**COMPLETED: Mutual Information Calculation of *B\_theta and M\_smithii* KBase Data**

**Public Narrative Links at KBase Data:**

[**https://narrative.kbase.us/narrative/ws.14662.obj.2**](https://narrative.kbase.us/narrative/ws.14662.obj.2)

[**https://narrative.kbase.us/narrative/ws.14663.obj.1**](https://narrative.kbase.us/narrative/ws.14663.obj.1)

**INTRACELLULAR CALCULATIONS – STAGE I**

**MI\_Calculation\_Fig13\_plotvalues.py file : only for 7 input compound calculation**

**B\_theta\_MI Calculation (Stage I – Intracellular) – When all 7 compounds present**

B\_Theta

Reactions 212

FBAs 128

DetailsofDuplicateRows =

Total Duplicates Real Duplicates

1. 1,34,41,60,79,105,134,154,184,189,191,0,0,0,0,0,0 11 10
2. 2,178,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
3. 4,57,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
4. 5,15,17,32,74,78,95,108,111,112,130,135,164,167,171,195,198 17 16
5. 7,91,172,208,0,0,0,0,0,0,0,0,0,0,0,0,0 4 3
6. 10,56,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
7. 11,52,55,131,175,0,0,0,0,0,0,0,0,0,0,0,0 5 4
8. 12,72,143,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
9. 18,144,152,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
10. 20,142,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
11. 21,125,163,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
12. 23,201,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
13. 25,179,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
14. 26,36,102,149,0,0,0,0,0,0,0,0,0,0,0,0,0 4 3
15. 27,113,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
16. 29,151,187,193,197,0,0,0,0,0,0,0,0,0,0,0,0 5 4
17. 35,51,210,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
18. 38,59,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
19. 40,99,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
20. 42,64,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
21. 44,70,81,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
22. 47,71,109,136,0,0,0,0,0,0,0,0,0,0,0,0,0 4 3
23. 48,50,127,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
24. 58,94,119,138,169,0,0,0,0,0,0,0,0,0,0,0,0 5 4
25. 65,86,196,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
26. 66,96,157,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
27. 69,93,133,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
28. 73,140,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
29. 84,110,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
30. 88,106,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
31. 98,100,126,147,158,182,0,0,0,0,0,0,0,0,0,0,0 6 5
32. 116,132,148,153,159,0,0,0,0,0,0,0,0,0,0,0,0 5 4
33. 121,212,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
34. 122,162,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
35. 150,173,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
36. 156,209,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
37. 180,181,185,192,0,0,0,0,0,0,0,0,0,0,0,0,0 4 3
38. 183,188,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 2 1
39. 199,205,206,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2
40. 202,204,207,0,0,0,0,0,0,0,0,0,0,0,0,0,0 3 2

Sum 139 99

NumDuplicateRows = 99

Unique Reactions = 113 (212-99)

B\_Theta

FBAs 128

Reactions 113

DetailsofDuplicateColumns =

Total Duplicates Real Duplicates

1. 1,4,17,42,55,94,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 ---------------------------------------------------------- {6} {5}
2. 2,5,7,18,20,22,24,38,43,45,52,56,58,62,74,76,78,80,91,93,95,96,98,111,113,115,126,128,0,0,0,0----------------------- {28} {27}
3. 3,10,48,53,123,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 ---------------------------------------------------------- {5} {4}
4. 6,19,23,75,85,97,114,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0------------------------------------------------------------- {7} {6}
5. 8,12,25,64,99,103,116,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0----------------------------------------------------------- {7} {6}
6. 9,11,13,14,16,27,29,31,33,34,36,47,49,51,54,65,67,69,71,82,84,87,89,100,102,104,106,117,118,120,122,124--------- {32} {31}
7. 15,28,32,35,66,70,83,88,101,105,119,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 ----------------------------------------------- {11} {10}
8. 21,59,108,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 ------------------------------------------------------------ {3} {2}
9. 26,30,46,50,68,81,86,107,121,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0--------------------------------------------------------- {9} {8}
10. 37,77,90,112,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0------------------------------------------------------------------- {4} {3}
11. 39,44,61,79,110,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0----------------------------------------------------------------- {5} {4}
12. 40,60,73,109,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0------------------------------------------------------------------- {4} {3}
13. 41,57,92,127,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0------------------------------------------------------------------- {4} {3}
14. 63,72,125,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0--------------------------------------------------------------------- {3} {2}

