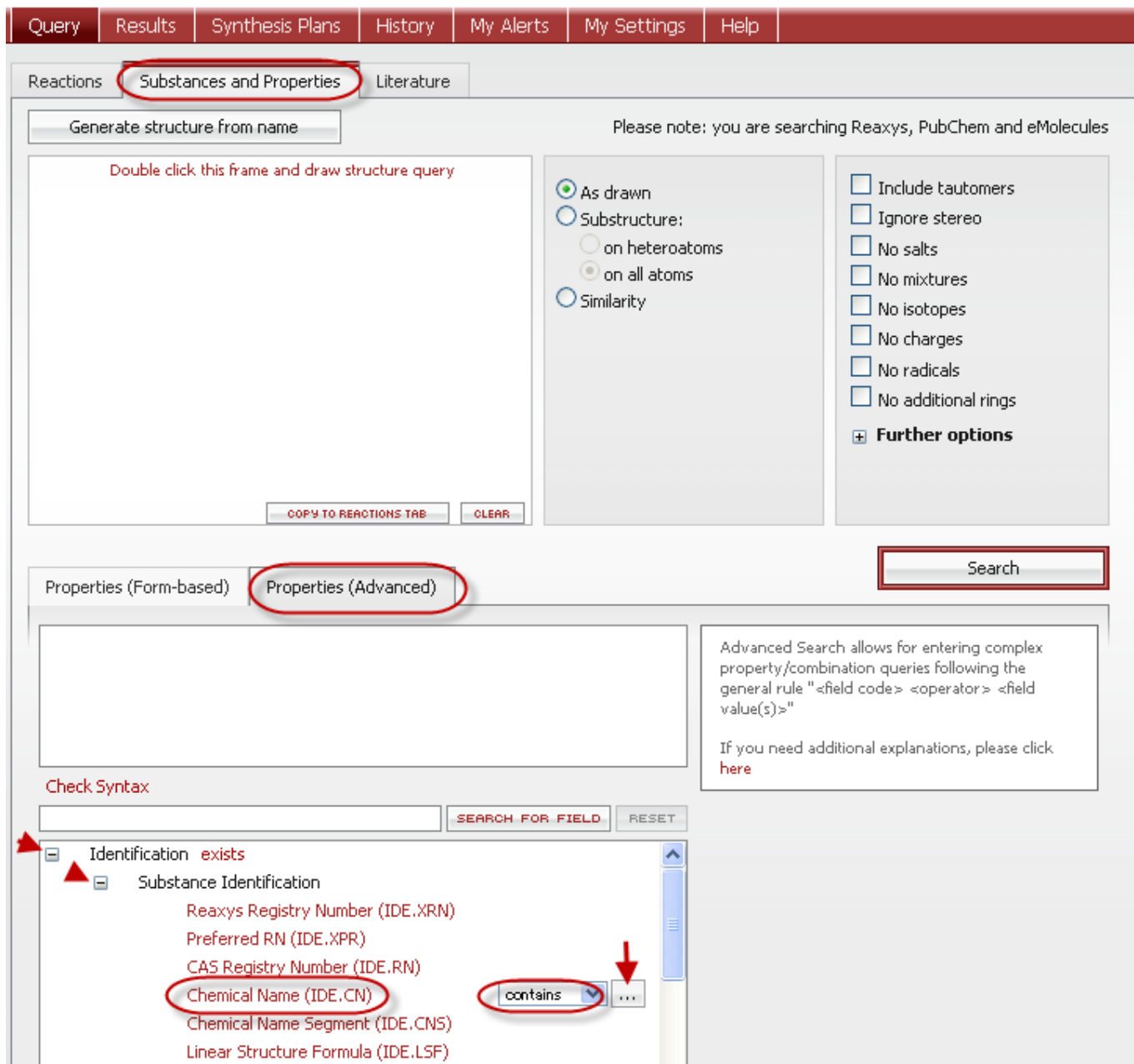


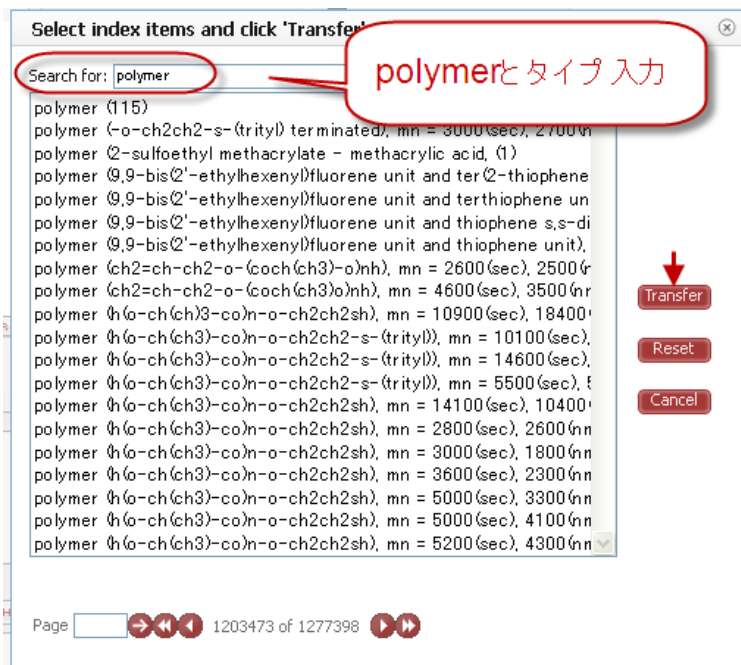
## Reaxys のポリマー検索

1. Query ページの Substances and Properties タブで Properties (Advanced) タブを選択します
2. Identification > Substance Identification > Chemical Name をクリックします
3. プルダウンメニューから contains を選択します



The screenshot shows the Reaxys search interface. At the top, there is a navigation bar with tabs: Query, Results, Synthesis Plans, History, My Alerts, My Settings, and Help. Below this, there are three sub-tabs: Reactions, **Substances and Properties** (highlighted with a red circle), and Literature. A button labeled 'Generate structure from name' is visible. A note states: 'Please note: you are searching Reaxys, PubChem and eMolecules'. The main search area contains a large empty box with the instruction 'Double click this frame and draw structure query'. To the right of this box are two panels of search options. The first panel has radio buttons for 'As drawn' (selected), 'Substructure: on heteroatoms', 'Substructure: on all atoms', and 'Similarity'. The second panel has checkboxes for 'Include tautomers', 'Ignore stereo', 'No salts', 'No mixtures', 'No isotopes', 'No charges', 'No radicals', and 'No additional rings', along with a '+ Further options' button. Below these panels is a 'Search' button (highlighted with a red box). Underneath the search area, there are two tabs: 'Properties (Form-based)' and **Properties (Advanced)** (highlighted with a red circle). A 'Check Syntax' section with a 'SEARCH FOR FIELD' button and a 'RESET' button is also present. The 'Properties (Advanced)' section is expanded to show a tree view: 'Identification exists' (expanded) -> 'Substance Identification' (expanded) -> 'Reaxys Registry Number (IDE.XRN)', 'Preferred RN (IDE.XPR)', 'CAS Registry Number (IDE.RN)', **Chemical Name (IDE.CN)** (highlighted with a red circle), 'Chemical Name Segment (IDE.CNS)', and 'Linear Structure Formula (IDE.LSF)'. A dropdown menu for the 'Chemical Name (IDE.CN)' field shows 'contains' selected (highlighted with a red circle) and a red arrow points to the dropdown arrow. A text box on the right explains the advanced search syntax: 'Advanced Search allows for entering complex property/combo queries following the general rule "<field code> <operator> <field value(s)>"' and provides a link for more information.

4. Search for テキストフィールドに polymer とタイプ入力した後、Transfer ボタンをクリックします



Select index items and click 'Transfer'

