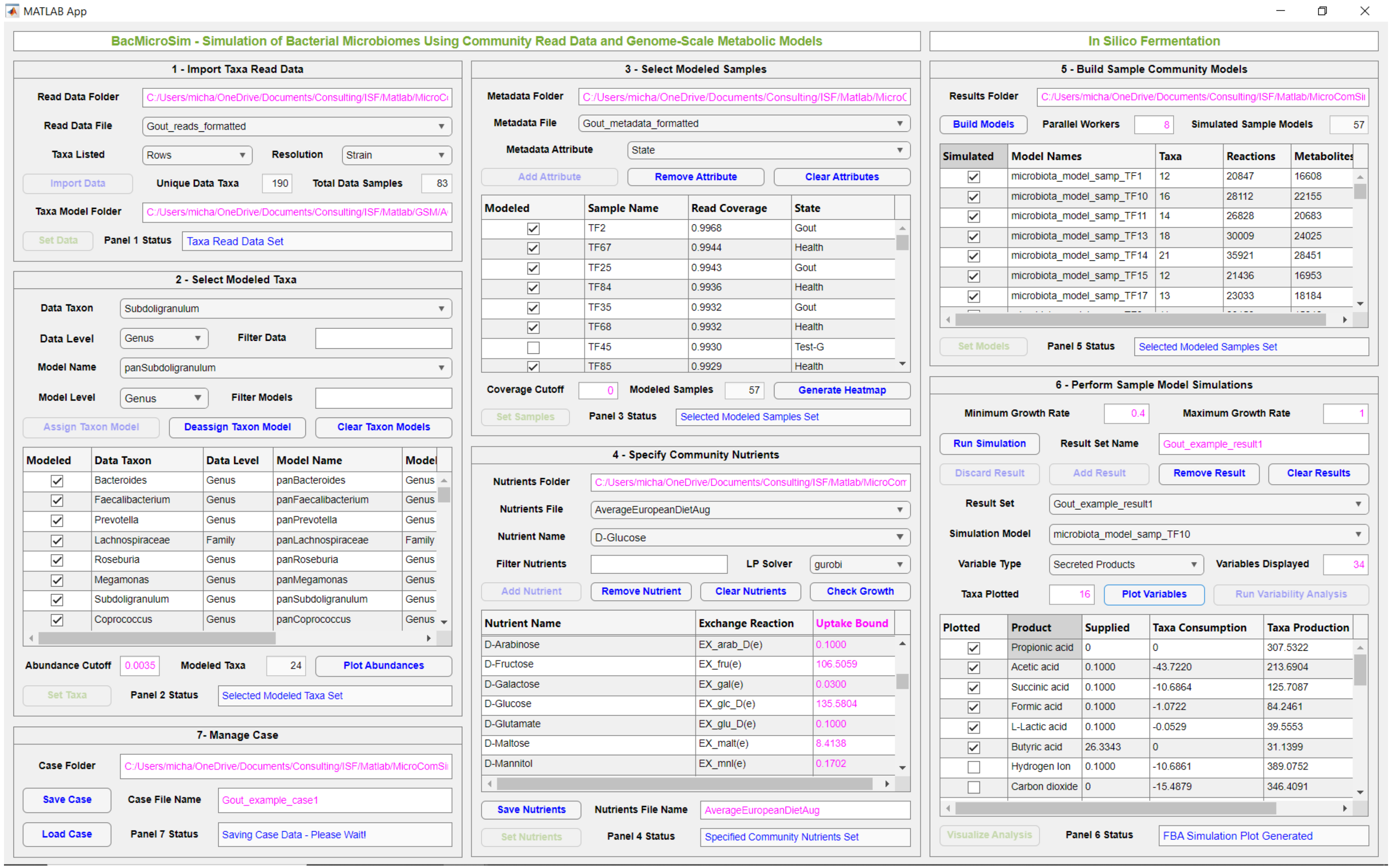
BacMicroSim – A MATLAB Application for Simulation of Bacterial Microbiomes



1 - Import Taxa Read Data

Read Data Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Read Data File: Gout_reads_formatted
Taxa Listed: Rows
Resolution: Strain
Unique Data Taxa: 190
Total Data Samples: 83
Taxa Model Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A
Panel 1 Status: Taxa Read Data Set

2 - Select Modeled Taxa

Data Taxon: Subdoligranulum
Data Level: Genus
Filter Data:
Model Name: panSubdoligranulum
Model Level: Genus
Filter Models:

Modeled	Data Taxon	Data Level	Model Name	Model
☑	Bacteroides	Genus	panBacteroides	Genus
☑	Faecalibacterium	Genus	panFaecalibacterium	Genus
☑	Prevotella	Genus	panPrevotella	Genus
☑	Lachnospiraceae	Family	panLachnospiraceae	Family
☑	Roseburia	Genus	panRoseburia	Genus
☑	Megamonas	Genus	panMegamonas	Genus
☑	Subdoligranulum	Genus	panSubdoligranulum	Genus
☑	Coprococcus	Genus	panCoprococcus	Genus

Abundance Cutoff: 0.0035
Modeled Taxa: 24
Panel 2 Status: Selected Modeled Taxa Set

7- Manage Case

Case Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi
Case File Name: Gout_example_case1
Panel 7 Status: Saving Case Data - Please Wait!

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Metadata File: Gout_metadata_formatted
Metadata Attribute: State

Modeled	Sample Name	Read Coverage	State
☑	TF2	0.9968	Gout
☑	TF67	0.9944	Health
☑	TF25	0.9943	Gout
☑	TF84	0.9936	Health
☑	TF35	0.9932	Gout
☑	TF68	0.9932	Health
☐	TF45	0.9930	Test-G
☑	TF85	0.9929	Health

Coverage Cutoff: 0
Modeled Samples: 57
Panel 3 Status: Selected Modeled Samples Set

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom
Nutrients File: AverageEuropeanDietAug
Nutrient Name: D-Glucose
Filter Nutrients:
LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
D-Arabinose	EX_arab_D(e)	0.1000
D-Fructose	EX_fru(e)	106.5059
D-Galactose	EX_gal(e)	0.0300
D-Glucose	EX_glc_D(e)	135.5804
D-Glutamate	EX_glu_D(e)	0.1000
D-Maltose	EX_malt(e)	8.4138
D-Mannitol	EX_mnl(e)	0.1702

Nutrients File Name: AverageEuropeanDietAug
Panel 4 Status: Specified Community Nutrients Set

5 - Build Sample Community Models

Results Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi
Parallel Workers: 8
Simulated Sample Models: 57

Simulated	Model Names	Taxa	Reactions	Metabolites
☑	microbiota_model_samp_TF1	12	20847	16608
☑	microbiota_model_samp_TF10	16	28112	22155
☑	microbiota_model_samp_TF11	14	26828	20683
☑	microbiota_model_samp_TF13	18	30009	24025
☑	microbiota_model_samp_TF14	21	35921	28451
☑	microbiota_model_samp_TF15	12	21436	16953
☑	microbiota_model_samp_TF17	13	23033	18184

Panel 5 Status: Selected Modeled Samples Set

6 - Perform Sample Model Simulations

Minimum Growth Rate: 0.4
Maximum Growth Rate: 1
Result Set Name: Gout_example_result1
Result Set: Gout_example_result1
Simulation Model: microbiota_model_samp_TF10
Variable Type: Secreted Products
Variables Displayed: 34
Taxa Plotted: 16

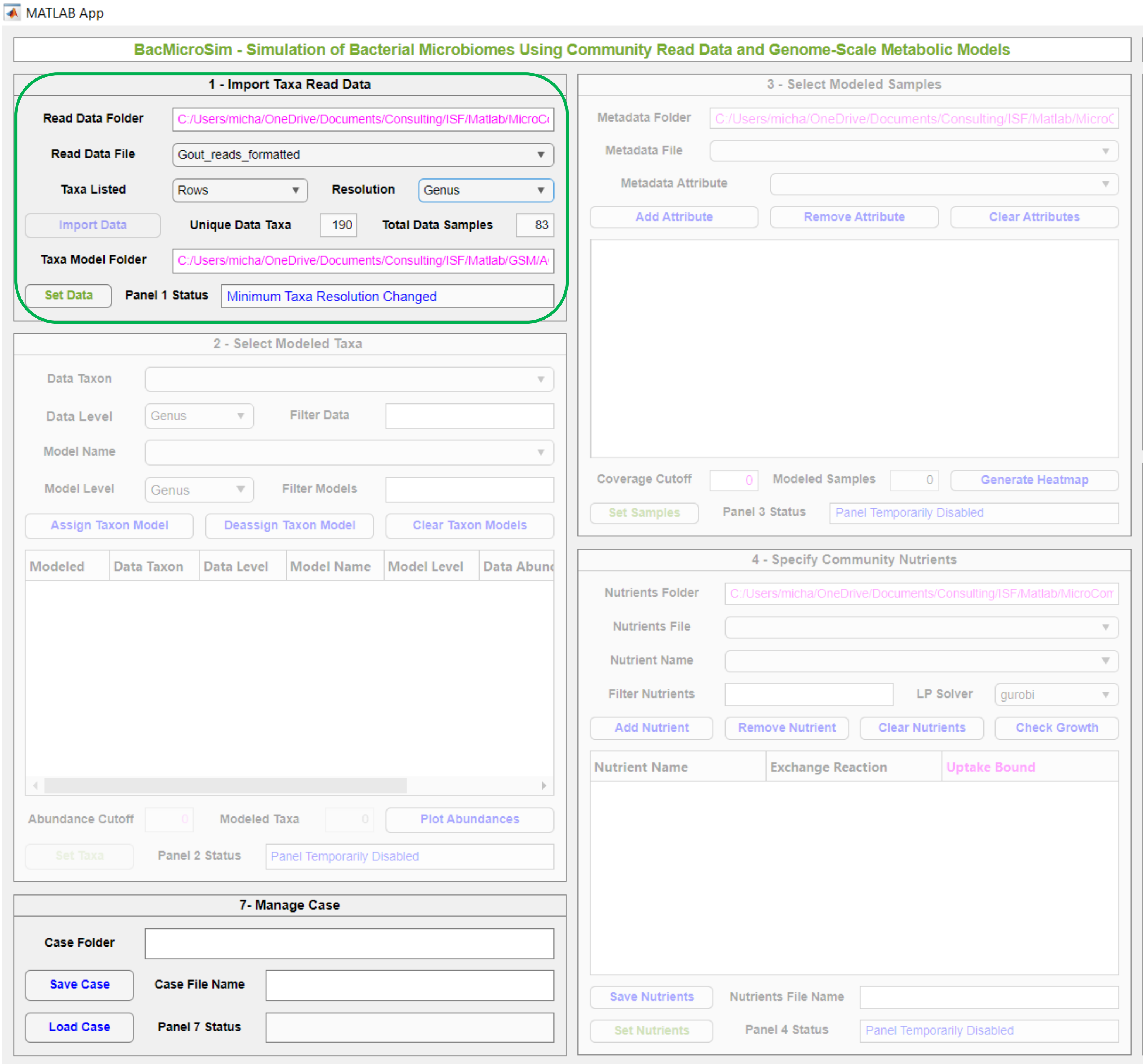
Plotted	Product	Supplied	Taxa Consumption	Taxa Production
☑	Propionic acid	0	0	307.5322
☑	Acetic acid	0.1000	-43.7220	213.6904
☑	Succinic acid	0.1000	-10.6864	125.7087
☑	Formic acid	0.1000	-1.0722	84.2461
☑	L-Lactic acid	0.1000	-0.0529	39.5553
☑	Butyric acid	26.3343	0	31.1399
☐	Hydrogen Ion	0.1000	-10.6861	389.0752
☐	Carbon dioxide	0	-15.4879	346.4091

Panel 6 Status: FBA Simulation Plot Generated

Example – Predict differential production of short chain fatty acids in the gut microbiomes of gouty arthritis and healthy patients

1. Import Taxa Read Data

- Read data is provided as an Excel spreadsheet containing the taxa-read matrix.
- The app will assemble the total reads for each unique taxon in each sample.
- The taxa model folder contains metabolic models covering different taxonomic levels.


