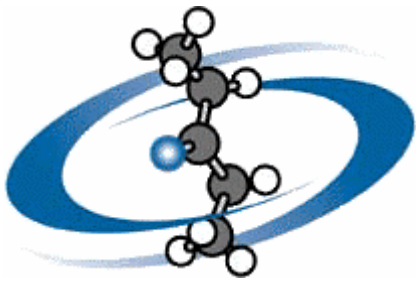

ACD/Column Selector

For ChemSketch

User's Guide

Version 9, Build: 01 May 2006

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1. ACD/Column Selector User Guide

1.1 Introduction

ACD/Column Selector helps chromatographers select the best column to use, when their particular chromatographic column is unavailable and they are faced with the dilemma of selecting the column that most closely matches the one they used previously. Since each parameter can be targeted individually, chromatographers can also search for columns that have high coefficients for a certain term, allowing them to change their columns to target a given structural aspect.

1.2 What's New

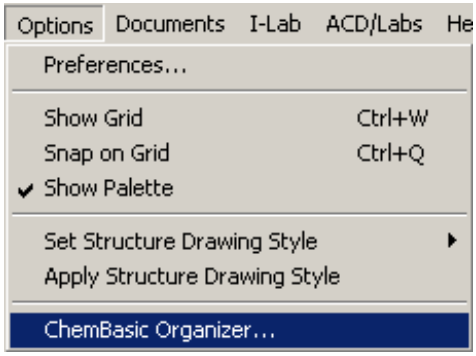
The number of columns has been increased to 187 from 153 in the previous version.

1.3 Installation

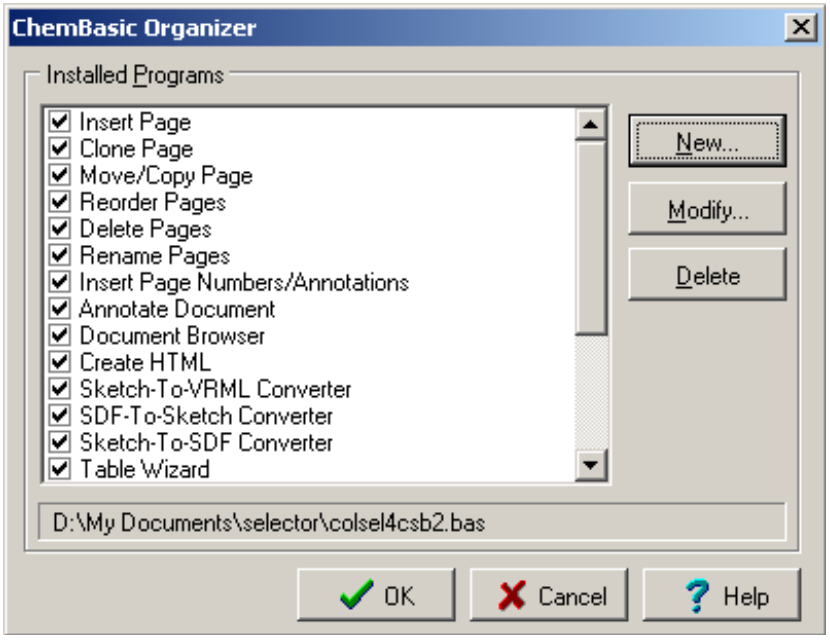
ACD/Column Selector is an ACD/ChemBasic application that runs within ACD/ChemSketch 5.0 or later. If you are using ChemSketch Freeware, you will need to download and install the ChemBasic add-on prior to installing Column Selector. Commercial versions of ChemSketch already include the ChemBasic program. Download ChemBasic from: http://www.acdlabs.com/download/chembas.html

Follow these instructions to install ACD/Column Selector.