Search for: polymer

polymer (115)

polymer (-o-ch2ch2-s-(trityl) terminated, mn = 3000(sec), 2700(n

polymer (2-sulfoethyl methacrylate - methacrylic acid, (1)

polymer (9,9-bis(2'-ethylhexenyl)fluorene unit and ter(2-thiophene

polymer (9,9-bis(2'-ethylhexenyl)fluorene unit and terthiophene un

polymer (9,9-bis(2'-ethylhexenyl)fluorene unit and thiophene s,s-di

polymer (9,9-bis(2'-ethylhexenyl)fluorene unit and thiophene unit),

polymer (ch2=ch-ch2-o-(coch(ch3)o)nh), mn = 2600(sec), 2500(n

polymer (ch2=ch-ch2-o-(coch(ch3)o)nh), mn = 4600(sec), 3500(n

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 10900(sec), 18400

polymer (h(o-ch(ch3)-co)n-o-ch2ch2-s-(trityl)), mn = 10100(sec),

polymer (h(o-ch(ch3)-co)n-o-ch2ch2-s-(trityl)), mn = 14600(sec),

polymer (h(o-ch(ch3)-co)n-o-ch2ch2-s-(trityl)), mn = 5500(sec),

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 14100(sec), 10400

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 2800(sec), 2600(n

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 3000(sec), 1800(n

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 3600(sec), 2300(n

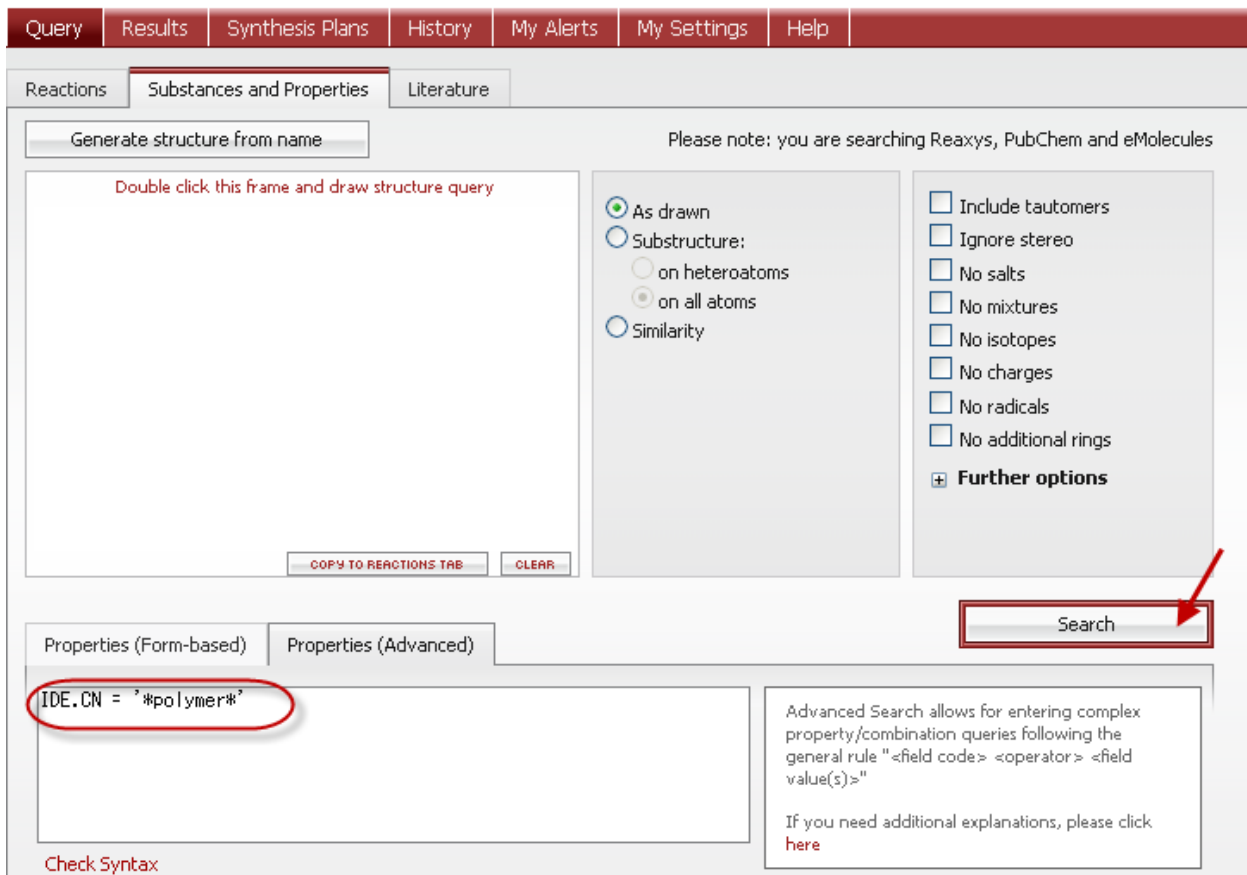
polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 5000(sec), 3300(n

