

Reaxys Predefined Generic Atoms & Groups

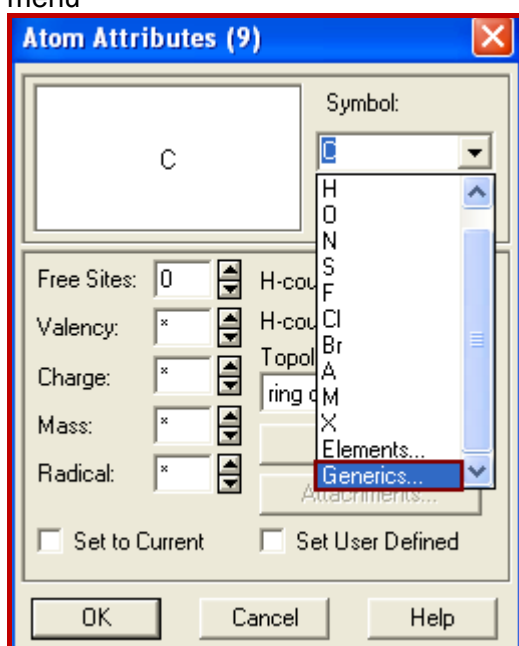
The Reaxys Generics are useful tools for researchers to rapidly define atoms and acyclic and cyclic groups.

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

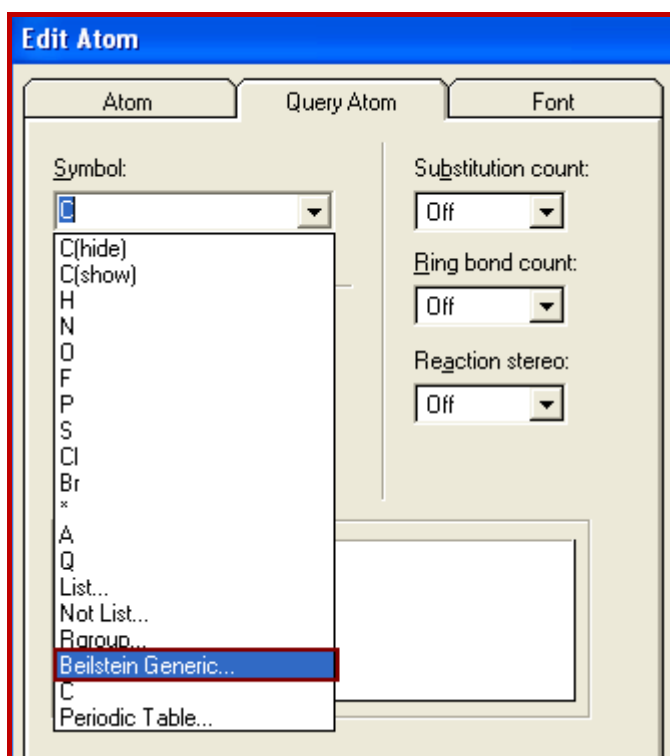
How to access Reaxys Generics from each structure editor

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

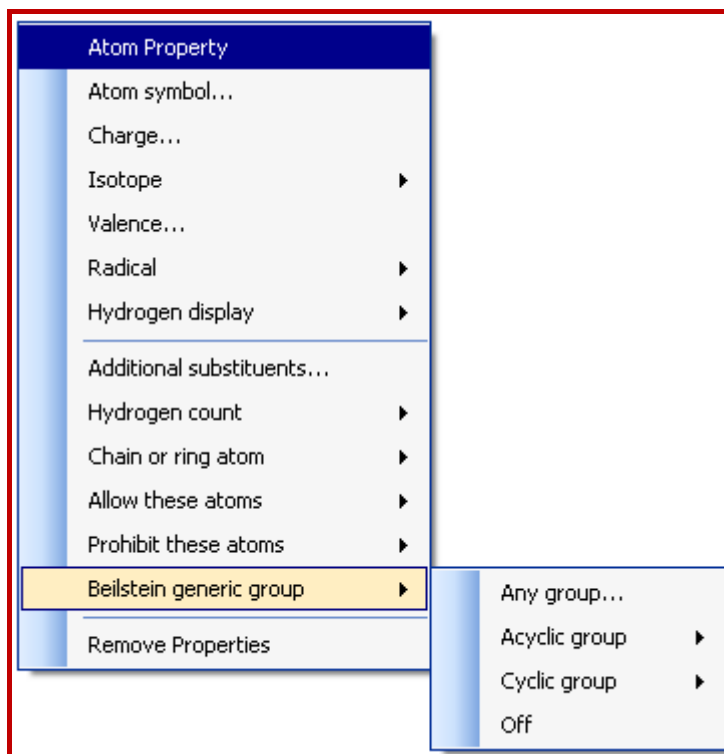
- In the **CrossFire Structure Editor**, click with the Edit tool on the attachment point for the future generic group and choose *Generics* on the Symbol menu of the *Atom Attributes* menu



