Technical report: CSVM dictionaries.

Extension of CSVM-1 specification: definition, usages, Python toolkit.

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Abstract

CSVM (CSV with Metadata) is a simple file format for tabular data. The possible application domain is the same as typical spreadsheets files, but CSVM is well suited for long term storage and the inter-conversion of RAW data. CSVM embeds different levels for data, metadata and annotations in human readable format and flat ASCII files. As a proof of concept, Perl and Python toolkits were designed in order to handle CSVM data and objects in workflows. These parsers can process CSVM files independently of data types, so it is possible to use same data format and parser for a lot of scientific purposes. CSVM-1 is the first version of CSVM specification, an extension of CSVM-1 for implementing a translation system between CSVM files is presented in this paper. The necessary data used to make the translation are also coded in another CSVM file. This particular kind of CSVM is called a CSVM dictionary, it is also readable by the current CSVM parser and it is fully supported by the Python toolkit. This report presents a proposal for CSVM dictionaries, a working example in chemistry, and some elements of Python toolkit usable to handle these files.

Keywords

CSVM; Tabular Data; Python; Specification; Data Conversion; Open Format; Open Data; Open Format; Dictionaries; Canonical Data Model.

Status

As CSVM itself, the dictionaries extension shown in this document must be considered as an Open format.

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1. Definition of a CSVM dictionary

The CSVM dictionary 1) must use the same basis than a CVM file defined by CSVM-1 specification; 2) must be processed by the same parser that a common CSVM file and 3) must embed all the information needed to transform a CSVM file in another.

We show in this section how we can define a translation set, encode it in a CSVM dictionary and how the translation set is used to transform or normalize data of data CSVM file.

1.1. Data structure of a CSVM dictionary

The following CSVM file shown below is a chemical inventory table limited to 6 rows and 5 columns for simplicity. This table codes for: a rank number (numero), a chemical structure (fichier), a molecular weight (masse_exacte), a common molecule name (nom), an amount (i.e. g or mg of product) of chemical in laboratory (vrac):

```
1  af01.mol  181.19293  Tyrosine  10  ...
5  af02.mol  155.15753  Histidine  20  ...
2  af03.mol  204.23049  Tryptophane  20  ...
3  af04.mol  115.13298  Proline  12  ...
4  af05.mol  267.24621  Adenosine  0  ...
6  af06.mol  661.90791  Ph-Choline  300  ...
```

![Figure 1. - CSVM file for a chemical inventory.](image)

The #HEADER, #TYPE, #WIDTH define a first system (SYS1) with particular types and column names, and this file is used as a data file.

Now we want to transfer the data in another system with different naming conventions (ie. to prepare import to a RDBMS), we call it SYS2 (second system). To do this task we have defined a new CSVM file called the dictionary:

```
numero  ID  number  #NUMERIC  #10
nom  Identificateur  name  TEXT  #100
fichier_mol  MOLSTRUCTURE  molfile  TEXT  #50
masse_exacte  mol.weight  #NUMERIC  #50
vrac  vrac  quanity  #NUMERIC  #10
...
```

![Figure 2. - CSVM dictionary for the table shown in Figure 1.](image)

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Now we want to transfer the data in another system with different naming conventions (ie. to prepare import to a RDBMS), we call it SYS2 (second system). To do this task we have defined a new CSVM file called the dictionary:

```
numero  ID  number  #NUMERIC  #10
nom  Identificateur  name  TEXT  #100
fichier_mol  MOLSTRUCTURE  molfile  TEXT  #50
masse_exacte  mol.weight  #NUMERIC  #50
vrac  vrac  quanity  #NUMERIC  #10
...
```

We see that obviously this is also a CSVM file. The only difference is that some keywords with the # character are present in the two last columns of data and metadata blocks. These two columns (order: 4,5 from left to right) are used to store data types of translation sets, while data columns (order: 1,2,3) are used to store the translation set data itself.
This CSVM dictionary stores the columns names used in SYS1 (orange column below) and expected in SYS2 (pink) or another name space/set (green). The dictionary stores also the #TYPE and #WITH fields of each name set (blue columns):

Table 1. – CSVM dictionary (Figure 2.) shown as colored table.

