

SUPPLEMENTARY MATERIAL

Two new flavone glycosides from the leaves of *Ochna afzelii* Oliv. (Ochnaceae)

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ABSTRACT

Two new glycosylflavones, 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**) and 8-C- β -D-galactopyranosylchrysoeriol (**2**) were isolated from the methanol extract of the leaves of *Ochna afzelii* Oliv., along with four known compounds namely 8-C- β -D-galactopyranosylapigenin (**3**), ochnaflavone (**4**), sitosterol-3-O- β -D-glucopyranoside (**5**) and D-mannitol (**6**). Isolation was performed chromatographically and the structures of the purified compounds were elucidated by analyzing their spectroscopic and mass spectrometric data. The antibacterial activity of extract, fractions, and compounds **1** - **4** was evaluated using broth microdilution method against Gram-positive and Gram-negative bacteria while the antioxidant capacity was performed using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) and the ferric reducing antioxidant power (FRAP) methods. The new flavones (**1** and **2**) displayed moderate antibacterial activities (MIC = 32 – 64 μ g/mL) and weak antioxidant properties.

Contents

Table SM1:	^1H (500 MHz), ^{13}C (125MHz) and selected HMBC data of compounds 1 and 2 in DMSO- d_6	4
Figure SM.1:	Key HMBC ($\text{H} \longrightarrow \text{C}$) and ROESY ($\text{H} \longleftrightarrow \text{H}$) correlations of compounds 1 and 2	5
Figure SM.2:	IR spectrum of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	6
Figure SM.3:	^1H NMR spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	7
Figure SM.4:	^{13}C NMR spectrum (125 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	8
Figure SM.5:	HSQC spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	9
Figure SM.6:	HMBC spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	10
Figure SM.7:	^1H - ^1H COSY spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	11
Figure SM.8:	ROESY spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	12
Figure SM.9:	HRESI-MS spectrum of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	13
Figure SM.10:	HRESI accurate data of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1).....	14
Figure SM.11:	IR spectrum of 8-C- β -D-galactopyranosylchrysoeriol (2).....	15
Figure SM.12:	^1H NMR spectrum (500 MHz, DMSO- d_6) of 8-C- β -D-galactopyranosylchrysoeriol (2).....	16
Figure SM.13:	^{13}C NMR spectrum (125 MHz, DMSO- d_6) of 8-C- β -D-galactopyranosylchrysoeriol (2).....	17
Figure SM.14:	HSQC spectrum (500 MHz, DMSO- d_6) of 8-C- β -D-galactopyranosylchrysoeriol (2).....	18
Figure SM.15:	HMBC spectrum (500 MHz, DMSO- d_6) of 8-C- β -D-galactopyranosylchrysoeriol (2).....	19

Figure SM.16:	^1H – ^1H COSY spectrum (500 MHz, DMSO- d_6) of 8- <i>C</i> - β - <i>D</i> -galactopyranosylchrysoeriol (2).....	20
Figure SM.17:	ROESY spectrum (500 MHz, DMSO- d_6) of 8- <i>C</i> - β - <i>D</i> -galactopyranosylchrysoeriol (2).....	21
Figure SM.18:	HRESI-MS spectrum of 8- <i>C</i> - β - <i>D</i> -galactopyranosylchrysoeriol (2).....	22
Figure SM.19:	HRESI accurate data of 8- <i>C</i> - β - <i>D</i> -galactopyranosylchrysoeriol (2).....	23

Table SM1: ^1H (500 MHz), ^{13}C (125MHz) and selected HMBC data of compounds **1** and **2** in DMSO- d_6

Position	1			2		
	δ_C	δ_H	HMBC	δ_C	δ_H	HMBC
2	164.6			164.6		
3	102.9	6.99, s	C-4, C-1'	102.9	6.82, s	C-4, C-1'
4	182.7			182.5		
5	161.0			161.6		
6	98.6	6.28, s	C-8, C-5	98.7	6.28, s	C-8, C-5
7	163.2			163.5		
8	104.8			105.1		
4a	104.7			104.4		
8a	156.6			156.7		
1'	121.8			121.6		
2'	110.5	7.56, d (2.2)	C-3', C-2	110.5	7.56, brs	
3'	148.3			148.4		
4'	151.3			151.2		
5'	116.4	6.89, d (8.4)	C-3', C-1'	116.4	6.89, d (8.9)	C-3', C-1'
6'	123.4	8.28, dd (8.5, 2.2)	C-2, C-4'	123.5	8.29, dd (8.9, 2.1)	
1''	74.3	4.68, d (7.8)	C-7, C-8a	74.4	4.66, m	C-7, C-8a
2''	68.3	4.22, m		68.6	4.22, m	
3''	75.6	3.45, m	C-2''	76.0	3.42, m	
4''	70.0	3.86, m		70.2	3.87, m	
5''	77.3	3.78, m		81.0	3.51, m	
6''	65.5	4.23, m ; 4.08, m	C-5'', C-4''	61.8	3.91, m ; 3.58, m	
5-OH		13.35, s			13.35, s	
3'-OCH ₃	56.6	3.89, s	C-3'	56.6	3.89, s	C-3'
6''-OAc	170.9					
	21.2	1.98, s				

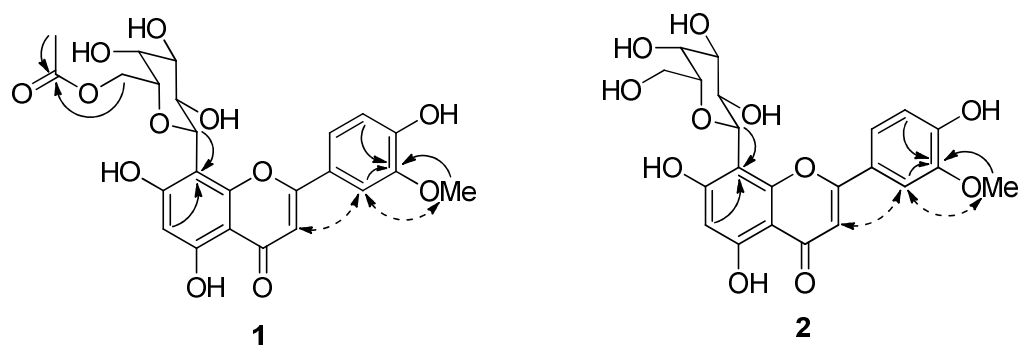


Figure SM.1: Key HMBC (H → C) and ROESY (H ↔ H) correlations of compounds **1** and **2**.

