

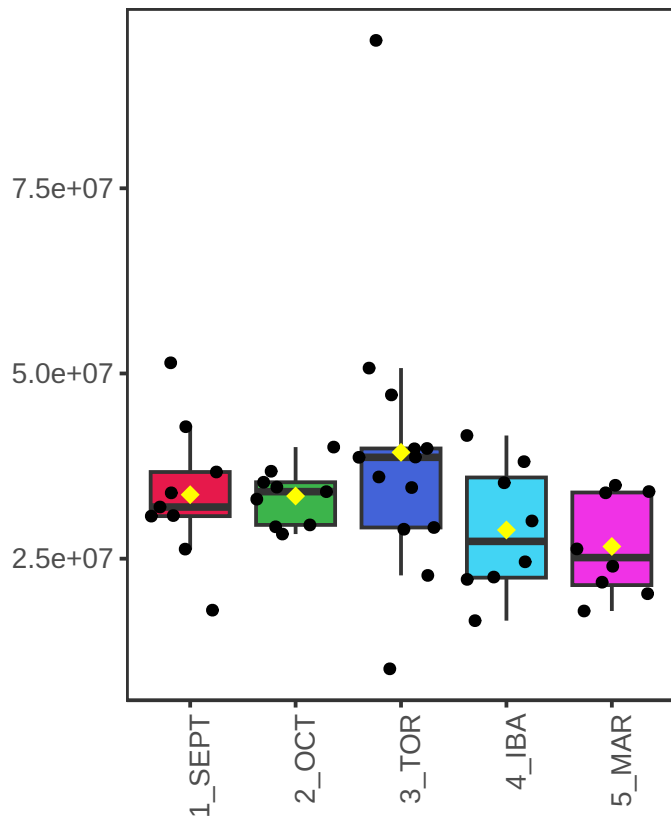
Figure S2

Supplementary Figure 2: Boxplot Representations of all Annotated Features from the Positive Ion Mode

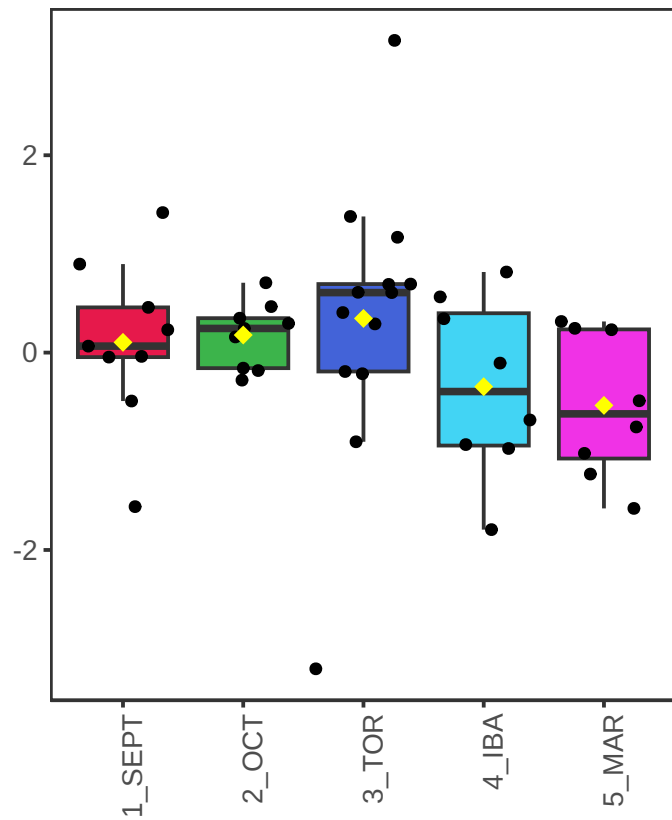
Collated feature intensity box plots for all annotated features in the positive ion mode. Left panel: original feature intensities from peak intensity table (Supplemental Table S2, tab 1). Right panel: feature intensities after \log_{10} transformation and auto scaling (values mean-centered and divided by the standard deviation).

1-Methyl-1,3-dihydro-2H-benzimidazole-2-thione

Original Conc.

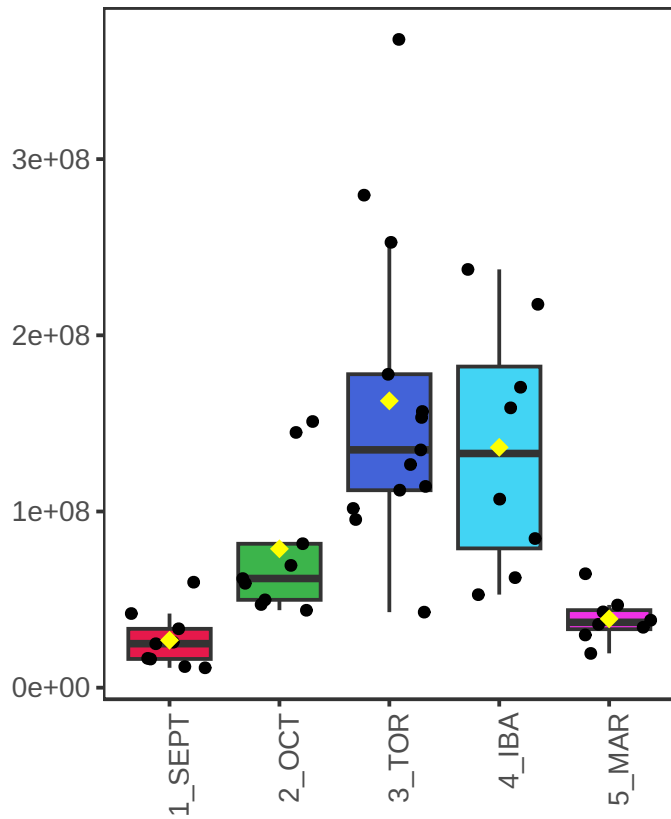


Normalized Conc.

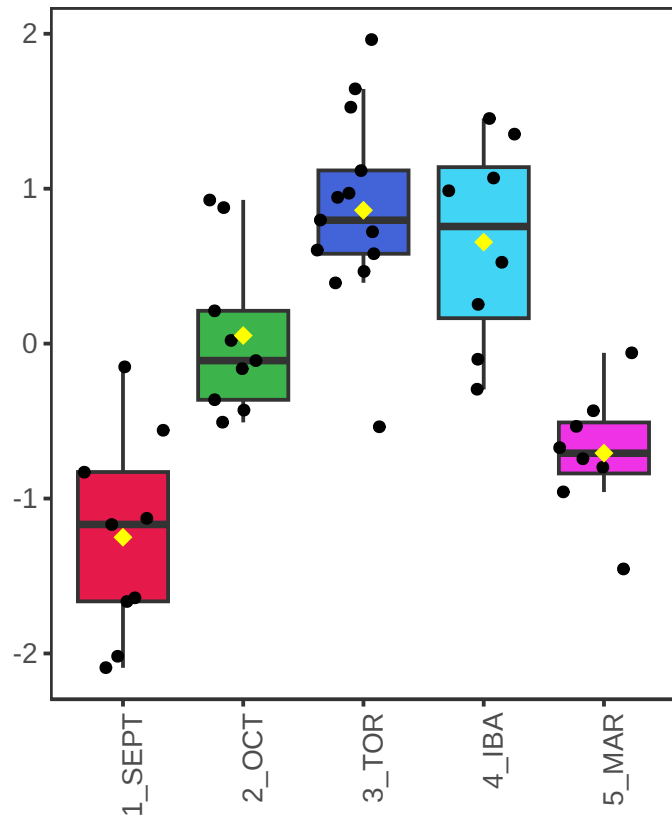


1-Methylhistidine

Original Conc.

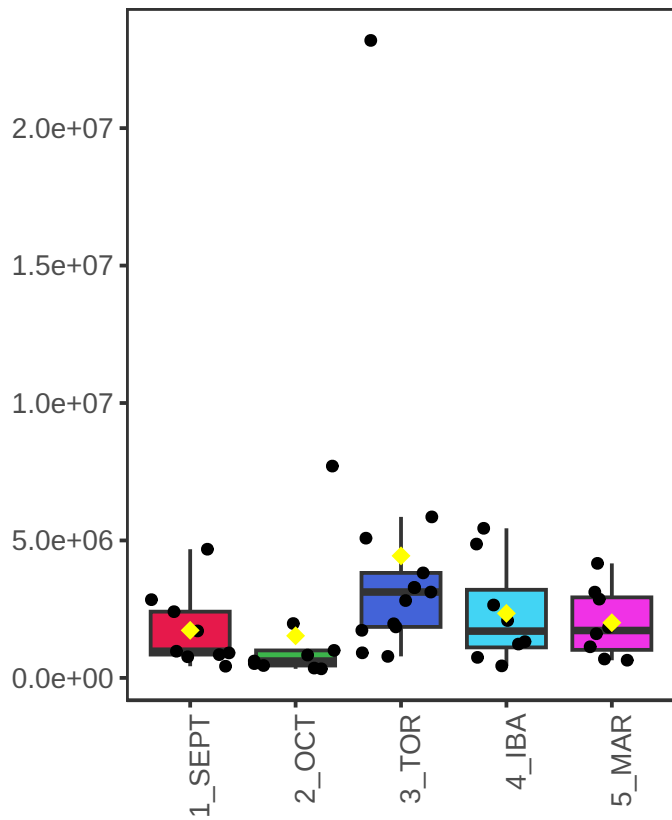


Normalized Conc.

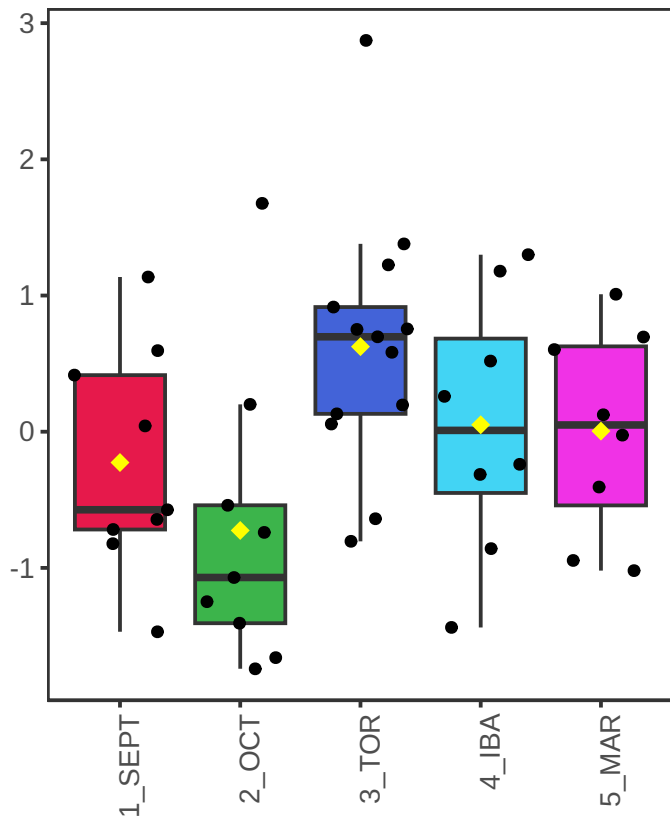


1-Methylimidazoleacetic acid

Original Conc.

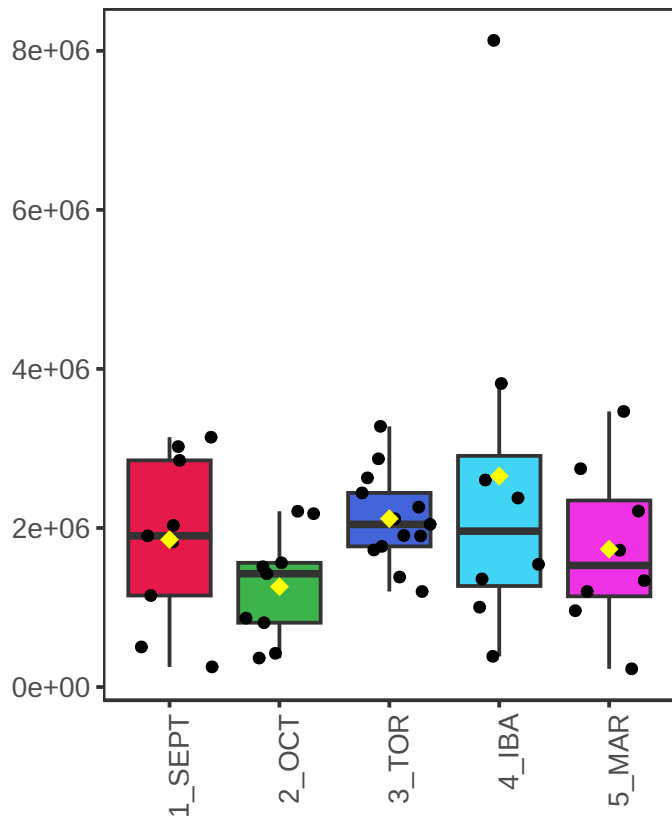


Normalized Conc.

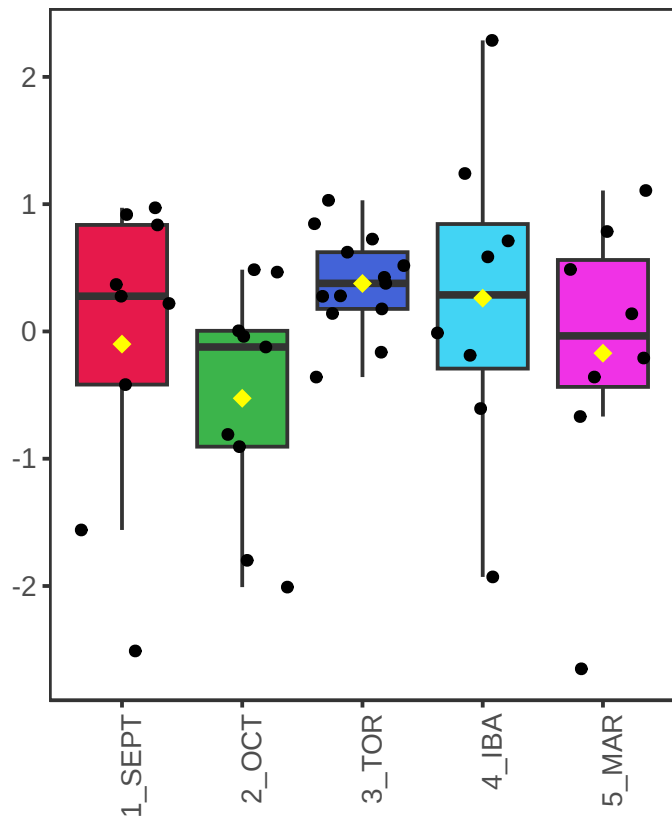


1-Palmitoyl-2-hydroxy-sn-glycero-3-PE

Original Conc.

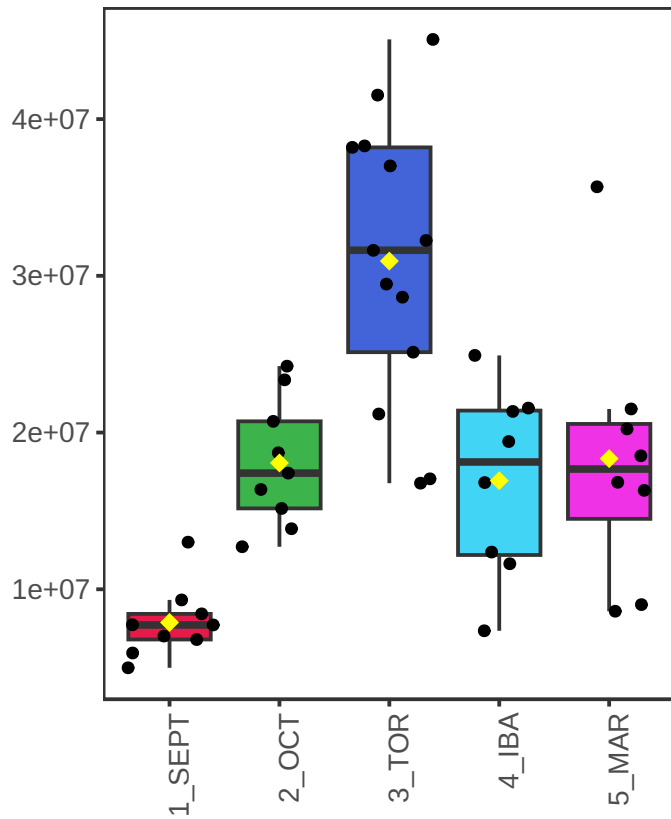


Normalized Conc.

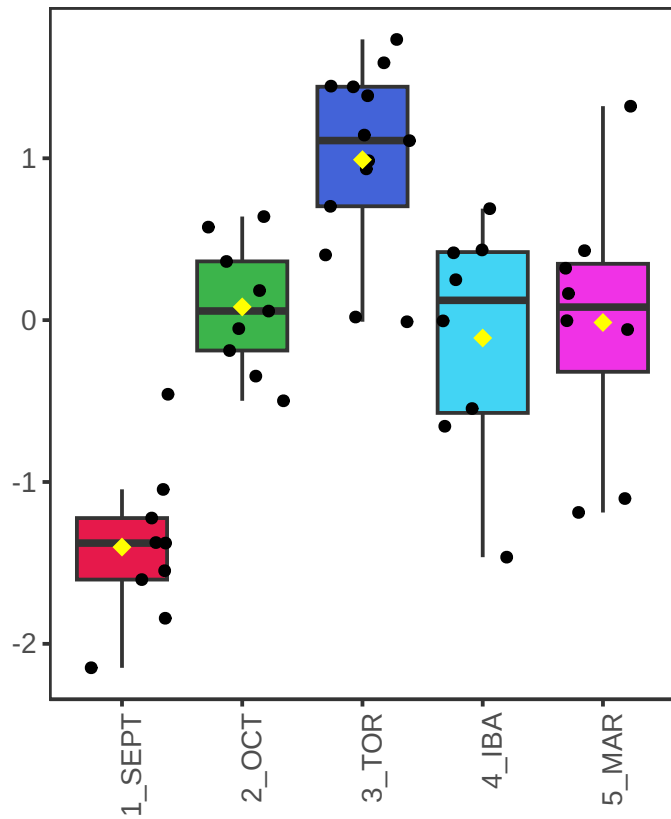


1-Piperidine

Original Conc.

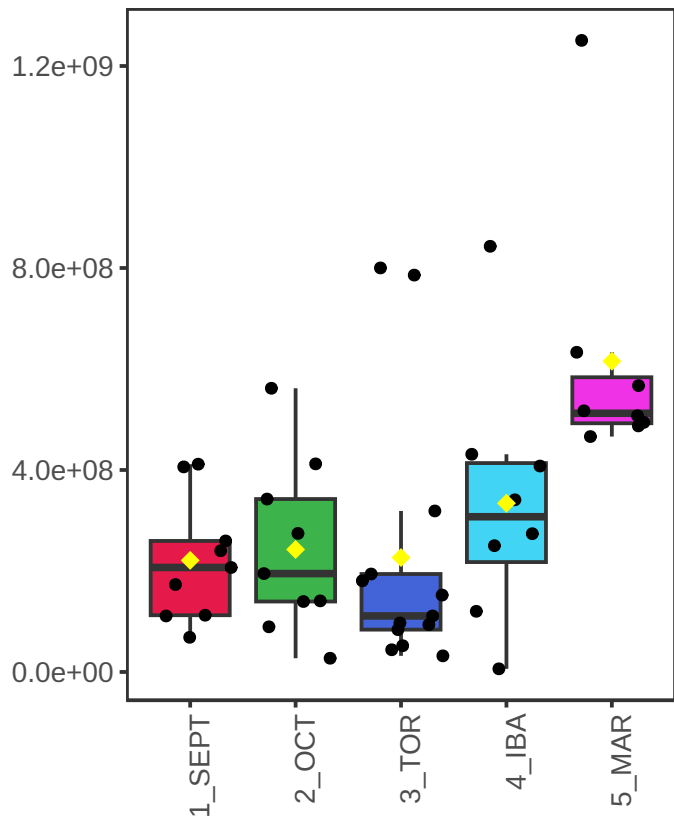


Normalized Conc.

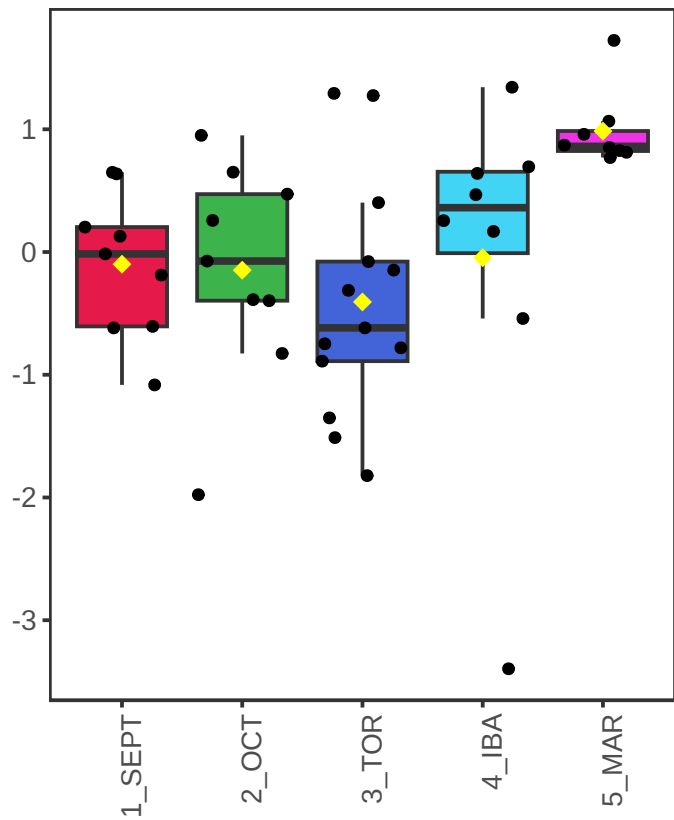


1-Vinylimidazole

Original Conc.

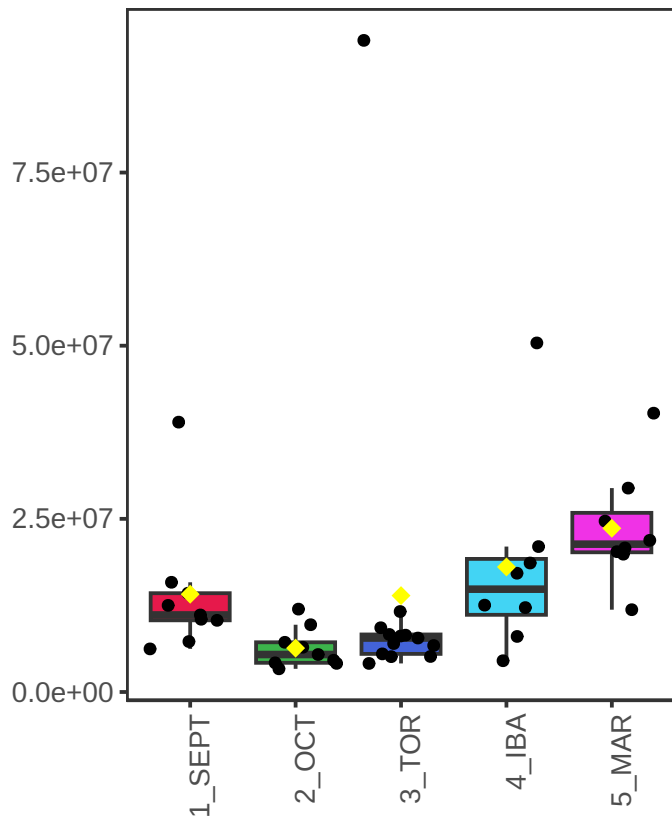


Normalized Conc.

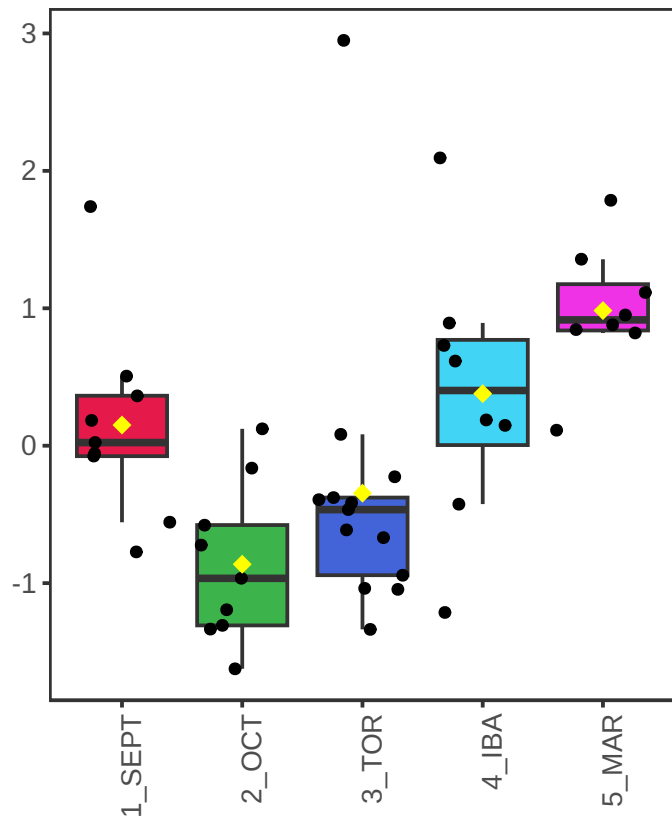


2-Aminoadipic acid

Original Conc.

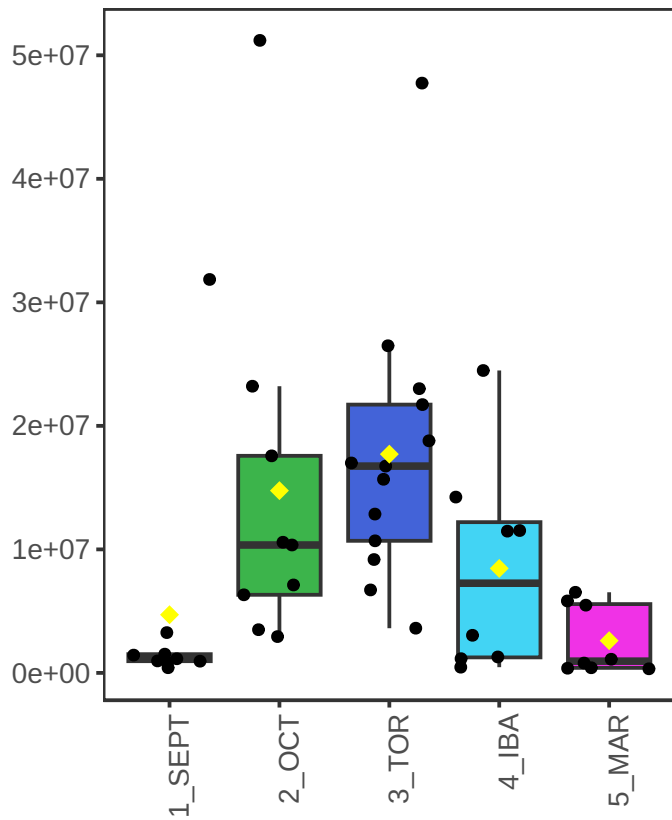


Normalized Conc.

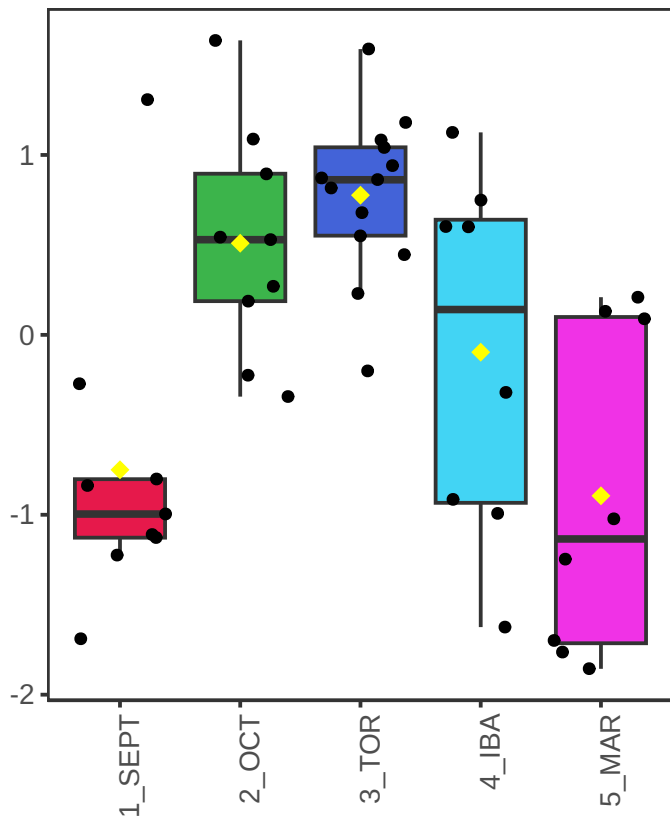


2-Aminonicotinic acid

Original Conc.

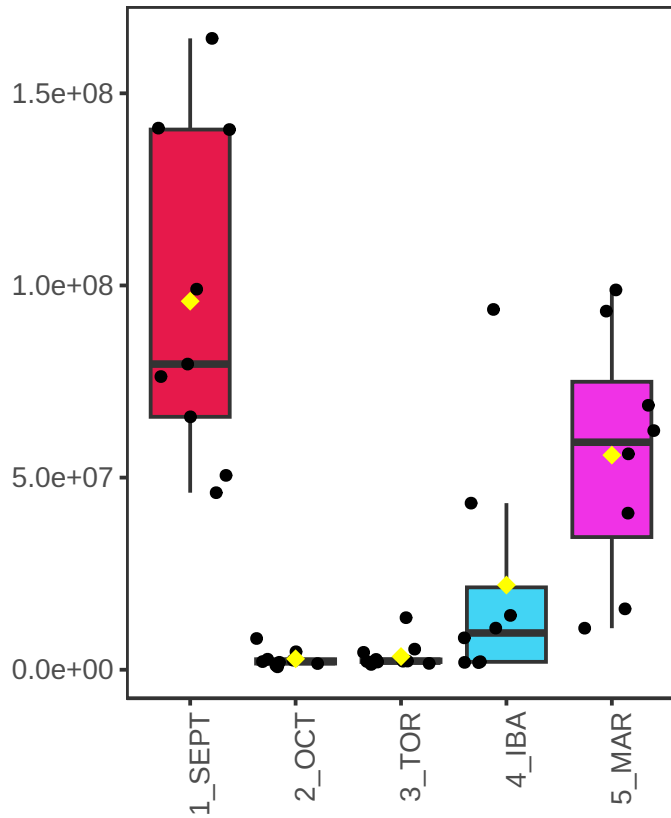


Normalized Conc.

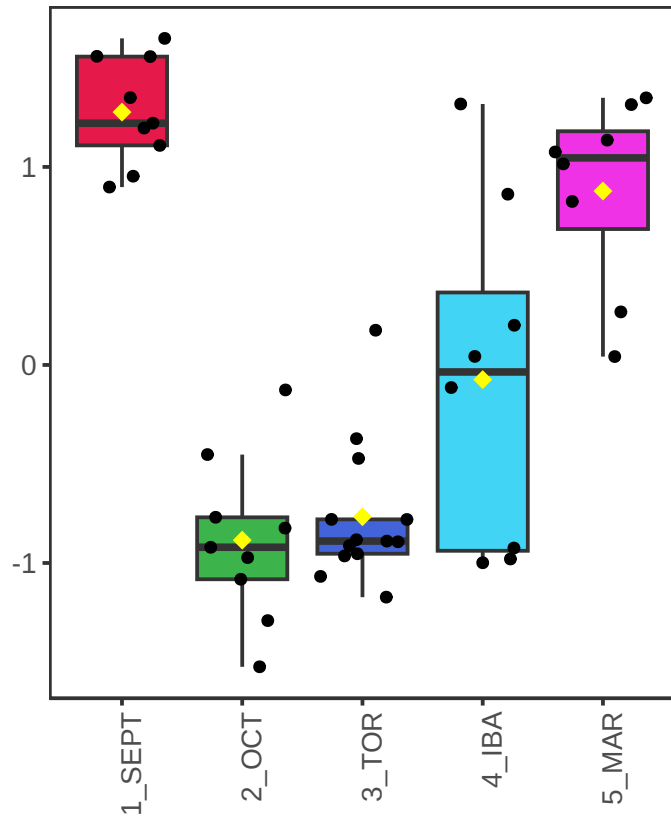


2-Methylbutyrylcarnitine

Original Conc.

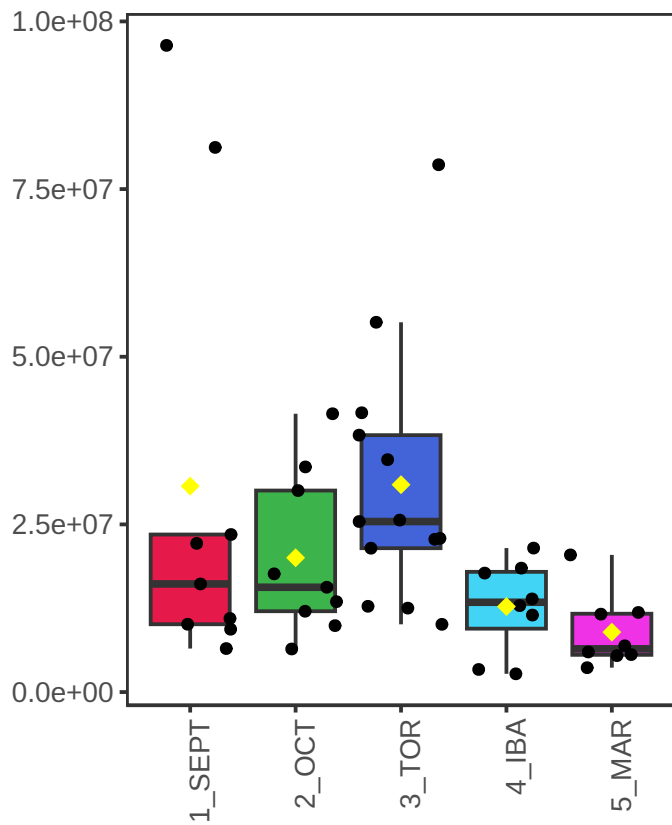


Normalized Conc.

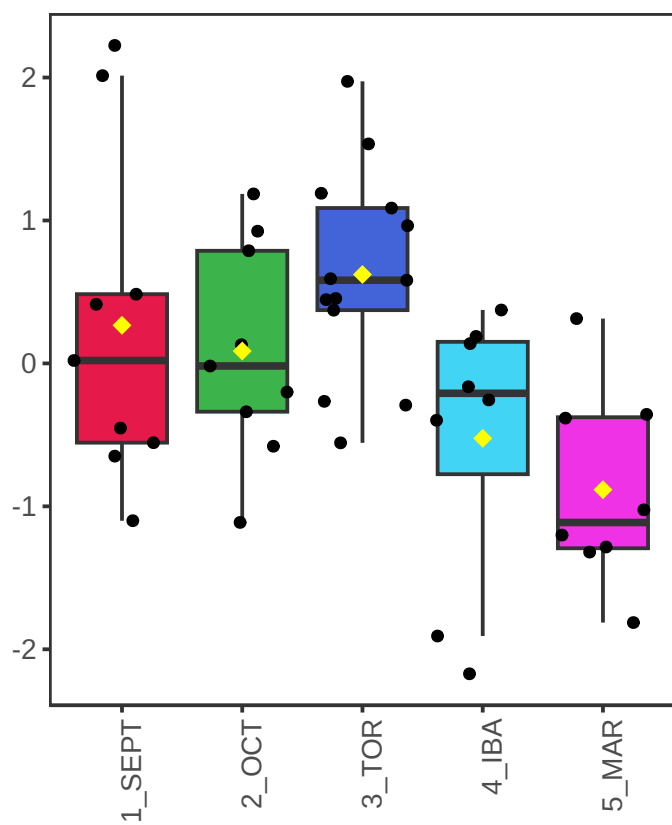


2-Oxindole

Original Conc.

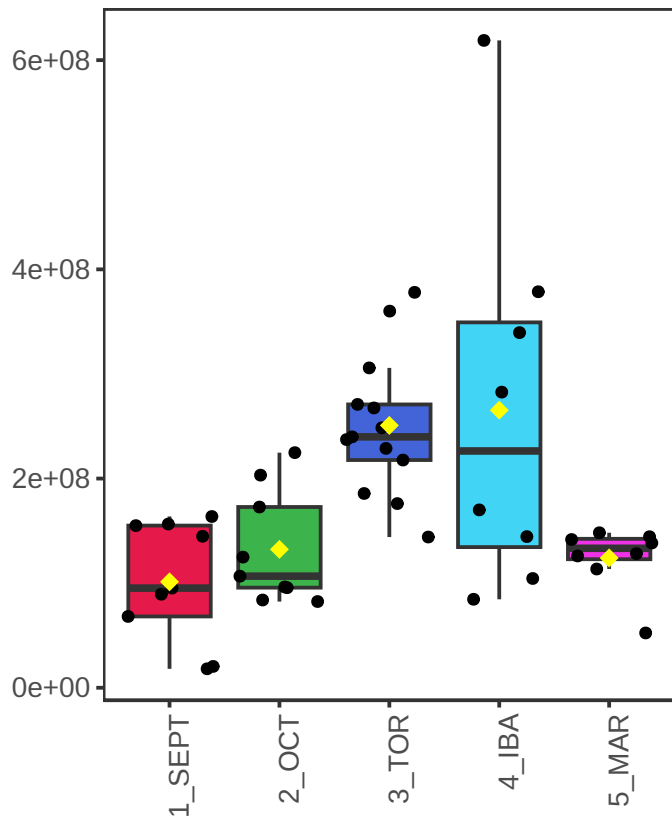


Normalized Conc.

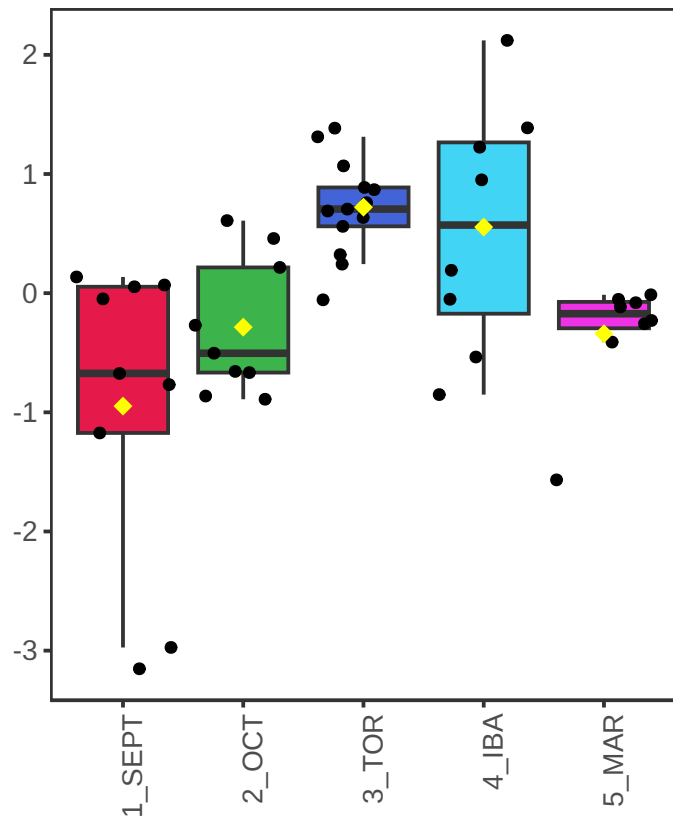


2-palmitoyl-sn-glycero-3-phosphocholine

Original Conc.

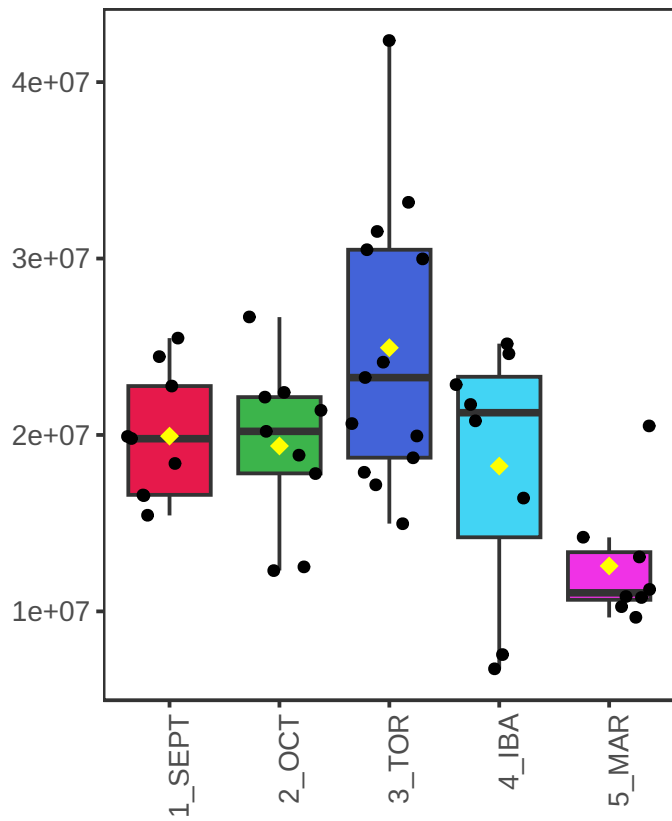


Normalized Conc.

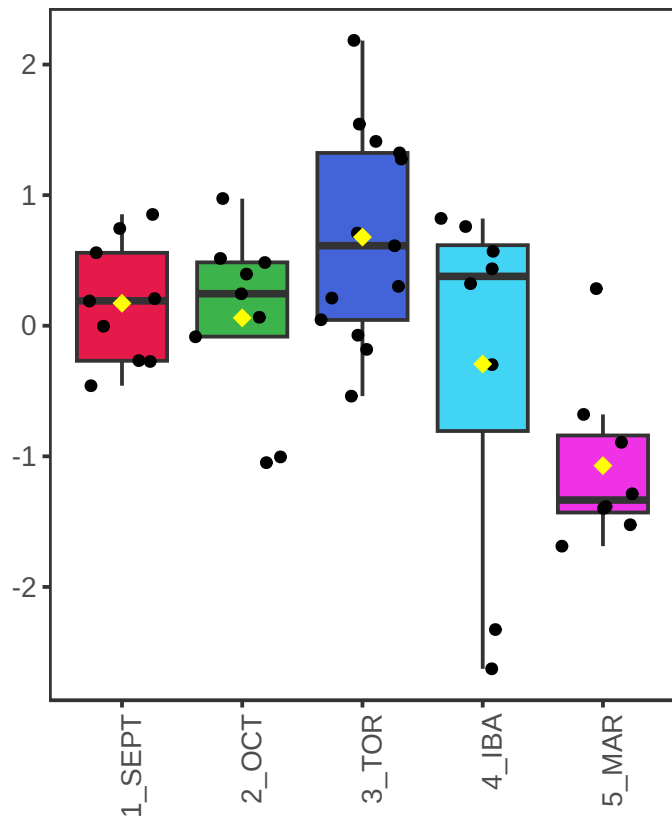


3'-CMP

Original Conc.

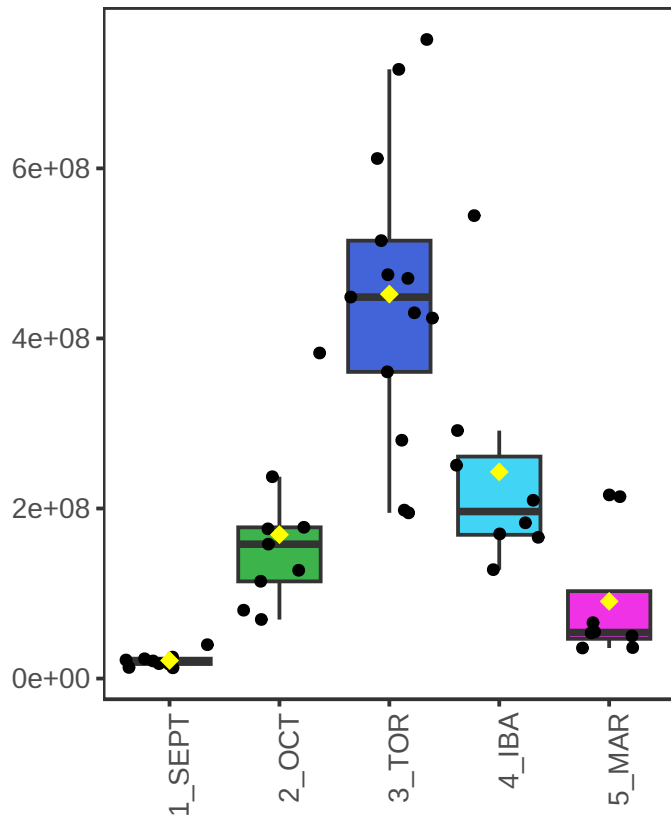


Normalized Conc.

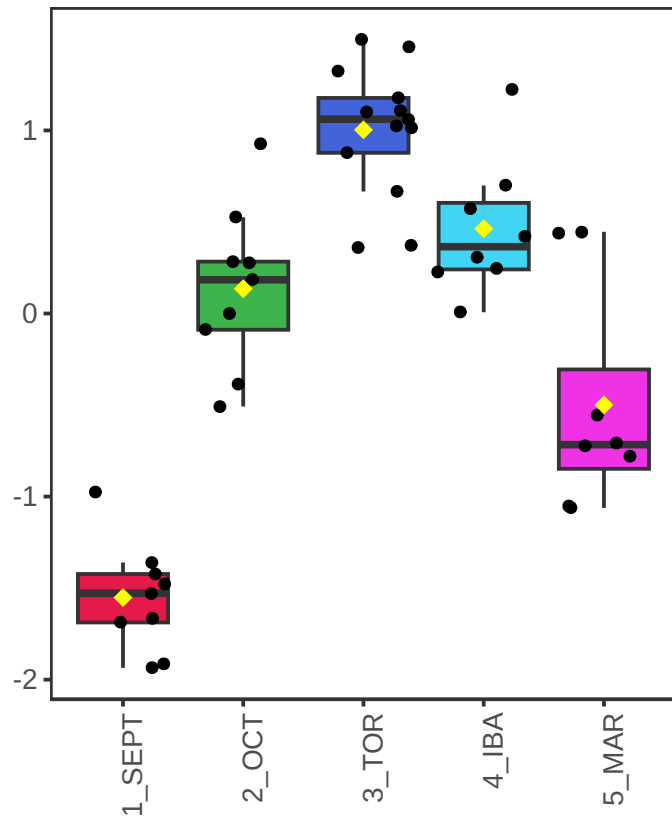


3-hydroxybutyrylcarnitine

Original Conc.

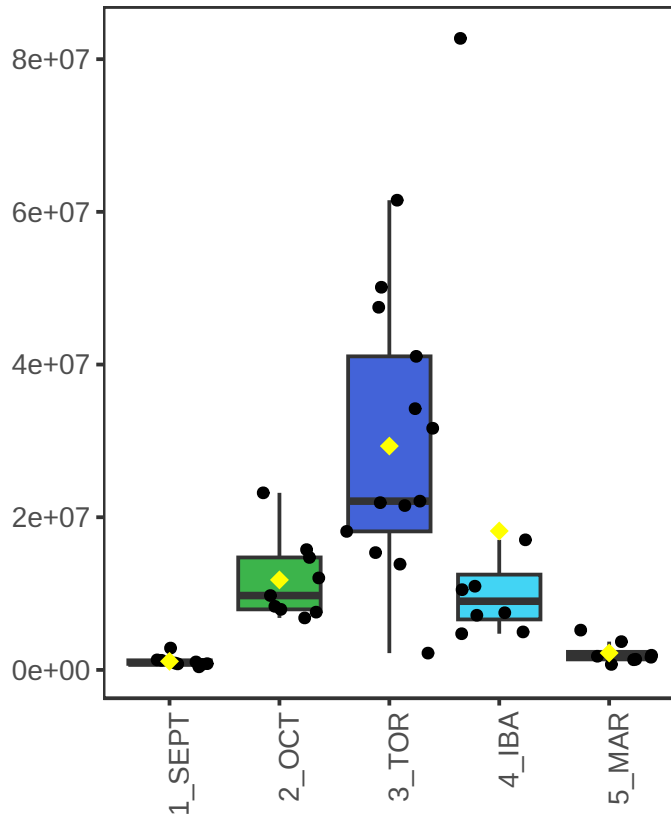


Normalized Conc.

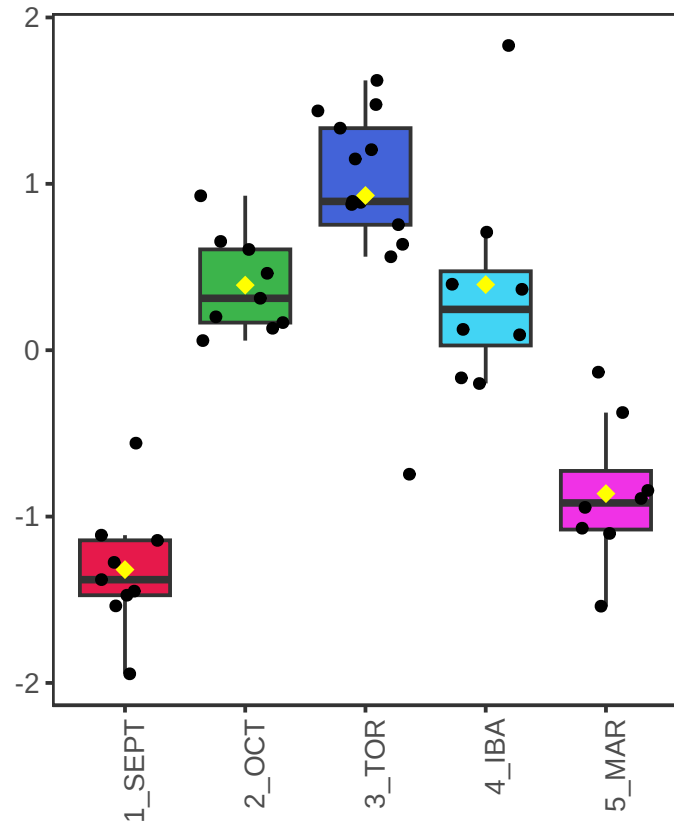


3-Hydroxy-cis-5-tetradecenoylcarnitine

Original Conc.

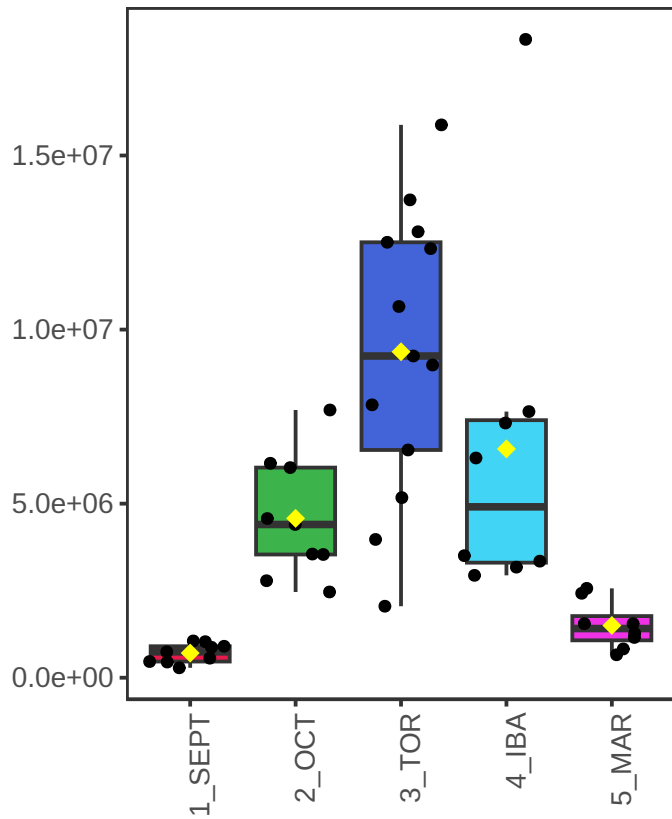


Normalized Conc.

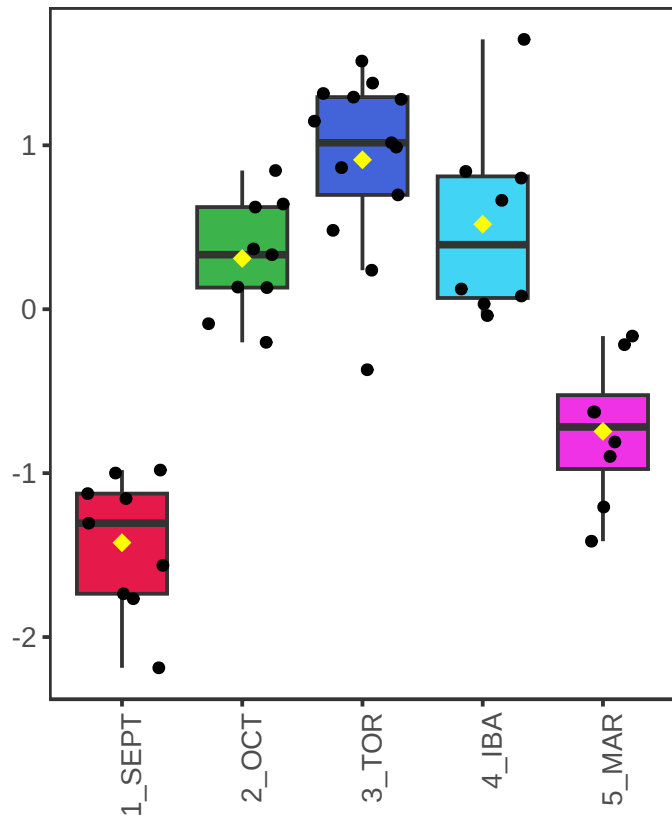


3-Hydroxydecanoylcarnitine

Original Conc.

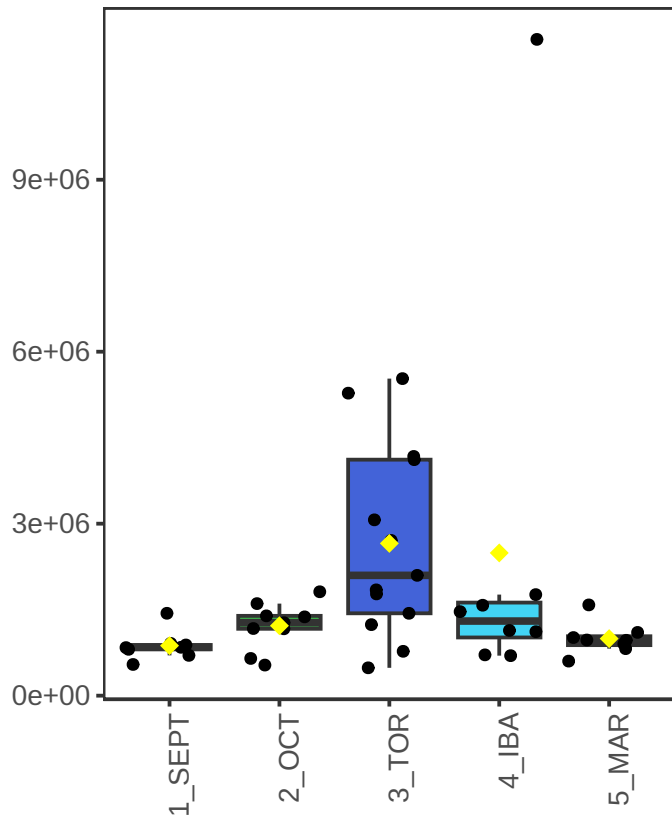


Normalized Conc.

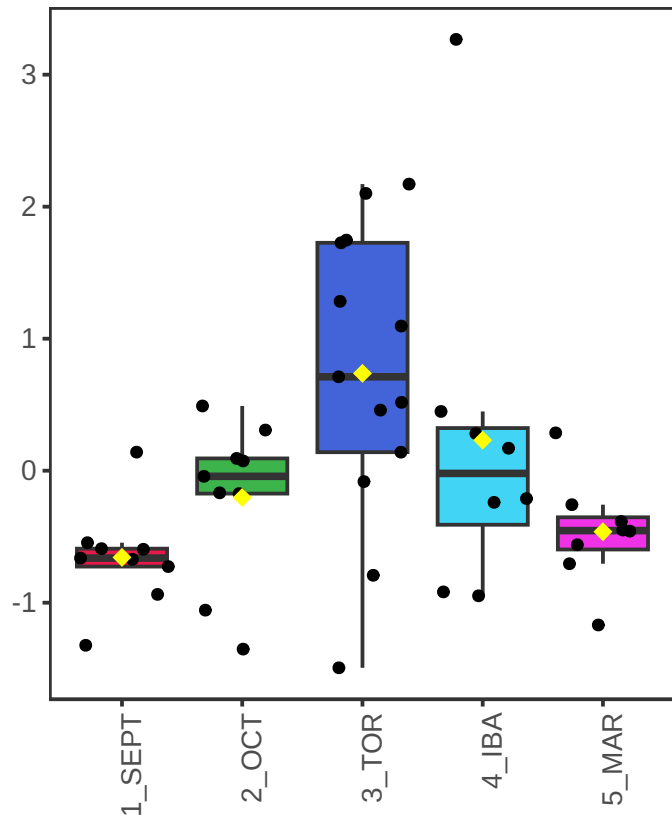


3-Hydroxydodecanoylcarnitine

Original Conc.

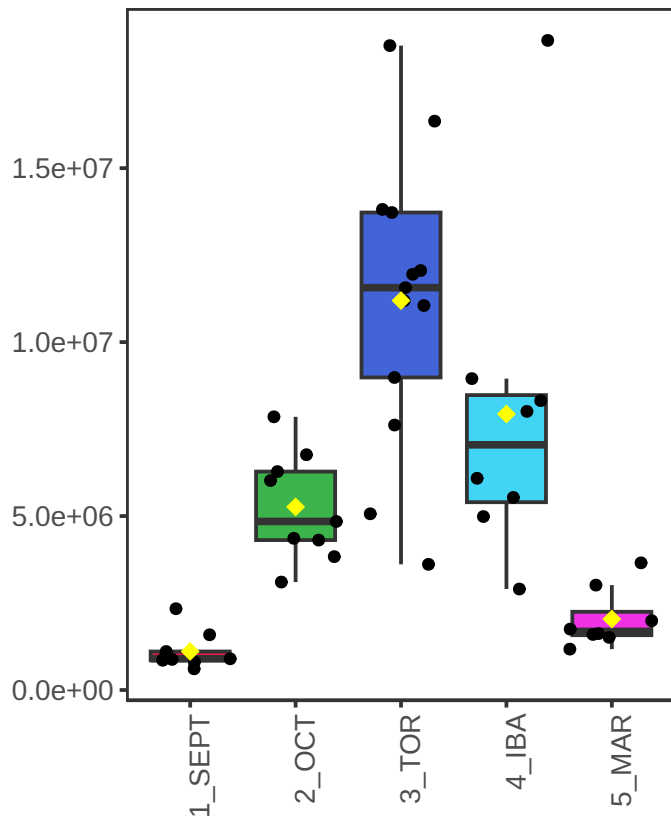


Normalized Conc.

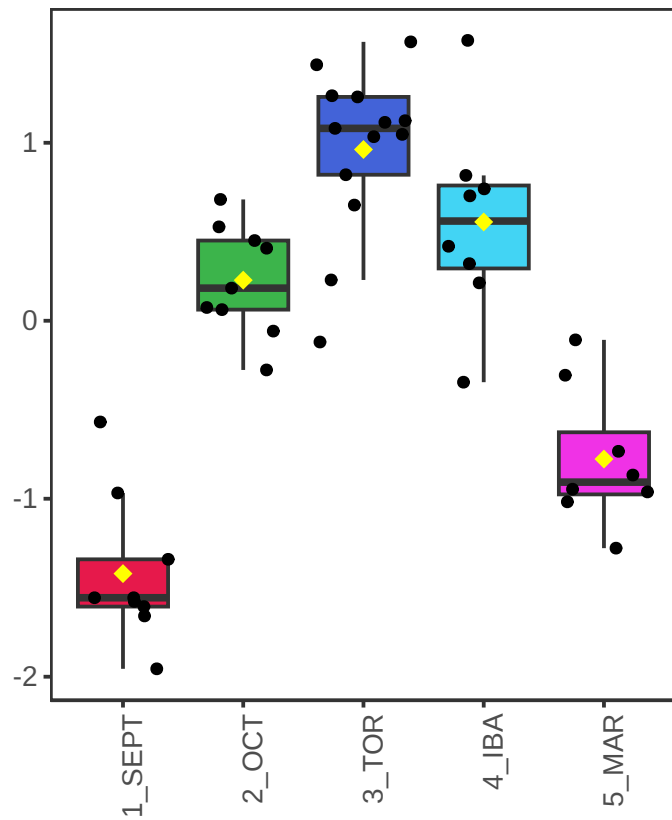


3-Hydroxyoctanoylcarnitine

Original Conc.

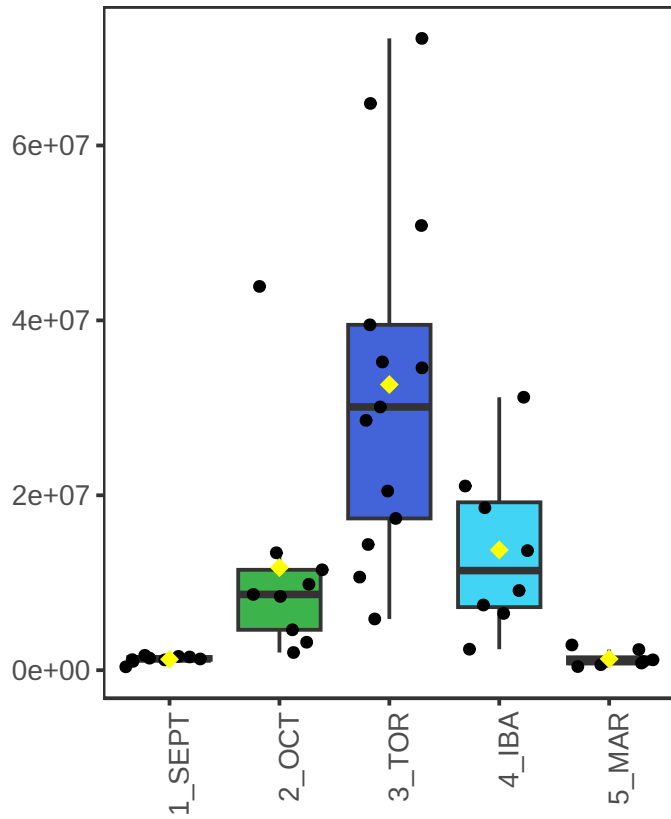


Normalized Conc.

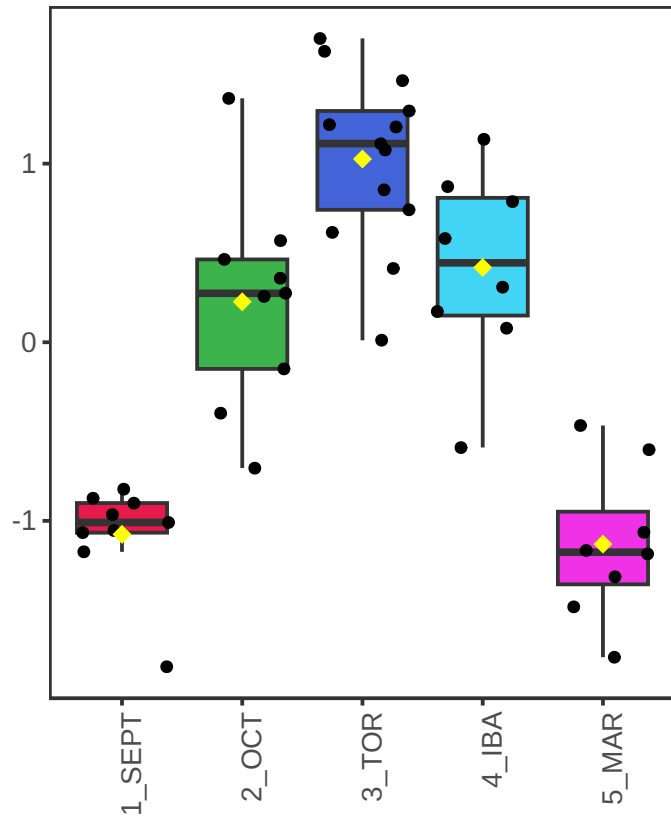


3-Hydroxyoctenoylcarnitine

Original Conc.

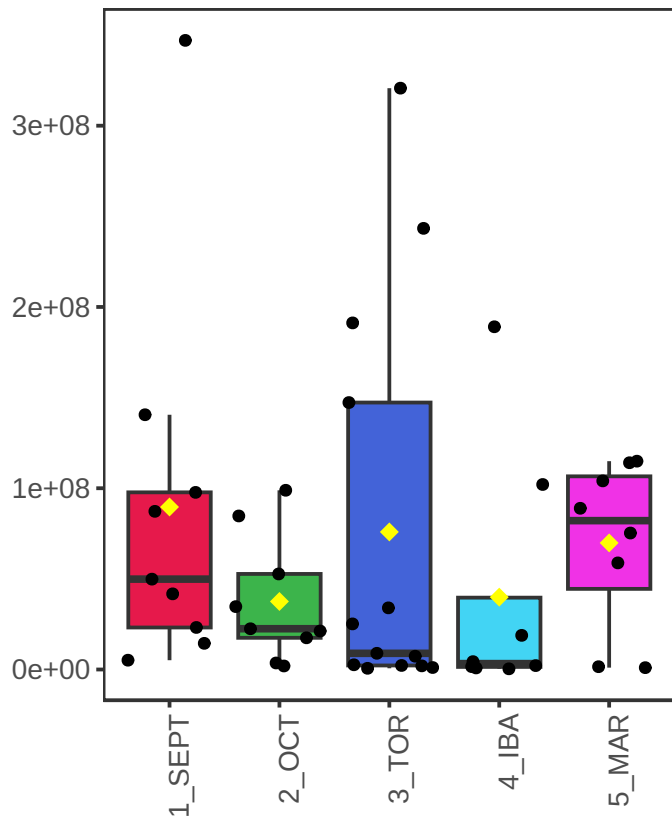


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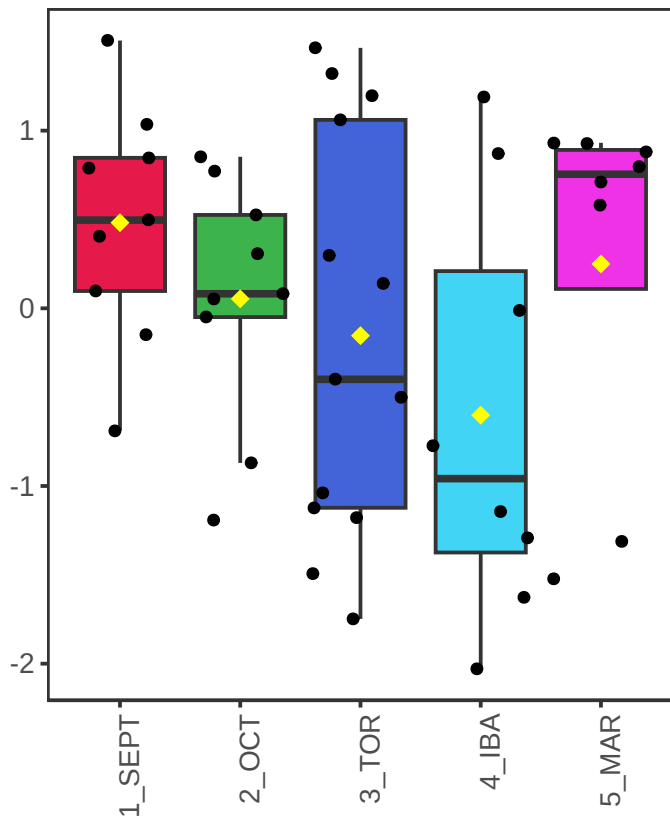


3-Methylenenorleucine

Original Conc.

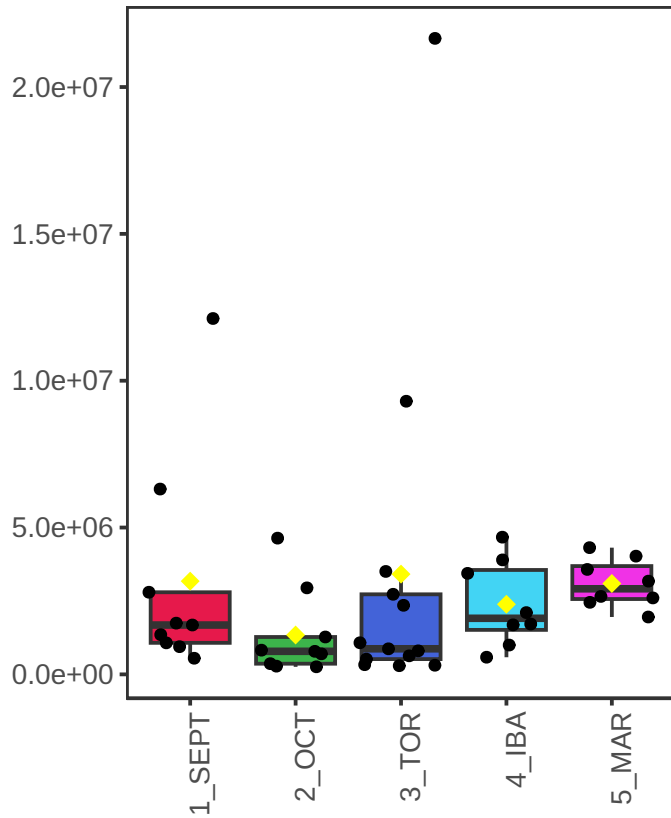


Normalized Conc.

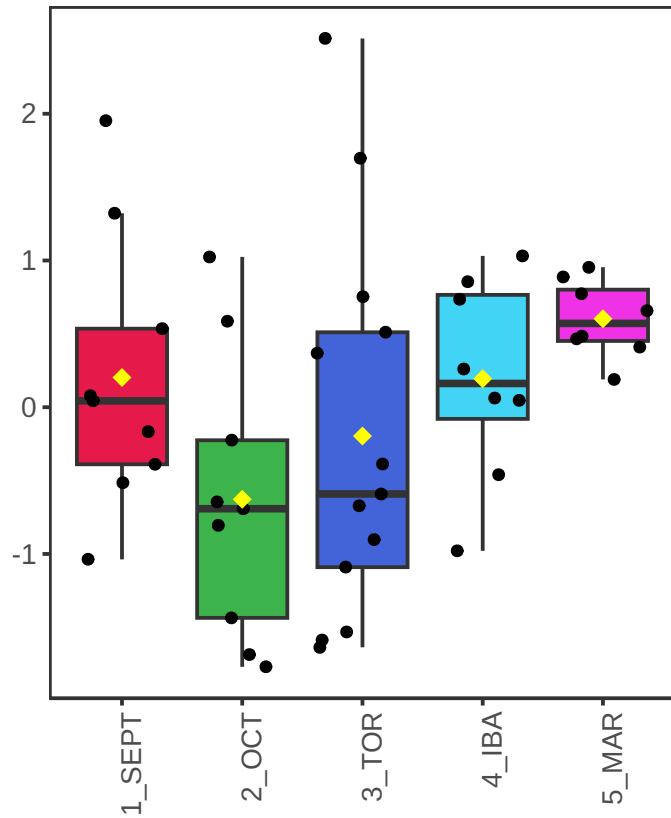


3-Methylguanine

Original Conc.

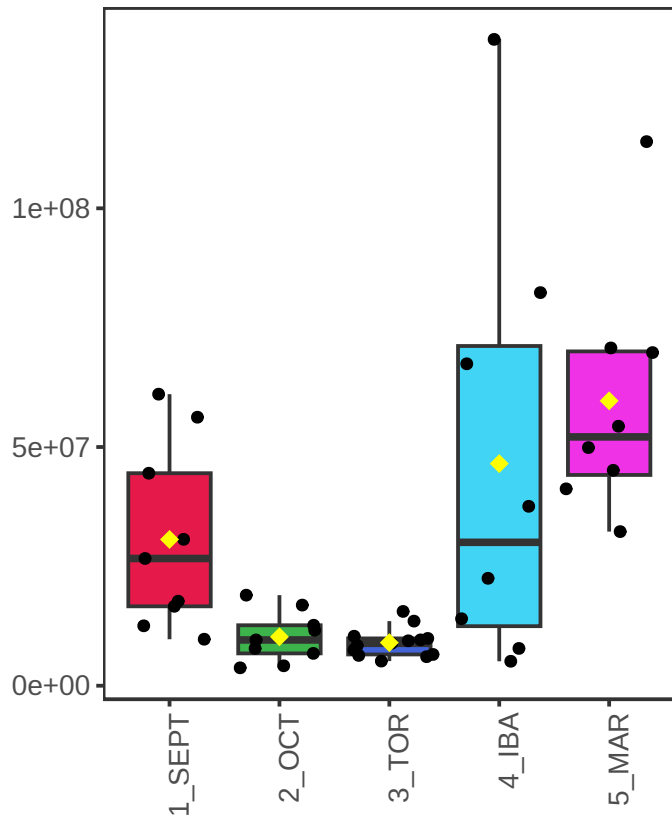


Normalized Conc.

