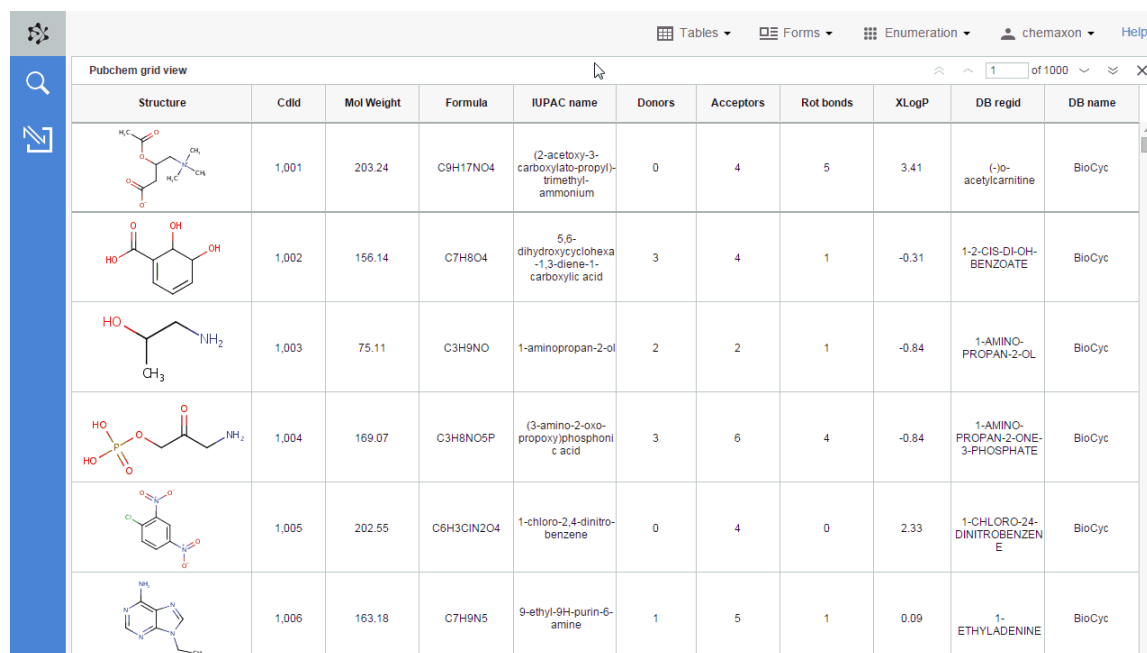


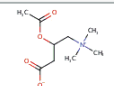
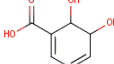
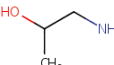
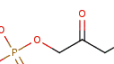
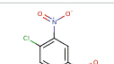
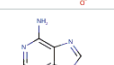
Exporting Your Data

Data in tables or forms can be exported to a variety of file formats

- ChemAxon MRV format (*.mrv)
- MDL SDF file (*.sdf)
- MDL RDF file (*.rdf)
- Tab separated text (*.txt)
- JChem for Excel with structures (*.xlsx)
- Microsoft Excel with structure images (*.xlsx)

In order to export the content of a table or a form, press the **Import & Export** button on the blue action bar on the left side of the application. As a result, the **Export** button slides down. Pressing this button opens the export panel, where you have to specify in which file format you want to export the data.



Structure	Cid	Mol Weight	Formula	IUPAC name	Donors	Acceptors	Rot bonds	XLogP	DB regid	DB name
	1,001	203.24	C9H17NO4	(2-acetoxy-3-carboxylato-propyl)-trimethylammonium	0	4	5	3.41	(-)-acetylcarfiline	BioCyc
	1,002	156.14	C7H8O4	5,6-dihydroxycyclohexa-1,3-diene-1-carboxylic acid	3	4	1	-0.31	1-2-CIS-DI-OH-BENZOATE	BioCyc
	1,003	75.11	C3H9NO	1-aminopropan-2-ol	2	2	1	-0.84	1-AMINO-PROPAN-2-OL	BioCyc
	1,004	169.07	C3H8NO5P	(3-amino-2-oxopropoxy)phosphonic acid	3	6	4	-0.84	1-AMINO-PROPAN-2-ONE-3-PHOSPHATE	BioCyc
	1,005	202.55	C6H3ClN2O4	1-chloro-2,4-dinitrobenzene	0	4	0	2.33	1-CHLORO-2,4-DINITROBENZENE	BioCyc
	1,006	163.18	C7H9N5	9-ethyl-9H-purin-6-amine	1	5	1	0.09	1-ETHYLADENINE	BioCyc

When the workspace contains more than one forms and tables, the export panel, similarly to the search panel, always refers to the currently active form or table. The name of the active form or table from which the data will be exported appears on the export panel as well.