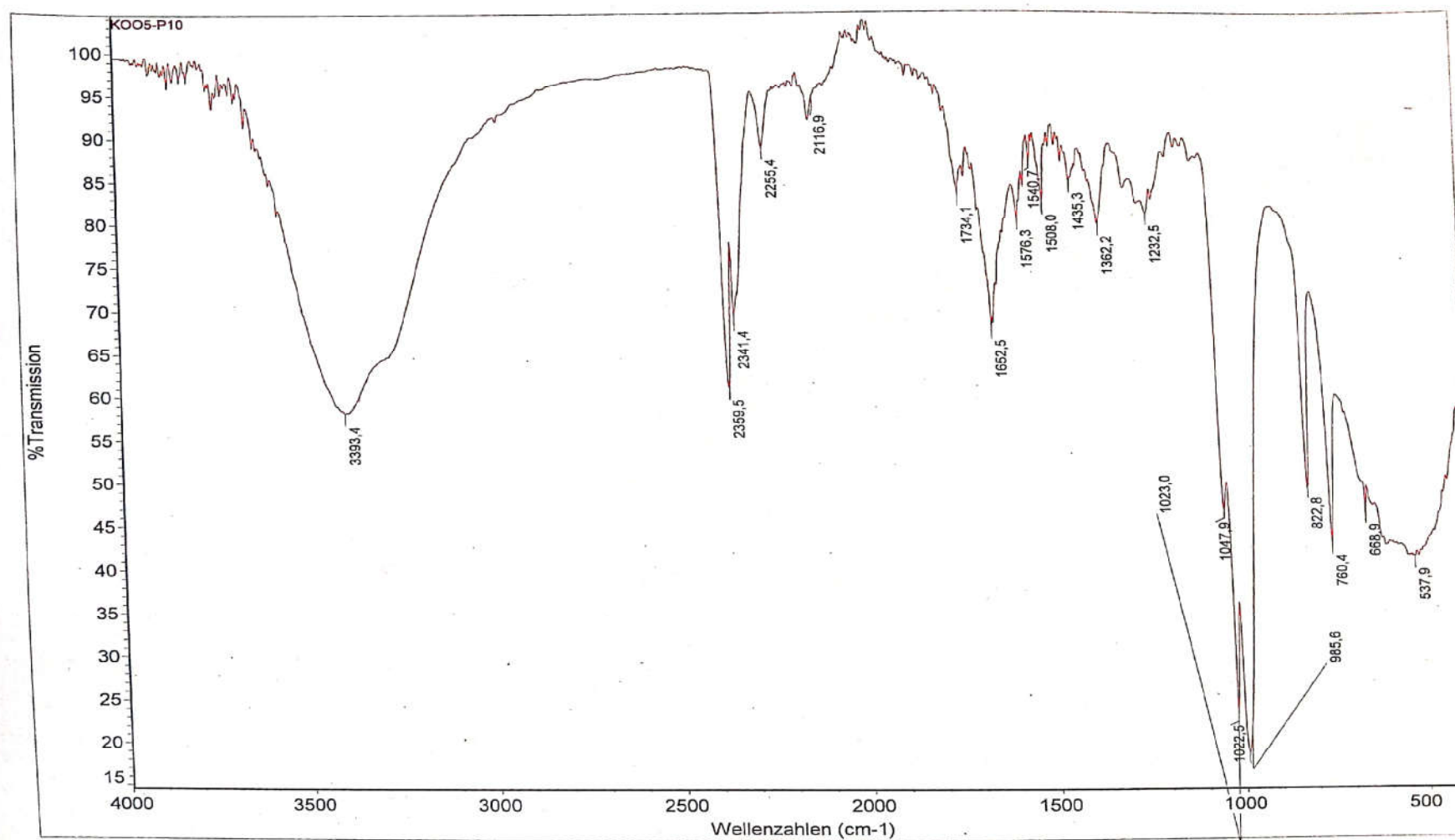


Figure SM.2: IR spectrum of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

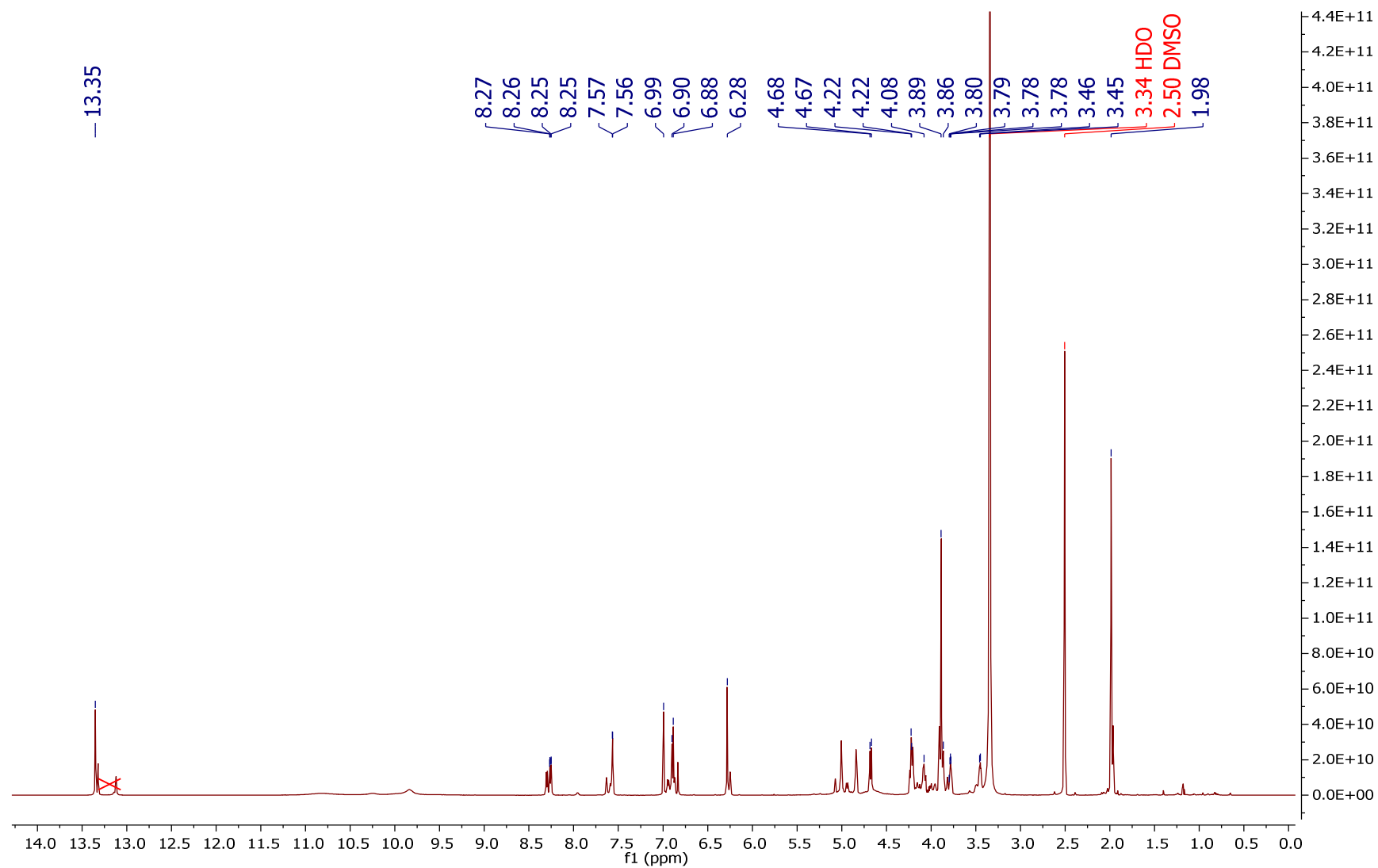


Figure SM.3: ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

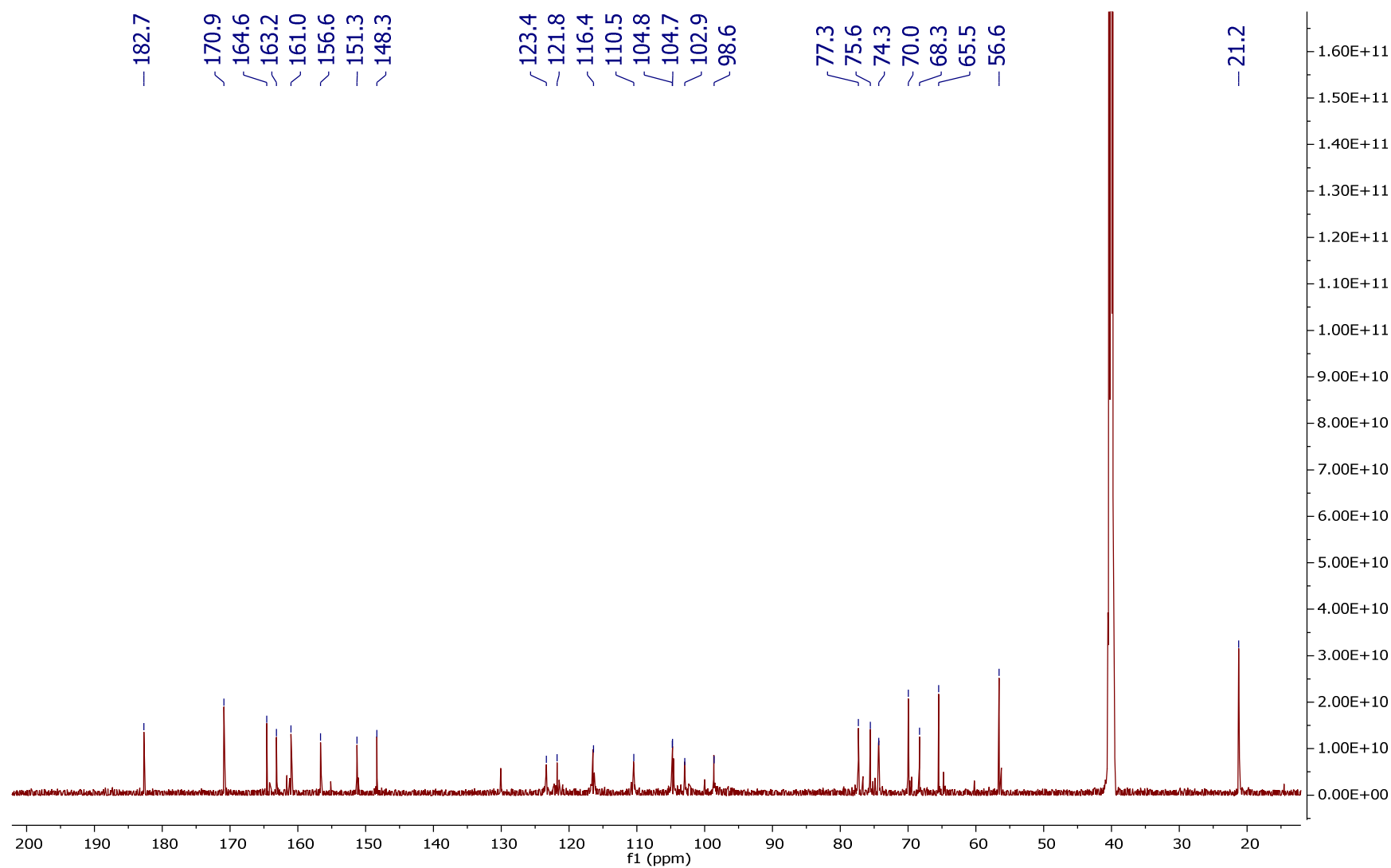


Figure SM.4: ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of $6''\text{-O-acetyl-8-C-}\beta\text{-D-galactopyranosylchrysoeriol}$ (**1**)

