

InChI V2

...a few thoughts and questions

What should go into InChI[Key] V2?

- More comprehensive handling of tautomerism
 - Making the FixedH layer mandatory
 - Add another layer to InChIKey: specific tautomer
 - Lengthening of InChIKey blocks?
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- In which sequence should other extensions be added?

Reduce collision risk



V2



Specific tautomer



HNDVDQJCIGZPNO**NE**-YFKPBYRVSB-N--LSKNCSLA

If molecule has no tautomers (e.g. benzene):

UHOVQNZJYSORNB**OB**-UHFFFAOYSB-N--NOTTAUTO

Searches with InChIKey V2

Full-tautomer search:

HNDVDQJCIGZPNO~~NE~~-YFKPBYRVSB-N--LSKNCSLA

Tautomer-invariant search:

HNDVDQJCIGZPNO~~NE~~-YFKPBYRVSB-N

InChIKey V1 search:

HNDVDQJCIGZPNO-YFKPBYRVSA-N

...Google should be able to handle this