



MedChemLens: An Interactive Visual Tool to Support Direction Selection in Interdisciplinary Experimental Research of Medicinal Chemistry



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Background

- Interdisciplinary experimental science
Integrate the data, methods, and theories from different scientific backgrounds and employ experiments as the key research approach
- Time-consuming and resource intensive



“What research direction will be feasible and promising?”

Motivation

Research direction selection in interdisciplinary experimental science is never an easy task...

Need to integrate and understand large-scale, heterogeneous data from all related disciplines

Current: Often focus on documentation organization, retrieval and discovery

Limitation: Decision-making in the research process?

Motivation

Research direction selection in interdisciplinary experimental science is never an easy task...

Need to integrate data in different perspectives

Current: Conventionally grouped and indexed by keywords, author network, and so forth

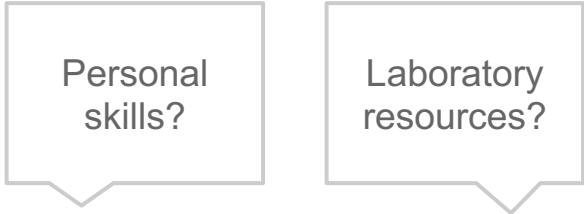
What about a medicinal chemists who commonly organize literature by the chemical structures of drug compounds?

Motivation

Research direction selection in interdisciplinary experimental science is never an easy task...

Need to estimate the feasibility and difficulties of future experimental testing stemming from their decisions

But different individuals or research groups may have different concerns



Personal
skills?

Laboratory
resources?

Select medicinal chemistry as a case

interdisciplinary of chemistry, pharmacology, and clinical pharmacy

Drug target:

Disease-linked proteins in the human body that can be agents being modulated by drugs to produce therapeutic effects

