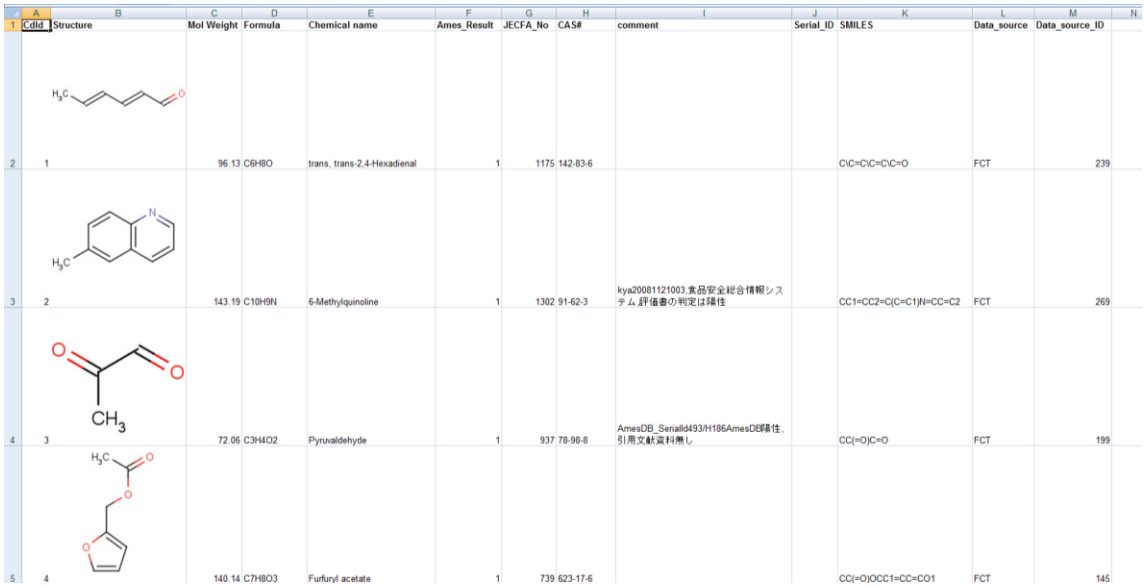
What is new in the Database Manager version 1.7.5

The system provides to users flexibility to create ODB databases starting from excel and tab files. If you collect your chemicals data in a software platform which allows you to make export to xls (Excel 2003) or tab files you can convert these data to ODB files and to use facilities provided by the Database Manager v. 1.7.5.

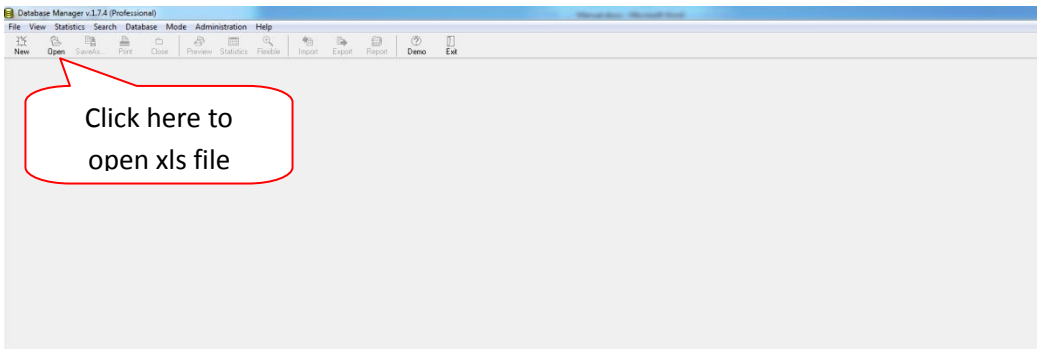
A. How to create ODB databases from excel files

Structure of the excel file exported from JChem software platform is illustrated below:



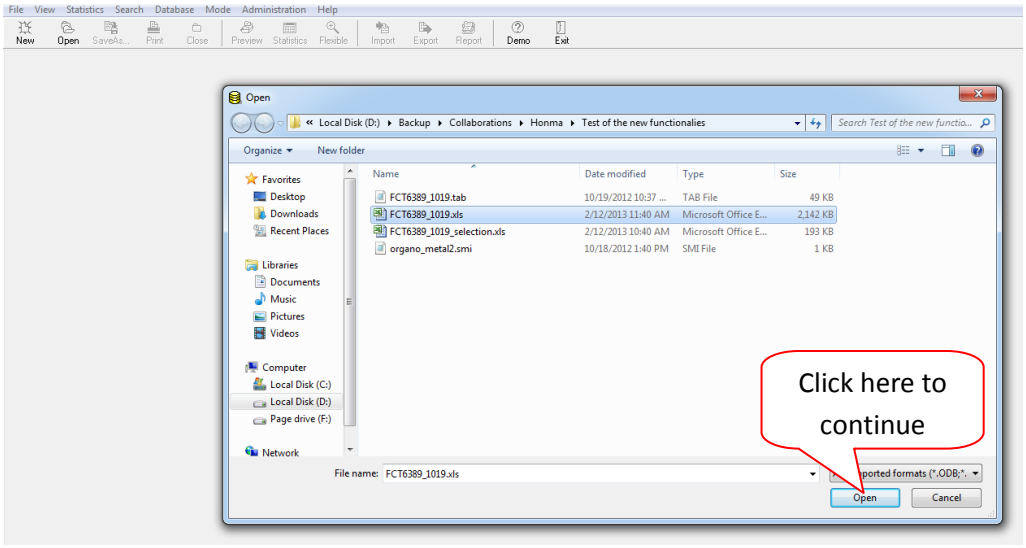
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	CdId	Structure	Mol Weight	Formula	Chemical name	Ames_Result	JECFA_No	CAS#	comment	Serial_ID	SMILES	Data_source	Data_source_ID	
2	1		96.13	C6H8O	trans, trans-2,4-Hexadienal	1	1175	142-83-6			C\C=C\C=C\C=O	FCT	239	
3	2		143.19	C10H9N	6-Methylquinoline	1	1302	91-62-3	kya20081121003,食品安全総合情報システム,評価書の判定は陽性		CC1=CC2=C(C=C1)N=CC=C2	FCT	269	
4	3		72.06	C3H4O2	Pyruvaldehyde	1	937	78-98-8	AmesDB_Serialld493/H186AmesDB陽性,引用文献資料無し		CC(=O)C=O	FCT	199	
5	4		140.14	C7H8O3	Furfuryl acetate	1	739	623-17-6			CC(=O)OCC1=CC=CO1	FCT	145	

Open this file directly in Database manager:

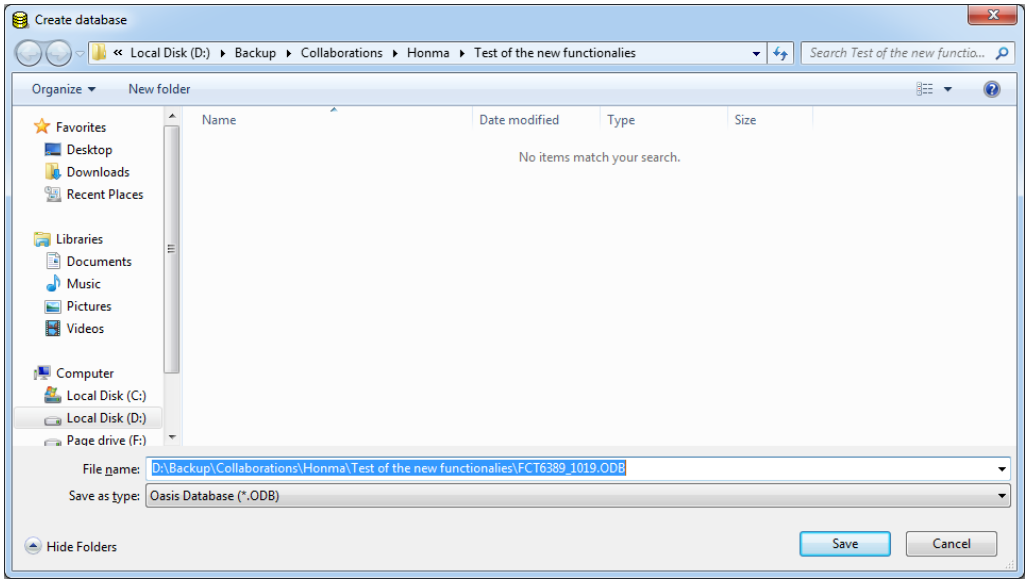


Note: the xls file should not be operating in your computer at this moment.

Select an xls file:

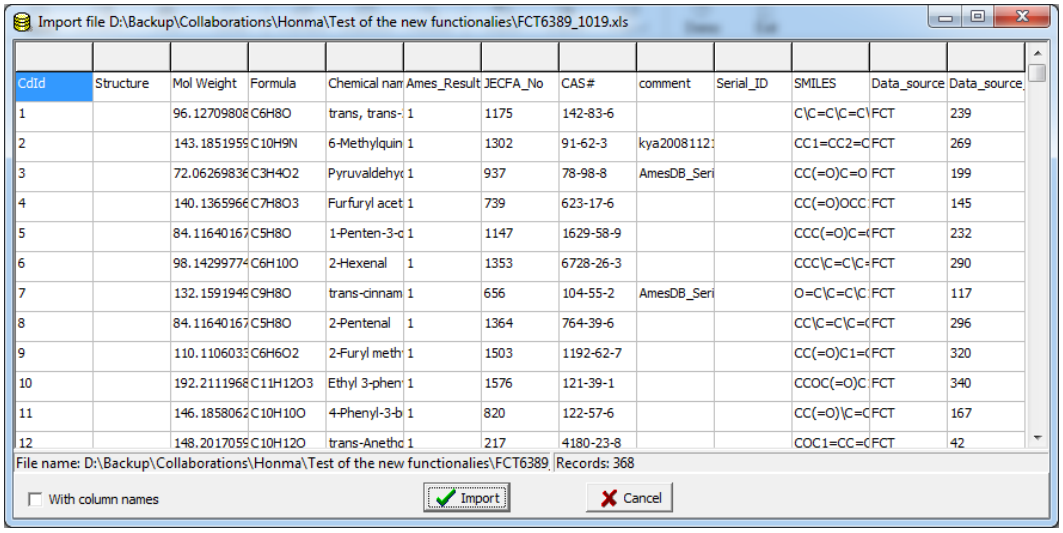


The system asks you to provide a directory where the ODB file will be created:



Confirm or change the ODB file name and click on Save to continue.

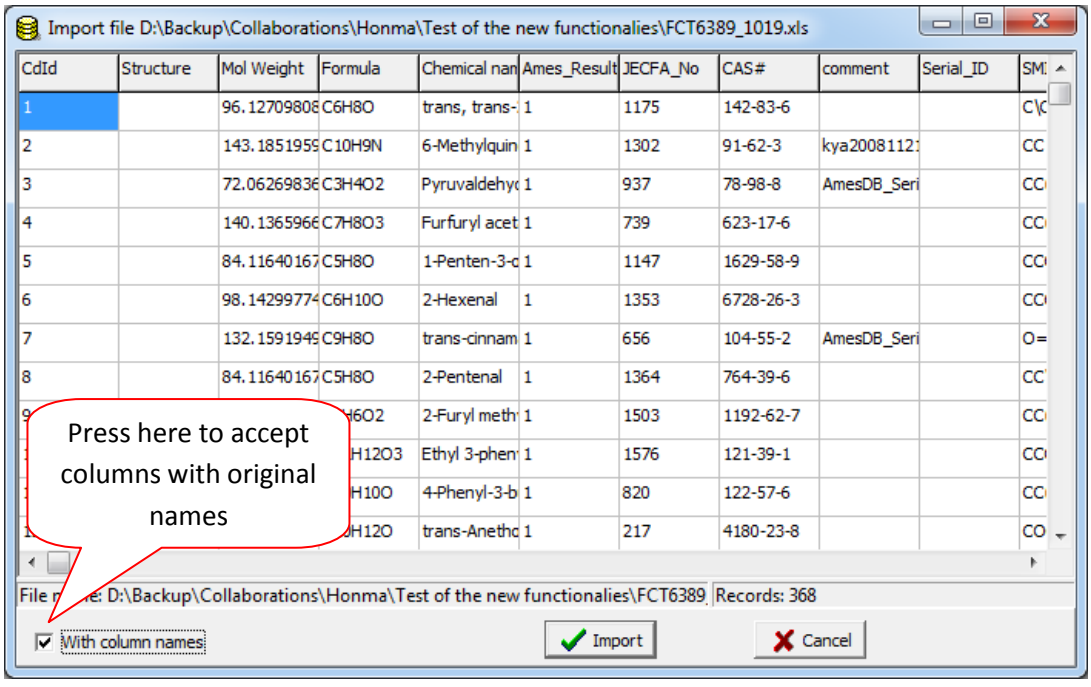
Then the following window will appear:



At this stage you should decide whether to accept the original columns names or you want to change them.

