Named Entity Resolution in OSCAR4

Daniel Lowe

Unilever Centre for Molecular Science Informatics

dl387@cam.ac.uk

13th April 2011, OSCAR4 Launch

Contents

- Named entity resolution architecture
- Systematic name resolution (OPSIN)
- Extending entity resolution
- Conclusions

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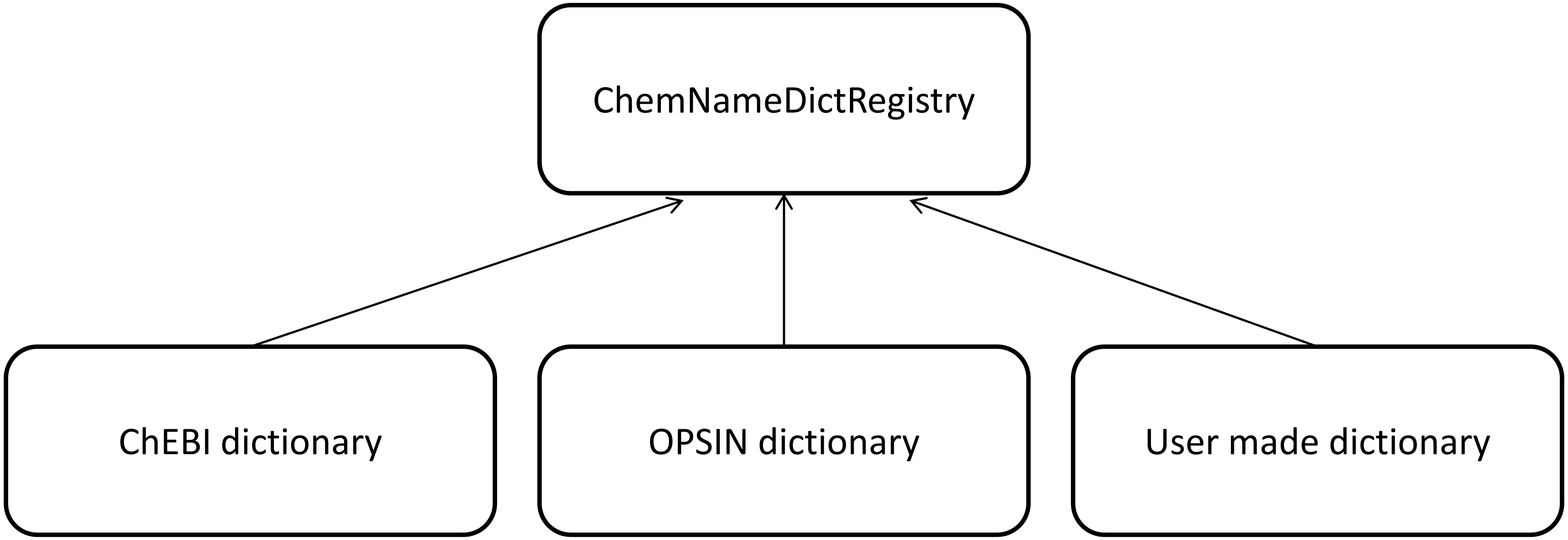
Dictionary Architecture

- Dictionaries are registered with a dictionary registry which then provides a central point of access
- To be registerable a class need only implement the ChemNameDict interface



Using dictionaries for Name to Structure

- Dictionaries that contain name to structure mappings implement the appropriate interface for that type of chemical identifier.

- IInChIProvider

  InChI=1/C6H12/c1-2-4-6-5-3-1/h1-6H2

- ISMILESProvider

  C1CCCCC1

- ICMLProvider

  <cml>…</cml>

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Implementing a provider

```
public interface IInChIProvider {
        /**
         * Returns a set containing all of the known InChIs for
         * the given query name.
         */
        public Set<String> getInchis(String queryName);
}
```

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Resolving entities against the dictionaries

ChemNameDictRegistry:

- resolveNamedEntity(NamedEntity ne)
- getInchis(String name)
- …

OSCAR API:

- findAndResolveNamedEntities(String input)
- findResolvableEntities(String input)

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Ontology Term Resolution

- ChEBI ontology, REX (physico-chemical process ontology), FIX (biophysical chemistry ontology)
- Ontology terms are stored as a multimap between terms and Ids.
- Ontology terms are found and resolved during the process of finding named entities or can be resolved using an OntologyTerms object's methods.