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 5000(sec), 4100(n

polymer (h(o-ch(ch3)-co)n-o-ch2ch2sh), mn = 5200(sec), 4300(n

Page 1203473 of 1277398

5. 下図赤丸のように表示されたことを確認した後、Search ボタンをクリックします



Query Results Synthesis Plans History My Alerts My Settings Help

Reactions Substances and Properties Literature

Generate structure from name

Please note: you are searching Reaxys, PubChem and eMolecules

Double click this frame and draw structure query

As drawn

Substructure:

on heteroatoms

on all atoms

Similarity

Include tautomers

Ignore stereo

No salts

No mixtures

No isotopes

No charges

No radicals

No additional rings

Further options

COPY TO REACTIONS TAB CLEAR

Properties (Form-based) Properties (Advanced)

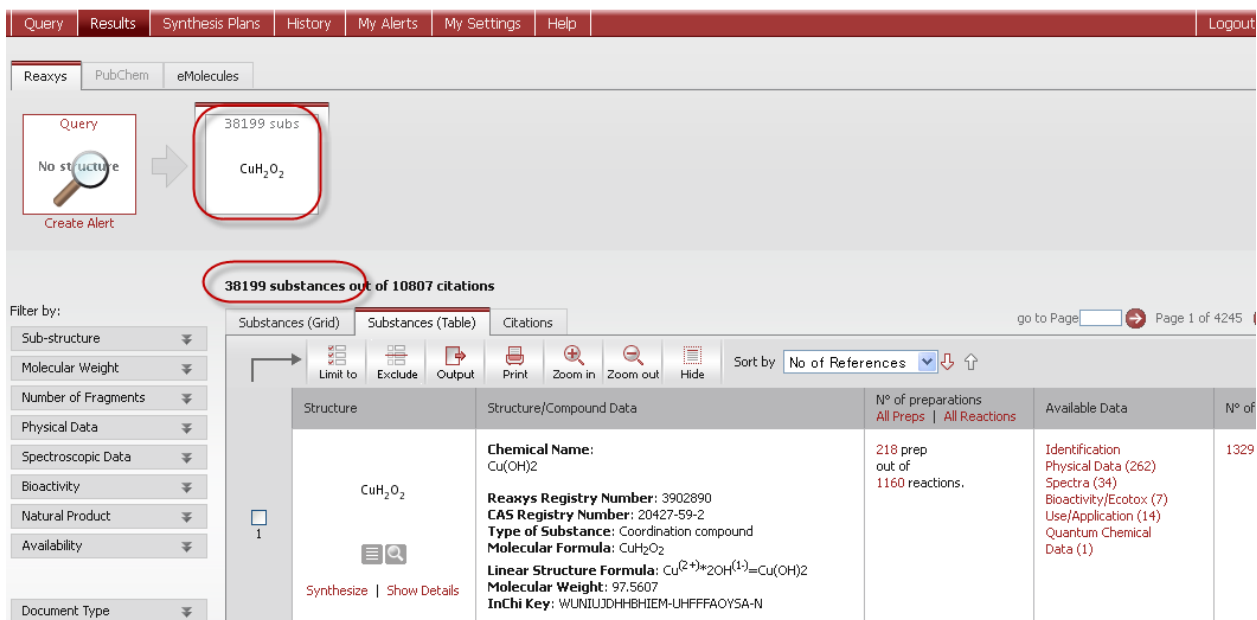
IDE.CN = '\*polymer\*'

Check Syntax

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

If you need additional explanations, please click [here](#)