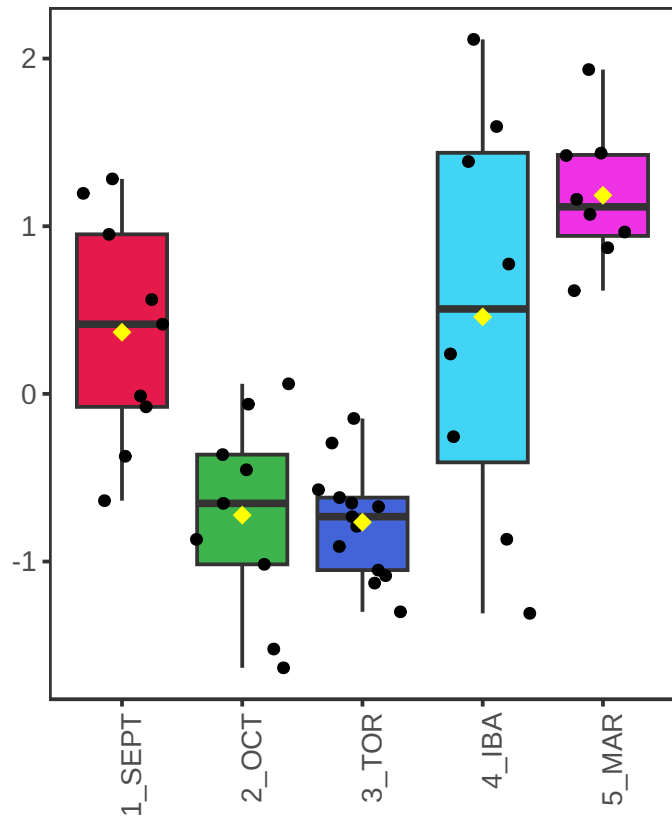


3-Ureidopropionic acid

Original Conc.

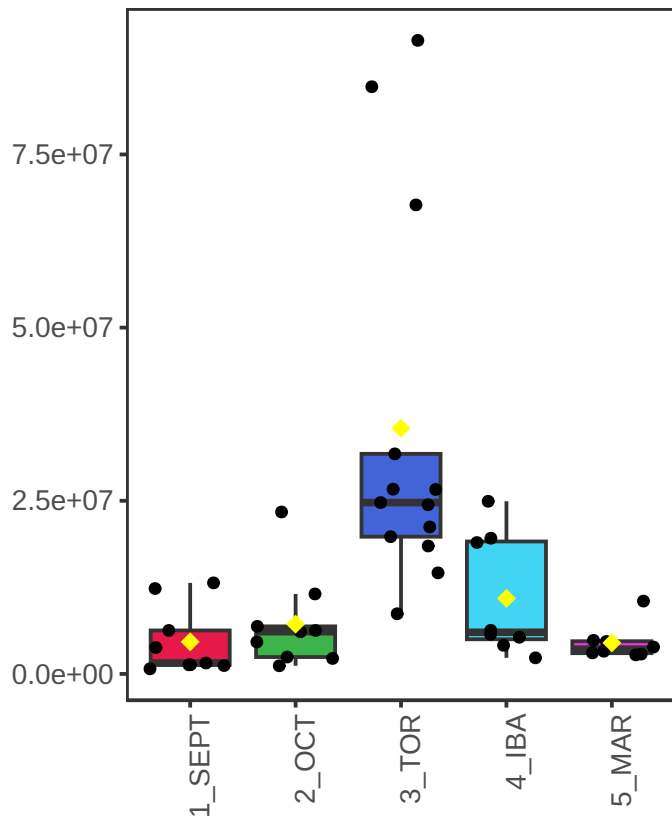


Normalized Conc.

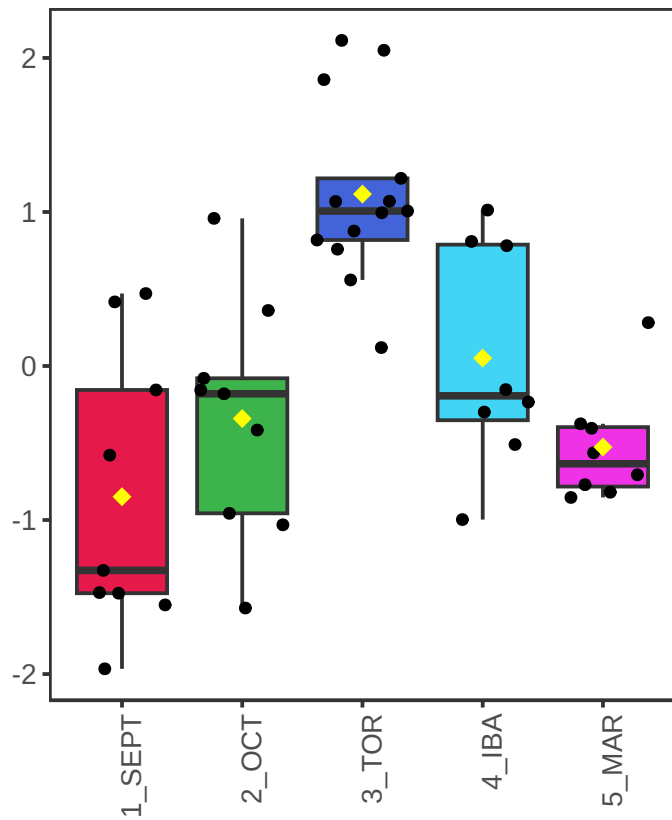


4-Acetamidobutanoic acid

Original Conc.

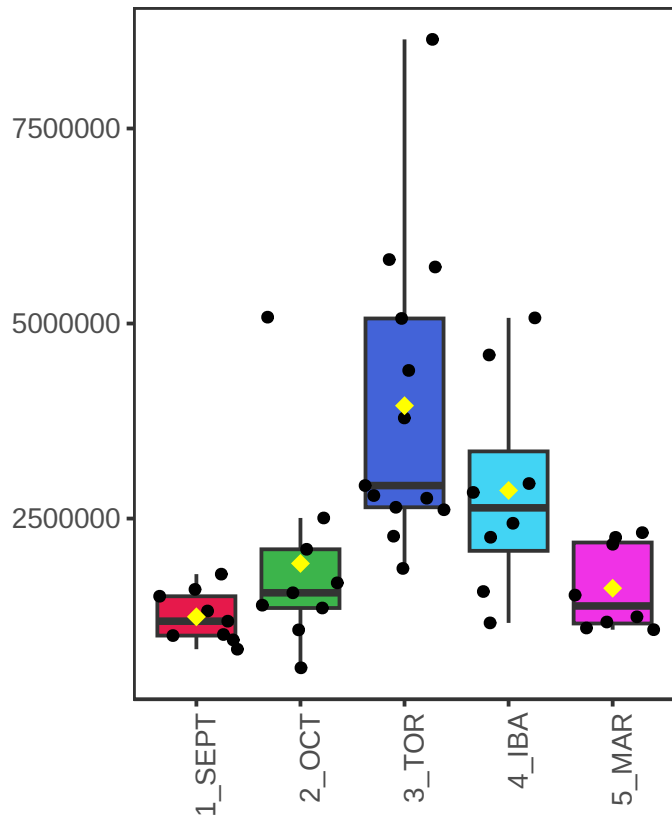


Normalized Conc.

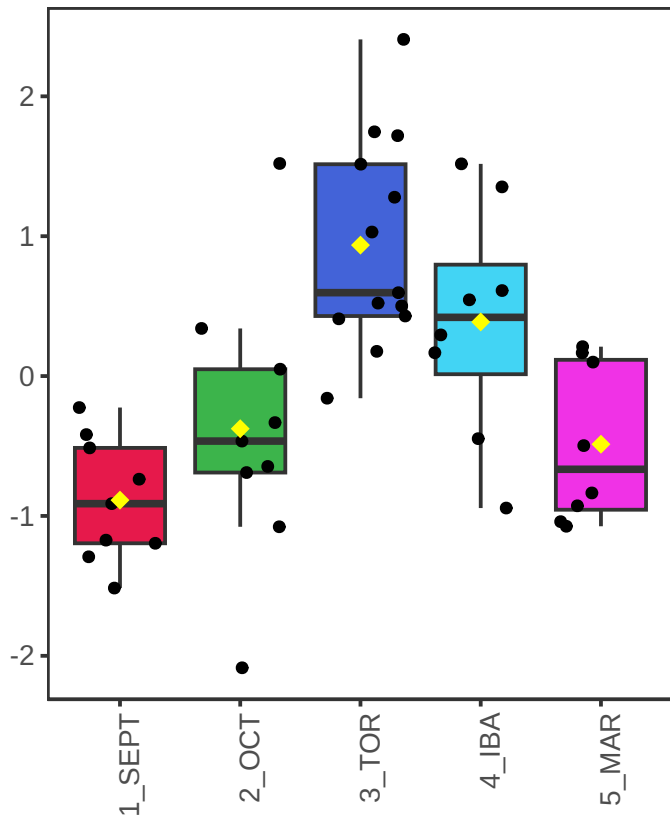


4-Amino-4-deoxypentopyranose

Original Conc.

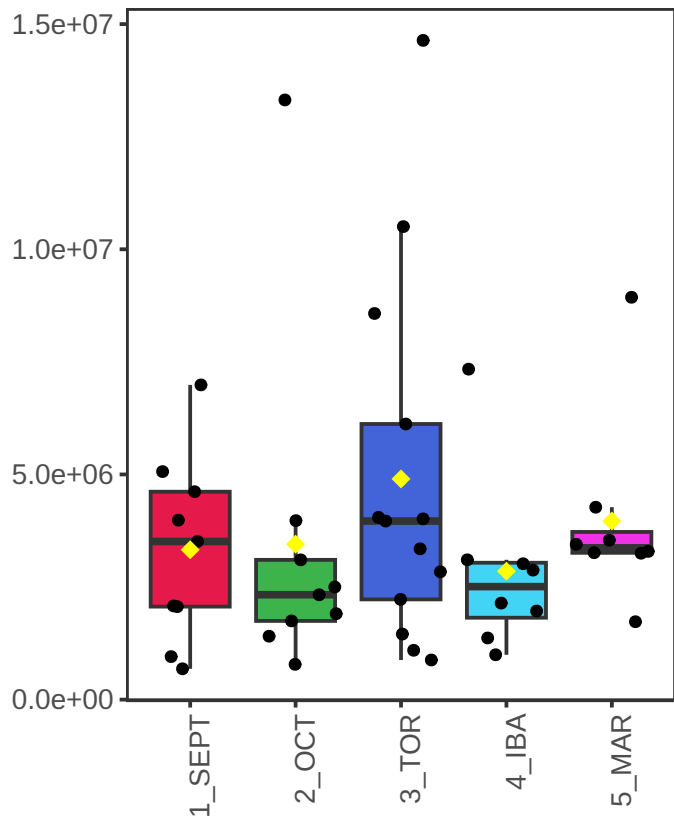


Normalized Conc.

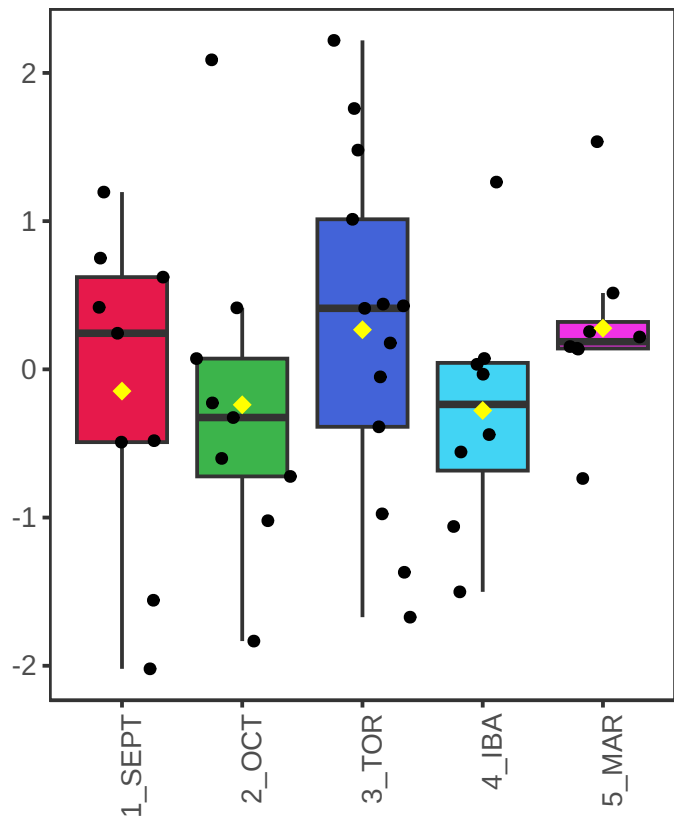


4-Guanidinobutyric acid

Original Conc.

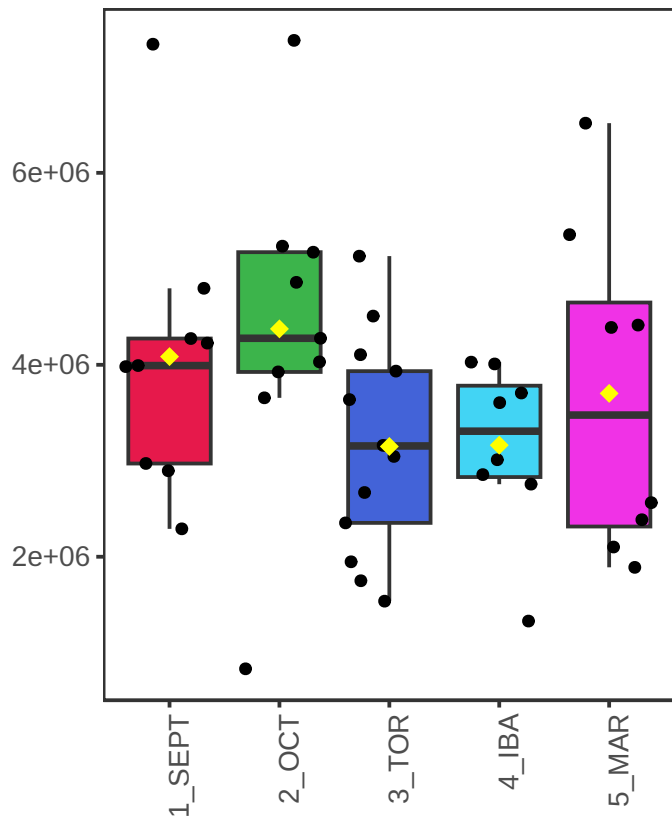


Normalized Conc.

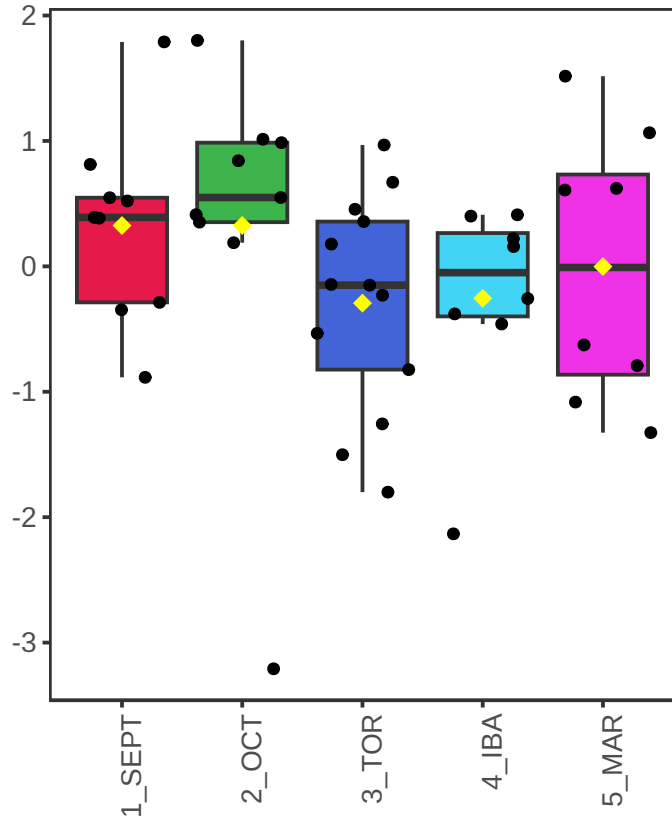


4'-Phosphopantetheine

Original Conc.

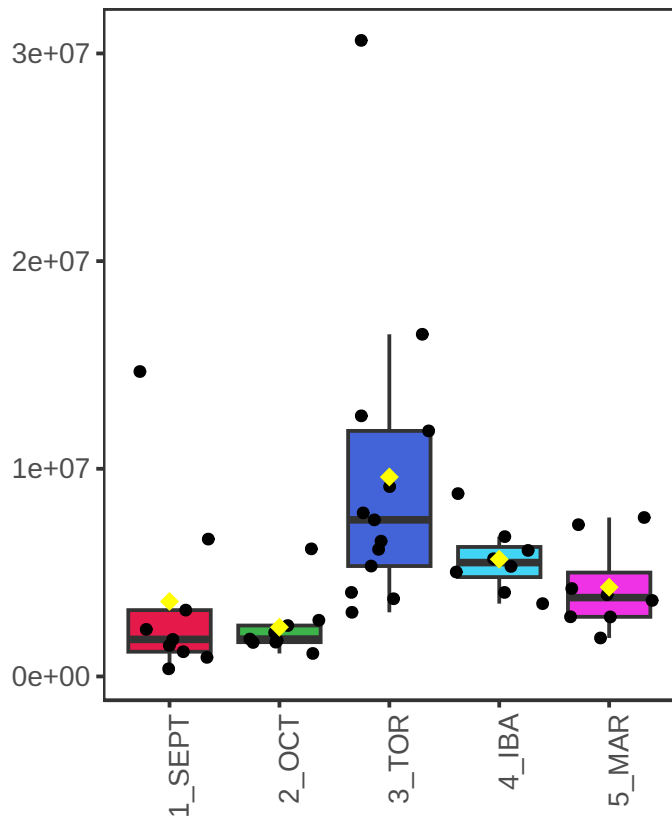


Normalized Conc.

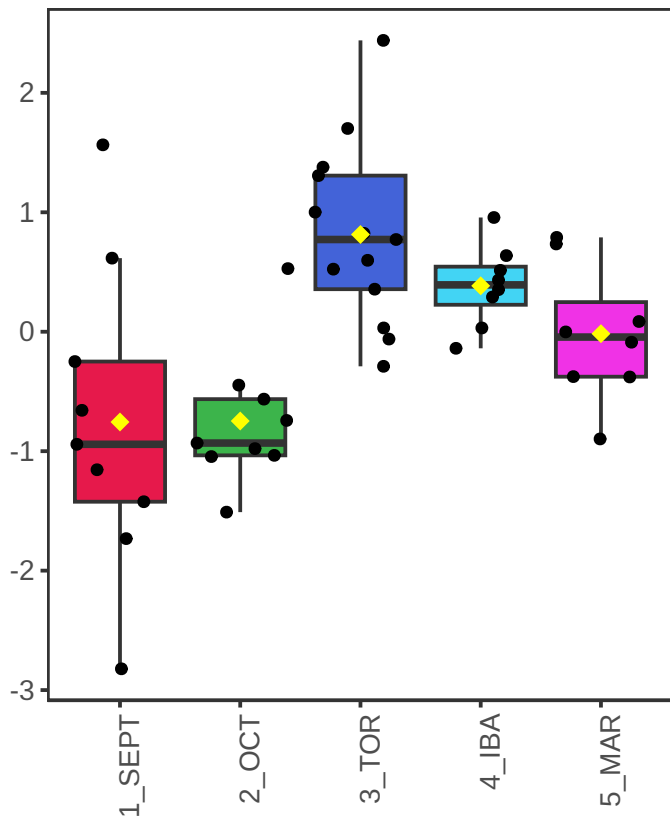


5-methylthioribose

Original Conc.

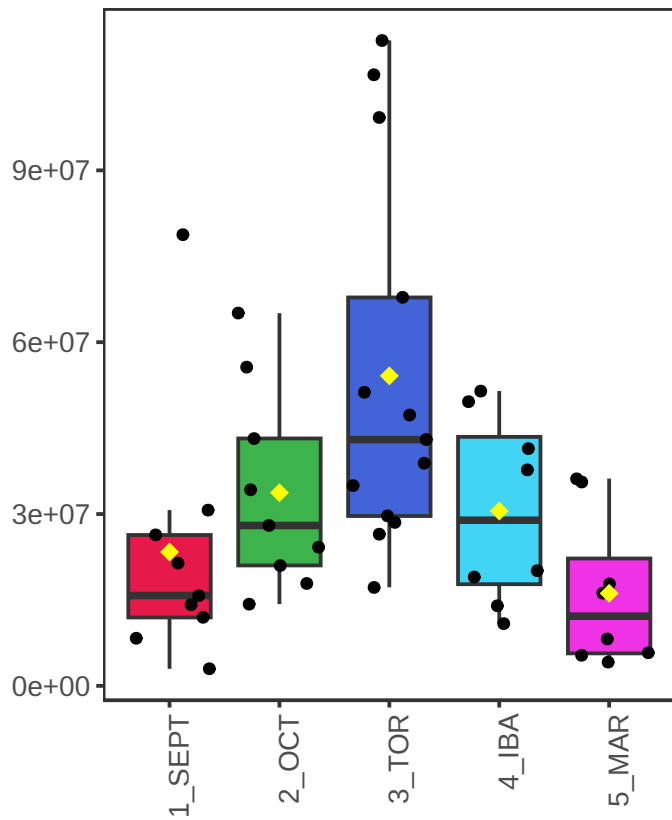


Normalized Conc.

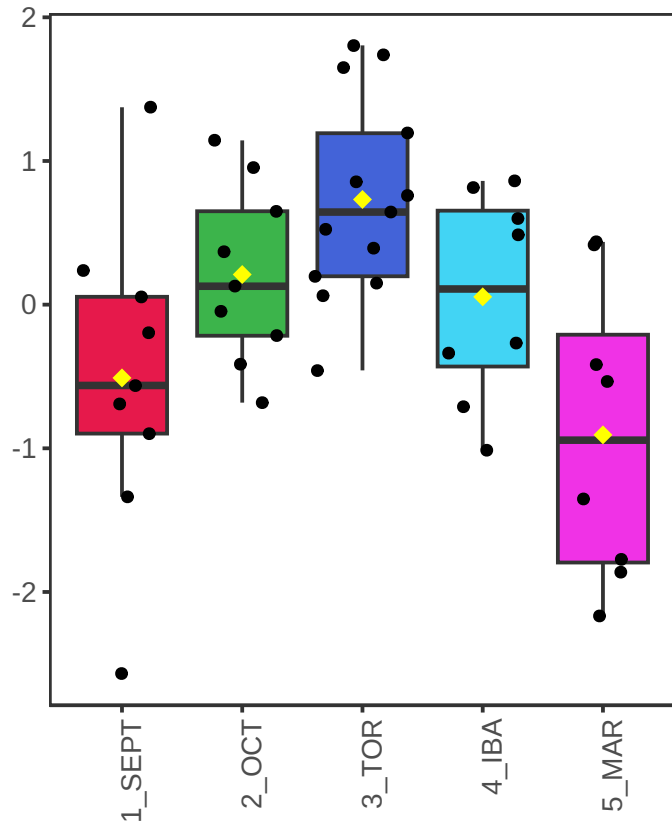


5-Nitro-o-toluidine

Original Conc.

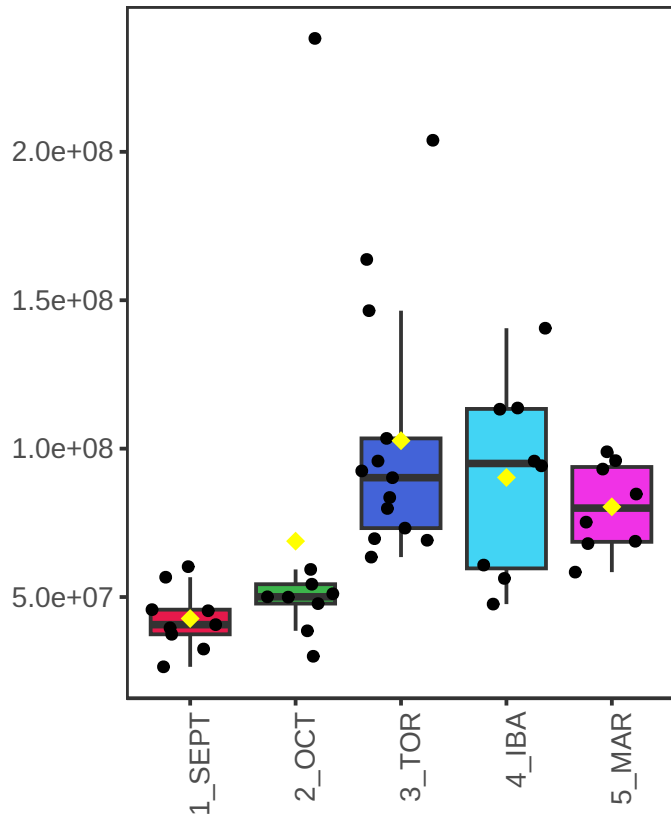


Normalized Conc.

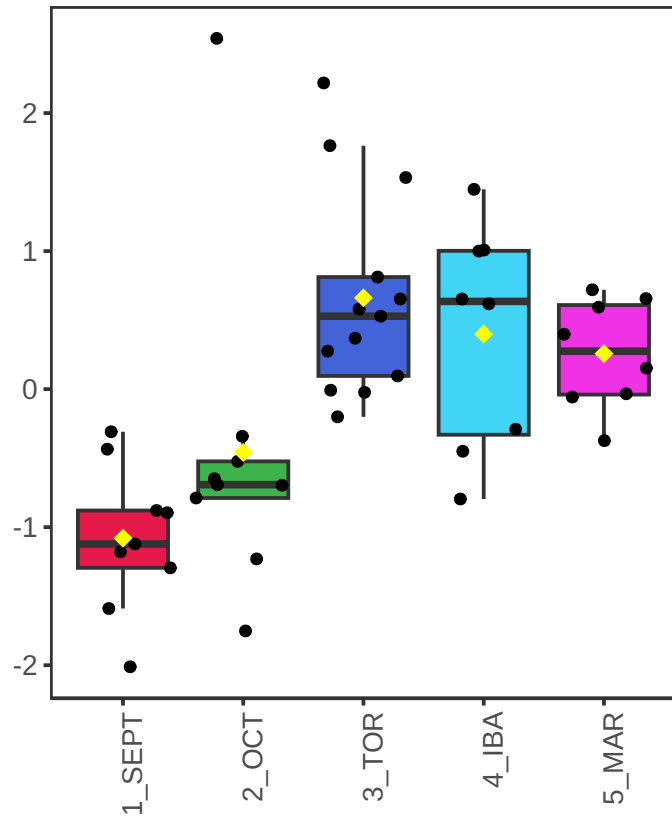


5'-S-Methyl-5'-thioadenosine

Original Conc.

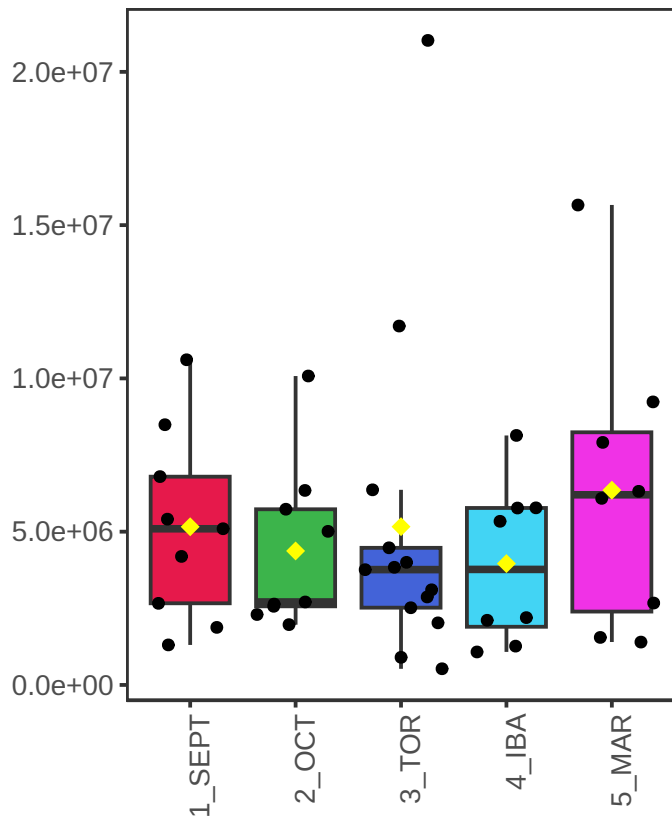


Normalized Conc.

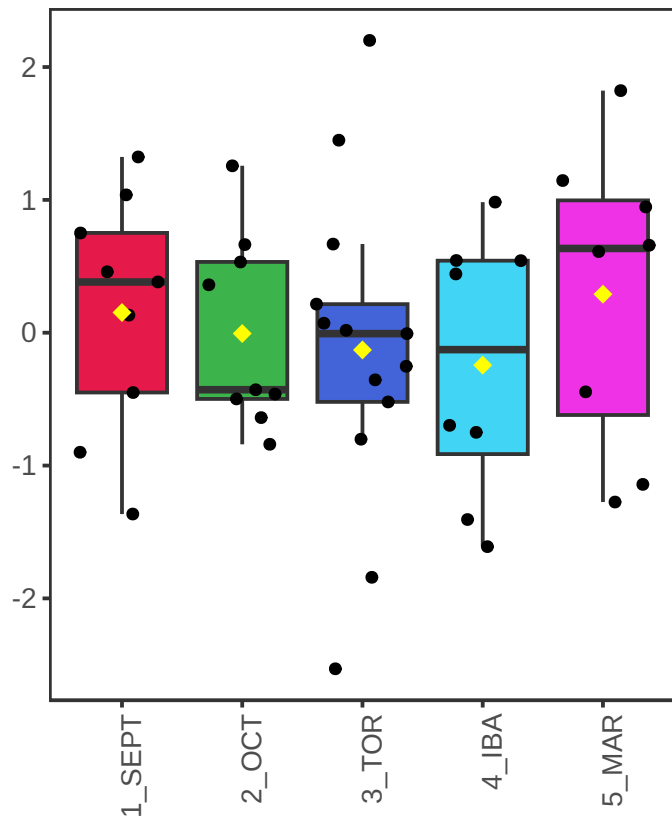


6-Aminocaproic acid

Original Conc.

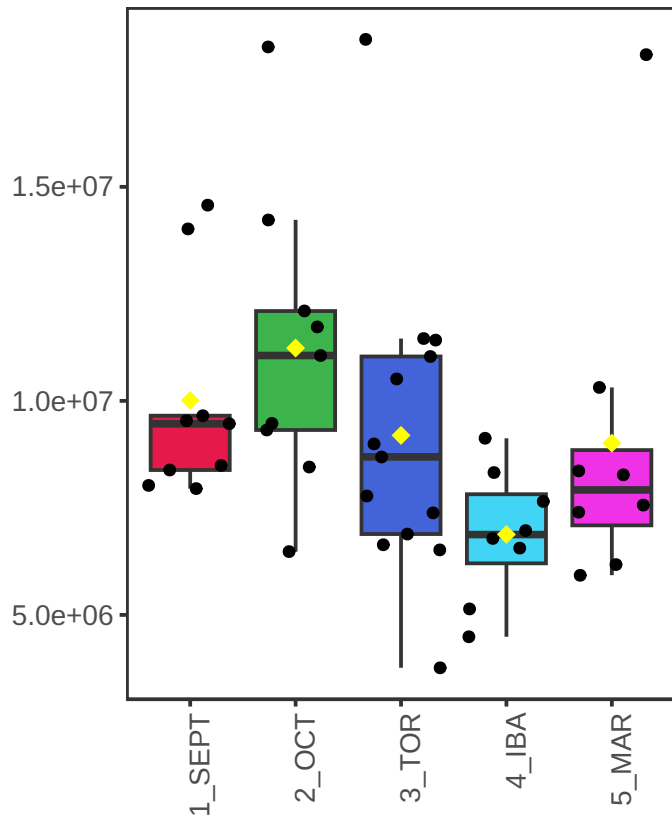


Normalized Conc.

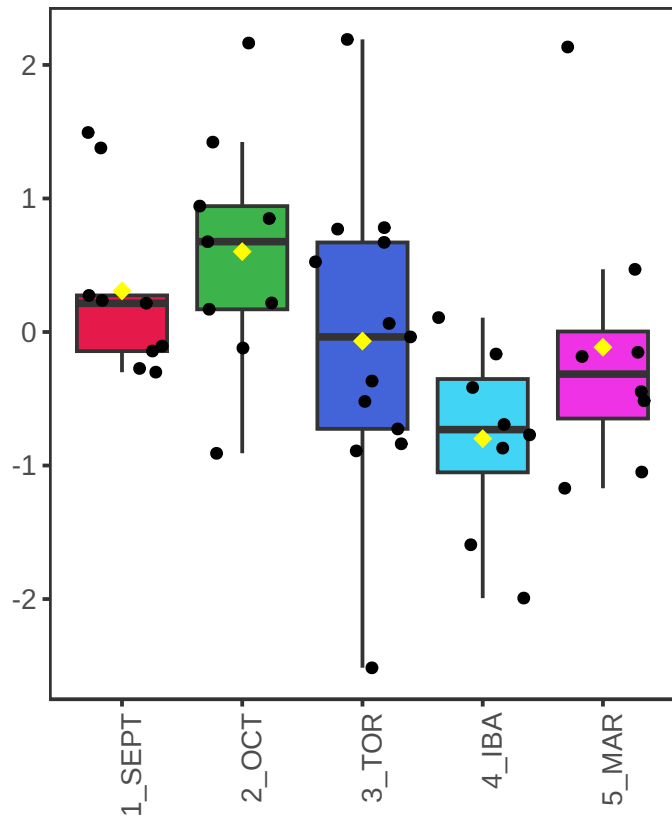


6-Hydroxycaproic acid

Original Conc.

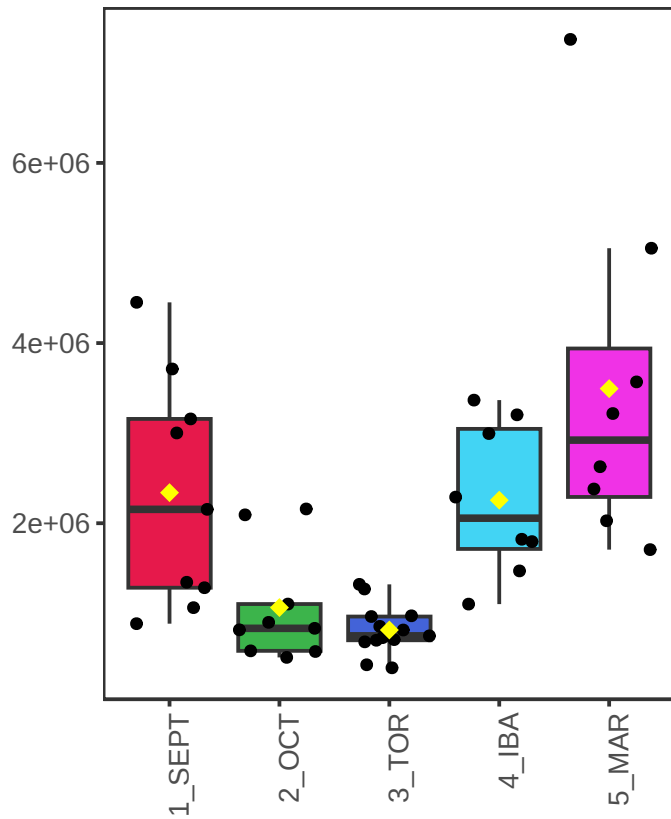


Normalized Conc.

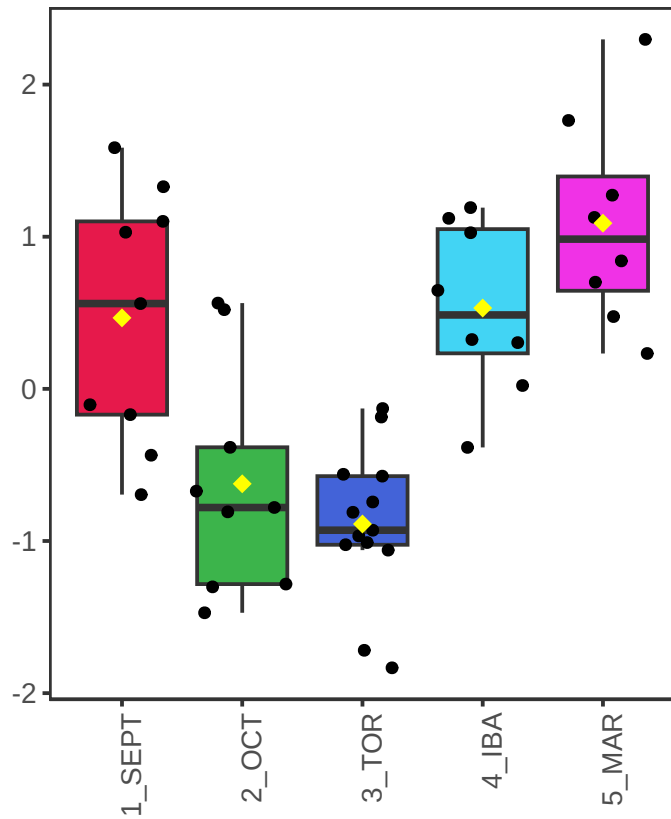


6-Ketoprostaglandin F1a

Original Conc.

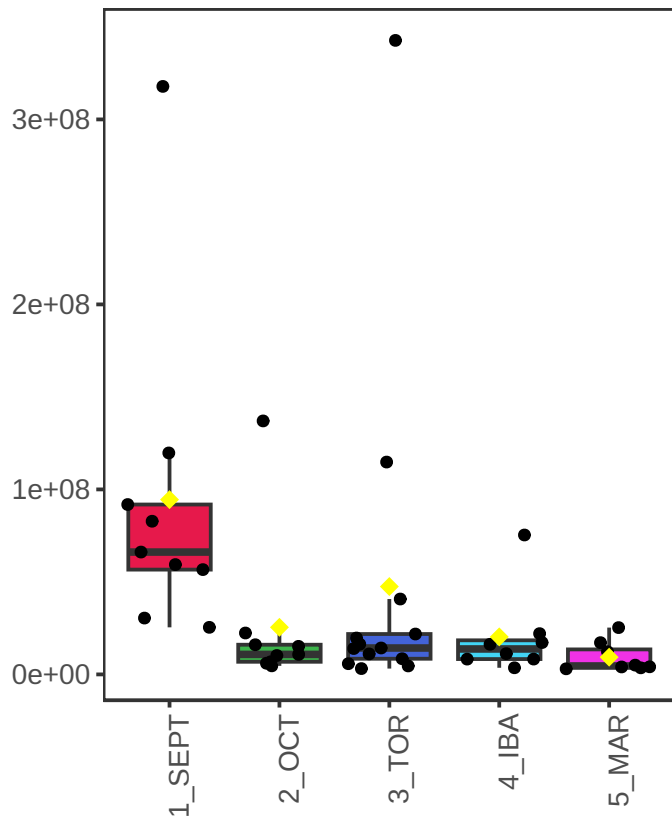


Normalized Conc.

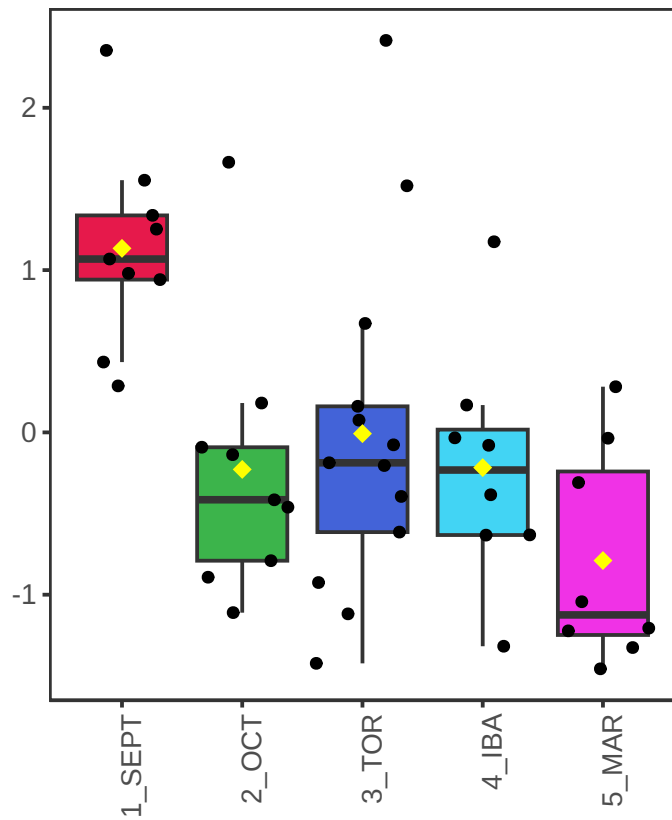


6-Methylnicotinamide

Original Conc.

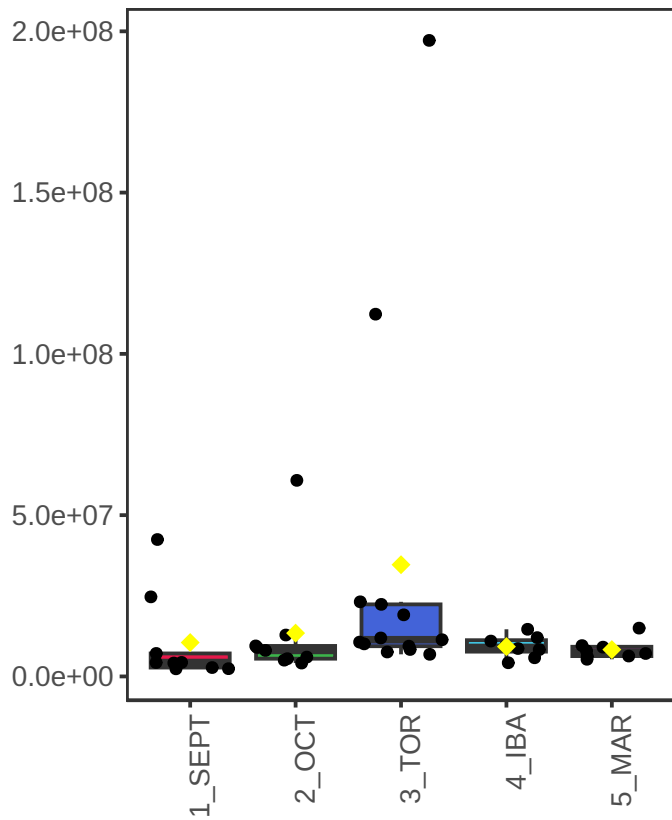


Normalized Conc.

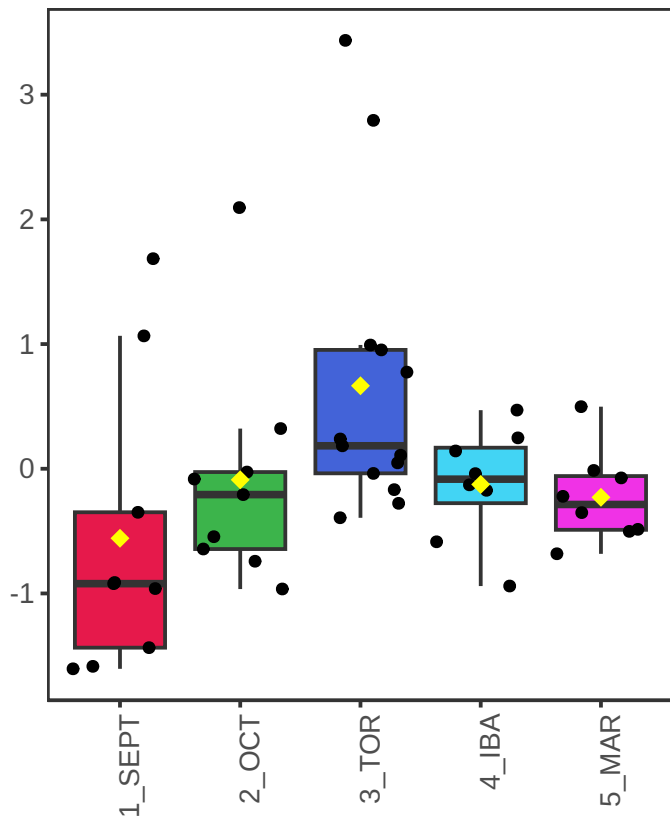


7-Methylguanine

Original Conc.

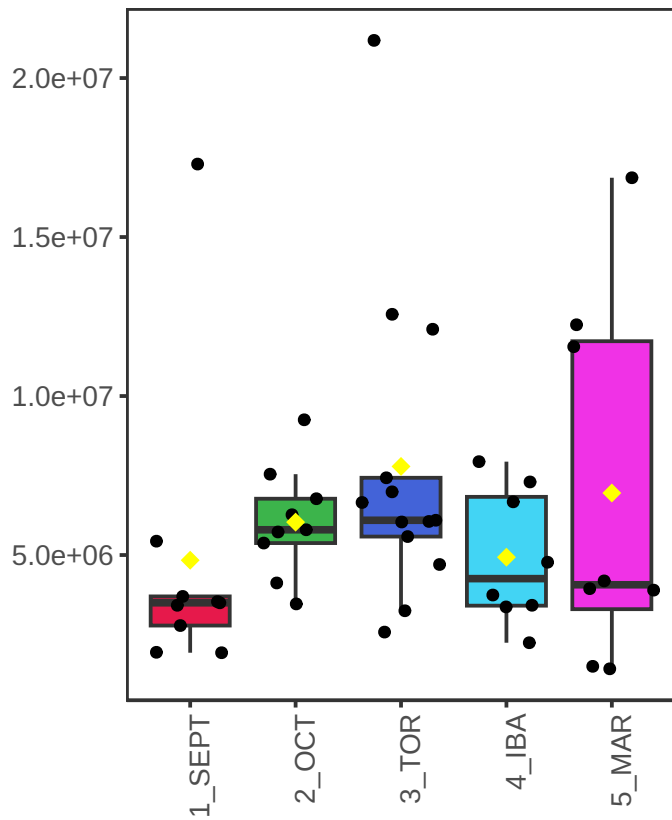


Normalized Conc.

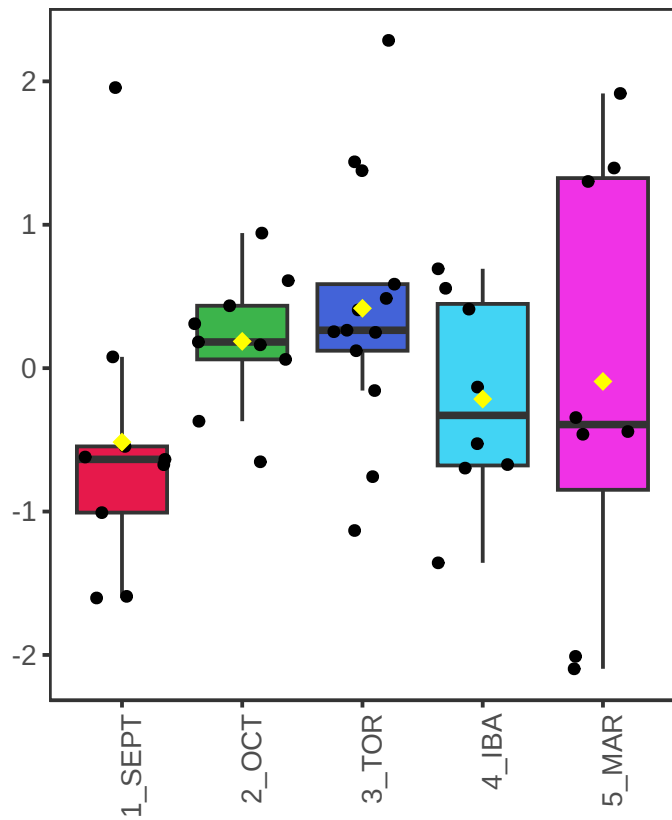


12-Aminododecanoic acid

Original Conc.

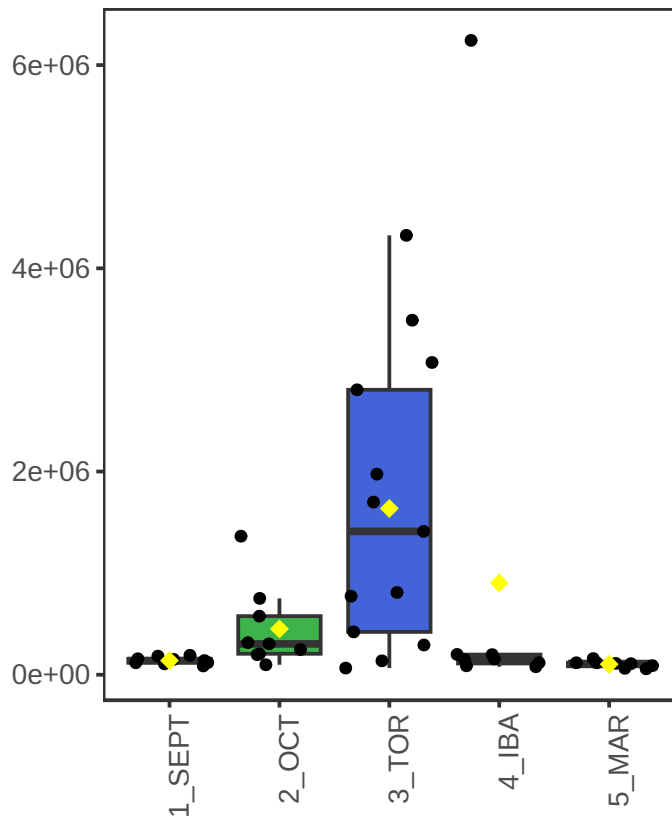


Normalized Conc.

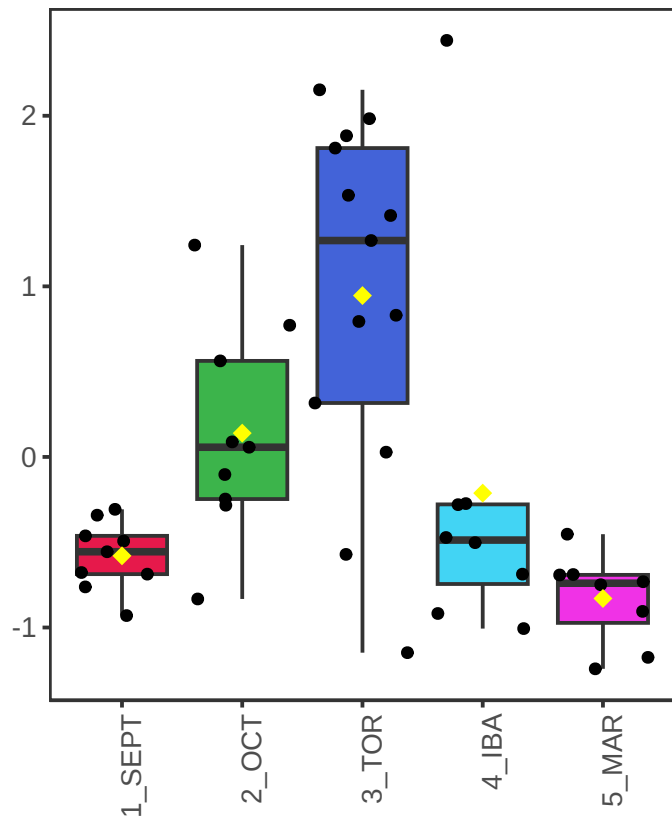


(15-Carboxypentadecanoyl)carnitine

Original Conc.

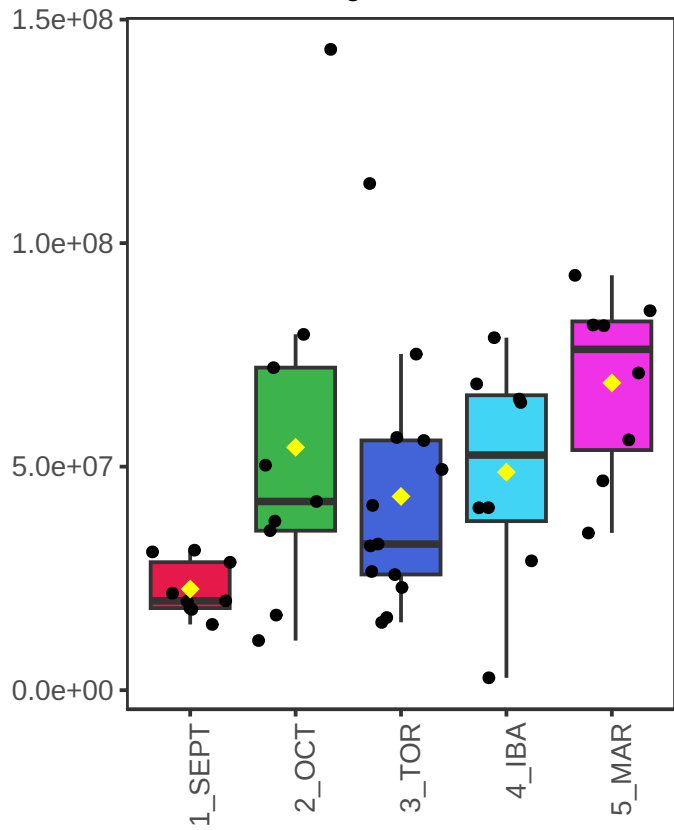


Normalized Conc.

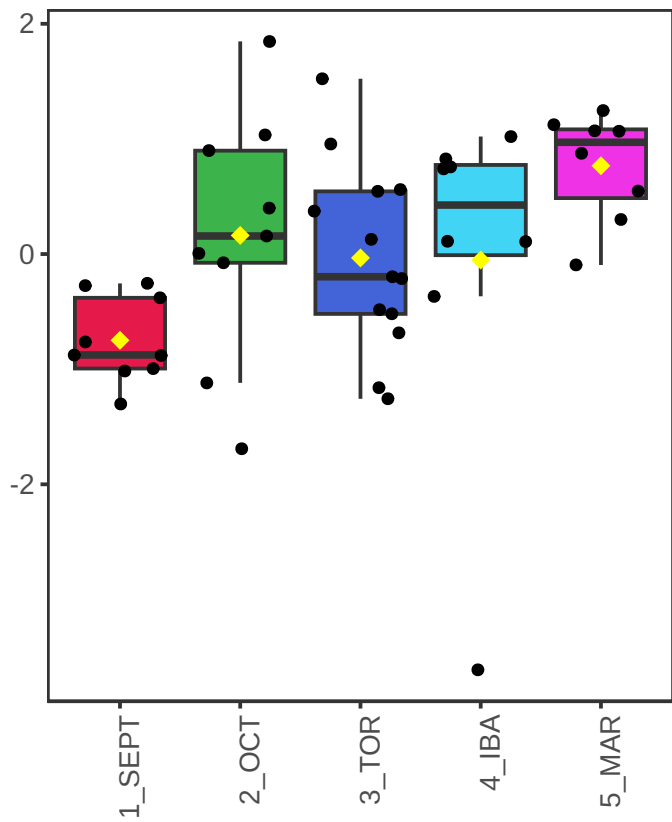


2,6-Dimethylpyrazine

Original Conc.

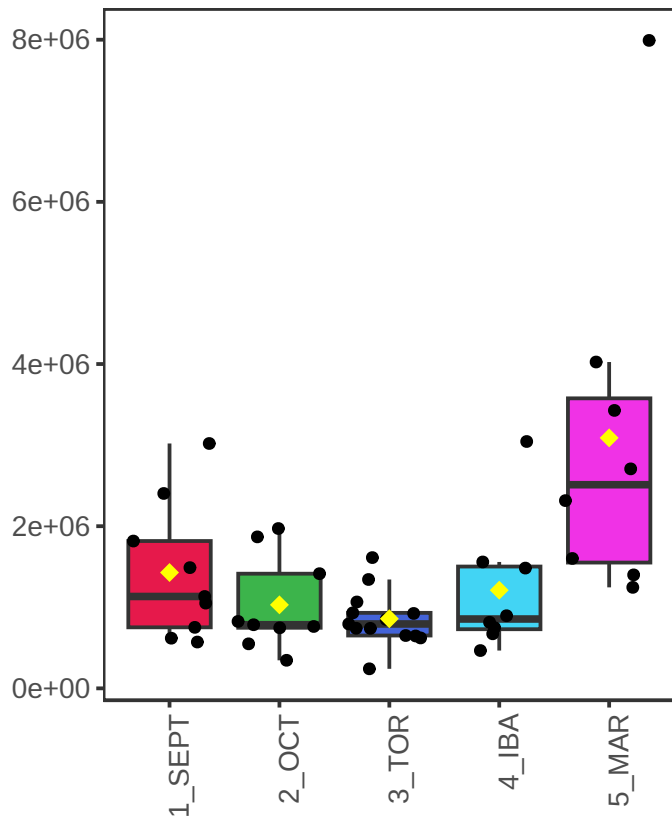


Normalized Conc.

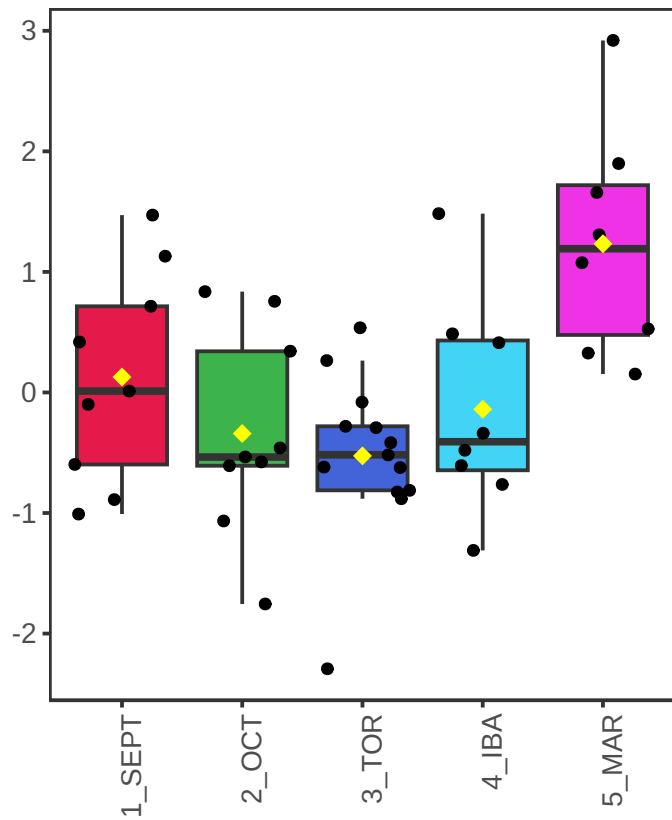


3,4-Methylenesebacic acid

Original Conc.

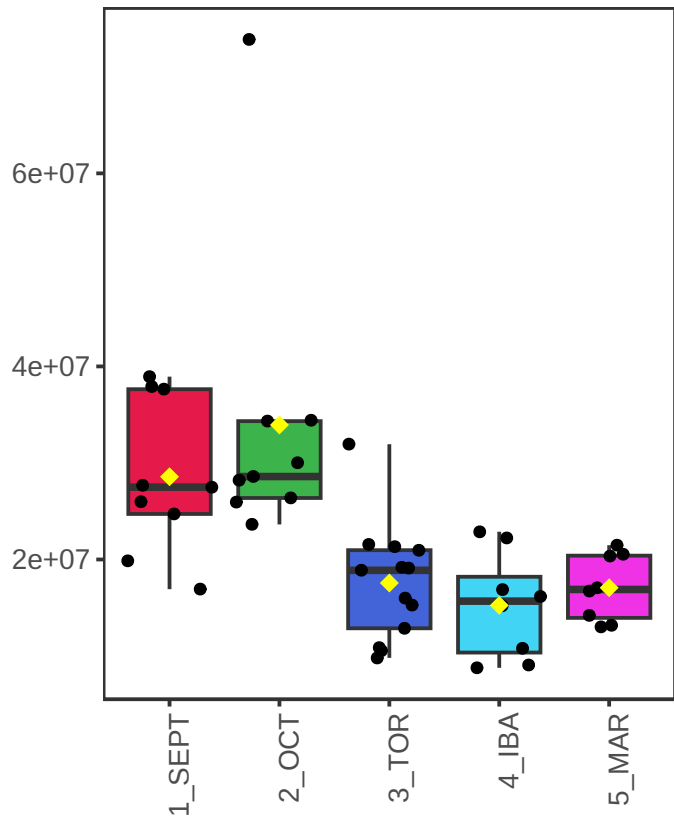


Normalized Conc.

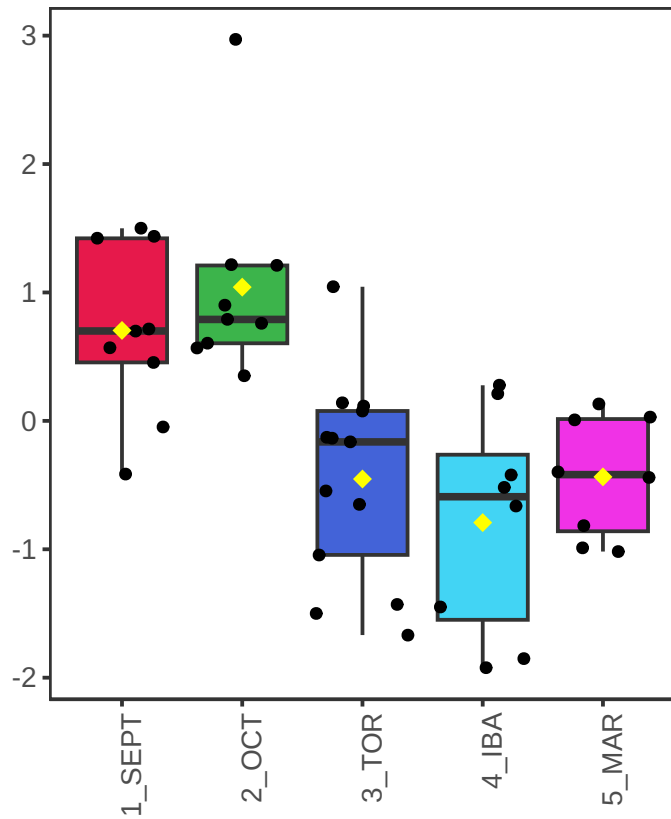


2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)

Original Conc.

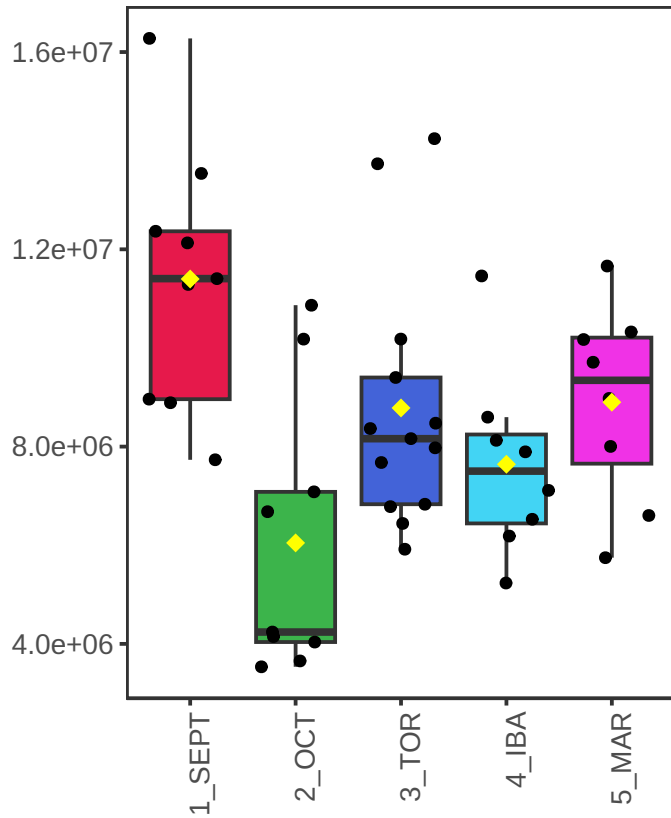


Normalized Conc.

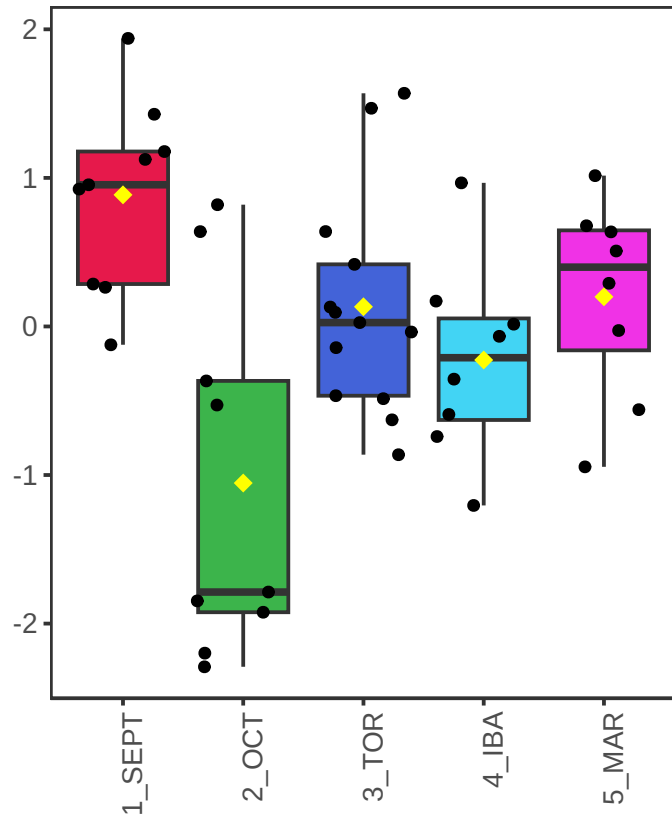


1-Aminocyclopropanecarboxylate

Original Conc.

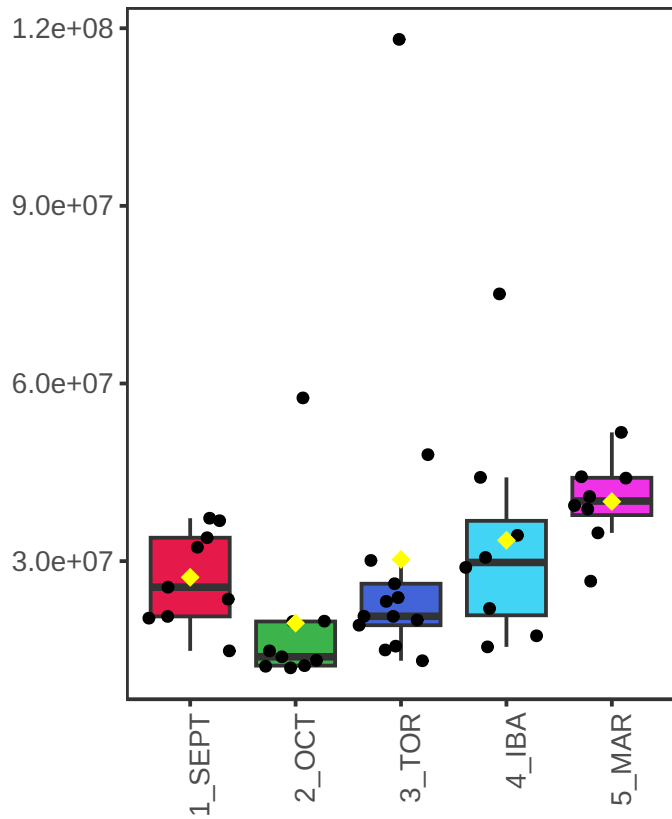


Normalized Conc.

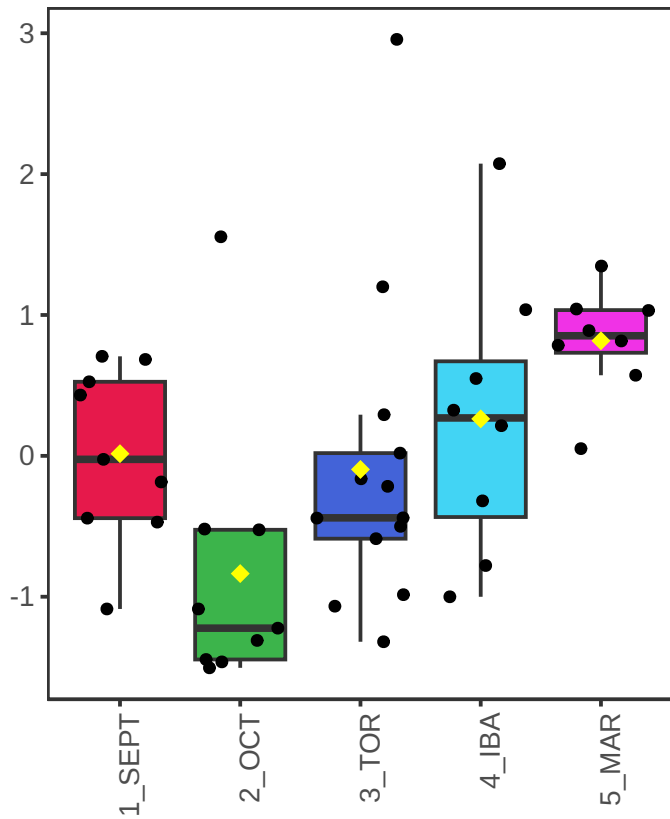


Acetohydroxamic acid

Original Conc.

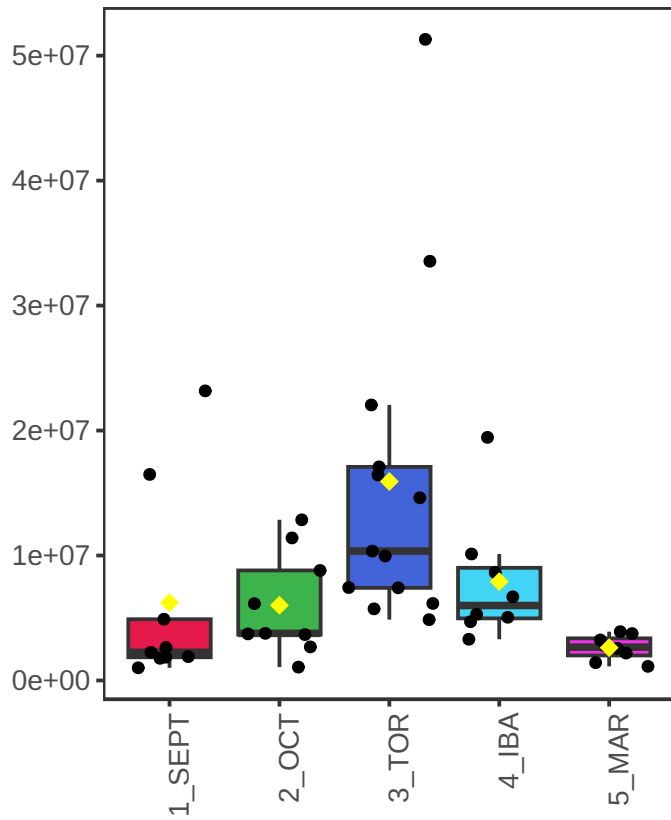


Normalized Conc.

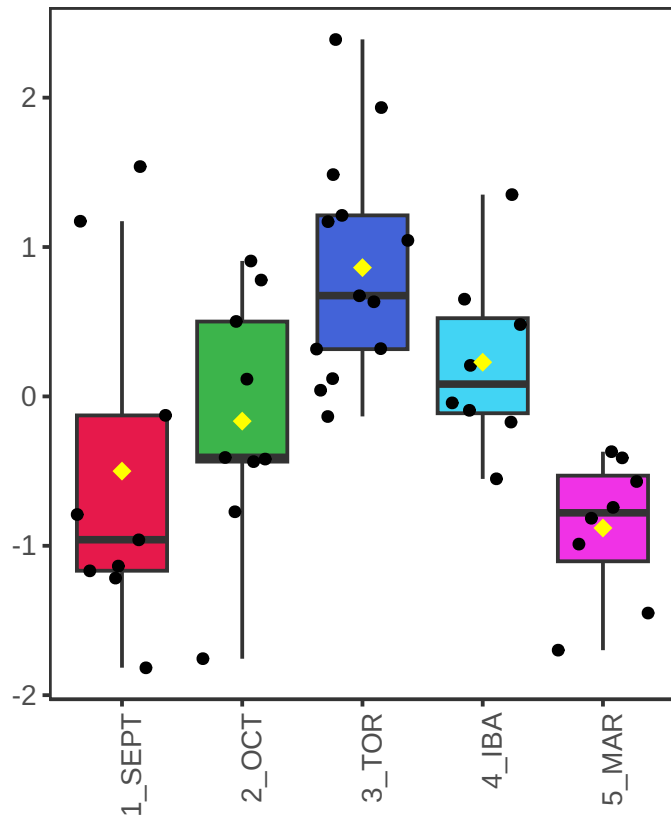


Acetylarginine

Original Conc.

