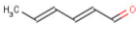
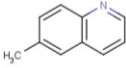
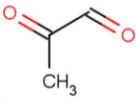
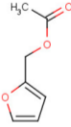


What is new in the Database Manager version 1.7.5

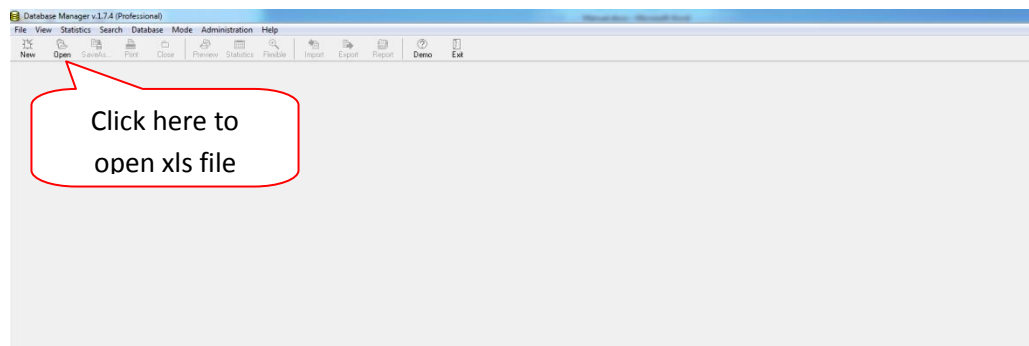
The system provides to users flexibility to create ODB databases starting from excel and tab files. If you collect your chemicals data in a software platform which allows you to make export to xls (Excel 2003) or tab files you can convert these data to ODB files and to use facilities provided by the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

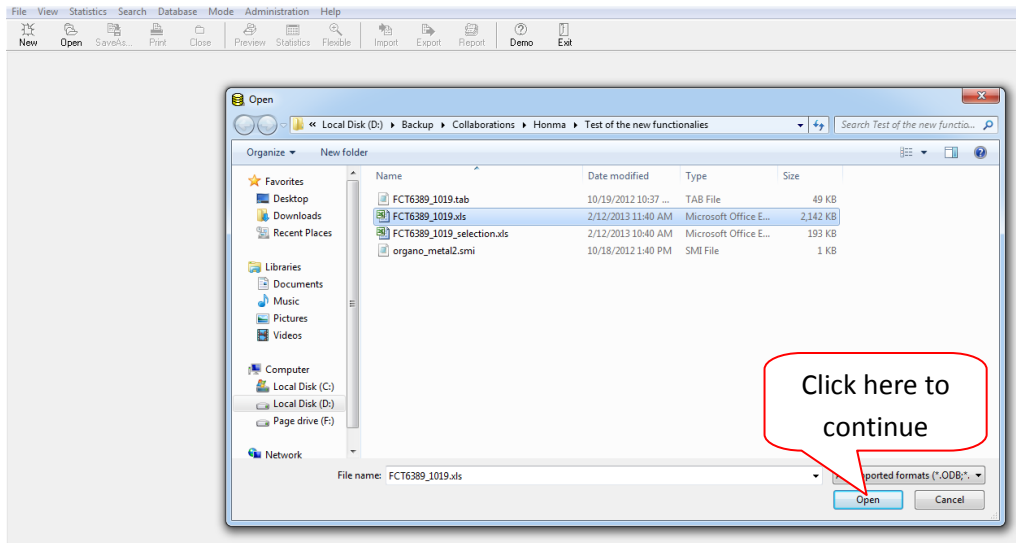
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	ColId	Structure	Mol Weight	Formula	Chemical name	Ames_Result	JECFA_No	CAS#	comment	Serial_ID	SMILES	Data_source	Data_source_ID	
2	1		96.13	C6H8O	trans, trans-2,4-Hexadienal	1	1175	142-83-6			C/C=C/C=C/O	FCT	239	
3	2		143.19	C10H9N	6-Methylquinoline	1	1302	91-62-3	kya20081121003 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_SerialId4931186AmesDB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:

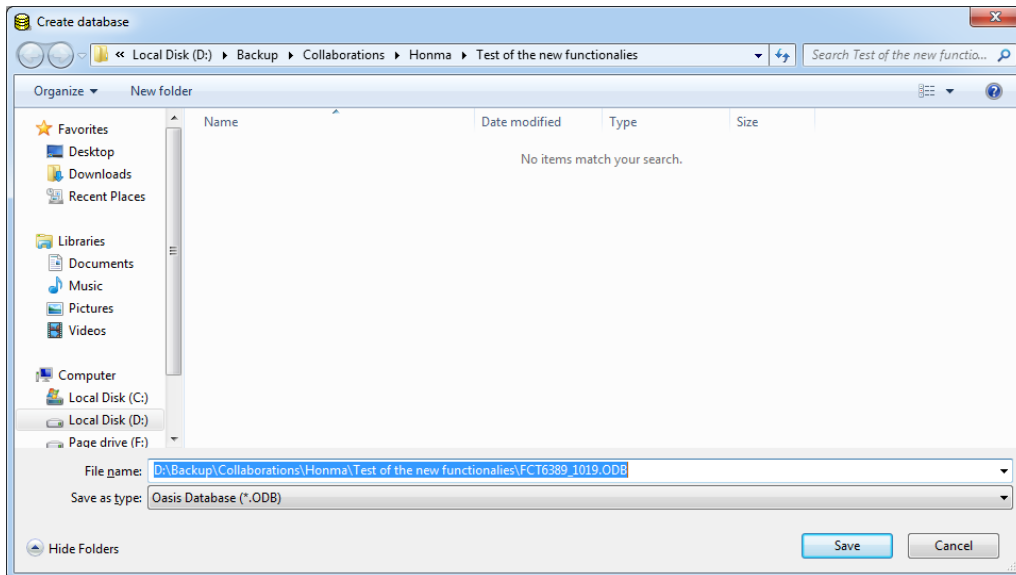


Note: the xls file should not be operating in your computer at this moment.

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:

Import file D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.xls

Cdid	Structure	Mol Weight	Formula	Chemical name	Ames_Result	JECFA_No	CAS#	comment	Serial_ID	SMILES	Data_source	Data_source
1		96.12709808	C6H8O	trans, trans-	1	1175	142-83-6			C/C=C/C=C\FCT	239	
2		143.1851955	C10H9N	6-Methylquin	1	1302	91-62-3	kya2008112		CC1=CC2=C\FCT	269	
3		72.06269836	C3H4O2	Pyruvaldehyc	1	937	78-98-8	AmesDB_Seri		CC(=O)C=O\FCT	199	
4		140.1365966	C7H8O3	Furfuryl acet	1	739	623-17-6			CC(=O)OCC\FCT	145	
5		84.11640167	C5H8O	1-Penten-3-c	1	1147	1629-58-9			CCC(=O)C=O\FCT	232	
6		98.14299774	C6H10O	2-Hexenal	1	1353	6728-26-3			CCC/C=C/C\FCT	290	
7		132.1591945	C9H8O	trans-cinnam	1	656	104-55-2	AmesDB_Seri		O=C/C=C/C\FCT	117	
8		84.11640167	C5H8O	2-Pentalen	1	1364	764-39-6			CC/C=C/C=C\FCT	296	
9		110.1106035	C6H6O2	2-Furyl meth	1	1503	1192-62-7			CC(=O)C1=O\FCT	320	
10		192.2111968	C11H12O3	Ethyl 3-phen	1	1576	121-39-1			CCOC(=O)C\FCT	340	
11		146.1858062	C10H10O	4-Phenyl-3-b	1	820	122-57-6			CC(=O)C=C\FCT	167	
12		148.2017055	C10H12O	trans-Anetho	1	217	4180-23-8			COC1=CC=C\FCT	42	

File name: D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.xls Records: 368

☐ With column names

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:

Import file D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.xls

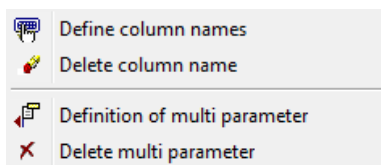
Cdid	Structure	Mol Weight	Formula	Chemical name	Ames_Result	JECFA_No	CAS#	comment	Serial_ID	SMILES
1		96.12709808	C6H8O	trans, trans-	1	1175	142-83-6			C/C=C/C=C\FCT
2		143.1851955	C10H9N	6-Methylquin	1	1302	91-62-3	kya2008112		CC1=CC2=C\FCT
3		72.06269836	C3H4O2	Pyruvaldehyc	1	937	78-98-8	AmesDB_Seri		CC(=O)C=O\FCT
4		140.1365966	C7H8O3	Furfuryl acet	1	739	623-17-6			CC(=O)OCC\FCT
5		84.11640167	C5H8O	1-Penten-3-c	1	1147	1629-58-9			CCC(=O)C=O\FCT
6		98.14299774	C6H10O	2-Hexenal	1	1353	6728-26-3			CCC/C=C/C\FCT
7		132.1591945	C9H8O	trans-cinnam	1	656	104-55-2	AmesDB_Seri		O=C/C=C/C\FCT
8		84.11640167	C5H8O	2-Pentalen	1	1364	764-39-6			CC/C=C/C=C\FCT
9		110.1106035	C6H6O2	2-Furyl meth	1	1503	1192-62-7			CC(=O)C1=O\FCT
10		192.2111968	C11H12O3	Ethyl 3-phen	1	1576	121-39-1			CCOC(=O)C\FCT
11		146.1858062	C10H10O	4-Phenyl-3-b	1	820	122-57-6			CC(=O)C=C\FCT
12		148.2017055	C10H12O	trans-Anetho	1	217	4180-23-8			COC1=CC=C\FCT