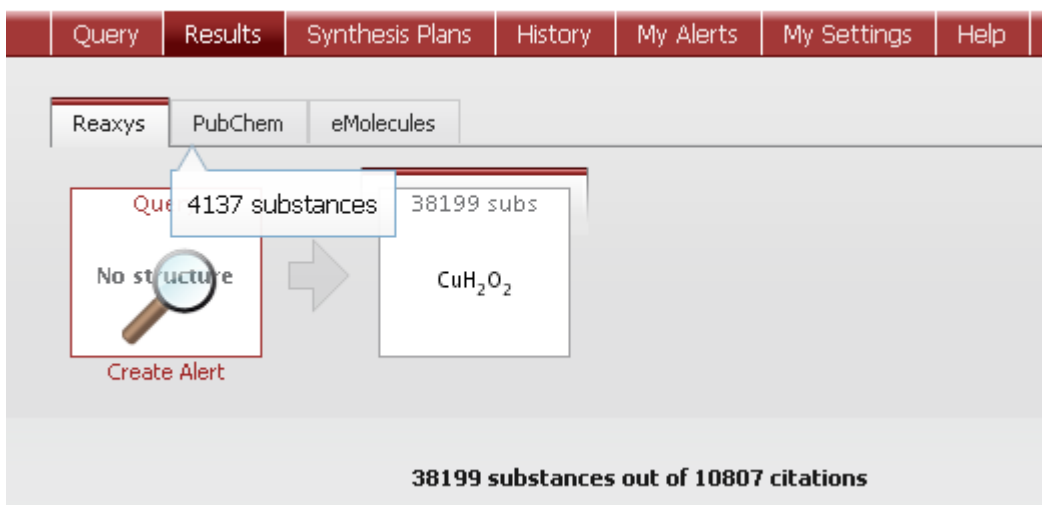
6. Result ページの Reaxys タブに Chemical Name で polymer を含む 38199 個の収載化合物があることが表示される



The screenshot shows the Reaxys search results page for the query CuH2O2. The search results are displayed in a table with the following columns: Structure, Structure/Compound Data, N° of preparations, Available Data, and N° of Citations. The first result is for Cu(OH)2.

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	N° of Citations
<chem>CuH2O2</chem>	<b>Chemical Name:</b> Cu(OH) <sub>2</sub> <b>Reaxys Registry Number:</b> 3902890 <b>CAS Registry Number:</b> 20427-59-2 <b>Type of Substance:</b> Coordination compound <b>Molecular Formula:</b> CuH <sub>2</sub> O <sub>2</sub> <b>Linear Structure Formula:</b> Cu <sup>(2+)</sup> +2OH <sup>(1-)</sup> =Cu(OH) <sub>2</sub> <b>Molecular Weight:</b> 97.5607 <b>InChi Key:</b> WUNIUJDHFBHIEM-UHFFFAOYSA-N	218 prep out of 1160 reactions.	Identification Physical Data (262) Spectra (34) Bioactivity/ECotox (7) Use/Application (14) Quantum Chemical Data (1)	1329

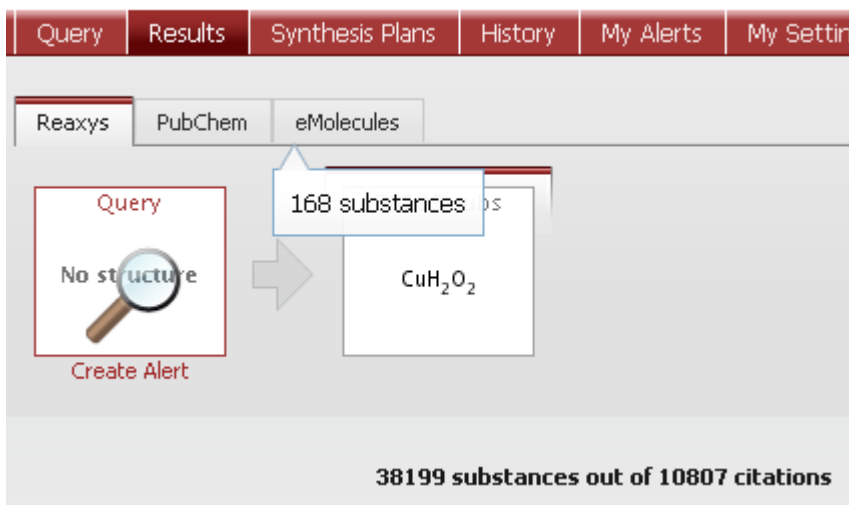
7. PubChem タブ上にポインターを合わせると、PubChem 由来で Chemical Name に polymer を含むの収載化合物が 4137 個であることがわかります。



The screenshot shows the Reaxys search results page for the query CuH2O2. A tooltip is visible over the search results, indicating that there are 4137 substances from PubChem. The search results are displayed in a table with the following columns: Structure, Structure/Compound Data, N° of preparations, Available Data, and N° of Citations. The first result is for Cu(OH)2.

