

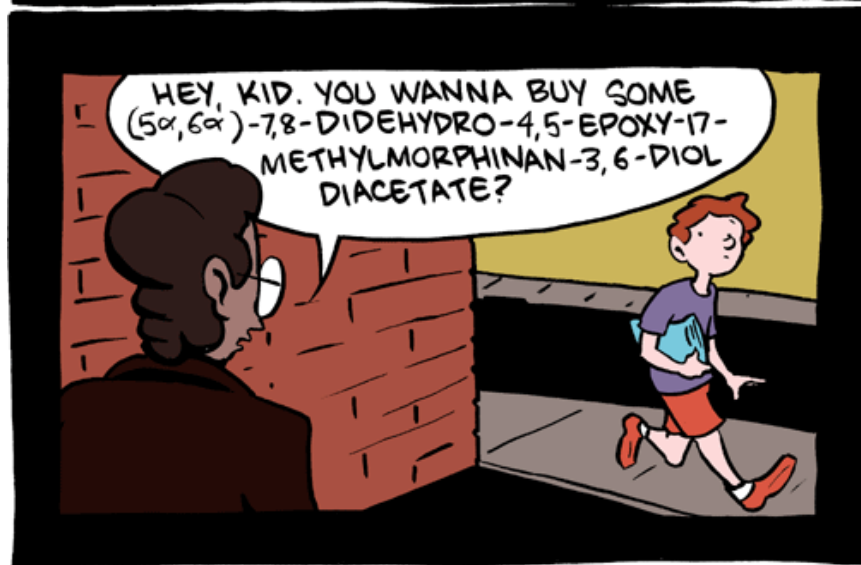
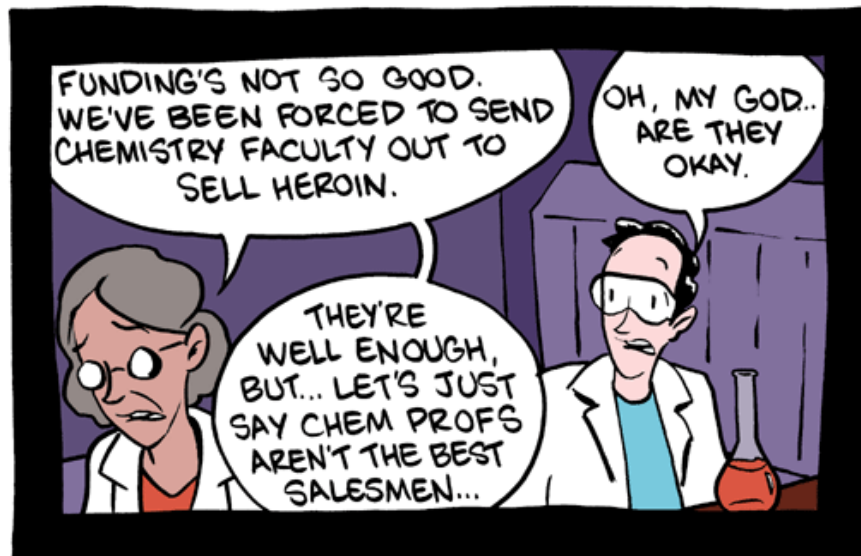
# Reliably converting names to structures with ChemAxon tools

