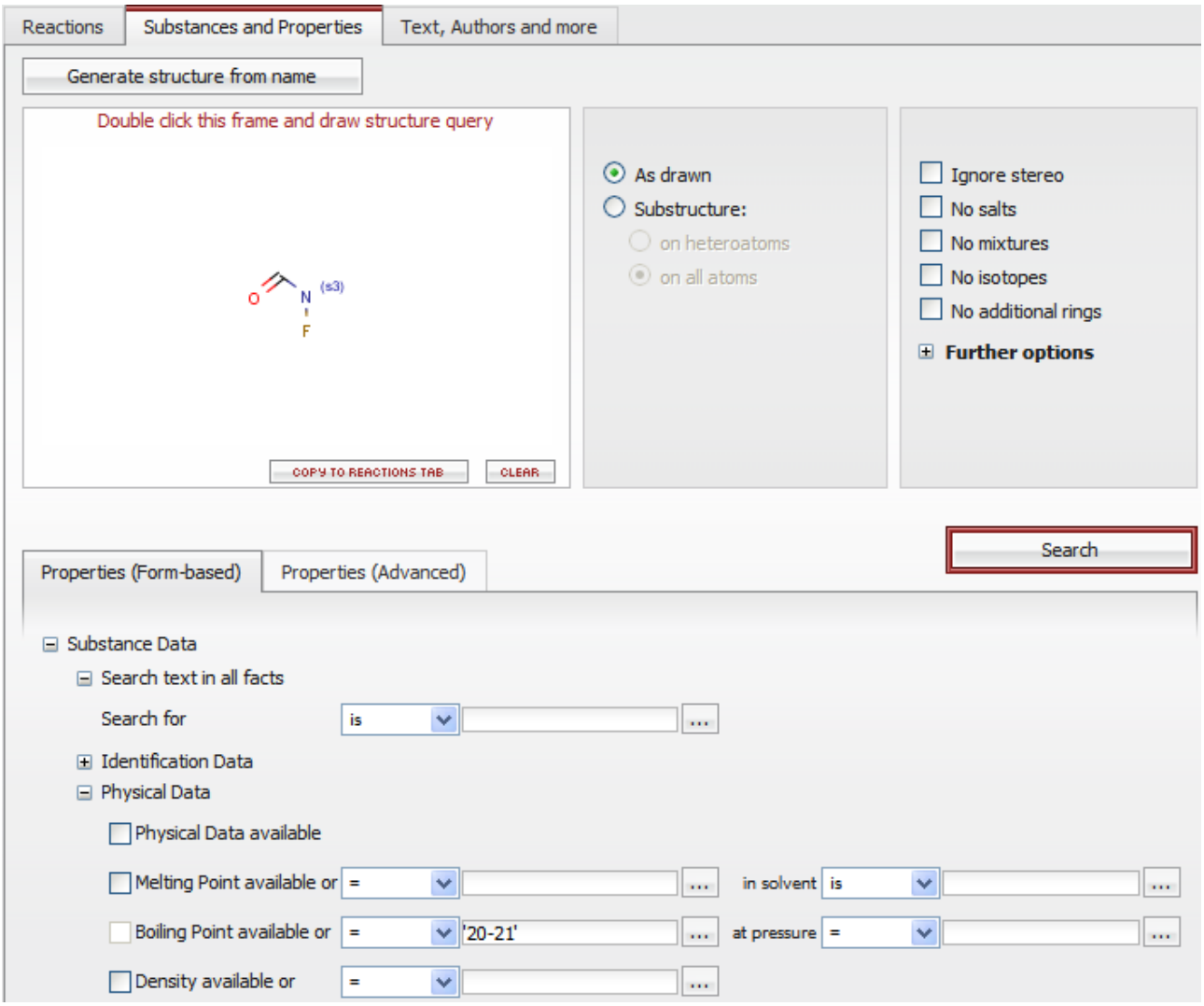
Reaxys Proximity Operator

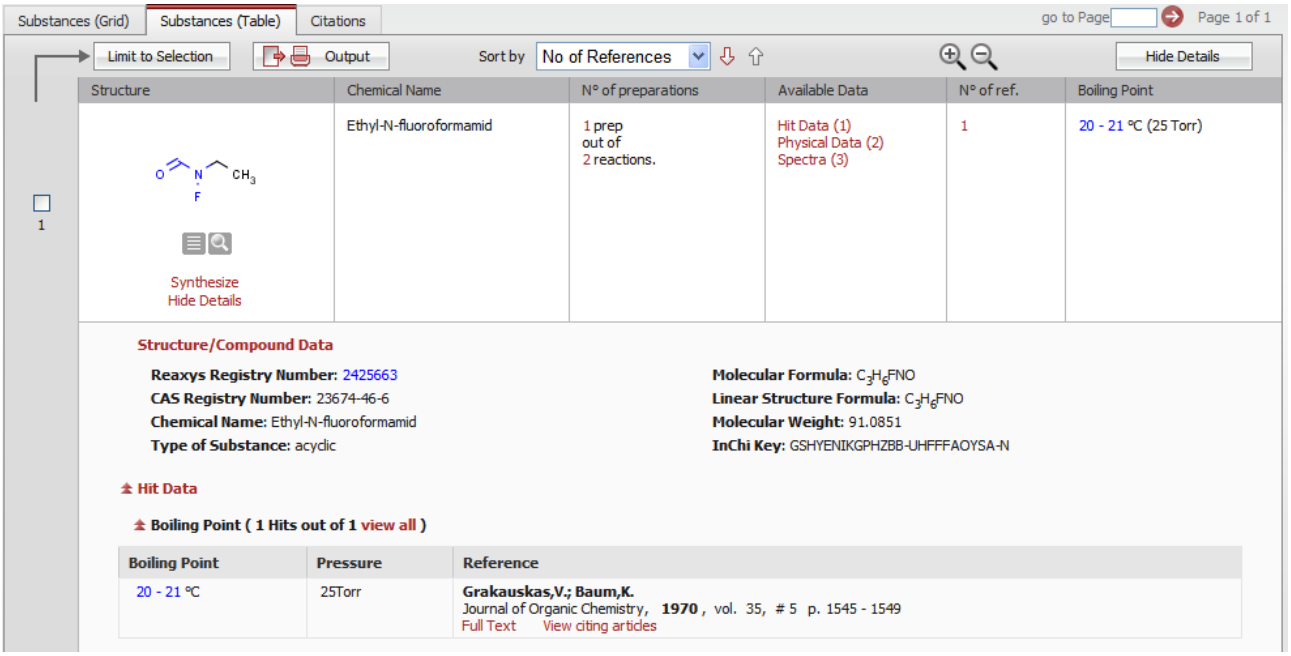
The January 2010 release saw the addition of the PROXIMITY operator - learn here how to best use this option.

Imagine that you need to rapidly find out which N-substituted-fluoroformamide has a boiling point of 20-21°C under a pressure of 25mmHg (25 Torr). How can you do this rapidly? The PROXIMITY operator gives you the solution - you can use this advanced search operator when you need to find correlated properties:

In the Properties (Form-based) tab:
Expand the substance data properties by clicking the '+' sign and then expand the *Physical Data* section. Here enter the required boiling point range value needed and the correlated pressure data. Click on Search to display the found substance.



The core substructure and the required information are highlighted; a click on the black part of the Boiling Point (1 Hit out of 1 view all) hyperlink will display the information and its citation.