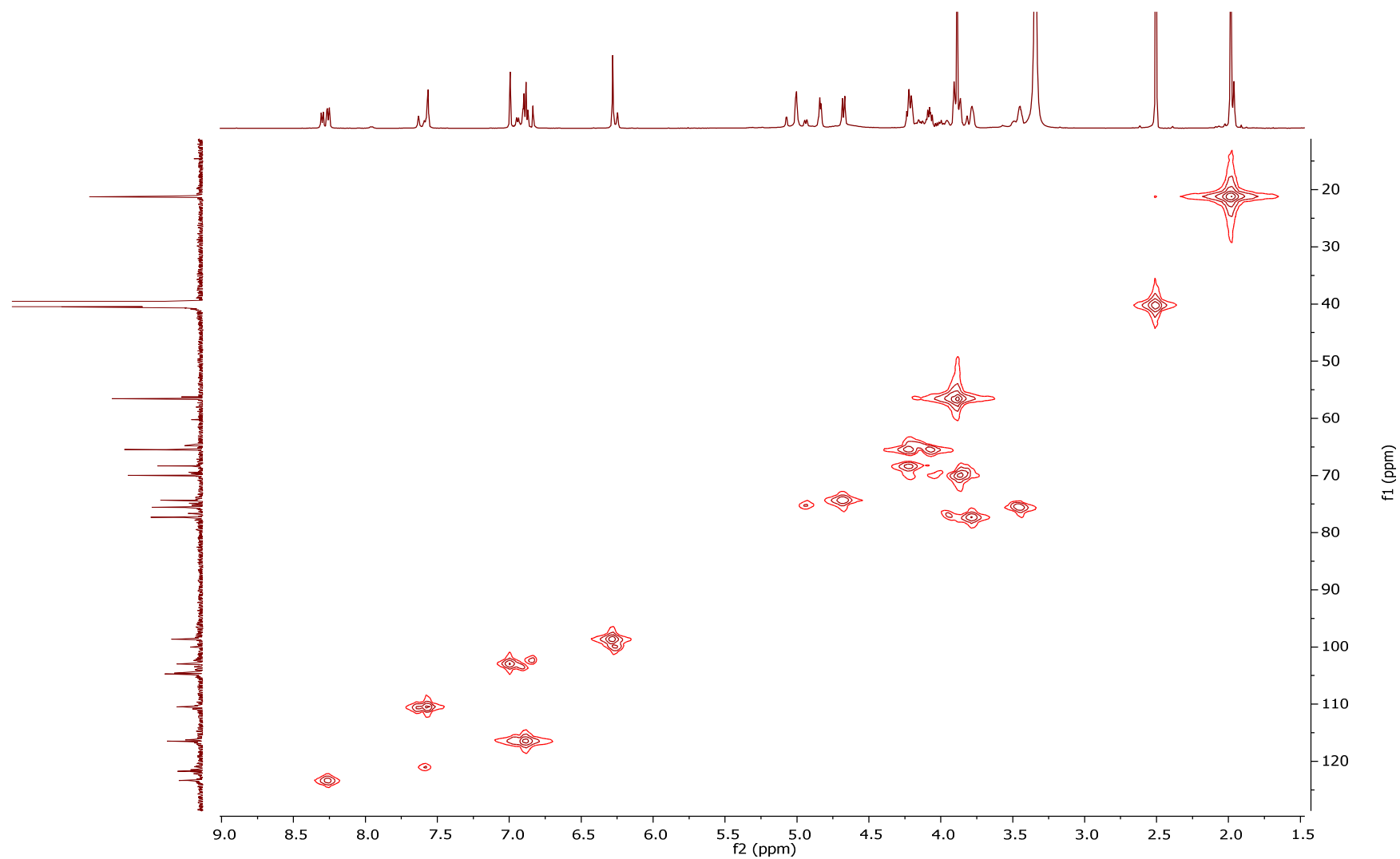


Figure SM.5: HSQC spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

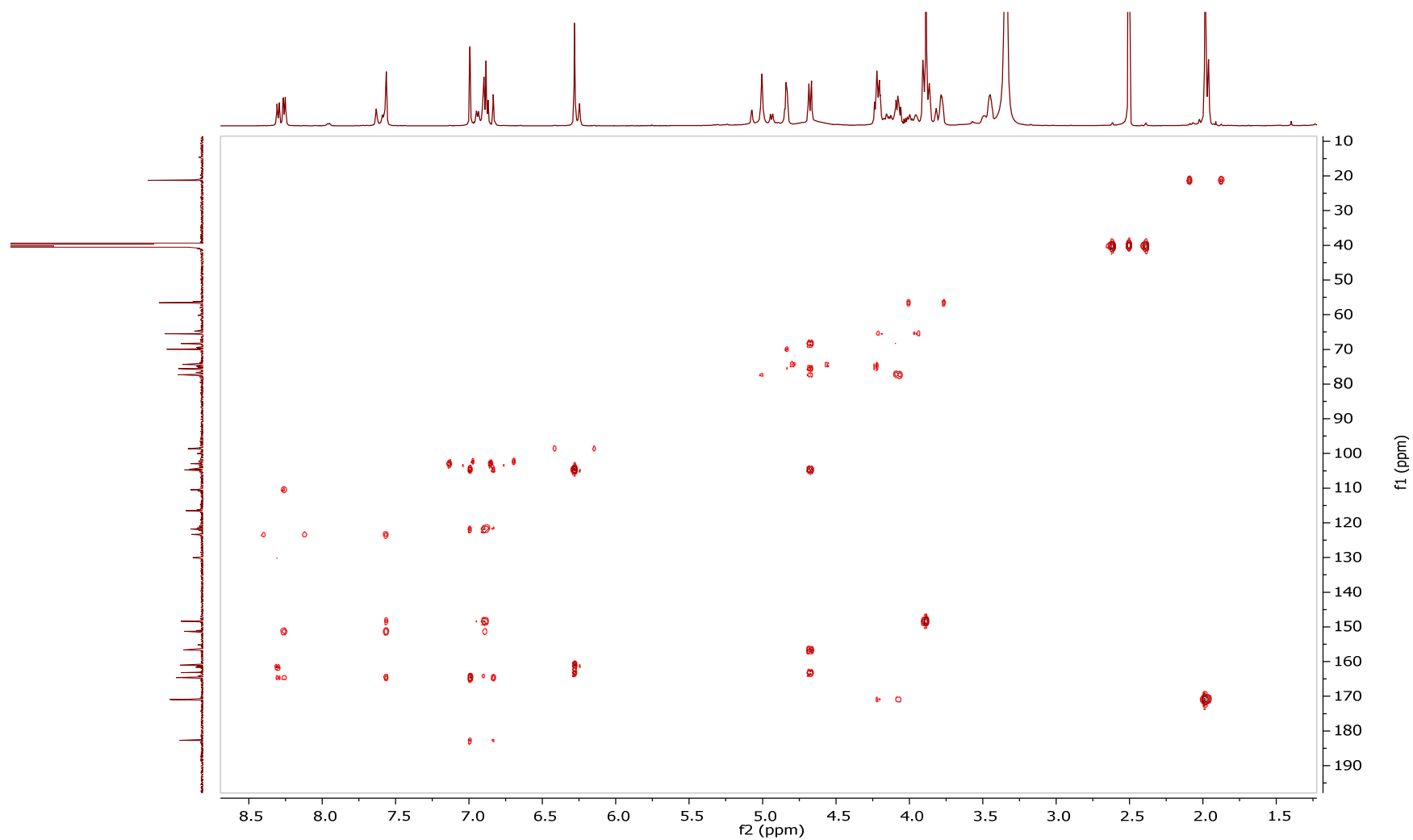


Figure SM.6: HMBC spectrum (500 MHz, $\text{DMSO}-d_6$) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

