

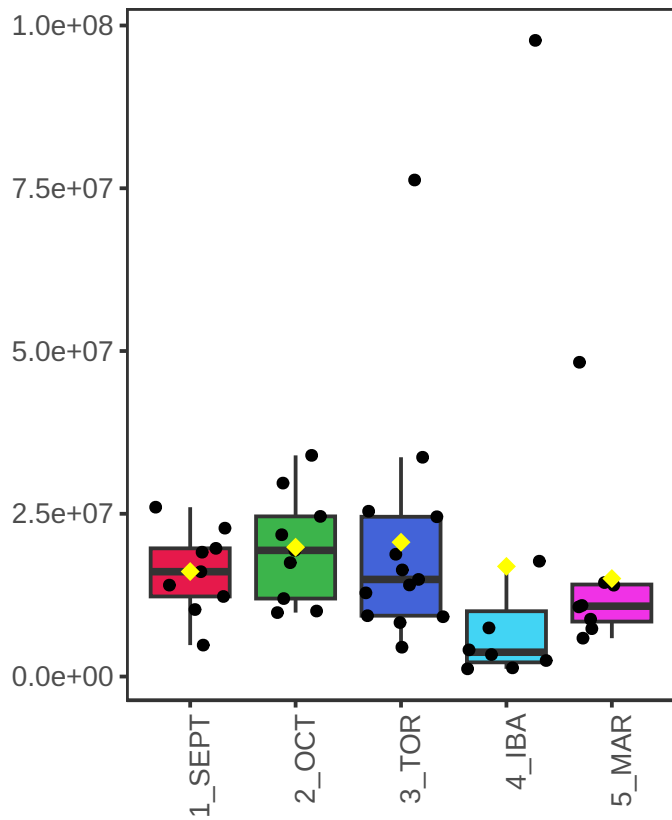
Figure S3

Supplementary Figure 3: Boxplot Representations of all Annotated Features from the Negative Ion Mode

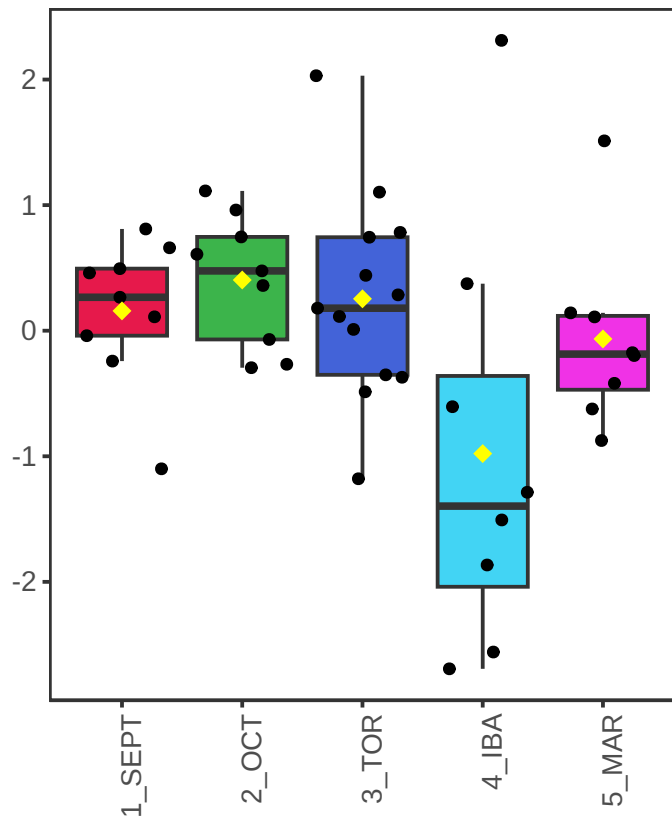
Collated feature intensity box plots for all annotated features in the negative ion mode. Left panel: original feature intensities from peak intensity table (Supplemental Table S2, tab 2). Right panel: feature intensities after \log_{10} transformation and auto scaling (values mean-centered and divided by the standard deviation).

2-Aminonicotinic acid

Original Conc.

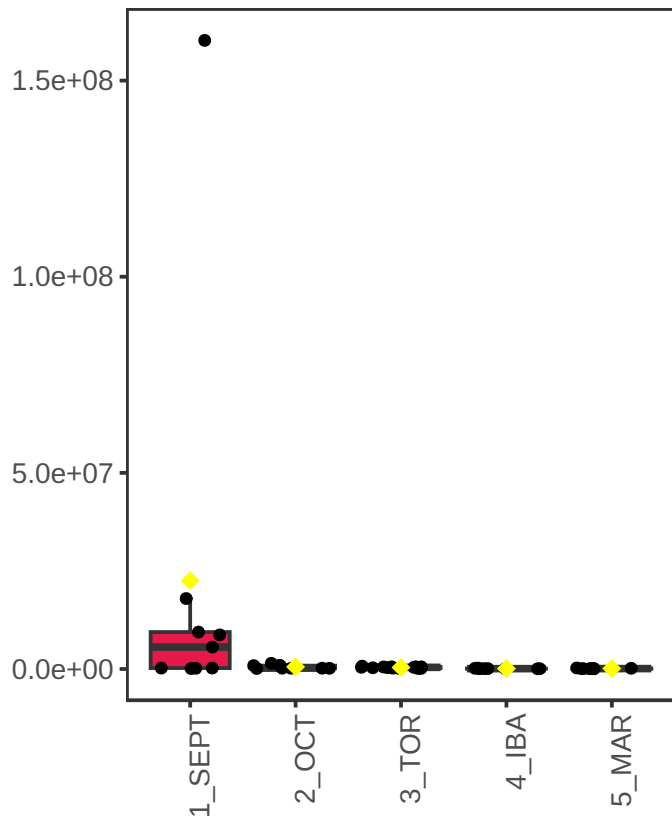


Normalized Conc.

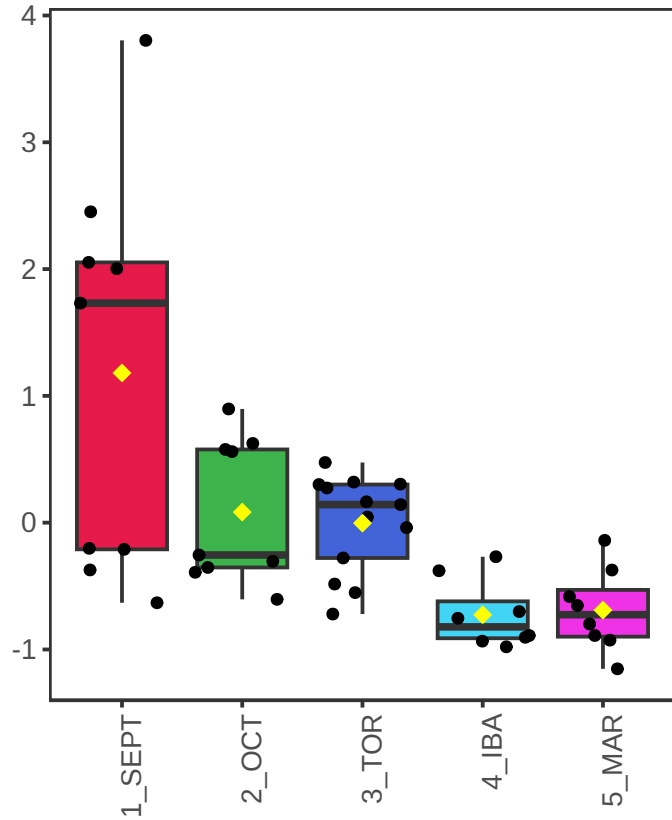


2-Hydroxyhippuric acid

Original Conc.

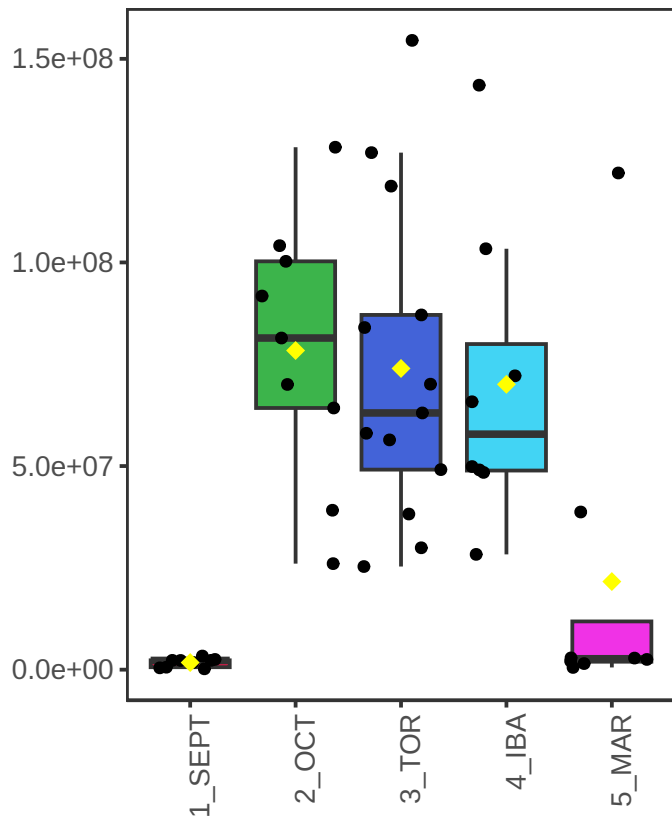


Normalized Conc.

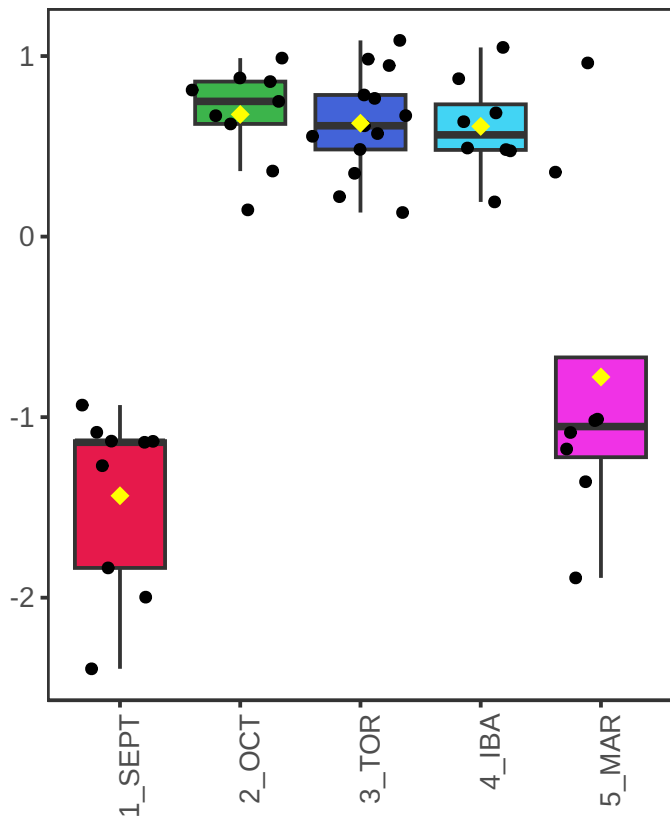


2-Oxobutyric acid

Original Conc.

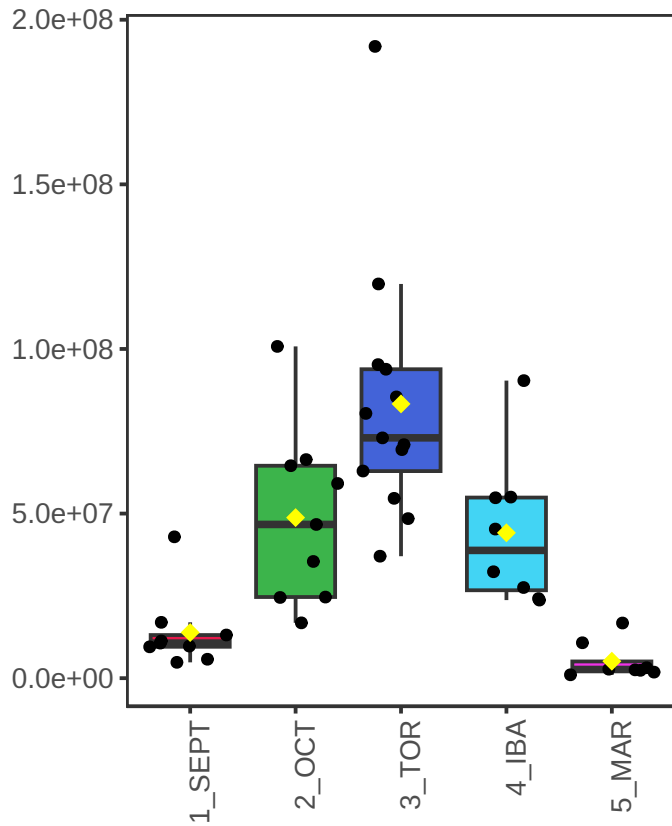


Normalized Conc.

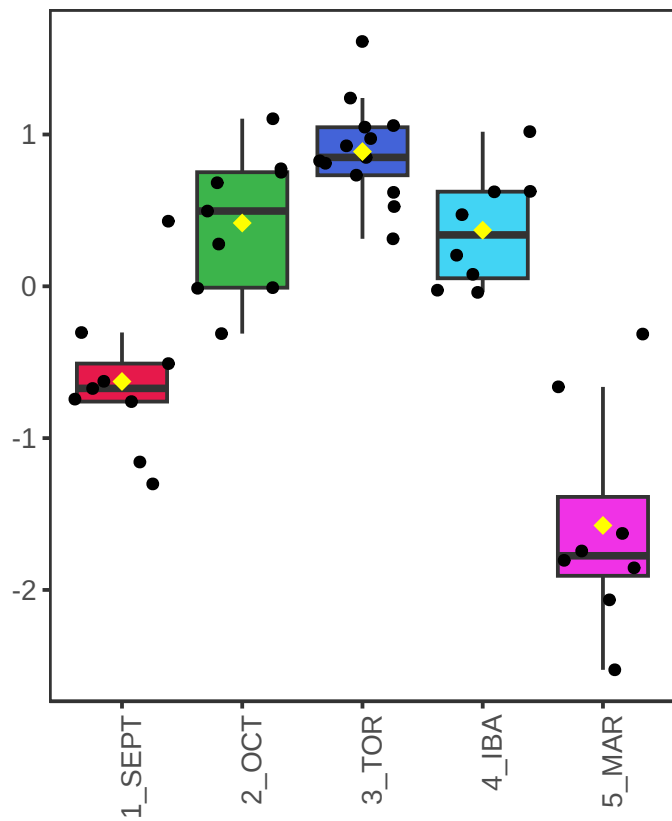


3-Hydroxyvaleric acid

Original Conc.

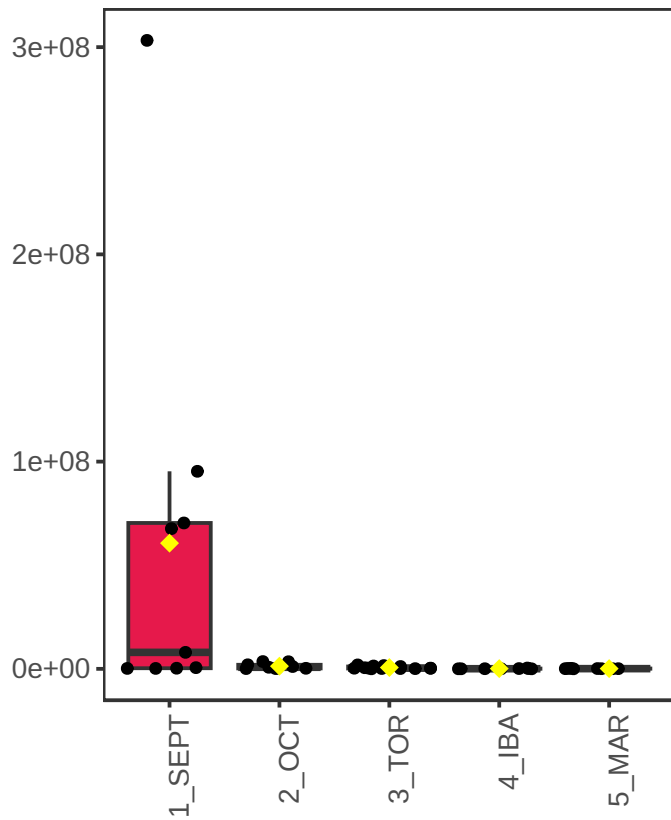


Normalized Conc.

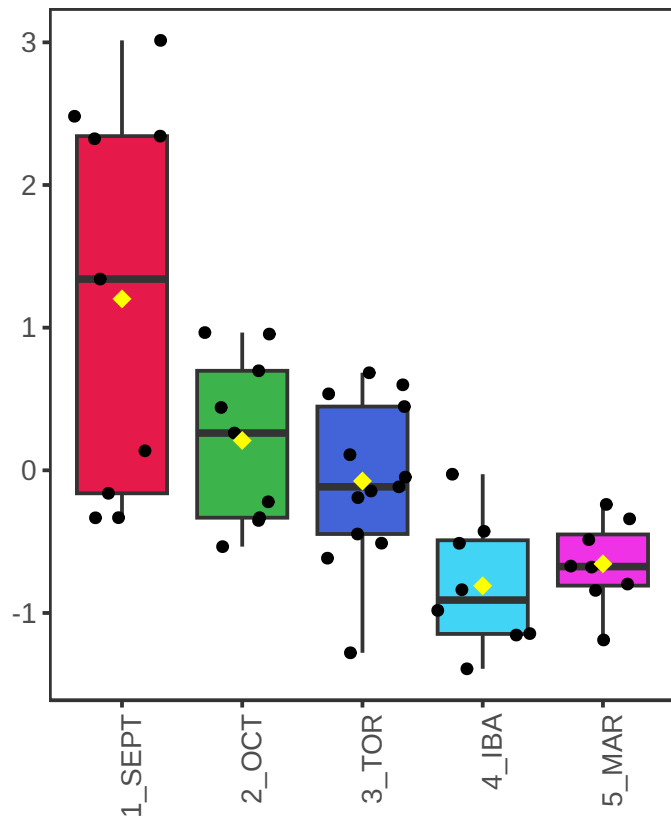


3-Methoxyphenylacetic acid

Original Conc.

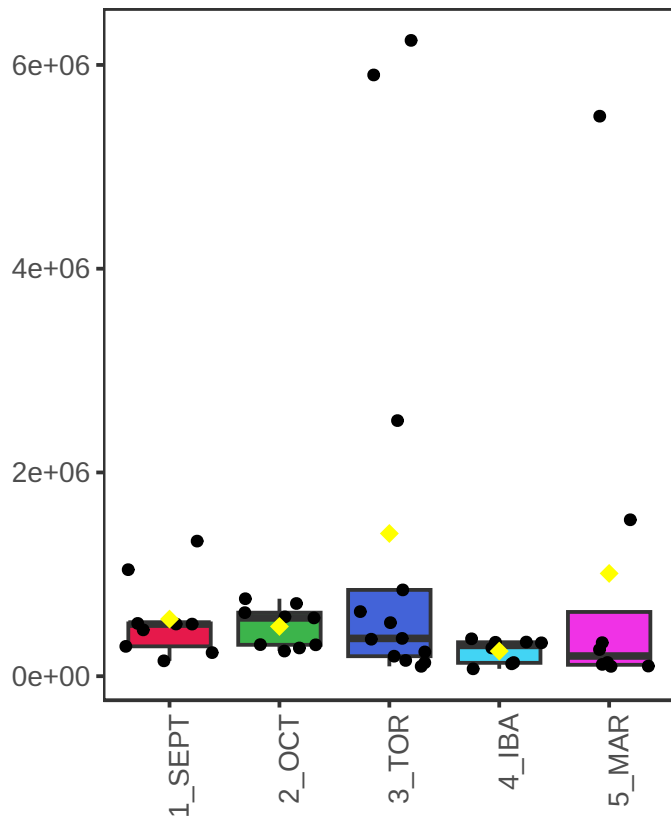


Normalized Conc.

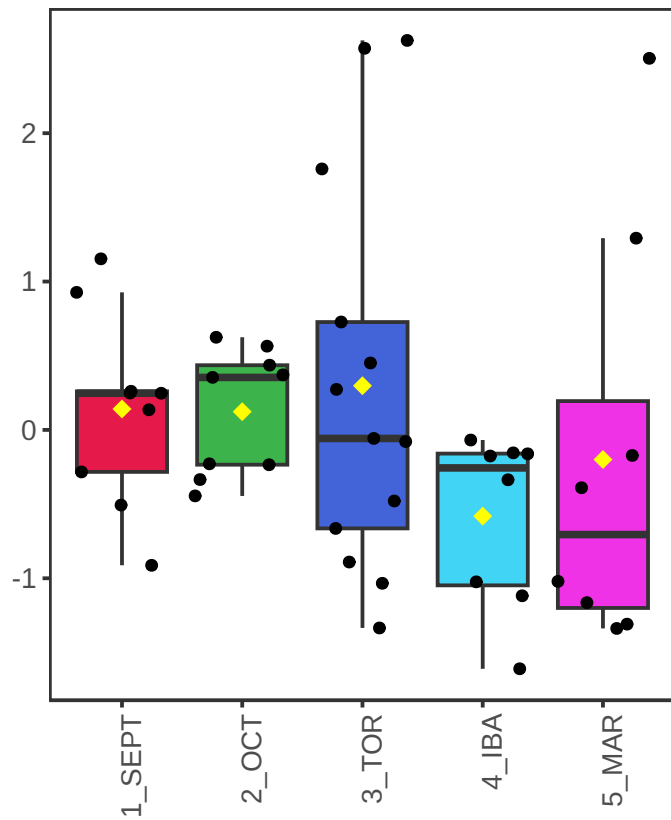


3-Octenedioic acid

Original Conc.

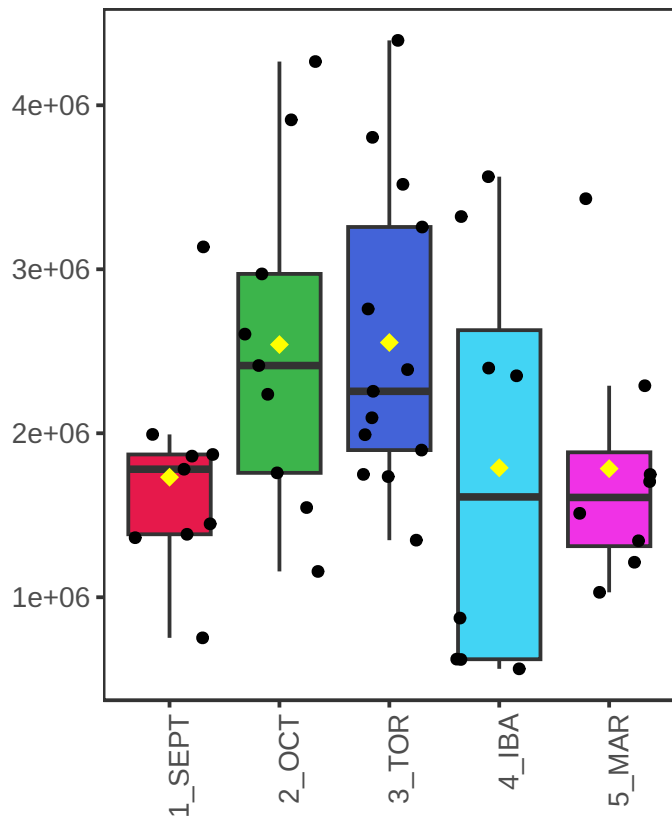


Normalized Conc.

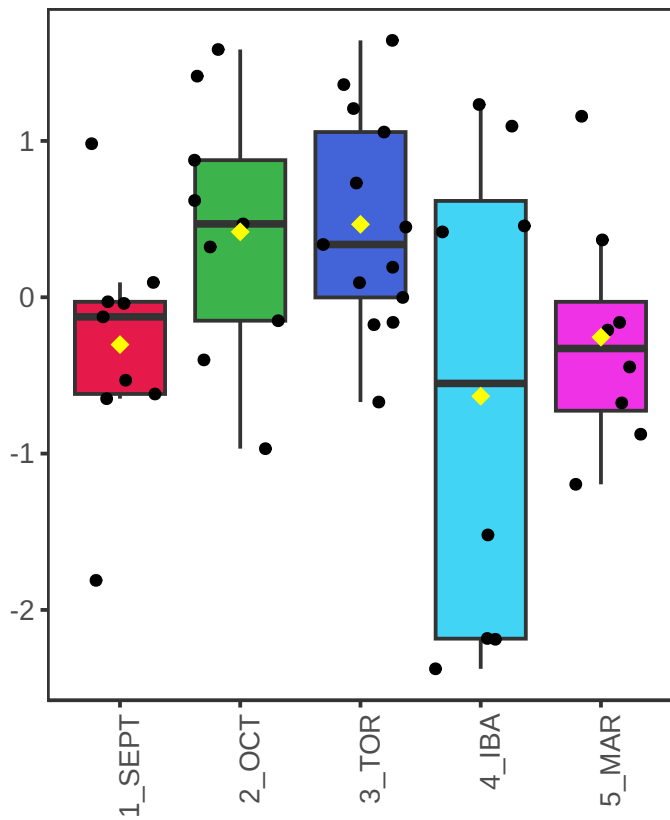


3-tert-Butyladipic acid

Original Conc.

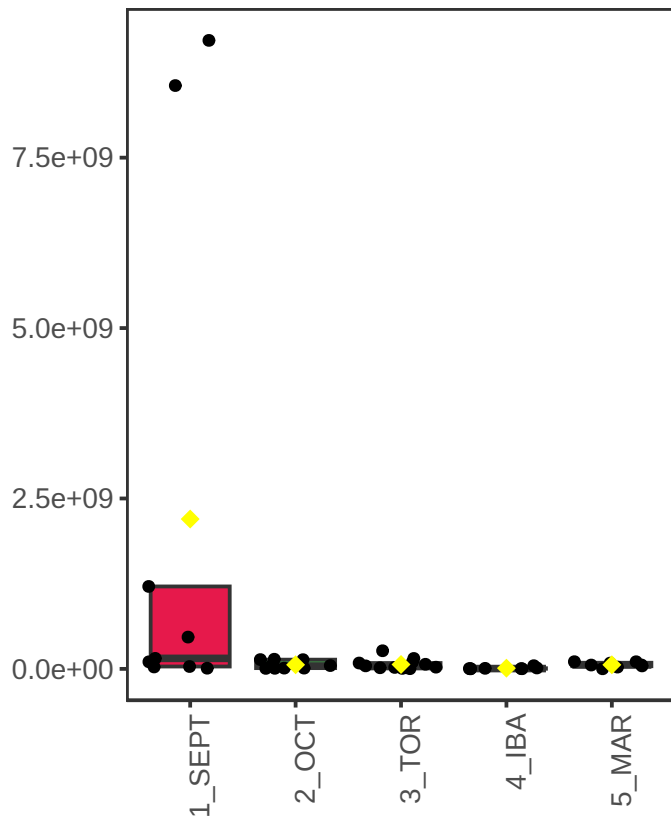


Normalized Conc.

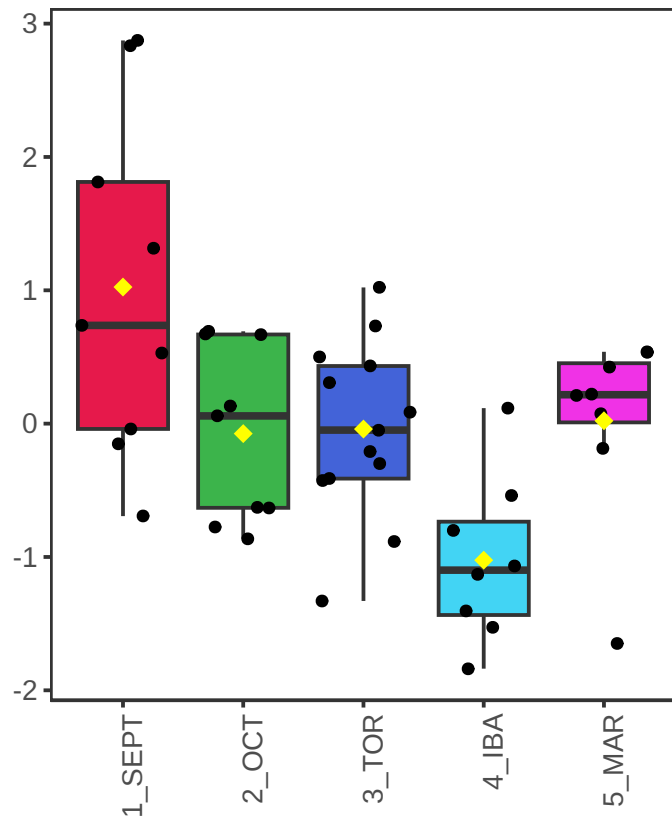


4-Acetamidobenzoic acid

Original Conc.

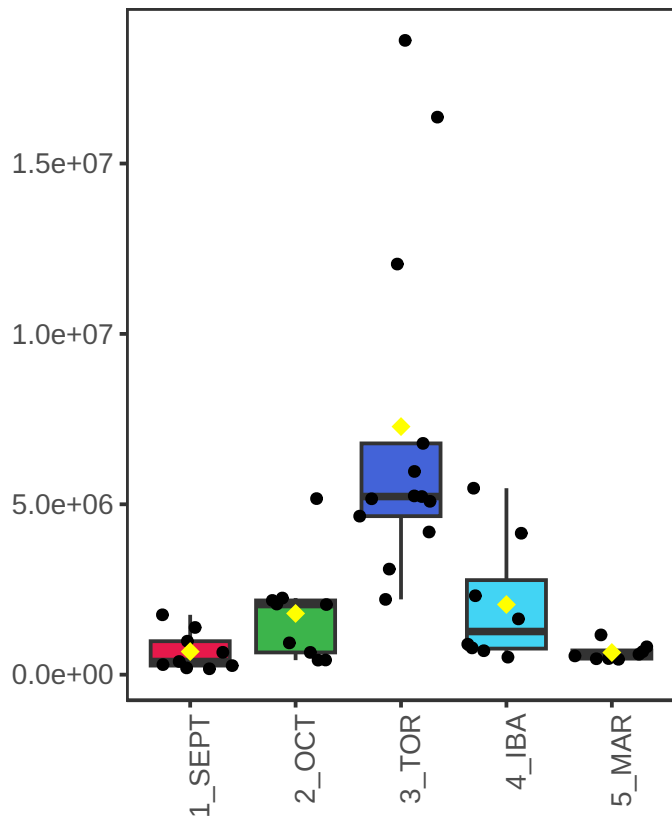


Normalized Conc.

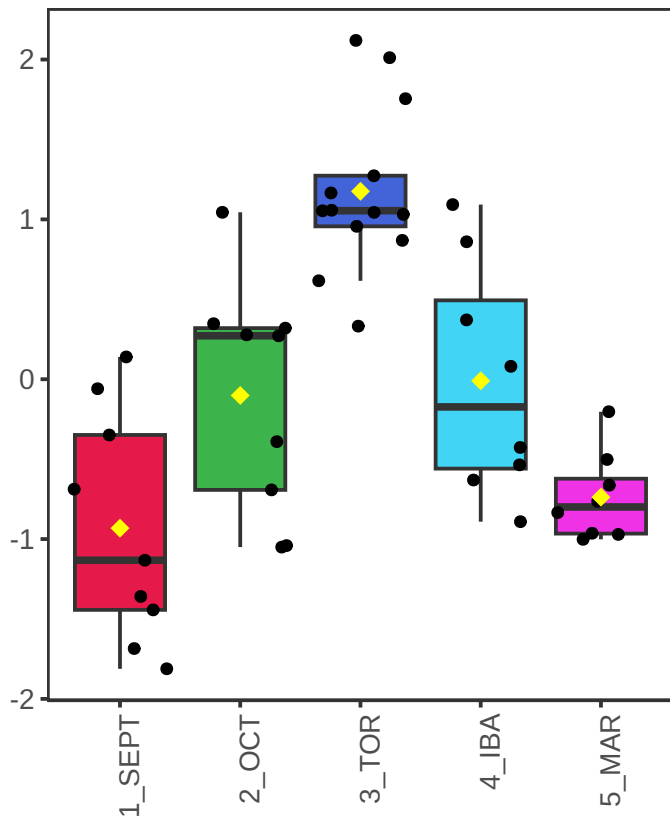


4-Acetamidobutanoic acid

Original Conc.

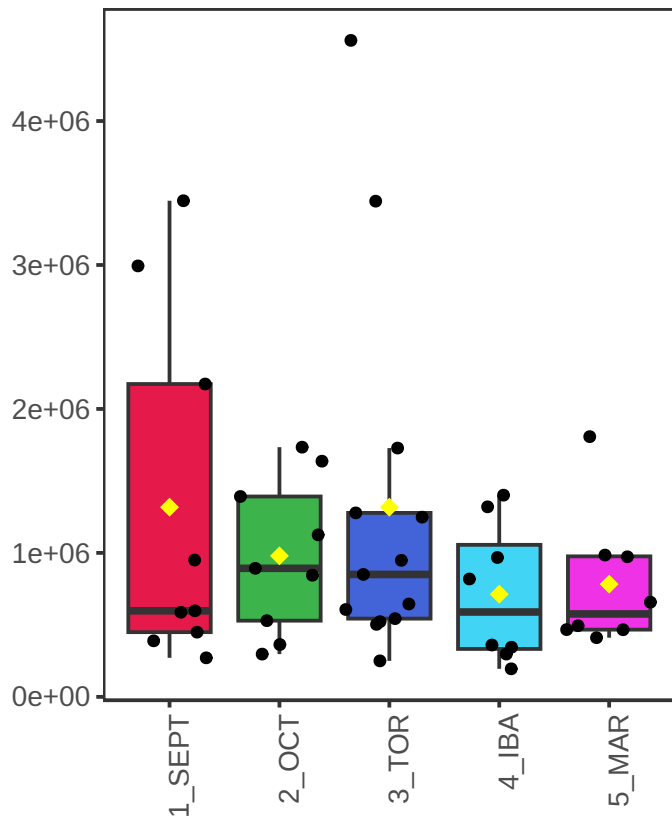


Normalized Conc.

