

# AI-assisted lead optimization with SynSpace

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Pharma R&D Informatics & AI Congress

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# ChemPass

- Founded 01/2016
- Location: Budapest, Hungary



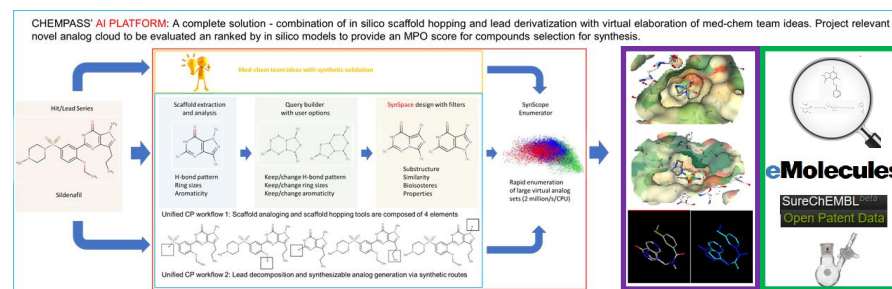
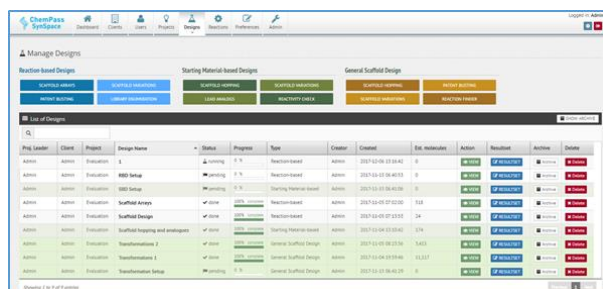
- Creating a **synthesis-based design concept** and software for medicinal chemists and AI-powered drug discovery
- Built an **AI-powered lead discovery platform**
- SynSpace availability



- Aims: reduce cycle time, optimization time, expand idea and IP space

# Key technologies

- ChemPass has both AI-based software for medicinal or computational chemists AND a complete AI-assisted lead discovery platform

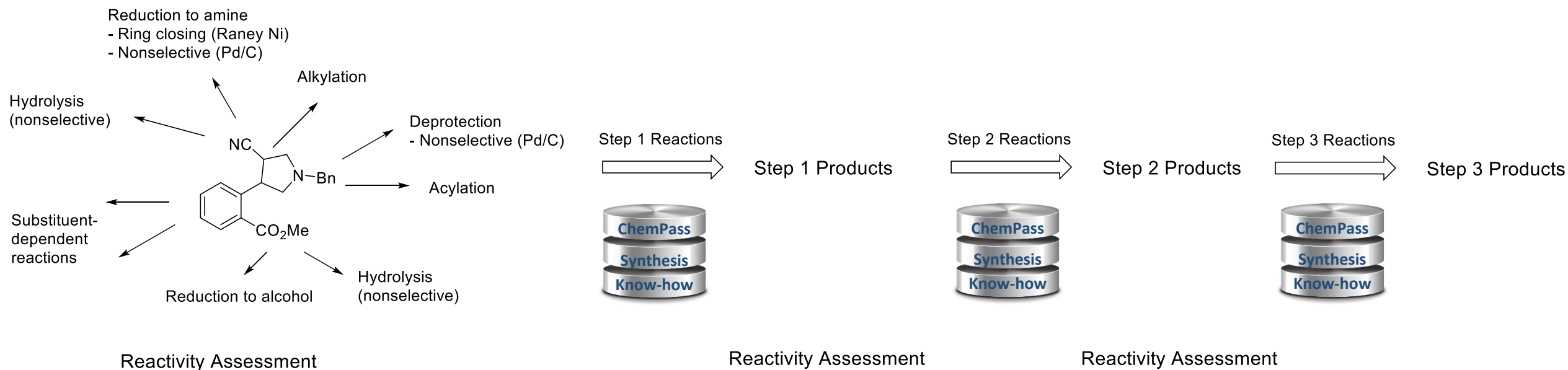


- ChemPass has AI-based technologies and software for both design of novel leads or lead analogs AND retrosynthesis



# ChemPass design concept

- ChemPass Design Technology: What can be synthesized from starting materials, intermediates or lead structures?



- **Unique proprietary technologies**

- Rule-based AI for forward in silico synthesis
- Molecule design based on multistep in silico synthesis
- Control of combinatorial explosion

# Comparison to a popular DL design method

Feature	Generative deep learning*	ChemPass SynSpace
Can design focused but diverse novel structures for lead analog design	Yes	Yes
Fully controllable scaffold design	No	Yes
Fully controllable side-chain design	No	Yes
Design can be limited to structural areas	No	Yes
Required prior art	Significant	Little (1-)
Synthetic feasibility considered	No	Yes
Bottleneck – expert synthesis evaluation	Yes	No

Why use methods that incorporate no synthesis information?

ChemPass has the technology to generate lead analog space with synthetic chemistry incorporated!

\*Ref: 1. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology. Vol 1038,37,1038–1040, 2019.  
 2. Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks. ACS Cent. Sci. 4, 120–131, 2018.  
 3. Generative Recurrent Networks for De Novo Drug Design. Mol. Inf. 2018, 37, 1700111.

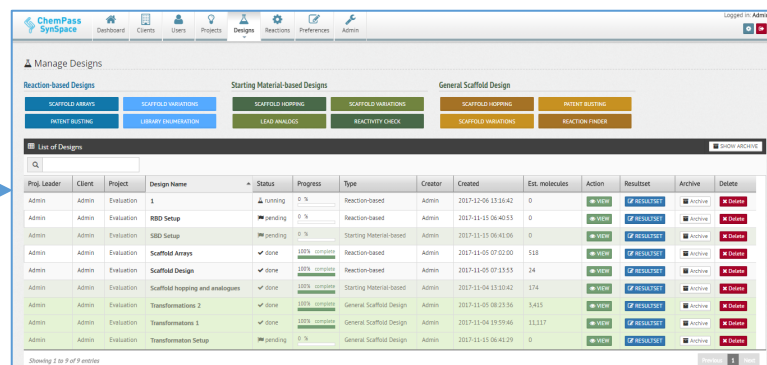
# Products/services

- Software license:
  - SynSpace for medicinal chemists and computational chemists
  - SynSpace API for computational chemists
  - SynSpace modules
    - Library design (e.g. DEL)
    - Side-chain design
    - Scaffold and lead analog design modules (new fully automated AI modules)
    - Retrosynthesis module (new)



- Services:
  - Design and problem-solving medicinal chemistry support
  - AI-driven lead optimization platform for lead generation and lead optimization

# SynSpace software availability and uses

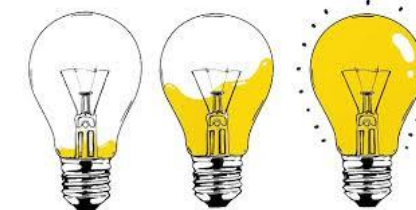


Lead discovery project support

**SYNSPACE Software**  
Scaffold, scaffold analog, lead analog design by chemists and cheminformaticians

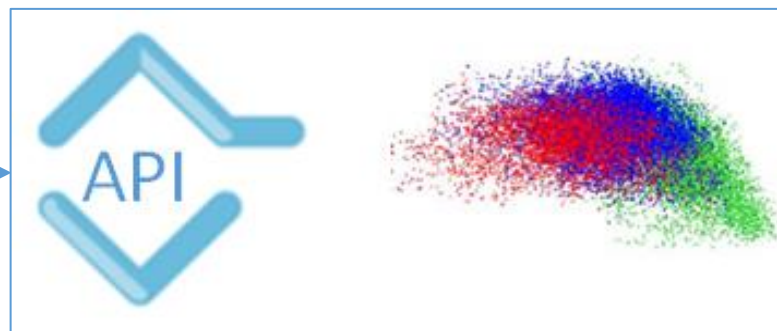


Reduce cycle time



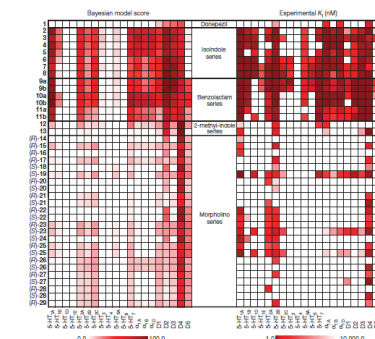
Expand idea space

**ChemPass Designer Technology**



Machine learning project support

**SYNSPACE API**  
Synthetically enabled scaffold and vast virtual library design from available reagents



Deep learning, AI-powered drug discovery

## Lead optimization support: 36 projects in 2018-2019

- Scaffold hopping for many different scaffold types
- Side-chain design for specific scaffolds
- Side-chain design in combination with scaffold hopping
- Hit expansion
- Probe molecule to lead
- Patent to new lead (busting)
- ADMET liability removal in late stage lead optimization
- Monocycle to bicycle lead transformation
- Create freedom of operation in crowded IP space against a target
- Create follow-on secondary series from primary series after candidate designation

