

# ChemicalToolBoX

## a Galaxy for Cheminformatics

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# ChemicalToolBoX



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**Paint your structure and add it to Galaxy!**

**Editor:**

**Mol. Weight: Formula:**

**Export Molfile to Galaxy**   **Export Smiles to Galaxy**

**History**

- Unnamed history 162.0 Mb
- 130: Convert MOL2 to FPS on data 129 10 molecules format: fps, database: ?
- #FPS1  
#num\_bits=1021  
#type=OpenBabel-FP2/1  
#software=OpenBabel/2.3.90  
#source=/home/ctb/galaxy-central/dat  
#date=2012-07-20T09:56:02
- 129: Select first on data 123
- 128: Remove counterions and fragments on data 122 1397 molecules format: sdf, database: ?
- [NO NAME]  
OpenBabel@7191219313D  
100105 0 0 1 0 0 0 0 0 0999 V2  
40.6155 0.7802 0.8512 0 0

# Integrated Tools

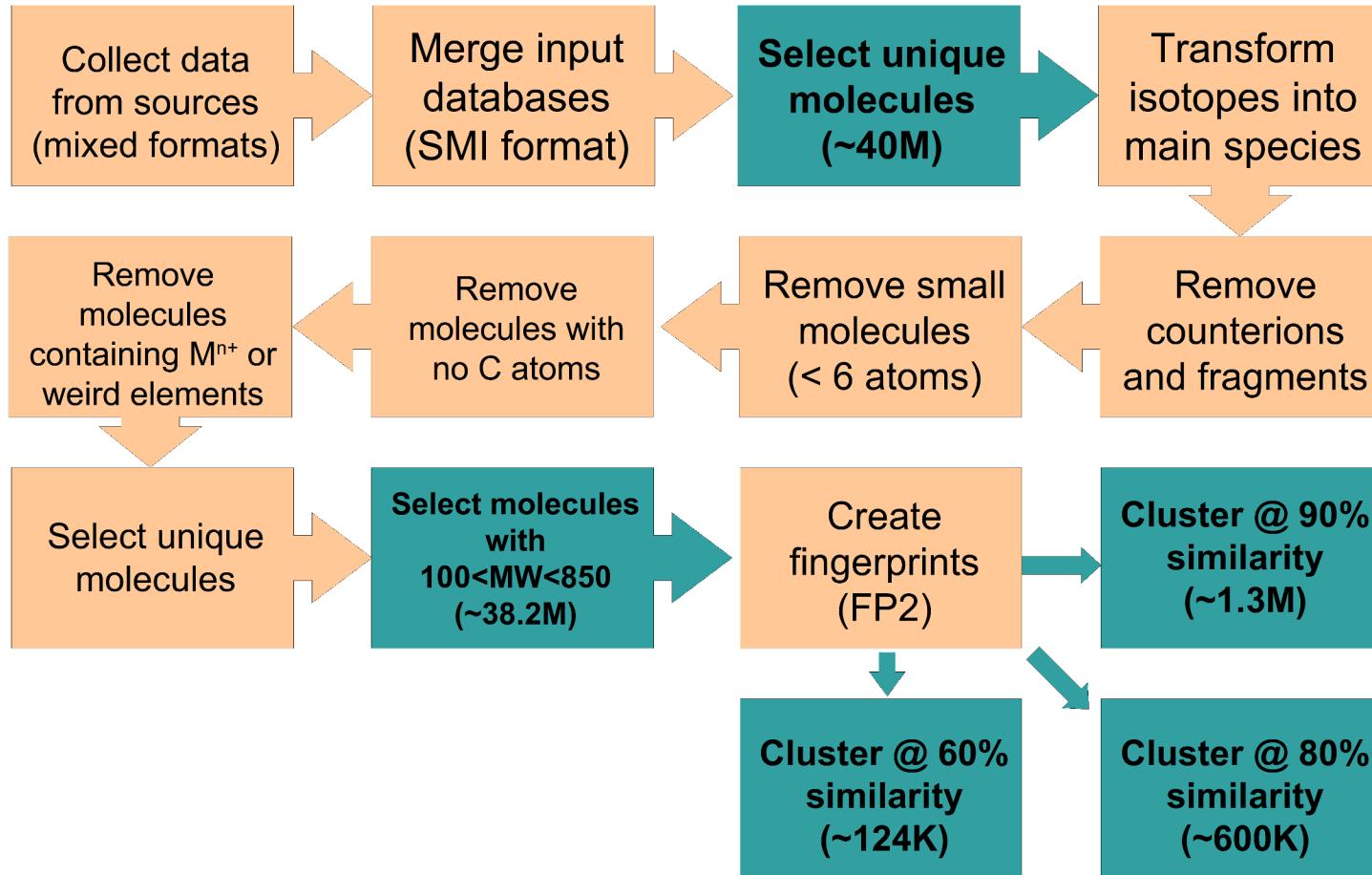


- filters
- physico-chemical properties
- Drug-likeness prediction
- Conformer
- 2D/3D coordinate
- converters + filetypes
- similarity and substructure search
- Clustering
- spectrophore and pharmacophore search
- Remove duplicates
- molecule modification
- remove ions
- plotting of compounds
- Compound-DB integration
- fragmentation of compounds

# ChemicalBoX: a workflow inside the ChemicalToolBoX



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# ChemicalBoX



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- PubChem ~ 32.5M\*
- ZINC ~ 12M
- ChEMBL ~ 1.1M
- BindingDB ~ 300K\*
- NCI ~ 260K
- ChEBI ~ 22K
- PDB ligand ~ 14K
- DrugBank ~ 6K\*

# Current features of the BoXes



## ChemicalBoX

- Largest freely available chemical library
- Workflow FULLY automatized using tools from the ChemicalToolBoX
- Weird compounds filtered out
- Monthly updated
- Pre-clustered sets at 90, 80 and 60% similarity thresholds

## PurchasableBoX

- ~ 40 companies are being fetched
- Largest filtered purchasable space known (~37M)

- <ftp://pharmaceutical-bioinformatics.org/chemicaltoolbox/>
- <ftp://pharmaceutical-bioinformatics.org/chemicalbox/>
- `$ git clone http://chemicalbox.pharmaceutical-bioinformatics.org/chemicalbox.git`

# Thanks



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