Table S1. Correlation coefficients of Gibbs energy values of ligand–receptor complexation

Epoch	20	21	22	23	24	25	26	27	28	29
ConA	0.74	0.58	0.63	0.45	0.46	**0.82***	**0.69***	**0.78***	0.69	0.69
CD206	0.82	0.77	0.73	0.59	0.43	0.55	**0.83***	**0.80***	0.55	0.72

Note. Values obtained by the neural network analysis in comparison with the literature data, which confirm relevance of the Pafnucy neural network training on the PDBbind2020 set. The epochs 20-29 are chosen (Fig. S1).
* The most accurate sequential predictions are marked in bold.

Table S2. Thermodynamic parameters of ConA complexation with carbohydrate ligands

No.	Name of ligand, PDB code of the complex with ConA, and Fig. number	Energies of ConA–ligand complexation, kcal/mol															
		MD1				MD2				MD3				MD – mean	MD – stand. error	REF.	NN
		A	B	C	D	A	B	C	D	A	B	C	D				
1	α-mannopyranose [5CNA]	10.7	24.0	10.6	11.8	19.8	12.2	11.1	30.0	13.5	20.6	19.3	10.5	16.2	2.0	4.0	6.0
2	Me-mannopyranoside [5CNA]; Fig. S3	21.5	21.5	26.8	22.0	18.3	22.3	25.5	15.3	22.0	20.6	21.2	12.7	20.8	2.0	5.2	6.4
3	Me-α(1→2)-dimannopyranoside [1BXH]; Fig. 4	43.8		47.7		39.2		19.4		29.5		42.0		36.9	8.3	7.0	7.2
4	α(1→2)-dimannopyranoside [1BXH]; Fig. S4	38.9		39.4		25.8		31.5		41.2		31.7		34.8	5.5	6.3	6.4
5	Me-α(1→3)-dimannopyranoside [1QDO/C]; Fig. 4	47.4	44.8	46.9	44.6	37.9	39.6	37.4	38.1	36.6	39.7	37.2	40.2	40.9	4.4	6.2	7.2
6	α(1→3)-dimannopyranoside; Fig. S4	42.0	43.4	40.6	42.2	39.8	40.3	37.0	33.7	39.0	37.9	36.1	47.6	39.9	2.2	5.7	7.0
7	α(1→6)-dimannopyranoside; Fig. S4, S7	34.4	40.5	36.6	38.4	28.7	42.2	32.2	43.9	33.8	29.5	37.4	32.6	35.8	2.2	5.6	6.6
8	Me-α(1→6)-dimannopyranoside; Fig. 4	35.8	35.9	36.4	37.8	27.7	39.6	42.9	37.6	43.8	37.2	24.8	47.4	37.2	1.0	5.3	7.0
9	Me-3,6-di-O-(mannopyranosyl)-α-mannopyranoside [1ONA]	53.9	46.7	52.6	44.3	34.5	36.3	44.4	52.7	38.4	53.2	43.8	39.8	45.1	3.9	7.8	7.0
10	3,6-di-O-(mannopyranosyl)-α-mannopyranose; Fig. 2	42.9	48.2	45.6	45.6	33.9	37.2	39.0	38.3	31.4	40.8	37.1	39.4	40.0	4.9	7.5	7.4
11	3,6-di-O-(α(1→2)-N-acetylglucosamino-mannopyranosyl)-α-mannopyranose [1TEI]; Fig. S6	50.9	50.1	48.6	60.2	42.0	50.1	48.8	69.4	48.2	50.1	46.1	60.6	52.1	0.7	8.4	7.8
12	Me-α-glucopyranoside [1GIC]	16.0		23.7		21.6		17.2		23.7		23.6		20.9	2.3	4.4	5.1
13	Me-α-galactopyranoside [1GIC]	33.7	43.4	30.1	28.7	34.1	25.2	33.9	33.7	26.6	41.6	28.0	28.1	32.3	1.5	4.5	6.0
14	Me-GlcNAc	41.4	36.9	45.4	45.1	43.7	42.4	43.8	40.0	40.8	41.5	42.0	42.6	42.1	0.4	3.9	6.6
15	Fuc-α(1→3)-GlcNAc	52.0	49.9	43.7	51.4	42.7	43.6	52.2	48.8	53.4	53.9	51.5	49.9	49.4	2.7	–	6.5

Note. The values were calculated using computer simulation (Pafnucy neural network, 10-ns molecular dynamics simulation – Amber20 and mm/pbsa) in comparison with the literature data (REF) [20-21, 26]. The initial values of energies (kcal/mol) after three cycles of molecular dynamics simulation (MD) and data of neural network analysis (NN) are presented. The energy values obtained by the MD method are presented for four subunits.

Table S3. Thermodynamic parameters of complexation of CRD4 of CD206 with carbohydrate ligands

No.	Name of ligand and Fig. number	Complexation energies of CD206–ligand, kcal/mol						
		MD1	MD2	MD3	MD – mean	MD – stand. error	REF	NN
1	α-mannopyranose [5CNA]; Fig. 5, Fig. S5	25.6	27.3	27.2	26.7	1.0		5.2
2	Me-mannopyranoside [5CNA]	32.8	32.5	34.5	33.3	1.1	3.6	5.9
3	Me-α(1→2)-dimannopyranoside [1BXH]	54.7	56.4	54.4	55.2	1.1		13.3
4	α(1→2)-dimannopyranoside [1BXH]	50.9	41.9	37.6	43.5	6.8	4.0	6.4
5	Me-α(1→3)-dimannopyranoside [1QDO/C]	66.7	51.2	45.1	54.3	11.1		5.6
6	α(1→3)-dimannopyranoside	63.2	51.3	59.0	57.8	6.0	3.6	6.3
7	α(1→6)-dimannopyranoside	41.9	41.5	40.9	41.4	0.5	4.1	6.5
8	Me-α(1→6)-dimannopyranoside; Fig. S2	59.9	75.8	46.8	60.8	14.5		6.6
9	Me-3,6-di-O-(mannopyranosyl)-α-mannopyranoside [1ONA]	76.9	86.4	57.8	73.7	14.6		5.6
10	3,6-di-O-(mannopyranosyl)-α-mannopyranose	76.9	92.1	92.5	87.2	8.9	4.2	7.9
11	3,6-di-O-(β(1→2)-N-acetylglucosamino-mannopyranosyl)-α-mannopyranose [1TEI]	120.1	112.9	88.7	107.2	16.5		7.2
12	Me-α-glucopyranoside [1GIC]; Fig. S2	37.4	37.3	34.6	36.5	1.6		4.2
13	Me-α-galactopyranoside [1GIC]; Fig. 3, Fig. S2	38.9	34.6	35.4	36.3	2.3		5.3
14	Me-GlcNAc	41.7	41.9	39.7	41.1	1.2	3.1	5.0
15	Fuc-α(1→3)-GlcNAc	44.6	43.5	42.7	43.6	1.0		6.7

Note. The values were calculated using computer simulation (Pafnucy neural network, 100-ns molecular dynamics simulation – Amber20 and mm/pbsa) in comparison with the literature data (REF) [13, 52-53]. The initial values of energies (kcal/mol) of three cycles of molecular dynamics (MD) and data of neural network analysis (NN) are presented.