SUPPLEMENTARY MATERIAL

Docking linear and branched ligands to Glucose oxidase

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Table S1. The final lamarckian genetic algorithm docked state – Binding energy of PEI ligand to the active sites of type of 3QVR during the nine explored conformations. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

Ligand	1	2	3	4	5	6	7	8	9	Best Docking Energy (kcal/mol)	Localization
LIG_PEI_C2N2_01_0Linear_1	-3	-3	-2.9	-2.9	-2.9	-2.8	-2.8	-2.8	-2.8	-3	inside of enzyme
LIG_PEI_C4N3_01_0Linear_1	-3.9	-3.8	-3.6	-3.4	-3.4	-3.1	-3	-3	-2.9	-3.9	inside of enzyme
LIG_PEI_C6N4_01_0Linear_1	-4.8	-4.5	-4.2	-4.2	-4.1	-4.1	-4	-4	-4	-4.8	inside of enzyme
LIG_PEI_C8N5_01_0Linear_1	-5.2	-4.9	-4.9	-4.9	-4.8	-4.8	-4.8	-4.8	-4.7	-5.2	inside of enzyme
LIG_PEI_C10N6_01_0Linear_1	-5.3	-5.2	-5.2	-5.2	-5	-5	-5	-4.9	-4.9	-5.3	inside of enzyme
LIG_PEI_C10N6_01_0Linear_3.	-4.3	-4.2	-4.1	-4.1	-4.1	-4.1	-4	-4	-4	-4.3	on surface of enzyme
LIG_PEI_C12N7_01_0Linear_2	-5.5	-5.3	-5.2	-4.9	-4.9	-4.9	-4.8	-4.7	-4.7	-5.5	inside of enzyme
LIG_PEI_C14N8_01_0Linear_2	-5.7	-5.4	-5.2	-5.2	-5.1	-5.1	-5.1	-5.1	-4.9	-5.7	inside of enzyme
LIG_PEI_C18N10_01_0Linear_2	-6	-5.6	-5.6	-5.6	-5.5	-5.5	-5.4	-5.4	-5.3	-6	inside of enzyme

Table S2. The final lamarckian genetic algorithm docked state – Binding energy of Chr ligand to the active sites of type of 3QVR during the nine explored conformations. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

Ligand	1	2	3	4	5	6	7	8	9	Best Docking Energy (kcal/mol)	Localization
LIG_Chr_6(6)_0_24_Chr_1	-6.8	-6.8	-6.8	-6.8	-6.8	-6.5	-6.4	-6.4	-6.4	-6.8	inside of enzyme
LIG_Chr_6(6)_1_39_Chr_1	-9.5	-9.5	-6.6	-6.5	-6.5	-6.5	-6.5	-6.5	-6.5	-9.5	inside of enzyme
LIG_Chr_6(6)_2_54_Chr_1	-8.3	-8.3	-8.3	-8.3	-8.2	-7.5	-7.4	-7.4	-7.4	-8.3	on surface of enzyme
LIG_Chr_6(6)_3_69_Chr_1	-9.1	-9.1	-9.1	-9.1	-9	-8.9	-8.4	-8.4	-8.4	-9.1	on surface of enzyme
LIG_Chr_6(6)_4_84_Chr_1	-10.2	-10.1	-10.1	-10.1	-10.1	-9.7	-9.7	-9.7	-9.7	-10.2	on surface of enzyme
LIG_Chr_6(6)_5_99_Chr_1	-11.6	-11.5	-11.5	-11.5	-11.5	-11.5	-11.1	-11.1	-11.1	-11.6	on surface of enzyme
LIG_Chr_6(6)_6_114_Chr_1	-13.5	-13.5	-13.5	-13.4	-13.4	-13.4	-11.7	-11.7	-11.7	-13.5	on surface of enzyme
LIG_Chr_6(6)_7_129_Chr_1	-13.2	-13.2	-13.2	-13.2	-13.2	-12.7	-12.6	-12.6	-12.6	-13.2	on surface of enzyme