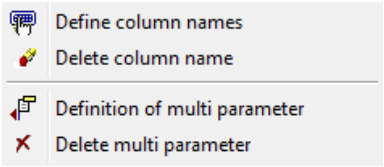
Note: Benefit of using xls instead of tab files is that the columns already have names which can be imported directly.

Accept the columns with their names:

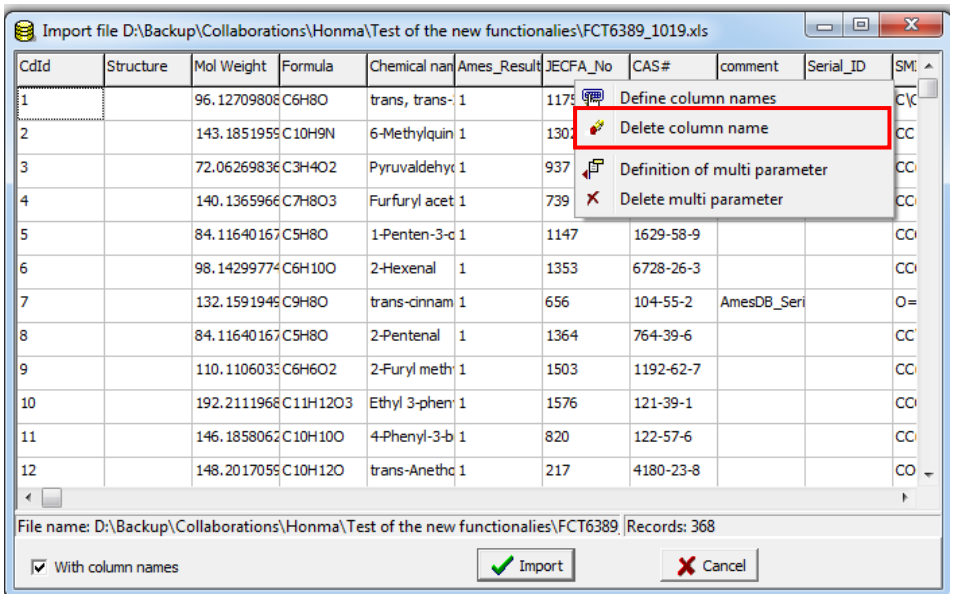


List of names will be saved automatically and loaded next time when a new file is imported.

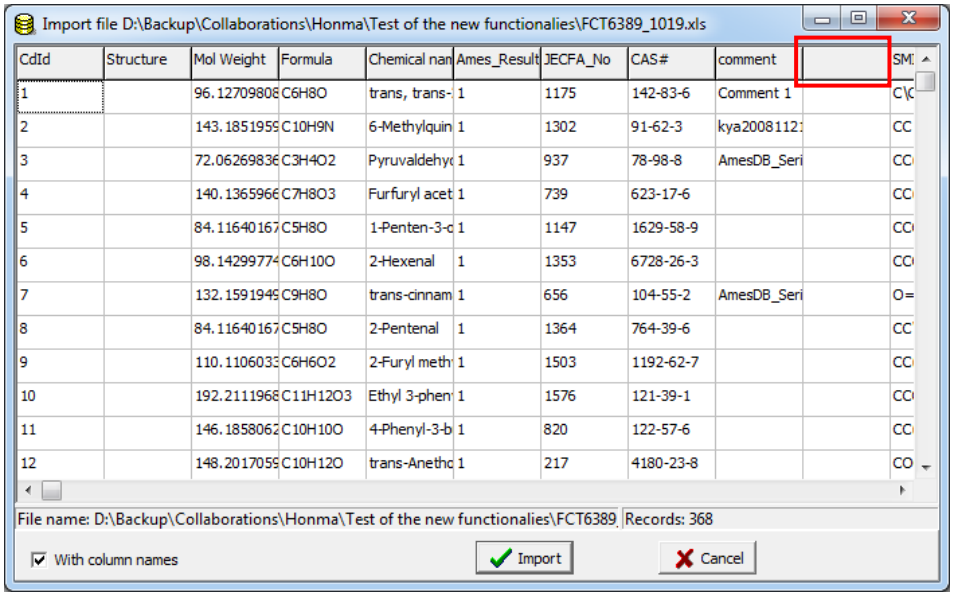
The system also allows you to edit existing columns names or to delete and define new names. Make right mouse click on the name. This window appears:



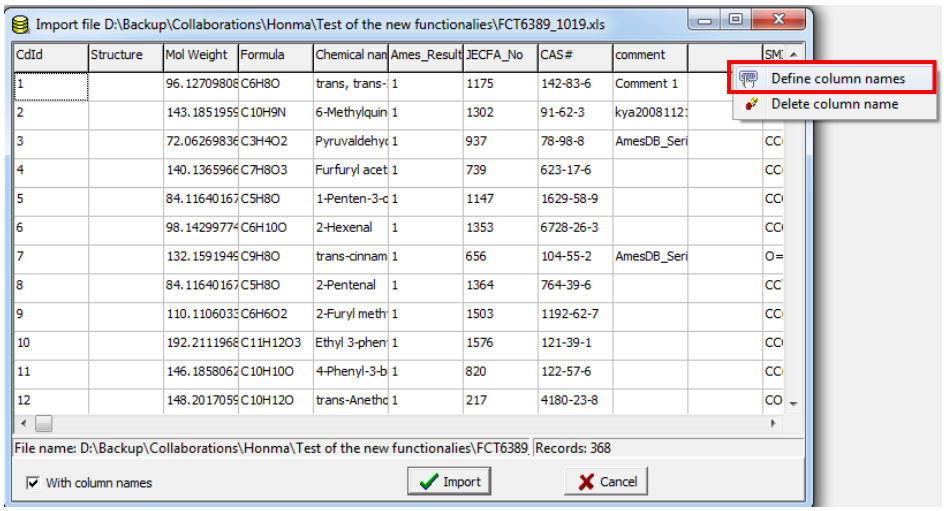
Choose Delete column name:



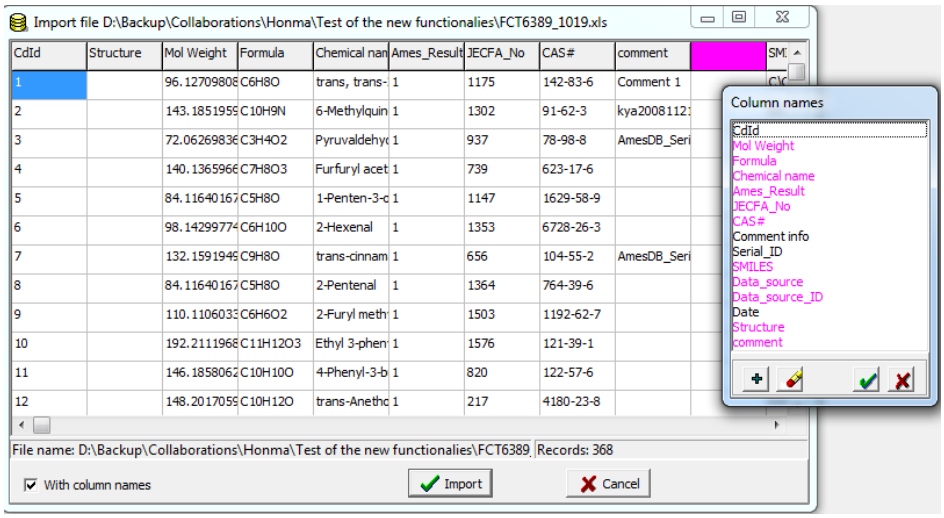
The column name disappear:



Now you can defile new column name:

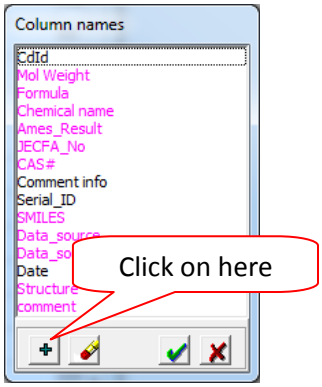


The following window appears:

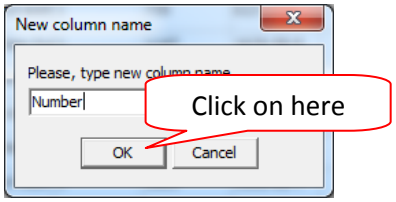


Names colored in pink have already been used as captions of the other columns. Black colored names are free to use. Choose the corresponding name and confirm by  button.

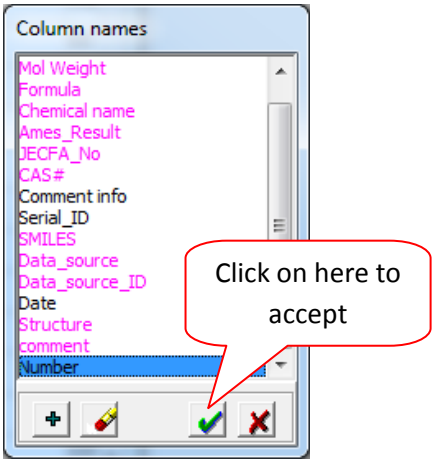
Nevertheless, you can define name which does not exist in the list of names:



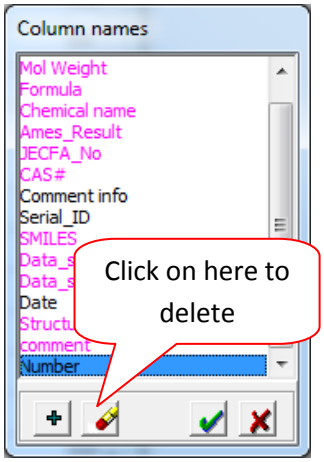
This window appears:



The new column name is listed along with the other names. Find it in the list and confirm to accept it:



Users are allowed also to remove permanently names from the list. Select the name and delete it:

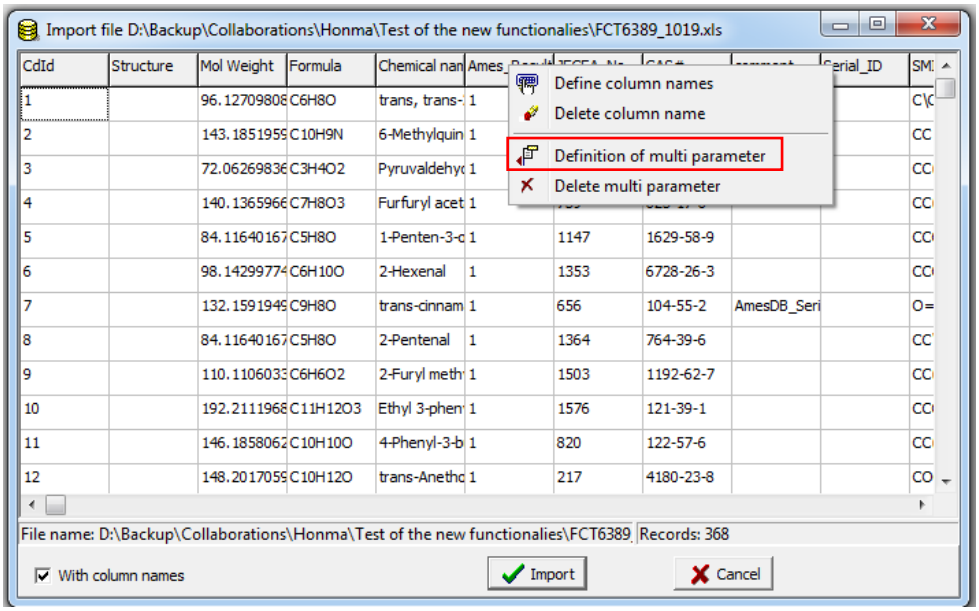


If you want to close the Column names window press  button.

