Stanislav
Geidl

geidl.stanislav@gmail.com | Czech nationality | 32 years old

Education and Academic Qualifications

Ph.D. 2013 – now
Chemoinformatical methods for prediction of physico-chemical properties of molecules
Biomolecular Chemistry and Bioinformatics
Supervisor: Prof. RNDr. Jaroslav Koča, DrSc.
Faculty of Science, Masaryk University,
Brno, Czech Republic

Advanced Master's study (2016)
Influence of molecular 3D structure on quality of pKa prediction
Biomolecular Chemistry
Faculty of Science, Masaryk University,
Brno, Czech Republic

Master study (2011 – 2013)
Predicting pKa values from EEM atomic charges
Chemoinformatics and Bioinformatics
Supervisor: Prof. RNDr. Jaroslav Koča, DrSc.
Faculty of Science, Masaryk University,
Brno, Czech Republic

Bachelor study (2009 – 2011)
pKa prediction based on atomic charges
Chemoinformatics and Bioinformatics
Supervisor: Prof. RNDr. Jaroslav Koča, DrSc.
Faculty of Science, Masaryk University,
Brno, Czech Republic

Working Experiences

- Senior Software Engineer (Sep 2020 - now) at Kiwi.com
- Technical Team Lead (Jan 2020 - Sep 2020) at Kiwi.com
- Automation Developer (Oct 2018 - Jan 2020) at Kiwi.com
- Automation Junior Developer (Jan 2018 - Oct 2018) at Kiwi.com

Scientific and Research Activities

Chemoinformatics (QSPR prediction of physico-chemical properties, quantum mechanical and empirical charge calculation approaches)

Structural bioinformatics (superimposition and validation of molecular structures)

Skills

Chemoinformatics and bioinformatics

Methods: QSPR and QSAR modeling, quantum mechanical calculations, docking, superimposition of molecular structures, atomic charge calculation
Software: Gaussian, Corina, RDKit, AIMAll, OpenBabel, R, PyMol, AutoDock Vina, Balloon

IT skills

Python, C++, C#, Perl, PHP, SQL, bash, R, Windows, Mac OS X, Unix, Microsoft Office, LaTeX

Language skills

English – professional working proficiency, German – elementary proficiency, Czech – native

Awards

- Best poster prize (2014) in *20th EuroQSAR - Understanding Chemical-Biological Interactions*
- Dean's price (2013)
- Student bursary (2013) for *6th Joint Sheffield Conference on Chemoinformatics*

Teaching Activities

Seminar tutor

- *WWW publishing* (in czech, autumn 2010 – autumn 2012)
- *Advanced Chemoinformatics* (in czech, spring 2014 - autumn 2018)
- *Introduction to programming in Python* (in czech, autumn 2014 - autumn 2018)

Supervisor of thesis

- Václav Hejret: *Prediction of physico-chemical properties via charge descriptors* (Master's thesis, 2017)
- Alžběta Türková: *Parametrization of EEM Approach for Calculation of Charges in Proteins* (Bachelor's thesis, 2015)
- Václav Hejret: *Charge Descriptors Application in Chemoinformatics* (Bachelor's thesis, 2015)
- Lukáš Petrusek: *Influence of structure optimization on the quality of QSPR models for pKa prediction* (Bachelor's thesis, 2014)

Consultant of thesis

- Adam Midlik: *Selection of protein fragments using minimal bond breaking* (Bachelor's thesis, 2014)
- Kateřina Beková: *Data preparation for creating of plant alkaloids structure database* (Bachelor's thesis, 2014)
- Tomáš Bouchal: *QSPR models for pKa prediction* (Bachelor's thesis, 2012)

Publications

Books

- Koča J, Svobodová Vařeková R, Pravda L, Berka K, Geidl S, Otyepka M: **Structural Bioinformatics Tools for Drug Design.** *Springer International Publishing, Cham* 2016.

