

Supplementary materials

Advanced settings	Observed chemical shifts in spin system ?	Examples
Offsets Specified values will be subtracted from 1H and 13C shifts provided in the search form. For experimental data that are referenced to DSS, profile DSS should be used. C offset: <input type="text" value="-1.8"/> H offset: <input type="text" value="0.0"/> Profile: <input type="text" value="Custom"/>	C1 101.63 — H1 4.447 0.0 C2 53.13 — H2 3.985 0.0 C3 71.589 — H3 3.698 0.0 C4 68.216 — H4 3.889 0.0 C5 75.851 — H5 3.564 0.0 C6 62.445 — H6 3.765 0.0 C7 0.0 — H7 0.0 0.0 C8 0.0 — H8 0.0 0.0 C9 0.0 — H9 0.0 0.0	α-L-Galp β-D-GlepNAc β-D-Quip3NAc
Number of matches Search domain Error measure		

Fig. S1. Typical search, using six C-H correlations that are found in a ^{13}C -HSQC, illustrated by a search with six C-H chemical shift pairs of GalNAc of LDNF trisaccharide. For the case of an CH_2 group a second ^1H chemical shift could be added next to the first one. However in this particular case only one of the two H6 chemical shifts is used and the second field is empty. Additional search options can be selected on the left, for example offsets and the number of matches

Top 73 matches out of 15525 database records (result generated in 60 ms.)

LinucsID	Residue	Linkage	Match																																																																																																																																																								
13039	β-D-GalpNAc	4,6	99,820																																																																																																																																																								
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Fig. S2. Typical results illustrated by a search with six C-H chemical shift pairs of GalNAc of LDNF trisaccharide. Highlighted is the score on the top right, and the different output lines with a description on the left.

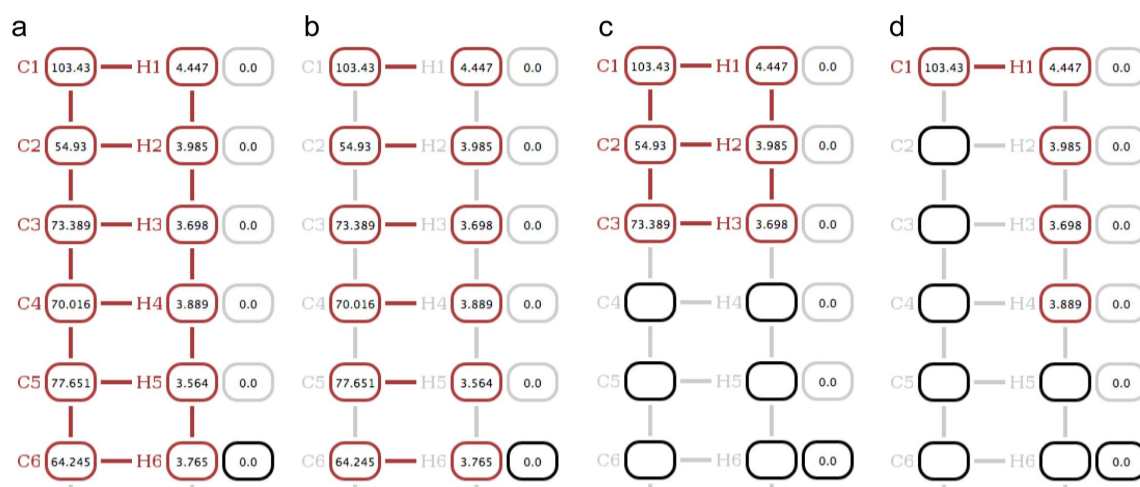


Fig. S3. Tested search patterns illustrated with the chemical shifts of GalNAc of the LDNF trisaccharide. a) Completely assigned spin system with chemical shifts for carbons C1 to C6 and the associated protons H1 to H6. H6 can be any of the two methylen protons (H61 and H62 or H6 and H6'). b) Six unassigned C-H chemical shift pairs. c) Partially assigned spin system with chemical shifts for carbons C1 to C3 and the associated protons H1 to H3. d) C1-H1 chemical shift pair together with proton resonances correlating with H1 in a 2D TOCSY.

