NOVEMBER 2014

REAXYS R101

BASIC SUBSTANCE QUERIES

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NOTES ON REAXYS R101
BASIC SUBSTANCE SEARCHING

THIS PRESENTATION

- Outlines basic ways to find specific substances by:
  - Name
  - Formula
  - Structure
- For an outline of other presentations in this series, go here

SUMMARY

- Searches by Name are performed through **Ask Reaxys** and through the **Chemical Name Querylet**
  - Works well if the substance has a simple name
- Searches by Formula are performed through the **Molecular Formula Querylet** or the **Formula Builder**
  - However many substances may have the same formula, and more precise answers may be obtained if terms are added in additional fields (e.g., the **Chemical Name Segment Querylet**)
- Searches by structure "**As drawn**" give precise answers without further substituents
  - Answers include isotopes, stereoisomers and salts

- Reaxys R101 level training module for substances describes how to search for specific substances
- Reaxys R201 level training modules describe how to search for groups of substances through (sub)structure, (part)name or (part)formula searches

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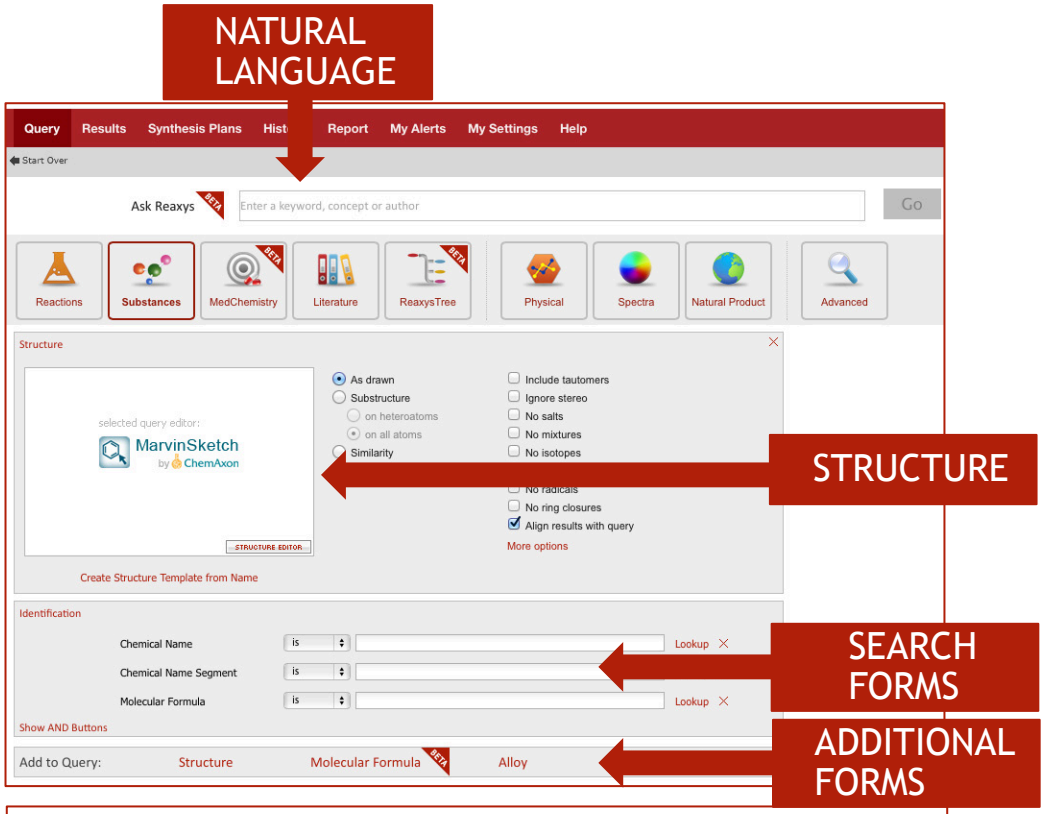
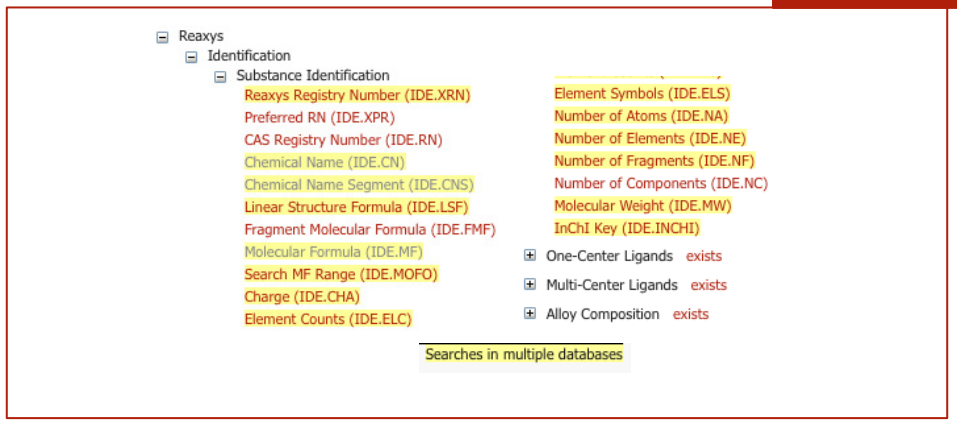
SEARCHING FOR SUBSTANCES

