

**Supporting Information: Neopetrosiquinones A and B, Sesquiterpene Benzoquinones Isolated from a Deep-water Sponge *Neopetrosia cf. proxima***

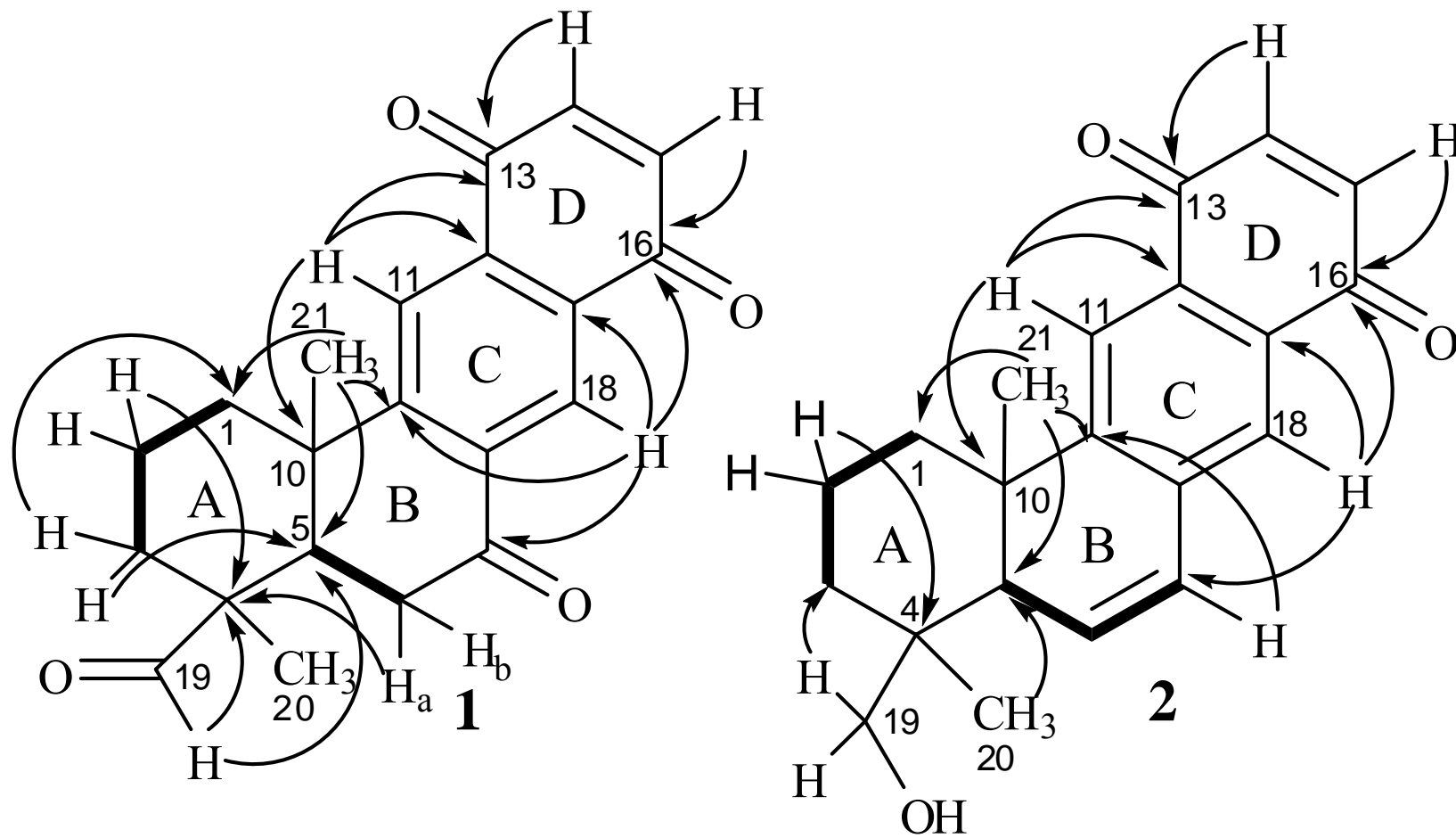
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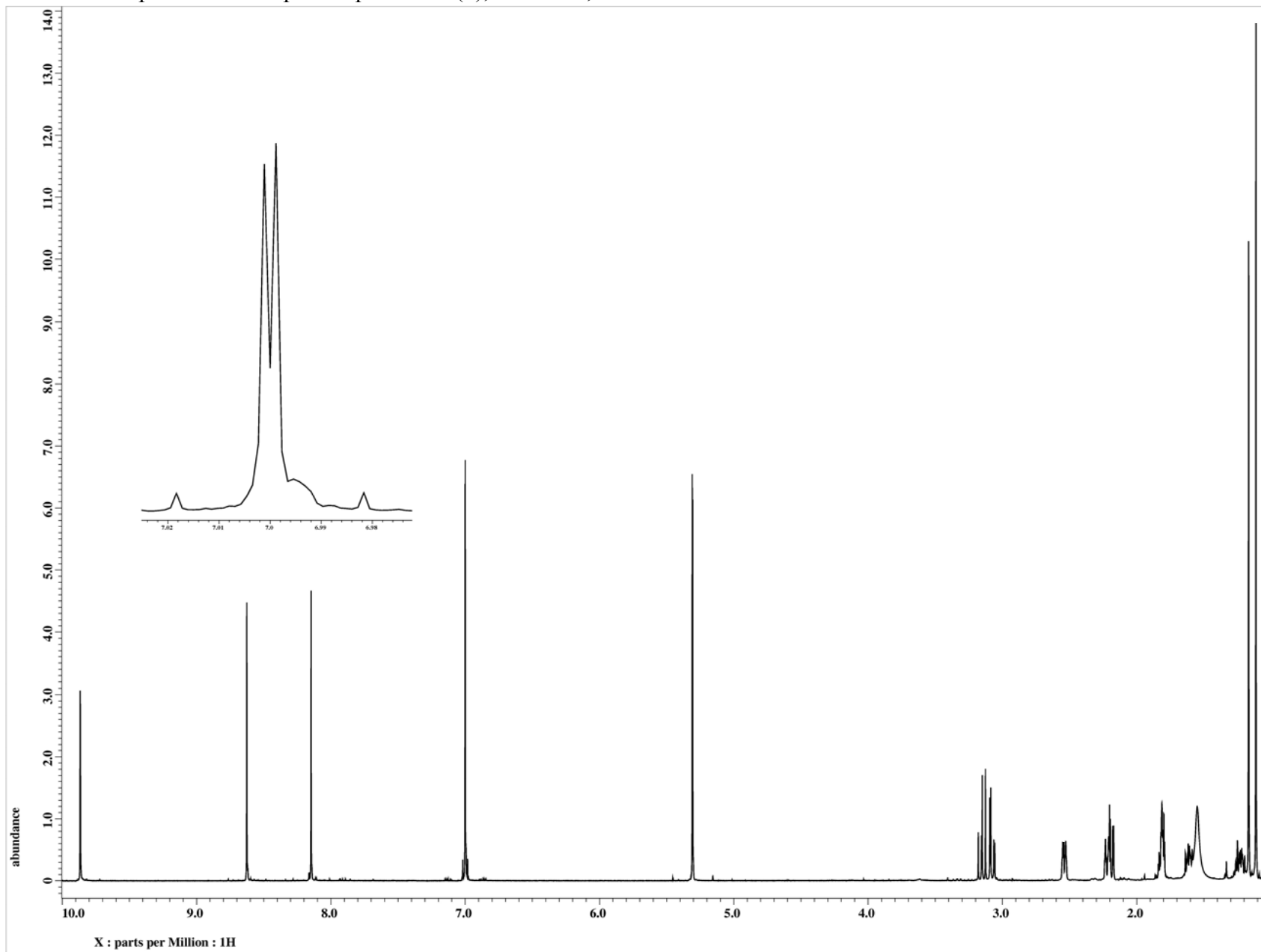
<sup>2</sup> Museo Marino de Margarita, Nueva Esparta, Venezuela

- S1: Planar structure of neopetrosiquinone A (**1**) and B (**2**) derived from gDQF-COSY and key gHMBC correlations, 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>
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- S3: Expansion of <sup>1</sup>H NMR spectrum of neopetrosiquinone A (**1**), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>
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- S9: gHMBC spectrum of neopetrosiquinone A (**1**), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>
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- S25: <sup>1</sup>H and <sup>13</sup>C NMR Data for neopetrosiquinone B (**2**)
- S26: Structure of neopetrosiquinone B (**2**) with chemical shifts on structure

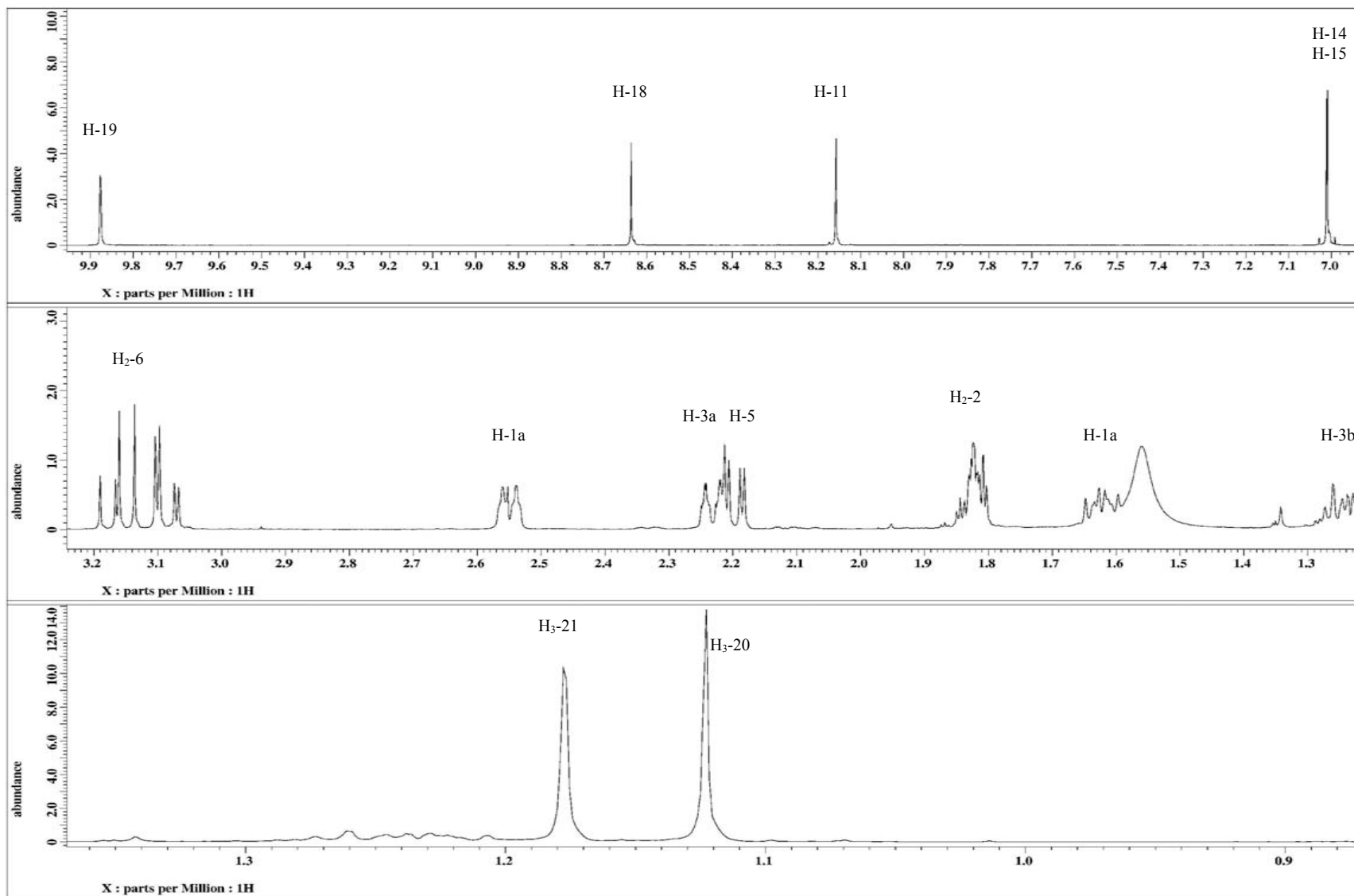
S1: Planar structure of neopetrosiquinones A (**1**) and B (**2**) derived from gDQF-COSY and key gHMBC correlations, 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



