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Possibilities for Searching with Chemical Structures in Conjunction with *esp@cenet*®

Nigel Clarke,
Vesna Hassler,
Marek Szubert

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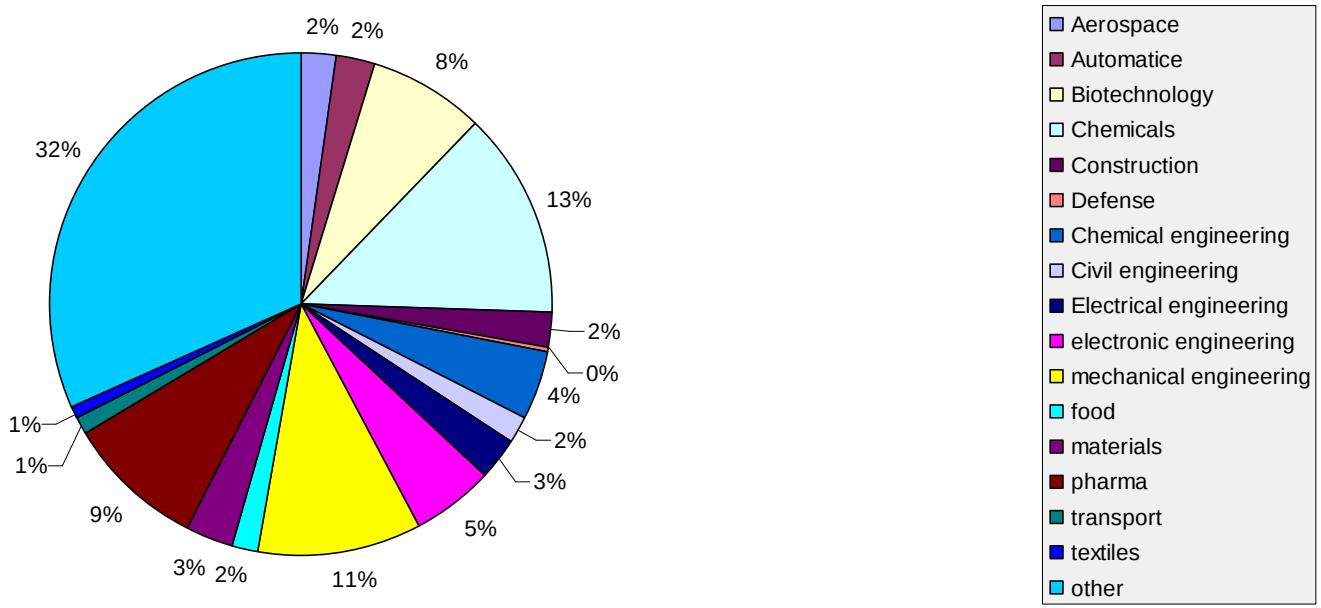
I wouldn't start from here if I were you

