

Using UHPLC-MS profiling for the discovery of new dihydro- β -agarofurans from Australian Celastraceae plant extracts

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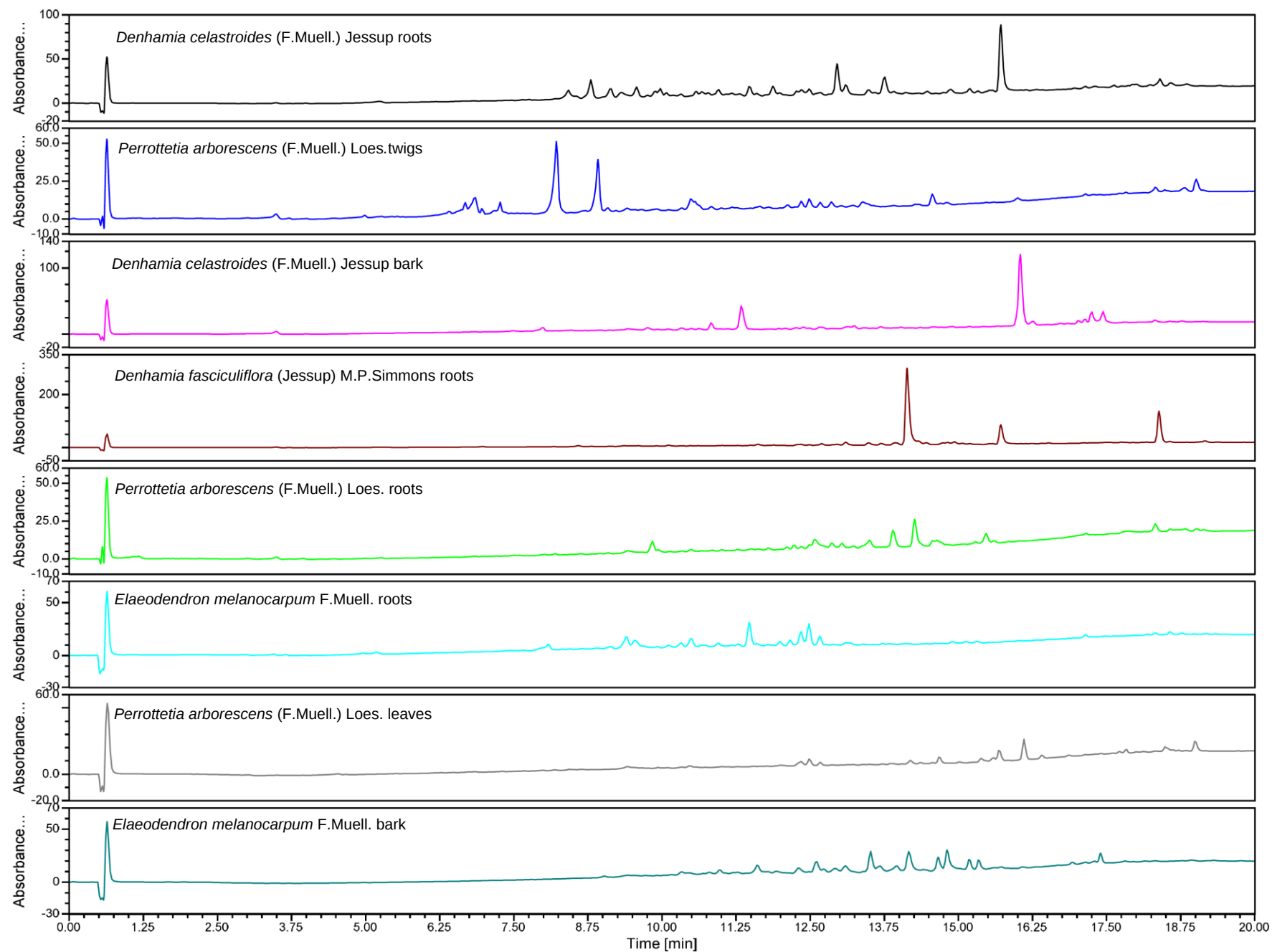
S24. HSQC spectrum of denhaminol R (**4**) in CDCl₃

S25. HMBC spectrum of denhaminol R (**4**) in CDCl₃

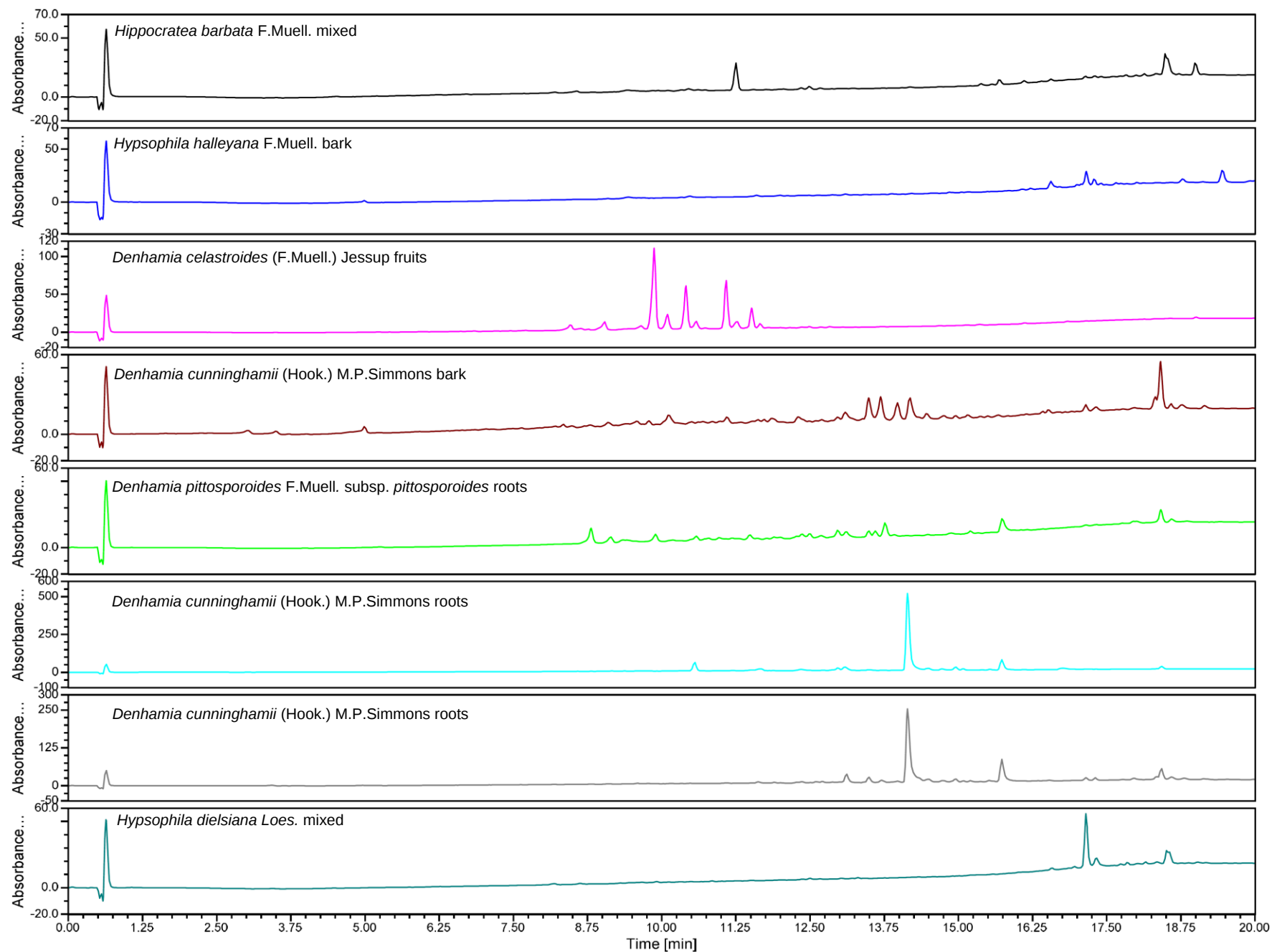
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S1 UHPLC chromatograms of 16 CH₂Cl₂ extracts of Australian Celastraceae plants



S1 Cont'd UHPLC chromatograms of 16 CH₂Cl₂ extracts of Australian Celastraceae plants



S2 UHPLC-MS data of the major UV peaks of 16 CH₂Cl₂ extracts of Australian Celastraceae and scientific database analyses

Scientific name	Sample type	Retention (t _R , min)	time	[M+H] ⁺ m/z	[M-H] ⁻ m/z	Molecular weight	No. of Scholar hits ^a	SciFinder	No. of hits ^a	DNP
<i>Denhamia celastroides</i> (F.Muell.) Jessup	Roots	12.96		497	—	496	6		0	
		13.11		481	—	480	8		0	
		13.77		481	—	480	8		0	
		15.72		465	—	464	17		0	
<i>Perrottetia arborescens</i> (F.Muell.) Loes	Twigs	8.20		457	—	456	29		0	
		8.92		441	—	440	21		0	
<i>Denhamia celastroides</i> (F.Muell.) Jessup	Bark	11.32		—	315	316	6		0	
		16.04		—	603	604	4		0	
<i>Denhamia fasciculiflora</i> (Jessup) M.P.Simmons	Roots	14.15		451	—	450	9		0	
		15.72		465	—	464	17		0	
		18.40		303	—	302	13		0	
<i>Perrottetia arborescens</i> (F.Muell.) Loes.	Roots	13.49		—	569	570	3		0	
		13.92		—	617	618	1		0	

		14.26	—	615	616	3	0
		15.45	—	573	573	0	0
<i>Elaeodendron melanocarpum</i> F.Muell.	Roots	11.49	—	471	472	28	0
		12.32	—	—	—	—	—
		12.94	—	—	—	—	—
		12.66	—	—	—	—	—
<i>Perrottetia arborescens</i> (F.Muell.) Loes.	Leaves	—	—	—	—	—	—
		—	—	—	—	—	—
		16.10	593	—	592	9	0
<i>Elaeodendron melanocarpum</i> F.Muell.	Bark	14.17	—	621	622	4	0
		14.64	—	471	472	28	0
<i>Hippocratea barbata</i> F.Muell.	Mixed	11.24	507	—	506	8	0
		18.48	—	—	—	—	—
		18.99	—	—	—	—	—
<i>Hypsophila halleyana</i> F.Muell.	Bark	17.17	615	—	614	1	0
		17.29	629	—	628	0	0
<i>Denhamia</i>	Fruits	9.87	615	—	614	1	0

celastroides
(F.Muell.) Jessup

10.09	657	—	656	0	0
10.41	673	—	672	10	0
11.03	631	—	630	4	0
11.51	653	—	652	17	0

Denhamia
cunninghamii
(Hook.)
M.P.Simmons

Bark

13.70	—	447	448	7	0
13.96	—	547	548	11	0
14.17	—	469	470	14	0
18.4	—	383	384	6	0

Denhamia
pittosporoides
F.Muell. subsp.
pittosporoides

Roots

8.82	—	361	362	5	0
13.75	—	497	498	10	0
15.72	465	—	464	17	0

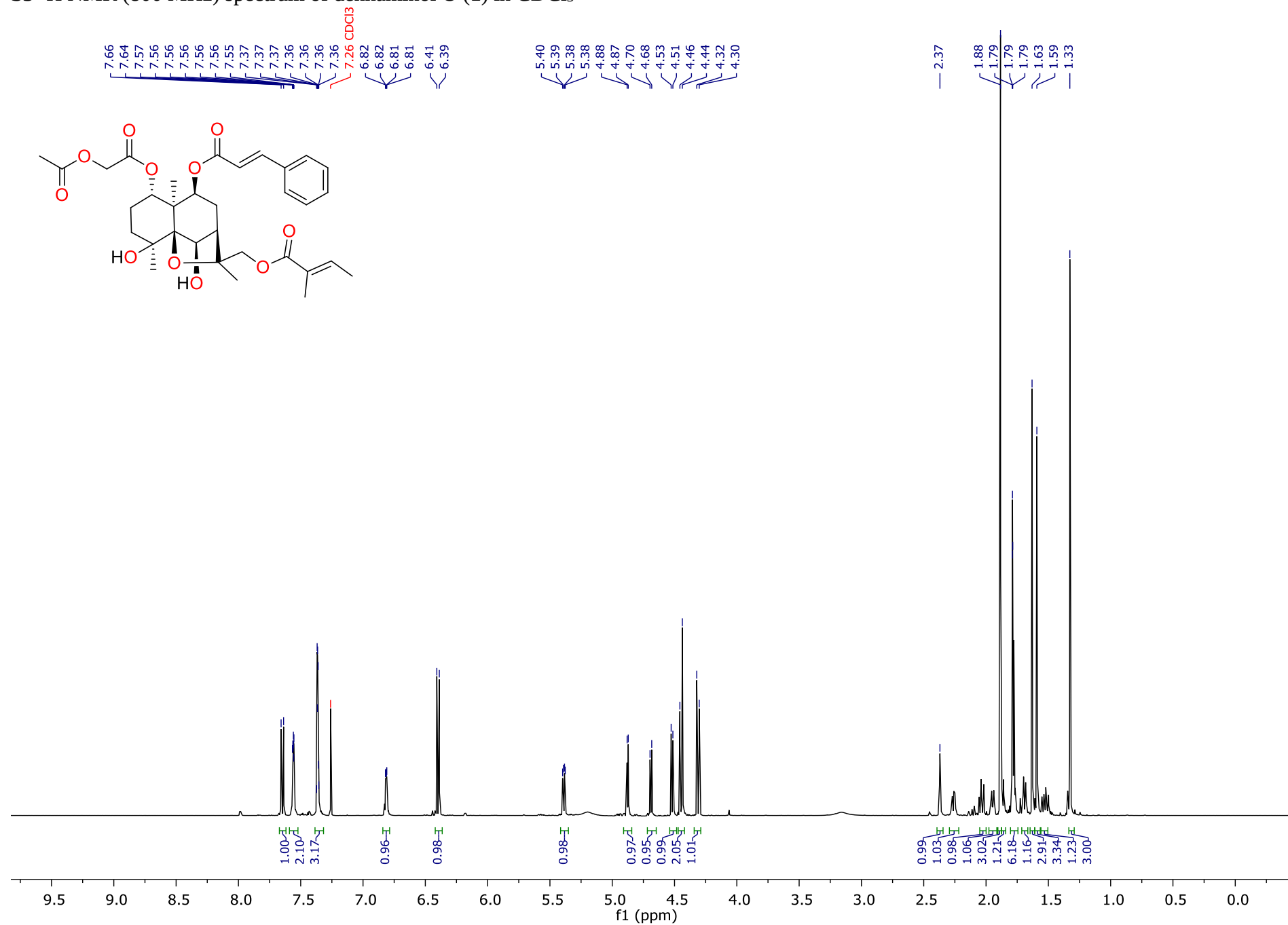
Denhamia
cunninghamii
(Hook.)
M.P.Simmons

