

Ochraceopetalin, a Mixed-Biogenetic Salt of Polyketide and Amino Acid Origins from a Marine-Derived *Aspergillus ochraceopetaliformis* Fungus

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† Equal contribution.

Contents

Figure S1. The ^1H NMR (500 MHz, DMSO- d_6) spectrum of 1	S3
Figure S2. The ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of 1	S4
Figure S3. The COSY (500 MHz, DMSO- d_6) spectrum of 1	S5
Figure S4. The HSQC (500 MHz, DMSO- d_6) spectrum of 1	S6
Figure S5. The HMBC (500 MHz, DMSO- d_6) spectrum of 1	S7
Figure S6. HR-ESI-MS data of 1	S8
Figure S7. The ^1H NMR (600 MHz, DMSO- d_6) spectrum of 2	S9
Figure S8. The ^{13}C NMR (150 MHz, DMSO- d_6) spectrum of 2	S10
Figure S9. The COSY (600 MHz, DMSO- d_6) spectrum of 2	S11
Figure S10. The HSQC (600 MHz, DMSO- d_6) spectrum of 2	S12
Figure S11. The HMBC (600 MHz, DMSO- d_6) spectrum of 2	S13
Figure S12. The ^1H NMR (600 MHz, DMSO- d_6) spectrum of 3	S14
Figure S13. The ^{13}C NMR (150 MHz, DMSO- d_6) spectrum of 3	S15
Figure S14. The COSY (600 MHz, DMSO- d_6) spectrum of 3	S16
Figure S15. The HSQC (600 MHz, DMSO- d_6) spectrum of 3	S17
Figure S16. The HMBC (600 MHz, DMSO- d_6) spectrum of 3	S18
Figure S17. The ^1H NMR (400 MHz, CDCl_3) spectrum of 4	S19
Figure S18. The ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4	S20
Figure S19. The ^1H NMR (400 MHz, DMSO- d_6) spectrum of 3a	S21
Figure S20. The ^1H NMR (400 MHz, CDCl_3) spectrum of 3b	S22
Figure S21. The ^1H NMR (800 MHz, Methanol- d_4) spectrum of 3aS	S23
Figure S22. The ^1H NMR (800 MHz, Methanol- d_4) spectrum of 3aR	S24
Figure S23. The LC/MS chromatogram data of 3b-L-FDAA adduct	S25
Figure S24. The time-scale LC-MS analysis of YMM liquid media extracts	S25
Figure S25. The time-scale LC-MS analysis of YMM-rice semi-solid media extracts	S26
Figure S26. The MTT assay against K562 and A549 cancer cells	S27
Table S1. Results of cytotoxicity tests	S27
Figure S27. The ^{13}C NMR (25 MHz, D_2O) spectra of guanidine and guanidine hydrochloride	S28
Figure S28. The HPLC analysis of 1	S29
Figure S29. The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of 3c	S30
Figure S30. The ^{13}C NMR (125 MHz, MeOH- d_4) spectrum of 1	S31
Figure S31. The ^{13}C NMR (200 MHz, MeOH- d_4) spectrum of 3	S32
Table S2. The ^{13}C NMR data of 1–3 and 3c	S33