- The main functions needed to search for substances are shown on the right, i.e.,
  - **Ask Reaxys**
    - Natural Language query input
  - The Structure Editor
  - The **Querylets**
    - **Chemical Name**
    - **Chemical Name Segment**
    - **Molecular Formula**
  - The **Additional Forms**
    - **Structure** (which opens the Structure Editor Screen)
    - **Molecular Formula** (which opens the **Formula Builder**)
    - **Alloy** (which opens the interface to input information for searching alloys/ceramics)



- There are other Querylets to find substances; these are used mainly to search for groups of substances
  - Reaxys R201 – for substructure queries
  - Reaxys R201 – for advanced name/formula queries



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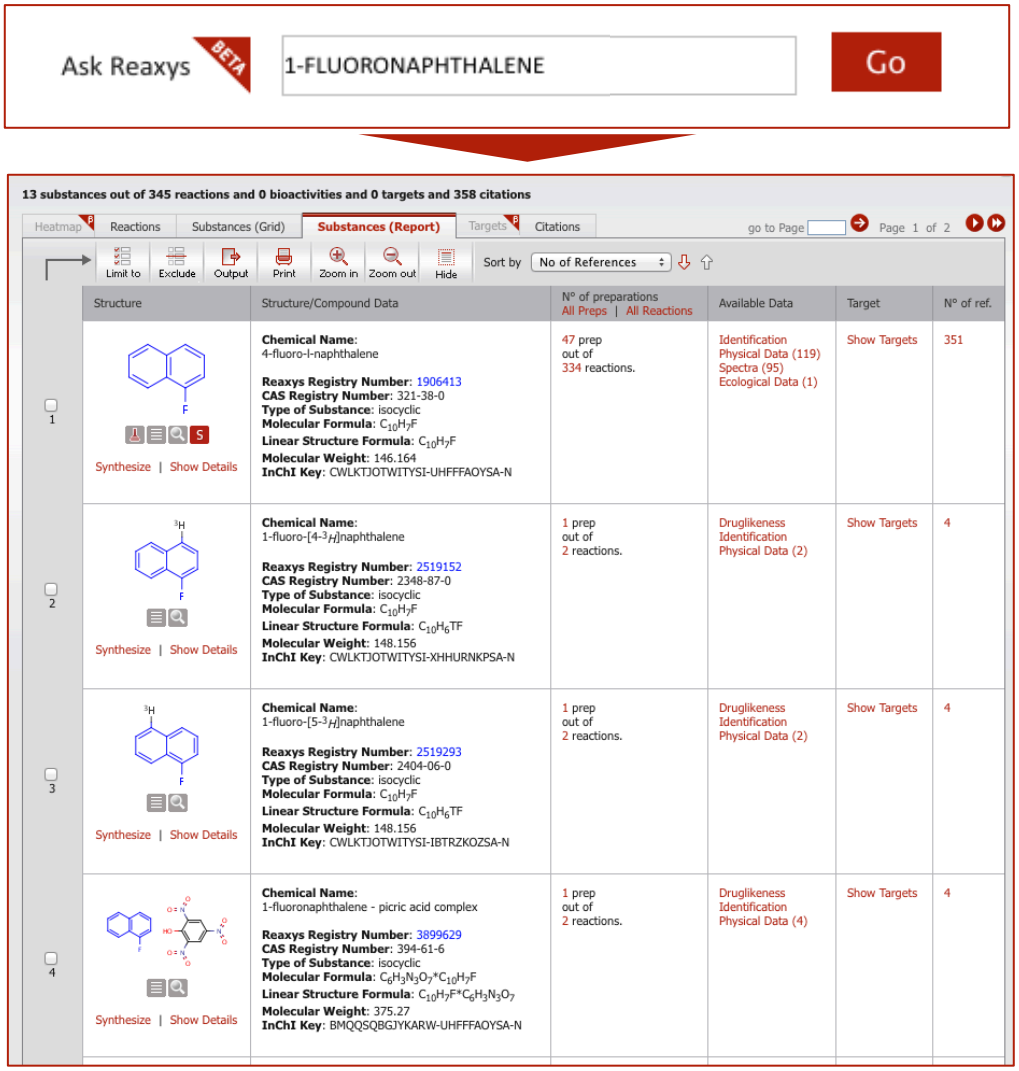
SEARCHING FOR SUBSTANCES BY NAME

ASK REAXYS

- **Ask Reaxys** can be a very good way to find substances where the name is not too complex
  - For example, one way to find 1-fluoronaphthalene is shown
- Behind **Ask Reaxys** are several algorithms to help Reaxys interpret your query, and in this case 13 substances are found
  - Each has "1-fluoronaphthalene" in one of the names listed for the substance in the database
- In many cases the ones of most interest will appear at the top of the list
  - The list is sorted by default by

