

Supporting Information

For

Enzymatic modular assembly of hybrid Lewis antigens

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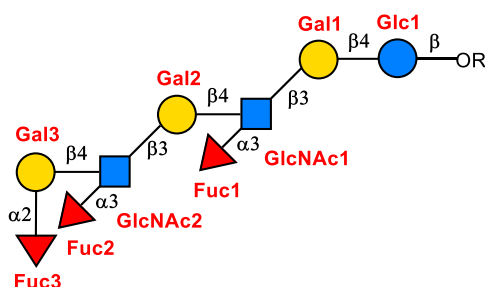
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1 NMR assignment of final products 1, 2, and 3.

1.1 NMR assignment data for final products

NMR signals were assigned on the basis of ^1H NMR, ^{13}C NMR, COSY (Correlated Spectroscopy), HMBC (Heteronuclear Multiple Bond Correlation), HSQC (^1H - ^{13}C Heteronuclear Single Quantum Coherence), and HSQC-TOCSY (Heteronuclear Single Quantum Coherence-Total Correlation Spectroscopy) experiments.

NMR assignment of compound 1



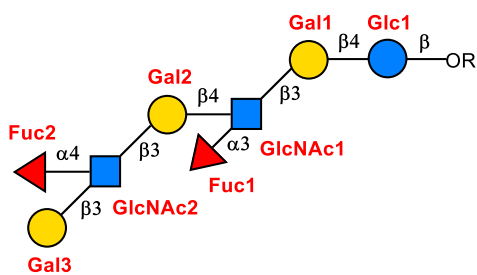
	H1	H2	H3	H4	H5	H6	NAc	Anomeric Carbon
Glc1	4.48	3.31	3.64	3.64	3.86	3.97, 3.79	- ^[a]	101.99
Gal1	4.43	3.57	3.70	4.15	N/A ^[b]	N/A	-	102.81
Gal2	4.44	3.51	3.68	4.09	N/A	N/A	-	101.60
Gal3	4.51	3.65	3.85	3.86	N/A	N/A	-	100.06
GlcNAc1	4.71	3.95	3.59	3.92	N/A	3.95, 3.85	2.02	102.42
GlcNAc2	4.71	3.95	3.57	3.94	N/A	3.98, 3.83	2.02	102.33
Fuc1	5.11	3.69	3.90	3.77	4.81	1.14	-	98.60
Fuc2	5.12	3.69	3.90	3.81	4.88	1.23	-	98.49
Fuc3	5.27	3.79	3.78	3.82	4.25	1.26	-	99.30

^[a] Not applicable

^[b] Not assigned

Linker	<u>O</u> CH ₂ CH ₂ CH ₂ N ₃	OCH ₂ <u>C</u> H ₂ CH ₂ N ₃	OCH ₂ CH ₂ <u>C</u> H ₂ N ₃
C	67.25	28.11	47.75
H	4.00, 3.76	1.91	3.46

NMR assignment of compound 2



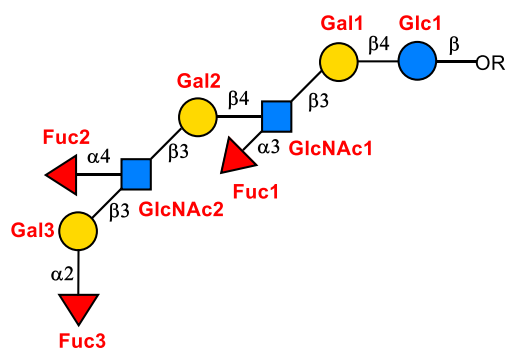
	H1	H2	H3	H4	H5	H6	NAc	Anomeric Carbon
Glc1	4.45	3.27	3.60	3.60	3.54	3.94, 3.76	- ^[a]	101.99
Gal1	4.39	3.54	3.67	4.06	N/A ^[b]	N/A	-	102.80
Gal2	4.40	3.47	3.67	4.12	N/A	N/A	-	101.63
Gal3	4.48	3.44	3.58	3.84	N/A	N/A	-	102.74
GlcNAc1	4.67	3.93	3.54	3.91	N/A	N/A	1.99 or 1.98	102.42
GlcNAc2	4.65	3.92	4.03	3.70	3.50	N/A	1.99 or 1.98	102.48
Fuc1	5.08	3.65	3.85	3.75	4.78	1.11	-	98.60
Fuc2	4.99	3.76	3.86	3.75	4.85	1.14	-	97.87

^[a] Not applicable

^[b] Not assigned

Linker	<u>O</u> CH ₂ CH ₂ CH ₂ N ₃	OCH ₂ <u>C</u> H ₂ CH ₂ N ₃	OCH ₂ CH ₂ <u>C</u> H ₂ N ₃
C	67.23	28.07	47.72
H	3.96, 3.72	1.87	3.42

NMR assignment of compound 3



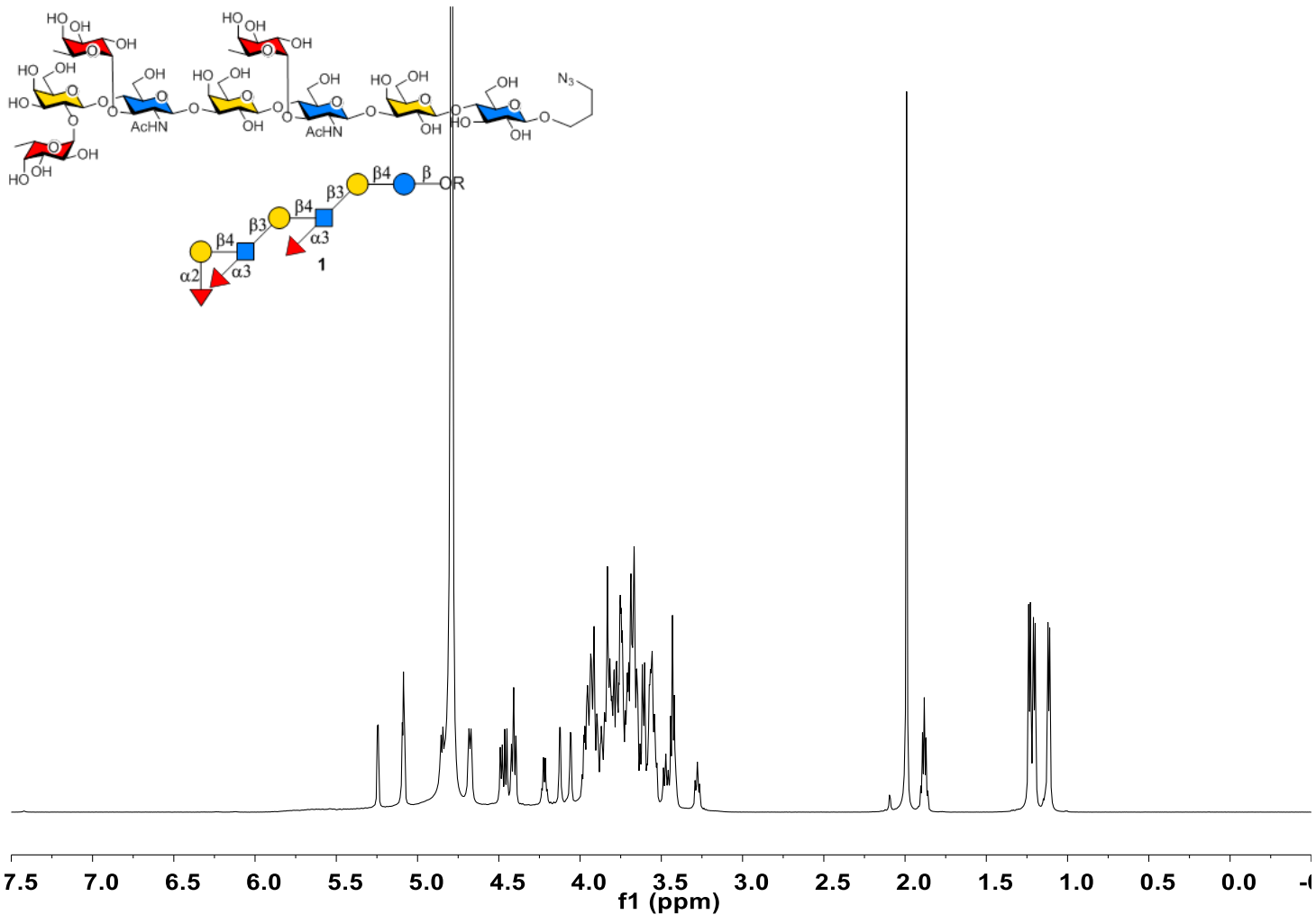
	H1	H2	H3	H4	H5	H6	NAc	Anomeric Carbon
Glc1	4.44	3.26	3.59	3.59	3.53	3.93,3.74	-[a]	101.96
Gal1	4.38	3.52	3.65	4.10	N/A ^[b]	N/A	-	102.78
Gal2	4.38	3.42	3.65	4.03	N/A	N/A	-	101.59
Gal3	4.61	3.56	3.76	3.81	N/A	N/A		100.45
GlcNAc1	4.66	3.90	3.81	3.89	N/A	N/A	2.00 or 1.97	102.39
GlcNAc2	4.55	3.78	4.08	3.68	3.52	N/A	2.00 or 1.97	103.07
Fuc1	5.06	3.64	3.82	3.72	4.77	1.10	-	98.66
Fuc2	5.00	3.75	3.86	3.77	4.82	1.21	-	97.61
Fuc3	5.10	3.69	3.63	3.66	4.29	1.22	-	99.38

^[a] Not applicable

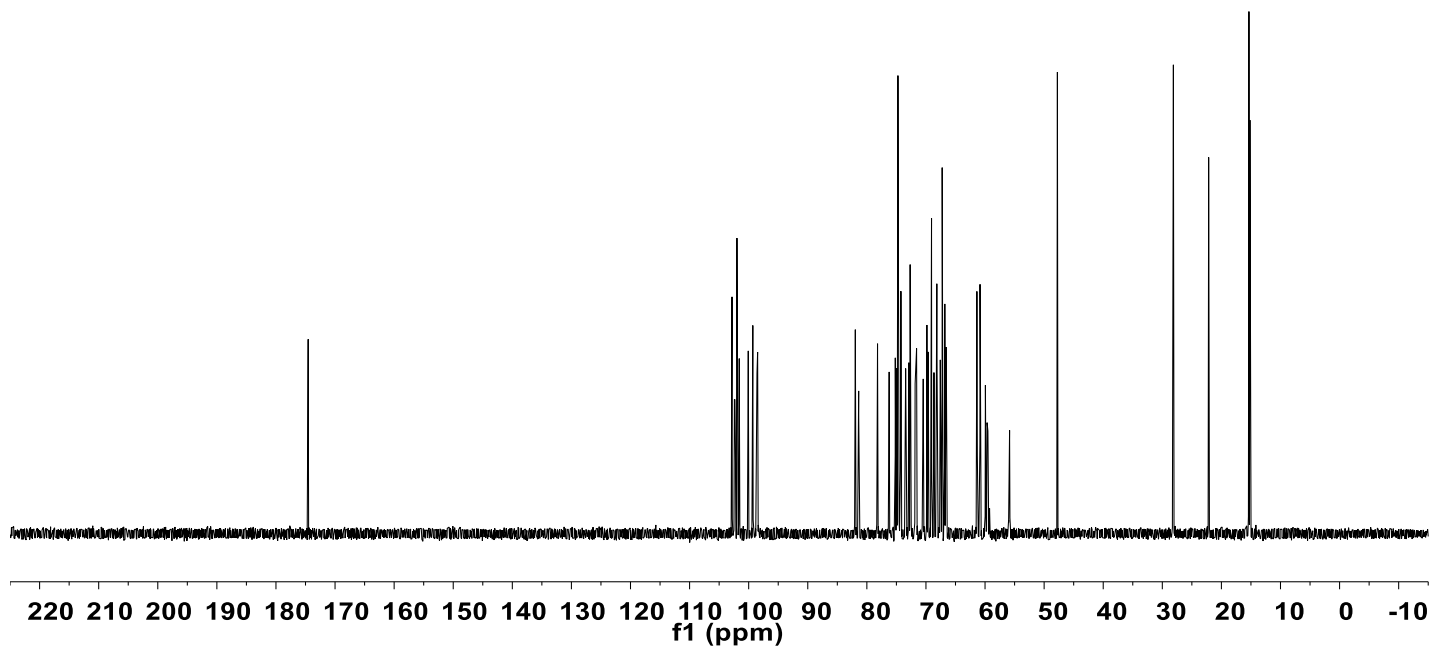
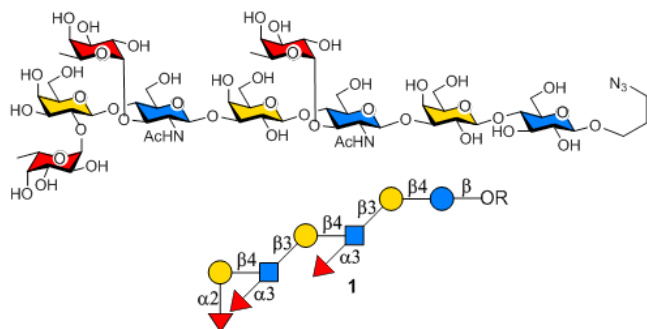
^[b] Not assigned

