A serendipitous formation of a cysteine-bridged disaccharide

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Instruments and spectra

^{1}H and ^{13}C NMR spectra were recorded on Varian Gemini 400 at ambient temperature, in $CDCl_3$. The splitting patterns are reported as follows: singlet (s), doublet (d), triplet (t), doublet of doublets (dd), multiplet (m) and broad singlet (br s). High resolution mass spectra were obtained on a Waters Synapt G2 mass spectrometer in the positive mode.

Figure 1: ^{1}H NMR spectrum of compound **6**

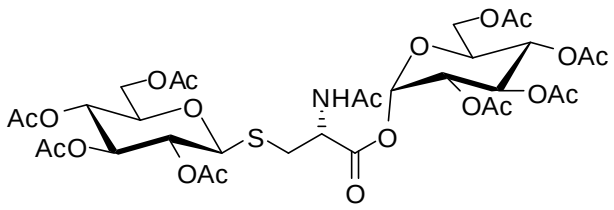

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Figure 2: ^{13}C NMR spectrum of compound **6**

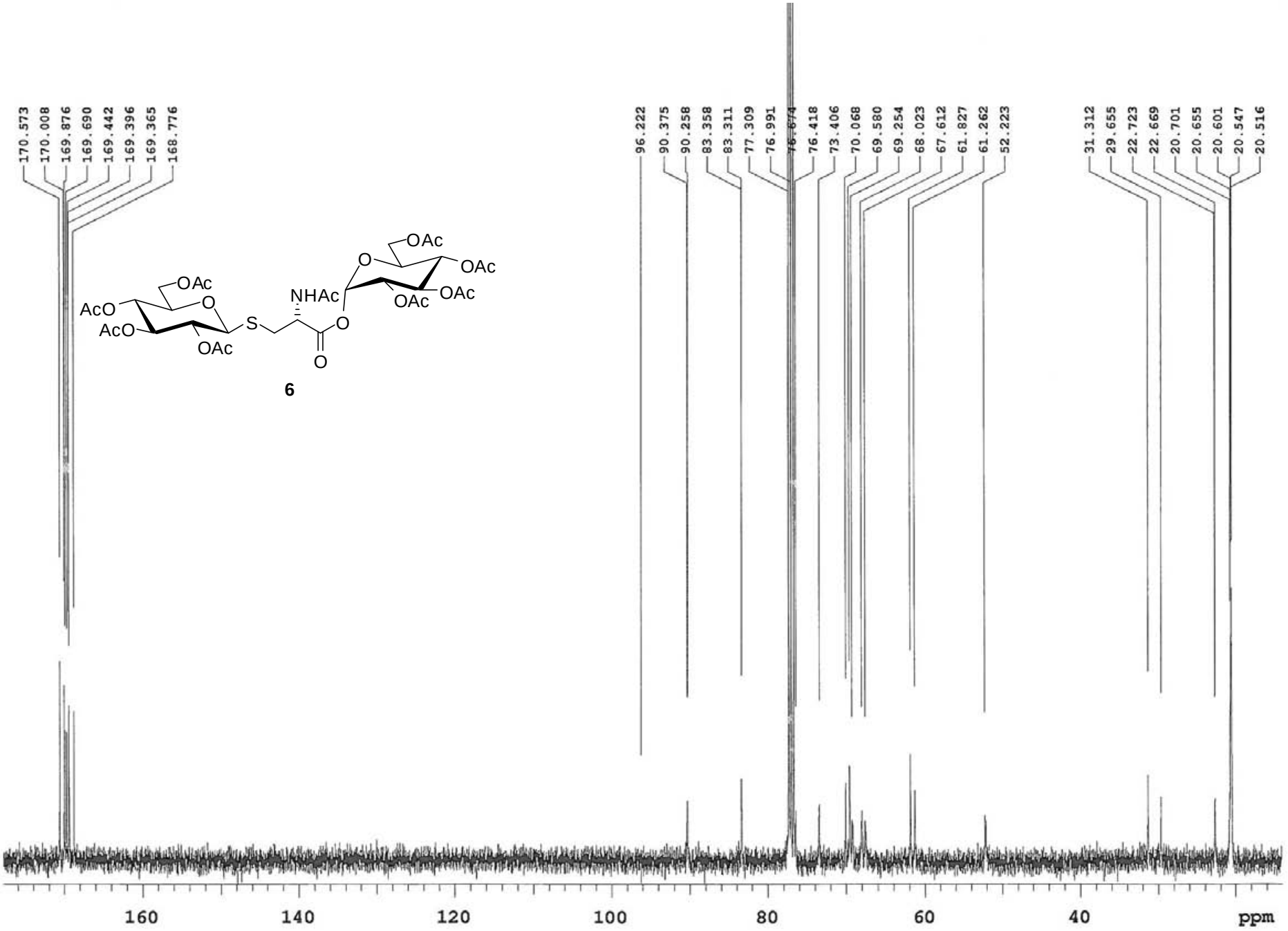

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Figure 3: COSY spectrum of compound **6**

