Beyond the plain text file format

How a relational database file can take us beyond the plain text file format

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Topics

- Text file formats
- Atoms, bonds, coordinates, properties, ...
- Relational database tables and SQL
- SQLite is a relational database in a single file
- Chemical and biological data
- Extensibility of SQL schemas
- Using SQLite files, programming

Molecular text file formats

Multiple formats commonly used

- Small molecules
- Proteins
- Nucleic acids
- Proprietary formats
- Chemical and biological data

Most can be interconverted – Problem solved!?

- OpenBabel supports 118 formats

PDB plain text

```
COMPND    1-1
AUTHOR    GENERATED BY OPEN BABEL 2.3.2
HETATM    1  C   LIG     1       27.705  22.040  17.024  1.00  0.00           C
HETATM    2  N   LIG     1       26.440  22.098  16.432  1.00  0.00           N
HETATM    3  C   LIG     1       25.538  21.442  17.283  1.00  0.00           C
HETATM    4  C   LIG     1       26.253  20.975  18.375  1.00  0.00           C
HETATM    5  C   LIG     1       27.594  21.361  18.222  1.00  0.00           C
HETATM    6  C   LIG     1       24.082  21.367  17.108  1.00  0.00           C
HETATM    7  C   LIG     1       26.132  22.682  15.163  1.00  0.00           C
HETATM    8  C   LIG     1       23.410  22.267  16.267  1.00  0.00           C
HETATM    9  C   LIG     1       22.022  22.201  16.120  1.00  0.00           C
HETATM   10  C   LIG     1       21.298  21.241  16.831  1.00  0.00           C
HETATM   11  C   LIG     1       21.951  20.340  17.675  1.00  0.00           C
HETATM   12  C   LIG     1       23.340  20.412  17.817  1.00  0.00           C
HETATM   13  C   LIG     1       26.369  24.046  14.936  1.00  0.00           C
HETATM   14  C   LIG     1       26.063  24.612  13.696  1.00  0.00           C
HETATM   15  C   LIG     1       25.524  23.818  12.691  1.00  0.00           C
...
CONECT    1    2    5   19
CONECT    2    1    3    7
CONECT    3    2    4    6
CONECT    4    3    5   24
CONECT    5    1    4   25
CONECT    6    3    8   12
CONECT    7    2   13   17
CONECT    8    6    9   26
CONECT    9    8   10   27
CONECT   10    9   11   20
CONECT   11   10   12   28
CONECT   12    6   11   29
CONECT   13    7   14   30
CONECT   14   13   15   31
CONECT   15   14   16   18
CONECT   16   15   17   32
 ...
MASTER        0    0    0    0    0    0    0    0   39    0   39    0
END
```

SDF plain text

```
1-1
  Cerius2 12120216093D 1   1.00000
 Structure written by MMmdl.
 39 41  0  0  0  0  0  0  0  0999 V2000
   27.7051   22.0403   17.0243 C   0  0  0  0  0  0
   26.4399   22.0976   16.4318 N   0  0  0  0  0  0
   25.5381   21.4424   17.2831 C   0  0  0  0  0  0
   26.2525   20.9753   18.3748 C   0  0  0  0  0  0
   27.5943   21.3608   18.2218 C   0  0  0  0  0  0
   24.0821   21.3670   17.1082 C   0  0  0  0  0  0
   26.1324   22.6824   15.1634 C   0  0  0  0  0  0
...
  1  2  1  0  0  0
  1  5  2  0  0  0
  1 19  1  0  0  0
  2  3  1  0  0  0
  2  7  1  0  0  0
  3  4  2  0  0  0
  3  6  1  0  0  0
  4  5  1  0  0  0
  4 24  1  0  0  0
  5 25  1  0  0  0
  6  8  2  0  0  0
  6 12  1  0  0  0
...
M  END
>  <Name>
1-1

>  <Family>
A.1

>  <IC50_uM>
0.06

>  <set>
1

$$$$
```