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Extending Ontology Support

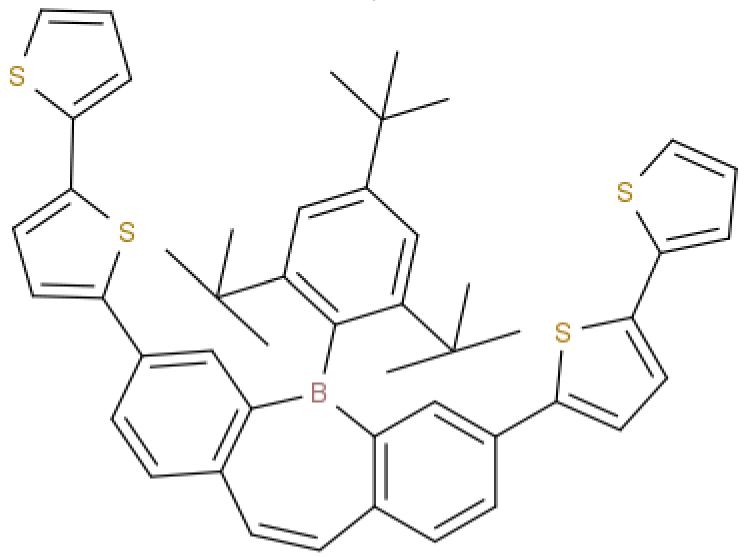
- A custom OntologyTerms can be created from a multimap of terms and ids.

```
OntologyTerms myCustomOntologyTerms = new
OntologyTerms(myTermIdMappings);
Oscar oscar = new Oscar();
oscar.setOntologyTerms(myCustomOntologyTerms);
```

OPSIN

(Open Parser for Systematic IUPAC Nomenclature)

3,7-Di([2,2′-bithiophen]-5-yl)-5-(2,4,6-tri-tert-butylphenyl)dibenzo[b,f]borepin



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Why is dictionary lookup insufficient?

- Infinite number of chemical compounds

- Many different ways of naming the same compound even if names are computer generated

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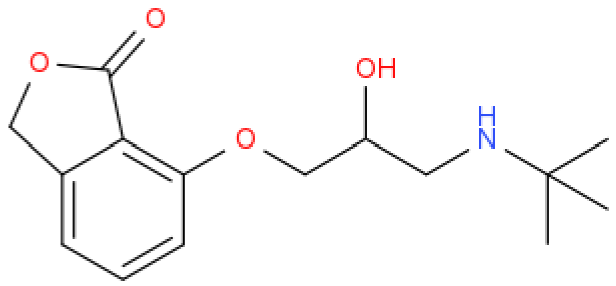


Name on Wikipedia and in dictionaries:
7-[3-(tert-butylamino)-2-hydroxy-propoxy]-3H-isobenzofuran-1-one

Other suitable names generated by structure to name programs:

7-(3-(tert-butylamino)-2-hydroxypropoxy)isobenzofuran-1(3H)-one

7-[3-(tert-butylamino)-2-hydroxypropoxy]-1,3-dihydro-2-benzofuran-1-one

7-[3-(tert-butylamino)-2-hydroxypropoxy]-2-benzofuran-1(3H)-one

Why is dictionary lookup insufficient?

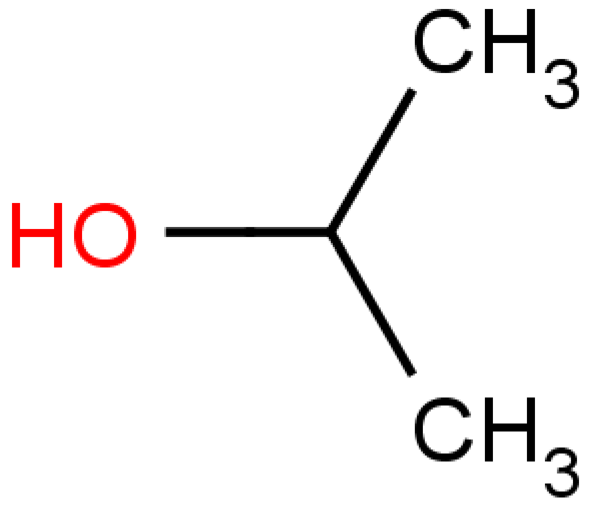
- Infinite number of chemical compounds
- Many different ways of naming the same compound even if names are computer generated
- Names for the same compound can have very little in common if different nomenclature is employed