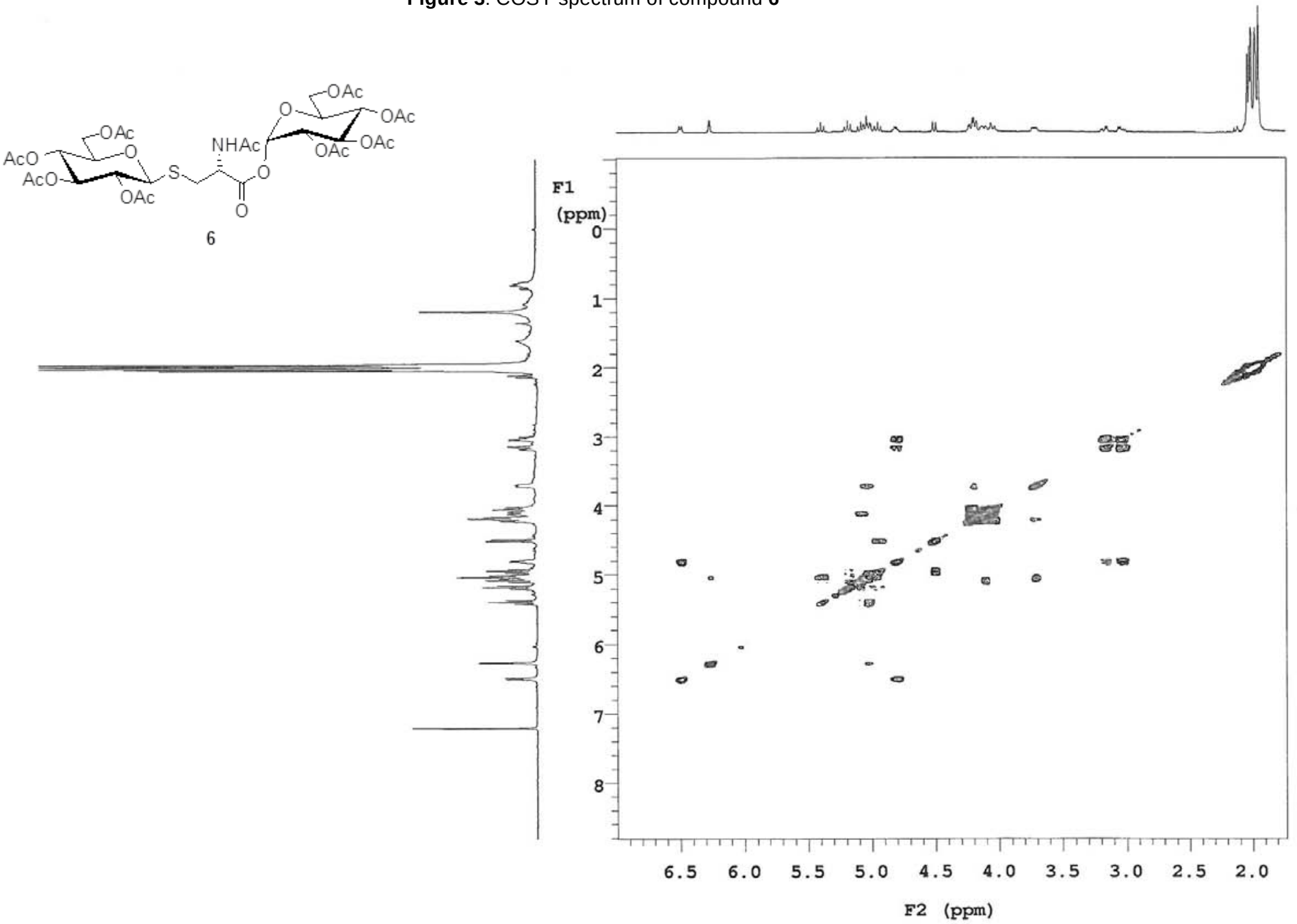

Figure 4: HMQC spectrum of compound **6**

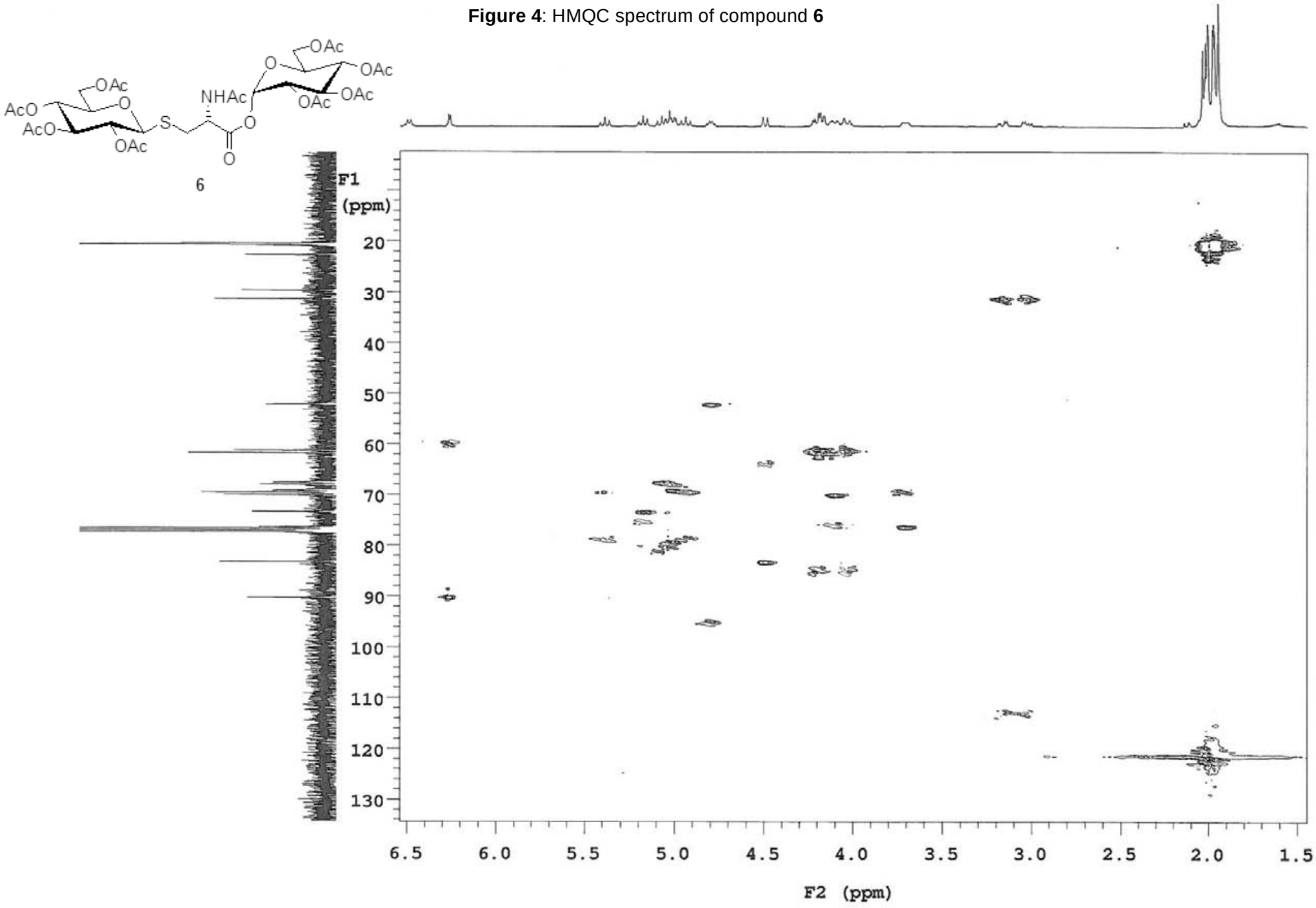

Figure 5: ^{1}H NMR spectrum of compound **7**

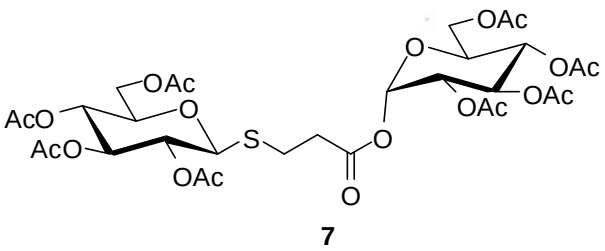

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Figure 6: ^{13}C NMR spectrum of compound **7**

