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Galaxie [™] Column and Solvent Database Plug-in

User's Guide

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Using the Column and Solvent Database Plug-in

This document describes the functions of the Column and Solvent Database Plug-in for Galaxie.

Overview

The Column and Solvent Database Plug-in enables users to manage columns and solvents that are used in chromatographic systems. The columns and solvents and their properties are defined in a database that is available from Galaxie Chromatography Data Systems. The Column and Solvent database is used for all chromatography types.

The Column and Solvent Database Plug-in permits users to increment automatically column parameters at each system injection. The Generic Column Tracker driver must be added to the Galaxie chromatographic system and a column from the list must be chosen in the method.

It can also manage solvent miscibility for Column Valve Modules.

A common audit trail lists all modifications in columns and solvents properties. The audit trail, the column and solvent properties and lists are exportable and printable.

Software functions

Chromatographic Column Management

In Galaxie, open the Chromatographic column management by selecting the corresponding option in the Plug-ins menu. The following screen is displayed:

Chromato	graphic column mana	gement								
File Edition	Audit-trail									
	🛛 🛛 🖓 🚰									
Short name :	Column name	Chromatography type	Serial number	Injection number	Solvent	Length	ID	OD	Phase type	~
▶ 61	CP-Sil 5CB	GC	XXXXXX	0		15 m	0,32 mm	0 mm	bounded 100% dimethylp	<u> </u>
HPLC 1	Microsorb BDS	LC		0		250 mm	0 mm	0 mm	C18-like reverse phase c	
LC 2	Pursuit C18	LC		0		30 cm	2 mm	0 mm	High bonded purity silica	
nb1	CP-Sil 88	GC	XXXX	0		100 m	0,25 mm	0 mm	non-bonded (88% cyapro	
packed 1	stainless steel	Packed	XXX	0		10 m	0 mm	315 mm		
PREP1	Omnispher C18	PREP	XXX	0		50 mm	10 mm	0 mm	reversed	
										×
Column de	escription									
hydrocarbons, h	ydrocarbons, ketones, organ	ic acids, oxygenates, PAHs,	pesticides, poly	mers, steriods, solve	nts, sulfur	compound	\$			

It contains the list of all defined columns of the database. When selecting a column line, the *Column description* is displayed at the bottom of the screen.

Adding a New Column and Modifying Column Parameters

Define a new column in the column database by pressing the button, selecting *EDITION / NEW* menu or in the contextual

menu. Modify the properties of a selected column by pressing, double-clicking, selecting **EDITION / EDIT** or in the contextual menu. Enter or modify the column parameters in the displayed column properties screen:

🖍 Column propertie	95	
Column properties		Chemical parameters
Column name	liquide column 2	Phase type Reverse phase Carbonyl C8
Short name	PAH1	Unit
Column description	column for HPLC application : PAH	Phase thickness 1,25 um
		Particle size 124 um
Pre column name	no pre column	Pore size 10 A
Pre column description		Storage solvent ACN
Manufacturer	varian	
Serial number	22222	Physical parameters Min May Unit
Chromatography type	LC _ Iypes	pH 4 10
Injection number	153	Pressure 400
1	Unit	
		Flow 5 ml/min
Internal diameter	2 um	
Uutside diameter	4,5 mm	
		l
	X Cancel	<u>√ DK</u>

Only the column short name field must be entered, all other fields are optional.

Validate the new settings clicking on _____ or cancel them.

Column Properties Parameter Group

In the Column name field, enter the entire column name.

In the *Short name* field, enter a short name or click on the button to automatically define the 10 first characters of the Column name as *Short name*. The *Short name* is used for the Galaxie column identification and is mandatory.

Fill in the *Column description*, the *Pre column name*, the *Pre column description*, the *Manufacturer* name and the *Serial number* of the column.

