

**Assessing the Impact of Semiconductor Wastewater Brine on Biological Nutrient Removal
Wastewater Treatment**

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Supplemental Data

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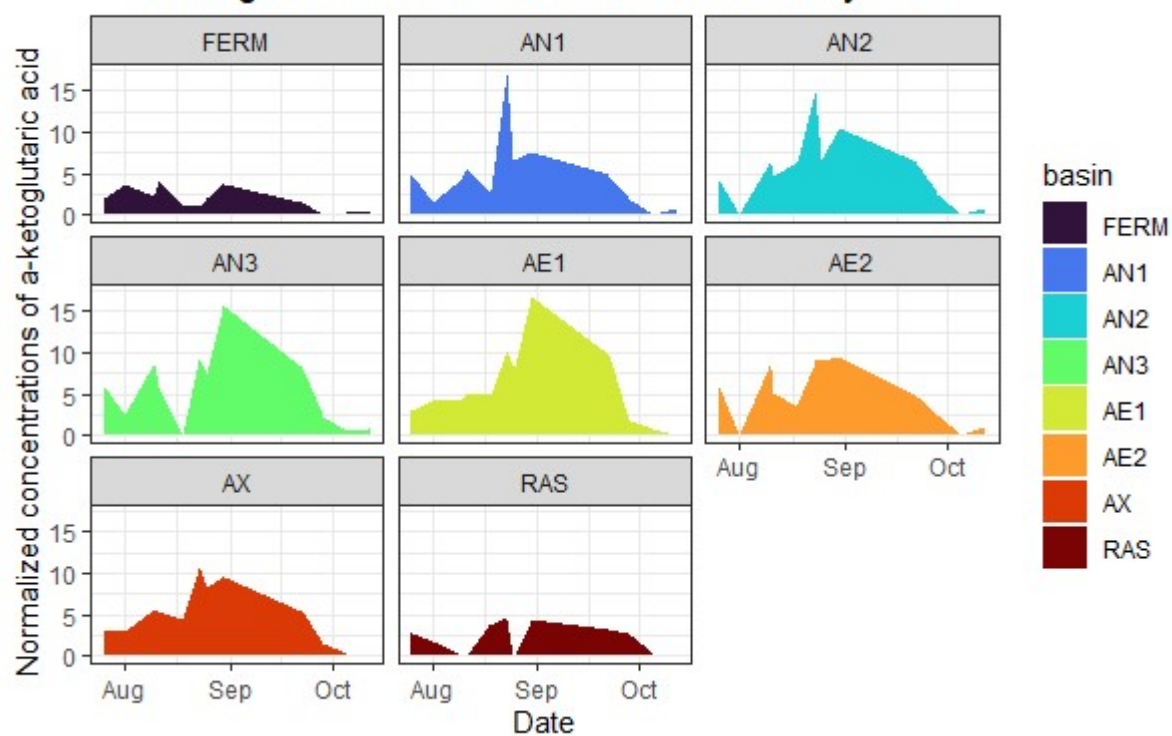
Table S1: Solvent Gradient for Metabolomic LC/MS

Time Point, minutes	%Solvent A	%Solvent B
0	99.95	0.05
1	99.95	0.05
3.5	10	90
5	10	90
5.1	99.95	0.05
7	99.95	0.05

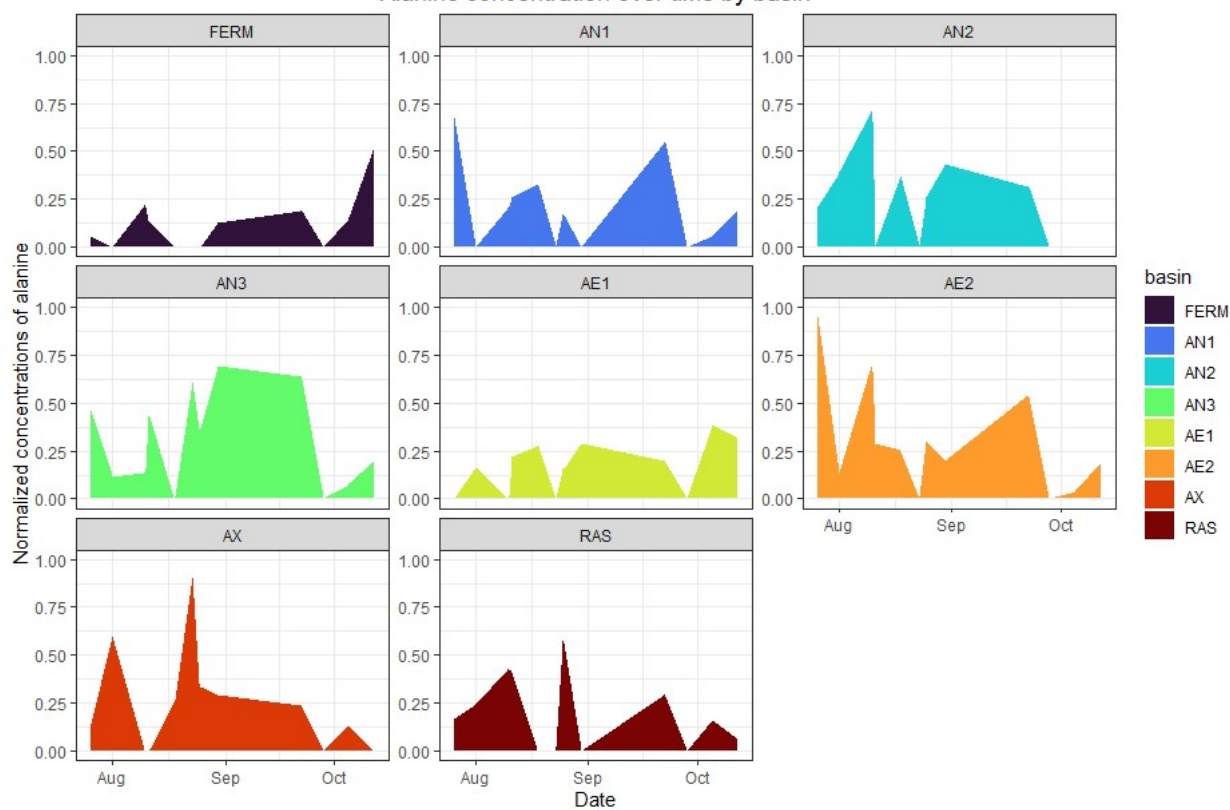
Table S2: Targeted Metabolites

Metabolite	Standard ID	Targeted m/z	Retention time, min	Potential biological roles [1, 2]
Acetyl CoA	CAS 102029-73-2	808.0-809.0	2.58	PHA synthesis, Glycolysis, Gluconeogenesis
Isovaleryl CoA	CAS 6244-91-3	850.0-850.2	2.78	PHA synthesis
Propionyl CoA	CAS 108321-21-7	822.0-823.0	2.70	PHA synthesis
Hydroxybutyryl CoA	CAS 103404-51-9	852.0-852.5	2.77	PHA synthesis
Citric acid	CAS 77-92-9	191.0-191.2	0.64	TCA cycle
Succinic acid	CAS 150-90-3	117.0-117.2	0.66	TCA cycle
α -Ketoglutaric acid	CAS 328-50-7	145.0-145.2	0.68	TCA cycle, Amino acid transformations
Malic acid		132.9-133.1	0.66	TCA cycle
Glyoxylate	CAS 918149-31-2	72.8-73.0	0.73	Glyoxylate cycle
D-Fructose 1, 6-Biphosphate	CAS 38099-82-0	338.8-339.0	0.62	Glycolysis, Gluconeogenesis
Pyruvate	CAS 113-24-6	87.0-87.5	0.79	TCA cycle, Glycolysis, Gluconeogenesis, Amino acid transformations
(-)-Methyl (R)-3-hydroxyvalerate	CAS 60793-22-8	115.0-115.5	0.66	PHA synthesis
NADH	CAS 606-68-8	664.0-665.0	0.84	Energy transfer
NADPH	CAS 2646-71-1	744.0-744.5	0.83	Energy transfer
3-Phosphoglyceric acid	CAS 80731-10-8	184.8-185.2	0.64	Calvin Benson cycle, Glycolysis, Gluconeogenesis
L-alanine	Sigma SN: AAS18	88.0-88.1	0.70	Protein biosynthesis, Peptidoglycan synthesis
L-arginine		173.0-173.4	0.80	Protein biosynthesis
L-aspartic acid		132.0-132.2	0.70	Protein biosynthesis, Gluconeogenesis
L-cystine		239.0-239.4	0.76	CoA precursor
L-glutamic acid		147.0-147.2	2.64	Protein biosynthesis, Amino acid transformations
Glycine		74.0-74.2	0.76	Protein biosynthesis
L-histidine		154.0-154.2	0.84	Protein biosynthesis
L-isoleucine		130.0-130.4	1.74	Protein biosynthesis
L-leucine		130.0-130.4	1.60	Protein biosynthesis
L-lysine		146.0-146.4	0.70	Protein biosynthesis
L-methionine		148.0-148.4	1.23	Protein biosynthesis
L-phenylalanine		164.0-164.2	2.64	Protein biosynthesis
L-proline		114.0-114.15	0.87	Protein biosynthesis
L-serine		104.0-104.2	0.74	Protein biosynthesis
L-threonine		118.0-118.2	0.76	Protein biosynthesis
L-tyrosine		180.0-180.4	1.54	Protein biosynthesis
L-valine		116.0-116.15	1.02	Protein biosynthesis

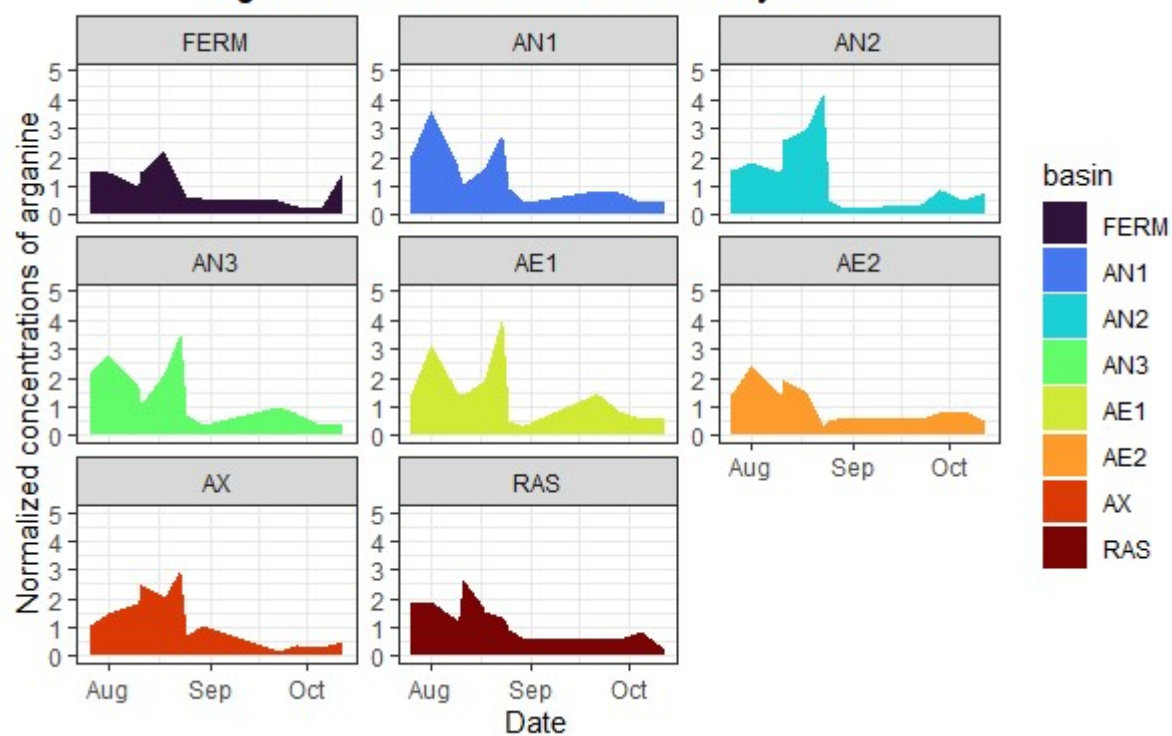
a-Ketoglutaric acid concentration over time by basin



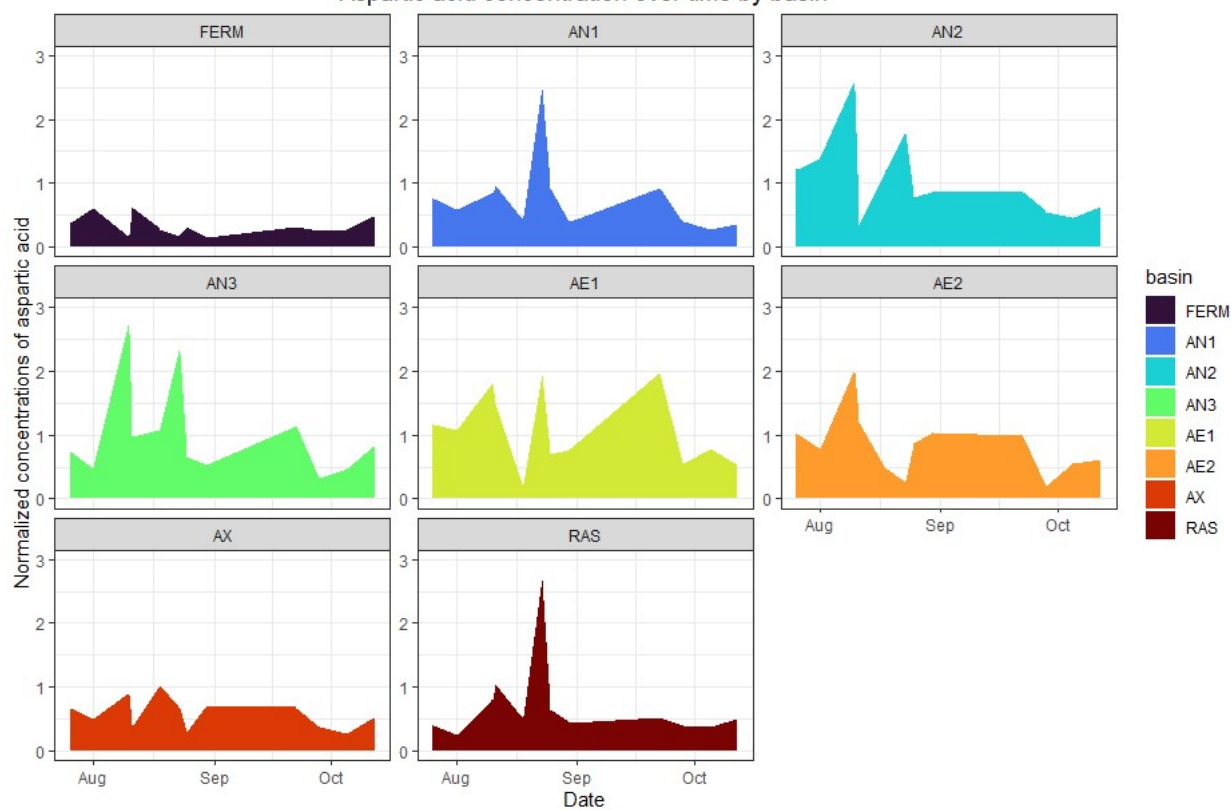
Alanine concentration over time by basin



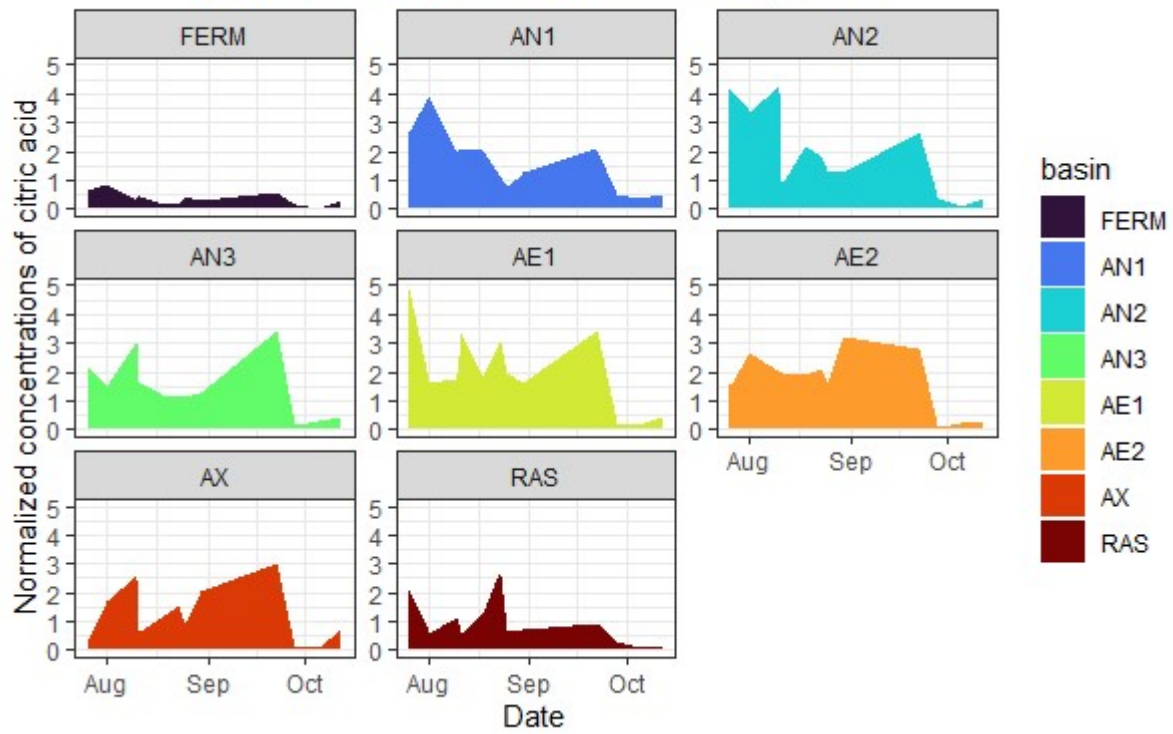
Arginine concentration over time by basin



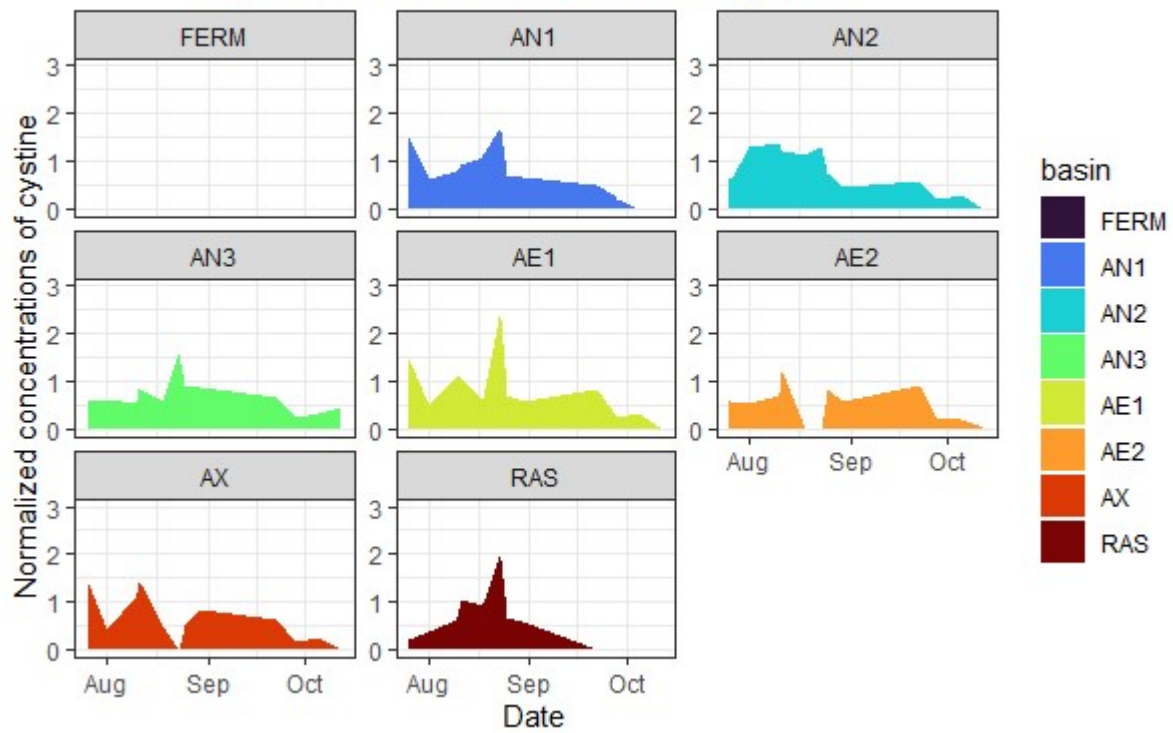
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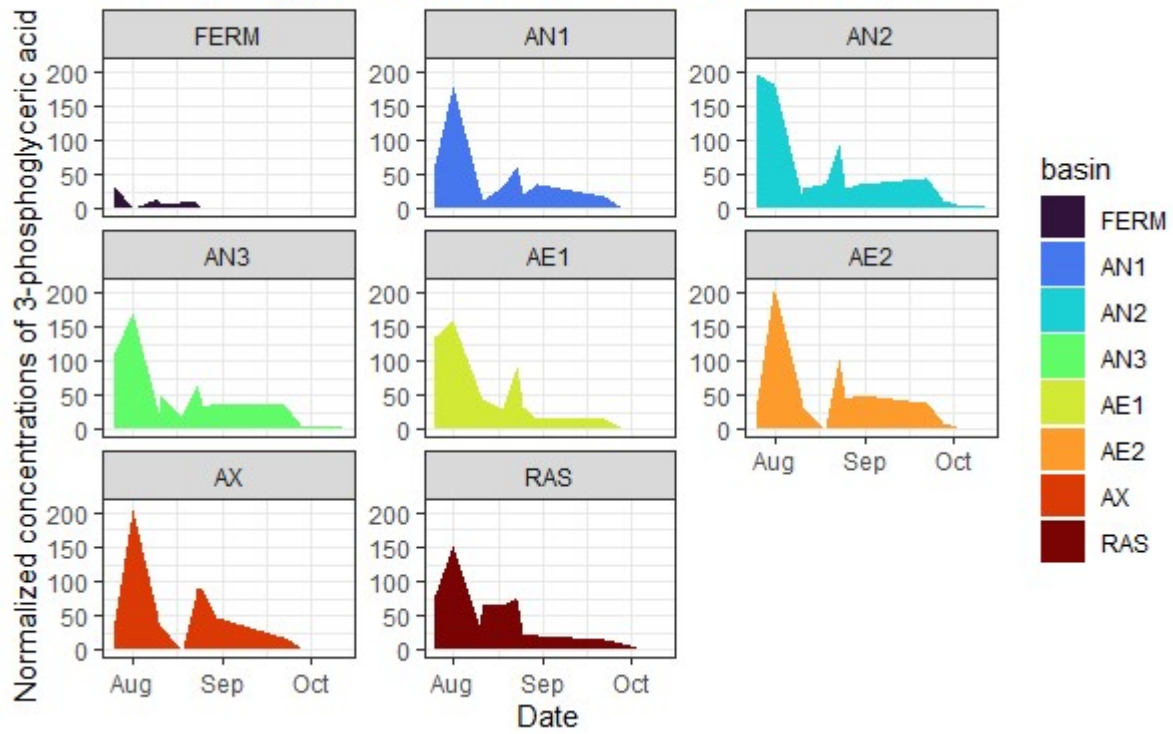
Citric acid concentration over time by basin