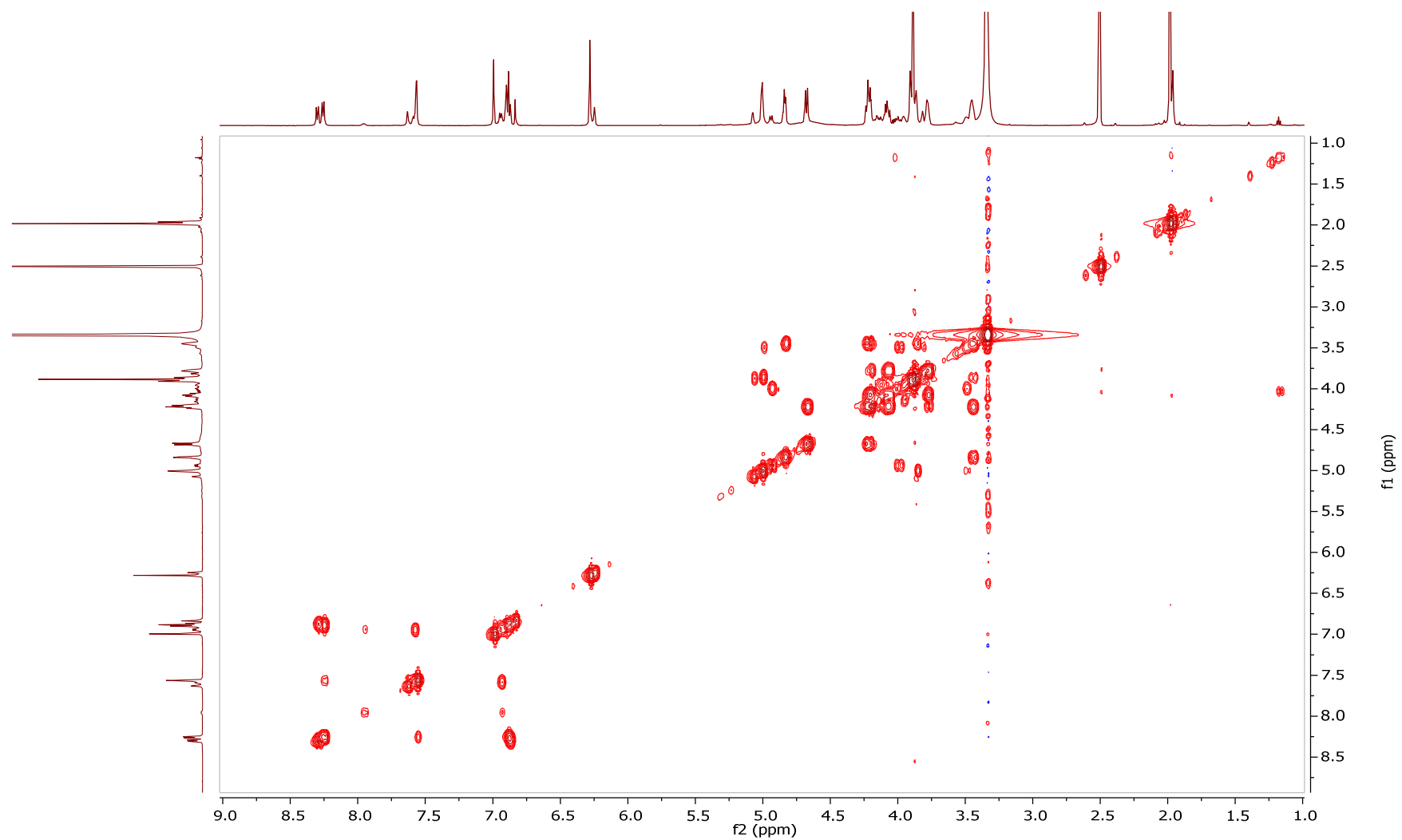


Figure SM.7: ^1H - ^1H COSY spectrum (500 MHz, $\text{DMSO}-d_6$) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

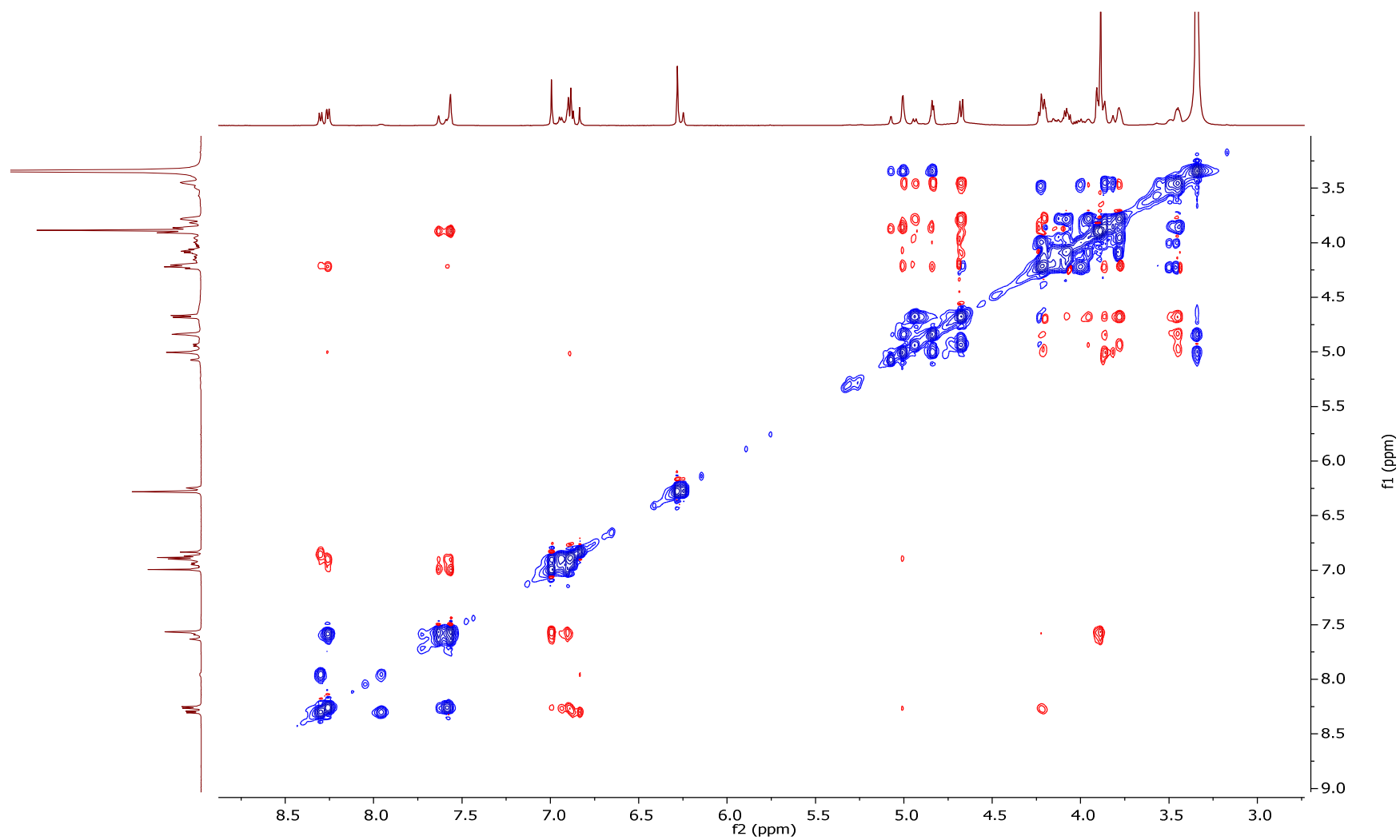


Figure SM.8: ROESY spectrum (500 MHz, DMSO- d_6) of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

