IChem: a toolkit for rational drug design

- **Accelerating and rationalizing hit to lead**
- **Enables in silico target fishing and early safety profiles**
- **Fast and cost-efficient**

KEYWORDS

In silico screening
Drug discovery
Target identification

REFERENCES

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LABORATORY

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TECHNOLOGY

1D fingerprinting of protein-ligand 3D structures
- Binding mode fingerprints
- Cavity fingerprints
- Cavity detection and druggability estimates
- In silico target screening
- Target family-based compound screening

APPLICATION

- Hit identification by virtual screening
- In silico target prioritization (Phenotypic screen follow-up)
- Early preclinical safety profile (most likely targets)
- Detection and screening of protein-protein interfaces

INNOVATION ADVANTAGES

- ultrafast
- relies on experimental data to post-process complex virtual screening matrices
- enables both compound and/or target libraries in silico screening

DEVELOPMENT STATUS

- Validated on difficult targets (e.g. GPCRs, RTKs; PPIs) either in-house or in collaboration with biotech/pharma partners
- Tool for automated identification of protein-protein interaction modulators under development

***Partnership** : licensing-out, fee for services, collaboration*

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