Supporting Information

Rhodocomatulin-type Anthraquinones from the Australian Marine Invertebrates *Clathria hirsuta* and *Comatula rotalaria*

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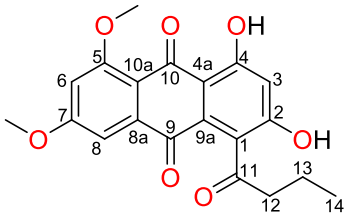
S1 NMR Table of Rhodocomatulin 5,7-dimethyl ether (**1**)[a] in DMSO-d_6

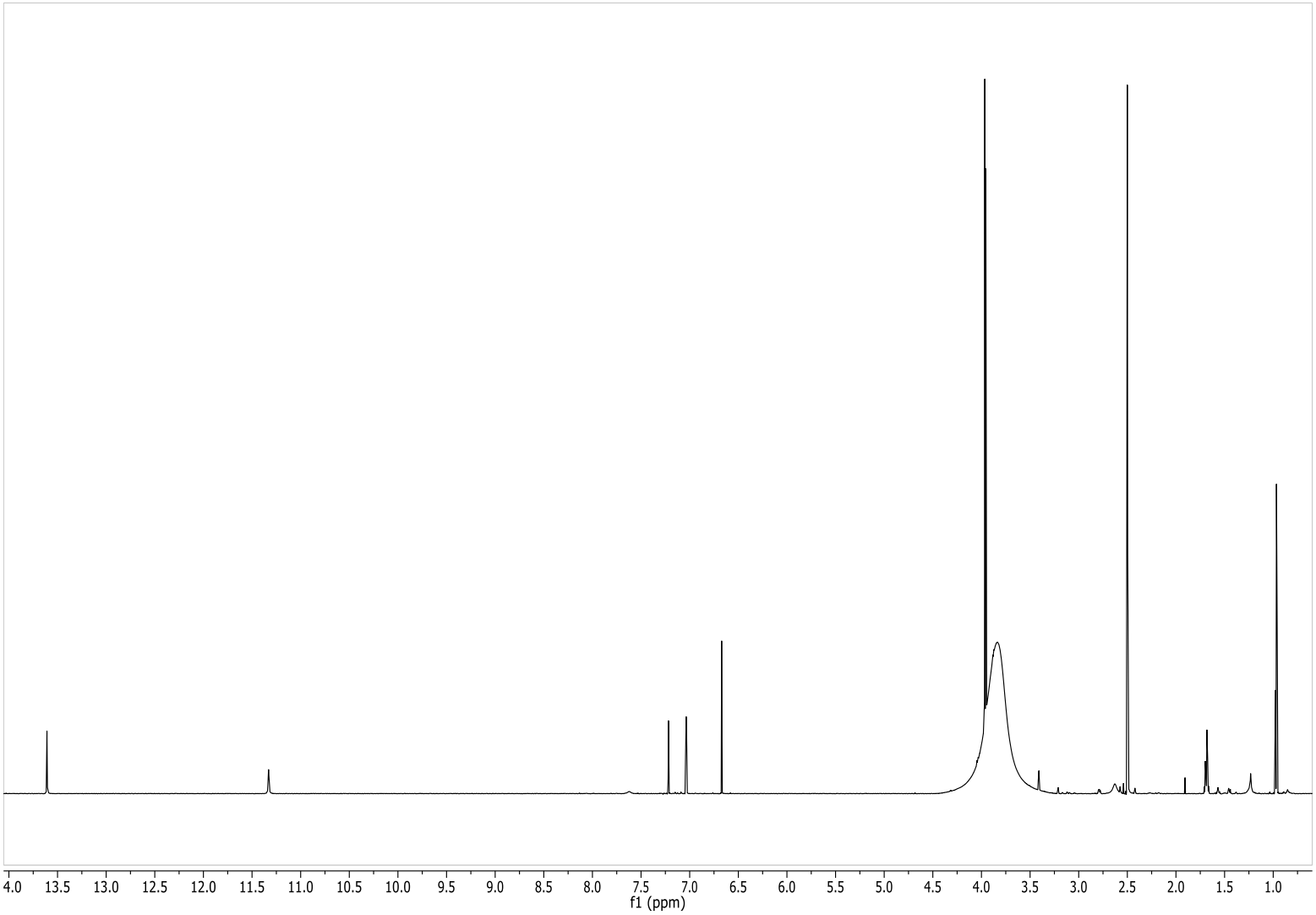
Position	**^{1}H, mult. (*J* in Hz)**	**^{13}C, type**	**HMBC**	**ROESY**
1		124.9, C		
2		159.9, C		
2-OH	11.33, br s	-		3
3	6.66, s	108.6, CH	1, 2, 4a	2-OH, 4-OH
4		163.8, C		
4-OH	13.61, s	-	3, 4, 4a	3
4a		109.8, C		
5		162.8, C		
5-OMe	3.96, s	56.2, CH_3	5	6
6	7.04, d (2.5)	105.1, CH	5, 7, 8, 10a	5-OMe, 7-OMe
7		164.8, C		
7-OMe	3.97, s	56.7, CH_3	7	6, 8
8	7.22, d (2.5)	104.7, CH	6, 7, 9, 9a, 10a	7-OMe
8a		130.2, C[b]		
9		182.5, C		
9a		136.2, C[b]		
10		185.2, C		
10a		113.6, C		
11		203.4, C		
12	2.64, br t (7.6)	44.7, CH_2		13
13	1.67, qt (7.6, 7.6)	16.2, CH_2	11, 12, 14	12, 14
14	0.98, t (7.6)	13.6, CH_3	12, 13	13

[a] Spectrum recorded in DMSO-d_6 + trace TFA (^{1}H at 900 MHz, ^{13}C at 225 MHz) at 25°C
[b] Signals are interchangeable

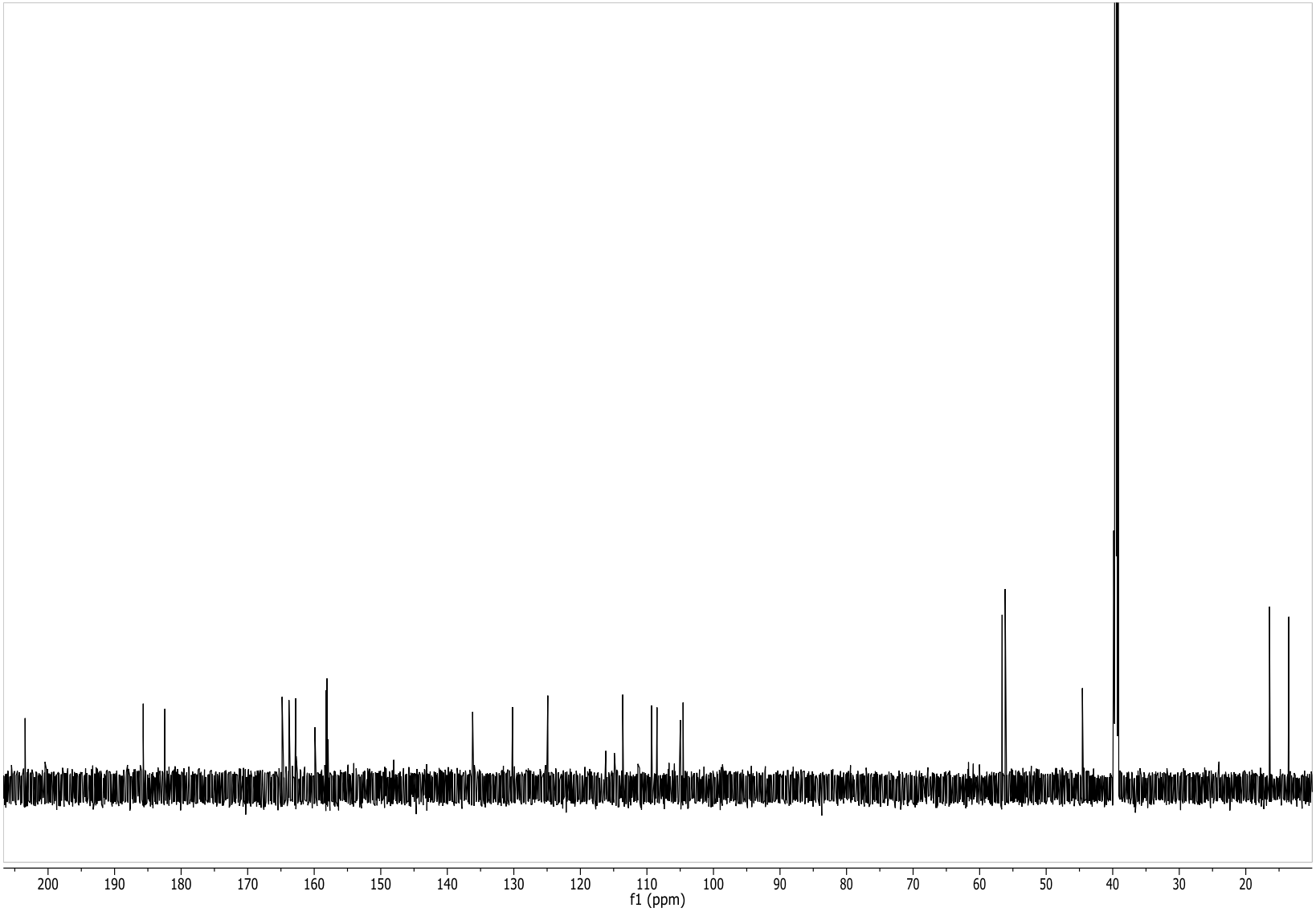


1

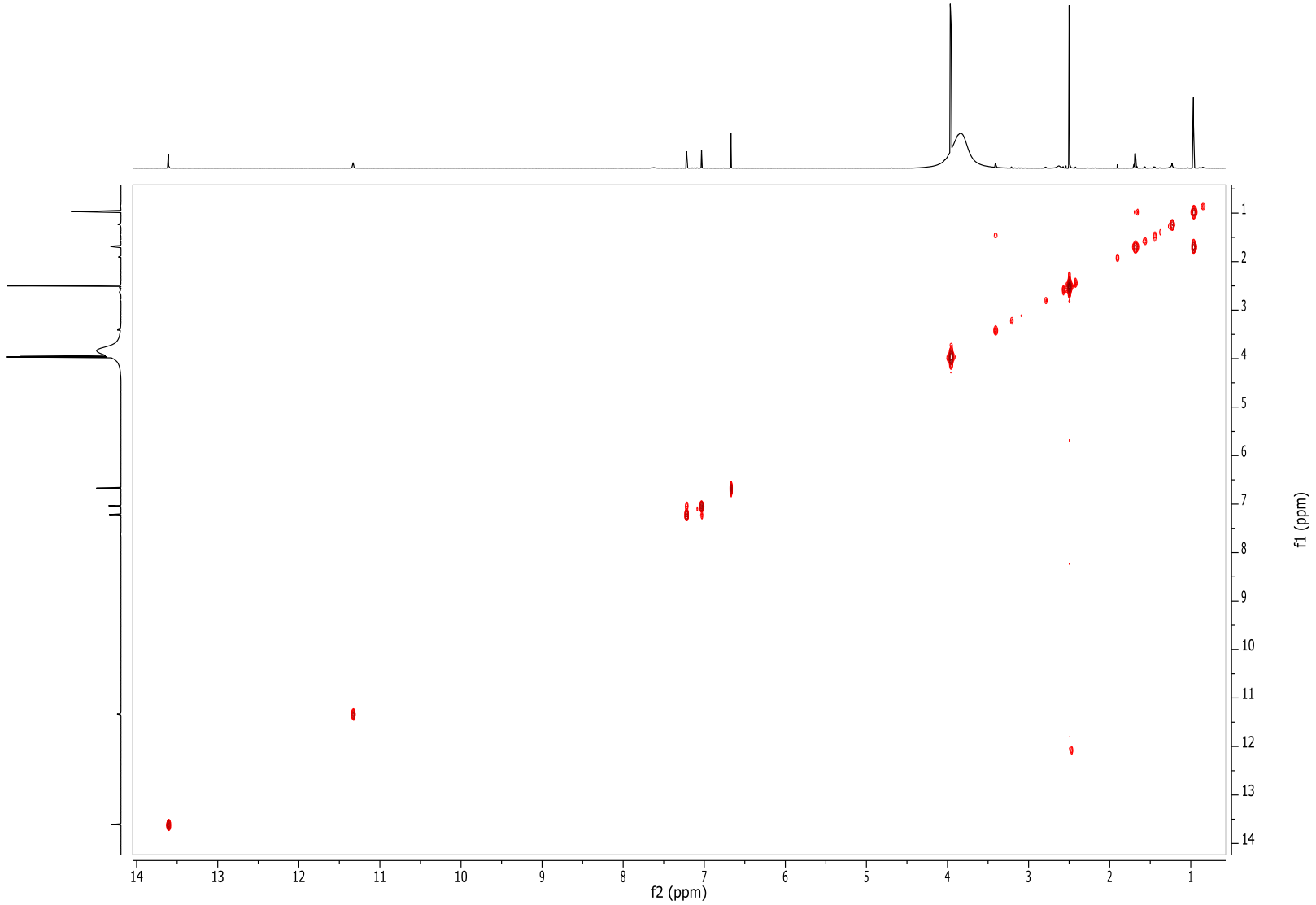
S2 ^{1}H NMR Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



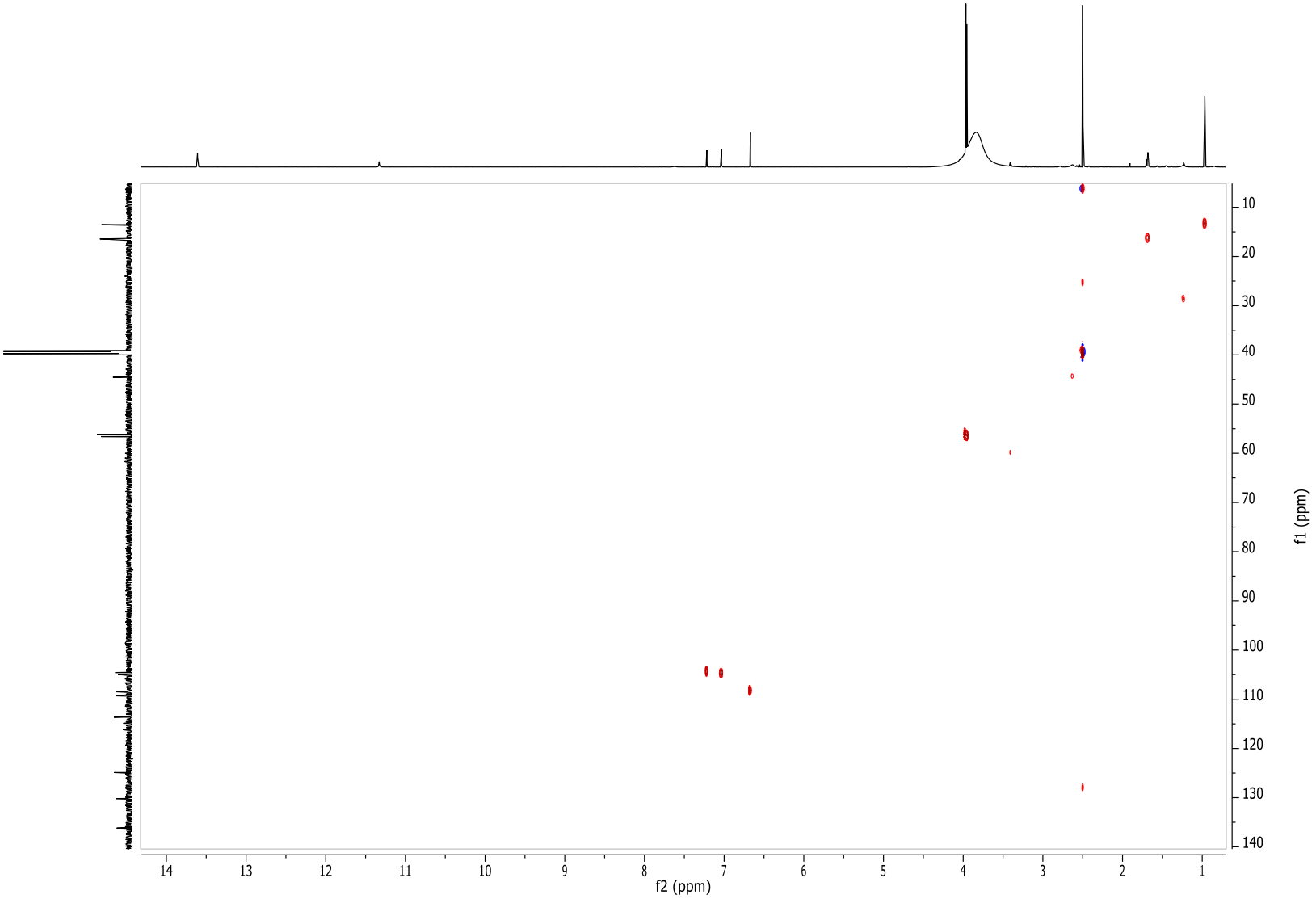
S3 ^{13}C NMR Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



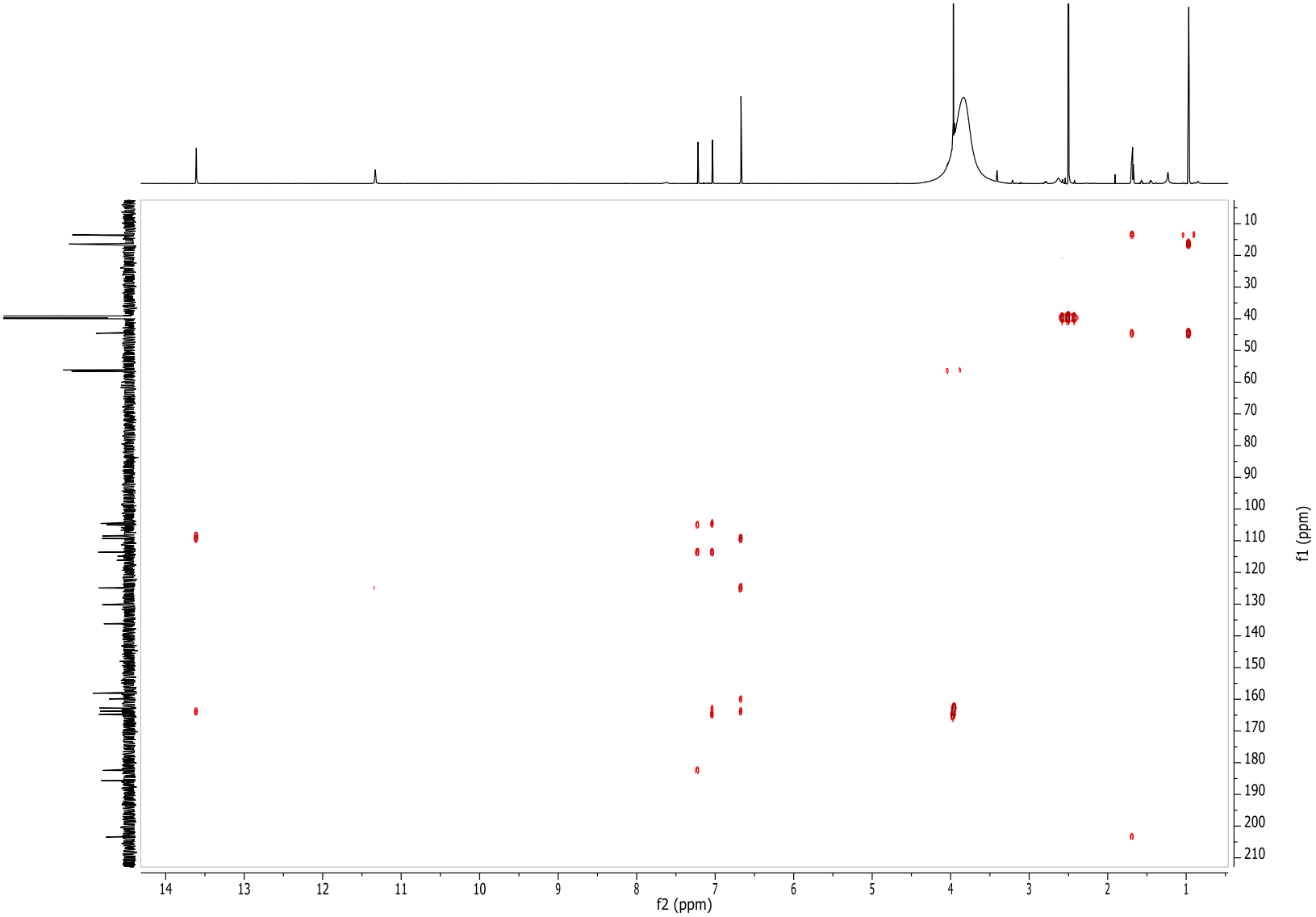
S4 COSY Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



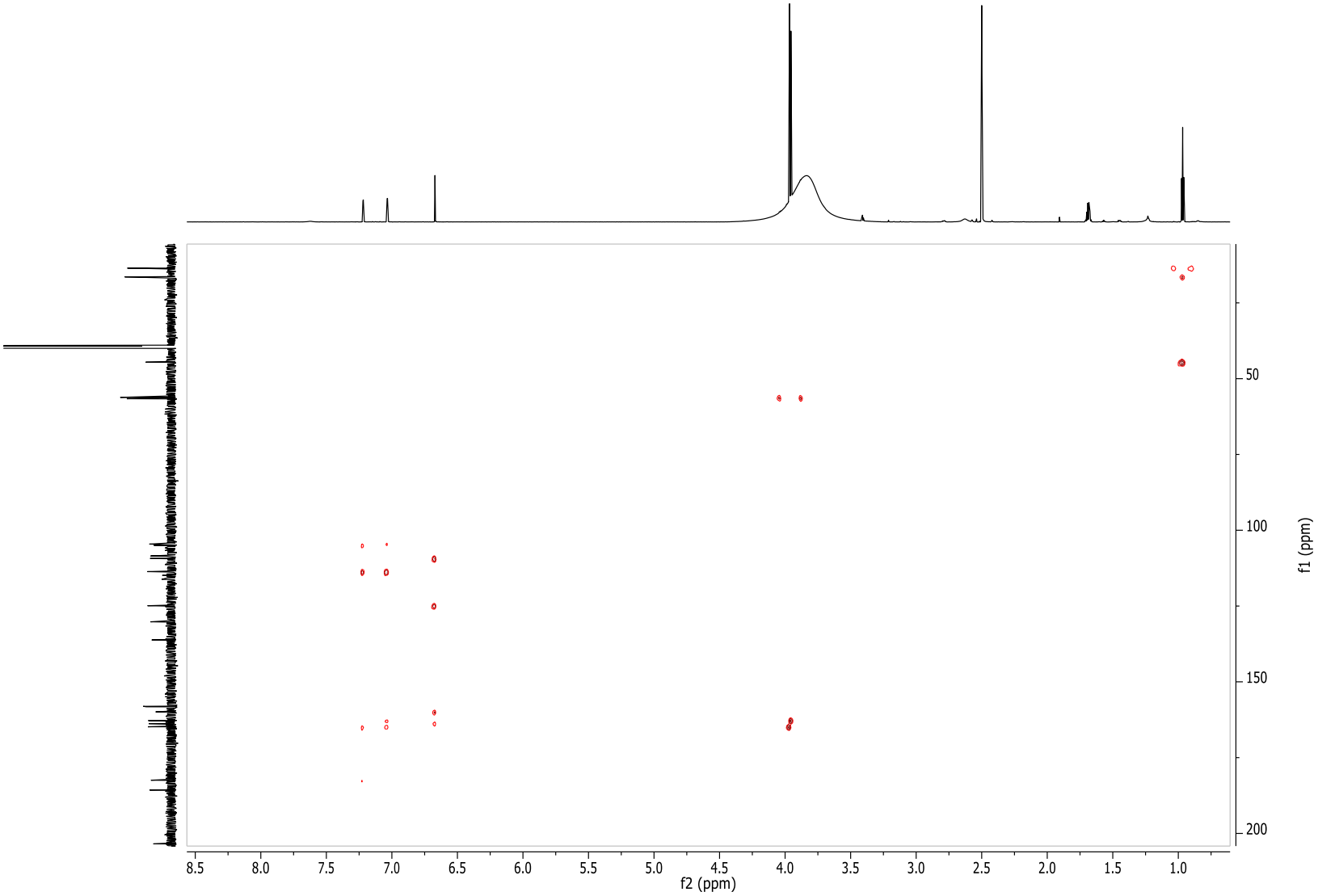
S5 HSQC Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



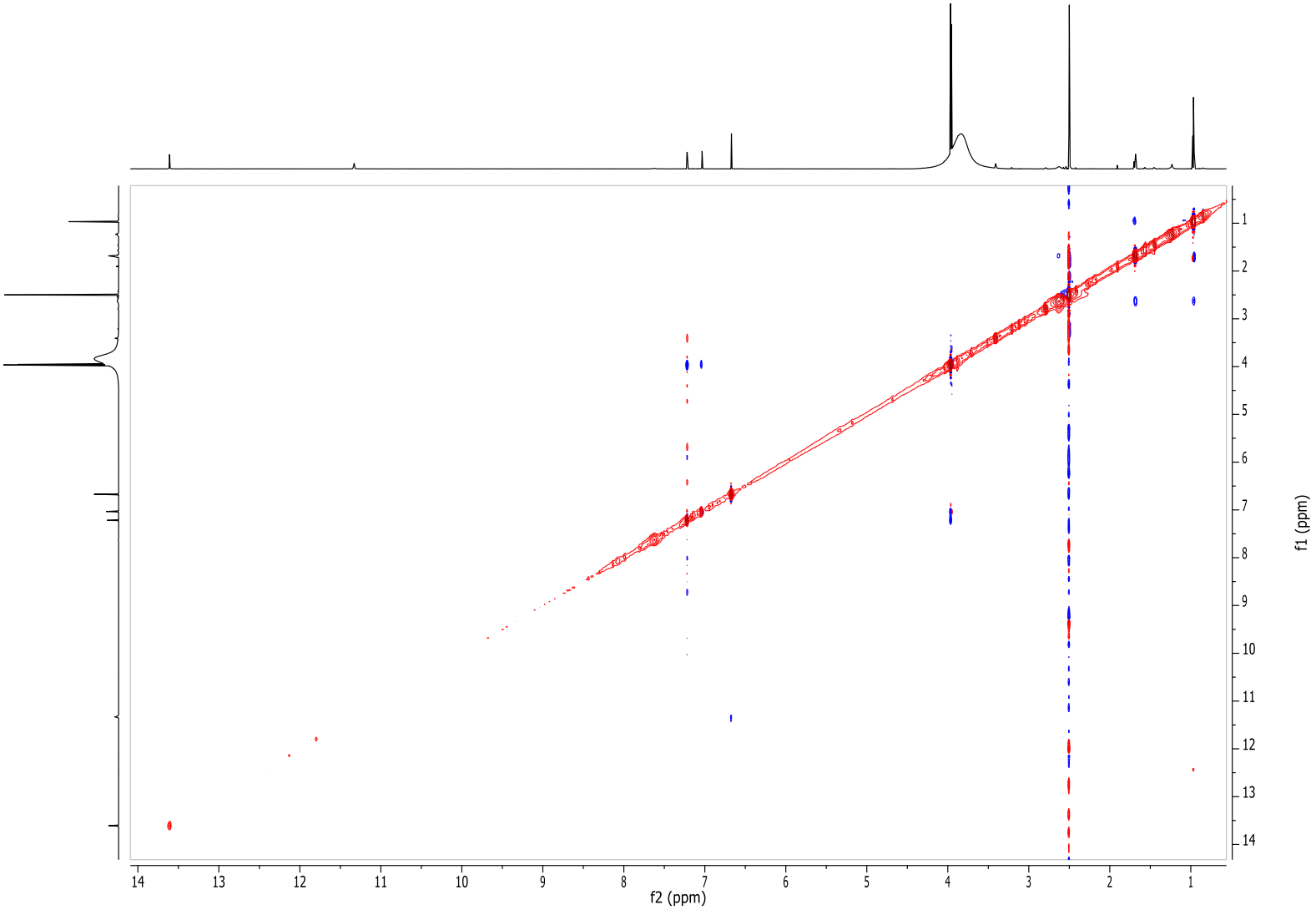
S6 HMBC ($^{n}J_{CH}$ = 8 Hz) Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



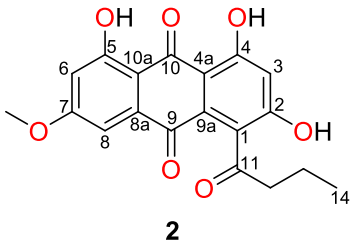
S7 HMBC ($^{n}J_{CH}$ = 2 Hz) Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