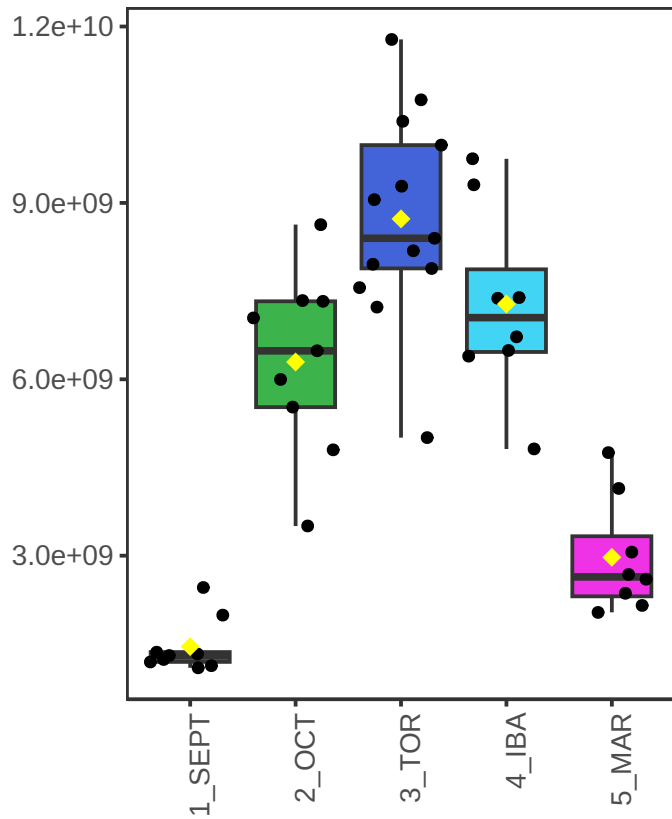


Normalized Conc.

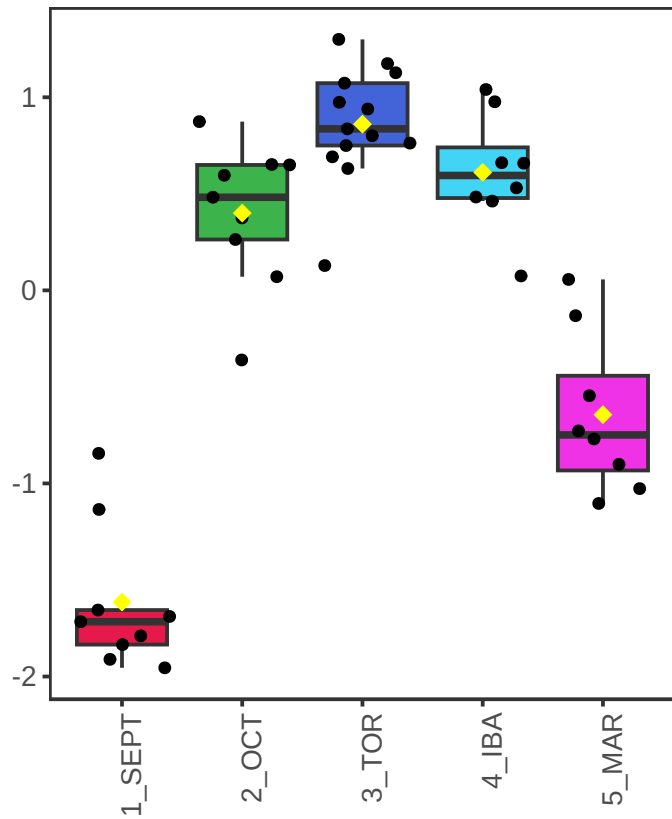


Acetylcarnitine

Original Conc.

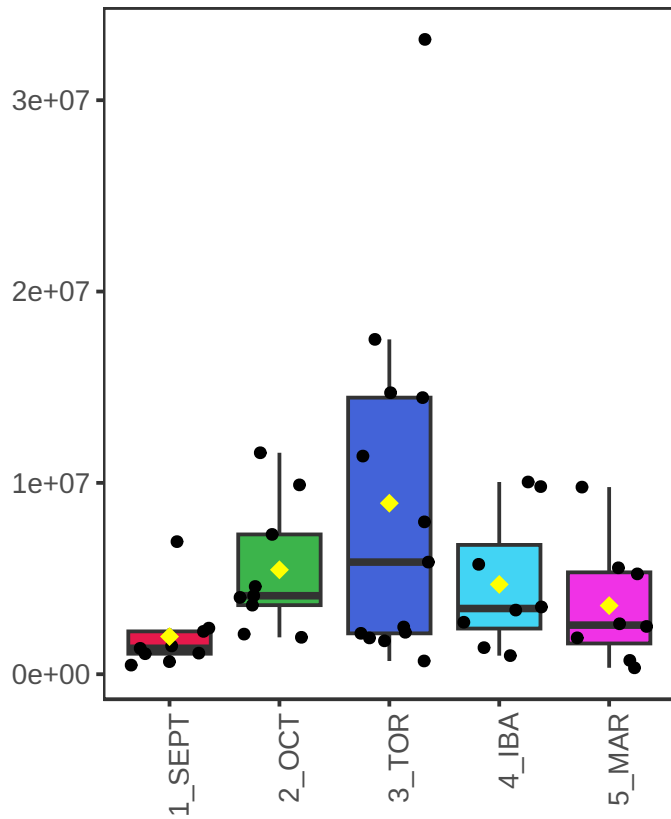


Normalized Conc.

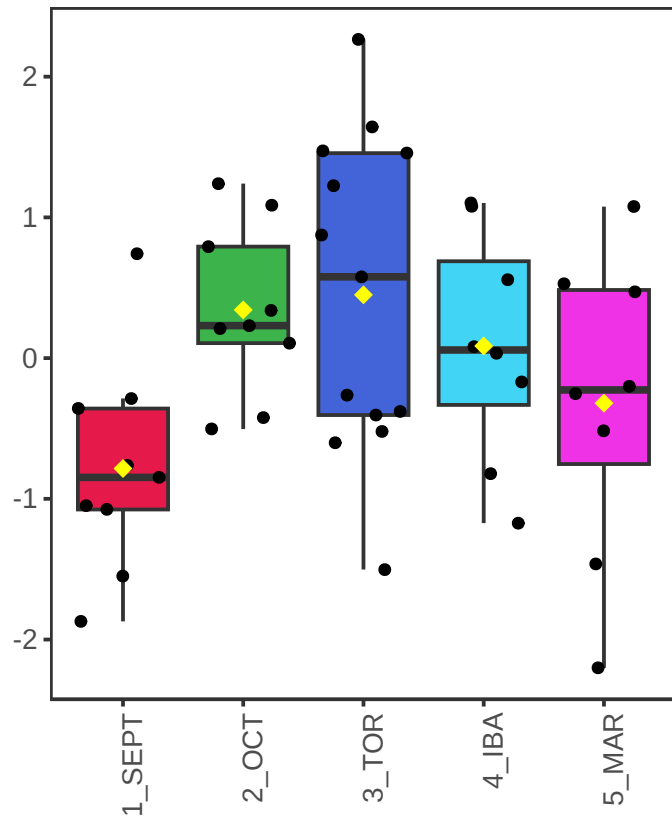


Acetylcholine

Original Conc.

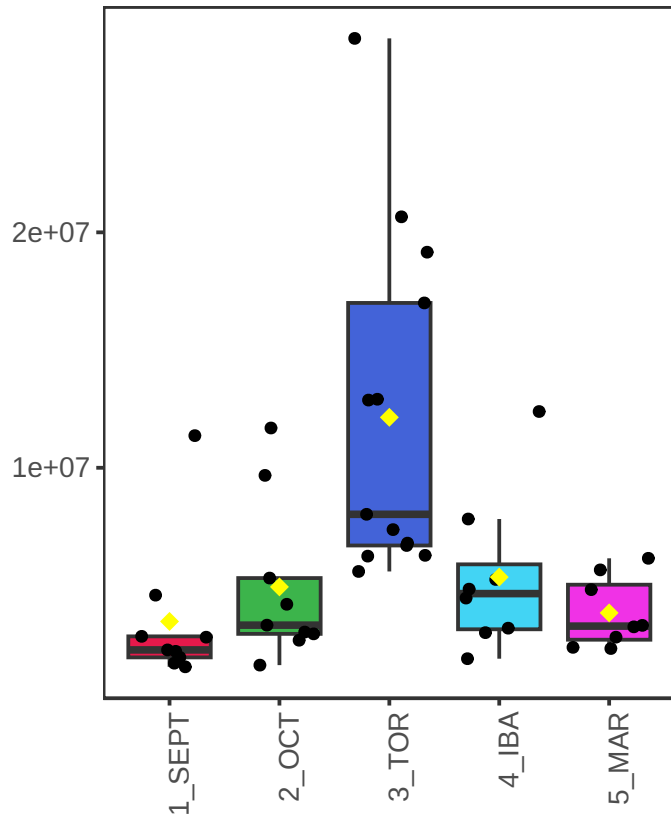


Normalized Conc.

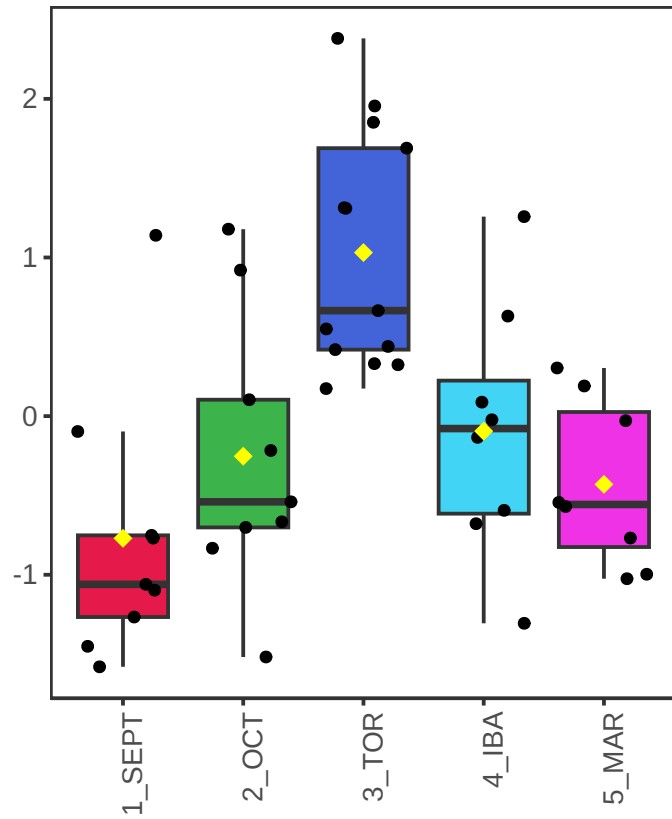


Acetylproline

Original Conc.

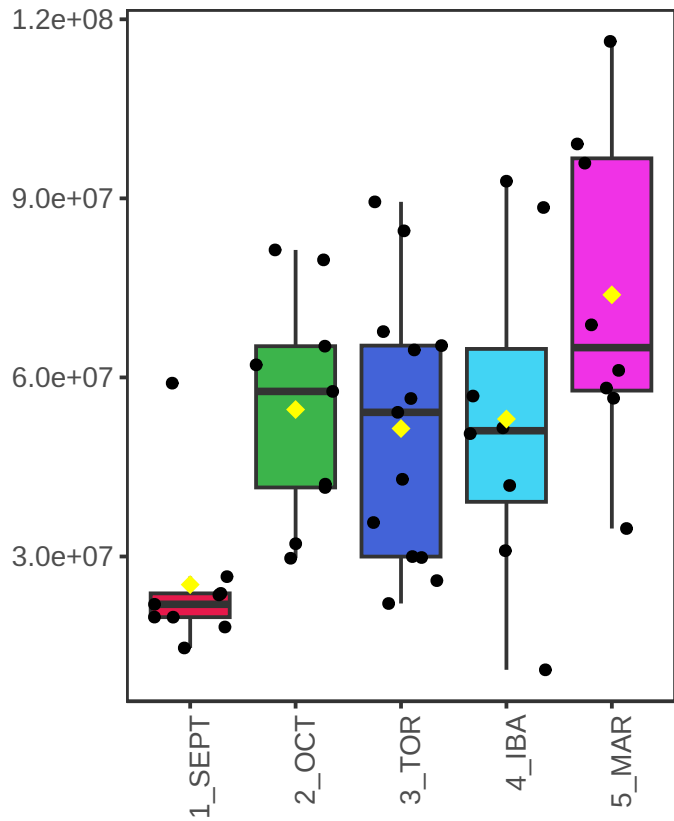


Normalized Conc.

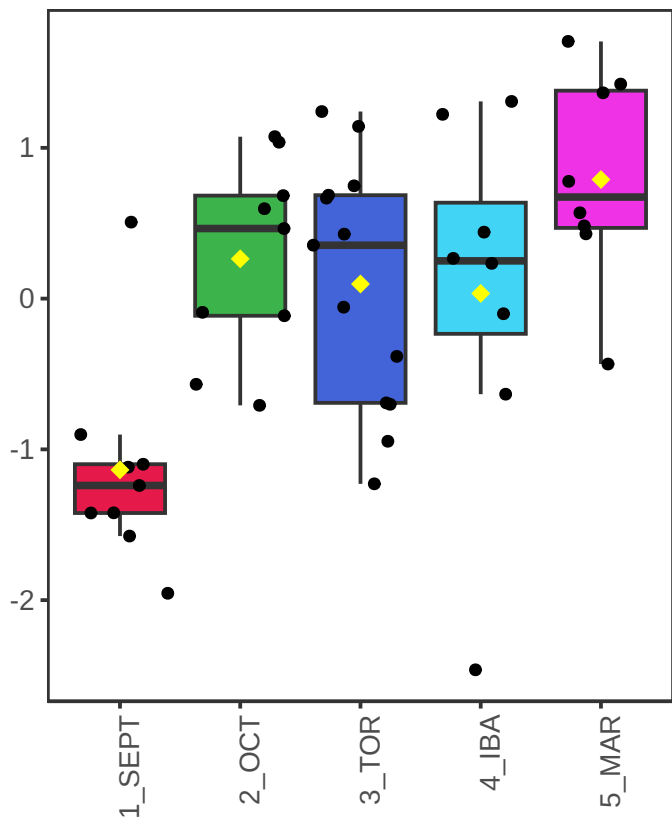


Adenine

Original Conc.

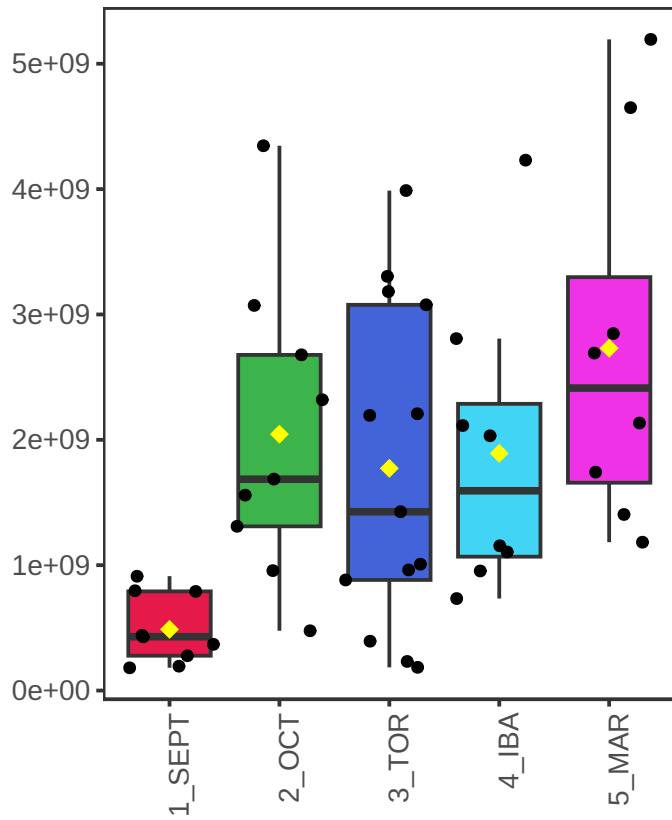


Normalized Conc.

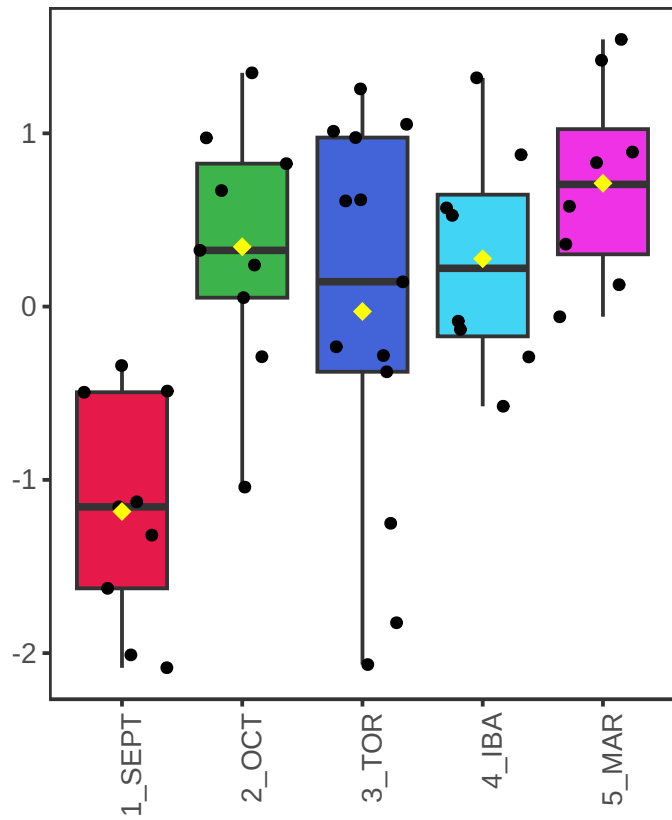


Adenosine

Original Conc.

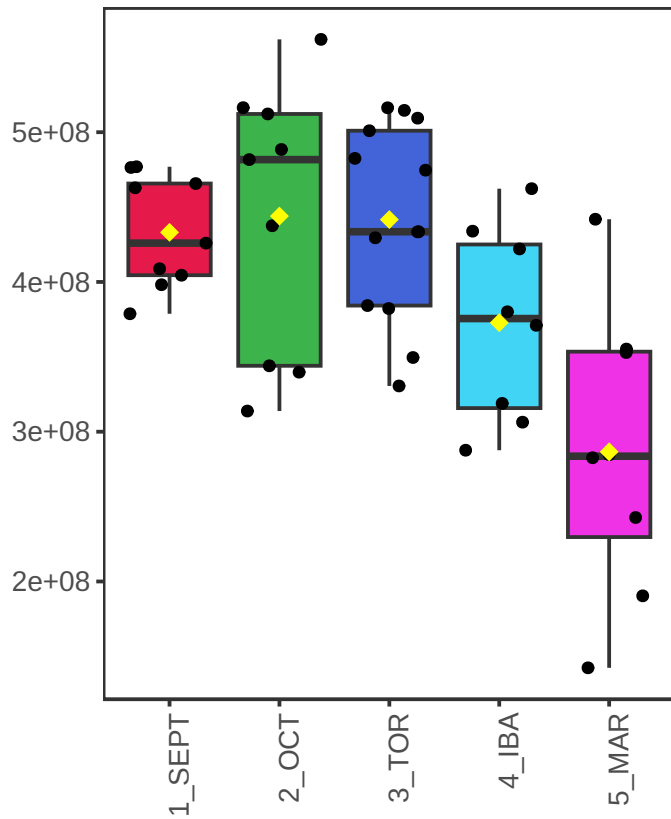


Normalized Conc.

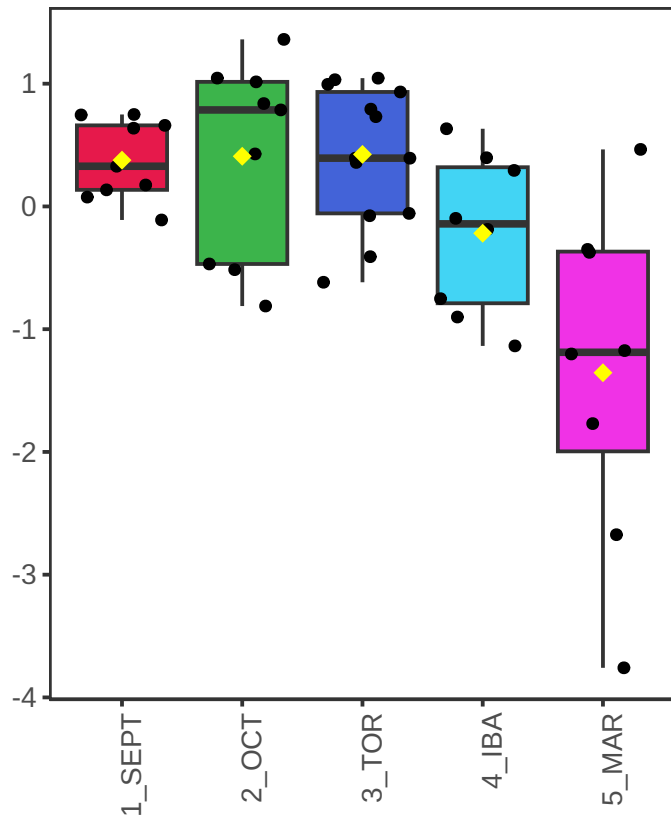


Adenosine 5'-monophosphate

Original Conc.

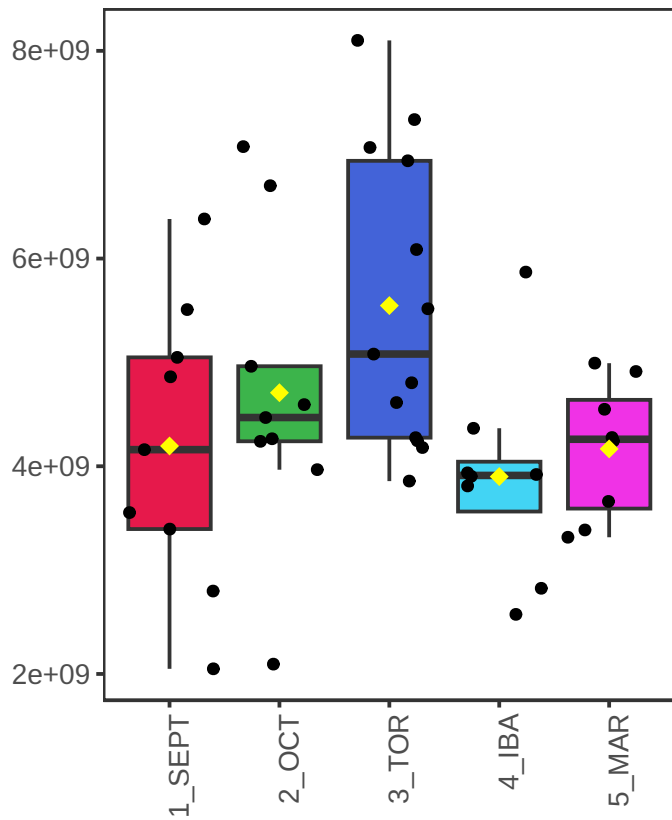


Normalized Conc.

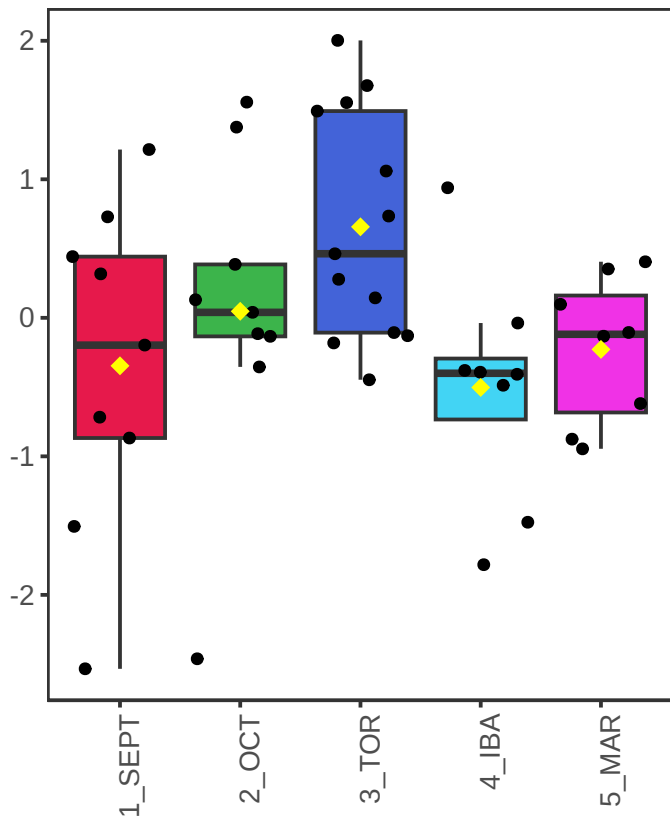


alpha-Glycerolphosphorylcholine

Original Conc.

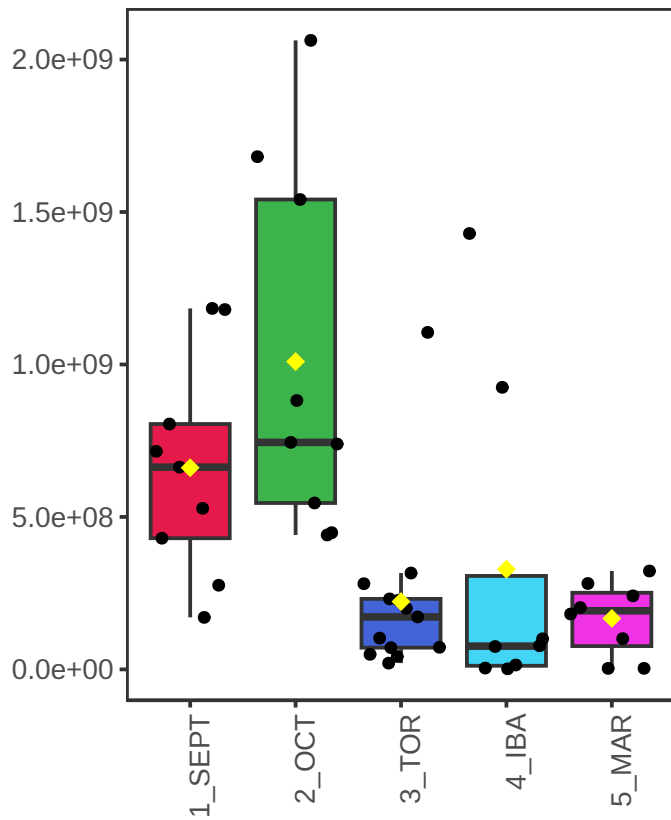


Normalized Conc.

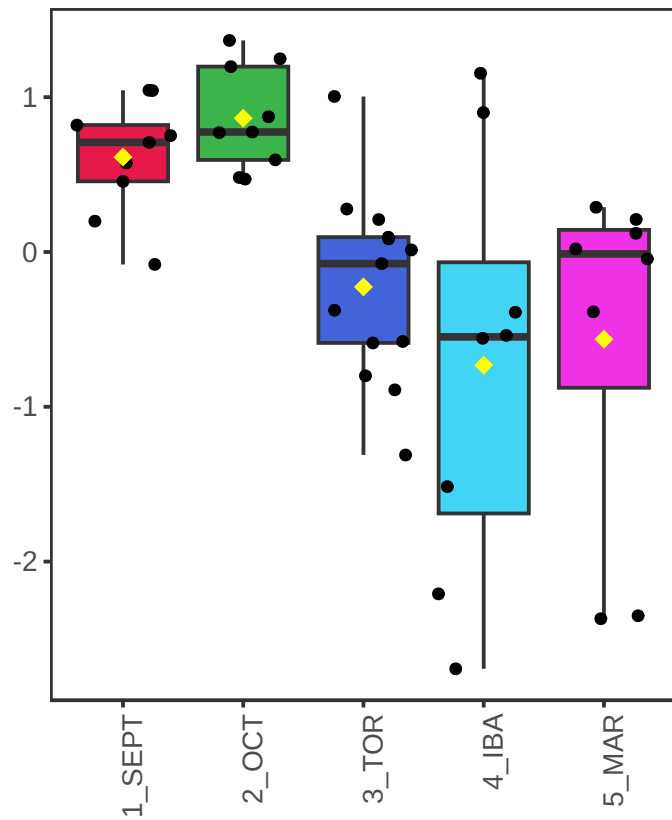


Anthranilic acid

Original Conc.

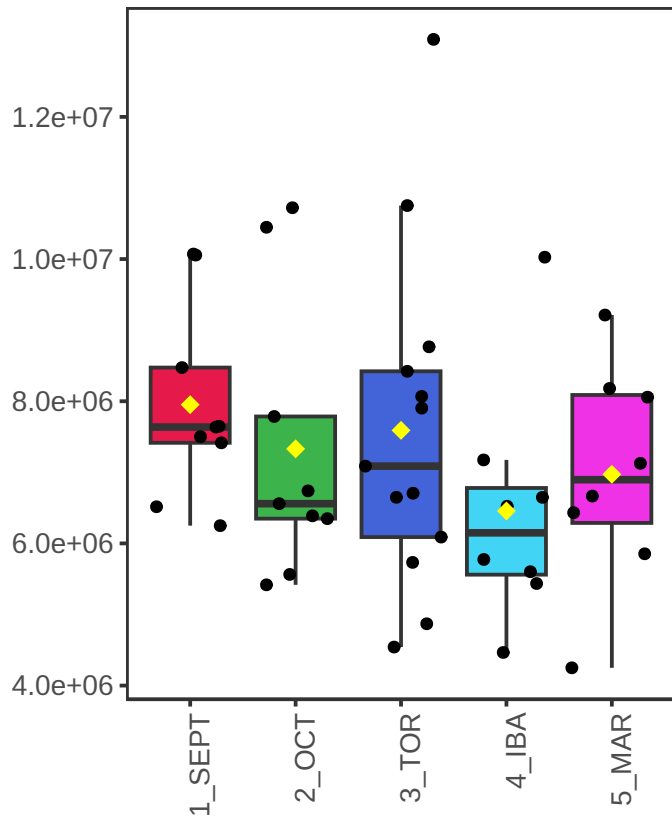


Normalized Conc.

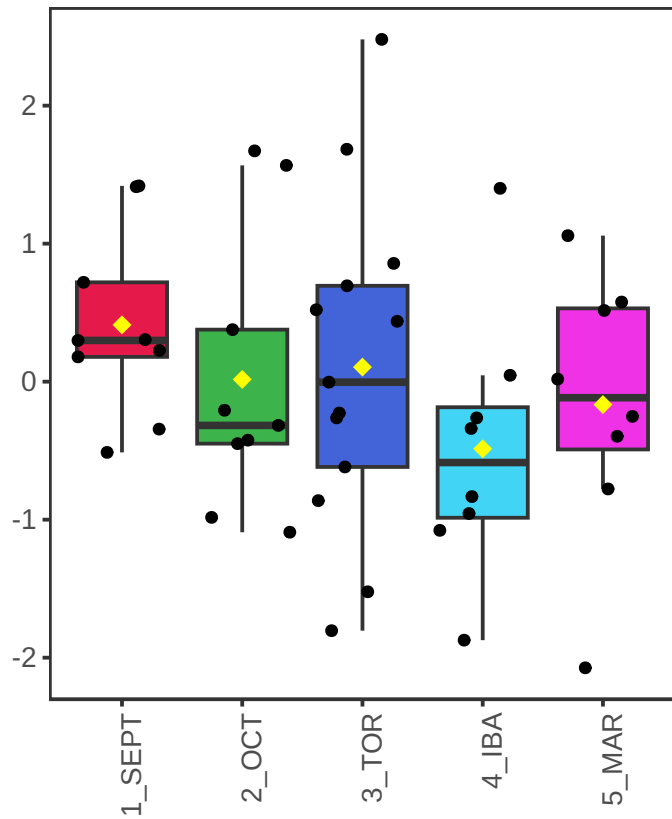


Argininosuccinic acid

Original Conc.

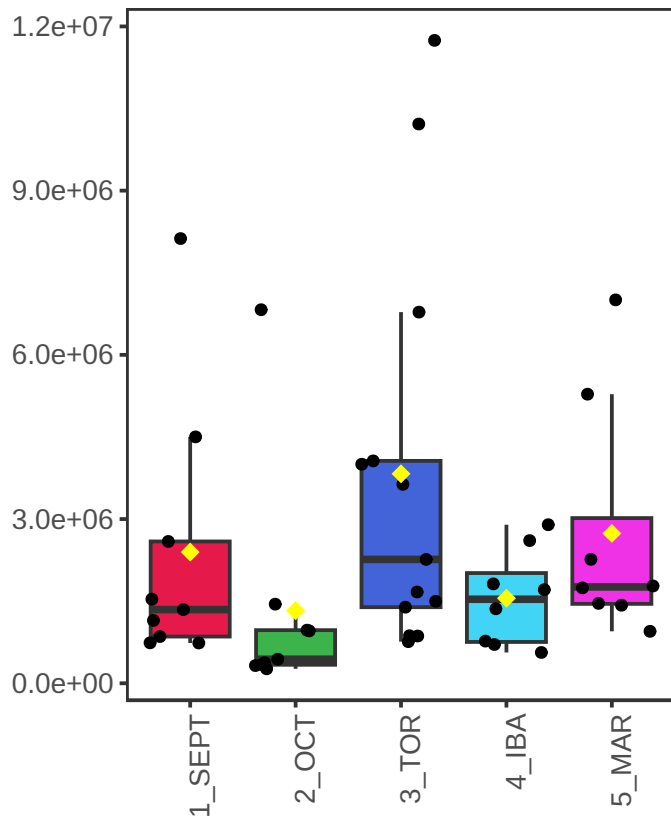


Normalized Conc.

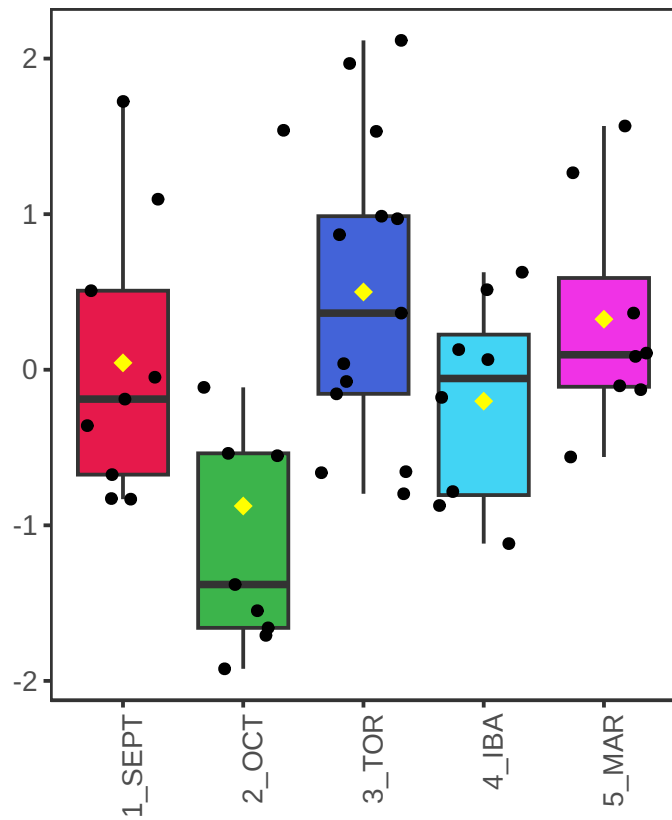


Ascorbate

Original Conc.

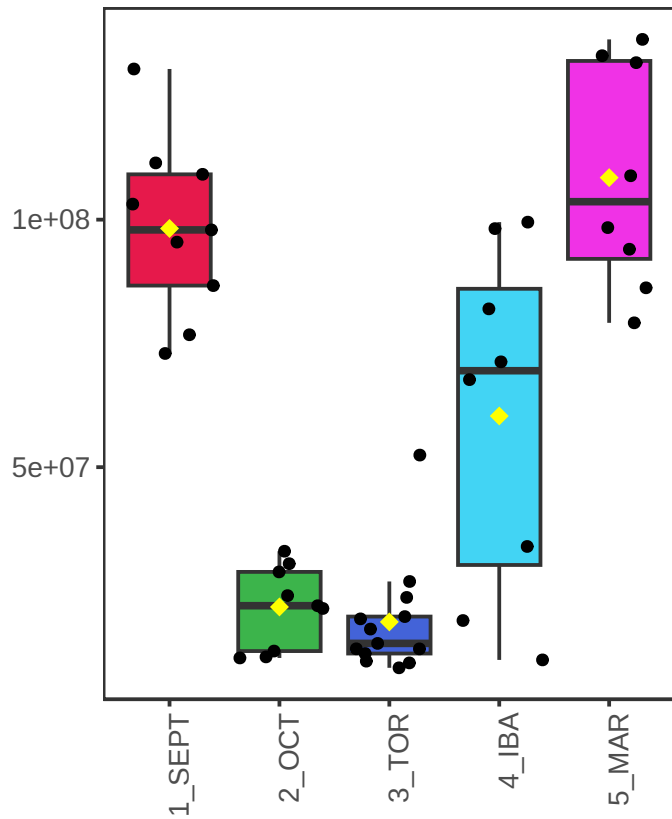


Normalized Conc.

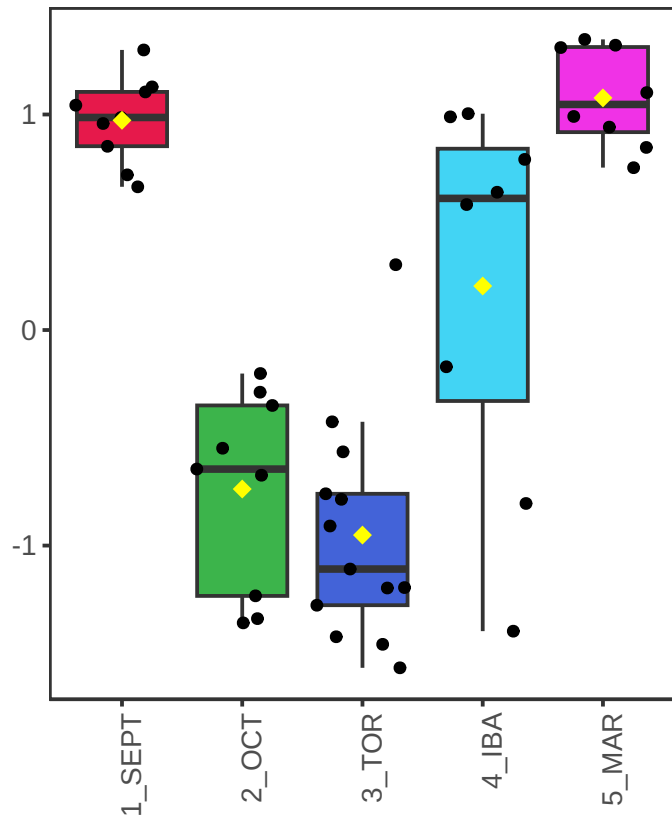


Asparagine

Original Conc.

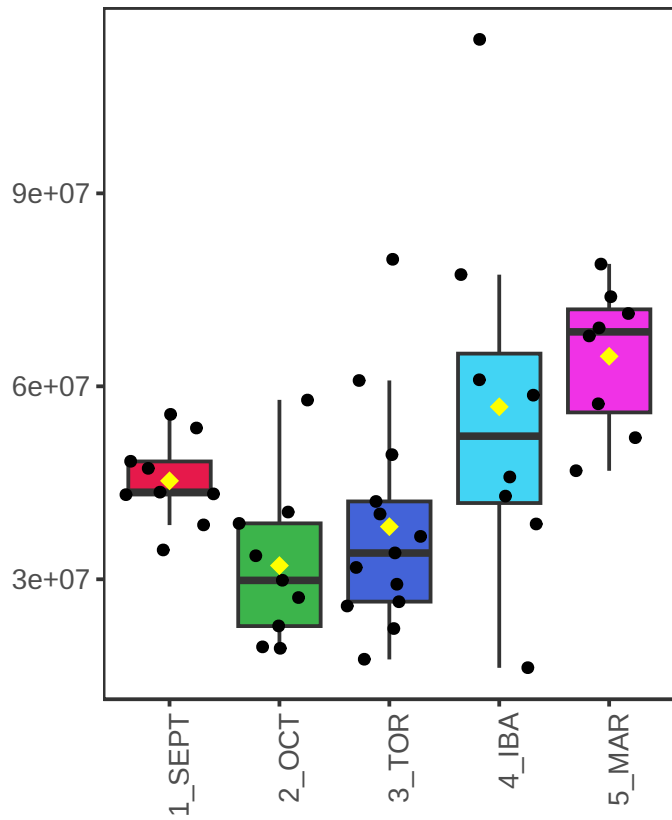


Normalized Conc.

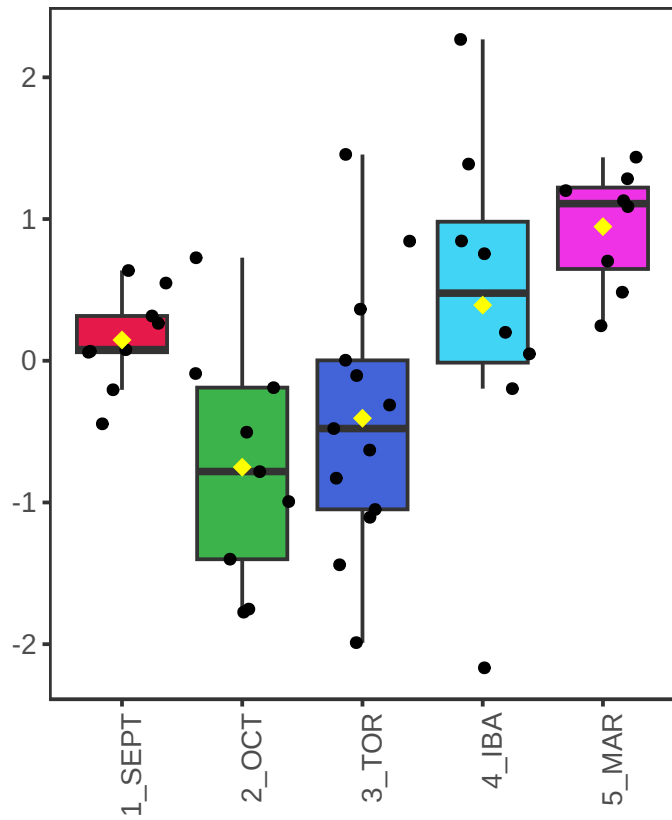


Aspartic acid

Original Conc.

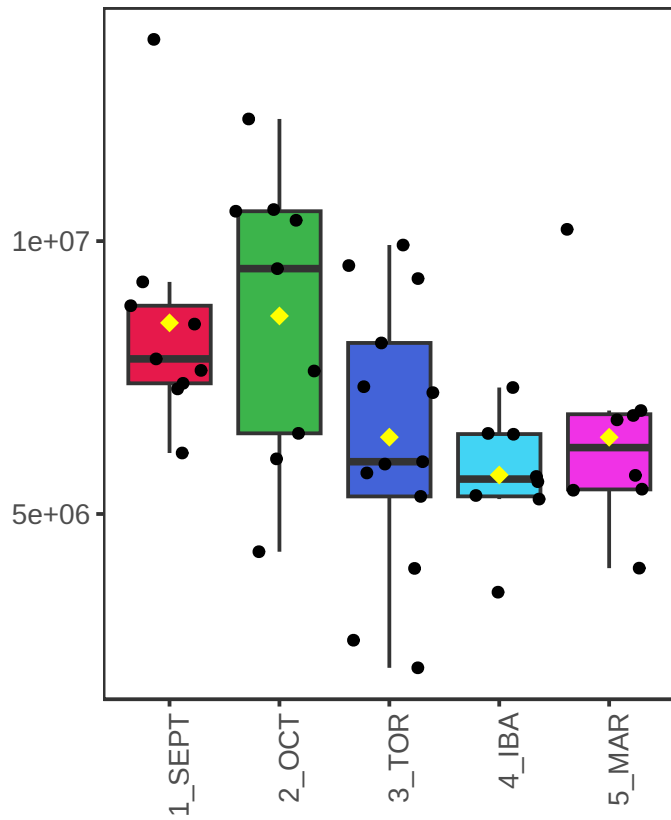


Normalized Conc.

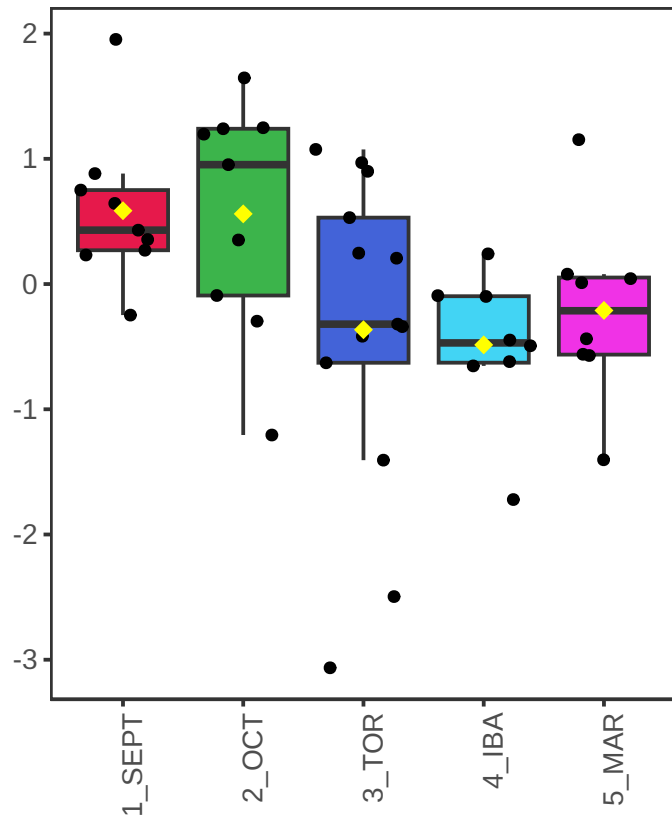


Asp-lys

Original Conc.

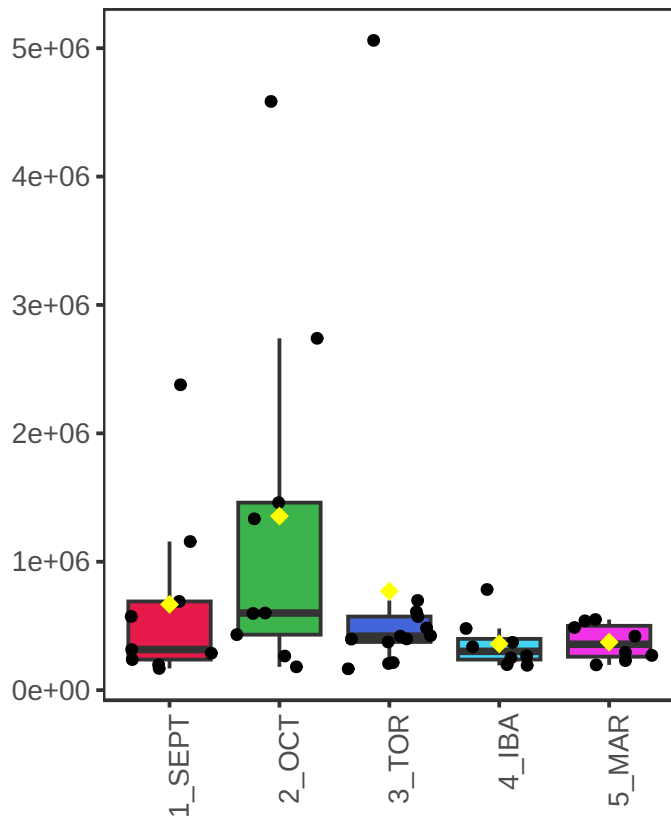


Normalized Conc.

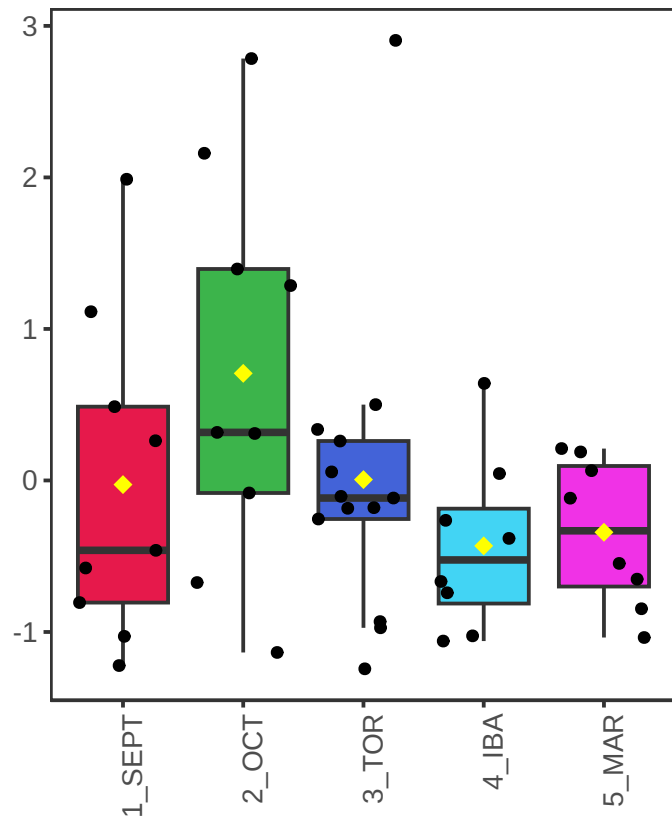


Australine

Original Conc.

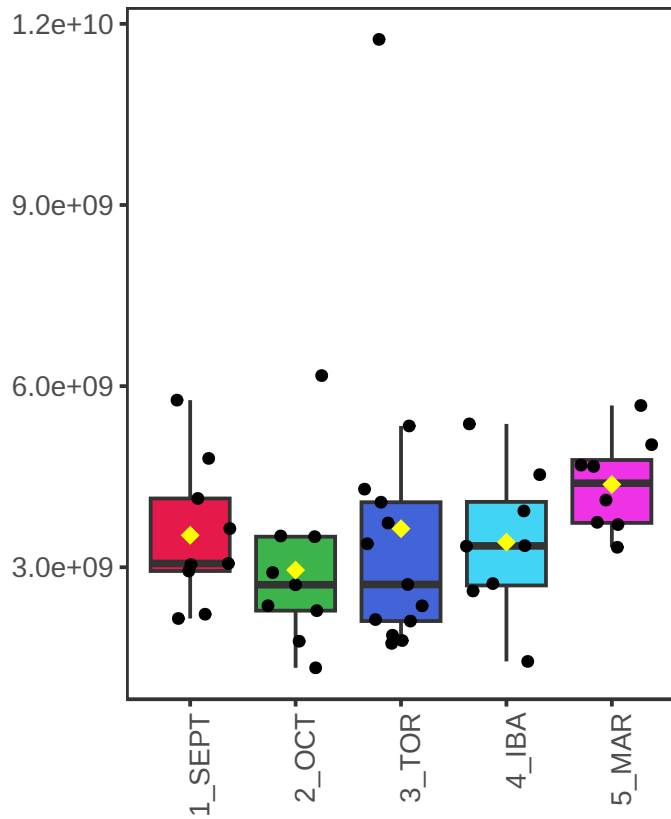


Normalized Conc.

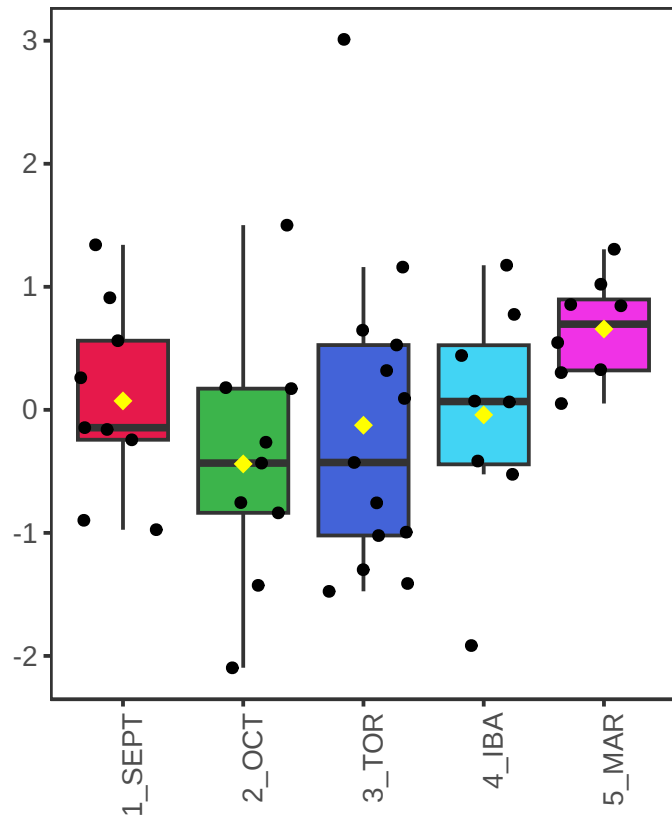


Betaine

Original Conc.

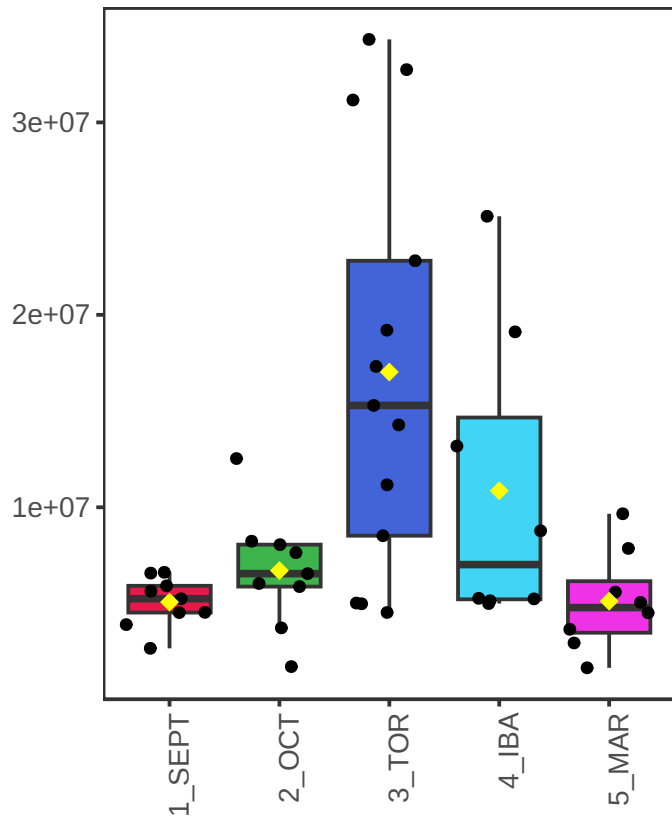


Normalized Conc.

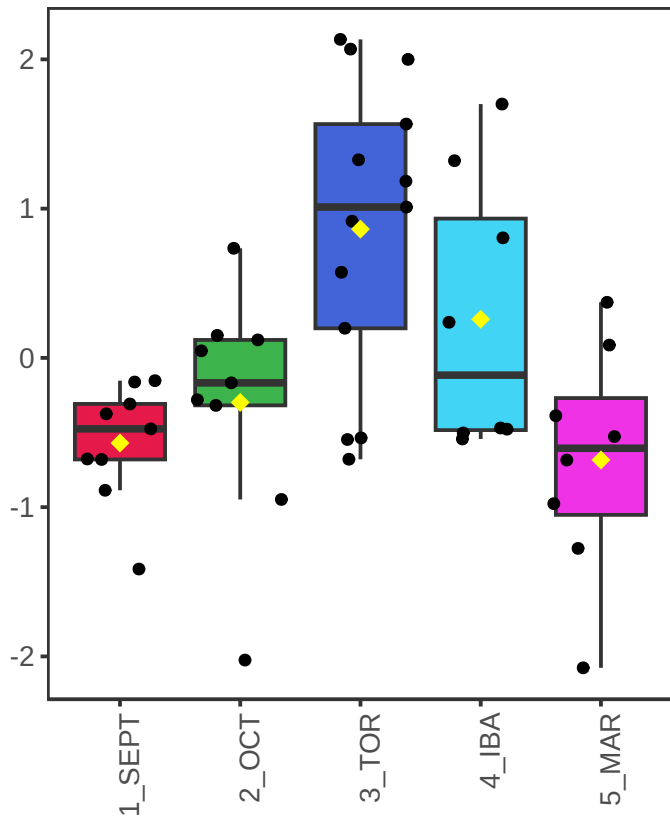


Biotinamide

Original Conc.

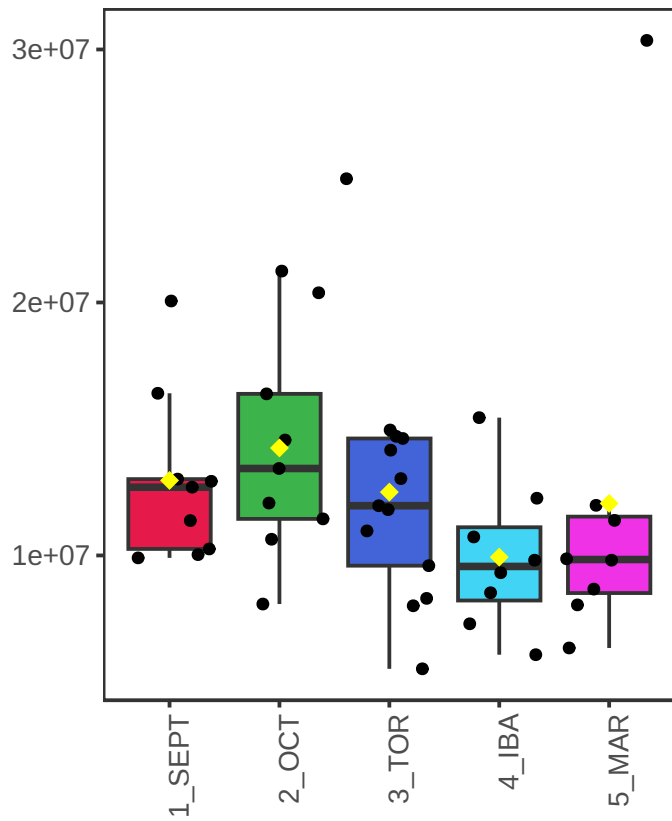


Normalized Conc.

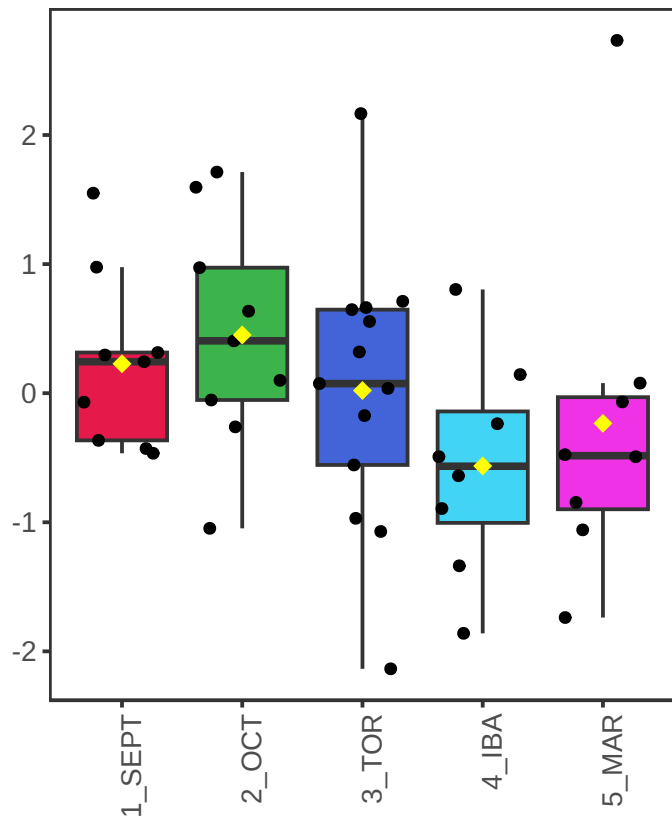


Butyric acid

Original Conc.

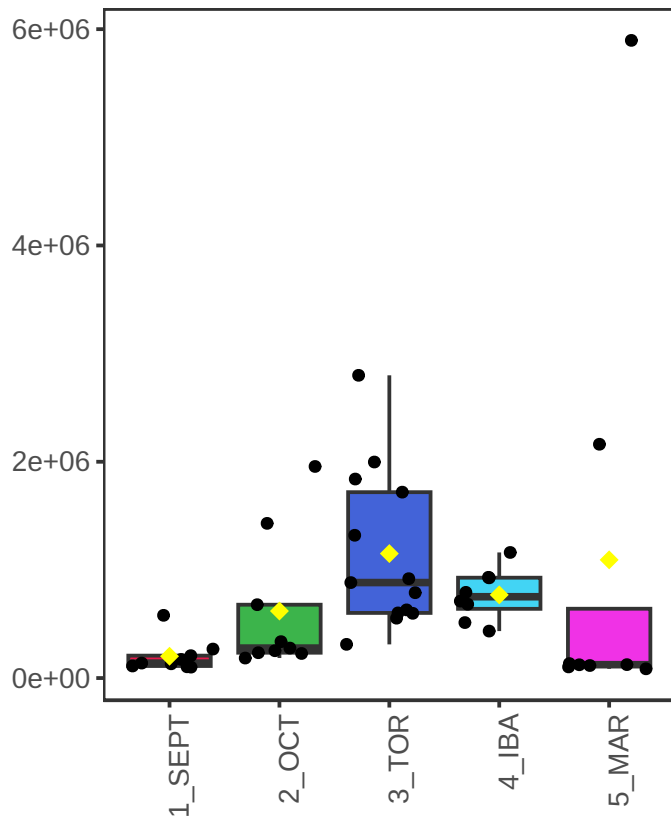


Normalized Conc.

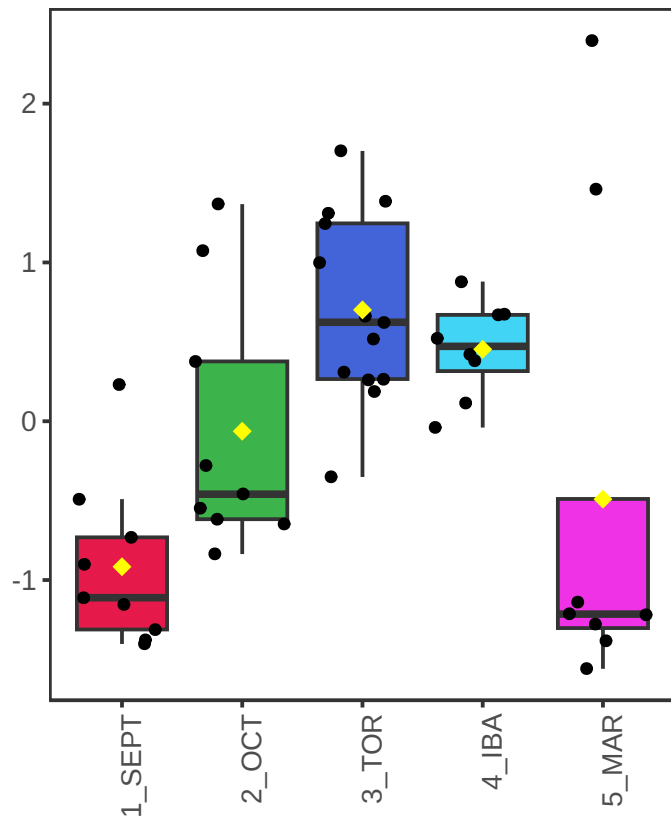


Butyryl-homoserine lactone

Original Conc.

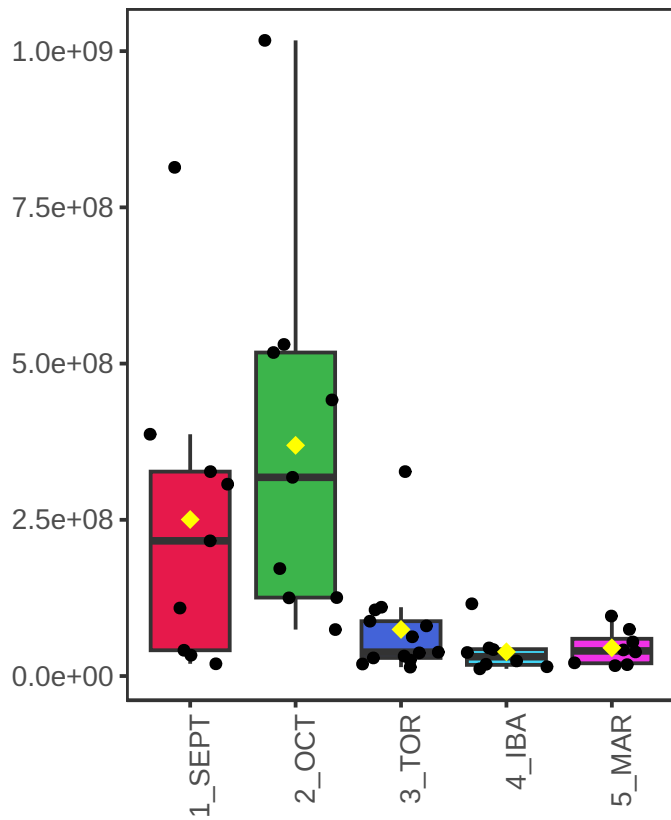


Normalized Conc.

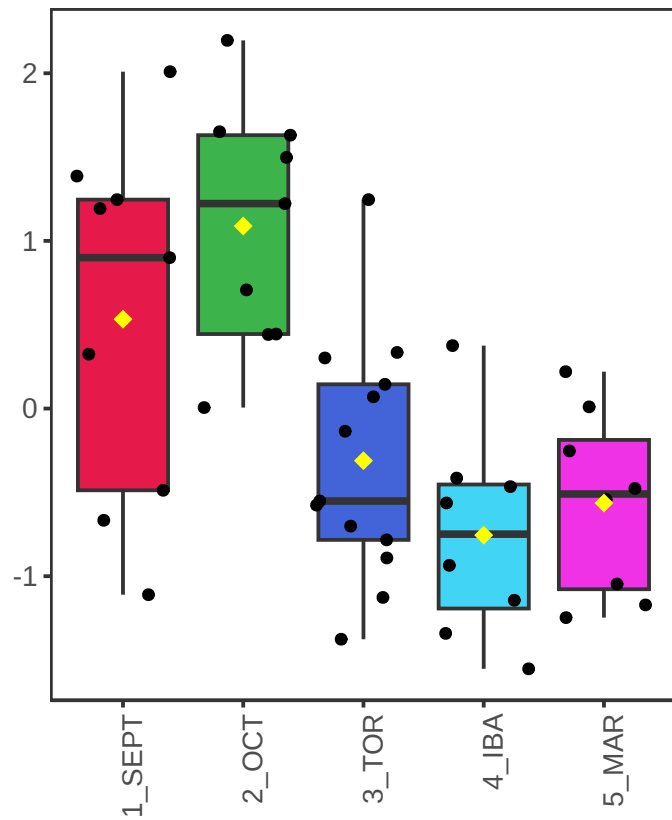


Caprolactam

Original Conc.

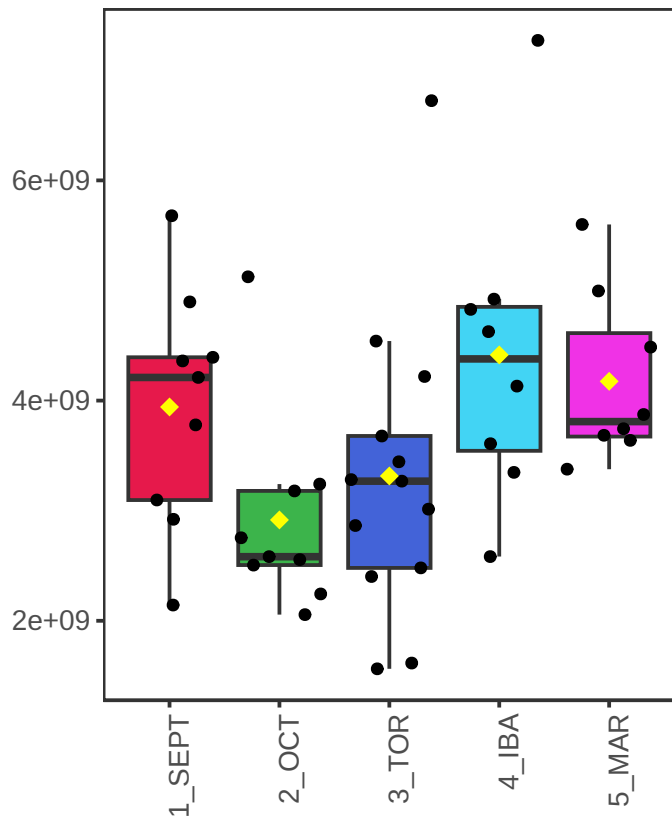


Normalized Conc.

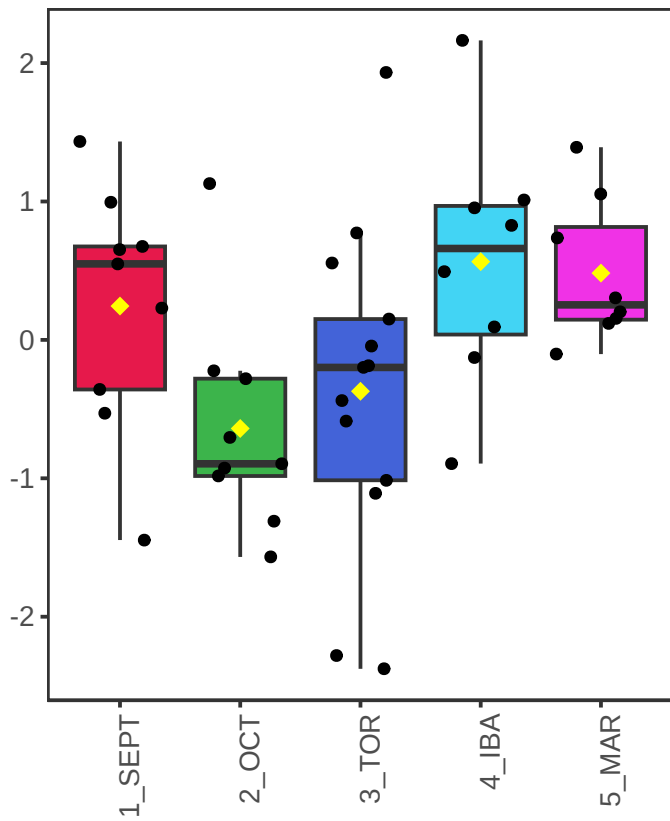


Carnitine

Original Conc.

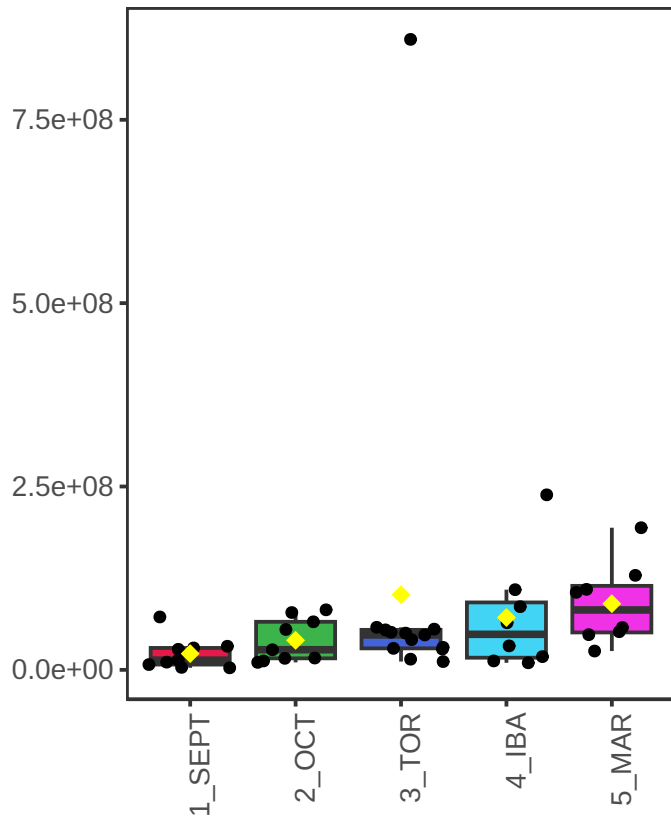


Normalized Conc.

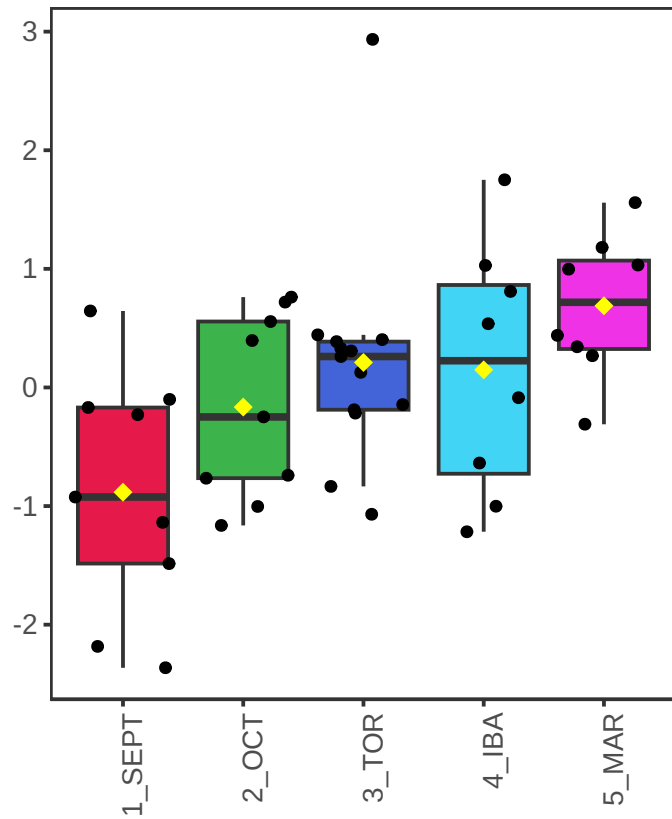


Carnosine

Original Conc.

