SEARCHING IN CHEMBL

Michał Nowotka
ChEMBL Group
EMBL-EBI

WHAT'S CHEMBL?

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"The majority of the ChEMBL data is derived by manual abstraction and curation from the primary scientific literature."

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CHEMBL DJANGO ORM MODEL

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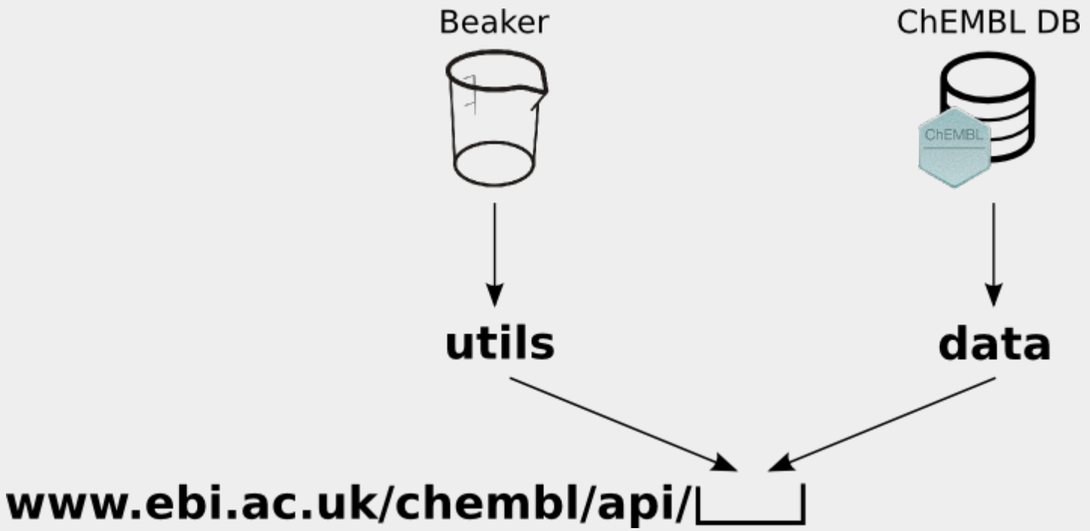
UTILITIES AND DATA



FILTERING

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molecule?max_phase=4

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Select all targets with name starting from 'serotonin':
target?pref_name__istartswith=serotonin

ORDERING

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Order molecules by weight, ascending:

molecule?order_by=molecule_properties__full_mwt

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Order by aromatic rings ascending and then by weight descending: **molecule?
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molecule_properties__full_mwt**

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- Search compounds by pref_name and synonyms

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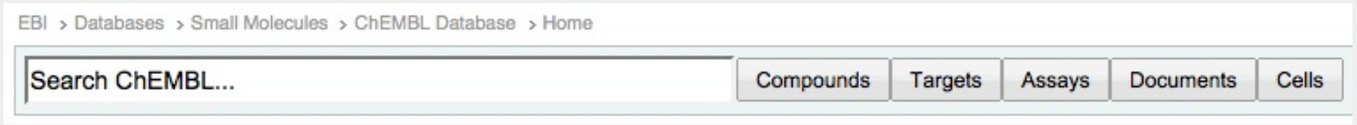

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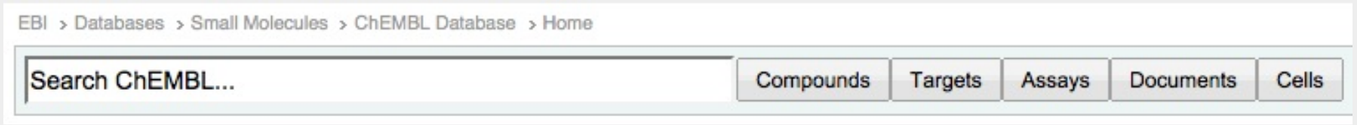

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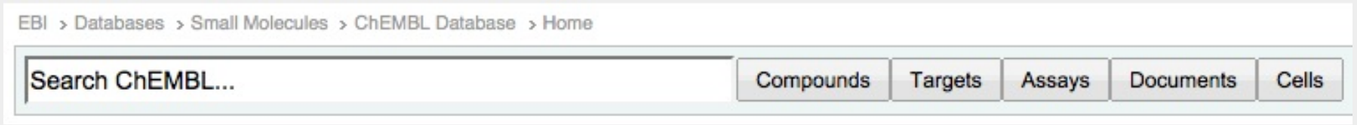

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- web widgets

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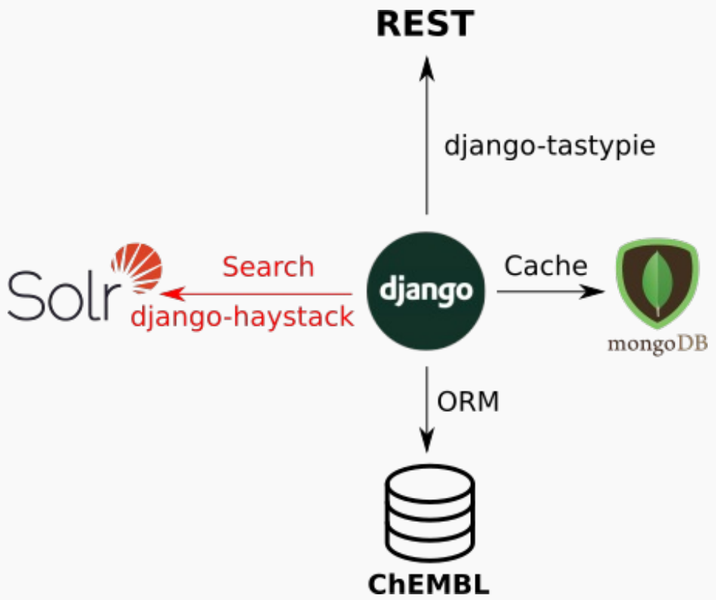
- Filtering simultaneously on many columns results in a long filter

