

POSTER PRESENTATION

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Homology modelling of metabotropic glutamate receptor 2

S Mordalski^{1*}, T Kosciolk¹, A Ravna², I Sylte², AJ Bojarski¹

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Many studies show involvement of metabotropic glutamate receptors (mGluRs) in synaptic excitation transduction. The mGluR family consists of eight proteins divided into three groups corresponding to sequence similarities, pharmacology and physiological role. These groups are: I (mGluR1, -5), II (mGluR2, -3) and III (mGluR4, -6, -7, -8). Group II lies in field of our interest due to its potential as therapeutic target for stroke and pain drugs. Primary goal of this research is to create viable virtual model of transmembrane domain of mGluR2 receptor capable of binding reference ligands. This model will be used for further research.

Our approach is based on homology modeling. Rhodopsin crystal structure has been used as a template for creating mGluR2 models. Due to inconsistencies between sequence alignments found in literature our alignment has been prepared basing on experimental secondary structure prediction for mGluR1 and mGluR3 [1]. So created models were then tested against available mutational data [2,3] and by flexible docking of known active/inactive compounds.

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Author details

¹Department of Medicinal Chemistry, Institute of Pharmacology Polish Academy of Sciences, Krakow, 31-343, Poland. ²Medical Pharmacology and Toxicology, Department of Medical Biology, Faculty of Health Science, University of Tromsø, N-9037 Tromsø, Norway.

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* Correspondence: stefanm@if-pan.krakow.pl

¹Department of Medicinal Chemistry, Institute of Pharmacology Polish Academy of Sciences, Krakow, 31-343, Poland
Full list of author information is available at the end of the article

References

1. Pin JP, Joly C, Heinemann SF, Bockaert J: Domains involved in the specificity of G protein activation in phospholipase C-coupled metabotropic glutamate receptors. *EMBO J* 1994, **13**:342-348.
2. Hu J, McLarnon SJ, Mora S, Jiang J, Thomas C, Jacobson KA, Spiegel AM: A region in the seven-transmembrane domain of the human Ca²⁺ receptor critical for response to Ca²⁺. *J Biol Chem* 2005, **280**:5113-5120.
3. Yanagawa M, Yamashita T, Shichida Y: Activation Switch in the Transmembrane Domain of Metabotropic glutamate receptor. *Mol Pharmacol* 2009, **76**:201-207.

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