

Preliminary Schedule Workshop LSERD

Monday, 14. November 2016

09:30 – 10:30 Welcome and introduction to the concept of pp-LFERs *Kai-Uwe Goss*

10:30 – 11:00 Coffee break

11:00 – 12:00 Introduction and demonstration of the on-line database *Nadin Ulrich*

12:00 – 14:00 Lunch, discussions, time to practice

14:00 – 15:00 Biopartitioning *Satoshi Endo*

15:00 – 15:30 QSARs for predicting missing descriptors *Trevor Brown*

15:30 – 17:00 Coffee and time to practice, discussions in smaller groups

17:00 – 18:00 Pitfalls, exceptions *Kai-Uwe Goss/Satoshi Endo*

19:00 Dinner in the city

Tuesday, 15. November 2016

9:00 – 10:00 Partitioning of Ions: experimental data, concepts predictive models

- Partitioning of organic ions to proteins *Luise Henneberger*
- Partitioning to membranes *Kai Bittermann*

10:00 - 10:15 Coffee break

10:15 – 12:00 Partitioning of ionics: experimental data, concepts predictive models

- Chemical space partitioning for ions *Nadin Ulrich*

12:00 – 14:00 Lunch and time for discussions

End of workshop