File name: D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.xls Records: 368

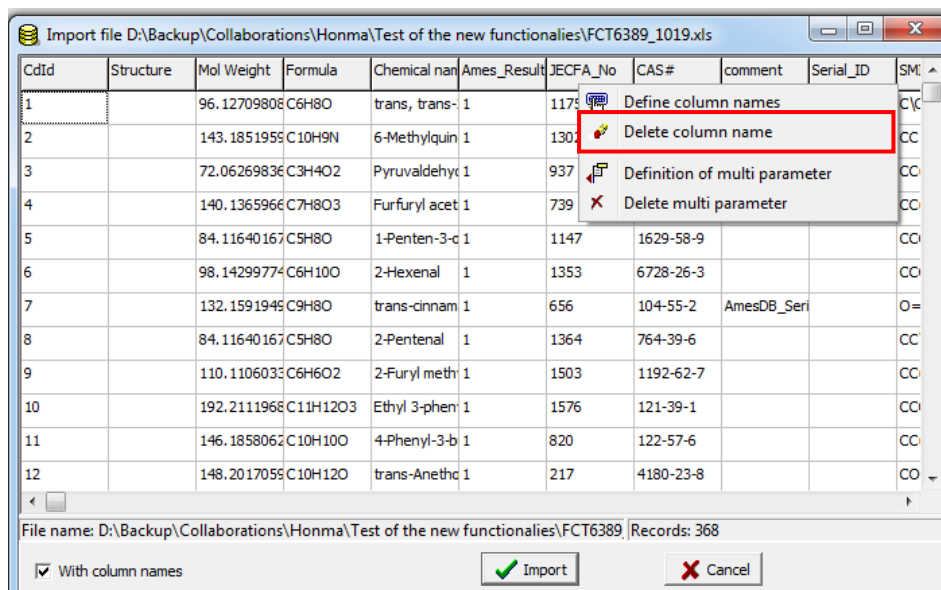
☒ With column names

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

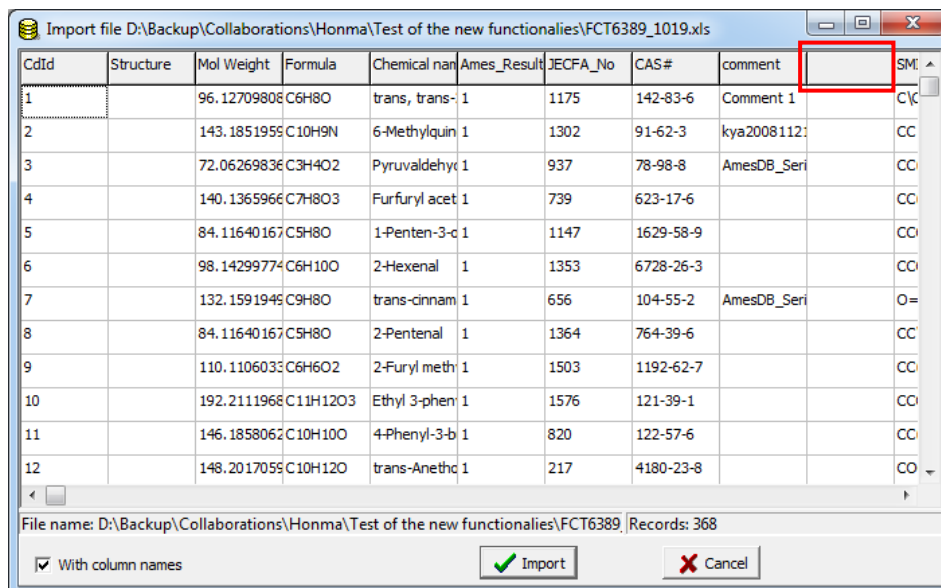
The system also allows you to edit existing columns names or to delete and define new names. Make right mouse click on the name. This window appears:



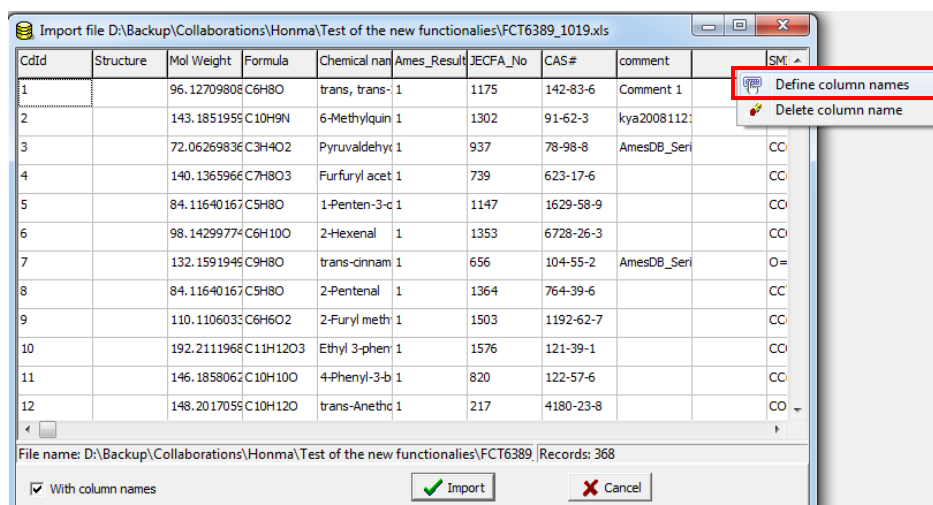
Choose **Delete column name**:



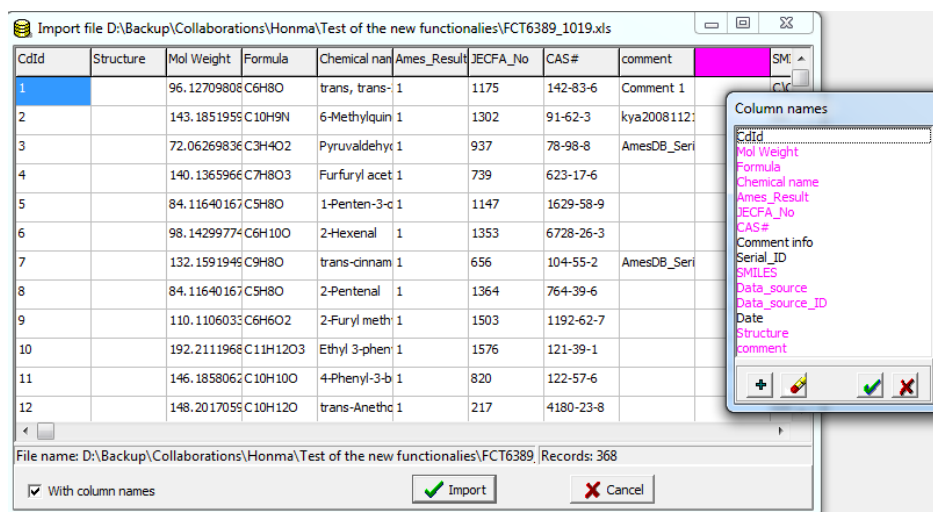
The column name disappear:



Now you can define new column name:

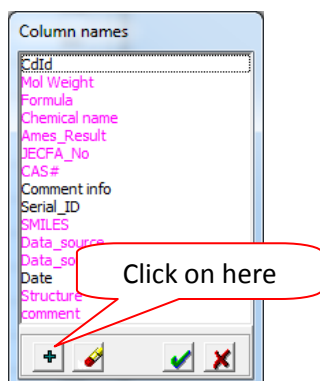


The following window appears:

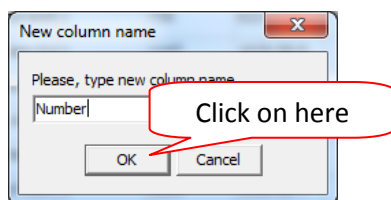


Names colored in pink have already been used as captions of the other columns. Black colored names are free to use. Choose the corresponding name and confirm by button.

