REAXYS®

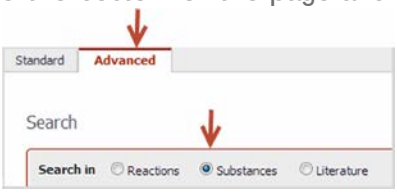
HOW YOU THINK HOW YOU WORK

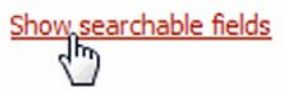
I'd like to explore the relationship between the density and refractive index of inorganic substances.

You can mine Reaxys and export the results to Excel to uncover correlations between certain properties.

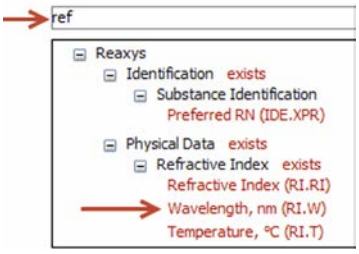
Set up the query so that only the relevant fields will be displayed under the "Hit Data" link in the results. Since density is temperature-dependent, and the refractive index is related to temperature and wavelength, it is critical to set up the query with these relationships in mind.

1. Begin by selecting the **Advanced** tab. Click the **Substances** radio button. Scroll to the bottom of the page and click the **Show searchable fields** link.

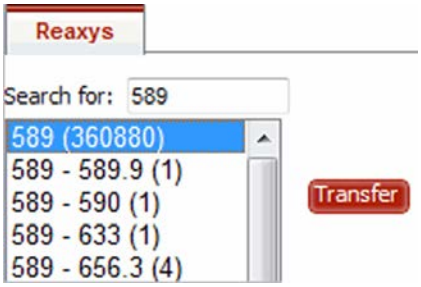




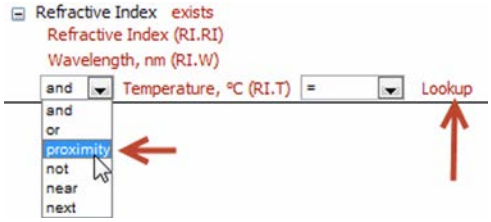
2. Find the **refractive index** fields by typing *ref* into the search box. Select the **Wavelength** field.

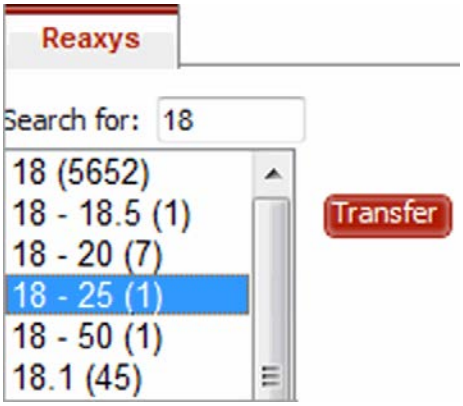


3. Click the **Lookup** link to open the index for the wavelength field. Type *589* into the box, select **589** from the list, and then click the **Transfer** button.

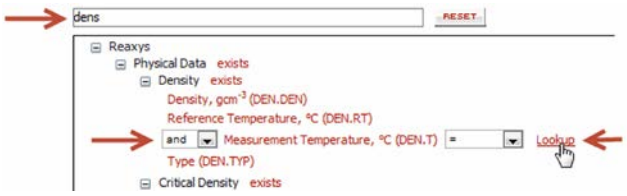


4. Now click the **Temperature** link. Select **Proximity** from the dropdown menu, click the **Lookup** link, type *18* into the box and select **18 – 25** from the list. Click **Transfer**.





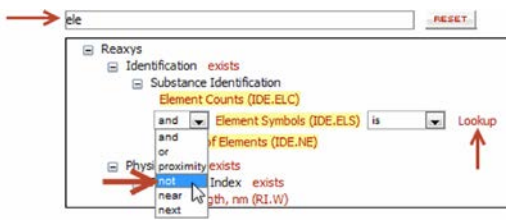
5. Density is next. Begin typing *dens* into the box, select **AND** from the dropdown menu, click the **Lookup** link, type *18* into the box, select **18 – 25** from the list, and then click **Transfer**.



The query, so far, looks like this:

```
RI.W='589' PROXIMITY RI.T='18 - 25' AND DEN.T='18 - 25'
```

6. Since you are only looking for inorganics, you can exclude carbon-containing substances. Look for the **Element Symbols** field by typing *ele* into the box. Select **Not** from the drop down menu, click **Lookup**, type *c* into the box, select **C** from the list, and click **Transfer**.



The final query looks like this:

```
RI.W='589' PROXIMITY RI.T='18 - 25' AND DEN.T='18 - 25' NOT IDE.ELS='c'
```

