

Supplementary Information

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The 16S rRNA Gene Sequences Data of *Streptomyces* sp. FXJ7.328

TCGAAGAAGAAAGCCGCTTCGGTGGTGGATTAGTGGCGAACGGGTGAGTAACACGTGGG
CAATCTGCCCTGCACTCTGGGACAAGCCCTGGAAACGGGTCTAATACCGGATATGACACG
GGATCGCATGGTCCGTGTCTGGAAAGCTCCGGCGGTGCAGGATGAGCCCGGGCCTATCAC
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GGTGTACAGGTGGTGCATGGCTGTCGTCAGCTCGTGTGTCGTGAGATGTTGGGTAAAGTCCC
GCAACGAGCGCAACCCTT GTCCTGTGTTGCCAGCAACTCCTTTC

The Physicochemical Data of the Known Compounds 7–10

Compound 7: White solid; $^1\text{H NMR}$ (600 MHz, $\text{C}_5\text{H}_5\text{N}-d_5$): δ 11.33 (1H, s, H-1), 10.97 (1H, s, H-4), 6.32 (1H, d, $J = 10.4$ Hz, H-7), 3.21 (1H, m, H-8), 1.09 (6H, d, $J = 6.6$ Hz, CH_3 -9/10), 7.32 (1H, s, H-11), 7.65 (2H, d, $J = 7.6$ Hz, H-13/17), 7.33 (2H, t, $J = 7.6$ Hz, H-14/16), 7.24 (1H, t, $J = 7.3$ Hz, H-15). $^{13}\text{C NMR}$ (150 MHz, $\text{C}_5\text{H}_5\text{N}-d_5$): δ 156.9 (C_q , C-2), 126.5 (C_q , C-3), 157.1 (C_q , C-5), 125.1 (C_q , C-6), 124.0 (C_q , C-7), 23.8 (CH, C-8), 20.7×2 (CH_3 , C-9/10), 113.1 (CH, C-11), 133.0 (C_q , C-12), 127.6×2 (CH, C-13/17), 127.9×2 (CH, C-14/16), 126.6 (CH, C-15). ESIMS m/z 257 [$\text{M} + \text{H}$] $^+$.

Compound 8: Yellow solid; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 3.29 (3H, s, NCH_3 -1), 8.02 (1H, s, H-4), 5.49 (1H, d, $J = 9.66$ Hz, H-7), 3.76 (1H, m, H-8), 1.08 (6H, d, $J = 6.6$ Hz, CH_3 -9/10), 6.98 (1H, s, H-11), 7.38 (2H, d, $J = 7.5$ Hz, H-13/17), 7.41 (2H, t, $J = 7.4$ Hz, H-14/16), 7.32 (1H, t, $J = 7.4$ Hz, H-15). $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 31.1 (CH_3 , NCH_3 -1), 157.8 (C_q , C-2), 125.8 (C_q , C-3), 157.6 (C_q , C-5), 128.1 (C_q , C-6), 134.8 (C_q , C-7), 26.8 (CH, C-8), 24.4×2 (CH_3 , C-9/10), 115.8 (CH, C-11), 133.4 (C_q , C-12), 128.5×2 (CH, C-13/17), 129.5×2 (CH, C-14/16), 128.6 (CH, C-15). ESIMS m/z 271 [$\text{M} + \text{H}$] $^+$.

Compound 9: White solid; $[\alpha]_D^{25} -88$ (c 0.03, $\text{DMSO}-d_6$), $^1\text{H NMR}$ (600 MHz, $\text{DMSO}-d_6$): δ 8.50 (1H, s, NH-1), 9.96 (1H, s, NH-4), 3.78 (1H, t, $J = 3.8$ Hz, H-6), 2.07 (1H, m, H-7), 0.93 (3H, d, $J = 6.8$ Hz, CH_3 -8), 0.87 (3H, d, $J = 6.6$ Hz, CH_3 -9), 6.66 (1H, s, H-10), 7.45 (2H, d, $J = 7.6$ Hz, H-12/16), 7.39 (2H, t, $J = 7.6$ Hz, H-13/15), 7.29 (1H, t, $J = 7.4$ Hz, H-14). $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO}-d_6$): δ 161.2 (C_q , C-2), 127.1 (C_q , C-3), 167.2 (C_q , C-5), 61.1 (CH, C-6), 34.1 (CH, C-7), 18.7 (CH_3 , C-8), 17.5 (CH_3 , C-9), 114.9 (CH, C-10), 133.8 (C_q , C-11), 129.6×2 (CH, C-12/16), 129.3×2 (CH, C-13/15), 128.6 (CH, C-14). ESIMS m/z 245 [$\text{M} + \text{H}$] $^+$.

Compound 10: Yellow solid; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 3.21 (3H, s, NCH_3 -1), 9.67 (1H, s, H-4), 5.47 (1H, d, $J = 10.4$ Hz, H-7), 3.81 (1H, m, H-8), 1.10 (6H, d, $J = 6.7$ Hz, CH_3 -9/10), 6.46 (1H, s, H-11), 7.52 (2H, d, $J = 7.6$ Hz, H-13/17), 7.33 (2H, t, $J = 7.6$ Hz, H-14/16), 7.27 (1H, t, $J = 7.4$ Hz, H-15). $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 31.1 (CH_3 , NCH_3 -1), 156.9 (C_q , C-2), 125.4 (C_q , C-3), 159.9 (C_q , C-5), 128.1 (C_q , C-6), 134.5 (CH, C-7), 26.8 (CH, C-8), 23.4×2 (CH_3 , C-9/10), 122.4 (CH, C-11), 134.1 (C_q , C-12), 127.9×2 (CH, C-13/17), 130.1×2 (CH, C-14/16), 128.4 (CH, C-15). ESIMS m/z 271 [$\text{M} + \text{H}$] $^+$.

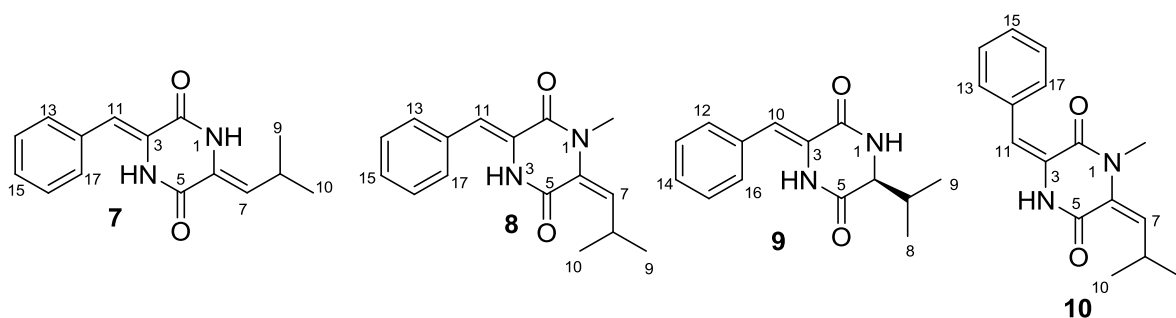


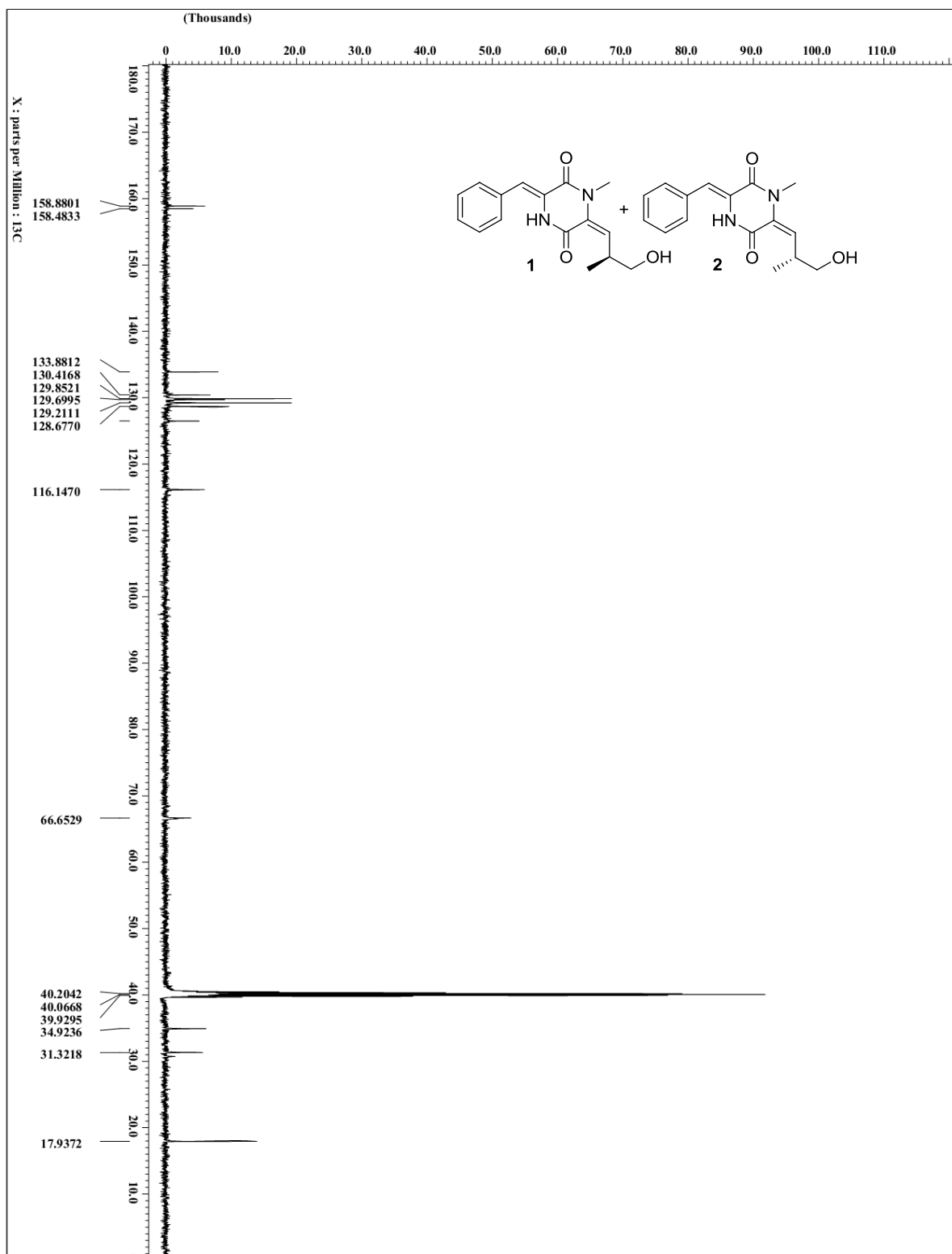
Figure S2. The ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compounds 1 and 2.

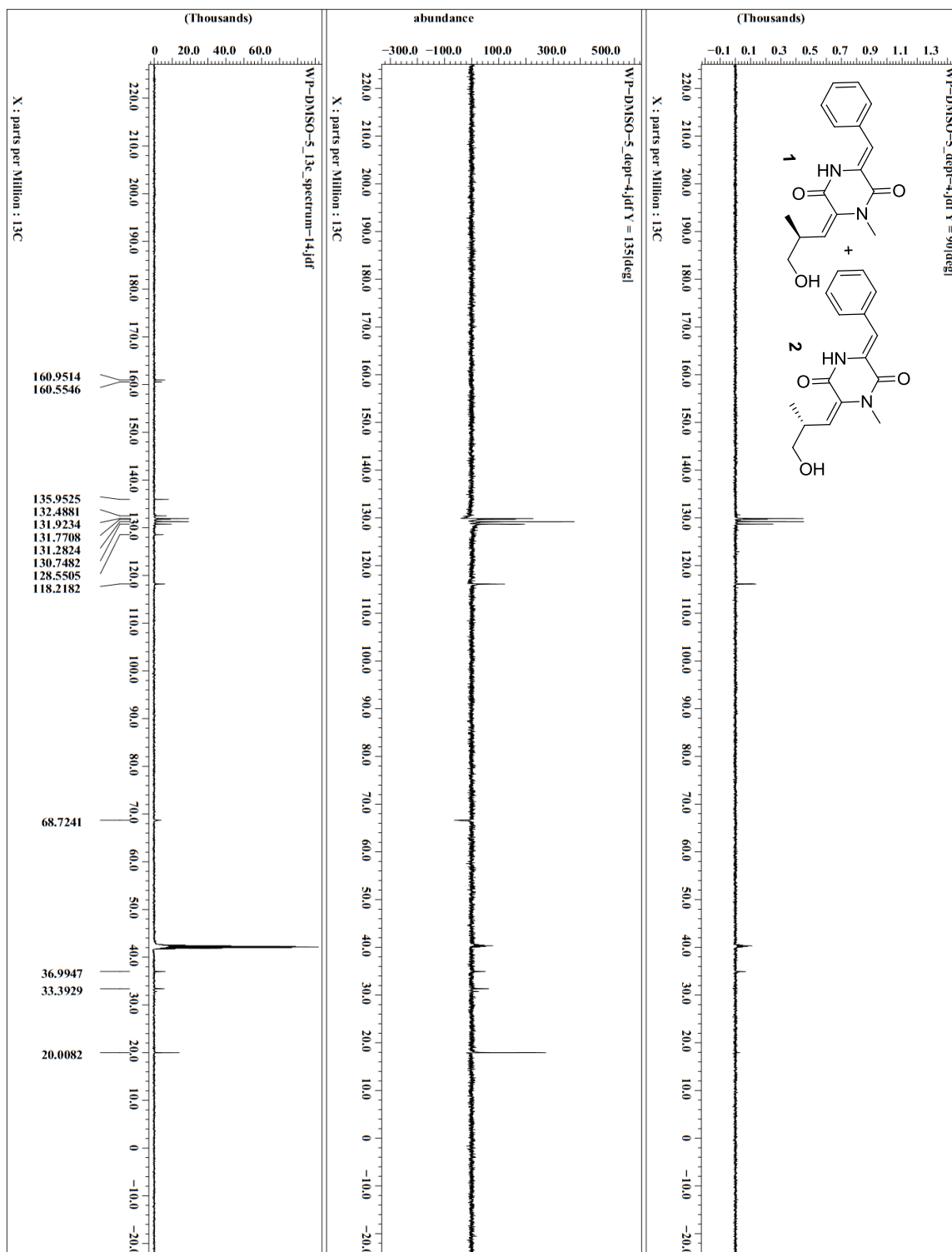
Figure S3. The DEPT (150 MHz, DMSO- d_6) spectrum of compounds 1 and 2.

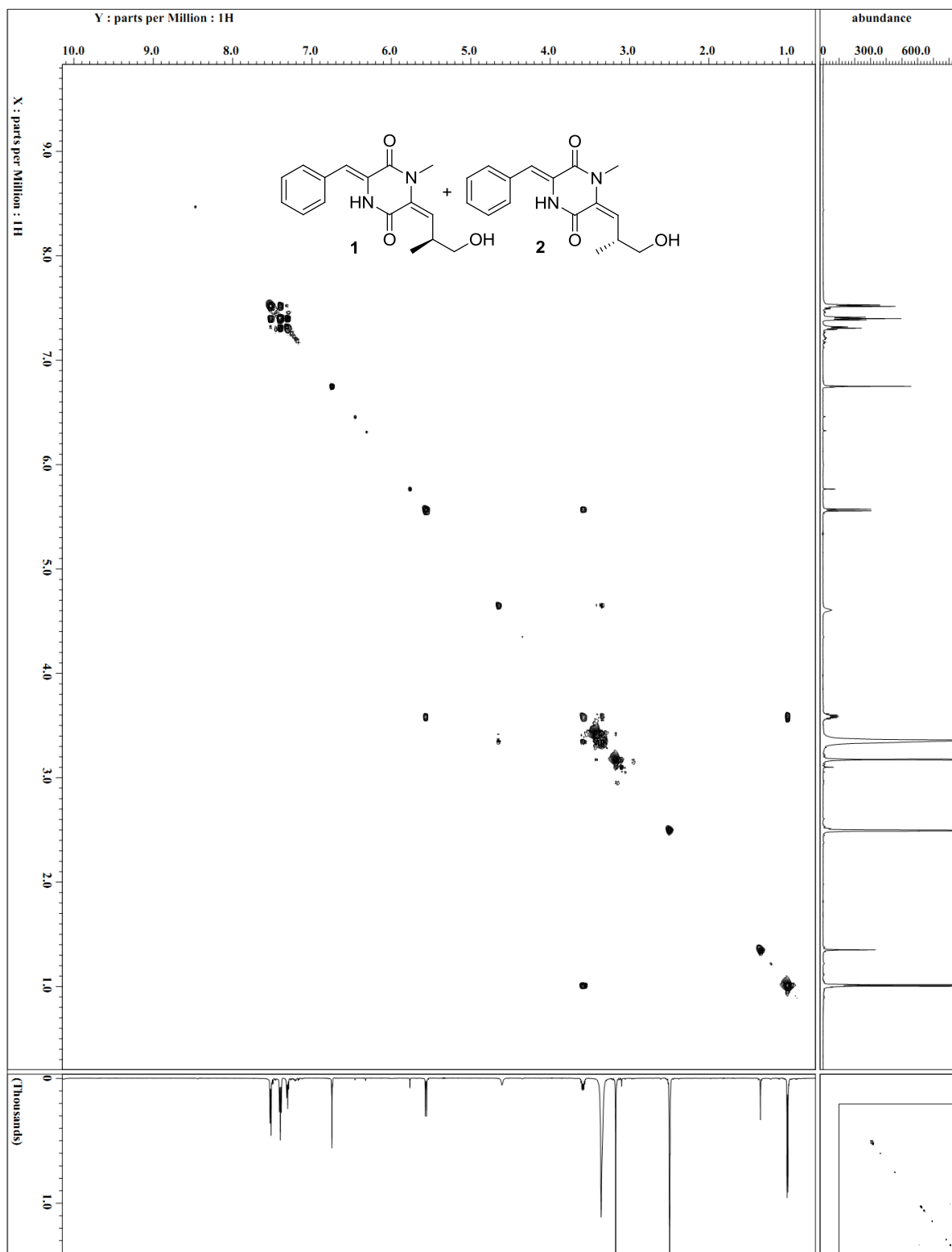
Figure S4. The ^1H - ^1H COSY (600 MHz, $\text{DMSO-}d_6$) spectrum of compounds **1** and **2**.