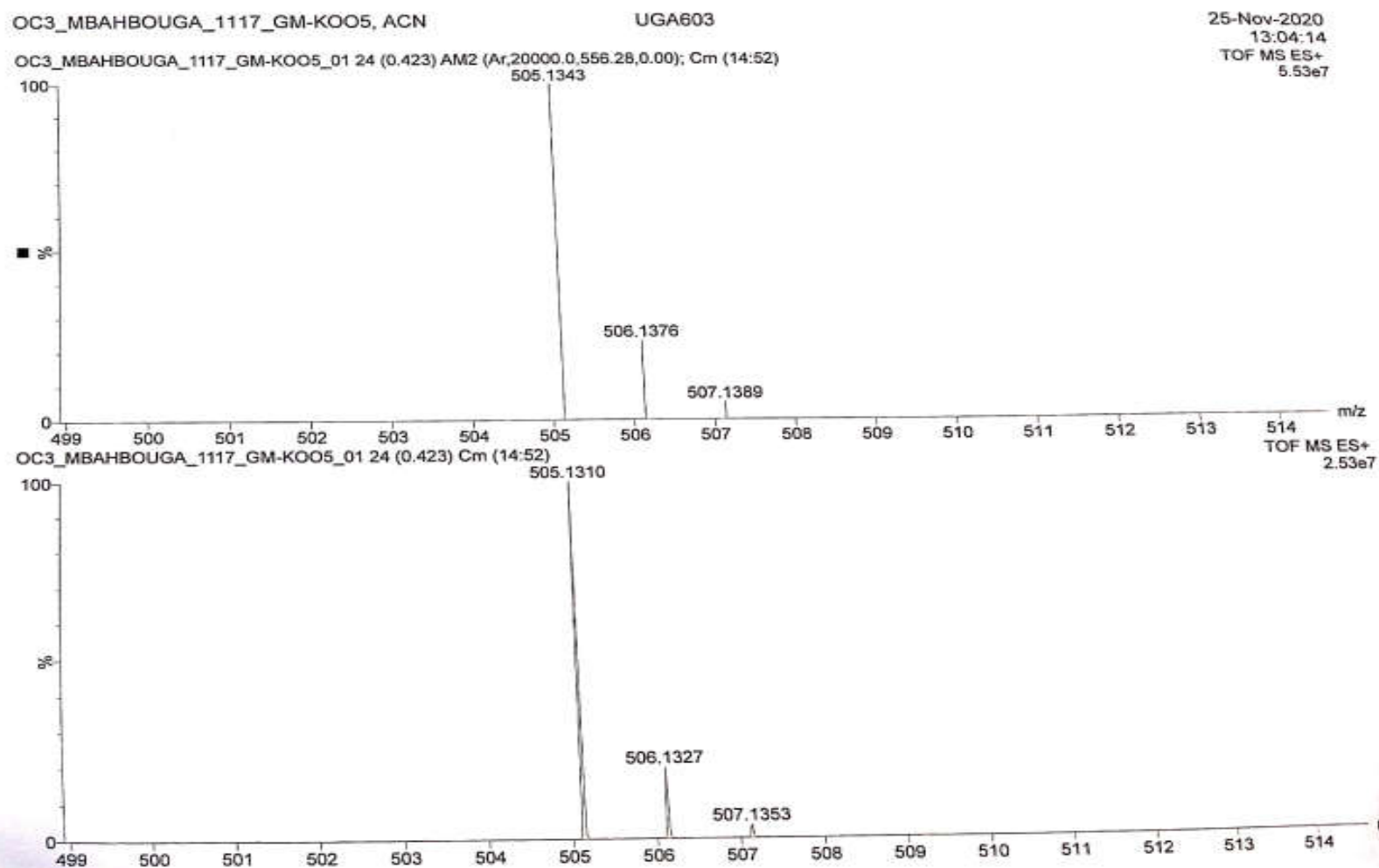


Figure SM.9: HRESI-MS spectrum of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (**1**)

Accurate Mass Measurement

Sample Name :	GM-KOO5	Group : OC3
Sample Supplier :	MBAHBOUGA	
Sample Filename :	OC3_MBAHBOUGA_1117_GM-KOO5_01.raw	
Sample Date :	11/25/2020	

Instrument :	Synapt G2Si
Ionisation Method :	ESI
Matching Method :	HR with cal.intern LeuEnk (m/z 556.2766)
Resolution :	> 20000
Substance Inlet :	nano ESI-Emitter

Measured Ion Mass(es) :	505.1343	Deviation [mmu] :	0.24 [mmu]
Calculated Ion Mass(es) :	505.13406	Deviation [ppm] :	0.48 [ppm]
Potential Molecular Formula :	C24H24O12H +		

Scanned with CamScanner

Figure SM.10: HRESI accurate data of 6''-O-acetyl-8-C- β -D-galactopyranosylchrysoeriol (1)

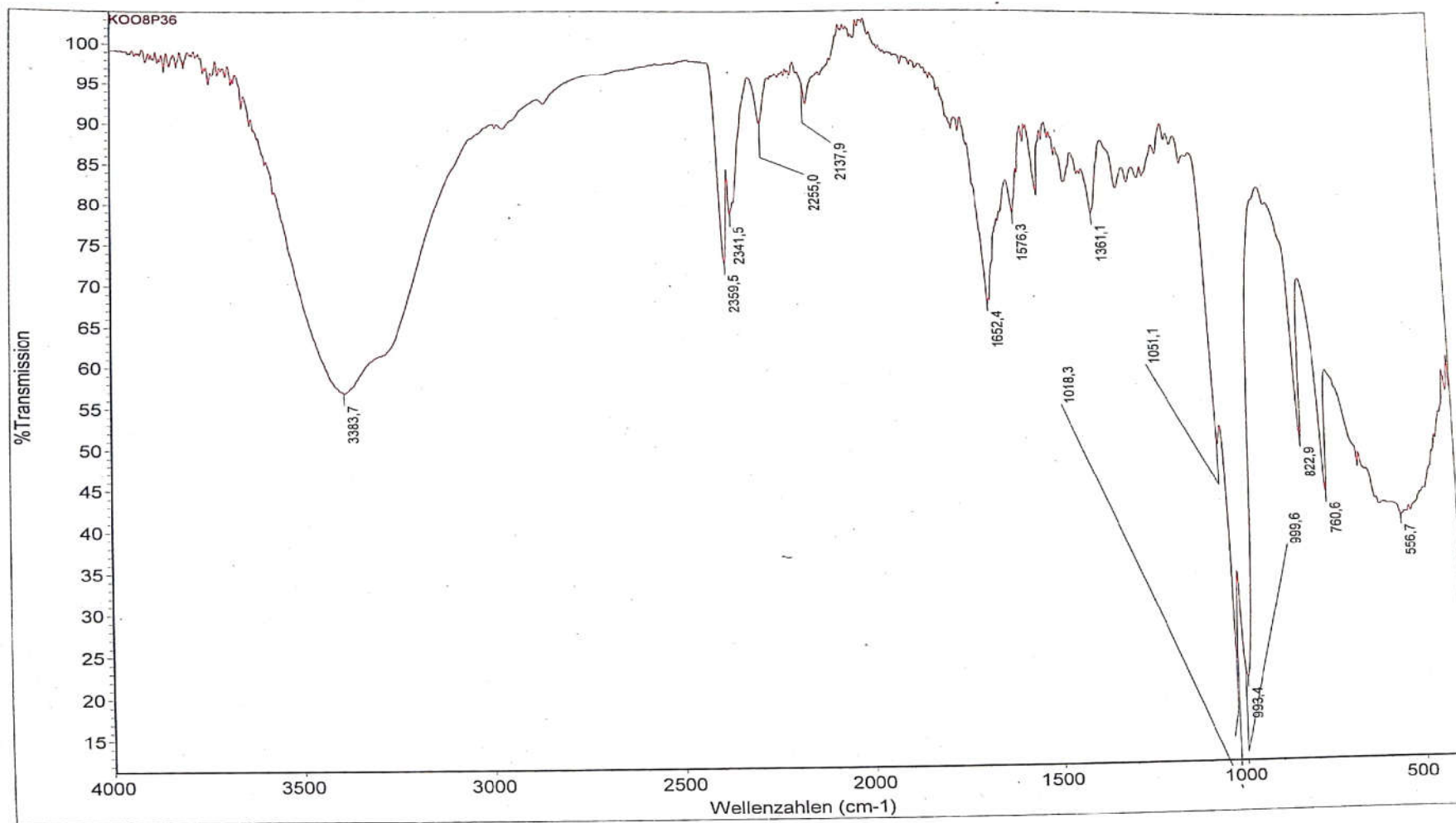


Figure SM.11: IR spectrum of 8-C- β -D-galactopyranosylchrysoeriol (2)