The screenshot displays the ChemAxon software interface. On the left, a sidebar contains an 'Export' button and a list of file formats: ChemAxon MRV format (*.mrv), MDL RDF file (*.rdf), Tab separated text (*.txt), JChem for Excel with structures (*.xlsx), and Microsoft Excel with structure images (*.xlsx). The main area shows a table with 8 rows of chemical reactions. The first row shows the reaction of styrene with ethylene to form cyclohexene. The second row shows the reaction of acetic acid with methanol to form methyl acetate and water. The third row shows the reaction of benzene with acetyl chloride to form acetophenone and HCl. The fourth row shows the reaction of 2-methyl-2-butene with bromine to form 2-bromo-2-methylbutane. The fifth row shows the reaction of 1-butene with HBr to form 1-bromobutane. The sixth row shows the reaction of 2-methyl-2-butene with HBr to form 2-bromo-2-methylbutane. The seventh row shows the reaction of 2-bromo-2-methylbutane with sodium hydroxide to form 2-methyl-2-butene and HBr. The eighth row shows the reaction of 1,2-dibromoethane with HI to form 1,2-ethanediol and HI. On the right, a 'Compact fields' panel displays the following data: CPO ID: 1, Mol weight: 330.81, Formula: C18H19ClN2O2, LOGKOW: 4.98, and LOGWSOL: -5.97. Below the compact fields, there is a note: 'More traditional ISIS/Base-style form look. This is done by changing the borders to a line border and setting the padding between the widgets to zero. Label widgets are used and background and border properties set. Also, form background colour is changed.'

By default, every column/field on the active table/form is exported, and the exported file will contain each record of the table. However, if you run a search on a table or form, or open a previously saved list, and then export it, the file will contain only the search hits or the records saved in the list. Similarly, if you select certain columns or widgets before the export, the exported file will contain only these fields. In order to select multiple widgets and/or columns, you have to hold down the **CTRL** or the **SHIFT** key while you click on the widgets and column headers.

It should be noted that if the database view does not have a structure field or if it is not part of the selection then only the non-chemical file formats, such as *Tab separated text (*.txt)* and *Microsoft Excel (*.xlsx)*, will be available.

When you have selected the file format and the fields you want to export to a file, click on the **Export** button of the panel. As a result, the exported file will be downloaded to your computer, and the file name will be the same as the name of the table or form from which the data has been exported.

Please note that the actual list of available file formats depends on the type of data in a particular table or form.

In the case of a **molecule table**, the records can be exported to:

- *ChemAxon MRV format (*.mrv)*
- *MDL SDF file (*.sdf)*
- *Tab separated text (*.txt)* where the structures are represented by their SMILES strings.
- *JChem for Excel with structures (*.xlsx)*
- *Microsoft Excel with structure images (*.xlsx)*

In the case of a **reaction table**, the records can be exported to:

- *ChemAxon MRV format (*.mrv)*
- *MDL RDF file (*.rdf)*

- *Tab separated text (*.txt)* where the reactions are represented by their SMILES strings.
- *JChem for Excel with structures (*.xlsx)*
- *Microsoft Excel with structure images (*.xlsx)*

In the case of a **query structure table**, the records can be exported to:

- *ChemAxon MRV format (*.mrv)*
- *MDL SDF file (*.sdf)*
- *Tab separated text (*.txt)* where the reactions are represented by their SMARTS strings.
- *JChem for Excel with structures (*.xlsx)*
- *Microsoft Excel with structure images (*.xlsx)*

In the case of **Markush libraries**, the records can be exported to:

- *ChemAxon MRV format (*.mrv)*
- *MDL SDF file (*.sdf)*
- *Tab separated text (*.txt)* where the reactions are represented by their ChemAxon Extended SMILES strings.
- *JChem for Excel with structures (*.xlsx)*
- *Microsoft Excel with structure images (*.xlsx)*

Exporting relational data

With Plexus Connect, you can export complex, relational data as well into each supported file type. Since, by default, Plexus Connect exports every field of a database view; when a form contains data from more than one database table, fields will be exported both from the root and from the child table.