esp@cenet® User Profile; Industry Sector



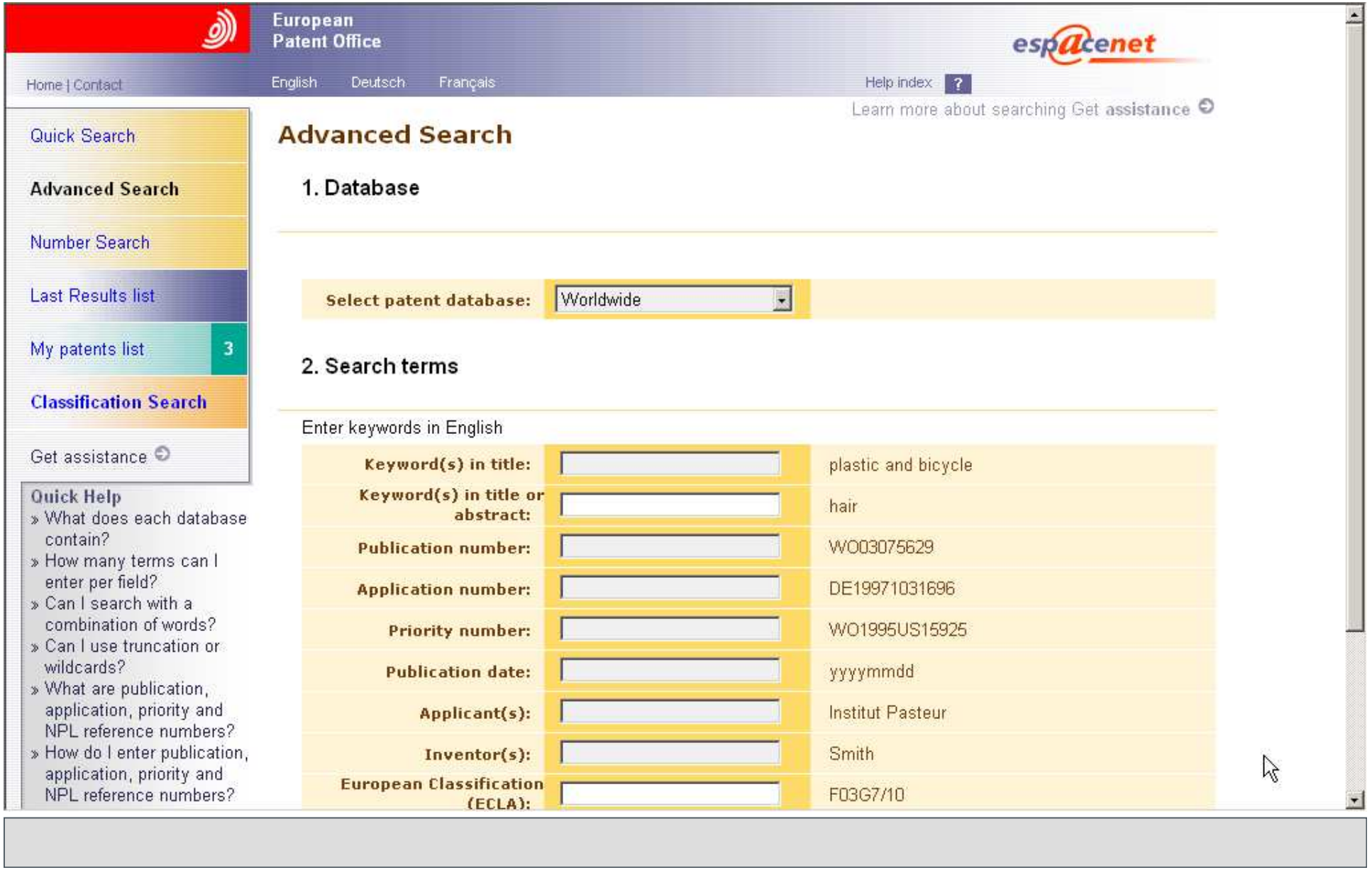
esp@cenet®

- Chemical Structure Search

- Why?

- Large User Group (chemistry and pharma)

esp@cenet® advanced search



esp@cenet® classification

esp@cenet® allowed inputs

- Words:
  - Keywords
  - Inventor names
  - Applicant names

esp@cenet® allowed inputs

- "Parameters"
  - Priority Number
  - Application Number
  - Publication Number

esp@cenet® allowed inputs

- Dates
  - Publication Date

esp@cenet® allowed inputs

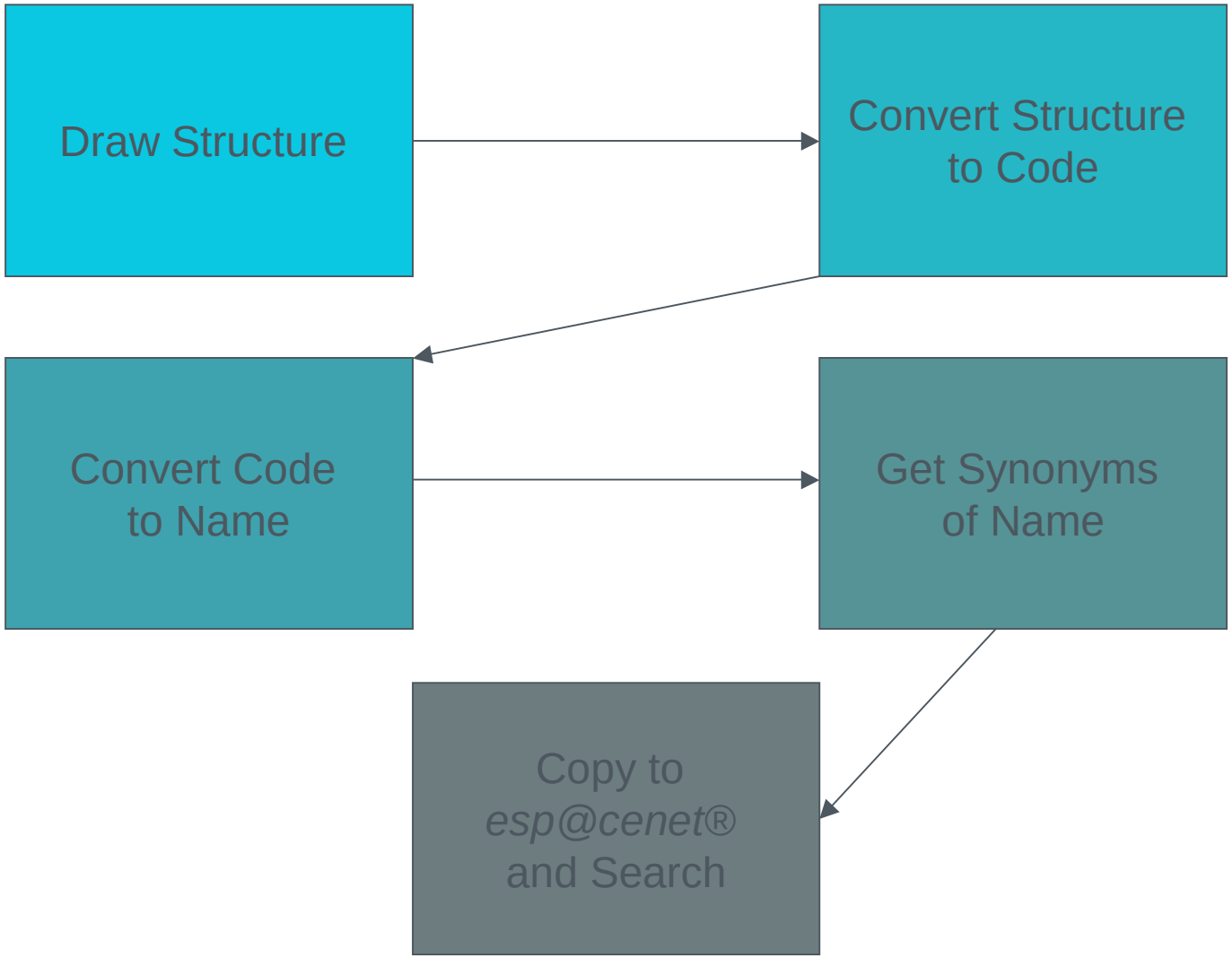
- Classifications
  - IPC
  - ECLA

esp@cenet® allowed inputs

- Only alphanumeric

- (wildcards allowed)

