Reaxys Predefined Generic Atoms & Groups

The Reaxys Generics are useful tools for researchers to rapidly define atoms and acyclic and cyclic groups.

Reaxys Generics are easily accessible via all the structure editors available in Reaxys, with the exception of ChemDraw, where this is not supported.

How to access Reaxys Generics from each structure editor

- In MarvinSketch, simply click this button to open Generics.

- In the CrossFire Structure Editor, click with the Edit tool on the attachment point for the future generic group and choose Generics on the Symbol menu of the Atom Attributes menu.
• In **Symyx Isis Draw**, right click with the lasso tool on the attachment point of the future generic group and select *Edit atom*; then on the *Query atom* tab choose *Beilstein Generic* on the Symbol menu

![Edit Atom](image1)

• In **Symyx Draw**, right click with the lasso tool on the attachment point of the future generic group and select *Beilstein generic group* in the *Atom Property* menu

![Atom Property](image2)
The pre-defined generic atoms and groups are recognized by Reaxys regardless of the structure editor which created the query.

The following table displays all the Reaxys Generics available.

On the first line are the Generic Atoms and then the Generic Groups. The groups are divided in Acyclic (Carbocyclic and Heteroacyclic) and in Cyclic (Carbocyclic, Heterocyclic and containing No Carbon) derivatives.

**Atom Generics**

The following Generic Atoms are available for searching in Reaxys:

- **A**: any atom except hydrogen
- **AH**: any atom, including hydrogen
- **Q**: any atom except C or H, so any heteroatom
- **QH**: any atom except C
- **M**: any metal
- **MH**: any metal or hydrogen
- **X**: any halogen
- **XH**: any halogen or hydrogen

**Group Generics**

The Generic Groups **G** and **GH** will retrieve any group (**G**) and any group or hydrogen (**GH**). The Group names which are marked with an asterisk (**G***, **GH***) retrieve the same as **G** and **GH**, but they also retrieve structures in which an atom in the group can be linked with an atom in the original structure to form a ring (ring closure). **G** and **GH** will not allow such implicit ring closures.

Please note: the Reaxys Query Form setting *No additional rings* should not be checked if you want to allow **G*** or **GH*** to form a ring with the rest of the structure. It is recommended that you perform a substructure search if you want to retrieve substances with this type of ring closure.
It is also important to remember that G, GH, G*, GH* are the unique Generic Groups which can have more than one attachment point.

For example, a simple substance query such as this one (‘exact match’, no other conditions)

![Diagram of a molecule]

will retrieve more than 1.6 million molecules beyond them:

**Acyclic Generic Groups**

This section contains the acyclic derivatives. Those groups can only have one attachment point.

- **ACY**: acyclic
- **ABC**: carbocyclic
- **AYL**: alkynyl
- **ALK**: alkyl
- **AEL**: alkenyl
- **AHC**: heteroacyclic
- **AOX**: alkoxy

The Group names that end in H allow either the group or hydrogen at that position. For example, **ALK** represents an alkyl group, while **ALH** represents an alkyl group or hydrogen.

In case of heteroacyclic group, the fragment can be linked by C atom or by any heteroatom being part of the derivative.

For example, a simple substance query such as this one (‘exact match’, no other conditions)
Cyclic Generic Groups

This group contains all the cyclic fragments, and is divided in three sections with the Carbocyclic, the Heterocyclic and the cycle containing No Carbon at all.

**CYC:** any cyclic group (can be Carbocyclic, heterocyclic, or with no C atoms)

As previously, group names that end in H allow either the group or hydrogen at that position. For example, **CYC** represents a cyclic group, while **CYH** represents a cyclic group or hydrogen. This applies of course also for all the following groups

1. **Carbocyclic**
   - **CBC:** carbocyclic derivatives
   - **ARY:** any aryl group
   - **CAL:** any cycloalkyl group
   - **CEL:** any cyloalkenyl group

2. **Heterocyclic**
   - **CHC:** Heterocyclic group
   - **HAR:** Heteroaryl group
   
   In case of heterocyclic/heteroaryl groups, the fragment can be linked by C atom or by any heteroatom of the fragment

3. **No Carbon**
   - **CXX:** cyclic group with no Carbon atoms

All those Cyclic Generic groups can only have one attachment point.
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