

# Reaction InChI Workshop Results

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# Agenda

- Introduction to Reaction – InChI
- Status – Implementations
  - Feedback for additional vendors to be contacted
- Requirement gathering
  - Technical enhancements
    - Potential overlap with the usage of special characters in some search systems
  - Input/export formats
  - Handling of equilibrium reactions

# Agenda

- **Requirement gathering**
  - **Reaction representation**
    - Reaction normalization
    - Stereochemistry and tautomer issue
      - Preferred parameter settings
  - **Recalculation of reactions from RInChI**
    - InChI based problem to rebuild stereoisomers and tautomers
  - **ProcAuxInfo**
    - Presentation of ideas described in paper by Philipp-Maximilian Jacob et al, University of Cambridge
  - **Generic transformations**
    - Starting to search for solution for simple generic reactions
  - **MInChI compatibility**

# Feedback to RInChI group

Please, send your feedback and ideas for the next RInChI release to

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