An Idea For Chemical Structure Searching



An Idea For Chemical Structure Searching

- Based on Public Domain Tools
  - Open Source
  - Freeware
  - Shareware
  - Proprietary

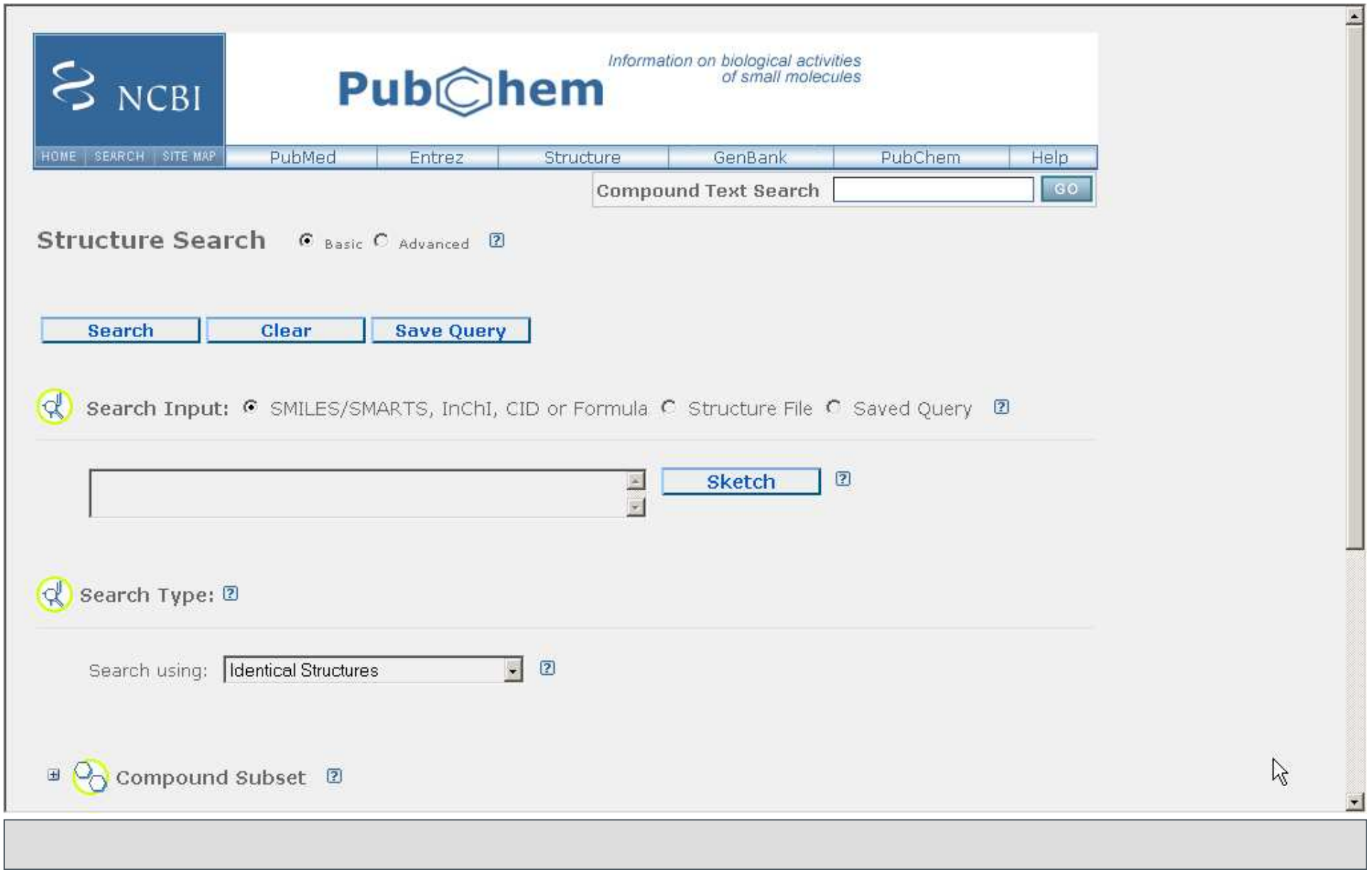
An Idea For Chemical Structure Searching

- Stand alone
- Does not alter the *esp@cenet*® application
  - c.f. translation engine
  - ECLA search