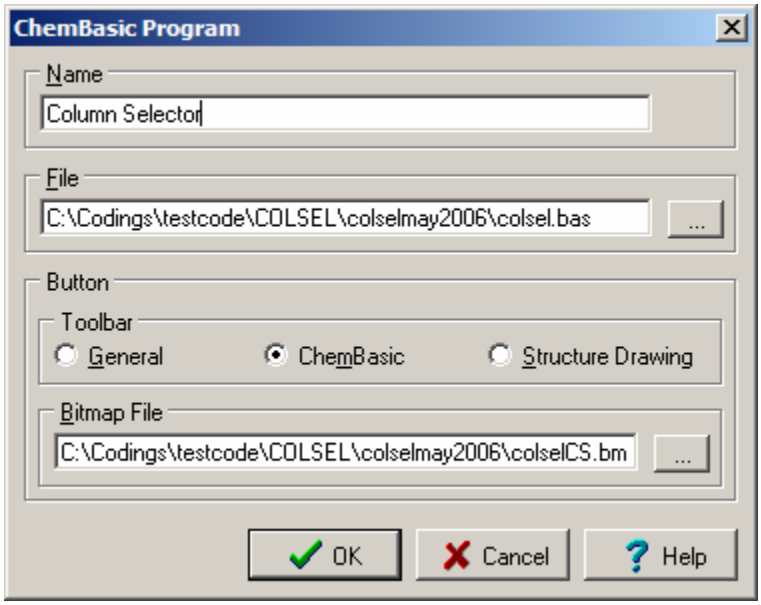
1. Make sure all the files for the Column Selector program are placed in the same directory.
2. In ChemSketch, from the **Options** menu, choose **ChemBasic Organizer**.



3. In the **ChemBasic Organizer** dialog box, click **New**.



4. In the **Name** box, type a name for the new icon, such as "Column Selector". This text will show up when the mouse pointer passes over the icon that is placed in the ChemBasic Toolbar in ChemSketch.



5. In the **File** box, enter the path where the "colsel.bas" file is located. Use the navigation button to locate this file in the directory it was placed in from step 1.
6. Under **Button**, click ChemBasic.
7. In the **Bitmap File** box, enter the path where the "colselCS.bmp" file is located. This will be the same directory as the "colsel.bas" file.
8. Click **OK**.
9. Scroll down the list of installed programs to the bottom and make sure the "Column Selector" (or whatever name you used in step 4) is checked.

10. Click **OK**.

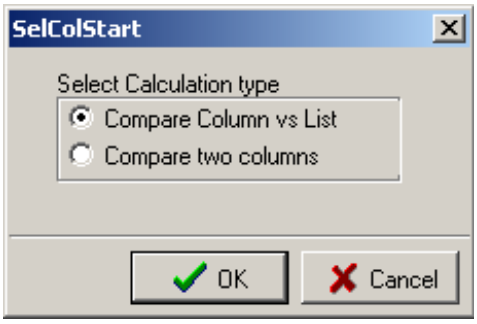
11. The new button should be visible on the ChemBasic toolbar. It will be the last one on the right side.

1.4 Getting Started

From the ChemSketch Window, click **Column Selector** to start the program.

In the **SelColStart** dialog box, you can choose from the following two features:

- **Compare Column vs. List**
- **Compare two columns**

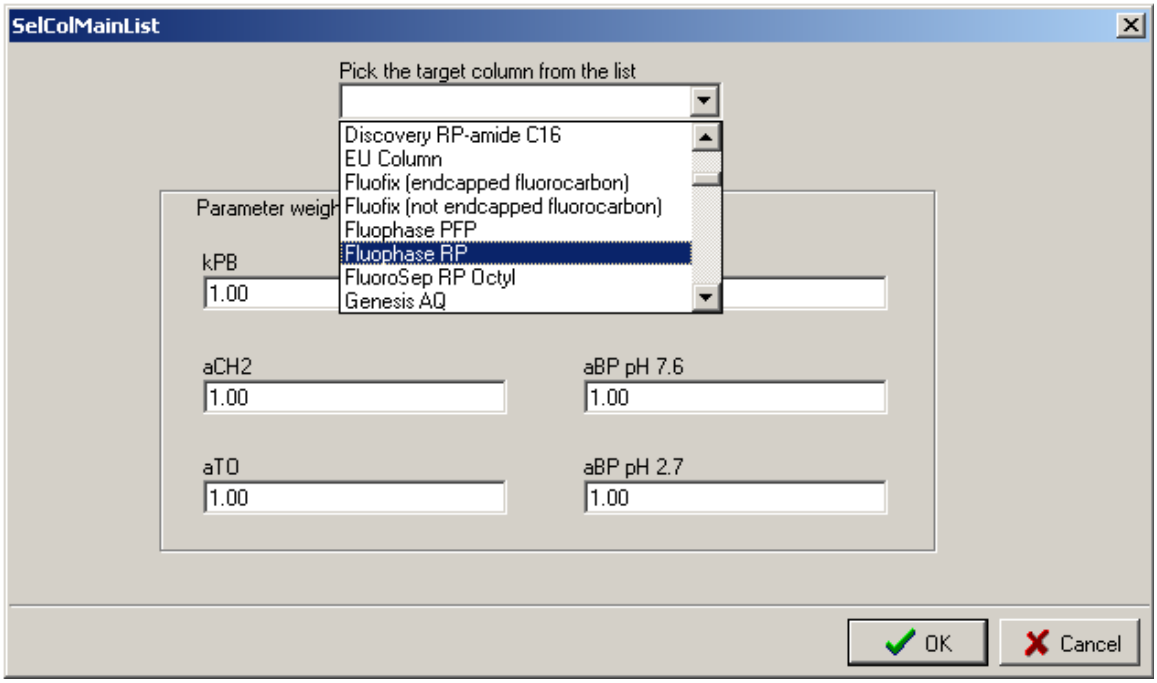


1.4.1 Compare Column Versus List

The most common application of Column Selector will be to find a match for a given column. There are 187 characterized columns in Column Selector. Each of these can be matched to any of the other columns.

This calculation mode works with only the 187 columns contained within the database.

1. Choose **Compare Column vs List**.
2. The parameters weighting screen appears. More information about this screen can be found in section 1.4.2.

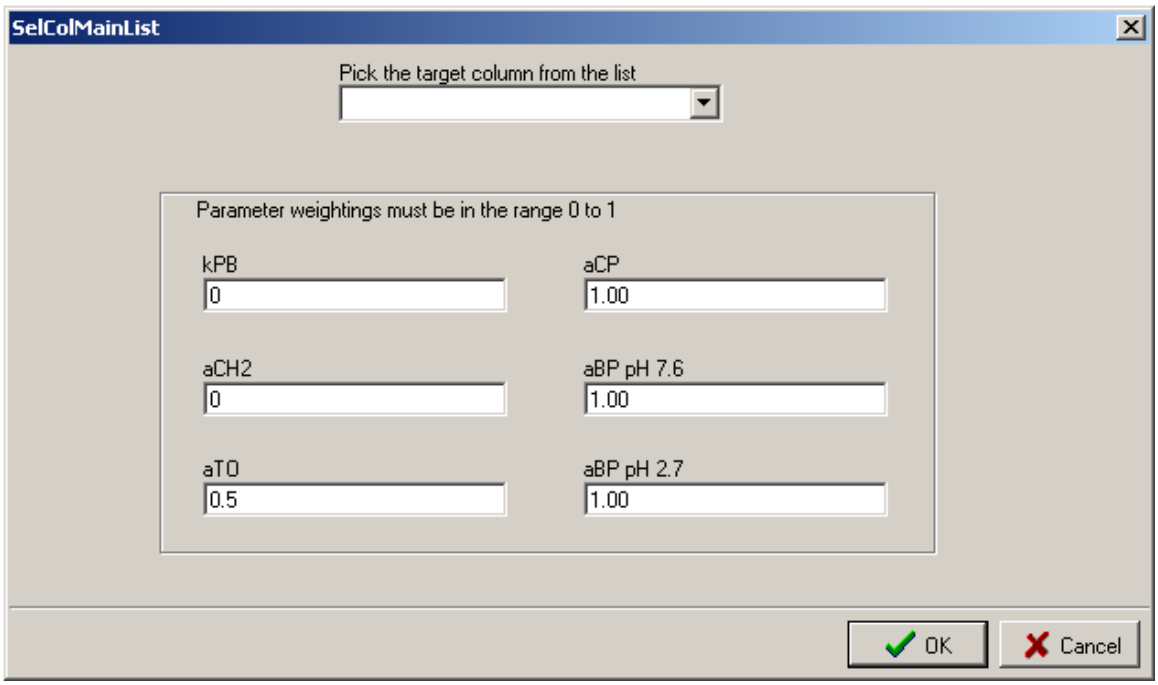


3. In the **Pick the target column from the list** box, type the name of or select a column to begin the calculation.
4. A list ranking the columns according to "column difference factor" (CDF) that most closely matches your selected column is generated. The column with the lowest CDF is the one that best matches your chromatographic column. Every column is shown, so you can not only locate the most similar columns, but you can also find the most *dissimilar*.

