Supplementary Table 1. Untargeted metabolites identified in CCCU (cow urine extract of *C. citratus*) by LC-MS/MS

Ionization mode	Relative intensity %	M/Z	Compound name	Chemical class
[M-H]-	14.61	197.01	syringic acid	Phenolic acid
[M-H]-	44.36	198.96	gallocatechin	Flavan-3-ol
[M-H]-	33.65	298.36	kaempferide	Flavonol
[M-H]-	15.83	250.36	derivatives of hydroxybenzoic acids	Phenolic acids
[M-H]-	6.66	299.31	diosmetin-7-O-rutinoside	Flavonoid
[M-H]-	100	312.36	diosmetin-6,8-di-C-glucoside, a flavonoid	Flavonoid
[M-H]-	23.77	313.31	apigenin 6-C-glucoside, a flavone	Flavonoid
[M-H]-	9.62	314.26	caffeoyl quinic acids	Hydroxycinnamic acid derivatives
[M-H]-	76.25	326.41	p-hydroxy phenylacetic acid	Phenolic acid
[M-H]-	18.79	327.36	luteolin-8-C-β-D-glucopyranoside	Flavonoid
[M-H]-	8.92	331.96	caffeic acid derivative	Phenolic acid
[M-H]-	26.13	556.31	phospholipids	Lipid
[M-H]-	8.92	331.96	caffeic acid derivative	Phenolic acid
[M+H]+	5.32	184.19	3-O-methylgallic acid	Phenolic acid
[M+H]+	29.08	208.24	sinapic acid	Phenolic acid
[M+H]+	17.06	209.24	zingerone	Phenolic ketone
[M+H]+	42.19	211.29	heroin	Alkaloid
[M+H]+	12.01	218.24	protocatechuic acid	Phenolic acid
[M+H]+	13.95	224.19	sinapoyl-hexoside	Phenolic glycoside
[M+H]+	13.98	227.24	myricitrin	Flavonol glycoside
[M+H]+	11.75	229.29	furanocoumarins	Phenolic compounds
[M+H]+	10.51	334.29	gibberellic acid	Diterpenoid
[M+H]+	5.06	356.29	feruloylglycoside	Phenolic glycoside
[M+H]+	42.23	387.34	luteolin-7-O-rutinoside	Flavonoid
[M+H]+	12.87	388.34	3-galloylquinic acid	Phenolic acid derivative
[M+H]+	72.46	431.34	3-methoxynobiletin	Flavonoid
[M+H]+	19.54	432.34	kaempferol 3-O-rhamnoside	Flavonoid
[M+H]+	16.29	452.29	catechin 3-O-glucoside	Flavonoid
[M+H]+	25.03	476.39	hesperetin 30-O-glucuronide	Flavonoid

[M+H]+	13.66	480.34	myricetin 3-O-glucoside	Flavonoid
[M+H]+	6.88	505.39	quercetin acetyl hexose	Flavonoid
[M+H]+	32.54	607.44	diosmetin C hexoside deoxyhexoside	Flavonoid
[M+H]+	9	608.44	rutin	Flavonol glycoside
[M+H]+	5.25	716.44	salvianolic acid	Polyphenol

Supplementary Table 2. Untargeted metabolites identified in CCW (water extract of *C. citratus*) by LC-MS/MS