Linker	<u>O</u> CH ₂ CH ₂ CH ₂ N ₃	OCH ₂ <u>C</u> H ₂ CH ₂ N ₃	OCH ₂ CH ₂ <u>C</u> H ₂ N ₃
C	67.22	28.08	47.72
H	3.95, 3.71	1.86	3.41

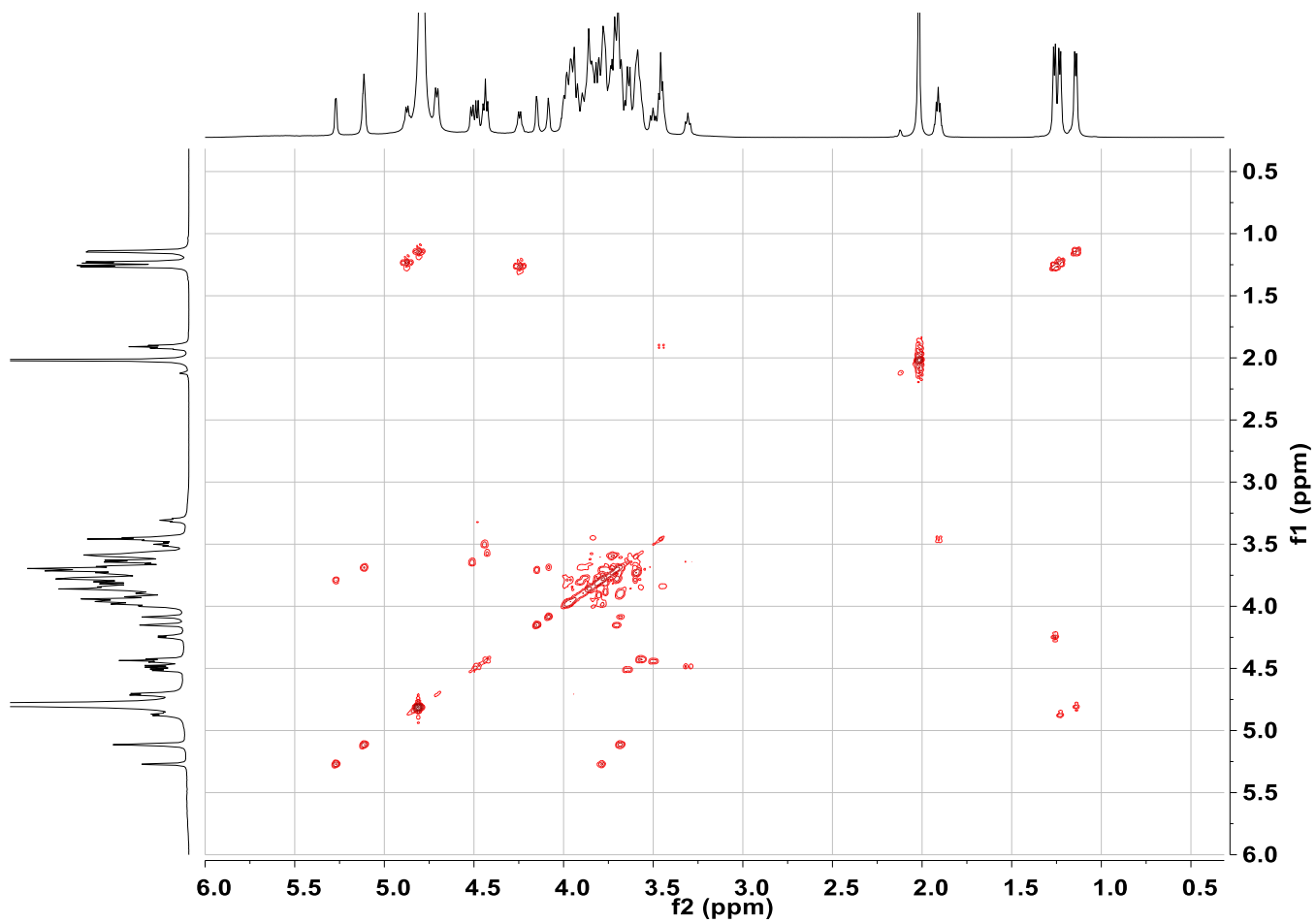
¹H NMR of compound 1



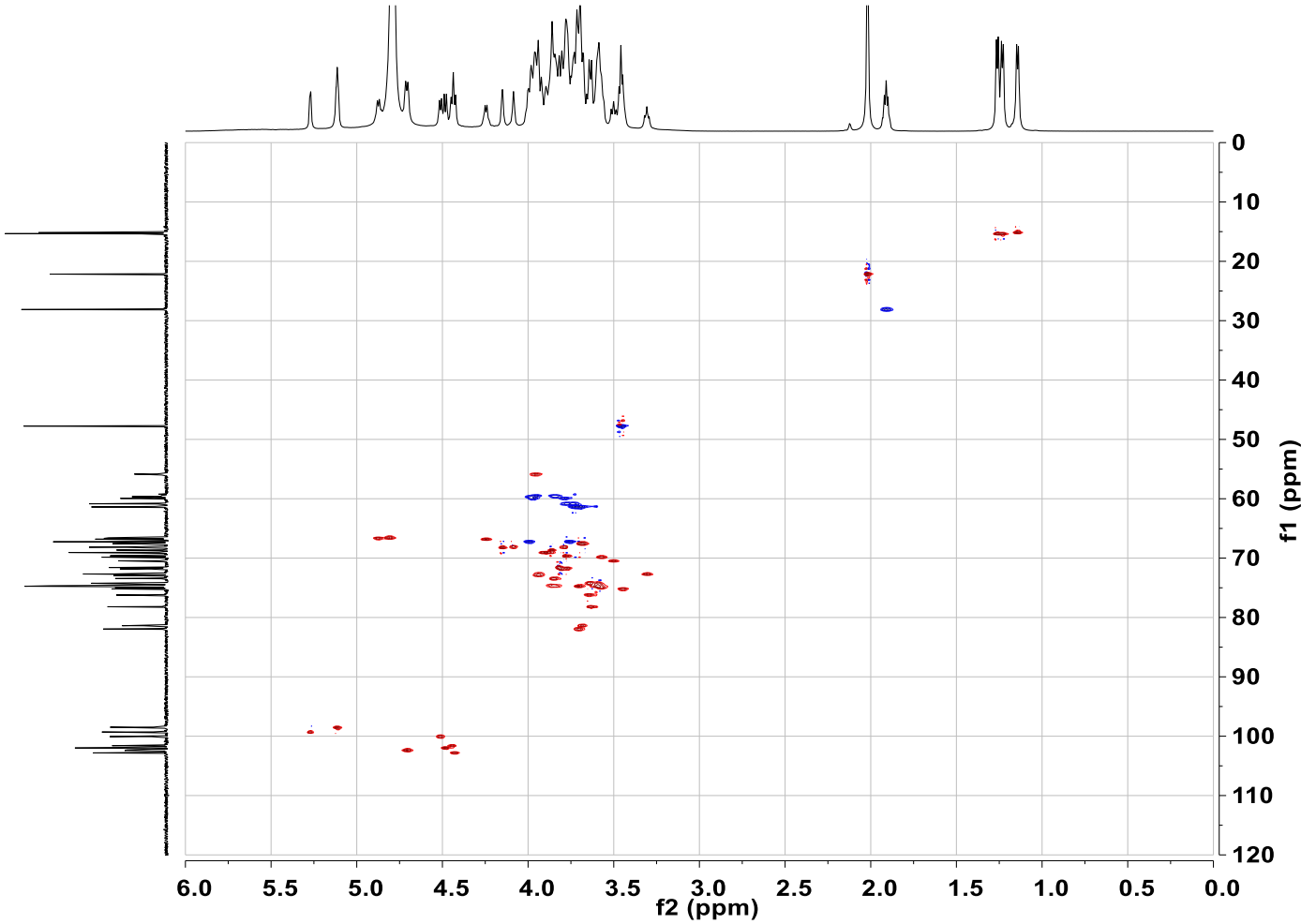
^{13}C NMR of compound 1



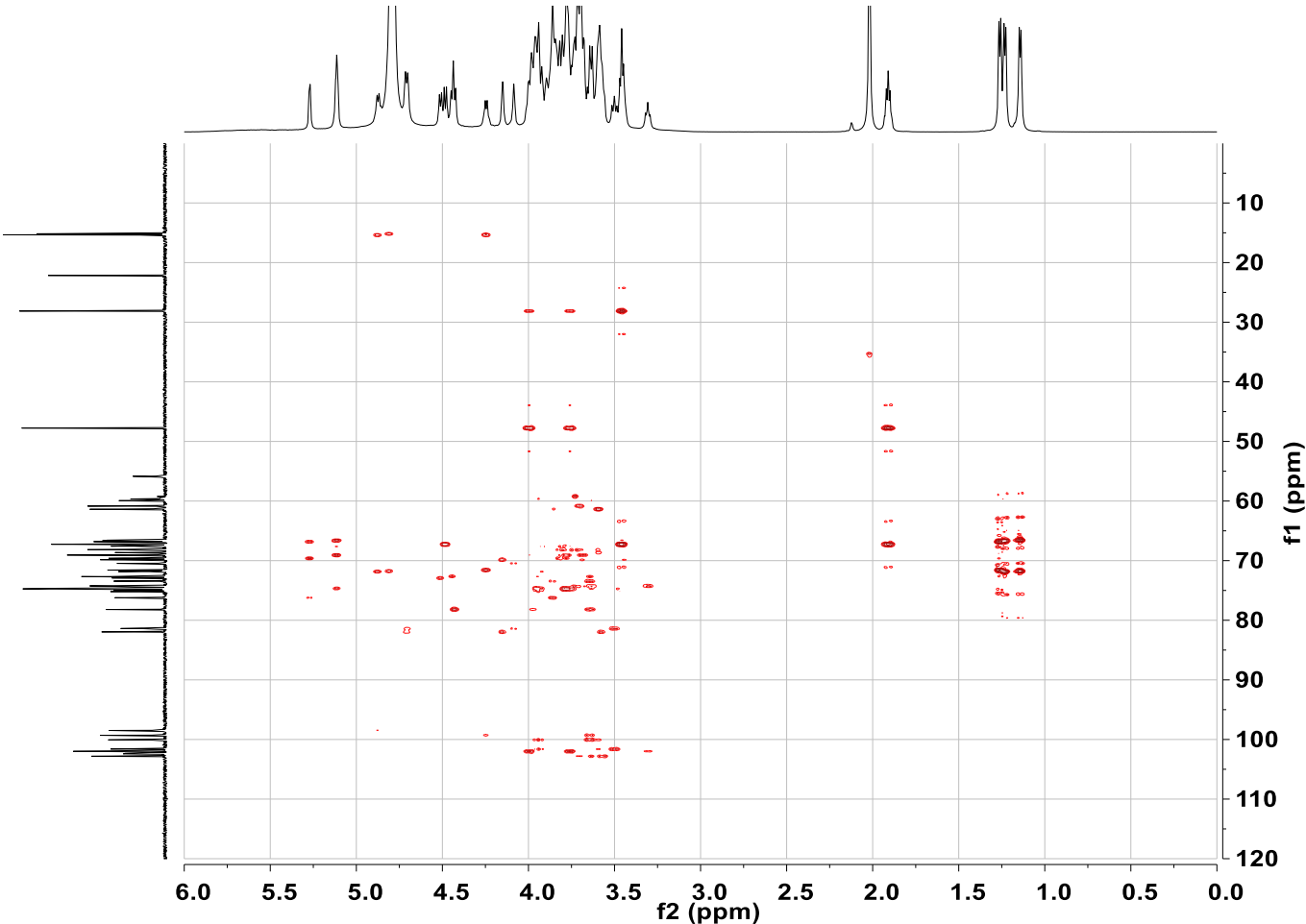
