Supporting Information

Bromopyrrole alkaloids from the sponge Agelas kosrae

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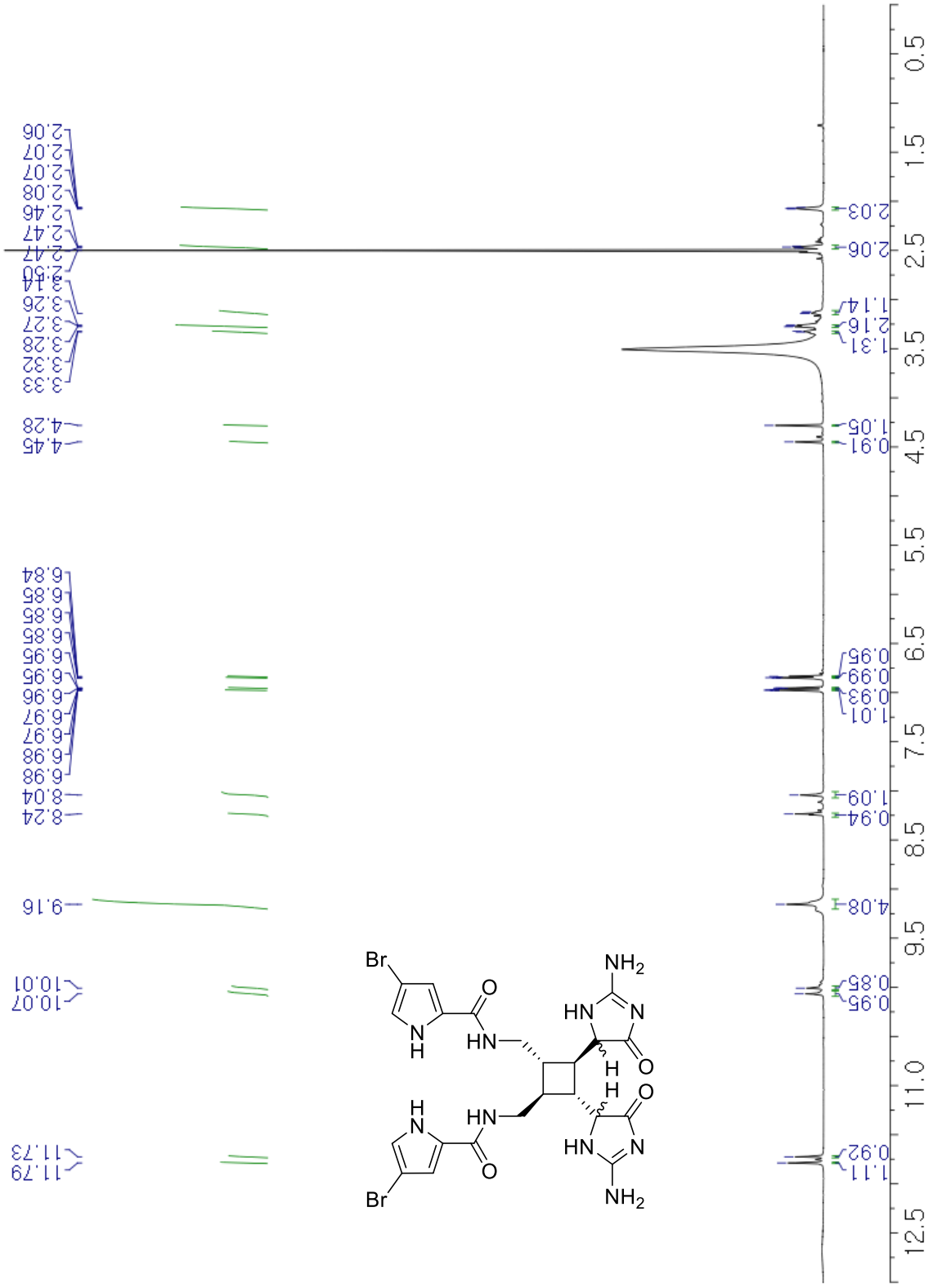