Sort by | No of References



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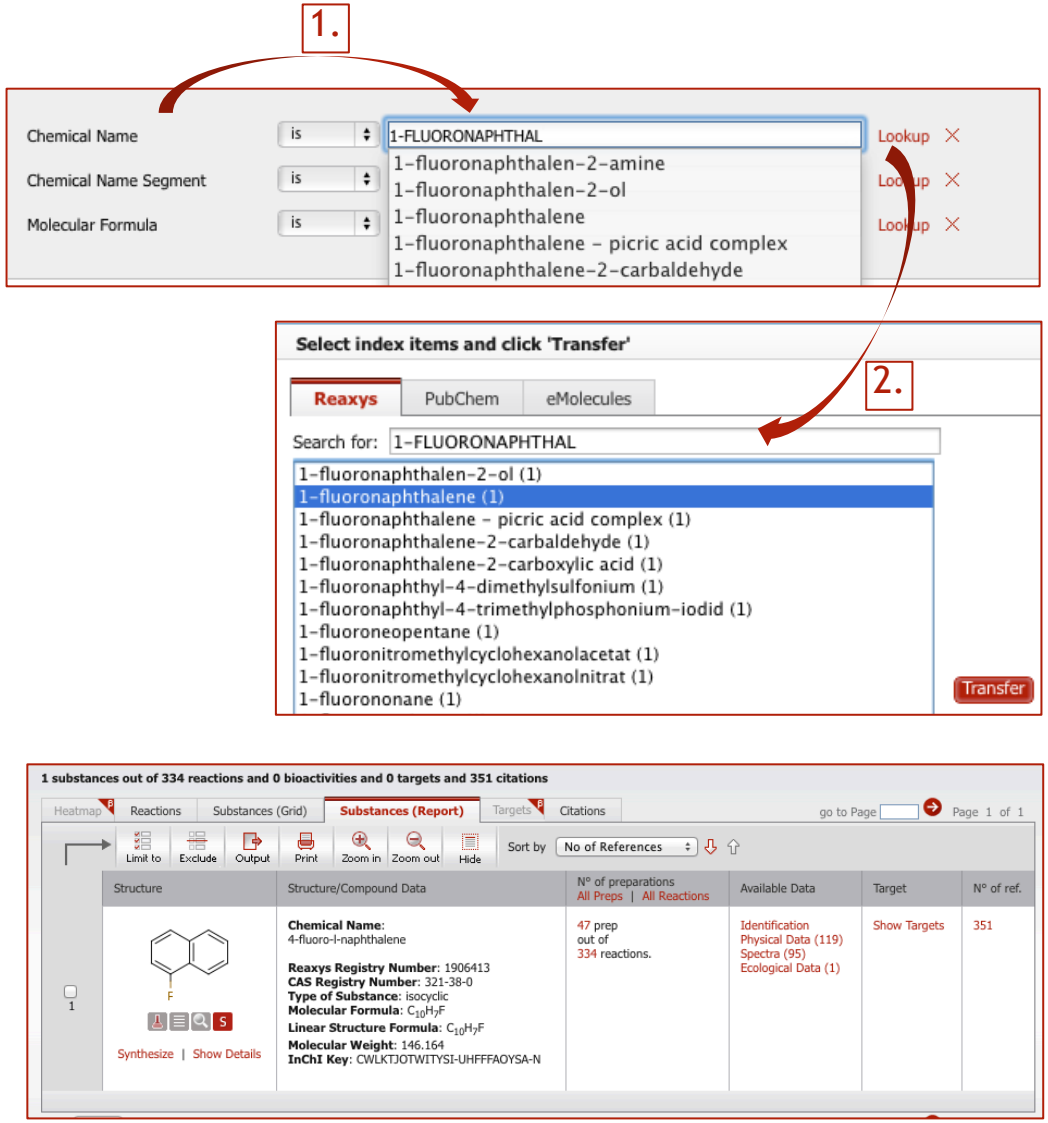
SEARCHING FOR SUBSTANCES BY NAME

CHEMICAL NAME QUERYLET

- The **Chemical Name Querylet** may be searched in two ways:
  1. Just start typing in the input field, then click on the name of the substance you want to search (e.g., on 1-fluoronaphthalene) *or*
  2. Click on Lookup , start typing, then click on the name of the substance(s) you want to search and finally click Transfer
- In either case, just one substance is retrieved
- An advantage of using the **Chemical Name Querylet** is that you see names in the database as you type
  - Finding substances with more complex names can be quite challenging, but seeing options as you type helps significantly



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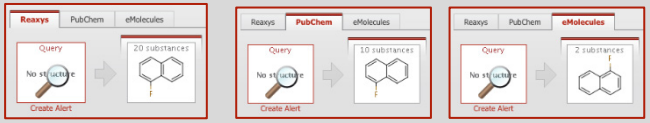
SEARCHING FOR SUBSTANCES BY FORMULA