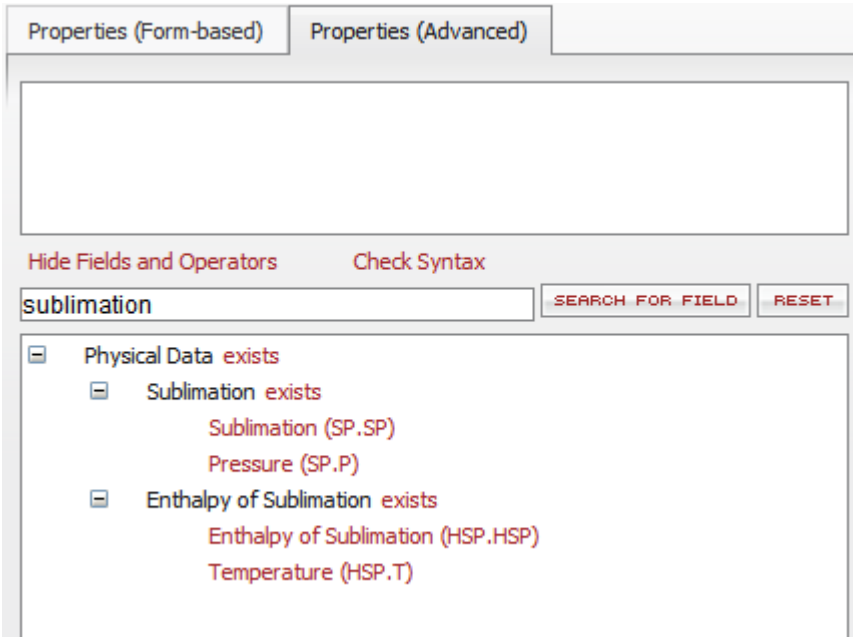


Imagine that you now need to purify by sublimation some 2,3-disubstituted-1,4-diazanaphtalene under reduced pressure and you'd like to work at a max temperature of 130°C and under a reduced pressure between 1 and 2 mmHg.

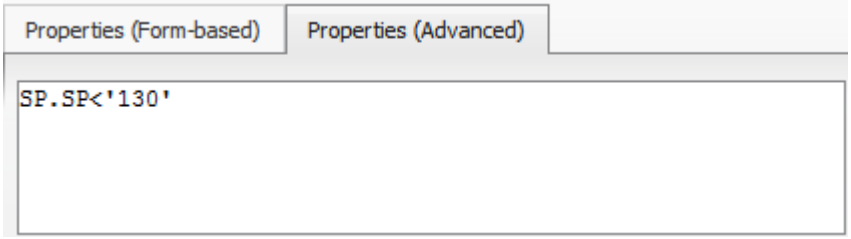
First draw the required scaffold and then check "no additional rings" to avoid any phenazine or other cyclic annelated derivatives that you don't want. To add the sublimation constraint, jump to the Properties (Advanced) tab.

In the Properties (Advanced) tab:

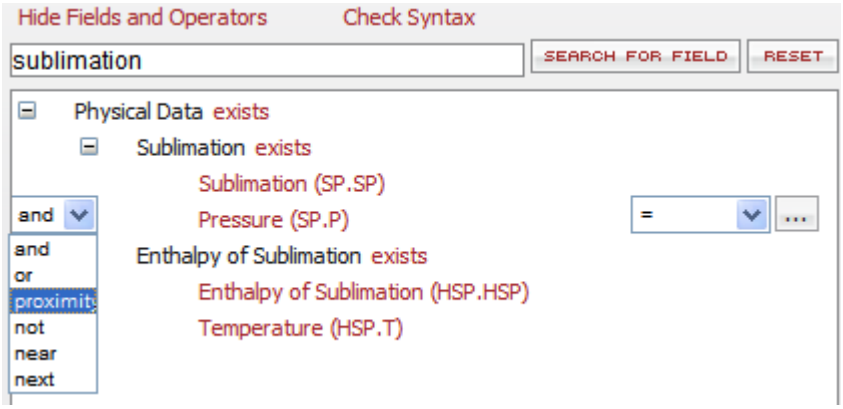
You first need to located the required field; click on Show Fields and Operators hyperlink and simply type sublimation in the *Search For Field* box and click on the corresponding button to locate the fields. These fields are then immediately displayed:



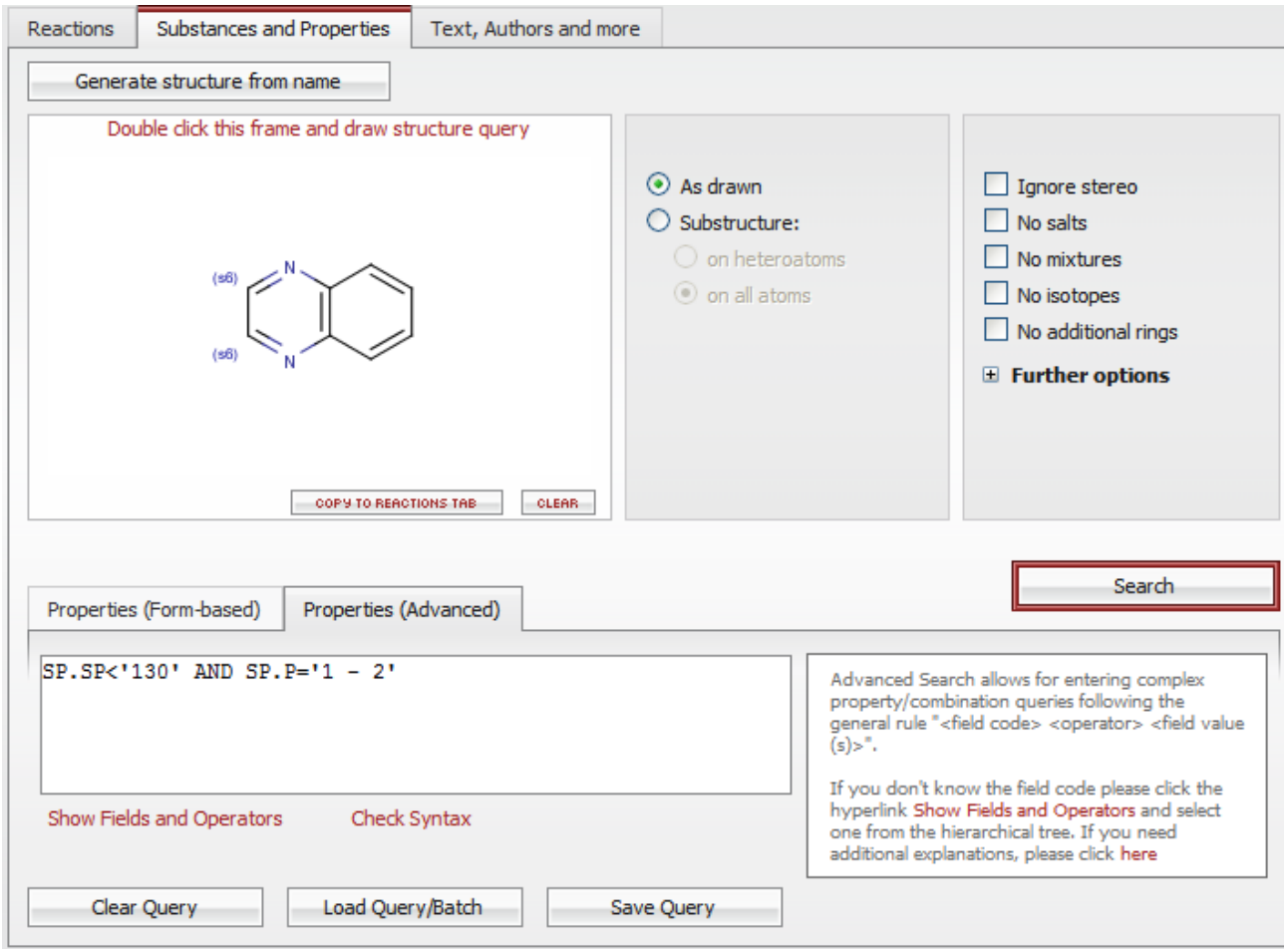
Click the Sublimation (SP.SP) field, chose '<' as an operator and add the needed value (130). The query is automatically written with the right Syntax in the upper box.