COSY NMR of compound 1



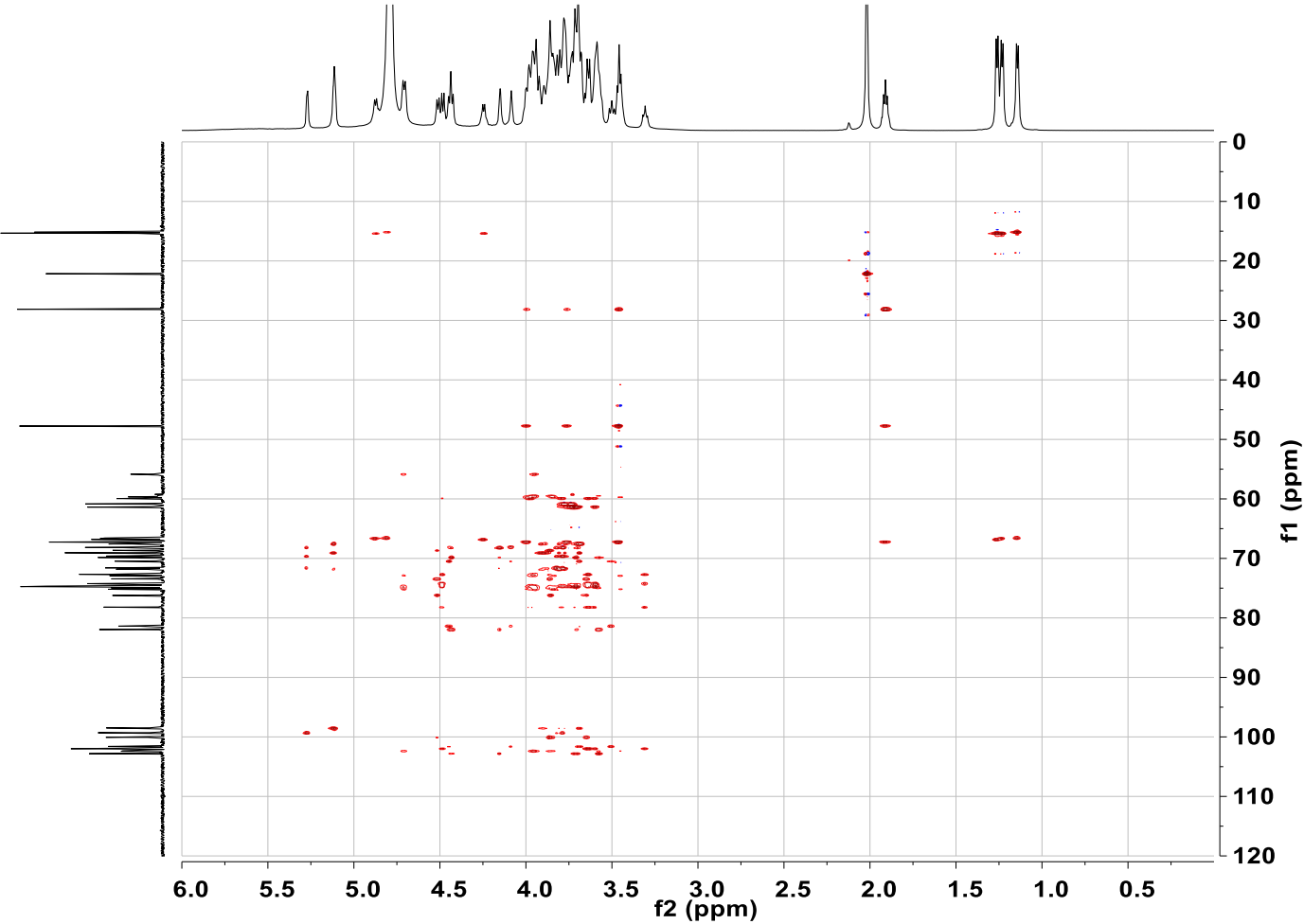
HSQC NMR of compound 1



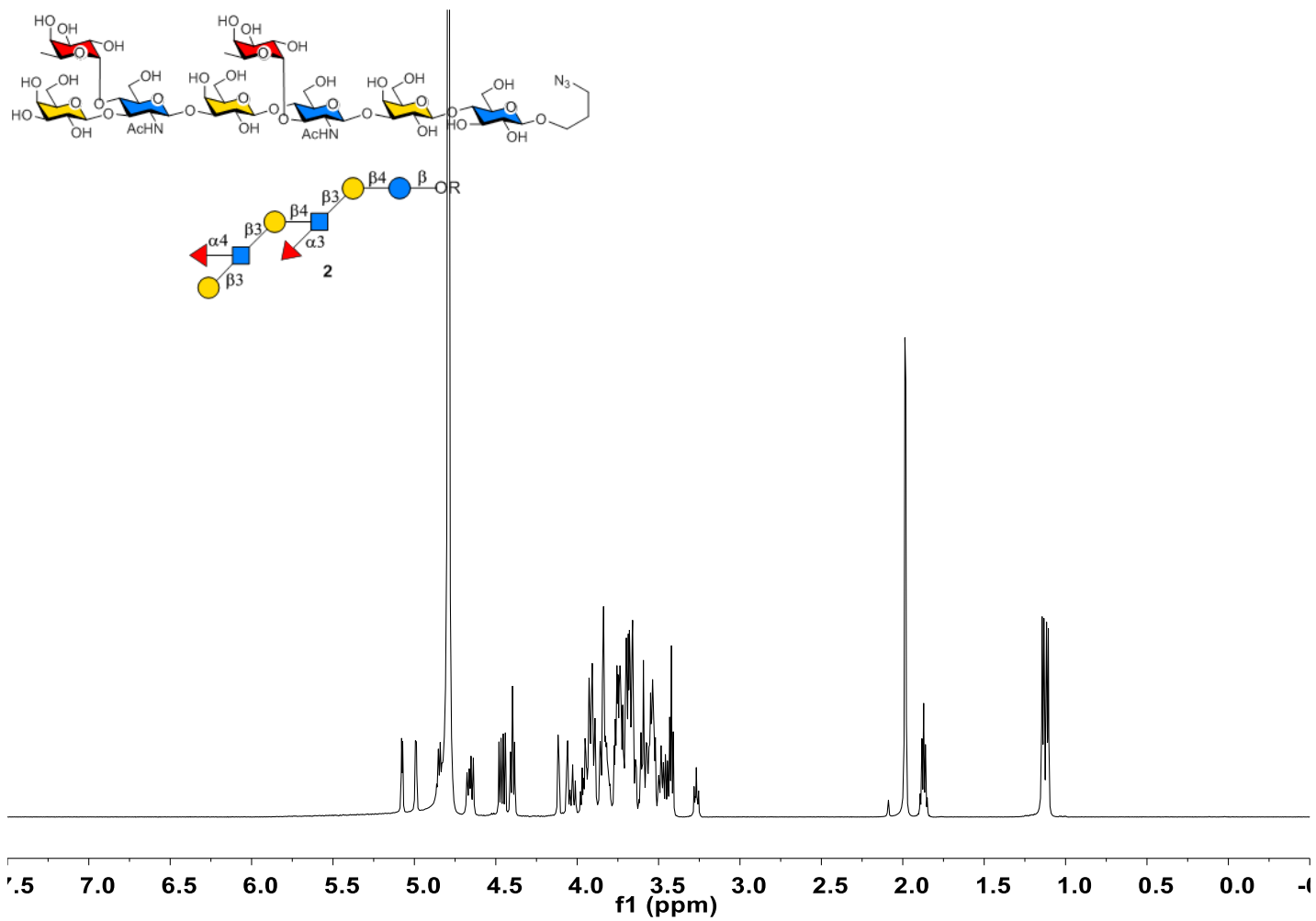
HMBC NMR of compound 1



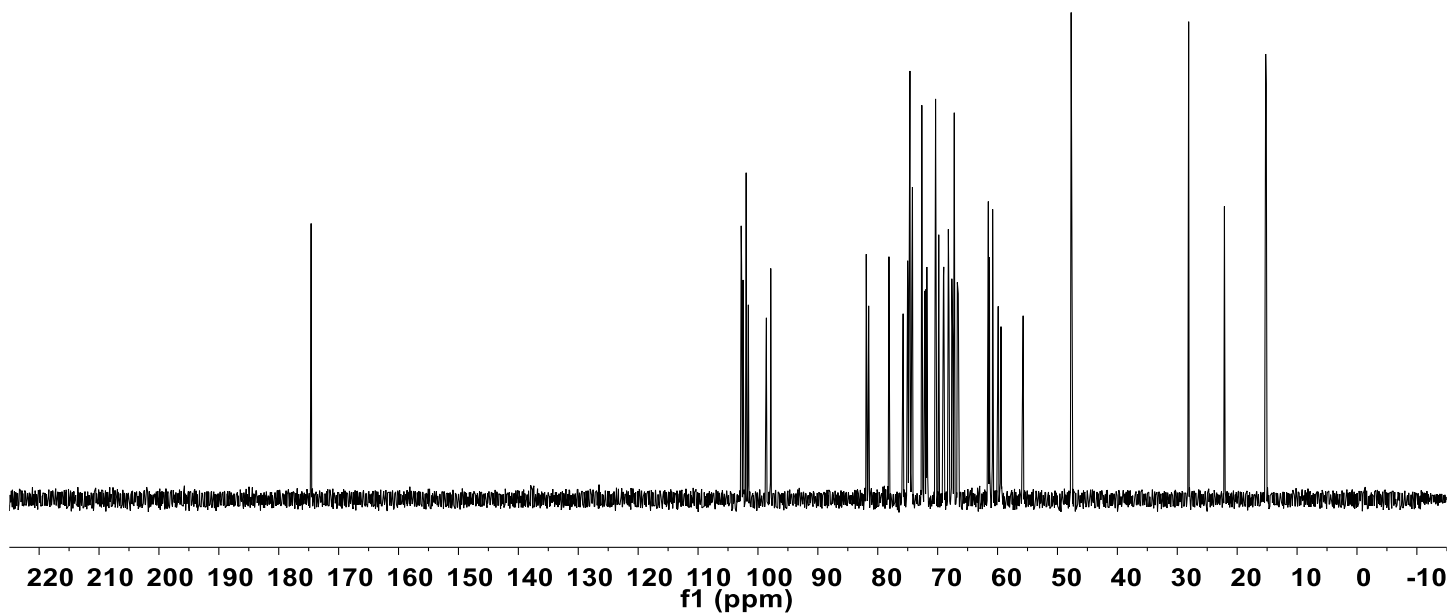
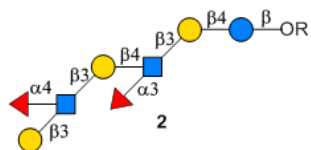
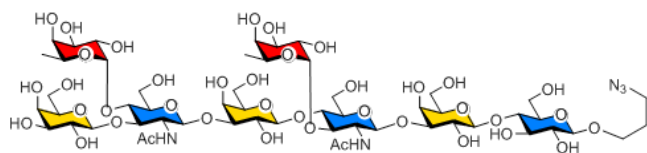
HSQC-TOCSY NMR of compound 1