**Daniel Bonniot**

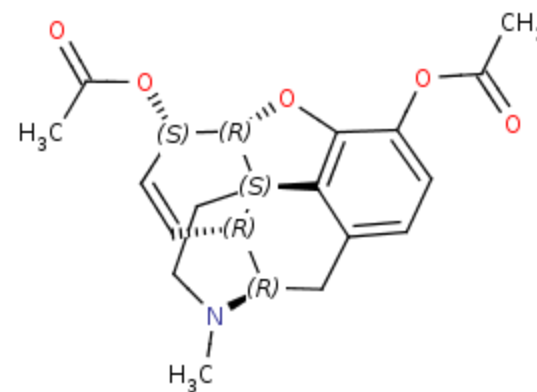
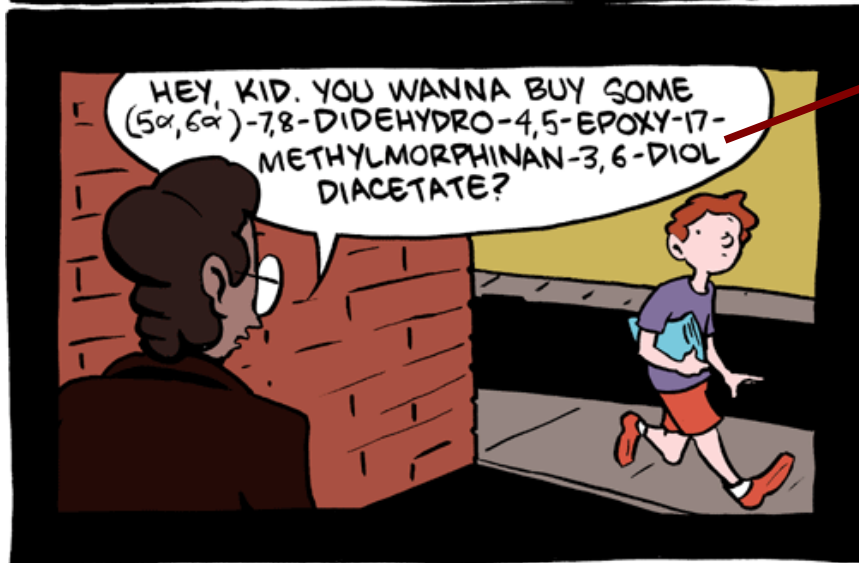
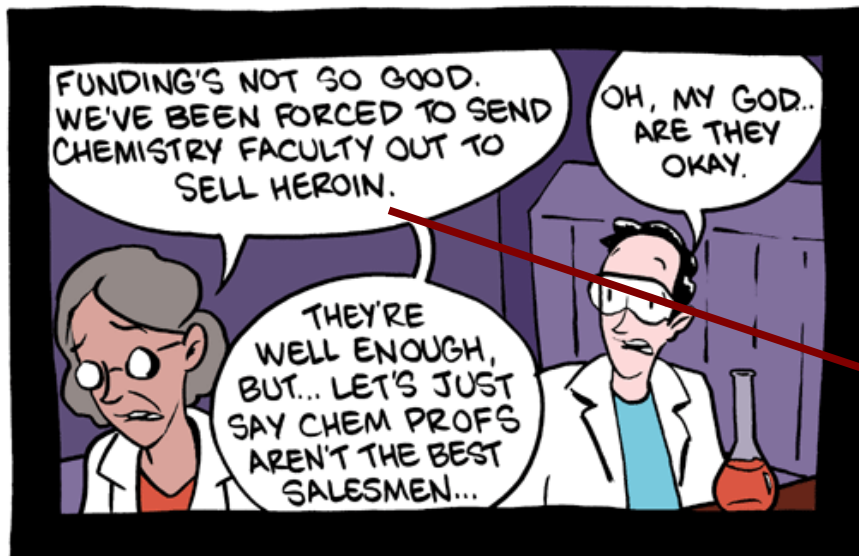