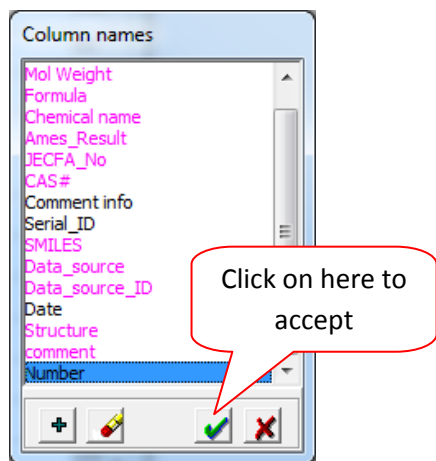
Nevertheless, you can define name which does not exist in the list of names:



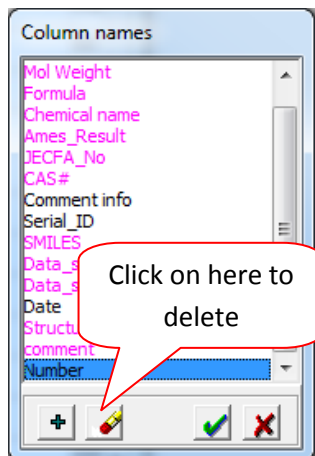
This window appears:



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:

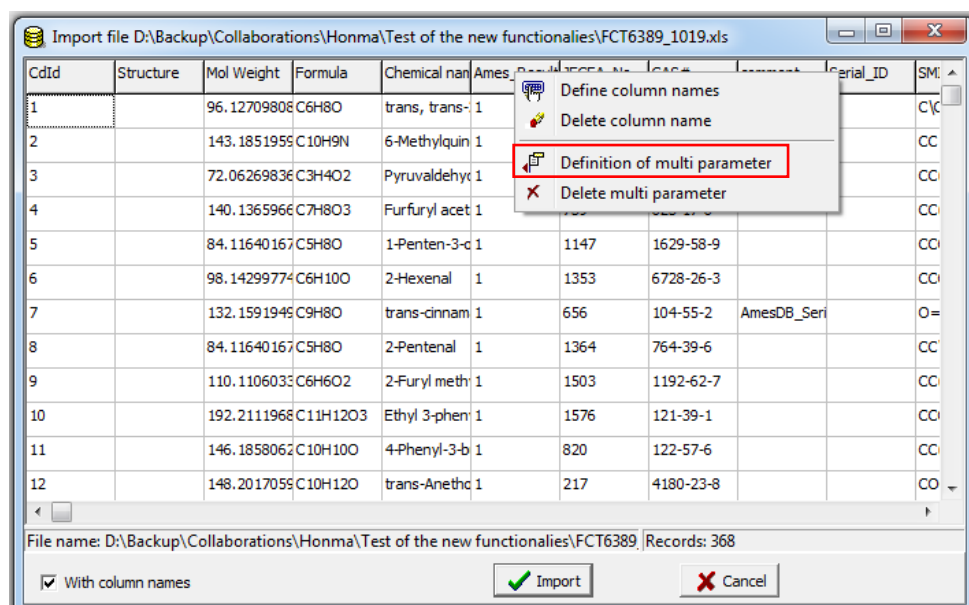


If you want to close the **Column names** window press  button.

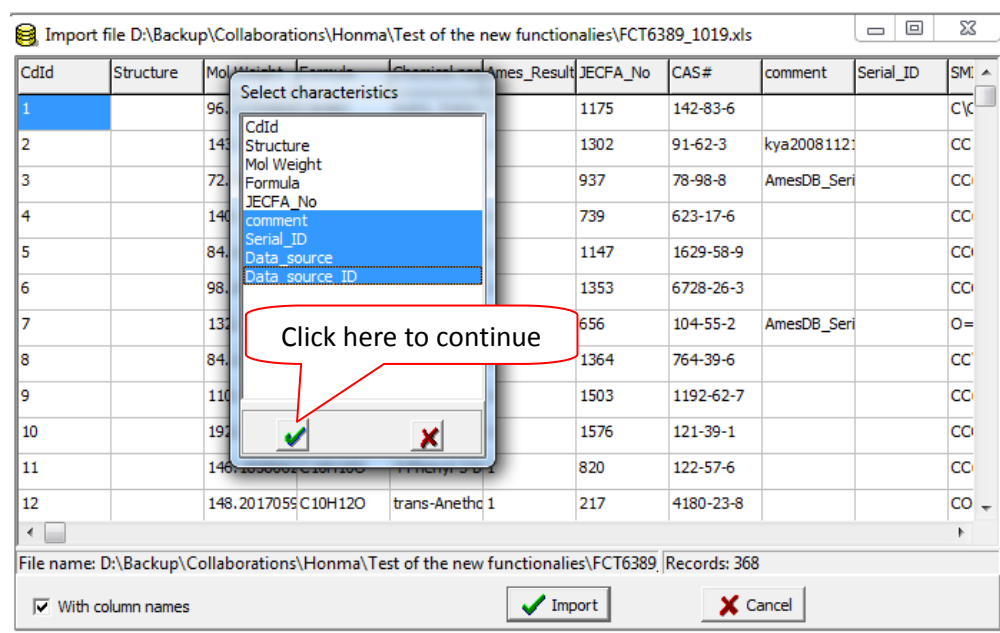
Now you should select a multi parameter. This is the parameter for which different integer values could be provided in the database. Here, the multi parameter is the **Ames_Result** because it may possess negative (0), positive (1) or equivocal (2) data.

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.

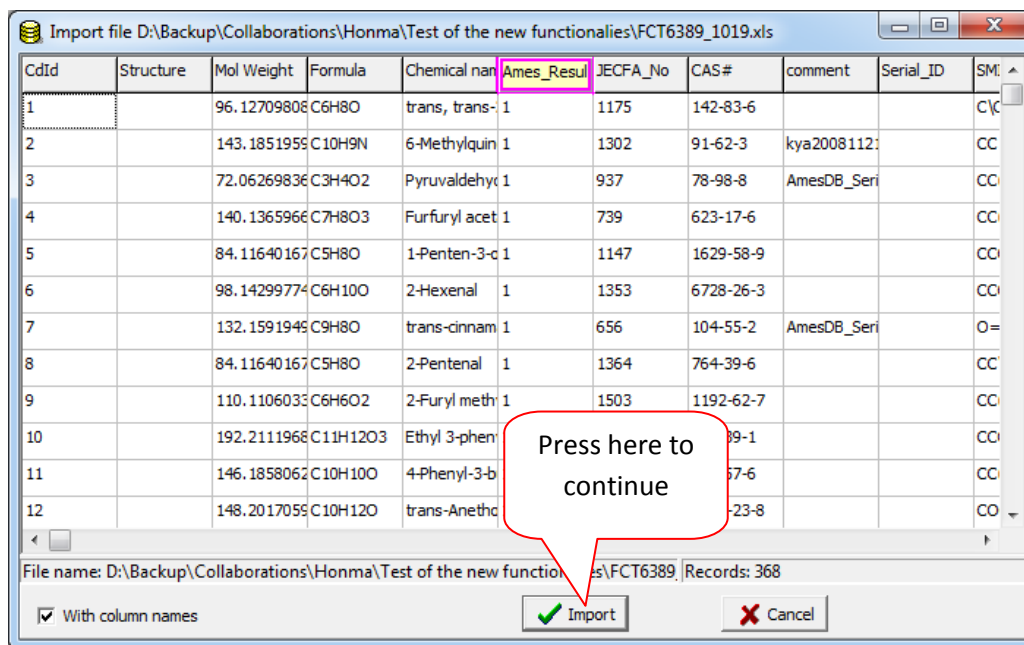
Selected the multi parameter by making right mouse click on the **Ames Result** column name:



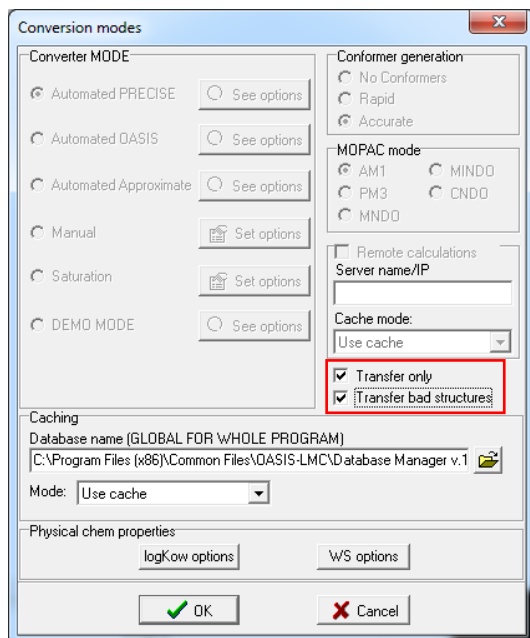
Along with selection of the multi parameter users need to define parameters which are associated to this parameter. These are any specific characteristics supporting the multi parameter, e.g. comment, Serial ID, etc:



When defined, the multi parameter will be yellow colored:

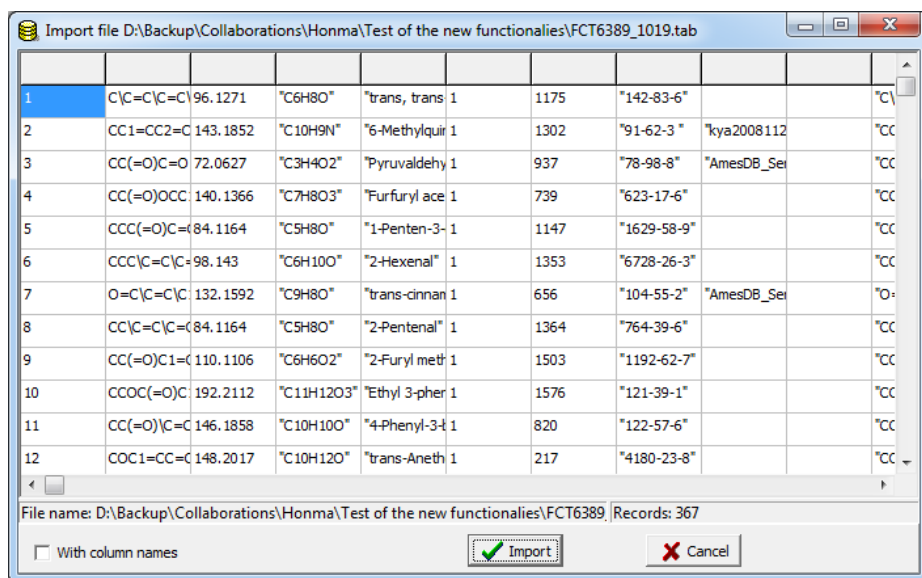


The following window appears:



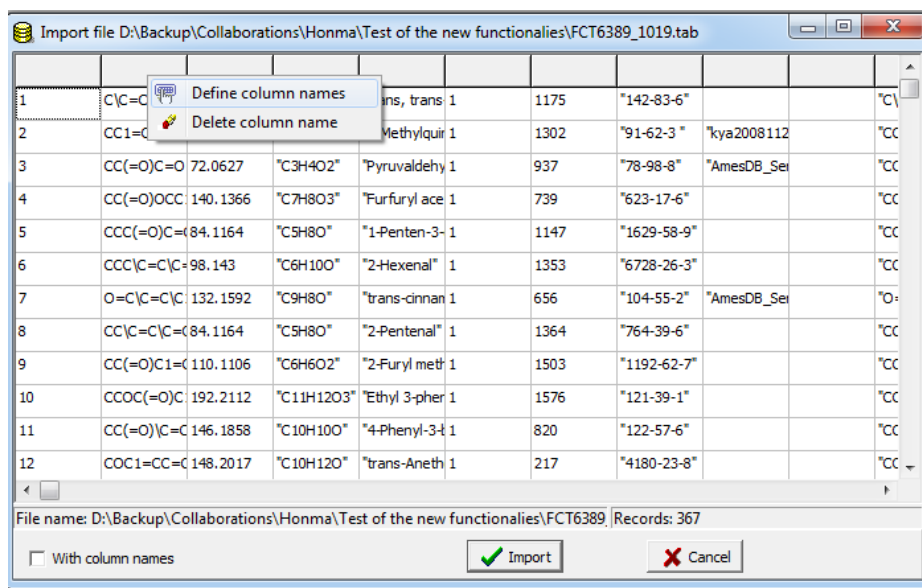
Do not forget to choose the option **Transfer bad structures**. This option allows you to import chemicals with errors in smiles, which can be edited manually. These structures can be inorganic chemicals, organo-metals, etc. Press OK.

The following window will appear:

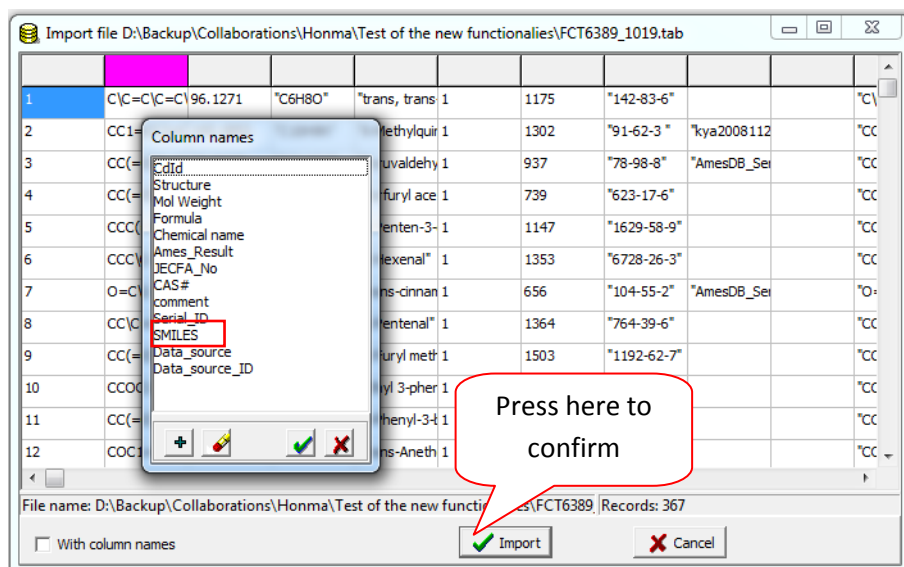


As seen, the columns names are empty and you need to define them manually:

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

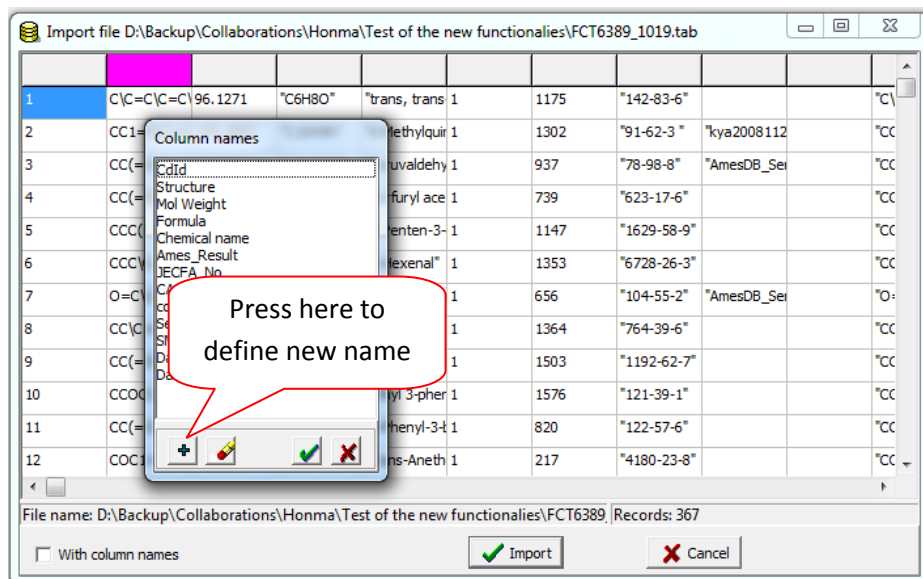


Select the corresponding name from a list of names:

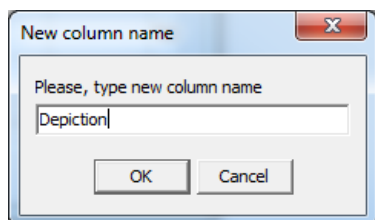


Select the corresponding name of each of the columns.

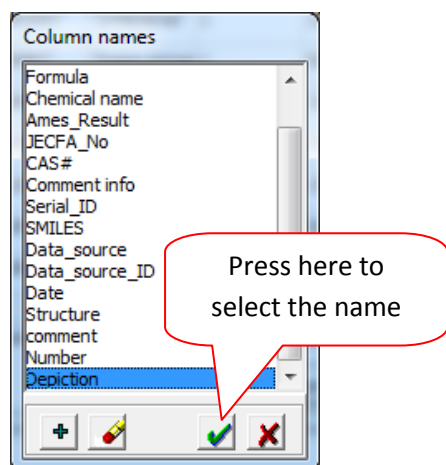
User is also allowed to type a new column name:



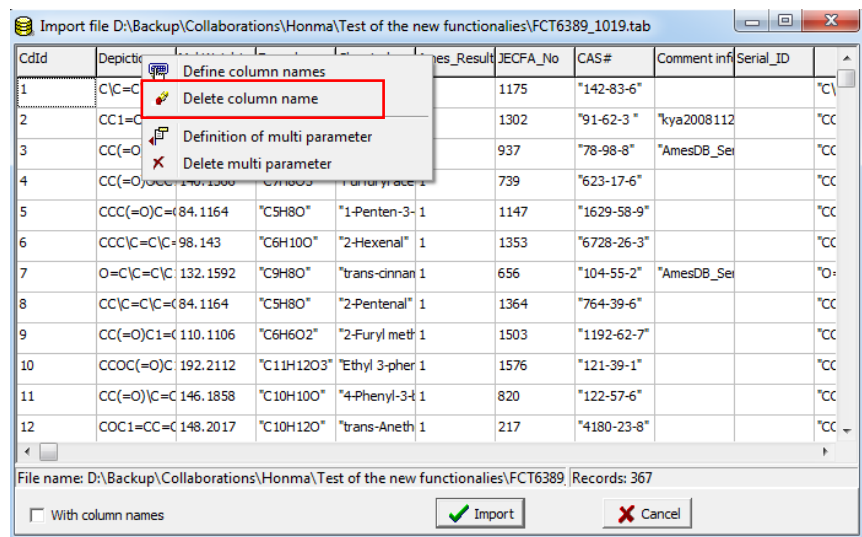
Type a name which will be new in the list:



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:

Import file D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.tab

CdId	Depiction	Mol Weight	Formula	Chemical name	Ames_Result	JECFA_No	CAS#	Comment info	Serial_ID
1	C/C=C/C=C	96.1271	"C6H8O"	"trans, trans	1	1175	"142-83-6"		"C\
2	CC1=CC2=C	143.1852	"C10H9N"	"6-Methylqui	1	1302	"91-62-3 "	"kya2008112	"CC
3	CC(=O)C=O	72.0627	"C3H4O2"	"Pyruvaldehy	1	937	"78-98-8"	"AmesDB_Ser	"CC
4	CC(=O)OCC	140.1366	"C7H8O3"	"Furfuryl ace	1	739	"623-17-6"		"CC
5	CCC(=O)C=C	84.1164	"C5H8O"	"1-Penten-3-	1	1147	"1629-58-9"		"CC
6	CCC/C=C/C=C	98.143	"C6H10O"	"2-Hexenal"	1	1353	"6728-26-3"		"CC
7	O=C/C=C/C=C	132.1592	"C9H8O"	"trans-cinnan	1	656	"104-55-2"	"AmesDB_Ser	"O-
8	CC/C=C/C=C	84.1164	"C5H8O"	"2-Pentenal"	1	1364	"764-39-6"		"CC
9	CC(=O)C1=C	110.1106	"C6H6O2"	"2-Furyl meth	1	1503	"1192-62-7"		"CC
10	CCOC(=O)C	192.2112	"C11H12O3"	"Ethyl 3-pher	1	1576	"121-39-1"		"CC
11	CC(=O)/C=C	146.1858	"C10H10O"	"4-Phenyl-3-4	1	820	"122-57-6"		"CC
12	COC1=CC=C	148.2017	"C10H12O"	"trans-Aneth	1	217	"4180-23-8"		"CC