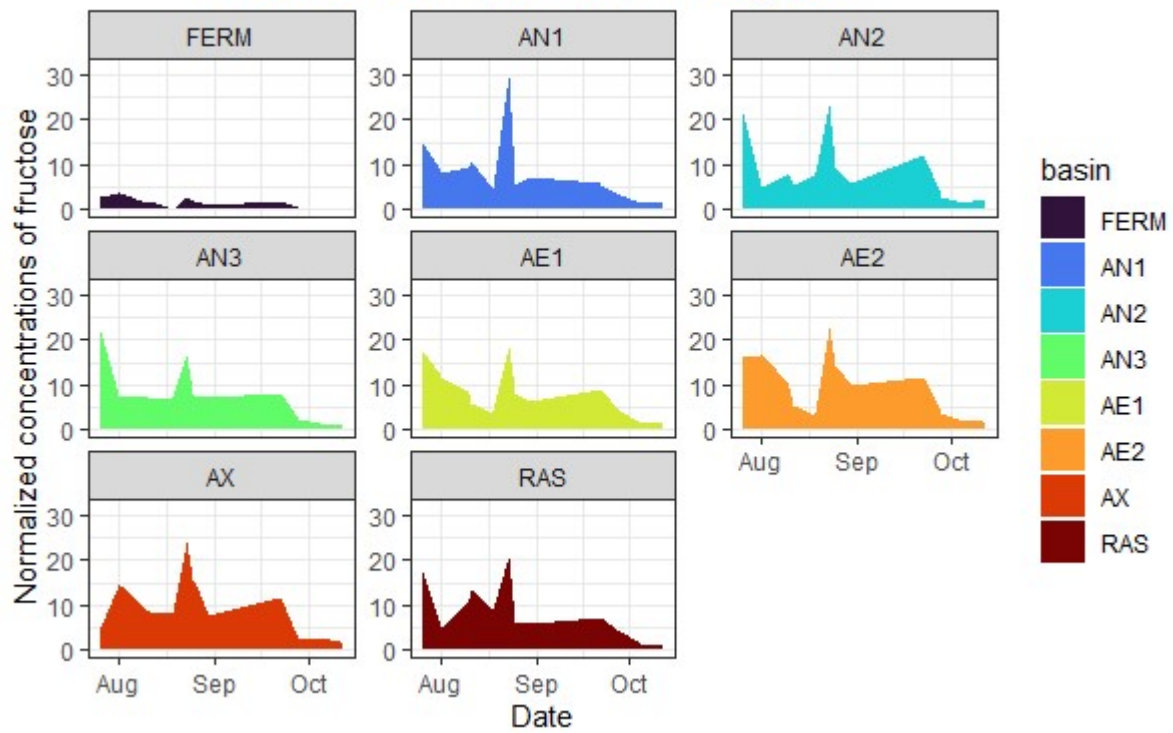
Cystine concentration over time by basin



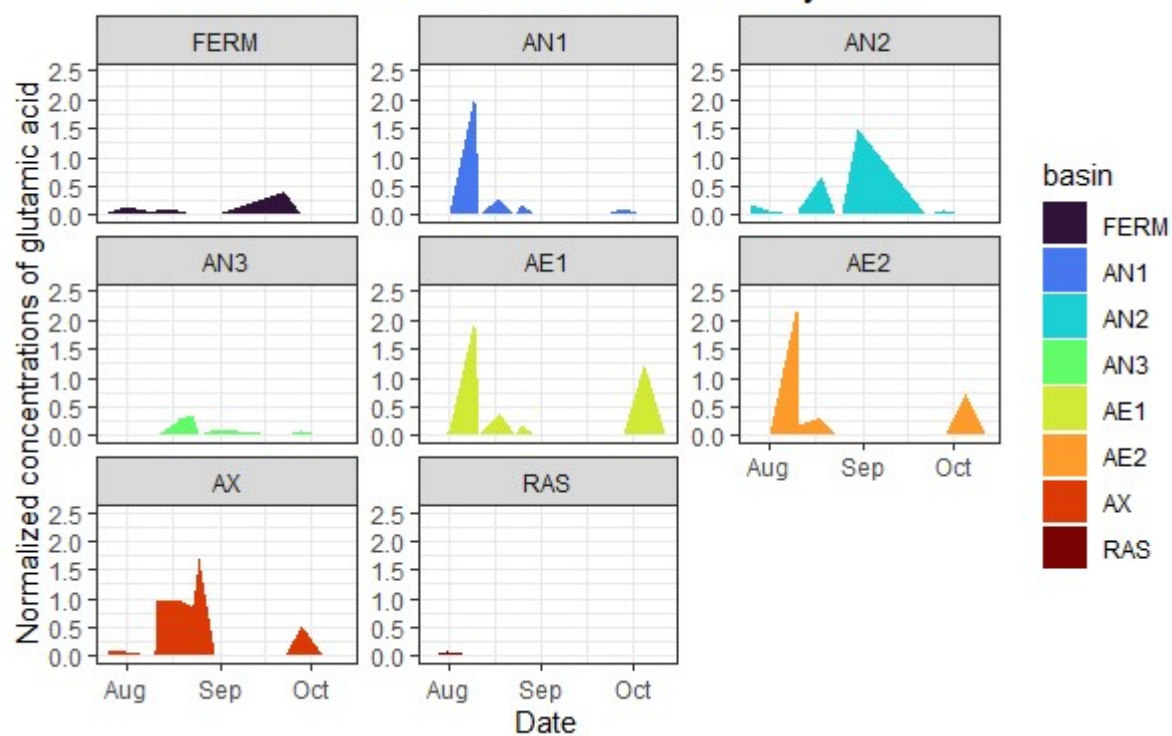
3-Phosphoglyceric acid concentration over time by basin



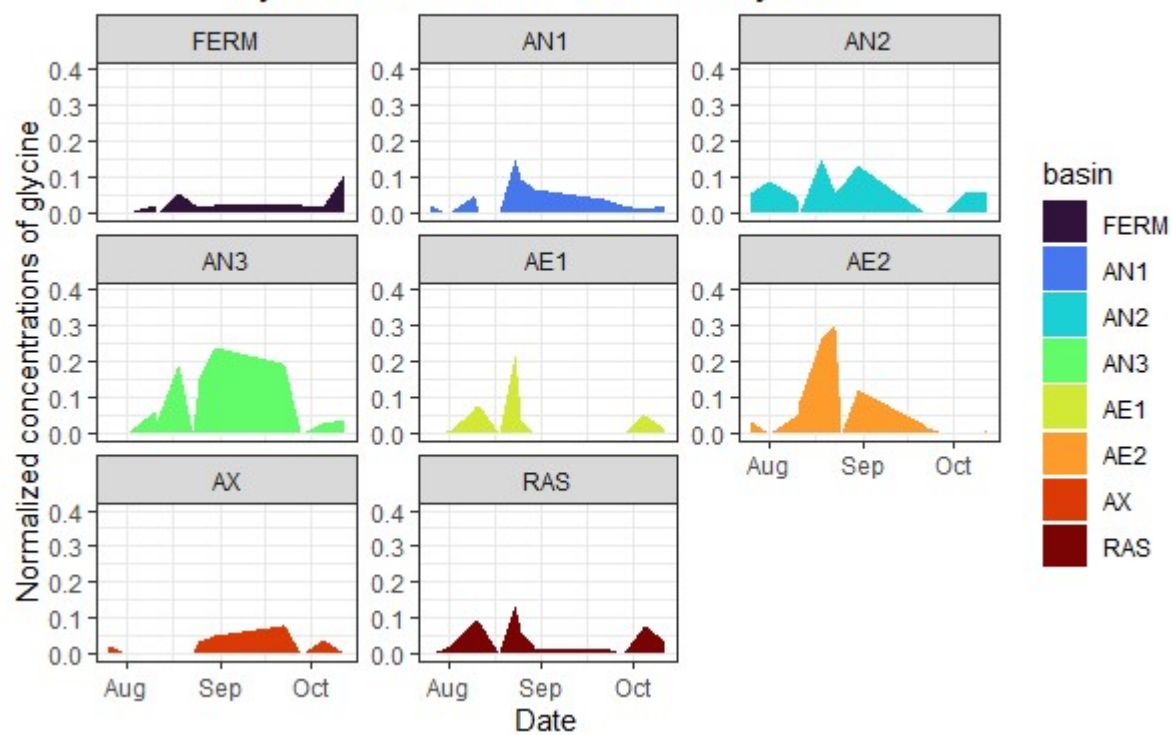
Fructose concentration over time by basin



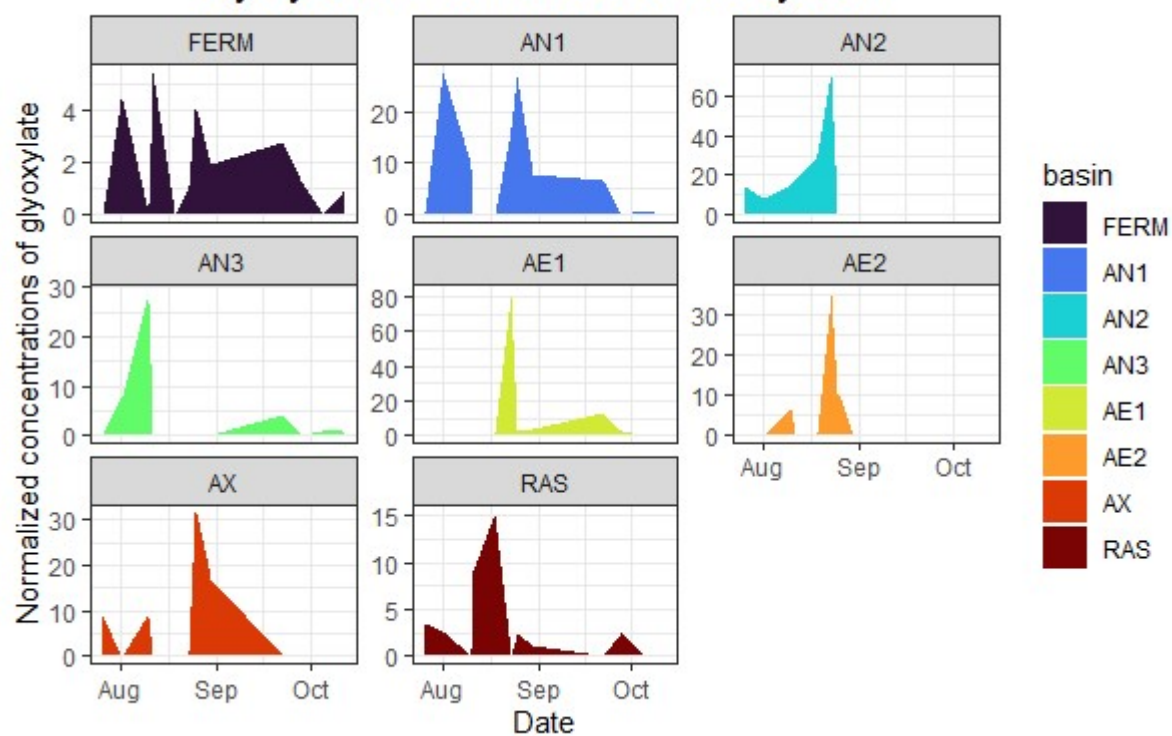
Glutamic acid concentration over time by basin



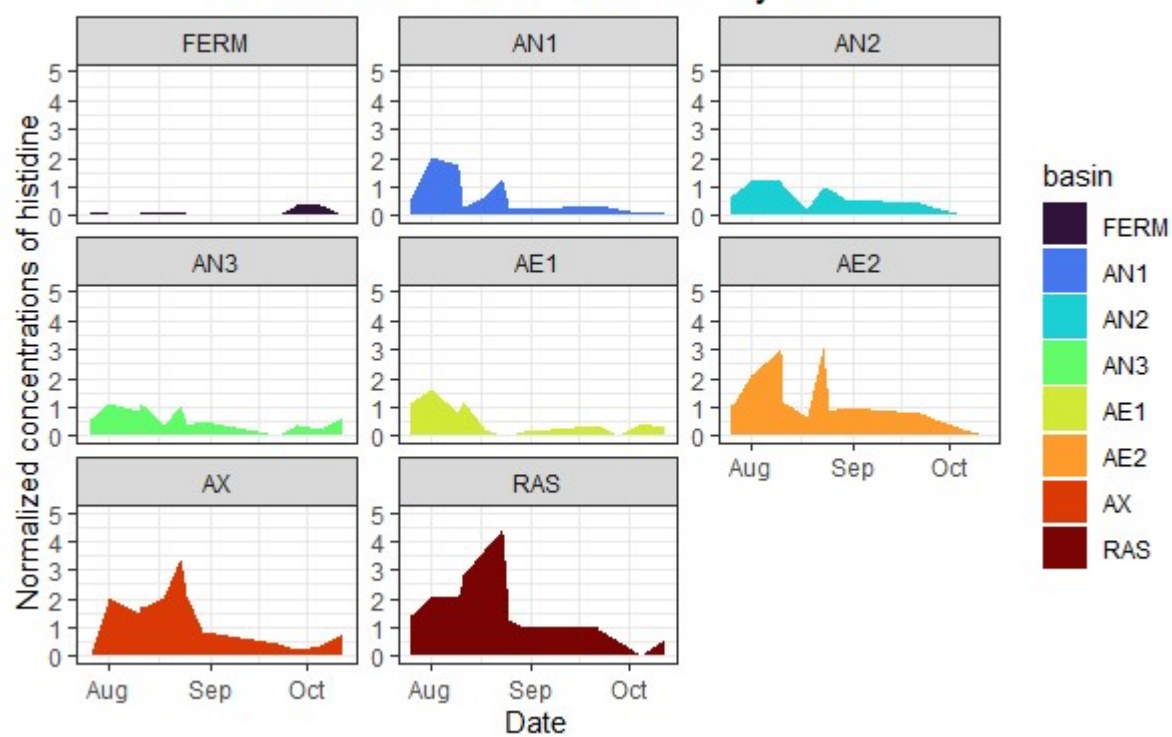
Glycine concentration over time by basin

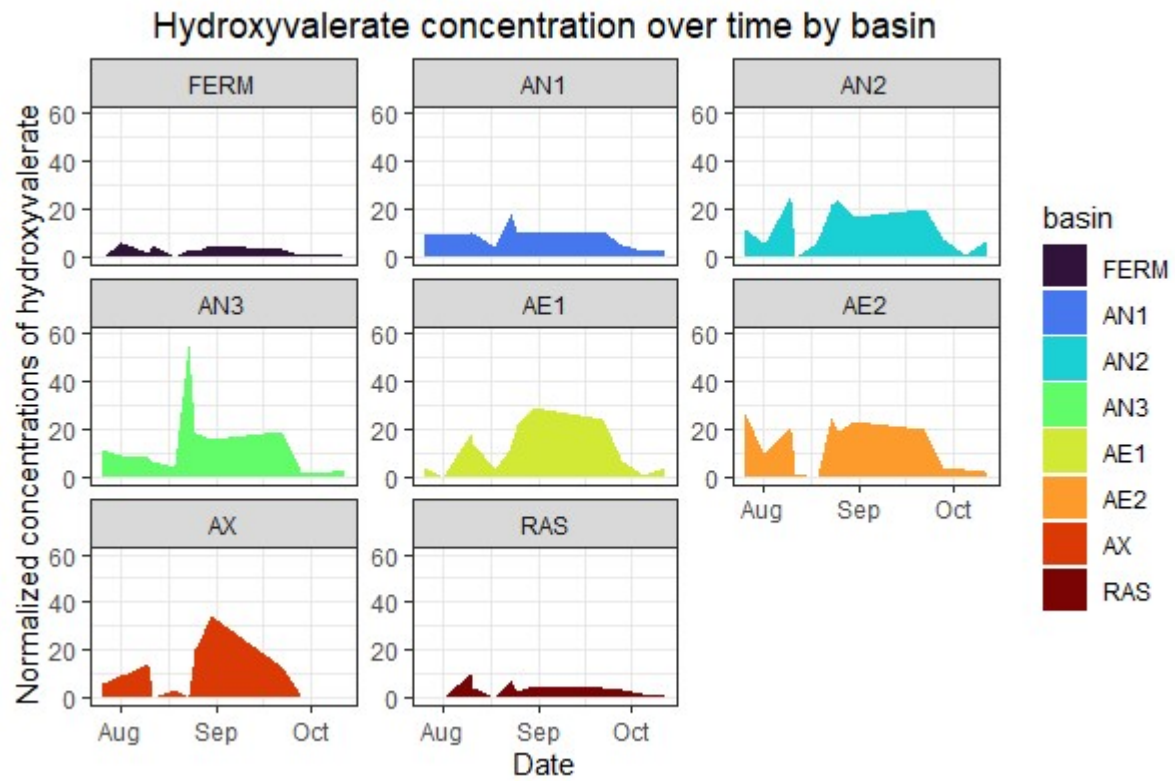
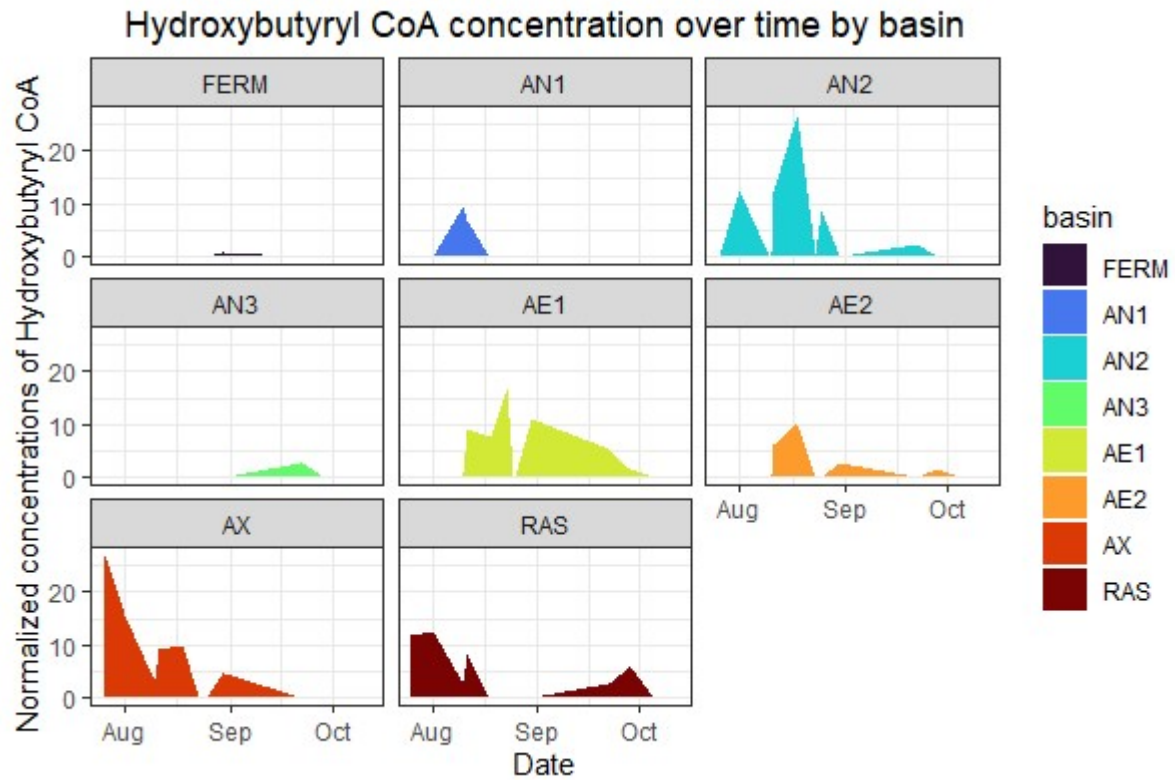


