

JRC QSAR Model Database

EURL ECVAM DataBase service on ALternative
Methods to animal experimentation

*To promote the development and uptake of alternative and
advanced methods in toxicology and biomedical sciences*

**SDF - STRUCTURE DATA
FORMAT:
How to create from
SMILES**



**The European Commission's science
and knowledge service**

Joint Research Centre

Directorate F

Health, Consumers & Reference Materials

Chemicals Safety & Alternative Methods Unit



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Contact information

Email:

JRC-COMPUTOX@ec.europa.eu

JRC Science Hub

<https://ec.europa.eu/jrc>

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Structure Data File format; description

Structure Data Format (SDF) is a chemical file format to represent multiple chemical structure records and associated data fields. SDF was developed and published by Molecular Design Limited (MDL) and became the most widely used standard for importing and exporting information on chemicals. A chemical data file created in the Structure Data File (SDF) format is saved in plain text and contains chemical structure records. Molecular Design Limited was renamed to MDL Information Systems and then later was acquired by Symyx Technologies, the organization that now maintains the SDF format.

Sample chemical record in SDF format

```
benzene
ACD/Labs0812062058

6 6 0 0 0 0 0 0 0 0 1 V2000
 1.9050 -0.7932 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
 1.9050 -2.1232 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
 0.7531 -0.1282 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
 0.7531 -2.7882 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.3987 -0.7932 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.3987 -2.1232 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
 2 1 1 0 0 0 0
 3 1 2 0 0 0 0
 4 2 2 0 0 0 0
 5 3 1 0 0 0 0
 6 4 1 0 0 0 0
 6 5 2 0 0 0 0
M END
$$$$
```

A feature of the SDF format is its ability to include associated data. Associated data items are denoted as follows:

```
> <Unique_ID>
XCA3464366

> <ClogP>
5.825

> <Vendor>
Sigma

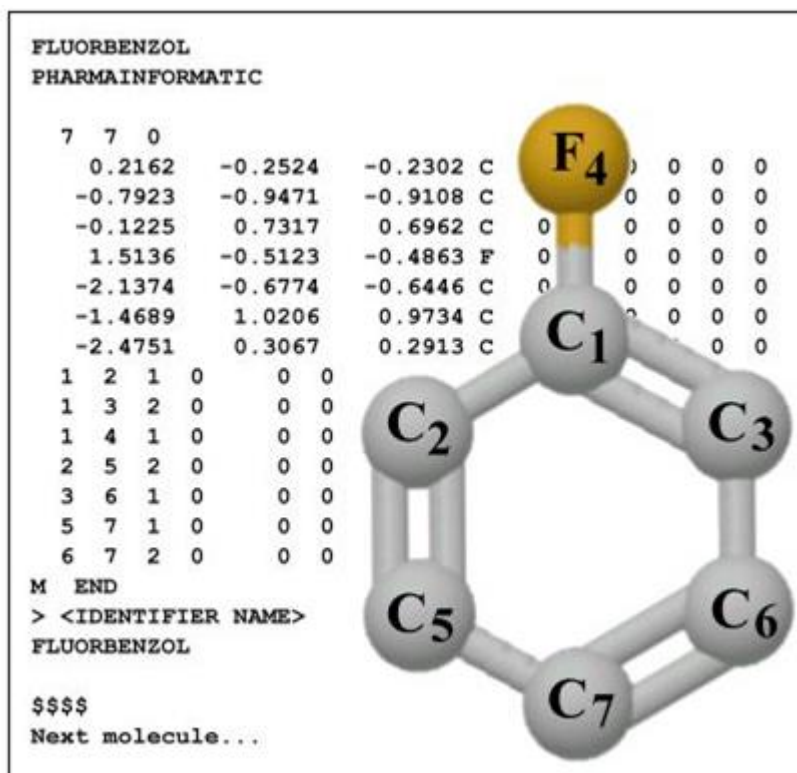
> <Molecular Weight>
499.611
```

Lines	Section	Description
1-3	Header	
1		Molecule name (" benzene ")
2		User/Program/Date/etc information
3		Comment (blank)
4-17	Connection table (Ctab)	
4		Counts line: 6 atoms, 6 bonds, ..., V2000 standard
5-10		Atom block (1 line for each atom): x, y, z (in angstroms), element, etc.
11-16		Bond block (1 line for each bond): 1st atom, 2nd atom, type, etc.
17		Properties block (empty)
18	\$\$\$\$	See note

Multiple-lines data items are also supported. The MDL SDF-format specification requires that a hard-carriage-return character be inserted if a single line of any text field exceeds 200 characters. This requirement is frequently violated in practice, as many SMILES and InChI (International Chemical Identifier) strings exceed that length.