Figure S1. The ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **1**

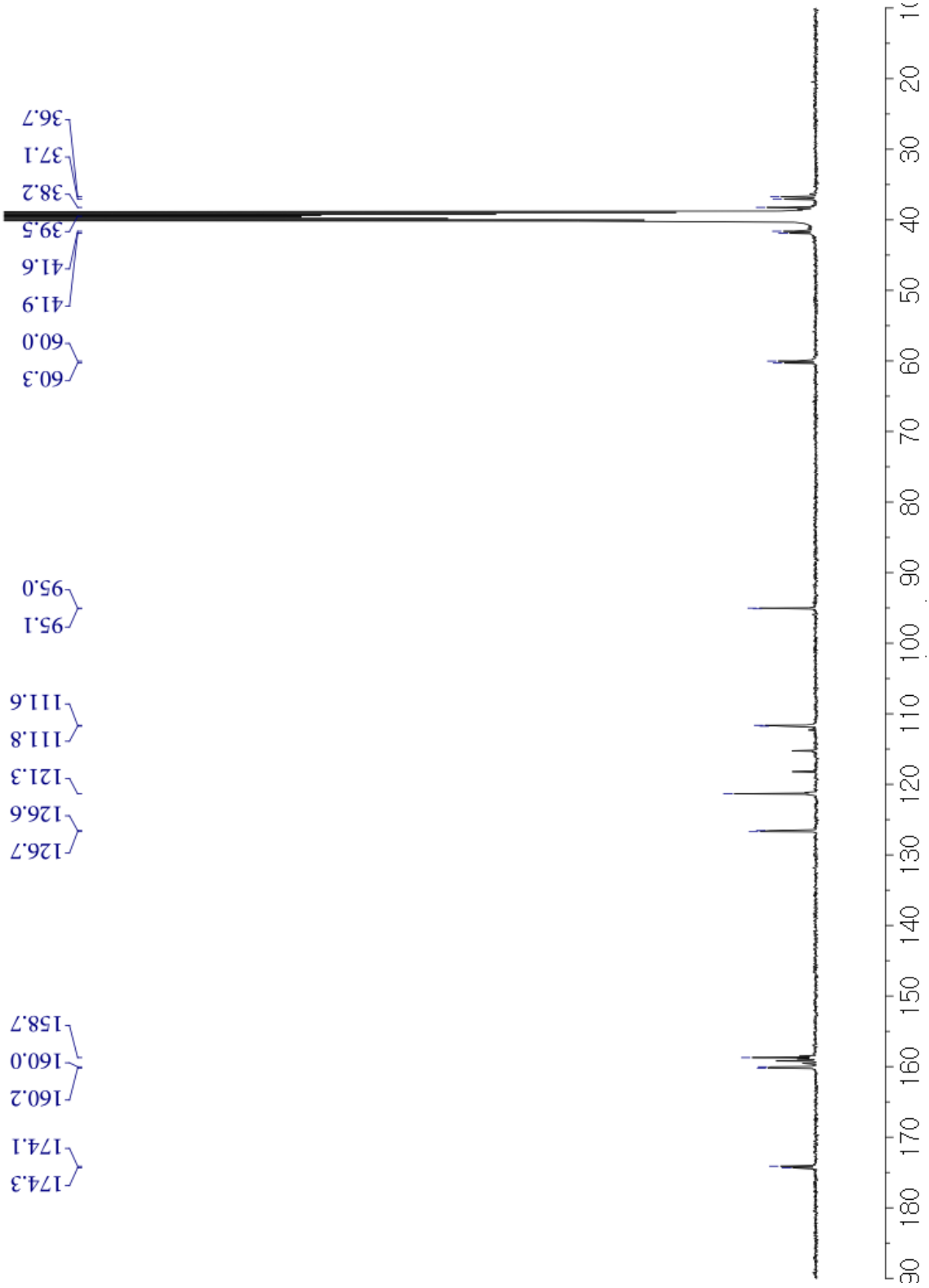


Figure S2. The ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **1**

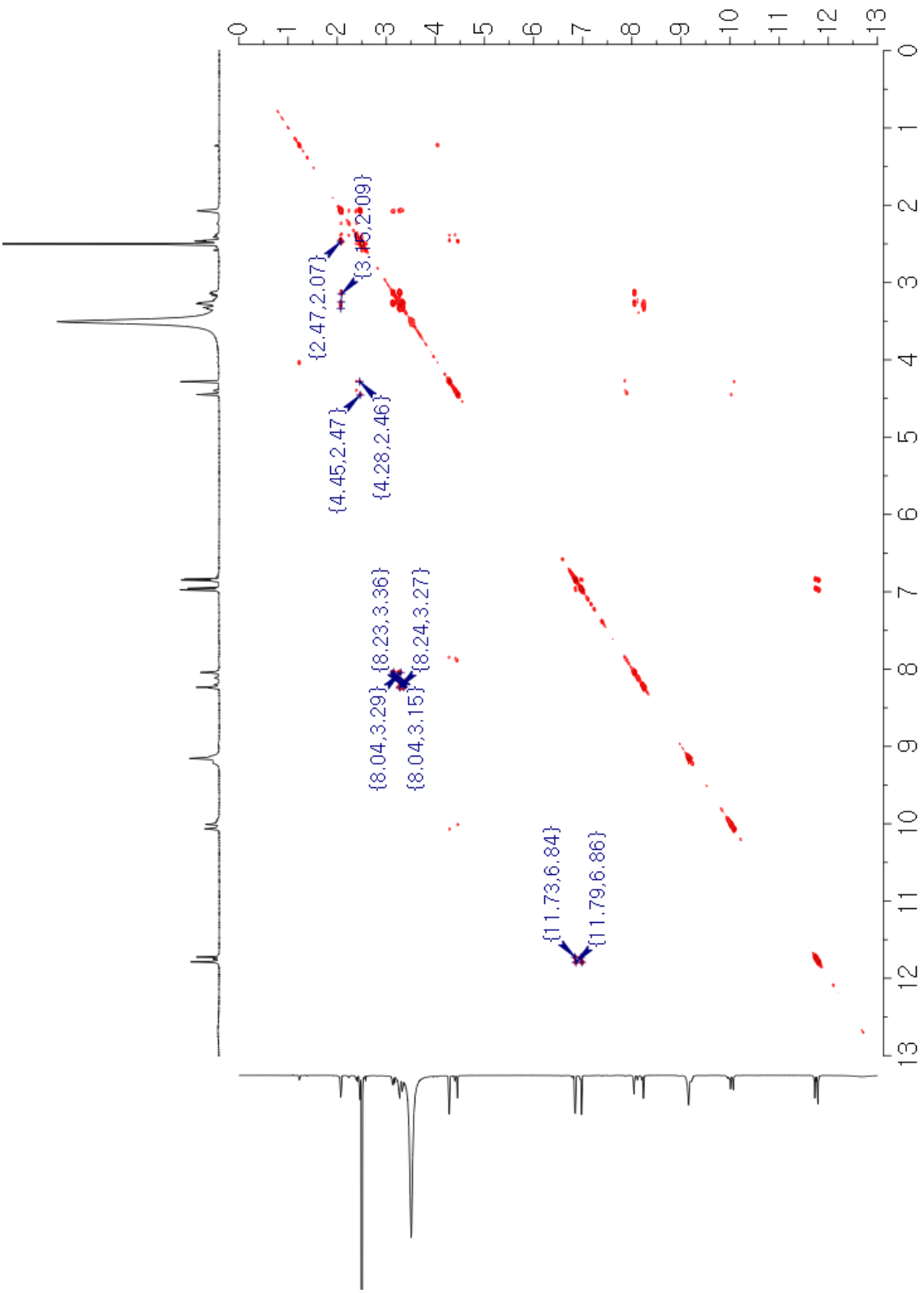


Figure S3. The COSY (600 MHz, DMSO-d_6) spectrum of **1**

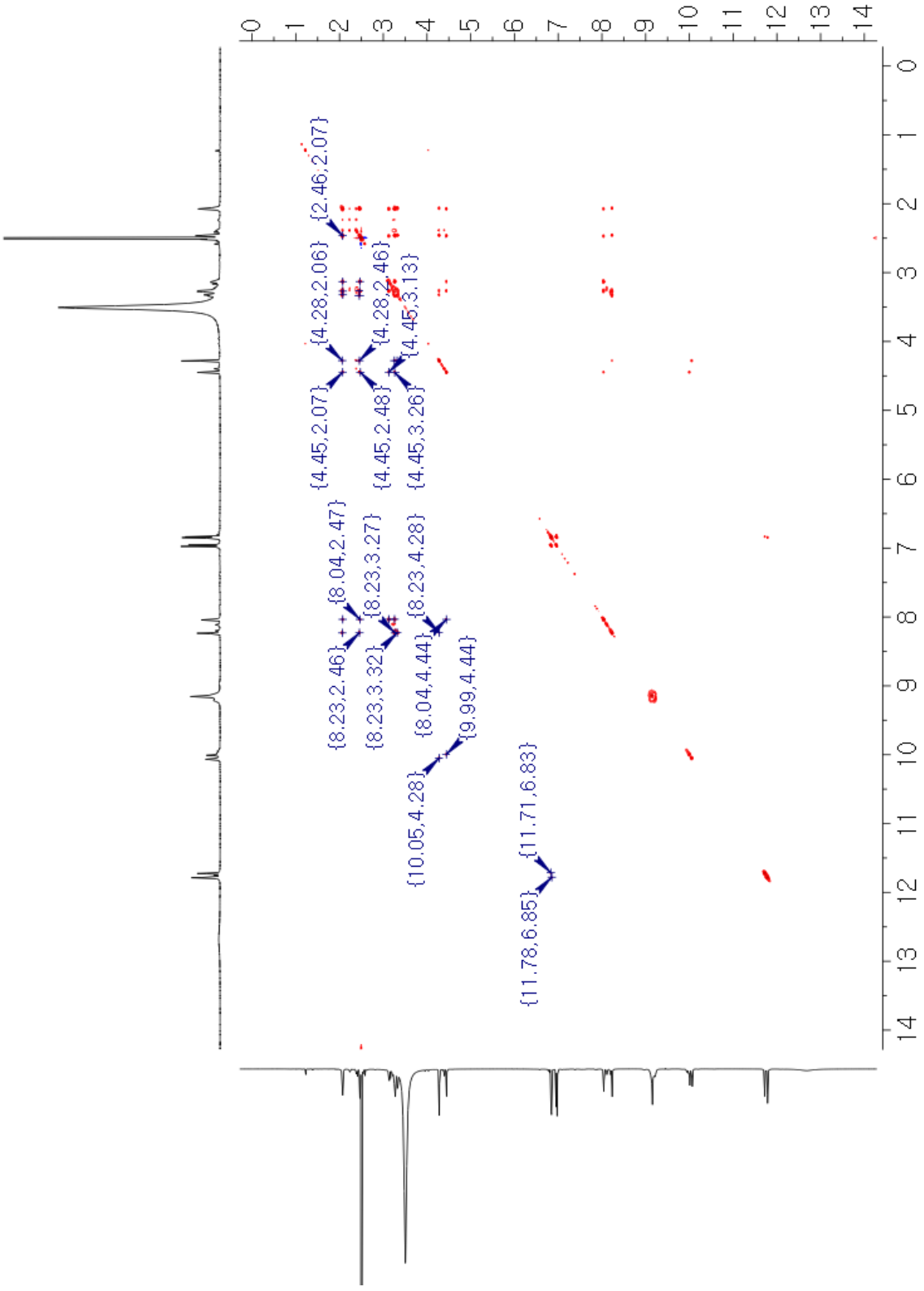


