

## Supplementary Materials: In Vitro Investigations of Human Bioaccessibility from Reference Materials Using Simulated Lung Fluids

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**Table S1.** Bioaccessibility values (%; mean  $\pm$  SD;  $n = 3$ ) of metallic elements in BCR-723 obtained through the four lung fluid extractions according to the four solid-to-liquid (S/L) ratios.

S/L Ratios	Ba	Cd	Co	Cr	Cu	Mn	Ni	Pb	Sr	Zn
PBS										
1/1000	0.6 $\pm$ 0.1	<LD	3.6 $\pm$ 3.5	0.4 $\pm$ 0.1	9.8 $\pm$ 0.8	0.1 $\pm$ 0.0	2.5 $\pm$ 0.5	<LD	9.0 $\pm$ 0.3	1.0 $\pm$ 0.0
1/2000	0.1 $\pm$ 0.0	<LD	8.2 $\pm$ 4.4	0.4 $\pm$ 0.0	8.9 $\pm$ 2.2	0.8 $\pm$ 0.0	1.5 $\pm$ 0.3	<LD	20.2 $\pm$ 1.2	2.1 $\pm$ 0.2
1/5000	0.5 $\pm$ 0.3	<LD	14.0 $\pm$ 6.0	0.8 $\pm$ 0.5	4.1 $\pm$ 1.5	0.9 $\pm$ 0.0	<LD	<LD	22.1 $\pm$ 1.2	6.8 $\pm$ 0.8
1/10,000	1.1 $\pm$ 0.5	<LD	16.0 $\pm$ 4.0	1.6 $\pm$ 1.4	1.0 $\pm$ 0.0	1.3 $\pm$ 0.1	<LD	<LD	24.2 $\pm$ 2.2	12.6 $\pm$ 0.6
Gamble										
1/1000	<LD	<LD	9.8 $\pm$ 0.1	0.8 $\pm$ 0.1	49.3 $\pm$ 2.1	0.5 $\pm$ 0.1	6.2 $\pm$ 0.8	<LD	15.7 $\pm$ 0.8	2.7 $\pm$ 2.0
1/2000	8.4 $\pm$ 0.3	<LD	11.8 $\pm$ 1.8	0.8 $\pm$ 0.3	54.4 $\pm$ 3.4	1.3 $\pm$ 0.0	7.1 $\pm$ 0.4	1.7 $\pm$ 0.8	18.6 $\pm$ 0.4	30.8 $\pm$ 0.3
1/5000	13.6 $\pm$ 0.4	<LD	8.2 $\pm$ 0.0	0.5 $\pm$ 0.3	49.9 $\pm$ 5.6	1.7 $\pm$ 0.0	0.8 $\pm$ 0.0	7.8 $\pm$ 0.6	18.5 $\pm$ 0.4	44.6 $\pm$ 0.8
