

Design Hub for Drug Discovery

Drug Design – Decision Making

Identify the goal

Gather information

Identify alternatives

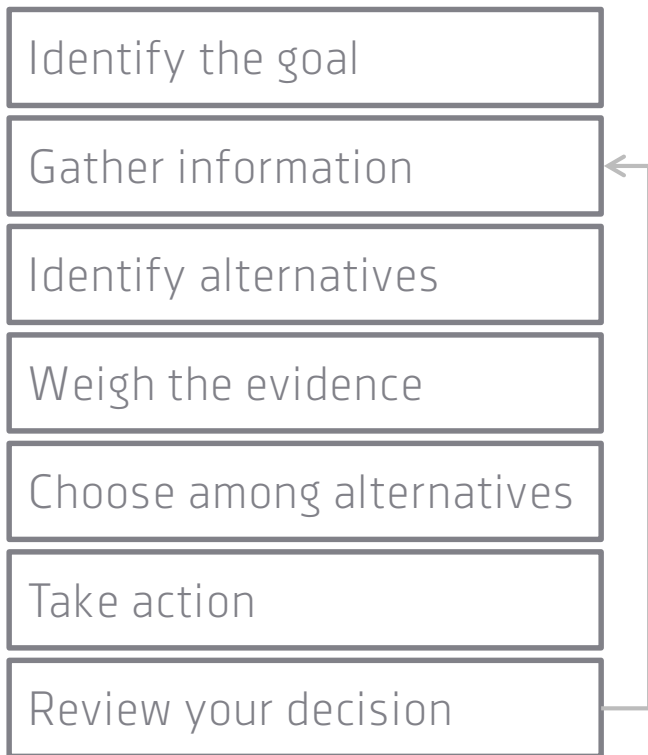
Weigh the evidence

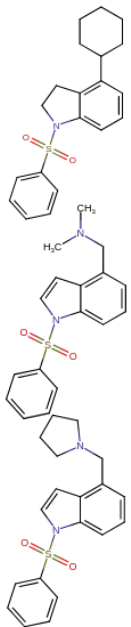
Choose among alternatives

Take action

Review your decision

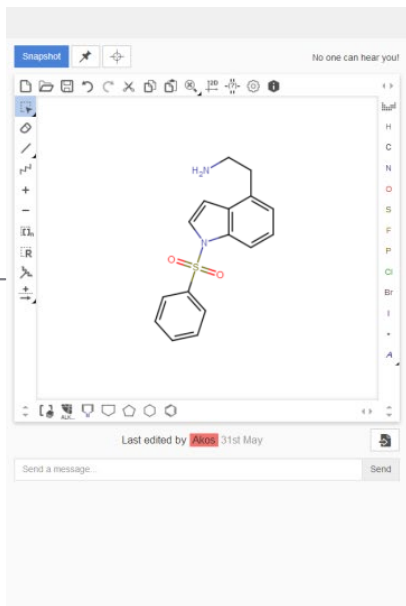
Drug Design – Decision Making





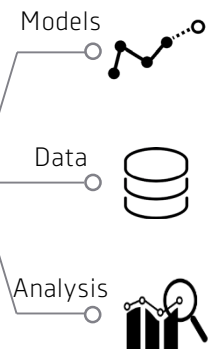
Variations

Idea
repository



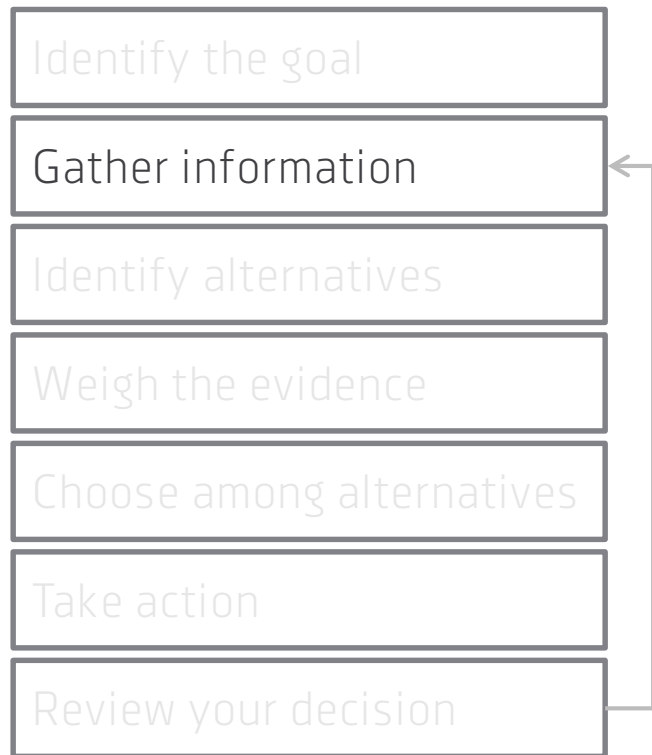
Brainstorming
space

Information



Plugin
results

Drug Design – Decision Making

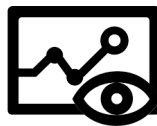


Gather information: Plugin system



Service-agnostic

Easy to extend
(REST, SQL, CLI)



Real-time