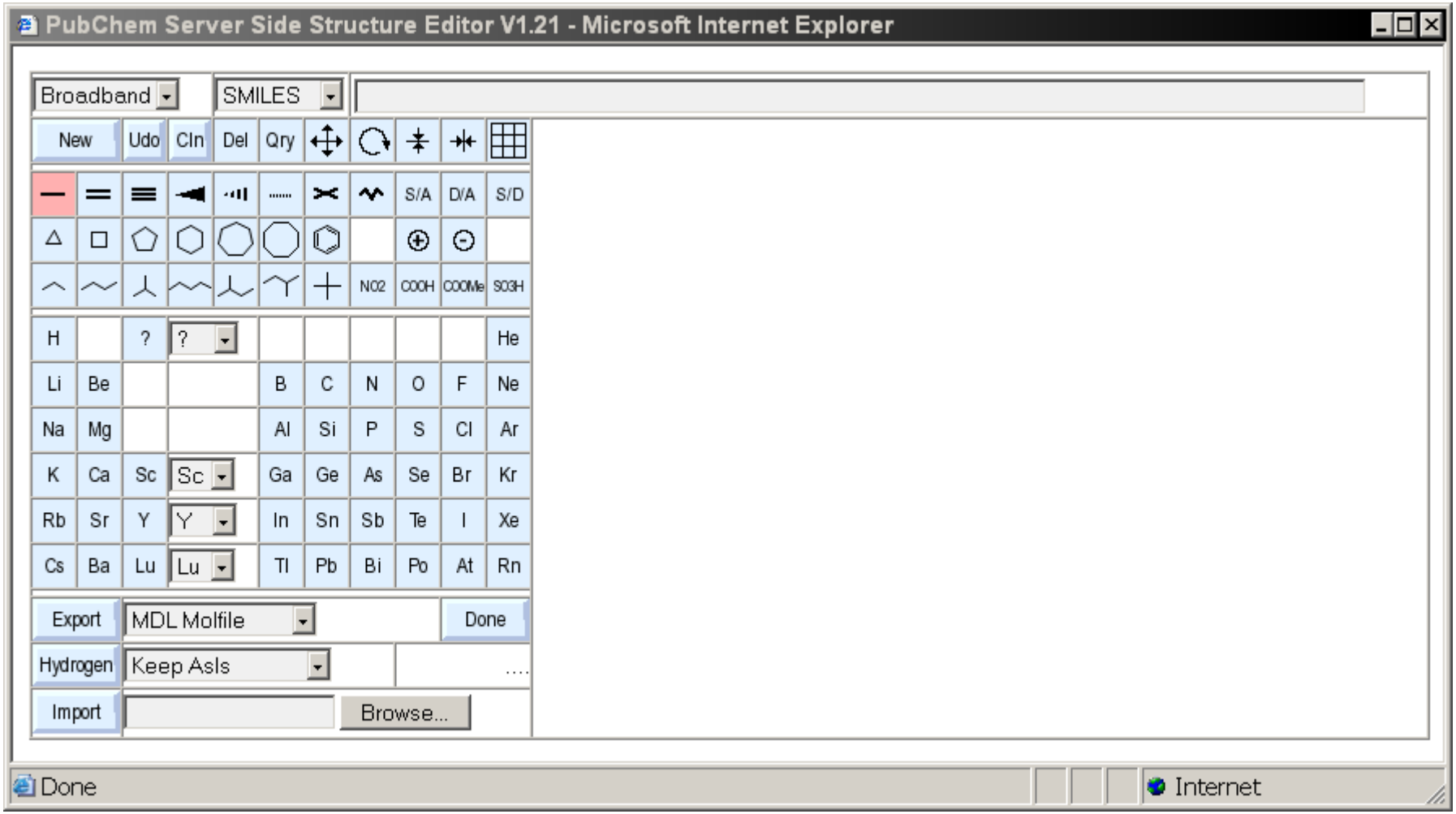
An Idea For Chemical Structure Searching

- Entry level
- To keep *esp@cenet*® attractive in the free sector
- Commercial suppliers can readily develop more sophisticated, added value tools