Partners:

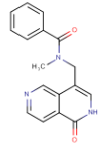

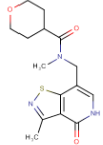
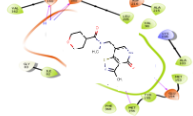
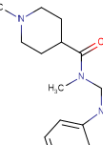
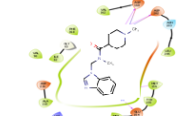
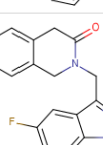
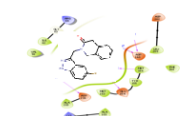
- Big Pharma
- Big Biotech
- Small biotech



# Example collaboration report for lead optimization

## Key information for rapid decision making:

- Structure
- ID
- Docking pose
- Docking interactions
- Docking scores
- Selectivity assessment
- Synthesis score
- Reagent availability score
- Synthesis scheme
- Lead likeness
- Selected properties (not shown)
- Flags
- Novelty assessment
- Commercial availability assessment

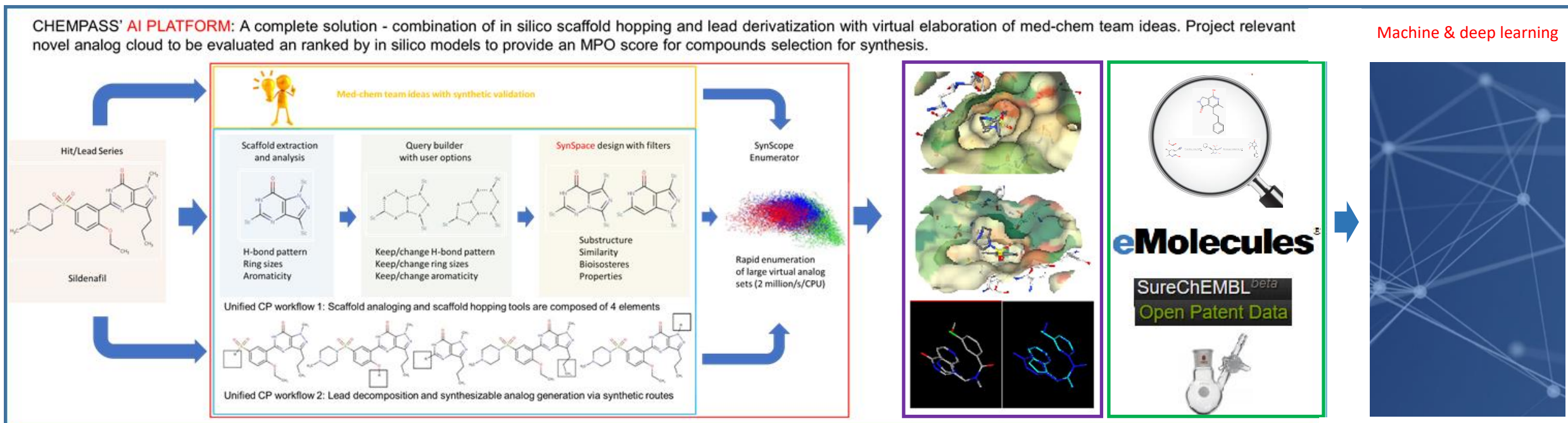
Molecule	Compound_id	Target_docking_pose_interactions	Target_docking_score	Off_target_docking_score	Docking_selectivity	Synthesis_score_(1-5)	BB_avail_score_(1-5)	Synthesis_route	Lead-likeness	Structural_Flag	Novelty_in_patent	Novelty_in_eMolecules
	"[[X14+#4-C62]-S9]"		-10.05	-7.78	2.27	2	2	Aryl_ketone_synthesis_Rxn62(62), Catalytic_reduction_50oC/30bar_Rxn9(9)	true	1	N	N
	"[#6+X4-C64]"		-10.01	-7.74	2.27	2	2	Ullmann_reaction_Rxn64(64)	true	0	N	N
	"[[#3+X55-C64]-S8]"		-9.98	-6.46	3.52	2	2	Ullmann_reaction_Rxn64(64), Catalytic_reduction_rt/1bar_Rxn8(8)	true	0	N	N
	"[[X14+#4-C62]-S9]"		-9.85	-8.96	0.89	2	2	Aryl_ketone_synthesis_Rxn62(62), Catalytic_reduction_50oC/30bar_Rxn9(9)	true	1	N	N

Extracted from real report with altered structures

Report format and data types are fully customizable

A detailed table is also available with synthesis scheme, reagent structures, ids, cost etc., hundreds of customizable properties

# Complete AI-driven lead optimization platform

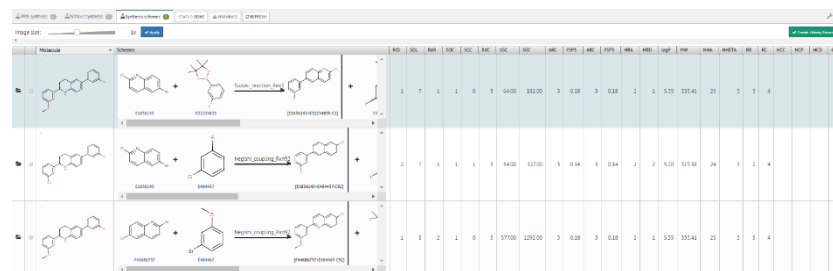


AI-powered ideation: scaffold hopping, substituent designs  
 Property predictions  
 Potency, selectivity predictions: semi-automated protein or ligand-based methods

Full synthesis and reagent availability assessment  
 Novelty assessment  
 Synthesis outsourcing

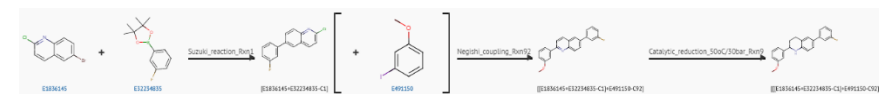
MPO scores  
 Ranking  
 Selection

# Med-chem team ideas

Reaction	Rank	Score	Yield	Time	Cost	...
<chem>CC1=CC=C(C=C1)C2=CC=CC=C2</chem> + <chem>CC(C)C</chem> → <chem>CC(C)C1=CC=C(C=C1)C2=CC=CC=C2</chem>	1	0.95	90%	1h	\$10	...
<chem>CC1=CC=C(C=C1)C2=CC=CC=C2</chem> + <chem>CC(C)C</chem> → <chem>CC(C)C1=CC=C(C=C1)C2=CC=CC=C2</chem>	2	0.85	80%	1h	\$10	...
<chem>CC1=CC=C(C=C1)C2=CC=CC=C2</chem> + <chem>CC(C)C</chem> → <chem>CC(C)C1=CC=C(C=C1)C2=CC=CC=C2</chem>	3	0.75	70%	1h	\$10	...

SynSpace retrosynthesis module



- Synthetic schemes, rankings
- Reagent structures, IDs

- Retrosynthesis enables human ideas to enter the design workflow

# Retrosynthesis example 1

## Retrosynthesis Planner (improved speed): done!

[Click here to be redirected to the old depth-first search planner](#)

Target compound:

Parsed structure:

Quick settings:

- 
- 
- 
- 

Expansion settings:

- Max. depth (1-9):
- Min. retro template count:
- Num. templates:
- Max cum. prob:
- Max. branching factor:
- Expansion time (s):

Stop criteria:

- Maximum chemical price (\$/g):
- Chemical property logic:
- Chemical popularity logic:

Evaluation settings:

- Min. plausibility:
- Manual forward prediction:

Controls:

- 
- Return as soon as any pathway found

After expanding (with 0 banned reactions, 0 banned chemicals), 744 total chemicals and 3565 total reactions

No trees resulting in buyable chemicals found! If the program is having trouble with your target, you may want to explore the One-Step Retrosynthesis options and help guide the search.

