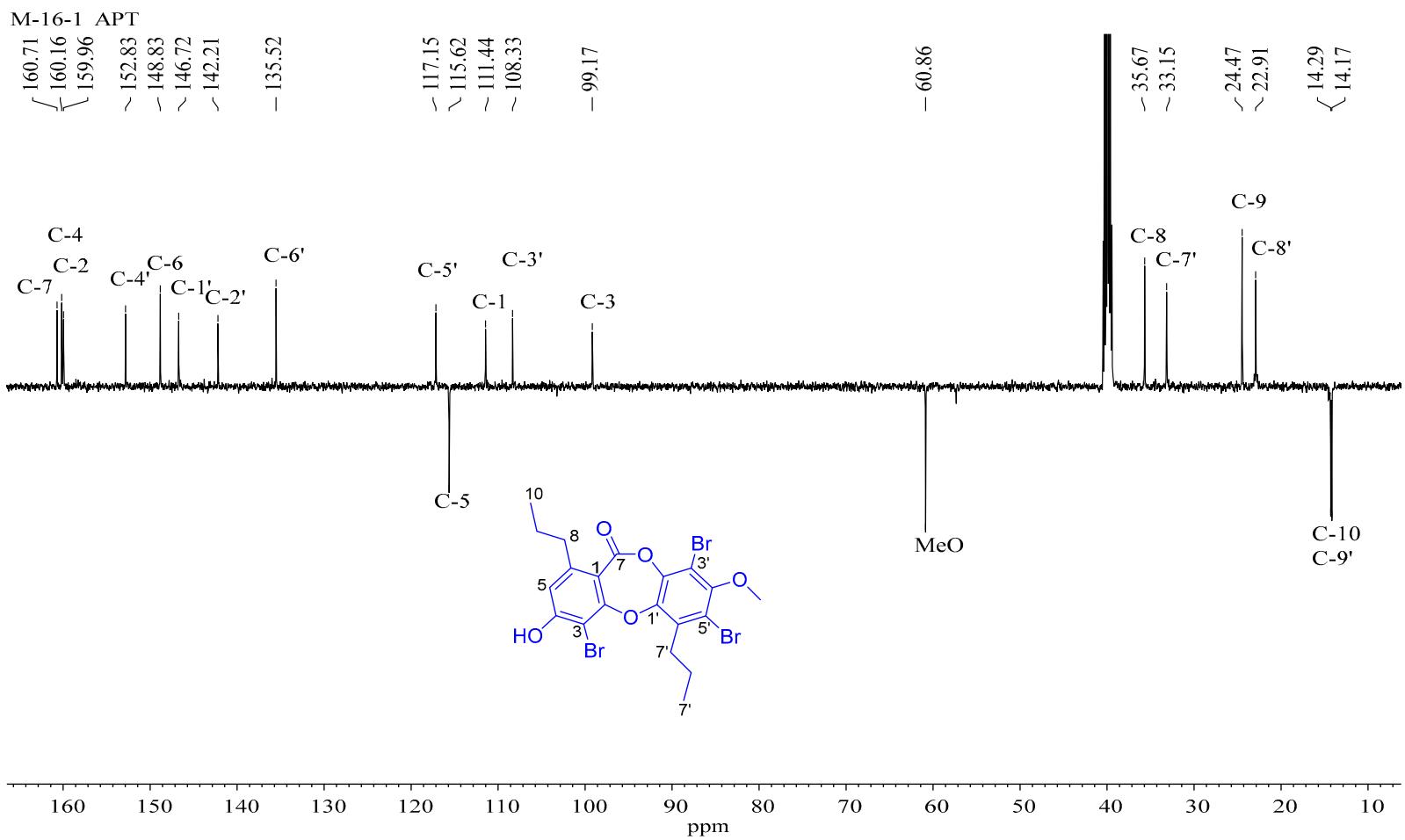


Figure S50. APT spectrum of **7** in $\text{DMSO}-d_6$ (125 MHz)

M-16-1 HSQC

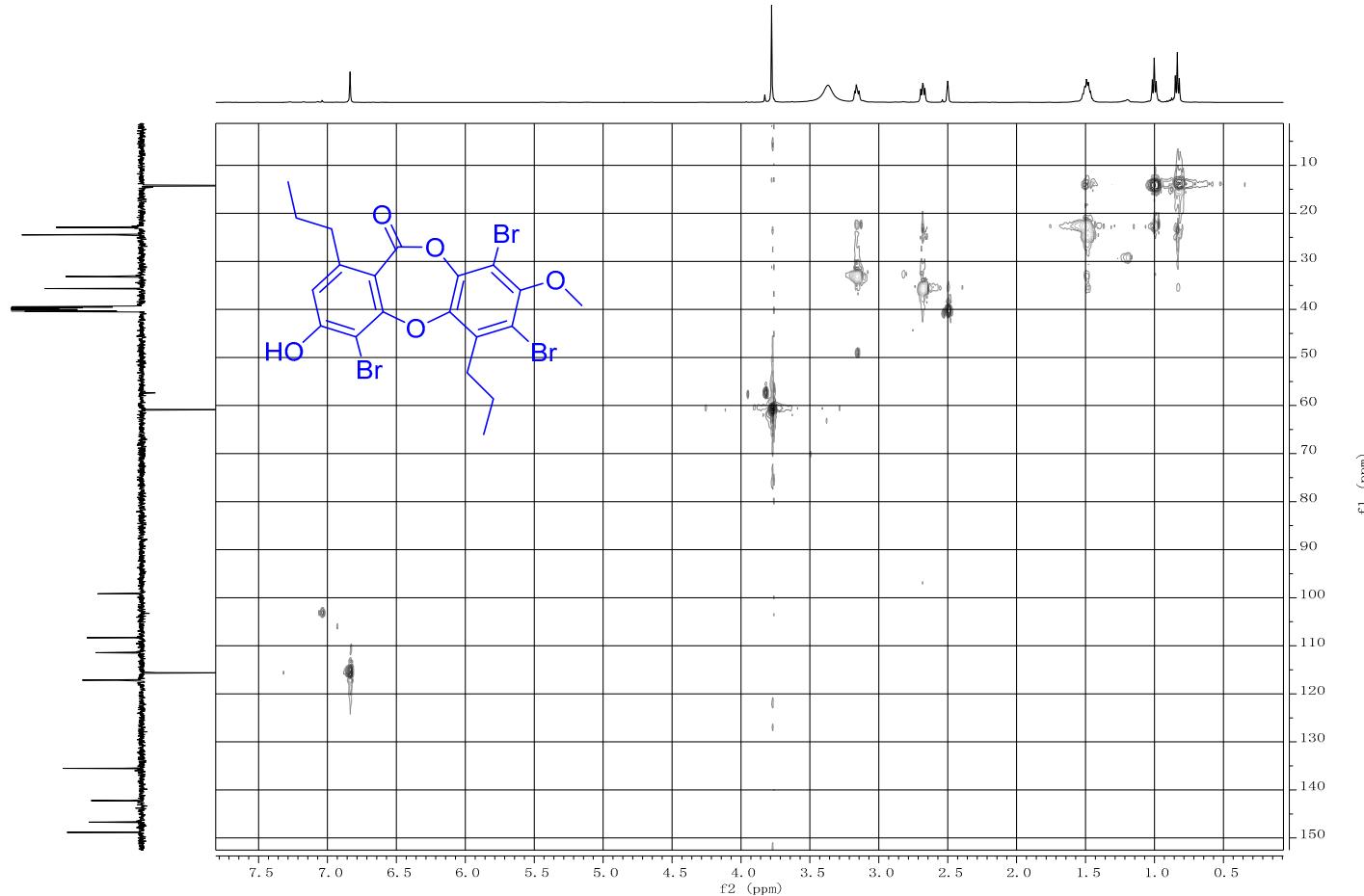


Figure S51. HSQC spectrum of **7** in $\text{DMSO}-d_6$

M-16-1 COSY

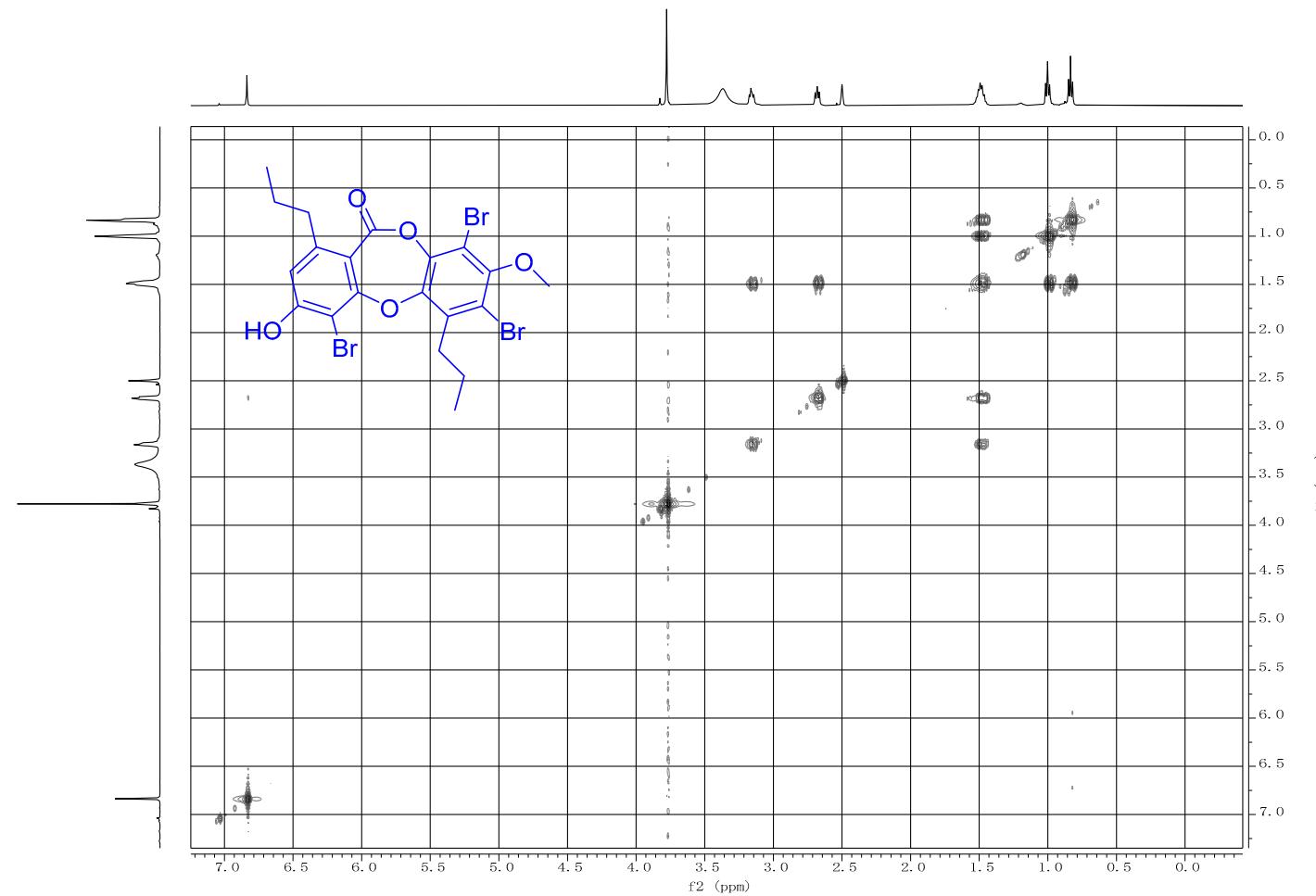


Figure S52. ^1H - ^1H COSY spectrum of **7** in $\text{DMSO}-d_6$

M-16-1 HMBC

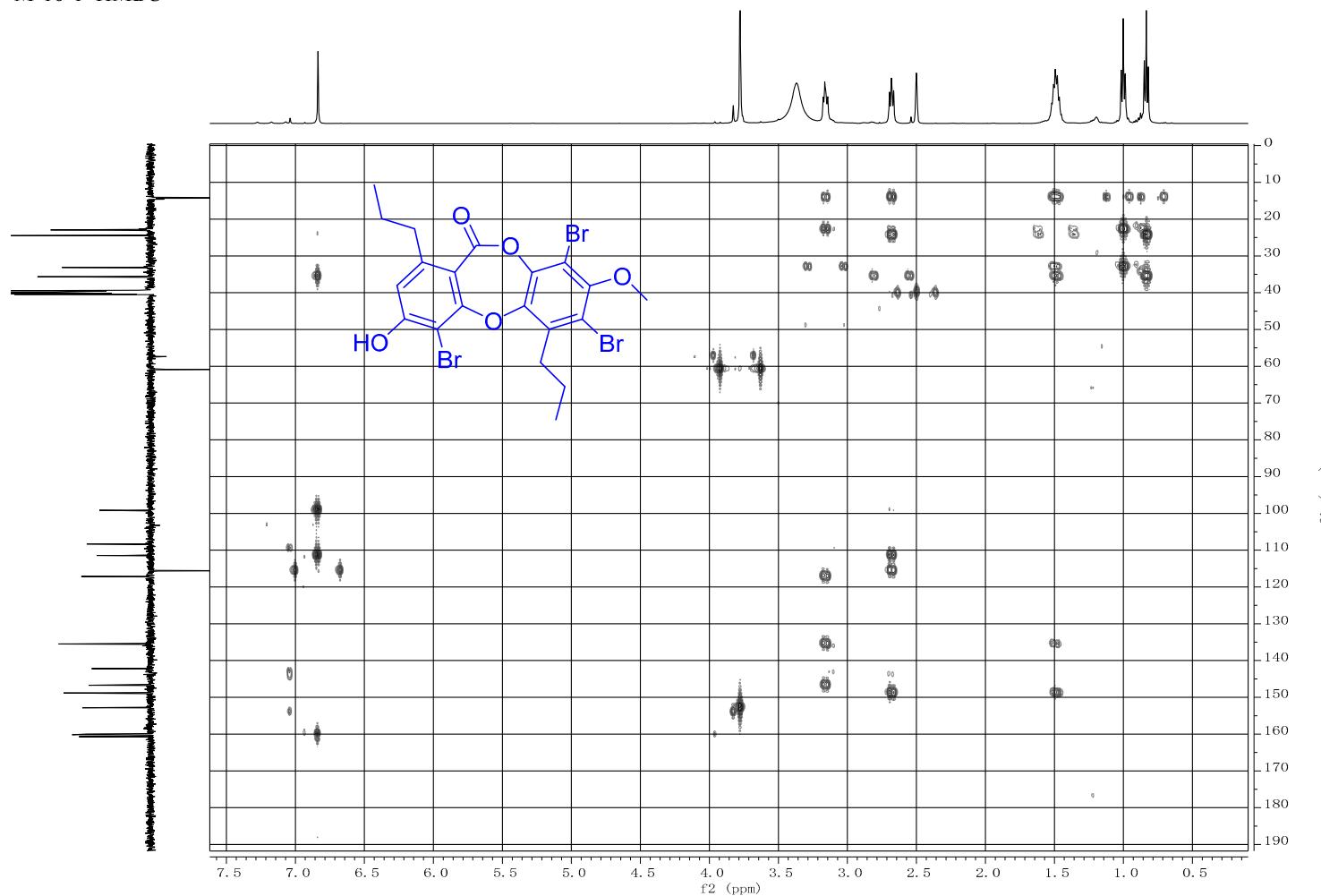


Figure S53. HMBC spectrum of 7 in $\text{DMSO}-d_6$

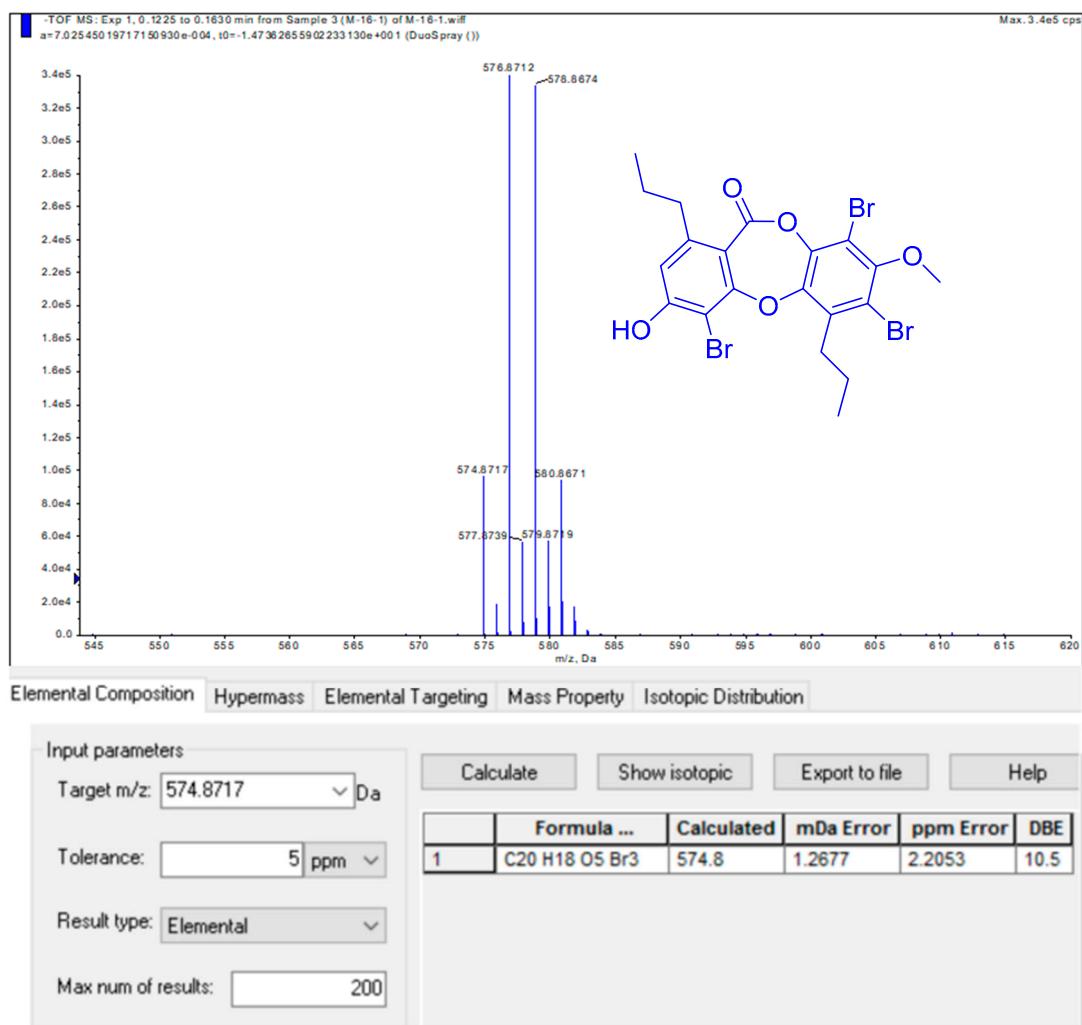


Figure S54. HRESIMS spectrum of 7

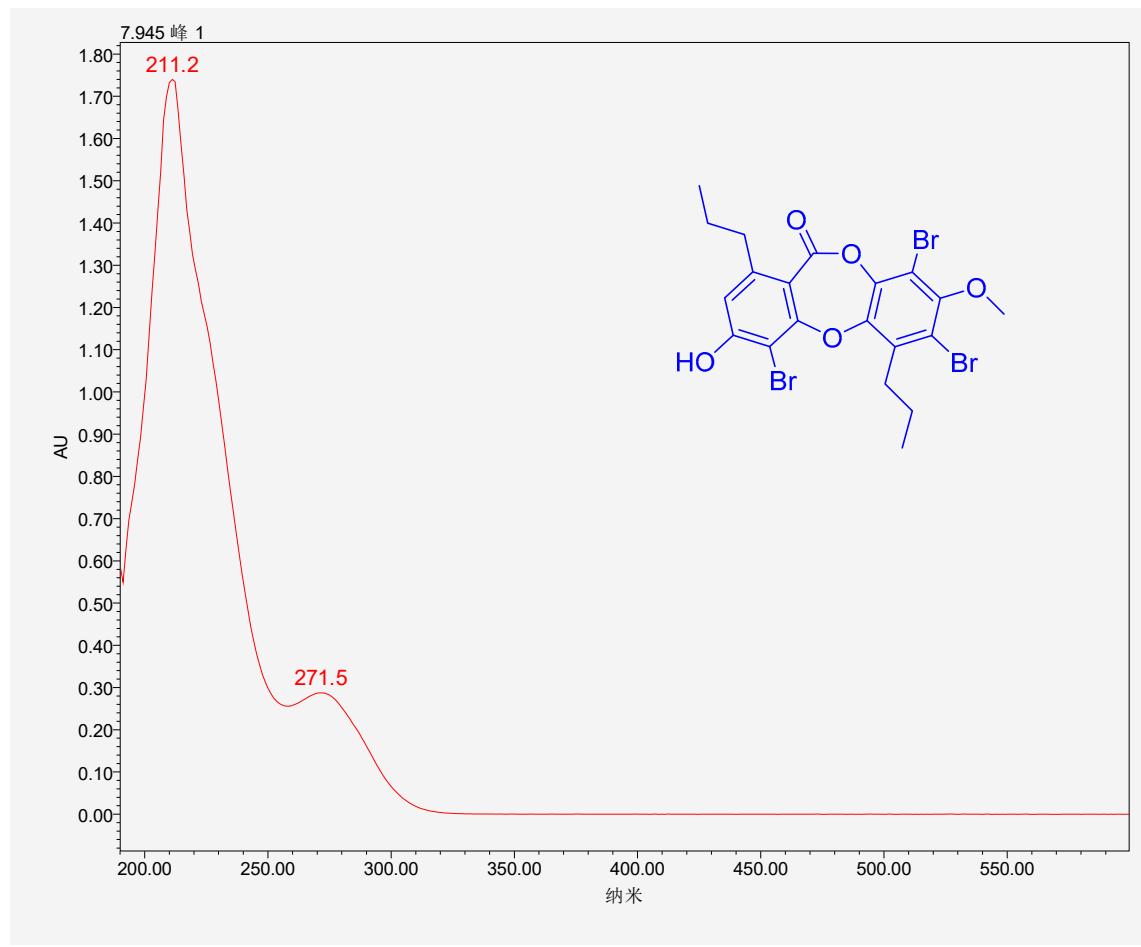


Figure S55. UV spectrum of 7

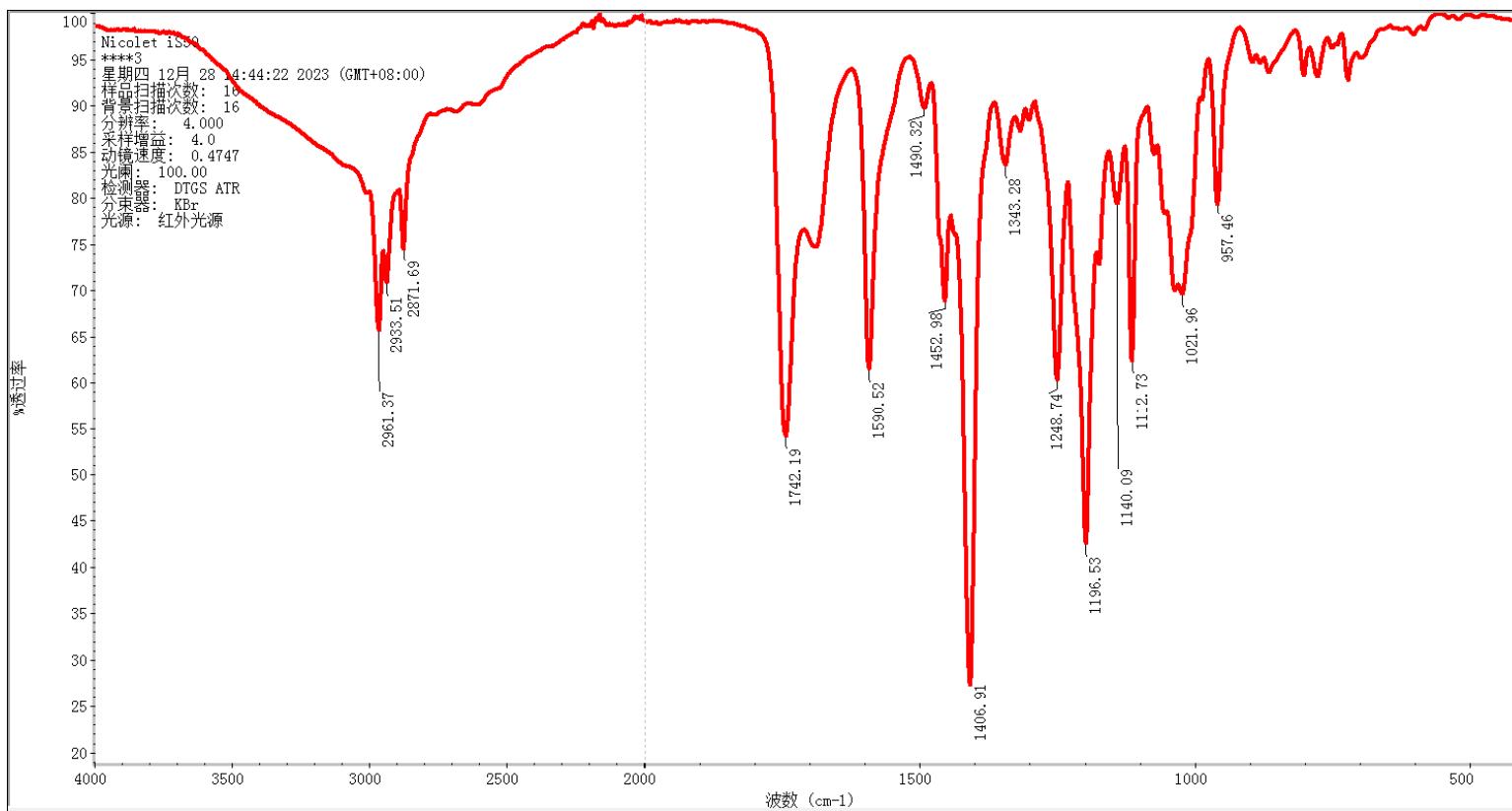


Figure S56. IR spectrum of 7

Table S8. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 8

No.	δ_{H}	δ_{C}	COSY	HMBC
1		111.7, C		
2		161.0, C		
3	6.84, s	105.7, CH		C-1, C-2, C-3, C-4
4		158.4, C		
5		112.4, C		
6		147.3, C		
7		161.2, C		
8	2.85, m	35.7, CH_2	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.55, m	22.8, CH_2	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.88, t (7.2)	14.2, CH_3	H ₂ -9	C-8, C-9
1'		146.1, C		
2'		142.5, C		
3'		108.0, C		
4'		152.5, C		
5'		116.6, C		
6'		135.2, C		
7'	2.87, m	32.5, CH_2	H ₂ -8'	C-1', C-5', C-6', C-8', C-9'
8'	1.55, m	22.5, CH_2	H ₂ -7', H ₃ -9'	C-6', C-7', C-9'
9'	1.04, t (7.2)	14.5, CH_3	H ₂ -8'	C-7', C-8'
MeO	3.76, s	60.9, CH_3		C-4'

M-16-2 500 MHz DMSO

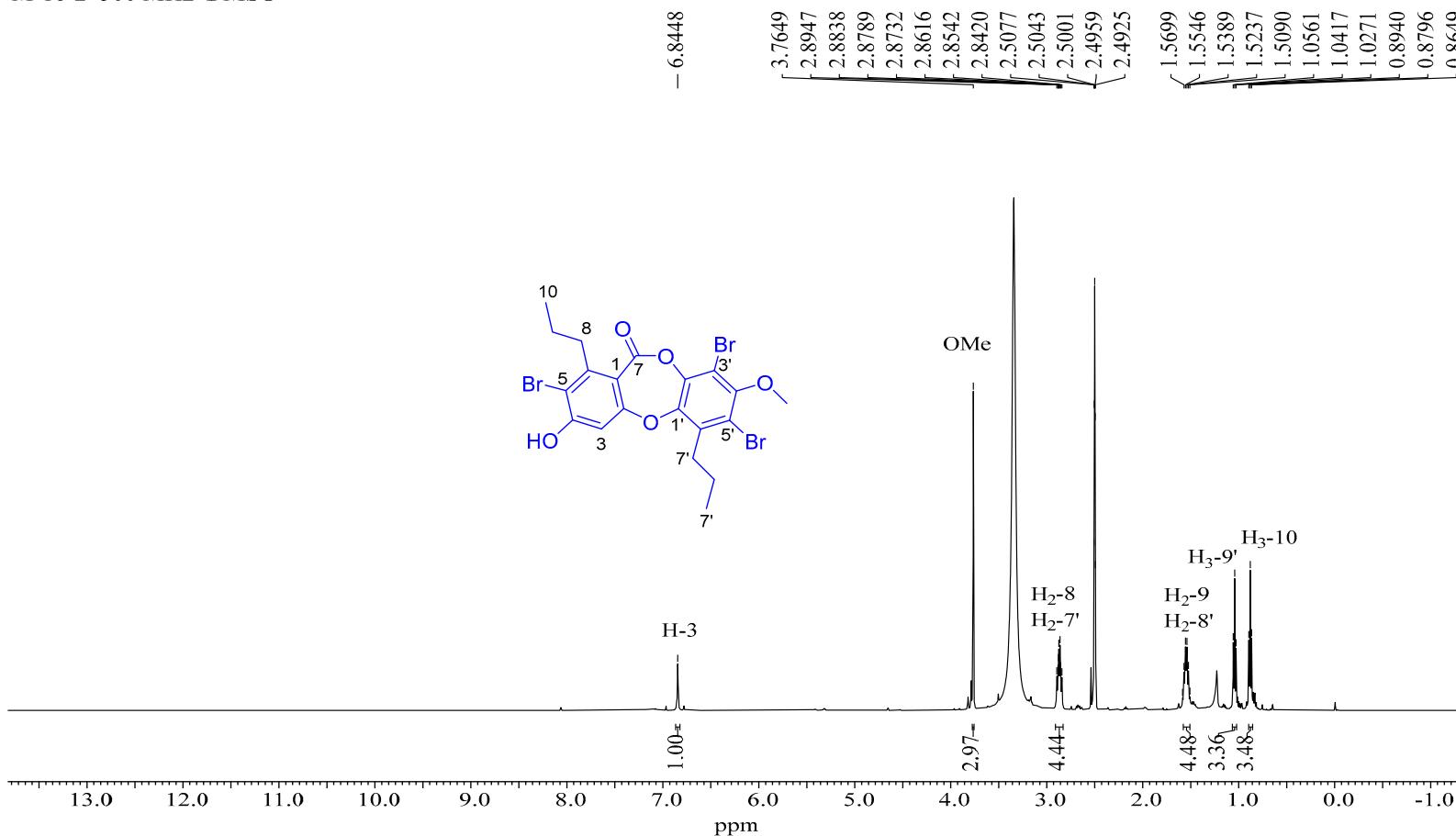


Figure S57. ^1H -NMR spectrum of **8** in $\text{DMSO}-d_6$ (500 MHz)

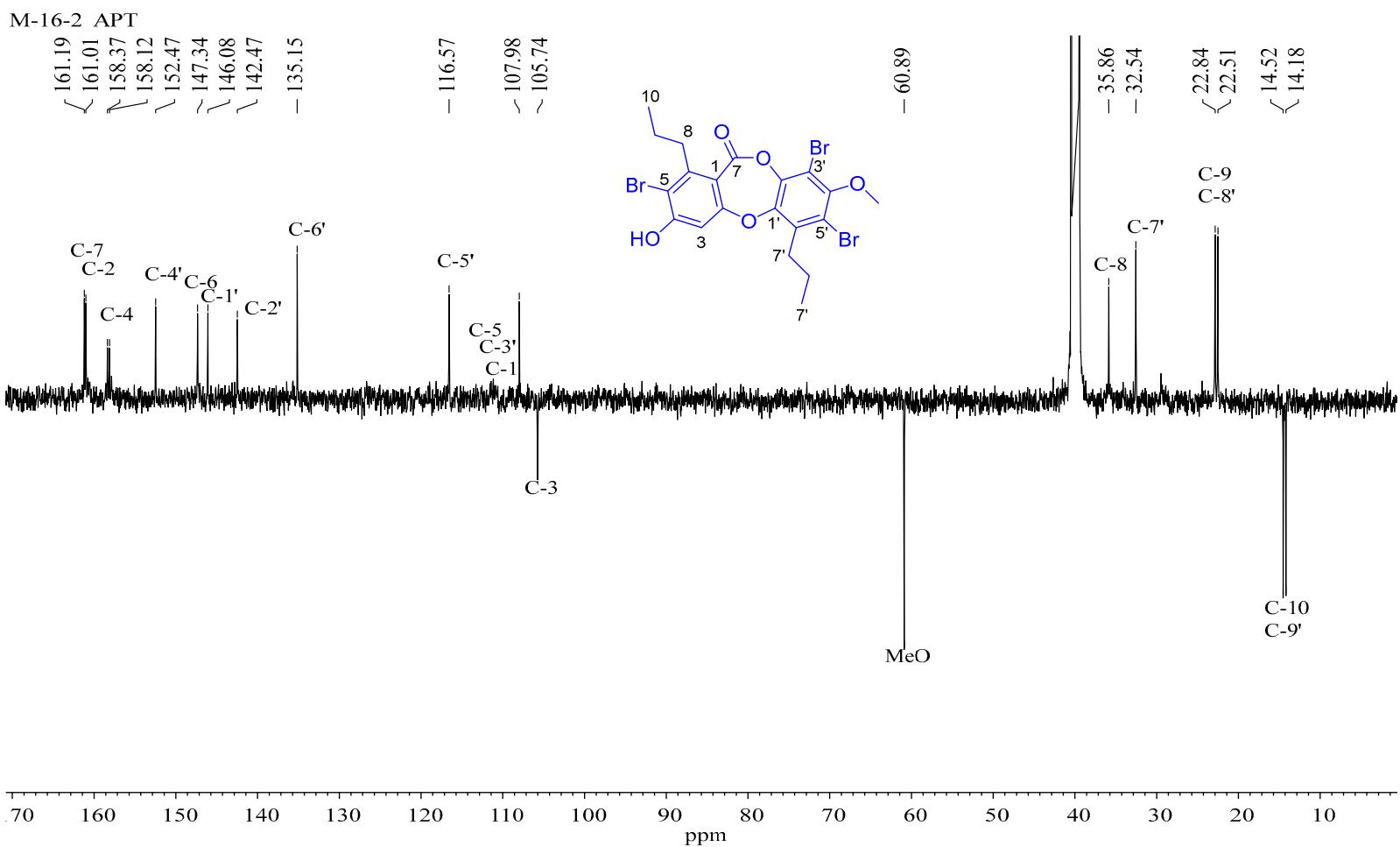


Figure S58. APT spectrum of **8** in DMSO-*d*₆ (125 MHz)