S8 ROESY Spectrum of Rhodocomatulin 5,7-dimethyl ether (**1**) in DMSO-d_6



S9 NMR Table of Rhodocomatulin 7-methyl ether (**2**)[a] in DMSO-d_6

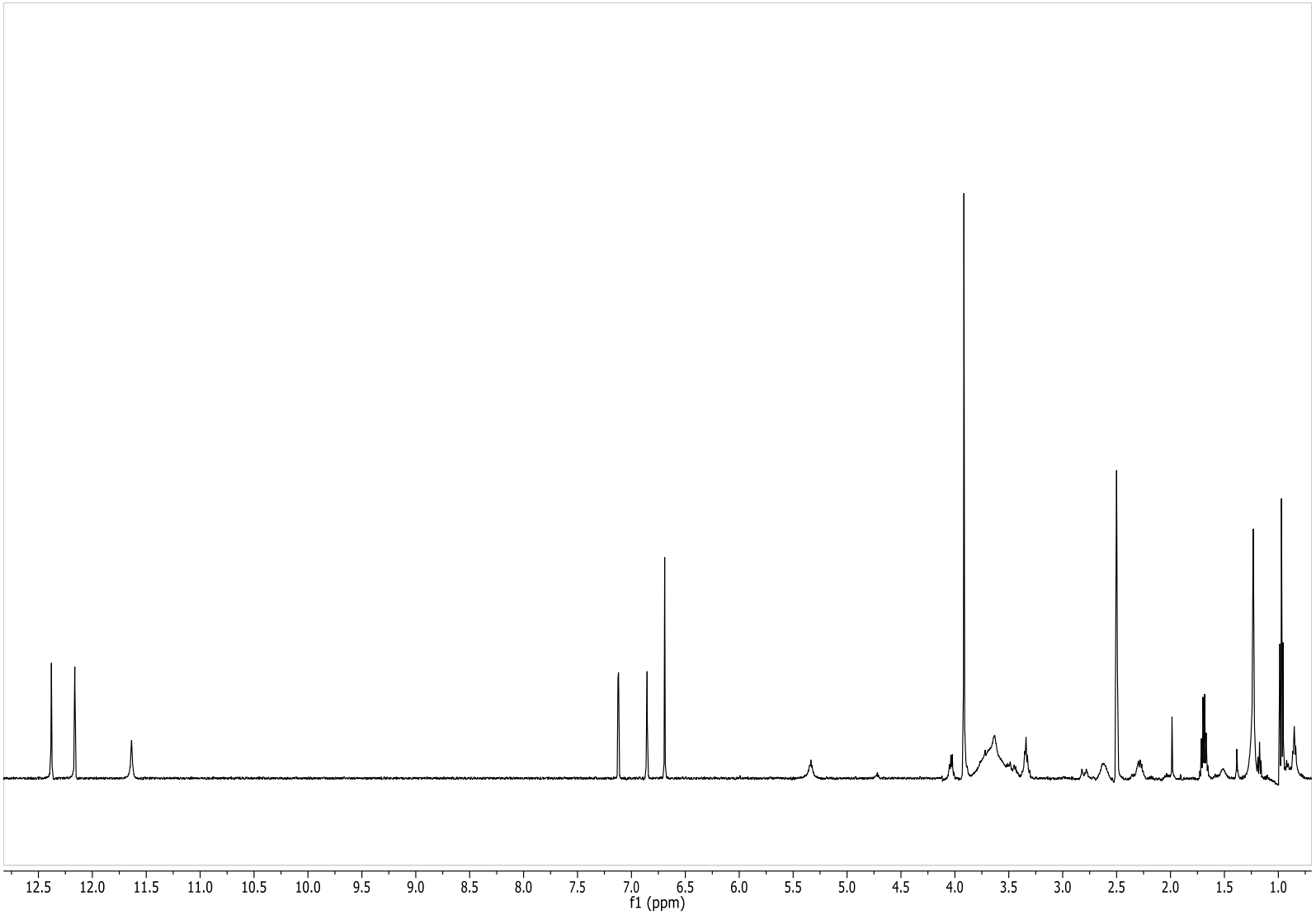


2

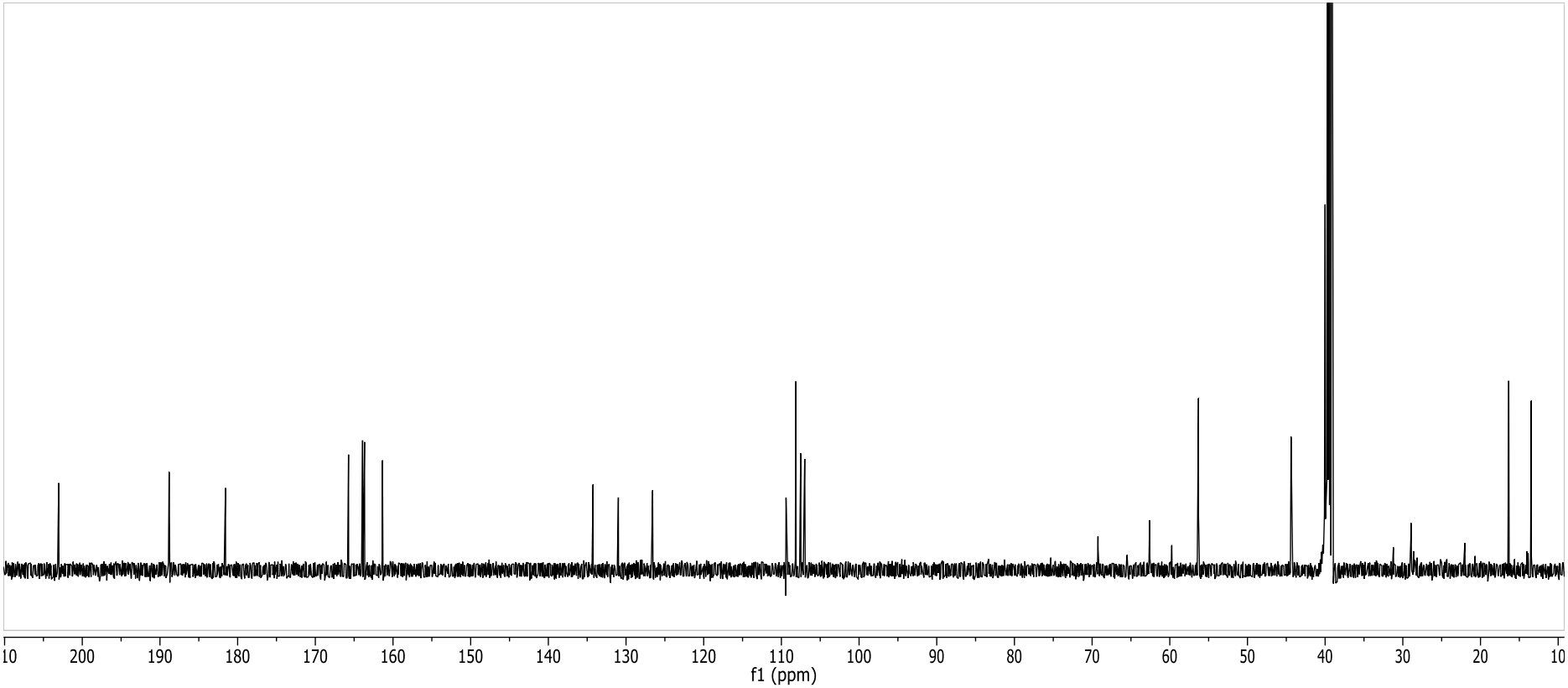
Position	^{1}H, mult. (*J* in Hz)	^{13}C, type	HMBC	ROESY
1		126.6, C		
2		161.5, C		
2-OH	11.64, br s			3
3	6.69, s	108.0, CH	1, 2, 4, 4a	2-OH, 4-OH
4		163.7, C		
4-OH	12.38, s		3, 4, 4a	3
4a		108.2, C		
5		163.9, C		
5-OH	12.15, s		5, 6, 10a	6
6	6.86, d (2.6)	106.9, CH	5, 7, 8, 10a	5-OH, 7-OMe
7		165.8, C		
7-OMe	3.92, s	56.1, CH_3	7	6, 8
8	7.12, d (2.6)	107.4, CH	9, 10a	7-OMe
8a		131.0, C[b]		
9		181.6, C		
9a		134.3, C[b]		
10		188.8, C		
10a		109.4, C		
11		203.1, C		
12	2.62, br t (7.6)	44.4, CH_2		13
13	1.69, qt (7.6, 7.6)	16.4, CH_2	11, 12, 14	12, 14
14	0.97, t (7.6)	13.5, CH_3	12, 13	13

[a] Spectrum recorded in DMSO-d_6 + trace TFA (^{1}H at 500 MHz, ^{13}C at 125 MHz) at 30°C
[b] Signals are interchangeable

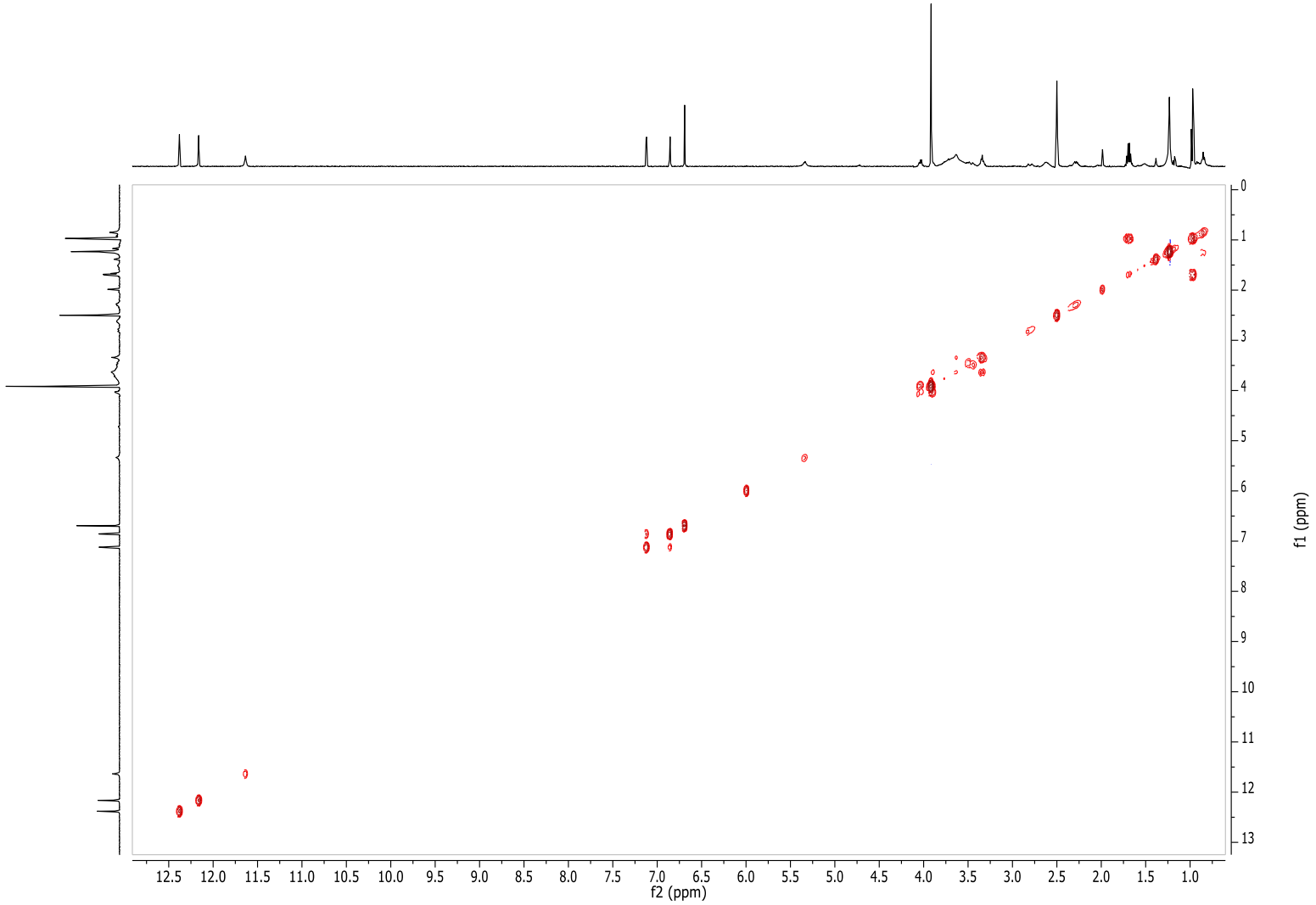
S10 ^{1}H NMR Spectrum of Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



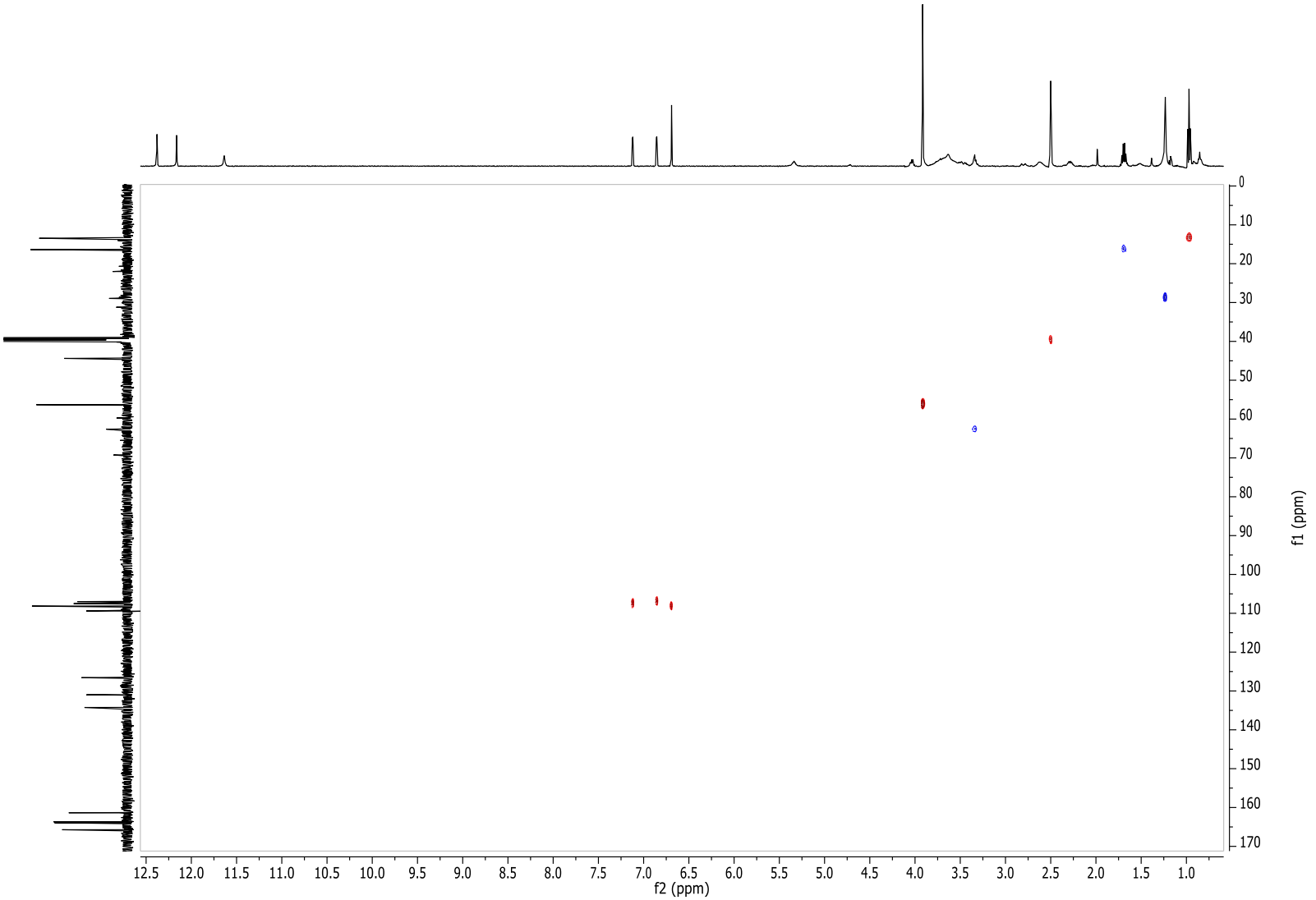
S11 ^{13}C NMR Spectrum of Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



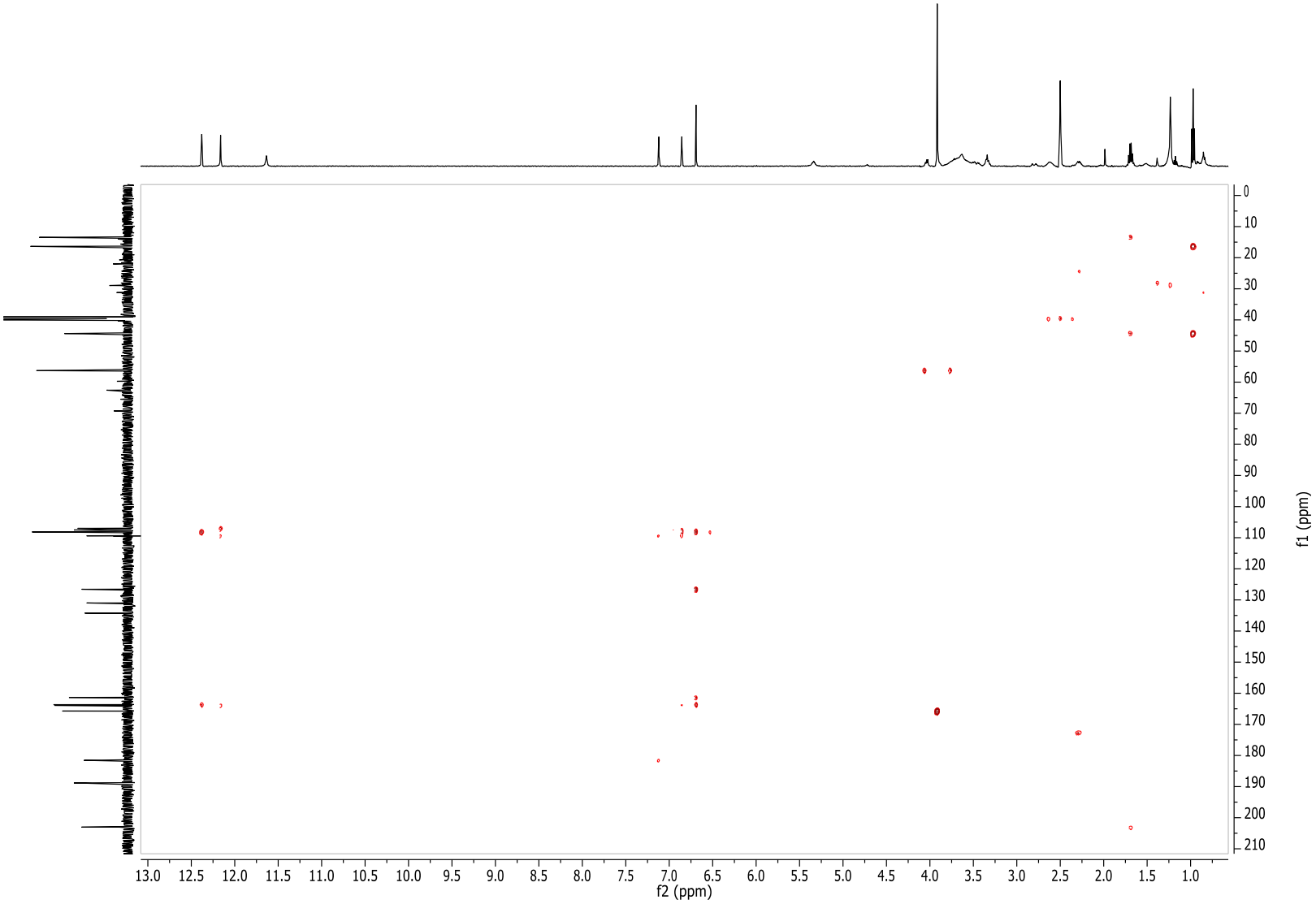
S12 COSY Spectrum of Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



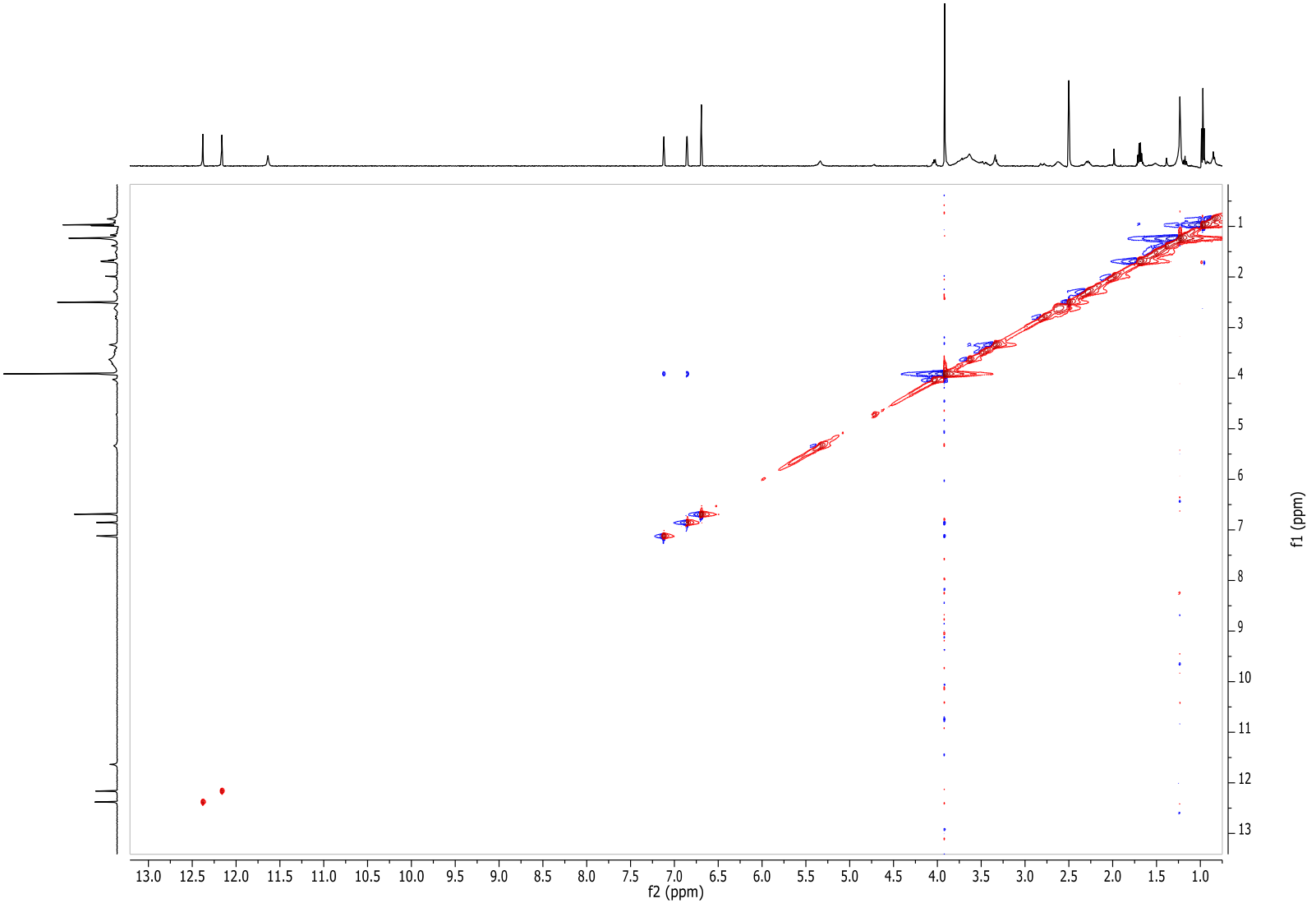
S13 HSQC Spectrum of Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



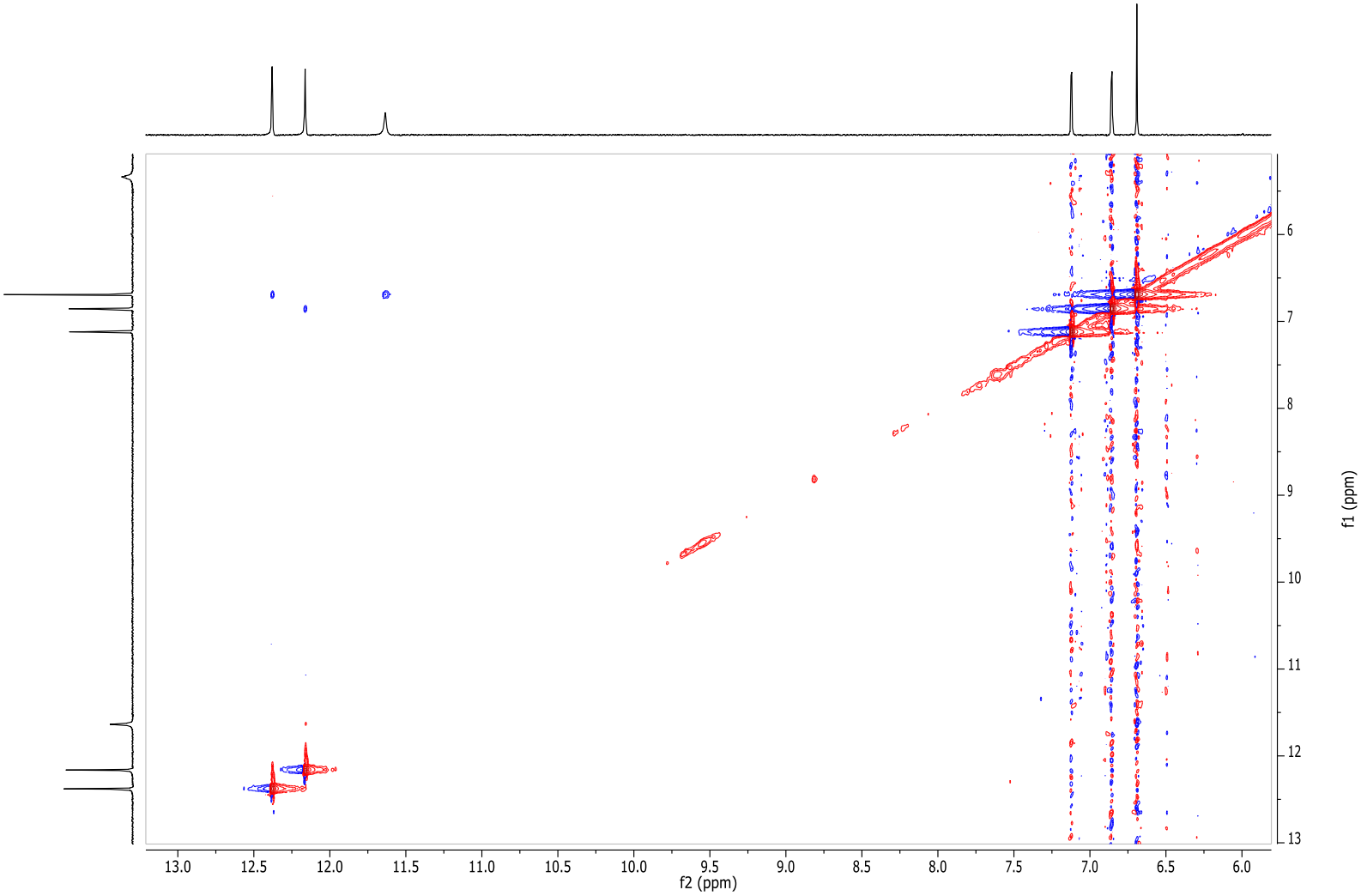
S14 HMBC Spectrum of Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



S15 ROESY Spectrum Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



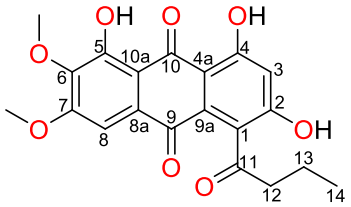
S16 Expansion of ROESY Spectrum of Rhodocomatulin 7-methyl ether (**2**) in DMSO-d_6



S17 NMR Table of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**)[a] in DMSO-d_6