Alternatively, please use the "Chemical popularity logic" setting above to give a more generous termination criterion to the search. Our buyables database is very sparse, so many pathways

https://rxn.res.ibm.com/rxn/projects/5db6a652bc67d20001772d74/Retro- 80%

Retro-1 < Retrosynthesis outcome

Confidence: 0.641 Optimization score: 0.821 Medium confidence

Predictions: B 2/F 27 Optimisation time: 37 s  Molecule commercially available on eMolecules.com  Not able to find a synthetic path

Sequences Generated

- Sequence 0

Parameters

MSSR	15
MRP	50
FAP	0.65
SbP	3

Help us improve! Send us your feedback.  
What do you think about this sequence?

© IBM RXN

# Retrosynthesis example 1

ChemPass SynSpace Dashboard | Projects | Designs | Reactions | Preferences

RESULTLIST - RETRO-1

With synthesis | Without synthesis | Synthesis schemes | STATUS: DONE | WARNINGS | REFRESH

Image size: 1x

Molecule	Schemes	RID	SOL	RAR	SOC	SCC	RXC	IGC	SGC	ARC	FSP3	ARC
	 Negishi_coupling_RxnQ2 Catalytic	1	11	1	1	0	5	396.00	1345.00	3	0.24	3
	 Sonogashira_reaction_Rxn35	1	11	1	1	0	5	417.00	1394.00	3	0.24	3
	 Suzuki_reaction_Rxn1 Catalytic_re	1	10	2	1	0	4	640.00	2316.00	3	0.24	3
	 Negishi_coupling_RxnQ2	1	11	1	1	0	5	434.00	1418.00	3	0.24	3
	 Negishi_coupling_RxnQ2	1	11	1	1	0	5	434.00	1418.00	3	0.24	3

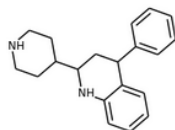
# Retrosynthesis example 2

Retrosynthesis Planner (improved speed): done!

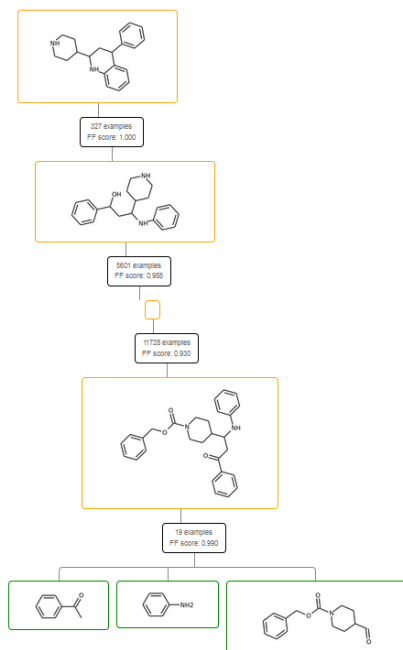
[Click here to be redirected to the old depth-first search planner](#)

Target compound:  [Draw](#)

Parsed structure:



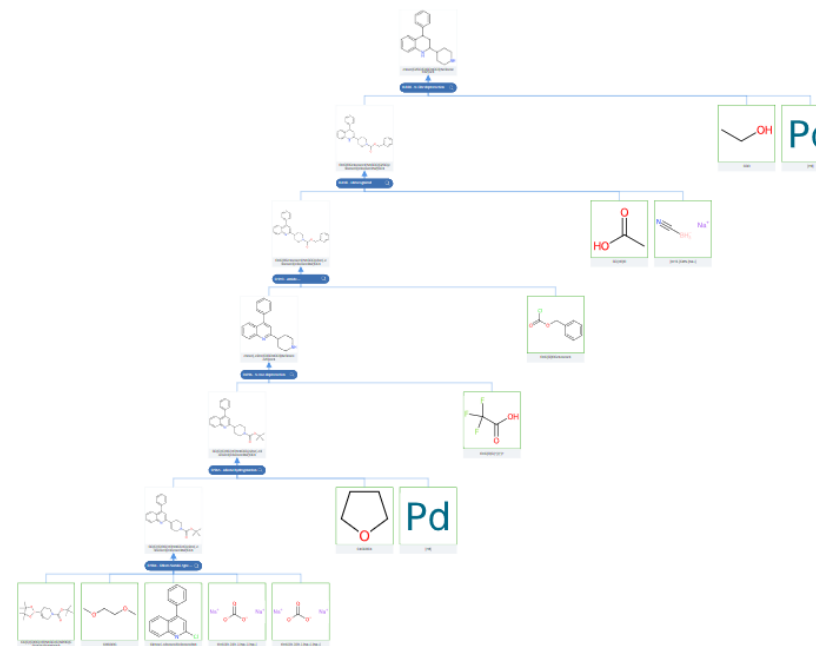
Option 1 [hide](#)



IBM RXN Projects < Retro-2 < Retrosynthesis outcome

Retro-2 Sequence 1 Confidence: 0.457 Optimization score: 0.345 Medium confidence

Predictions: B 81/F 244 Optimisation time: 630 s ■ Molecule commercially available on eMolecules.com



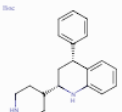
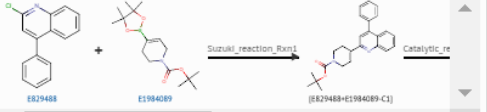
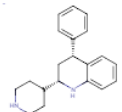

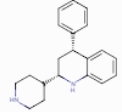

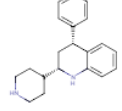
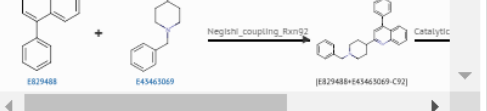
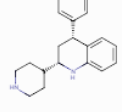
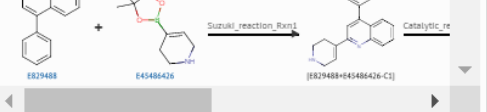
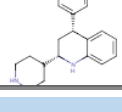
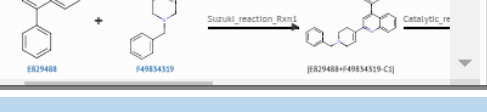
# Retrosynthesis example 2

ChemPass SynSpace Dashboard Projects Designs Reactions Preferences

RESULTLIST-RETRO-2

With synthesis Without synthesis Synthesis schemes STATUS: DONE WARNINGS REFRESH

Image size: 1x Apply

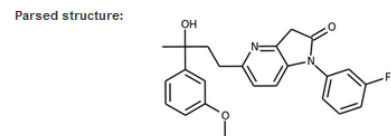
Molecule	Schemes	RID	SOL	RAR	SOC	SCC	RXC	SGC	SGC	ARC	FSP3	ARC	FSP3	HBA
		1	7	1	1	0	3	336.00	1297.00	2	0.40	2	0.40	2
		1	8	2	1	0	3	436.00	1596.00	2	0.40	2	0.40	2
		1	3	1	1	0	2	387.00	1455.00	2	0.40	2	0.40	2
		1	3	1	1	0	2	673.00	2838.00	2	0.40	2	0.40	2
		1	7	1	1	0	3	436.00	1596.00	2	0.40	2	0.40	2
		1	8	2	1	0	3	423.00	1660.00	2	0.40	2	0.40	2

# Retrosynthesis example 3

## Retrosynthesis Planner (improved speed): done!

[Click here to be redirected to the old depth-first search planner](#)

Target compound:



**Quick settings:**

- 
- 
- 
- 

**Expansion settings:**

- Max. depth (1-9):  Max. branching factor:
- Min. retro template count:  Expansion time (s):
- Num. templates:
- Max cum. prob:

**Stop criteria:**

- Maximum chemical price (\$/g):
- Chemical property logic:
- Chemical popularity logic:

**Evaluation settings:**

- Min. plausibility:
- Manual forward prediction:

**Controls:**   Return as soon as any pathway found

After expanding (with 0 banned reactions, 0 banned chemicals), 537 total chemicals and 3914 total reactions

No trees resulting in buyable chemicals found! If the program is having trouble with your target, you may want to explore the One-Step Retrosynthesis options and help guide the search.