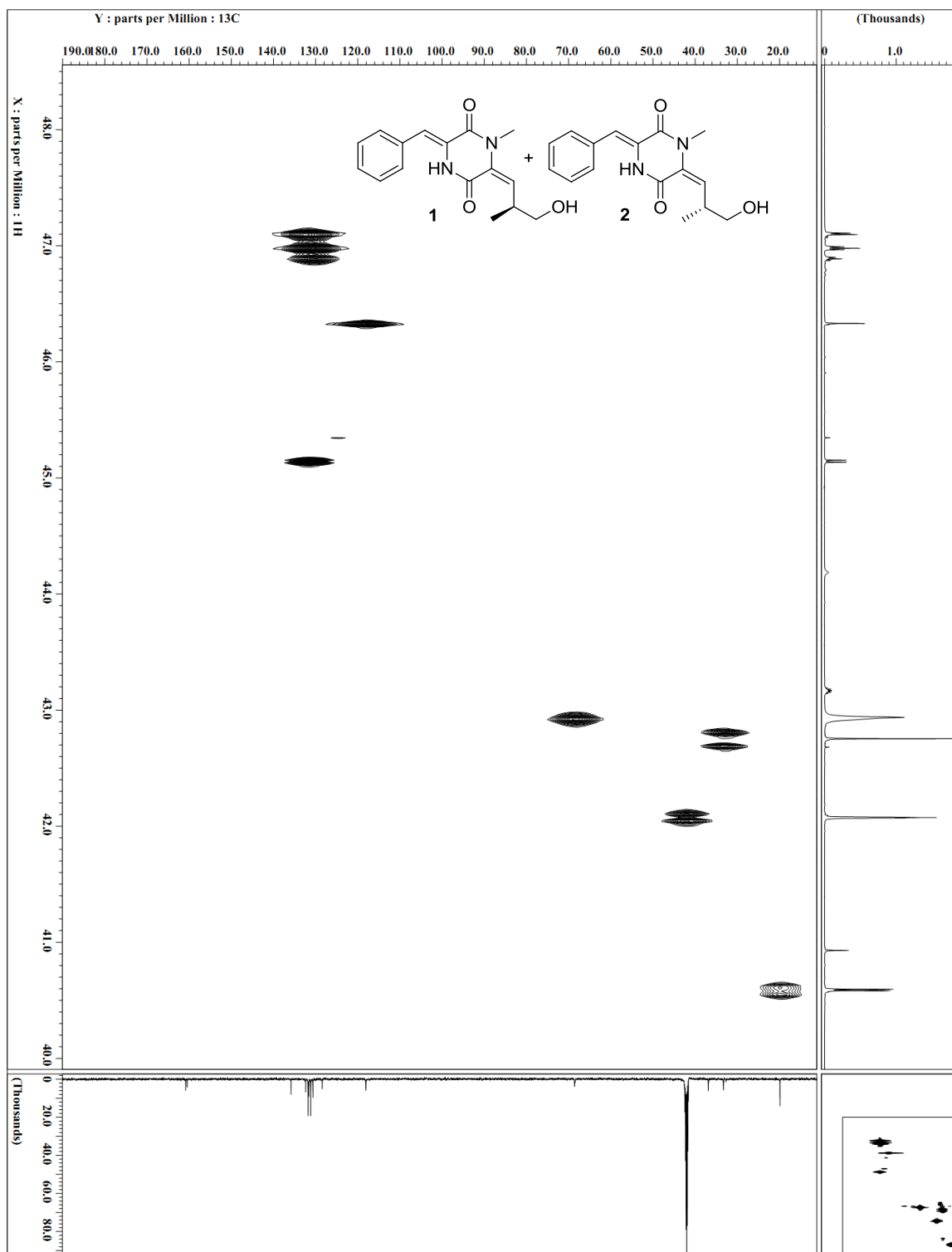
Figure S5. The HMQC (600 MHz, DMSO-*d*₆) spectrum of compounds **1** and **2**.

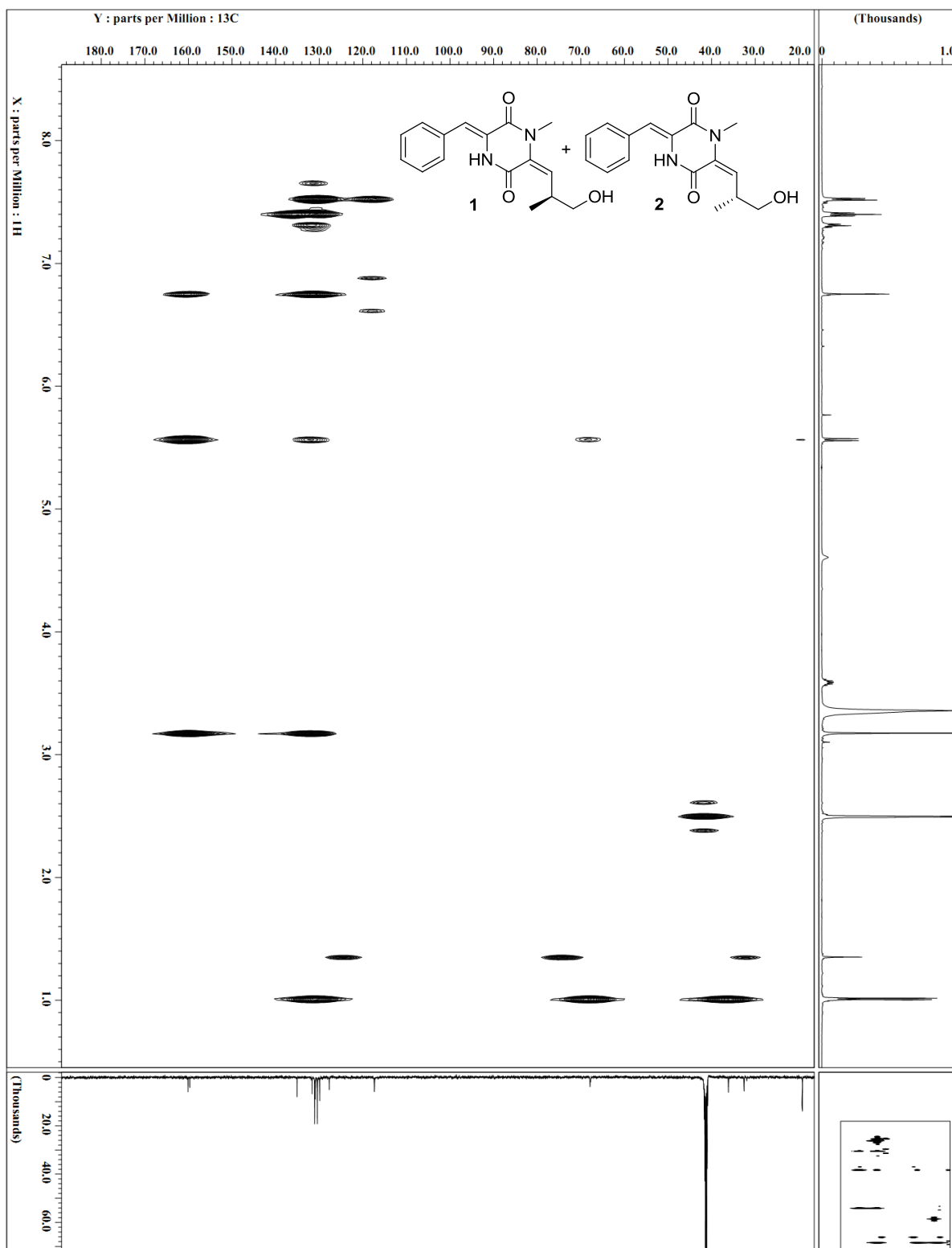
Figure S6. The HMBC (600 MHz, DMSO-*d*₆) spectrum of compounds **1** and **2**.

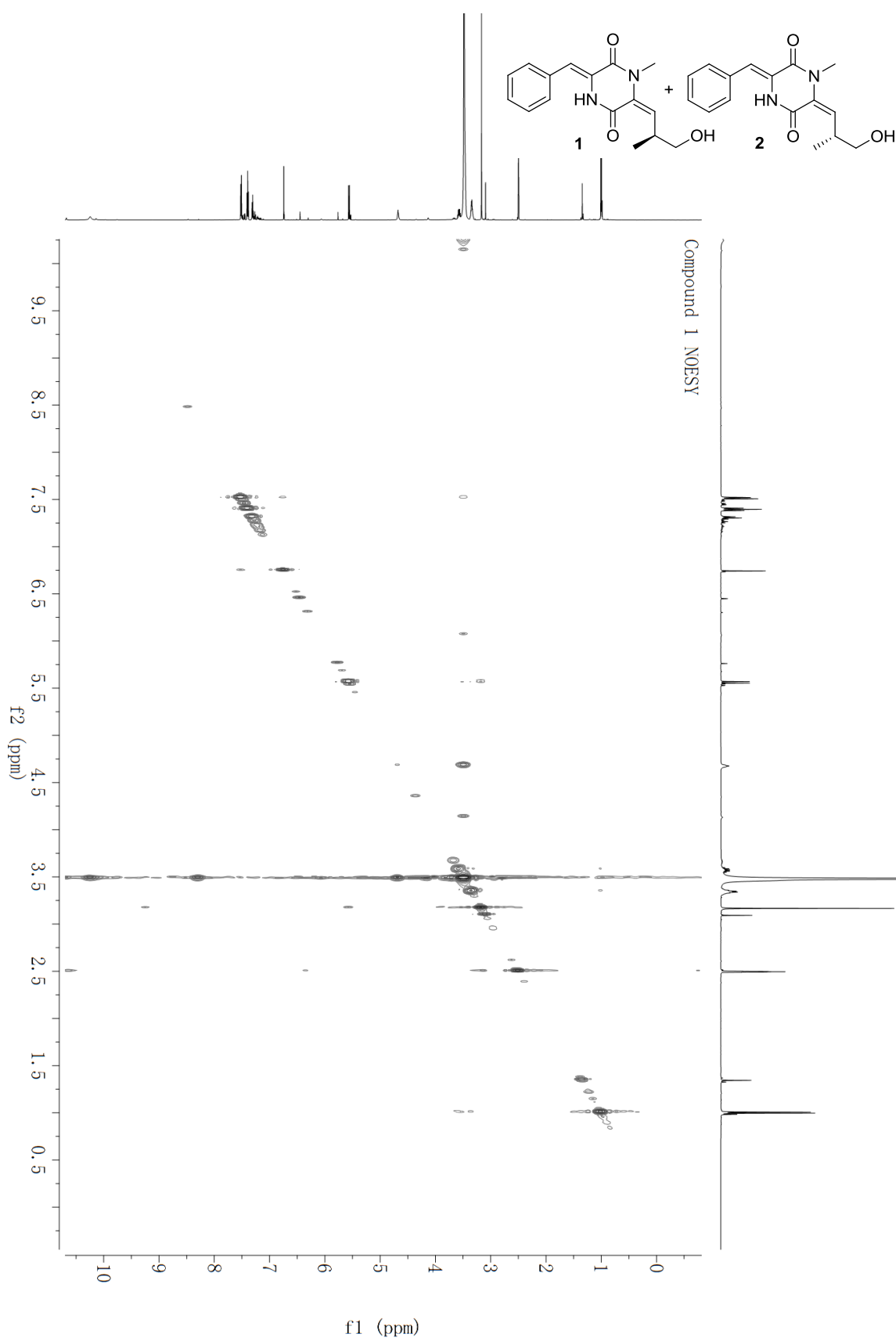
Figure S7. The NOESY (600 MHz, DMSO-*d*₆) spectrum of compounds **1** and **2**.

Figure S8. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**.

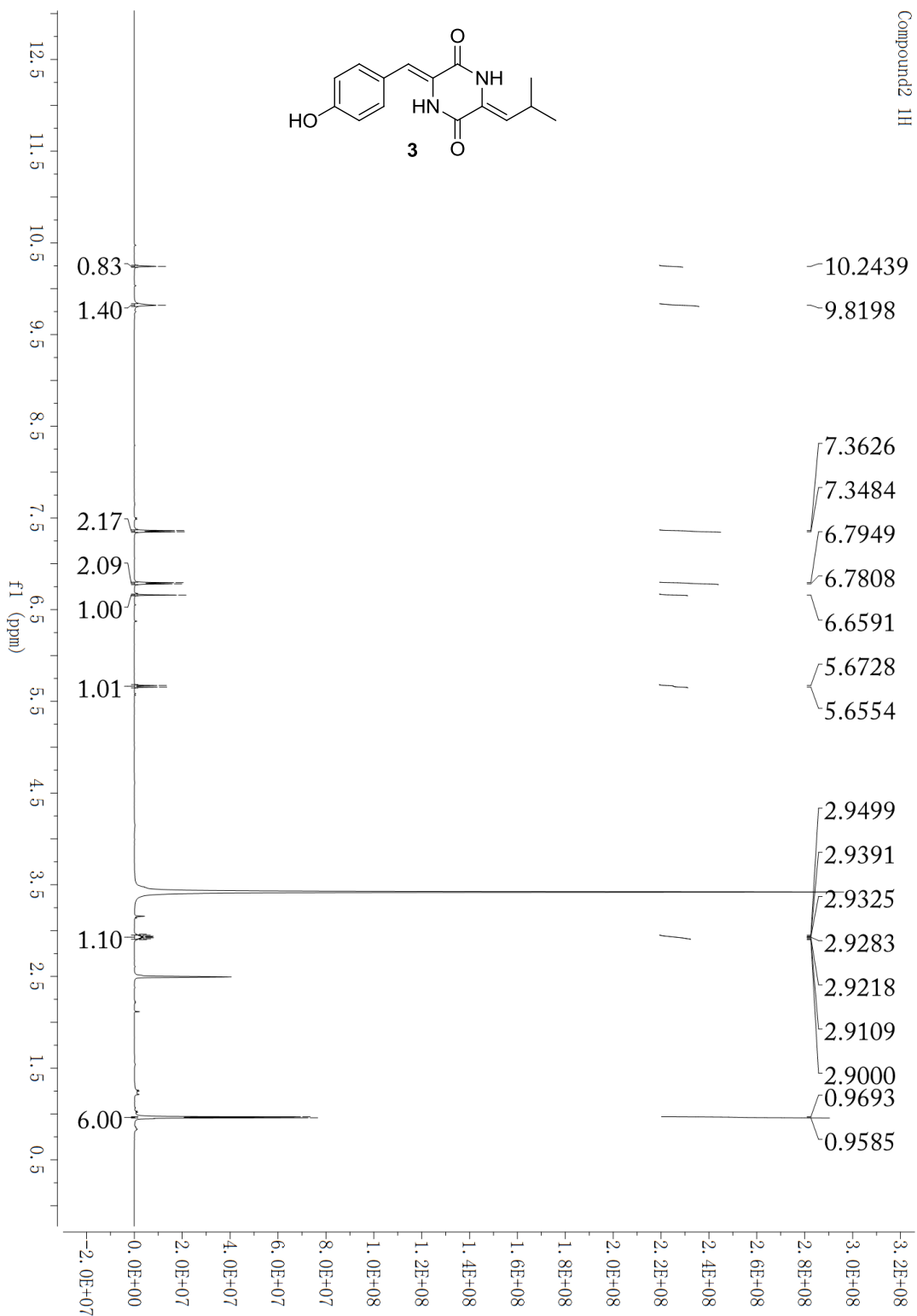


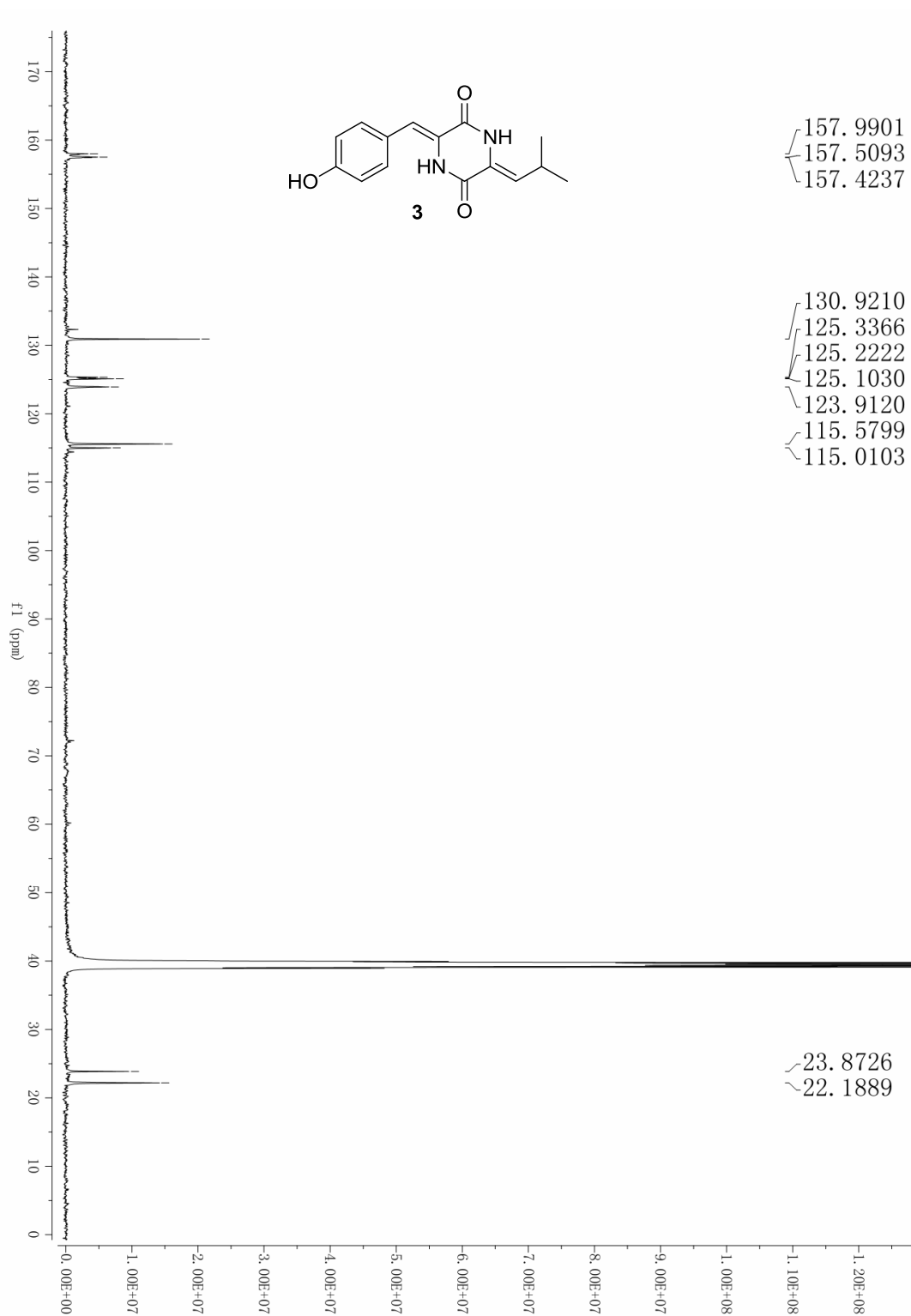
Figure S9. The ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**.

