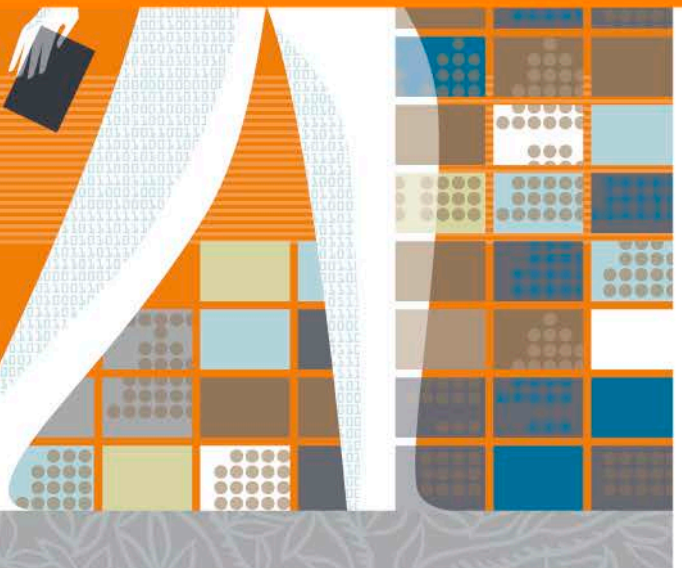
InChI @ Elsevier/Reaxys

August 2017



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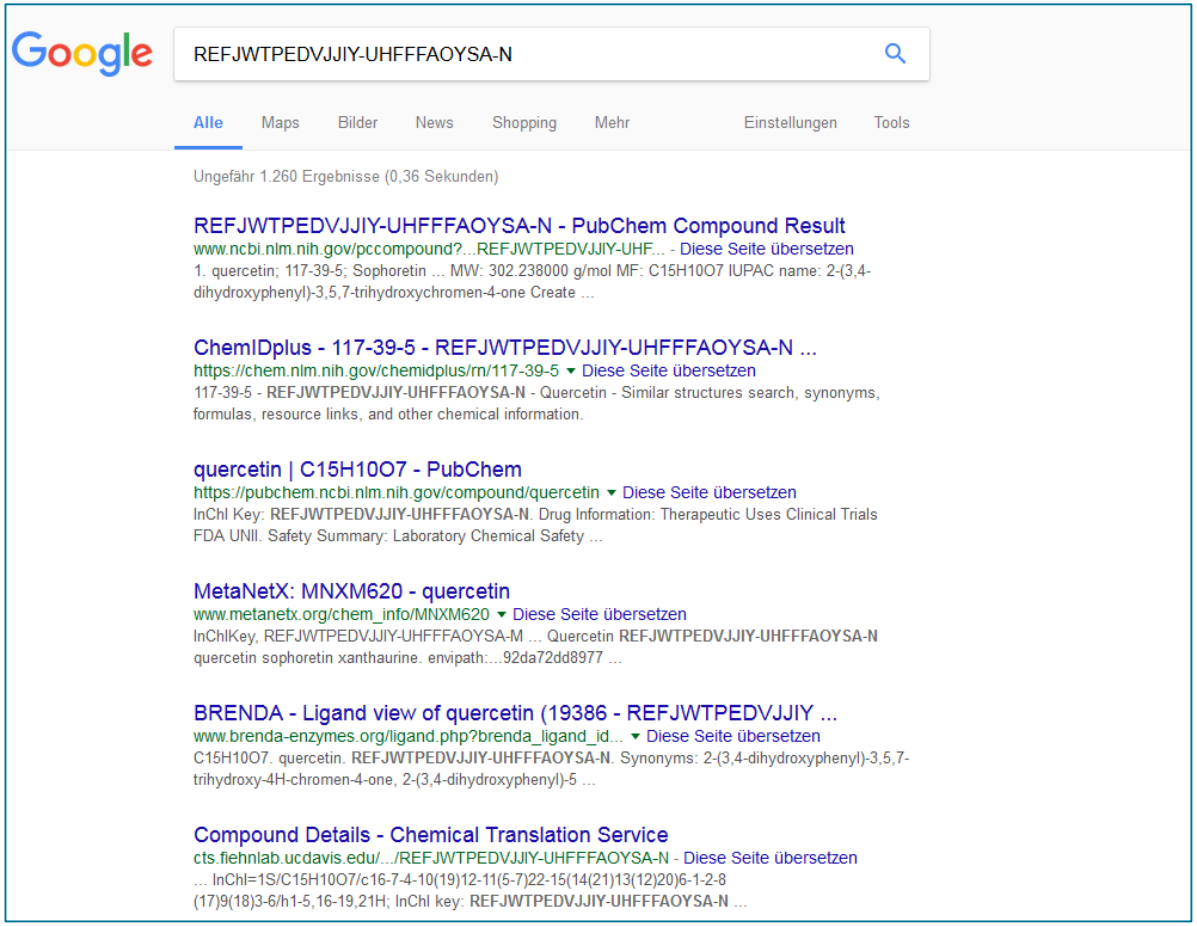
August 2017