Alternatively, please use the "Chemical popularity logic" setting above to give a more generous termination criterion to the search. Our buyables database is very sparse, so many pathways n

https://rxn.res.ibm.com/rxn/projects/5dc13664bc67d2000177dd34/Retrosynthesis/retrosynthesis/5dc13c2ebc67d2000177e250

XN Projects < Retrosynthesis < Retrosynthesis outcome

Retrosynthesis Sequence 0.928 Confidence: 0.449 Optimization score: 0.928 High confidence

Molecule commercially available on eMolecules.com  Not able to find

HH Pd



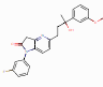
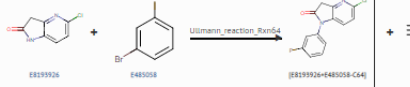
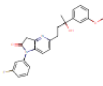
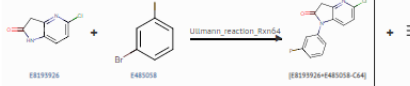
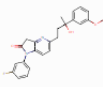
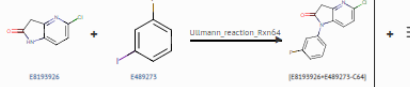
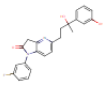
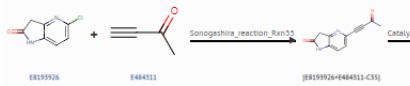
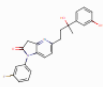
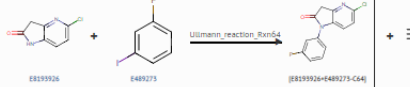
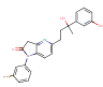
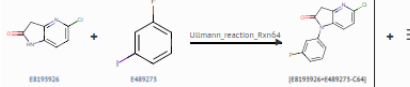
# Retrosynthesis example 3

ChemPass SynSpace Dashboard Clients Users Projects Design Reactors Preferences Admin

RESULTLIST-1

With synthesis Without synthesis Synthesis schemes STATUS: DONE WARNINGS REFRESH

Image size: 1x Apply

Molecule	Schemes	RID	SOL	RAR	SOC	SCC	RKC	SCC	SGC	ARC	PSP3	ARC	PSP3	HBA	HBD	logP	MW	NNA	NHETA	RB	RC	HCC	NCP	HCD
	 E819926 + E485058 → Ullmann_reaction_Bun54 → [E819926+4485058-C64]	1	9	1	1	0	4	538.00	1831.00	3	0.25	3	0.25	4	1	3.65	406.46	30	6	6	4			
	 E819926 + E485058 → Ullmann_reaction_Bun54 → [E819926+4485058-C64]	1	9	1	1	0	4	538.00	1827.00	3	0.25	3	0.25	4	1	3.65	406.46	30	6	6	4			
	 E819926 + E489273 → Ullmann_reaction_Bun54 → [E819926+4489273-C64]	1	9	1	1	0	4	538.00	1827.00	3	0.23	3	0.23	4	1	3.65	406.46	30	6	6	4			
	 E819926 + E484911 → Sonogashira_reaction_Bun72 → [E819926+4484911-C35]	2	9	1	1	1	4	553.00	1905.00	3	0.22	3	0.22	4	2	3.51	392.43	29	6	5	4			
	 E819926 + E489273 → Ullmann_reaction_Bun54 → [E819926+4489273-C64]	2	9	1	1	1	4	553.00	1905.00	3	0.22	3	0.22	4	2	3.51	392.43	29	6	5	4			
	 E819926 + E489273 → Ullmann_reaction_Bun54 → [E819926+4489273-C64]	2	9	1	1	1	4	538.00	1827.00	3	0.22	3	0.22	4	2	3.51	392.43	29	6	5	4			

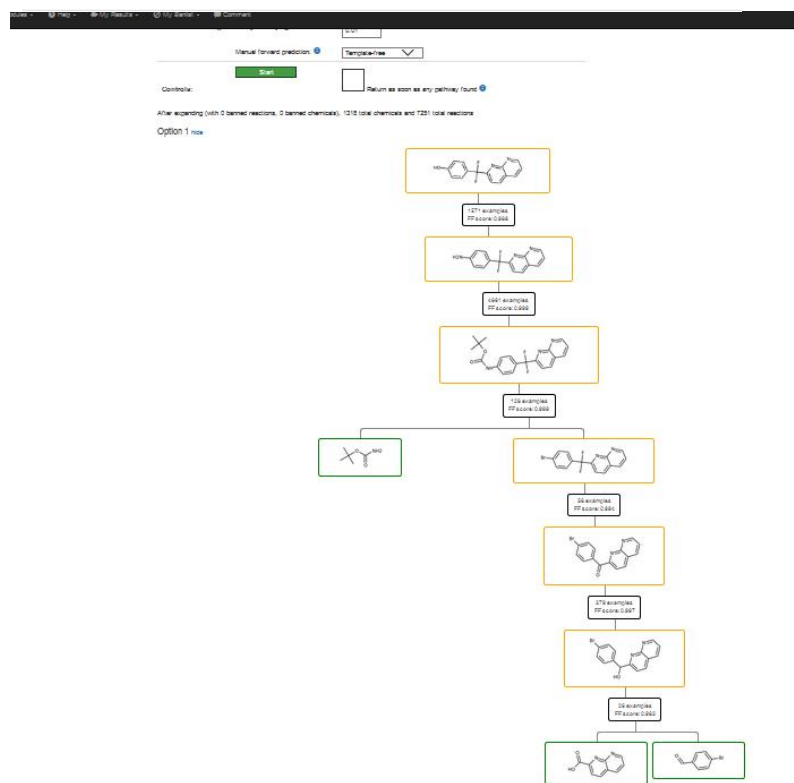
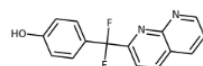
# Retrosynthesis example 4

Retrosynthesis Planner (improved speed): done!

[Click here to be redirected to the old depth-first search planner](#)

Target compound:

Parsed structure:



https://rxn.res.ibm.com/rxn/projects/5db6a652bc67d20001772d74/Retrosynthesis outcome

80%

Retrosynthesis outcome

Confidence: 0.916 Optimization score: 1.13 High confidence

Predictions: B 37/F 121 Optimisation time: 282 s  Molecule commercially available on eMolecules.com  Not able to find a synthetic path

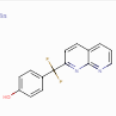
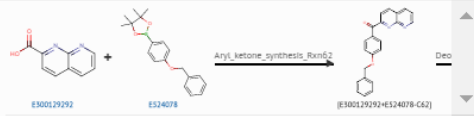
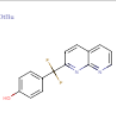
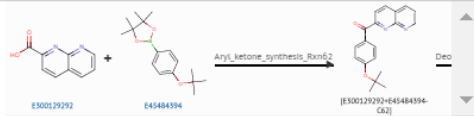
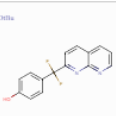

