



Cheminformatics: Supporting innovation through open data

Skylight Hall, Expocentre, Moscow

Friday 24th October

9.00-9.30	Registration
9.30-10.30	An introduction to data and cheminformatics at the Royal Society of Chemistry: Building a Global Chemistry Network at the RSC Valery Tkachenko, <i>Royal Society of Chemistry</i>
10.30-11.00	Exposing Russian science to the rest of the world: Publishing, micropublishing, data sharing, and collaborating with the RSC Sergey Vatsadze, <i>Moscow State University</i>
11:00-11:30	Tea and coffee break
11:30-12:00	Open components as a part of roadmap for RSC cheminformatics Valery Tkachenko, <i>Royal Society of Chemistry</i>
12:00-12:30	The condensed graph of reaction approach for different tasks of reaction mining Timur Madzhidov, <i>Kazan Federal University</i>
12:30-13:00	Universal Organic Chemistry Toolkit: Indigo, Bingo, Imago, Ketcher Alexander Savelyev, <i>EPAM</i>
13:00-14:00	Lunch
14:00-14:45	Prediction of Activity Spectra for Substances (PASS): From biological activity profiling to computation chemical systems biology Vladimir Poroiko, <i>Institute of Biomedical Chemistry</i>
14:45-15:15	Software for prediction and identification of components in complex LC-MS runs: Impurities, Metabolites and Degradants Vitaly Lashin, <i>Advanced Chemistry Development</i>
15:15-15:45	Computer-Assisted Structure Elucidation (CASE) – Quicker ways to novel chemical structures that don't require correction Mikhail Elyashberg, <i>Advanced Chemistry Development</i>
15:45-17:00	Open Discussion
17:00-17:30	Networking