Roots

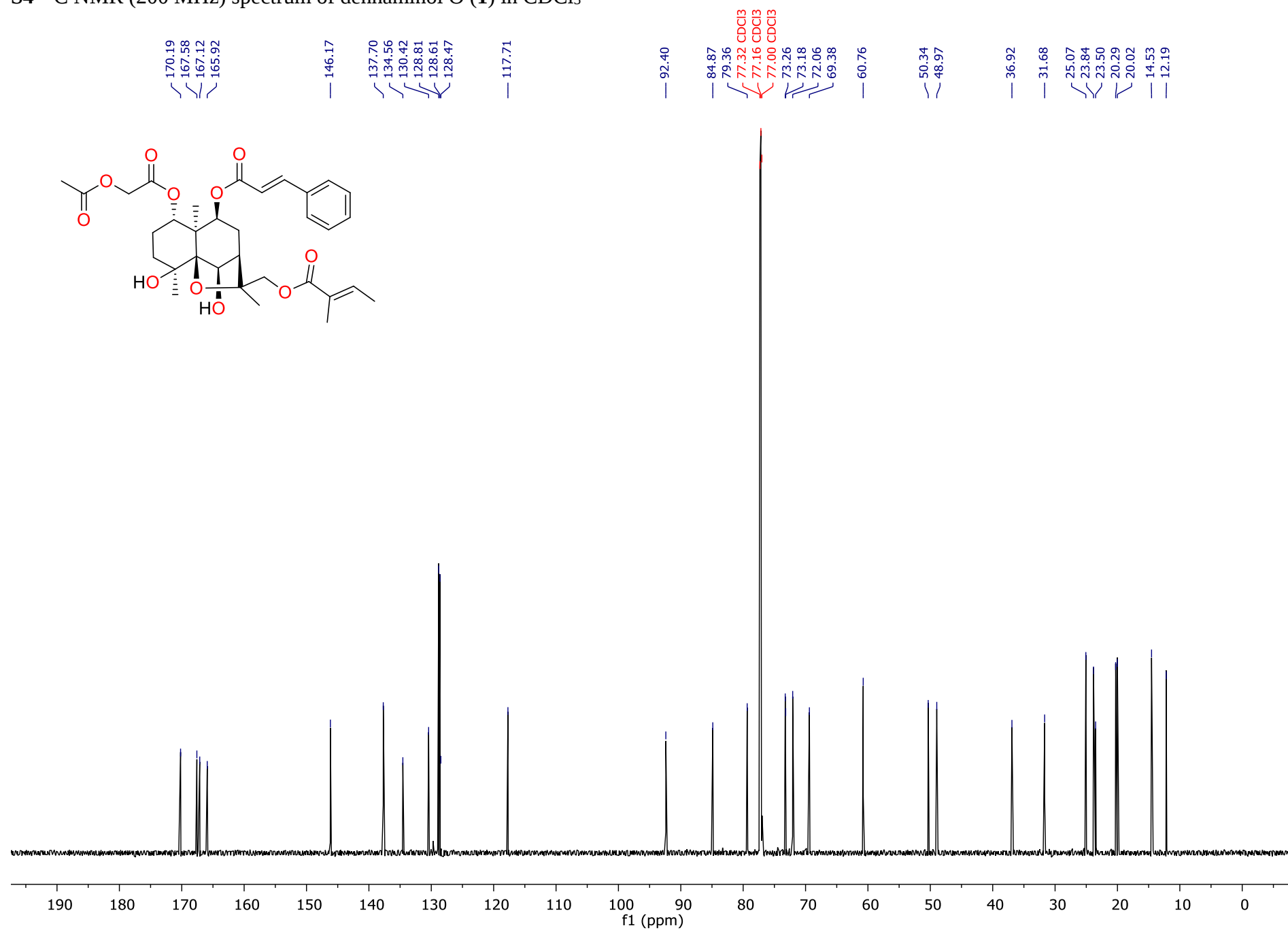
10.54	319	—	318	7	0
14.15	451	—	450	9	0
15.72	465	—	464	17	0

<i>Denhamia</i>	Roots	14.15	451	—	450	9	0
<i>cunninghamii</i>							
(Hook.)							
M.P.Simmons							
		15.72	465	—	464	17	0
		18.40	429	—	428	12	0
<i>Hypsophila</i>	Mixed	17.17	441	—	440	21	0
<i>dielsiana</i> Loes.							

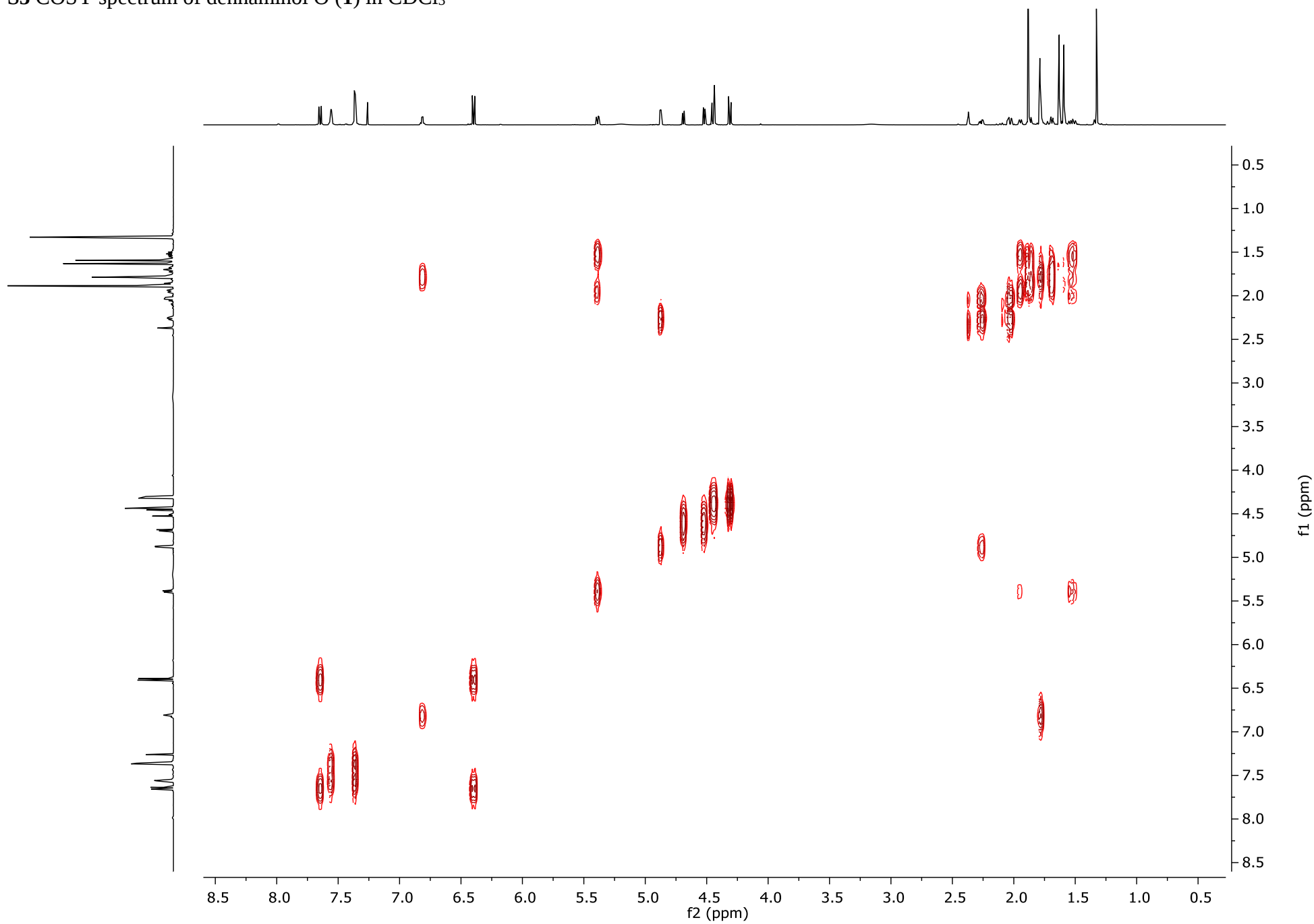
S3 ^1H NMR (800 MHz) spectrum of denhaminol O (**1**) in CDCl_3



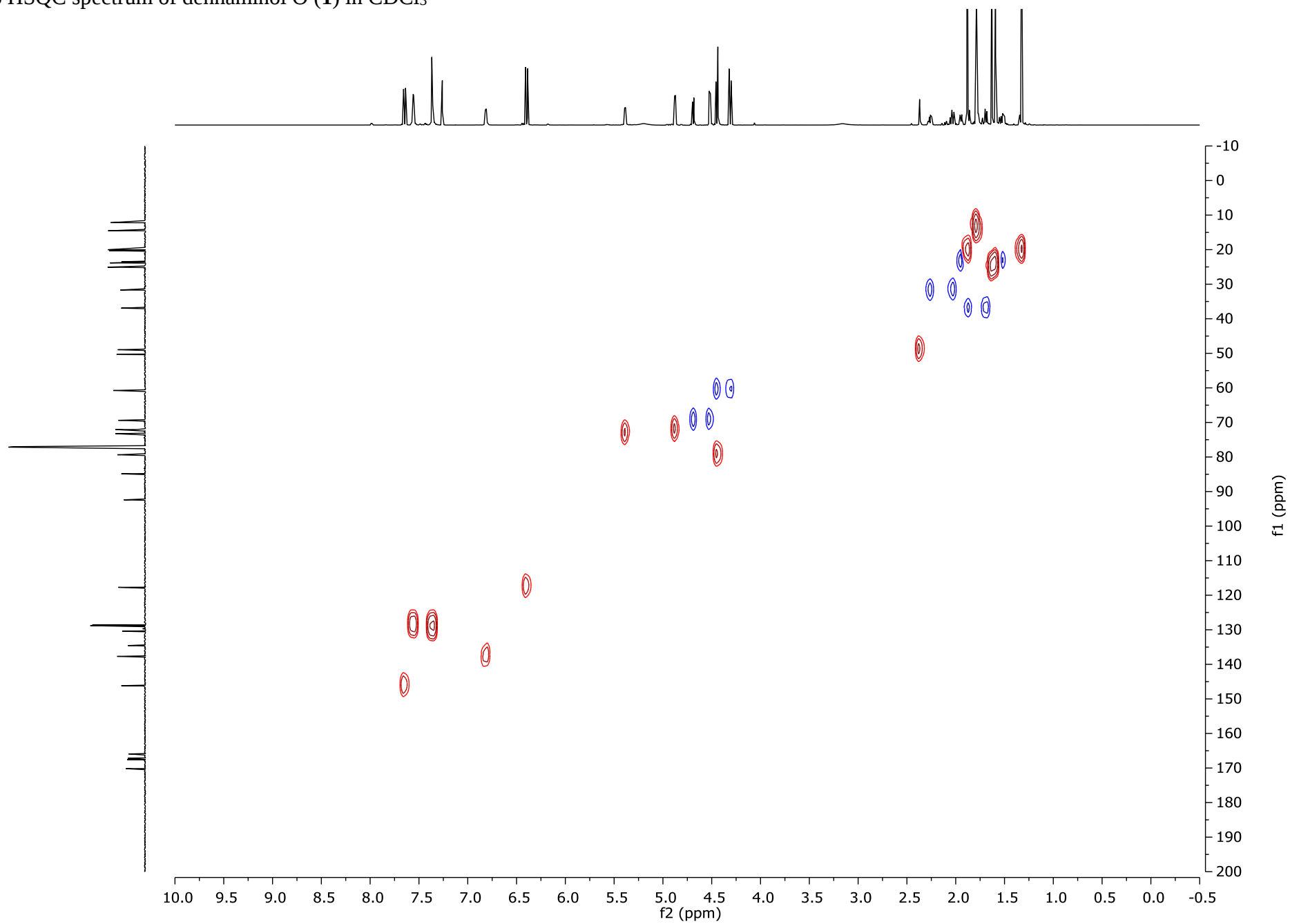
S4 ^{13}C NMR (200 MHz) spectrum of denhaminol O (**1**) in CDCl_3