MATLAB App

BacMicroSim - Simulation of Bacterial Microbiomes Using Community Read Data and Genome-Scale Metabolic Models

1 - Import Taxa Read Data

Read Data Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Read Data File: Gout_reads_formatted
Taxa Listed: Rows
Resolution: Genus
Unique Data Taxa: 190
Total Data Samples: 83
Taxa Model Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A
Panel 1 Status: Minimum Taxa Resolution Changed

2 - Select Modeled Taxa

Data Level: Genus
Model Level: Genus
Abundance Cutoff: 0
Modeled Taxa: 0
Panel 2 Status: Panel Temporarily Disabled

Modeled	Data Taxon	Data Level	Model Name	Model Level	Data Abund

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Coverage Cutoff: 0
Modeled Samples: 0
Panel 3 Status: Panel Temporarily Disabled

4 - Specify Community Nutrients

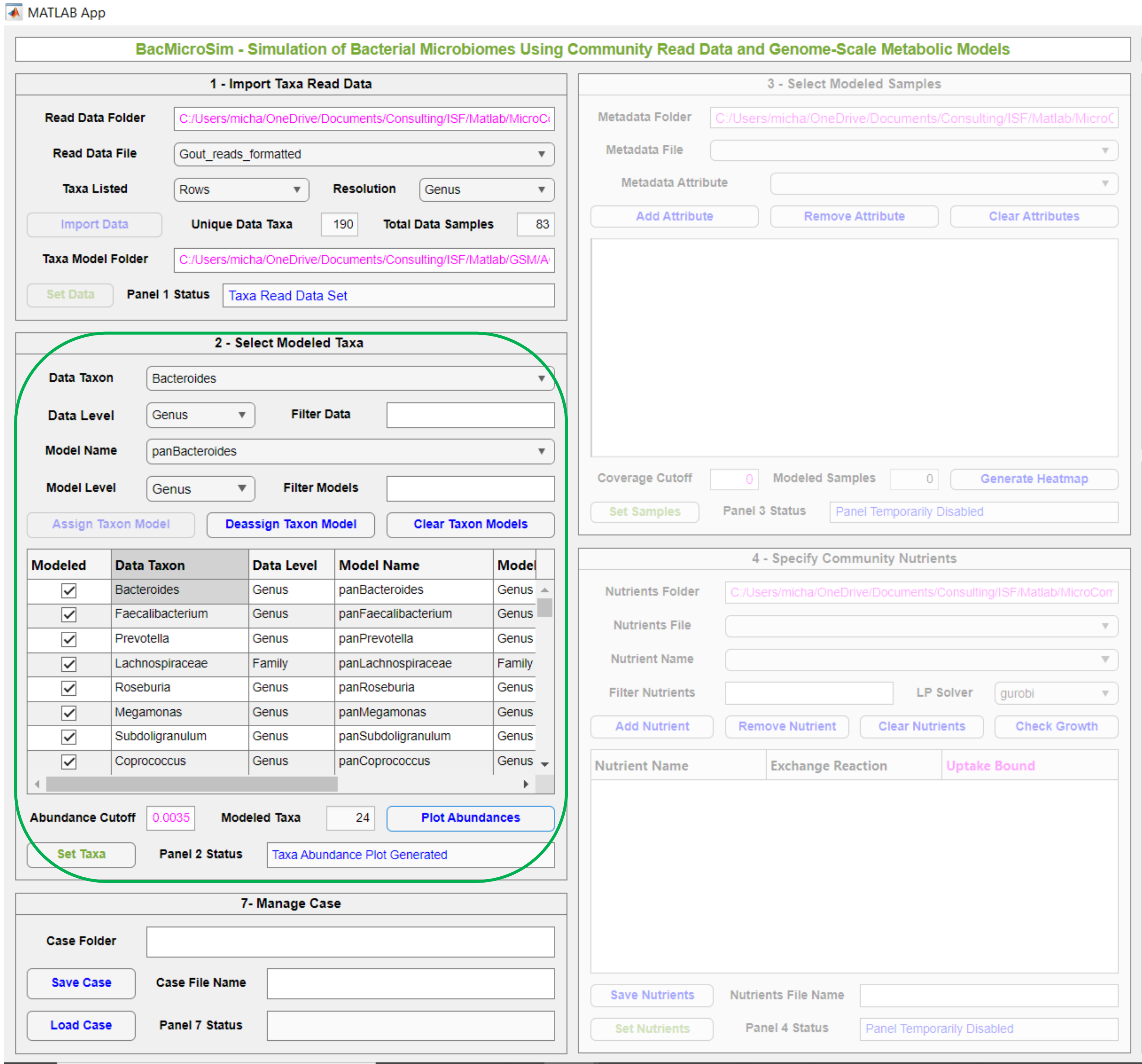
Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom
LP Solver: gurobi
Panel 4 Status: Panel Temporarily Disabled

Nutrient Name	Exchange Reaction	Uptake Bound

7- Manage Case

2. Select Modeled Taxa

- Taxa are ordered by their average abundance across all samples.
- The app will attempt to match each taxon to a corresponding metabolic model at the same taxonomic level.
- Unmatched taxa can be manually assigned models.
- The cutoff value allows selection of only taxa with an average abundance above the cutoff.
- Only the selected taxa can be included in sample community models.



MATLAB App

BacMicroSim - Simulation of Bacterial Microbiomes Using Community Read Data and Genome-Scale Metabolic Models

1 - Import Taxa Read Data

Read Data Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Read Data File: Gout_reads_formatted

Taxa Listed: Rows

Resolution: Genus

Unique Data Taxa: 190

Total Data Samples: 83

Taxa Model Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A

Panel 1 Status: Taxa Read Data Set

2 - Select Modeled Taxa

Data Taxon: Bacteroides

Data Level: Genus

Filter Data:

Model Name: panBacteroides

Model Level: Genus

Filter Models:

Modeled	Data Taxon	Data Level	Model Name	Model
☑	Bacteroides	Genus	panBacteroides	Genus
☑	Faecalibacterium	Genus	panFaecalibacterium	Genus
☑	Prevotella	Genus	panPrevotella	Genus
☑	Lachnospiraceae	Family	panLachnospiraceae	Family
☑	Roseburia	Genus	panRoseburia	Genus
☑	Megamonas	Genus	panMegamonas	Genus
☑	Subdoligranulum	Genus	panSubdoligranulum	Genus
☑	Coprococcus	Genus	panCoprococcus	Genus

Abundance Cutoff: 0.0035

Modeled Taxa: 24

Panel 2 Status: Taxa Abundance Plot Generated

7- Manage Case

Case Folder:

Case File Name:

Panel 7 Status:

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Metadata File:

Metadata Attribute:

Coverage Cutoff: 0

Modeled Samples: 0

Panel 3 Status: Panel Temporarily Disabled

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom

Nutrients File:

Nutrient Name:

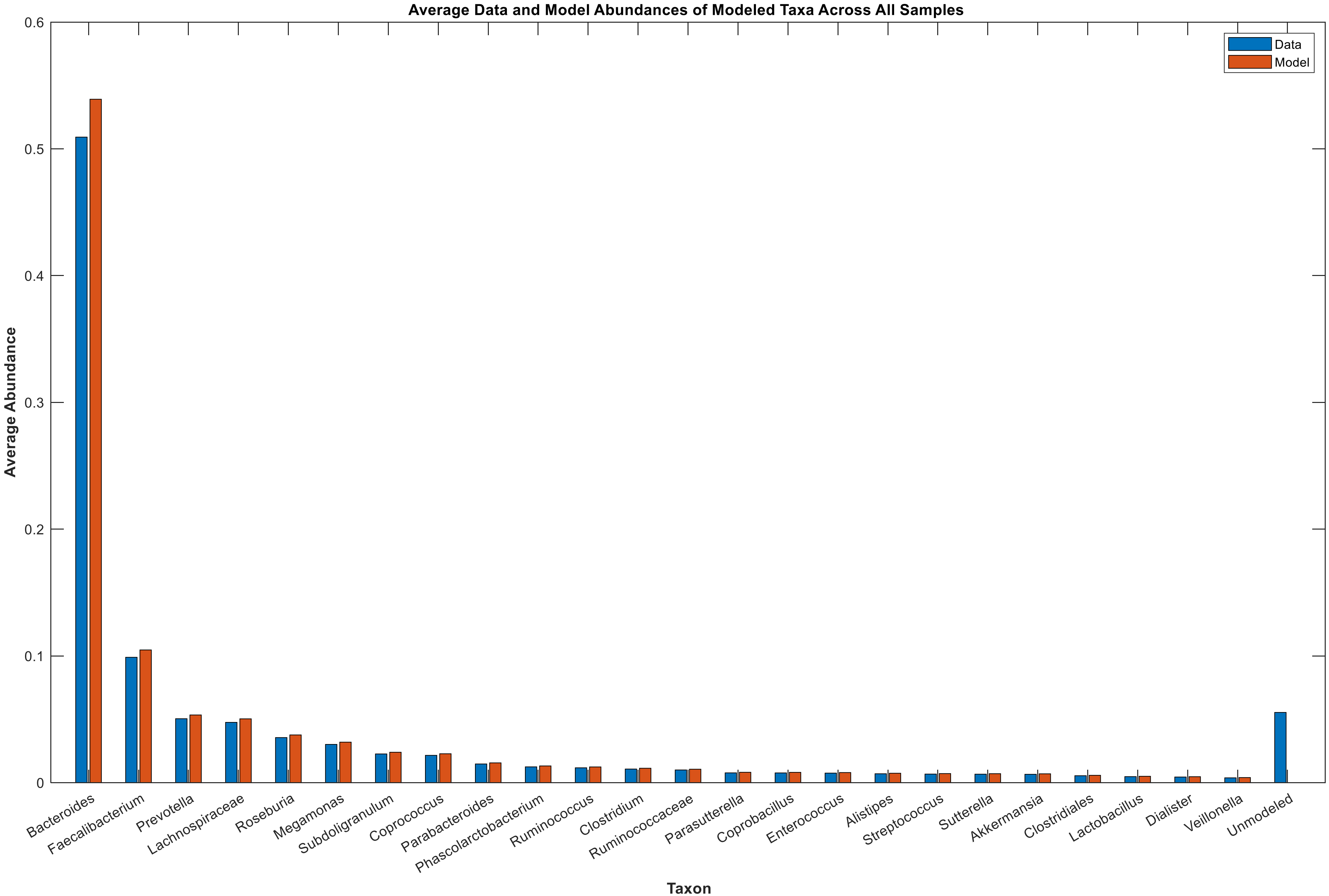
Filter Nutrients:

LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound

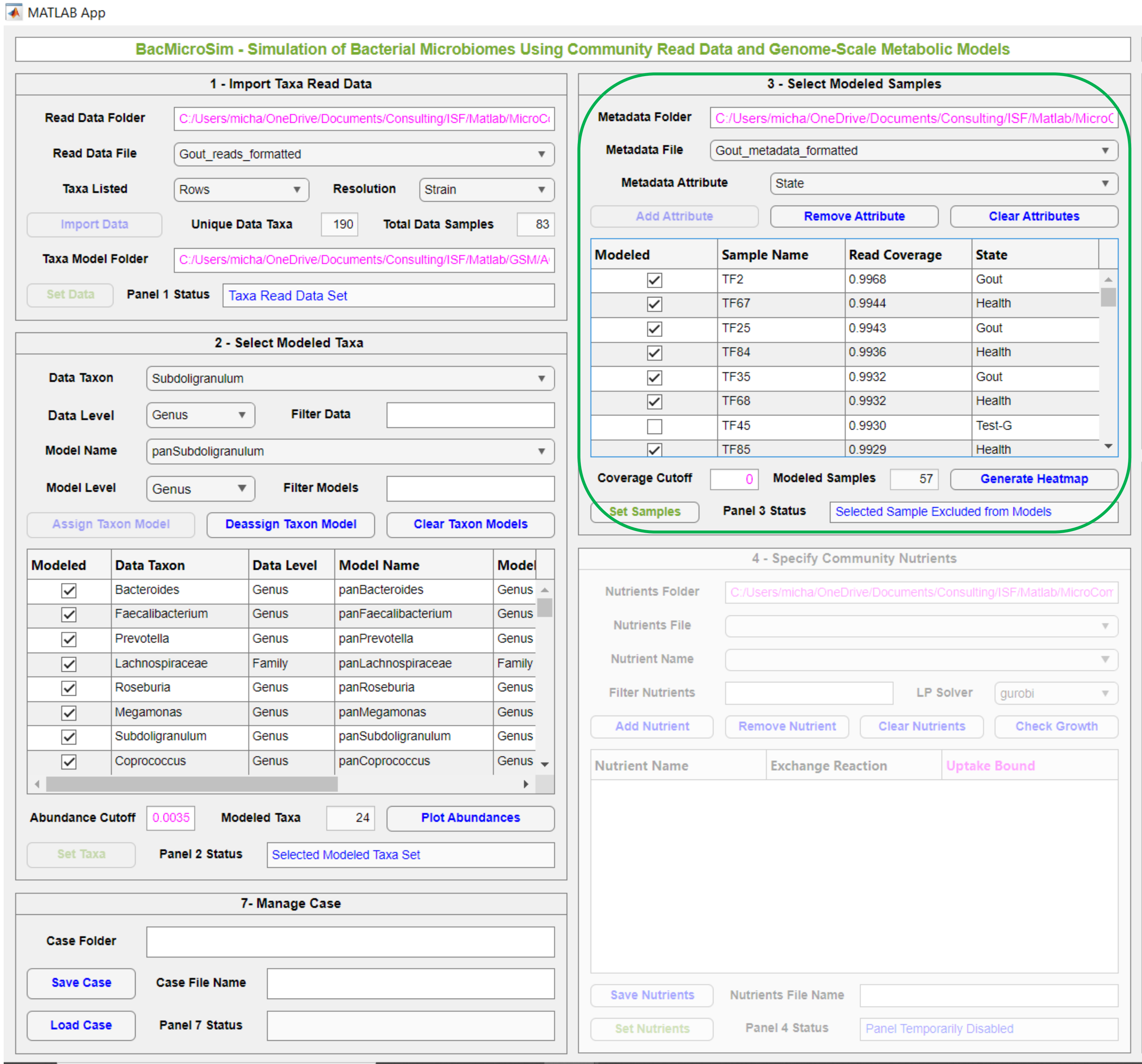
Nutrients File Name:

Panel 4 Status: Panel Temporarily Disabled


Average Data and Model Abundances of Modeled Taxa Across All Samples
Data
Model
Average Abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
Bacteroides
Faecalibacterium
Prevotella
Lachnospiraceae
Roseburia
Megamonas
Subdoligranulum
Coprococcus
Parabacteroides
Phascolarctobacterium
Ruminococcus
Clostridium
Ruminococcaceae
Parasutterella
Coprobacillus
Enterococcus
Alistipes
Streptococcus
Sutterella
Akkermansia
Clostridiales
Lactobacillus
Dialister
Veillonella
Unmodeled
Taxon

3. Select Modeled Samples

- Samples are ordered according to their read coverage by the modeled taxa.
- Sample metadata are uploaded as an Excel spreadsheet.
- The cutoff value allows selection of only samples with a modeled read coverage above the cutoff.
- Only the selected sample can have community models built.



MATLAB App

BacMicroSim - Simulation of Bacterial Microbiomes Using Community Read Data and Genome-Scale Metabolic Models

1 - Import Taxa Read Data

Read Data Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Read Data File: Gout_reads_formatted

Taxa Listed: Rows   Resolution: Strain

Unique Data Taxa: 190   Total Data Samples: 83

Taxa Model Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A

Panel 1 Status: Taxa Read Data Set

2 - Select Modeled Taxa

Data Taxon: Subdoligranulum

Data Level: Genus   Filter Data:

Model Name: panSubdoligranulum

Model Level: Genus   Filter Models:

Modeled	Data Taxon	Data Level	Model Name	Model
☑	Bacteroides	Genus	panBacteroides	Genus
☑	Faecalibacterium	Genus	panFaecalibacterium	Genus
☑	Prevotella	Genus	panPrevotella	Genus
☑	Lachnospiraceae	Family	panLachnospiraceae	Family
☑	Roseburia	Genus	panRoseburia	Genus
☑	Megamonas	Genus	panMegamonas	Genus
☑	Subdoligranulum	Genus	panSubdoligranulum	Genus
☑	Coprococcus	Genus	panCoprococcus	Genus

Abundance Cutoff: 0.0035   Modeled Taxa: 24

Panel 2 Status: Selected Modeled Taxa Set

7- Manage Case

Case Folder:

Case File Name:

Panel 7 Status:

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Metadata File: Gout_metadata_formatted

Metadata Attribute: State

Modeled	Sample Name	Read Coverage	State
☑	TF2	0.9968	Gout
☑	TF67	0.9944	Health
☑	TF25	0.9943	Gout
☑	TF84	0.9936	Health
☑	TF35	0.9932	Gout
☑	TF68	0.9932	Health
☐	TF45	0.9930	Test-G
☑	TF85	0.9929	Health

Coverage Cutoff: 0   Modeled Samples: 57

Panel 3 Status: Selected Sample Excluded from Models

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom

Nutrients File:

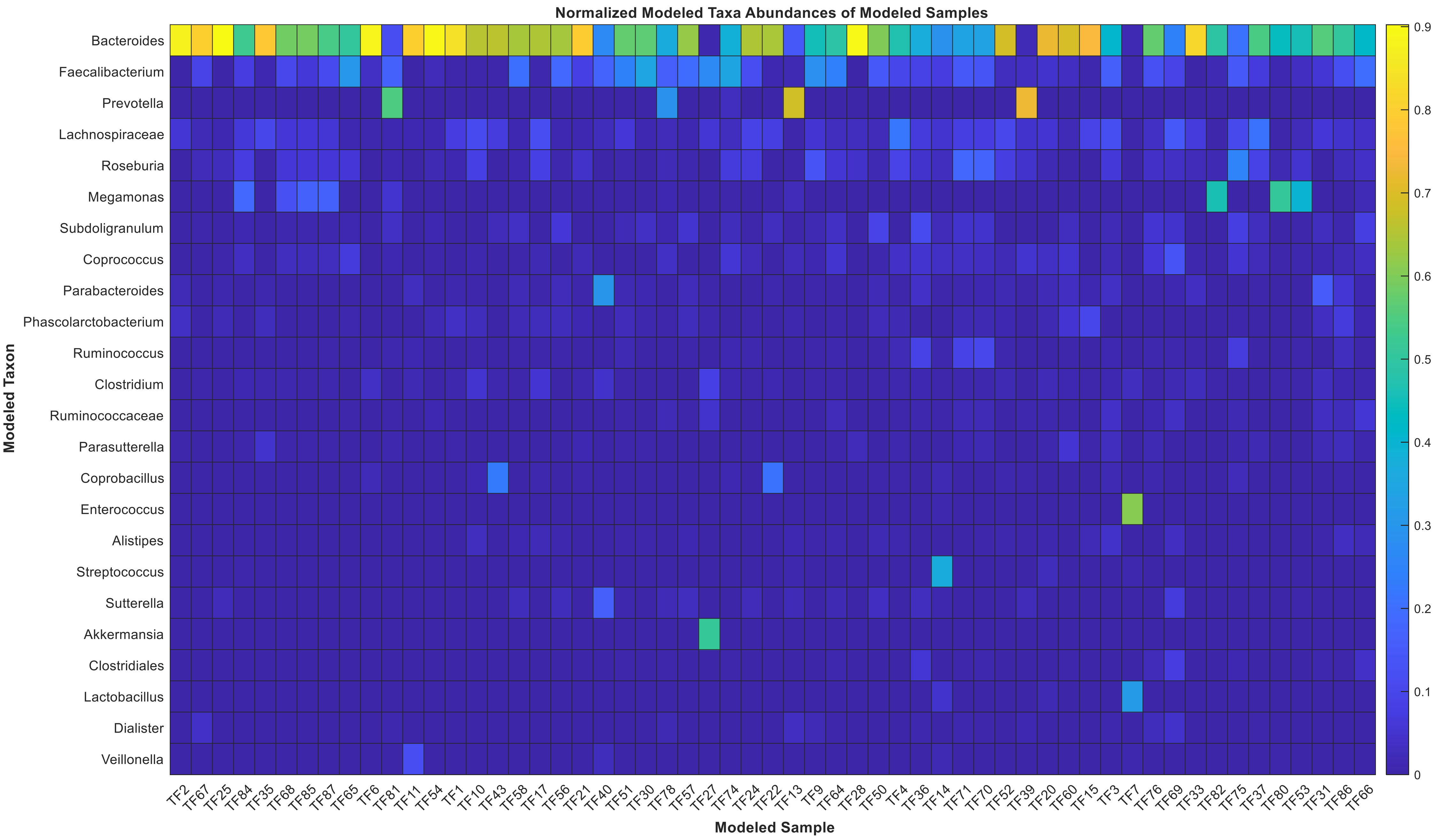
Nutrient Name:

Filter Nutrients: LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound

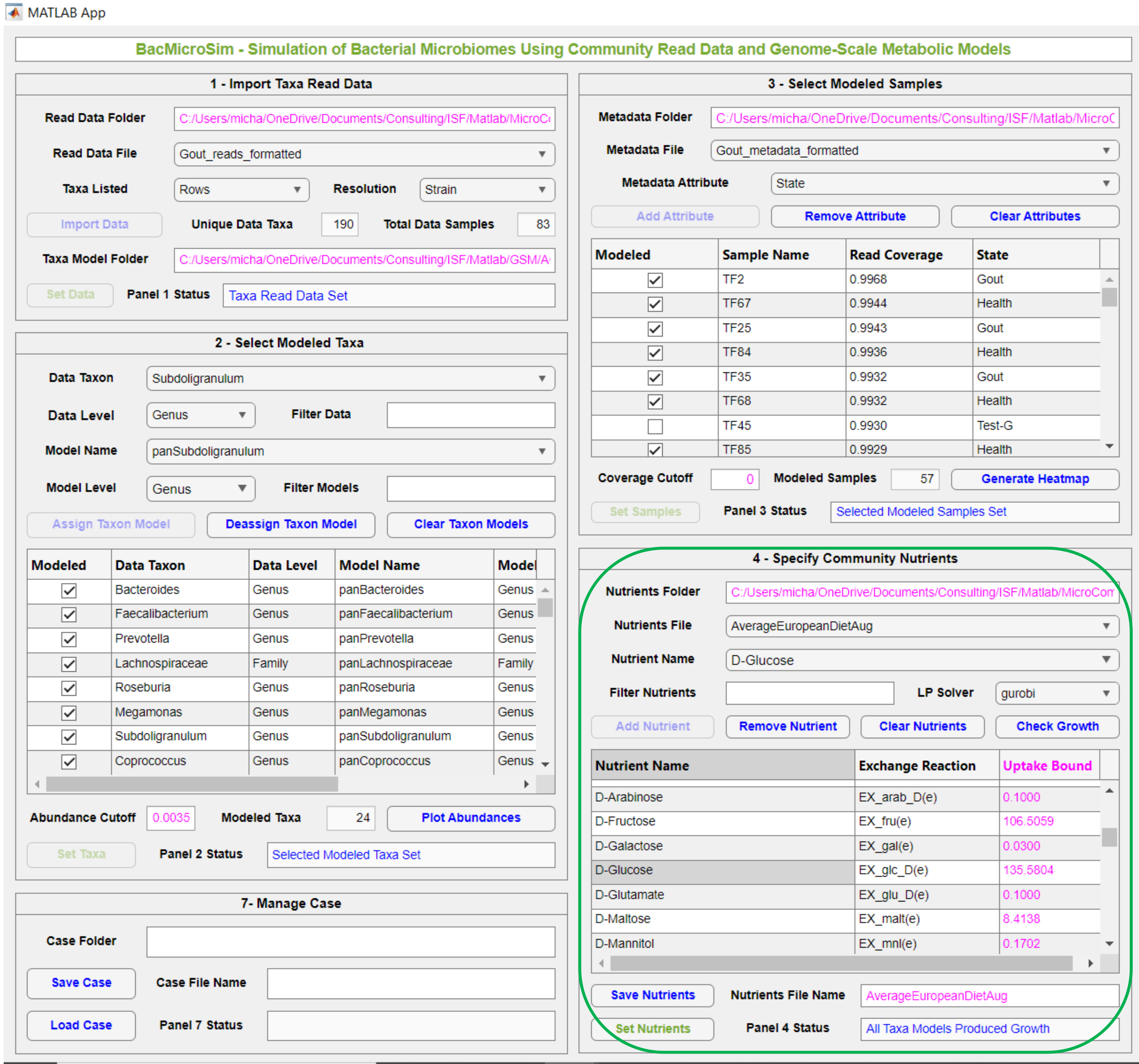
Nutrients File Name:

Panel 4 Status: Panel Temporarily Disabled


Normalized Modeled Taxa Abundances of Modeled Samples
Modeled Taxon
Bacteroides
Faecalibacterium
Prevotella
Lachnospiraceae
Roseburia
Megamonas
Subdoligranulum
Coprococcus
Parabacteroides
Phascolarctobacterium
Ruminococcus
Clostridium
Ruminococcaceae
Parasutterella
Coprobacillus
Enterococcus
Alistipes
Streptococcus
Sutterella
Akkermansia
Clostridiales
Lactobacillus
Dialister
Veillonella
TF2
TF67
TF25
TF84
TF35
TF68
TF85
TF87
TF65
TF6
TF81
TF11
TF54
TF1
TF10
TF43
TF58
TF17
TF56
TF21
TF40
TF51
TF30
TF78
TF57
TF27
TF74
TF24
TF22
TF13
TF9
TF64
TF28
TF50
TF4
TF36
TF14
TF71
TF70
TF52
TF39
TF20
TF60
TF15
TF3
TF7
TF76
TF69
TF33
TF82
TF75
TF37
TF80
TF53
TF31
TF86
TF66
Modeled Sample
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

4. Specify Supplied Nutrients

- Nutrients can be specified by loading a saved text file and/or by defining nutrients manually.
- Individual nutrient uptake bounds can be altered.
- Monoculture growth of each modeled taxon can be ensured by augmenting the current nutrients with any missing essential nutrients.
- Only the specified nutrients and other crossfed metabolites are available to support community growth.



BacMicroSim - Simulation of Bacterial Microbiomes Using Community Read Data and Genome-Scale Metabolic Models

1 - Import Taxa Read Data

Read Data Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Read Data File Gout_reads_formatted

Taxa Listed Rows **Resolution** Strain

Unique Data Taxa 190 **Total Data Samples** 83

Taxa Model Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A

Panel 1 Status Taxa Read Data Set

2 - Select Modeled Taxa

Data Taxon Subdoligranulum

Data Level Genus **Filter Data**

Model Name panSubdoligranulum

Model Level Genus **Filter Models**

Modeled	Data Taxon	Data Level	Model Name	Model
☑	Bacteroides	Genus	panBacteroides	Genus
☑	Faecalibacterium	Genus	panFaecalibacterium	Genus
☑	Prevotella	Genus	panPrevotella	Genus
☑	Lachnospiraceae	Family	panLachnospiraceae	Family
☑	Roseburia	Genus	panRoseburia	Genus
☑	Megamonas	Genus	panMegamonas	Genus
☑	Subdoligranulum	Genus	panSubdoligranulum	Genus
☑	Coprococcus	Genus	panCoprococcus	Genus

Abundance Cutoff 0.0035 **Modeled Taxa** 24

Panel 2 Status Selected Modeled Taxa Set

7- Manage Case

Case Folder

Case File Name

Panel 7 Status

3 - Select Modeled Samples

Metadata Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Metadata File Gout_metadata_formatted

Metadata Attribute State

Modeled	Sample Name	Read Coverage	State
☑	TF2	0.9968	Gout
☑	TF67	0.9944	Health
☑	TF25	0.9943	Gout
☑	TF84	0.9936	Health
☑	TF35	0.9932	Gout
☑	TF68	0.9932	Health
☐	TF45	0.9930	Test-G
☑	TF85	0.9929	Health

