Identify Conserved Moieties

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INTRODUCTION

Given an atom transition multgraph for a metabolic model, this tutorial identifies its conserved moieties, as described elsewhere [1,2].

These tutorials should generally be used in the following order:

1. Initialise and set the paths to inputs and outputs

COBRA.tutorials/driver_initConservedMoietyPaths.mlx

2. Build an atom transition graph

tutorial_buildAtomTransitionMultigraph.mlx

3. Identify conserved moieties, given an atom transition graph

tutorial_identifyConservedMoieties.mlx

4. Analyse the output of #3

tutorial_analyseConservedMoieties.mlx

5. Prepare for visualisation of individual conserved moieties (beta)

tutorial_visualiseConservedMoieties.mlx

```
if ~exist('resultsDir','var')
    driver_initConservedMoietyPaths
end
```

```
if ~recompute %|| isequal(modelName,'iDopaNeuro1')
    load([resultsDir modelName '_arm.mat'])
    return
end
```

1.2.3. Conserved moieties

With the atom mappings we obtained, we can compute the conserved moieties for the iDopaNeuro metabolic network using the atom transition network and the COBRA function `identifyConservedMoieties`.

```
switch modelName
    case 'DAS'
```

```
        load([dataDir filesep 'models' filesep modelName '.mat'])
        load([resultsDir filesep modelName '_dATM.mat'])
    case 'iDopaNeuro1'
        load([resultsDir filesep modelName '.mat'])
        load([resultsDir filesep modelName '_dATM.mat'])

    case
{'centralMetabolism','centralMetabolism_fastCore','centralMetabolism_thermoKe
rnel'}
        load([resultsDir filesep modelName '.mat'])
        load([resultsDir filesep modelName '_dATM.mat'])
    otherwise
        load([dataDir filesep modelName '.mat'])
end
```

```
options.sanityChecks=1;
[arm, moietyFormulae] = identifyConservedMoieties(model, dATM, options);
```

```
save([resultsDir filesep modelName '_arm.mat'],'arm',
'moietyFormulae','options')
```


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REFERENCES

1. Ghaderi, S., Haraldsdóttir, H. S., Ahookhosh, M., Arreckx, S., & Fleming, R. M. T. (2020). Structural conserved moiety splitting of a stoichiometric matrix. Journal of Theoretical Biology, 499, 110276. https://doi.org/10.1016/j.jtbi.2020.110276
2. Rahou, H., Haraldsdóttir, H. S., Martinelli, F., Thiele, I., & Fleming, R. M. T. (2026). Characterisation of conserved and reacting moieties in chemical reaction networks. Journal of Theoretical Biology, 112348. https://doi.org/10.1016/j.jtbi.2025.112348