

Methicillin-resistant *Staphylococcus aureus* (MRSA)-active Metabolites from *Platanus occidentalis* (American Sycamore)

Supporting Information

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Key words: Selective anti MRSA, *Platanus occidentalis*, American Sycamore.

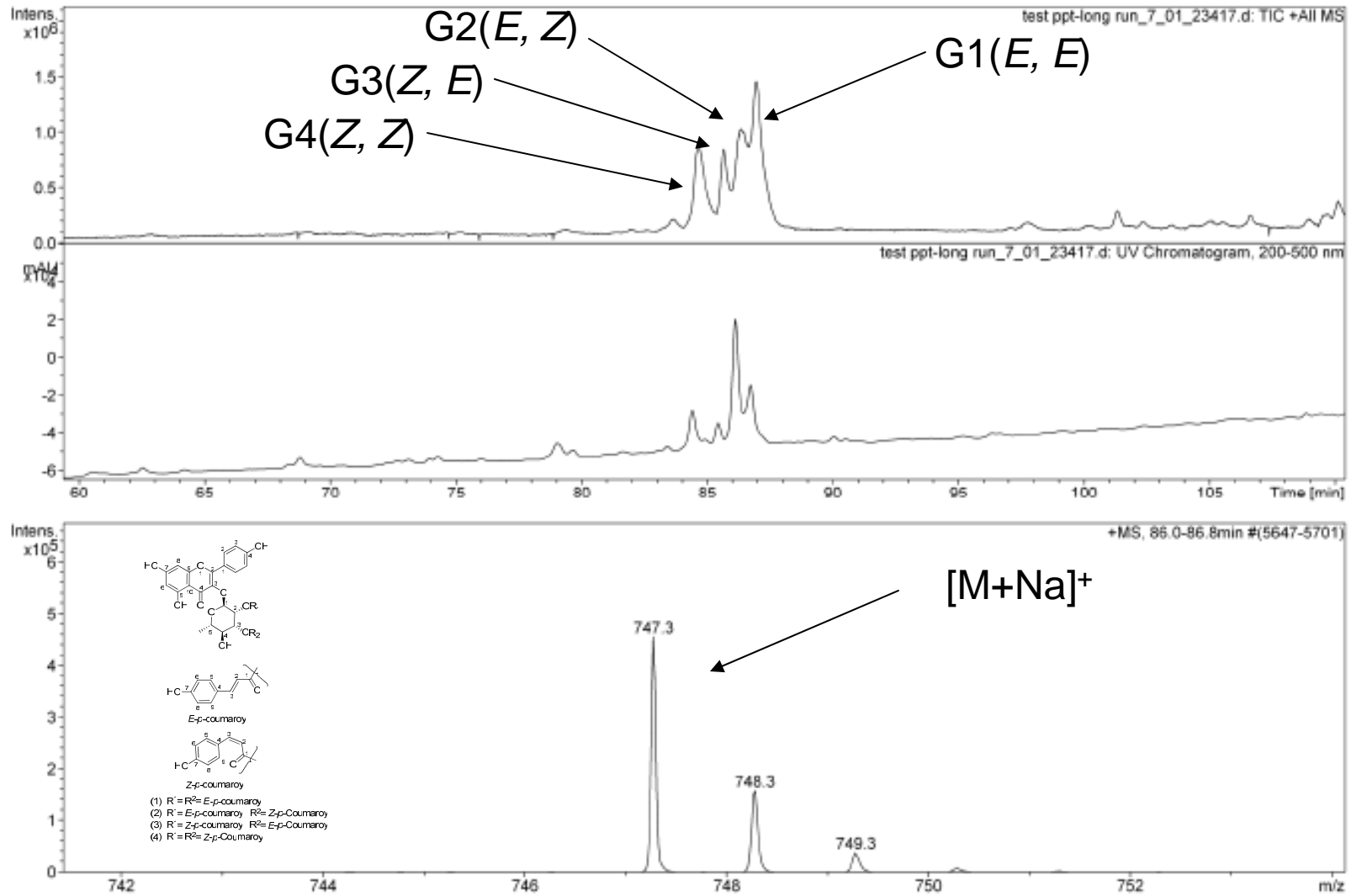
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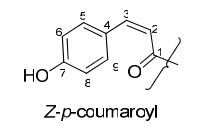
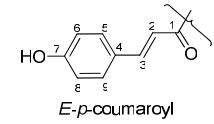
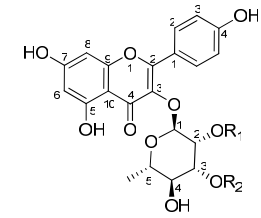
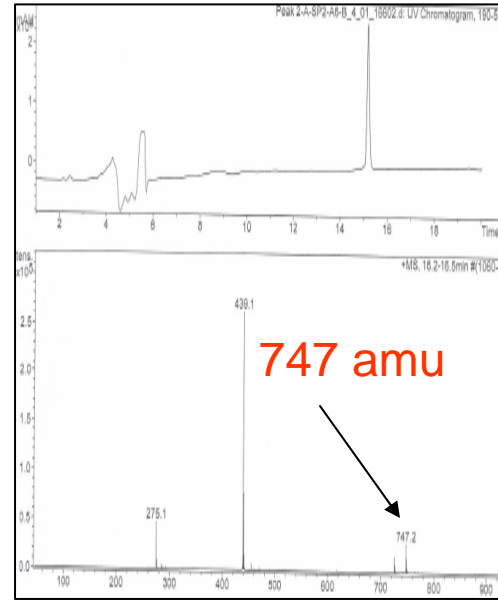
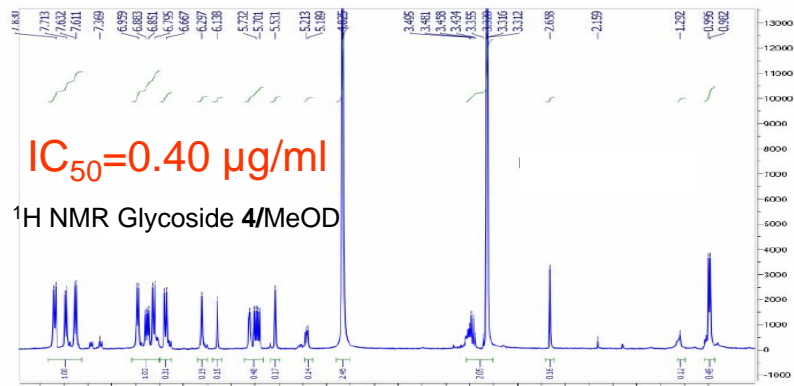
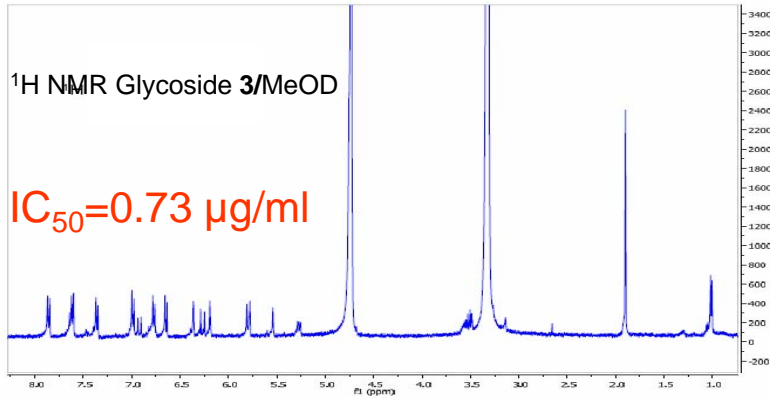
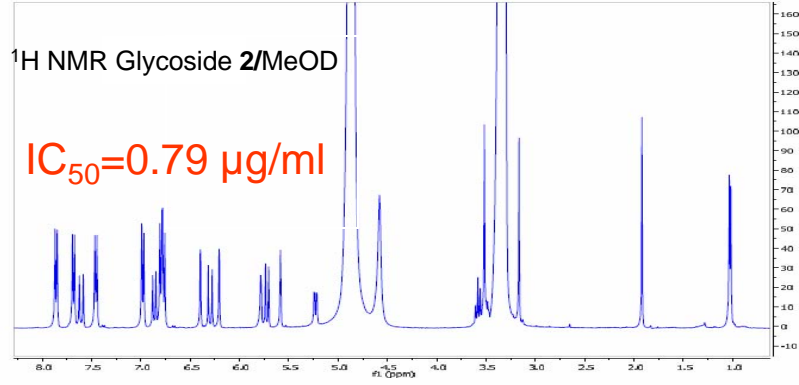
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Crude mixture after simple one step extraction