Figure S3. The TOCSY (600 MHz, DMSO-d_6) spectrum of **1**

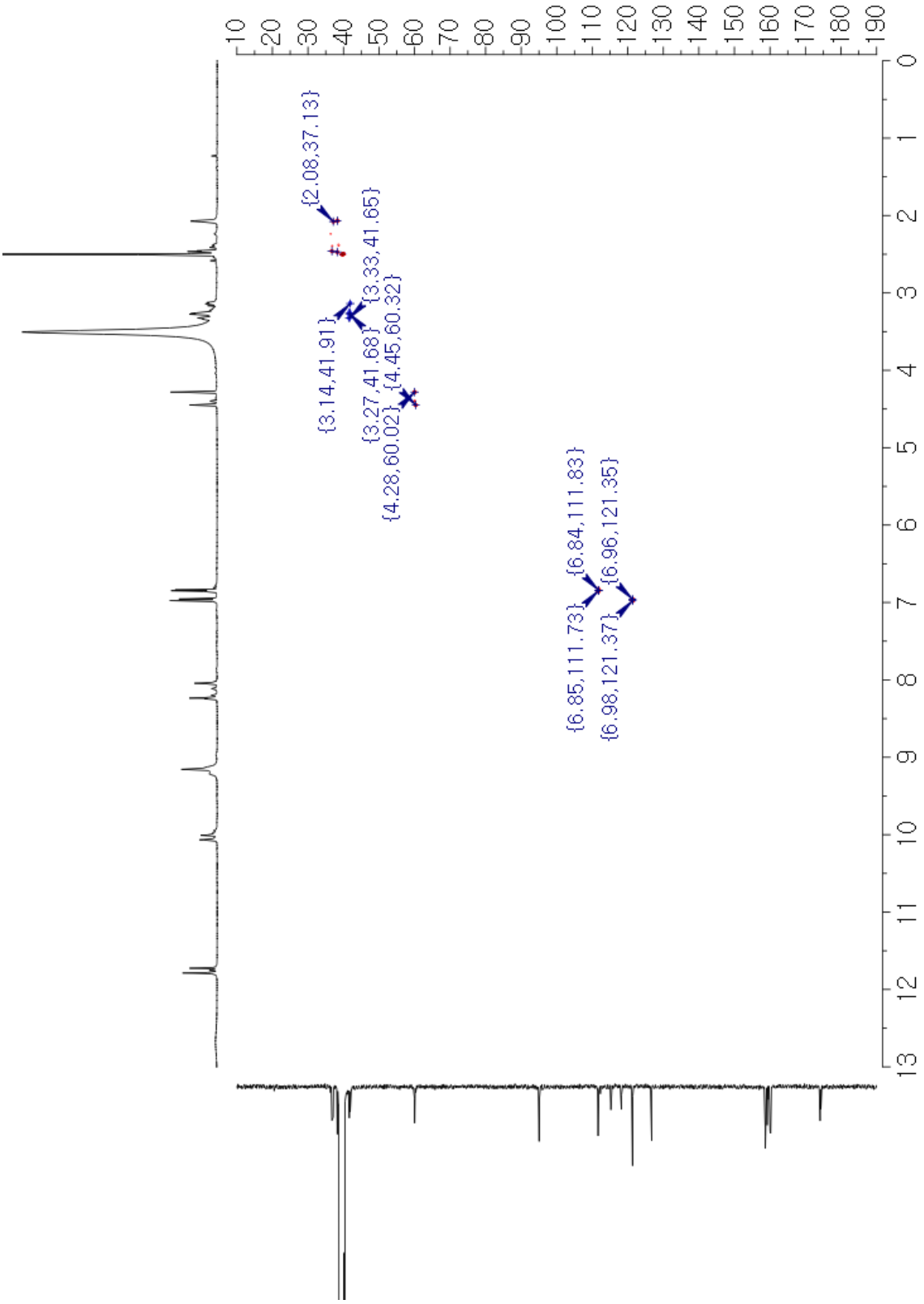


Figure S4. The eHSQC (600 MHz, DMSO-d_6) spectrum of **1**

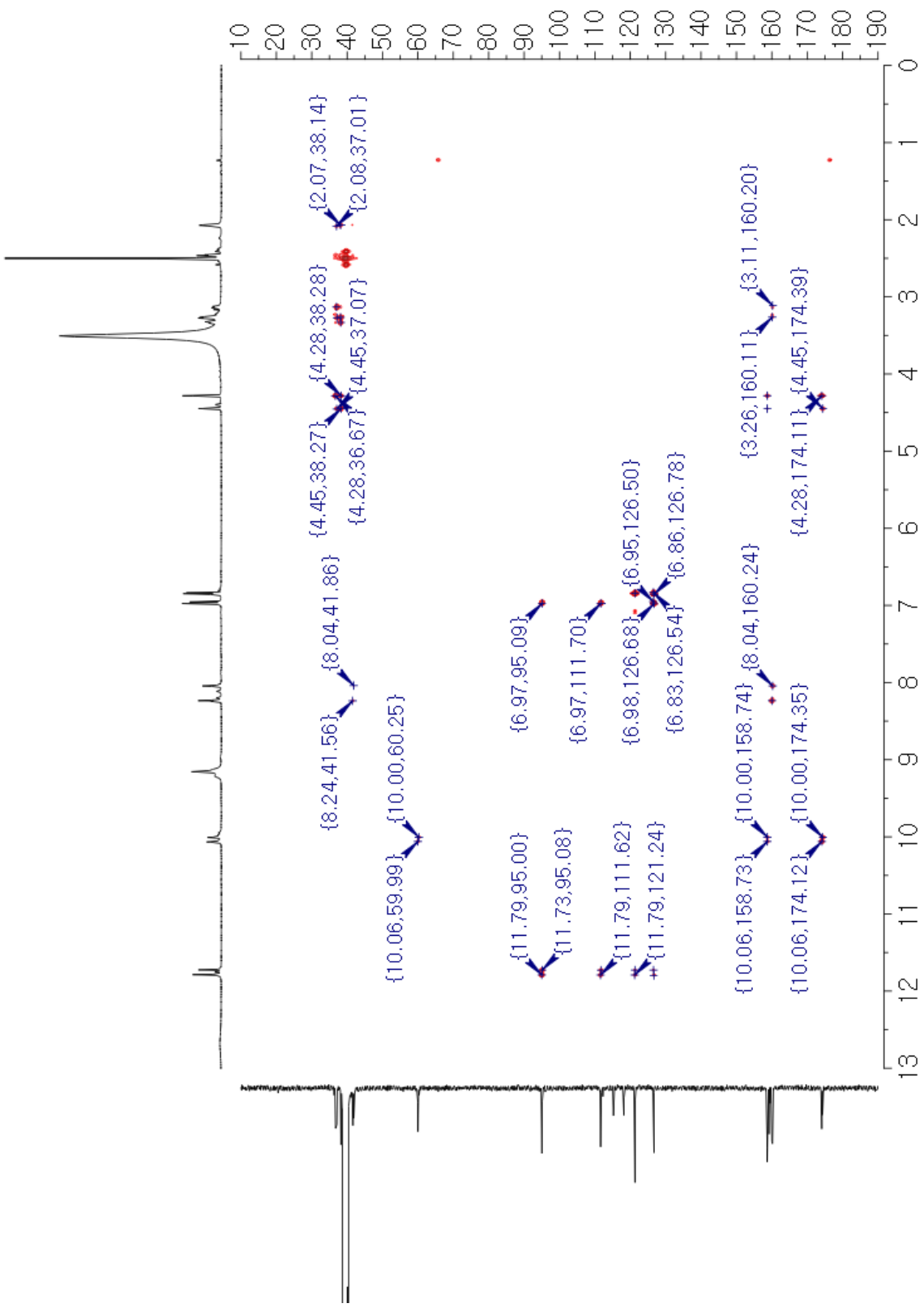


Figure S5. The HMBC (600 MHz, DMSO-d_6) spectrum of **1**

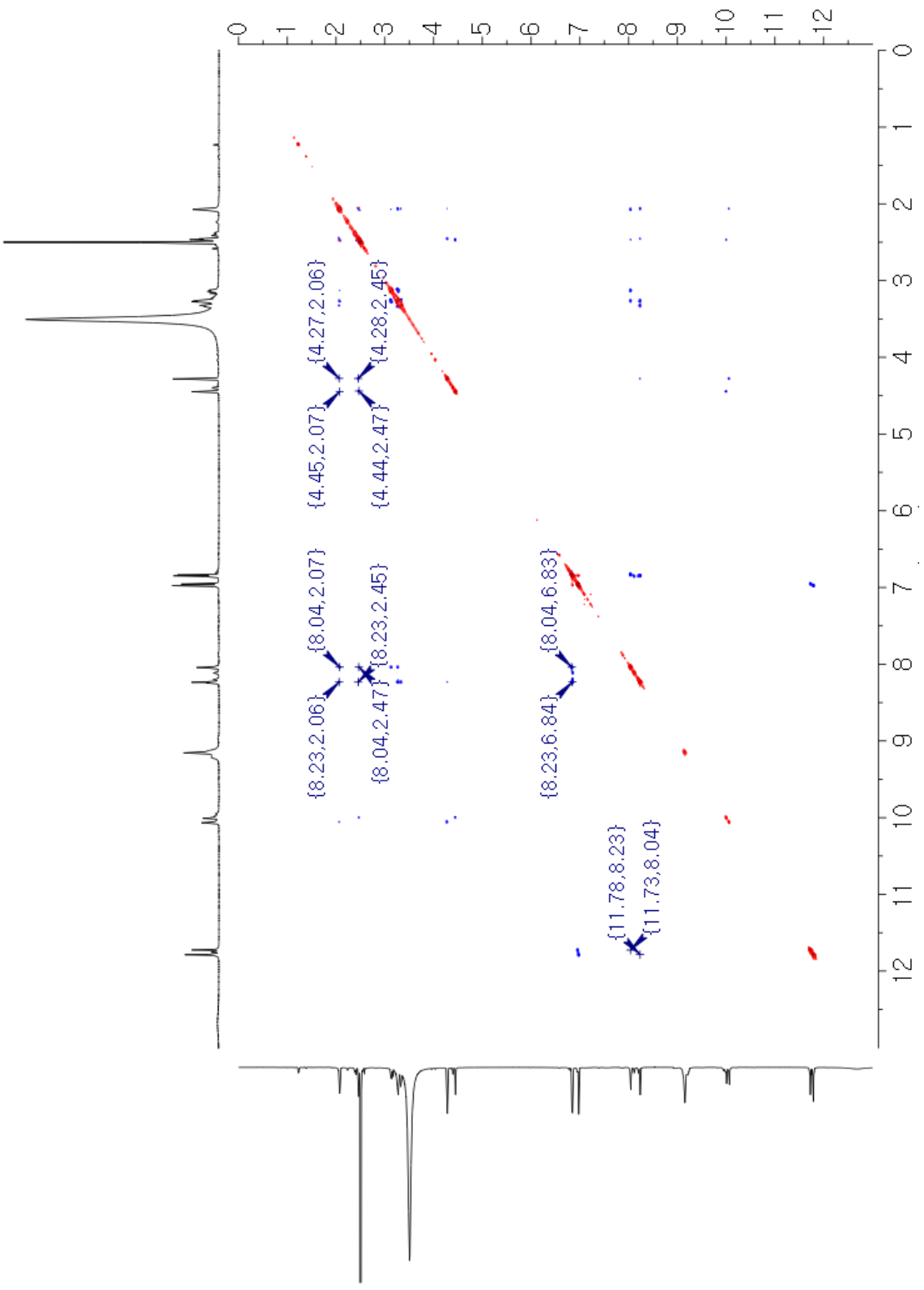


Figure S6. The ROESY (600 MHz, DMSO-d_6) spectrum of **1**