Select the Chromatography type in the corresponding scrolling list. By default, GC, LC, PREP, Packed and Not defined are the available types. Press Ivpes... to modify the chromatography types list. The following screen is displayed:

	Chromatography types				
	Name	Technique	Description	^	
•	Not defined	Not defined			
	GC	GC	Gaz chromatography		New
	LC	LC	Liquid chromatography		
	PREP	LC	Preparative chromatography		🧾 <u>E</u> dit
	Packed	GC			
					Delete
					<u> 0</u> K
<			>		

Press New... to add a new type and press Edit ... to modify the selected one. Choose the *Technique* and fill in the new *Description* and *Name* field in the displayed Chromatography type properties edition screen:

Chromatog	raphy type (properties edition)
Name	E
Technique	LC
Description	Liquid chromatography
	Cancel V DK

Validate the new settings clicking on



Fill in the column *Length*, *Internal diameter*, *outside diameter* and *units* in the corresponding fields.

Chemical Parameters Parameter Group

Enter the *Phase type*, the *Film thickness*, the *Granulometry*, the *Pore size* and *units* in the corresponding fields. Choose the *Storage solvent* among the whole Solvent database list.

Note that the *Granulometry*, the *Pore size* and the *Storage solvent* fields are only available when the Chromatography technique is LC.

Physical Parameters Parameter Group

Enter the *pH* minimum and maximum values tolerated by the column in the *Min* and *Max* fields.

Enter the maximum *Pressure* and *Flow* with the units that the column can stand.

It is possible to fill in the pH and Flow fields only when the chromatography technique is LC.

Enter the column minimum and maximum temperatures when used in isothermal or programmed mode.

Managing the Columns List

Delete a selected column of the list by pressing the button, selecting **EDITION / DELETE** menu or from the contextual menu.

To duplicate a column entry in the list, select it and then the *EDITION / DUPLICATE* menu or from the contextual menu. A new column entry is created with exactly the same parameters except the *Column name* and the *Short name*. The column name of the created column entry begins with "copy of " and ends with the name of the duplicated column entry. The *Short name* of the created column entry corresponds to the first 9 characters of the duplicated *Column name* ended by a number suffix.

Print or Export in HTML the columns list by selecting *EDITION / PRINT LIST* or *EDITION / EXPORT LIST*. Choose the path to export and the file is automatically displayed at screen. The

column parameters that are printed and exported are the currently displayed in the table and the *Column description*.

Print or Export in HTML each column parameters by selecting *EDITION / PRINT PROPERTIES* or *EDITION / EXPORT PROPERTIES* or from the contextual menu. Choose the path to export and the file is automatically displayed at screen.

Displaying Columns Parameters

Click on the database that can be modified from different stations at the same time when in Client/Server configuration.

Click on the button or select *Properties* in the contextual menu to change the parameters to display in the column table. The following screen is then displayed:

🖉 Properties		
Column properties		Chromatography type
	 Phase type Phase/Film thickness Storage solvent Particle size Pore Size Temp min/max pH min/max 	 ✓ Chromatography type ✓ Not defined ✓ GC ✓ LC ✓ PREP ✓ Packed ✓ amino acids
Length	∫ Max flow	y <u>S</u> elect all <u>↓</u> Inselect all
	<u>√</u> <u>□</u> K	

To display a parameter in the column list table, check the corresponding box in the *Column properties* part. Choose also to display particular columns in the list depending on their chromatography types by selecting the type in the

Chromatography type part. Press

to select all available chromatography types or to unselect all checked types.

Displaying Column and Solvent Database Audit Trail

Press the ^{SOS} button or select the **AUDIT TRAIL / VIEW AUDIT TRAIL** menu to display the column and solvent database audit trail.