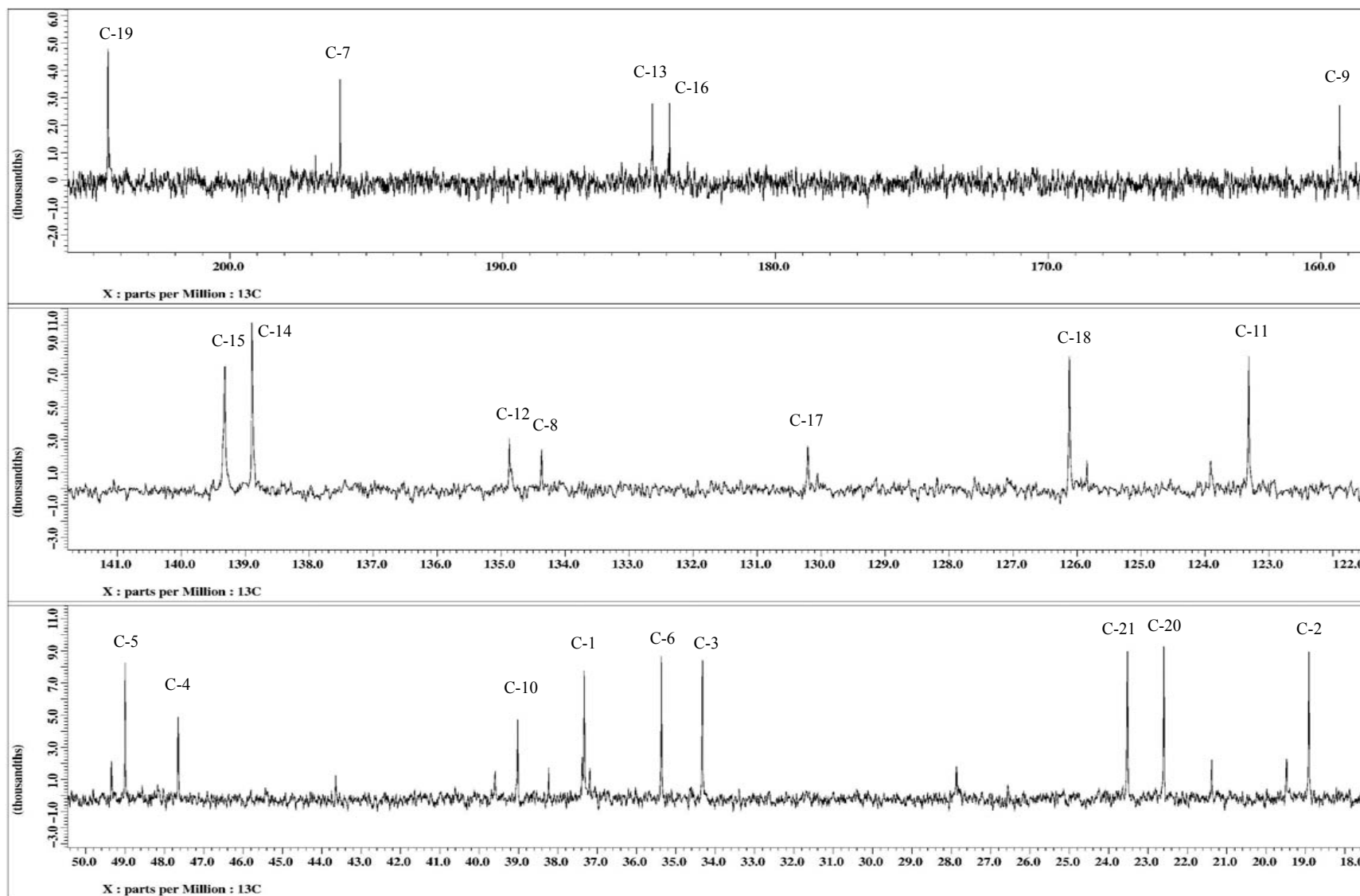
S2:  $^1\text{H}$  NMR spectrum of neopetrosiquinone A (**1**), 600 MHz,  $\text{CD}_2\text{Cl}_2$



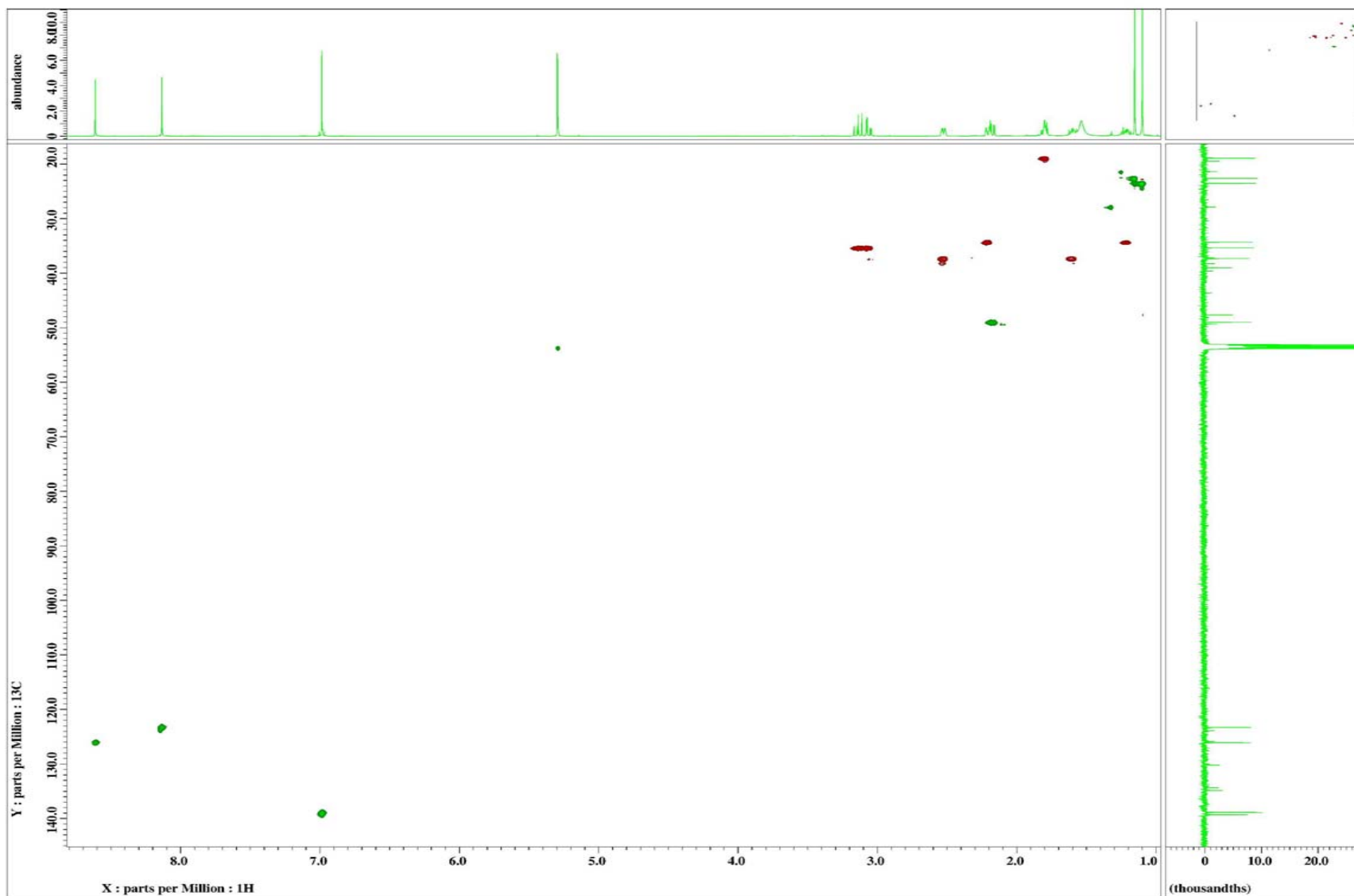
S3: Expansion of  $^1\text{H}$  NMR spectrum of neopetrosiquinone A (**1**), 600 MHz,  $\text{CD}_2\text{Cl}_2$



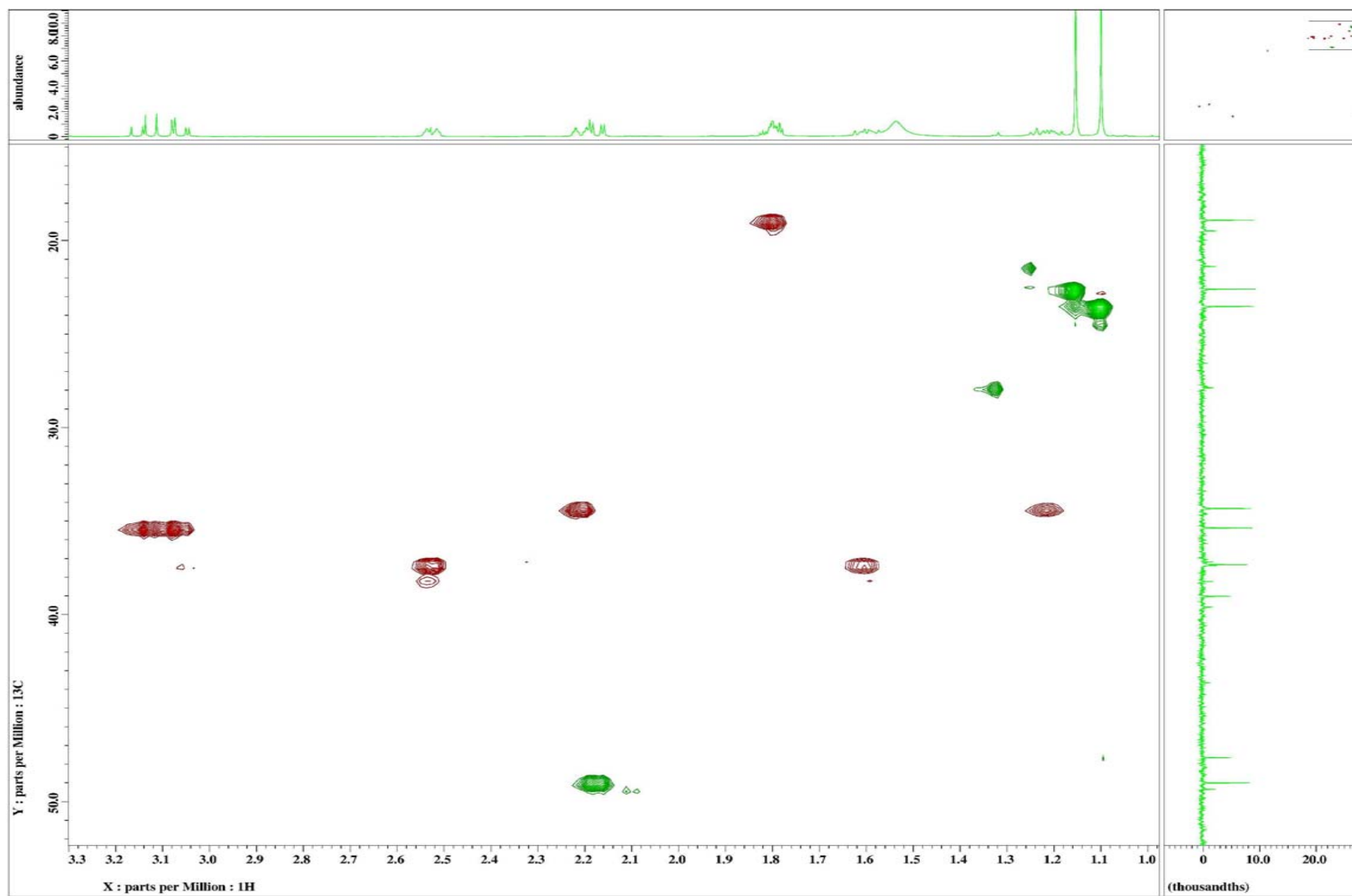
S4:  $^{13}\text{C}$  NMR spectrum of neopetrosiquinone A (**1**), 600 MHz,  $\text{CD}_2\text{Cl}_2$