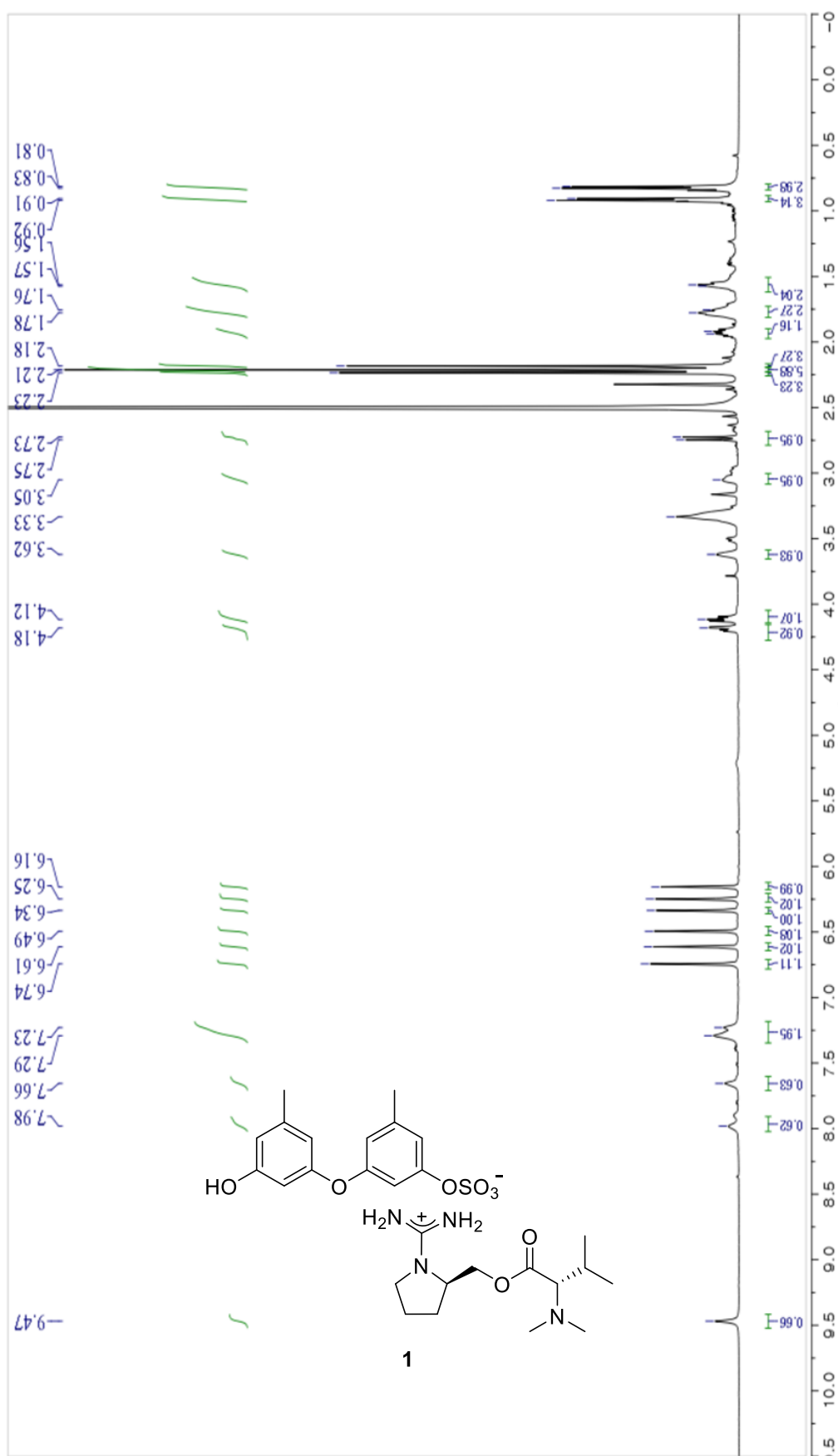


Figure S1. The ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **1**

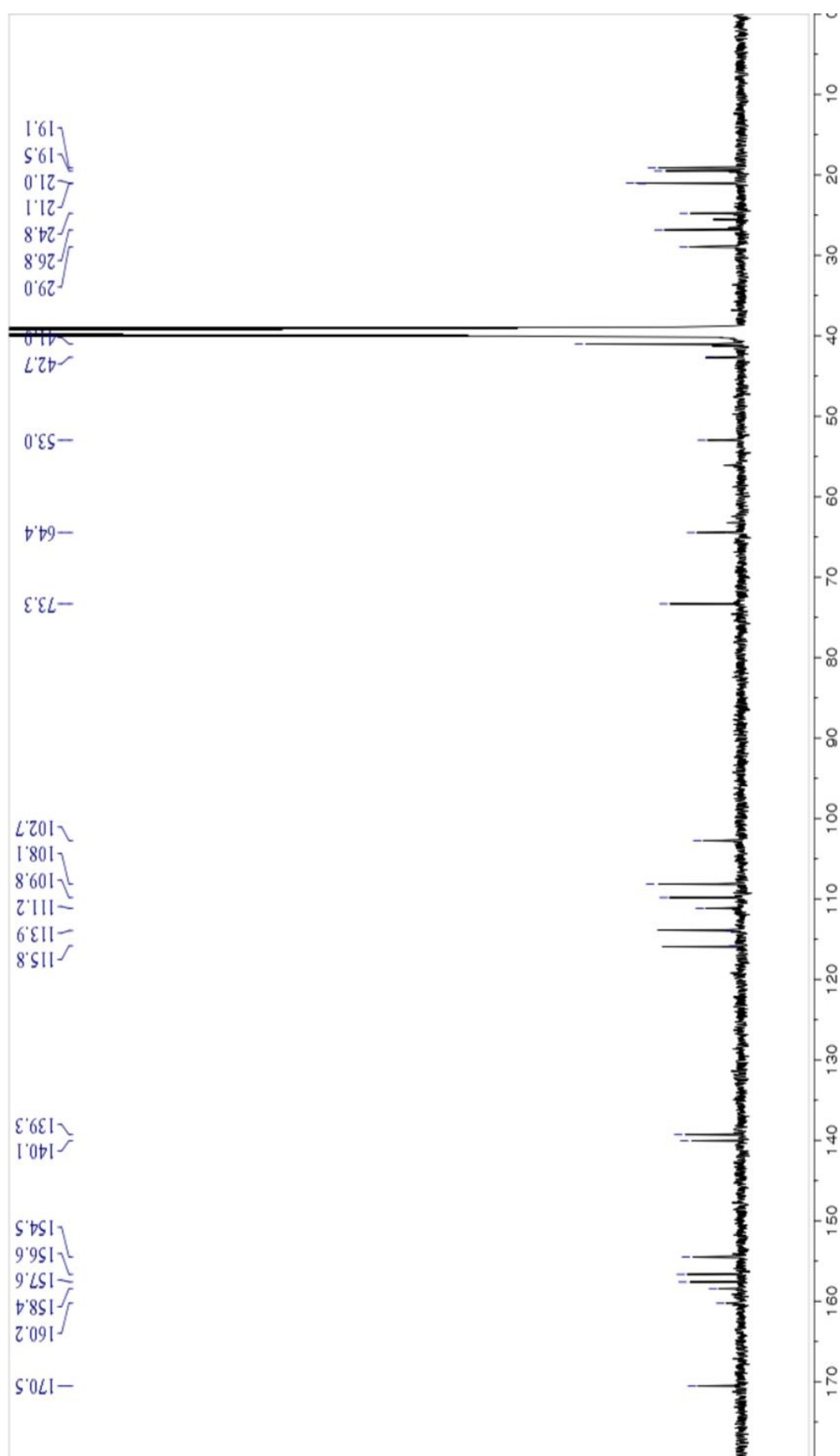


Figure S2. The ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of **1**

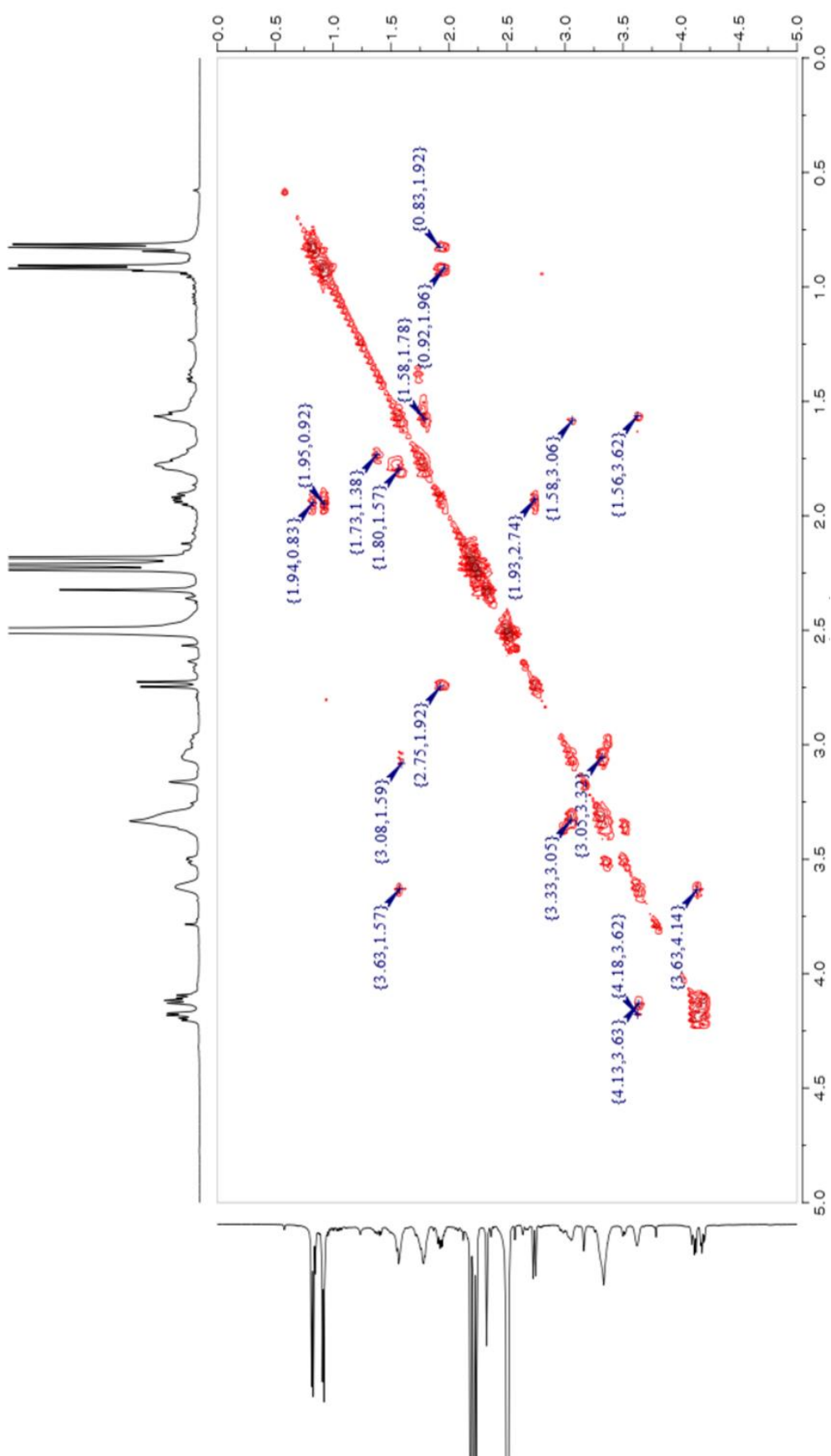


Figure S3. The COSY (500 MHz, $\text{DMSO-}d_6$) spectrum of **1**

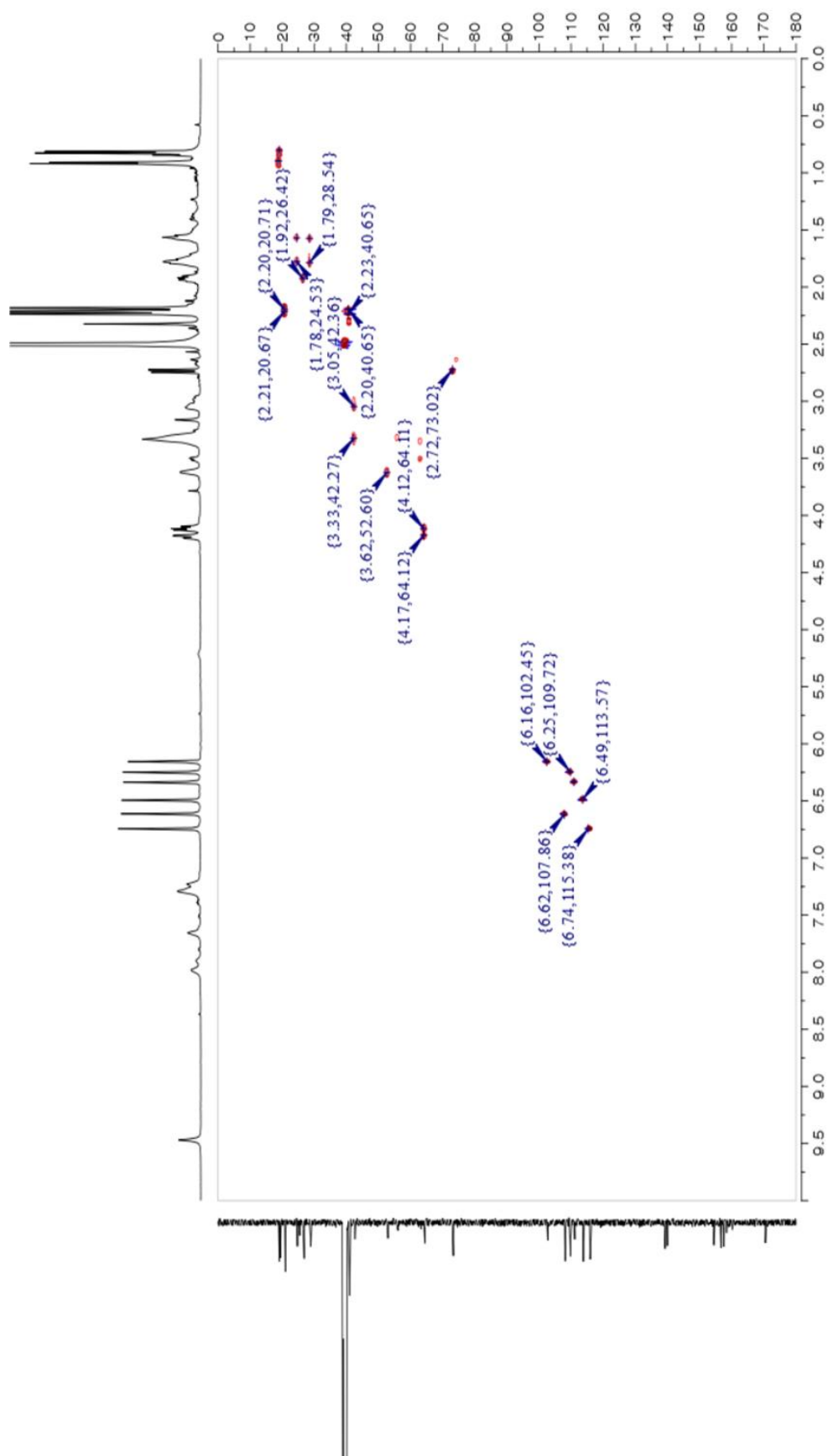


Figure S4. The HSQC (500 MHz, DMSO-*d*₆) spectrum of **1**

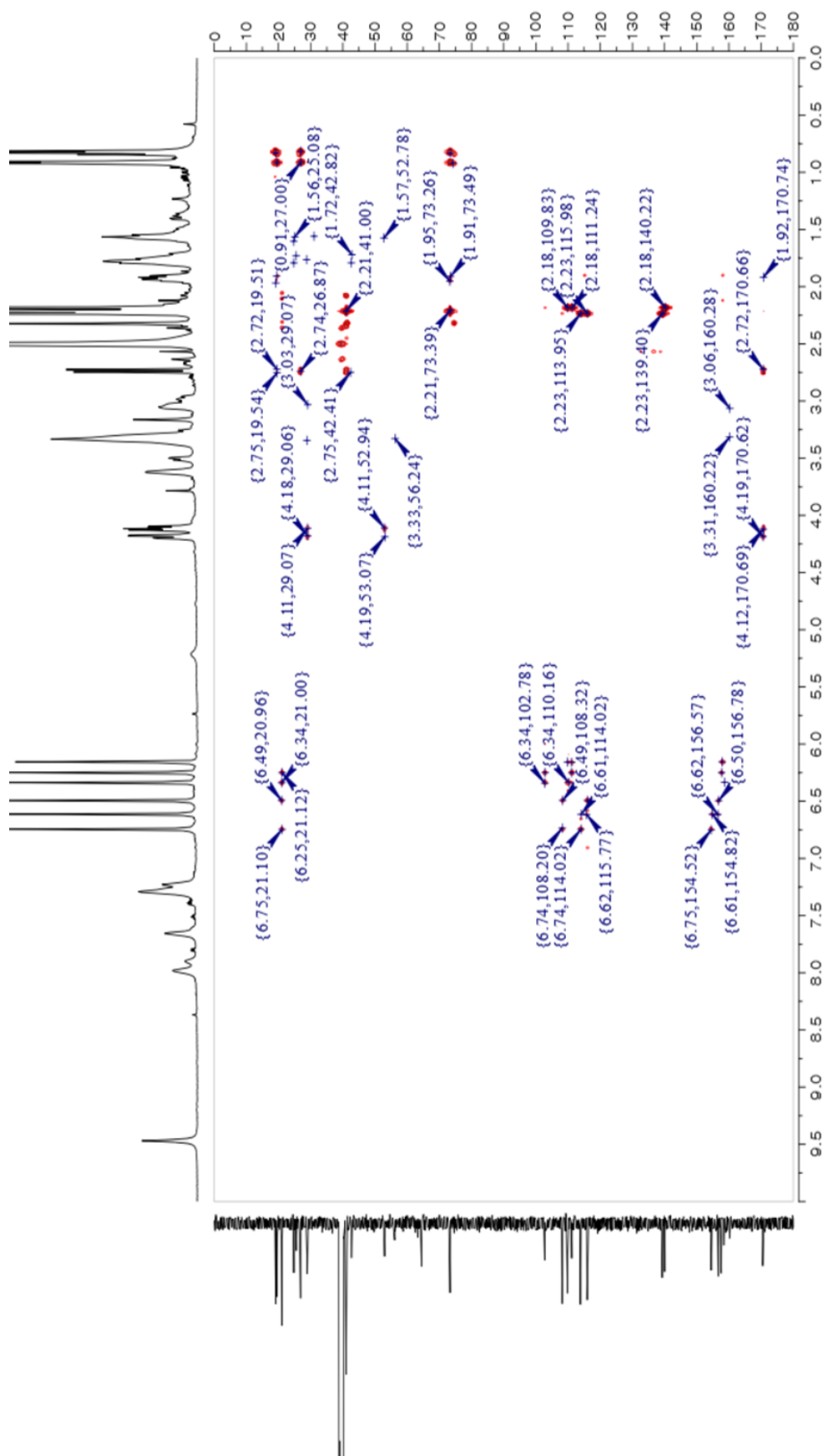


Figure S5. The HMBC (500 MHz, DMSO- d_6) spectrum of **1**

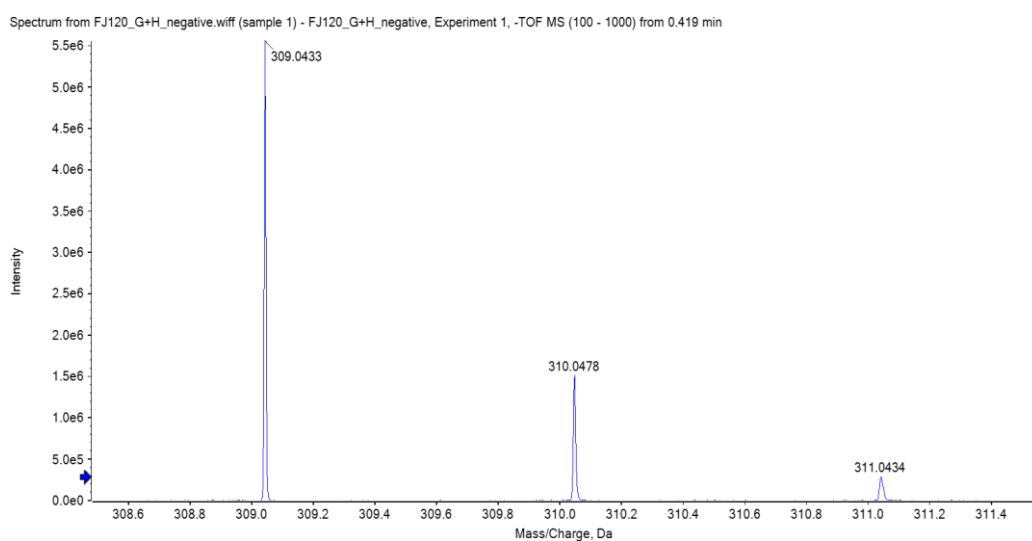
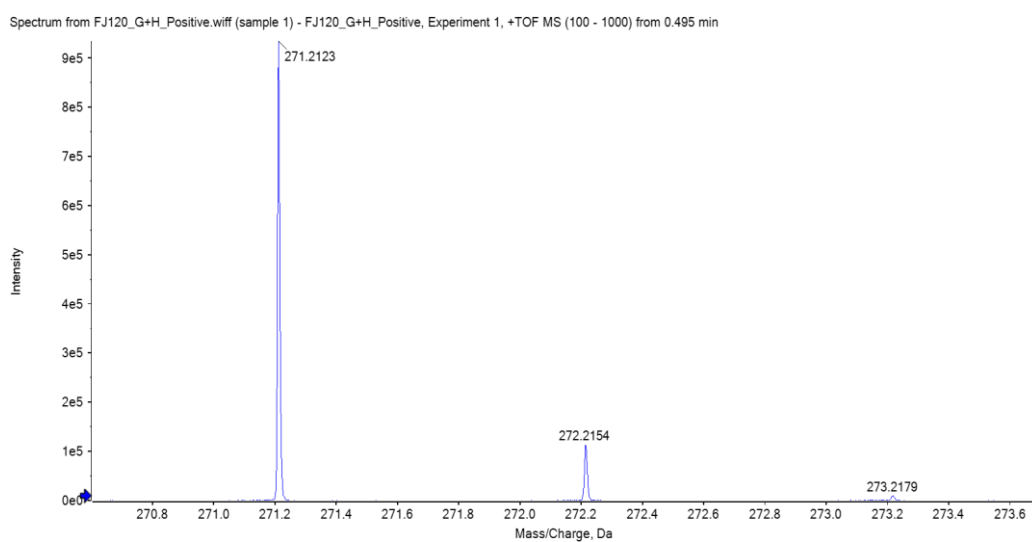
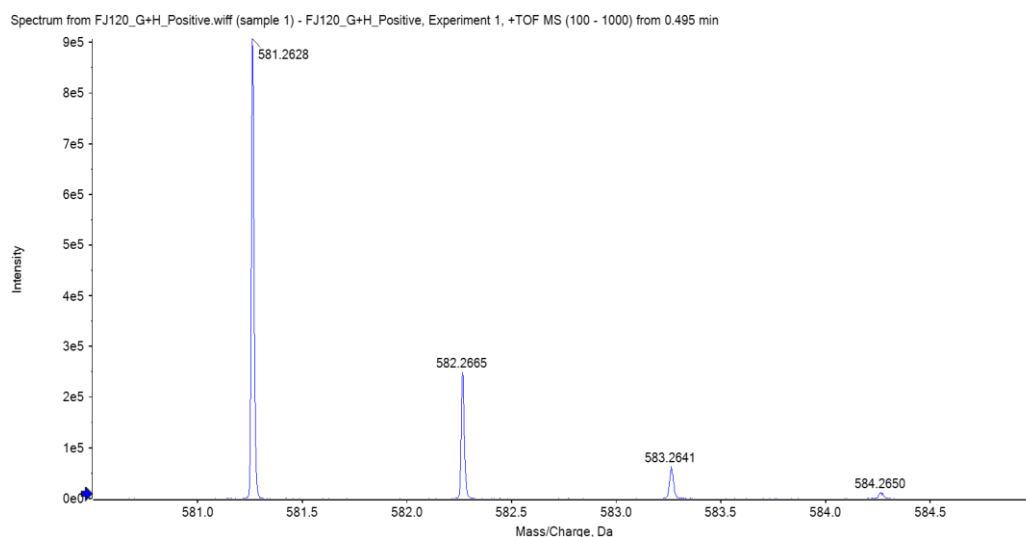