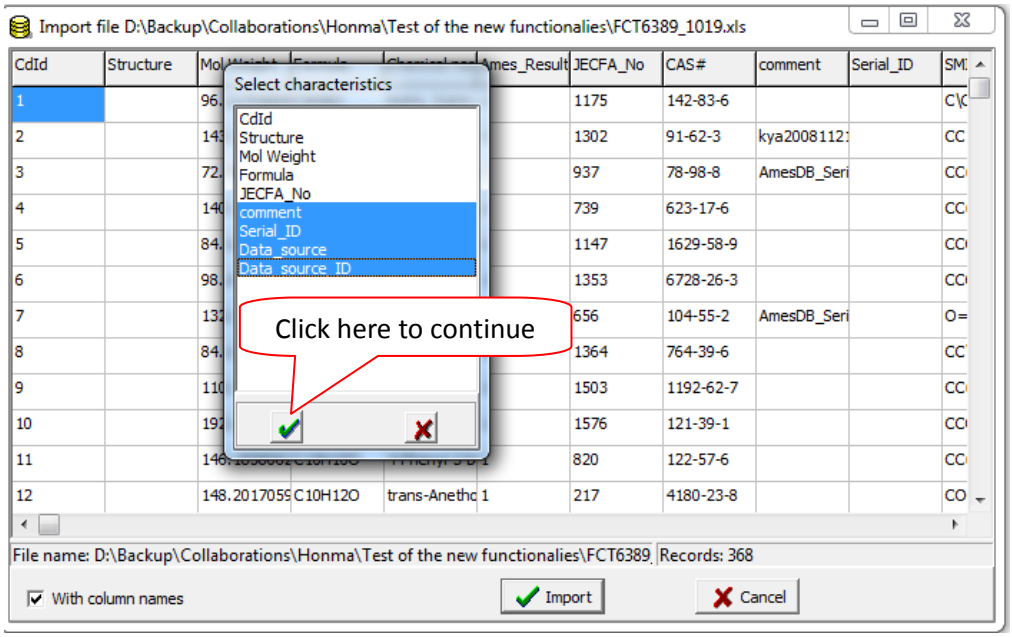
Now you should select a multi parameter. This is the parameter for which different integer values could be provided in the database. Here, the multi parameter is the Ames_Result because it may possess negative (0), positive (1) or equivocal (2) data.

Note: System allows you to use integer values only, i.e. 0, 1, 2, etc. Please do not use text, e.g. negative, positive and equivocal.

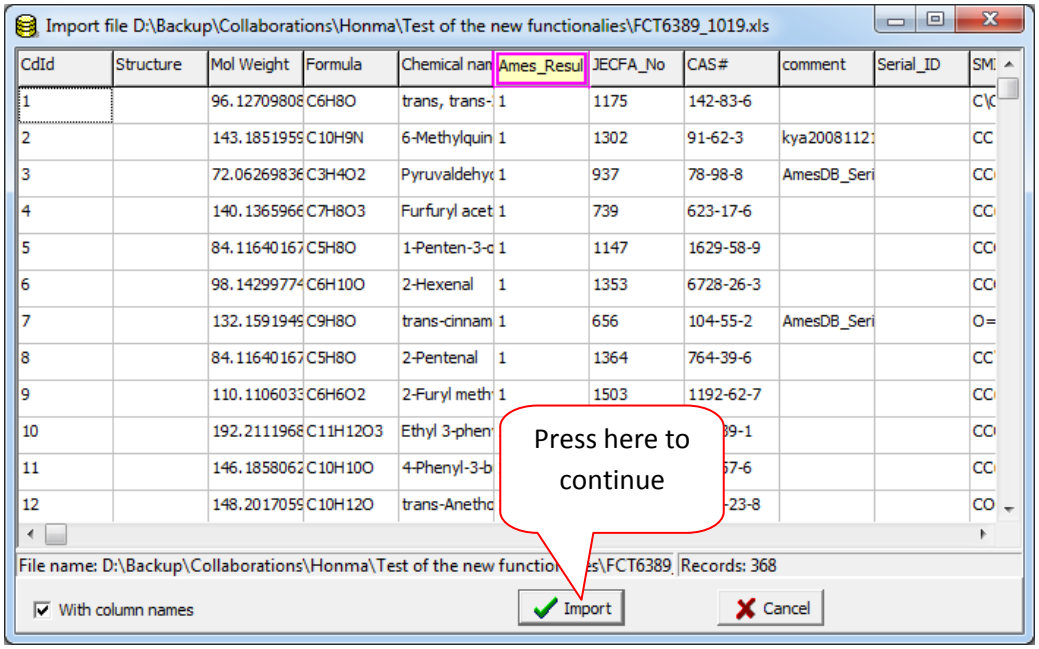
Selected the multi parameter by making right mouse click on the Ames Result column name:



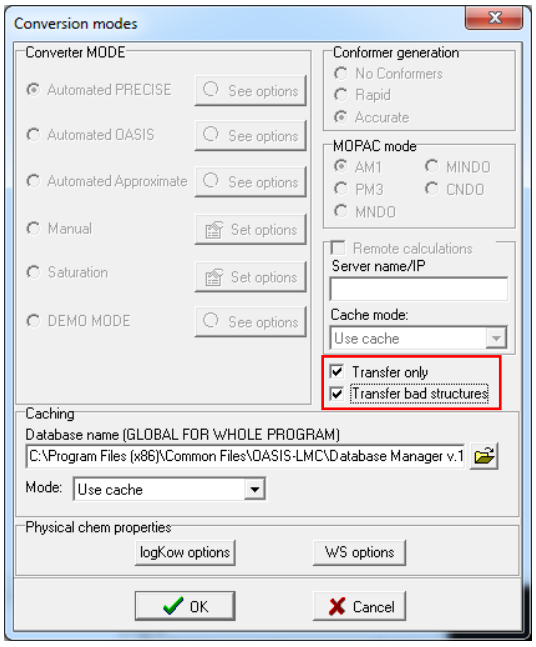
Along with selection of the multi parameter users need to define parameters which are associated to this parameter. These are any specific characteristics supporting the multi parameter, e.g. comment, Serial ID, etc:



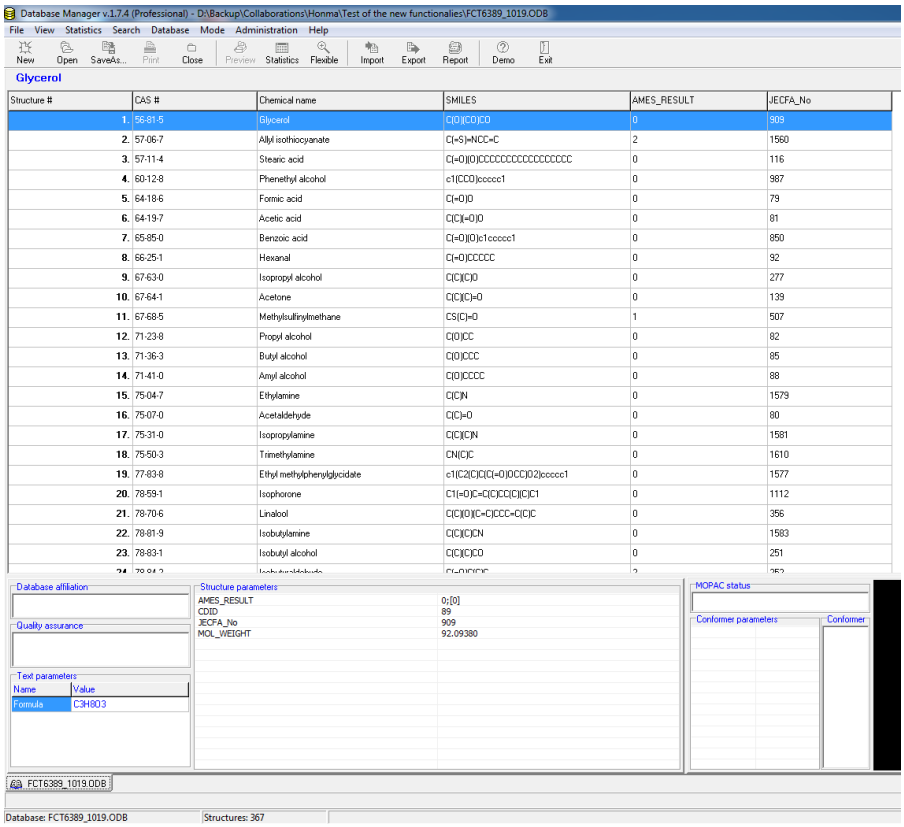
When defined, the multi parameter will be yellow colored:



The following window appears:



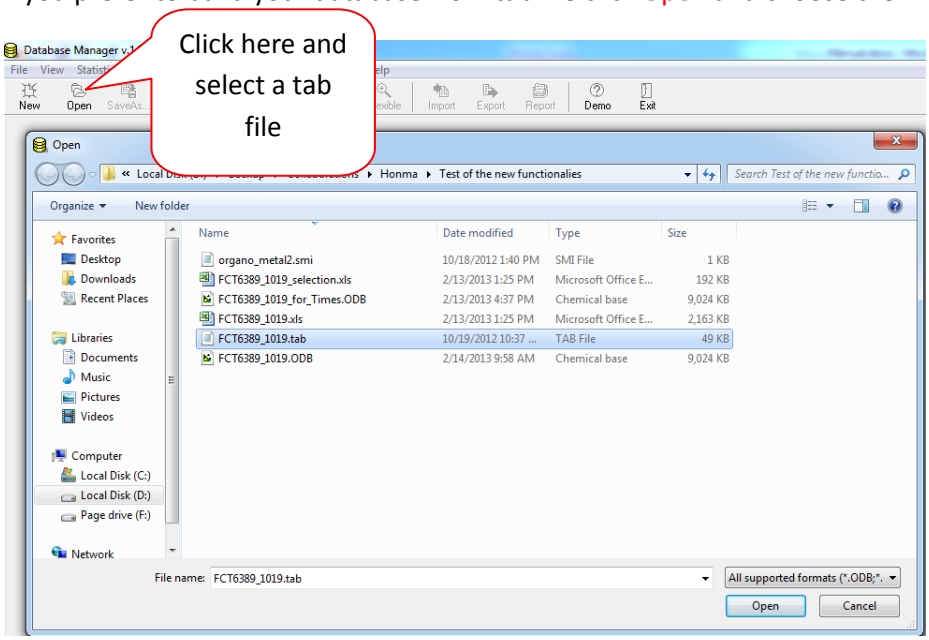
Do not forget to choose the option Transfer bad structures. This option allows you to import chemicals with errors in smiles, which can be edited manually. These structures can be inorganic chemicals, organo-metals, etc. Press OK.



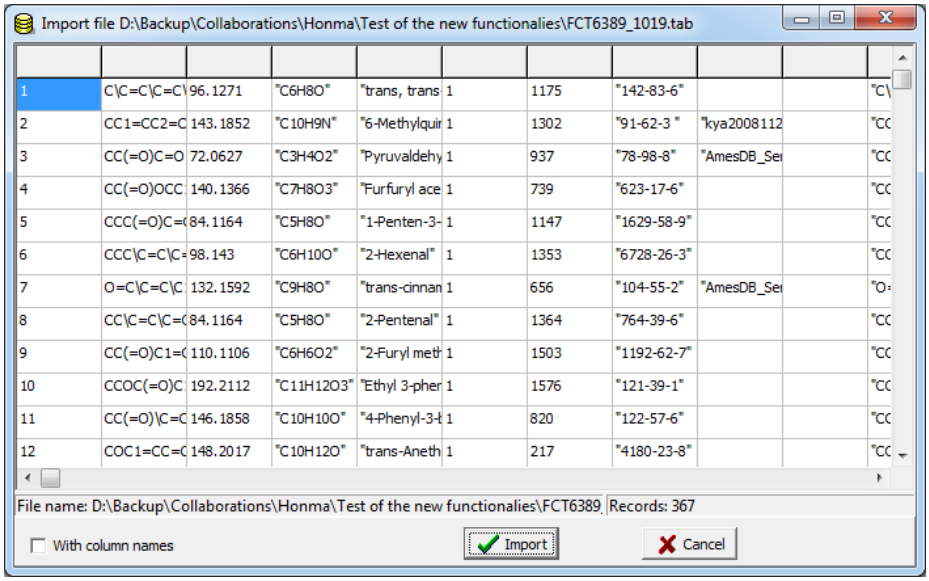
The ODB is already created.