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	N° of Citations
<chem>CuH2O2</chem>	<b>Chemical Name:</b> Cu(OH) <sub>2</sub> <b>Reaxys Registry Number:</b> 3902890 <b>CAS Registry Number:</b> 20427-59-2 <b>Type of Substance:</b> Coordination compound <b>Molecular Formula:</b> CuH <sub>2</sub> O <sub>2</sub> <b>Linear Structure Formula:</b> Cu <sup>(2+)</sup> +2OH <sup>(1-)</sup> =Cu(OH) <sub>2</sub> <b>Molecular Weight:</b> 97.5607 <b>InChi Key:</b> WUNIUJDHFBHIEM-UHFFFAOYSA-N	218 prep out of 1160 reactions.	Identification Physical Data (262) Spectra (34) Bioactivity/ECotox (7) Use/Application (14) Quantum Chemical Data (1)	1329

8. 同様に eMolecules タブ上にポインターを合わせると、eMolecules データベース由来で Chemical Name に polymer を含むの収載化合物が 168 個であることがわかります



Query Results Synthesis Plans History My Alerts My Settings

Reaxys PubChem eMolecules

Query  
No structure  
Create Alert

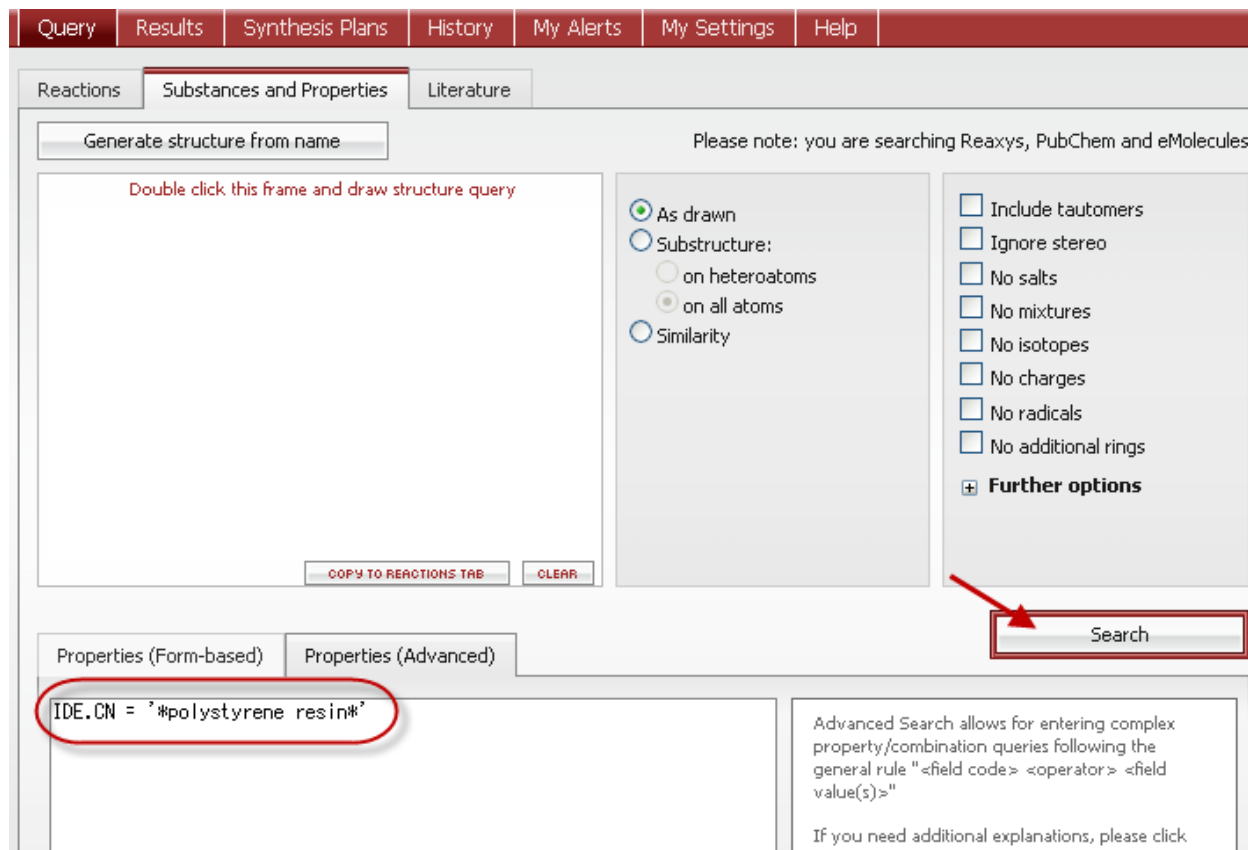
168 substances  
CuH<sub>2</sub>O<sub>2</sub>