Glyoxylate concentration over time by basin

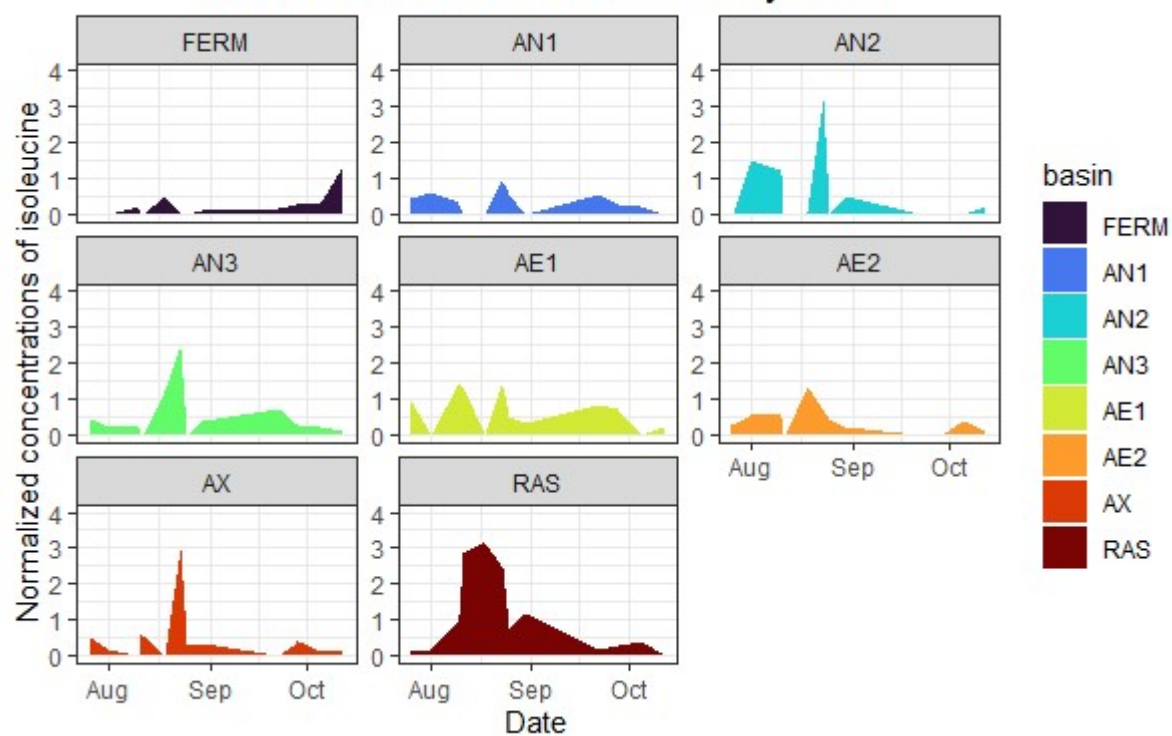


Histidine concentration over time by basin

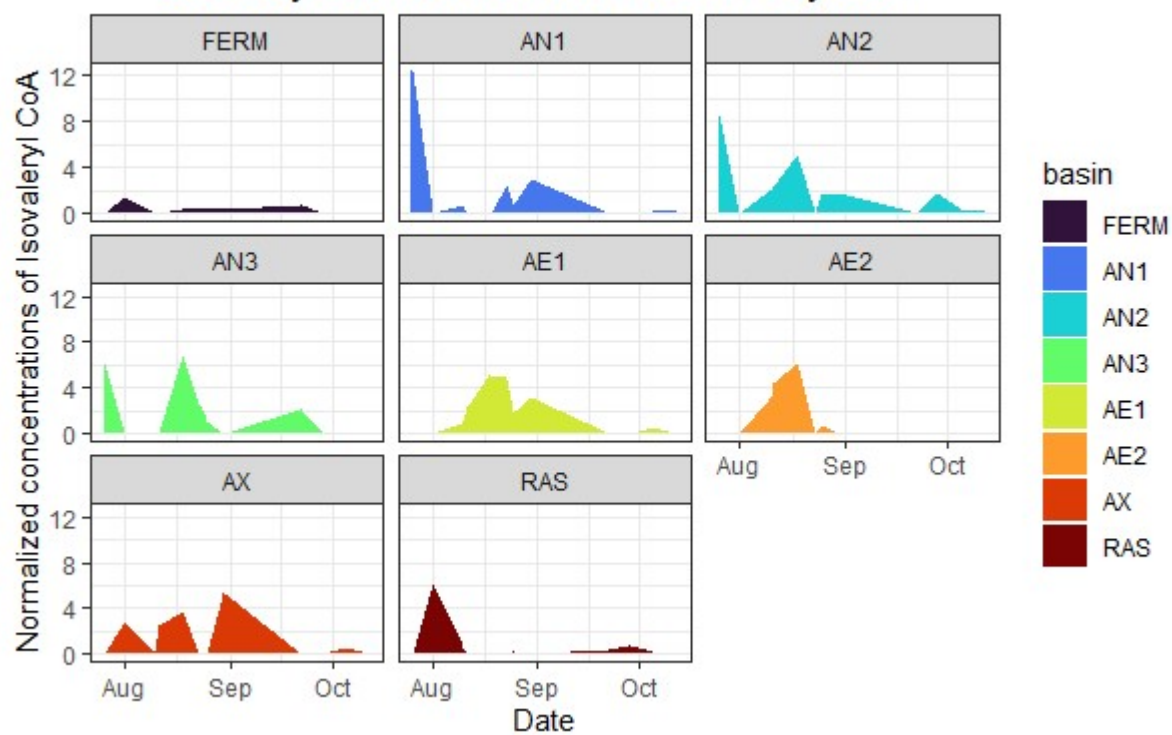




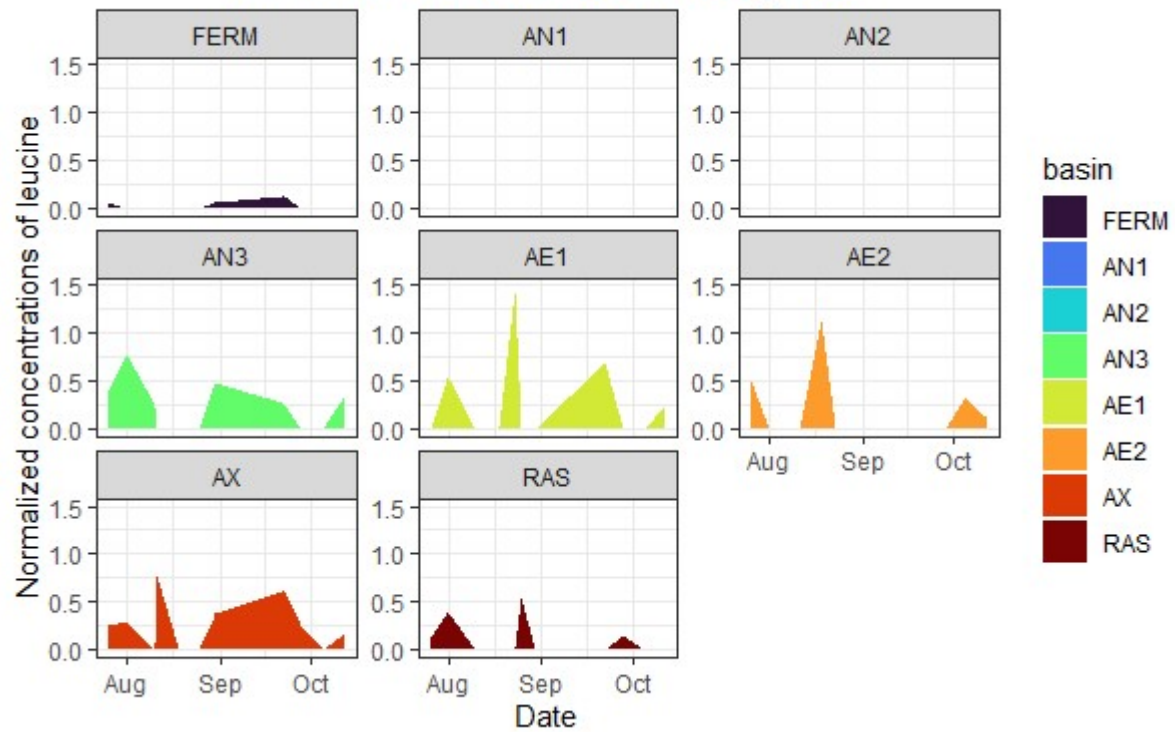
Isoleucine concentration over time by basin



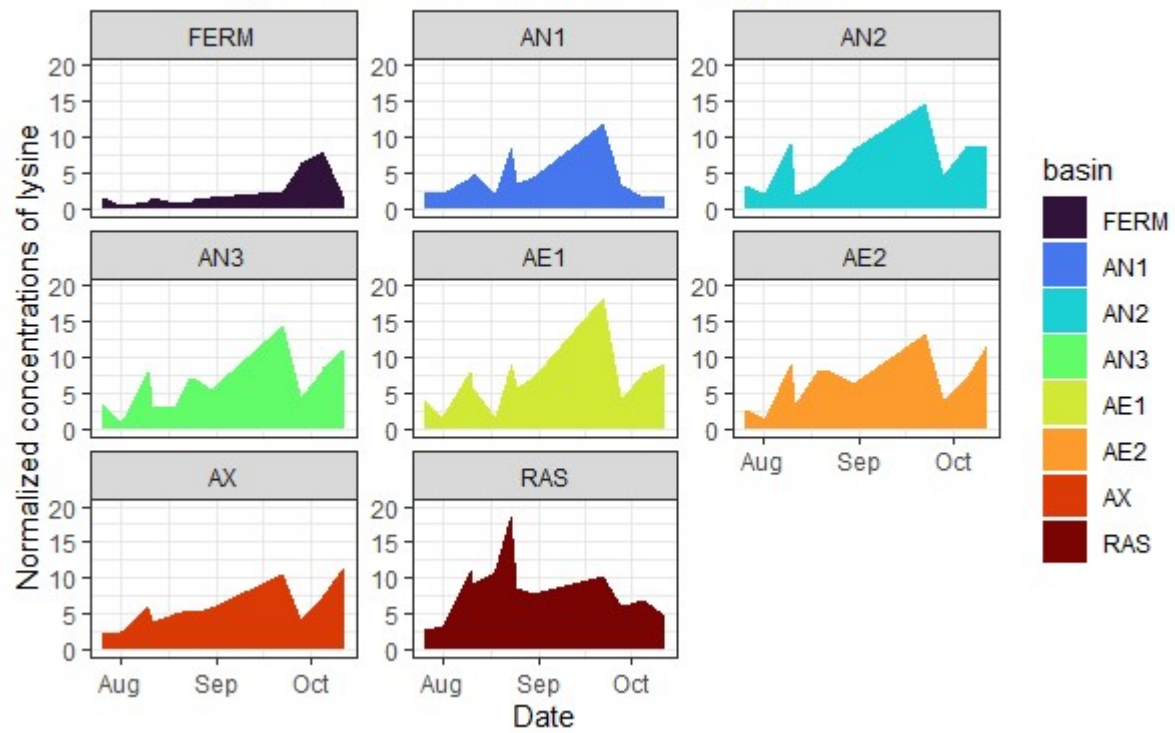
Isovaleryl CoA concentration over time by basin



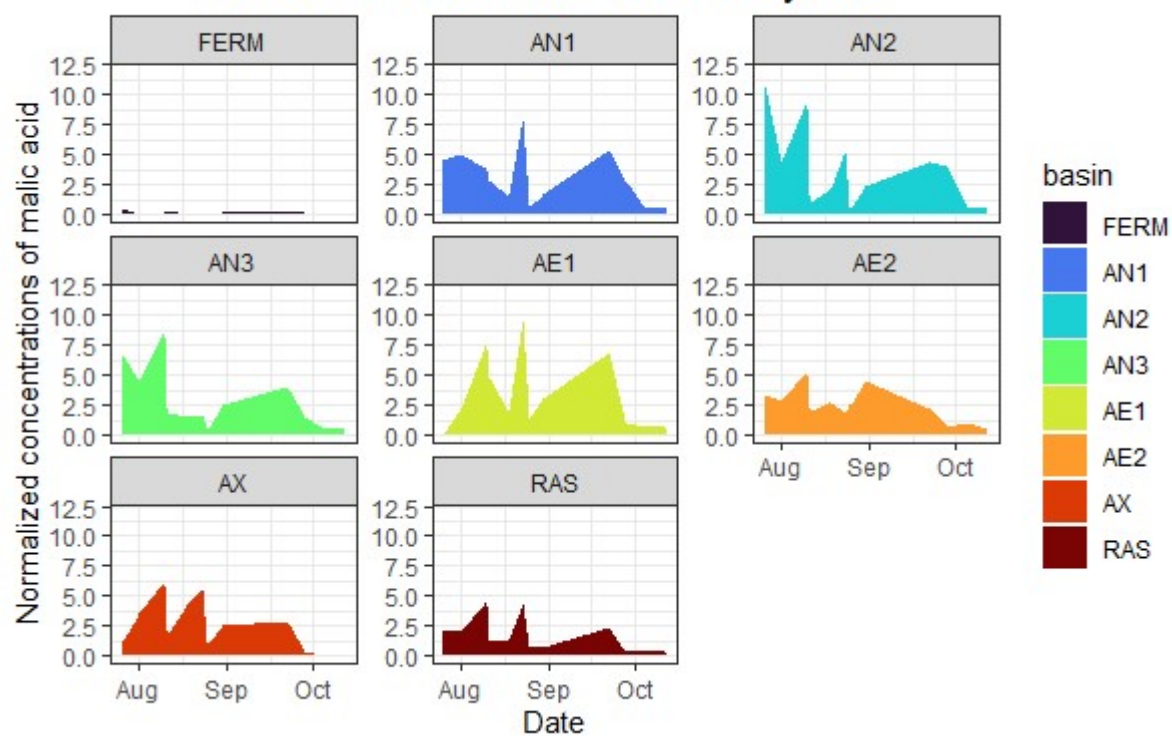
Leucine concentration over time by basin



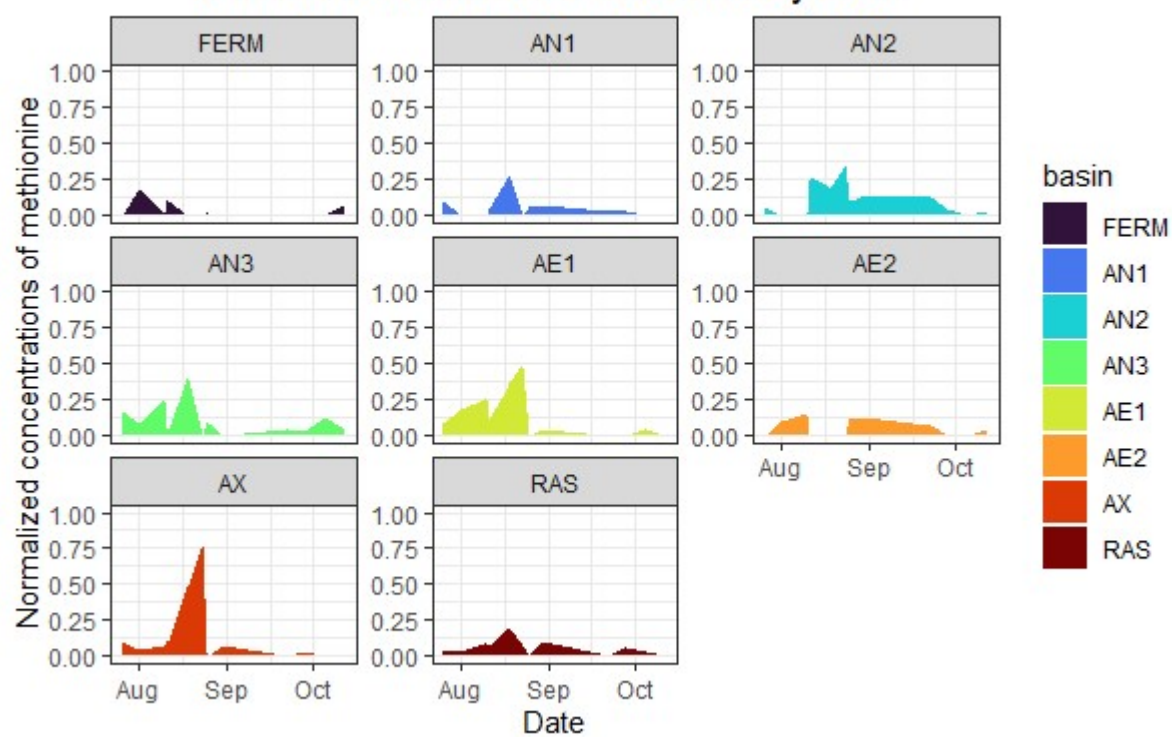
Lysine concentration over time by basin



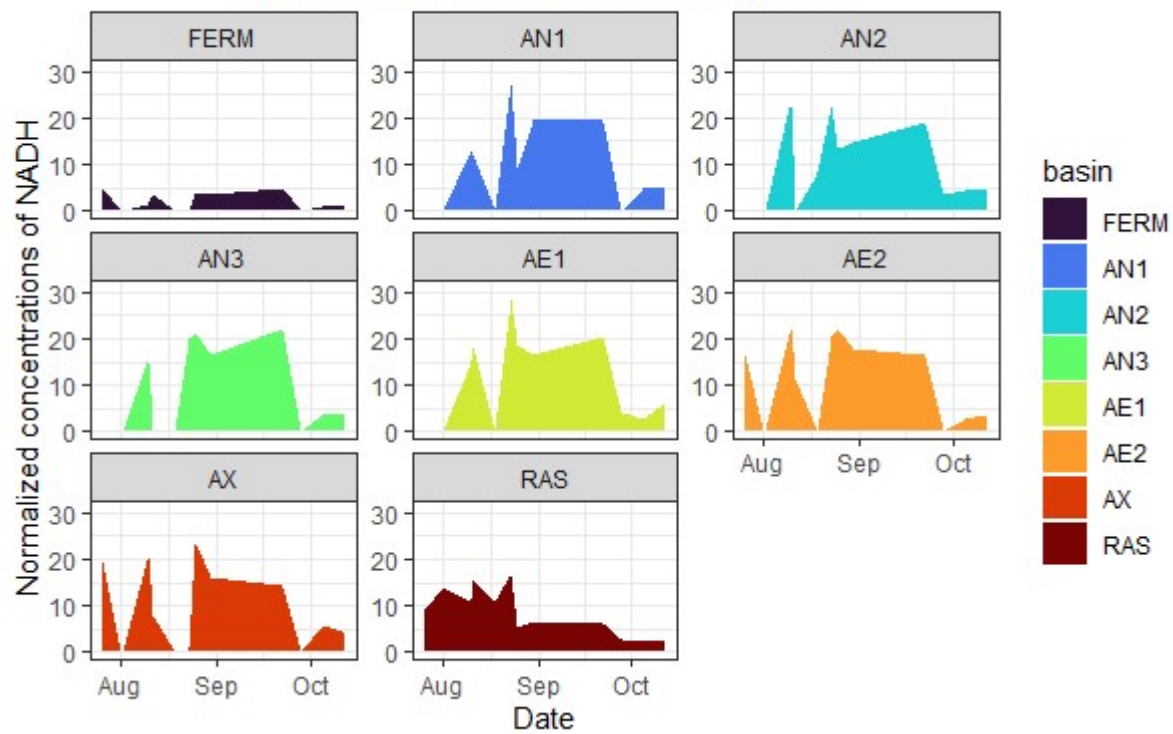
Malic acid concentration over time by basin



