Reaction InChI
Workshop
Results

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InChI workshop at the NIH, Bethesda (MD)
August 16th to 18th, 2017
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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