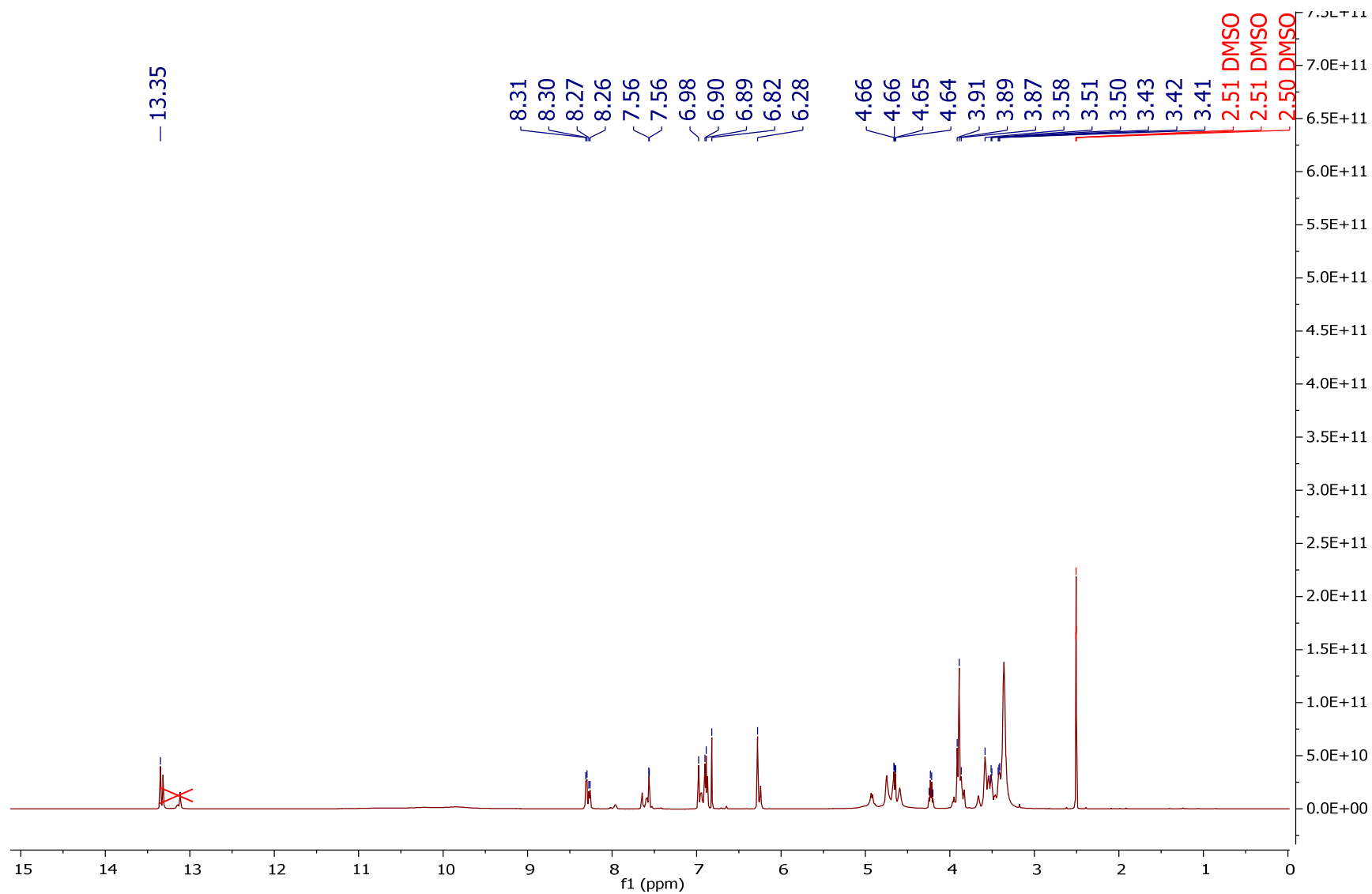


Figure SM.12: ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 8-C- β -D-galactopyranosylchrysoeriol (**2**)

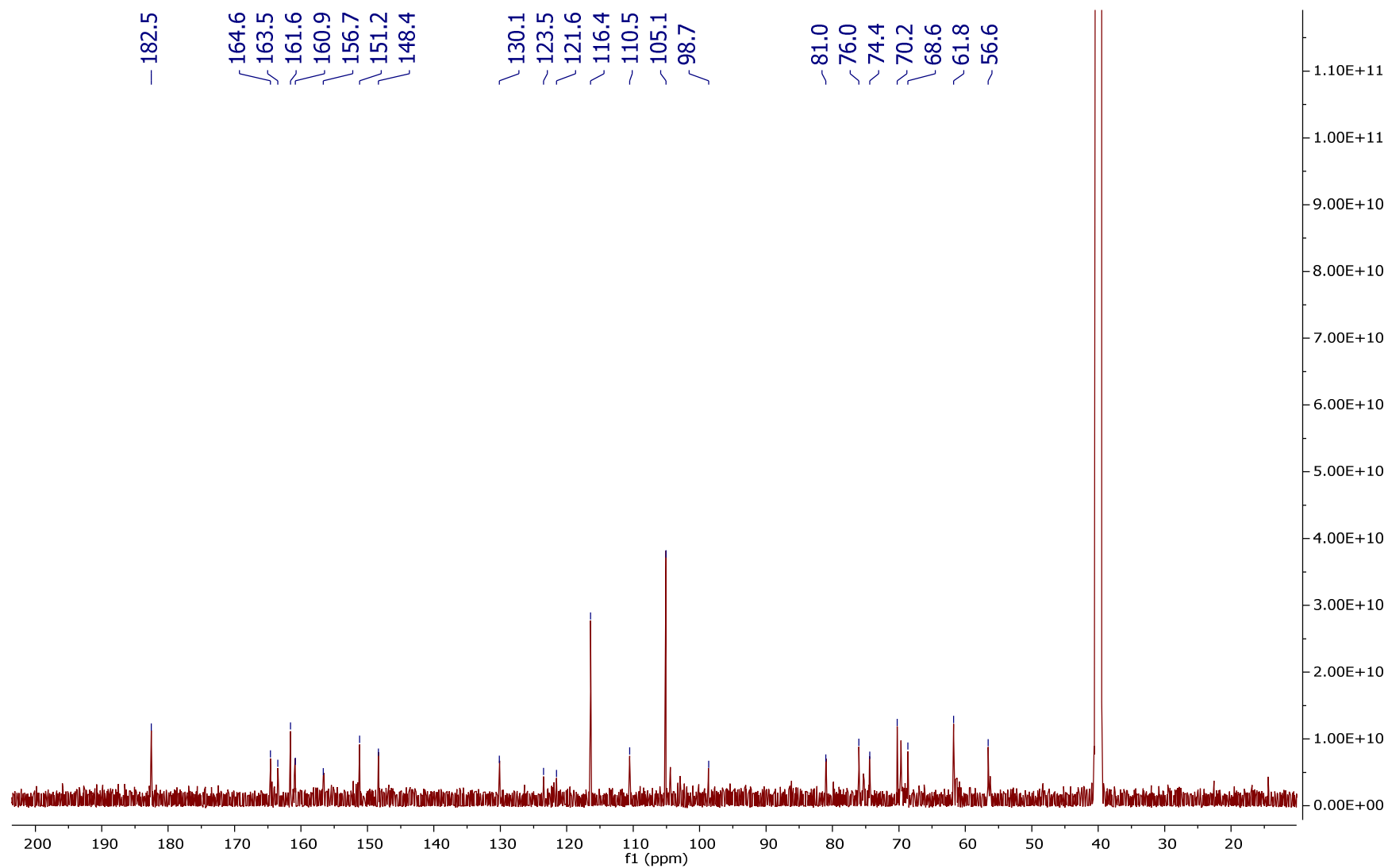


Figure SM.13: ^{13}C NMR spectrum (125 MHz, $\text{DMSO-}d_6$) of 8-C- β -D-galactopyranosylchrysoeriol (**2**)

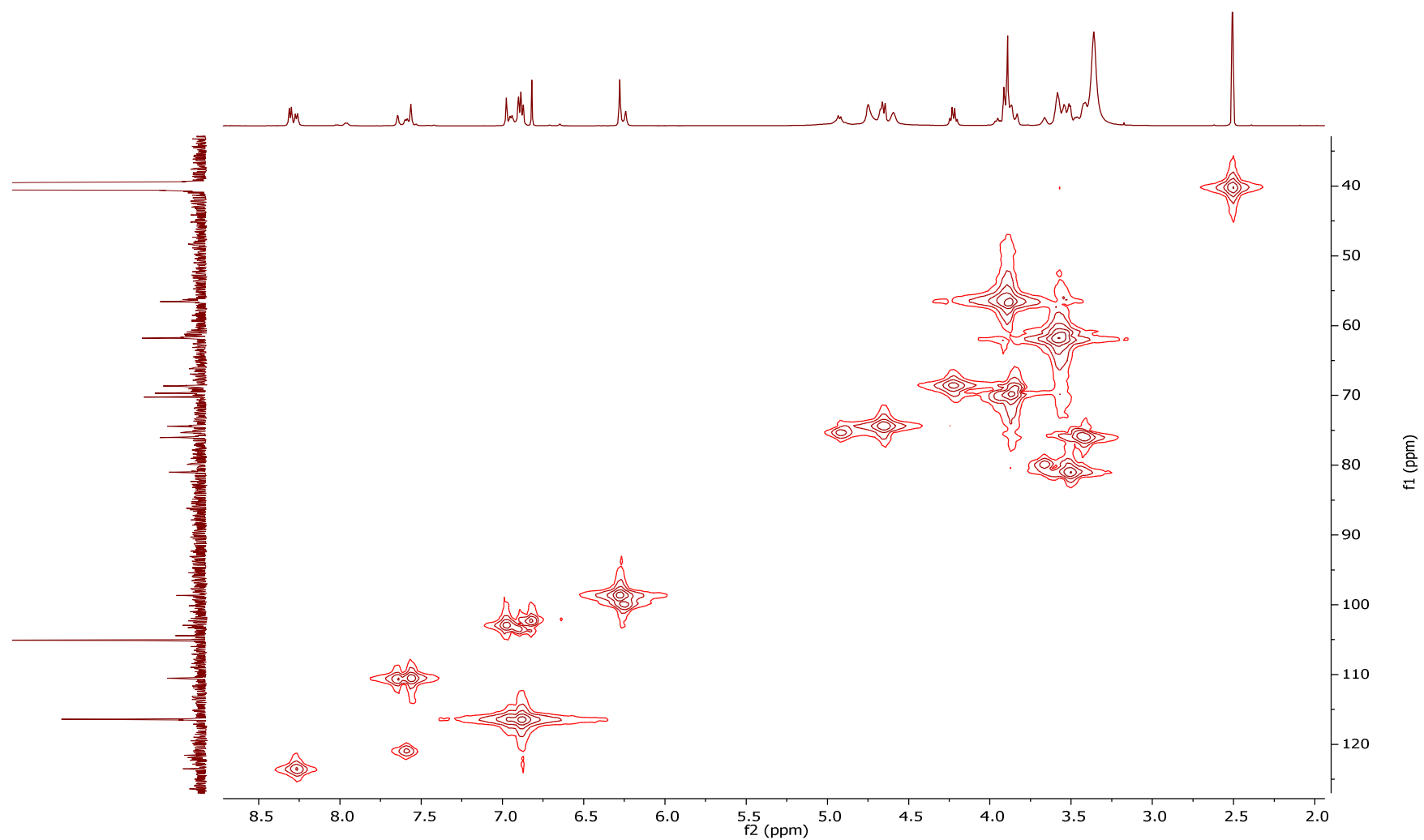


Figure SM.14: HSQC spectrum (500 MHz, DMSO- d_6) of 8-*C*- β -*D*-galactopyranosylchrysoeriol (**2**)