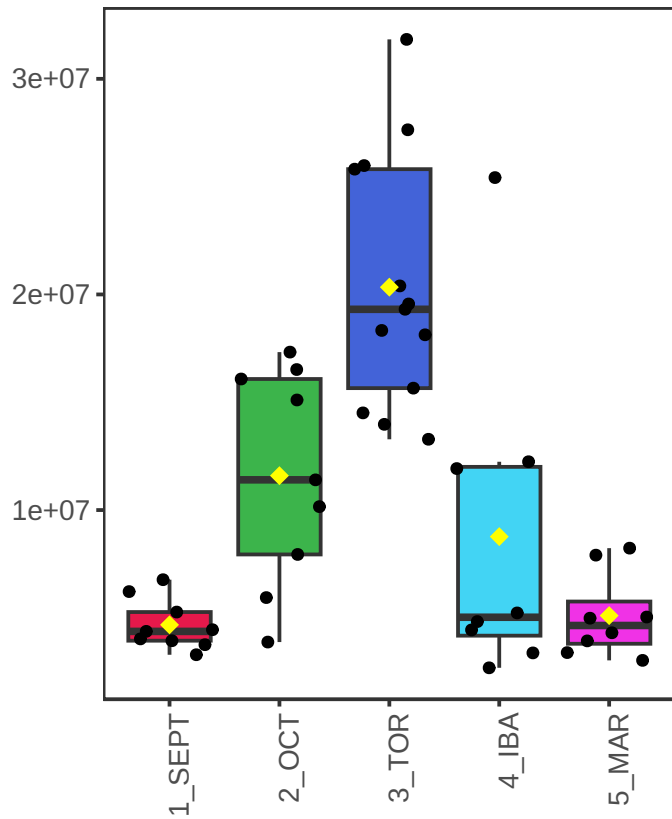


Normalized Conc.

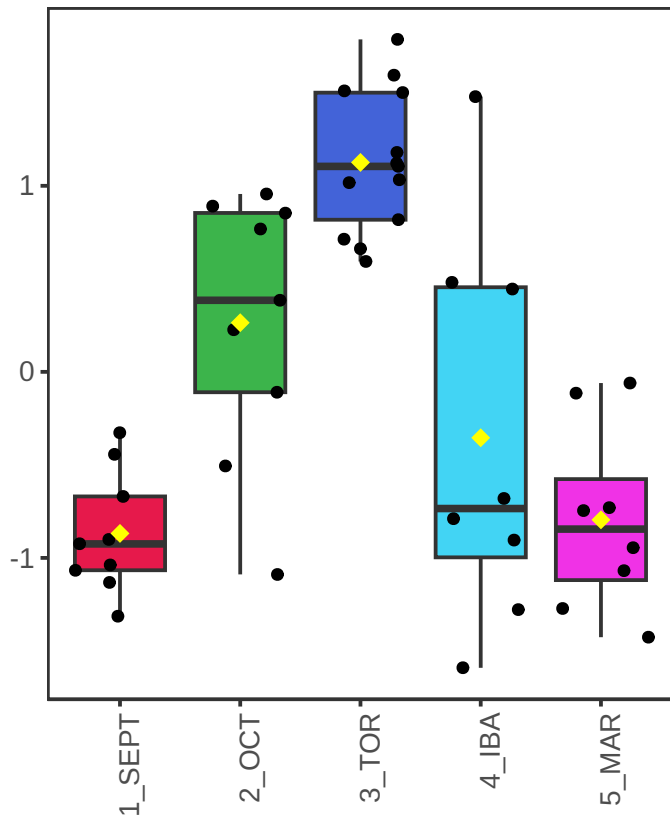


CDP-ethanolamine

Original Conc.

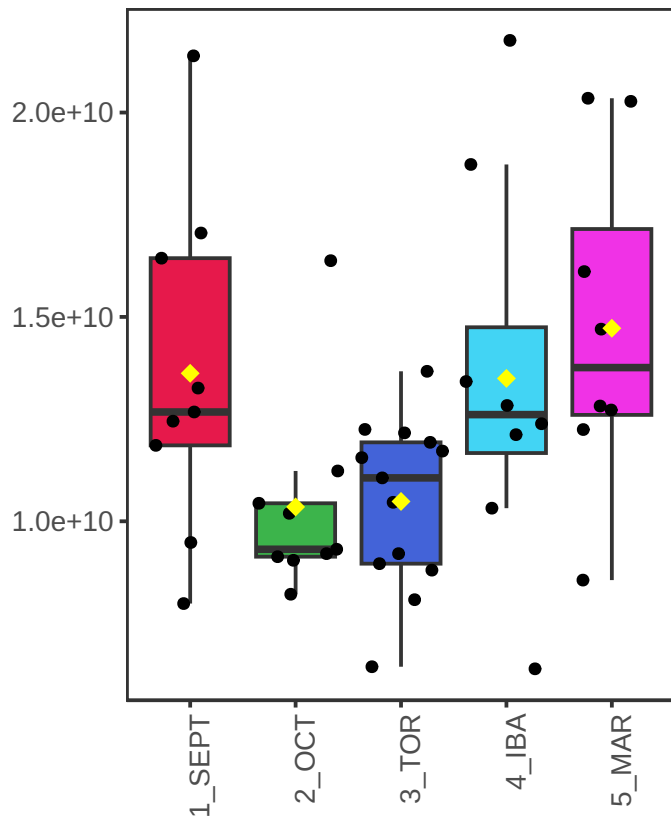


Normalized Conc.

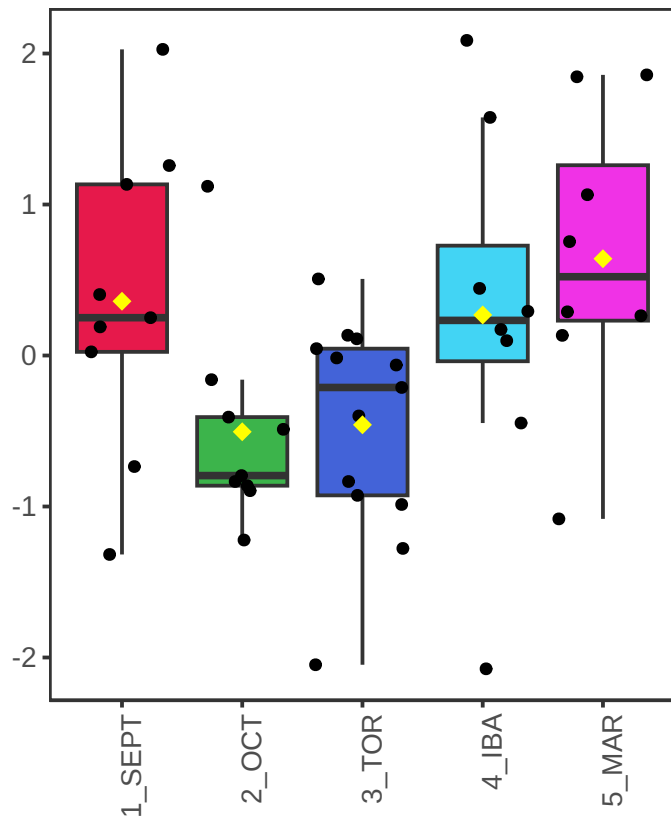


Choline

Original Conc.

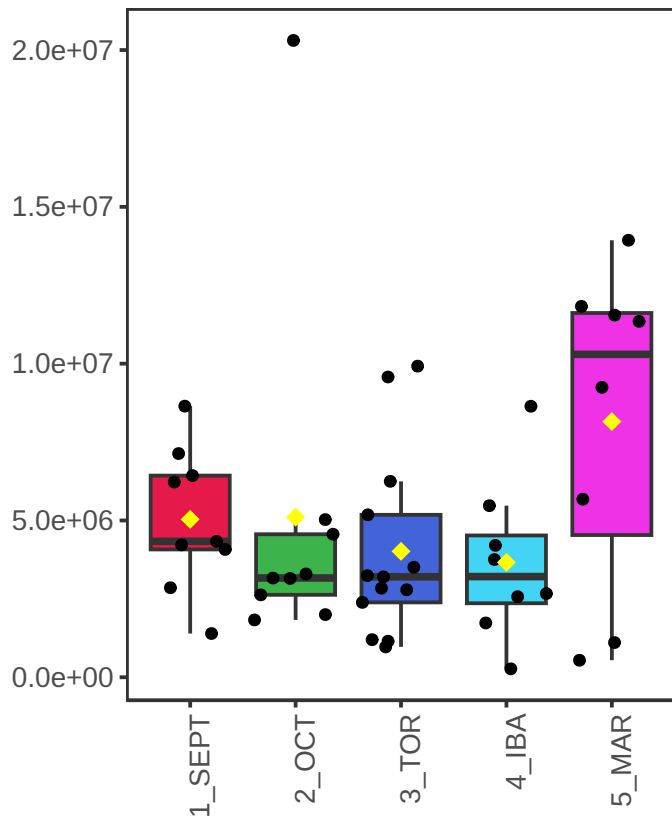


Normalized Conc.

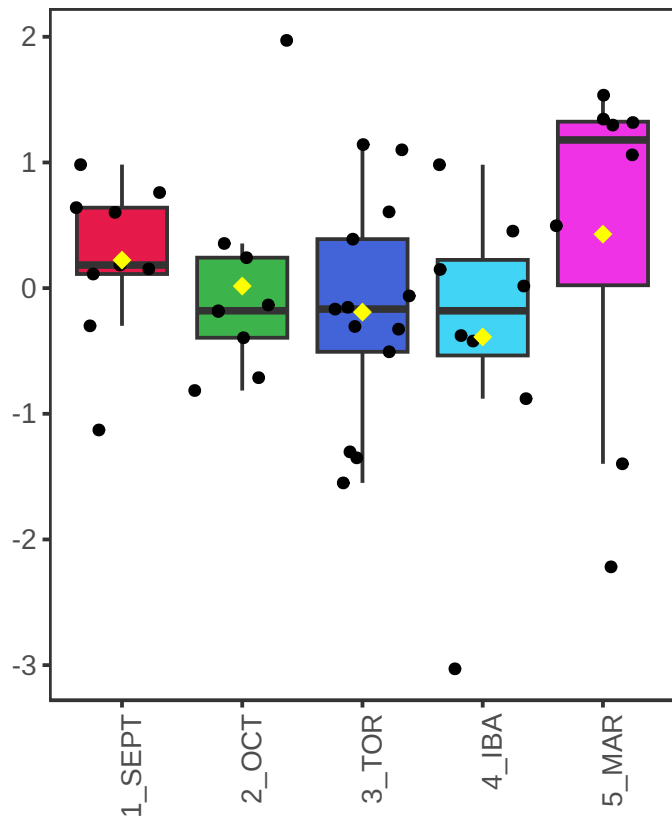


Choline O-Sulfate

Original Conc.

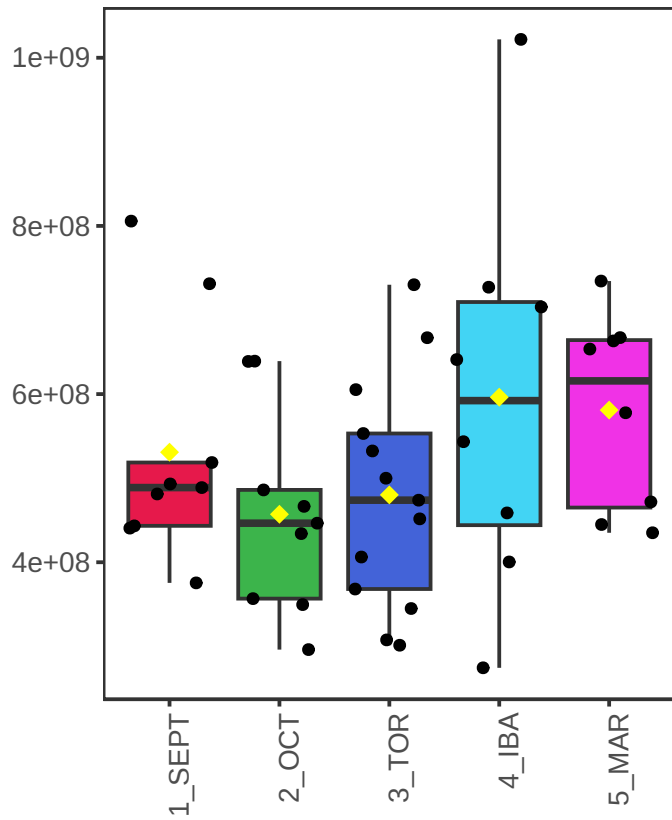


Normalized Conc.

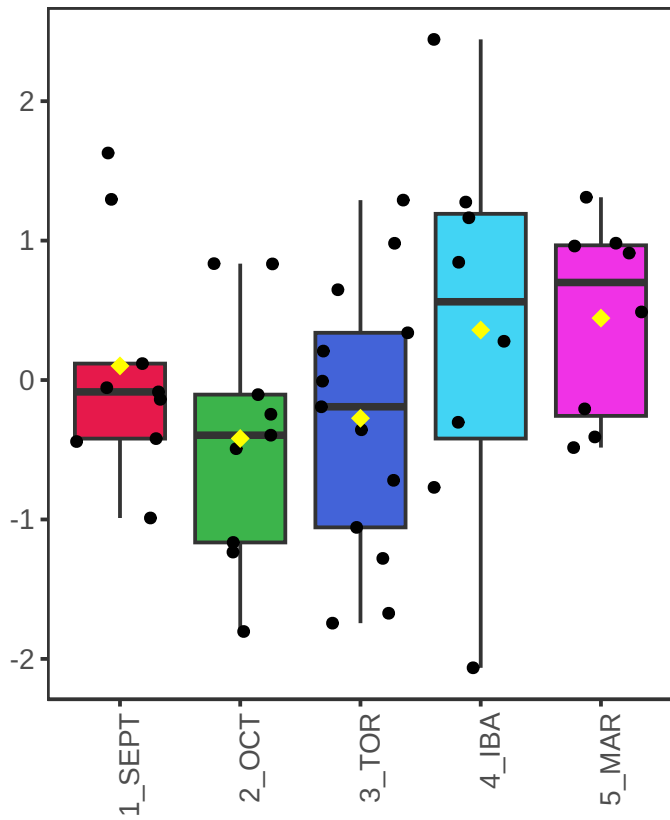


Citrulline

Original Conc.

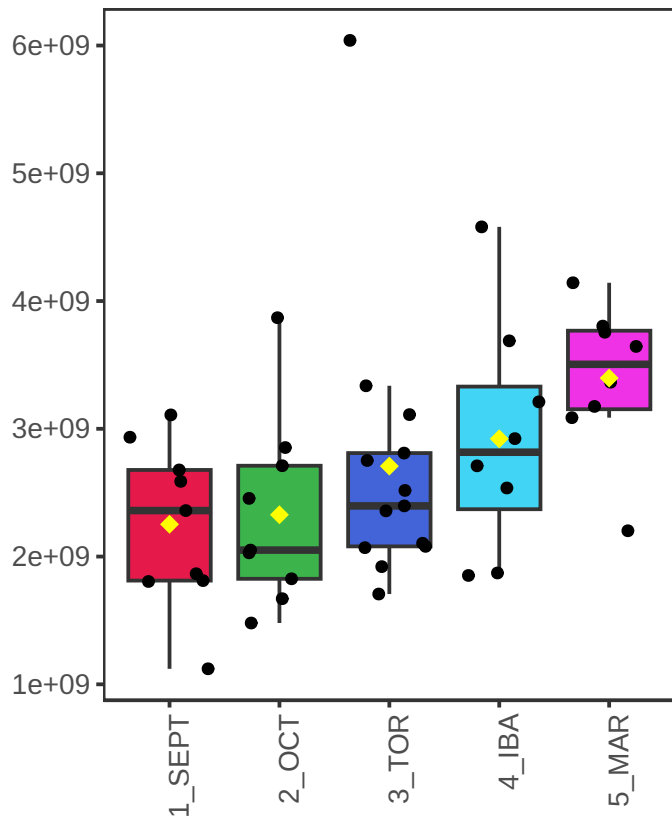


Normalized Conc.

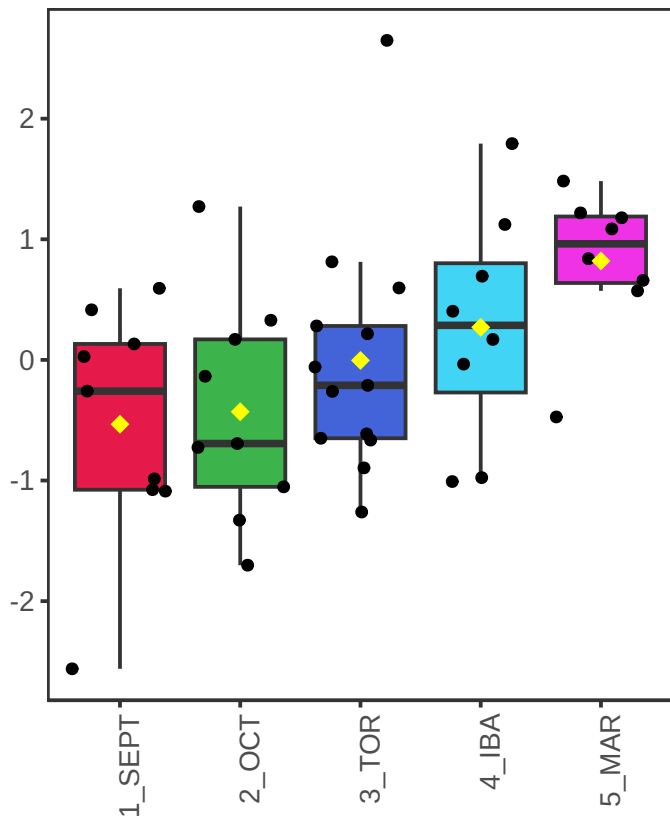


Creatine

Original Conc.

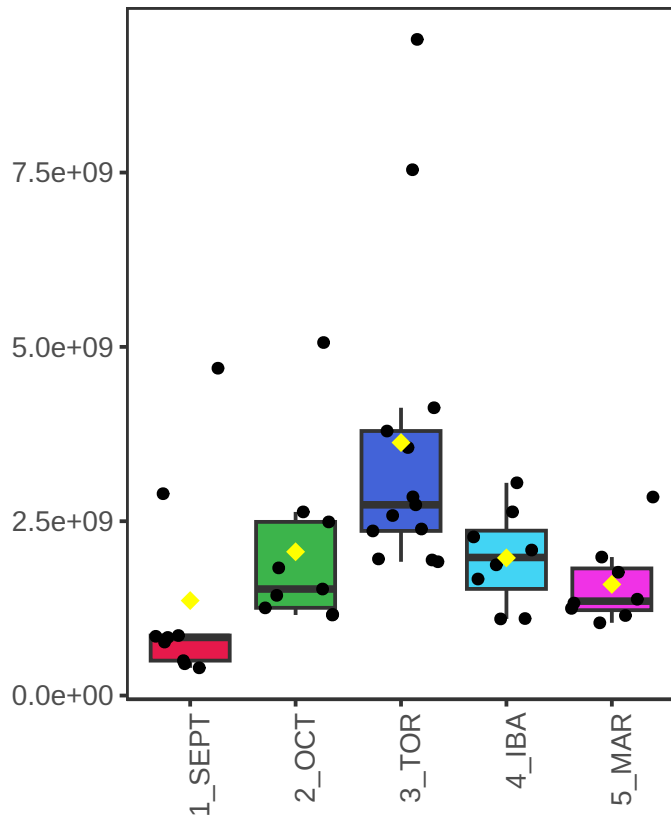


Normalized Conc.

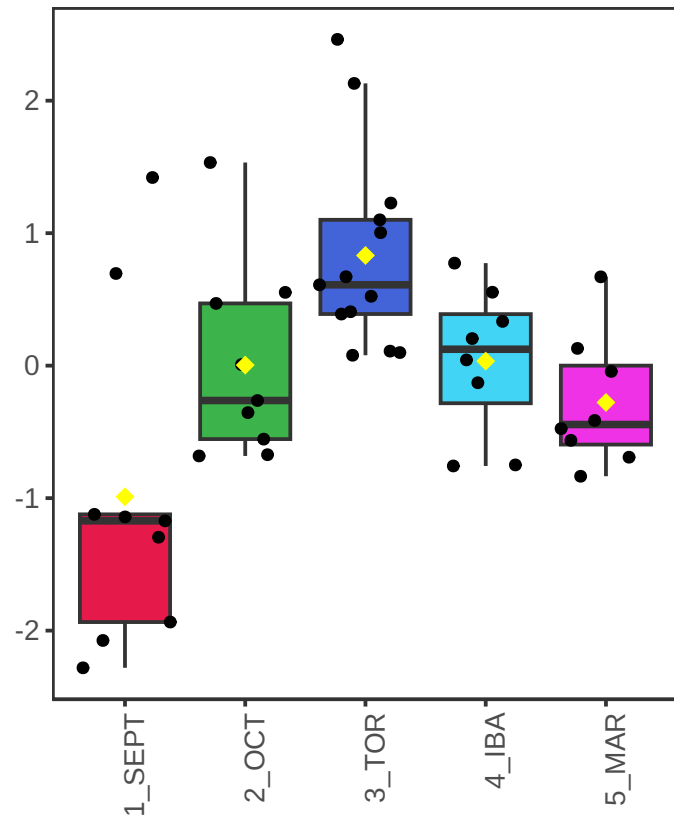


Creatinine

Original Conc.

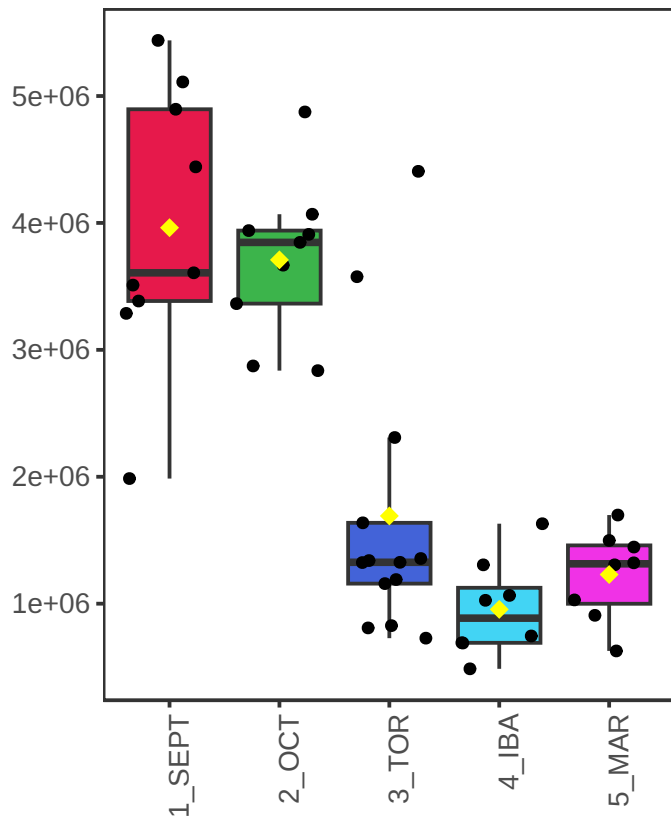


Normalized Conc.

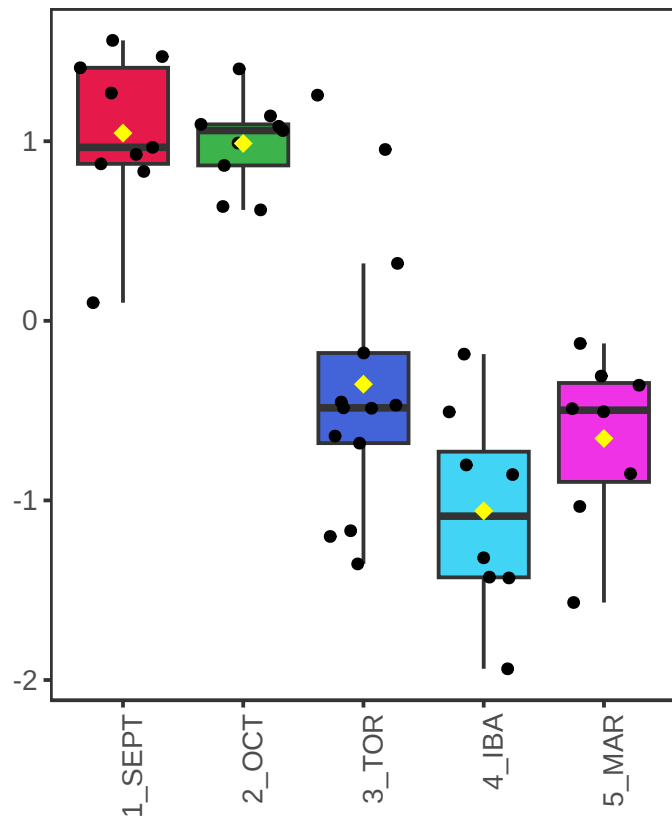


Crotonic acid

Original Conc.

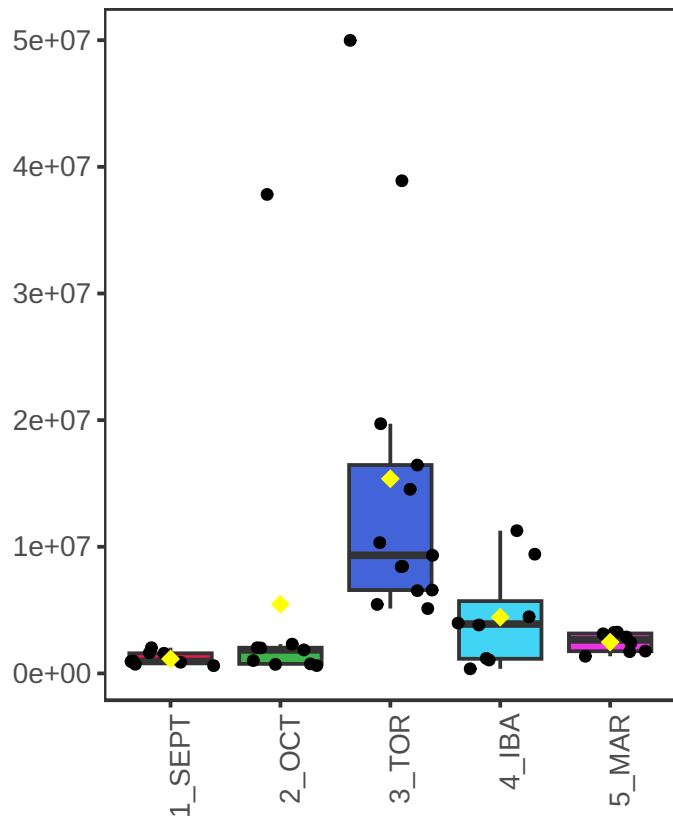


Normalized Conc.

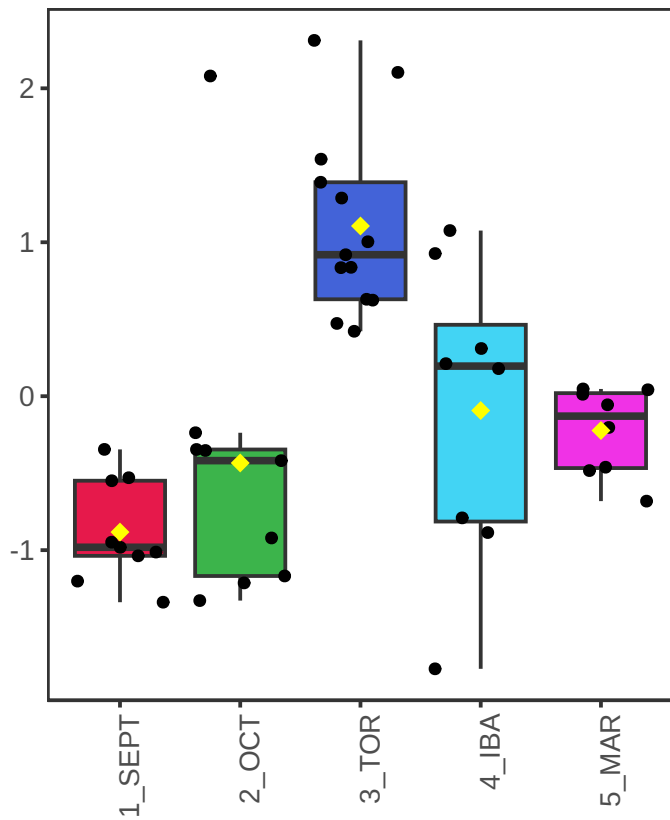


Cystathionine

Original Conc.

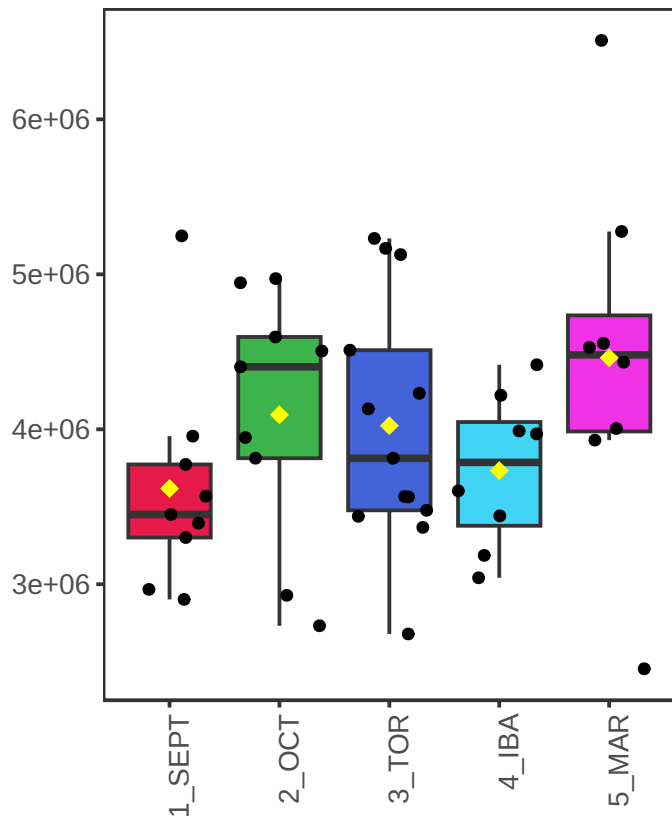


Normalized Conc.

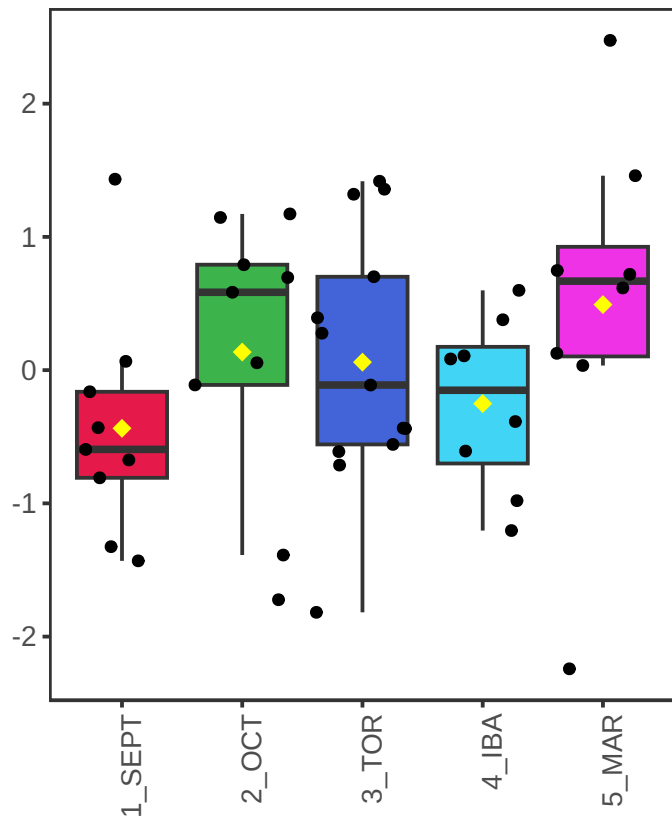


Cysteinylglycine

Original Conc.

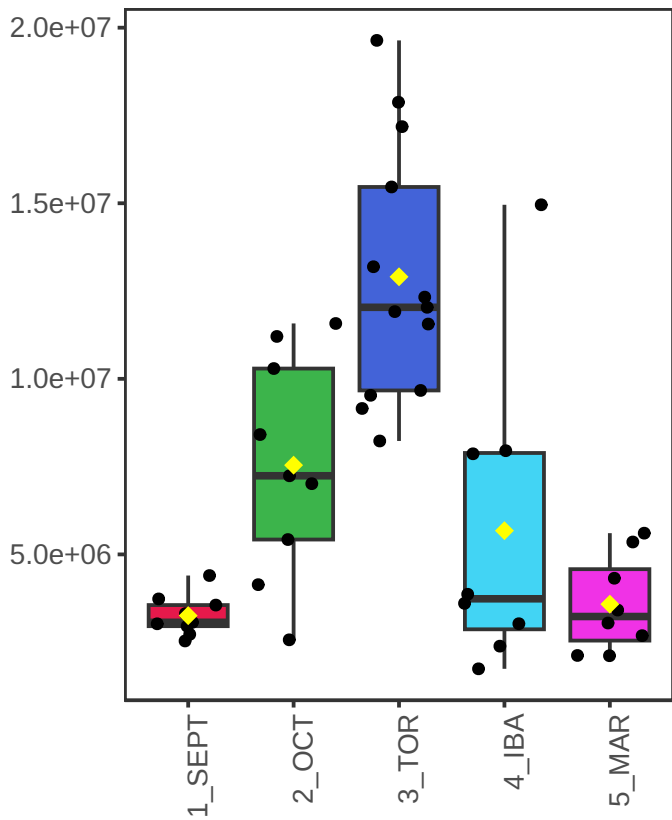


Normalized Conc.

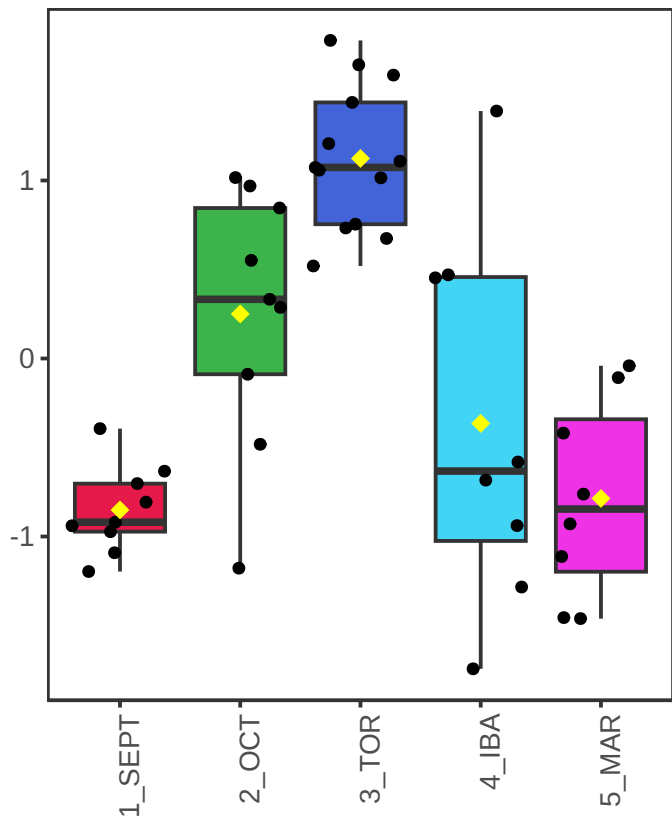


Cytidine 5'-monophosphate (hydrate)

Original Conc.

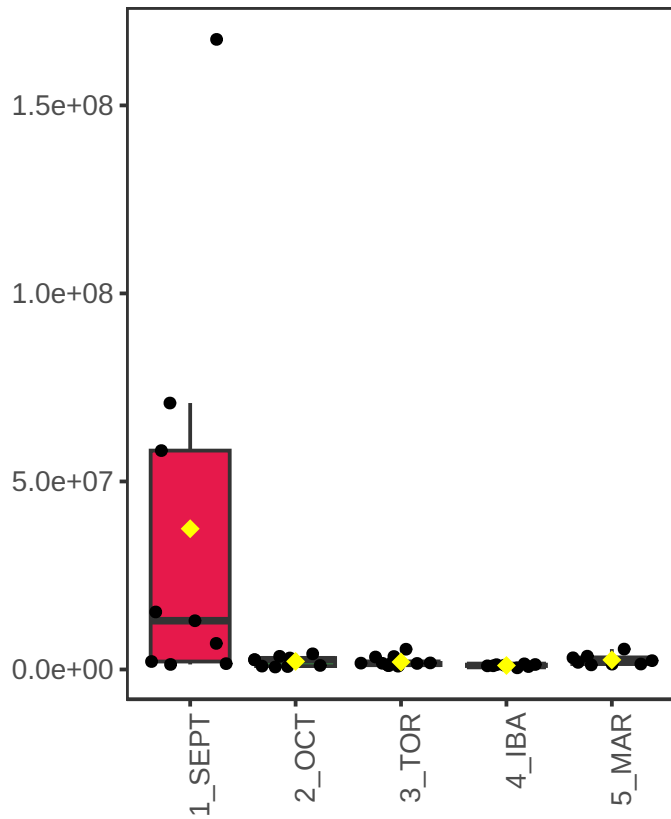


Normalized Conc.

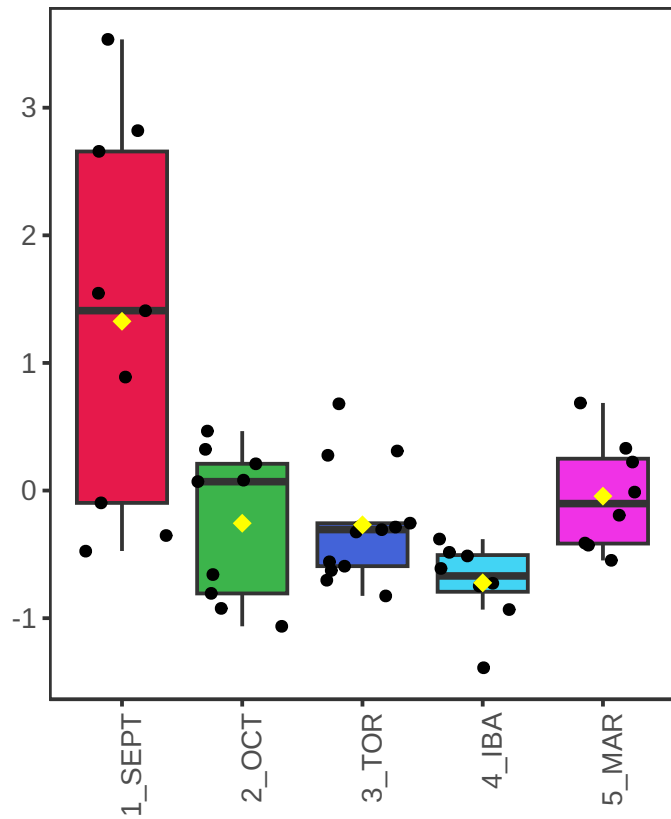


Cytosine

Original Conc.

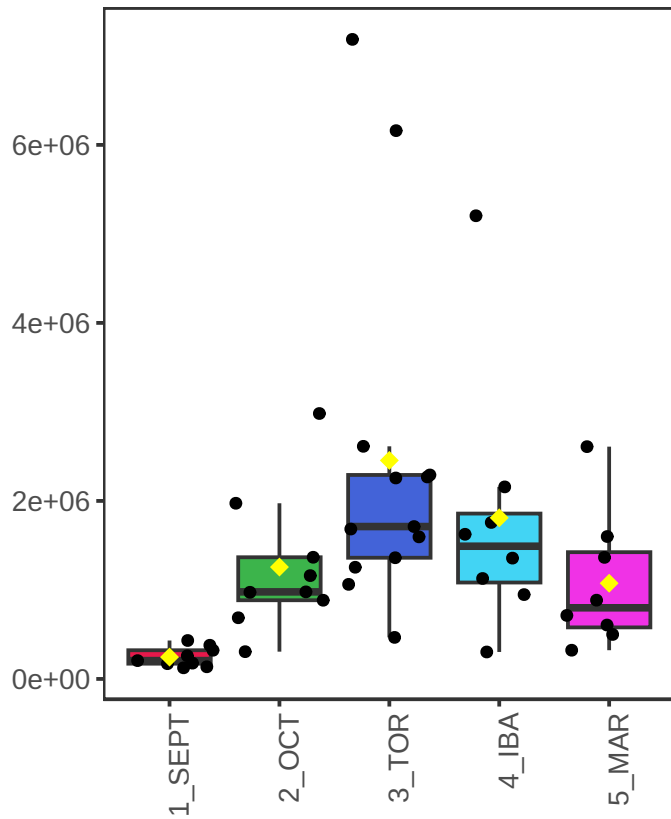


Normalized Conc.

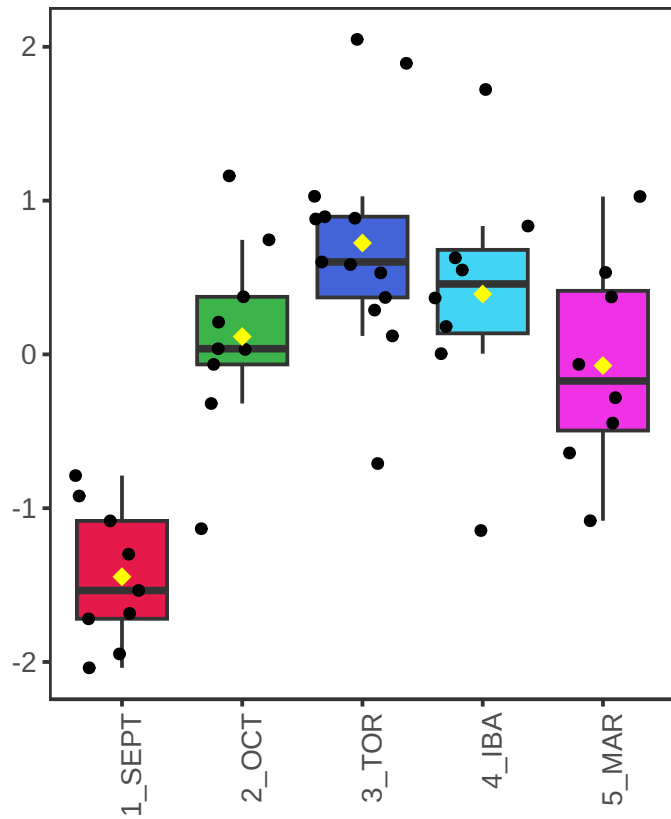


delta-Guanidinovaleric acid

Original Conc.

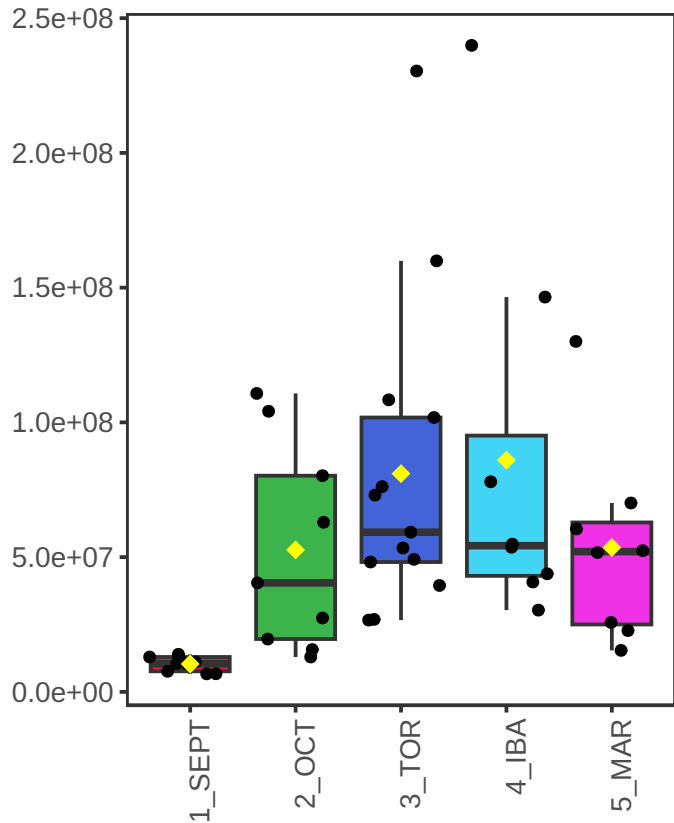


Normalized Conc.

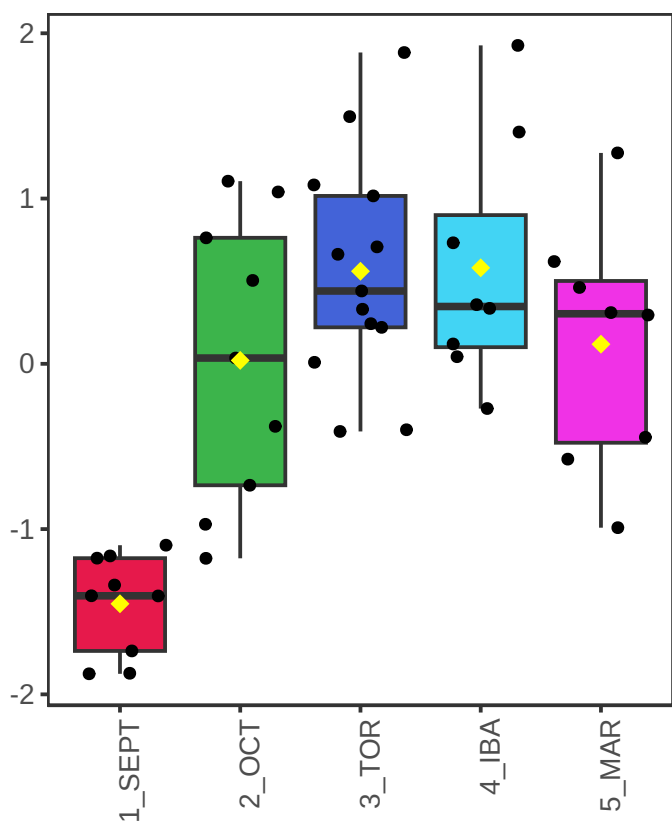


Dihydrothymine

Original Conc.

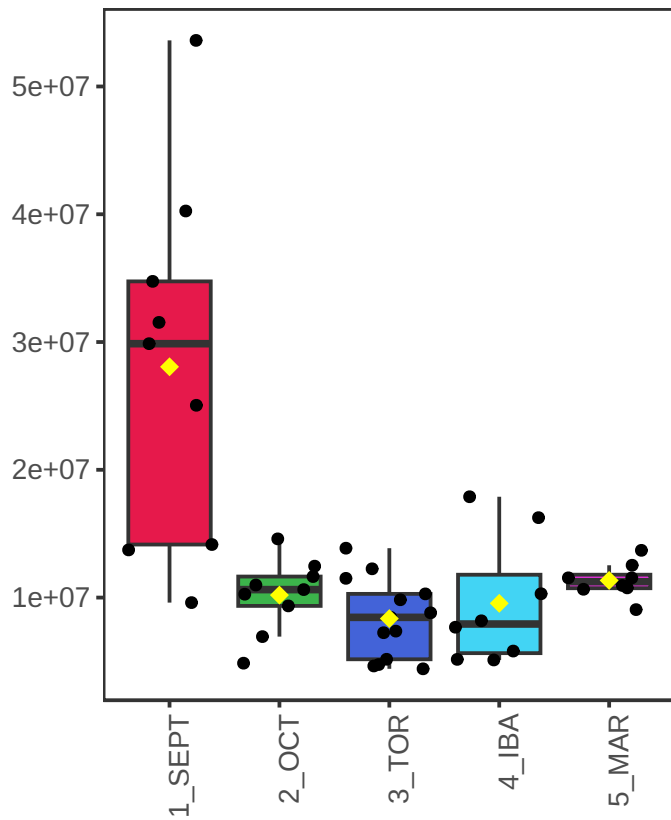


Normalized Conc.

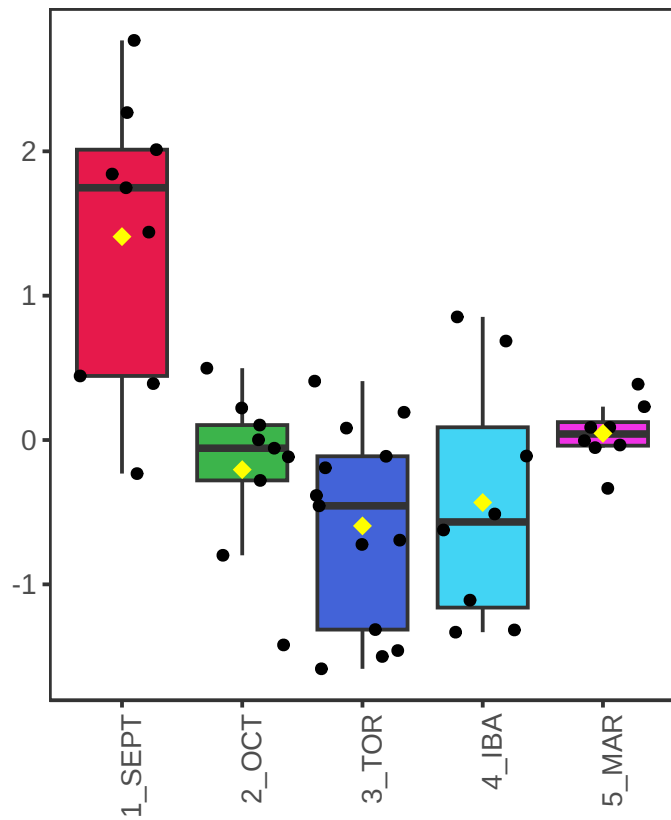


Dimethylethanolamine

Original Conc.

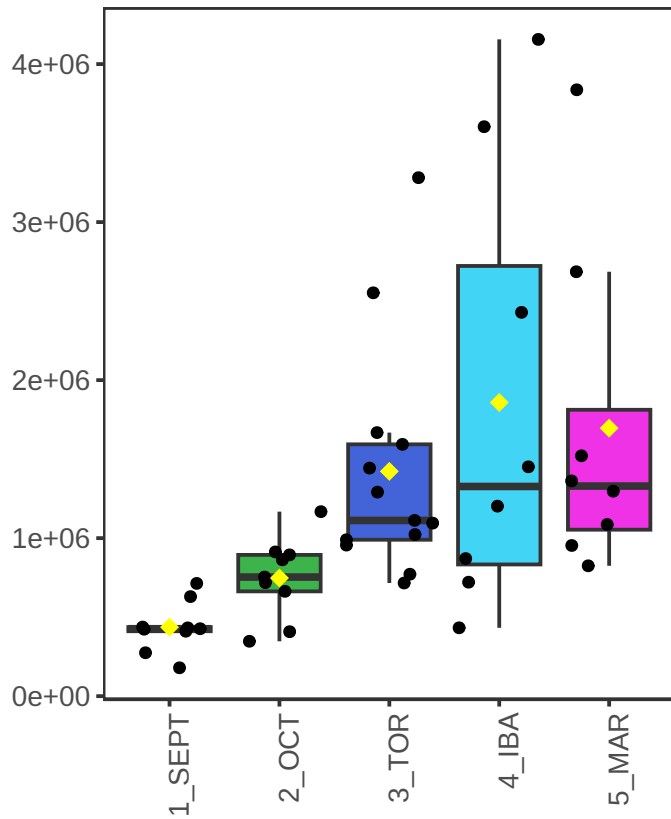


Normalized Conc.

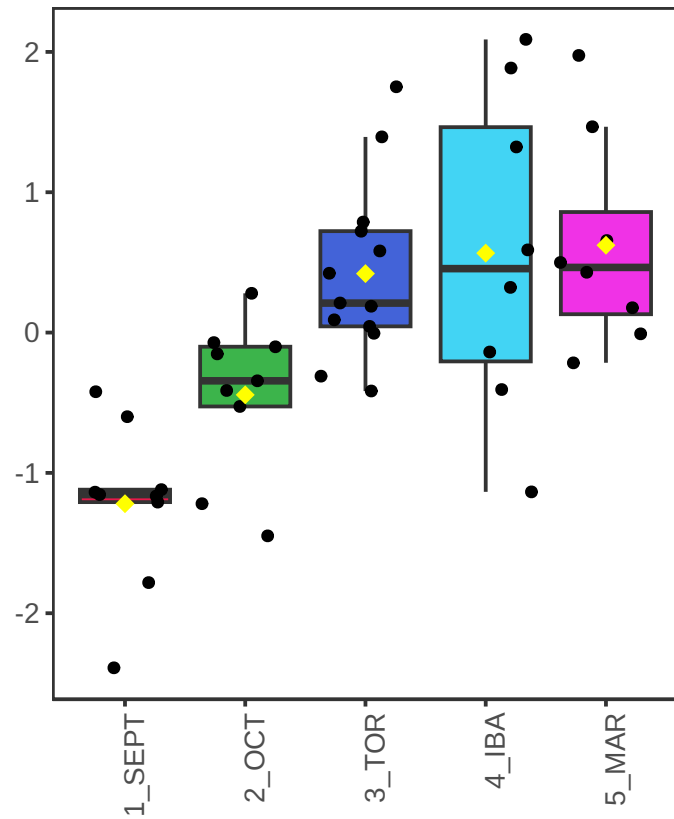


Epsilon-(gamma-Glutamyl)-lysine

Original Conc.

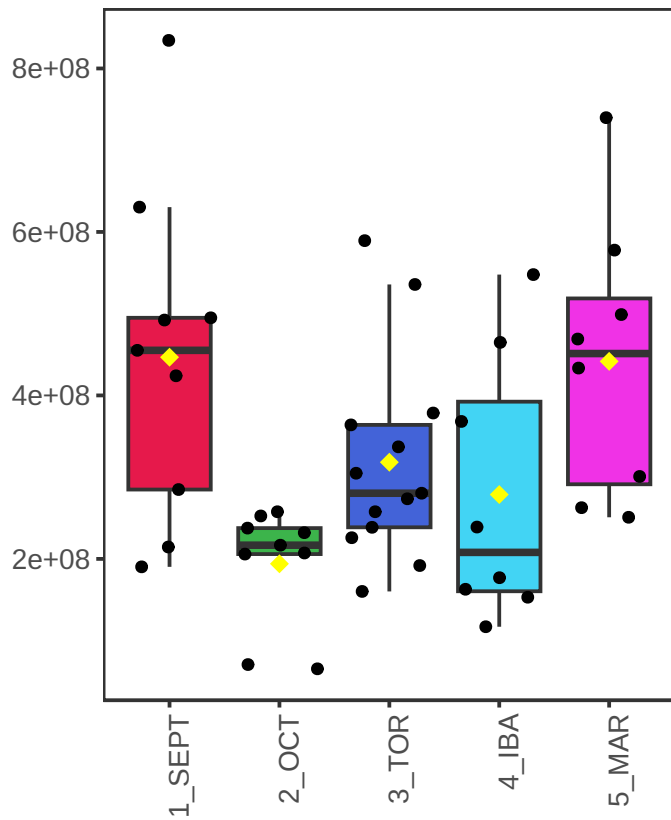


Normalized Conc.

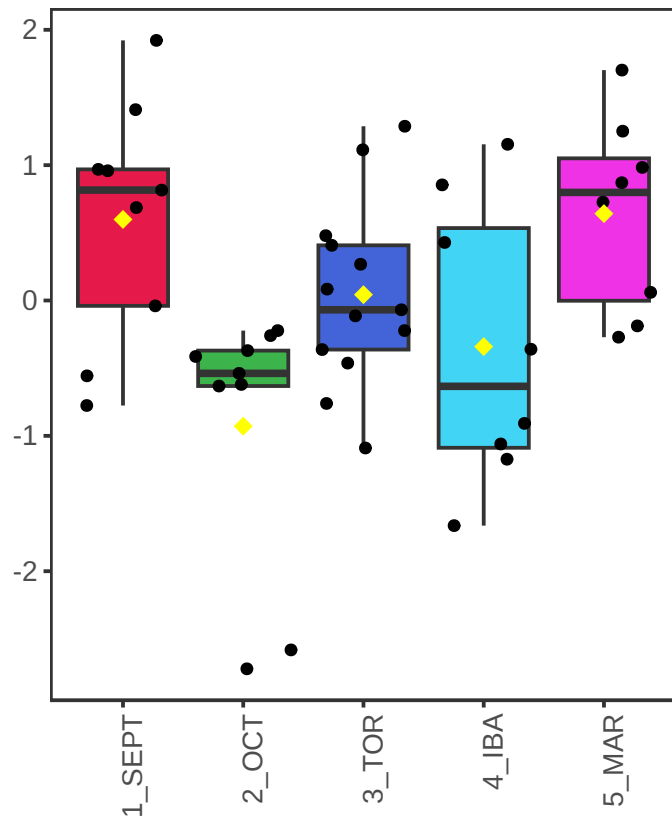


Ergothioneine

Original Conc.

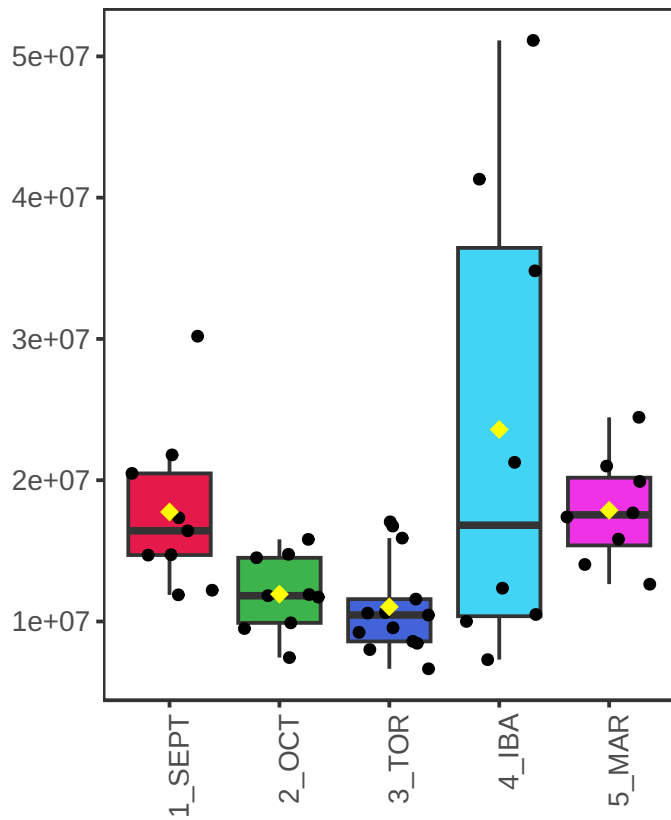


Normalized Conc.

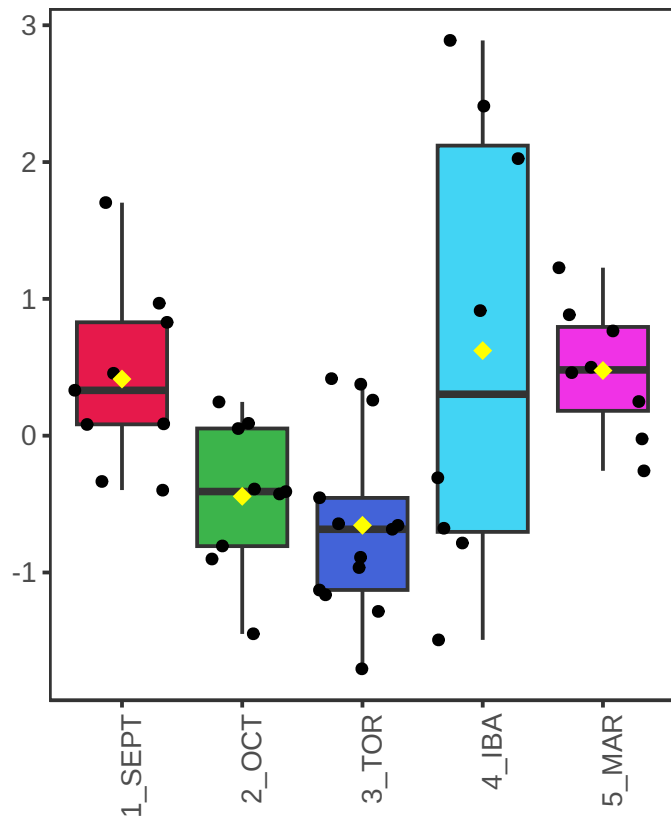


Ethanolamine

Original Conc.

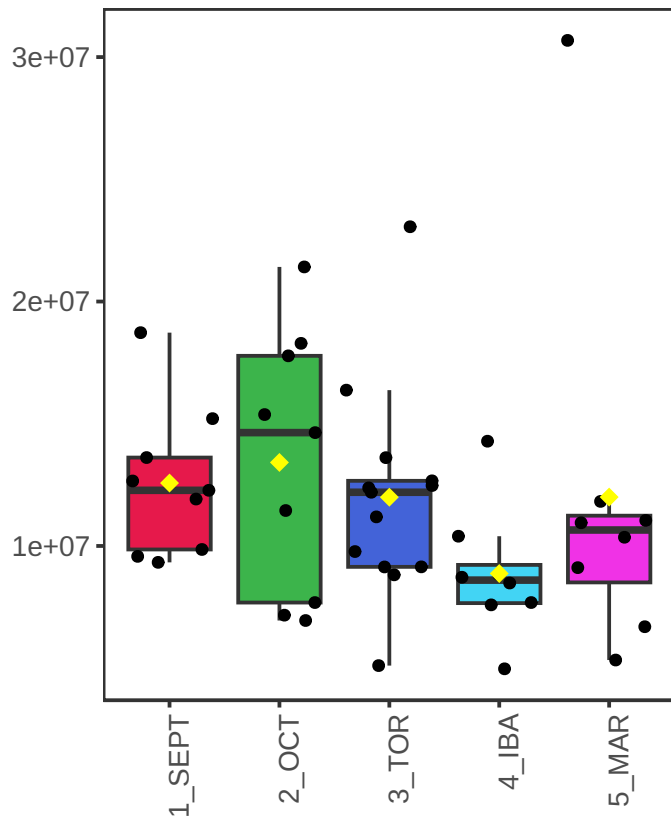


Normalized Conc.

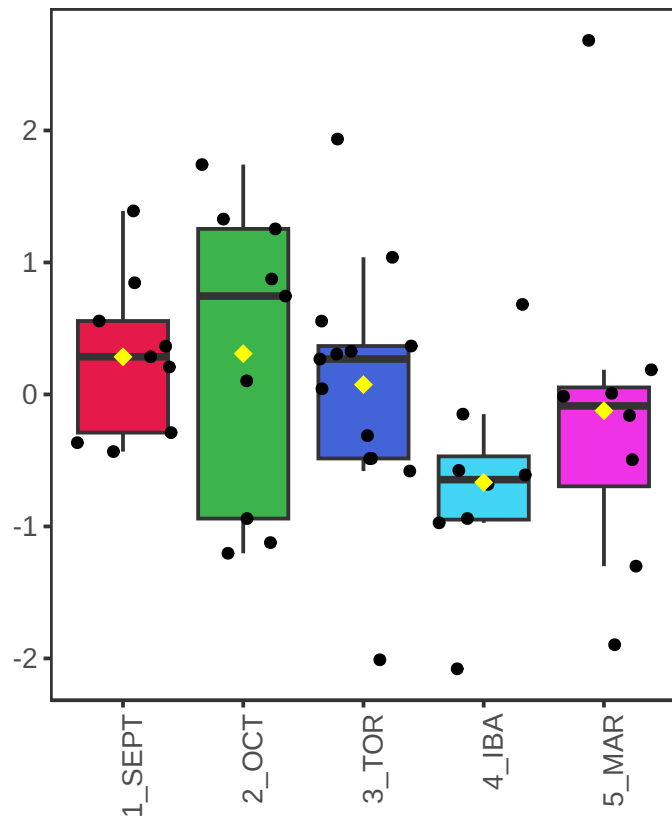


Ethyl acetate

Original Conc.

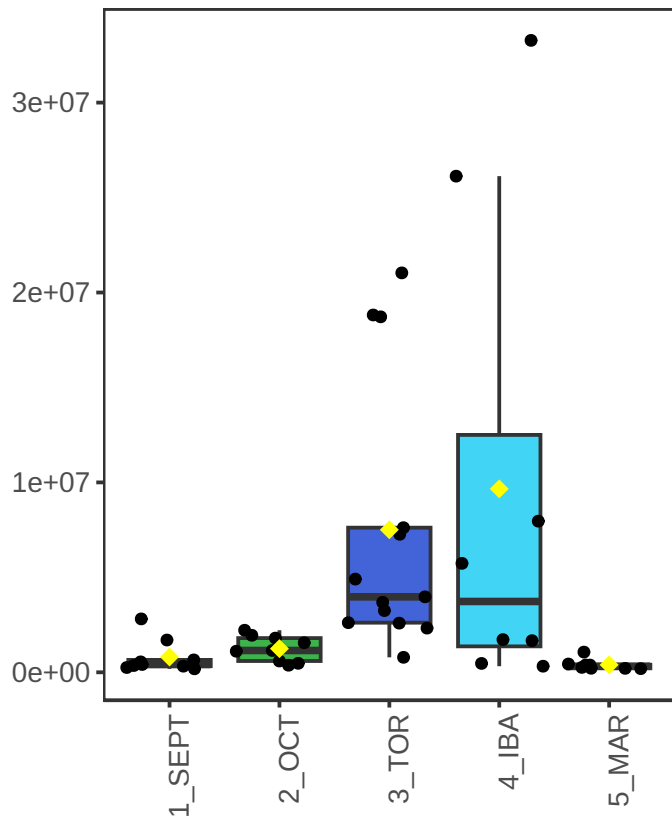


Normalized Conc.

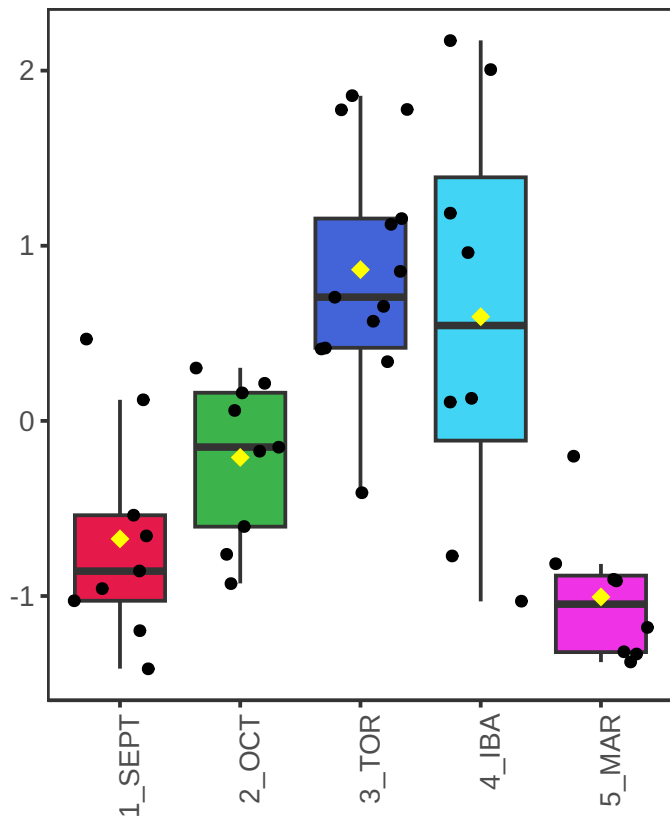


Formiminoglutamic Acid

Original Conc.

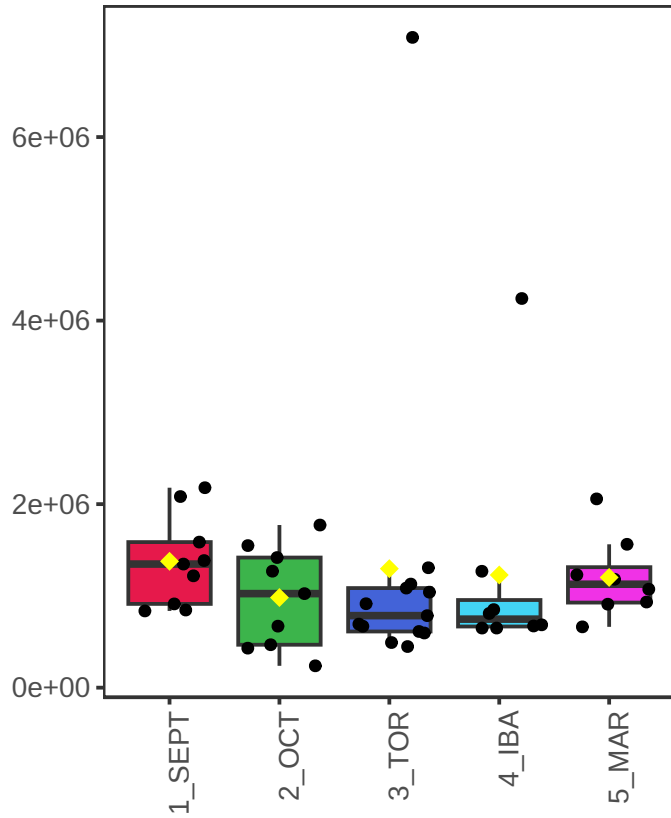


Normalized Conc.

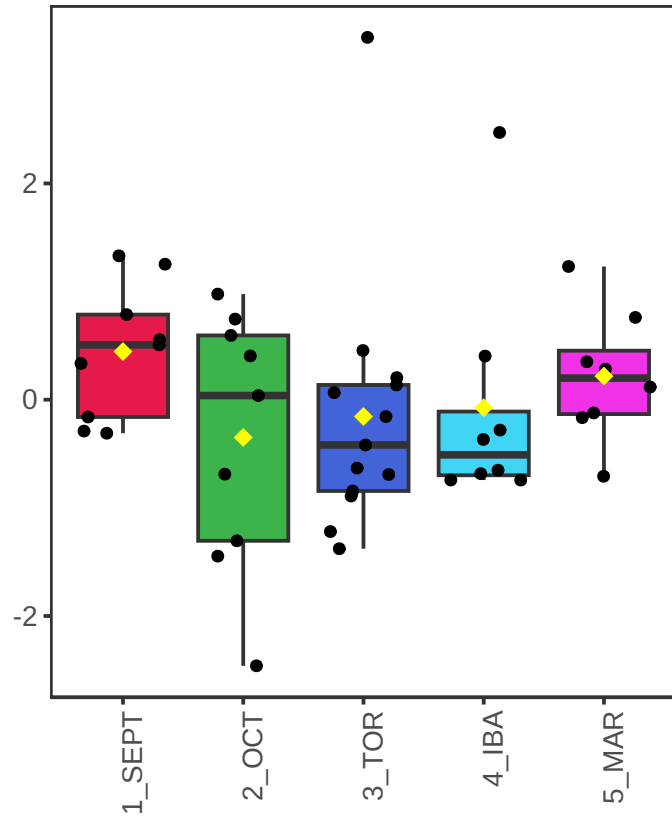


gamma-Glutamylleucine

Original Conc.

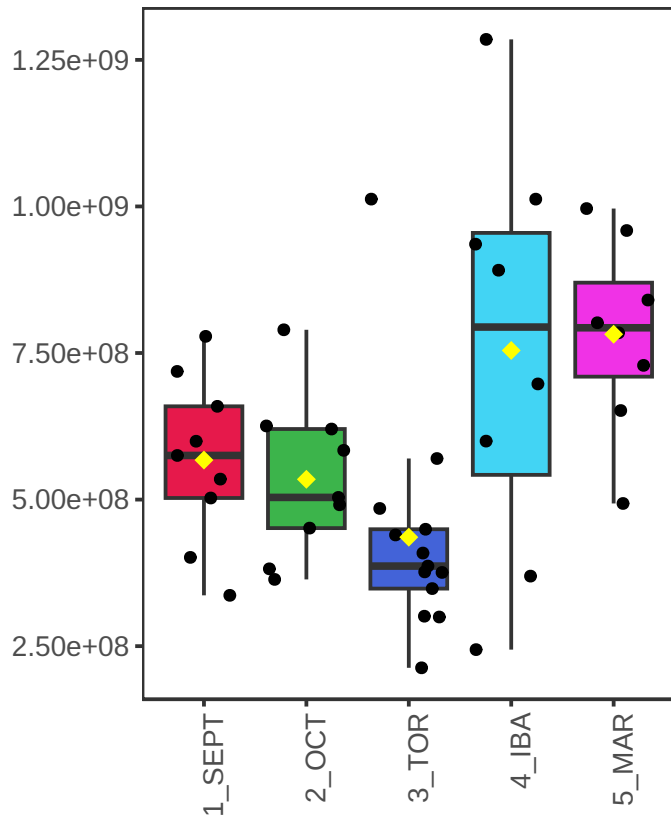


Normalized Conc.

