

Questionnaire for InChI/InChIKey Users and Manufacturers

Prepared by GGA Software Services LLC, Cambridge, Massachusetts, on November 24, 2010

- 1. How do you use InChI/InChIKey in your work?**
 - Storing chemical structures*
 - Searching chemical structures*
 - Normalizing chemical structures*
 - Linking to publications or web sites*
 - Having other web sites or publications linked to you*
- 2. Do you use standard or non-standard InChI/InChIKeys or both?**
 - Standard*
 - "SNon"*
 - "FixedH"*
 - Other (if so, which parameters do you use?)*
- 3. What computer operating system do you use?**
 - Windows*
 - Linux*
 - Mac OS*
 - Other (specify)*
- 4. Is InChI input allowed in your software system?**
 - Yes*
 - No*
- 5. What, if any, other input is used for chemical structures?**
 - Molfile*
 - SMILES*
 - CML*
 - other (specify)*
- 6. Do you provide an InChI/InChIKey lookup?**
 - Yes*
 - No*
- 7. Are there any instances in which only an InChIKey is provided?**
 - Yes (if so, how do you obtain the actual InChI/structure?)*
 - No*

8. Which programming platform do you use for your software?

Portable C/C++

Java

.NET

Python

Ruby

Other (specify)

9. Is your InChI software based on the existing IUPAC InChI implementation?

Yes

No (if so, what implementation is used?)

10. What features would you like to be added to the InChI format?

Markush structures

Pseudo-atoms

Polymers

Organometallics

Special kinds of stereochemistry (specify)

Other (specify)

11. What user interface would you prefer for the InChI implementation?

Command-line desktop application

GUI desktop application

Mobile application

Web interface

Other (specify)

12. What kind of API would you prefer for the InChI implementation?

Plain C interface

C++ library

Java library

.NET library

Python library

Ruby library

Javascript library

SOAP web service

REST web service

Other (specify)