As you draw



Dynamic

Right amount of information

Gather information

Array of services



- Data access
- Preprocessed data
 - MMPA
- Derived models
 - QSAR
 - AI, Machine Learning

Gather information

Migrate to the system



Gather information

Service-agnostic integration



Gather information

Dynamic



Gather information

Dynamic



Gather information



Gather information: Matched Molecular Pair Analysis

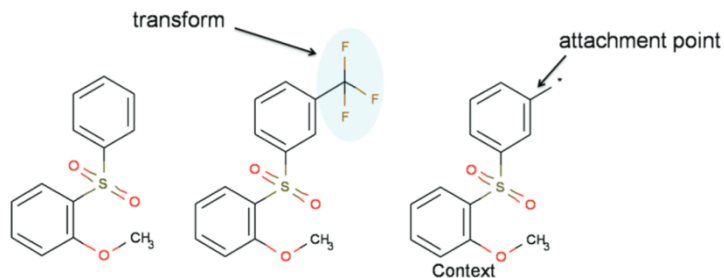
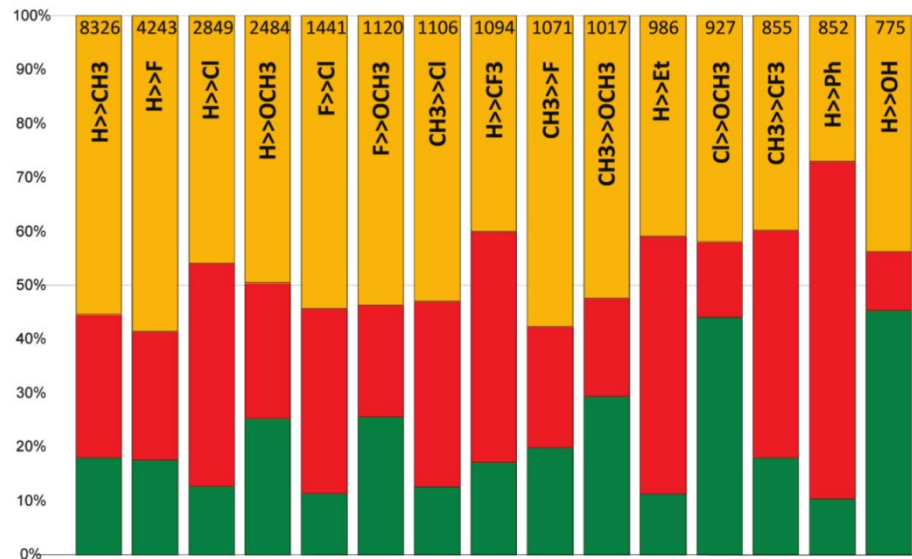


Figure 1. One matched molecular pair and its context. The transformation is $H \rightarrow CF_3$ (a single-point change) and is highlighted in yellow. The asterisk in the context denotes the attachment point.