M-16-2 HSQC

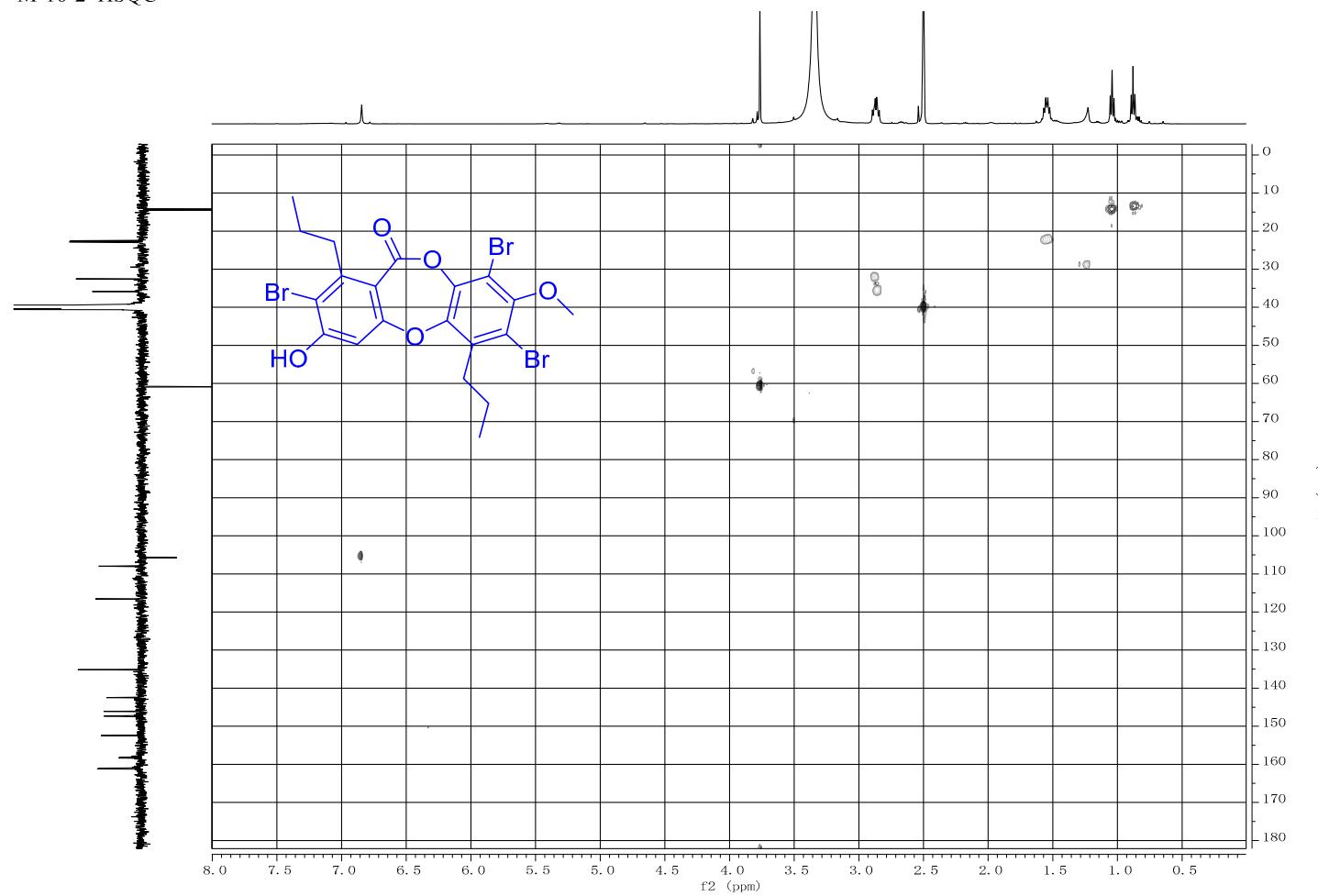


Figure S59. HSQC spectrum of **8** in $\text{DMSO}-d_6$

M-16-2 COSY

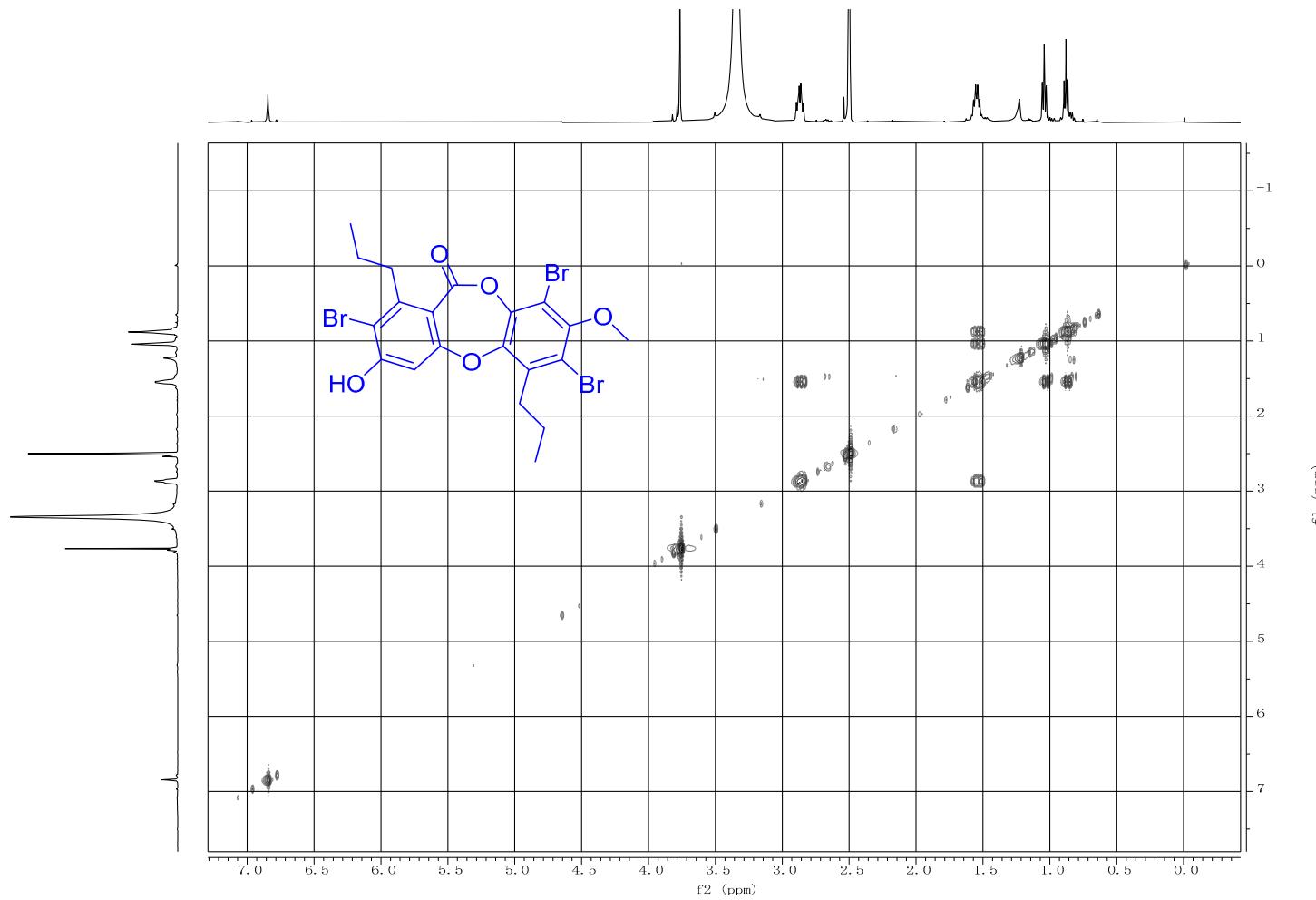


Figure S60. ^1H - ^1H COSY spectrum of **8** in $\text{DMSO}-d_6$

M-16-2 HMBC

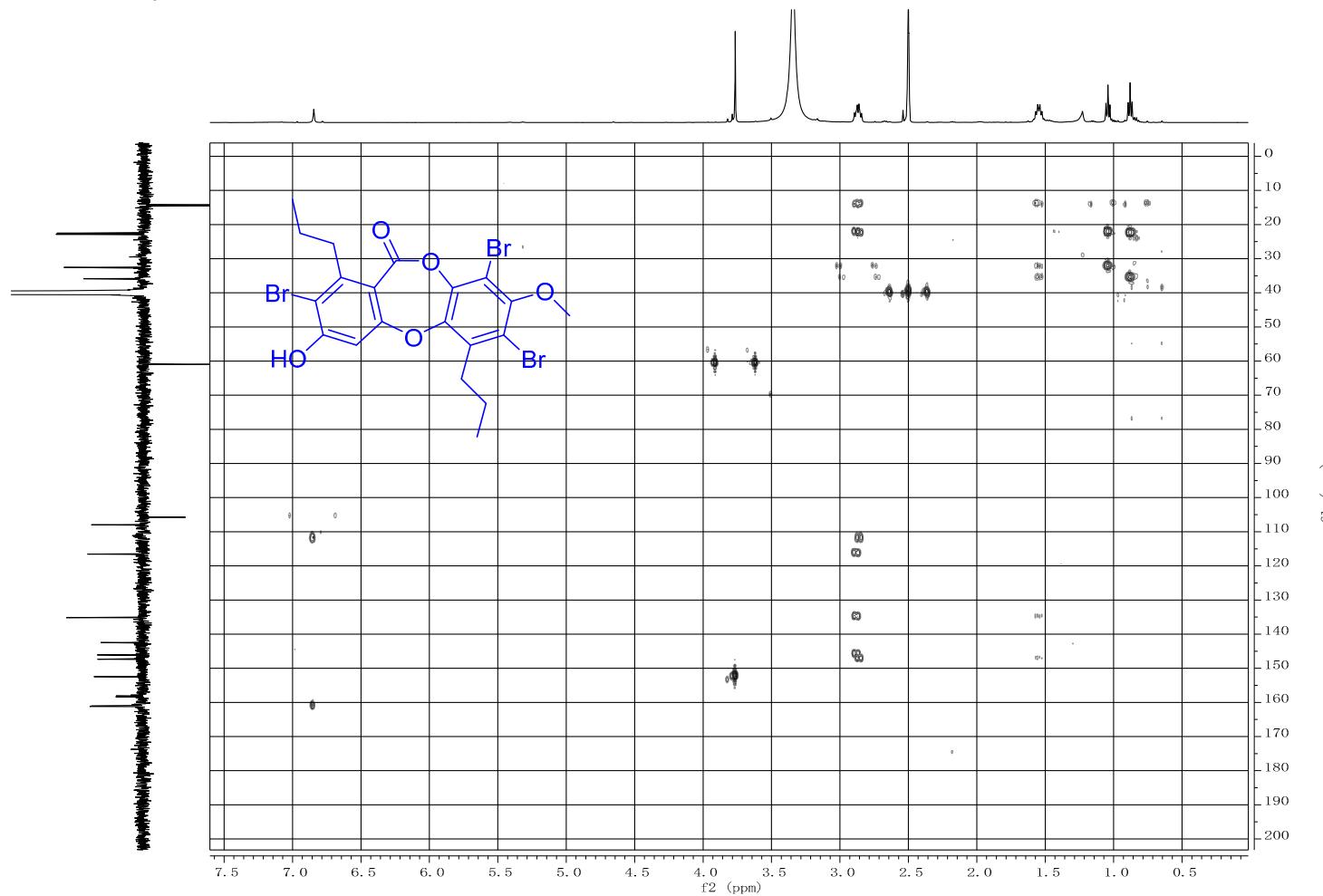


Figure S61. HMBC spectrum of **8** in $\text{DMSO}-d_6$

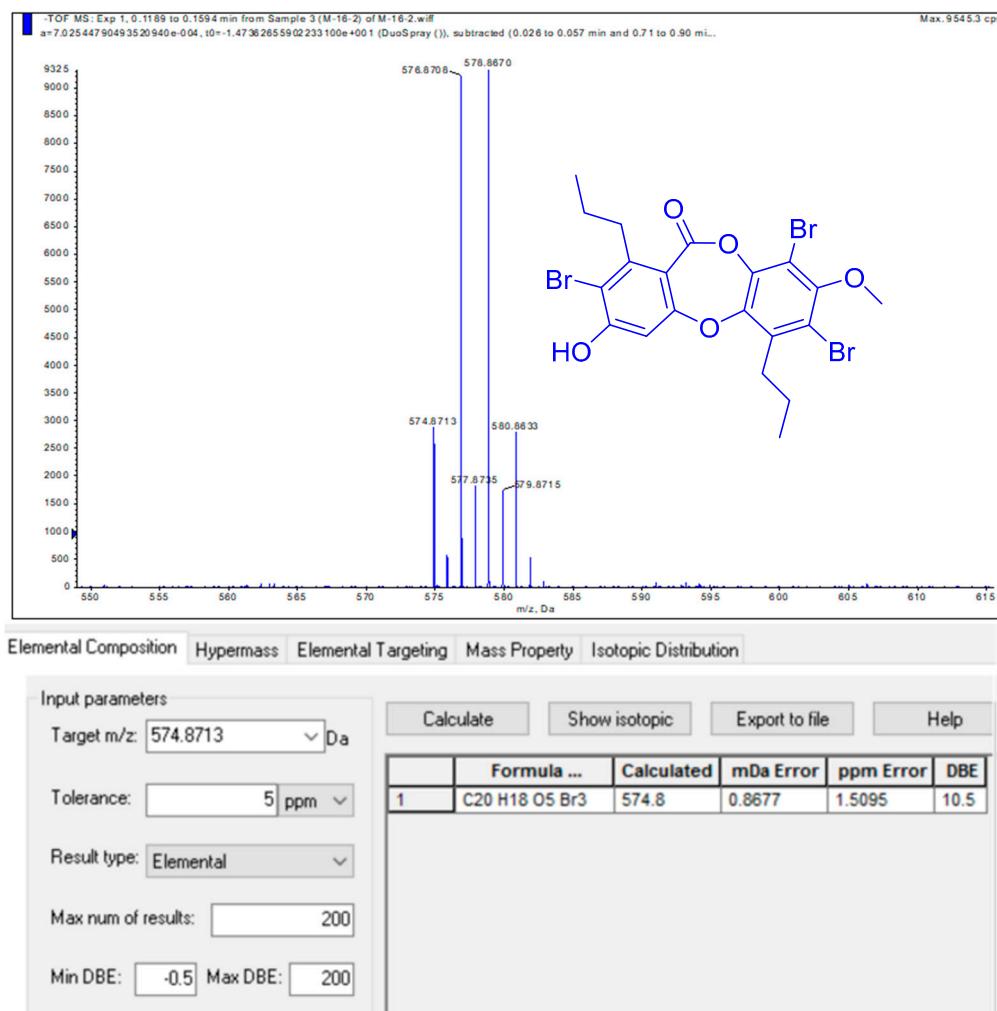


Figure S62. HRESIMS spectrum of **8**

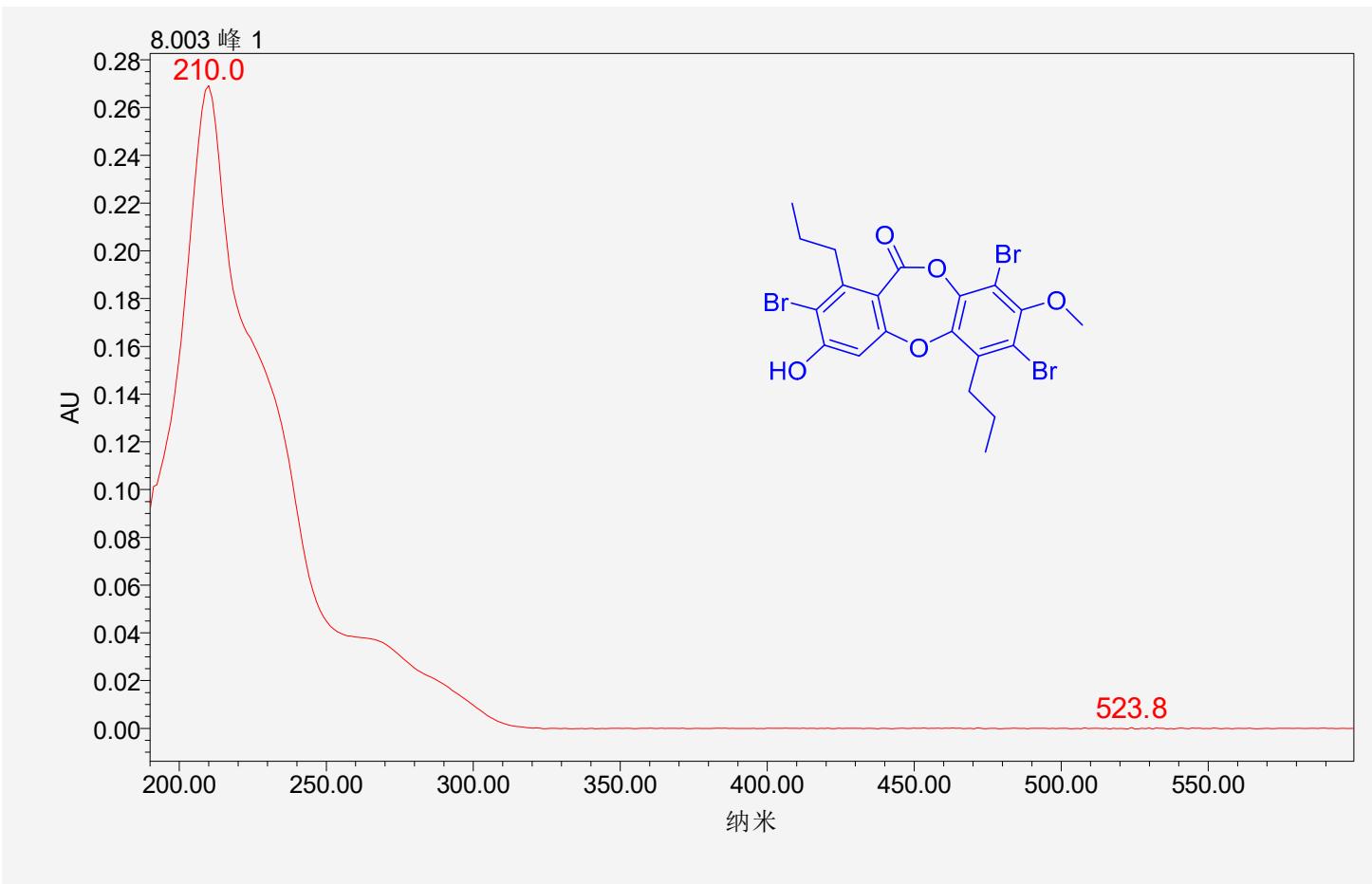


Figure S63. UV spectrum of **8**

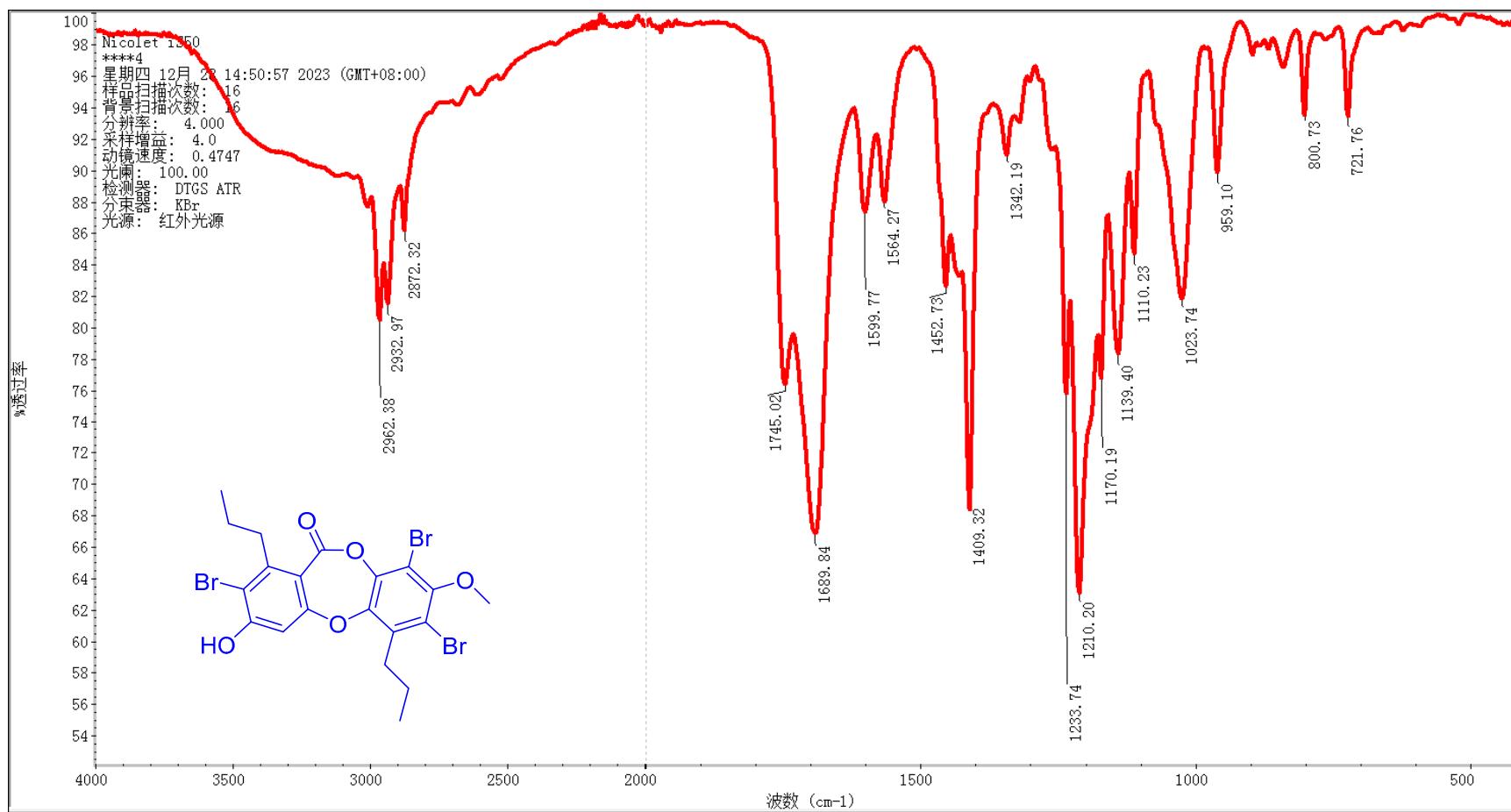


Figure S64. IR spectrum of 8

Table S9. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 9

No.	δ_{H}	δ_{C}	COSY	HMBC
1		112.7, C		
2		158.8, C		
3		101.5, C		
4		158.8, C		
5		113.8, C		
6		146.1, C		
7		160.6, C		
8	2.81, t (7.7)	36.6, CH ₂	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.58, m	22.7, CH ₂	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.87, t (7.3)	14.1, CH ₃	H ₂ -9	C-8, C-9
1'		146.6, C		
2'		142.2, C		
3'		108.3, C		
4'		152.9, C		
5'		117.2, C		
6'		135.5, C		
7'	3.15, t (7.9)	33.2, CH ₂	H ₂ -8'	C-1', C-5', C-6', C-8', C-9'
8'	1.50, m	22.9, CH ₂	H ₂ -7', H ₃ -9'	C-6', C-7', C-9'
9'	1.02, t (7.3)	14.3, CH ₃	H ₂ -8'	C-7', C-8'
MeO	3.78, s	60.8, CH ₃		C-4'

Fr.C-2 400 MHz DMSO

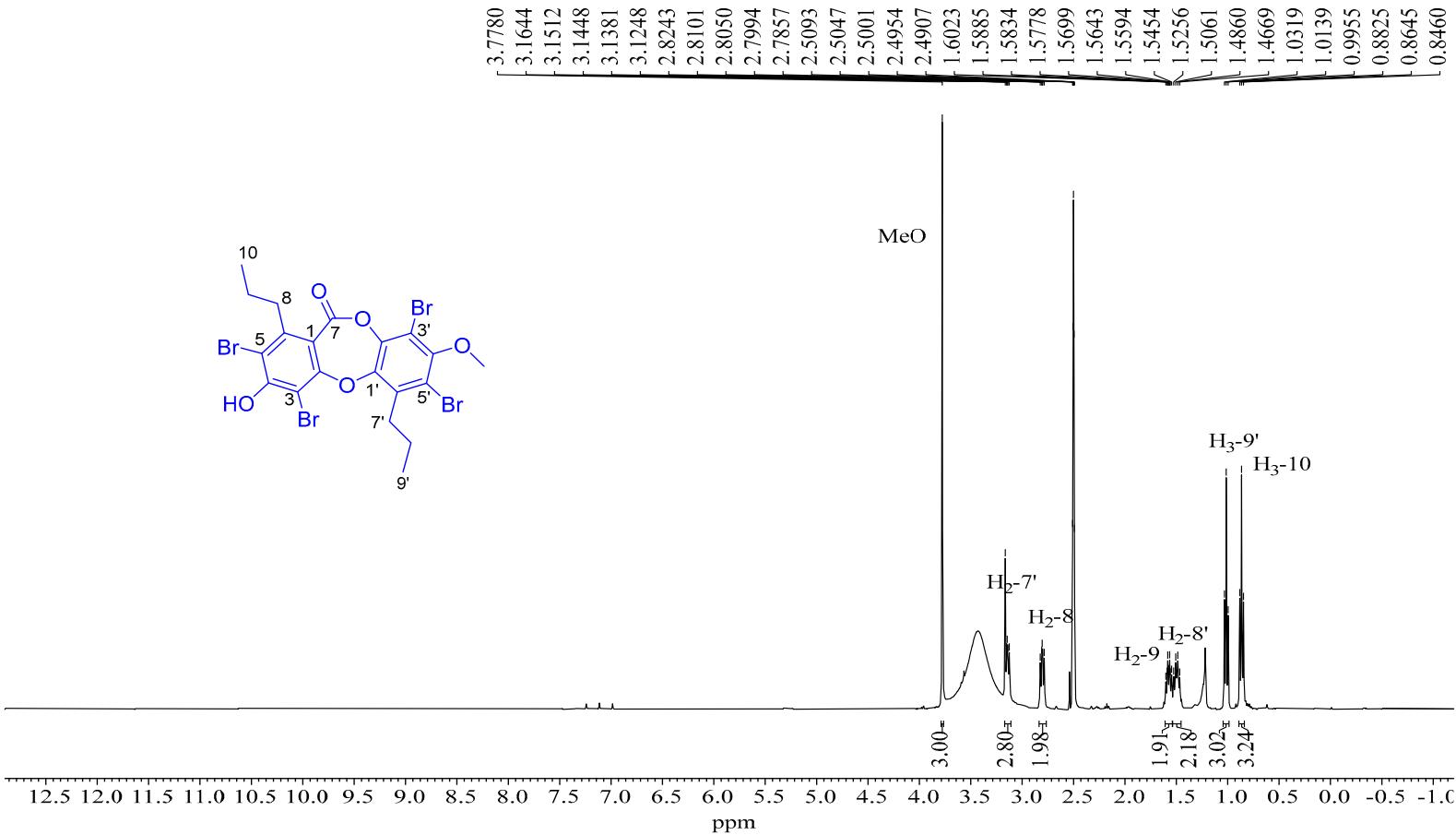


Figure S65. ^1H -NMR spectrum of **9** in $\text{DMSO}-d_6$ (400 MHz)

Fr.C-2 C

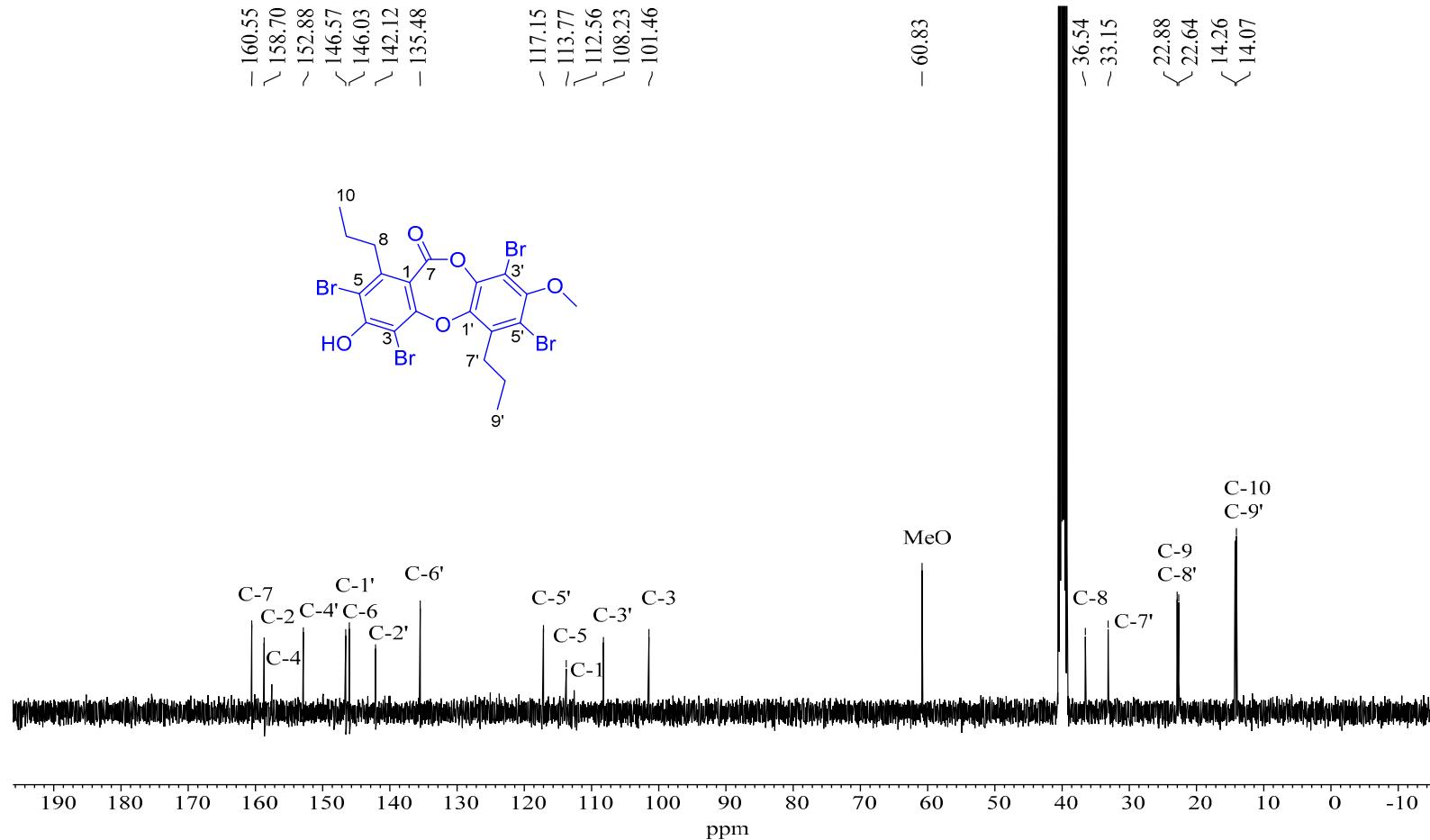


Figure S66. ^{13}C -NMR spectrum of **9** in $\text{DMSO}-d_6$ (100 MHz)

Fr.C-2 HSQC

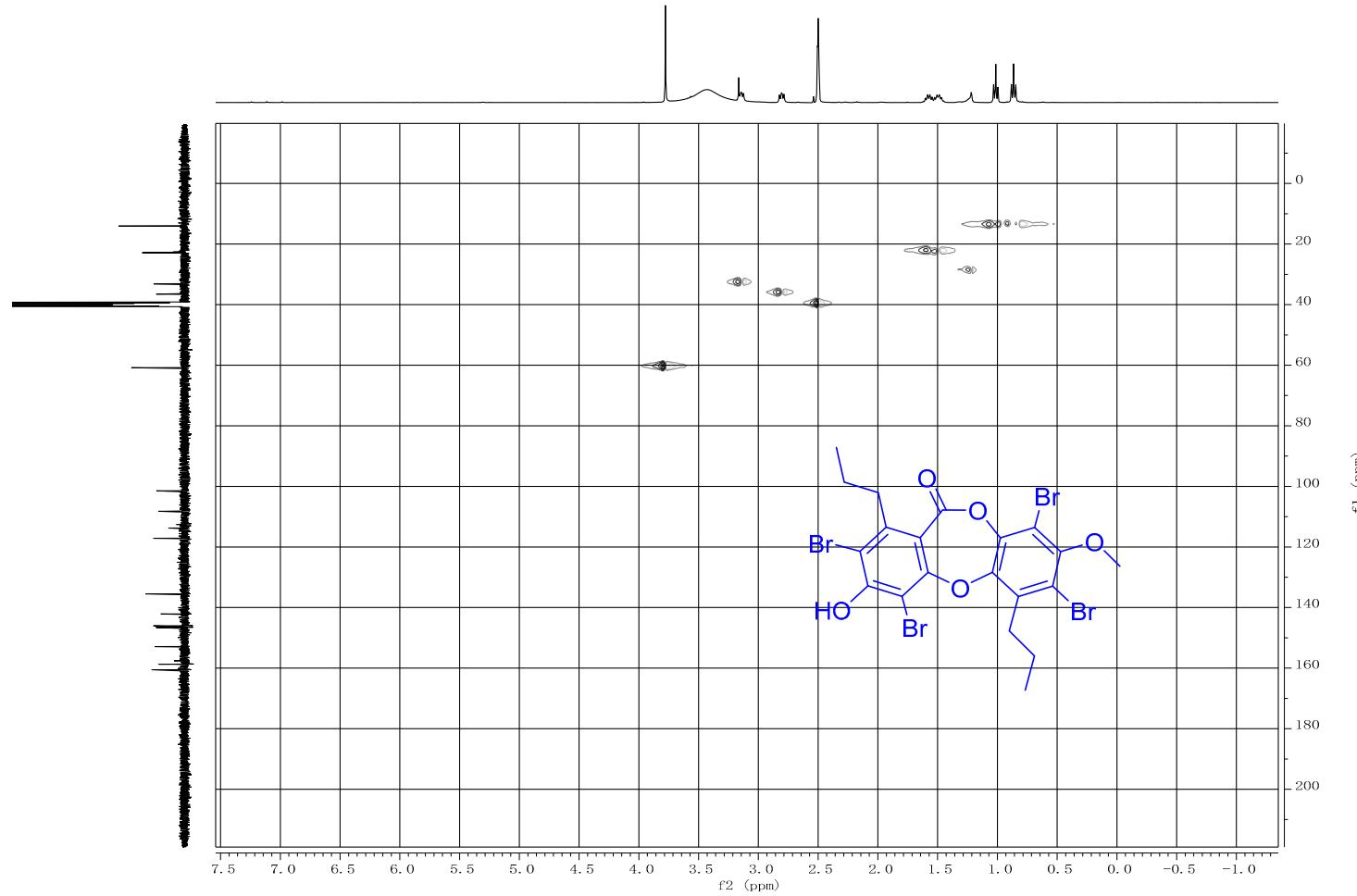


Figure S67. HSQC spectrum of **9** in $\text{DMSO}-d_6$

Fr.C-2 COSY

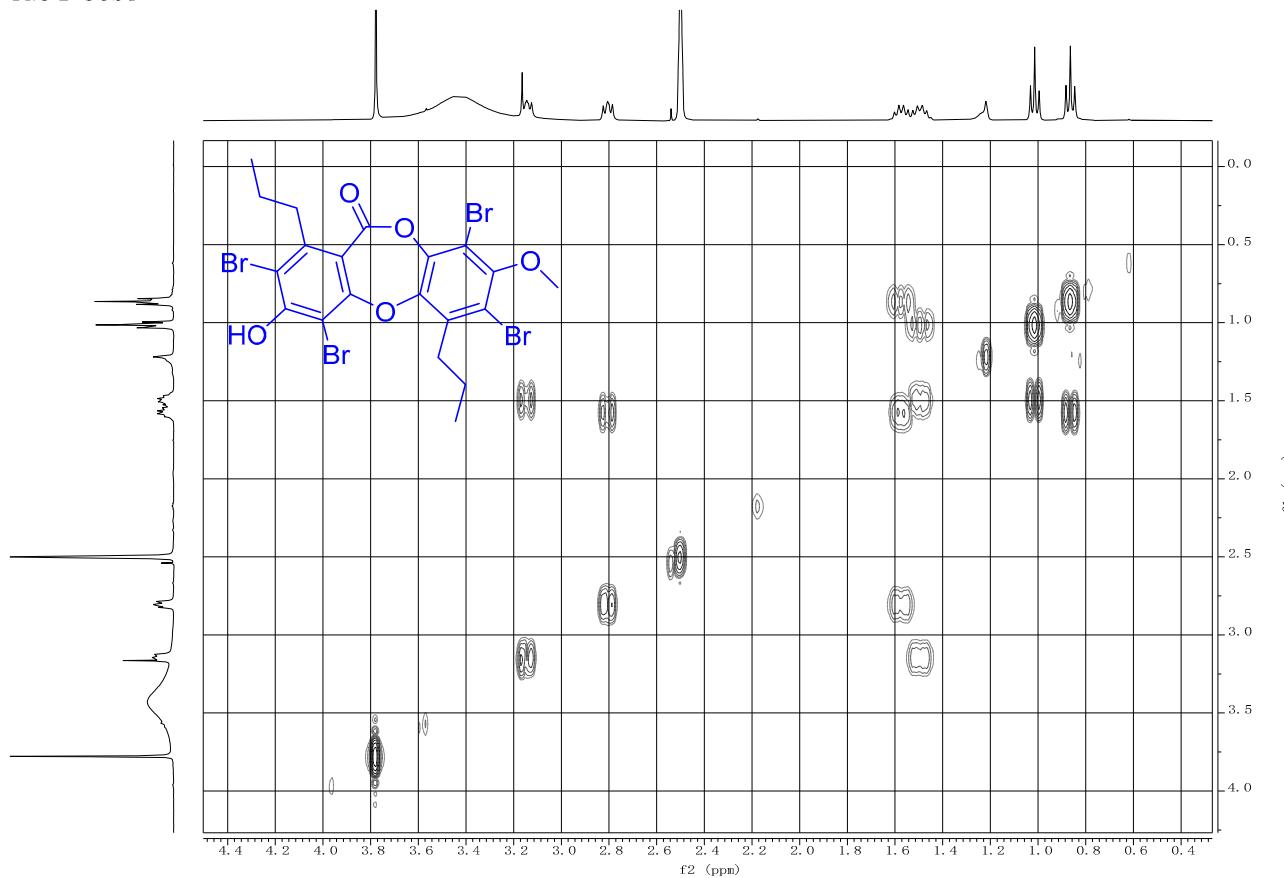


Figure S68. ^1H - ^1H COSY spectrum of **9** in $\text{DMSO}-d_6$

Fr.C-2 HMBC

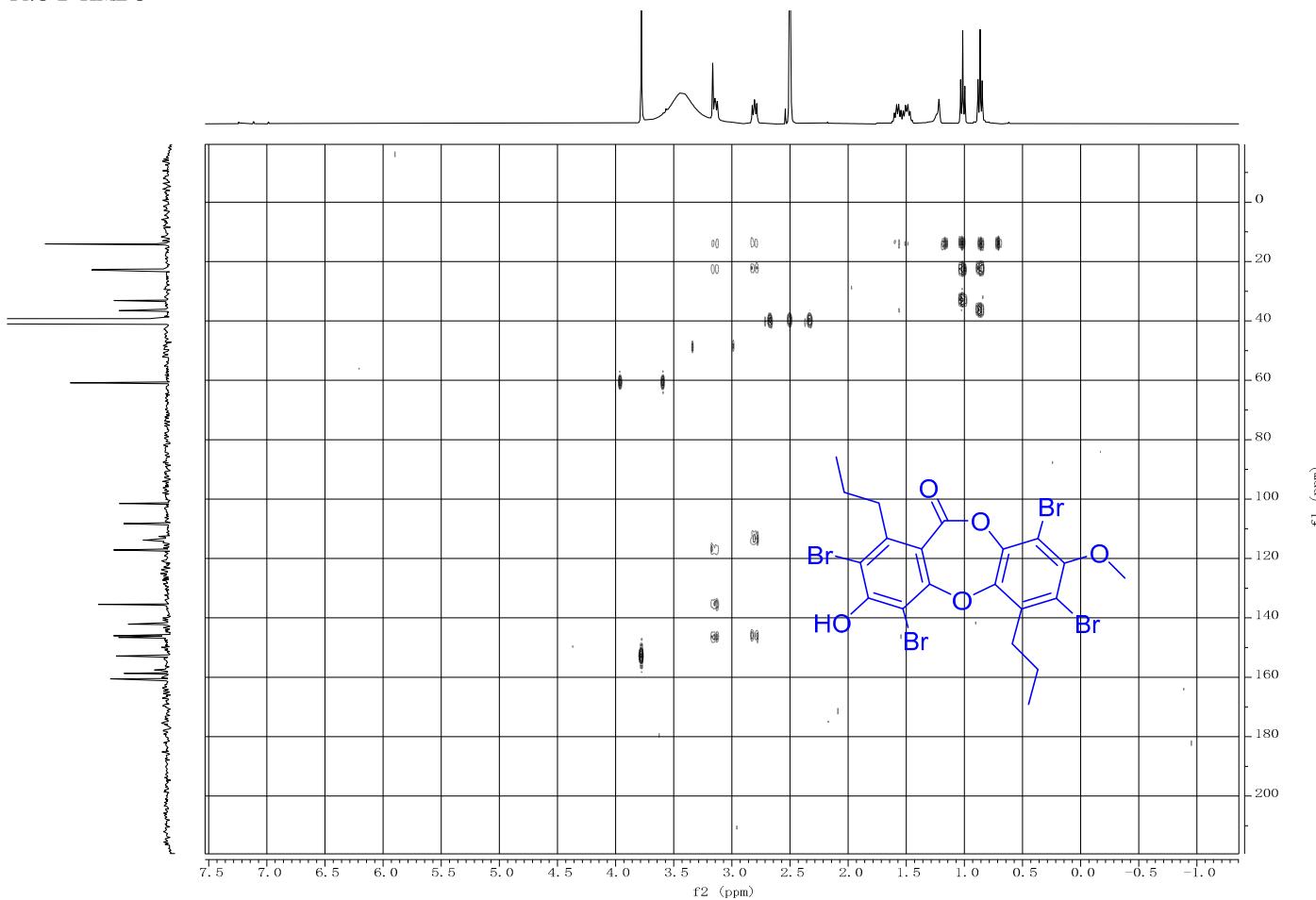
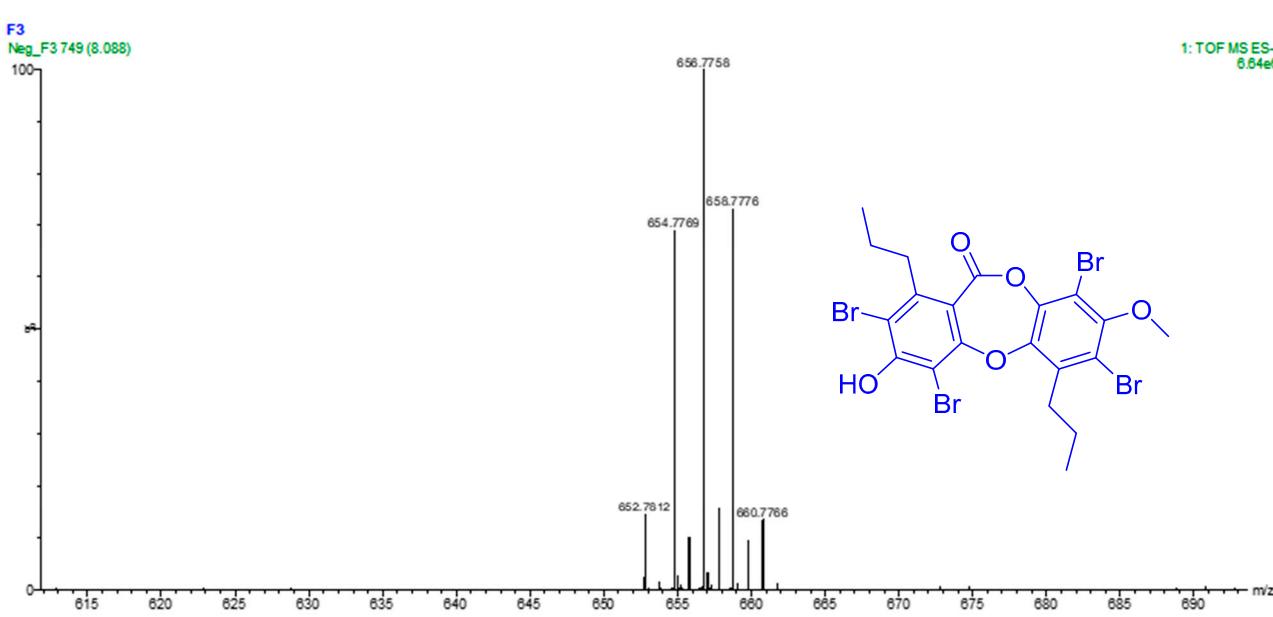