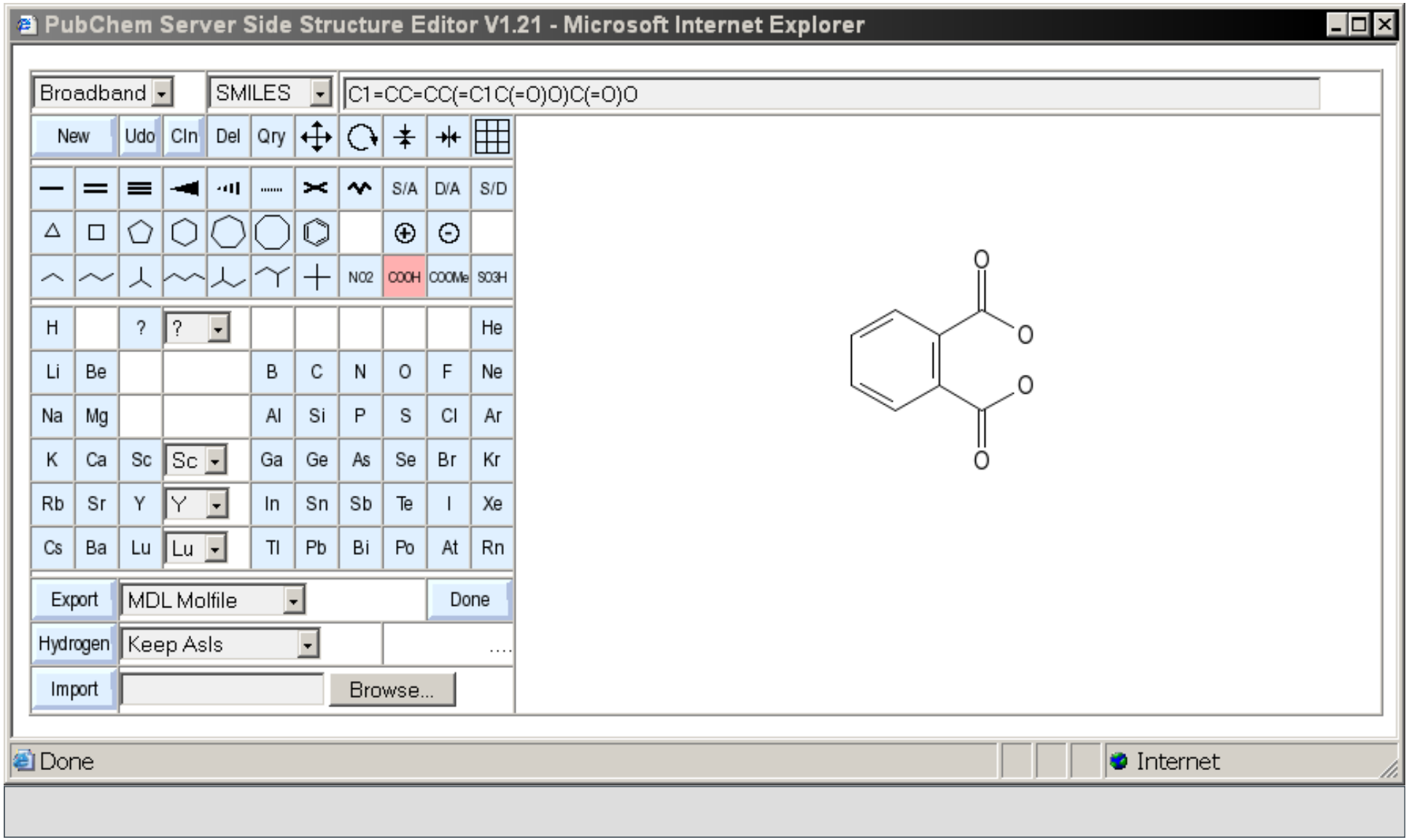
An open-source application



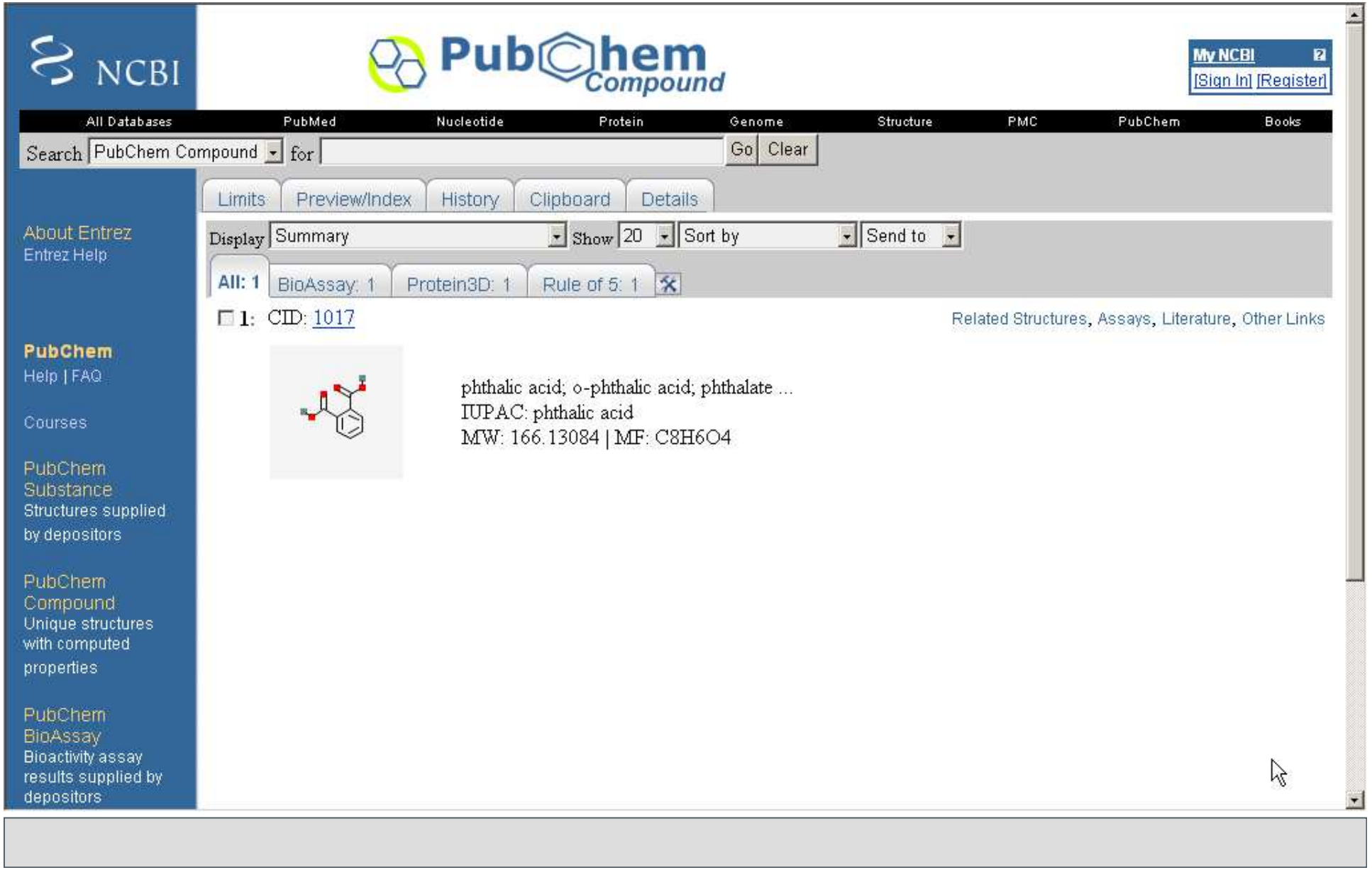
Draw structure using open source structure editor