File name: D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.tab Records: 367

☐ With column names

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

Import file D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.tab

CdId	Depiction	Mol Weight	Formula	Chemical name	Ames_Result	JECFA_No	CAS#	Comment info	Serial_ID
1	C/C=C/C=C	96.1271	"C6H8O"	"trans, trans	1	1175	"142-83-6"		"C\
2	CC1=CC2=C	143.1852	"C10H9N"	"6-Methylqui	1	1302	"91-62-3 "	"kya2008112	"CC
3	CC(=O)C=O	72.0627	"C3H4O2"	"Pyruvaldehy	1	937	"78-98-8"	"AmesDB_Ser	"CC
4	CC(=O)OCC	140.1366	"C7H8O3"	"Furfuryl ace	1	739	"623-17-6"		"CC
5	CCC(=O)C=C	84.1164	"C5H8O"	"1-Penten-3-	1	1147	"1629-58-9"		"CC
6	CCC/C=C/C=C	98.143	"C6H10O"	"2-Hexenal"	1	1353	"6728-26-3"		"CC
7	O=C/C=C/C=C	132.1592	"C9H8O"	"trans-cinnan	1	656	"104-55-2"	"AmesDB_Ser	"O-
8	CC/C=C/C=C	84.1164	"C5H8O"	"2-Pentenal"	1	1364	"764-39-6"		"CC
9	CC(=O)C1=C	110.1106	"C6H6O2"	"2-Furyl meth	1				"CC
10	CCOC(=O)C	192.2112	"C11H12O3"	"Ethyl 3-pher	1				"CC
11	CC(=O)/C=C	146.1858	"C10H10O"	"4-Phenyl-3-4	1				"CC
12	COC1=CC=C	148.2017	"C10H12O"	"trans-Aneth	1				"CC

File name: D:\Backup\Collaborations\Honma\Test of the new functionalities\FCT6389_1019.tab Records: 367

☐ With column names

Press here to continue

Then, the ODB is created.

C. What can we do with created ODB file

When imported the ODB looks like that:

The screenshot shows the Glycerol browser interface. The main table displays chemical data for various compounds. The chemical structure of Glycerol is shown on the right.

Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	JECFA_No
1	57-05-7	Glycerol	C(C(CO)CO)CO	0	909
2	57-05-7	Allyl isothiocyanate	C=C(S)=NCC=C	2	1560
3	57-11-4	Stearic acid	C1=O)CCCCCCCCCCCCCCCC	0	116
4	60-12-8	Phenethyl alcohol	c1(CCO)ccccc1	0	987
5	64-19-6	Formic acid	C=O)O	0	79
6	64-19-7	Acetic acid	C(C)=O)O	0	81
7	65-85-0	Benzoic acid	C=O)O)c1ccccc1	0	850
8	66-25-1	Hexanal	C=O)CCCC	0	92
9	67-63-0	Isopropyl alcohol	C(C)C)O	0	277
10	67-64-1	Acetone	C(C)C)=O	0	139
11	67-68-5	Methylsulfinylmethane	CS(C)=O	1	507
12	71-23-8	Propyl alcohol	C)O)CC	0	82
13	71-36-3	Butyl alcohol	C)O)CCC	0	85
14	71-41-0	Amyl alcohol	C)O)CCCC	0	88
15	75-04-7	Ethylamine	C)CN	0	1579
16	75-07-0	Acetobutyrol	C=O)CC(C)O	0	80

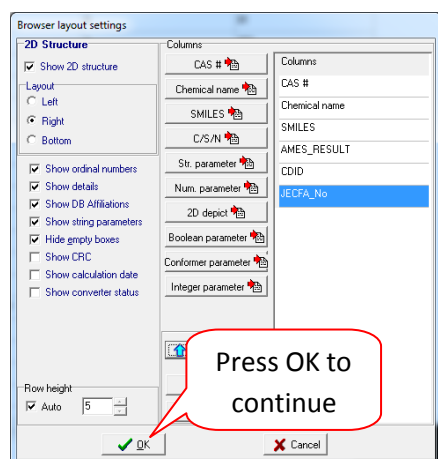
Press view and configure your browser:

The screenshot shows the Database Manager v.1.7.4 (Professional) interface. The Glycerol browser is configured to show the following columns:

Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	JECFA_No
1	57-05-7	Glycerol	C(C(CO)CO)CO	0	909
2	57-05-7	Allyl isothiocyanate	C=C(S)=NCC=C	2	1560
3	57-11-4	Stearic acid	C1=O)CCCCCCCCCCCCCCCC	0	116
4	60-12-8	Phenethyl alcohol	c1(CCO)ccccc1	0	987
5	64-19-6	Formic acid	C=O)O	0	79
6	64-19-7	Acetic acid	C(C)=O)O	0	81
7	65-85-0	Benzoic acid	C=O)O)c1ccccc1	0	850
8	66-25-1	Hexanal	C=O)CCCC	0	92
9	67-63-0	Isopropyl alcohol	C(C)C)O	0	277
10	67-64-1	Acetone	C(C)C)=O	0	139
11	67-68-5	Methylsulfinylmethane	CS(C)=O	1	507
12	71-23-8	Propyl alcohol	C)O)CC	0	82
13	71-36-3	Butyl alcohol	C)O)CCC	0	85
14	71-41-0	Amyl alcohol	C)O)CCCC	0	88
15	75-04-7	Ethylamine	C)CN	0	1579
16	75-07-0	Acetobutyrol	C=O)CC(C)O	0	80

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 screenshot shows the Browser layout settings dialog box. The 'Columns' tab is selected, and a red box highlights the 'Up' and 'Down' buttons. A callout box points to these buttons with the text: "Click here to change order of columns".



The newly configure browser appears:

Database Manager v.17.4 (Professional) - D:\Backup\Collaborations\Normal\Test of the new functionalities\FC16389_1019.ODB

File View Statistics Search Database Mode Administration Help

New Open Save As... Print Close Preview Statistics Flexible Import Export Report Demo Exit

Glycerol

Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	CCID	JECFA_No
1	56-81-5	Glycerol	<chem>OCC(O)CO</chem>	0	89	909
2	57-06-7	Allyl isothiocyanate	<chem>C=CSCC=C</chem>	2	25	1560
3	57-11-4	Stearic acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>	0	135	116
4	60-12-8	Phenethyl alcohol	<chem>c1ccc(cc1)CCO</chem>	0	261	987
5	64-19-6	Formic acid	<chem>C=O</chem>	0	111	79
6	64-19-7	Acetic acid	<chem>CC(=O)O</chem>	0	113	81
7	65-85-0	Benzoic acid	<chem>C1=CC=C(C=C1)C(=O)O</chem>	0	239	950
8	66-25-1	Hexanal	<chem>CCCCCC=O</chem>	0	120	92
9	67-63-0	Isopropyl alcohol	<chem>CC(C)CO</chem>	0	153	277
10	67-64-1	Acetone	<chem>CC(C)=O</chem>	0	138	139
11	67-68-5	Methylsulfinylmethane	<chem>CS(C)=O</chem>	1	15	507
12	71-23-8	Propyl alcohol	<chem>CCCOC</chem>	0	114	82
13	71-36-3	Butyl alcohol	<chem>CCCCOC</chem>	0	116	85
14	71-41-0	Amyl alcohol	<chem>CCCCCOC</chem>	0	119	88
15	75-04-7	Ethylamine	<chem>CCN</chem>	0	349	1579
16	75-07-0	Acetaldehyde	<chem>CC=O</chem>	0	112	80
17	75-31-0	Isopropylamine	<chem>CC(C)N</chem>	0	350	1581
18	75-50-3	Trimethylamine	<chem>CN(C)C</chem>	0	360	1610
19	77-83-8	Ethyl methylphenylglycidate	<chem>c1cc(ccc1)C1OC(=O)CC1</chem>	0	59	1577
20	78-59-1	Isophorone	<chem>CC1(C)CC(C)CC1</chem>	0	278	1112
21	78-70-6	Linalool	<chem>CC1=CC(C)CC1C</chem>	0	161	356
22	78-81-8	Isobutylamine	<chem>CC(C)CN</chem>	0	352	1583
23	78-83-1	Isobutyl alcohol	<chem>CC(C)CO</chem>	0	147	251

Database affiliation: Structure parameters: AMES_RESULT 0:01
CCID 89
JECFA_No 909
MOL_WEIGHT 92.09380

Quality assurance

Text parameters:
Name Value
Structure OCC(O)CO
Formula C3H8O3

MOPAC status

Conformer parameters: Conformer

FC16389_1019.ODB

Database: FC16389_1019.ODB Structures: 367

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:

Database Manager v.1.7.4 (Professional) - D:\Backup\Collaborations\Honna\Test of the new functionalities\FCT6389_1019.ODB

File View Statistics Search Database Mode Administration Help

New Open SaveAs... Print Close Preview Statistics Flexible Import Export Report Demo Exit