B. How to create ODB database from tab files

If you prefer to build your database from tab file click Open and choose the file:

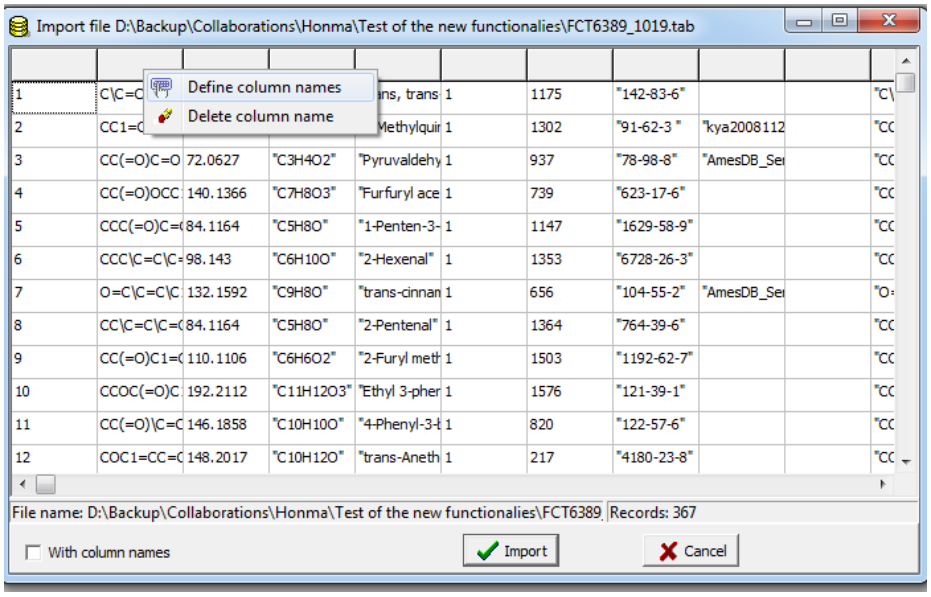


The following window will appear:

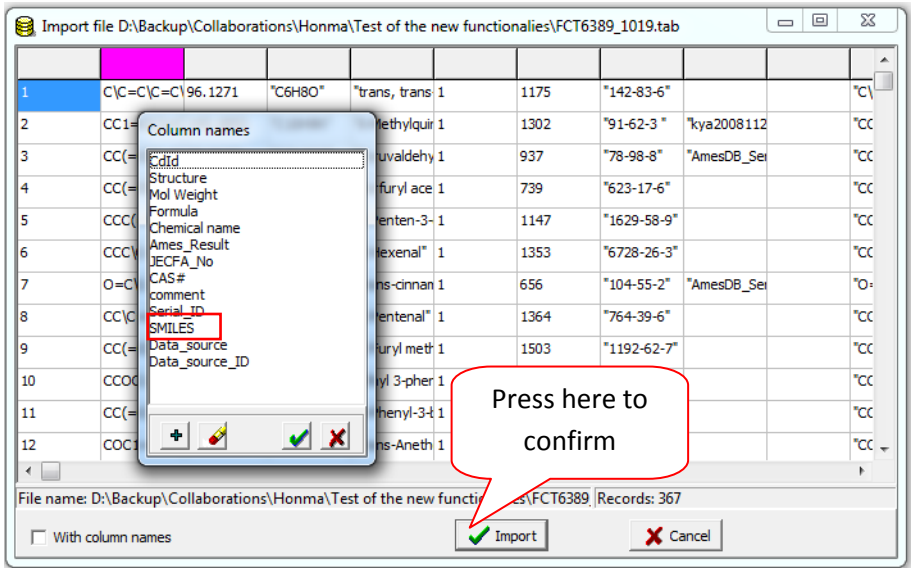


As seen, the columns names are empty and you need to define them manually:

Make right mouse click on an empty column and select Define column names:

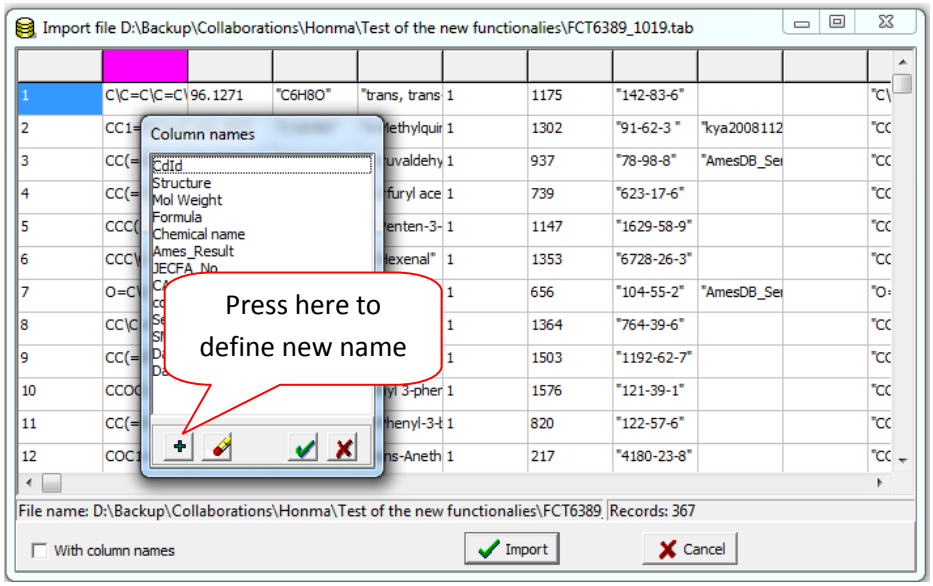


Select the corresponding name from a list of names:

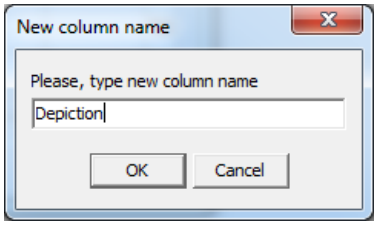


Select the corresponding name of each of the columns.

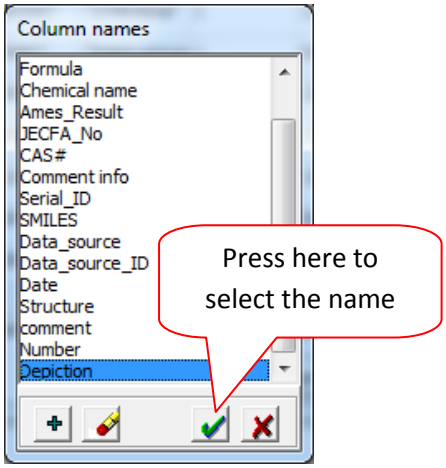
User is also allowed to type a new column name:



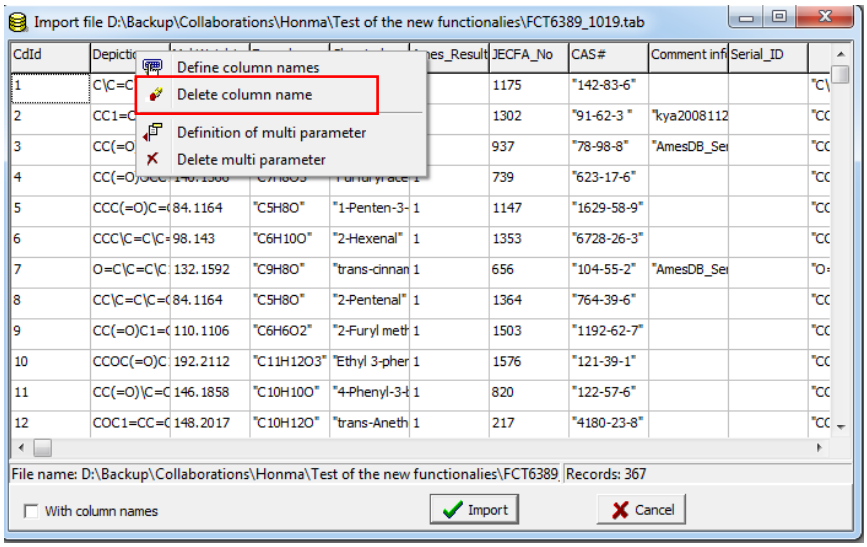
Type a name which will be new in the list:



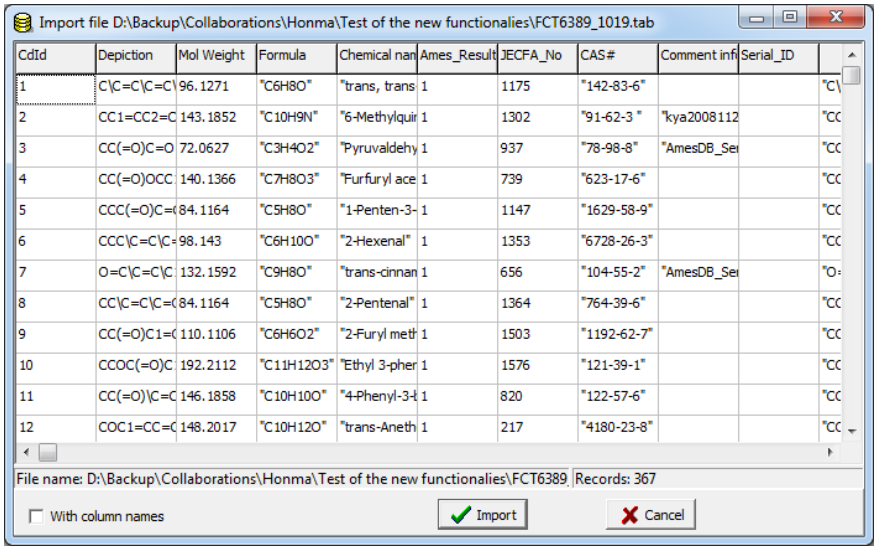
Press OK and find listed the new name:



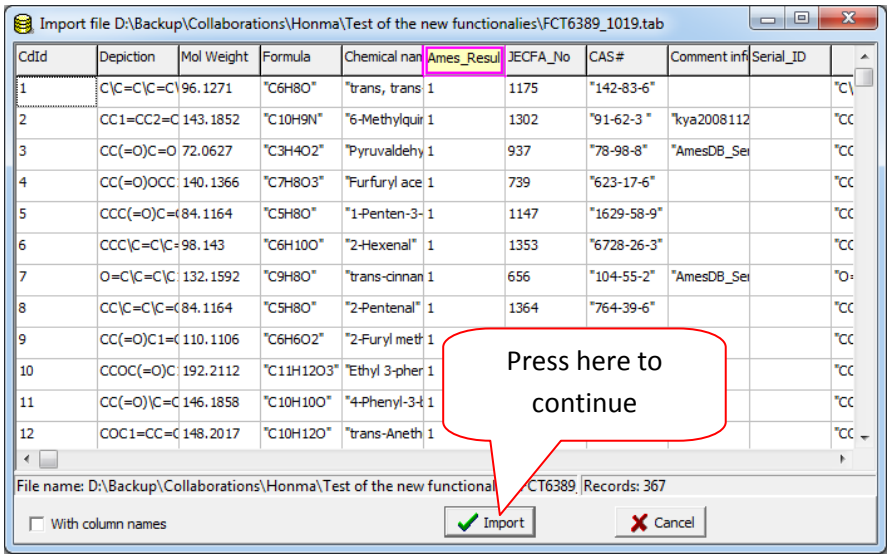
You can also delete a column name:



When all column names are defined the window looks like that:



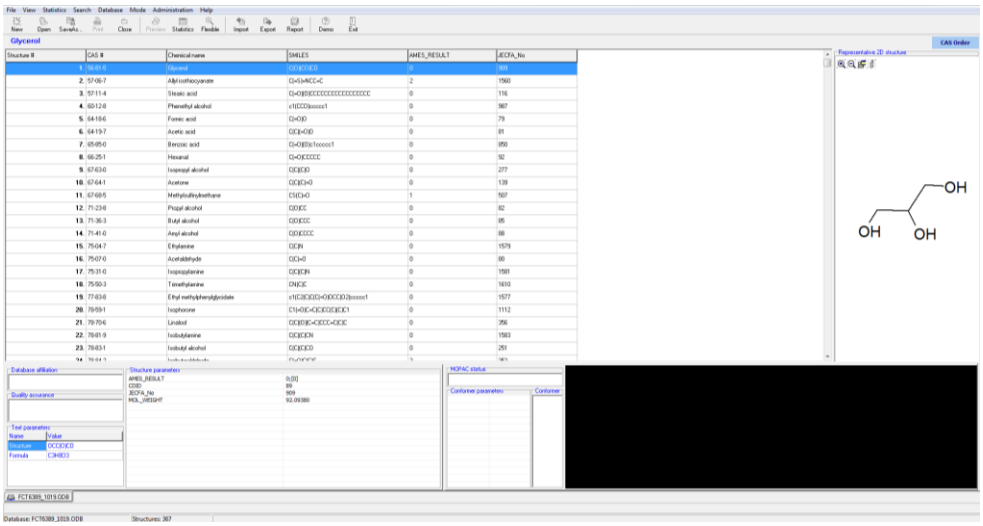
Now, the multi parameter Ames_result and its characteristics need to be defined:



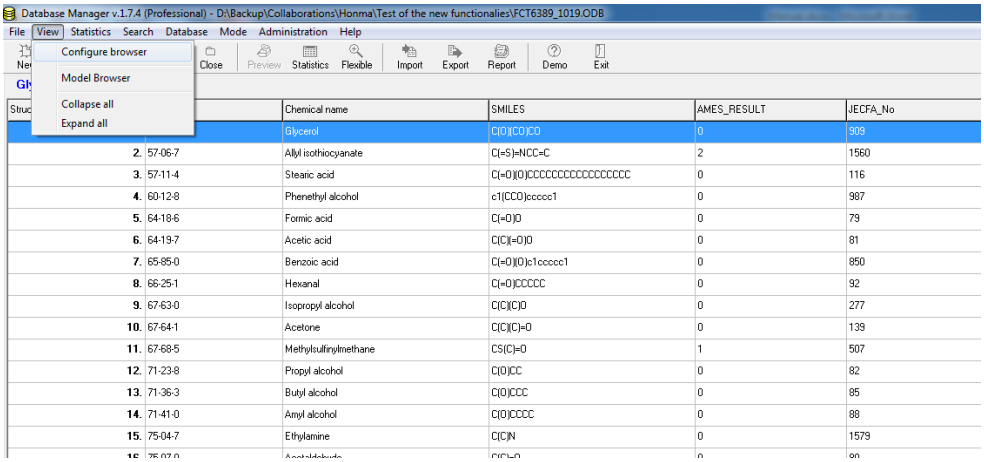
Then, the ODB is created.

C. What can we do with created ODB file

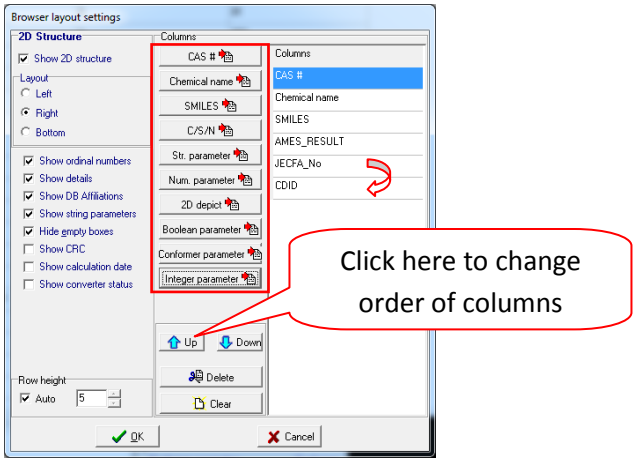
When imported the OBD looks like that:

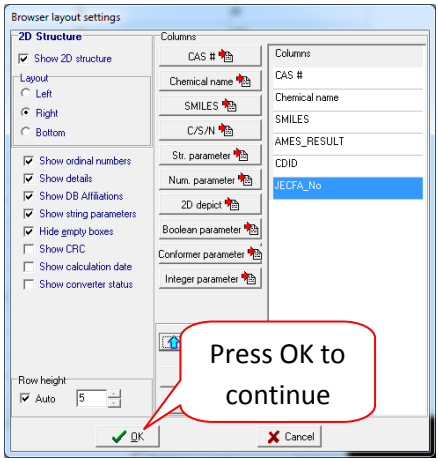


Press view and configure your browser:

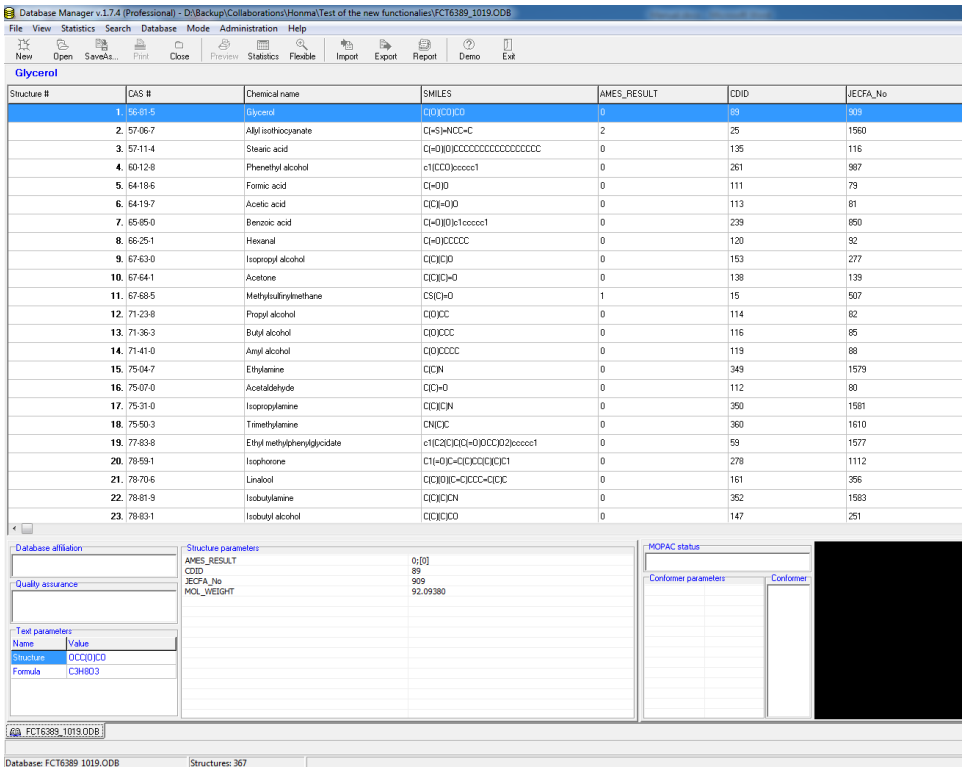


The red colored box includes the buttons which allow you to arrange the view of your browser. New functionalities here are **Up** and **Down** buttons. They give you possibility to change order of columns:



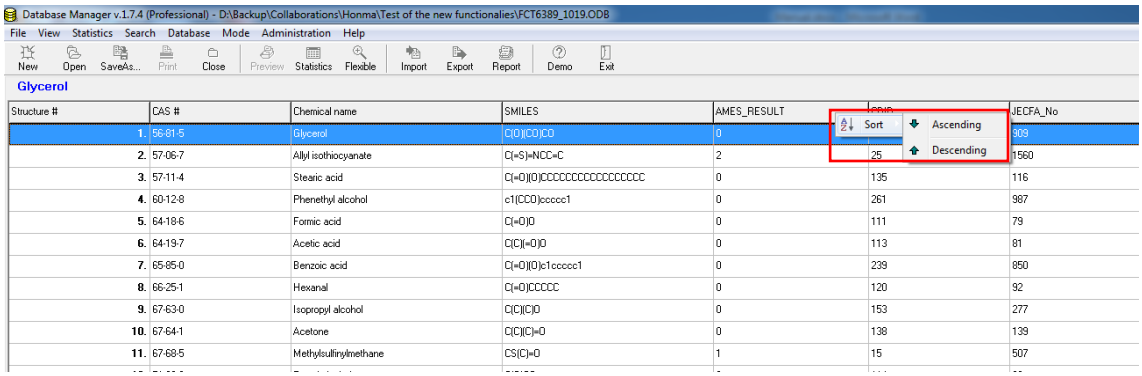


The newly configure browser appears:

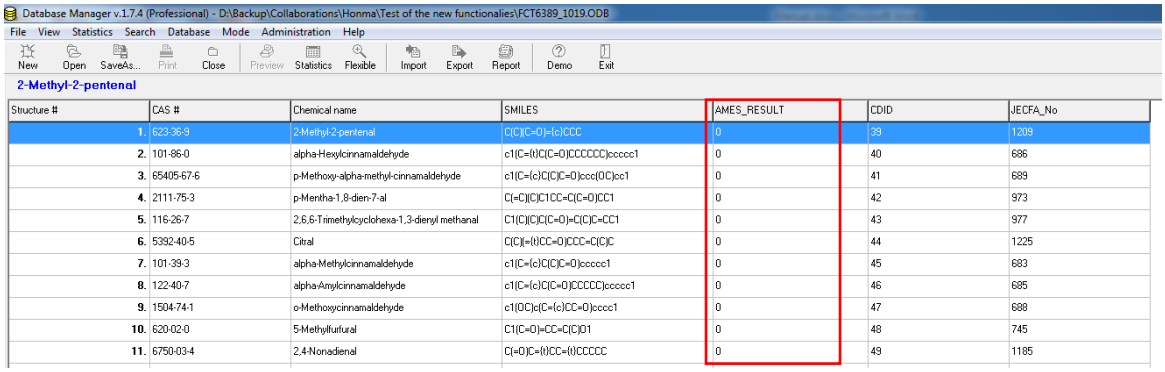


There is a new functionality which allows you to sort the information included in each of the columns.