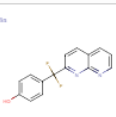

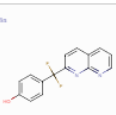

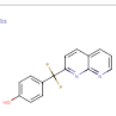

# Retrosynthesis example 4

ChemPass SynSpace Dashboard Projects Designs Reactors Preferences

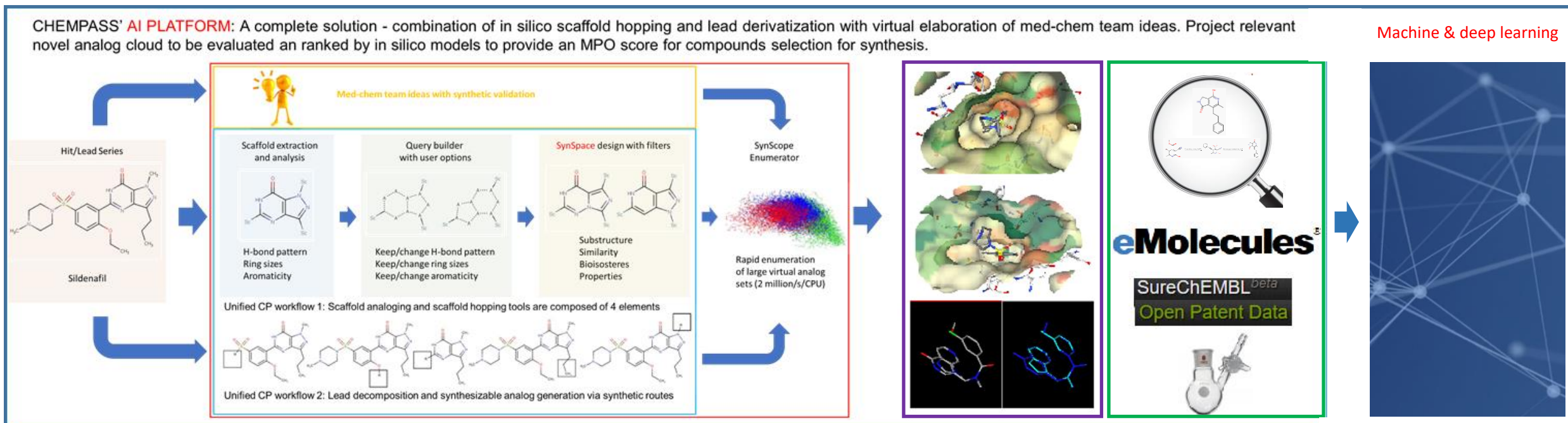
RESULTLIST-RETRO-4

With synthesis Without synthesis Synthesis schemes STATUS DONE WARNINGS REFRESH

Image size: 1x Apply

Molecule	Schemes	RID	SOL	RAR	SOC	SCC	RXC	IGC	SGC	ARC	FSP3	ARC	FSP3	HBA
	 Aryl ketone synthesis_Rxn62 E300129292 E524078 (E300129292-E524078-C62)	1	3	1	1	0	2	182.00	540.00	3	0.07	3	0.07	3
	 Aryl ketone synthesis_Rxn62 E300129292 E45484394 (E300129292-E45484394-C62)	1	3	1	1	0	2	268.00	767.00	3	0.07	3	0.07	3
	 Aryl ketone synthesis_Rxn62 E300129292 E45478359 (E300129292-E45478359-C62)	1	3	1	1	0	2	308.00	900.00	3	0.07	3	0.07	3
	 Negishi_coupling_Rxn62 E55453801 F887731 (E55453801-F887731-C92)	1	6	2	1	0	2	649.00	3096.00	3	0.07	3	0.07	3
	 Aryl ketone synthesis_Rxn62 E300129292 E717325 (E300129292-E717325-C62)	1	3	1	1	0	2	175.00	490.00	3	0.07	3	0.07	3
	 Negishi_coupling_Rxn62 F35510392 F887731 (F35510392-F887731-C92)	1	8	4	1	0	2	648.00	1902.00	3	0.07	3	0.07	3

# Complete AI-driven lead optimization platform



AI-powered ideation: scaffold hopping, substituent designs  
 Property predictions  
 Potency, selectivity predictions: semi-automated protein or ligand-based methods

Full synthesis and reagent availability assessment  
 Novelty assessment  
 Synthesis outsourcing

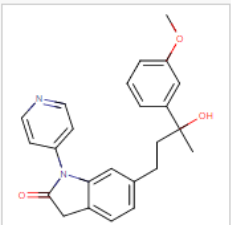
MPO scores  
 Ranking  
 Selection

# Scaffold analog design/hit generation with SynSpace

**Target molecule**

+ INSERT
Upload

all items: 1
<< < > >>
current page:



✖ delete
☐
↻ update

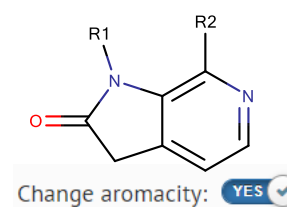
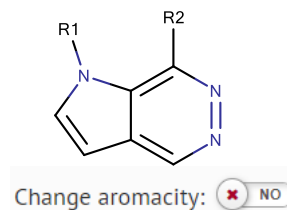
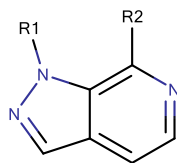
- A very simple solution for
  - scaffold hopping
  - ring exploration
  - novel hit generation from known hits

Change aromaticity:  YES
Enforce keeping H-bond sites:  All  No  Selected atoms
Change ring sizes:  NO
Close rings:  YES
Stringency:  HIGH
Show protected:  NO

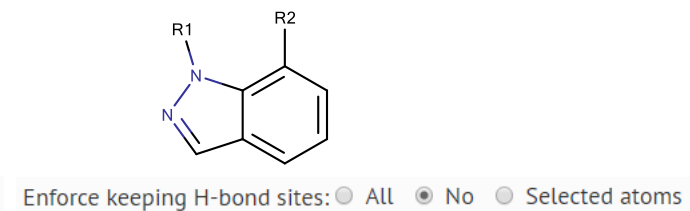
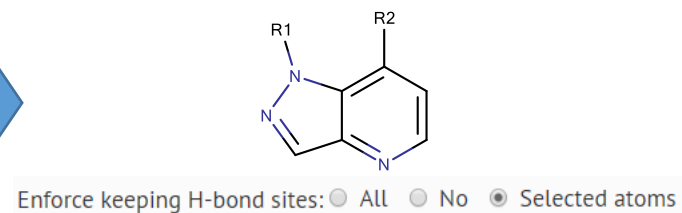
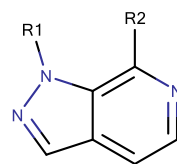
- Fully automated design of scaffold analogs containing the desired side-chains
- Intelligent ring closing mechanisms included
- Intelligent explorations of alternative ring sizes with same side-chain vectors

# Automated scaffold design options

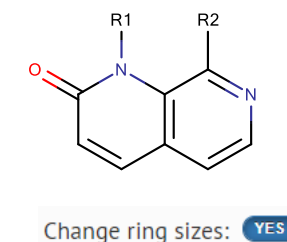
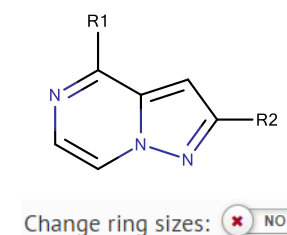
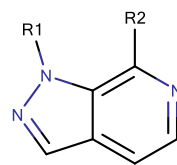
- Scaffold aromaticity:



- Scaffold H-bonding:

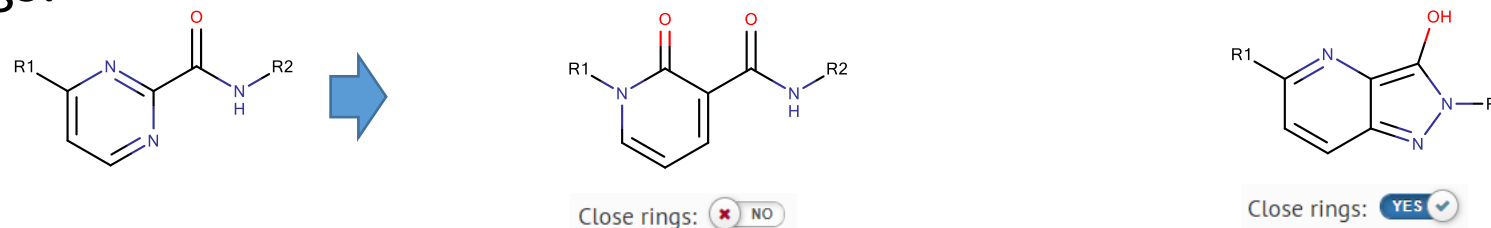


- Scaffold ring size:

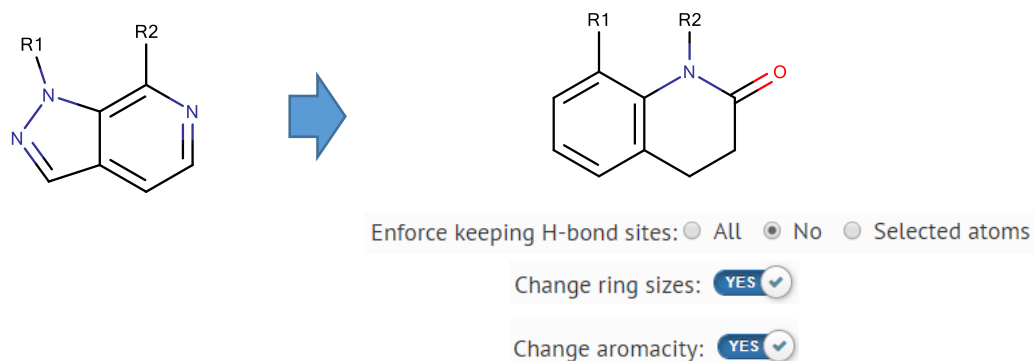


# Automated scaffold design options

- Close new rings:

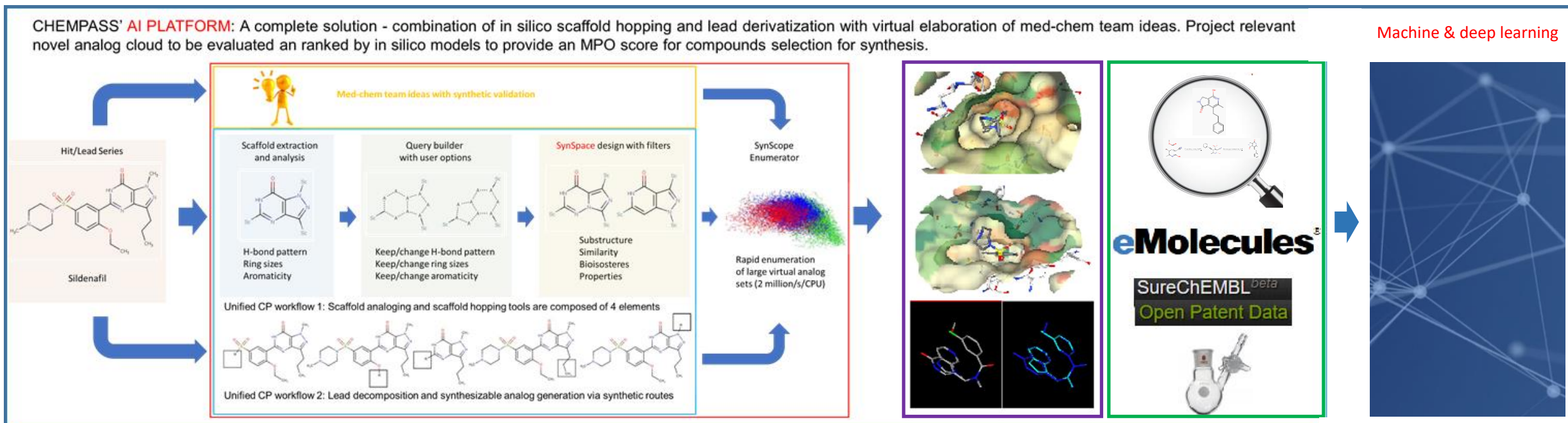


- Major change example: Side-chains and their vector remain similar



Lost both ring H-bond acceptors  
Modified ring size  
Modified aromaticity

# Complete AI-driven lead optimization platform



AI-powered ideation: scaffold hopping, substituent designs  
 Property predictions  
 Potency, selectivity predictions: semi-automated protein or ligand-based methods

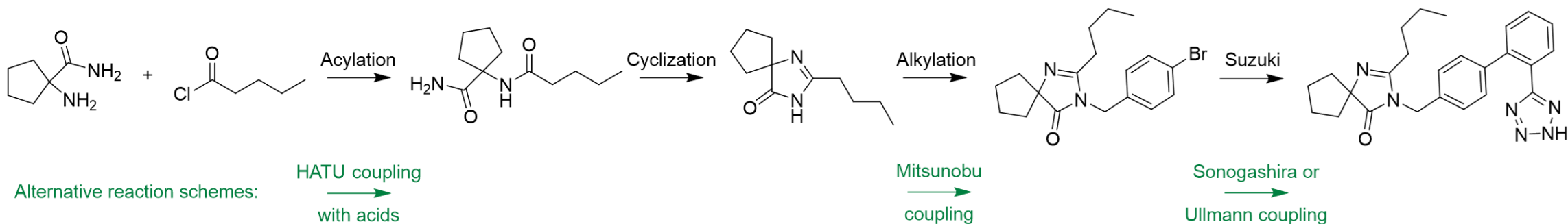
Full synthesis and reagent availability assessment  
 Novelty assessment  
 Synthesis outsourcing

MPO scores  
 Ranking  
 Selection



# Derivatization design: side-chain, connectivity and scaffold design with SynSpace API

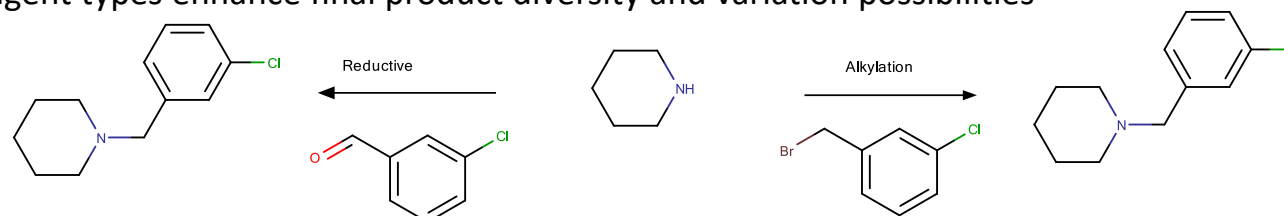
- User settings needed:
  - How many total variations per compound
  - How many total compounds
  - Minimum similarity
- Derivatization of side-chains via synthetic routes: Irbesartan analog design via a 4-step synthetic sequence



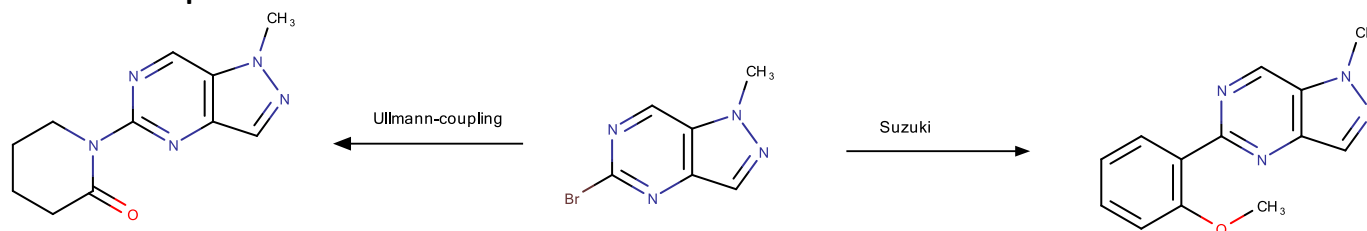
- Analog selection by multiple similarity methods, bioisosteres and substructures:
  - >90K analogs generated before property filtration

# Countless variation possibilities: related reactions

- Each synthetic step has 2 types of „related reactions”
  - Different reaction(s) that can lead to the same product type using different reagent classes (i.e. alkylation with halides or reductive amination)
    - Different reagent types enhance final product diversity and variation possibilities

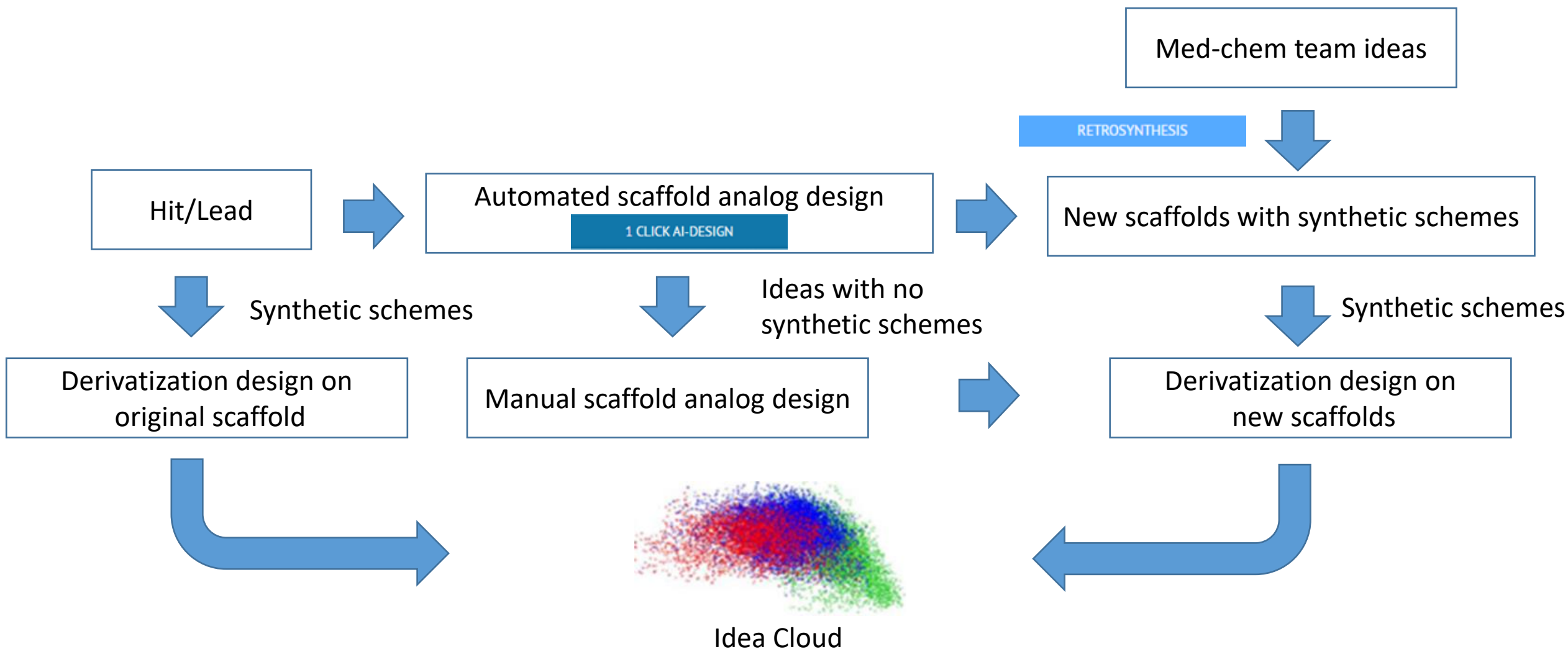


- Different reaction(s) that use functional groups found at least in one of the reagents and can produce a similar product motif