- 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



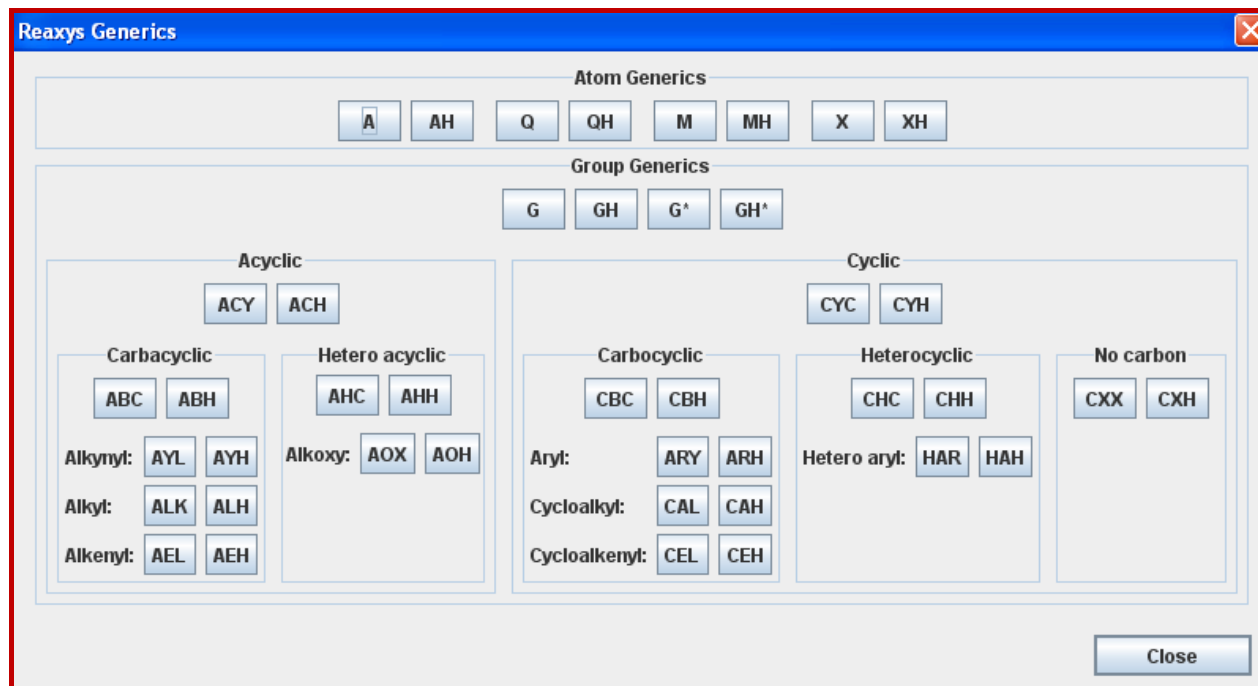
- In **Symyx Draw**, right click with the lasso tool on the attachment point of the future generic group and select *Beilstein generic group* in the *Atom Property* menu



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

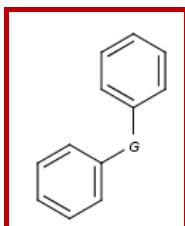
Group Generics

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)



will retrieve more than 1.6 million molecules beyond them:

<p>16</p> <p>Synthesize</p>	<p>17</p> <p>Synthesize</p>	<p>18</p> <p>Synthesize</p>
<p>19</p> <p>Synthesize</p>	<p>20</p> <p>Synthesize</p>	<p>21</p> <p>Synthesize</p>
<p>22</p> <p>Synthesize</p>	<p>23</p> <p>Synthesize</p>	<p>24</p> <p>Synthesize</p>

Acyclic Generic Groups

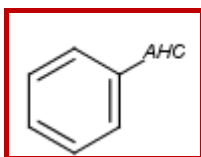
This section contains the acyclic derivatives. Those groups can only have one attachment point.

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)



will retrieve more than 410,000 molecules beyond them:

<p>1</p> <p>Identification Physical Data (187) Spectra (86) Bioactivity/Ecotox (9) Use/Application (5)</p> <p>Synthesize</p>	<p>2</p> <p>Identification Physical Data (7) Spectra (17)</p> <p>Synthesize</p>	<p>3</p> <p>Identification Physical Data (9) Spectra (10)</p> <p>Synthesize</p>
<p>4</p> <p>Identification Physical Data (551) Spectra (166) Bioactivity/Ecotox (9) Use/Application (2)</p> <p>Synthesize</p>	<p>5</p> <p>Identification Physical Data (1031) Spectra (268) Bioactivity/Ecotox (52) Use/Application (20) Natural Product (2)</p> <p>Synthesize</p>	<p>6</p> <p>Identification Physical Data (1141) Spectra (264) Bioactivity/Ecotox (60) Use/Application (17) Natural Product (1)</p> <p>Synthesize</p>
<p>7</p> <p>Identification Physical Data (158) Spectra (95) Bioactivity/Ecotox (73) Use/Application (19) Natural Product (1)</p> <p>Synthesize</p>	<p>8</p> <p>Identification Physical Data (32) Spectra (36) Use/Application (3)</p> <p>Synthesize</p>	<p>9</p> <p>Identification Physical Data (84) Spectra (75) Bioactivity/Ecotox (7) Use/Application (1)</p> <p>Synthesize</p>

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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