1.4.2 Adjust Parameter Weighting

Each of the six parameters is given the same weighting by default in the column search. However, for your situation, certain terms will not be as important. For example, for uncharged analytes, the ion-exchange capacity (silanol activity) will be of no interest. You can lower the coefficient for this search term accordingly.

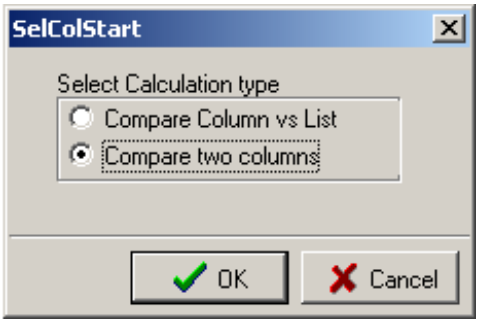
1. To adjust the weightings of the six parameters before performing a calculation, simply enter a parameter weighting between 0 and 1. A weighting of 0 will ensure that this parameter is not used.
2. To reset all parameter weightings to 1.0, simply close the application and restart it.



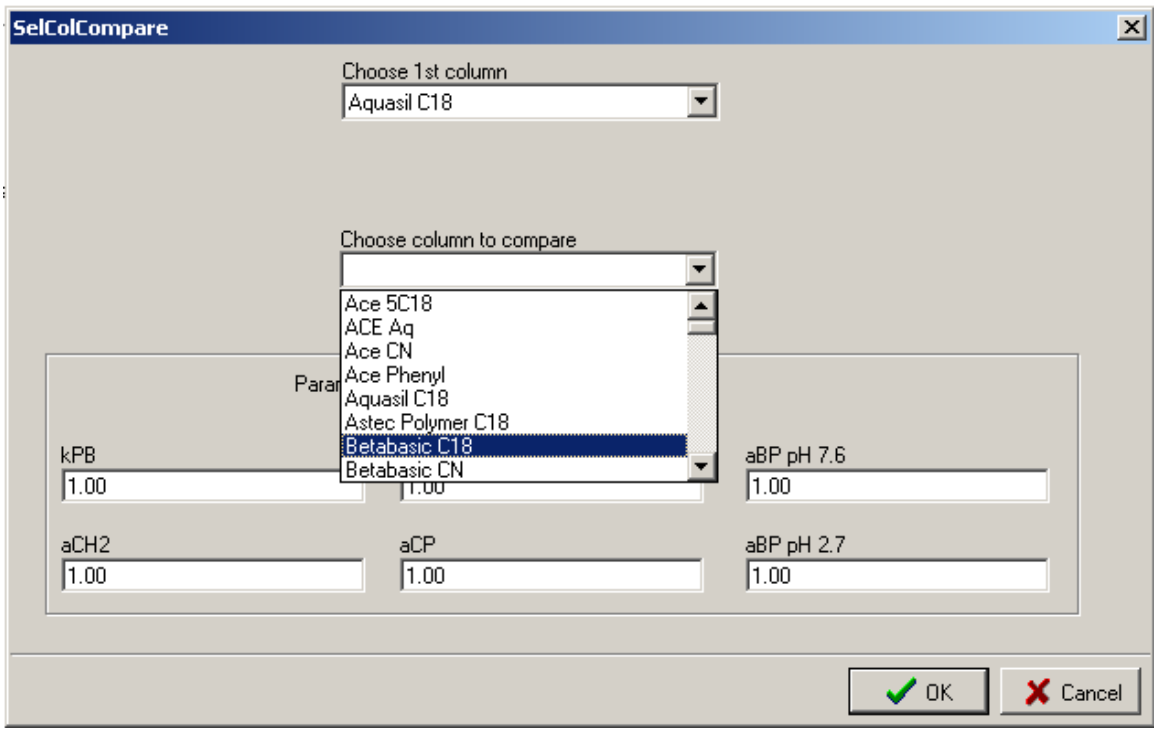
1.4.3 Comparing Two Columns

If you wish to evaluate the similarities of a specific pair of columns, you can do this individual calculation, and also include a table of the parameters of each. This can offer insights into chemical structures and retention time differences.