Ionization mode	**Relative intensity %**	**M/Z**	**Compound name**	**Chemical class**
[M-H]-	13.92	161.96	umbelliferone	Coumarin
[M-H]-	11.46	164.01	p-hydroxybenzoic acid	Phenolic acid
[M-H]-	19.04	166.06	3-O-galloyl quinic acid	Phenolic acid derivative
[M-H]-	6.89	168.16	gallic acid	Phenolic acid
[M-H]-	9.41	172.11	2-chloro-1,4-dimethoxybenzene.	Aromatic compound
[M-H]-	5.2	174.11	dehydroascorbic acid	Organic acid
[M-H]-	19.68	182.11	syringic acid fragment	Phenolic acid
[M-H]-	10.93	183.21	fragment of phenolic or hydroxyl groups	Phenolic fragment
[M-H]-	58.38	198.96	8-O-methyl-11-deoxy alkannin	Naphthoquinone
[M-H]-	37.6	201.01	4-hydroxybenzoic acid 4-O-glucoside	Phenolic glycoside
[M-H]-	8.98	202.96	phenolic acid fragments	Phenolic fragment
[M-H]-	12.35	228.11	fragment of kaempferol	Flavonol fragment
[M-H]-	12.65	238.11	3-0-feruloylquinic acid II	Phenolic acid derivative
[M-H]-	8.46	256.06	fragment of kaempferol	Flavonol fragment
[M-H]-	6.25	270.96	apigenin	Flavone
[M-H]-	9.19	272.91	naringenin	Flavanone
[M-H]-	8.91	286.01	luteolin	Flavone
[M-H]-	5.05	288.11	kaempferol	Flavonol
[M-H]-	41.44	298.36	kaempferide	Flavonol
[M-H]-	10.58	299.31	sativanone	Isoflavone
[M-H]-	6.5	300.16	ellagic acid	Polyphenol
[M-H]-	6.26	302.06	quercetin	Flavonol
[M-H]-	13.3	308.01	caffeoyl derivative (caffeoyl-hexose-deoxyhexoside)	Phenolic acid derivative
[M-H]-	100	312.36	diosmetin-6,8-di-C-glucoside	Flavone glycoside
[M-H]-	22.57	313.36	apigenin 6-C-glucoside	Flavone glycoside
[M-H]-	13.65	314.21	caffeoyl quinic acids	Phenolic acid

				derivative
[M-H]-	36.35	326.41	p-hydroxyphenylacetic acid	Phenolic acid
[M-H]-	27.52	331.96	carnosic acid	Diterpenoid
[M-H]-	10.73	334.11	gibberellic acid	Diterpenoid
[M-H]-	8.57	353.91	chlorogenic acid	Phenolic acid derivative
[M-H]-	7.31	356.01	feruloylglycoside	Phenolic glycoside
[M-H]-	14.14	369.96	ferulic acid 4-O-glucuronide	Phenolic acid derivative
[M-H]-	6.69	449.91	myricetin 3-O-arabinoside	Flavonol glycoside
[M-H]-	10.92	467.91	4"-O-methylepigallocatechin	Flavan-3-ol derivative
[M-H]-	10.58	505.81	quercetin acetyl hexose	Flavanol glycoside
[M+H]+	6.7	152.19	citral	Terpenoid
[M+H]+	5.71	168.14	gallic acid	Phenolic acid
[M+H]+	16.13	180.09	phenolic acids	Phenolic acid
[M+H]+	6.25	205.19	alpha-1-cadinene	Sesquiterpene
[M+H]+	14.7	216.14	hydroxylated derivatives	Hydroxylated compounds
[M+H]+	9.49	272.24	naringenin	Flavanone
[M+H]+	6.52	288.19	phlorin	Phenolic glycoside
[M+H]+	11.61	300.19	isokaempferide	Flavonol
[M+H]+	20.34	317.24	6,8-dihydroxykaempferol	Flavonol
[M+H]+	9.96	344.84	rosmanol	Diterpenoid
[M+H]+	17.18	378.34	caffeic acid dimer	Phenolic acid derivative
[M+H]+	32.88	387.34	luteolin-7-O-rutinoside	Flavone glycoside
[M+H]+	10.75	388.49	3-galloylquinic acid	Phenolic acid derivative
[M+H]+	47.22	431.34	3-methoxynobiletin	Flavone
[M+H]+	16.69	432.29	kaempferol 3-O-rhamnoside	Flavonol glycoside
[M+H]+	42.24	452.24	Catechin 3-O-glucoside	Flavan-3-ol glycoside
[M+H]+	16.39	476.39	hesperetin 30-O-glucuronide	Flavanone glycoside
[M+H]+	9.5	480.34	myricetin 3-O-glucoside	Flavonol glycoside
[M+H]+	57.42	563.44	apigenin C pentoside hexoside (isoschaftoside)	Flavone glycoside
[M+H]+	47.23	607.44	diosmetin C hexoside deoxyhexoside	Flavone glycoside
[M+H]+	12.64	608.44	rutin	Flavonol glycoside
[M+H]+	16.43	716.44	salvianolic acid	Polyphenol
[M+H]+	6.18	717.49	salvianolic acid	Polyphenol

Supplementary Table 3. Untargeted metabolites identified in LCCU (cow urine extract of *L. camara*) by LC-MS/MS