Figure S69. HMBC spectrum of **9** in $\text{DMSO}-d_6$



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

694 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500

H: 0-1000

O: 0-200

Br: 0-8

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O	Br	
652.7812	652.7810	0.2	0.3	10.5	C20 H17 O5 Br4	20	17	5	4	

Figure S70. HRESIMS spectrum of 9

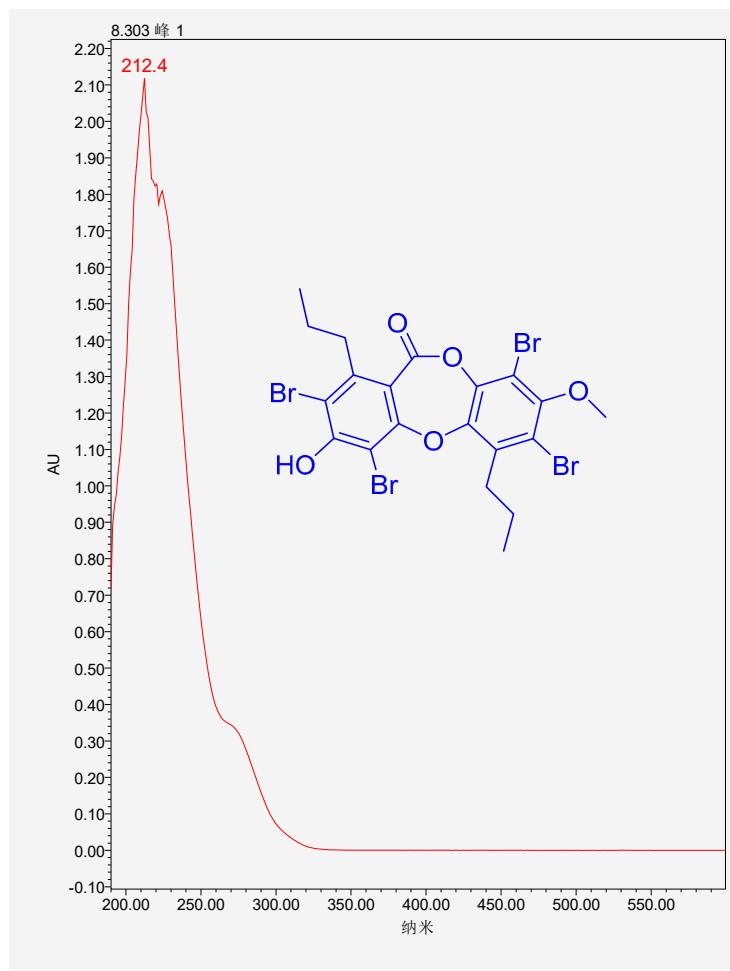


Figure S71. UV spectrum of **9**

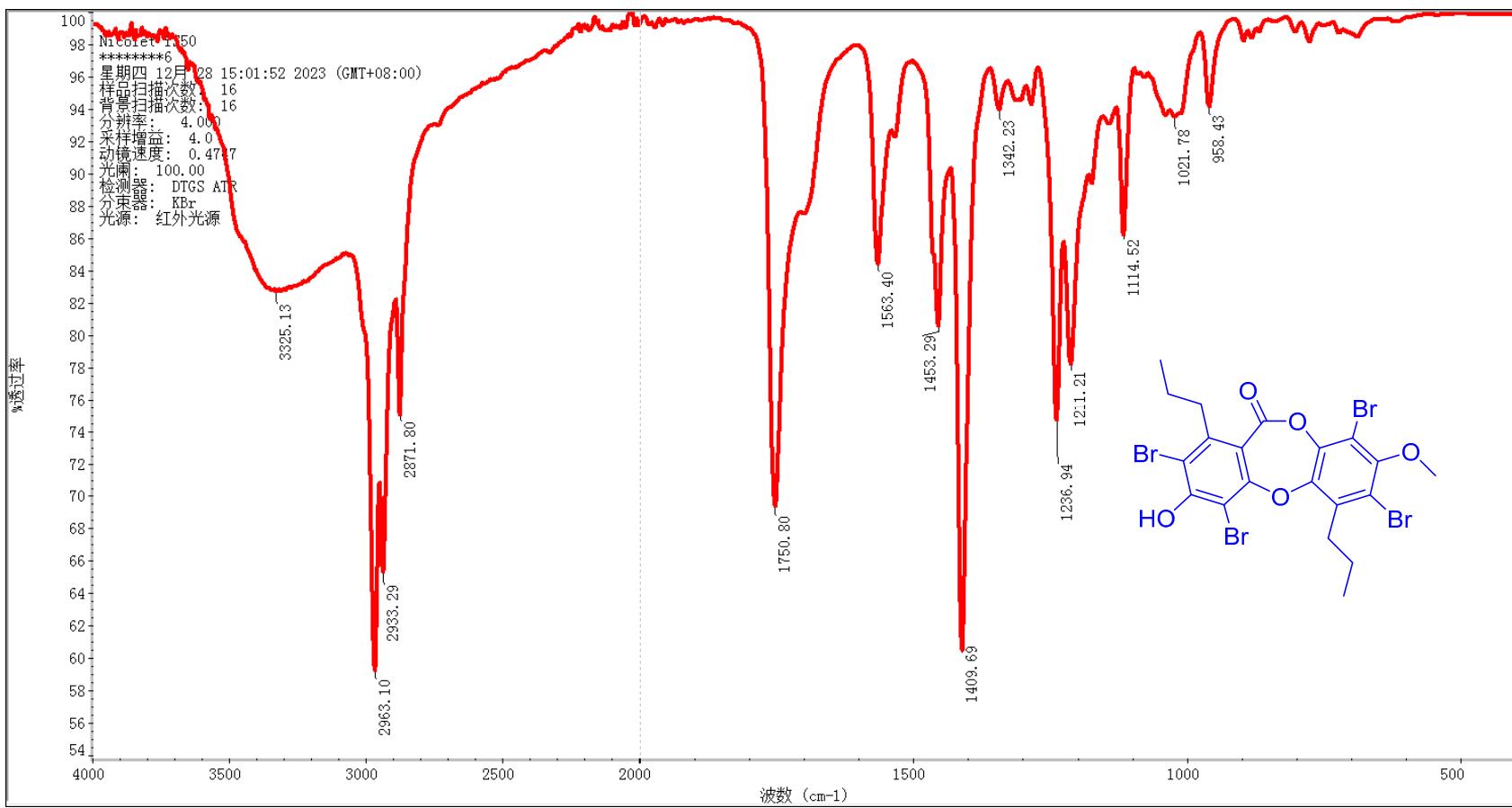


Figure S72. IR spectrum of 9

Table S10. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 10

No.	δ_{H}	δ_{C}	COSY	HMBC
1		112.6, C		
2		157.6, C		
3		102.5, C		
4		157.6, C		
5		114.1, C		
6		144.6, C		
7		161.9, C		
8	2.79, m	36.1, CH ₂	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.53, m	23.0, CH ₂	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.90, t (7.2)	14.1, CH ₃	H ₂ -9	C-8, C-9
1'		150.1, C		
2'		136.5, C		
3'		135.2, C		
4'		110.8, C		
5'		153.9, C		
6'	7.07, s	103.6, C		C-1', C-2', C-4', C-5'
7'	2.81, m	32.3, CH ₂	H ₂ -8'	C-2', C-3', C-4', C-8', C-9'
8'	1.50, m	22.1, CH ₂	H ₂ -7', H ₃ -9'	C-3', C-7', C-9'
9'	0.90, t (7.2)	14.4, CH ₃	H ₂ -8'	C-7', C-8'
MeO	3.85, s	57.3, CH ₃		C-5'

M-16-5 500 MHz DMSO

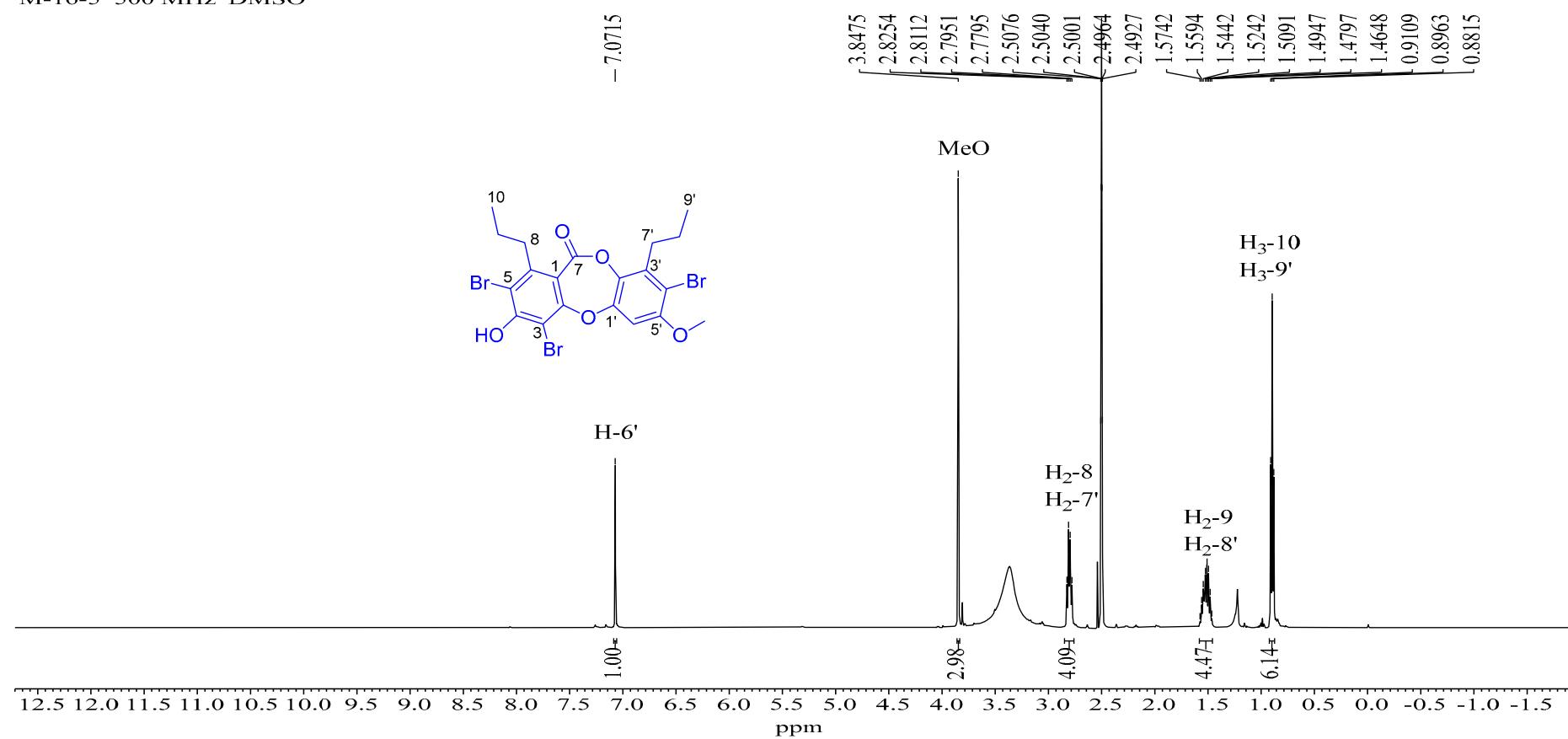


Figure S73. ¹H-NMR spectrum of **10** in DMSO-*d*₆ (500 MHz)

M-16-5 C

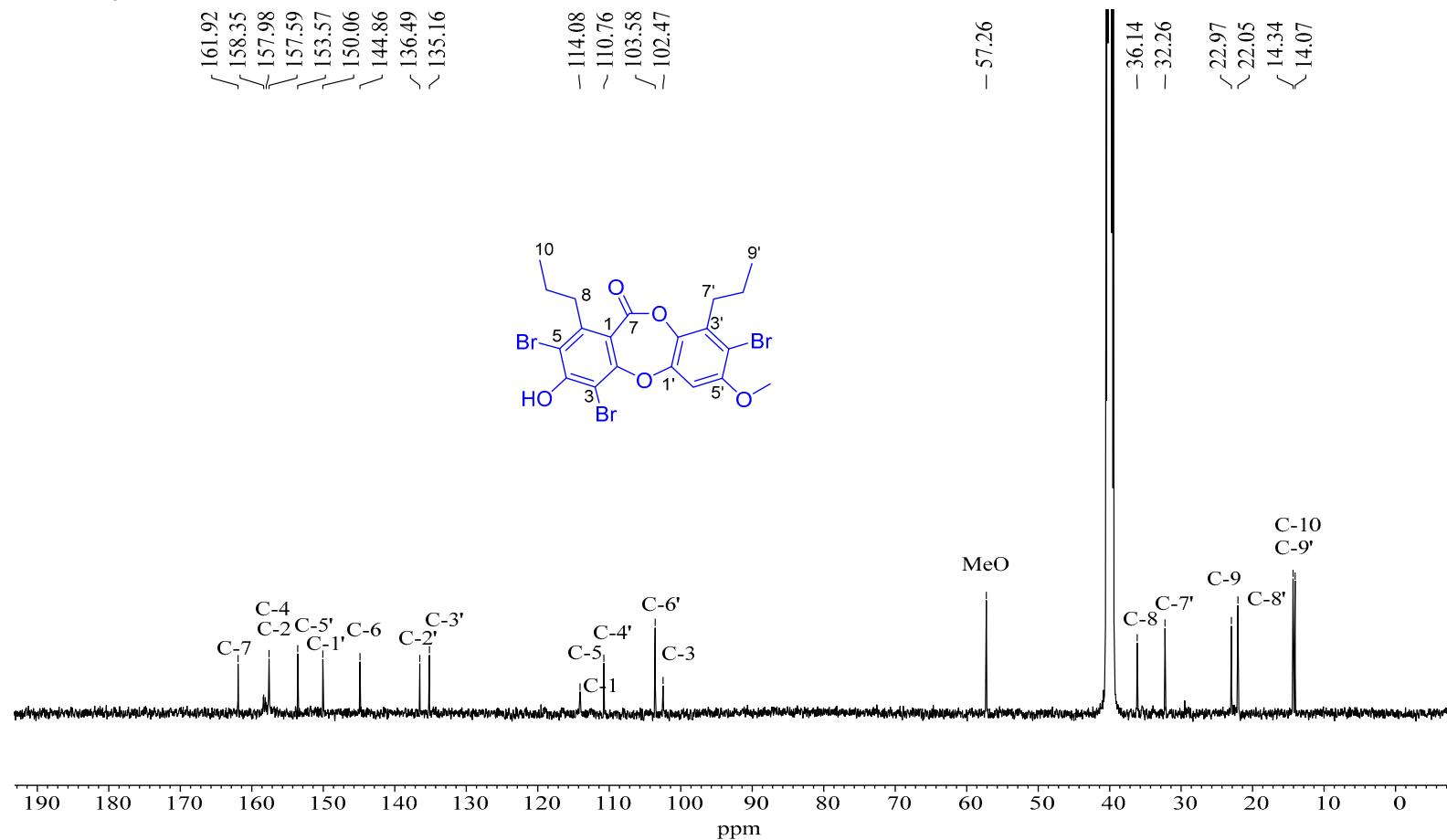


Figure S74. ^{13}C -NMR spectrum of **10** in $\text{DMSO}-d_6$ (125 MHz)

M-16-5 HSQC

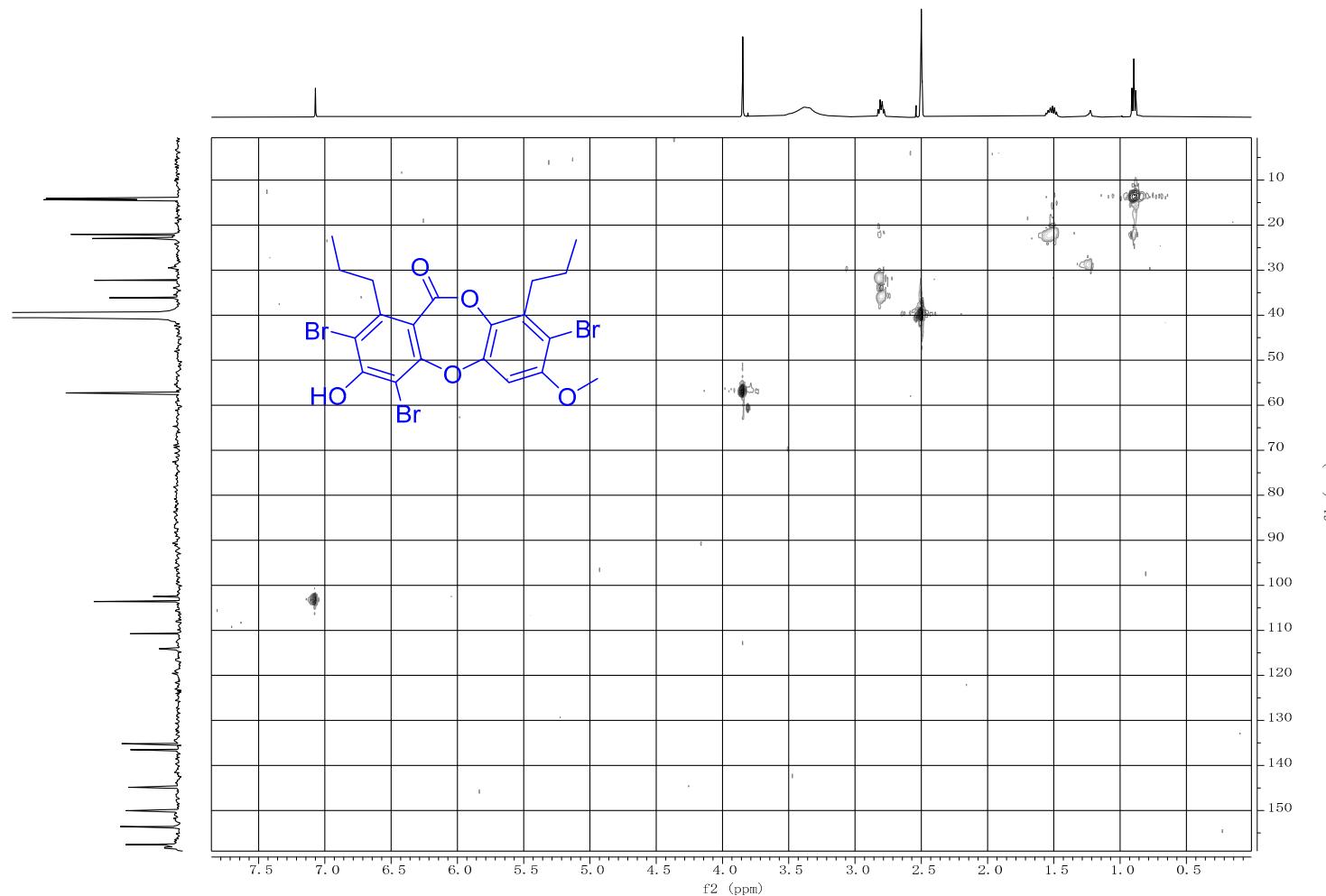


Figure S75. HSQC spectrum of **10** in $\text{DMSO}-d_6$

M-16-5 COSY

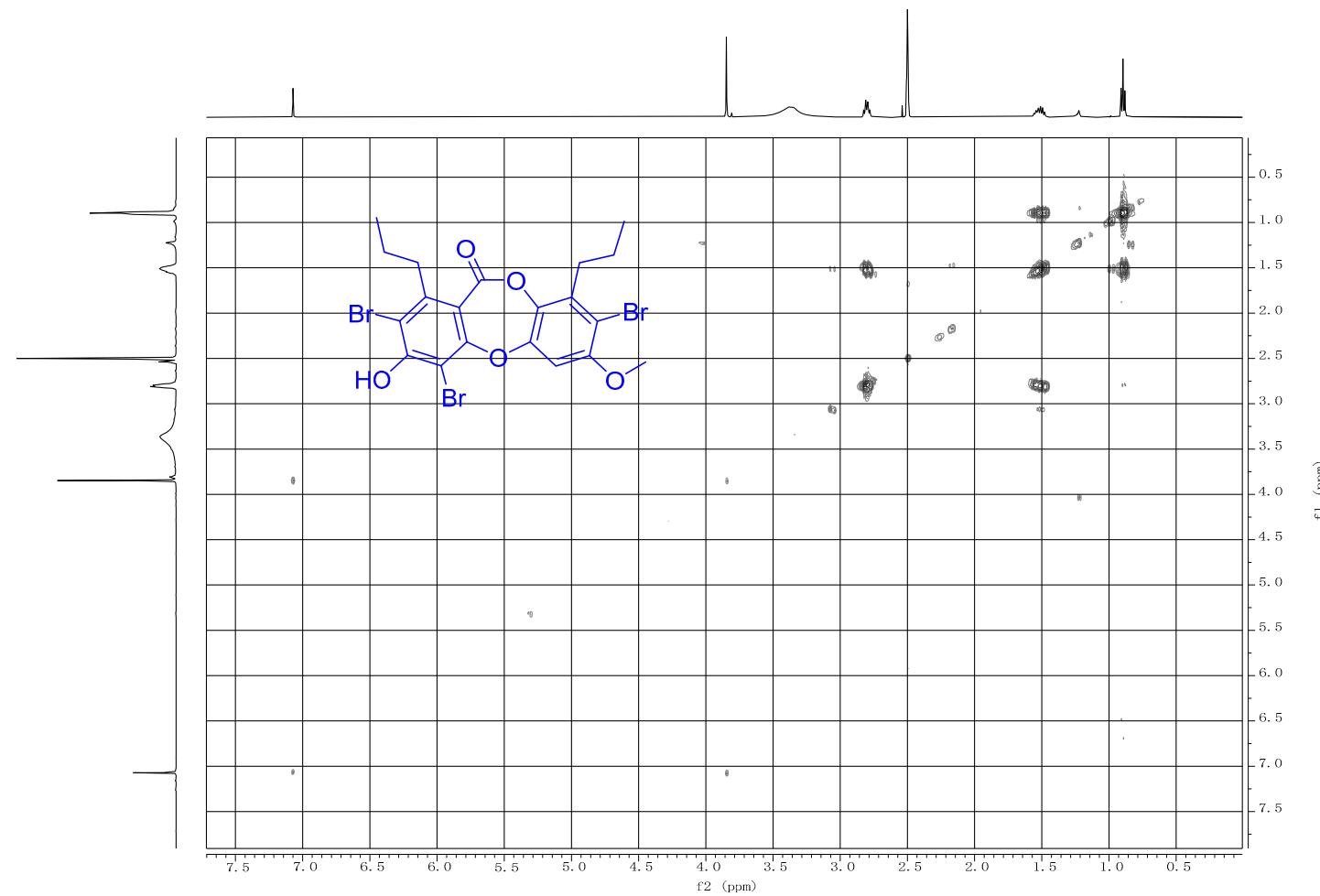


Figure S76. ^1H - ^1H COSY spectrum of **10** in $\text{DMSO}-d_6$

M-16-5 HMBC

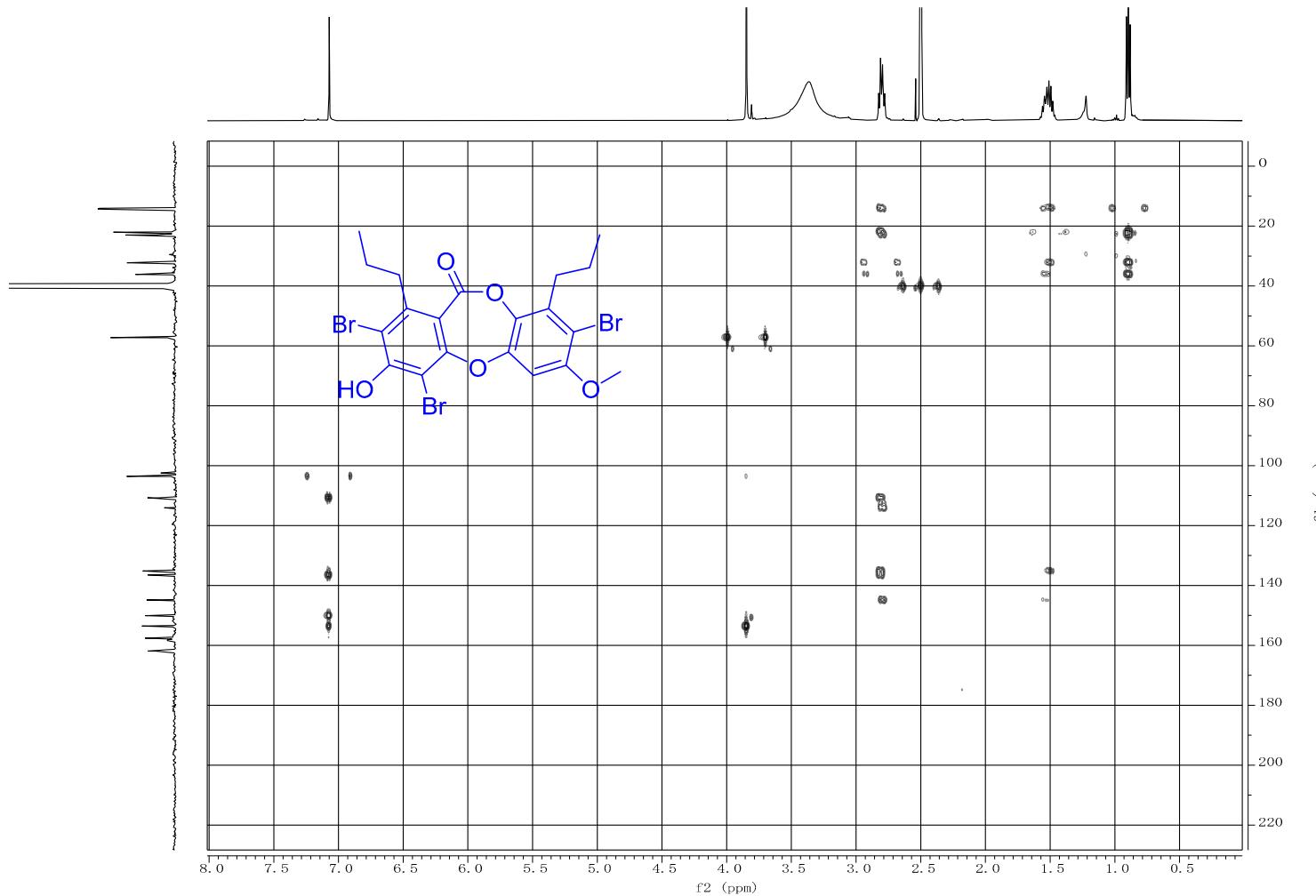
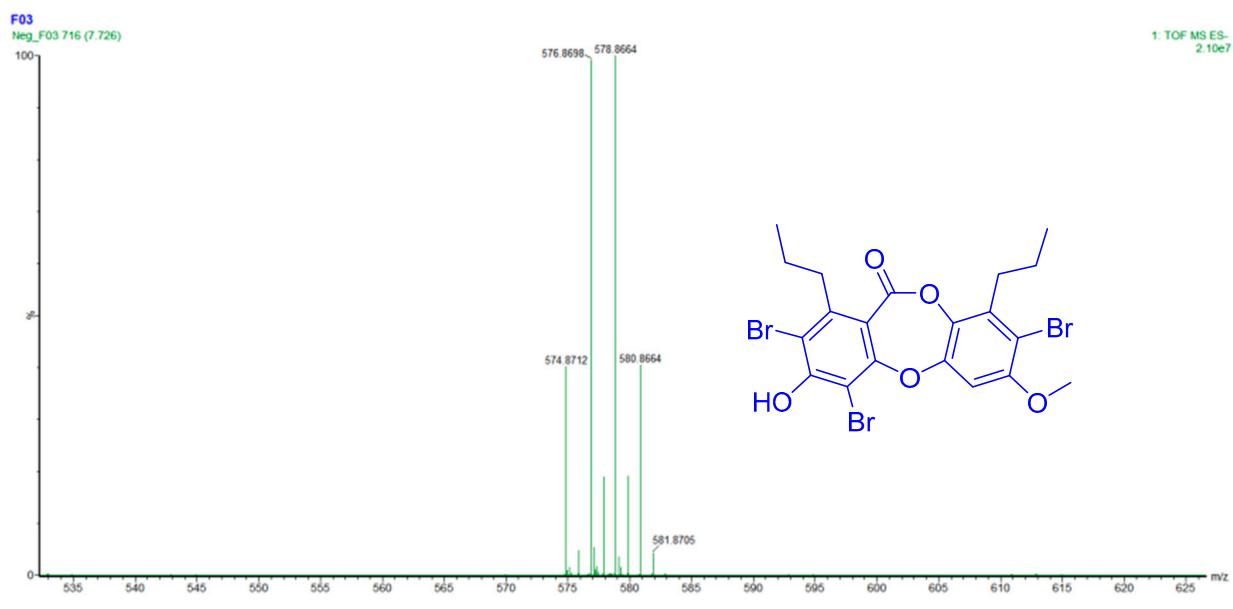


Figure S77. HMBC spectrum of **10** in $\text{DMSO}-d_6$



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

510 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Br: 0-8

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O	Br	
574.8712	574.8704	0.8	1.4	10.5	C20 H18 O5 Br3	20	18	5	3	