Figure S6. HR-ESI-MS data of 1

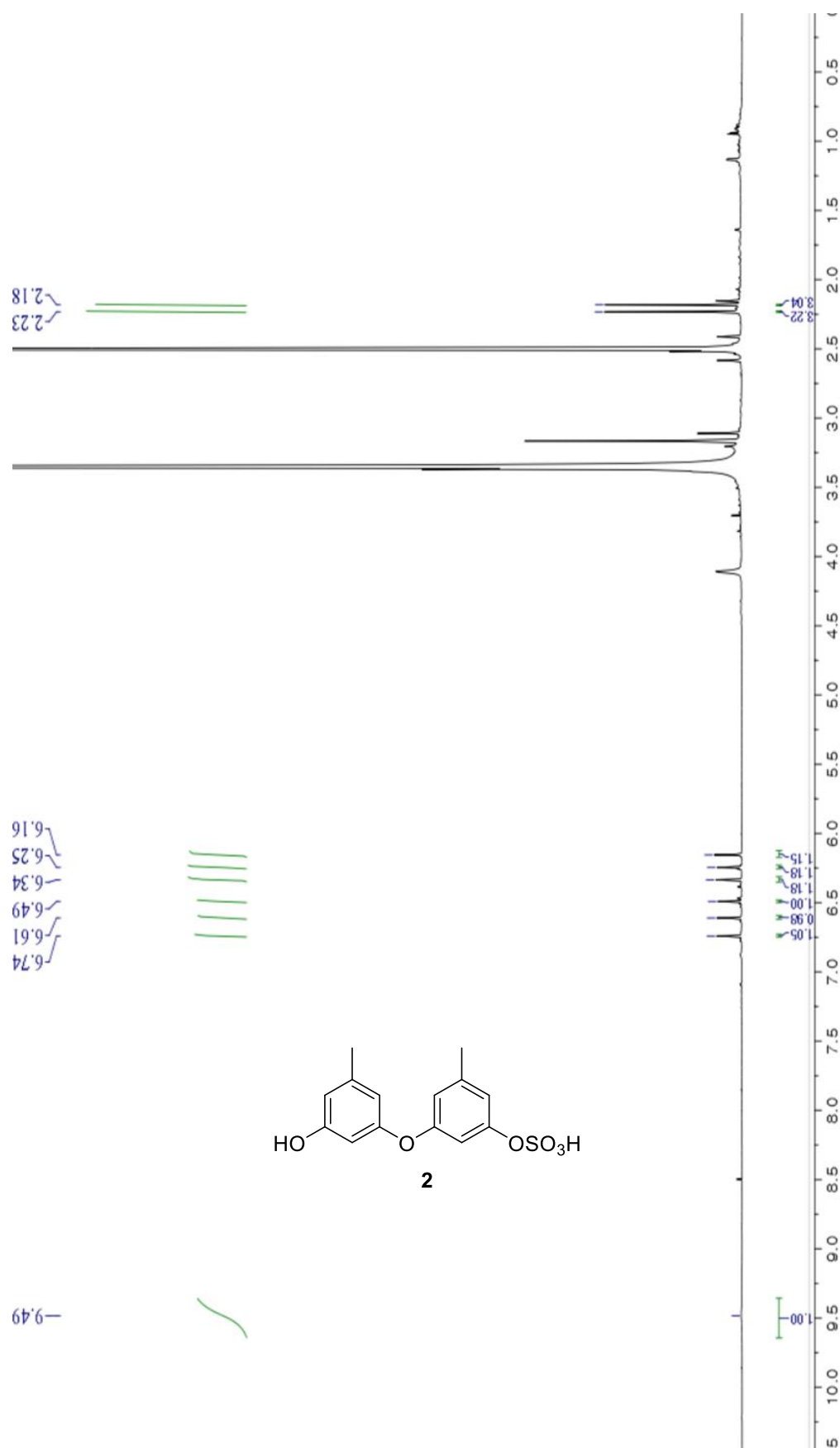


Figure S7. The ¹H NMR (600 MHz, DMSO- *d*₆) spectrum of **2**

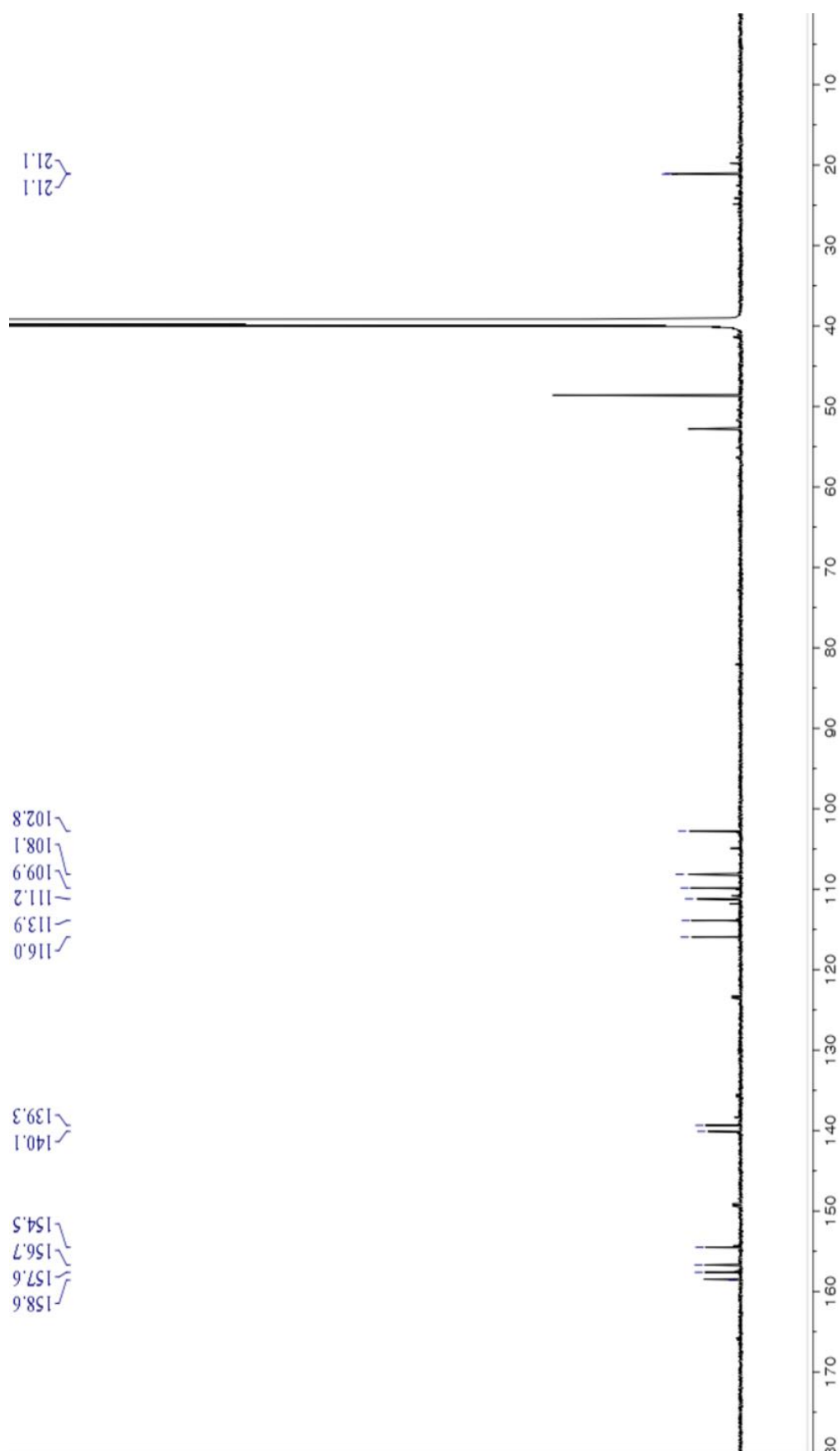


Figure S8. The ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of **2**

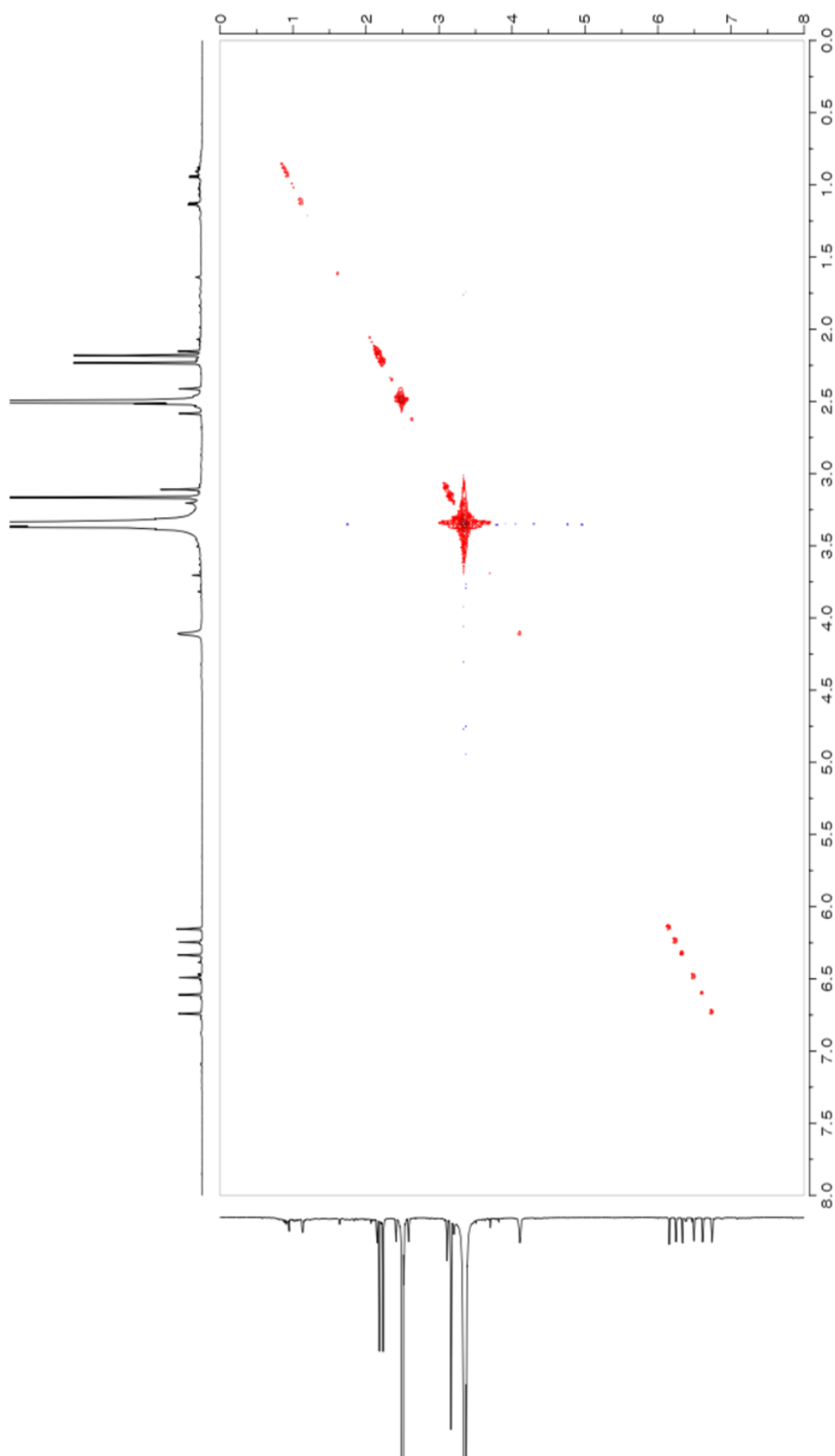


Figure S9. The COSY (600 MHz, DMSO- d_6) spectrum of **2**

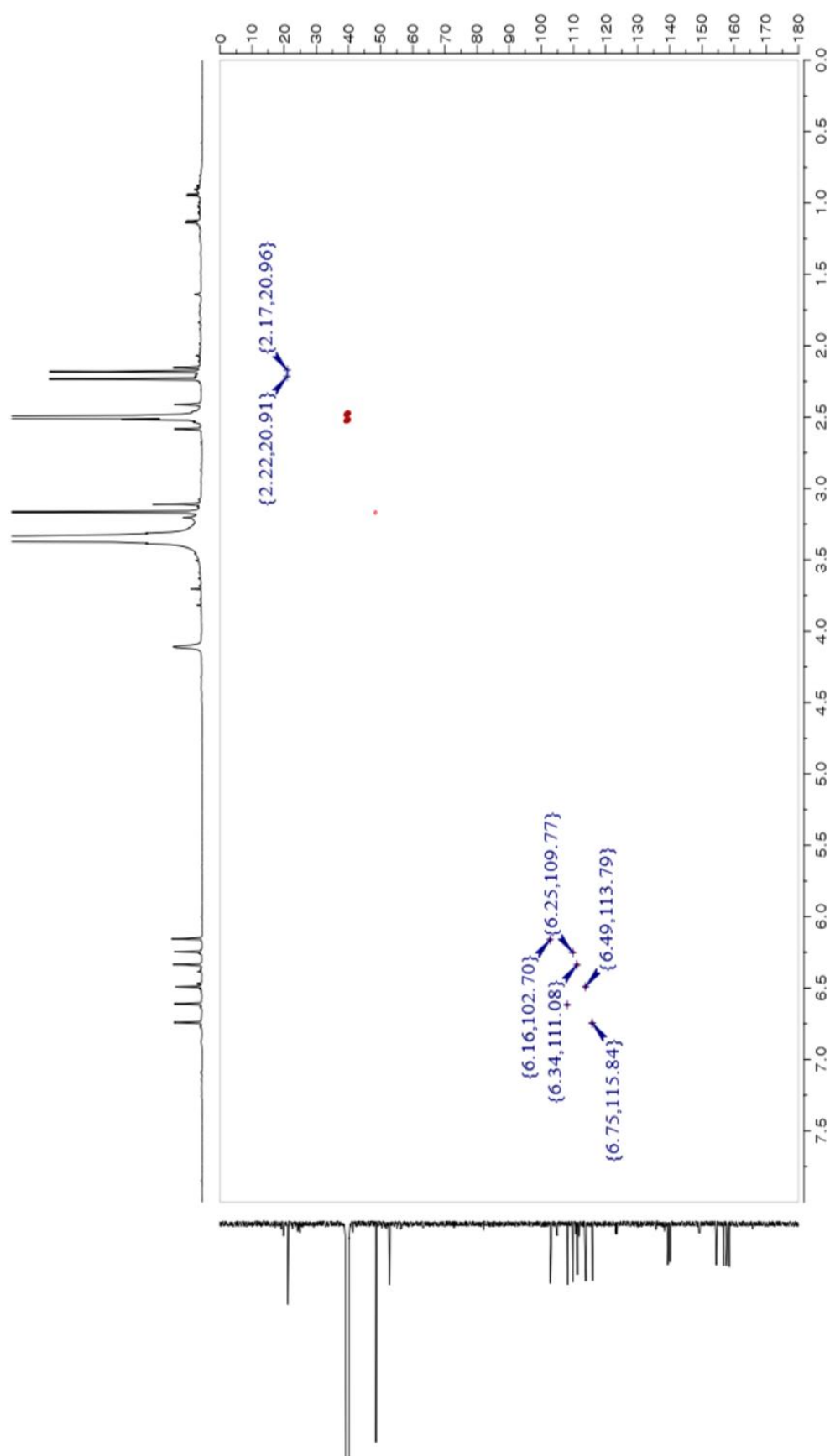


Figure S10. The HSQC (600 MHz, DMSO- d_6) spectrum of **2**

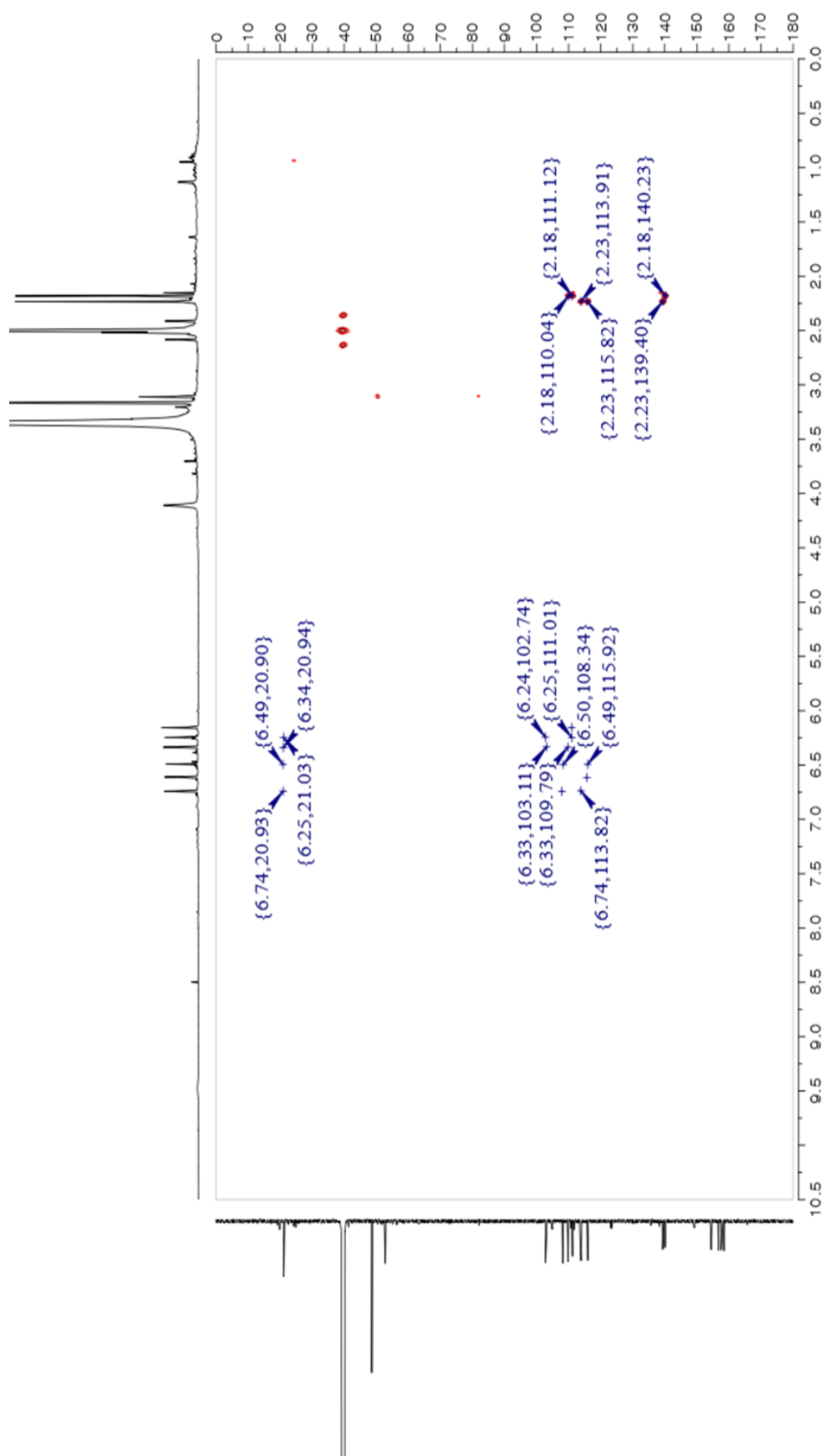


Figure S11. The HMBC (600 MHz, DMSO- d_6) spectrum of **2**