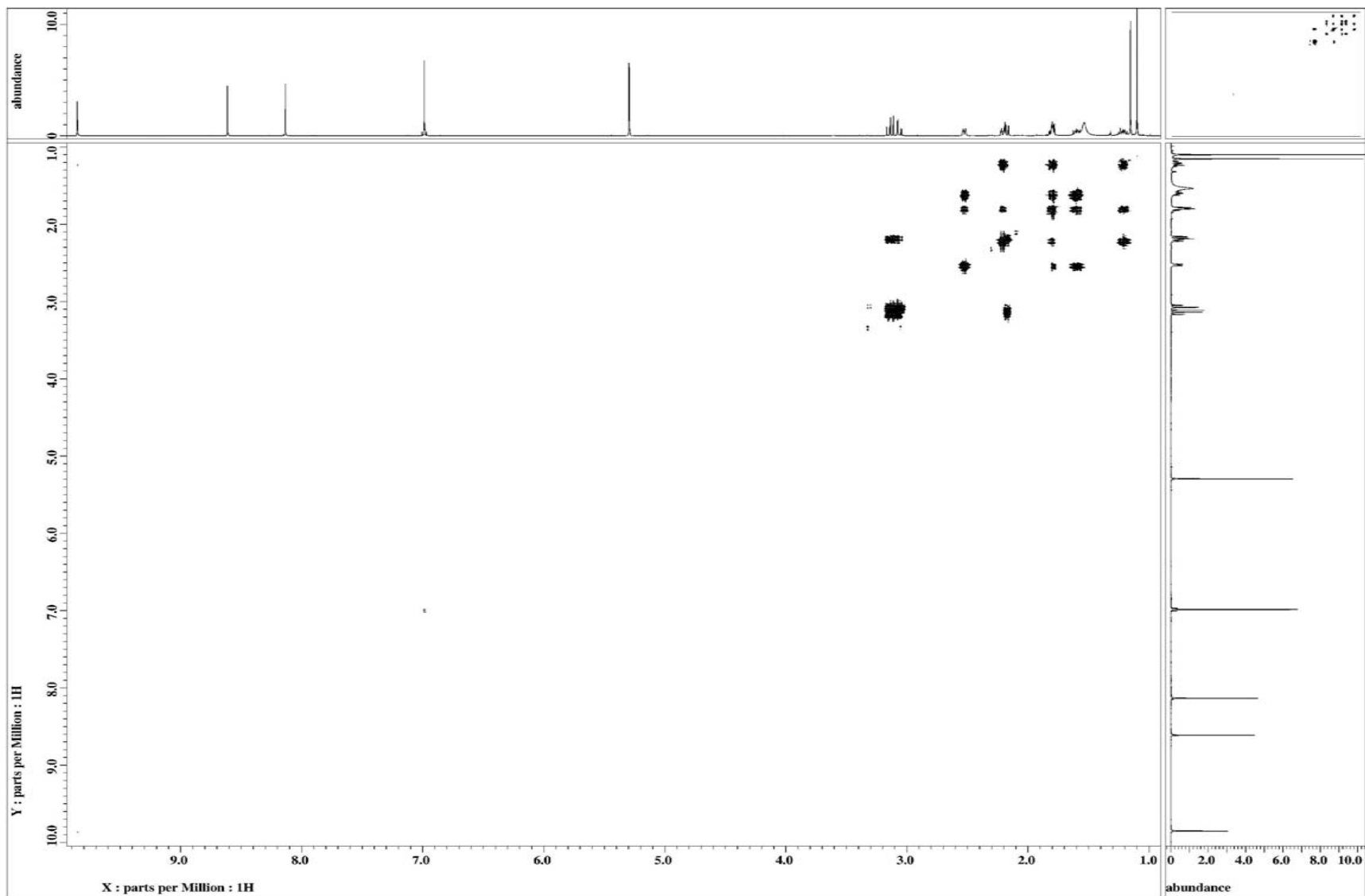
S5: edited gHSQC spectrum of neopetrosiquinone A (**1**), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



S6: Expansion of gHSQC spectrum of neopetrosiquinone A (**1**), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>

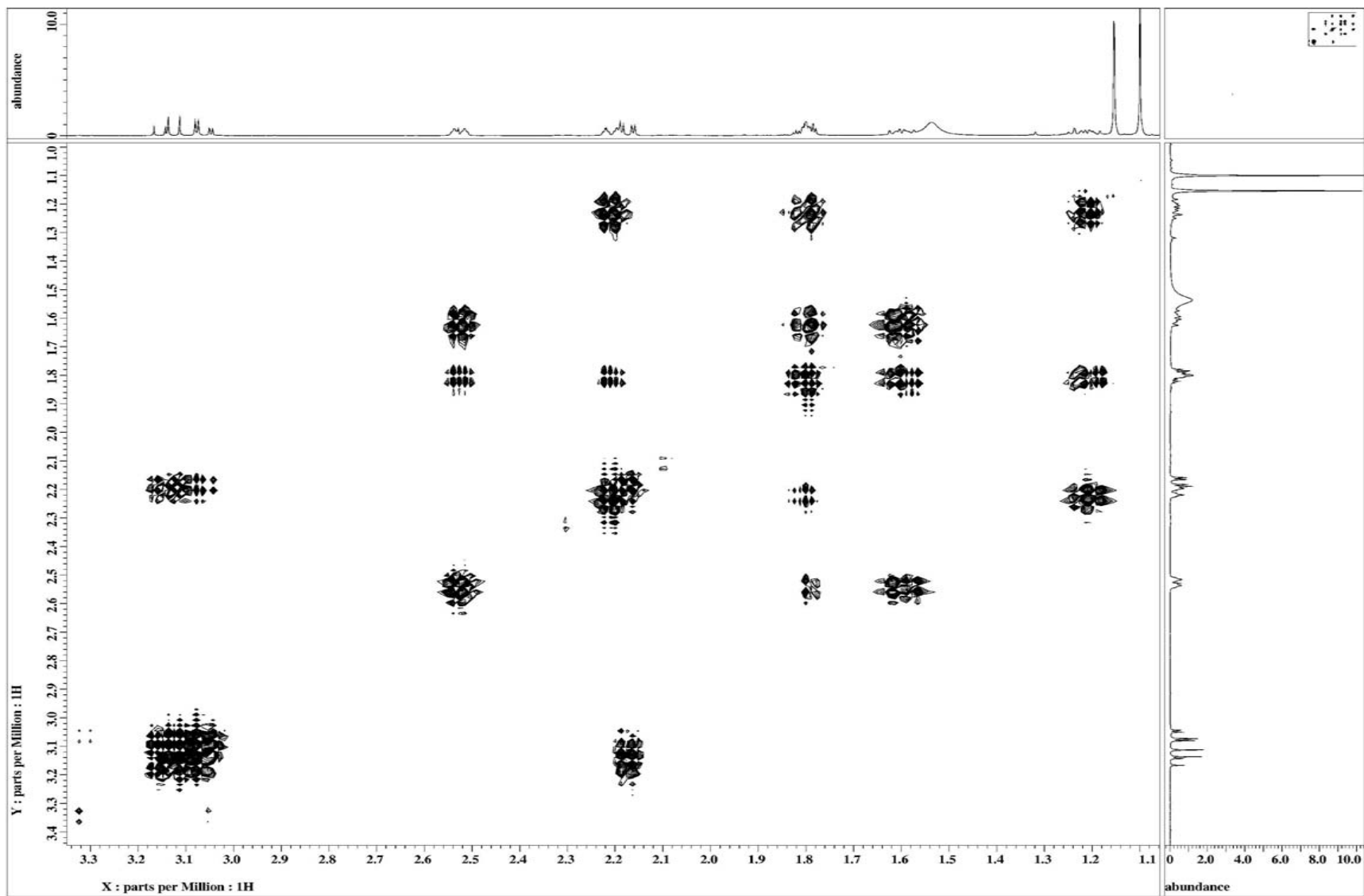


S7: gDQF-COSY spectrum of neopetrosiquinone A (1), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>