Sum 128 114

NumDuplicateColumns = 114 (128-14)

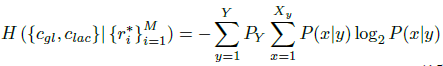
Unique FBAs = 14 (128-114) **Hence 14 Groups in BT**



**(1)**



= log2(128) = 7 bits



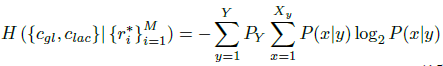
No.of.Members in each group 3 4 5 6 7 9 11 28 32

| | | | | | | | |

No. Groups 2 3 2 1 2 1 1 1 1

+ + +

= -0.1814



= 3.6933 bits

Implement the values to equation (1),



**MI = 7 bits - 3.6933 bits**

**MI = 3.3068 bits**

**MI\_Calculation\_Fig14\_plotvalues.py file : only for 7 input compound calculation**

**M\_smithii GROUP\_MI Calculation (Stage I)– When all 7 compounds present**

NumDuplicateRows = 420

Unique Reactions = 136 (556-420) P.S = Matrix information is excluded, because the size of the matrix is large to fit on a page

DetailsofDuplicateColumns =

Total Duplicates Real Duplicates

1. 1,108,0,0,0,0,0,0,0,0,0,0,0,0 2 1
2. 2,38,0,0,0,0,0,0,0,0,0,0,0,0 2 1
3. 4,21,59,63,77,112,0,0,0,0,0,0,0,0 6 5
4. 5,22,74,0,0,0,0,0,0,0,0,0,0,0 3 2
5. 6,44,79,85,97,114,0,0,0,0,0,0,0,0 6 5
6. 7,24,60,78,98,0,0,0,0,0,0,0,0,0 5 4
7. 8,26,46,81,99,107,116,0,0,0,0,0,0,0 7 6
8. 9,47,65,100,117,118,0,0,0,0,0,0,0,0 6 5
9. 10,28,48,66,83,101,119,0,0,0,0,0,0,0 7 6
10. 11,14,29,49,67,84,102,120,0,0,0,0,0,0 8 7
11. 12,25,50,68,86,103,121,0,0,0,0,0,0,0 7 6
12. 13,16,33,34,36,51,69,104,0,0,0,0,0,0 8 7
13. 15,32,35,53,70,88,105,123,0,0,0,0,0,0 8 7
14. 17,37,55,72,125,0,0,0,0,0,0,0,0,0 5 4
15. 18,20,40,52,56,58,73,76,91,93,109,111,126,128 14 13
16. 27,82,0,0,0,0,0,0,0,0,0,0,0,0 2 1
17. 31,54,71,87,89,106,122,124,0,0,0,0,0,0 8 7
18. 39,41,57,75,92,110,127,0,0,0,0,0,0,0 7 6
19. 42,94,0,0,0,0,0,0,0,0,0,0,0,0 2 1
20. 43,113,0,0,0,0,0,0,0,0,0,0,0,0 2 1
21. 45,62,80,0,0,0,0,0,0,0,0,0,0,0 3 2

Sum 118 97

NumDuplicateColumns = 97 (118-21)

Unique FBAs = 31 (128-97) **Hence 31 Groups in MS**



= log2(128) = 7 bits

No.of.Members in each group 1 2 3 5 6 7 8 14

| | | | | | | |

No. Groups 10 5 2 2 3 4 4 1

+

+ = -0.0781

= = -0.0743

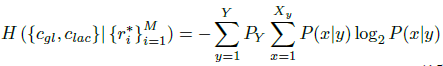
=

=

=

=

=



Implement the values to equation (1),



**MI = 7 bits - bits**

**MI = 4.5222 bits**

**STAGE II : Figure 17, Upper bounds of the steady-state mutual information for all the different combinations of seven compounds (extracellular) in E2E in B. theta with respect to Biomass only**

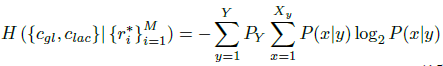
**B\_theta\_MI between 7 most influential factors and Biomass (Stage II) – zero values for all 14 groups for compound is eliminated**

