RInChI Status

InChI meeting San Diego
August 23rd to 24th, 2019

David Nicolaides, Gerd Blanke, Günter Grethe, Hans Kraut, István Öri, Jan Holst Jensen, Jonathan Goodman
Current status

- RInChI 1.0 released in March 2017
- Since summer 2018 the RInChI group has been working on the next release.
  - The currently active members are

<table>
<thead>
<tr>
<th>Name</th>
<th>Company/Location</th>
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<tbody>
<tr>
<td>David Nicolaides</td>
<td>Biovia, Cambridge, UK</td>
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<tr>
<td>Gerd Blanke</td>
<td>StructurePendium Technology GmbH, Essen</td>
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<td>Günter Grethe</td>
<td>Poway, CA</td>
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<td>Hans Kraut</td>
<td>InfoChem GmbH, Munich</td>
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<td>István Öri</td>
<td>ChemAxon Ltd, Budapest</td>
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<td>Jan Holst Jensen</td>
<td>Biochemfusion ApS, Copenhagen</td>
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<tr>
<td>Jonathan M. Goodman</td>
<td>University of Cambridge, UK</td>
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Current Status

• Public RInChI presentations in 2018/19:
  • Talk at the Biovia community days in Brussels by David Nicolaides and Gerd Blanke, November 2018
    • Presentation of RInChI in Biovia/Draw
  • Talk at the ChemAxon UGM in Budapest by István Öri and Gerd Blanke, May 2019
    • Presentation of RInChI in Marvin by István Öri
  • Talk at the ACS Fall meeting by Gerd Blanke, August 2019

• Publications
  • International chemical identifier for reactions (RInChI), Grethe et al. J Cheminform (2018) 10:22 (May 2018)
    • https://doi.org/10.1186/s13321-018-0277-8
Current Status

• Group meetings
  • Biweekly Skype conferences
  • Group meeting during the InChI Meeting in Cambridge, February 2019
  • Group meeting during the RDKit UGM in Cambridge, October 2018
    • Most of the group members were present
    • Exchange with Jarek Tomczak for the UDM project of Pistoia Alliance
  • Experiences:
    • A one day personal meeting may save up to 4 months of biweekly phone conferences
Current Status

• RInChI implementations by cheminformatics software vendors
  • The Biovia software packages Draw, Direct and Pipeline Pilot (version 2019, released in December 2018) include RInChI
Current Status

• RInChI implementations by cheminformatics software vendors
  • ChemAxon introduced RInChI into its 2019 rlass
Current Status

- First publisher introducing RInChI
  - Beilstein Institute, Frankfurt (Main), Germany
Planned enhancements for the next RInChI release

- Defined for next release
  - Technical issues
  - Additional input and output formats
  - Reaction mapping (MapAuxInfo)
  - Workaround for stereochemistry restrictions
  - Support for AI/ML in reaction prediction
    - Class code layer for reaction similarity clustering and pathway optimization, InfoChem tool
Atom mapping (Example Quinone reduction)

Quinone reduction
RInChI=1.00.1S/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H<>C6H6O2/c7-5-1-2-6(8)4-3-5/h1-4,7-8H/d+

Mapping for each atom (including layer and molecule)
2-1-1 <> 3-1-1  2-1-5 <> 3-1-5
2-1-2 <> 3-1-2  2-1-6 <> 3-1-6
2-1-3 <> 3-1-3  2-1-7 <> 3-1-7
2-1-4 <> 3-1-4

Skip the trailing 2 and 3 as they are defined by the reaction separator “<>” and the 4th layer is not available
1-1 <> 1-1  1-5 <> 1-5
1-2 <> 1-2  1-6 <> 1-6
1-3 <> 1-3  1-7 <> 1-7
1-4 <> 1-4

MapAuxInfo=1.00.1/1-1<>1-1;1-2<>1-2;1-3<>1-3;1-4<>1-4;1-5<>1-5;1-6<>1-6;1-7<>1-7
Stereochemistry example

- **Standard InChI**
- **Additional stereo layer at the of the RInChI string marked by “/st”**
- **Use atom identification developed for atom mapping**
- **Group related centers by brackets**
  - Use “mix” to indicate mixtures including racemates
  - Use “pu” to identify pure but unknown centers
Planned enhancements for the next RInChI release

• To be discussed (in the breakout session)
  • How to handle tautomer restrictions
    • Need exchange with Marc’s tautomer group
  • Failing reactions
    • Format has not yet been defined
• Support for AI/ML in reaction prediction
  • Class codes by InfoChem
  • Reaxys formats (discussion with Elena Herzog and Markus Fischer if any and which data formats of Reaxys may be suitable)
  • Reaction properties (ProcAuxInfo)
Planned enhancements for later releases

• Depending on InChI progress
  • Make use of positional isomers and Markush representations for InChI
  • InChI support for enhanced stereochemistry
Thank you