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A System for Automated Validation of GPCRs Homology Models Against Mutational Data.

Stefan Mordalski [a], *Tomasz Kosciolek* [a], *Kurt Kristiansen* [b], *Ingebrigt Sylte* [b], *Zdzisław Chilmonczyk* [c], *Andrzej J. Bojarski* [a]

[a]*Department of Medicinal Chemistry, Institute of Pharmacology, Polish Academy of Sciences, Smętna 12, 31-343 Krakow*
[b]*Medical Pharmacology and Toxicology, Department of Medical Biology, Faculty of Health Science, University of Tromsø, N-9037 Tromsø, Norway*
[c] *Department of Cell Biology, National Medicines Institute, Chełmska 30/34, 00-725 Warszawa*
e-mail: stefanm@if-pan.krakow.pl

Sequence alignment between target and template sequence is the most troublesome stage of homology modeling protocol. Misplacing amino acids responsible for interactions with ligands may lead to improper binding mode of so created model and render it useless. This is the reason of wide usage of mutational data in either aligning sequences or models verification.

In this study we present a tool allowing automated comparison of mutagenesis data retrieved from tinyGRAP [1] database with corresponding residues of the model. tinyGRAP dataset is queried for the investigated sequence and its close homologs (i.e. group members), and substitution mutations are retrieved. Query results are then checked whether appropriate residues face inside of the receptor (with some margin), and if not, the tool produces report in PyMol .pse file pointing amino acids violating mutational „constrains".

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[1] Beukers M. W., Kristiansen K., Jzerman A. P., Edvardsen I.: *Trends Pharmacol. Sci.* 1999 20 (12) (1999), 475-7.