Ø Audit trail					
Date <	Action	Actor	Station name	~	
08/11/2005 17:14:13	Column b1 modified.	Column Tracker	BEAGLE		J OK
08/11/2005 17:13:29	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:12:46	Column b1 modified.	Column Tracker	BEAGLE		🕼 <u>R</u> efresh
08/11/2005 17:12:04	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:11:23	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:10:41	Column b1 modified.	Column Tracker	BEAGLE		A Evport
08/11/2005 17:10:02	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:09:22	Column b1 modified.	Column Tracker	BEAGLE		🚔 Print
08/11/2005 17:08:43	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:08:00	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:07:18	Column b1 modified.	Column Tracker	BEAGLE		Reason
08/11/2005 17:06:37	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:05:53	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:05:10	Column b1 modified.	Column Tracker	BEAGLE		
08/11/2005 17:04:29	Column b1 modified.	Column Tracker	BEAGLE	12121	
Injection number = 100					
Reason User comment					

All modifications in the column parameters are listed in the audit trail with the corresponding date, actor and station. Each time an acquisition is done using a column that is defined in the Column and Solvent Database and in a system using the column tracker driver, the injection number of the column is automatically incremented in the column parameters. In that case, the actor listed in the audit trail is the name of the system and the system acquisition server is listed as station name.

Click on the 🔯 button to refresh the audit trail.
Click on the Export button to export the current audit trail. Choose the path to export and the file is automatically displayed at screen.
Click on the Erint button to print the current audit trail.
Press the Reason button to display user reasons and comments.

Chromatographic Solvent Management

In Galaxie, open the Chromatographic Solvent Management by selecting the selecting the selecting the selecting the following screen is displayed:

Solvent								
olvent lis								
ype 1 : Hydro	phobic Type 2 : Intermediate Type	3 : Hydrophilic	A Type 4 : H	ydrophilic B	Type 5 : Hydr	ophilic C 💧		
Short name	Name >		Concentration					<u>N</u> ew
HSA	Hexane Sulfonic Acid							🖬 Edit
P04-4.5	Potassium Phosphate buffe	r pH4.5	100 mmol					
P04-7.0	Potassium Phosphate buffe	r pH7.0	100 mmol					🔀 <u>D</u> elete
TEA	Triethylamine Acetate		50 mmol	1				
								Export
								C Print
								😡 <u>A</u> udit tra
								Betres
								J OK
pe com	patibility							
pe com	patibility Type Name	Type 1	Туре 2	Type 3	Type 4	Type 5		
rpe com Type 1	patibility Type Name Hydrophobic	Type 1	Туре 2	Туре 3	Type 4	Type 5		
ре сот Туре 1 Туре 2	Datibility Type Name Hydrophobic Intermediate	Туре 1	Type 2	Туре 3	Туре 4	Туре 5		
г ре сот Туре 1 Туре 2 Туре 3	Datibility Type Name Hydrophobic Intermediate Hydrophilic A	Type 1	Type 2	Туре 3	Туре 4	Туре 5		
pe com Type 1 Type 2 Type 3 Type 4	Datibility Type Name Hydrophobic Intermediate Hydrophilic A Hydrophilic B	Type 1	Type 2	Type 3	Туре 4	Type 5		

It contains the list of all defined solvents that are distributed into 5 different tabs depending on their hydrophobia. The hydrophilic solvents are dispensed into tree different types: the more hydrophilic corresponds to *Type 5*, the less hydrophilic to *Type 3* and the moderately well hydrophilic to *Type 4*. The hydrophobic solvents are listed in the *Type 1* tab and the solvents of intermediate hydrophobia in the *Type 2* tab.

At the bottom of the screen, the *Type compatibility* table indicates the miscibility between solvents of different solvent types.

Adding a New Solvent and Modifying Solvent Parameters

Define a new solvent in the solvent type database by pressing

the wew button or from the contextual menu. Modify the

properties of a selected solvent by pressing <u>Edit</u> ... or from the contextual menu. Enter or modify the solvent parameters in the displayed column properties screen:

Name	J	
Short name	<u> </u>	
Concentration		
Туре	Туре 5 💌	

Enter the solvent Name and Concentration.

In the *Short name* field, enter a short name or click on the **b**utton to automatically define the 10 first characters of the solvent name as *Short name*. The *Short name* is used for the Galaxie solvent identification.