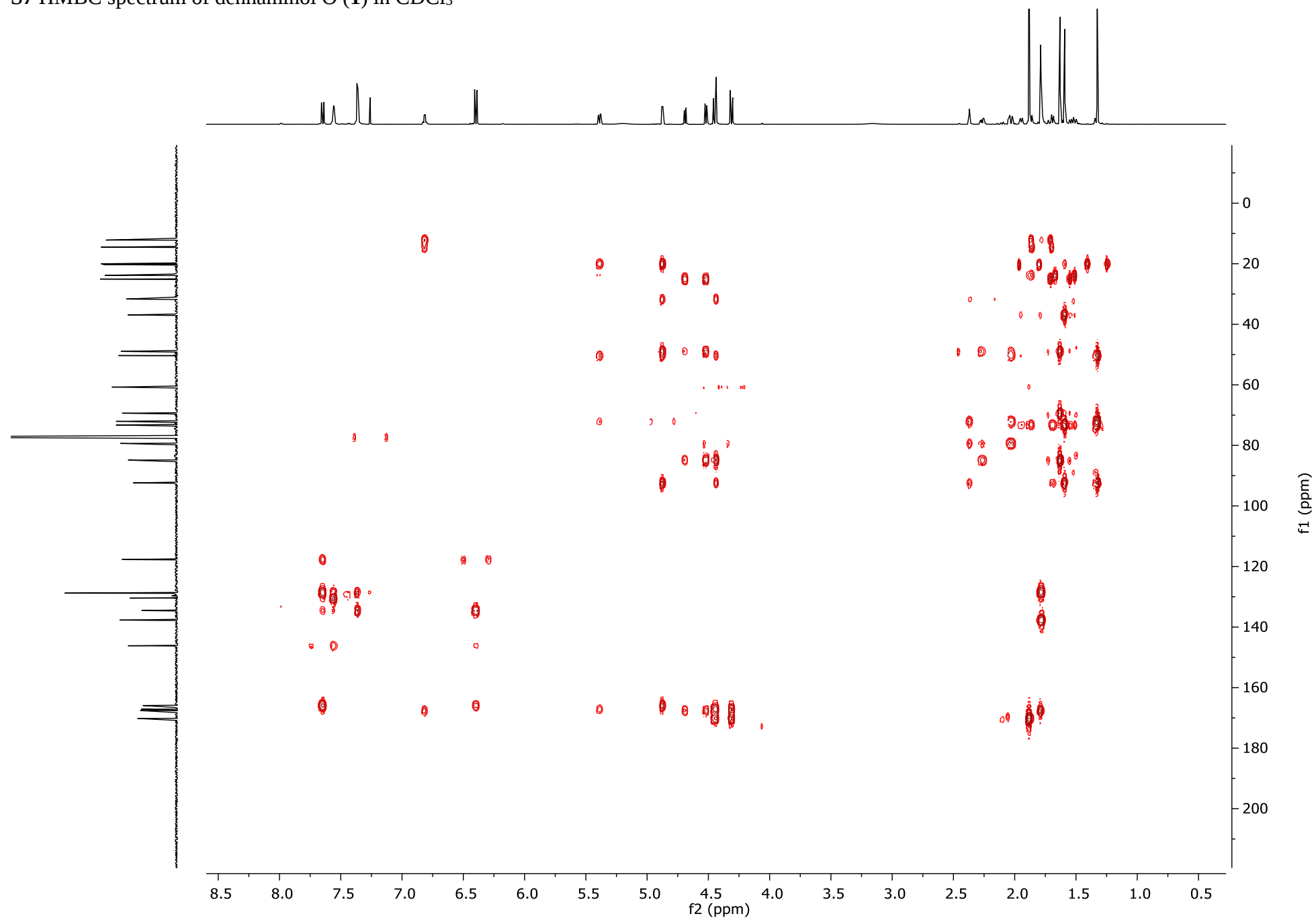
S5 COSY spectrum of denhaminol O (**1**) in CDCl₃



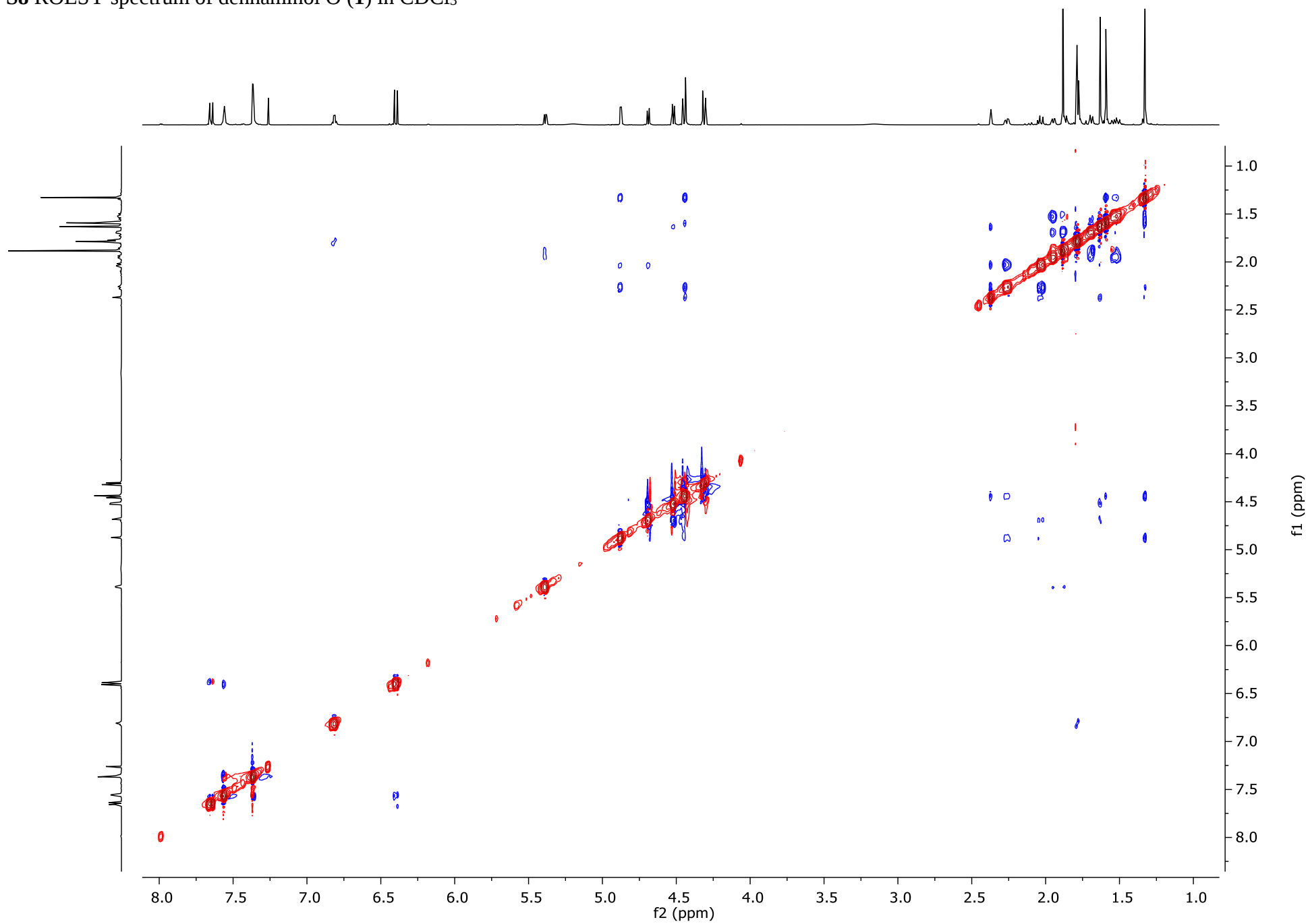
S6 HSQC spectrum of denhaminol O (**1**) in CDCl₃



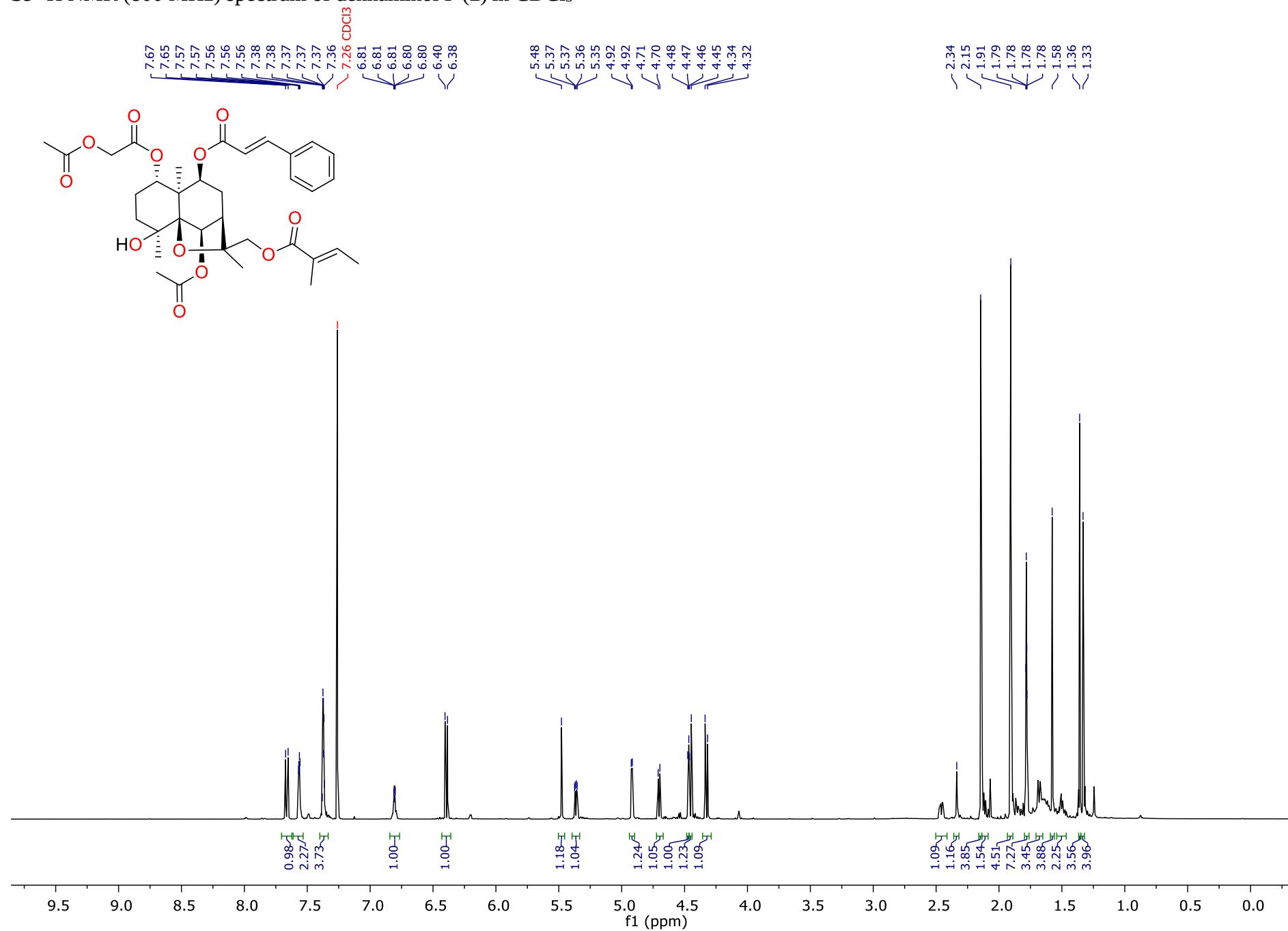
S7 HMBC spectrum of denhaminol O (**1**) in CDCl₃



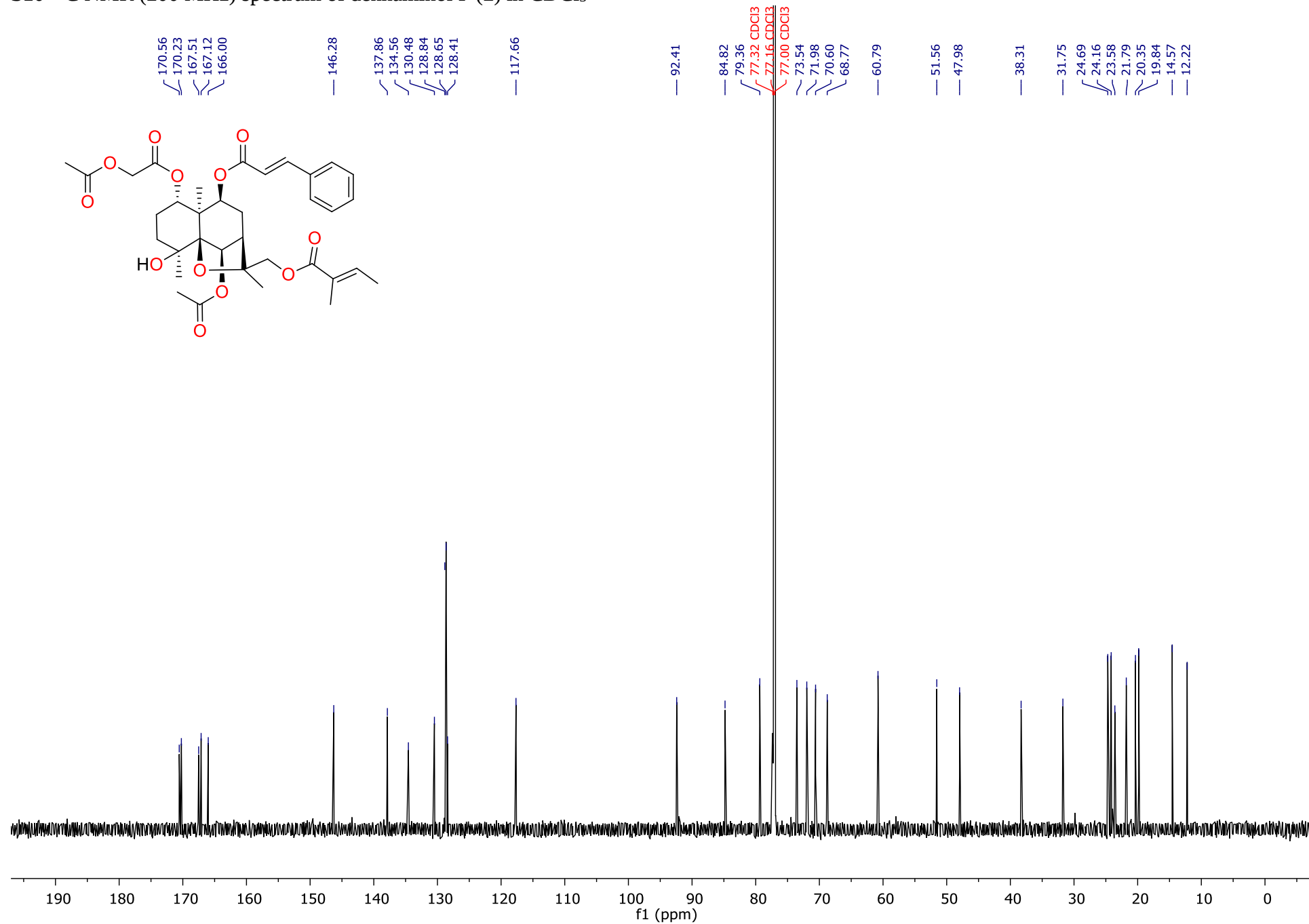
S8 ROESY spectrum of denhaminol O (**1**) in CDCl₃