Different naming styles

- isopropanol
- Isopropyl alcohol
- 2-Propanol
- Propan-2-ol
- 2-Hydroxypropane
- sec-Propyl alcohol
- 1-Methylethanol
- i-Propanol
- i-Propyl alcohol
- n-Propan-2-ol
- sec-Propanol
- 2-Propyl alcohol
- 1-Methylethyl alcohol
- Iso-propyl alcohol
- iso-propylalcohol
- Dimethylcarbinol

$\longrightarrow$

InChI=1/C3H8O/c1-3(2)4/h3-4H,1-2H3



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Key Facts

- Outputs to CML, InChI or SMILES
- Provides high precision conversions
- Offers comparable recall to commercial offerings on systematic names

Chemical Name to Structure: OPSIN, an Open Source Solution
Daniel M. Lowe, Peter T. Corbett, Peter Murray-Rust, Robert C. Glen
Journal of Chemical Information and Modeling **2011** *51* (3), 739-753

Most Read Paper in JCIM in the previous month!

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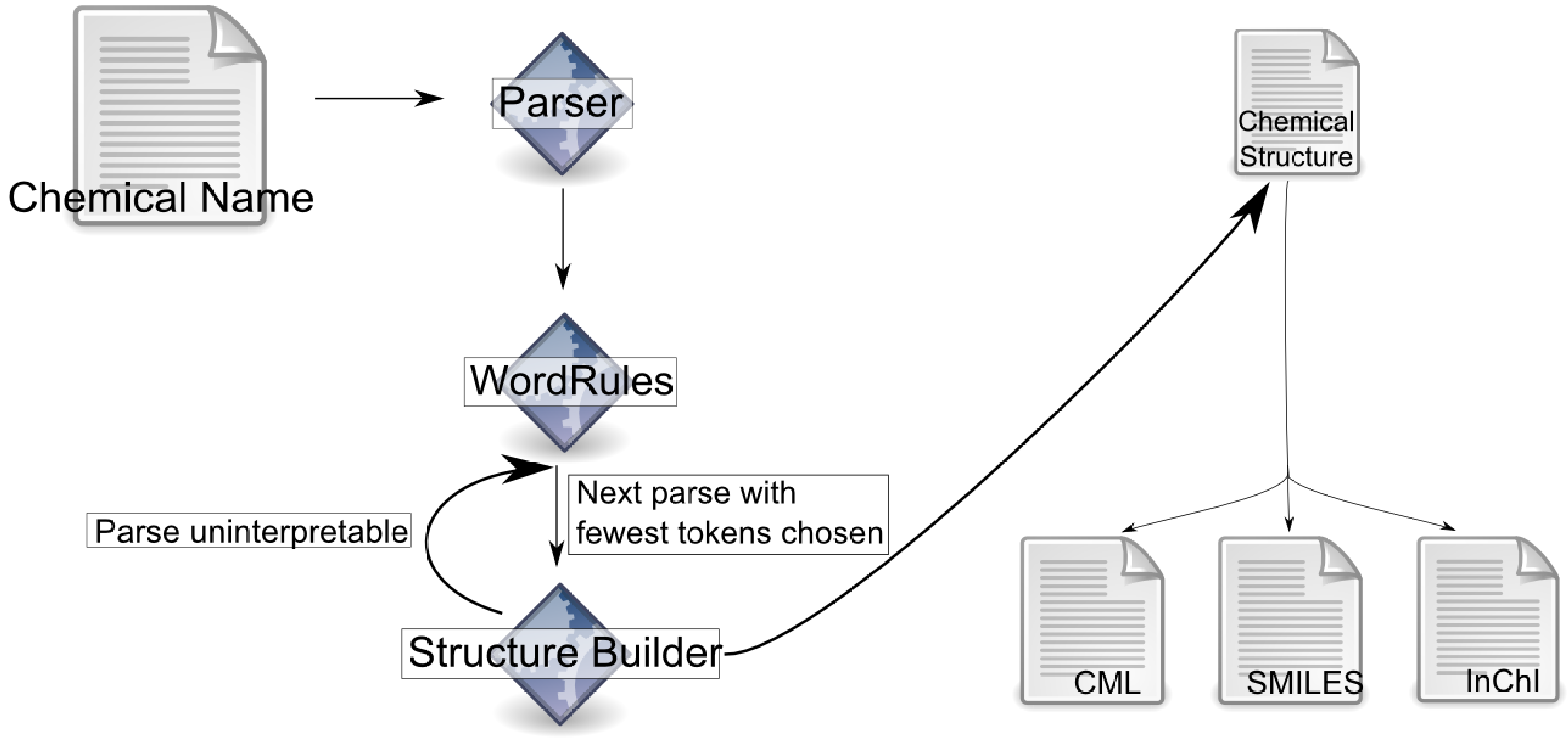
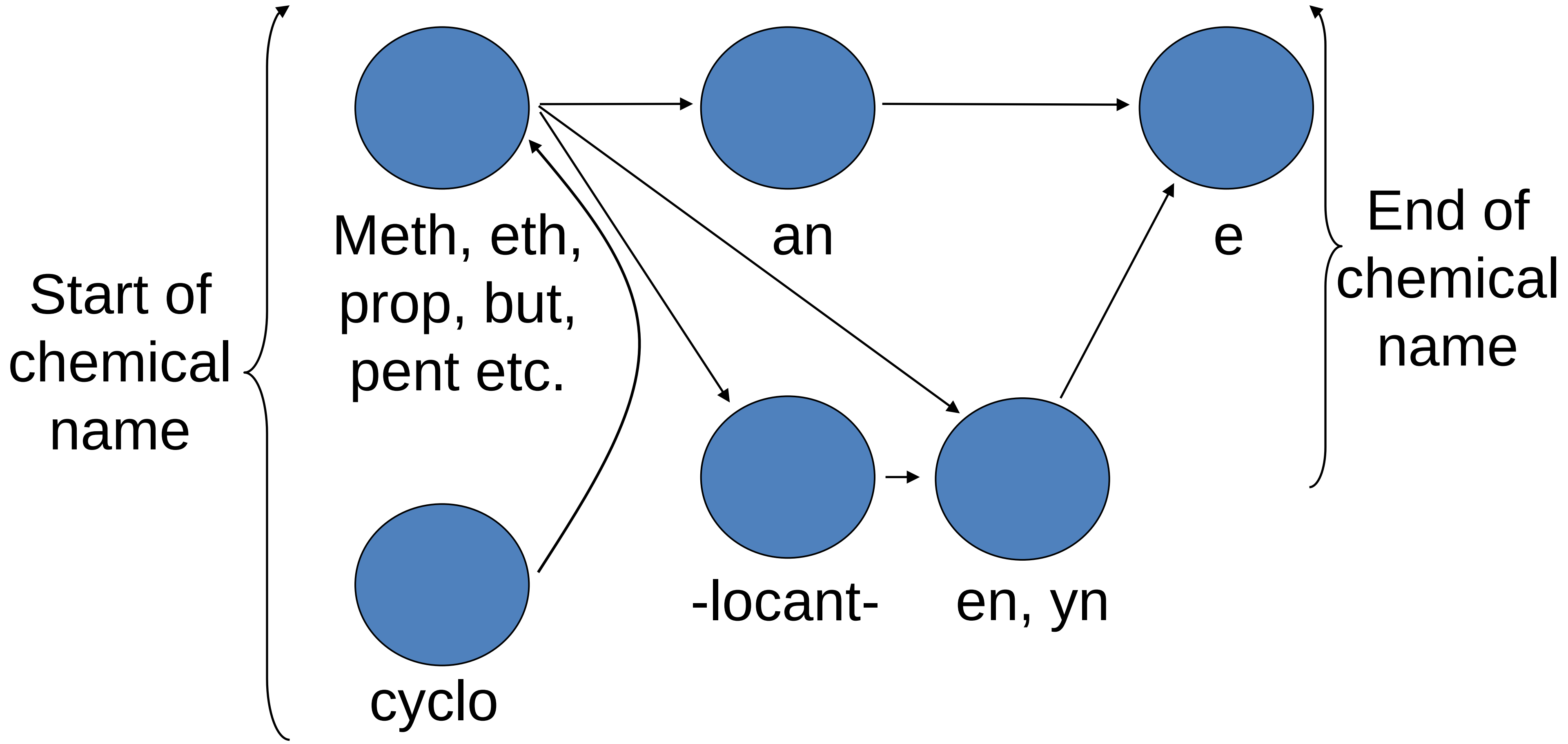
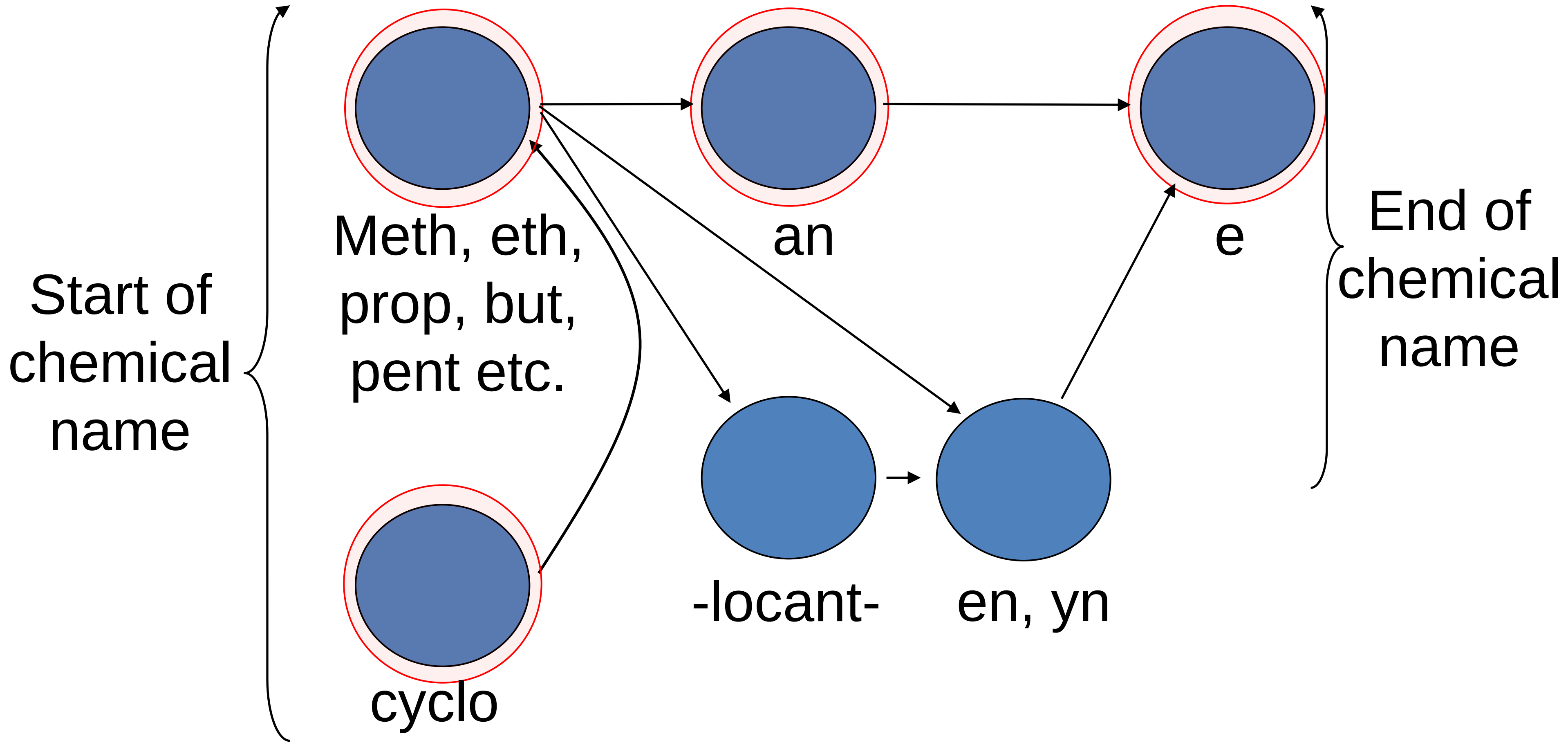
Schematic of program