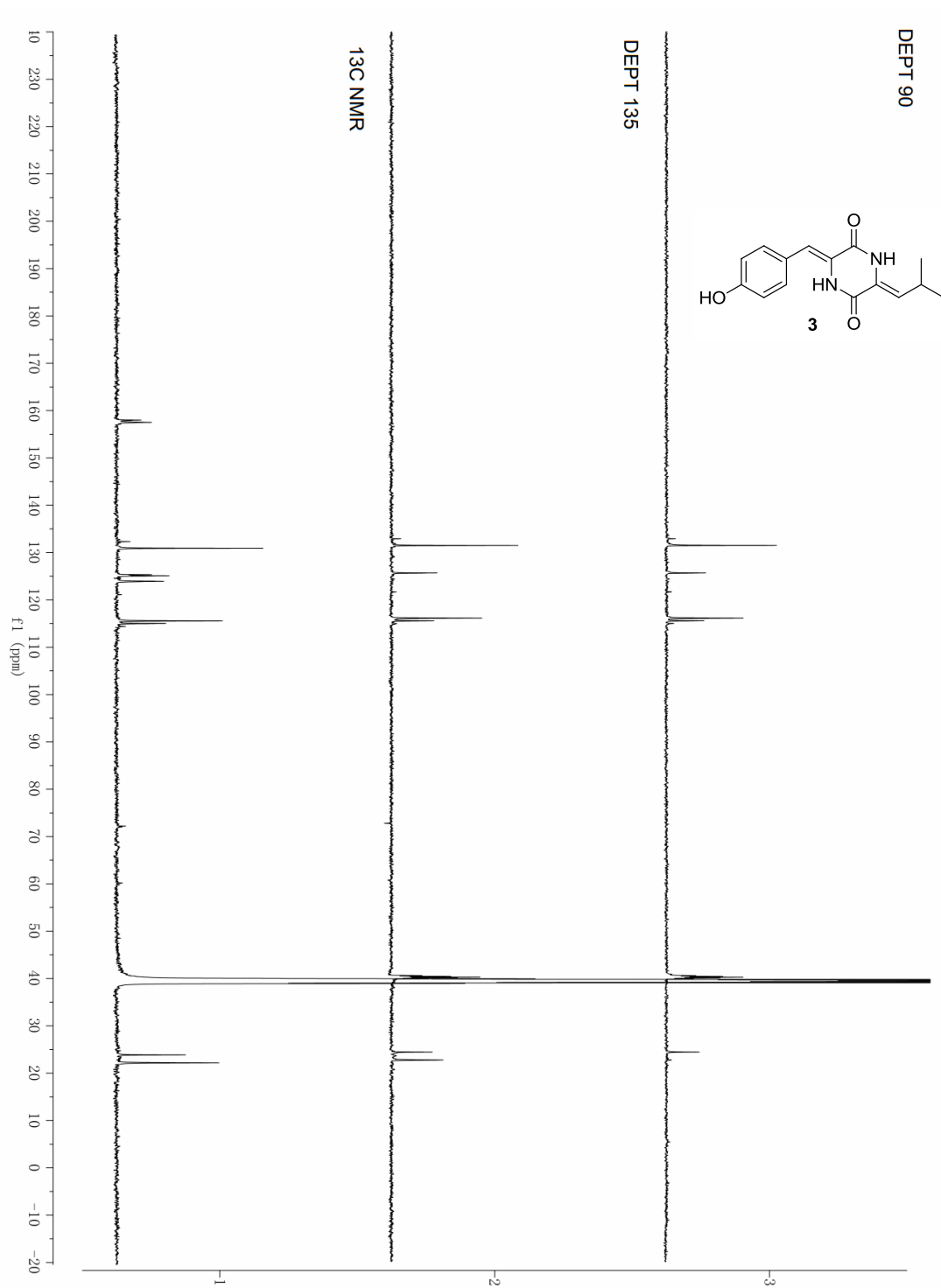
Figure S10. The DEPT (150 MHz, DMSO-*d*₆) spectrum of compound **3**.

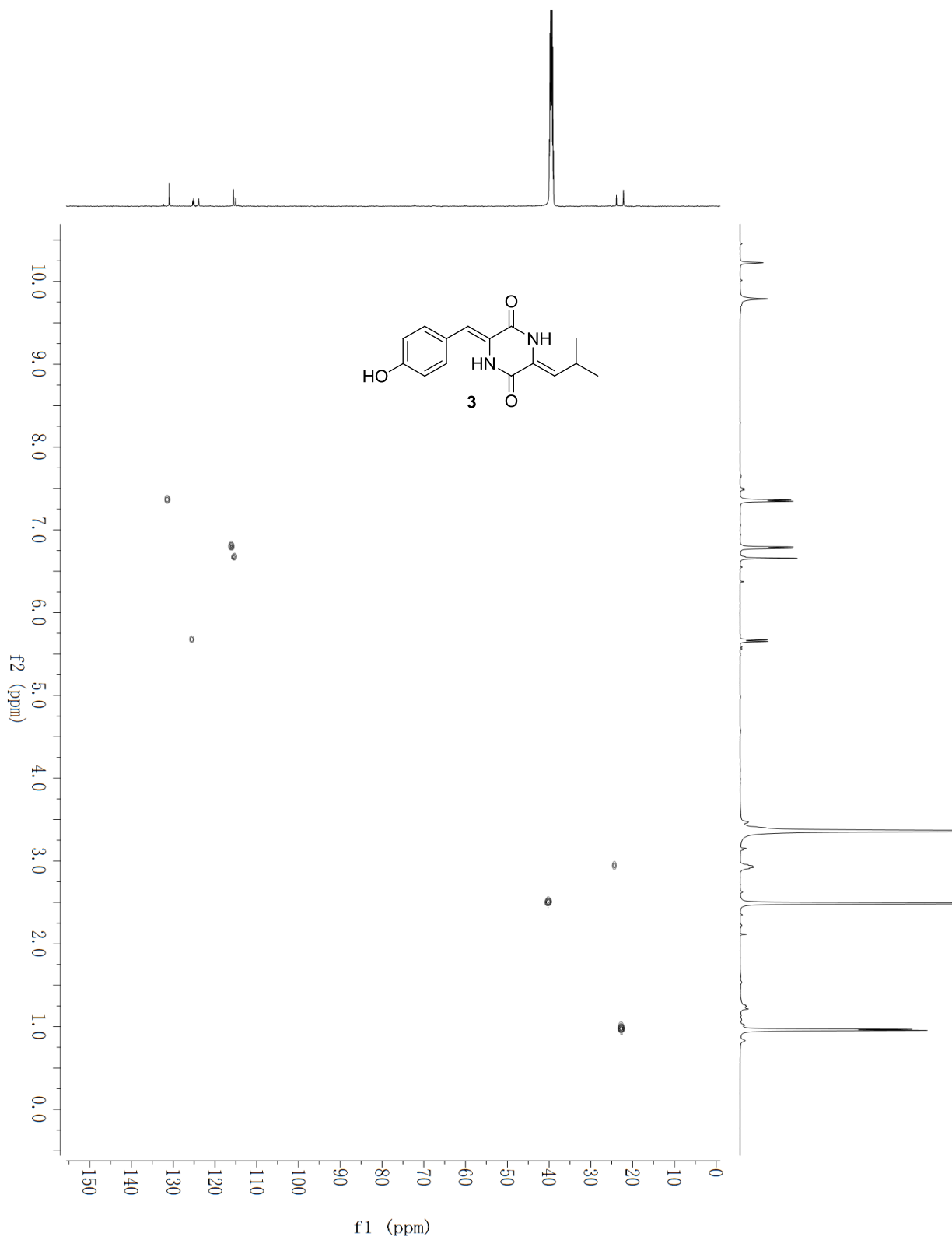
Figure S11. The HMQC (6000 MHz, DMSO- d_6) spectrum of compound **3**.

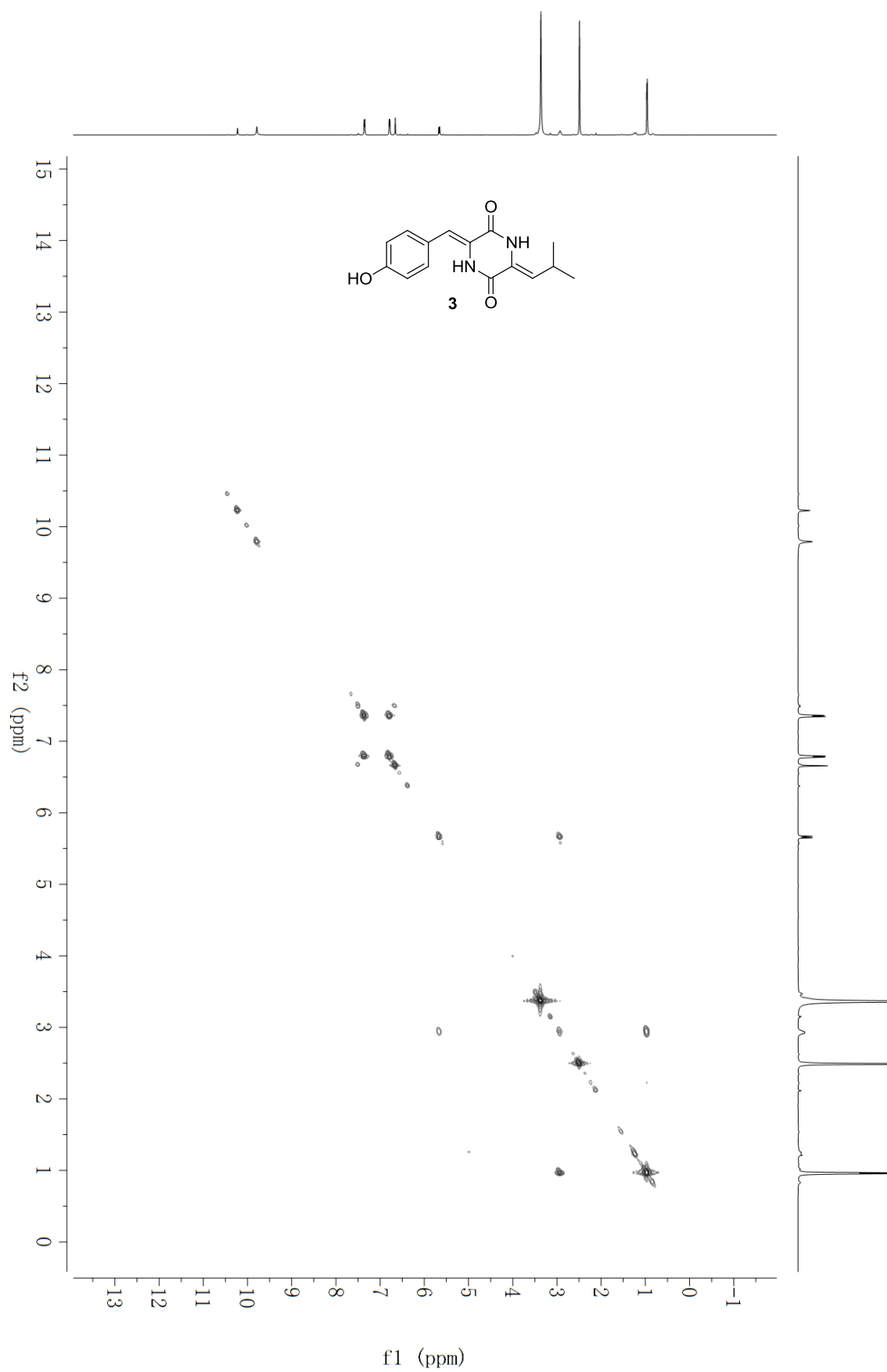
Figure S12. The ^1H - ^1H COSY (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**.

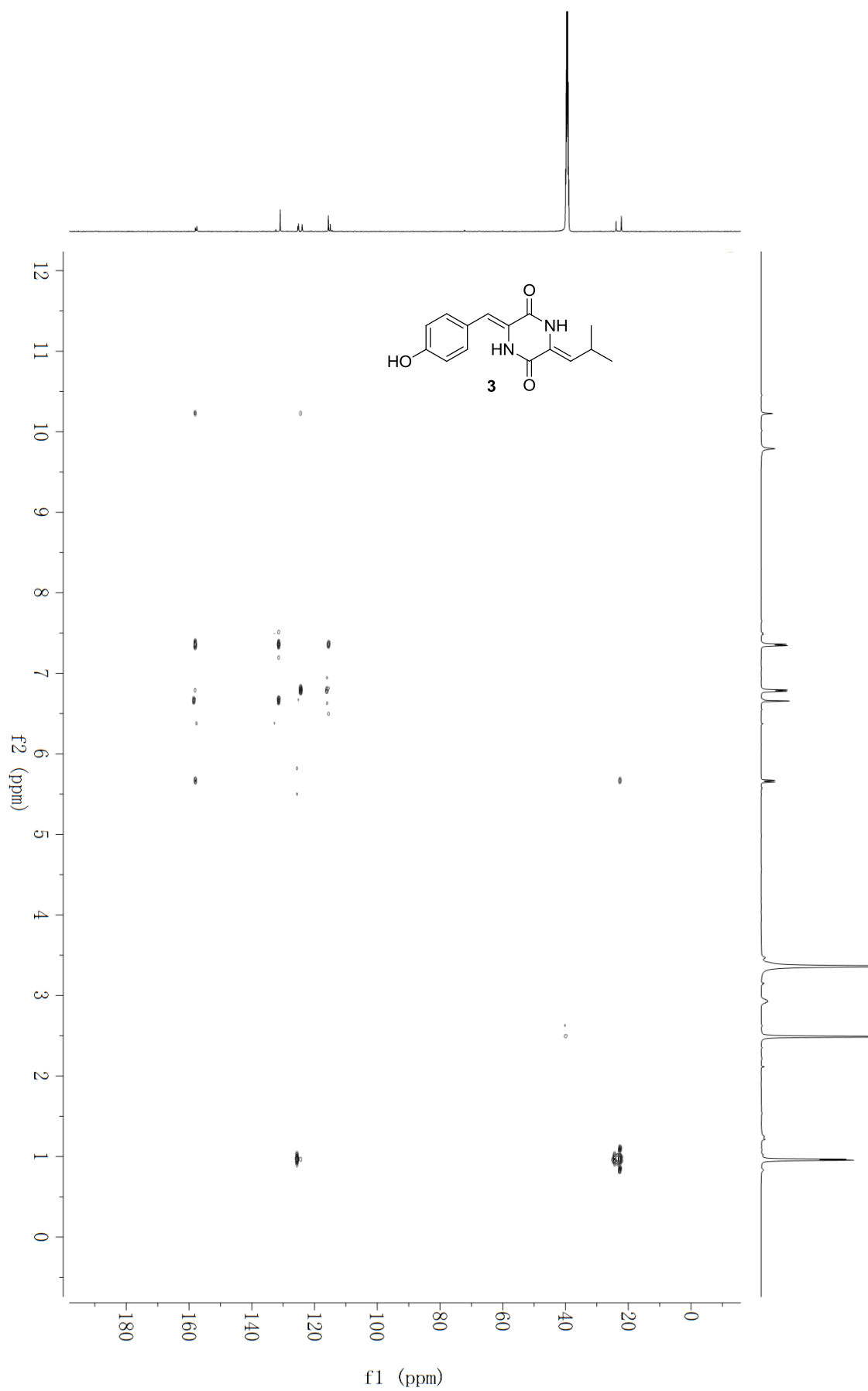
Figure S13. The HMBC (600 MHz, DMSO- d_6) spectrum of compound **3**.