Gather information



Gather information



ChEMBL23

hERG
Drug-like
Standardization

RDKit MMPDB
Hussain and Rea
SQLite DB

Import
JWS search

NodeJS

Gather information



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JWS search

NodeJS



~1 day

Gather information



ChEMBL23

hERG
Drug-like
Standardization

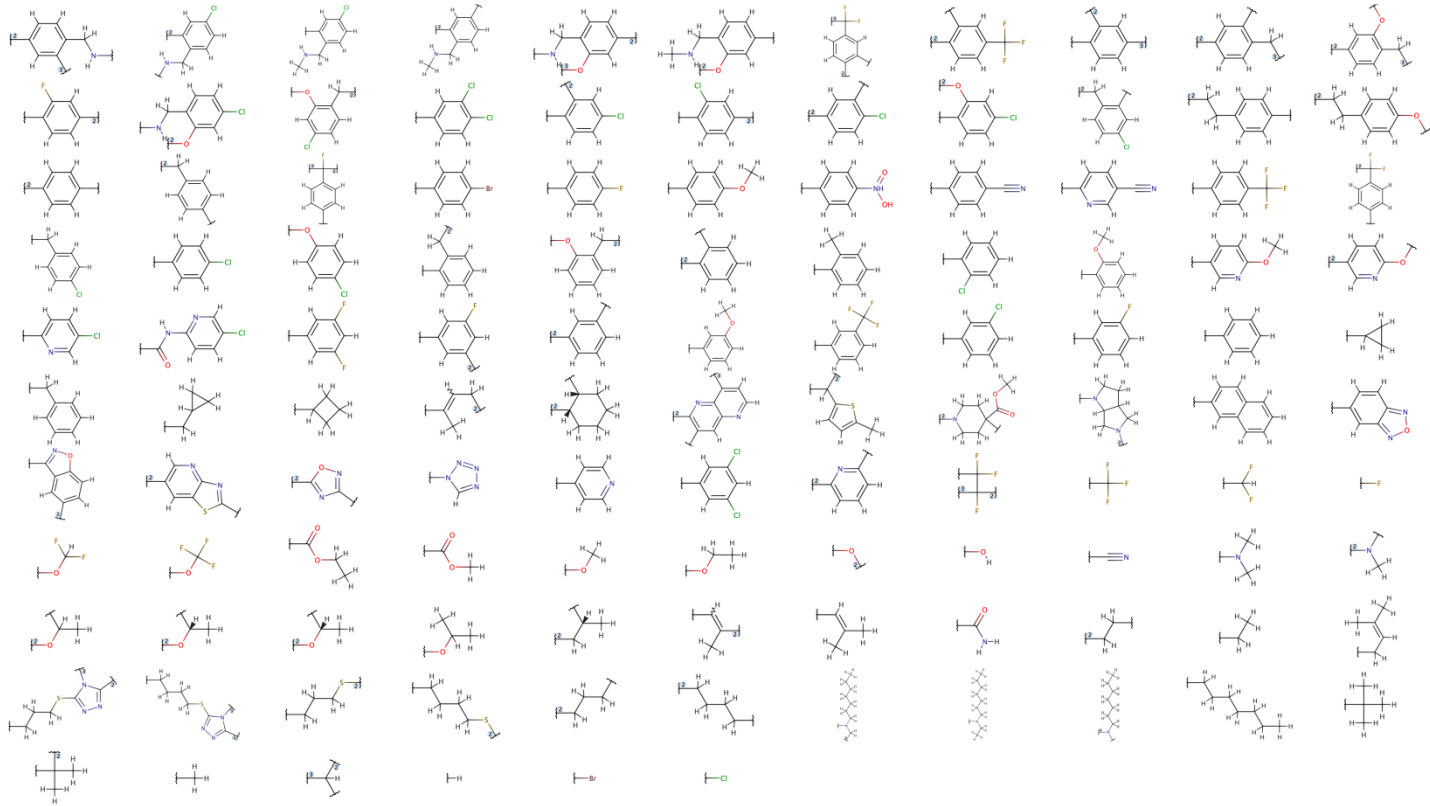
RDKit MMPDB
Hussain and Rea
SQLite DB

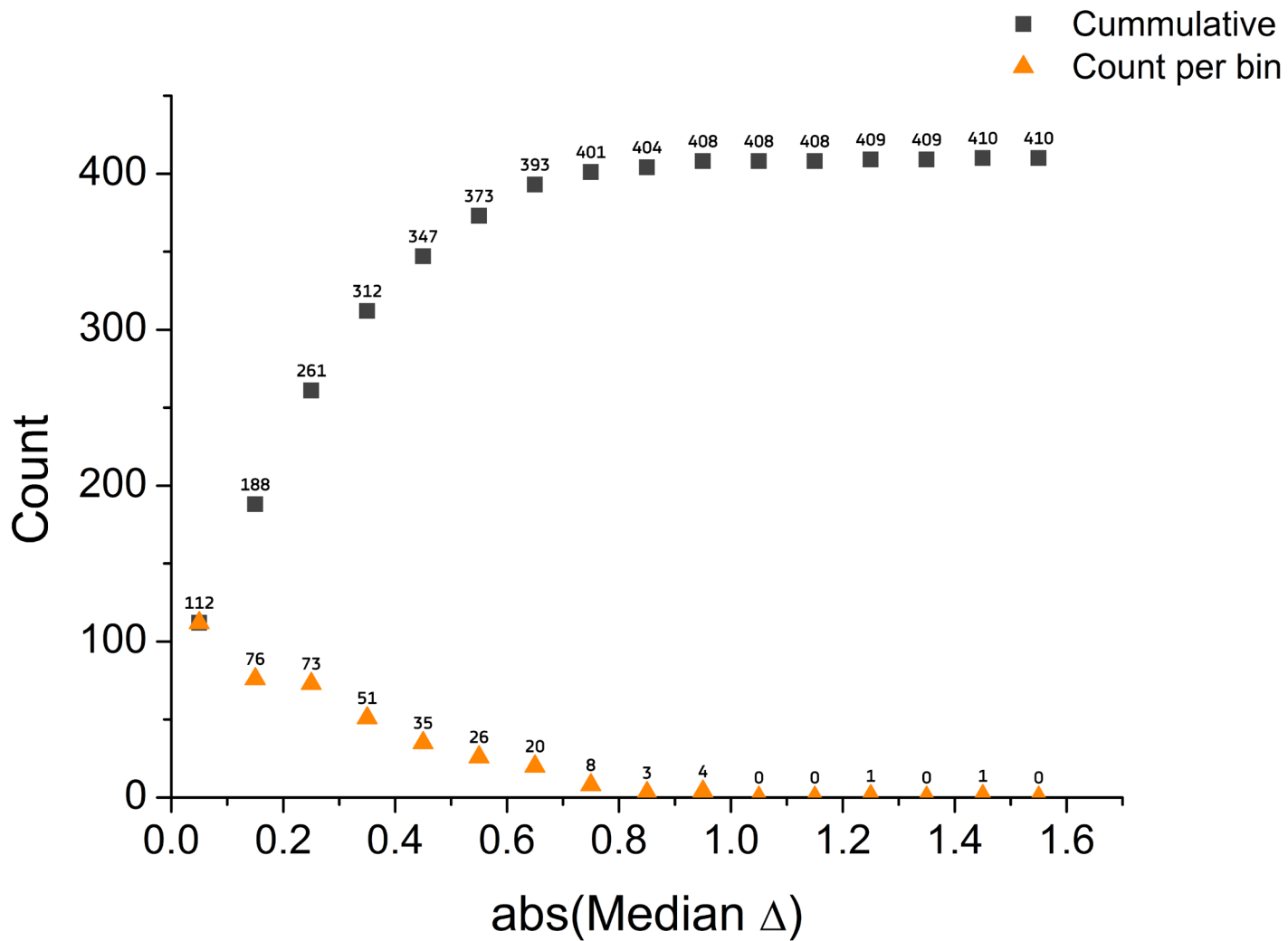
Import
JWS search

