

Interpret query features with "Generate Structure from Name"

As you know already, this feature available from the Reaction- and from the Substances & Properties- Query pages is very simple to use, and allows a rapid transformation of any type of name (chemical name, generic name, InChI key, CAS registry number, Smiles string) into a chemical structure, which will then serve as query templates for further refinement using the editors and saving time in drawing complex molecules, such as steroids.

But did you know that this feature is also able to interpret query features to some extent? Type for example 3-alkyl-indole, and see what happens: this general name is translated into a substructure query containing the 'ALK' generic group on the 3 position of the molecule.

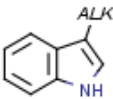
Please enter a chemical identifier and then click "Submit" ✕

Chemical Name: aspirin
 InChI-Key: BSYNRYMUTXBXSQ-UHFFFAOYSA-N Submit
 CAS-No: 50-78-2 Cancel
 Smiles: CC(=O)OC1=C(C=CC=C1)C(O)=O

Reactions **Substances and Properties** Text, Authors and more

Generate structure from name

Double click this frame and draw structure query



COPY TO REACTIONS TAB CLEAR

As drawn

Substructure:

on heteroatoms

on all atoms

Ignore stereo

No salts

No mixtures

No isotopes

No additional rings

Further options

Search

Properties (Form-based) **Properties (Advanced)**

Show Fields and Operators Check Syntax

Clear Query Load Query/Batch Save Query

Advanced Search allows for entering complex property/combination queries following the general rule "<field code> <operator> <field value (s)>".

If you don't know the field code please click the hyperlink [Show Fields and Operators](#) and select one from the hierarchical tree. If you need additional explanations, please click [here](#)

This may not work in all cases, but where this works, this method of searching can be a significant help.

For more information please visit

www.reaxys.com

Americas:

E-Customer Service
360 Park Avenue South
New York
NY 10010-1710
Toll Free: +1 888 615 4500
Tel: +1 212 462 1978
Fax: +1 212 462 1974
Email: usinfo@reaxys.com

Europe and all other regions:

E-Customer Service
Theodor-Heuss-Allee 108
60486 Frankfurt/Main, Germany
Tel: +49 69 5050 4268
Fax: +49 69 5050 4213
Email: nlinfo@reaxys.com

Japan:

E-Customer Service
1-9-15 Higashi-Azabu
Minato-ku Tokyo
106-0044 Japan
Tel: +81 3 5564 5034
Fax: +81 3 5561 5047
Email: jpinfo@reaxys.com



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