

# PubPharm - the search engine for pharmacology, toxicology & pharmacy-specific literature

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## PubPharm Search Platform

The screenshot shows the search interface for 'Capmatinib'. At the top, there's a search bar with the query 'Capmatinib', a 'Structure Search' button, and a 'Search History' link. Below the search bar are three search results:

- Phase I dose-escalation study of capmatinib (INC280) in patients with advanced solid tumors. In *Cancer science* | (02 2019) by Esaki, T.; Hirai, F.; Makiyama, A. | +9
- MET Inhibitors Promote Liver Tumor Evasion of the Immune Response by Stabilizing PDL1. In *Gastroenterology* | (01 2019) by Li, H.; Lu, C.; Xie, X. | +16
- Phase II Multicenter Randomized Two-arm Study of Capmatinib/Spartalatinib Combination Therapy vs Dovasertaxel in Patients With EGFR Wild-type ALK Rearrangement Non-Small Cell Lung Cancer. In *Cancer discovery* | (02 2019) by Hwang, J.; Kim, J.; Cho, J. | +16

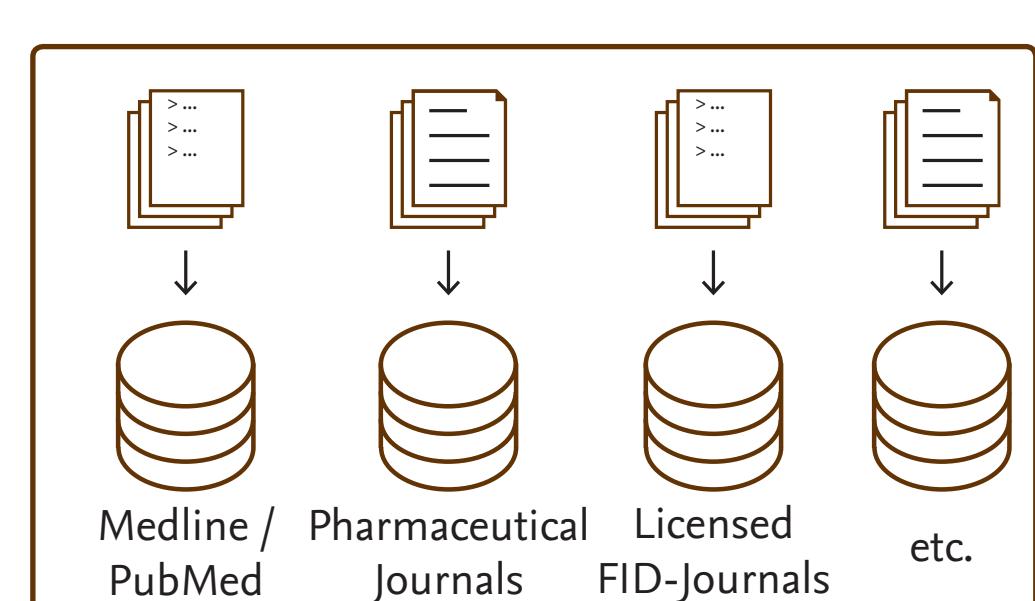
On the right side of the search results, there's a 'Structure Editor and Name Search' panel where a chemical structure of Capmatinib is shown.

PubPharm is a free pharmacy-specific search platform.

- PubPharm contains more than 50 million references
  - Including 28 million Medline (PubMed) publications



- Content beyond Medline
  - Journal articles from adjacent scientific disciplines (e.g. chemistry)
  - Pharmaceutical books (e-books, dissertations)
  - Conference papers
  - Information on clinical trials