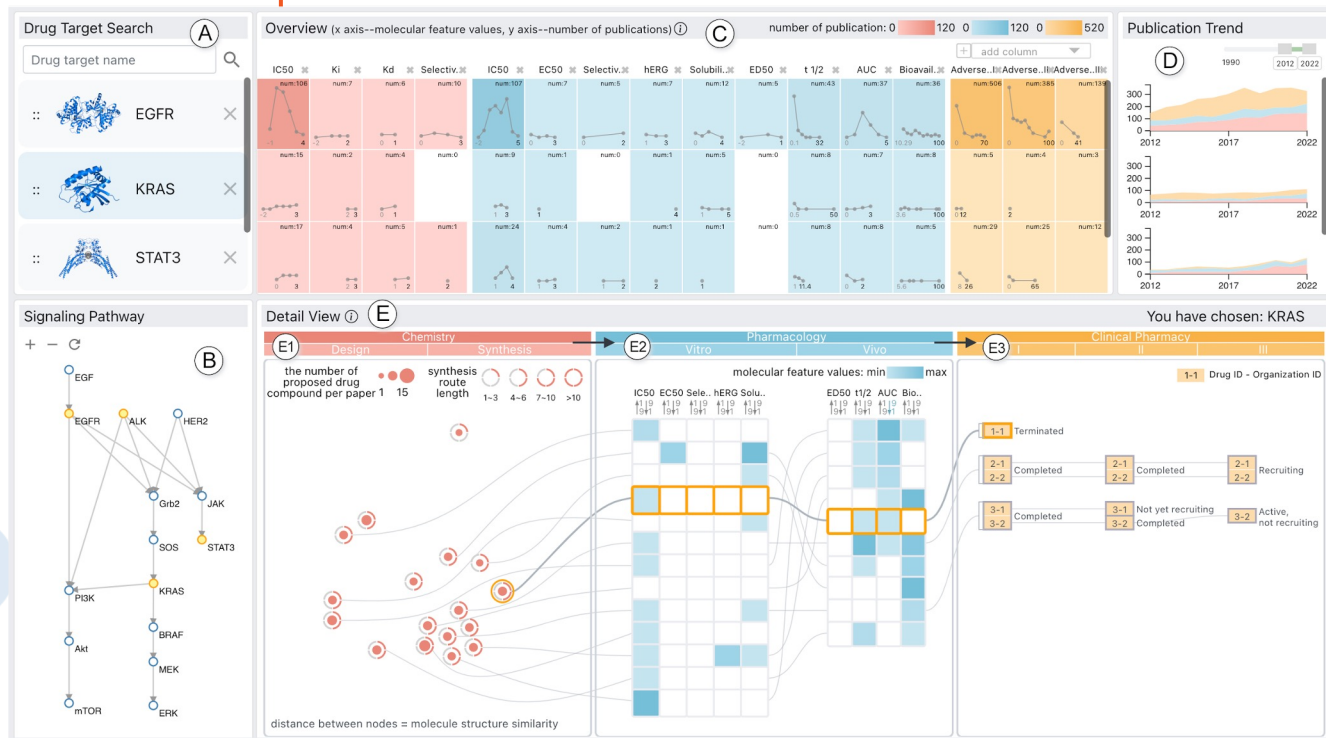
Pool of drug candidates for a disease

Select one particular

Design and test out drug compounds against it

Research direction selection

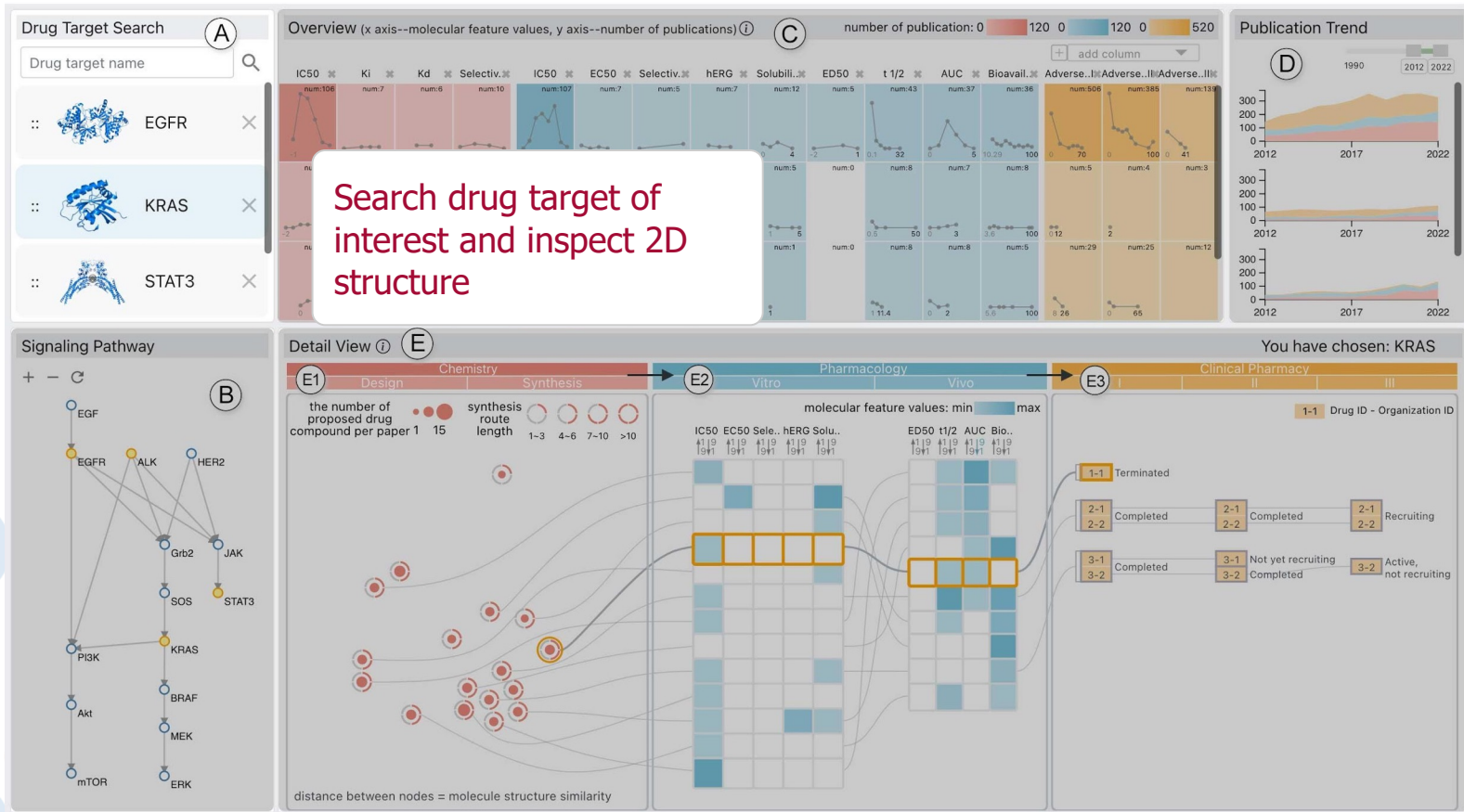
Our solution: MedChemLens for drug target selection in medicinal chemistry



- Drug Target Search View
- Signaling Pathway View
- Publication Trend View
- Overview
- Detail view

MedChemLens

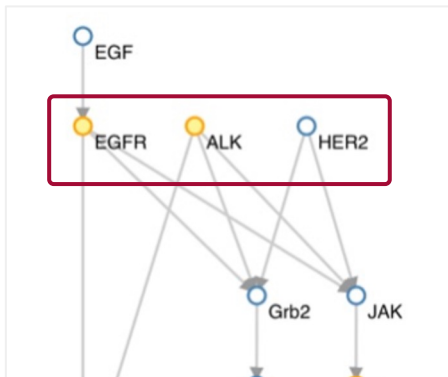
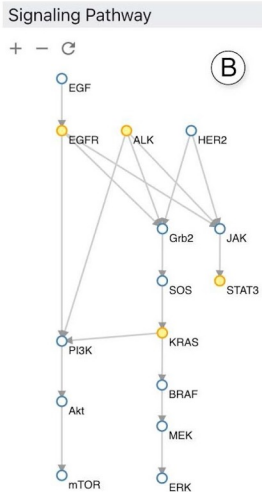
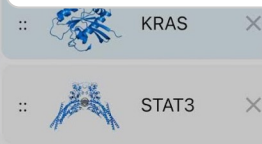
Drug Target Search View



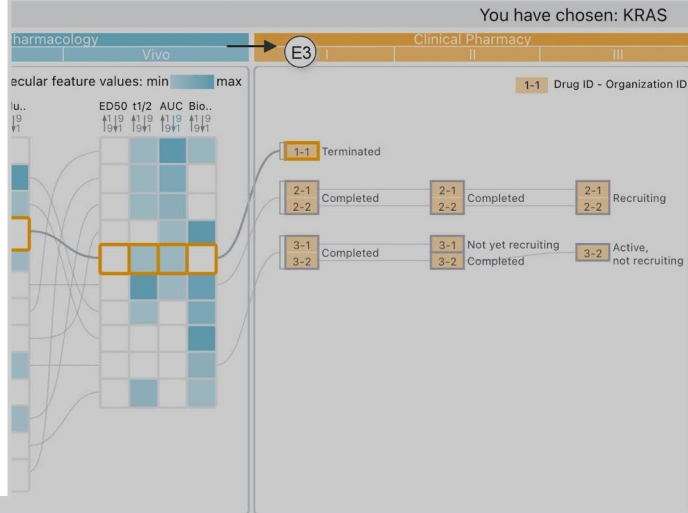
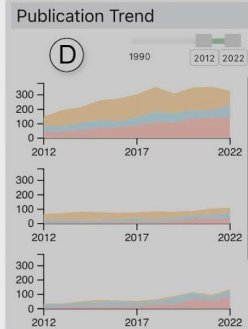
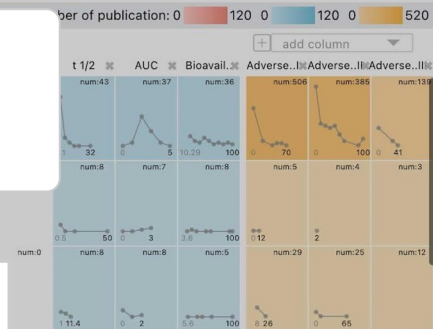
Signaling Pathway View

Signaling Pathway

A chain of proteins activated by drug compounds binding with drug targets and often contains several drug targets