Coverage Cutoff 0 **Modeled Samples** 57

Panel 3 Status Selected Modeled Samples Set

4 - Specify Community Nutrients

Nutrients Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom

Nutrients File AverageEuropeanDietAug

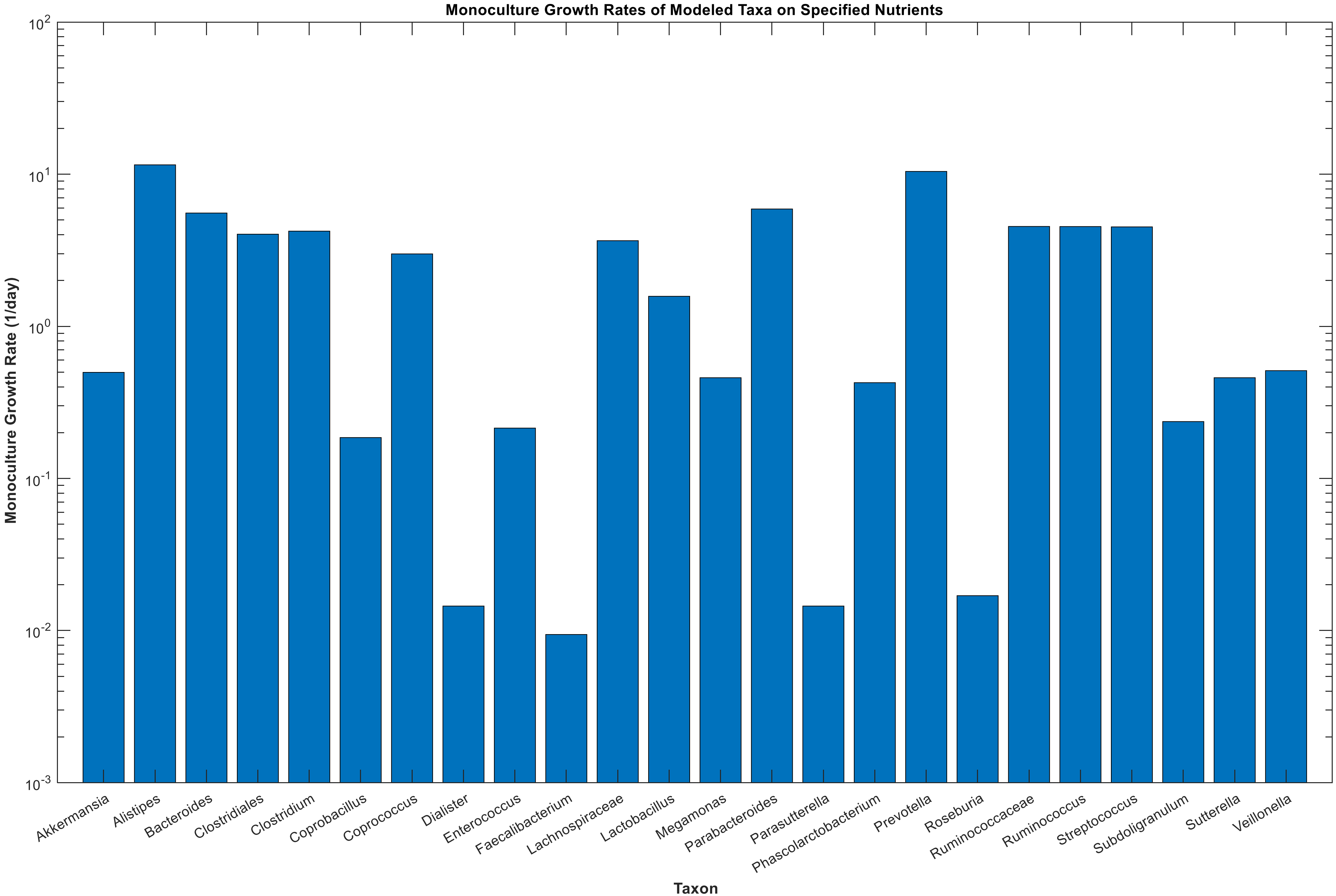
Nutrient Name D-Glucose

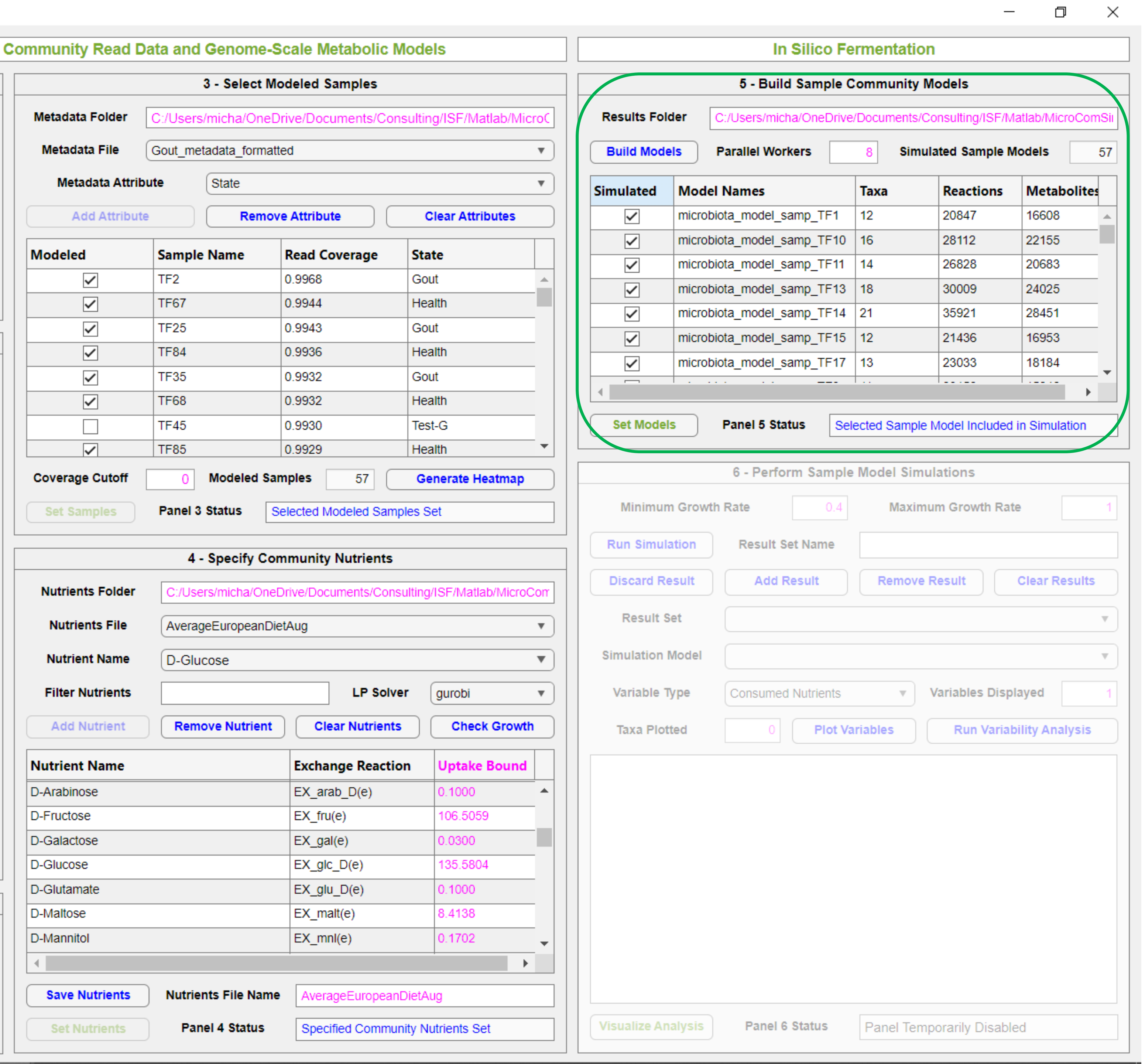
Filter Nutrients **LP Solver** gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
D-Arabinose	EX_arab_D(e)	0.1000
D-Fructose	EX_fru(e)	106.5059
D-Galactose	EX_gal(e)	0.0300
D-Glucose	EX_glc_D(e)	135.5804
D-Glutamate	EX_glu_D(e)	0.1000
D-Maltose	EX_malt(e)	8.4138
D-Mannitol	EX_mnl(e)	0.1702

Nutrients File Name AverageEuropeanDietAug

Panel 4 Status All Taxa Models Produced Growth


Monoculture Growth Rates of Modeled Taxa on Specified Nutrients
Monoculture Growth Rate (1/day)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
Akkermansia
Alistipes
Bacteroides
Clostridiales
Clostridium
Coprobacillus
Coprococcus
Dialister
Enterococcus
Faecalibacterium
Lachnospiraceae
Lactobacillus
Megamonas
Parabacteroides
Parasutterella
Phascolarctobacterium
Prevotella
Roseburia
Ruminococcaceae
Ruminococcus
Streptococcus
Subdoligranulum
Sutterella
Veillonella
Taxon



Community Read Data and Genome-Scale Metabolic Models

3 - Select Modeled Samples

Metadata Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Metadata File Gout_metadata_formatted

Metadata Attribute State

Modeled	Sample Name	Read Coverage	State
☑	TF2	0.9968	Gout
☑	TF67	0.9944	Health
☑	TF25	0.9943	Gout
☑	TF84	0.9936	Health
☑	TF35	0.9932	Gout
☑	TF68	0.9932	Health
☐	TF45	0.9930	Test-G
☑	TF85	0.9929	Health

Coverage Cutoff 0 **Modeled Samples** 57

Panel 3 Status Selected Modeled Samples Set

4 - Specify Community Nutrients

Nutrients Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom

Nutrients File AverageEuropeanDietAug

Nutrient Name D-Glucose

Filter Nutrients

LP Solver gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
D-Arabinose	EX_arab_D(e)	0.1000
D-Fructose	EX_fru(e)	106.5059
D-Galactose	EX_gal(e)	0.0300
D-Glucose	EX_glc_D(e)	135.5804
D-Glutamate	EX_glu_D(e)	0.1000
D-Maltose	EX_malt(e)	8.4138
D-Mannitol	EX_mnl(e)	0.1702

Nutrients File Name AverageEuropeanDietAug

Panel 4 Status Specified Community Nutrients Set

In Silico Fermentation

5 - Build Sample Community Models

Results Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi

Parallel Workers 8 **Simulated Sample Models** 57

Simulated	Model Names	Taxa	Reactions	Metabolites
☑	microbiota_model_samp_TF1	12	20847	16608
☑	microbiota_model_samp_TF10	16	28112	22155
☑	microbiota_model_samp_TF11	14	26828	20683
☑	microbiota_model_samp_TF13	18	30009	24025
☑	microbiota_model_samp_TF14	21	35921	28451
☑	microbiota_model_samp_TF15	12	21436	16953
☑	microbiota_model_samp_TF17	13	23033	18184

Panel 5 Status Selected Sample Model Included in Simulation

6 - Perform Sample Model Simulations

Minimum Growth Rate 0.4 **Maximum Growth Rate** 1

Result Set Name

Result Set

Simulation Model

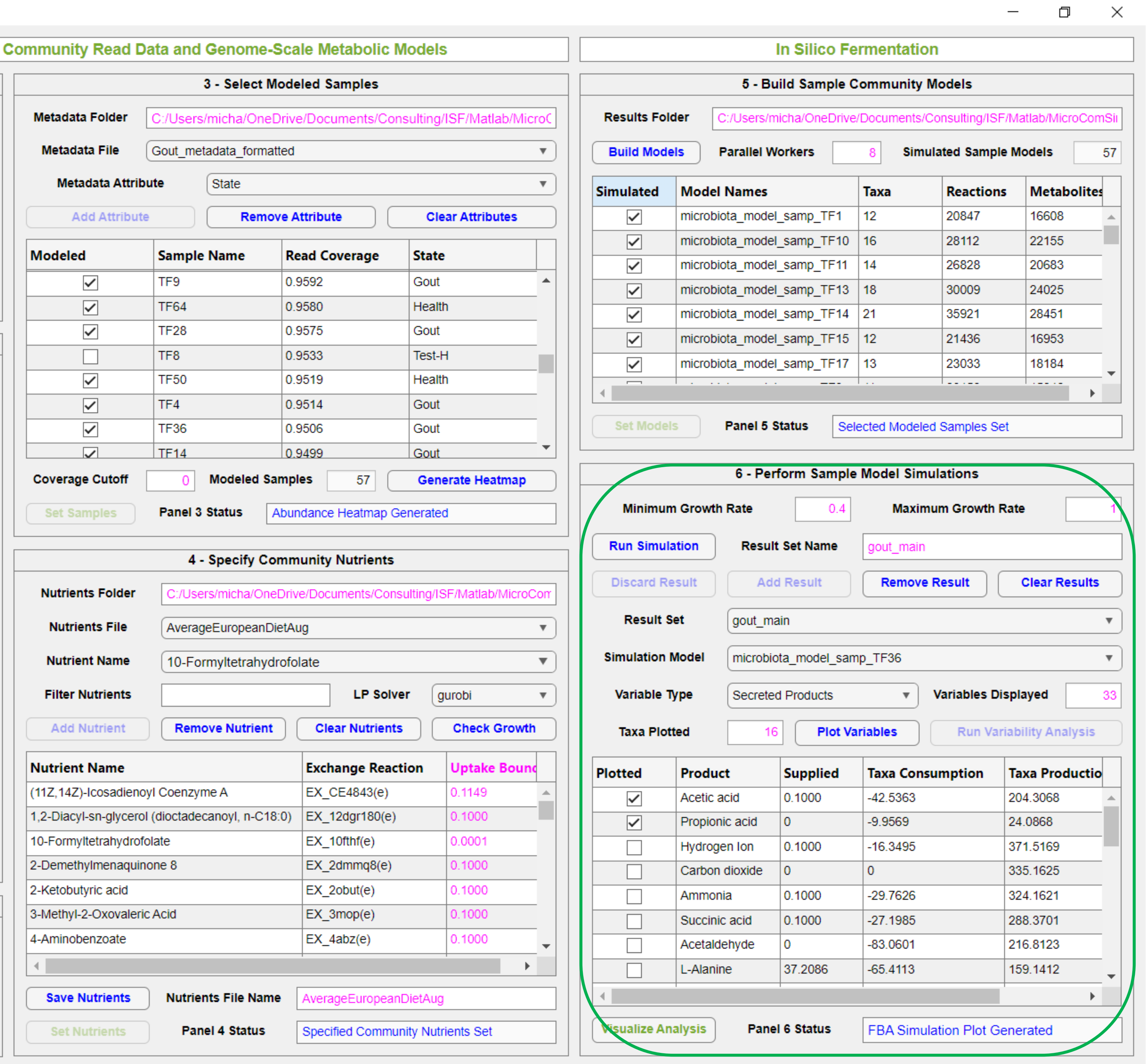
Variable Type Consumed Nutrients **Variables Displayed** 1

Taxa Plotted 0

Panel 6 Status Panel Temporarily Disabled

5. Build Sample Models

- Sample community models are built from normalized taxa abundances and nutrient uptake rate bounds.
- Only non-existing models are built for the selected samples.
- Any subset of the available models can be selected for simulation.