FBAGroups Value No.of.FBAs Number of groups

1. C,G 0.202862 C=4,G=5🡪9 2 (index: 4,8)
2. L 0.203778 L=11🡪 11 1 (index: 13)
3. I 0.205694 I=7🡪 7 1 (index: 10)
4. F 0.206636 F=5🡪 5 1 (index: 7)
5. E,M 0.396393 E=4,M=28🡪32 2 (index: 6,14)
6. N 0.398741 N=32🡪 32 1 (index: 15)
7. A,B,D,H 0.87827 A=3,B=3,D=4,H=6🡪16 4 (index: 2,3,5,9)
8. J,K 0.883073 J=7,K=9🡪16 2 (index: 11,12)



= log2(128) = 7 bits



No.of.Members in each group 1(11,7,5,32) 2(4,5,4,28,7,9) 4(3,3,4,6)

| | |

No. Groups 4 3 1

=

=

=

=

= = -2.5000

=

= 4.2644



**MI = 7 bits – 4.2644 bits**

**MI = 2.7356 bits**

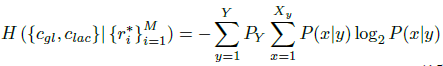
**B\_theta \_ONLY BIOMASS (Stage II) – with respect to intracellular metabolism as inputs and only biomass out put14 groups**

FBAGroups Value Number of groups

1. C,G 0.202862 2 (index: 4,8)
2. L 0.203778 1 (index: 13)
3. I 0.205694 1 (index: 10)
4. F 0.206636 1 (index: 7)
5. E,M 0.396393 2 (index: 6,14)
6. N 0.398741 1 (index: 15)
7. A,B,D,H 0.87827 4 (index: 2,3,5,9)
8. J,K 0.883073 2 (index: 11,12)



= log2(14) = 3.8074 bits



=

No.of.Members in each group 1 2 4

| | |

No. Groups 4 3 1

=

= = 0

=

=

=

= 1.0000



**MI = 3.8074 bits - 1.0000 bits**

**MI = 2.8074 bits**

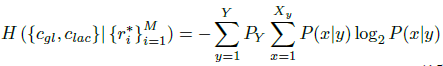
**BT \_MI of all excreted and up-taken, secreted compounds including Biomass (Stage II) – 14 Groups (with respect to intracellular metabolism as inputs and excreted and up-taken, secreted, and biomass**

FBAGroups Value Number of groups

1. C,G 0.202862 2 (index: 4,8)
2. L 0.203778 1 (index: 13)
3. I 0.205694 1 (index: 10)
4. F 0.206636 1 (index: 7)
5. E 0.396393 1 (index: 6)
6. M 0.396393 1 (index: 14)
7. N 0.398741 1 (index: 15)
8. A 0.87827 1 (index: 2)
9. B 0.87827 1 (index: 3)
10. D 0.87827 1 (index: 5)
11. H 0.87827 1 (index: 2,3,5,9)
12. J 0.883073 1 (index: 11)
13. K 0.883073 1 (index: 12)



= log2(14) = 3.8074 bits



=

No.of.Members in each group 1 2

| |

No. Groups 12 1

=

=

=

=

= 0.1429



**MI =** **3.8074 bits – 0.1429 bits**

**MI = 3.6645 bit**

**P.S.: Exactly same result is obtained as above for MI of all excreted and up-taken compounds excluding Biomass**

**STAGE II : Figur 18, Upper bounds of the steady-state mutual information for all the different combinations of seven compounds (extracellular) in E2E in M. smithii with respect to Biomass only**

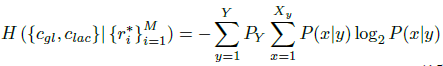
**M\_Smitti\_MI between 7 most influential factors and Biomass (Stage II) – zero values for all 31 groups for compound is eliminated**