Table S3. The length of the hydrogen bond formed between the PEI and Chr ligands and the protein 3QVR in cases of the interactions with the best binding energy. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

ligand	Best Docking Energy (kcal/mol)	H-bonds							
LIG_PEI_C10N6_01_0Linear_1.log	-5.3	2.05	2.13	2.55	2.64	2.68	2.76		
LIG_PEI_C12N7_01_0Linear_2.log	-5.5	2.09	2.51	2.54	2.67	2.75	2.93	2.98	
LIG_PEI_C14N8_01_0Linear_2.log	-5.7	2.31	2.60	2.61	2.69	2.73	2.78	2.93	2.98
LIG_PEI_C18N10_01_0Linear_2.log	-6.0	1.93	2.07	2.13	2.13	2.18	2.30	2.41	
LIG_Chr_6(6)_1_39_Chr_1.log	-9.5	1.79	1.96	2.17	2.32	2.38	2.42	2.59	
LIG_Chr_6(6)_6_114_Chr_3.log	-13.5	2.15	2.68	2.71	2.79				
LIG_Chr_6(6)_7_129_Chr_1.log	-13.2	1.91	2.09	2.64					

Table S4. The final lamarckian genetic algorithm docked state – Binding energy of PEI ligand to the active sites of type of 3QVR on the first surface of docking (Figure 13) during the nine explored conformations. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

Ligand	1	2	3	4	5	6	7	8	9	Best Docking Energy (kcal/mol)
LIG_PEI_C2N2_01_0Linear_1.log	-2.6	-2.6	-2.5	-2.4	-2.3	-2.2	-2.1	-2.1	-2	-2.6
LIG_PEI_C4N3_01_0Linear_1.log	-3.2	-3.1	-3	-3	-2.9	-2.9	-2.8	-2.8	-2.7	-3.2
LIG_PEI_C6N4_01_0Linear_1.log	-3.7	-3.4	-3.4	-3.4	-3.4	-3.4	-3.4	-3.3	-3.3	-3.7
LIG_PEI_C8N5_01_0Linear_2.log	-3.8	-3.8	-3.7	-3.7	-3.7	-3.7	-3.6	-3.5	-3.5	-3.8
LIG_PEI_C10N6_01_0Linear_3.log	-4	-3.8	-3.8	-3.7	-3.7	-3.7	-3.7	-3.6	-3.6	-4
LIG_PEI_C12N7_01_0Linear_1.log	-4	-3.9	-3.9	-3.9	-3.8	-3.8	-3.8	-3.8	-3.8	-4
LIG_PEI_C14N8_01_0Linear_1.log	-4	-3.8	-3.8	-3.8	-3.8	-3.8	-3.8	-3.7	-3.7	-4
LIG_PEI_C18N10_01_0Linear_3.log	-4	-3.9	-3.8	-3.8	-3.8	-3.8	-3.8	-3.7	-3.7	-4

Table S5. The final lamarckian genetic algorithm docked state – Binding energy of PEI ligand to the active sites of type of 3QVR on the second surface of docking (Figure 13) during the nine explored conformations. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

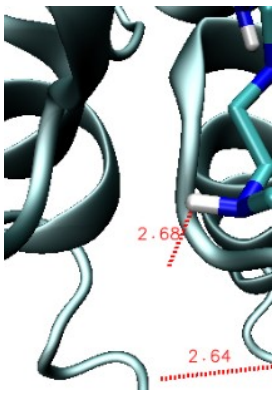
Ligand	1	2	3	4	5	6	7	8	9	Best Docking Energy (kcal/mol)
LIG_Str_6(6)_0_24_Str_1.log	-4.7	-4.6	-4.6	-4.6	-4.6	-4.6	-4.5	-4.5	-4.3	-4.7
LIG_Str_6(6)_1_39_Str_1.log	-5.1	-5.1	-5.1	-5.1	-5.1	-5.1	-4.8	-4.8	-4.6	-5.1
LIG_Str_6(6)_2_54_Str_1.log	-6.1	-6.1	-6.1	-6.1	-6.1	-6.1	-6.1	-6.1	-6.1	-6.1
LIG_Str_6(6)_3_69_Str_1.log	-7.5	-7.5	-7.5	-7.5	-7.5	-7.5	-7.1	-7.1	-7.1	-7.5
LIG_Str_6(6)_4_84_Str_1.log	-8	-8	-8	-8	-8	-8	-7.9	-7.9	-7.9	-8
LIG_Str_6(6)_5_99_Str_1.log	-8.7	-8.7	-8.6	-8.6	-8.6	-8.6	-8.5	-8.5	-8.5	-8.7
LIG_Str_6(6)_6_114_Str_1.log	-9.3	-9.3	-9.3	-9.3	-9.3	-8.9	-8.9	-8.9	-8.9	-9.3
LIG_Str_6(6)_7_129_Str_1.log	-9.6	-9.5	-9.5	-9.5	-9.5	-9.5	-9.3	-9.3	-9.3	-9.6

