

**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  $\mu\text{M}$  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	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		
	fructose-6-phosphate	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		
	glucose	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		
	pyruvate	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	11.0	11.1	10.8	11.0	10.7	9.4	10.7	11.6	11.6			
	lactate	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		
	maltose	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		
	maltotetraose	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		
	maltotriose	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		
	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		
	Lipid	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	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		