Figure S78. HRESIMS spectrum of 10

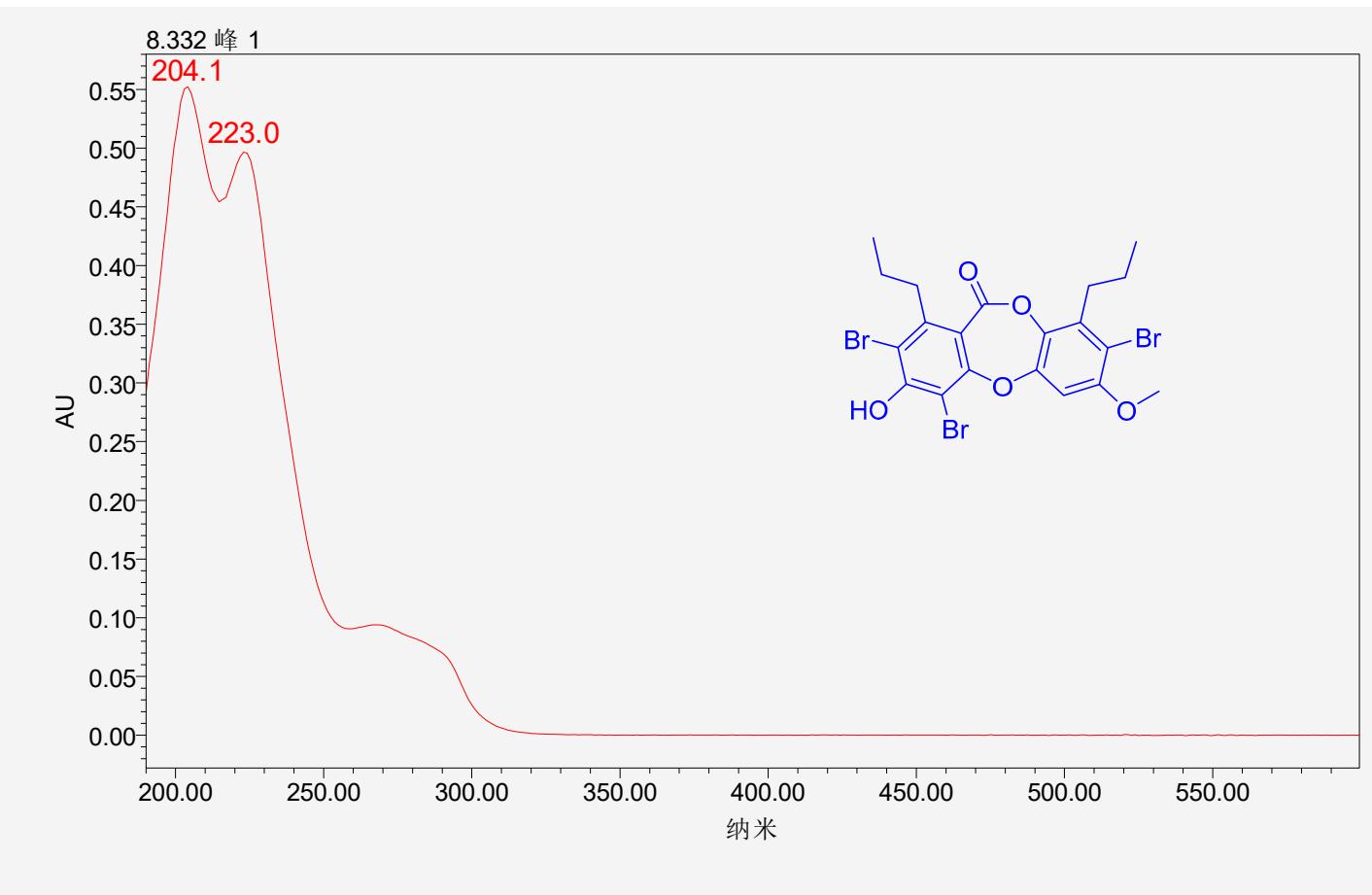


Figure S79. UV spectrum of **10**

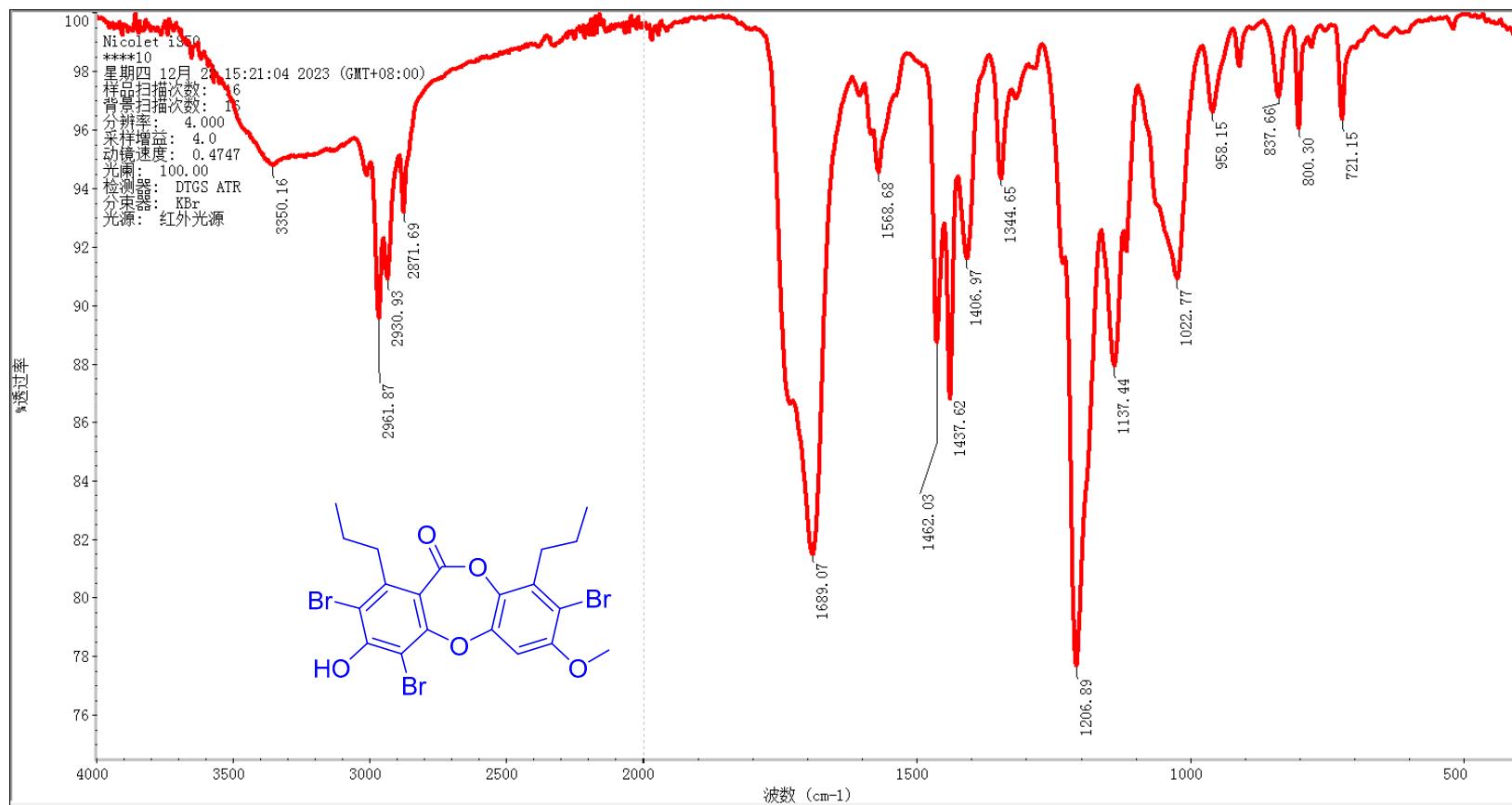


Figure S80. IR spectrum of **10**

Table S11. ^1H and ^{13}C NMR data and key COSY and HMBC correlations of 11

No.	δ_{H}	δ_{C}	COSY	HMBC
1		112.2, C		
2		158.9, C		
3		102.2, C		
4		151.1, C		
5		116.2, C		
6		145.7, C		
7		161.6, C		
8	2.72, t (8.0)	36.9, CH ₂	H ₂ -9	C-1, C-5, C-6, C-9, C-10
9	1.56, m	23.0, CH ₂	H ₂ -8, H ₃ -10	C-6, C-8, C-10
10	0.87, t (7.2)	14.5, CH ₃	H ₂ -9	C-8, C-9
1'		149.1, C		
2'		141.9, C		
3'		134.0, C		
4'		117.5, C		
5'		152.0, C		
6'		108.3, C		
7'	2.83, t (7.5)	32.5, CH ₂	H ₂ -8'	C-2', C-3', C-4', C-8', C-9'
8'	1.54, m	22.0, CH ₂	H ₂ -7', H ₃ -9'	C-3', C-7', C-9'
9'	0.92, t (7.2)	14.0, CH ₃	H ₂ -8'	C-7', C-8'
MeO	3.78, s	60.8, CH ₃		C-5'

Fr.C-3 600 MHz DMSO

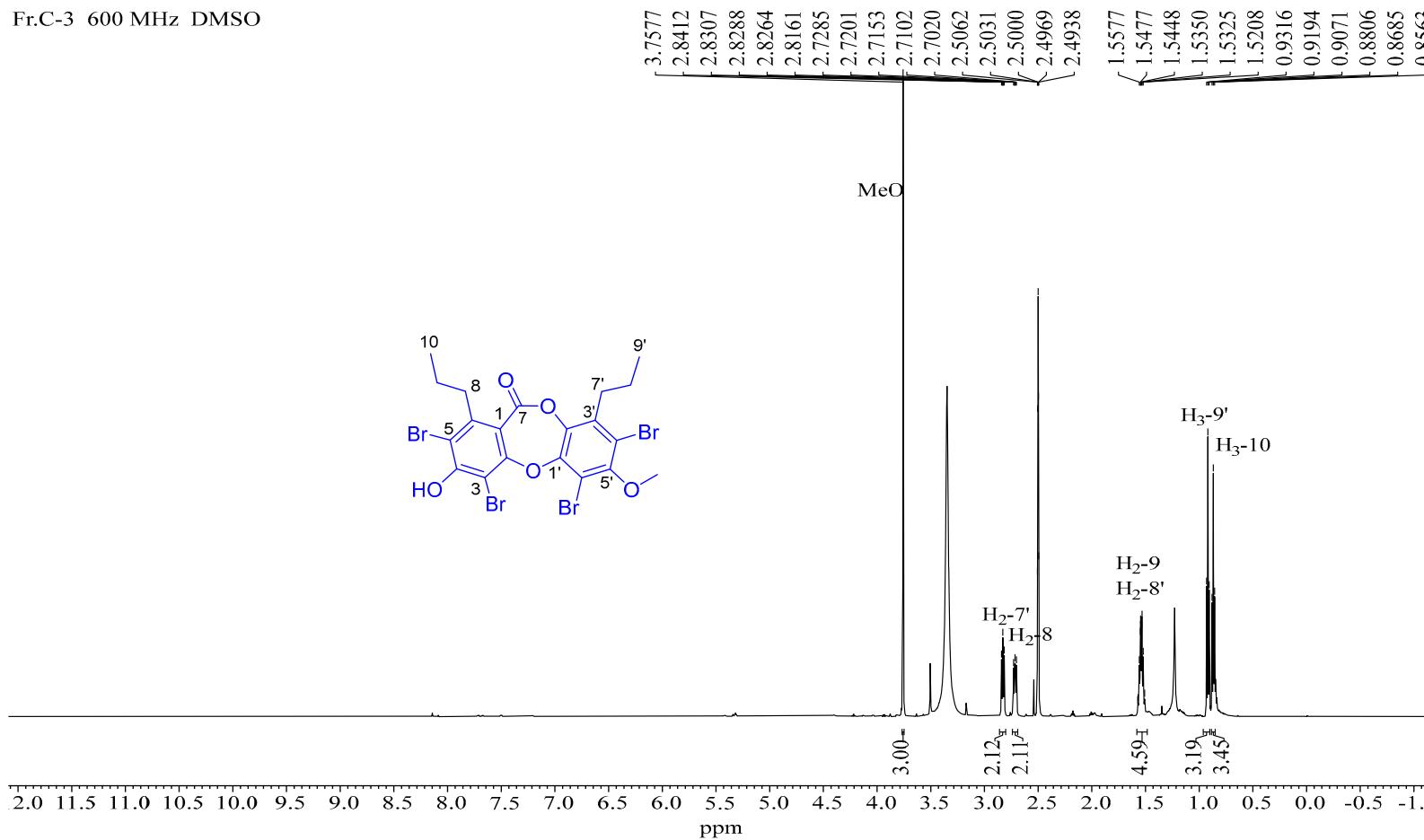


Figure S81. ^1H -NMR spectrum of **11** in $\text{DMSO}-d_6$ (600 MHz)

Fr.C-3 C

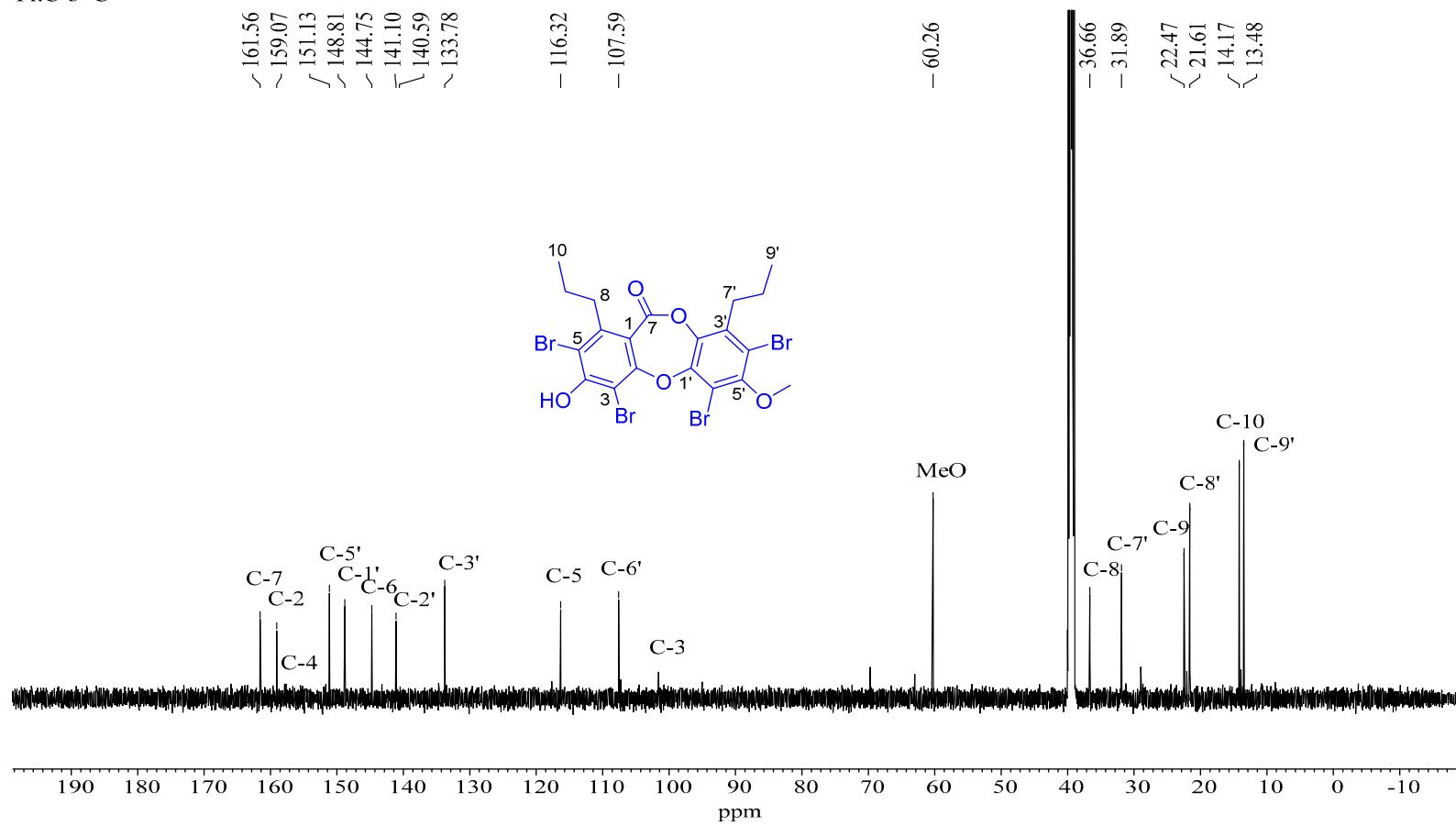


Figure S82. ^{13}C -NMR spectrum of **11** in $\text{DMSO}-d_6$ (150 MHz)

Fr.C-3 HSQC

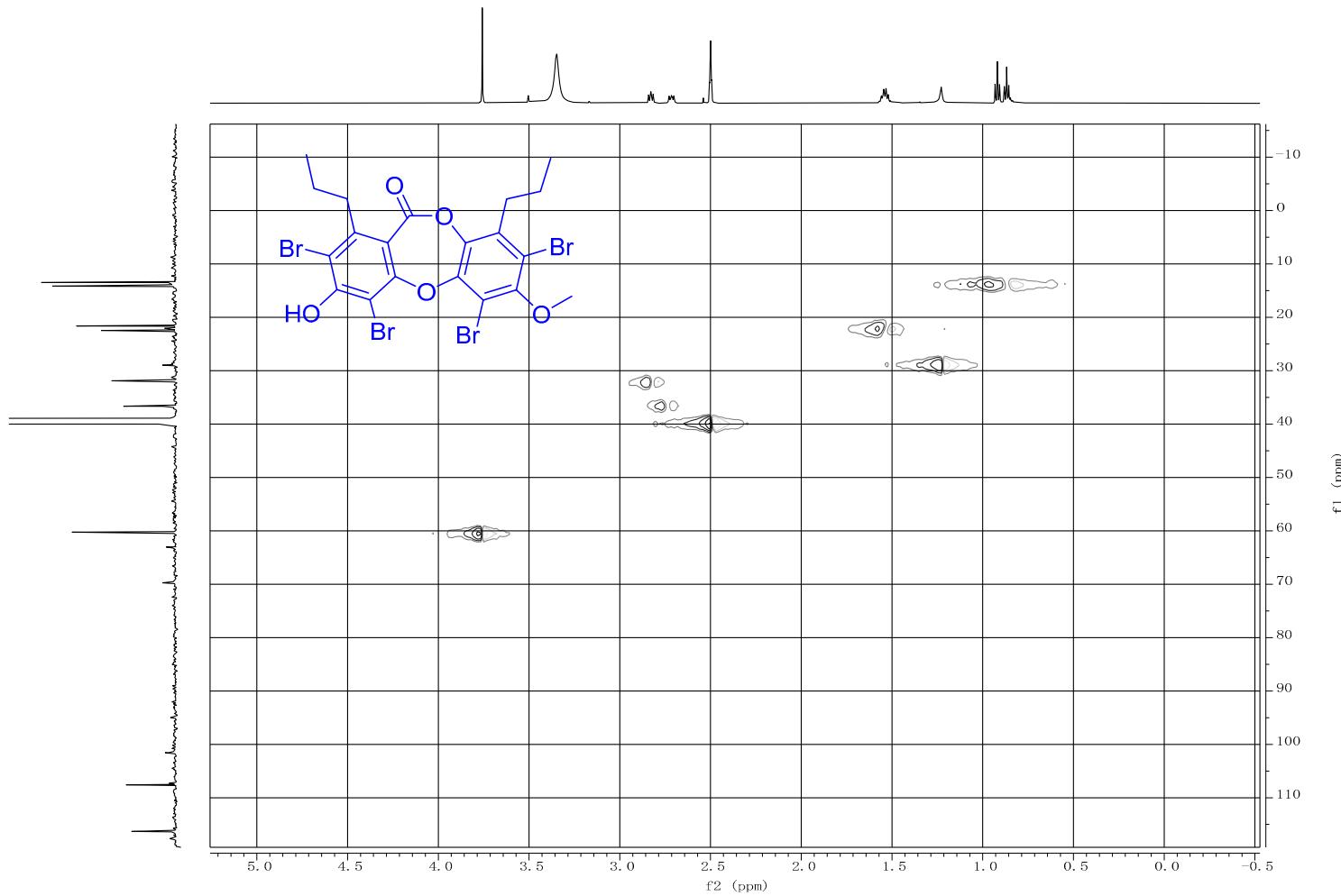


Figure S83. HSQC spectrum of **11** in $\text{DMSO}-d_6$

Fr.C-3 COSY

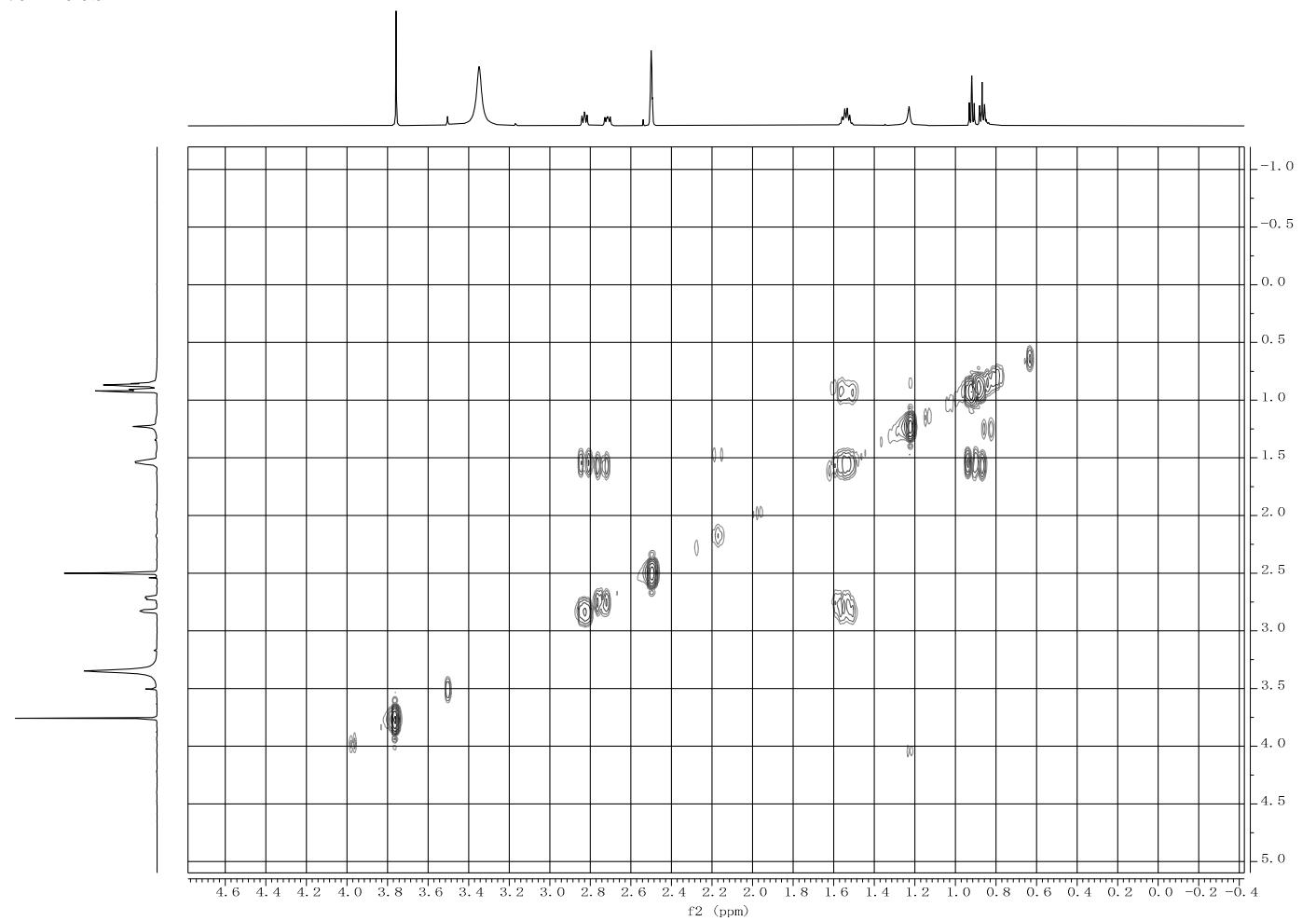


Figure S84. ^1H - ^1H COSY spectrum of **11** in $\text{DMSO}-d_6$

Fr.C-3 HMBC

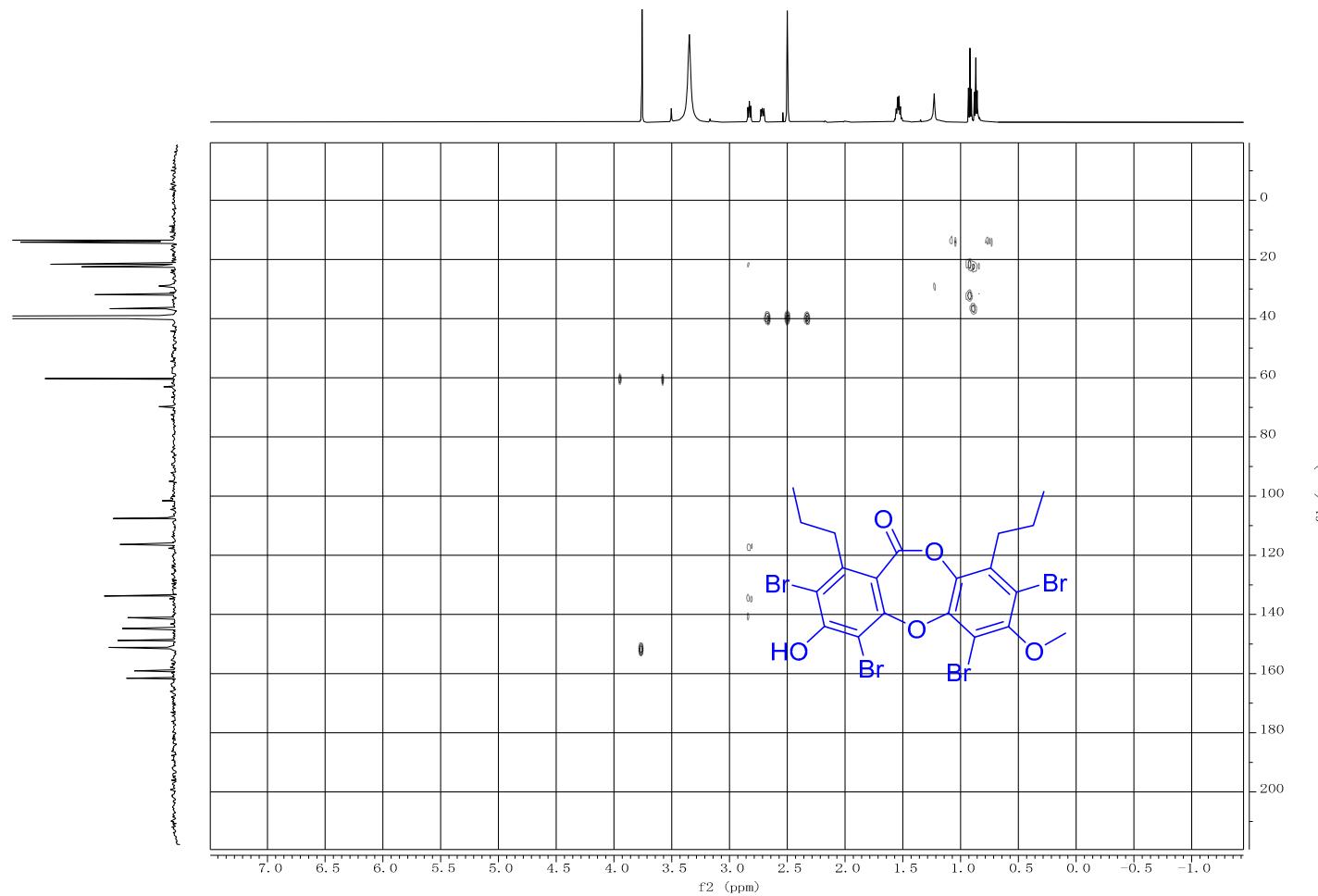
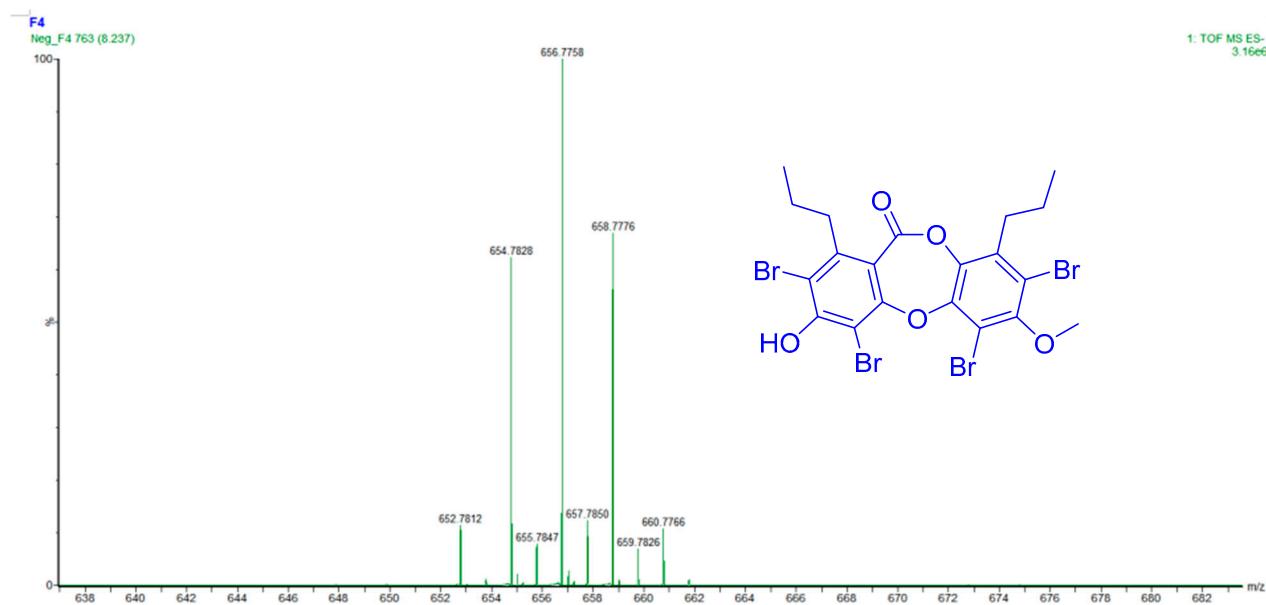


Figure S85. HMBC spectrum of **11** in $\text{DMSO}-d_6$



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

694 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Br: 0-8

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O	Br	
652.7812	652.7810	0.2	0.3	10.5	C20 H17 O5 Br4	20	17	5	4	

Figure S86. HRESIMS spectrum of 11

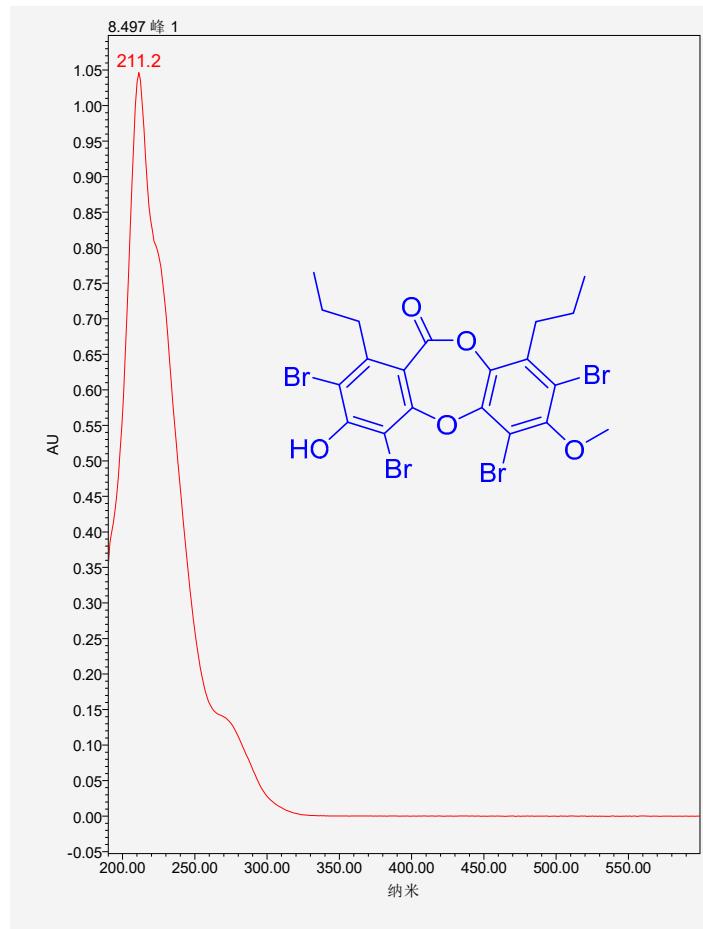


Figure S87. UV spectrum of **11**

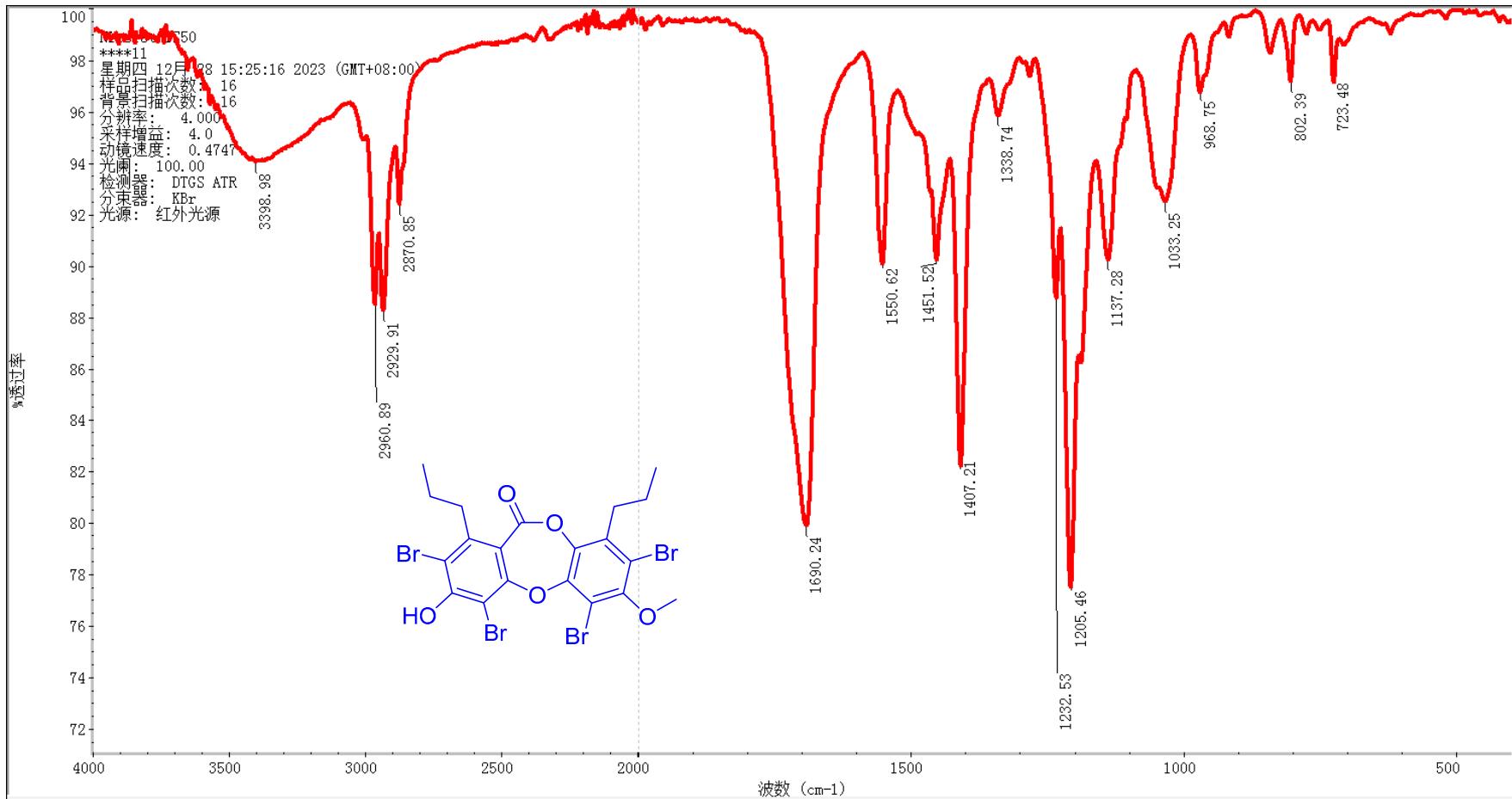


Figure S88. IR spectrum of 11

N-3-4 500 MHz DMSO

- 10.6260

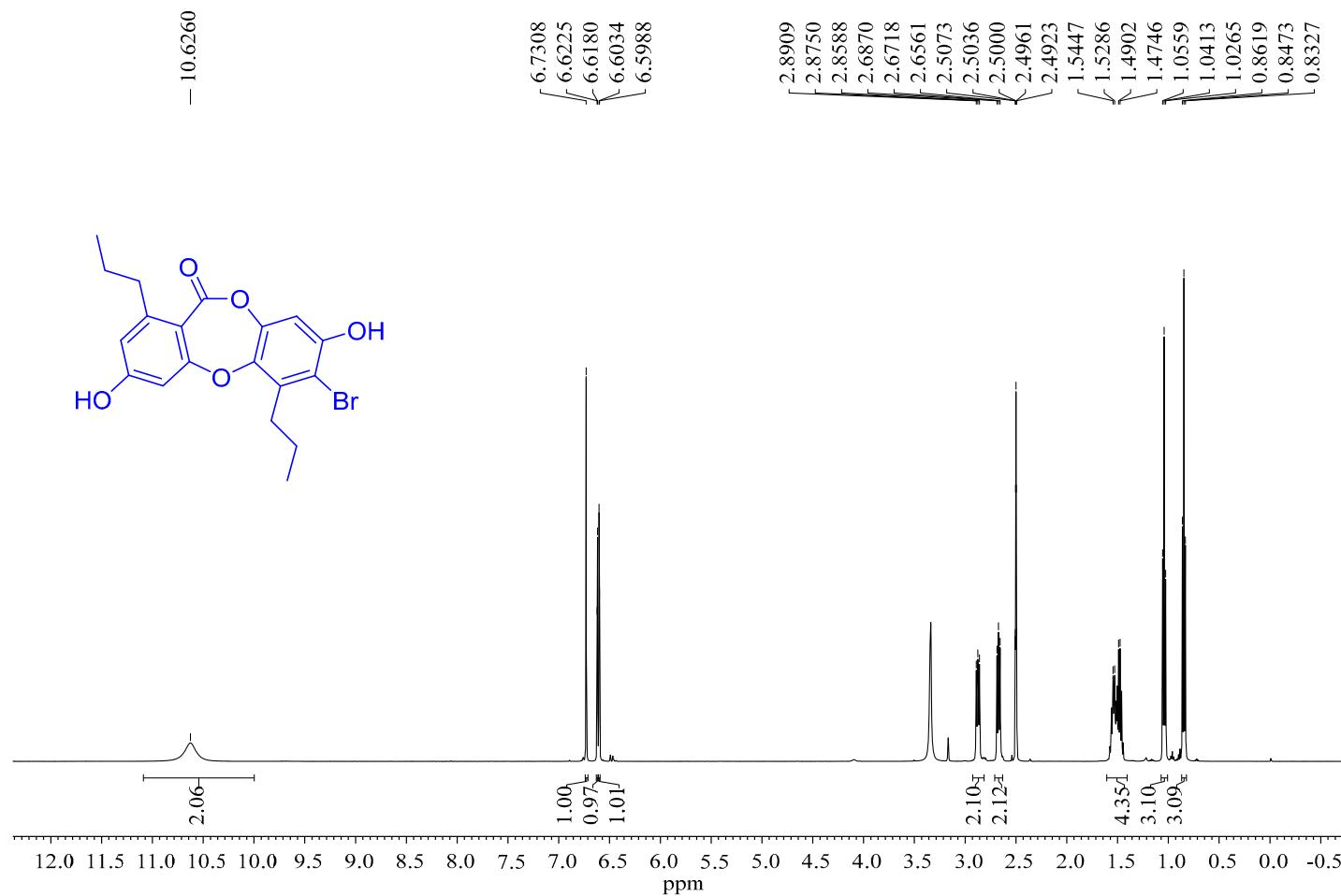
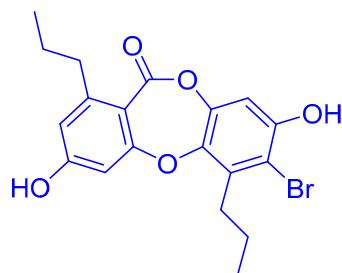


Figure S89. ¹H-NMR spectrum of **12** in DMSO-d₆ (500 MHz)

