

Supplementary Materials: Article

Untargeted Metabolite Profiling for Screening Bioactive Compounds in Digestate of Manure under Anaerobic Digestion

Jiaxin Lu, Atif Muhmood, Wojciech Czekala, Jakub Mazurkiewicz, Jacek Dach and Renjie Dong

Table S1. The shared significant features from paired-comparison between manures and digestates.

Atomic Number (z)	Retention Time (min)	Mass Accuracy	Compounds	Data Base (Metlin)
241.2	39.87	0	Sodium pantothenate	317283
248.3	38.65	0	6-azido-N-ethyl-N'-methyl-1,3,5-Triazine-2,4-diamine	446410
104.2	46.75	2	1-Pentanethiol	88476
102.1	15.85	6	1-Norbornyllithium	341945
164.1	38.65	0	N-Methyl-4-phenylbutan-1-amine--hydrogen chloride	270195
385.4	48.97	2	2,4,6-Trioctyl-1,3,5,2,4,6-trioxatriborinane	835524
231.2	46.75	3	2-(Azocan-1-yl)-N,N-diethylethan-1-amine--hydrogen chloride (1/1)	788429
221.1	39.04	0	Propionic acid, 3-((2,3,5,6-tetramethylphenyl)thio)-	380677
315.3	46.77	1	Octanamide, N-[2-[[2-[(2-aminoethyl)amino]ethyl]amino]ethyl]-	374577
71.1	15.85	2	(Ethyne-1,2-diyl)bis(dimethylborane)	854286
130.1	21.27	2	1-Pentanamine, hydrofluoride	637280
131.1	21.26	1	(Trimethylsilyl)methyl isocyanide	331308
162.1	46.75	1	N,N-Dimethyl-2-(1H-pyrazol-1-yl)ethan-1-amine	272493
430.4	46.89	1	Octadecanamide, N-[2-[(2-aminoethyl)amino]ethyl]-, monoacetate	378459
232.2	47.57	1	Esaprazole	314167
231.2	48.96	3	2-(Azocan-1-yl)-N,N-diethylethan-1-amine--hydrogen chloride (1/1)	788429
231.2	47.59	3	2-(Azocan-1-yl)-N,N-diethylethan-1-amine--hydrogen chloride (1/1)	788429
96.1	32.54	1	Dimethylaminoethanol	265670
190.2	17.23		heptyl(trimethyl)silane	545122
85.1	17.99	6	Lithium, bicyclo[2.2.1]hept-1-yl-	341945
203.2	46.76	1	2-[(2-[2-(Dimethylamino)ethyl](methyl)amino)ethyl](methyl)amino]ethan-1-ol	770923
163.1	24.21	0	Ethyl N,N,N',N'-tetramethyldiamidophosphate	345898
191.8	35.01	5	Vanadium--yttrium (2/1)	959761
127.9	35	4	Arsenic monoxide monochloride	428853
255.8	35.01	3	Dibromonitromethane	269303
55.1	32.3	36	lithium; azanide; boron	609818
64	35	15	Allyl isothiocyanate	73027
71.1	36.05	2	(Ethyne-1,2-diyl)bis(dimethylborane)	854286
221.1	41.23	0	Propionic acid, 3-thio-2,3,5,6-tetramethylphenyl	380677
84.1	30.61	1	Trimethylamine, hydrate	435419

Mass accuracy value <10 is validated to efficiently capture data points to describe chromatographic peak.

Table S2. Metabolic pathways involved in the formation of bioactive compounds during anaerobic digestion of chicken, cow and pig manure.

Metabolic Pathway	No.	Fisher's P	EASE	Metabolites	Bioactivity
Chicken manure digestate					
Tryptophan metabolism	22	0.532	0.83	Tetrahydrobiopterin Tryptamine Serotonin	Vitamins and Cofactors Indole alkaloids derived from tryptophan and anthranilic acid
Linoleate metabolism	6	0.390	1	Azelaic acid Nonionic acid	Fatty Acids and Conjugates
Hexose phosphorylation	3	0.217	1	Sorbitol	Carbohydrates
Vitamin B5 - CoA biosynthesis from pantothenate	2	0.150	1	D-Glucosamine; L-Cysteine Pantothenate	Amino sugars, anti-inflammatory, Peptides, Cysteine Vitamins and Cofactors
Androgen and estrogen biosynthesis and metabolism	18	0.781	1	19-Hydroxy testosterone 19-Hydroxy androstenedione	Steroids derivatives ,Hormones, Steroids derivatives, Sterol Lipids.
Vitamin B9 (folate) metabolism	4	0.280	1	Serine	Peptides, Serine
CoA Catabolism	1	0.078	1	Pantothenate	Vitamins and Cofactors
Pyrimidine metabolism	7	0.439	1	Thymidine L-Asp L-Arg	Nucleic acids Peptides, Aspartic acid Peptides, Arginine
Aspartate and asparagine metabolism	18	0.781	1	L-Orniyhine L-Cysteine L-Cysteine	Peptides, L-Ornithine Peptides, Cysteine Peptides, Cysteine
Tyrosine metabolism	18	0.781	1	L-Adrenaline N-Methyltyramine Tetrahydrobiopterin	Adrenaline, anti-aging Alkaloids derived from tyrosine Vitamins and Cofactors
C21-steroid hormone biosynthesis and metabolism	9	0.526	1	5beta-Cholestane-26-tetrol Estrone	Sterol Lipids, Bile acids derivatives Steroid hormones, Terpenoids derivatives
Cow manure digestate					
Hexose phosphorylation	3	0.145	1	Sorbitol	Carbohydrates
Vitamin E metabolism	3	0.145	1	Vitamin E	Vitamins and Cofactors
Glycerophospholipid metabolism	5	0.231	1	L-Adrenaline DHA	Adrenaline, anti-aging Steroid derivatives hormones
C21-steroid hormone biosynthesis and metabolism	13	0.505	1	Cortodoxone Corticosterone	Steroid derivatives hormones Steroid derivatives hormones
Swine manure digestate					
Lysine degradation	7	0.374	1	Citrulline L-Arg	Peptides, L-Citrulline Peptides, Arginine (Arg)
Arginine and proline metabolism	13	0.584	1	L-Ornithine L-Adrenaline	Peptides-Ornithine Adrenaline, anti-aging

Table Table S2 . Cont.

Tyrosine metabolism	7	0.374	1	Acetoacetate	Fatty Acids and Conjugates
				4-Oxobutanoate	Organic acids, Carboxylic acids
				Tryptamine	Indole alkaloids
				Serotonin	Indole alkaloids
Tryptophan metabolism	14	0.612	1	Vitamin L1	Anthranilate
				Indole acetic acid	Indole alkaloids
				Pantothenate	Vitamins and Cofactors
beta-Alanine metabolism	3	0.182	1	Carosine	Peptides, Dipeptides
				L-Arg	Peptides, Arginine (Arg)
				L-Ornithine	Peptides, L-Ornithine
D-Arginine and D-ornithine metabolism	6	0.330	1	D-Arginine	Peptides, D-Arginine
				2-Ketovaline	Organic acids, Carboxylic acids
Pantothenate and CoA biosynthesis	2	0.124	1	Pantothenate	Vitamins and Cofactors

Fisher's $P > 0.05$ means significant.

© 2019 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).