ChemAxon

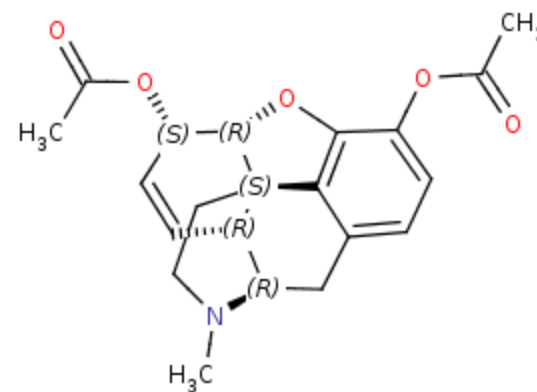
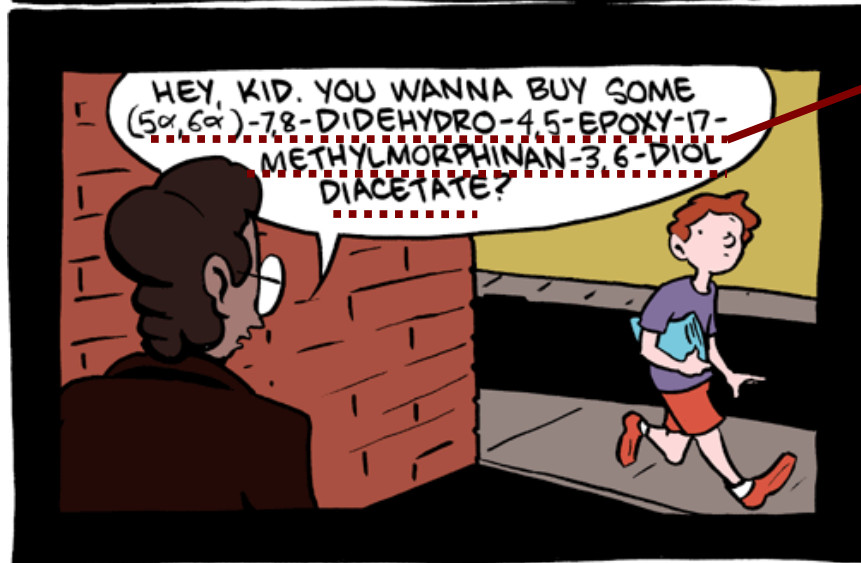
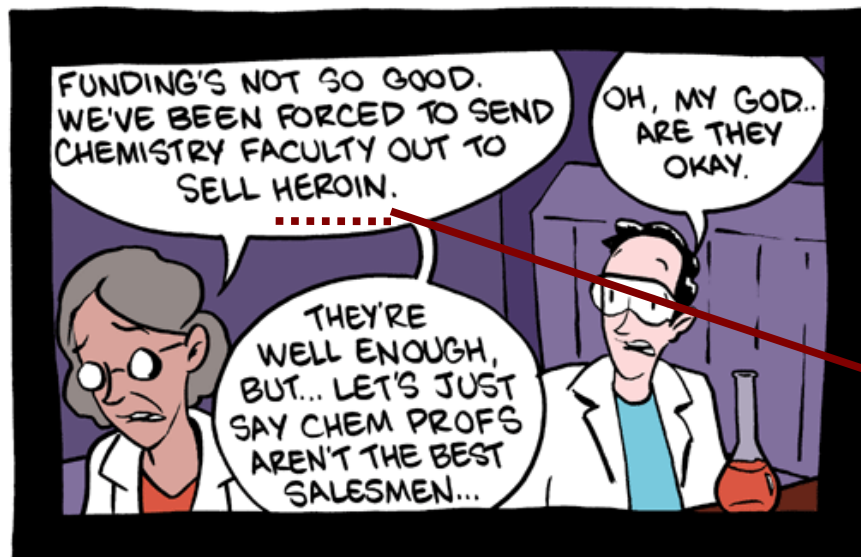
# A look at chemical literature