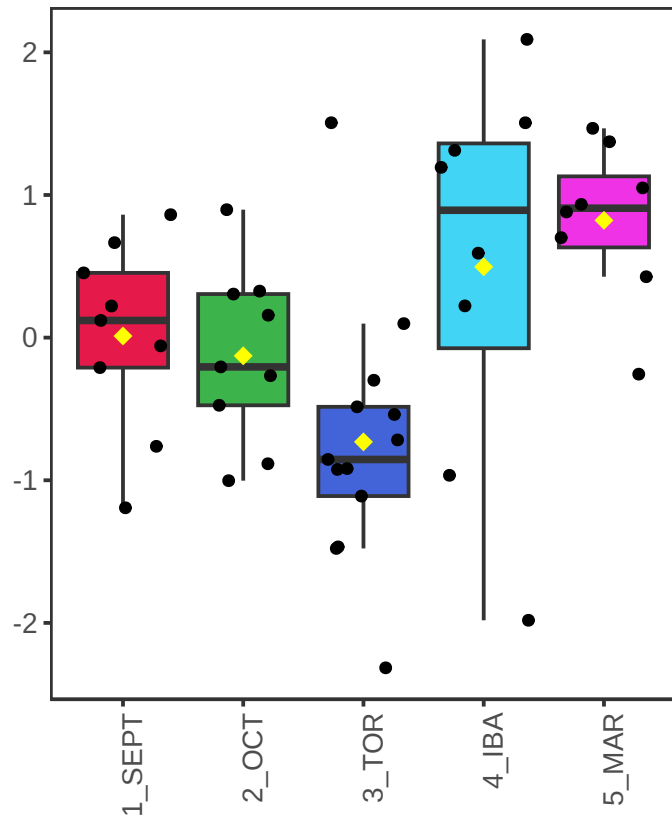


Glutamic acid

Original Conc.

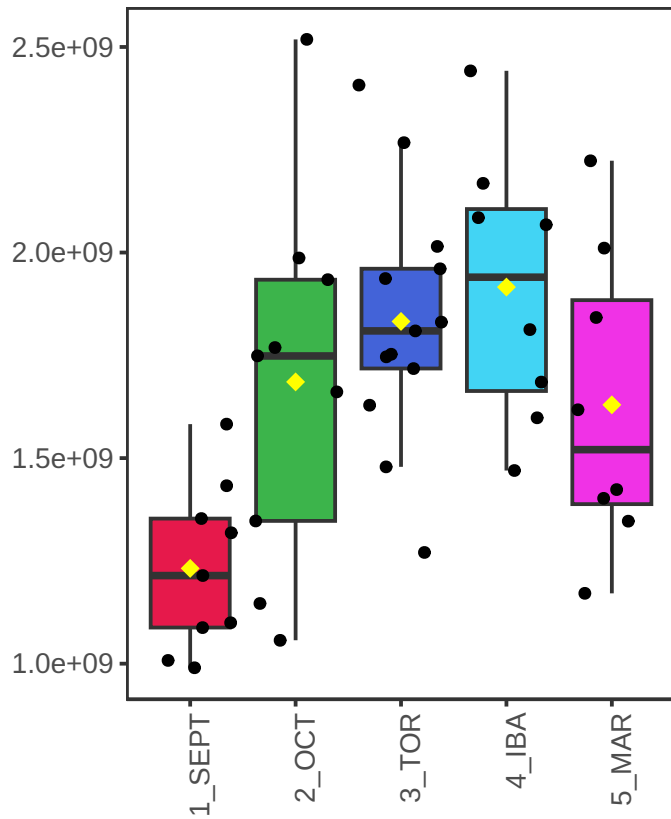


Normalized Conc.

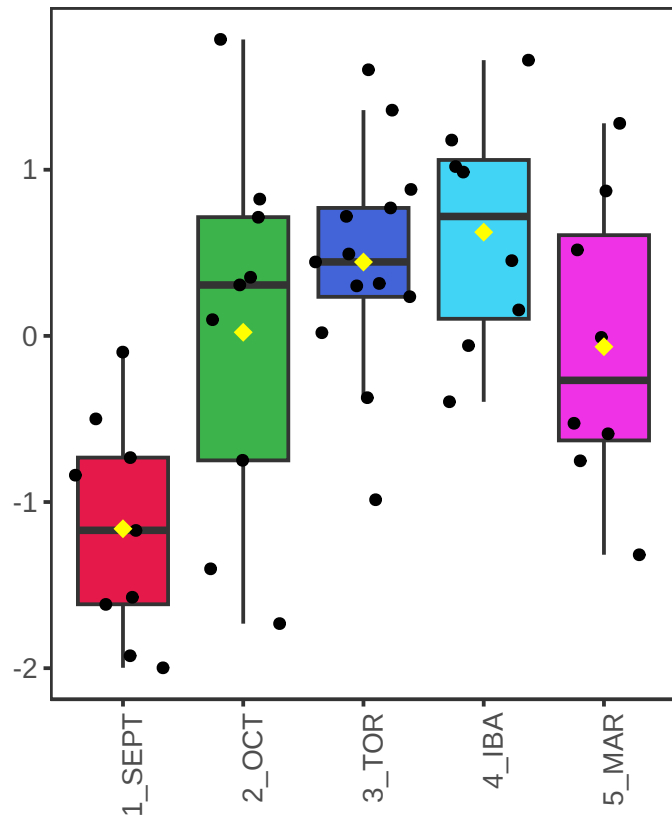


Glutamine

Original Conc.

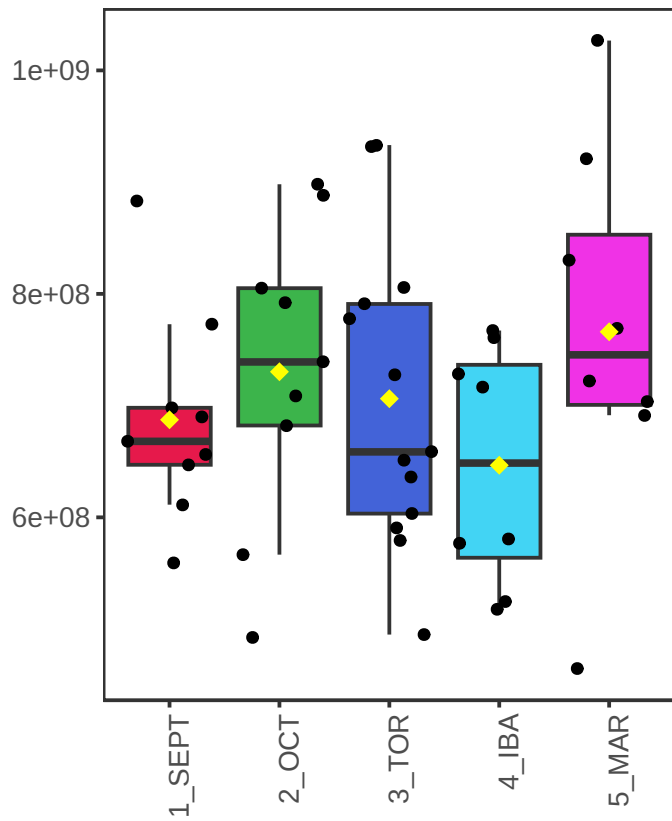


Normalized Conc.

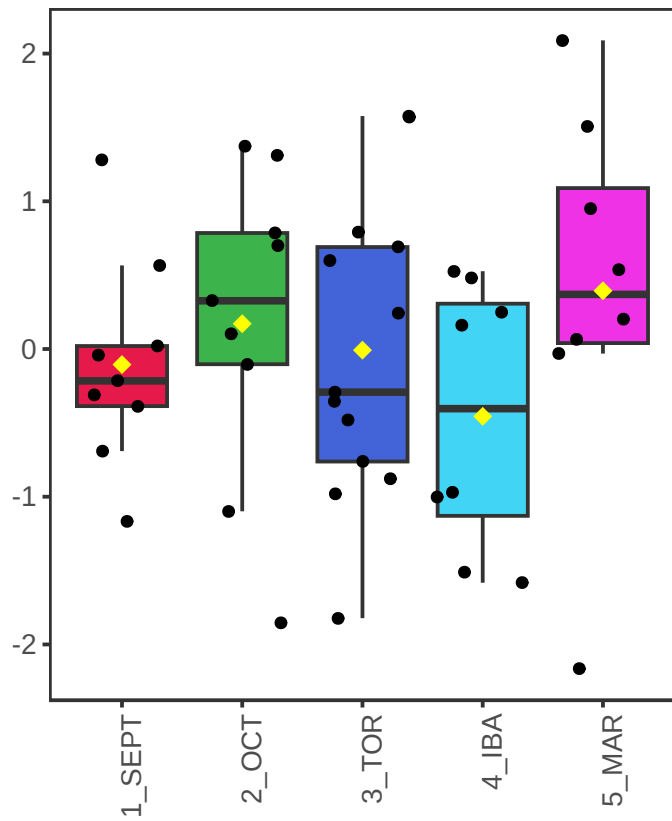


Glutathione (reduced)

Original Conc.

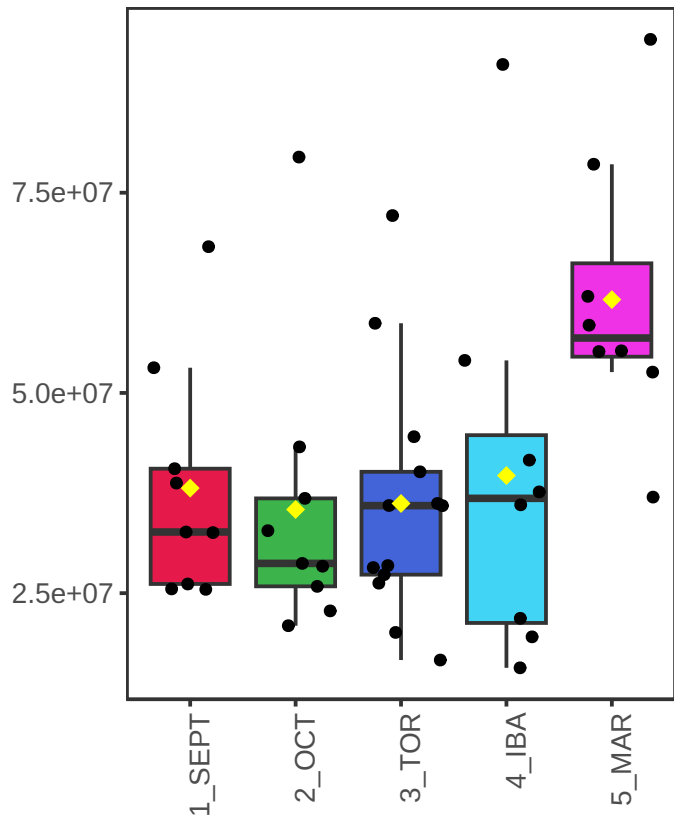


Normalized Conc.

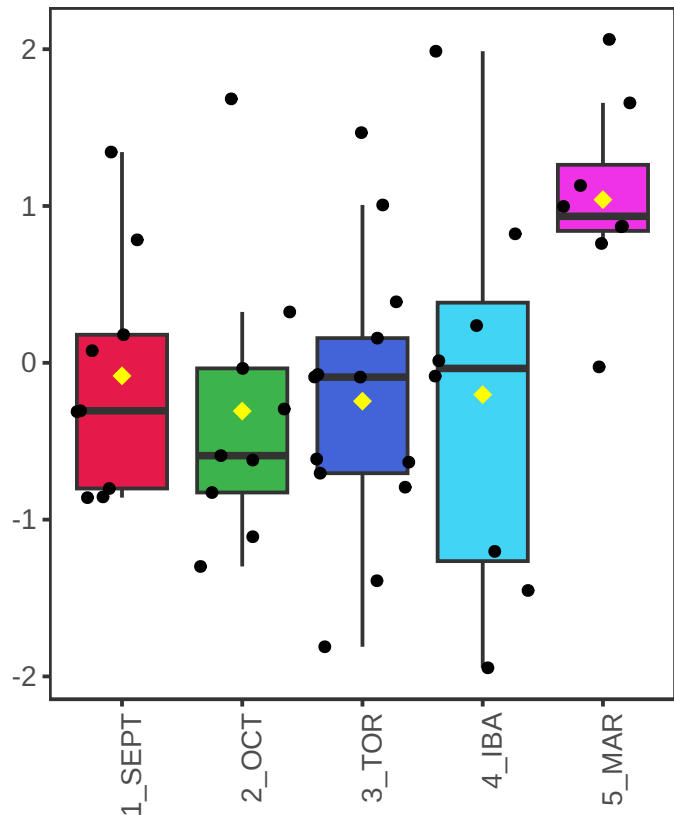


Glycerol 3-phosphate

Original Conc.

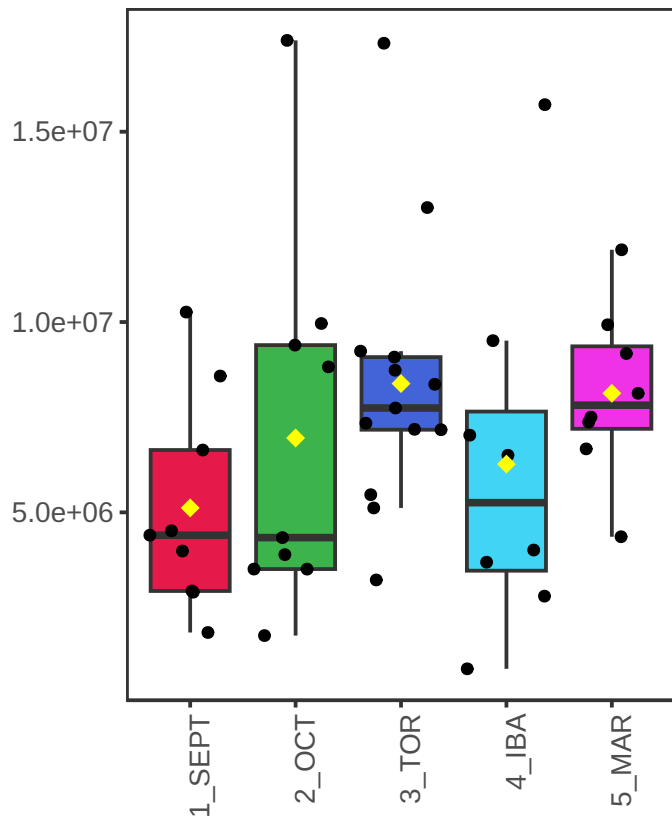


Normalized Conc.

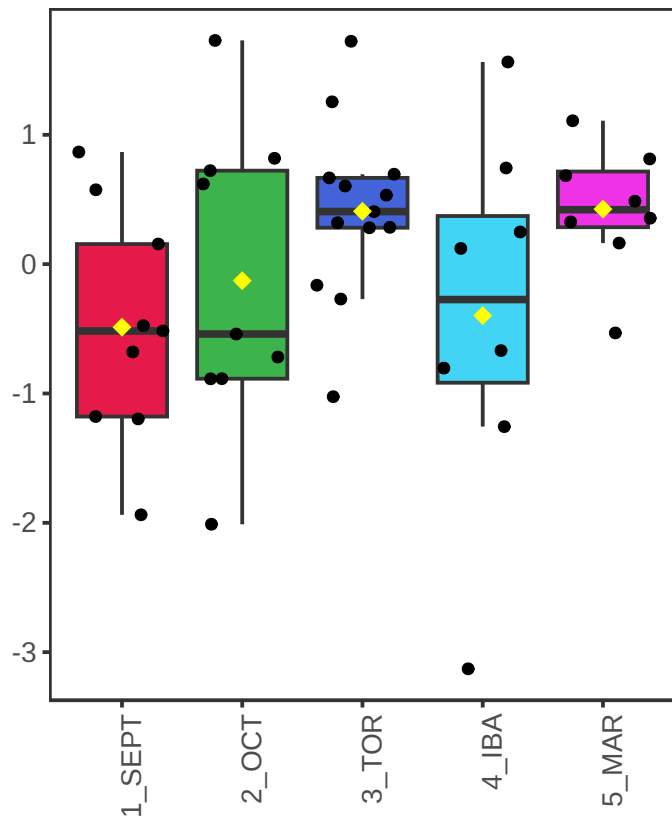


Glycerophosphoinositol

Original Conc.

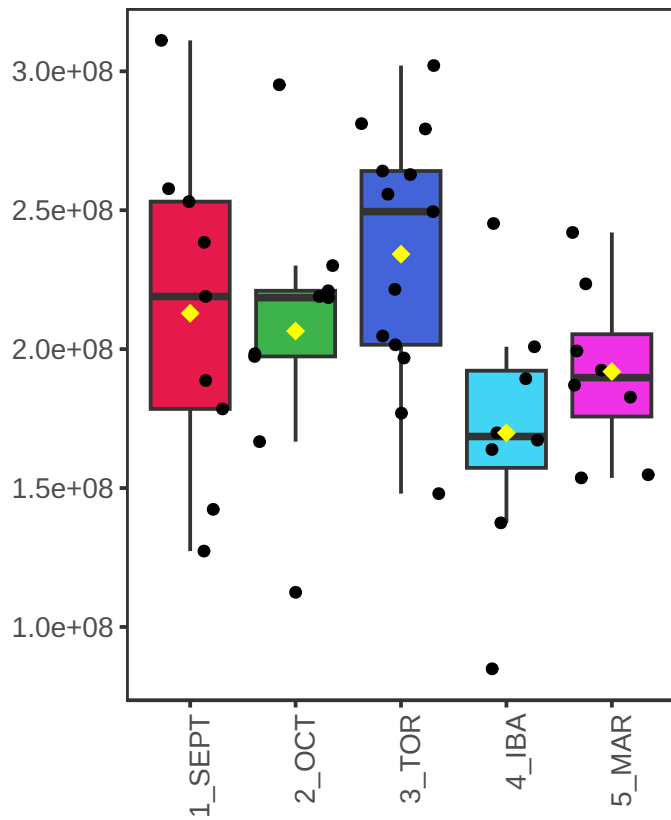


Normalized Conc.

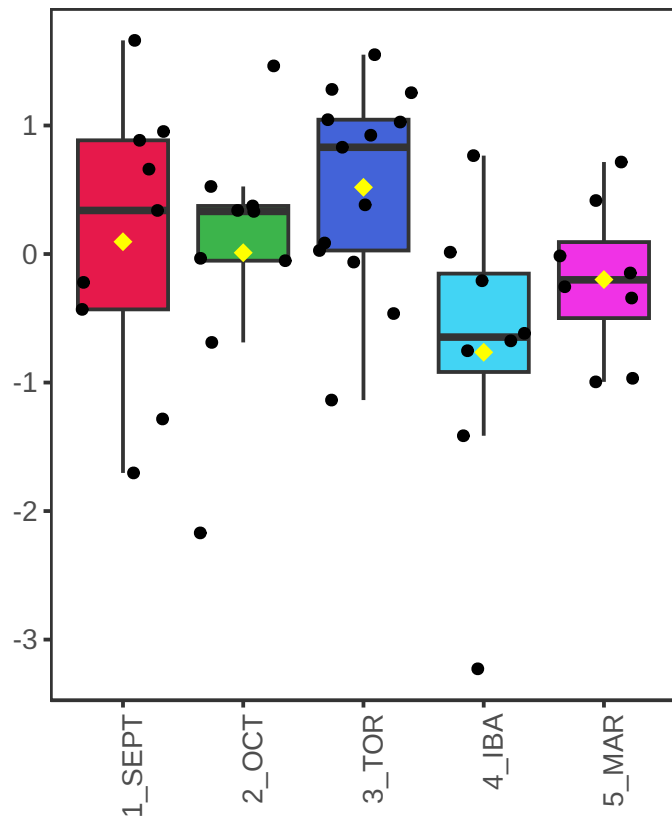


Glycerolphosphorylethanolamine

Original Conc.

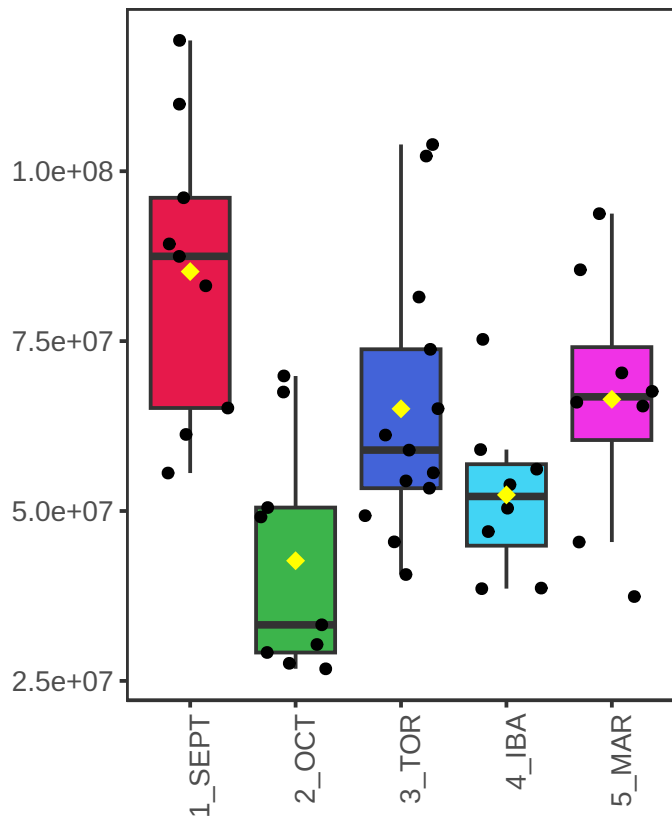


Normalized Conc.

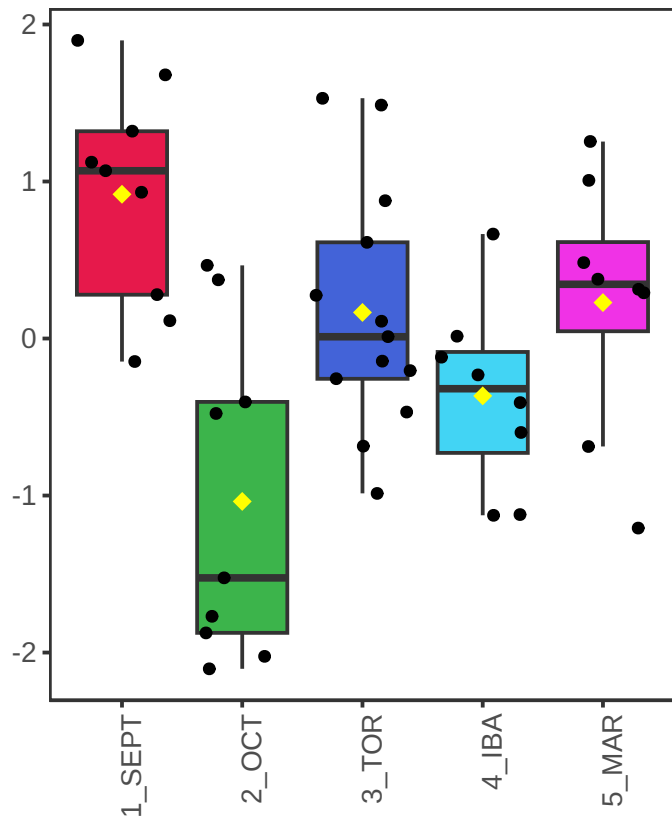


Guanidineacetic acid

Original Conc.

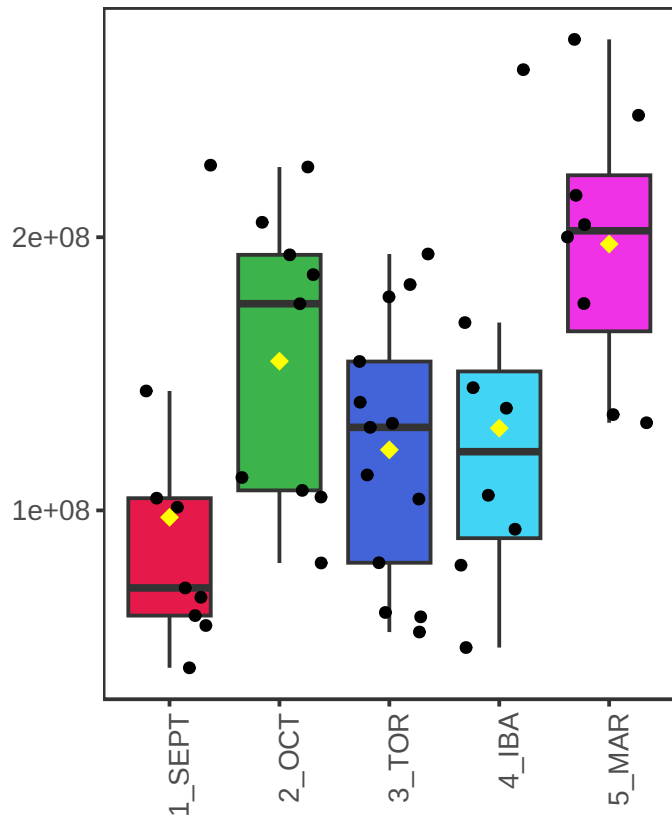


Normalized Conc.

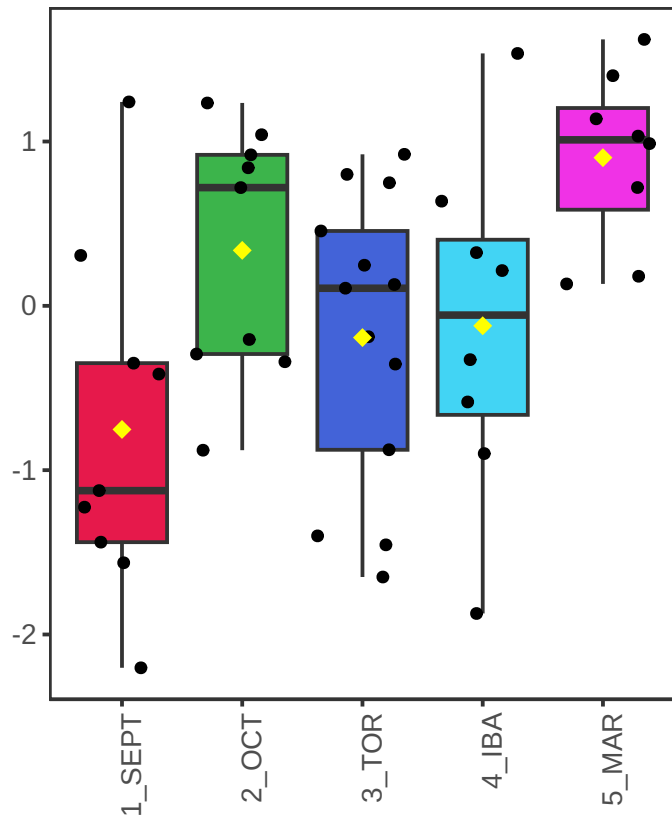


Guanine

Original Conc.

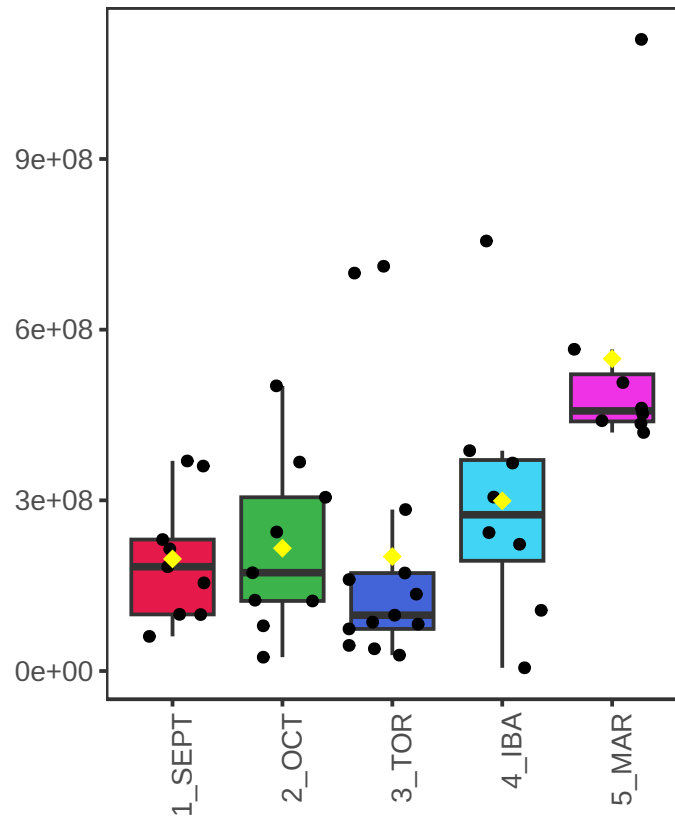


Normalized Conc.

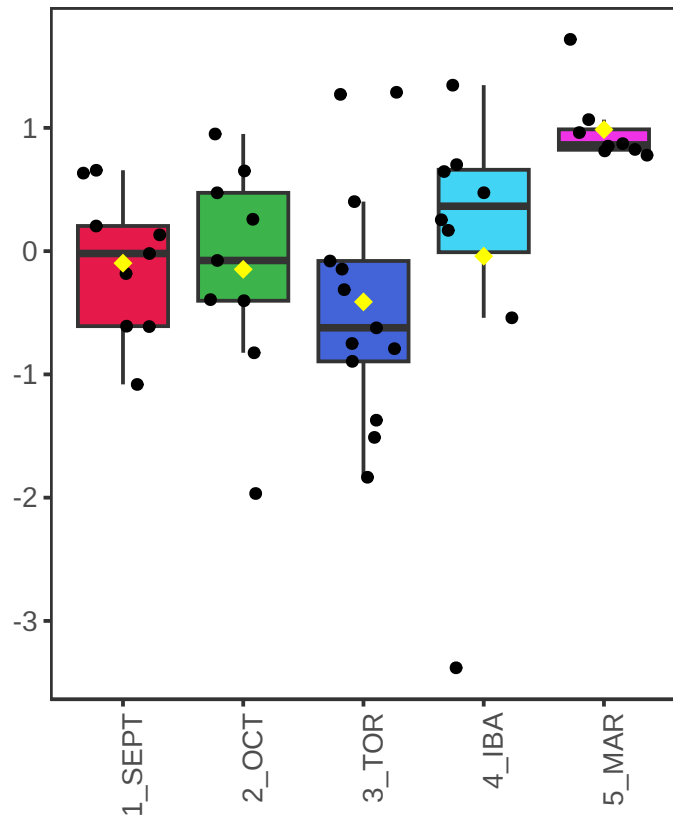


Histamine

Original Conc.

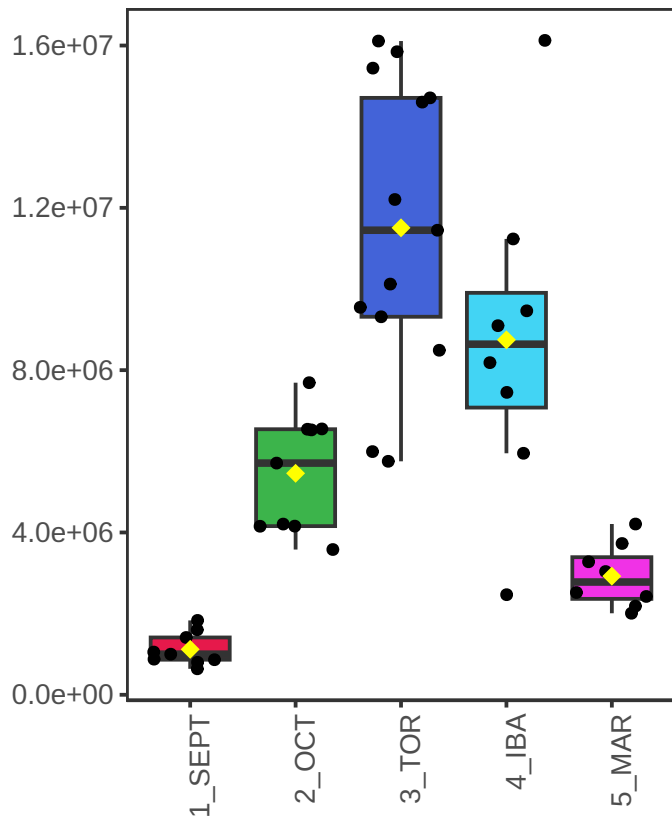


Normalized Conc.

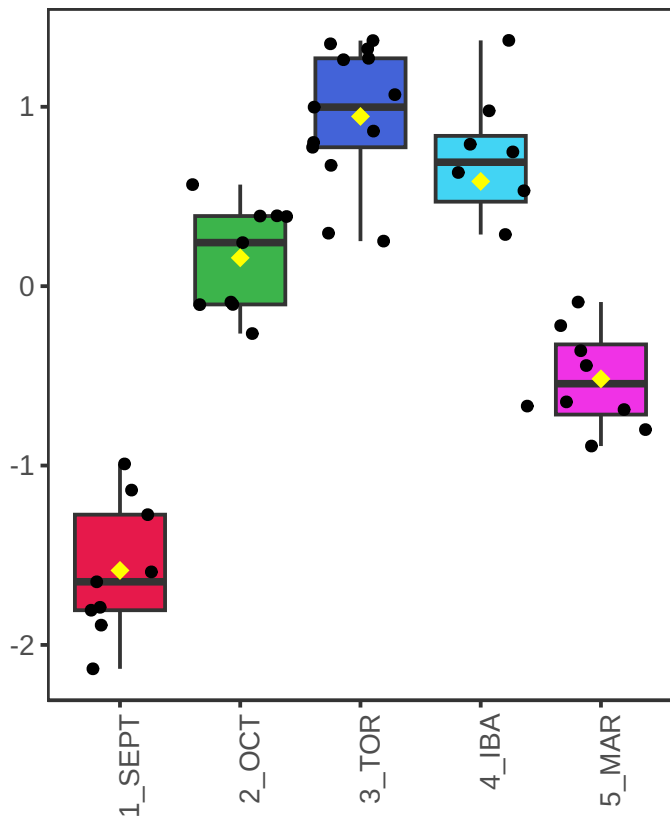


Hydroxyhexanoylcarnitine

Original Conc.

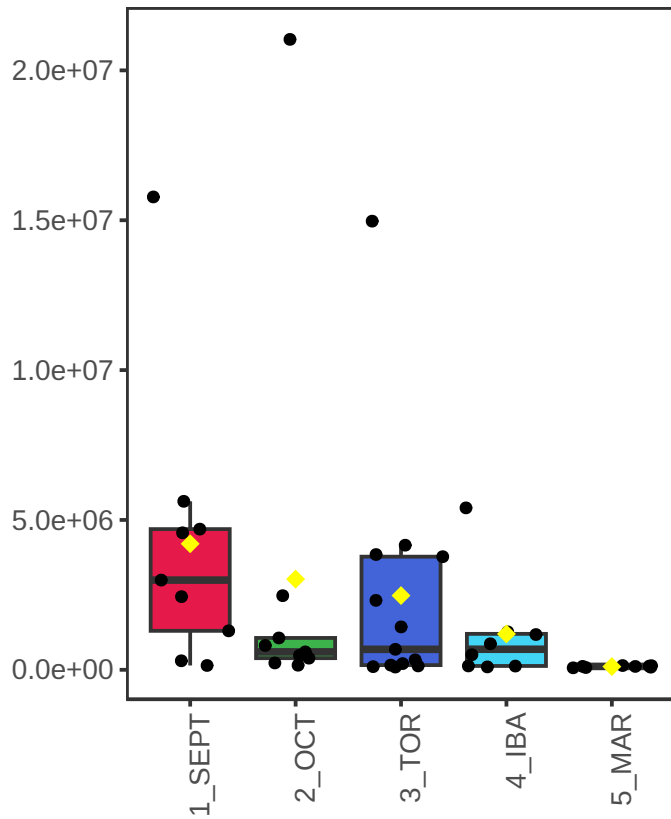


Normalized Conc.

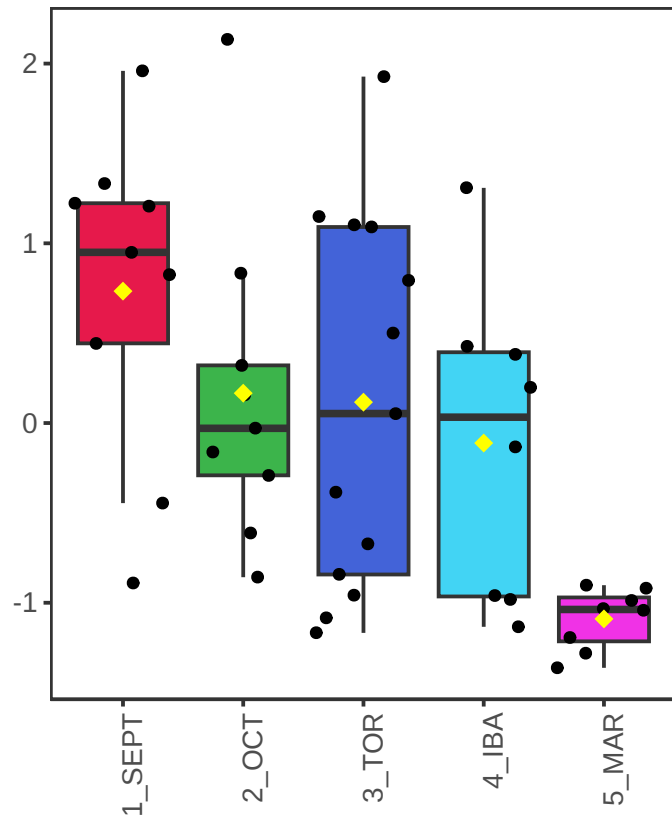


Hypaphorine

Original Conc.

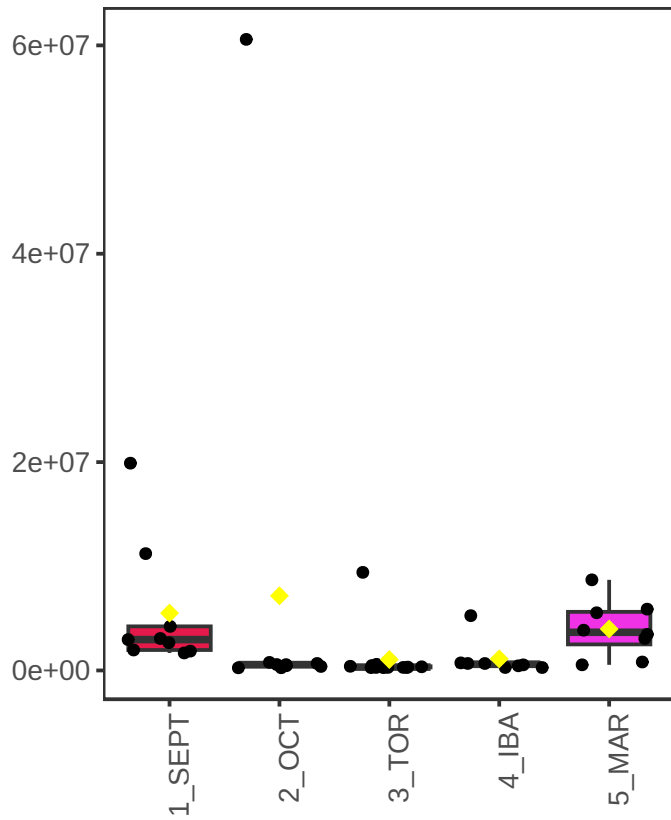


Normalized Conc.

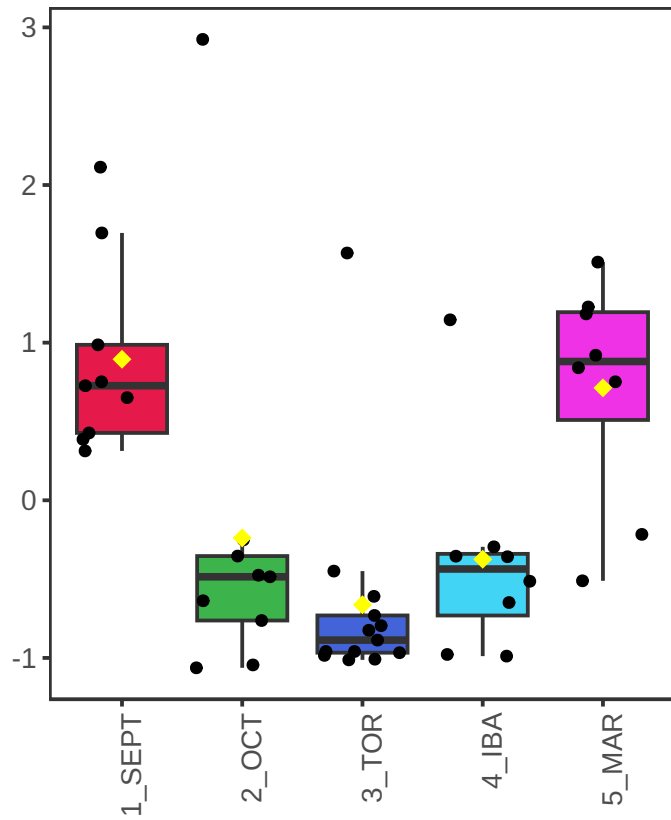


Hypotaurine

Original Conc.

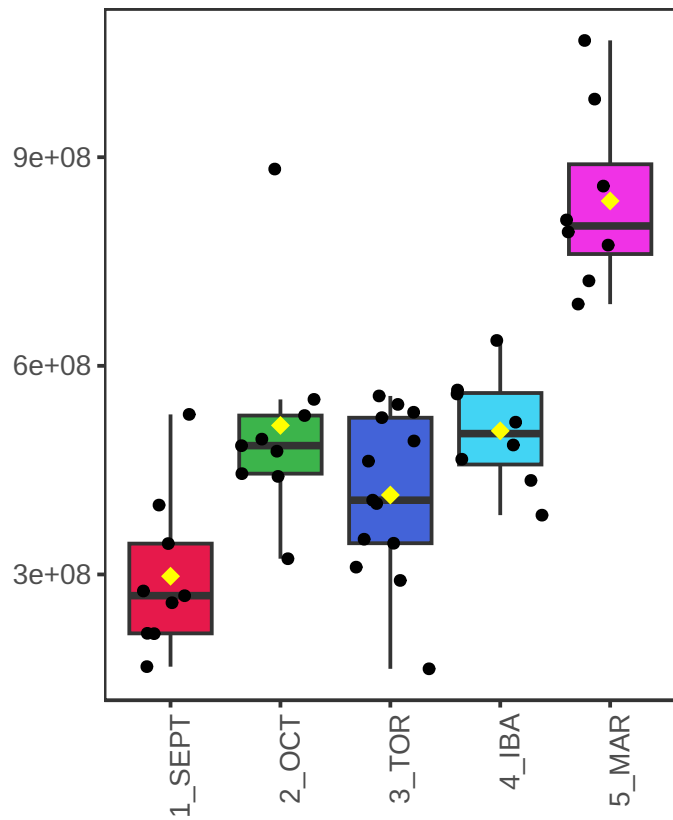


Normalized Conc.

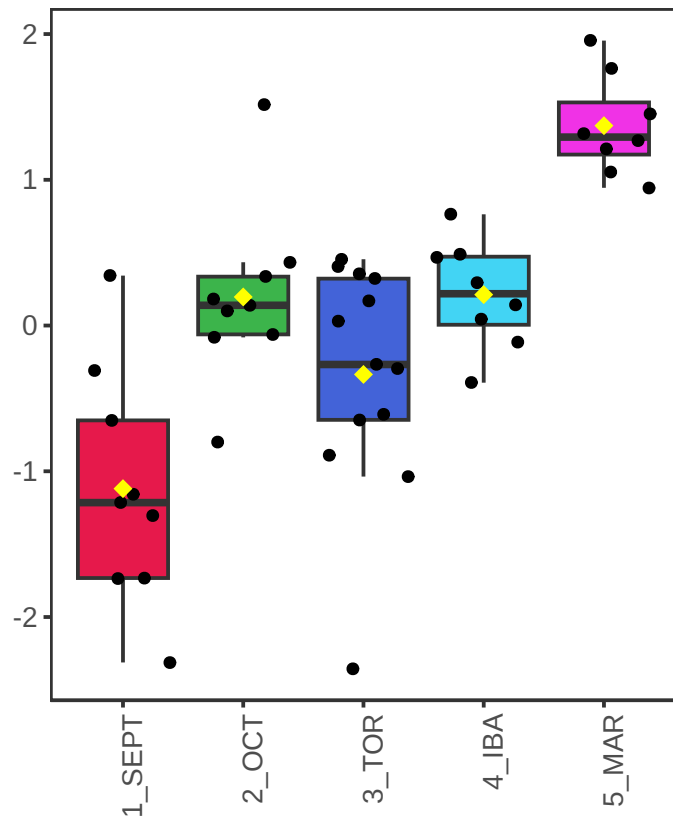


Hypoxanthine

Original Conc.

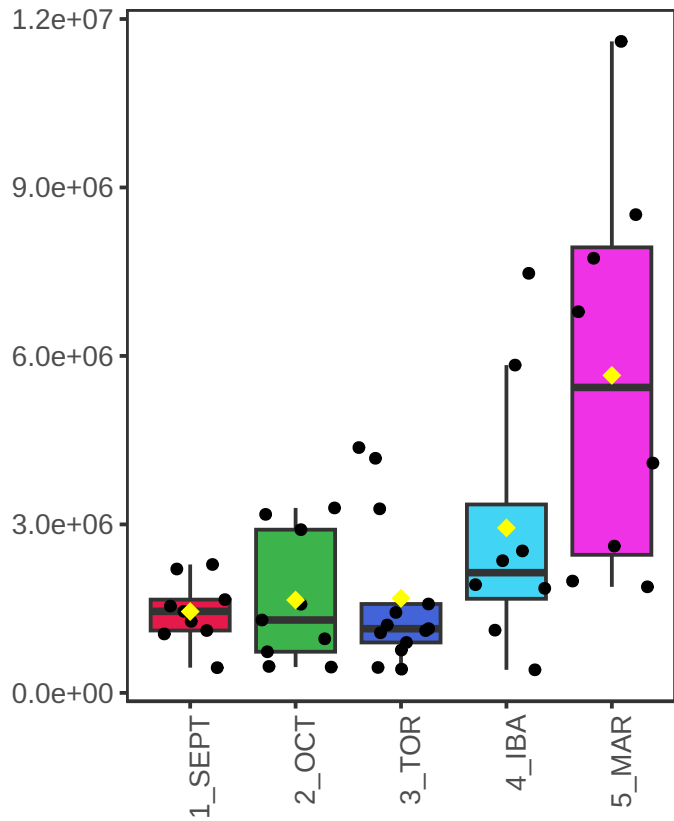


Normalized Conc.

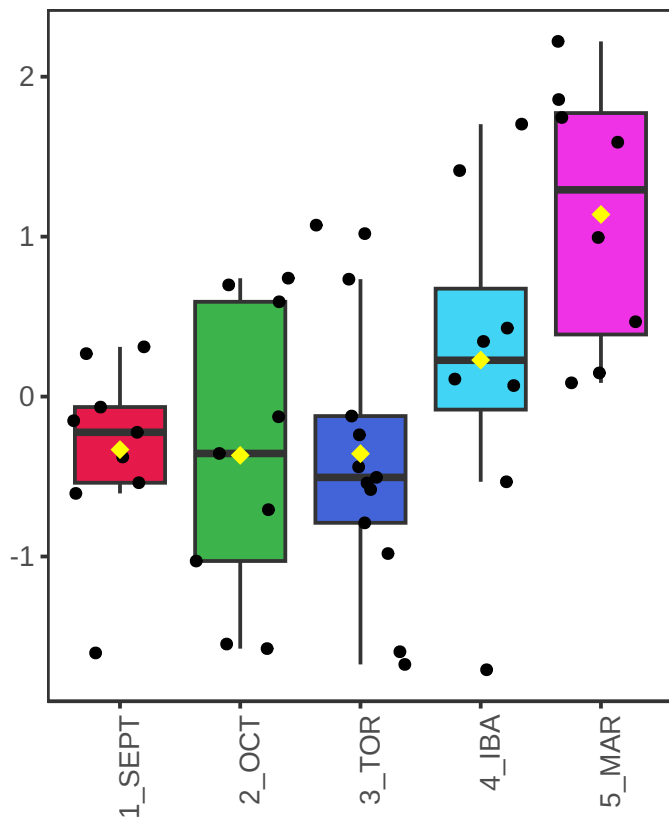


Imidazoleacetic acid

Original Conc.

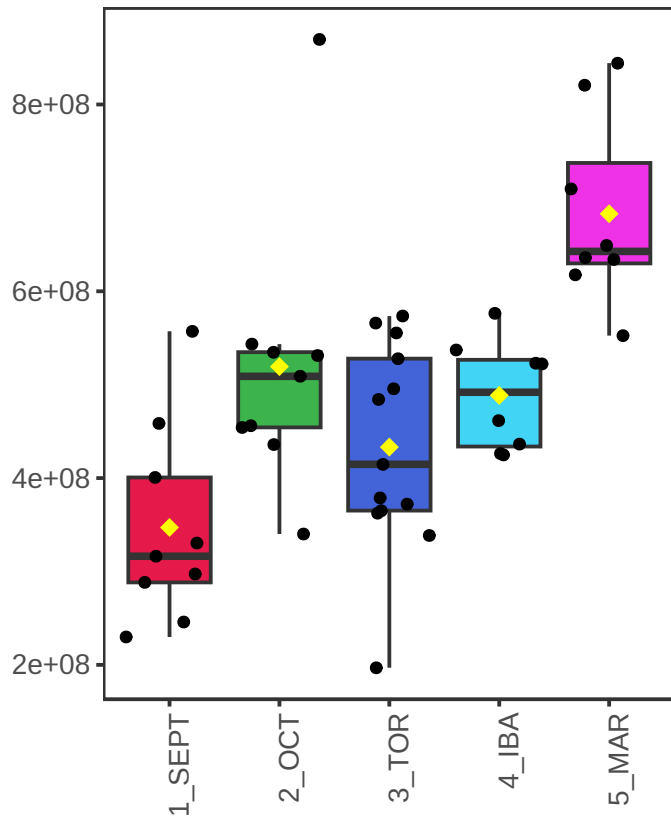


Normalized Conc.

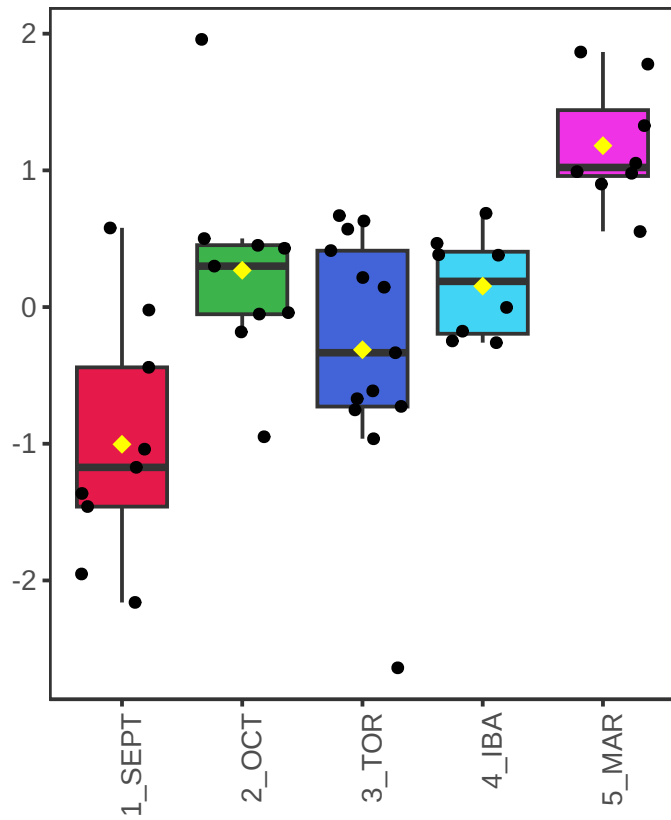


Inosine

Original Conc.

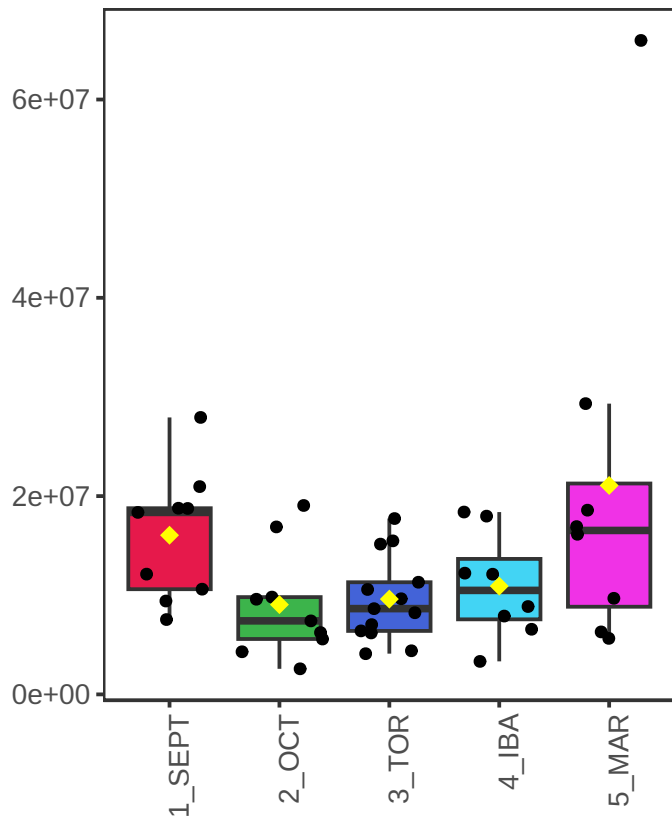


Normalized Conc.

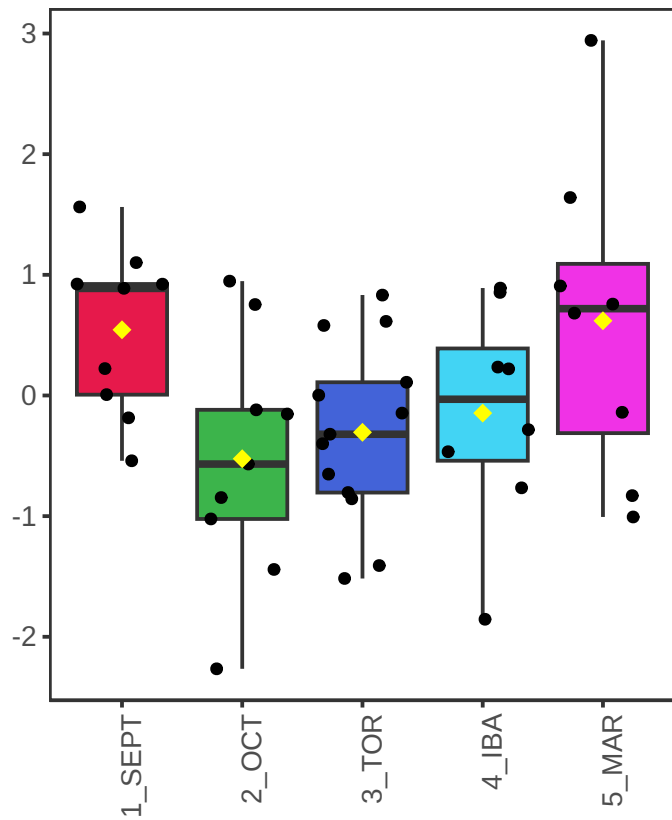


Inosine-5'-monophosphate (IMP)

Original Conc.

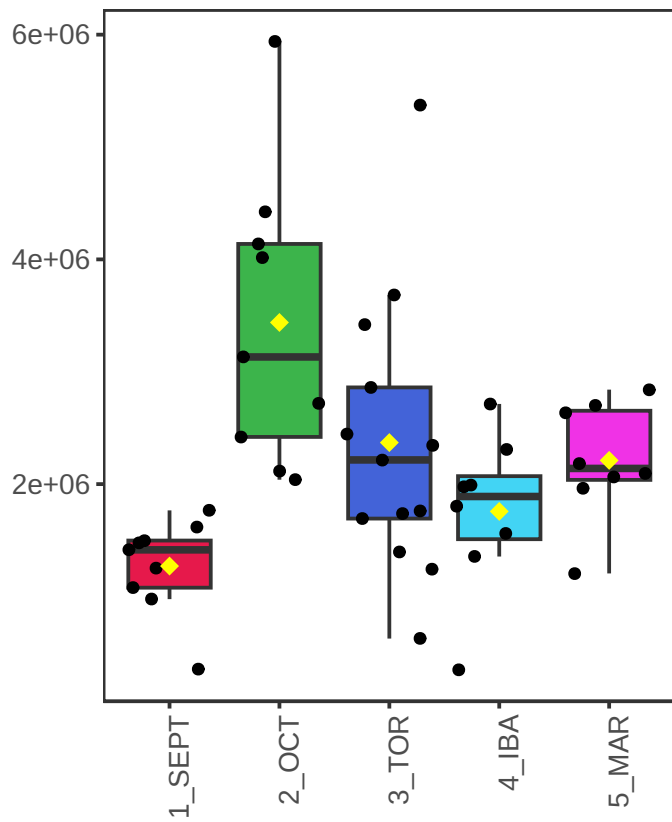


Normalized Conc.

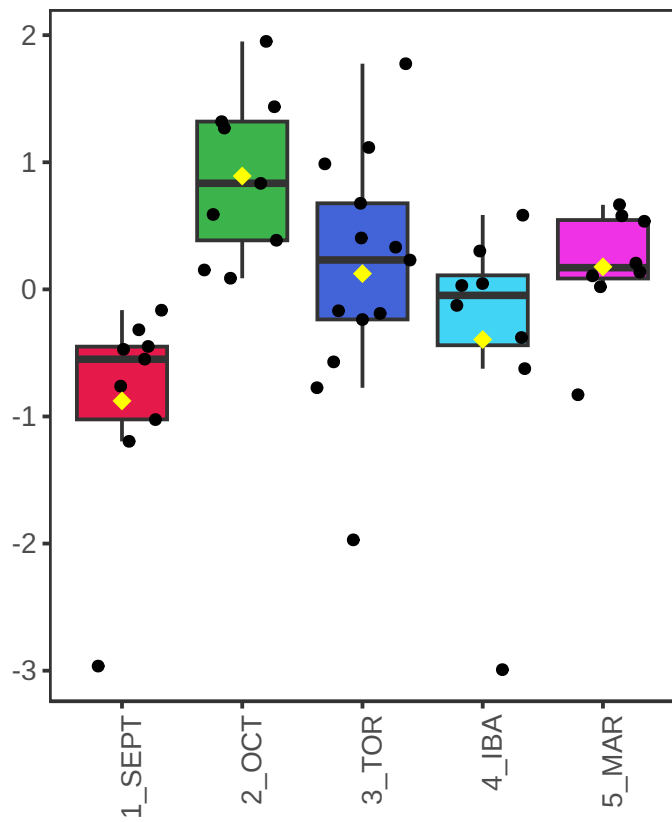


Inositol cyclic phosphate

Original Conc.

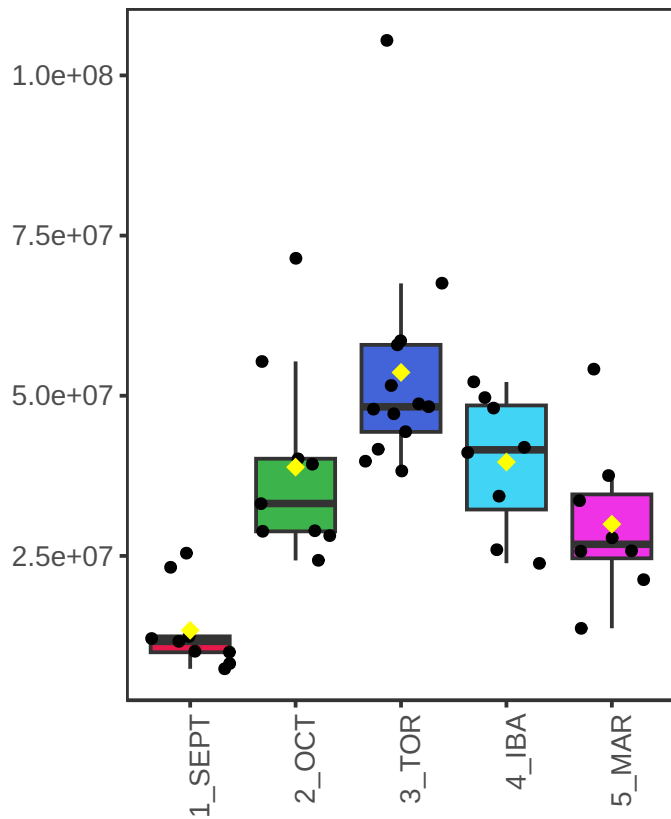


Normalized Conc.

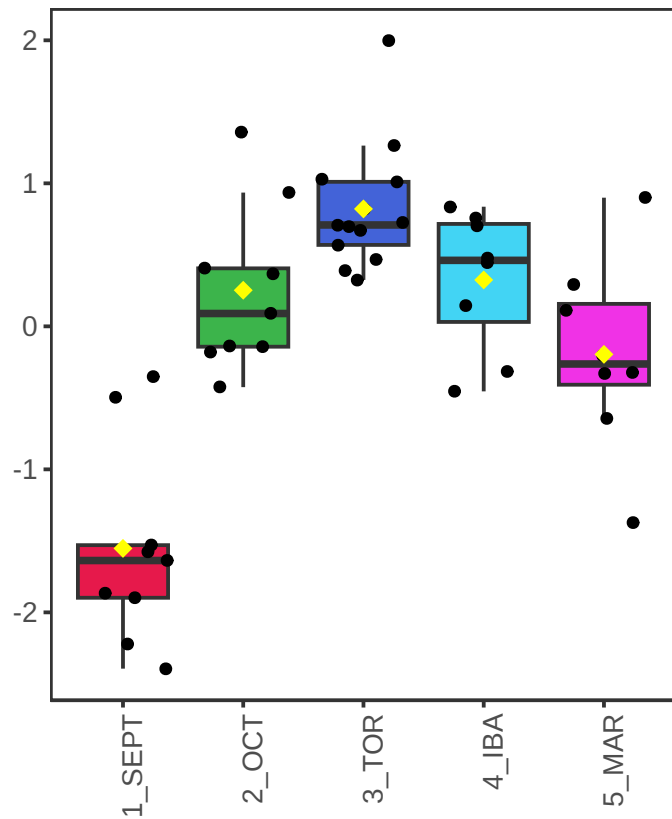


Isoleucine

Original Conc.

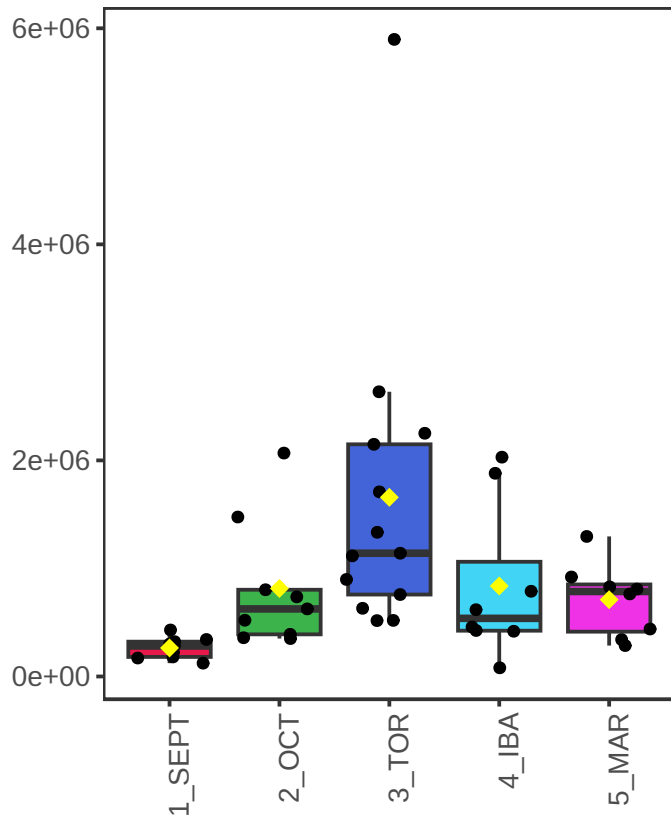


Normalized Conc.

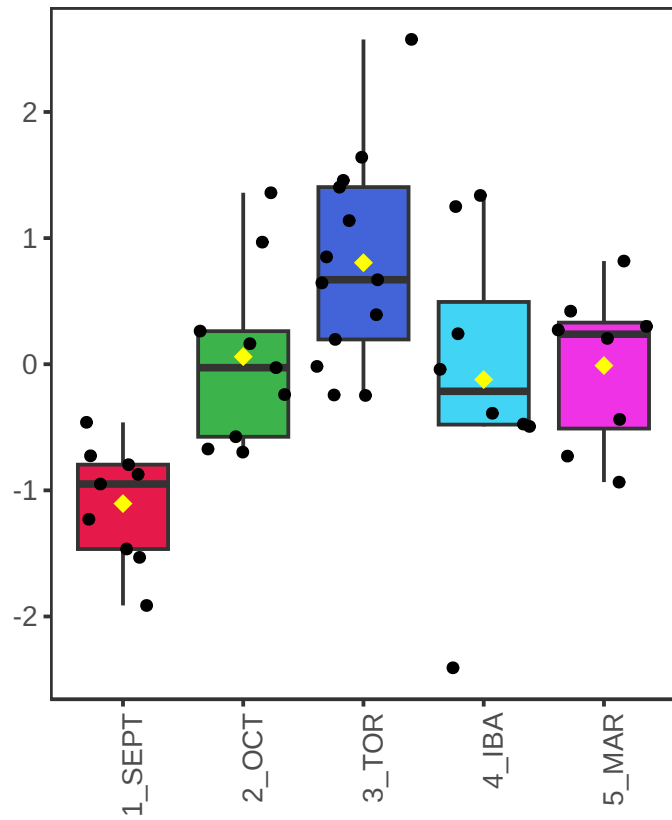


Kynurenine

Original Conc.

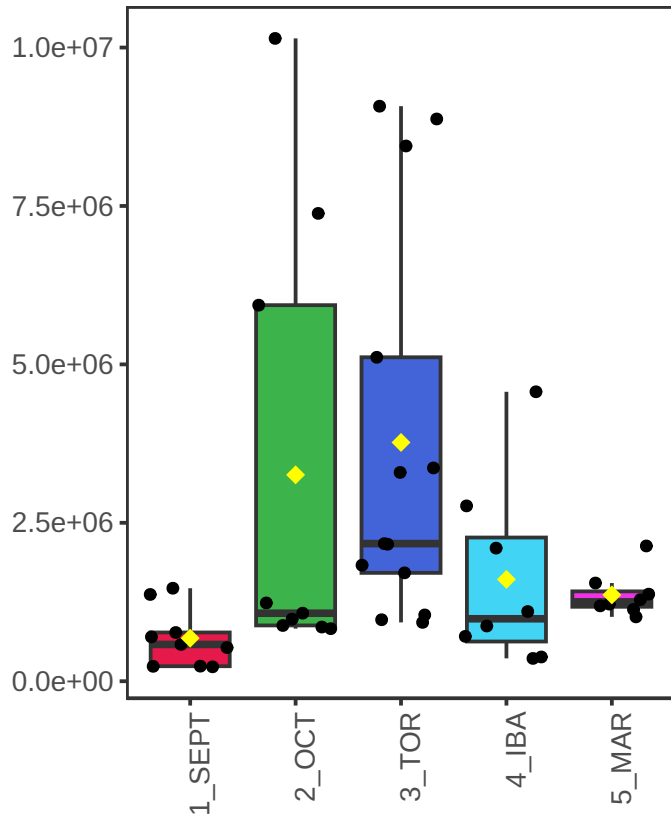


Normalized Conc.

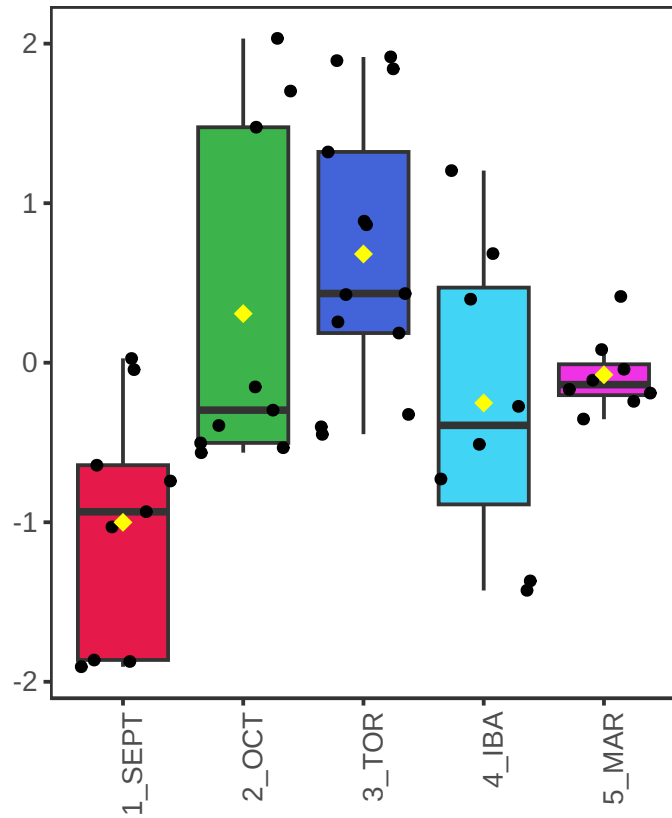


Lactose

Original Conc.

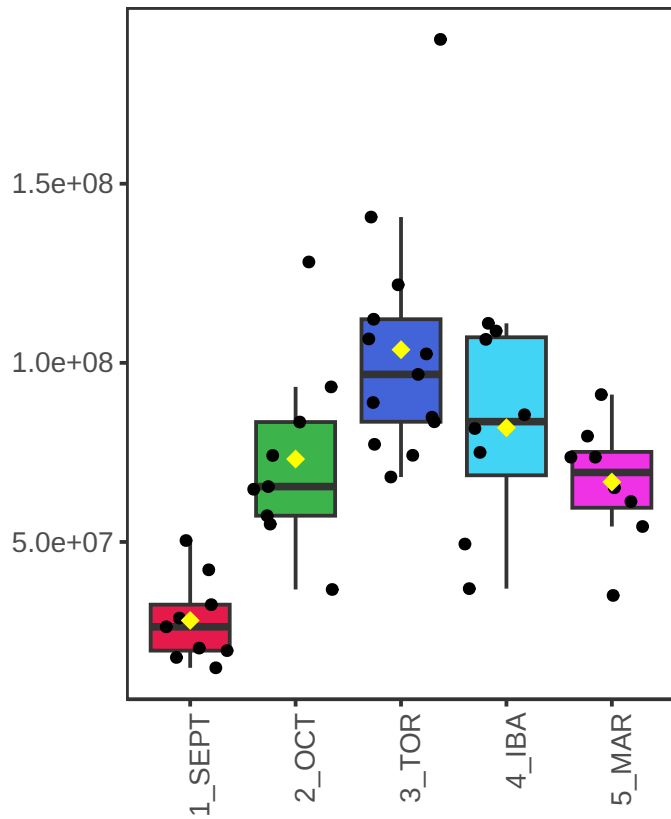


Normalized Conc.

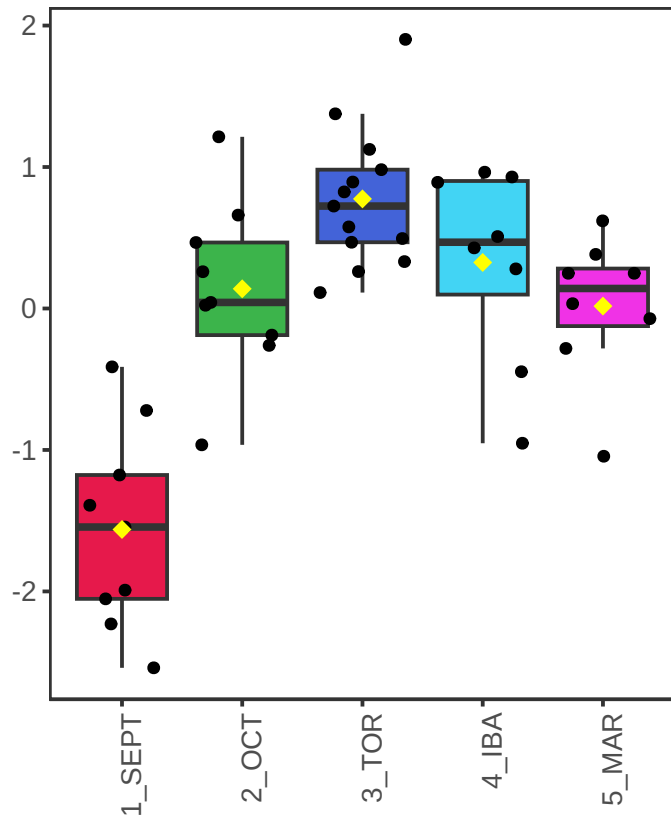


Leucine

Original Conc.

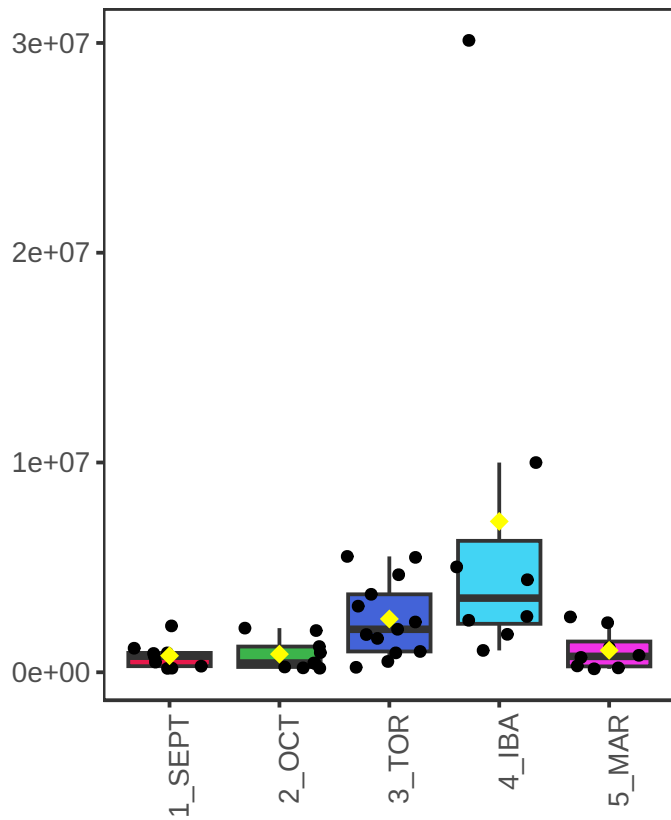


Normalized Conc.