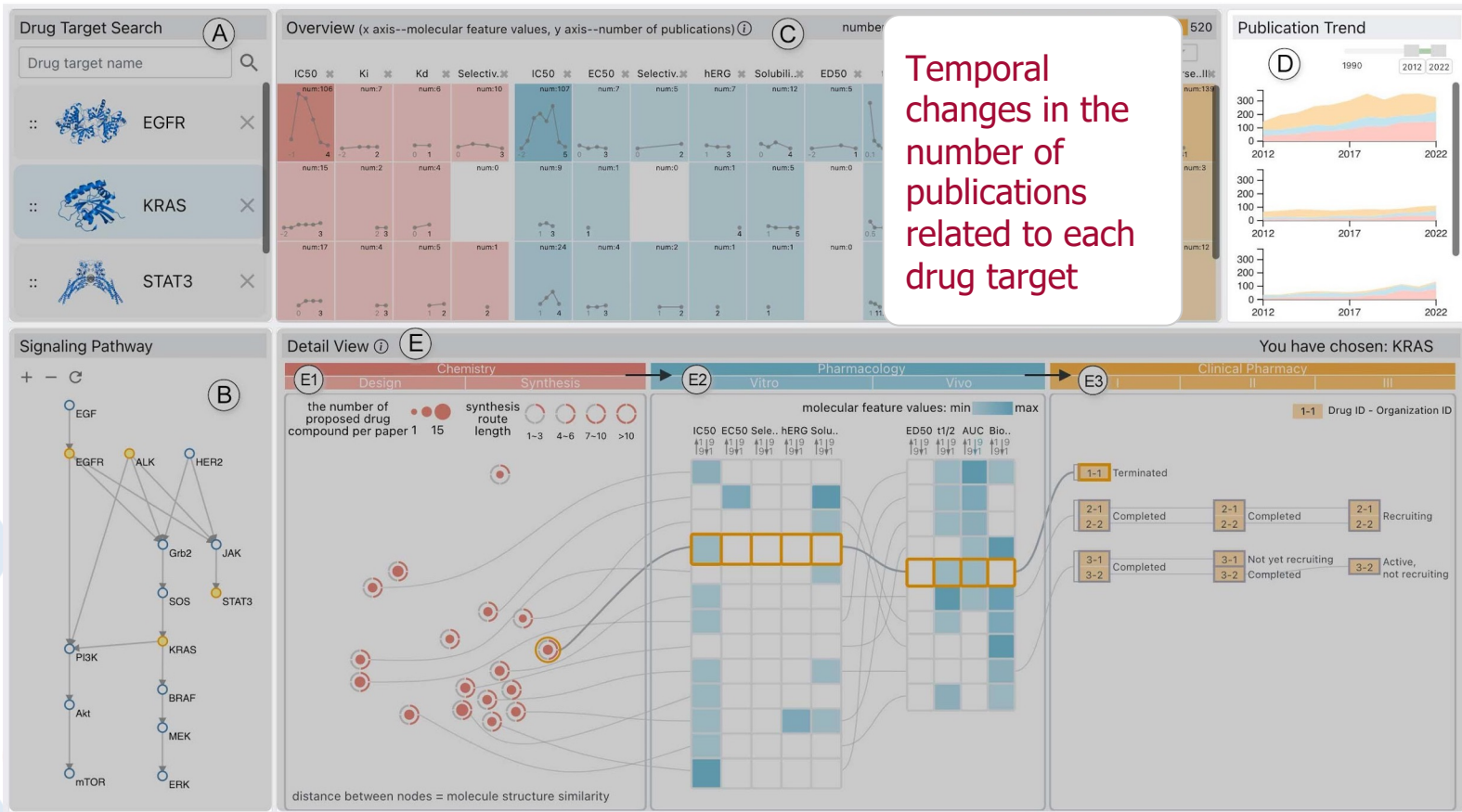


HER2 is similar to EGFR and ALK but is missed by users



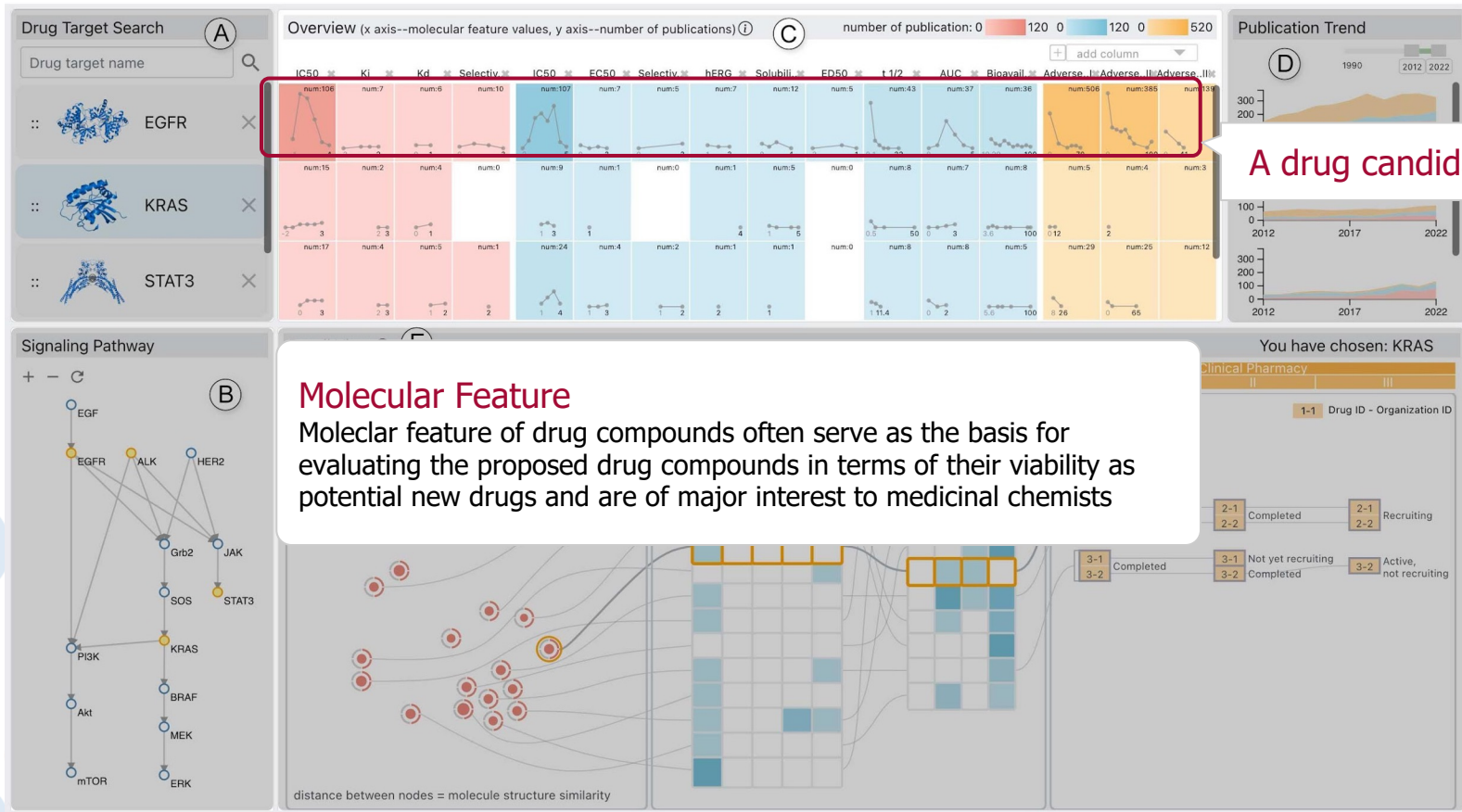
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Publication Trend View



