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Supplementary information

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Host metabolism can produce many indoles and phenols independently of the microbiome

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Metabolite name	Standard RT (min)	Sample RT (min)	Ion	Measured m/z	Matching fragment m/z in MS/MS
Indole-3-pyruvic acid	2.6	2.6	[M-H]-	202.051	73.029; 158.0603
Indole-3-lactic acid	4.74	4.74	[M-H]-	204.0666	72.9931; 116.0506; 128.0505; 130.0663; 158.0611; 186.0560
Indole-3-acetate	2.74	2.74	[M-H]-	174.06	130.0696
Indole-3-carboxylic acid	3.24	3.24	[M-H]-	160.0404	116.0506
Indole-3-propionic acid	4.73	4.73	[M-H]-	188.0717	59.0138; 116.0506; 142.0663
Indole sulfate	2.15	2.15	[M-H]-	212.0023	79.9574; 80.9652; 92.0507; 120.0454; 132.0457; 203.0854
Phenylpyruvate	2.38	2.38	[M-H]-	163.04	91.0553; 120.045; 135.0453
Phenyllactate	2.62	2.62	[M-H]-	165.06	72.9931; 91.0553; 119.0503; 147.0452
Cinnamic acid	4.3	4.3	[M-H]-	147.0452	119.0506; 57.0347
Benzoic acid	2.73	2.73	[M-H]-	121.03	No fragments detected
3-Phenylpropionic acid	2.47	2.47	[M-H]-	149.0609	101.0243; 105.0710
Hydroxyphenyllactate	2.77	2.77	[M-H]-	181.0506	135.0451; 163.0405
Phenol sulfate	2.07	2.07	[M-H]-	172.9914	79.9573; 93.0345; 109.0295
Cresol sulfate	2.08	2.08	[M-H]-	187.01	107.0502

Supplementary Table 1: Spectral data for indole and phenol metabolites as measured by Orbitrap Exploris 240 mass spectrometer

Name	Q1 (m/z)	Q3 (m/z)	Retention Time
Tryptophan	205.1	188	5.112
^{13}C11-Tryptophan	216.14	199.1	5.112
Indole-3-lactic acid	206.1	130	6.14
Indole-3-acetic acid	176.1	137	6.8
Indole-3-propionic acid	190.1	130	7.27
Melatonin	233.1	174	7.26
D3-Melatonin	236.15	174	7.26

Supplementary Table 2: Spectral data for indole metabolites via targeted analysis on Agilent 6470 triple quadrupole mass spectrometer

Compound	CAS	[M-H]-	RT on IQX
Phenylpyruvate	156-06-9	163.0408	4.07
Phenyllactate	20312-36-1	165.0563	4.60
Hydroxyphenyllactate	306-23-0	181.0512	2.92
Cresol sulfate	3233-58-7	187.0076	4.09
Indole-3-carboxylic acid	771-50-6	160.0410	4.99

Supplementary Table 3: Spectral data for phenol metabolites via targeted analysis on Orbitrap IQ-X mass spectrometer