N-3-4 APT

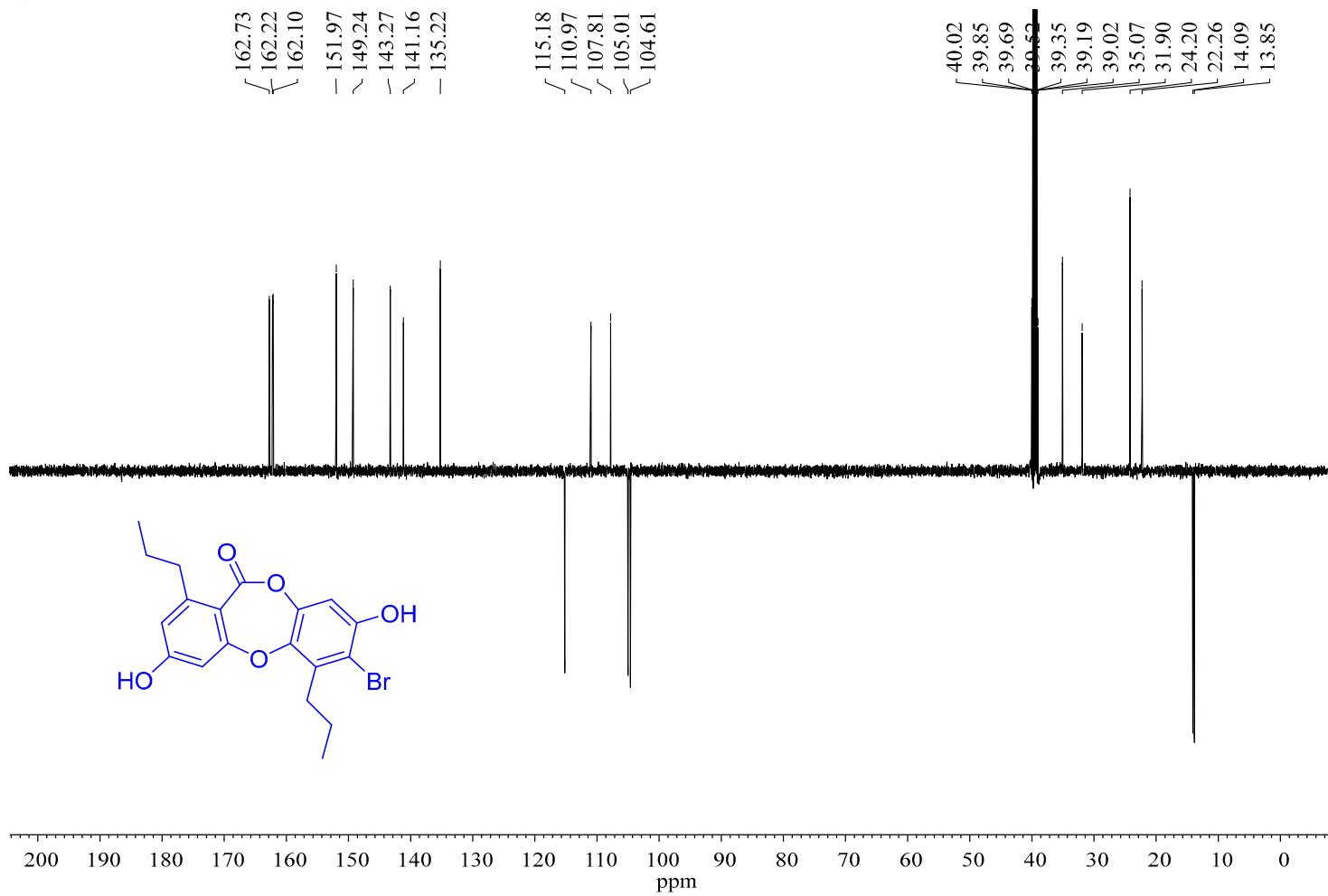


Figure S90. APT spectrum of **12** in $\text{DMSO}-d_6$ (125 MHz)

N-3-4 HSQC

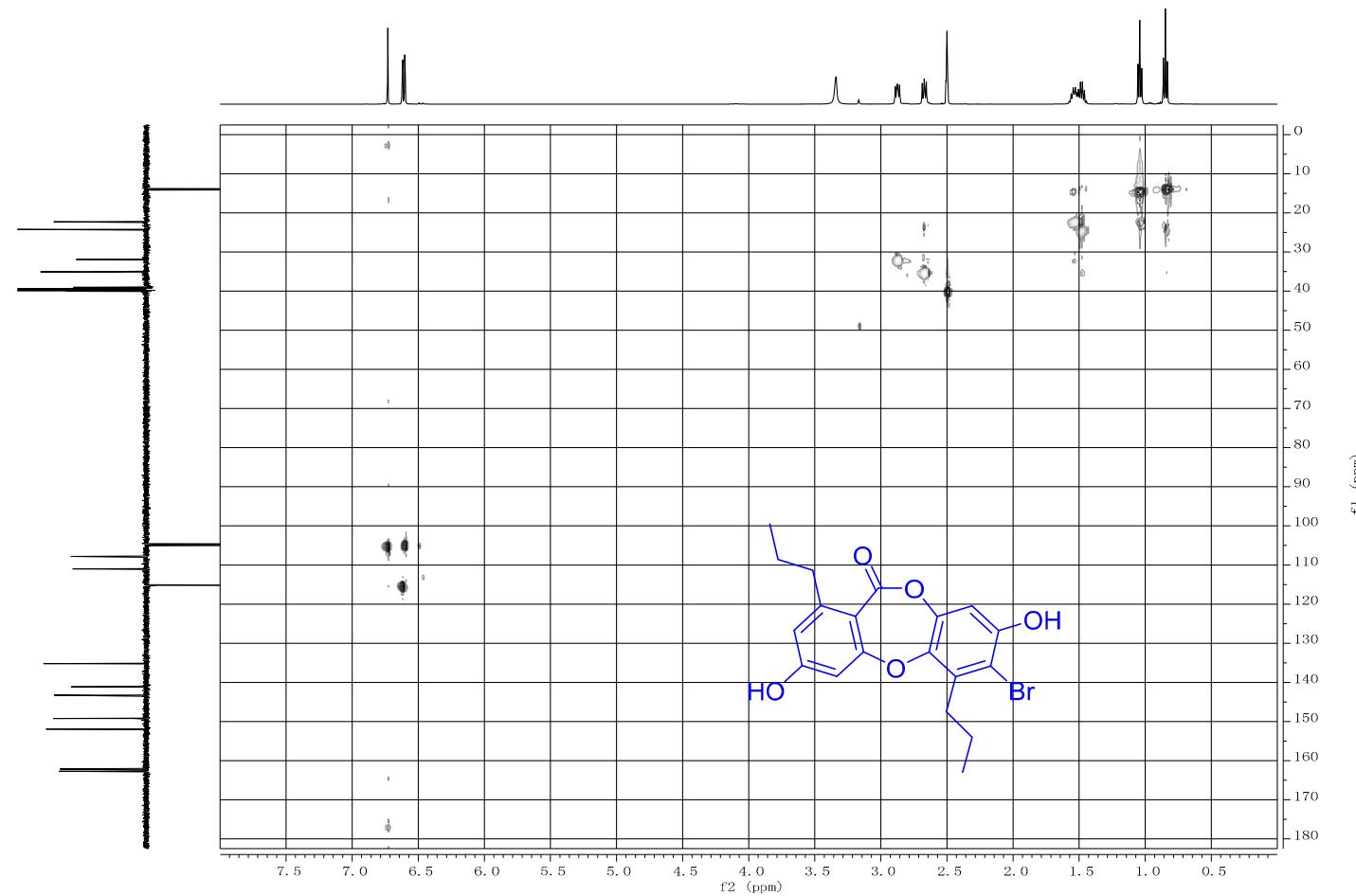


Figure S91. HSQC spectrum of **12** in $\text{DMSO}-d_6$

N-3-4 COSY

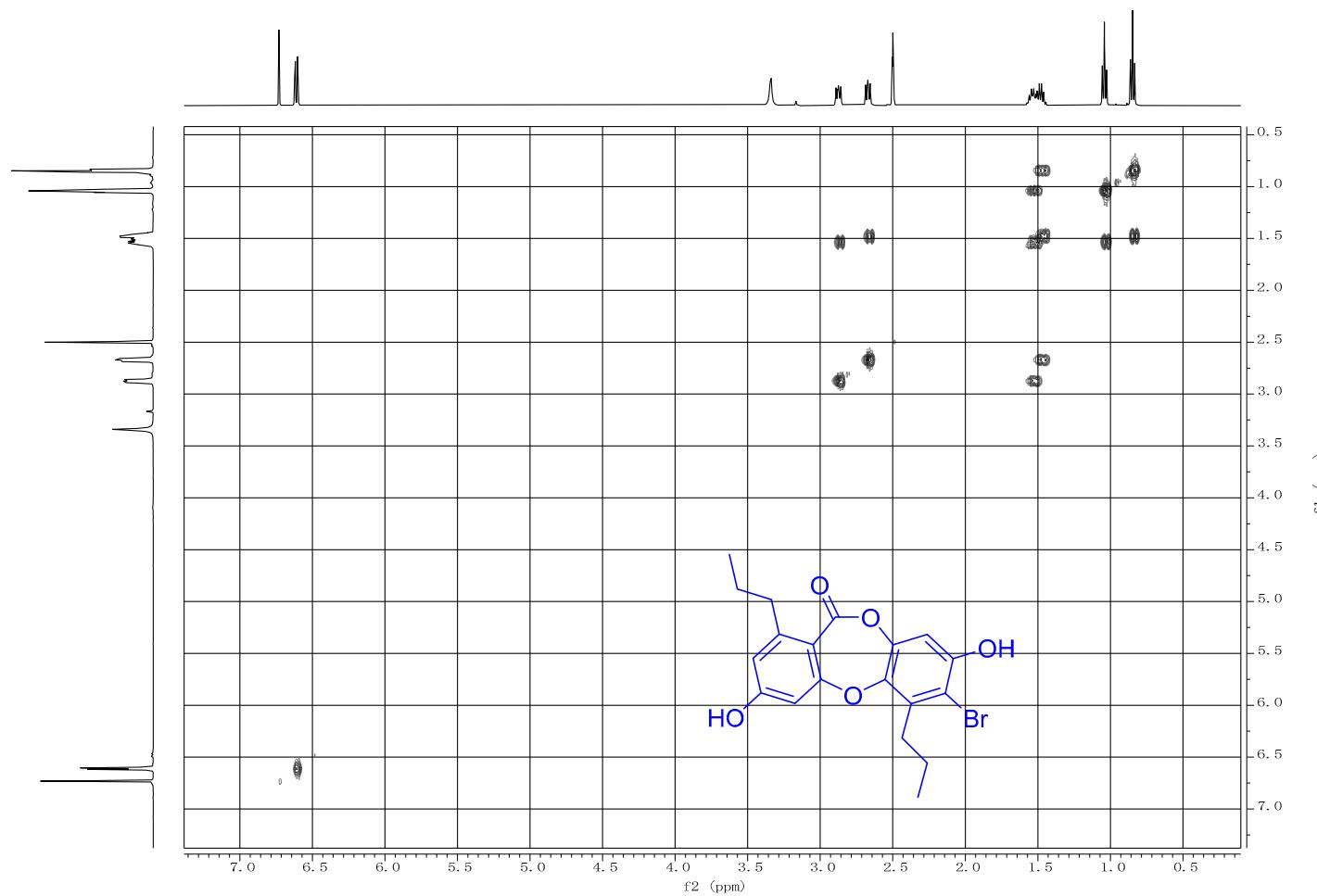


Figure S92. ^1H - ^1H COSY spectrum of **12** in $\text{DMSO}-d_6$

N-3-4 HMBC

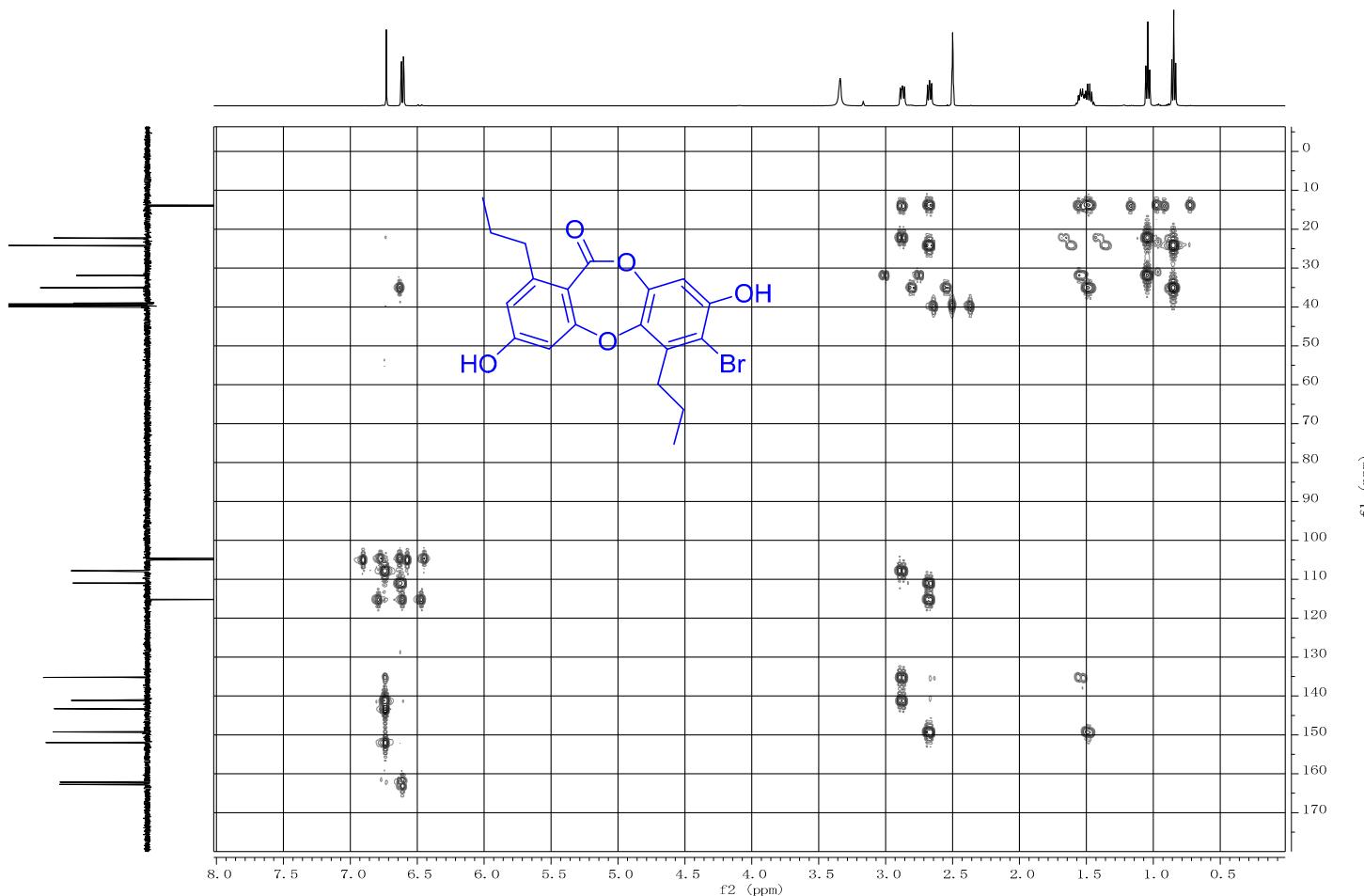
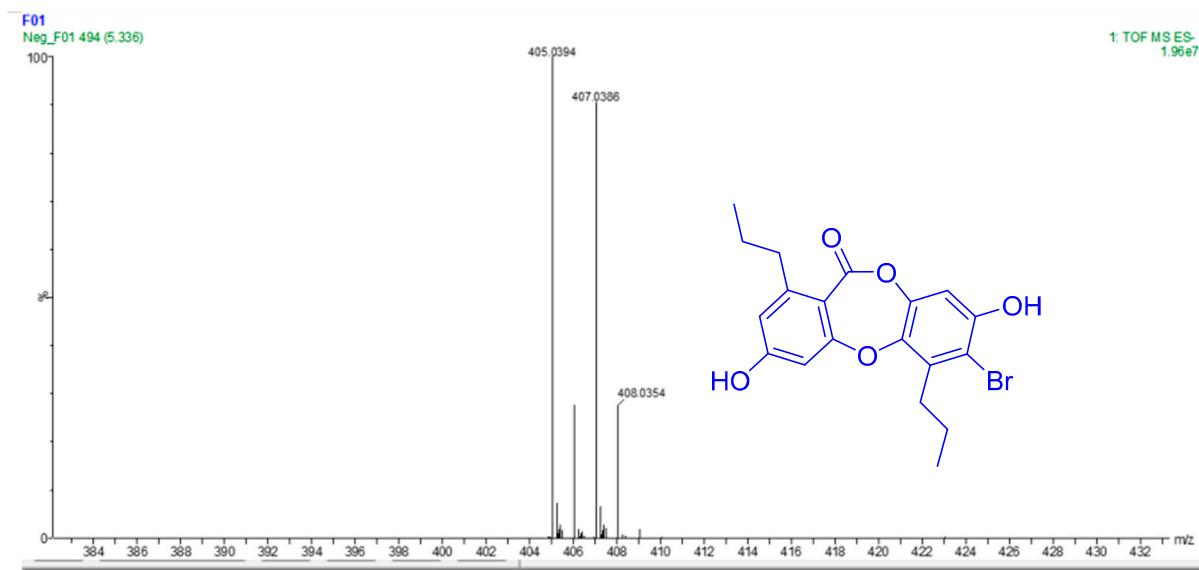


Figure S93. HMBC spectrum of **12** in $\text{DMSO}-d_6$



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

213 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500

H: 0-1000

O: 0-200

Br: 0-8

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O	Br
405.0348	405.0396	-4.8	-11.9	1.5	C12 H22 O10...	12	22	10	1
	405.0338	1.0	2.5	10.5	C19 H18 O5 Br	19	18	5	1
	405.0340	0.8	2.0	30.5	C32 H5 O	32	5	1	

Figure S94. HRESIMS spectrum of 12

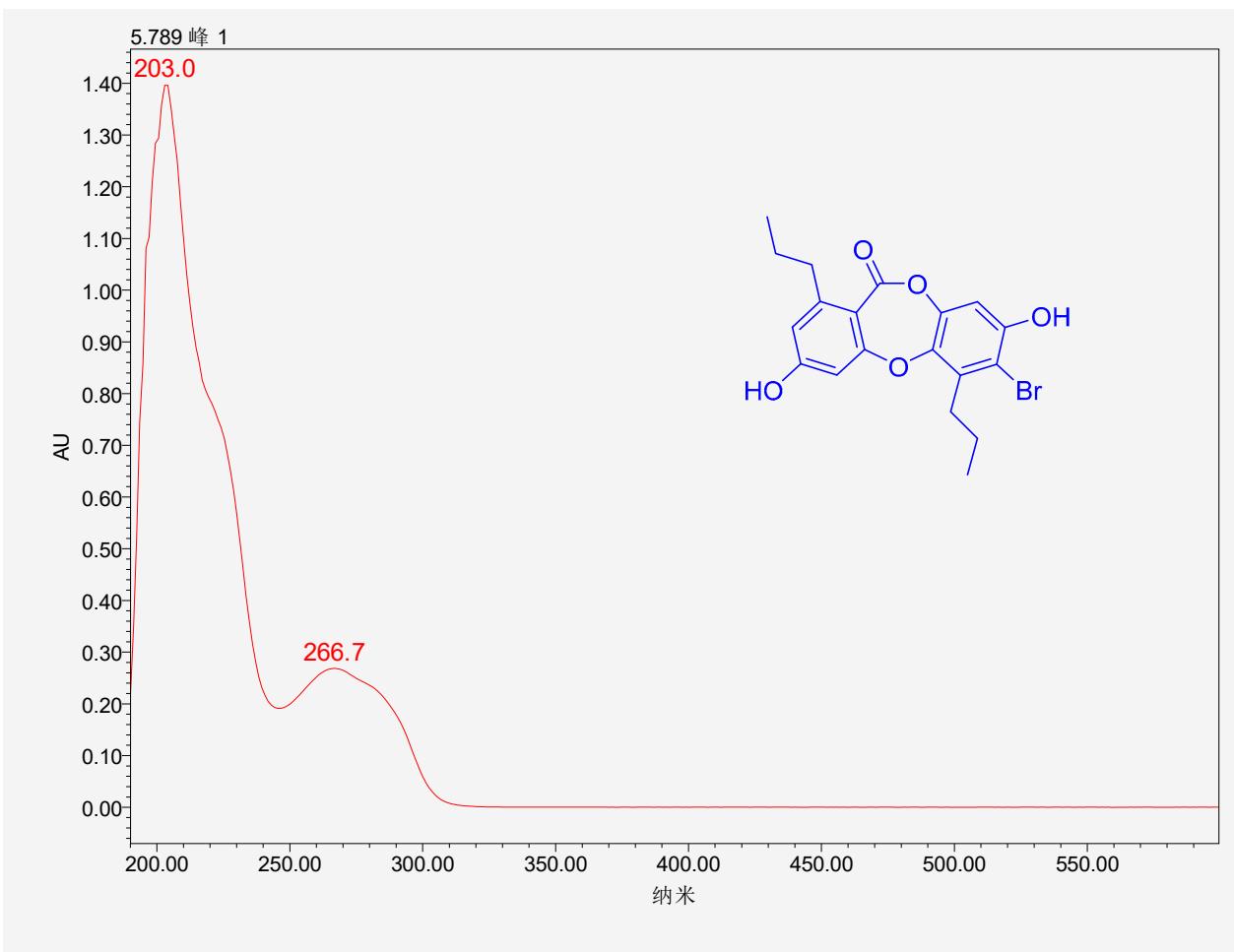


Figure S95. UV spectrum of **12**

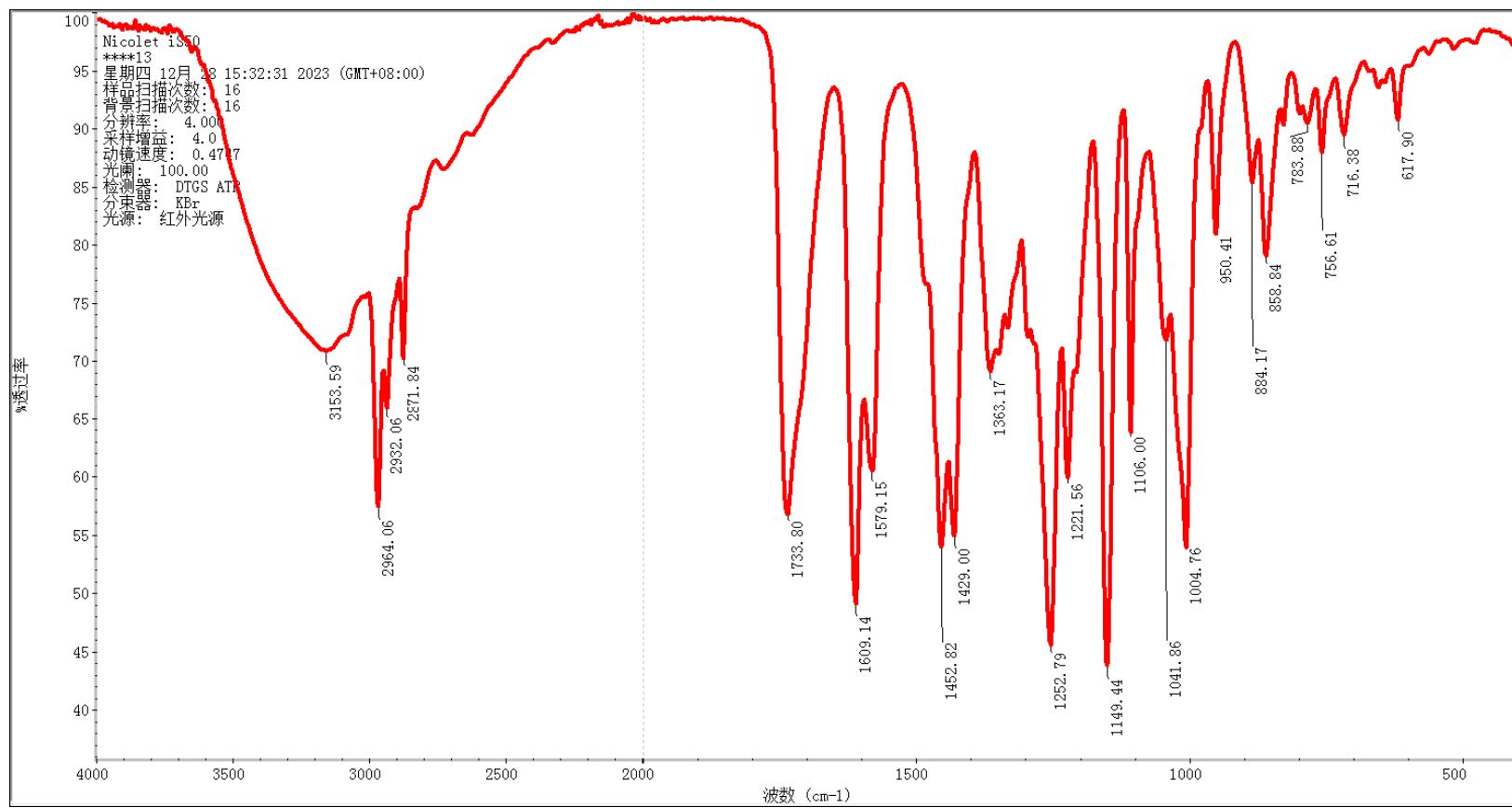


Figure S96. IR spectrum of **12**

I-6-1-1 500 MHz DMSO

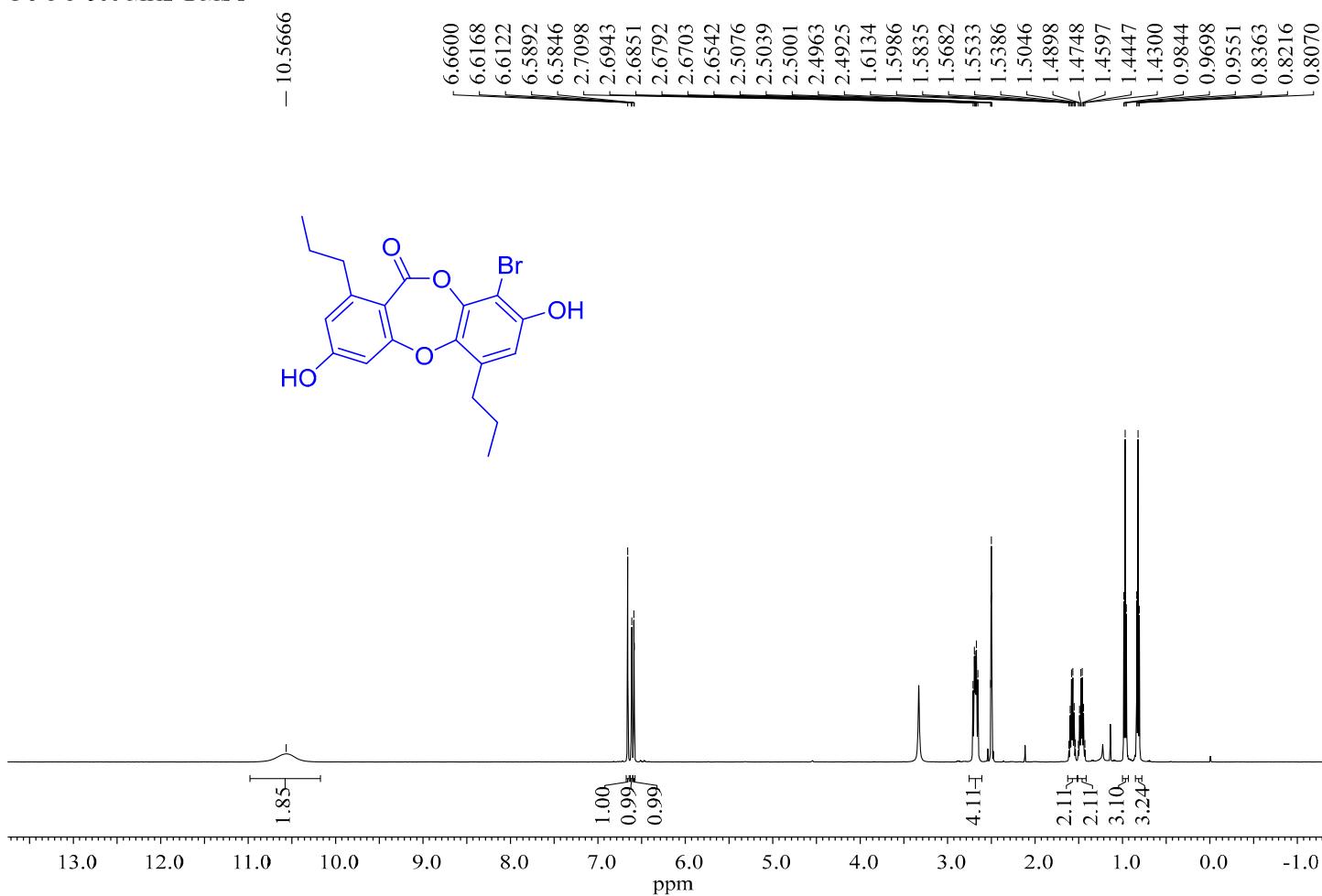


Figure S97. ^1H -NMR spectrum of **13** in $\text{DMSO}-d_6$ (500 MHz)

I-6-1-1 APT

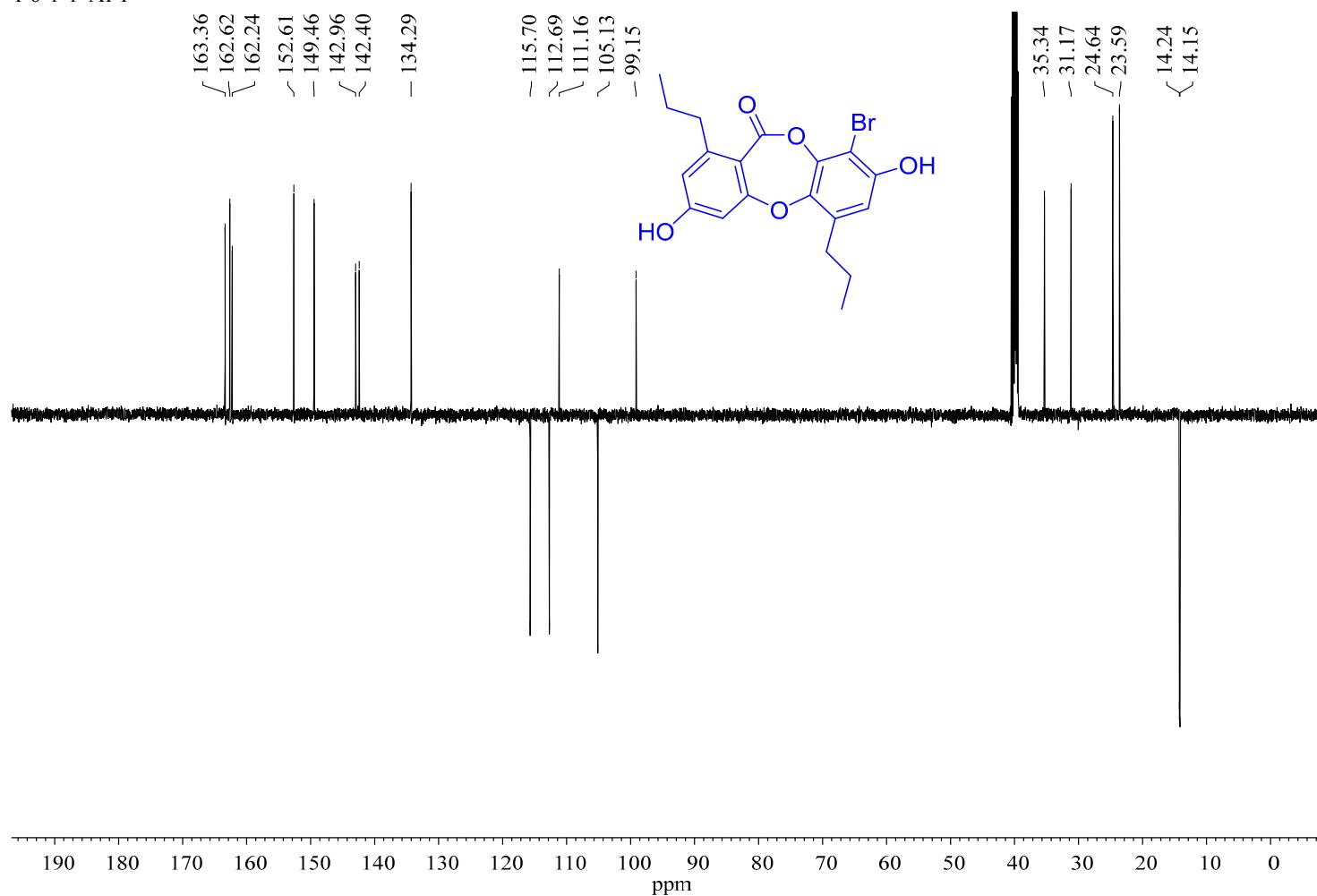


Figure S98. APT spectrum of **13** in $\text{DMSO}-d_6$ (125 MHz)

I-6-1-1 HSQC

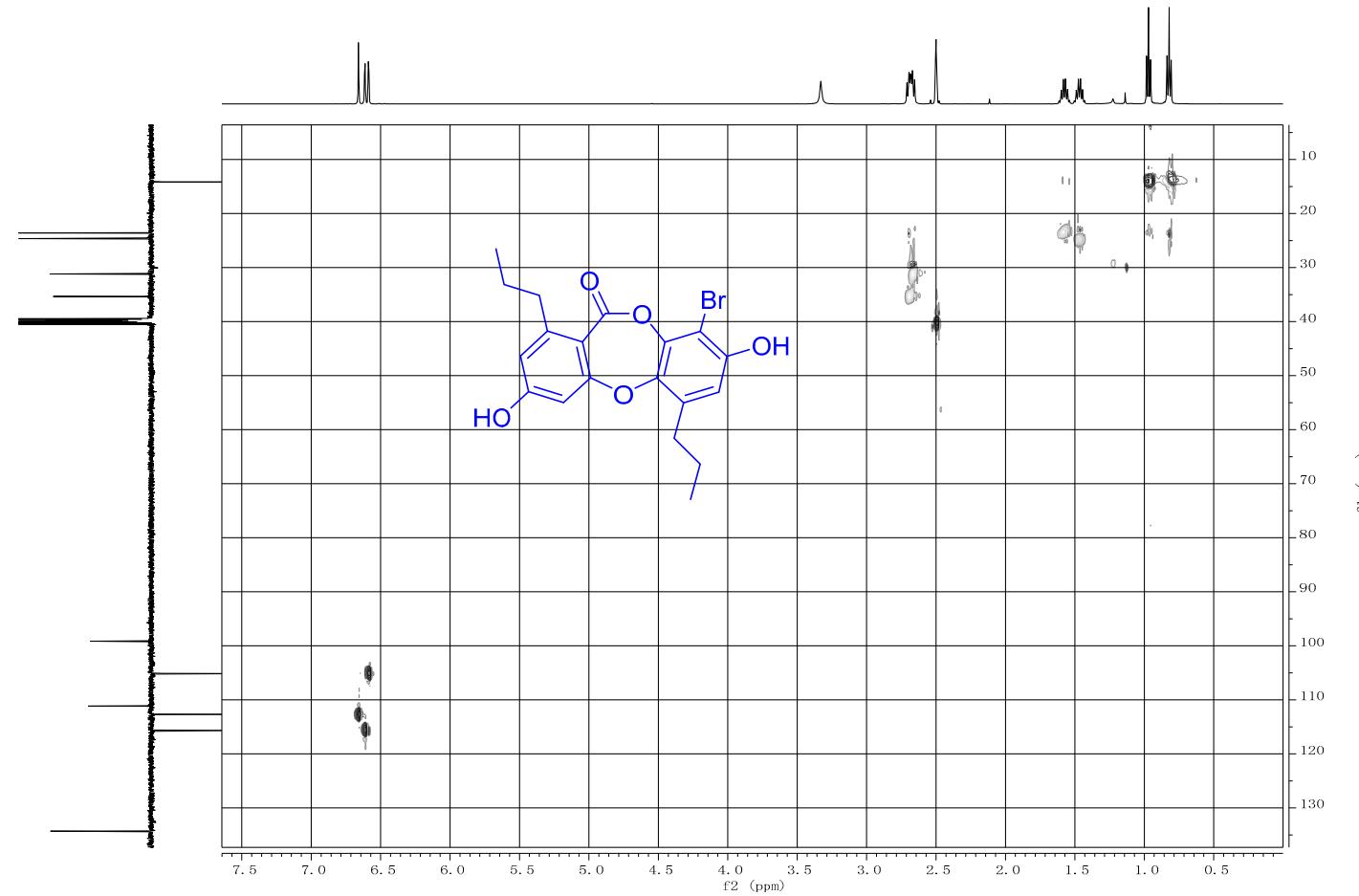
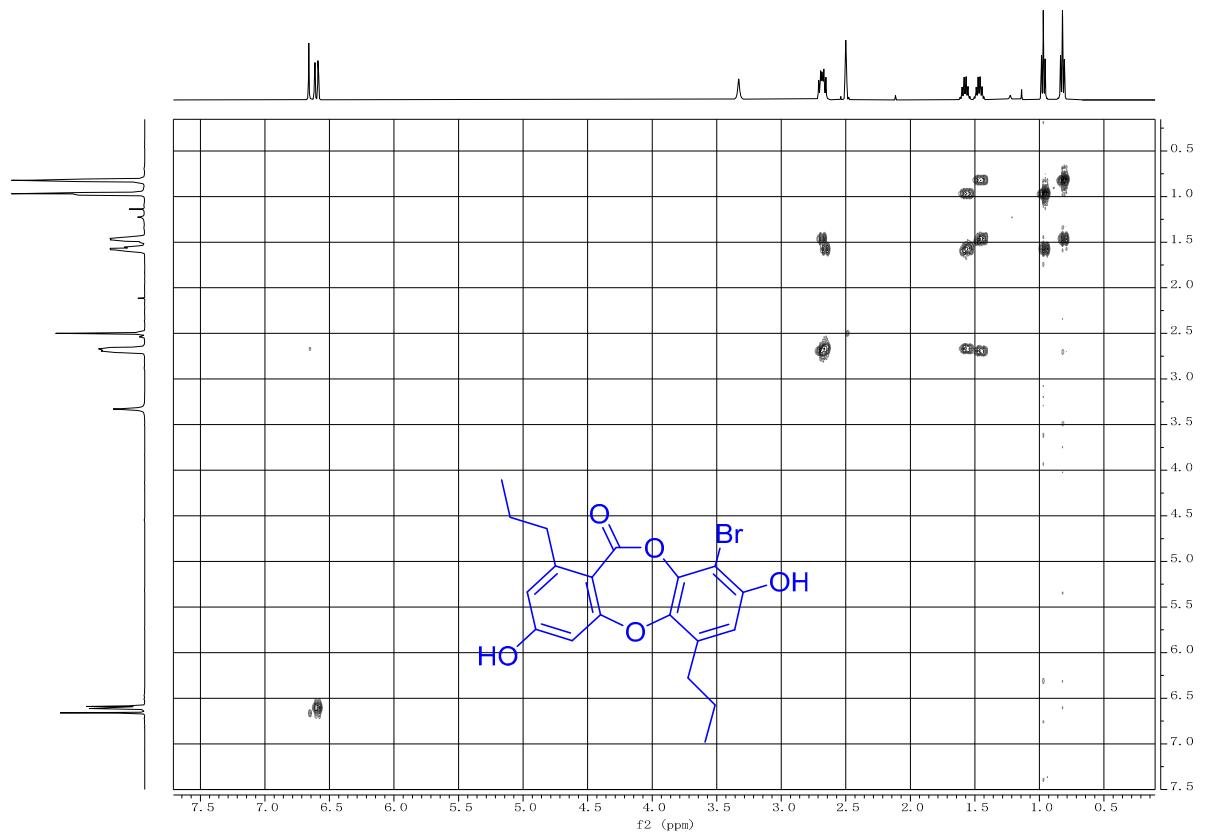