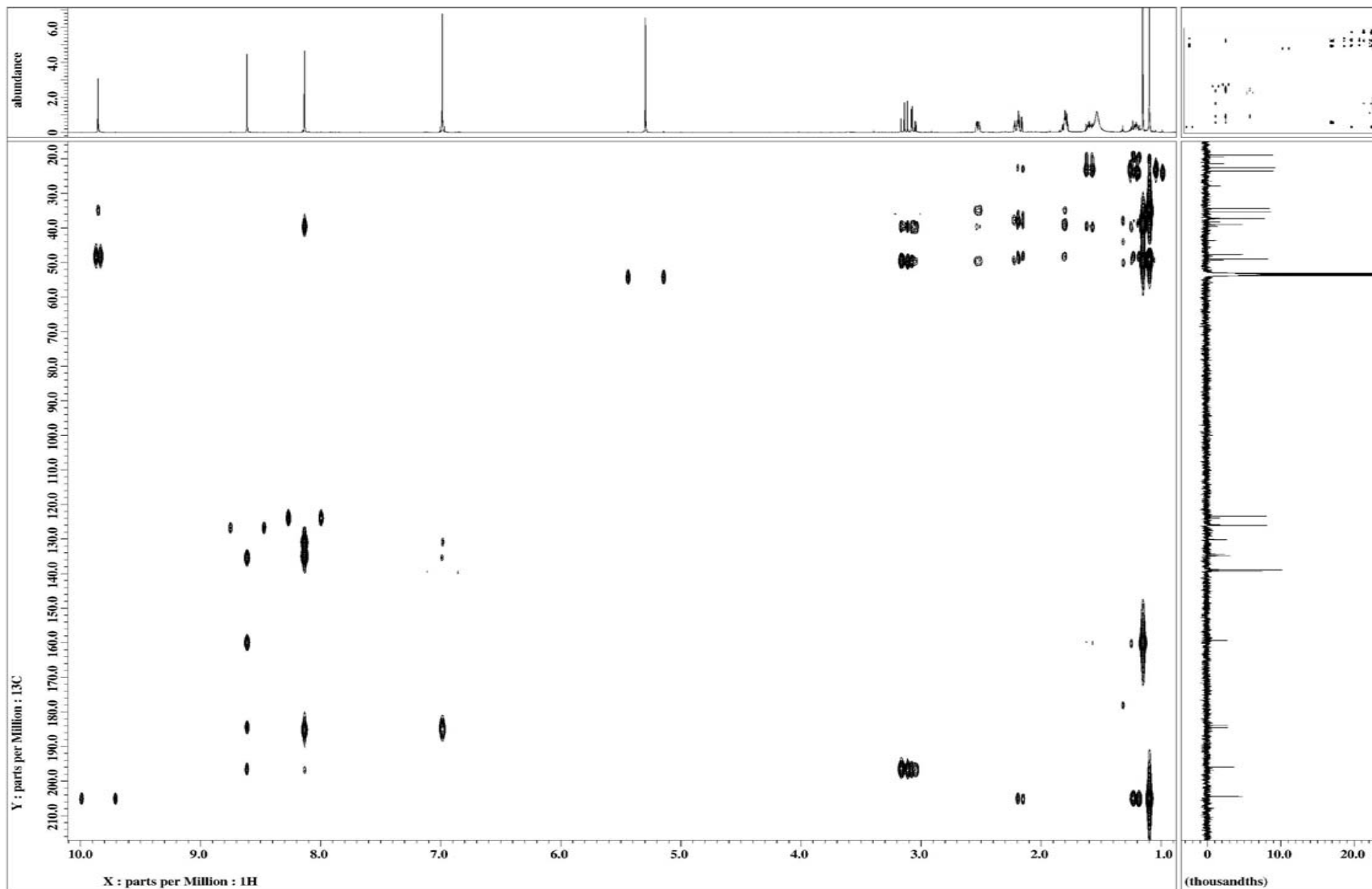




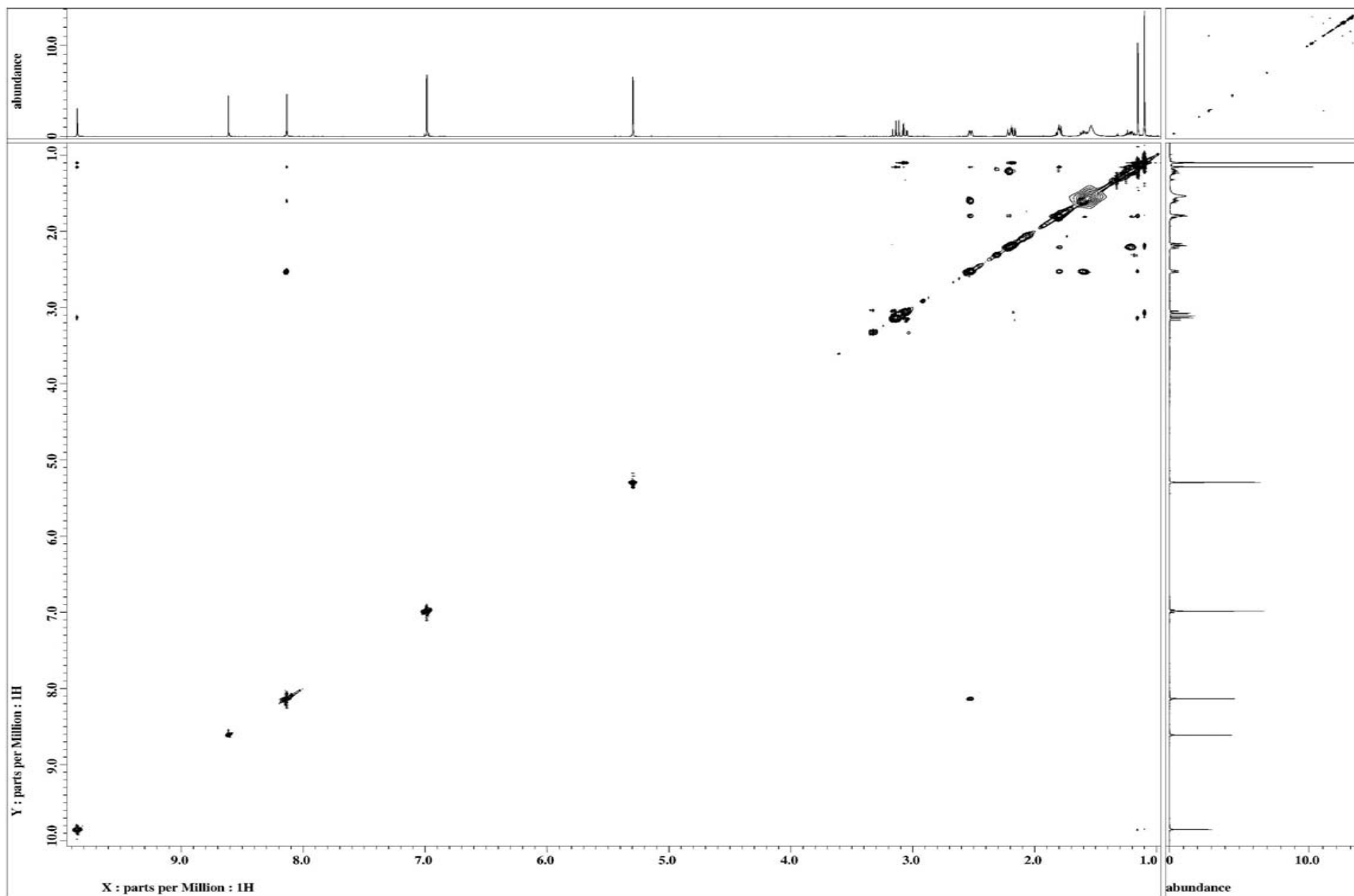
S8: Expansion of gDQF-COSY spectrum of neopetrosiquinone A (**1**), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



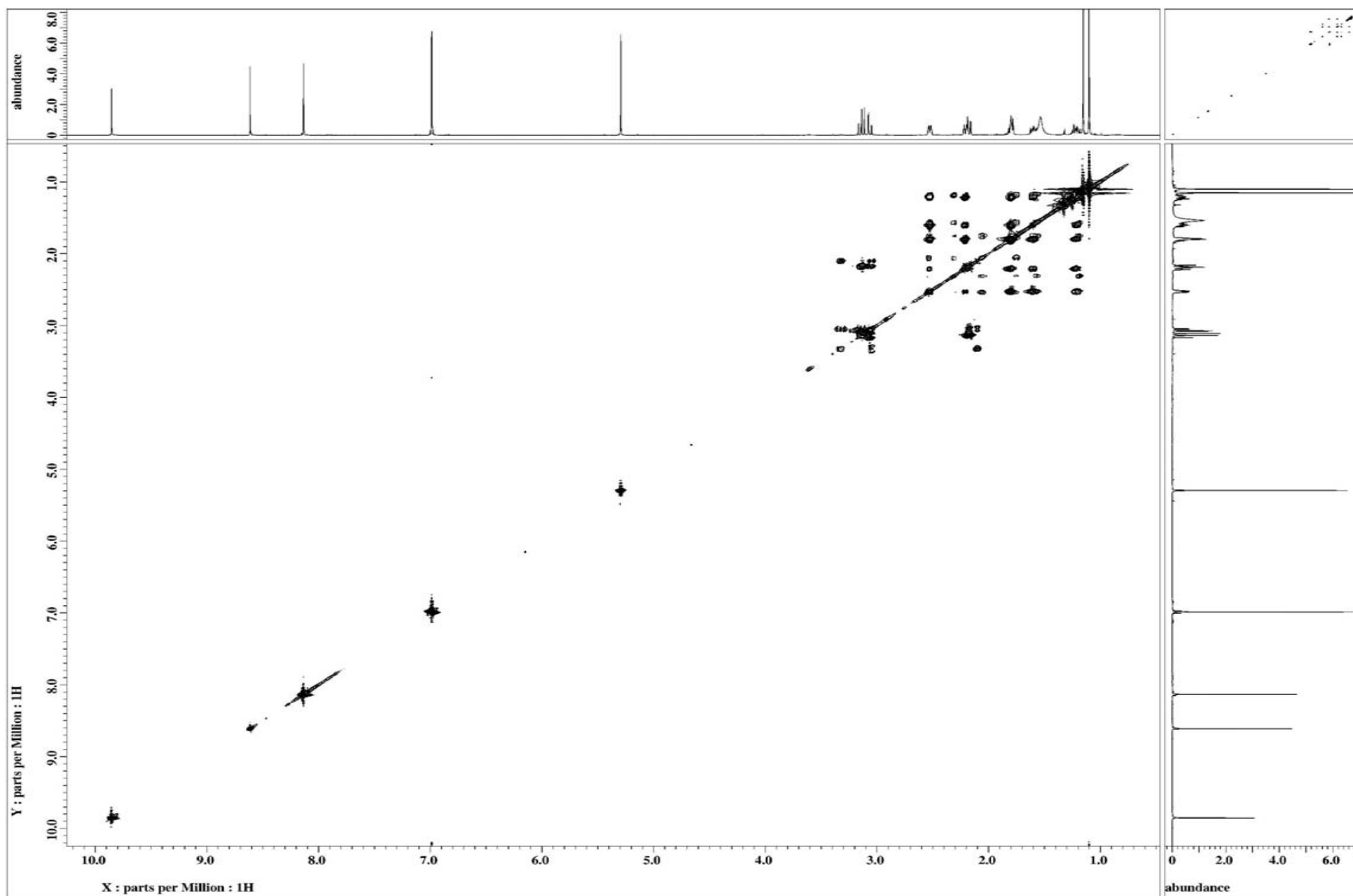
S9: gHMBC spectrum of neopetrosiquinone A (1), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



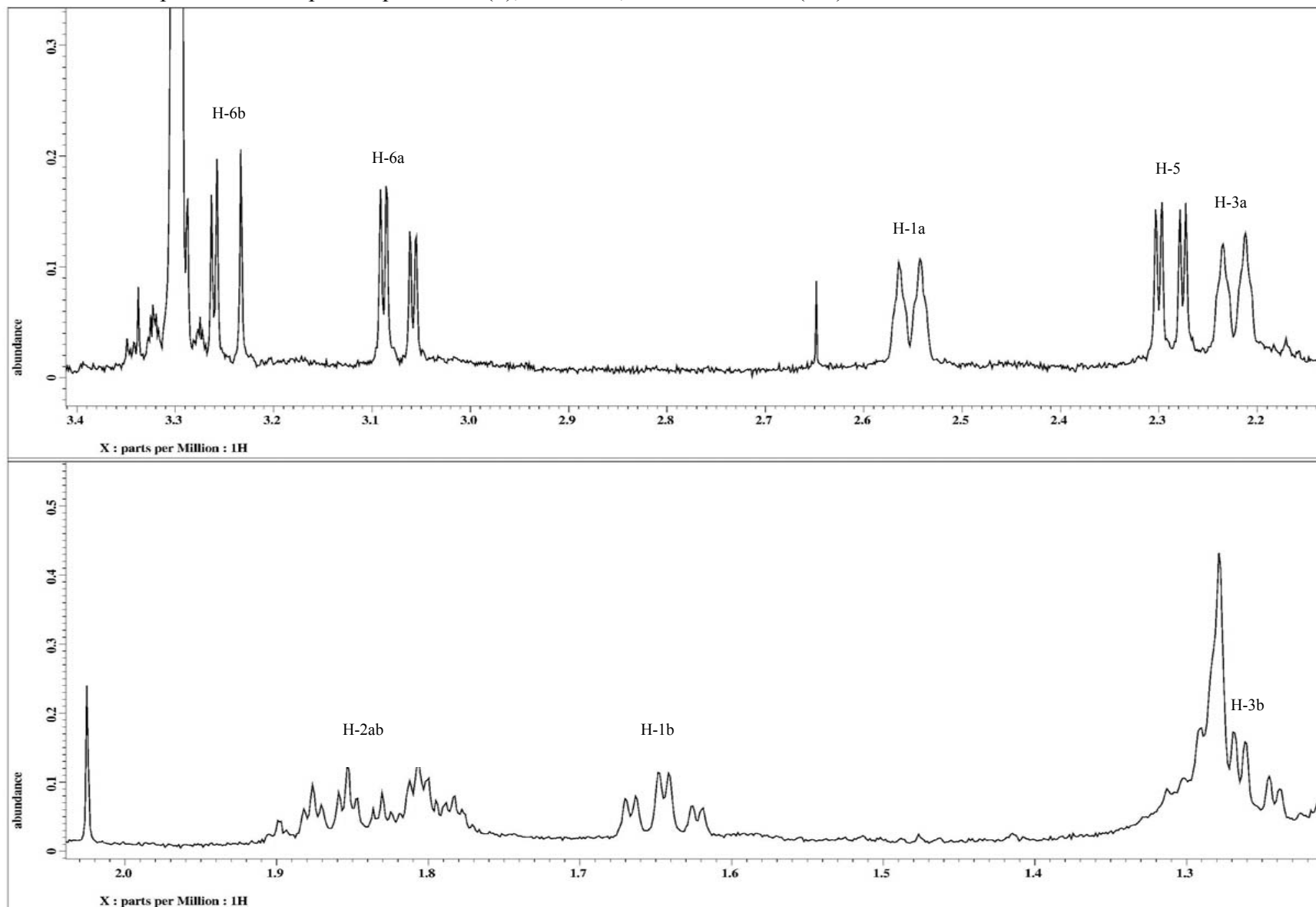
S10: NOESY spectrum of neopetrosiquinone A (1), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



S11: TOCSY spectrum of neopetrosiquinone A (1), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



S12:  $^1\text{H}$  NMR spectrum of neopetrosiquinone A (**1**), 600 MHz,  $\text{CH}_2\text{Cl}_2:\text{CD}_3\text{OD}$  (1:1)