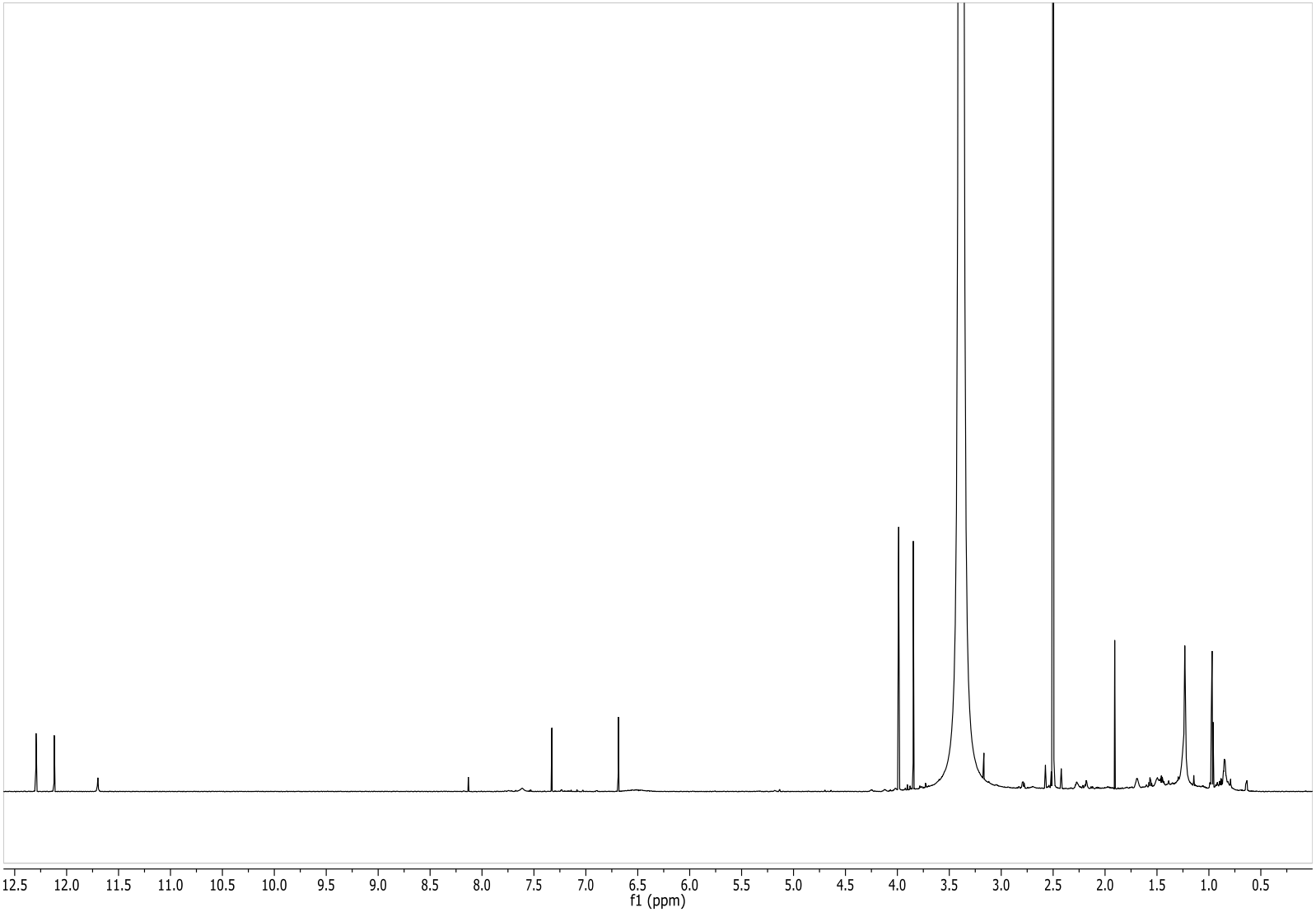
Position	**^{1}H, mult. (*J* in Hz)**	**^{13}C[b], type**	**HMBC**	**ROESY**
1		126.8, C		
2		[c]		
2-OH	11.70, br s	-		3
3	6.69, s	107.8, CH	1, 4a	2-OH, 4-OH
4		163.7, C		
4-OH	12.29, s	-	3, 4	3
4a		108.4, C		
5		155.3, C		
5-OH	12.10, s	-	5, 6, 10a	
6		141.2, C		
6-OMe	3.85, s	60.1, CH_3	6	
7		158.0, C		
7-OMe	3.99, s	56.3, CH_3	7	8
8	7.33, s	104.4, CH	6, 9, 10a	7-OMe
8a		[c]		
9		180.9, C		
9a		[c]		
10		[c]		
10a		111.0, C		
11		[c]		
12	2.62, t (7.6)	44.2, CH_2		13
13	1.70, qt (7.6, 7.6)	16.2, CH_2		12, 14
14	0.97, t (7.6)	13.3, CH_3	12, 13	13

[a] Spectra recorded in DMSO-d_6 + trace TFA (^{1}H at 900 MHz) at 25°C
[b] ^{13}C chemical shift obtained through 2D HSQC and HMBC experiments
[c] Not observed

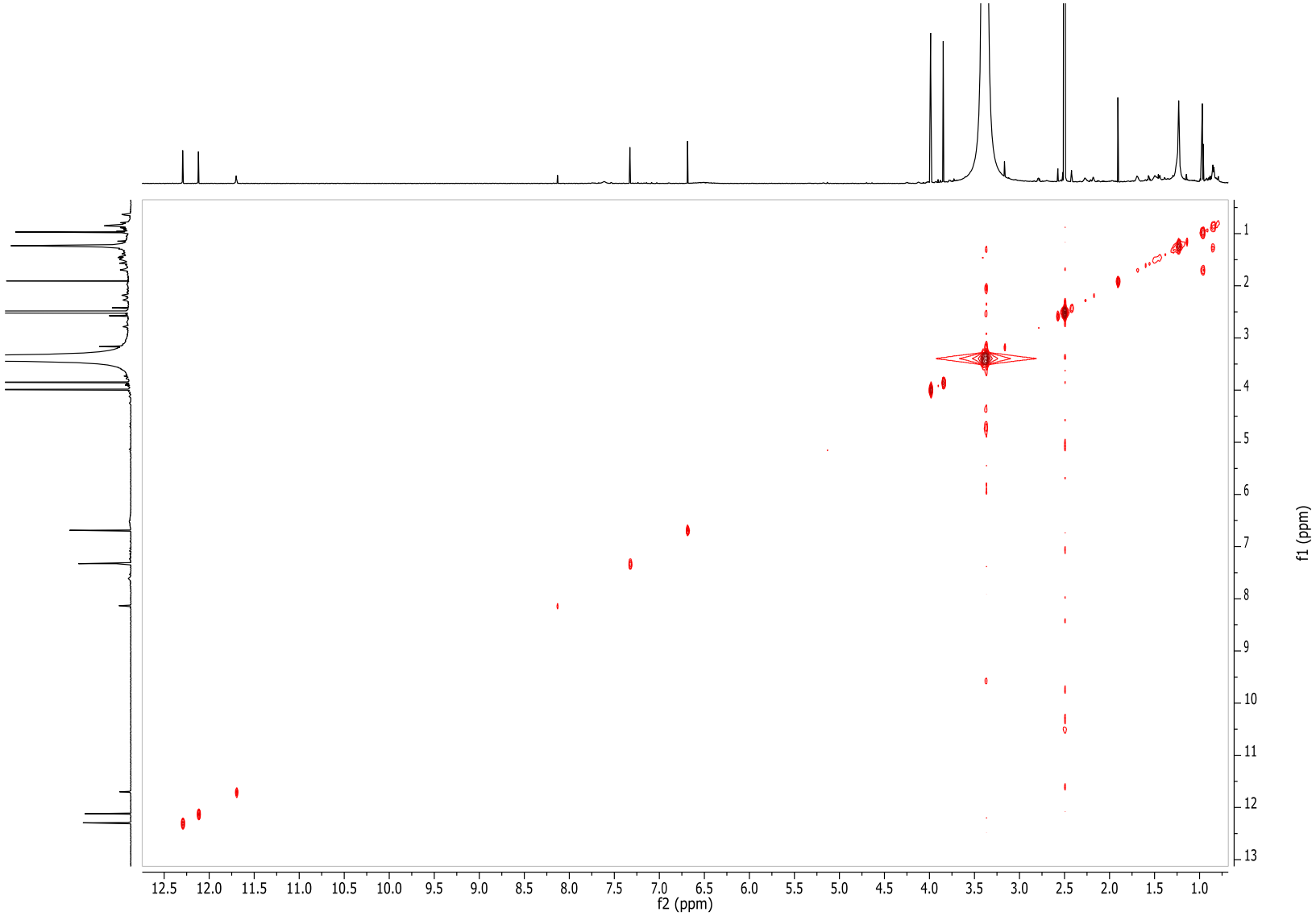


3

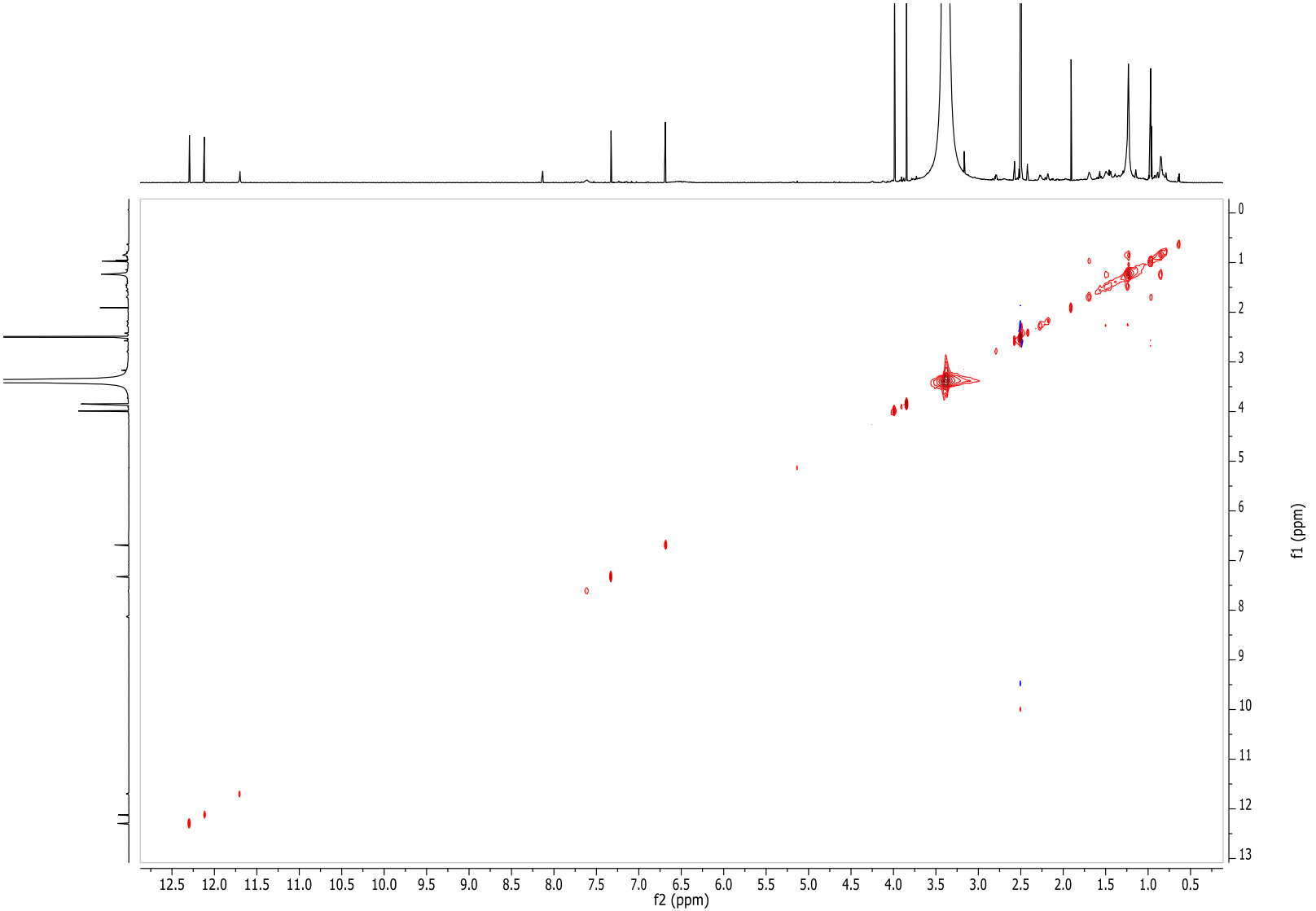
S18 ^{1}H NMR Spectrum of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**) in DMSO-d_6



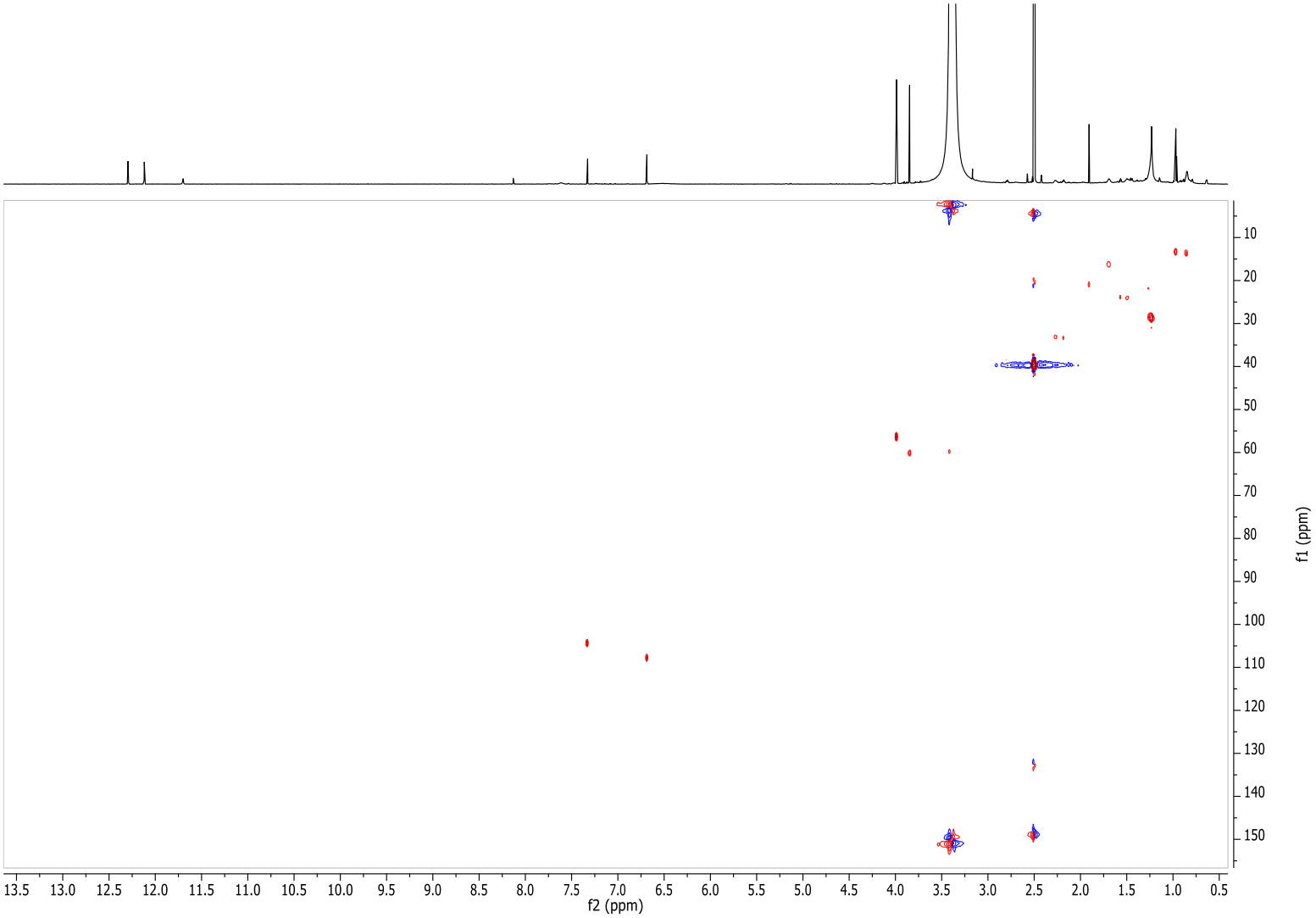
S19 COSY Spectrum of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**) in DMSO-d_6



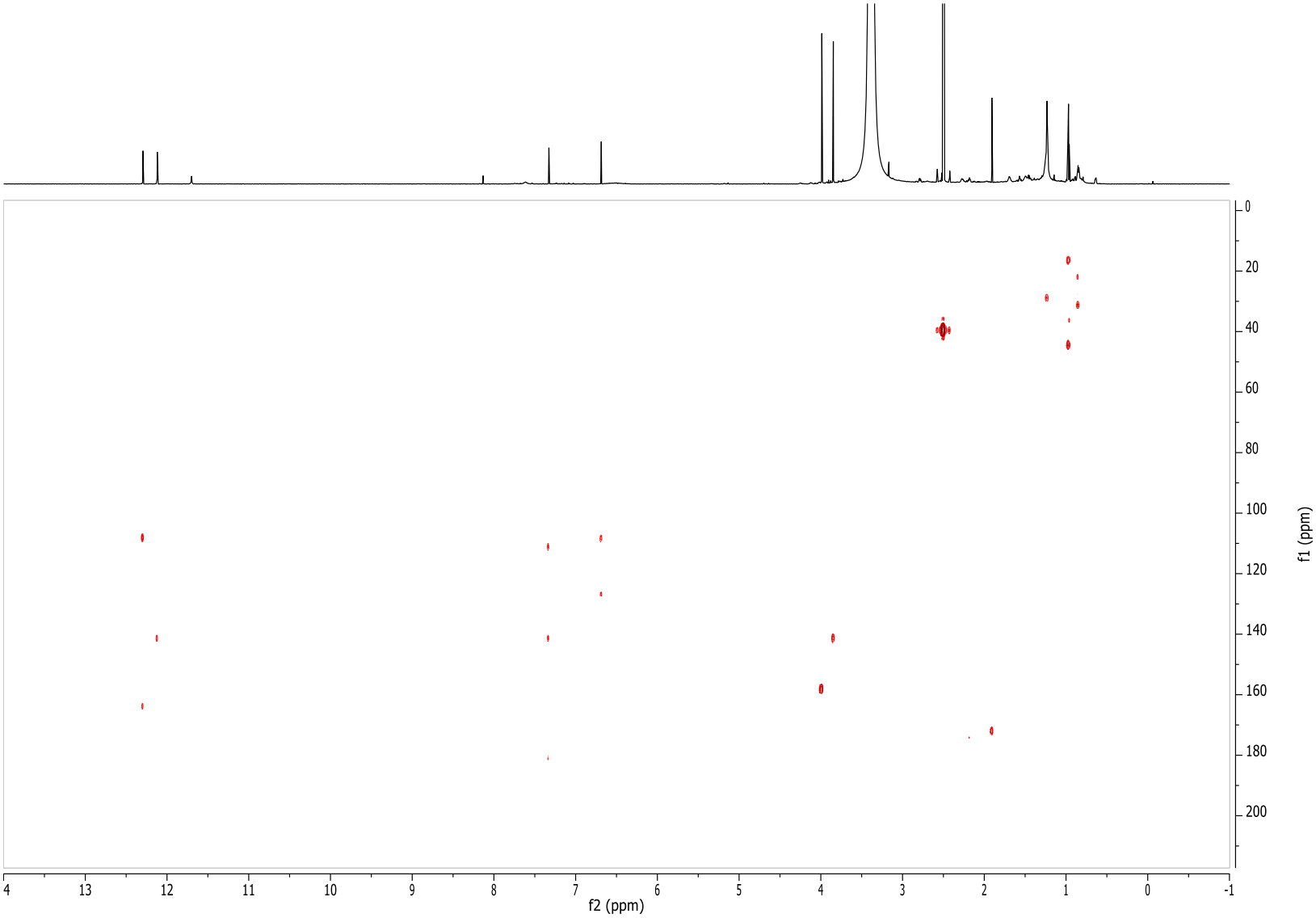
S20 2D-TOCSY Spectrum of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**) in DMSO-d_6



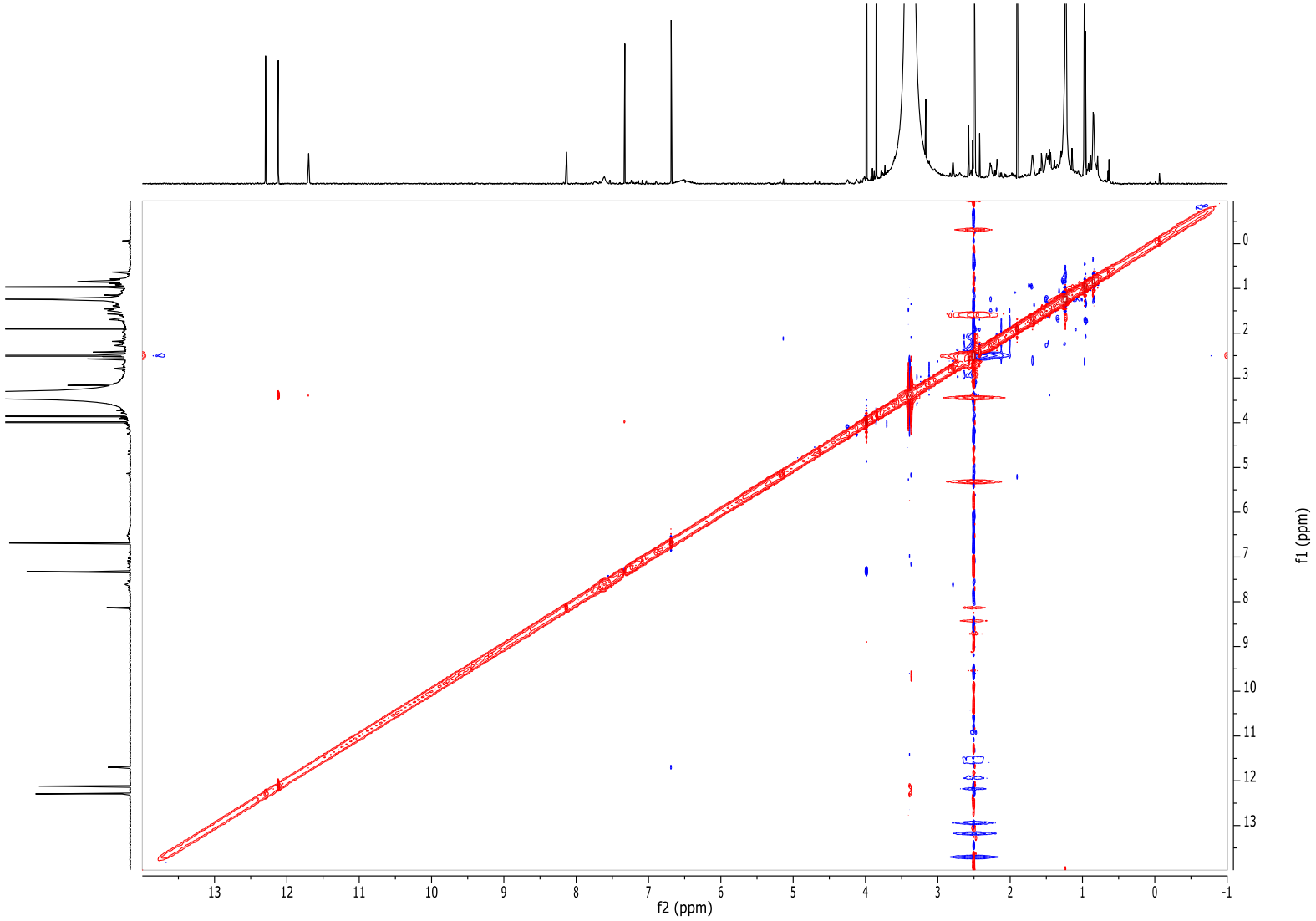
S21 HSQC Spectrum of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**) in DMSO-d_6



S22 HMBC Spectrum of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**) in DMSO-d_6

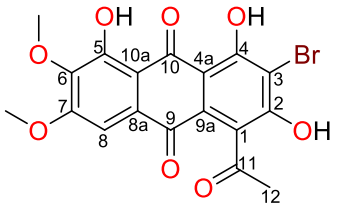


S23 ROESY Spectrum of 6-Methoxy-Rhodocomatulin 7-methyl ether (**3**) in DMSO-d_6



S24 NMR Table of 3-Bromo-6-methoxy-12-desethyl-rhodocomatulin 7-methyl ether (**4**)[a] in DMSO-d_6

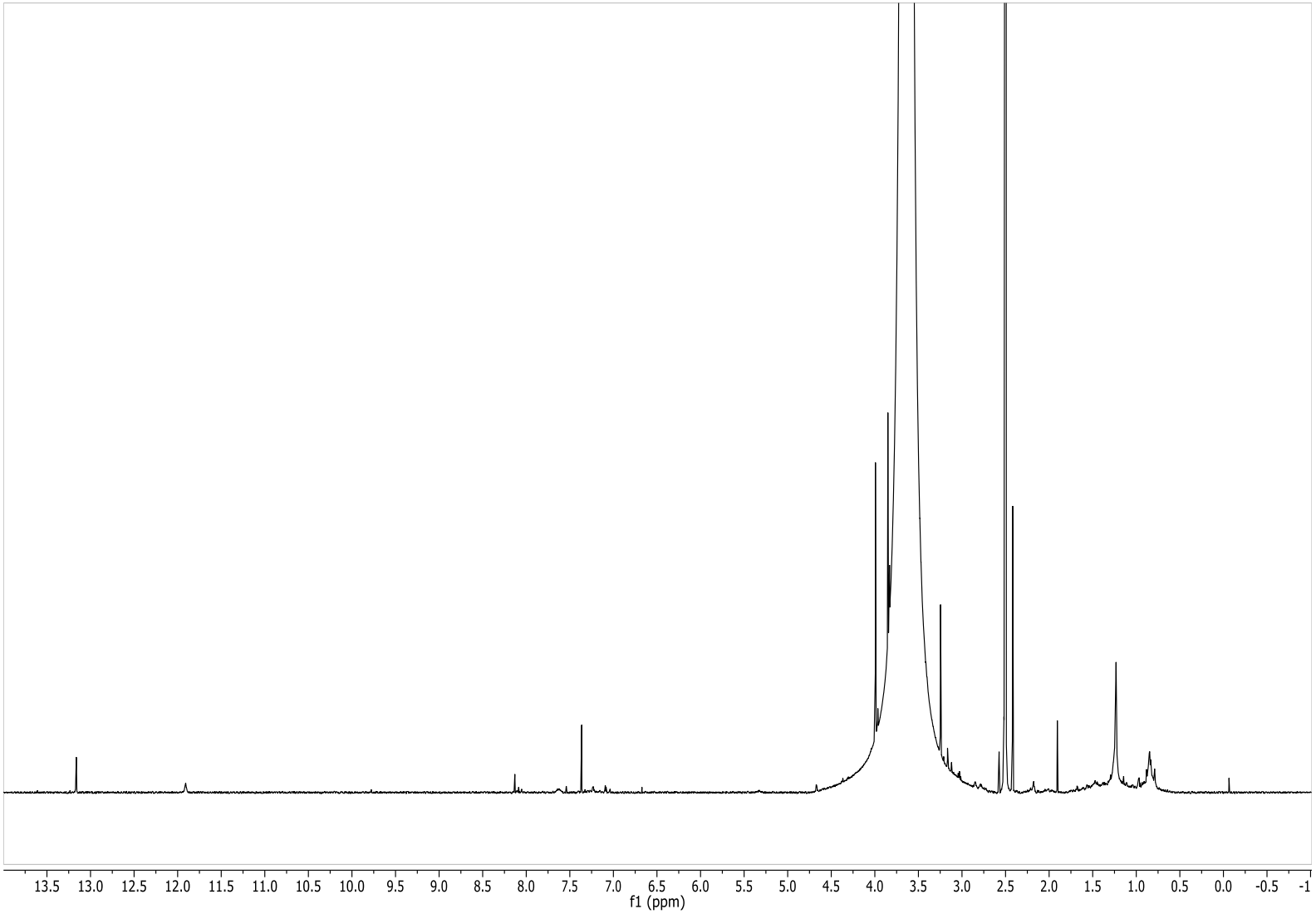
Position	**^{1}H, mult. (*J* in Hz)**	**^{13}C[b], type**	**HMBC**	**ROESY**
1		[c]		
2		[c]		
2-OH	11.93, br s	-		
3		106.1, C[d]		
4		160.3, C		
4-OH	12.29, s	-	3, 4, 4a	
4a		108.8, C[d]		
5		[c]		
5-OH	[c]	-		
6		141.5, C		
6-OMe	3.85, s	60.6, CH_3	6	
7		158.3, C		
7-OMe	3.99, s	56.7, CH_3	7	8
8	7.37, s	105.0, CH	6, 9, 10a	7-OMe
8a		[c]		
9		181.1, C		
9a		[c]		
10		[c]		
10a		111.3, C		
11		200.4, C		
12	2.42, s	31.0, CH_3	11	