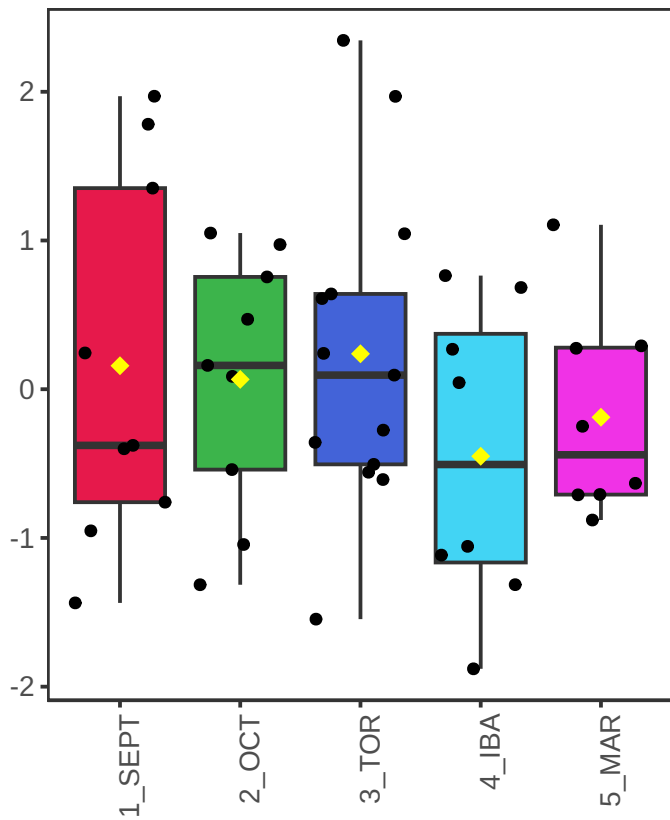


5-Decenedioic acid

Original Conc.

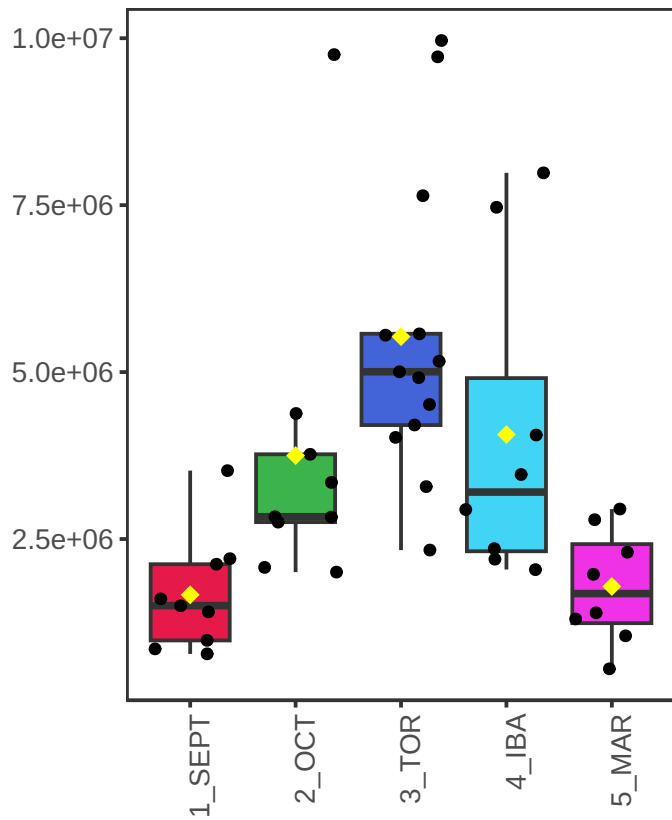


Normalized Conc.

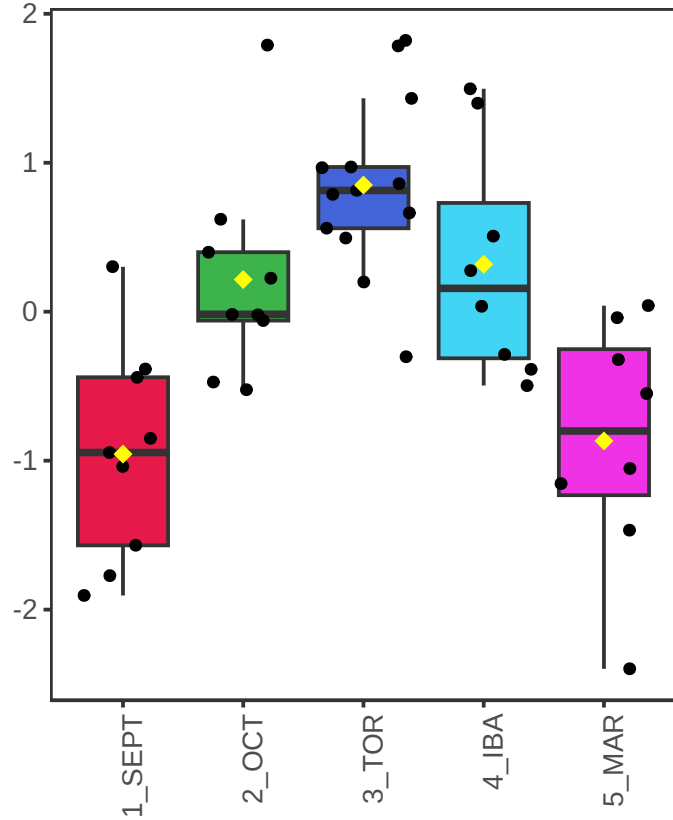


5-Hydroxycaproic acid

Original Conc.

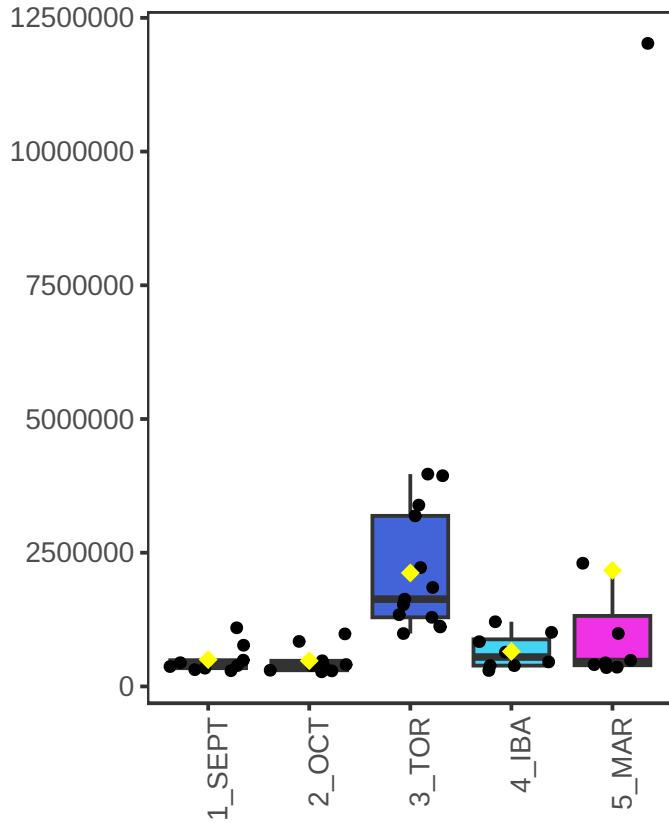


Normalized Conc.

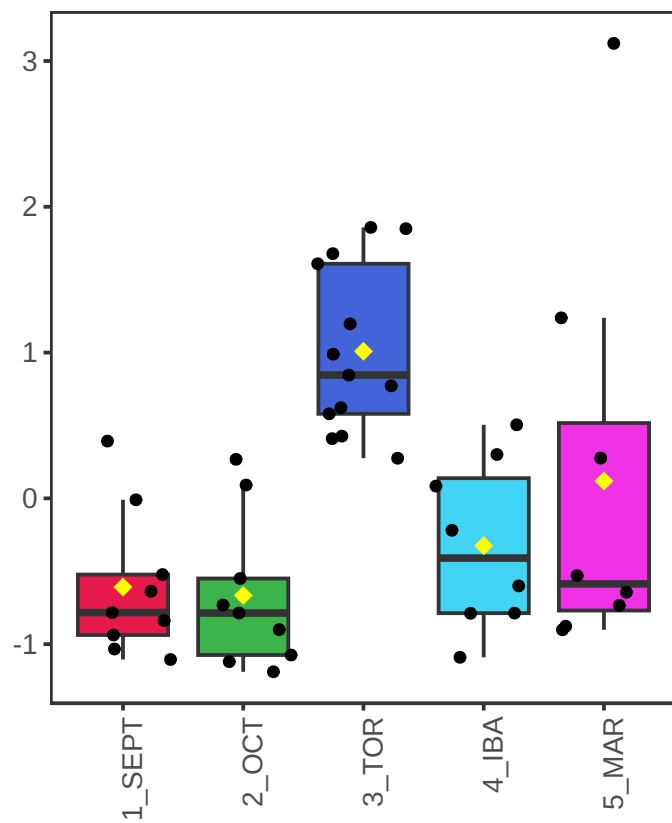


5-Hydroxytryptophan

Original Conc.

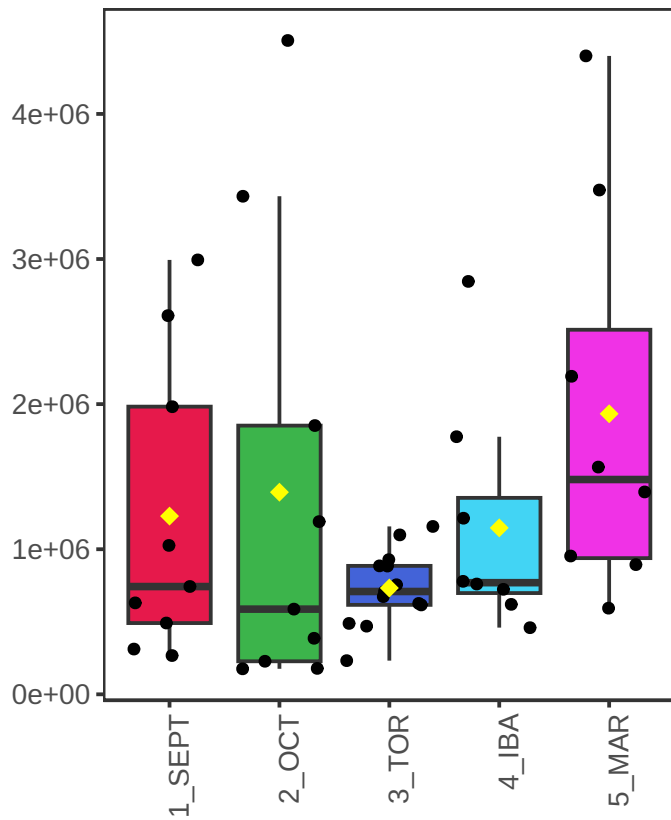


Normalized Conc.

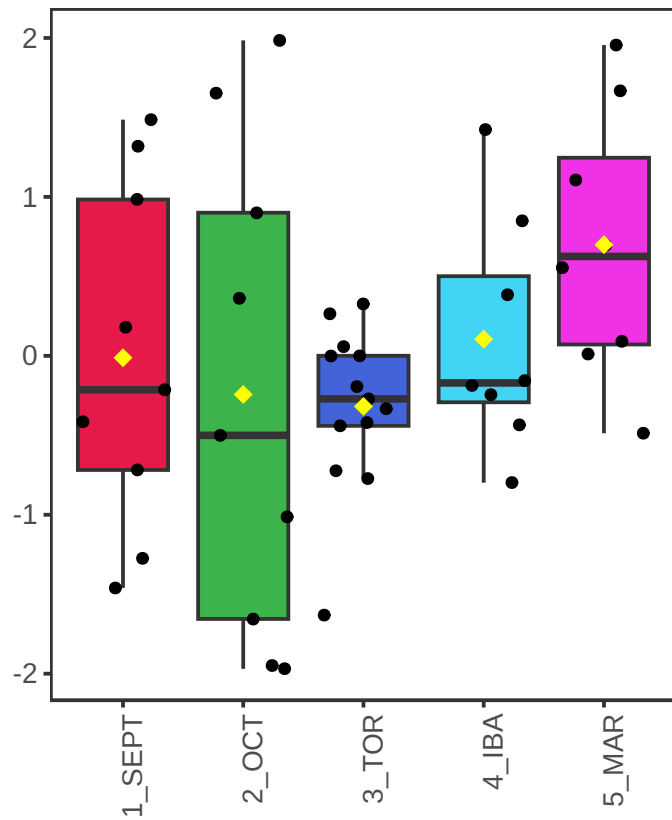


9,12,13-Trihydroxy-15-octadecenoic acid

Original Conc.

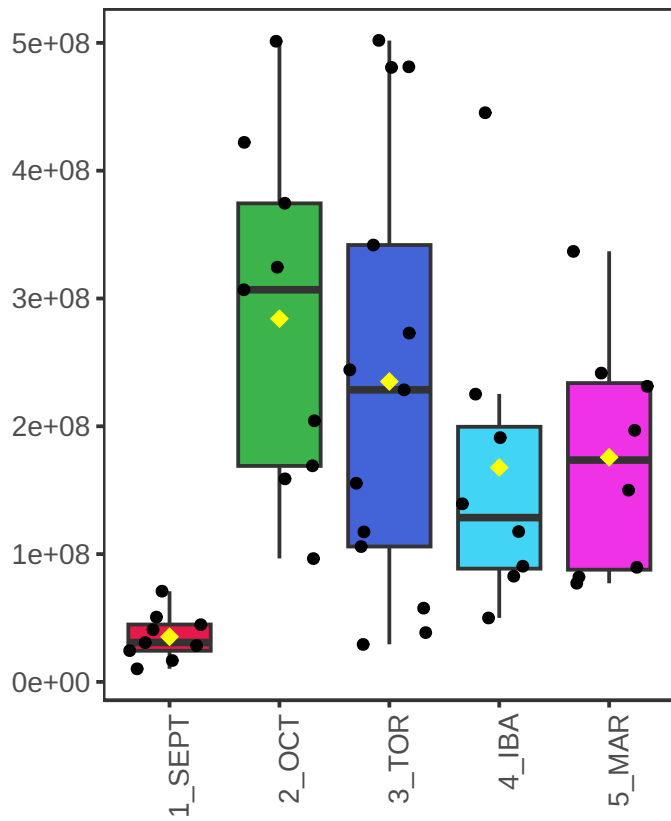


Normalized Conc.

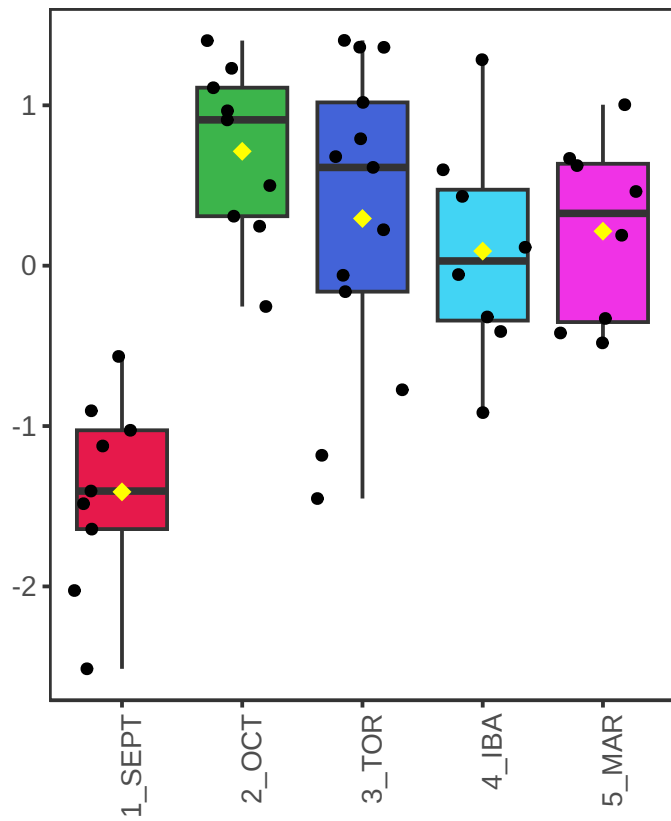


Adenosine

Original Conc.

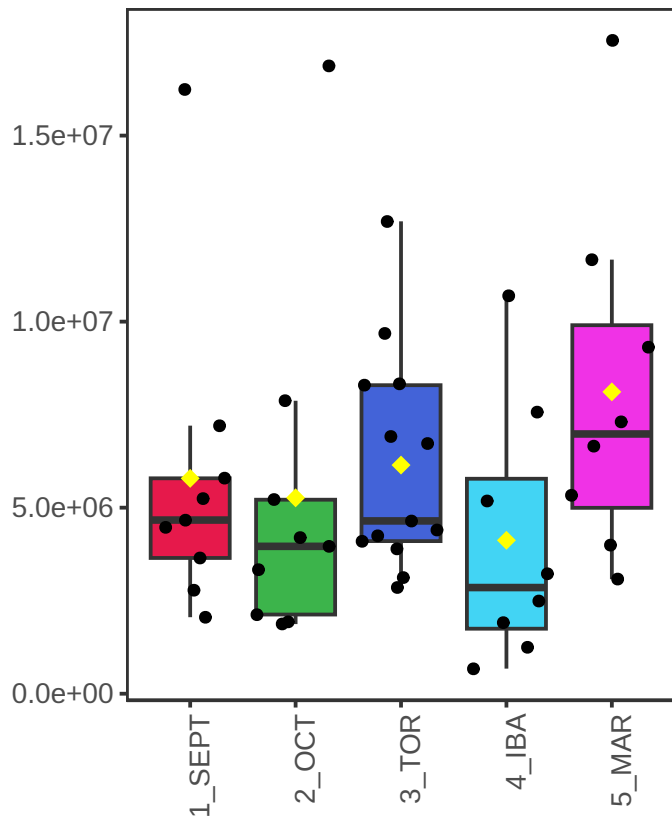


Normalized Conc.

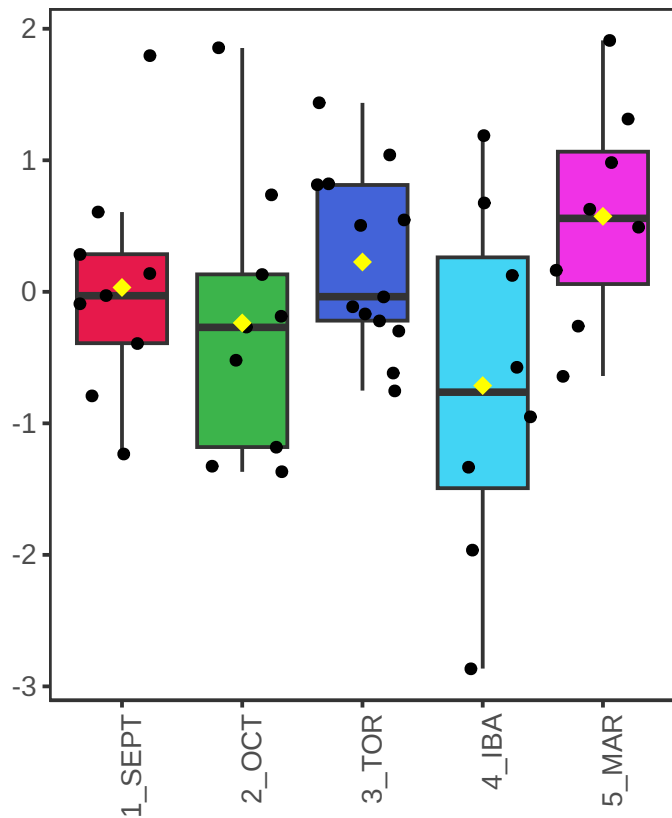


Adipic acid

Original Conc.

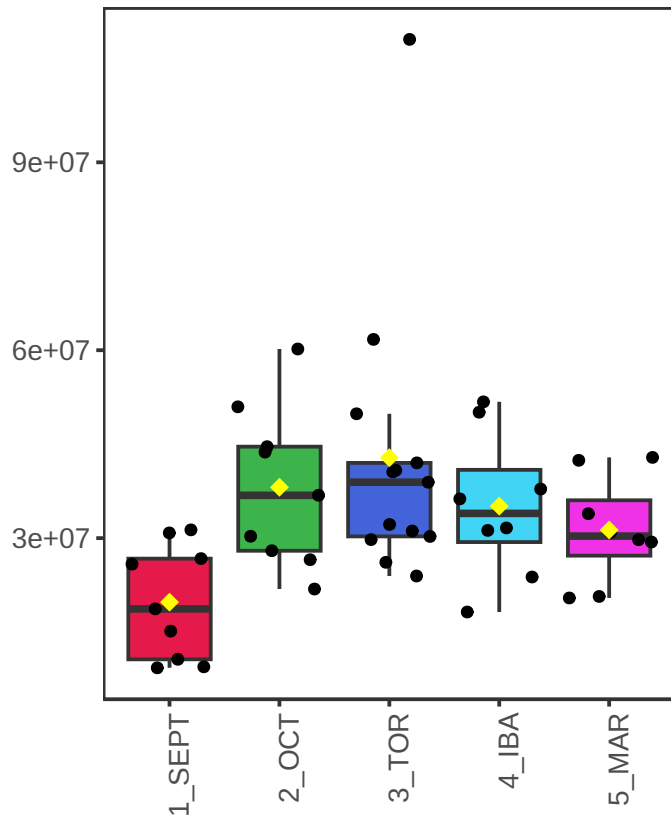


Normalized Conc.

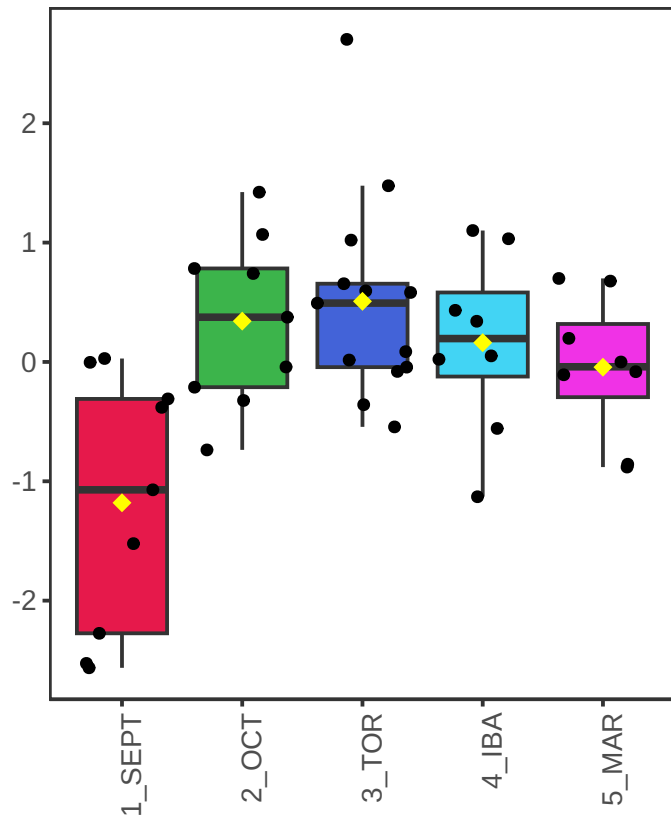


Alanine

Original Conc.

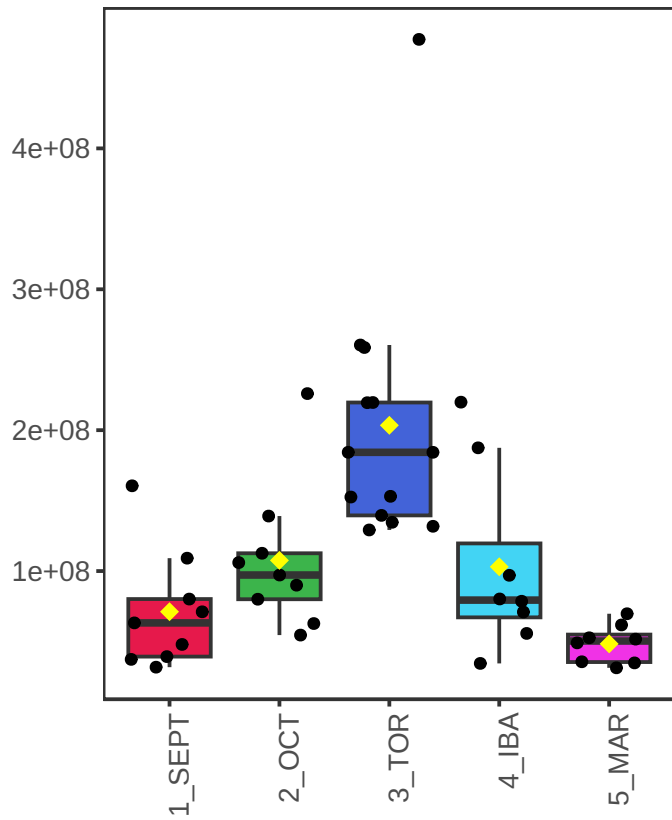


Normalized Conc.

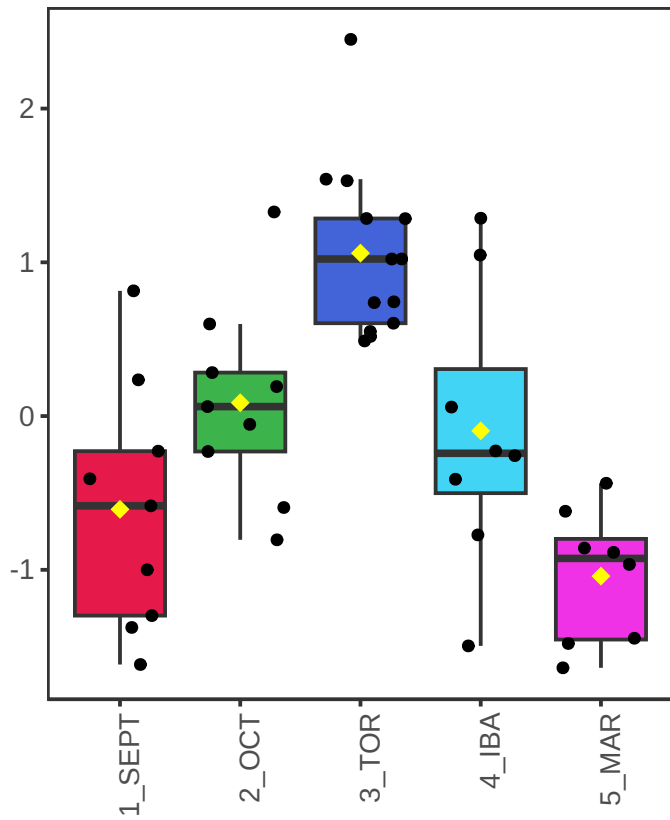


Allantoin

Original Conc.

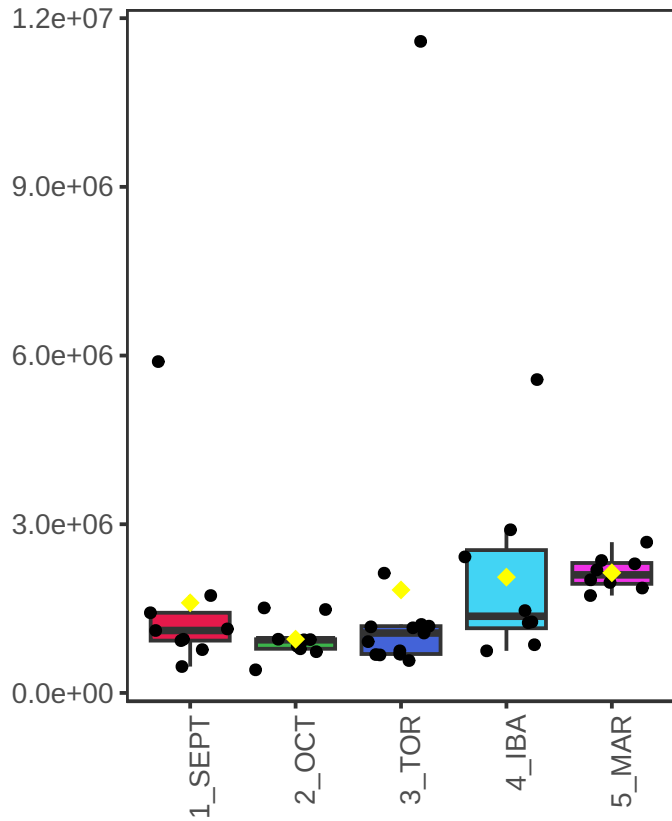


Normalized Conc.

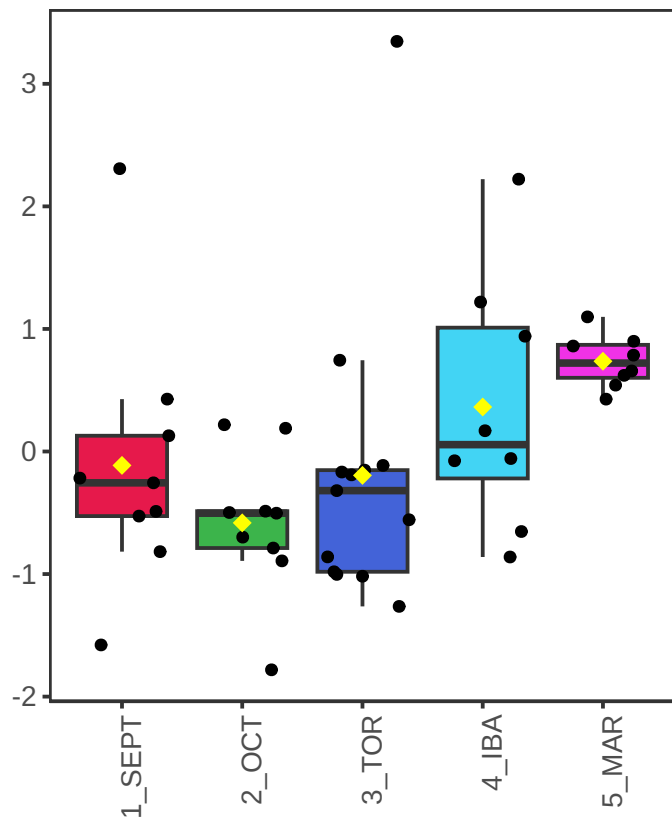


alpha-Aminoacidic acid

Original Conc.

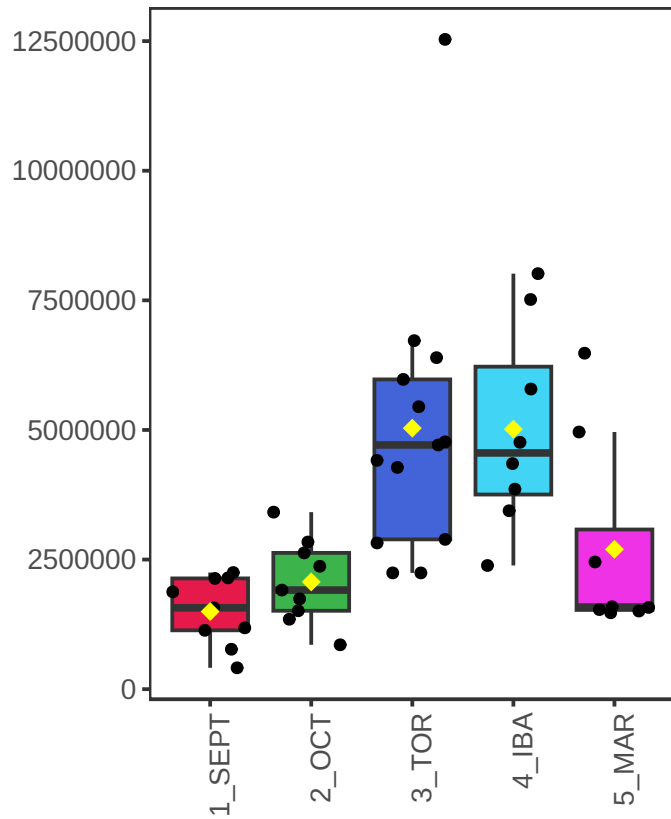


Normalized Conc.

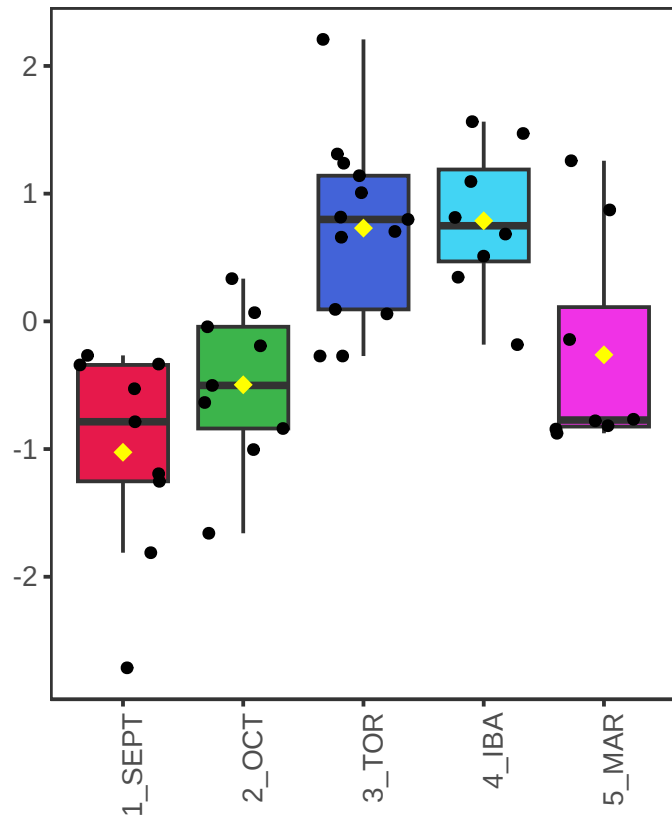


Aminolevulinic acid

Original Conc.

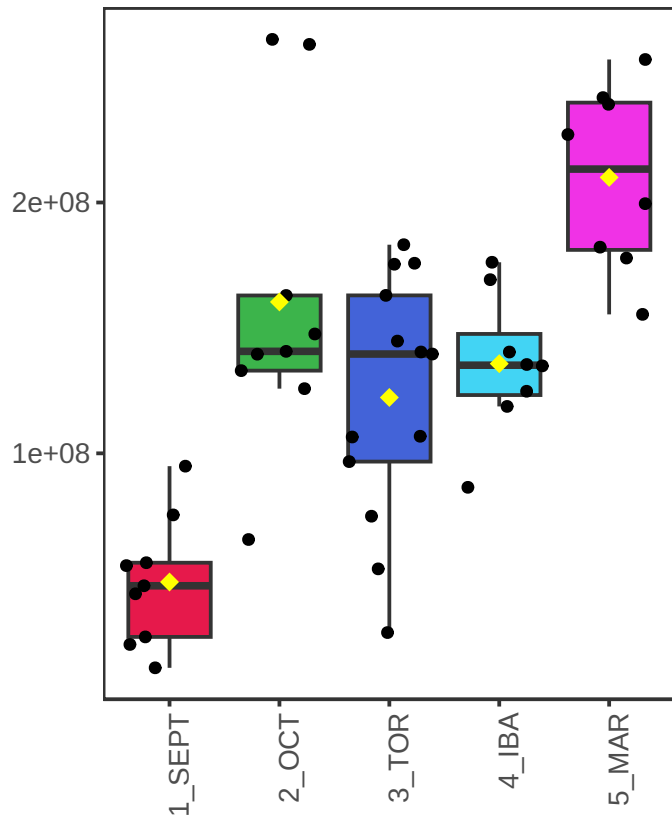


Normalized Conc.