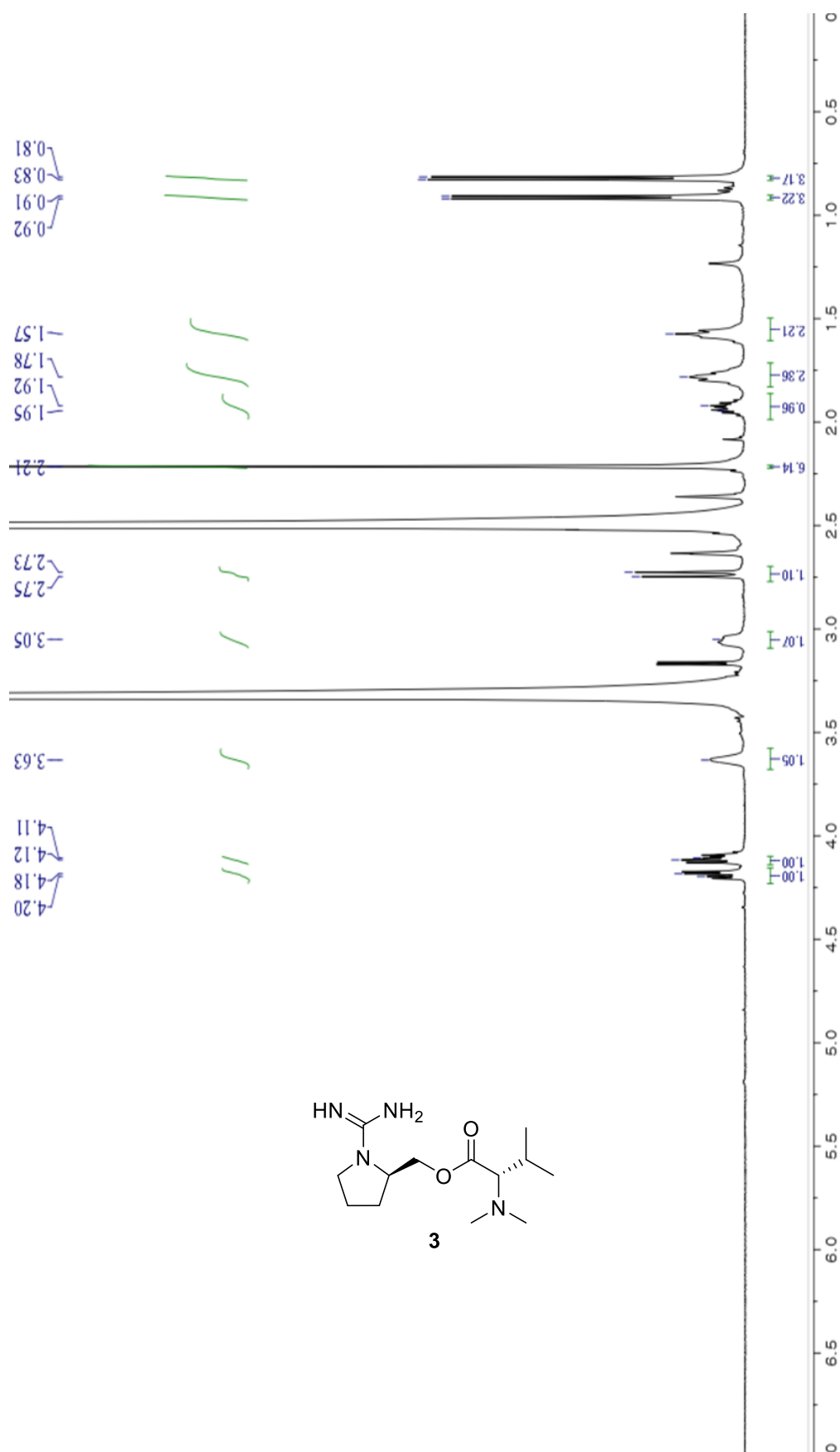


Figure S12. The ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of **3**

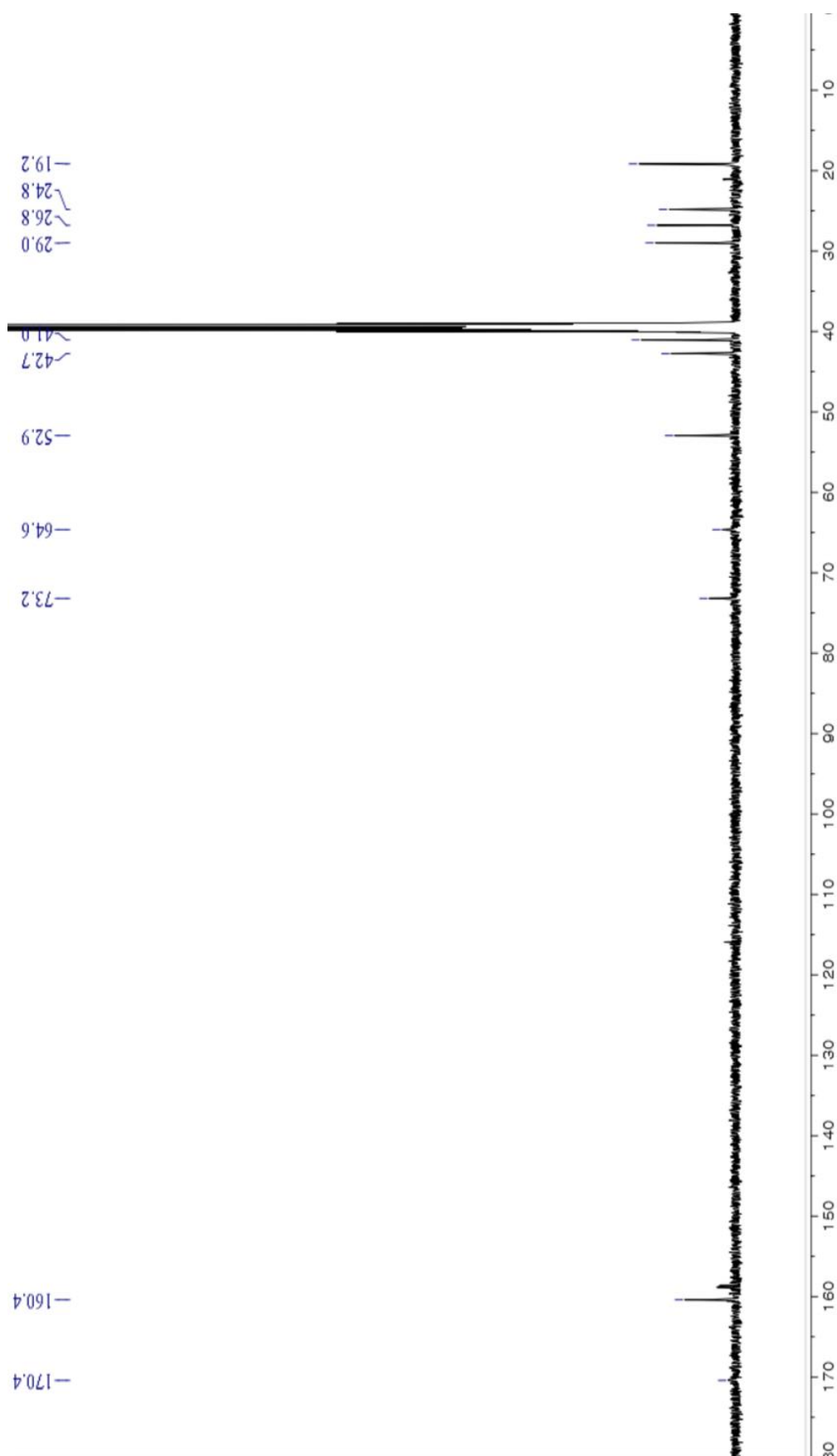


Figure S13. The ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of **3**

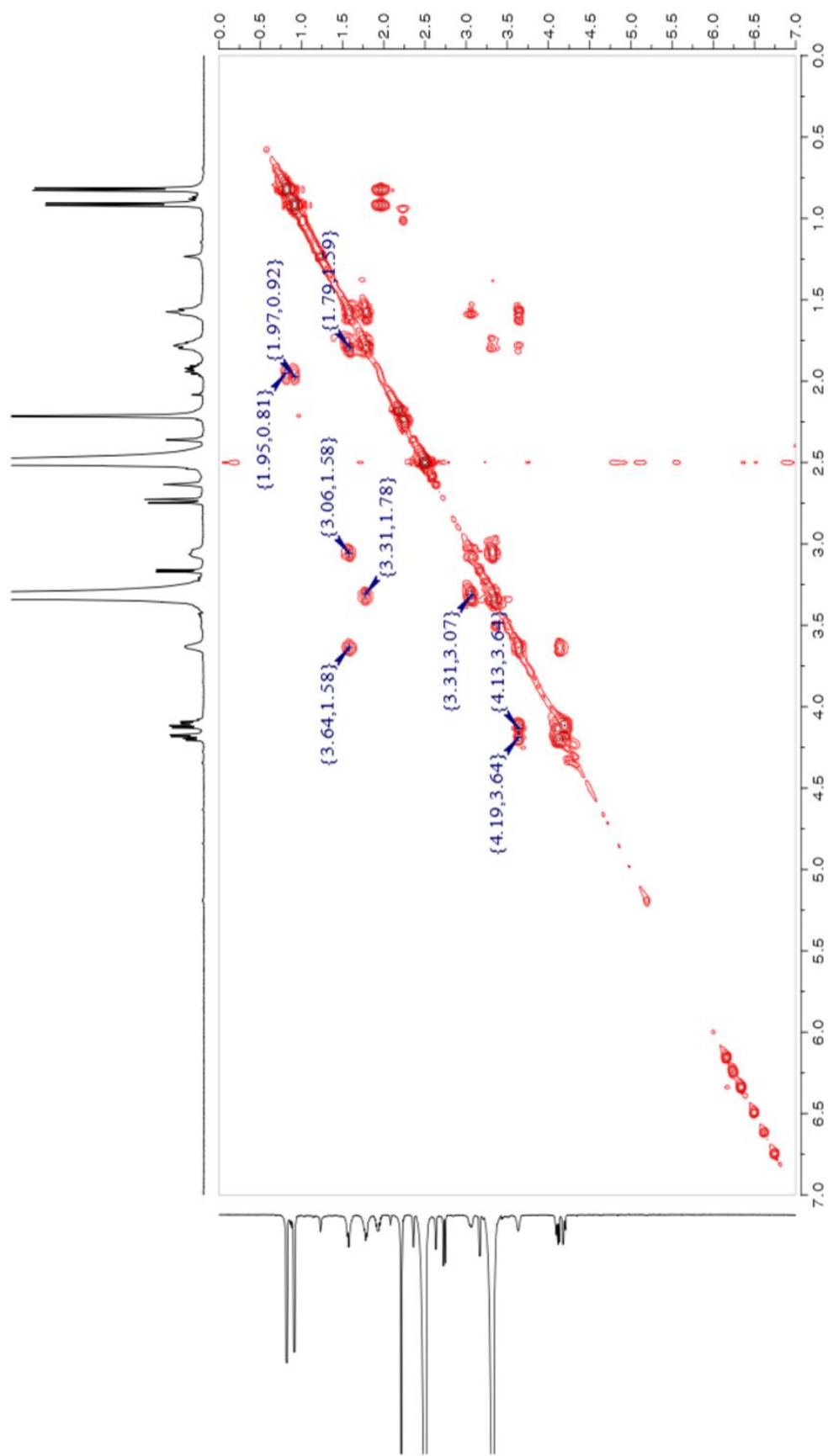


Figure S14. The COSY (600 MHz, DMSO- d_6) spectrum of **3**

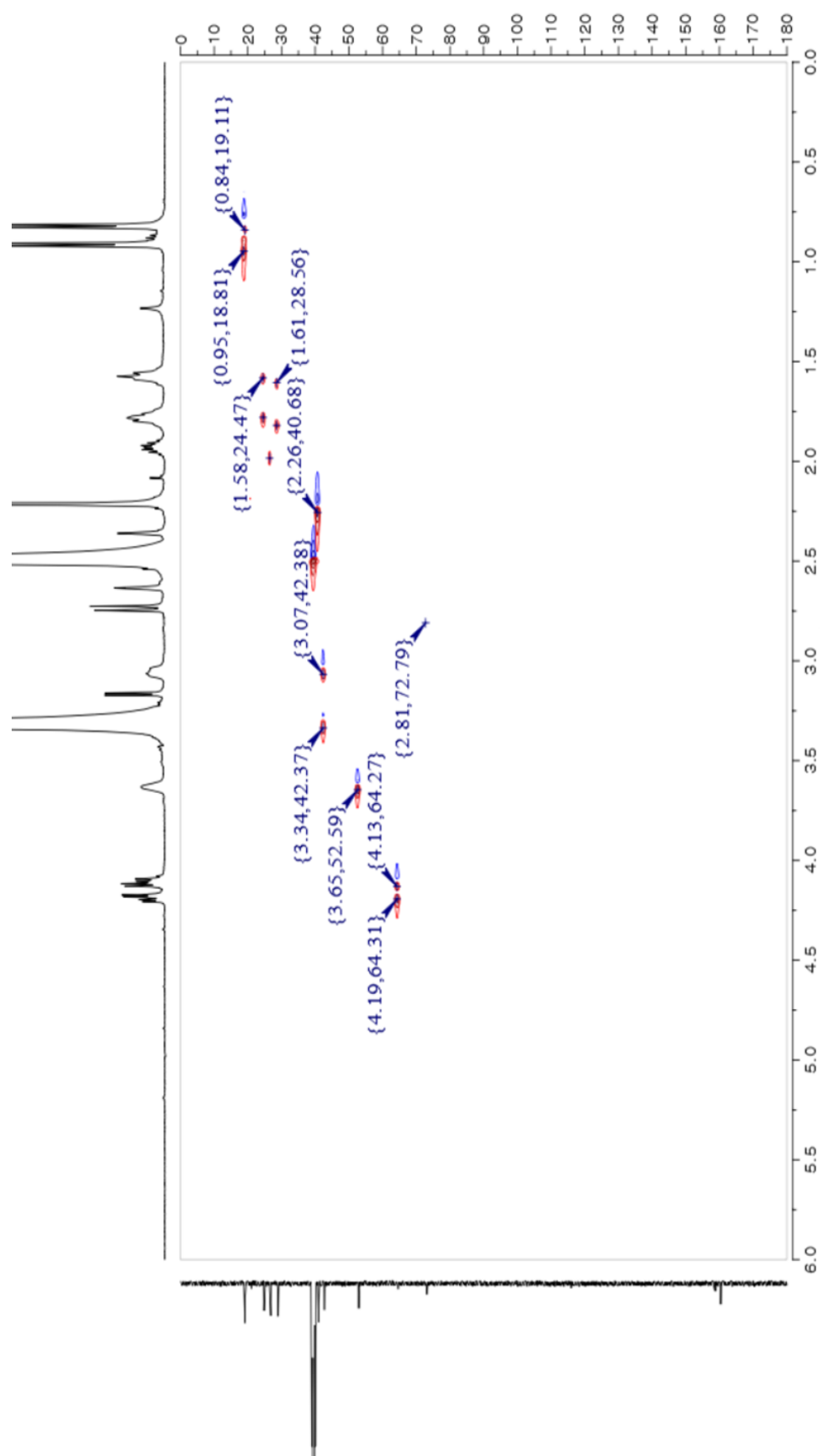


Figure S15. The HSQC (600 MHz, DMSO- d_6) spectrum of **3**

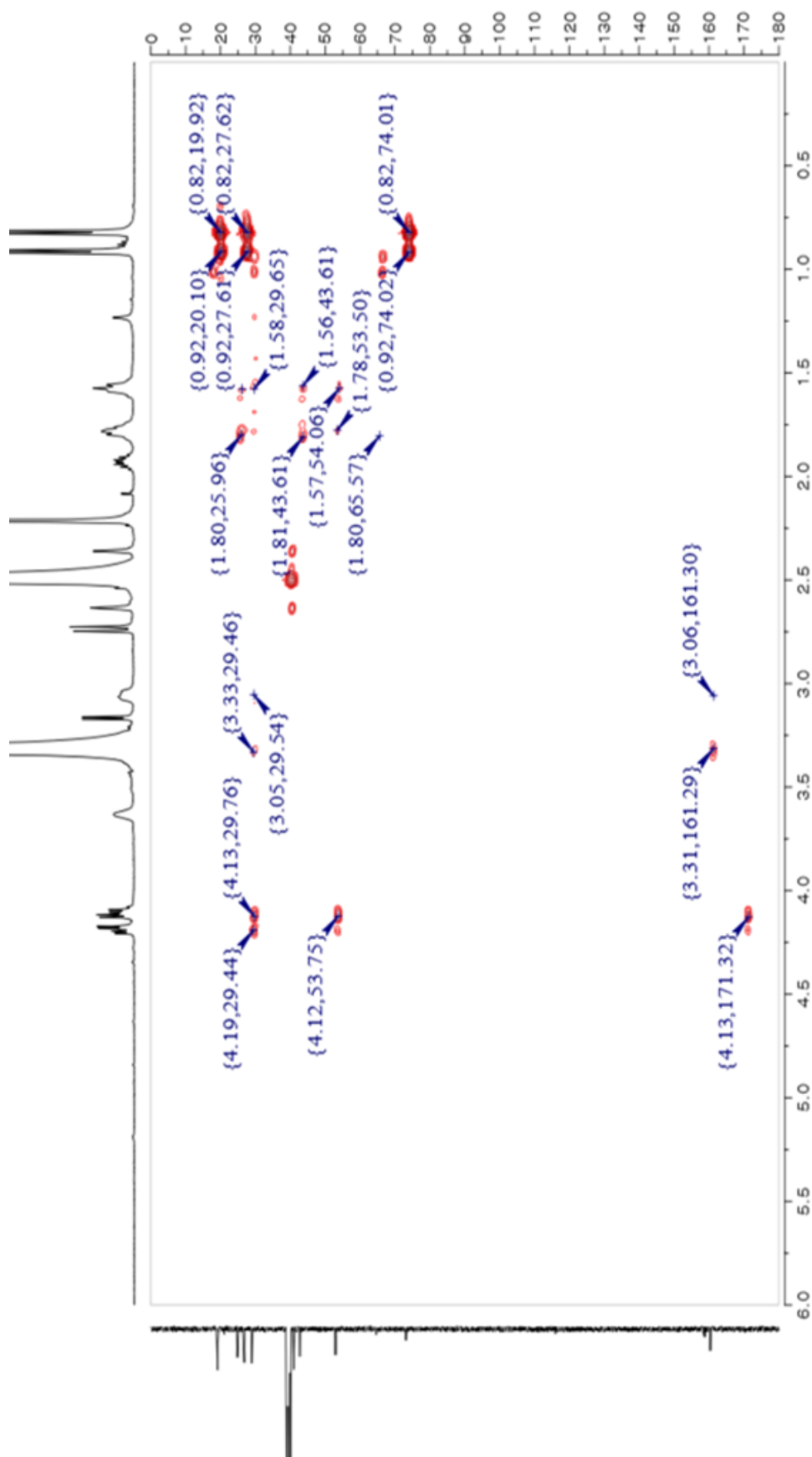


Figure S16. The HMBC (600 MHz, DMSO-*d*₆) spectrum of **3**