| numero | ID     | number | #NUMERIC | #10 |
|--------|--------|--------|----------|-----|
| nom    | identificateur | name   | #TEXT    | #100|
| fichier_mol | MOLSTRUCTURE | molfile | #TEXT    | #50 |
| masse_exacte | - | mol.weight | #NUMERIC | #50 |
| vrac  | crac   | qttity | #NUMERIC | #10 |

| #TITLE | CSV dictionary for SYS1, SYS2 and SYS1_UK |
|--------|----------------------------------------|
| #HEADER | SYS1 TEXT | SYS2 TEXT | SYS1_UK TEXT | #TYPE TEXT | #TYPE TEXT | #WIDTH TEXT |
| #WIDTH  | 50 | 50 | 50 | #50 | #50 |

So we have here all data needed to convert a CSV file using SYS1 in another naming space because we have the #HEADER, #TYPE, #WIDTH values of SYS1 and SYS2 in this dictionary. The case of a column (#HEADER value) named TYPE or WIDTH is possible, so have chosen to mark type and width metadata in data block (blue columns) with # character to avoid confusions.

A CSV dictionary could be defined as a way to store Metadata of n CSV files in the data block of another CSV file.

1.2. Translation sets

If we read the first row dictionary file, we find a value ‘numero’ that is the contents of #HEADER first column in data file. The second and third values of the row (‘ID’ and ‘number’) are alternate values of ‘numero’. If we read the first column of dictionary file, we find ‘numero’, ‘nom’, ‘fichier_mol’, ‘masse_exacte’, ‘vrac’. All are values used in data file and corresponding to SYS1, we call this ensemble a translation set. The previous dictionary defines 3 translation sets:

- The SYS1 set : [numero, nom, fichier_mol, masse_exacte, vrac]
- The SYS2 set : [ID, identificateur, MOLSTRUCTURE, , vrac]
- The SYS1_UK set : English translation of SYS1 [number, name, molfile, mol.weight, qttity]

1.3. Guidelines for Standards and data transformation

So we can use one translation set defined in a dictionary to change values of #HEADERS of a CSVM file/object. But what about the data of target CSVM file?

First, take in account that the perimeter of CSV-1 covers only the syntax of a CSV file, not the value of keywords. The recommendation about values of #TYPE fields (i.e. TEXT, NUMERIC …) must be considered only as a good practice. So, it is possible to include a lot of values for #TYPE and #WIDTH keywords, typically information to make data conversions.

The previous CSVM table shows that only one column #TYPE or #WIDTH is included in the dictionary for the all 3 translation sets. This is what we call a Standard, with this dictionary it is possible to convert all data type of each CSV file processed into the units defined by the standard.

Consider a current case in a laboratory, some columns of a CSV file prepared by a first scientific team (encoded by translation set TEAM1) must have column names changed before data transfer to another team (translation set TEAM2). But the second team uses also different units (i.e. mass concentration unit rather than molar units).
The transformation of data units into a standard is resumed by the following figure:

*Figure 3. - Schematics of transformation of a CSVM file using a CSVM dictionary.*

A software component knowing a rule to transform Mol.1 in g/L (gram per liter) could make the data transformation, but this operation must be let out of CSVM parser’s range. The corresponding coding part of dictionary for this #HEADER is given by the Table 2.

**Table 2. – Data normalization using a standard as data type in a CSVM dictionary.**

| concentration | CONC | #GR/L | #10 |
|---------------|------|-------|-----|
| #TITLE        | Example |       |     |
| #HEADER       | TEAM1 | TEAM2 | #TYPE |
| #TYPE         | TEXT  | TEXT  | #TEXT |
| #WIDTH        | 50    | 50    | #50  |

1.4 Guidelines for data transformation

Now if a data conversion (not the Standard) is planned for a particular column of a CSVM table ? In CSVM’s context, different approaches are available. In example, if a CSVM dictionary is used ¹, it is possible to add columns (TEAM1_UNITS, TEAM2_UNITS) coding for local units used by TEAM1 and TEAM2 as shown in the following table:

¹ If a dictionary is not used, the programmer could make all transformations on the target CSVM using information picked manually in another CSVM and organized in columns or rows (this approach is often used when the transformations/rules defined in dictionary must be applied sequentially). For more complex case, it could be interesting to split information in more than one CSVM file (dictionaries of common files).
Table 3. – Adding specific columns for multi-standards.

| concentration | MOLAR | CONC | GR/L | #NUMERIC | #10 |
|---------------|-------|------|------|----------|-----|
| #TITLE        | Example |      |      |          |     |
| #HEADER       | TEAM1 | TEAM1_UNITS | TEAM2 | TEAM2_UNITS | #TYPE | #WIDTH |
| #TYPE         | TEXT  | TEXT    | TEXT  | TEXT     | #TEXT | #TEXT  |
| #WIDTH        | 50    | 10      | 50    | 10       | #50   | #50    |

In the example shown in Table 3 no Standard is defined, but it is also possible to add one. It is also possible to extend this approach to #WIDTH columns. In dictionary file, the columns defined by values #TEAM1_UNITS and #TEAM2_UNITS are not used by the conversion functions defined in toolkits. The reason is simple: the #TEAM1_UNITS and #TEAM2_UNITS are not defined as #HEADER keywords in data files. But it is not a problem for making conversions outside the CSVVM parser range, the dictionary could be read as a CSVVM object and its contents used as it is a common CSVVM file.

A CSVVM dictionary could also used to save knowledge about a data space of CSVVM files, including supplemental fields.

1.5 Lost words in translation sets

The first table (Table 1.) shows that keyword defined by ‘masse_exacte’ in first translation set (SYS1 set) is not defined in SYS2 set (the char ‘-’ is used here to mark an empty cell).

No particular processing is done about that, because the CSVVM parser doesn’t make interpretation about data or metadata values. Holes in tables are very often found in real data and can be taken in account, if a #HEADER value is not defined in the translation set, the corresponding column can be suppressed (or not) in the resulting CSVVM file 2 after CSVVM dictionary application.

For advanced uses, it is also possible to make a union between two CSVVM files in order to restore all missing empty columns (a specific CSVVM file can be forged and used as a data mask). Unions, Intersections, Additions of tables are implemented in CSVVM Python toolkit, given an example:

```python
print "\n*** Test CSVVM files with equivalent, different, missing columns"
c1 = csvm_ptr()
c1 = csvm_ptr_read_extended_csvm(c1,"test/test1.csvm","\t")
c2 = csvm_ptr()
c2 = csvm_ptr_read_extended_csvm(c2,"test/test2.csvm","\t")
print "\n=> Compute INTERSECTION"
r = csvm_ptr_intersect(c1, c2)
if (r != None):
    r.csvm_ptr_dump(0,0)
    r.csvm_ptr_clear()
else:
    print "None data found"
print "\n=> compute UNION"
r = csvm_ptr_union(c1, c2)
r.csvm_ptr_dump(0,0)
r.csvm_ptr_clear()
c1.csvm_ptr_clear()
c2.csvm_ptr_clear()
```

Using CSVVM paradigm, table unions or tables intersection are easy to implement, even if the two files have not exactly the same number of columns or columns names (an intermediate step using CSVVM dictionaries could be added to the process).

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2 A typical use is the generation of a subset of RAW data (one or n CSVVM files) prior to a RDBMS import.
1.6 Annotation of dictionaries

Dictionaries are CSVM files and can be annotated in the same way that standard CSVM. Remark lines tagged by a # character in data block (or metadata block) are used. The only rule is that a CSVM keyword (#TITLE, #HEADER, #TYPE, #WIDTH, #META) cannot be used (but combinations such as # TITLE, #_HEADER, # HEADER, #HEADER ... are allowed). The level of annotation of a CSVM file can be very high because the corresponding rows are not taken in account by the CSVM parser.

The following figure shows annotation of a CSVM file, in the case of a commented parameter’s set for doing calculations using AMBER\textsuperscript{3} package.