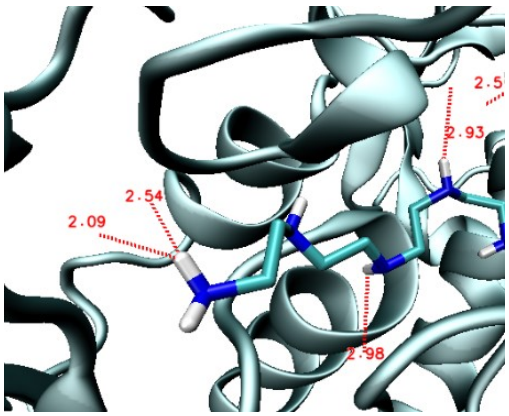
Table S6. The final lamarckian genetic algorithm docked state – Binding energy of PEI ligand to the active sites of type of 3QVR on the second surface of docking (Figure 13) during the nine explored conformations. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

Ligand	1	2	3	4	5	6	7	8	9	Best Docking Energy (kcal/mol)
LIG_PEI_C2N2_01_0Linear_1.log	-2.8	-2.8	-2.7	-2.7	-2.7	-2.7	-2.6	-2.5	-2.8	-2.8
LIG_PEI_C4N3_01_0Linear_3.log	-3.8	-3.7	-3.5	-3.4	-3.4	-3.2	-3.1	-3.1	-3.8	-3.7
LIG_PEI_C6N4_01_0Linear_1.log	-3.8	-3.7	-3.7	-3.7	-3.6	-3.6	-3.5	-3.5	-3.8	-3.8
LIG_PEI_C8N5_01_0Linear_2.log	-4.1	-3.8	-3.8	-3.7	-3.7	-3.7	-3.6	-3.6	-4.1	-3.6
LIG_PEI_C10N6_01_0Linear_1.log	-3.9	-3.9	-3.7	-3.7	-3.7	-3.7	-3.7	-3.7	-3.9	-3.9
LIG_PEI_C12N7_01_0Linear_1.log	-4	-3.8	-3.7	-3.7	-3.7	-3.7	-3.6	-3.6	-4	-4
LIG_PEI_C14N8_01_0Linear_3.log	-4.2	-4.2	-4.1	-4	-4	-4	-3.9	-3.9	-4.2	-4.2
LIG_PEI_C18N10_01_0Linear_2.log	-4.2	-4	-4	-3.9	-3.9	-3.9	-3.8	-3.8	-4.2	-4.2

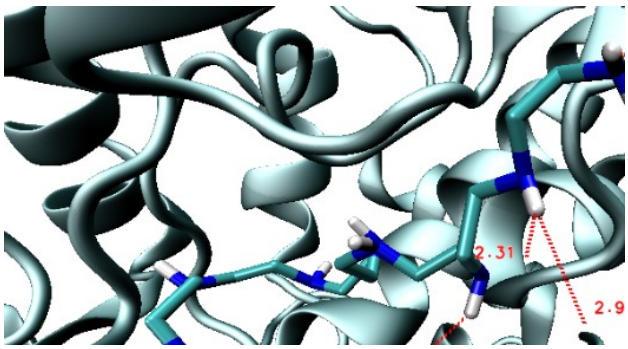
Table S7. The final lamarckian genetic algorithm docked state – Binding energy of Chr ligand to the active sites of type of 3QVR on the second surface of docking (Figure 13) during the nine explored conformations. The number 1,2,3 in the ligand name means the use of another random variable in the docking procedure.

Ligand	1	2	3	4	5	6	7	8	9	Best Docking Energy (kcal/mol)
LIG_Str_6(6)_0_24_Str_1.log	-3.9	-3.9	-3.9	-3.9	-3.9	-3.9	-3.9	-3.9	-3.9	-3.9
LIG_Str_6(6)_1_39_Str_1.log	-5	-5	-5	-5	-5	-4.9	-4.8	-4.8	-4.8	-4.8
LIG_Str_6(6)_2_54_Str_1.log	-6.2	-6.2	-6.2	-6.2	-6.2	-6.1	-5.9	-5.9	-5.9	-5.9
LIG_Str_6(6)_3_69_Str_3.log	-6.8	-6.7	-6.7	-6.7	-6.7	-6.7	-6.7	-6.7	-6.6	-6.6
LIG_Str_6(6)_4_84_Str_1.log	-8.2	-8.1	-8.1	-8.1	-8.1	-8.1	-7.7	-7.6	-7.5	-7.5
LIG_Str_6(6)_5_99_Str_2.log	-9	-8.9	-8.9	-8.9	-8.9	-8.9	-8.6	-8.6	-8.6	-8.6
LIG_Str_6(6)_6_114_Str_1.log	-9.5	-9.5	-9.4	-9.4	-9.4	-9.4	-9.2	-9.2	-9.2	-9.2
LIG_Str_6(6)_7_129_Str_1.log	-10.2	-10.2	-10.2	-10.2	-10.2	-10.2	-9.9	-9.9	-9.6	-9.6