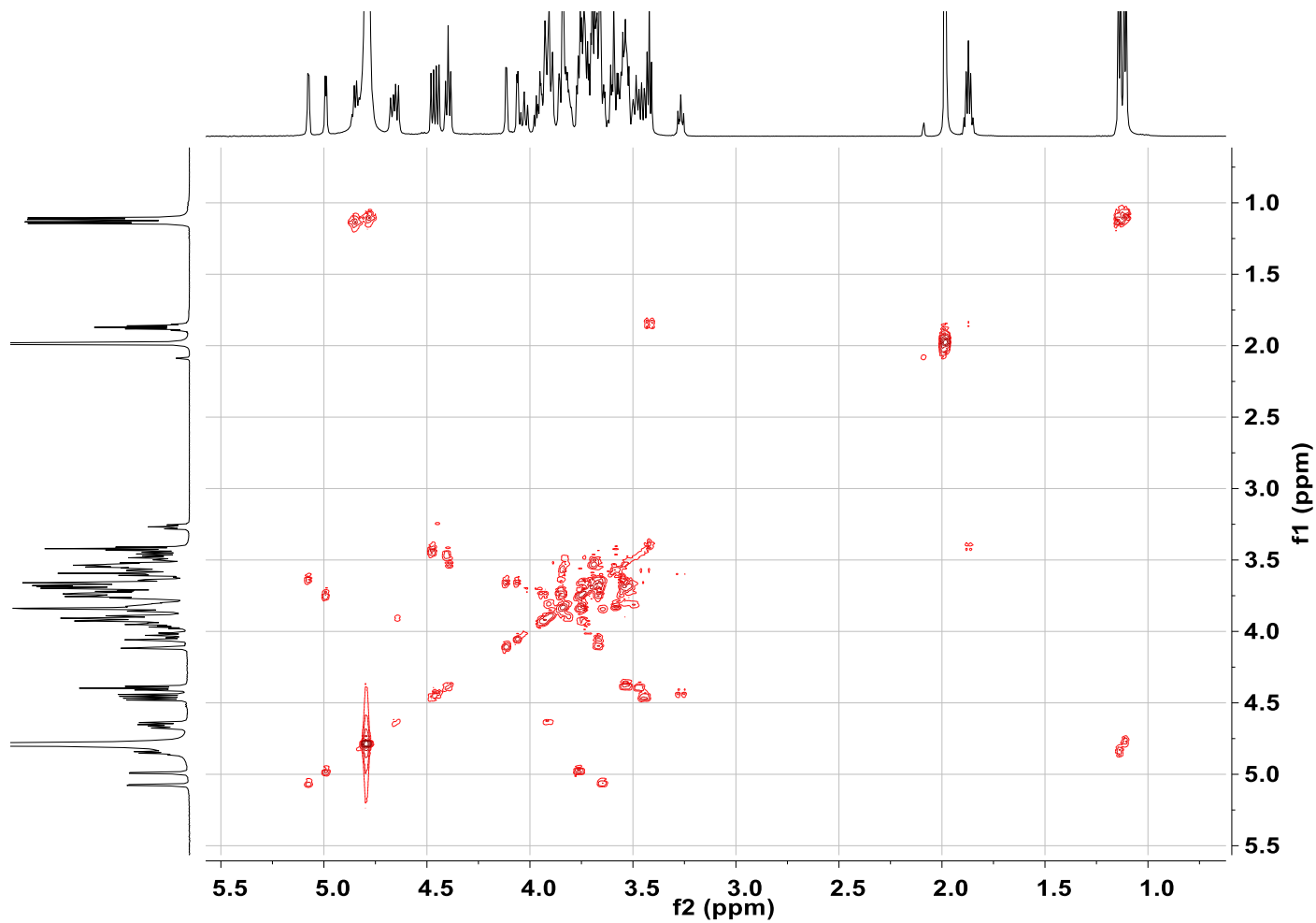
¹H NMR of compound 2



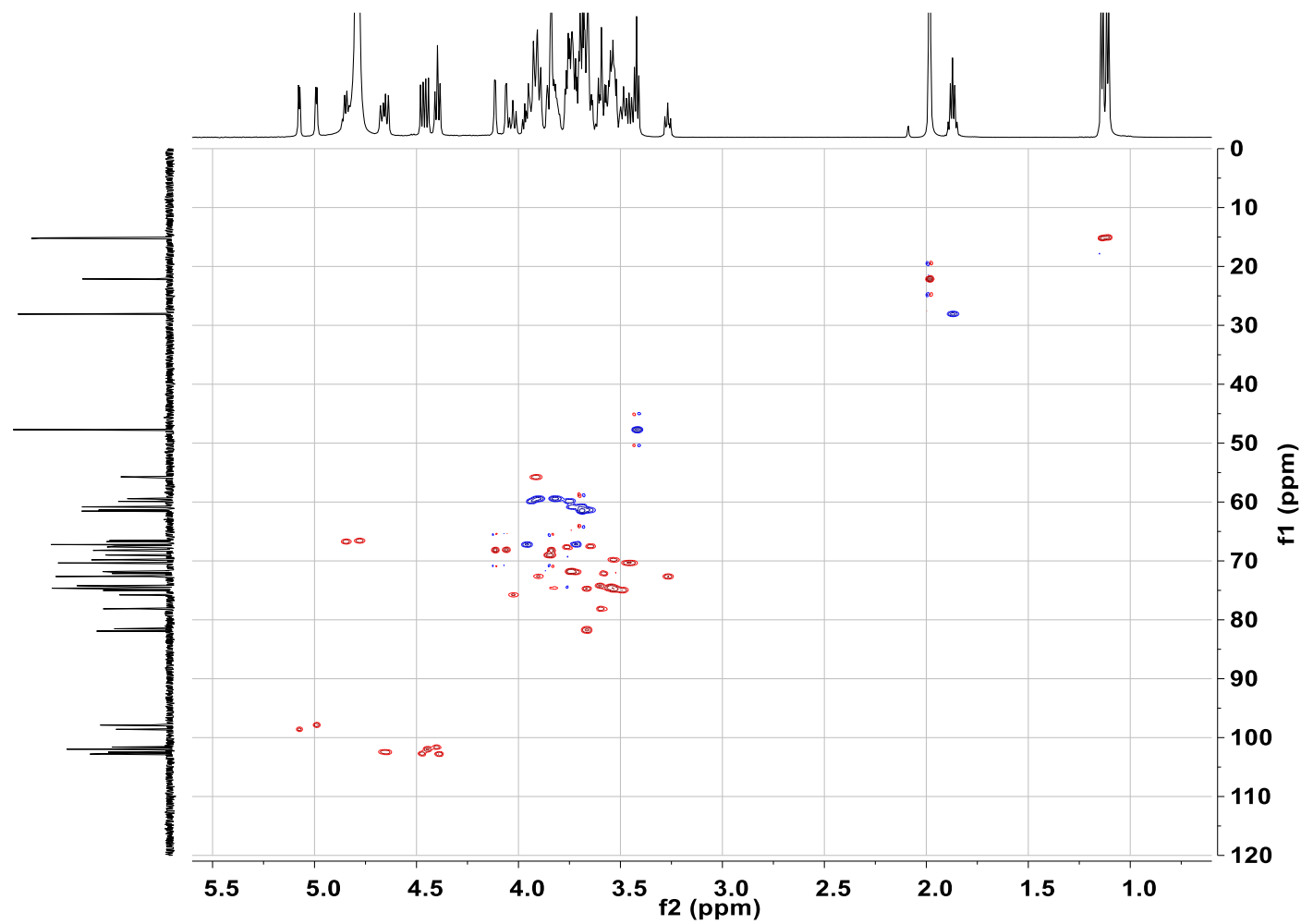
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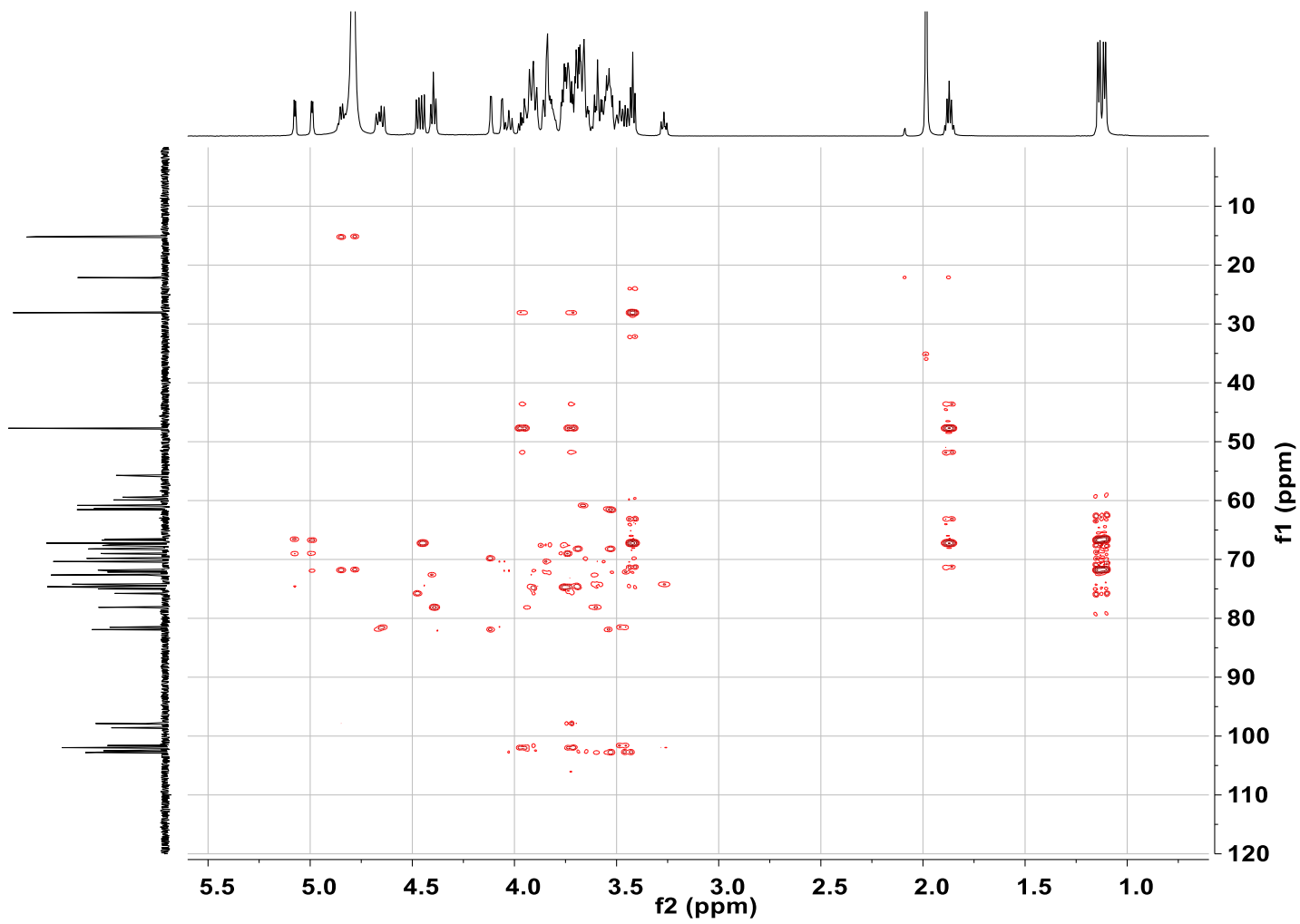
COSY NMR of compound 2