Ionization	Relative intensity %	M/Z	Compound Name	Chemical class
[M-H]-	16.49	166.11	p-Coumaric acid	Phenolic acid
[M-H]-	7.02	202.96	α-humulene	Monocyclic sesquiterpene
[M-H]-	5.14	226.11	myristoleic acid	Unsaturated fatty acid
[M-H]-	6.64	286.01	kaempferol	Flavonoid
[M-H]-	7.68	298.21	3',4'-dimethoxy-7-hydroxyflavanone	Flavonoid
[M-H]-	5.13	312.36	arachidic acid	Saturated fatty acid
[M-H]-	5.27	314.06	pectolinarigenin	Flavonoid
[M-H]-	11.67	331.96	trihydroxy- dimethoxyflavone	Flavonoid
[M-H]-	5.88	467.96	amyrin	Triterpene
[M-H]-	7.83	552.56	durantoside I	Iridoid glycosides
[M-H]-	12.05	568.56	icterogenin, lantanilic acid, camaric acid	Oleane-type triterpene
[M-H]-	53.15	570.31	lantacin, icterogenin/lantacin	Ursane-type triterpene, Triterpene
[M+H]+	11.8	148.19	cinnamic acid	Aromatic monocarboxylic acid
[M+H]+	12	166.19	p-coumaricacid	Phenolic acid
[M+H]+	9.37	194.19	ferulic acid, isoferulic acid	Phenolic acid
[M+H]+	19.03	202.24	α-humulene	Monocyclic sesquiterpene
[M+H]+	11.38	221.19	copaenol	Sesquiterpene
[M+H]+	40.38	226.19	myristoleic acid	Unsaturated fatty acid
[M+H]+	9.29	244.19	6- methoxy-5-hydroxynaphtho[2,3-b] furan-4,9-dione	Furanonaphthoquinone
[M+H]+	6.57	274.24	afzelechin	Flavonoid
[M+H]+	14.53	286.29	kaempferol	Flavonoid
[M+H]+	23.66	294.24	1-cinnamoyl rhamnoside	Aromatic acid glycoside
[M+H]+	23.8	298.19	3',4'-dimethoxy-7-hydroxyflavanone	Flavonoid
[M+H]+	21.5	300.19	chrysoeriol	Flavonoid
[M+H]+	67.77	304.29	benzalkonium chloride	Ammonium Compound
[M+H]+	22.46	312.29	arachidic acid	Saturated fatty acid
[M+H]+	5.59	314.34	pectolinarigenin	Flavonoid
[M+H]+	9.34	318.29	myricetin, hexahydroxyflavone (gossypetin)	Flavonoid
[M+H]+	5.28	340.29	behenic acid	Saturated fatty acid
[M+H]+	12.93	344.69	penduletin	Flavonoid
[M+H]+	9.34	388.49	geniposide	Iridoid glycosides
[M+H]+	20.98	390.29	8-epiloganin	Iridoid glycosides
[M+H]+	5.55	441.39	momorodol	Triterpene

[M+H]+	19.99	454.39	stigmasterol acetate	Triterpene
[M+H]+	25.55	468.39	3,24-dioxo-12-ursen-28-oic acid	Ursane-type triterpene
[M+H]+	15.73	469.39	pomonic acid	Triterpene
[M+H]+	8.97	470.39	lantic acid	Ursane-type triterpene
[M+H]+	5.87	471.34	camarin	Triterpene
[M+H]+	5.68	472.39	pomolic acid	Ursane-type triterpene
[M+H]+	5.27	473.39	dihydroxyolean-enoic acid	Triterpene
[M+H]+	22.85	476.39	linaroside	Flavonoid
[M+H]+	7.86	477.44	dihydroxy-dimethoxyflavone-O-glucopyranoside (camaroside)	Flavonoid
[M+H]+	5.08	486.39	3,22,24-trihydroxy-12-oleanen-28-oic acid (3β,22β)-form, 3-ketone	Oleane-type triterpene
[M+H]+	6.4	488.44	3,12,13-trihydroxy-28-oleananoic acid (3β,12β,13β)-form, 3-ketone	Oleane-type triterpene
[M+H]+	6.58	500.39	methyl-hydroxylantanolate	Triterpeme
[M+H]+	5.49	512.39	lantanone	Triterpene
[M+H]+	93.59	519.44	lantanoside	Flavonoid
[M+H]+	13.86	541.39	lantadene D	Triterpene
[M+H]+	45.93	552.29	lantadene A	Triterpene
[M+H]+	20.9	553.29	lantadene C	Triterpene
[M+H]+	8.08	554.34	dihydrorehmannic acid	Oleane-type triterpene
[M+H]+	36.23	568.49	lantanilic acid	Oleane-type triterpene
[M+H]+	96.85	570.29	lantacin	Ursane-type triterpene
[M+H]+	7.91	592.24	osmanthuside B	Phenolic acid
[M+H]+	9.67	609.39	lipedoside A	Phenolic acid
[M+H]+	7.51	610.34	isonuomioside A	Phenolic acid
[M+H]+	6.12	647.54	triterpenes glycoside derivative	Triterpene glycoside