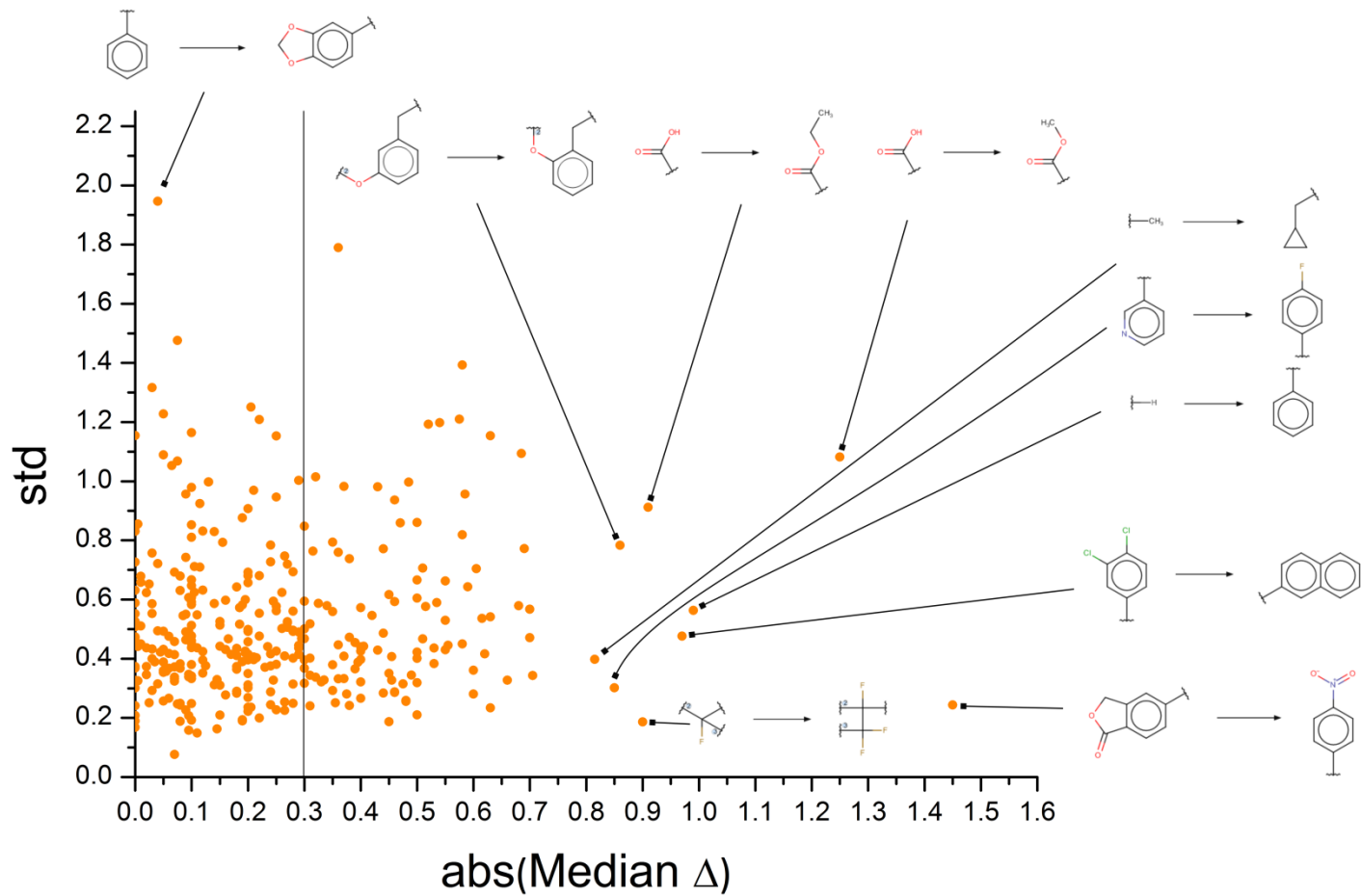
NodeJS



~1 day







MMP case study

ChEMBL

Filters

MMPDB

JChemWS

Plugin



hERG assistant

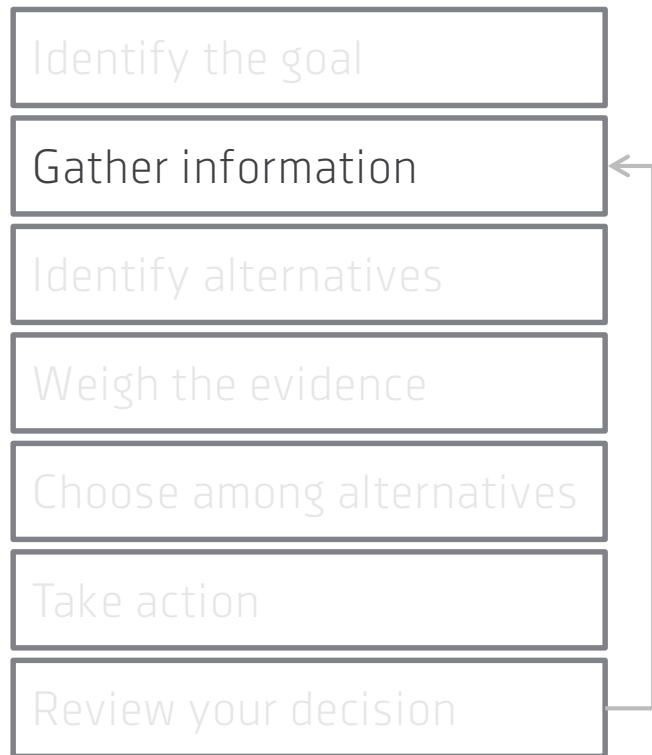
Suggestions total: 28. Showing page 3 of 10. [Prev](#) [Next](#)

