MOMS-PI

2018-11-24

Settings

HMP2 Data

https://ibdmdb.org/tunnel/public/summary.html - 178 samples

16S

- \bullet Summary: mapping statistics, https://ibdmdb.org/tunnel/dataset_summary/HMP2/16S/1806/summary/summary.html
- Raw files: .tar files with bgzipped FASTq paired-end files, https://ibdmdb.org/tunnel/public/HMP2/ 16S/1806/rawfiles
- Products:
 - Taxonomic profiles (BIOM): 178 BIOM files
 - Taxonomic Profiles (Text): 178 .tsv files. Example:

Taxonomy	206719
Bacteria;Firmicutes;Bacilli;Bacillales;Alicyclobacillaceae;Tumebacillus	0
Bacteria;Firmicutes;Clostridia;Clostridiales;Lachnospiraceae;	0
Lachnospiraceae_FCS020_group	
Bacteria;Proteobacteria;Betaproteobacteria;Burkholderiales;Comamonadaceae;	0
Ramlibacter	
Bacteria;Cyanobacteria;Melainabacteria;Obscuribacterales;f;g	0
Bacteria;Proteobacteria;Rhizobiales;Rhizobiaceae;	0
Rhizobium	

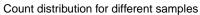
- **Merged Tables: ** `taxonomic_profiles.biom.gz` and `taxonomic_profiles.tsv.gz`. Content is the same,
 [1] "Data dimensions"
- [1] 982 178

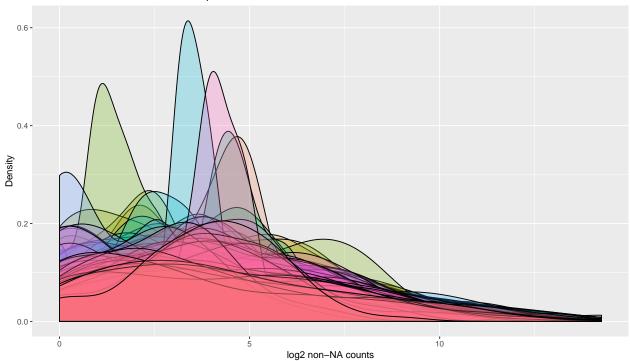
	206646	224324	206619	224326	206624
IP8BSoli	0	0	0	0	17
${f UncTepi3}$	0	0	0	0	0
${ m Unc}004{ m ii}$	0	0	0	0	0
${f Unc 00re 8}$	0	0	0	0	0
Unc018j2	1	0	0	0	0

Count distribution

[1] "Summary of count data"

```
Min. 1st Qu. Median Mean 3rd Qu. Max. 0.0 0.0 0.0 15.4 0.0 19572.0
```





Distribution of sample medians

Min. 1st Qu. Median Mean 3rd Qu. Max. 0 0 0 0 0 0 0

Sparsity

Sparsity distribution 7.52.50.80 0.85 0.90 pct_nas

```
Min. 1st Qu. Median Mean 3rd Qu. Max. 0.7821 0.8872 0.9221 0.9166 0.9440 0.9939
```

Questions

- What are the row IDs?
- Most sample counts are very small, median = 0. Is it expected?
- There are outliers, like a sample with maximum count = 19572 (while mean is \sim 15). Shall we remove such samples?
- The data is very sparse (\sim 92% zeros) is it expected?

Serology

 $\verb|hmp2_serology_Compiled_ELISA_Data.tsv|, columns are samples$

- [1] "Data dimensions"
- [1] 14 212

Serum ID	206454	206458	206459	206460
Site	Harvard	Harvard	Harvard	Harvard
Plate	1	1	1	1
Sample	1	2	3	4
IgA ASCA EU	0	0	0	49
IgA ASCA Pos.	0	0	0	1

Metagenomes

 $Lots\ of\ files.\ Look\ at\ Products,\ Merged\ Tables,\ https://ibdmdb.org/tunnel/public/HMP2/WGS/1818/products$

$taxonomic_profiles.tsv$

- [1] "Data dimensions"
- [1] 1479 1639

$\#\mathrm{SampleID}$	CSM5FZ	4MSM5M	C W9 M5MC	CVOSM5MCVN
kArchaea	0	0	0	0
kArchaea pEuryarchaeota	0	0	0	0
kArchaea $ p$ Euryarchaeota $ c$ Methanobacteria	0	0	0	0
${\tt k__Archaea p__Euryarchaeota c__Methanobacteria o__Methanobacteria o__Methanobacteria$	anob@cteria	ales 0	0	0
lem:lem:lem:lem:lem:lem:lem:lem:lem:lem:	anob@cteria	$ales f0_N$	Iethanobact	eria@ae

