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Title	Microbiota and metabolite profiling reveal specific alterations in bacterial community structure and environment in the cystic fibrosis airway during exacerbation
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Table S4. Concentrations of metabolites identified in CF sputum taken from 26 stable CF patients. Data are given as the average values measured in triplicate (metabolite concentrations are described as μM unless otherwise stated and means \pm standard deviations are reported).

Metabolite	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25		
Amino acids																											
alanine	2500.0	2510.0	2555.0	2589.0	2572.0	2589.0	2549.0	2533.0	2554.0	2579.0	2577.0	2588.0	2555.0	2577.0	2599.0	2599.0	2545.0	2533.0	2500.0	2570.0	2513.0	2595.0	2955.0	2600.0	2400.0		
aspartate	64.7	63.9	64.1	65.4	64.6	66.0	65.4	64.5	64.4	65.1	64.7	65.8	64.4	64.4	65.0	66.4	65.3	65.9	63.2	66.5	62.9	57.1	73.9	70.4	53.8		
cysteine	20.3	19.9	19.6	20.3	19.6	20.2	20.3	20.0	19.8	20.1	19.7	20.4	20.0	19.8	19.6	20.3	19.8	20.8	19.0	21.1	22.1	15.5	21.0	26.2	16.6		
glycine	75.4	76.2	72.6	77.7	72.7	74.6	76.0	75.9	73.8	76.7	72.2	76.6	75.6	75.9	72.3	76.9	71.4	82.1	67.6	71.8	107.0	55.2	60.1	118.6	62.1		
glutamate	114.4	119.6	106.5	121.9	111.1	111.9	114.1	117.2	109.8	121.1	107.4	115.5	113.5	119.8	107.2	122.7	99.1	138.6	107.2	76.5	220.9	104.8	57.8	217.9	94.3		
histidine	66.0	77.5	60.3	75.7	68.5	67.7	67.2	73.7	62.5	77.8	64.1	70.2	65.4	77.2	60.2	85.4	49.3	89.2	96.7	23.9	145.5	125.1	18.3	159.4	57.1		
lysine	127.6	192.9	119.4	165.9	151.8	151.1	136.9	176.7	120.5	182.0	137.1	161.0	127.1	192.1	105.8	259.7	83.0	138.3	607.2	24.6	174.4	1026.2	17.2	418.6	124.1		
phenylalanine	26.5	64.6	28.8	43.7	40.2	44.2	31.0	58.6	26.5	53.1	34.0	50.7	26.5	72.6	16.3	125.2	24.0	9.1	986.0	5.6	6.8	2384.0	1.6	134.9	33.1		
tyrosine	49.8	49.1	49.3	50.3	49.7	50.8	50.3	49.6	49.5	50.0	49.8	50.6	49.6	49.6	50.0	51.1	50.2	50.7	48.6	51.1	48.4	43.9	56.8	54.2	41.4		
tryptophan	34.5	33.8	33.3	34.5	33.3	34.3	34.5	34.1	33.6	34.2	33.4	34.7	34.0	33.7	33.3	34.6	33.7	35.4	32.3	35.9	37.5	26.3	35.7	44.5	28.1		
arginine	91.7	91.4	87.1	93.2	87.2	89.5	91.2	91.1	88.6	92.0	86.6	92.0	86.6	92.0	90.8	91.1	86.7	92.2	85.7	98.6	81.1	86.2	128.4	66.3	72.1	142.4	74.5
proline	150.5	157.4	140.1	160.4	146.1	147.3	150.2	154.2	144.5	159.4	141.3	152.0	149.4	157.7	141.0	161.5	130.4	182.4	141.1	100.7	290.7	137.8	76.0	286.7	124.1		
valine	1244.5	1463.0	1137.5	1428.8	1291.9	1277.0	1268.0	1389.8	1180.1	1468.9	1210.3	1324.5	1233.8	1455.8	1136.8	1612.1	931.1	1683.0	1824.9	450.9	2745.5	2361.4	345.2	3006.9	1077.5		
Polyamines																											
putrescine	21.0	17.9	23.0	18.3	20.2	20.5	20.6	18.8	22.1	17.8	21.6	19.7	21.2	18.0	23.0	16.2	28.1	15.5	14.3	58.0	9.5	11.1	75.7	8.7	24.3		
spermine	10.0	9.8	9.9	10.1	9.9	10.2	10.1	9.9	9.9	10.0	10.0	10.1	9.9	9.9	10.0	10.2	10.0	10.1	9.7	10.2	9.7	8.8	11.4	10.8	8.3		