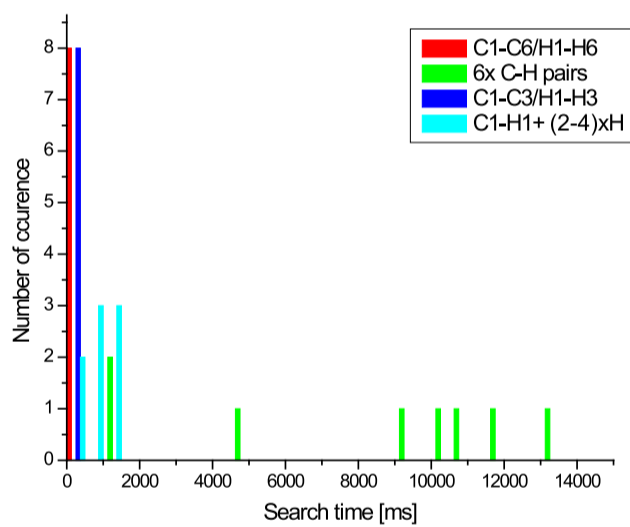


Fig. S4. Search times of the different strategies illustrated with the 32 test searches of Figure 3.

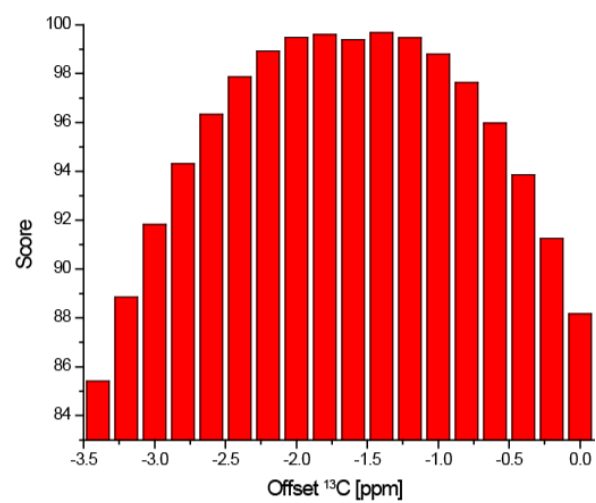


Fig. S5. Offset dependency of the ^{13}C chemical shifts illustrated with a search of the chemical shifts of Fuc within Bv9 (C1 to C6 and H1 to H6). An offset of -1.8 ppm means, that 1.8 ppm needs to be subtracted from the experimental values in order to fit to the database.