SOFTWARE STACK



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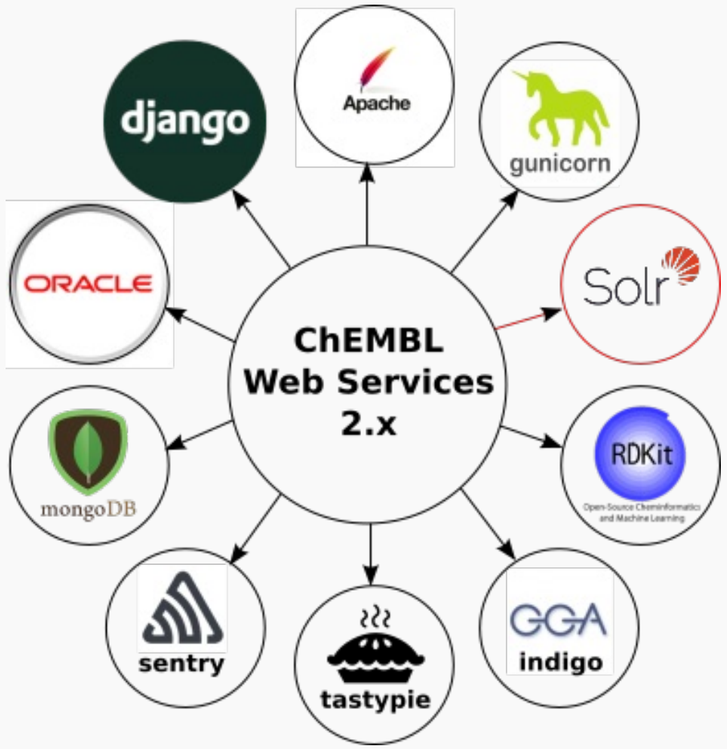
TECHNOLOGIES USED



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- BioSolr, compound similarity

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- Good performance, good results

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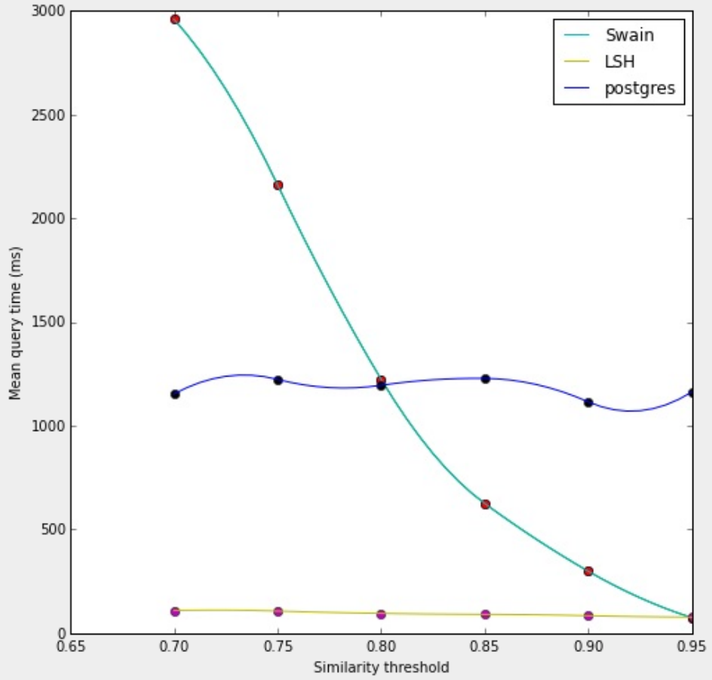
- Cache should be shared across many production machines
- Available from python, supported by EBI
- Failproof, timeout

LSH-BASED SIMILARITY SEARCH



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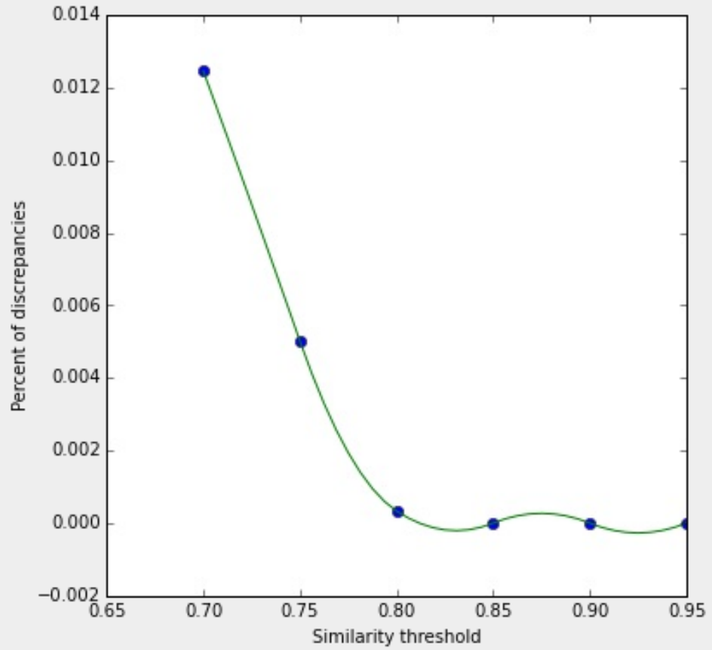

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- Very new idea (to us)

THANK YOU!

Questions?