spermidine	8.1	8.0	7.8	8.1	7.8	8.1	8.1	8.0	7.9	8.0	7.9	8.2	8.0	7.9	7.8	8.1	7.9	8.3	7.6	8.4	8.8	6.2	8.4	10.5	6.6		
Carbohydrate																											
fructose-6-phosphate	81.5	81.2	77.4	82.9	77.5	79.6	81.1	81.0	78.8	81.8	77.0	81.7	80.7	81.0	77.1	82.0	76.2	87.6	72.1	76.6	114.2	58.9	64.1	126.5	66.2		
glucose	90.3	94.4	84.1	96.2	87.7	88.4	90.1	92.5	86.7	95.6	84.8	91.2	89.6	94.6	84.6	96.9	78.3	109.4	84.6	60.4	174.4	82.7	45.6	172.0	74.5		
pyruvate	99.4	116.9	90.9	114.1	103.2	102.0	101.3	111.0	94.3	117.3	96.7	105.8	98.5	116.3	90.8	128.8	74.4	134.4	145.8	36.0	219.3	188.6	27.6	240.2	86.1		
lactate	11.1	11.1	10.9	10.7	10.8	10.7	10.9	11.0	10.9	10.8	10.7	10.9	10.8	10.7	10.9	10.7	10.9	11.0	11.1	10.8	11.0	10.7	9.4	10.7	11.6		
maltose	26.1	26.5	26.3	25.8	26.2	25.6	25.8	26.2	26.3	26.0	26.1	25.7	26.2	26.2	26.0	25.5	25.9	25.7	26.7	25.4	26.8	29.6	22.9	24.0	31.4		
maltotetraose	89.6	88.4	88.8	90.6	89.4	91.4	90.6	89.3	89.1	90.1	89.6	91.2	89.2	89.2	90.0	91.9	90.4	91.2	87.5	92.0	87.2	79.0	102.3	97.5	74.5		
maltotriose	71.0	69.7	68.6	70.9	68.5	70.7	71.0	70.1	69.3	70.4	68.8	71.5	70.0	69.4	68.5	71.1	69.4	72.9	66.6	73.9	77.2	54.1	73.4	91.6	57.9		
lipid																											
glycerol	5.1	5.0	4.9	5.1	4.9	5.0	5.1	5.0	4.9	5.0	4.9	5.1	5.0	5.0	4.9	5.1	5.0	5.2	4.8	5.3	5.5	3.9	5.2	6.5	4.1		
glycerol 3-phosphate (G3P)	5.0	4.9	4.9	5.0	5.0	5.1	5.0	5.0	5.0	5.0	5.0	5.1	5.0	5.0	5.0	5.1	5.0	5.1	4.9	5.1	4.8	4.4	5.7	5.4	4.1		
cholesterol	4.1	4.0	3.9	4.1	3.9	4.0	4.1	4.0	4.0	4.0	3.9	4.1	4.0	4.0	3.9	4.1	4.0	4.2	3.8	4.2	4.4	3.1	4.2	5.2	3.3		
7-beta-hydroxycholesterol	32.9	32.4	32.6	33.2	32.8	33.5	33.2	32.7	32.7	33.0	32.9	33.4	32.7	32.7	33.0	33.7	33.2	33.4	32.1	33.7	32.0	29.0	37.5	35.8	27.3		
lathosterol	22.9	22.6	22.7	23.2	22.8	23.4	23.1	22.8	22.8	23.0	22.9	23.3	22.8	22.8	23.0	23.5	23.1	23.3	22.4	23.5	22.3	20.2	26.1	24.9	19.0		
oleate (18:1n9)	13.9	13.8	13.8	14.1	13.9	14.2	14.1	13.9	13.9	14.0	13.9	14.2	13.9	13.9	14.0	14.3	14.1	14.2	13.6	14.3	13.6	12.3	15.9	15.2	11.6		
palmitate (16:0)	35.0	45.0	40.0	27.0	40.0	56.0	40.0	35.0	29.0	61.0	23.0	34.0	45.0	45.0	35.0	39.0	41.0	40.0	47.0	32.0	60.0	61.0	34.0	42.0	37.0		
caproate (6:0)	117.5	119.5	118.7	119.5	117.6	116.9	117.9	119.0	118.9	119.4	117.9	118.9	120.0	120.0	117.5	116.9	115.4	118.6	116.0	119.8	136.4	120.0	110.8	133.8	133.8		
heptanoate (7:0)	7.0	6.9	6.9	7.0	7.0	7.1	7.0	6.9	6.9	7.0	7.0	7.1	6.9	6.9	7.0	7.1	7.0	7.1	6.8	7.2	6.8	6.1	8.0	7.6	5.8		
Nucleotide																											
inosine	6.0	5.9	5.9	6.0	6.0	6.1	6.0	6.0	5.9	6.0	6.0	6.1	5.9	6.0	6.1	6.0	6.1	6.0	6.1	5.8	6.1	5.8	5.3	6.8	6.5	5.0	
adenosine	4.0	3.9	3.9	4.0	4.0	4.1	4.0	4.0	4.0	4.0	4.0	4.1	4.0	4.0	4.0	4.1	4.0	4.1	3.9	4.1	3.9	3.5	4.5	4.3	3.3		
guanosine	30.9	30.5	30.6	31.2	30.8	31.5	31.2	30.7	30.7	31.0	30.9	31.4	30.7	30.7	31.0	31.7	31.1	31.4	30.2	31.7	30.0	27.2	35.2	33.6	25.7		
cytidine	25.9	25.5	25.7	26.2	25.8	26.4	26.2	25.8	25.7	26.0	25.9	26.3	25.8	25.8	26.0	26.6	26.1	26.3	25.3	26.6	25.2	22.8	29.6	28.2	21.5		