


Reaxys Training for New Users

Demonstration & Workshop

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Search substances, reactions, documents and bioactivity data

In Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork, SigmaAldrich and Commercial Substances

Import

Search Reaxys

Find >

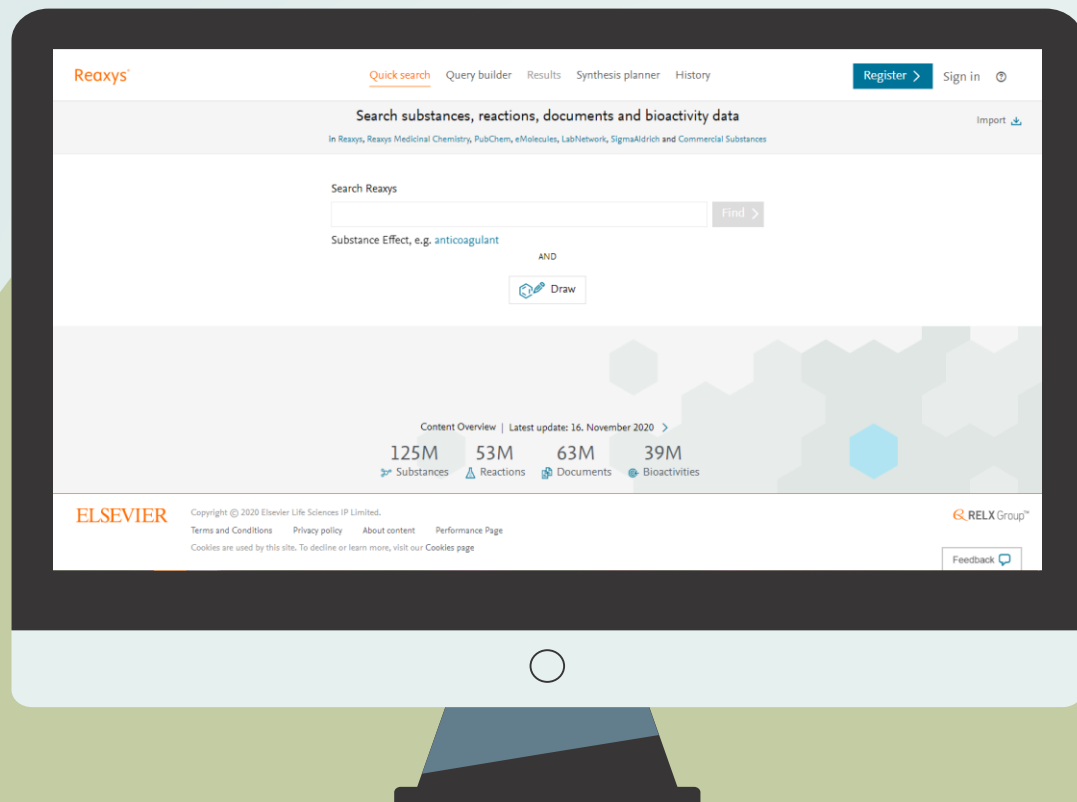
Substance Names, e.g. [Atenolol](#)

AND



Draw

What is Reaxys?



Reaxys supports:

- **Substances**
(including physical and spectral data)
- **Reactions**
- **Documents**
- **Bioactivity data**
(Available in Reaxys Medicinal Chemistry)

Database Overview

Reaxys Content

Reactions: 57 329 603
Substances: 35 675 069
Documents: 86 941 143

Reaxys Medicinal Chemistry Content

Bioactivities: 41 596 186
Targets: 34 543
Substances: 7 866 511
Documents: 578 893

Molecules

Content
Substances:
15 900 580

Commercial Substances Content

Substances:
93 403 279
Products: 220
427 545



LabNetwork
Content
Substances:
1 647 146



Content
Substances:
400 495

PubChem Content

Substances:
111 050 698

Reaxys Group Generics

Atom Generics

A: Any atom except hydrogen

AH: Any atom

Q: Any atom except carbon or hydrogen

QH: Any atom except carbon

M: Any metal

MH: Any metal or hydrogen

X: Any halogen

XH: Any halogen or hydrogen

Group Generics

G/G*: Any group

GH/GH*: Any group or hydrogen
(* ring closure between group allowed)