Glycerol

Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	Sort	CDID	JECFA_No
1. 56-81-5		Glycerol	<chem>OCC(O)CO</chem>	0	Sort	39	909
2. 57-06-7		Allyl isothiocyanate	<chem>CS(=S)NCC=C</chem>	2	Ascending	25	1560
3. 57-11-4		Stearic acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>	0	Descending	135	116
4. 60-12-8		Phenethyl alcohol	<chem>c1ccc(cc1)CCO</chem>	0		261	987
5. 64-18-6		Formic acid	<chem>OC=O</chem>	0		111	79
6. 64-19-7		Acetic acid	<chem>CC(=O)O</chem>	0		113	81
7. 65-85-0		Benzoic acid	<chem>c1ccccc1C(=O)O</chem>	0		239	850
8. 66-25-1		Hexanal	<chem>CCCCCC=O</chem>	0		120	92
9. 67-63-0		Isopropyl alcohol	<chem>CC(C)CO</chem>	0		153	277
10. 67-64-1		Acetone	<chem>CC(C)=O</chem>	0		138	139
11. 67-68-5		Methylsulfinylmethane	<chem>CS(C)=O</chem>	1		15	507

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

Database Manager v.1.7.4 (Professional) - D:\Backup\Collaborations\Honna\Test of the new functionalities\FCT6389_1019.ODB

File View Statistics Search Database Mode Administration Help

New Open SaveAs... Print Close Preview Statistics Flexible Import Export Report Demo Exit

2-Methyl-2-pentenal

Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	CDID	JECFA_No
1. 623-36-9		2-Methyl-2-pentenal	<chem>CC(C)=C/C=C/C</chem>	0	39	1209
2. 101-86-0		alpha-Hexylcinnamaldehyde	<chem>c1cc(ccc1)/C=C/C(CCCCC)C=O</chem>	0	40	686
3. 65405-67-6		p-Methoxy-alpha-methyl-cinnamaldehyde	<chem>COc1ccc(cc1)/C=C/C(C)C=O</chem>	0	41	689
4. 2111-75-3		p-Mentha-1,8-dien-7-al	<chem>CC1=CC(C=C(C=C1)C=O)CC</chem>	0	42	973
5. 116-26-7		2,6,8-Trimethylcyclohexa-1,3-dienyl methanal	<chem>CC1=CC(C=C(C=C1)C=O)CC</chem>	0	43	977
6. 5392-40-5		Citral	<chem>CC(=C)CC=CC=CC=O</chem>	0	44	1225
7. 101-39-3		alpha-Methylcinnamaldehyde	<chem>CC1=CC(C=C(C=C1)C=O)C=O</chem>	0	45	683
8. 122-40-7		alpha-Amylcinnamaldehyde	<chem>c1cc(ccc1)/C=C/C(CCCC)C=O</chem>	0	46	685
9. 1504-74-1		o-Methoxycinnamaldehyde	<chem>c1cc(ccc1)/C=C/C(C=O)C=O</chem>	0	47	688
10. 620-02-0		5-Methylfurfural	<chem>CC1=C(C=CC=C1)C=O</chem>	0	48	745
11. 6750-03-4		2,4-Nonadienal	<chem>CCCC=CC=CC=CC=O</chem>	0	49	1185

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**:

Database Manager v.1.7.4 (Professional) - D:\Backup\Collaborations\Honna\Test of the new functionalities\FCT6389_1019.ODB

File View Statistics Search Database Mode Administration Help

New Open SaveAs... Print Close Preview Statistics Flexible Import Export Report Demo Exit

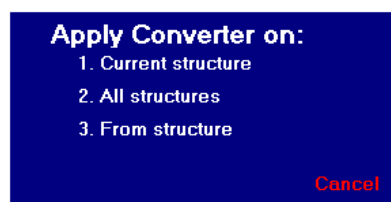
Glycerol

Structure #	CAS #	Chemical name	SMILES	AMES_RESULT	CDID	JECFA_No
1. 56-81-5		Glycerol	<chem>OCC(O)CO</chem>	0	39	909
2. 57-06-7		Allyl isothiocyanate	<chem>CS(=S)NCC=C</chem>	2	25	1560
3. 57-11-4		Stearic acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>	0	135	116
4. 60-12-8		Phenethyl alcohol	<chem>c1ccc(cc1)CCO</chem>	0	261	987
5. 64-18-6		Formic acid	<chem>OC=O</chem>	0	111	79
6. 64-19-7		Acetic acid	<chem>CC(=O)O</chem>	0	113	81
7. 65-85-0		Benzoic acid	<chem>c1ccccc1C(=O)O</chem>	0	239	850
8. 66-25-1		Hexanal	<chem>CCCCCC=O</chem>	0	120	92
9. 67-63-0		Isopropyl alcohol	<chem>CC(C)CO</chem>	0	153	277
10. 67-64-1		Acetone	<chem>CC(C)=O</chem>	0	138	139
11. 67-68-5		Methylsulfinylmethane	<chem>CS(C)=O</chem>	1	15	507
12. 75-29-8		Propanol alcohol	<chem>CCCO</chem>	0	114	82

Press OK to continue

CAS Order

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



After calculations:

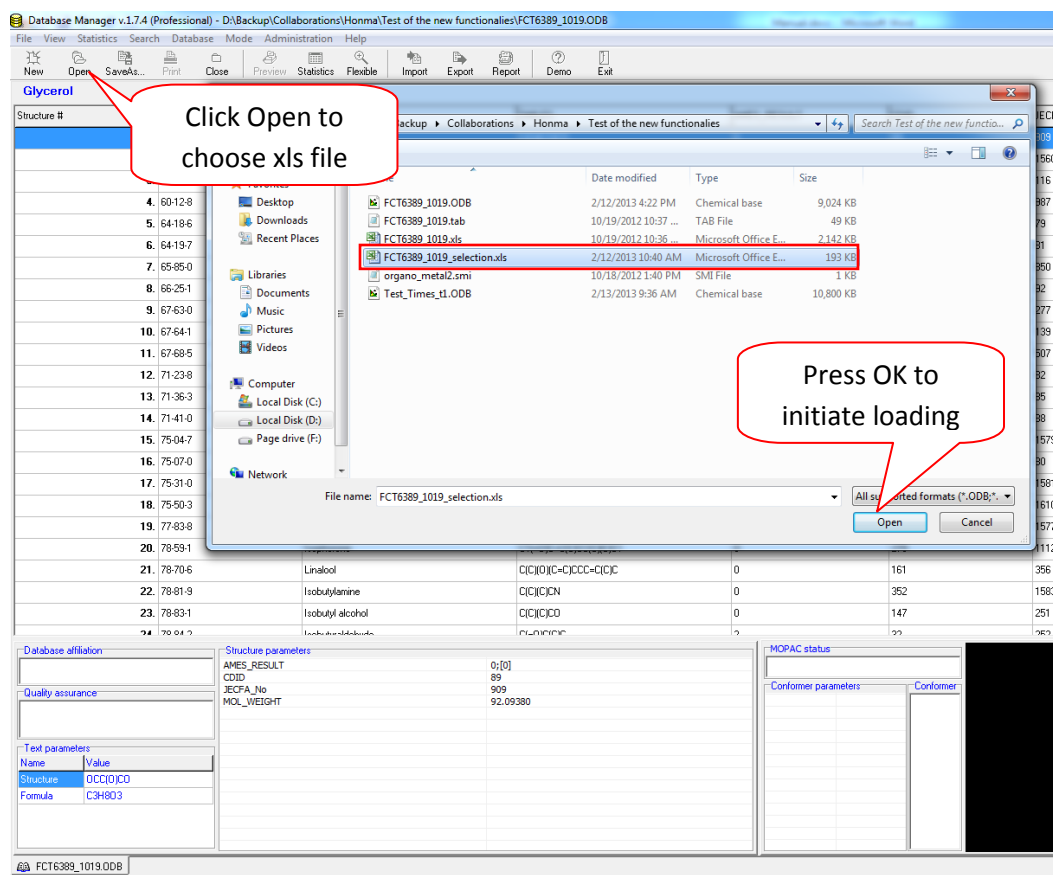
16.	75-04-7	Ethylamine	C/CN		
17.	75-07-0	Acetaldehyde	C(C)=O		
18.	75-31-0	Isopropylamine	C(C)CN		
19.	75-50-3	Trimethylamine	CN(C)C		
20.	77-83-8	Ethyl methylphenylglycidate	c1(C2(C)C(C=O)OCC)O2)ccccc1		
21.	78-59-1	Isophorone	CC1(=O)C=C(C)CC(C)C1		
22.	78-70-6	Linalool	C(C)O(C=C)CC=C(C)C		
23.	78-81-9	Isobutylamine	C(C)CN		

Database affiliation		Structure parameters		MOPAC status	
Quality assurance		AMES_RESULT	0:[0]	Precise	
Structure quality: High		BALABAN_D2	3.165751	Conformer parameters	
Converter mode: AutoPrecise		BALABAN_J	5.176409	A_max [(a.u.)]	0.25911
Text parameters		CDID	89	BCF_Covera...	0
Name	Value	ENTROPY	4.200542	CALC_HEAT...	-153.43460
Formula	C3H8O3	Exp_log(Kow)	-1.76000	D_max [(a.u.)]	0.24672
CalcTrace_CM		INFO_CHI	1.922023	Diameff [A]	5.454559
		INFO_WIENER	6.37570	Diammax [A]	7.004294
		JECHA_No	909	Diammin [A]	4.846617
		Log(Kow) [mol.Lg-1mol-1Lw]	-1.65240	DIPOLE_MO...	1.85408
		log_Kp	-4.11389	E_GAP [eV]	13.73490
		logBCF	0.4260407	E_HOMO [eV]	-10.69791
		logBCF_MaxTox	-1.23269	ELECTRONE...	-3.83046
		logBCFmax	0.9641899	Electrochil...	1.068769
		logBCFmax...	-2.60074		