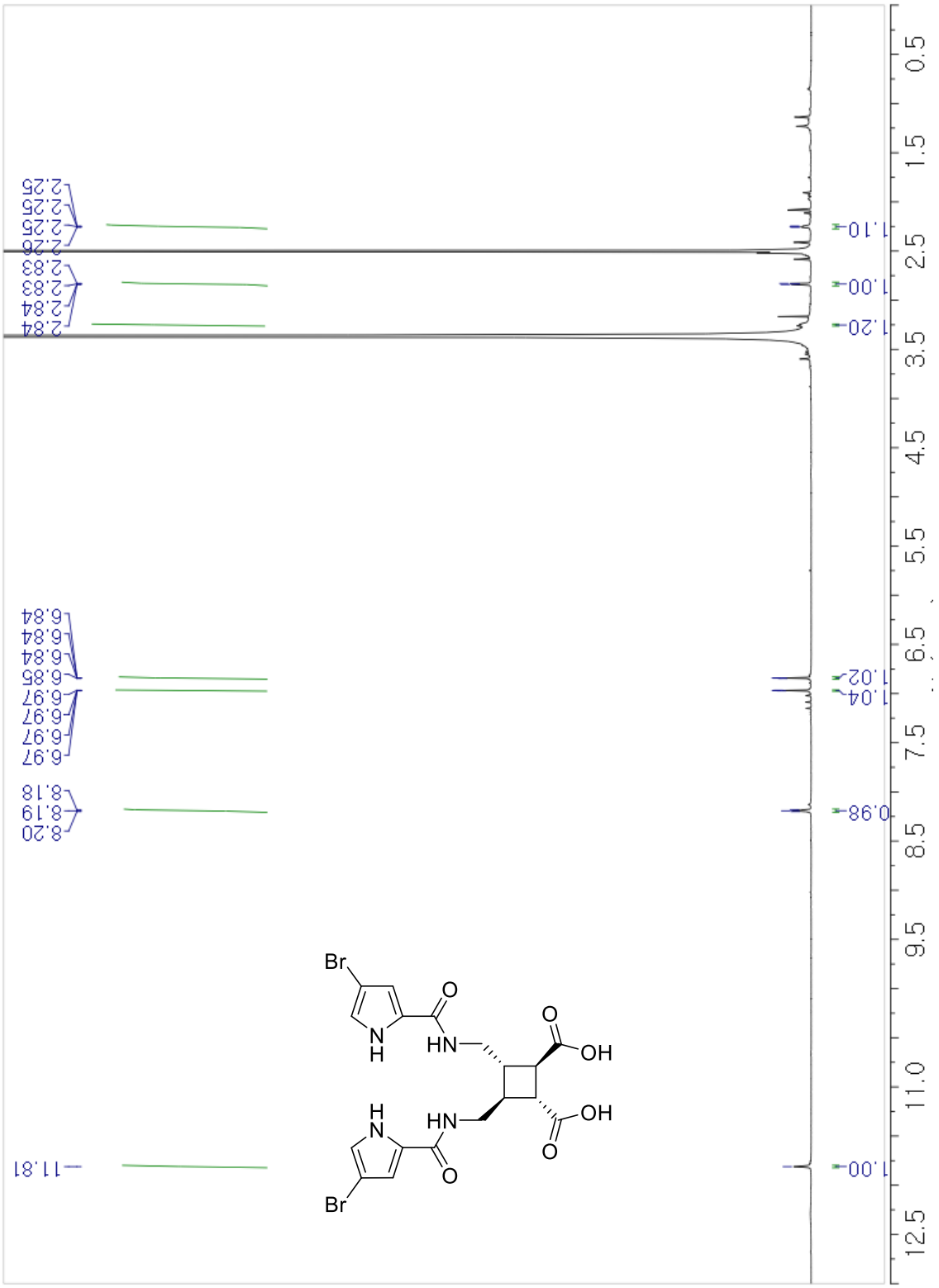


Figure S7. The ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **2**

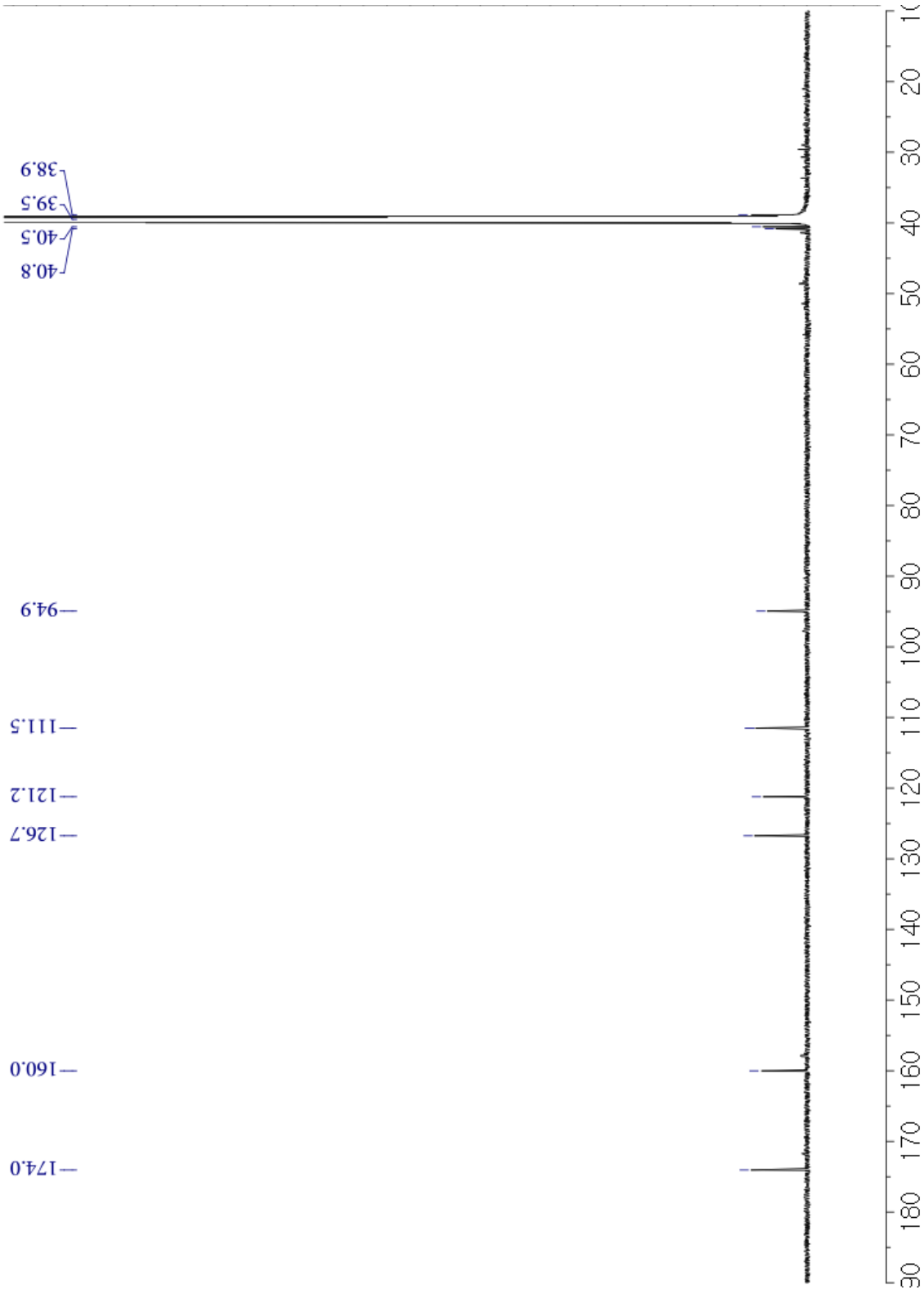


Figure S8. The ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **2**

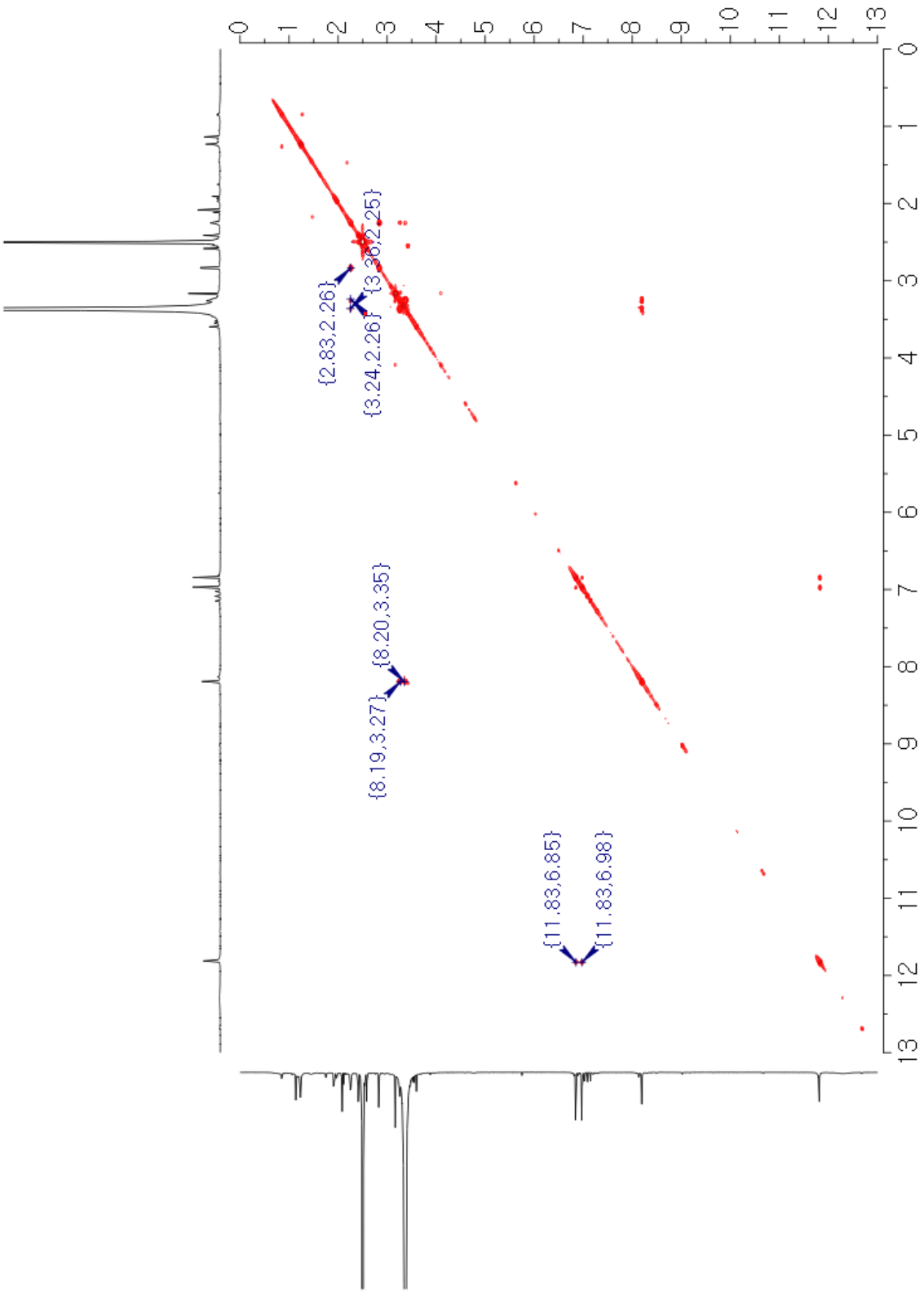


Figure S9. The COSY (600 MHz, DMSO-d_6) spectrum of **2**