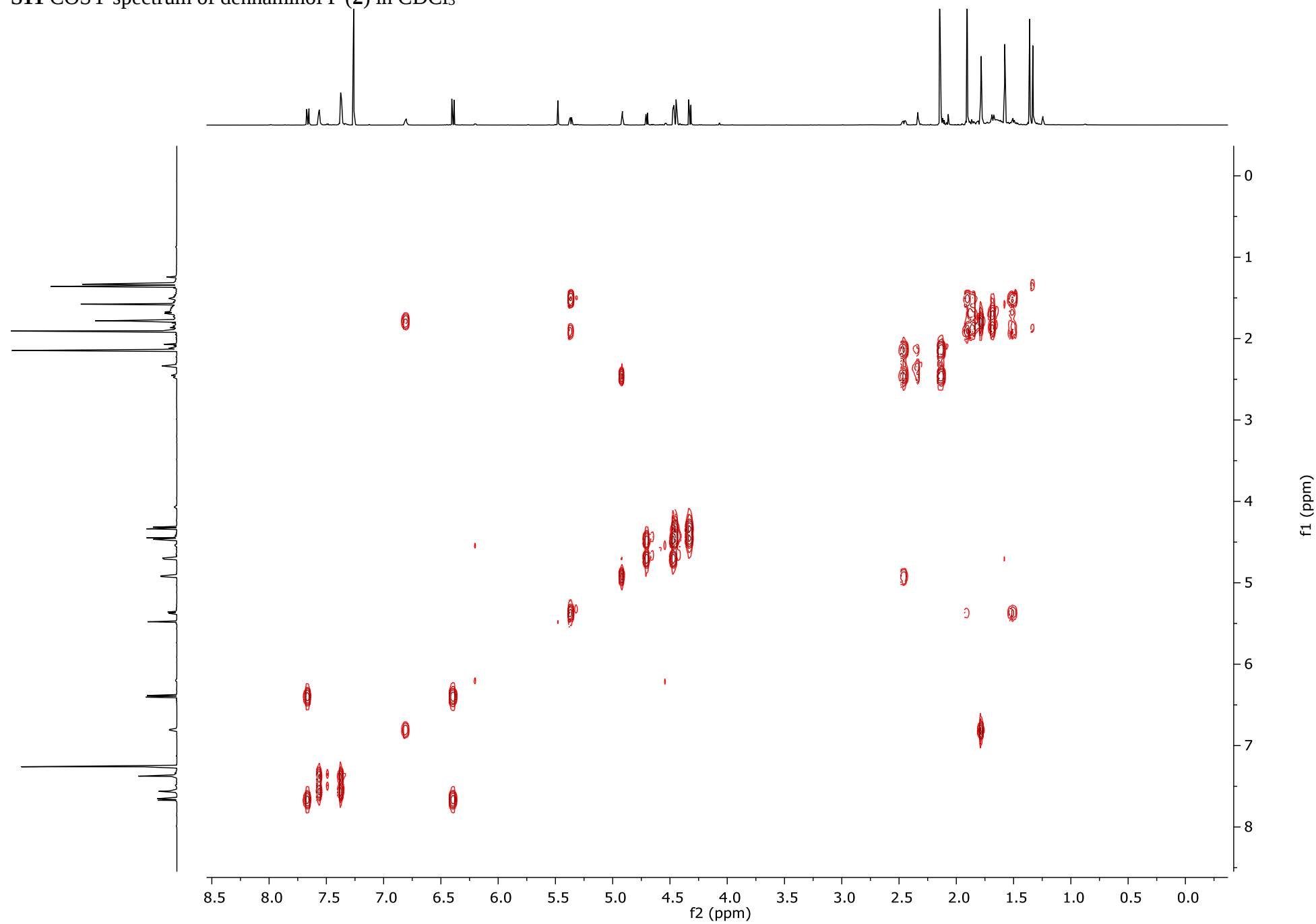
S9 ^1H NMR (800 MHz) spectrum of denhaminol P (**2**) in CDCl_3



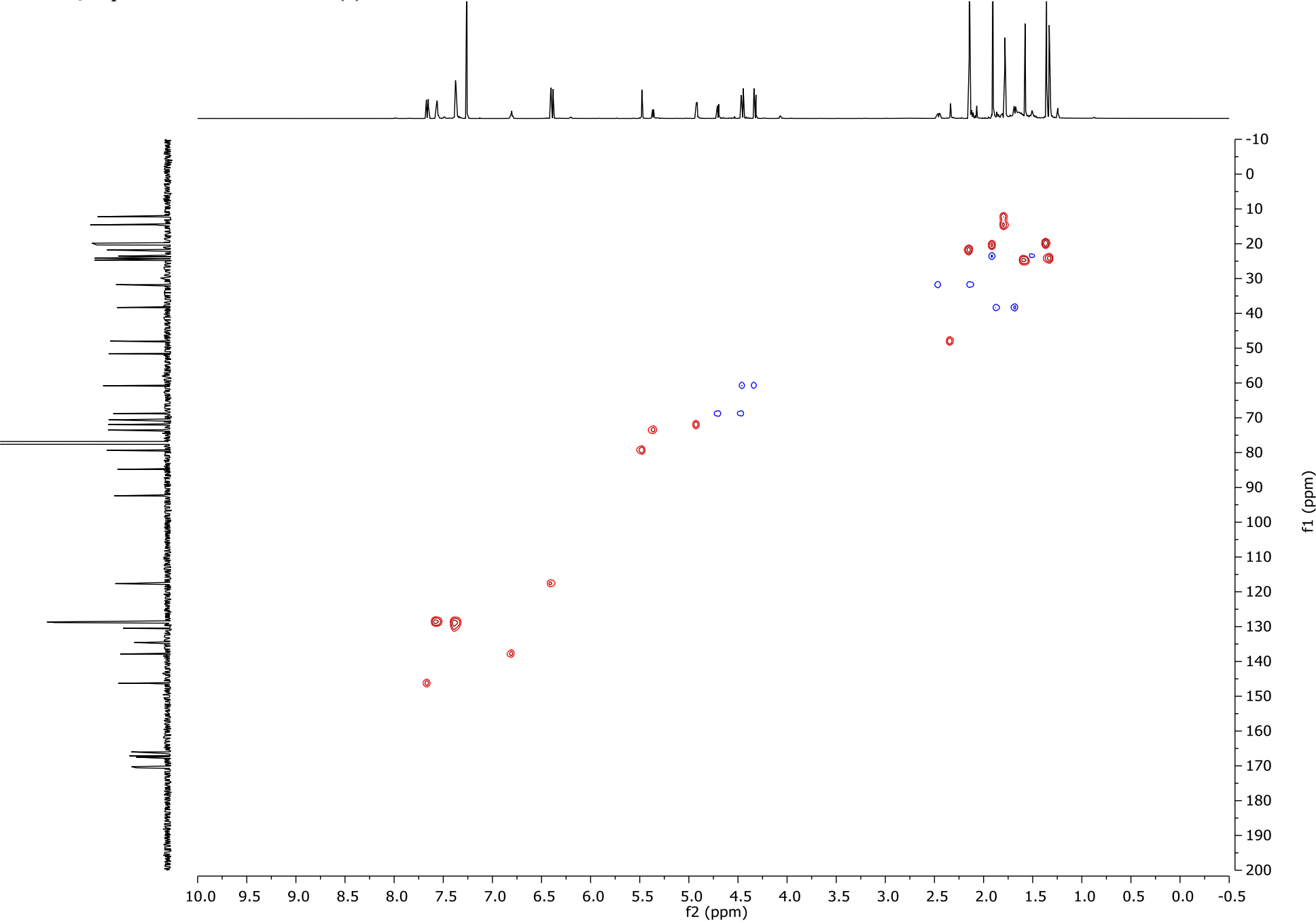
S10 ^{13}C NMR (200 MHz) spectrum of denhaminol P (**2**) in CDCl_3



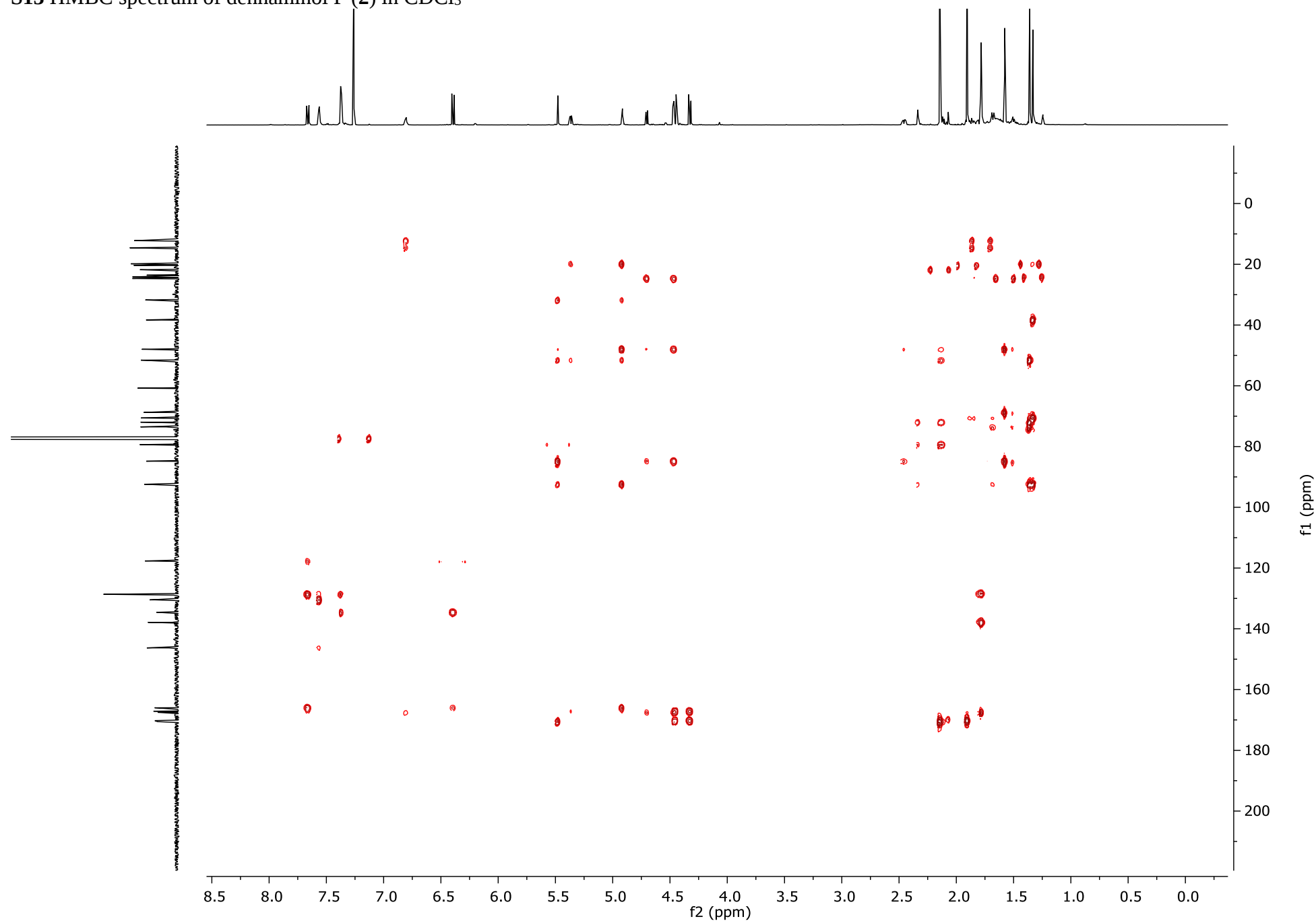
S11 COSY spectrum of denhaminol P (2) in CDCl₃



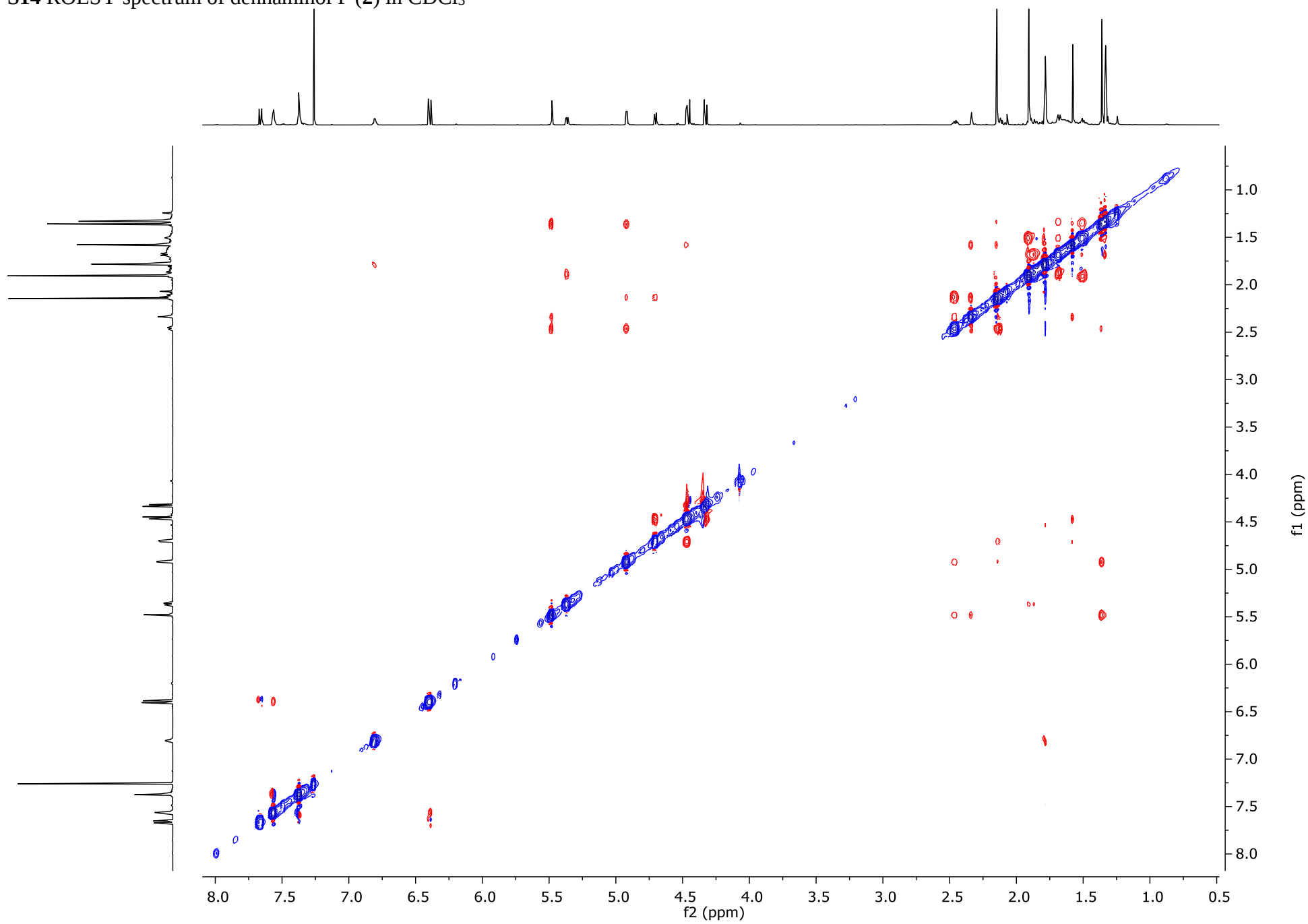
S12 HSQC spectrum of denhaminol P (2) in CDCl₃