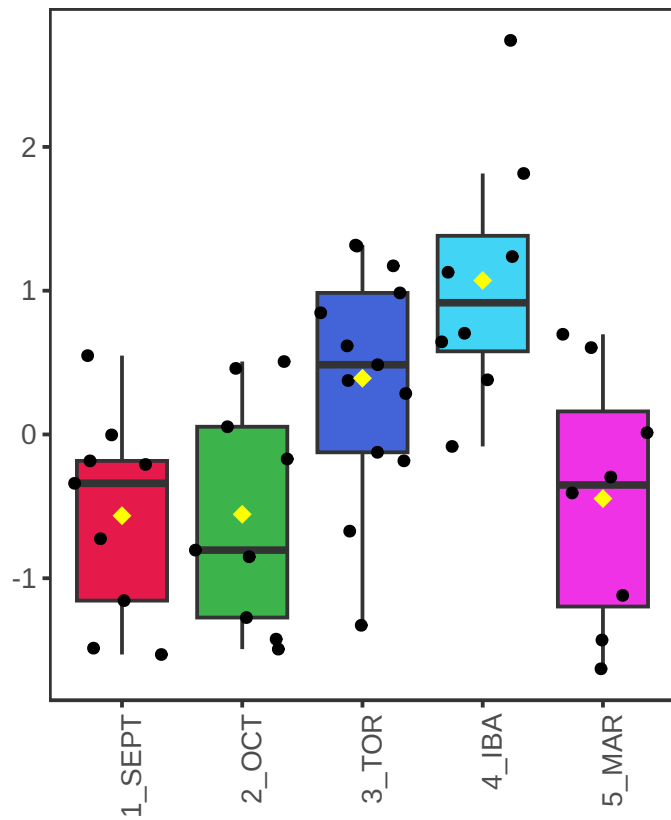


Linoleyl carnitine

Original Conc.

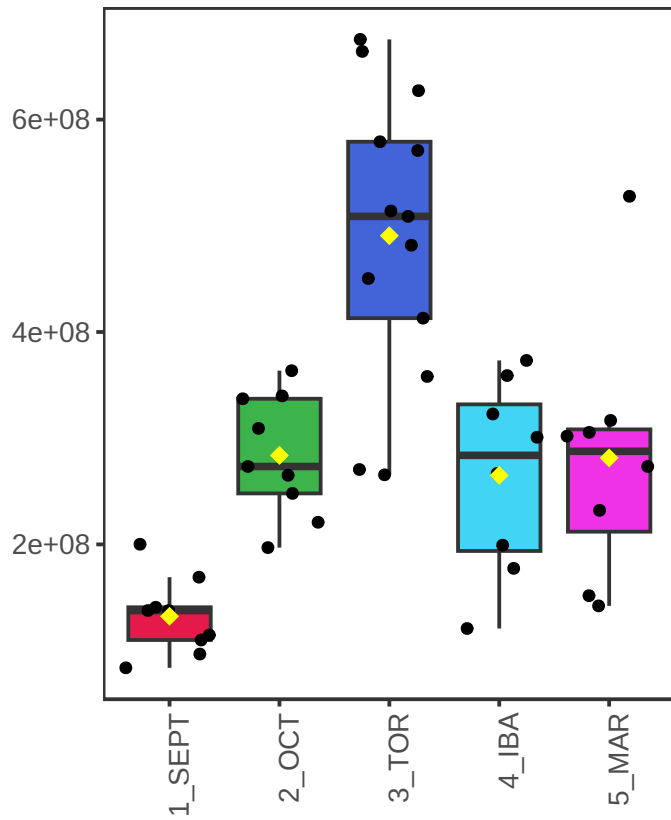


Normalized Conc.

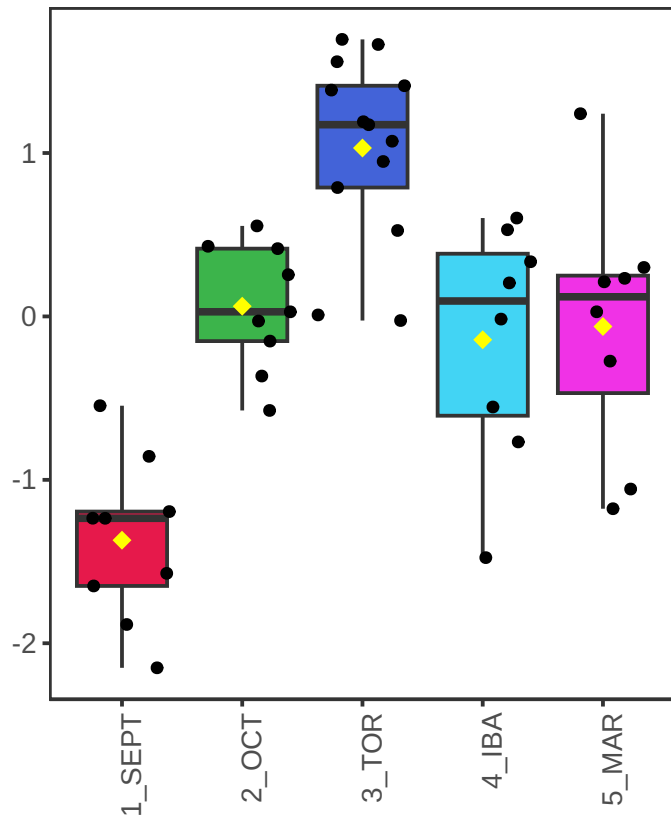


Lysine

Original Conc.

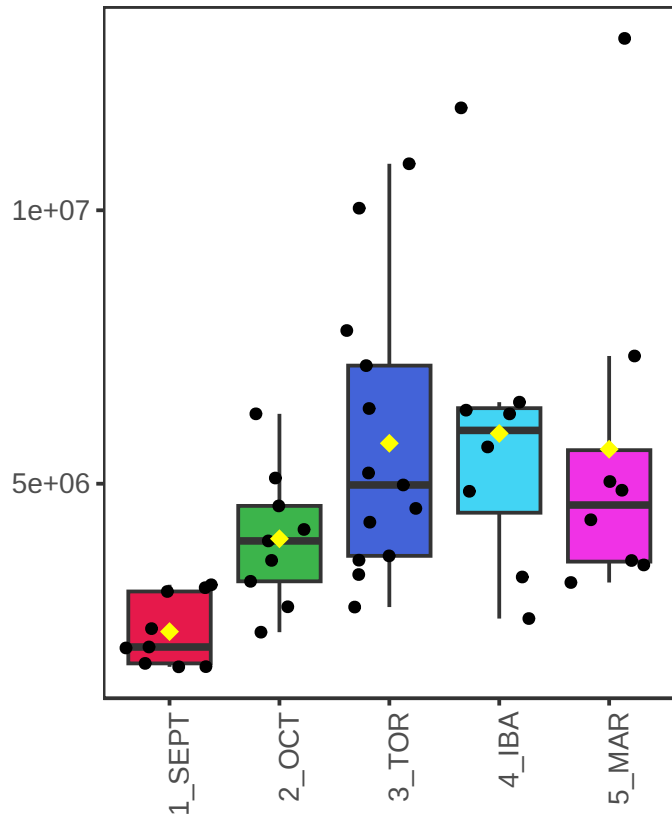


Normalized Conc.

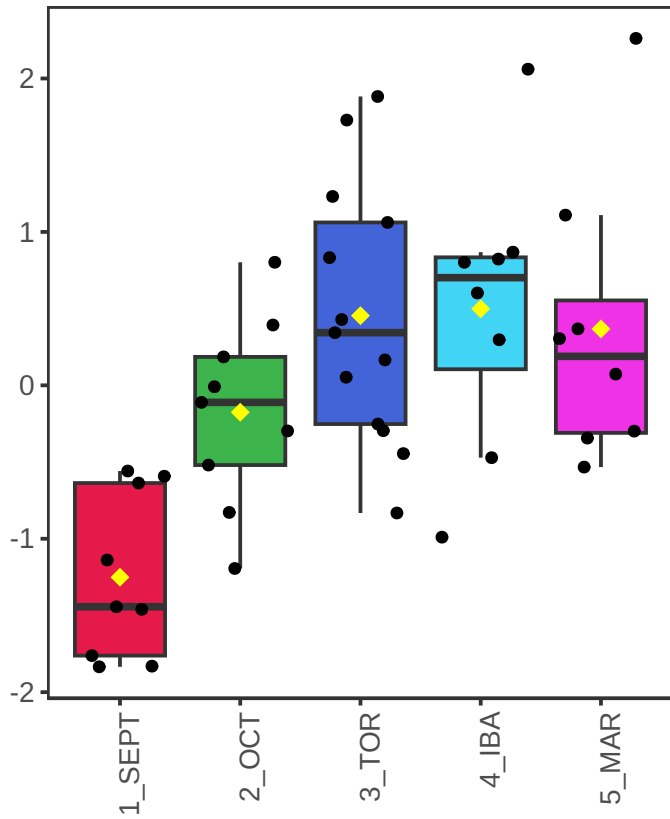


Lys-leu

Original Conc.

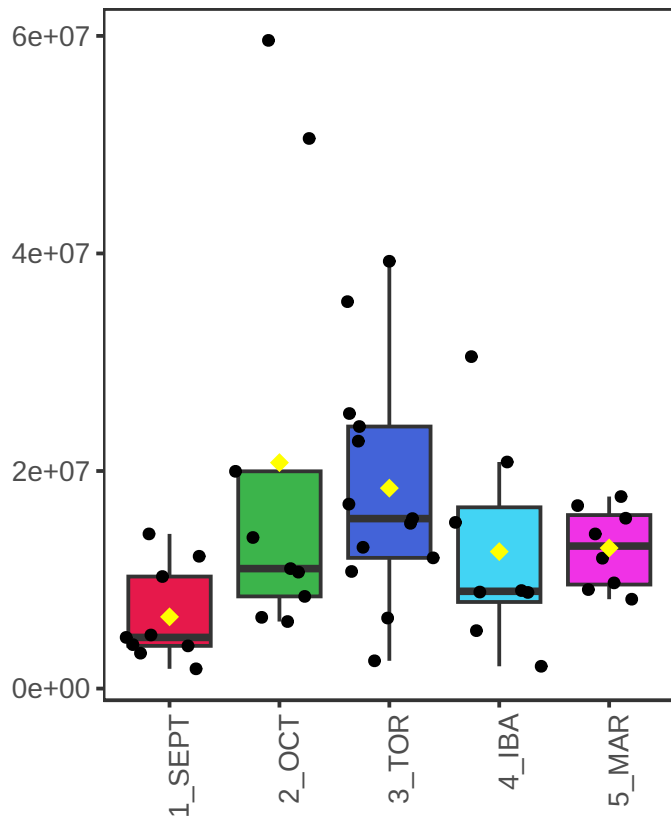


Normalized Conc.

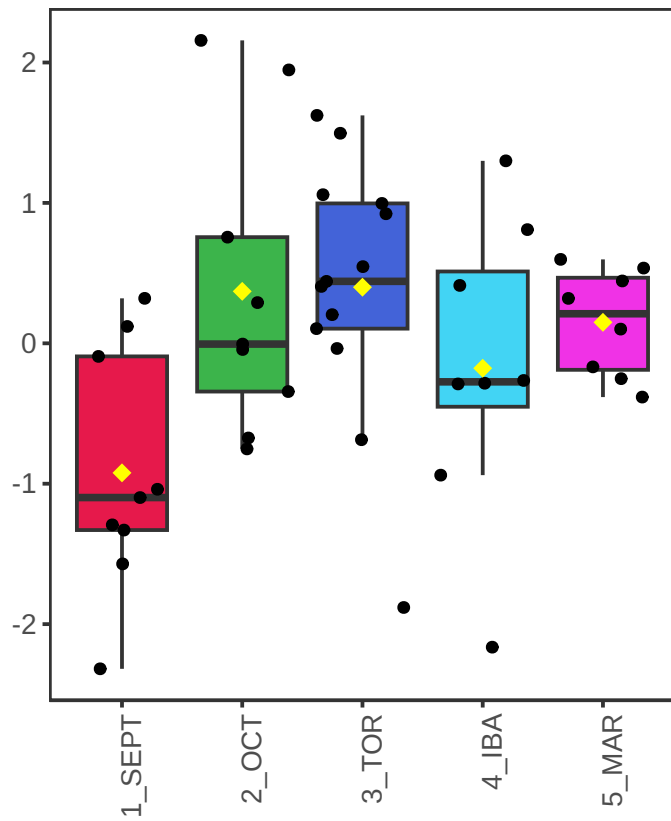


Maltose

Original Conc.

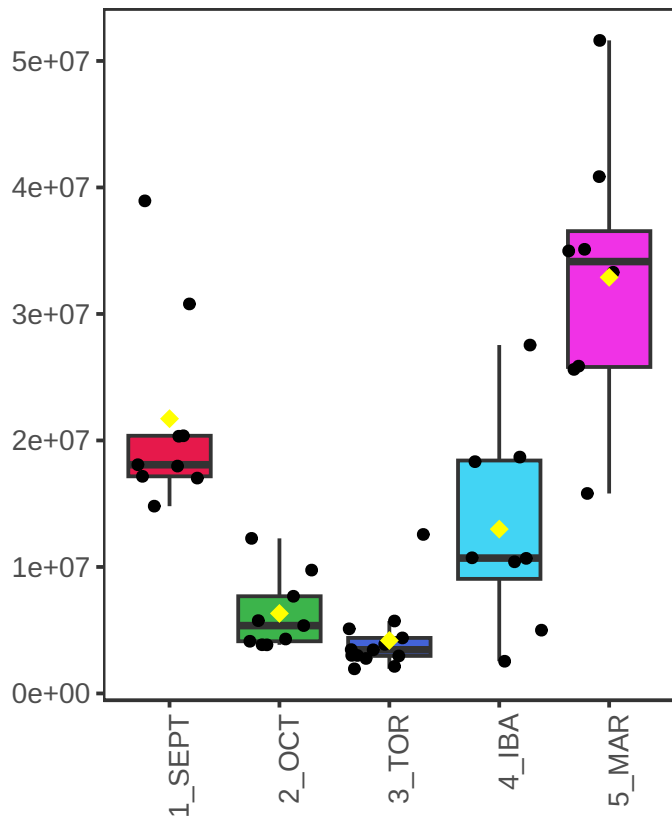


Normalized Conc.

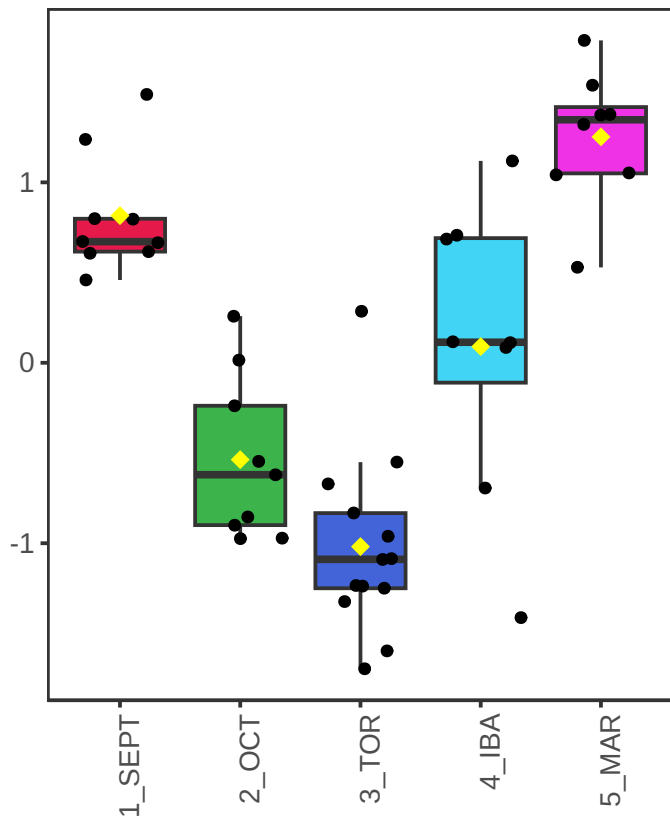


Methionine

Original Conc.

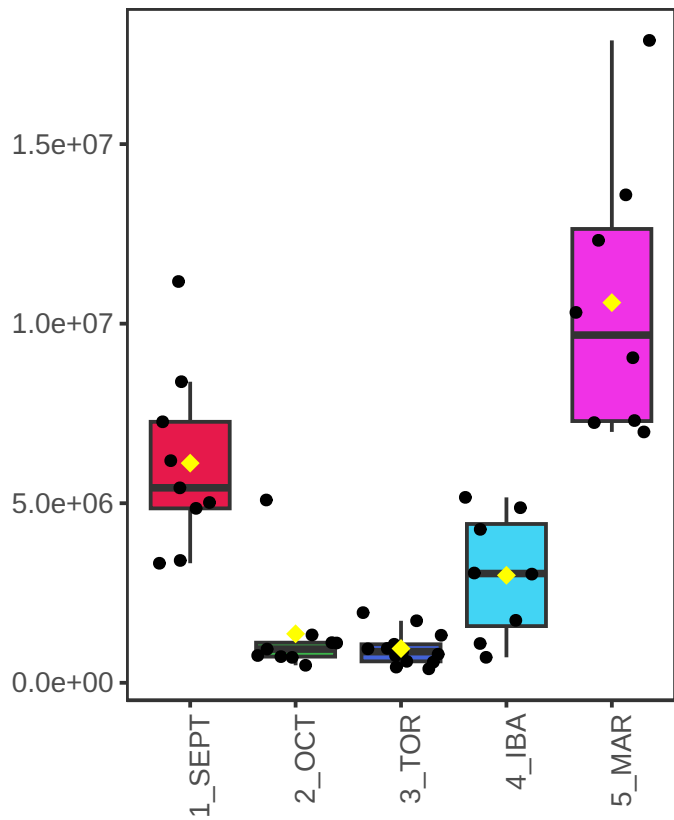


Normalized Conc.

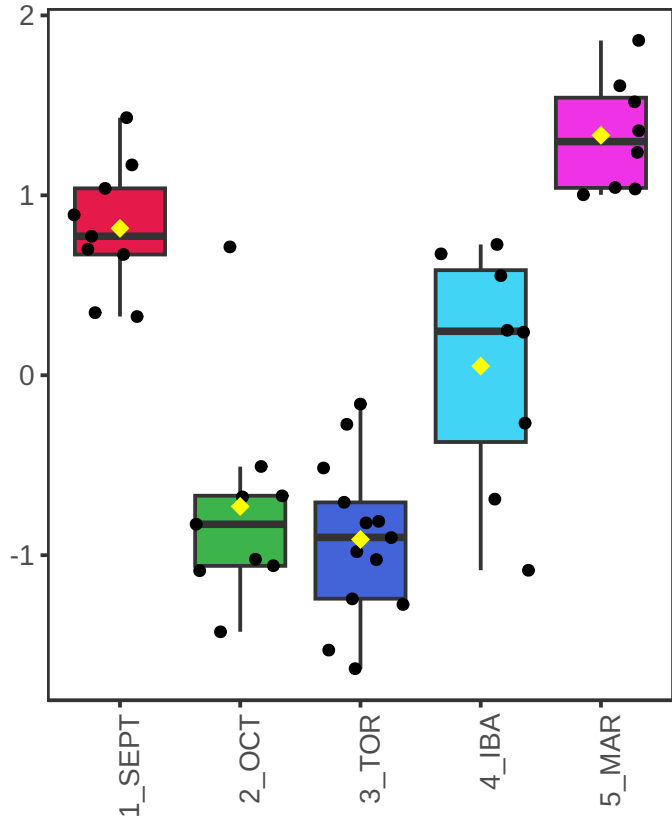


Methionine sulfoxide

Original Conc.

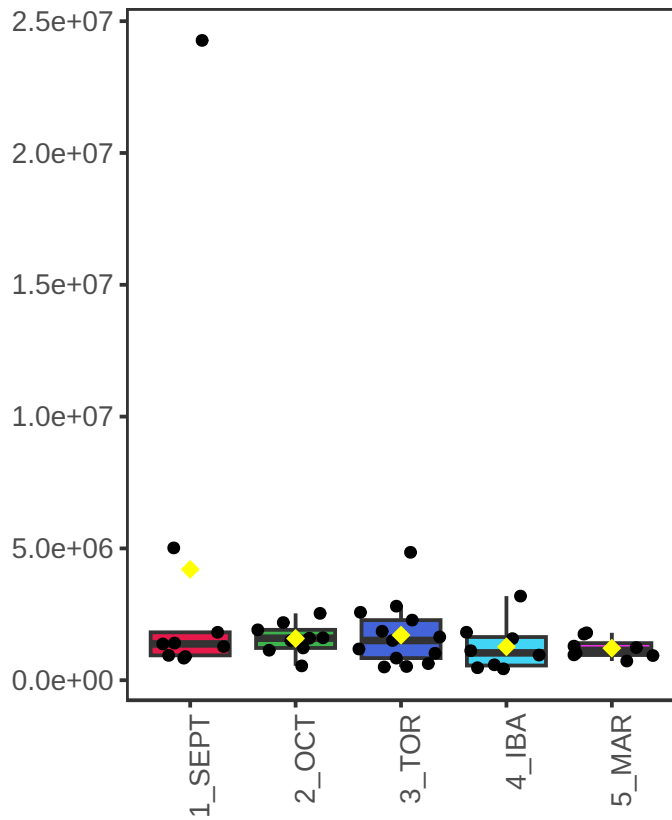


Normalized Conc.

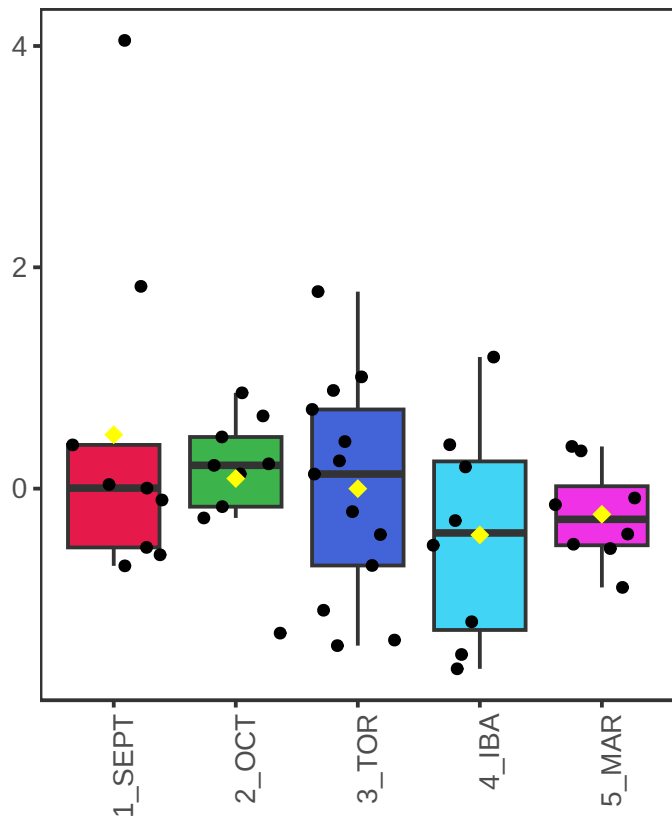


Methylenediurea

Original Conc.

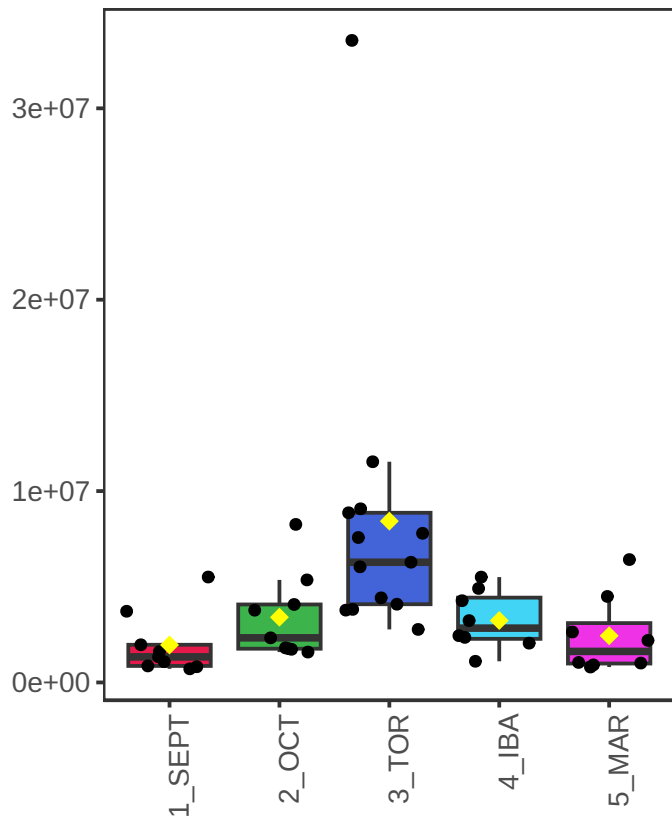


Normalized Conc.

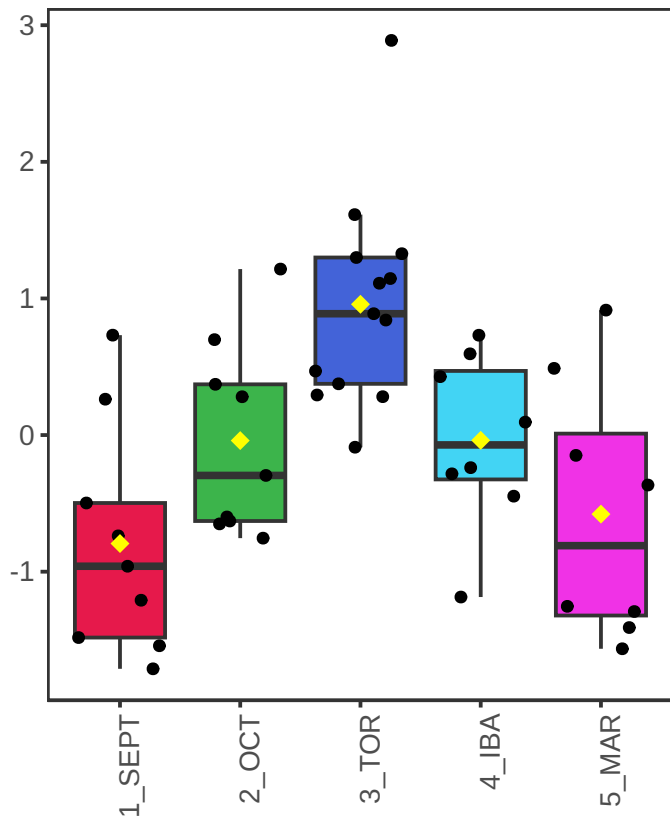


Methylguanidine

Original Conc.

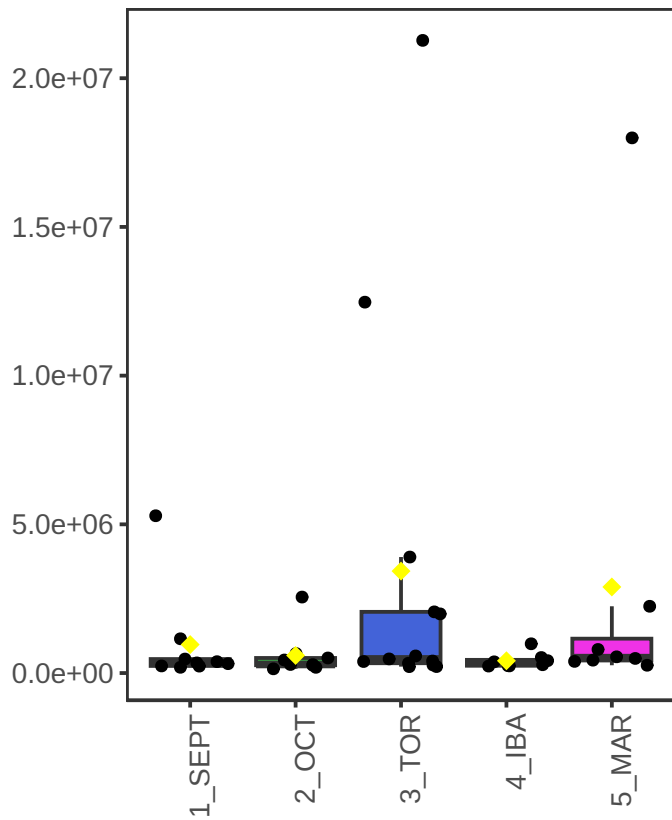


Normalized Conc.

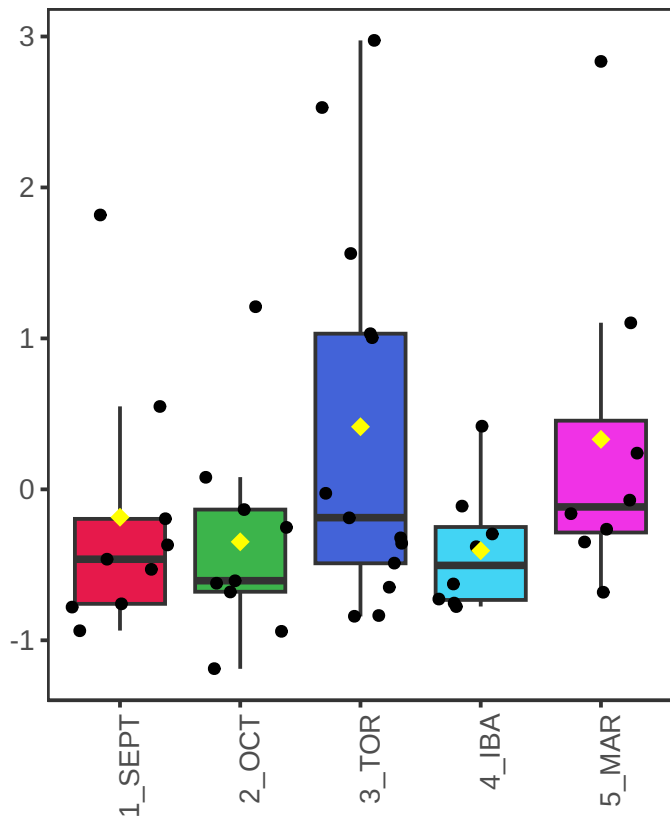


Methylimidazoleacetic acid

Original Conc.

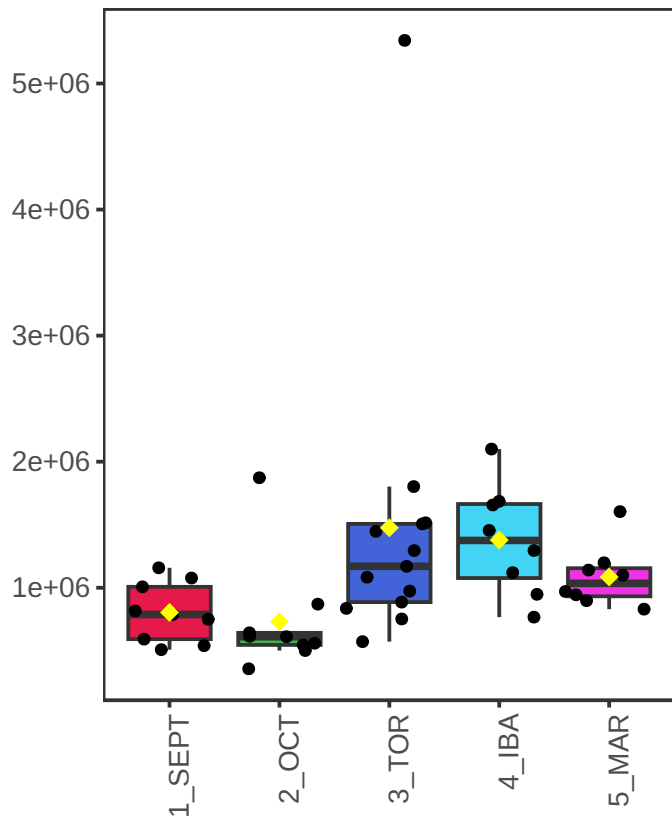


Normalized Conc.

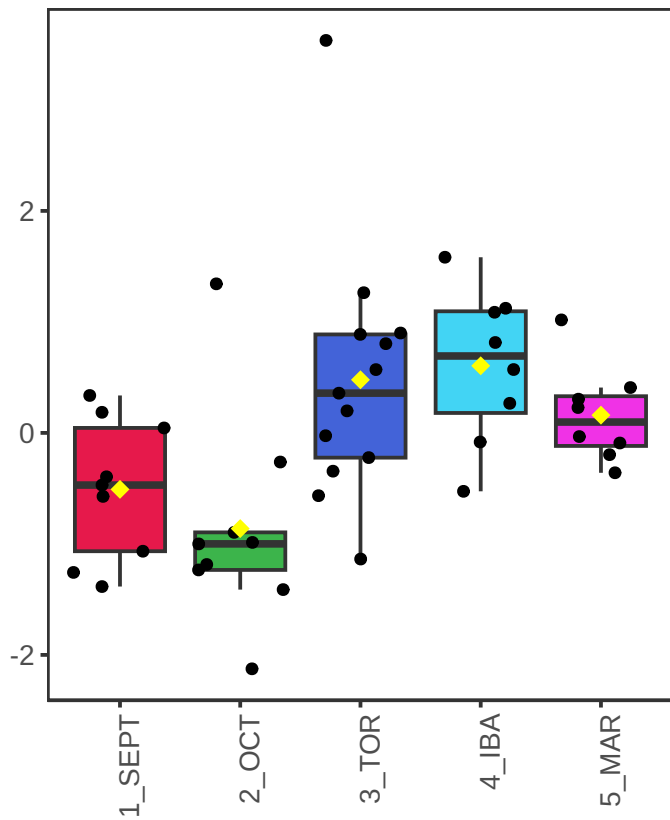


N-(2-Hydroxyethyl)glutamine

Original Conc.

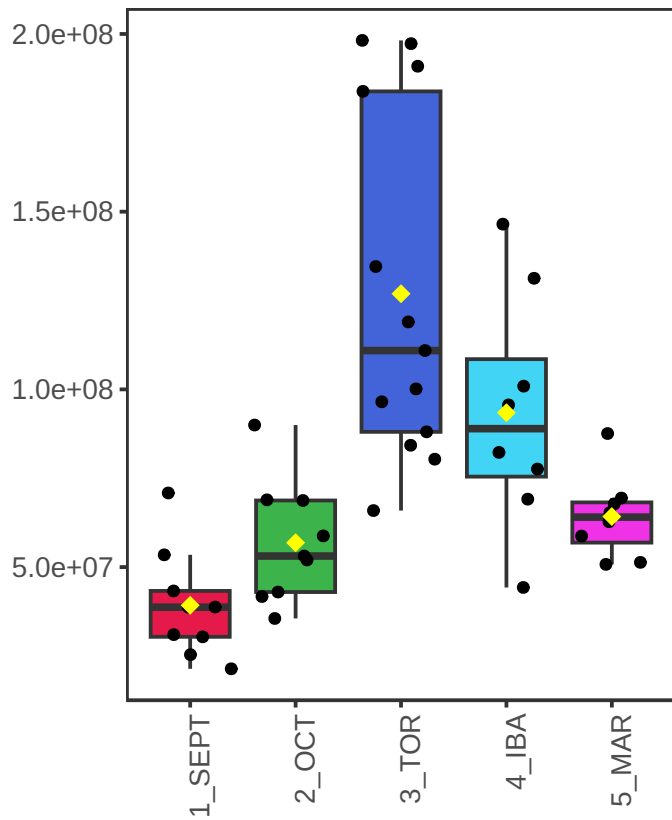


Normalized Conc.

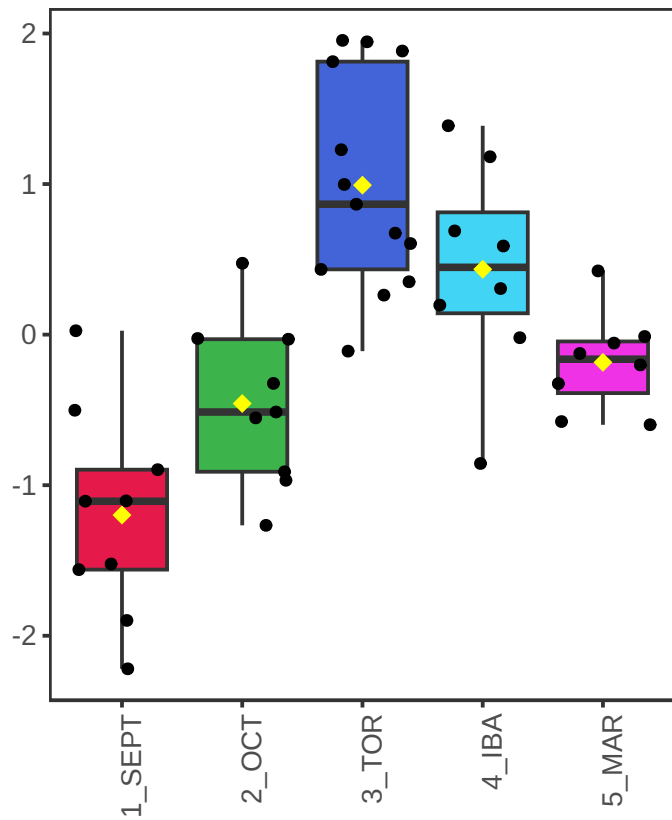


N3,N4-Dimethylarginine

Original Conc.

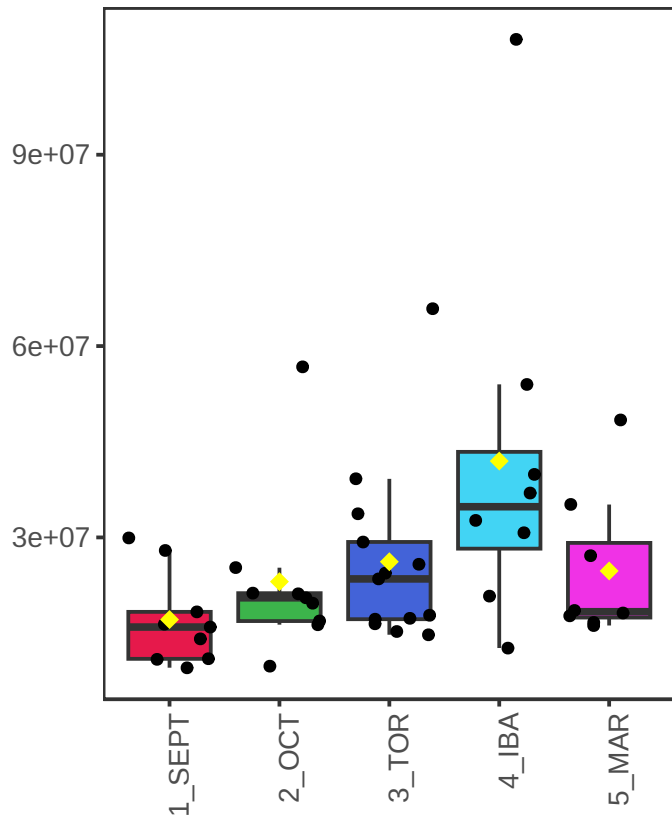


Normalized Conc.

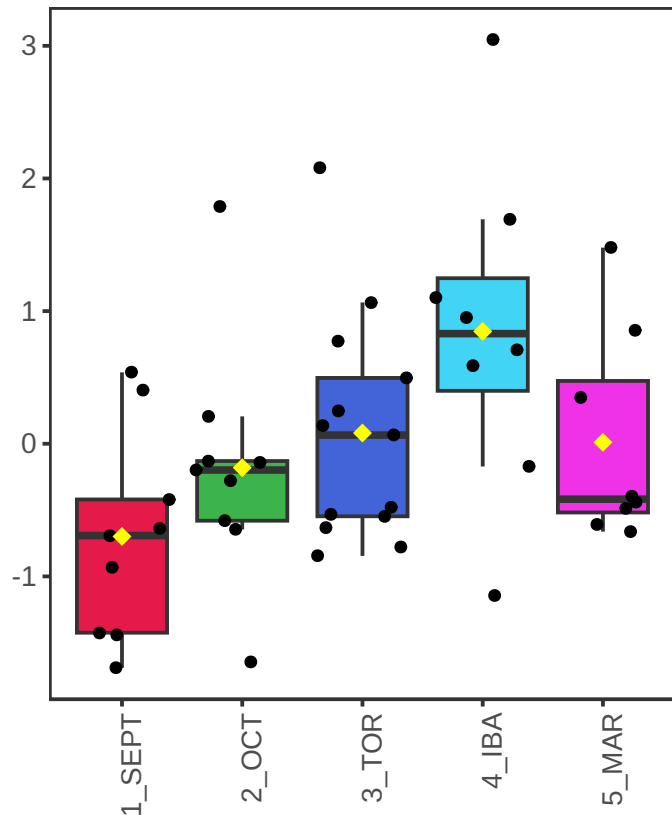


N8-Acetylspemidine

Original Conc.

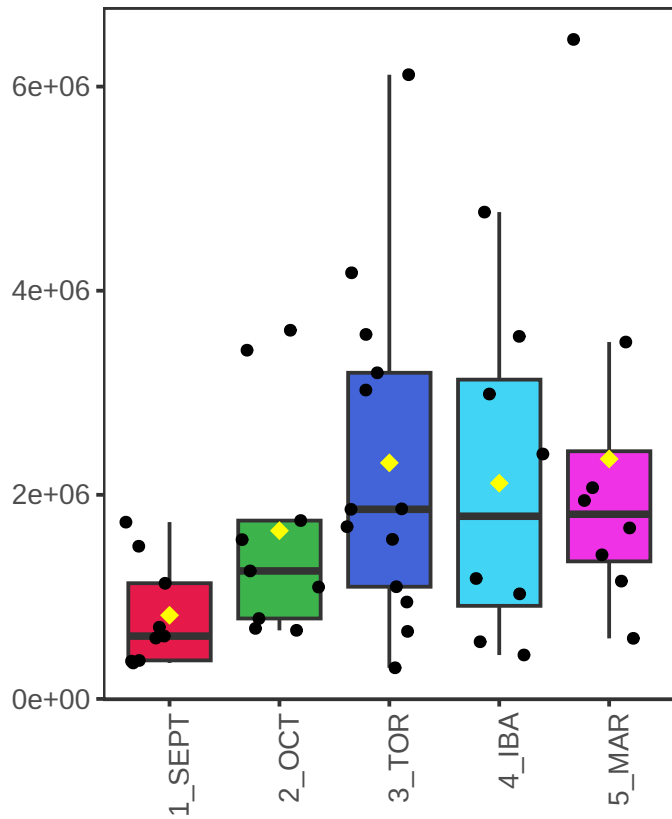


Normalized Conc.

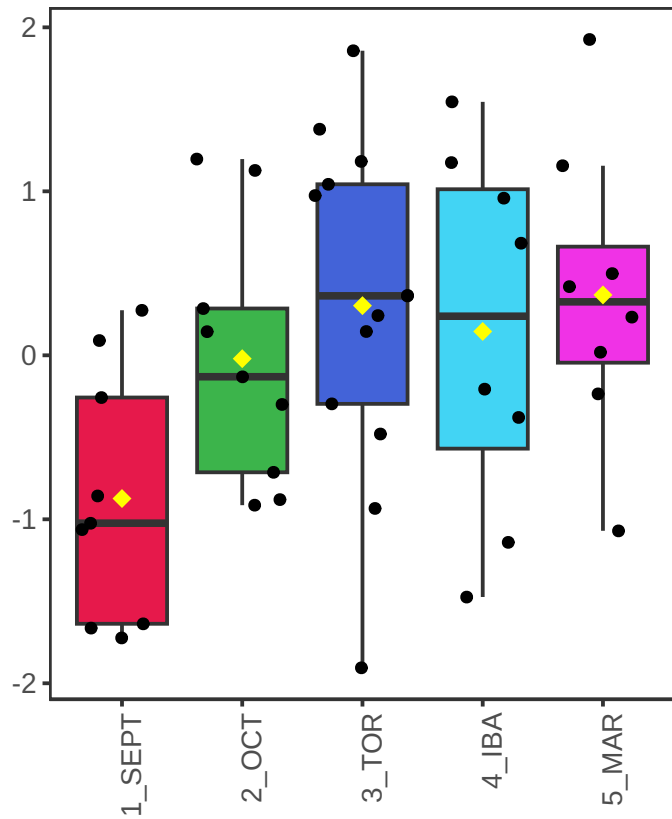


N-(3,4-Dihydroxyphenyl)glutamine

Original Conc.

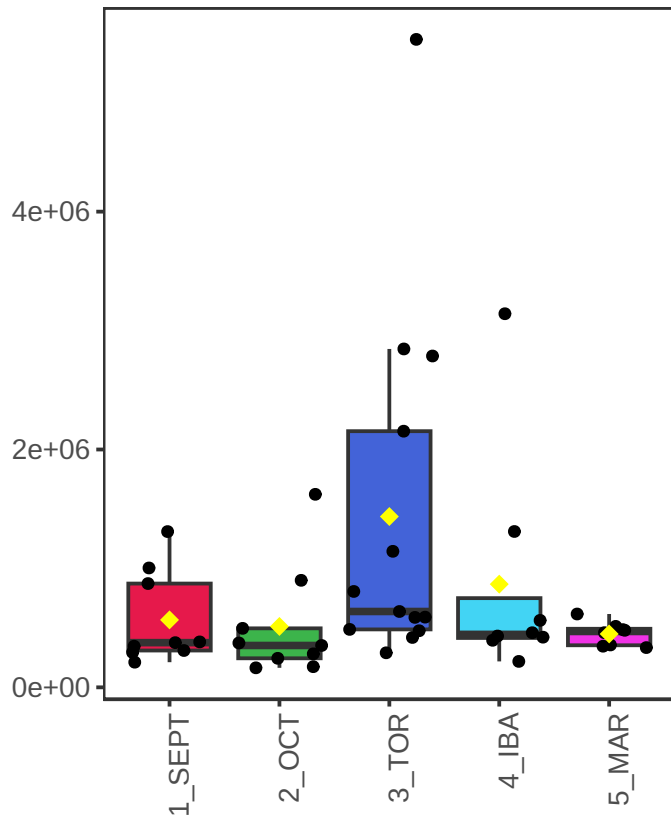


Normalized Conc.

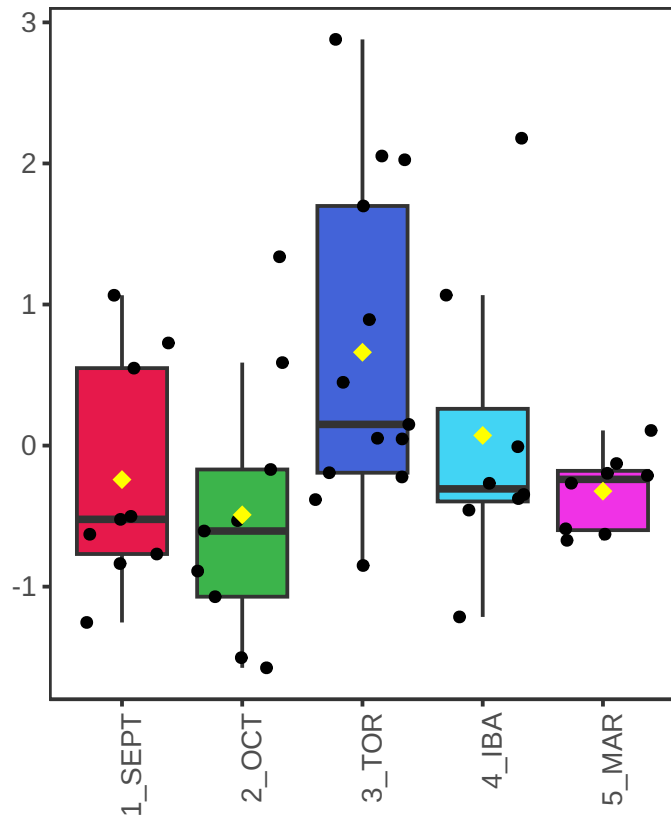


N-Acetylputrescine

Original Conc.

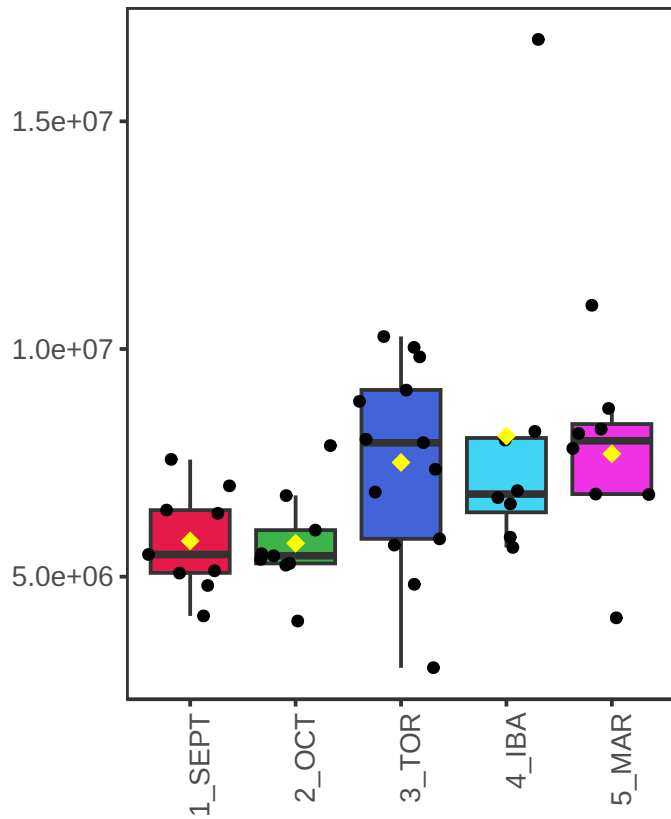


Normalized Conc.

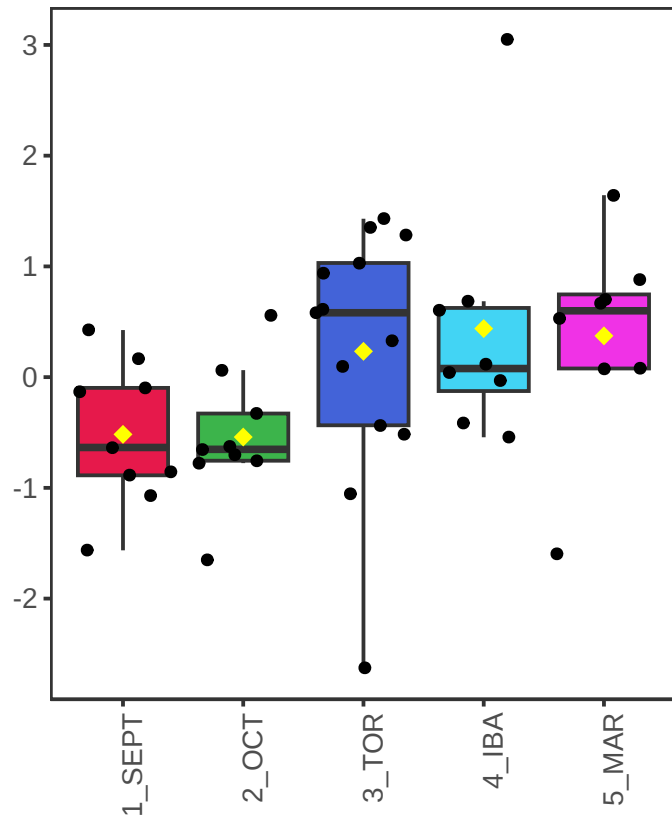


N-Acetyserotonin

Original Conc.

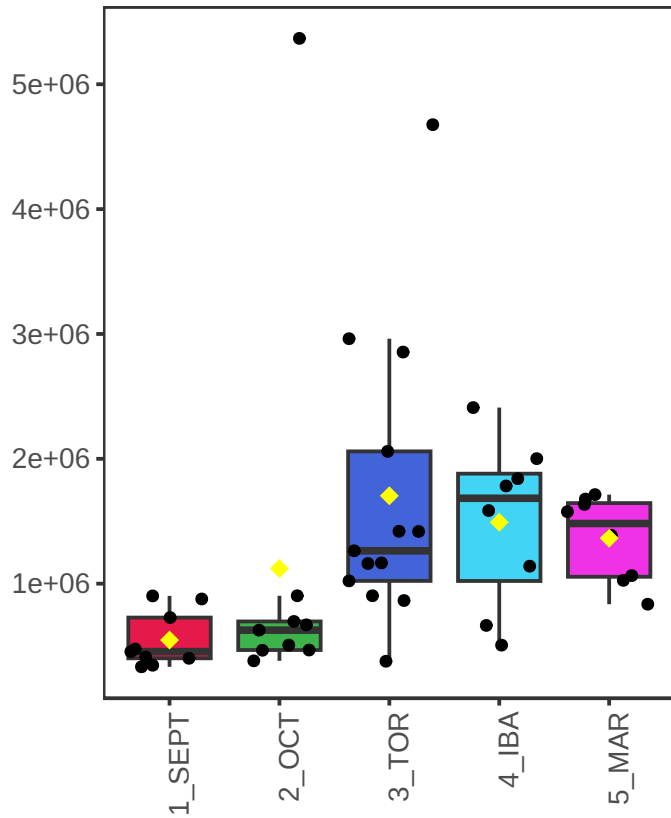


Normalized Conc.

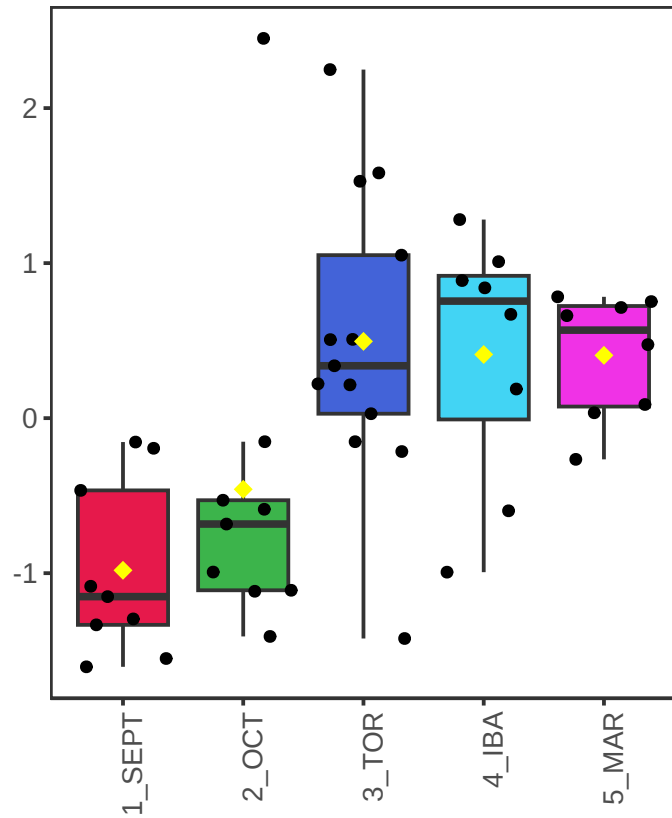


N-Lactoyl ethanolamine

Original Conc.

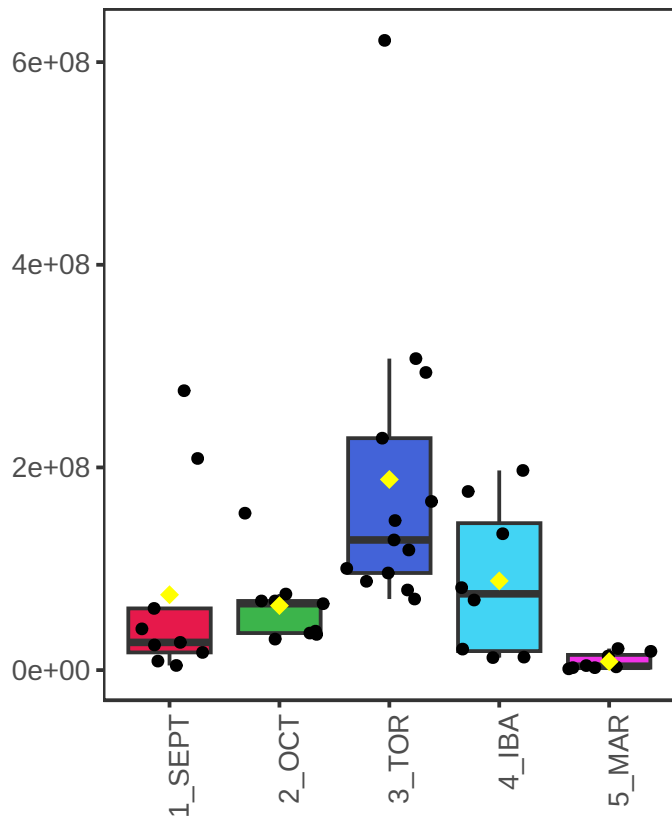


Normalized Conc.

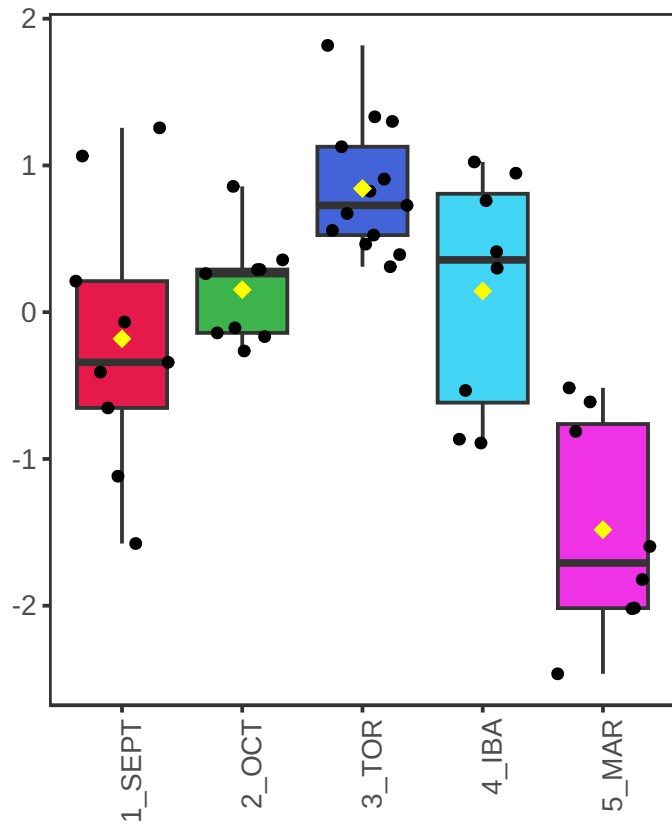


Nicotinamide 1-oxide

Original Conc.

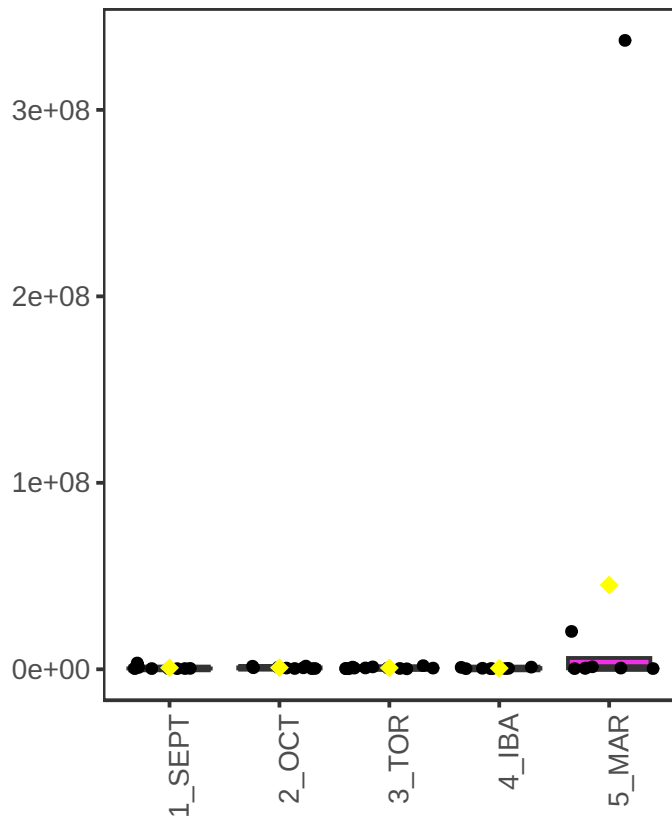


Normalized Conc.

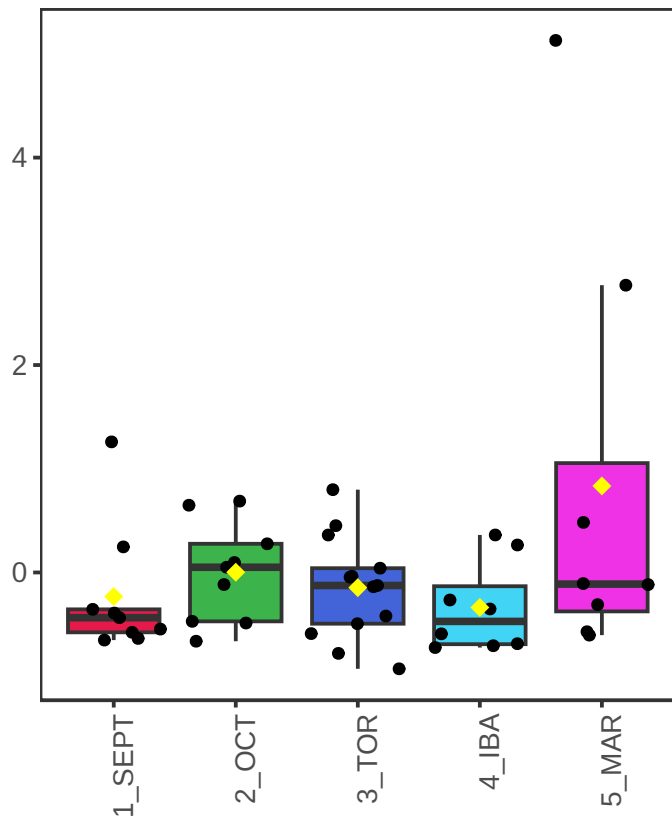


Nicotinic acid

Original Conc.

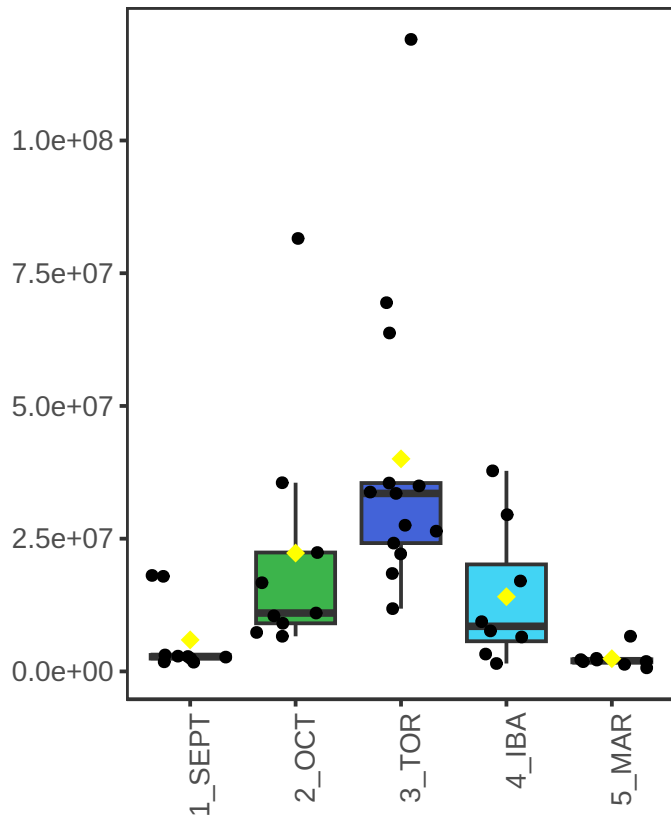


Normalized Conc.

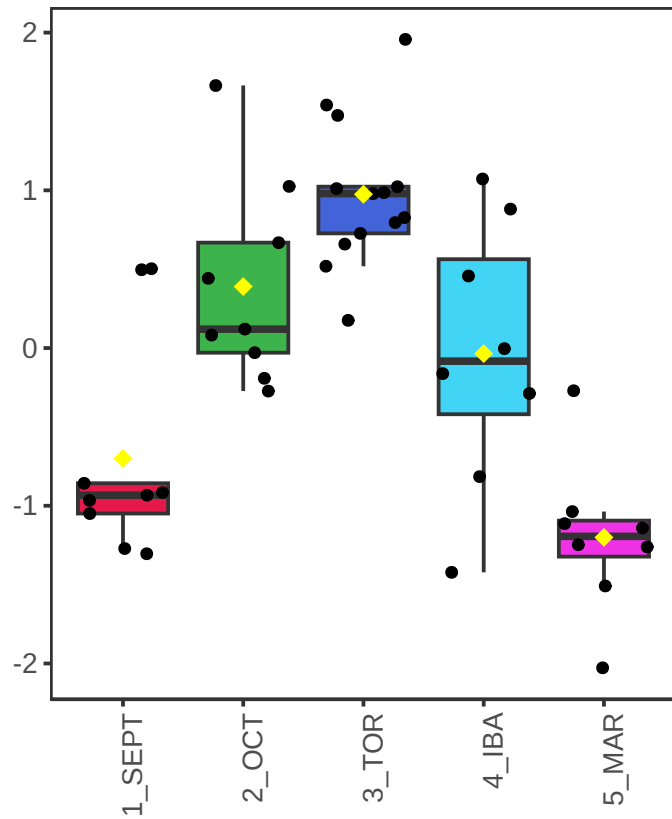


N-Isobutyrylacetamide

Original Conc.

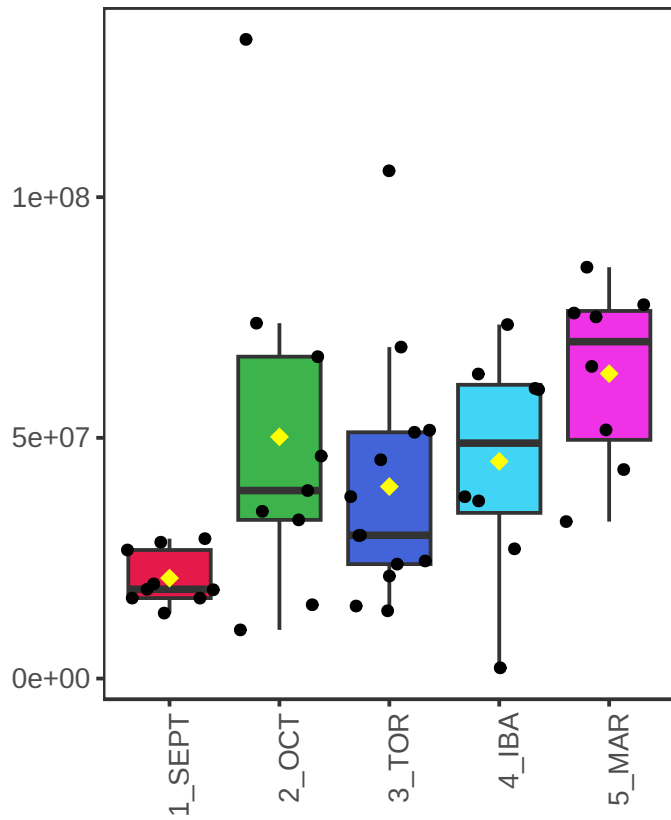


Normalized Conc.

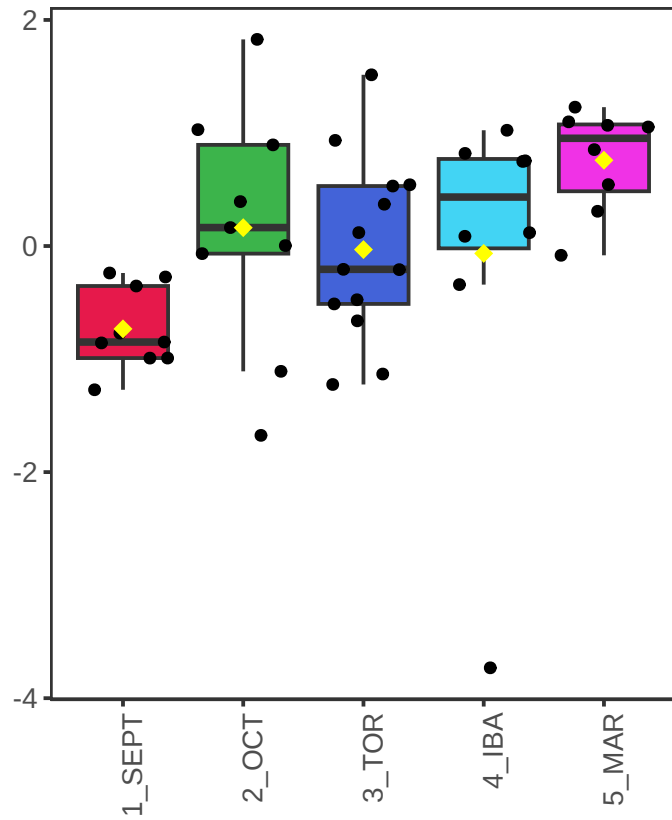


N-Methylhistamine

Original Conc.

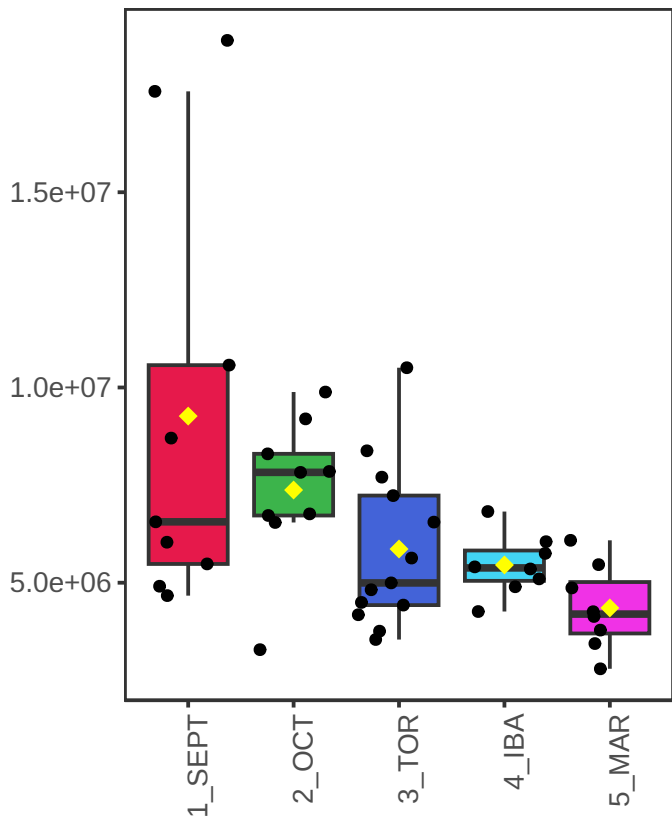


Normalized Conc.

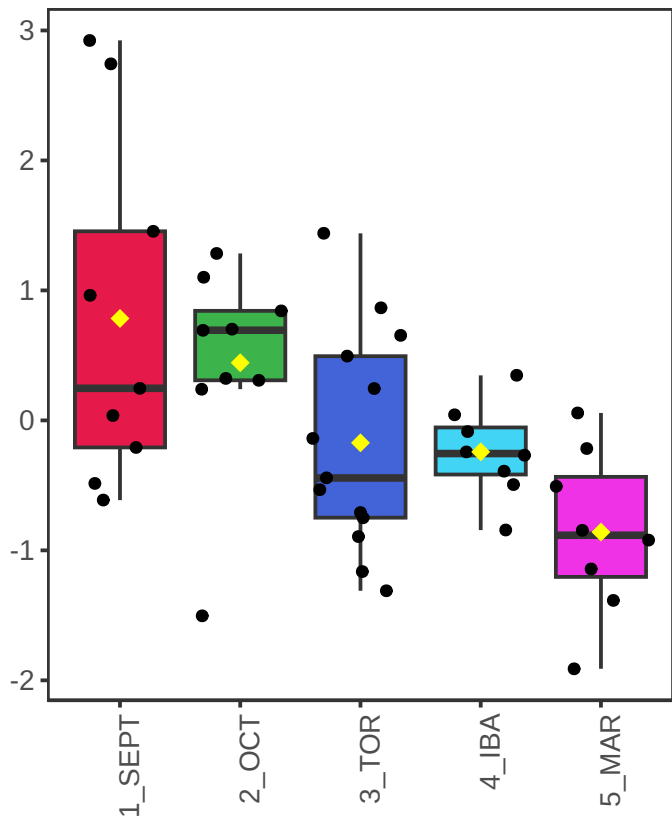


N-Nonanoylglycine

Original Conc.