Short explanation of SDF format

- The first three lines can contain general information about the molecule (e.g. substance name, version number, software used).
- The overall number of the atoms and of the bonds is stated in the fourth line in this case 7 atoms and 7 bonds.
- The following lines contain the x-, y-, and z-coordinates and the atom types of each atom in the molecule.
- At the end, the bonds between the atoms are described. The use of delocalised bond types can lead to misunderstandings. This bond type is not recommended and should not be used.



Resources on SDF

1. **CHEMFILEBROWSER** [ChemFileBrowser - A win32 free software for chemistry](#) - is a win32 free software for chemistry designed to visualize and works with SDF file (MDL® format) to exchange and analyse information associated with chemical structure. It includes descriptors calculation like TPSA, molecular weight, HBd,...
2. **WIKIPEDIA** [Chemical file format - Wikipedia, the free encyclopedia](#) List of commonly used chemical MIME file formats including SDF...

3. **CHEMTOOL** [Chemtool development page](#) is a small program for drawing chemical structures on Linux and Unix systems using the GTK toolkit under X11. A short and possibly outdated description of the available functions is available [here](#). Chemtool relies on transfig by Brian Smith for postscript printing and exporting files in PicTeX and EPS formats. Its companion program, XFig, is recommended for enhancing the output of chemtool, and for creation of 2D diagrams and schematics in general. Both are included with most distributions of Linux, and are available through a number of websites including,

www.xfig.org. If you want to import chemtool drawings into word processing programs other than LaTeX you will probably want to add a preview bitmap to them, as neither StarOffice/OpenOffice nor that software from Redmond seem to be able to display postscript inserts on screen without them. For this purpose, using either ps2epsi, which comes with [ghostscript](#), or epstool, a part of [gsview](#) is recommended. Since chemtool-1.6, this option is supported directly (through the equivalent function offered by recent versions of transfig).

4. **OPEN BABEL** [Main Page - Open Babel](#) is a project designed to pick up where Babel left off, as a cross-platform program and library designed to interconvert between many file formats used in molecular modeling, computational chemistry, and many related areas.

Features:

Open Babel is a chemical toolbox designed to speak the many languages of chemical data. It's an open, collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.

- Open Source Chemistry Toolbox
- [Ready-to-use programs](#), and [complete programmer's toolkit](#)
- Read, write and convert over [110 chemical file formats](#)
- Filter and search molecular files using [SMARTS](#) and other methods
- Supports molecular modeling, cheminformatics, bioinformatics
- Organic chemistry, inorganic chemistry, solid-state materials, nuclear chemistry

5. **CONVERT** [MN.CONVERT: Conversion of chemical file formats \(SDF, MOL, MOL2,](#) recognizes about 40 formats either by analyzing of the file's content or by using the file's extension (e.g. .mol, .smi, .sdf...), or the input format can also be specified...

6. **CHEMFILE BROWSER** <http://www.hyleos.net/index.php> is a win32 free software which was designed to visualize and work with SDF file (MDL® format). A format which is used by chemists to exchange and store compounds as well as associated data. Produced by HYLEOS.

Features:

- ability to navigate forward and backward through an SDF
- introduce SDI file (SDF File index) for direct mapping
- adding and editing field names
- the option to export selected compounds
- exporting SDF with selected fields
- renaming structures with a given field value
- export the data as *.csv file
- copy to clipboard (compatible with IsisDraw, ChemDraw, ViewerPro and others)
- bookmark compound manager to create an SDF file from a selection
- splitting and merging of SDF
- chemical descriptors : TPSA, Hydrogen Bond donor and acceptor number, molecular weight



[Download](#)

Programs that open SDF files

Windows

[Avogadro](#)
[OpenEye Scientific VIDA](#)
[Advanced Chemistry Development ACD/ChemFolder](#)
[ChemD](#)

MacOS and Linux

[Avogadro](#)
[OpenEye Scientific VIDA](#)

How to: Step by Step

How to create SD/SDF files from Simplified Molecular Input Line Entry Specification (SMILES)

One of the most significant steps during QSAR Model Reporting Formats (QMRFs) completing is to generate and provide SDF files including all necessary information about training/test set molecules (i.e. identifiers of all compounds, e.g. CAS/InChI/name/formula; visualised 3D structures; experimental and predicted values of target properties/parameters; the values of utilized molecular descriptors).