JSON structured file

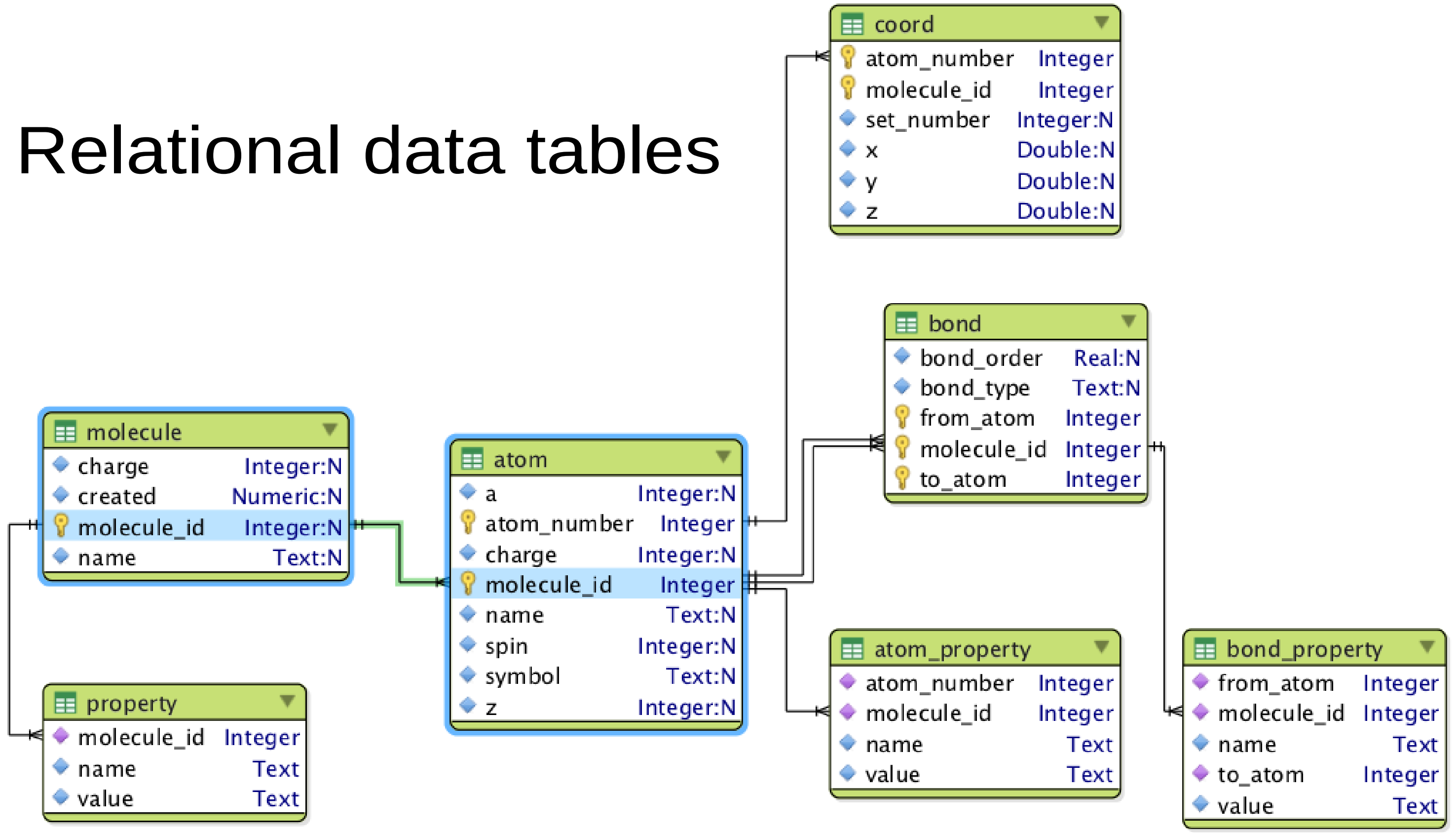
```
{
    "name": "1-1",
    "charge": null,
    "atoms": [
        {
            "idx": 1,
            "symbol": "C",
            "atomic_number": 6,
            "charge": 0,
            "x": 27.7051,
            "y": 22.0403,
            "z": 17.0243
        },
        {
            "idx": 2,
            "symbol": "N",
            "atomic_number": 7,
            "charge": 0,
            "x": 26.4399,
            "y": 22.0976,
            "z": 16.4318
        },
...],
    "bonds": [
            [1,19,1],
            [1,2,1],
            [1,5,2],
            [2,3,1],
            [2,7,1],
...],
    "properties":
       {
          "Family": "A.1",
          "IC50_uM": 0.06,
          "set": 1
       }
}
```

CML/XML structured file

```
<?xml version="1.0"?>
<molecule id="id1-1" xmlns="http://www.xml-cml.org/schema">
 <atomArray>
  <atom id="a1" elementType="C" x3="27.705100" y3="22.040300" z3="17.024300"/>
  <atom id="a2" elementType="N" x3="26.439900" y3="22.097600" z3="16.431800"/>
  <atom id="a3" elementType="C" x3="25.538100" y3="21.442400" z3="17.283100"/>
  <atom id="a4" elementType="C" x3="26.252500" y3="20.975300" z3="18.374800"/>
  <atom id="a5" elementType="C" x3="27.594300" y3="21.360800" z3="18.221800"/>
  <atom id="a6" elementType="C" x3="24.082100" y3="21.367000" z3="17.108200"/>
...
 </atomArray>

 <bondArray>
  <bond atomRefs2="a1 a2" order="1"/>
  <bond atomRefs2="a1 a5" order="2"/>
  <bond atomRefs2="a1 a19" order="1"/>
  <bond atomRefs2="a2 a3" order="1"/>
  <bond atomRefs2="a2 a7" order="1"/>
  <bond atomRefs2="a3 a4" order="2"/>
...
 </bondArray>

 <propertyList>
  <property title="Name">
   <scalar>1-1</scalar>
  </property>
  <property title="Family">
   <scalar>A.1</scalar>
  </property>
  <property title="IC50_uM">
   <scalar>0.06</scalar>
  </property>
  <property title="set">
   <scalar>1</scalar>
  </property>
 </propertyList>
</molecule>
```

SQLite structured file .umdb

Relational data tables



coord

atom_number	Integer
molecule_id	Integer
set_number	Integer:N
x	Double:N
y	Double:N
z	Double:N

bond

bond_order	Real:N
bond_type	Text:N
from_atom	Integer
molecule_id	Integer
to_atom	Integer

molecule

charge	Integer:N
created	Numeric:N
molecule_id	Integer:N
name	Text:N

atom

a	Integer:N
atom_number	Integer
charge	Integer:N
molecule_id	Integer
name	Text:N
spin	Integer:N
symbol	Text:N
z	Integer:N