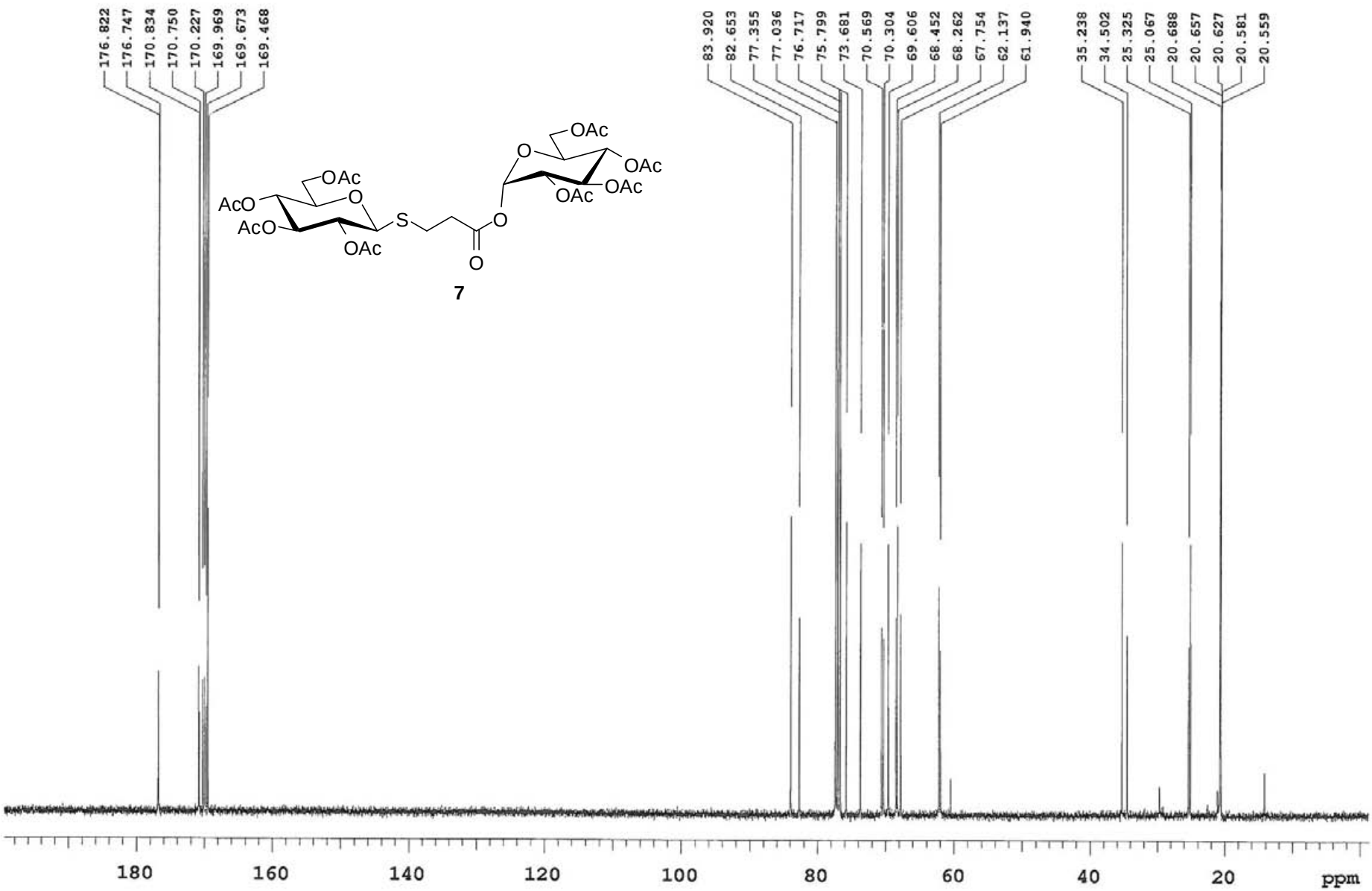

Figure 7: COSY spectrum of compound **7**

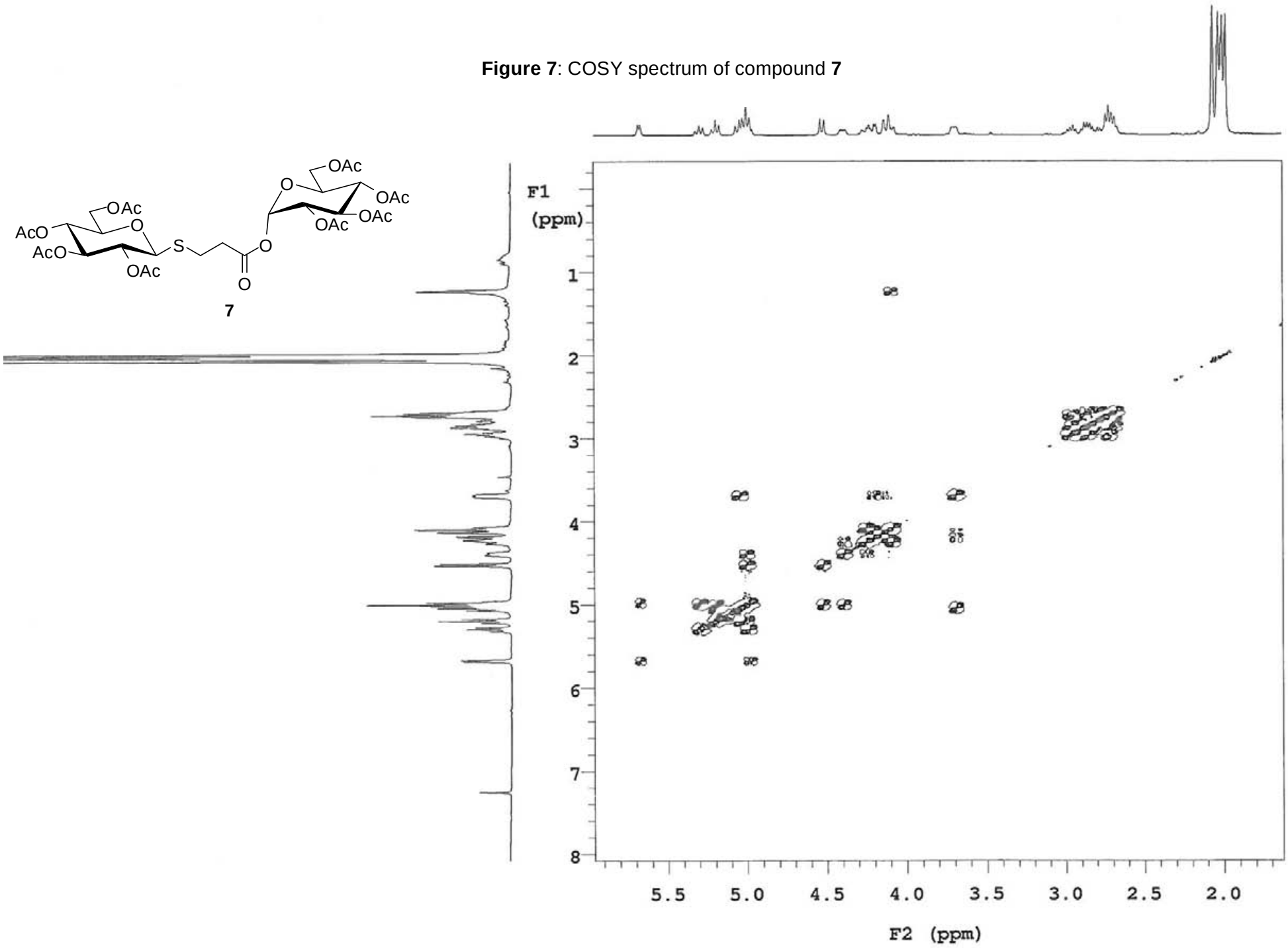

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