The solvent Name and Short name must be filled in.

Managing the Solvents List

Delete a selected solvent entry of the list by pressing the

Delete button or from the contextual menu.

To duplicate a selected solvent entry in the list, press

Duplicate or select it from the contextual menu. A new solvent entry is created with exactly the same parameters except the solvent *Name* and the *Short name*. The solvent *Name* of the

created solvent entry begins with "copy of" and ends with the name of the duplicated solvent entry. The *Short name* of the created solvent entry corresponds to the first 9 characters of the duplicated solvent name ended by a number suffix.

Print or Export the solvent list and parameters by pressing the <u>Export</u> or <u>Export</u> button. Choose the path to export and the file is automatically displayed at screen.

Click on the Befresh button to refresh the database that can be modified from different stations at the same time when in Client/Server configuration.

Displaying Solvents and Columns Database Audit Trail

Press the <u>Audit trail</u> button to display the column and solvent database audit trail.

Date V	Action	Actor	Station name
)/11/2005 09:38:36	Solvent 'Dichloromethane' duplicated in 'Copy of Dic	av (rtrtrt)	BEAGLE
/11/2005 17:14:13	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:13:29	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:12:46	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:12:04	Column b1 modified.	Column Tracker	BEAGLE
08/11/2005 17:11:23	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:10:41	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:10:02	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:09:22	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:08:43	Column b1 modified.	Column Tracker	BEAGLE
3/11/2005 17:08:00	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:07:18	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:06:37	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:05:53	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:05:10	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:04:29	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:03:46	Column b1 modified.	Column Tracker	BEAGLE
08/11/2005 17:03:04	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:02:24	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:01:41	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:00:59	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 17:00:16	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 16:59:34	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 16:58:53	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 16:58:10	Column b1 modified.	Column Tracker	BEAGLE
8/11/2005 16:57:27	Column b1 modified.	Column Tracker	BEAGLE
08/11/2005 16:56:44	Column b1 modified.	Column Tracker	BEAGLE
	Column b1 modified.	Column Tracker	BEAGLE

All modifications in the solvent parameters are listed in the audit trail with the corresponding date, actor and station.

Click on the Dutton to refresh the audit trail.

Click on the Export ... button to export the current audit trail. Choose the path to export and the file is automatically displayed at screen.

Click on the Frint ... button to print the current audit trail.

Press the **Beason** ... button to display user reasons and comments.

Using the Generic Column Tracker Driver

Use the Generic Column Tracker Driver to use the Column and Solvent Management Plug-in to automatically increment column parameters.

Configuring the Generic Column Tracker

The driver software configuration is done in the Galaxie Configuration Manager when a new chromatographic system is created.

NOTE: If the system is equipped with several columns, it is necessary that system driver list contains the column tracker driver as many times as the columns number of the system.

Click on the solution corresponding to the Generic Column Tracker driver and the configuration screen appears.

Co 📽	nfigure system				
Over View		Column Tra	acker Module		√ <u>o</u> ĸ
		Column Tracker Name: Chromatography Type:	GC		
colum	n tracker	Generic Column Tracker #1	Idle	Free	

In case the system contains several columns, enter a *Column Tracker Name* to differentiate each column of the system. This *Column Tracker Name* should be different for each Column tracker module of the system.

Choose the *Chromatography Type* of each column of the system in the corresponding scrolling list. All the defined chromatography types of the column database are available.

Configuring the Synopsis

In the *Overview* part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

Right click on the system name in the bottom part of the *Galaxie Configuration Manager* screen. A pop-up menu appears: click on *Stop.* Then right click on the system name again, and click on *Start.*



The synopsis will be displayed in the Galaxie Chromatography Data System, in the *Systems* tab. In this tab, the *Overview* will show the synopsis of the system.