1/10,000	19.8 $\pm$ 6.3	<LD	<LD	0.5 $\pm$ 0.1	56.3 $\pm$ 4.9	2.8 $\pm$ 0.7	5.9 $\pm$ 0.0	12.3 $\pm$ 3.6	19.8 $\pm$ 0.1	57.7 $\pm$ 0.8
Modified Gamble										
1/1000	1.0 $\pm$ 0.3	26.5 $\pm$ 1.9	16.0 $\pm$ 4.9	1.3 $\pm$ 0.8	51.5 $\pm$ 0.7	0.4 $\pm$ 0.1	6.7 $\pm$ 1.0	1.0 $\pm$ 0.5	28.5 $\pm$ 2.2	3.0 $\pm$ 1.7
1/2000	7.7 $\pm$ 3.5	17.1 $\pm$ 15.4	22.1 $\pm$ 3.9	1.2 $\pm$ 0.2	51.7 $\pm$ 5.4	1.2 $\pm$ 0.2	6.3 $\pm$ 0.8	3.8 $\pm$ 2.2	45.8 $\pm$ 1.7	27.2 $\pm$ 5.9
1/5000	16.2 $\pm$ 4.5	79.4 $\pm$ 14.4	24.9 $\pm$ 6.4	0.9 $\pm$ 0.8	51.4 $\pm$ 7.2	1.8 $\pm$ 0.1	1.1 $\pm$ 0.0	11.9 $\pm$ 4.8	66.7 $\pm$ 18.6	42.0 $\pm$ 6.3
1/10,000	21.9 $\pm$ 2.3	95.0 $\pm$ 0.1	29.6 $\pm$ 7.4	1.9 $\pm$ 0.7	63.0 $\pm$ 5.1	2.0 $\pm$ 0.0	<LD	22.1 $\pm$ 11.4	85.5 $\pm$ 3.6	53.9 $\pm$ 1.5
ALF										
1/1000	42.0 $\pm$ 13.7	75.4 $\pm$ 10.2	52.0 $\pm$ 16.8	12.4 $\pm$ 4.6	71.1 $\pm$ 8.8	5.5 $\pm$ 0.2	34.8 $\pm$ 2.3	67.2 $\pm$ 1.8	50.7 $\pm$ 1.8	77.8 $\pm$ 1.8
1/2000	47.5 $\pm$ 19.8	77.4 $\pm$ 8.0	59.7 $\pm$ 27.2	12.7 $\pm$ 5.9	75.6 $\pm$ 4.3	5.6 $\pm$ 0.0	33.8 $\pm$ 0.5	66.4 $\pm$ 0.4	52.8 $\pm$ 0.3	79.2 $\pm$ 0.8
1/5000	35.7 $\pm$ 0.5	81.4 $\pm$ 7.6	39.8 $\pm$ 15.3	8.7 $\pm$ 0.0	65.2 $\pm$ 3.7	5.5 $\pm$ 0.1	24.1 $\pm$ 3.7	62.0 $\pm$ 3.2	56.2 $\pm$ 3.2	76.8 $\pm$ 2.2
1/10,000	39.0 $\pm$ 0.1	74.4 $\pm$ 3.0	51.8 $\pm$ 0.1	8.3 $\pm$ 0.1	75.8 $\pm$ 0.1	5.6 $\pm$ 0.0	47.3 $\pm$ 0.1	59.7 $\pm$ 0.1	63.5 $\pm$ 0.1	74.9 $\pm$ 0.1