Community Read Data and Genome-Scale Metabolic Models

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Metadata File: Gout_metadata_formatted
Metadata Attribute: State

Modeled	Sample Name	Read Coverage	State
☑	TF9	0.9592	Gout
☑	TF64	0.9580	Health
☑	TF28	0.9575	Gout
☐	TF8	0.9533	Test-H
☑	TF50	0.9519	Health
☑	TF4	0.9514	Gout
☑	TF36	0.9506	Gout
☑	TF14	0.9499	Gout

Coverage Cutoff: 0
Modeled Samples: 57
Panel 3 Status: Abundance Heatmap Generated

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom
Nutrients File: AverageEuropeanDietAug
Nutrient Name: 10-Formyltetrahydrofolate
Filter Nutrients:
LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
(11Z,14Z)-Icosadienoyl Coenzyme A	EX_CE4843(e)	0.1149
1,2-Diacyl-sn-glycerol (dioctadecanoyl, n-C18:0)	EX_12dgr180(e)	0.1000
10-Formyltetrahydrofolate	EX_10fthf(e)	0.0001
2-Demethylmenaquinone 8	EX_2dmmq8(e)	0.1000
2-Ketobutyric acid	EX_2obut(e)	0.1000
3-Methyl-2-Oxovaleric Acid	EX_3mop(e)	0.1000
4-Aminobenzoate	EX_4abz(e)	0.1000

Nutrients File Name: AverageEuropeanDietAug
Panel 4 Status: Specified Community Nutrients Set

In Silico Fermentation

5 - Build Sample Community Models

Results Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi
Parallel Workers: 8
Simulated Sample Models: 57

Simulated	Model Names	Taxa	Reactions	Metabolites
☑	microbiota_model_samp_TF1	12	20847	16608
☑	microbiota_model_samp_TF10	16	28112	22155
☑	microbiota_model_samp_TF11	14	26828	20683
☑	microbiota_model_samp_TF13	18	30009	24025
☑	microbiota_model_samp_TF14	21	35921	28451
☑	microbiota_model_samp_TF15	12	21436	16953
☑	microbiota_model_samp_TF17	13	23033	18184

Panel 5 Status: Selected Modeled Samples Set

6 - Perform Sample Model Simulations

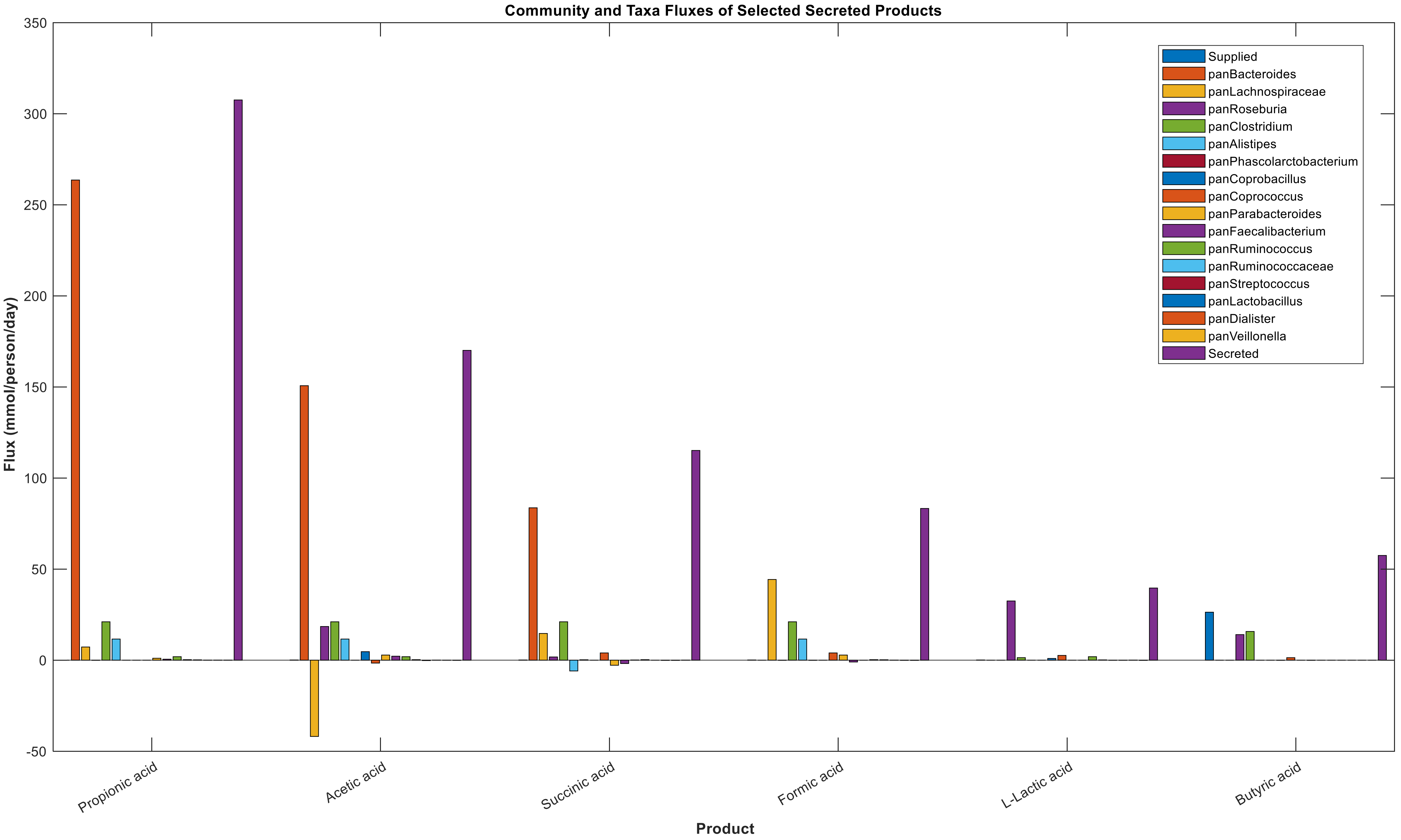
Minimum Growth Rate: 0.4
Maximum Growth Rate: 1
Result Set Name: gout_main
Result Set: gout_main
Simulation Model: microbiota_model_samp_TF36
Variable Type: Secreted Products
Variables Displayed: 33
Taxa Plotted: 16

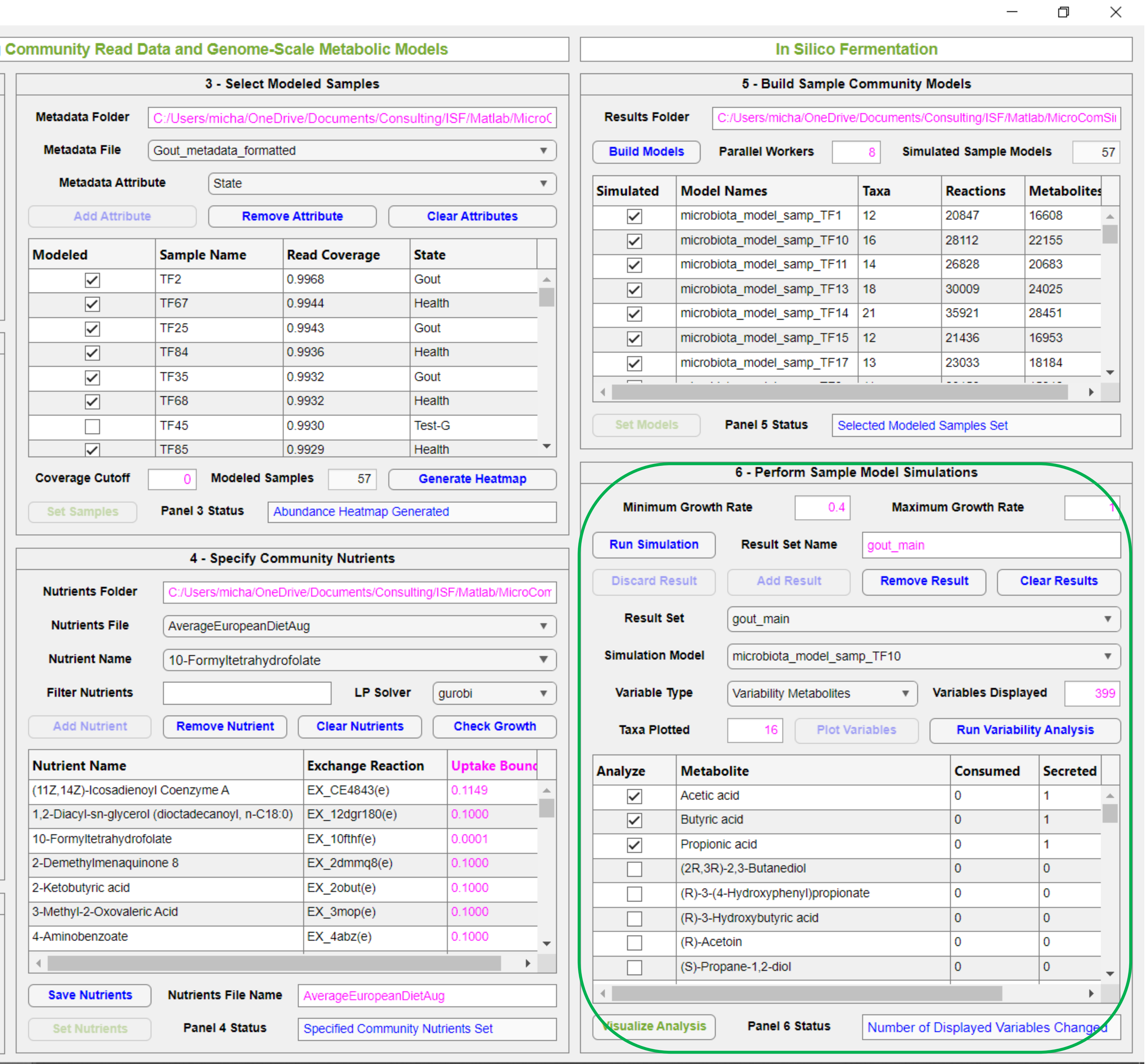
Plotted	Product	Supplied	Taxa Consumption	Taxa Productio
☑	Acetic acid	0.1000	-42.5363	204.3068
☑	Propionic acid	0	-9.9569	24.0868
☐	Hydrogen Ion	0.1000	-16.3495	371.5169
☐	Carbon dioxide	0	0	335.1625
☐	Ammonia	0.1000	-29.7626	324.1621
☐	Succinic acid	0.1000	-27.1985	288.3701
☐	Acetaldehyde	0	-83.0601	216.8123
☐	L-Alanine	37.2086	-65.4113	159.1412

Panel 6 Status: FBA Simulation Plot Generated

5a. Perform FBA Simulations

- Flux balance (FBA) simulations are performed for all selected models.
- Lower and upper bounds can be imposed on the community growth rate.
- Consumed nutrient, secreted product and crossfed metabolite fluxes can be viewed for each model.
- Result sets for different nutrients bounds and/or models can be stored and reloaded.