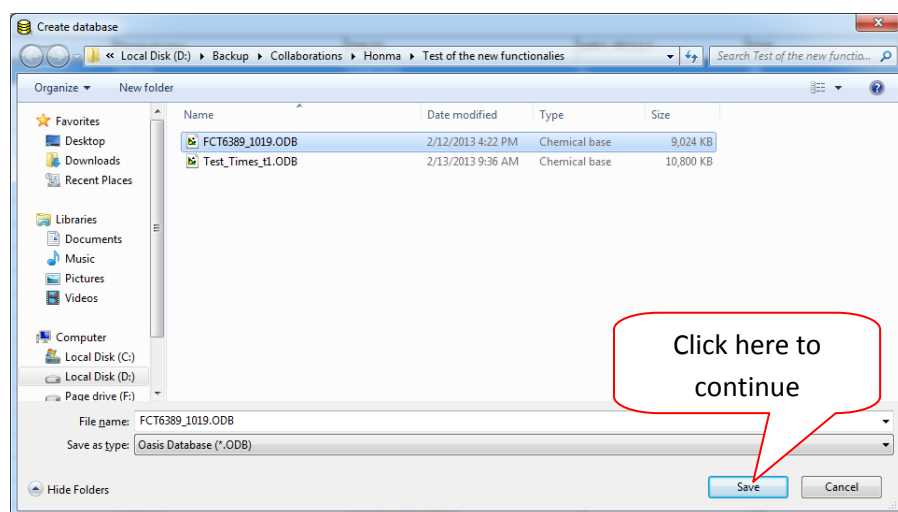
Database: FCT6389_1019.ODB Structures: 368

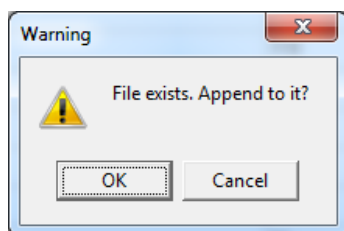
D. Append new data to existing ODB database

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

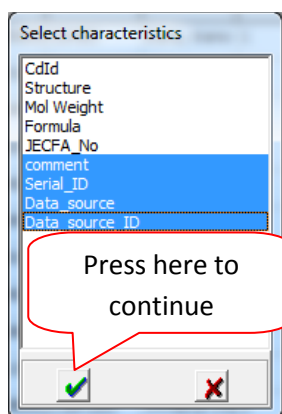
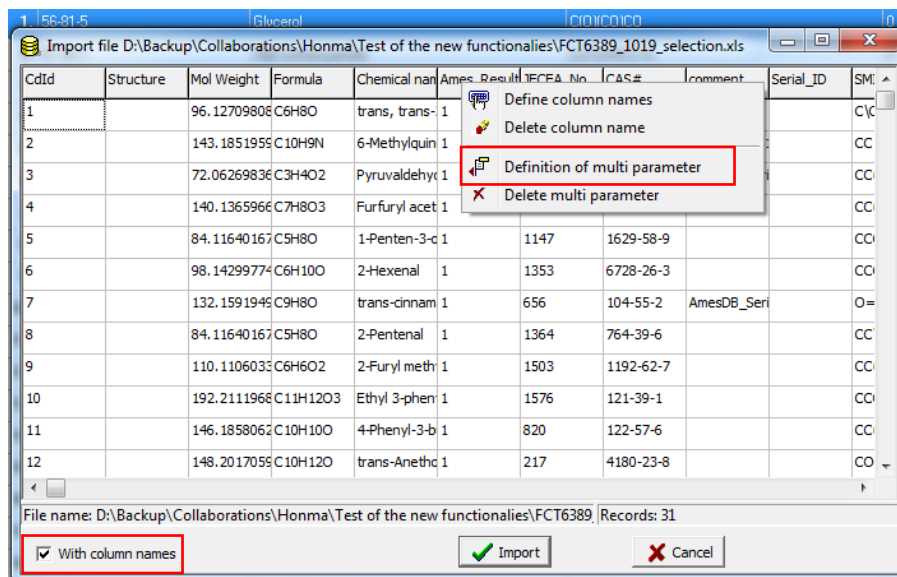


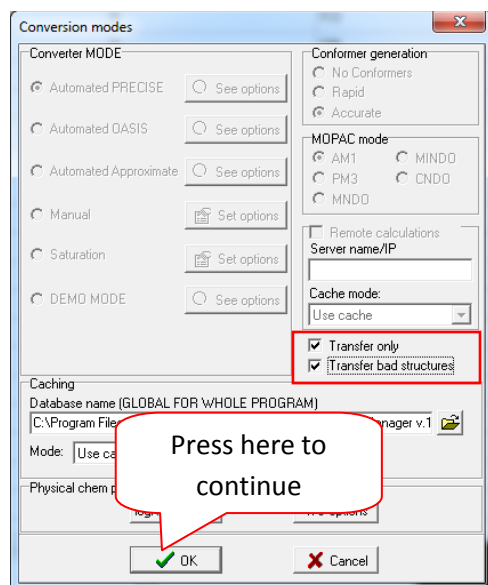
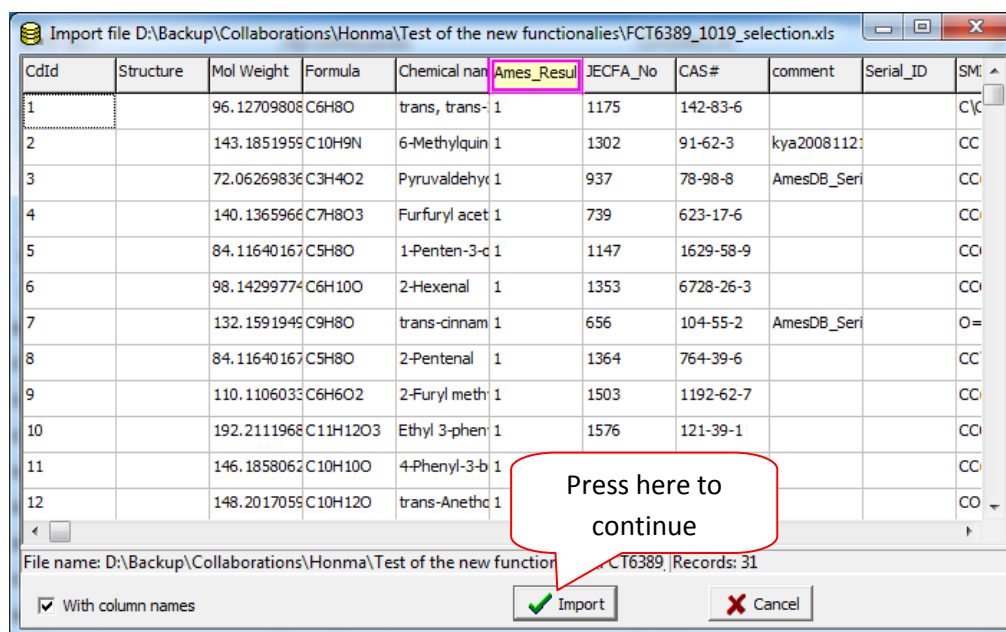
Select ODB which already exists and append the new chemicals to this file.



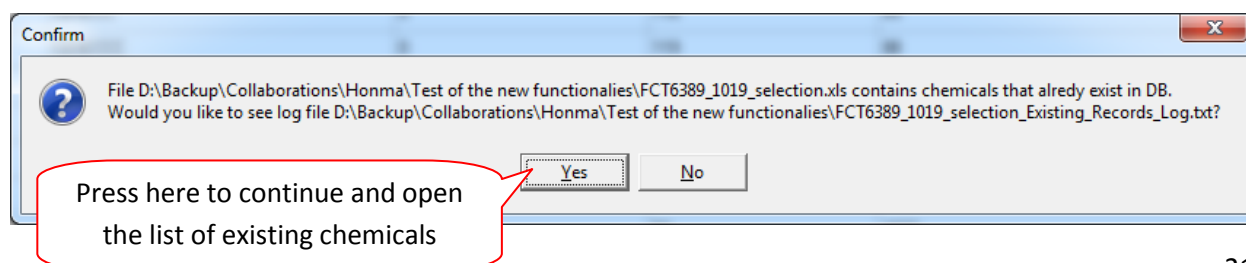


If you do not want to change columns names check in **With column names** option. Then, define the multi parameter and its characteristics:





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



The list of existing chemicals in Excel:

	A	B	C	D	E	F	G	H	I	J	K
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	Pyrvalde	C(C)(=O)C		The same chemical exist in DB. The total number of records will be decreased.						
4	623-17-6	Furfuryl al	C(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-Penten-	C(=O)C=	t	The same chemical exist in DB. The total number of records will be decreased.						
9	1192-62-7	2-Furyl m	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)COCO	0	89
2.	57-06-7	Allyl isothiocyanate	C1=S)NCC=C	2	25
3.	57-11-4	Stearic acid	C1=O)OCCCCCCCCCCCCCCCC	0	135
4.	60-12-8	Phenethyl alcohol	c1(CCO)ccccc1	0	261
5.	64-19-6	Formic acid	C1=O)O	0	111
6.	64-19-7	Acetic acid	C(C1=O)O	0	113
7.	65-85-0	Benzoic acid	C1=O)O)c1ccccc1	0	239
8.	66-25-1	Hexanal	C1=O)CCCCC	0	120
9.	67-63-0	Isopropyl alcohol	C(C)CO	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)CCCC	0	116
14.	71-41-0	Amyl alcohol	C(O)CCCCC	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)CN	0	
18.	75-50-3	Trimethylamine	CN(C)C	0	
19.	77-83-8	Ethyl methylphenylglycidate	c1(C2C(C)C(=O)OCCO2)ccccc1	0	
20.	78-59-1	Isophorone	C1=O)C=C(C)C(C)C(C)C1	0	
21.	78-70-6	1-Isobutyl	CCCC(C)C	0	

Find the chemical in the ODB

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

212.	141-32-4	Hydroxycitronellal dimethyl acetal	C(C)(C)OCCCC(C)C(C)C(C)C	0
213.	141-97-9	Ethyl acetoacetate	C(=O)CC(C)=O)OCC	0
214.	142-62-1	Hexanoic acid	C(=O)O)CCCCC	0
215.	142-83-6	trans, trans-2,4-Hexadienal	C(=O)C=(O)CC=(O)CC	1
216.	143-07-7	Lauric acid	C(=O)O)CCCCCCCCCCCC	0
217.	150-60-7	Benzyl disulfide	c1(CSSCc2ccccc2)ccccc1	0
218.	150-78-7	p-Dimethoxybenzene	c1(OC)ccc(OC)cc1	0
219.	151-10-0	m-Dimethoxybenzene	c1(OC)cc(OC)ccc1	0
220.	288-47-1	Thiazole	C1=CN=CS1	1
221.	290-37-9	Pyrazine	c1cnccn1	0
222.	301-00-8	Methyl linolenate	C(=O)O)CCCCCCCC=(c)CCC=(c)CCC=(c)CCC)OC	0
223.	326-61-4	Piperonyl acetate	c12c(cc(COC(C)=O)cc1)OCCO2	0
224.	334-48-5	Decanoic acid	C(=O)O)CCCCCCCCC	0
225.	350-03-8	3-Acetylpyridine	C(C)(=O)c1ccccn1	0
226.	421-02-0	Disobutyl	CC(C)C(C)C	1

Database affiliation	Structure parameters
	AMES_RESULT 1:[0;1]
	CDID 1
Quality assurance	JECFA_No 1175
	MOL_WEIGHT 96.12710

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

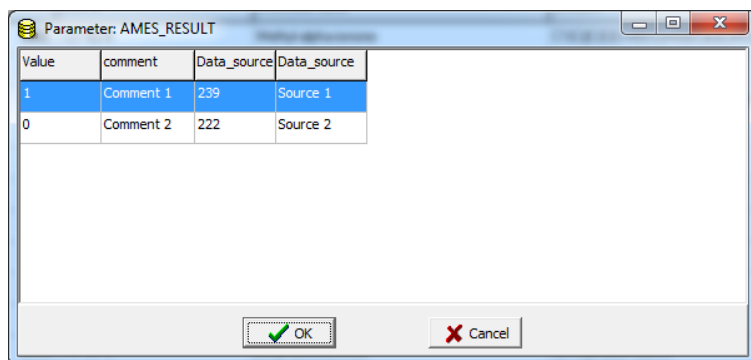
E. How to select a default value of the multi parameter

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:

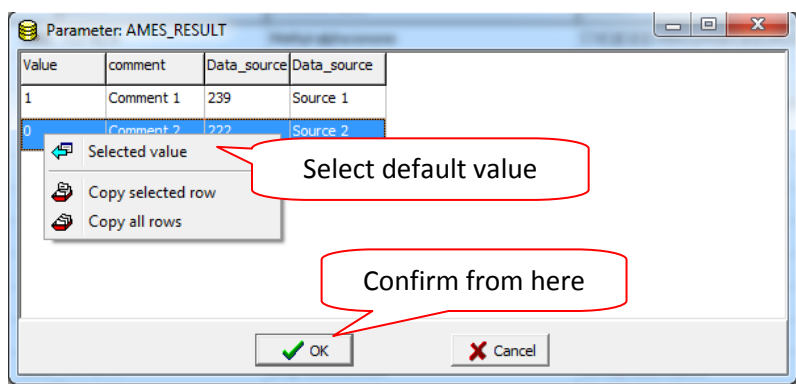
215.	142-83-6	trans, trans-2,4-Hexadienal	C(=O)C=(O)CC=(O)CC	1
216.	143-07-7	Lauric acid	C(=O)O)CCCCCCCCCCCC	0
217.	150-60-7	Benzyl disulfide	c1(CSSCc2ccccc2)ccccc1	0
218.	150-78-7	p-Dimethoxybenzene	c1(OC)ccc(OC)cc1	0
219.	151-10-0	m-Dimethoxybenzene	c1(OC)cc(OC)ccc1	0
220.	288-47-1	Thiazole	C1=CN=CS1	1
221.	290-37-9	Pyrazine	c1cnccn1	0
222.	301-00-8	Methyl linolenate	C(=O)O)CCCCCCCC=(c)CCC=(c)CCC=(c)CCC)OC	0
223.	326-61-4	Piperonyl	C(=O)O)CC(C(C)=O)cc1)OCCO2	0
224.	334-48-5	Decanoic	CCCCCCCC	0
225.	350-03-8	3-Acetyl	ccccn1	0
226.	421-02-0	Disobutyl	CC(C)C(C)C	1

Database affiliation	Structure parameters
	AMES_RESULT 1:[0;1]
	CDID 1
Quality assurance	JECFA_No 1175
	MOL_WEIGHT 96.12710

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:

215.	142-83-6	trans, trans-2,4-Hexadienal	C1=O)C=O)CC=O)CC	0	1
216.	143-07-7	Lauric acid	C1=O)O)CCCCCCCCCCCC	0	132
217.	150-60-7	Benzyl disulfide	c1(CSSCc2ccccc2)ccccc1	0	184
218.	150-78-7	p-Dimethoxybenzene	c1(OC)cc(OC)cc1	0	297
219.	151-10-0	m-Dimethoxybenzene	c1(OC)cc(OC)ccc1	0	296
220.	288-47-1	Thiazole	C1=CN=CS1	1	19
221.	290-37-9	Pyrazine	c1ccnnc1	0	259
222.	301-00-8	Methyl linolenate	C1=O)CCCCCCCCC=C)CCC=C)CCC=C)CCC)OC	0	160
223.	326-61-4	Piperonyl acetate	c12c(cc(COC(C)=O)cc1)OC2	0	250
224.	334-48-5	Decanoic acid	C1=O)O)CCCCCCCC	0	129
225.	350-03-8	3-Acetylpyridine	C(C)=O)c1cccc1	0	312
226.	421-02-0	Dibenzodioxin	c1ccc2c(c1)ccc3ccccc23	1	12

Database affiliation		Structure parameters		MOPAC status	
AMES_RESULT	0;[0;1]				
CID	1				
JECFA_No	1175				
MOL_WEIGHT	96.12710				

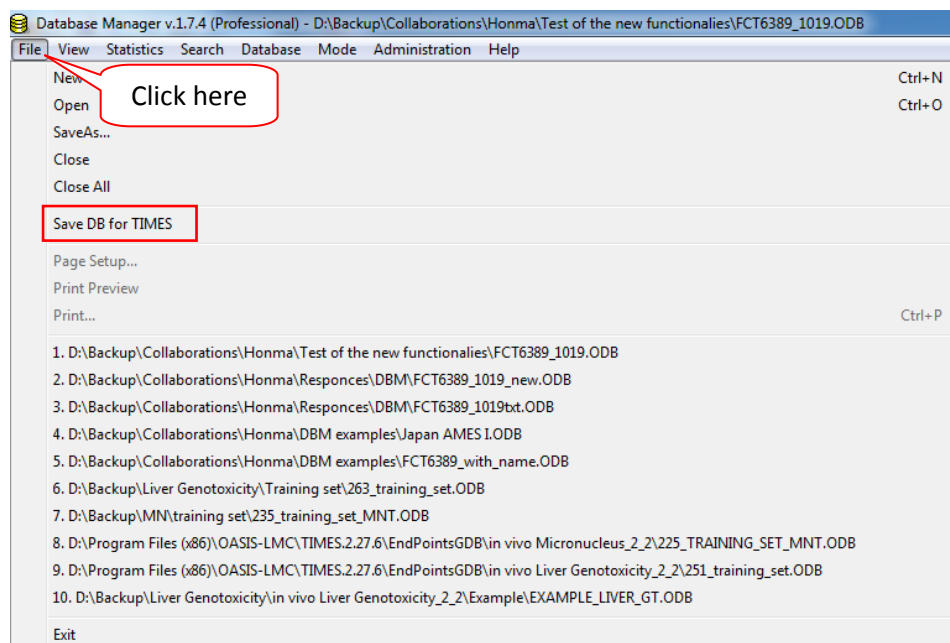
Text parameters	
Name	Value
Formula	C8H8O

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

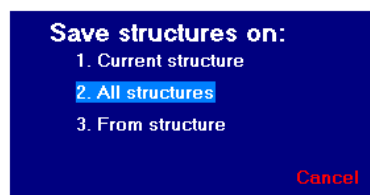
Note: flexible search by Ames result in the database is provided for the selected default value only.

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.