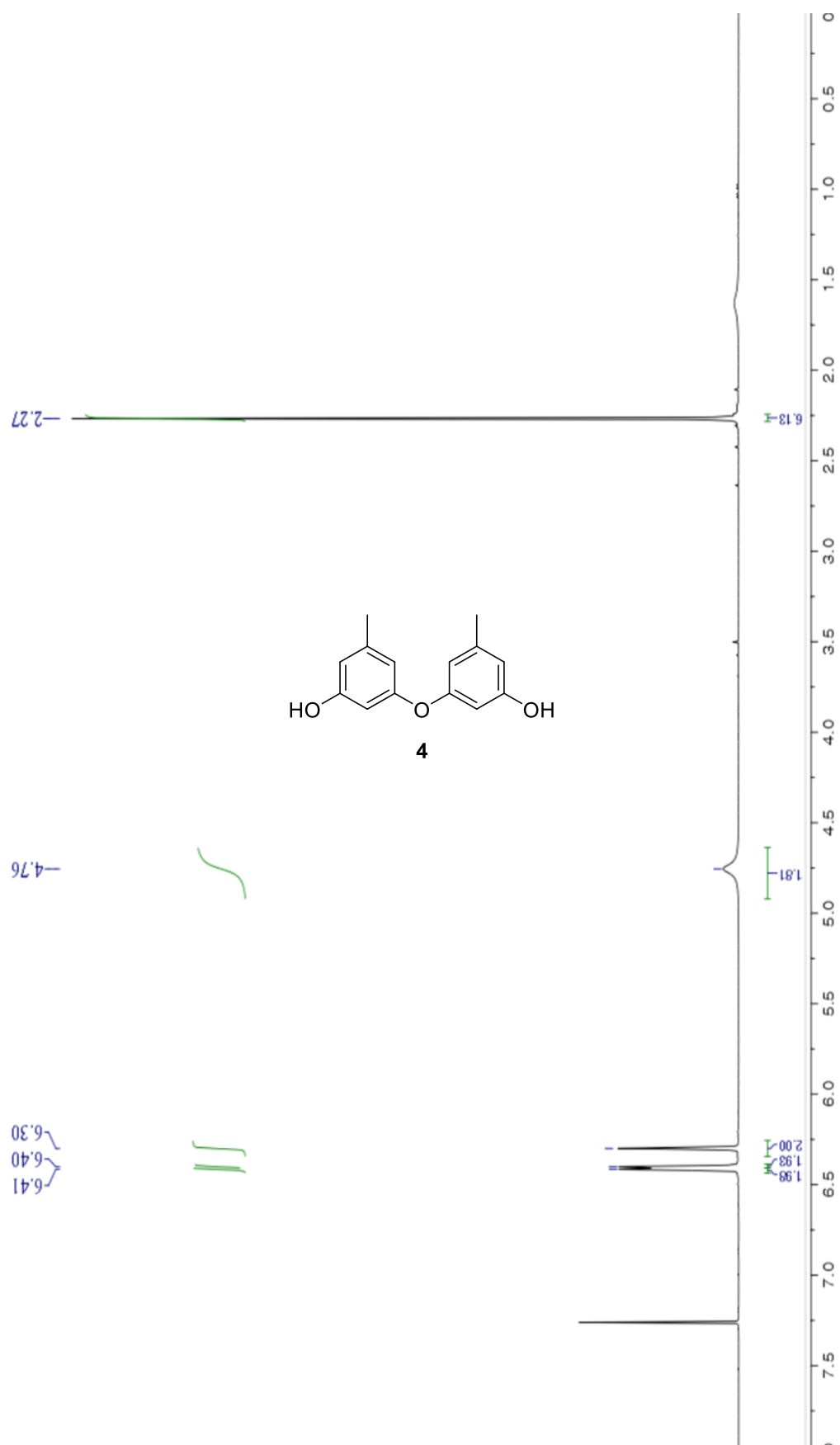


Figure S17. The ¹H NMR (400 MHz, CDCl₃) spectrum of **4**

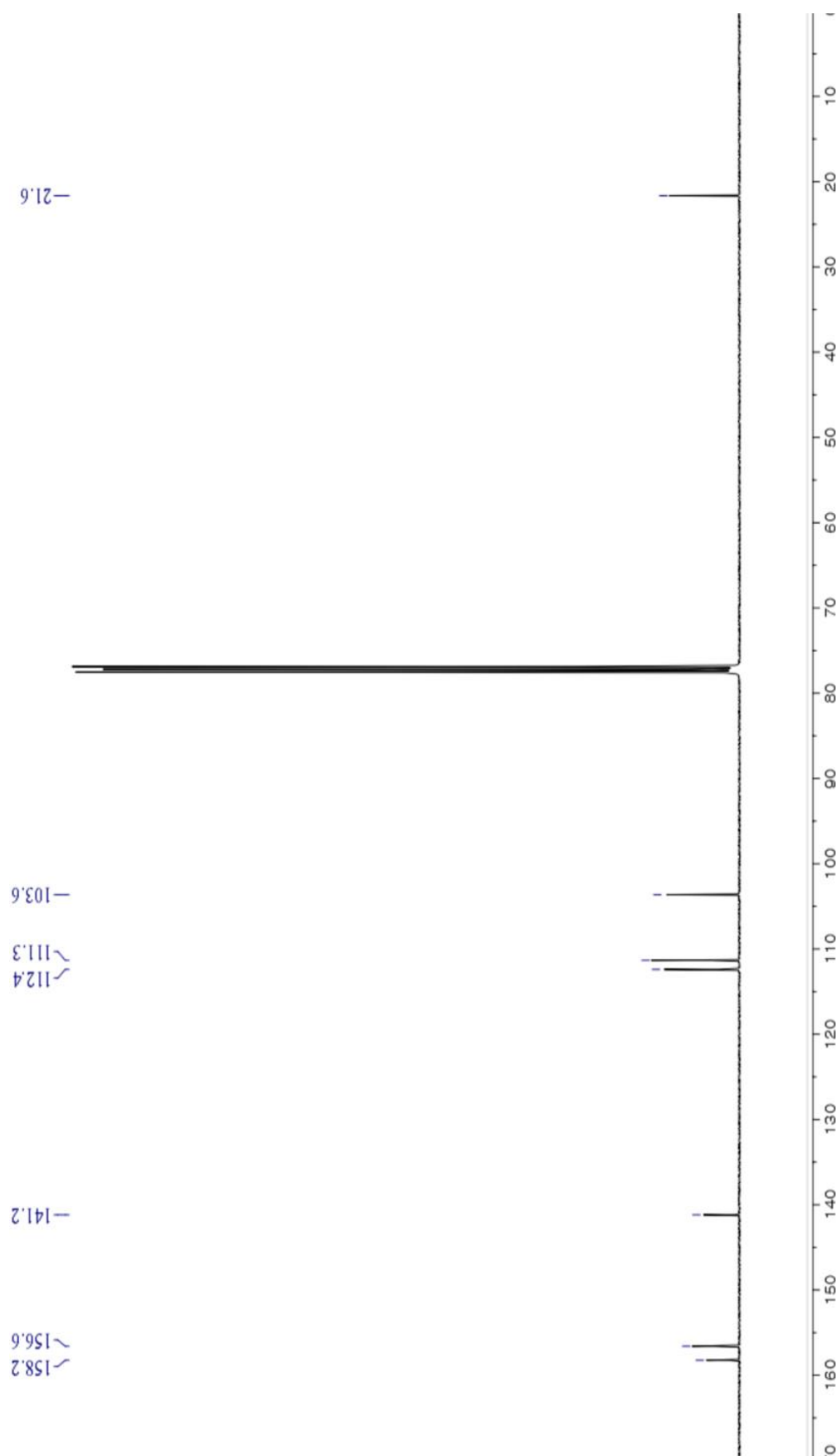


Figure S18. The ^{13}C NMR (100 MHz, CDCl_3) spectrum of **4**

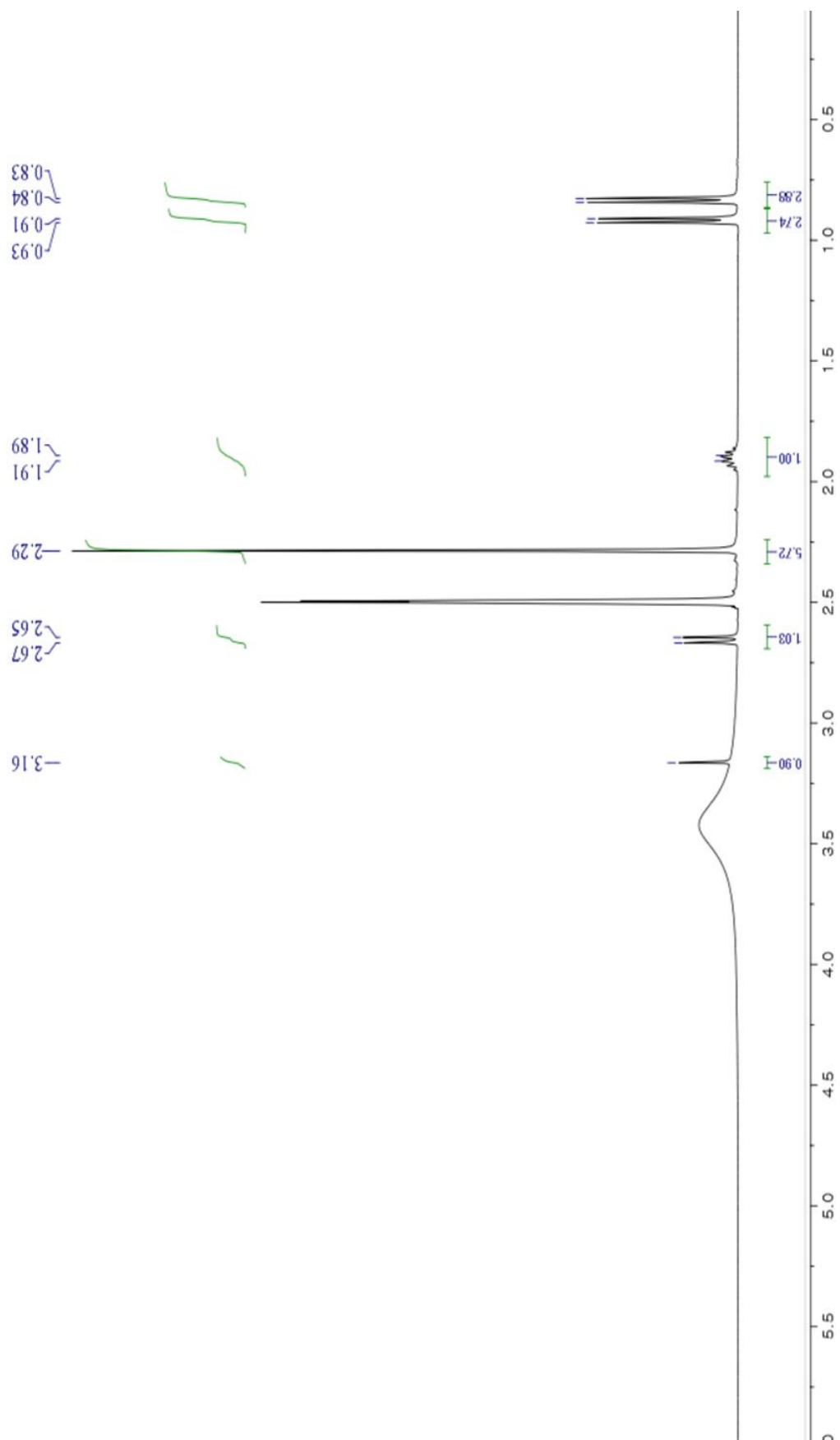


Figure S19. The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of **3a**

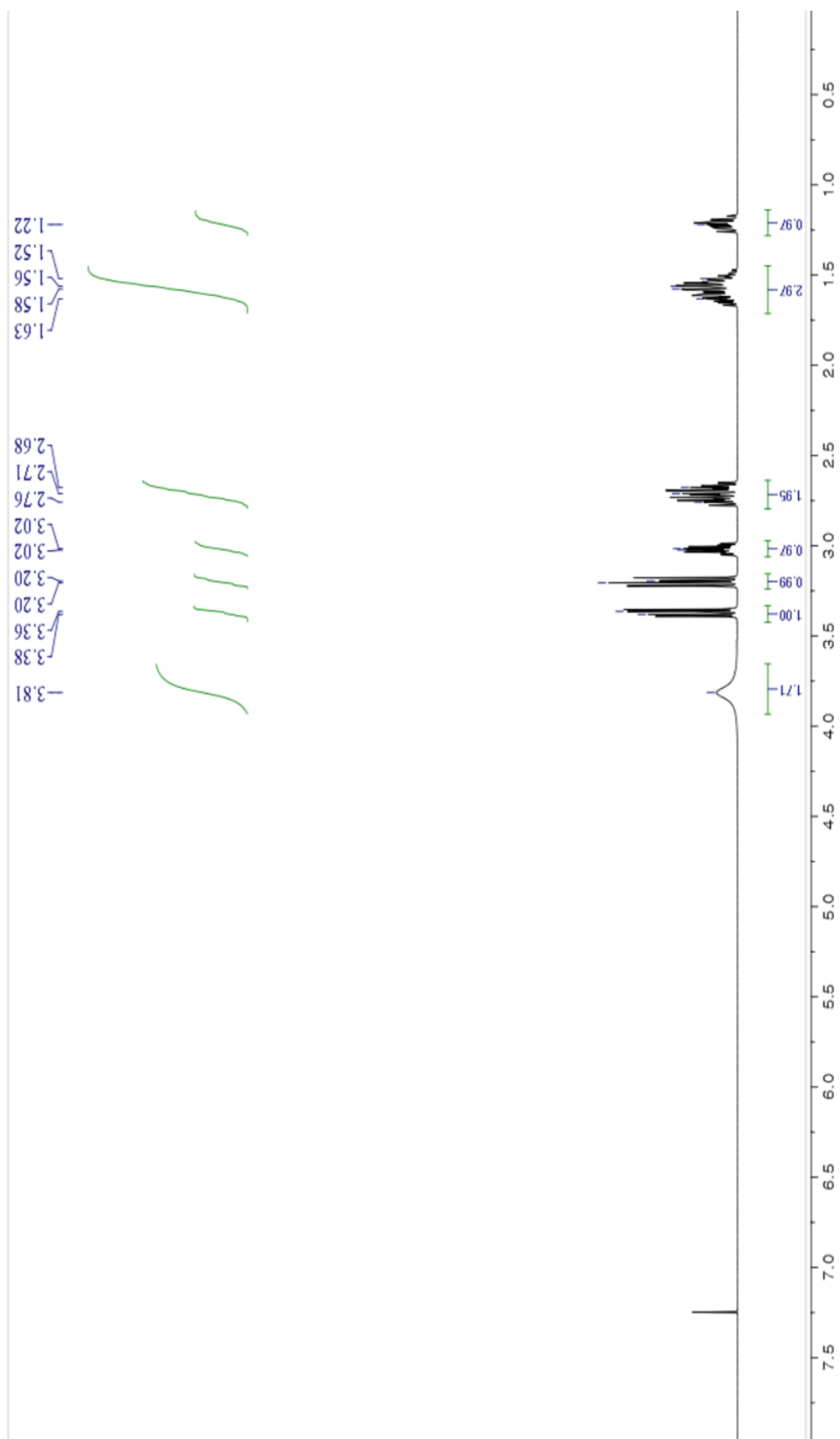


Figure S20. The ^1H NMR (400 MHz, CDCl_3) spectrum of **3b**

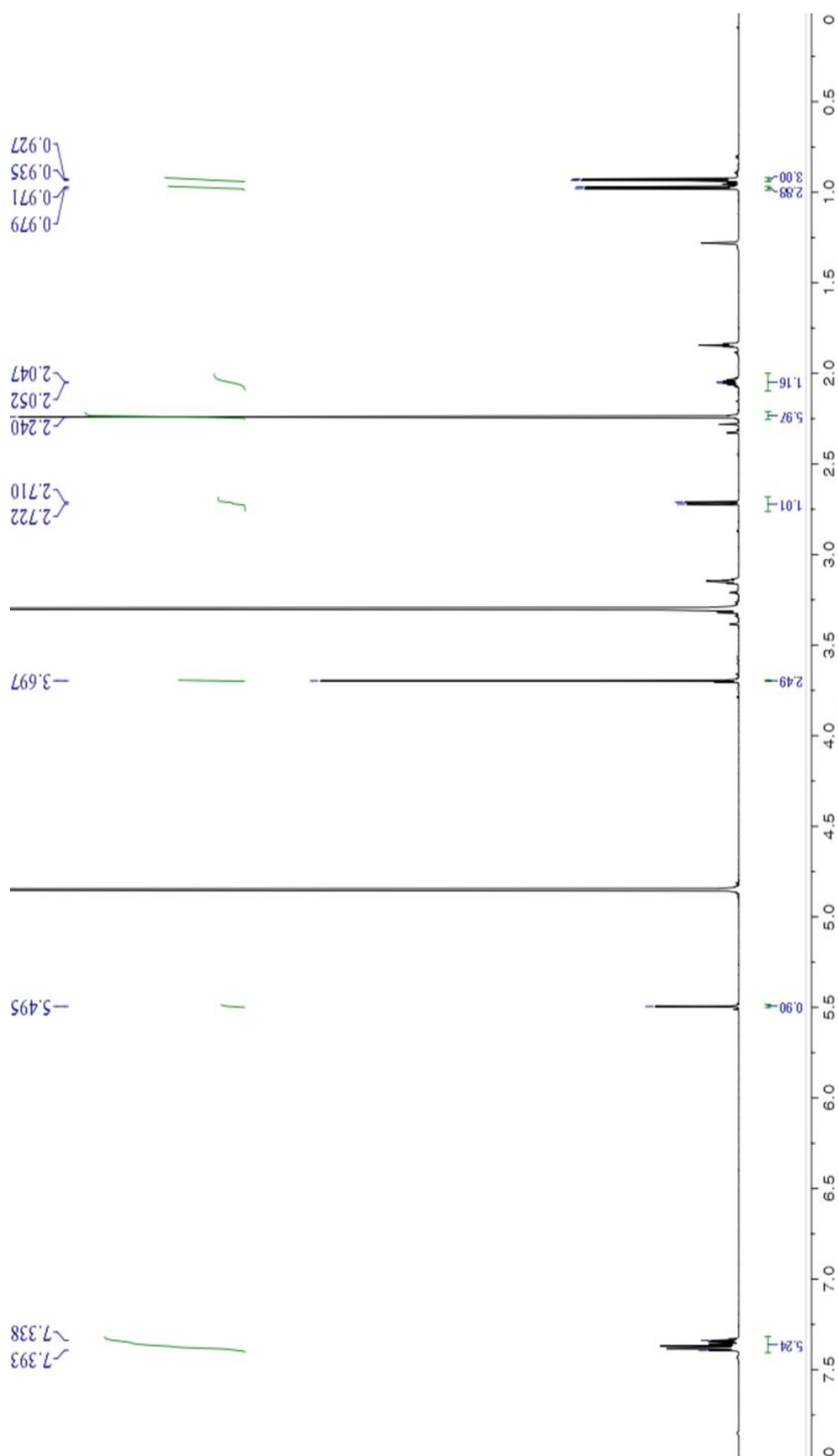


Figure S21. The ^1H NMR (800 MHz, $\text{Methanol-}d_4$) spectrum of **3aS**

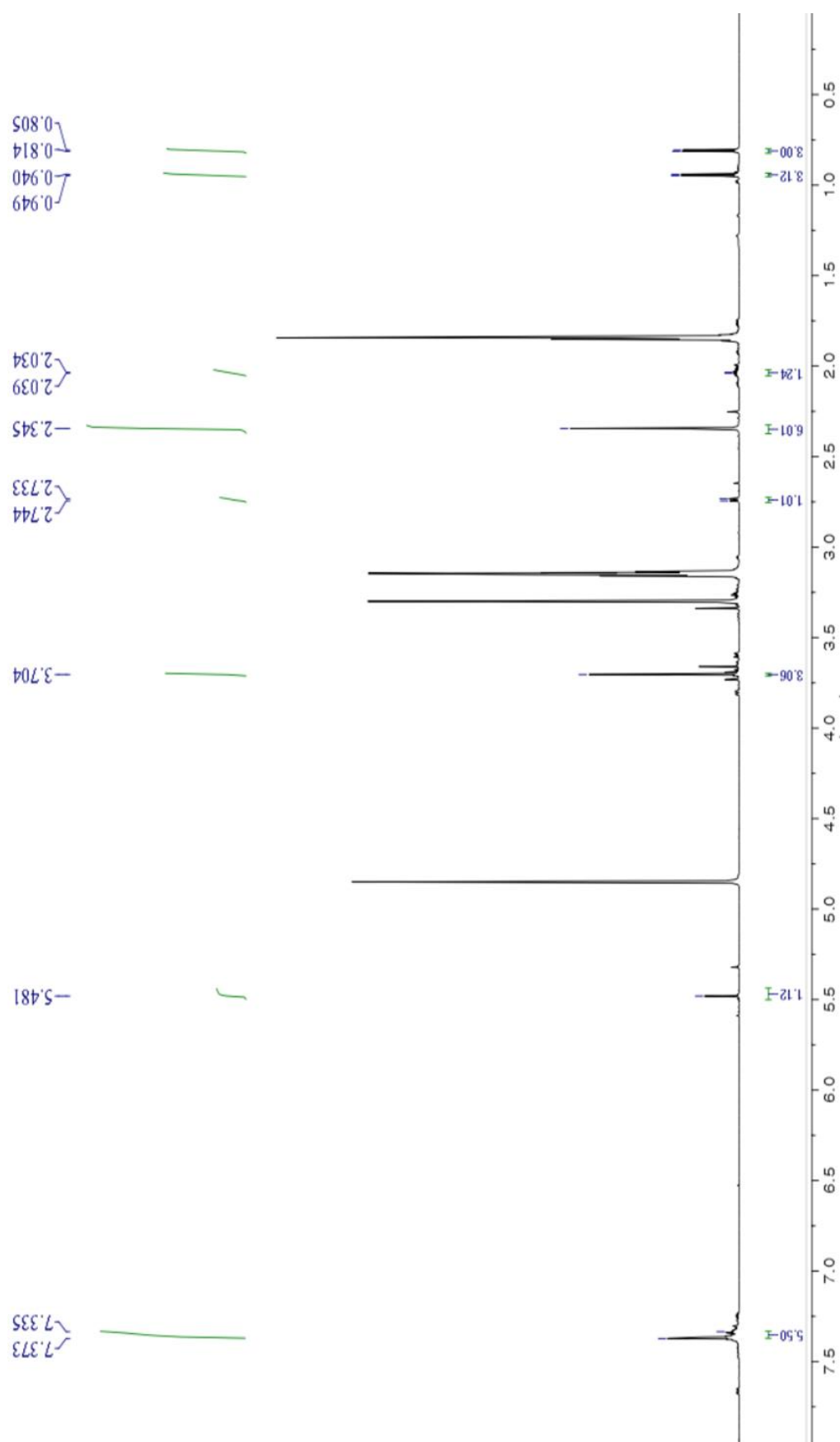


