Publications and lectures – Dávid Bajusz

Publications

1. Discovery of a Novel Kinase Hinge Binder Fragment by Dynamic Undocking
   Moira Rachman, Dávid Bajusz, Anasztázia Hetényi, Andrea Scarpino, Balázs Merő, Attila Egyed, László Buday, Xavier Barril, György M. Keserű, *RSC Medicinal Chemistry*, **2020** *(in press)* IF(2018, as *MedChemComm*): 2.394

2. Human serum albumin binding in a vial: a novel UV-pH titration method to assist drug design
   Gergő Dargó, Dávid Bajusz, Kristóf Simon, Judit Müller, György T. Balogh, *Journal of Medicinal Chemistry*, **2020**, *63 (4),* 1763-1774. IF(2018): 6.054

3. Direct Targeting Options for STAT3 and STAT5 in Cancer
   Anna Orlova, Christina Wagner, Elvin D. de Araujo, Dávid Bajusz, Heidi A. Neubauer, Marco Herling, Patrick T. Gunning, György M. Keserű, Richard Moriggl, *Cancers*, **2019**, *11 (12),* 1930. IF(2018): 6.162

4. Structural Implications of STAT3 and STAT5 SH2 Domain Mutations
   Elvin D. de Araujo, Anna Orlova, Heidi A. Neubauer, Dávid Bajusz, Hyuk-Soo Seo, Sirano Dhe-Paganon, György M. Keserű, Richard Moriggl, Patrick T. Gunning, *Cancers*, **2019**, *11 (11),* 1757. IF(2018): 6.162

5. Multi-Level Comparison of Machine Learning Classifiers and Their Performance Metrics
   A. Rácz, D. Bajusz, K. Héberger, *Molecules*, **2019**, *24 (15),* 2811. IF(2018): 3.060

6. Comparison of Data Fusion Methods as Consensus Scores for Ensemble Docking
   D. Bajusz, A. Rácz, K. Héberger, *Molecules*, **2019**, *24 (15),* 2690. IF(2018): 3.060

7. Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening
   A. Scarpino, D. Bajusz, M. Proj, M. Gobec, I. Sosič, S. Gobec, G. G. Ferenczy, G. M. Keserű, *Molecules*, **2019**, *24 (14),* 2590. IF(2018): 3.060

8. Intercorrelation Limits in Molecular Descriptor Preselection for QSAR/QSPR
   A. Rácz, D. Bajusz, K. Héberger, *Molecular Informatics*, **2019**, *38 (8-9),* 1800154. IF(2018): 2.375

9. DUckCov: a Dynamic Undocking‐based Virtual Screening Protocol for Covalent Binders
   M. Rachman, A. Scarpino, D. Bajusz, G. Pálfy, I. Vida, A. Perczel, X. Barril, G. M. Keserű, *ChemMedChem*, **2019**, *14 (10),* 1011-1021. IF(2018): 3.016

10. The impact of binding site waters on the activity/selectivity trade-off of Janus kinase 2 (JAK2) inhibitors
    A. Egyed, D. Bajusz, G. M. Keserű, *Bioorganic and Medicinal Chemistry*, **2019**, *27 (8),*

1497-1508. IF(2018): 2.802

11. Life beyond the Tanimoto coefficient: similarity measures for interaction fingerprints
A. Rácz, D. Bajusz, K. Héberger, *Journal of Cheminformatics*, **2018**, *10*, 48. IF(2018): 4.154

12. Modelling methods and cross-validation variants in QSAR: a multi-level analysis
A. Rácz, D. Bajusz, K. Héberger, *SAR and QSAR in Environmental Research*, **2018**, *29 (9)*, 661-674. IF(2018): 2.287

13. Pharmacologic inhibition of STAT5 in acute myeloid leukemia
B. Wingelhofer, A. C. Cumaraswamy, B. Maurer, E. C. Heyes, A. Orlova, P. Freund, F. Ruge, A. Berger, E. D. de Araujo, J. Park, G. Tin, S. Ahmar, C-H. Lardeau, I. Sadovnik, D. Bajusz, G. M. Keserű, F. Grebien, S. Kubicek, P. Valent, P. T. Gunning, R. Moriggl, *Leukemia*, **2018**, *32*, 1135-1146. IF(2018): 9.944

14. Validation of tautomeric and protomeric binding modes by free energy calculations. A case study for the structure based optimization of D-amino acid oxidase inhibitors
Z. Orgován, G. G. Ferenczy, T. Steinbrecher, B. Szilágyi, D. Bajusz, G. M. Keserű, *Journal of Computer-Aided Molecular Design*, **2018**, *32 (2)*, 331-345. IF(2018): 3.250