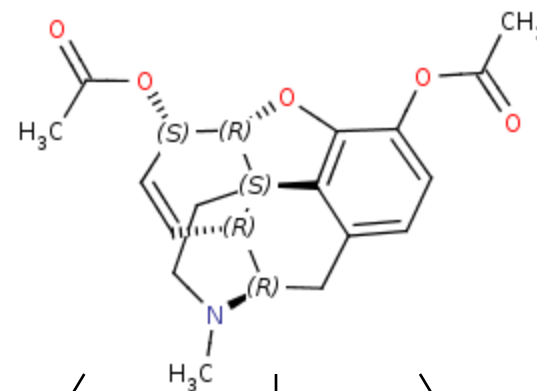
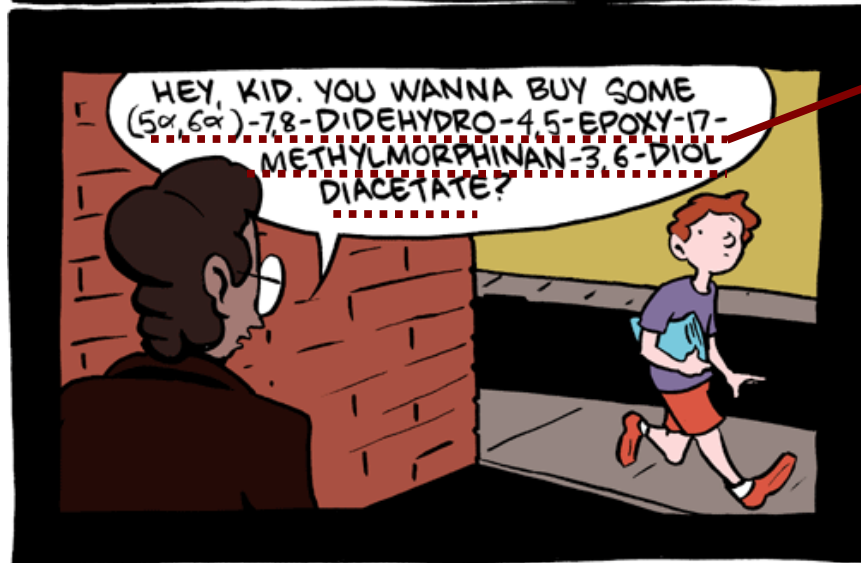
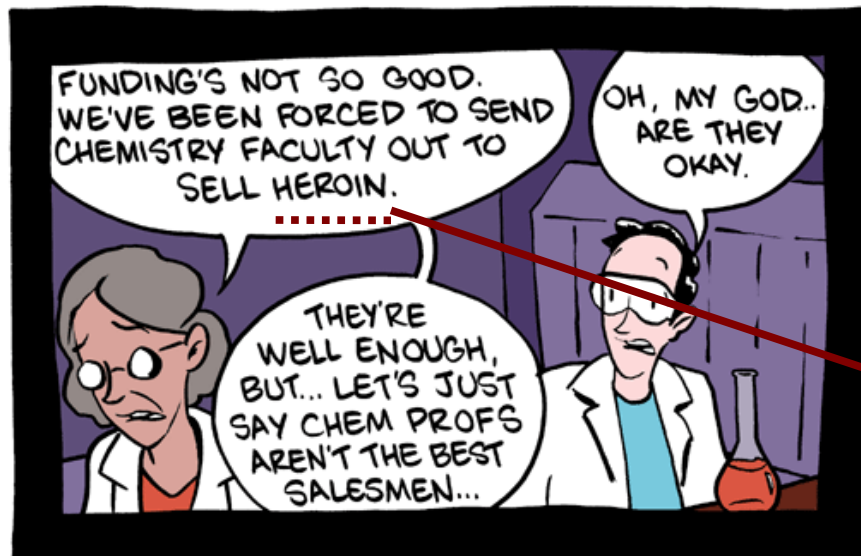
# Name to structure



# Name extraction from document



# Name extraction from document

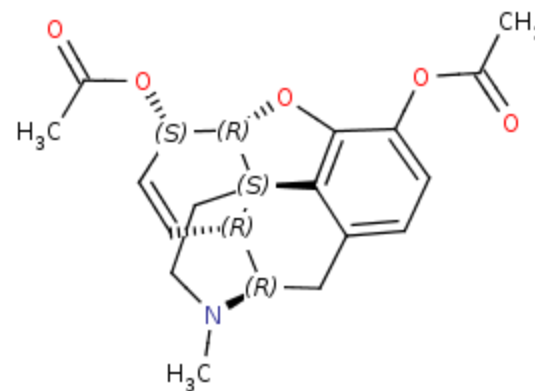
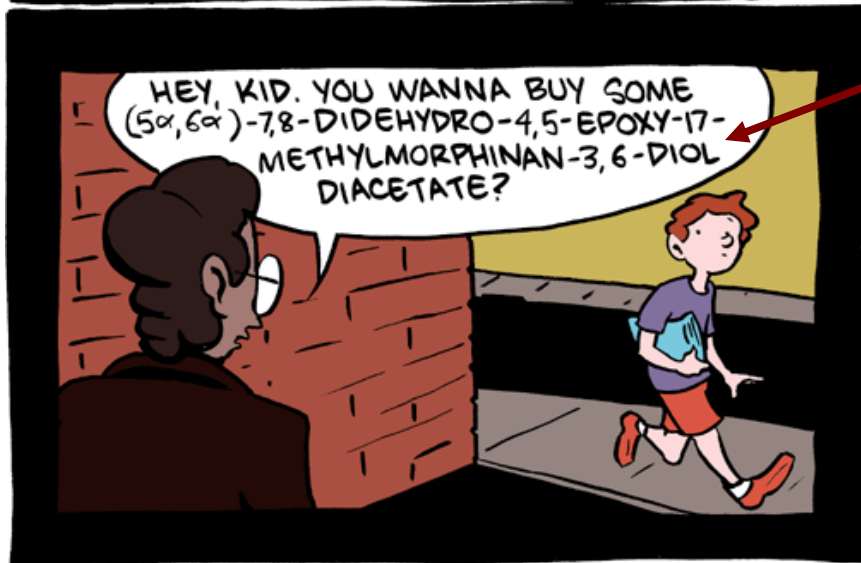
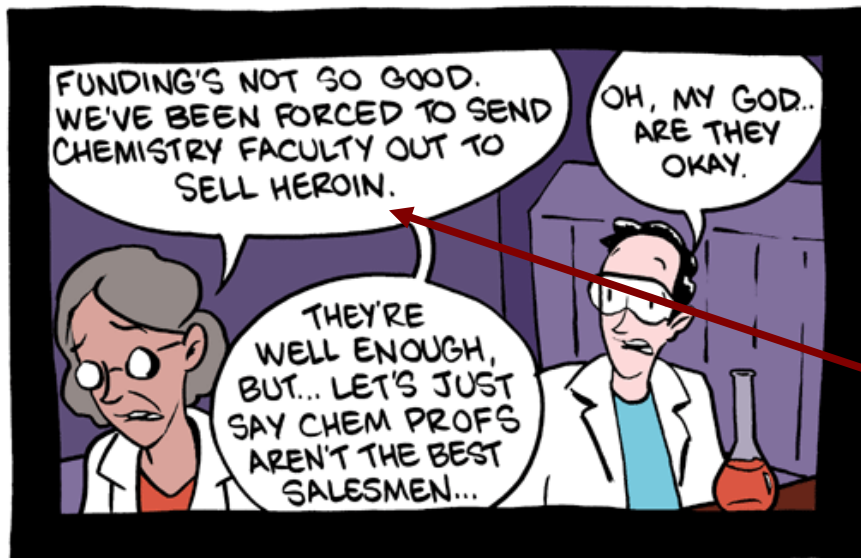


