Table S1. Study design and metabolomic data description for all analyzed datasets.

Dataset	Organism and site	Study type	Data used	# samples	# subjects	# metabolites	# KEGG metabolites	# analyzed metabolites	Ref
1	Human, vagina	Case-control (BV)	16S qPCR, metabolomics	67 (42/25/0)[*]	59 (40/23/0)[*]	279	197	82	(22)
2	Human, vagina	Case-control (BV)[a]	16S sequencing, targeted metabolomics	70 (40/20/10)[*]	70 (40/20/10)[*]	101	96	58	(22)
3	Mouse, gut	Perturbation (antibiotics)	16S sequencing, metabolomics	29		480	297	116	(23)
4	Human, gut (fecal)	Case-control (CD)[b]	Shotgun sequencing, metabolomics	12		1113	136	31	(15, 40)
E. coli	*E. coli* cultures	Perturbation (stress)[c]	Microarray, metabolomics	28		196	87	42	(44)

[*] (BV+/BV-/ intermediate)
[a] Bacterial vaginosis with intermediate samples
[b] Twins discordant and concordant for Crohn's disease
[c] E. coli cultures treated with heat, cold, oxidative stress, glucose-lactose shift