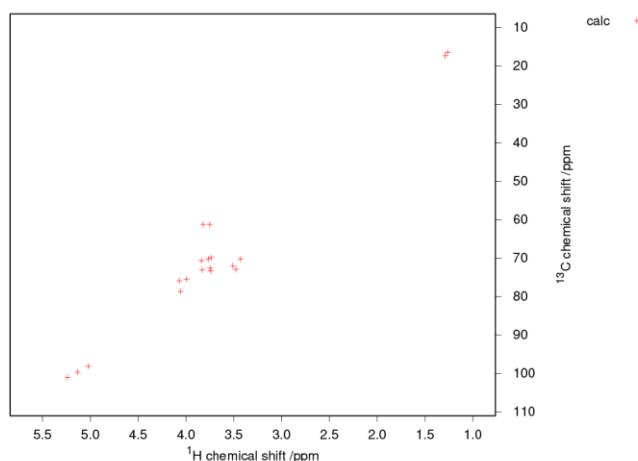


Additional file 6 NMR chemical shift prediction of the repeating unit structure of *S. uberis* RPS

CASPER report

Streptococcus uberis RPS branched



Predicted ^{13}C and ^1H NMR chemical shifts

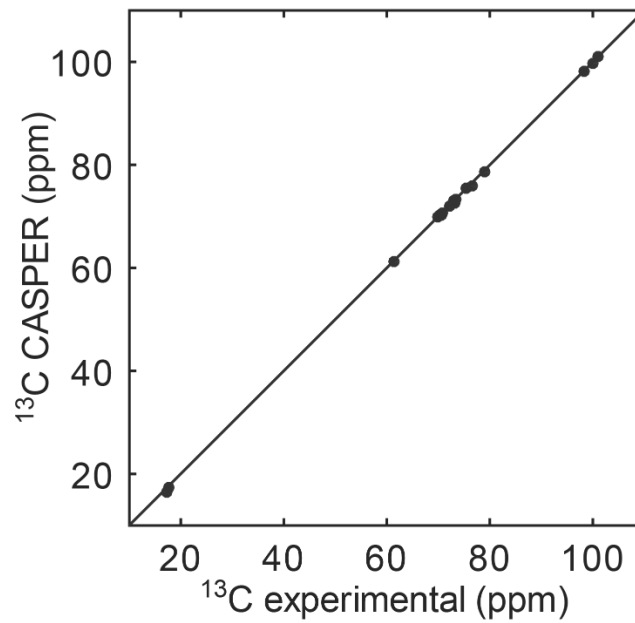
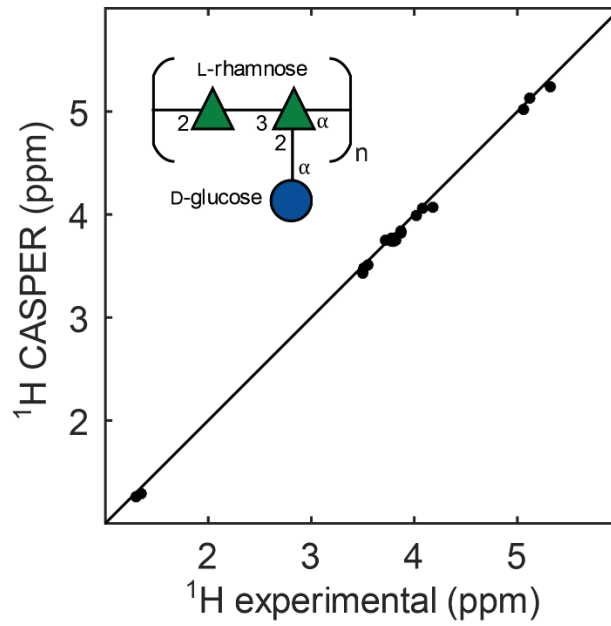
Structure

