Distribution of charged and hydrophobic amino acids on the surfaces of two types of beta-fructosidase from *Thermotoga maritima*

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Materials and methods

- Beta-fructosidases from *Thermotoga maritima* PDB ID: 1UYP and PDB ID: 1W2T was chosen as objects of this work. Molecular structures were visualized using the Maestro 10.3 software.
- The degree of remoteness of amino acid residues from each other was a criterion for the grouping of amino acid residues into a local cluster. The residues were assigned to a certain cluster if the distance between the nearest atoms of these amino acids did not exceed 10 Å. The distance was calculated based on the formula:

$$r = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$$

The composition of charged amino acid clusters on the surface of beta-fructosidase 1UYP

No. 1	Lys3, Arg37, Lys38, Glu40, His59, Asp67, Asp68, Glu69, Lys269, Arg270, Glu271
No. 2	Lys25, Lys27, Asp52, His56, Arg58, Glu80, Asp82, Lys84, Glu111, Asp115, Arg143
No. 3	Arg93, His97, Lys99, Glu101, Lys102, Lys127
No. 4	Glu130, Glu131, Glu147, Lys156, Asp157, Glu158, Lys159, Asp169, His173, Lys175, Glu177, Glu182, Glu184, Lys187, Arg196, Glu199, Lys221, Glu222, Lys224, Glu228, Lys229, Arg230
No. 5	Glu286, Glu289, Asp296, Arg302, Lys303, Arg304, Lys305, Glu308, Lys311, Asp318, Lys320, Glu321, Glu333, Arg337, Arg351, Asp352, Glu353, Arg369, Lys370, Glu374, Asp375, Glu376, Arg380, Asp396, Lys416, Lys421
No. 6	Glu341, Glu344, Arg360, Glu407

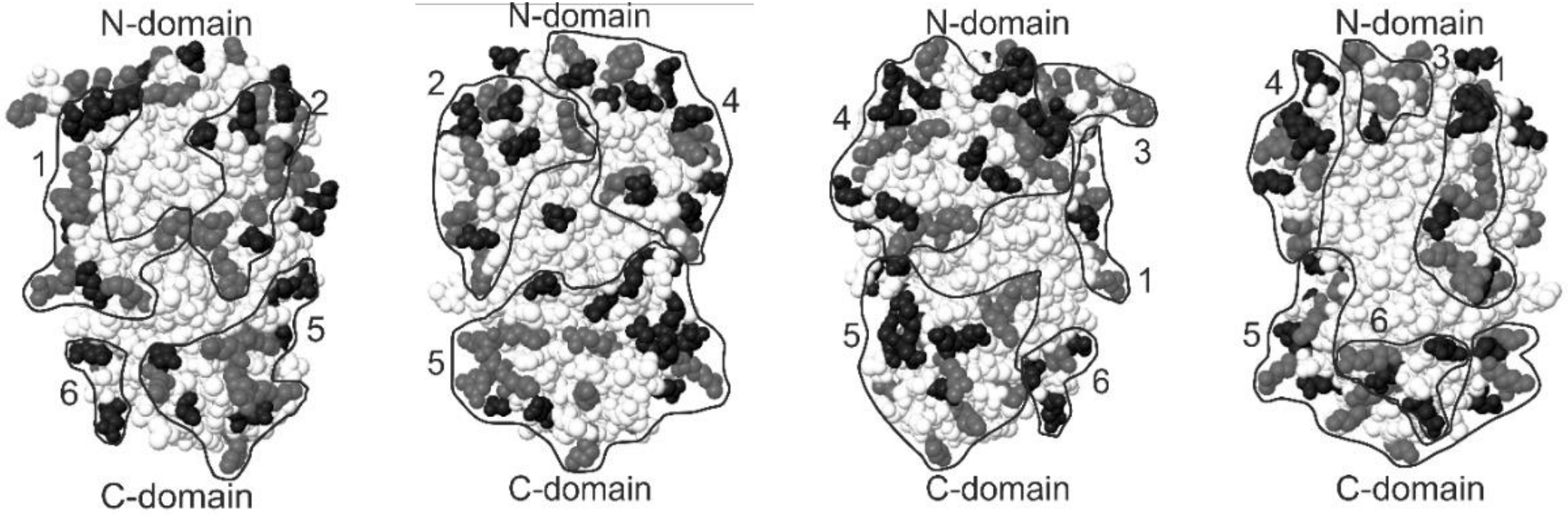
The composition of charged amino acid clusters on the surface of beta-fructosidase 1W2T