MedChemLens

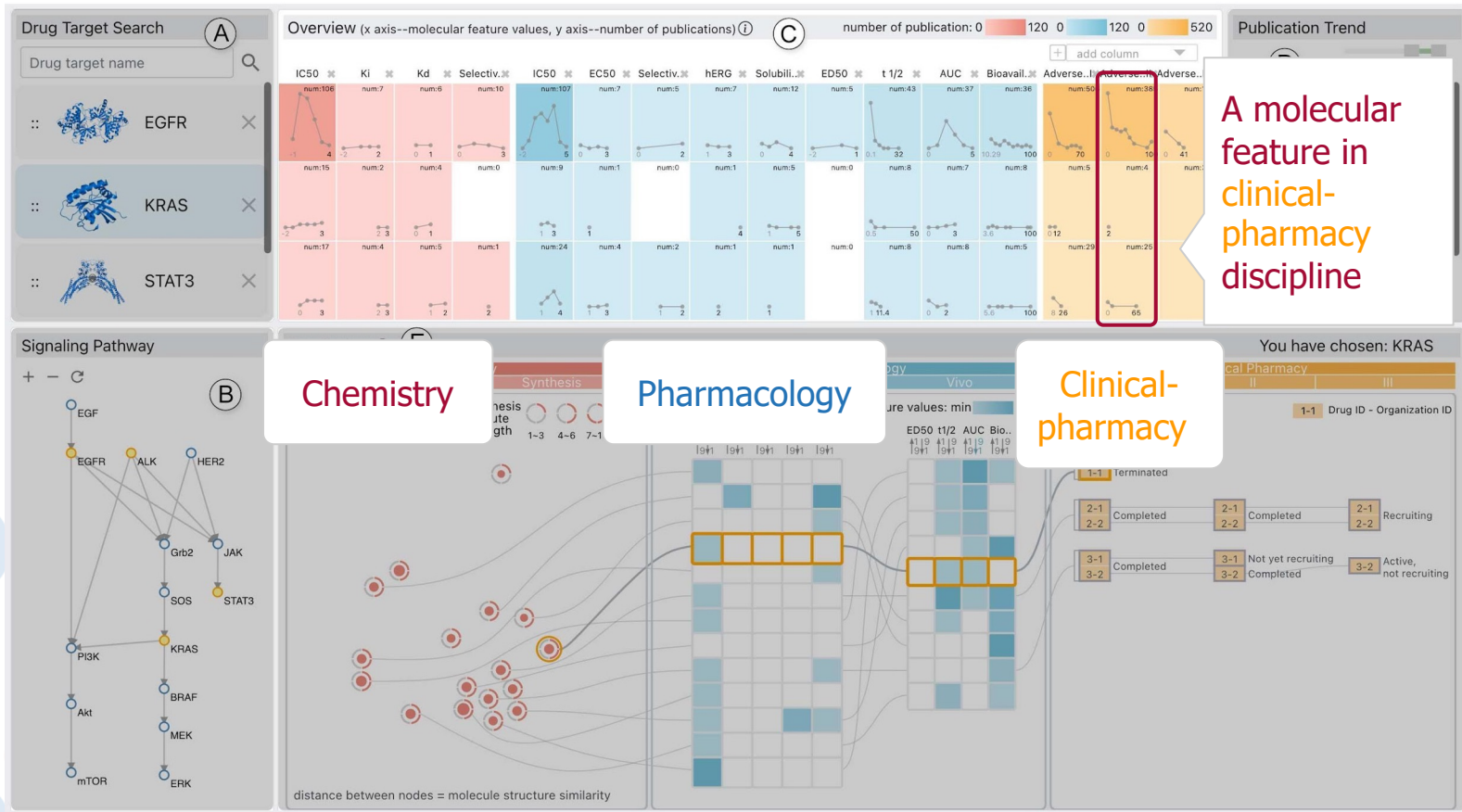
Overview



A drug candidate target

MedChemLens

Overview



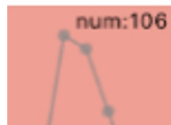
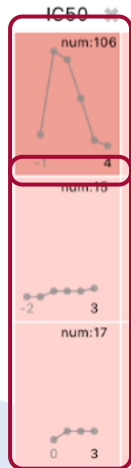
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Overview

Overview (x axis--molecular feature values, y axis--number of publications) ⓘ

number of publication: 0 120 0 120 0 520

+ add column ▼



Line chart: Distribution of the feature value in publications
X-Axis: Feature value



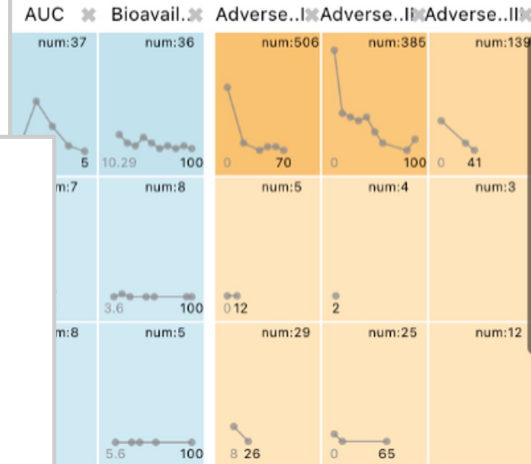
KARS



STAT3

Comparison
 Drug compounds against KARS achieved better (lower value is better) IC_{50} than those against STAT3 though there are more related works

Improving the potency of STAT3 may be challenging!