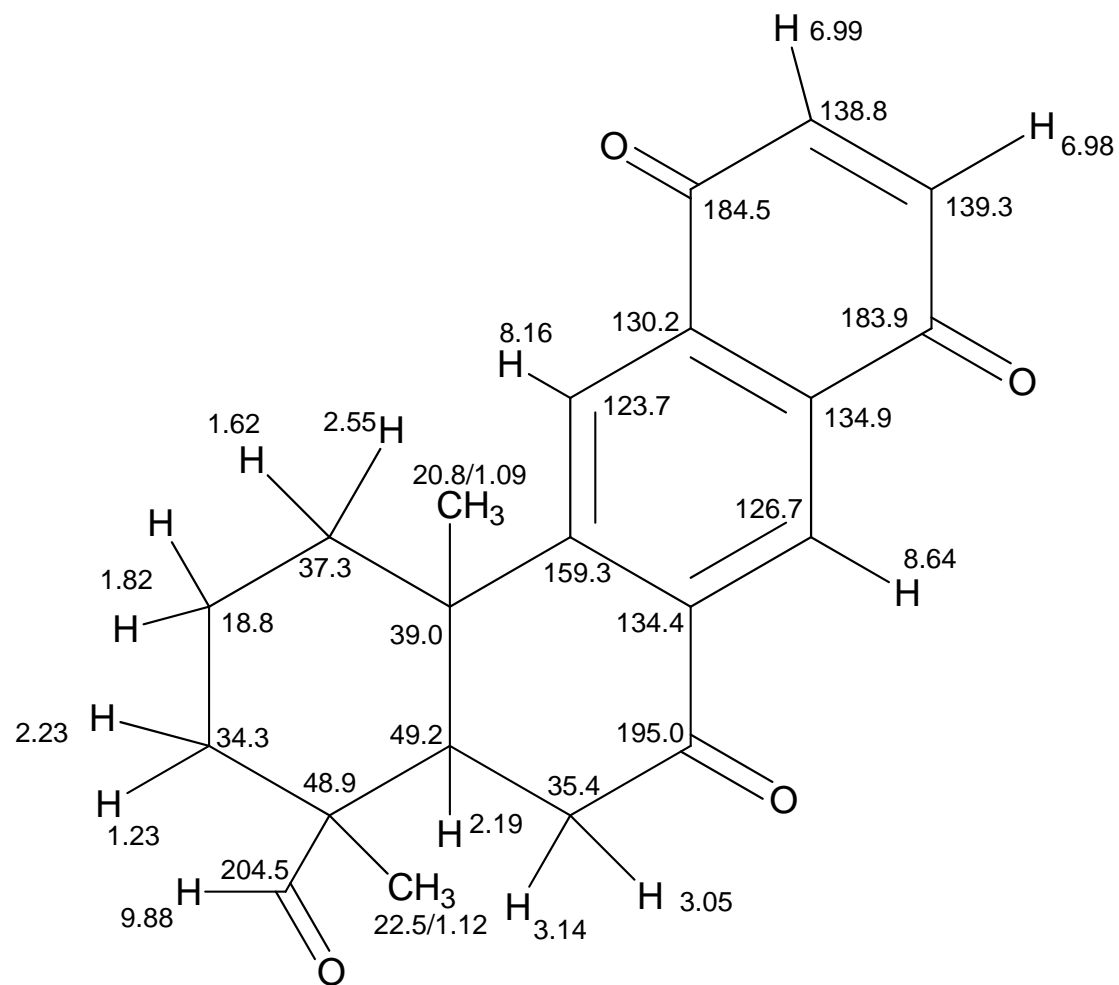


S13:  $^1\text{H}$  and  $^{13}\text{C}$  NMR data for neopetrosiquinone A (**1**),  $\text{CD}_2\text{Cl}_2$ , 600 MHz

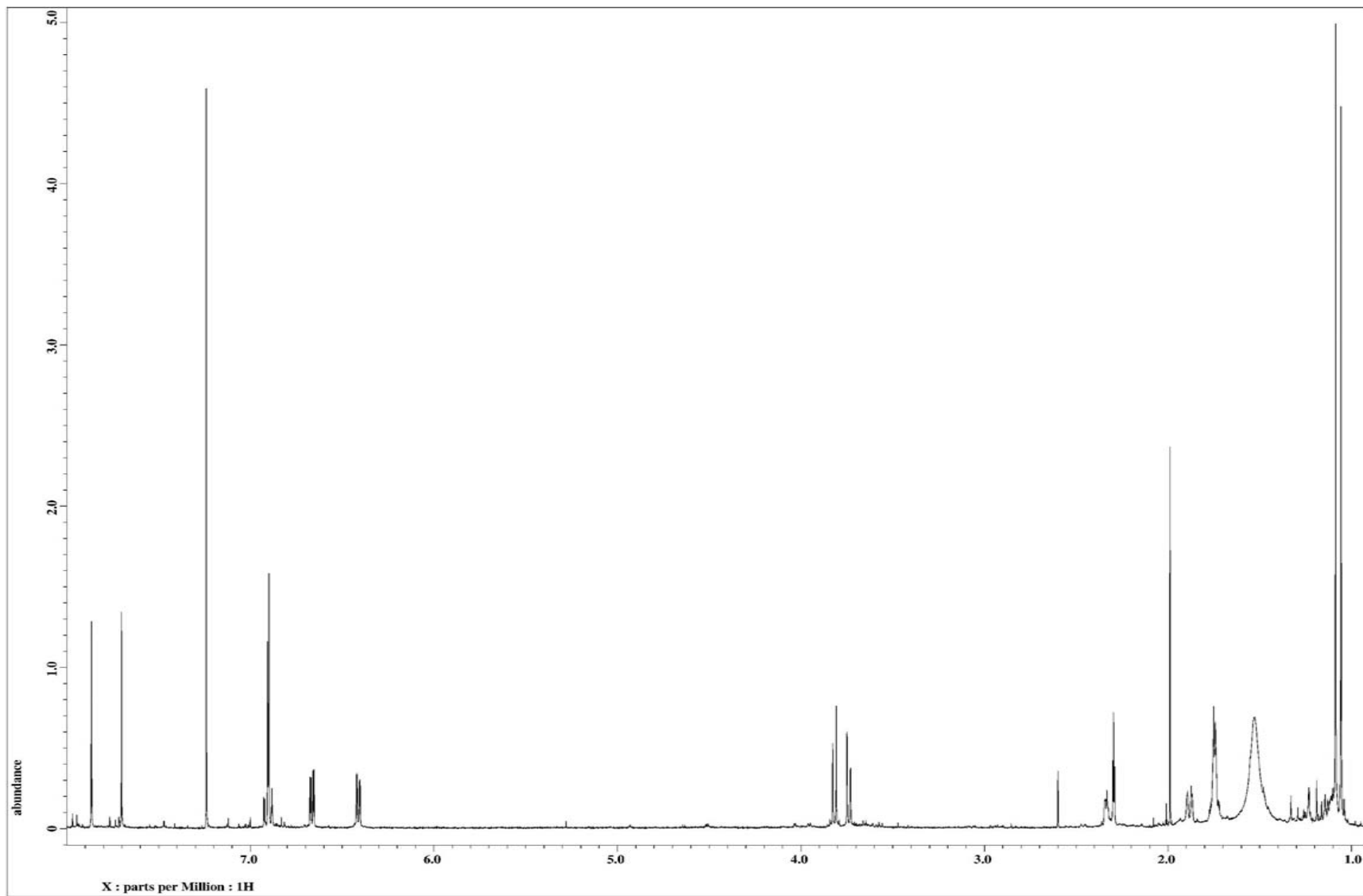
position		$\delta\text{C}$ , mult.	$\delta\text{H}$ , J (Hz)	COSY	HMBC <sup>a</sup>	NOESY	TOCSY
1	A	37.3, CH <sub>2</sub>	2.55, br dt (13.1, 3.4) <sup>f</sup>	1B, 2	2,5,10	1B, 11, 21	1B, 2, 3AB
	B		1.62, m	1A, 2	2,10	1A	1A, 2, 3AB
2		18.8, CH <sub>2</sub>	1.82, m	1AB, 3AB	4	21	1AB, 3AB
3	A	34.3, CH <sub>2</sub>	2.23, dt (14.4, 3.4) <sup>f</sup>	2, 3B	1,5,19	1B, 20	1B, 2, 3B
	B		1.23, m	2, 3A	2,4,19, 20	1AB, 2, 3A	3A
4		48.9, qC					
5		49.2, CH	2.19, dd (14.8, 4.8)	6	3,4,6,19,20	1B, 2, 20	6
6	A <sup>b</sup>	35.4, CH <sub>2</sub>	3.14, dd (17.9, 3.4)	5	4,7,8,10	20	5
	B <sup>c</sup>		3.05, dd (17.9, 14.4)			19, 21	
7		195.0, qC					
8		134.4, qC					
9		159.3, qC					
10		39.0, qC					
11		123.7, CH	8.16, s		7,8,10,12, 13	1AB, 21	
12		134.9, qC <sup>d</sup>					
13		184.5, qC					
14		138.8, CH <sup>e</sup>	6.99, d (10.3) <sup>e</sup>		12, 13, 16, 17		
15		139.3, CH <sup>e</sup>	6.98, d (10.3) <sup>e</sup>		12, 13, 16, 17		
16		183.9, qC					
17		130.2, qC <sup>d</sup>					
18		126.7, CH	8.64, s		7,9,16, 17		
19		204.5, CH	9.88, s		3,4, 5	1B, 2, 6B, 20, 21	
20		22.5, CH <sub>3</sub>	1.12, s		3,4,19	5, 6A, 19	
21		23.5, CH <sub>3</sub>	1.18, s		1,5,9	1A, 2, 6B, 11, 19	

<sup>a</sup>HMBC correlations, optimized for 8 Hz, are from proton(s) stated to the indicated carbon; <sup>b</sup>Equatorial proton; <sup>c</sup>Axial proton; <sup>d</sup>Assignments may be interchanged; <sup>e</sup>AB spin system, assignments may be interchanged; <sup>f</sup>Coupling constants were defined for H-1a and H-3a from  $^1\text{H}$  NMR spectrum performed in a 1:1 mixture of  $\text{CD}_2\text{Cl}_2$ :  $\text{CD}_3\text{OD}$ .