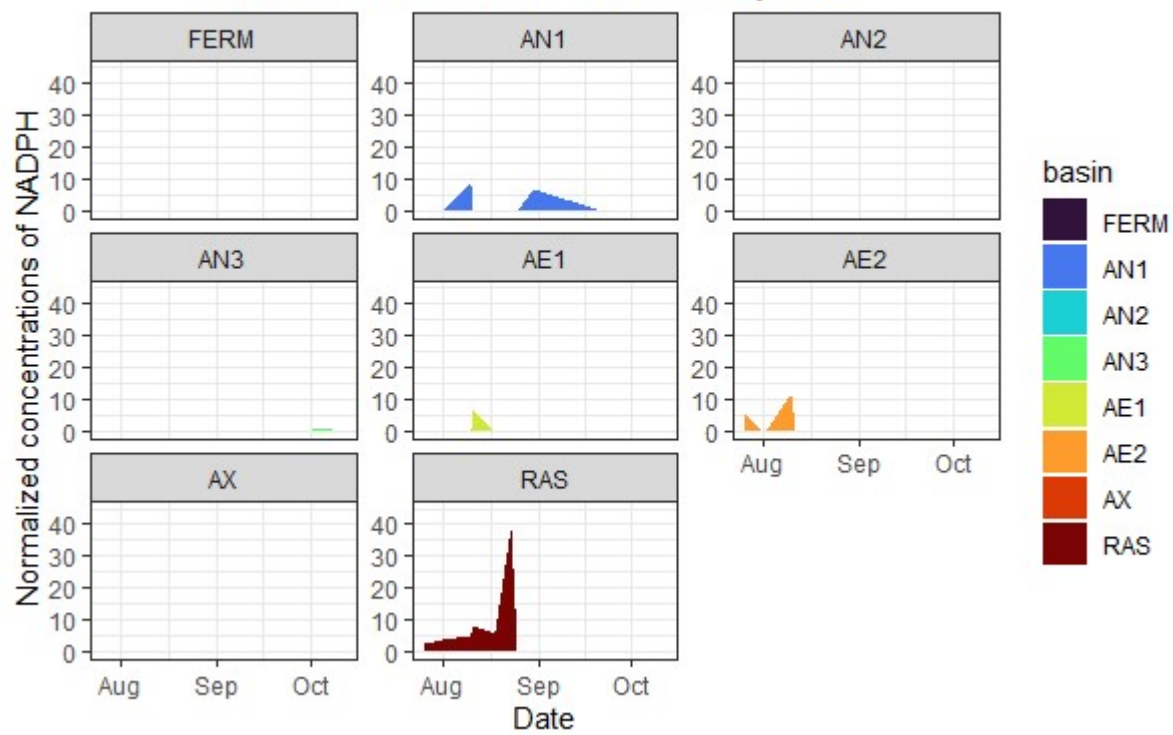
Methionine concentration over time by basin



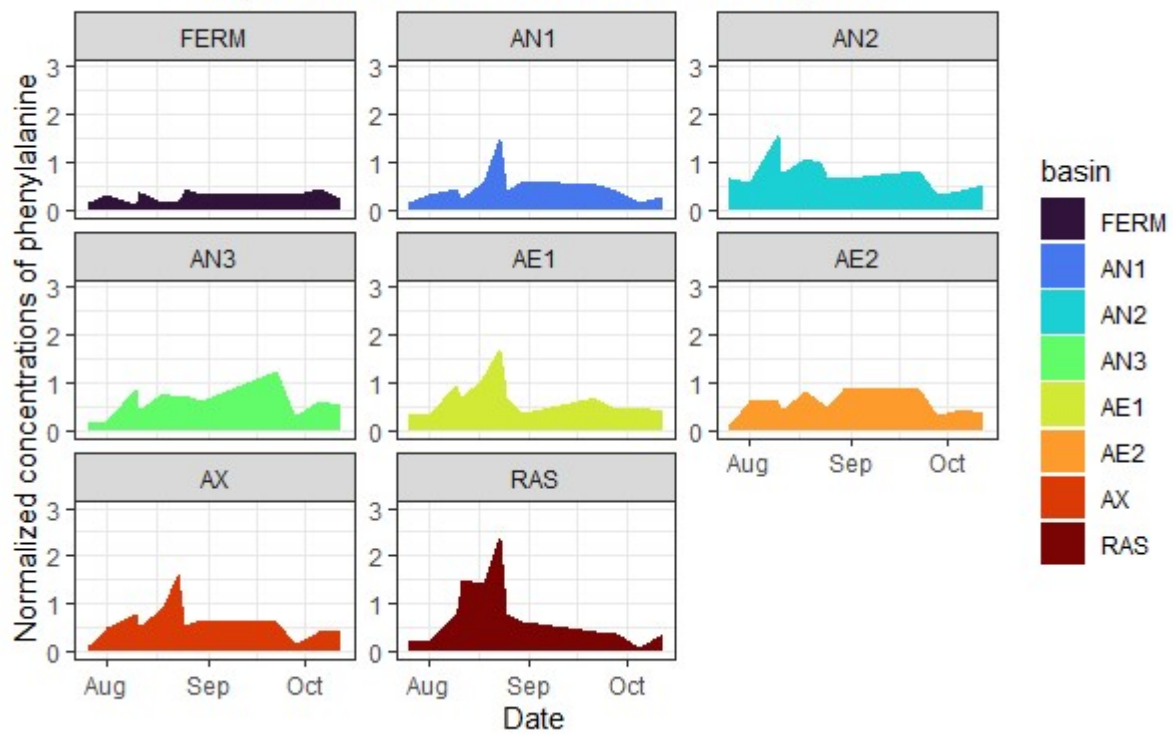
NADH concentration over time by basin



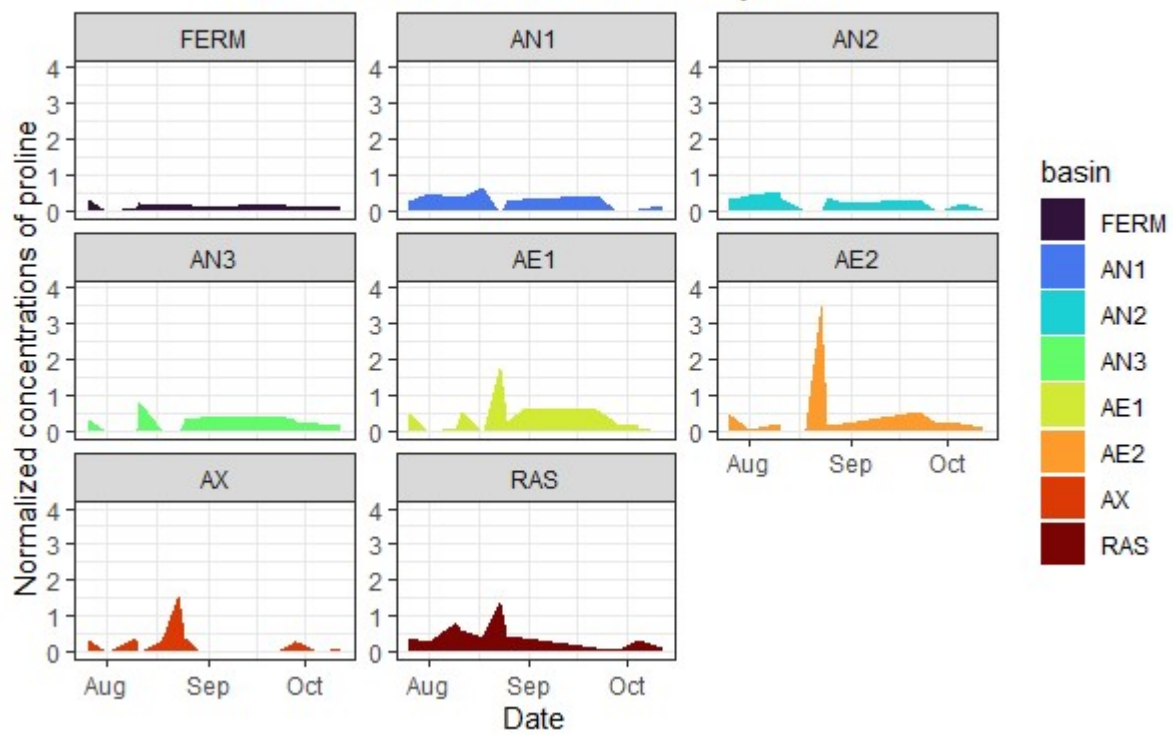
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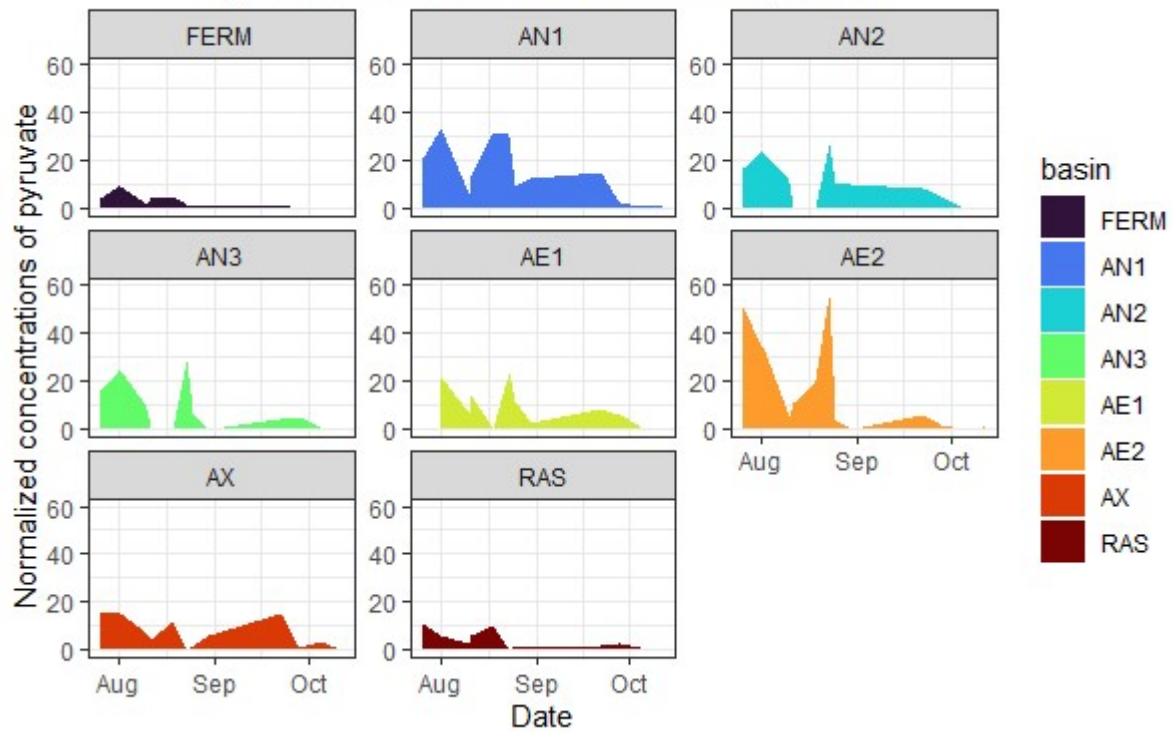
Phenylalanine concentration over time by basin



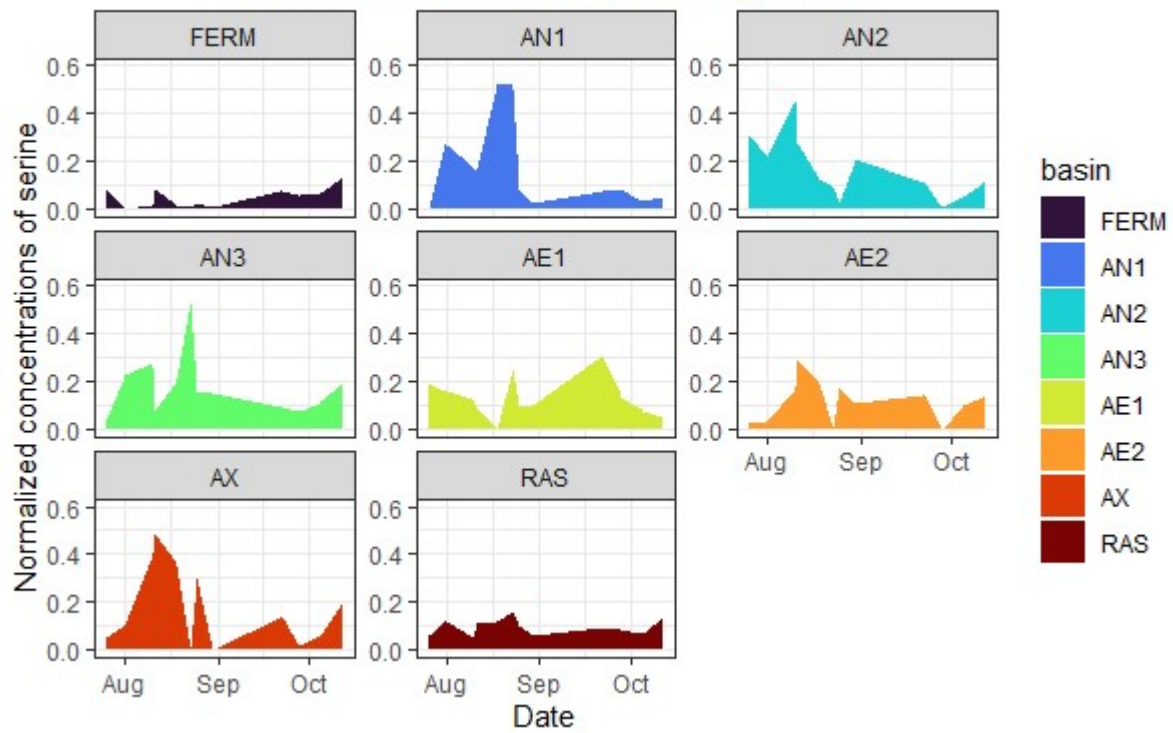
Proline concentration over time by basin



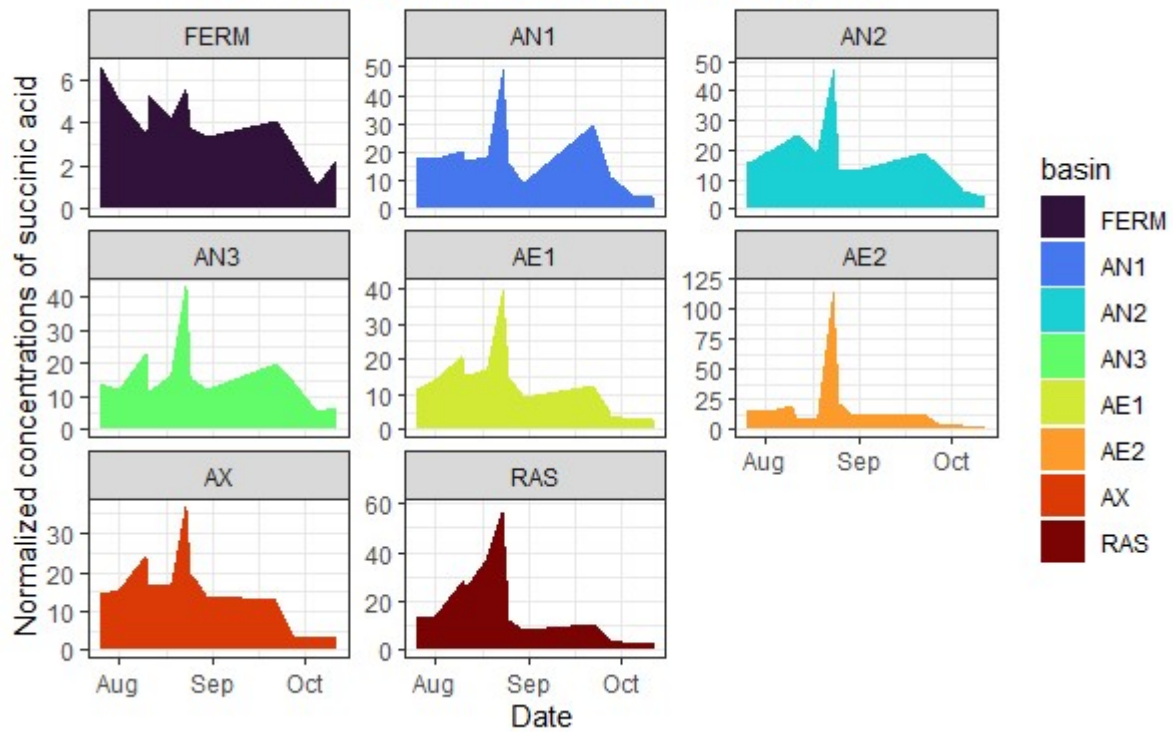
Pyruvate concentration over time by basin