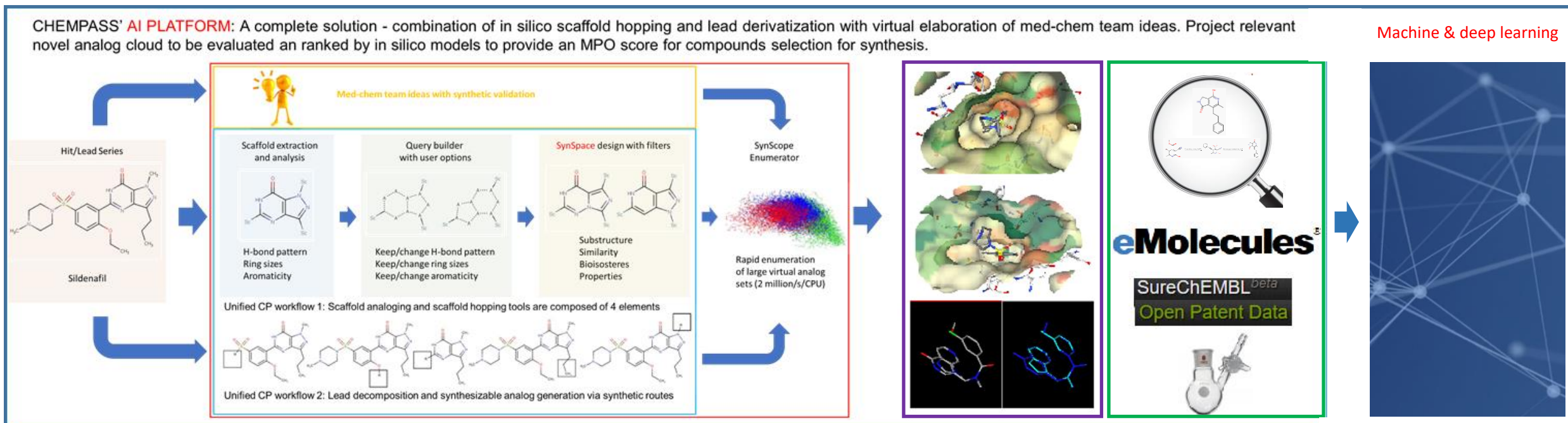


- The above synthetic knowledge is naturally encoded in our synthetic know-how

# Complete design cycle



# Complete AI-driven lead optimization platform

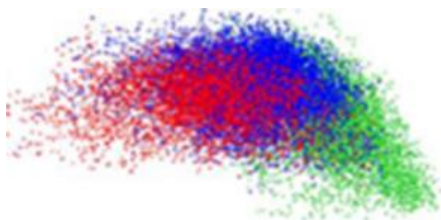


AI-powered ideation: scaffold hopping, substituent designs  
 Property predictions  
 Potency, selectivity predictions: semi-automated protein or ligand-based methods

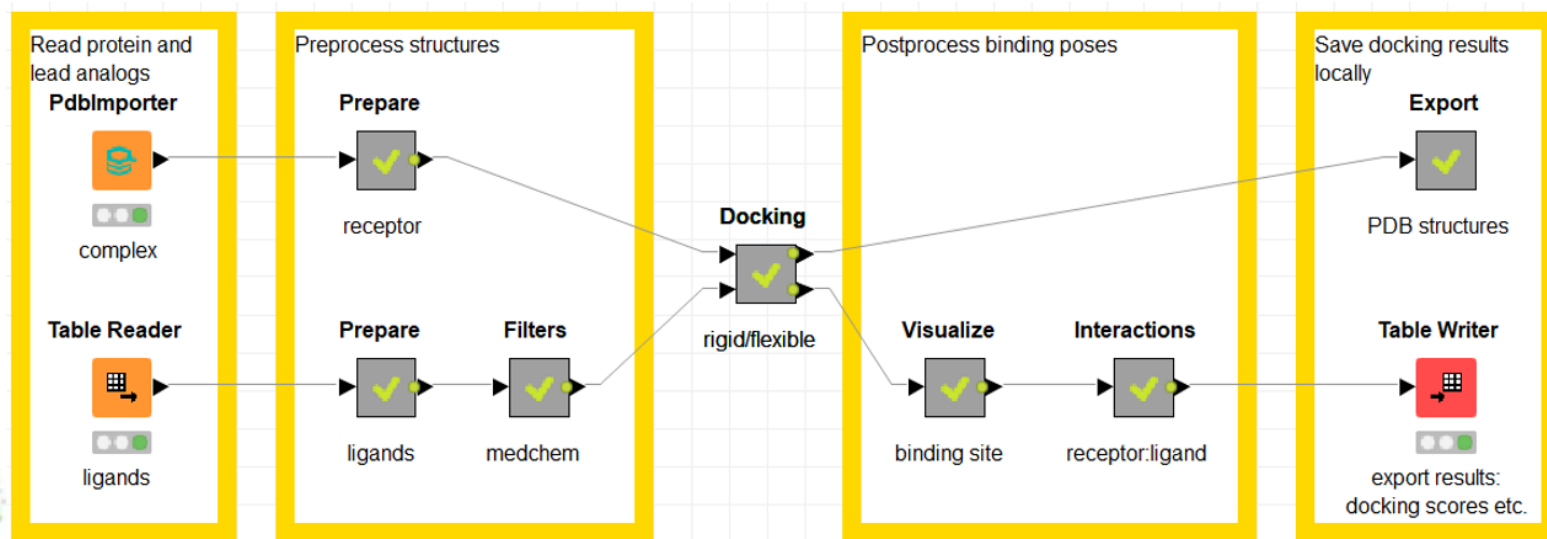
Full synthesis and reagent availability assessment  
 Novelty assessment  
 Synthesis outsourcing

MPO scores  
 Ranking  
 Selection

# Binding predictions



Idea Cloud



Output:

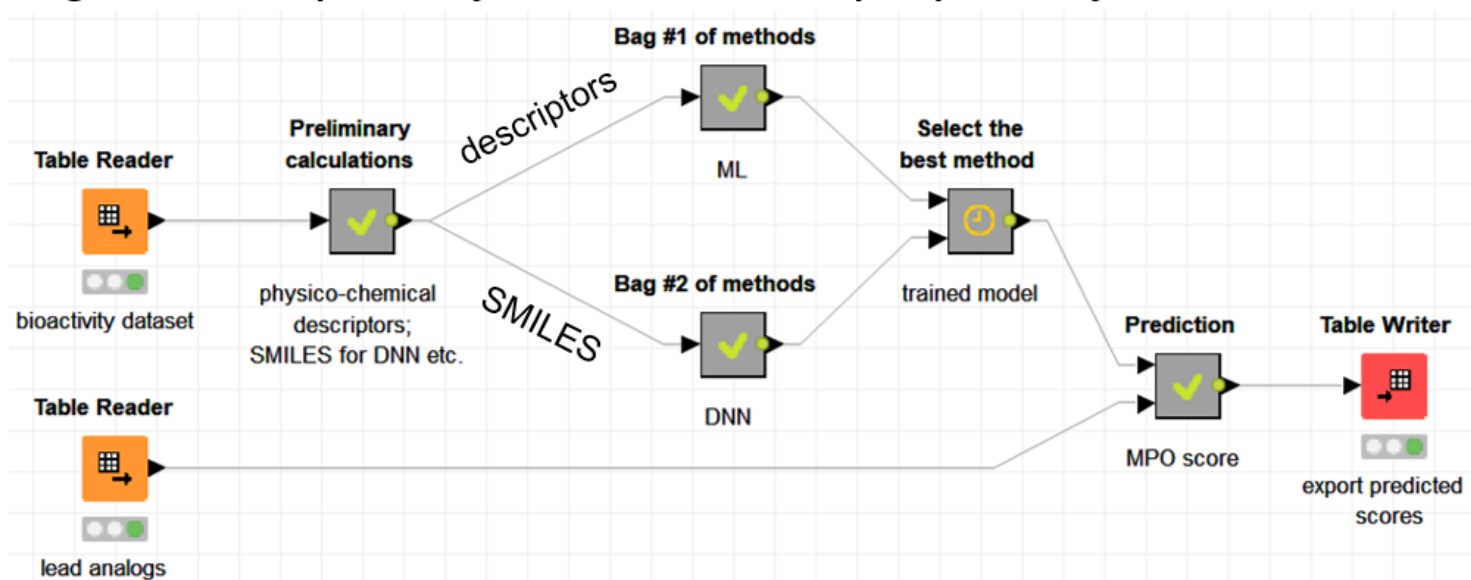
- Docking pose
- Docking interactions
- Docking scores
- Selectivity assessment

Built-in

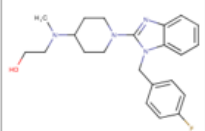
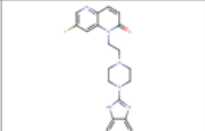
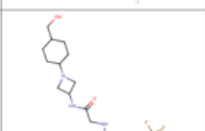
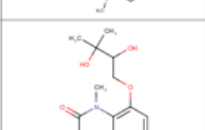
- SuCOS for pose analysis
- Clash analysis
- Interaction analysis

# ML and deep learning models for an MPO score

Predictive models trained with various ML and DNN methods using a mix of publicly available and proprietary datasets.