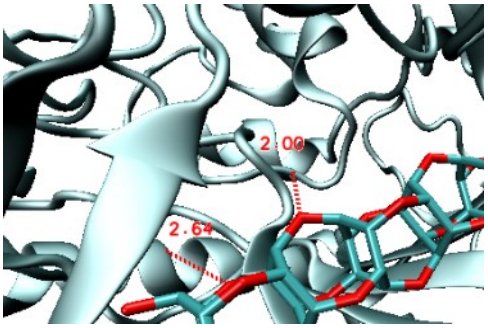


3QVR - LIG_PEI_C10N6_01_0Linear_1 complex 3QVR - LIG_PEI_C12N7_01_0Linear_2 complex

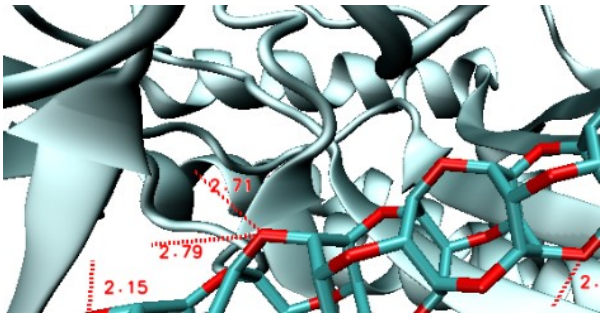


3QVR - LIG_PEI_C14N8_01_0Linear_2 complex

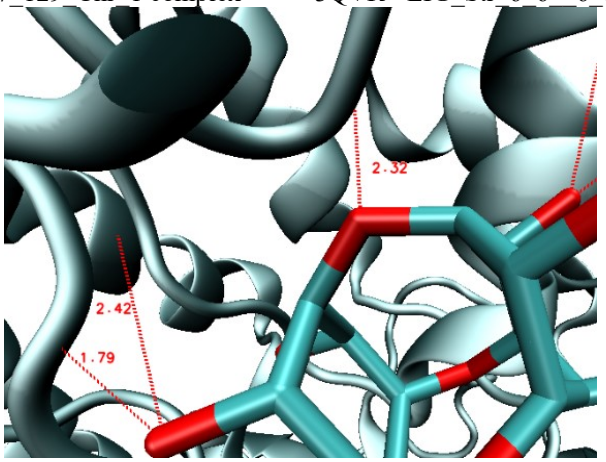
Figure S1. The length of hydrogen bonds in Å formed between ligands PEI and GOX enzyme.