pathabundances.tsv

- [1] "Data dimensions"
- [1] 10884 1639

# Pathway	CSM5FZ4I	M CSM5MCUC	O CSM5MCV	LCSM5MCV
1CMET2-PWY: N10-formyl-tetrahydrofolate	0.01581	0.01017	0.01674	0.018
biosynthesis				
1CMET2-PWY: N10-formyl-tetrahydrofolate	0	0	0	0
$biosynthesis \underline{\mathbf{g}} \underline{\hspace{0.5cm}} Akkermansia.s \underline{\hspace{0.5cm}} Akkermansia\underline{\hspace{0.5cm}} mucin \underline{\hspace{0.5cm}}$	iphila			
1CMET2-PWY: N10-formyl-tetrahydrofolate	0	0	0	0
$biosynthesis \underline{\mathbf{g}} \underline{\hspace{0.5cm}} Bacteroides. \underline{\hspace{0.5cm}} Bacteroides \underline{\hspace{0.5cm}} barnesiae$,			
1CMET2-PWY: N10-formyl-tetrahydrofolate	0	0.0001569	0	0
$biosynthesis g__Bacteroides.s__Bacteroides_caccae$				
1CMET2-PWY: N10-formyl-tetrahydrofolate	0	0	0	0
$biosynthesis {\tt g}__Bacteroides.s__Bacteroides_cellulosily$	yticus			

ecs.tsv

- [1] "Data dimensions"
- [1] 108433 1639

# Gene Family	CSM5FZ4N	M CSM5MCU	JCSM5MCV	/LCSM5MCVN
1.1.1.100: 3-oxoacyl-[acyl-carrier-protein] reductase	0.001835	0.001472	0.001571	0.001173
1.1.1.100: 3-oxoacyl-[acyl-carrier-protein]	0	0	0	0
reductase gAggregatibacter.sAggregatibacter_s	segnis			
1.1.1.100: 3-oxoacyl-[acyl-carrier-protein]	0	0	0	0
$reductase \underline{g} \underline{\hspace{0.5cm}} Alloprevotella.\underline{s} \underline{\hspace{0.5cm}} Alloprevotella\underline{\hspace{0.5cm}} tann$	erae			
1.1.1.100: 3-oxoacyl-[acyl-carrier-protein]	0	0	0	0
reductase gAnaerococcus_obesi	iensis			
1.1.1.100: 3-oxoacyl-[acyl-carrier-protein]	0	0	0	0
$reductase \underline{g} \underline{\hspace{0.5cm}} Anaerococcus.\underline{\hspace{0.5cm}} \underline{\hspace{0.5cm}} Anaerococcus\underline{\hspace{0.5cm}} \underline{\hspace{0.5cm}} vagin$	nalis			

Proteomics

https://ibdmdb.org/tunnel/public/HMP2/Proteomics/1633/products

$HMP2_proteomics_ecs.tsv$

- [1] "Data dimensions"
- [1] 910 451

Gene	CSM5FZ3N	CSM5FZ3T	CSM5FZ44	CSM5FZ48
UNGROUPED	1769	1128	2765	1183
1.1.1.1: Alcohol dehydrogenase	0	0	0	0
1.1.1.100: 3-oxoacyl-[acyl-carrier-protein]	0	0	0	0
reductase				
1.1.1.103: L-threonine 3-dehydrogenase	0	0	0	0
1.1.1.127: 2-dehydro-3-deoxy-D-gluconate	0	0	0	0
5-dehydrogenase				

$HMP2_proteomics_kos.tsv.gz$

- [1] "Data dimensions"
- [1] 1823 451

KO	CSM5FZ3N	CSM5FZ3T	CSM5FZ44	CSM5FZ48
UNGROUPED	1595	1134	2771	954
K00003: homoserine dehydrogenase	0	0	0	0
[EC:1.1.1.3]				
K00005: glycerol dehydrogenase	0	0	0	0
[EC:1.1.1.6]				
K00008: L-iditol 2-dehydrogenase	0	0	0	0
[EC:1.1.1.14]				
K00009: mannitol-1-phosphate	0	0	0	0
5-dehydrogenase [EC:1.1.1.17]				