property

molecule_id	Integer
name	Text
value	Text

atom_property

atom_number	Integer
molecule_id	Integer
name	Text
value	Text

bond_property

from_atom	Integer
molecule_id	Integer
name	Text
to_atom	Integer
value	Text

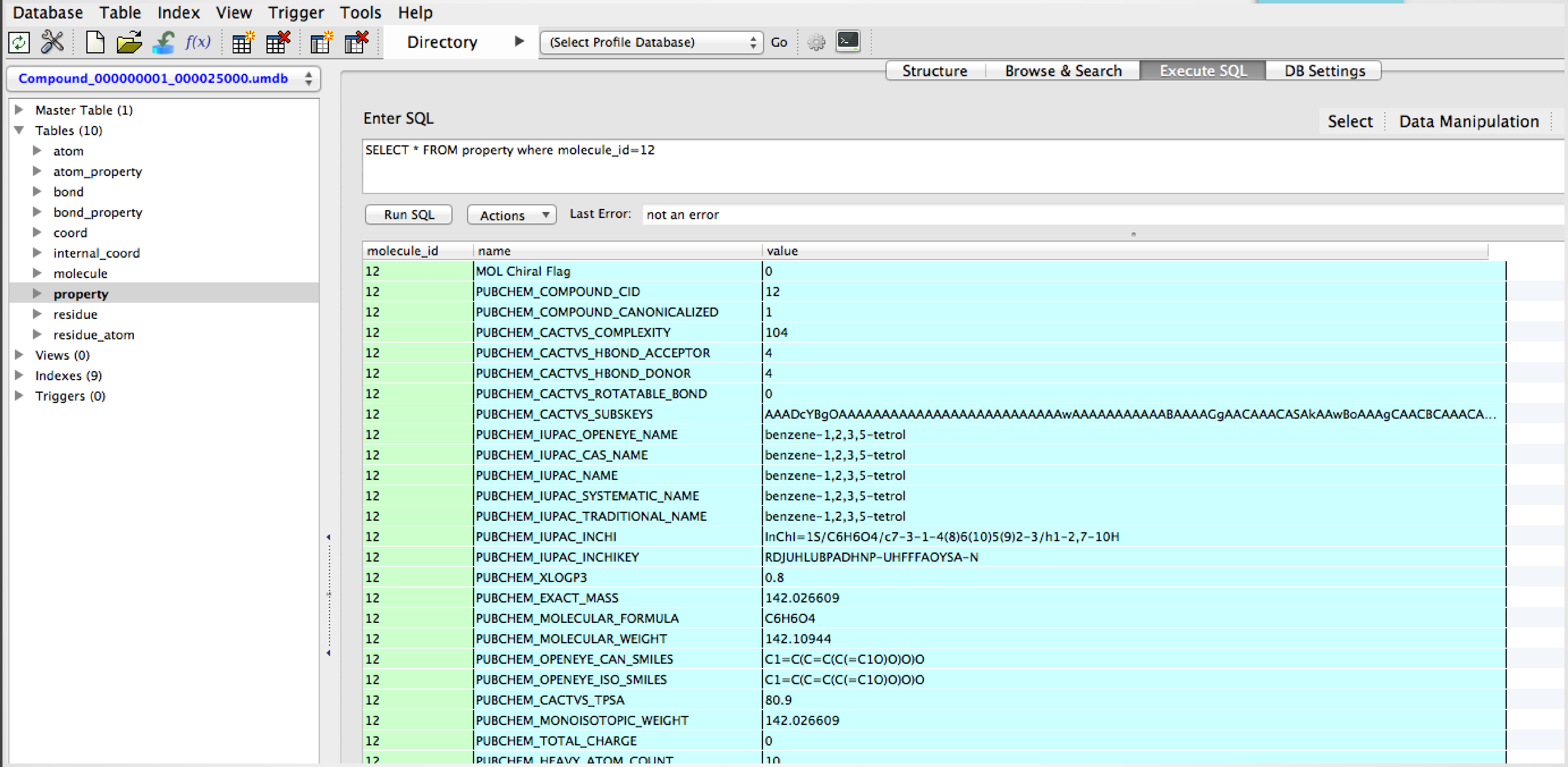
What's in a SQLite file?

```
Select atom.atom_number, atom.symbol, coord.x, coord.y, coord.z, atom.charge
   From atom Join coord Using (molecule_id, atom_number)
   Where molecule_id=1 Order By atom.atom_number;

atom_number  symbol      x           y           z           charge
-----------  ----------  ----------  ----------  ----------  ----------
1            C           27.7051     22.0403     17.0243     0
2            N           26.4399     22.0976     16.4318     0
3            C           25.5381     21.4424     17.2831     0
4            C           26.2525     20.9753     18.3748     0
5            C           27.5943     21.3608     18.2218     0
6            C           24.0821     21.367      17.1082     0
7            C           26.1324     22.6824     15.1634     0
8            C           23.4105     22.2668     16.2675     0
9            C           22.022      22.2007     16.1197     0
10           C           21.2976     21.2409     16.8307     0
11           C           21.9509     20.3402     17.675      0
12           C           23.3399     20.4115     17.8175     0
13           C           26.3695     24.0457     14.9358     0
14           C           26.0627     24.6119     13.6959     0
15           C           25.5236     23.8179     12.691      0
16           C           25.2821     22.466      12.901      0
17           C           25.5848     21.8942     14.1391     0
18           F           25.2311     24.3643     11.5034     0
...
```

Viewing and editing SQLite files

- Command line (built-in, all platforms)
- DB Browser for SQLite (open source on github)
- SQLite Manager Firefox addin
- SQLite Administrator (freeware, windows)
- Toad v4.2+ (not Mac)

SQLite Manager Firefox addin



Compound_000000001_000025000.umdb

- Master Table (1)
- Tables (10)
  - atom
  - atom_property
  - bond
  - bond_property
  - coord
  - internal_coord
  - molecule
  - **property**
  - residue
  - residue_atom
- Views (0)
- Indexes (9)
- Triggers (0)