STARTING WITH example.xls

The most common **starting point** is a table in **EXCEL**. Microsoft Excel is a spreadsheet developed by Microsoft for Windows, macOS, Android and iOS. It features calculation, graphing tools, pivot tables, and a macro programming language called Visual Basic for Applications. It has been a very widely applied spreadsheet for these platforms, especially since version 5 in 1993, and it has replaced Lotus 1-2-3 as the industry standard for spreadsheets. Excel forms part of Microsoft Office.

The table should list the compounds in separate rows and associated data in columns (e.g. example.xls table). It must include one or more molecular structures (each structure represented by SMILES should be placed in a separate row, e.g. a file containing 50 structures should have 50 rows), beginning with the list of compounds (SMILES), without any heading or empty lines. It can contain the IDs of molecules (in columns), but they have to be separated from the SMILES by TAB or SPACE. Also other information can be optionally added (e.g. to which set (training/test) the compound belongs, if the compound is active or inactive, what are the values of descriptors, etc.) and each column (information) has to be TAB/SPACE delimited

□ This could be a starting point:

	A	B	C	D	E	F
1	O=C=Nc1cccc(N=C=O)c1C	2,6-Diisocyanatotoluene				
2	O=NN(c1ccccc1)C	N-Methyl-N-nitrosoaniline				
3	O=C(OCCOC)C(=C)C	Pentyl methacrylate				
4	O=C(OCCOC)C(=O)C(=C)C(=C)C	Ethylene dimethacrylate				
5	O(c1ccc2N(C(=C(c2(c1)C)C)C)CC	Ethoxyquin				
6	O=[N+][O-]c2ccc1ccc3c1c2CC3	Acenaphthene, 3-nitro-				
7	O=C(O)C1(OC1(O)C(O)C(C)C)C(=O)N	1-Carbamoyl-2,4-dimethyl-1,2-epoxy-3-hydroxy-1-(methoxycarbonyl)pentane				
8	O=C(O)C4=CC3=CCC1(CCC2(O)C(C(=O)NC(C)C)C)C	Epristeride				
9	c1cc(ccc1C)Br	4-Bromotoluene				
10	O=C2Oc3c(OC)c1ccc1c(OC)c3(C=C2)	Isopimpinellin				
11	Nc1ccc(cc1)c2ccc(cc2)Cl	4-Amino-4'-chlorodiphenyl				
12	O=C(Oc1ccc(cc1)CC)C	Phenol, 4-(chloromethyl)-, acetate				
13	O=C(OCCOC)C	Isoamyl acetate				
14	O=[N+][O-]c1ccc(cc1)c2ccc(cc2[N+]=O)[O-][N+]=C	1,1'-Biphenyl, 2,4,4'-trinitro-				
15	O=[N+][O-]c1ccc(cc1)[N+]=O[O-]Cl[N+]=O[O-]	Picryl chloride				
16	O=C1c5cccc(OC)c5(C(=O)c2c(O)c4c(c(O)c12)CC(O)C	4'-O-Methyldoxorubicin				
17	Fc2ccc3c1ccc(F)c1C(c3(c2))C	9H-Fluorene, 2,7-difluoro-9-methyl-				

□ Or this:

□ In this case, please delete the headings and move the SMILES column to the beginning (first column), followed by the name (second column),.....