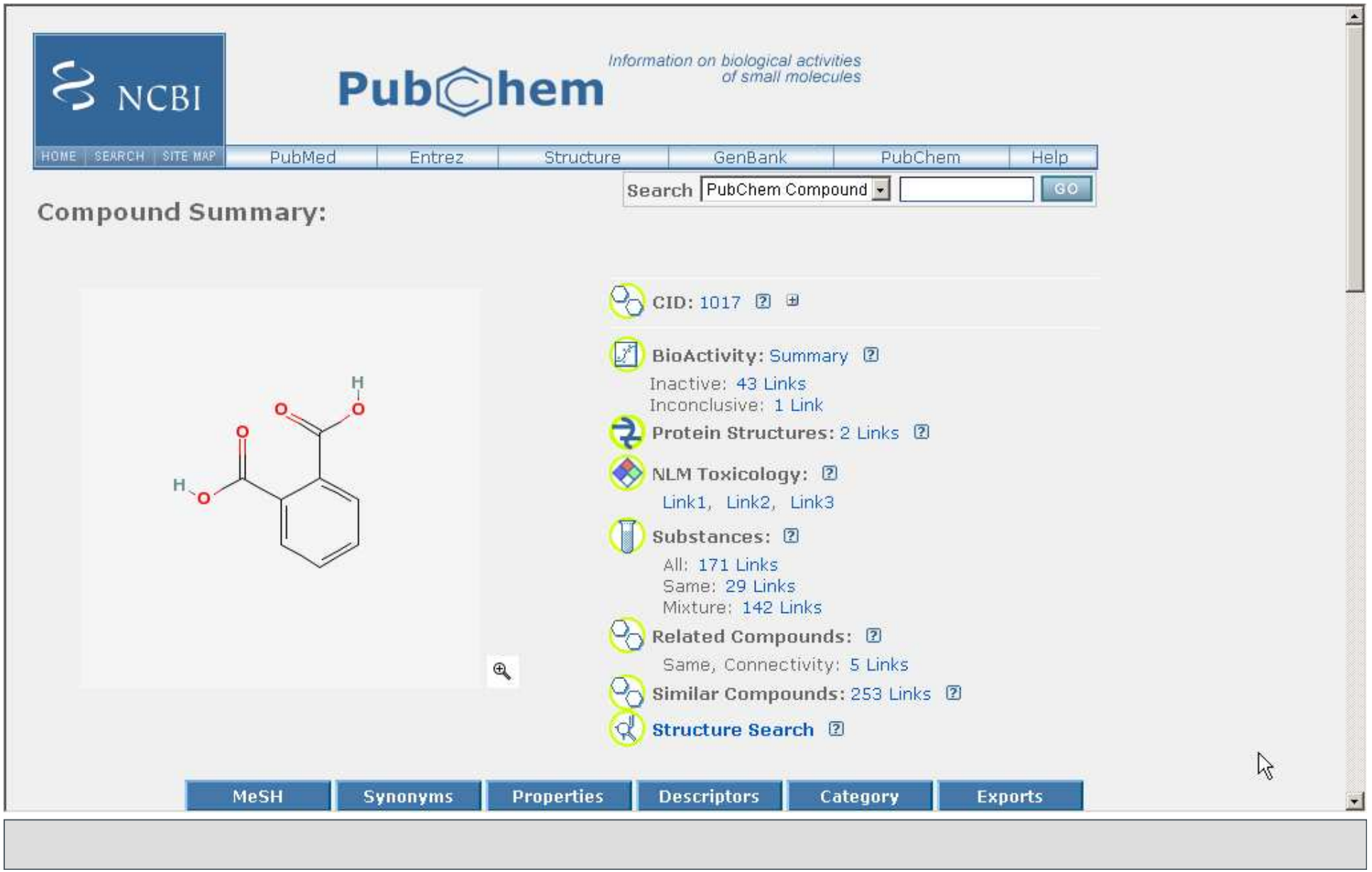
Structure gives code - open source



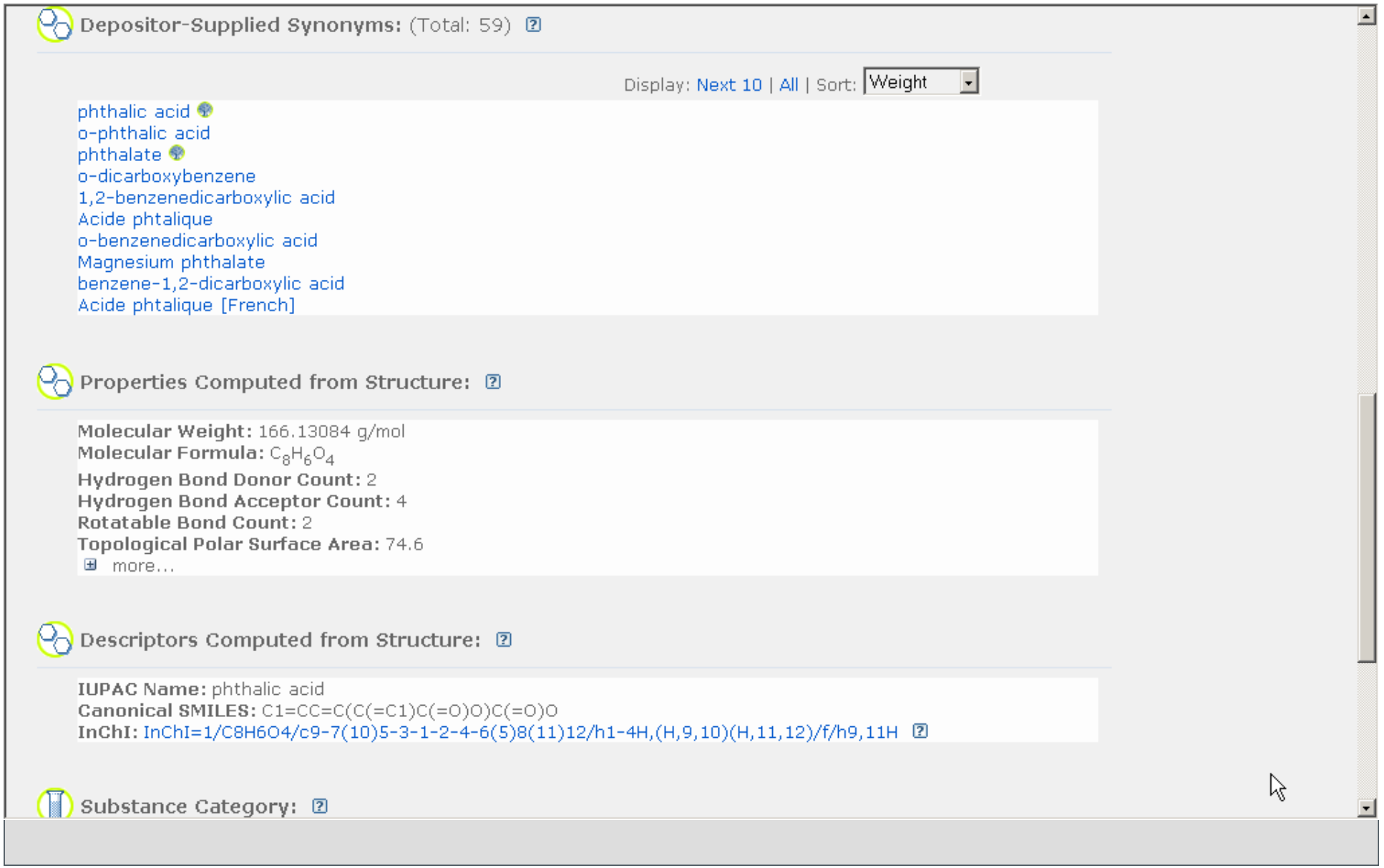
Code Gives Chemical Name - open source



Chemical Name Has Synonyms - open source



Get Synonyms - open source



Depositor-Supplied Synonyms: (Total: 59)

Display: Next 10 | All | Sort: Weight

phthalic acid
o-phthalic acid
phthalate
o-dicarboxybenzene
1,2-benzenedicarboxylic acid