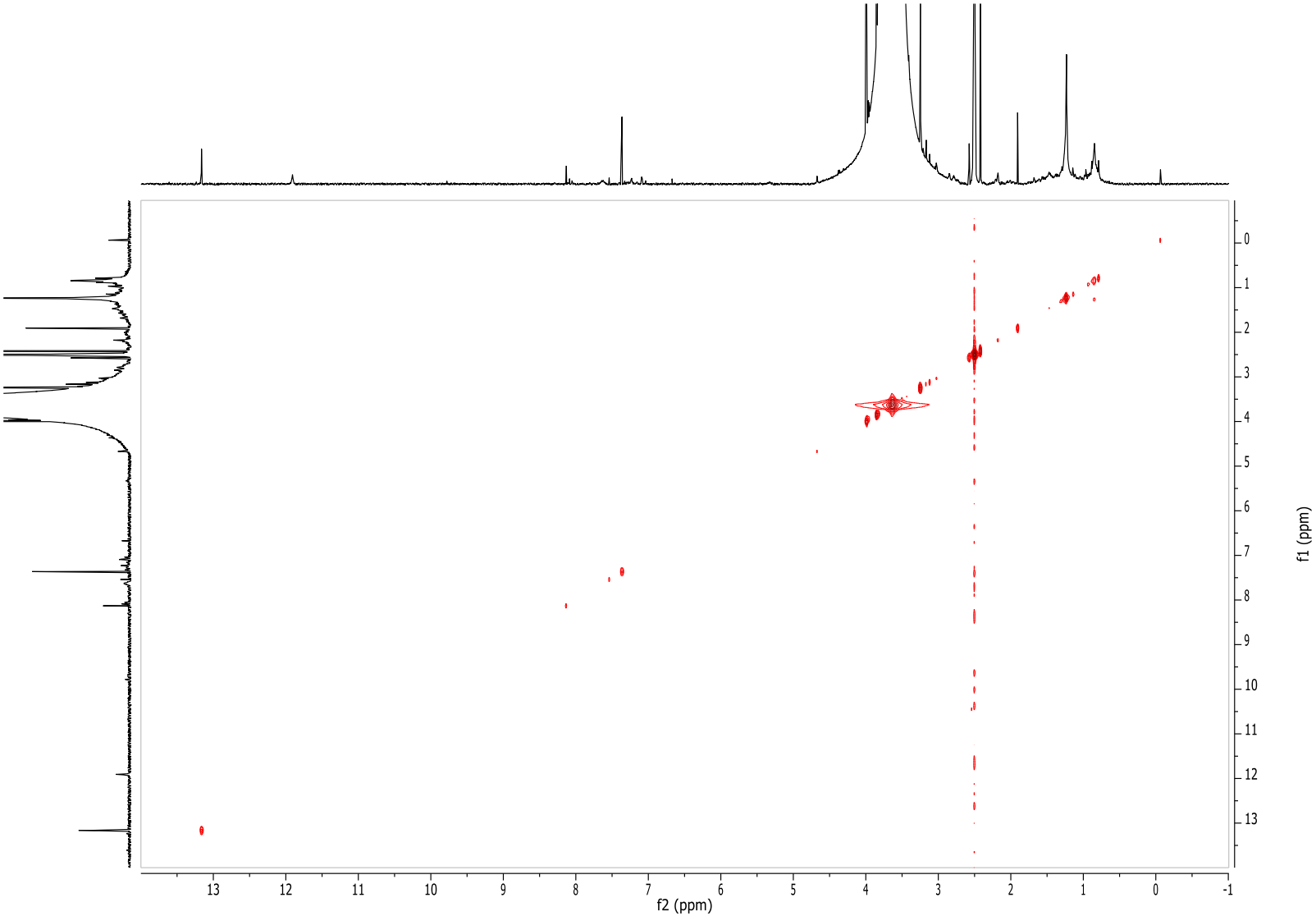
4

[a] Spectra recorded in DMSO-d_6 + trace TFA (^{1}H at 900 MHz) at 25°C
[b] ^{13}C chemical shift obtained through 2D HSQC and HMBC experiments
[c] Not observed
[d] Signals are interchangeable

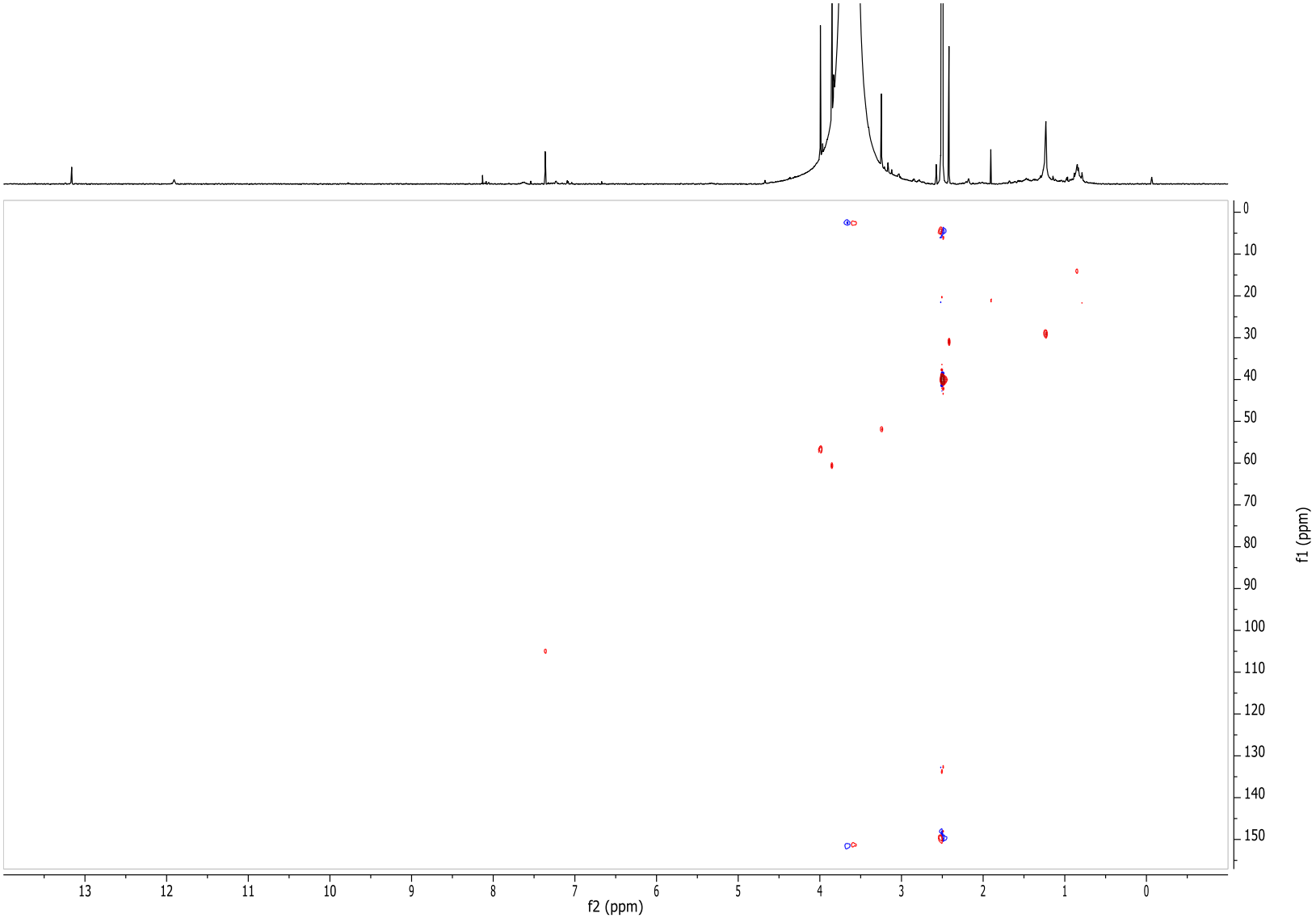
S25 ^{1}H NMR Spectrum of 3-Bromo-6-methoxy-12-desethyl-rhodocomatulin 7-methyl ether (**4**) in DMSO-d_6



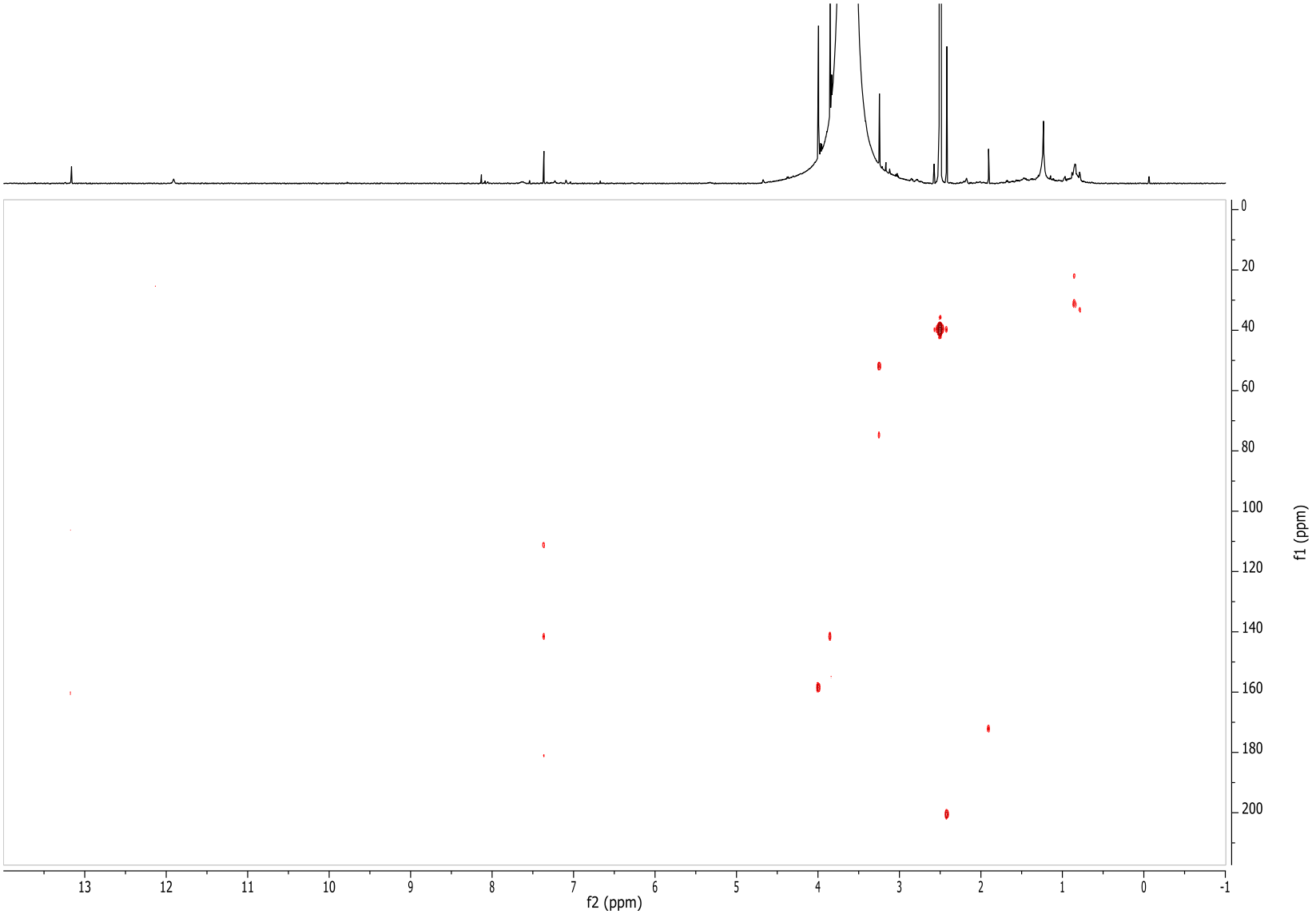
S26 COSY Spectrum of 3-Bromo-6-methoxy-12-desethyl-rhodocomatulin 7-methyl ether (**4**) in DMSO-d_6



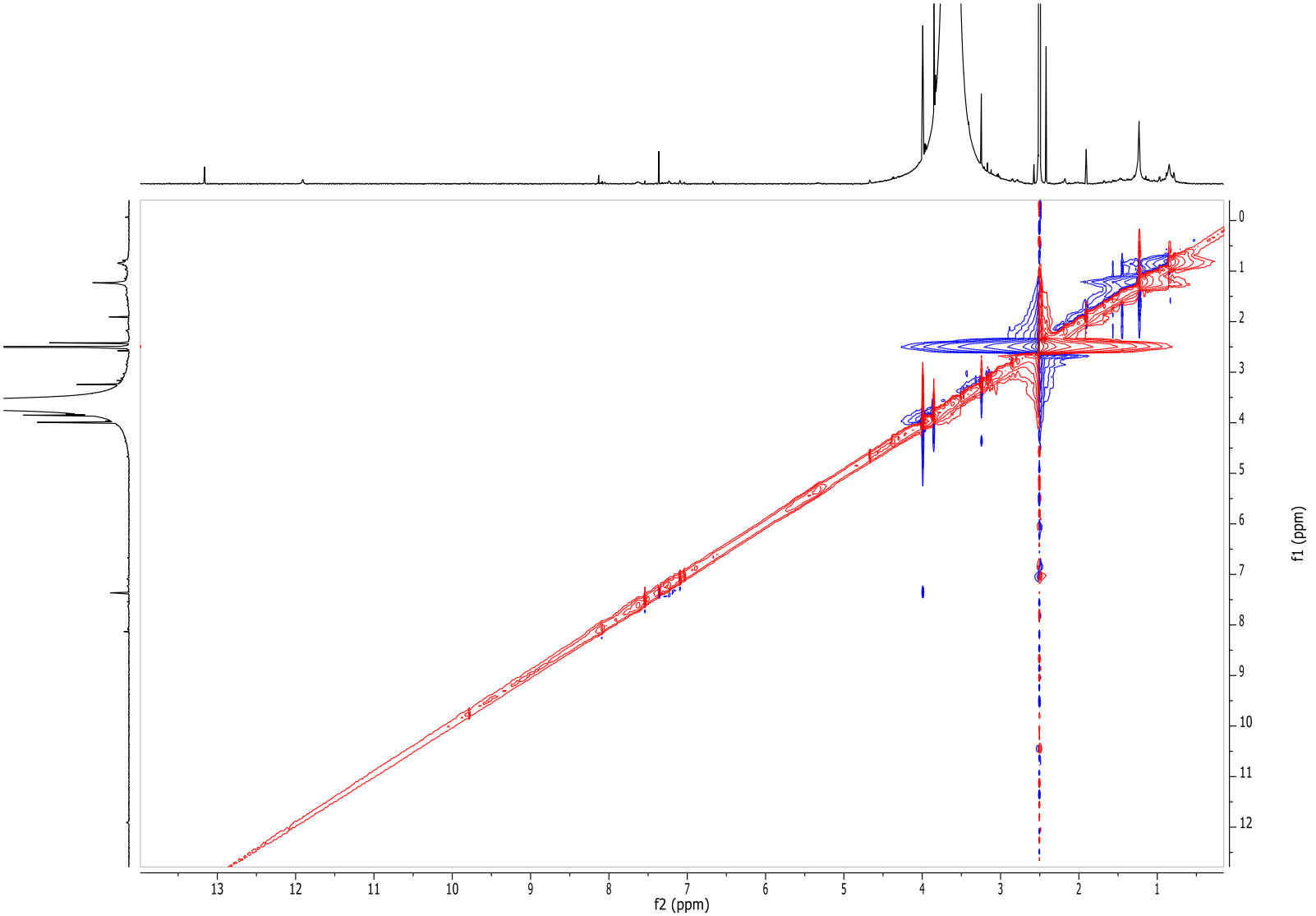
S27 HSQC Spectrum of 3-Bromo-6-methoxy-12-desethyl-rhodocomatulin 7-methyl ether (**4**) in DMSO-d_6



S28 HMBC Spectrum of 3-Bromo-6-methoxy-12-desethyl-rhodocomatulin 7-methyl ether (**4**) in DMSO-d_6

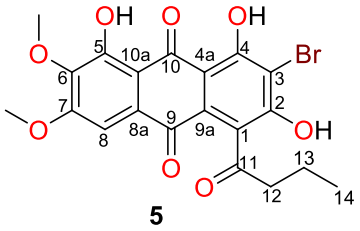


S29 ROESY Spectrum of 3-Bromo-6-methoxy-12-desethyl-rhodocomatulin 7-methyl ether (**4**) in DMSO-d_6



S30 NMR Table of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**)[a] in DMSO-d_6

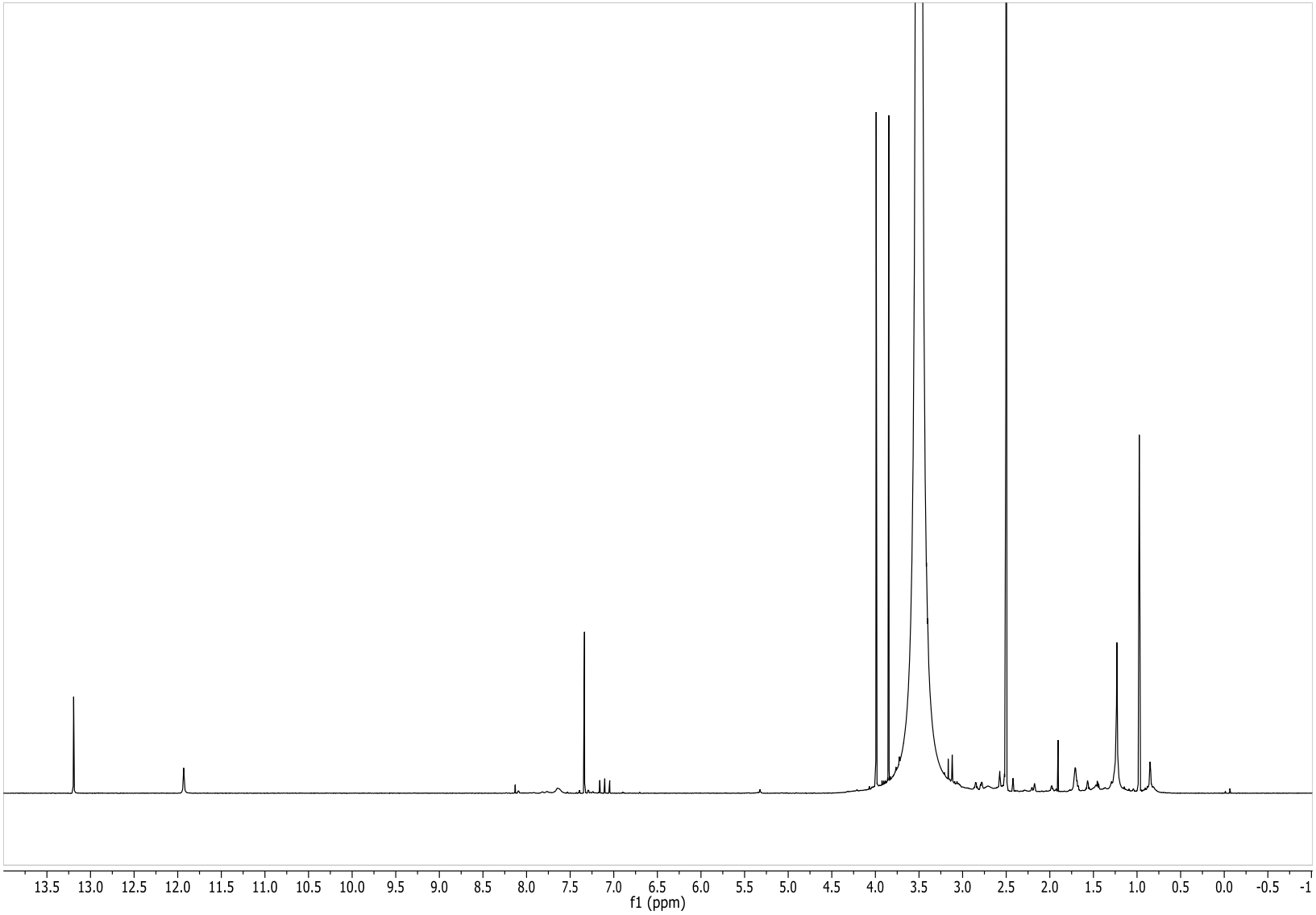
Position	^{1}H, mult. (*J* in Hz)	^{13}C,[b] type	HMBC	ROESY
1		[c]		
2		[c]		
2-OH	11.94, br s	-		
3		105.9, C[d]		
4		160.7, C		
4-OH	13.19, s	-	3, 4, 4a	
4a		108.8, C[d]		
5		[c]		
5-OH	[c]	-		
6		141.4, C		
6-OMe	3.85, s	60.1, CH_3	6	
7		158.2, C		
7-OMe	3.99, s	56.8, CH_3	7	8
8	7.34, s	104.9, CH	6, 7, 8a, 9, 10a	7-OMe
8a		128.4, C		
9		181.0, C		
9a		[c]		
10		[c]		
10a		111.2, C		
11		[c]		
12	2.65, br t (7.6)	44.5, CH_2		13
13	1.71, qt (7.6, 7.6)	16.6, CH_2		12, 14
14	0.97, t (7.6)	13.7, CH_3	12, 13	13



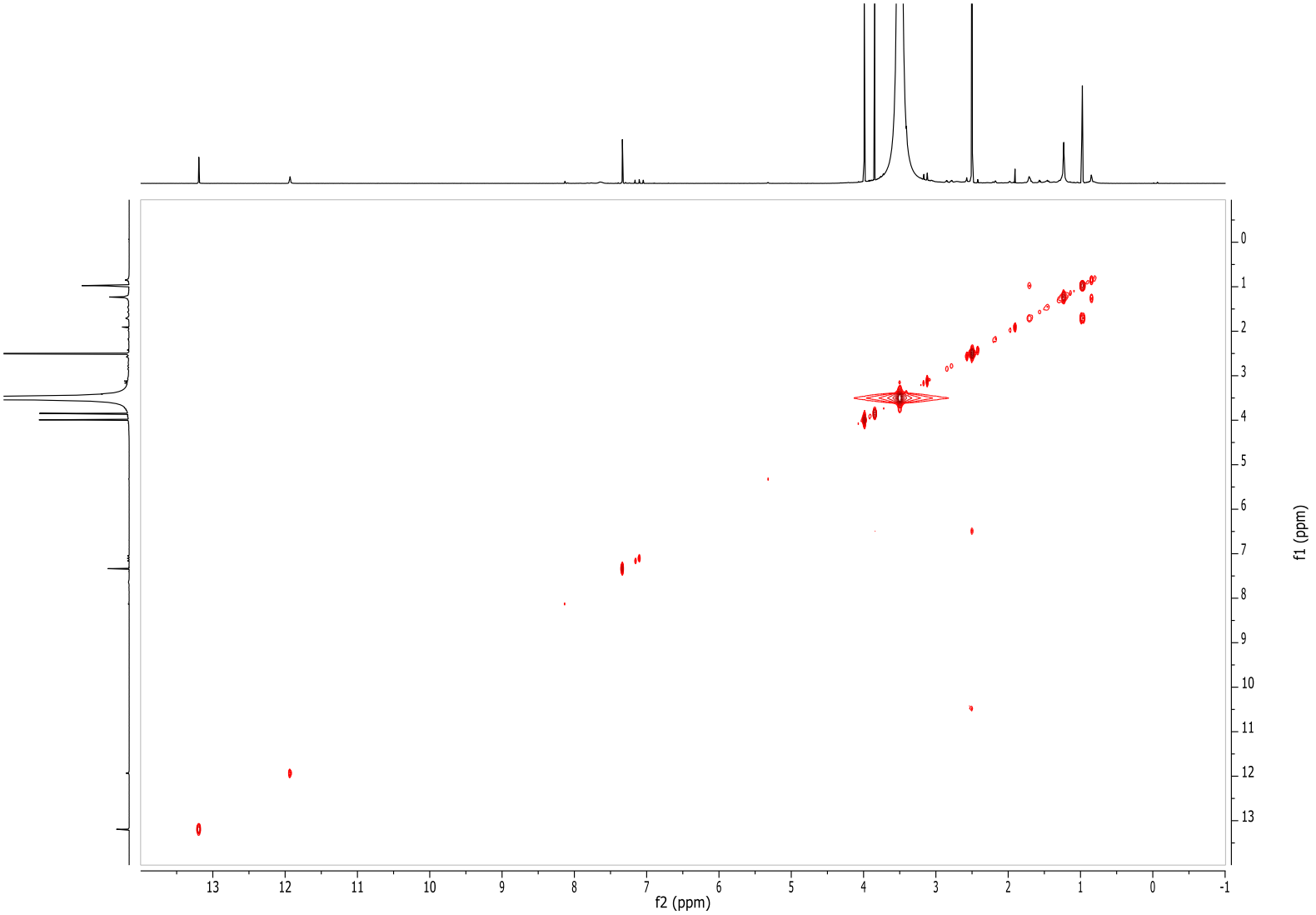
5

[a] Spectra recorded in DMSO-d_6 (^{1}H at 900 MHz) at 25°C
[b] ^{13}C chemical shift obtained through 2D HSQC and HMBC experiments
[c] Not observed
[d] Signals are interchangeable

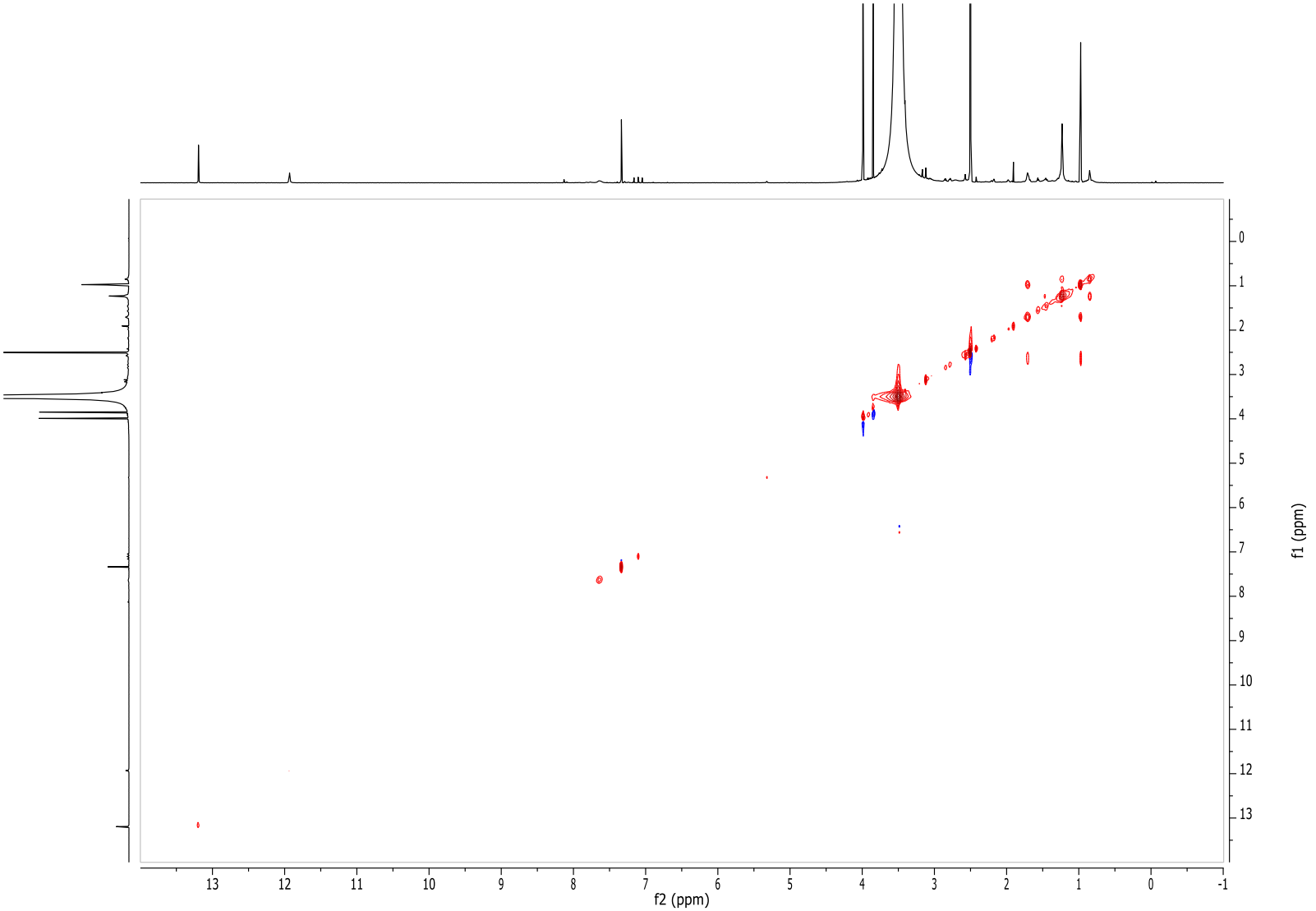
S31 ^{1}H NMR Spectrum of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**) in DMSO-d_6