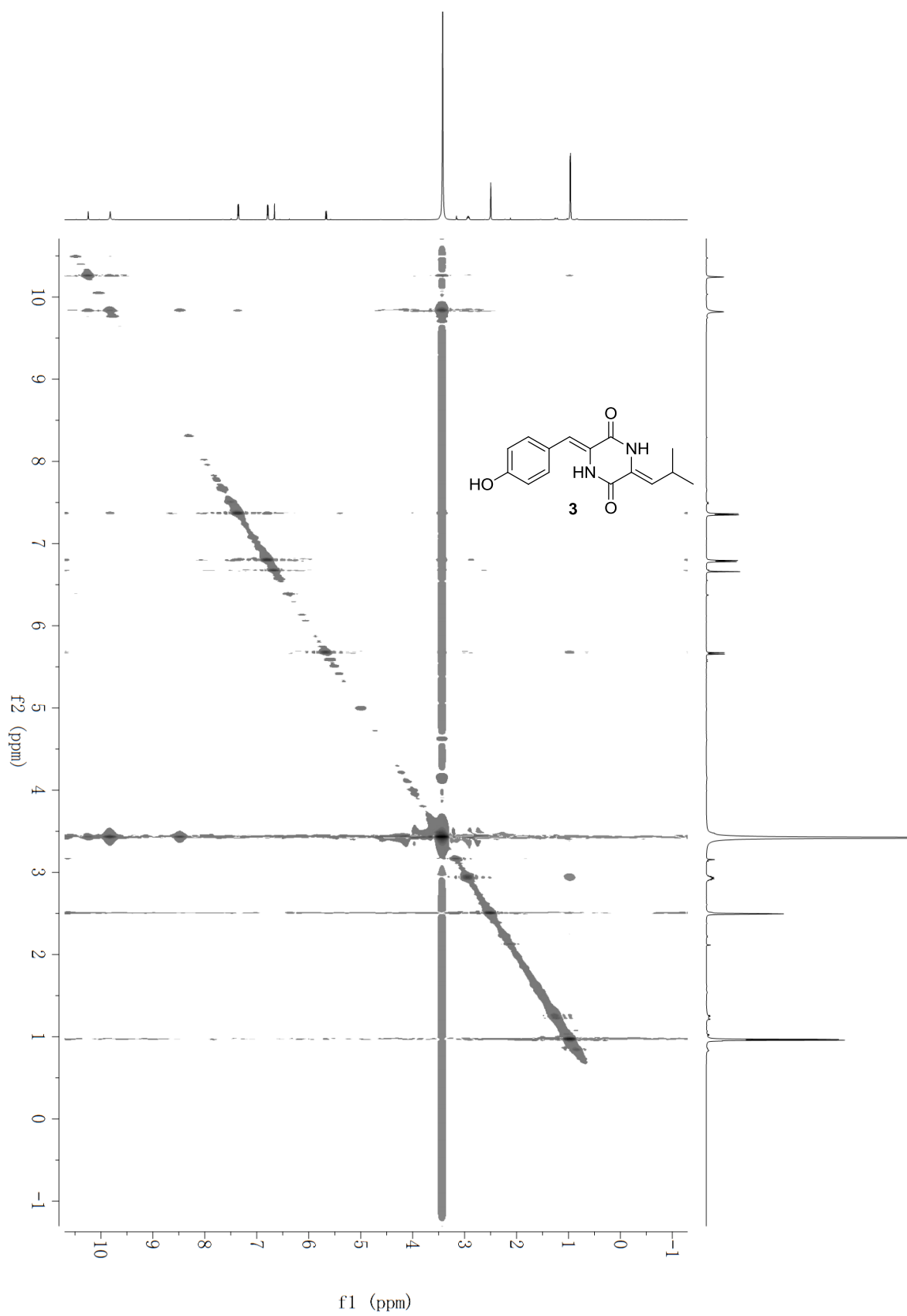
Figure S14. The NOESY (600 MHz, DMSO-*d*₆) spectrum of compound **3**.

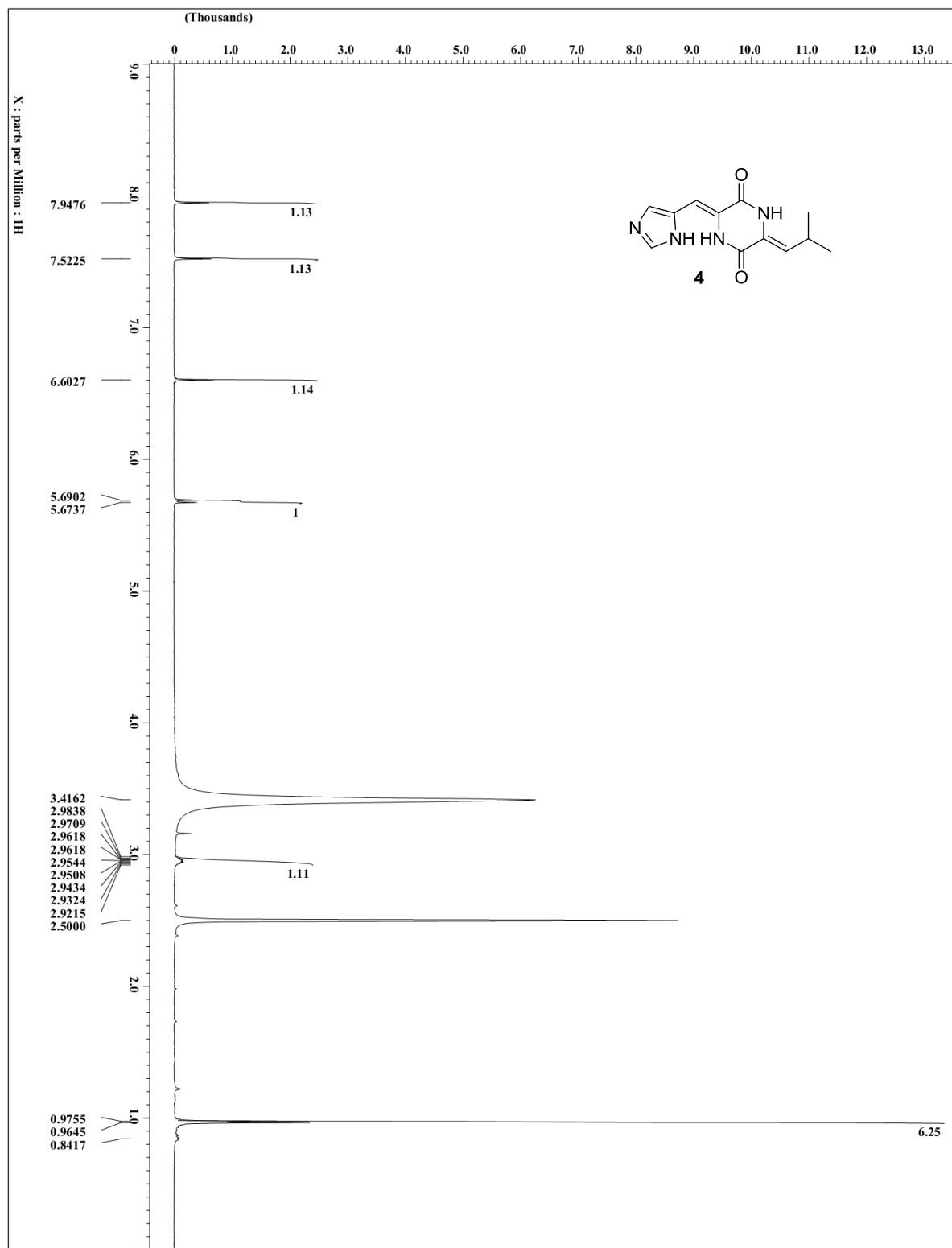
Figure S15. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **4**.

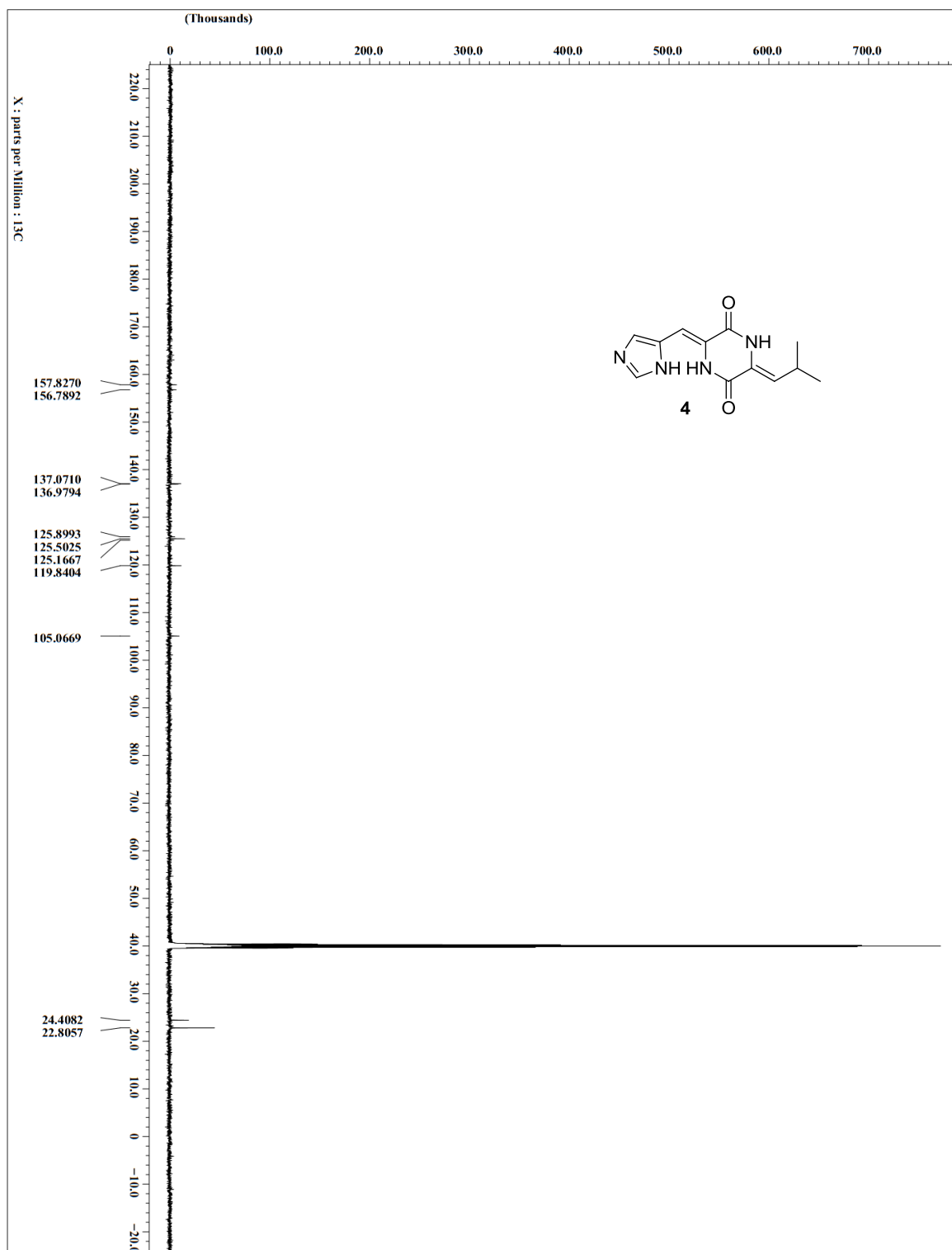
Figure S16. The ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound **4**.

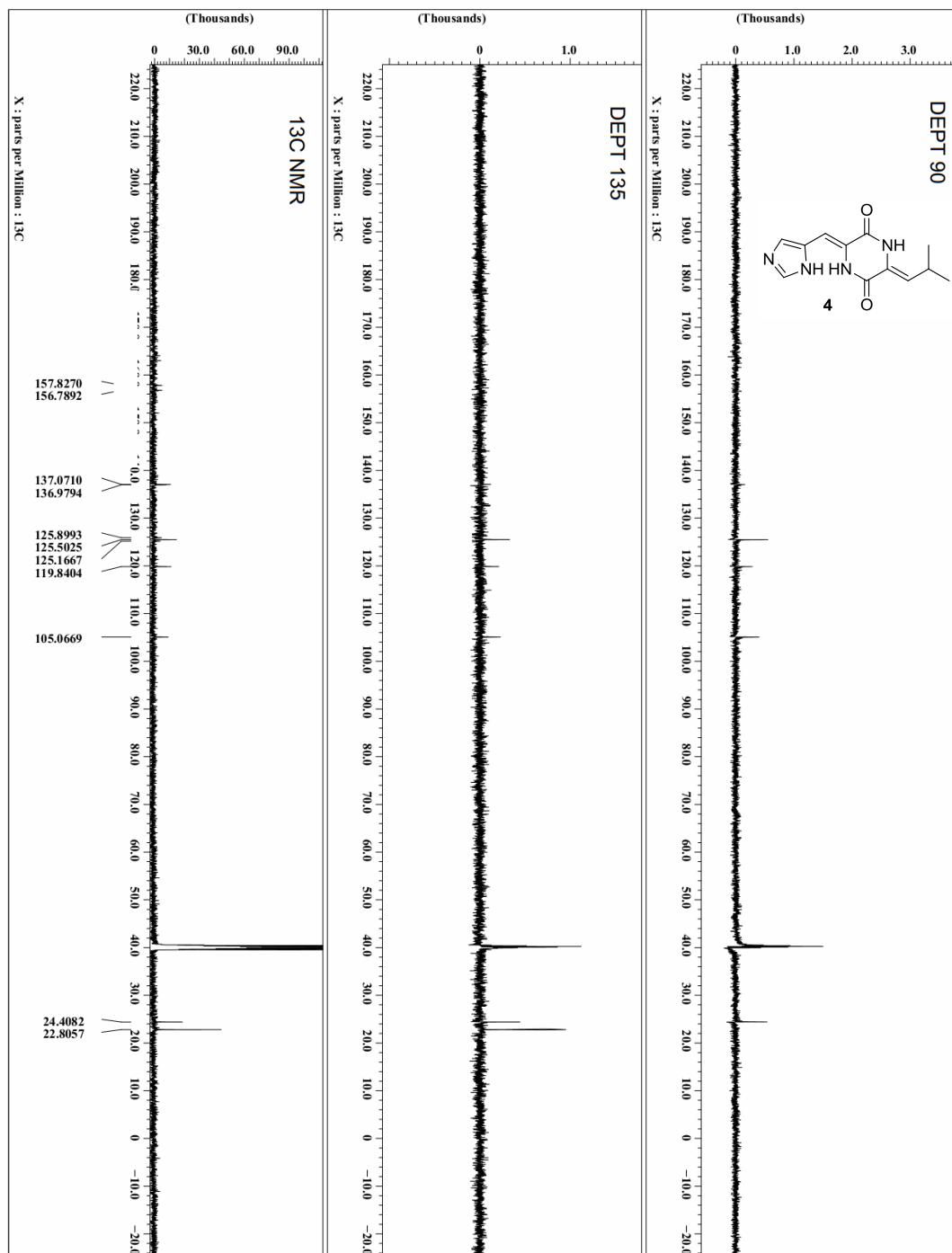
Figure S17. The DEPT (150 MHz, DMSO-*d*₆) spectrum of compound 4.

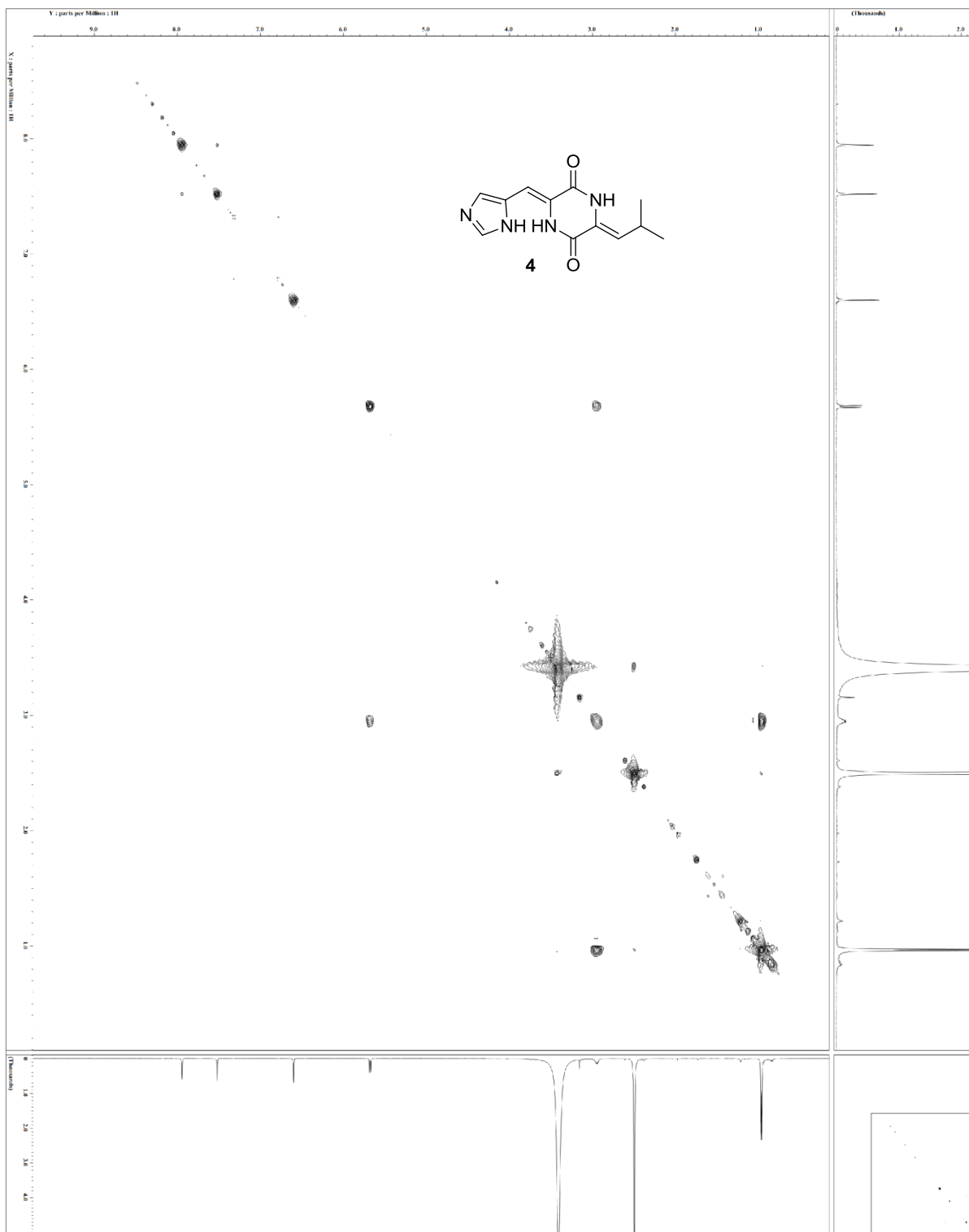
Figure S18. The ^1H - ^1H COSY (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **4**.

