# Targeted Small Molecules Analysis at ARC-BIO center

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Contact us: <a href="https://www.research.colostate.edu/pmf/team/">https://www.research.colostate.edu/pmf/team/</a>

# • Phytohormones in leaf, rachis, root, bud, grain

trans-zeatin (tZ), trans-zeatin riboside (tZR), indole-3-acetamide (IAM), indole-3-acetyl-alanine (IAA-ala), indole-3-carboxylic acid (ICA), indole-3-acetic acid (ICA), indole-3-acrylic acid (IACA), indole-3-butyric acid (IBA), indole-3-acetonitrile (IAN), jasmonic acid (JA), dihydrophaseic acid (DPA), gibberellic acid GA3 (GA3), phaseic acid (PA), salicylic acid (SA), abscisic acid (ABA), gibberellic acid GA4 (GA4), 12-oxo-phytodienoic acid (OPDA), indole-3-acetic acid (IAA)

Note: The compounds on the phytohormone panel change with the availability of commercial standards.

### Uremic toxins in serum

trimethylamine N-oxide (TMAO), indoxyl sulfate, p-cresol sulfate

# • <u>Cannabinoids</u>

- In plasma/serum: cannabidiol (CBD), cannabidiolic acid (CBDA), delta-9-tetrahydrocannabinol (delta-9-THC)
- In plant tissues: cannabichromeorcin (CBCO), cannabichromevarin (CBCV), cannabidivarin (CBDV), tetrahydrocannabivarin (THCV), cannabinol (CBN), cannanbichromene (CBC), cannabidiol (CBD), cannabicyclol (CBL), delta-8-tetrahydrocannabinol (delta-8-THC), delta-9-tetrahydrocannabinol (delta-9-THC), cannabigerol (CBG), cannabidivarinic acid (CBDVA), cannabinolic acid (CBNA), cannabichromenic acid (CBCA), cannabidiolic acid (CBDA), cannabicyclolic acid (CBLA), delta-9-tetrahydrocannabinolic acid (delta-9-THCA), cannabigerolic acid (CBGA)

  Note: method development in progress

# Drugs/antibotics in whole blood/plasma

cefepime, flucloxacillin, vancomycin

# • Circadian rhythm related neurotransmitter and hormones in plasma/serum

melatonin, serotonin, cortisol

#### • **Sex hormones** in plasma/serum

estradiol, progesterone, testosterone, dihydrotestosterone (DHT), dehydroepiandrosterone sulfate (DHEA-S)

Note: method development in progress

#### Tryptophan metabolites

In feces: 5-hydroxyindole-3-acetic acid (5-HIAA), melatonin, Serotonin, anthranilic acid, indole-3-propionic acid (IPA), 3-methylindole, tryptophan, kynurenic acid, kynurenine, tryptamine, indole-3-acetic acid (IAA)

In plant root: tryptophan, indole-3-acetic acid (IAA), indole-3-pyruvic acid (IPyA)

#### Bile acids in feces

serotonin, tryptamine, taurocholic acid (TCA), taurodeoxycholic acid (TDCA),  $\beta$ -muricholic Acid ((5 $\beta$ )-3 $\alpha$ ,6 $\beta$ ,7 $\beta$ -trihydroxy-cholan-24-oic acid), glycocholic acid (GCA), 3-oxocholic acid (OCA), ursodeoxycholic acid (UDCA), hyodeoxycholic acid (HDCA), nutriacholic acid (NCA), glycodeoxycholic acid (GDCA), glycochenodeoxycholic acid (GCDCA), cholic acid (CA), 7 $\alpha$ -hydroxy-3-oxo-5 $\beta$ -cholanoic acid (OCDCA), cholenic acid (3 $\beta$ -hydroxy-5-cholenoic acid), chenodeoxycholic acid (CDCA), deoxycholic acid (DCA), lithocholic acid (LCA)