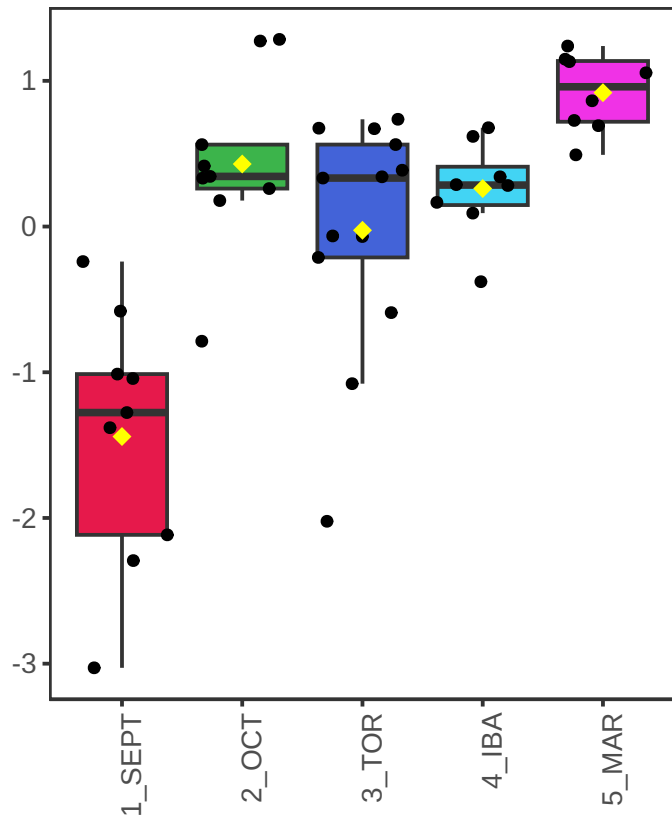


Arabinosylhypoxanthine

Original Conc.

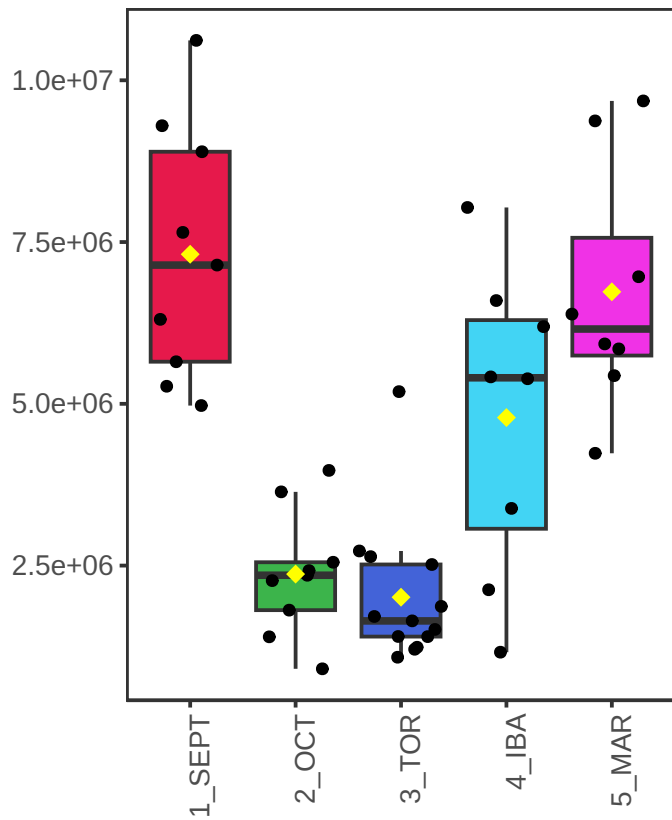


Normalized Conc.

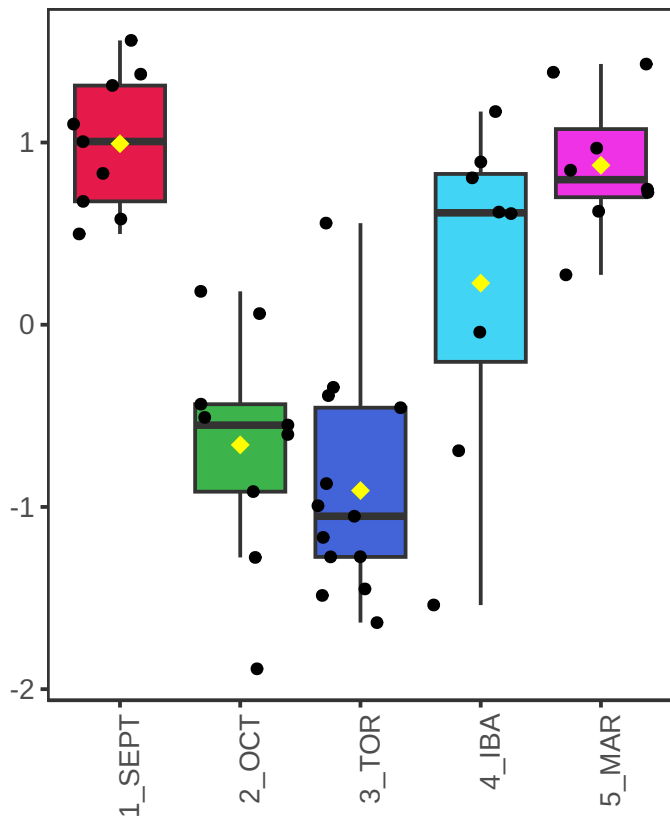


Asparagine

Original Conc.

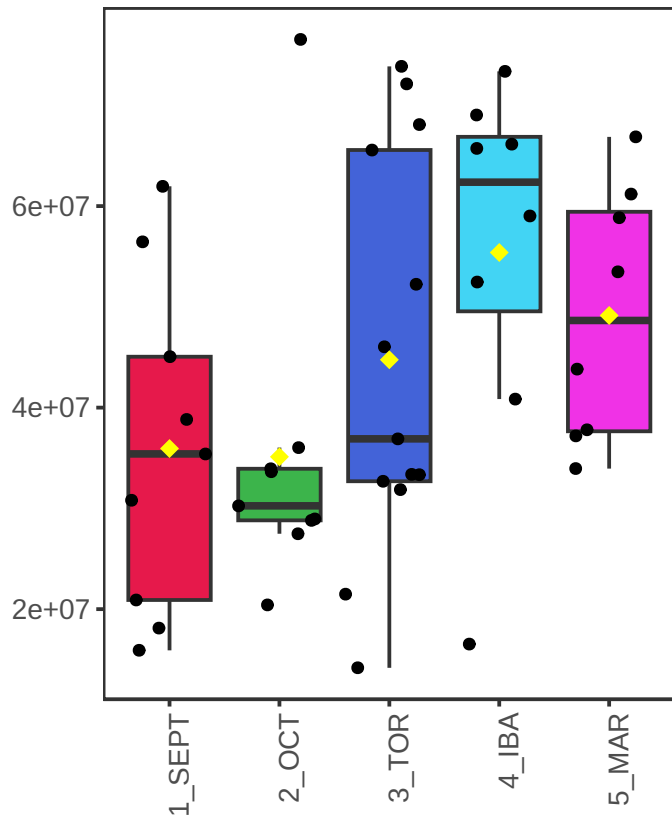


Normalized Conc.

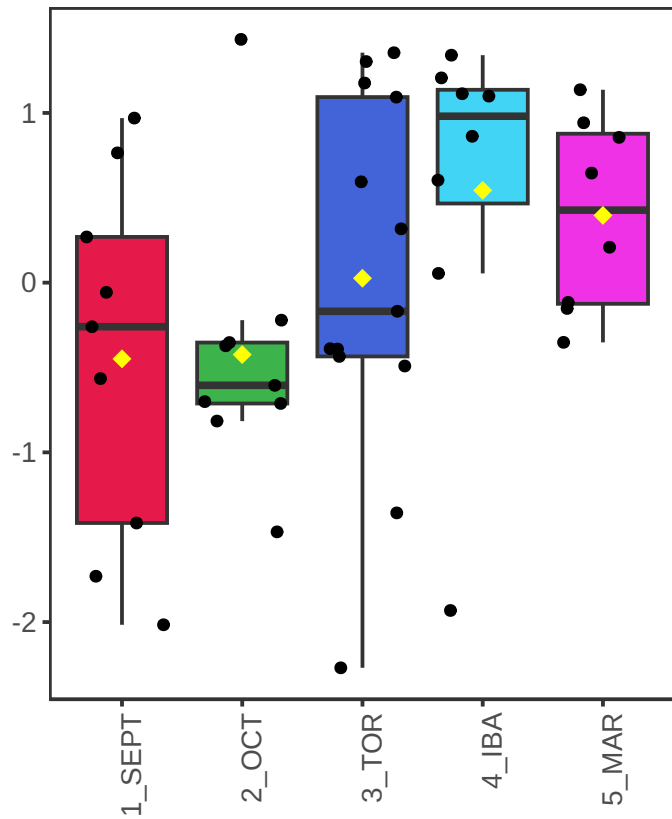


Aspartic acid

Original Conc.

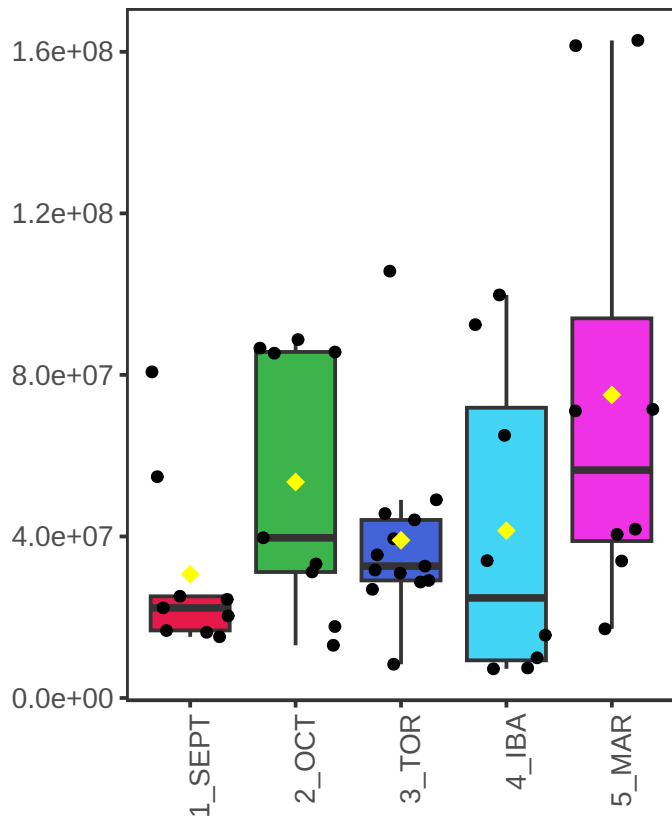


Normalized Conc.

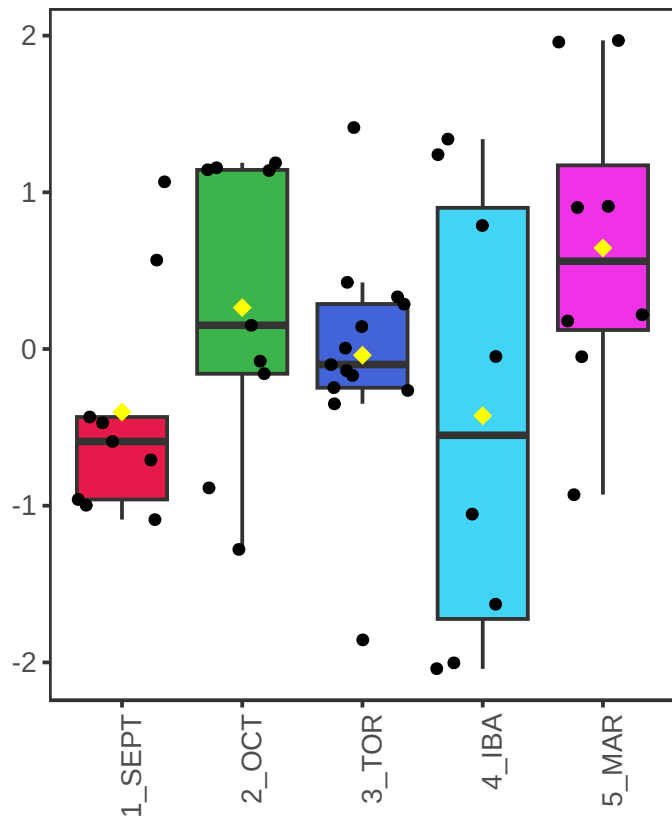


Azelaic acid

Original Conc.

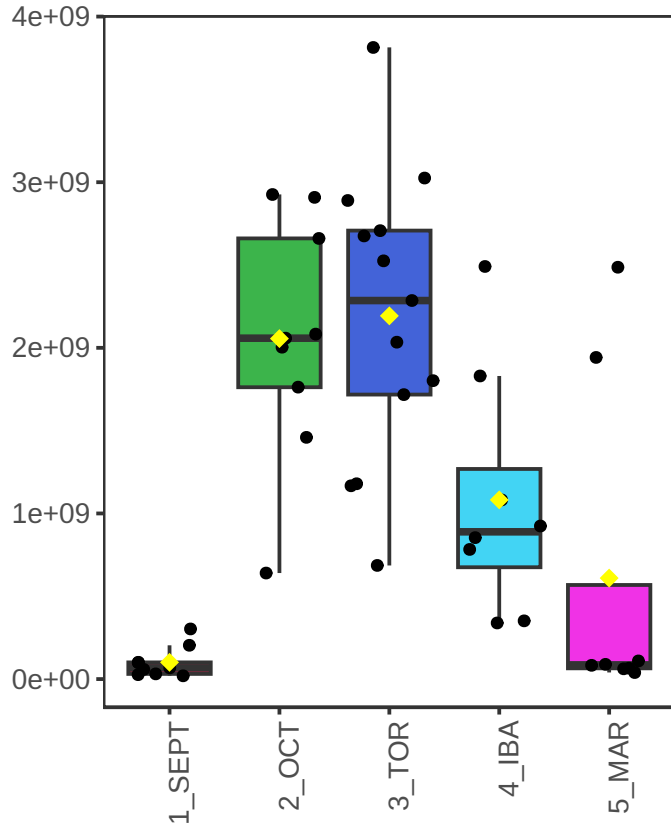


Normalized Conc.

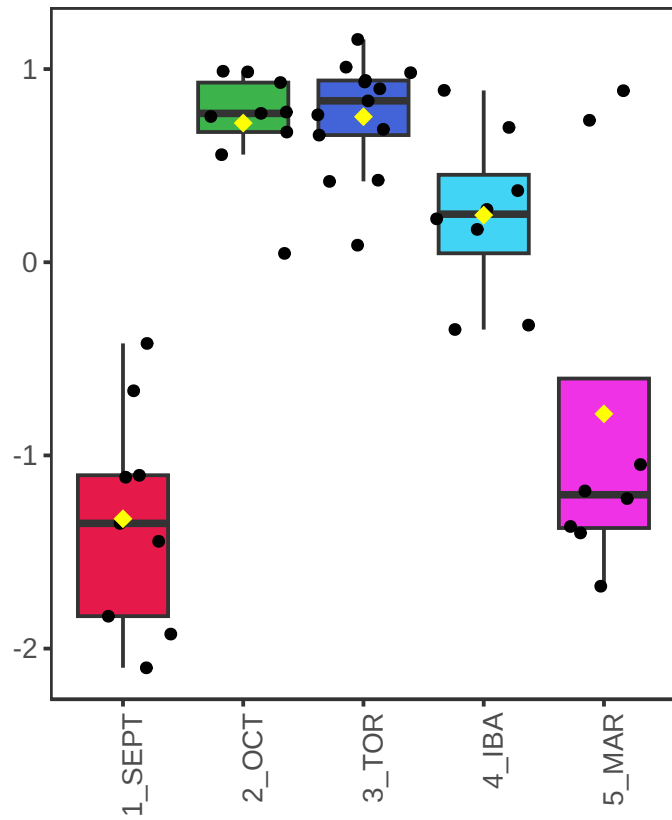


beta-Hydroxybutyric acid

Original Conc.

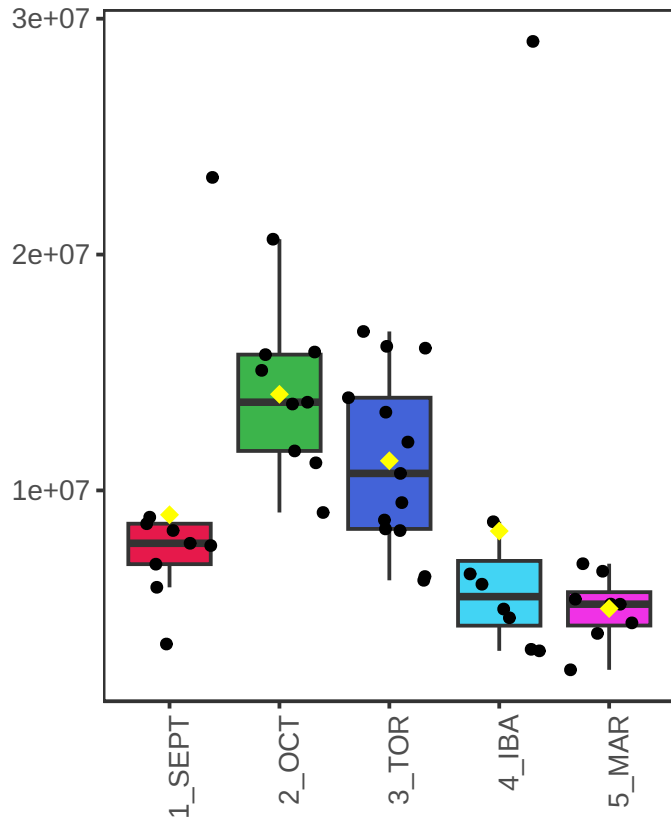


Normalized Conc.

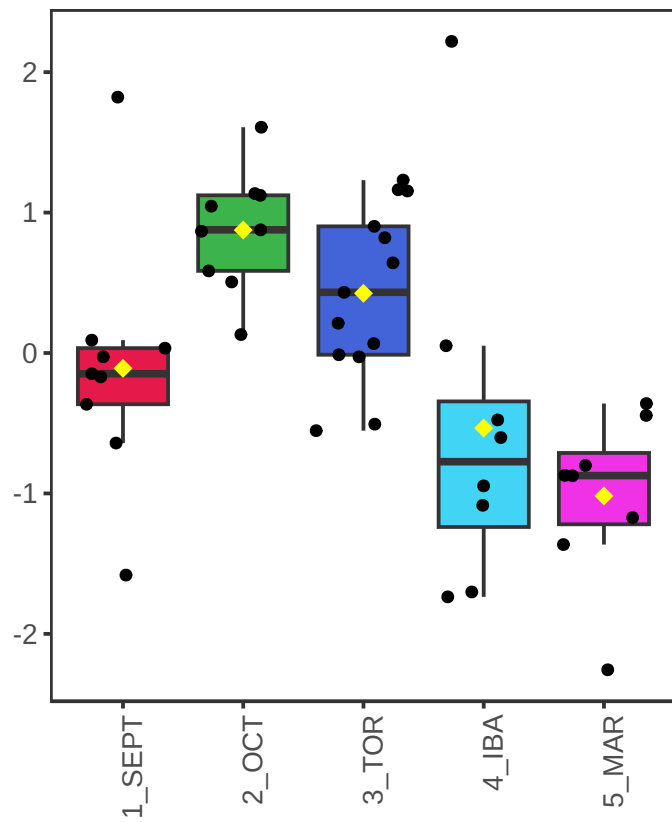


Benzoic acid

Original Conc.

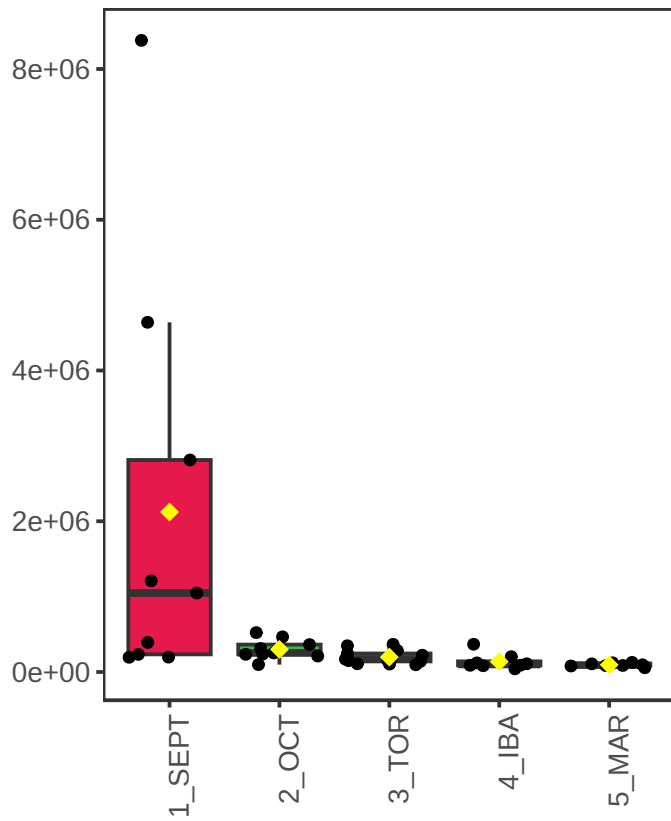


Normalized Conc.

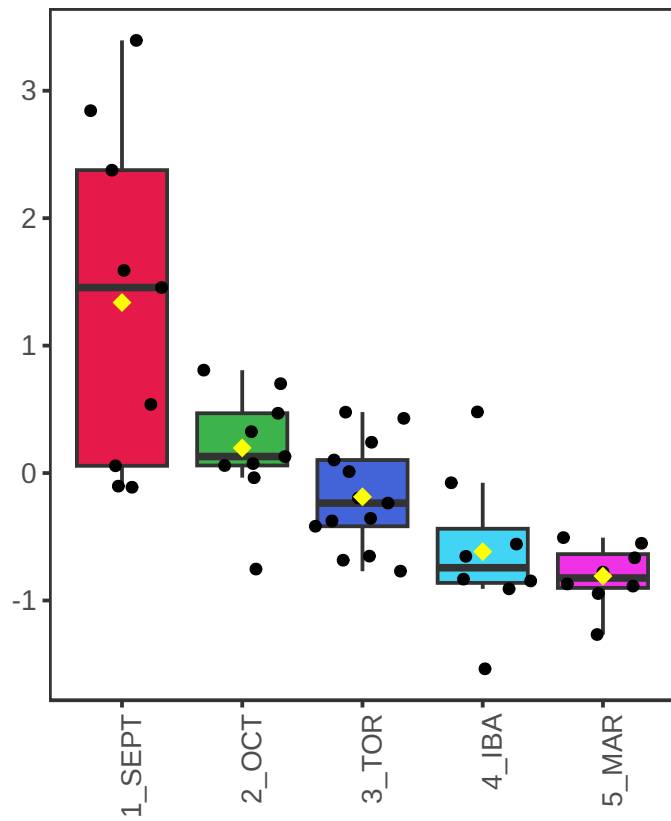


Caffeic acid

Original Conc.

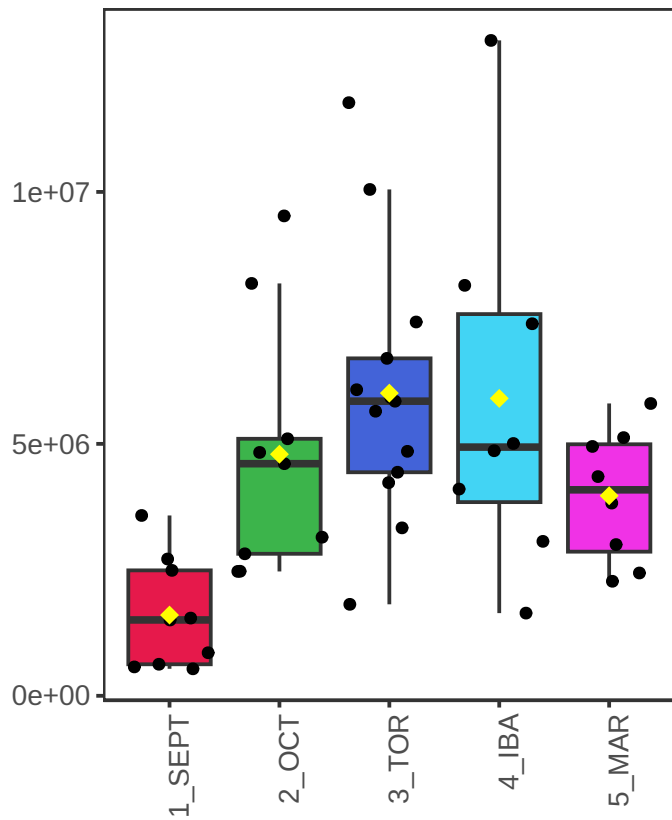


Normalized Conc.

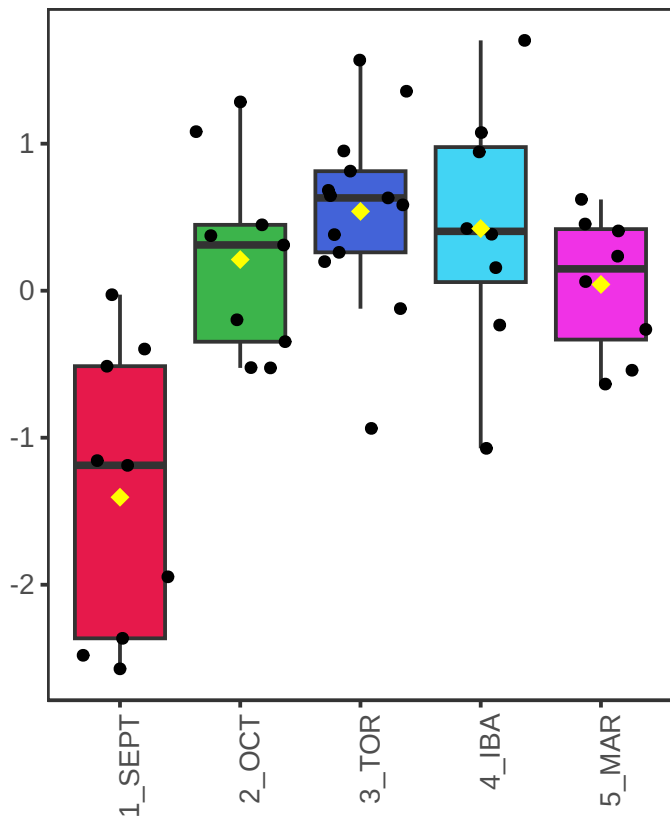


cis-Acetylacrylic acid

Original Conc.

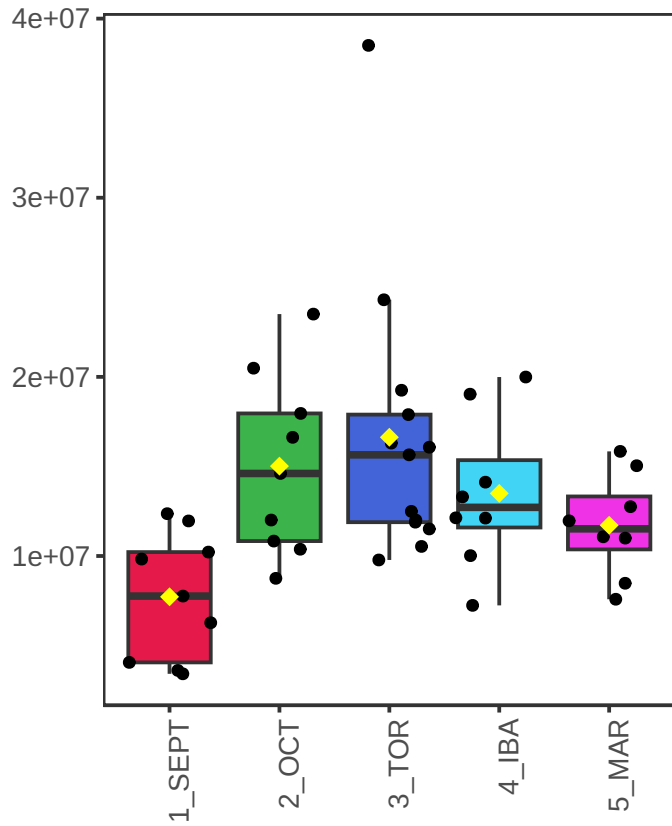


Normalized Conc.

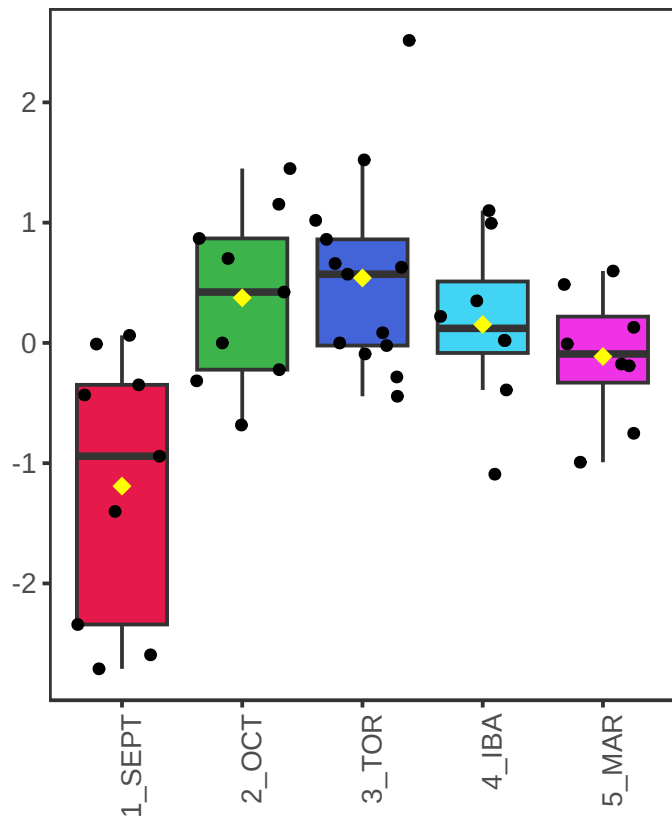


Creatine

Original Conc.

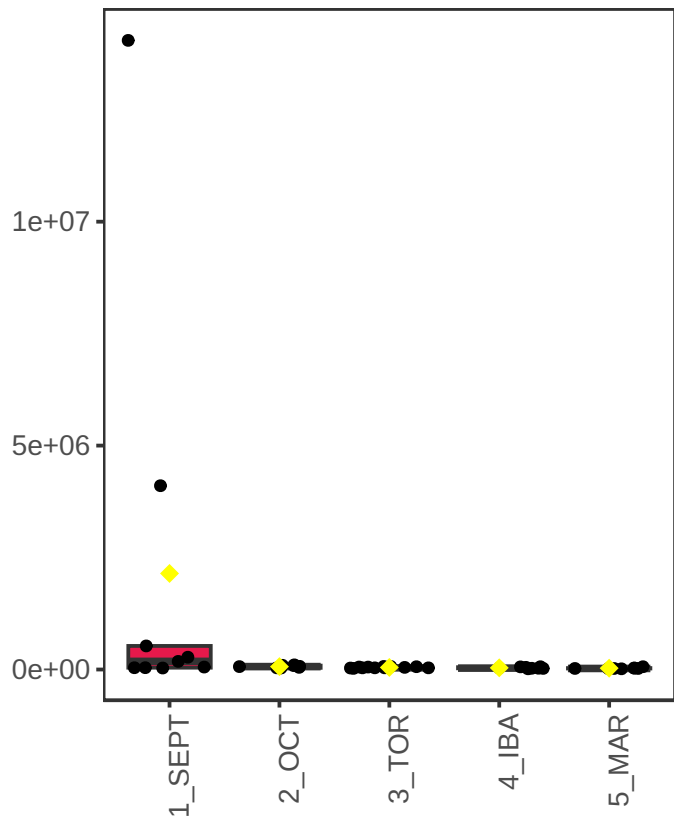


Normalized Conc.

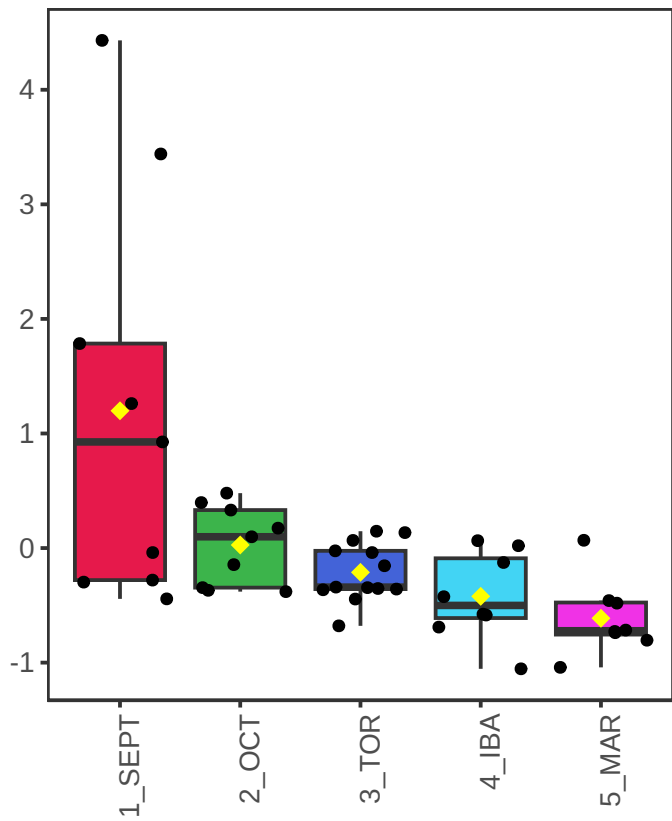


Cyclo(Seryltyrosyl)

Original Conc.