No. 1	Lys3, Arg37, Lys38, Glu40, His59, Glu69, Asp94, Lys269, Arg270, Glu271
No. 2	Lys25, Lys27, Asp52, His56, Arg58, Asp67, Asp68, Glu80, Asp82, Lys84, Arg93, Lys99, Glu101, Lys102, Glu111, Asp115, Lys118, Asp120, Lys127, Glu130, Glu131, His134, Arg143, Glu147, Asp157, Glu158, Lys159, Asp169, His173, Lys175, Glu177, Glu182, Glu184, Lys187, Lys224, Arg230
No. 3	Arg196, Glu199, Lys221, Glu222, Glu228, Lys229, Glu286, Glu289, Glu333, Arg351, Asp352, Glu353, Lys370, Glu374, Asp375, Glu376, Arg380, Asp396, Lys416, Lys421
No. 4	Asp296, Arg302, Lys303, Arg304, Lys305, Glu308, Asp318, Lys320, Glu321, Glu426
No. 5	Glu335, Arg337, Glu341, Arg360, Glu407

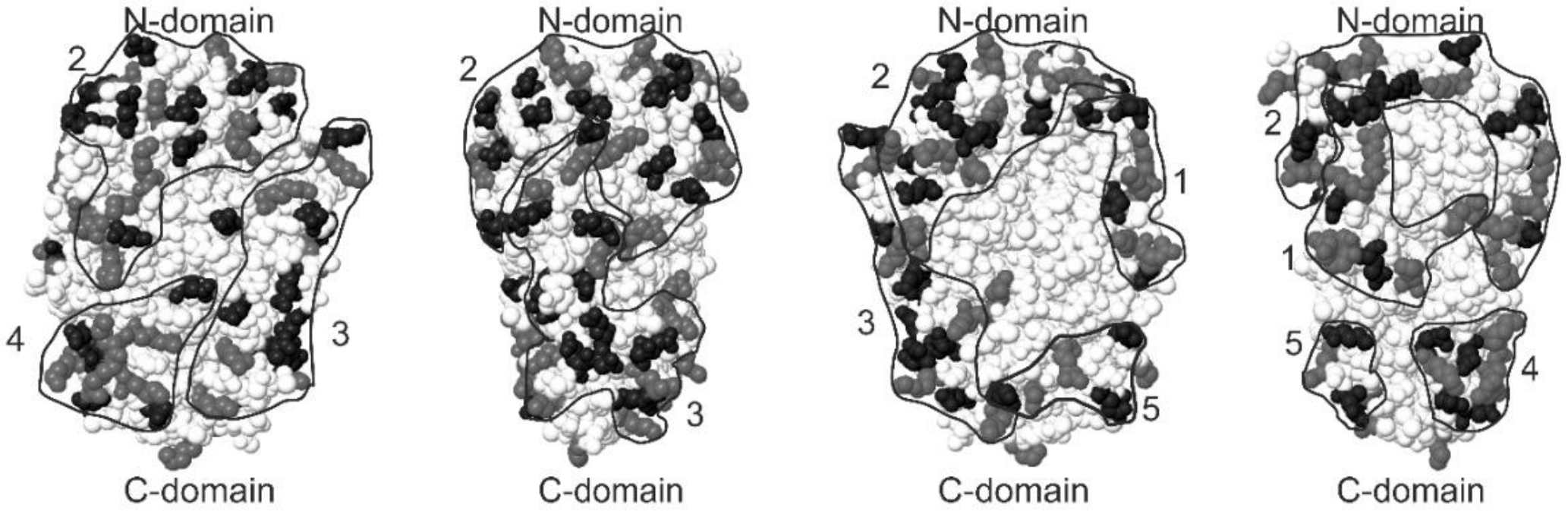
The composition of hydrophobic amino acid clusters on the surface of beta-fructosidases 1UYP and 1W2T respectively

No. 1	Ile11, Pro36, Pro61, Tyr65, Leu114, Val117, Trp431	Ile11, Pro61, Tyr65, Leu114, Val117, Tyr119, Gly121, Pro123
No. 2	Pro123, Pro128, Pro129, Gly132, Tyr176	Trp41, Trp260, Leu261, Gly264, Leu265, Val363
No. 3	Trp41, Trp260, Leu261, Gly264, Leu265, Val363	

