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## Список научных трудов

### Публикации в рецензируемых журналах:

1. Kireeva, N and Pervov, V.S. Materials Space of Solid-State Electrolytes: Unraveling Chemical Composition- Structure-Li Ionic Conductivity Relationships in Garnet-Type Metal Oxides Using Cheminformatics Virtual Screening Approaches. Submitted to *PhysChemChemPhys*
2. Pervov, V.S., Ovchinnikova, S.I., Medvedeva, A.E., Makhonina, E.V., Kireeva N.V. *Inorg Mater* (2016) 52: 83. doi:10.1134/S002016851601012X
3. Solov'ev, V., Kireeva, N., Ovchinnikova, S. and Tsivadze, A.Yu. *J Incl Phenom Macrocycl Chem* (2015) 83: 89. doi:10.1007/s10847-015-0543-6
4. Kireeva NV, Ovchinnikova SI, Tetko IV, Asiri AM, Balakin KV, Tsivadze AY Nonlinear Dimensionality Reduction for Visualizing Toxicity Data: Distance-Based Versus Topology-Based Approaches. *ChemMedChem* 9 (5):1047-1059. doi:10.1002/cmdc.201400027 Impact factor: 3.075 <http://onlinelibrary.wiley.com/doi/10.1002/cmdc.201400027/abstract>
5. Ovchinnikova S, Bykov A, Tsivadze A, Dyachkov E, Kireeva N Supervised extensions of chemography approaches: case studies of chemical liabilities assessment. *Journal of Cheminformatics* 6 (1):20 (2014) Impact factor: 3.59 <http://www.jcheminf.com/content/6/1/20/abstract>
6. Natalia V. Kireeva, Svetlana I. Ovchinnikova, Sergey L. Kuznetsov, Andrey M. Kazennov and Aslan Yu. Tsivadze Large Margin Nearest Neighbors Classifier as an Approach to Metric Learning. *Journal of Computer-Aided Molecular Design. Early View* (2014). Impact factor: 3.2 <http://www.springer.com/chemistry/physical+chemistry/journal/10822>
7. Baskin I.I., Kireeva N. and Varnek A. The One-Class Classification Approach to Data Description and to Models Applicability Domain. *Molecular Informatics*, 29, pp. 581-587 (2010). Impact factor: 2.338 <http://onlinelibrary.wiley.com/doi/10.1002/minf.201000063/abstract>
8. Kireeva N., Baskin I.I., Gaspar H.A., Horvath D., Marcou G. and Varnek A. Generative Topographic Maps (GTM) as a Universal Tool for Data Visualization, Predicting Activity Profiles and Comparison of Databases. *Molecular Informatics*, 31, pp.301-312 (2012). Impact factor: 2.338 <http://onlinelibrary.wiley.com/doi/10.1002/minf.201100163/abstract>
9. Bonachera, F., Marcou, G., Kireeva, N., Varnek, A., Horvath D. Using Self-Organizing Maps to Accelerate Similarity Search. *Bioorganic and Medicinal Chemistry*, 20, pp. 5396-5409 (2012). Impact factor: 2.903 <http://www.sciencedirect.com/science/article/pii/S0968089612002994>
10. Kireeva N. , Kuznetsov S.L. and Tsivadze A.Yu. Toward Navigating Chemical Space of Ionic Liquids: Prediction of Melting Points Using Generative Topographic Maps. *Industrial & Engineering Chemistry Research*, 51, pp. 14337-14343 (2012). Impact factor: 2.206 <http://pubs.acs.org/doi/abs/10.1021/ie3021895>
11. Solov'ev V. P., Kireeva N, Tsivadze A.Yu and Varnek A. QSPR Ensemble Modeling of Alkaline-Earth Metal Complexation. *J. Inc.Phenom. and Macrocycl. Chem.*, 76, pp 159-171 (2013) Impact factor: 1.399 <http://link.springer.com/article/10.1007/s10847-012-0185-x>
12. Kireeva N. , Kuznetsov S.L., Bykov A.A. and Tsivadze A.Yu. Towards in silico identification of the human ether-a-go-go-related gene channel blockers: discriminative vs. generative classification models. *SAR & QSAR in Environmental Research*, 24 (2013) 103-117. Impact factor: 1.667 <http://www.tandfonline.com/doi/full/10.1080/1062936X.2012.742135>