FBAGroups BiomassValue No.of.FBAs Number of groups

1. S 0 S=5🡪5 1 (index: 20) - Data start from row index2, row 1 is title of the compounds)
2. J,Z 0.102111 J=1,Z=7🡪8 2 (index: 11,27)
3. W 0.102548 W=8🡪8 1 (index: 24)
4. E,K,R 0.129823 E=1,K=2,R=5🡪8 3 (index: 6,12,19)
5. D,Y 0.154711 D=1,Y=7🡪8 2 (index:5,26)
6. C 0.162135 C=1🡪1 1 (index:4)
7. M,T 0.170735 M=2, T=6🡪8 2 (index:14,21)
8. I,U 0.182998 I=1, U=6🡪7 2 (index:10,22)
9. O,V,AB 0.23574 O=2,V=6,AB=8🡪16 3 (index:6,23,29)
10. L,AE 0.259537 L=2,AE=14🡪16 2( index:13,32)
11. B, AA 0.289634 B=1, AA=7🡪8 2 (index:3,28)
12. H,X 0.306145 H=1,X=7🡪8 2 (index:9,25)
13. A,N,P,Q 0.417114 A=1,N=2,P=3,Q=3🡪9 4 (index: 2,15,17,18) - matlab index(1,14, 16, 17)
14. AC,AD 0.422201 AC =8, AD=8🡪16 2 (index: 30,31)
15. F,G 0.433068 F=1,G=1🡪2 2 (index: 7,8)



= log2(128) = 7 bits



=

No.of.Members in each group 1(5,8,1) 2(8,8,8,7,16,8,816,2) 3(8,16) 4(9)

| | | |

No. Groups 3 9 2 1

++ +

0.0156

= -0.0907

= -0.1535

=

=

=

=

= 3.2952



**MI = 7 bits- 3.2952bits**

**MI = 3.7048 bits**

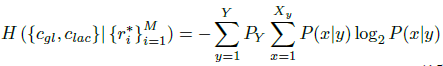
**M\_Smitti \_ONLY BIOMASS (Stage II) – 31 Groups**

FBAGroups Value Number of groups

1. S 0 1 (index: 20) - Data start from row index2, row 1 is title of the compounds)
2. J,Z 0.102111 2 (index: 11,27)
3. W 0.102548 1 (index: 24)
4. E,K,R 0.129823 3 (index: 6,12,19)
5. D,Y 0.154711 2 (index:5,26)
6. C 0.162135 1 (index:4)
7. M,T 0.170735 2 (index:14,21)
8. I,U 0.182998 2 (index:10,22)
9. O,V,AB 0.23574 3 (index:6,23,29)
10. L,AE 0.259537 2( index:13,32)
11. B, AA 0.289634 2 (index:3,28)
12. H,X 0.306145 2 (index:9,25)
13. A,N,P,Q 0.417114 4 (index: 2,15,17,18) - matlab index(1,14, 16, 17)
14. AC,AD 0.422201 2 (index: 30,31)
15. F,G 0.433068 2 (index: 7,8)



= log2(31) = 4.9542 bits



=

No.of.Members in each group 1 2 3 4

| | | |

No. Groups 3 9 2 1

+

=

=

=-0.3068

= = -0.2581

=

= 1.1455



**MI = 4.9542 bits - 1.1455 bits**

**MI = 3.8087 bit**

**M\_Smitti \_MI of all excreted and up-taken compounds including Biomass (Stage II) – 31 Groups**

FBAGroups Indexes Number of groups

1) A,N,P,Q 1 14 16 17 4 -matlab index

2) B,AA 2 27 2

3) D,Y 4 25 2

4) E,K,R 5 11 18 3

5) F,G 6 7 2

6) H,X 8 24 2

7) I, U 9 21 2

8) J,Z 10 26 2

9) L,AE 12 31 2

10) M,T 13 20 2

11) O,V,AB 15 22 28 3

12) C 3 1

13) S 19 1

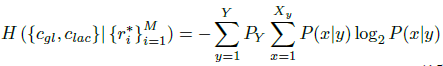
14) W 23 1

15) AC 29 1

16) AD 30 1



= log2(31) = 4.9542 bits



No.of.Members in each group 1 2 3 4

| | | |

No.of groups 5 8 2 1

+

=

=

=-0.3068

= = -0.2581

=

= 1.0810



**MI = 4.9542 bits - 1.0810 bits**

**MI = 3.8732 bit**

**P.S.: Exactly same result is obtained as above for MI of all excreted and up-taken compounds excluding Biomass**