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Author: Michal Grulich Jan Brezovský Václav Štěpánek Andrea Palyzová Helena Marešová Jiří Zahradník Eva Kyslíková Pavel Kyslík

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In-silico driven engineering of enantioselectivity of a penicillin G acylase towards active pharmaceutical ingredients

Michal Grulich[1*] Jan Brezovský[2,3] Václav Štěpánek[1] Andrea Palyzová[1] Helena Marešová[1] Jiří Zahradník[1,4] Eva Kyslíková[1] Pavel Kyslík[1]

[1] Laboratory of Enzyme Technology, Institute of Microbiology of the CAS, v.v.i., Vídeňská 1083, 142 20 Prague 4, Czech Republic
[2] Laboratory of Biomolecular Interactions and Transport, Department of Gene Expression, Institute of Molecular Biology and Biotechnology Faculty of Biology, Adam Mickiewicz University, Umultowska 89, 61-614 Poznan, Poland
[3] International Institute of Molecular and Cell Biology in Warsaw, Ks Trojdena 4, 02-109, Warsaw, Poland
[4] Department of Genetics and Microbiology, Faculty of Science, Charles University Prague, Viničná 5, CZ-128 44 Prague 2, Czech Republic

***Corresponding author**
Michal Grulich
Tel.: +420 241062657
Fax: +420 296442347
E-mail address: grulich@biomed.cas.cz

Co-authors
Václav Štěpánek, Andrea Palyzová, Helena Marešová, Jiří Zahradník, Eva Kyslíková, Pavel Kyslík: Laboratory of Enzyme Technology, Institute of Microbiology of the CAS, v.v.i., Prague, Czech Republic
Jan Brezovský: Laboratory of Biomolecular Interactions and Transport, Department of Gene Expression, Institute of Molecular Biology and Biotechnology, Faculty of Biology, Adam Mickiewicz University, Poznan, Poland and International Institute of Molecular and Cell Biology in Warsaw, Warsaw, Poland

Graphical abstract