Figure S22. The ^1H NMR (800 MHz, $\text{Methanol-}d_4$) spectrum of **3aR**

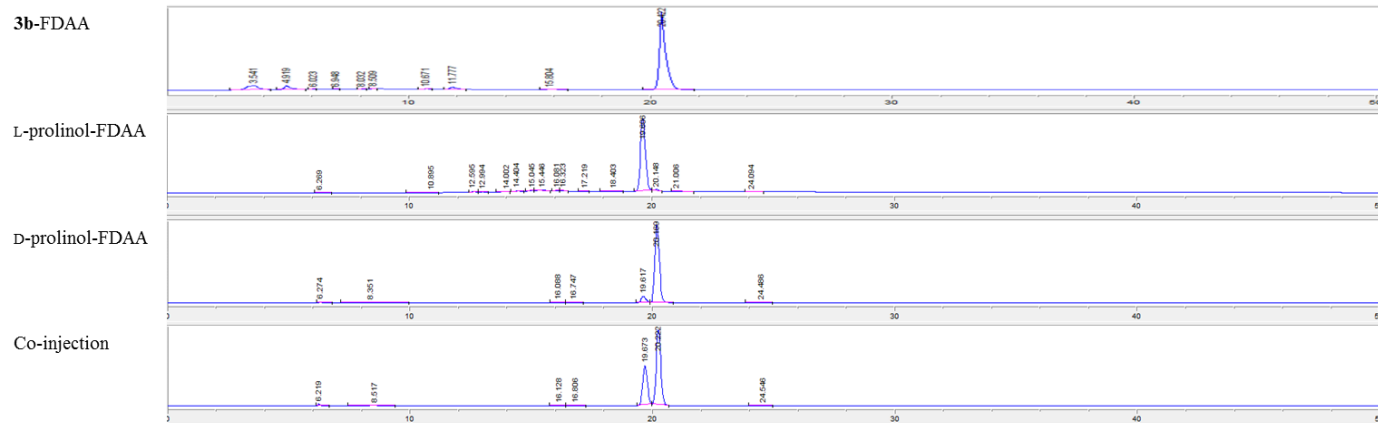


Figure S23. The LC/MS chromatogram data of **3b-L-FDAA** adduct

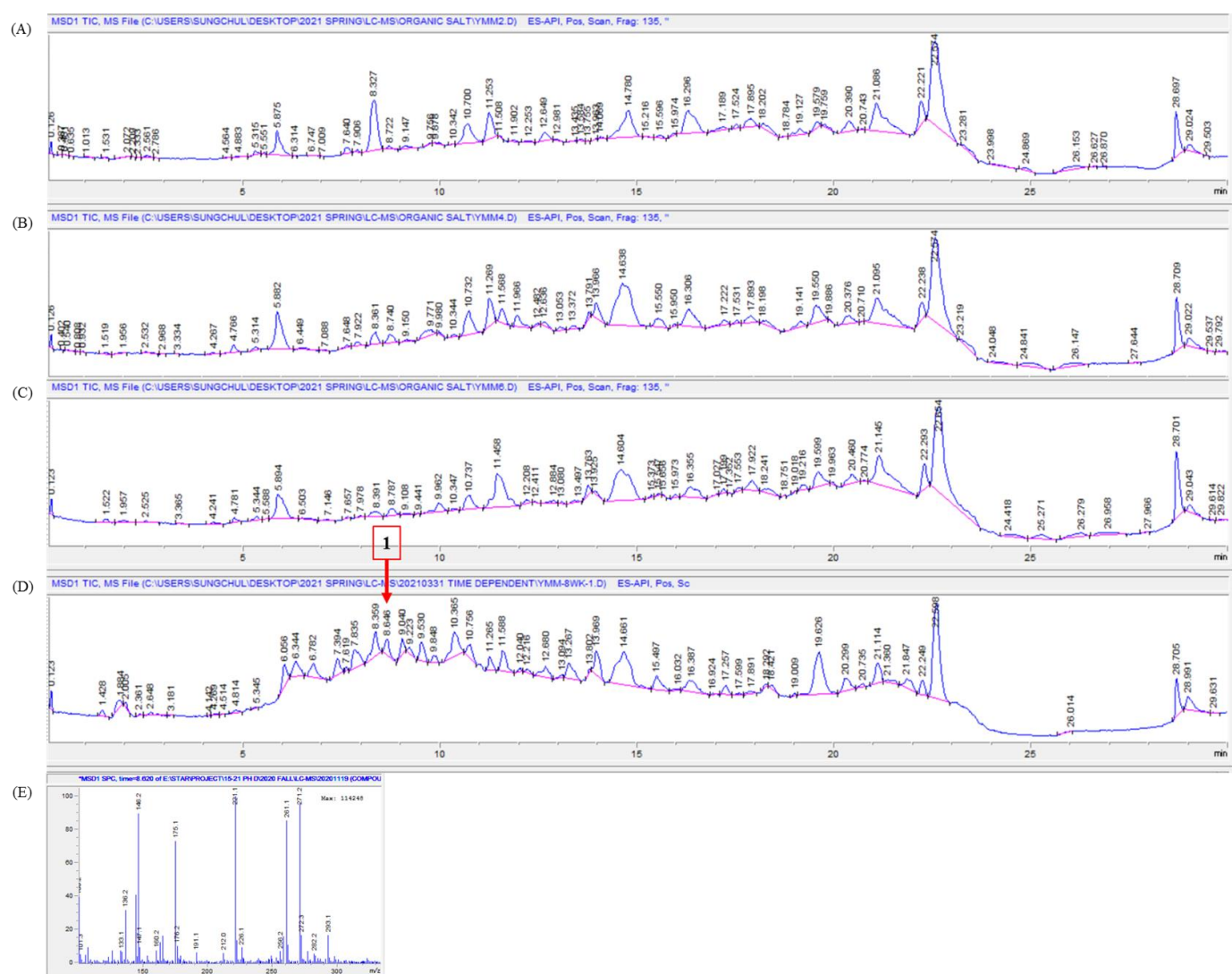


Figure S24. The time-scale LC-MS analysis of YMM liquid media extracts. (A)–(D) Extracts from 2, 4, 6, and 8 weeks of incubation, respectively. (E) The MS data on $t_R = 8.641$. *Condition:* YMC-ODS-A column, 250 x 4.6 mm; 10–100% MeCN–H₂O gradient over 20 min with 0.1% trifluoroacetic acid. Compound **1** ($t_R = 8.646$).