Supplementary Table 4. Untargeted metabolites identified in LCW (water extract of *L. camara*) by LC-MS/MS

Ionization	Relative intensity %	M/Z	Compound name	Chemical class
[M-H]-	38.6	148.21	cinnamic acid	Aromatic monocarboxylic acid
[M-H]-	30.87	170.01	gallic acid	Phenolic acid
[M-H]-	7.93	193.66	ferulic acid	Phenolic acid
[M-H]-	8.69	194.91	ferulic acid	Phenolic acid
[M-H]-	16.6	226.26	myristoleic acid	Unsaturated fatty acid
[M-H]-	18.9	257.11	palmitamide	Fatty amide amide
[M-H]-	14.26	291.96	catechin	Flavonoid
[M-H]-	20.38	294.16	1-cinnamoyl rhamnoside	Aromatic acid glycoside
[M-H]-	21.74	304.21	benzalkonium chloride	Ammonium compound
[M-H]-	10.11	312.96	arachidic acid	Saturated fatty acid
[M-H]-	7.91	318.71	myricetin	Flavonoid
[M-H]-	20.17	330.61	cirsiliol	Flavonoid
[M-H]-	38.4	340.61	behenic acid	Saturated fatty acid
[M-H]-	11.91	344.76	penduletin	Flavonoid
[M-H]-	31.12	354.66	chlorogenic acid	Phenolic acid
[M-H]-	23.08	391.06	theveside	Iridoid
[M-H]-	8.69	442.01	catechin gallate	Flavonoid gallic acid ester
[M-H]-	8.69	473.11	dihydrixyolean-enoic acid (hederagenin)	Triterpene
[M-H]-	12.25	486.91	3,22,24-trihydroxy-12-oleanen-28-oic acid; (3β,22β)-form, 3-ketone	Oleane-type triterpene
[M-H]-	8.69	488.31	3,12,13-trihydroxy- 28-oleananoic acid; (3β,12β,13β)-form, 3-ketone	Oleane-type triterpene
[M-H]-	8.69	491.01	carminic acid	Flavonoid
[M-H]-	11.67	529.16	camarinic acid	Triterpene
[M-H]-	8.69	553.41	lantadene C	Triterpene
[M-H]-	8.3	568.46	22-tigloyloxylantanolic acid	Oleane-type triterpene
[M-H]-	8.3	583.26	ursangilic acid	Triterpene
[M-H]-	8.69	589.01	triterpene glycoside derivative	Triterpene glycoside
[M-H]-	26.09	593.31	pheophorbide A	Chlorophyll derivative
[M-H]-	8.3	594.06	apigenin-6,8-di-C-glycoside (vicenin 2)	Flavonoid
[M-H]-	13.04	785.41	triterpene glycoside derivative	Triterpene glycoside
[M-H]-	8.69	901.81	triterpene glycoside derivative	Triterpene glycoside

Supplementary Table 5. Untargeted metabolites identified in MICU (cow urine extract of M. indica) by LC-MS/MS