Figure 4. – Example of CSVM annotations inside the data block. The image is truncated after the 80\textsuperscript{th} column (vertical grey line at right). Some lines (7, 19, 21, 31) are wrapped by the text editor\textsuperscript{5}.

```plaintext
1 # MIN Flag to run minimization.
2 #******************************************************************************
3 # 0 no minimization (only do molecular dynamics; default).
4 # 1 perform minimization (and no molecular dynamics).
5 # 5 read-in a trajectory for analysis.
6 # althoughamber will write energy information in the output files (using ntraj),
7 # to post-process a set of structures using a different energy function than was used
8 # replaced with a continuum model, when min is set to 5amber will expect to read
9 # described in the mdin file for each of the structures in the trajectory file. The
10 maxcyc=0000,amber will minimize each structure in the trajectory for 1000 steps to
11 extract the energies of each of the coordinate sets in the inptrafile
12 #ctrl = min =
13 # MAXCyc the maximum number of cycles of minimization. Default 1
14 #******************************************************************************
15 #ctrl = maxcyc
16 # NOYC if MINMIN is 1 then the method of minimization will be switched from steepest
17 #ctrl = noyc
18 # NTB Periodic-boundary.
19 #******************************************************************************
20 # if NTB is 0 then a boundary is not applied regardless of any boundary condition
21 # will be used. options for constant pressure are described in a separate section be-
22 # if NTB is 0, there must be a periodic boundary in the topology file. Constant
23 # for a periodic system, constant pressure is the only way to equilibrate density-
24 # when solvent molecules are subtracted which can aggregate into “vacuum bubbles” in
25 # every system needs to be equilibrated at constant pressure (ntb=2, ntp=0) to get to
26 # temperature, before turning on constant pressure.
27 #ctrl = ntb
28 # GB Flag for using the generalized born or poisson-boltzmann implicit solvent max
29 #******************************************************************************
30 # see sections 6.1 and 6.2 for information about using this option, default is 0
31 #ctrl = gb
32 # cut This is used to specify the nonbonded cutoff, in Angstroms.
33 #******************************************************************************
34 # TITLE --CNA minimization mask
35 #HEADER BNUM --BTYPE --KEY
36 #TYPE --NUMERIC TEXT --TEXT
37 #WIDTH = 10 --10--10
38 #META = 03/June/07
```

\textsuperscript{3} The Amber Molecular Dynamics Package - \url{http://ambermd.org/}

\textsuperscript{4} Watson-Crick base-pairing properties of nucleic acid analogues with stereocontrolled alpha and beta torsion
angles (alpha,beta-D-CNAs). C. Dupouy, N. Iché-Tarrat, M.P. Durrieu, F. Rodriguez, J.M. Escudier, A. Vigroux.
Angewandte Chemie (2006) 45:22, 3623-3627.

\textsuperscript{5} Scintilla and SciTE - \url{http://www.scintilla.org/}
2. A working example in Chemistry

A SDF \(^6\) file is a collection of \(n\) data blocks. For each block, one can find a molecules (coded using MDL Molfile format) and \([0..m]\) descriptors stored as key/values pairs, in another terms, it is a serialized molecular data table. Given a such molecular collection \(^7\), we want to transform the descriptor space: removing or renaming some of them in order to export the collection to a chemical RDBMS.

Figure 5. – Molecular collection (displayed using a SDF viewer \(^9\)). The molecular formulas for each compound are shown at top part of each record. The descriptors (key/values pairs) are shown in bottom.

The corresponding CSVM table has one row for each compound and a column for each descriptor key (number, name, plate, chemist, amount, ref_product, ref_labbook, id_lab, id_team, id_box, rights, chr_row_box, num_col_box). Another column is used to store the 2D chemical structure at SMILES \(^10\) format.

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\(^6\) Chemical table file [Wikipedia] - [http://en.wikipedia.org/wiki/Chemical_table_file](http://en.wikipedia.org/wiki/Chemical_table_file)

\(^7\) L. Hammal, S. Bouzroura, C. André, B. Nedjar-Kolli, P. Hoffmann (2007) Versatile Cyclization of Aminoanilino Lactones: Access to Benzotriazoles and Condensed Benzodiazepin-2-thione. *Synthetic Commun.*, 37:3, 501-511.

\(^8\) M. Fodili, M. Amari, B. Nedjar-Kolli, B. Garrigues, C. Lherbet, P. Hoffmann (2009) Synthesis of Imidazoles from Ketimines Using Tosylmethyl Isocyanide (TosMIC) Catalyzed by Bismuth Triflate. *Lett. Org. Chem.*, 6, 354-358.