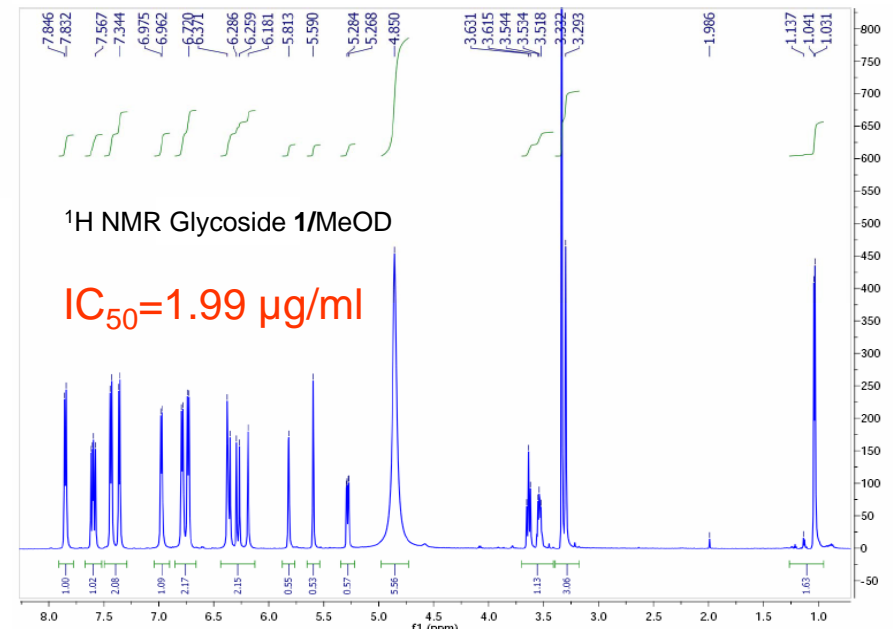
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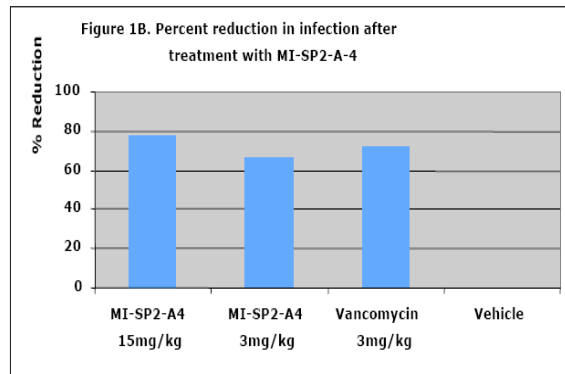
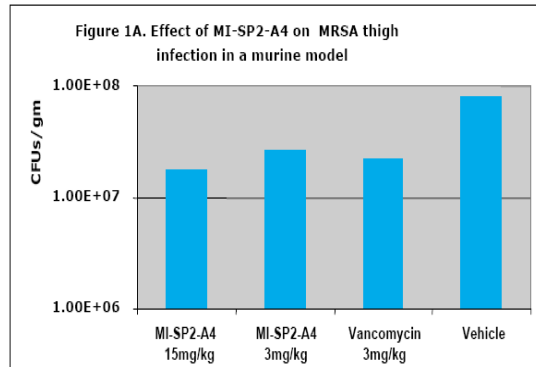
G1: glycoside 1, G2: glycoside 2, G3: glycoside 3, G4: glycoside 4



- (1), R¹ = R² = *E-p-coumaroyl*
- (2), R¹ = *E-p-coumaroyl*, R² = *Z-p-coumaroyl*
- (3), R¹ = *Z-p-coumaroyl*, R² = *E-p-coumaroyl*
- (4), R¹ = R² = *Z-p-coumaroyl*



In vivo assay



NC = no cytotoxicity up to 100 µg/ml

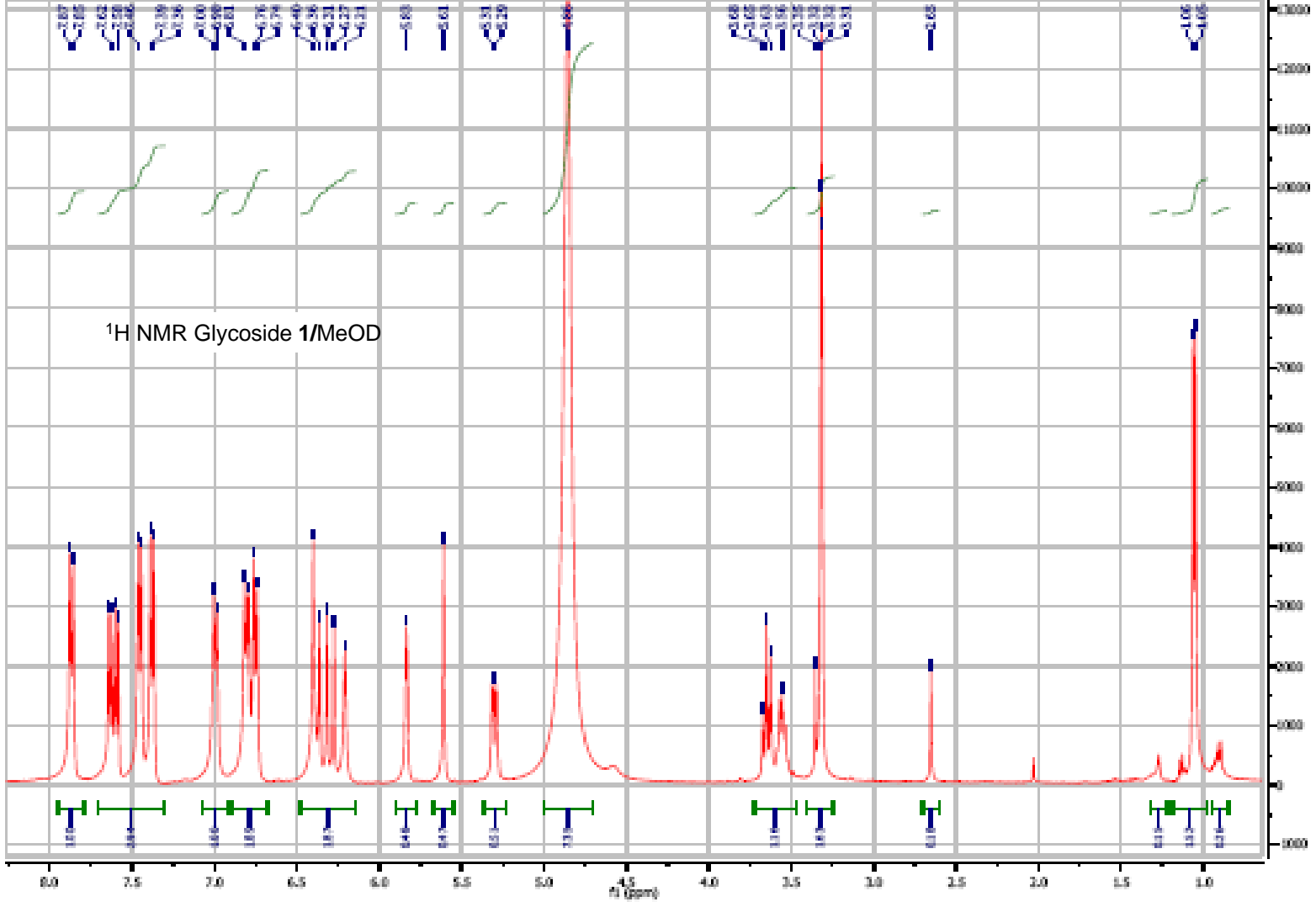
Cancer Cells:

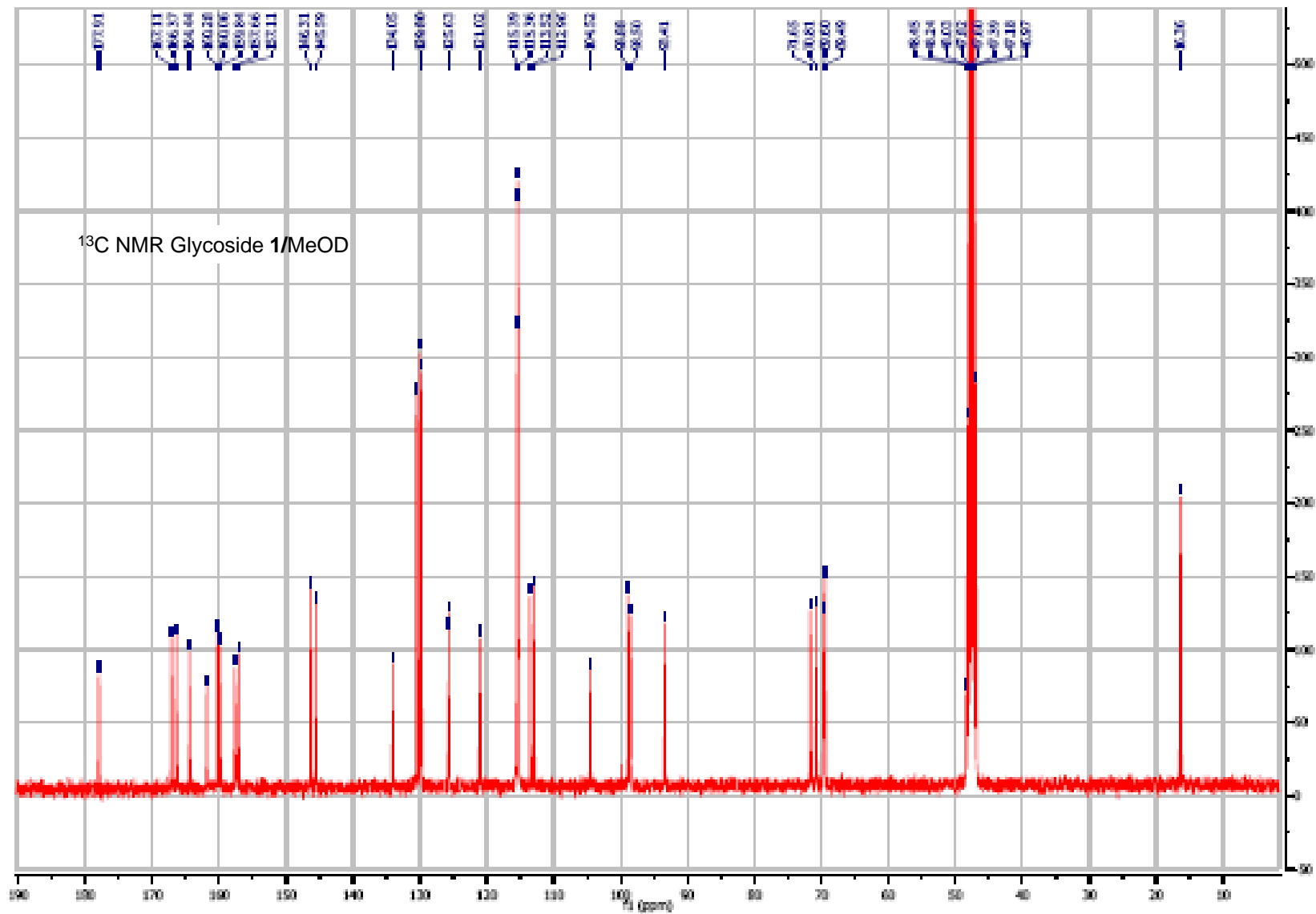
KB Human Epidermal Carcinoma, Oral
BT-549 Ductal Carcinoma, Breast
SK-OV -3 Human Ovary carcinoma