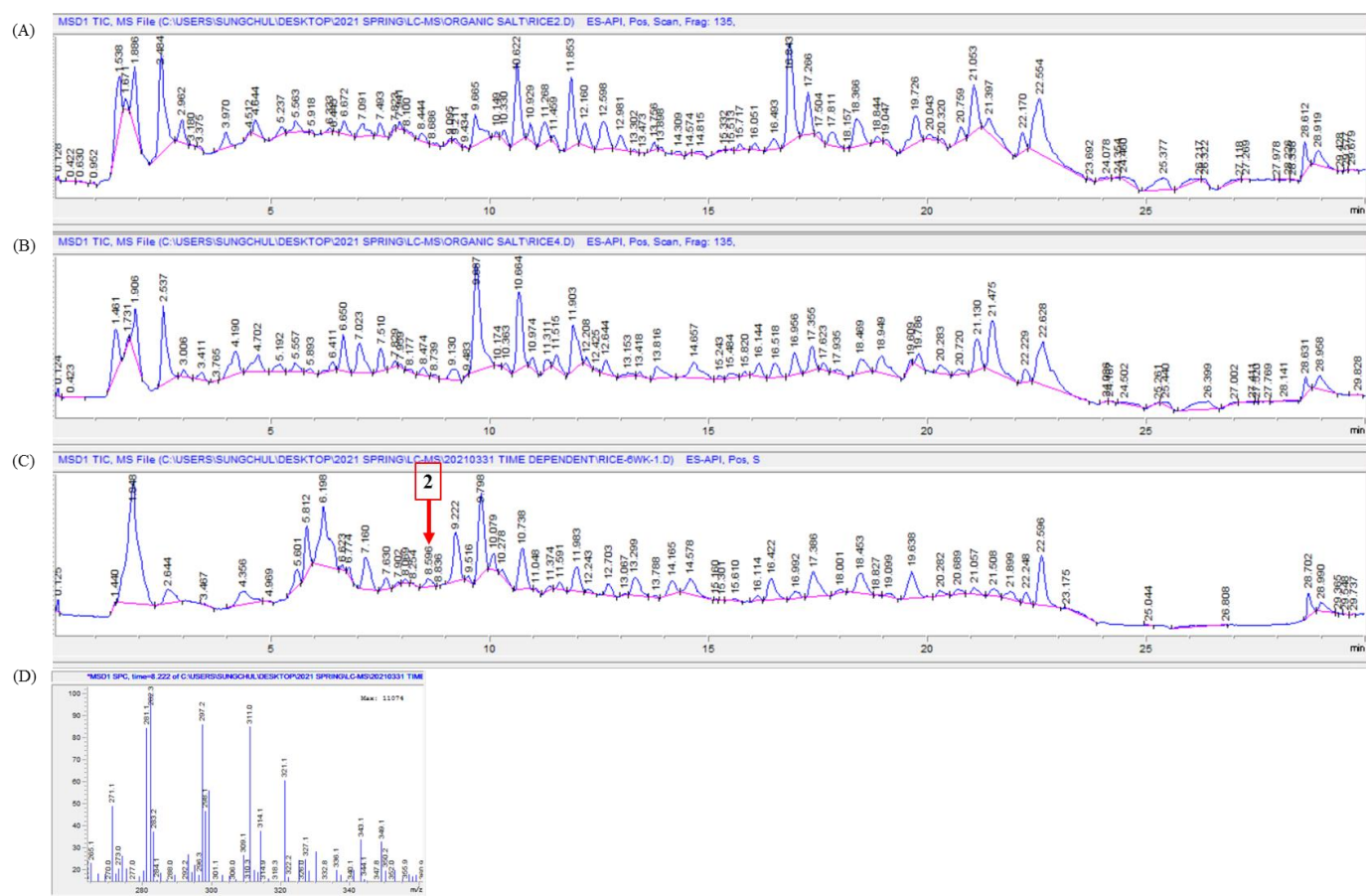


Figure S25. The time-scale LC-MS analysis of YMM-rice semi-solid media extracts. (A)–(C) Extracts from 2, 4 and 6 weeks of incubation, respectively. (D) The MS data on $t_R = 8.596$. *Condition:* YMC-ODS-A column, 250 x 4.6 mm; 10–100% MeCN–H₂O gradient over 20 min with 0.1% trifluoroacetic acid. Compound **2** ($t_R = 8.596$).

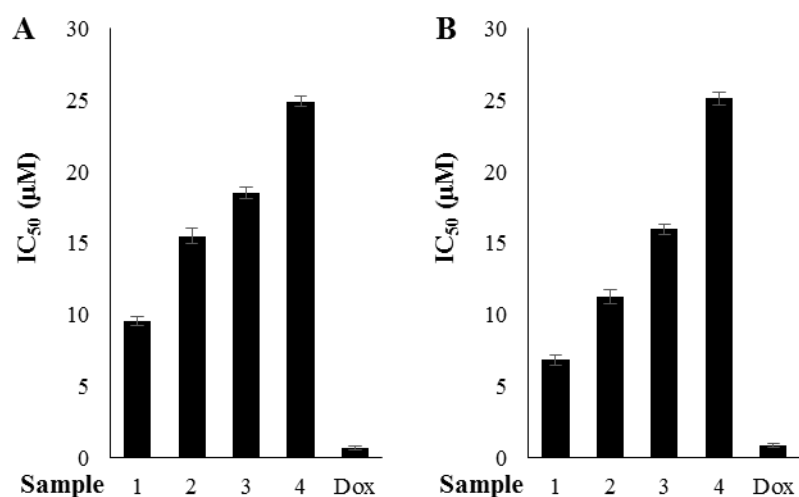


Figure S26. The MTT assay against K562 and A549 cancer cells. (A) IC₅₀ values were calculated by MTT assay results against K562 cancer cell. (B) IC₅₀ values were calculated by MTT assay results against A549 cancer cell. Doxorubicin was used as a positive control. The values are expressed as the mean \pm SD of triplicate tests.

Table S1. Results of cytotoxicity tests

Compounds	IC ₅₀ (μM)	
	K562	A549
1	9.5	6.8
2	16	11
3	19	16
4	25	25
Doxorubicin	0.72	0.90

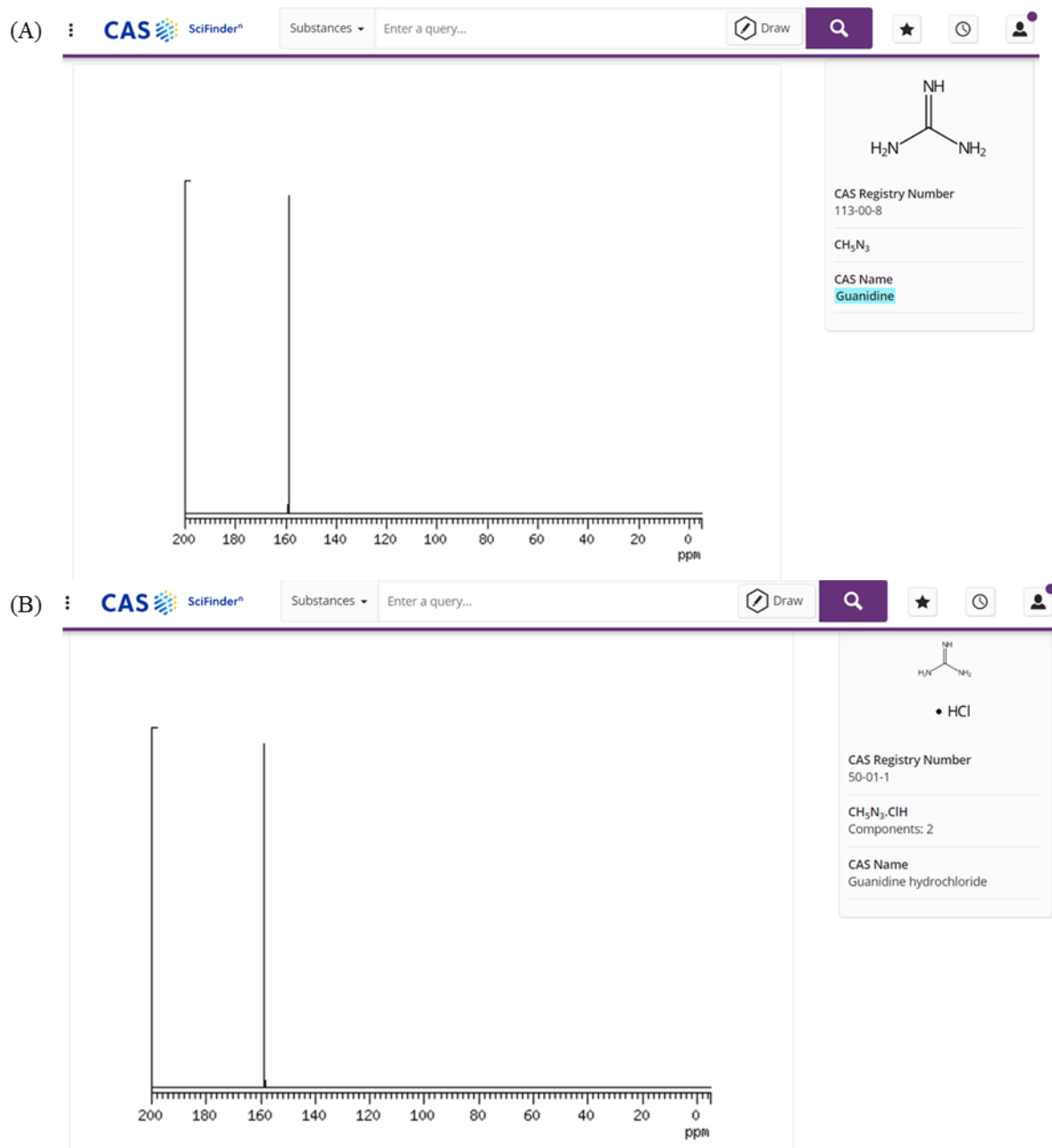


Figure S27. The ^{13}C NMR (25 MHz, D_2O) spectra of guanidine and guanidine hydrochloride. (A) The ^{13}C NMR (25 MHz, D_2O) spectrum of guanidine (CAS 113-00-8). The ^{13}C NMR (25 MHz, D_2O) spectrum of guanidine hydrochloride (CAS 50-01-1). The SciFinder provides experimental carbon NMR spectra of both guanidine (CAS 113-00-8) and guanidine hydrochloride (CAS 50-01-1) obtained from the National Institute of Advanced Industrial Science and Technology (Japan).

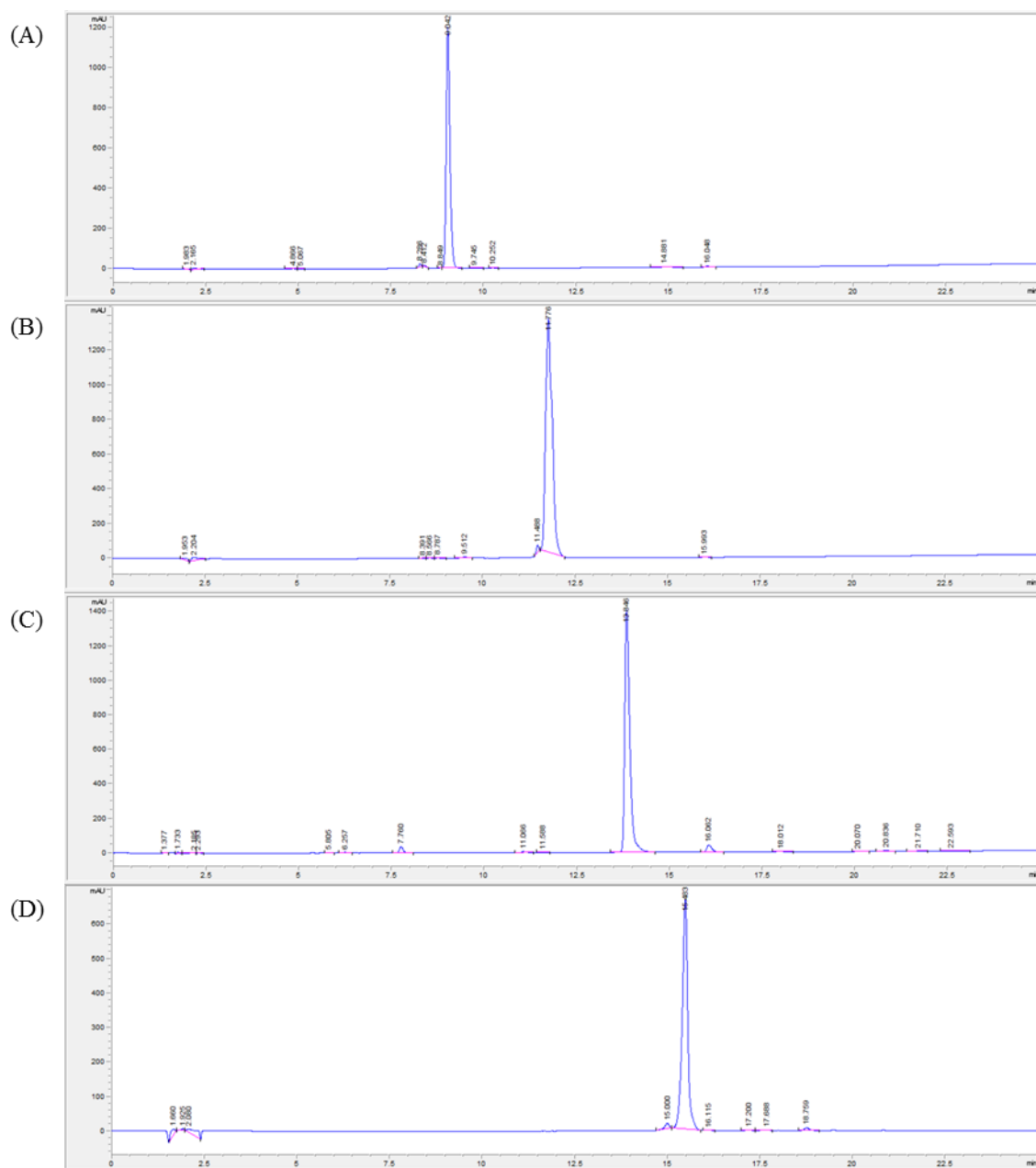


Figure S28. The HPLC analysis of **1**. *Condition:* (A) YMC-ODS-A column, 250 x 4.6 mm; 20–100% MeCN–H₂O gradient over 25 min; 0.5 mL/min; UV detection at 210 nm; $t_R = 9.042$ min. (B) YMC-ODS-A column, 250 x 4.6 mm; 10–100% MeCN–H₂O gradient over 25 min; 0.5 mL/min; UV detection at 210 nm; $t_R = 11.776$ min. (C) YMC-ODS-A column, 250 x 4.6 mm; H₂O–MeOH, 60:40; 0.5 mL/min; UV detection at 210 nm; $t_R = 13.846$ min. (D) YMC-ODS-A column, 250 x 4.6 mm; H₂O–MeCN, 69:31; 0.5 mL/min; UV detection at 210 nm; $t_R = 15.483$ min.