Enter SQL

```
SELECT * FROM property where molecule_id=12
```

Last Error: not an error

molecule_id	name	value
12	MOL Chiral Flag	0
12	PUBCHEM_COMPOUND_CID	12
12	PUBCHEM_COMPOUND_CANONICALIZED	1
12	PUBCHEM_CACTVS_COMPLEXITY	104
12	PUBCHEM_CACTVS_HBOND_ACCEPTOR	4
12	PUBCHEM_CACTVS_HBOND_DONOR	4
12	PUBCHEM_CACTVS_ROTATABLE_BOND	0
12	PUBCHEM_CACTVS_SUBSKEYS	AAADcYBgOAAAAAAAAAAAAAAAAAAAAAAAAAAAwAAAAAAAAAAAABAAAAGgAACAAACASAkAAwBoAAAgCAACBCAAACA...
12	PUBCHEM_IUPAC_OPENEYE_NAME	benzene-1,2,3,5-tetrol
12	PUBCHEM_IUPAC_CAS_NAME	benzene-1,2,3,5-tetrol
12	PUBCHEM_IUPAC_NAME	benzene-1,2,3,5-tetrol
12	PUBCHEM_IUPAC_SYSTEMATIC_NAME	benzene-1,2,3,5-tetrol
12	PUBCHEM_IUPAC_TRADITIONAL_NAME	benzene-1,2,3,5-tetrol
12	PUBCHEM_IUPAC_INCHI	InChI=1S/C6H6O4/c7-3-1-4(8)6(10)5(9)2-3/h1-2,7-10H
12	PUBCHEM_IUPAC_INCHIKEY	RDJUHLUBPADHNP-UHFFFAOYSA-N
12	PUBCHEM_XLOGP3	0.8
12	PUBCHEM_EXACT_MASS	142.026609
12	PUBCHEM_MOLECULAR_FORMULA	C6H6O4
12	PUBCHEM_MOLECULAR_WEIGHT	142.10944
12	PUBCHEM_OPENEYE_CAN_SMILES	C1=C(C=C(C(=C1O)O)O)O
12	PUBCHEM_OPENEYE_ISO_SMILES	C1=C(C=C(C(=C1O)O)O)O
12	PUBCHEM_CACTVS_TPSA	80.9
12	PUBCHEM_MONOISOTOPIC_WEIGHT	142.026609
12	PUBCHEM_TOTAL_CHARGE	0
12	PUBCHEM_HEAVY_ATOM_COUNT	10

SQLite (www.sqlite.org)

- All the advantages of a flat-file; all the features of a relational database
- Self-contained, serverless, zero configuration
- Included in Python standard library
- Bindings for 43 languages
- Most widely deployed database engine in the world
- Public domain, free to use for any purpose

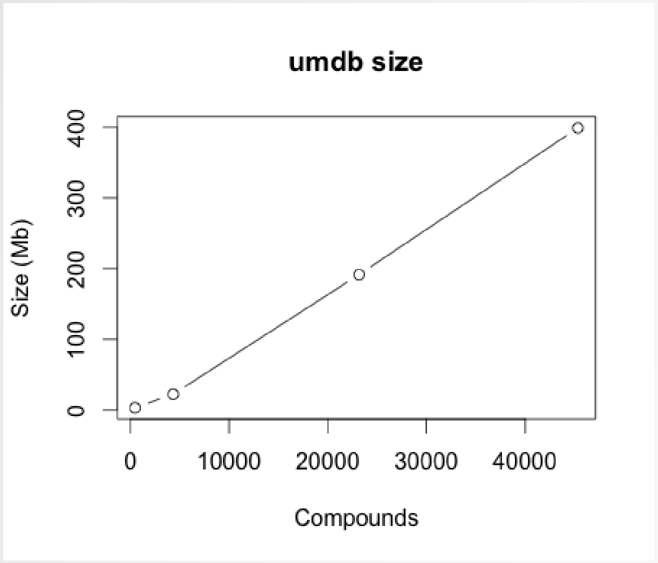
How large are SQLite files?

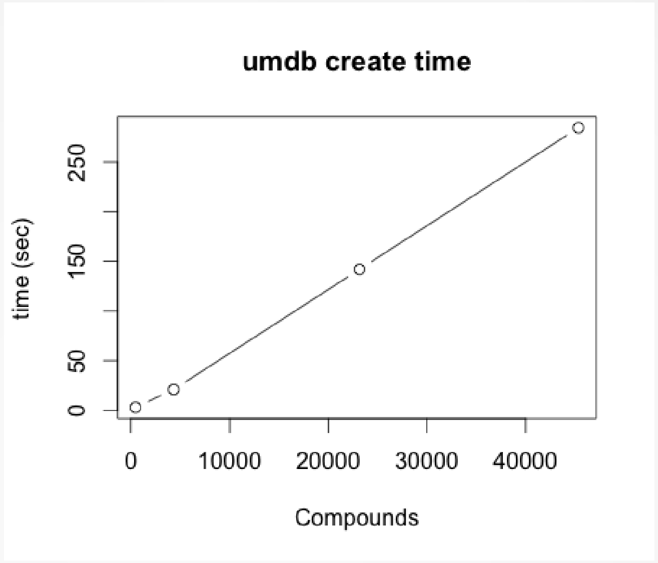
Original SDF contains 467 molecules

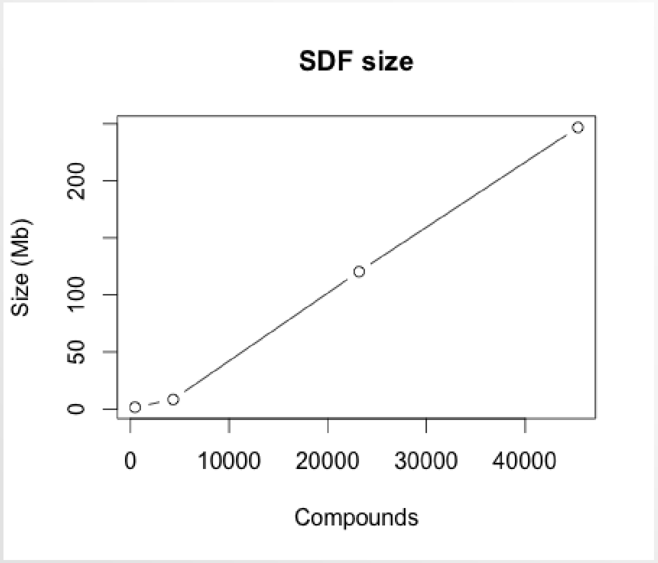
```
$ babel cox2_3d.sdf cox2_3d.pdb
$ babel cox2_3d.sdf cox2_3d.cml
$ python obmol.py cox2_3d.sdf cox2_3d.umdb

$ wc -c cox* | sort -n
 1486991 cox2_3d.sdf
 2419255 cox2_3d.cml
 2444870 cox2_3d.js
 2994176 cox2_3d.umdb
 3115692 cox2_3d.pdb

$ gzip cox*; wc -c cox* | sort -n
  247045 cox2_3d.sdf.gz    (16%)
  262544 cox2_3d.pdb.gz    ( 8%)
  273579 cox2_3d.js.gz     (11%)
  284060 cox2_3d.cml.gz    (11%)
 1293529 cox2_3d.umdb.gz   (37%)
```