# • Thyroid hormones in meat ingredients

Triiodothyronine (T3), thyroxine (T4)

• Amino acids in plant tissues, biofluids, cell extracts

#### Short chain fatty acids

- In plasma/serum: acetate, propionate, butyrate
- In feces: acetate, propionate, butyrate, isobutyrate, valerate, isovalerate

#### Fatty acids

- Standard/common fatty acids: palmitic acid (C16:0), stearic acid (C18:0), oleic acid (C18:1cis). linoleic acid (C18:2, linolenic acid (C18:3), arachidic acid (C20:0)
  Note: We can add most of the non-conjugated saturated/unsaturated fatty acids from C12:0 to C24:0 including EPA (C20:5ω3) and DHA (C22:6ω3) to the standard panel.
- Conjugated linoleic acids (CLA)

#### Mono- and disaccharides

In root exudates: arabinose, xylose, glucose, mannose, galactose, sucrose, maltose, trehalose

#### • Photorespiration metabolites in leaf tissues

Glyceric acid, glycolic acid, glycine, phosphoglycolic acid, glyoxylic acid, hydroxypyruvic acid, glutathione (by LC-MS/MS)

- Ethyl carbamate (urethane) in plasma and ethanol distillers' grain co-products
- Organic acids in plant tissues, root exudate, biofluids

# Nutrition biomarkers in plasma, urine, stool

Pipecolic acid, methyl pipecolate, S-methyl-L-cysteine, S-methyl cysteine sulfoxide, trigonelline, pyridoxal, xanthurenic acid, apigenin, salicylic acid, myo-inositol, salicyluric acid

# • Central carbon metabolism (See Table 1)

Note: Profiling of all the compounds involved in central carbon metabolism is semi-quantitative or nontargeted (i.e., peak intensities are reported). Absolute quantification (i.e., ng/mL) is available for custom subsets if internal standards are available.

Table 1. Central carbon metabolism or other small polar molecules assays

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Amino acids and	Alanine, Arginine, Asparagine, Aspartic acid, Cysteine, Glutamate,
related	Glutamine, Glycine, Hydroxyproline, Isoleucine, Leucine, Lysine,
	Methionine, Ornithine, Phenylalanine, Proline, Serine, Taurine,
	Threonine, Tryptophan, Tyrosine, Valine, beta-alanine, Betaine,
	Carnitine, Carnosine, Citrulline, Creatine, Cystathionine, Cysteine-
	glutathione disulfide-CySSG, Cystine, Glutathione, Kynurenine,
	Oxiglutatione-GSSG, S-adenosylmethionine
Organic acids and related	2-methylglutarate, 2-phosphoglycerate, 3-hydroxymethylglutarate, 6-phosphogluconate, cis-aconitate, Citrate, Fumarate, Glucuronate,
	Glycerate, Isocitrate, Kynurenate, Lactate, Malate, Methylmalonate,
	Orotate, Phosphoenolpyruvate, Pipecolate, Pyruvate, Succinate, trans-
	aconitate, Allantoate, alpha-ketoglutarate, Aminoadipate,
	Arginosuccinate, Dihydroorotate
Nucleotides and	NADH, NADP, NADPH, Adenine, Adenosine, ADP, AMP, ATP, CMP, CTP,
related	Cytosine, Deoxycytidine, Deoxyguanosine, Deoxyuridine, GDP, GTP,
	Inosine, Inosine monophosphate, Uridine, 5-methyluridine, 7-
	methylguanosine, cyclic AMP, cyclic GMP, Cytidine, FAD, Flavin
	mononucleotide, Hypoxanthine, UDP-glucose, UMP, Uracil, Xanthine
Sugar phosphates	Pentose monophosphate, Hexose monophosphate
Others	Acetyl-CoA, allantoin, Choline, Glycerol-3-P, Glycerophosphocholine,
	Phosphocholine, Trigonelline, Tryptamine, Gln-6-P, Myo-inositol,
	Urea, Acetylcholine