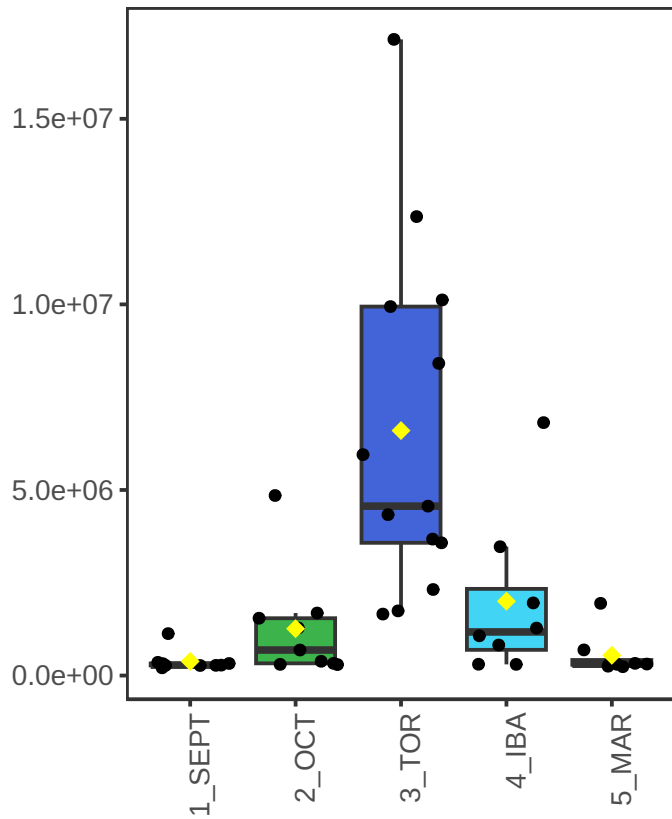


Normalized Conc.

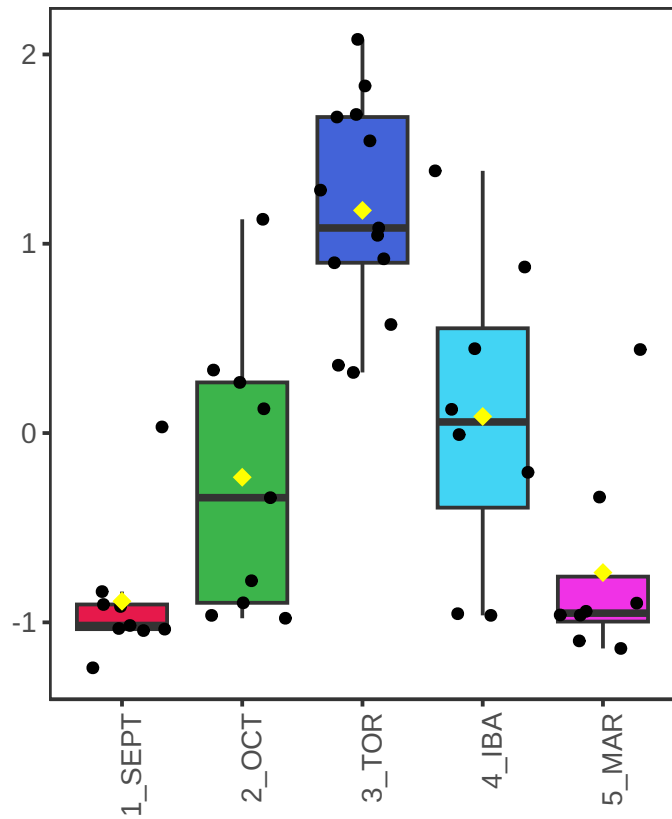


N-Propionylmethionine

Original Conc.

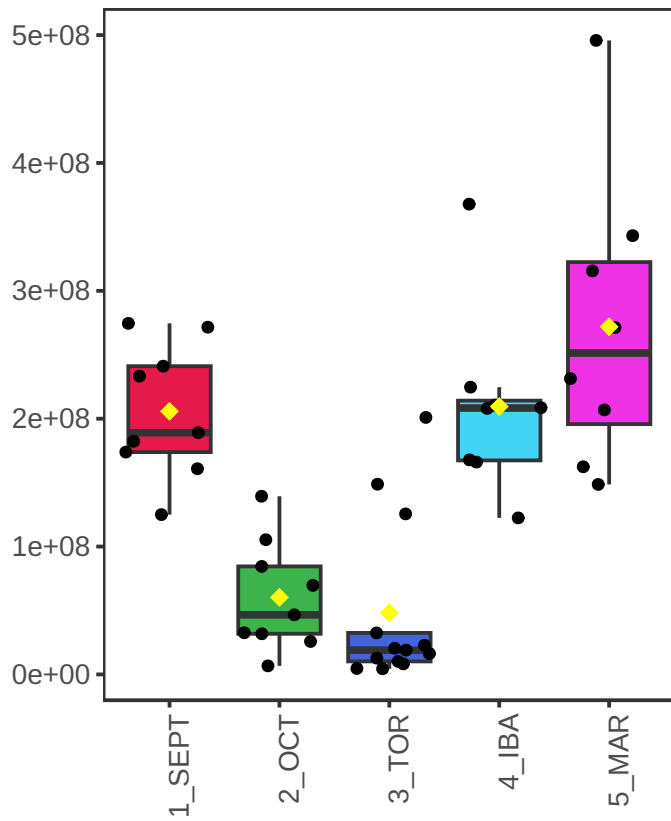


Normalized Conc.

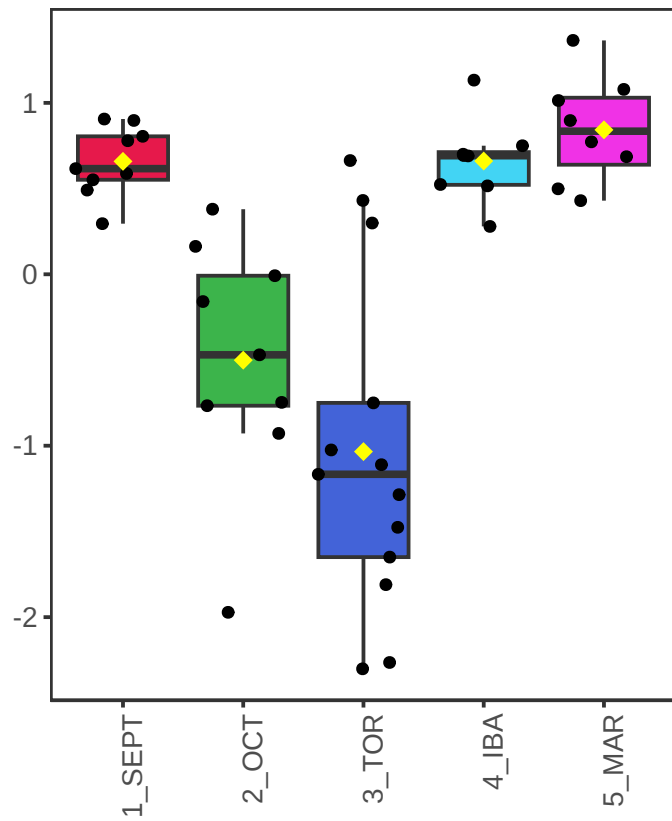


N-Succinyl-L,L-2,6-diaminopimelate

Original Conc.

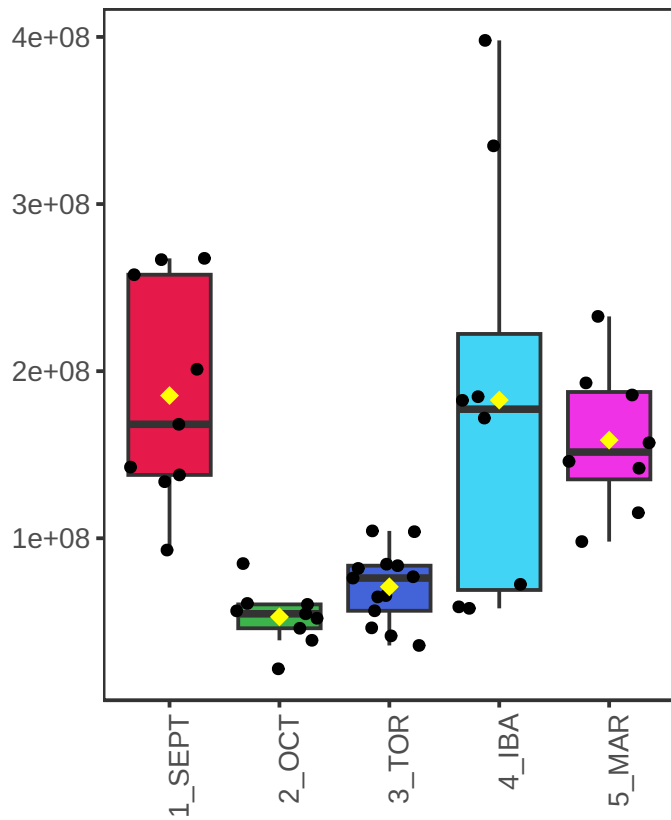


Normalized Conc.

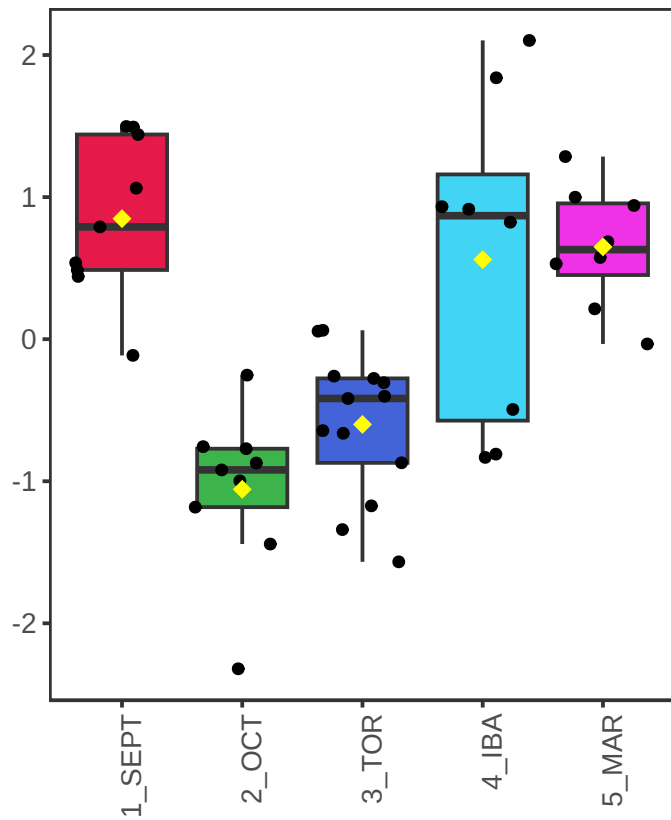


N-(tert-Butoxycarbonyl)leucine

Original Conc.

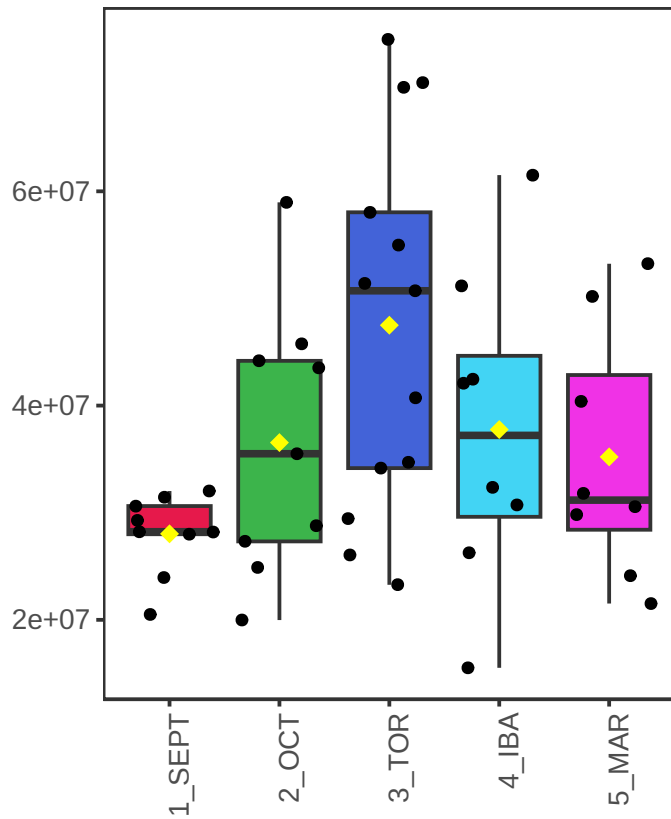


Normalized Conc.

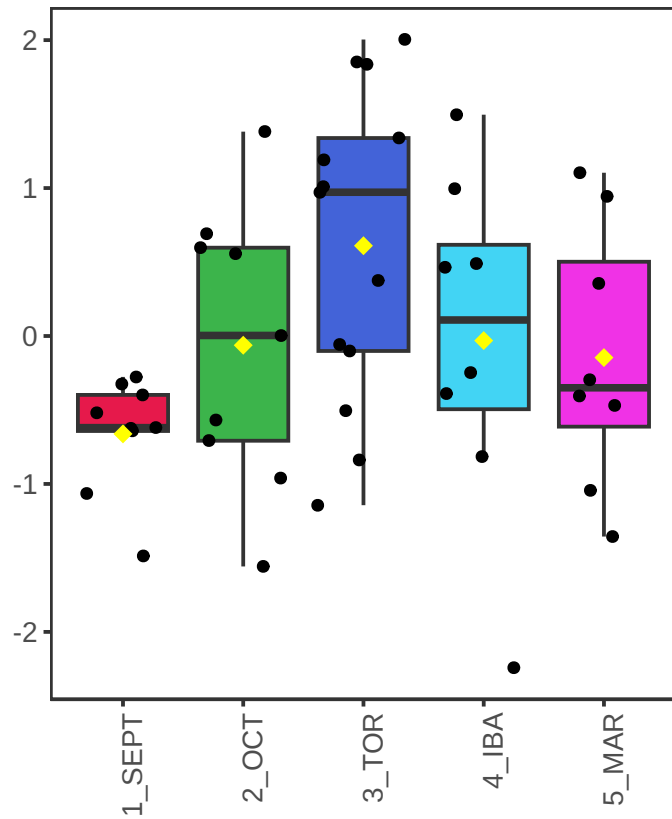


N6,N6,N6-Trimethyllysine

Original Conc.

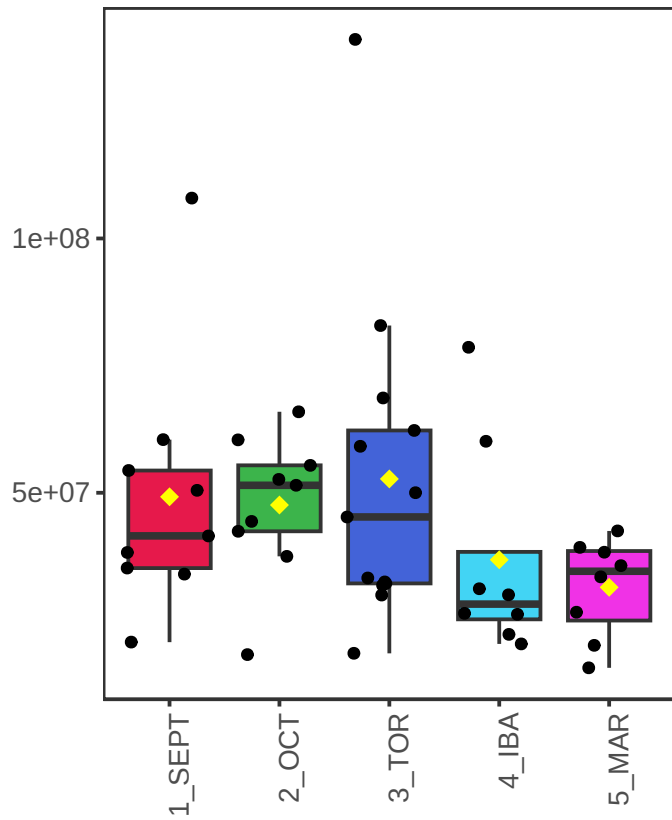


Normalized Conc.

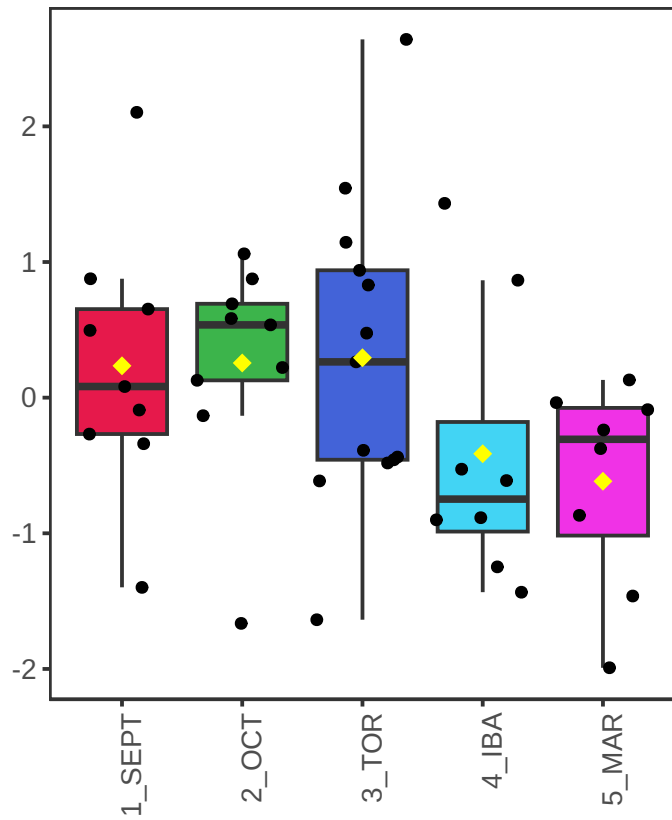


N-Undecanoylglycine

Original Conc.

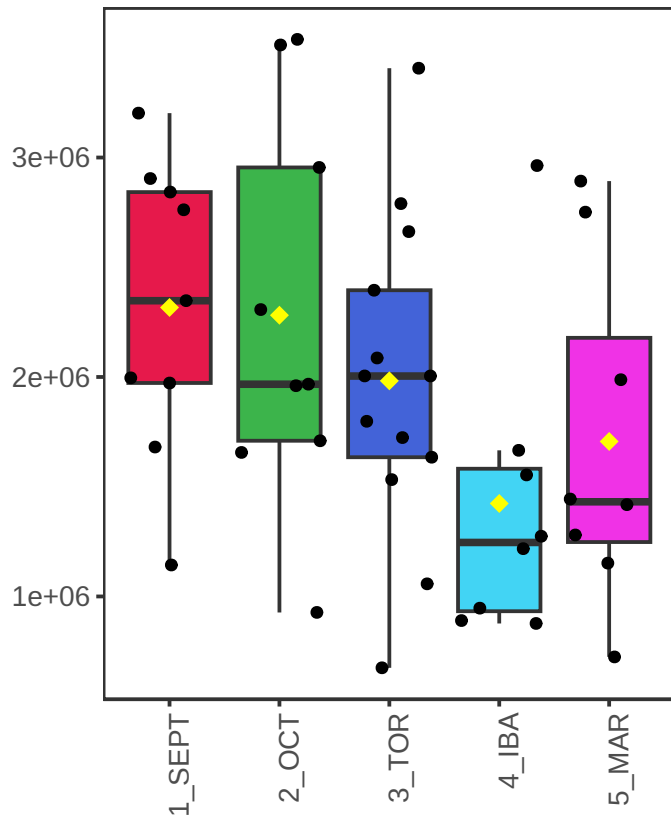


Normalized Conc.

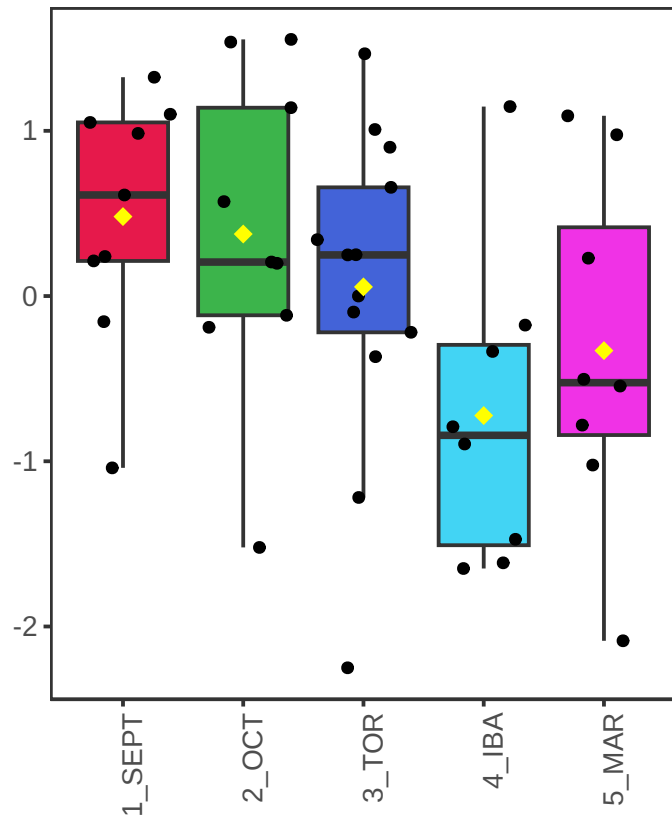


Octanedioic acid

Original Conc.

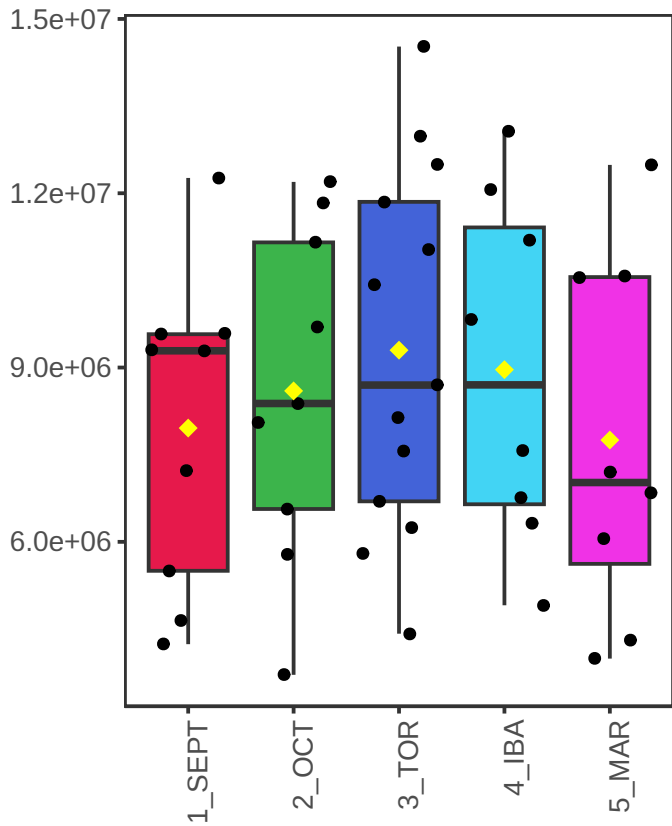


Normalized Conc.

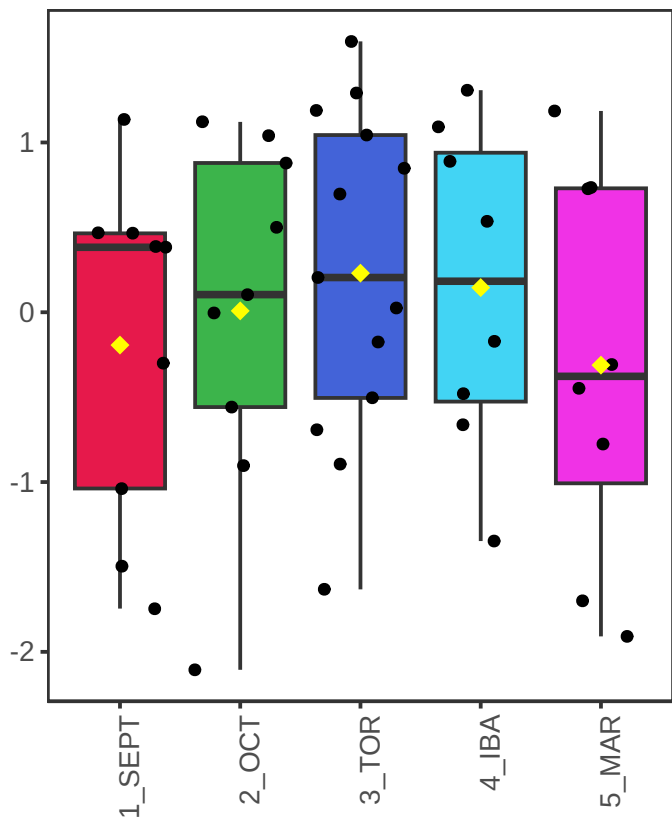


O-ureido-(DL)-serine

Original Conc.

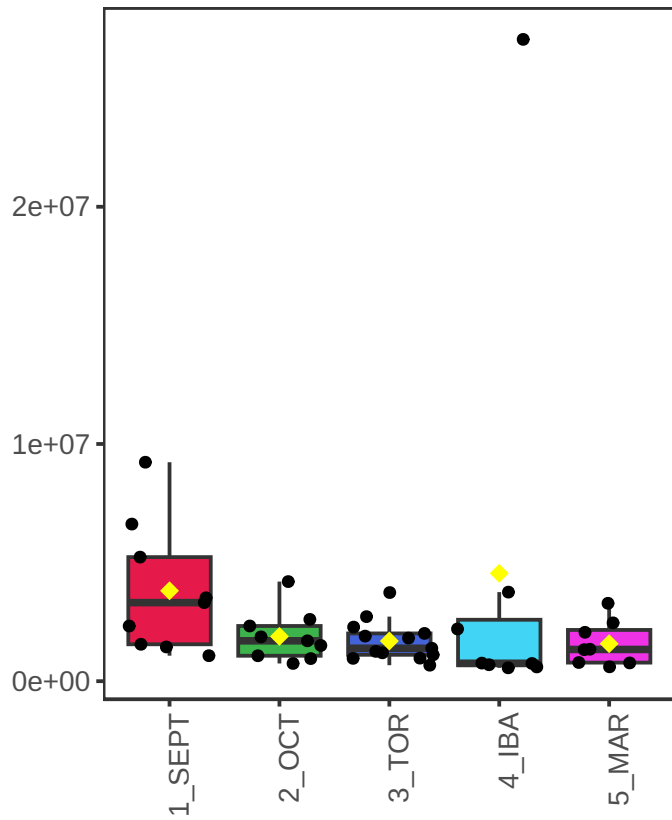


Normalized Conc.

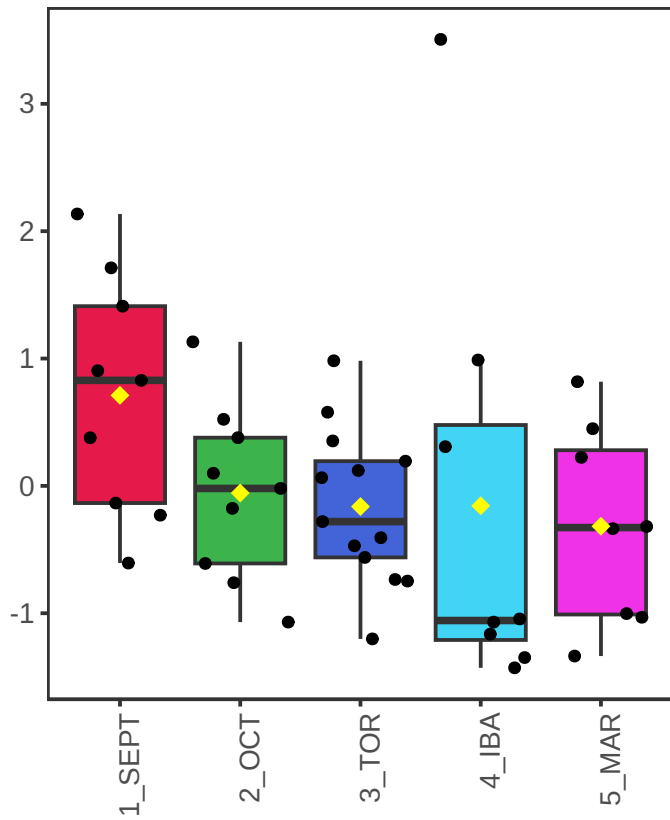


Panthenol

Original Conc.

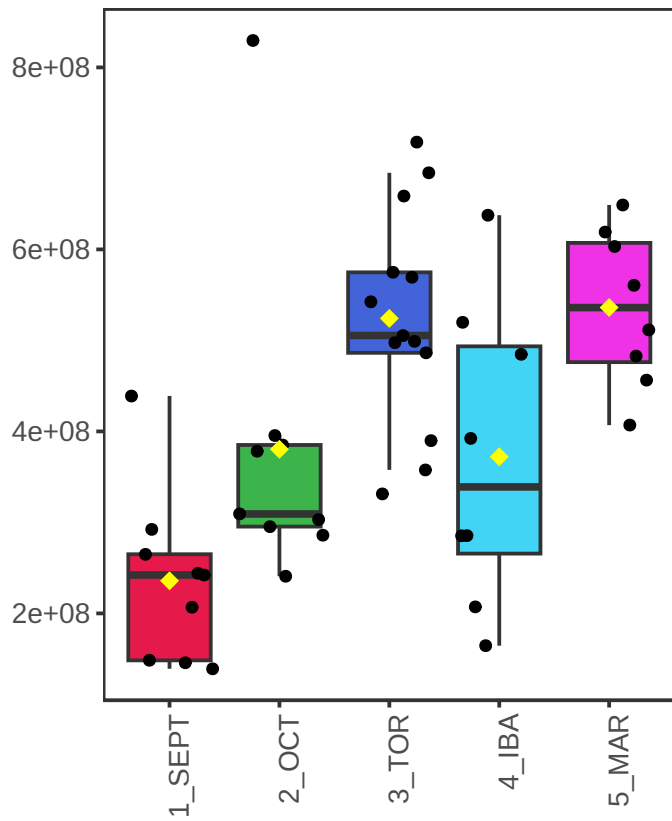


Normalized Conc.

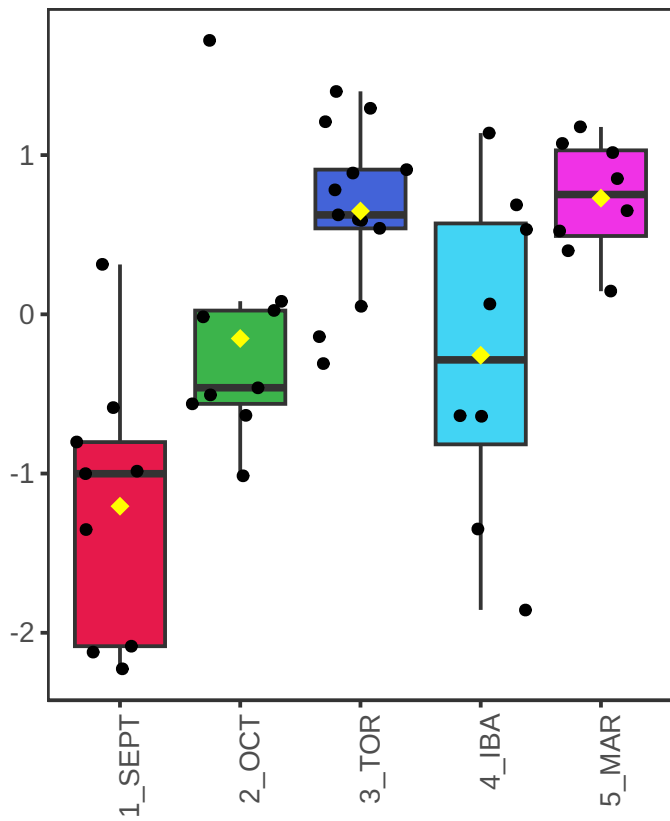


Pantothenic acid

Original Conc.

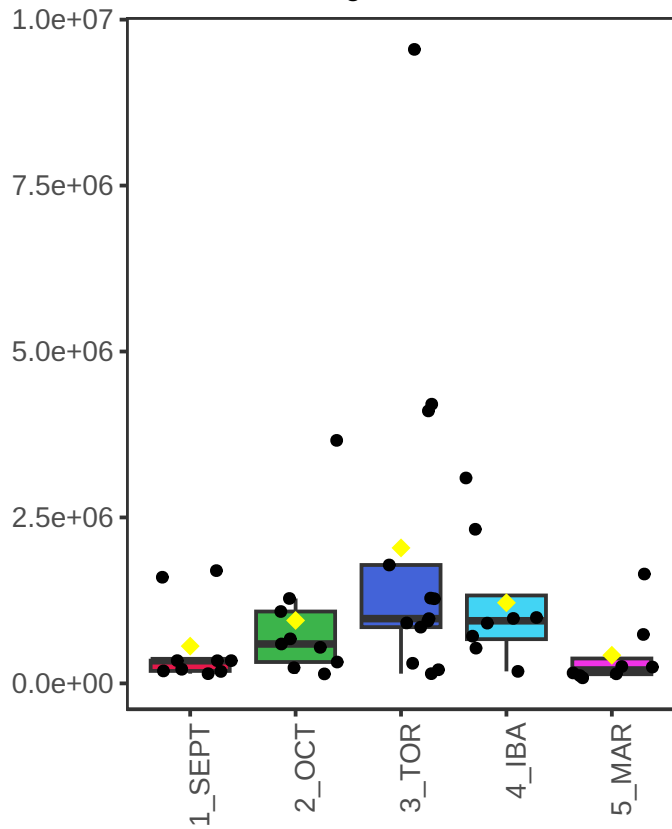


Normalized Conc.

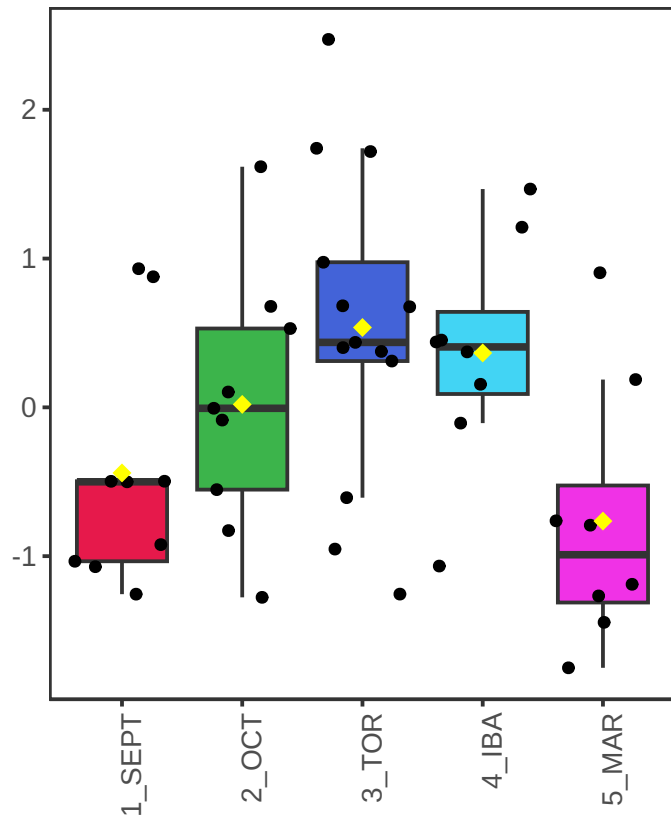


Pentahomomethionine

Original Conc.

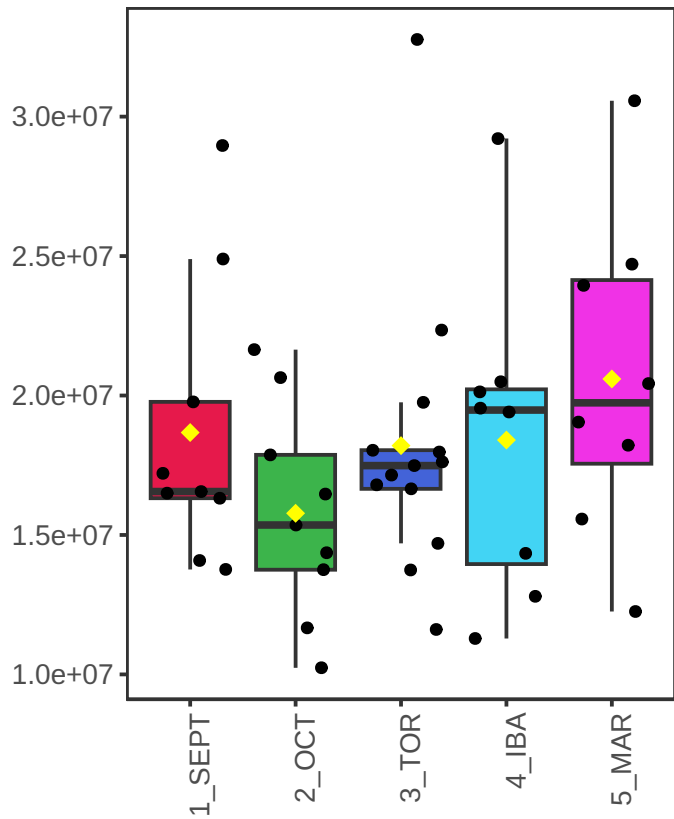


Normalized Conc.

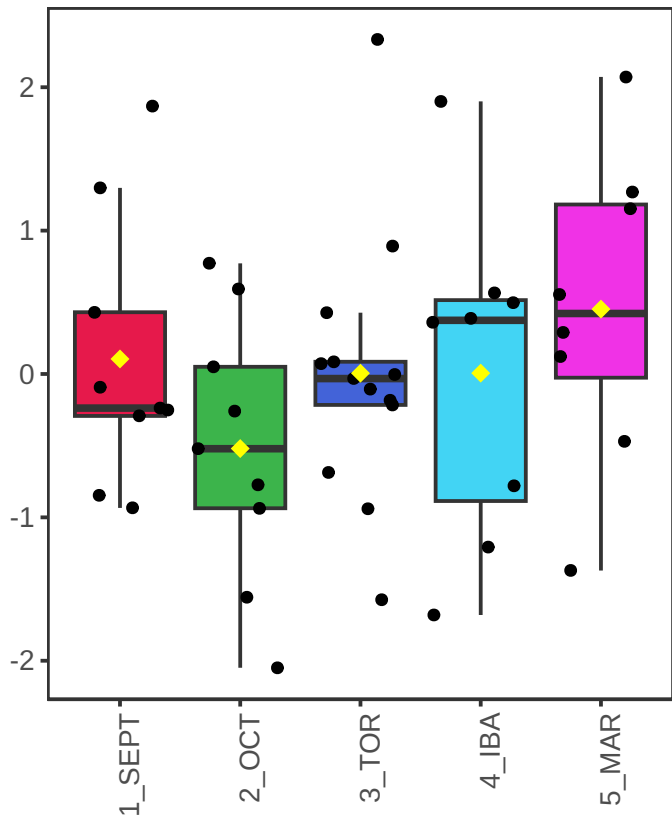


Phenylalanine

Original Conc.

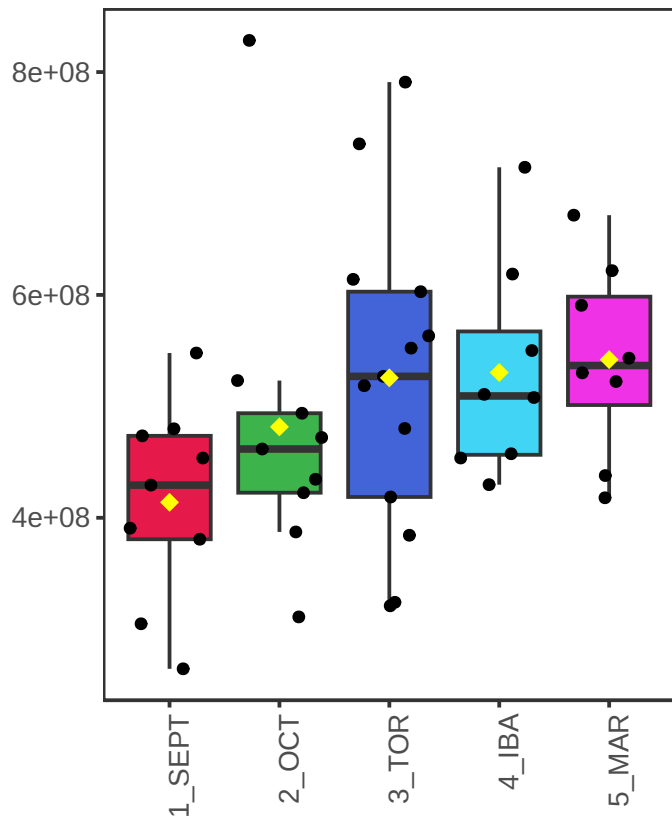


Normalized Conc.

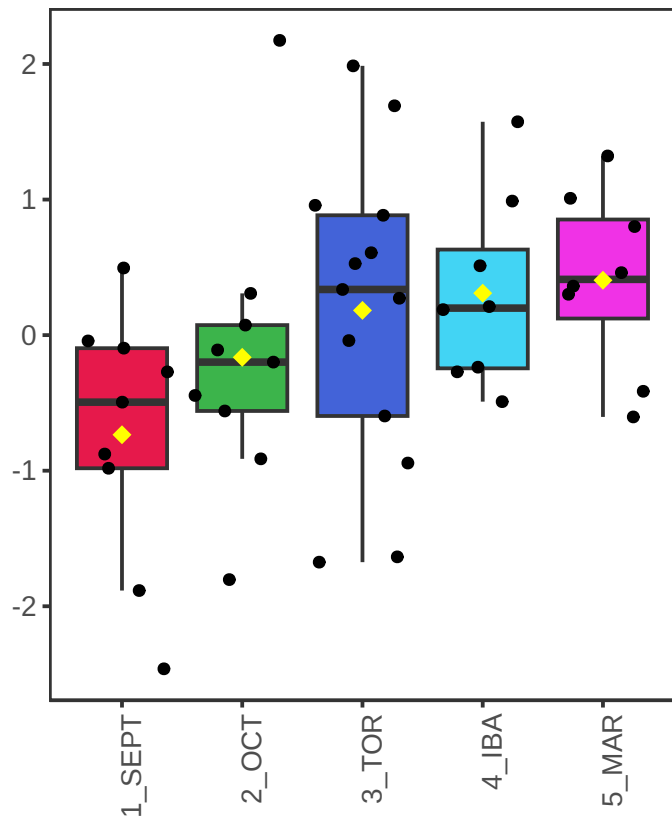


Phosphoethanolamine

Original Conc.

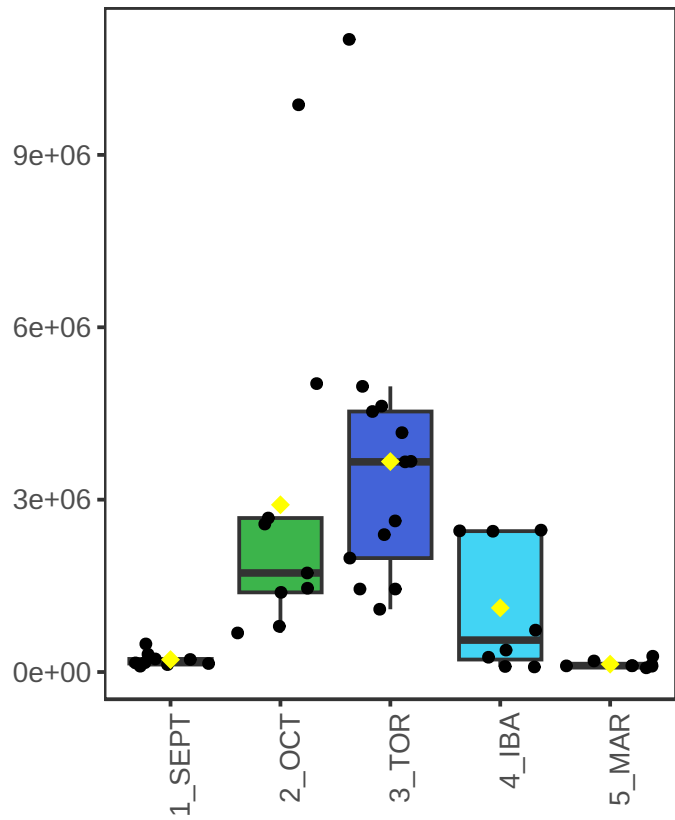


Normalized Conc.

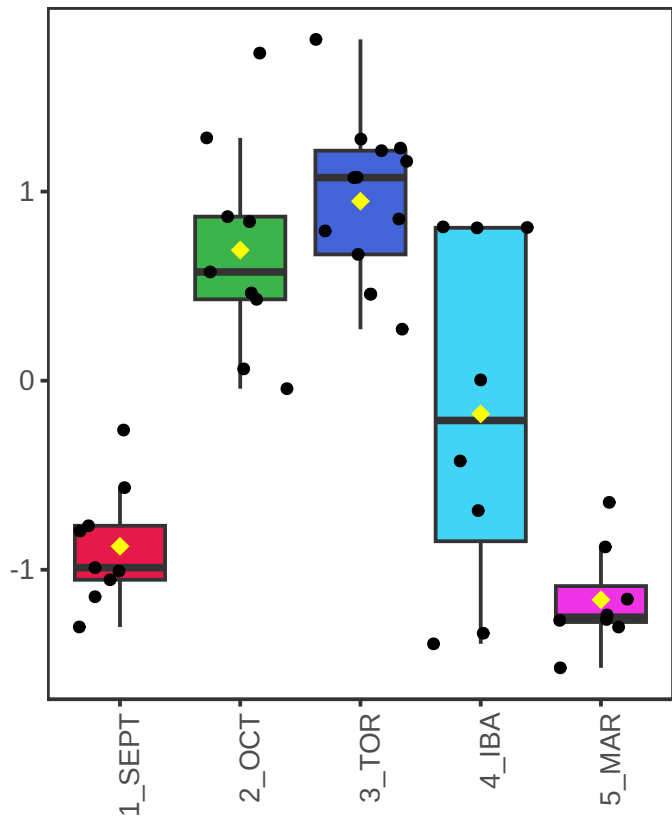


Picolinic acid N-oxide

Original Conc.

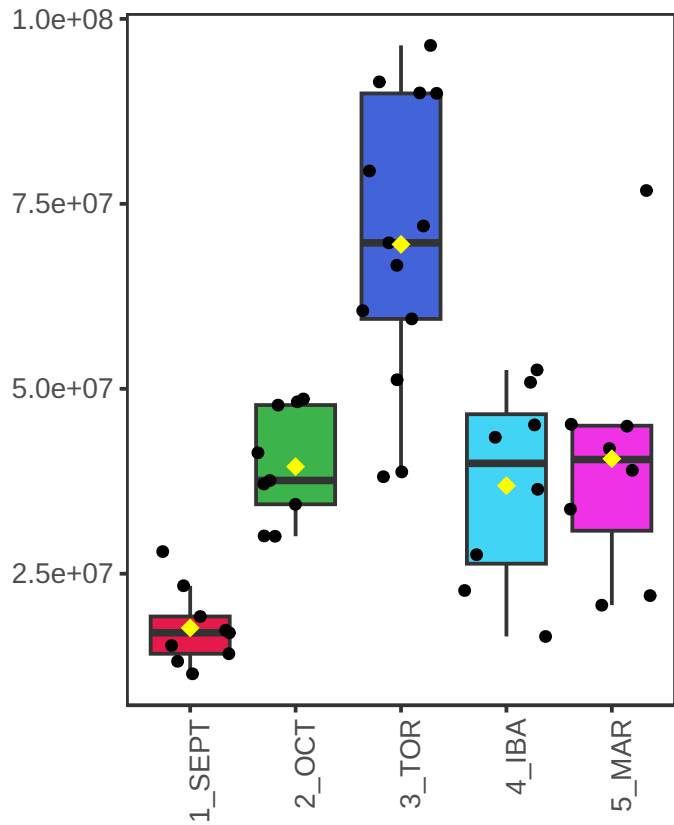


Normalized Conc.

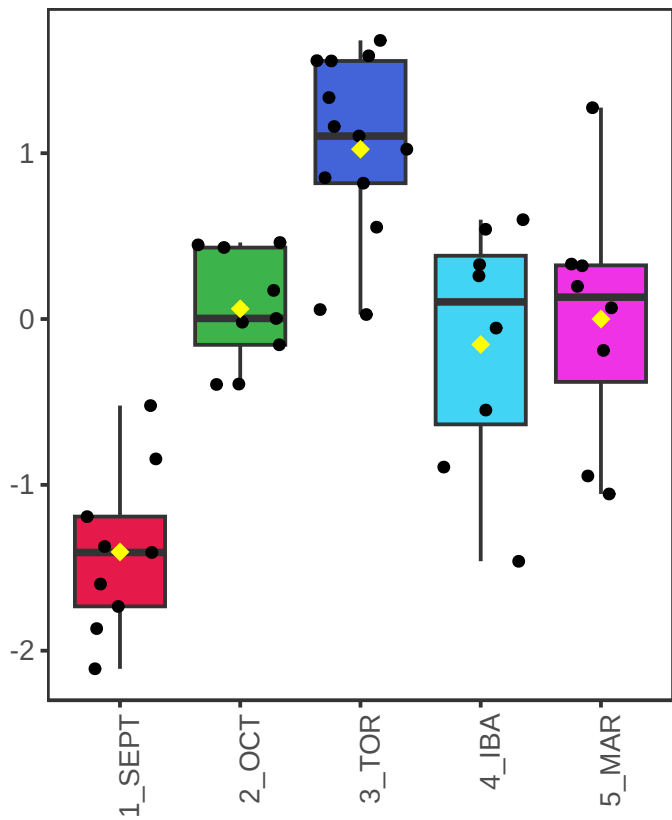


Pipecolinic acid

Original Conc.

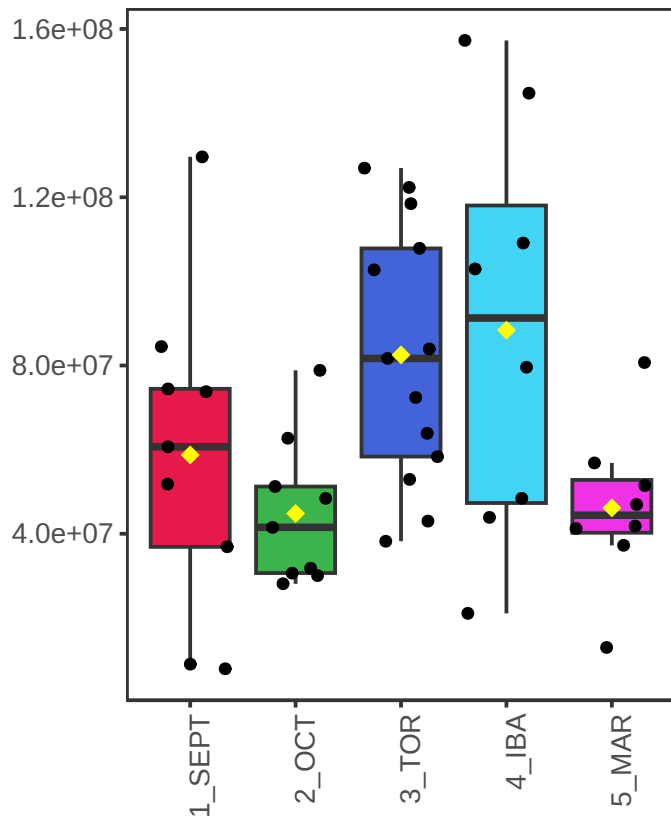


Normalized Conc.

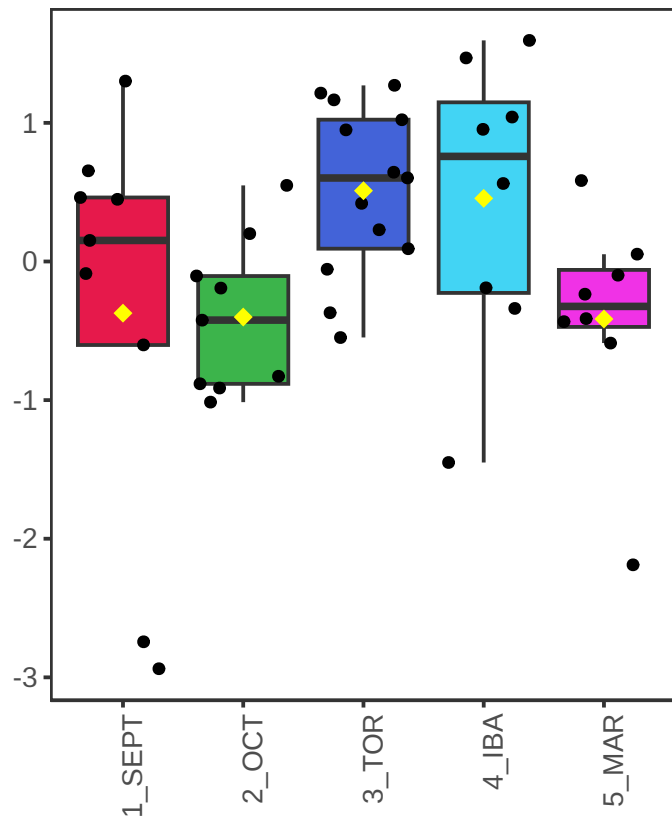


Platelet-activating factor

Original Conc.

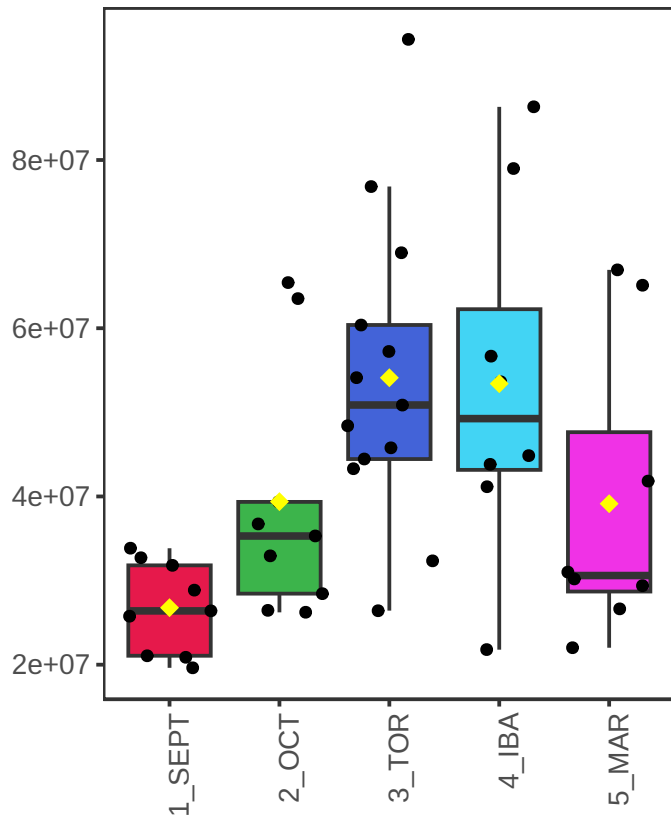


Normalized Conc.

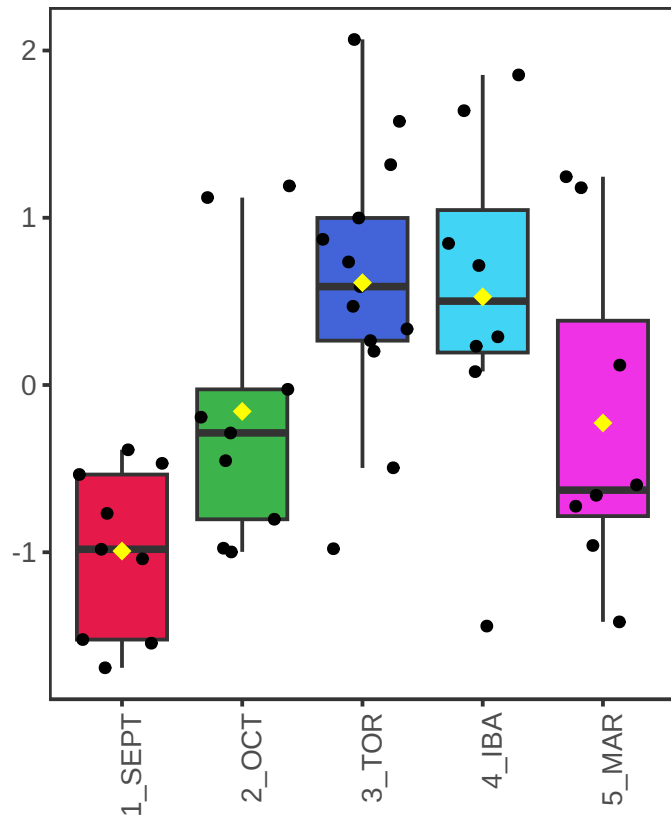


Pro-Leu-Lys

Original Conc.

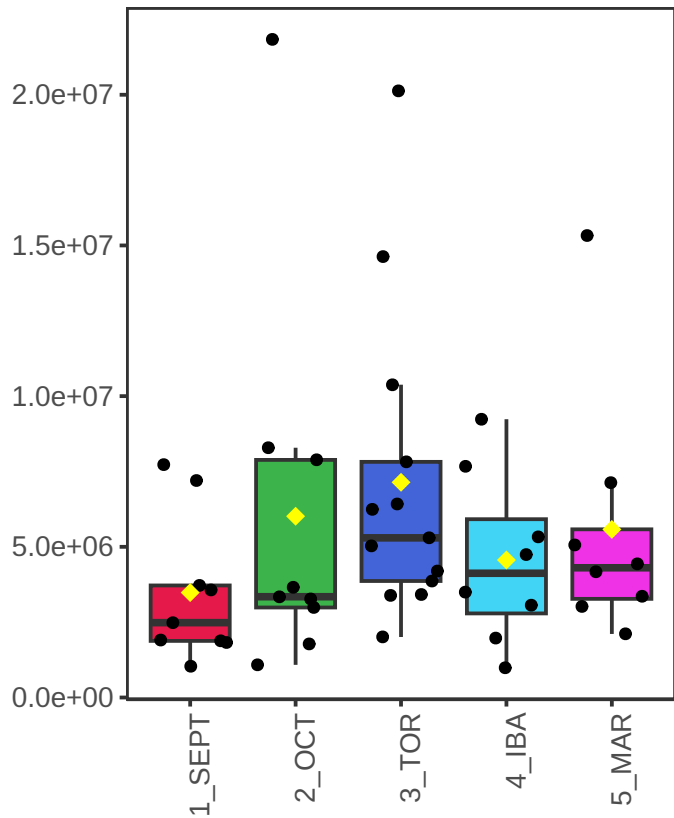


Normalized Conc.

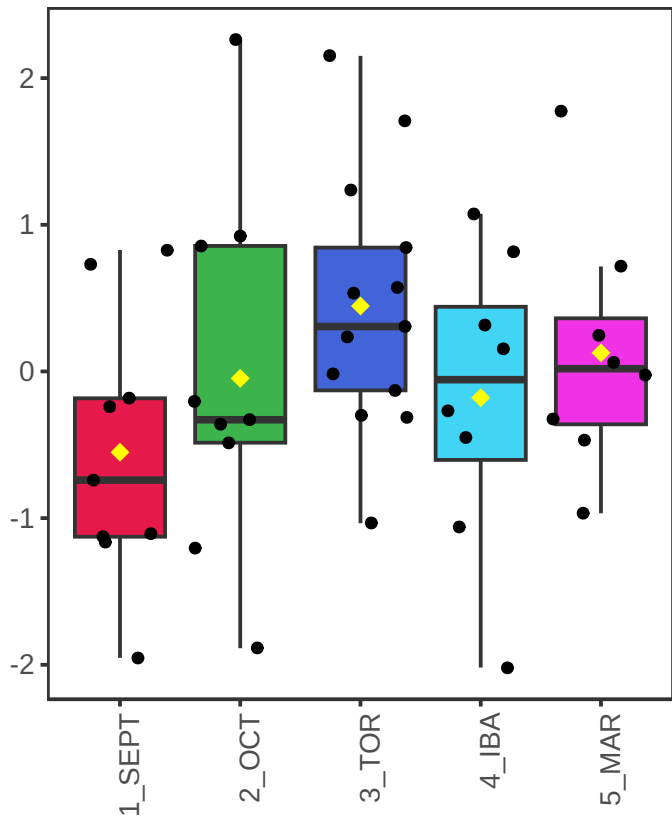


Prolinamide

Original Conc.

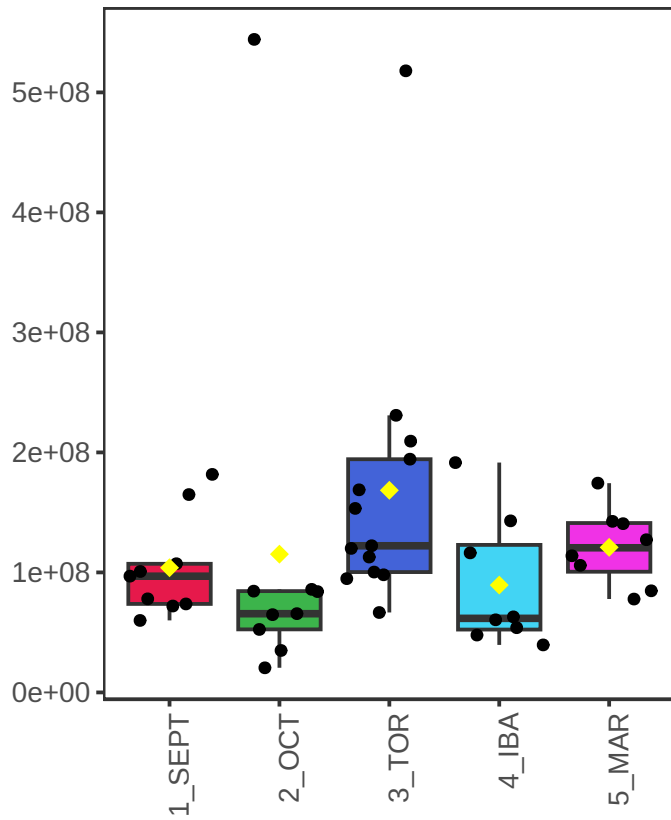


Normalized Conc.

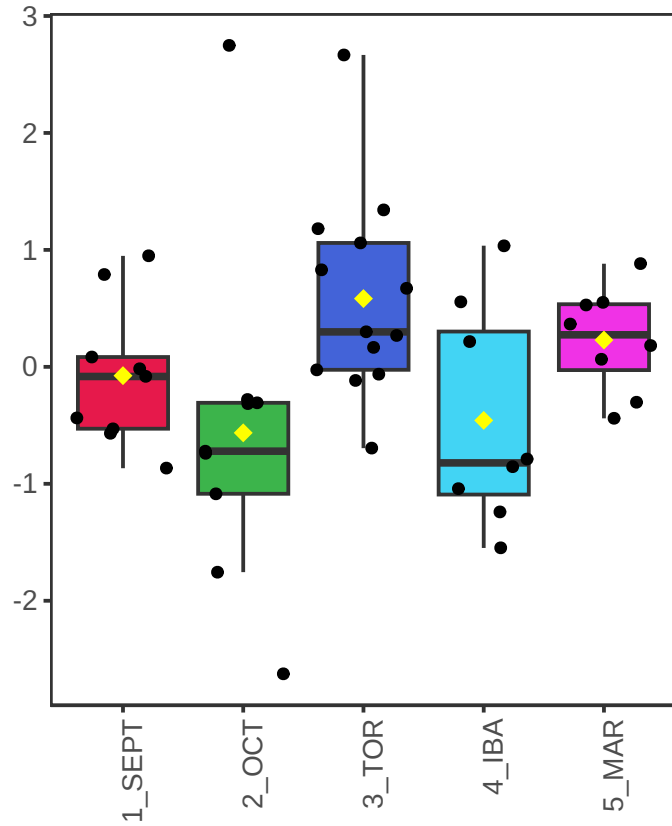


Proline

Original Conc.

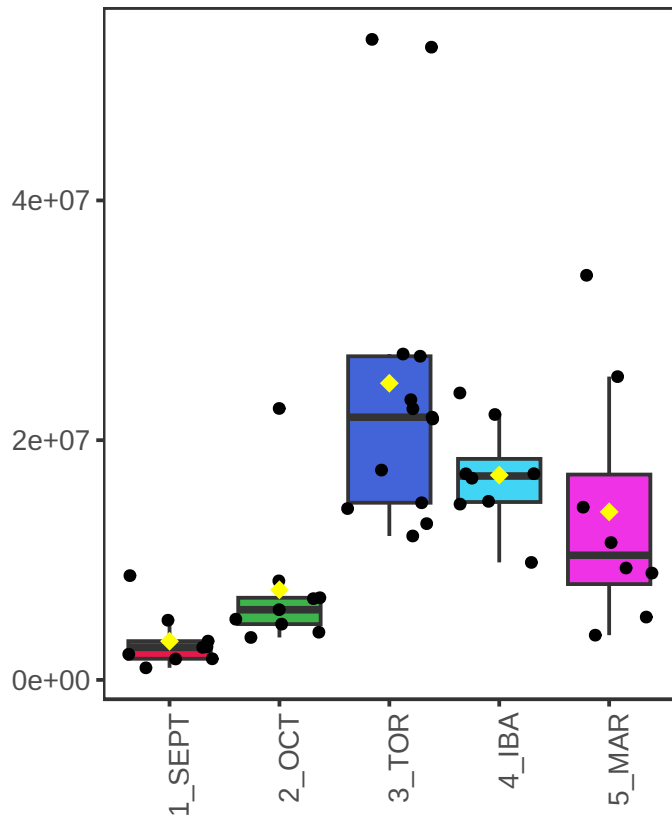


Normalized Conc.

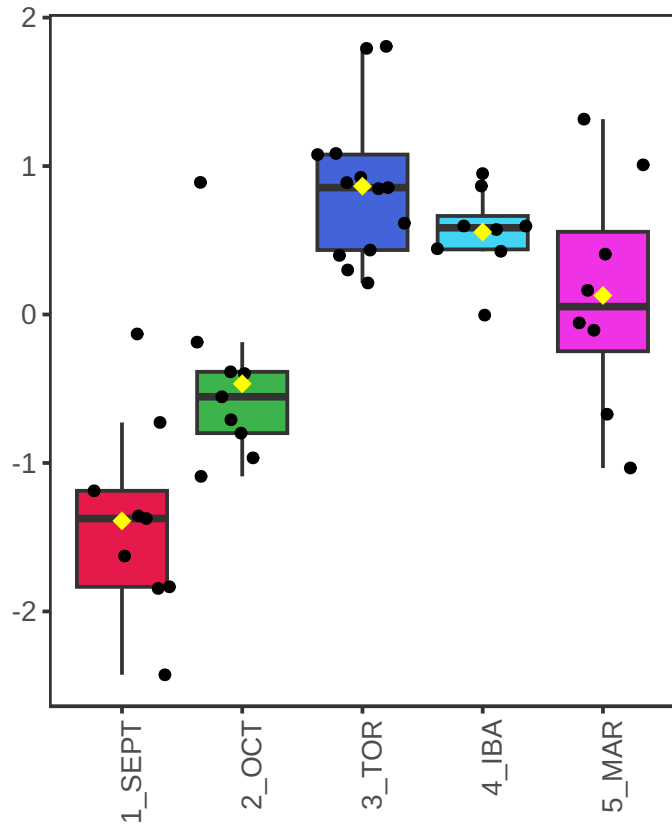


Prolylleucine

Original Conc.

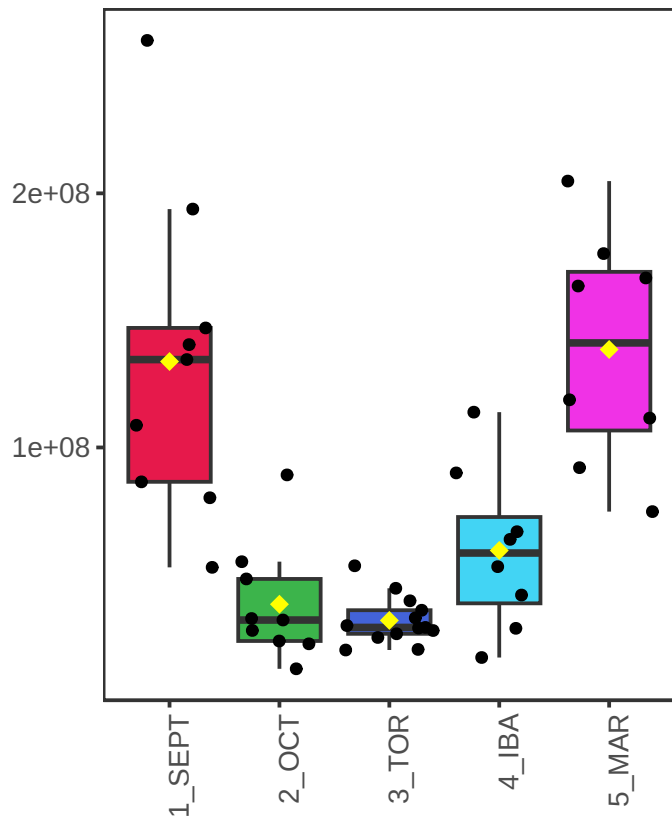


Normalized Conc.

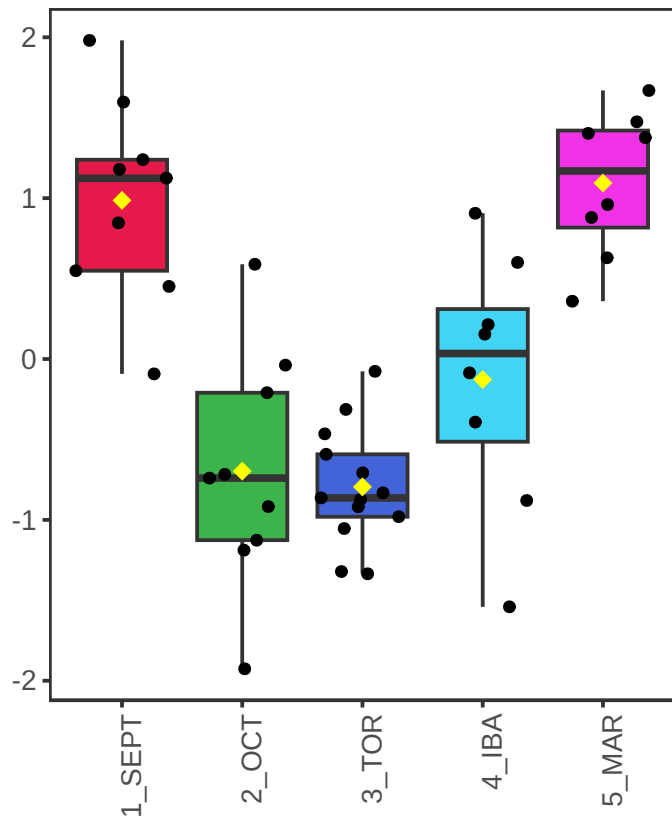


Propionylcarnitine

Original Conc.

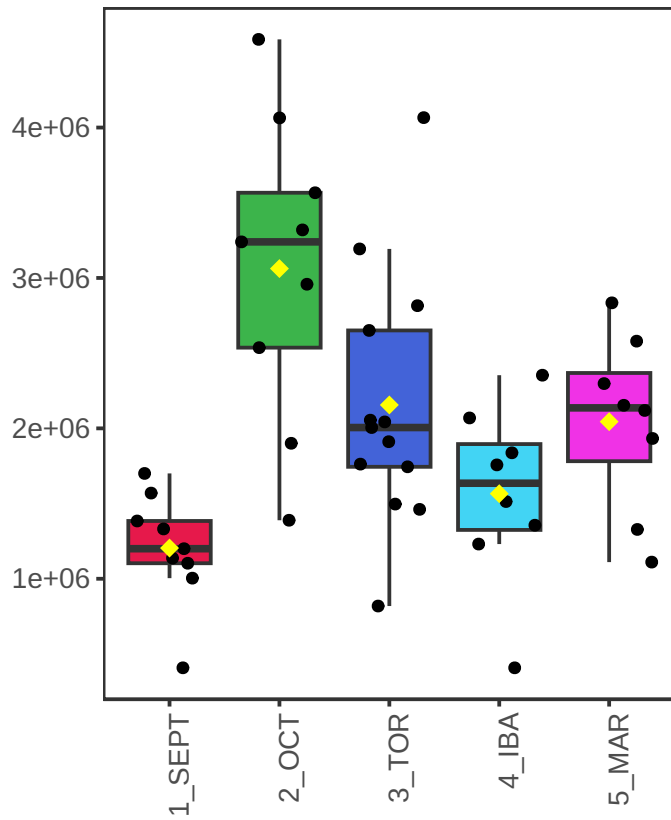


Normalized Conc.

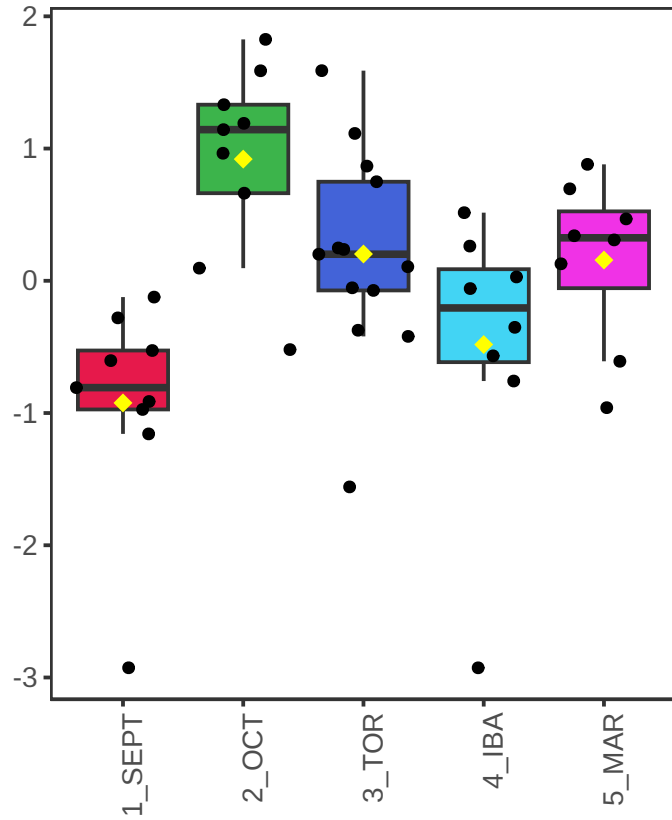


Pyrogallol

Original Conc.