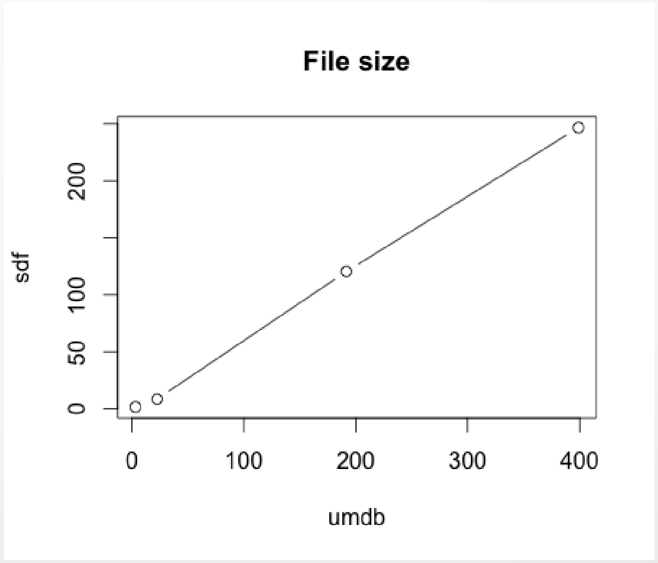
Maximum size allowed by filesystem

How do SQLite files scale?









cox2	467
cas	4337
pubchem	23170
pubchem	45353

How efficient is using SQLite files?

Compute center of mass for 467 molecules

OpenBabel python vs. SQLite

```
$ time python cm.py
...
14-15 397.4194432 24.5140548807 22.1725456909 15.9736236732
14-16 412.88598 24.5963886245 22.3002506939 15.8502371715
14-17 413.87404 24.5813303532 22.2904584772 15.8464177326
7-39 328.3607232 23.7537457692 21.924262208 15.9951401499

real    0m0.842s
user    0m0.811s
 sys    0m0.026s


$ time python cm-select.py
...
14-15 397.4194432 24.5140548807 22.1725456909 15.9736236732
14-16 412.88598 24.5963886245 22.3002506939 15.8502371715
14-17 413.87404 24.5813303532 22.2904584772 15.8464177326
7-39 328.3607232 23.7537457692 21.924262208 15.9951401499

real    0m0.166s
user    0m0.136s
 sys    0m0.027s
```

SQLite is *fast* random access file

Any table can be indexed for fast access

Select data for first molecule

```
sqlite> select molecule_id,name,value from property
  where name in ('PUBCHEM_IUPAC_CAS_NAME', 'PUBCHEM_IUPAC_INCHI') And molecule_id=1;

molecule_id|name|value
1|PUBCHEM_IUPAC_CAS_NAME|3-acetyloxy-4-(trimethylammonio)butanoate
1|PUBCHEM_IUPAC_INCHI|InChI=1S/C9H17NO4/c1-7(11)14-8(5-9(12)13)6-10(2,3)4/h8H,5-6H2,1-4H3
Run Time: real 0.001 user 0.000293 sys 0.000087
```

Select data for molecule 20000

```
sqlite> select molecule_id,name,value from property
  where name in ('PUBCHEM_IUPAC_CAS_NAME', 'PUBCHEM_IUPAC_INCHI') And molecule_id=20000;

molecule_id|name|value
20000|PUBCHEM_IUPAC_CAS_NAME|2-thiocyanatoacetic acid butyl ester
20000|PUBCHEM_IUPAC_INCHI|InChI=1S/C7H11NO2S/c1-2-3-4-10-7(9)5-11-6-8/h2-5H2,1H3
Run Time: real 0.000 user 0.000279 sys 0.000089
```

Create SQLite .umdb files

Row by row, table by table taking data from anywhere

```
Insert into molecule (name, charge, created) Values ('aspirin', 0, datetime());
Insert Into atom (molecule_id, atom_number, z) Values (1,1,6),(1,2,6),(1,3,7);
Insert Into coord (molecule_id, atom_number, x, y, z) Values (1,1,0.0,0.0,0.0);
...
```

467 molecules; python program using OpenBabel

```
$ time python obmol.py cox2_3d.sdf cox2_3d.umdb
```

```
real 0m2.854s
user 0m2.252s
sys  0m0.400s
```

Update SQLite .umdb files

```
sqlite> .timer on
sqlite> .mode csv
sqlite> .import newprop.csv newprop

sqlite> Insert Into property (molecule_id,name,value)
 Select molecule_id,'gnova_glogp',gnova_glogp From molecule
 Join newprop On (molecule.name=newprop.pubchem_id) ;
Run Time: real 0.807 user 0.283474 sys 0.469584

sqlite> Insert Into property (molecule_id,name,value)
 Select molecule_id,'gnova_tpsa',gnova_tpsa From molecule
 Join newprop On (molecule.name=newprop.pubchem_id) ;
Run Time: real 0.830 user 0.296428 sys 0.481289

sqlite> drop table newprop;
Run Time: real 0.038 user 0.006310 sys 0.021853

$ head newprop.csv
pubchem_id,gnova_glogp,gnova_tpsa
384,0.6933,86.63
385,1.1061,74.6
391,3.7655,132.91
399,-0.2772,111.9
409,1.8197,42.32
413,1.3615,41.99
416,-1.7999,149.65
420,7.3887,20.23
422,-3.3761,194.79
```

