Rafał Kurczab

Lista publikacji

- październik 2011

I. Prace oryginalne (rozdziały w książkach zbiorowych, artykuły w czasopismach):

1. Gabrielsen M., **Kurczab R**., Ravna A. W., Kufareva I., Abagyan R., Chilmonczyk Z., Bojarski A. J., Sylte I., 2011, ***Molecular mechanism of serotonin transporter inhibition elucidated by a new flexible docking protocol***, *Eur. J. Med. Chem.*

2. **Kurczab R**., Nowak M., Chilmonczyk Z., Sylte I., Bojarski A. J., 2010, ***The Development and Validation of a Novel Virtual Screening Cascade Protocol to Identify Potential Serotonin 5-HT7R Antagonists***, *Bioorg. & Med. Chem. Lett.* 20: 2465-2468.

3. Mitoraj M. P., **Kurczab R**., Boczar M., Michalak A., 2010, ***Theoretical description of hydrogen bonding in oxalic acid dimer and trimer based on the combined extended-transition-state energy decomposition analysis and natural orbitals for chemical valence (ETS-NOCV)***, *J. Mol. Mod.* 16: 1789-1795.

4. **Kurczab R**., Mitoraj M. P., Michalak A., Ziegler T., 2010, ***Theoretical Analysis of the Resonance Assisted Hydrogen Bond Based on the Combined Extended Transition State Method and Natural Orbitals for Chemical Valence Scheme***, *J. Phys. Chem. A* 114(33): 8581-8590.

5. Boczar M., **Kurczab R**., Wójcik M. J., 2010, ***Theoretical and spectroscopic studies of vibrational spectra of hydrogen bonds in molecular crystal of β-oxalic acid***, *Vibrational Spectroscopy* 52: 39-47.

II. Prace przeglądowe (raporty, suplementy, recenzje naukowe, opracowania źródłowe):

1. **Kurczab R.**, 2011, ***Znaleźć igłę w stogu siana***, *BPM Przemysł Farmaceutyczny* 5/2011: 88-92.

2. **Kurczab R.**, 2011, ***Projektowanie leków „in silico”***, *BPM Przemysł Farmaceutyczny*, 1/2011: 32-34.

3. Nowak M., **Kurczab R.**, Mordalski S., Bugno R., ***Badania nad modelowaniem receptorów mGlu***, XXVI Zimowa Szkoła Instytutu Farmakologii PAN „Pobudzające aminokwasy III”, Kraków 2009, s: 117.

III. Prace pokonferencyjne i doniesienia zjazdowe:

1. **Kurczab R.**, Zajdel P., Pawłowski M., Bojarski A. J., ***Development and Validation of Methodology for Designing and Analysis of Virtual Combinatorial Libraries Based on Defined Reaction Pathways***, IV Konwersatorium Chemii Medycznej, 8.-10.09.2011, Lublin, Book of Abstracts, 29 s.

2. Warszycki D., Kristiansen K., **Kurczab R.**, Mordalski S., Sylte I., Bojarski A. J., ***Linear Combination of Pharmacophore Hypotheses as a New Tool in Search of New 5-HT1A***

Receptor Ligands, IV Konwersatorium Chemii Medycznej, 8.-10.09.2011, Lublin, Book of Abstracts, 4 s.

3. Smusz S., **Kurczab R.**, Bojarski A. J., ***Meta-Learning as an Improvement of Machine Learning Methods Performance in Virtual Screening***, IV Konwersatorium Chemii Medycznej, 8.-10.09.2011, Lublin, Book of Abstracts, 57 s.

4. Trela M., Bugno R., **Kurczab R.**, Brański P., Bojarski A. J., ***New heterocyclic derivatives as potential allosteric modulators of group III metabotropic glutamate receptors***, 4th International Symposium on Advances in Synthetic and Medicinal Chemistry, 21.-25.08.2011, St. Petersburg, Rosja, Book of Abstracts, 220 s.

5. **Kurczab R.**, Mordalski S., Kosciolek T., Bojarski A. J., ***The new strategy in structure-based pharmacophore model generation and its applications in virtual screening***, VII Joint Meeting on Medicinal Chemistry, 29.06-02.07.2011, Katania, Włochy, Book of Abstracts, 187 s.

6. Warszycki D., Kristiansen K., **Kurczab R.**, Satała G., Mordalski S., Sylte I., Bojarski A. J., ***Extensive pharmacophore modeling studies on 5-HT1A receptor ligands – single hypothesis vs. linear combinations***, VII Joint Meeting on Medicinal Chemistry, 29.06-02.07.2011, Katania, Włochy, Book of Abstracts, 186 s.

7. **Kurczab R.**, Bojarski A. J., ***The Multi-Conformations-Receptor-Based Pharmacophore Model Generation Schema and Its Potential Applications in Virtual Screening***, 9th International Conference on Chemical Structures, 5.-9.06.2011, Noordwijkerhout, Holandia, Book of Abstracts, s. 126-7.

8. Warszycki D., Kristiansen K., Mordalski S., **Kurczab R.**, Sylte I., Bojarski A. J., ***Comparison of various strategies in pharmacophore models generation – application to 5-HT1A receptor ligands***, 9th International Conference on Chemical Structures, 5.-9.06.2011, Noordwijkerhout, Holandia, Book of Abstracts, s. 95-6.

9. Smusz S., **Kurczab R.**, Warszycki D., Kościółek T., Mordalski S., Bojarski A. J., ***Hybridization of ligands as a way of generating combinatorial libraries of drug candidates***, Spring Congress of Polish Chemical Society Student Section, 13.-17.04.2011, Murzasichle, Polska, Book of Abstracts, 130 s.