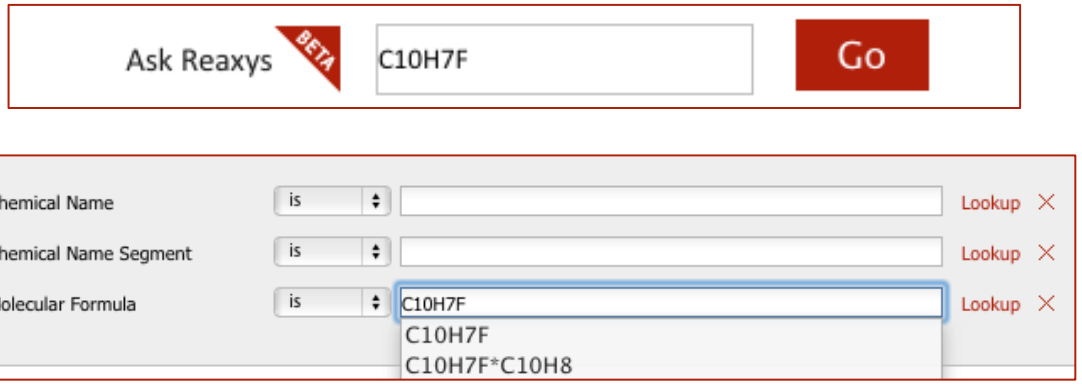
ASK REAXYS AND THE MOLECULAR FORMULA QUERYLET

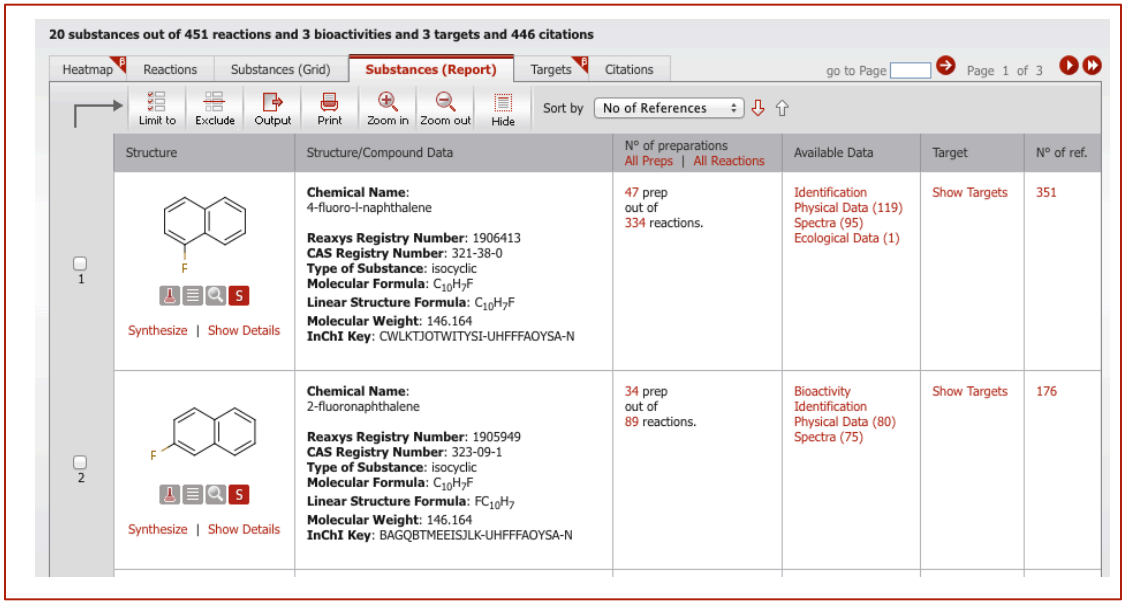
- **Ask Reaxys** and the **Molecular Formula Querylet** may be used to find substances by formula
- In this case both methods give the same number of substances in Reaxys
- However, there are three substance databases in Reaxys…
  - Reaxys, PubChem, eMolecules

  …and the answers may be viewed separately



- In many cases information on the substances you want will be in Reaxys, but on occasions there may be some unique substances in the other databases and it may be of value to check them
- Note also that while the substance of interest may occur in two or three of the databases, the information on the substance may be quite different in the different databases





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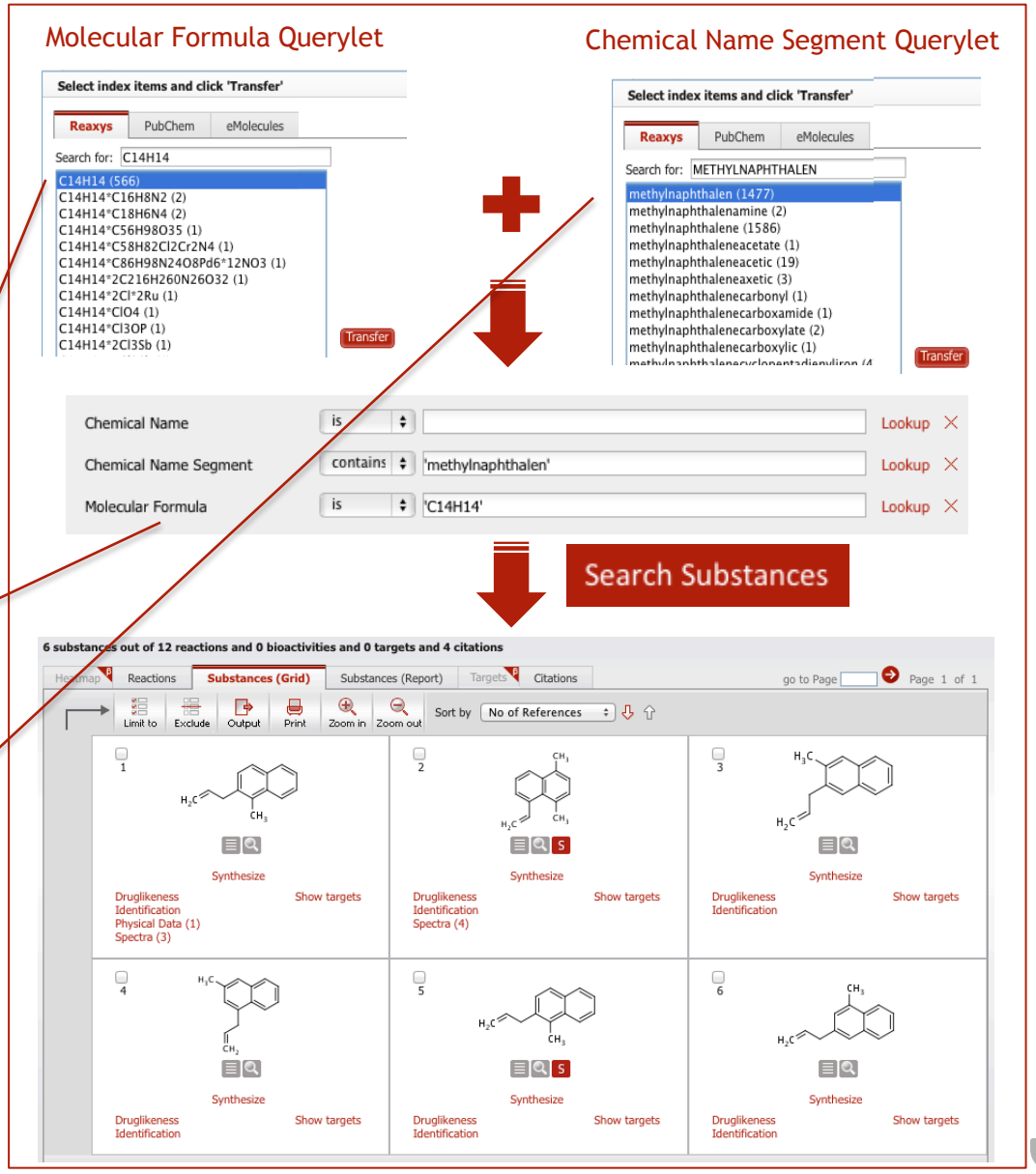
SEARCHING FOR SUBSTANCES BY NAME