Chemistry

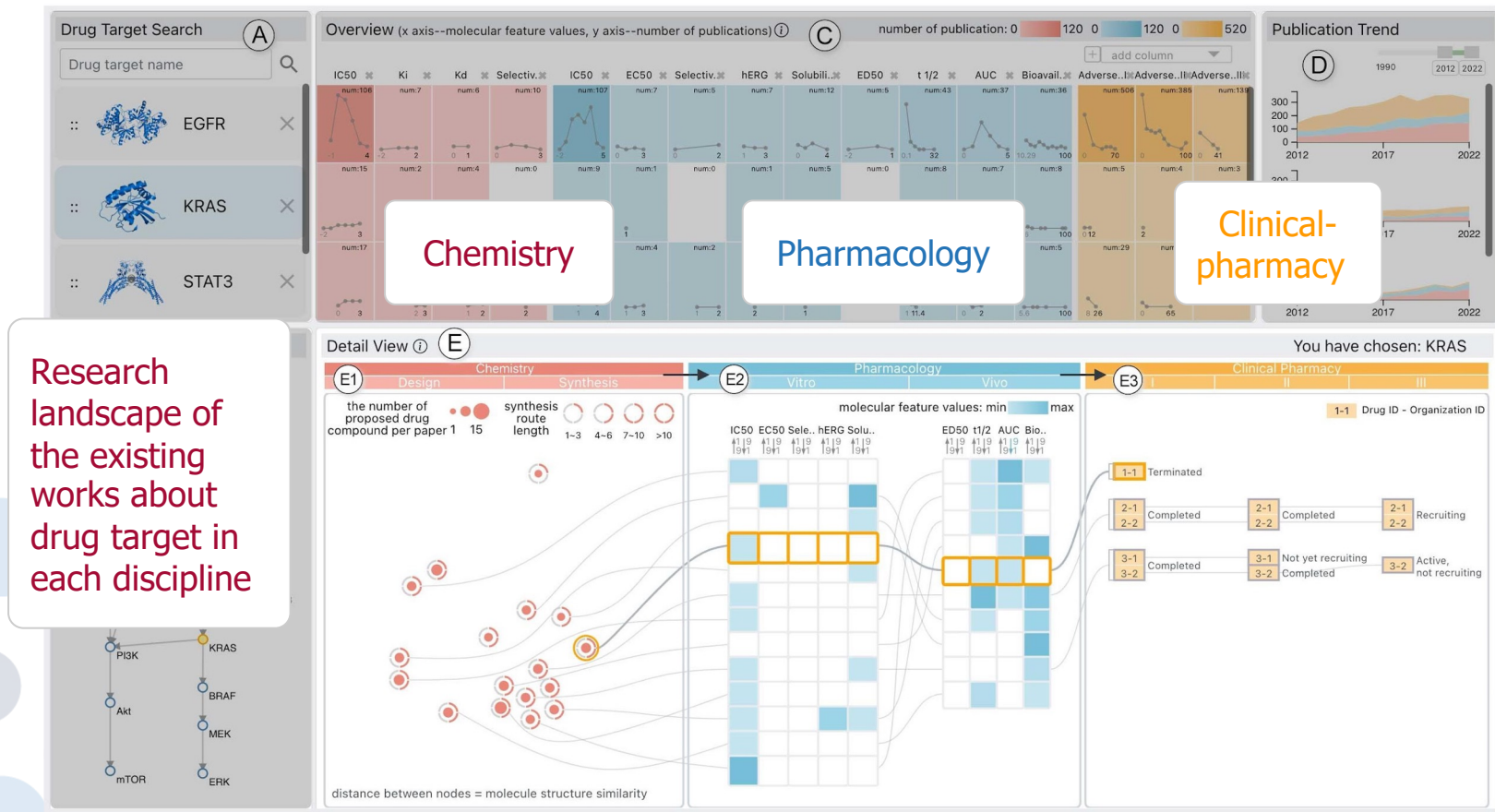
The number of publications whose proposed compounds improved the corresponding molecular feature

Pharmacology-related columns:

The number of clinical studies in each phase of clinical trials

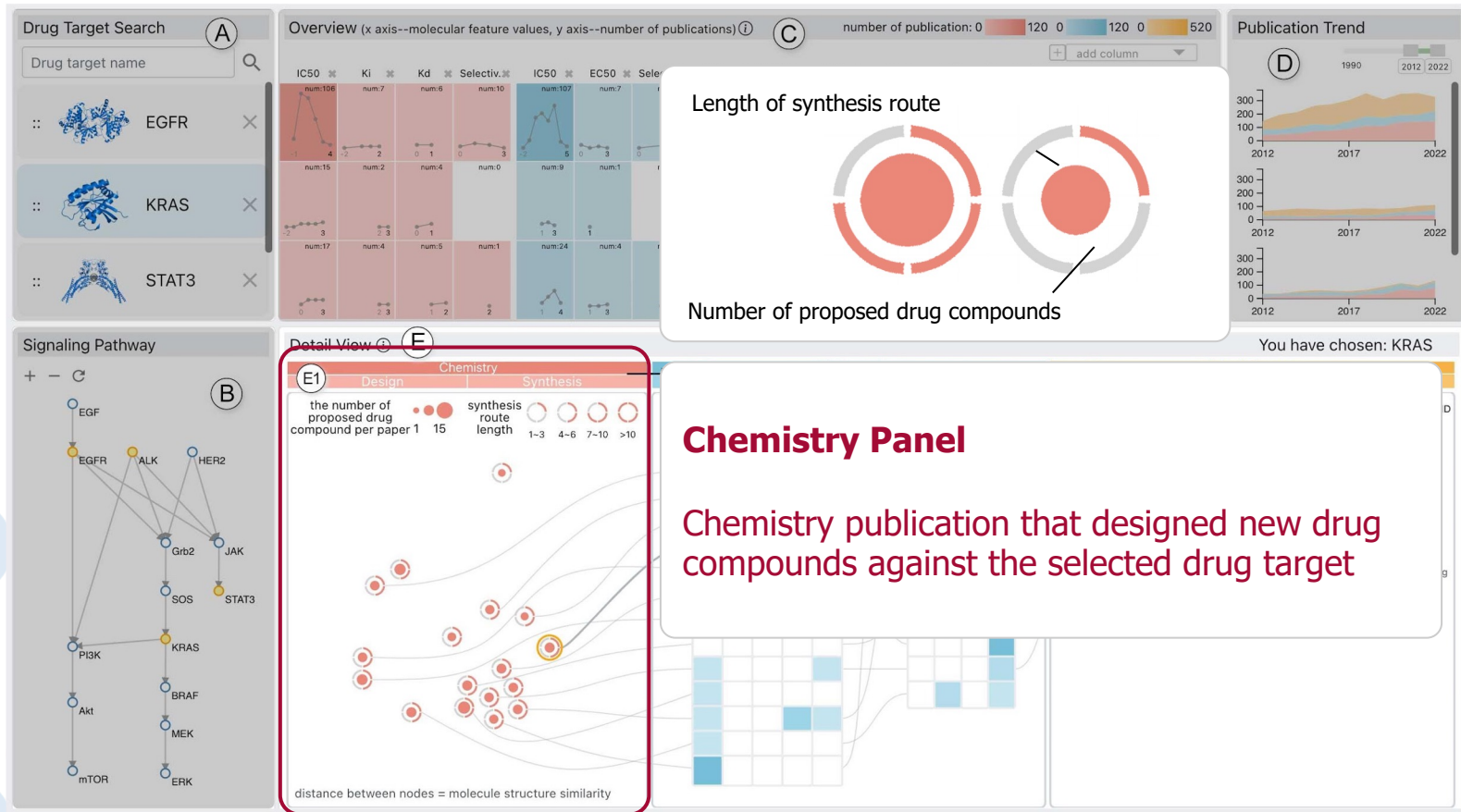
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Detail View



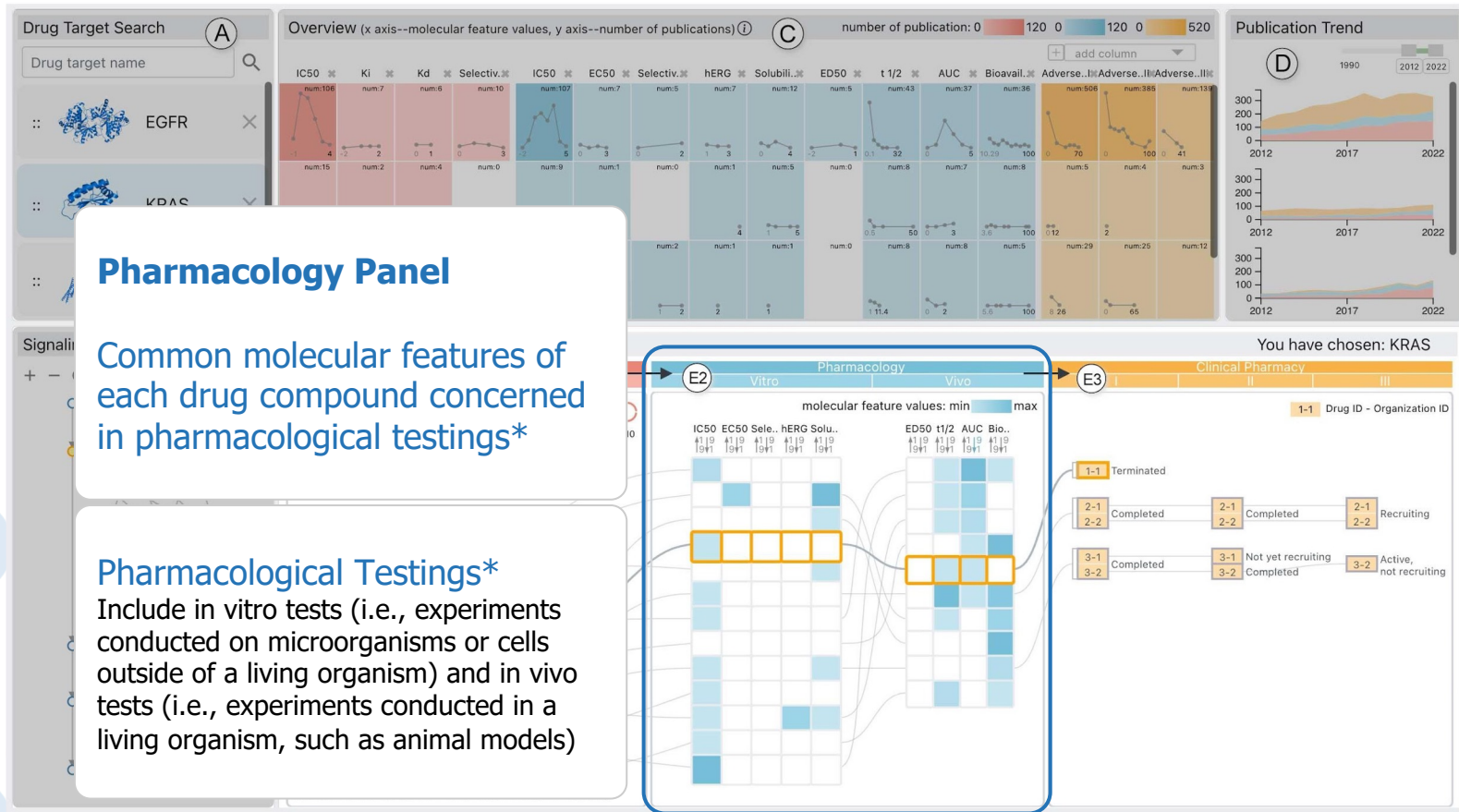
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Detail View