LD: Limit of detection; PBS: phosphate-buffered saline; ALF: artificial lysosomal fluid.

**Table S2.** Bioaccessibility values (%; mean  $\pm$  SD;  $n = 3$ ) of metallic elements in NIST 2710a obtained through the four lung fluid extractions according to the four S/L ratios.

S/L Ratios	Ba	Cd	Co	Cr	Cu	Mn	Ni	Pb	Sr	Zn
PBS										
1/1000	<LD	28.9 $\pm$ 10.3	5.9 $\pm$ 1.7	<LD	3.4 $\pm$ 0.4	21.6 $\pm$ 3.0	<LD	<LD	0.2 $\pm$ 0.0	2.1 $\pm$ 0.3
1/2000	<LD	43.8 $\pm$ 6.4	27.5 $\pm$ 12.5	1.4 $\pm$ 1.0	5.9 $\pm$ 0.1	31.9 $\pm$ 1.2	<LD	0.2 $\pm$ 0.0	3.3 $\pm$ 0.1	4.1 $\pm$ 0.4
1/5000	<LD	44.2 $\pm$ 21.2	95.1 $\pm$ 52.7	7.8 $\pm$ 0.0	8.3 $\pm$ 0.2	28.7 $\pm$ 0.4	<LD	0.04 $\pm$ 0.00	2.8 $\pm$ 0.0	6.2 $\pm$ 0.1
1/10,000	<LD	69.7 $\pm$ 11.5	61.9 $\pm$ 0.1	5.5 $\pm$ 0.0	11.7 $\pm$ 3.6	33.1 $\pm$ 8.8	<LD	0.1 $\pm$ 0.1	<LD	8.6 $\pm$ 2.0
Gamble										
1/1000	<LD	56.8 $\pm$ 9.0	<LD	<LD	55.3 $\pm$ 4.2	33.0 $\pm$ 2.3	<LD	2.3 $\pm$ 0.3	1.3 $\pm$ 0.6	13.7 $\pm$ 2.2
1/2000	<LD	61.9 $\pm$ 10.4	<LD	<LD	52.1 $\pm$ 3.0	37.3 $\pm$ 1.8	<LD	3.7 $\pm$ 0.2	0.8 $\pm$ 0.0	18.0 $\pm$ 0.9
1/5000	<LD	86.0 $\pm$ 2.8	<LD	<LD	47.6 $\pm$ 1.4	40.1 $\pm$ 0.7	<LD	7.9 $\pm$ 0.4	0.8 $\pm$ 0.2	23.7 $\pm$ 0.1
1/10,000	<LD	82.7 $\pm$ 16.1	<LD	<LD	62.4 $\pm$ 1.4	56.9 $\pm$ 12.5	<LD	12.5 $\pm$ 0.6	1.4 $\pm$ 0.1	34.0 $\pm$ 6.8
Modified Gamble										
1/1000	0.1 $\pm$ 0.0	76.1 $\pm$ 2.4	22.9 $\pm$ 23.4	<LD	49.4 $\pm$ 2.9	31.8 $\pm$ 1.7	<LD	2.2 $\pm$ 0.1	7.0 $\pm$ 0.3	13.2 $\pm$ 1.0
1/2000	0.3 $\pm$ 0.1	77.3 $\pm$ 0.1	32.5 $\pm$ 0.1	<LD	47.4 $\pm$ 2.0	36.6 $\pm$ 1.6	<LD	3.8 $\pm$ 0.1	13.9 $\pm$ 1.4	18.6 $\pm$ 0.4
1/5000	1.0 $\pm$ 0.0	97.2 $\pm$ 11.7	47.5 $\pm$ 0.1	<LD	39.4 $\pm$ 2.2	41.3 $\pm$ 2.0	<LD	7.1 $\pm$ 1.5	35.0 $\pm$ 1.1	25.5 $\pm$ 0.4
1/10,000	1.4 $\pm$ 2.0	88.1 $\pm$ 0.1	55.6 $\pm$ 25.8	<LD	36.9 $\pm$ 4.9	40.9 $\pm$ 2.2	<LD	11.8 $\pm$ 1.1	46.7 $\pm$ 5.8	25.9 $\pm$ 4.2
ALF										
1/1000	23.2 $\pm$ 0.4	94.4 $\pm$ 5.1	22.2 $\pm$ 9.3	<LD	62.0 $\pm$ 0.6	43.4 $\pm$ 1.6	<LD	51.4 $\pm$ 1.1	2.9 $\pm$ 0.3	36.7 $\pm$ 1.6
1/2000	24.9 $\pm$ 0.9	93.5 $\pm$ 5.8	32.3 $\pm$ 22.9	<LD	61.2 $\pm$ 1.8	43.1 $\pm$ 1.2	<LD	55.0 $\pm$ 1.4	2.6 $\pm$ 0.5	36.1 $\pm$ 0.7
1/5000	25.3 $\pm$ 0.4	85.3 $\pm$ 8.4	35.1 $\pm$ 0.0	<LD	59.7 $\pm$ 1.4	44.3 $\pm$ 0.2	<LD	55.0 $\pm$ 0.5	2.3 $\pm$ 0.5	35.3 $\pm$ 0.1
1/10,000	26.8 $\pm$ 0.0	89.4 $\pm$ 0.1	36.5 $\pm$ 0.1	<LD	61.8 $\pm$ 0.3	45.7 $\pm$ 0.1	<LD	56.1 $\pm$ 0.1	3.1 $\pm$ 0.1	35.9 $\pm$ 0.1

**Table S3.** Bioaccessibility values (%; mean  $\pm$  SD;  $n = 3$ ) of metallic elements in NIST 1648a obtained through the four lung fluid extractions according to the four S/L ratios.