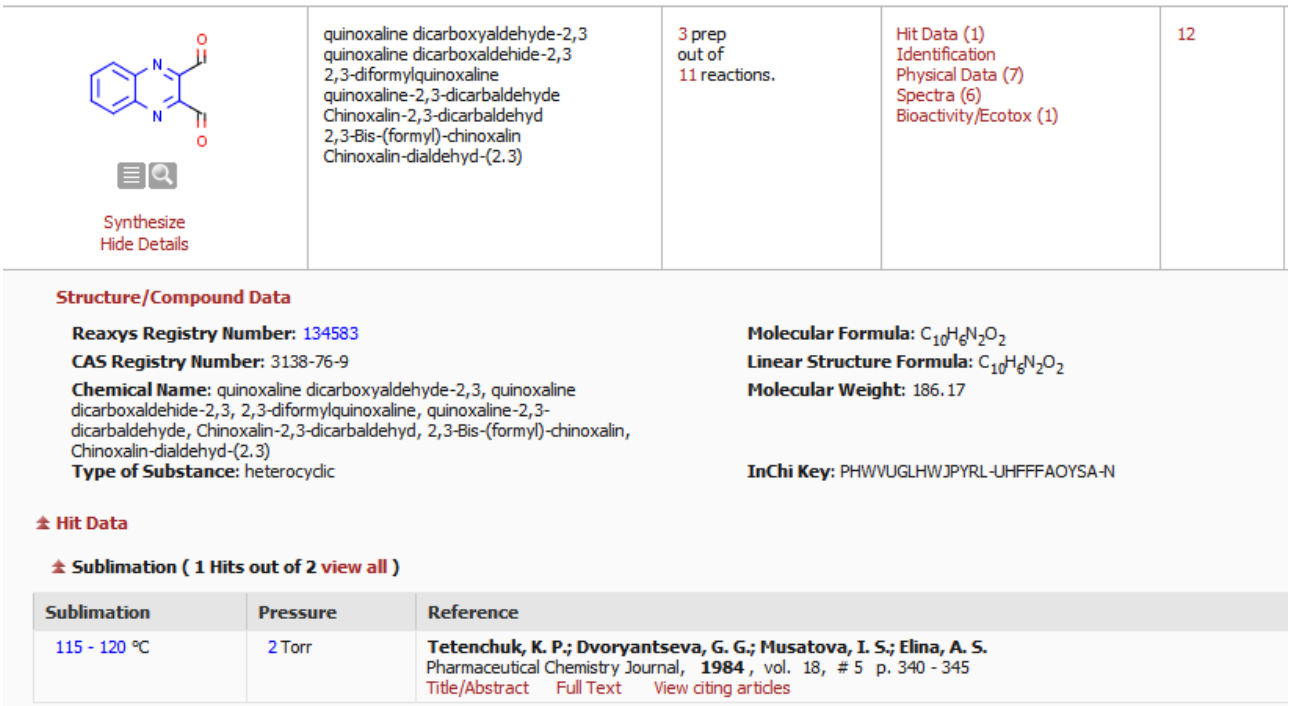
You can now add the correlated constraint - the fact the the sublimation temperature must be linked to a pressure between 1 and 2 Torr. Click the Pressure (SP.P) field and a menu with the possible operators is then displayed. Choose proximity.



Select '=' as the operator and enter the needed range. The query appears as below:



Click on Search to display the found results: two substituted quinoxalines are found. For example, the sublimation details for the second hit are as shown below:



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