Using .umdb files in programs

- Compared to traditional object-oriented C++ or python
- Replacing object iterators with SQL select
- Replacing entire program with SQL computation

Structured data in programs

```
class OBAPI OBMol: public OBBase
 {
 protected:
   int                           _flags;        //!< bitfield of flags
   bool                          _autoPartialCharge;//!< Assign partial charges
   bool                          _autoFormalCharge;//!< Assign formal charges
   std::string                   _title;        //!< Molecule title
   std::vector<OBAtom*>          _vatom;        //!< vector of atoms
   std::vector<OBAtom*>          _atomIds;      //!< vector of atoms indexed by id
   std::vector<OBBond*>          _vbond;        //!< vector of bonds
   std::vector<OBBond*>          _bondIds;      //!< vector of bonds
   unsigned short int            _dimension;    //!< Dimensionality of coordinates
   int                           _totalCharge;  //!< Total charge on the molecule
   unsigned int                  _totalSpin;    //!< Total spin on the molecule
   double                        *_c;           //!< coordinate array
   std::vector<double*>          _vconf;        //!< vector of conformers
   double                        _energy;       //!< heat of formation
   unsigned int                  _natoms;       //!< Number of atoms
   unsigned int                  _nbonds;       //!< Number of bonds
   std::vector<OBResidue*>       _residue;      //!< Residue information (if applicable)
   std::vector<OBInternalCoord*> _internals;    //!< Internal Coordinates (if applicable)
...
```

Read text file into program objects

```
# compute center of mass

import openbabel

mol = openbabel.OBMol()
conv = openbabel.OBConversion()
conv.SetInFormat("sdf")

notatend = conv.ReadFile(mol,"cox2_3d.sdf")
while notatend:
   total_mass = 0.0
   cm_x = 0.0
   cm_y = 0.0
   cm_z = 0.0
   for atom in openbabel.OBMolAtomIter(mol):
      m = atom.GetAtomicMass()
      total_mass += m
      cm_x += m * atom.GetX()
      cm_y += m * atom.GetY()
      cm_z += m * atom.GetZ()

   print mol.GetTitle(), total_mass, \
   cm_x/total_mass, cm_y/total_mass, cm_z/total_mass
   mol.Clear()
   notatend = conv.Read(mol)
```

Read SQLite tables into program objects

Open the database file

Select all molecule, atoms, bonds, properties into program objects, corresponding to traditional reading of plain text file

```
Select molecule_id, molecule.name, atom.atom_number, atom.symbol, atom.charge, coord.x,
coord.y, coord.z, group_concat(to_atom) As bonds From molecule Join atom Using(molecule_id)
Join coord Using (molecule_id,atom_number) Join bond Using (molecule_id) Where
atom.atom_number=bond.from_atom Group by molecule_id, atom_number;
```

Iterate over objects to carry out program algorithms

```
total_mass = 0.0
cm_x = 0.0
cm_y = 0.0
cm_z = 0.0
for atom in openbabel.OBMolAtomIter(mol):
      m = atom.GetAtomicMass()
      total_mass += m
      cm_x += m * atom.GetX()
      cm_y += m * atom.GetY()
      cm_z += m * atom.GetZ()

print mol.GetTitle(), total_mass, mol.GetMolWt(), cm_x/total_mass,
cm_y/total_mass, cm_z/total_mass
```

Use SQL *select* as object *iterators*

Connect database file replaces file open and read

Database tables replace program objects

SQL select replaces object iterator

```
import sqlite3

conn = sqlite3.connect('cox2_3d.umdb')
conn.row_factory = sqlite3.Row
curs = conn.cursor()
curs.execute("Attach 'element.sqlite' As element")
sql = "Select molecule.name, mass, coord.x, coord.y,coord.z From molecule \
 Join atom Using (molecule_id)\
 Join element.element Using(z) \
 Join coord Using (molecule_id,atom_number) \
 Where molecule_id = ?"
for imol in range(467):
      total_mass = 0.0
      cm_x = 0.0
      cm_y = 0.0
      cm_z = 0.0
      for row in curs.execute(sql, [imol+1]):
         name = row['name']
         m = row['mass']
         total_mass += m
         cm_x += m * row['x']
         cm_y += m * row['y']
         cm_z += m * row['z']

      print name, total_mass, cm_x/total_mass, cm_y/total_mass, cm_z/total_mass
```

Using SQL for entire computation

Compute center of mass for 467 molecules using SQL

```
Attach "element.sqlite" As element;
Select molecule.name, sum(mass),
 sum(mass*coord.x)/sum(mass),
 sum(mass*coord.y)/sum(mass),
 sum(mass*coord.z)/sum(mass)
 From molecule Join atom Using (molecule_id)
  Join element.element Using(z)
  Join coord Using (molecule_id,atom_number)
 Group By molecule_id;

$ time sqlite3 cox2_3d.umdb <cm.sql

real    0m0.058s
user    0m0.046s
sys     0m0.008s

$ sqlite3 element.sqlite
sqlite> select z,symbol,mass from element limit 10;
z           symbol      mass
----------  ----------  ----------
1           H           1.00794
2           He          4.002602
3           Li          6.941
4           Be          9.012182
5           B           10.811
6           C           12.0107
7           N           14.0067
8           O           15.9994
9           F           18.9984032
10          Ne          20.1797
```

How efficient can SQLite be?

