

# Initialisation of conserved moiety decomposition

Conserved moiety decomposition consists of several sequential live scripts

1. tutorial\_initConservedMoietyPaths.mlx (this script)
2. tutorial\_buildAtomTransitionMultigraph.mlx
3. tutorial\_identifyConservedMoieties.mlx
4. tutorial\_analyseConservedMoieties.mlx
5. tutorial\_visualiseConservedMoieties.mlx

Define the model that will be used for conserved moiety decomposition

```
if ~exist('modelName','var')
    modelName = 'iDopaNeuro1';
    %modelName = 'DAS'
```

```
modelName =
'DAS'
```

```
end
```

Setup the paths

```
switch modelName
    case 'DAS'
        projectDir = strrep(which('tutorial_identifyConservedMoieties'),'tutorial_iden
    case 'iDopaNeuro1'
        projectDir = ['~' filesep 'work' filesep 'sbgCloud' filesep 'programExperimenta
end
```

```
projectDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties'
```

```
dataDir = [projectDir filesep 'data' filesep]
```

```
dataDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/'
```

```
addpath(genpath(dataDir));
softwareDir = [projectDir filesep 'software' filesep]
```

```
softwareDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/software/'
```

```
visDataDir = [projectDir filesep 'data' filesep 'visualisation' filesep]
```

```
visDataDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/visualisation/'
```

```
resultsDir = [projectDir filesep 'results' filesep modelName '_ConservedMoieties' files
```

```
resultsDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/results/DAS_ConservedMo'
```

A collection of pre-existing chemical table files in vmh namespace, including atom mapped reactions are here:  
<https://github.com/opencobra/ctf>, otherwise use a local directory.

```
switch modelName
  case 'DAS'
    rxnfileDir = [projectDir filesep 'data' filesep 'mini-ctf' filesep 'rxns' filesep 'atomMapped']
  case 'iDopaNeuro1'

    %rxnfileDir = [resultsDir 'fluxCobra' filesep 'dataBase' filesep 'rxn', filesep 'atomMapped']
    %rxnfileDir = '~/work/sbgCloud/programReconstruction/projects/exoMetDN/papers/vmh/atomMapped'
    %rxnfileDir = '~/work/sbgCloud/data/rxnDatabase/explicitH/atomMapped/RDT/rxnFile'

    %system('git clone git@github.com:opencobra/ctf.git ~/work/sbgCloud/code/fork-cobra-ctf')
    rxnfileDir = '~/work/sbgCloud/code/fork-ctf/rxns/atomMapped'
end
```

```
rxnfileDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/mini-ctf/rxns/atomMapped'
```

```
if ~exist(resultsDir, 'dir')
  mkdir(resultsDir)
end
cd(resultsDir)
```

Decide whether to recompute everything from scratch or try to load cached intermediate results

```
recompute = 1;
```