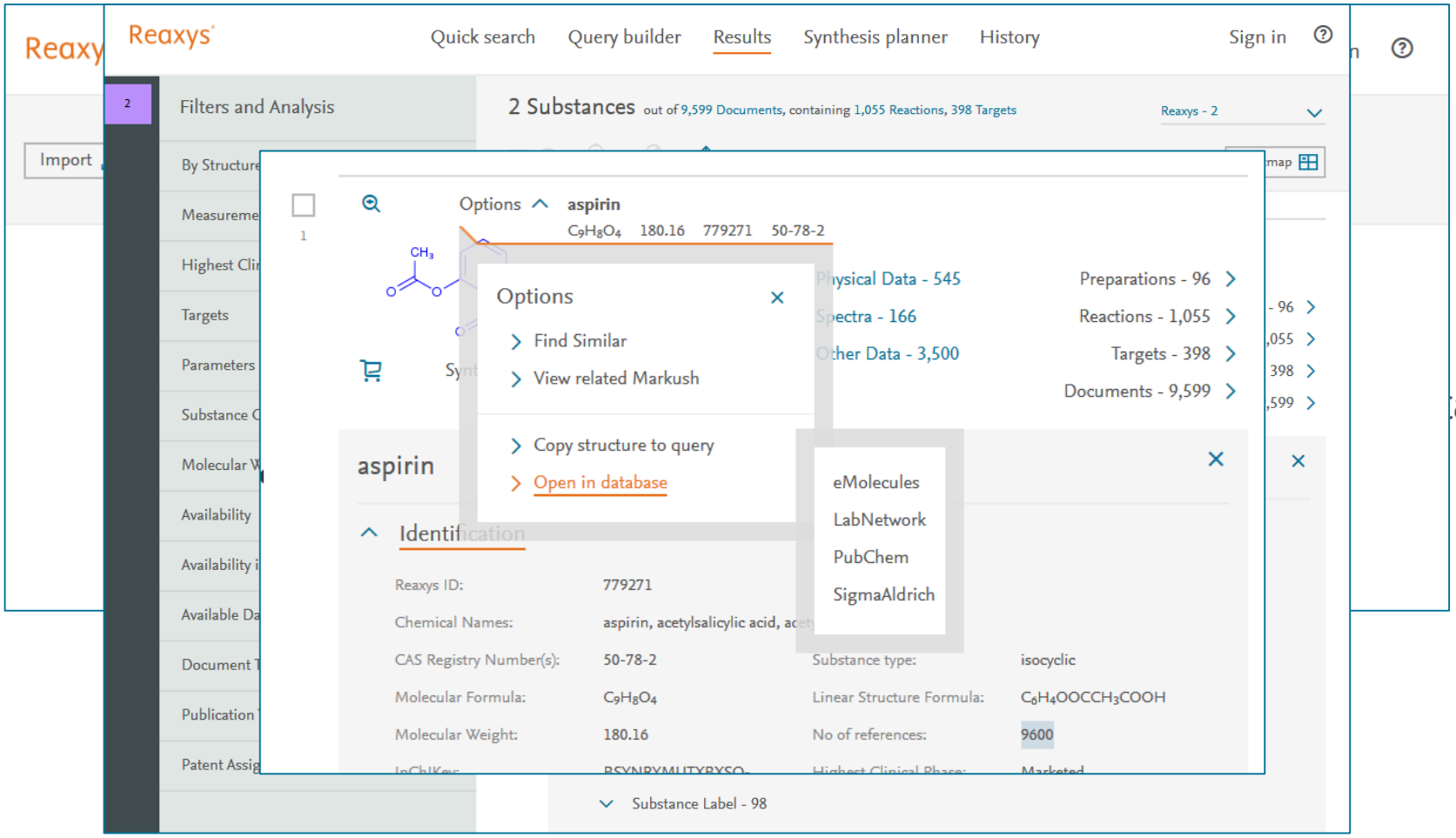
Introduction - Why InChI?