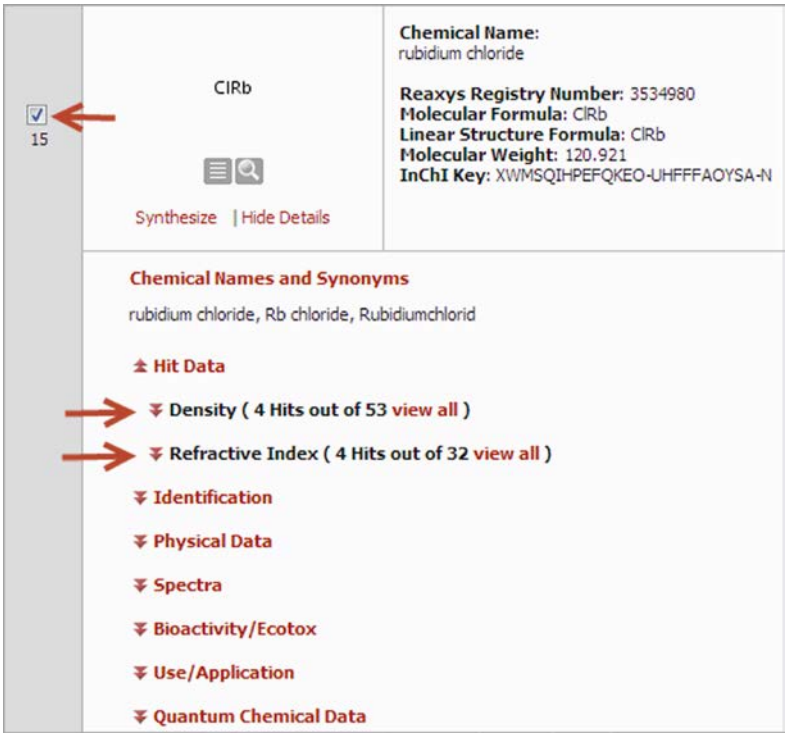
Click **Search**.

Hint: If you'd like to, you can just copy/paste this into the query box:

RI.W='589' PROXIMITY RI.T='18 - 25' AND DEN.T='18 - 25' NOT IDE.ELS='c'

Results:

About 193 substances are retrieved. The hit data fields are separated from the rest. You can select the desired hits by clicking the check boxes near each structure and then clicking the **Limit to** button.

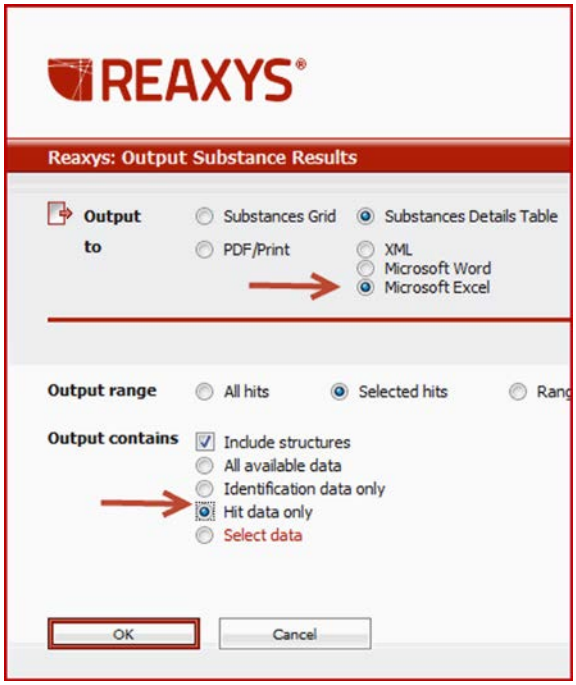


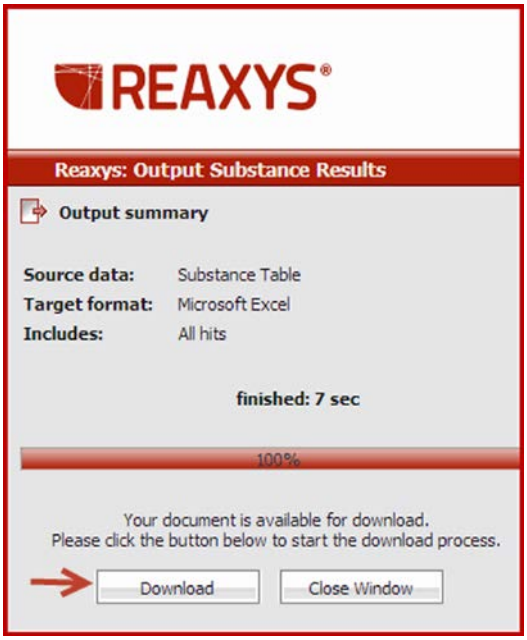
REAXYS®

HOW YOU THINK HOW YOU WORK

Export selections to Excel

Click the **Output** button and make the appropriate selections in the output box. Click **OK**. Click **Download**.





REAXYS®

HOW YOU THINK HOW YOU WORK

You can easily view the data for each substance:

R	S	T	U	V
Refractive Index	**Wavelength [nm]**	**Temperature [°C]**	**References**	**Density: Density [gcm-3]**
1.4186	589	20	Article; Chernyshev, E. A.; Krasnova, T.	1.4798
1.4245	589	20	Article; Baturina, L. S.; Gol'din, G. S.; Fedorov, S.	1.608
1.4295	589	20	Article; Baturina, L. S.; Gol'din, G. S.; Fedorov, S.	1.609
1.45648	589	20	Article; Blanc, M. Le; Z. phys. Ch.; vol. 10; (1892); p.	1.8813 - 1.8827
1.4566	589	7 - 21	Article; Soret, Ch.; Arch. Sci. Phys. Nat.; vol.	1.88 - 1.888
1.7233	589	20	Article; Baroni, A.; Atti della Accademia	2.1593
3.5 - 6.4	380 - 780	25 - 400	Article; Shokr, E. Kh.; Wakkad, M. M.; Journal of Materials	7.93

Do you have an idea for a workflow example?

Please contact me:

Christine Flemming

c.flemming@elsevier.com

Sept. 16, 2013