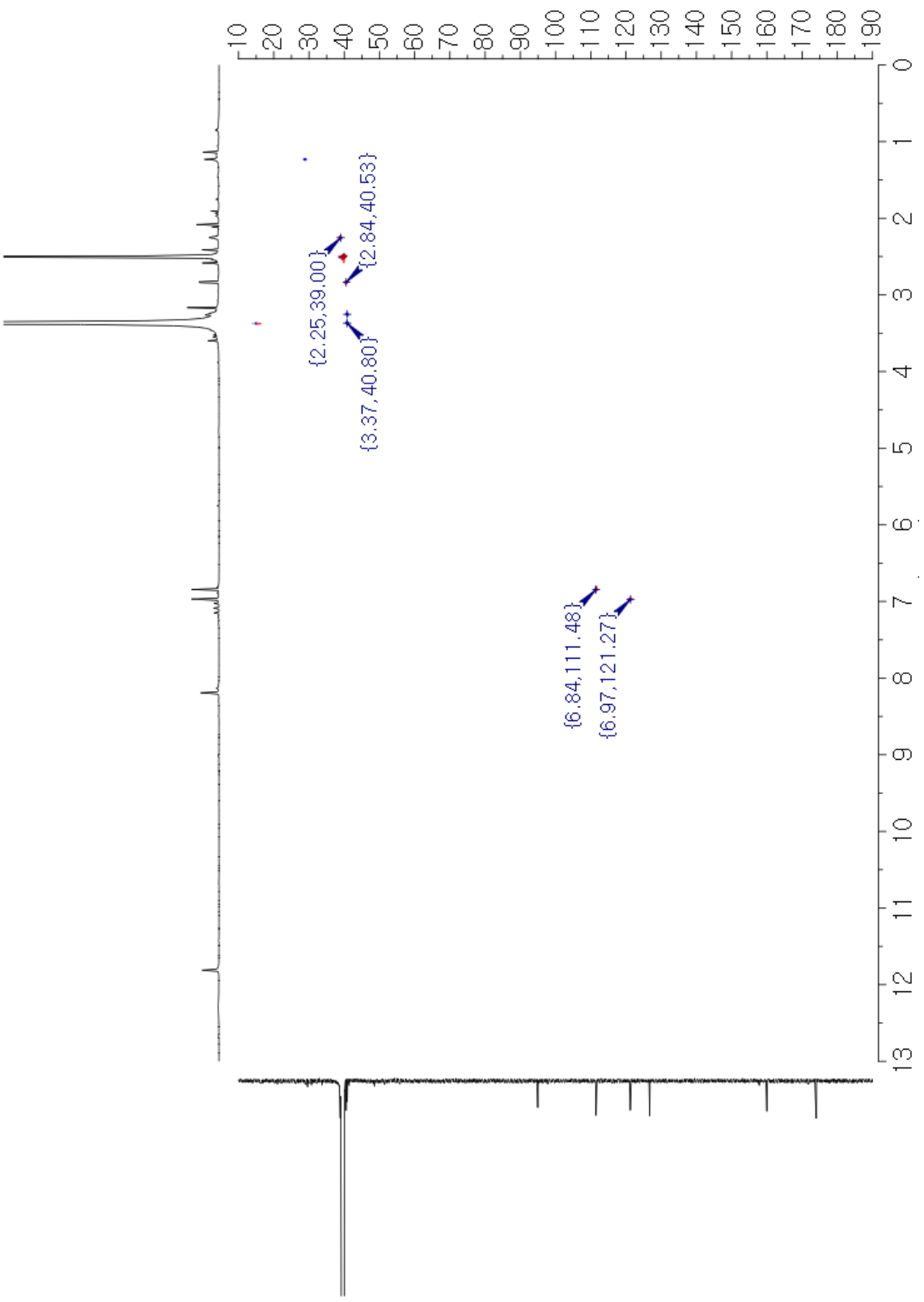


Figure S10. The eHSQC (600 MHz, DMSO-d_6) spectrum of **2**

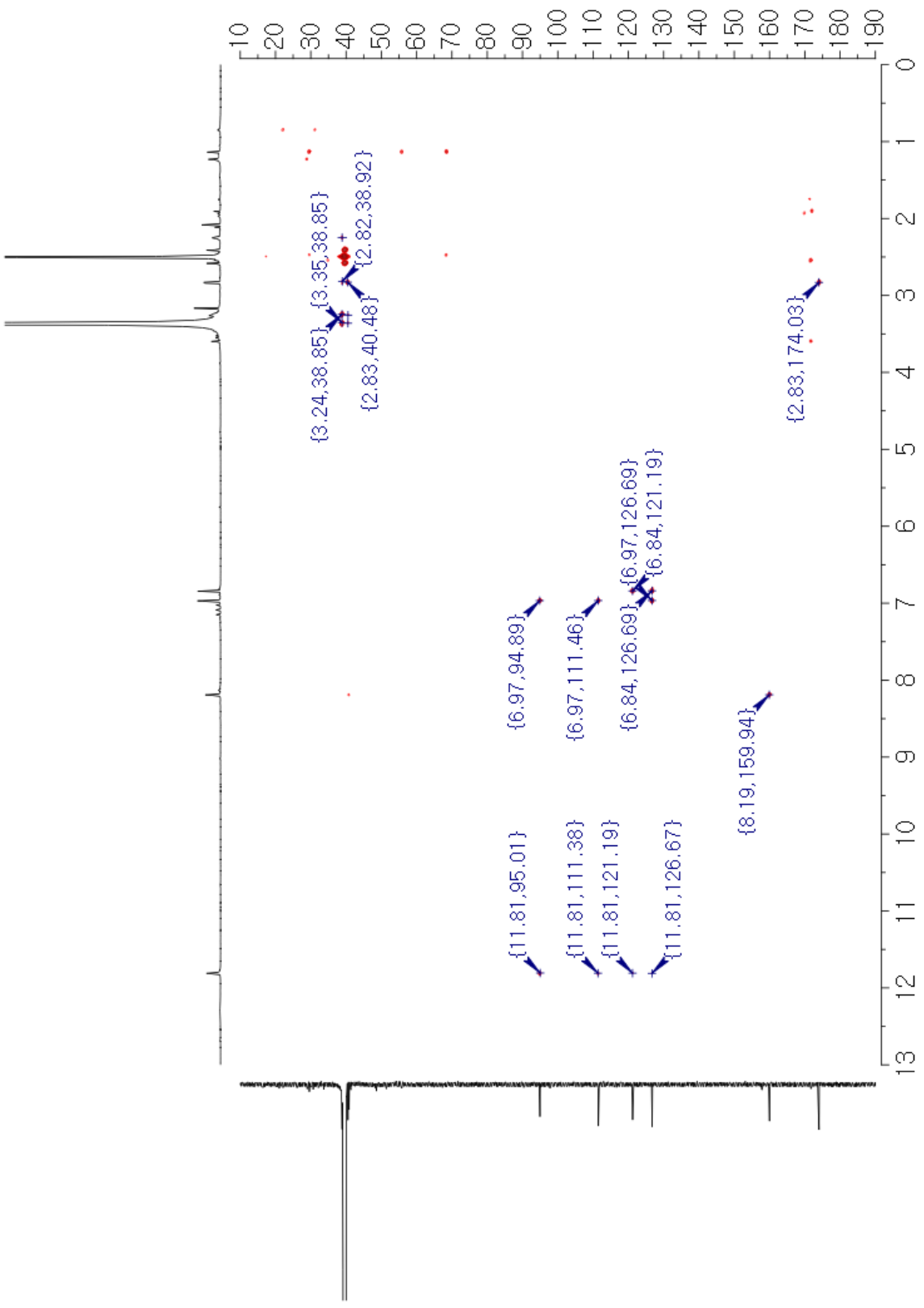


Figure S11. The HMBC (600 MHz, DMSO-d_6) spectrum of **2**

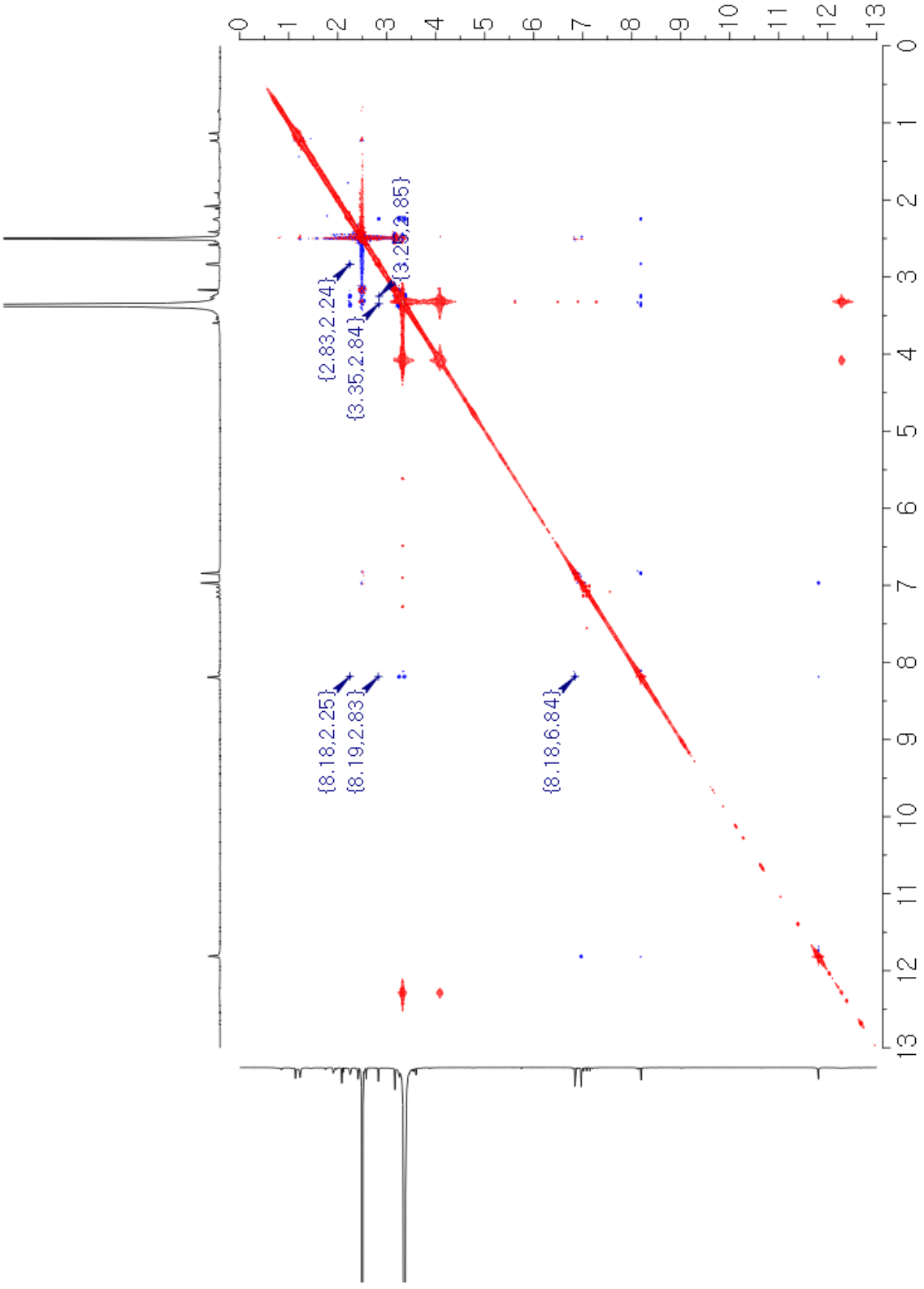


Figure S12. The ROESY (600 MHz, DMSO-d_6) spectrum of **2**

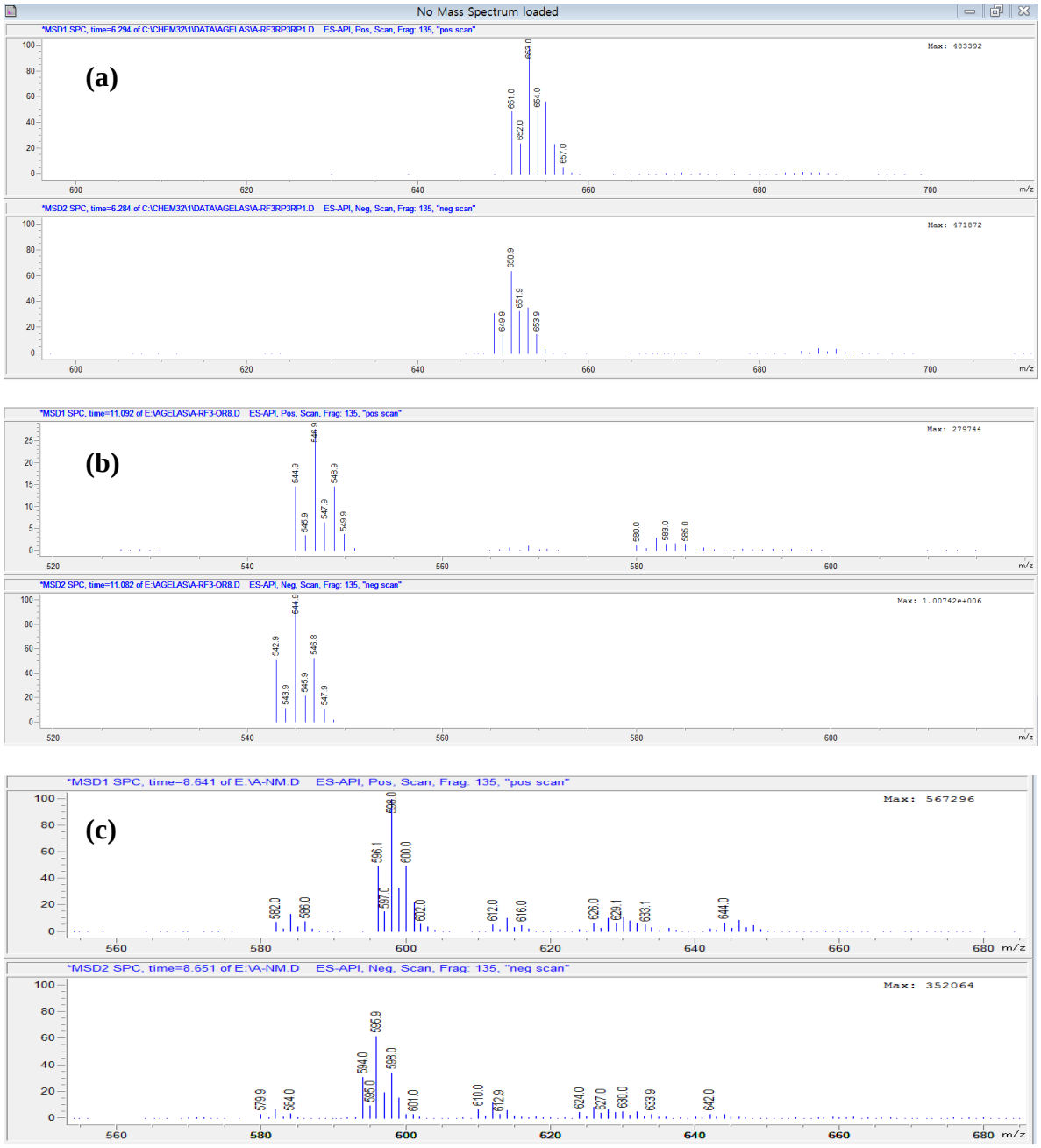