Noncancer Cells:

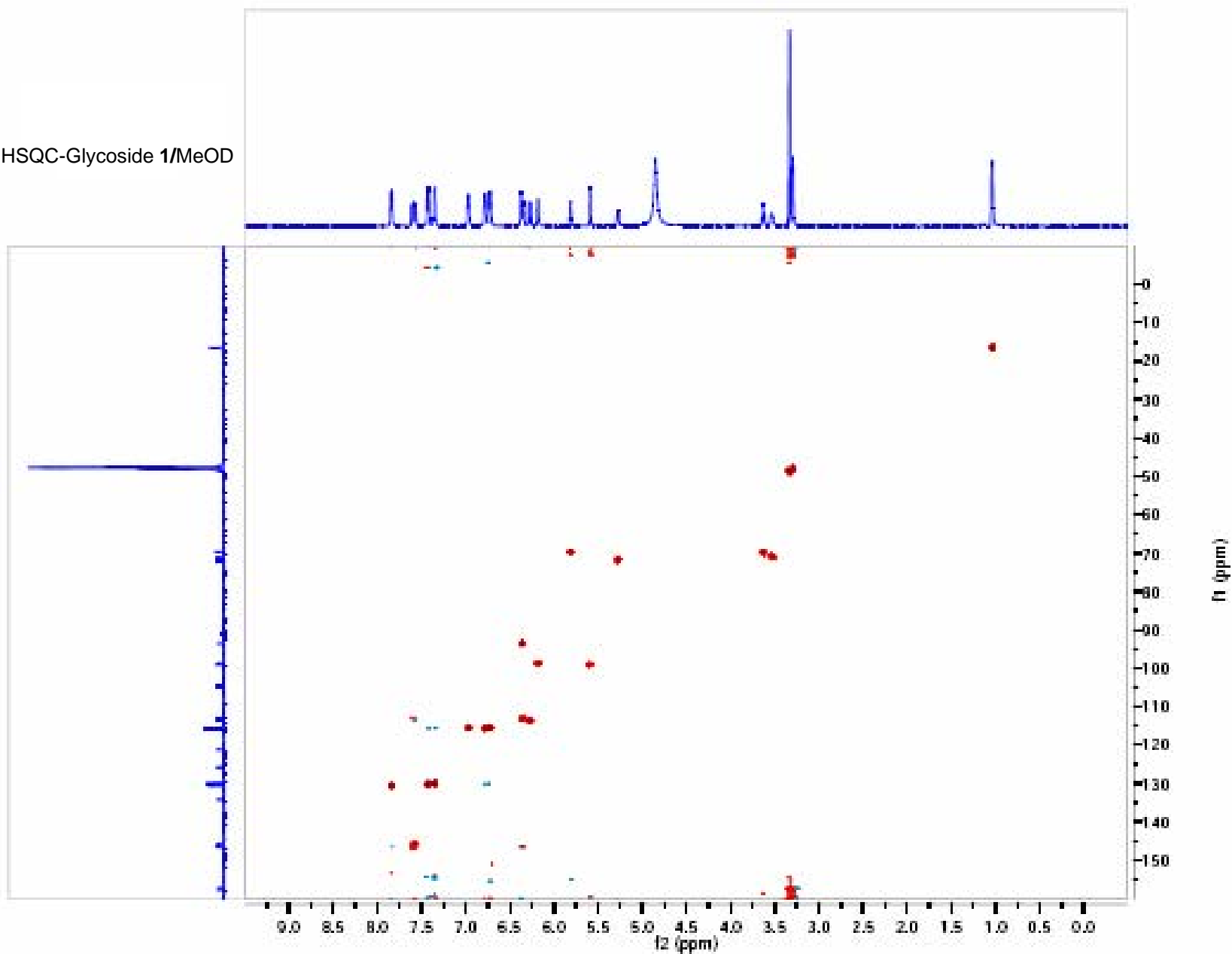
Vero Monkey Kidney Fibroblasts
LLC-PK11 Pig Kidney Epithelial Cells