Acide phtalique
o-benzenedicarboxylic acid
Magnesium phthalate
benzene-1,2-dicarboxylic acid
Acide phtalique [French]

Properties Computed from Structure:

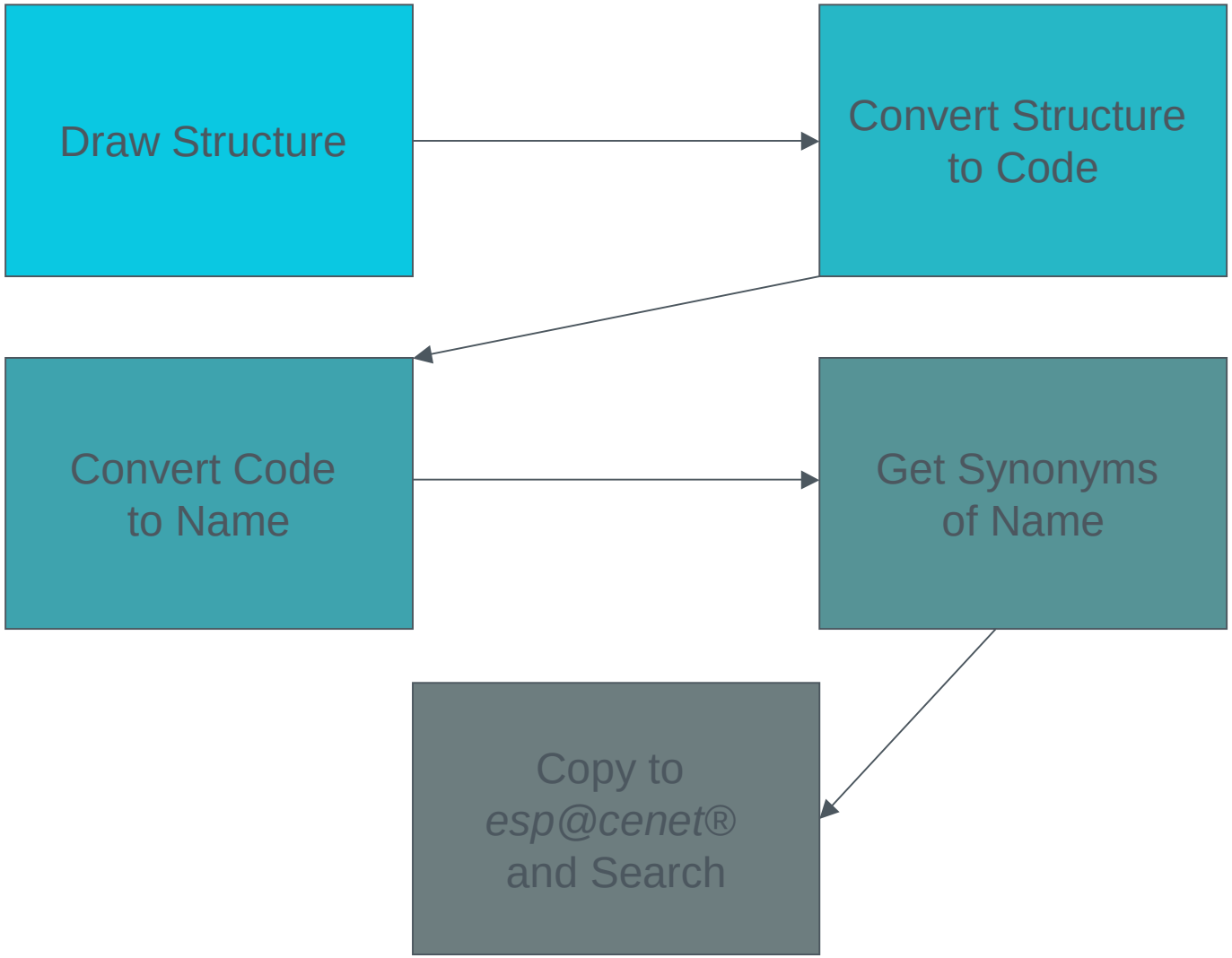
Molecular Weight: 166.13084 g/mol
Molecular Formula: $C_8H_6O_4$
Hydrogen Bond Donor Count: 2
Hydrogen Bond Acceptor Count: 4
Rotatable Bond Count: 2
Topological Polar Surface Area: 74.6
more...