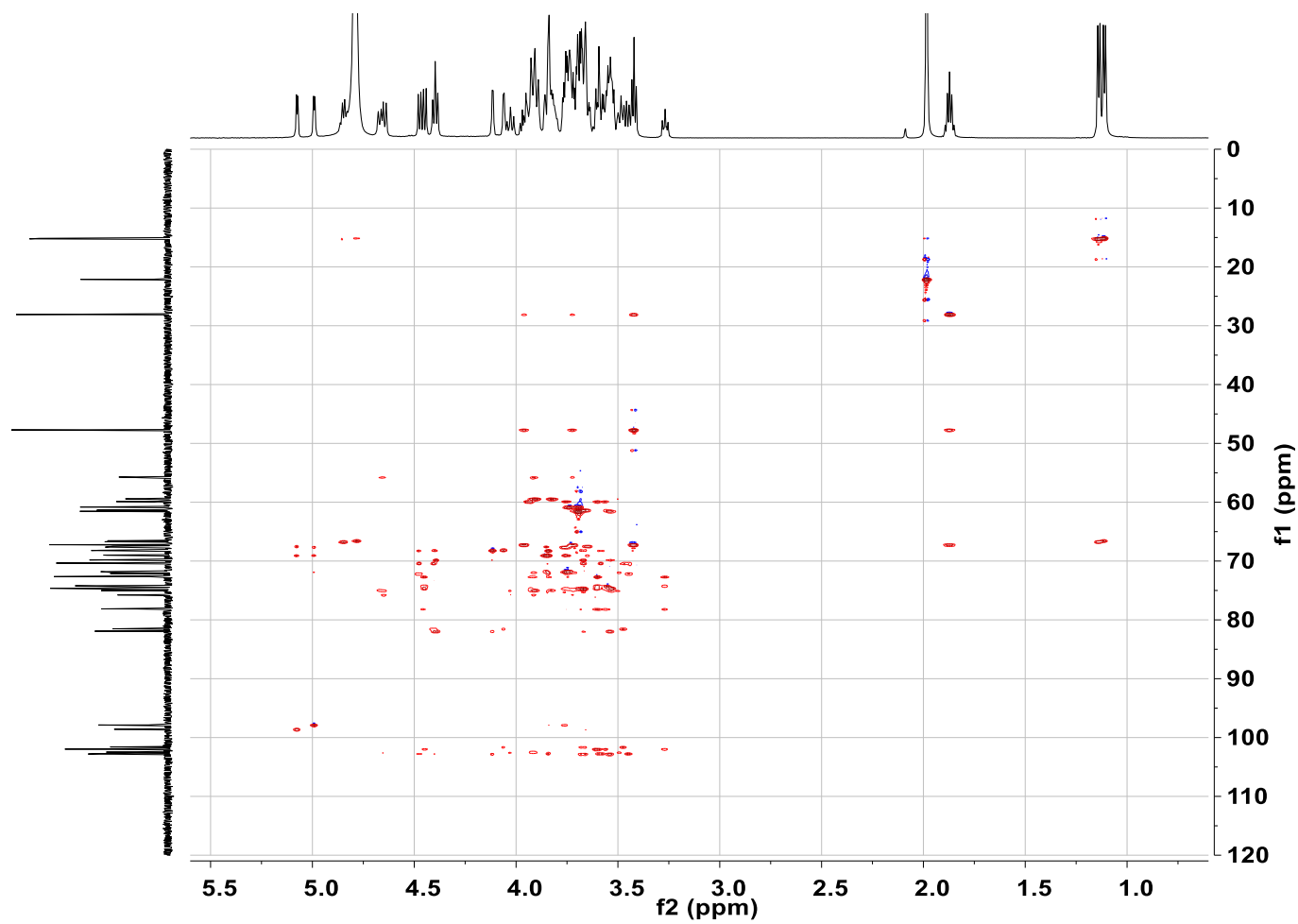
HSQC NMR of compound 2



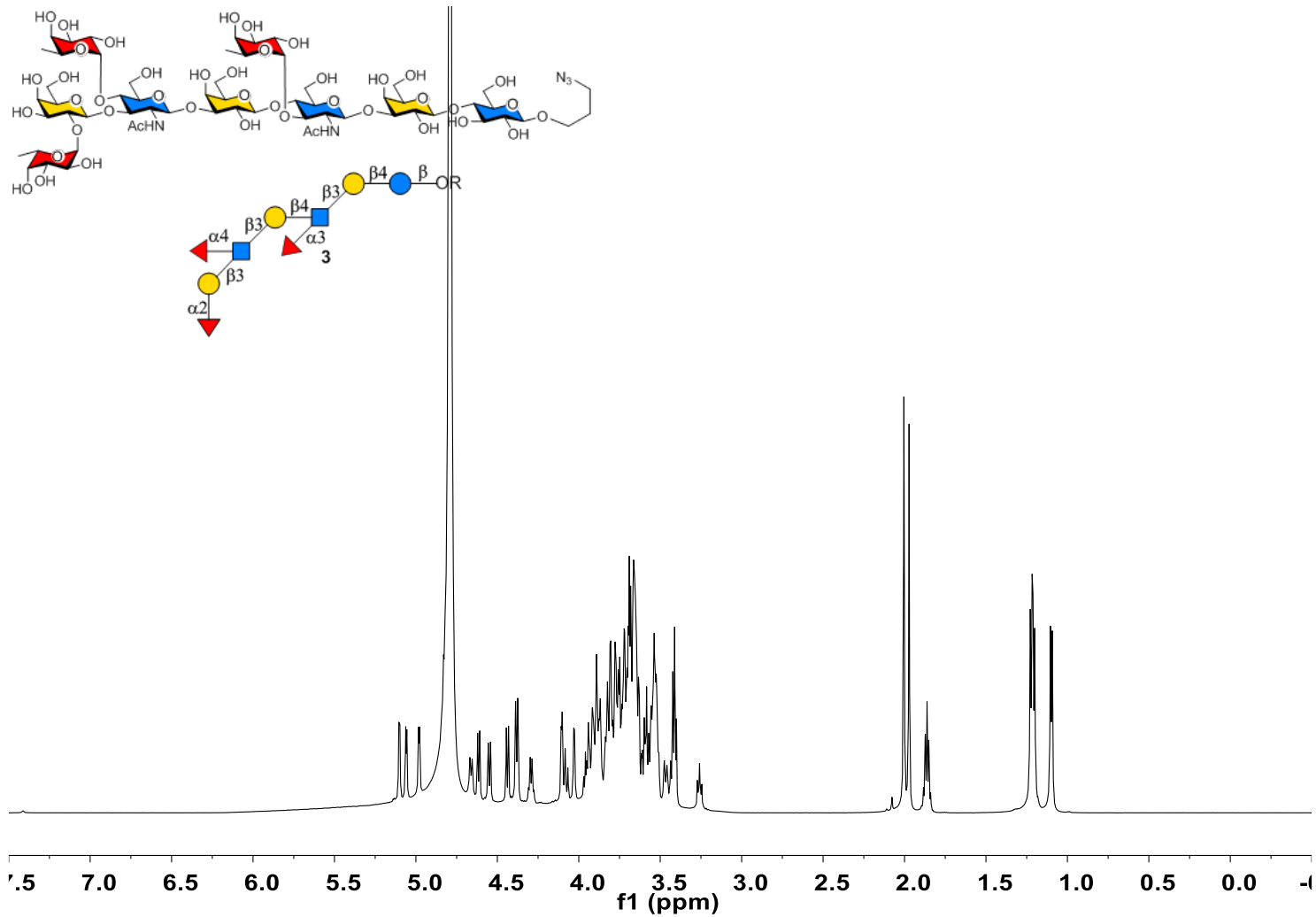
HMBC NMR of compound 2



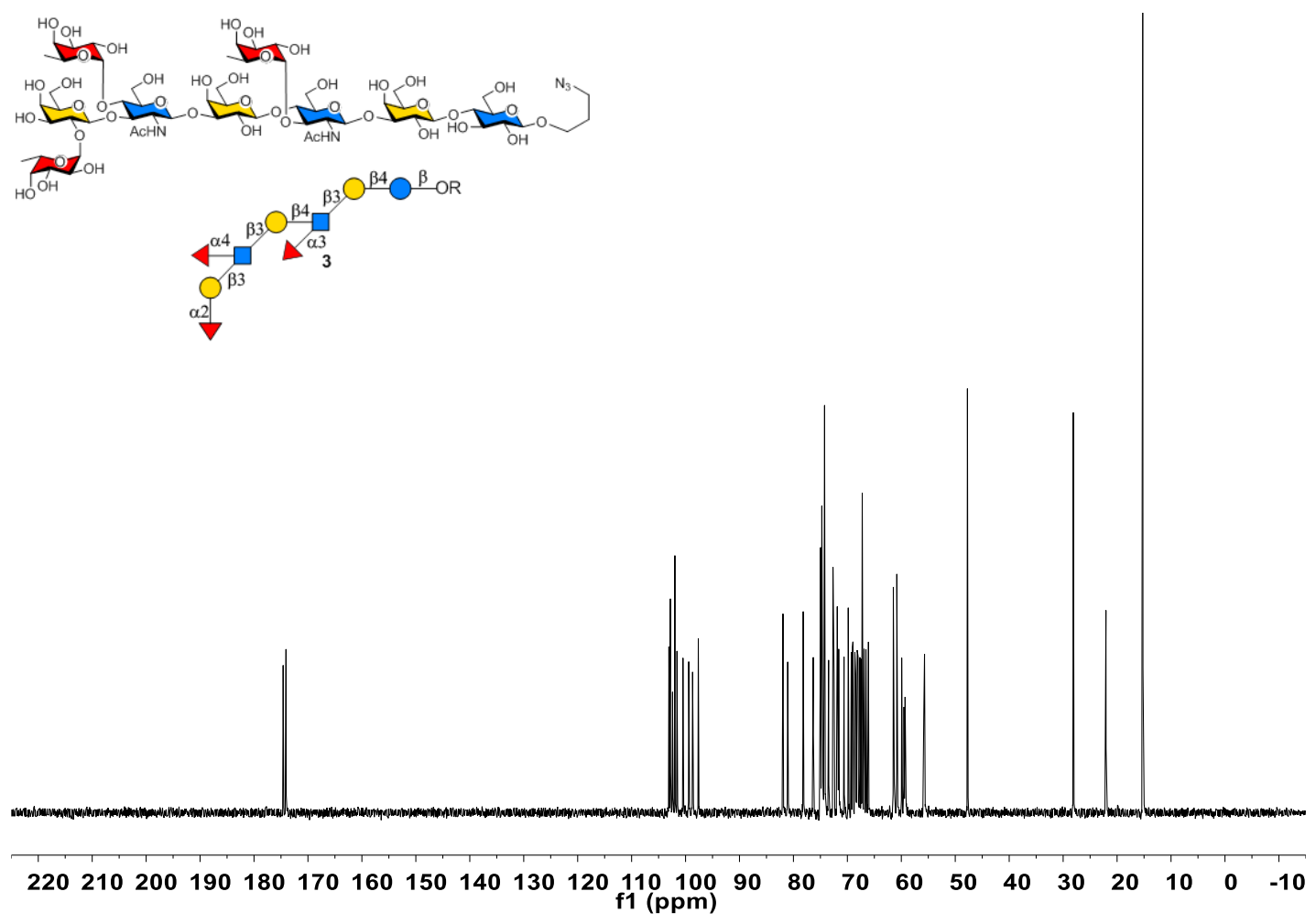
HSQC-TOCSY NMR of compound 2



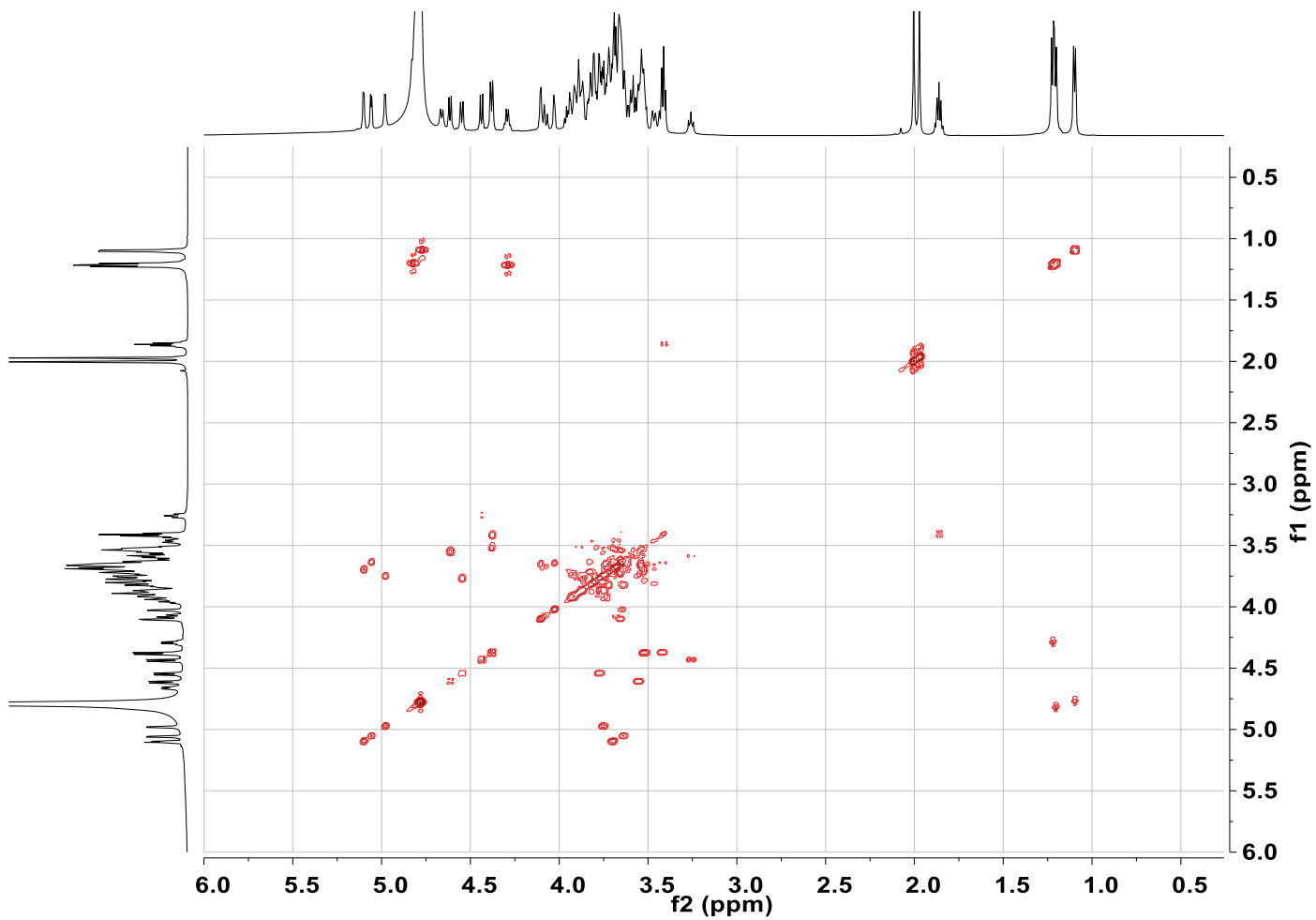
¹H NMR of compound 3



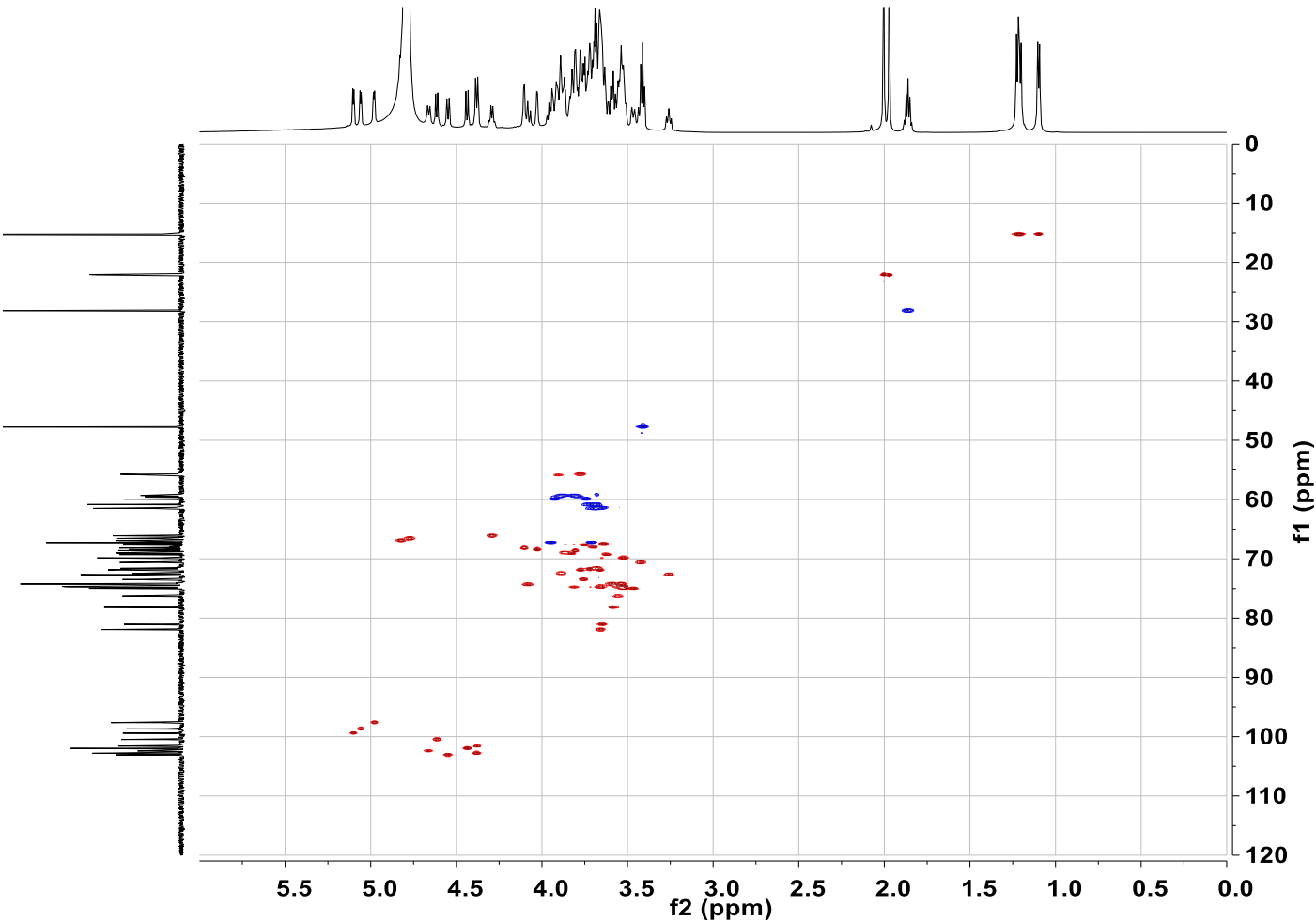
¹³C NMR of compound 3