Id	Status	SMILES	Formula	CAS RN	Chemical_I	SmCH3	SaCH2	ae	SsaCH2	SsdCH	SaaCH	SssaCH	SdssC	SsaasC	SsaasC	SssasC	SsN	SdN	SaaN	SssaN	SdaaN	SsOH	SdO	SsO	SaaO	SHCHn	Gmin	ldwbr	nrings	ALOGP	Exp	Muta	class
2	2	Test	O=C=Nc1c9HN2O2	91-08-7	2,6-Diisocya	1	0	0	0	3	0	0	3	0	0	0	0	0	2	0	0	0	0	0	0	0	0.464	6.092	1	2.037	1	1	
9	9	Test	O=NN(c1c7H8ZQ	614-06-6	N-Methyl-N-	1	0	0	0	5	0	0	1	0	0	0	0	1	0	1	0	0	0	2	0	0	0.803	5.313	1	1.667	1	1	
21	21	Test	O=C(OCCOC)C(=	2949-99-1	Pentyl meth	2	1	4	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0.28	5.541	0	2.95	0	0	
23	23	Test	O=C(OCCOC)C(=	97-90-5	Ethylene dir	2	2	2	0	0	0	4	0	0	0	0	0	0	0	0	0	2	2	0	0	0	0.49	6.257	0	2.149	0	0	
29	29	Test	O(c1ccc2N(C(=	91-63-2	Ethoxyquin	4	0	1	1	3	0	1	3	0	1	0	0	0	0	0	0	0	0	1	0	0	0.032	6.694	2	3.221	0	0	
38	38	Test	O=[N+][O-]c2	3807-77-0	Acenaphthe	0	0	2	0	5	0	0	3	2	0	0	0	0	0	0	0	0	2	0	0	0	0.299	6.541	3	3.234	1	1	
43	43	Test	O=C(O)C1(O)C	142438-73-	1-Carbamoy	4	0	0	0	2	2	0	0	2	1	0	0	0	0	0	0	1	2	2	0	0	0.186	6.746	1	0.343	1	1	
52	52	Test	O=C(O)C2S(H3	119169-78-	Epristeride	5	0	7	2	0	4	4	0	0	3	0	0	0	0	0	0	0	1	2	0	0	0.77	8.413	4	4.391	0	0	
54	54	Test	c1ccc(cc1C)H7	106-38-7	4-Bromotolu	1	0	0	0	4	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1.142	4.649	1	3.065	0	0	
56	56	Test	O=C2Oc3C13H	1005-482-27-9	Isopimpinell	2	0	0	2	2	0	1	4	2	0	0	0	0	0	0	0	0	1	3	1	0	0.45	7.094	3	2.171	0	1	
72	72	Test	Nc1ccc(cc1C1	12100N135-68-2	4-Amino-4-c	0	0	0	0	8	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0.754	6.278	2	3.266	1	1	
76	76	Test	O=C(O)c1c9H9	0202-39720-7-9	Phenol, 4-(1	0	1	0	4	0	1	2	0	0	0	0	0	0	0	0	0	1	1	0	0	1.31	5.817	1	2.197	1	1	
78	78	Test	O=C(OCCOC)C(=	123-92-2	Isoamyl ace	3	0	2	0	0	1	1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0.19	4.949	0	1.602	0	0	
79	79	Test	O=[N+][O-]c1	36712-34-2	1,1'-Bipheny	0	0	0	0	7	0	0	5	0	0	0	0	0	0	0	0	0	6	0	0	0	0.38	7.485	2	3.032	1	1	
86	86	Test	O=[N+][O-]C	88-88-0	Picryl chloro	0	0	0	0	2	0	0	4	0	0	0	0	0	0	0	0	0	6	0	0	0	0.81	6.745	1	2.178	1	1	
95	95	Test	O=C1c5cC2B(H	17121-90-5	4-O-Methyl	3	0	4	0	3	5	3	9	0	1	1	0	0	0	0	0	0	4	3	4	0	0.22	9.399	5	0.387	1	1	
98	98	Test	Fc2ccc3c1c4H	96563-10-9	9H-Fluorene	1	0	0	0	6	1	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0.24	6.721	3	4.156	1	1	
99	99	Test	O=Nc2ccc1c3H	9NO 2568-20-5	2-Nitrosodf	0	0	1	0	7	0	0	5	0	0	0	0	1	0	0	0	0	1	0	0	0	0.515	6.509	3	3.739	1	1	
104	104	Test	O=C(O)c1c7H9	96-99-1	4-Chloro-3-m	0	0	0	0	3	0	1	3	0	0	0	0	0	0	0	0	0	1	3	0	0	0.121	6.111	1	1.993	1	1	
112	112	Test	c1ccc(cc1)C(O	108-70-3	1,5,5-Trichlo	0	0	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0.563	5.026	1	3.823	0	0	
115	115	Test	O=[N+][O-]C	141414NO 2012-00-2	Epin oxon	1	0	1	0	9	0	0	3	0	0	0	0	0	0	0	0	0	0	3	2	0	0.349	7.487	2	3.078	1	1	