“MI-SP2-A4” is glycoside 1

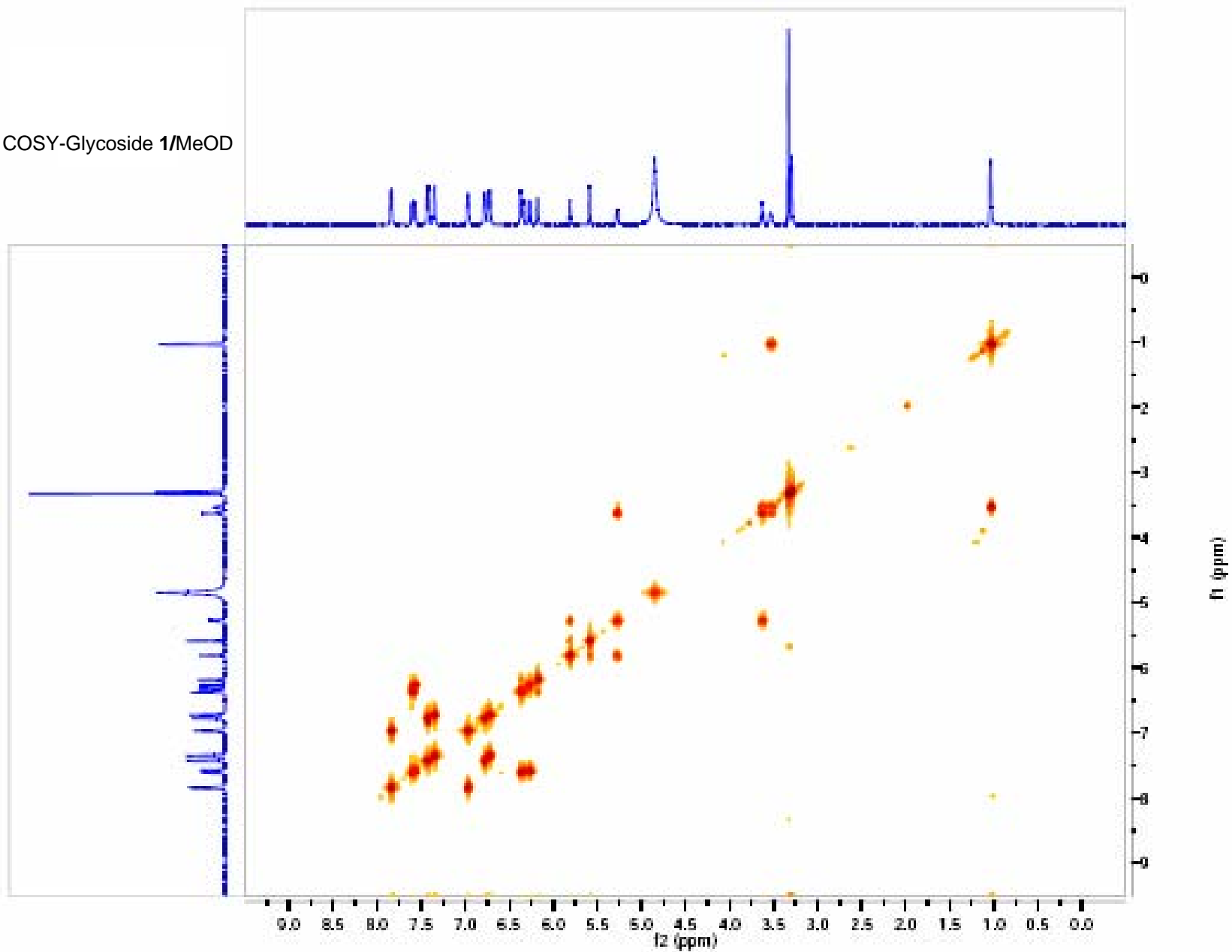




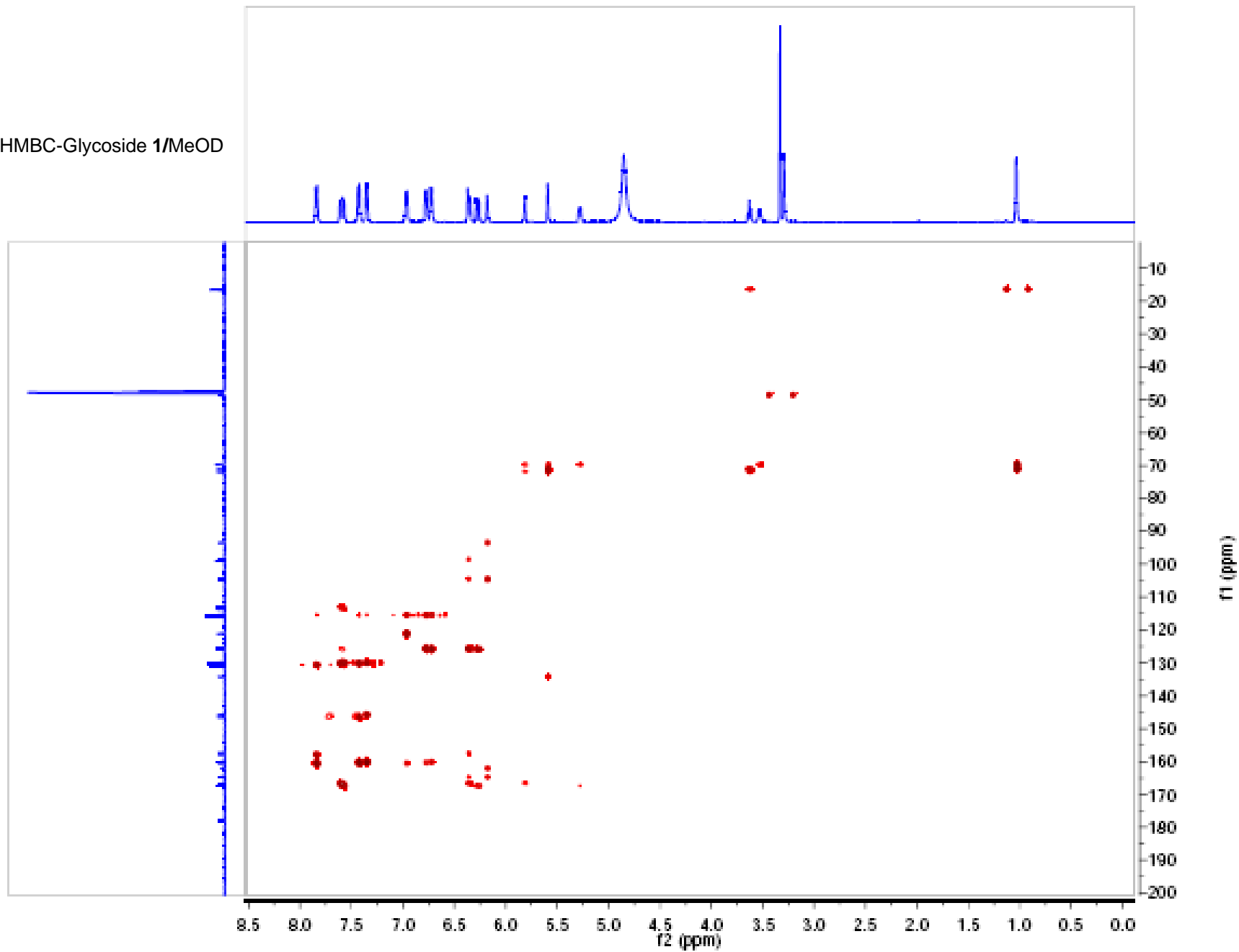
HSQC-Glycoside 1/MeOD

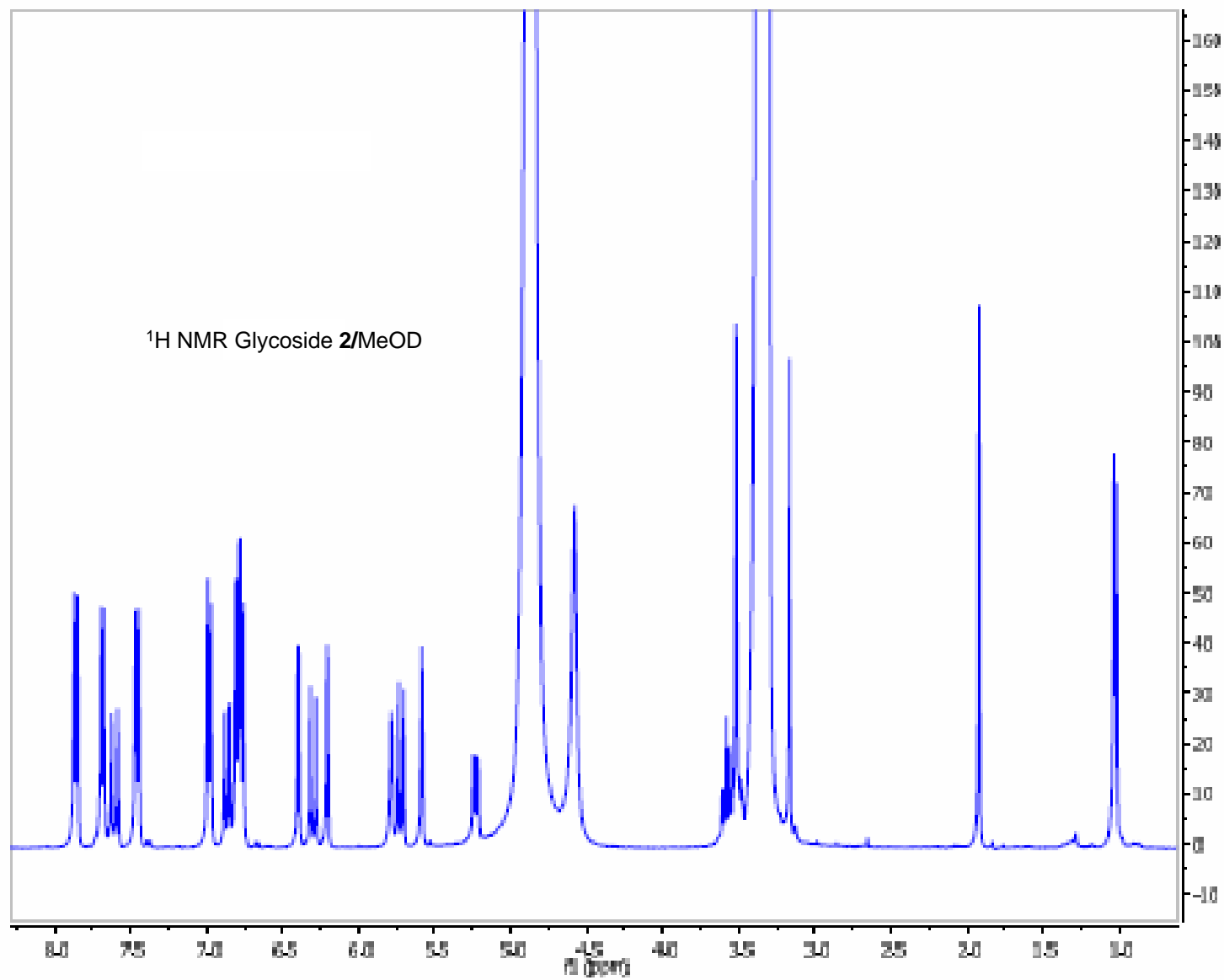


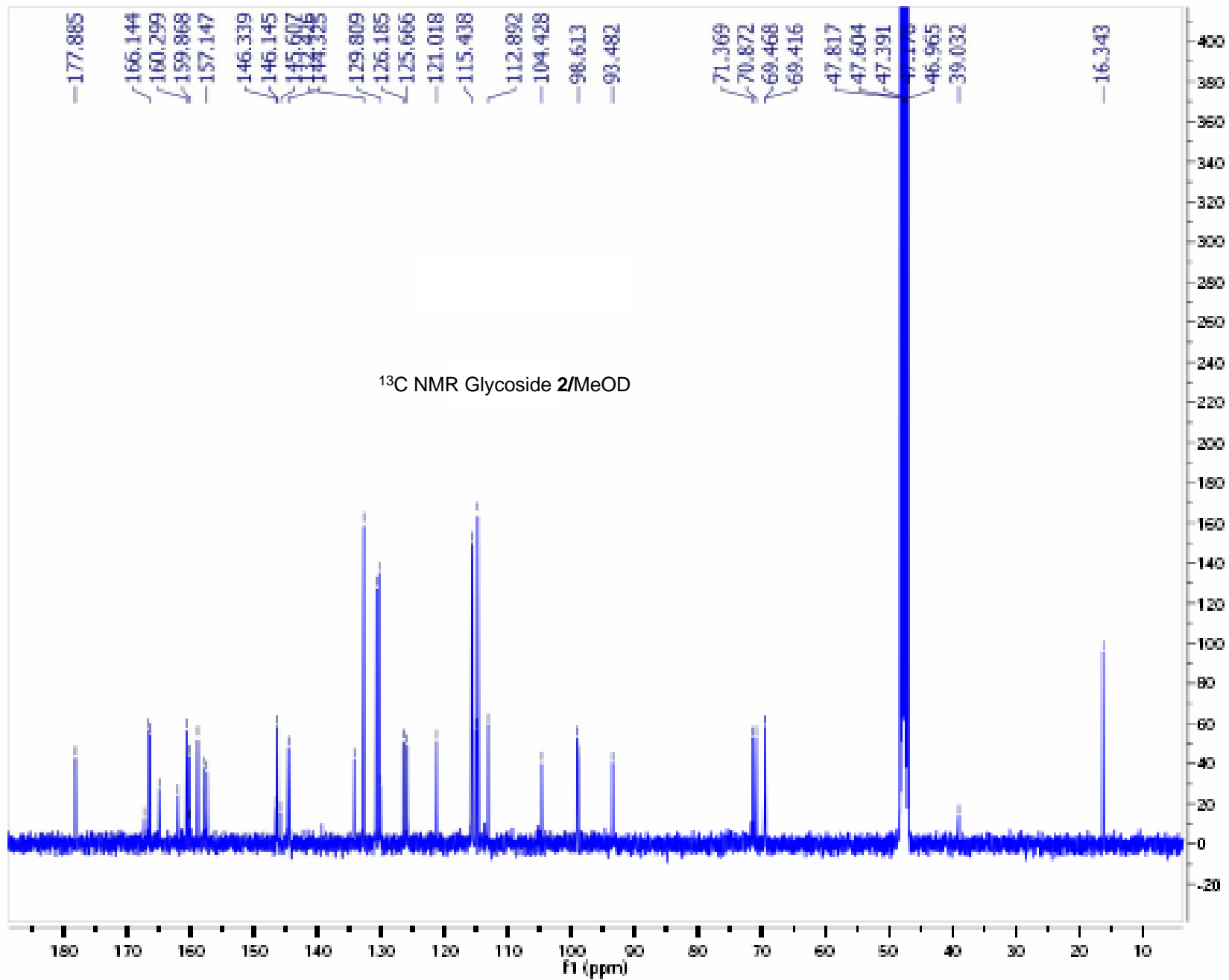
COSY-Glycoside 1/MeOD



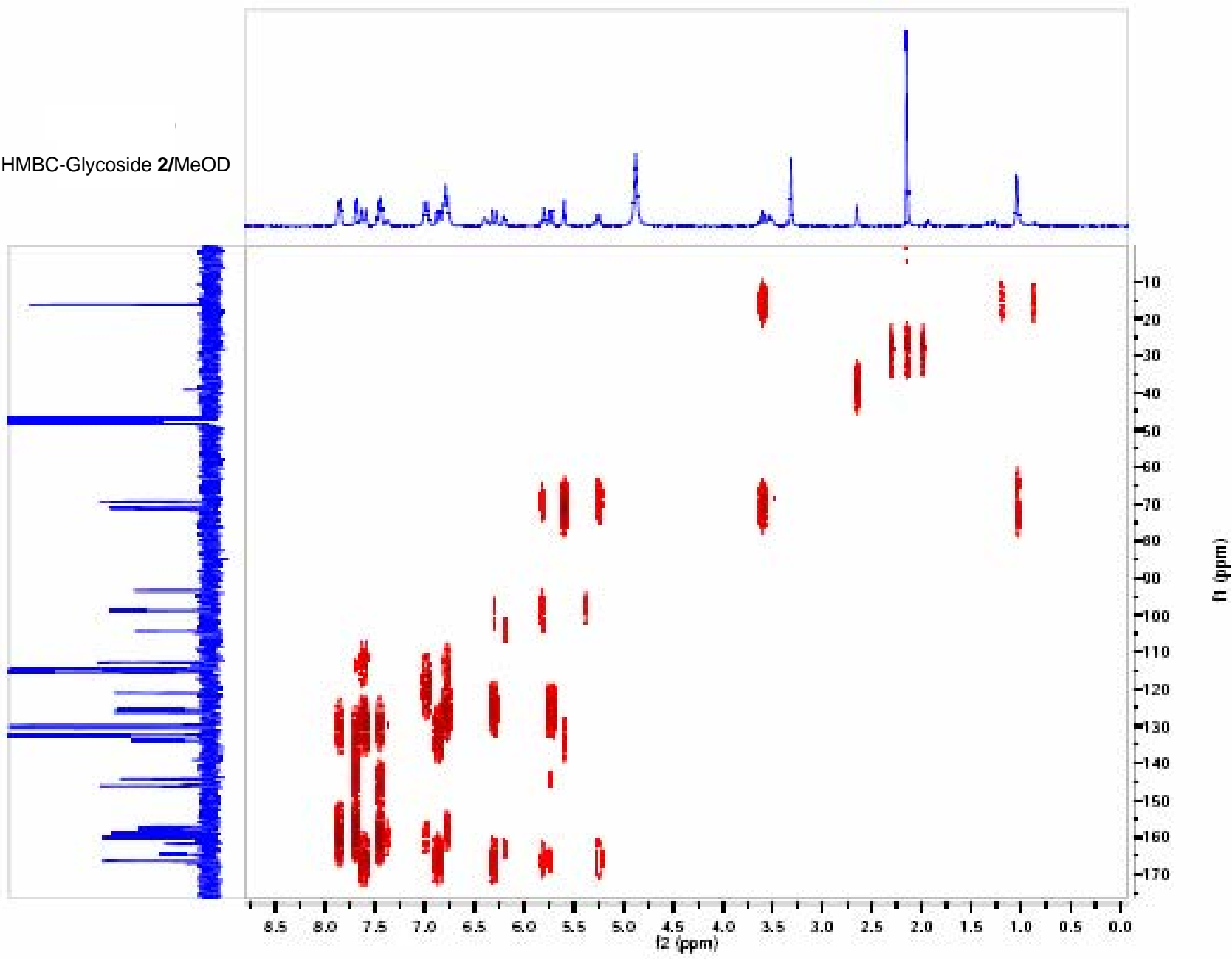
HMBC-Glycoside 1/MeOD



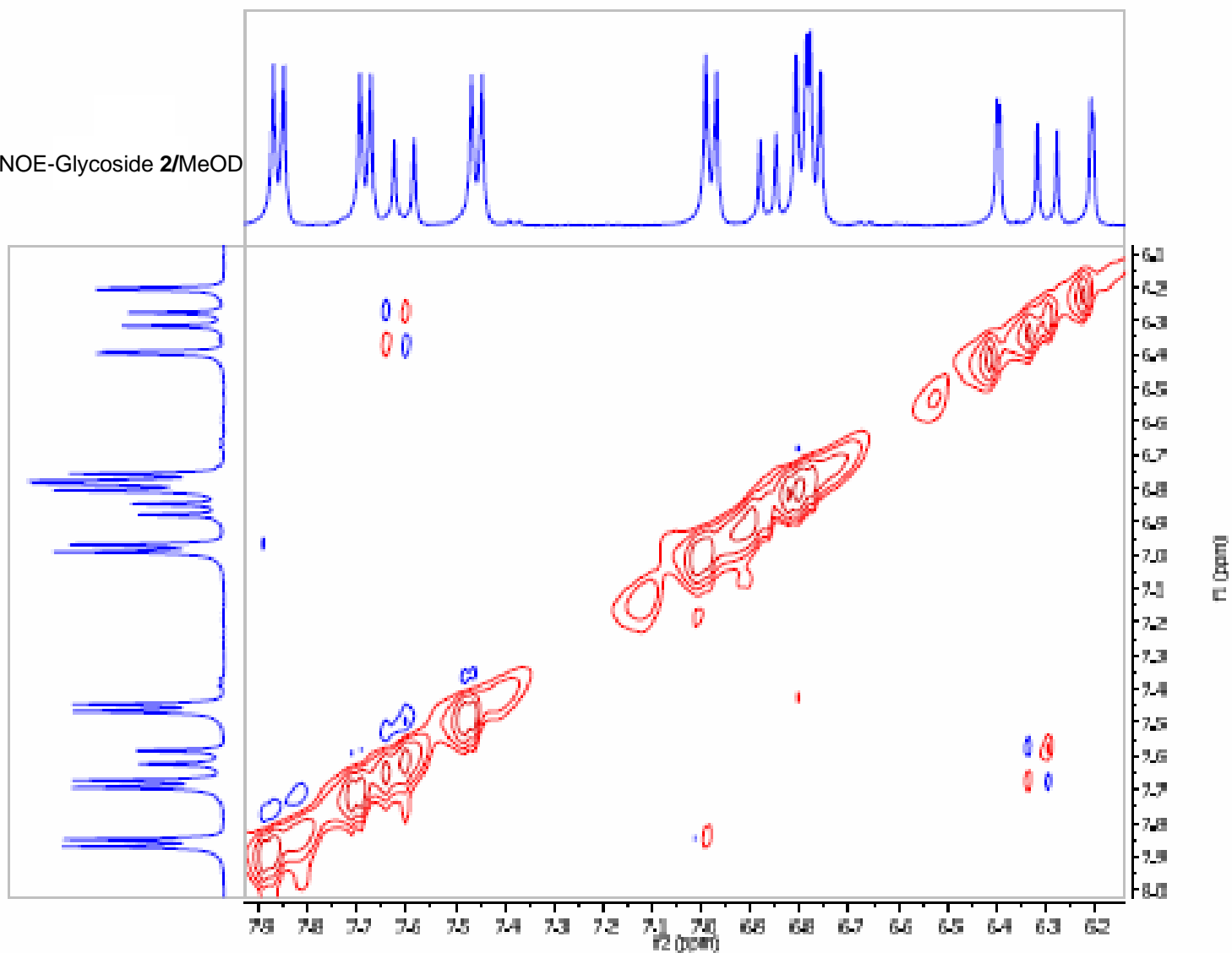




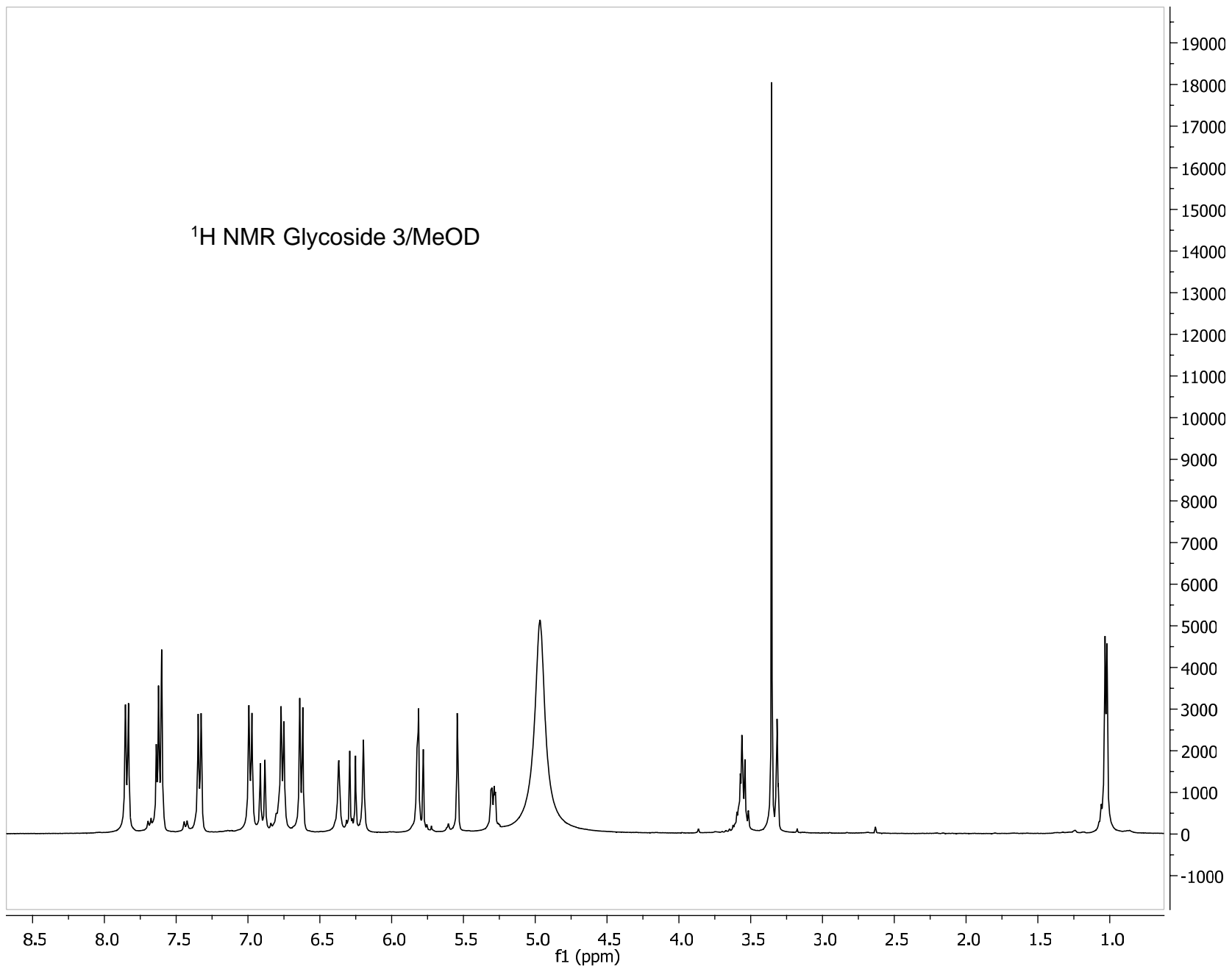
HMBC-Glycoside 2/MeOD



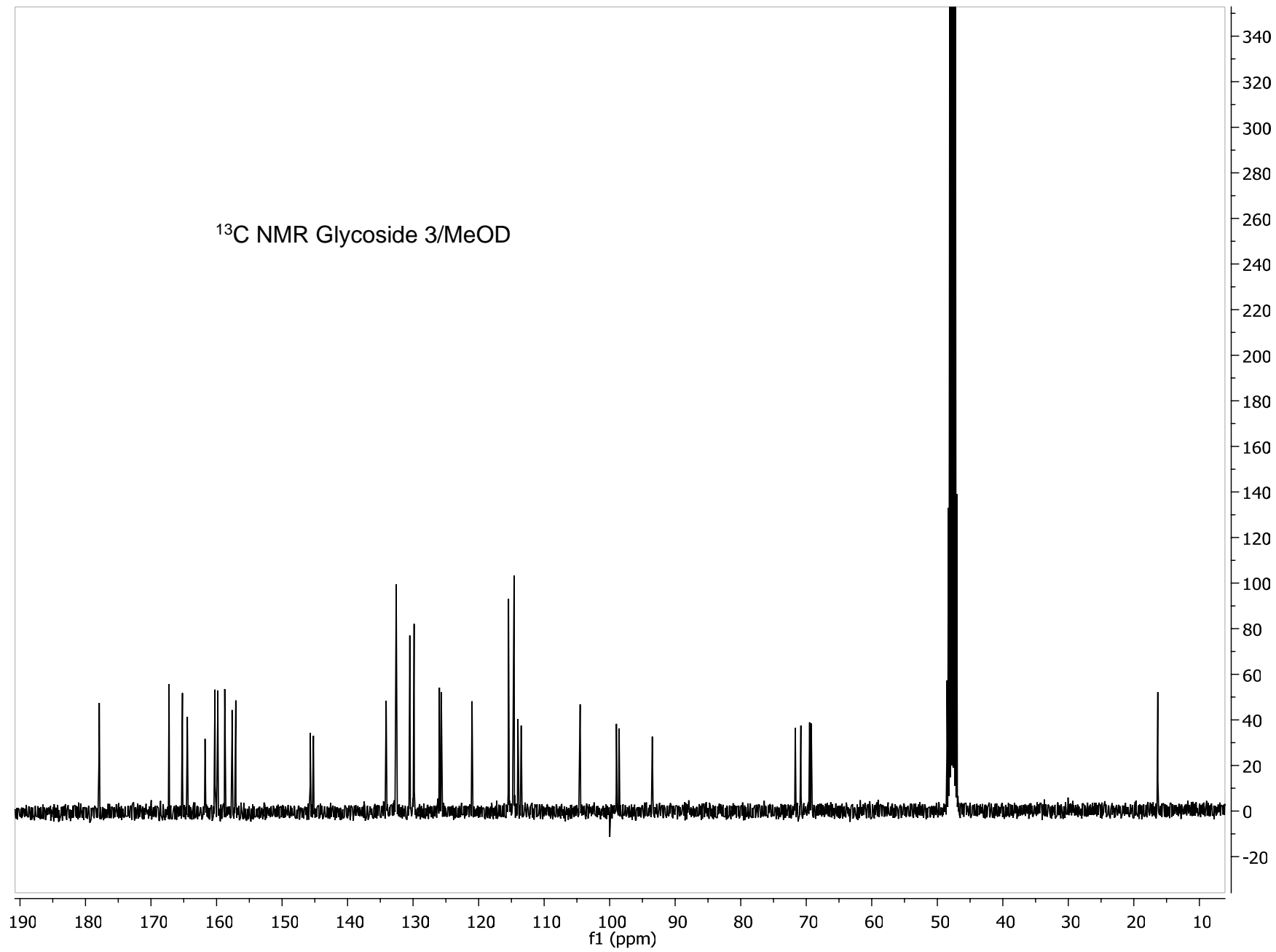
NOE-Glycoside **2**/MeOD

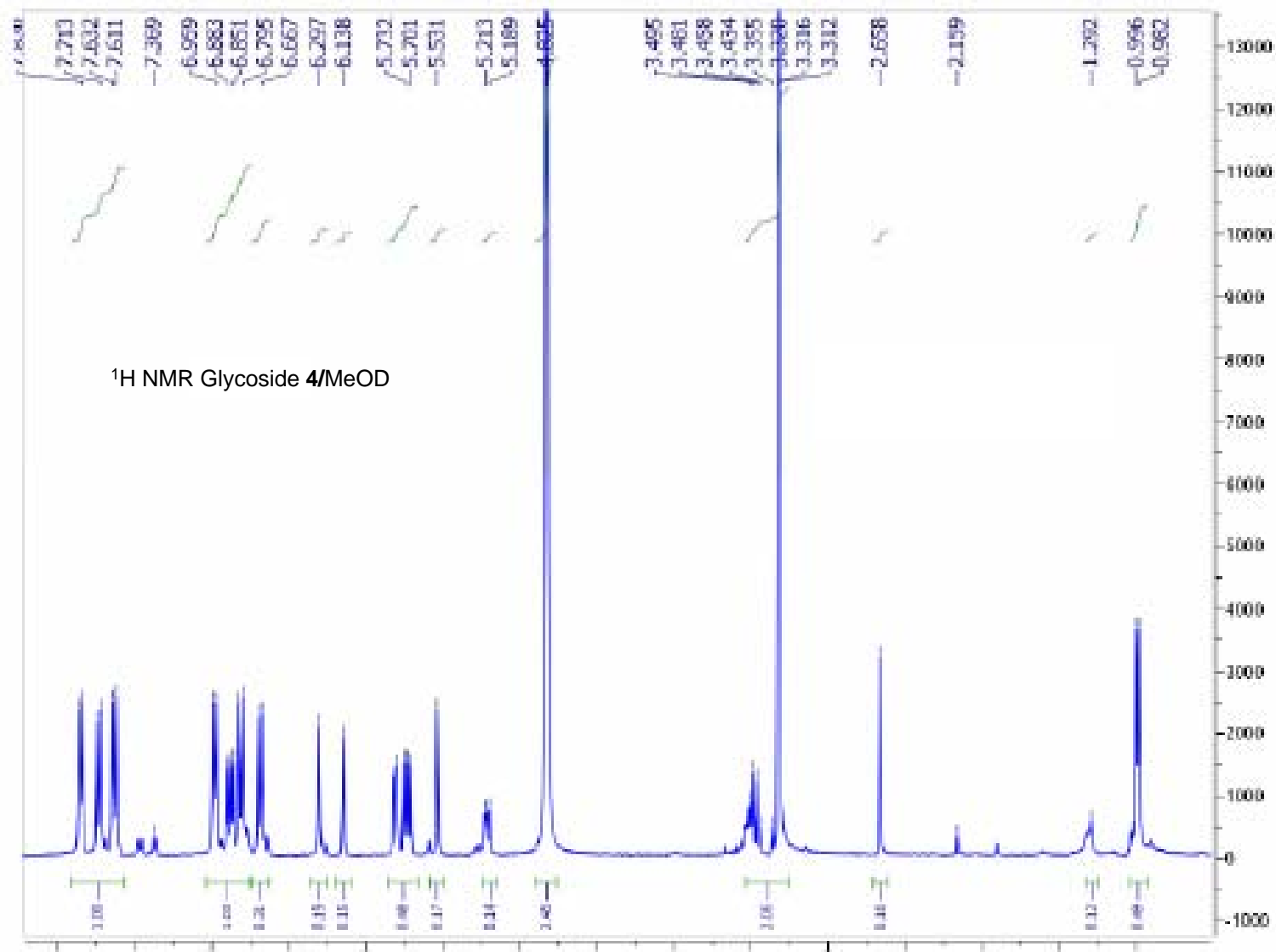


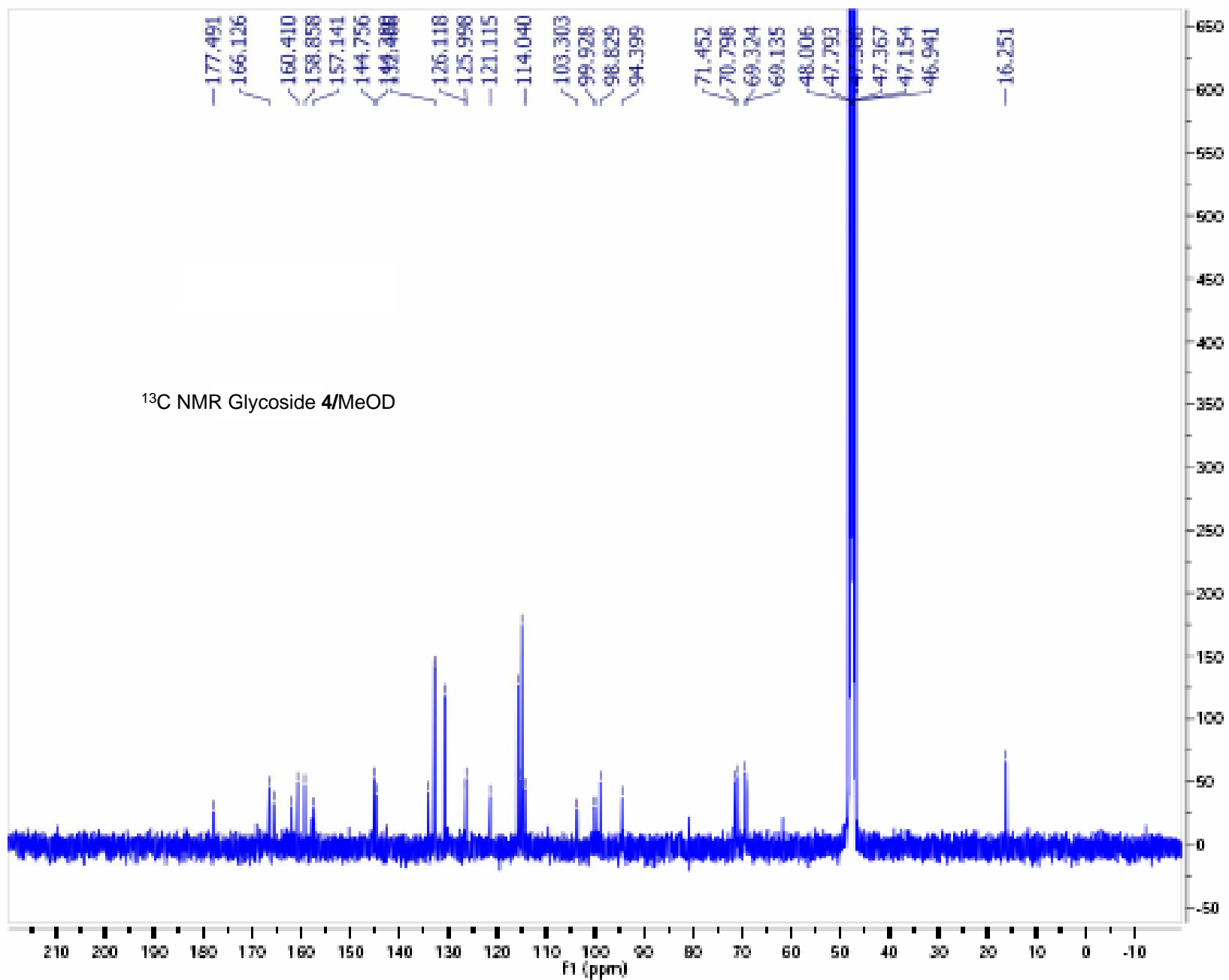
^1H NMR Glycoside 3/MeOD



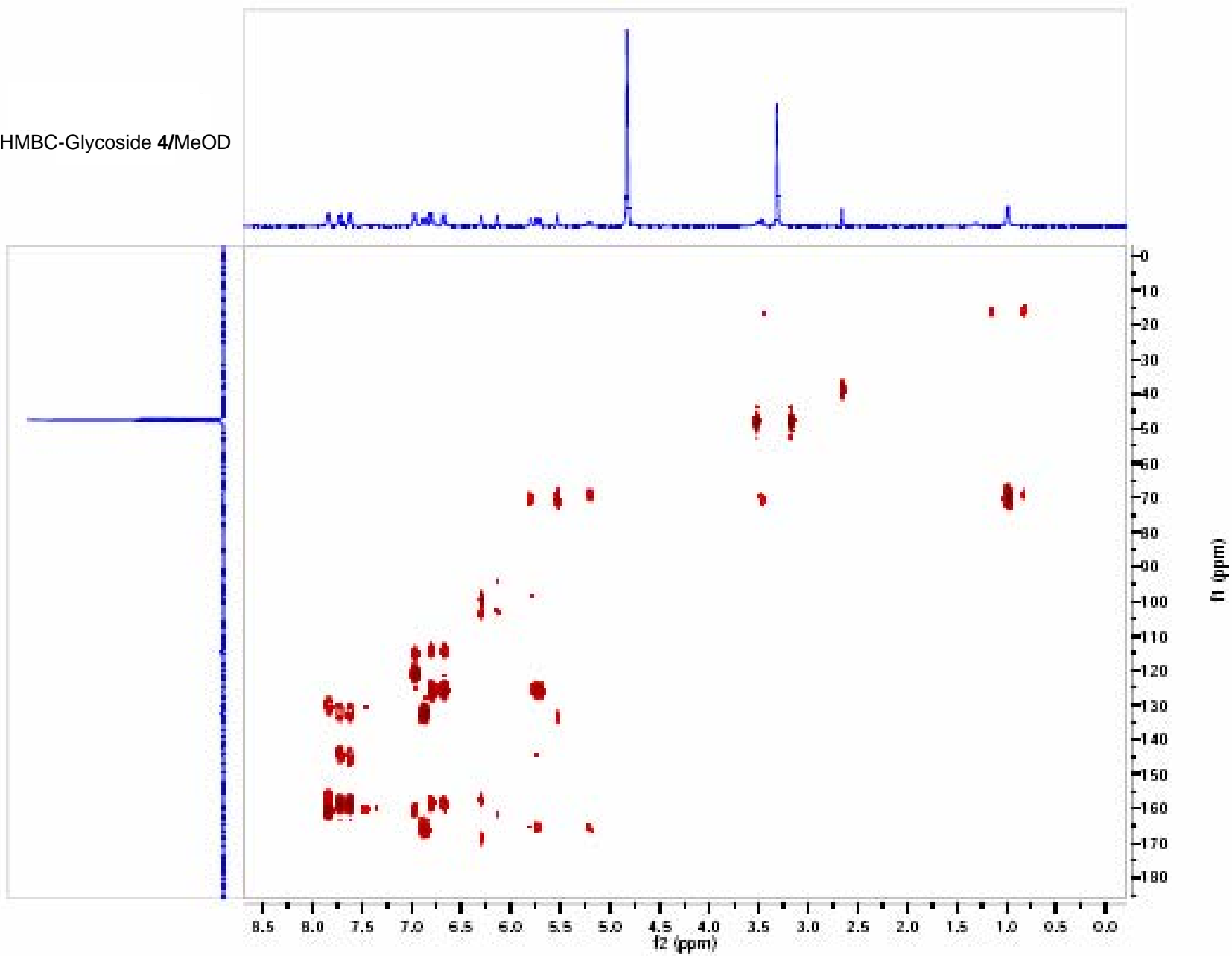
^{13}C NMR Glycoside 3/MeOD

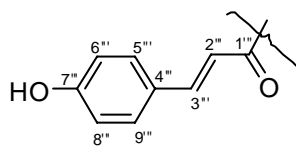
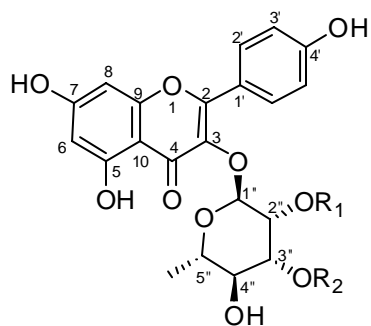




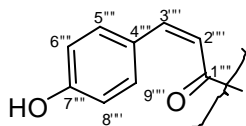


HMBC-Glycoside **4**/MeOD





E-p-coumaroyl



Z-p-coumaroyl

- 1, $R^1 = R^2 = E-p\text{-coumaroyl}$
