

Reaction InChI

Status

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InChI workshop at the NIH, Bethesda (MD)

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Status

- First release in March 2017
- First tests based on the SAVI project by Marc Niklaus and Wolf-Dieter Ihlenfelder
- RInChIs for 4.5 million reaction of SPRESI generated by InfoChem (Hans Kraus and colleagues)

Status - Implementations

- **Drawing tool implementations**
 - Discussions for Biovia/Draw and Marvin (ChemAxon)
 - Open: ChemDraw, OpenEye
- **Publishers**
 - SpringerNature very active
 - Elsevier: contacted but no feedback
 - Clarivate Analytics (Former IP & Science business of Thomson Reuters): started testing with release 0.03 but no feedback

Status – Requirements gathering for next release

- **Technical enhancements**
 - Adapt to latest InChI release (currently 1.05)
 - Remove hurdles for C compiler
 - Tread safe
 - Rework Apple make file / RInChI for Mac
- **Additional input formats**
 - Especially InChI with reaction roles
- **Additional export formats**
 - Include InChI with roles

Status – Requirements gathering for next release

- **Reaction representation:**
 - Details of reaction normalization
 - Restrictions by Standard InChIs
 - Stereochemistry
 - Tautomers
 - Introduction of ProcAuxInfo
 - Extension to generic transformations
- **Make sure that Mixture-InChIs can be used within Reactions**