Extraction of a submap from a Cell Designer map (PART 3)

Authors: Ronan M.T. Fleming, Leiden University

Reviewer(s):

INTRODUCTION
Given a generic map of metabolism, creat a derivative map by removing a subset of the reactions.

EQUIPMENT SETUP
To visualise the metabolic maps it is necessary to obtain the version 4.4 of CellDesigner. This software can be freely downloaded from:

http://www.celldesigner.org/download.html

PROCEDURE

1. Import a CellDesigner XML file to MATLAB environment
The `transformXML2Map` function parses an XML file from Cell Designer (CD) into a Matlab structure. This structure is organised similarly to the structure found in the COnstraint-Base and Reconstruction Analysis (COBRA) models.

Read in a map

```
[GlyXml, GlyMap] = transformXML2Map('glycolysisAndTCA.xml');
```

```
Elapsed time is 1.834226 seconds.
```

2. Remove some reactions from the map

```
if 1
    rxnRemoveList={'ENO';'PFK';'PGMT';'ABC'};
else
    rxnRemoveList={'PGMT'};
end
printLevel=1;
[GlyXmlStructSubset,GlyMapSubset,rxnNotInMap] = removeMapReactions(GlyXml,GlyMap,rxnRem
```

```
ABC not present in the map
```

There is no reaction 'ABC' in the map, so the function alerts that it has not been removed.

```
rxnRemoveList(rxnNotInMap)
```

```
ans = 1×1 cell array

    {'ABC'}
```

3. Export the modified map

```
transformMap2XML(GlyXmlStructSubset,GlyMapSubset,'glycolysisAndTCA_subset.xml');
```

```
Elapsed time is 1.317182 seconds.
```

4. Import the modified map and compare it with the matlab structures

```
[GlyXmlStructSubset2,GlyMapSubset2] = transformXML2Map('glycolysisAndTCA_subset.xml');
```

```
Elapsed time is 1.667602 seconds.
ans = struct with fields:
        id: 're2'
    metaid: 're57'
      name: 'DPGM'
ans = struct with fields:
          id: 're2'
      metaid: 're57'
        name: 'DPGM'
  reversible: 'true'
```

Compare xml structure

```
[resultXml, whyXml] = structeq(GlyXmlStructSubset, GlyXmlStructSubset2)
```

```
resultXml = logical

   0
whyXml = struct with fields:
    Reason: 'Properties are different <- Unequal Subcell <- Properties are different <- Unequal Subcell <-
     Where: '(1).sbml(1).model(1).listOfReactions(1).reaction{2}(1).Attributes'
```

```
GlyXmlStructSubset.sbml(1).model(1).listOfReactions(1).reaction{2}(1).Attributes
```

```
ans = struct with fields:
        id: 're2'
    metaid: 're57'
      name: 'DPGM'
```

```
GlyXmlStructSubset2.sbml(1).model(1).listOfReactions(1).reaction{2}(1).Attributes
```

```
ans = struct with fields:
          id: 're2'
      metaid: 're57'
        name: 'DPGM'
  reversible: 'true'
```

Compare map structure

```
[resultMap, whyMap] = structeq(GlyMapSubset, GlyMapSubset2)
```

```
resultMap = logical

   1
whyMap = struct with fields:
    Reason: ''
     Where: ''
```

```
    return
```

4. Remove reactions from the map directly

```
fileName = 'glycolysisAndTCA.xml';
printLevel=1;
removeCDReactions(fileName,rxnRemoveList,printLevel)
```