- 2, $R^1 = E-p\text{-coumaroyl}$, $R^2 = Z-p\text{-coumaroyl}$
- 3, $R^1 = Z-p\text{-coumaroyl}$, $R^2 = E-p\text{-coumaroyl}$
- 4, $R^1 = R^2 = Z-p\text{-coumaroyl}$

Table 1. The ^{13}C NMR for the four glycosides **1-4**:

Carbon no.	^{13}C NMR (Ref.) δ_{C}, mult.	^{13}C NMR (1), δ_{C}	^{13}C NMR (2), δ_{C}	^{13}C NMR (3), δ_{C}	^{13}C NMR (4), δ_{C}
2	158.8, qC	157.9	157.7	157.6	157.5
3	135.2, qC	134.2	134.0	134.1	133.7
4	178.9, qC	178.1	177.9	177.9	177.5
5	163.0, qC	162.0	161.8	161.8	161.6
6	100.2, CH	98.7	98.6	98.6	99.9
7	165.8, qC	164.7	164.8	164.5	165.3
8	95.7, CH	93.6	93.48	93.5	94.4
9	158.8, qC	157.3	157.1	157.1	157.1
10	104.8, qC	104.7	104.4	104.6	103.3
1'	122.5, qC	121.2	121.0	121.2	121.1
2', 6'	131.8, CH	130.7	130.5	130.5	130.4
3', 5'	116.9a, CH	115.6	115.4	115.4	115.4
4'	161.5, qC	160.5	160.3	160.2	160.4
1''	101.2, CH	99.1	98.8	98.9	98.9
2''	72.2, CH	69.7	69.4	69.3	69.1
3''	73.1, CH	71.9	71.4	71.7	71.5