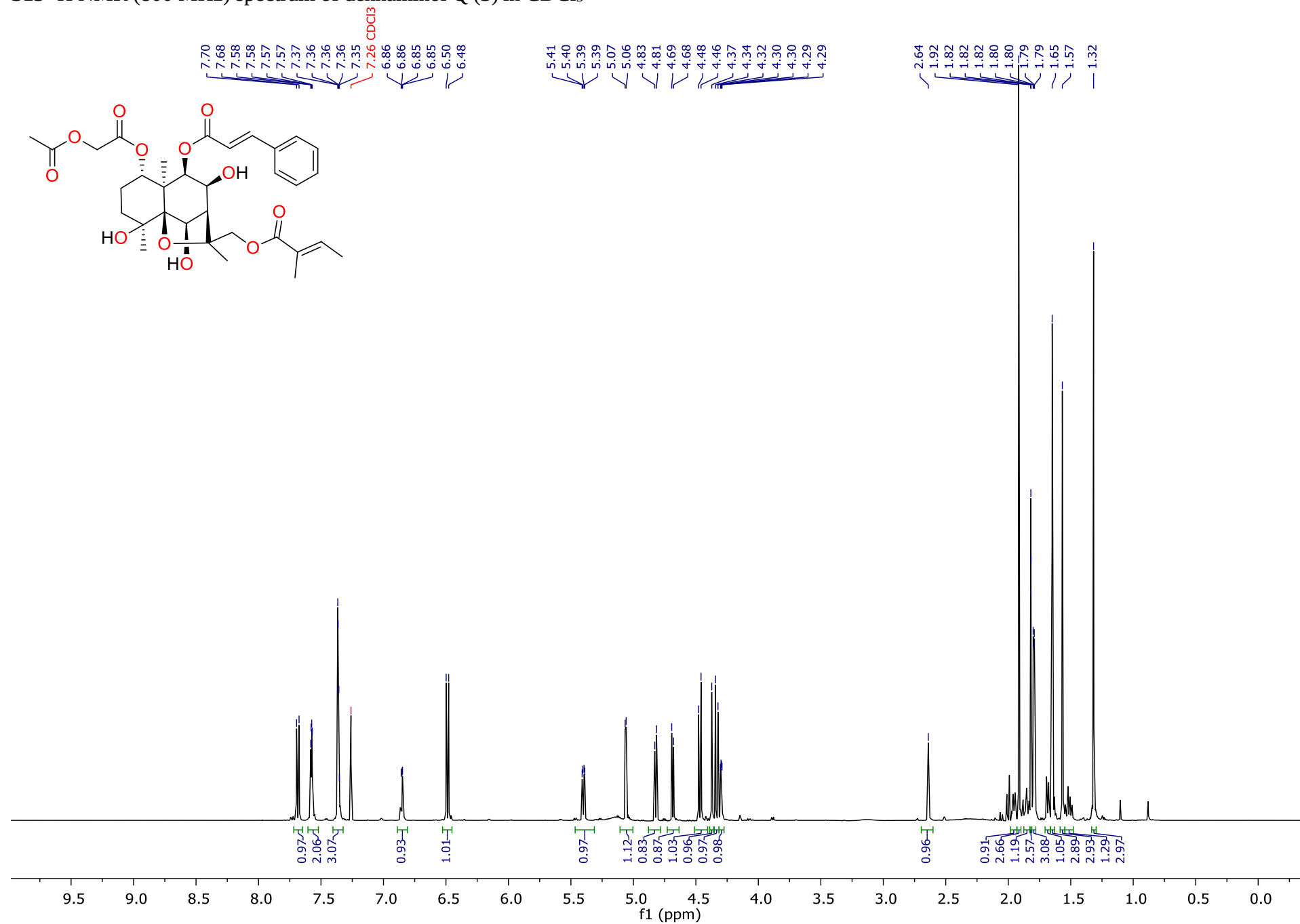
S13 HMBC spectrum of denhaminol P (2) in CDCl₃



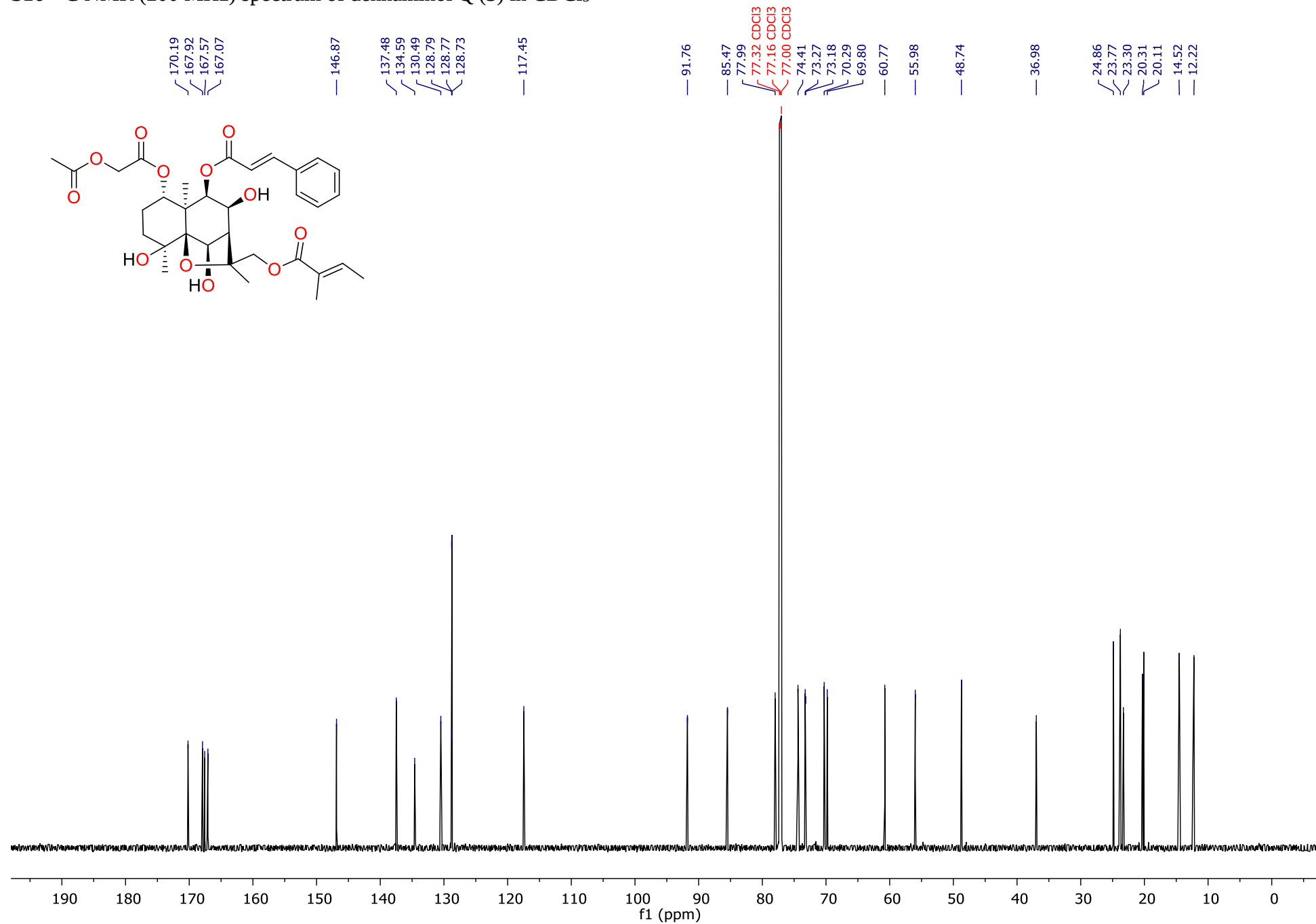
S14 ROESY spectrum of denhaminol P (2) in CDCl₃



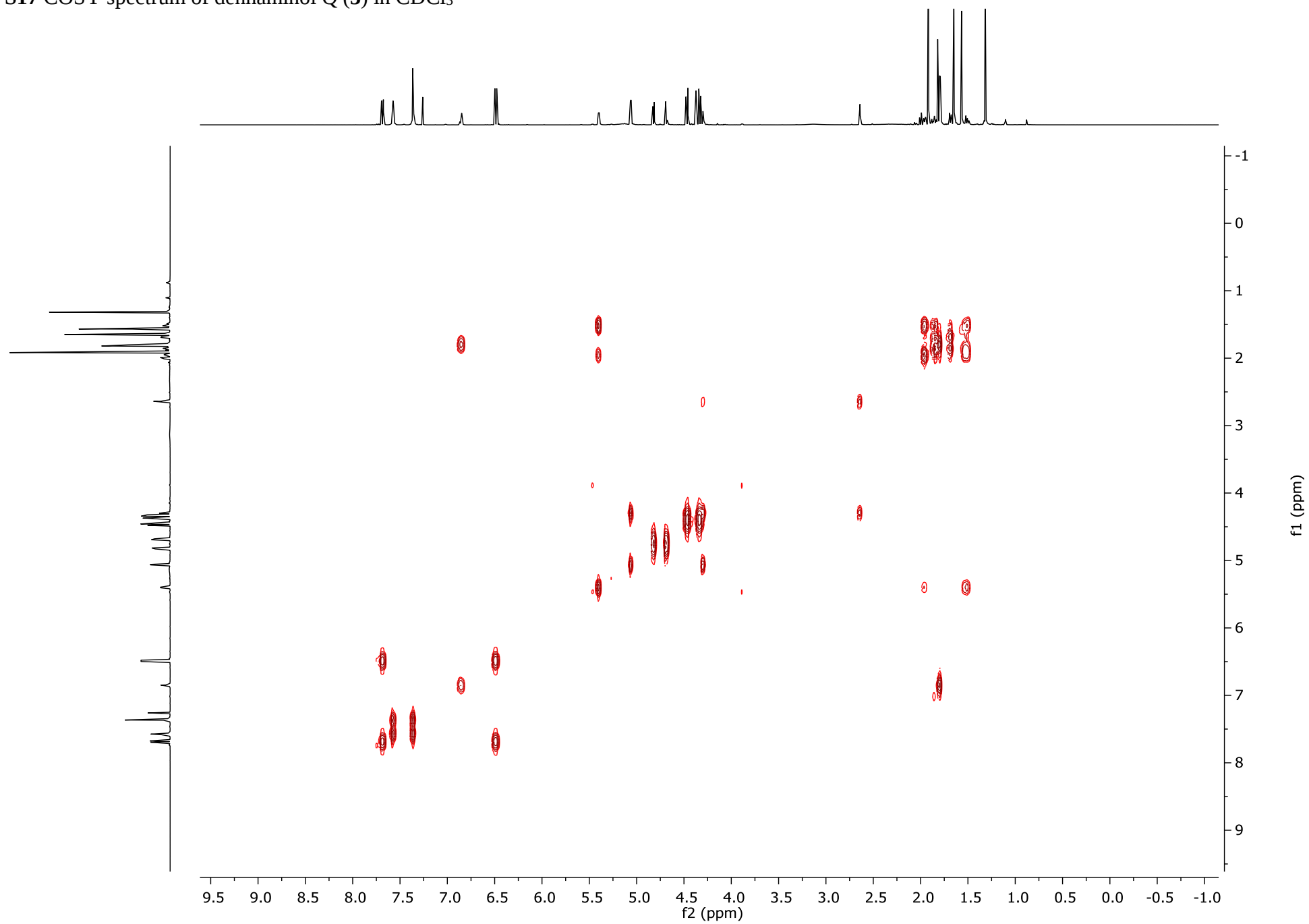
S15 ^1H NMR (800 MHz) spectrum of denhaminol Q (**3**) in CDCl_3