COMBINING MOLECULAR FORMULA AND CHEMICAL NAME SEGMENT QUERYLETS

- In cases where there are many substances with the same molecular formula, you may consider combining a molecular formula search with a chemical name segment search
- For example, if you wish to find a specific naphthalene which has a methyl (CH3) and a propenyl (CH2-CH=CH2) attachment, you would determine that the molecular formula of the substance is C14H14
- When you enter this formula (in the **Molecular Formula Querylet**) Lookup ind there are over 500 substances with this formula
- Click to enter this in the querylet
- Next, go to Transfer in the **Chemical Name Segment Qu** Lookup **t**, and type some alternatives (you could try METHYL or NAPHTHALENE or even METHYLNAPHTHALEN – as shown)
- Click to enter information in the query Transfer
- After you click you find a number of subs Search Substances erest



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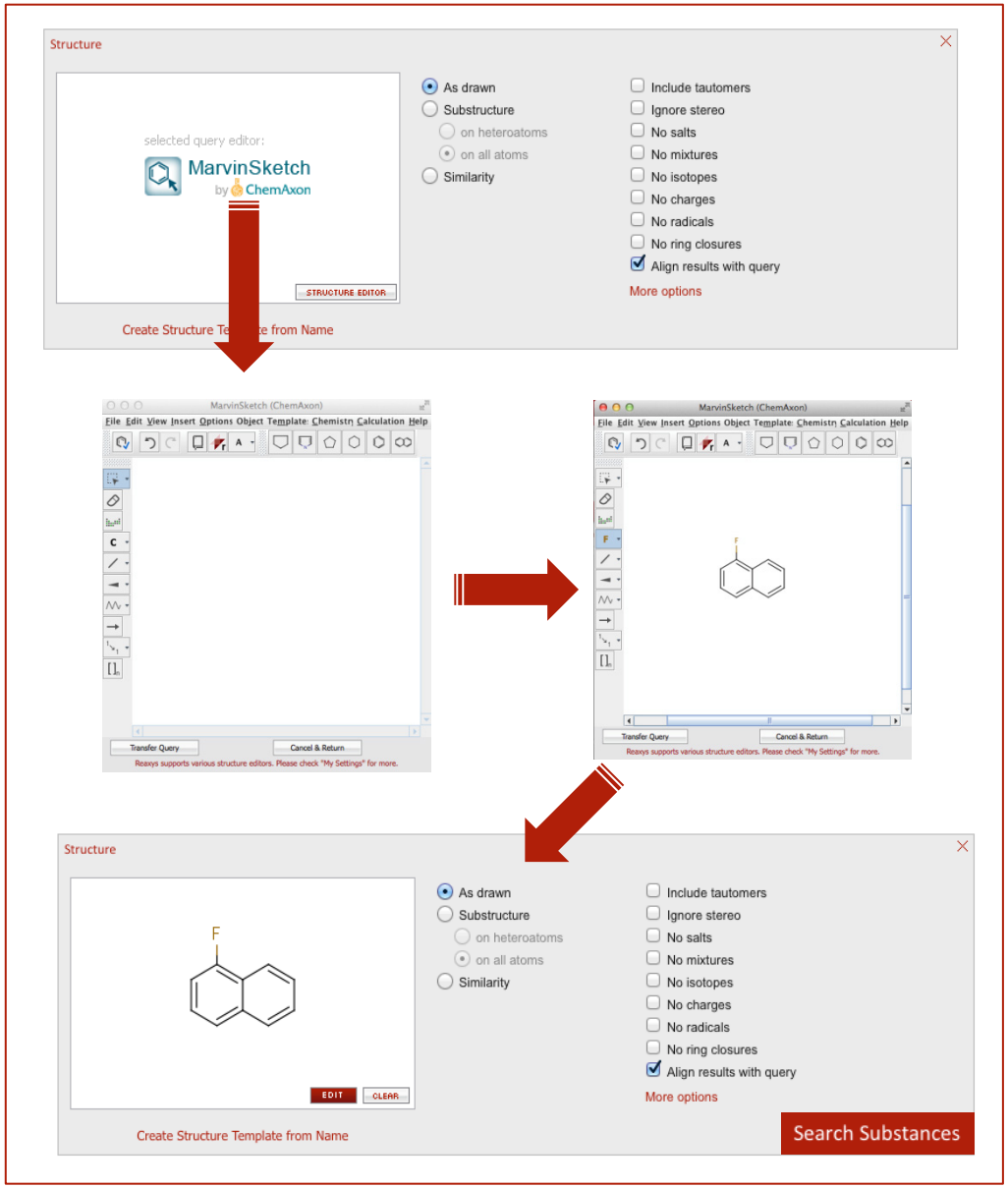
SEARCHING FOR SUBSTANCES BY STRUCTURE