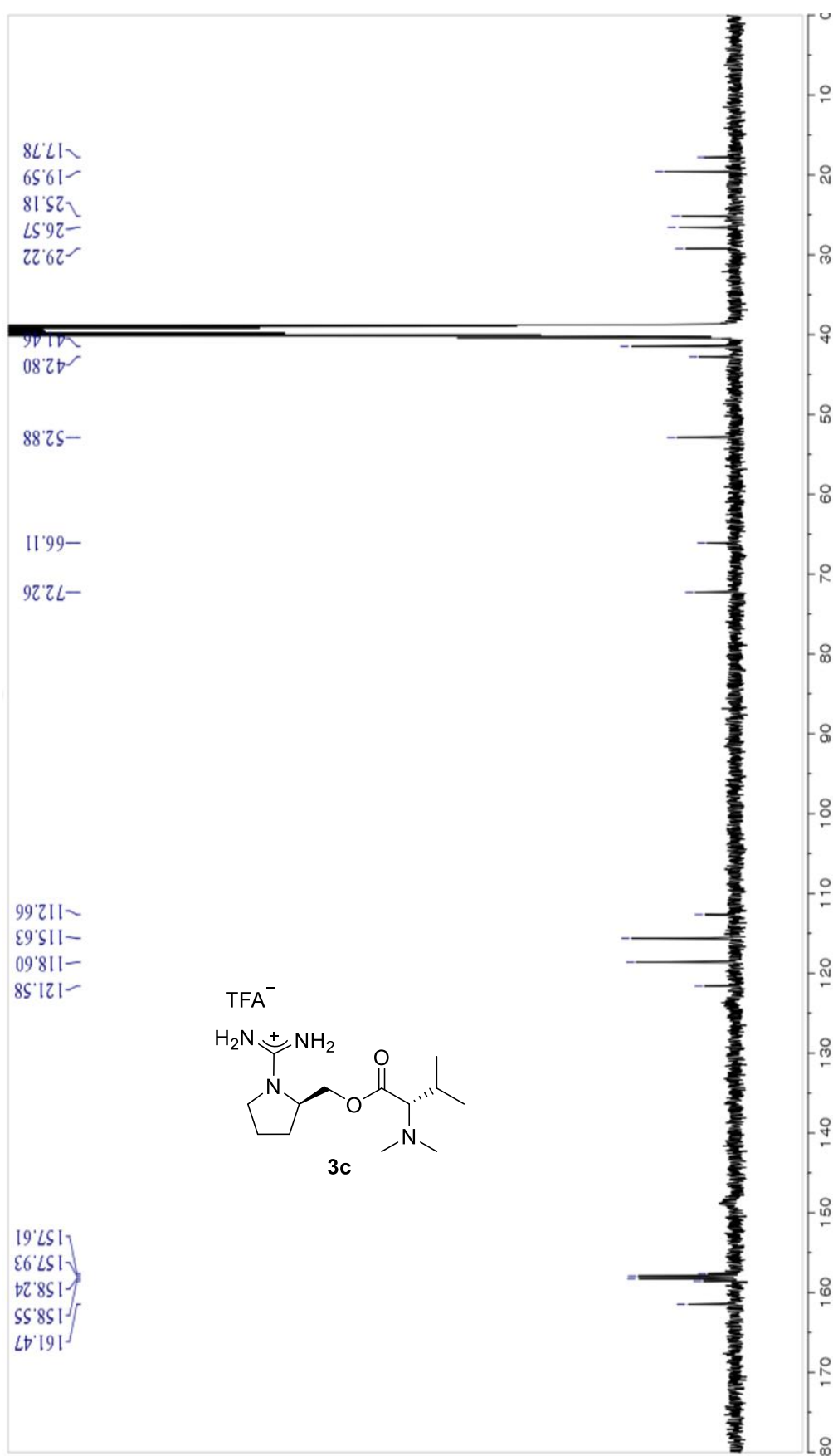


Figure S29. The ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **3c**

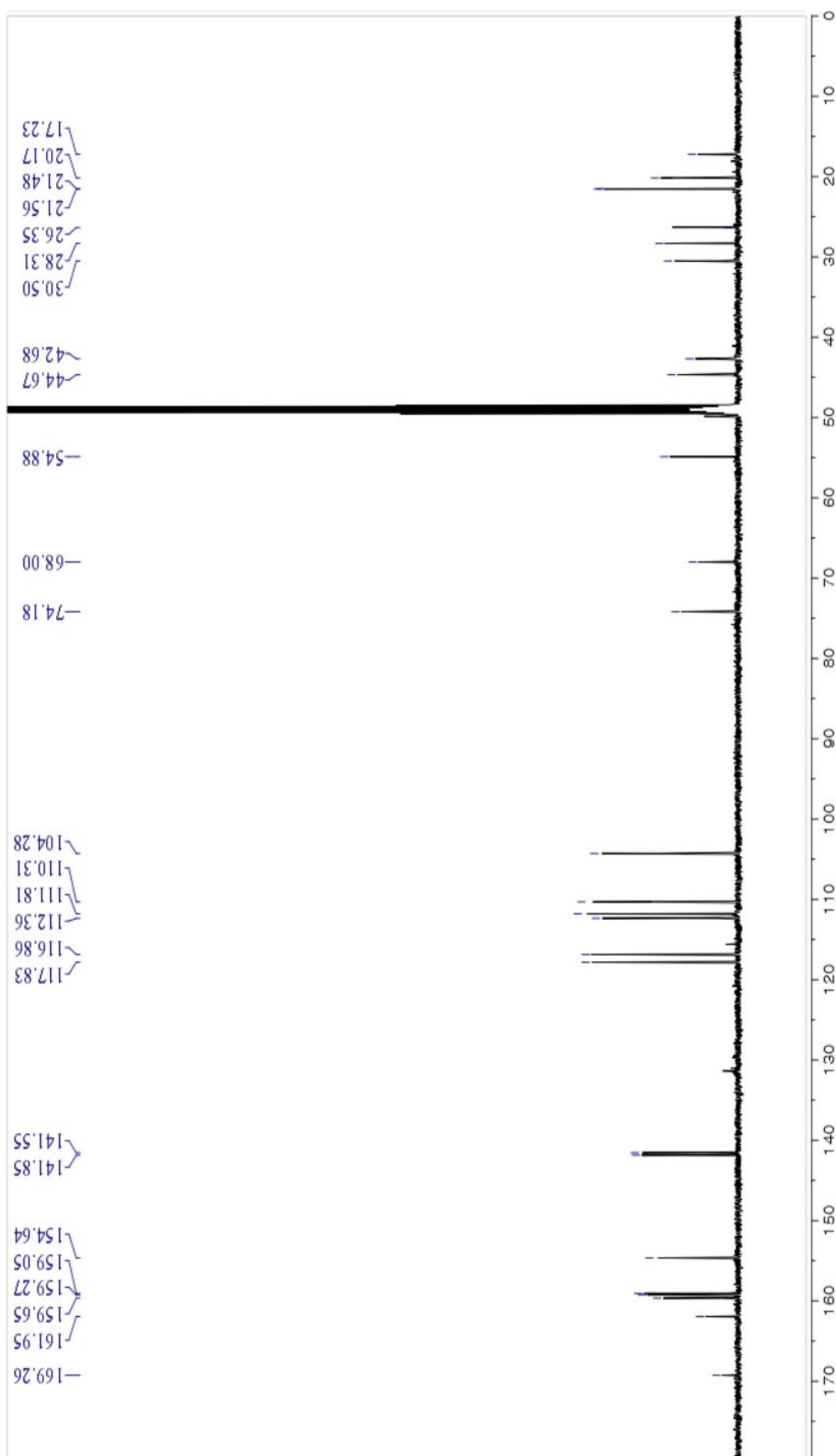


Figure S30. The ^{13}C NMR (125 MHz, $\text{MeOH-}d_4$) spectrum of **1**

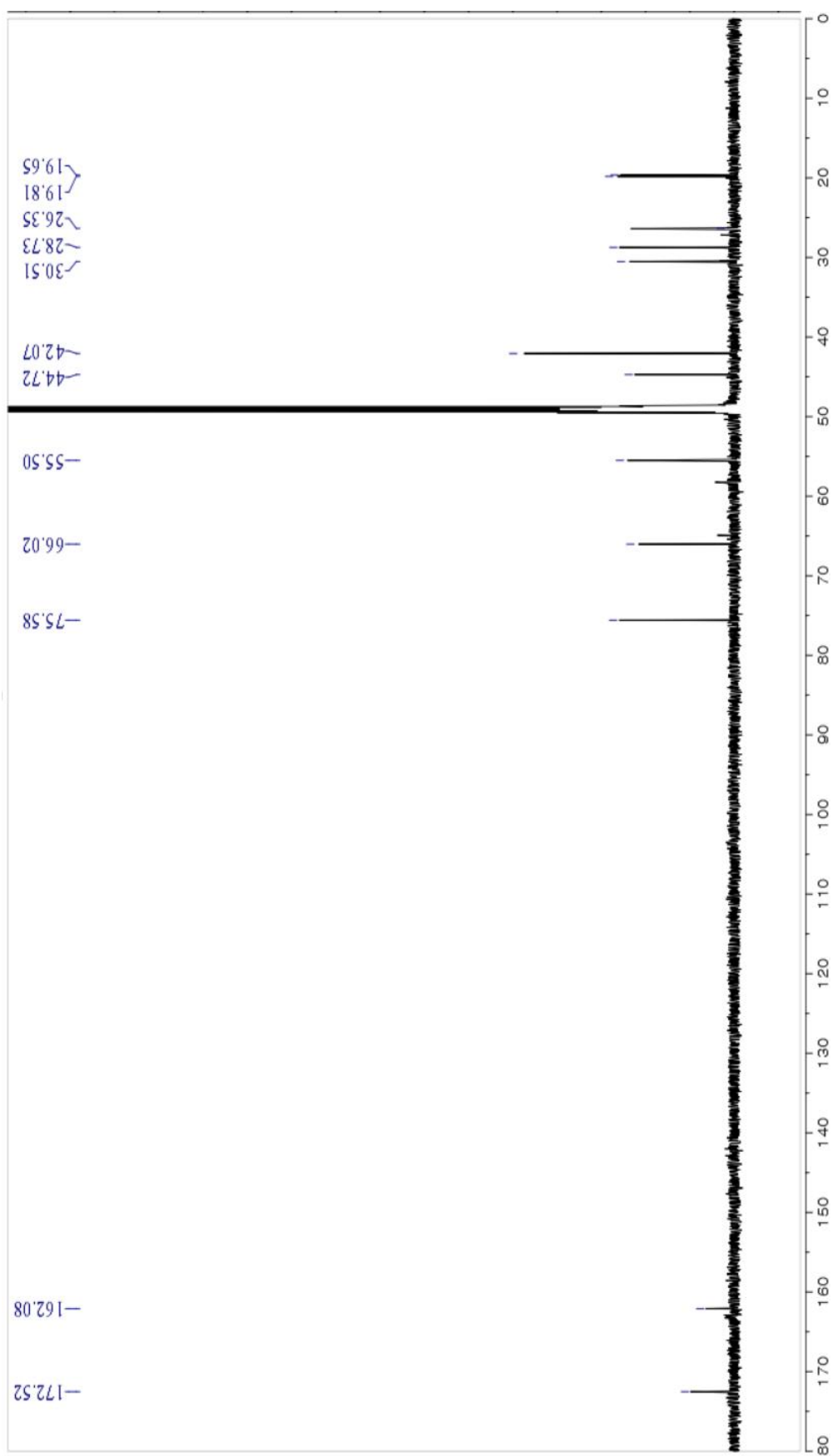


Figure S31. The ^{13}C NMR (200 MHz, $\text{MeOH-}d_4$) spectrum of **3**

Table S2. The ^{13}C NMR data of **1–3** and **3c**

No	1 ^a	2 ^a	3 ^a	3c ^a	1 ^b	3 ^b
	δ_{C} , type	δ_{C} , type	δ_{C} , type	δ_{C} , type	δ_{C} , type	δ_{C} , type
1	154.50, C	154.50, C			154.64, C	
2	108.13, CH	108.15, CH			110.31, CH	
3	156.65, C	156.69, C			154.64, C	
4	113.93, CH	113.89, CH			116.86, CH	
5	139.28, C	139.34, C			141.55, C	
6	115.83, CH	115.95, CH			117.83, CH	
7	157.59, C	157.60, C			159.05, C	
8	102.74, CH	102.79, CH			104.28, CH	
9	158.43, C	158.47, C			159.27, C	
10	109.82, CH	109.85, CH			111.81, CH	
11	140.05, C	140.10, C			141.85, C	
12	111.15, CH	111.21, CH			112.36, CH	
13	21.02, CH ₃	21.13, CH ₃			21.48, CH ₃	
14	21.09, CH ₃	21.06, CH ₃			21.56, CH ₃	
1'	42.67, CH ₂		42.74, CH ₂	42.80, CH ₂	44.67, CH ₂	44.72, CH ₂
2'	24.78, CH ₂		24.82, CH ₂	25.18, CH ₂	26.35, CH ₂	26.35, CH ₂
3'	28.96, CH ₂		28.98, CH ₂	29.22, CH ₂	30.50, CH ₂	30.51, CH ₂
4'	52.98, CH		52.95, CH	52.88, CH	54.88, CH	55.50, CH
5'	64.45, CH ₂		64.64, CH ₂	66.11, CH ₂	68.00, CH ₂	66.02, CH ₂
6'	170.53, C		170.37, C	ND	169.26, C	172.52, C
7'	73.31, CH		73.19, CH	72.26, CH	74.18, CH	75.58, CH
8'	26.84, CH		26.80, CH	26.57, CH	28.31, CH	28.73, CH
9'	19.13, CH ₃		19.16, CH ₃	17.78, CH ₃	17.23, CH ₃	19.65, CH ₃
10'	19.51, CH ₃		19.16, CH ₃	19.57, CH ₃	20.17, CH ₃	19.81, CH ₃
11'	41.01, CH ₃		41.05, CH ₃	41.46, CH ₃	42.68, CH ₃	42.07, CH ₃
12'	41.01, CH ₃		41.05, CH ₃	41.46, CH ₃	42.68, CH ₃	42.07, CH ₃
13'	160.24, C		160.39, C	161.47, C	161.95, C	162.08, C

^a Data were obtained in DMSO-*d*₆. ^b Data were obtained in MeOH-*d*₄.