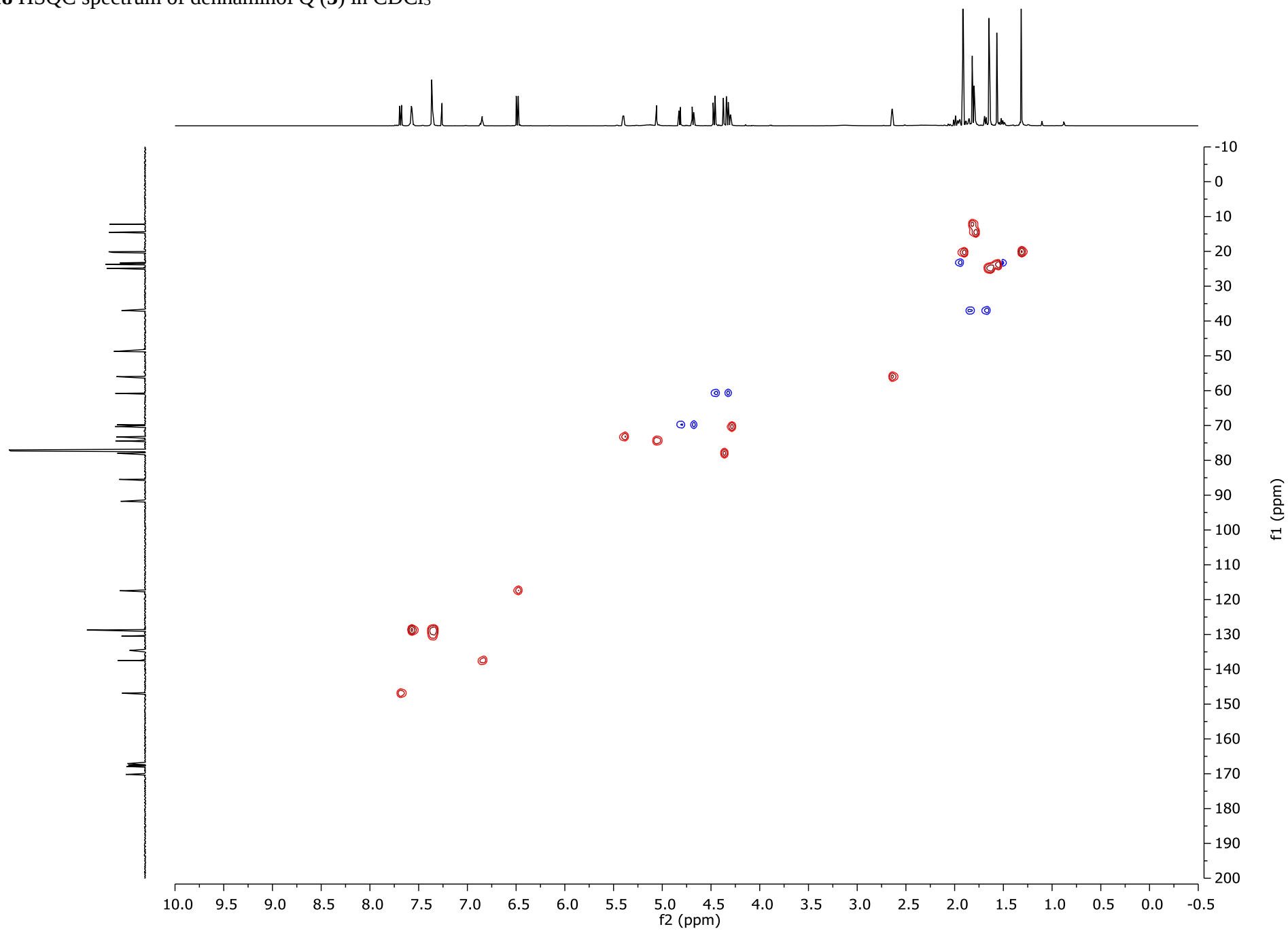
S16 ^{13}C NMR (200 MHz) spectrum of denhaminol Q (**3**) in CDCl_3



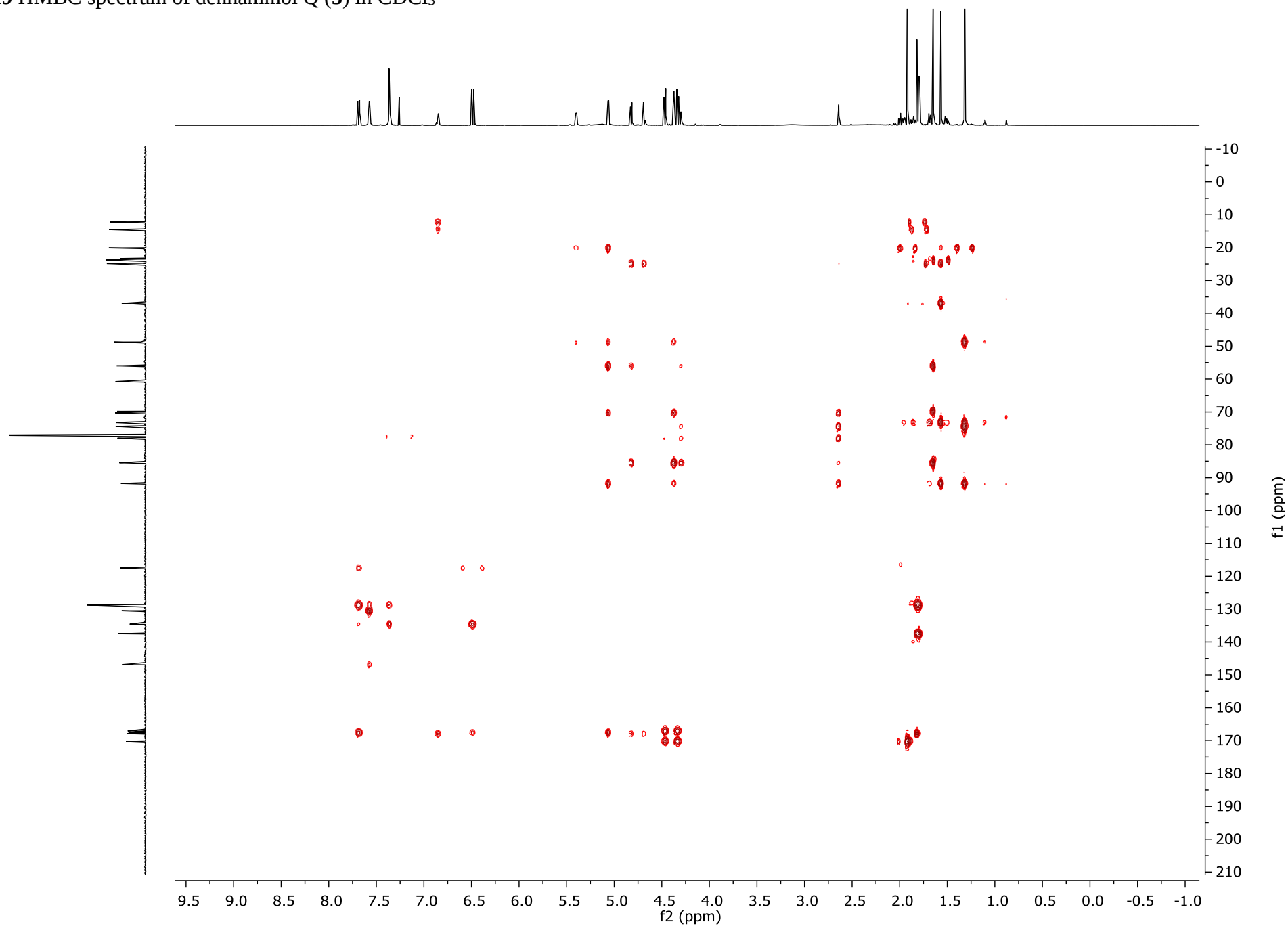
S17 COSY spectrum of denhaminol Q (3) in CDCl₃



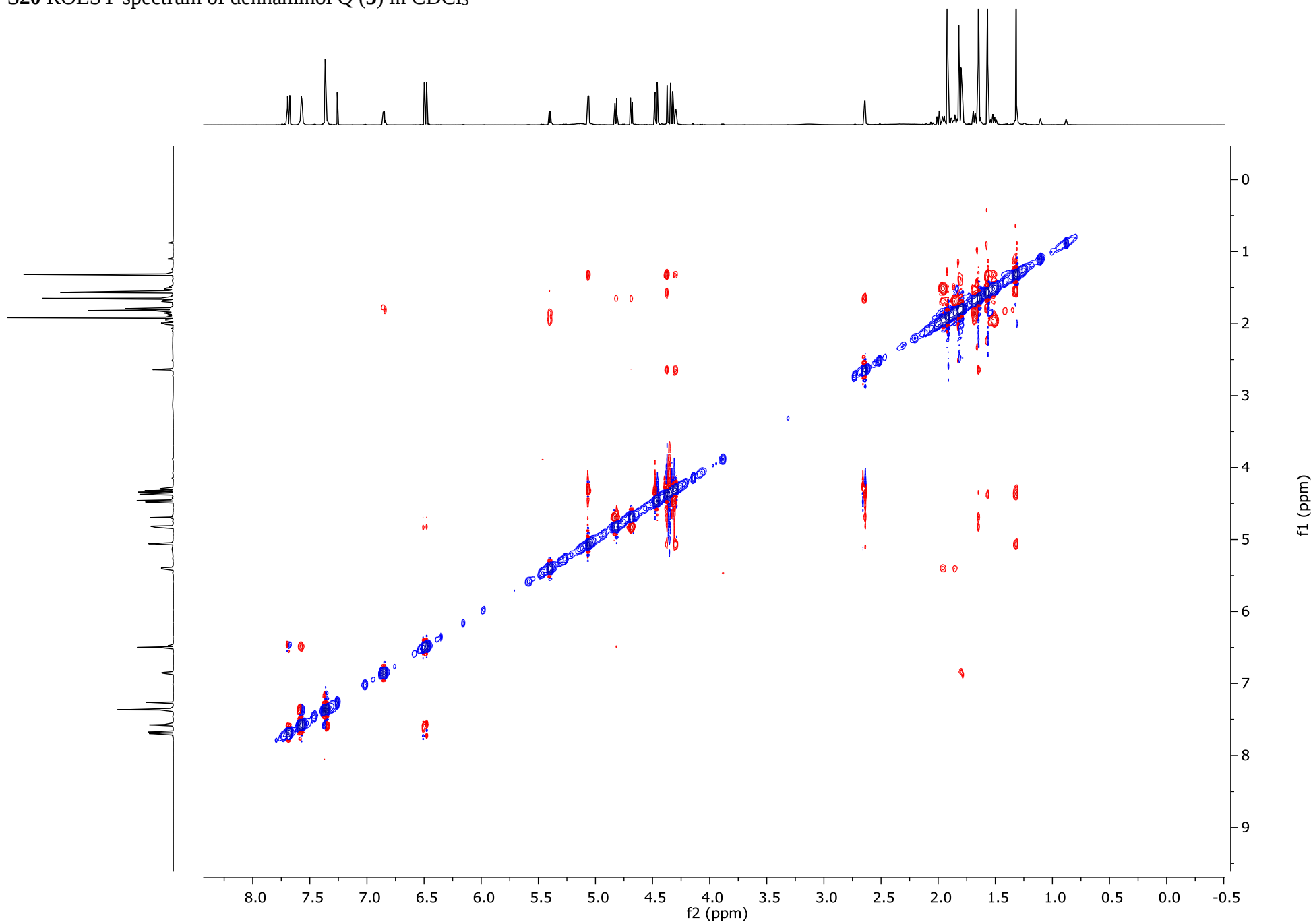
S18 HSQC spectrum of denhaminol Q (**3**) in CDCl₃



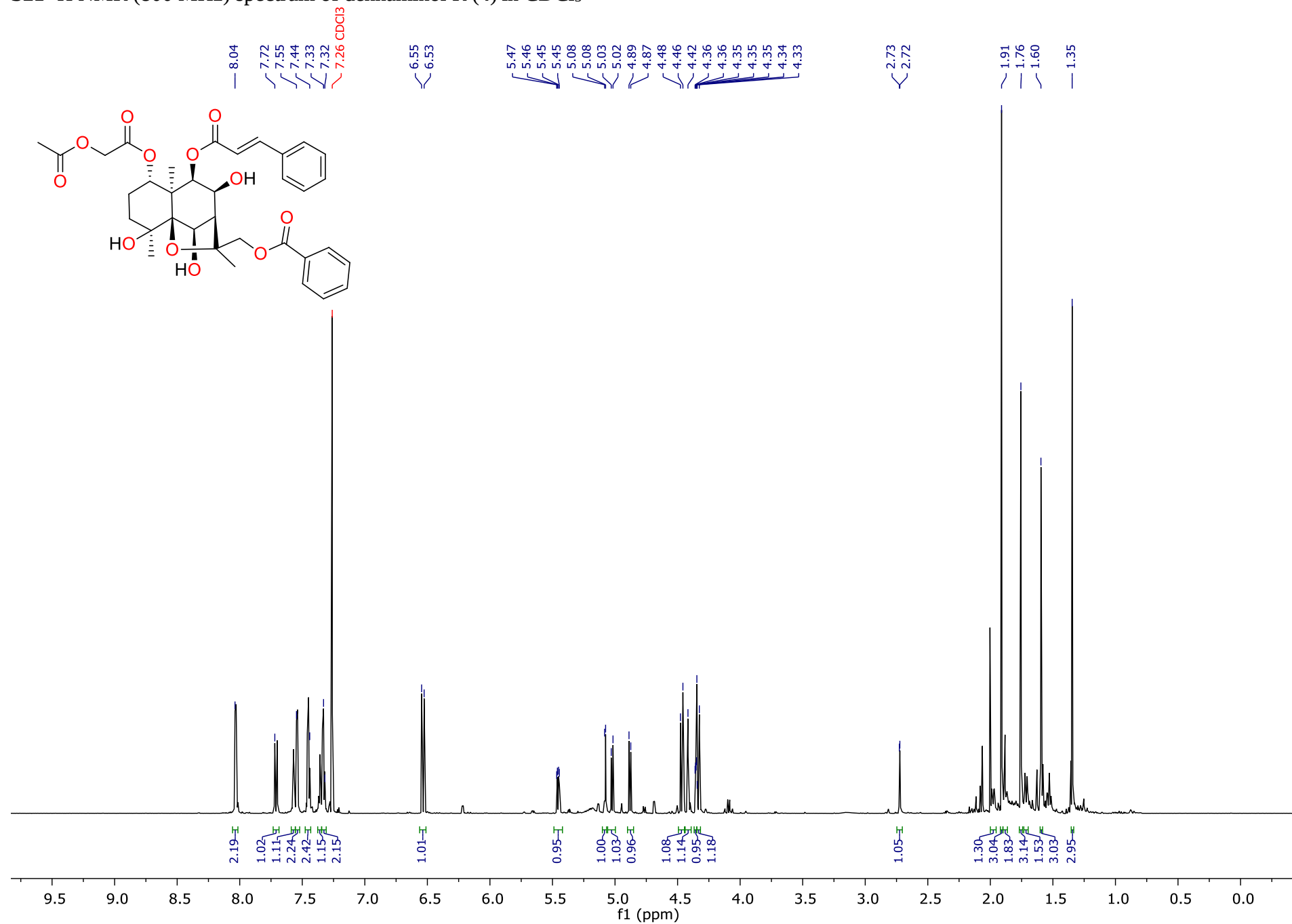
S19 HMBC spectrum of denhaminol Q (3) in CDCl₃