Descriptors Computed from Structure:

IUPAC Name: phthalic acid
Canonical SMILES: C1=CC=C(C(=C1)C(=O)O)C(=O)O
InChI: InChI=1/C8H6O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H,(H,9,10)(H,11,12)/f/h9,11H

Substance Category:

An Idea For Chemical Structure Searching



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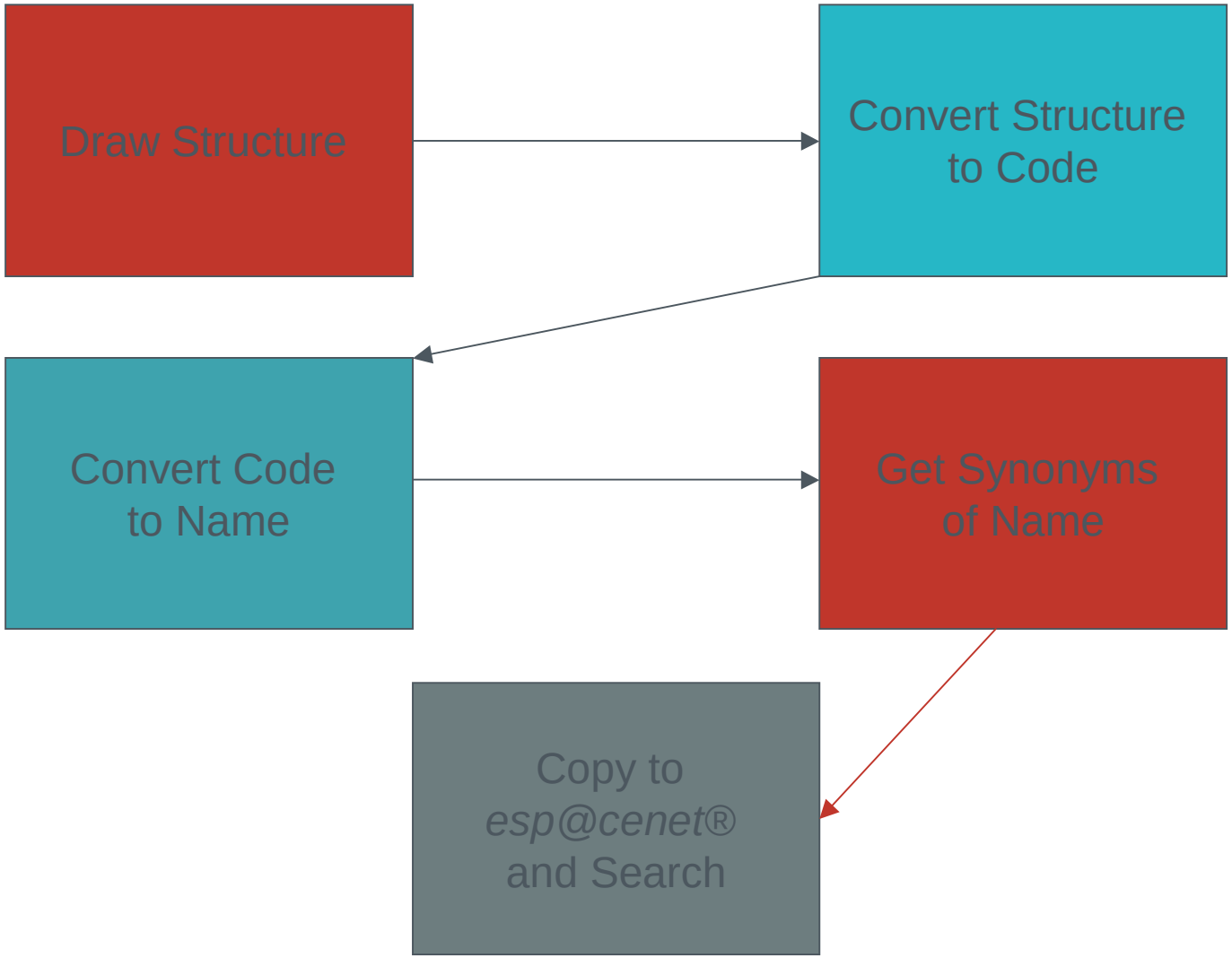

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