SCIFINDER DEMONSTRATION EXAMPLES IMPERIAL COLLEGE - MAY 2019

RESEARCH TOPIC SEARCH

1. Find references for “Cycloadditions for the synthesis of alkaloids”.
   Take the first set of answers to view.

   Look at the options for analysing and refining your answer set.

   Refine your answers to Journals only.

   Sort your answers in order of citing references. How many publications cite the top answer?

   Use the analyse function and select “Analyse by Concept Heading”. Are there publications where Crystal Structures are also a main feature of the publication?

   Set up a Keep Me Posted on this search.
   Export a selection of answers (put a mark on the check box next to the answer) and export. Chose any export format you wish.

   Use Categorise, select Synthetic Chemistry and then Reactions. Look for the specific types of cycloaddition reactions in this list.

2. Find all journals with the term ‘inorganic’ in the title.

SUBSTANCE SEARCH

1. Search for the drug ibuprofen (CAS RN 15687-27-1)

   Display the substance detail for this

   View the "Other Names" for Ibuprofen. View the different categories of information available for this substance. Using the CAS Reference Roles, how many publications in total relate to analytical studies of ibuprofen?

   What experimental spectra are available?

   How many commercial sources are available for ibuprofen? Click on commercial sources then "analyse" by country. How many suppliers are located in, or will ship to the UK? Select these and use 'Keep analysis", then export this list.

SEARCHES USING CHEMICAL STRUCTURES

Based on substance search

Search for the substance Celecoxib (CAS RN 169590-42-5) then click on the chevron in the structure image and select "explore by structure", then chose "Chemical Structure".

Choose an "exact search" and explore what is retrieved in the answer set.

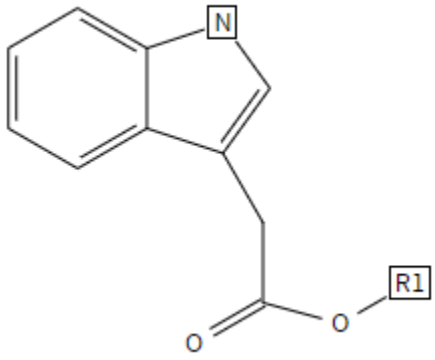
Change to "Substructure" then run the search. How many substances in total are now received in the answer set?

Use the Refine tab to limit structures to those containing isotopes. How many are there?

Can we make this search broader by making the structure generic? – Be as inventive as you wish!

Based on drawn structure

1. Draw the following structure in the Chemical Structure window



R1 = Ak (alkyl) or Hy (heterocycle)
The R1 and the Nitrogen in the ring are blocked from any further substitution

Search the structure as a substructure (this is the default setting)

Analyse by bioactivity indicators and view how many substances are linked to anti-tumour agents in publications. Use “Keep analysis” and then see if any of these are commercially available.
What is the CAS RN for the oldest substance in this answer set?

Get the references for these substances and the refine to patent as the document type.

REACTION SEARCHING

Based on substance search

Search for the drug Celecoxib.

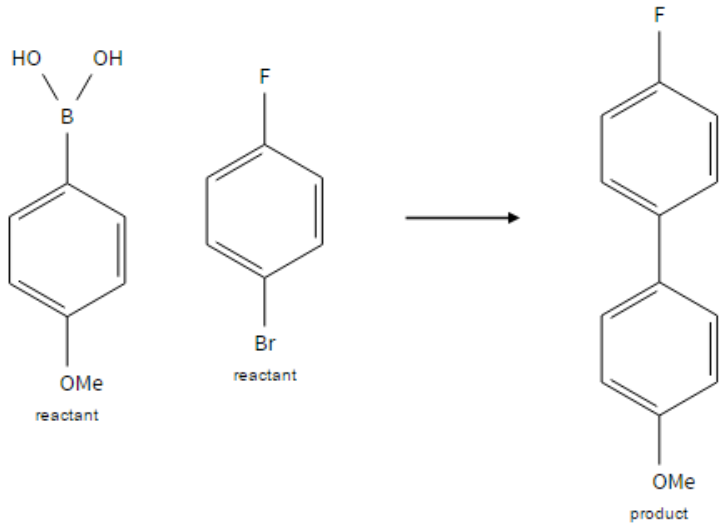
Display the substance record and then click on the chevron in the structure window and select "Synthesize this". How many reactions are there for synthesizing this drug?

Analyse by "solvent", how many reactions involve water as a solvent?

Go back to the substance record and list how many reactions has Celecoxib listed as a reactant.

Based on chemical structure

Draw the following reaction



Find reactions within your answers that have experimental procedures available and give a high product yield.

Of these reactions, how many of them use disodium carbonate as a reagent?