In the case of a One-to-Many relationship, when you want to export every field from the form, or you have selected at least one field from the child table, the rows of the parent table will be repeated for each record of the child table.

However, when the selected fields are all from the root table, the exported file will not contain any child table data, and the records of the root table will not be repeated.

Wombat (calc fields)

SMDEL-0000470

logP / MW

65.43

Num assay vals

3

Formula C18H19ClN2O2

EST.LOGWSOL -5.97

EST.LOGKOW 4.98

EXP.LOGKOW

EXP.LOGWSOL

Assay values

IC50 [5-HT2A] 8.7200

IC50 [5-HT2C] 8.4200

IC50 [H1] 6.9900

Wombat activities

TYPE	VALUE	VALUEMIN	VALUEMAX	TARGETTYPE	TARGETNAME	BIO.SPECIES
IC50	8.7200	8.72	8.72	receptor	5-HT2A	human
IC50	8.4200	8.42	8.42	receptor	5-HT2C	human
IC50	6.9900	6.99	6.99	receptor	H1	human

Printing

Printing functionality is part of Plexus Connect since version 17.16.0. Print feature enables you to generate *.pdf document which can be than paper printed. The printed representation of the information is often more restrictive than exploring your data in the form or grid view. For instance you can't use scroll bars in a printout. For this reason, all the columns presented in the grid view or table widget are squeezed on the printed page. Page breaks are added between rows, so that better readability is achieved, printing the content over multiple sheets.

Printing functionality is available under the **Export and Import** button on the blue action bar on the left side of the application.

ID	Structure	Mol Weight	Formula	Cid	IUPAC name	Donors	Acceptors	Rot bonds	DB regio	DB name	XLogP	Google	NCBI	ChemSpide	New Calculated Integer Field
1		203.24	C9H17NO4	1,001	2-acetyl-3-carboxypropyltrimethylammonium	0	4	5	(2-acetyl)amide	BioCyc	3.41	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=203.24	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=203.24	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=203.24	4
2		156.14	C7H8O4	1,002	5,6-dihydroxyoctane-1,3-diene-1-carboxylic acid	3	4	1	1,2-CIS-DI-OH-BENZOATE	BioCyc	-0.31	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=156.14	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=156.14	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=156.14	7
3		75.11	C3H9NO	1,003	1-aminopropan-2-ol	2	2	1	1-AMINO-PROPAN-2-OL	BioCyc	-0.84	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=75.11	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=75.11	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=75.11	4
6		163.18	C7H9N5	1,006	9-ethyl-9H-purin-6-amine	1	5	1	1-ETHYLADE-NINE	BioCyc	0.09	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=163.18	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=163.18	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=163.18	6
7		148.16	C6H12O4	1,007	2,3-dihydro-3-methylpentanoic acid	3	4	3	1-KETO-2-METHYLAERATE	BioCyc	0.22	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=148.16	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=148.16	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=148.16	7
8		260.13	C6H13O9P	1,008	2,3,4,5,6-pentahydroxycyclohexanecarboxylic acid	7	9	2	14-MYO-INOSITOL-1-P	BioCyc	0.22	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=260.13	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=260.13	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=260.13	16
9		473.45	C20H23N7O7	1,009	2-[4-(2-amino-4-hydroxy-5,6,7,8-tetrahydroimidazo[6,5-f]pyridin-2-yl)phenyl]ethane-1-thiol	7	12	9	10-FORMYL-THF	BioCyc	-1.04	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=473.45	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=473.45	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=473.45	19
10		98.95	C2H4Cl2	1,010	1,2-dichloroethane	0	0	0	12-DICHLOROETHANE	BioCyc	1.52	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=98.95	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=98.95	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=98.95	0
11		181.44	C6H3Cl3	1,011	1,2,4-trichlorobenzene	0	0	0	124-TCB	BioCyc	3.82	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=181.44	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=181.44	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=181.44	0
12		290.45	C18H30O2	1,012	17-hydroxy-10,13-dimethyl-1,2,4,5,6,7,8,9,10,11,12,13-dioxolane	1	2	1	17-BETA-HYDROXYA-NDIOSTAN-0,3-ONE	BioCyc	3.08	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=290.45	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=290.45	http://www.ncbi.nlm.nih.gov/ncbi/om/Search.aspx?q=290.45	3