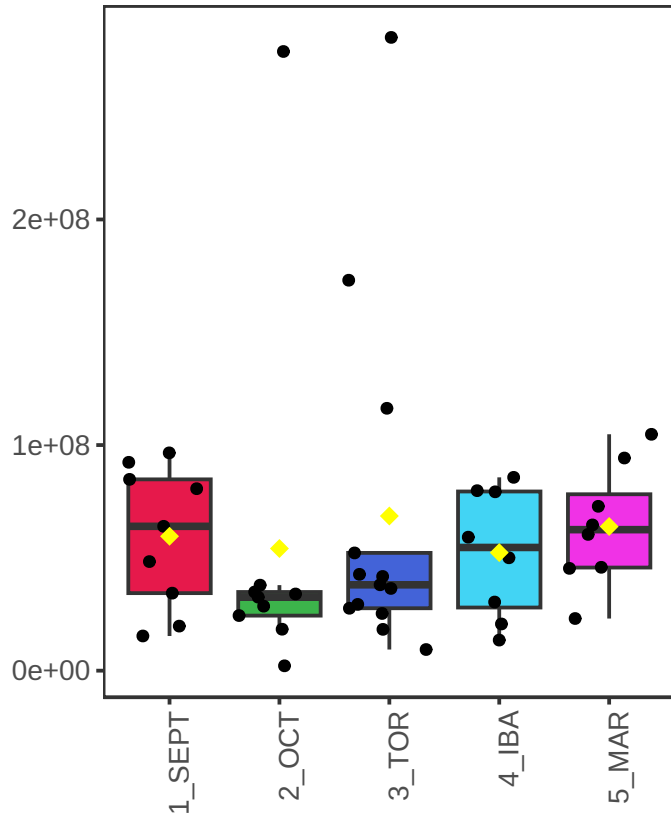


Normalized Conc.

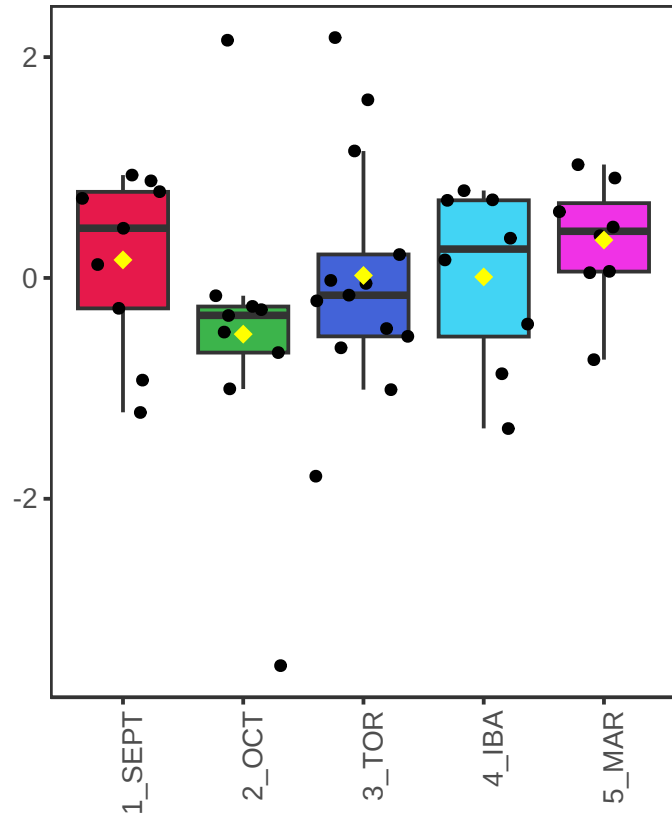


Dehydroascorbic acid

Original Conc.

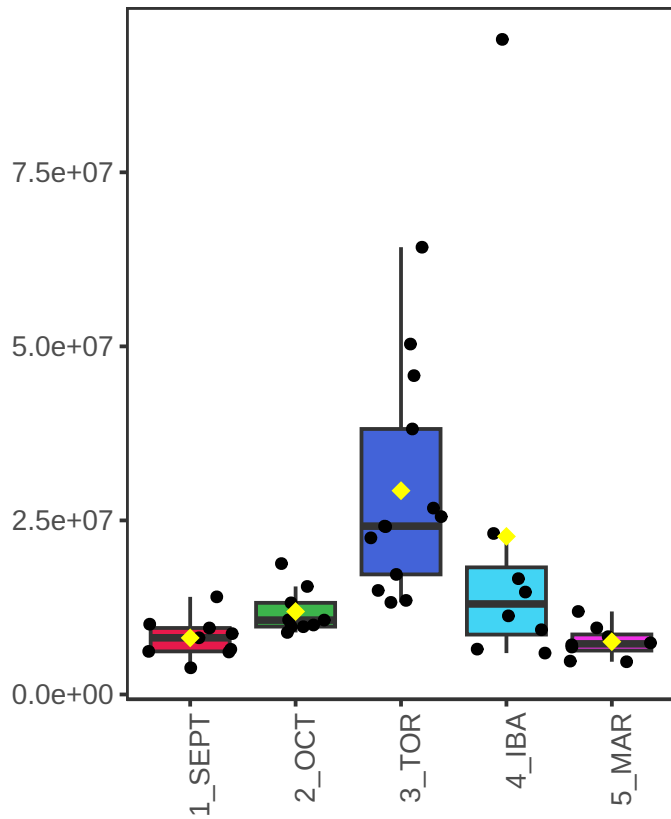


Normalized Conc.

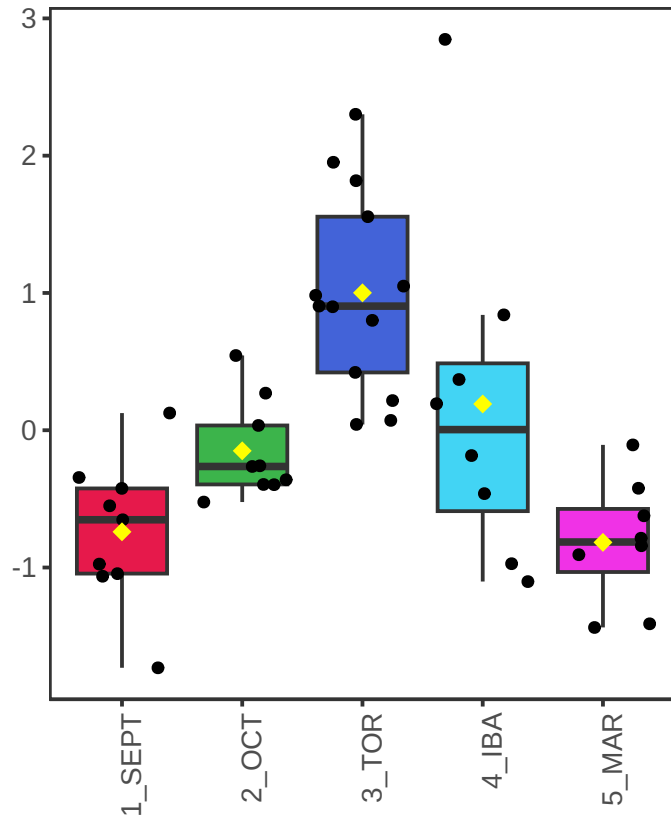


Ethyl lactate

Original Conc.

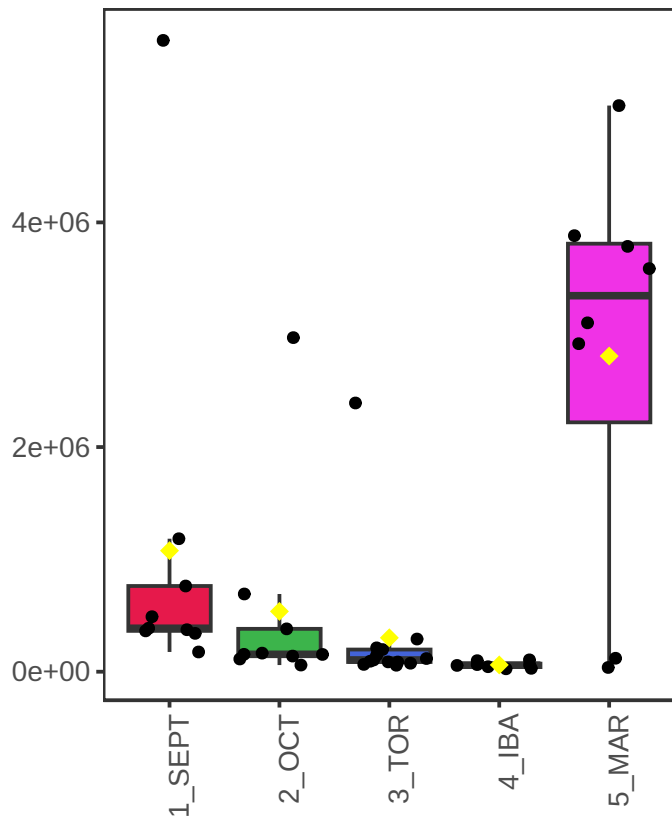


Normalized Conc.

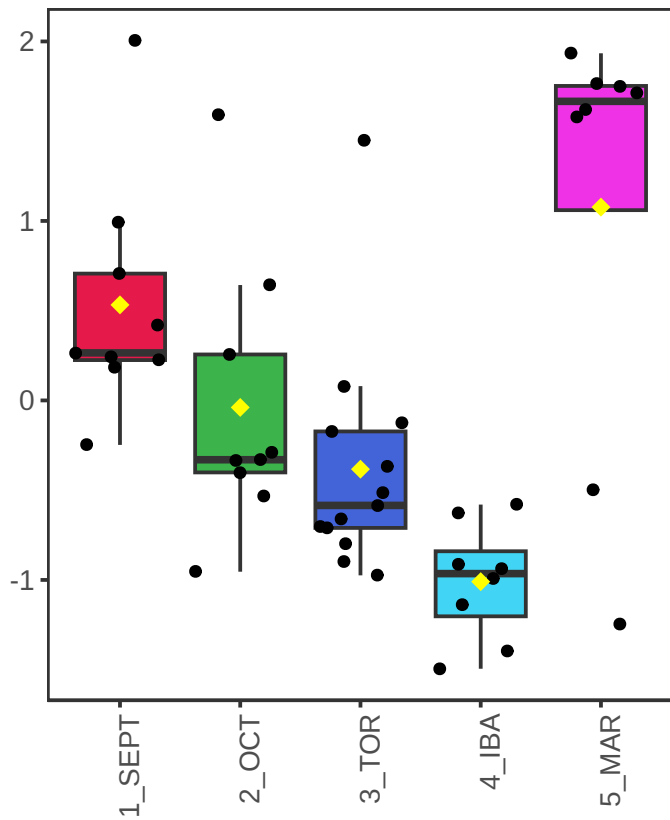


Gentisic acid

Original Conc.

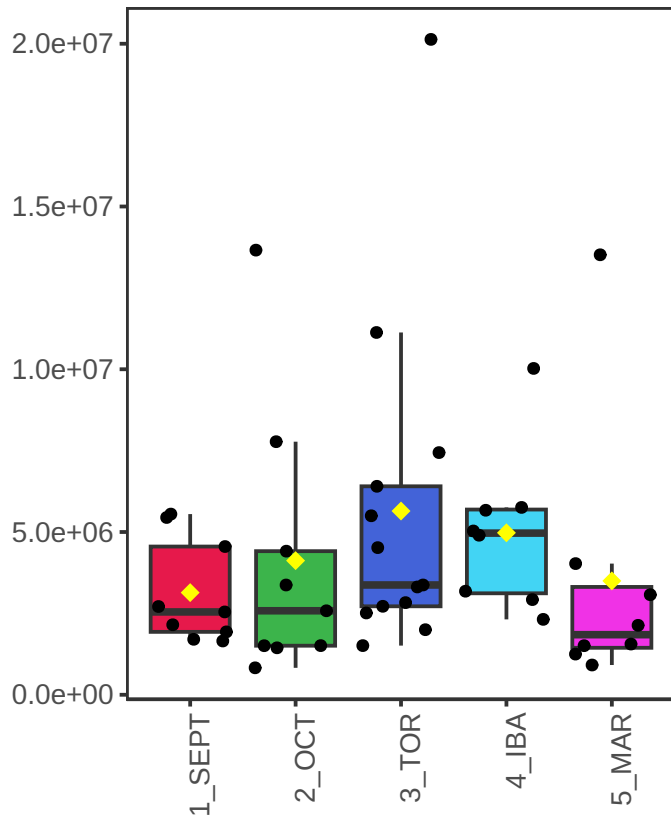


Normalized Conc.

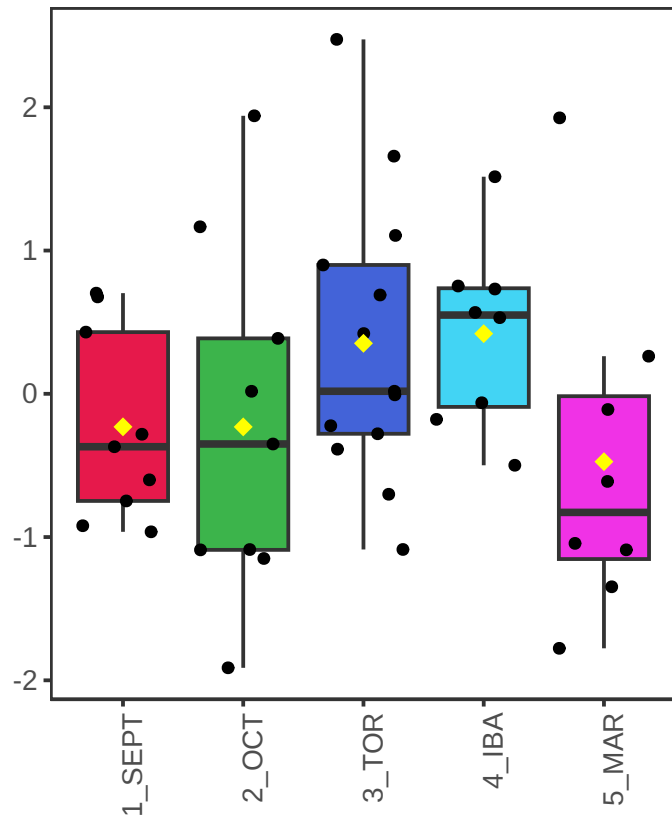


Gluconic acid

Original Conc.

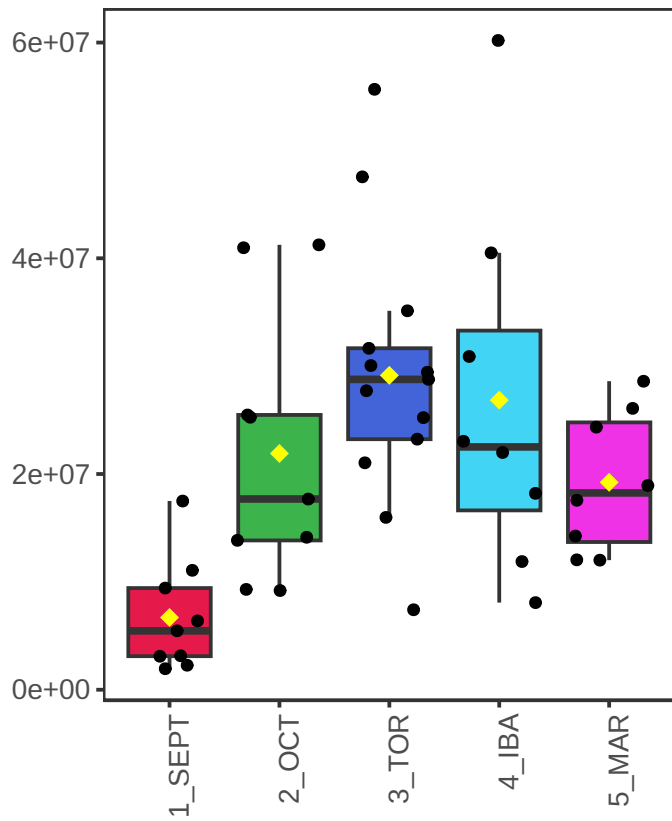


Normalized Conc.

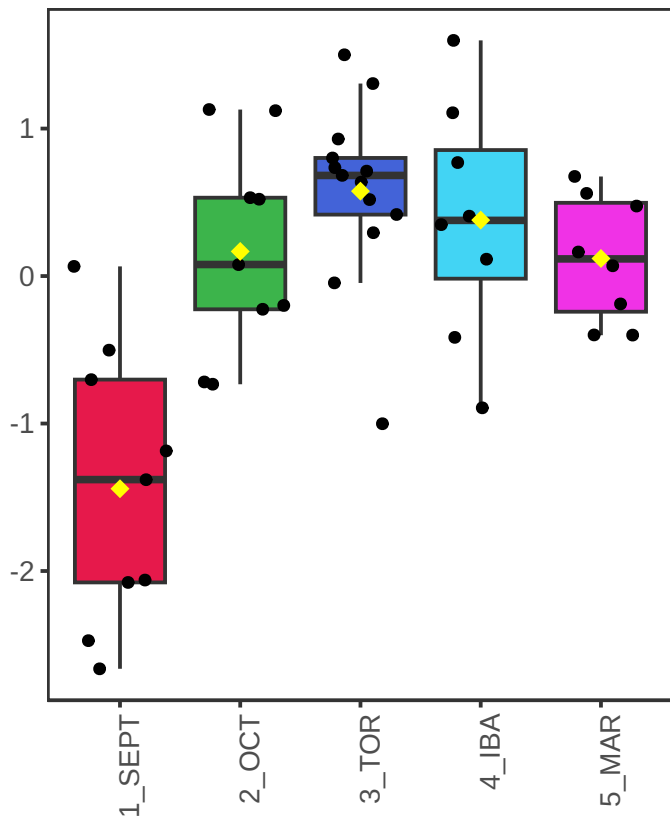


Glucose

Original Conc.

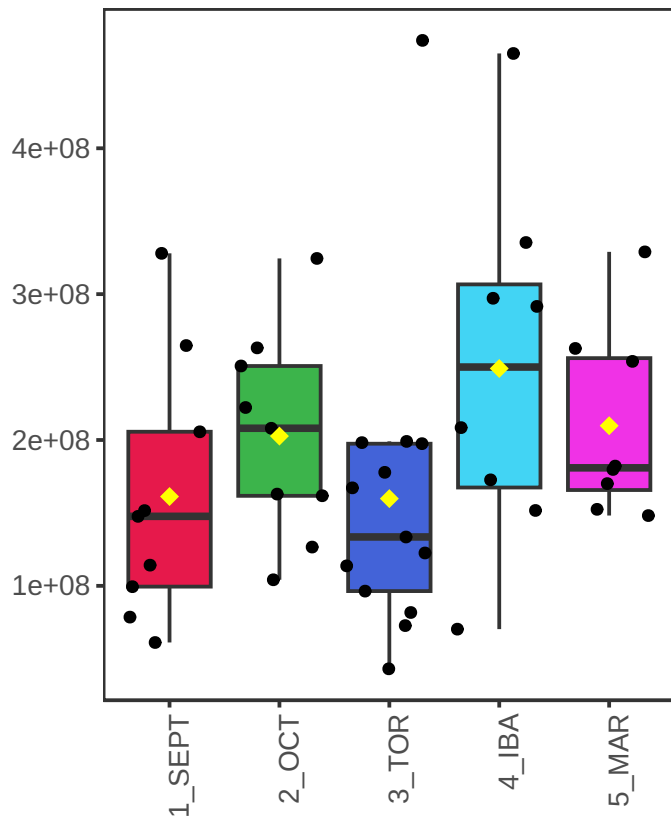


Normalized Conc.

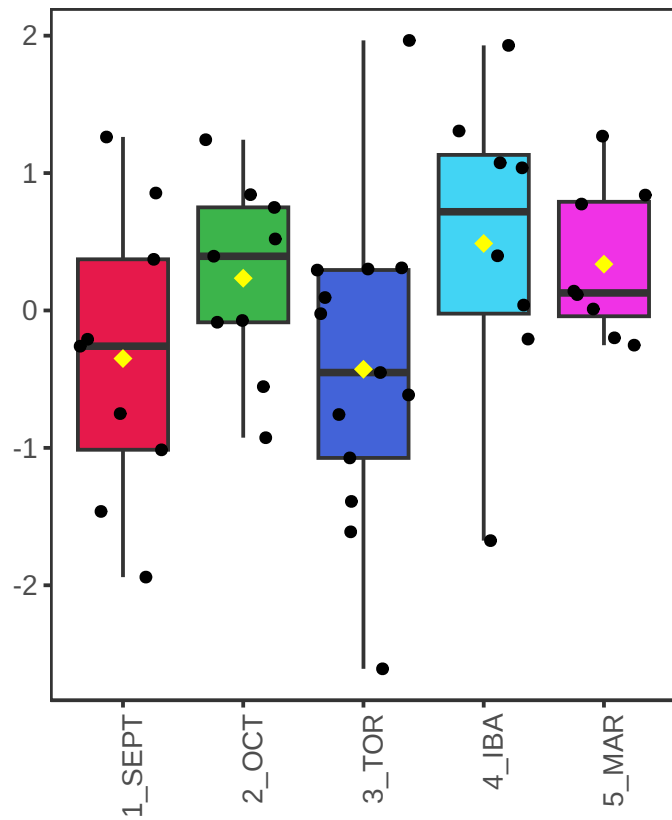


Glutamic acid

Original Conc.

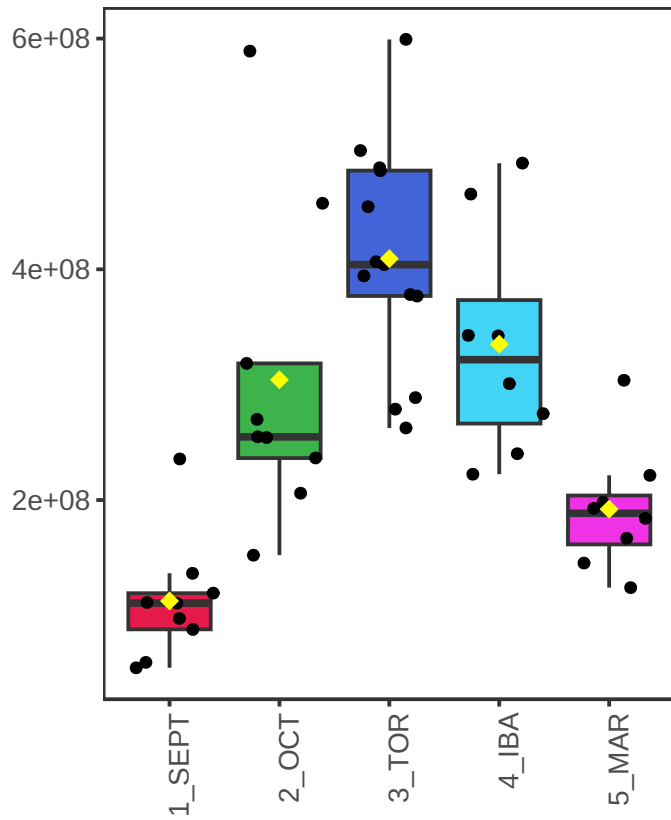


Normalized Conc.

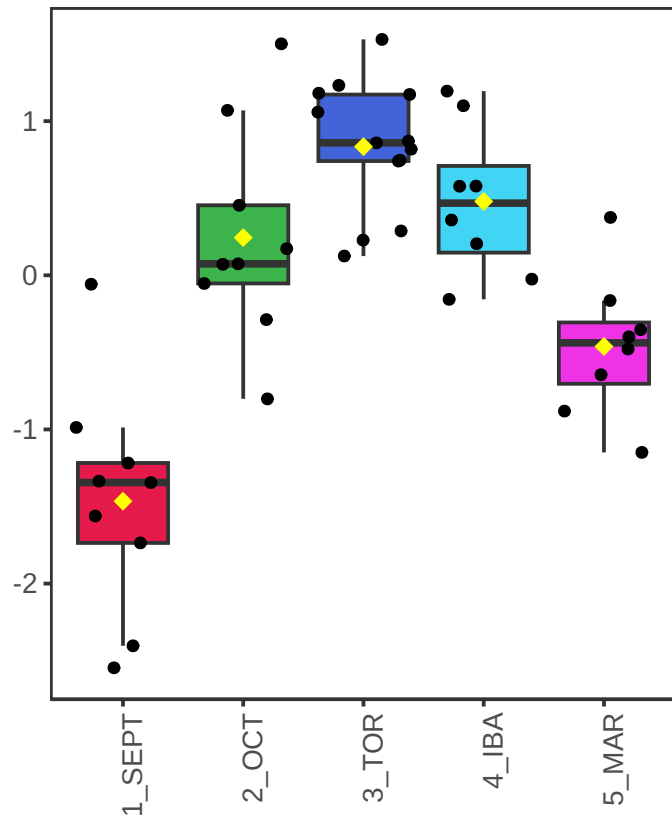


Glutamine

Original Conc.

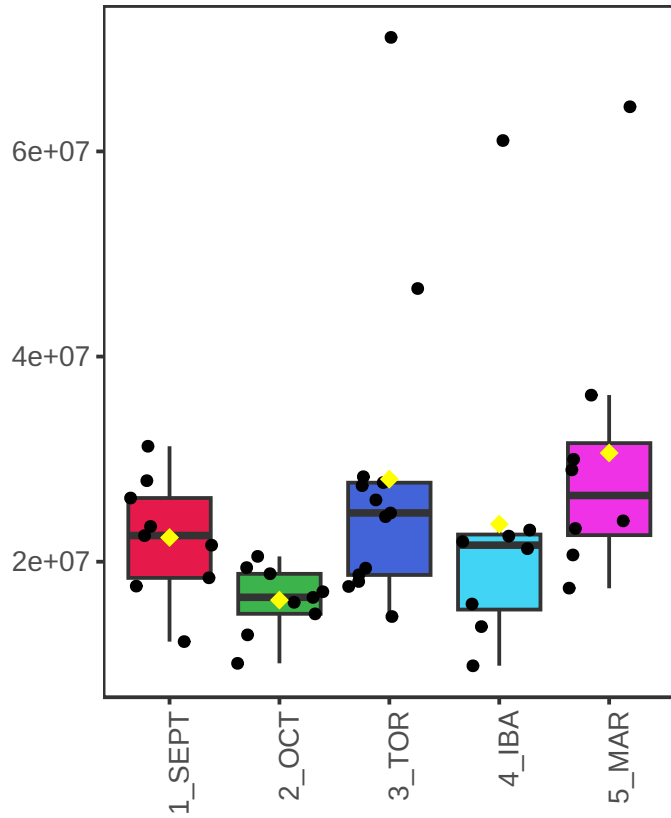


Normalized Conc.

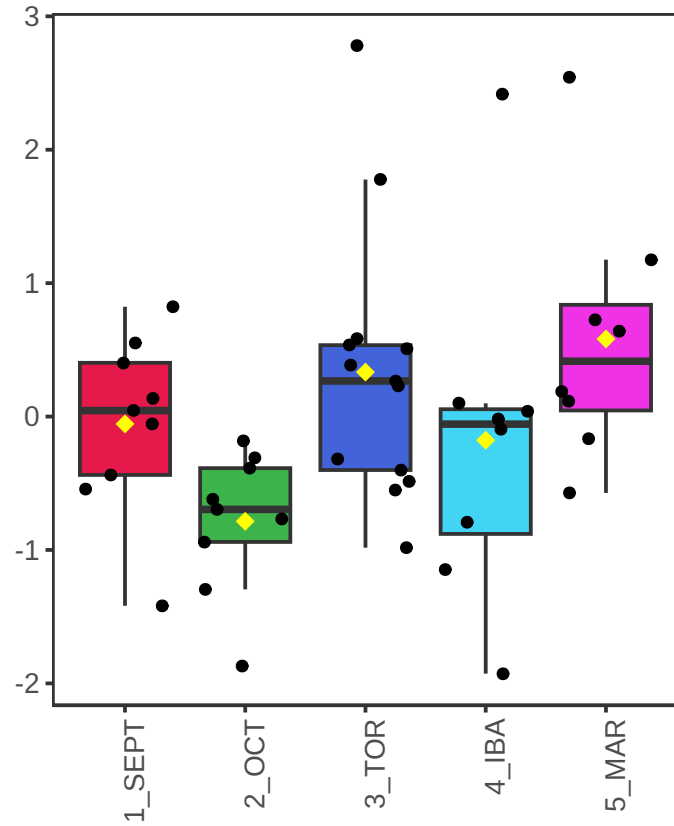


Glutaric acid

Original Conc.

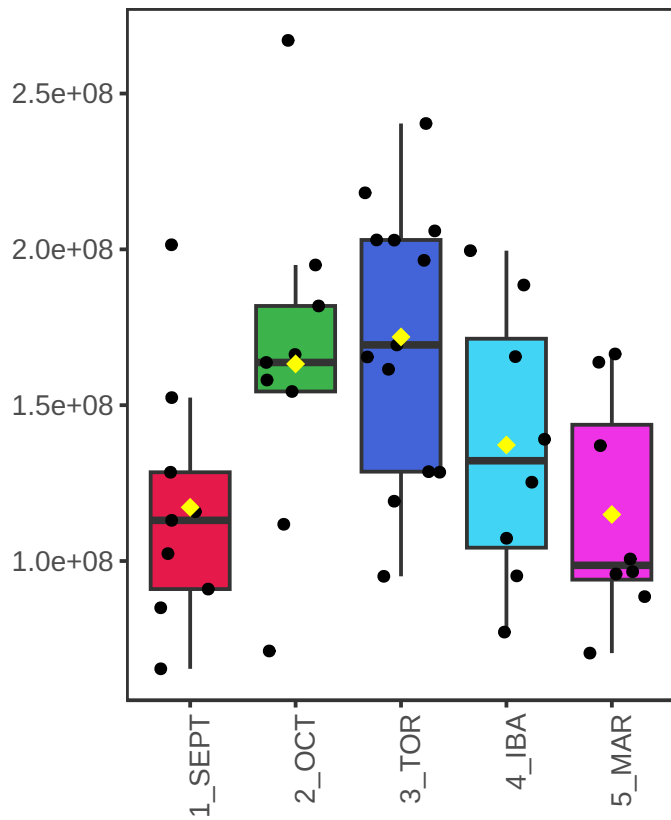


Normalized Conc.

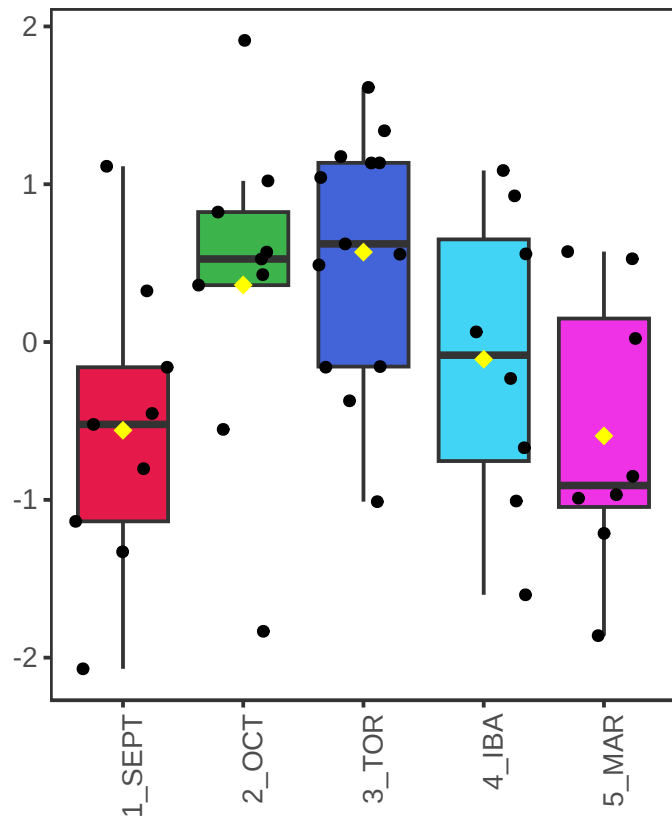


Glutathione

Original Conc.

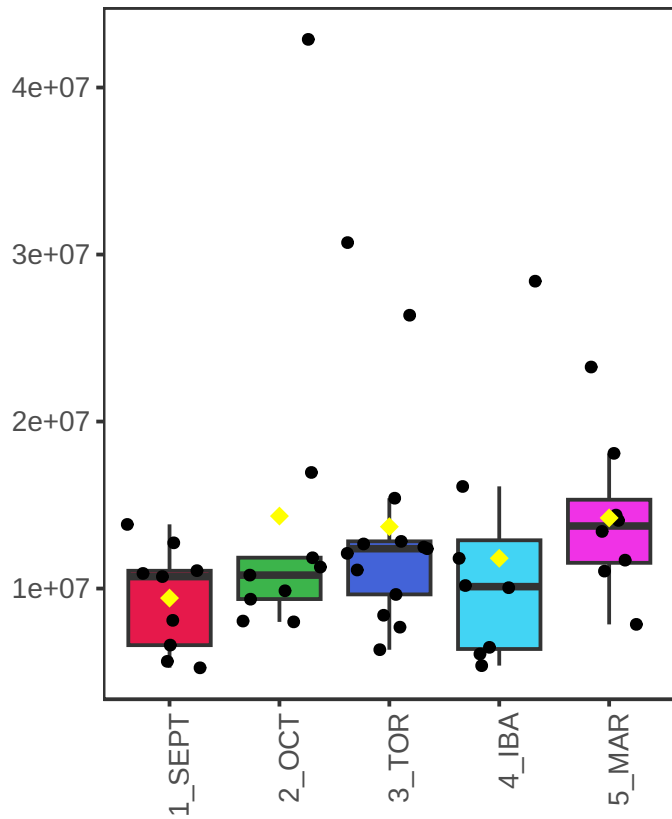


Normalized Conc.