Figure S99. HSQC spectrum of **13** in $\text{DMSO}-d_6$

I-6-1-1 COSY



I-6-1-1 HMBC

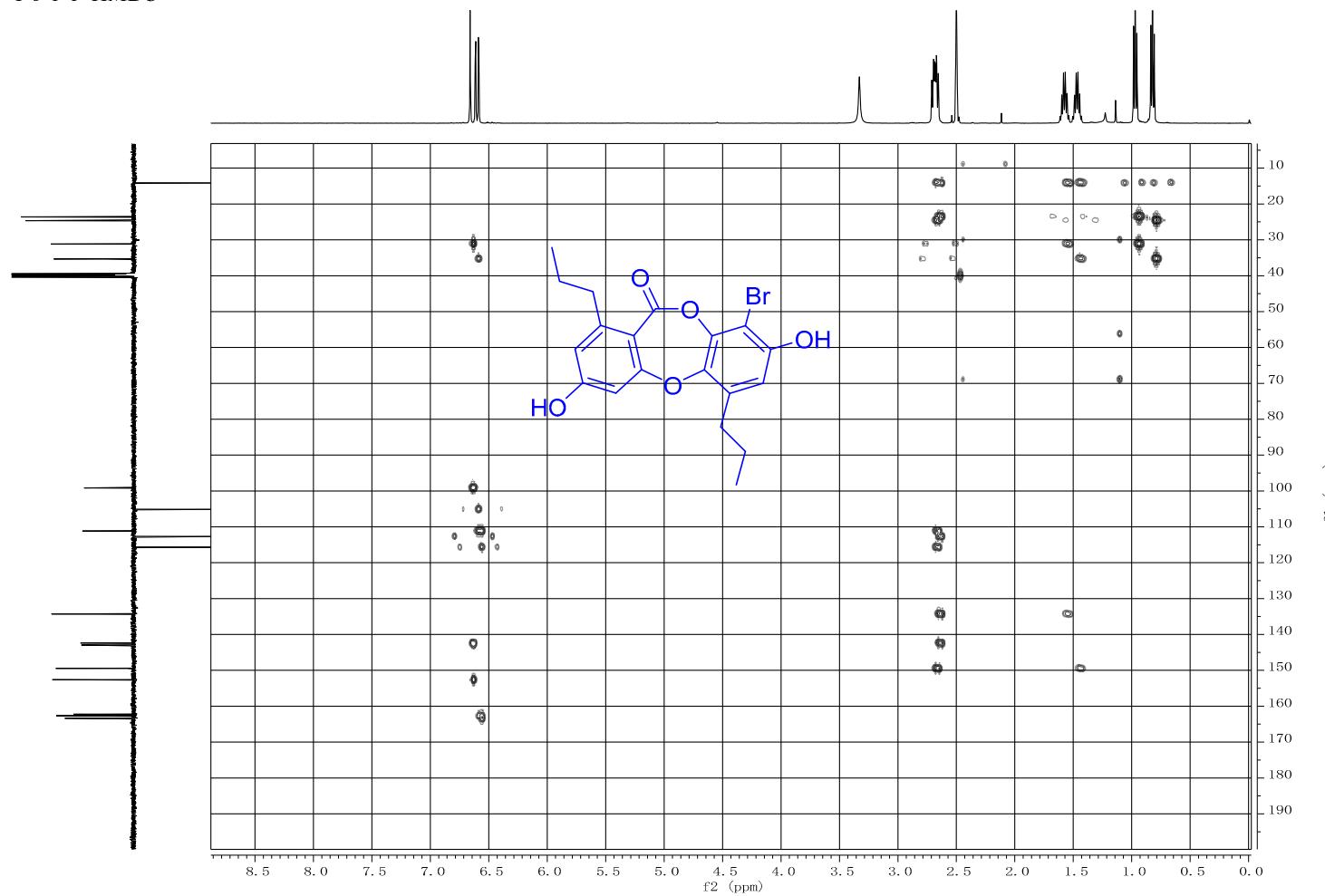


Figure S101. HMBC spectrum of **13** in $\text{DMSO}-d_6$

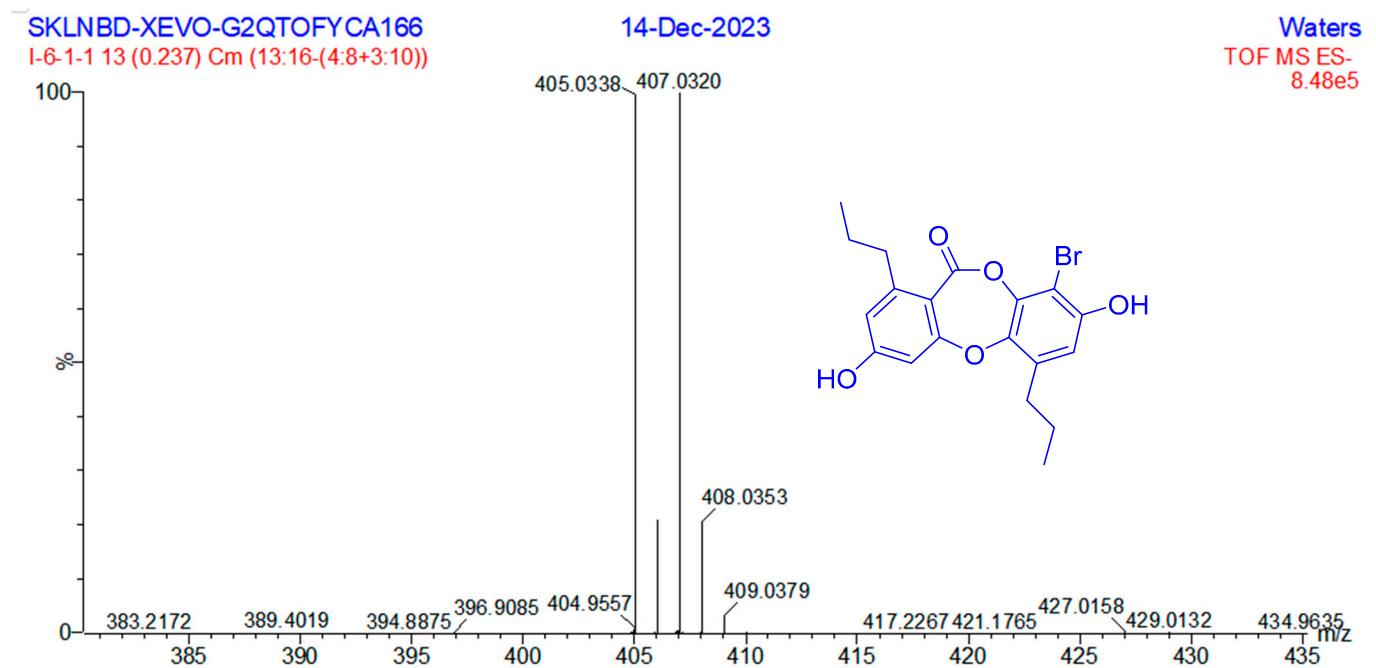


Figure S102. HRESIMS spectrum of 13

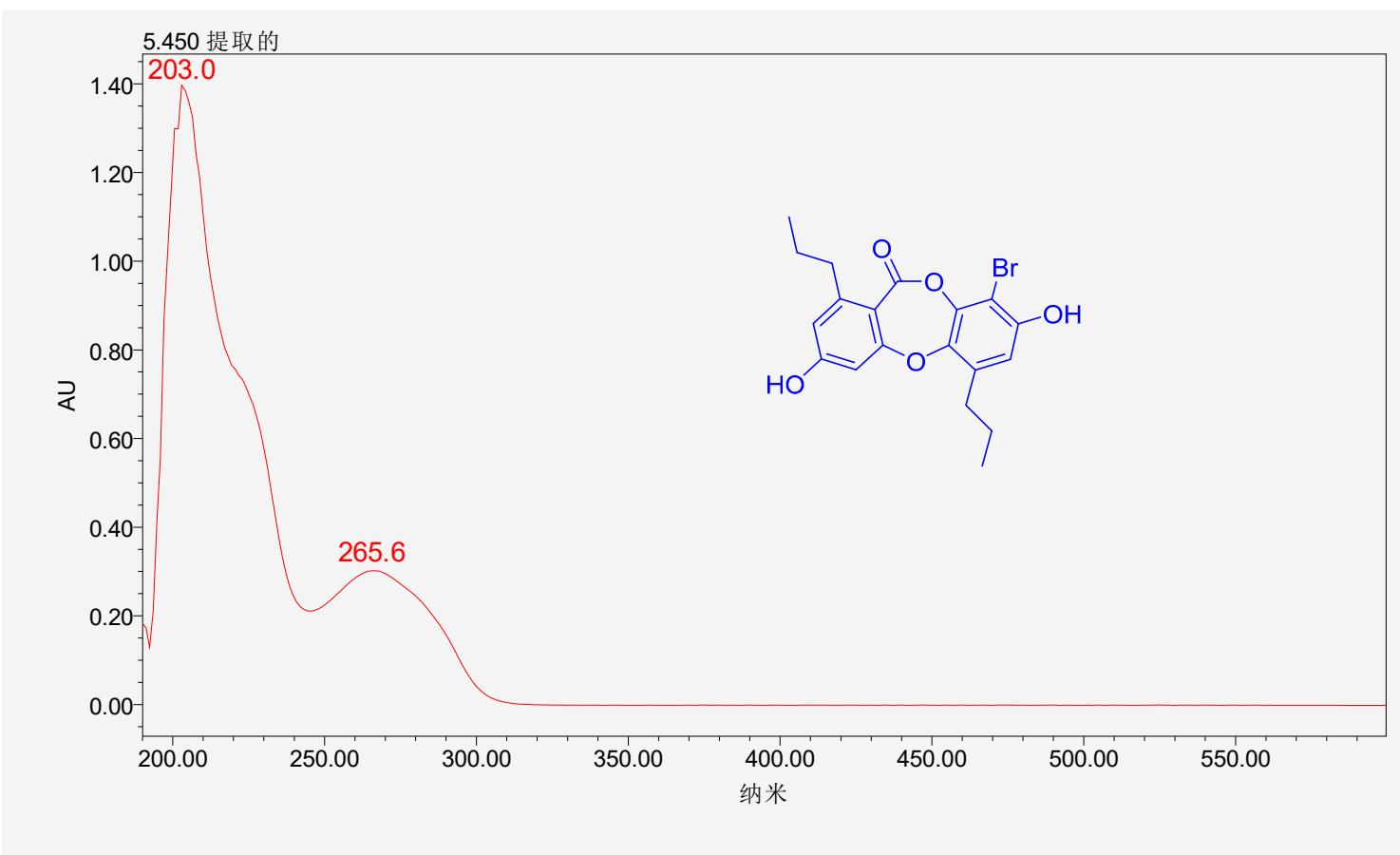


Figure S103. UV spectrum of **13**

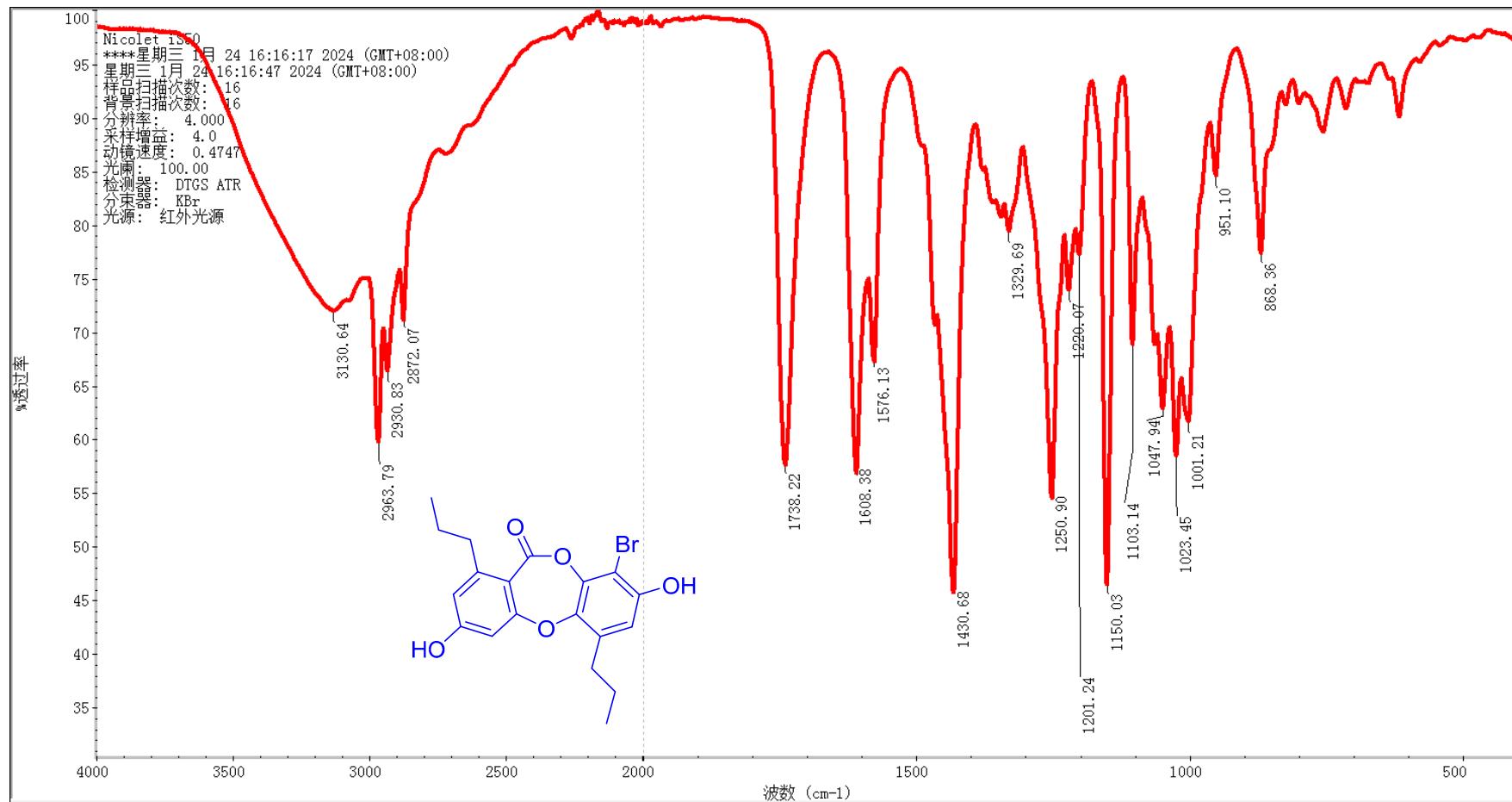


Figure S104. IR spectrum of 13

N-3-2 500 MHz DMSO

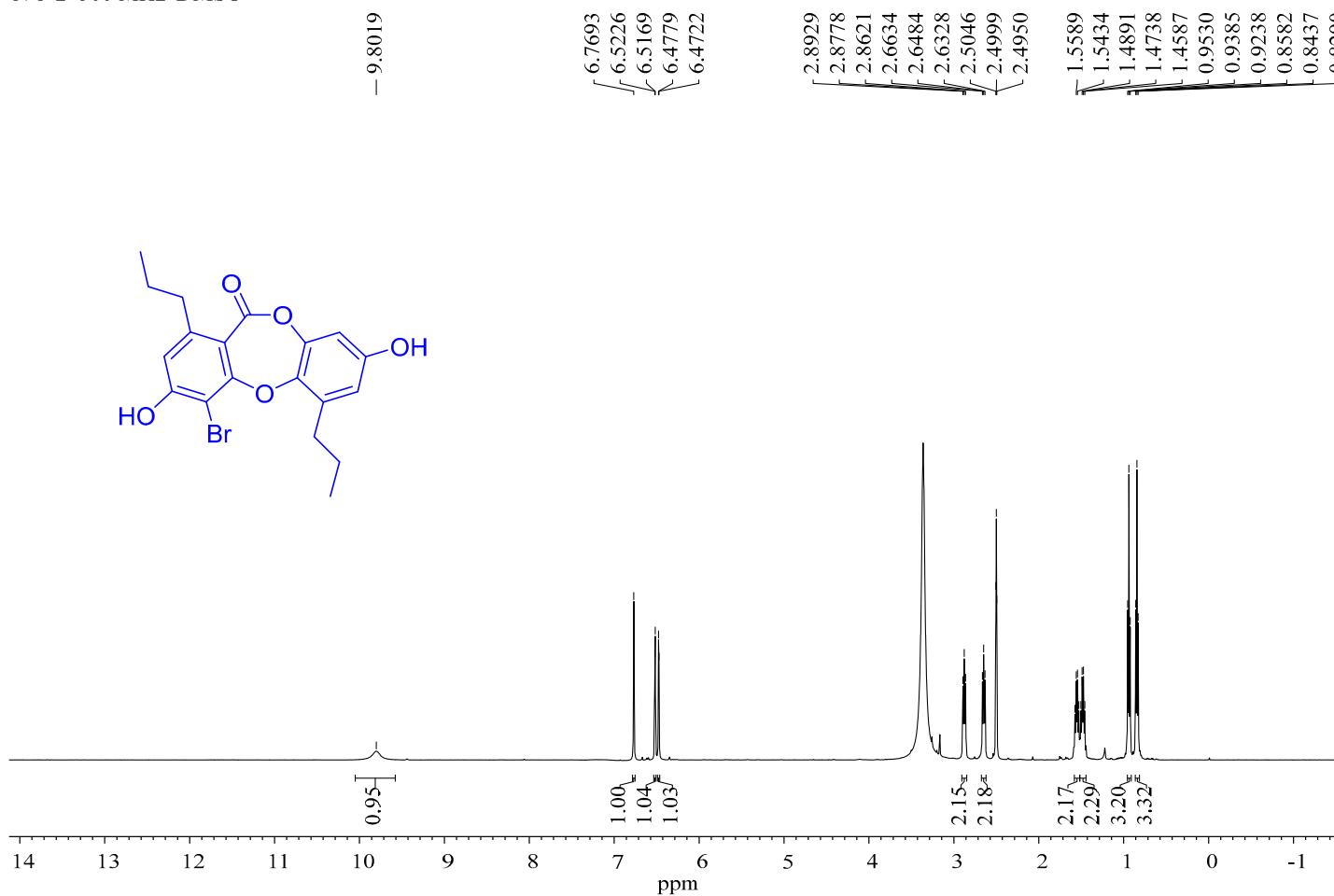


Figure S105. ^1H -NMR spectrum of **14** in $\text{DMSO}-d_6$ (500 MHz)

N-3-2 APT

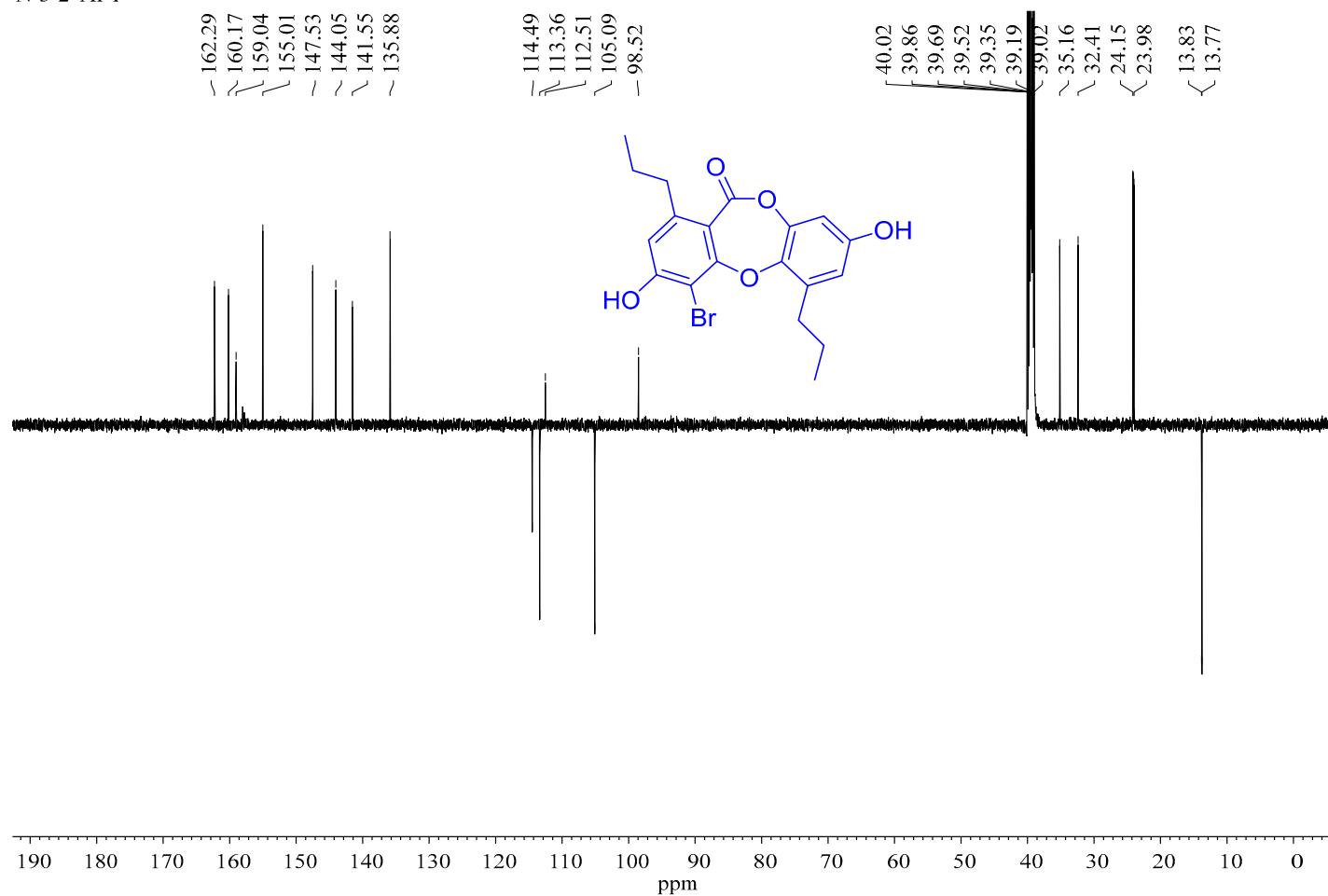


Figure S106. APT spectrum of **14** in $\text{DMSO}-d_6$ (125 MHz)

N-3-2 HSQC

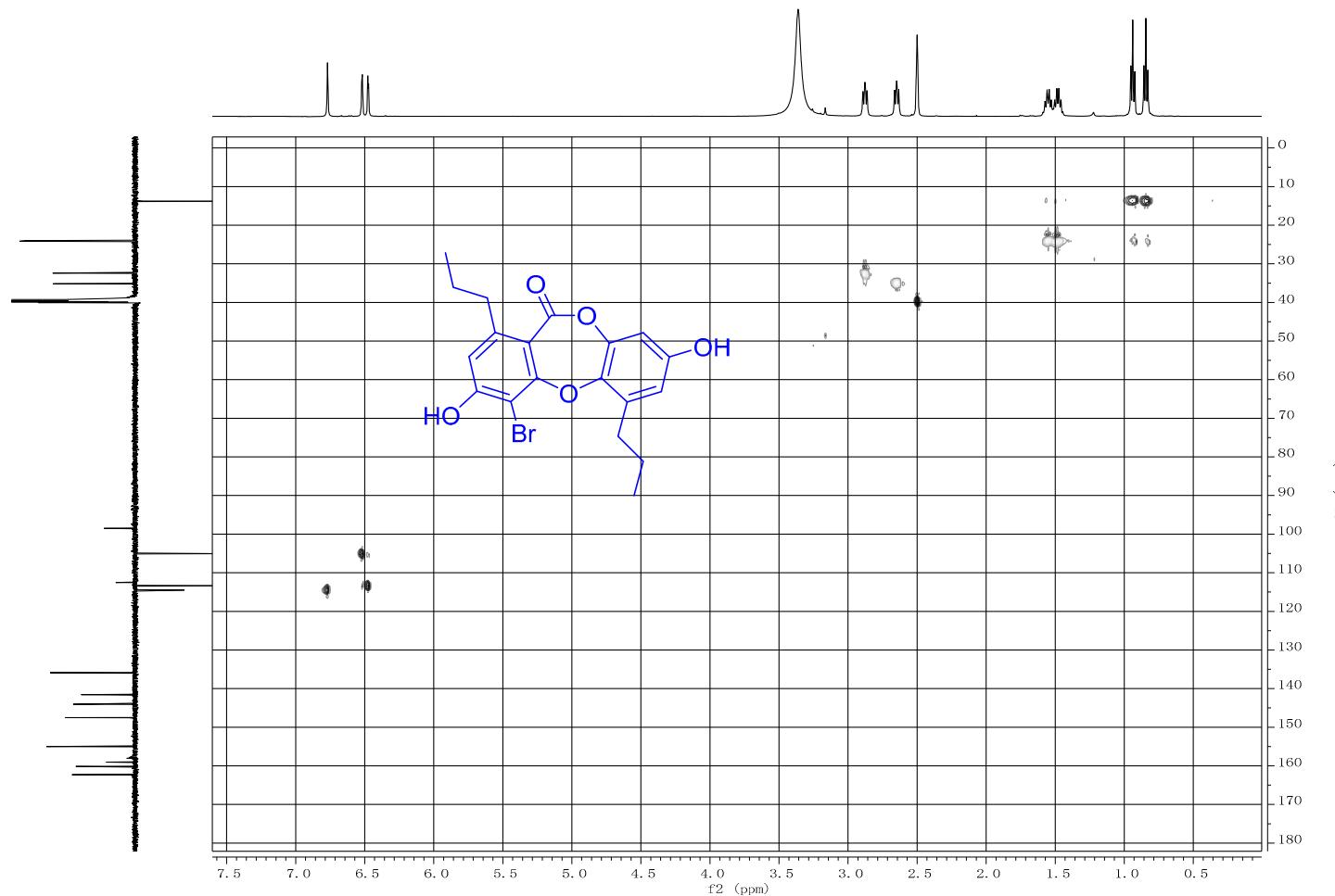


Figure S107. HSQC spectrum of **14** in $\text{DMSO}-d_6$

N-3-2 COSY

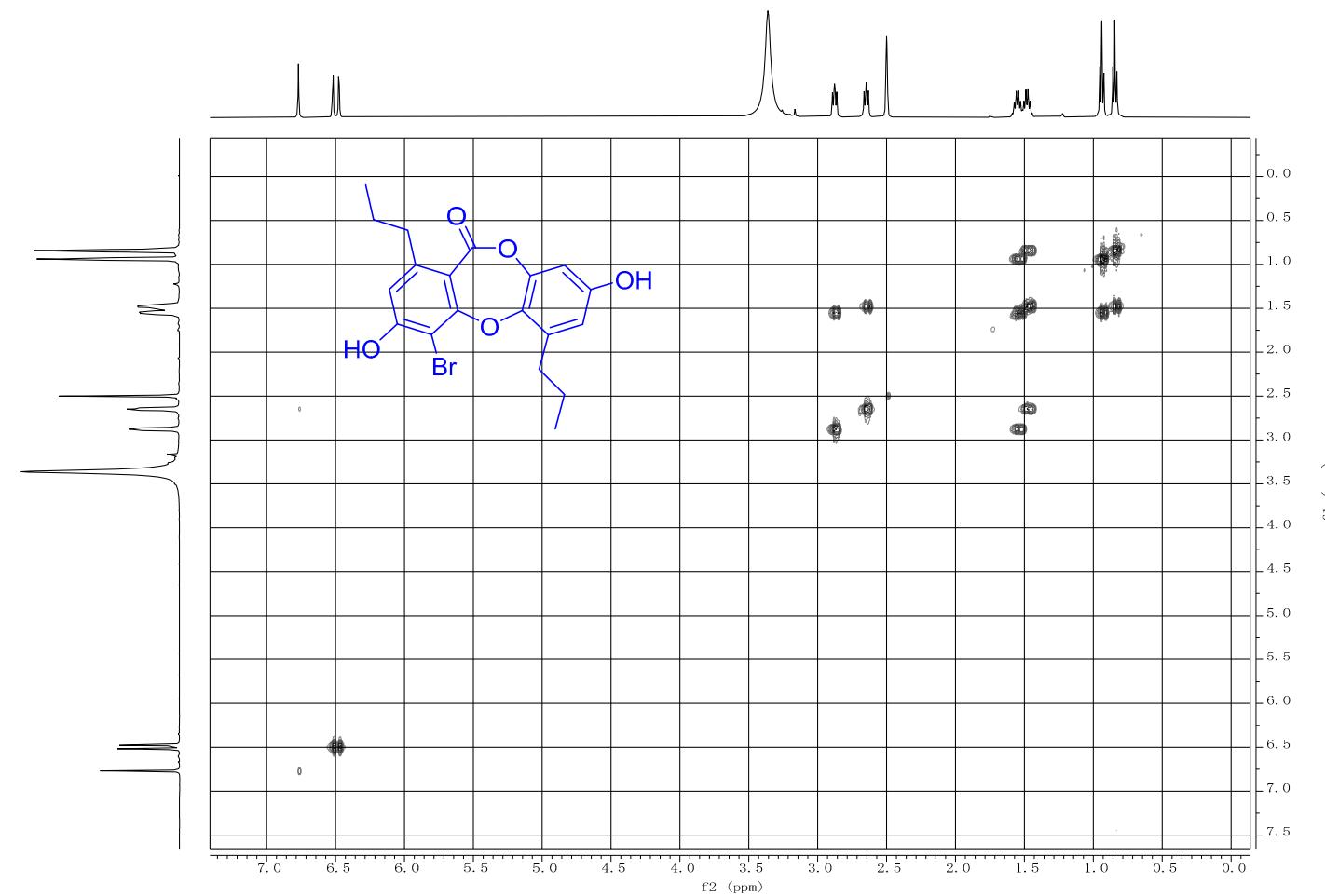


Figure S108. ^1H - ^1H COSY spectrum of **14** in $\text{DMSO}-d_6$

N-3-2 HMBC

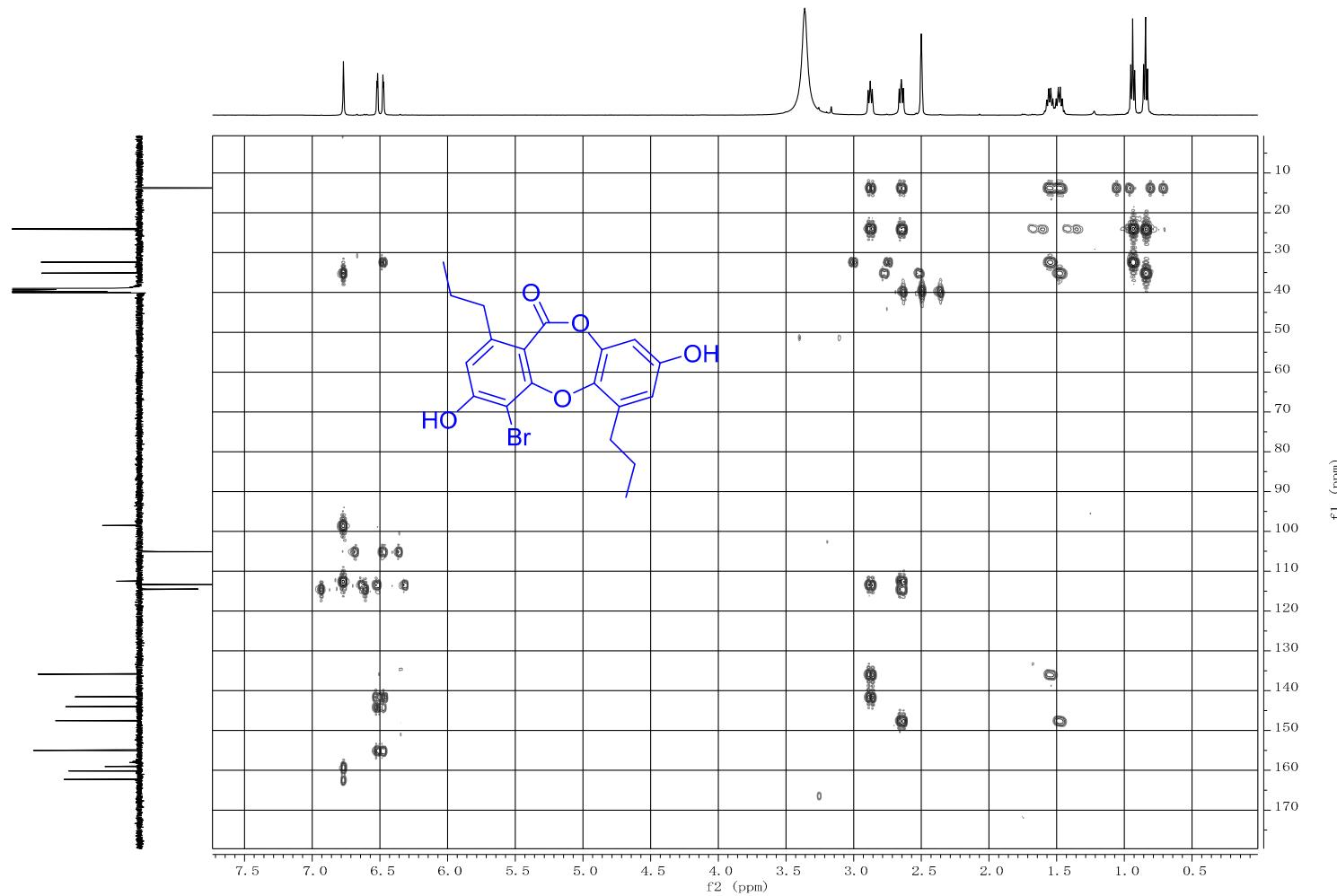


Figure S109. HMBC spectrum of **14** in $\text{DMSO}-d_6$

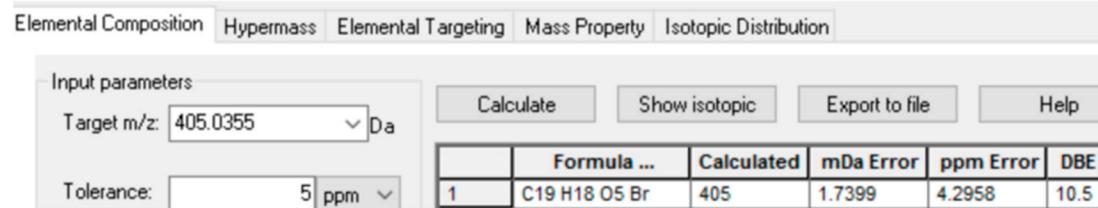
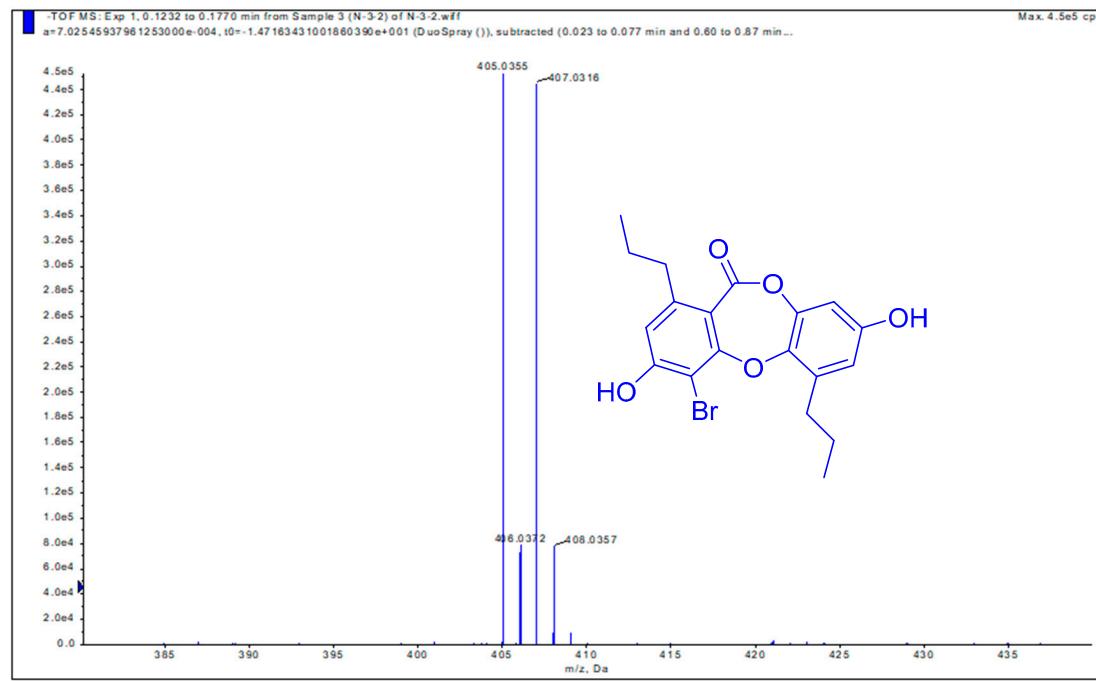