S14: Structure of neopetrosiquinone A (1) with chemical shifts on structure

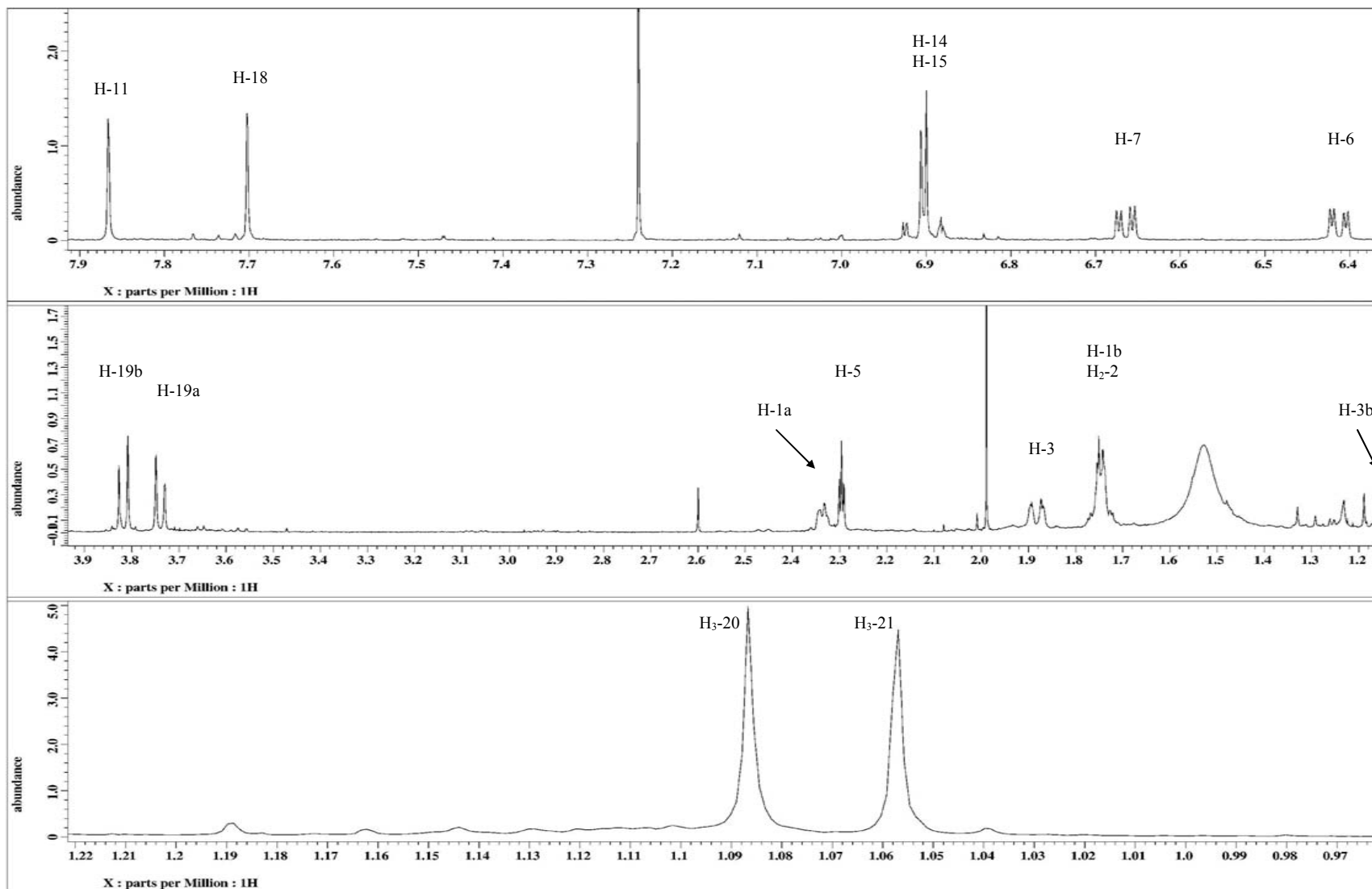


S15:  $^1\text{H}$  NMR spectrum of neopetrosiquinone B (2), 600 MHz,  $\text{CDCl}_3$

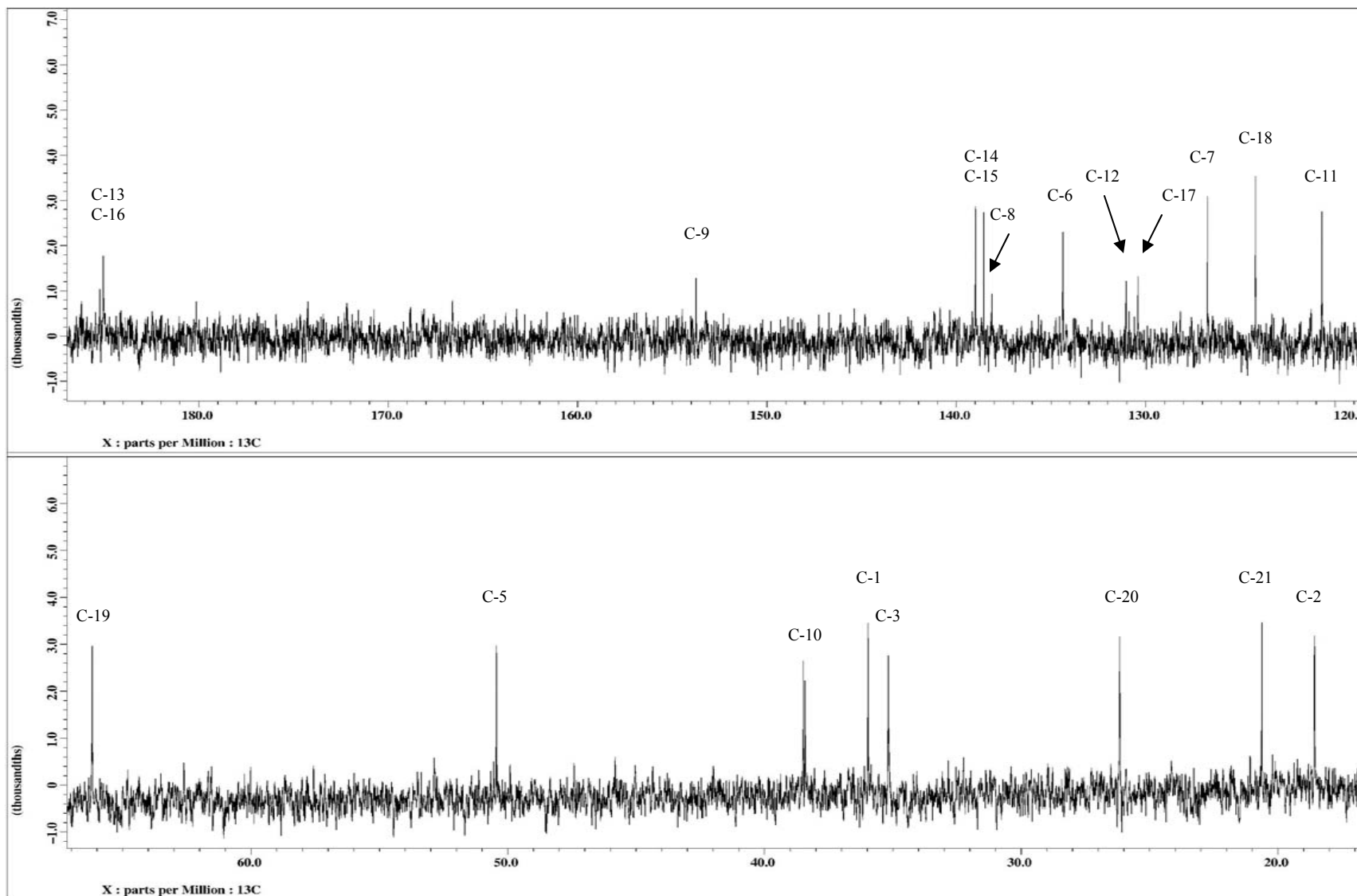




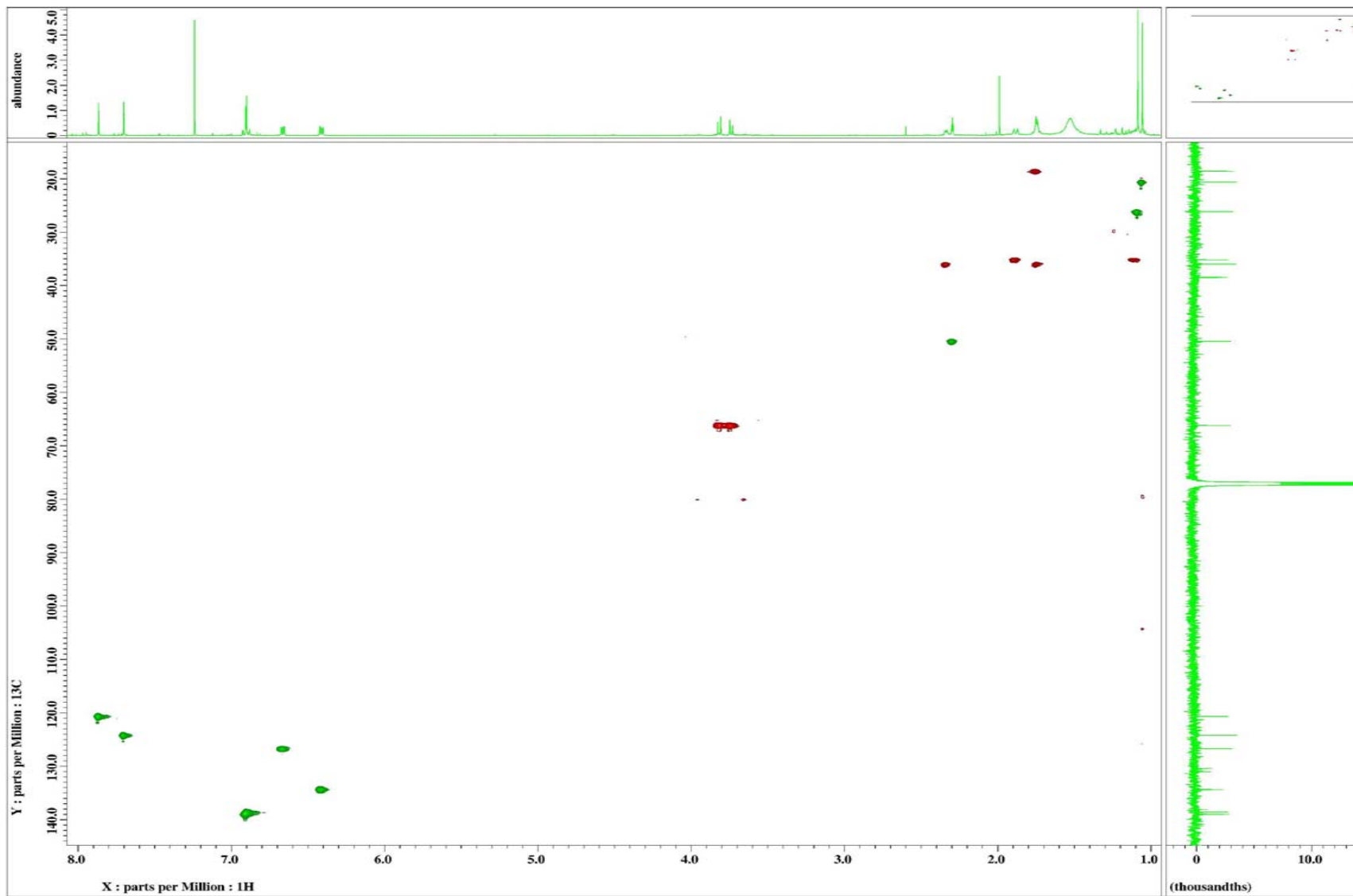
S16: Expansion of  $^1\text{H}$  NMR spectrum of neopetrosiquinone B (**2**), 600 MHz,  $\text{CDCl}_3$



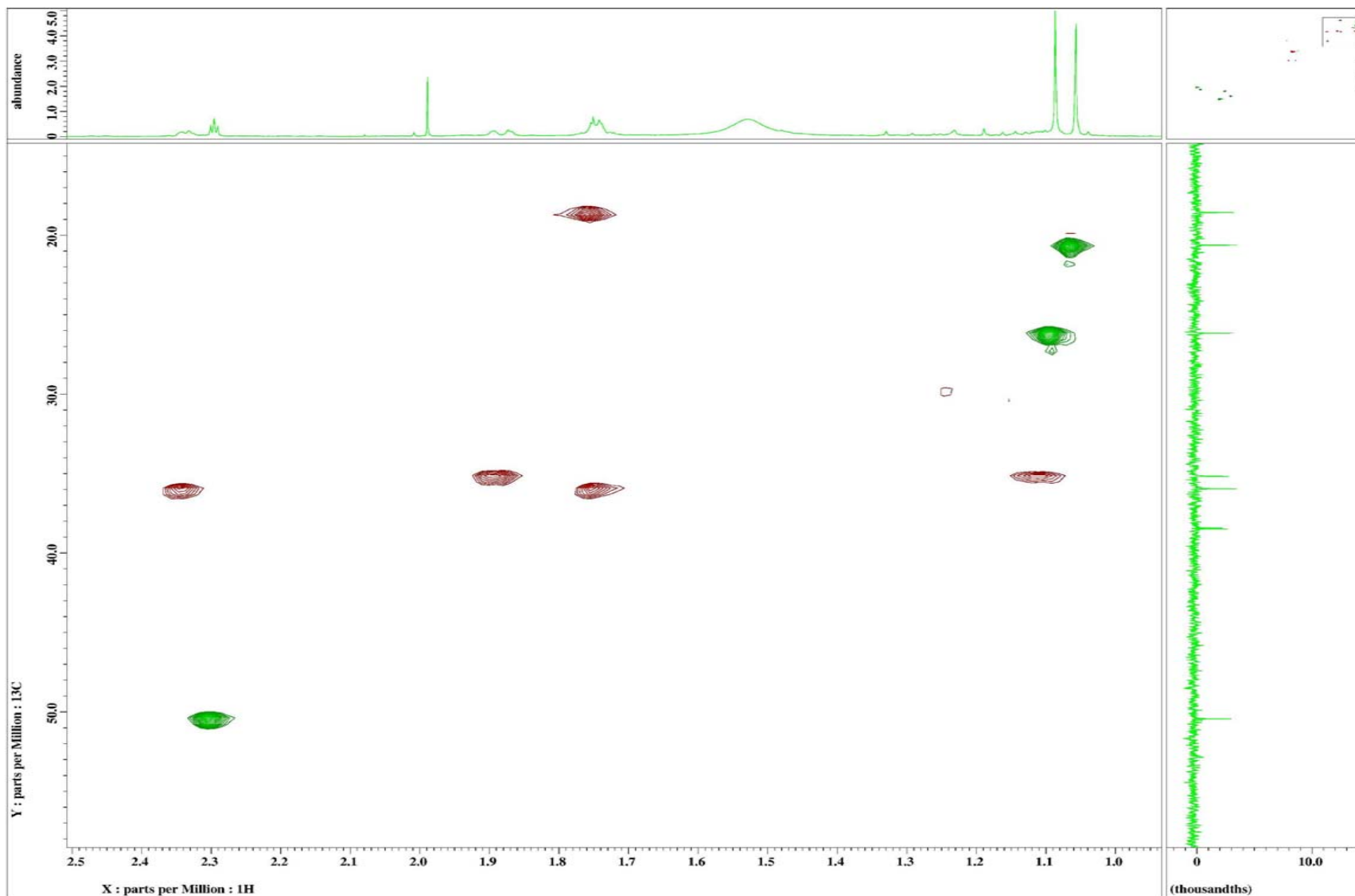
S17:  $^{13}\text{C}$  NMR spectrum of neopetrosiquinone B (**2**), 150.1 MHz,  $\text{CDCl}_3$