$\rightarrow 3) [\alpha\text{-D-Glc}^{\text{iii}} (1\rightarrow 2)]\alpha\text{-L-Rha}^{\text{ii}} (1\rightarrow 2) \alpha\text{-L-Rha}^{\text{i}} (1\rightarrow$

$\rightarrow 2) \alpha\text{-L-Rha}^{\text{i}} (1\rightarrow$	1	2	3	4	5	6	
Expected Calc. Error: 8.73	101.04	78.66	70.66	72.92	69.91	17.36	
	5.24	4.06	3.84	3.48	3.74	1.29	
$\rightarrow 2,3) \alpha\text{-L-Rha}^{\text{ii}} (1\rightarrow$	1	2	3	4	5	6	
Expected Calc. Error: 9.66	99.70	75.93	75.47	72.59	70.25	16.45	
	5.13	4.07	3.99	3.75	3.77	1.26	
$\alpha\text{-D-Glc}^{\text{iii}} (1\rightarrow$	1	2	3	4	5	6	6
Expected Calc. Error: 6.61	98.17	72.00	73.31	70.27	73.07	61.23	
	5.02	3.51	3.74	3.43	3.83	3.75	3.82

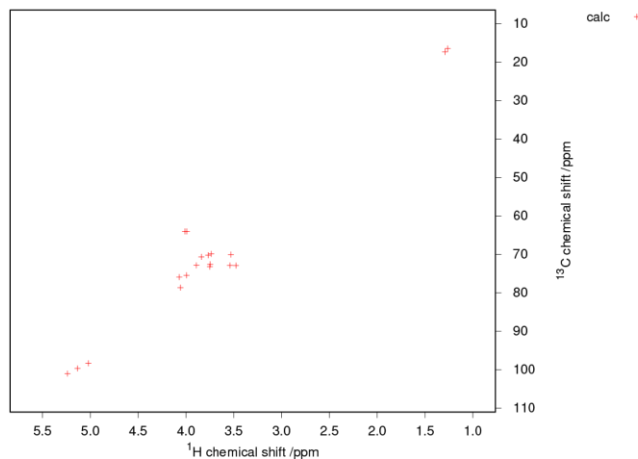
Generated 2024-11-29 10:21:12+01:00.

Additional file 6A NMR chemical shift prediction by CASPER of the repeating unit structure of the RPS from *S. uberis* containing an $\alpha\text{-D-Glc}p\text{-(1}\rightarrow 2\text{)}$ -linked side-chain residue.



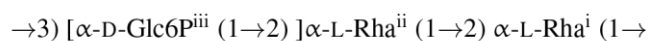
Additional file 6B Comparison of ^1H (top) and ^{13}C (bottom) NMR chemical shifts predicted by CASPER versus assigned by NMR experiments for the repeating unit structure (schematically inserted in the top panel) containing the α -D-Glcp-(1 \rightarrow 2)-linked side-chain residue of the RPS from *S. uberris*.

Streptococcus uberis RPS branched P-substituent



Predicted ¹³C and ¹H NMR chemical shifts

Structure



→2) α-L-Rha ⁱ (1→	1	2	3	4	5	6	
Expected Calc. Error: 8.73	101.04	78.66	70.66	72.92	69.91	17.36	
	5.24	4.06	3.84	3.48	3.74	1.29	
→2,3) α-L-Rha ⁱⁱ (1→	1	2	3	4	5	6	
Expected Calc. Error: 9.66	99.70	75.93	75.47	72.59	70.25	16.45	
	5.13	4.07	3.99	3.75	3.77	1.26	
α-D-Glc6P ⁱⁱⁱ (1→	1	2	3	4	5	6	6
Expected Calc. Error: 6.61	98.37	72.90	73.21	70.07	72.87	64.03	
	5.02	3.54	3.75	3.53	3.89	3.99	4.01

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Additional file 6C NMR chemical shift prediction by CASPER of a repeating unit structure corresponding to the RPS from *S. uberis* containing an α-D-Glcp-(1→2)-linked side-chain residue carrying a phosphate group at O6.