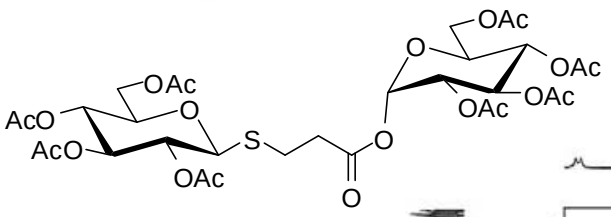
Figure 8: HMQC spectrum of compound **7**



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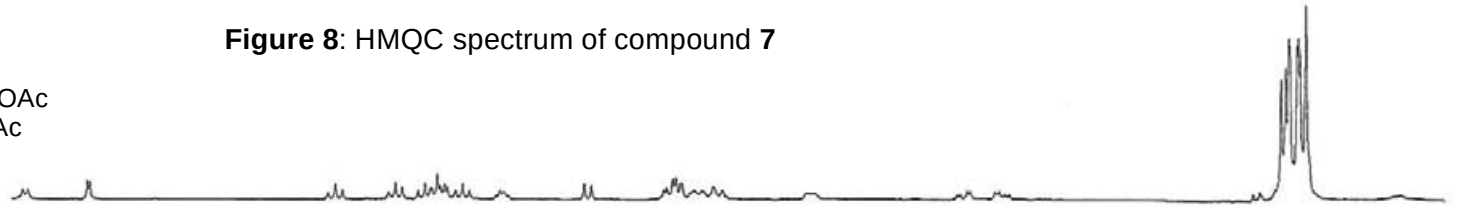