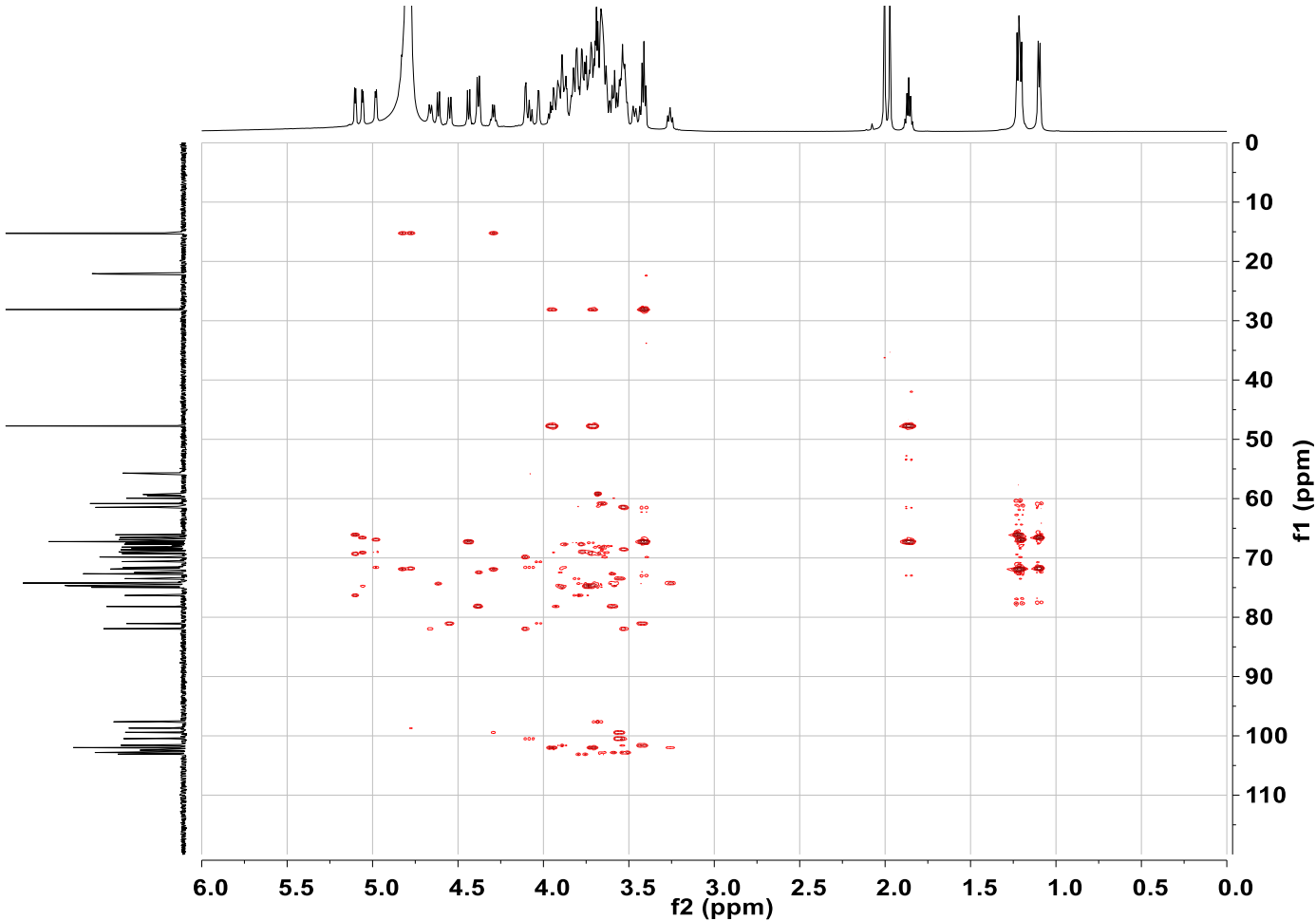
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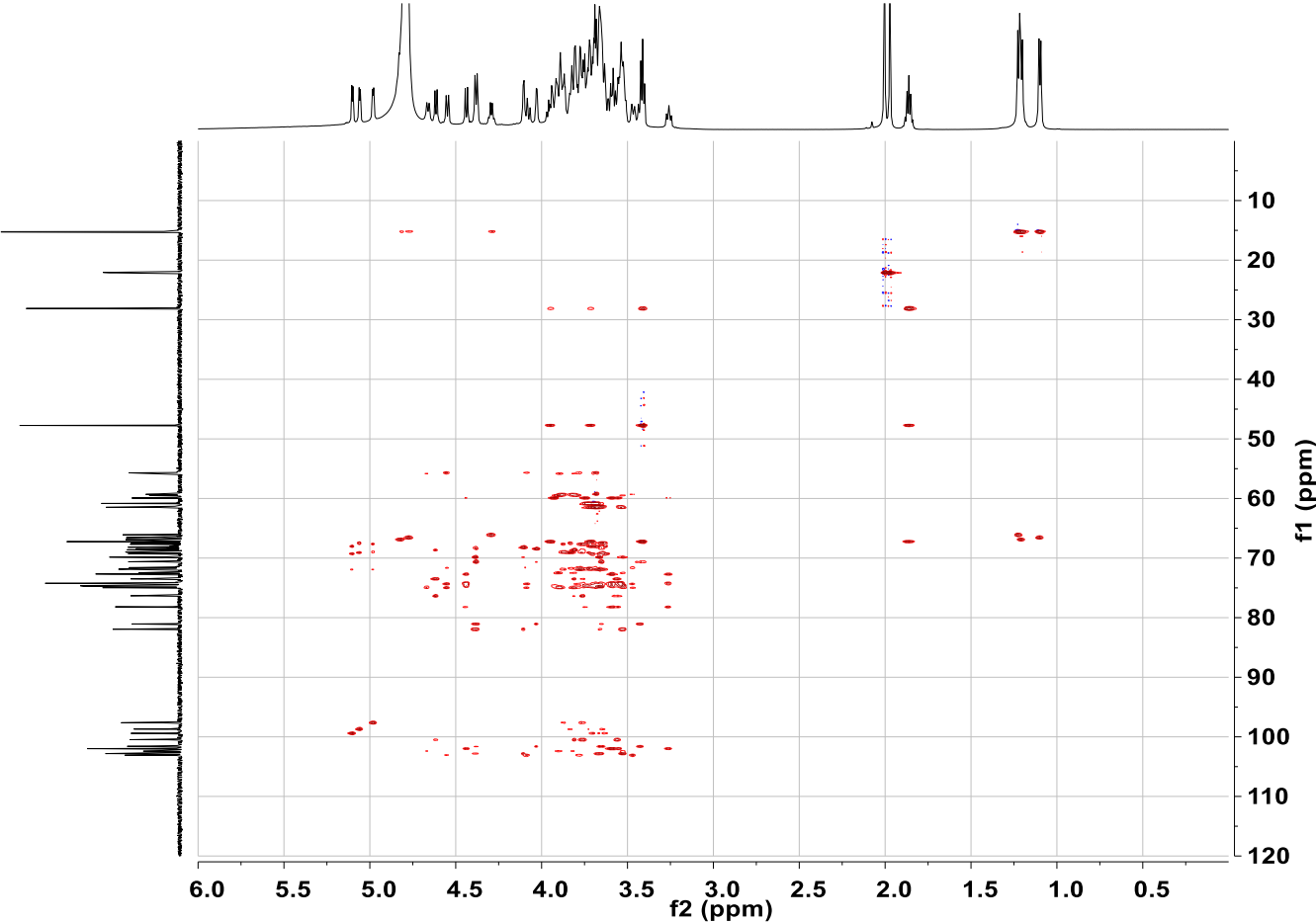
HSQC NMR of compound 3



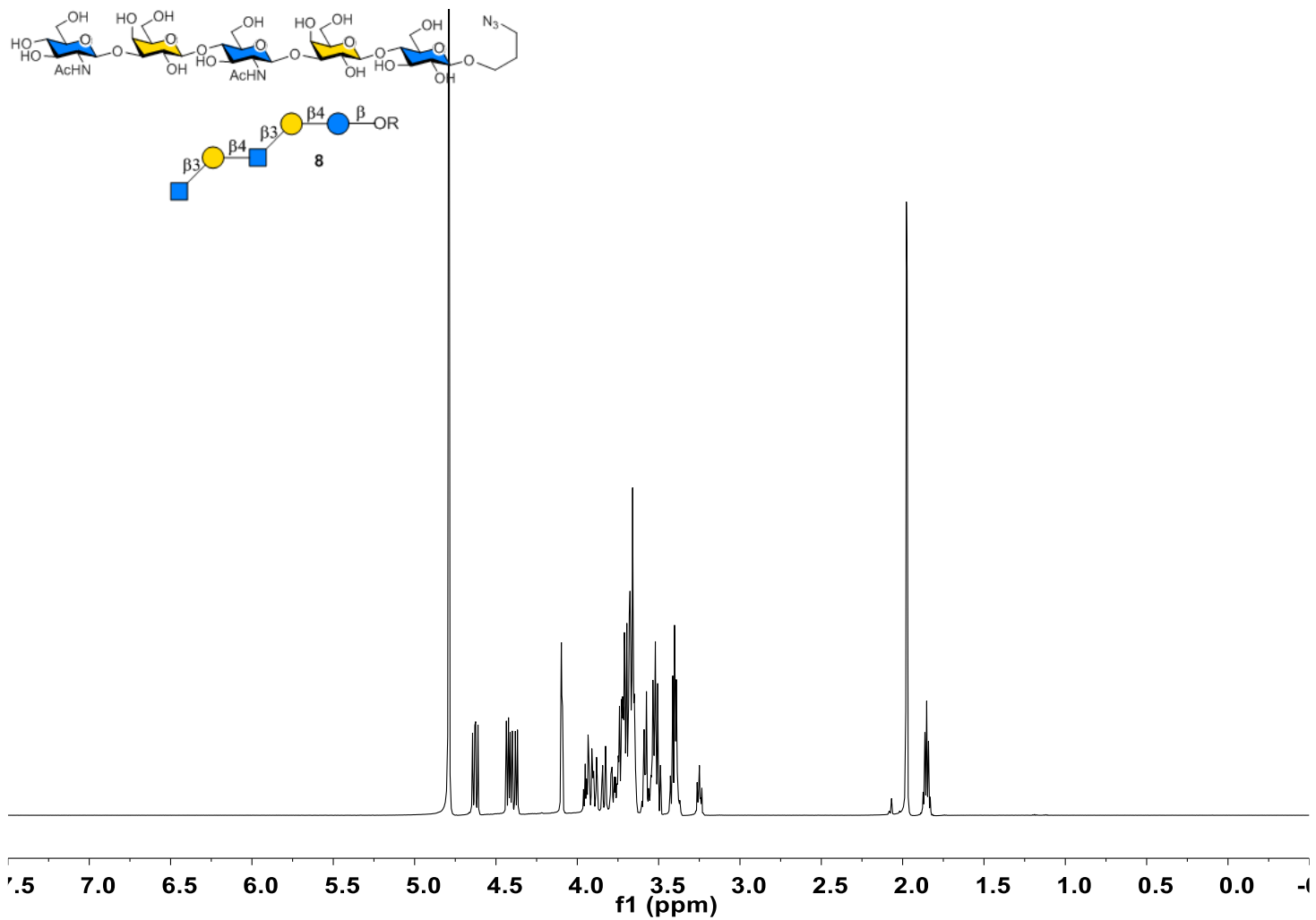
HMBC NMR of compound 3



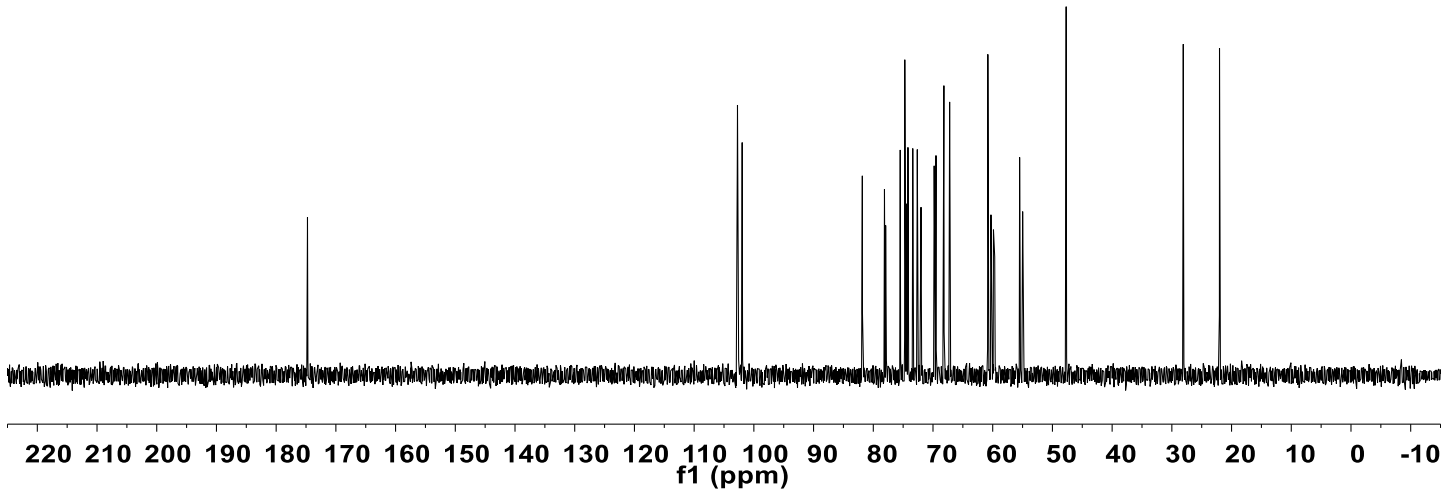
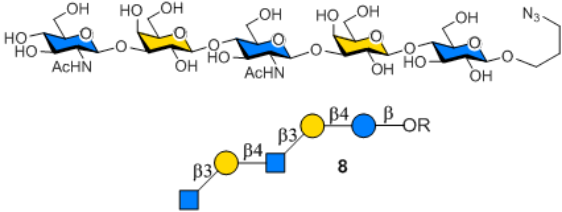
HSQC-TOCSY NMR of compound 3