3QVR - LIG_Str_6_6__7_129_Chr_1 complex

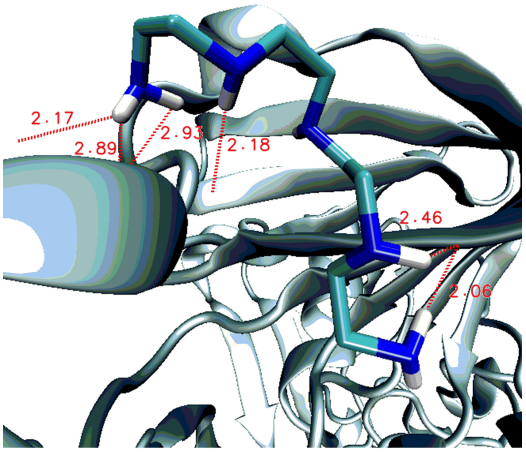


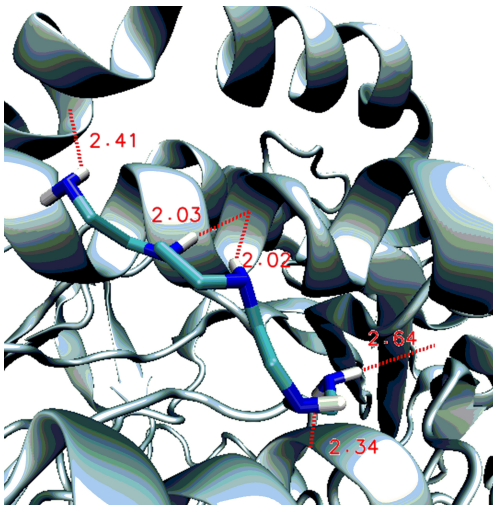
3QVR - LIG_Str_6_6__6_114_Chr_1 complex



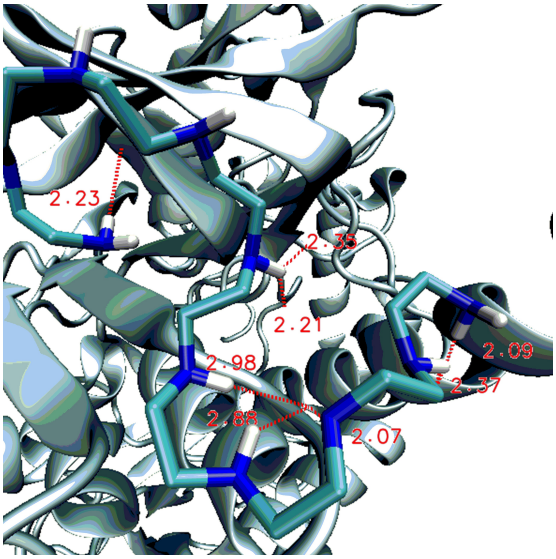
3QVR - LIG_Str_6_6__1_39_Chr_1 complex

Figure S2. The length of hydrogen bonds in Å formed between ligands Chr and GOX enzyme.





LIG_PEI_C8N5_01_0Linear_2



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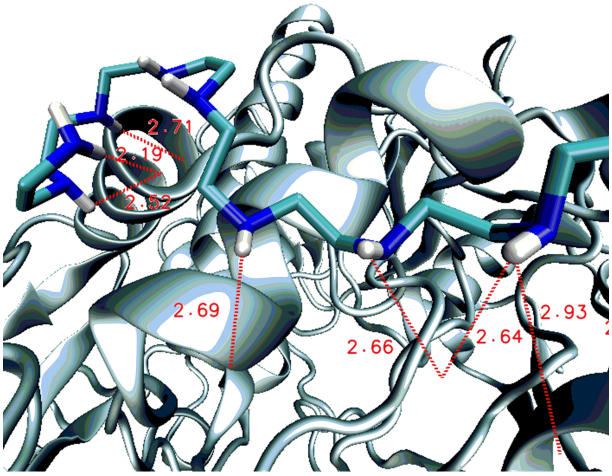
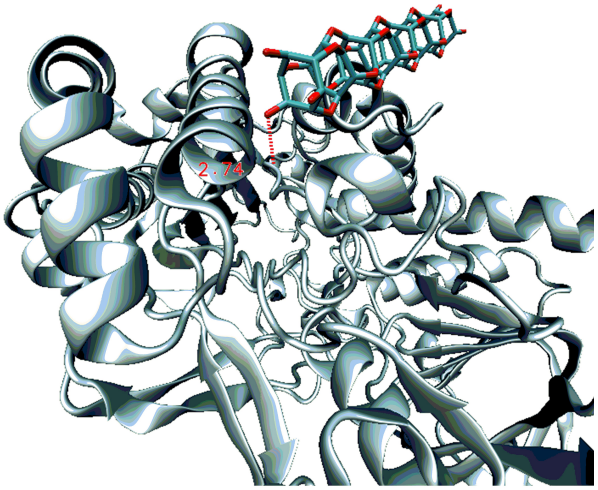


LIG_PEI_C18N10_01_0Linear_2



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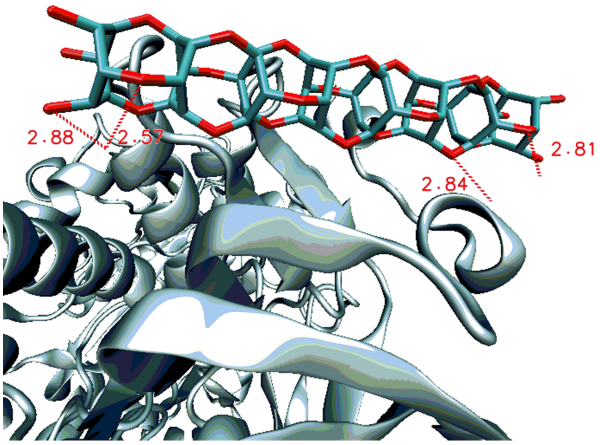

LIG_Str_6(6)_7_129_Str_1

LIG_Str_6(6)_7_129_Str_1

Figure S3. The length of hydrogen bonds (Å) formed between ligands PEI, Chr and GOX as differences between first (right) and second (left) surface of enzyme.