\(^9\) ChemAxon marvinView - [http://www.chemaxon.com/products/marvin/marvinview/](http://www.chemaxon.com/products/marvin/marvinview/)

\(^10\) Chemical file format [Wikipedia] - [http://en.wikipedia.org/wiki/Chemical_file_format](http://en.wikipedia.org/wiki/Chemical_file_format)
The following image shows the end of data block of the CSVM file and metadata block:

Figure 6. – The molecular collection of Figure 4. encoded in a CSVM table, details only: last compounds, some rows [73 .. 80] are cut off at right. Tabs are used as field separator and are shown as red arrows.

A first CSVM dictionary (dict1, Figure 7) will be used to filter CSVM columns of the molecular collection (Figure 6). In dict1, the columns 1-3 of data block, list the keywords of CSVM files allowed in corresponding translation sets LOCAL, LOCAL2, CN. If the translation occurs from LOCAL to LOCAL2, all columns of the molecular table that are named num_col_box will be renamed to ccol.

Figure 7. – A CSVM dictionary (dict1).

Some values in dict1.CN are set to DEL string: if translation occurs from LOCAL/LOCAL2 to CN, all columns tagged with DEL will be deleted in the resulting collection.

Figure 8. – Molecular collection after application of dict1.CN filter.
The corresponding SDF file is shown in Figure 9. The molecular formulas are regenerated and some keywords are missing or are renamed (number -> ID, name -> Identificateur, plate -> plaque, amount -> vrac) in the new SDF file.

Figure 9. – Molecular collection after filtering by dict1.CN set.

This example shows how to use CSVM as intermediate format in order to make operations (here a simple filtering) on tables. This kind of operation is very often done in a lot of scientific fields and using CSVM let us integrate table in scientific workflows and normalize data. CSVM’s paradigm permits a real data management and storage of RAW data. Eventually these RAW data will be integrated in a RDBMS, if this job is done by another team, the CSVM files are enough documented, and the producer’s team will be very little demand. If the RAW data will not be integrated in a RDBMS: all that is needed (metadata, annotations) to use these files some years later is embedded inside (event is a CSVM parser is not available, all information is human readable).
3. Python toolkit

The CSVM dictionaries are fully supported in the Python toolkit for CSVM, the following code was used for the translation shown in previous section:

```python
if __name__ == '__main__':
    from build_file import file2str, file_str2file, file_cleanpath
    print "*** CSVM dictionary test"
    print
    print "*** TEST1: using a dictionary in which __DEL__ are included."
    print "*** strong mode IS NOT used"
    print "\n=> A new blank CSVM object"
    c = csvm_ptr()
    print "\n=> Populates it with a CSVM file ... "
    c = csvm_ptr_read_extended_csvm(c, file_cleanpath("test/hoffmann.csvm"), "\t")
    c.csvm_ptr_dump(0,0)
    print "\n=> Apply a filter using a dictionary"
    dict_file = file_cleanpath("test/dictionary_test1.csvm")
    print "\n=> dictionary file is [%s]\n" % (dict_file)
    c = csvm_dict_file_filter(c, dict_file, 'CN', 0)
    print "\n=> resulting output"
    c.csvm_ptr_dump(0,0)
    print "\n=> save new CSV file"
    s = csvm_ptr_make_csvm(c,"\n","\t")
    file_str2file(file_cleanpath("test/hofmann_test1.csvm"), s)
    print "\n=> Clear CSVM object"
    c.csvm_ptr_clear()
```

The `csvm_ptr_read_extended_csvm` functions make a CSVM object (c) in memory, using a CSVM file. The method `csvm_dict_file_filter` make the filter operation. It uses the name of the `dict1` dictionary file ("dictionary_test1.csvm" stored in argument `dict_file`) and the translation set ‘CN’. Then the CSVM object is converted in a file and the memory cleared.