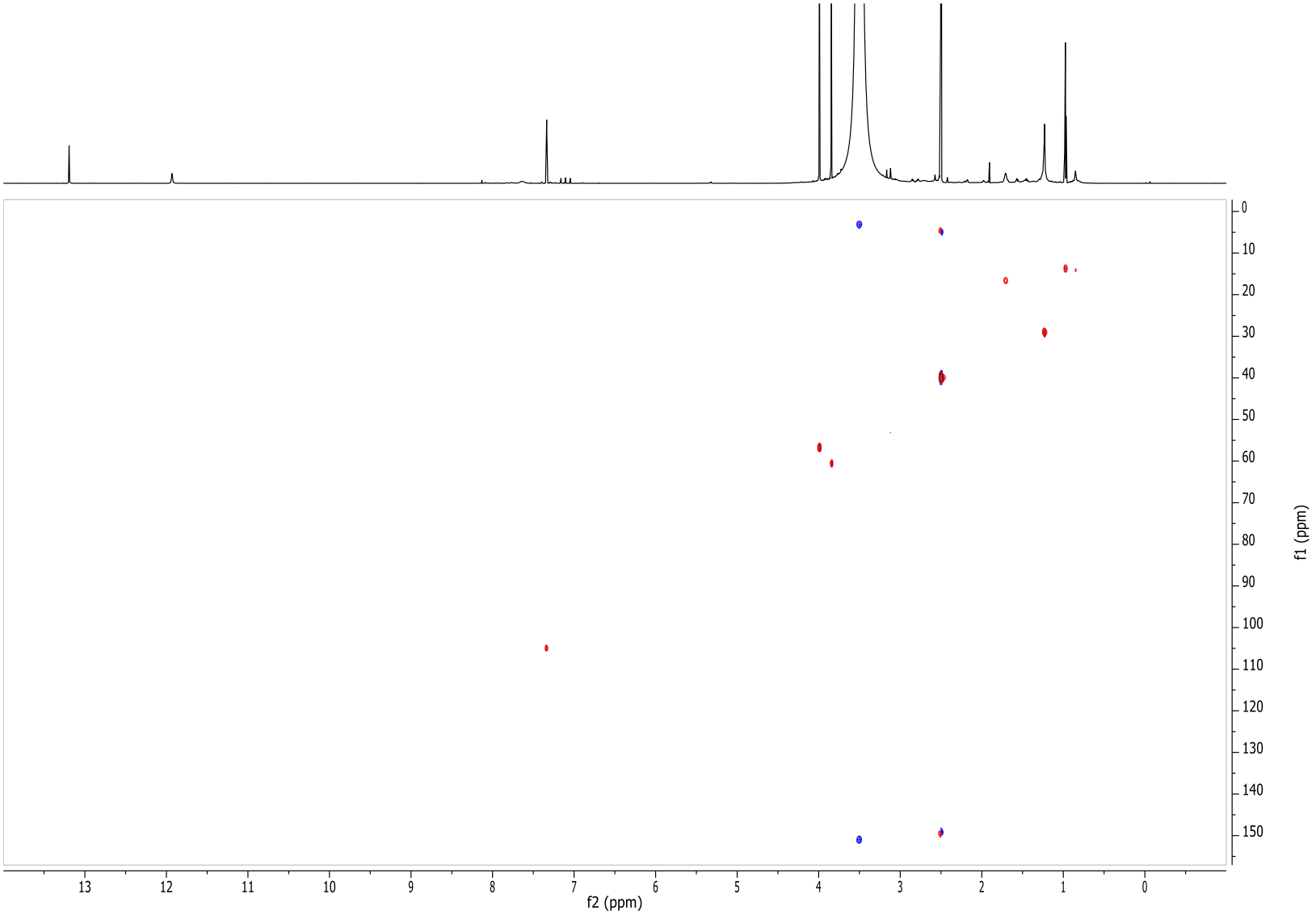
S32 COSY Spectrum of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**) in DMSO-d_6



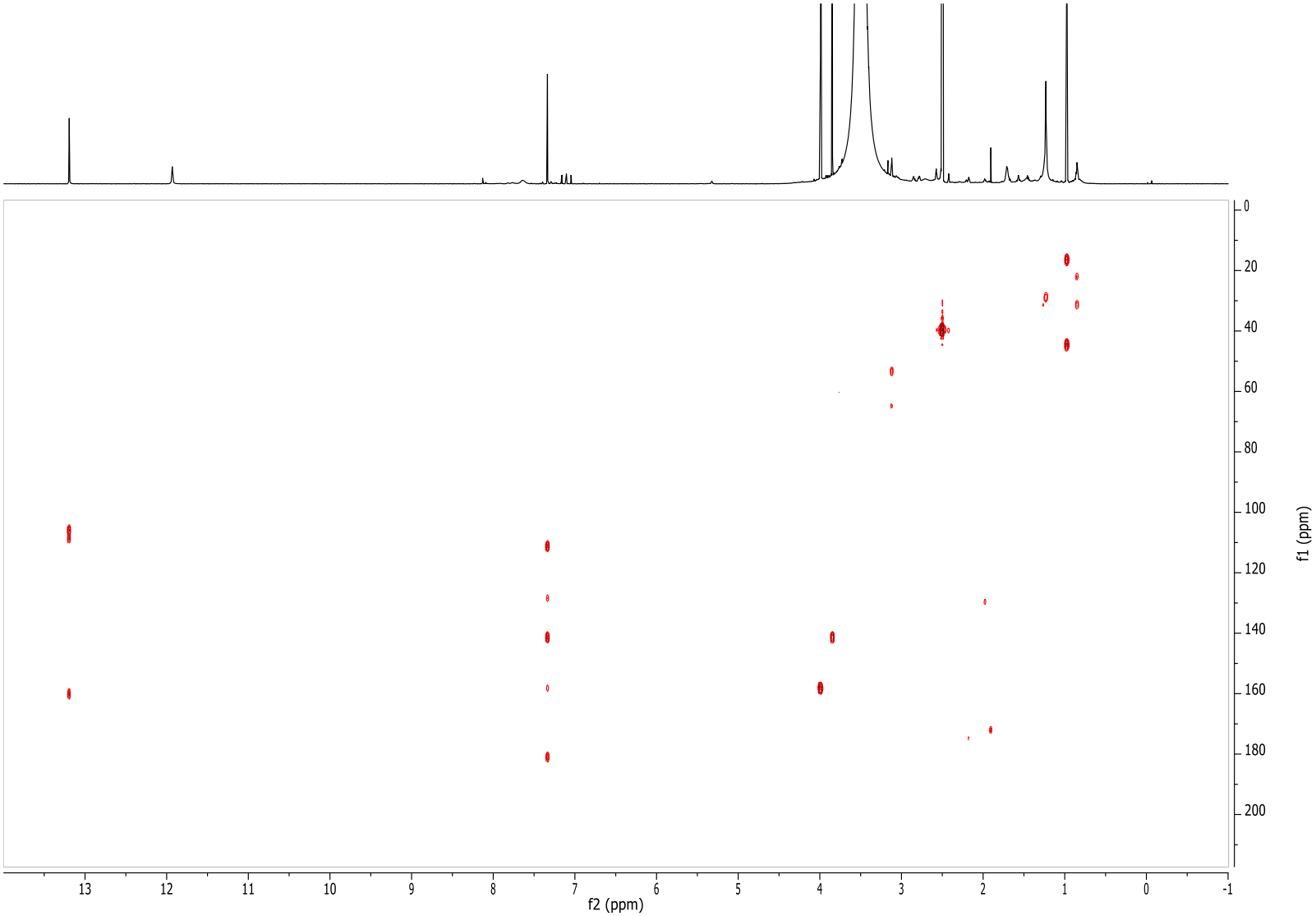
S33 2D-TOCSY Spectrum of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**) in DMSO-d_6



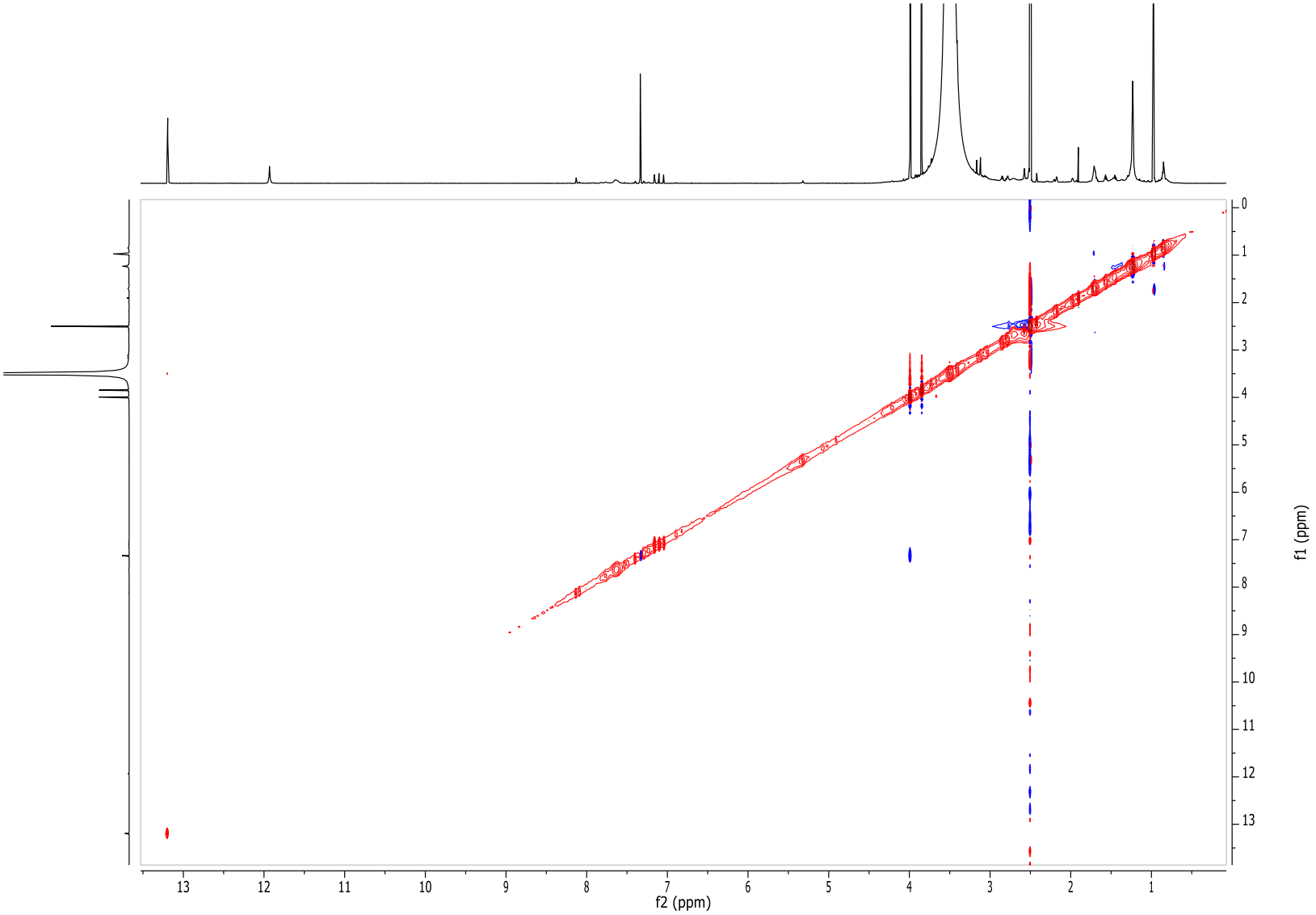
S34 HSQC Spectrum of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**) in DMSO-d_6



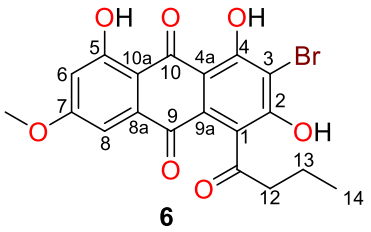
S35 HMBC Spectrum of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**) in DMSO-d_6



S36 ROESY Spectrum of 3-Bromo-6-methoxy-rhodocomatulin 7-methyl ether (**5**) in DMSO-d_6



S37 NMR Table of 3-Bromo-rhodocomatulin 7-methyl ether (**6**)[a] in DMSO-d_6

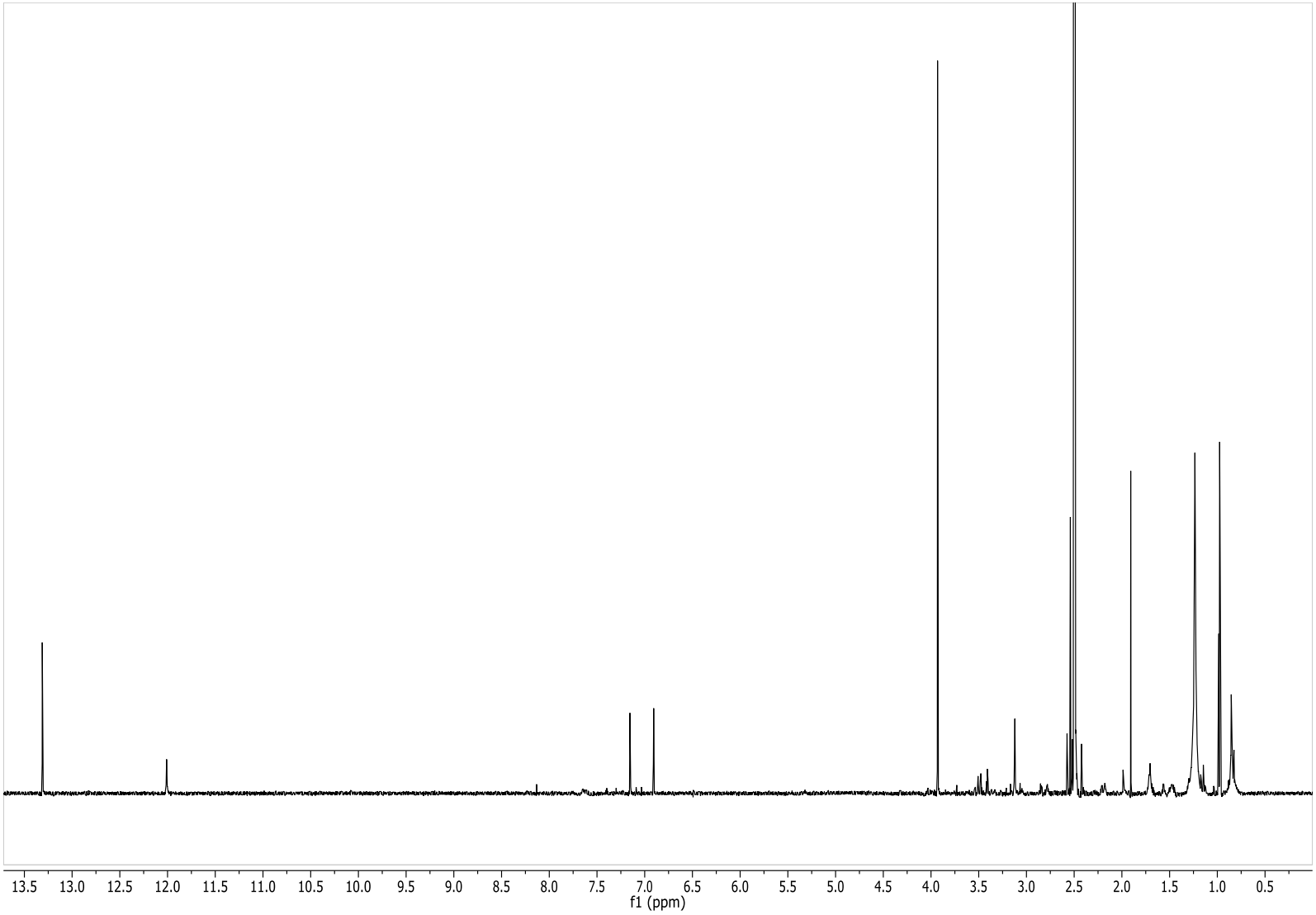


6

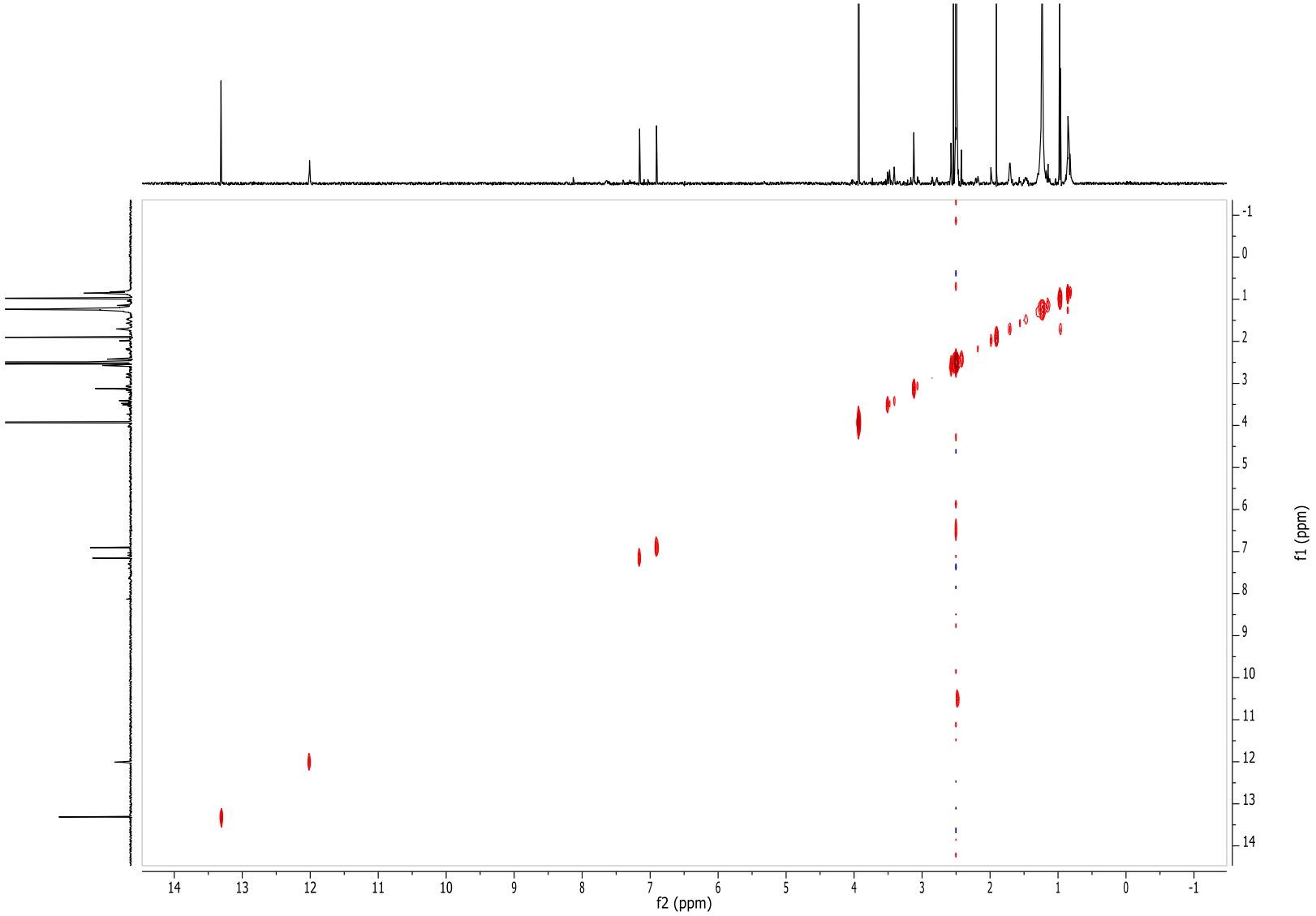
Position	^{1}H, mult. (*J* in Hz)	^{13}C,[b] type	HMBC	ROESY
1		[c]		
2		[c]		
2-OH	12.01, br s	-		
3		105.9, C[d]		
4		160.7, C		
4-OH	13.31, s	-	3, 4, 4a	
4a		108.8, C[d]		
5		[c]		
5-OH	[c]	-		
6	6.91, d (2.5)	107.3, CH	8, 10a	7-OMe
7		166.0, C		
7-OMe	3.93, s	56.7, CH_3	7	6, 8
8	7.16, d (2.5)	108.0, CH		7-OMe
8a		[c]		
9		[c]		
9a		[c]		
10		[c]		
10a		108.6, C		
11		[c]		
12	2.64, br t (7.6)	44.5, CH_2		13
13	1.71, qt (7.6, 7.6)	16.7, CH_2		12, 14
14	0.98, t (7.6)	13.7, CH_3	12, 13	13

[a] Spectra recorded in DMSO-d_6 + trace TFA (^{1}H at 900 MHz) at 25°C
[b] ^{13}C chemical shift obtained through 2D HSQC and HMBC experiments
[c] Not observed
[d] Signals are interchangeable

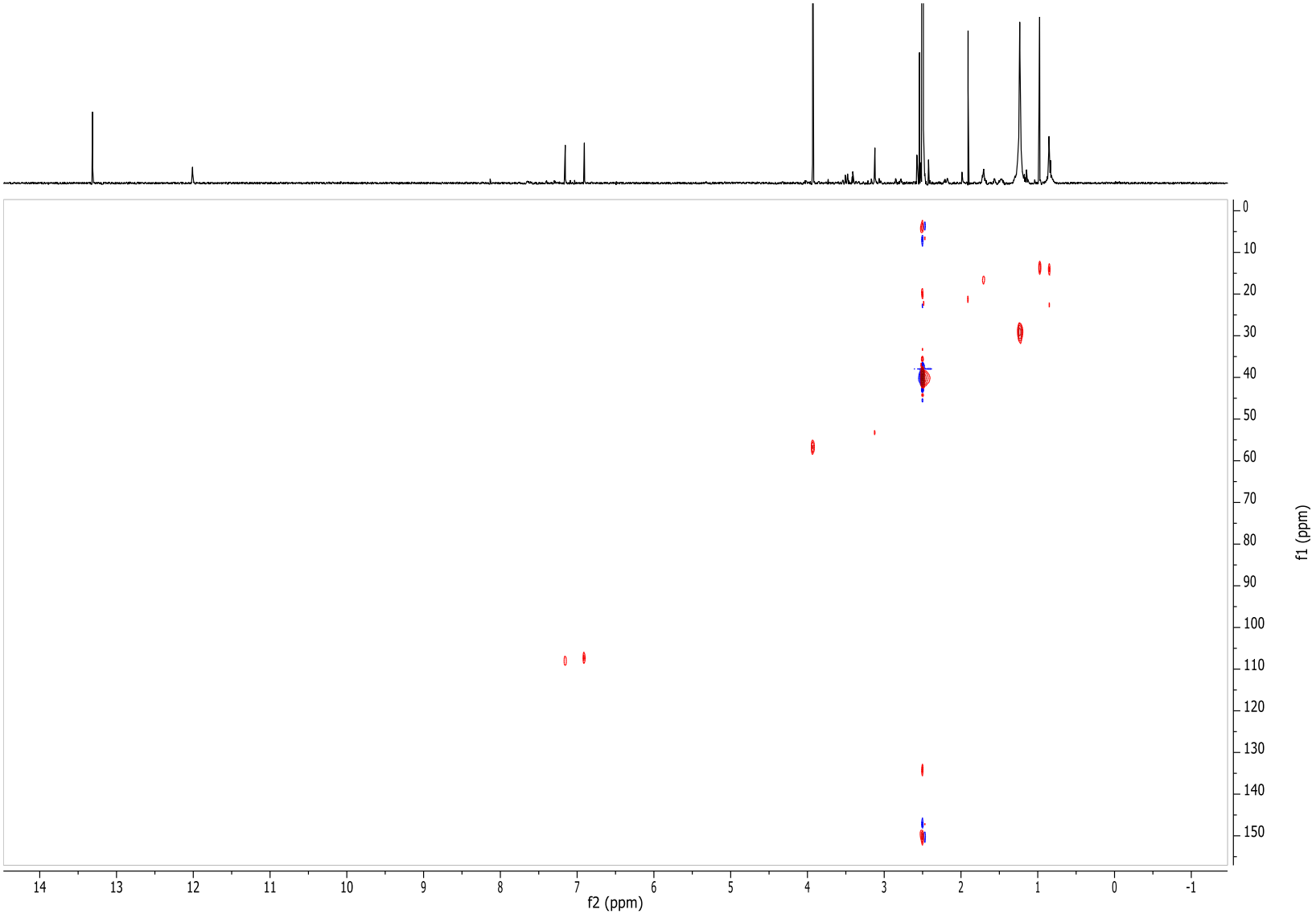
S38 ^{1}H NMR Spectrum of 3-Bromo-rhodocomatulin 7-methyl ether (**6**) in DMSO-d_6



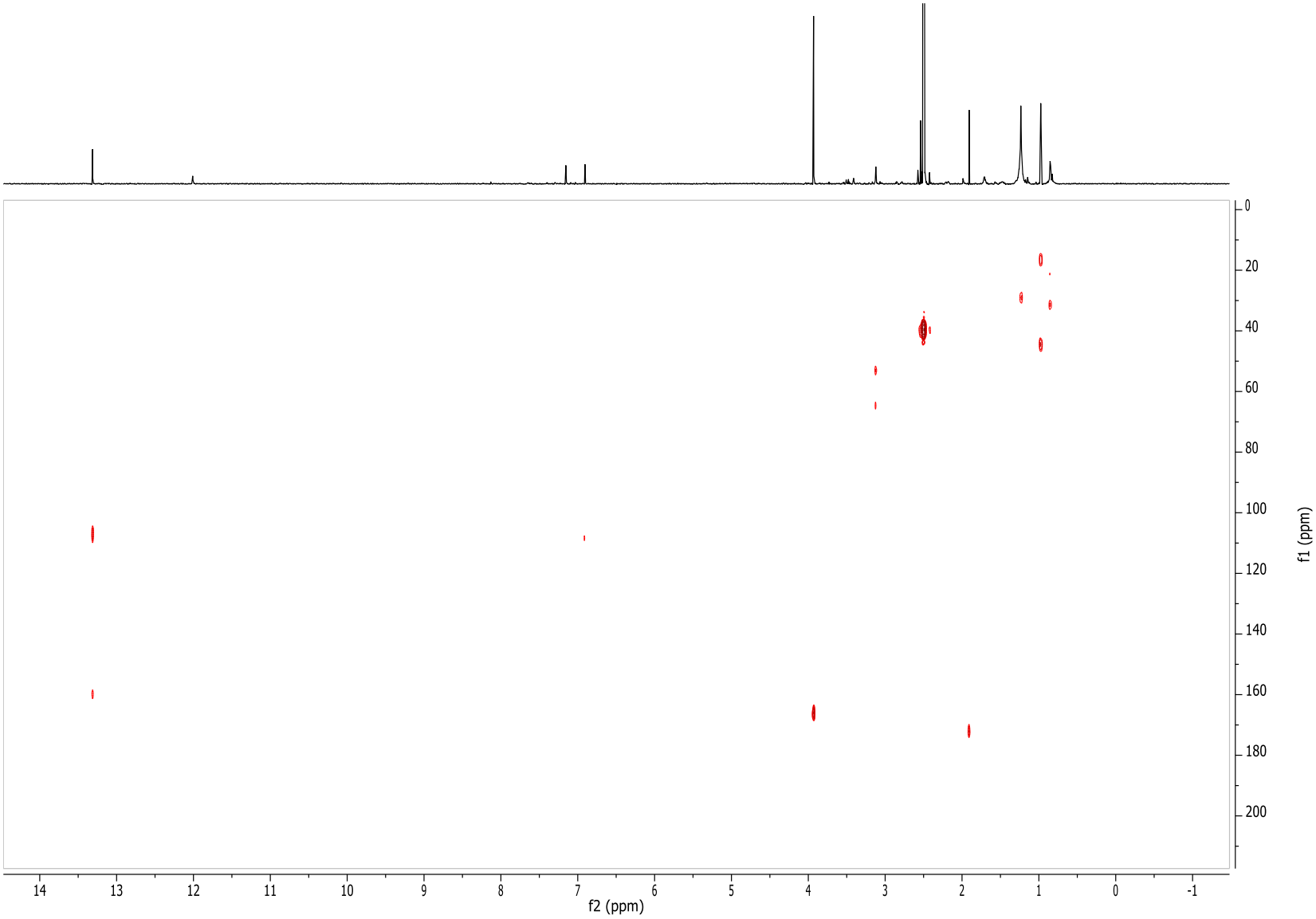
S39 COSY Spectrum of 3-Bromo-rhodocomatulin 7-methyl ether (**6**) in DMSO-d_6