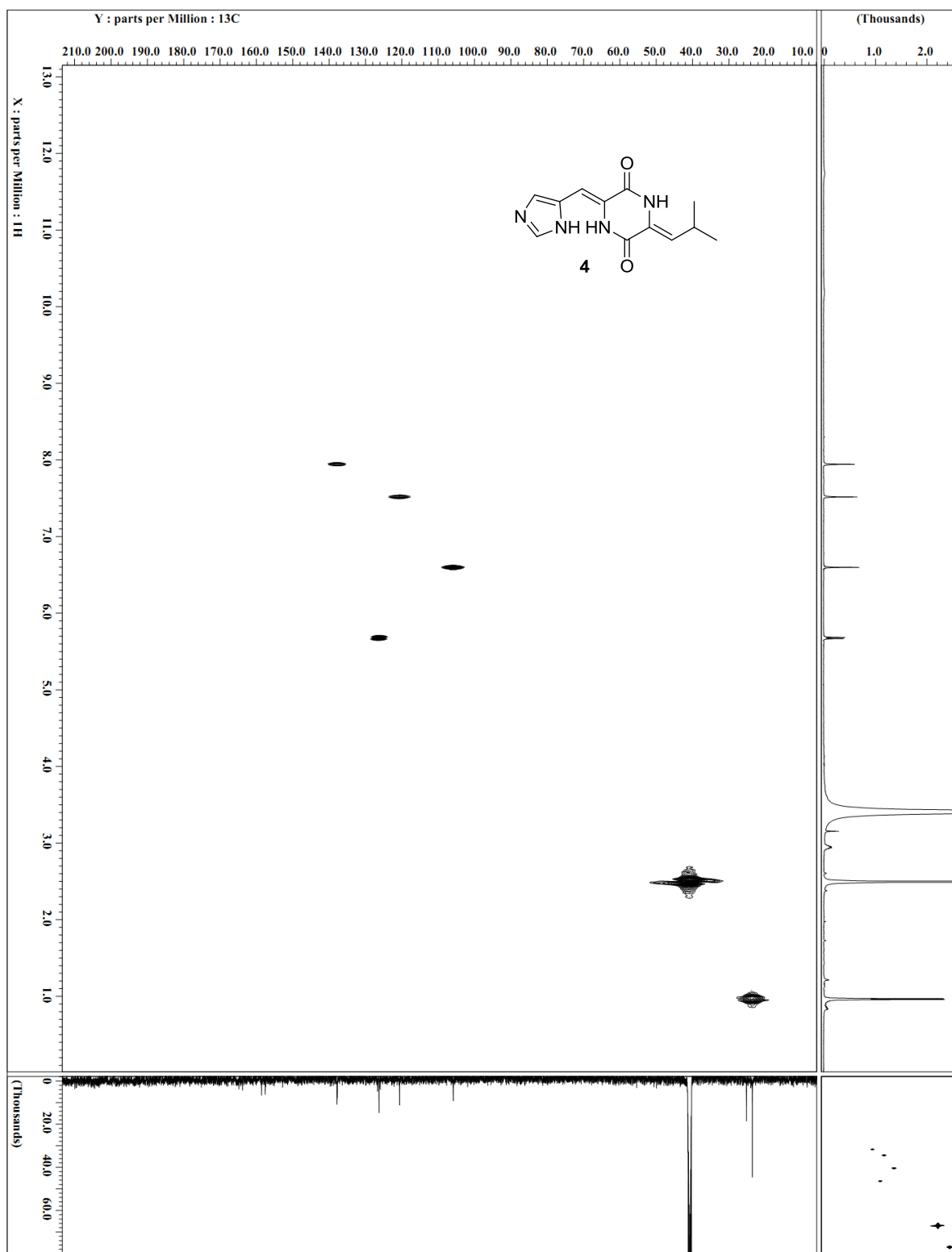
Figure S19. The HMQC (600 MHz, DMSO-*d*₆) spectrum of compound **4**.

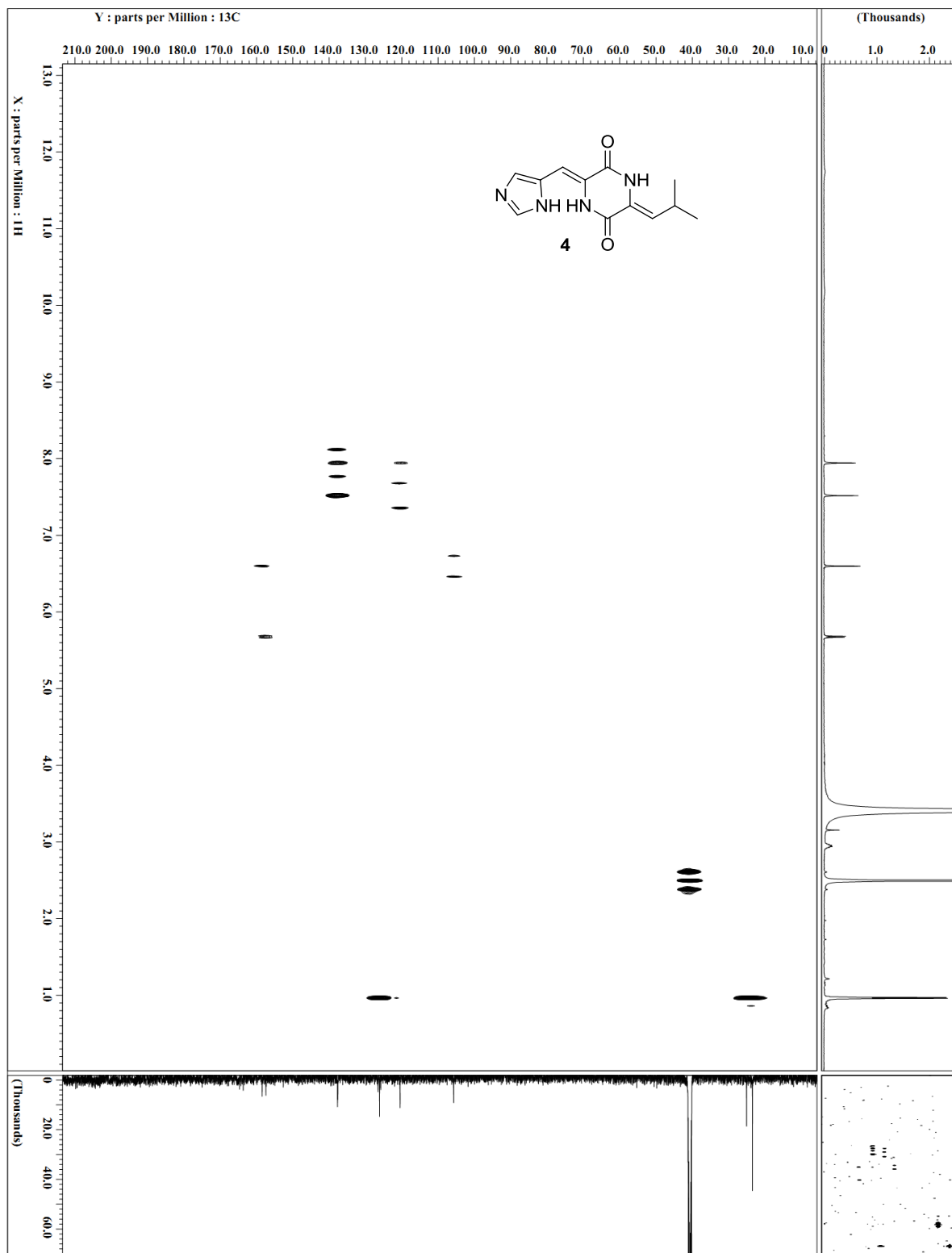
Figure S20. The HMBC (600 MHz, DMSO- d_6) spectrum of compound **4**.

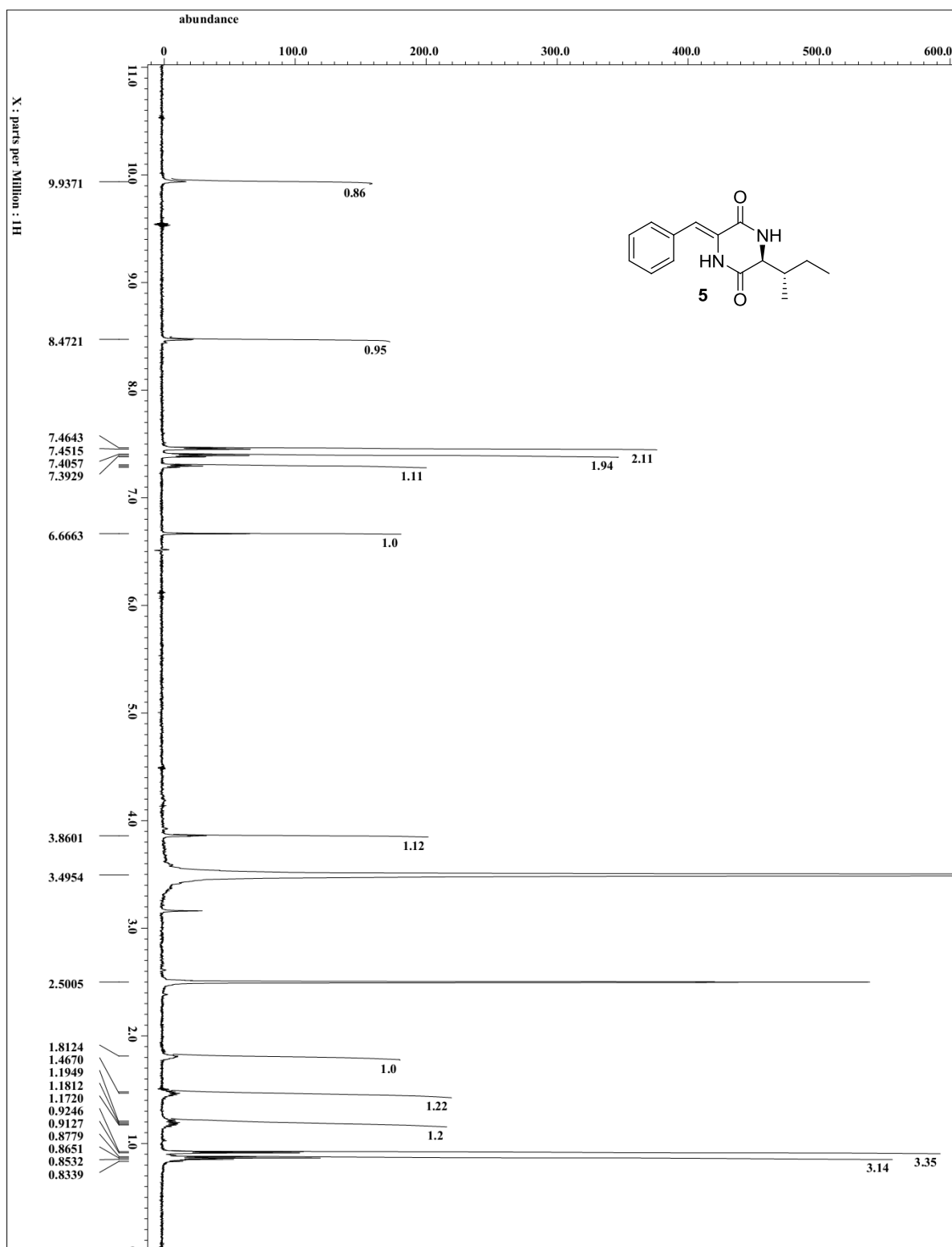
Figure S21. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of compound 5.

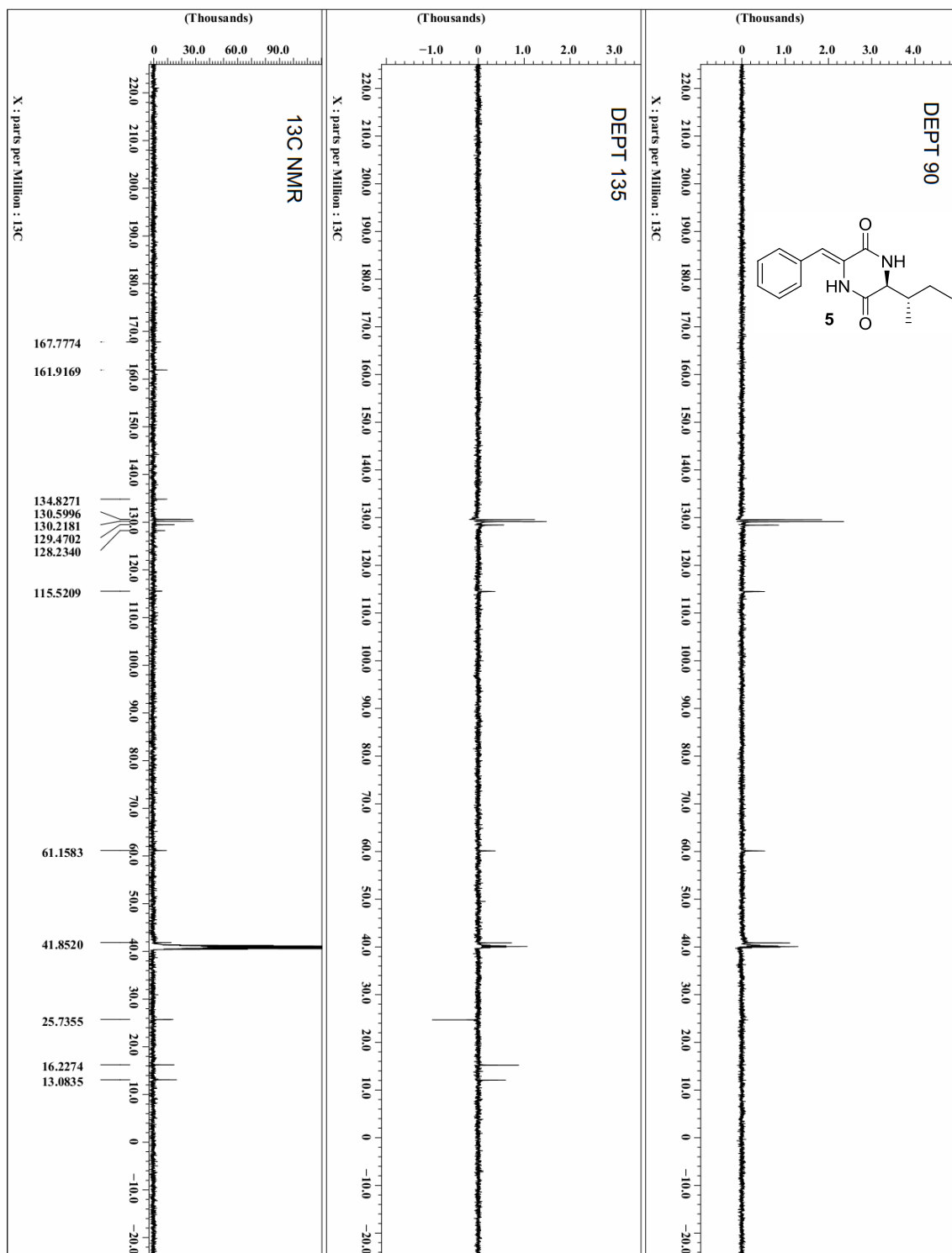
Figure S23. The DEPT (150 MHz, DMSO-*d*₆) spectrum of compound 5.

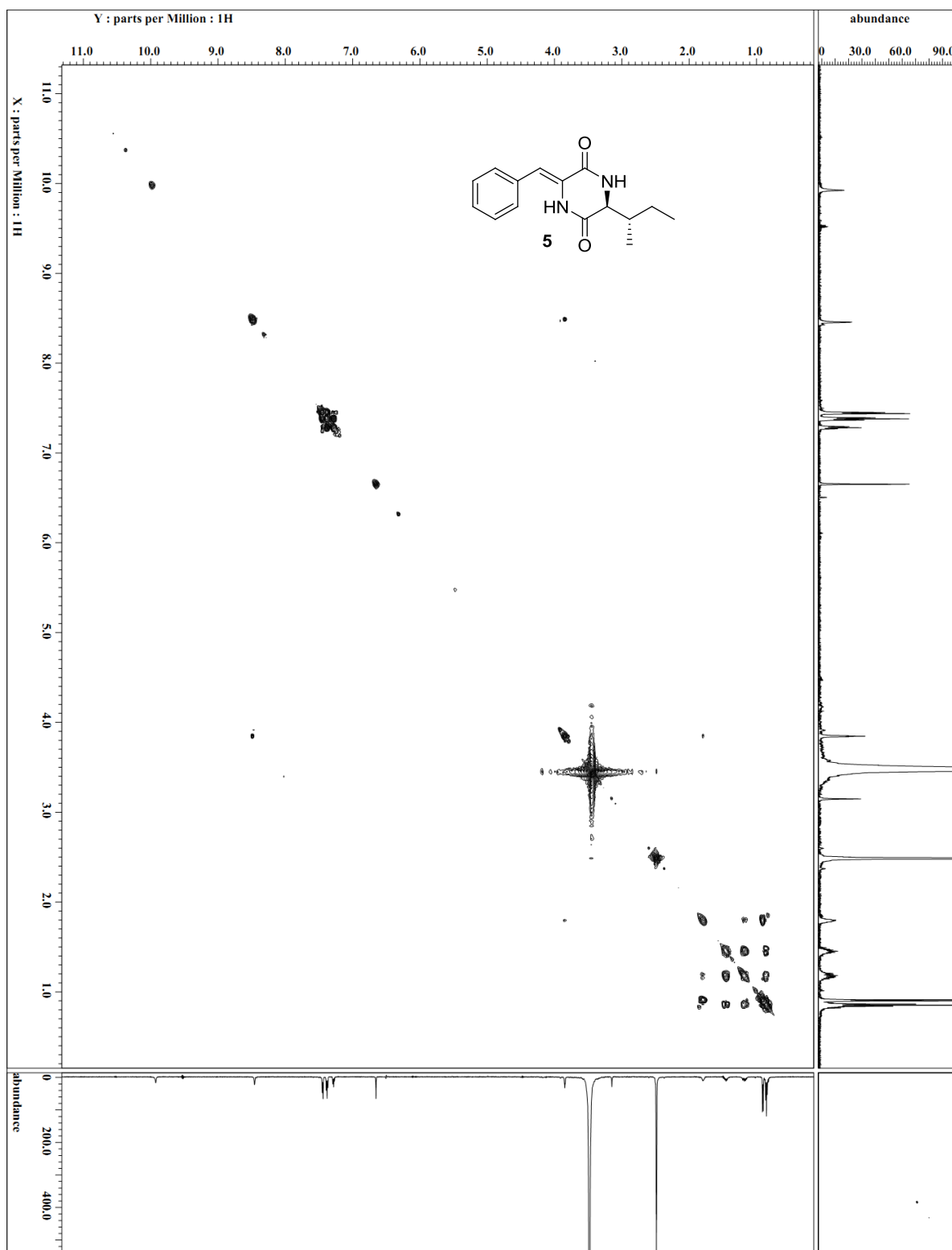
Figure S24. The ^1H - ^1H COSY (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **5**.