In order to compare two columns, select the appropriate box in Column Selector.



Next select the two columns to compare, and change the parameters as desired.



Column Selector will output a column difference factor, and a table comparing each of the terms. Select “copy to ChemSketch” if you want to create a printed report.

2. Appendix

2.1 Chromatographic Column Parameters

The six chromatographic column parameters are determined experimentally.

2.1.1 Retention factor for pentylbenzene, kPB

A measurement of the surface area and surface coverage (ligand density).

Chromatographic Conditions: MeOH-H_2O (8:2, v/v), 1.0mL/min, 40°C, 5µL injection of pentylbenzene (0.6µg/mL). Injections and flowrates have been scaled for 4.6 mm i.d. columns. The first disturbance of the base-line when injecting methanol has been used as a dead time marker.

2.1.2 Hydrophobicity or hydrophobic selectivity, aCH2

The retention factor ratio between pentylbenzene and butylbenzene, aCH2 = kPB/kBB, is a measure of the surface coverage of the stationary phase as the selectivity between alkylbenzenes differentiated by a single methyl group depends on ligand density.

Chromatographic Conditions: All conditions as for kPB determinations, except individual injections of pentylbenzene (0.6µg/mL) and butylbenzene (0.3µg/mL) are performed.

2.1.3 Shape selectivity, aT/O

The retention factor ratio between triphenylene and *o*-terphenyl, aT/O = kT/kO, is a measure of the shape selectivity, which depends on ligand spacing and the shape/functionality of the silylating reagent.

Chromatographic Conditions: All conditions as for aCH2 determinations, except 5µL injection of o-terphenyl and triphenylene both at 0.05mg/mL.

2.1.4 Hydrogen bonding capacity, aC/P

The retention factor ratio between caffeine and phenol, aC/P = kC/kP, is a measure of the number of available silanol groups and the degree of endcapping.

Chromatographic Conditions: MeOH-H_2O (3:7, v/v), 1.0ml/min, 40°C, individual 5µL of phenol (1mg/mL) and caffeine (0.5mg/mL).

2.1.5 Total ion-exchange capacity, aB/P pH 7.6

The retention factor ratio between benzylamine and phenol, aB/P pH 7.6 = kB/kP, is a measure of the total silanol activity.

Chromatographic Conditions: 20mM KH_2PO_4, pH 7.6, in MeOH-H_2O (3:7, v/v), 1.0mL/min, 40°C, individual 5µL injections of phenol and benzylamine HCl both at 0.5mg/mL.

2.1.6 Acidic ion-exchange capacity, aB/P pH 2.7

The retention factor ratio between benzylamine and phenol, aB/P pH 2.7 = kB/kP, is a measure of the acidic activity of the silanol groups.

Chromatographic Conditions: All conditions as for total ion-exchanged determinations above, except using a pH 2.7 KH_2PO_4 buffer.

2.2 Calculation Methods

The Chromatographic Column Selector program contains the above six parameters for 135 chromatographic columns. The mean (μ) and standard deviation (SD) for these six parameters are calculated using all of the 135 columns. For each column, a normalized value (xn_1 to xn_6) is calculated for each of the six parameters, $xn_x = (x_x - \mu_x)/SD$, where x_x is the value raw value for the parameter. The Euclidean distance is then used to calculate the column difference factor (CDF) between the target column and the rest of the columns.

$$CDF = \sqrt{[(xn_{t1}-xn_1)^2 + (xn_{t2}-xn_2)^2 + (xn_{t3}-xn_3)^2 + (xn_{t4}-xn_4)^2 + (xn_{t5}-xn_5)^2 + (xn_{t6}-xn_6)^2]}$$

where xn_{t1} to xn_{t6} are the normalized values of the six chromatographic parameters for the target column. The CDF values are ranked in ascending order, with the lowest CDF indicating the best column match.

2.3 References

1. Euerby, MR; Petersson, P. “Chromatographic classification and comparison of commercially available reversed-phase liquid chromatographic columns using principal component analysis.” *J. Chromatogr. A* **2003**; *994*: 13-36.