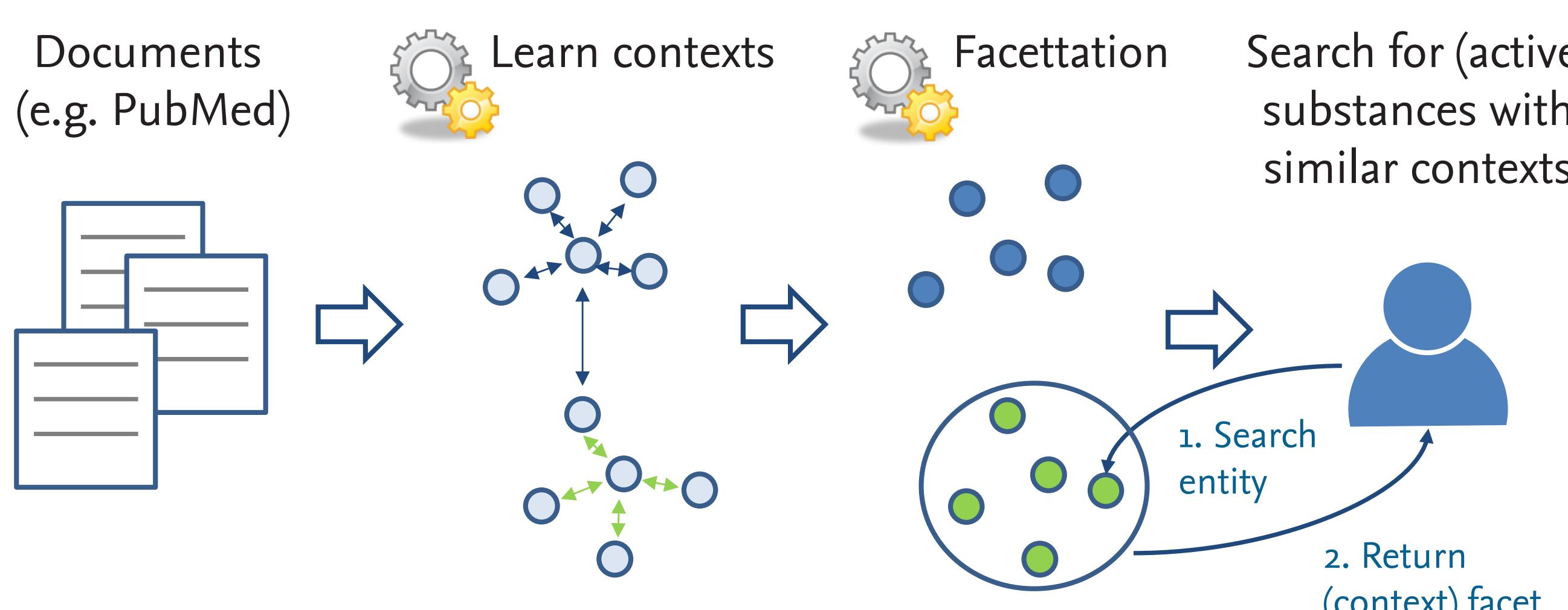


## Development of Search Tools

Semantic facettation in pharmaceutical collections using deep learning for active substance contextualization

- Aim: Prediction of possible (active) substance effects
- Hypothesis: Similar effect = similar (deep learned) context
- Provides: Alternative access paths to literature beyond mere keyword or bibliographic search

### Process Overview



References:  
Wawrzinek, J., Balke, W.-T.: Semantic Facettation in Pharmaceutical Collections Using Deep Learning for Active Substance Contextualization. In International Conference on Asian Digital Libraries. Springer, Cham, 2017; 41-53.  
Keßler, K., Krüger, A.T., Ghammed, Y., Wulle, S., Balke, W.-T., Stump, K.: PubPharm - Der Fachinformationsdienst Pharmazie. o.b.b. Das offene Bibliotheksjournal 2016; 3(3):1-23.

[www.pubpharm.de](http://www.pubpharm.de)



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## Structure Search

Structure editor      SMILES / InChI      Name

PubChem database  
97 million structures

DrugBank database  
11,938 drug entries

Name IUPAC, Mol. Weight, Description

Links

→ ChEMBL

→ PubChem

→ DrugBank

→ EPO Patents

Search in PubPharm  
for publications

The effects of simvastatin...  
Drug Treatment of Hyperlipidemia ...  
Safety of statin drugs...

Substructure search

Similarity search  
880 bit fingerprint,  
Tanimoto score > 90



## Innovative Search Tools

### Implementation in PubPharm

The screenshot shows the search results for 'Sitagliptin'. The first result is an electronic article titled 'Enzymatic synthesis of sitagliptin intermediate using a novel  $\omega$ -transaminase' by Kim, G.; Jeon, H.; Khobragade, T. | +6. The second result is another electronic article titled 'Modulating impacts of quercetin/sitagliptin combination on streptozotocin-induced diabetes mellitus in rats' by Elsh, H.; Maledi, Y.; Mokbelauer, N. | +3. The third result is an electronic article titled 'UPLC-MS/MS method for the quantification of erugliflozin and sitagliptin in rat plasma' by Qiu, X.; Xie, S.; Yu, L. | +1. The interface includes a 'Related Substances' section with links to BRENDA, a 'Related Diseases' section with links to BRENDA, and a 'Related Genes' section with links to KEGG.

In PubPharm lists of semantically related substances, diseases and genes were generated when searching for a drug substance.