Export

Database

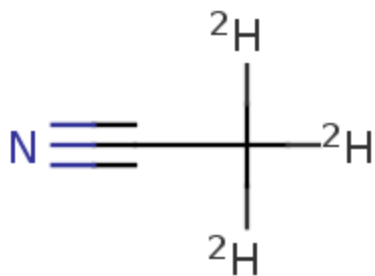
...

# Structure to Name

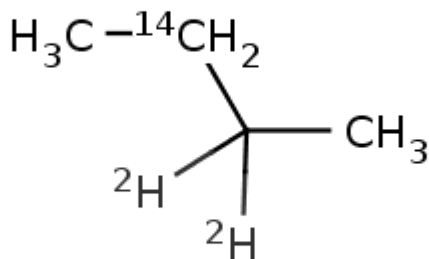


# Structure to Name

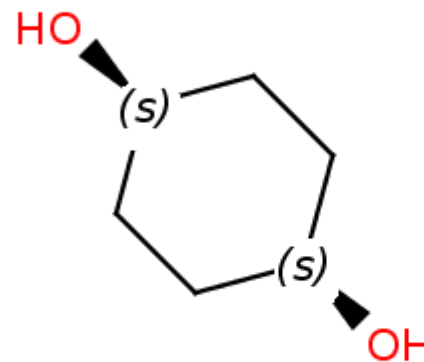
- Support for Isotopes, pseudo-asymmetric stereocenters, ...:



(<sup>2</sup>H<sub>3</sub>)acetonitrile



(3-<sup>14</sup>C,2,2-<sup>2</sup>H<sub>2</sub>)butane



(1s,4s)-cyclohexane-1,4-diol

- Generates more traditional names (optional)
- 2x speedup in 5.4.0 (november 2010)
- Various fixes and smaller improvements



# Name to Structure

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Continuous improvements since last year:

- Coverage (how many names we understand correctly)
- Correction (few errors)

5.4.0 and 5.5.0 both include major upgrades:

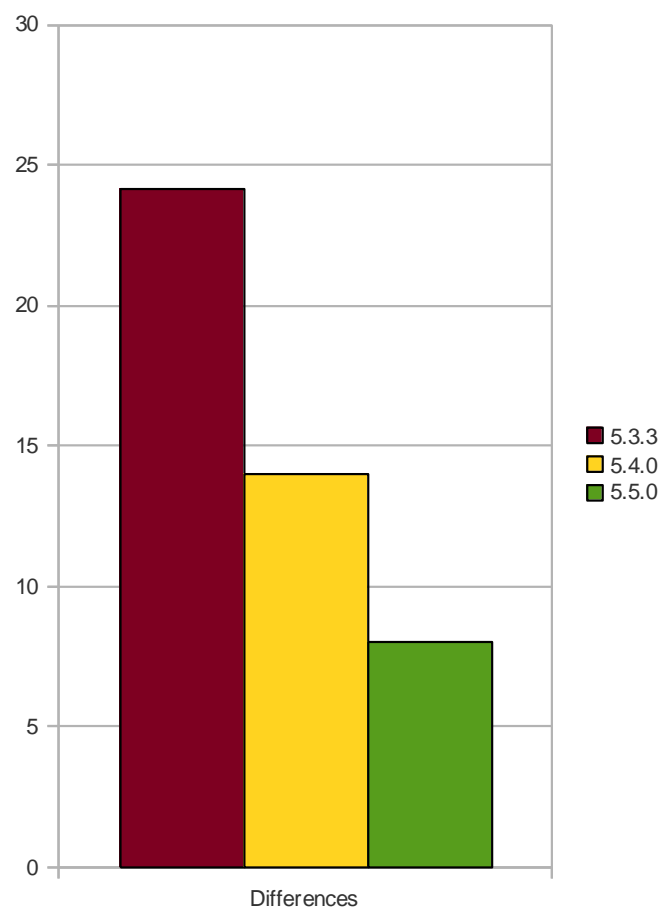
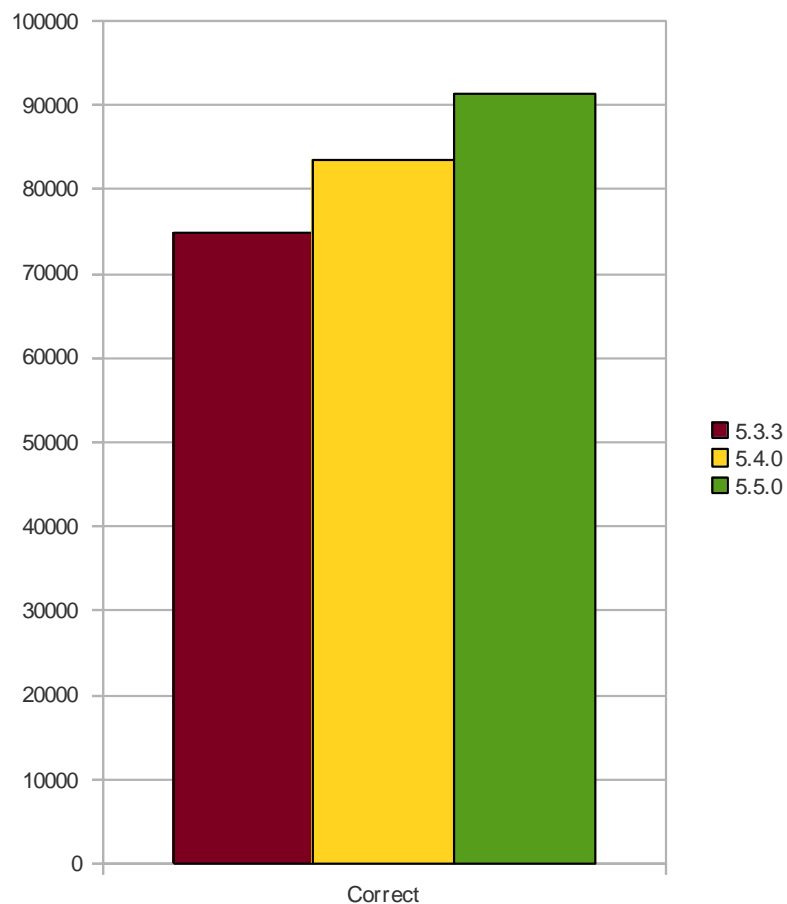
- Coverage+
- Correction++





# Name to Structure improvements

Various names, mixed nomenclatures (hard)



# Document to Structure

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- Extracts names from text documents
- Returns the discovered structures and their location
- OCR and syntax correction constantly developed
  - 3-methyl-1-methoxynaphthalene
  - 3-methyl-1-methoxynaphthalene
- Since 5.4: extraction from **PDF** documents



# Summary

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Structure to Name: incremental improvements, mature

Name to Structure: improving steadily, major upgrades in 5.4 and 5.5

Document to Structure: improves with n2s, PDF support, more OCR and syntax correction

*Try them, get support, ask questions!*