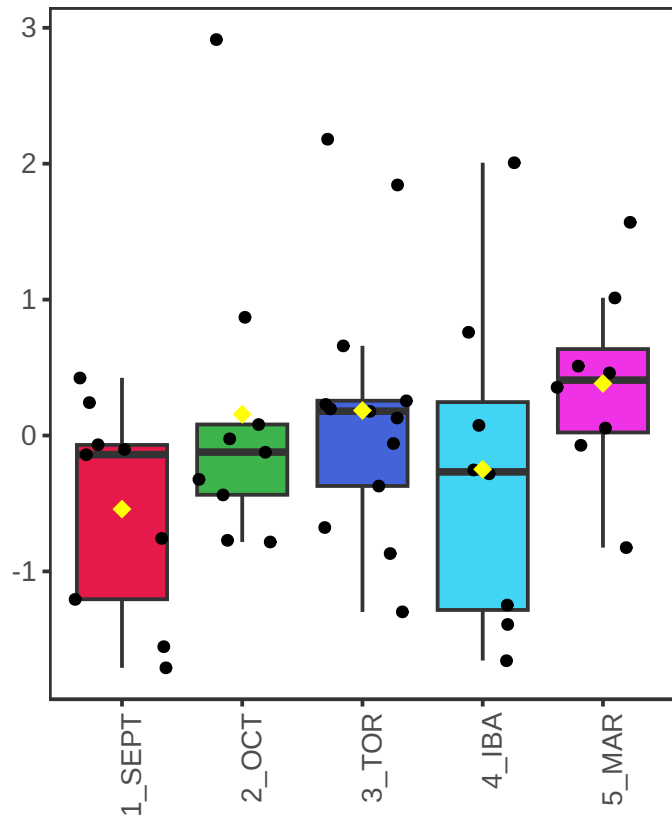


Glycerol 3-phosphate

Original Conc.

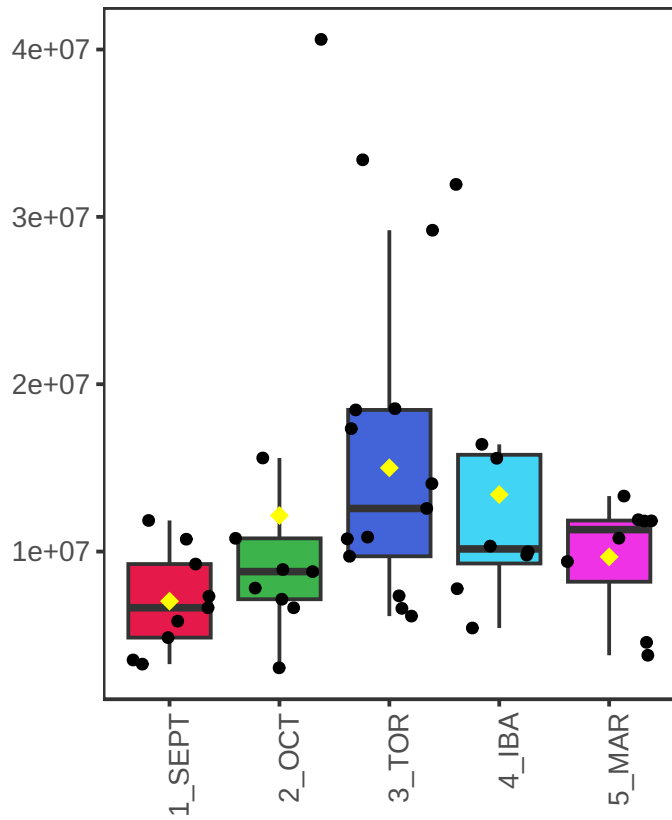


Normalized Conc.

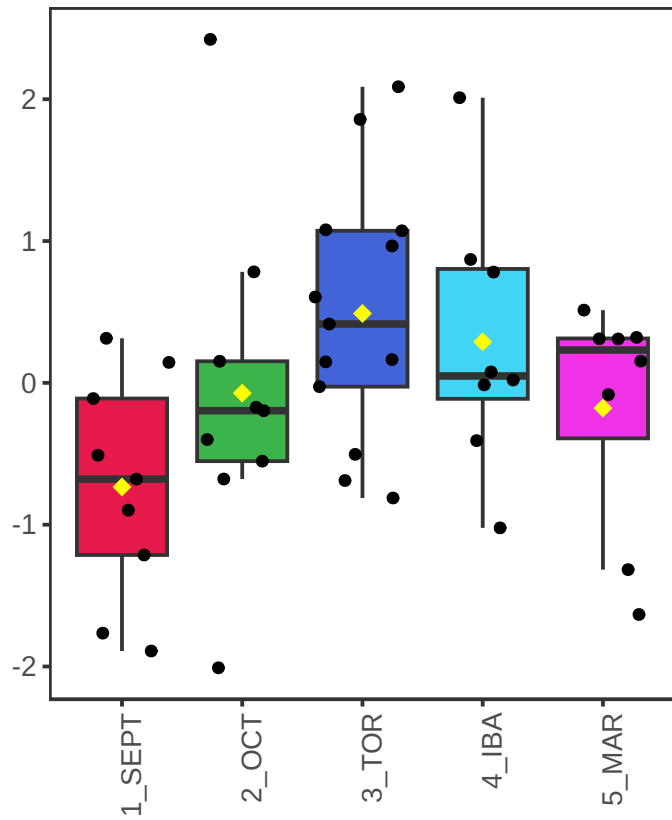


Glycerophosphoglycerol

Original Conc.

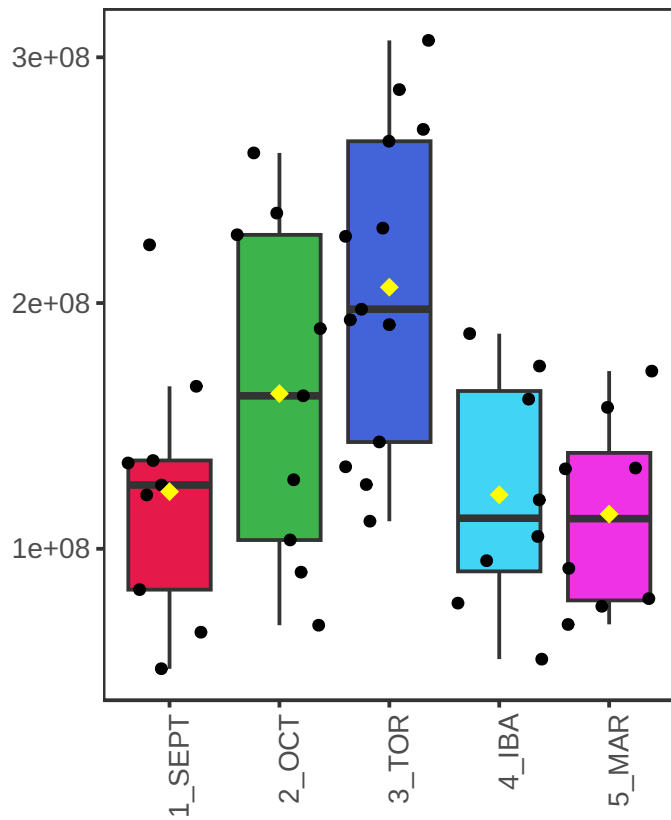


Normalized Conc.

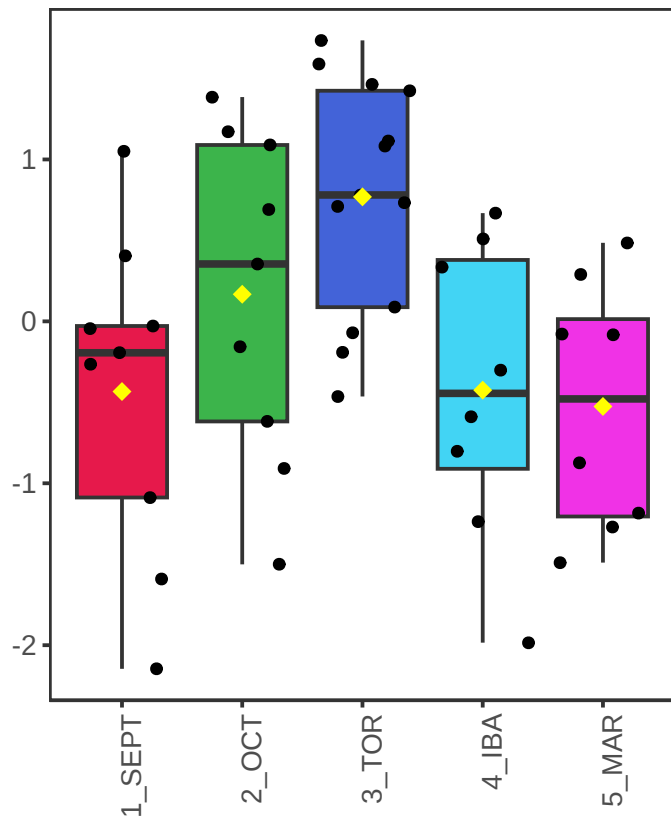


Glycerolphosphorylethanolamine

Original Conc.

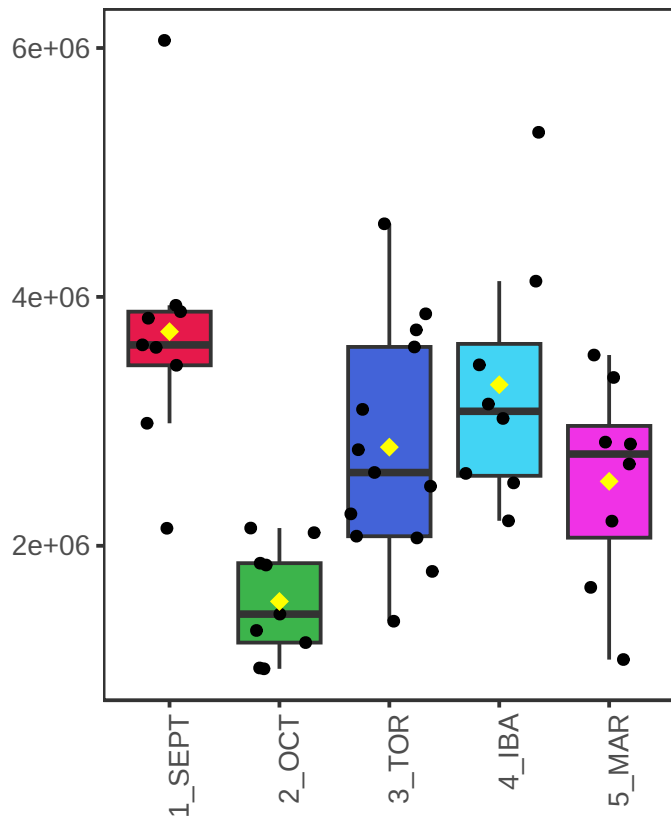


Normalized Conc.

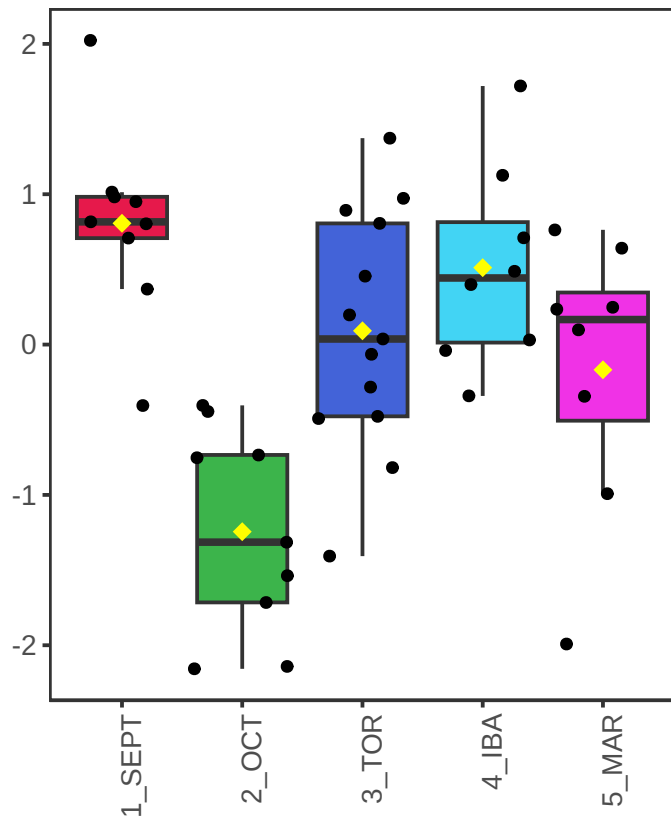


Glycine

Original Conc.

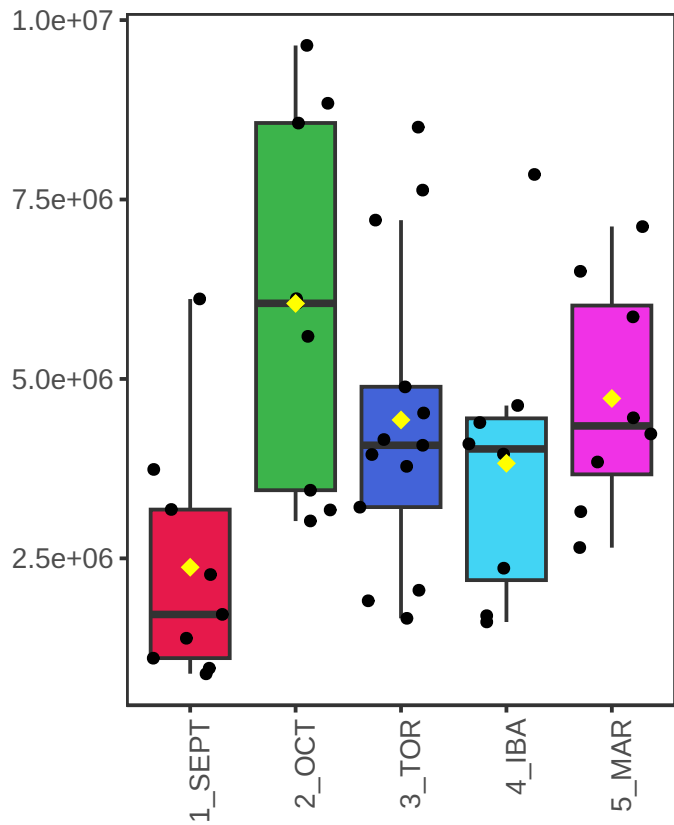


Normalized Conc.

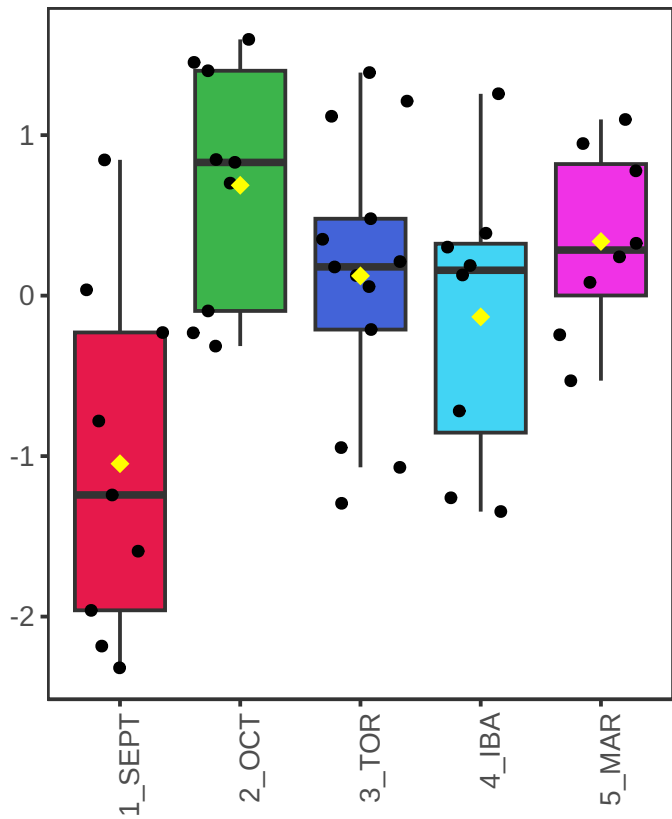


Guanine

Original Conc.

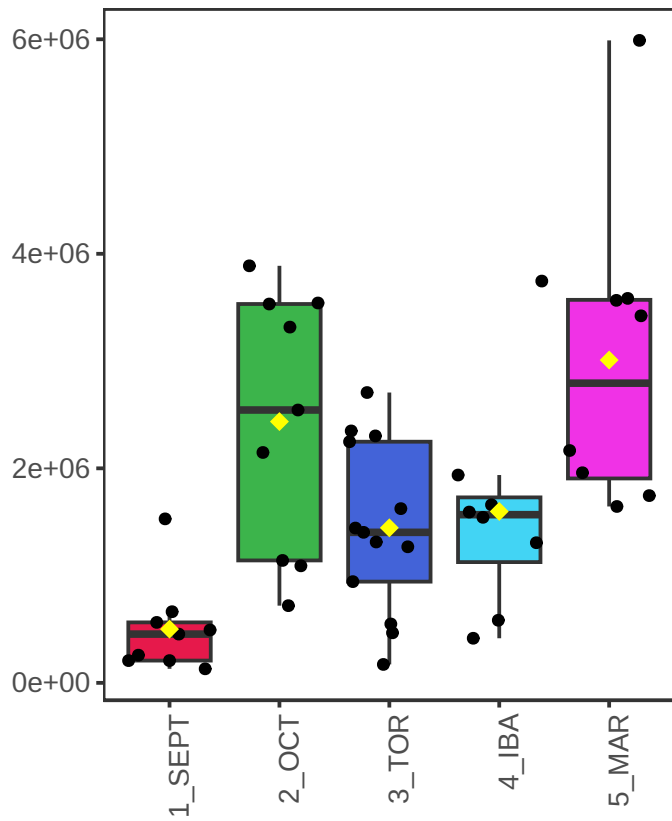


Normalized Conc.

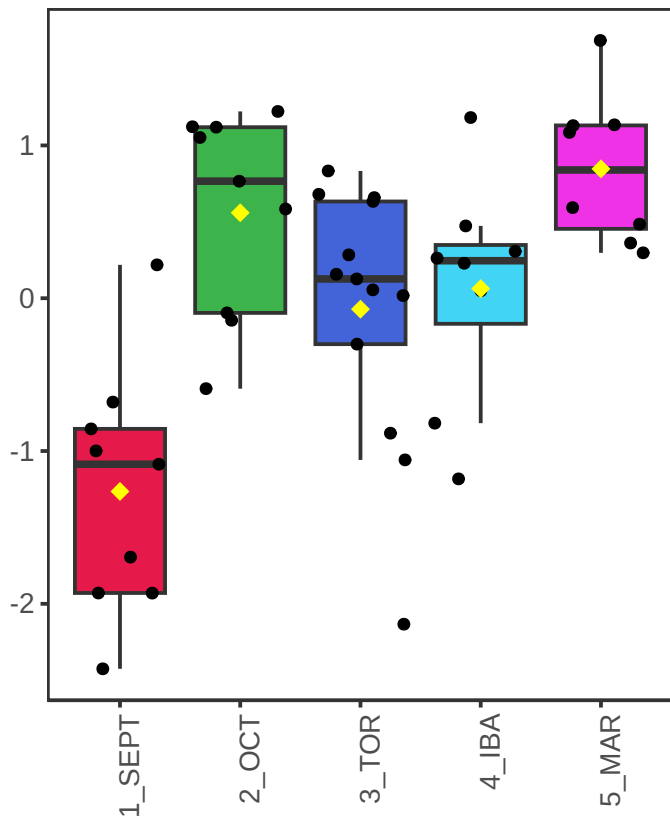


Guanosine

Original Conc.

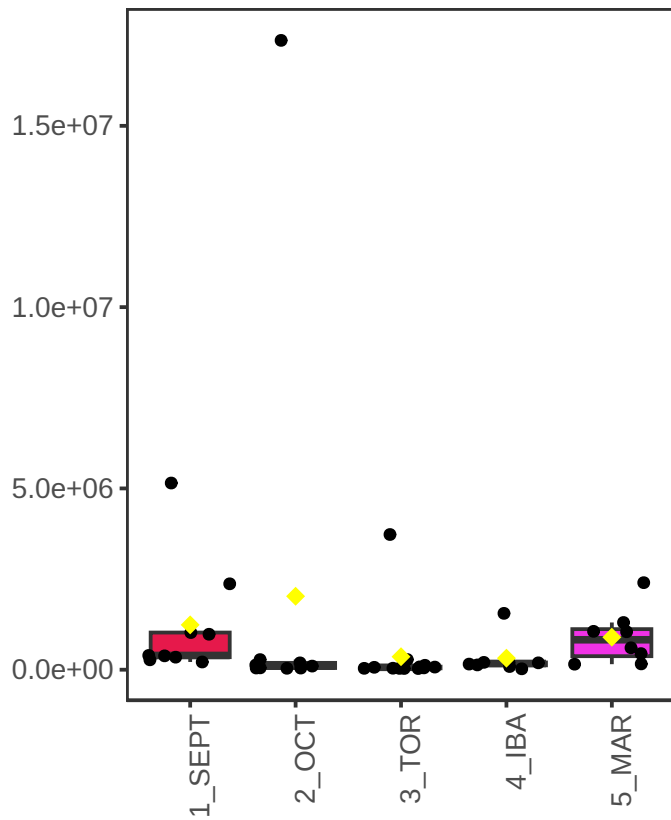


Normalized Conc.

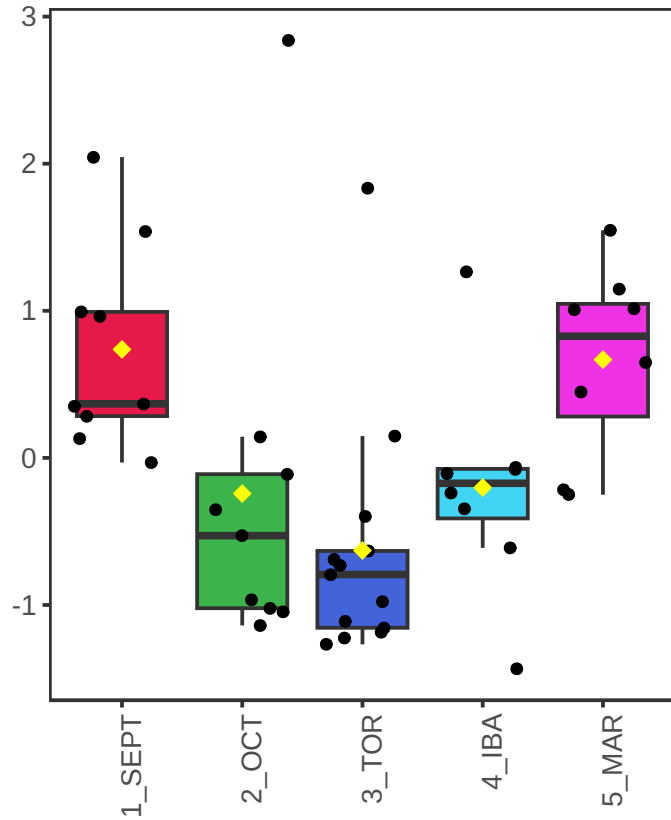


Hypotaurine

Original Conc.

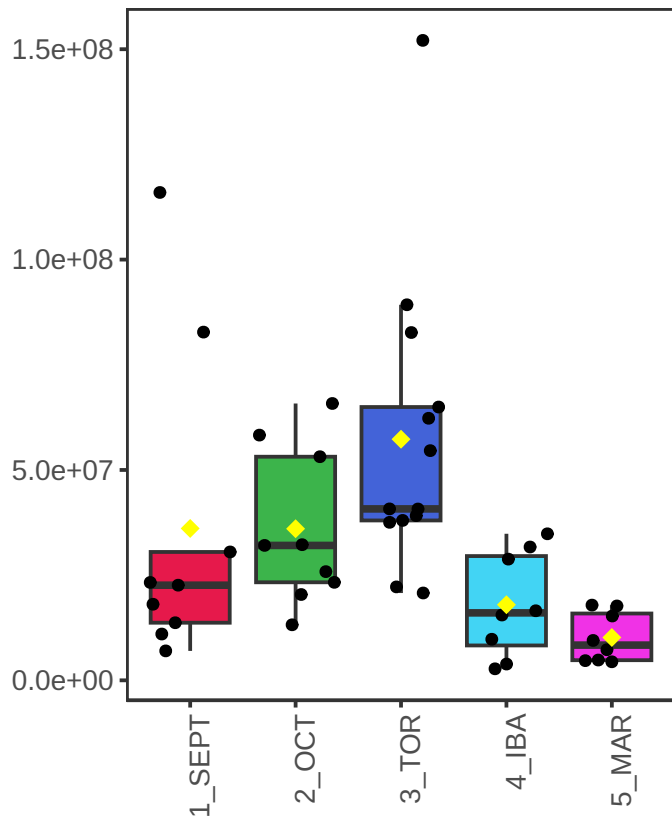


Normalized Conc.

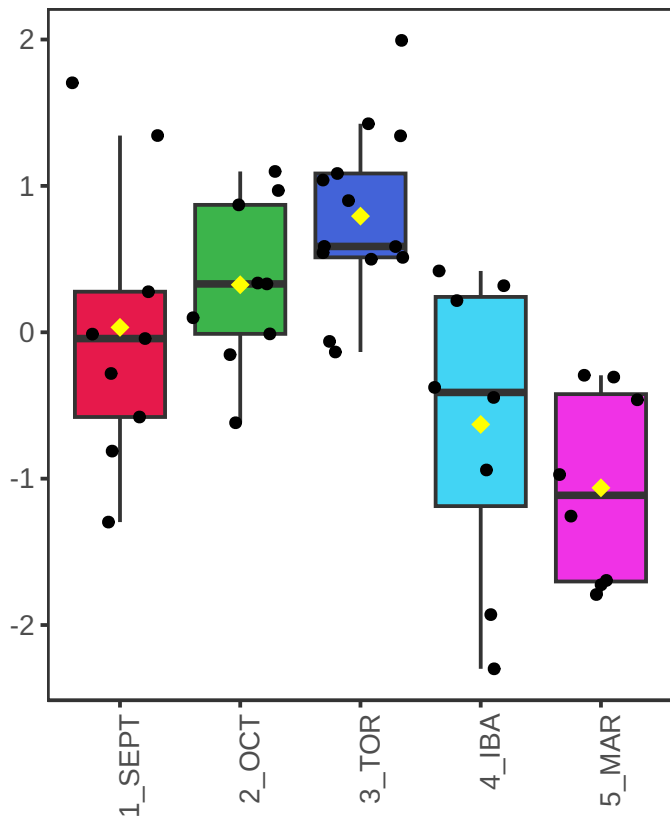


Indoxyl sulfate

Original Conc.

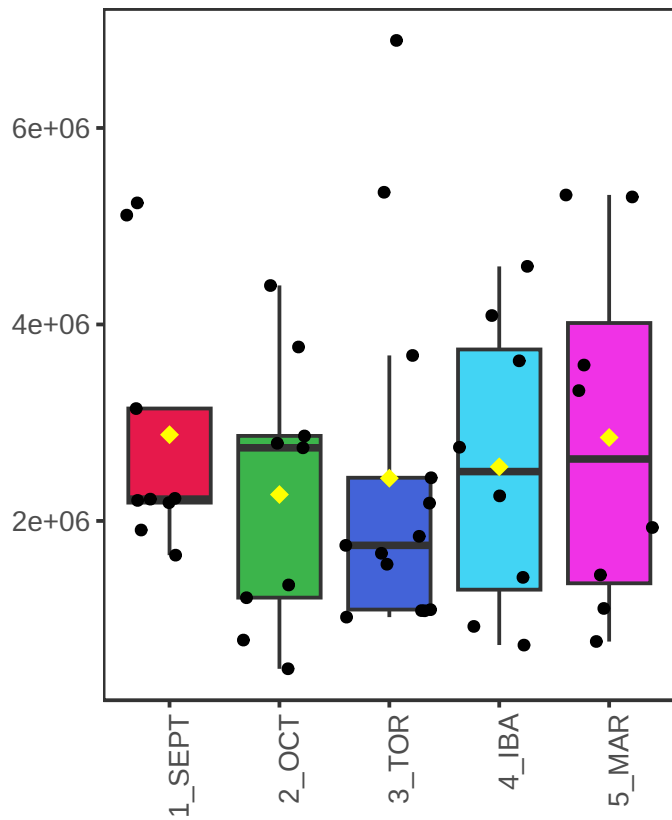


Normalized Conc.

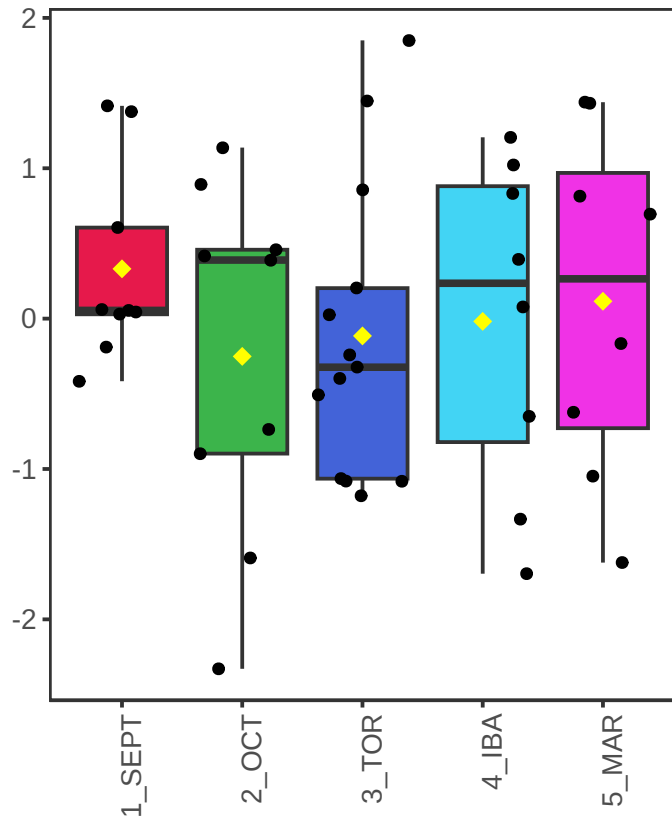


Inosine-5'-monophosphate (IMP)

Original Conc.

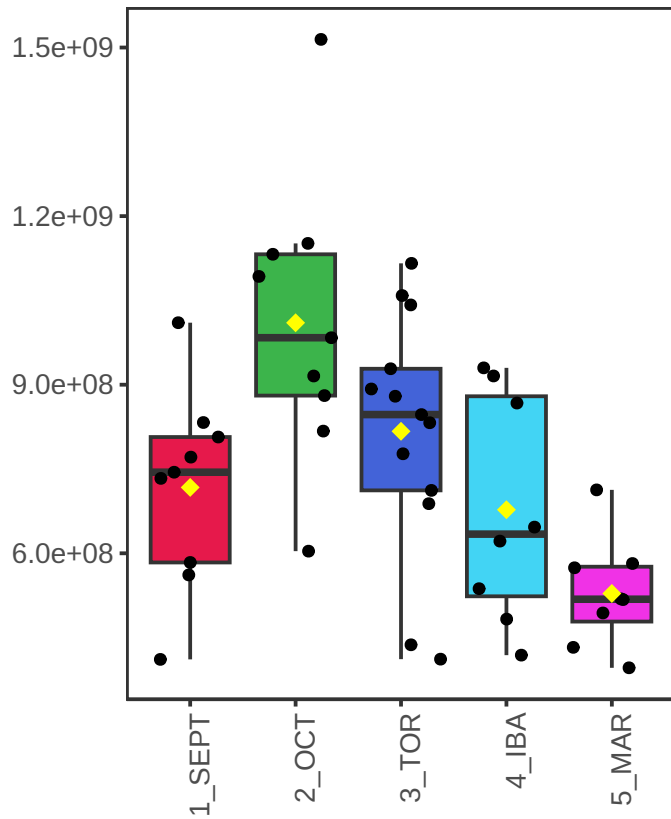


Normalized Conc.

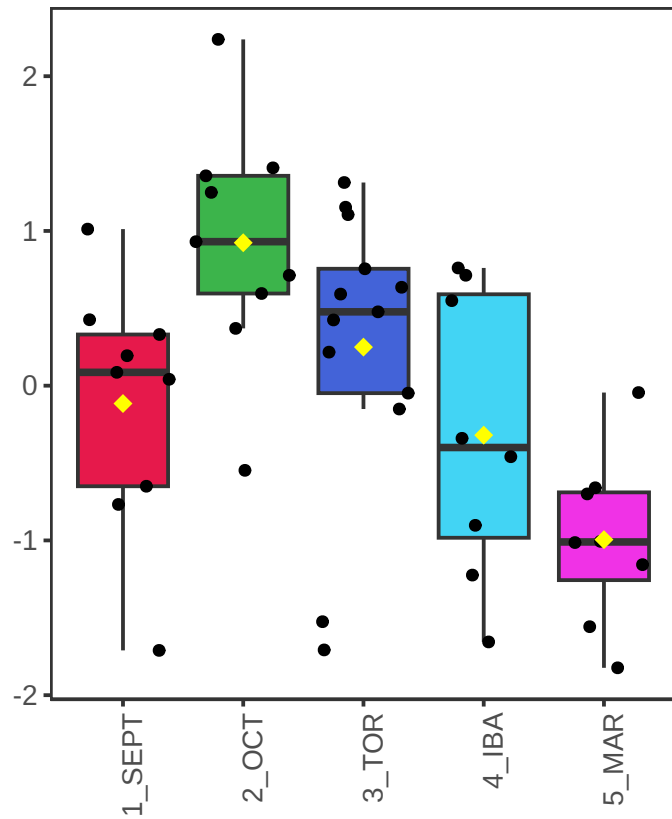


Inositol

Original Conc.

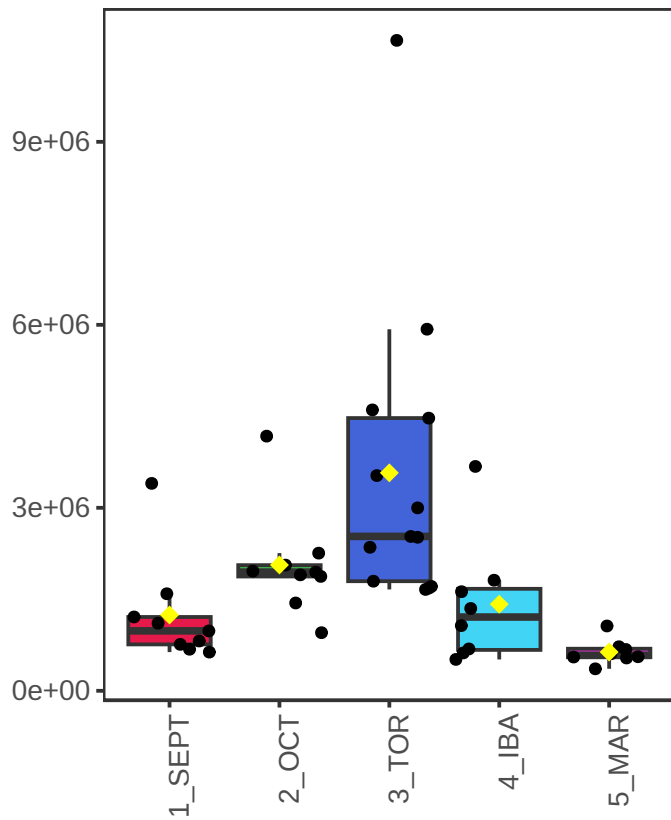


Normalized Conc.