Create SMI file -> example.txt -> example.smi

The next step is to create a SMI file (i.e. a file with extension *.smi). The extension of obtained TXT file should be changed into SMI (by simply opening the example.txt file and saving it again but as an example.smi file). The content of each SMI file can be browsed by opening the file with Notepad/WordPad, etc..

```
example.txt - Notepad
File Edit Format View Help
O=C=Nc1cccc(N=C=O)c1C 2,6-Diisocyanatotoluene
O=NN(c1ccccc1)C N-Methyl-N-nitrosoaniline
O=C(OCCOC)C(=C)C Pentyl methacrylate
O=C(OCCOC)C(=O)C(=C)C(=C)C Ethylene dimethacrylate
O(c1ccc2N(C(=C(c2(c1)C)C)C)CC Ethoxyquin
O=[N+][O-]c2ccc1ccc3c1c2CC3 Acenaphthene, 3-nitro-
O=C(O)C1(OC1(O)C(O)C(C)C)C(=O)N 1-Carbamoyl-2,4-dimethyl-
1,2-epoxy-3-hydroxy-1-(methoxycarbonyl)pentane
O=C(O)C4=CC3=CCC1(CCC2(O)C(C(=O)NC(C)C)C)C)CC4 Epristeride
c1cc(ccc1C)Br 4-Bromotoluene
O=C2Oc3c(OC)c1ccc1c(OC)c3(C=C2) Isopimpinellin
Nc1ccc(cc1)c2ccc(cc2)Cl 4-Amino-4'-chlorodiphenyl
O=C(Oc1ccc(cc1)CC)C Phenol, 4-(chloromethyl)-, acetate
O=C(OCCOC)C Isoamyl acetate
O=[N+][O-]c1ccc(cc1)c2ccc(cc2[N+]=O)[O-][N+]=C 1,1'-Biphenyl, 2,4,4'-trinitro-
O=[N+][O-]c1ccc(cc1)[N+]=O[O-]Cl[N+]=O[O-] Picryl chloride
O=C1c5cccc(OC)c5(C(=O)c2c(O)c4c(c(O)c12)CC(O)C(=O)CO)CC4(OC3OC(C)C(O)C(N)C3) 4'-O-Methyldoxorubicin
Fc2ccc3c1ccc(F)c1C(c3(c2))C 9H-Fluorene, 2,7-difluoro-9-methyl-
O=Nc2ccc3c1ccccc1Cc3(c2) 2-Nitrosodfluorene
O=C(O)c1ccc(cc1)[N+]=O[O-]Cl 4-Chloro-3-nitrobenzoic acid
```

File name:
Save as type:

File name:
Save as type:

- **Saving as .smi** The **Simplified Molecular Input line Entry Specification (SMILES)** is a line notation for molecules. SMILES strings include connectivity but do not include 2D or 3D coordinates.

Hydrogen atoms are not represented. Other atoms are represented by their element symbols B, C, N, O, F, P, S, Cl, Br, and I. The symbol "=" represents double bonds and "#" represents triple bonds. Branching is indicated by (). Rings are indicated by pairs of digits.

Name	Formula	SMILES String
Methane	CH ₄	C
Ethanol	C ₂ H ₆ O	CCO
Benzene	C ₆ H ₆	C1=CC=CC=C1 or c1ccccc1
Ethylene	C ₂ H ₄	C=C



File conversion to example.sdf

Properly prepared SMI file can be subjected to conversion. Currently there are several software tools which can operate SMI to SD/SDF transformation; two freely available ones will be discussed here:

OpenBabel version 2.3.2 for Windows, freely available at <http://openbabel.org/>

A properly prepared SMI file has to be indicated as OpenBabel input – its content is visualised if the file is properly recognized.

Open Babel does not generate coordinates, unless the box "Generate 3D coordinates" is ticked. It is necessary to select this option, as the SDF files without calculated coordinates (x, y and z coordinates are equal 0) cannot be recognized by the overwhelming majority of software as well as by the SDF files browser (recommended in point 3).

Before the conversion it is necessary to specify the path to and the name of the output file in order to save the results.

The conversion procedure can be a bit time consuming due to calculation of 3D coordinates (about 3 minutes for 60 relatively small molecules).