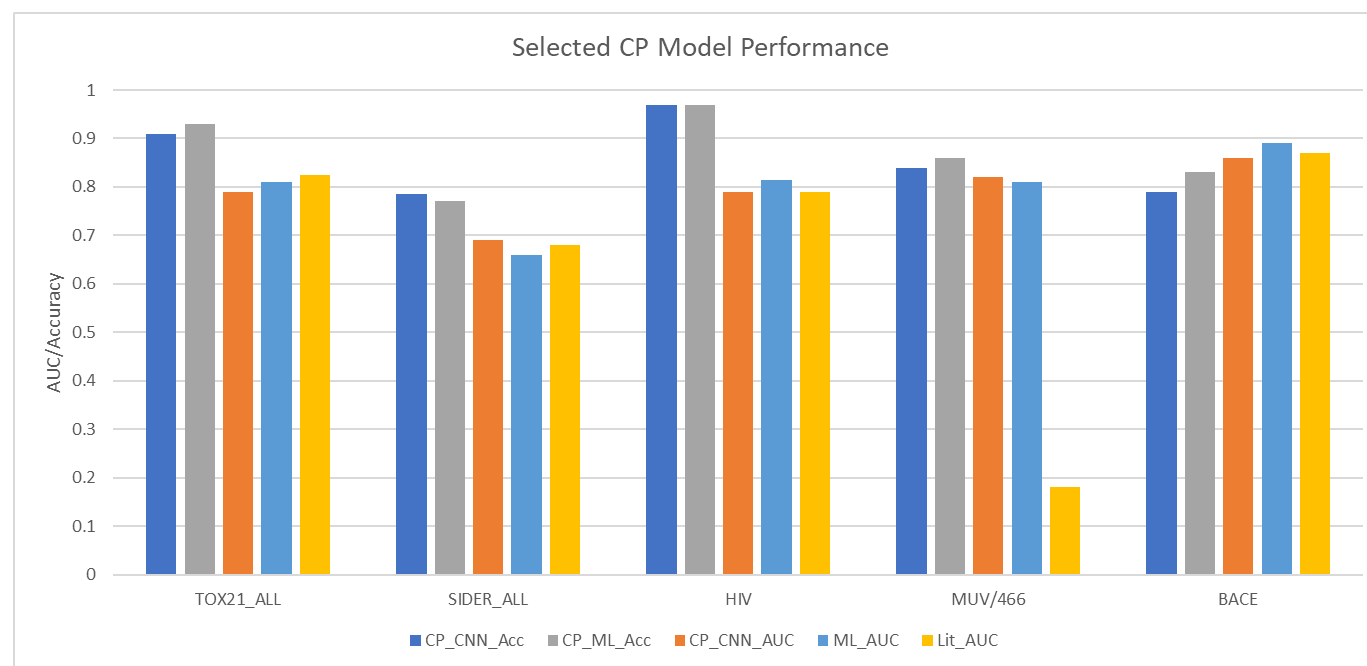
Models are automatically re-trained in each design cycle

Row ID	SMILES	S Activity	S Prediction	D Confidence
Row0		Active	Active	0.975
Row1		Active	Active	0.97
Row2		Inactive	Active	0.515
Row3		Inactive	Inactive	0.835

Training set data

# ChemPass predictive AI and ML models

- Several deep learning and machine learning (ML) methods automatically refined in each optimization cycle
- Deep learning methods with smiles or property inputs
  - ChemPass' smiles-based CNN appears to be string-independent
- Comparison to literature models
  - M. Hirohara et al. BMC Bioinform. 19, 526 (2018)
  - Z. Wu, et al. Chem. Sci. 9, 513 (2018)
  - **CP models perform well**



ML methods tested: Tree Ensemble, Random Forest

ML\_acc: obtained in a 5-fold validation with optimal hyperparameters (number of models, maximum number of levels) to maximize the accuracy

Tox21: average of 12 sub-datasets

SIDER: average of 27 sub-datasets

# A typical use of the AI-driven lead optimization platform

- ChemPass
  - design, in silico profiling (traditional and ML methods)
  - ranking of newly designed analogs
  - management of chemistry and biology CROs (if requested)
- Joint selection with project owner partner of compounds for synthesis
- Objectives:
  - H2L in 6 months or
  - Hit generation and H2L in 8 months
  - Lead to advanced lead in 8-12 months



# Current lead optimization tasks in the design-make process

Ideation



Literature check for prior art



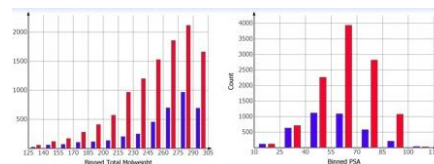
Idea sharing



Focused library enumeration



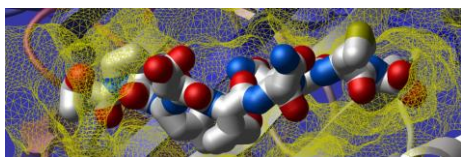
Property calculations



Predictions



Modelling, comp-chem



Selection



Synthesis planning



Reagent search

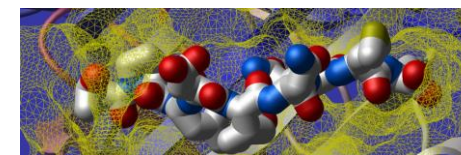


# Lead optimization with SynSpace AI-assisted platform


**ChemPass** Ideation Literature check for prior art  
**SynSpace** Idea sharing Focused library enumeration  
 Property calculations Synthesis planning Reagent search


**ChemPass**  
**AI Platform**

Modelling, comp-chem



Predictions



Selection



ChemPass SynSpace Dashboard Clients Users Projects Designs Reactions Preferences Admin Logged in: Admin

Manage Designs

Reaction-based Designs: SCAFFOLD ARRAYS, SCAFFOLD VARIATIONS, PATENT BUSTING, LIBRARY ENUMERATION

Starting Material-based Designs: SCAFFOLD HOPPING, SCAFFOLD VARIATIONS, LEAD ANALOGS, REACTIVITY CHECK

General Scaffold Design: SCAFFOLD HOPPING, PATENT BUSTING, SCAFFOLD VARIATIONS, REACTION FINDER

List of Designs

Proj. Leader	Client	Project	Design Name	Status	Progress	Type	Creator	Created	Est. molecules	Action	Resultset	Archive	Delete
Admin	Admin	Evaluation	1	running	0 %	Reaction-based	Admin	2017-12-06 13:16:42	0	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	RBD Setup	pending	0 %	Reaction-based	Admin	2017-11-15 06:40:53	0	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	SBD Setup	pending	0 %	Starting Material-based	Admin	2017-11-15 06:41:06	0	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	Scaffold Arrays	done	100% complete	Reaction-based	Admin	2017-11-05 07:02:00	518	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	Scaffold Design	done	100% complete	Reaction-based	Admin	2017-11-05 07:13:53	24	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	Scaffold hopping and analogues	done	100% complete	Starting Material-based	Admin	2017-11-04 13:10:42	174	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	Transformations 2	done	100% complete	General Scaffold Design	Admin	2017-11-05 08:23:36	3,415	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	Transformations 1	done	100% complete	General Scaffold Design	Admin	2017-11-04 19:59:46	11,117	VIEW	RESULTSET	Archive	Delete
Admin	Admin	Evaluation	Transformaton Setup	pending	0 %	General Scaffold Design	Admin	2017-11-15 06:41:29	0	VIEW	RESULTSET	Archive	Delete

Showing 1 to 9 of 9 entries

Thank you for your attention!