The `csvm_dict_file_filter` launch a simple function `csvm_dict_ptr_filter` to do the filtering:

```python
def csvm_dict_ptr_filter(self, dict, set, delcol='__DEL__'):
    ""
    The subroutine filters a CSVM file (a csvm_ptr object self) using a
dictionary (another csvm_ptr object, dict). The HEADER values (columns names
of CSVM structure) are translated using the set of dictionary given as
argument. If the HEADER values are explicitly translated to '__DEL__' value,
the corresponding columns of CSVM structure are deleted.
The argument set is a string used as the identifier (column name, element
of #HEADER list) of a translate set included in dict (a csvm_ptr object).
*** we call 'standard' this filtering mode.
    ""
    if (dict.HEADER_N <= 0): return self
dict.csvm_ptr_dump(0,0)
    if (len(set) <= 0): return self
    if ((set in dict.HEADER) == False): return self
    self = csvm_ptr_colfilter(self, dict, set)
    self = csvm_ptr_delcol(self, delcol)
    return self
```

One function does the filtering (`csvm_ptr_colfilter`) and the other (`csvm_ptr_delcol`) does the column removal.

3.1 Special cases: strong mode

Sometimes user cannot define if columns must be removed explicitly in a translation set, or if columns have a corresponding value in another translation set.

The Figure 10 illustrates this case for a CSVM dictionary (dict2) derived from previous dict1. The values __DEL__ have disappeared from the table and are replaced by characters ’-’ currently used to mark empty cells in the CSVM files.
In this case another approach could be used, first the calling code similar to Code 1 example, but using strong mode: the last argument of csvm_dict_file_filter function is set to 1 rather than zero.

**Code 3.** Advanced filtering.

```
print "*** TEST2: using a dictionary without __DEL__ or meta commands."
print "*** strong mode IS used"
c = csvm_ptr()
p = "A new blank CSVM object"
c = csvm_ptr_read_extended_csvm(c, file_cleanpath("test/hoffmann.csvm"), "\t")
c = csvm_dict_file_filter(c, dict_file, 'CN', 1)
print "\n=> resulting output"
c = csvm_ptr_dump(0, 0)
```

The csvm_dict_ptr_filter_blank function is called and could be taken as a basis to make more advanced filtering subroutines.

**Code 4.** Evolution of csvm_dict_ptr_filter subroutine.

```
def csvm_dict_ptr_filter_blank(self, dict, set, blank_list=[', '-'], delcol=__DEL__):
    The subroutine filters a CSVM file like csvm_dict_ptr_filter subroutine but using another approach to destroy columns. A csvm_ptr object (self) is given in input and filtered using a set (set) of a CSVM dictionary (dict).
    The argument set is a string used as the identifier (column name, element of #HEADER list) of a translate set included in dict (a csvm_ptr object).
    If a column name of self, is not found in the list defined by set, the corresponding column must be deleted in self. The argument blank_list is used to store the values used in cells for no data (empty string or a special char as '-').
    If the argument delcol is set (and its length is > 1), the destruction of corresponding columns (same as csvm_dict_ptr_filter) is applied before destruction of columns with data of blank_list.
    The values of blank_list are case sensitive and compared in equal (not include) mode for security reasons about data.
    if (dict.HEADER_N <= 0): return self
    if (len(set) <= 0): return self
    if ((set in dict.HEADER) == False): return self
    if (len(delcol) > 1):
        self = csvm_ptr_delcol(self, delcol)
```


The first part (## apply filter) is the same as code shown in Code 2 example. The isset variable is used to store the index of translation set selected in the dict2, in this case isset = [2] because it is the third element of #HEADER list.

The kwlist Python list (mono-dimensional array) is used to store the column names corresponding to the translation set: kwlist = ['ID', 'identificateur', 'vrac', 'plaque', 'smi', 'mdl']. This list is filtered using the argument blank_list of the function. With default values the empty cells or cell tagged by '-' are removed from kwlist, and now, kwlist = ['ID', 'identificateur', 'vrac', 'plaque', 'smi', 'mdl']

Knowing this information, it is possible to get the column names (in this case indexes are returned) of molecular table that are not found in kwlist. And we have dist = [3, 5, 6, 7, 8, 9, 10, 11, 12, 13]. The corresponding column names are stored in hlist, in this case hlist = ['plaque', 'laboratoire'] and all columns with names included in hlist will be deleted.