4''	71.0b, CH	69.8	69.5	69.5	69.3
5''	70.9b, CH	71.0	70.9	70.8	70.8
6''	17.8, CH ₃	16.6	16.3	16.30	16.3
1''', 1''''	167.8, 168.5, qC	166.6, 167.3	166.4, 166.1	167.3, 165.2	166.1, 166.2
2''', 2''''	114.2, 114.8, CH	113.1, 113.7	112.9, 114.8	113.5, 114.1	114.0, 114.8
3''', 3''''	147.0, 147.8, CH	145.8, 146.5	146.2, 144.3	145.6, 145.2	144.4, 144.8
4''', 4''''	126.9, 127.0, qC	125.8, 125.9	125.7, 126.2	125.7, 126.0	126.0, 126.1
5''', 9''', 5'''', 9''''	131.2, 131.4, CH	130.0, 130.2	130.0, 132.4	129.8, 132.4	132.5, 132.5
6''', 8''', 6'''', 8''''	116.8a, 117.0a, CH	115.6, 115.7	114.5, 115.4	114.6, 115.5	114.5, 114.6
7''', 7''''	161.8, 161.8, qC	160.1, 160.3	160.0, 158.7	159.8, 158.7	158.8, 158.9

^{a, b} Assignments bearing the same superscript in any one spectrum may be reversed. Reference compound measured at 300 MHz / MeOD.¹⁷ Compounds (**1-4**) measured at 400 MHz / MeOD.