Make double left mouse click in a column name and sort by:

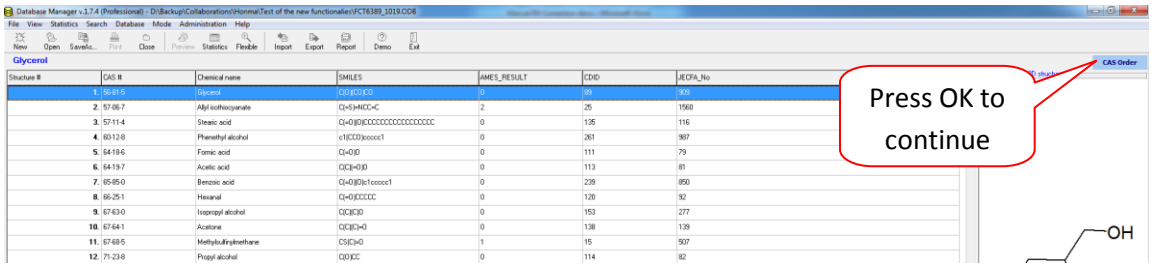


In this case, Ascending sort of the Ames Result is chosen:

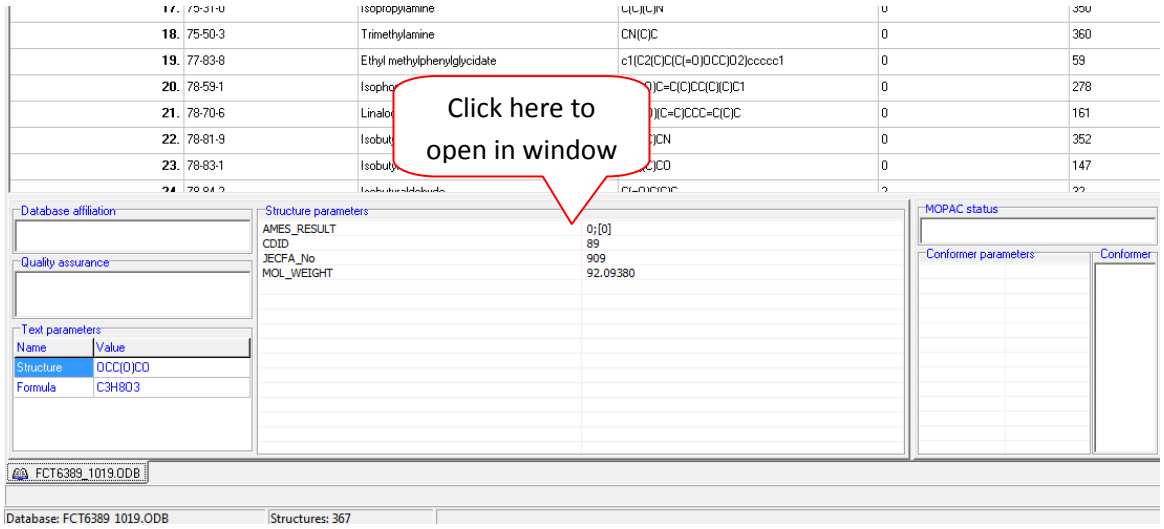


This option is available for all columns in the database.

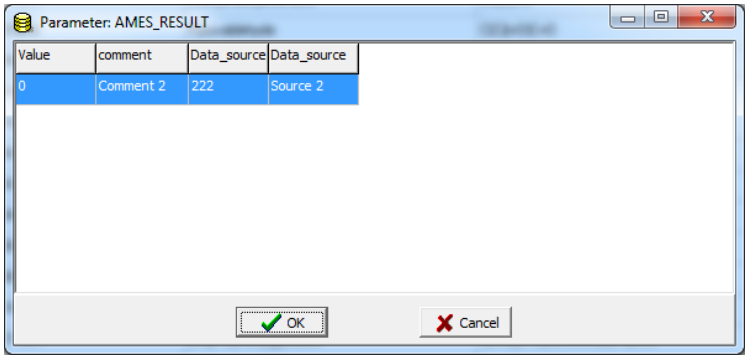
CAS order and Natural order also allow you to sort chemicals. Use CAS order to sort chemicals by increasing of their CAS number and Natural order to sort chemicals by their order of receipt. Double left mouse click allows you to switch from CAS to Natural order:



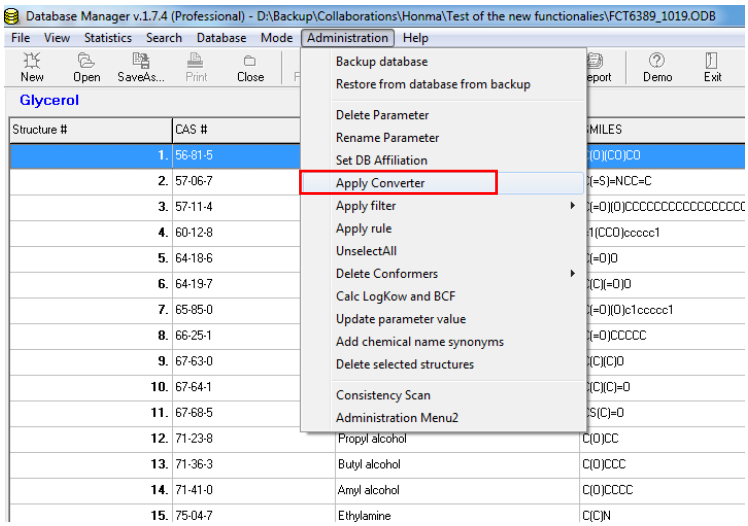
If you want to see the supporting characteristics of the multi parameter make left mouse click on the Ames_Result:



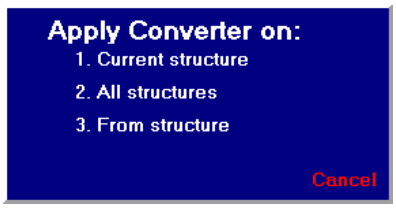
Window appears:



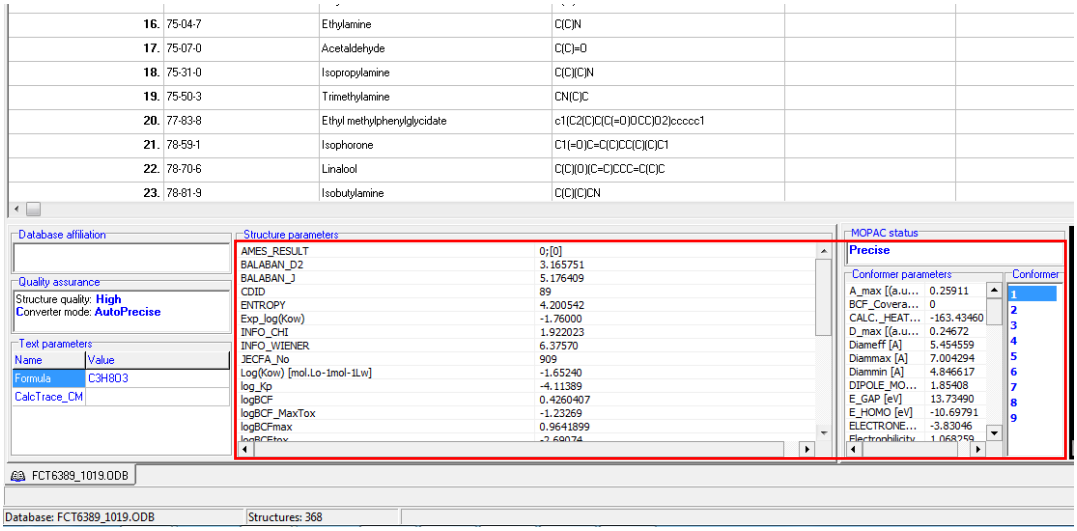
The system allows you to calculate structural and conformational parameters:



Choose to apply converter to the current structure, all structures or from structure # to the last structure in the file.

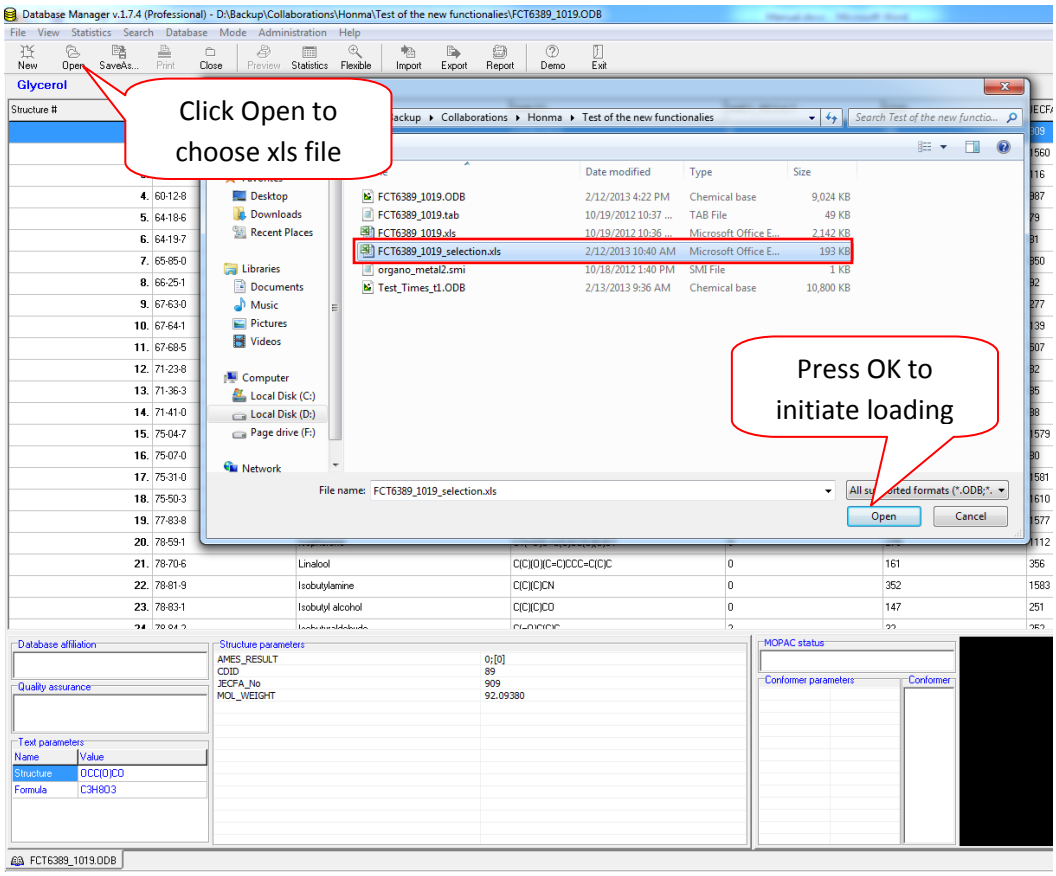


After calculations:

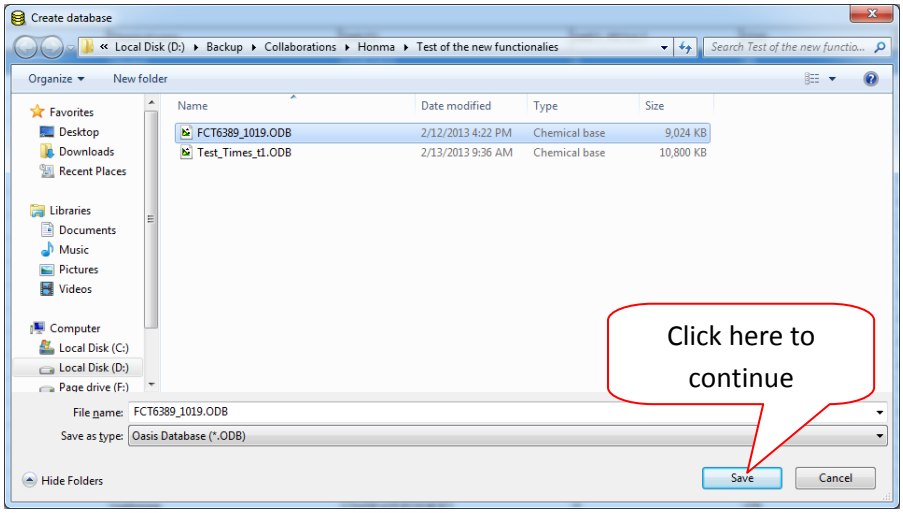


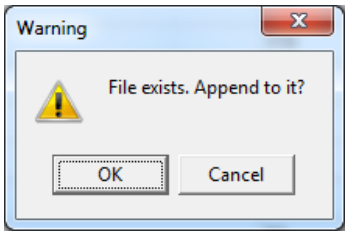
D. Append new data to existing ODB database

To append data to already existing database you need to repeat the procedure for conversion of xls or tab to ODB file:

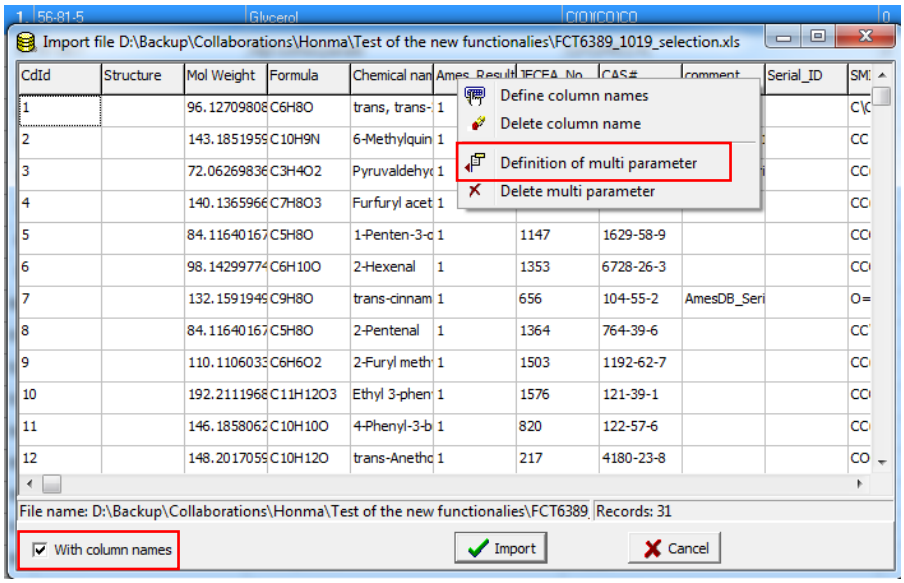


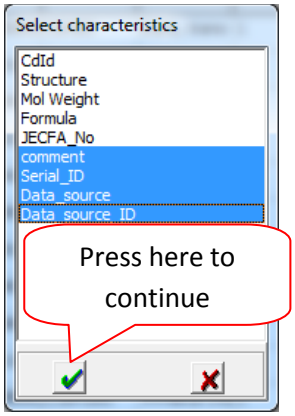
Select ODB which already exists and append the new chemicals to this file.