When you click on this button, it slides down revealing the **Print** button. Pressing this button opens the print panel, where you have to specify which of your open forms or tables you want to print out. The name of the selected form or table from which the data will be printed appears on the print panel as well.

The screenshot shows the software interface with the print panel open. The print panel contains two tables for selection:

child 1-4				
ID	Number	data	link_45	Column1
1	1	ABCD 1	1	2
2	2	ABCD 2	1	8
3	3	ABCD 3	1	7
4	4	ABCD 4	1	2
5	5	ABCD 5	1	3
6	6	ABCD 6	1	8
7	7	ABCD 7	1	1
8	8	ABCD 8	1	9
9	9	ABCD 9	1	2
10	10	ABCD 10	1	2
11	11	ABCD 11	1	6

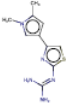
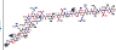
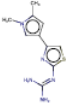
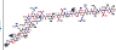
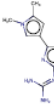

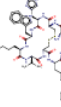

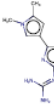

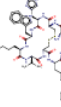

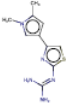
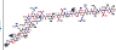
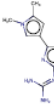

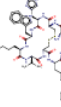

chembl_20_chemreps						
ID	Structure	Mol Weight	Formula	chembl_id	link 4.1	Structure link 3D
1		235.31	C16H13N5	CHEMBL153534	1	1
2		2,863.38	C123H212N44O34S	CHEMBL440660	1	2
3			C52H73N1	CHEMBL44		

The right side of the interface shows a grid of reaction structures, including various chemical transformations and syntheses.

On print panel, you also have two printing options:

- **Fit to widgets** option will print out only those child data, which can fit into their table widget.
- **Print all data** option will print out all child data, even though it might overflow widget size.

Pressing **Print** button will export your data in *.pdf format into your computer.

Fit to widgets	Print all data																															
<p>Parent data table</p> <p>child 1:4</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Number data</th> <th>link_45</th> <th>Column1</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>1 ABCD 1</td> <td>1</td> <td>2</td> </tr> </tbody> </table>	ID	Number data	link_45	Column1	1	1 ABCD 1	1	2	<p>Parent data table</p> <p>child 1:4</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Numb</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> </tr> </tbody> </table>	ID	Numb	1																				
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1	1 ABCD 1	1	2																													
ID	Numb																															
1																																
<p>Child data table</p> <p>chembl_20_chemreps</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Structure</th> <th>Mol Weight</th> <th>Formula</th> <th>chembl_id</th> <th>link 4-1</th> <th>Structure link 3D</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> <td>235.31</td> <td>C10H13N5S</td> <td>CHEMBL153534</td> <td>1</td> <td>1</td> </tr> <tr> <td>4</td> <td></td> <td>3,548.21</td> <td>C160H268N50O41</td> <td>CHEMBL440245</td> <td>1</td> <td>4</td> </tr> </tbody> </table>	ID	Structure	Mol Weight	Formula	chembl_id	link 4-1	Structure link 3D	1		235.31	C10H13N5S	CHEMBL153534	1	1	4		3,548.21	C160H268N50O41	CHEMBL440245	1	4	<p>Child data table</p> <p>chembl_20_chemreps</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> </tr> <tr> <td>4</td> <td></td> </tr> <tr> <td>3</td> <td></td> </tr> <tr> <td>2</td> <td></td> </tr> </tbody> </table>	ID	Structure	1		4		3		2	
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2																																

✔ Need more help? Check out our [tutorial video](#) about filtering a data set by using a saved query and exporting the search hits into a file.