15. Binary similarity measures for fingerprint analysis of qualitative metabolomics profiles
A. Rácz, F. Andrić, D. Bajusz, K. Héberger, *Metabolomics*, **2018**, *14*, 29. IF(2018): 3.167

16. Is soft independent modeling of class analogies a reasonable choice for supervised pattern recognition?
A. Rácz, A. Gere, D. Bajusz, K. Héberger, *RSC Advances*, **2018**, *8*, 10-21. IF(2018): 3.049

17. Structure-based virtual screening approaches in kinase-directed drug discovery
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Current Topics in Medicinal Chemistry*, **2017**, *17 (20)*, 2235-2259. IF(2017): 3.374

18. Identification of 8-Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1 Dependent Cells
R. Kiss, D. Bajusz, R. Baskin, K. Tóth, K. Monostory, P. Sayeski, G. M. Keserű, *Archiv der Pharmazie*, **2016**, *349 (12)*, 925-933. IF(2016): 1.994

19. Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Journal of Molecular Graphics and Modelling*, **2016**, *70*, 275-283. IF(2016): 1.754

20. Multivariate assessment of lipophilicity scales—computational and reversed phase thin-layer chromatographic indices
F. Andrić, D. Bajusz, A. Rácz, S. Šegan, K.Héberger, *Journal of Pharmaceutical and Biomedical Analysis*, **2016**, *127*, 81-93. IF(2016): 3.255

21. Discovery of subtype selective Janus kinase (JAK) inhibitors by structure-based virtual screening

D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Journal of Chemical Information and Modeling*, **2016**, *56 (1)*, 234-247. IF(2016): 3.760

22. Comparison of classification methods with "n-class" receiver operating characteristic curves: a case study of energy drinks
A. Rácz, D. Bajusz, M. Fodor, K. Héberger, *Chemometrics and Intelligent Laboratory Systems*, **2016**, *151*, 34-43. IF(2016): 2.303

23. Property-based characterization of kinase-like ligand space for library design and virtual screening
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Medicinal Chemistry Communications*, **2015**, *6*, 1898-1904. IF(2015): 2.319

24. Consistency of QSAR models: Correct split of training and test sets, ranking of models and performance parameters
A. Rácz, D. Bajusz, K. Héberger, *SAR and QSAR in Environmental Research,* **2015**, *26*, 683-700. IF(2015): 1.897

25. Why is Tanimoto index an appropriate choice for fingerprint-based similarity calculations?
D. Bajusz, A. Rácz, K. Héberger, *Journal of Cheminformatics*, **2015**, *7*, 20. IF(2015): 3.949

26. One vs. Two Electron Oxidation with Peroxomonosulfate Ion: Reactions with Iron(II), Vanadium(IV), Halide ions and Photoreaction with Cerium(III)
G. Lente, J. Kalmár, Zs. Baranyai, A. Kun, I. Kék, D. Bajusz, M. Takács, L. Veres, I. Fábián, *Inorganic Chemistry*, **2009**, *48*, 1763-1773. IF(2009): 4.657

Book chapters

1. Chemoinformatics/Chemometrics in Analytical Chemistry
A. Rácz, D. Bajusz, K. Héberger, in *Applied Chemoinformatics: Achievements and Future Opportunities* (Eds.: J. Gasteiger, T. Engel), Wiley, **2018**, 471-499.

2. Which performance parameters are best suited to assess the predictive ability of models?
K. Héberger, A. Rácz, D. Bajusz, in *Advances in QSAR modeling with applications in Pharmaceutical, Chemical, Food, Agricultural and Environmental Sciences* (Ed.: K. Roy), Springer, **2017**, 89-104.

3. Chemical data formats, fingerprints and other molecular descriptions for database analysis and searching
D. Bajusz, A. Rácz, K. Héberger, in *Comprehensive Medicinal Chemistry 3rd edition* (Eds.: S. Chackalamannil, D. Rotella, S. Ward), Elsevier, **2017**, 329-378.