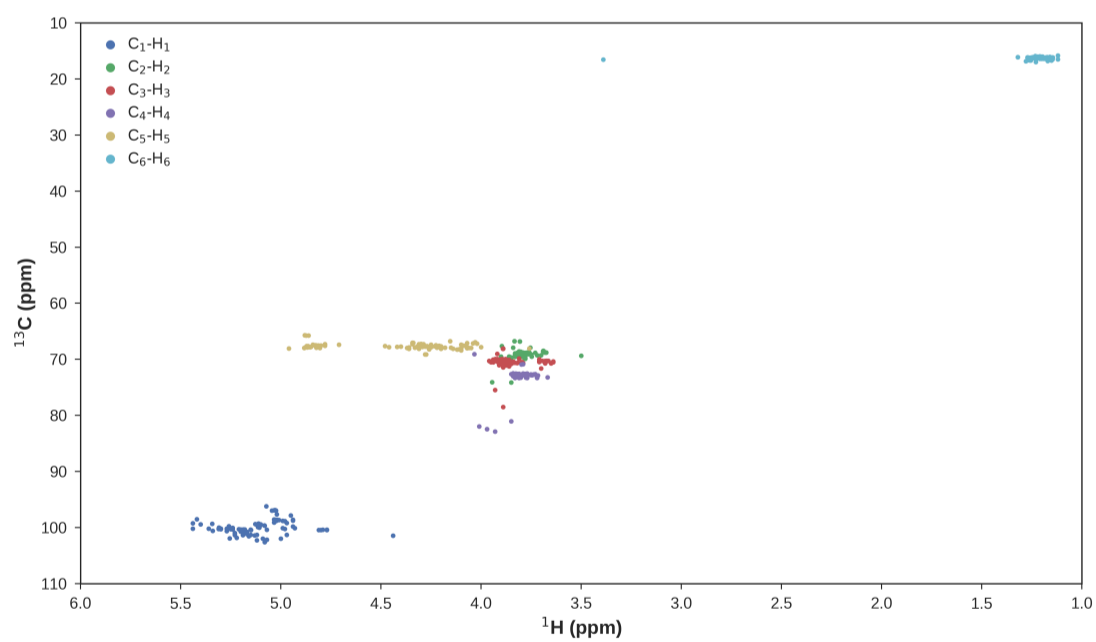


Fig. S6. Visualization of C-H chemical shift pairs of α -L Fuc pyranoses in the glycosciences.de database.

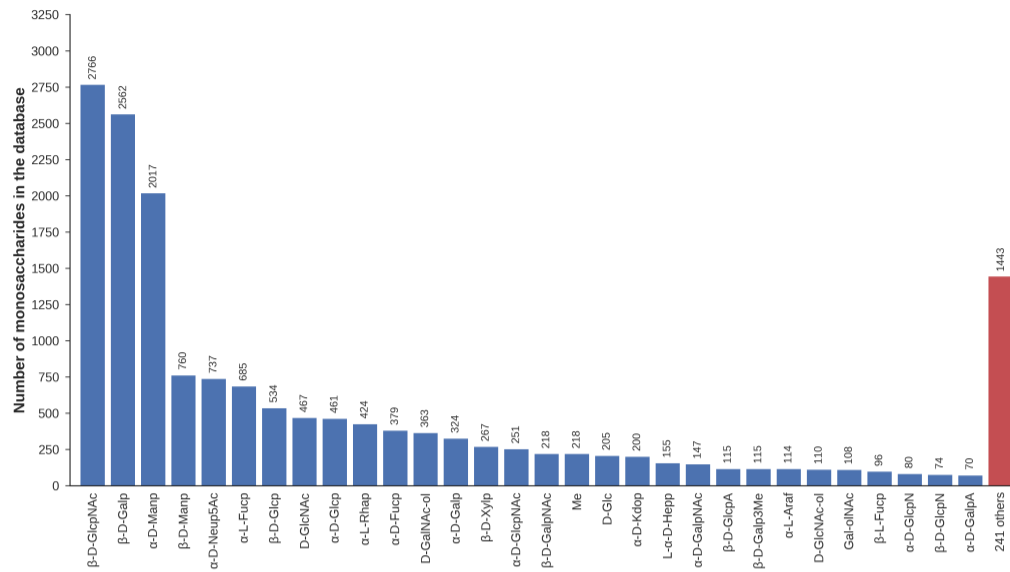


Fig. S7. Most frequent types of monosaccharides in the glycosciences.de database

Top 134 matches out of 16465 database records (result generated in 683 ms.)