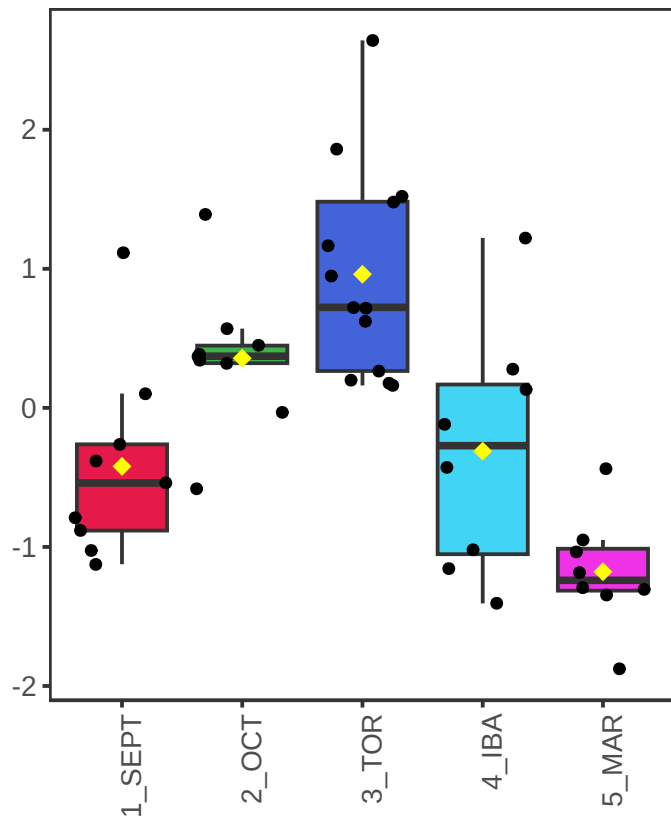


Isethionic acid

Original Conc.

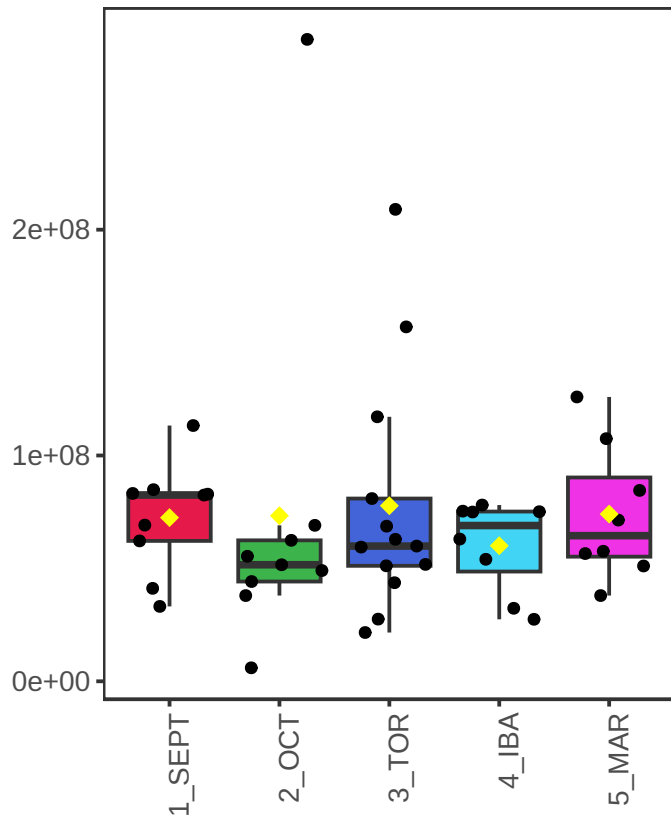


Normalized Conc.

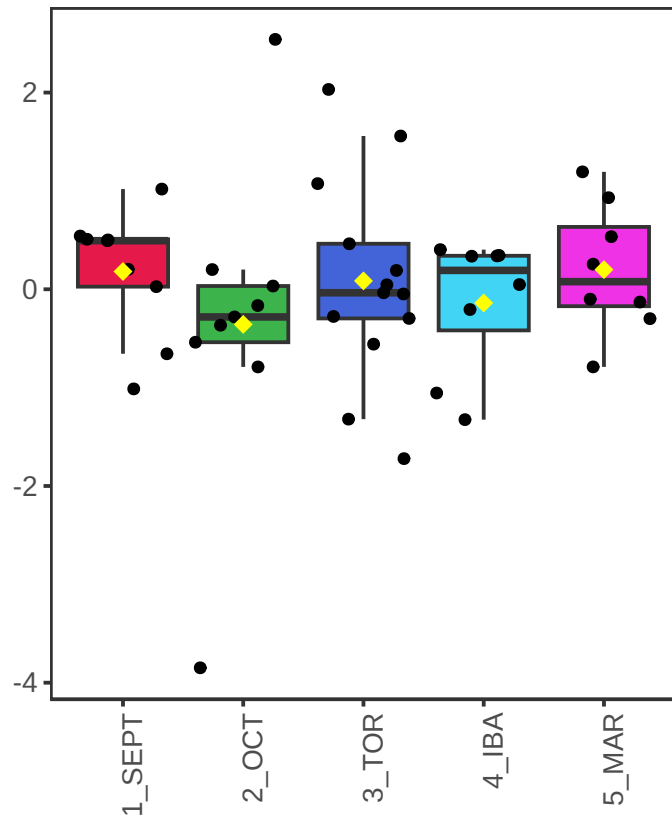


Itaconic acid

Original Conc.

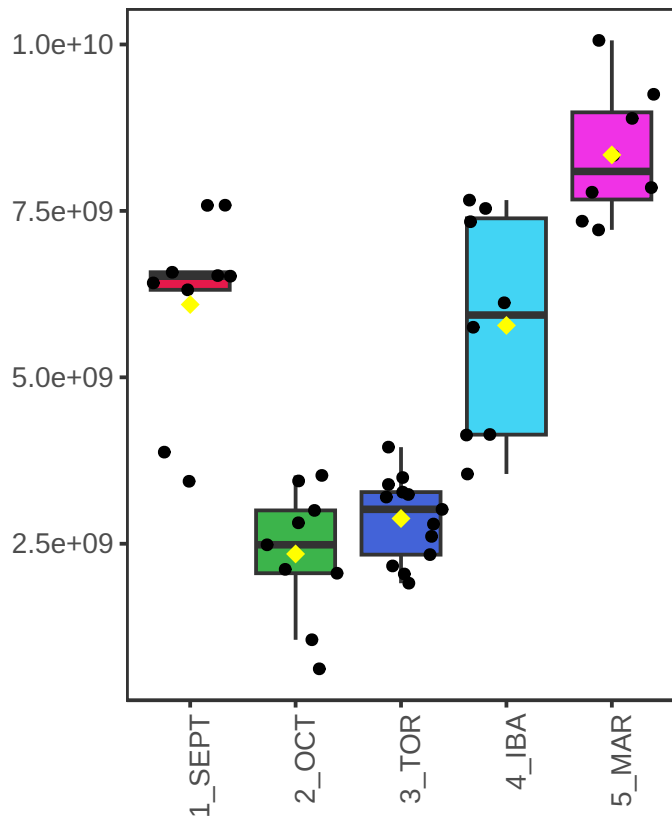


Normalized Conc.

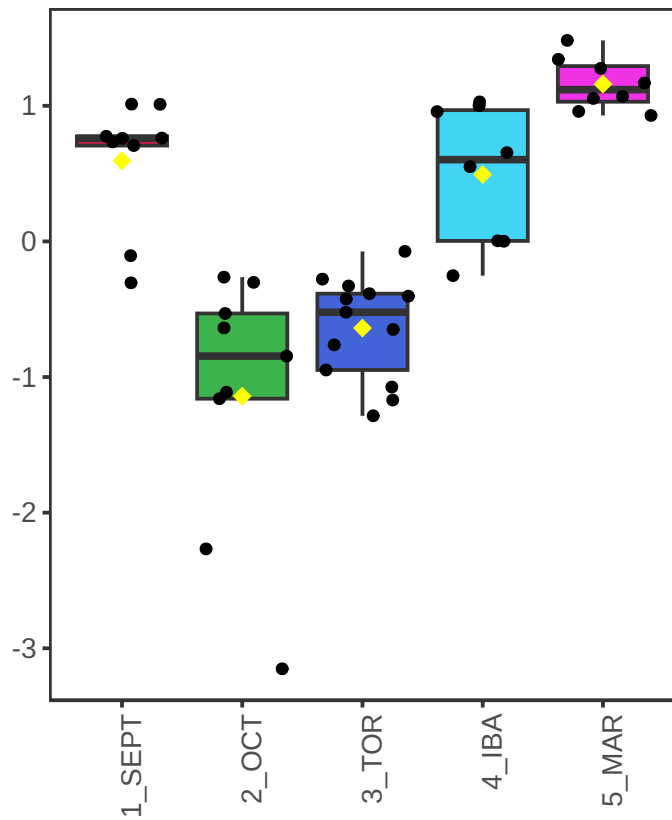


Lactic acid

Original Conc.

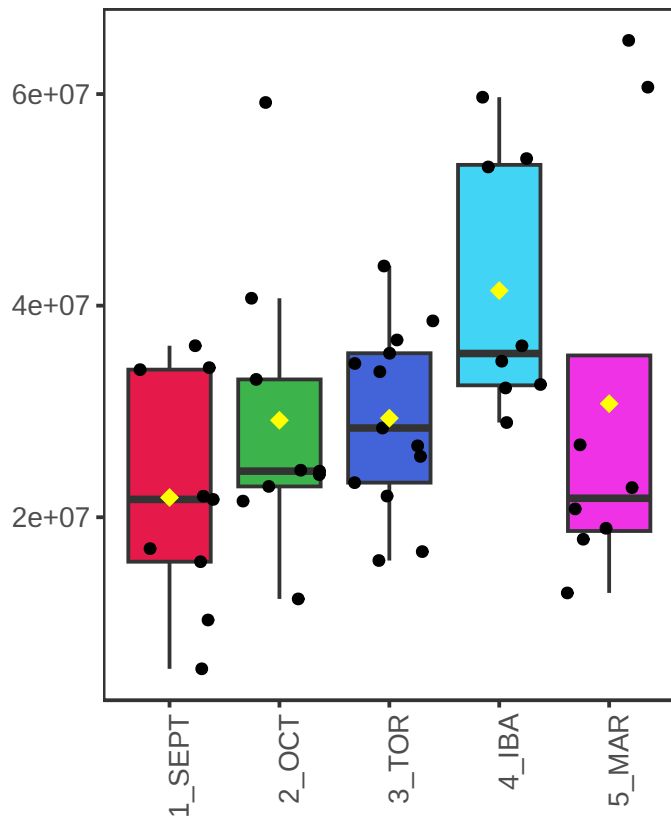


Normalized Conc.

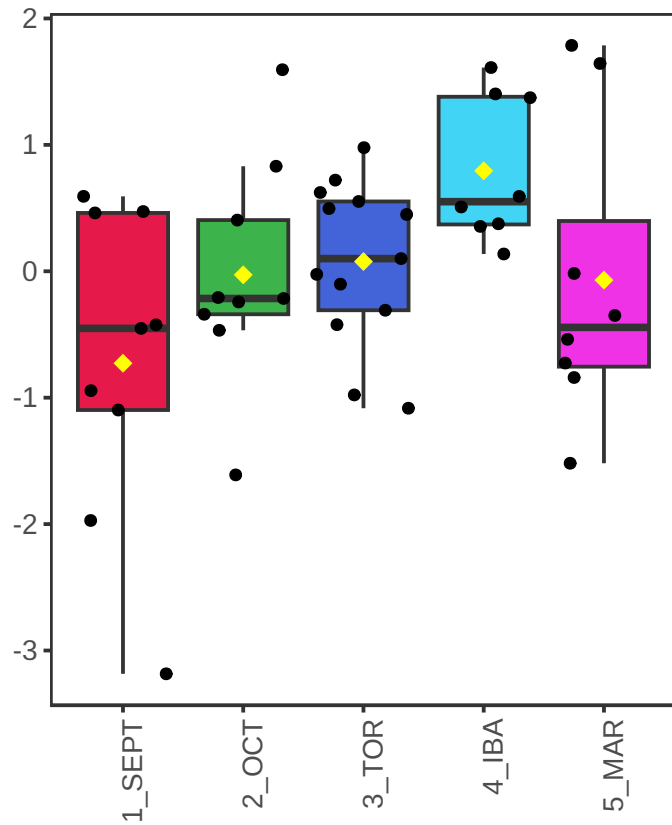


Levulinic acid

Original Conc.

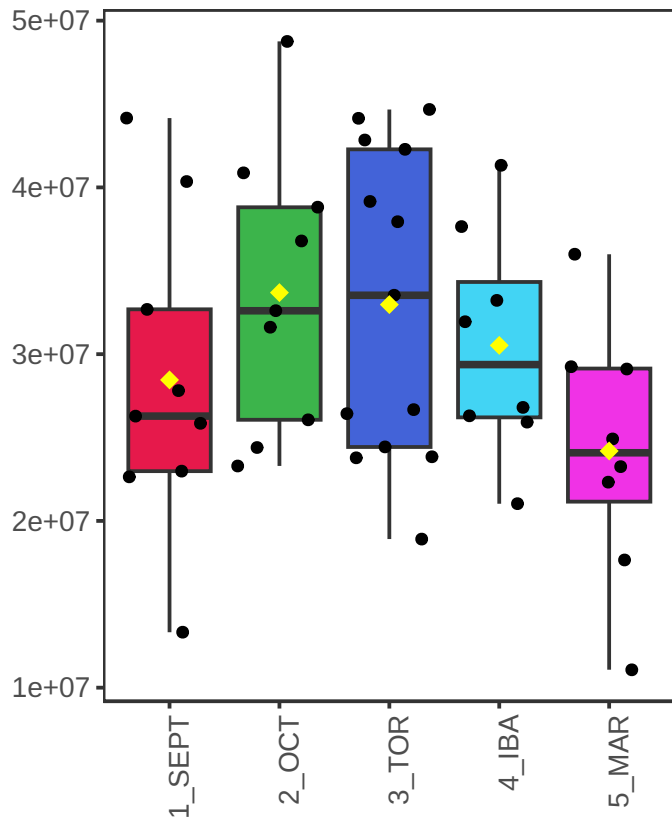


Normalized Conc.

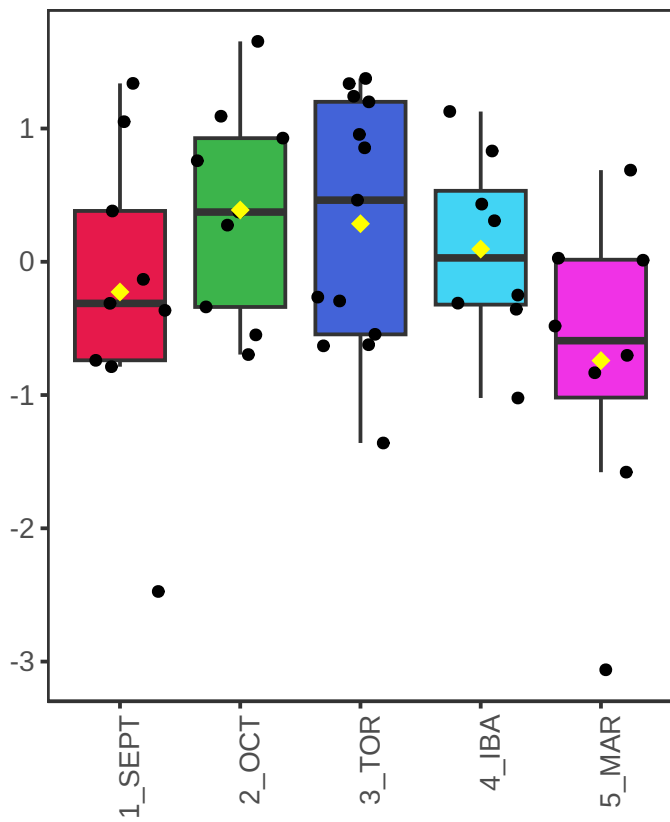


Meglumine

Original Conc.

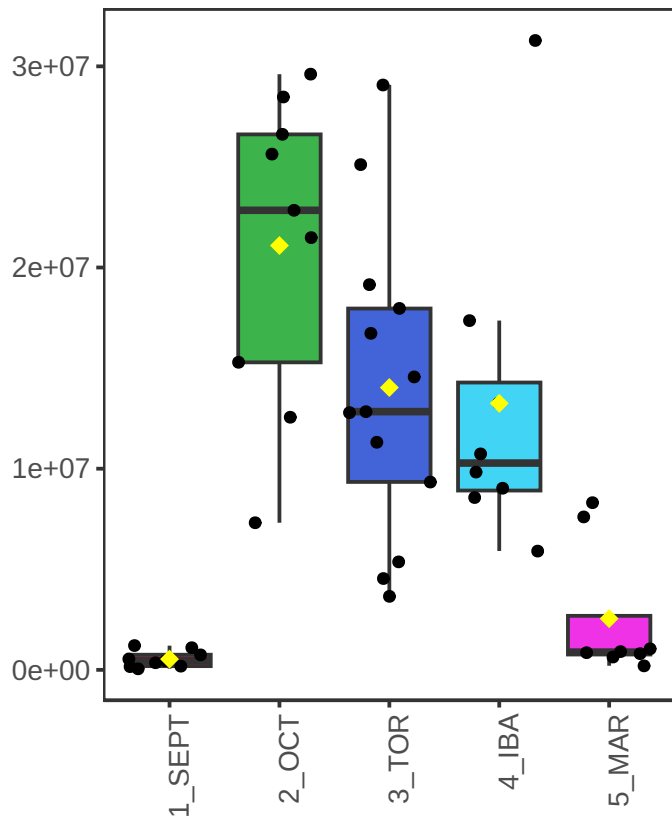


Normalized Conc.

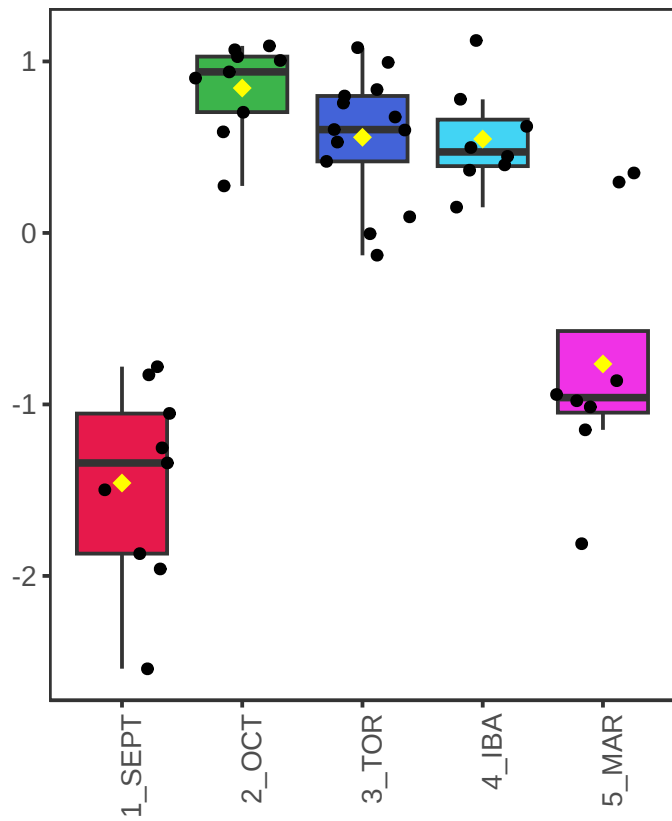


Methanesulfonic acid

Original Conc.

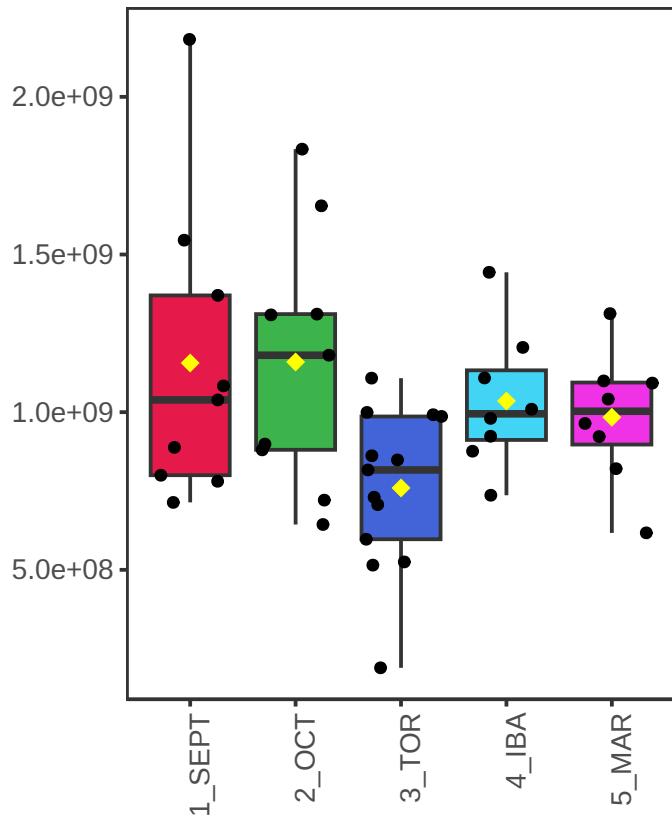


Normalized Conc.

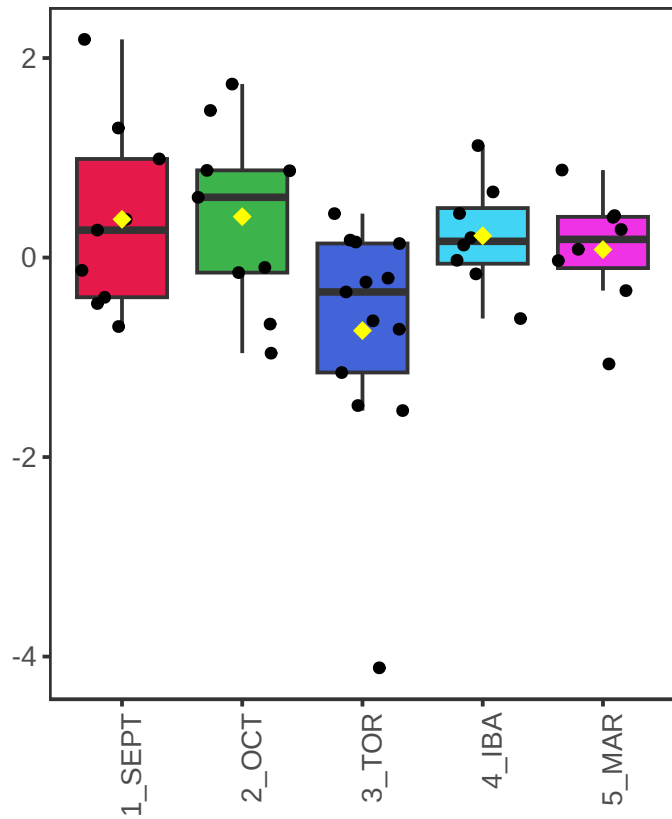


Methylmalonic acid

Original Conc.

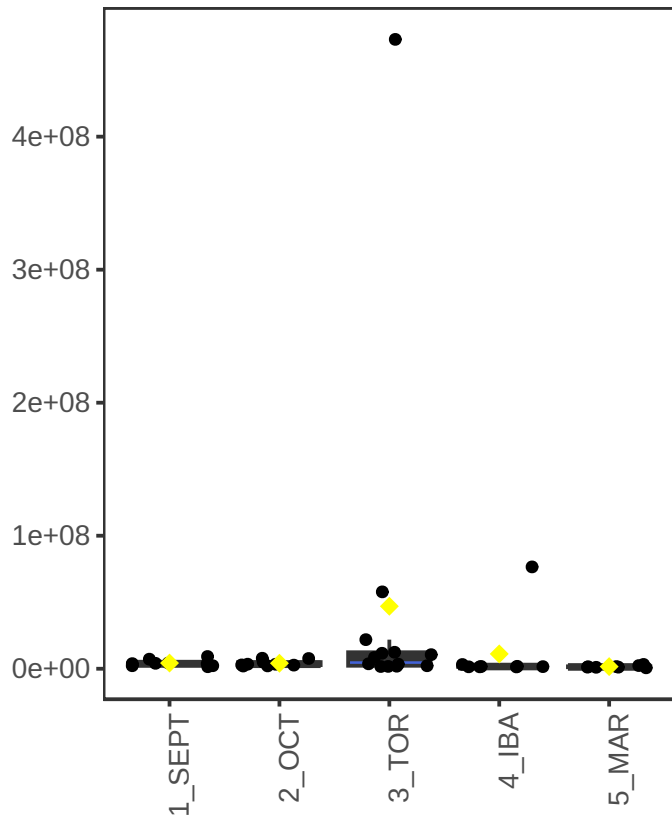


Normalized Conc.

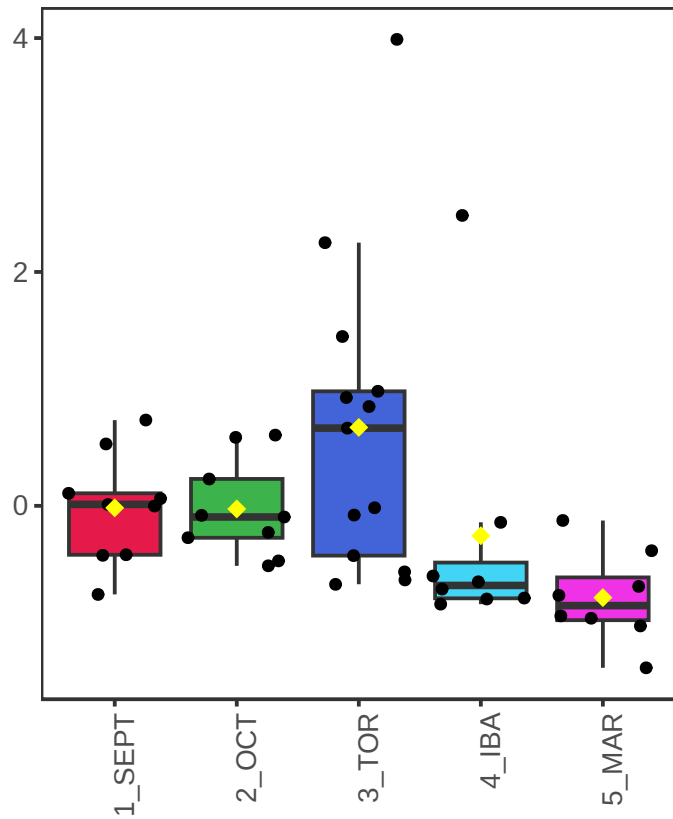


Methyl salicylate

Original Conc.

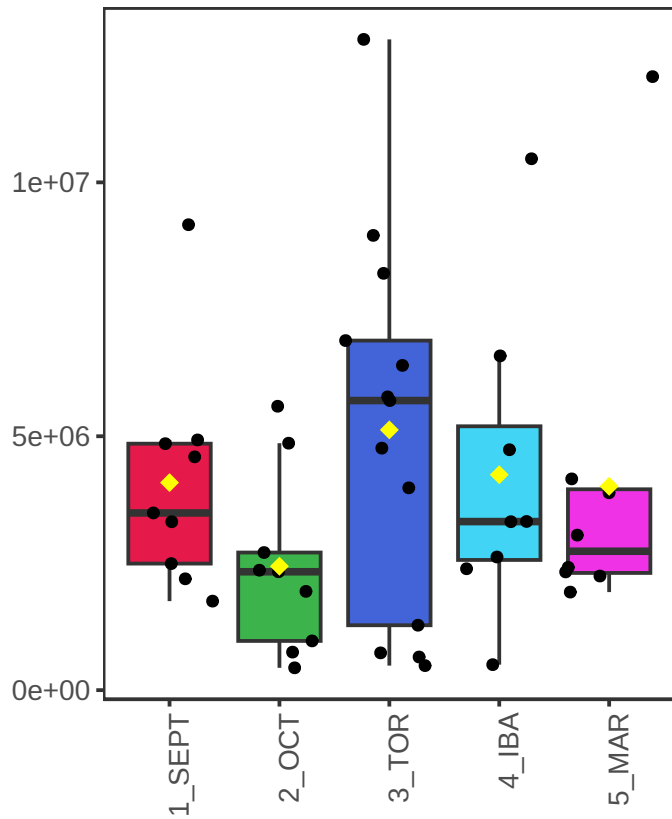


Normalized Conc.

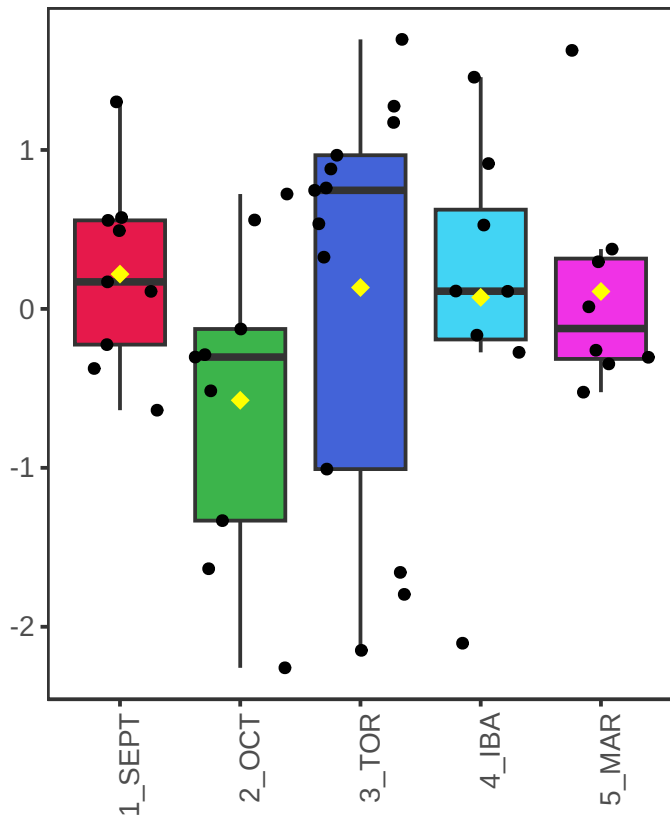


Mevalonic acid

Original Conc.

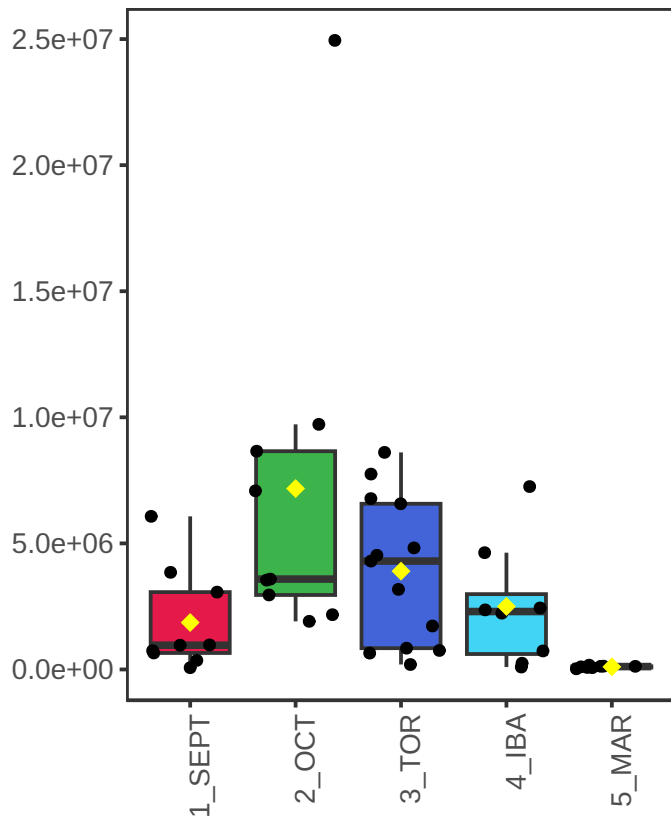


Normalized Conc.

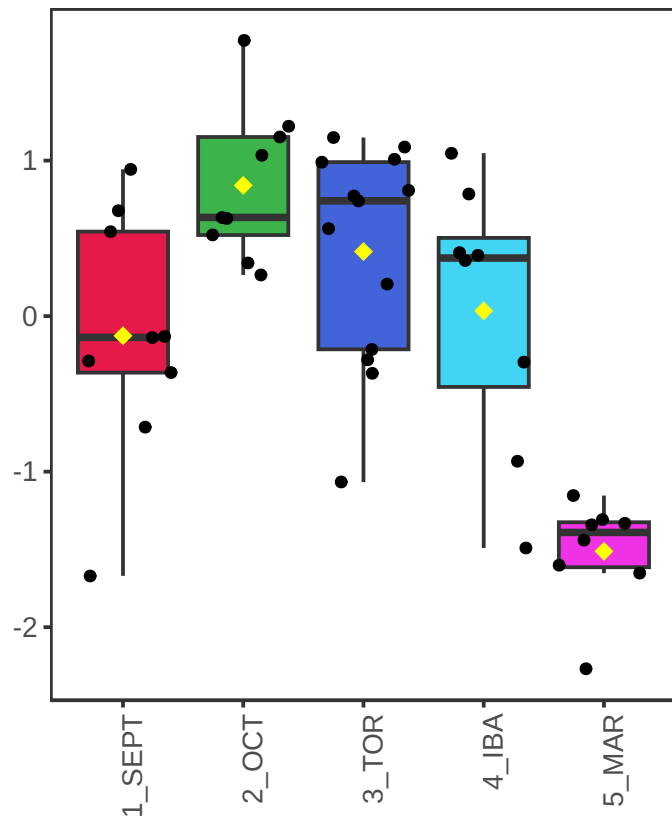


Myristyl sulfate

Original Conc.