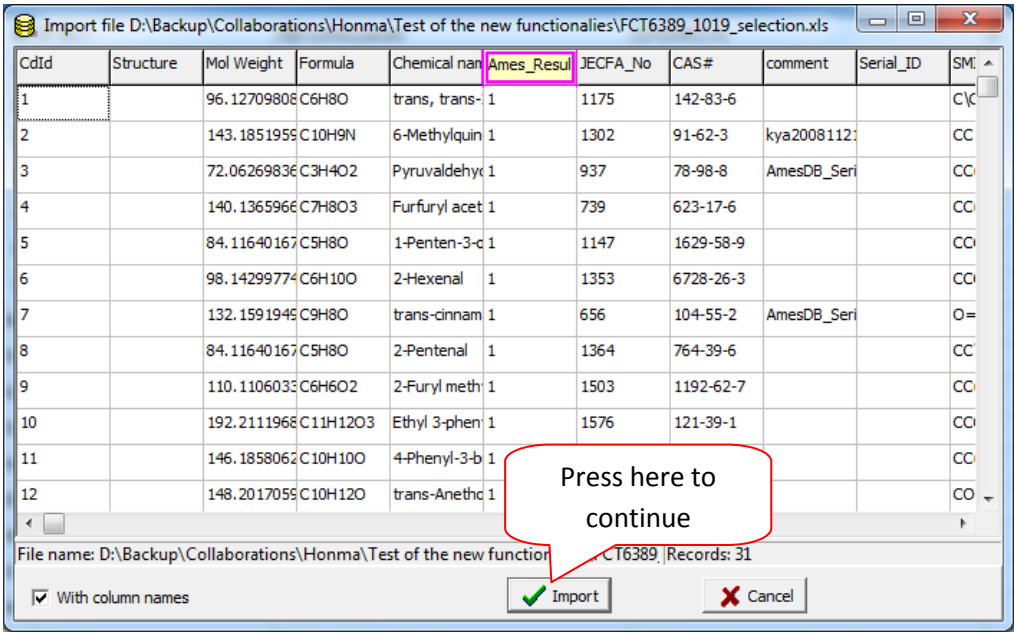


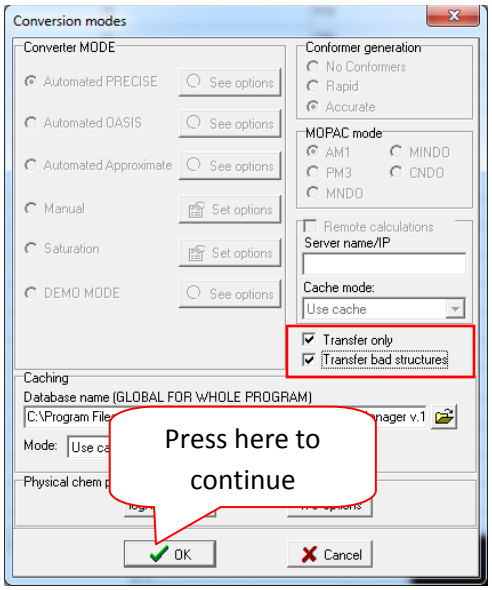


If you do not want to change columns names check in With column names option. Then, define the multi parameter and its characteristics:

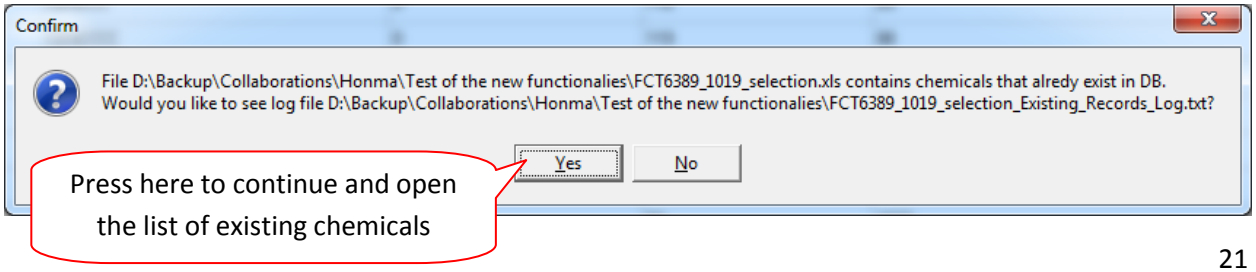




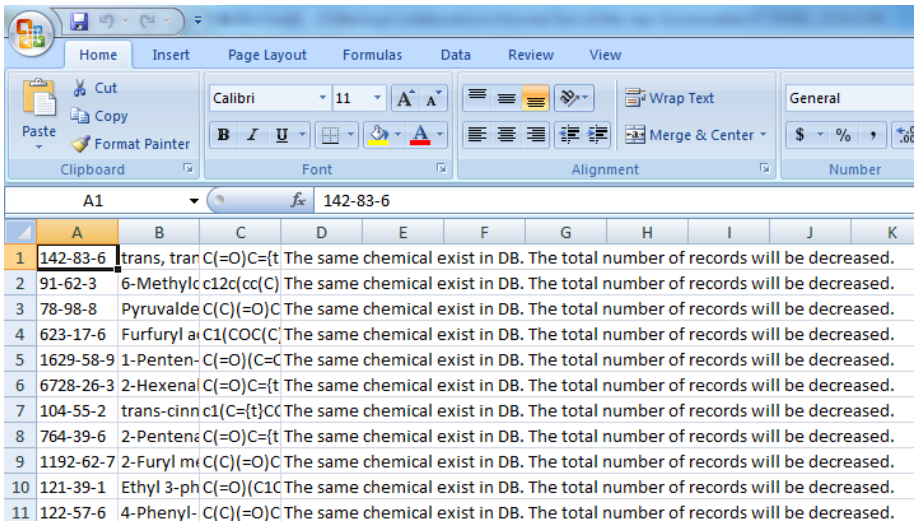




When imported, the system immediately identifies chemicals which exist in the current database:

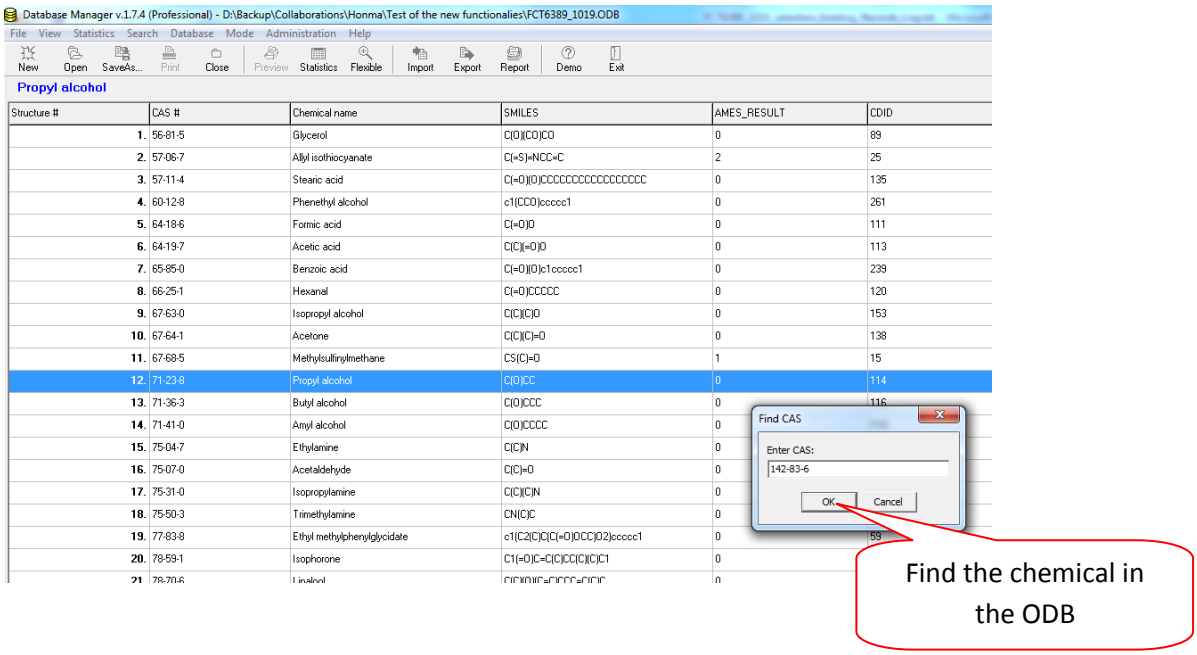


The list of existing chemicals in Excel:



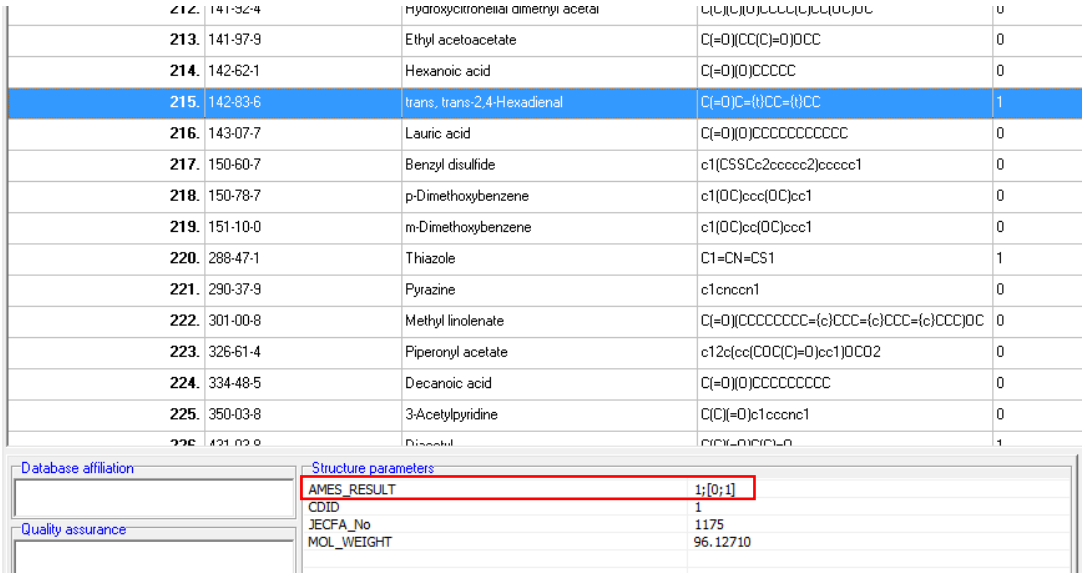
	A	B	C	D
1	142-83-6	trans, tran	C(=O)C={t	The same chemical exist in DB. The total number of records will be decreased.
2	91-62-3	6-Methylc	c12c(cc(C)	The same chemical exist in DB. The total number of records will be decreased.
3	78-98-8	Pyruvalde	C(C)(=O)C	The same chemical exist in DB. The total number of records will be decreased.
4	623-17-6	Furfuryl a	C1(COC(C	The same chemical exist in DB. The total number of records will be decreased.
5	1629-58-9	1-Penten-	C(=O)(C=C	The same chemical exist in DB. The total number of records will be decreased.
6	6728-26-3	2-Hexenal	C(=O)C={t	The same chemical exist in DB. The total number of records will be decreased.
7	104-55-2	trans-cinn	c1(C={t}CC	The same chemical exist in DB. The total number of records will be decreased.
8	764-39-6	2-Pentena	C(=O)C={t	The same chemical exist in DB. The total number of records will be decreased.
9	1192-62-7	2-Furyl me	C(C)(=O)C	The same chemical exist in DB. The total number of records will be decreased.
10	121-39-1	Ethyl 3-ph	C(=O)(C1C	The same chemical exist in DB. The total number of records will be decreased.
11	122-57-6	4-Phenyl-	C(C)(=O)C	The same chemical exist in DB. The total number of records will be decreased.