Here all columns names of molecular collection are specified in the dictionary (using a value or a '–'). In the general case, a dictionary may not have all possible column names that can be found in data files. To illustrate this remark, we can comment two rows in dict2 dictionary, one that is included in target translation set (plate row) and one that is not included (chemist). These two rows are tagged using the ‘##’ character in first position and will not be read by the CSV parser (they are considered now like annotations in the data block of the dictionary):

```plaintext
#plate plaque plaque #TEXT #10
#chemist laboratoire - #TEXT #50
```

The corresponding values of intermediate variables are:

```plaintext
isset = [2]
kwlist = ['ID', 'identificateur', '–', 'vrac', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', 'smi', 'mdl', '–', '–']
dist = [2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13]
hlist = ['plate', 'chemist', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–', '–']
```

And the column ‘plate’ is not added to the final molecular collection. The following lines are the dump of the corresponding CSVM object (only the ten first lines of the data block are shown):

=> resulting output
DUMP: CSVM info {
SOURCE test\hoffmann.csvm
CSV  CSV
META [ ]
TITLE_N 1
TITLE HEADER_N 4
TYPE_N 4
WIDTH_N 4
0 -10 TEXT {ID}
1 -10 TEXT {identificateur}
DATA_R 80
DATA_C 4

\[ [01] \text{[af01]}[114]\text{[C1C(OC(O)C=ClNc1ccccc1N)C]} \\
[02] \text{[af02]}[85]\text{[c1(cccc(c1)[N+]\text{[O]}\text{[O]}\text{[N]}]} / \text{N=C(C1=C(O)CC(OCl=O)C)N} \\
[03] \text{[af03]}[60]\text{[n12nc(scinc(C)c/c/2=C/1\text{C}\text{[=O]}\text{=N}(N=C1)c1cccc1cSc]} \\
[04] \text{[af04]}[50]\text{[c1(cccc(c1)C1Nc2c(N=C(c3c(=O)oc(cc3O)C)C1)cccc2]} \\
[05] \text{[af05]}[100]\text{[C1(=CC(=O)OC1)Nc1ccccc1N]} \\
[06] \text{[af06]}[71]\text{[C1(=CC(=O)OC1)Nc1ccccc1cCl]} \\
[07] \text{[af07]}[60]\text{[c1(cccc(c1)OC)C1Nc2c(N=C(c3c(=O)oc(cc3O)C)C1)cccc2]} \\
[08] \text{[af08]}[50]\text{[C1(=CC(=O)OC1)Nc1ccccc1cN] [N+]\text{[O]}\text{[O]}\text{[N]}]} \\
[09] \text{[af09]}[60]\text{[c12c(cccc2)n(cnl)C1=CC(=O)OC(C1)C]} \\
[10] \text{[af10]}[45]\text{[c12c(cccc(c2)c)n(cnl)C1=CC(=O)OC(C1)C]} \\
[11] \text{[af11]}[43]\text{[c12c(cccc(c2)c)n(cnl)C1=CC(=O)OC(C1)C]} \\
\]
5. Conclusion and perspectives

One typical tedious task is to develop software in order to convert different data flows. The combined use of text components and CSVM dictionaries has helped us to reduce greatly the number of lines of code. The use of dictionaries rather than UNIX filters has considerably helped all users to design-debug-share filters. All the steps of data flows can be documented: the data itself, the dictionaries, the indexes of collections (data, files), the intermediate files used in interchange flows … allowing re-using information at high level, even for RAW data.

The CSVM files are easy to generate, not only for automatic processes but also for humans. The only need is to add a metadata block at the bottom of a spreadsheet file and to save it using a ASCII/CSVM format and a well chosen field delimiter.

For these reasons CSVM seems a good candidate for being a canonical data model in a lot of applications for science and industry.

Supporting information

Please contact corresponding author for support on the Python (Pybuild) CSVM toolkit or data format. The CSVM-1 specification details can be found in the following reference:

G. Beyries, F. Rodriguez (2012) Technical Report: CSVM format for scientific tabular data - arXiv:1207.5711v1 [http://fr.arxiv.org/abs/1207.5711v1].

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