Table 2. ¹H NMR, COSY and HMBC for glycoside **1** and ¹H NMR for glycosides **2-4**.

Proton no.	glycoside (1)				glycoside (2)	glycoside (3)	glycoside (4)
	¹ H NMR (Ref) δ _H , mult.	¹ H NMR δ _H (J value in Hz)	COSY	HMBC	¹ H NMR δ _H (J value in Hz)	¹ H NMR δ _H (J value in Hz)	¹ H NMR δ _H (J value in Hz)
6	6.10, br s	6.16, s	--	93.6, 104.7, 162.0, 164.7	6.26, s	6.22, s	6.13, S
8	6.26, br s	6.36, s	-	98.7, 104.7, 157.3, 164.7	6.39, bs	6.41, bs	6.30, Bs
2', 6'	7.81, d	7.83, d (8.4)	6.96	157.9, 160.5	7.87, d (8.4)	7.86, d (8.8)	7.83, d (8.4)
3', 5'	6.93, d	6.96, d (7.8)	7.84	121.2, 130.7, 160.5	7.01, d (8.4)	6.98, d (8.8)	6.96, d (8.4)
1''	5.55 (d)	5.57, s	-	71.0, 134.2	5.56, s	5.54, s	5.52, S
2''	5.77 (dd)	5.81, brs	5.27	166.6, 71.9	5.78, brs	5.78, brs	5.79, brs
3''	5.25 (dd)	5.27, dd (9.6, 3.2)	5.81, 3.62	69.7, 167.3	5.27, dd (9.6, 3.2)	5.27, dd (9.2, 3.2)	5.21, dd (9.2, 3.2)
4''	3.59 (t)	3.62, t, (9.6)	5.27, 3.53	16.6, 71.0	3.58, t, (9.6)	3.49, t (9.2)	3.48, t, (9.6)