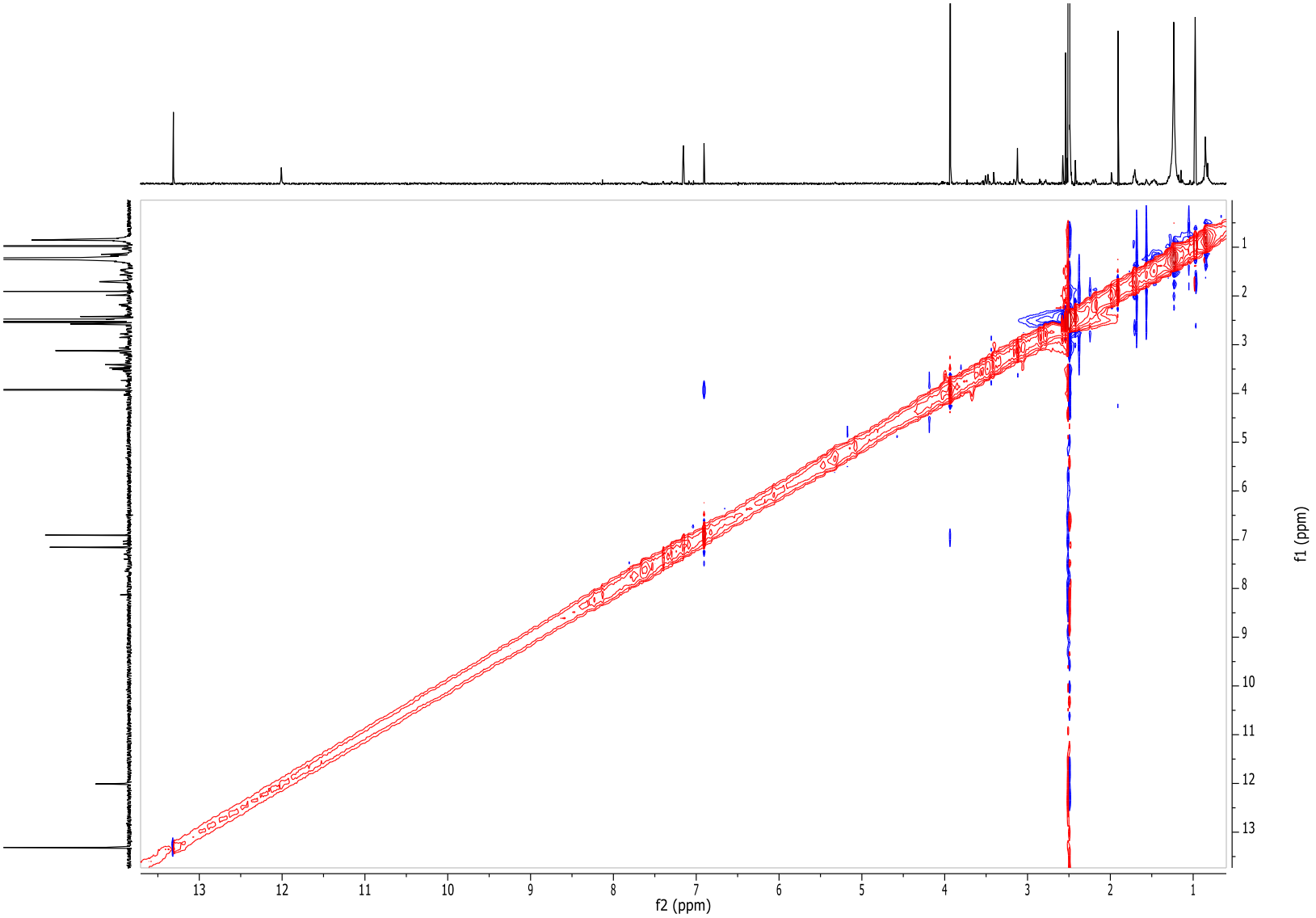
S40 HSQC Spectrum of 3-Bromo-rhodocomatulin 7-methyl ether (**6**) in DMSO-d_6



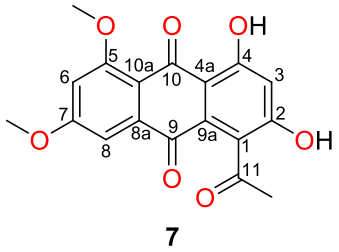
S41 HMBC Spectrum of 3-Bromo-rhodocomatulin 7-methyl ether (**6**) in DMSO-d_6



S42 ROESY Spectrum of 3-Bromo-rhodocomatulin 7-methyl ether (**6**) in DMSO-d_6



S43 NMR Table of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**)[a] in DMSO-d_6

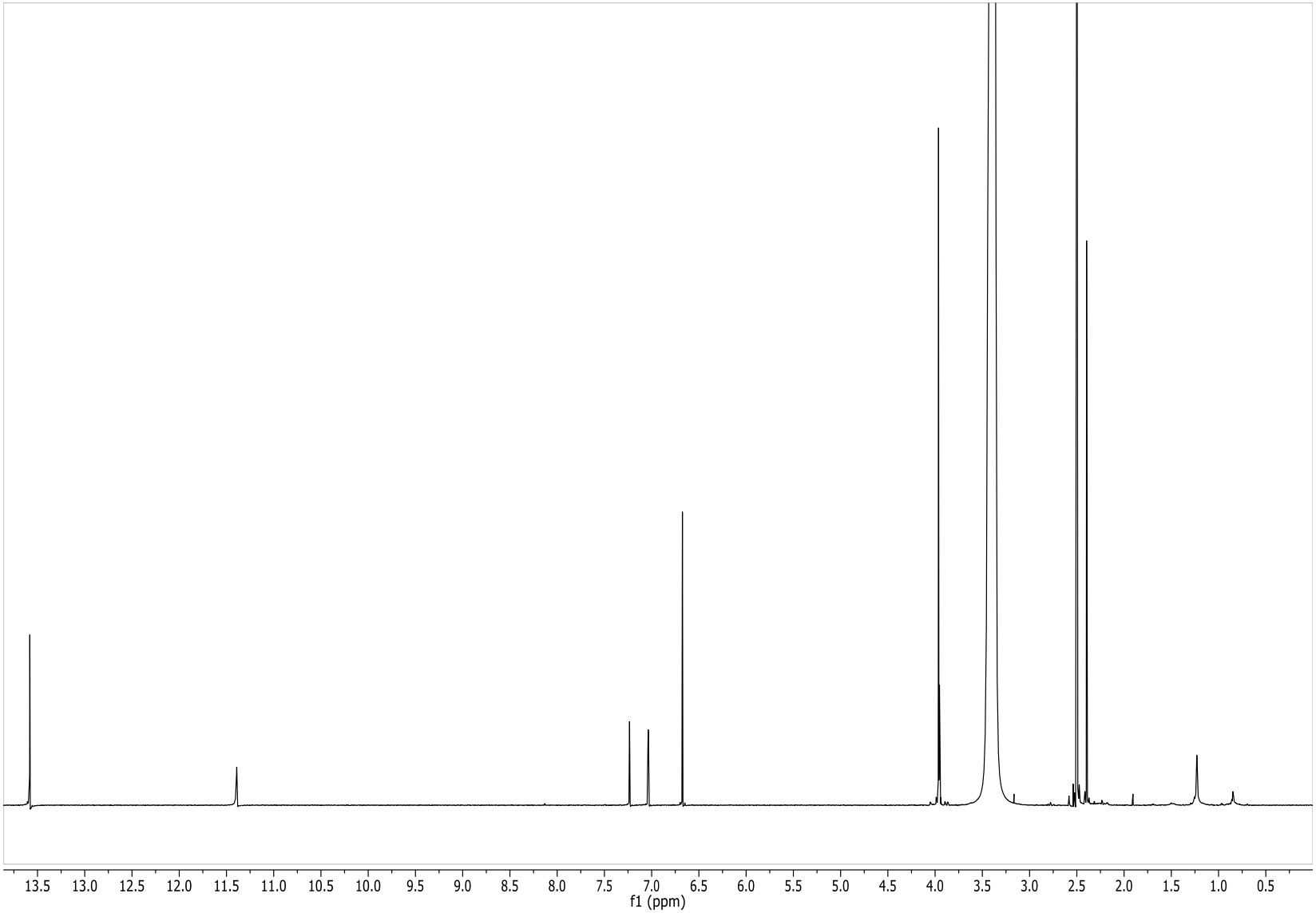


7

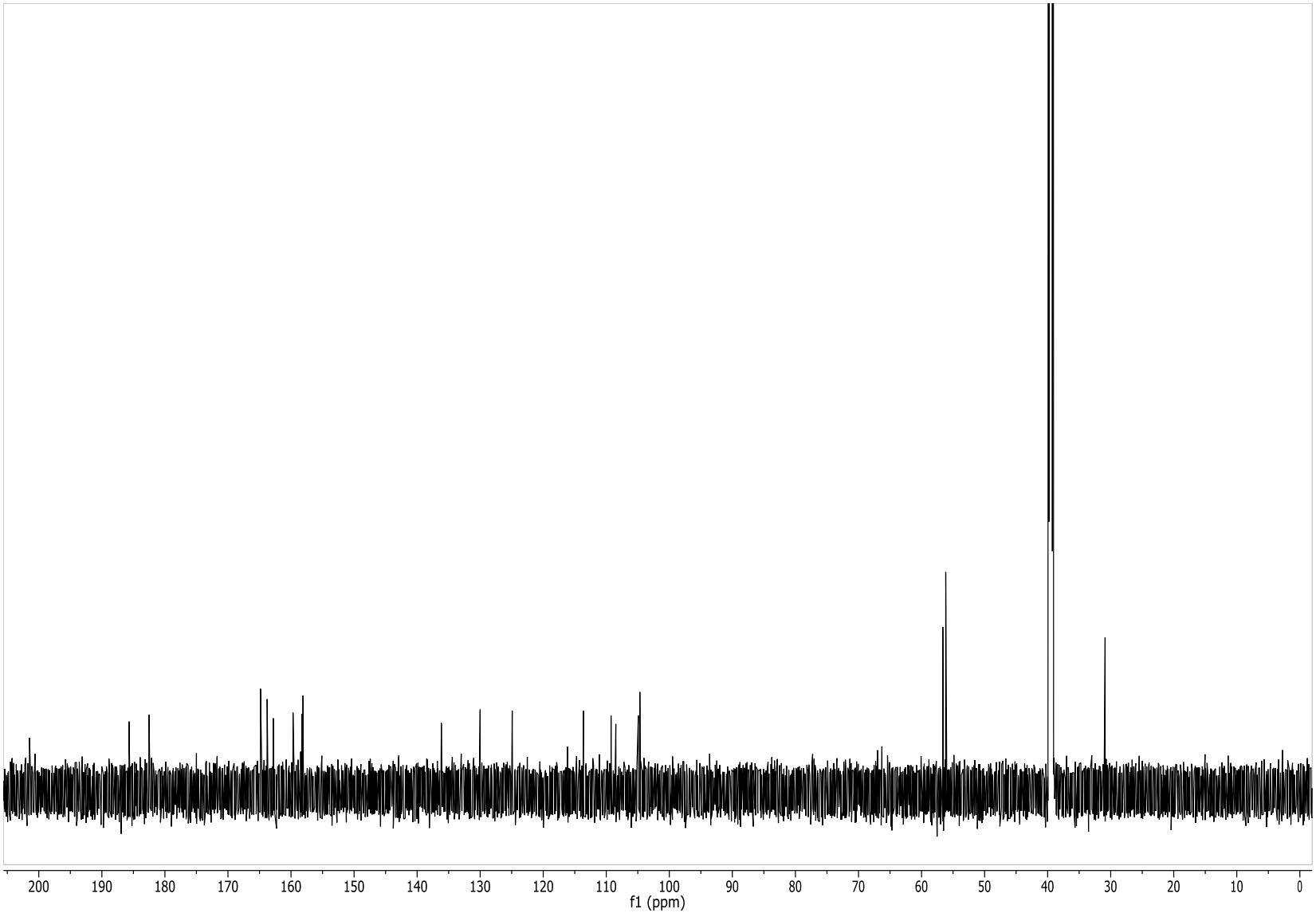
Position	^{1}H, mult. (*J* in Hz)	^{13}C, type	HMBC	ROESY
1		124.9, C		
2		159.7, C		
2-OH	11.37, br s	-		3
3	6.67, s	108.5, CH	1, 2, 4, 4a	2-OH, 4-OH
4		163.8, C		
4-OH	13.58, s	-	3, 4, 4a	3
4a		109.3, C		
5		162.8, C		
5-OMe	3.96, s	56.1, CH_3	5	6
6	7.04, d (2.5)	104.9, CH	5, 7, 8, 10a	5-OMe, 7-OMe
7		164.8, C		
7-OMe	3.97, s	56.6, CH_3	7	6, 8
8	7.24, d (2.5)	104.6, CH	6, 9, 10a	7-OMe
8a		130.0, C[b]		
9		182.5, C		
9a		136.1, C[b]		
10		185.7, C		
10a		113.4		
11		201.2, C		
12	2.39, s	30.5, CH_3	1, 11	

[a] ^{1}H NMR spectrum recorded in DMSO-d_6 + trace TFA (^{1}H at 800 MHz, ^{13}C at 200 MHz) at 25°C
[b] Signals are interchangeable

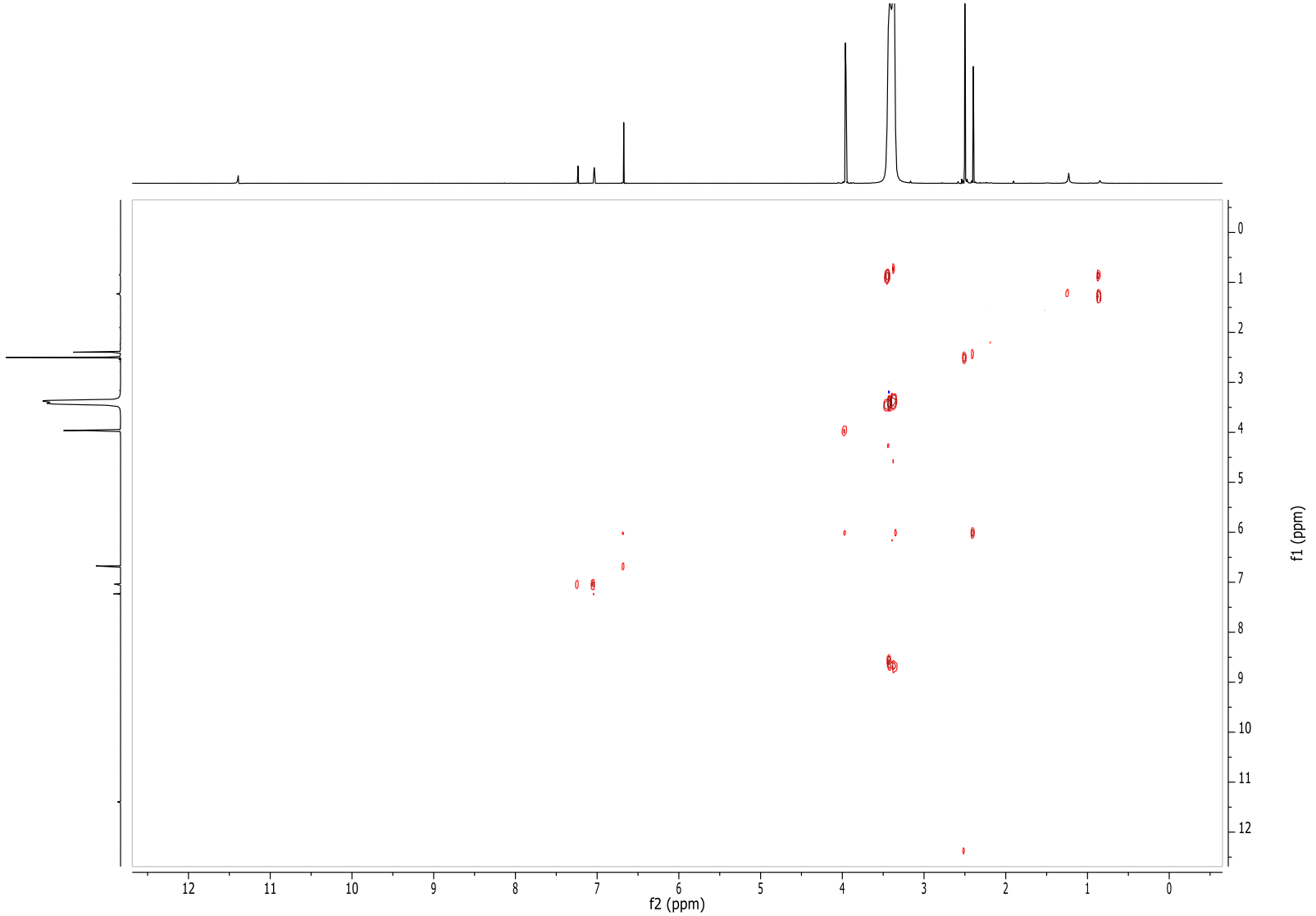
S44 ^{1}H NMR Spectrum of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**) in DMSO-d_6



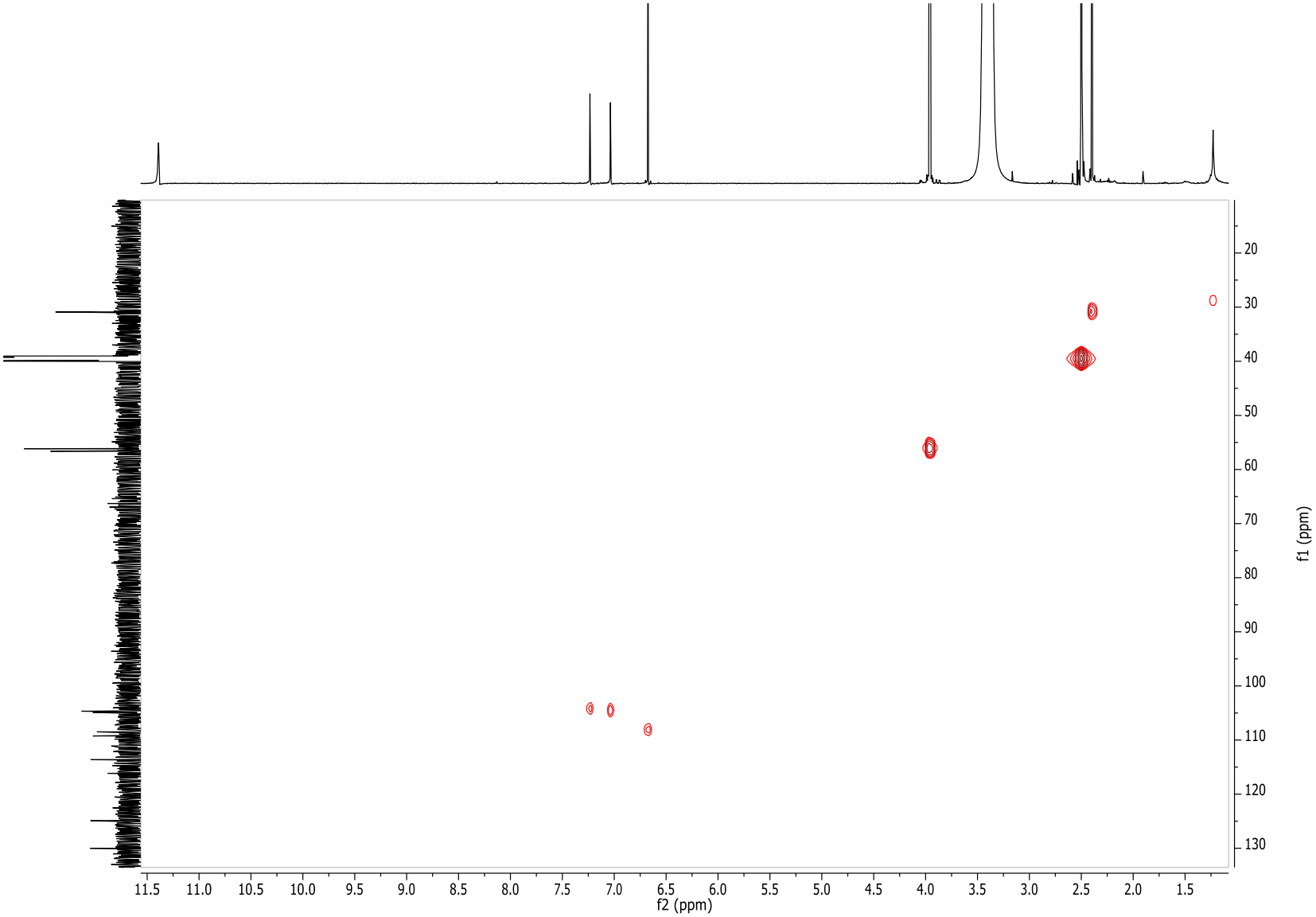
S45 ^{13}C NMR Spectrum of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**) in DMSO-d_6



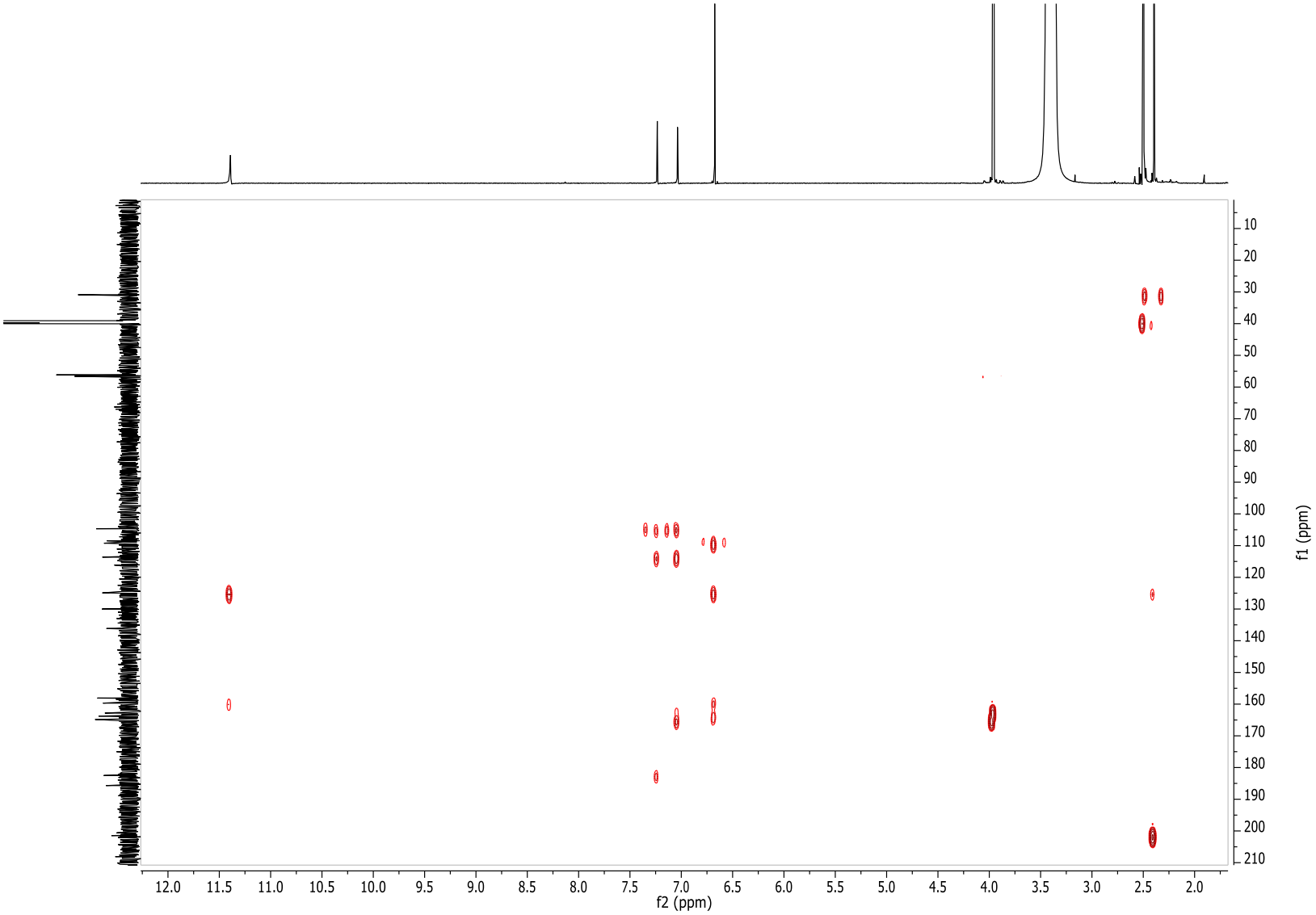
S46 COSY Spectrum of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**) in DMSO-d_6



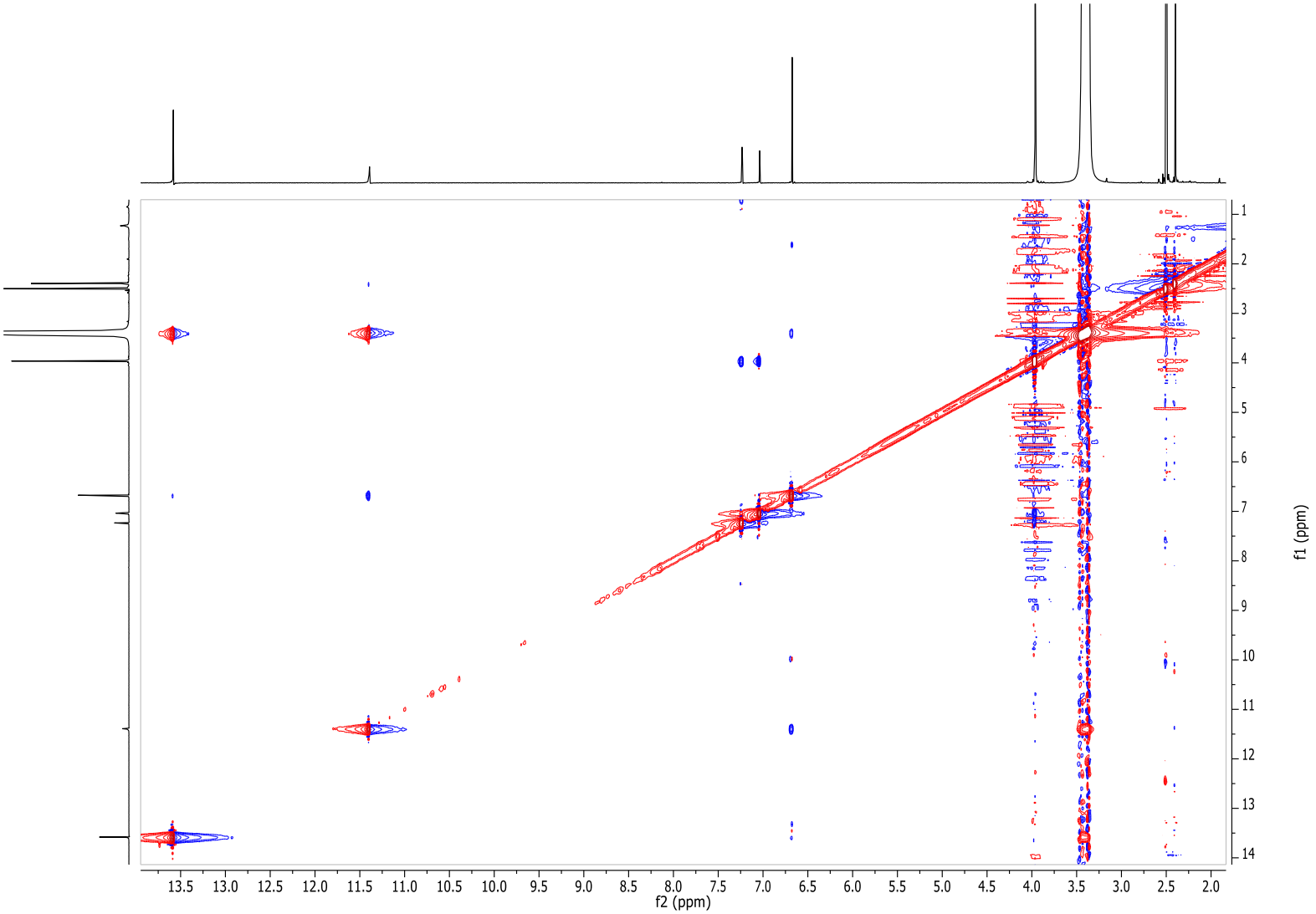
S47 HSQC Spectrum of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**) in DMSO-d_6



S48 HMBC Spectrum of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**) in DMSO-d_6

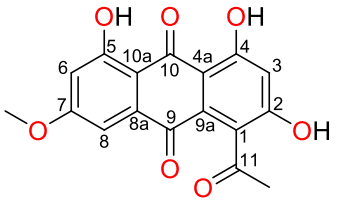


S49 ROESY Spectrum of 12-Desethyl-rhodocomatulin 5,7-dimethyl ether (**7**) in DMSO-d_6



S50 NMR Table of 12-Desethyl-rhodocomatulin 7-methyl ether (**8**)[a] in DMSO-d_6