Community and Taxa Fluxes of Selected Secreted Products
Flux (mmol/person/day)
350
300
250
200
150
100
50
0
-50
Product
Propionic acid
Acetic acid
Succinic acid
Formic acid
L-Lactic acid
Butyric acid
Supplied
panBacteroides
panLachnospiraceae
panRoseburia
panClostridium
panAlistipes
panPhascolarctobacterium
panCoprobacillus
panCoprococcus
panParabacteroides
panFaecalibacterium
panRuminococcus
panRuminococcaceae
panStreptococcus
panLactobacillus
panDialister
panVeillonella
Secreted



3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Metadata File: Gout_metadata_formatted

Metadata Attribute: State

Modeled	Sample Name	Read Coverage	State
☑	TF2	0.9968	Gout
☑	TF67	0.9944	Health
☑	TF25	0.9943	Gout
☑	TF84	0.9936	Health
☑	TF35	0.9932	Gout
☑	TF68	0.9932	Health
☐	TF45	0.9930	Test-G
☑	TF85	0.9929	Health

Coverage Cutoff: 0

Modeled Samples: 57

Panel 3 Status: Abundance Heatmap Generated

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom

Nutrients File: AverageEuropeanDietAug

Nutrient Name: 10-Formyltetrahydrofolate

Filter Nutrients:

LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
(11Z,14Z)-Icosadienoyl Coenzyme A	EX_CE4843(e)	0.1149
1,2-Diacyl-sn-glycerol (dioctadecanoyl, n-C18:0)	EX_12dgr180(e)	0.1000
10-Formyltetrahydrofolate	EX_10fthf(e)	0.0001
2-Demethylmenaquinone 8	EX_2dmmq8(e)	0.1000
2-Ketobutyric acid	EX_2obut(e)	0.1000
3-Methyl-2-Oxovaleric Acid	EX_3mop(e)	0.1000
4-Aminobenzoate	EX_4abz(e)	0.1000

Nutrients File Name: AverageEuropeanDietAug

Panel 4 Status: Specified Community Nutrients Set

5 - Build Sample Community Models

Results Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi

Parallel Workers: 8

Simulated Sample Models: 57

Simulated	Model Names	Taxa	Reactions	Metabolites
☑	microbiota_model_samp_TF1	12	20847	16608
☑	microbiota_model_samp_TF10	16	28112	22155
☑	microbiota_model_samp_TF11	14	26828	20683
☑	microbiota_model_samp_TF13	18	30009	24025
☑	microbiota_model_samp_TF14	21	35921	28451
☑	microbiota_model_samp_TF15	12	21436	16953
☑	microbiota_model_samp_TF17	13	23033	18184

Panel 5 Status: Selected Modeled Samples Set

6 - Perform Sample Model Simulations

Minimum Growth Rate: 0.4

Maximum Growth Rate: 1

Result Set Name: gout_main

Result Set: gout_main

Simulation Model: microbiota_model_samp_TF10

Variable Type: Variability Metabolites

Variables Displayed: 399

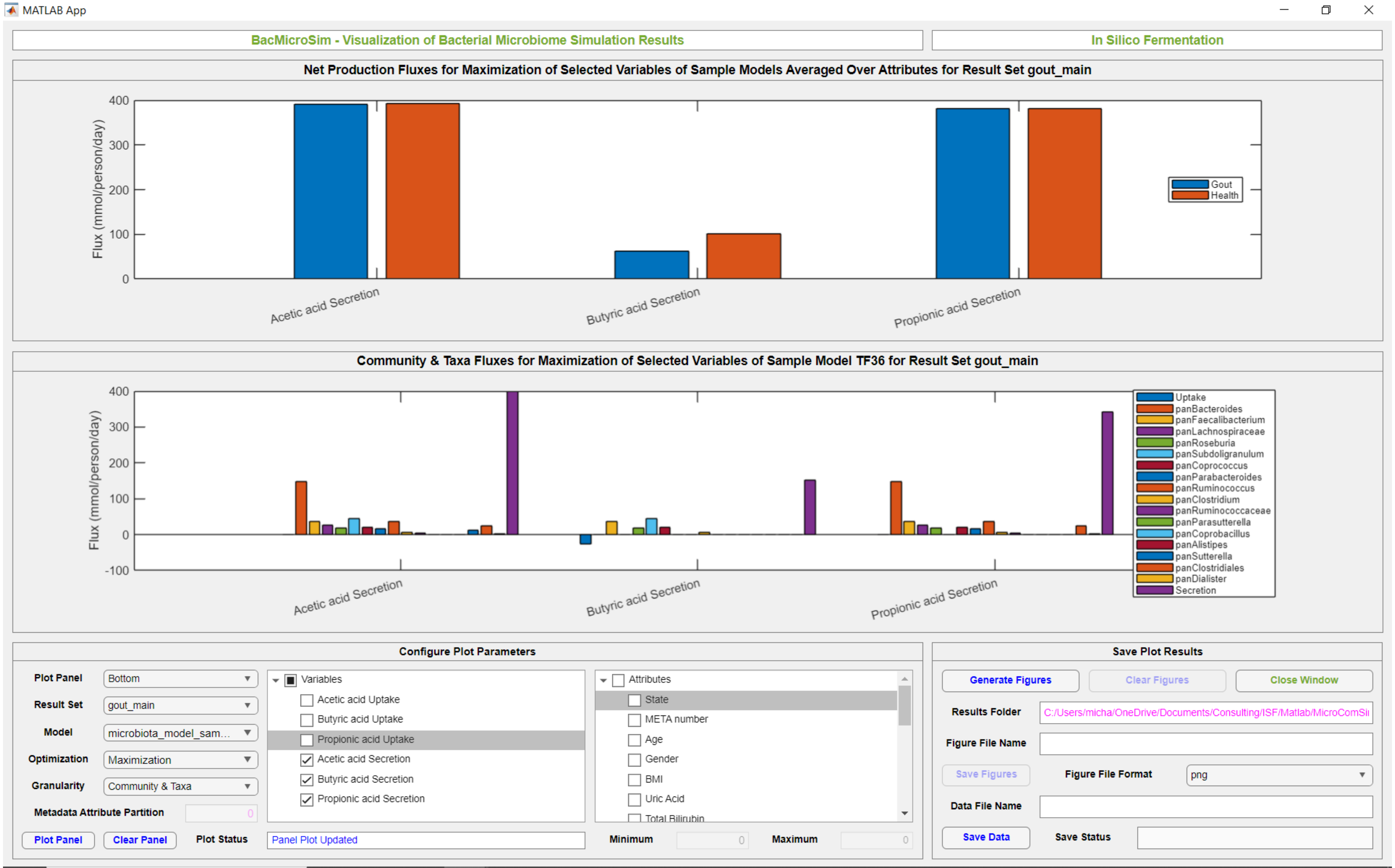
Taxa Plotted: 16

Analyze	Metabolite	Consumed	Secreted
☑	Acetic acid	0	1
☑	Butyric acid	0	1
☑	Propionic acid	0	1
☐	(2R,3R)-2,3-Butanediol	0	0
☐	(R)-3-(4-Hydroxyphenyl)propionate	0	0
☐	(R)-3-Hydroxybutyric acid	0	0
☐	(R)-Acetoin	0	0
☐	(S)-Propane-1,2-diol	0	0

Panel 6 Status: Number of Displayed Variables Changed

5b. Perform FVA Simulations

- Flux balance (FVA) simulations are performed for all models in the current result set.
- Any combination of extracellular fluxes can be selected for FVA simulations.
- FVA simulation results can be plotted and saved in the companion visualization app.
- The FVA results can be parsed according to the flux variable, sample model, metadata attribute, optimization type and flux granularity.



Net Production Fluxes for Maximization of Selected Variables of Sample Models Averaged Over Attributes for Result Set gout_main

Community & Taxa Fluxes for Maximization of Selected Variables of Sample Model TF36 for Result Set gout_main

Plot Panel Bottom

Result Set gout_main

Model microbiota_model_sam...

Optimization Maximization

Granularity Community & Taxa

Metadata Attribute Partition 0

- ■ Variables
  - ☐ Acetic acid Uptake
  - ☐ Butyric acid Uptake
  - ☐ Propionic acid Uptake
  - ☑ Acetic acid Secretion
  - ☑ Butyric acid Secretion
  - ☑ Propionic acid Secretion

- ☐ Attributes
  - ☐ State
  - ☐ META number
  - ☐ Age
  - ☐ Gender
  - ☐ BMI
  - ☐ Uric Acid
  - ☐ Total Bilirubin

Plot Status Panel Plot Updated

Minimum 0

Maximum 0

Results Folder C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi

Figure File Name

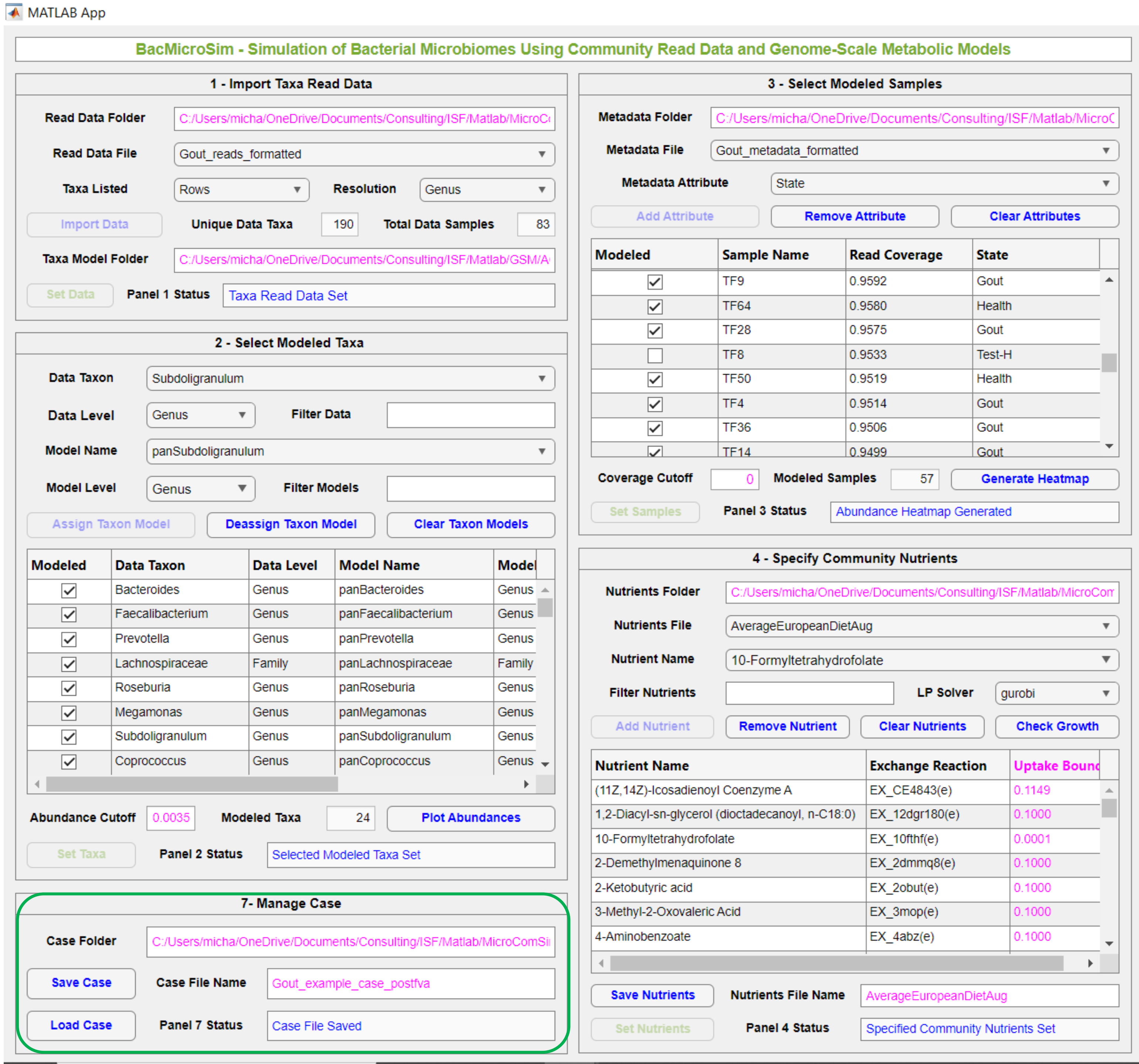
Figure File Format png

Data File Name

Save Status

7. Manage Case

- The current app state can be saved and later reloaded.
- Neither models or results need to be saved to reduce file size.
- All app panels are updated when a new state is loaded.
- All stored results are retained regardless of the results present when the state was saved.