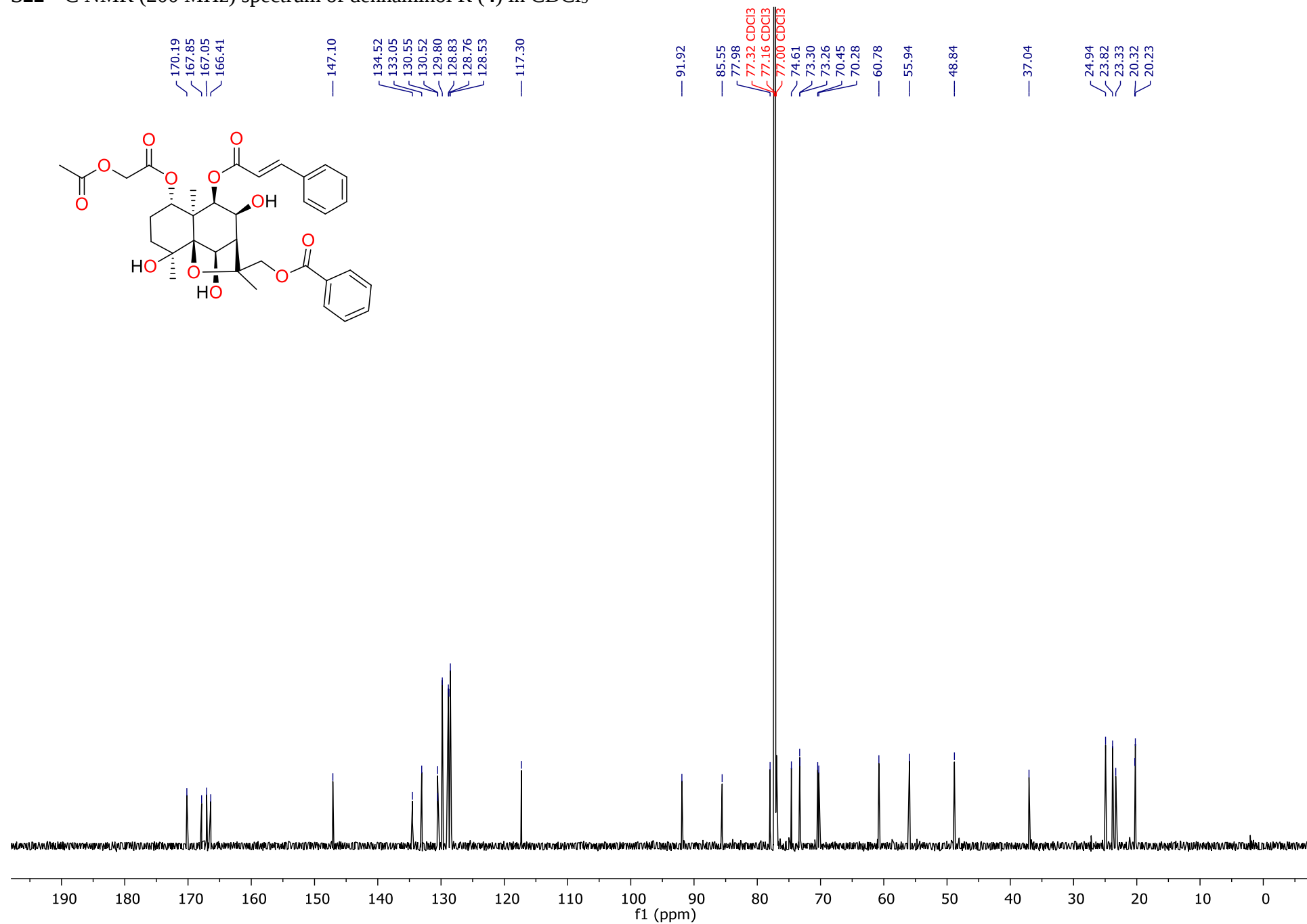
S20 ROESY spectrum of denhaminol Q (3) in CDCl₃



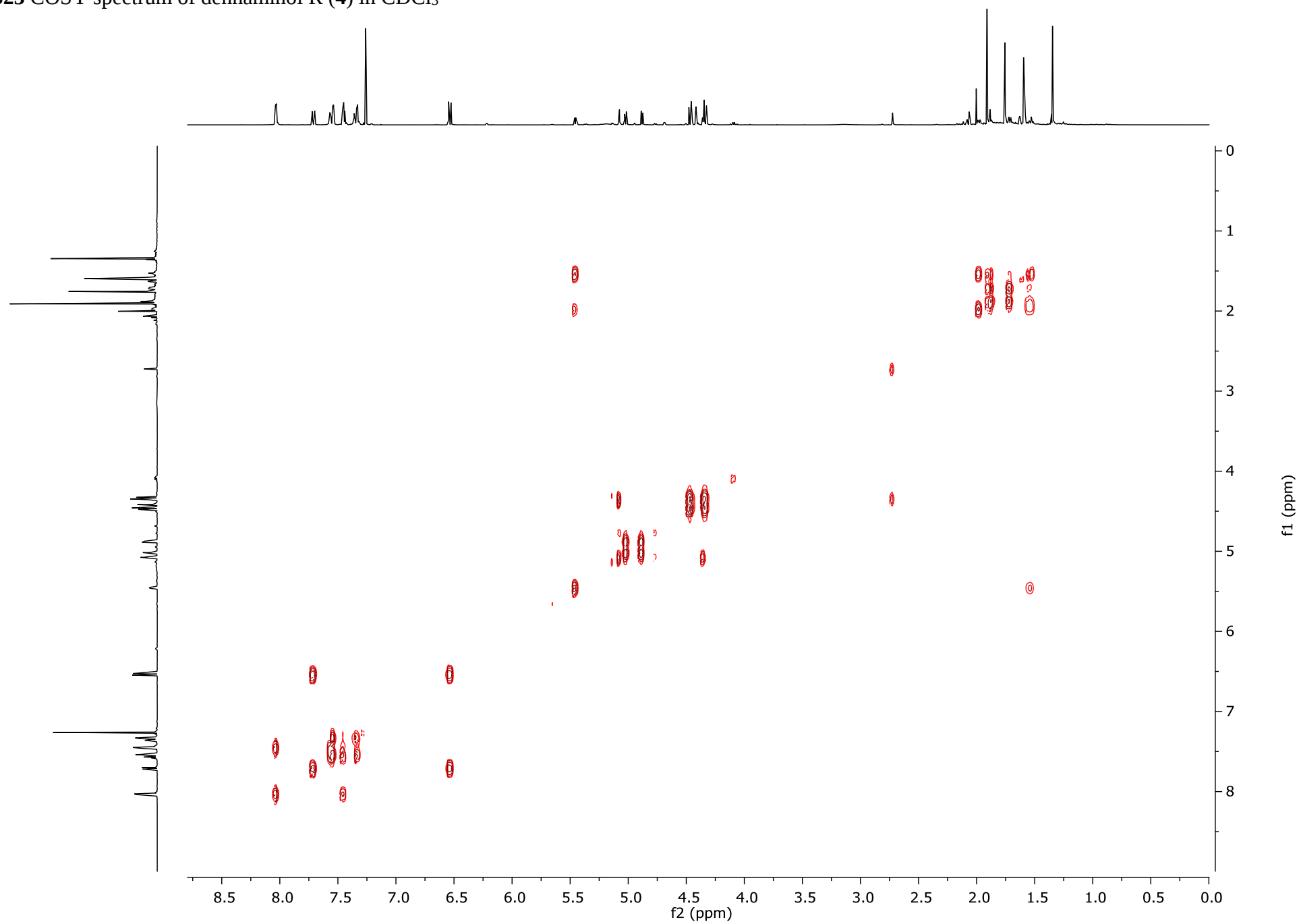
S21 ^1H NMR (800 MHz) spectrum of denhaminol R (**4**) in CDCl_3



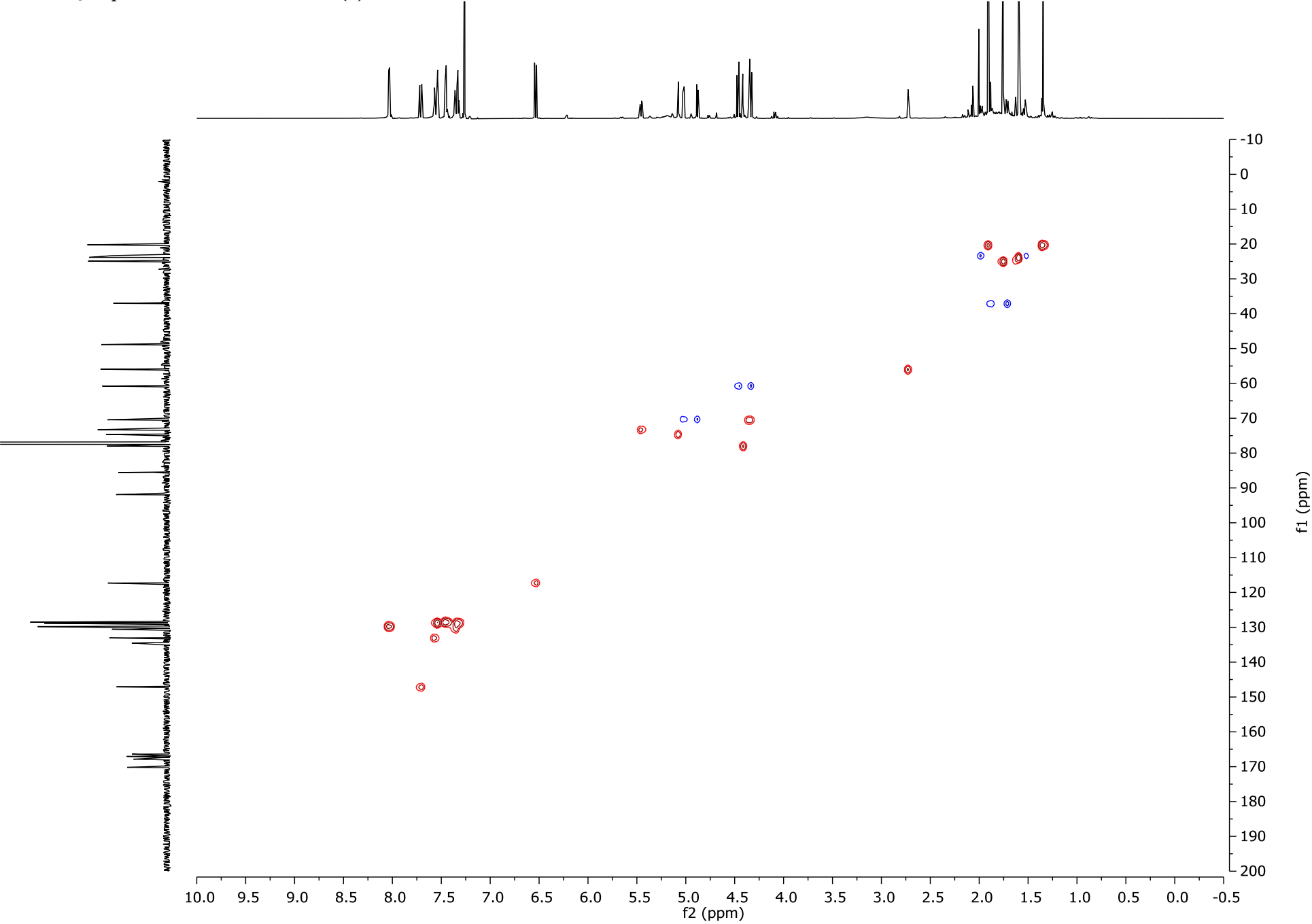
S22 ^{13}C NMR (200 MHz) spectrum of denhaminol R (**4**) in CDCl_3



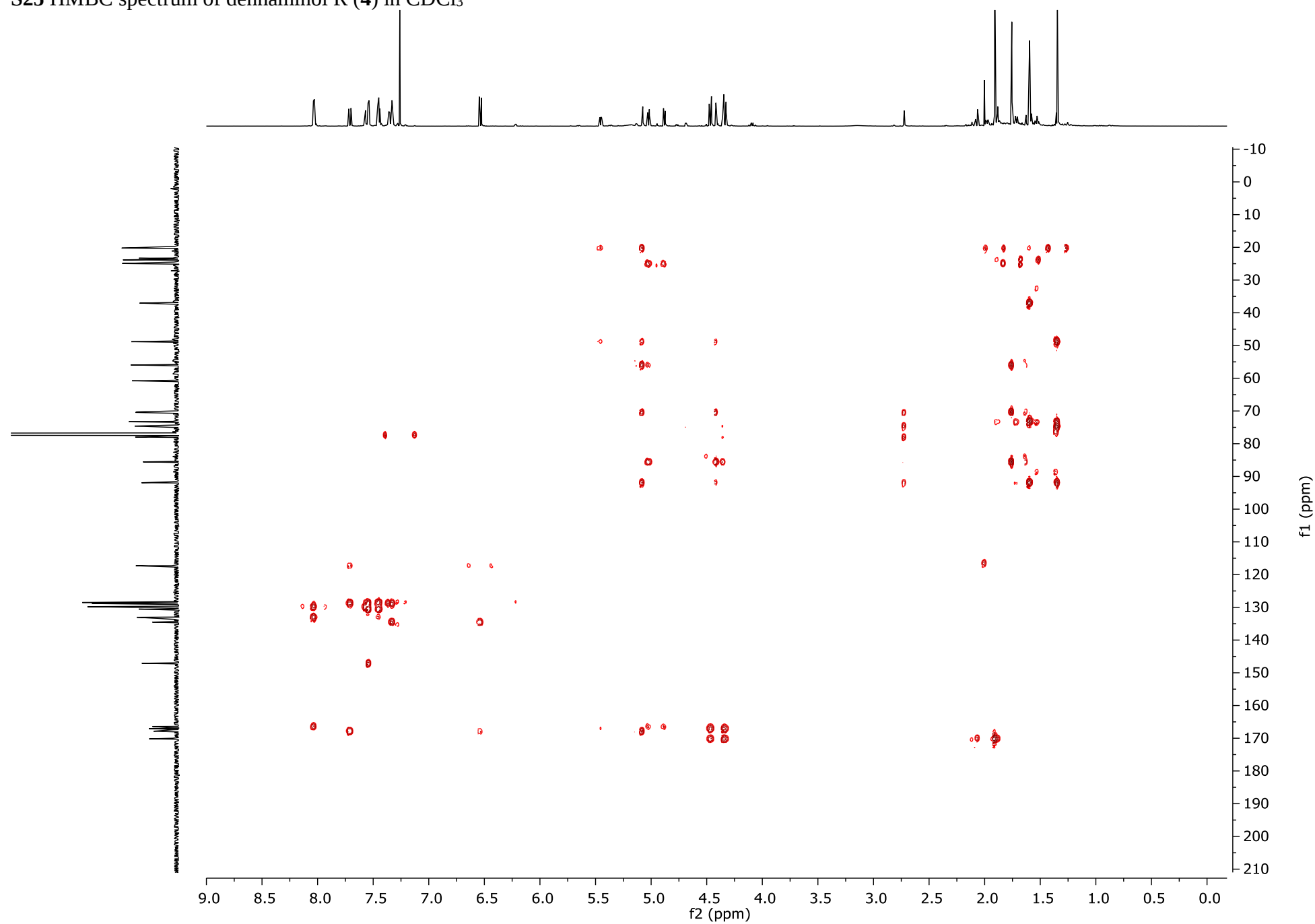
S23 COSY spectrum of denhaminol R (**4**) in CDCl₃