Number of matched pairs 6

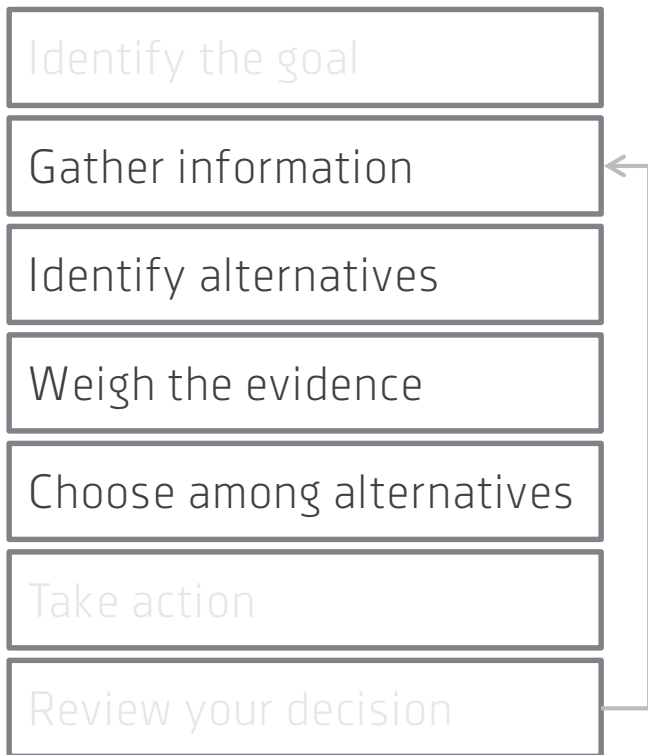
Min value (ΔpIC_{50})	-1.77
Max value (ΔpIC_{50})	0.92
Median value (ΔpIC_{50})	-0.91

Example compounds:

Drug Design – Decision Making



Drug Design – Decision Making

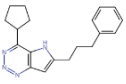
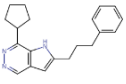
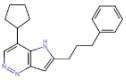
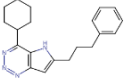
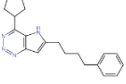
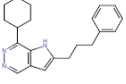


Weigh the evidence

H3: Linker length variations (private) 29d
Test linker length variations.

CREATE OVERVIEW

Showing 9 of 64 snapshots.

ID	Molecule	Author	Create date	Task	Priority	Chemist	Status	cLogP	TPSA	H-bond acceptors	Highest similarity
<input type="checkbox"/> #8		Akos	21st Nov	Synthesize	High	Jon	Synthesized	3.6	54.46	3	0.64
<input type="checkbox"/> #7		Akos	21st Nov	Synthesize	High	Jon	Approved	3.65	41.57	2	0.71
<input type="checkbox"/> #4		Akos	21st Nov	Synthesize	High	Jon	Approved	3.88	41.57	2	0.7
<input type="checkbox"/> #16		Akos	21st Nov	Synthetic feasibility ch...	Medium	Linda	Ready for review	3.99	54.46	3	0.63
<input type="checkbox"/> #24		Akos	21st Nov	Synthetic feasibility ch...	Medium	Linda	Ready for review	3.99	54.46	3	0.64
<input type="checkbox"/> #15		Akos	21st Nov	Synthetic feasibility ch...	Medium	Linda	Ready for review	4.04	41.57	2	0.7

ADD PROPERTY

Calculated Properties

- Mass
- cLogP 3.6 - 4.3
- TPSA
- pKa (str. acidic)
- FSP3
- Solubility
- H-bond acceptors
- H-bond donors
- pKa (str. basic)

SureChEMBL

- Highest similarity
- ID

Molport

- Compound IDs

Snapshot details

- ID
- Molecule
- Author
- Create date
- Task
- Priority
- Chemist
- Status

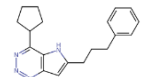
Choose among alternatives

H3: Linker length variations (private) 29d
Test linker length variations.