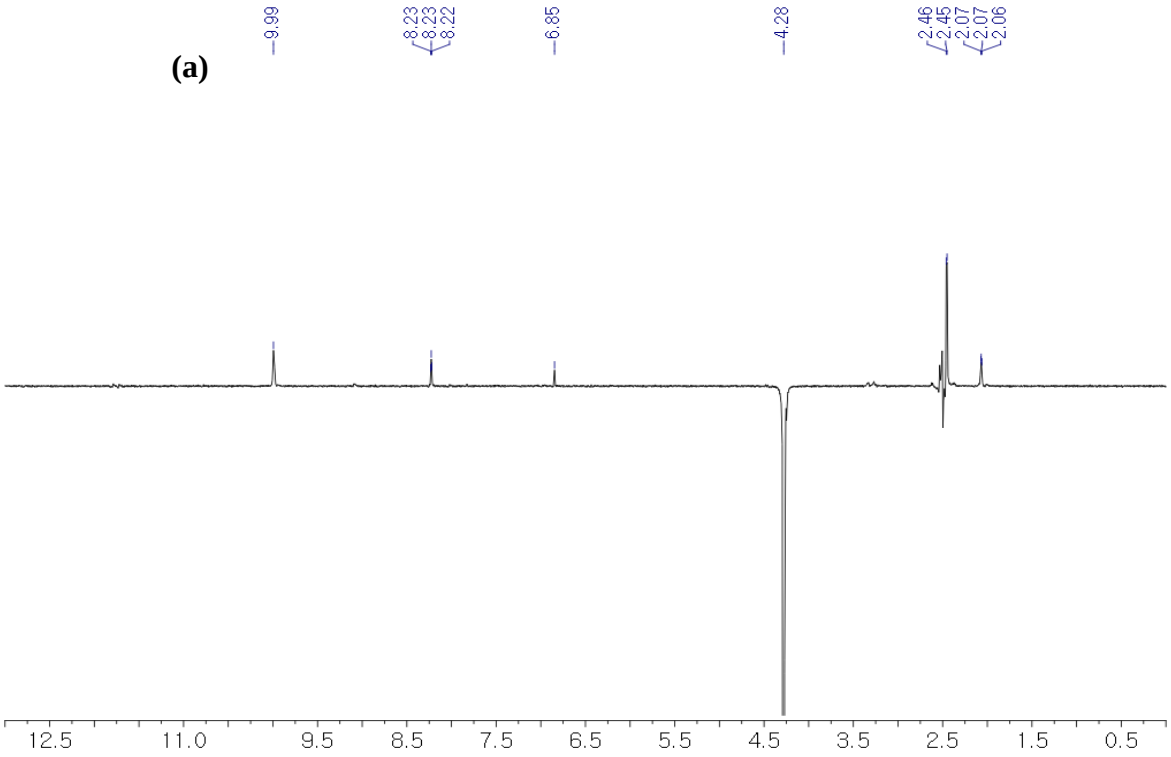
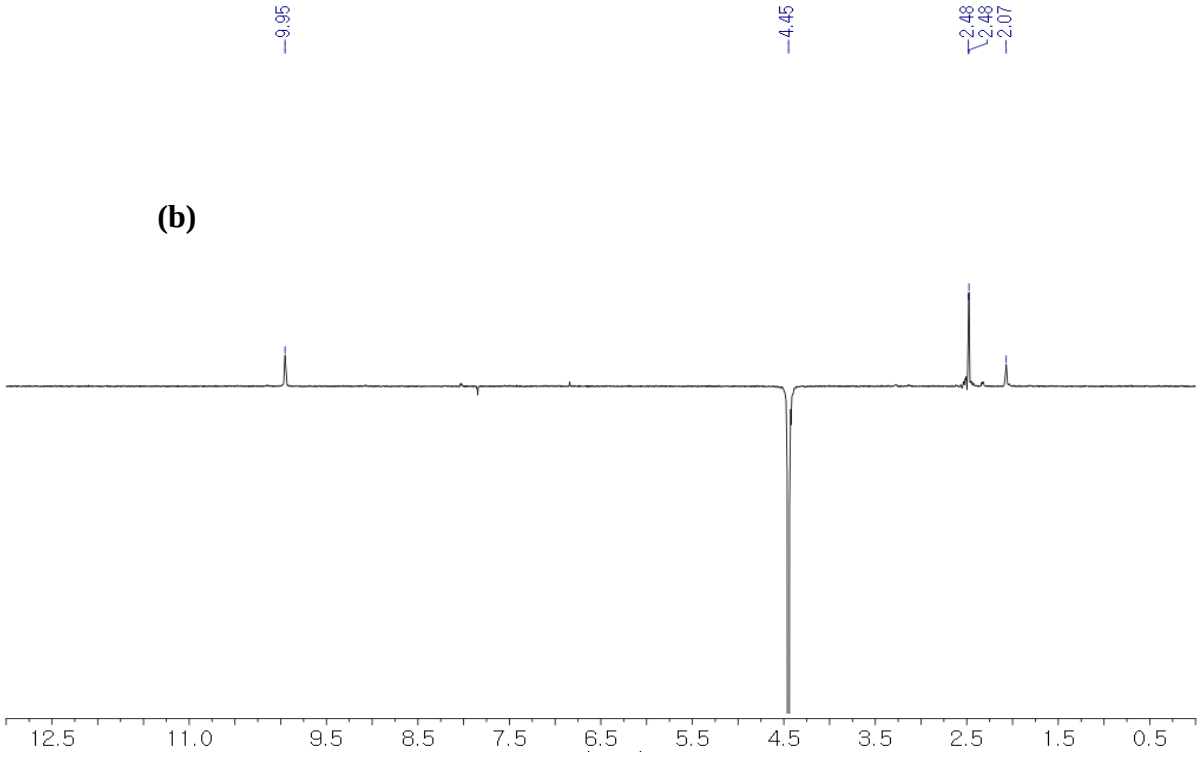


Figure S13. ESI/MS isotopic cluster patterns of compounds **1**, **2** and **6** ((a)-(c)) in positive and negative ion modes

(a)


9.99
8.23
8.23
8.22
6.85
4.28
2.46
2.45
2.07
2.07
2.06
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

(b)