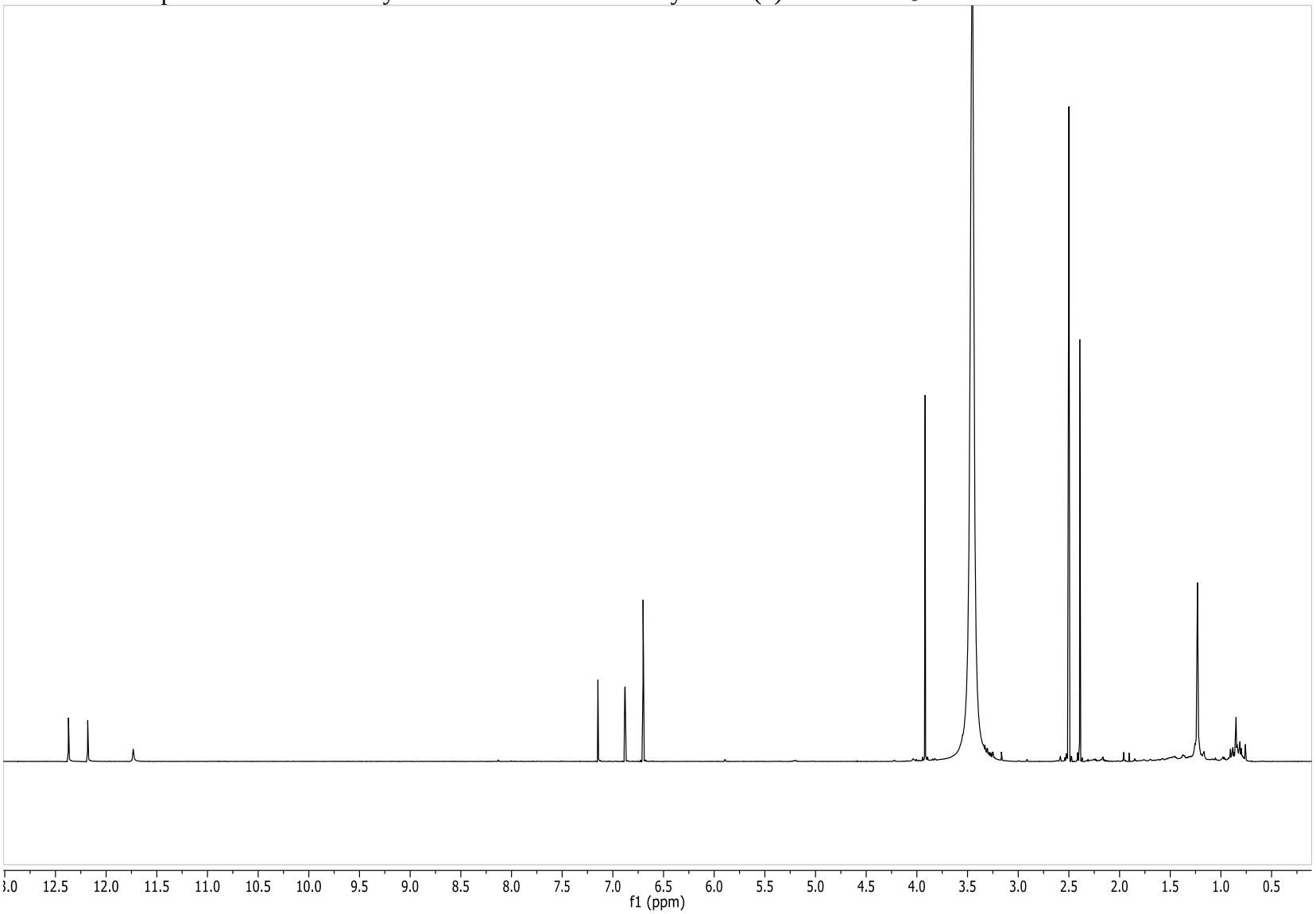
Position	^{1}H, mult. (*J* in Hz)	^{13}C, type	HMBC	ROESY
1		126.6, C		
2		161.2, C		
2-OH	11.68, br s	-		3
3	6.70, s	108.1, CH	1, 2, 4, 4a	2-OH, 4-OH
4		163.5, C		
4-OH	12.37, s	-	3, 4, 4a	3
4a		108.1, C		
5		163.8, C		
5-OH	12.18, s		5, 6, 10a	6
6	6.89, d (2.5)	107.0, CH	5, 7, 8, 10a	5-OH, 7-OMe
7		165.7, C		
7-OMe	3.92, s	56.1, CH_3	7	6, 8
8	7.16, d (2.5)	107.4, CH	6, 9, 10a	7-OMe
8a		130.9, C[b]		
9		181.8, C		
9a		134.3, C[b]		
10		188.9, C		
10a		109.5, C		
11		201.2, C		
12	2.40, s	30.8, CH_3	1, 11	



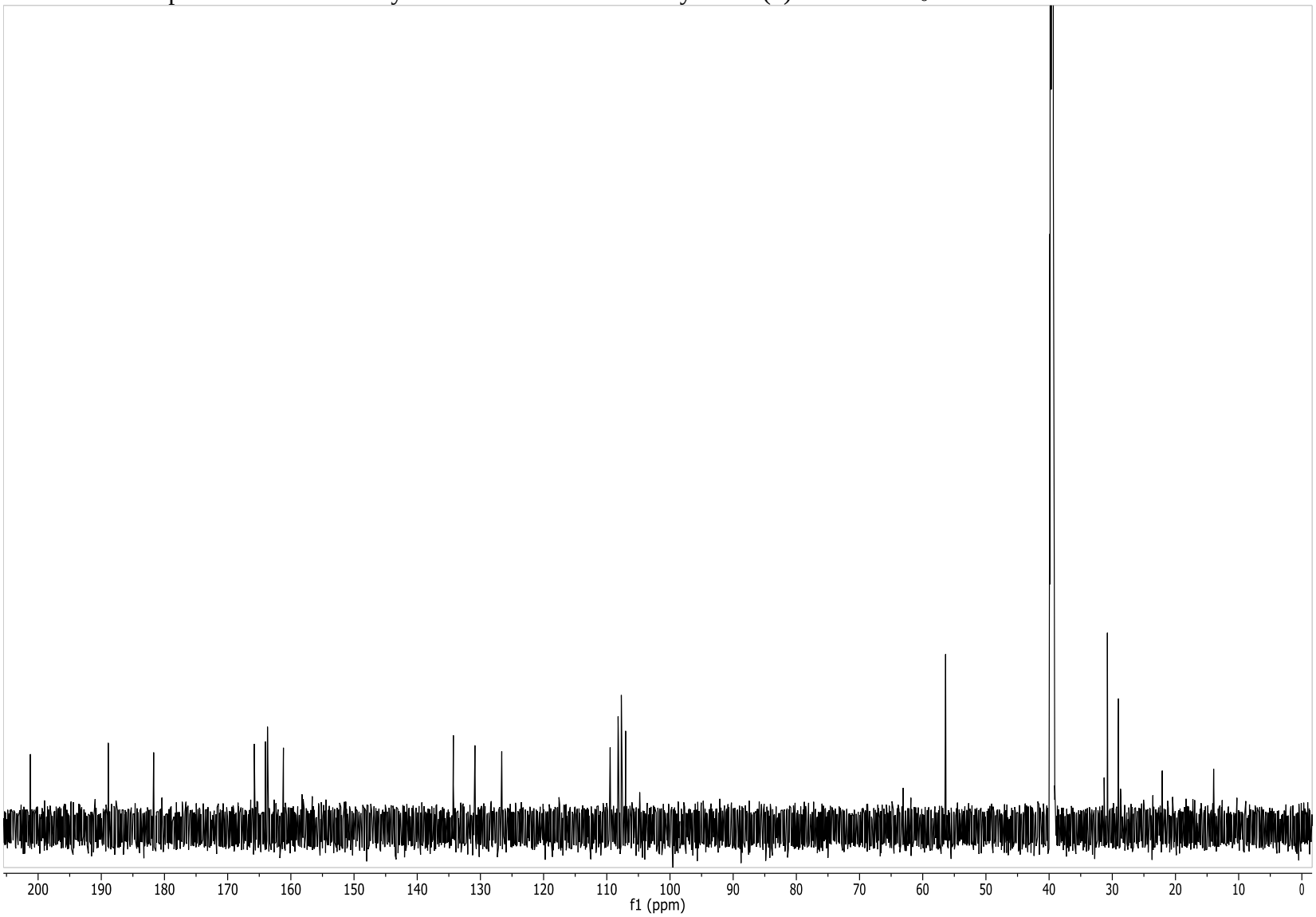
8

[a] Spectra recorded in DMSO-d_6 + trace TFA (^{1}H at 800 MHz, ^{13}C NMR at 200 MHz)
[b] Signals are interchangeable

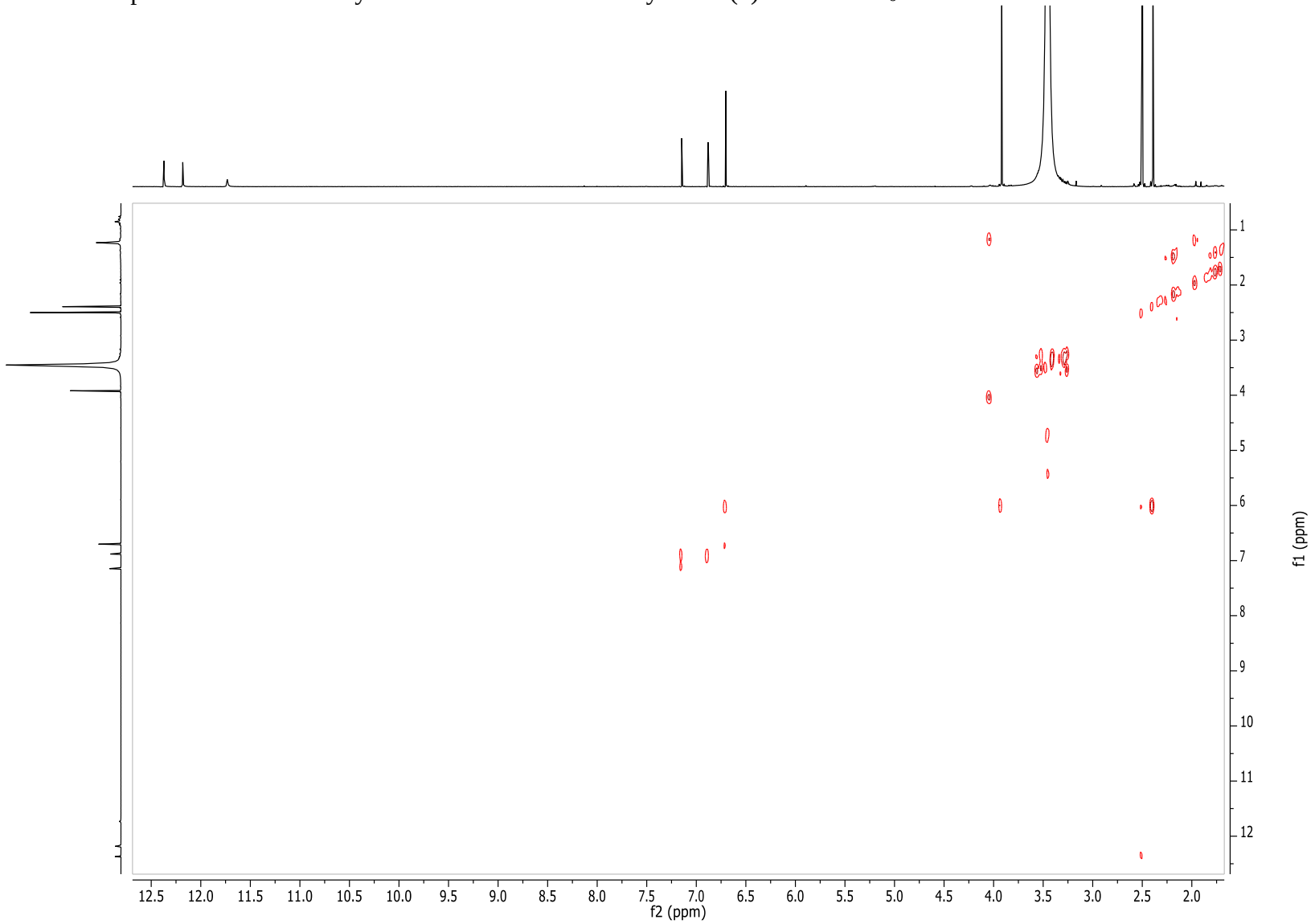
S51 ^{1}H NMR Spectrum of 12-Desethyl-rhodocomatulin 7-dimethyl ether (**8**) in DMSO-d_6



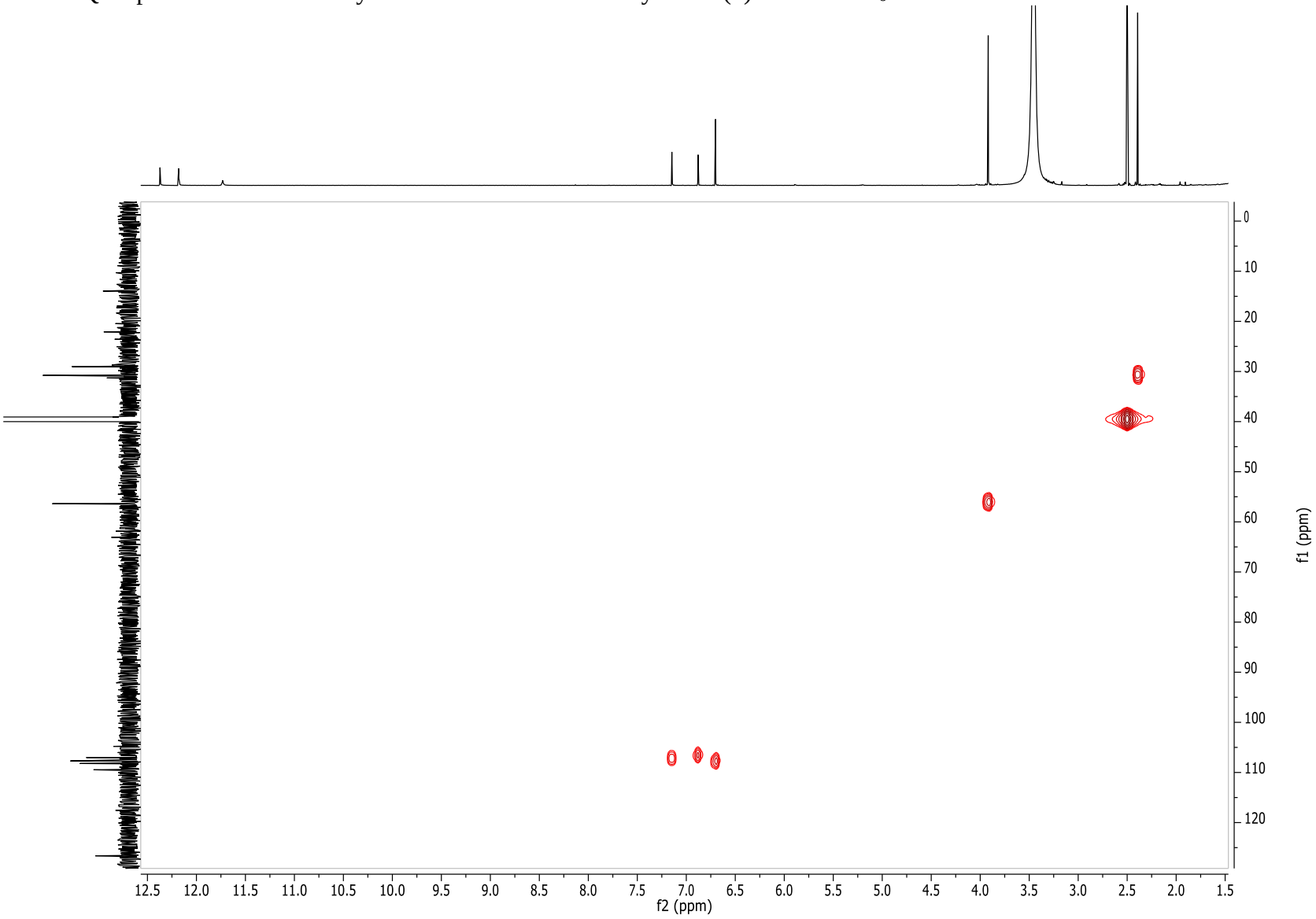
S52 ^{13}C NMR Spectrum of 12-Desethyl-rhodocomatulin 7-dimethyl ether (**8**) in DMSO-d_6



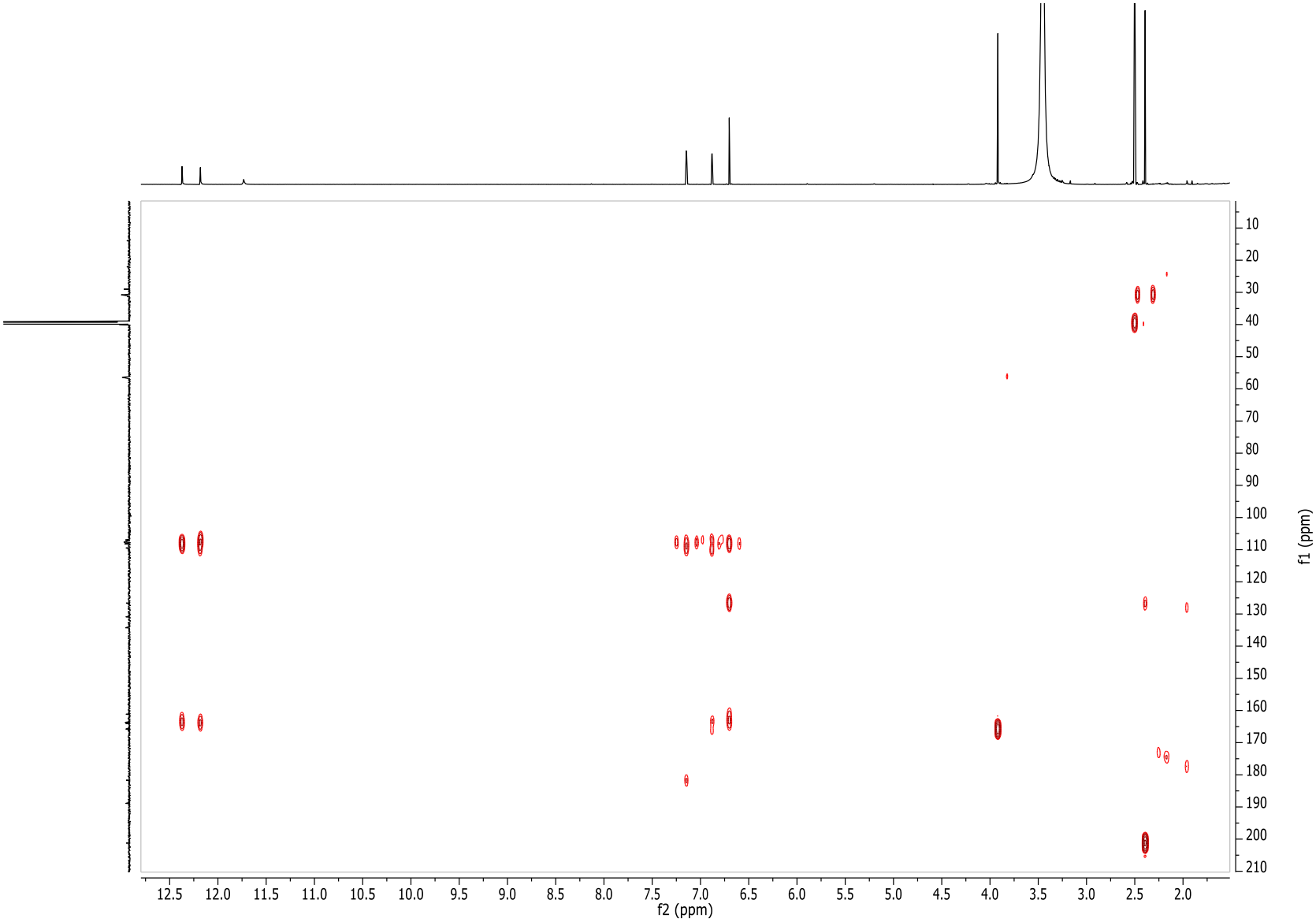
S53 COSY Spectrum of 12-Desethyl-rhodocomatulin 7-dimethyl ether (**8**) in DMSO-d_6



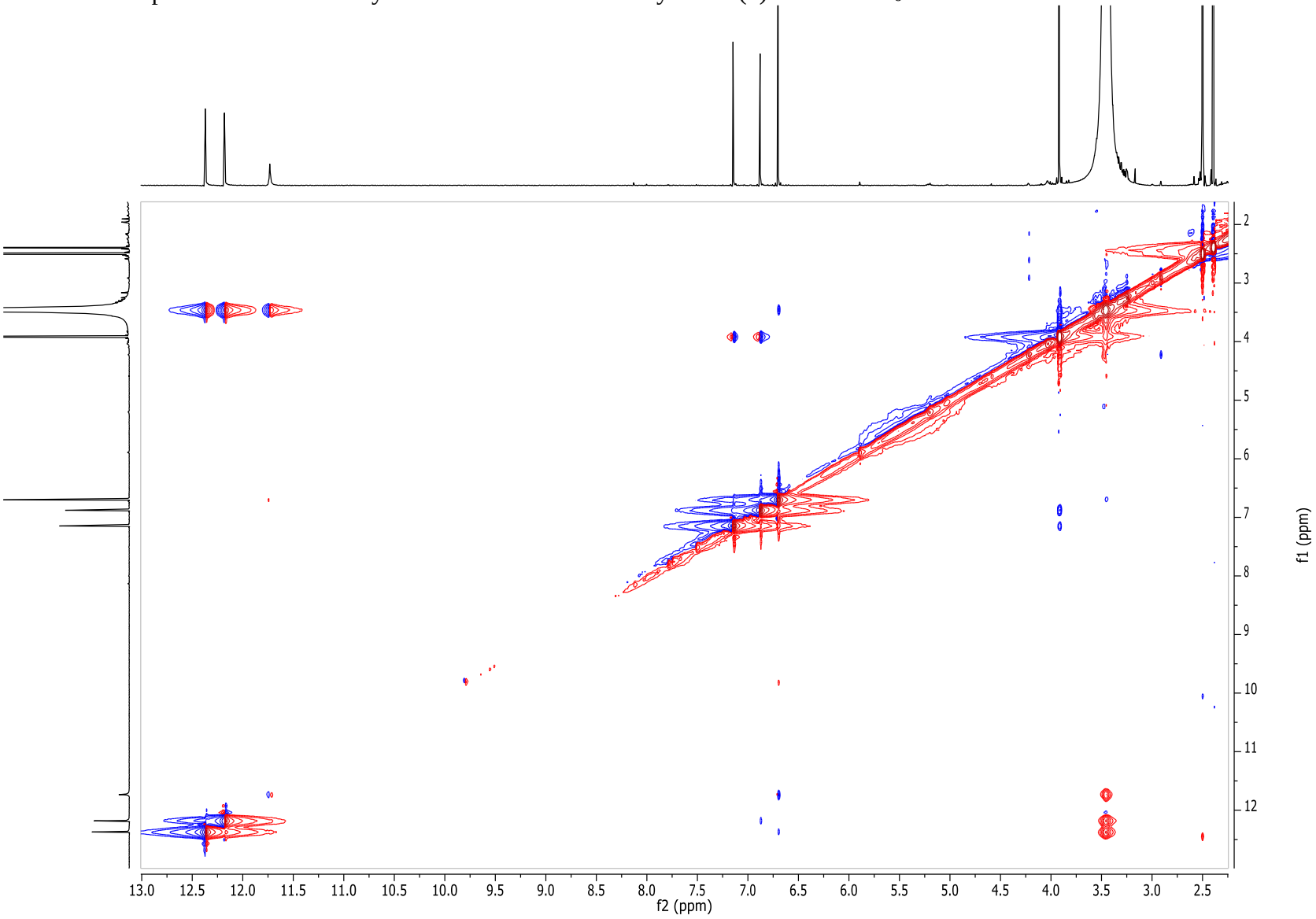
S54 HSQC Spectrum of 12-Desethyl-rhodocomatulin 7-dimethyl ether (**8**) in DMSO-d_6



S55 HMBC Spectrum of 12-Desethyl-rhodocomatulin 7-dimethyl ether (**8**) in DMSO-d_6

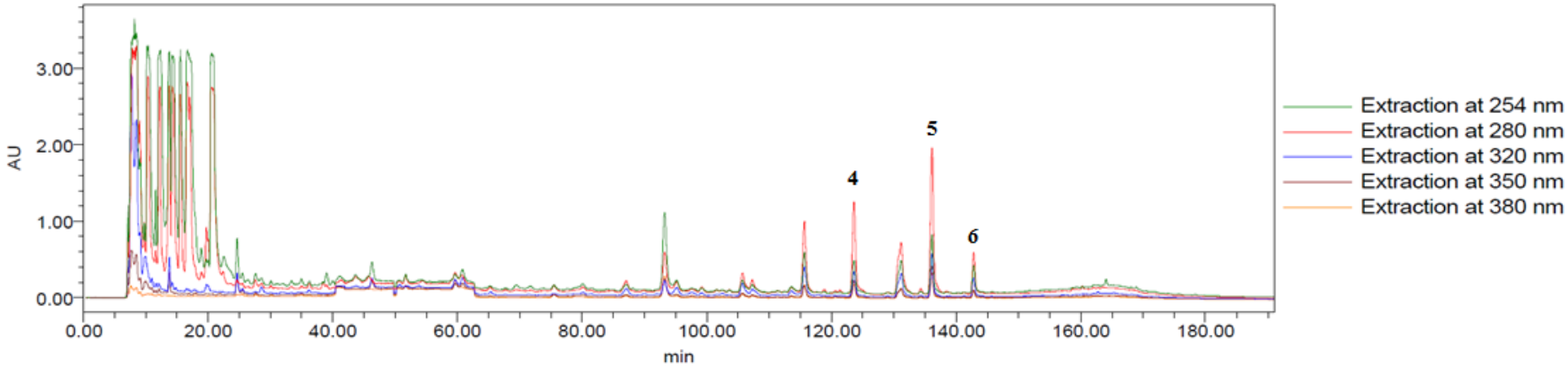

12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

S56 ROESY Spectrum of 12-Desethyl-rhodocomatulin 7-dimethyl ether (**8**) in DMSO-d_6



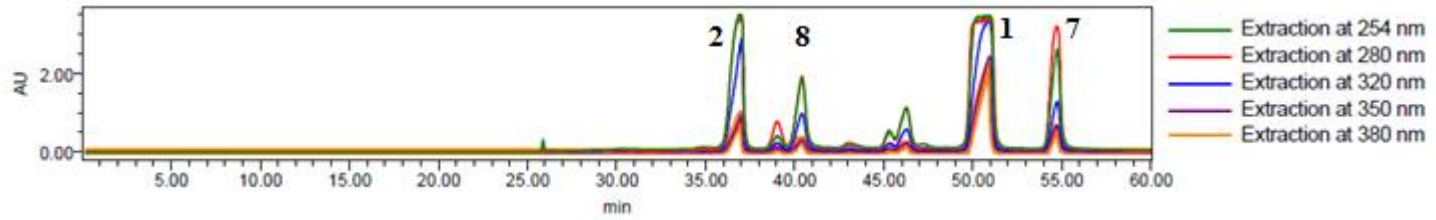
S57 HPLC Chromatograms for the Isolation of **1**–**8**[a]

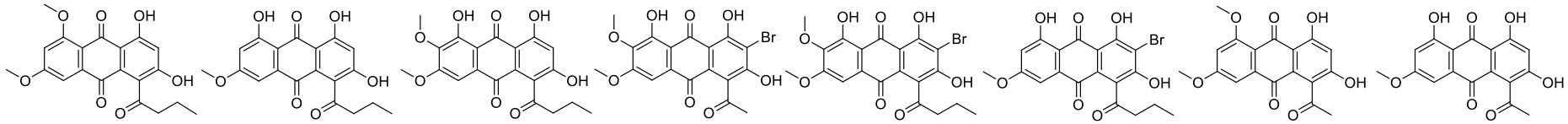
RP HPLC trace of combined *Clathria hirsuta* fractions 4–6, with compounds **4**, **5** and **6** labelled.



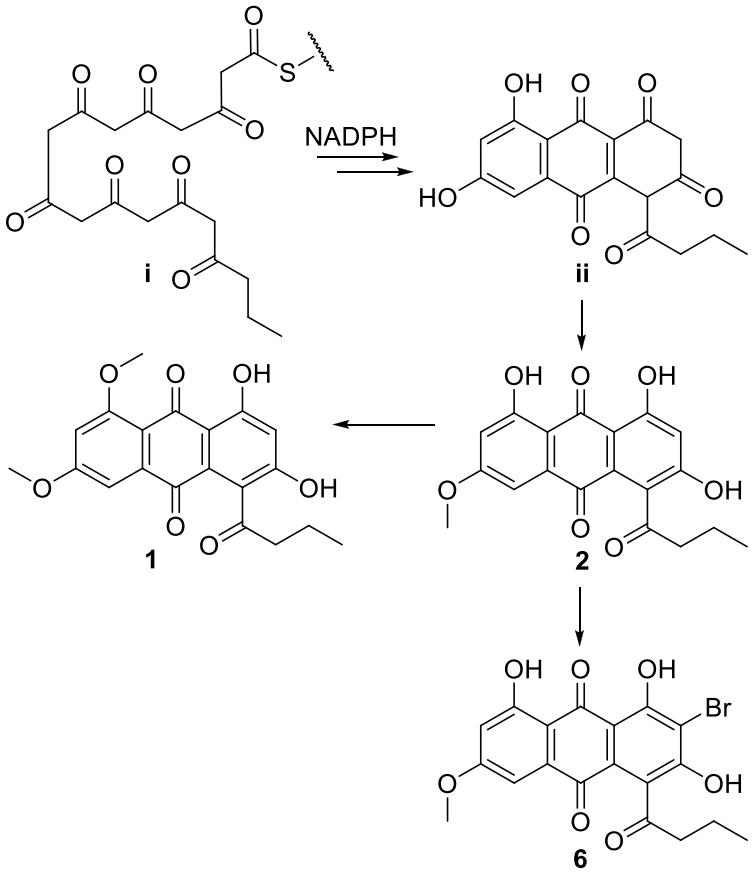
[a] The UV/Vis Spectrophotometer was malfunctioning at the time of purification of the *Clathria* extract by DIOL HPLC, and so this trace is not shown.