Figure S110. HRESIMS spectrum of 14

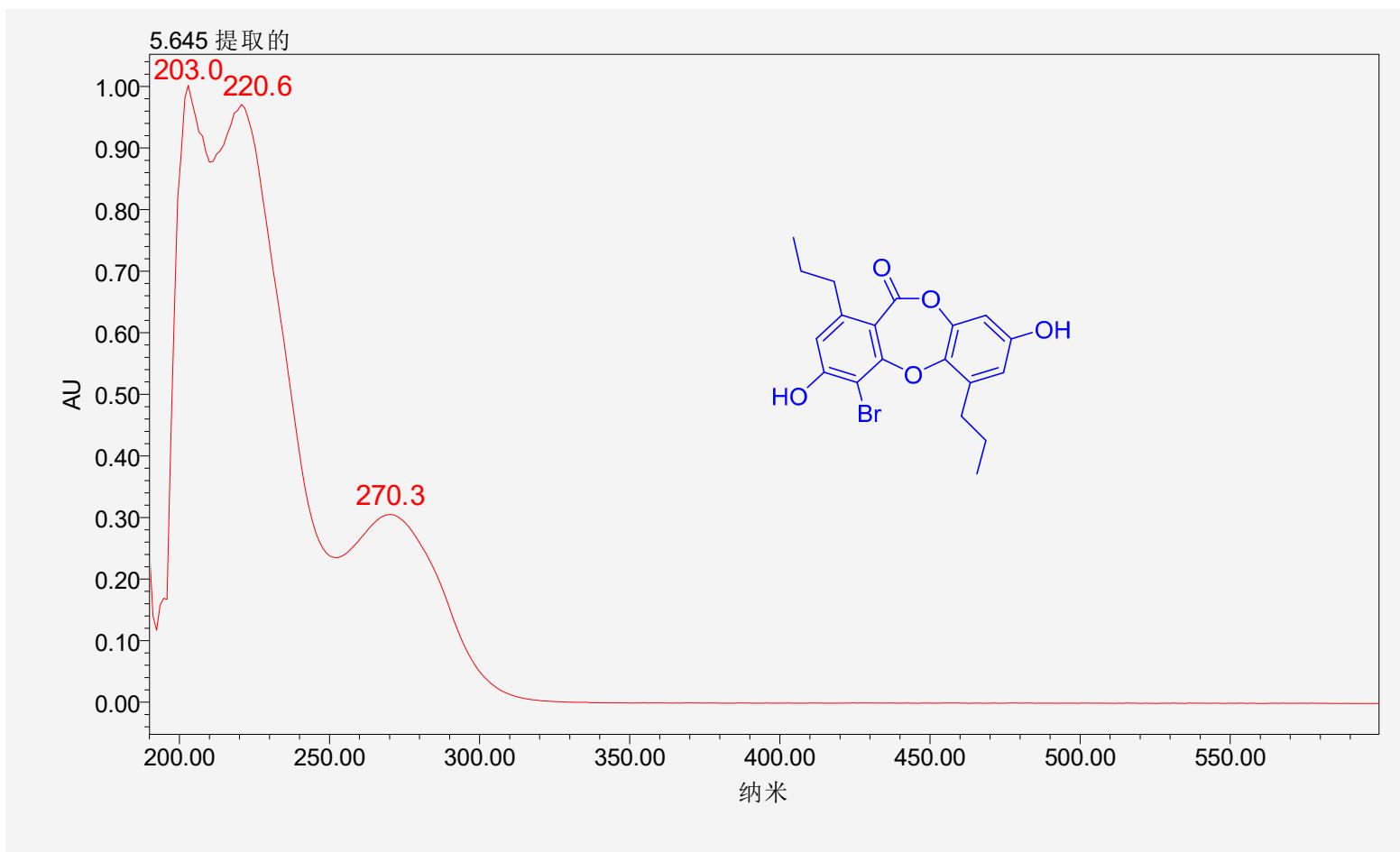


Figure S111. UV spectrum of **14**

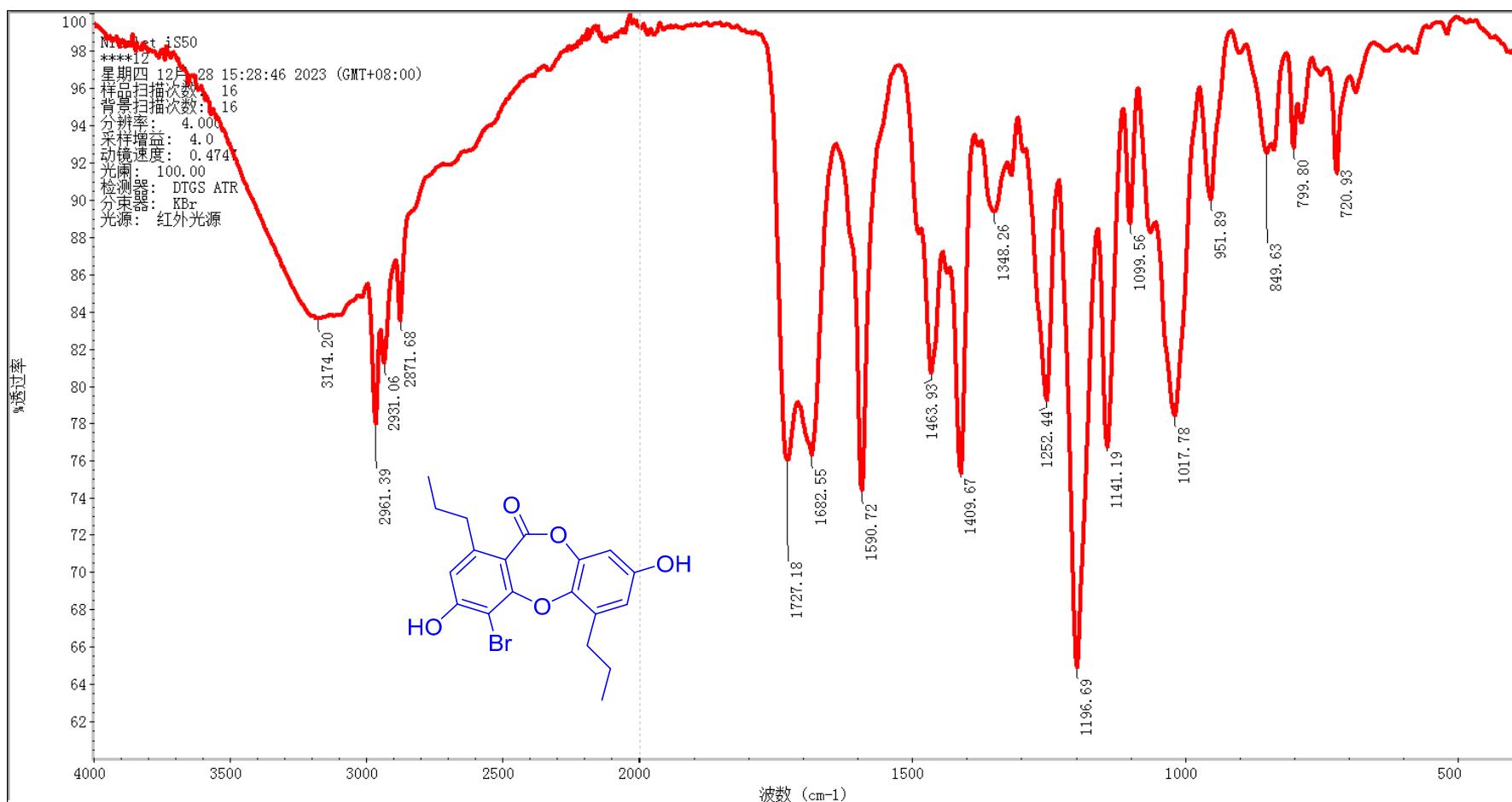


Figure S112. IR spectrum of 14

N-5-4 500 MHz DMSO

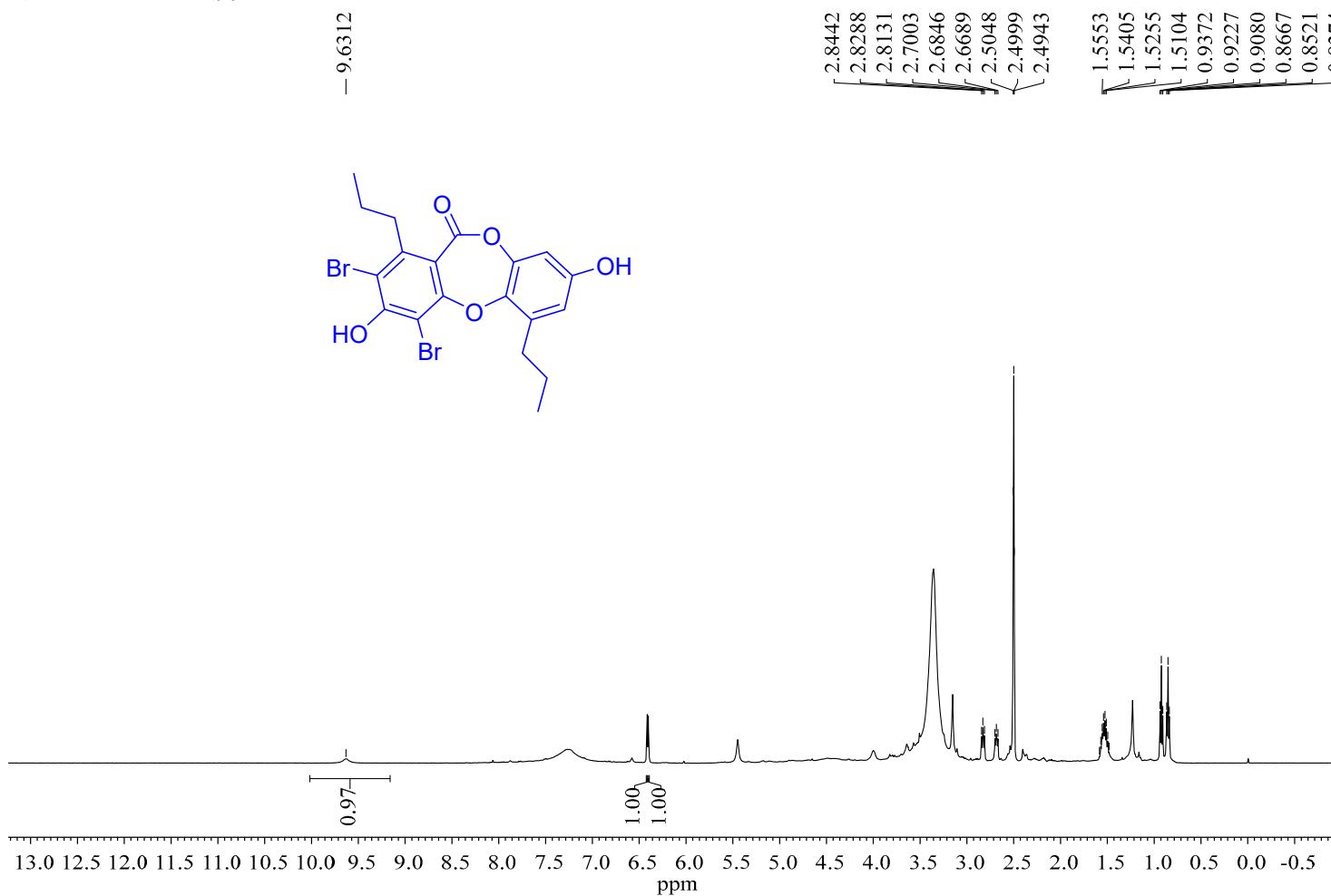


Figure S113. ^1H -NMR spectrum of **15** in $\text{DMSO}-d_6$ (500 MHz)

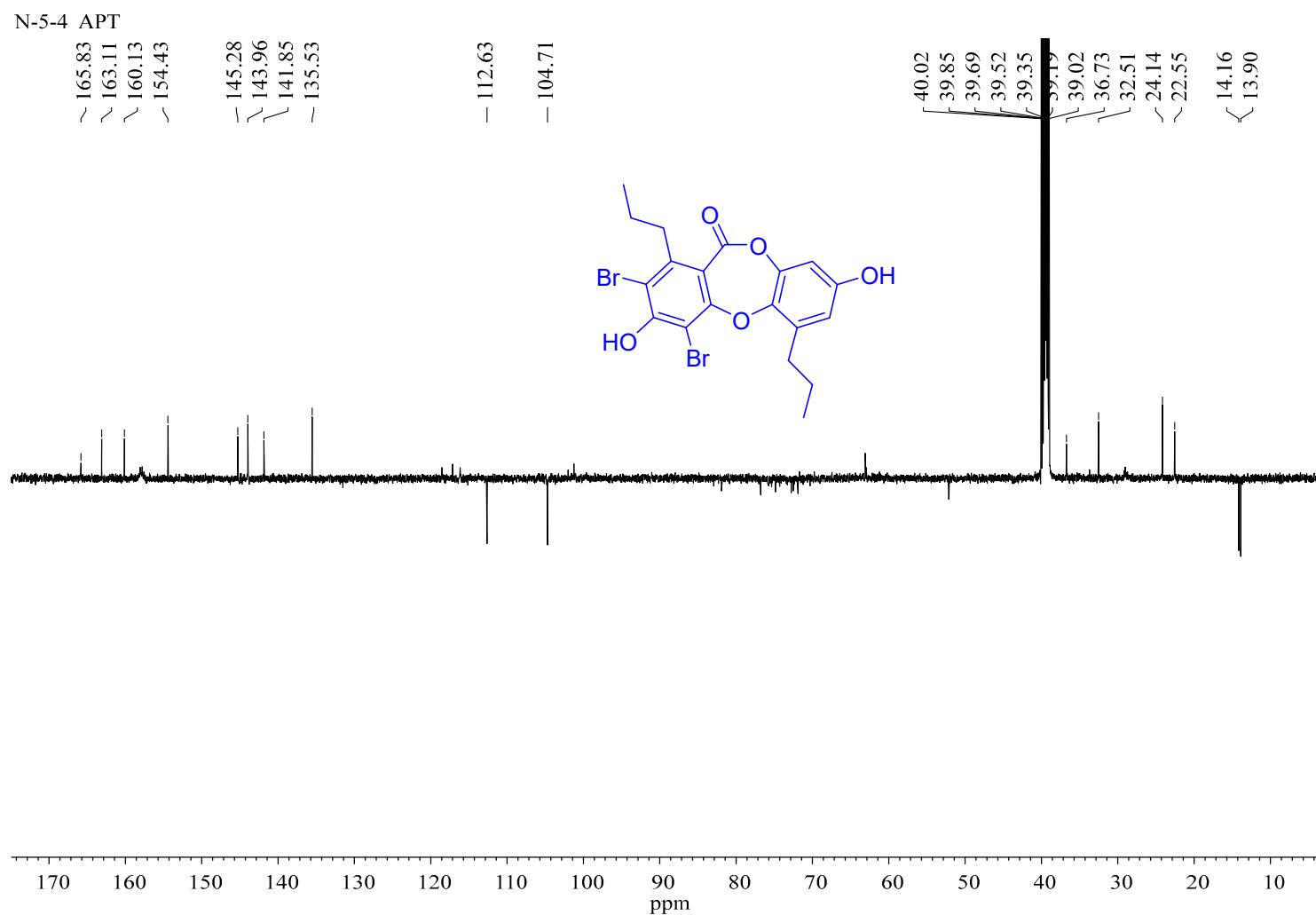


Figure S114. APT spectrum of **15** in DMSO-d₆ (125 MHz)

N-5-4 HSQC

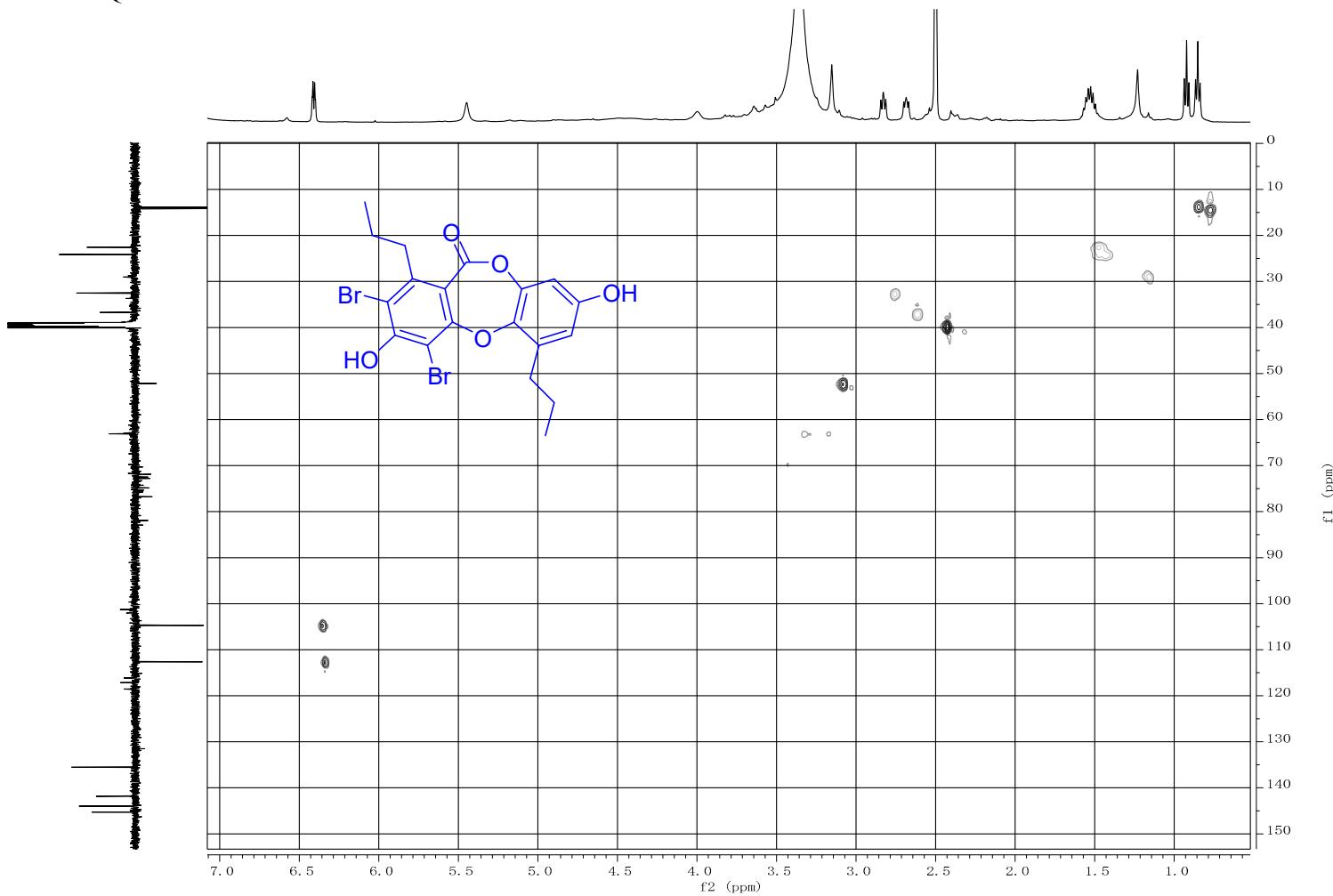


Figure S115. HSQC spectrum of **15** in $\text{DMSO}-d_6$

N-5-4 COSY

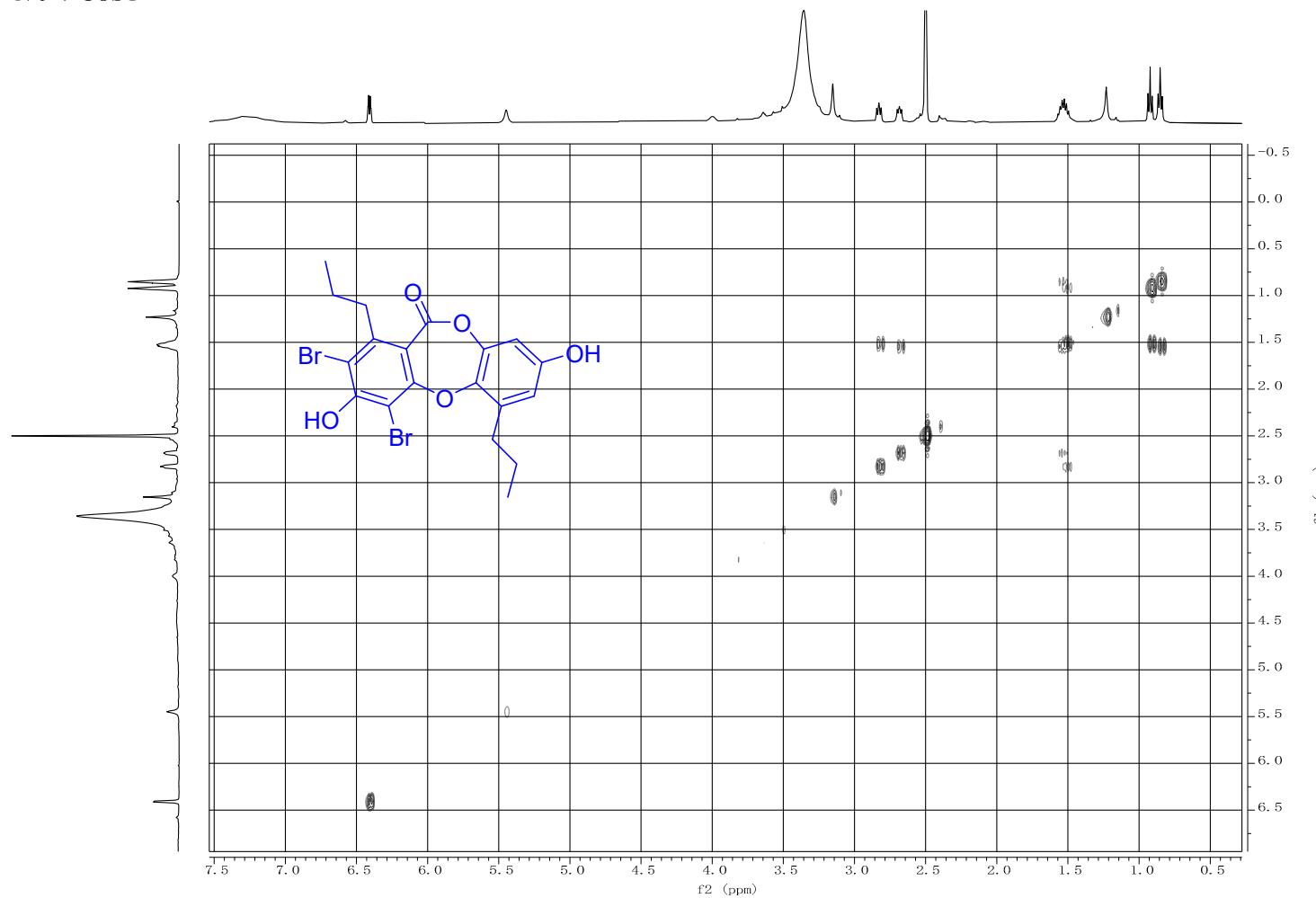


Figure S116. ^1H - ^1H COSY spectrum of **15** in $\text{DMSO}-d_6$

N-5-4 HMBC

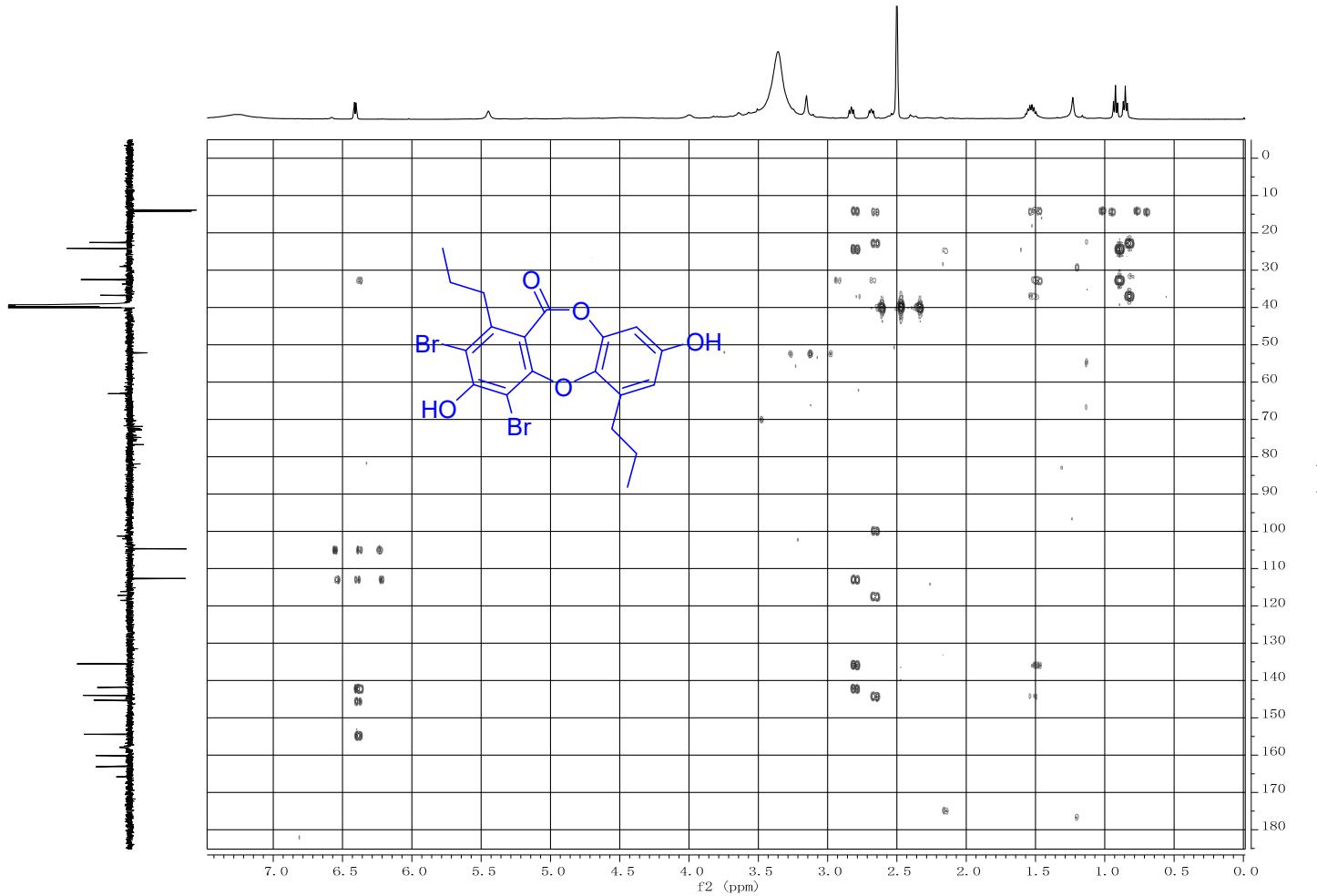


Figure S117. HMBC spectrum of **15** in $\text{DMSO}-d_6$

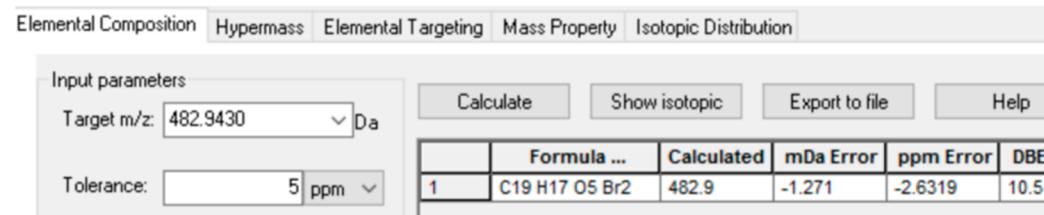
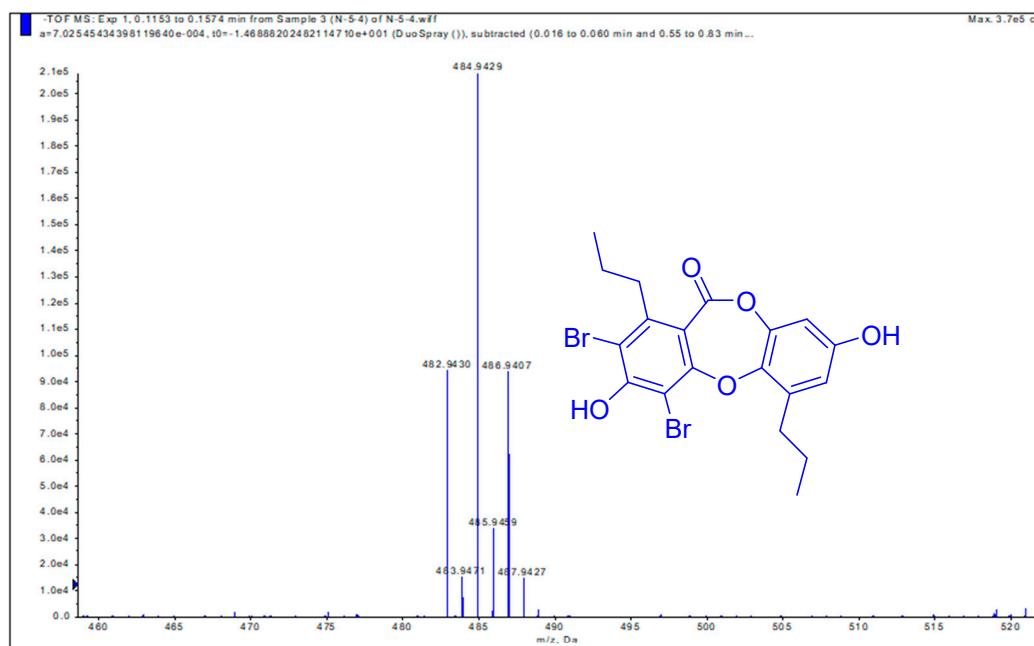


Figure S118. HRESIMS spectrum of 15

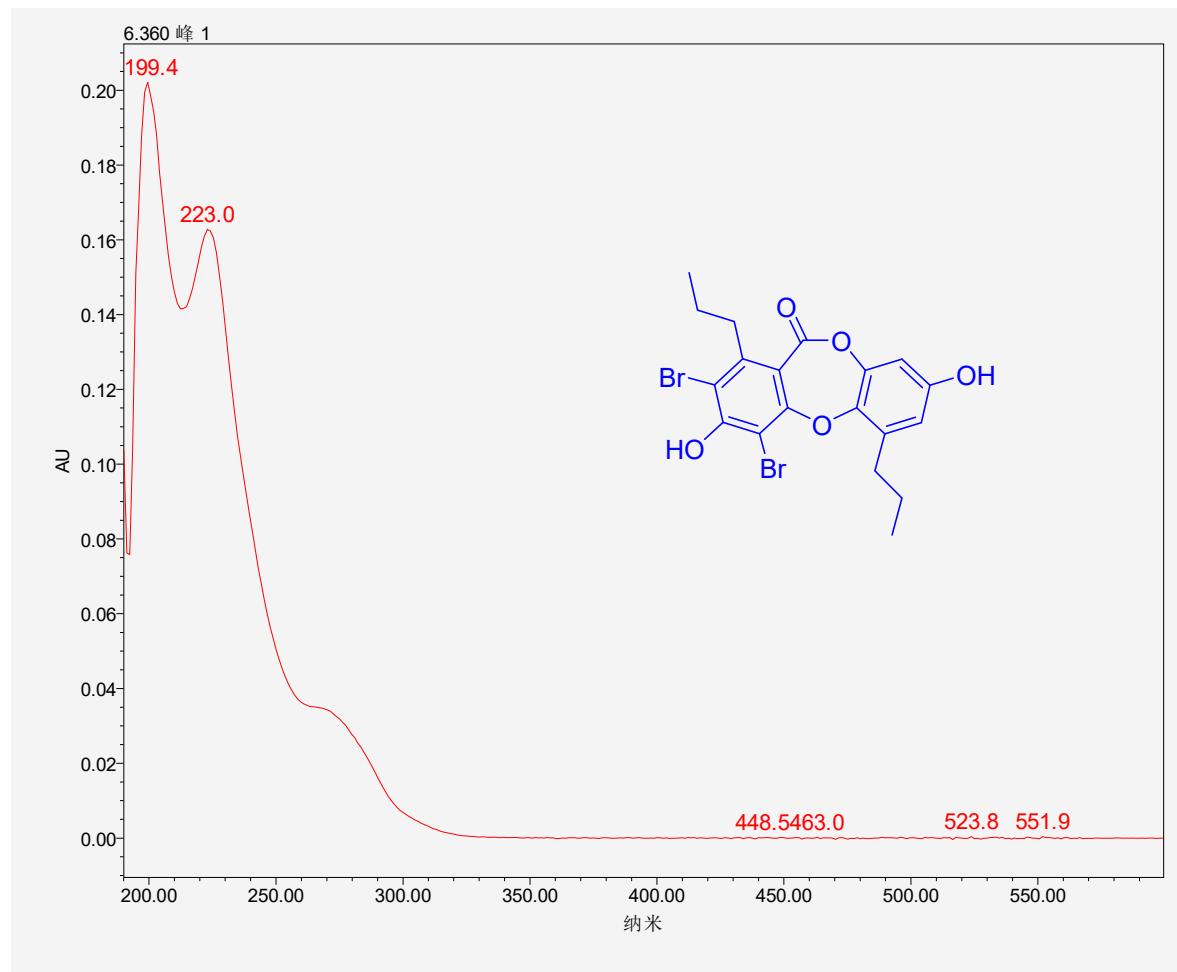


Figure S119. UV spectrum of **15**

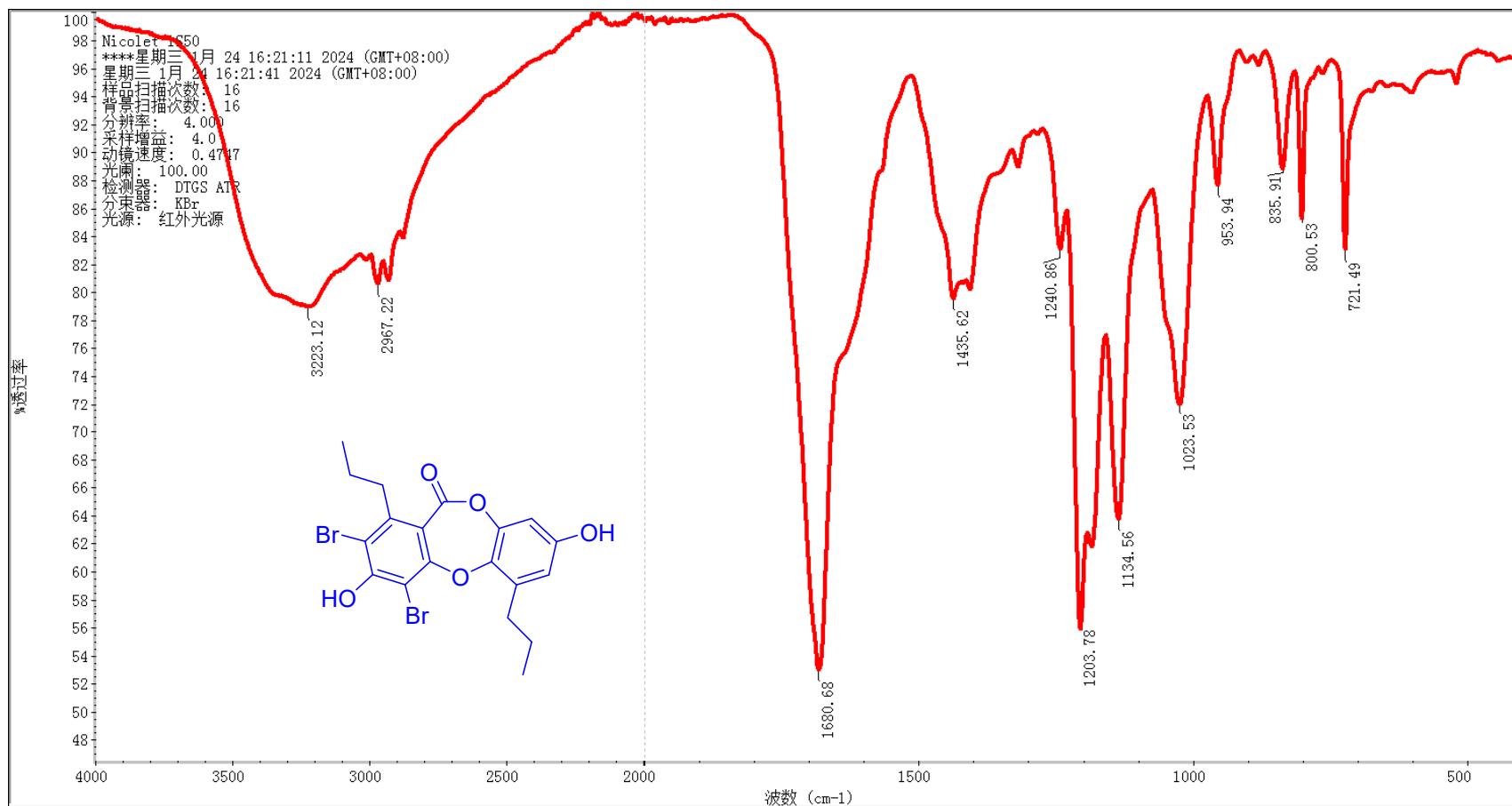


Figure S120. IR spectrum of 15

Fr.M-2 500 MHz DMSO

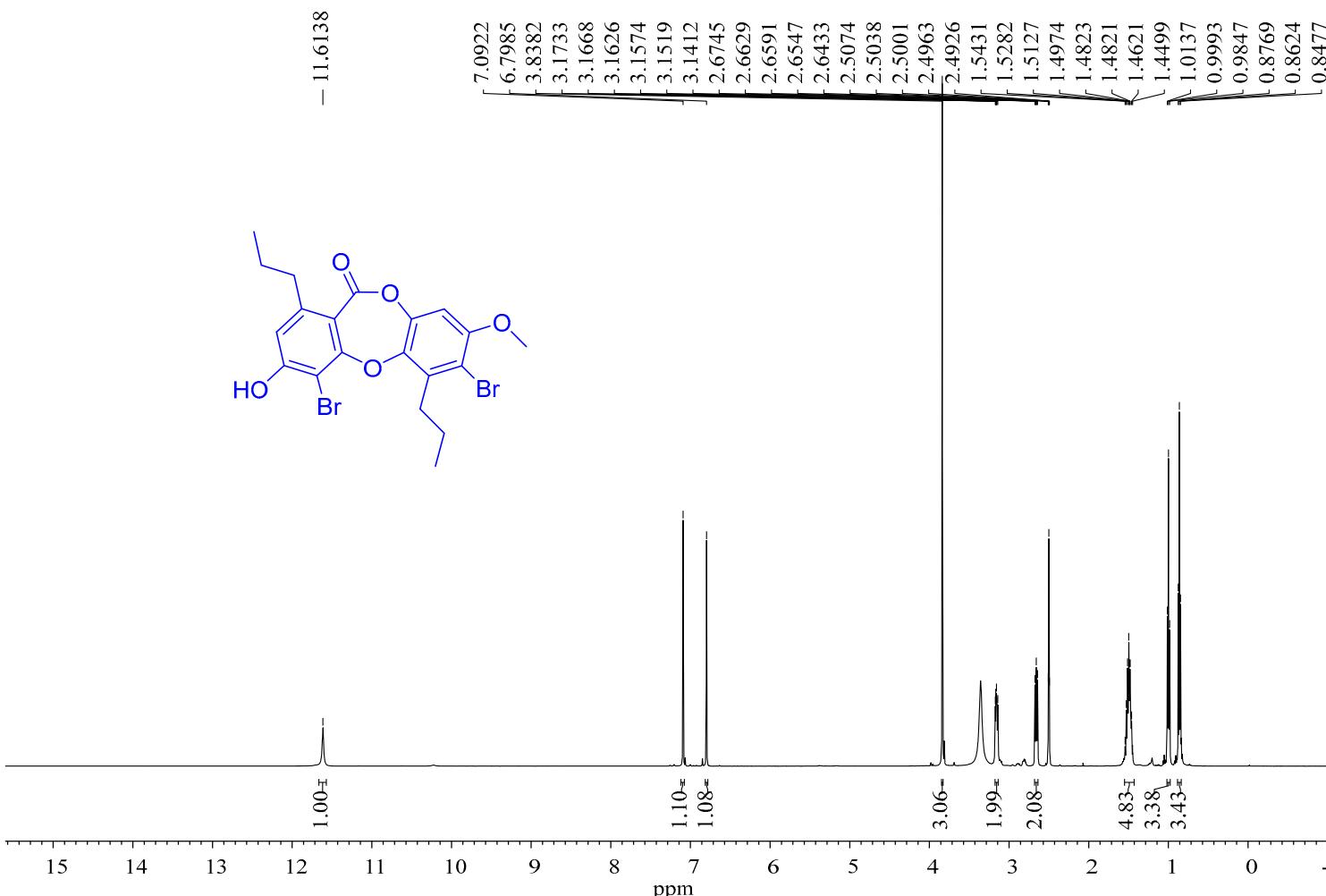


Figure S121. ¹H-NMR spectrum of **16** in DMSO-*d*₆ (500 MHz)