For example, the following pictures represent the synopsis of the Generic Column Tracker:

2	
	0 Inj.
Column Tracker	

Galaxie Configuration Manager screen



Galaxie Chromatography Data System screen

NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the Galaxie Configuration Manager User's Guide.

Press the button to print the current configuration.

Building a Method

Create a new method for the system using the Generic Column Tracker driver.

The control section must be defined in order to start an acquisition. In the following part of this guide, only the control section for the Generic Column Tracker is detailed.

NOTE: For more details about the programming of each method section, turn to the Galaxie Chromatography Data System User's Guide.

Control Method Section for the Generic Column Tracker

In the method, select the control section in the lower part of the browser.

The following screen appears:

🖉 Galaxie Chromatography Data Sy	stem	
File Display Acquisition Method Data	Session Processing Plug-ins Help	
\$\$ • \$\$ • \$\$ • \$ • \$ • \$		
📄 Data Files :	System Control Mathod Advanced Tools	
 ■ meth1.METH ✓ ● back ● Channel 2 ✓ ● front ✓ ● channel 1 		
<u> </u>		
ଟଟ' meth1.METH		
Control		
acquisition pre processing		
integration events		
peak identification		
• group identification		
····· • calibration		
• formats		
• suitability tests		
export post processing		
post processing report style		
• summary		
🖥 Data 📖 Systems 🔛 Calibration	column tracker system Overview Idle Free	
meth1[Channel 1]	stephanie validation column tracker	0 f //

Click on the button to display the Generic Column Tracker control method section.

Column Tracker Module Control

Over			Column Tracke	r Module - 5890-bac	:k		
5890			Column type	GC	-		
			Column Short name	GC 3	•		
7673	Column properties	GC 3					
	Column name	Gas column 3		Manufacturer	VARIAN		
	Column description	column for gas chromatograp	γ	Serial number	ххххууу		
				Chromatography type	GC		
1		J		Injection number	12227		
	Pre column name	no pre column				Unit	
	Dre ook een dooorie	line MA		Length	60.00	m	
	Fie column descrip			Internal diameter	0.53	um	
				Outside diameter	1.00	mm	
	Chemical parameters Phase type silanol phase à 40%			Physical parameters			
					Min	Мах	Unit
		Unit		pH 0.	00	0.00	
	Phase thickness	42.50 um		Breathing	F	150.00	Res
				Flessule		100.00	Ddl
				Flow		0.00	ml/min
	Pore size	0.00 A				lso Prog	
				Temperature 10	0.00	250.00 250.00	
	storage solvent	J				1	
0	OLUMN TRACKER IHM	DLL 1.0.1.1					
5890+7	673	Generic Column Tracker #2	Running	anais (VALIDAT	FION] 58	90 column 1.ME	ETH

The *Chromatography type* chosen while configuring the system is displayed at the top of the control screen.

Select the *Column Short name* to be used in the system in the corresponding scrolling list just above. Only the columns defined for this *Chromatography type* are available in the scrolling list.

Once a column is selected, its *Column properties*, *Chemical parameters* and *Physical parameters* are automatically displayed on screen.

Starting and Viewing an Acquisition

To view a running acquisition, click on the *Systems* tab then select the running system.

Status of the Generic Column Tracker

Click on the button corresponding to the Generic Column Tracker driver and the Generic Column Tracker status screen will appear.

Status Window

Over	er Column Tracker Module - 5890-back						
View	Column properties GC 3						
5890	Column name	Gas column 3	Manufacturer	VARIAN			
76738	Column description	column for gas chromatography	Serial number	ххххууу			
			Chromatography type	GC	-		
P		J	Injection number	12228			
	Pre column name	no pre column	Length	60.00 m	-		
1	Pre column description	NA	Internal diameter	0.53 um	-		
			Outside diameter	1.00 mm	-		
						1	
0	COLUMNI_TRACKER_HMA.DLL 1.0.1.1						

The *Status* window displays the column properties as defined in the column database. All fields are in read-only mode. The *Injection number* is incremented at each injection.