Lectures and posters

1. Discovery of new, covalent JAK3 inhibitors with innovative medicinal chemical approaches
Dávid Bajusz, György M. Keserű, *Onkoplatform 2019*, **Mátraháza**, Hungary, Nov 20,

2019

2. Comparison of performance parameters for machine learning classifiers
   Anita Rácz, Dávid Bajusz, Károly Héberger, *Conferentia Chemometrica 2019*, **Karcag**, Hungary, Sept 12, 2019

3. Data Fusion Methods as Consensus Scores for Ensemble Docking
   Dávid Bajusz, Anita Rácz, Károly Héberger, *Conferentia Chemometrica 2019*, **Karcag**, Hungary, Sept 12, 2019

4. Fingerprint similarity metrics in cheminformatics, metabolomics and other fields (poster)
   Dávid Bajusz, Anita Rácz, Károly Héberger, *Conferentia Chemometrica 2019*, **Karcag**, Hungary, Sept 8-12, 2019

5. Unsupervised data reduction: How to set the intercorrelation limits optimally? (poster)
   Anita Rácz, Dávid Bajusz, Károly Héberger, *Conferentia Chemometrica 2019*, **Karcag**, Hungary, Sept 8-12, 2019

6. Gyógyszerhatóanyagok szérum albumin kötődése és fajspecifikus vonatkozása
   György Tibor Balogh, Gergő Dargó, Dávid Bajusz, *Gyógyszerkémiai és Gyógyszertechnológiai Szimpózium*, **Kecskemét**, Hungary, Sept 6, 2019

7. QSAR behind the curtains: best practices by multi-level comparisons
   A. Rácz, D. Bajusz, K. Héberger, *SSC16: Scandinavian Symposium on Chemometrics*, **Oslo**, Norway, June 20, 2019

8. Similarity metrics for binary data structures in cheminformatics, metabolomics and other fields (poster)
   D. Bajusz, A. Rácz, K. Héberger, *SSC16: Scandinavian Symposium on Chemometrics*, **Oslo**, Norway, June 17-20, 2019

9. Chemometrics in cheminformatics – statistical evaluation of similarity metrics for interaction fingerprints (in Hungarian)
   A. Rácz, D. Bajusz, K. Héberger, *KeMoMo-QSAR 2019 symposium*, **Szeged**, Hungary, June 6, 2019

10. Similarity metrics and interaction fingerprints in rational drug design (in Hungarian)
    D. Bajusz, A. Rácz, K. Héberger, *Young Analysts' Conference 2018*, **Budapest**, Hungary, Nov 12, 2018

11. Similarity metrics under the magnifying glass: comparative study on metabolomic fingerprints (poster)
    A. Rácz, F. Andrić, D. Bajusz, K. Héberger, *Copenhagen School of Chemometrics 2018*, **Copenhagen**, Denmark, May 15-30, 2018

12. Comparison of similarity metrics for binary fingerprints (in Hungarian)
    D. Bajusz, A. Rácz, F. Andrić, K. Héberger, *Analytics Days 2018*, **Balatonszemes**, Hungary, Apr 24, 2018

13. Large-scale comparison of similarity metrics for metabolomic, molecular and interaction fingerprints (awarded lecture)
D. Bajusz, A. Rácz, F. Andrić, K. Héberger, *11th Winter Symposium on Chemometrics*, **St. Petersburg**, Russia, Mar 1, 2018

14. Similarity metrics under the magnifying glass: comparative study on metabolomic fingerprints (awarded poster)
A. Rácz, F. Andrić, D. Bajusz, K. Héberger, *11th Winter Symposium on Chemometrics*, **St. Petersburg**, Russia, Feb 26-Mar 2, 2018

15. Investigation of a protein-protein interaction (PPI) inhibitor with molecular dynamics
D. Bajusz, B. Wingelhofer, G. M. Keserű, R. Moriggl, 8*th Hungarian Schrödinger User Group Meeting*, **Budapest**, Hungary, Nov 22, 2017

16. Binary (dis)similarity measures for fingerprint analysis of plant extracts based on qualitative metabolomic data (poster)
F. Andrić, D. Bajusz, A. Rácz, K. Héberger, *Conferentia Chemometrica 2017*, **Gyöngyös-Farkasmály**, Hungary, Sept 3-6, 2017

17. Discovery of novel JAK1 and JAK2 inhibitors by customized virtual screening strategies (poster)
D. Bajusz, R. Kiss, A. Egyed, G. G. Ferenczy, G. M. Keserű, *Conferentia Chemometrica 2017*, **Gyöngyös-Farkasmály**, Hungary, Sept 3-6, 2017

18. Similarity metrics for molecular fingerprints: a large-scale comparison (poster)
D. Bajusz, A. Rácz, K. Héberger, *Conferentia Chemometrica 2017*, **Gyöngyös-Farkasmály**, Hungary, Sept 3-6, 2017