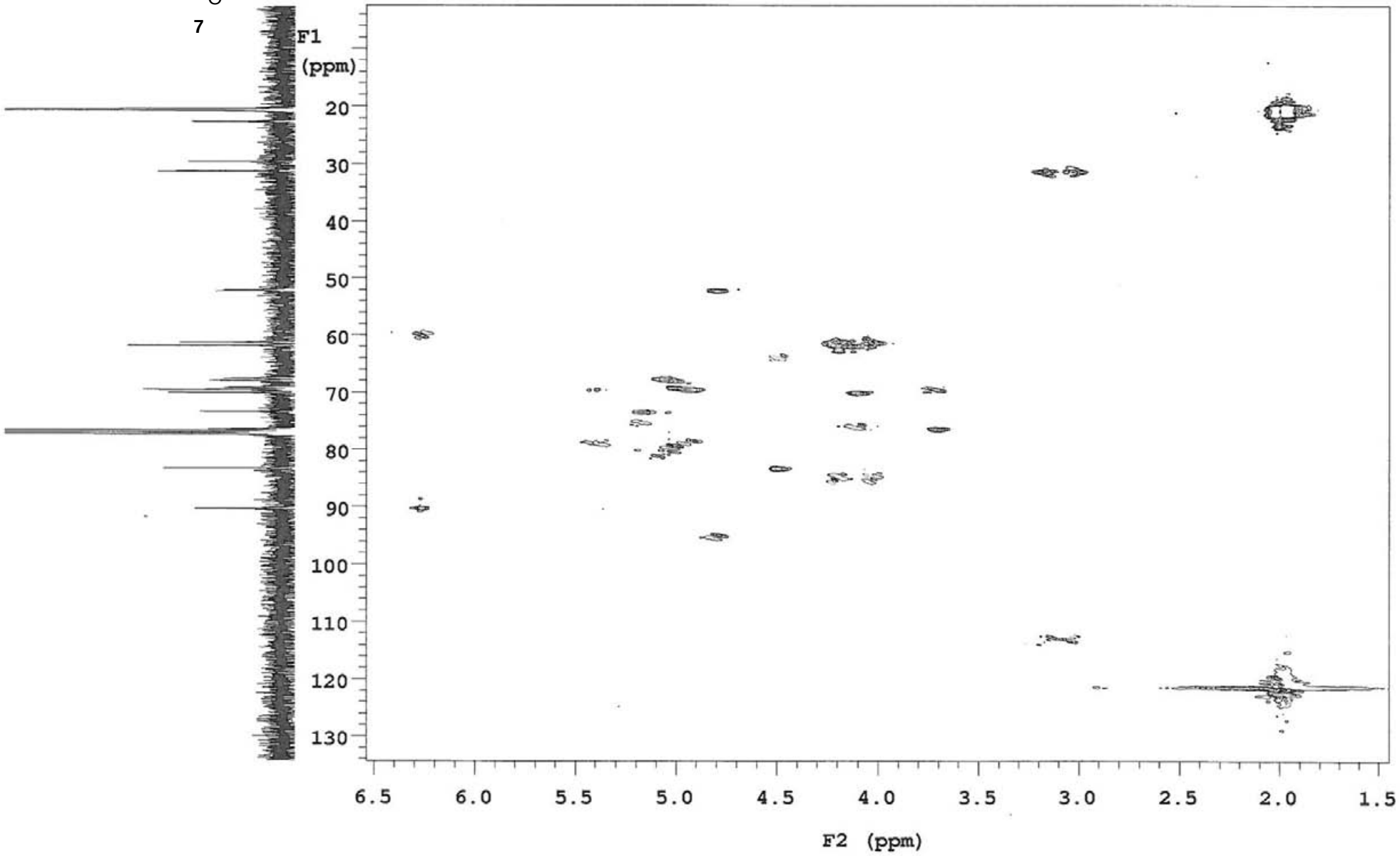

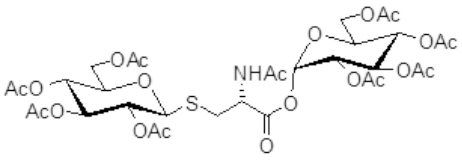

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Figure 9: HRMS of compound **6**