DRAW THE STRUCTURE

- Currently there are 8 Structure Editors that can be used in Reaxys
- For information on the Structure Editors, go to http://help.elsevier.com/app/answers/list/p/9459/c/9432 (the page can also be accessed through the Help messages in Reaxys)
- The default Structure Editor is MarvinSketch
- After you click this editor, you are taken to the structure drawing program and you draw your structure
  - Drawing the basic structure is easy; you simply need to be familiar with the structure drawing program of your choice
- Next click Transfer Query and your query is entered into the Structure Query Screen
- Finally, click Search Substances and you retrieve all substances with exactly the 1-fluoronaphthalene structure (including substances with C and H isotopes, and substances where 1-fluoronaphthalene is one structure in a multi-component substance)
- Answers are similar to those shown on Slide 5
- Note that there are a number of search options to the right of the Structure Query Screen
  - For a simple structure search you choose the default, **As drawn**, where answers have no additional non-hydrogen atoms



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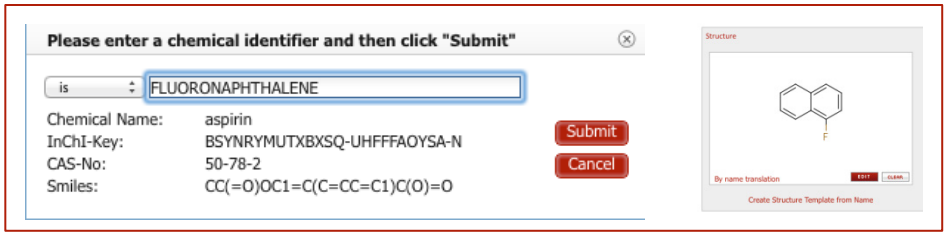
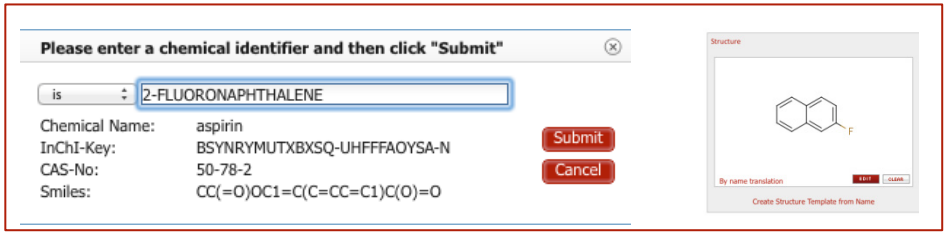
SEARCHING FOR SUBSTANCES BY STRUCTURE

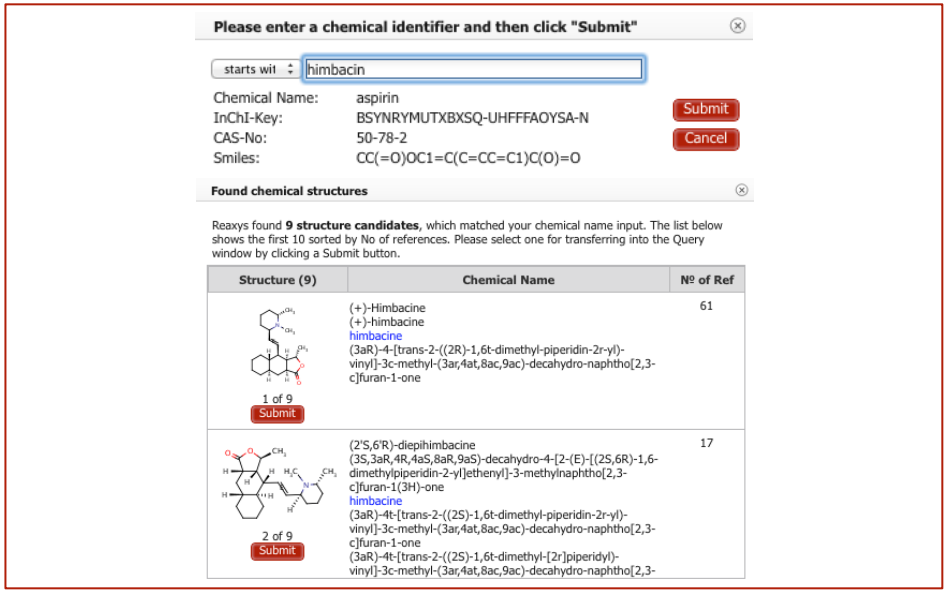
CREATE STRUCTURE TEMPLATE FROM NAME

- Another, quick approach is to click Create Structure Template from Name that appears under the Structure Query Screen
- A screen that asks for a chemical identifier is displayed; enter information as required
  - Note that Reaxys will try to find the "best match", which in the first example is 1-fluoronaphthalene
  - 2-fluoronaphthalene is retrieved if the locator (2-) is specified
- Note also that the operators: is, starts with, ends with, and contains may be used
  - Remember that you do not enter any truncation symbols in these fields (although you can with "is")