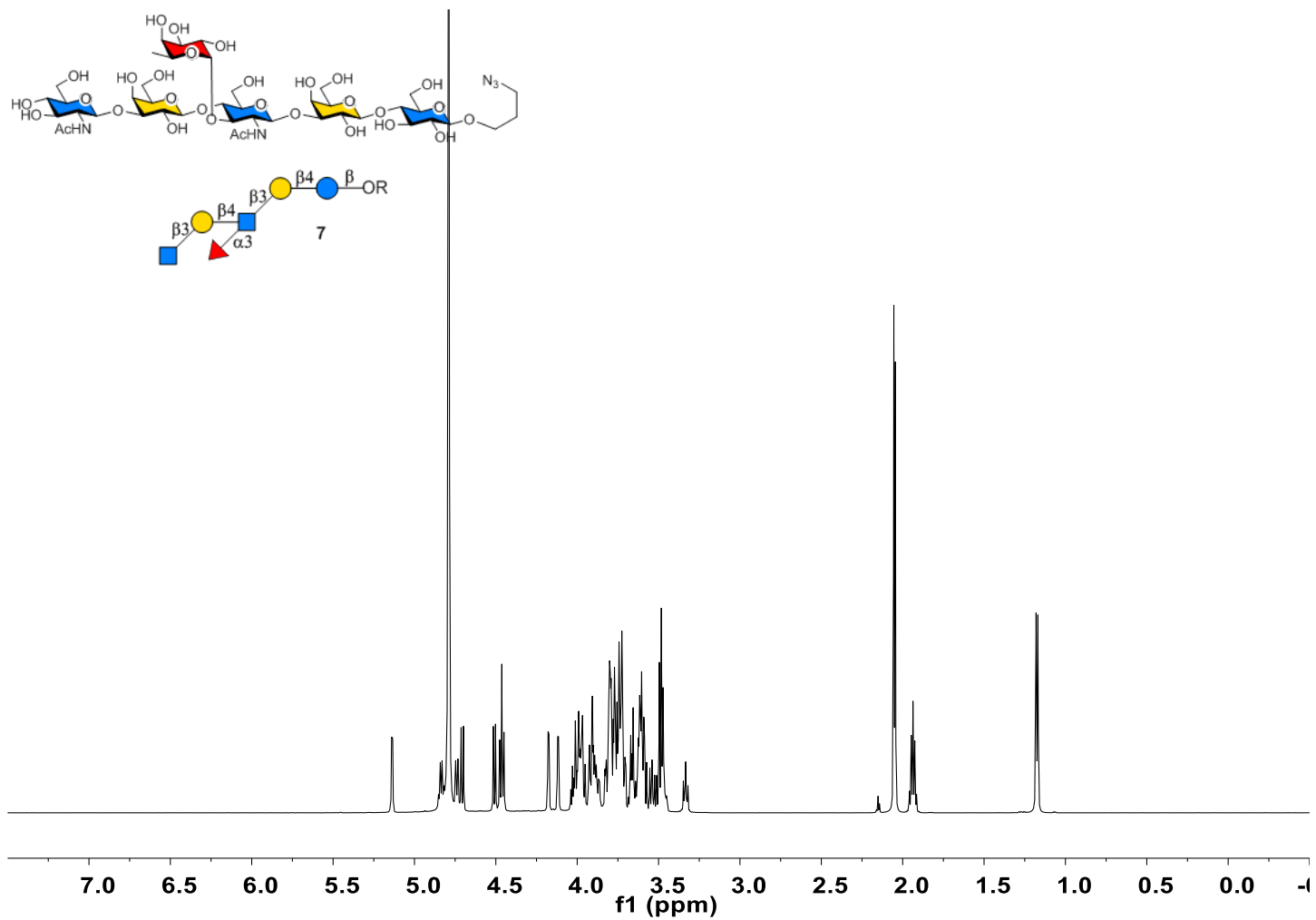
¹H NMR of compound 8



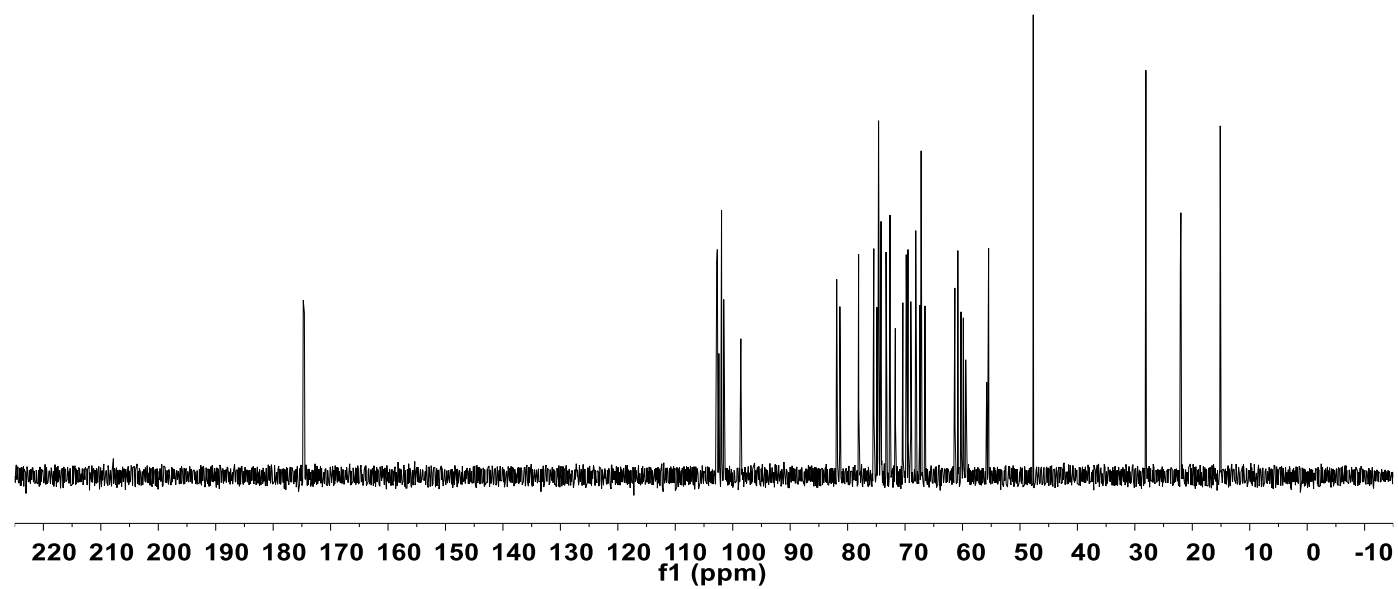
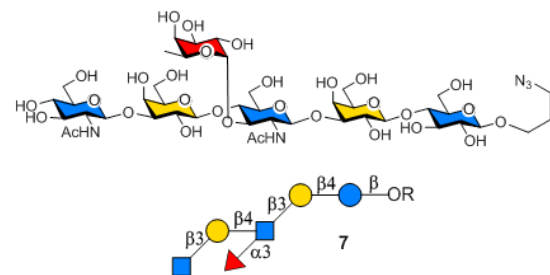
¹³C NMR of compound 8



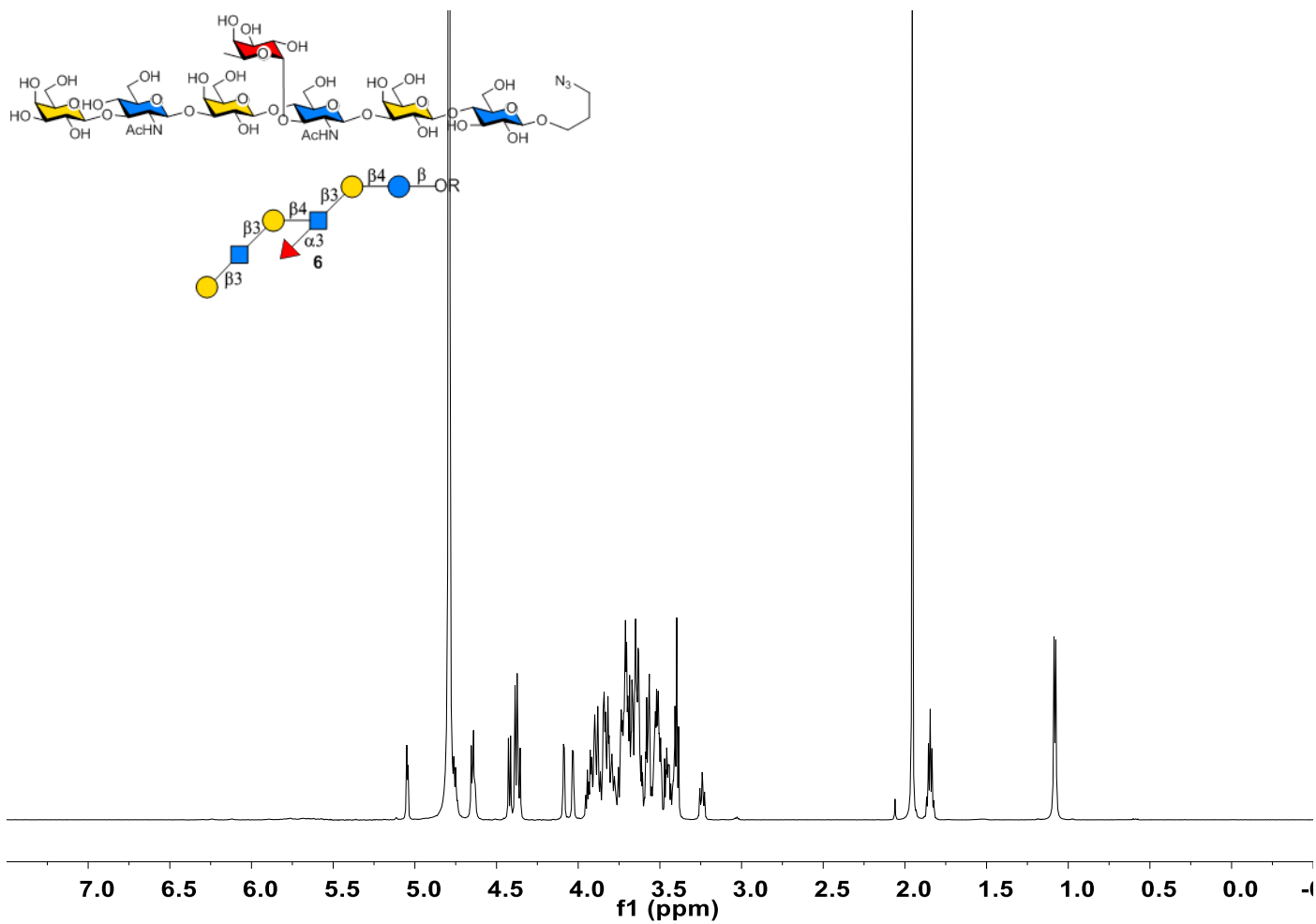
¹H NMR of compound 7



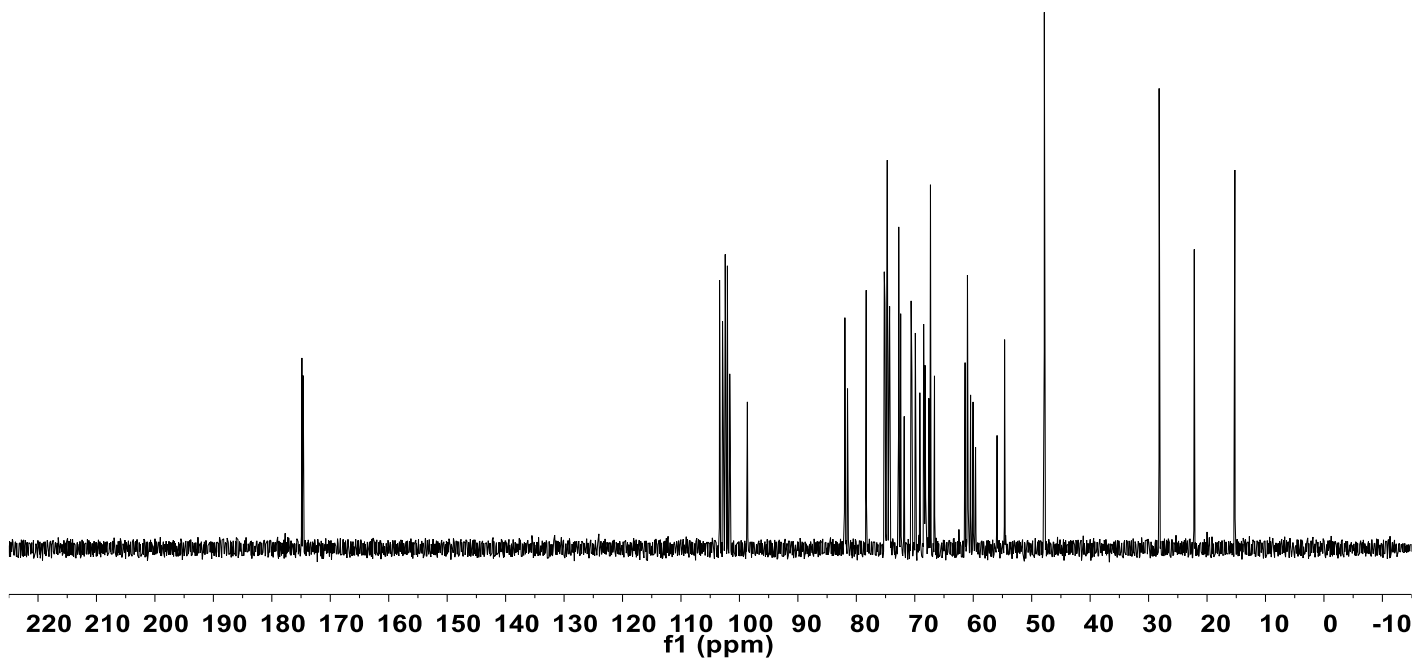
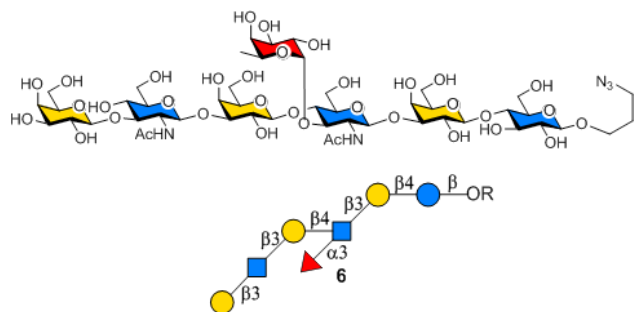
^{13}C NMR of compound 7