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

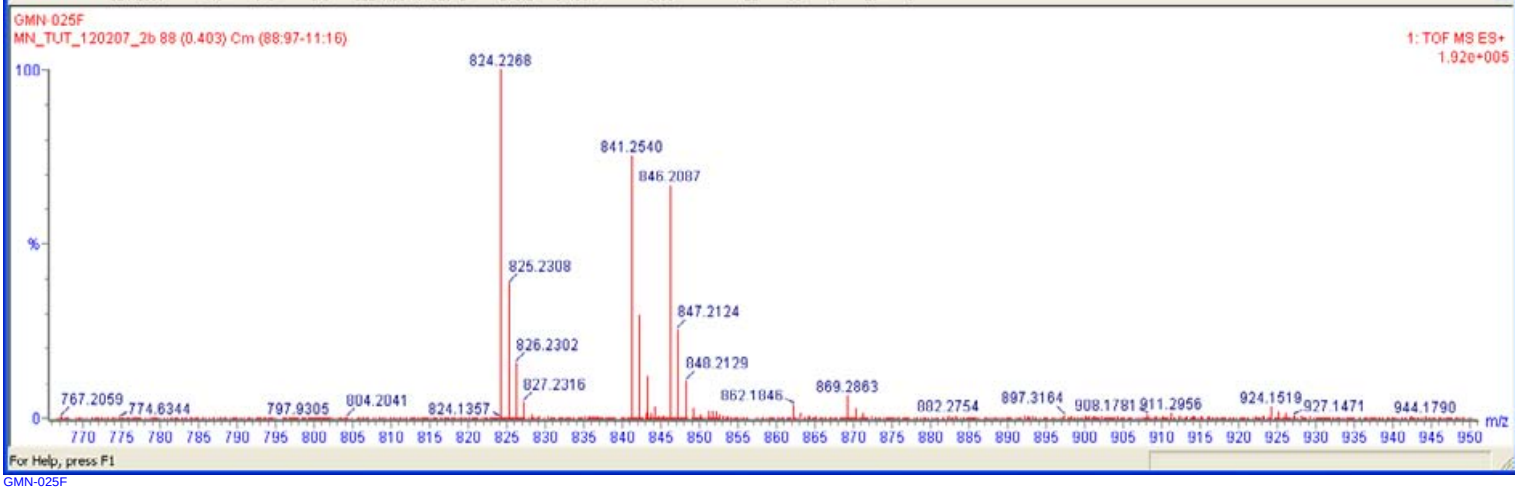
Number of isotope peaks used for i-FIT = 3