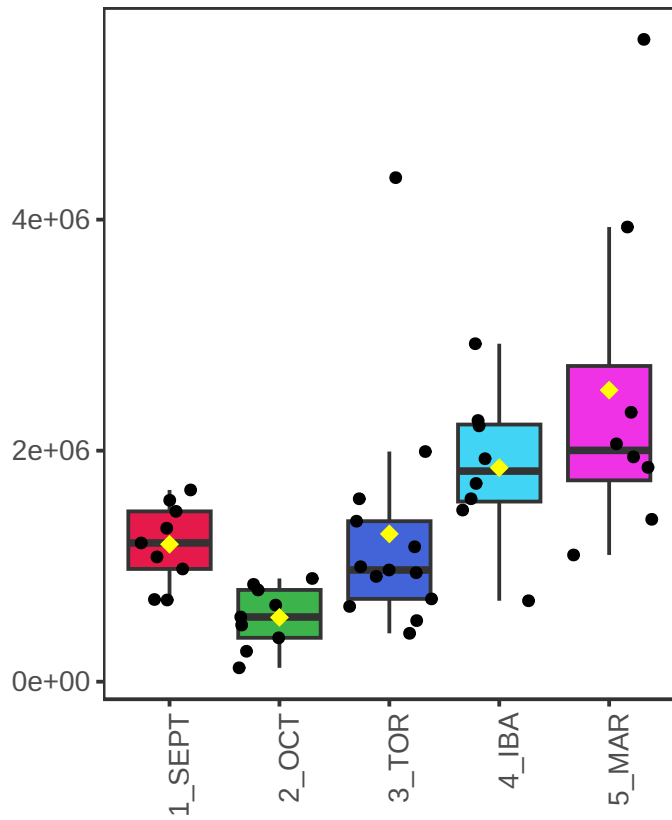


Normalized Conc.

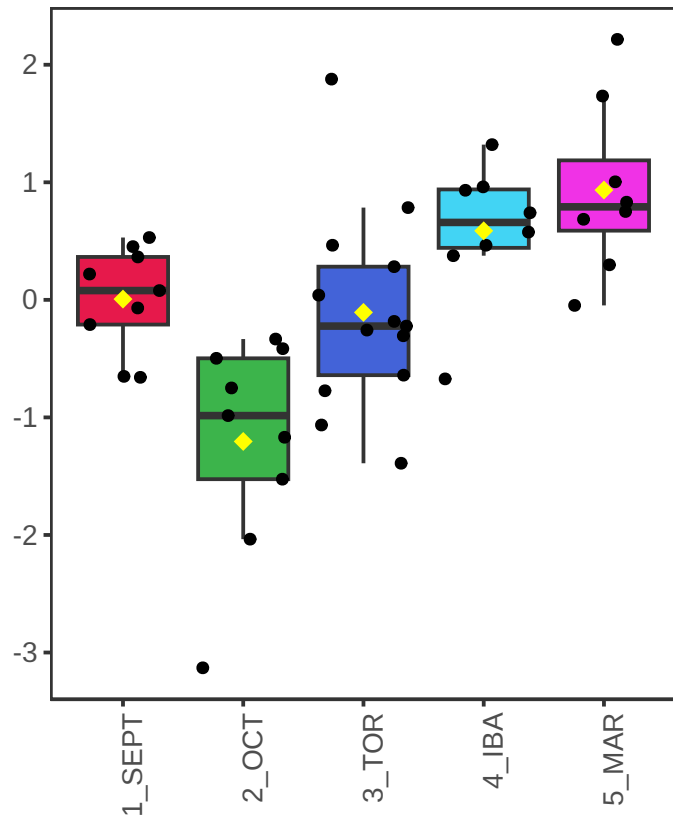


N-Acetylalanine

Original Conc.

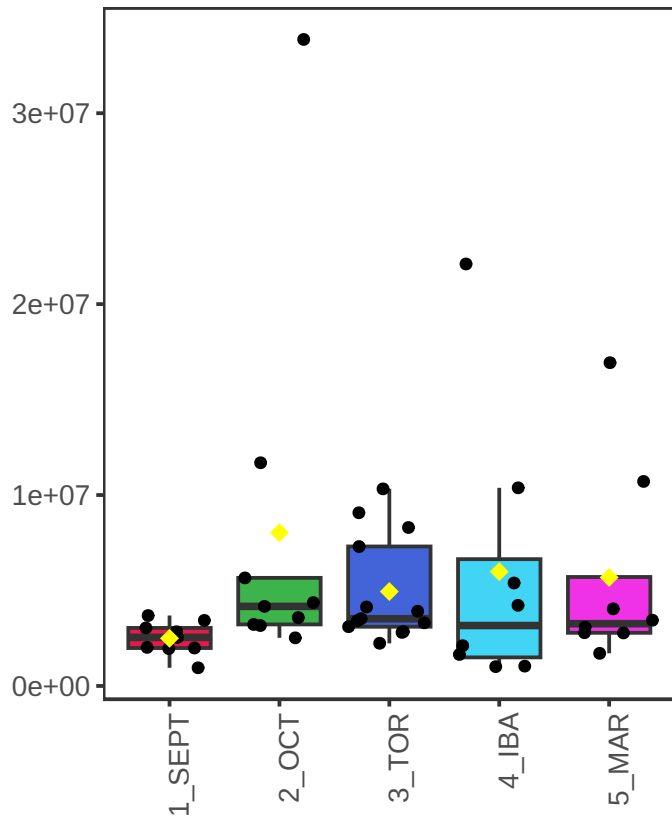


Normalized Conc.

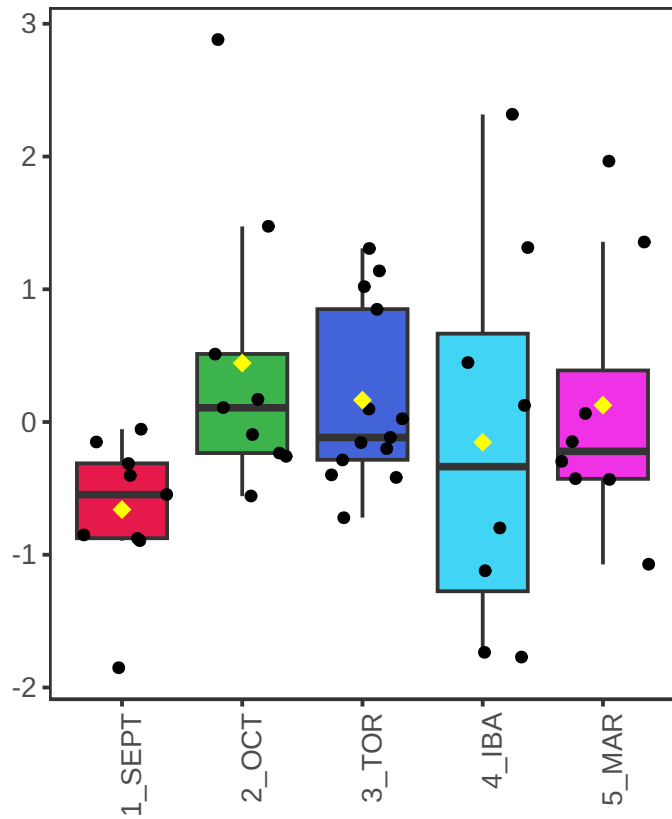


n-Butyl lactate

Original Conc.

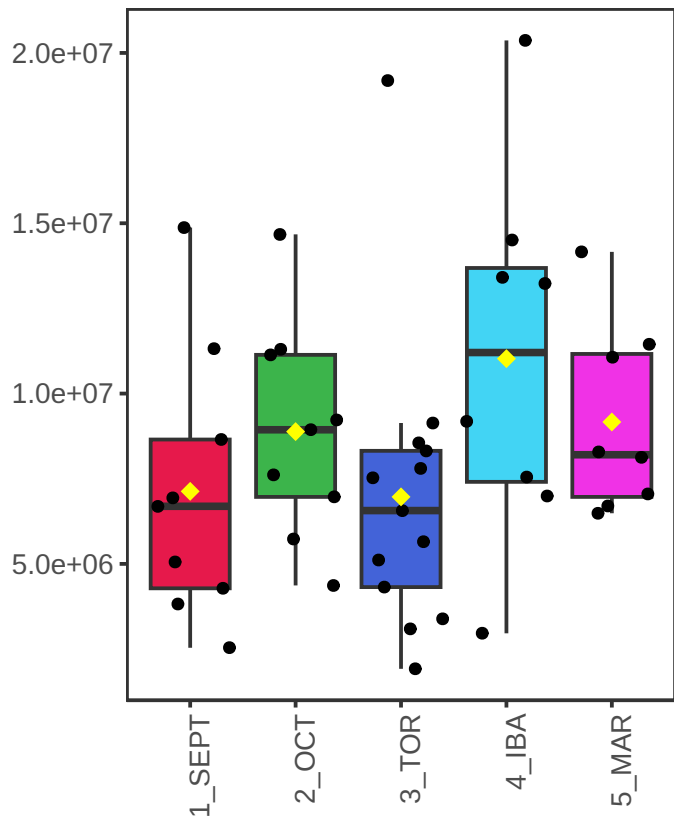


Normalized Conc.

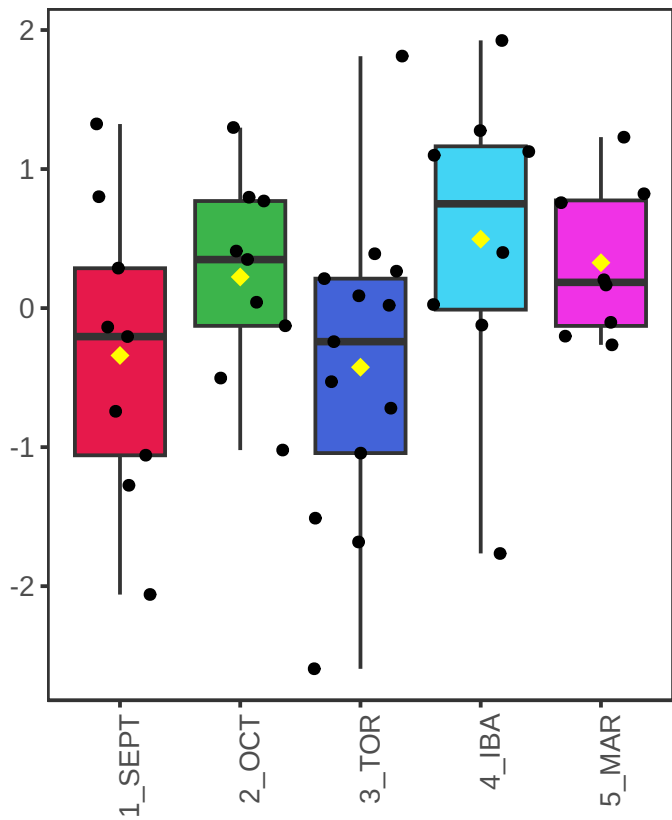


N-Ethylglycine

Original Conc.

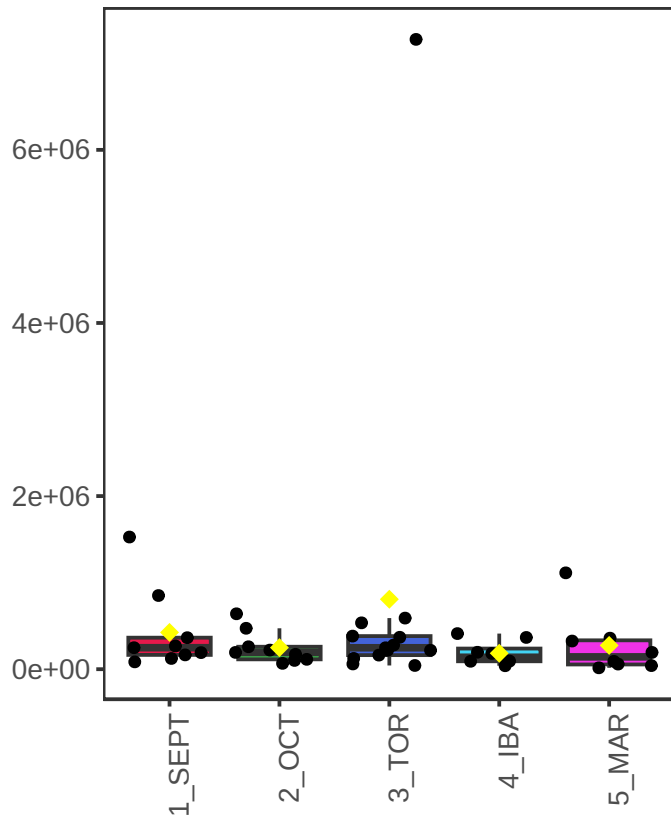


Normalized Conc.

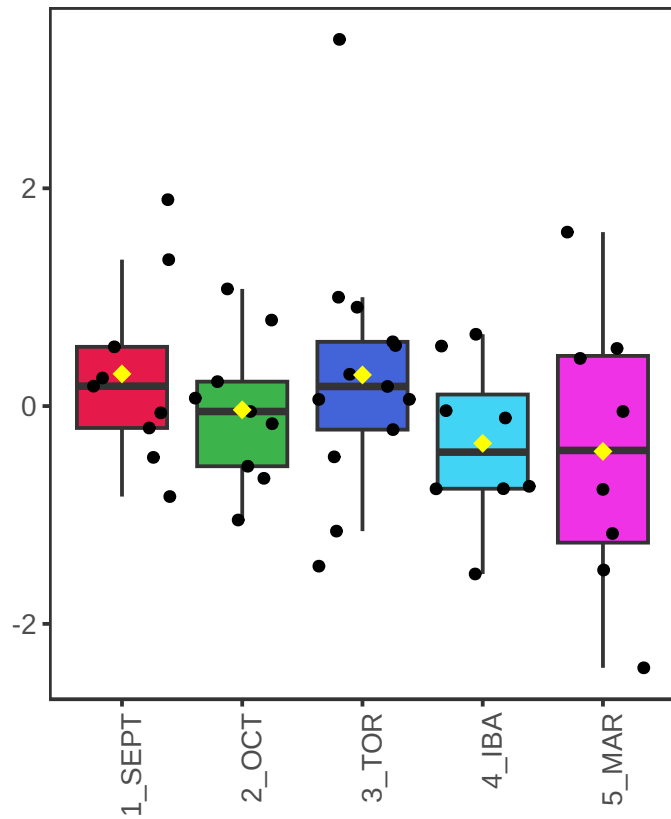


N-methyl-2-oxoglutaramic acid

Original Conc.

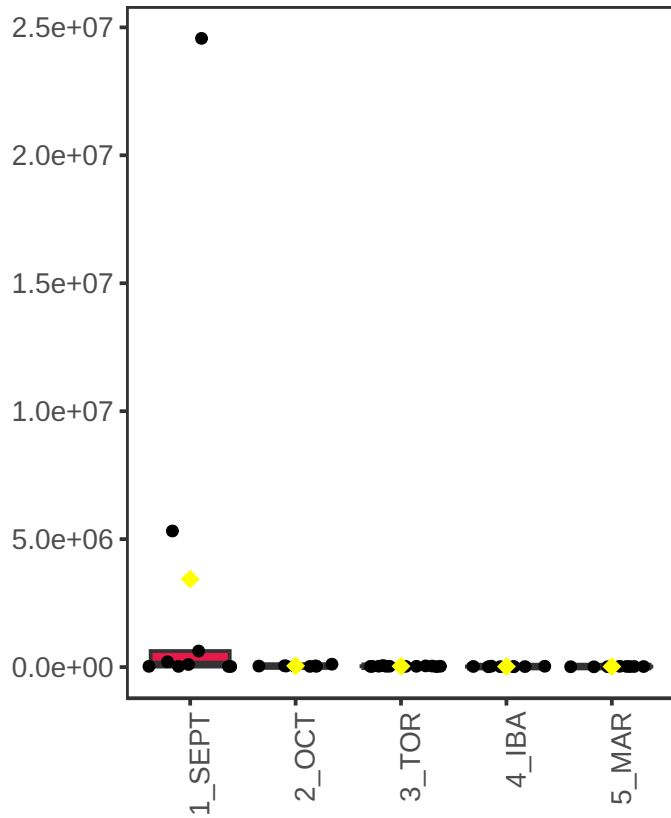


Normalized Conc.

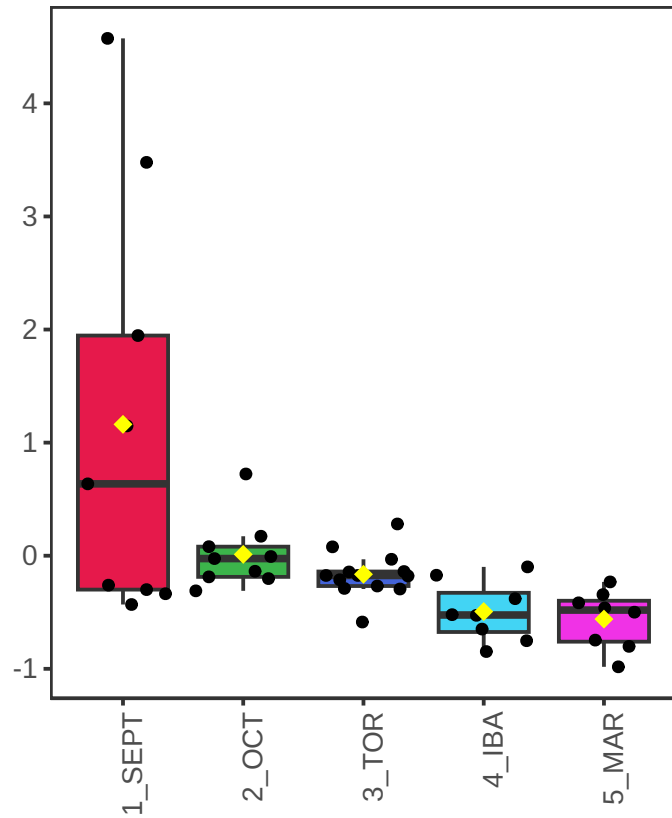


N,N-Dihydroxy-L-tryptophan

Original Conc.

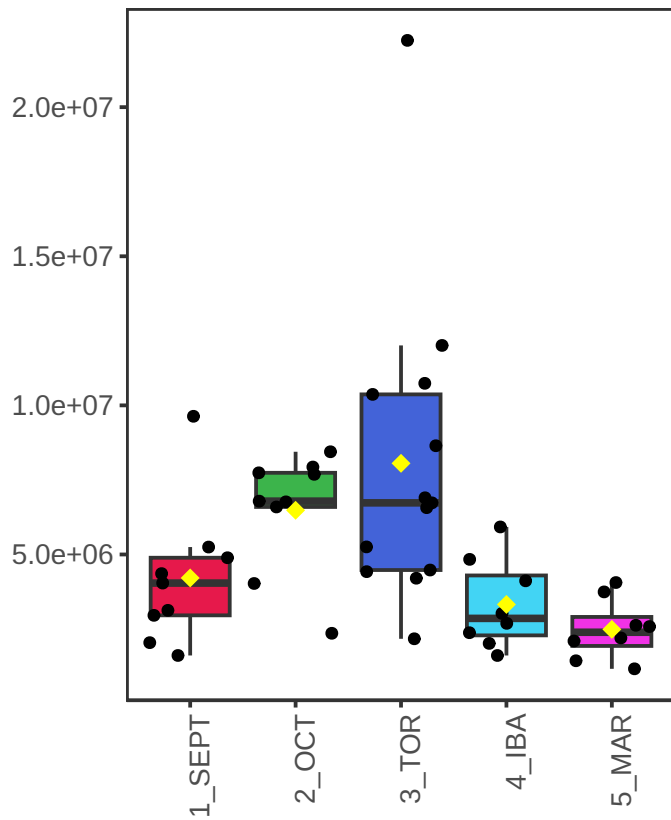


Normalized Conc.

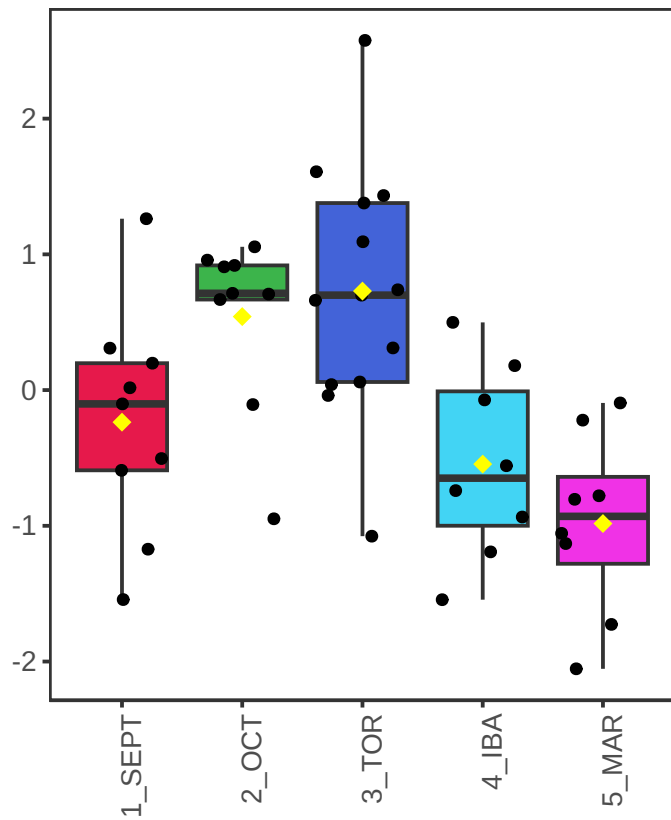


N-Undecanoylglycine

Original Conc.

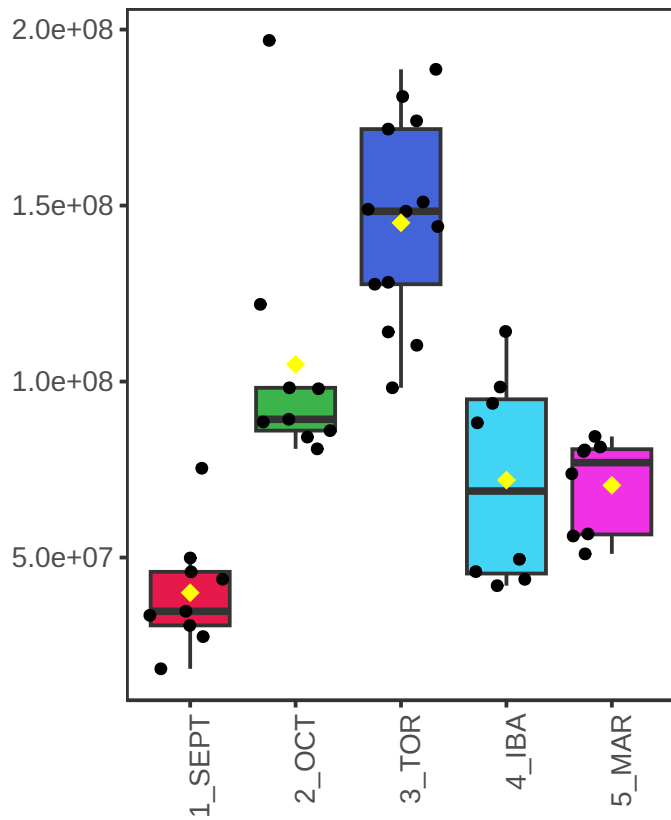


Normalized Conc.

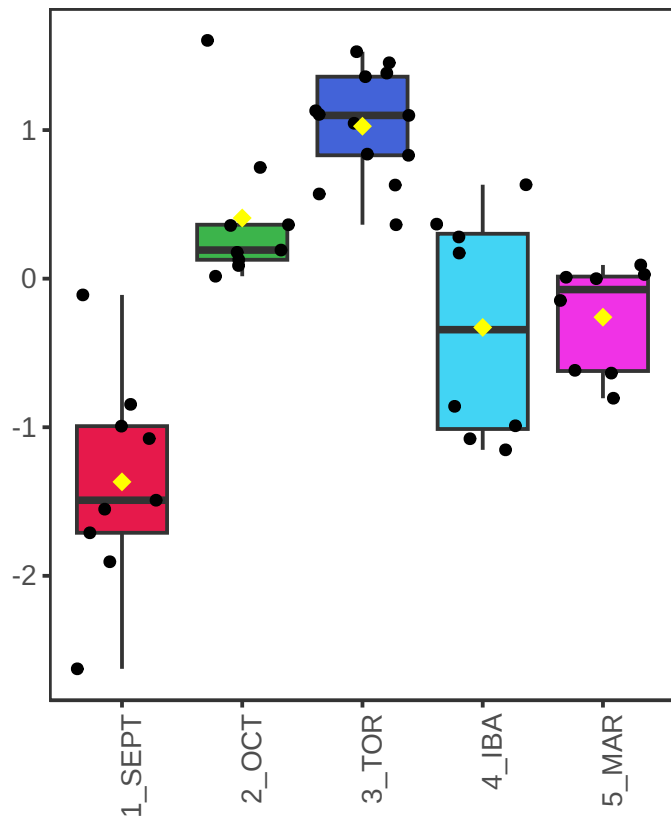


Pantothenic acid

Original Conc.

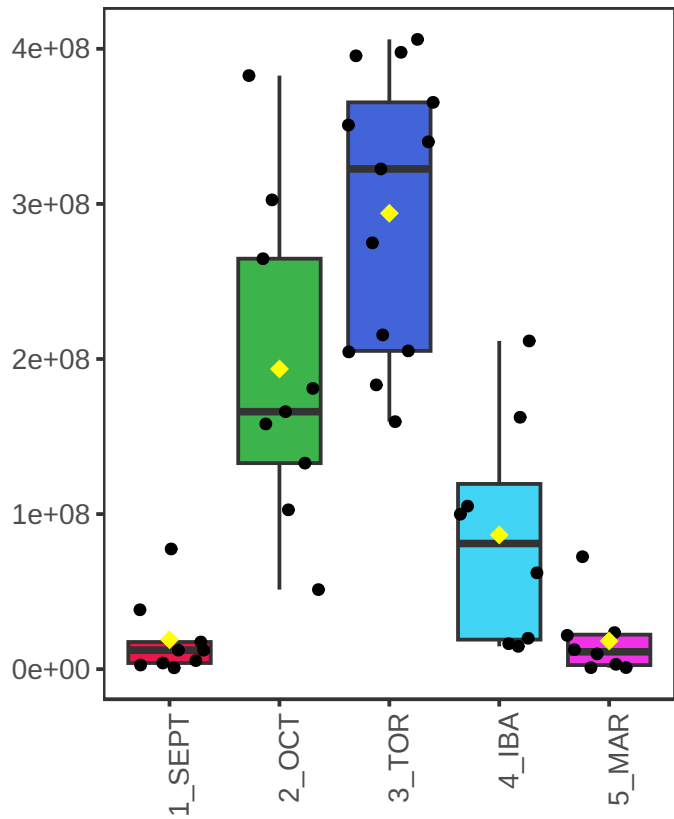


Normalized Conc.

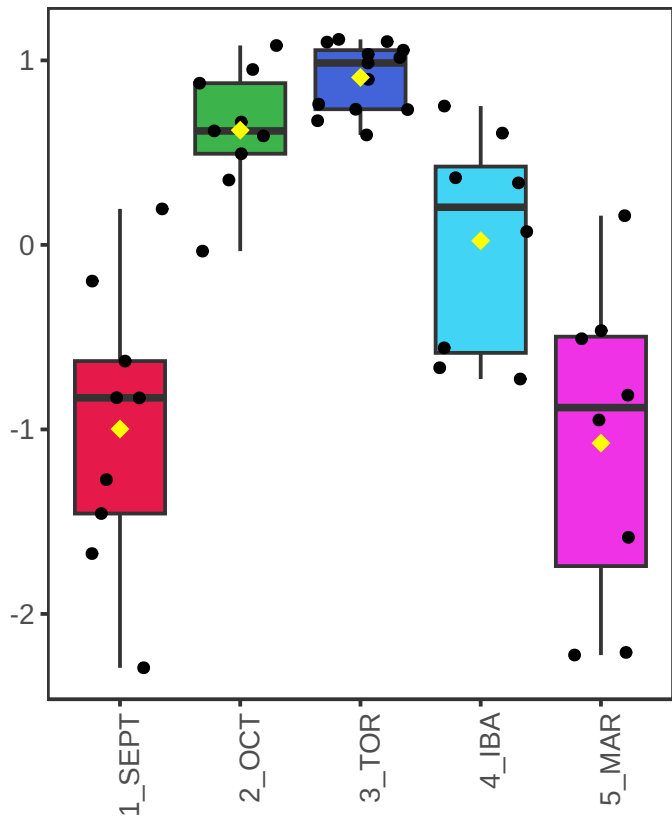


p-Cresylsulfate

Original Conc.

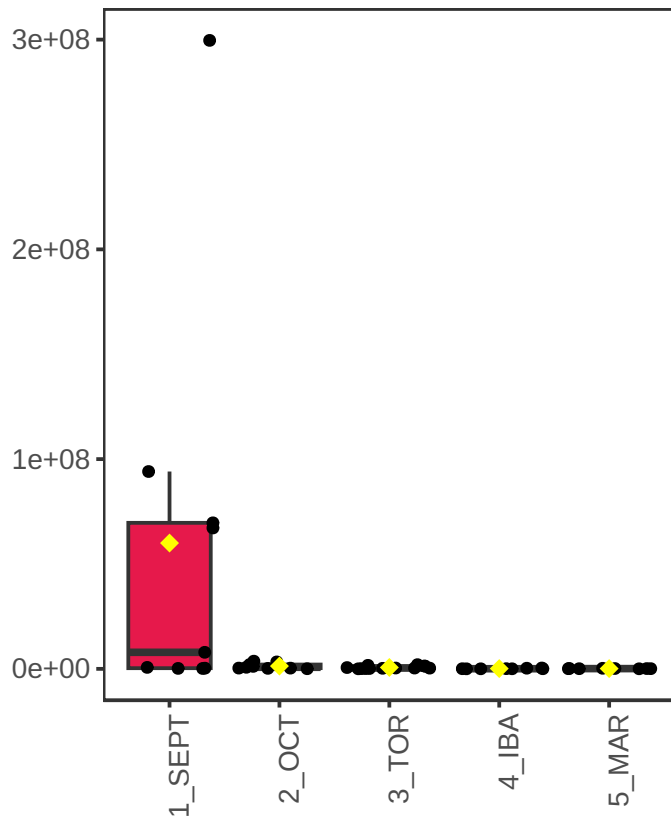


Normalized Conc.

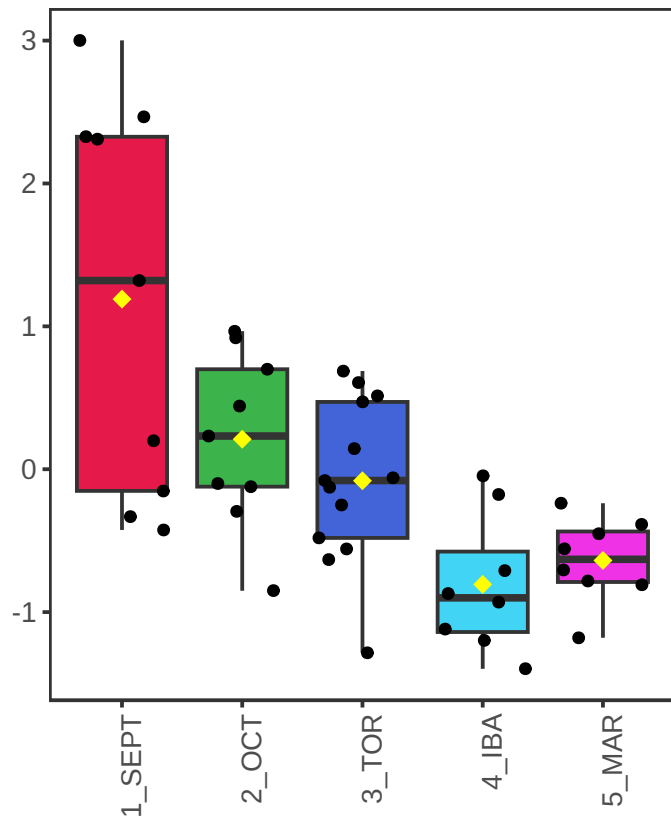


Phenylacetaldehyde

Original Conc.

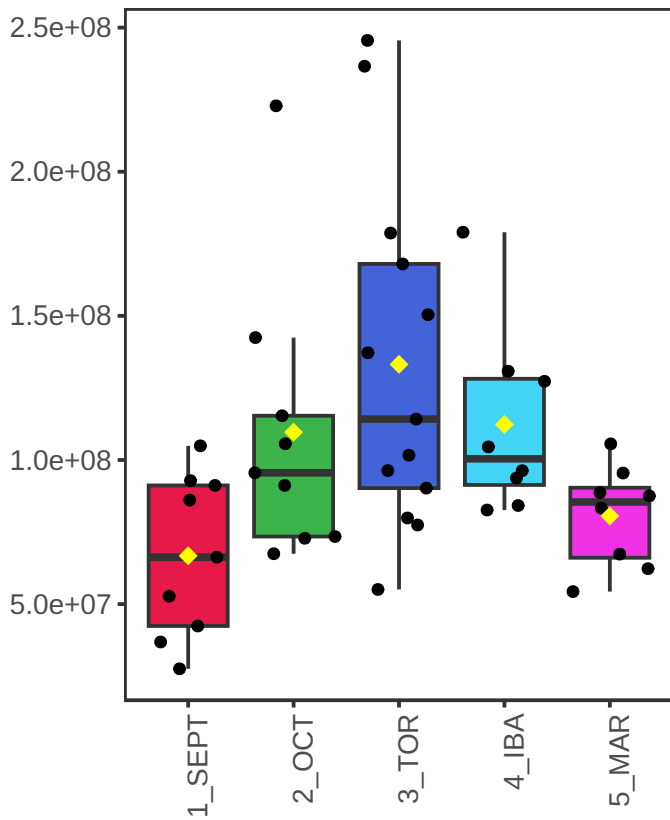


Normalized Conc.

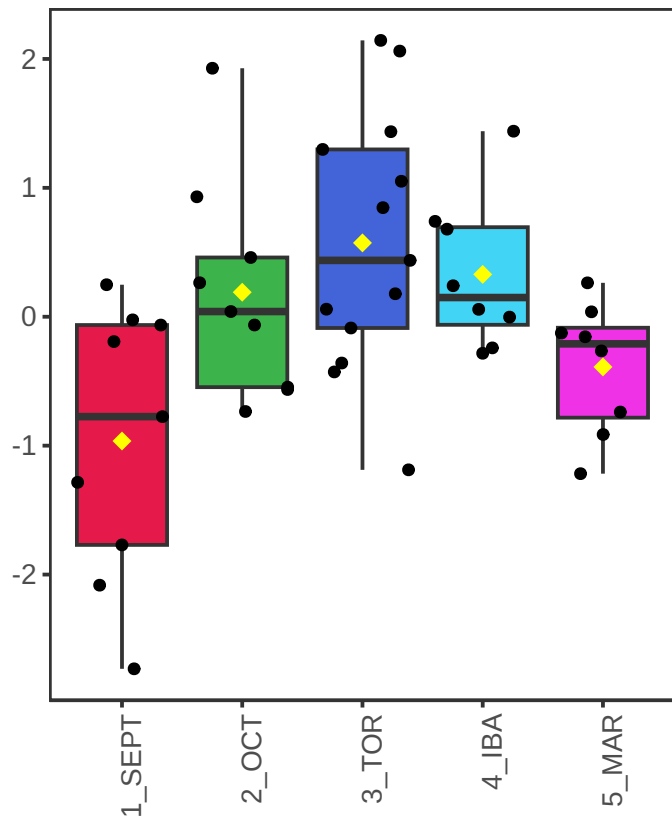


Phosphoethanolamine

Original Conc.

