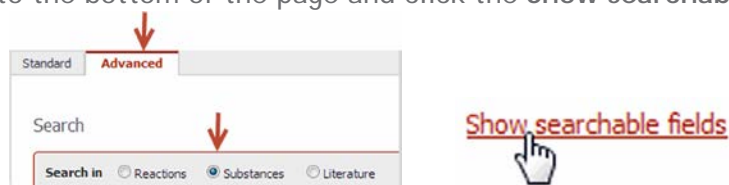


I'd like to explore the relationship between the density and refractive index of inorganic substances.

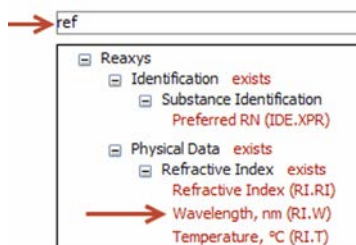
You can mine Reaxys and export the results to Excel to uncover correlations between certain properties.

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.

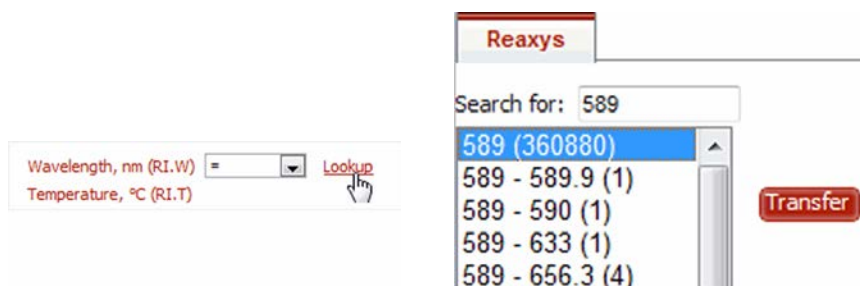
1. Begin by selecting the **Advanced** tab. Click the **Substances** radio button. Scroll to the bottom of the page and click the **Show searchable fields** link.



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.



- 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**.

The screenshot shows the Reaxys search interface. The main query is: **Refractive Index exists** **Refractive Index (RI.RI)** **Wavelength, nm (RI.W)** **and** **Temperature, °C (RI.T) =** **Lookup**. The dropdown menu for the equals sign is open, showing options: **and**, **or**, **proximity** (highlighted), **not**, **near**, **next**. A search box for '18' is open, showing results: **18 (5652)**, **18 - 18.5 (1)**, **18 - 20 (7)**, **18 - 25 (1)** (highlighted), **18 - 50 (1)**, **18.1 (45)**. A **Transfer** button is visible to the right.

- 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 screenshot shows the Reaxys search interface. The main query is: **Physical Data exists** **Density exists** **Density, gcm⁻³ (DEN.DEN)** **Reference Temperature, °C (DEN.RT)** **and** **Measurement Temperature, °C (DEN.T) =** **Lookup**. The dropdown menu for the equals sign is open, showing options: **and** (highlighted), **or**, **proximity**, **not**, **near**, **next**. A search box for '18' is open, showing results: **18 (5652)**, **18 - 18.5 (1)**, **18 - 20 (7)**, **18 - 25 (1)** (highlighted), **18 - 50 (1)**, **18.1 (45)**. A **Transfer** button is visible to the right.

The query, so far, looks like this:

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

- 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 screenshot shows the Reaxys search interface. The main query is: **Identification exists** **Substance Identification** **Element Counts (IDE.ELC)** **and** **Element Symbols (IDE.ELS) is** **and** **Refractive Index exists** **Refractive Index (RI.RI)** **Wavelength, nm (RI.W)** **and** **Measurement Temperature, °C (DEN.T) =** **Lookup**. The dropdown menu for the 'is' operator is open, showing options: **and**, **or**, **proximity**, **not** (highlighted), **near**, **next**. A search box for 'c' is open, showing results: **C (1)**. A **Transfer** button is visible to the right.

The final query looks like this:

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

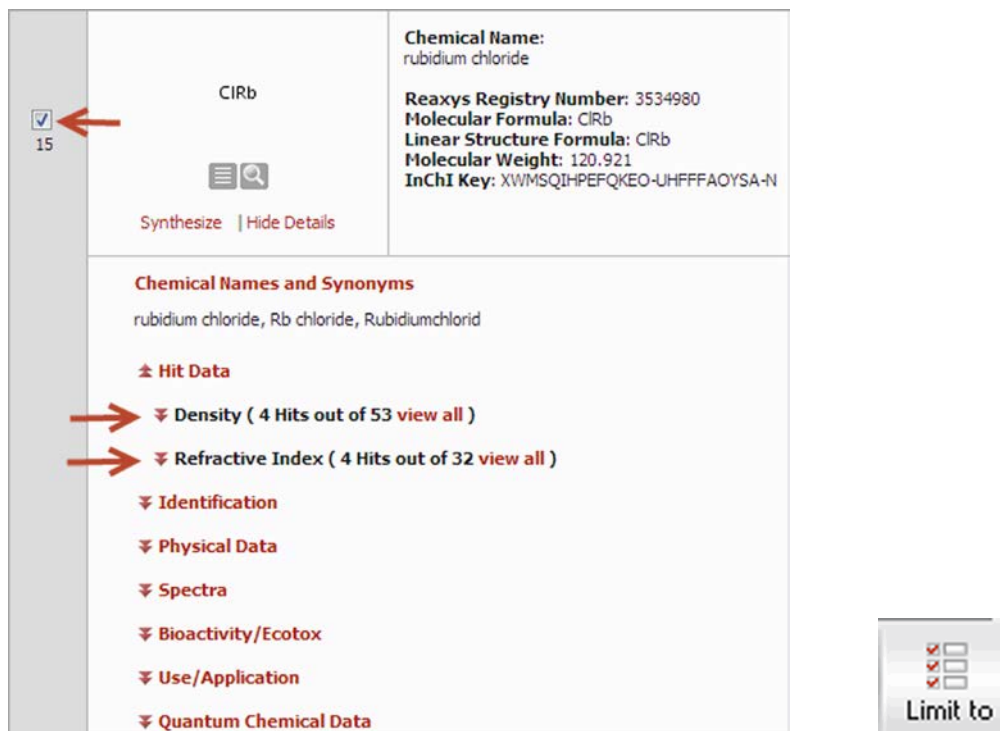
Click Search.

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.



15

ClRb

Synthesize | Hide Details

Chemical Name:
rubidium chloride

Reaxys Registry Number: 3534980
Molecular Formula: ClRb
Linear Structure Formula: ClRb
Molecular Weight: 120.921
InChI Key: XWMSQIHPEFQKEO-UHFFFAOYSA-N

Chemical Names and Synonyms
rubidium chloride, Rb chloride, Rubidiumchlorid

Hit Data

↕ Density (4 Hits out of 53 view all)

↕ Refractive Index (4 Hits out of 32 view all)

↕ Identification

↕ Physical Data

↕ Spectra

↕ Bioactivity/Ecotox

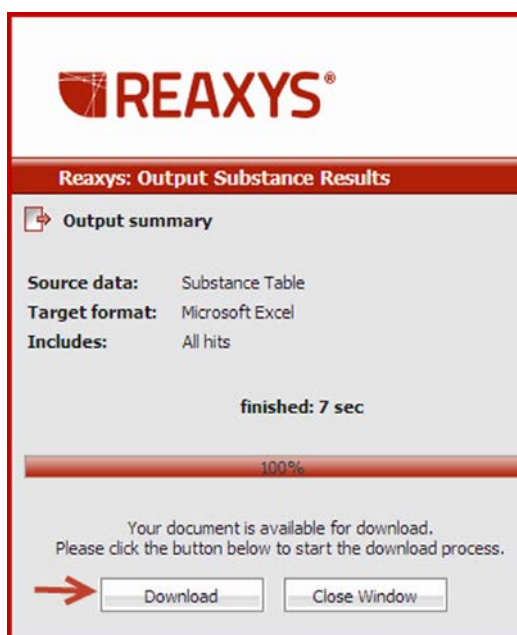
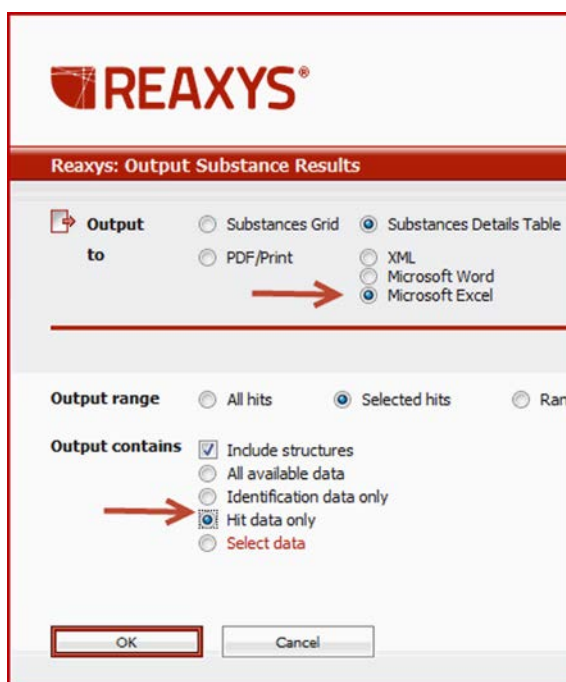
↕ Use/Application

↕ Quantum Chemical Data

Limit to

Export selections to Excel

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



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. 448-449.	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:

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