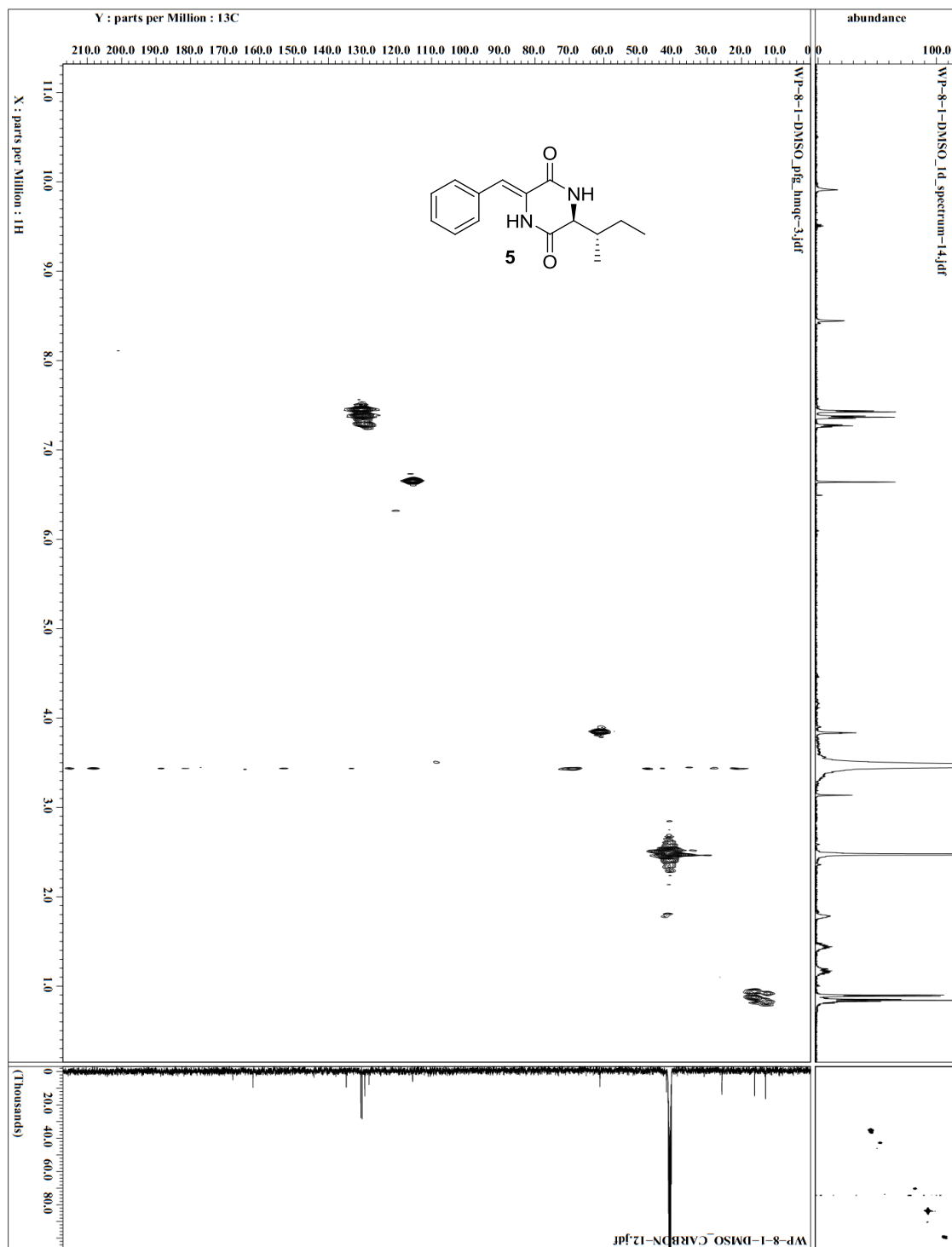
Figure S25. The HMQC (600 MHz, DMSO-*d*₆) spectrum of compound **5**.

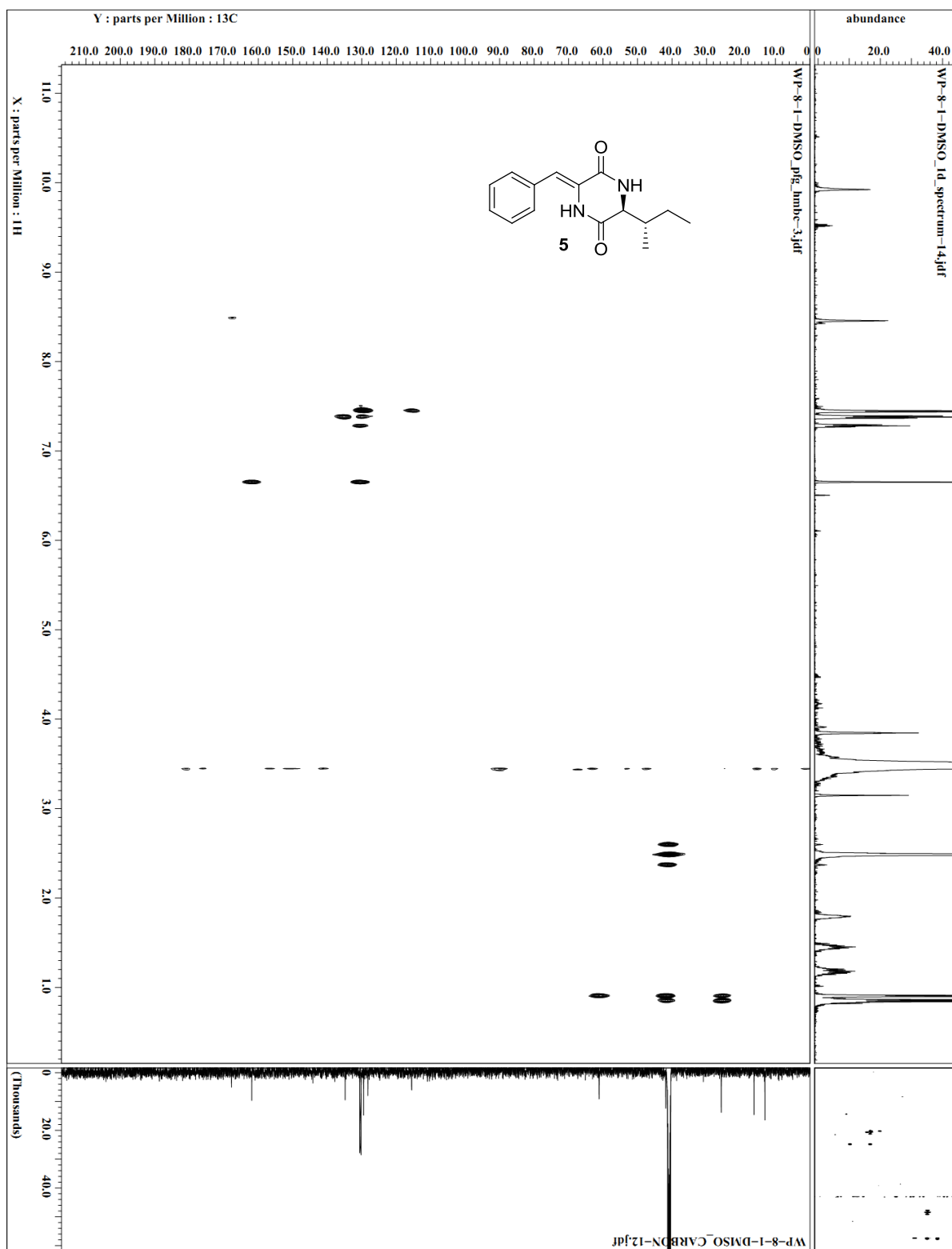
Figure S26. The HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **5**.

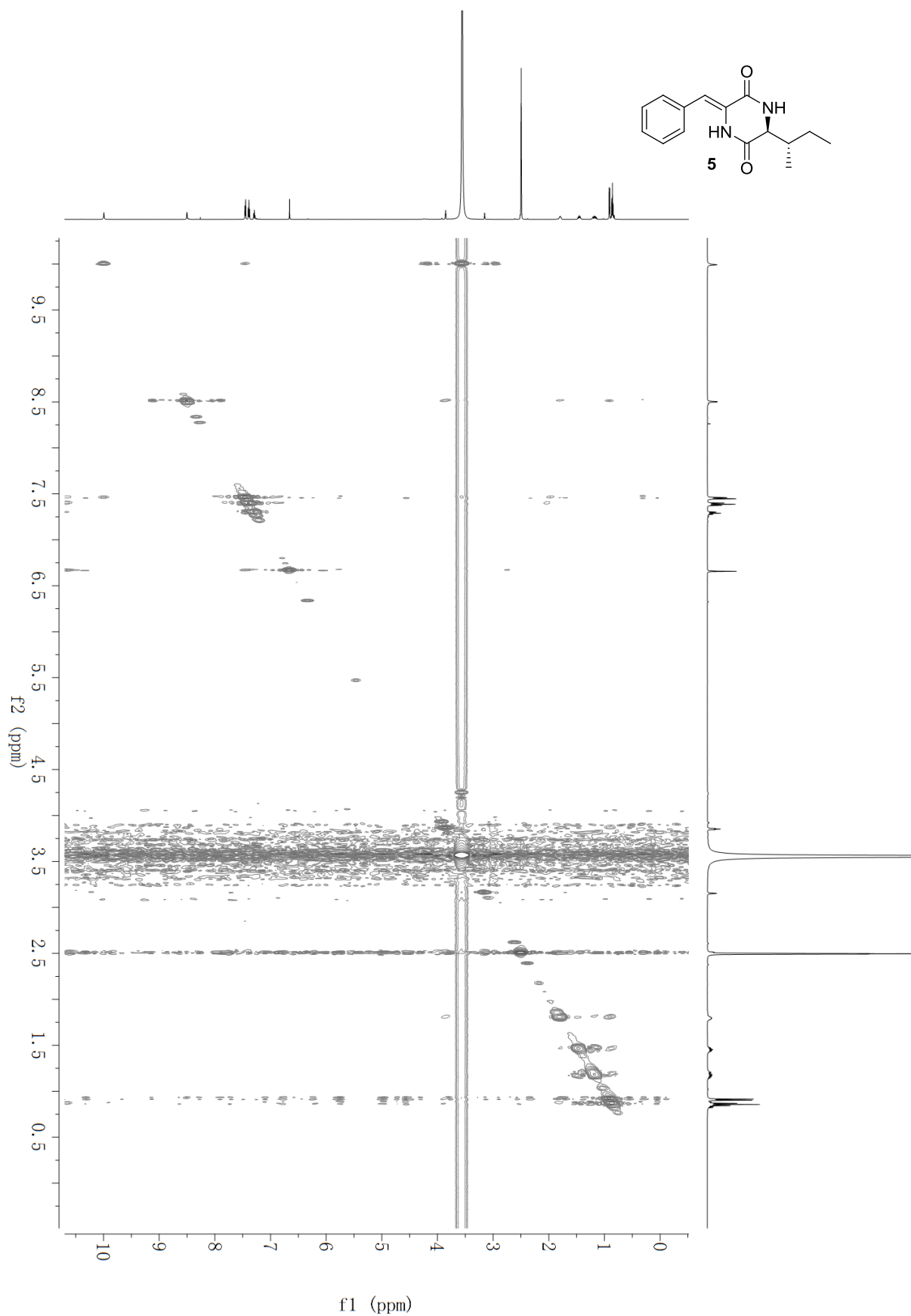
Figure S27. The NOESY (600 MHz, DMSO- d_6) spectrum of compound **5**.

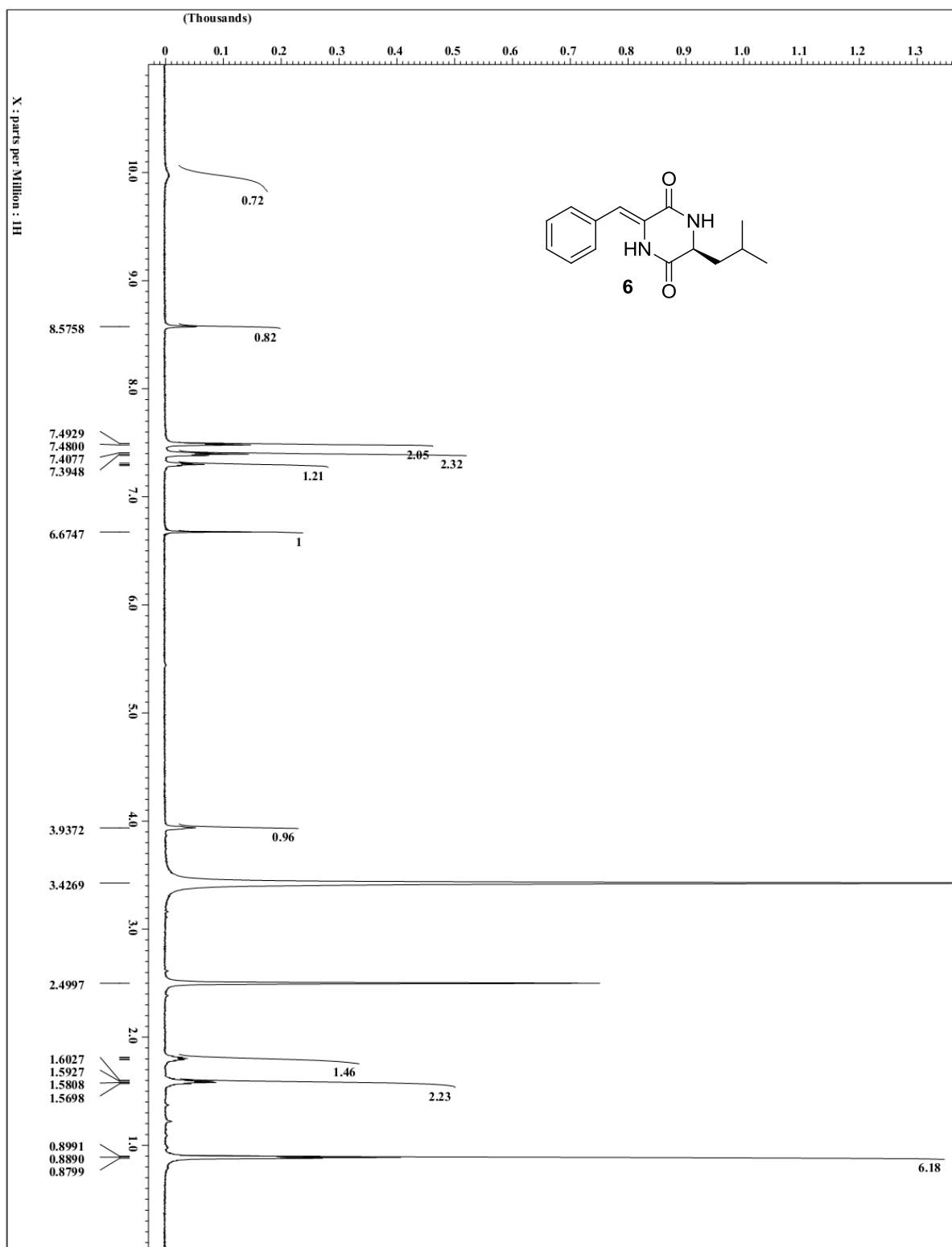
Figure S28. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **6**.

Figure S29. The ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound **6** in $\text{DMSO-}d_6$.