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2690	α-D-Neup5Ac	3,4,6,3	99,973																																																																																																																																																
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Error	-	-	0,000	0,000	0,006	0,002	0,010	-	-	-	-	0,011	-	-	-	-	-	-	-	-	-	0,030	-	-	-	-	-	-																																																																																																																							
26396	α-D-NeupAc	4, 6, 4, 3	99,896																																																																																																																																																
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Query	-	-	1,800	3,700	3,840	3,640	3,610	-	-	-	-	2,780	-	-	-	-	-	-	-	-	-	40,700	-	-	-	-	-	-																																																																																																																							
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527	α-D-Neup5Ac	3,3,3,4	99,839																																																																																																																																																
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Sugar	-	-	1,783	3,702	3,834	3,665	3,590	3,875	3,660	-	-	2,760	-	-	-	-	-	-	3,820	174,630	100,470	40,610	69,160	52,510	73,620	68,890	72,640	63,310																																																																																																																							
Query	-	-	1,800	3,700	3,840	-	3,610	-	3,640	-	-	2,780	-	-	-	-	-	-	-	-	-	40,700	-	-	-	-	-	-																																																																																																																							
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2838	α-D-Neup5Ac	3,3,4	99,838																																																																																																																																																
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Sugar	-	-	1,801	3,680	3,850	3,630	3,590	3,880	3,640	-	-	2,762	-	-	-	-	-	-	3,870	174,600	100,200	40,500	69,200	52,500	73,700	68,900	72,600	63,400																																																																																																																							
Query	-	-	1,800	3,700	3,840	3,610	-	-	3,640	-	-	2,780	-	-	-	-	-	-	-	-	-	40,700	-	-	-	-	-	-																																																																																																																							
Error	-	-	0,001	0,020	0,010	0,020	-	-	0,000	-	-	0,018	-	-	-	-	-	-	-	-	-	0,200	-	-	-	-	-	-																																																																																																																							

Fig. S8. Top 4 results for the first sialic acid spin system observed in a commercial human serum albumin sample.

Top 128 matches out of 16465 database records (result generated in 1224 ms.)

LinusID	Residue	Linkage	Match
<u>2836</u>	α -D-Neup5Ac	6,4,6,4	99,736
	H	H'	C
ID	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9
Sugar	- - 1,712 3,660 3,790 3,710 3,560 3,890 -	- - 2,669 - - - - -	174,100 - 40,900 69,000 52,700 73,400 69,200 72,500 63,500
Query	- - 1,710 3,670 3,790 3,690 3,590 3,870 -	- - 2,690 - - - - -	- - 41,100 - - - - -
Error	- - 0,002 0,010 0,000 0,020 0,030 0,020 -	- - 0,021 - - - - -	- - 0,200 - - - - -
LinusID	Residue	Linkage	Match
<u>529</u>	α -D-Neup5Ac	6,4,3,4	99,732
	H	H'	C
ID	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9
Sugar	- - 1,713 3,666 3,810 3,670 3,560 3,870 3,670	- - 2,668 - - - - 3,860	174,260 100,940 40,880 68,980 52,710 73,230 69,210 72,510 63,480
Query	- - 1,710 - 3,790 3,670 3,590 3,870 3,690	- - 2,690 - - - - -	- - 41,100 - - - - -
Error	- - 0,003 - 0,020 0,000 0,030 0,000 0,020	- - 0,022 - - - - -	- - 0,220 - - - - -
LinusID	Residue	Linkage	Match
<u>2839</u>	α -D-Neup5Ac	6,4,6,4	99,691
	H	H'	C
ID	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9
Sugar	- - 1,712 3,650 3,790 3,700 3,550 3,880 3,640	- - 2,668 - - - - 3,880	174,100 - 40,900 69,100 52,700 73,400 69,300 72,600 63,500
Query	- - 1,710 3,670 3,790 3,690 3,590 3,870 -	- - 2,690 - - - - -	- - 41,100 - - - - -
Error	- - 0,002 0,020 0,000 0,010 0,040 0,010 -	- - 0,022 - - - - -	- - 0,200 - - - - -
LinusID	Residue	Linkage	Match
<u>1166</u>	α -D-Neup5Ac	6,3,4	99,536
	H	H'	C
ID	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9	1 2 3 4 5 6 7 8 9
Sugar	- - 1,685 3,680 3,816 3,680 3,590 3,880 3,750	- - 2,741 - - - - 3,820	174,200 101,010 40,890 69,080 52,700 73,300 69,080 72,500 63,420
Query	- - 1,710 3,670 3,790 3,690 3,590 3,870 -	- - 2,690 - - - - -	- - 41,100 - - - - -
Error	- - 0,025 0,010 0,026 0,010 0,000 0,010 -	- - 0,051 - - - - -	- - 0,210 - - - - -

Fig. S9. Top 4 results for the second sialic acid spin system observed in a commercial human serum albumin sample.