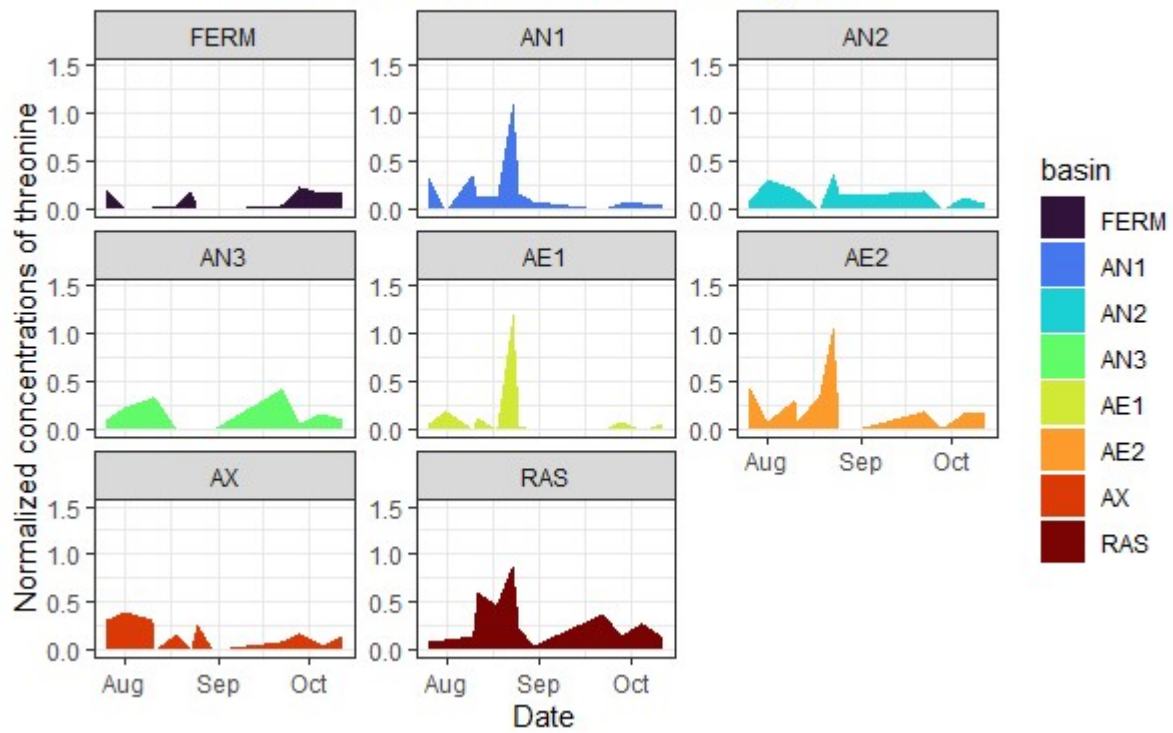
Serine concentration over time by basin



Succinic acid concentration over time by basin



Threonine concentration over time by basin



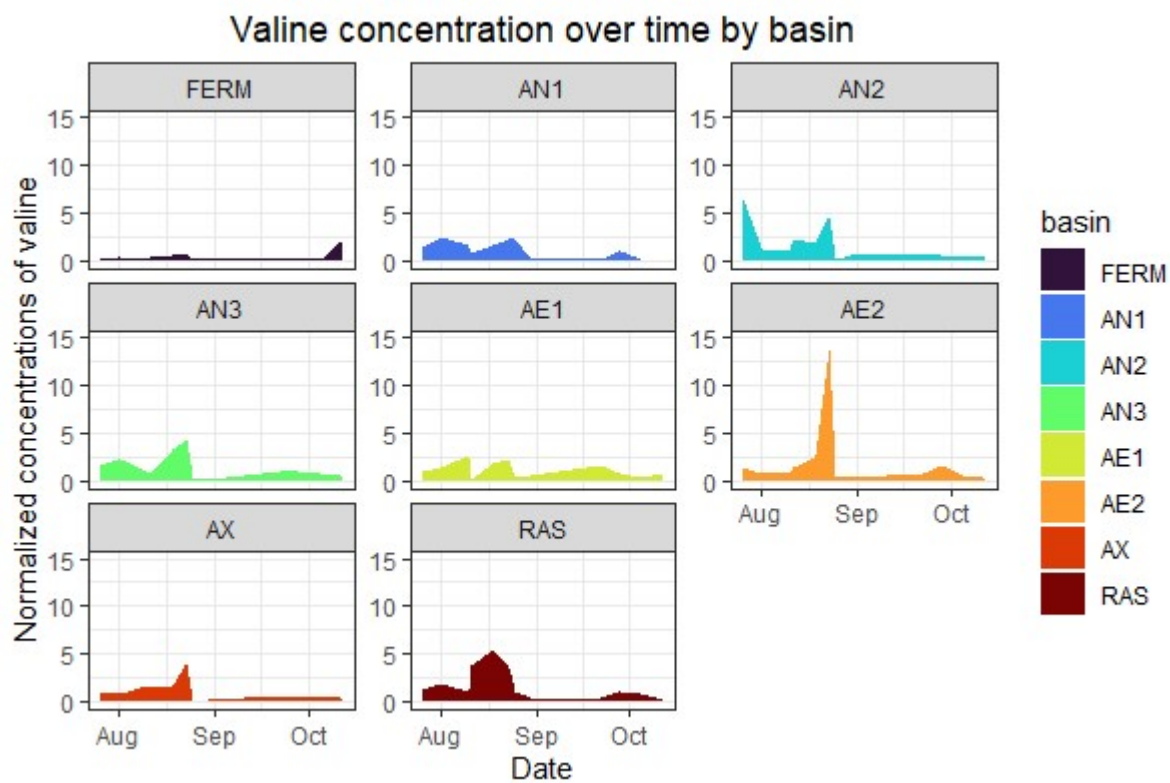
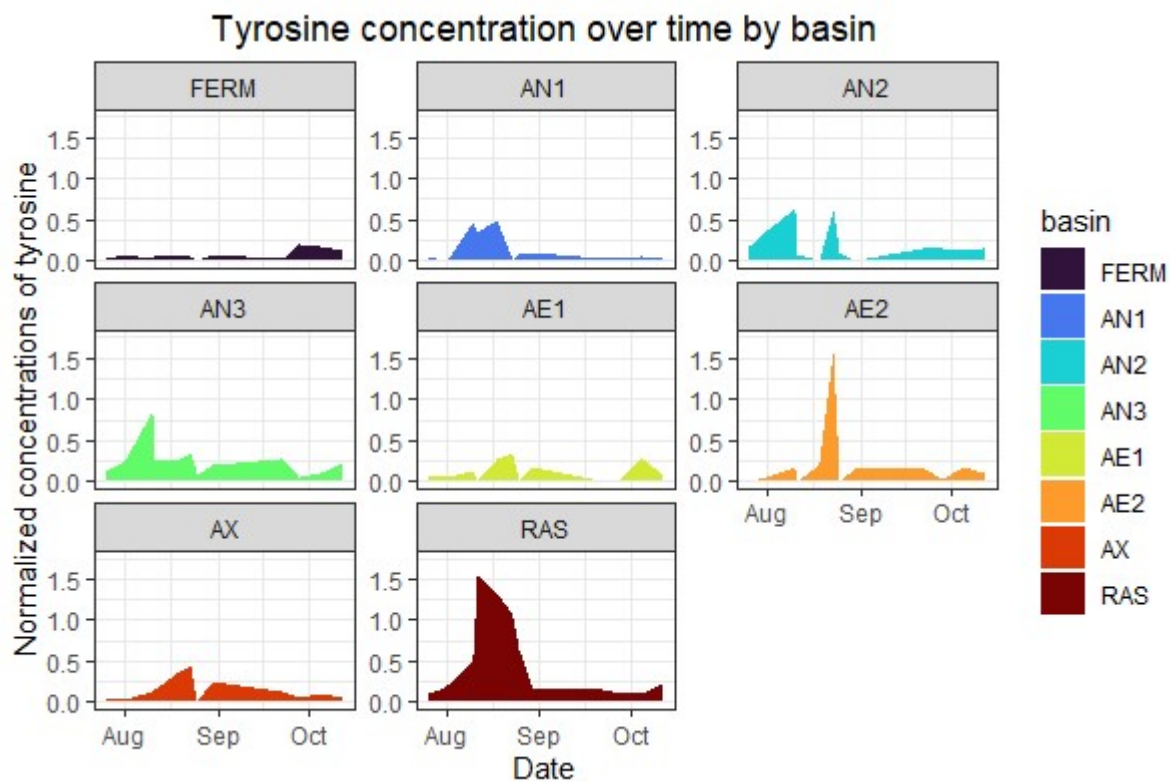
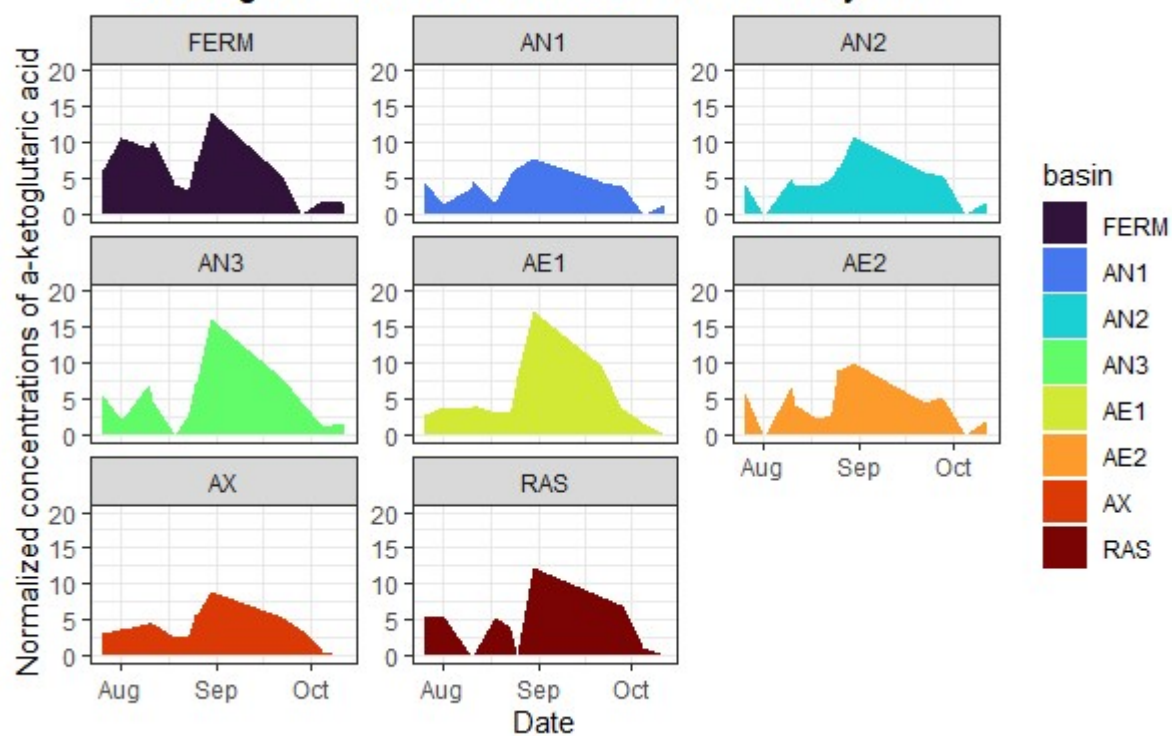
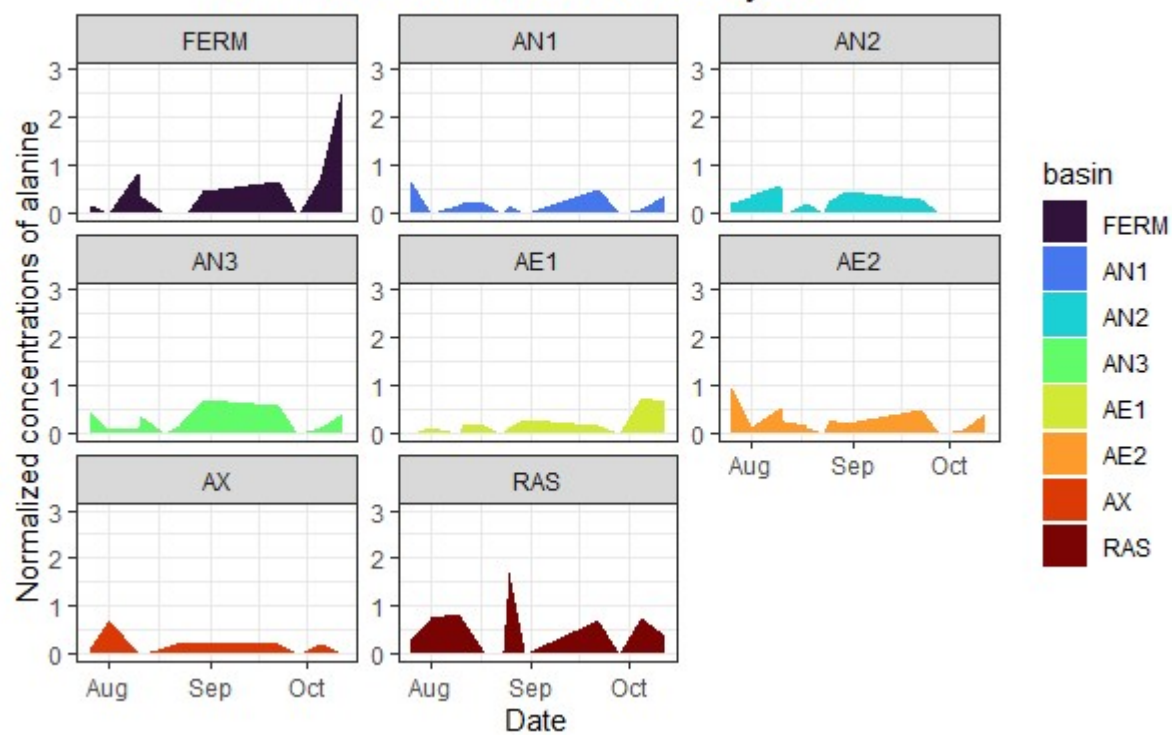


Figure S1: Temporal metabolome trends by basin, normalized to MLSS. Data up to and including Aug. 1st was pre-ROC; Aug. 2-Sept. 28 represents data for a ROC augmented WRRF; Sept. 29-Oct. 13 represents post-ROC loading.

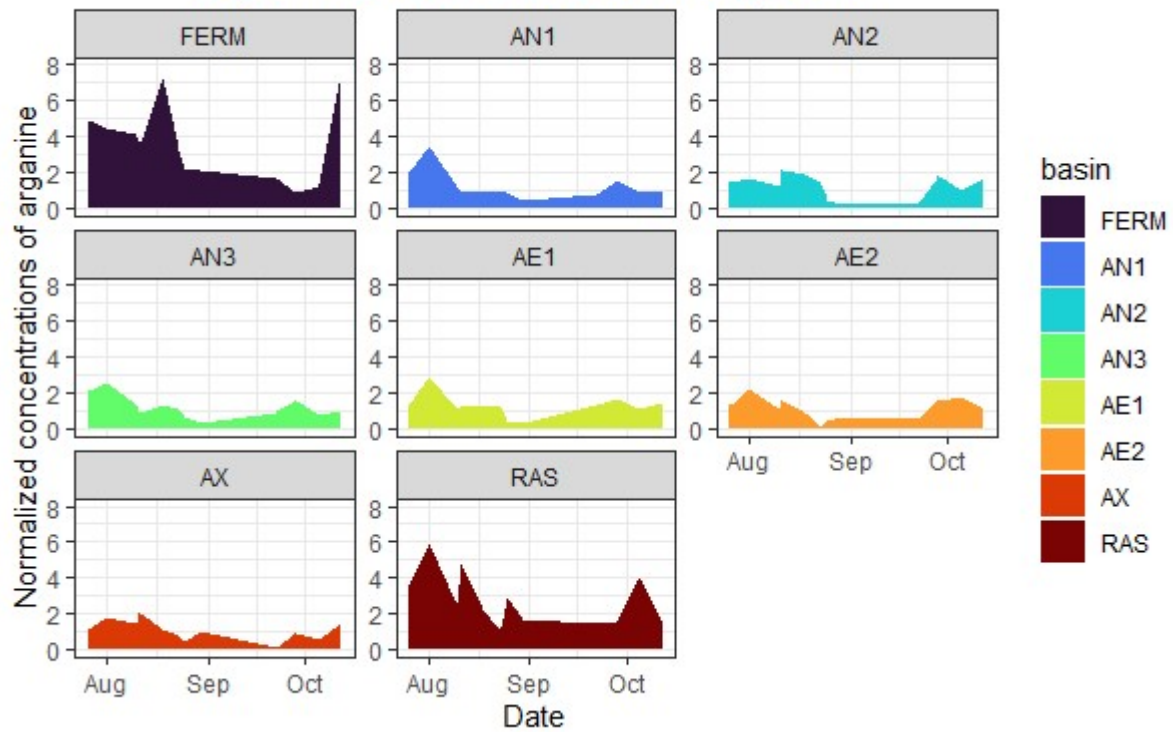
a-Ketoglutaric acid concentration over time by basin



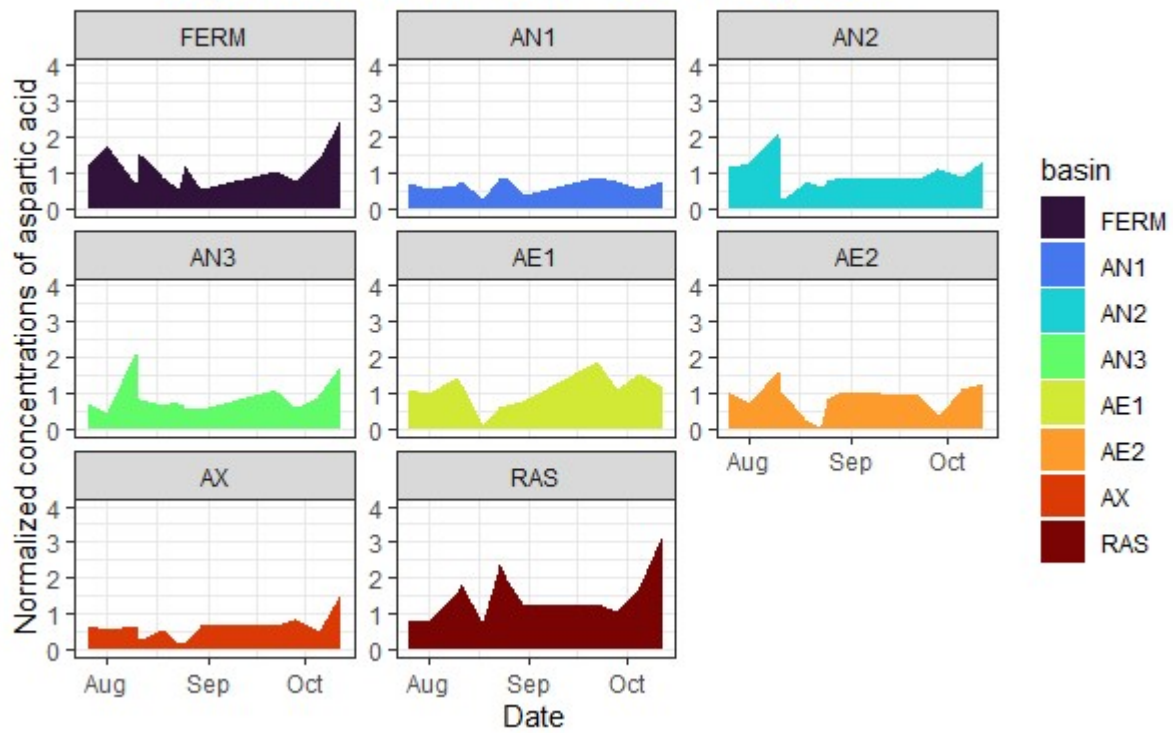
Alanine concentration over time by basin



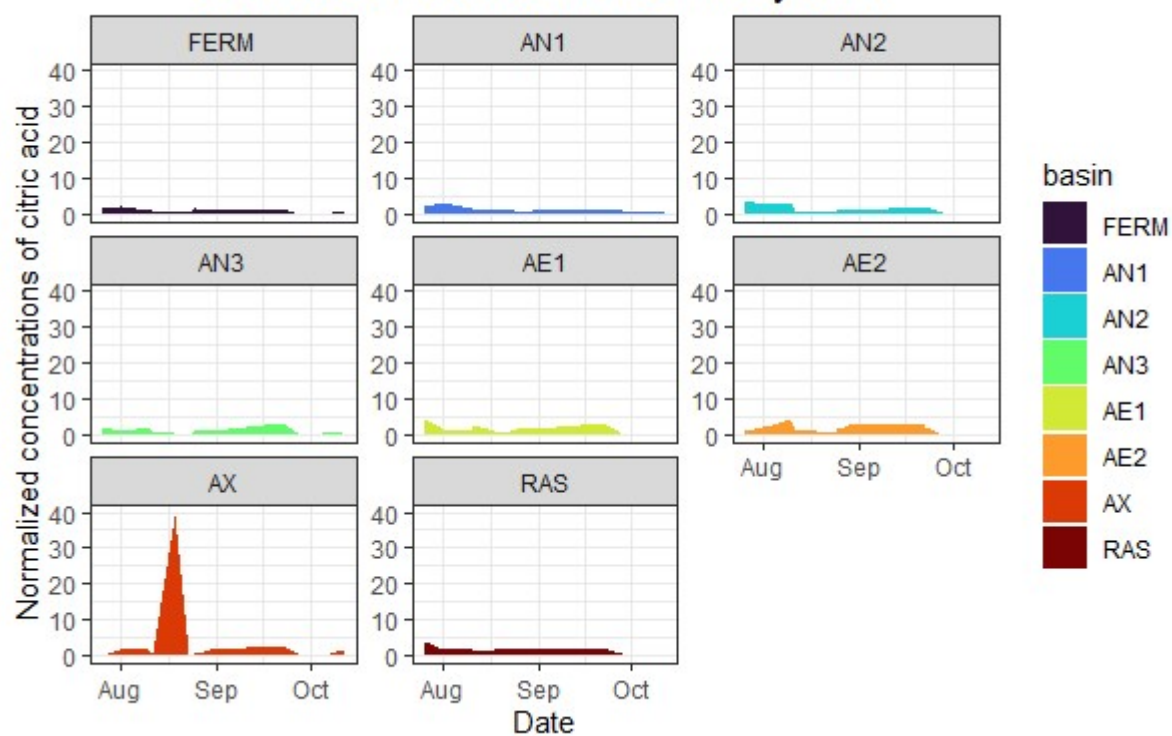
Arginine concentration over time by basin



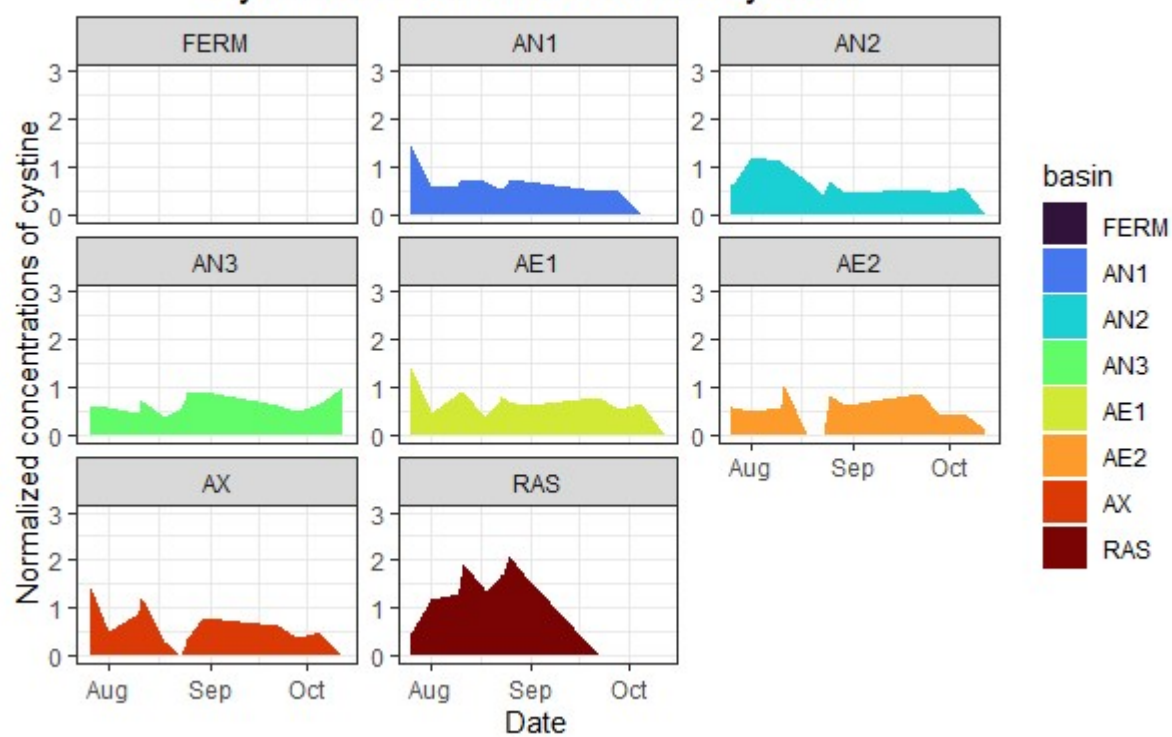
Aspartic acid concentration over time by basin