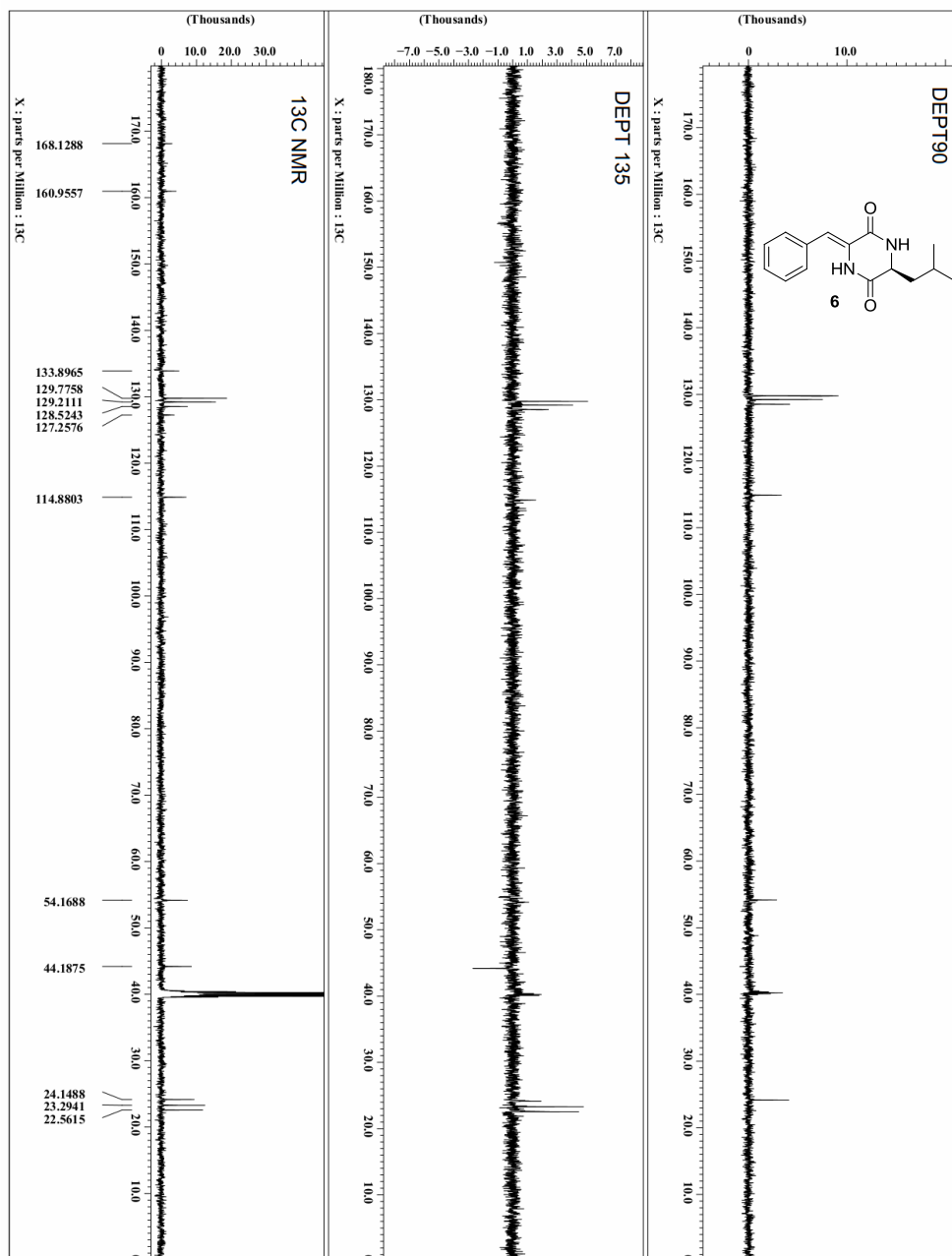
Figure S30. The DEPT (150 MHz, DMSO-*d*₆) spectrum of compound 6.

Figure S31. The ¹H NMR (600 MHz, DMSO-d₆) spectrum of (S)-1 MTPA ester (1a).

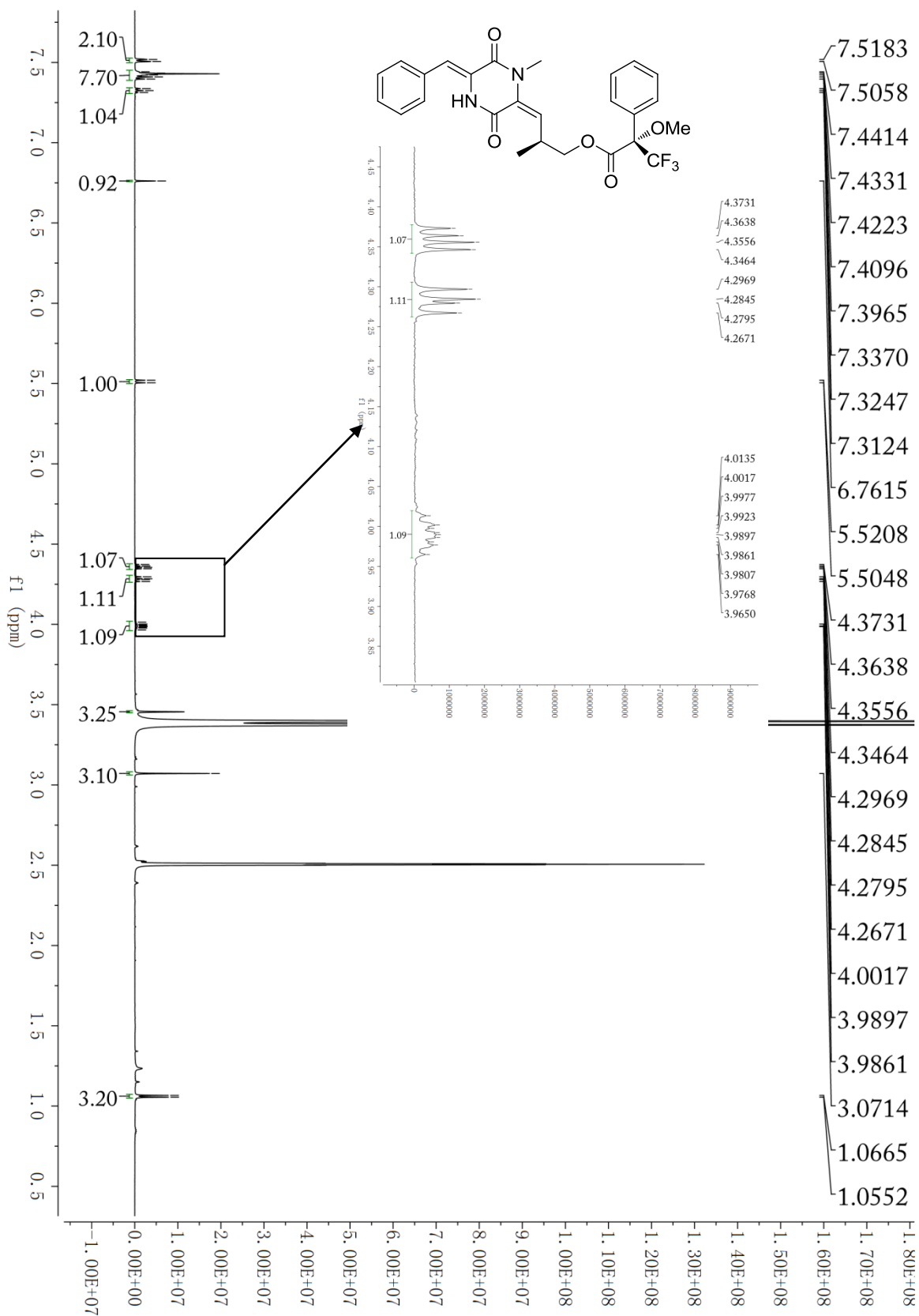


Figure S32. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of (*R*)-1 MTPA ester (**1b**) in $\text{DMSO-}d_6$.

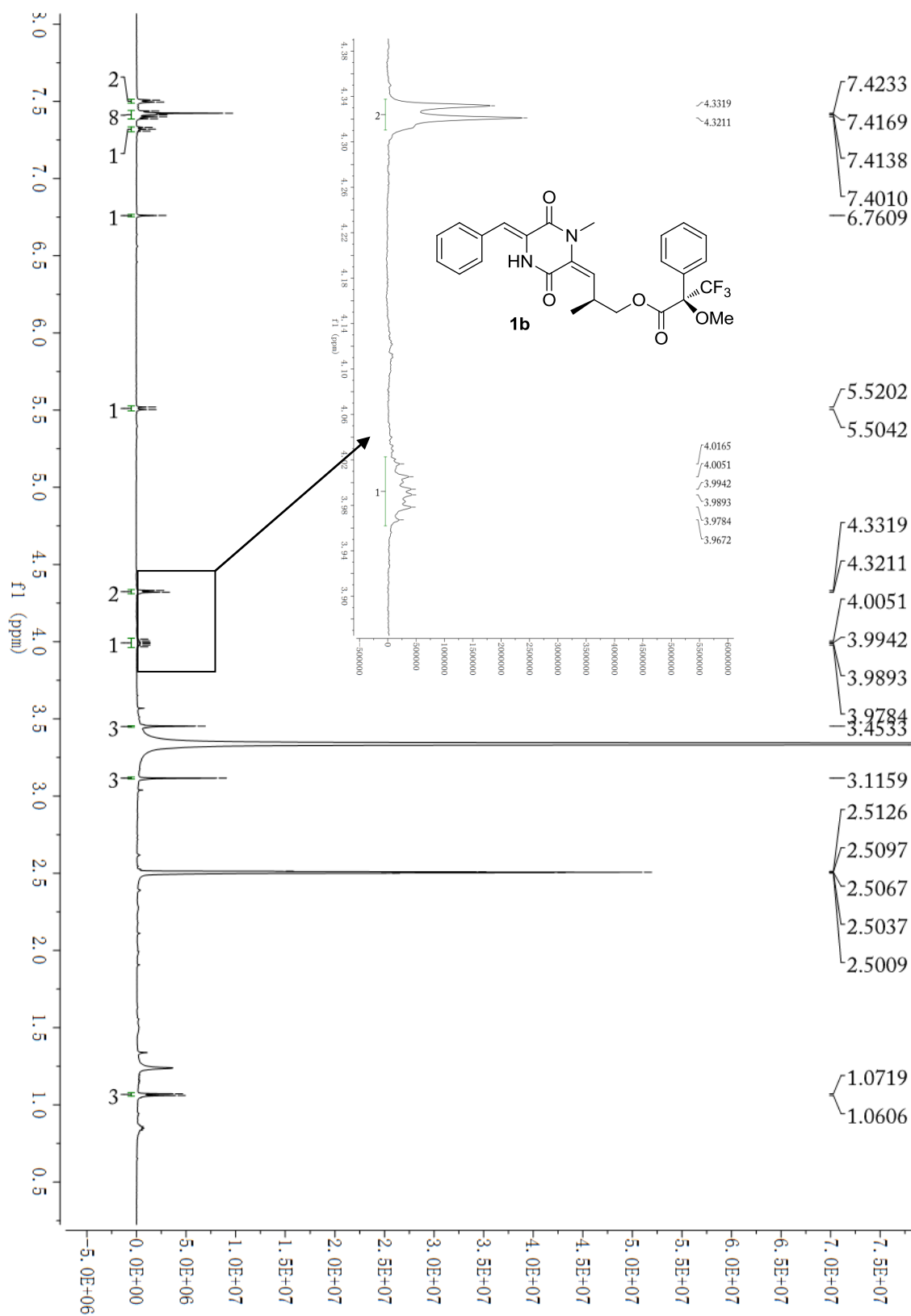


Figure S34. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of (*R*)-**2** MTPA ester (**2b**) in $\text{DMSO-}d_6$.

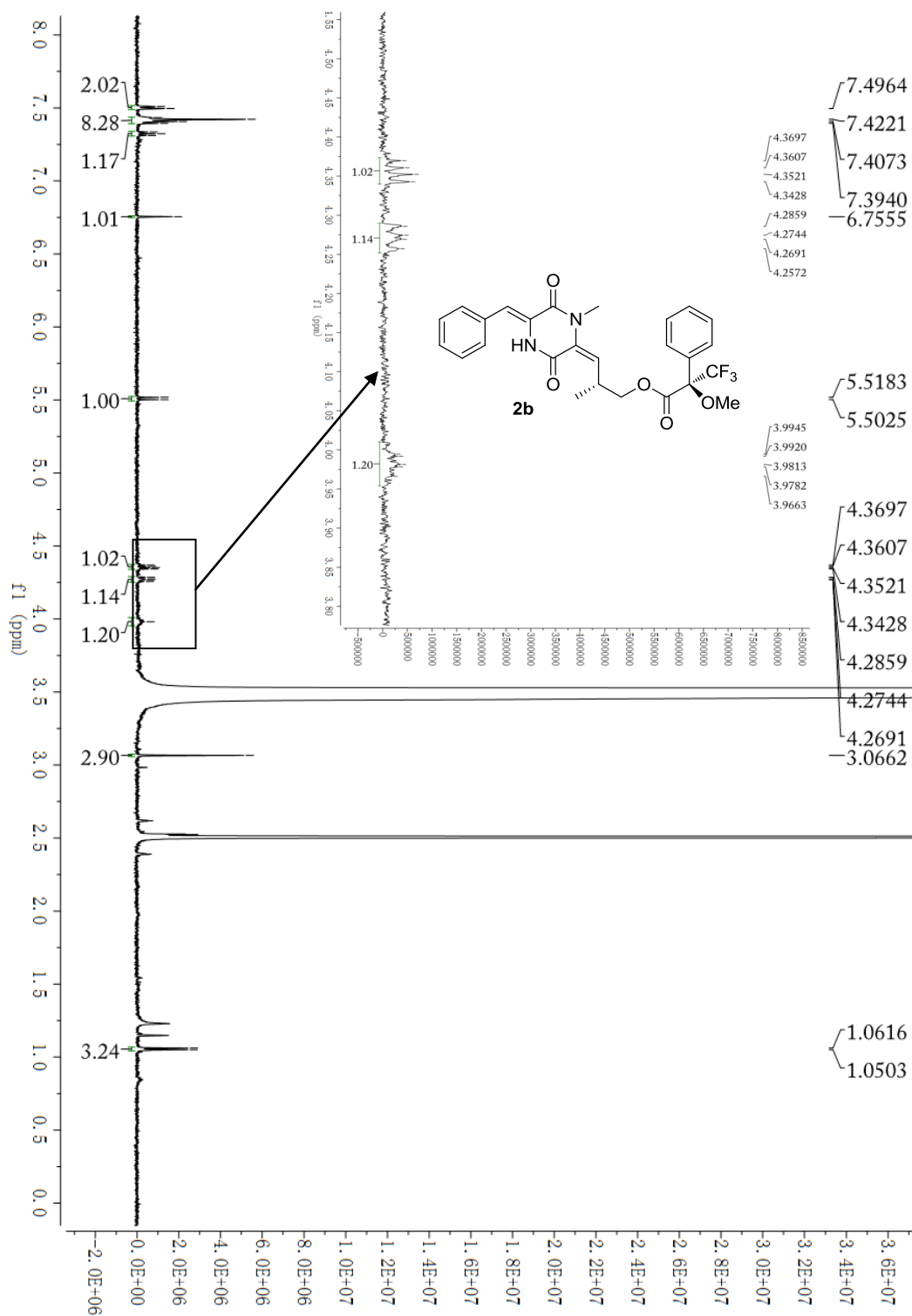


Figure S35. The ¹H NMR (600 MHz, DMSO-d₆) spectrum of *p*-bromobenzoate (**1c**).

