TUTORIALS with InstantJChem

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Datasets

All files are to found in the IJC directory.

SC100.sdf: A database of 99 diverse compounds from Chemaxon

ISICCRsm.mrv/ISICCRsm.RDF: A database of 239 reactions in both RDF and MRV formats.

Exercise 1.

Create a new Project named ***IJCExercises*** and import the file SC100.sdf in it. Customize a browser for it. A new database table should be created named ***SC100***.

Exercise 2.

In the ***SC100*** database, perform a search on fluorobenzene and pyridine molecules using *Substructure* or *Similarity* options. Compare results of these two types of search.

Exercise 3.

Combine the compound 89 and 25 into one query editor and create a bond between them. Search the database with the resulting query with the option *superstructure*. Comment the result compared to the previous exercise.

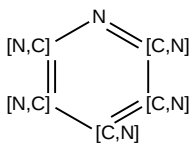
Exercise 4.

Use the entry 46 as a query. Edit the query and remove the Bromide. Perform a search setting the query as *Exact search* first, then as *Exact fragment*.

Exercise 5. *Combined Searching*
Perform a search on benzene as substructure and 'pyrimidin' containing *Product name* field and *Aq Sol* being Good.

Exercise 6.

Perform a substructural search on cyclic aromatic fragments of 6 atoms containing at least one nitrogen atoms.



Exercise 7.

Perform a search on molecules for which MolWeight > 200 and which don't contain the benzene ring.

Exercise 8.

Same question as in Exercise 7, but perform the search on two steps (*i*) search for compounds for which MolWeight > 200 then (*ii*) search for compounds containing benzene ring. Cross the two result lists.

Exercise 9.

Use the Chemical Term field to search compounds possessing more than 4 microspecies at pH=4.0. Export your hit list in an SDF file called **HitList.sdf**.

Exercise 10.

Import into your project, the file ISICCRsm.RDF. Customize a browser for it. A new database table should be created named ***ISICCRsm***.

Exercise 11.

In the ***ISICCRsm*** table, perform a search of imydazole as a substructure of the reactant then as a substructure of the product.

Exercise 12.

Edit the Schema of your project and add a new Data Tree and structure entity called ***AlkanBoilingPoint***. The new table must contain a field names BoilingPoint receiving floating point values.

Exercise 13.

Add to the ***AlkanBoilingPoint*** table the following compounds along with their boiling point temperature.

Alkan	**Boiling Point (in K)**
Pentane	231.05
Butane	272.65
Cyclopentane	322.4
1,1-dimethyl cyclopropane	293.75

Tableau 1: Boiling point for sample alkans

Exercise 14.

Add a new field named Date, for the date of the entry and fill it.

Exercise 15.

Add a Chemical Term field to add an automatically estimated value of the logP to each entry.