Fr.M-2 C

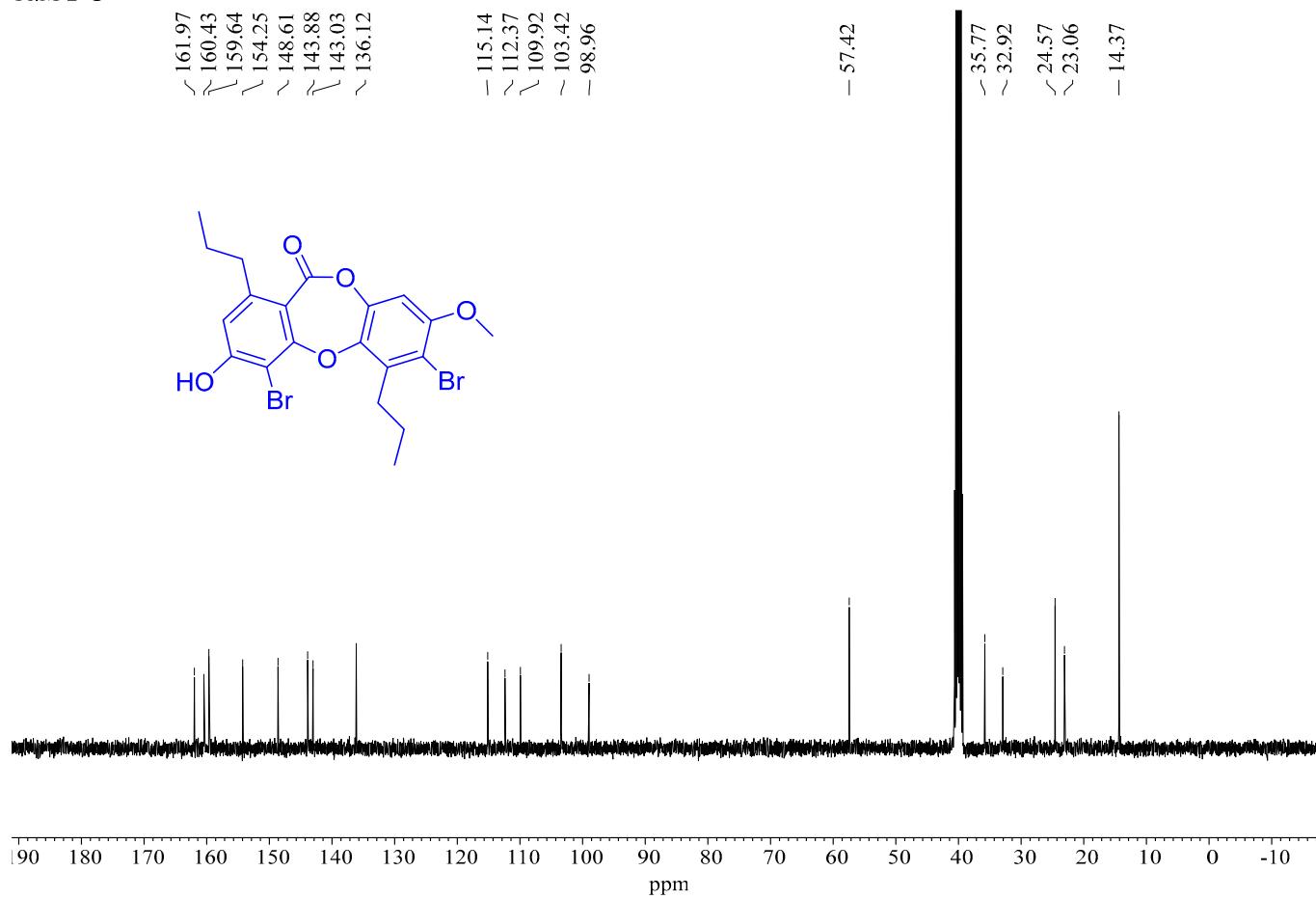


Figure S122. ^{13}C -NMR spectrum of **16** in $\text{DMSO}-d_6$ (125 MHz)

Fr.M-2 HSQC

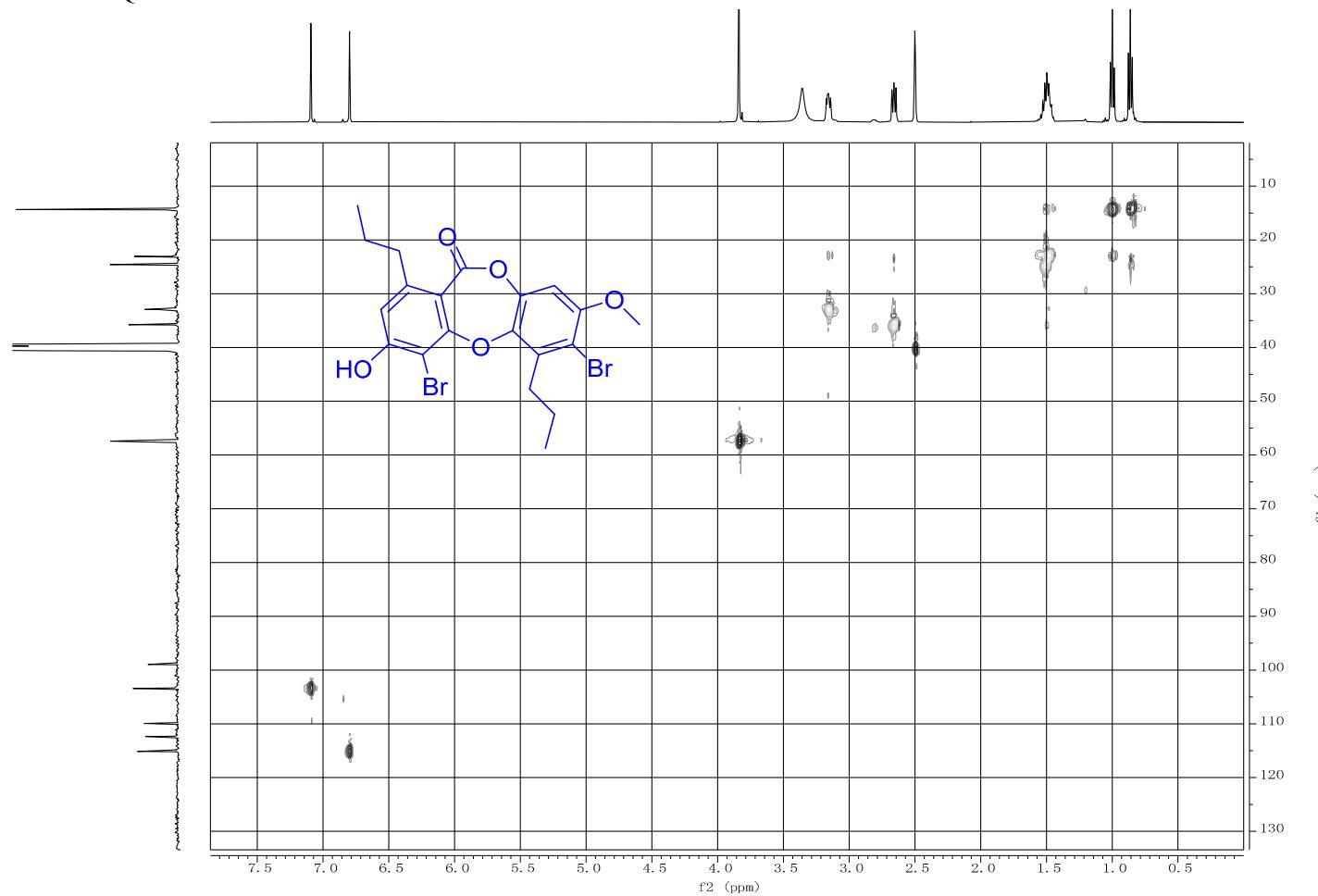


Figure S123. HSQC spectrum of **16** in DMSO-*d*₆

Fr.M-2 COSY

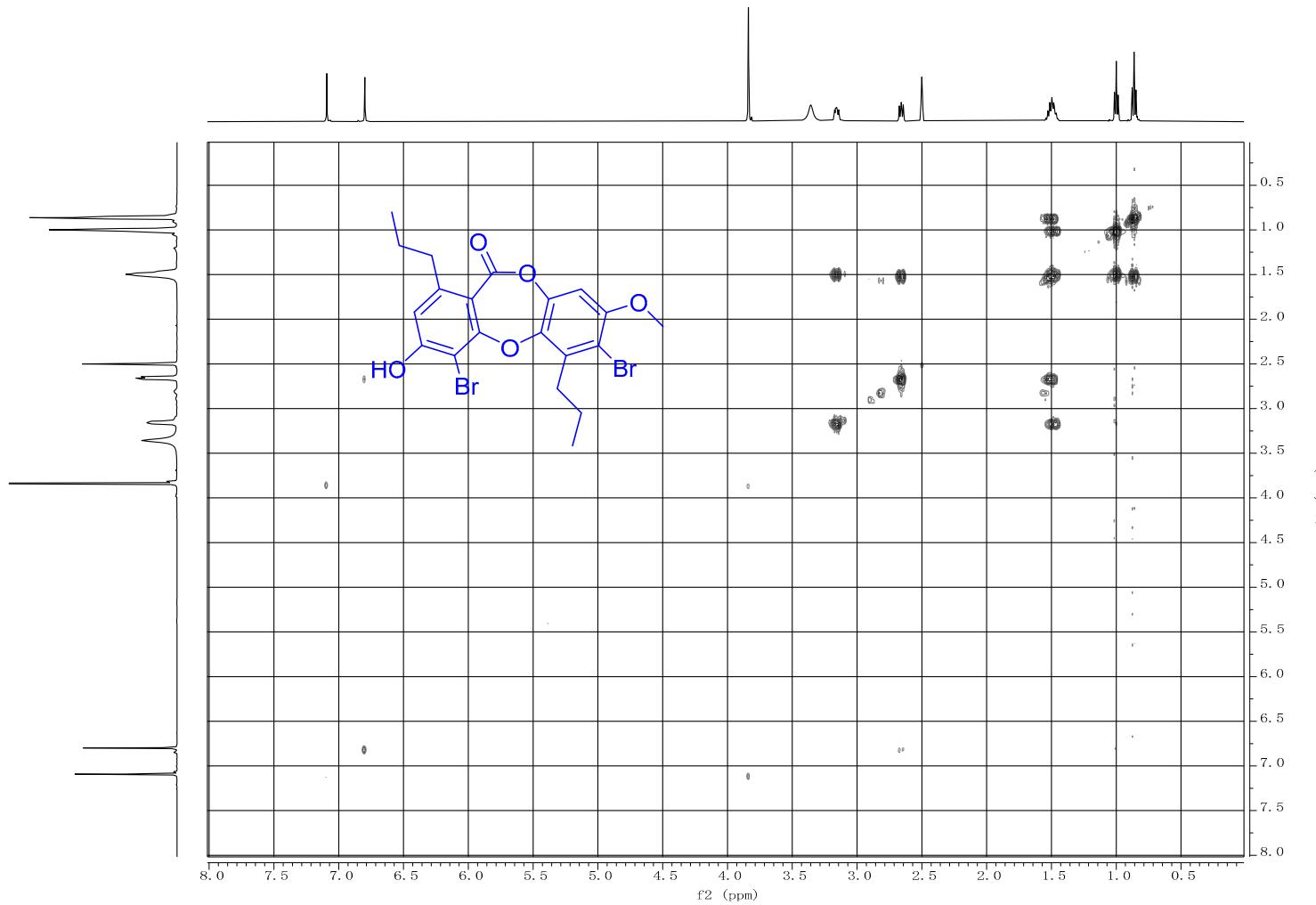


Figure S124. ^1H - ^1H COSY spectrum of **16** in $\text{DMSO}-d_6$

Fr.M-2 HMBC

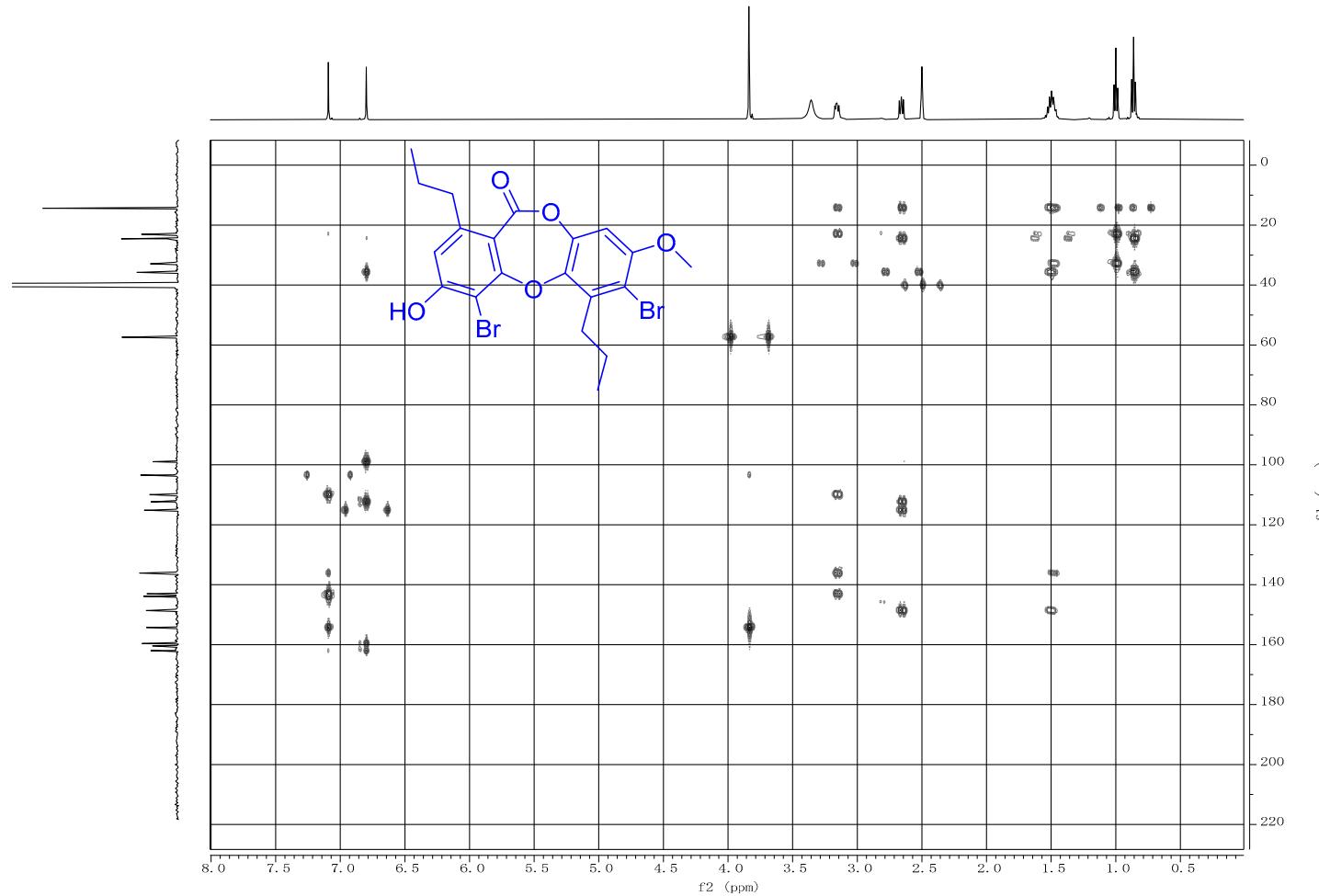
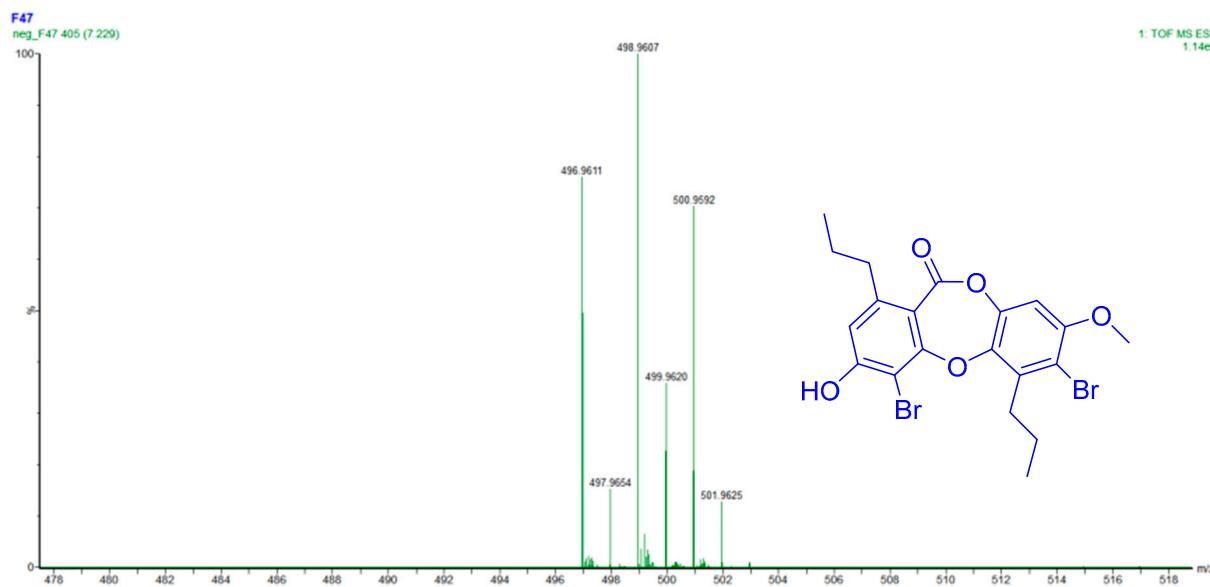


Figure S125. HMBC spectrum of **16** in $\text{DMSO}-d_6$



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

351 formula(e) evaluated with 8 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Br: 0-8

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O	Br	
496.9611	496.9658	-4.7	-9.5	1.5	C13 H23 O10 Br2	13	23	10	2	
	496.9599	1.2	2.4	10.5	C20 H19 O5 Br2	20	19	5	2	

Figure S126. HRESIMS spectrum of 16

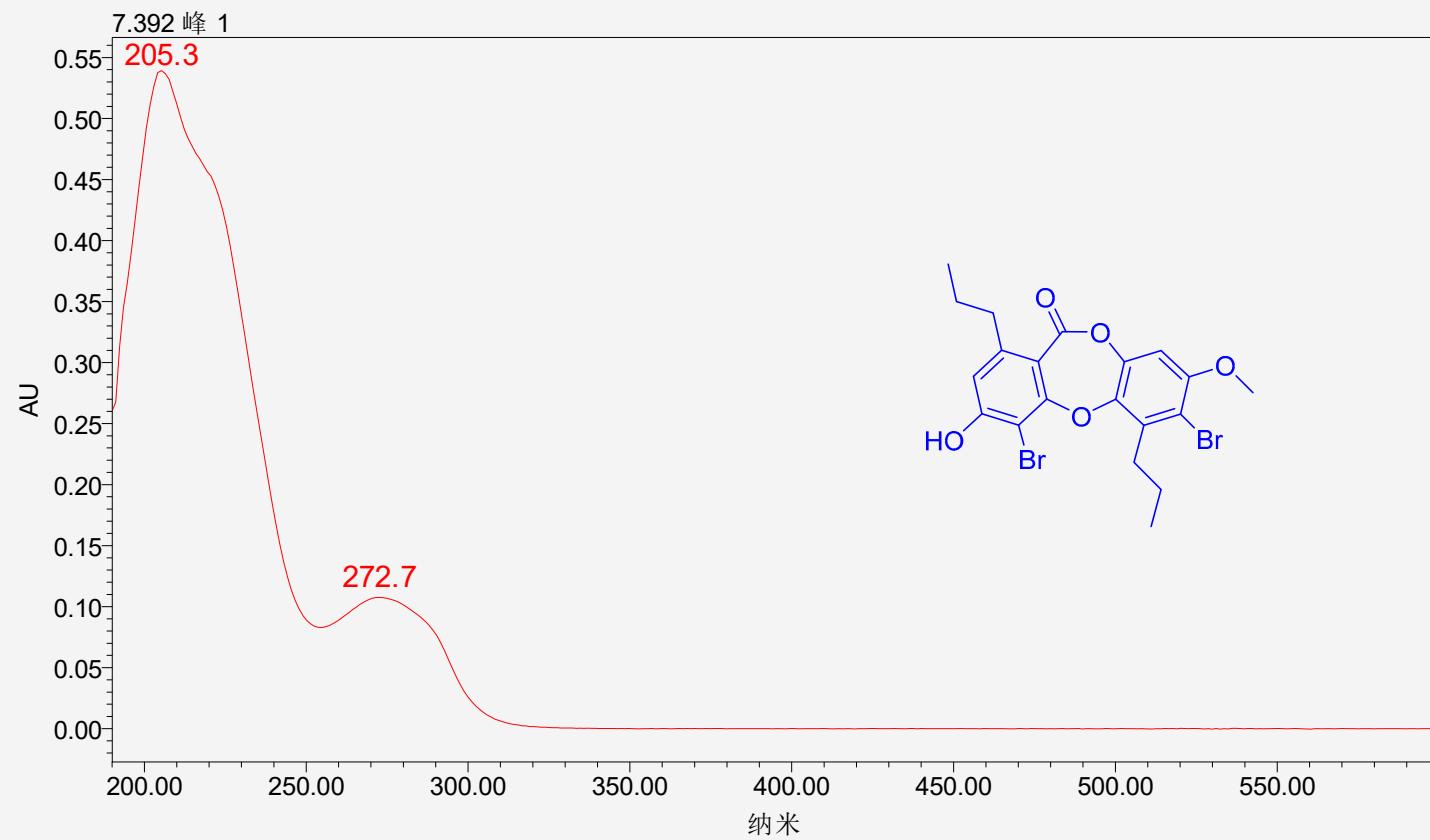


Figure S127. UV spectrum of **16**

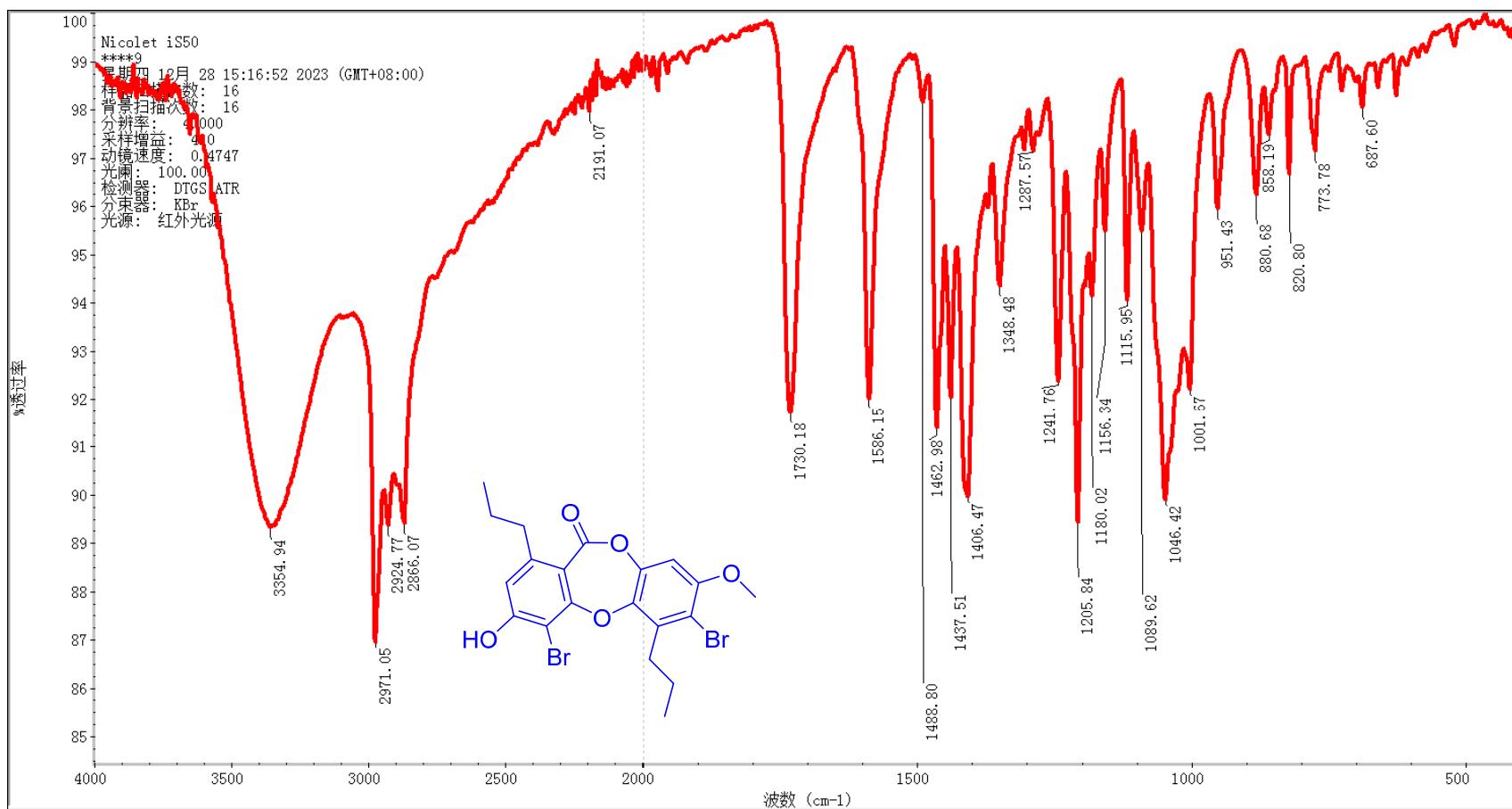


Figure S128. IR spectrum of **16**

Table S12. Comparison of the ^1H NMR data of **12-16** to spiromastixones P-T (δ_{H} ppm, J in Hz)

Position	12^{a,d}	P^{b,e}	13^{a,d}	Q^{a,e}	14^{a,d}	R^{b,e}	15^{a,d}	S^{a,f}	16^{a,d}	T^{a,e}
3	6.60, d (2.3)	6.73, d (2.0)	6.59, d (2.3)	6.72, d (2.0)	-	-	-	-	-	-
5	6.62, d (2.3)	6.72, d (2.0)	6.62, d (2.3)	6.71, d (2.0)	6.77, s	6.90, s	-	-	6.80, s	6.93, s
8	2.68, t (7.9)	2.76, t (7.8)	2.69, m	2.79, t (7.8)	2.65, t (7.8)	2.73, t (9.8)	2.68, t (7.9)	2.90, t (7.8)	2.66, t (7.9)	2.74, t (7.8)
9	1.48, m	1.57, m	1.47, m	1.57, m	1.48, m	1.57, m	1.55, m	1.64, m	1.50, m	1.58, m
10	0.85, t (7.3)	0.89, t (7.5)	0.82, t (7.3)	0.88, t (7.5)	0.84, t (7.4)	0.88, t (7.3)	0.85, t (7.4)	0.93, t (7.5)	0.86, t (7.4)	0.89, t (7.5)
3'	6.73, s	6.81, s	-	-	6.52, d (2.9)	6.57, d (3.0)	6.42, d (2.9)	6.49, d (2.5)	7.09, s	6.94, s
5'	-	-	6.66, s	6.79, s	6.47, d (2.9)	6.58, d (3.0)	6.40, d (2.9)	6.48, d (2.5)	-	-
6'	-	-	-	-	-	-	-	2.94, t (7.8)	-	-
7'	2.88, t (8.1)	2.99, t (8.0)	2.67, m	2.75, t (7.8)	2.88, t (7.9)	2.98, t (9.8)	2.83, t (7.9)	2.94, t (7.8)	3.16, t (8.1)	3.28, t (8.0)
8'	1.54, m	1.66, m	1.55, m	1.66, m	1.55, m	1.66, m	1.52, m	1.66, m	1.48, m	1.61, m
9'	1.04, t (7.4)	1.09, t (7.5)	0.97, t (7.4)	1.01, t (7.5)	0.94, t (7.4)	1.08, t (7.3)	0.92, t (7.4)	1.00, t (7.5)	1.00, t (7.3)	1.07, t (7.5)
OMe	-	-	-	-	-	-	-	-	3.84, s	3.92, s

^a500 MHz; ^b400 MHz; ^c600 MHz; ^dRecorded in DMSO-*d*₆; ^eRecorded in acetone-*d*₆; ^fRecorded in methanol-*d*₄ P: spiromastixone P, Q: spiromastixone Q, R: spiromastixone R, S: spiromastixone S, T: spiromastixone T. The NMR data of known analogues are cited from the literature (Guo, Z.; Zhu, W.; Zhao, L.; Chen, Y.; Li, S.; Cheng, P.; Ge, H.; Tan, R.; Jiao, R. New antibacterial depsidones from an ant-derived fungus Spiromastix sp. MY-1, Chin. J. Nat. Med. 2022, 20, 627-632).

P

Table S13. Comparison of the ^{13}C NMR data of **12-16** to spiromastixones P-T (δ_{C} ppm)

Position	12^{a,d}	P^{b,e}	13^{a,d}	Q^{a,e}	14^{a,d}	R^{b,e}	15^{a,d}	S^{a,f}	16^{a,d}	T^{a,e}
1	111.4, C	113.1, C	111.2, C	113.1, C	112.9, C	114.8, C	100.0, C	116.7, C	112.4, C	114.0, C
2	162.7, C	162.8, C	162.6, C	162.7, C	160.6, C	159.4, C	160.6, C	156.9, C	160.5, C	159.9, C
3	105.1, CH	105.7, CH	105.1, CH	105.8, CH	98.9, C	99.4, C	101.7, C	101.1, C	98.9, C	99.4, C
4	162.6, C	163.1, C	162.3, C	163.1, C	159.5, C	161.5, C	160.6, C	160.8, C	159.6, C	161.4, C
5	115.6, CH	116.1, CH	115.7, CH	116.2, CH	114.9, CH	115.5, CH	117.6, C	112.2, C	115.2, CH	115.8, CH
6	149.7, C	150.7, C	149.5, C	150.4, C	147.9, C	149.0, C	144.4, C	147.2, C	148.6, C	149.6, C
7	163.2, C	164.3, C	163.4, C	164.3, C	162.7, C	163.1, C	163.5, C	164.1, C	161.9, C	162.4, C
8	35.5, CH ₂	36.4, CH ₂	35.3, CH ₂	36.3, CH ₂	36.6, CH ₂	36.5, CH ₂	37.2, CH ₂	37.4, CH ₂	35.8, CH ₂	36.6, CH ₂
9	24.7, CH ₂	25.4, CH ₂	24.7, CH ₂	25.4, CH ₂	24.6, CH ₂	25.3, CH ₂	22.9, CH ₂	24.1, CH ₂	24.6, CH ₂	25.3, CH ₂
10	14.3, CH ₃	14.3, CH ₃	14.2, CH ₃	14.3, CH ₃	14.3, CH ₃	14.4, CH ₃	14.6, CH ₃	14.2, CH ₃	14.4, CH ₃	14.3, CH ₃
1'	141.6, C	143.1, C	142.4, C	143.8, C	141.9, C	143.3, C	142.3, C	143.5, C	143.0, C	144.1, C
2'	143.7, C	145.1, C	142.9, C	144.1, C	144.5, C	145.6, C	145.7, C	145.7, C	143.9, C	144.9, C
3'	105.5, CH	106.2, CH	99.2, C	99.8, C	105.5, CH	106.0, CH	105.2, CH	106.0, CH	103.9, CH	103.4, CH
4'	152.4, C	152.8, C	152.6, C	153.0, C	155.4, C	155.9, C	154.9, C	156.6, C	154.3, C	155.3, C
5'	108.3, C	108.7, C	112.7, CH	113.3, CH	113.8, CH	114.2, CH	113.1, C	114.7, C	110.2, C	110.7, C
6'	135.7, C	136.7, C	134.3, C	135.4, C	136.3, C	137.4, C	135.9, C	137.7, C	136.1, C	137.4, C
7'	32.4, CH ₂	33.1, CH ₂	31.2, CH ₂	32.2, CH ₂	32.8, CH ₂	33.8, CH ₂	32.9, CH ₂	34.2, CH ₂	32.9, CH ₂	33.8, CH ₂
8'	22.7, CH ₂	23.4, CH ₂	23.6, CH ₂	24.2, CH ₂	24.4, CH ₂	25.0, CH ₂	24.6, CH ₂	25.4, CH ₂	23.1, CH ₂	23.7, CH ₂
9'	14.5, CH ₃	14.4, CH ₃	14.3, CH ₃	14.2, CH ₃	14.2, CH ₃	14.3, CH ₃	14.3, CH ₃	14.2, CH ₃	14.4, CH ₃	14.2, CH ₃
OMe	-	-	-	-	-	-	-	-	-	57.4, CH ₃
										57.3, CH ₃

^a500 MHz; ^b400 MHz; ^c600 MHz; ^dRecorded in DMSO-*d*₆; ^eRecorded in acetone-*d*₆; ^fRecorded in methanol-*d*₄ P: spiomastixone P, Q: spiomastixone Q, R: spiomastixone R, S: spiomastixone S, T: spiomastixone T. The NMR data of known analogues are cited from the literature (Guo, Z.; Zhu, W.; Zhao, L.; Chen, Y.; Li, S.; Cheng, P.; Ge, H.; Tan, R.; Jiao, R. New antibacterial depsidones from an ant-derived fungus Spiromastix sp. MY-1, Chin. J. Nat. Med. 2022, 20, 627-632).