Supplementary Data for

Modeled structural basis for the recognition of α2-3-sialyllactose by soluble klotho

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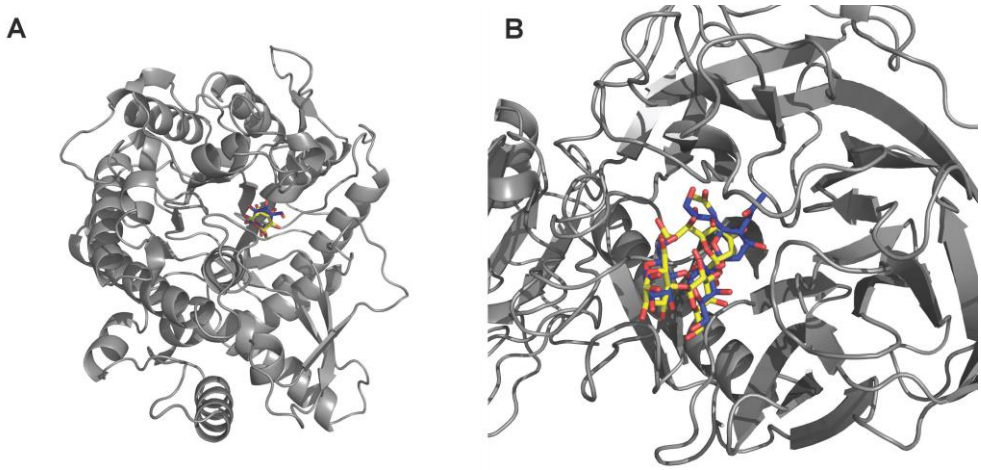
Supplementary Table S1. Pairwise sequence alignment between the PDB structures containing α2-3-sialyllactose and the klotho KL1 and KL2 domains.[a]

	N[b]	1s0i	1z4x	4c1w	4wvw	4yz5	KL1	KL2
1s0i	642		107/22%	161/19%	48/21%	185/22%	87/23%	175/20
1z4x	456	110/22%		37/32%	19/38%	74/26%	71/21%	64/26%
4c1w	196	159/19%	33/32%		22/27%	183/27%	53/21%	41/24%
4wvw	152	47/21%	21/38%	21/27%		52/24%	30/33%	43/21%
4yz5	665	181/21%	65/26%	181/27%	58/24%		80/22%	68/20%
KL1	450	80/23%	70/21%	55/21%	28/33%	74/22%		450/33%
KL2	439	167/21%	60/26%	42/24%	45/21%	74/20%	439/33%	

[a]Each pair of sequences was aligned using the Lalign program (X. Huang and W. Miller (1991) Adv. Appl. Math. 12:373-381). The entries in column 3 to 9 correspond to the maximum number of residues in the template sequence that was aligned with the target sequence followed by the percentage sequence identity of the longest aligned amino acid sequence; e.g., in the 2nd row and 4th column, 107 denotes that a maximum of 107 out of 642 residues in 1s0i template sequence was aligned with the 1z4x protein sequence and 22% denotes the sequence identity of the longest aligned amino acid sequence.
[b]N is the total number of amino acid residues in the template protein.

Supplementary Figure S1.



Supplementary Figure S1. (A) Comparison of the top-ranked docked glucose configuration (yellow) with the X-ray structure (PDB entry 2e91) of glucose (dark blue) bound to KLrP (grey). (B) Comparison of the top-ranked docked α2-3-sialyllactose configuration (yellow) with the X-ray structure (PDB entry 1s0i) of α2-3-sialyllactose (dark blue) bound to *Trypanosoma cruzi* trans-sialidase (grey).