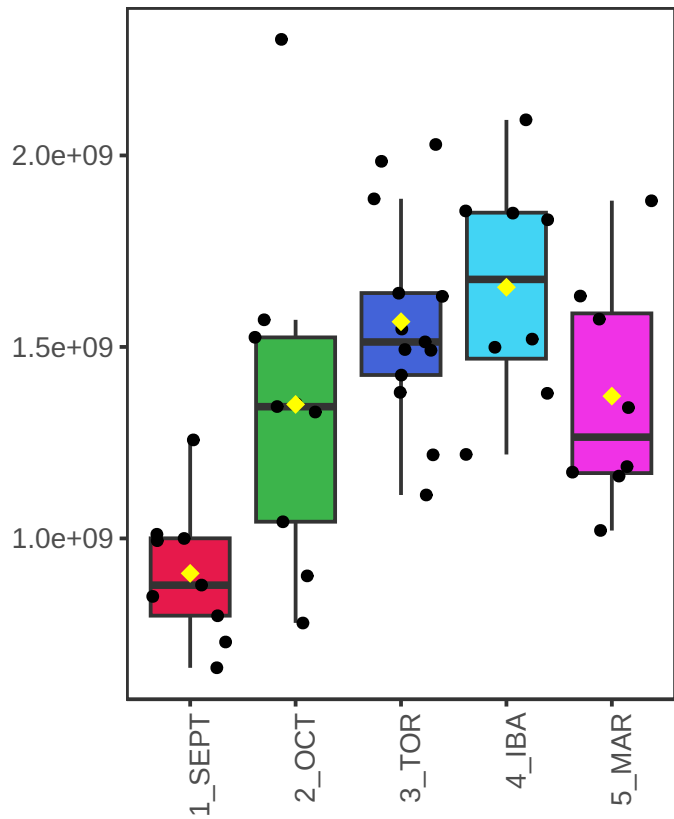


Normalized Conc.

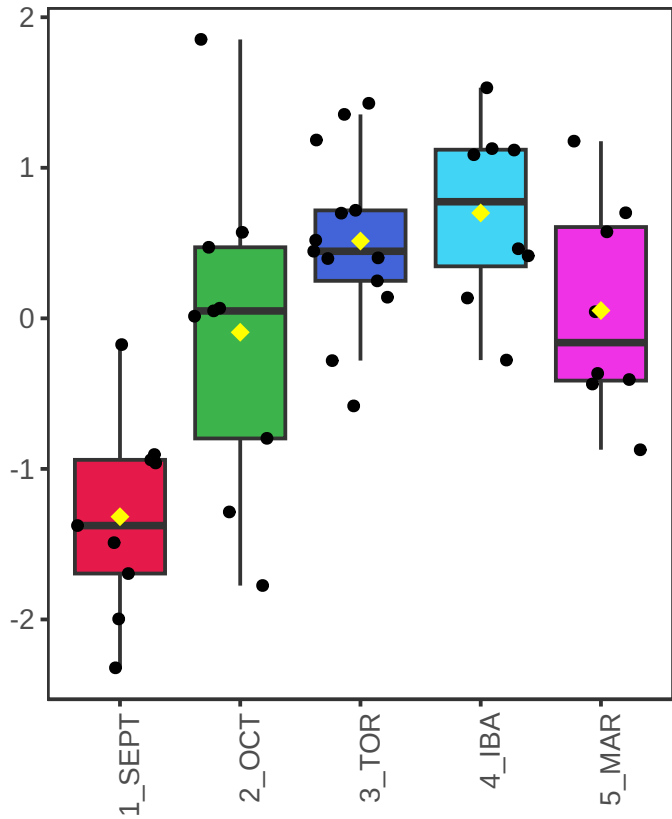


Pyroglutamic acid

Original Conc.

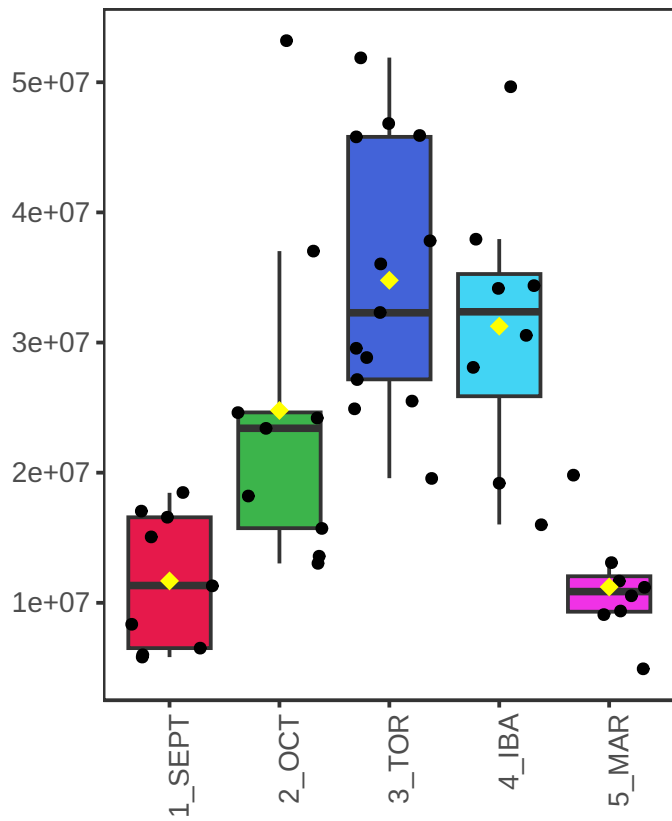


Normalized Conc.

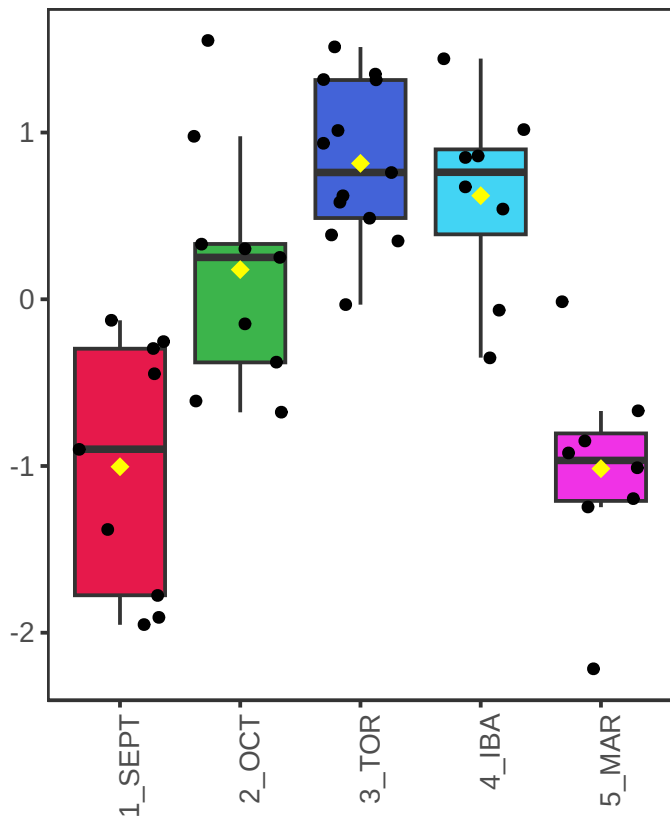


Pyrrolidine

Original Conc.

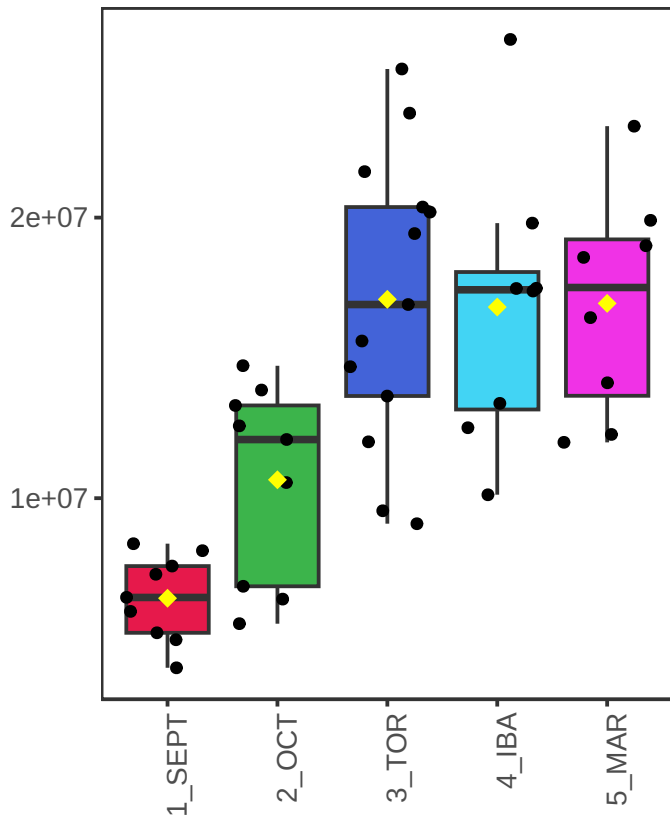


Normalized Conc.

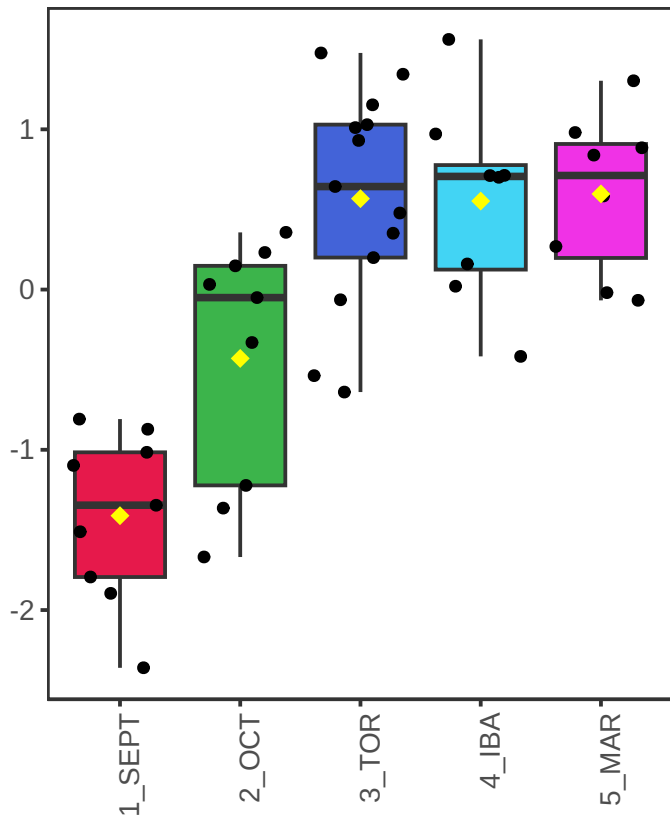


S-Adenosylhomocysteine

Original Conc.

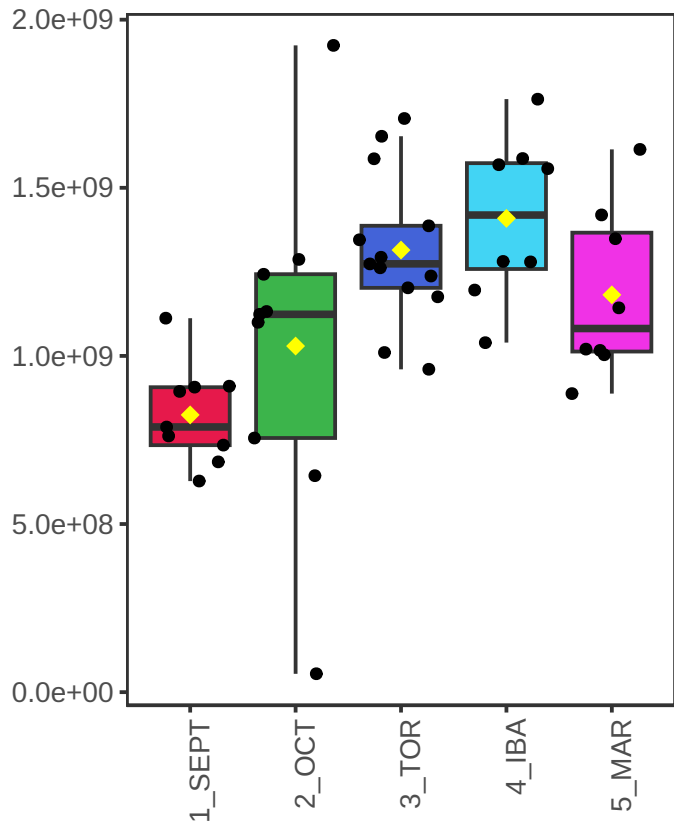


Normalized Conc.

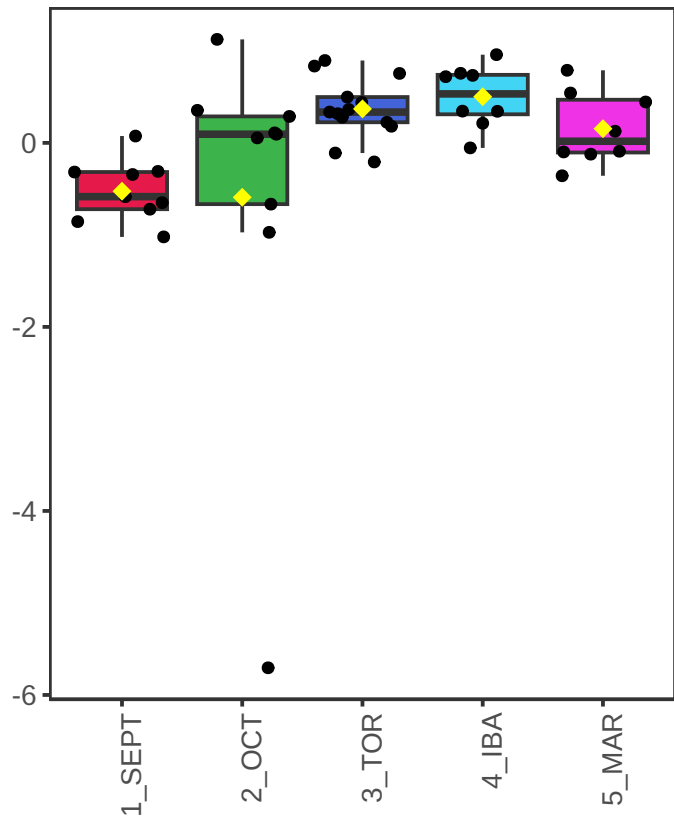


Serine

Original Conc.

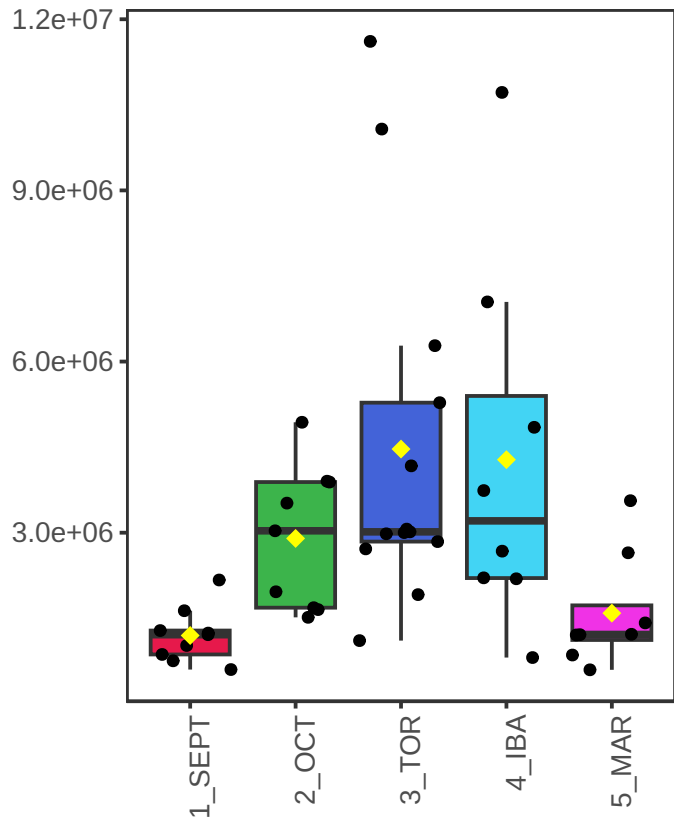


Normalized Conc.

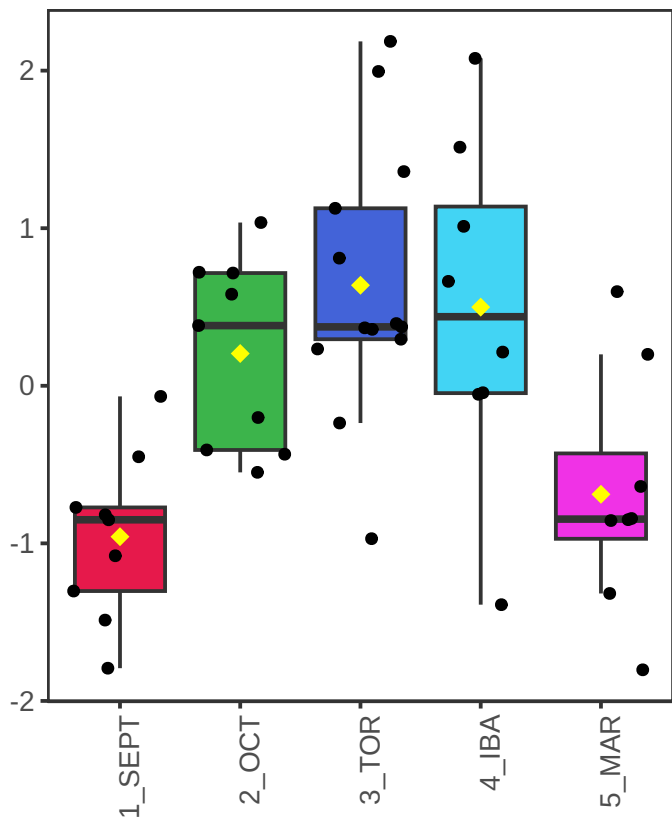


Stachydrine

Original Conc.

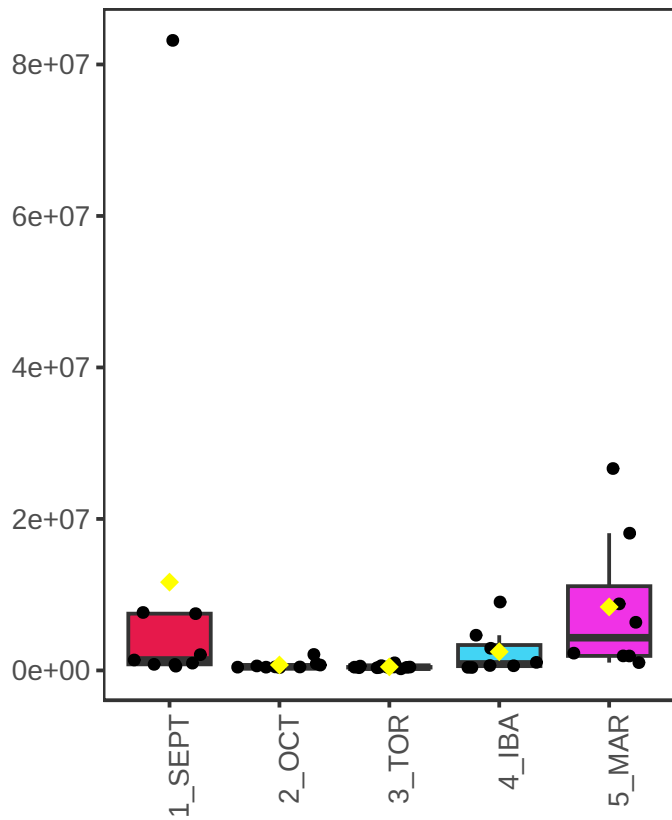


Normalized Conc.

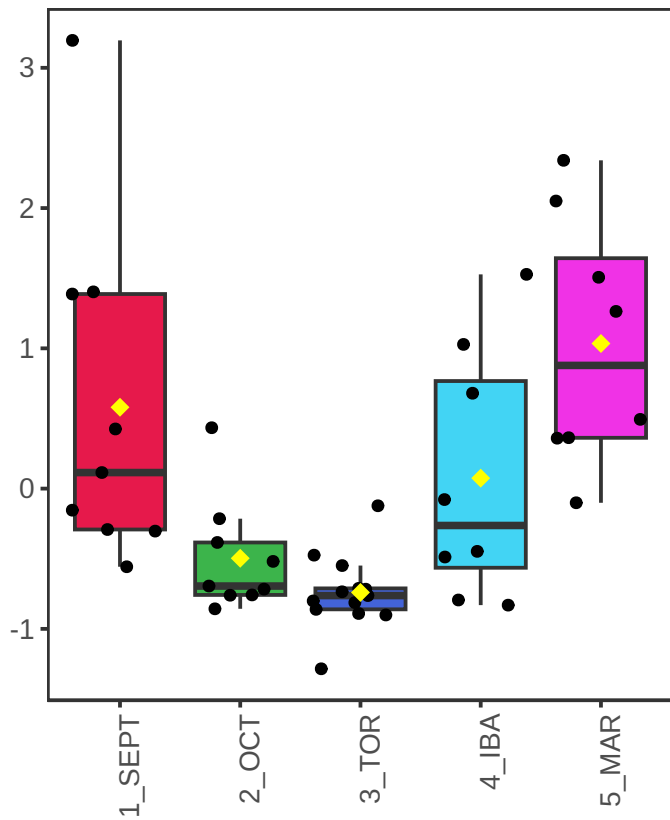


Taurocholic acid

Original Conc.

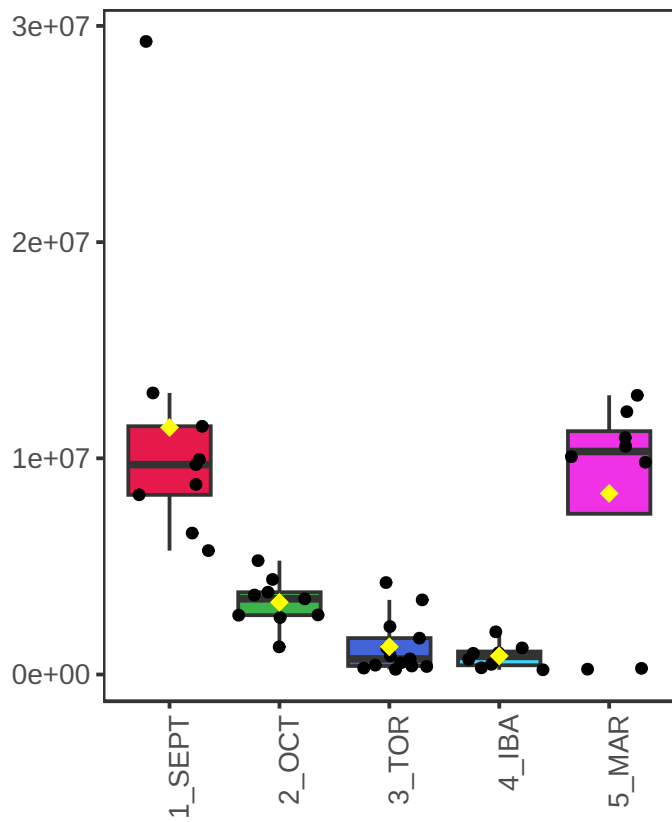


Normalized Conc.

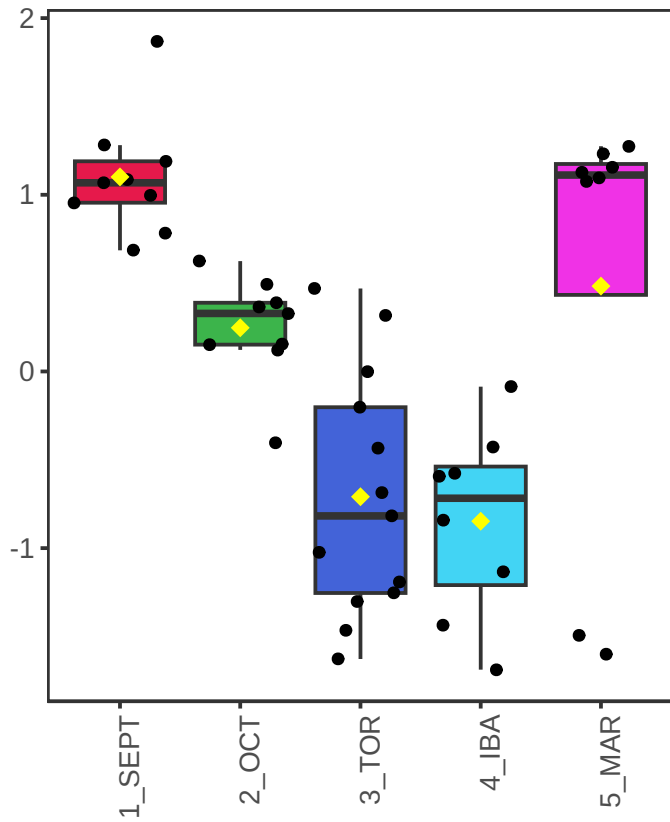


Thiamine

Original Conc.

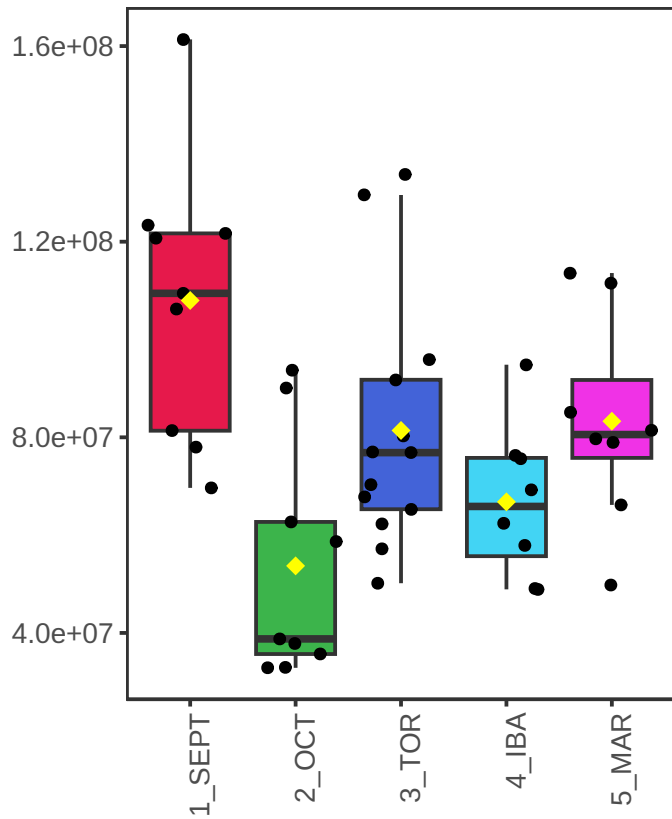


Normalized Conc.

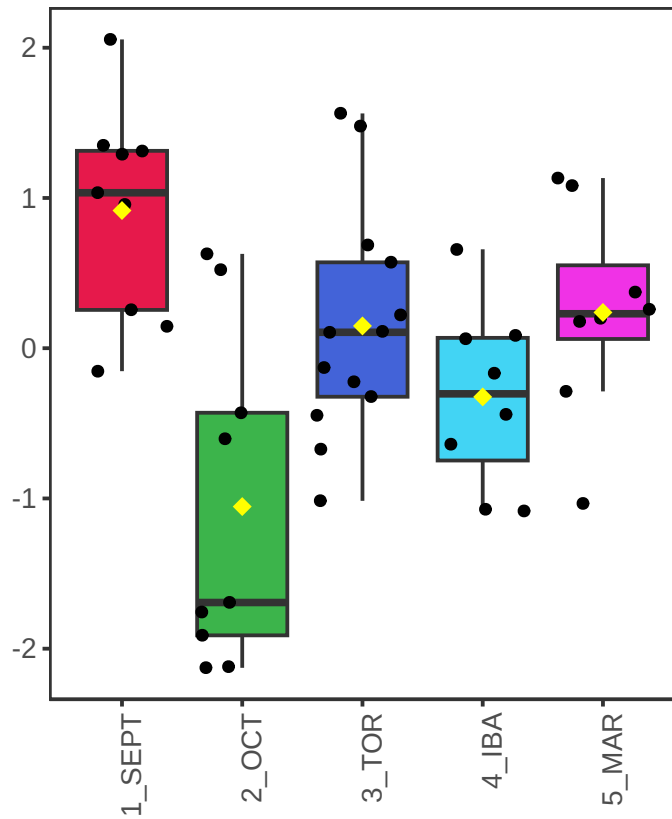


Threonine

Original Conc.

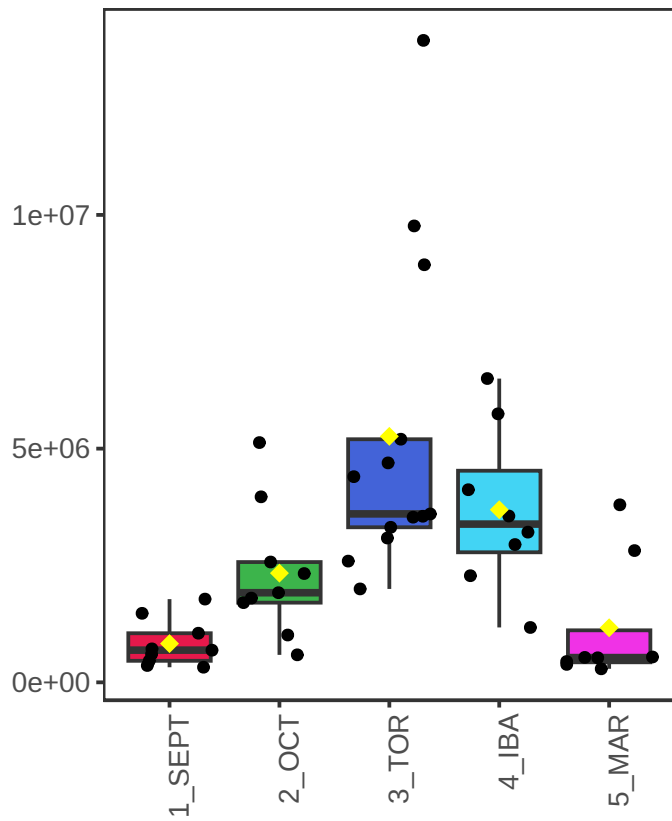


Normalized Conc.

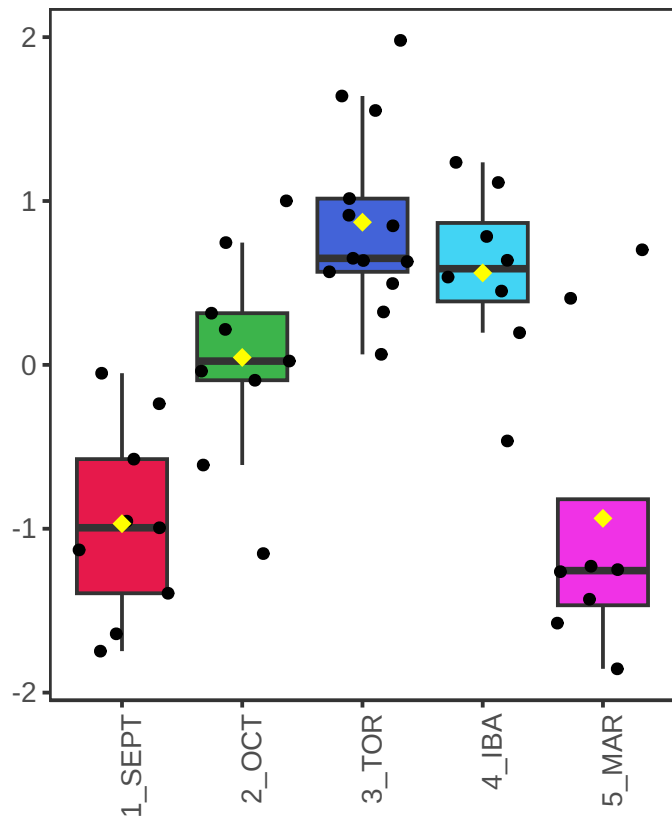


THTA

Original Conc.

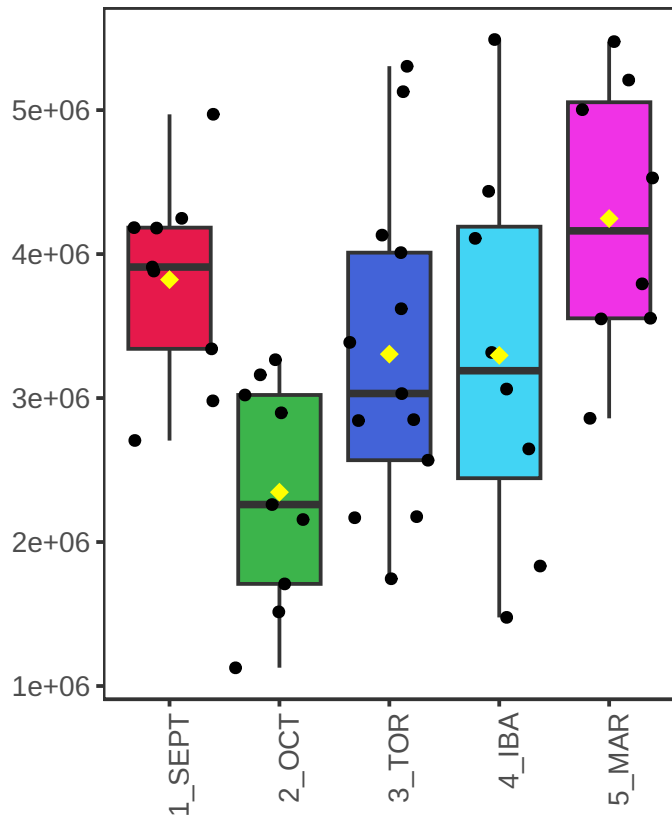


Normalized Conc.

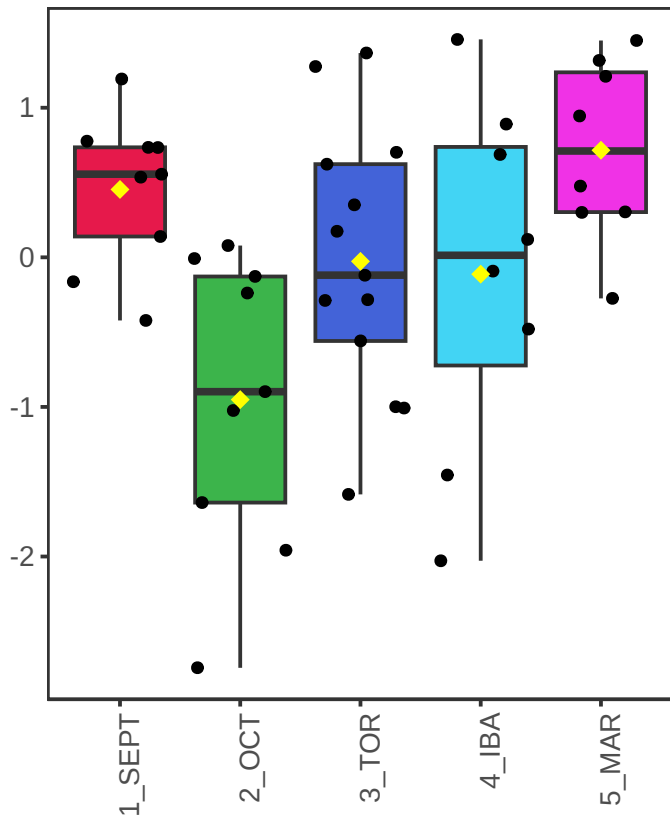


Tilarginine

Original Conc.

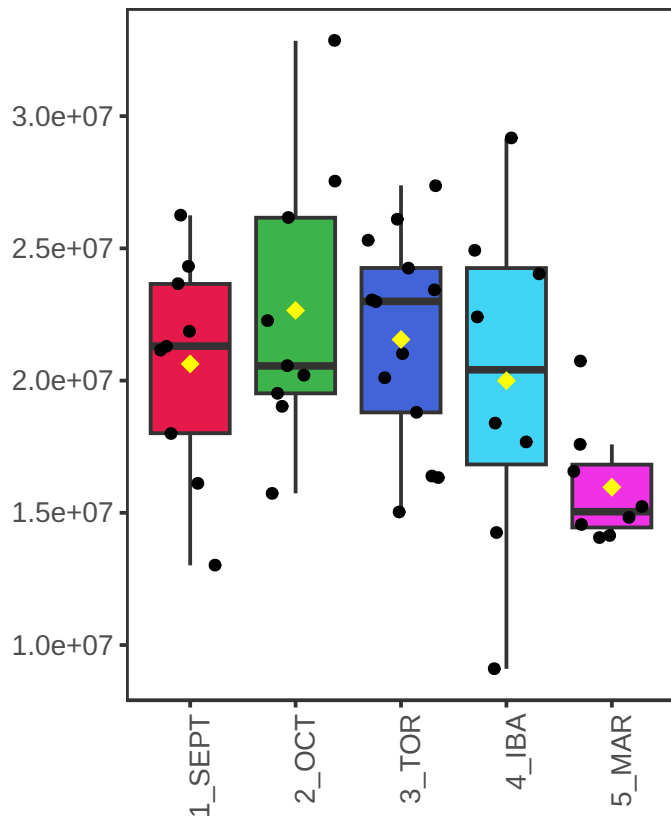


Normalized Conc.

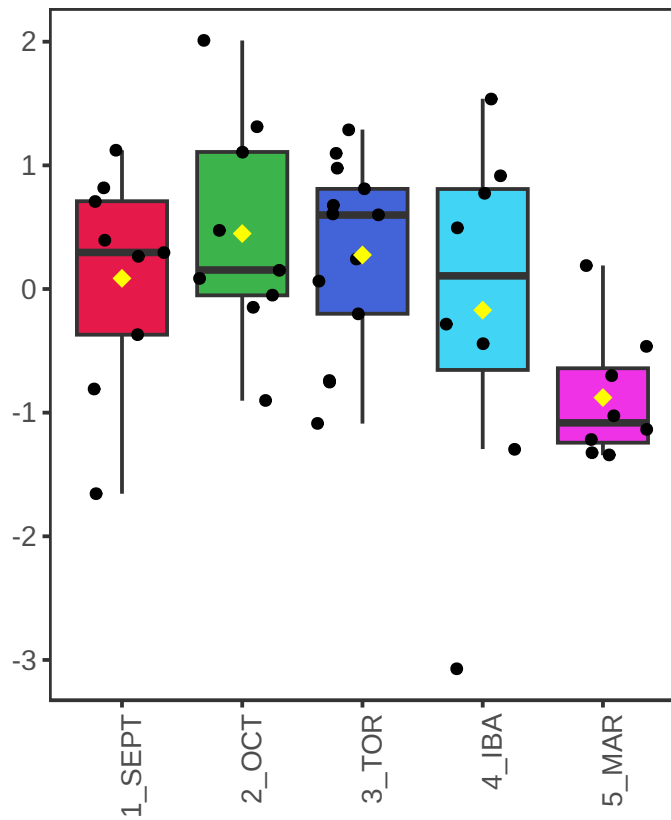


Trans-3-Indoleacrylic acid

Original Conc.

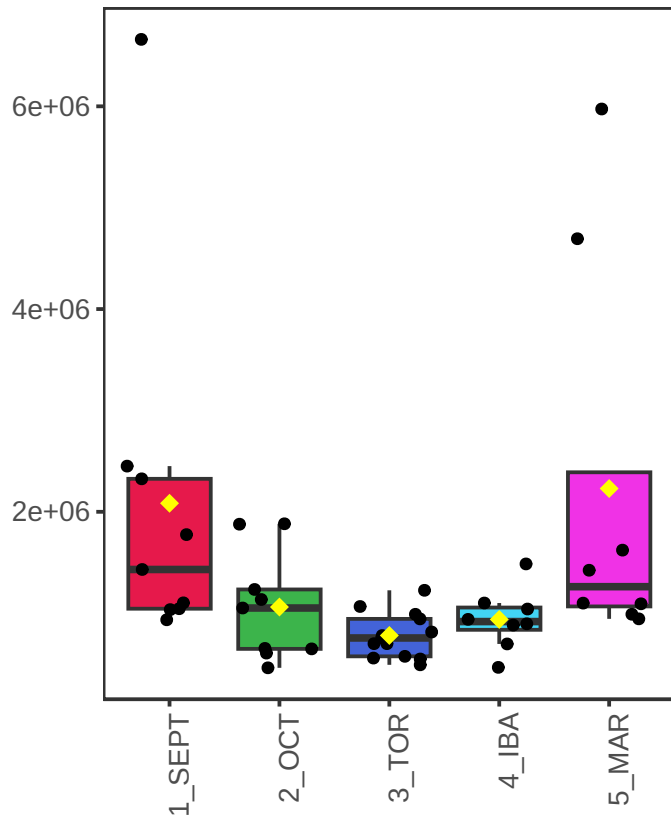


Normalized Conc.

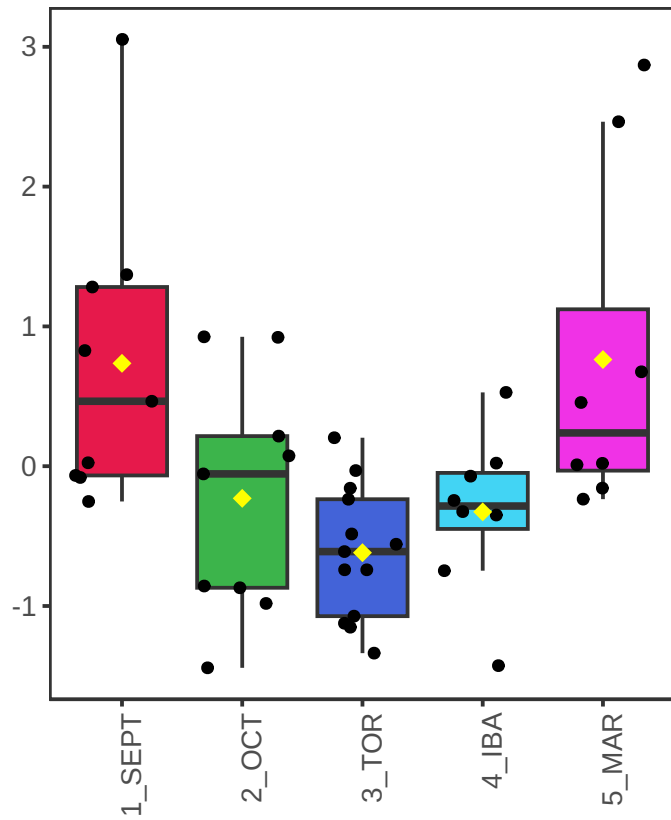


Traumatin

Original Conc.

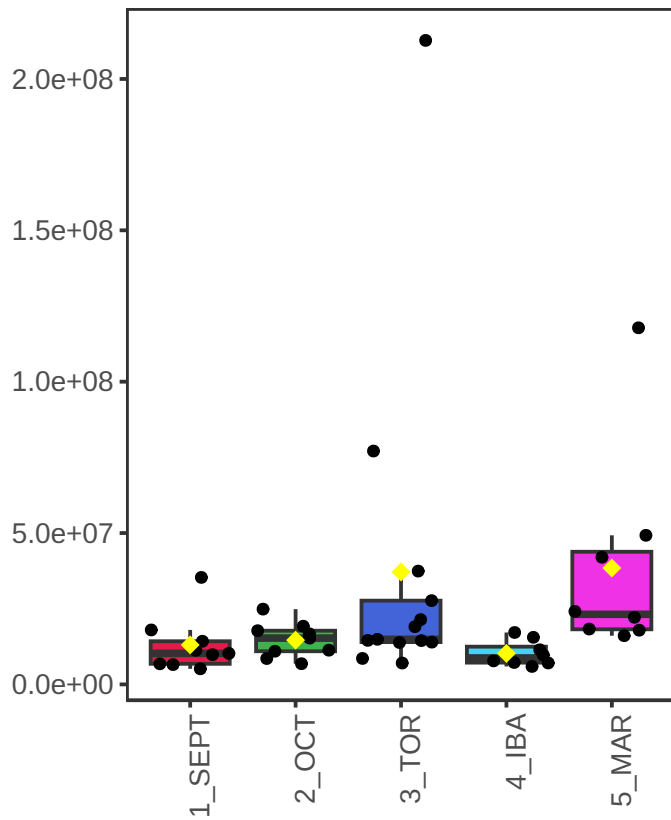


Normalized Conc.

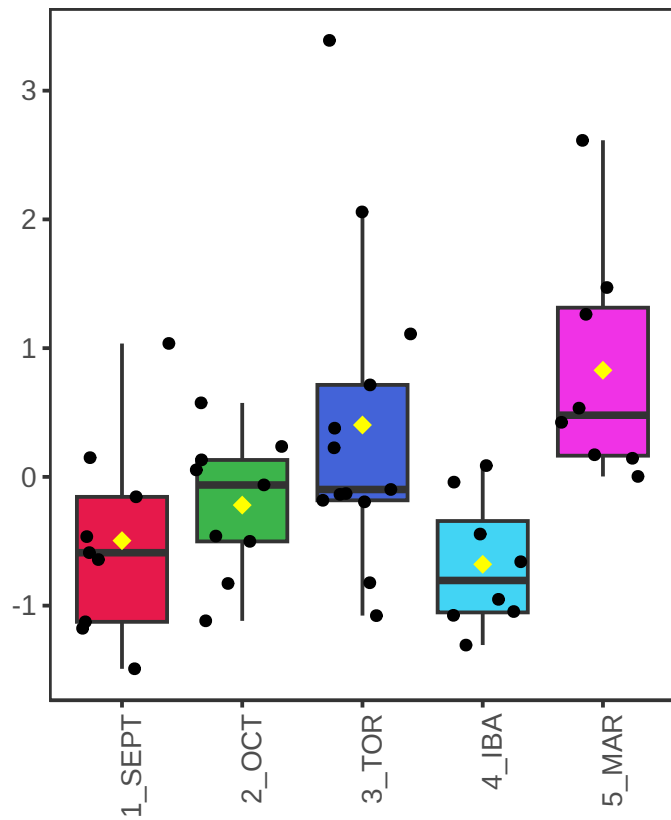


Triethanolamine

Original Conc.

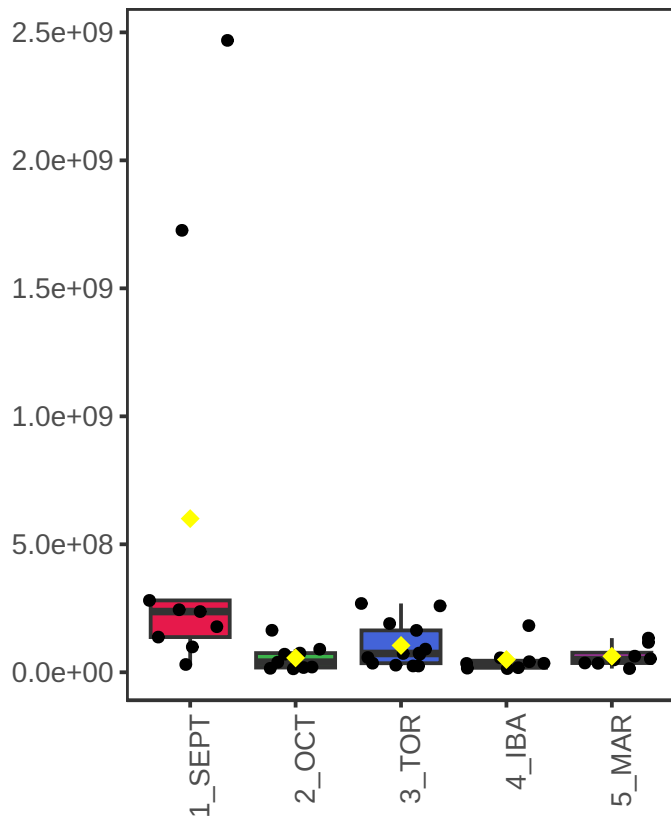


Normalized Conc.

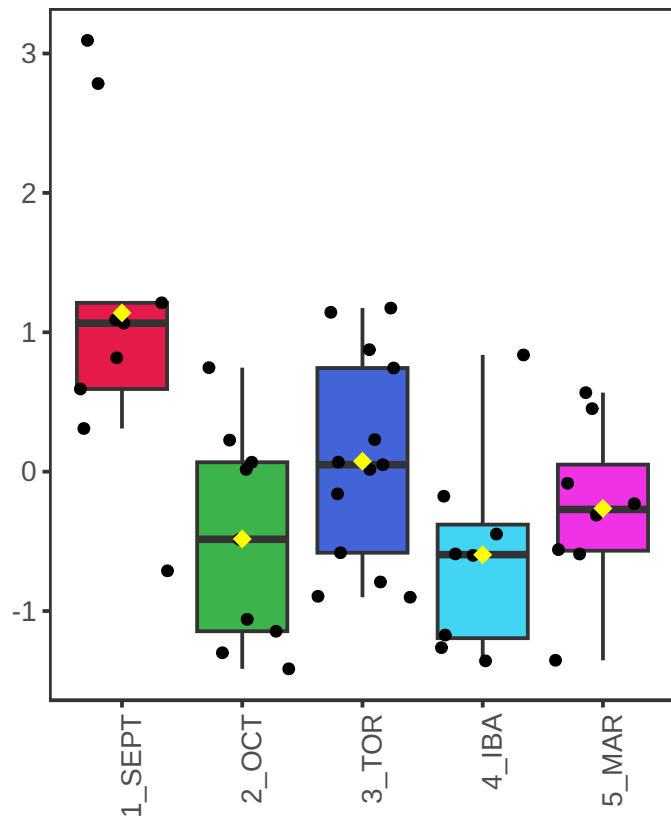


Trimethylamine N-oxide

Original Conc.

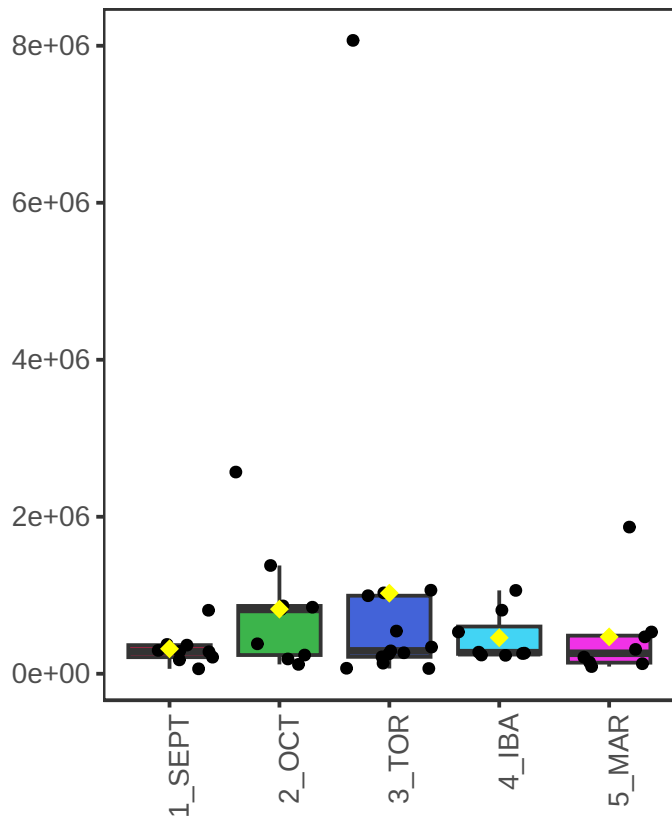


Normalized Conc.

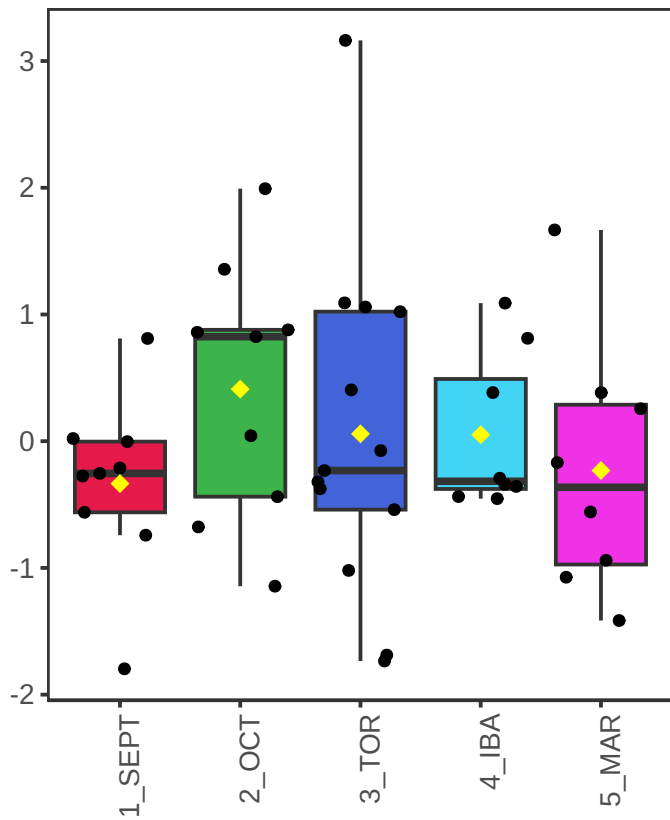


Tris(2-butoxyethyl) phosphate

Original Conc.

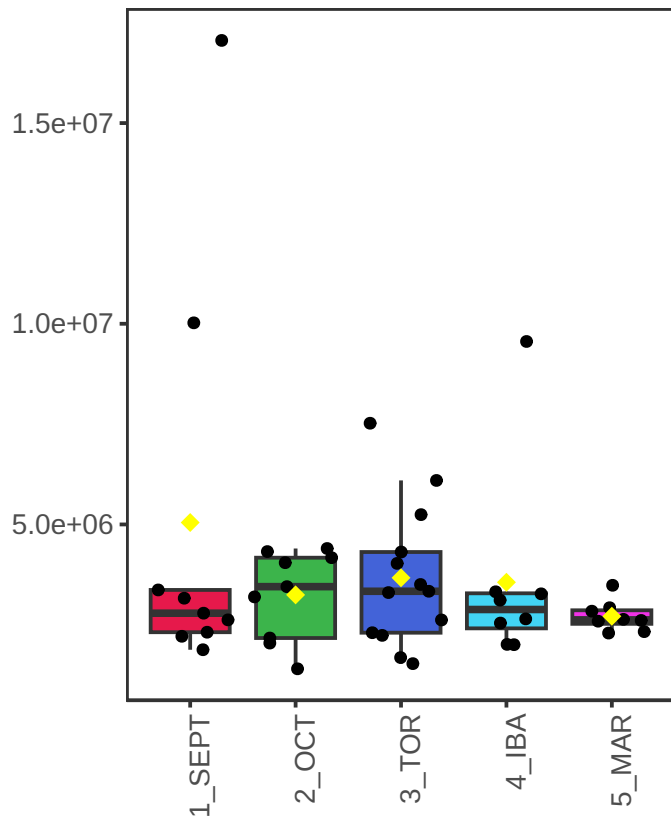


Normalized Conc.

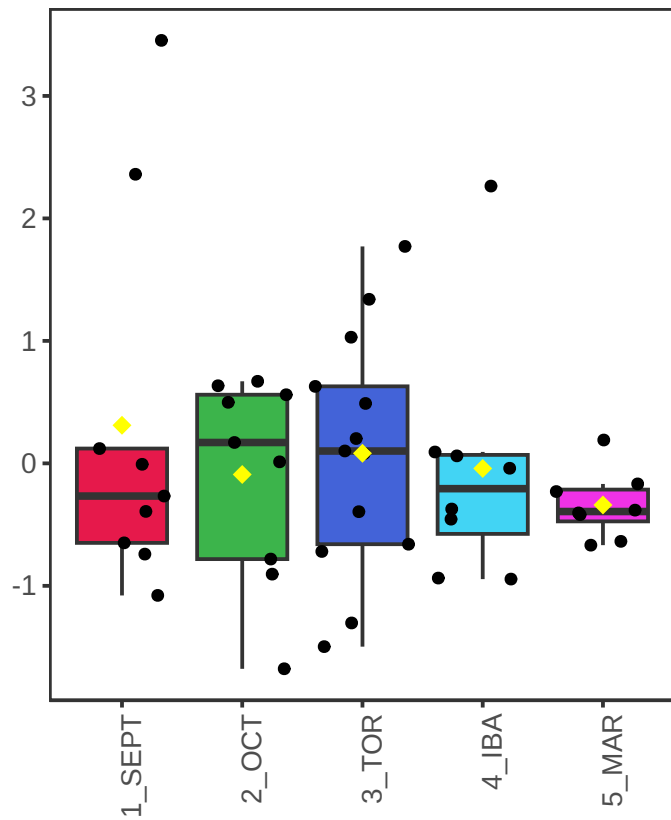


Tris(hydroxymethyl)aminomethane

Original Conc.

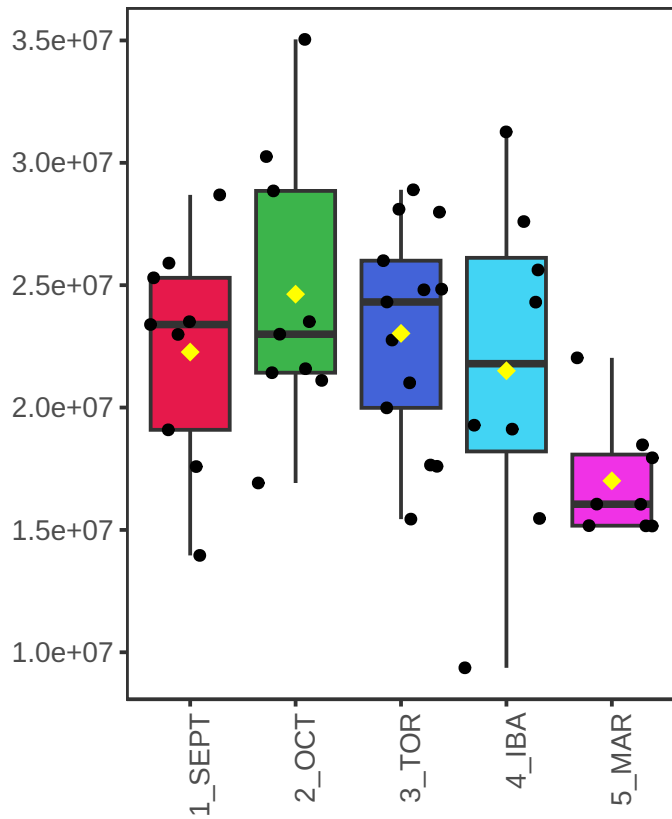


Normalized Conc.

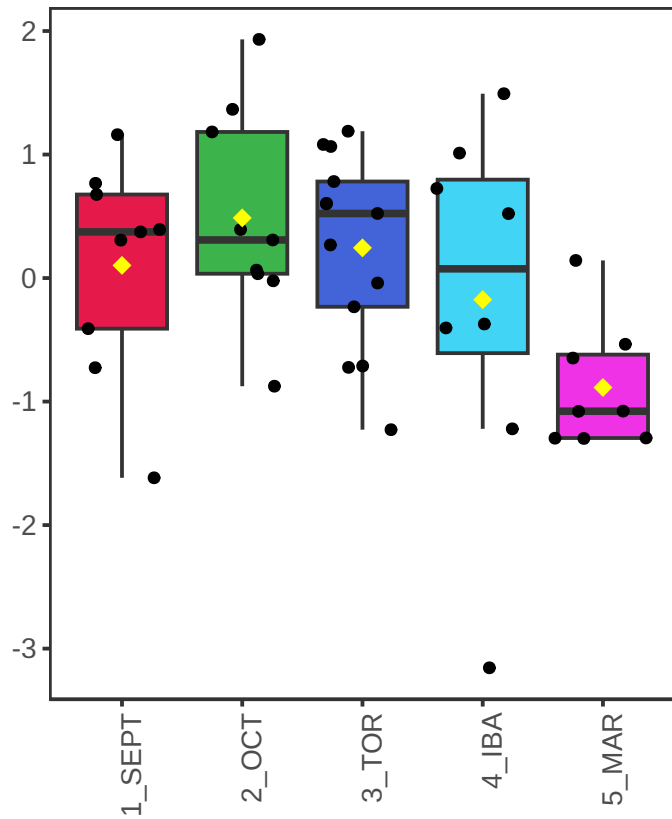


Tryptophan

Original Conc.

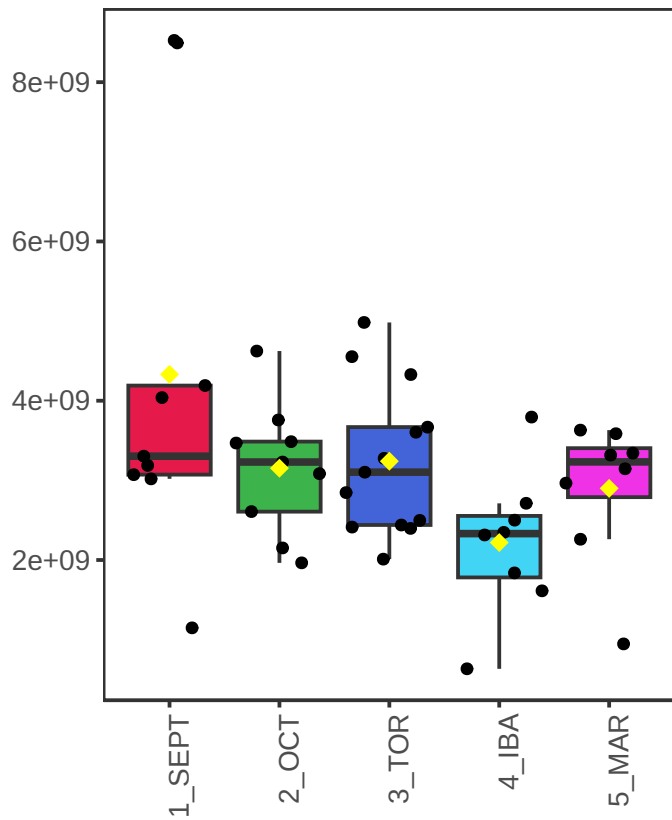


Normalized Conc.

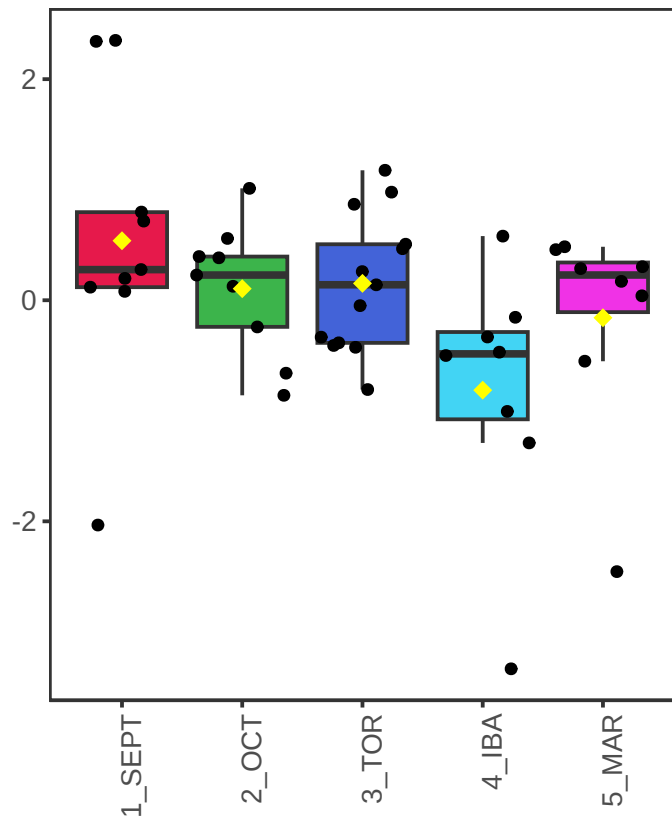


Urea

Original Conc.

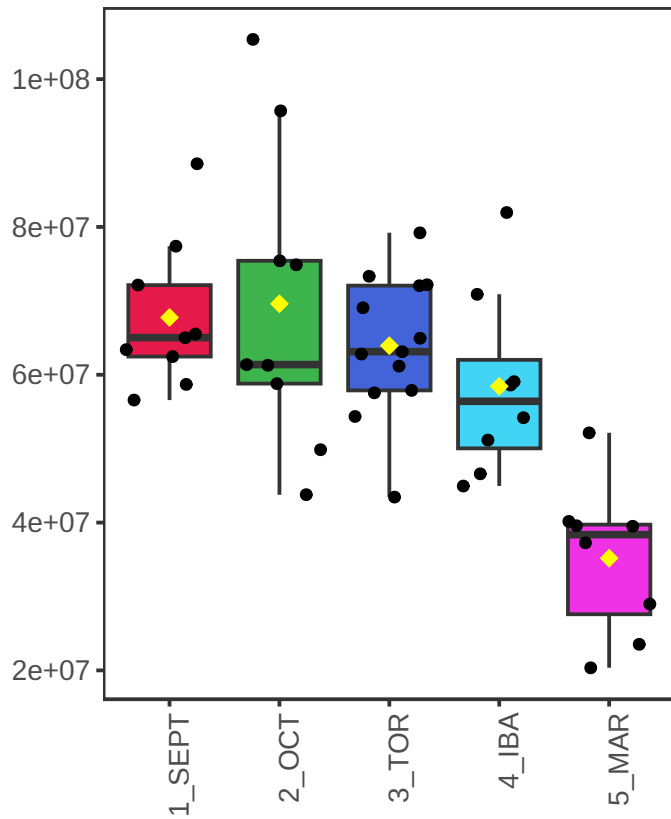


Normalized Conc.

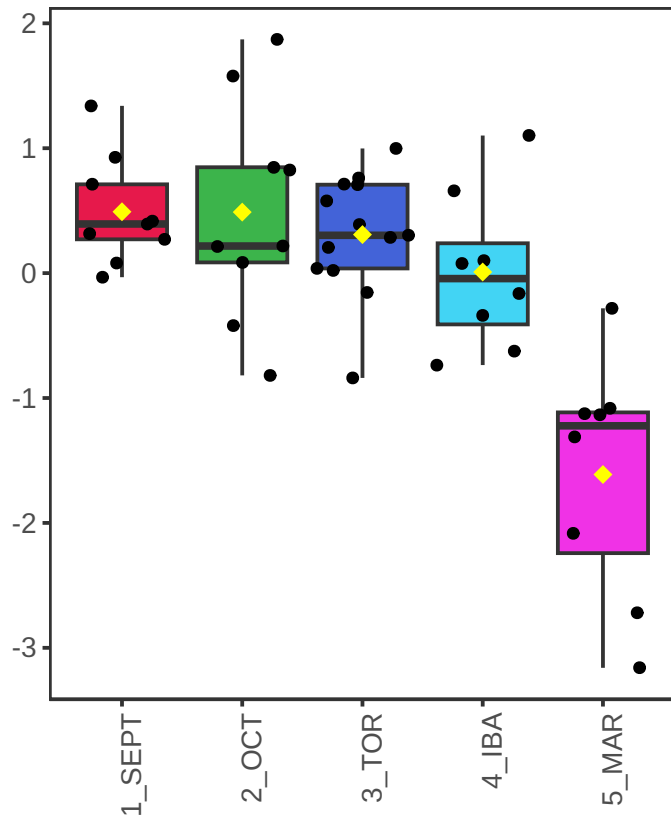


Uridine monophosphate

Original Conc.

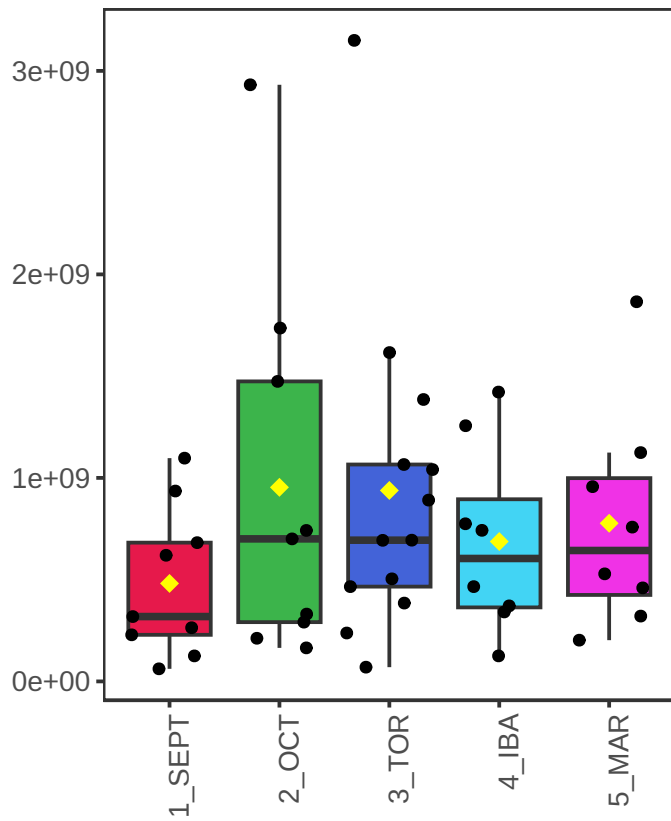


Normalized Conc.

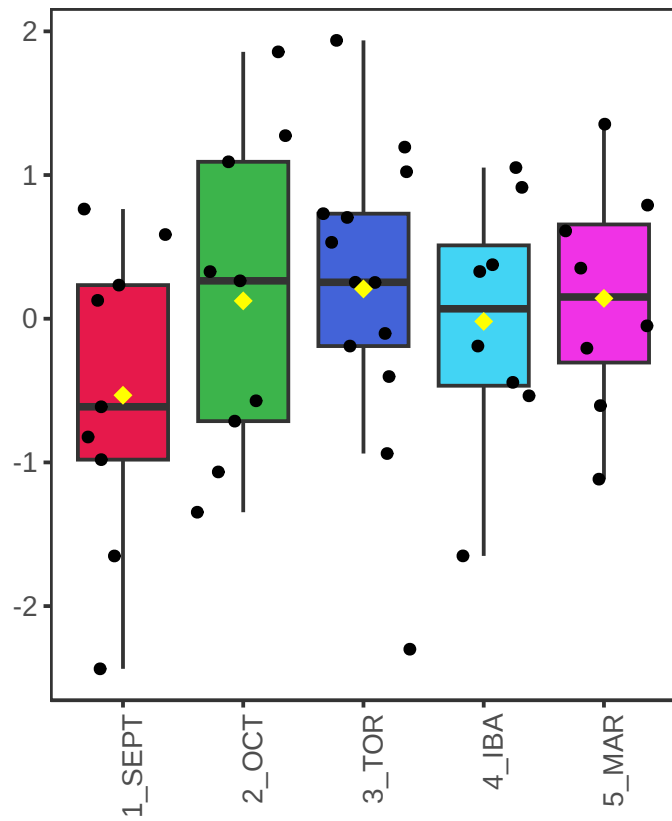


Urocanic acid

Original Conc.

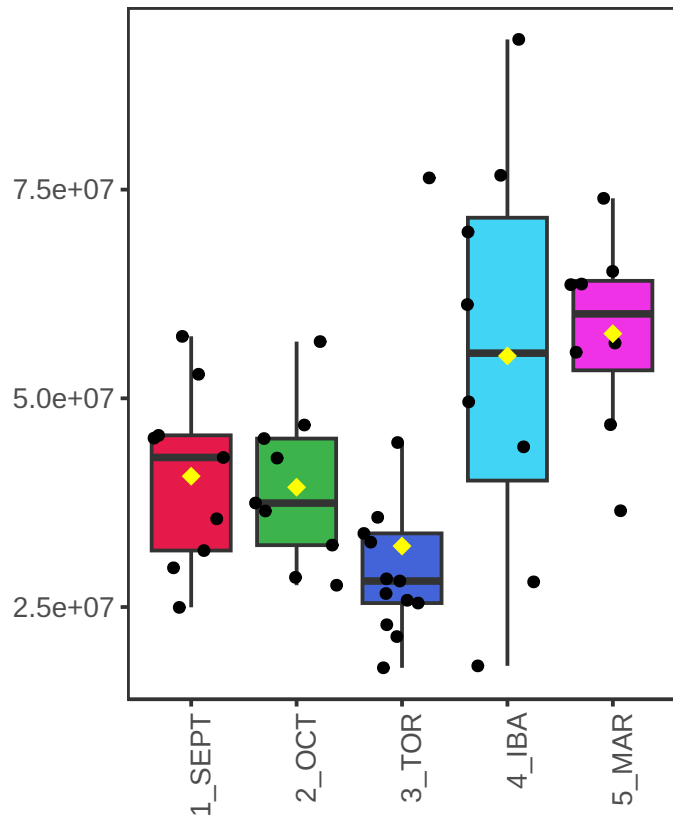


Normalized Conc.



Vinylglycine

Original Conc.



Normalized Conc.