The disadvantage of OpenBabel is that it does not allow to add various attributes of compounds (different IDs, values of descriptors, etc.) to the output file. The only way to include all information in SDF seems to be to prepare the input SMI file containing TAB/SPACE delimited columns with all necessary information about the molecules. Thus, the SMI file should consist of all rows (except the heading row) and columns from the initial (XLS) data table. However, in the output file all attributes are placed in one row without heading and it is difficult to recognize the meaning of particular textual/numerical information. Hence, OpenBabel could be recommended to produce SDF files including 3D structures with only one ID (e.g. name) associated. As far as QMRFs are concerned, providing the remaining data in a separate attachment (e.g. XLS file) would be necessary.

Accelrys Discovery Studio Visualizer version 2.5, freely available at <http://accelrys.com/>

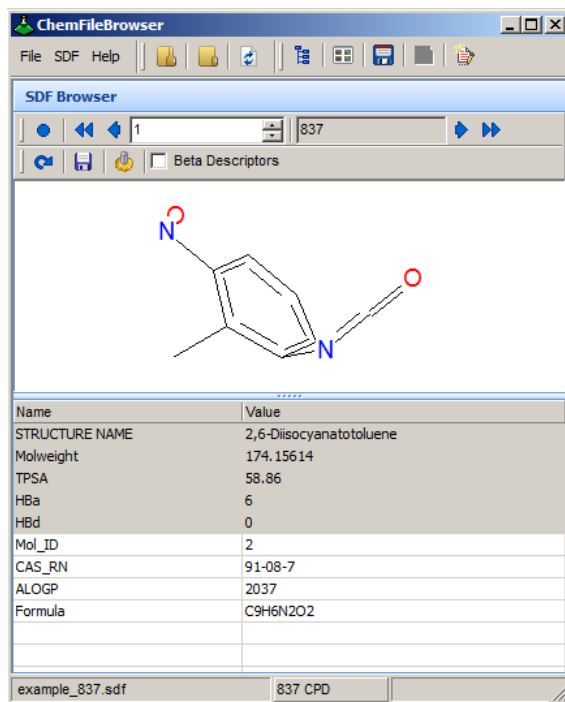
The input SMI file should include SMILES and – optionally – one structure ID (preferably name since the software, by default, will recognize this initial ID as name).

Other attributes (like CAS, InChI, descriptors values, etc.) can be easily added (Edit à Add Attribute...) and copy-pasted from the XLS data table. They will be transparently placed in separate rows in the output SDF file

The file can be subsequently saved as SDF (File à Save as... à MDL MOL/SD files). The software generates 3D coordinates, but the procedure is much faster than the one performed by OpenBabel.

Accelrys Discovery Studio is able to produce SDF files including 3D structures as well as all other textual/numerical information about studied compounds (additional attachments are not necessary).

- **Saving as .sdf structure-data format** file wrap the molfile (MDL Molfile) format. Multiple compounds are delimited by lines consisting of four dollar signs (\$\$\$\$)



SDF files browser

The content of the final SDF files can be browsed either with *Accelrys Discovery Studio* or with easy to use SDF files browser *Hyleos* (currently version 0.2.9.3), freely available at <http://www.hyleos.net/>

With the Hyleos application it is possible to screen the content of SDFs (visualised 3Dstructures and all associated data) as well as to merge/split the files.

Template for SDF files

12	11	10	9	8	7	6	5	4	3	2	1
											Id
											Status
											SMILES
											Formula
											CAS_RN
											Chemical_Name
											SsCH3_acnt
											SdCH2_acnt
											SssCH2_acnt
											SdsCH_acnt
											SaaCH_acnt
											SsssCH_acnt
											SdssC_acnt
											SaasC_acnt
											SaaaC_acnt
											SssssC_acnt
											SsNH2_acnt
											StN_acnt
											SdsN_acnt
											SaaN_acnt
											SsssN_acnt
											SdaaN_acnt
											SsOH_acnt
											SdO_acnt
											SssO_acnt
											SaaO_acnt
											SHCHnX_Acnt
											Gmin
											idwbar
											nrings
											ALOGP
											Exp class
											Muta class

KEEP IN MIND TO DELETE the **HEADINGS** and move the **SMILES** column to the beginning (**first column**), followed by the name (second column),.....

For preparation of the sdf file this is **essential!**

GETTING IN TOUCH WITH THE EU

In person

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