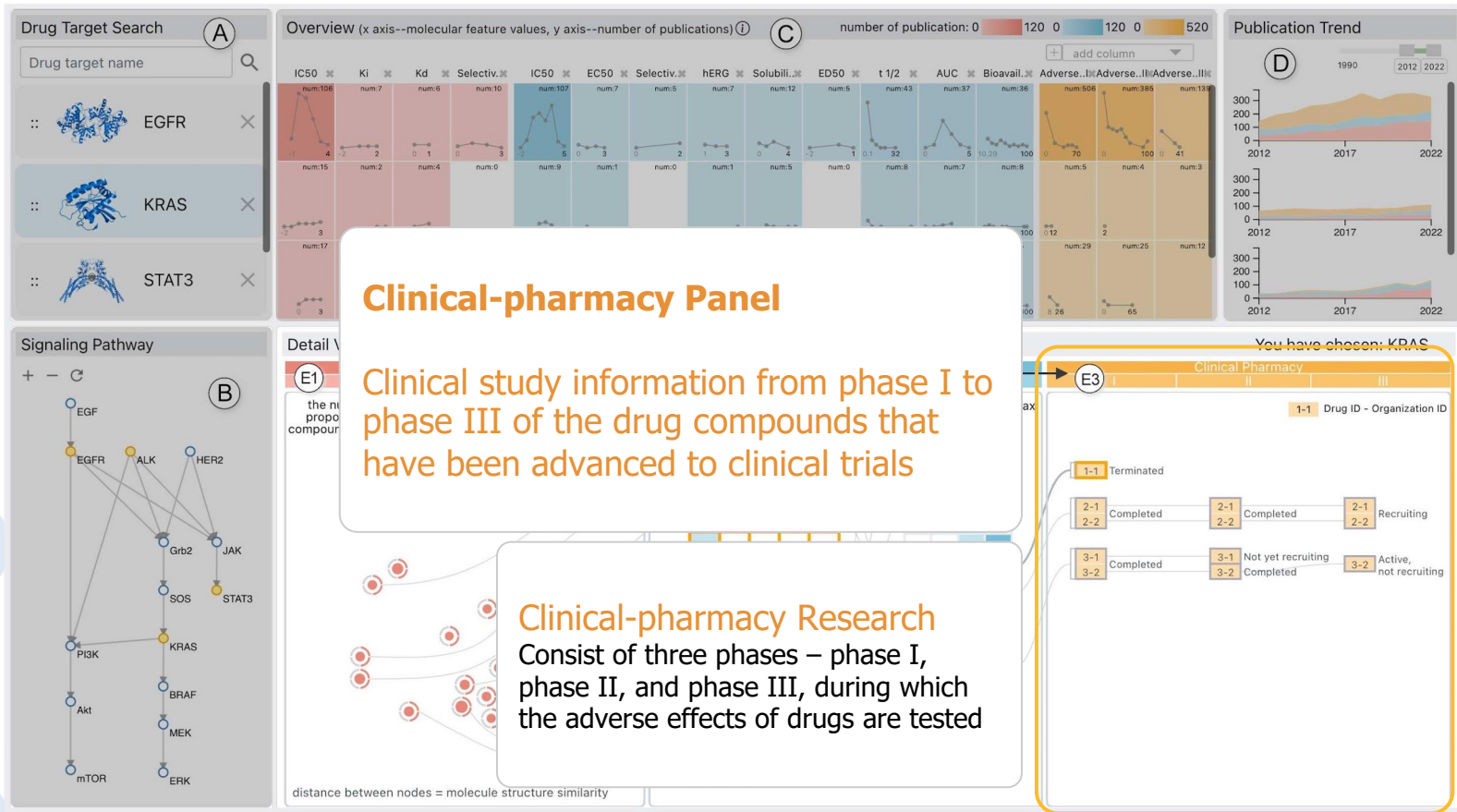
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Detail View



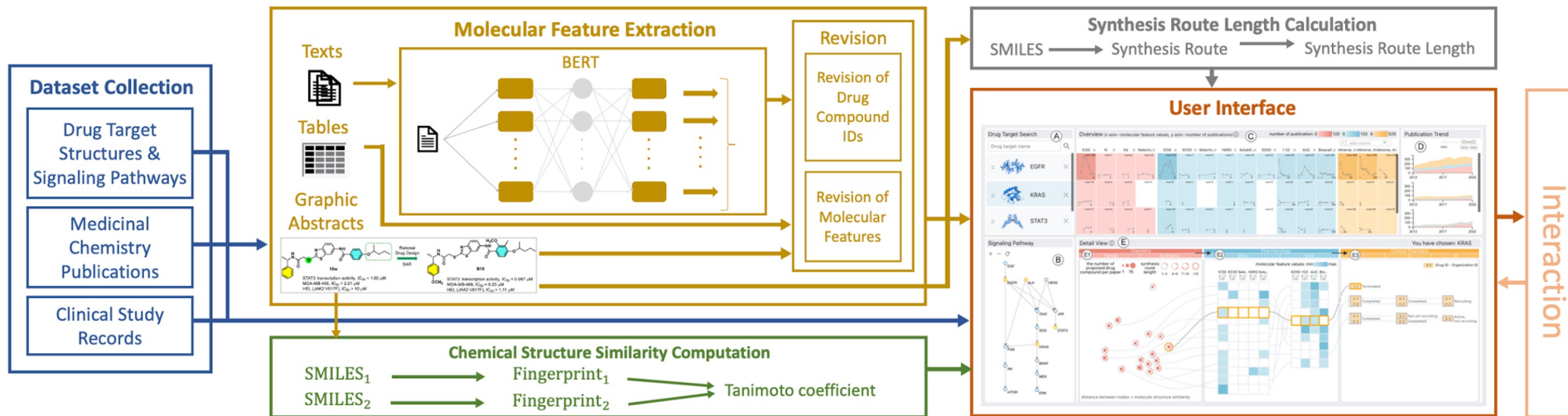
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Detail View