CREATE OVERVIEW

Showing 9 of 64 snapshots.

#8



cLogP: 3.6
TPSA: 54.46
Highest similarity: 0.64
H-bond acceptors: 3

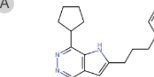
Synthesize

High

Jon

Synthesized

#7



cLogP: 3.65
TPSA: 41.57
Highest similarity: 0.71
H-bond acceptors: 2

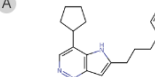
Synthesize

High

Jon

Approved

#4



cLogP: 3.88
TPSA: 41.57
Highest similarity: 0.7
H-bond acceptors: 2

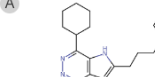
Synthesize

High

Jon

Approved

#16



cLogP: 3.99
TPSA: 54.46
Highest similarity: 0.63
H-bond acceptors: 3

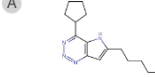
Synthetic feasibility check

Medium

Linda

Ready for review

#24



cLogP: 3.99
TPSA: 54.46
Highest similarity: 0.64
H-bond acceptors: 3

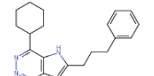
Synthetic feasibility check

Medium

Linda

Ready for review

#15



cLogP: 4.04
TPSA: 41.57
Highest similarity: 0.7
H-bond acceptors: 2

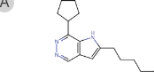
Synthetic feasibility check

Medium

Linda

Ready for review

#23



cLogP: 4.04
TPSA: 41.57
Highest similarity: 0.71
H-bond acceptors: 2

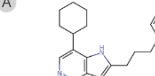
Task

Priority

Chemist

Status

#12



cLogP: 4.28
TPSA: 41.57
Highest similarity: 0.71
H-bond acceptors: 2

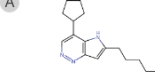
Task

Priority

Chemist

Status

#20



cLogP: 4.28
TPSA: 41.57
Highest similarity: 0.72
H-bond acceptors: 2

Task

Priority

Chemist

Status

ADD PROPERTY

Calculated Properties

- Mass
- cLogP

3.6 - 4.3

TPSA

- pKa (str. acidic)
- FSP3
- Solubility
- H-bond acceptors
- H-bond donors
- pKa (str. basic)

SureChEMBL

- Highest similarity
- ID

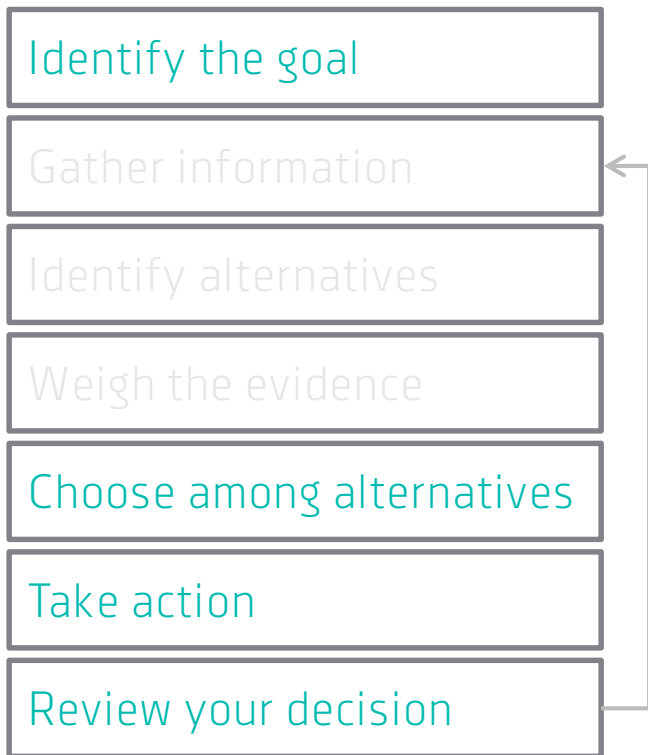
Molport

- Compound IDs

Snapshot details

- ID
- Molecule
- Author
- Create date
- Task
- Priority
- Chemist
- Status

Design Hub: Marvin Live Roadmap





THANK YOU