You are informed that these chemicals exist in the ODB. Copy CAS, make right mouse click and find the chemical in the database:



Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	CDID
1.	56-81-5	Glycerol	C(O)(CO)CO	0	89
2.	57-06-7	Allyl isothiocyanate	C(=S)=NCC=C	2	25
3.	57-11-4	Stearic acid	C(=O)(O)CCCCCCCCCCCCCCCCC	0	135
4.	60-12-8	Phenethyl alcohol	c1(CCO)ccccc1	0	261
5.	64-18-6	Formic acid	C(=O)O	0	111
6.	64-19-7	Acetic acid	C(C)(=O)O	0	113
7.	65-85-0	Benzoic acid	C(=O)(O)c1ccccc1	0	239
8.	66-25-1	Hexanal	C(=O)CCCCC	0	120
9.	67-63-0	Isopropyl alcohol	C(C)(C)O	0	153
10.	67-64-1	Acetone	C(C)(C)=O	0	138
11.	67-68-5	Methylsulfinylmethane	CS(C)=O	1	15
12.	71-23-8	Propyl alcohol	C(O)CC	0	114
13.	71-36-3	Butyl alcohol	C(O)CCC	0	116
14.	71-41-0	Amyl alcohol	C(O)CCCC	0	
15.	75-04-7	Ethylamine	C(C)N	0	
16.	75-07-0	Acetaldehyde	C(C)=O	0	
17.	75-31-0	Isopropylamine	C(C)(C)N	0	
18.	75-50-3	Trimethylamine	CN(C)C	0	
19.	77-83-8	Ethyl methylphenylglycidate	c1(C2(C)C(C(=O)OCC)O2)ccccc1	0	59
20.	78-59-1	Isophorone	C1(=O)C=C(C)CC(C)(C)C1	0	
21.	78-70-6	Linalool	C(C)(O)(C=CCCC=C(C)C	0	

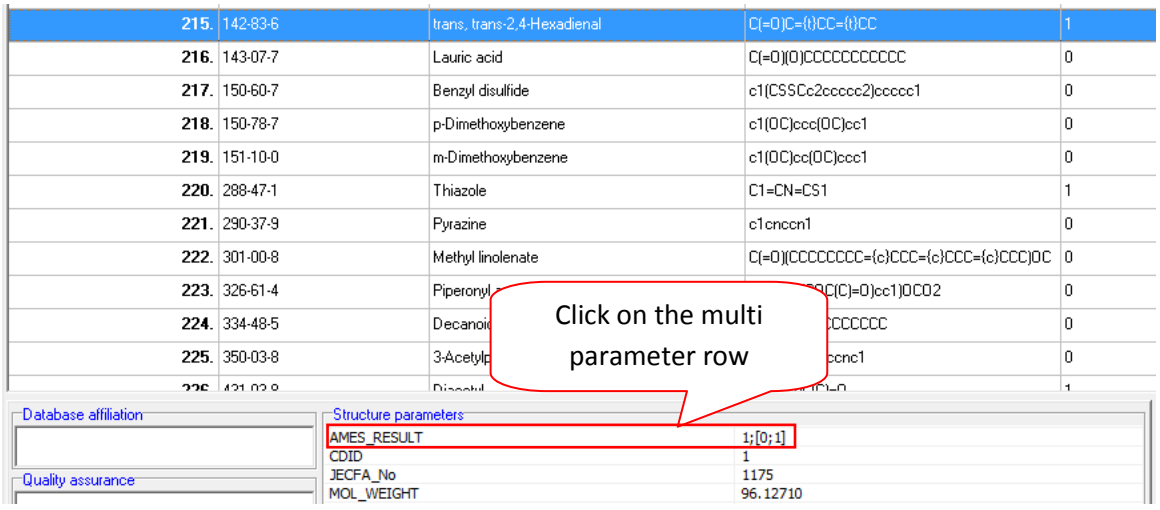
Have a look at the multi parameter values of the selected existing chemicals:



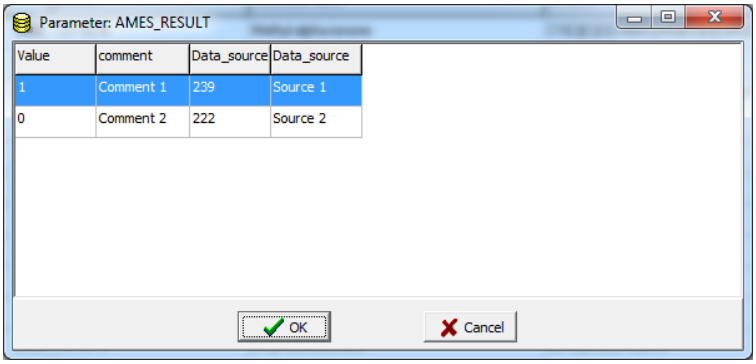
In this case, the multi parameter Ames_Result has now two different values.

E. How to select a default value of the multi parameter

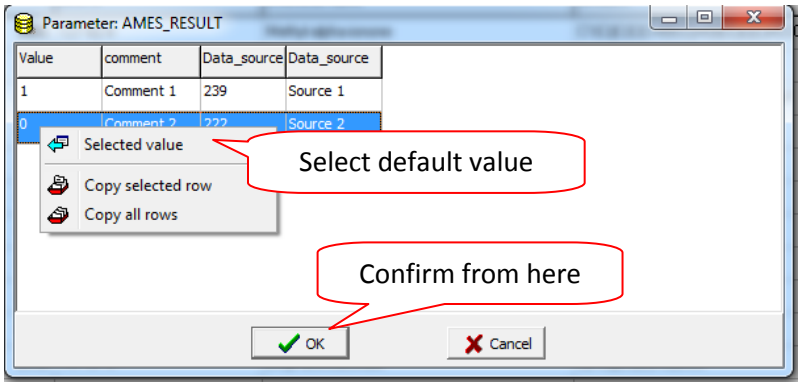
One of the most notable modifications of the DBM is that users have flexibility to select default value of the multi parameter when more than one value is available:



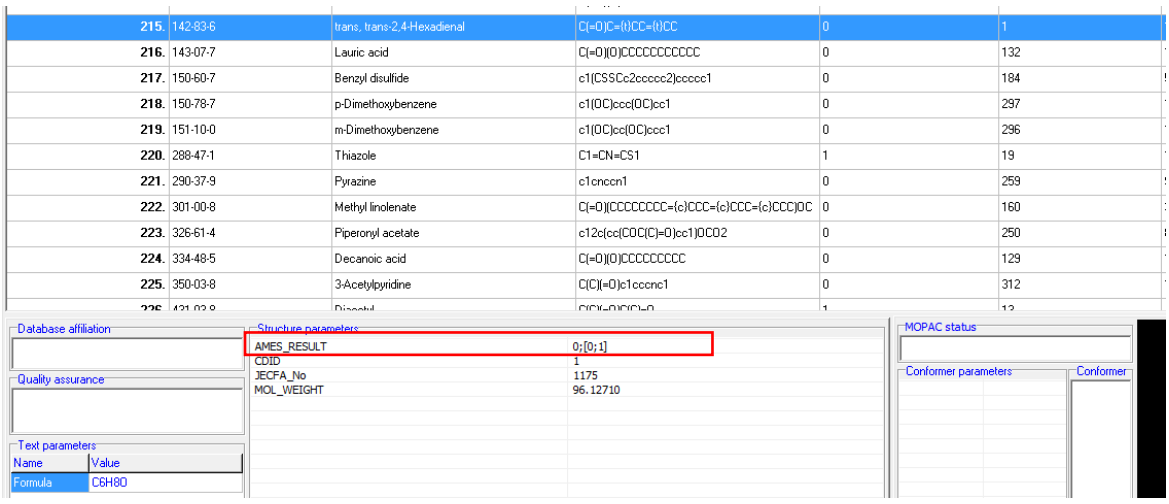
Window appears to show you the characteristics supporting both conflicting values:



Users have given the opportunity to consider which of the existing values of the multi parameter is more reliable. Using the supporting information included in the comments (Japan language is supported) user should be able to decide which value to be considered as default. Make right mouse click on the selected value:



For example, negative Ames result is considered to be more reliable. Default value is always written out of the square brackets:

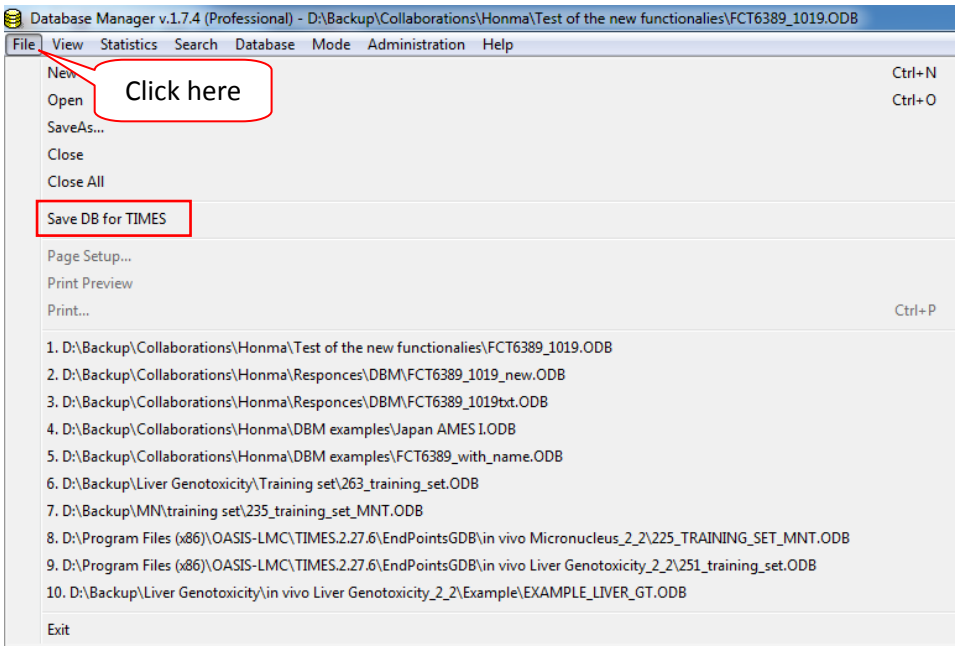


System allows you to change the selected default value. This is important option when acquire new Ames data which need to be reevaluated.

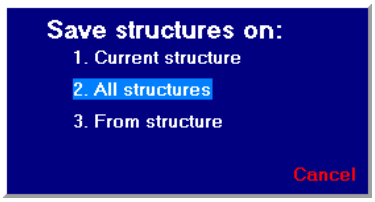
Note: flexible search by Ames result in the database is provided for the selected default value only.

F. How to prepare ODB suitable for TIMES

The DBM gives you the option to save created database and load it in TIMES:



This window appears:



When Save is performed you can load the ODB file in the TIMES. Chose models to make predictions of chemicals with or without metabolic activation.