S/L Ratios	Ba	Cd	Co	Cr	Cu	Mn	Ni	Pb	Sr	Zn
PBS										
1/1000	<LD	9.1 $\pm$ 0.5	9.5 $\pm$ 3.7	0.4 $\pm$ 0.1	9.6 $\pm$ 0.4	7.4 $\pm$ 0.3	6.6 $\pm$ 1.8	<LD	14.1 $\pm$ 0.5	0.7 $\pm$ 0.0
1/2000	<LD	15.4 $\pm$ 1.5	8.2 $\pm$ 0.9	0.6 $\pm$ 0.3	11.4 $\pm$ 1.0	13.5 $\pm$ 0.5	5.6 $\pm$ 2.6	<LD	16.5 $\pm$ 0.6	2.0 $\pm$ 0.1
1/5000	<LD	24.1 $\pm$ 6.2	3.3 $\pm$ 0.0	1.3 $\pm$ 0.4	7.3 $\pm$ 1.8	16.4 $\pm$ 1.4	<LD	<LD	29.0 $\pm$ 23.8	4.3 $\pm$ 0.2
1/10,000	<LD	29.6 $\pm$ 1.2	8.9 $\pm$ 0.1	1.8 $\pm$ 0.3	8.4 $\pm$ 4.5	23.0 $\pm$ 0.9	<LD	<LD	32.1 $\pm$ 2.2	7.1 $\pm$ 0.1
Gamble										
1/1000	<LD	11.0 $\pm$ 2.0	16.5 $\pm$ 5.9	1.4 $\pm$ 0.4	52.0 $\pm$ 13.2	8.5 $\pm$ 2.8	26.7 $\pm$ 8.8	0.4 $\pm$ 0.1	15.8 $\pm$ 0.7	4.3 $\pm$ 1.3
1/2000	<LD	34.2 $\pm$ 7.5	17.4 $\pm$ 4.0	1.8 $\pm$ 0.5	51.9 $\pm$ 6.1	23.4 $\pm$ 2.4	18.9 $\pm$ 0.9	2.6 $\pm$ 0.1	32.0 $\pm$ 9.2	25.4 $\pm$ 0.4
1/5000	<LD	45.2 $\pm$ 4.0	38.8 $\pm$ 4.3	2.7 $\pm$ 1.0	49.9 $\pm$ 2.7	29.6 $\pm$ 0.2	3.3 $\pm$ 1.2	9.1 $\pm$ 0.9	31.5 $\pm$ 0.9	43.2 $\pm$ 0.2
1/10,000	<LD	49.7 $\pm$ 2.1	56.7 $\pm$ 2.0	3.7 $\pm$ 0.0	45.7 $\pm$ 11.6	29.4 $\pm$ 5.4	<LD	16.3 $\pm$ 0.4	37.4 $\pm$ 0.1	49.2 $\pm$ 6.9
Modified Gamble										
1/1000	0.1 $\pm$ 0.0	15.2 $\pm$ 0.4	26.7 $\pm$ 5.4	1.4 $\pm$ 0.1	46.0 $\pm$ 2.7	12.2 $\pm$ 0.6	22.2 $\pm$ 2.1	0.9 $\pm$ 0.1	28.2 $\pm$ 2.5	7.0 $\pm$ 0.5
1/2000	0.4 $\pm$ 0.1	33.2 $\pm$ 1.8	34.9 $\pm$ 11.9	1.9 $\pm$ 0.5	48.4 $\pm$ 1.7	22.4 $\pm$ 0.6	18.2 $\pm$ 3.6	3.1 $\pm$ 0.0	40.9 $\pm$ 1.7	27.3 $\pm$ 0.4
1/5000	2.4 $\pm$ 0.5	50.7 $\pm$ 3.1	56.5 $\pm$ 6.9	2.4 $\pm$ 0.2	44.0 $\pm$ 0.4	28.1 $\pm$ 0.8	<LD	11.2 $\pm$ 0.5	68.9 $\pm$ 1.4	43.0 $\pm$ 1.2
1/10,000	2.3 $\pm$ 0.3	64.9 $\pm$ 16.0	74.8 $\pm$ 8.5	2.5 $\pm$ 0.9	53.3 $\pm$ 4.7	33.4 $\pm$ 1.4	<LD	16.3 $\pm$ 3.9	41.9 $\pm$ 1.2	55.3 $\pm$ 3.5
ALF										
1/1000	38.9 $\pm$ 1.2	69.9 $\pm$ 2.0	33.9 $\pm$ 2.1	8.9 $\pm$ 0.5	57.5 $\pm$ 1.6	45.9 $\pm$ 0.6	30.9 $\pm$ 1.8	74.0 $\pm$ 2.8	51.0 $\pm$ 3.6	67.4 $\pm$ 2.1
1/2000	46.7 $\pm$ 1.8	68.4 $\pm$ 3.8	40.6 $\pm$ 9.6	8.5 $\pm$ 0.6	52.6 $\pm$ 3.7	45.2 $\pm$ 2.5	25.2 $\pm$ 5.7	72.3 $\pm$ 2.6	49.9 $\pm$ 4.1	65.7 $\pm$ 2.8
1/5000	52.8 $\pm$ 1.9	65.6 $\pm$ 5.5	35.0 $\pm$ 16.5	8.7 $\pm$ 0.9	55.0 $\pm$ 1.1	46.8 $\pm$ 2.6	12.2 $\pm$ 4.1	75.9 $\pm$ 2.2	50.9 $\pm$ 3.2	66.2 $\pm$ 2.3
1/10,000	52.7 $\pm$ 1.9	72.2 $\pm$ 6.4	52.9 $\pm$ 45.1	7.0 $\pm$ 0.9	52.7 $\pm$ 3.1	46.1 $\pm$ 1.3	<LD	76.0 $\pm$ 2.3	52.8 $\pm$ 2.7	66.1 $\pm$ 1.9



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