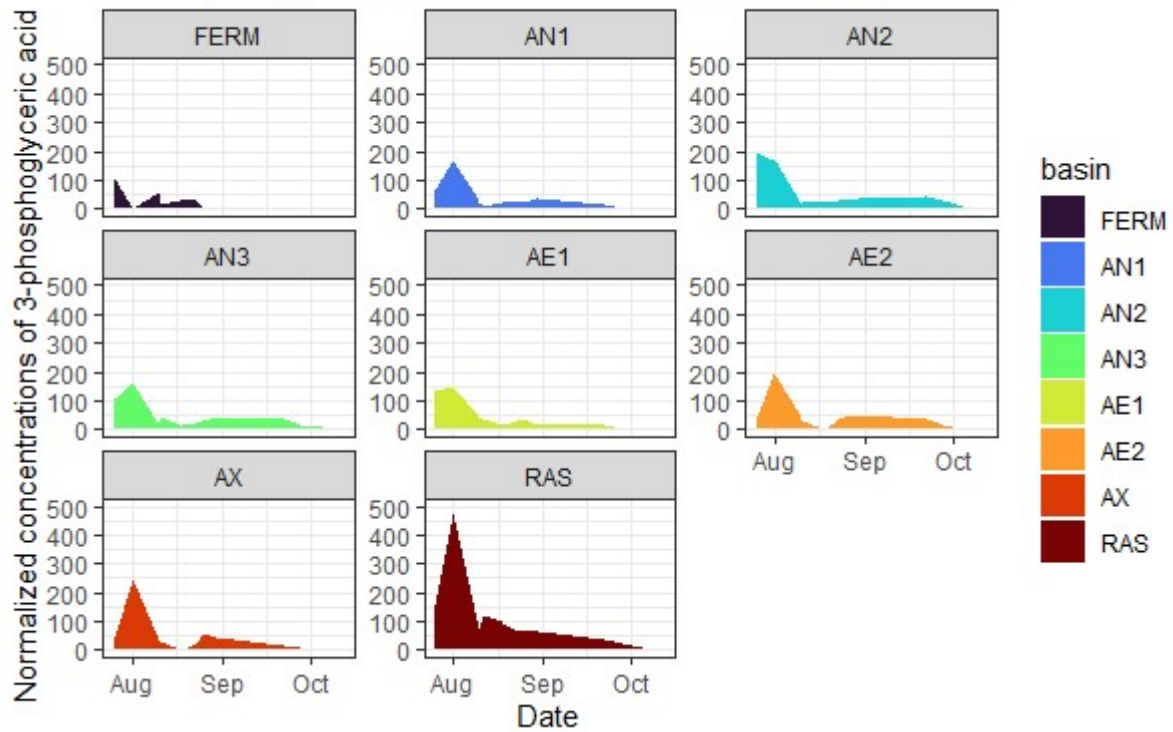
Citric acid concentration over time by basin



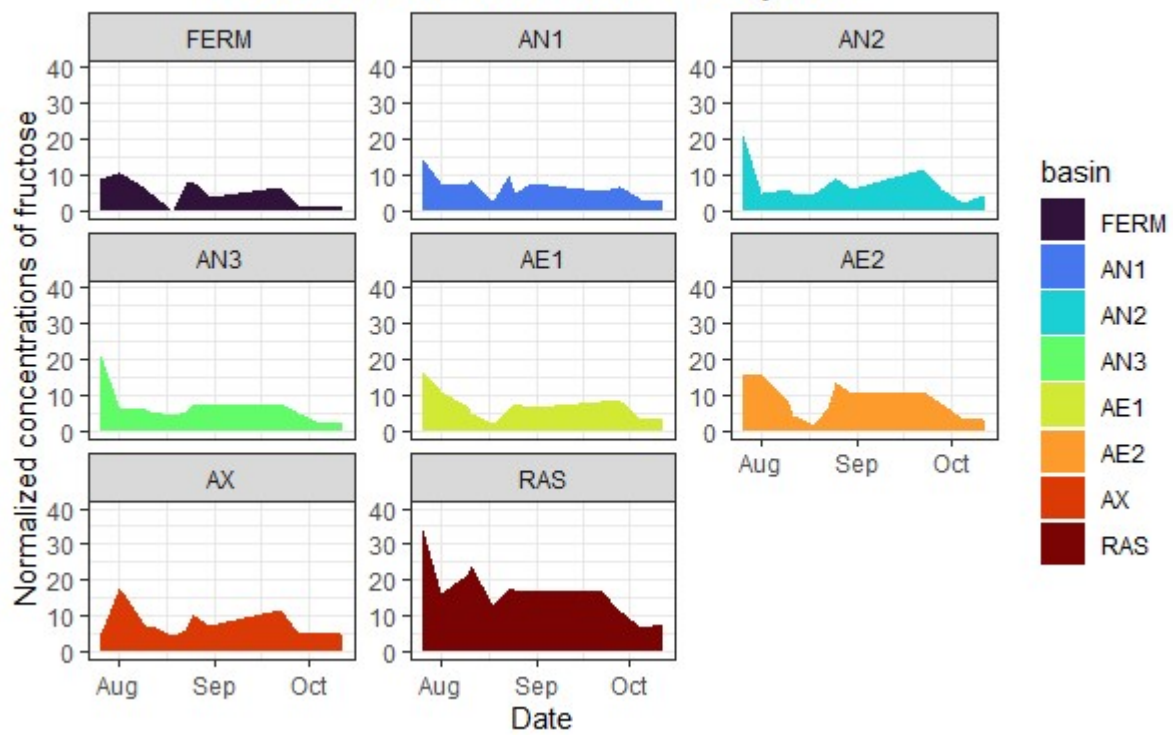
Cystine concentration over time by basin



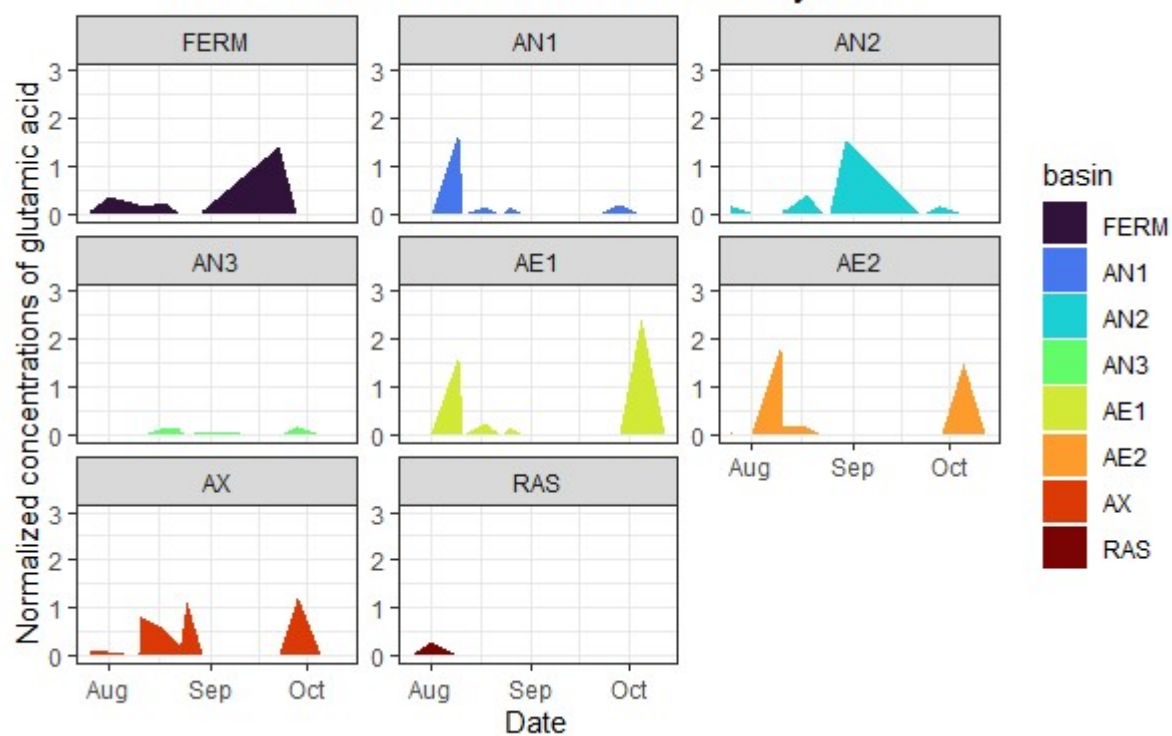
3-Phosphoglyceric acid concentration over time by basin



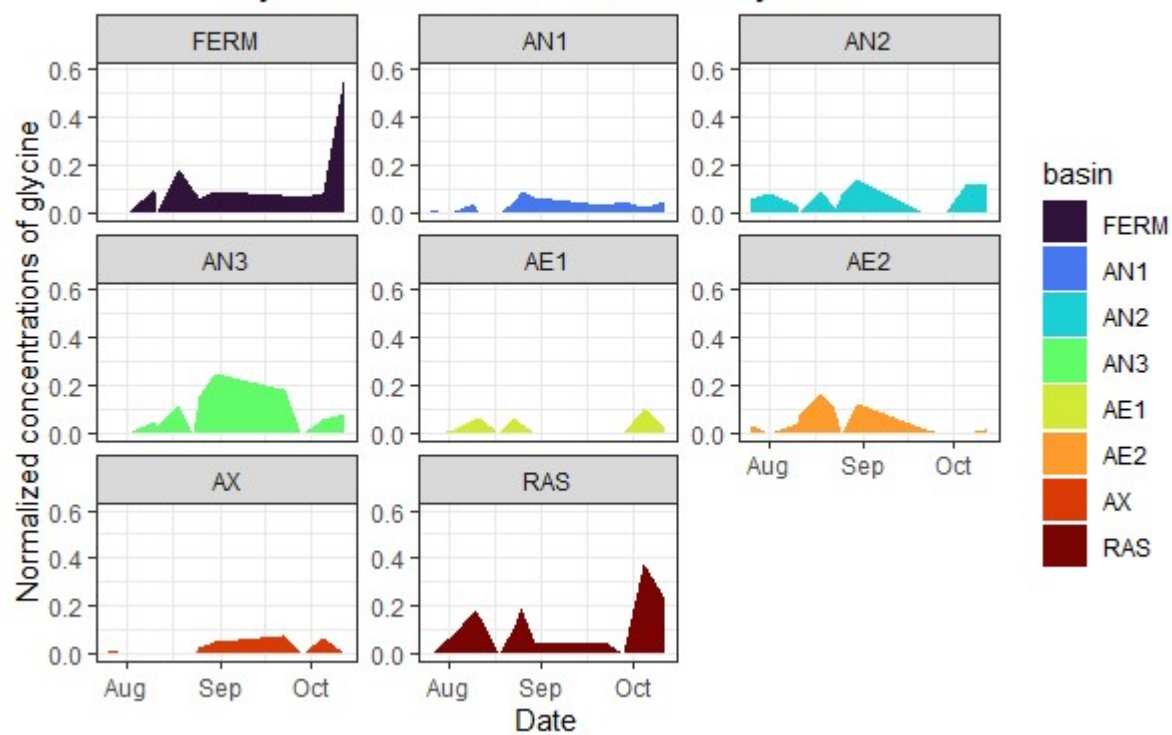
Fructose concentration over time by basin



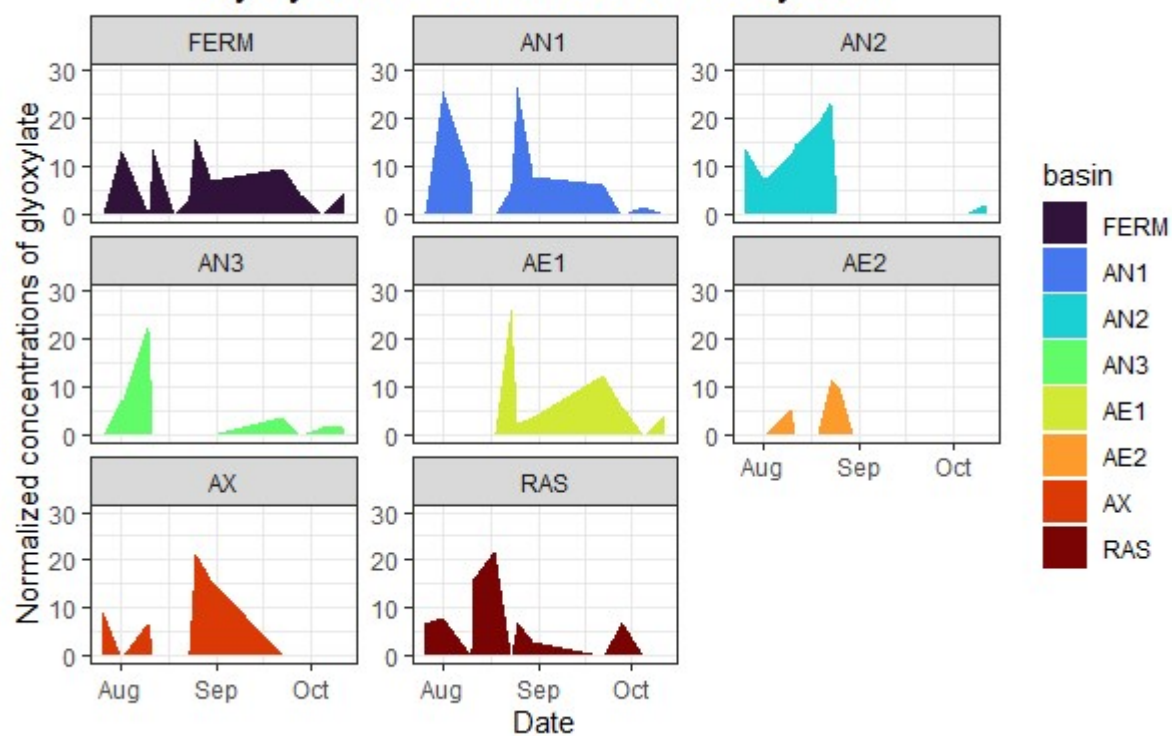
Glutamic acid concentration over time by basin



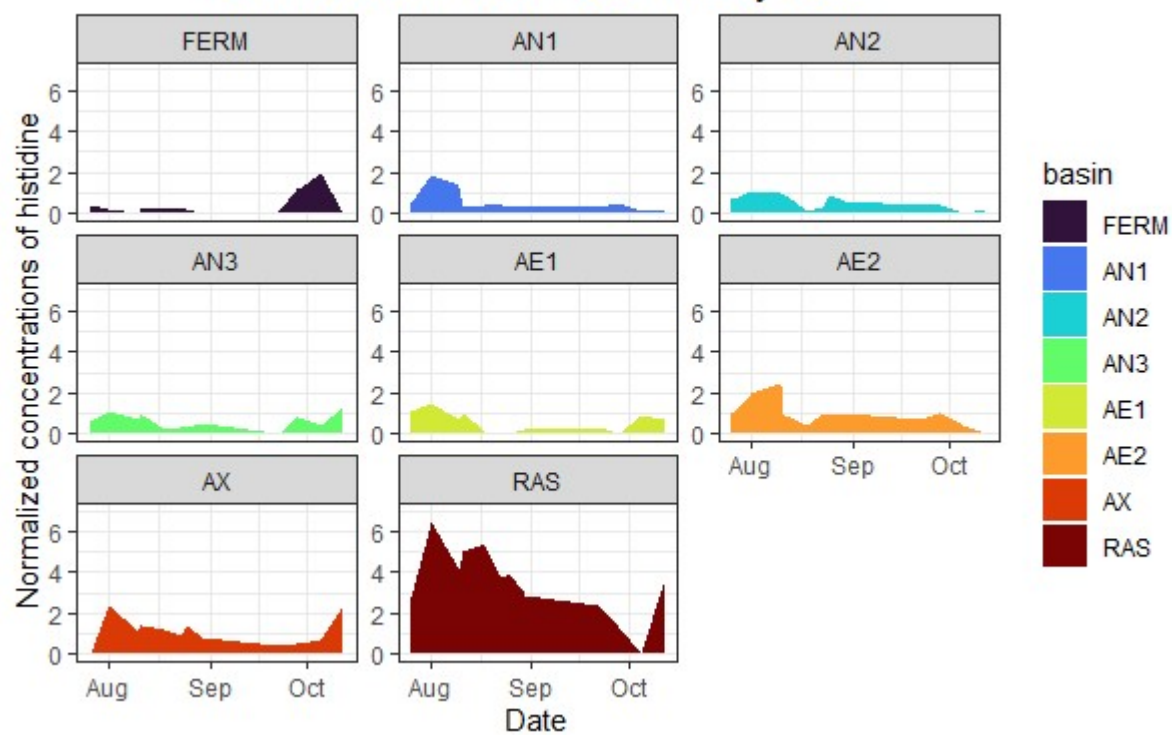
Glycine concentration over time by basin



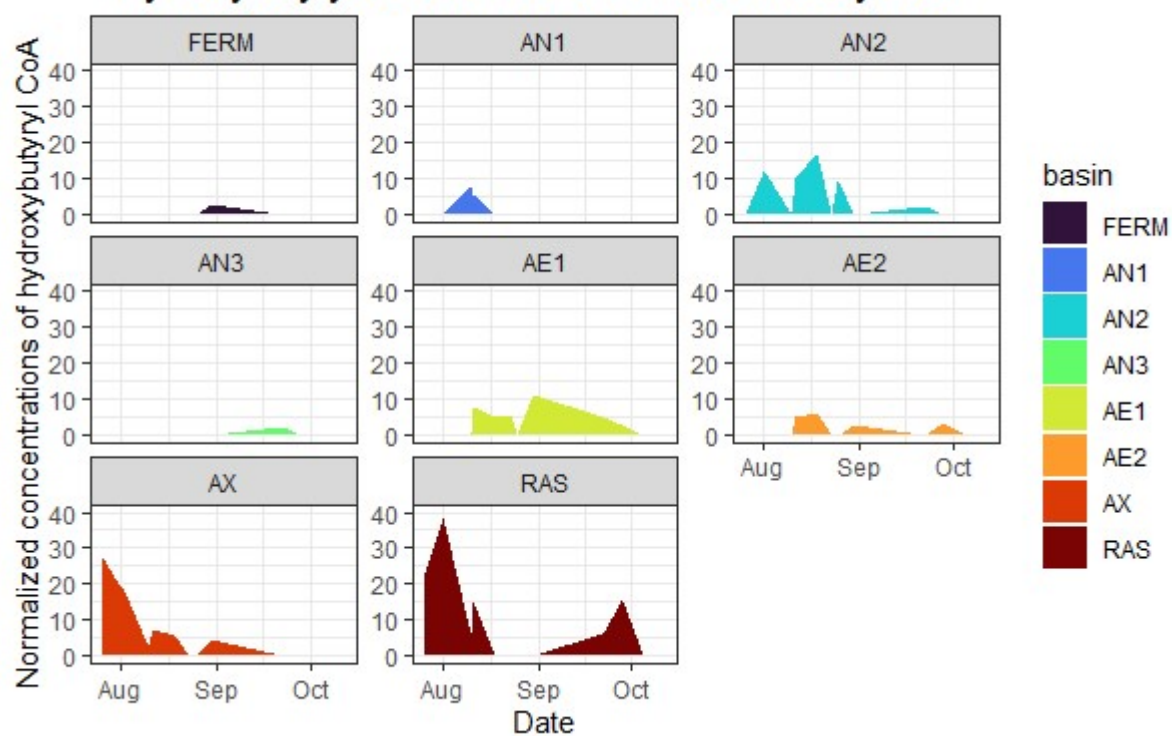
Glyoxylate concentration over time by basin