### Публикации в научных сборниках и материалах научных мероприятий:

1. N.Kireeva and V.S. Pervov "Unraveling Composition-Structure-Ionic Conductivity Relationships in Garnet-Type Solid Electrolytes Using Cheminformatics Approaches" 41st International Conference and Exposition Advanced Ceramics and Composites, January 22-27, 2017, Daytona Beach, Florida, USA
2. Natalia Kireeva, Alexandre Petrov, Denis Ostroumov, Vitaly P. Solov'ev, Vladislav S. Pervov Prediction of the functional properties of electroceramic materials using cheminformatics approaches 11th German Conference on Cheminformatics (GCC 2015) Fulda, Germany. 8–10 November 2015
3. Kireeva N., Ovchinnikova S.I., Pervov V.S., Zotova A.E and Tsivadze A.Yu. *Prediction of the functional properties of electroceramic materials for SOFCs using cheminformatics approaches* 248th National Meeting and Exposition August 10-14, 2014, San Francisco, USA
4. Natalia Kireeva, Svetlana Ovchinnikova, Anna Zotova, Aslan Tsivadze *Prediction of transport properties of electroceramic oxide systems for SOFCs using cheminformatics approaches* EuroQSAR 2014, August 31 - September 4, St-Petersbourg, Russia
5. Svetlana Ovchinnikova, Vladimir Chupakhin, Natalia Kireeva, Vladimir Talismanov, Aslan Tsivadze *Mining with imbalanced data: modeling strategies for classification and visualization* EuroQSAR 2014, August 31 - September 4, St-Petersbourg, Russia
6. Natalia Kireeva, Svetlana Ovchinnikova, Sergey Kuznetsov, Andrey Kazennov, Aslan Tsivadze *Impact of distance-based metric learning on classification and visualization model performance and structure-activity landscapes* EuroQSAR 2014, August 31 - September 4, St-Petersbourg, Russia
7. Ovchinnikova S.I., Tsivadze A.Yu. and Kireeva N. *Applying Methods of Machine Learning for Assessment of Chemical Liabilities*, 9th AFMC International Medicinal Chemistry Symposium, October 15-18, 2013, Taipei, Taiwan.
8. Kireeva N., Ovchinnikova S.I. and Tsivadze A.Yu. *Nonlinear Dimensionality Reduction for Visualizing Toxicity Data: Distance-Based vs Topology-Based Approaches*, 9th AFMC International Medicinal Chemistry Symposium, October 15-18, 2013, Taipei, Taiwan.
9. Kireeva N., Ovchinnikova S.I. and Tsivadze A.Yu. *Supervised Generative Topographic Mapping for In Silico Assessment of Chemical Liabilities*, 246th National Meeting and Exposition "Chemistry In Motion", September 8-12, 2013, Indianapolis, USA.
10. Kireeva N., Varnek A., Baskin I.I., Kuznetsov S.L. and Tsivadze A.Yu. *Large Margin Nearest Neighbors Classifier as an Approach to Metric Learning*. 13th Tetrahedron Symposium. 27 - 30 November 2012, Taipei, Taiwan.
11. Kireeva N., Baskin I.I., Gaspar H.A. and Varnek A. *Generative Topographic Mapping: an Universal Approach for Data Processing in Cheminformatics*. 22nd International Symposium on Medicinal Chemistry. September 2 - 6, 2012, Berlin, Germany.
12. Kireeva N., Baskin I.I. and Varnek A. *Design of "Optimal" Descriptor Spaces for Data Visualization and Modeling*. 3rd Strasbourg Summer School on Cheminformatics. 25-29 June 2012, Strasbourg, France.
13. Kireeva N, Baskin I.I., Kuznetsov S.L., Dyachkov E.P. and Varnek A. *Generative Topographic Maps (GTM) as a universal tool for data visualization, applicability domain analysis, structure-activity modeling and comparison of databases*. 8th Winter Symposium on Chemometrics (WSC-8 Symposium) February 27–March 2, 2012, Drakino, Russia.