9.95
4.45
2.48
2.48
2.07
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

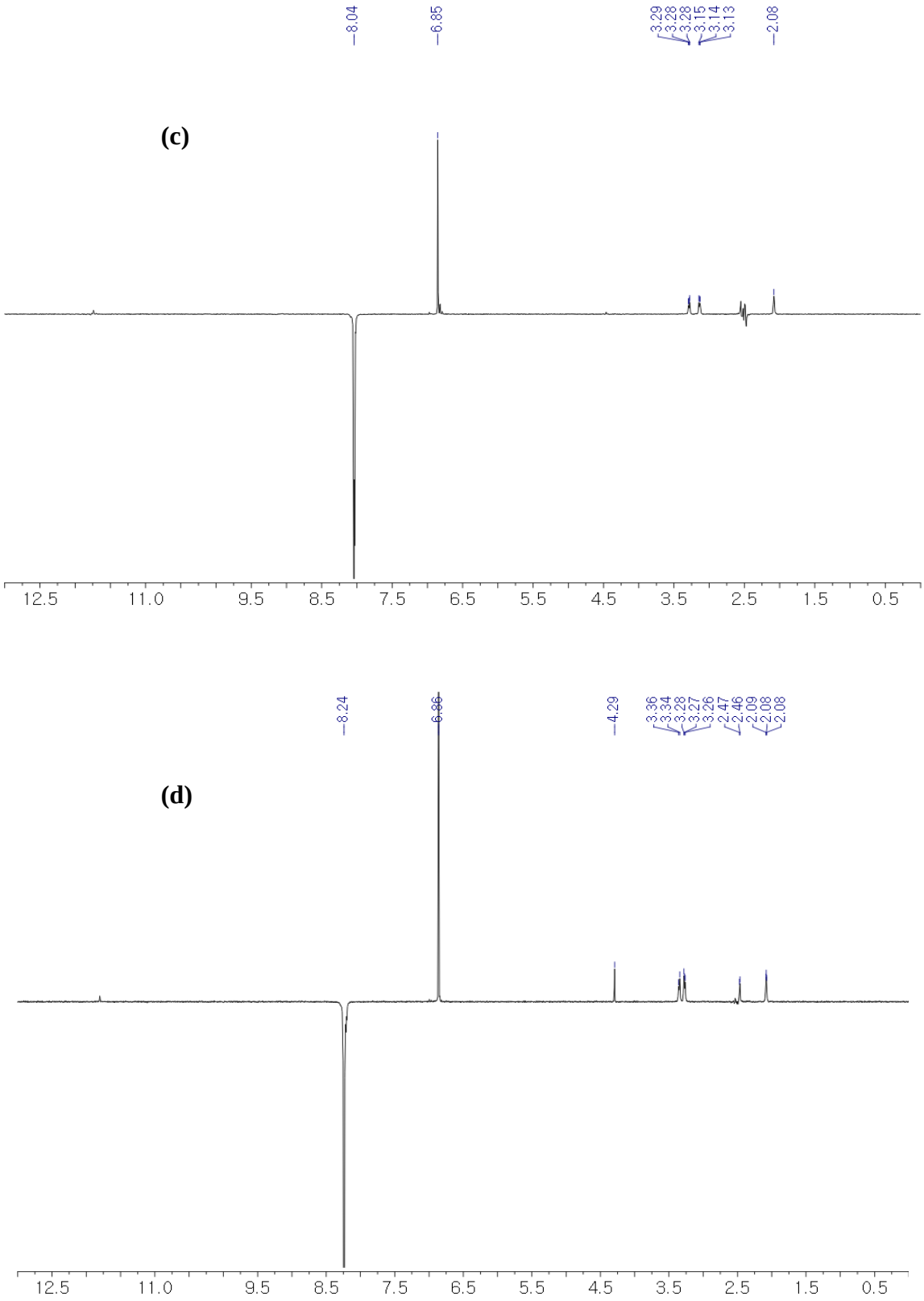
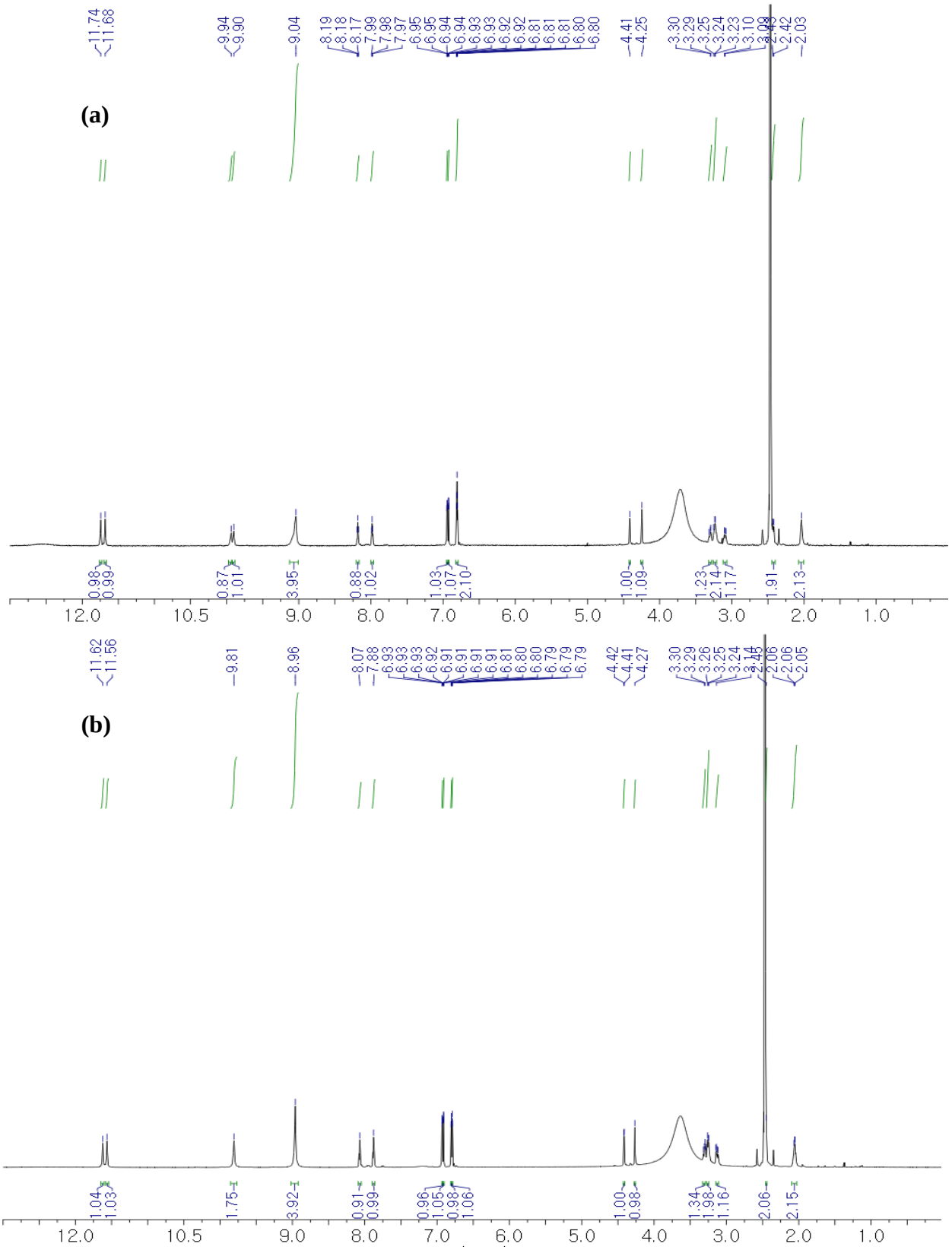
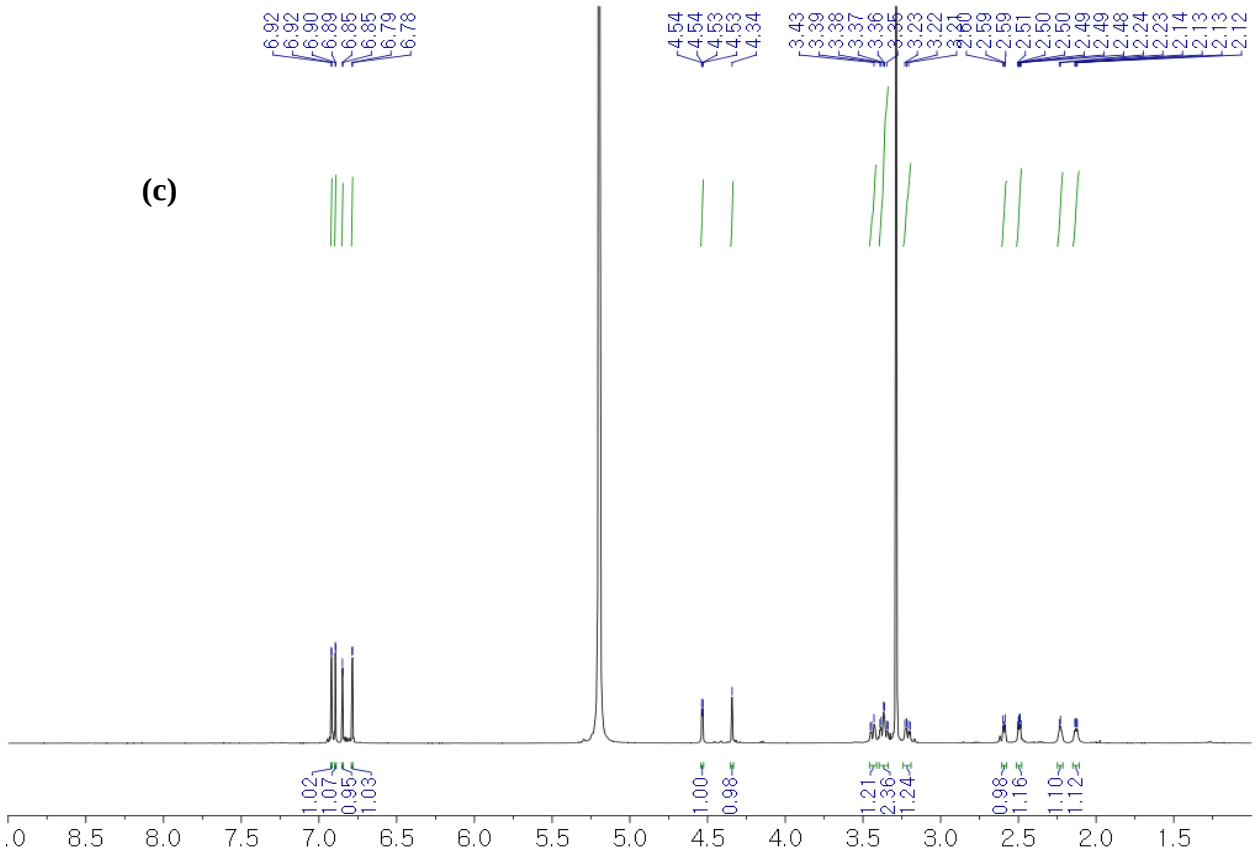
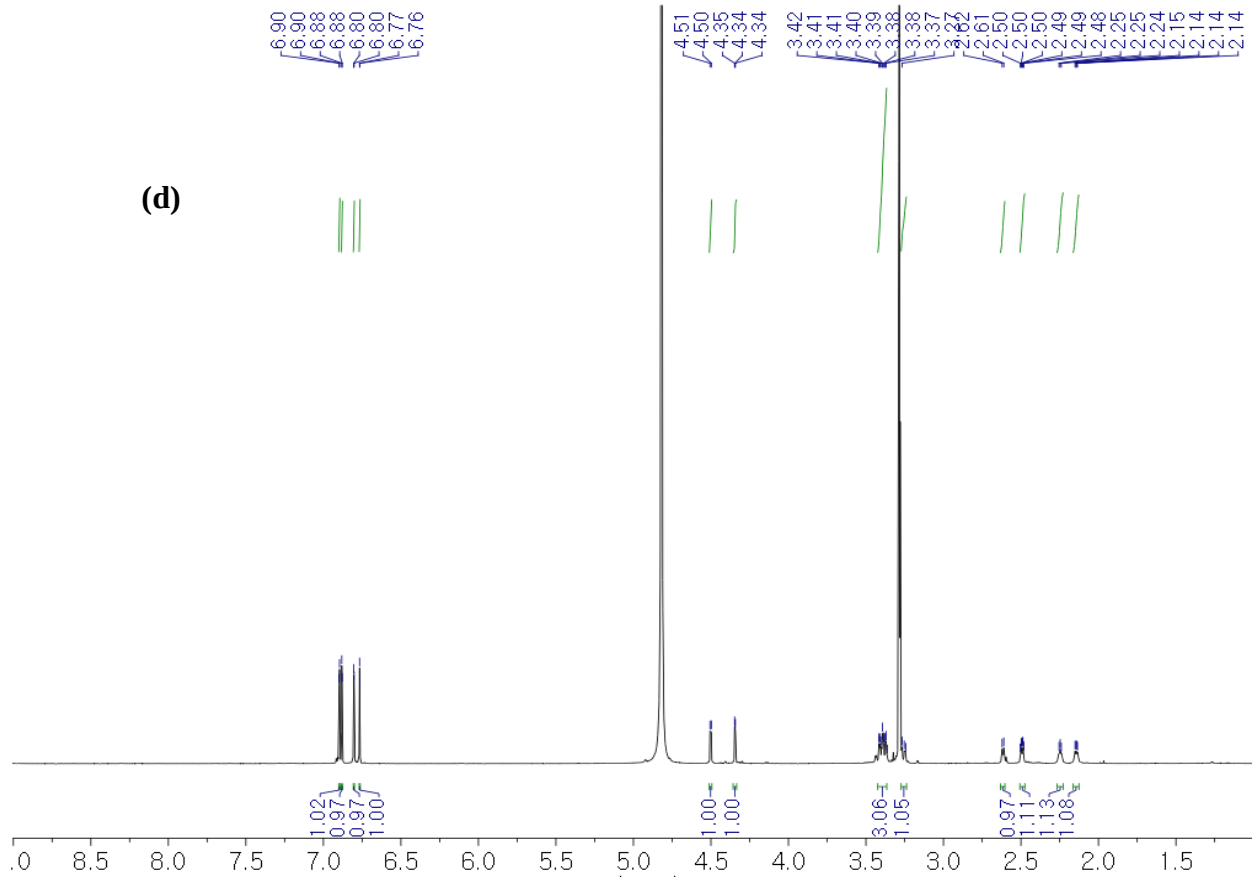


Figure S14. 1D selective gradient ROESY experiments (600 MHz, DMSO-d_6) of **1**: Irradiation of the protons at δ_H 4.28, 4.45, 8.04, and 8.24 for (a)-(d), respectively.