DIOL HPLC trace of combined *Comatula rotalaria* fractions 3–5, with compounds **1**, **2**, **7** and **8** labelled.





S58 Proposed Biosynthesis for Compounds **1**, **2** and **6**



The rhodocomatulin class of anthraquinones are produced by a polyketide biosynthetic pathway (**S57**). These polyketide pathways are often initially based on the successive addition of malonyl-SCoA units to a single unit of acetyl-SCoA through a polyketide synthetase and acyl-carrier protein.[1] For example, in the case of the proposed biosynthesis of compounds **1**, **2** and **6,** thioester hydrolysis of the polyketide chain (**i**) via NAPDH cleaves the enzyme from the polyketide chain, and this chain can undergo intramolecular aldol-ring closures to yield an anthraquinone core (**ii**).[1] Re-aromatization of this core could then yield **2**.[1] *S*-adenosyl methionine is then capable of selectively methylating hydroxyl groups under enzymatic control, which could lead to the formation of **1**. Alternatively, a bromo-peroxidase enzyme could feasibly introduce a bromine atom at the appropriate position in **2**, yielding **6**.[2]

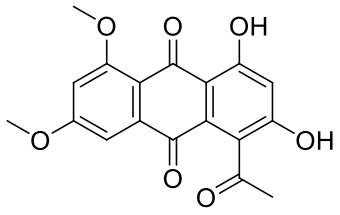
(1) Dewick, P. M. *Medicinal Natural Products*; 3rd ed.; John Wiley & Sons: Chichester, 2009.

(2) Butler, A.; Carter-Franklin, J. N. *Nat. Prod. Rep.* **2004**, *21*, 180-188.

S59 Computational Chemistry: Boltzmann Distributions for Each Conformer of *para* and *ortho* **7**

For the *para* form of compound **7**, nine conformers were identified by MCMM.

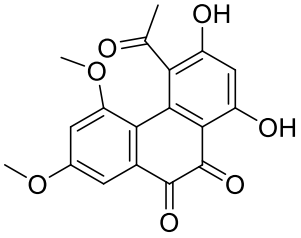
Conformer Number	Boltzmann Population (%)	Energies (Hartrees)
Conformer 1	20.32%	-1221.034969
Conformer 2	14.01%	-1221.034618
Conformer 3	0.08%	-1221.029685
Conformer 4	0.09%	-1221.029897
Conformer 5	0.11%	-1221.030065
Conformer 6	32.74%	-1221.035419
Conformer 7	32.26%	-1221.035405
Conformer 8	0.2%	-1221.030626
Conformer 9	0%	-1221.030498



para form

For the *ortho* form of compound **7**, five conformers were identified by MCMM.

Conformer Number	Boltzmann Population (%)	Energies (Hartrees)
Conformer 1	36.79 %	-1221.259448
Conformer 2	31.75 %	-1221.259072
Conformer 3	31.45 %	-1221.254798
Conformer 4	0.01 %	-1221.250489
Conformer 5	0 %	-1221.249860



ortho form

Para **7**, Conformer 1

C	-2.14140	-1.59550	-0.09360
C	-1.11590	-0.63660	-0.11860
C	-1.40000	0.72210	0.04410
C	-2.73300	1.12980	0.25620
C	-3.74540	0.15890	0.28580
C	-3.45850	-1.19870	0.10850
C	0.27200	-1.09320	-0.33850
C	1.39140	-0.16880	-0.06120
C	1.12270	1.20050	0.02460
C	-0.27480	1.69140	-0.03510
C	2.71830	-0.62180	0.05260
C	3.76820	0.29380	0.20320
C	3.50700	1.65890	0.25320
C	2.18950	2.10670	0.17110
O	-0.45530	2.90180	-0.14570
O	0.47630	-2.21620	-0.78720
O	2.01700	3.46550	0.24280
O	5.05590	-0.15600	0.31020
C	3.04360	-2.06150	0.10480
O	2.77680	-2.70260	1.12080
C	3.72620	-2.66270	-1.09460
O	-2.96880	2.46660	0.44570
O	-4.54830	-2.02420	0.15920
C	-4.31380	-3.41890	-0.02590
C	-4.31820	2.89910	0.59900
H	-1.88260	-2.64210	-0.22970
H	-4.78530	0.43070	0.45050
H	4.31180	2.38110	0.36770
H	1.05540	3.65440	0.11480
H	5.65620	0.61150	0.42230
H	3.17730	-3.55430	-1.40980
H	3.74440	-1.96030	-1.93290
H	4.75320	-2.92930	-0.83190
H	-5.27950	-3.92980	0.03630
H	-3.89290	-3.61890	-1.01670
H	-3.67280	-3.81800	0.76700
H	-4.76150	2.48580	1.51060
H	-4.30850	3.98870	0.69850
H	-4.91530	2.65080	-0.28450

Para **7**, Conformer 2

C	-2.13990	-1.58970	-0.06930
C	-1.11000	-0.65490	0.09480
C	-1.39750	0.70840	0.17880
C	-2.73730	1.14150	0.07630
C	-3.75940	0.19100	-0.09700
C	-3.46540	-1.17240	-0.16560
C	0.28060	-1.14170	0.19390
C	1.39460	-0.18000	0.05590
C	1.12600	1.18270	0.21750
C	-0.26900	1.65230	0.39660
C	2.71760	-0.60240	-0.16780
C	3.76490	0.32840	-0.18150
C	3.50470	1.68060	0.01420
C	2.19030	2.10340	0.20550
O	-0.44440	2.82460	0.72040
O	0.49320	-2.32610	0.43070
O	2.01840	3.45350	0.37670
O	5.04890	-0.09220	-0.39670
C	3.03980	-2.00980	-0.47850
O	2.75020	-2.46380	-1.58510
C	3.74860	-2.80960	0.58160
O	-2.97040	2.49220	0.12820
O	-4.37010	-2.18540	-0.32870
C	-5.74570	-1.82130	-0.42200
C	-4.31980	2.95030	0.11420
H	-1.91030	-2.65270	-0.12740
H	-4.79010	0.51600	-0.18380
H	4.30760	2.41380	0.00810
H	1.06050	3.61460	0.55900
H	5.64750	0.68480	-0.38760
H	4.76930	-3.02260	0.25370
H	3.78590	-2.26490	1.52940
H	3.20640	-3.74450	0.74770
H	-6.32620	-2.74150	-0.53890
H	-6.08480	-1.32640	0.49390
H	-5.92790	-1.19730	-1.30300
H	-4.88350	2.54600	0.96130
H	-4.30180	4.03960	0.21610
H	-4.80400	2.71350	-0.83860

Para **7**, Conformer 3

C	-2.14930	-1.58790	-0.06760
C	-1.11070	-0.65700	0.09010
C	-1.39040	0.70550	0.17650
C	-2.72800	1.12490	0.09800
C	-3.76250	0.19490	-0.09090
C	-3.47670	-1.16670	-0.16260
C	0.28060	-1.14450	0.17720
C	1.39580	-0.17990	0.05050
C	1.12620	1.18430	0.20770
C	-0.26950	1.65470	0.37310
C	2.72140	-0.60090	-0.16090
C	3.76820	0.33090	-0.16620
C	3.50560	1.68330	0.02460
C	2.18950	2.10590	0.20280
O	-0.45850	2.83180	0.67030
O	0.49200	-2.33250	0.39620
O	2.01480	3.45620	0.36880
O	5.05460	-0.08950	-0.36790
C	3.04960	-2.00820	-0.46600
O	2.78320	-2.46130	-1.57870
C	3.73690	-2.80830	0.60800
O	-3.05430	2.45850	0.10170
O	-4.38660	-2.17300	-0.33240
C	-5.75930	-1.79500	-0.41820
C	-3.67460	2.82900	1.33800
H	-1.92380	-2.65180	-0.12830
H	-4.77880	0.56560	-0.19060
H	4.30830	2.41690	0.02440
H	1.05390	3.61870	0.53300
H	5.65260	0.68780	-0.35450
H	4.76400	-3.02110	0.30070
H	3.75510	-2.26370	1.55640
H	3.19150	-3.74320	0.76300
H	-6.34940	-2.70900	-0.53460
H	-6.08920	-1.29850	0.50030
H	-5.93910	-1.16680	-1.29670
H	-3.72560	3.92130	1.37090
H	-4.69640	2.43990	1.39350

Para **7**, Conformer 4

C	-2.15320	-1.58590	-0.08690
C	-1.11350	-0.64150	-0.08250
C	-1.39310	0.71490	0.07100
C	-2.73060	1.10990	0.23870
C	-3.76960	0.16660	0.21590
C	-3.48270	-1.18700	0.06040
C	0.27490	-1.10810	-0.27260
C	1.39740	-0.17200	-0.03910
C	1.12580	1.19780	0.05290
C	-0.27420	1.68620	0.04360
C	2.73100	-0.61640	0.03350
C	3.78070	0.30520	0.14670
C	3.51450	1.66860	0.20430
C	2.19290	2.10910	0.16670
O	-0.46820	2.89940	0.03180
O	0.47630	-2.25190	-0.66670
O	2.01770	3.46730	0.24770
O	5.07380	-0.13780	0.20850
C	3.07220	-2.05270	0.07580
O	2.88250	-2.68700	1.11310
C	3.67990	-2.65670	-1.16190
O	-3.08430	2.43150	0.35210
O	-4.39420	-2.20540	0.02850
C	-5.76670	-1.84850	0.18190
C	-3.32290	2.77150	1.72240
H	-1.92810	-2.64430	-0.21200
H	-4.79110	0.52350	0.31420
H	4.31900	2.39500	0.29180
H	1.04880	3.65140	0.18280
H	5.67370	0.63300	0.29910
H	3.12130	-3.55670	-1.43340
H	3.63480	-1.96070	-2.00450
H	4.72500	-2.91010	-0.96620
H	-6.35640	-2.76940	0.14270
H	-5.94460	-1.37850	1.15470
H	-6.09880	-1.20360	-0.63820
H	-2.46390	2.51550	2.35260
H	-3.47410	3.85370	1.77610
H	-4.22910	2.28240	2.09490

Para **7**, Conformer 5

C	-2.15340	-1.59430	-0.07910
C	-1.11480	-0.65420	0.06140
C	-1.39340	0.70940	0.15680
C	-2.73120	1.12800	0.09150
C	-3.76350	0.18890	-0.03050
C	-3.48080	-1.17400	-0.12330
C	0.27830	-1.14170	0.13510
C	1.39650	-0.17760	0.03670
C	1.12680	1.18660	0.19180
C	-0.27090	1.66310	0.32440
C	2.72600	-0.60060	-0.14930
C	3.77530	0.32800	-0.12980
C	3.51220	1.68020	0.05820
C	2.19340	2.10550	0.20860
O	-0.45970	2.85540	0.55400
O	0.48760	-2.33550	0.32370
O	2.02070	3.45680	0.36990
O	5.06460	-0.09550	-0.30410
C	3.06020	-2.00720	-0.45150
O	2.83700	-2.45100	-1.57740
C	3.70110	-2.81750	0.64320
O	-3.07370	2.44970	0.22390
O	-4.57810	-1.98020	-0.24640
C	-4.34220	-3.38370	-0.34180
C	-3.50770	2.99460	-1.02710
H	-1.89660	-2.64830	-0.14640
H	-4.80010	0.52140	-0.04270
H	4.31630	2.41200	0.07610
H	1.05470	3.62530	0.49280
H	5.66430	0.68010	-0.27580
H	3.14550	-3.75040	0.77120
H	4.73830	-3.03380	0.37460
H	3.68560	-2.27850	1.59490
H	-5.31340	-3.87880	-0.43540
H	-3.75670	-3.62400	-1.23530
H	-3.85930	-3.76340	0.56460
H	-4.50060	2.61760	-1.29480
H	-3.57760	4.08040	-0.91070
H	-2.78830	2.78350	-1.82700

Para **7**, Conformer 6

C	-2.14340	-1.59340	-0.10550
C	-1.11690	-0.63500	-0.11430
C	-1.40140	0.72210	0.05390
C	-2.73650	1.12960	0.25470
C	-3.75000	0.15950	0.26770
C	-3.46240	-1.19710	0.08490
C	0.27260	-1.09230	-0.31720
C	1.39550	-0.17530	-0.03160
C	1.12410	1.19720	0.04490
C	-0.27450	1.68940	-0.00890
C	2.72520	-0.63190	0.07370
C	3.77240	0.30140	0.16100
C	3.50660	1.66460	0.21860
C	2.18890	2.10840	0.17040
O	-0.45520	2.90130	-0.10330
O	0.48220	-2.22150	-0.74660
O	2.01550	3.46690	0.24030
O	5.09550	-0.05760	0.19870
C	3.10120	-2.06620	0.15340
O	4.02010	-2.47240	-0.56130
C	2.46640	-2.93210	1.21240
O	-2.97360	2.46550	0.44930
O	-4.55330	-2.02190	0.11910
C	-4.31830	-3.41550	-0.07360
C	-4.32420	2.89790	0.59230
H	-1.88470	-2.63950	-0.24520
H	-4.79140	0.43130	0.42300
H	4.32260	2.37900	0.29950
H	1.05080	3.65370	0.13310
H	5.17270	-0.98970	-0.11310
H	1.98200	-3.79200	0.74330
H	3.24800	-3.27980	1.89440
H	1.73090	-2.38100	1.80370
H	-5.28510	-3.92570	-0.02530
H	-3.88720	-3.60880	-1.06130
H	-3.68610	-3.82100	0.72300
H	-4.77650	2.47920	1.49710
H	-4.31470	3.98690	0.69880
H	-4.91290	2.65560	-0.29840

*Para **7***, Conformer 7

C	-2.14160	-1.58560	-0.10540
C	-1.11360	-0.63430	-0.11520
C	-1.40060	0.72040	0.05340
C	-2.73820	1.12560	0.25430
C	-3.75850	0.15760	0.26970
C	-3.46500	-1.19520	0.08610
C	0.27430	-1.09320	-0.31830
C	1.39680	-0.17580	-0.03210
C	1.12480	1.19670	0.04430
C	-0.27420	1.68860	-0.00980
C	2.72650	-0.63210	0.07420
C	3.77330	0.30160	0.16200
C	3.50710	1.66480	0.21900
C	2.18920	2.10820	0.17020
O	-0.45540	2.90030	-0.10490
O	0.48370	-2.22200	-0.74860
O	2.01530	3.46670	0.23980
O	5.09650	-0.05700	0.20070
C	3.10250	-2.06630	0.15510
O	4.02250	-2.47280	-0.55810
C	2.46610	-2.93180	1.21350
O	-2.97090	2.46300	0.45040
O	-4.36790	-2.22260	0.07840
C	-5.74150	-1.88410	0.25790
C	-4.31930	2.90840	0.57030
H	-1.91280	-2.64130	-0.24370
H	-4.78720	0.45970	0.43040
H	4.32280	2.37940	0.30030
H	1.05070	3.65310	0.13220
H	5.17410	-0.98930	-0.11030
H	1.98220	-3.79180	0.74400
H	3.24680	-3.27940	1.89660
H	1.73000	-2.38040	1.80370
H	-6.32090	-2.81140	0.21610
H	-5.90890	-1.42970	1.23990
H	-6.09480	-1.23260	-0.54810
H	-4.78730	2.50230	1.47280
H	-4.30170	3.99820	0.66670
H	-4.89800	2.66280	-0.32610

*Para **7***, Conformer 8

C	-2.15030	-1.58800	-0.05540
C	-1.11150	-0.65480	0.08780
C	-1.39180	0.70720	0.16790
C	-2.73070	1.12480	0.09850
C	-3.76580	0.19260	-0.07550
C	-3.47900	-1.16910	-0.14120
C	0.28070	-1.13970	0.16060
C	1.39880	-0.18090	0.02120
C	1.12700	1.18460	0.18830
C	-0.26980	1.65710	0.34980
C	2.72670	-0.60720	-0.18480
C	3.77200	0.33070	-0.12620
C	3.50520	1.68260	0.05770
C	2.18860	2.10750	0.20380
O	-0.45940	2.83740	0.63370
O	0.49690	-2.32910	0.36490
O	2.01320	3.45700	0.37200
O	5.09440	-0.01210	-0.24740
C	3.10240	-2.00400	-0.51970
O	4.02900	-2.52760	0.10280
C	2.45760	-2.67020	-1.70910
O	-3.05840	2.45800	0.09680
O	-4.38900	-2.17750	-0.29680
C	-5.76290	-1.80180	-0.37230
C	-3.67040	2.83540	1.33520
H	-1.92440	-2.65210	-0.11180
H	-4.78330	0.56150	-0.16870
H	4.31970	2.40260	0.08780
H	1.04940	3.62090	0.51710
H	5.17750	-0.98360	-0.10180
H	3.23130	-2.88310	-2.45270
H	1.98460	-3.60430	-1.39630
H	1.71040	-2.02760	-2.18150
H	-6.35290	-2.71720	-0.47770
H	-6.08510	-1.30010	0.54610
H	-5.95160	-1.17920	-1.25300
H	-3.07780	2.50090	2.19430
H	-3.72170	3.92790	1.36210
H	-4.69160	2.44610	1.40000

*Para **7***, Conformer 9

C	-2.15380	-1.58690	-0.06390
C	-1.11240	-0.65180	0.05450
C	-1.39340	0.70950	0.14220
C	-2.73500	1.12280	0.09210
C	-3.77520	0.18580	-0.00740
C	-3.48660	-1.17360	-0.09360
C	0.28010	-1.13870	0.10860
C	1.40150	-0.17910	0.00320
C	1.12830	1.18620	0.16940
C	-0.27090	1.66440	0.29280
C	2.73420	-0.60620	-0.17280
C	3.78000	0.32850	-0.08370
C	3.51140	1.67980	0.09880
C	2.19220	2.10670	0.21230
O	-0.46250	2.85980	0.50290
O	0.49360	-2.33450	0.27540
O	2.01720	3.45680	0.37730
O	5.10410	-0.01700	-0.17310
C	3.11710	-2.00110	-0.50650
O	4.01650	-2.53480	0.14620
C	2.51820	-2.65000	-1.72900
O	-3.08840	2.44340	0.21810
O	-4.39910	-2.18590	-0.20160
C	-5.77520	-1.81300	-0.24290
C	-3.38500	3.00880	-1.06360
H	-1.92760	-2.65060	-0.12800
H	-4.79860	0.55050	-0.00650
H	4.32620	2.39820	0.15140
H	1.04850	3.62650	0.47470
H	5.18210	-0.98850	-0.02570
H	3.31810	-2.84430	-2.44950
H	2.04150	-3.59270	-1.44890
H	1.78200	-2.00430	-2.21440
H	-6.36560	-2.72930	-0.33890
H	-6.07580	-1.31740	0.68600
H	-5.98690	-1.18580	-1.11510
H	-4.31030	2.58910	-1.47190
H	-3.53050	4.08460	-0.92800
H	-2.55660	2.86250	-1.76580

Ortho **7**, Conformer 1

C	-1.157377	-1.240684	-0.486405
C	-2.542768	-1.368675	-0.536005
C	-3.379742	-0.312205	-0.161773
C	-2.819495	0.909215	0.206748
O	-0.332844	-2.240168	-0.878870
H	-3.005287	-2.286891	-0.868051
O	-4.706414	-0.564547	-0.222614
H	-3.421184	1.776000	0.436554
C	-1.429749	1.036419	0.232069
C	-0.551827	-0.033330	-0.038446
C	0.545888	2.635182	-0.068632
C	-0.886187	2.396302	0.432918
O	0.908377	3.804613	-0.263683
O	-1.519036	3.322305	0.900313
C	1.408273	1.490998	-0.192403
C	0.914596	0.171546	0.038067
C	1.841300	-0.870862	0.241978
C	3.222981	-0.629110	-0.081936
C	3.688642	0.639513	-0.402942
C	2.803656	1.704685	-0.413321
O	4.120180	-1.618193	-0.069378
H	4.737999	0.792875	-0.616978
O	3.284801	2.928860	-0.649131
C	1.536861	-2.164809	0.902634
O	2.267264	-3.146376	0.712251
C	0.499686	-2.259723	1.994306
H	-0.197729	-1.428350	2.031423
H	-0.038487	-3.204502	1.909084
H	1.054232	-2.280626	2.938699
H	3.629861	-2.456113	0.139079
H	2.523589	3.561934	-0.602149
C	-5.624927	0.478356	0.134283
H	-6.615442	0.041909	0.030755
H	-5.469410	0.797754	1.167631
H	-5.527087	1.331832	-0.541045
C	-0.880841	-3.456308	-1.406489
H	-1.473383	-3.257066	-2.302307
H	-0.021250	-4.070501	-1.663852
H	-1.488882	-3.969271	-0.657858

Ortho **7**, Conformer 2

C	-1.403483	-0.845213	-0.406923
C	-2.793079	-0.667133	-0.422326
C	-3.357130	0.547440	-0.032404
C	-2.521863	1.612699	0.316258
O	-0.837898	-2.005226	-0.814247
H	-3.425955	-1.478867	-0.742980
O	-4.685475	0.791942	0.005728
H	-2.944240	2.580389	0.551568
C	-1.146148	1.434443	0.308318
C	-0.534538	0.190648	0.017042
C	1.121689	2.554959	-0.065770
C	-0.306887	2.638112	0.491444
O	1.725856	3.615441	-0.285886
O	-0.697165	3.675276	0.989073
C	1.705046	1.248201	-0.207242
C	0.940681	0.068738	0.047317
C	1.622604	-1.152479	0.228414
C	3.011112	-1.220598	-0.143545
C	3.733563	-0.085217	-0.489003
C	3.105378	1.148549	-0.476594
O	3.668968	-2.382704	-0.153181
H	4.783015	-0.166651	-0.738968
O	3.836169	2.236958	-0.735946
C	1.063701	-2.346706	0.908431
O	1.554628	-3.465262	0.703618
C	0.064925	-2.212254	2.031425
H	-0.426826	-1.245955	2.088013
H	-0.674141	-3.011493	1.963698
H	0.628578	-2.362883	2.958398
H	3.013807	-3.091957	0.079361
H	3.234485	3.022080	-0.669871
C	-5.599792	-0.254300	-0.349729
H	-6.592299	0.172678	-0.228022
H	-5.457674	-0.560946	-1.389081
H	-5.485484	-1.114107	0.315150
C	-1.651725	-3.067024	-1.332394
H	-2.206152	-2.736298	-2.213475
H	-0.953212	-3.851829	-1.612574
H	-2.338891	-3.442744	-0.570824

Ortho **7**, Conformer 3

C	1.403526	-0.845214	0.407109
C	2.793138	-0.667004	0.422553
C	3.357186	0.547510	0.032525
C	2.521824	1.612692	-0.316195
O	0.838038	-2.005158	0.814631
H	3.426040	-1.478612	0.743521
O	4.685494	0.792136	-0.005486
H	2.944117	2.580421	-0.551536
C	1.146150	1.434418	-0.308234
C	0.534546	0.190610	-0.017006
C	-1.121807	2.554852	0.065639
C	0.306883	2.638127	-0.491215
O	-1.726033	3.615338	0.285610
O	0.697251	3.675397	-0.988591
C	-1.705111	1.248088	0.207212
C	-0.940656	0.068642	-0.047196
C	-1.622638	-1.152534	-0.228397
C	-3.011162	-1.220674	0.143391
C	-3.733636	-0.085316	0.488965
C	-3.105437	1.148434	0.476572
O	-3.669160	-2.382736	0.152788
H	-4.783102	-0.166782	0.738848
O	-3.836304	2.236819	0.735959
C	-1.063753	-2.346650	-0.908523
O	-1.554718	-3.465232	-0.704104
C	-0.064707	-2.211922	-2.031309
H	0.426172	-1.245178	-2.088335
H	0.675128	-3.010427	-1.962896
H	-0.627808	-2.363821	-2.958415
H	-3.014123	-3.092067	-0.079838
H	-3.234630	3.021998	0.669911
C	5.599878	-0.254595	0.348608
H	6.592401	0.172040	0.225819
H	5.458874	-0.561425	1.388065
H	5.484387	-1.114178	-0.316343
C	1.651944	-3.066860	1.333095
H	2.206289	-2.735875	2.214127
H	0.953452	-3.851624	1.613401
H	2.339245	-3.442608	0.571646

Ortho **7**, Conformer 4

C	-1.183777	-1.217136	-0.496626
C	-2.568225	-1.353157	-0.460754
C	-3.386922	-0.296264	-0.044986
C	-2.813286	0.931160	0.268824
O	-0.376969	-2.194467	-0.976657
H	-3.046488	-2.272782	-0.765514
O	-4.715978	-0.557601	-0.024921
H	-3.403660	1.802788	0.509565
C	-1.420846	1.059869	0.223243
C	-0.559537	-0.016326	-0.067034
C	0.551473	2.636343	-0.195380
C	-0.870621	2.424324	0.348124
O	0.914112	3.791892	-0.457810
O	-1.489801	3.376258	0.783326
C	1.414757	1.486091	-0.257590
C	0.910842	0.173248	0.000888
C	1.816483	-0.857165	0.285283
C	3.208632	-0.593135	0.165424
C	3.702695	0.647820	-0.208688
C	2.814469	1.698642	-0.398040
O	4.050653	-1.607820	0.463802
H	4.768252	0.822663	-0.298099
O	3.312287	2.906388	-0.683827
C	1.381888	-2.167417	0.905928
O	0.622417	-2.139332	1.859855
C	1.942869	-3.476964	0.403777
H	2.274180	-3.420715	-0.632406
H	2.804100	-3.747252	1.019555
H	1.183380	-4.250326	0.522127
H	4.970136	-1.323555	0.380444
H	2.549712	3.537184	-0.728784
C	-5.614720	0.486191	0.372381
H	-6.608356	0.045600	0.337222
H	-5.397121	0.822480	1.389259
H	-5.563242	1.330741	-0.319452
C	-0.960943	-3.382126	-1.528831
H	-1.630285	-3.134584	-2.355933
H	-0.126036	-3.971647	-1.899340
H	-1.499718	-3.947123	-0.764456

Ortho **7**, Conformer 5

C	-1.426133	-0.808747	-0.420983
C	-2.813882	-0.632543	-0.354069
C	-3.355322	0.578734	0.079877
C	-2.502687	1.640427	0.383228
O	-0.879307	-1.945079	-0.916894
H	-3.464519	-1.438591	-0.652681
O	-4.682968	0.821594	0.192102
H	-2.908413	2.610893	0.635738
C	-1.126535	1.456749	0.308444
C	-0.537477	0.210473	-0.009371
C	1.133606	2.551726	-0.173460
C	-0.276391	2.659013	0.428068
O	1.735128	3.598725	-0.453451
O	-0.642129	3.714851	0.906815
C	1.713896	1.237456	-0.263823
C	0.938129	0.067566	0.012247
C	1.600944	-1.141306	0.264878
C	3.010868	-1.193912	0.093724
C	3.757104	-0.091173	-0.296668
C	3.120578	1.132634	-0.454058
O	3.615725	-2.373616	0.359396
H	4.830833	-0.158652	-0.424716
O	3.865394	2.201203	-0.757376
C	0.906962	-2.324890	0.903457
O	0.207463	-2.134323	1.884243
C	1.142506	-3.723929	0.384439
H	1.440461	-3.737593	-0.663217
H	1.943175	-4.183137	0.969265
H	0.234188	-4.308686	0.532733
H	4.571173	-2.301413	0.236895
H	3.261712	2.986543	-0.776718
C	-5.611929	-0.223029	-0.123401
H	-6.597827	0.198366	0.058229
H	-5.528283	-0.518200	-1.172708
H	-5.459243	-1.090843	0.523383
C	-1.727560	-2.966456	-1.459114
H	-2.338781	-2.570221	-2.273174
H	-1.054410	-3.726906	-1.847012
H	-2.364595	-3.401135	-0.685194