- In some cases, Reaxys will present a number of options (as in the himbacine option)
  - Scroll down the list until you find the one that best matches your requirements



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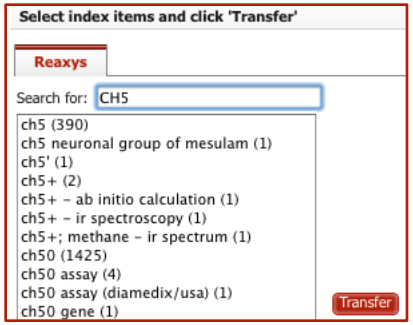
SEARCHING FOR SUBSTANCES IN LITERATURE

CH5+

- Further information on substances may be found through searching in the **Citation Basic Index Querylet**
- The advantage of this process is that over 48 million records are searched in the title, abstract, and keyword fields
- Searches may not be precise, e.g., a search: “benzoic acid” will retrieve records which refer to “benzoic acid esters”
- However, at other times this may be an easier way to find substances that may be challenging to find through other searches

- For example, if you wish to search for the substance CH5+, go to Lookup in the **Citation Basic Index Querylet**, start typing, highlight relevant terms, and click Transfer
- Click Search Literature



- Reaxys retrieves several hundred references; the titles of four of them, and the substance detail, are shown

A beam scattering study of the dynamics of CH4+ (CH4,CH3)CH5+ reaction in the eV collision energy range: three competing mechanisms of CH5+ formation

Vibrational spectroscopy and dynamics of ionic complexes of CH5+, CH5+ (A)x(B)y (A, B = Ar, N2, CH4; x, y = 0-5)

An MO Study on the Structure and the Stability of the CH5+(CH4)n Cluster (n = 0, 1, 2, and 3)

Infrared spectroscopy of the molecular hydrogen solvated carbonium ions, CH5+(H2)n (n=1-6)

Structure	Structure/Compound Data	N° of preparations All Preps | All Reactions
 Synthesize | Show Details	**Chemical Name**: methanium ion **Reaxys Registry Number**: 9329326 **CAS Registry Number**: 15135-49-6 **Type of Substance**: acyclic **Molecular Formula**: CH_5 **Linear Structure Formula**: $CH_5^{(1+)}$ **Molecular Weight**: 17.0507 **InChI Key**: PXOFOHGGCICFQD-UHFFFAOYSA-N	7 prep out of 17 reactions.

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SEARCHING FOR SUBSTANCES IN LITERATURE

OTHER EXAMPLES

CITATION BASIC INDEX SEARCH FOR A POLYMER AND A PHARMACEUTICAL

Citation Basic Index | is | ACRYLIC ACID STYRENE COPOLYMER | Lookup

Preparation of styrene/acrylic acid copolymer microspheres: Polymerization mechanism and carboxyl group distribution	Wang; Pan	2002	Colloid and Polymer Science, **2002** , vol. 280, # 2 p. 152 - 159 Full Text View citing articles	

Title/Abstract

Preparation of styrene/acrylic acid copolymer microspheres: Polymerization mechanism and carboxyl group distribution

Poly(styrene-co-acrylic acid) (St/AA) copolymer microspheres were prepared by batch emulsifier-free emulsion copolymerization of St with AA. The monomer conversion, the morphology and the composition of the particles along the polymerization process were monitored by a gravimetric method, transmission electron microscopy observation and Fourier transform IR analysis, respectively. A shift of the polymerization locus from inside the particles to "outside" the particles in the postnucleation stage was proposed. The results of the study of the distribution of carboxyl groups by a combination of elemental and X-ray photoelectron spectroscopy analyses implied a core/shell structure for the St/AA copolymer microspheres. By chemical metal deposition, nickel particles were formed and deposited on the surface of St/AA microspheres, forming polymer/metal composite particles.

Keywords:
EMTREE drug term: acrylic acid; carboxyl group; copolymer; metal; microsphere; monomer; nickel; poly(styrene co acrylic acid); styrene; unclassified drug
EMTREE medical term: article; chemical analysis; chemical composition; chemical modification; chemical structure; complex formation; controlled study; emulsion; gravimetry; infrared spectroscopy; polymerization; priority journal; surface property; synthesis; transmission electron microscopy; X ray photoelectron spectroscopy
Author: Core/shell structure; Polymerization locus; Styrene/acrylic acid copolymer microspheres
Reaxys Terms: Poly(styrene-co-acrylic acid); nickel particles; styrene - X-ray photoelectron spectroscopy; copolymerization; microsphere; transmission electron microscopy

Sono-assisted photocatalytic degradation of styrene-acrylic acid copolymer in aqueous media with nano titania particles and kinetic studies	Saien; Delavari; Solymani	2010	Journal of Hazardous Materials, **2010** , vol. 177, # 1-3 p. 1031 - 1038 Full Text View citing articles	13

Title/Abstract

Sono-assisted photocatalytic degradation of styrene-acrylic acid copolymer in aqueous media with nano titania particles and kinetic studies