(a)
11.74
11.68
9.94
9.90
9.04
8.19
8.18
8.17
7.99
7.98
7.97
6.95
6.95
6.94
6.94
6.93
6.93
6.92
6.92
6.81
6.81
6.80
6.80
4.41
4.25
3.30
3.29
3.25
3.24
3.23
3.10
2.43
2.42
2.03
0.98
0.99
0.87
1.01
3.95
0.88
1.02
1.03
1.07
2.10
1.00
1.09
1.23
2.14
1.17
1.91
2.13
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(b)
11.62
11.56
9.81
8.96
8.07
7.88
6.93
6.93
6.93
6.92
6.91
6.91
6.91
6.91
6.81
6.80
6.80
6.79
6.79
6.79
4.42
4.41
4.27
3.30
3.29
3.26
3.25
3.24
2.06
2.06
2.05
1.04
1.03
1.75
3.92
0.91
0.99
0.96
1.05
0.98
1.06
1.00
0.98
1.34
1.98
1.16
2.06
2.15
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0


(c)
6.92
6.92
6.90
6.89
6.85
6.85
6.79
6.78
4.54
4.54
4.53
4.53
4.34
3.43
3.39
3.38
3.37
3.36
3.35
3.23
3.22
2.60
2.59
2.59
2.51
2.50
2.50
2.49
2.49
2.48
2.24
2.23
2.14
2.13
2.13
2.12
1.02
1.07
0.95
1.03
1.00
0.98
1.21
2.36
1.24
0.98
1.16
1.10
1.12
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5


(d)
6.90
6.90
6.88
6.88
6.80
6.80
6.77
6.76
4.51
4.50
4.35
4.34
4.34
3.42
3.41
3.41
3.40
3.39
3.38
3.38
3.37
2.61
2.50
2.50
2.50
2.49
2.49
2.48
2.25
2.25
2.24
2.15
2.14
2.14
2.14
1.02
0.97
0.97
1.00
1.00
1.00
3.06
1.05
0.97
1.11
1.13
1.08
.0
8.5
8.0
7.5
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4.0
3.5
3.0
2.5
2.0
1.5

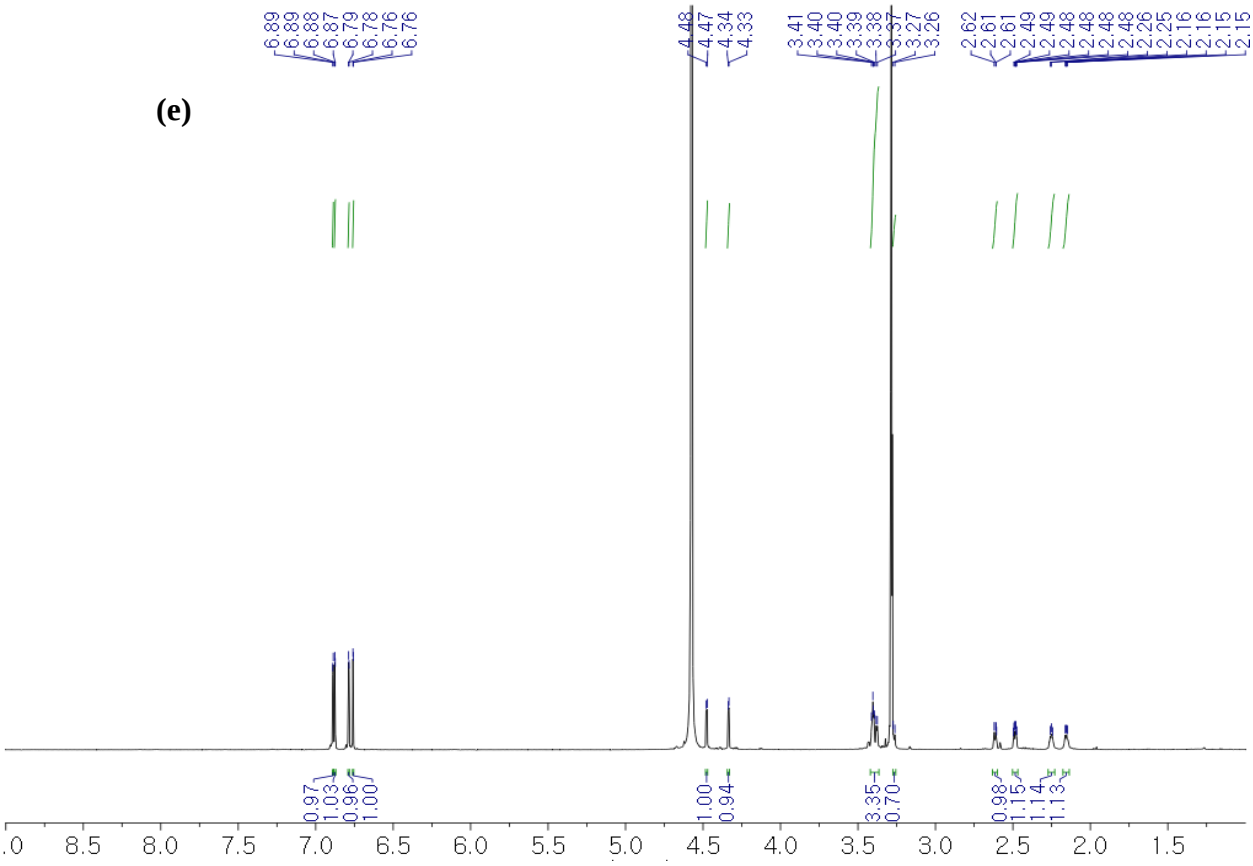

Figure S15. The variable temperature NMR experiments (DMSO-d_6) of **1**: (a) +25 ˚C and (b) +50 ˚C (MeOH-d_4) of **1**: (c) -15 ˚C, (d) +25 ˚C, and (e) +50 ˚C

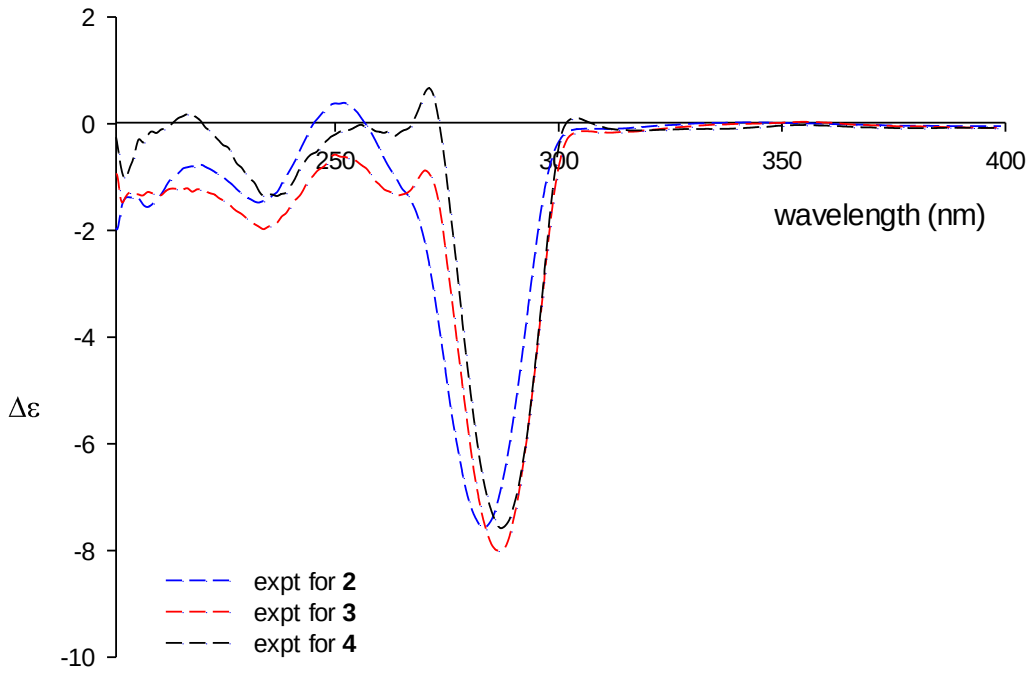

Figure S16. The CD spectra of **2-4**

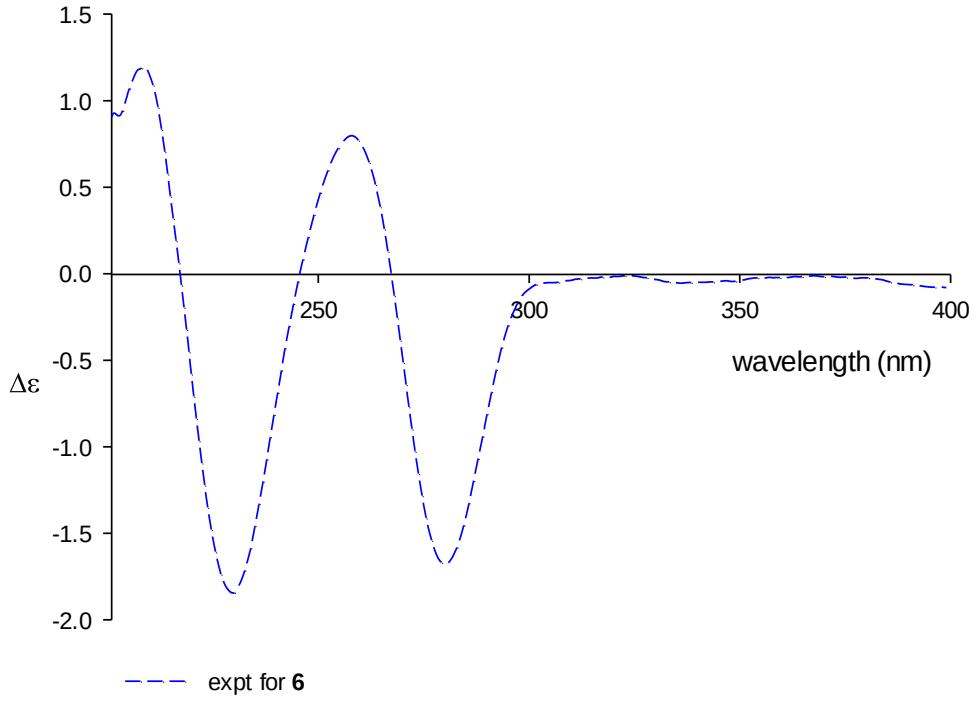

Figure S17. The CD spectrum of **6**