Ionization	Relative intensity %	M/Z	Compound name	Chemical class
[M-H]-	15.96	163.96	coumaric acid	Phenolic acid
[M-H]-	38.07	166.16	N-alkylamide	Alkamide
[M-H]-	7.09	182.06	methyl gallate	Phenolic acid ester
[M-H]-	11.89	224.11	ellagic acid	Polyphenol
[M-H]-	7.69	501.91	hypericin	Naphthodianthrone
[M+H]+	9.96	152.19	protocatechuic acid	Phenolic acid
[M+H]+	6.07	182.19	methyl gallate	Phenolic esters
[M+H]+	5.74	191.14	quinic acid	Organic acid (cyclitol)
[M+H]+	7.7	197.19	syringic acid	Phenolic acid
[M+H]+	84.43	206.19	epicatechin	Flavan-3-ol
[M+H]+	92.54	208.24	sinapic acid derivative	Phenolic acid derivative
[M+H]+	59.22	210.24	sterols	Lipid (Steroid)
[M+H]+	79.26	211.29	glucosides/glycosides	Glycosides
[M+H]+	12.79	216.19	phloretin-2′-O-glucoside	Flavonoid glycoside
[M+H]+	35.17	218.24	hydroxypyrenes	Phenolic derivative
[M+H]+	12.87	219.24	gallocatechin	Flavan-3-ol
[M+H]+	15.01	220.19	2,3-dihydroxybenzoic acid	Phenolic acid
[M+H]+	21.94	222.19	Methyl stearate	Fatty acid
[M+H]+	47.35	224.19	ellagic acid	Polyphenol
[M+H]+	41.45	225.19	methyl Jasmonate	Oxylipin
[M+H]+	6.2	259.24	bellidin (1,3,5,8-tetrahydroxyxanthone)	Polyphenolic compound
[M+H]+	21.03	271.29	rhamnocitrin	Flavanol
[M+H]+	13.06	272.24	naringenin	Flavanone
[M+H]+	16.06	290.24	catechin	Flavan-3-ol
[M+H]+	26.84	304.24	gallocatechin or epicatechin gallate	Flavan-3-ol
[M+H]+	17.64	317.29	quercetin carboxylic acid	Flavanol derivative
[M+H]+	23.25	387.34	5,8-dihydroxy-6,7,3-trimethoxy-30,40-methylenedioxyflavone	Flavanone derivative
[M+H]+	7.03	434.29	quercetin pentoside	Flavonol glycoside
[M+H]+	12.3	447.44	apigenin 7-O-glucuronide	Flavonoid glycoside

[M+H]+	6.47	448.34	quercetin 3-O-rhamnoside	Flavonol glycoside
[M+H]+	5.8	449.44	rhamnetin hexoside	Flavonol glycoside
[M+H]+	23.05	476.39	reynoutrin	Flavonol glycoside
[M+H]+	96.62	519.39	benzophenones	Aromatic ketone
[M+H]+	28.17	520.39	phospholipid	Lipid

SupplementaryTable 6. Untargeted metabolites identified in MIW (water extract of *M. indica*) by LC-MS/MS

Ionization	Relative intensity %	M/Z	Compound name	Chemical class
[M-H]-	17.22	114.36	N-hydroxy-lysine	Amino acid derivative
[M-H]-	17.22	118.16	indole	Heterocyclic compound
[M-H]-	18.71	131.46	2-acetylcyclobutanone	Ketone
[M-H]-	18.74	132.51	phenylpropanoic acid	Phenolic acid derivative
[M-H]-	89.06	138.16	salicylic acid	Phenolic acid
[M-H]-	93.57	146.21	acetylcholine	Neurotransmitter/Choline ester
[M-H]-	20.82	170.26	gallate	Phenolic acid derivative
[M-H]-	18.04	245.41	catechin/epicatechin	Flavan-3-ol
[M-H]-	14.79	256.96	quercetin 3-O-glycoside	Flavonol glycoside
[M-H]-	20.92	312.31	C-glycosyl flavone	Flavone glycoside
[M-H]-	9.01	343.01	eupatorin	Flavone
[M-H]-	18.04	420.61	isomangiferin	Xanthone glycoside
[M-H]-	9.01	437.51	mangiferin 3-methyl ether	Xanthone derivative
[M-H]-	18.04	465.11	phenolic aid derivatives	Phenolic acid derivative
[M-H]-	18.04	563.91	apigenin-6,8-C-pentoside-hexoside	Flavone glycoside
[M-H]-	18.04	605.21	flavonoid glycosides	Flavonoid glycoside
[M-H]-	18.04	754.71	3,4-dihydroxyphenylglycol	Phenolic compound