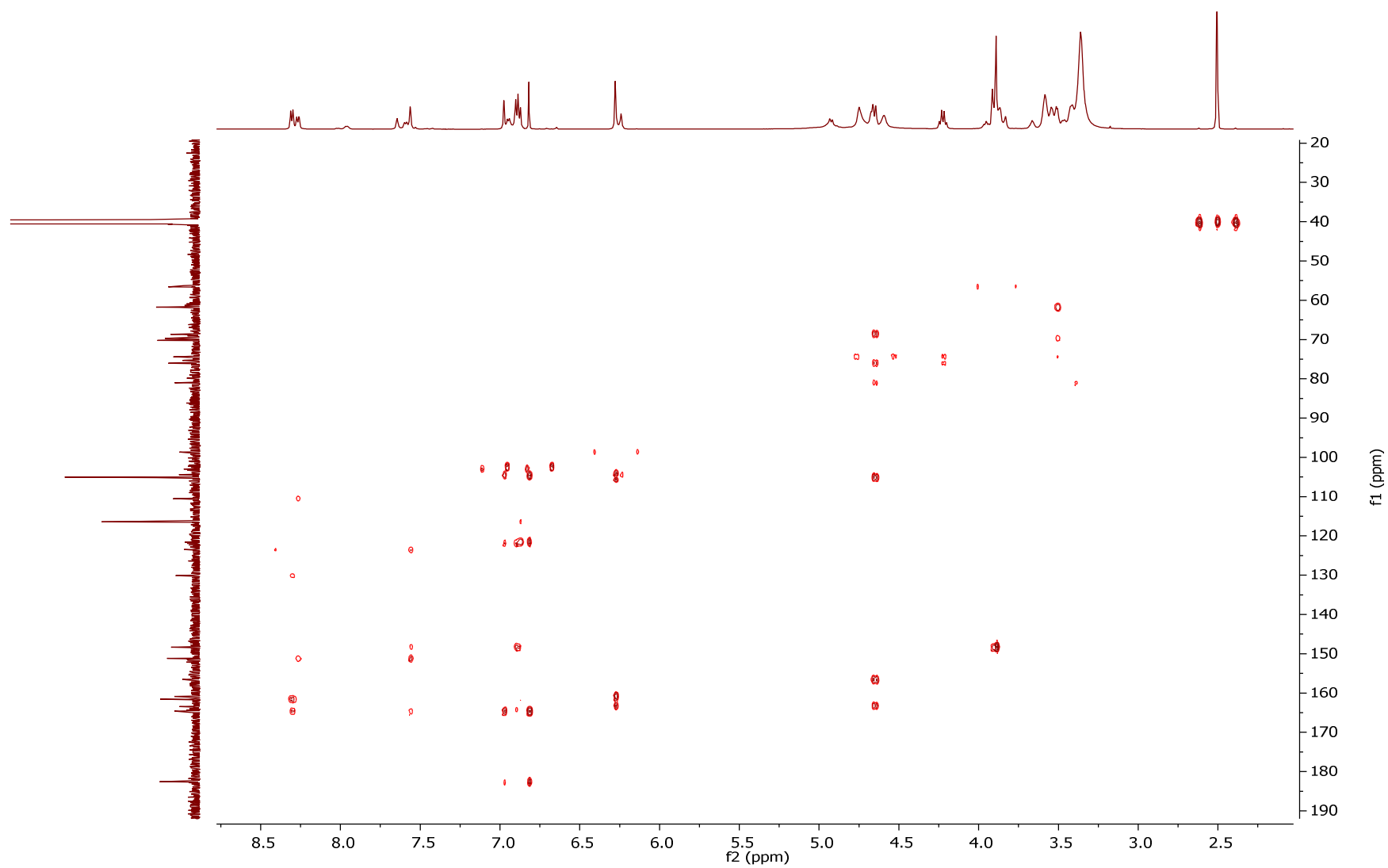


Figure SM.15: HMBC spectrum (500 MHz, DMSO- d_6) of 8-C- β -D-galactopyranosylchrysoeriol (**2**)

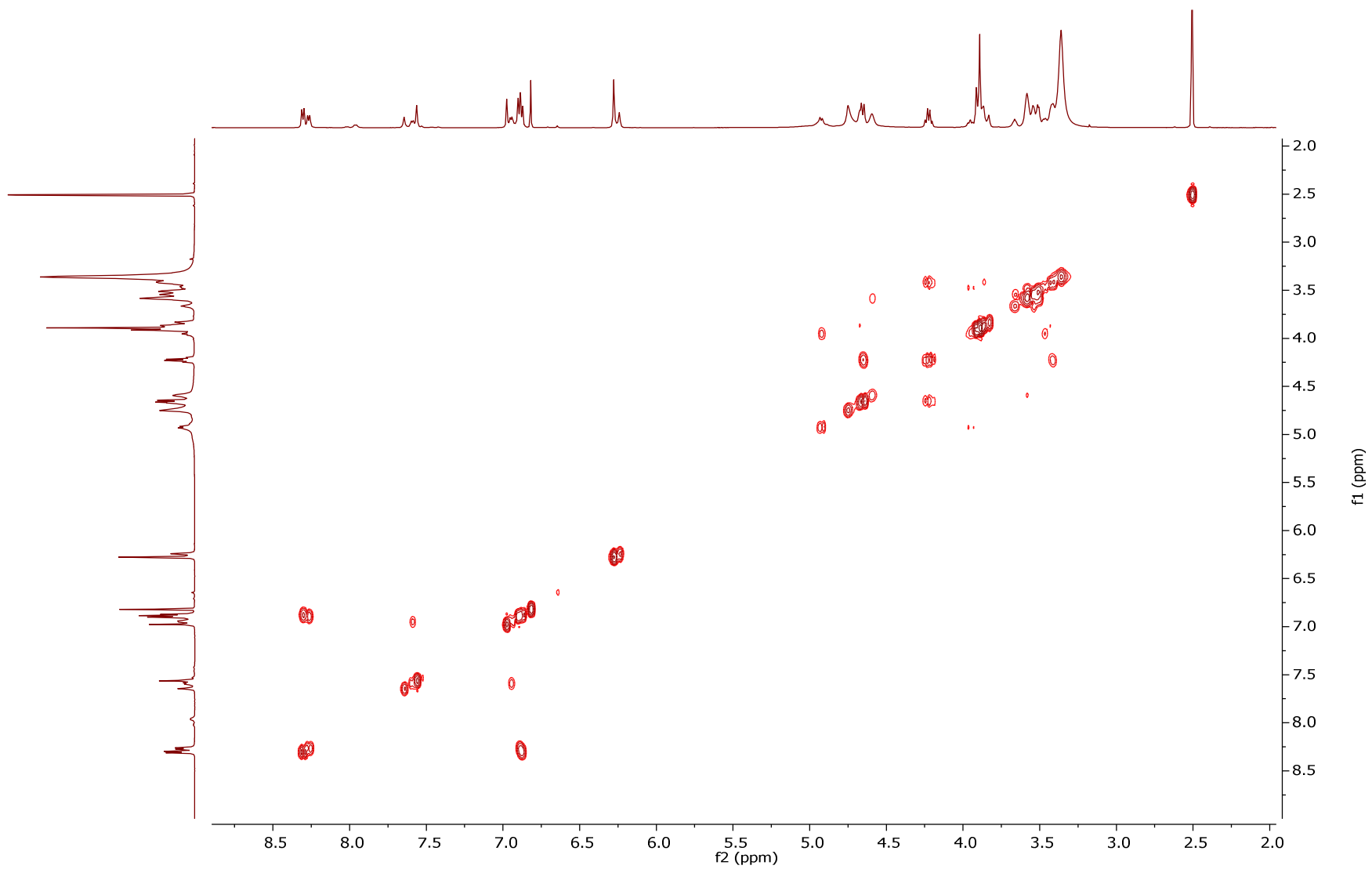


Figure SM.16: ^1H - ^1H COSY spectrum (500 MHz, $\text{DMSO}-d_6$) of 8-*C*- β -*D*-galactopyranosylchrysoeriol (**2**)