19. Is soft independent modeling of class analogies a reasonable choice for supervised pattern recognition? (poster)
A. Rácz, A. Gere, D. Bajusz, K. Héberger, *Conferentia Chemometrica 2017*, **Gyöngyös-Farkasmály**, Hungary, Sept 3-6, 2017

20. Interaction fingerprints and similarity metrics for virtual screening: a comparative study (poster)
A. Rácz, K. Héberger, D. Bajusz, *Conferentia Chemometrica 2017*, **Gyöngyös-Farkasmály**, Hungary, Sept 3-6, 2017

21. Large-scale comparison of interaction fingerprints and similarity metrics for virtual screening (poster)
A. Rácz, K. Héberger, D. Bajusz, *RICT 2017: Drug Discovery and Selection*, **Toulouse**, France, July 5-7, 2017

22. Ranking and grouping of computational and reversed phase thin-layer chromatographic lipophilicity indices (poster)
F. Andrić, D. Bajusz, A. Rácz, S. Šegan, K. Héberger, *RICT 2017: Drug Discovery and Selection*, **Toulouse**, France, July 5-7, 2017

23. Virtual screening in the discovery of novel JAK1 and JAK2 inhibitors (poster)
D. Bajusz, R. Kiss, A. Egyed, G. G. Ferenczy, G. M. Keserű, *RICT 2017: Drug Discovery*

and Selection, **Toulouse**, France, July 5-7, 2017

24. Large-scale comparison of similarity metrics for molecular fingerprints (poster)
D. Bajusz, A. Rácz, K. Héberger, *Math/Chem/Comp 2017*, **Dubrovnik**, Croatia, June 19-24, 2017

25. Why is soft independent modeling of class analogy no standard for classification? (poster)
A. Rácz, A. Gere, D. Bajusz, K. Héberger, *Math/Chem/Comp 2017*, **Dubrovnik**, Croatia, June 19-24, 2017

26. The jewel of class modeling techniques: why did SIMCA not become a standard? (in Hungarian)
A. Rácz, A. Gere, D. Bajusz, K. Héberger, *KeMoMo-QSAR 2017 symposium*, **Szeged**, Hungary, June 2, 2017

27. Investigation of a protein-protein interaction (PPI) inhibitor with equilibrium molecular dynamics (in Hungarian)
D. Bajusz, B. Wingelhofer, G. M. Keserű, R. Moriggl, *KeMoMo-QSAR 2017 symposium*, **Szeged**, Hungary, June 1, 2017

28. Similarity (or distance) metrics for molecular fingerprints (in Hungarian)
D. Bajusz, A. Rácz, K. Héberger, *Meeting of the Chemometrics Working Group of the Hungarian Academy of Sciences*, **Budapest**, Hungary, Apr 10, 2017

29. Identification of novel, selective Janus kinase inhibitors with computational methods
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Variations to four institutes*, **Budapest**, Hungary, Nov 24, 2016 (in Hungarian)

30. *n*-class ROC curves for the evaluation and visualization of classification methods – a case study of energy drinks
D. Bajusz, *Food Chemistry Day*, **Belgrade**, Serbia, Oct 25, 2016

31. Discovery of novel, potent inhibitors of Janus kinase 1 with virtual screening
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *KeMoMo-QSAR 2016 symposium*, **Miskolc**, Hungary, May 12, 2016 (in Hungarian)

32. Comparison of computational and thin layer chromatographic lipophilicity indices with chemometric methods
A. Rácz, F. Andrić, D. Bajusz, K. Héberger, *KeMoMo-QSAR 2016 symposium*, **Miskolc**, Hungary, May 12, 2016 (in Hungarian)

33. How to evaluate our models? Cross-validation vs. external validation
K. Héberger, D. Bajusz, A. Rácz, *Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences*, **Mátrafüred**, Hungary, Nov 5, 2015 (in Hungarian)

34. Revival of an Old Debate: Cross- vs. external validation in QSAR modeling
D. Bajusz, A. Rácz, K. Héberger, *Conferentia Chemometrica 2015*, **Budapest**, Hungary, Sept 16, 2015

35. Large Scale Statistical Comparison of Similarity Metrics for Fingerprint-based Calculations (poster)
A. Rácz, D. Bajusz, K. Héberger, *Conferentia Chemometrica 2015*, **Budapest**, Hungary, Sept 13-16, 2015