Viromics

https://ibdmdb.org/tunnel/public/HMP2/Viromics/1732/products

$taxonomic_profiles.tsv.gz$

- [1] "Data dimensions"
- [1] 56 330

		#ID		CSM5M @%M 5L M% M5L C9M 5MCXH	
k_	_Viruses p_	_Viruses_noname c	_Viruses_noname o_	_Caudovirales f_0_Myov i ridae g_0_Mulik @ virus s]	Escherichia_
k_{-}	$_$ Viruses $ p_$	$_{ m Viruses_noname} c\{ m }$	$_{ m Viruses_noname} _{ m o}$	_Caudovirales f <u>0</u> Myov i ridae g <u>0</u> Mulik @ virus s1	Mulikevirus
k_{-}	$_$ Viruses $ p_$	$_{ m Viruses_noname} c\{ m }$	$_{ m Viruses_noname} _{ m o}$	_Caudovirales f <u>0</u> Myov i ridae g <u>0</u> T4like@irus sF	Klebsiella_p
k_{-}	$_$ Viruses $ p_$	$_{ m Viruses_noname} c\{ m }$	$_{ m Viruses_noname} _{ m o}$	$\underline{\hspace{0.1cm}}\text{Caudovirales} \underline{\text{f}}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{Podov@ridae} \underline{\text{g}}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{Epsil}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{n}15\\ \text{likevirales} \underline{\text{f}}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{Podov}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{ridae} \underline{\text{g}}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{Epsil}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}}\text{n}15\\ \text{likevirales} \underline{\text{f}}\underline{\hspace{0.1cm}0}\hspace{0.1cm}\underline{\hspace{0.1cm}0$	ıs sEpsil
k_	$_$ Viruses $ p_$	$_{ m Viruses_noname} c\{ m }$	$_{ m Viruses_noname} _{{ m o}_}$	$_Caudovirales f_0_Sipho@iridae g_0_C2lil@virus s__$	C2likevirus

$virome_virmap_analysis.tsv.gz$

- [1] "Data dimensions"
- [1] 260 704

Virus	MSM5LI	LDSSM5FZ	4 M SM5FZ	BMSM5MD5B
superkingdom=Viruses;dsDNA viruses, no RNA	0	0	0	0
stage;family=Adenoviridae;genus=Mastadenovirus;species=Hu	ıman			
mastadenovirus A;taxId=129875				
superkingdom=Viruses;dsDNA viruses, no RNA	0	0	0	0
stage;family=Baculoviridae;genus=Alphabaculovirus;species=	stage;family=Baculoviridae;genus=Alphabaculovirus;species=Autographa			
californica multiple nucleopolyhedrovirus; tax $Id=307456$				
superkingdom=Viruses;dsDNA viruses, no RNA	0	0	0	0
stage;family=Baculoviridae;genus=Alphabaculovirus;taxId=55	58016			

Virus	MSM5L1	LD\$SM5FZ	4MSM5FZ	ZB M SM5MD5B
superkingdom=Viruses;dsDNA viruses, no RNA	0	0	0	0
stage;order=Caudovirales;family=Myoviridae;genus=Felixo1vi	irus;species	=Salmonel	la	
phage FelixO1;taxId=77775				
superkingdom=Viruses;dsDNA viruses, no RNA	0	0	0	0
stage;order=Caudovirales;family=Myoviridae;genus=Felixo1vi	irus;unclass	sified		
FelixO1likevirus;species=Escherichia phage				
$vB_EcoM_AYO145A; taxId=1636202$				

Metabolites

https://ibdmdb.org/tunnel/public/HMP2/Metabolites/1723/products

$HMP2_metabolomics.csv.gz$

[1] "Data dimensions"

[1] 81867 553

Method	Pooled QC sample CV	$\mathrm{m/z}$	RT	HMDB (*Representative ID)
C18-neg	0.02719	313.2	9.75	HMDB04705
C18-neg	0.02641	313.2	9.95	HMDB04704
C18-neg	0.04684	115.1	5.79	HMDB00535
C18-neg	0.07408	129.1	7.43	HMDB00666
C18-neg	0.02414	149.1	5.81	HMDB00764

HMP2_Pilot Data

16S

 $taxonomic_profiles.biom.gz$

[1] "Data dimensions"

[1] 503 58

	CSM5FZ3N	CSM5FZ3X	CSM5FZ3Z	CSM5FZ46	CSM5FZ4G
kBacteria;	0	0	0	0	0
${f p}$ Firmicutes;					
${ m c}$ Clostridia;					
oClostridiales; f;					
$g_{}; s_{}:390820$					
kBacteria;	0	0	0	0	0
${f p}$ Firmicutes;					
${f c}$ Clostridia;					
oClostridiales; f;					
$g_{}; s_{}:369429$					

	CSM5FZ3N	CSM5FZ3X	CSM5FZ3Z	CSM5FZ46	CSM5FZ4G
kBacteria;	0	0	0	0	0
${f p}$ Firmicutes;					
${f c}$ Clostridia;					
${ m o}$ Clostridiales;					
$f_{\underline{}}$ Ruminococcaceae;					
${f g}$ Ruminococcus;					
\mathbf{s} :363646					
kBacteria;	0	0	0	0	0
${f p}$ Bacteroidetes;					
${f c}$ Bacteroidia;					
${ m o}$ Bacteroidales;					
${f f}$ Bacteroidaceae;					
${f g}$ Bacteroides;					
scaccae:195508					
kBacteria;	0	0	0	0	0
pFirmicutes;					
cClostridia;					
oClostridiales;					
fLachnospiraceae;					
gDorea; s:577406					