Acyclic Groups

ACY: Any acyclic group

ACH: Any acyclic group or hydrogen

Cyclic Groups

CYC: Any cycle

CYH: Any cycle or hydrogen

Scenario #1

Find the physical and spectral data

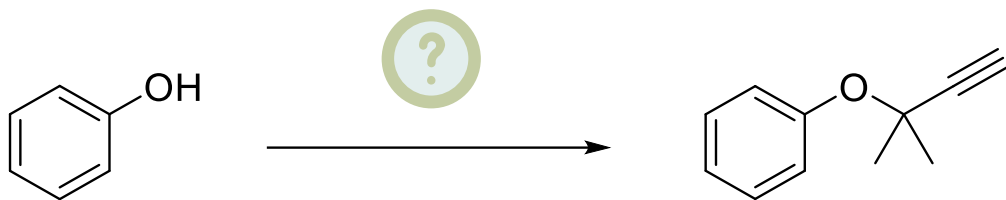
🔍 Ibuprofen

🔍 Manzamine A

🔍 Sildenafil

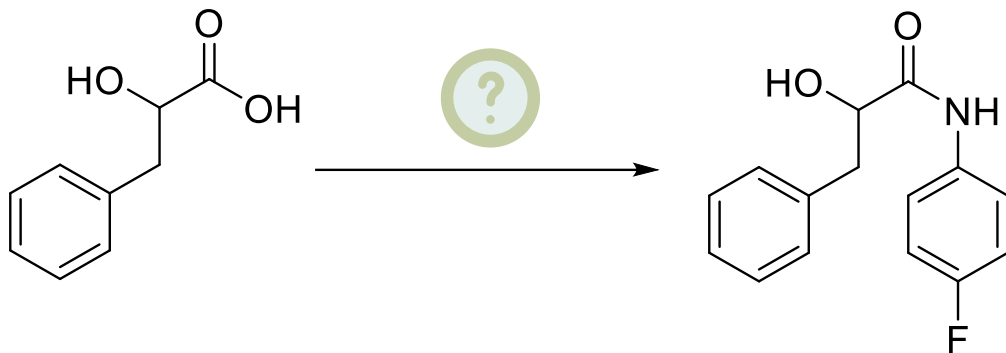
Scenario #2

Finding the appropriate conditions
for the following reaction



Scenario #3

Finding the appropriate conditions
for the following reaction



Scenario #4

Finding the appropriate conditions
for the following reaction



Scenario #5

Finding the appropriate conditions
for the following reaction

Note: the Boc protecting group must be remained intact



Scenario #6

Create the retrosynthetic plans



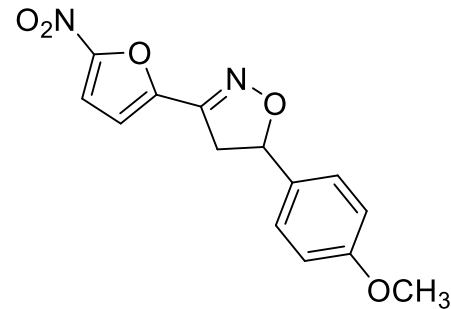
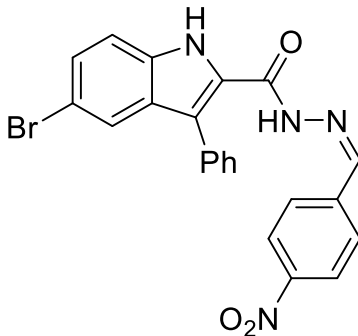
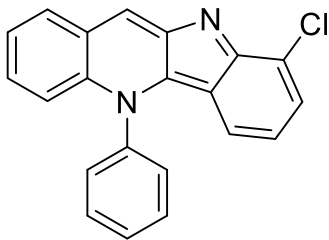
Ibuprofen



Epibatidine

Scenario #7

Use Query Builder to find the biological properties



antiviral

antibacterial

antifungal

antimalarial

antiparasitic

antiflam-
-matory



Thank you for your attention

Q&A