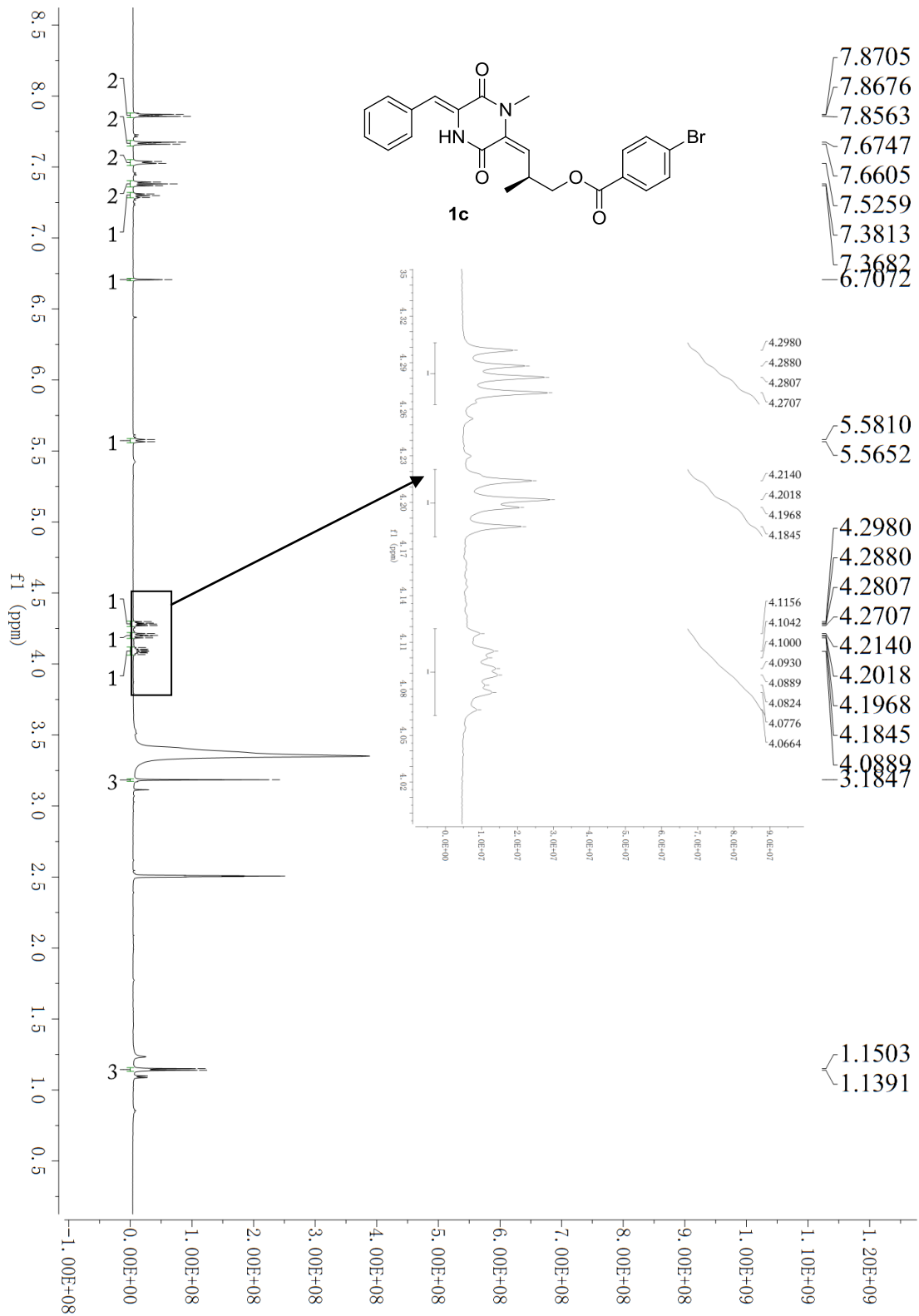


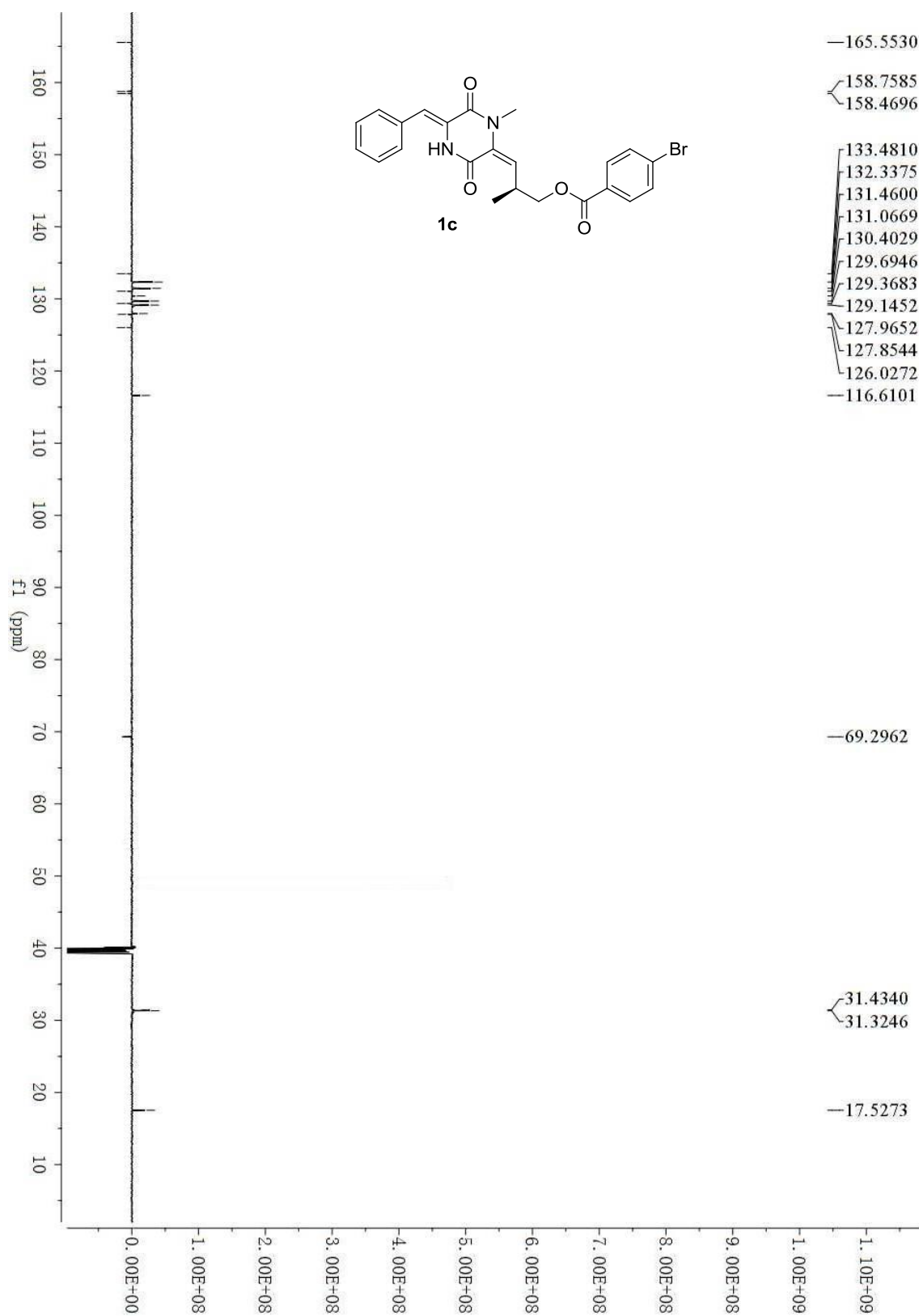
Figure S36. The DEPTQ (150 MHz, DMSO-*d*₆) spectrum of *p*-bromobenzoate (**1c**).

Figure S37. The resolution of the racemic mixture of **1/2** by chiral column (CHIRALPAK AY, 4.6 × 150 mm, 0.5 mL/min).

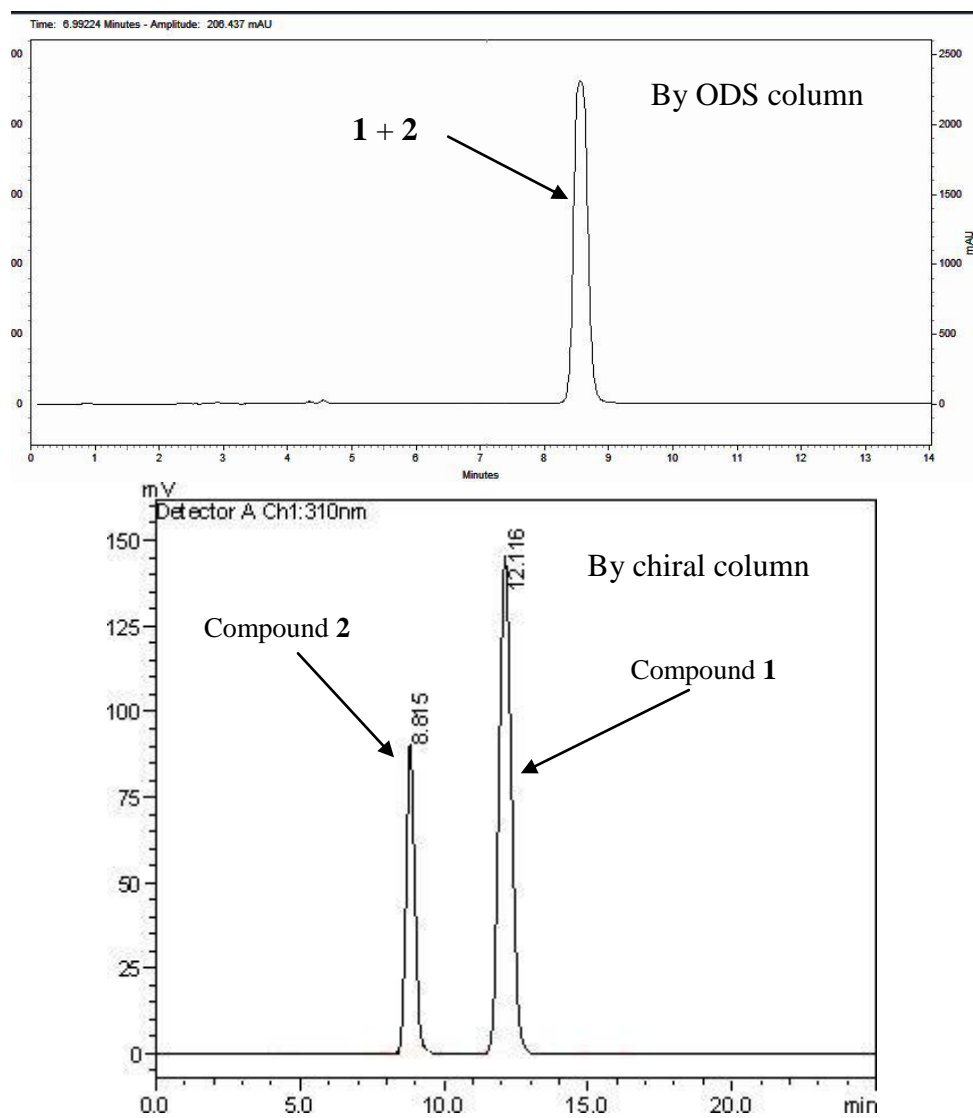
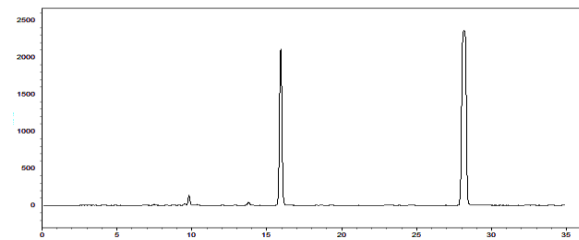
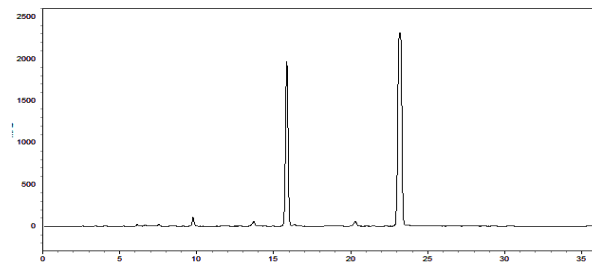


Figure S38. Marfey's method applying for compound **5** (ODS column; Solvents: (A) water + 0.2% TFA, (B) MeCN; linear gradient: 0 min, 75% A + 25% B; 40 min, 40% A + 60% B; 45 min, 100% B; temperature, 30 °C; flow rate, 1 mL/min; UV detection at λ_{\max} 340 nm; FDAA, 16.0 min).

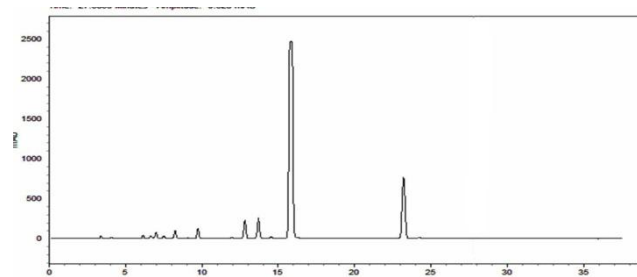
Co-injection of FDAA derivatives of standard D-Ile with standard D-*allo*-Ile by ODS column



Co-injection of FDAA derivatives of standard L-Ile with standard L-*allo*-Ile by ODS column



FDAA derivatives of the acid hydrolysate of **5** by ODS column



Co-injection of FDAA derivatives of the acid hydrolysates of **5** with standard L-Ile and L-*allo*-Ile by ODS column

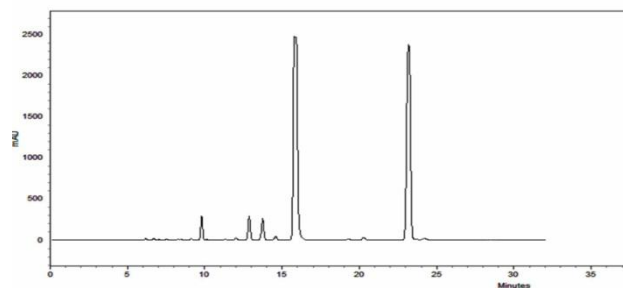
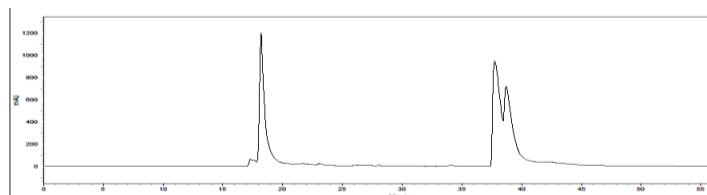
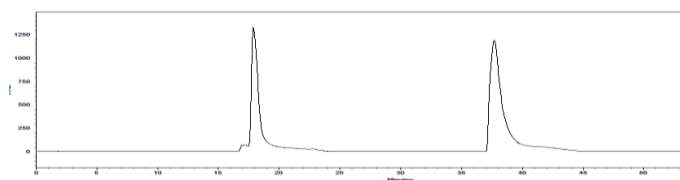


Figure S39. C₃ Marfey's method applying for compound **5** (C₃ column; The column was developed with a linear gradient of 15%–60% MeOH/water (+isocratic 5% of a 1% formic acid solution in MeCN, over 55 min; temperature, 50 °C; flow rate, 1 mL/min; UV detection at λ_{\max} 340 nm; FDAA, 17.95 min).

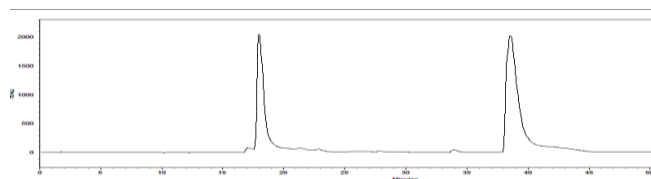
Co-injection of FDAA derivatives of standard L-Ile with standard L-*allo*-Ile by C₃ column



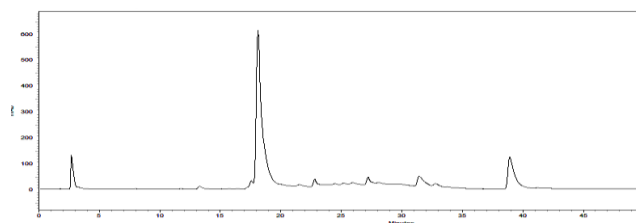
FDAA derivatives of standard L-*allo*-Ile by C₃ column



FDAA derivatives of standard L-Ile by C₃ column



FDAA derivatives of the acid hydrolysate of **5** by C₃ column



Co-injection of FDAA derivatives of the acid hydrolysates of **5** with standard L-Ile by C₃ column

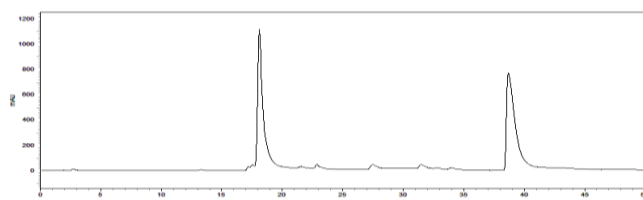
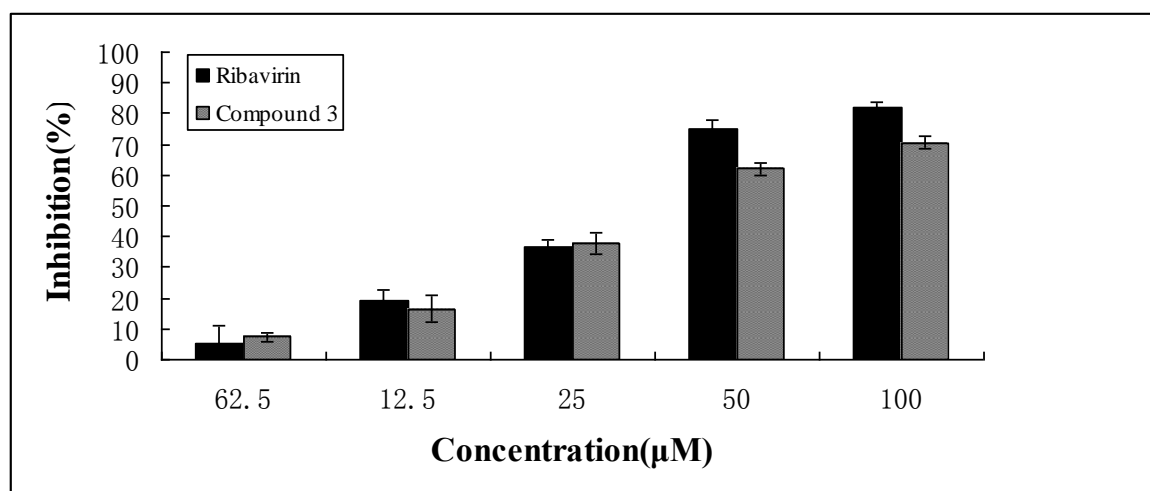


Figure S40. Dose-response histograms of antivirus activity for compound **3** and ribavirin ($p > 0.05$).**Table S1.** Cytotoxic, anti-virus, anti-microbial and anti-inflammatory activities of **1–10**.

Compounds	MIC (μg/mL)						IC ₅₀ (μM)				
	<i>E. coli</i>	<i>E. aerogenes</i>	<i>P. aeruginosa</i>	<i>B. subtilis</i>	<i>S. aureus</i>	<i>C. albicans</i>	HL-60	K562	A549	H1N1	RAW 264.7
1	>100	>100	>100	>100	>100	>100	>100	>100	>100	75.5 ± 2.2	>10
2	>100	>100	>100	>100	>100	>100	>100	>100	>100	>50	>10
3	>100	>100	>100	>100	>100	>100	>100	>100	>100	41.1 ± 4.5	>10
4	>100	>100	>100	>100	>100	>100	>100	>100	>100	62.6 ± 3.9	>10
5	>100	>100	>100	>100	>100	>100	>100	>100	>100	106.5 ± 4.2	>10
6	>100	>100	>100	>100	>100	>100	ND ^a	ND ^a	ND ^a	28.9 ± 2.2	ND ^a
7	>100	>100	>100	>100	>100	>100	ND ^a	ND ^a	ND ^a	6.8 ± 1.5	ND ^a
8	>100	>100	>100	>100	>100	>100	ND ^a	ND ^a	ND ^a	94.5 ± 3.0	ND ^a
9	>100	>100	>100	>100	>100	>100	ND ^a	ND ^a	ND ^a	113.8 ± 4.9	ND ^a
10	>100	>100	>100	>100	>100	>100	ND ^a	ND ^a	ND ^a	156.6 ± 4.0	ND ^a
Ciprofloxacin	0.05	0.19	0.1	0.39	3.12	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a
Ketoconazole	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	0.024	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a
PDTC	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	<0.1
Adriamycin	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	0.652	0.645	0.080	ND ^a	ND ^a
Ribavirin	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	ND ^a	38.8 ± 1.5	ND ^a

^a Not detected.

Table S2. The HMBC correlations (H → C) for compounds 1–5.

Proton (position)	Carbon (position)			
	1 and 2	3	4	5
1	2, 6	3, 5		5
2				
3				
4		2, 6		
5				
6				
7	5, 6, 9, 10	5, 6, 9, 10	5, 8	
8	7, 9, 10			
9	7, 10	7, 8	7, 8	7, 8
10	7, 8, 9	7, 8	7, 8	6, 7, 8
11	2, 13	2, 13/17	2, 12, 13	2, 13
12				
13/17	11, 15	11, 15	12, 15	11, 15
14/16	12, 15	12, 15		12, 15
15	13/17		12, 13	13