BacMicroSim - Simulation of Bacterial Microbiomes Using Community Read Data and Genome-Scale Metabolic Models

1 - Import Taxa Read Data

Read Data Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Read Data File: Gout_reads_formatted

Taxa Listed: Rows

Resolution: Genus

Unique Data Taxa: 190

Total Data Samples: 83

Taxa Model Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A

Panel 1 Status: Taxa Read Data Set

2 - Select Modeled Taxa

Data Taxon: Subdoligranulum

Data Level: Genus

Filter Data:

Model Name: panSubdoligranulum

Model Level: Genus

Filter Models:

Modeled	Data Taxon	Data Level	Model Name	Model
☑	Bacteroides	Genus	panBacteroides	Genus
☑	Faecalibacterium	Genus	panFaecalibacterium	Genus
☑	Prevotella	Genus	panPrevotella	Genus
☑	Lachnospiraceae	Family	panLachnospiraceae	Family
☑	Roseburia	Genus	panRoseburia	Genus
☑	Megamonas	Genus	panMegamonas	Genus
☑	Subdoligranulum	Genus	panSubdoligranulum	Genus
☑	Coprococcus	Genus	panCoprococcus	Genus

Abundance Cutoff: 0.0035

Modeled Taxa: 24

Panel 2 Status: Selected Modeled Taxa Set

7- Manage Case

Case Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi

Case File Name: Gout_example_case_postfva

Panel 7 Status: Case File Saved

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC

Metadata File: Gout_metadata_formatted

Metadata Attribute: State

Modeled	Sample Name	Read Coverage	State
☑	TF9	0.9592	Gout
☑	TF64	0.9580	Health
☑	TF28	0.9575	Gout
☐	TF8	0.9533	Test-H
☑	TF50	0.9519	Health
☑	TF4	0.9514	Gout
☑	TF36	0.9506	Gout
☑	TF14	0.9499	Gout

Coverage Cutoff: 0

Modeled Samples: 57

Panel 3 Status: Abundance Heatmap Generated

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom

Nutrients File: AverageEuropeanDietAug

Nutrient Name: 10-Formyltetrahydrofolate

Filter Nutrients:

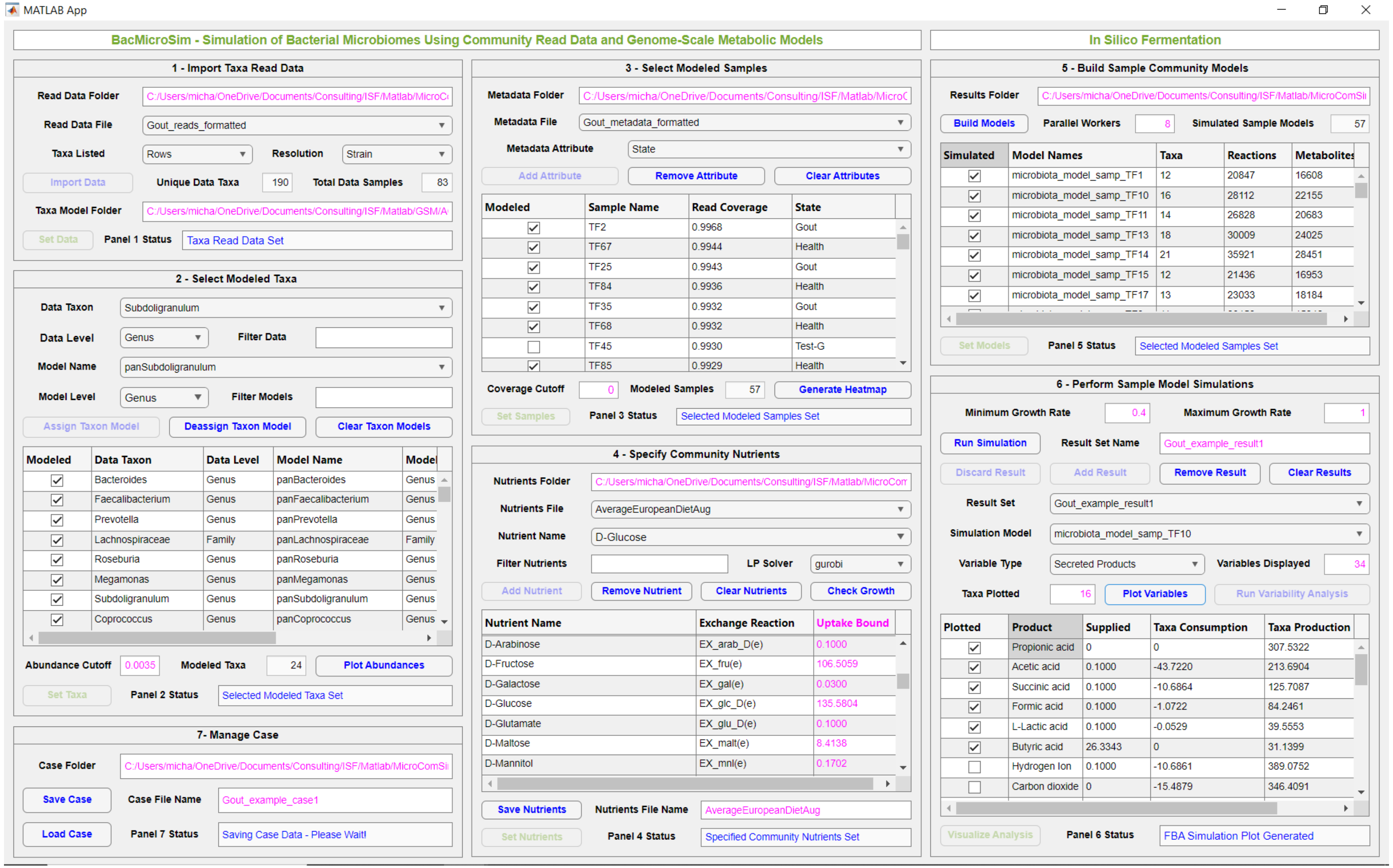
LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
(11Z,14Z)-Icosadienoyl Coenzyme A	EX_CE4843(e)	0.1149
1,2-Diacyl-sn-glycerol (dioctadecanoyl, n-C18:0)	EX_12dgr180(e)	0.1000
10-Formyltetrahydrofolate	EX_10fthf(e)	0.0001
2-Demethylmenaquinone 8	EX_2dmmq8(e)	0.1000
2-Ketobutyric acid	EX_2obut(e)	0.1000
3-Methyl-2-Oxovaleric Acid	EX_3mop(e)	0.1000
4-Aminobenzoate	EX_4abz(e)	0.1000

Nutrients File Name: AverageEuropeanDietAug

Panel 4 Status: Specified Community Nutrients Set

BacMicroSim – A MATLAB Application for Simulation of Bacterial Microbiomes



BacMicroSim - Simulation of Bacterial Microbiomes Using Community Read Data and Genome-Scale Metabolic Models

1 - Import Taxa Read Data

Read Data Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Read Data File: Gout_reads_formatted
Taxa Listed: Rows
Resolution: Strain
Unique Data Taxa: 190
Total Data Samples: 83
Taxa Model Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/A
Panel 1 Status: Taxa Read Data Set

2 - Select Modeled Taxa

Data Taxon: Subdoligranulum
Data Level: Genus
Filter Data:
Model Name: panSubdoligranulum
Model Level: Genus
Filter Models:

Modeled	Data Taxon	Data Level	Model Name	Model
☑	Bacteroides	Genus	panBacteroides	Genus
☑	Faecalibacterium	Genus	panFaecalibacterium	Genus
☑	Prevotella	Genus	panPrevotella	Genus
☑	Lachnospiraceae	Family	panLachnospiraceae	Family
☑	Roseburia	Genus	panRoseburia	Genus
☑	Megamonas	Genus	panMegamonas	Genus
☑	Subdoligranulum	Genus	panSubdoligranulum	Genus
☑	Coprococcus	Genus	panCoprococcus	Genus

Abundance Cutoff: 0.0035
Modeled Taxa: 24
Panel 2 Status: Selected Modeled Taxa Set

7- Manage Case

Case Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi
Case File Name: Gout_example_case1
Panel 7 Status: Saving Case Data - Please Wait!

3 - Select Modeled Samples

Metadata Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroC
Metadata File: Gout_metadata_formatted
Metadata Attribute: State

Modeled	Sample Name	Read Coverage	State
☑	TF2	0.9968	Gout
☑	TF67	0.9944	Health
☑	TF25	0.9943	Gout
☑	TF84	0.9936	Health
☑	TF35	0.9932	Gout
☑	TF68	0.9932	Health
☐	TF45	0.9930	Test-G
☑	TF85	0.9929	Health

Coverage Cutoff: 0
Modeled Samples: 57
Panel 3 Status: Selected Modeled Samples Set

4 - Specify Community Nutrients

Nutrients Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroCom
Nutrients File: AverageEuropeanDietAug
Nutrient Name: D-Glucose
Filter Nutrients:
LP Solver: gurobi

Nutrient Name	Exchange Reaction	Uptake Bound
D-Arabinose	EX_arab_D(e)	0.1000
D-Fructose	EX_fru(e)	106.5059
D-Galactose	EX_gal(e)	0.0300
D-Glucose	EX_glc_D(e)	135.5804
D-Glutamate	EX_glu_D(e)	0.1000
D-Maltose	EX_malt(e)	8.4138
D-Mannitol	EX_mnl(e)	0.1702

Nutrients File Name: AverageEuropeanDietAug
Panel 4 Status: Specified Community Nutrients Set

In Silico Fermentation

5 - Build Sample Community Models

Results Folder: C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/MicroComSi
Parallel Workers: 8
Simulated Sample Models: 57

Simulated	Model Names	Taxa	Reactions	Metabolites
☑	microbiota_model_samp_TF1	12	20847	16608
☑	microbiota_model_samp_TF10	16	28112	22155
☑	microbiota_model_samp_TF11	14	26828	20683
☑	microbiota_model_samp_TF13	18	30009	24025
☑	microbiota_model_samp_TF14	21	35921	28451
☑	microbiota_model_samp_TF15	12	21436	16953
☑	microbiota_model_samp_TF17	13	23033	18184

Panel 5 Status: Selected Modeled Samples Set

6 - Perform Sample Model Simulations

Minimum Growth Rate: 0.4
Maximum Growth Rate: 1
Result Set Name: Gout_example_result1
Result Set: Gout_example_result1
Simulation Model: microbiota_model_samp_TF10
Variable Type: Secreted Products
Variables Displayed: 34
Taxa Plotted: 16

Plotted	Product	Supplied	Taxa Consumption	Taxa Production
☑	Propionic acid	0	0	307.5322
☑	Acetic acid	0.1000	-43.7220	213.6904
☑	Succinic acid	0.1000	-10.6864	125.7087
☑	Formic acid	0.1000	-1.0722	84.2461
☑	L-Lactic acid	0.1000	-0.0529	39.5553
☑	Butyric acid	26.3343	0	31.1399
☐	Hydrogen Ion	0.1000	-10.6861	389.0752
☐	Carbon dioxide	0	-15.4879	346.4091

Panel 6 Status: FBA Simulation Plot Generated

Visit insilicofermentation.com for more information about BacMicroSim and instructions for downloading the app