Compute center of mass for 467 molecules

OpenBabel python vs. SQLite

```
$ time python cm.py

real    0m0.842s
user    0m0.811s
sys     0m0.026s

$ time python cm-select.py

real    0m0.166s
user    0m0.136s
sys     0m0.027s

$ time sqlite3 cox2_3d.umdb <cm.sql

real    0m0.059s
user    0m0.047s
sys     0m0.008s
```

Extending .umdb files

SQLite .umdb files can add new tables and relationships as well as update or add new data

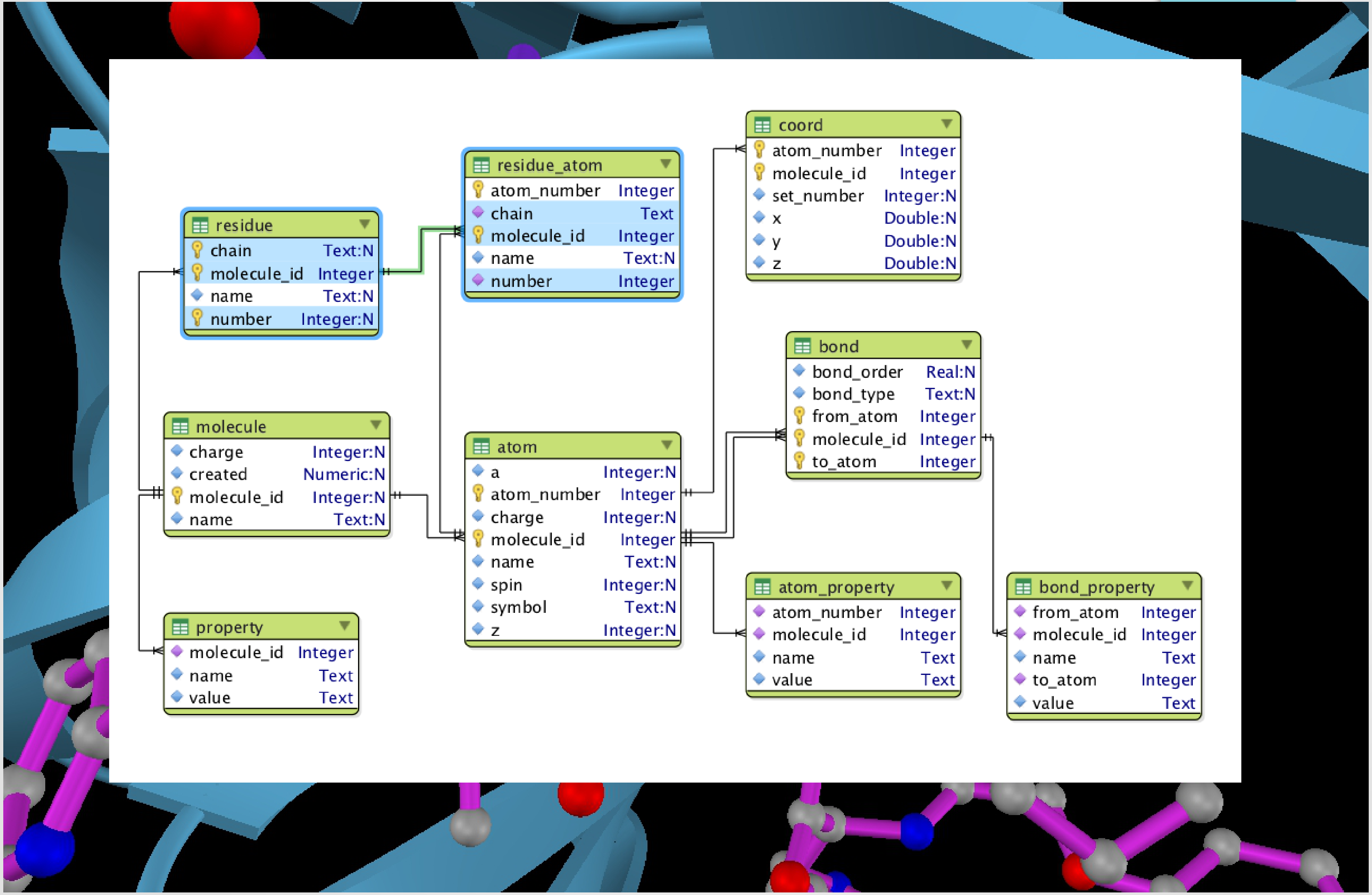
SD files v2000 limited to 999 atoms

- V3000 no atom limit, enhanced stereochemistry

PDB files limited to 99999 atoms, 1-character chain, 3-character residue

- PDBML/XML, mmCIF eliminate column-width limits and add data definitions

Extended schema for proteins



residue

chain	Text:N
molecule_id	Integer
name	Text:N
number	Integer:N

residue_atom

atom_number	Integer
chain	Text
molecule_id	Integer
name	Text:N
number	Integer

coord

atom_number	Integer
molecule_id	Integer
set_number	Integer:N
x	Double:N
y	Double:N
z	Double:N

bond

bond_order	Real:N
bond_type	Text:N
from_atom	Integer
molecule_id	Integer
to_atom	Integer

molecule

charge	Integer:N
created	Numeric:N
molecule_id	Integer:N
name	Text:N

atom

a	Integer:N
atom_number	Integer
charge	Integer:N
molecule_id	Integer
name	Text:N
spin	Integer:N
symbol	Text:N
z	Integer:N