A regular grammar for hydrocarbons



e.g. cyclopropane



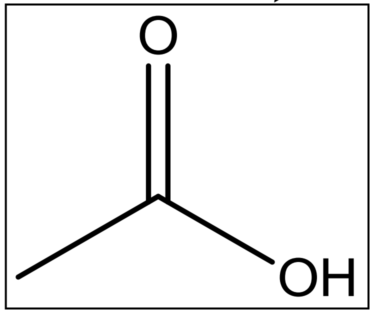
- OPSIN's grammar describes a finite state machine with 10091 states
- Around 3500 discrete morphemes form the program's vocabulary
- These are grouped into 117 morpheme classes e.g. multiplier (mono, di, tri, tetra, penta…), acidStem (acet, oxal, succin…)

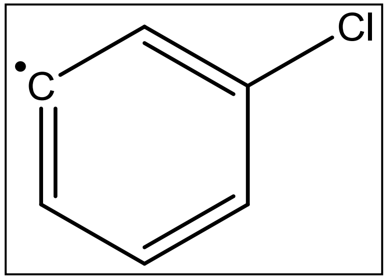
Example

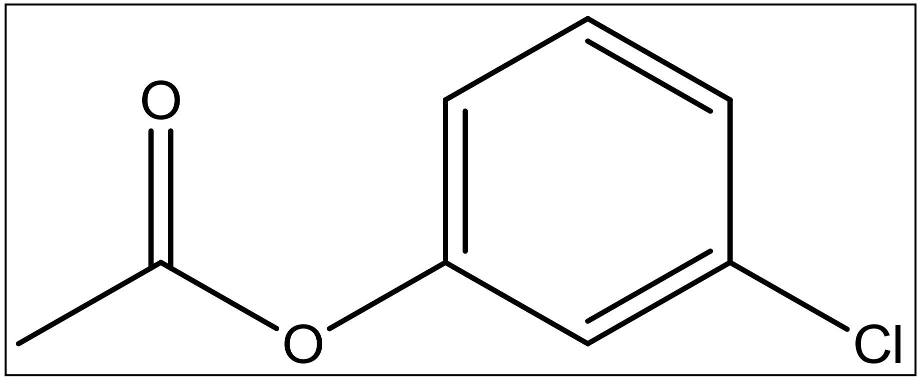
ethanoic acid m-chlorophenyl ester

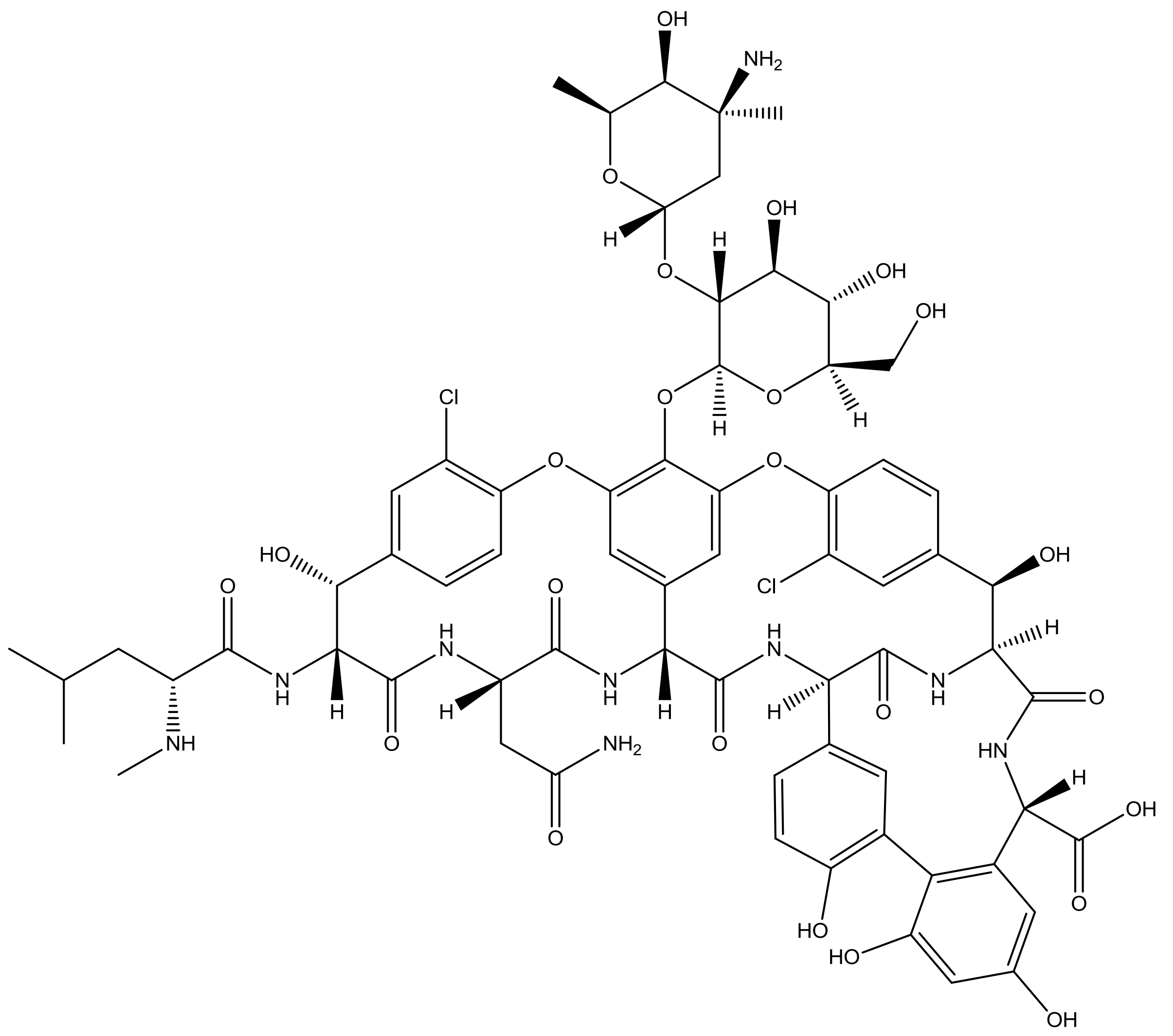
full substituent functionalTerm

WordRule="functionalClassEster"









(1S,2R,18R,19R,22S,25R,28R,40S)-48-{[(2S,3R,4S,5S,6R)-3-{[(2S,4S,5S,6S)-4-amino-5-hydroxy-4,6-dimethyloxan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-22-(carbamoylmethyl)-5,15-dichloro-2,18,32,35,37-pentahydroxy-19-[(2R)-4-methyl-2-(methylamino)pentanamido]-20,23,26,42,44-pentaoxo-7,13-dioxa-21,24,27,41,43-pentaazaoctacyclo[26.14.2.2^{3,6}.2^{14,17}.1^{8,12}.1^{29,33}.0^{10,25}.0^{34,39}]pentaconta-3,5,8(48),9,11,14,16,29(45),30,32,34,36,38,46,49-pentadecaene-40-carboxylic acid

Extending entity resolution

Proof of concept code for retrieving InChIs from the NIH's Chemical Identifier Resolver

```
public class CIRDictionary implements IChemNameDict, IInChIProvider{
 ........................................
public Set<String> getInchis(String queryName) {
    Set<String> inchis = new HashSet<String>();
    try{
        URI uri = new URI("http", null, "cactus.nci.nih.gov", 80, "/chemical/structure/" + queryName +"/stdinchi", null, null);
        URLConnection connection = uri.toURL().openConnection();
        BufferedReader in = new BufferedReader(new InputStreamReader(connection.getInputStream()));
        StringBuilder input = new StringBuilder();
        String inputLine = null;
        while ((inputLine = in.readLine()) != null){
            input.append(inputLine);
        }
        inchis.add(input.toString());
    }
    catch (Exception e) {
        LOG.debug("Request to CIR failed", e);
    }
    return inchis;
}

public boolean hasName(String queryName) {
    return getInchis(queryName).size()>0;
}

........................................

}
```

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```
Oscar oscar = new Oscar();

ChemNameDictRegistry myChemNameDictReg  = new ChemNameDictRegistry();

myChemNameDictReg.register(new CIRDictionary());

oscar.setDictionaryRegistry(myChemNameDictReg);

List<ResolvedNamedEntity> resolvedEntities =
oscar.findResolvableEntities("Cholecalciferol is not in ChEBI.");
```

Conclusions

- OSCAR4 provides out of the box named entity resolution through simple APIs.

- OPSIN's provides commercial level name to structure performance across a wide range of IUPAC chemical nomenclature.

- OSCAR4 contains a readily extensible system for adding custom dictionaries and ontology term/id pairs.

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Any Questions?

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