Provisional roadmap/milestones

Application of AI/Machine Learning in Chemical Discovery and Development

AI/ML methodology

- Interpretability of model
  - Validated with high throughput experimentation
  - Mathematical representation of research questions
- High quality benchmarking datasets
- Measurement of diversity in datasets
- Benchmarking and metrics tools
- Confidence and uncertainty
- Adaptive models which improves with more data
- Guidelines/standard practice
- Motivation for data deposition
- Community-owned-database

Data

- Standards and formats for data reporting
- Metadata
- Tools for data extraction and data curation
- Motivation for data deposition
- Community-owned-database
- Data sharing:
  - Sharing information and models based on in-house data
  - Standardised data structures and sharing agreements

Areas of application

- Route design/reaction outcome prediction
- Reaction/process optimisation including workup and purification
- Predicting reactivity, selectivity and properties
- Molecular and material discovery

Reaction prediction and optimisation

- Standard approaches to descriptors development
- Extrapolation outside the chemical space covered by the training set
- Prediction of relative reactivity
- Getting data from negative results
- Multi-objective optimisation
- Community challenges and competitions

Predicting properties and activity

- Solubility
- Formulation
- Crystal structure and lattice energy
- Biological activity
- Controlling protein-protein interaction

Wider engagement

- Summer school
- Secondments
- Community hub
- Showcasing