DOCUMENTATION

**Title: Molecular Communication Based on Cell Metabolism:
A Case Study with Human Gut Microbes**
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Requirements:

OS: window or Mac platform
- MATLAB: able to run the code with most of the latest versions
- Python: version 2 or 3. It's easy to run in PyCharm CE
- MS-Excel
- Hive plots constructed using this link: http://www.hiveplot.com/
- Link for Gephi: https://gephi.org/

MetabolicMC_Supplementary_Git_v1 consists of following folders:
(1) General_Docs
(2) Related_References
(3) B.theta_Data_Analysis
(4) M.smithii_Data_Analysis
(5) Mutual_Information_Analysis_Module_BT_MS
(6) Constellation
(7) Hive_plots_and_explanation
(8) Gephi

1. **General_Docs:** This folder contains,

FILES:
- *General_Example_MutualInformation_BitsCal_Demo.pdf:* general example on how to quantify Mutual Information (MI) in bits for one input and two input combination compounds. Same computation is applicable for 7,6,5,3,2,1 input compound combination

- Example_MI_Calculation_BT&MS_StageI&II_7inputs.pdf: This file consists of MI calculations associated with *B.theta* (BT) and *M.smithii* (MS)organisms. It has calculation steps for Upper bounds of the steady-state mutual information for all the different combinations of seven compounds in Stage I in both organisms **(Figures 13-14)** and Upper bounds of the steady-state mutual information for all the different combinations of seven compounds in E2E in organisms with respect to Biomass only

(Figures 17-18). E2E is calculated similar way **(Figures 19-20)** which we didn't include the workout in this document. Pdf/Docx files contain how the state changing reactions and other groupings are carried out for both organism

- BT_2states_groupings.xlsx
- MS_2states_groupings.xlsx,
- BT_2states_234567bits_intracellular.xlsx,
- MS_2states_234567bits_intracellular.xlsx, and
- BT_MS_Groups_U_S_Biomass(E2E).xlsx
- 14FBAGroups_BT.jpg **(Figure 15)**
- 31FBAGroups_MS.jpg **(Figure 16)**

2. *Related_Refer*

This folder contains, the papers and a master's thesis concept that associated with this journal manuscript

3. *B.theta*_Data_Analysis

This folder contains a subfolder named Active_InActive_State_Changing_Reactions for BT.

The MATLAB_R2018a scripts in this archive execute with three main functions.

a. FBAReactionMatrix_BT_ARIAR.m:
This folder contains the state changing reactions extracted from KBase (www.kbase.us) narrative link for *B.theta* in: https://narrative.kbase.us/narrative/ws.14662.obj.2. Downloaded data in the format of .json files(CompareFBA_JmmolBT.json, KBase_object_details_CompareFBA_JmmolBT2016-05-12T075536918.json)

3.a function will use CompareFBA_JmmolBT.json to construct CompareFBA_JmmolBT.mat. This .mat will use to create BT_Matrix.mat: on and off state changing reaction states of the metabolic network of BT, FBAorder.mat: various input combination labels correspond to state changing reactions and ReducedReactionLabel.mat: associated reaction ID's in the metabolic pathways

b. BT_2states_text.m: construct using three .mat files created in 3.a to build a text file named BT_2states.txt (the same file excel format also included in the folder). This file can be a source file

for various MI calculation in the other folders as well. We used this file in excel to sort and created the groups

c. MutualInfo_BT_2states.m: MI of stage I (intracellular with respect to extracellular input of 7 chemical compounds) is calculated

Apart from these files folder contains BT_ 2states.xlsx file and use it to construct **BT_Matrix_2states_imagesecs.fig or BT_Matrix_2states_imagesecs.jpgas in (Figure 11) in the manuscript.**

4. *M.smithii*_Data_Analysis
This folder contains, exactly the information contains as in the 3.a, 3.b, and 3.c. But this calculation is corresponding to *M.smithii* organisms. **MS_Matrix_2states_imagesecs.fig or MS_Matrix_2states_imagesecs.jpgas in (Figure 12) in the manuscript.**

5. Mutual_Information_Analysis_Module_BT_MS:

This folder contains, eleven excel files which are constructed using text file created in 3.b or 4.b. Associated biomass values for different groups in (BT-14 and MS 31) are extracted using CompareFBA_JmmolBT.mat structure. These 11 excels files are used for MI calculation for fig 13, 14, 17, 18, 19, and 20. Included three python functions to compute the values associated with these figures. Also included comments and purpose of these
functions. Here user needs to be careful of choosing the correct for an organism. Each time calculate the MI of one of the organisms. Pay attention
to comments in MI_Calculation_Fig13-14_plotvalues.py, 2 MI_Calculation_Fig17-18_plotvalues.py and MI_Calculation_Fig19-20_plotvalues.py python files

6. Constellation:
This folder contains two excel files which contain how the reduction of the models are accrued out for *B.theta* and *M.smithii*

7. Hive_plots_and_explanation
The folder consists of files extracted from the data file of *M. smithii* with 31 groups to construct the hive plots. Also, we included

Hive_plot_simple_explanation.pdf file to understand how we
constructed the hive plot for an organism

8. Gephi

The folder consists of subfolders that extracted from the data file
of *M. smithii* with 31 groups to construct the Gephi plot