36. *n*-class ROC Curves as Novel, Intuitive Tools for Method Comparison (poster)
A. Rácz, D. Bajusz, K. Héberger, *Conferentia Chemometrica 2015*, **Budapest**, Hungary, Sept 13-16, 2015

37. Ensemble docking-based virtual screening reveals novel, subtype selective JAK2 inhibitors (poster)
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Computer Aided Drug Desing: Gordon Research Conference*, **West Dover, VT**, USA, July 19-24, 2015

38. Similarity metrics under the magnifying glass: a comparative study for fingerprint-based similarity calculations (poster)
A. Rácz, D. Bajusz, K. Héberger, *Computer Aided Drug Desing: Gordon Research Conference*, **West Dover, VT**, USA, July 19-24, 2015

39. Property-based characterization of ATP-site kinase inhibitor space for virtual screening (poster)
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Computer Aided Drug Desing: Gordon Research Seminar*, **West Dover, VT**, USA, July 18-19, 2015

40. Comparison and ranking of QSAR models and performance parameters (poster)
A. Rácz, D. Bajusz, K. Héberger, *Computer Aided Drug Desing: Gordon Research Seminar*, **West Dover, VT**, USA, July 18-19, 2015

41. Consistency of QSAR models: Correct split of training and test sets, ranking of models and performance parameters
K. Héberger, D. Bajusz, A. Rácz, *8th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources,* **Chios**, Greece, June 23, 2015

42. Virtual screening reveals novel Janus kinase inhibitors
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *KeMoMo-QSAR 2015 symposium*, **Szeged**, Hungary, May 14, 2015

43. A multi-step virtual screening approach for the identification of novel Janus kinase inhibitors
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *5th Hungarian Schrödinger User Group Meeting*, **Budapest**, Hungary, Nov 25, 2014

44. On the lookout for new drug candidates: virtual screening in drug discovery (guest lecture)
D. Bajusz, *Poznań University of Technology, Department of Organic Chemistry*, **Poznań**, Poland, Sept 18, 2014

45. Desirability function-based scoring scheme for ATP-site kinase inhibitors (poster)
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *EFMC-YMCS 2014: 1st EFMC Young Medicinal Chemist Symposium*, **Lisbon**, Portugal, Sept 12, 2014

46. Large-scale screening of public chemical databases to identify novel selective Janus kinase inhibitors (poster)
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *EFMC-ISMC 2014: XXIII International Symposium on Medicinal Chemistry*, **Lisbon**, Portugal, Sept 7-11, 2014

47. Discovery of novel, selective Janus kinase inhibitors by virtual screening
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *KeMoMo-QSAR 2014 symposium*, **Szeged**, Hungary, May 22, 2014 (in Hungarian)

48. Development of a virtual screening protocol to identify Janus kinase inhibitors
D. Bajusz, G. G. Ferenczy, G. M. Keserű, *Schrödinger Hungarian User Group Meeting*, **Budapest**, Hungary, Nov 26, 2013

49. Theoretical model and dynamics of the $P2Y_{12}$ receptor
D. Bajusz, L. Muszbek, I. Komáromi, *KeMoMo-QSAR 2013 symposium*, **Szeged**, Hungary, Apr 29-30, 2013 (in Hungarian)

50. Chemical reactions in the Os(VI)-Os(VIII)-periodate-formate system
D. Bajusz (supervisor: Dr. Gábor Lente), *XXXI. National Scientific Students' Associations Conference*, **Eger**, Hungary, Apr 4-6, 2013 (in Hungarian)

51. Oxidation of formate ion with periodate and osmium-tetroxide
D. Bajusz (supervisor: Dr. Gábor Lente), *XXX. National Scientific Students' Associations Conference*, **Pécs**, Hungary, Apr 27-29, 2011 (in Hungarian)

52. Reactions of the peroxomonosulfate ion with iodide and bromide
D. Bajusz (supervisor: Dr. Gábor Lente), *XXIX. National Scientific Students' Associations Conference*, **Debrecen**, Hungary, Apr 6-8, 2009 (in Hungarian)

53. Reactions of the peroxomonosulfate ion with halide ions (poster)
G. Lente, D. Bajusz, M. Takács, L. Veres, I. Fábián, *37th Inorganic Reaction Mechanisms Group Meeting*, **Barcelona**, Spain, Jan 9-12, 2008

54. Reactions of the peroxomonosulfate ion with halide ions
G. Lente, D. Bajusz, M. Takács, L. Veres, I. Fábián, *Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences*, **Gyöngyöstarján**, Hungary, Oct 25-26, 2007 (in Hungarian)