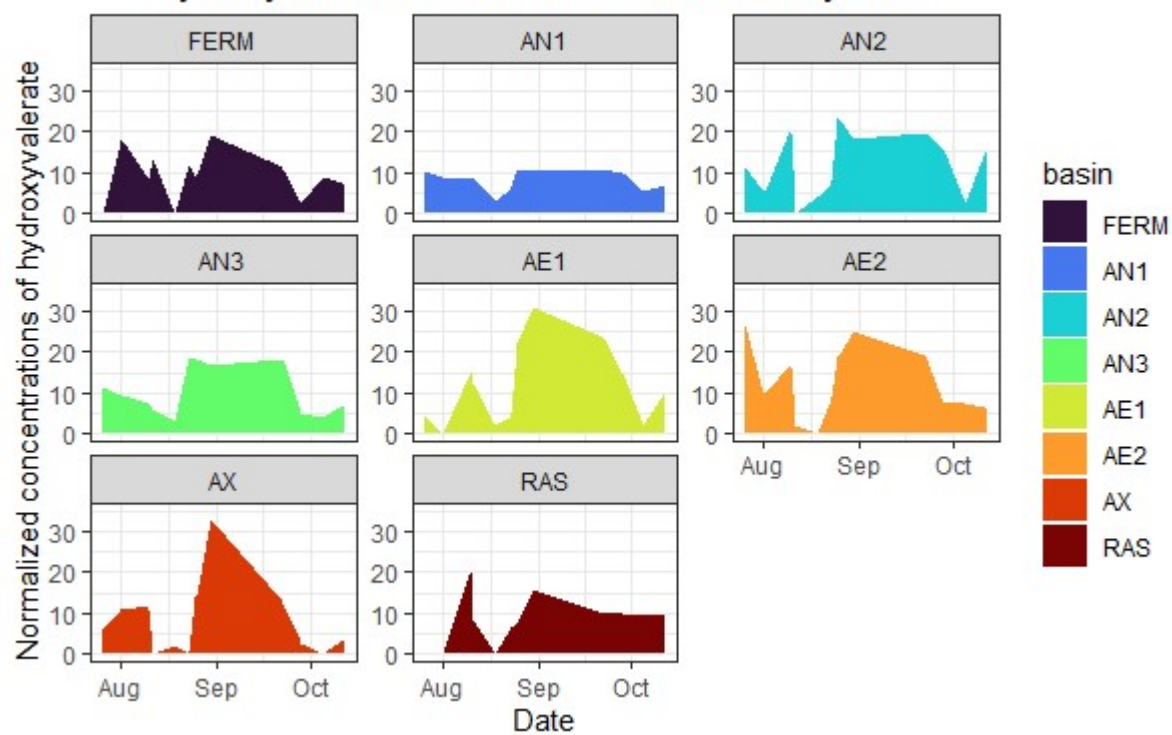
Histidine concentration over time by basin



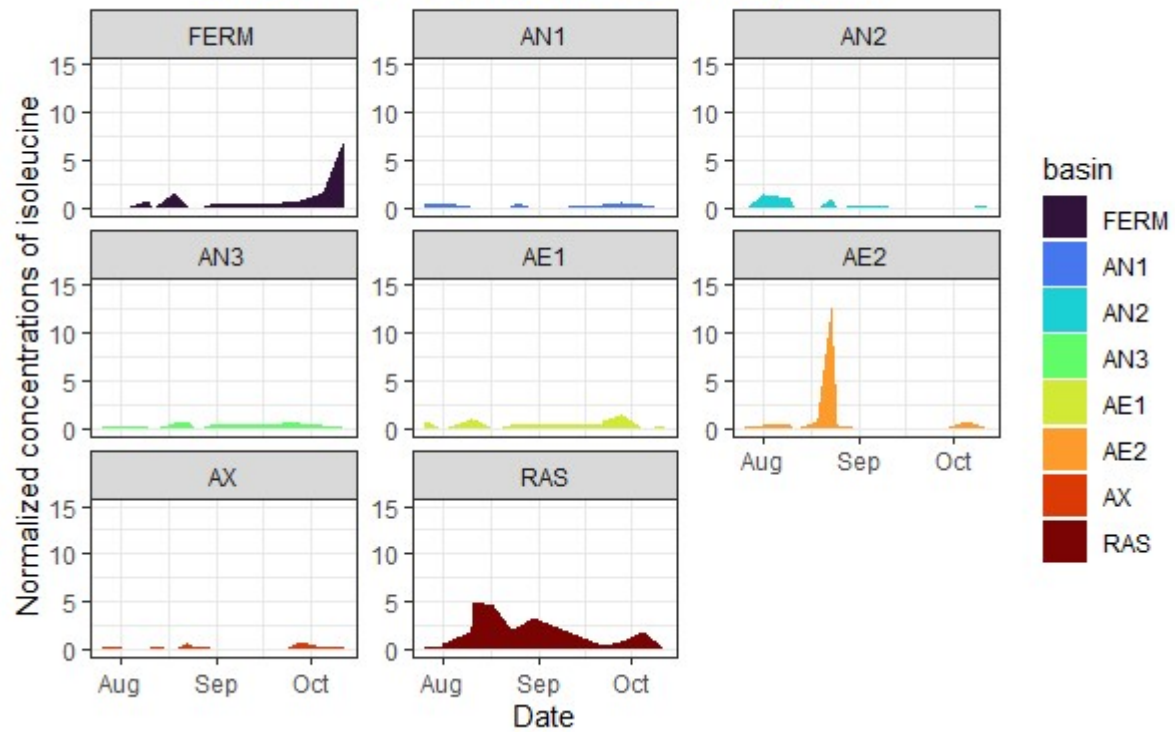
Hydroxybutyryl CoA concentration over time by basin



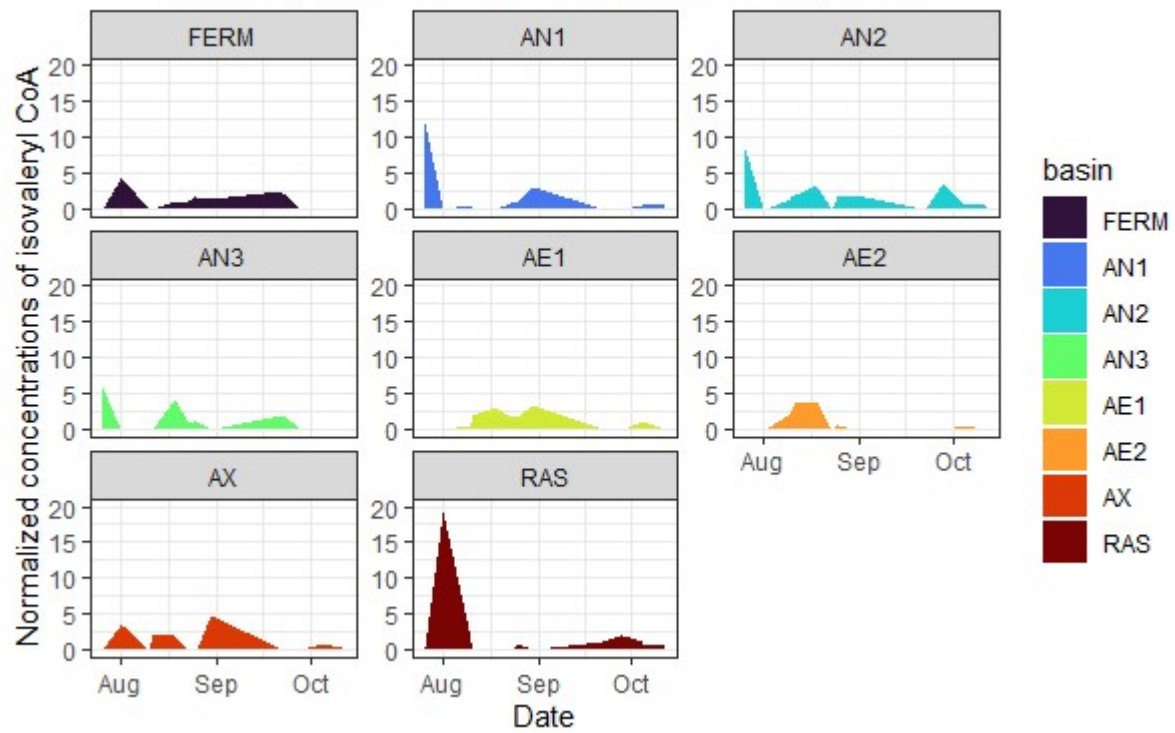
Hydroxyvalerate concentration over time by basin



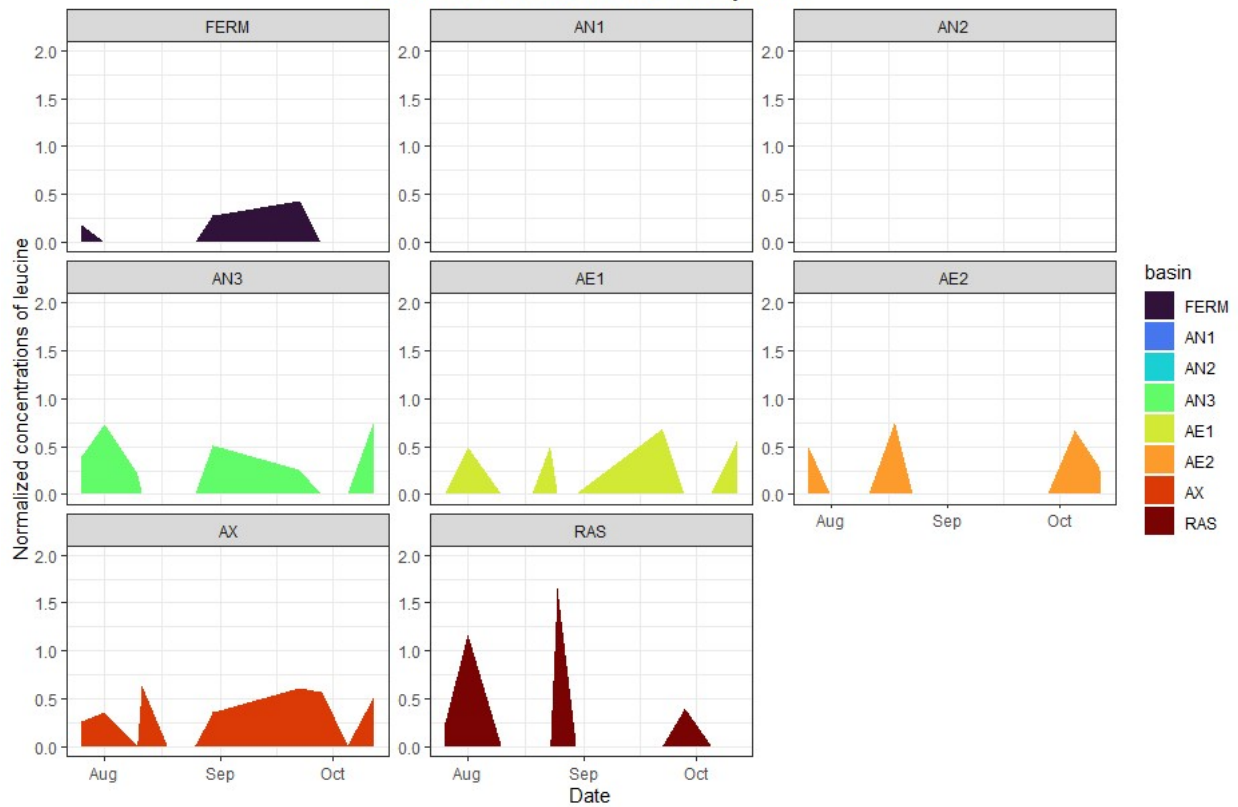
Isoleucine concentration over time by basin



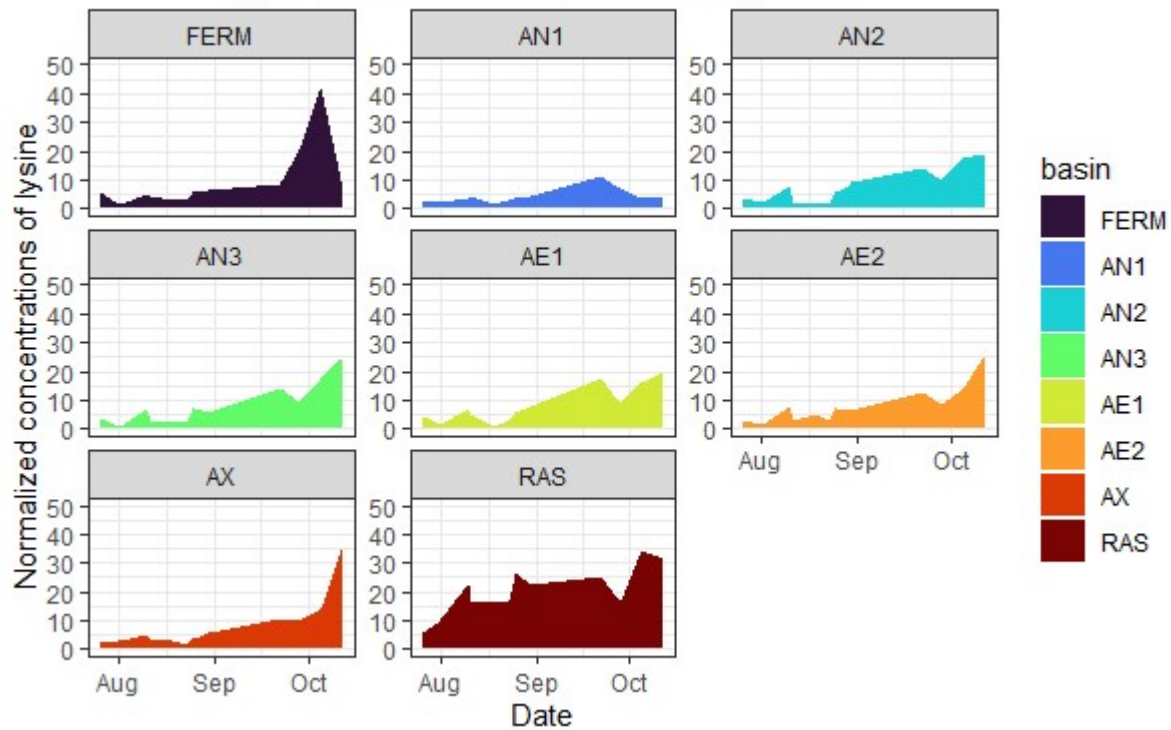
Isovaleryl CoA concentration over time by basin



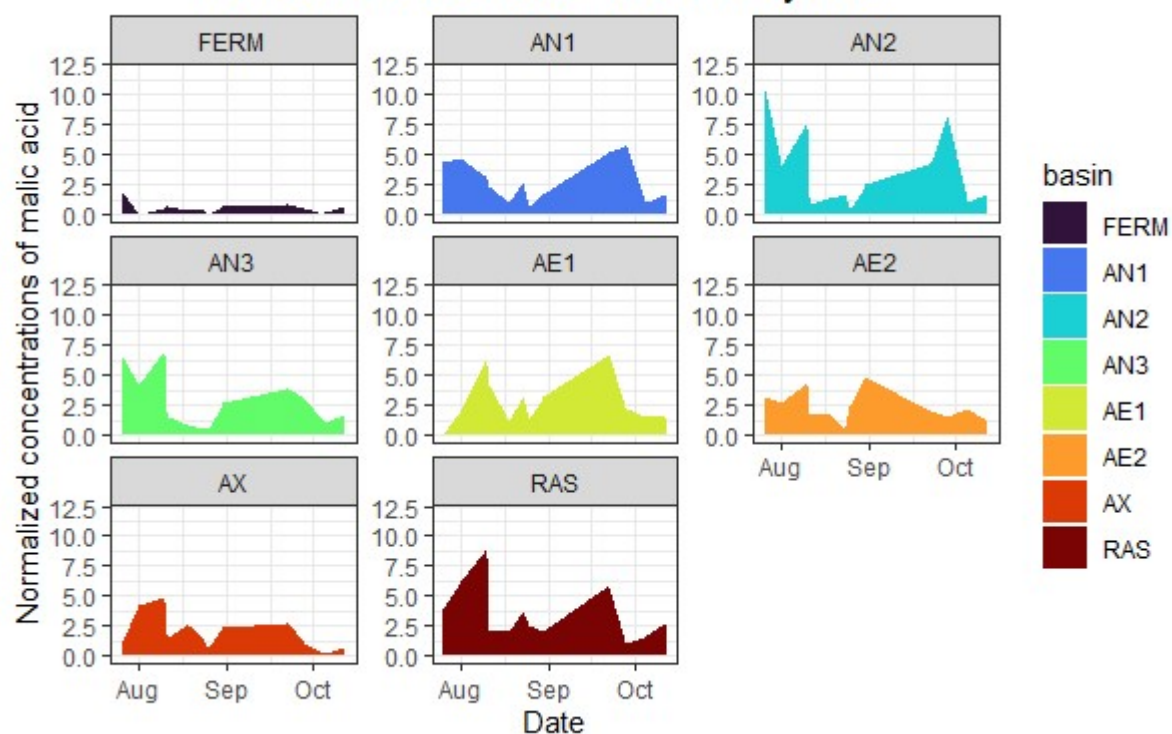
Leucine concentration over time by basin



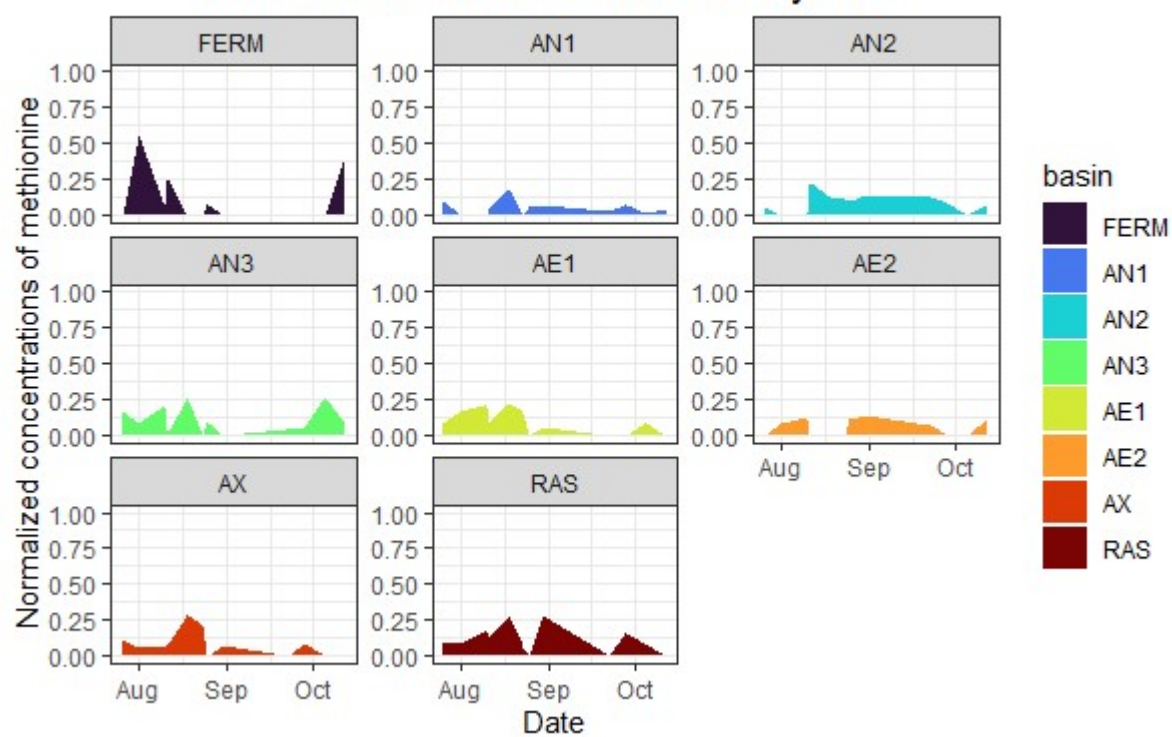
Lysine concentration over time by basin



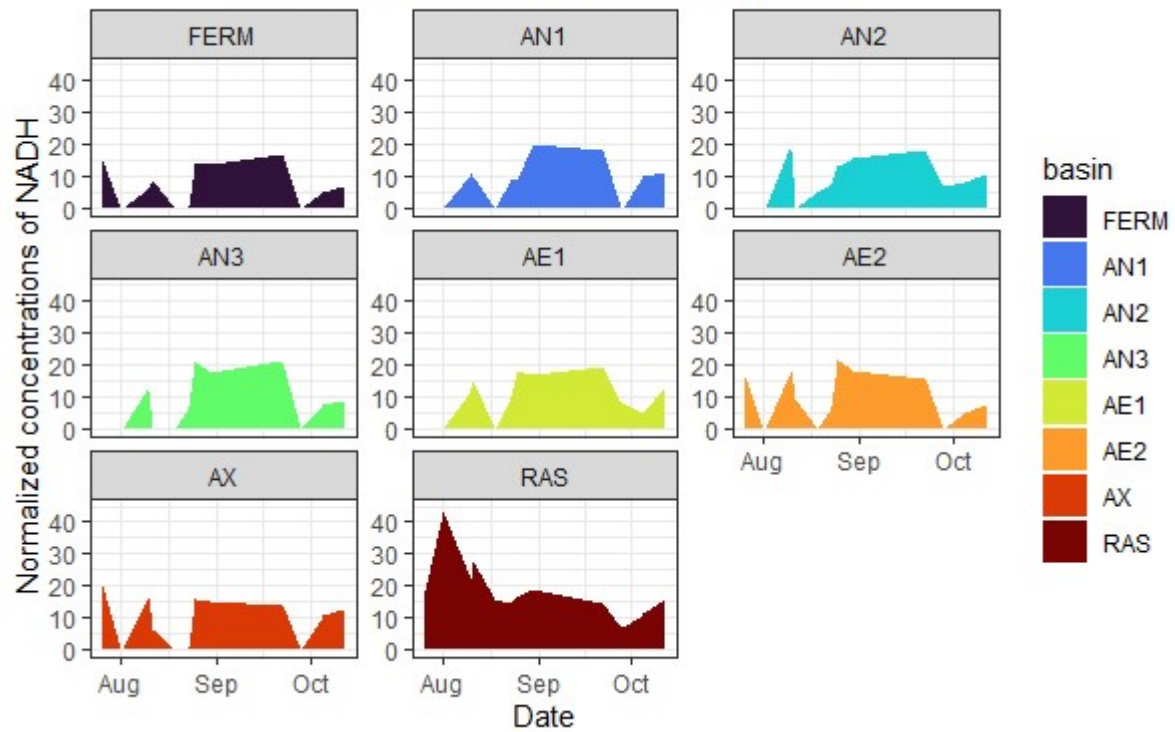
Malic acid concentration over time by basin