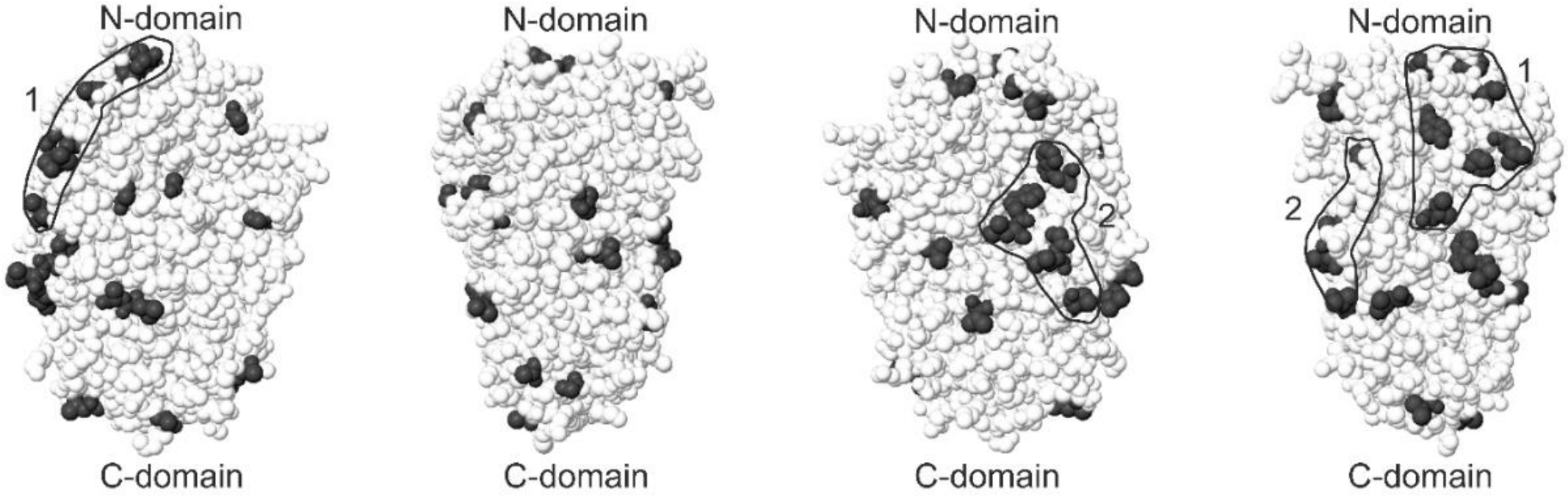
The distribution of charged amino acid clusters on the surface of beta-fructosidase 1UYP



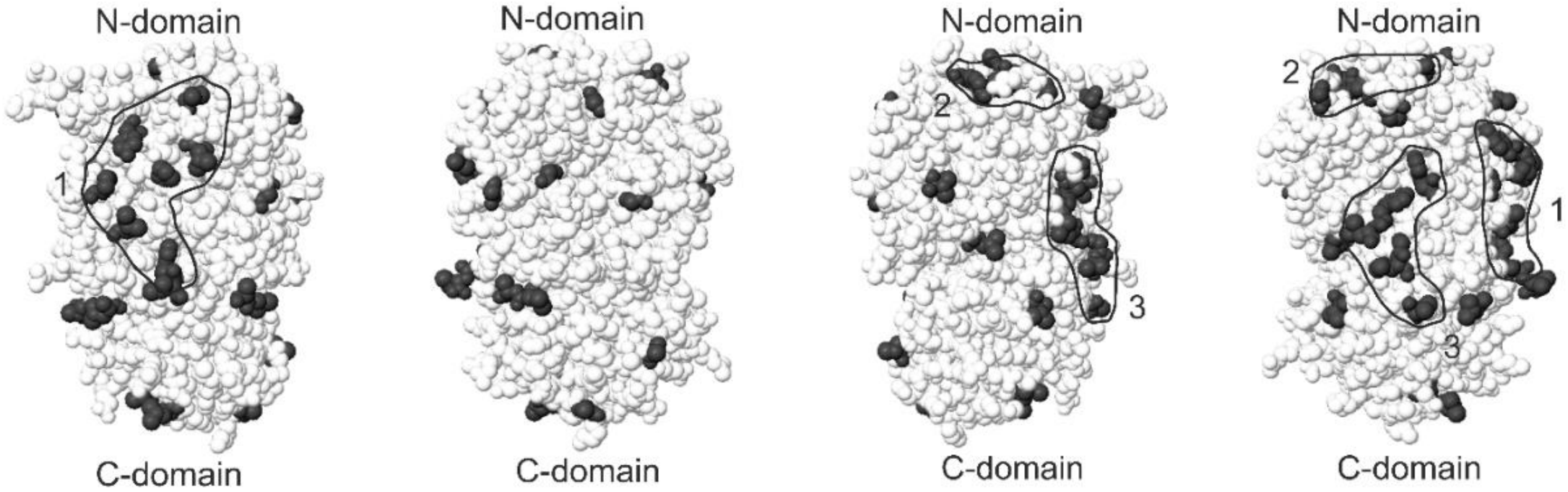
The distribution of charged amino acid clusters on the surface of beta-fructosidase 1W2T



The distribution of hydrophobic amino acid clusters on the surface of beta-fructosidase 1W2T



The distribution of hydrophobic amino acid clusters on the surface of beta-fructosidase 1UYP



Conclusion

- Insoluble biocatalysts based on immobilized enzymes are promising catalytic agents for industry and medicine due to high activity and stability. Immobilization based on weak interactions, such as hydrophobic and electrostatic interactions, make it possible to save more activity than covalent bonds.

- It was showed that charged carriers are more promising for immobilization of beta-fructosidases 1UYP and 1W2T from *Thermotoga maritima* because of presence on its surfaces several clusters remote from active site. Binding of carrier's matrix with such clusters may lead to immobilization of the enzymes without significant losses of activity.

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