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**INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY**

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QR Code InChI

IUPAC & InChI Trust Project

Connecting Physical & Digital worlds

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I U P A C VISION

IUPAC is an indispensable resource for chemistry.



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MISSION

The International Union of Pure and Applied Chemistry is the global organization that provides *objective scientific expertise* and *develops the essential tools for the application and communication of chemical knowledge* for the benefit of humankind and the world.



I**U****P****A****C****MISSION**

The International Union of Pure and Applied Chemistry accomplishes its mission by

- Fostering sustainable development
- Providing a common language for chemistry
- Advocating the free exchange of scientific information



QR Code Recommendations

- The InChI QR code should have the IUPAC name above the QR Code and InChI or InChIKey below.
- The use of the IUPAC logo in addition to IUPAC would be allowed.

IUPAC



InChIKey

QR Code Recommendations

- The InChI QR code will contain the InChI/InChIKey for the major or most significant component in the container.
- The compound name that would be expected to be on the bottle should be used.

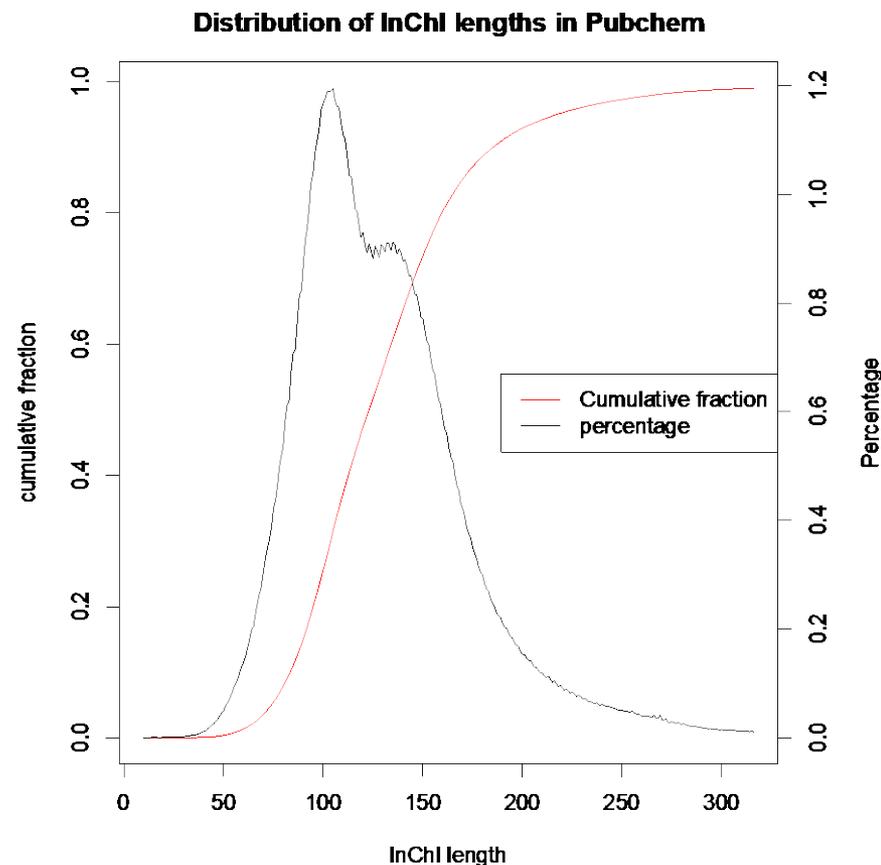
IUPAC



InChIKey

QR Code Recommendations

- For small molecules and those with a compact InChI (for example with less than about 150 Characters) the InChI QR Code may contain the actual InChI in the form of InChI = 'InChi text'.



QR Code Recommendations

- In the general case the InChI Key should be used to ensure that the whole InChI can be captured with a moderate sized QR code with good accuracy.
- The QR code should then contain a string of the form `InChIkey = 'InChI key text'`.

QR Code Recommendations

- The option to specify a resolver for the InChI Key, to ensure the InChI Key can be resolved is allowed, but...
- The search string should explicitly contain the text InChIkey = 'InChI key text' so that a QR code reader (or a specific InChI App) can recognise the presence of an InChI Key and provide alternative resolution and information if required.

QR Code Recommendations

- The direct use of a link to a specific entry on a web site or database would not be allowed if it by-passed:

InChIkey = 'InChI key text'

QR Code Recommendations

- Providing additional information alongside the InChI Key is allowed, subject to the information carry capacity of the chosen QR code.
 - Batch numbers
 - Sample/organisational code numbers
 - Purity

QR Code Recommendations

- The QR InChI code should as far as possible be constructed in a way that always does something useful when read by a general QR code reader that would offer the ability to look up a url or present the text in the QR code to a general search engine.

QR Code Recommendations

- IUPAC and the Trust should provide an easy to use and free web service to create the QR codes for the InChI and InChI Key. This would most simply be added as part of the existing service to create an InChI and InChI Key and to the InChI code.

QR Code Recommendations

- That IUPAC and the Trust commission a QR InChI app (ideally for IOS and Android) that would read the InChI QR code and then enable the users to make the most of the InChI enabled services that exist worldwide.

QR Code Status

- We have a near-final draft of the written recommendation.
- Coding and Apps
- Resolvers
- Engagement, as needed, with users.