38199 substances out of 10807 citations

また上記 4 の段階でより特異的に検索することができます。

例 polystyrene resin が Chemical Name に含まれる化合物の検索

上記 4 での Search for テキストフィールドに polystyrene resin をタイプ入力した後、Transfer ボタンをクリックし、下図赤枠のように表記されたら Search ボタンをクリックして検索を開始します。



Query Results Synthesis Plans History My Alerts My Settings Help

Reactions Substances and Properties Literature

Generate structure from name

Please note: you are searching Reaxys, PubChem and eMolecules

Double click this frame and draw structure query

As drawn  
 Substructure:  
 on heteroatoms  
 on all atoms  
 Similarity

Include tautomers  
 Ignore stereo  
 No salts  
 No mixtures  
 No isotopes  
 No charges  
 No radicals  
 No additional rings  
 Further options

COPY TO REACTIONS TAB CLEAR

Properties (Form-based) Properties (Advanced)

IDE.CN = '\*polystyrene resin\*'

Search

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

If you need additional explanations, please click

Results ページに下図のように Chemical Name が青色で表記されている場合は、その中に検索ワードである polystyrene resin が含まれております。


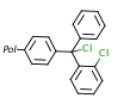

黒文字で表記されている場合は、下図赤枠のように Show Details をクリックしますと Chemical Names and Synonyms の欄に青文字で表記される化合物名を確認できます。

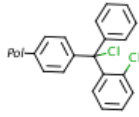
361 substances out of 656 citations

Substances (Grid) Substances (Table) Citations

go to Page  Page 1 of 41

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by No of References

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	N° of ref.
 Pol-NH <sub>2</sub> Synthesize   Show Details	<b>Chemical Name:</b> NovaPEG Rink amide resin <b>Reaxys Registry Number:</b> 11410842 <b>Molecular Formula:</b> H <sub>2</sub> NPol <b>Linear Structure Formula:</b> H <sub>2</sub> NPol	2 prep out of 351 reactions.	Identification	187
 Synthesize   Show Details	<b>Chemical Name:</b> 2-chlorotrityl chloride resin <b>Reaxys Registry Number:</b> 14200391 <b>Molecular Formula:</b> C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> Pol <b>Linear Structure Formula:</b> C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> Pol	1 prep out of 114 reactions.	Identification	87
 Pol-OH Synthesize   Show Details	<b>Chemical Name:</b> 4-(hydroxymethyl)phenoxyethyl polystyrene resin crosslinked with 1percent divinylbenzene <b>Reaxys Registry Number:</b> 14252365 <b>Molecular Formula:</b> HOPol <b>Linear Structure Formula:</b> HOPol	1 prep out of 120 reactions.	Identification	80

 Synthesize   Hide Details	<b>Chemical Name:</b> 2-chlorotrityl chloride resin <b>Reaxys Registry Number:</b> 14200391 <b>Molecular Formula:</b> C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> Pol <b>Linear Structure Formula:</b> C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> Pol	1 prep out of 114 reactions.
<b>Chemical Names and Synonyms</b> 2-chlorotrityl chloride resin, 2-chlorotritylchloride resin, 2-chlorotrityl resin, 2-chlorotrityl chloride polystyrene resin, 2-chlorotrityl chloride.(R). resin, chlorotrityl chloride resin, Barlos resin		
<b>Identification</b>		