10. Kristiansen K., Rueda M., Warszycki D., **Kurczab R.**, Gabrielsen M., Abagyan R., Bojarski A. J., Sylte I., ***Modeling of ligand interactions for the human 5-HT1A receptor. Docking, pharmacophores and virtual screening of databases containing drug-like compounds***, The 47th Norwegian Biochemical Society (NBS) contact meeting, 3.-6.02.2011, Tromsø, Norwegia, Book of Abstracts, 108 s.

11. Gabrielsen M., **Kurczab R.**, Jaronczyk M., Ravna A. W., Kristiansen K., Chilmonczyk Z., Bojarski A. J., Sylte I., ***Docking of substrates and inhibitors into the substrate binding site of two serotonin transporter models***, The 47th Norwegian Biochemical Society (NBS) contact meeting, 3.-6.02.2011, Tromsø, Norwegia, Book of Abstracts, 39 s.

12. **Kurczab R.**, ***How to find a needle in a haystack? Implementation of „in silico" methods in searching of a chemical space***, Mini Sympozjum kończące projekt z Polsko-Norweskiego Funduszu Badań Naukowych, 23.09.2011, Warszawa.

13. **Kurczab R.**, ***Jak znaleźć igłę w stogu siana? Zastosowanie metod „in silico" w poszukiwaniu nowych leków***, I Studencka Konferencja Matematyczno-Informatyczno-Biologiczna „Liczby-Nauka-Życie", 19.03.2011, Kraków.

14. Smusz S., **Kurczab R.**, Bojarski A. J., ***Machine learning methods as virtual screening tools in computer-aided drug design***, 23rd Polish School of Chemistry, 10.-14.11.2010, Jastrzębia Góra, Book of Abstracts, 35 s.

15. **Kurczab R.**, Smusz S., Bojarski A. J., ***Evaluation of different Machine Learning Methods for Ligand-based Virtual Screening***, 6th German Conference on Chemoinformatics, 7.-9.11.2010, Goslar-Niemcy, Book of Abstracts, 104 s.

16. Gabrielsen M., **Kurczab R.**, Ravna A. W., Kristiansen K., Chilmonczyk Z., Bojarski A. J., Sylte I., ***Docking of substrates and inhibitors into the substrate binding sites of two serotonin transporter models***, 21st International Symposium on Medicinal Chemistry (EFMC-ISMC), 5.-9.09.2010, Bruksela, Drugs of the Future 2010, 35 A, s. 81-2.

17. Gabrielsen M., Ravna A. W., Kristiansen K., **Kurczab R.**, Chilmonczyk Z., Bojarski A. J., Sylte I., ***Ligand Interactions and Ligand-Induced Conformational States of the Serotonin Transporter***, III Konwersatorium Chemii Medycznej, 20.-22.09.2010, Lublin, Book of Abstracts, K-1.

18. Warszycki D., Prymula K., **Kurczab R.**, Satała G., Bojarski A. J., ***The Implementation of an Expert System to Search for Novel Substances Acting on Serotonergic and Glutamatergic Systems***, III Konwersatorium Chemii Medycznej, 20.-22.09.2010, Lublin, Book of Abstracts, K-3.

19. Satała G., Bugno R., Duszyńska B., **Kurczab R.**, Bojarski A. J., ***Verification of Virtual Screening Results for 5-HT6 Receptor in In Vitro Experiments***, III Konwersatorium Chemii Medycznej, 20.-22.09.2010, Lublin, Book of Abstracts, 12 s.

20. Bugno R., Satała G., Duszyńska B., **Kurczab R.**, Bojarski A. J., ***Examination of 5-HT6 receptor affinity in the group of arylsulfonamide derivatives***, VII MKNOL, 10.-12.05.2010, Zakopane.

21. **Kurczab R.**, Gabrielsen M., Chilmonczyk Z., Sylte I., Bojarski A. J., ***Identification of Novel 5-HT$_7$R Ligands via Multistep Virtual Screening of Commercially Available Compounds Databases***, VII MKNOL, 10.-12.05.2010, Zakopane.

22. **Kurczab R.**, ***Zastosowanie metod bio- i chemoinformatycznych w nowoczesnym projektowaniu leków***, Uniwersytet Medyczny w Poznaniu, 6.12.2010, Poznań.

23. **Kurczab R.**, Gabrielsen M., Chilmonczyk Z., Sylte I., Bojarski A. J., ***Virtual Screening Approach as a Potent Technology in Drug Design Campaigns. Methods, Applications and Computational Perspectives***, III Konwersatorium Chemii Medycznej, 20.-22.09.2010, Lublin, Book of Abstracts, L-3.

24. **Kurczab R.**, ***Virtual Screening as a potent technology of computer-aided drug design. Methods and applications***, Sesja sprawozdawczo-szkoleniowa użytkowników KDM, 14.04.2010, Goniądz.

25. **Kurczab R.**, Nowak M., Jarończyk M., Chilmonczyk Z., Bojarski A. J., ***The Development and Validation of a Novel Virtual Screening Cascade Protocol to Identify Potential Serotonin 5-HT$_7$R Antagonists***, II Konwersatorium Chemii Medycznej, 8.-10.09.2009, Lublin.

26. **Kurczab R.**, Nowak M., Bojarski A. J., ***Comparison of FlexX and Surflex Docking Algorithms Based on Astex Diverse Set***, I Konwersatorium Chemii Medycznej, 19.-20.09.2008, Lublin.

27. **Kurczab R.**, Boczar M., Wójcik M. J., **The theoretical and spectroscopic studies of vibrational spectra of the hydrogen bond in molecular crystal of oxalic acid**, Current Trends in Theoretical Chemistry – CTTC V, 6.-8.07.2008, Kraków.