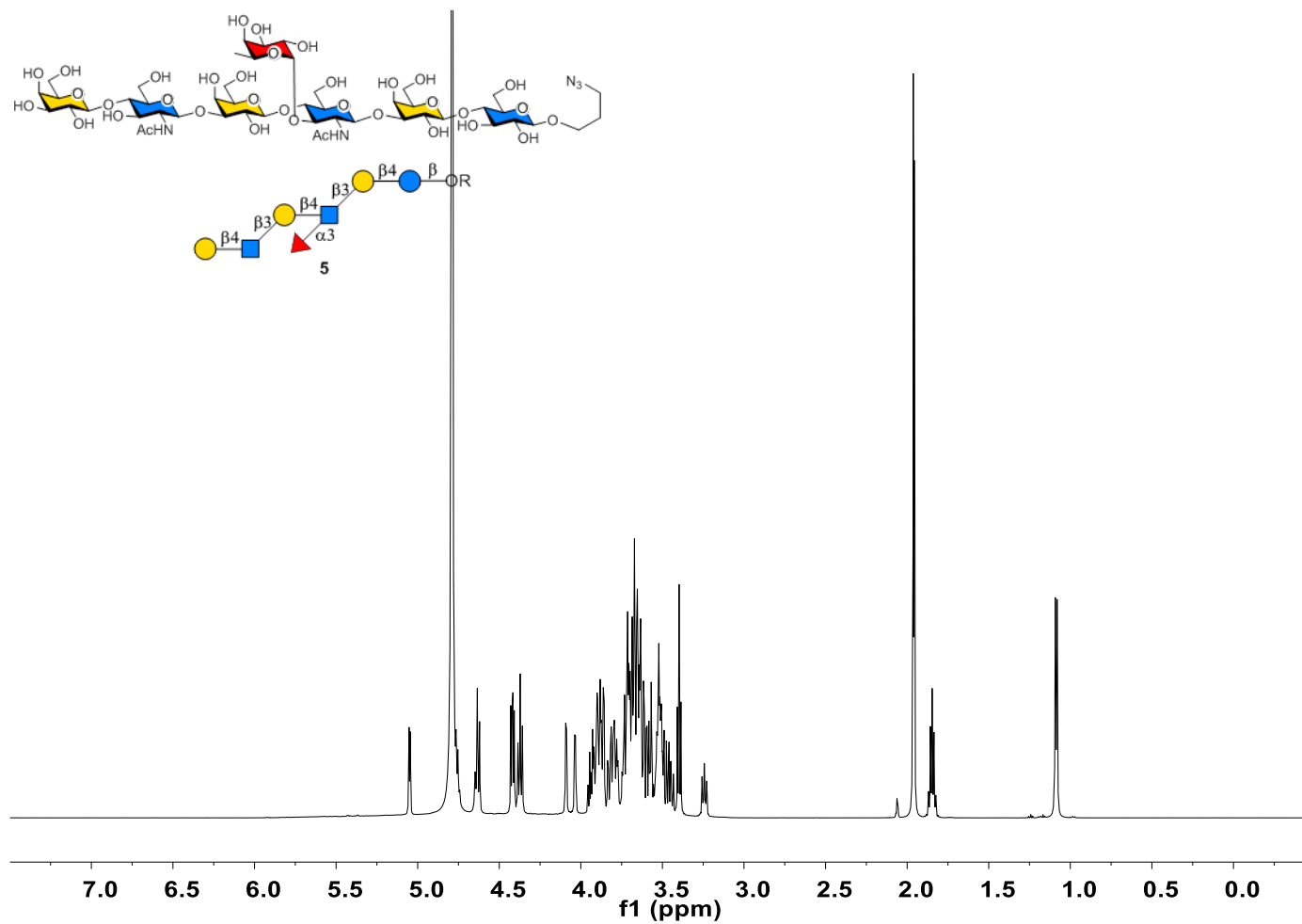
¹H NMR of compound 6



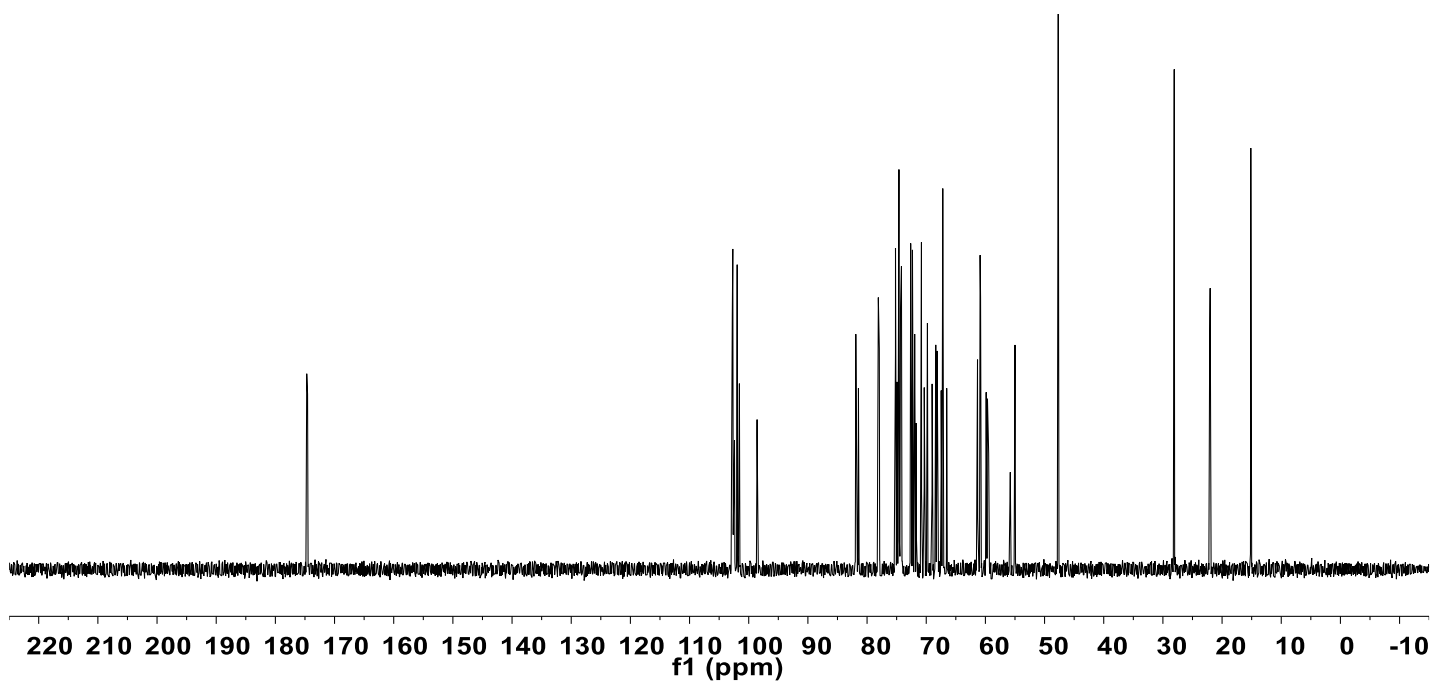
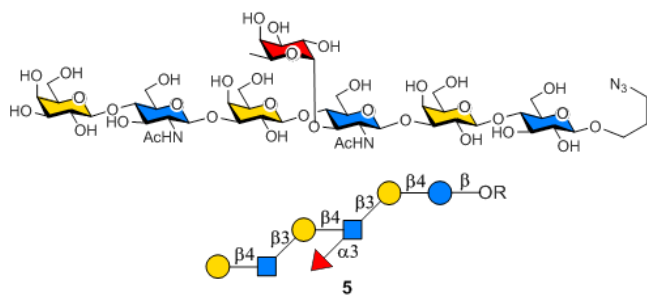
¹³C NMR of compound 6



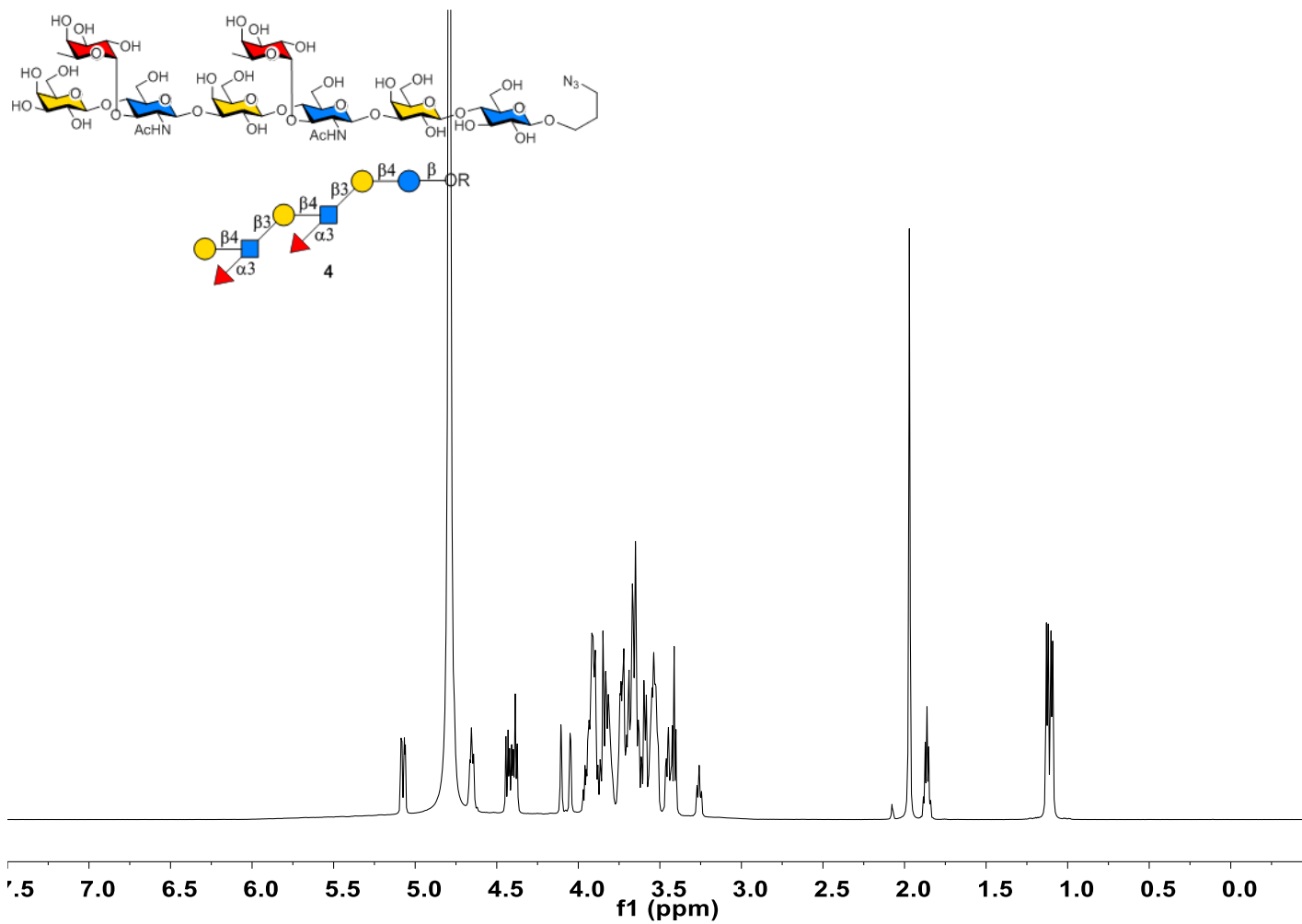
¹H NMR of compound 5



¹³C NMR of compound 5



¹H NMR of compound 4



^{13}C NMR of compound 4