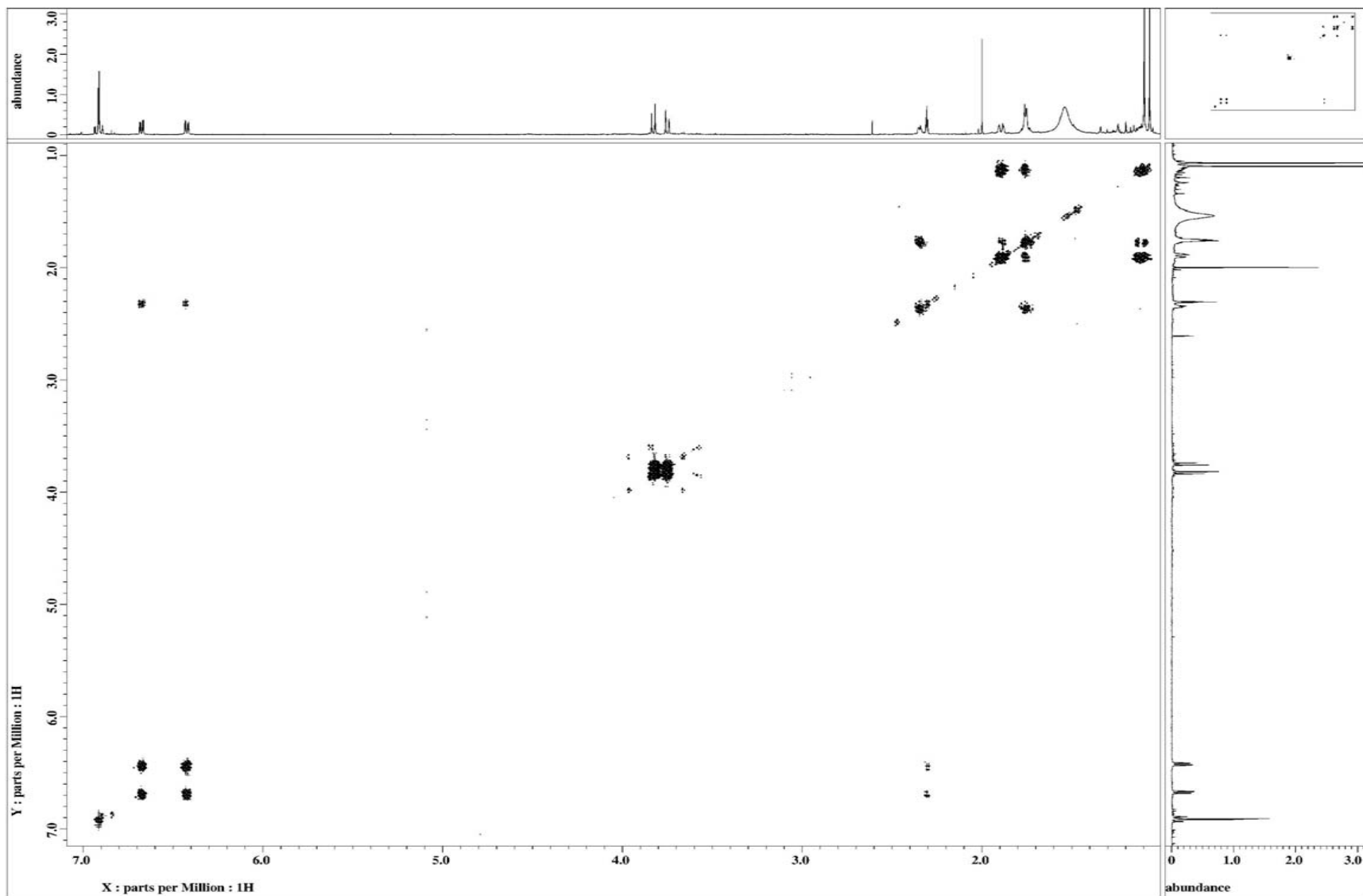
S18: edited gHSQC spectrum of neopetrosiquinone B (**2**), 600 MHz, CDCl<sub>3</sub>



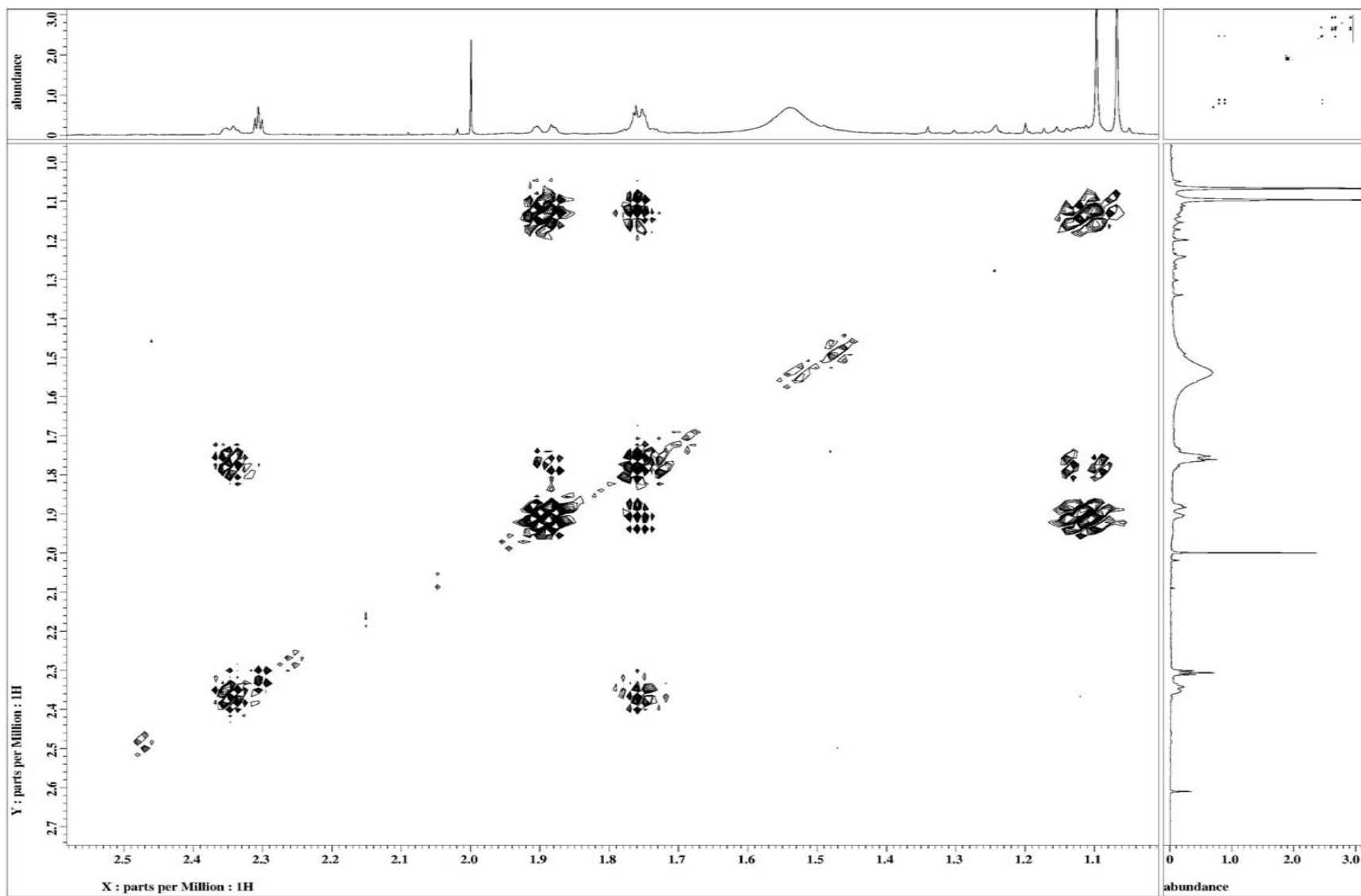
S19: Expansion of gHSQC spectrum of neopetrosiquinone B (2), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



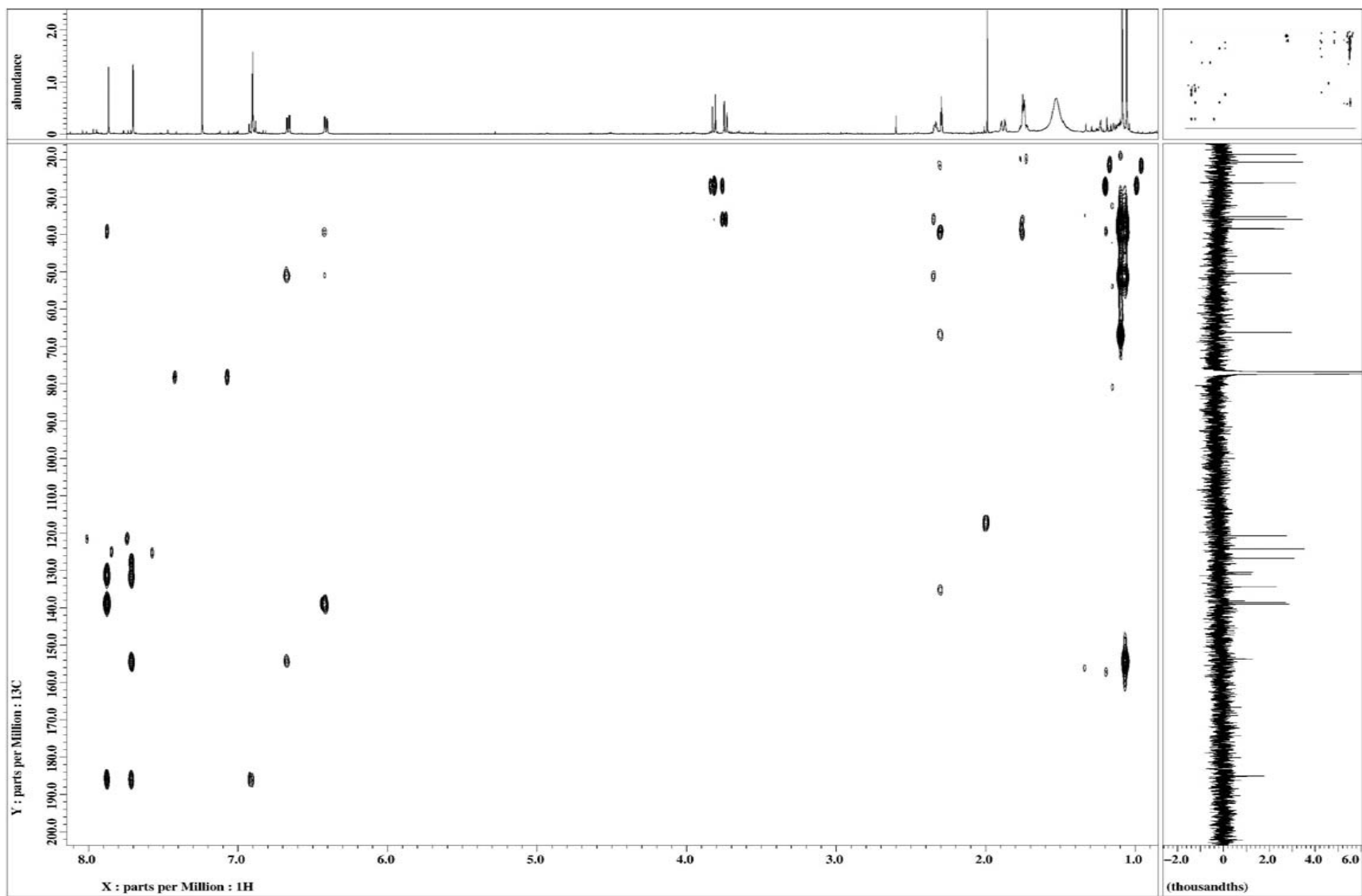
S20: gDQF-COSY spectrum of neopetrosiquinone B (2), 600 MHz, CDCl<sub>3</sub>