The ultrasonic irradiation (28kHz, 50W) in pre-cavitations regime was employed to enhance the degradation rate of styrene-acrylic acid copolymer in aqueous media with nano titania photocatalyst particles. A stainless steel cylindrical sono-photo reactor with capacity of about 1.25L, equipped with a UV lamp (250W) was used. The influence of operational parameters, i.e. catalyst concentration, pH and temperature was studied and the role of active species was also distinguished. For an initial substrate concentration of $30mgL^{-1}$, under mild applied conditions of $30mgL^{-1}$ of photocatalyst, 25°C and natural pH, a degradation and mineralization conversion of 96percent and 91percent, respectively, was achieved using sono-assisted photocatalysis process in about only 60min. These efficiencies are much higher than those obtained with only photocatalysis process. Meanwhile, the threshold of cavitations was found corresponded to catalyst concentration of about $70mgL^{-1}$. Kinetic studies based on Langmuir-Hinshelwood and power law models in addition to the results from radical scavenger usage revealed that for sono-assisted process, the substrate undergoes degradation mainly via electron-hole redox on the surface of titania particles. It is while for the only photocatalysis process, the reaction proceeds via hydroxyl radicals in the solution bulk.

Keywords:
Author: Active species; Kinetics; Mineralization; Photocatalysis; Sono-assisted process; Styrene-acrylic acid copolymer
Compendex Free Language: Active species; Aqueous media; Catalyst concentration; Degradation rate; Electron hole; Hydroxyl radicals; Kinetic study; Langmuir-Hinshelwood; Nano-titania; Operational parameters; Photo catalytic degradation; Photocatalysis process; Power law model; Radical scavengers; Styrene-acrylic acid; Substrate concentrations; Ultrasonic irradiation; UV lamps
Compendex Descriptor: Carboxylic acids; Catalysts; Cavitation; Copolymerization; Kinetic theory; Mineralogy; Organic acids; Photodegradation; Stainless steel; Styrene; Titanium dioxide
Compendex Mainhead: Photocatalysis
EMTREE drug term: copolymer; hydroxyl radical; styrene acrylic acid copolymer; titanium dioxide; unclassified drug
GEObase Subject Index: aqueous solution; catalysis; degradation; hydroxyl radical; mineralization; organic compound; polymer; power law; reaction kinetics
EMTREE medical term: aqueous solution; article; concentration (parameters); controlled study; degradation kinetics; mineralization; pH; photocatalysis; photodegradation; surface property; temperature; ultrasound
Medline descriptor: Acrylates; Catalysis; Hydroxyl Radical; Kinetics; Nanoparticles; Photolysis; Polystyrenes; Titanium; Ultrasonics; Water
Reaxys Terms: hydroxyl radicals; styrene-acrylic acid copolymer; titania - catalyst; degradation rate; irradiation; photocatalysis; radical scavenger

Citation Basic Index | is | LENALIDOMIDE | Lookup

Lenalidomide (REVLIMID)		2005	Type: Clinical Pharmacology Biopharmaceutics Review, Lab: NDA021880, Owner: CELGEN CORPORATION, Number: 000, Revision: 27.12.2005 00:00:00 **2005** Full Text

Title/Abstract

Show All Targets
Show All Substances (2)

S-LENALIDOMIDE, POLYMORPHIC FORMS THEREOF AND BLEND COMPRISING S- UND R-LENALIDOMIDE	RATIOPHARM GMBH; STRIEGEL, Hans-Guenter; ALBRECHT, Wolfgang; BRUECK, Sandra; HOLFINGER, Konstantin	2011	**Patent:** WO2011/69608 A1, **2011** ; **Patent Family:** WO2011/69608 A1; Full Text

Title/Abstract

Front page Information
Show All Reactions (3)
Show All Substances (4)

Desensitization to lenalidomide	Canamares Orbis; Cortijo Cascajares; Garcia Munoz; Mendez Esteban	2012	Farmacia Hospitalaria, **2012** , vol. 36, # 6 p. 542 - 544 Full Text View citing articles

Title/Abstract

Pulmonary toxicity after long-term treatment with lenalidomide in two myeloma patients	Amraoui, Kamel; Belhadj, Karim; Dupuis, Jehan; Jannier-Nartey, Caroline; Maitre, Bernard	2013	European Respiratory Review, **2013** , vol. 22, # 127 p. 93 - 95 Full Text View citing articles

Title/Abstract

Lenalidomide for multiple myeloma	Hutchinson, Lisa	2010	Nature Reviews Clinical Oncology, **2010** , vol. 7, # 5 p. 241 - 241 Full Text View citing articles

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SUPPLEMENTARY SLIDE

FURTHER PRESENTATIONS IN THIS SERIES

REAXYS R101

A QUICK GUIDE

An overview of the functions of Reaxys 2014

REAXYS R101

TIPS FOR LITERATURE SEARCHING

A quick guide to searching literature

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BASIC SUBSTANCE QUERIES

A quick guide to searching for specific substances by name, formula and structure

REAXYS R101

BASIC REACTION QUERIES

A quick guide to searching for chemical reactions

REAXYS R101

SEARCHING PROPERTIES

A quick guide to searching for properties

REAXYS R201

ADVANCED STRUCTURE QUERIES

Searching by substructure

REAXYS R201

ADVANCED NAME AND FORMULA SEARCHING

Searching for Substances by Names and Formulas

REAXYS R201

ADVANCED REACTION QUERIES

Additional ways to search for reactions