RDKit User Group Meeting 2013
October 2-4, European Bioinformatics Institute, Hinxton, UK

Open-Source Cheminformatics
and Machine Learning

Agenda

Day 1

9:15 Registration
9:45 Welcome + Introduction
10:00 Intro to the RDKit: History and Status
11:00 How is everyone using the RDKit? Lightning talks
12:00 Lunch
13:00 Sereina Riniker: Benchmarking of 2D Fingerprints and Machine-Learning Methods
13:30 Jameed Hussain: Fraggle, A New Similarity Algorithm
14:00 Gregori Gerebtzoff: LUCID: Supervised Multidimensional Optimization of Compounds Using Matched Molecular Pairs
14:30 Anthony Bradley: 3D Matched Molecular Pair tool using RDKit, the PDB and ChEMBL
15:00 Coffee break
15:30 Francis Atkinson: Compound Standardization
16:00 Roger Sayle: RDKit Gems
16:30 Greg Landrum: Not Just For Molecules: Reaction Fingerprints
17:00 End of day
Evening: Social Activity

Day 2

9:30 Nicholas Firth: Lessons Learnt Using RDKit for Multi-Objective Optimisation
10:00 Tjelvar Olsson: Creating A Conformer Validation Test Set Using RDKit And The Cambridge Structural Database
10:30 Paolo Tosco: Bringing MMFF to the RDKit
11:00 Coffee break
11:30 Michal Nowotka: Beaker - RDKit in the Bottle on Tornado
12:00 George Papadatos: Clippy - A Little wx Widget Based On RDKit Web Services
12:30 Lunch
13:30 Roundtable: What's missing, what needs to be improved?
14:30 Coffee break
15:00 Tutorials and free-form hacking
15:00 Christo Kannas: ESOL/Diversity Filter
15:30 Nikolas Fechner: Pandas and SciKit Learn
16:00 Jameed Hussain: MMPA
17:00 End of day
Evening: Social Activity

Day 3 (Optional)

Hackathon – Topics to be picked onsite