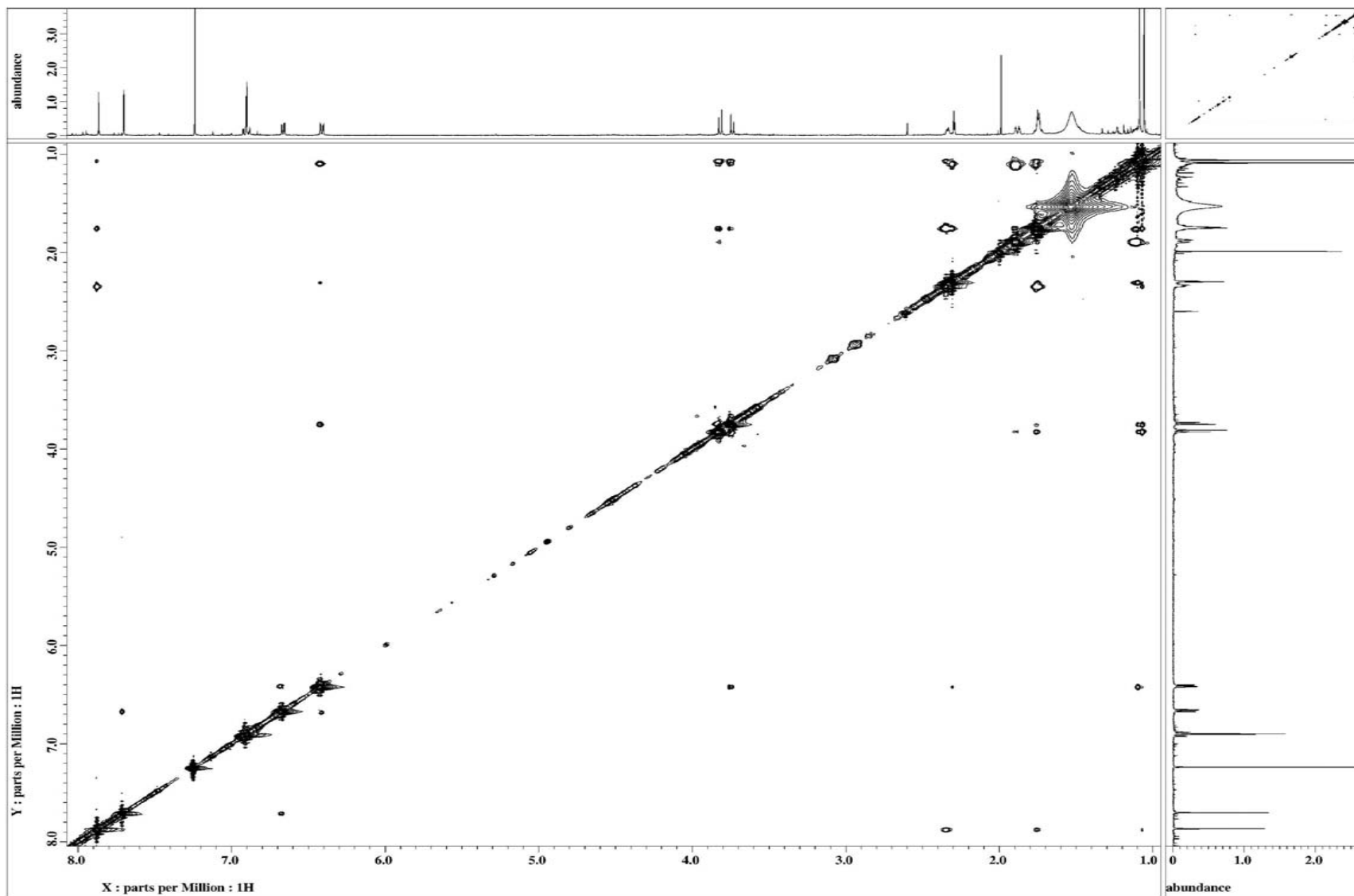
S21: Expansion of gDQF-COSY spectrum of neopetrosiquinone B (**2**), 600 MHz, CD<sub>2</sub>Cl<sub>2</sub>



S22: gHMBC spectrum of neopetrosiquinone B (2), 600 MHz, CDCl<sub>3</sub>

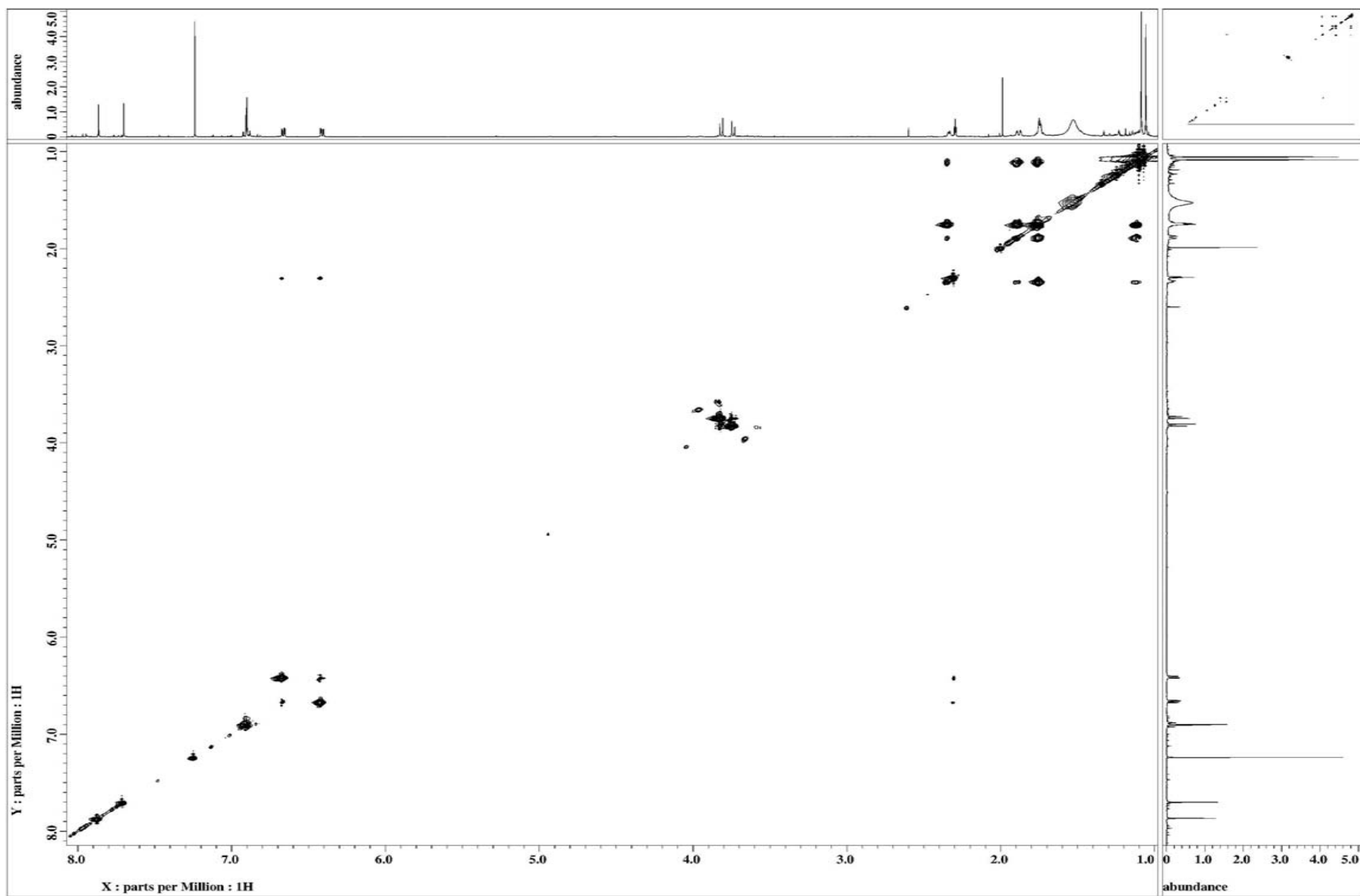


S23: NOESY spectrum of neopetrosiquinone B (**2**), 600 MHz, CDCl<sub>3</sub>





S24: TOCSY spectrum of neopetrosiquinone B (2), 600 MHz, CDCl<sub>3</sub>



S25: <sup>1</sup>H and <sup>13</sup>C NMR Data for neopetrosiquinone B (2)

Position		$\delta_C$ , mult.	$\delta_H$ , <i>J</i> (Hz)	COSY	HMBC <sup>a</sup>	NOESY	TOCSY
1	A	36.1, CH <sub>2</sub>	2.33, br m		3, 5, 21	11, 21	
	B		1.75, br m	1A			1A
2		18.7, CH <sub>2</sub>	1.75, br m	1A, 3A, 3A	4, 10		1A, 3AB
3	A	35.3, CH <sub>2</sub>	1.88, br d (15.1)	3A		3B	3B
	B		1.11, br m	3A	2	1A, 3A, 19AB	1A, 3A
4		38.6, qC					
5		50.6, CH	2.29, t (3.4)	6	4, 6, 19, 20, 21	6, 20	6, 20
6		134.5, CH	6.42, dd (9.6, 2.8)	5, 7	4, 5, 8	5, 7, 19, 20	7
7		126.9, CH	6.67 dd (9.6, 3.4)	5, 6	5, 9	6, 18	6
8		138.7, qC					
9		153.8, qC					
10		38.5, qC					
11		120.8, CH	7.87, s		8, 10, 13/16, 17	1A, 21	
12		131.2, qC <sup>c</sup>					
13		185.2, qC					
14		139.1, CH <sup>b</sup>	6.91, d (10.3) <sup>b</sup>		13/16		
15		138.6, CH <sup>b</sup>	6.89, d (10.3) <sup>b</sup>		13/16		
16		185.2, qC					
17		130.5, qC <sup>c</sup>					
18		124.3, CH	7.70, s		7, 9, 12, 13/16	7	
19	A	66.3, CH <sub>2</sub>	3.81, d (11.3)	19B	20	6, 19B, 21	19B
	B		3.74, d (11.3)	19A	3, 20	6, 19A, 21	19A
20		26.3, CH <sub>3</sub>	1.09, s		3, 4, 5, 19	3A, 5, 6, 19AB	
21		20.8, CH <sub>3</sub>	1.06, s		1, 5, 9, 10	1A, 11, 19AB	

<sup>a</sup>HMBC correlations, optimized for 8 Hz, are from proton(s) stated to the indicated carbon ; <sup>b</sup>AB spin system, assignments may be interchanged; <sup>c</sup>Assignments may be interchanged

S26: Structure of neopetrosiquinone B (2) with chemical shifts on structure