- “Identifiers” of chemical structures coded in common, but proprietary formats come with intrinsic issues
  - They may not be unique for a given structure (dependent on applied business rules)
  - Normalization needs to be applied to “register” compounds in databases leading to another, proprietary type of “structure descriptors”
  - proprietary registry numbers based on unique registry strings are too limited and too focused on just one system
    - e.g. Reaxys numbers are simple integers and Reaxys registry strings are not publicly available
- Ideally, there is one unique common identifier for any given substance that is
    - Short
    - Unique
    - Independent
    - human readability is a plus…
  - and that allows to connect disparate data sources (link-able)
- InChI and esp. the InChIKey answers some of those needs…

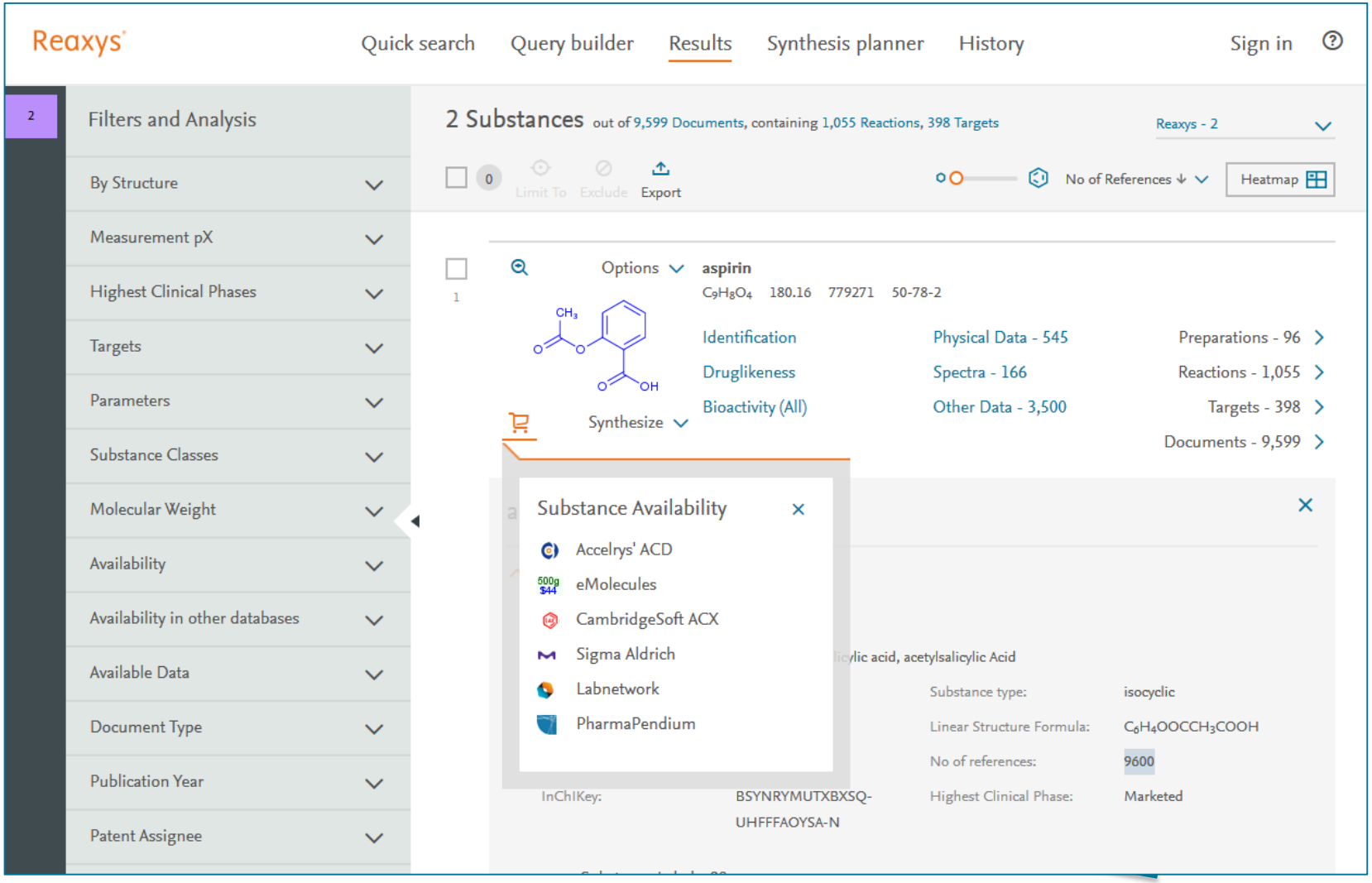
InChI at ScienceDirect



InChI @ Reaxys – Content Integration



InChI @ Reaxys – Link-Outs



Thank you very much for your attention…