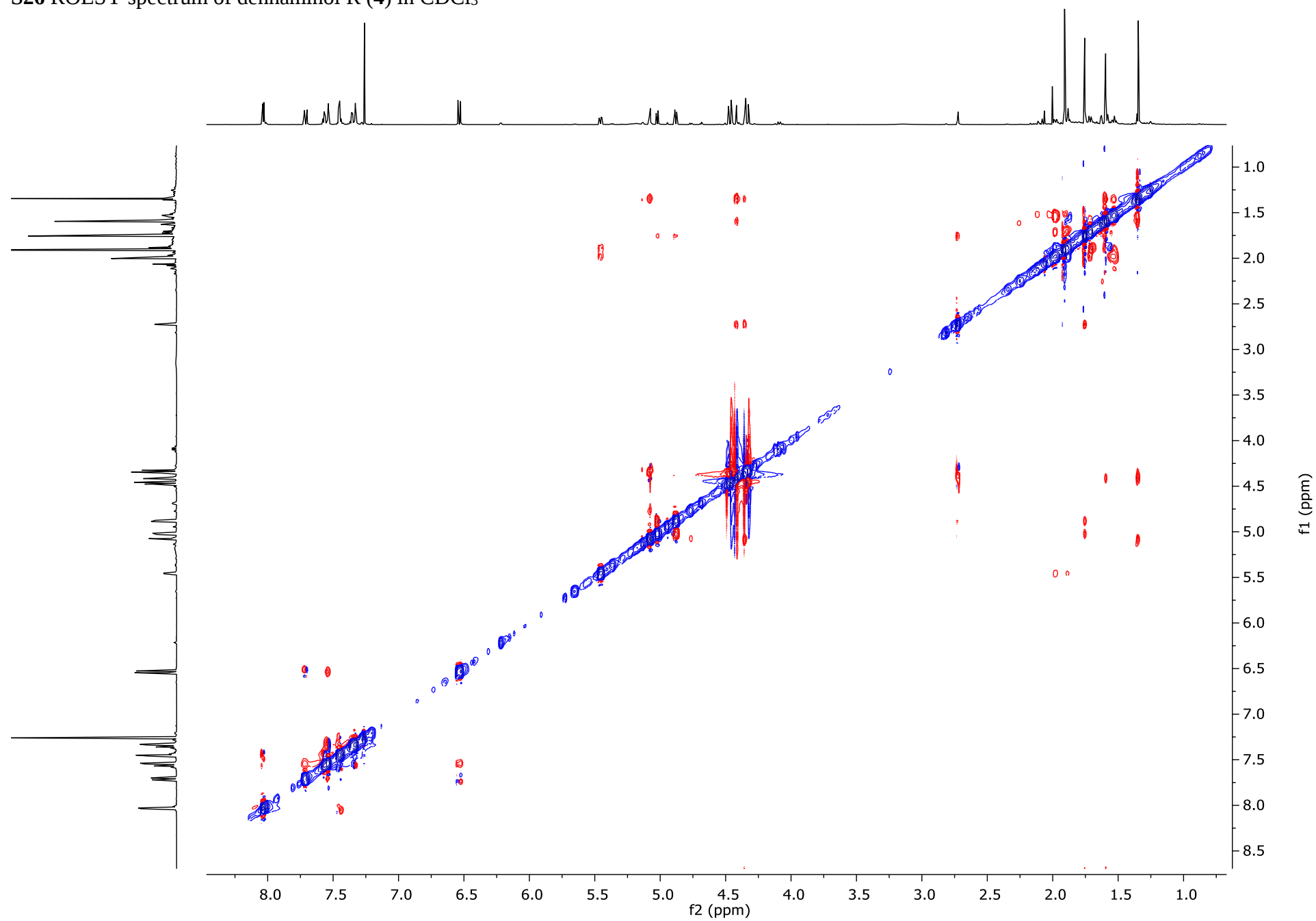
S24 HSQC spectrum of denhaminol R (4) in CDCl₃



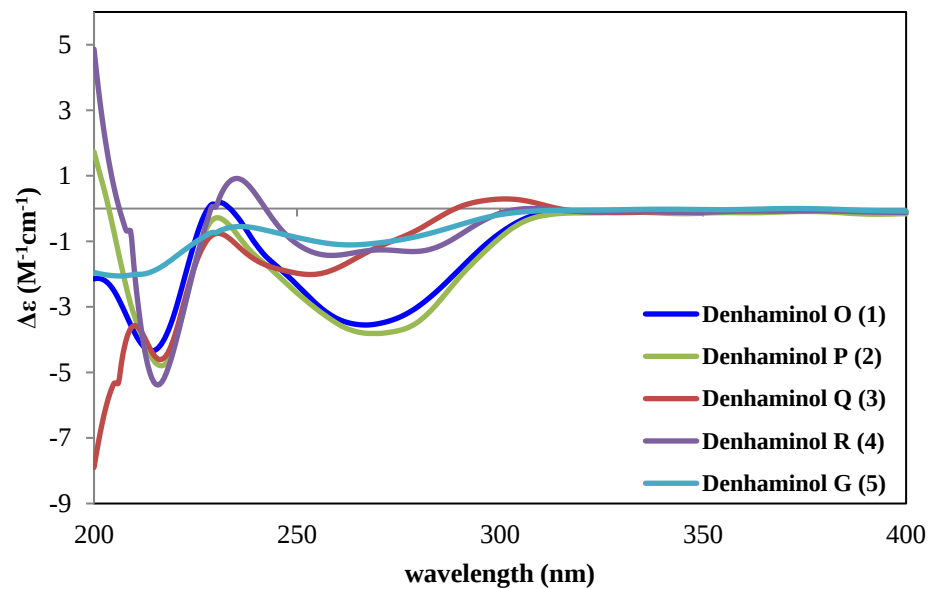
S25 HMBC spectrum of denhaminol R (**4**) in CDCl₃



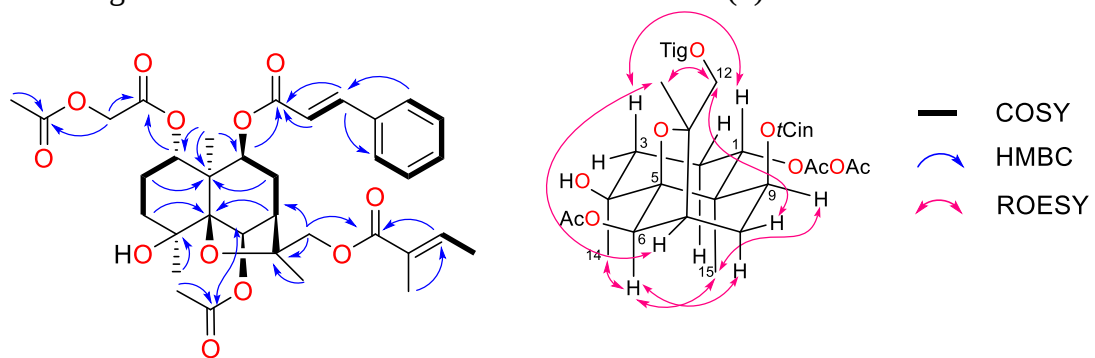
S26 ROESY spectrum of denhaminol R (**4**) in CDCl₃



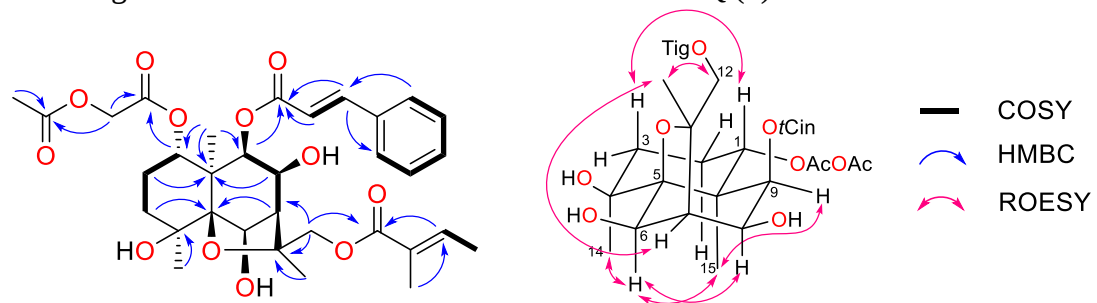
S27 ECD spectra of denhaminols O–R (1–4) and denhaminol G (5) in MeOH



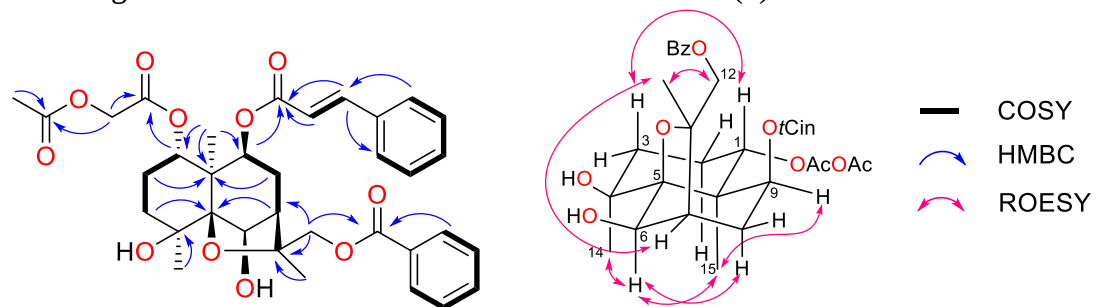
S28 Diagnostic 2D NMR correlations for denhaminol P (2)



S29 Diagnostic 2D NMR correlations for denhaminol Q (3)



S30 Diagnostic 2D NMR correlations for denhaminol R (4)



S31. Australian Celastraceae plant collection date, location, and voucher specimen codes

NatureBank (NB) code	Queensland Herbarium (BRI) voucher accession number	Sample type	Species name	Collection date	Collection site
NB019299	AQ605014	Roots	<i>Denhamia celastroides</i> (F.Muell.) Jessup	26 November 1997	Mt Windsor Tableland, Queensland, Australia
NB005745	AQ603214	Twigs	<i>Perrottetia arborescens</i> (F.Muell.) Loes.	10 June 1996	Longlands Gap, Queensland, Australia
NB015383	AQ605014	Bark	<i>Denhamia celastroides</i> (F.Muell.) Jessup	26 November 1997	Mt Windsor Tableland, Queensland, Australia
NB020738	AQ605523	Roots	<i>Denhamia fasciculiflora</i> (Jessup) M.P.Simmons	28 June 1998	Macrossan Range, Queensland, Australia
NB005757	AQ603214	Roots	<i>Perrottetia arborescens</i> (F.Muell.) Loes.	10 June 1996	Longlands Gap, Queensland, Australia
NB010702	AQ602529	Roots	<i>Elaeodendron melanocarpum</i> F.Muell.	29 December 1995	Wietalaba, Queensland, Australia
NB005647	AQ603214	Leaves	<i>Perrottetia arborescens</i> (F.Muell.) Loes.	10 June 1996	Longlands Gap, Queensland, Australia
NB016513	AQ604981	Bark	<i>Elaeodendron melanocarpum</i> F.Muell.	26 November 1997	Mt Windsor Tableland, Queensland, Australia
NB003376	AQ600521	Mixed	<i>Hippocratea barbata</i> F.Muell.	10 December 1993	Shiptons Flat, Queensland, Australia
NB013676	AQ604654	Bark	<i>Hypsophila halleyana</i> F.Muell.	25 October 1997	Bartle Frere, Queensland, Australia
NB004940	AQ602808	Bark	<i>Denhamia cunninghamii</i> (Hook.) M.P.Simmons	7 February 1996	Lappa, Queensland, Australia
NB022808	AQ605663	Roots	<i>Denhamia pittosporoides</i> F.Muell. subsp. <i>pittosporoides</i>	6 November 1998	Cannondale Scrub, Queensland, Australia
NB021847	AQ605691	Roots	<i>Denhamia cunninghamii</i> (Hook.) M.P.Simmons	3 November 1998	Bigge Range, Queensland, Australia
NB018975	AQ605133	Roots	<i>Denhamia cunninghamii</i> (Hook.) M.P.Simmons	17 March 1998	Surprise Creek, Queensland, Australia
NB001949	AQ601069	Mixed	<i>Hypsophila dielsiana</i> Loes.	16 July 1994	Danbulla, Queensland, Australia
NB016128	AQ605014	Fruits	<i>Denhamia celastroides</i> (F.Muell.) Jessup	26 November 1997	Mt Windsor Tableland, Queensland, Australia