Articles in impact journals

- Raček T, Pazúriková J, Svobodová Vařeková R, Geidl S, Křenek A, Falginella FL, Horský V, Hejret V, Koča J: **NEEMP: Software for validation, accurate cal- culation and fast parameterization of EEM charges**. *J Cheminf* 2016, **8**:1.
- Ionescu CM, Sehnal D, Falginella FL, Pant P, Pravda L, Bouchal T, Vařeková Svobodová R, Geidl S and Koča J: **AtomicChargeCalculator: Interactive Web-based calculation of atomic charges in large biomolecular complexes and drug like molecules**. *J Cheminf* 2015, **7**(50).
- Geidl S, Bouchal T, Raček T, Svobodová Vařeková R, Hejret V, Křenek A, Abagyan R and Koča J: **High-quality and universal empirical atomic charges for chemoinformatics applications**. *J Cheminf* 2015. (Shared first authorship of SG, TB and TR)
- Geidl S, Svobodová Vařeková R, Bendová V, Petrusek L, Ionescu CM, Jurka Z, Abagyan R and Koča J: **How Does the Methodology of 3D Structure Preparation Influence the Quality of pK(a) Prediction?** *J Chem Inf Model* 2015, **55**(6): 1088-1097. (Shared first authorship of SG and RSV)
- Sehnal D, Svobodová Vařeková R, Pravda L, Ionescu CM, Geidl S, Horský V, Jaiswal D, Wimmerová M and Koča J: **ValidatorDB: database of up-to-date validation results for ligands and non-standard residues from the Protein Data Bank**. *Nucleic Acids Res* 2015, **43**: D369-D375.

- Svobodová Vařeková R, Jaiswal D, Sehnal D, Ionescu CM, Geidl S, Pravda L, Horský V, Wimmerová M and Koča J: **MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes.** *Nucleic Acids Res* 2014, **42**: W227-W233.
- Ionescu CM, Geidl S, Svobodová Vařeková R, Koča J: **Rapid Calculation of Accurate Atomic Charges for Proteins via the Electronegativity Equalization Method.** *J Chem Inf Model* 2013, **53**(10): 2548-2558.
- Geidl S, Svobodová Vařeková R, Ionescu CM, Skřehota O, Bouchal T, Sehnal D, Abagyan RA and Koča J: **Predicting pK_a values from EEM atomic charges.** *J Cheminf* 2013, **5**(18). (Shared first authorship of SG and RSV)
- Sehnal D, Svobodová Vařeková R, Huber HJ, Geidl S, Ionescu CM, Wimmerová M and Koča J: **SiteBinder: An Improved Approach for Comparing Multiple Protein Structural Motifs.** *J Chem Inf Model* 2012, **52**(2): 343-359.
- Svobodová Vařeková R, Geidl S, Ionescu CM, Skřehota O, Kudera M, Sehnal D, Bouchal T, Abagyan R, Huber HJ, Koča J: **Predicting pK_a values of substituted phenols from atomic charges: Comparison of different quantum mechanical methods and charge distribution schemes.** *J Chem Inf Model* 2011, **51**(8): 1795-1806.

Selected posters

- Geidl S, Svobodová Vařeková R, Petrusek L, Ionescu CM, Sehnal D and Koča J: **How the methodology of 3D structure preparation influences the quality of pKa prediction?** 20th EuroQSAR - Understanding Chemical-Biological Interactions, St. Petersburg, Russia, 2014.
- Geidl S, Sehnal D, Ionescu CM, Svobodová Vařeková R, Pant P and Koča: **Web server for the rapid calculation of empirical atomic charges with QM accuracy.** 10th International Conference on Chemical Structures and the 10th German Conference on Chemoinformatics -Noordwijkerhout, Netherlands, 2014.
- Geidl S, Ionescu CM, Svobodová Vařeková R and Koča J: **QM quality atomic charges for proteins**. 9th German Conference on Chemoinformatics - Fulda, Germany, 2013.
- Bouchal T, Svobodová Vařeková R, Raček T, Ionescu CM, Geidl S, Krenek A and Koča J: **Empirical charges for chemoinformatics applications**. 9th German Conference on Chemoinformatics - Fulda, Germany, 2013.
- Geidl S, Svobodová Vařeková R, Ionescu CM, Skřehota O, Bouchal T, Sehnal D and Koča J: **Predicting pKa Values from EEM Atomic Charges**. 6th Joint Sheffield Conference on Chemoinformatics - Sheffield, United Kingdom, 2013.
- Geidl S, Svobodová Vařeková R, Ionescu CM, Skřehota O, Bouchal T, Kudera M, Sehnal D, Abagyan RA and Koča J: **Predicting pK_a values of substituted phenols by QSPR models which employ EEM atomic charges**. 3rd Strasbourg Summer School on Chemoinformatics - Strasbourg, France, 2012.
- Geidl S, Beránek R, Svobodová Vařeková R, Bouchal T, Brumovský M, Kudera M, Skřehota O and Koča J: **How the methodology of 3D structure preparation influences the quality of QSPR models?** 7th German Conference on Chemoinformatics - Goslar, Germany, 2011.