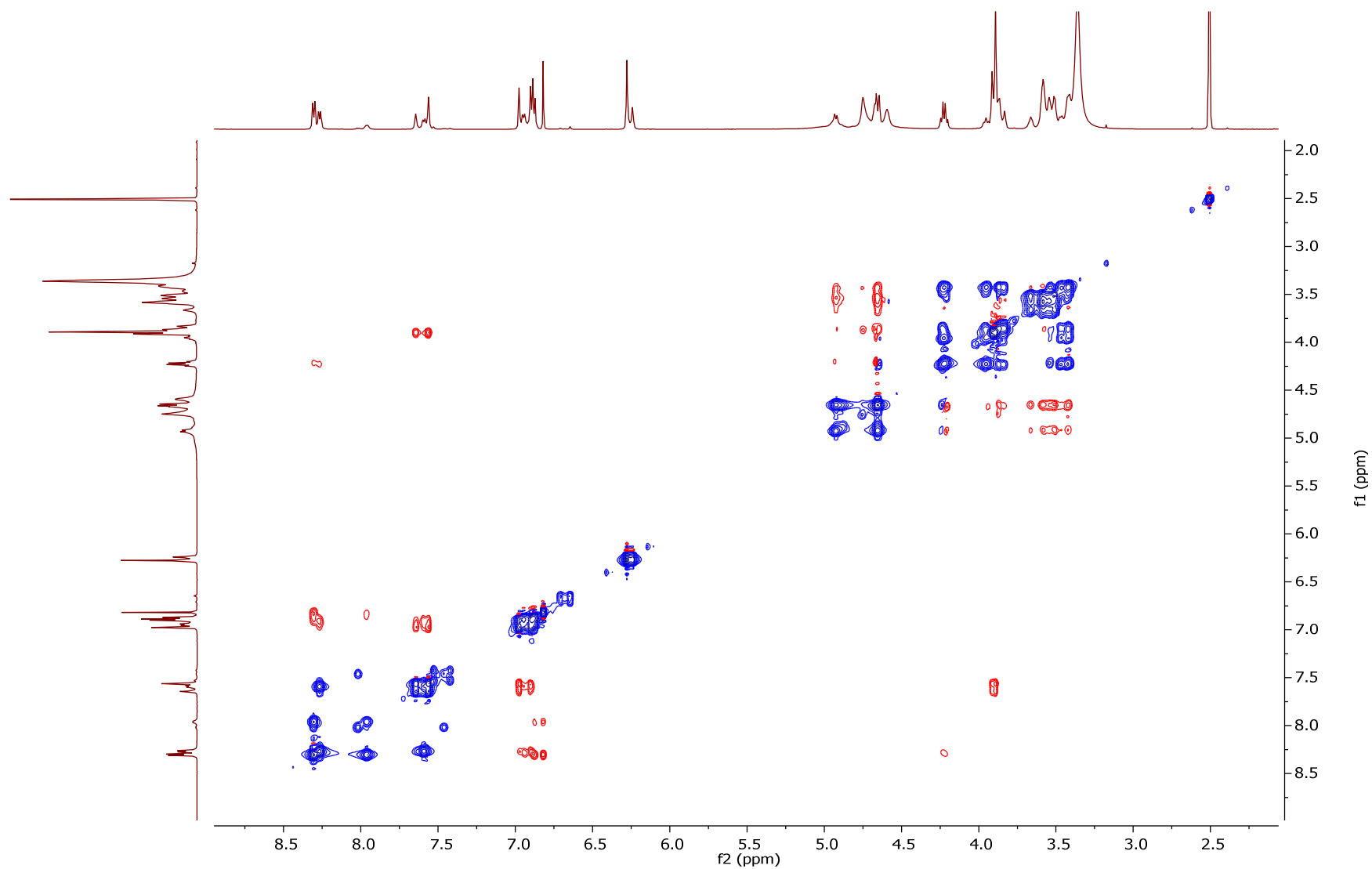


Figure SM.17: ROESY spectrum (500 MHz, DMSO- d_6) of 8-C- β -D-galactopyranosylchrysoeriol (**2**)

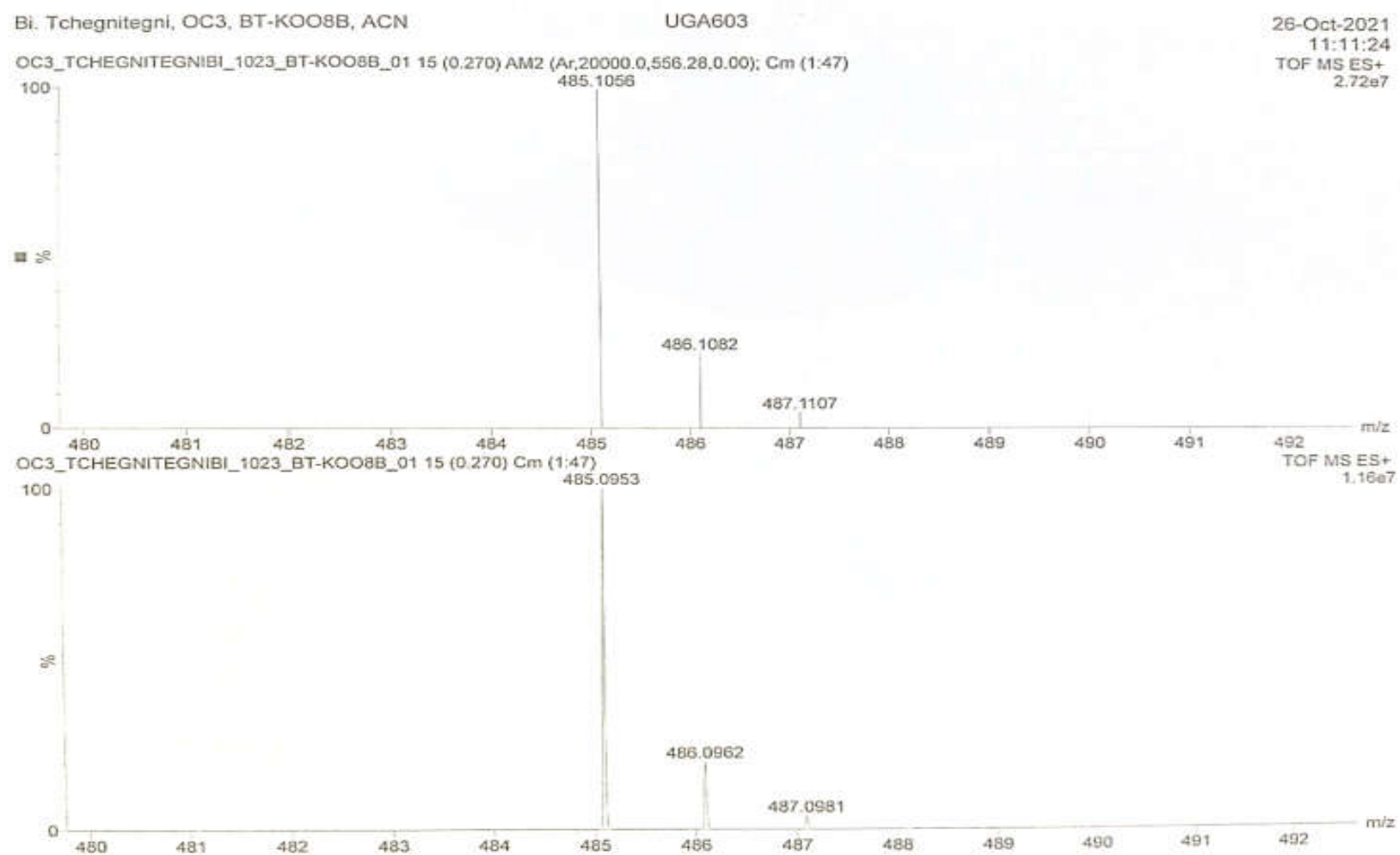


Figure SM.18: HRESI-MS spectrum of 8-C- β -D-galactopyranosylchrysoeriol (**2**)



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Accurate Mass Measurement

Sample Name :	BT-KOO8B	Group :	OC3
Sample Supplier :	TCHEGNITEGNIBI		
Sample Filename :	OC3_TCHEGNITEGNIBI_1023_BT-KOO8B_01.raw		
Sample Date :	10/26/2021		
Instrument :	Synapt G2Si		
Ionisation Method :	ESI		
Matching Method :	HR with cal.intern LeuEnk (m/z 556.2766)		
Resolution :	> 20000		
Substance Inlet :	nano ESI-Emitter		
Measured Ion Mass(es) :	485.1056	Deviation [mmu] :	0.16 [mmu]
Calculated Ion Mass(es) :	485.10544	Deviation [ppm] :	0.33 [ppm]
Potential Molecular Formula :	C22H22O11Na+		

Comment : Measured and calculated masses are true ion masses, taking into account the mass of lost (or added) electrons.

Bielefeld, 10/26/2021

Figure SM.19: HRESI accurate data of *8-C-β-D-galactopyranosylchrysoeriol* (**2**)