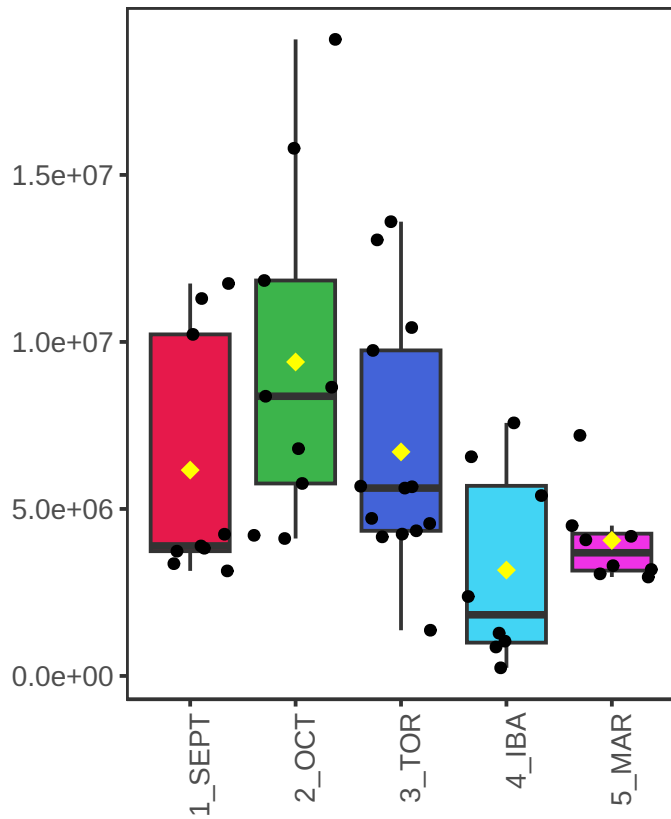


Normalized Conc.

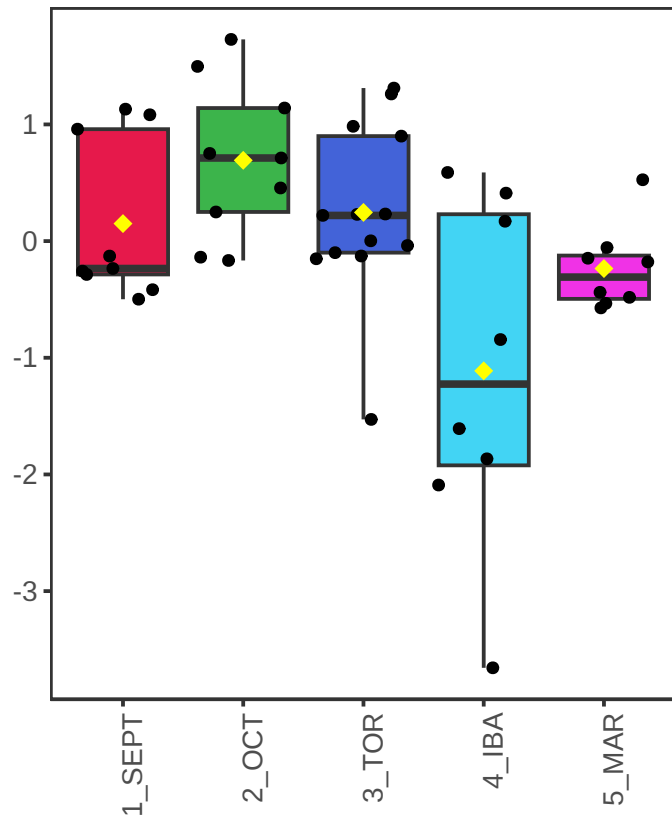


Pimelic acid

Original Conc.

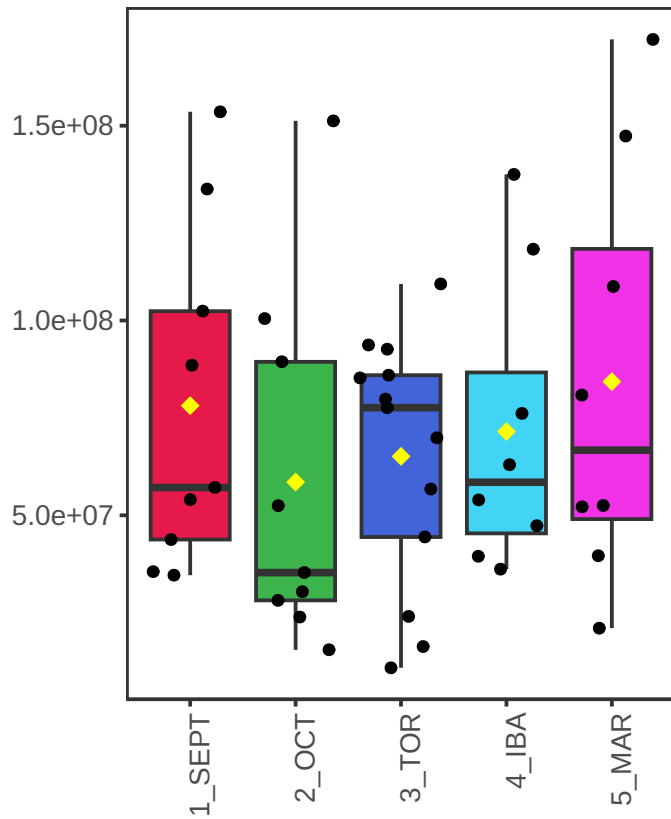


Normalized Conc.

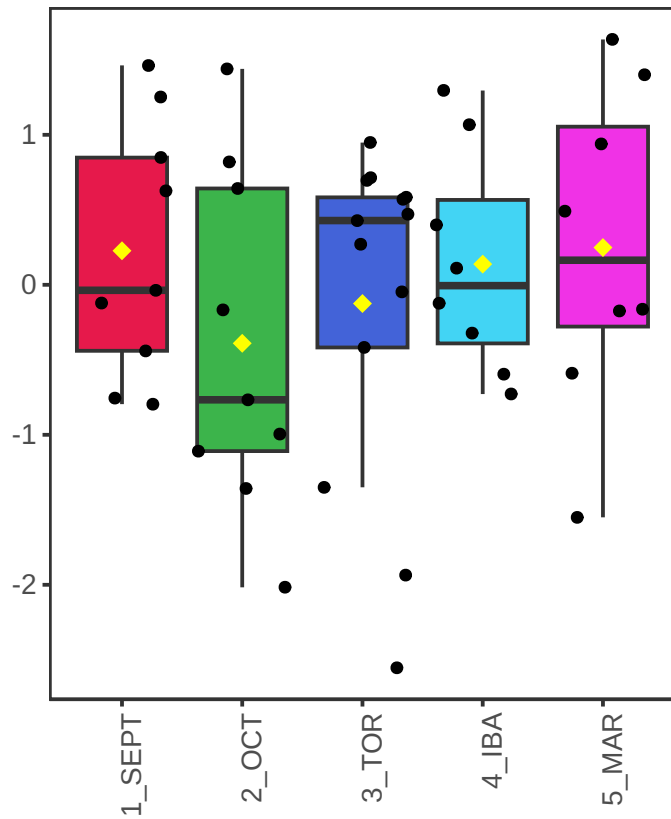


Pyruvic acid

Original Conc.

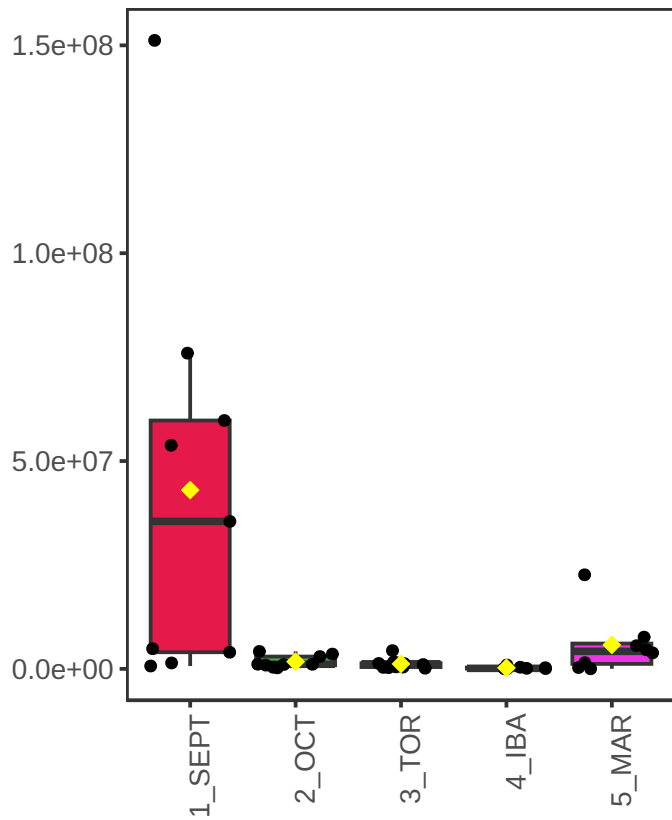


Normalized Conc.

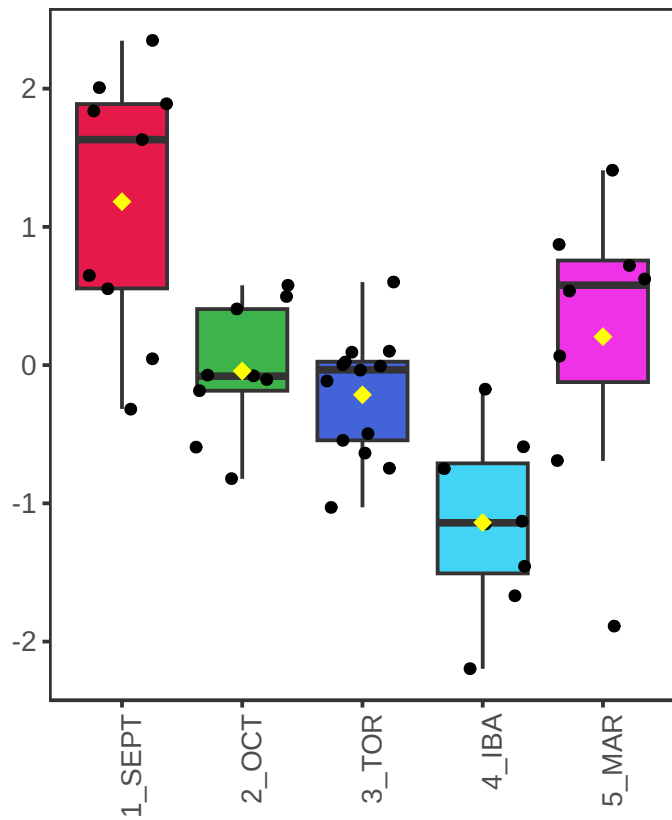


Quinol sulfate

Original Conc.

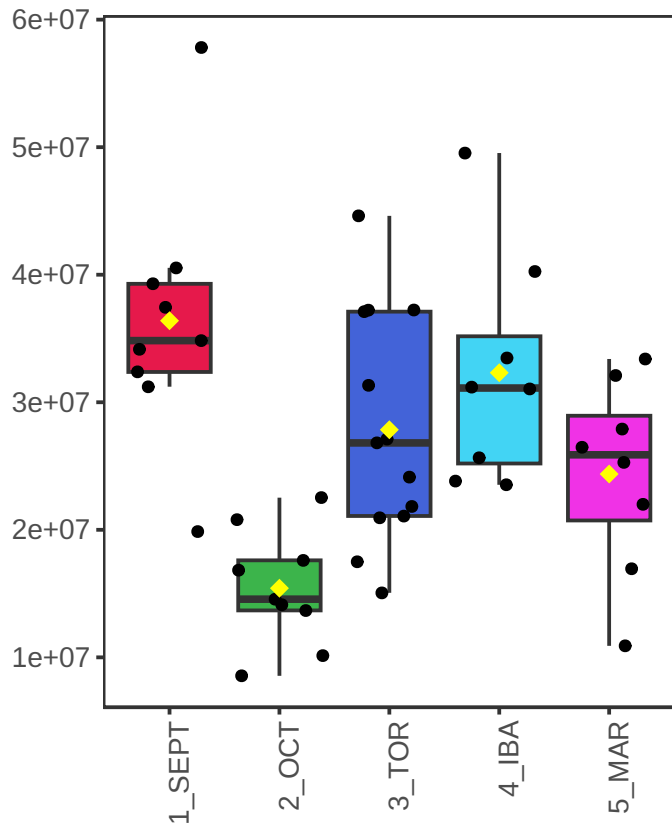


Normalized Conc.

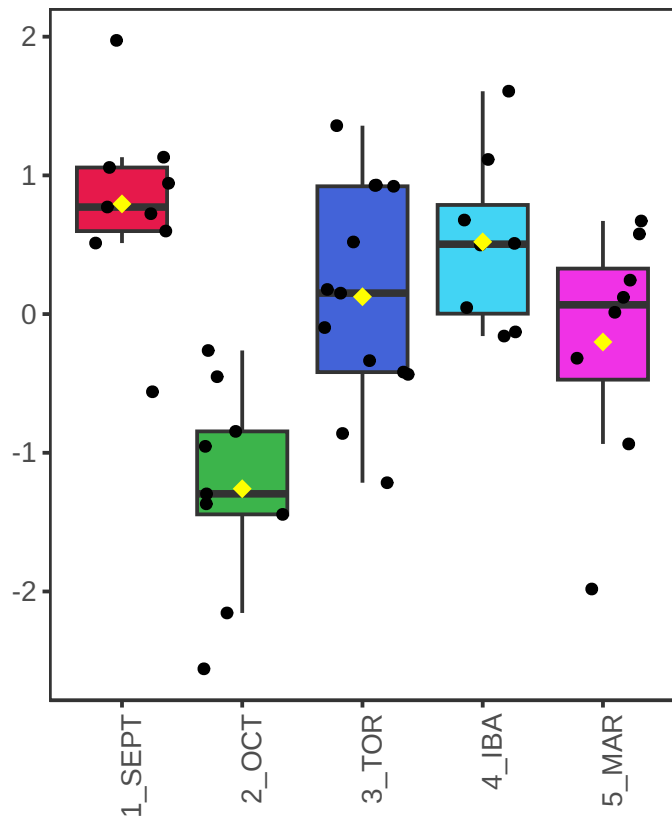


Serine

Original Conc.

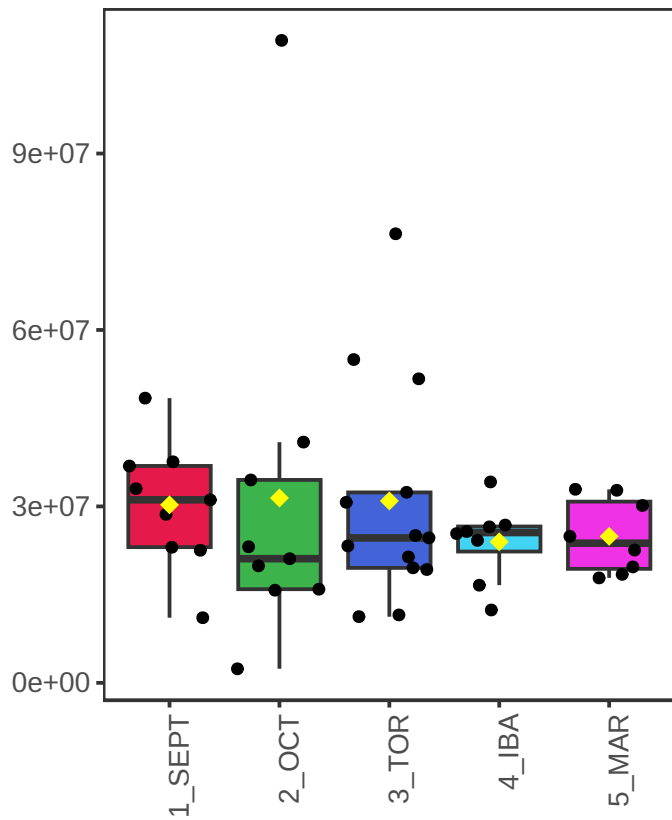


Normalized Conc.

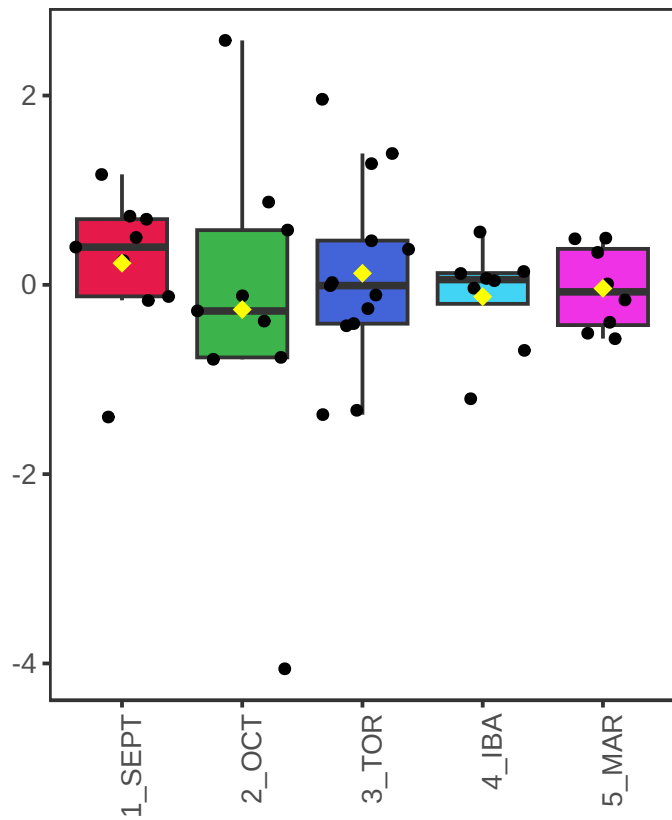


Succinic anhydride

Original Conc.

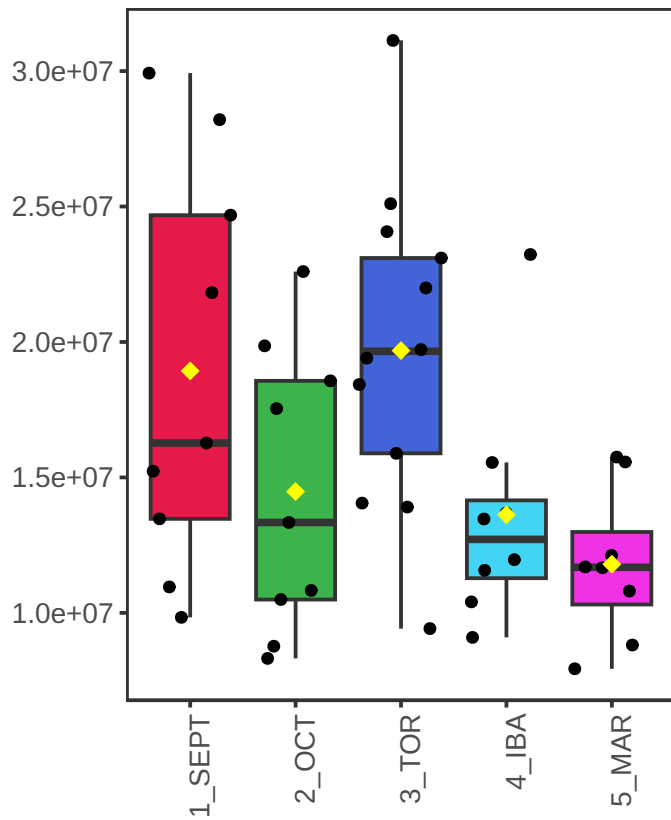


Normalized Conc.

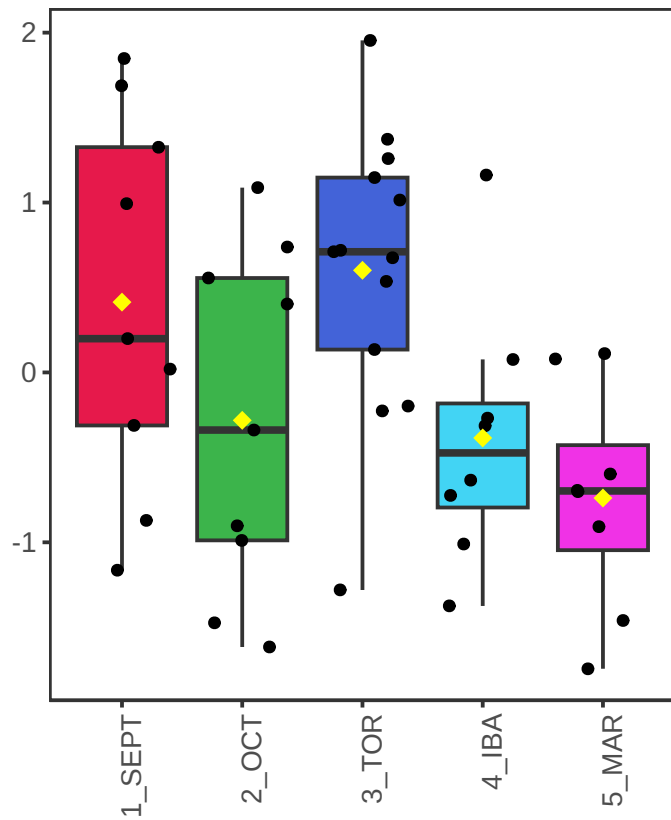


Threonine

Original Conc.

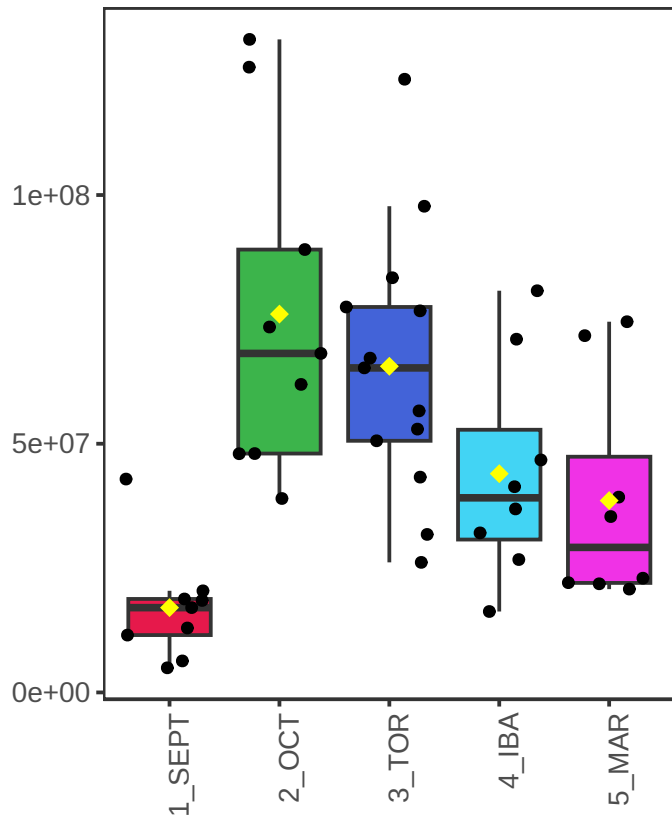


Normalized Conc.

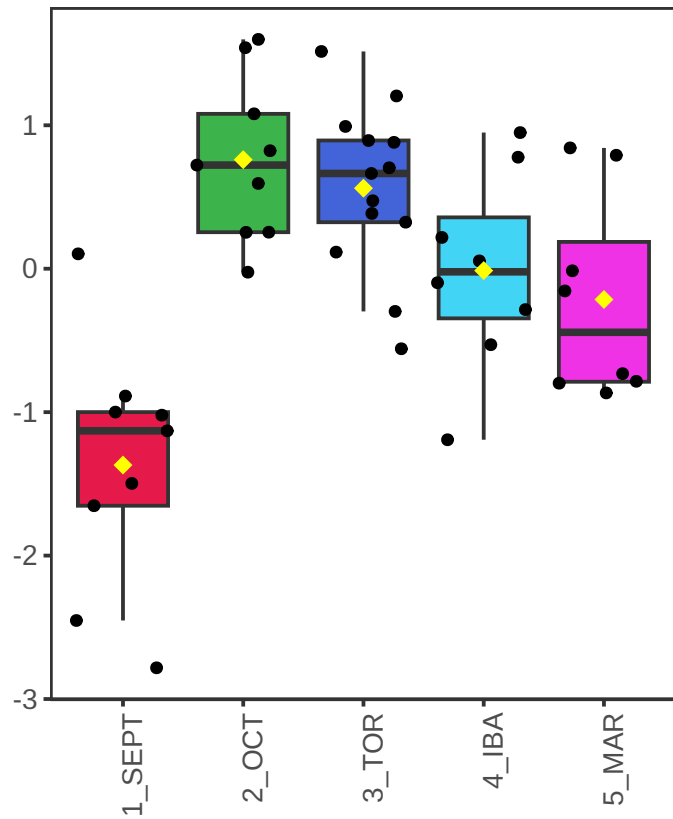


Uracil

Original Conc.

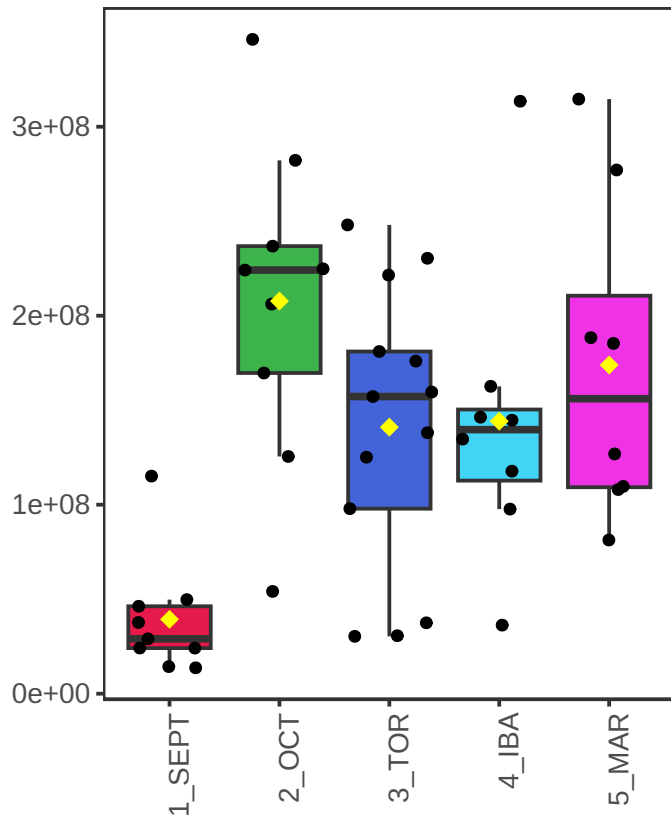


Normalized Conc.

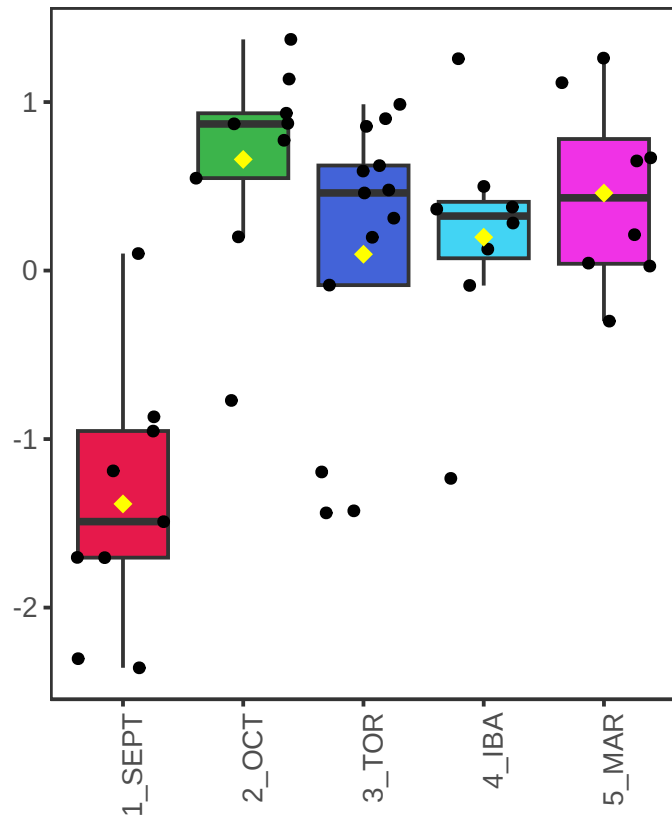


Uridine

Original Conc.

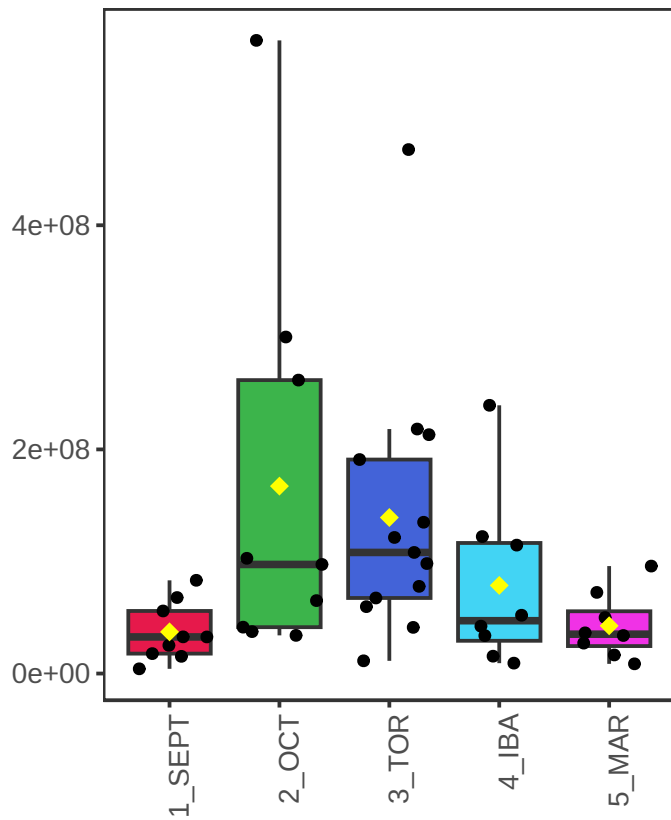


Normalized Conc.

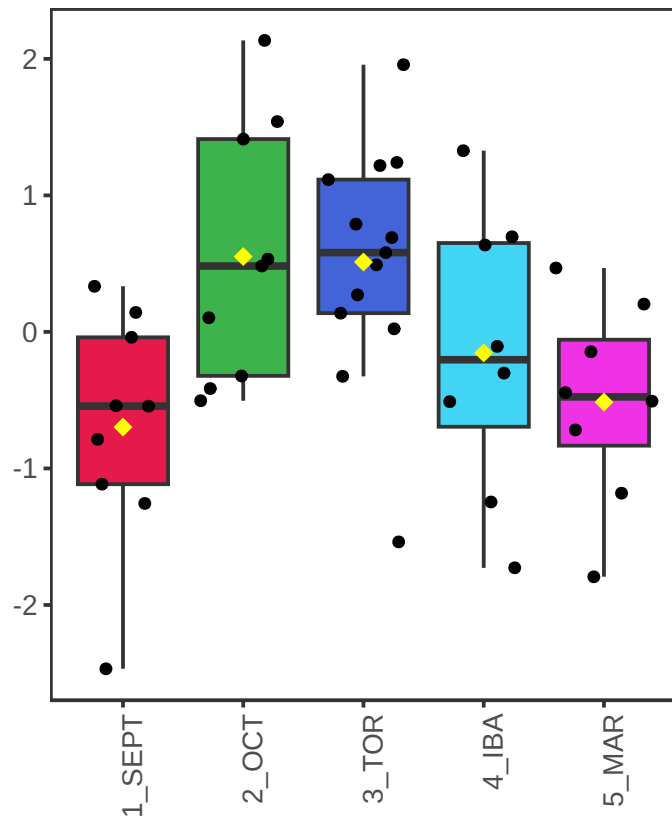


Urocanic acid

Original Conc.

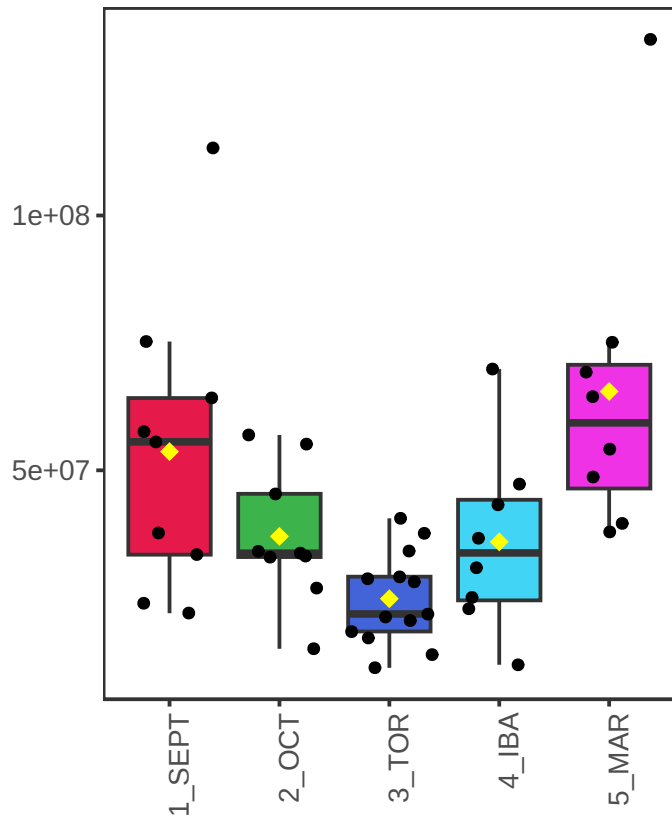


Normalized Conc.



Xanthine

Original Conc.



Normalized Conc.

