**NADH demand/ maximization analysis**

This folder contains the core scripts used to quantify and visualize the maximum NADH production (demand) capacity under NSD and HSD conditions using parsimonious flux balance analysis (pFBA). The analyses assess network-wide NADH production and consumption, verify mass balance, and visualize reaction-level contributions to NADH production and consumption.

All analyses were performed in MATLAB, with all figures and summary tables generated for publication and validation purposes.

**Notes**

For access to the full dataset or additional information, please contact: [sunjin\_moon@hms.harvard.edu](mailto:sunjin_moon@hms.harvard.edu)

**Summary of scripts**

1. **script\_01\_NADH\_demand\_pFBA.m**
   1. Purpose:  
      Perform parsimonious FBA (pFBA)–based analysis to estimate the maximum NADH production (demand) capacity under NSD and HSD conditions.
   2. Input:
      1. model\_out\_cbra\_u.mat (NSD and HSD models)
      2. Stoichiometric model structure with metabolite and reaction definitions
   3. Output: 01\_NADH\_demand\_pFBA foder
      1. enhanced\_FBA\_results.mat, comparative\_results.mat, model\_constrained\_out.mat — full pFBA and NADH demand results
      2. NADH\_Summary\_AllModels.xlsx — summarized NADH oxidation capacity, growth rate, and balance check across models
      3. NADH\_analysis\_summary.txt — comparative report of NADH oxidation capacities and pFBA validation summary
2. **script\_02\_NADH\_demand\_pFBA\_vis.m**
   1. Purpose:  
      Visualize NADH maximum (demand) capacity results from pFBA simulations.
   2. Input:
      1. enhanced\_FBA\_results.mat and comparative\_results.mat (from script\_01\_NADH\_demand\_pFBA)
   3. Output:
      1. NADH\_Oxidation\_Capacity\_Bar.pdf/png/svg — bar plots showing maximum NADH demand fluxes
      2. NADH\_Fold\_Changes.pdf/png/svg — fold-change comparison relative to control (if applicable)
      3. NADH\_Analysis\_Summary.csv — summary of NADH oxidation capacity, biomass rate, efficiency, and fold-change
3. **script\_03\_NADH\_demand\_pFBA\_indiv\_vis.m**
   1. Purpose:  
      Perform reaction- and gene-level analysis of NADH-producing and NADH-consuming reactions under NADH demand–maximized pFBA conditions. Quantifies reaction-specific fluxes, verifies NADH mass balance, and visualizes cumulative NADH production and oxidation by gene.
   2. Input:
      1. enhanced\_FBA\_results.mat and model\_constrained\_out.mat (from script\_01\_NADH\_demand\_pFBA)
   3. Output:
      1. NADH\_Prod\_Cons\_byCondition.pdf/png/svg
      2. Cumulative\_NADH\_Production\_Genes.pdf/png/svg/xlsx
      3. Cumulative\_NADH\_Consumption\_Genes.pdf/png/svg/xlsx