property

molecule_id	Integer
name	Text
value	Text

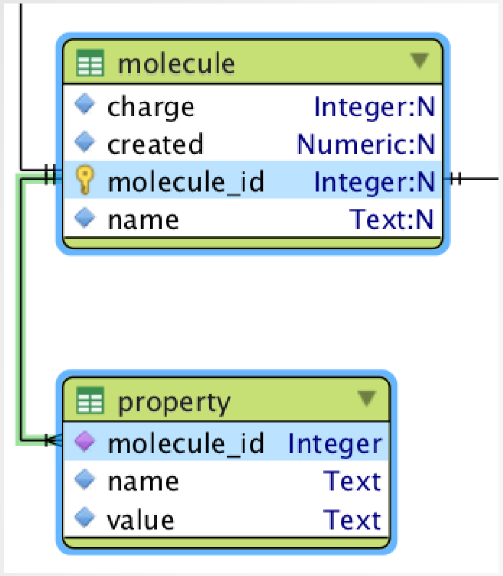
atom_property

atom_number	Integer
molecule_id	Integer
name	Text
value	Text

bond_property

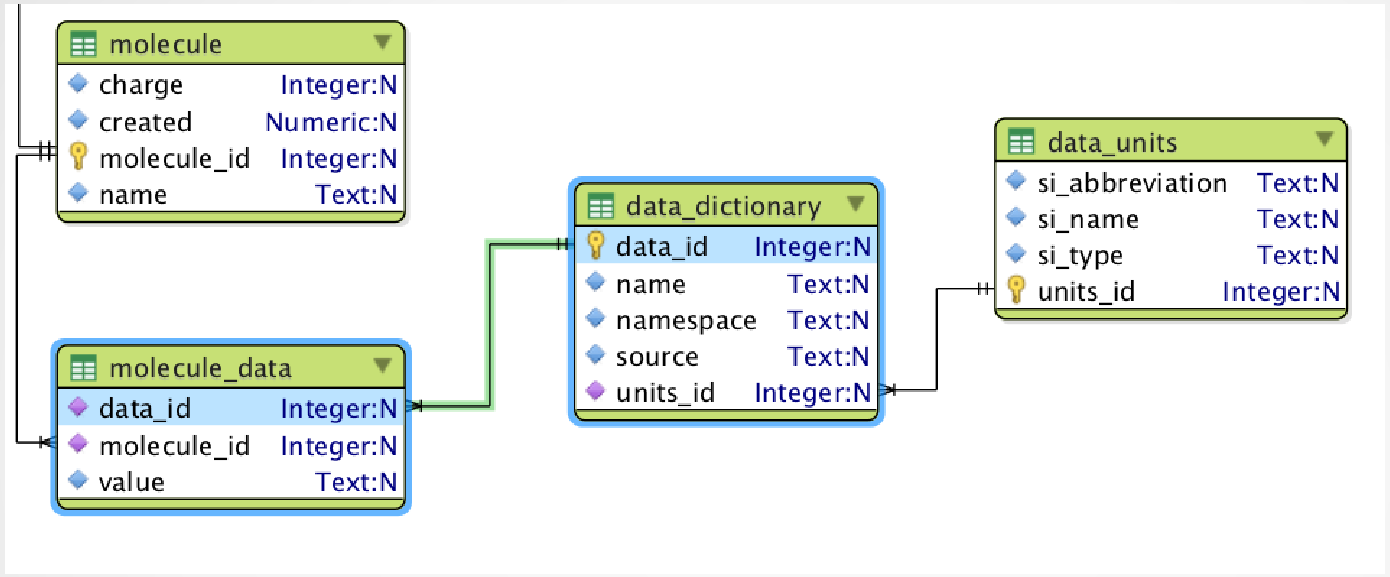
from_atom	Integer
molecule_id	Integer
name	Text
to_atom	Integer
value	Text

Chemical and biological data



```
Select property.name, property.value
 From property Where molecule_id=1;

Name                  value
--------------------  -----------
Name                  1-1
Family                A.1
IC50_uM               0.06
Set                   1
```

Extension for chemical/biological data



```
Select dict.name, data.value
 From molecule_data As data Join data_dictionary dict Using (data_id)
 Where molecule_id=1;
```

CML data dictionary

```
<?xml version="1.0" encoding="UTF-8" ?>
<dictionary xmlns="http://www.xml-cml.org/schema"
            xmlns:convention="http://www.xml-cml.org/convention/"
            xmlns:unit="http://www.xml-cml.org/unit/nonSi/"
            xmlns:unitType="http://www.xml-cml.org/unit/unitType/"
            xmlns:xhtml="http://www.w3.org/1999/xhtml"
            xmlns:xsd="http://www.w3.org/2001/XMLSchema"
            convention="convention:dictionary"
            title="fundamental chemistry concepts"
            namespace="http://www.xml-cml.org/dictionary/dummy/"
            dictionaryPrefix="dummy">
        <description>
            <xhtml:p>
                This is an example dictionary
            </xhtml:p>
        </description>

    <entry id="molecmass" term="Molecular Mass"
           dataType="xsd:double" unitType="unitType:amount" units="unit:dalton">
        <definition>
            <xhtml:p>
                The mass of one mole of a substance in unified atomic mass units (Dalton).
            </xhtml:p>
        </definition>
        <description>
            <xhtml:p>
                The molecular mass (m) of a substance is the mass of one molecule of that substance,
                in unified atomic mass unit(s) ...
            </xhtml:p>
        </description>
    </entry>

    <entry id="molarmass" term="Molar Mass"
           dataType="xsd:double" unitType="unitType:amount" units="unit:dalton">
        <definition>
            <xhtml:p>
                The mass per amount of substance.
            </xhtml:p>
        </definition>
        <description>
            <xhtml:p>
                Molar mass, symbol M, is a physical property characteristic of a given substance
                ...
            </xhtml:p>
        </description>
    </entry>

</dictionary>
```

Summary

Advantages

- Single-File documents
- Cross-platform
- Fast access
- SQL
- Easily updated
- Readily extensible and reducible
- Concurrent use by multiple processes
- Transactions
- Better applications; restart files

Future work, other extensions

- umdb project at http://github.com/tjod
- PDBML/XML
  - “Third, the straightforward mapping of PDB data to relational database systems is retained.”
- mmCIF
  - flexible and extensible tag-value format for representing macromolecular structural data
- Extension tables
  - New types of data, for example spectroscopic data
  - Supramolecular assemblies