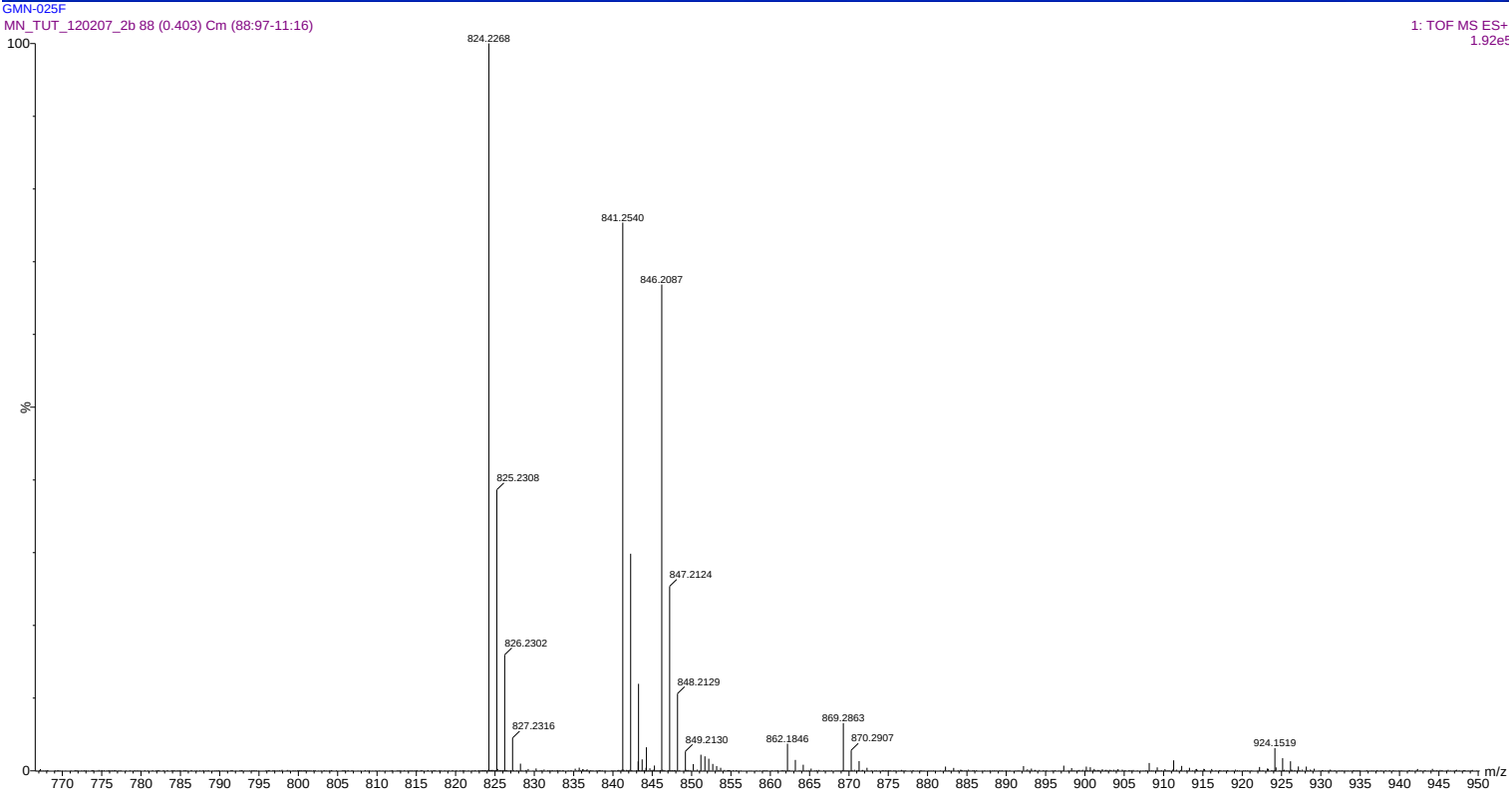
Monoisotopic Mass, Even Electron Ions

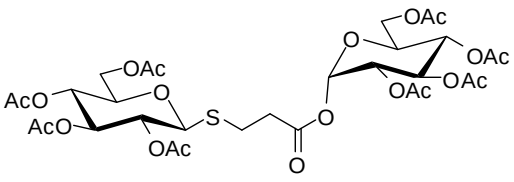
449 formula(e) evaluated with 68 results within limits (all results (up to 1000) for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S
824.2268	824.2283	-1.5	-1.8	11.5	C33 H46 N O21 S	262.2	0.463	62.97	33	46	1	21	1
	824.2243	2.5	3.0	7.5	C28 H46 N3 O23 S	272.3	10.630	0.00	28	46	3	23	1
	824.2296	-2.8	-3.4	16.5	C34 H42 N5 O17 S	268.0	6.277	0.19	34	42	5	17	1
	824.2302	-3.4	-4.1	-1.5	C21 H50 N3 O28 S	276.6	14.918	0.00	21	50	3	28	1
	824.2224	4.4	5.3	20.5	C40 H42 N O16 S	273.0	11.253	0.00	40	42	1	16	1
	824.2203	6.5	7.9	3.5	C23 H46 N5 O25 S	275.6	13.860	0.00	23	46	5	25	1
	824.2337	-6.9	-8.4	20.5	C39 H42 N3 O15 S	272.7	11.029	0.00	39	42	3	15	1
	824.2342	-7.4	-9.0	2.5	C26 H50 N O26 S	274.1	12.428	0.00	26	50	1	26	1
	824.2189	7.9	9.6	-1.5	C22 H50 N O29 S	276.2	14.501	0.00	22	50	1	29	1







7

Figure 10: HRMS of compound **7**

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1315 formula(e) evaluated with 189 results within limits (all results (up to 1000) for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S
	767.2030	0.7	0.9	33.5	C47 H31 N2 O9	111.3	5.206	0.55	47	31	2	9	
	767.2045	-0.8	-1.0	41.5	C56 H31 O2 S	113.4	7.251	0.07	56	31		2	1
	767.2028	0.9	1.2	6.5	C26 H43 N2 O22 S	110.8	4.730	0.88	26	43	2	22	1
	767.2053	-1.6	-2.1	2.5	C22 H43 N2 O27	111.7	5.605	0.37	22	43	2	27	
	767.2011	2.6	3.4	46.5	C59 H27 O2	112.5	6.337	0.18	59	27		2	
	767.2063	-2.6	-3.4	28.5	C44 H35 N2 O9 S	112.5	6.391	0.17	44	35	2	9	1
	767.2010	2.7	3.5	19.5	C38 H39 O15 S	111.1	4.990	0.68	38	39		15	1
	767.2068	-3.1	-4.0	10.5	C31 H43 O20 S	109.5	3.365	3.45	31	43		20	1
	767.2005	3.2	4.2	37.5	C51 H31 N2 O4 S	113.3	7.140	0.08	51	31	2	4	1