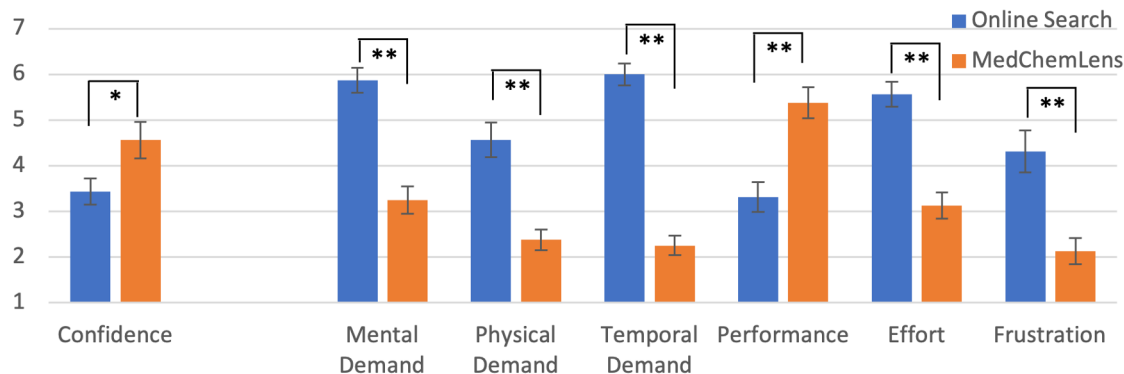
MedChemLens

How does it work?



User Study

- Performance
 - Less task completion time
 - More effective in inspecting relevant publications
 - More rational and comprehensive final selections
- Significantly more confidence and less cognitive load
- Positive responses to the usability ($M = 5.75$, $SD = 1.13$) and usefulness ($M = 5.75$, $SD = 1.13$)



Conclusion

- MedChemLens, an interactive visual tool to support medicinal chemists to evaluate possible research directions by analyzing and comparing relevant literature and experimental data.
- A within-subjects user study that demonstrates the effectiveness of our approach in helping users select research directions in the interdisciplinary experimental research of medicinal chemistry.

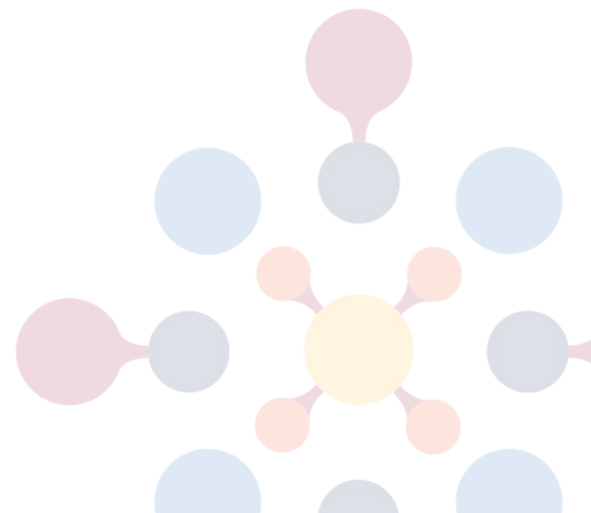
A decorative graphic on the left side of the slide. It features a vertical dashed orange line. To the left of this line are several overlapping circles in light blue, light pink, and light yellow. At the bottom left, there is a small logo consisting of a cluster of colored dots (blue, orange, yellow) next to the text 'VIS 2022'.

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Thank you!

Search Us: HCI HKUST <http://hci.cse.ust.hk/>

Contact Me: Chuhan Shi cshiag@connect.ust.hk



Motivation

Research direction selection in interdisciplinary experimental science is never an easy task

Often focus on documentation organization, retrieval and discovery

Decision-making in the research process?

Organize data in conventional ways

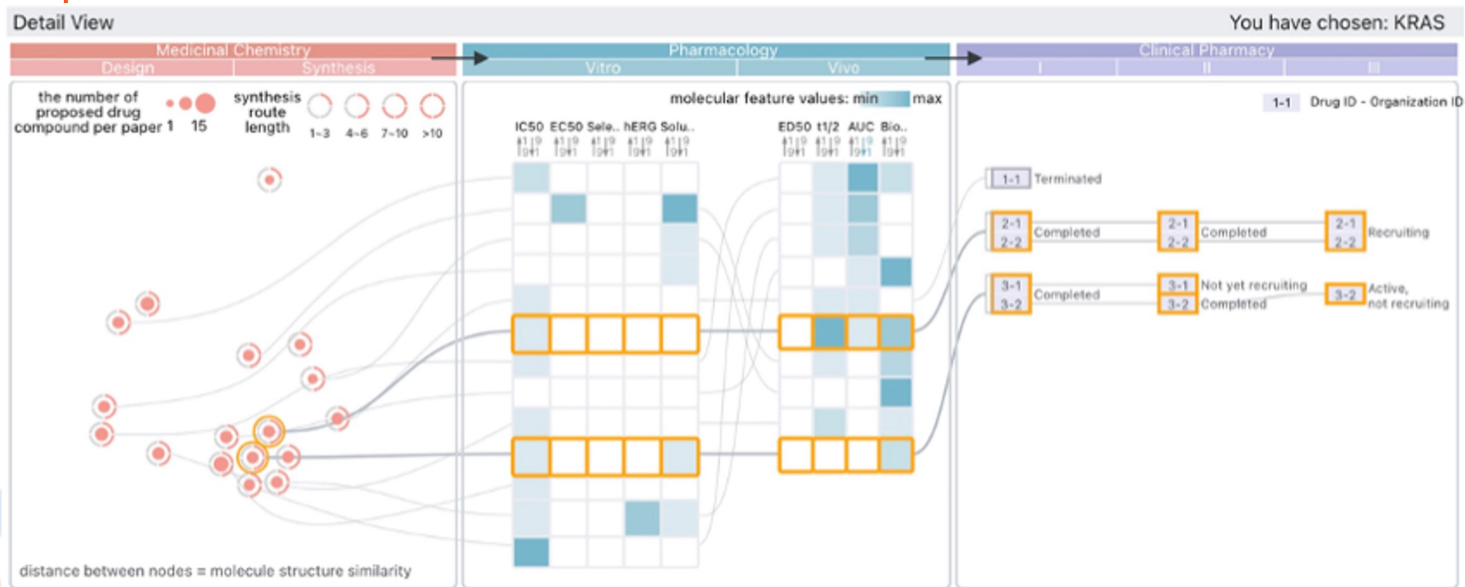
Data integration needs in the field?

Different concerns from different disciplines

Estimate the feasibility and difficulties?

MedChemLens

Detail View





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