5''	3.50 (m)	3.53, m	1.03, 3.62	69.8	3.52, m	3.53, m	3.52, m
6''	0.99 (d)	1.03, d (6.0)	3.53	71.0	1.04, d (6.0)	1.00, d (6.0)	0.97, d (5.6)
2''', 2''''	6.24 (d), 6.33 (d)	6.34, d (15.6), 6.28, d (15.6)	7.61, 7.56	(125.8, 166.6), (125, 167.3)	6.31, d (16.0), 5.72, d (12.8)	6.30, d (16.0), 5.81, d (12.8)	5.72, d (12.8), 5.74, d (12.8)
3''', 3''''	7.56 (d), 7.58 (d)	7.56, d (15.6), 7.61, d (15.6)	6.28, 6.34	167.3, 166.6	7.59, d (16.0), 6.88, d (12.8)	7.61, d (16.0), 6.94, d (12.8)	6.89, d (12.8), 6.86, d (12.8)
5''', 9''', 5'''', 9''''	7.33 (d), 7.42 (d)	7.34, d (8.4), 7.43, d (8.4)	6.72, 6.77	160.1, 160.3	7.47, d (8.4), 7.71, d (8.4)	7.36, d (8.8), 7.64, d (8.8)	7.71, d (8.4), 7.62, d (8.4)
6''', 8''', 6'''', 8''''	6.71 (d), 6.76 (d)	6.72, d (7.8), 6.77, d (8.4)	7.34, 7.43	(125.9, 130.0), (125.8)	6.81, m, 6.81, m	6.63, d (8.8), 6.78, d (8.8)	6.81, d (8.4), 6.69, d (8.4)