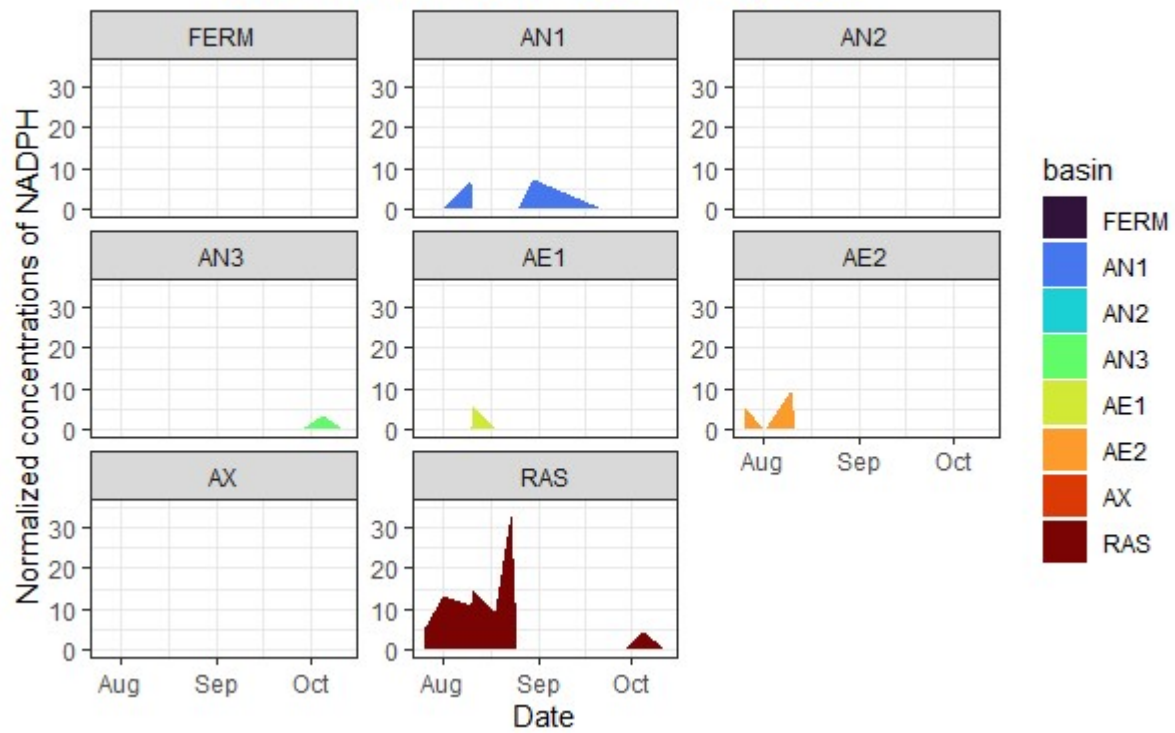
Methionine concentration over time by basin



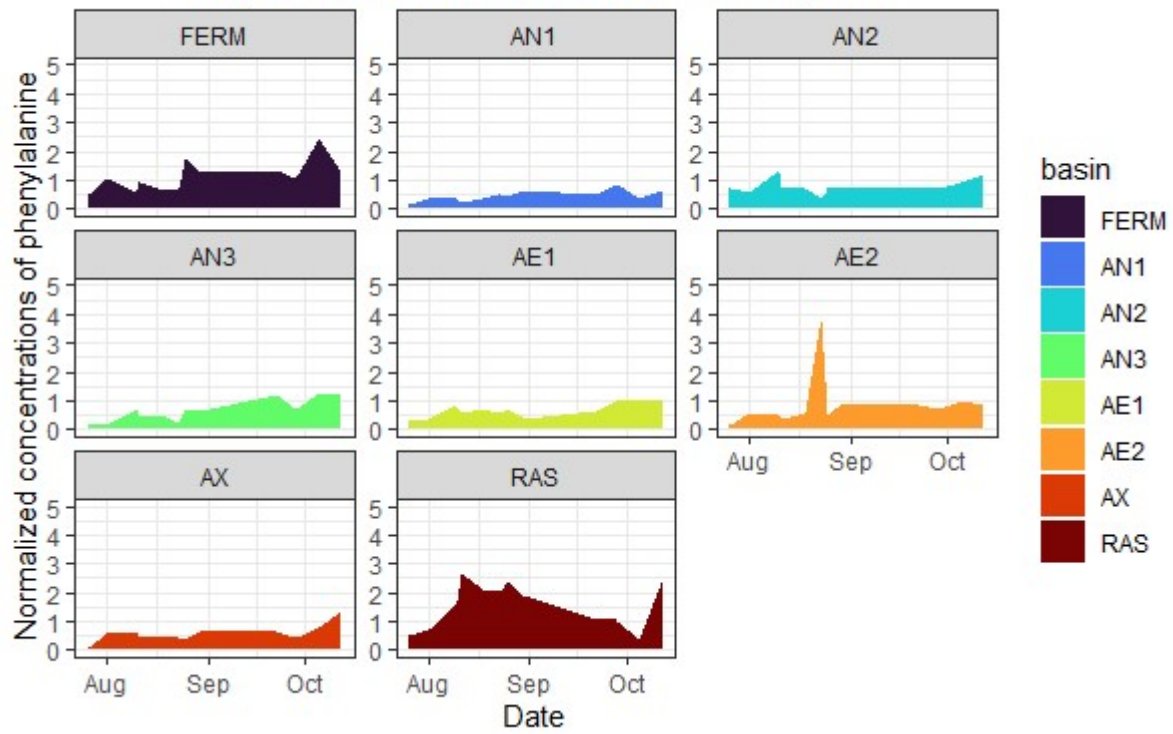
NADH concentration over time by basin



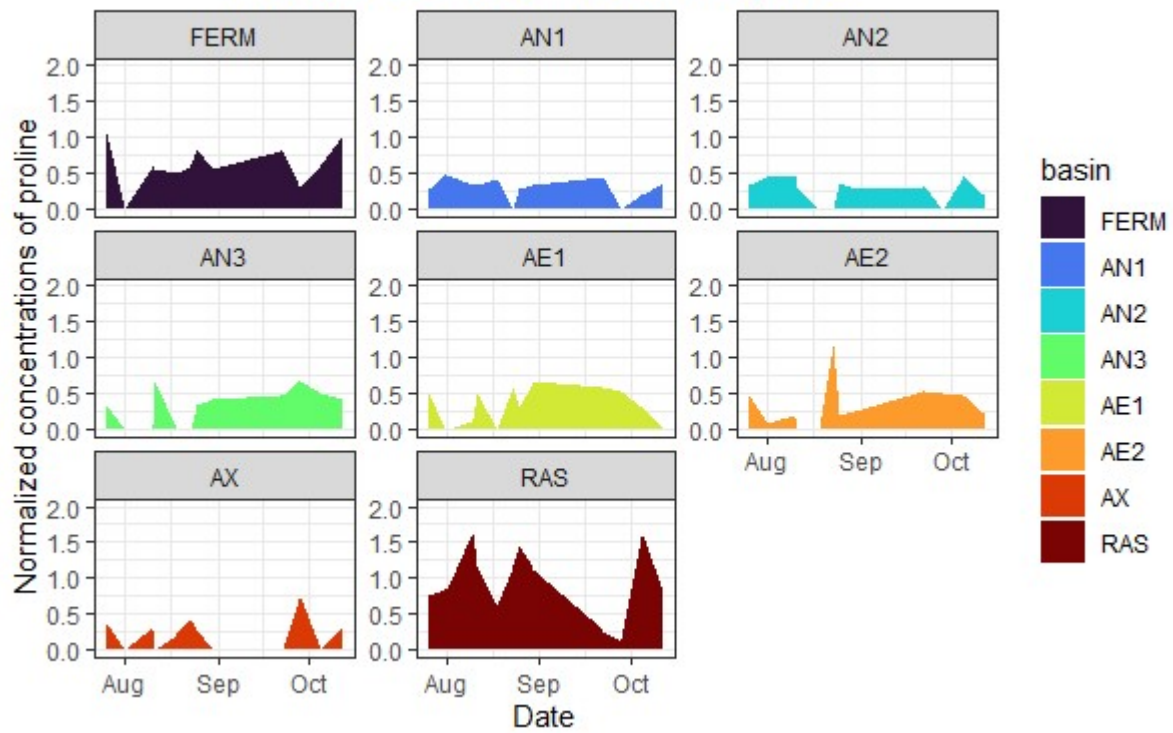
NADPH concentration over time by basin



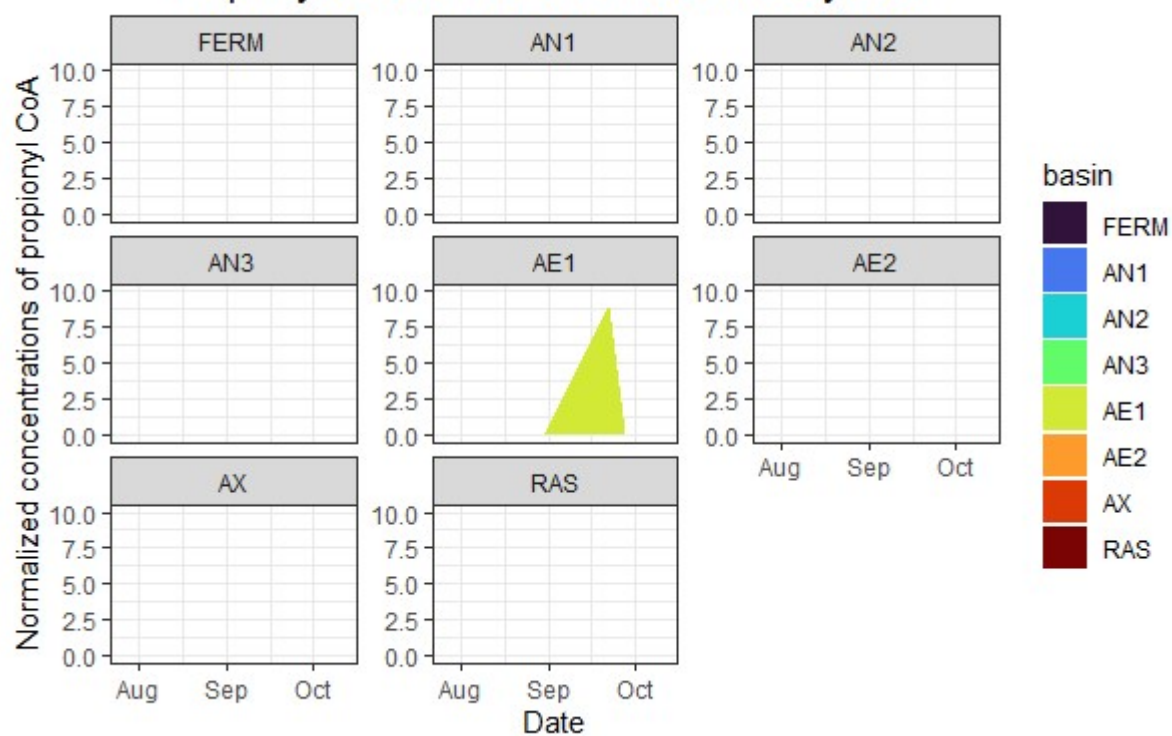
Phenylalanine concentration over time by basin



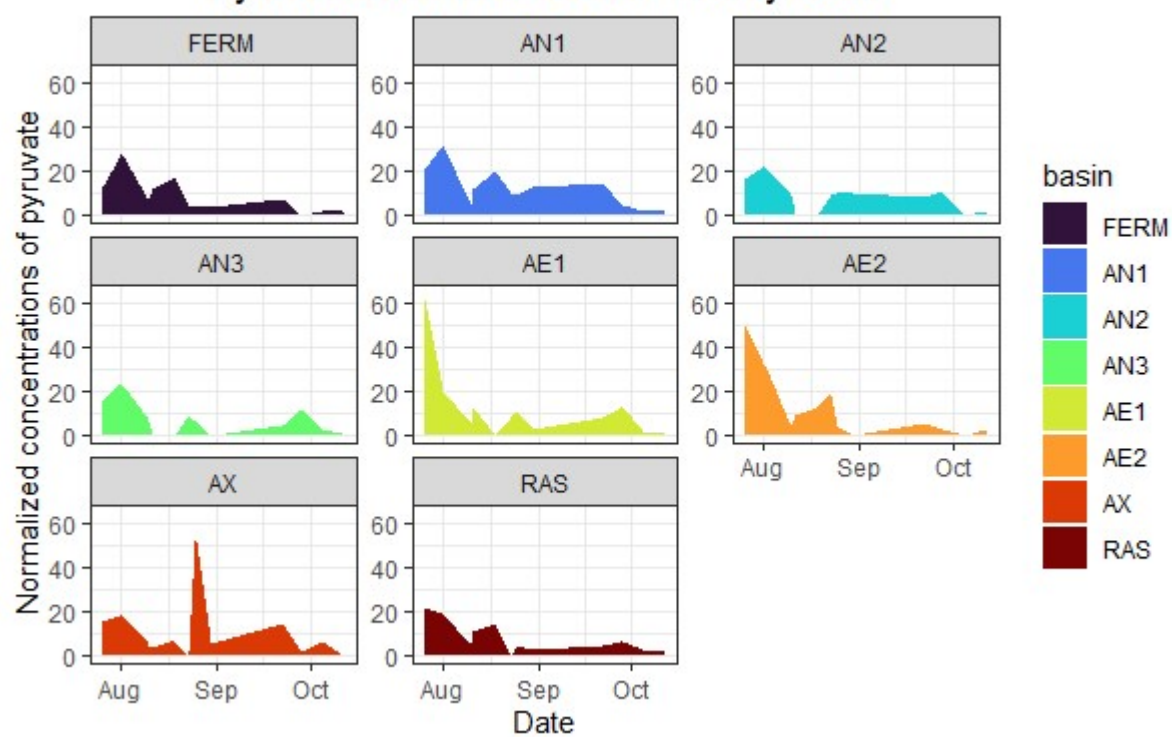
Proline concentration over time by basin



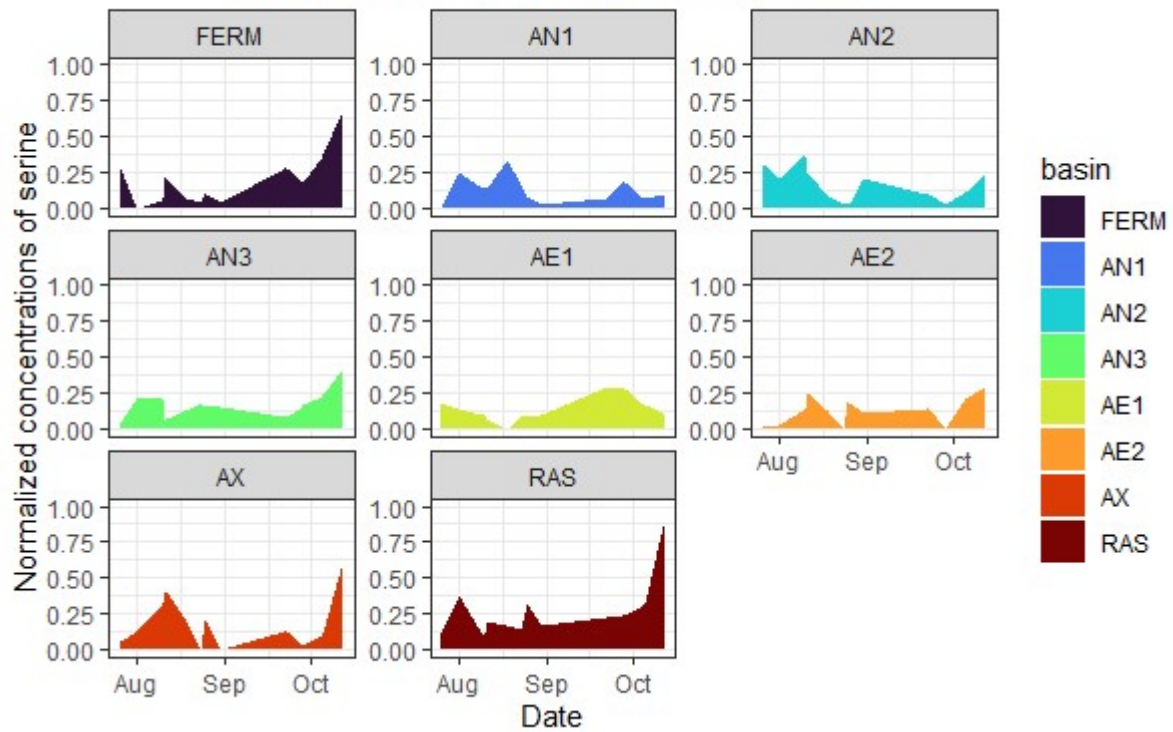
Propionyl CoA concentration over time by basin



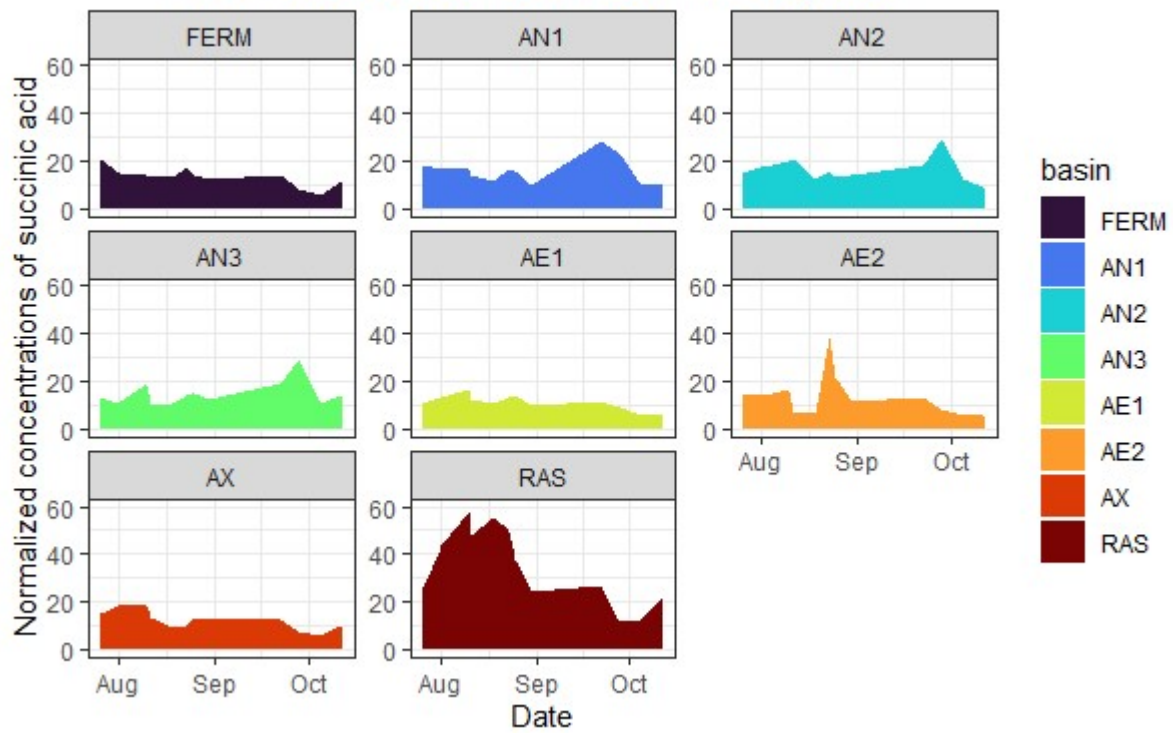
Pyruvate concentration over time by basin



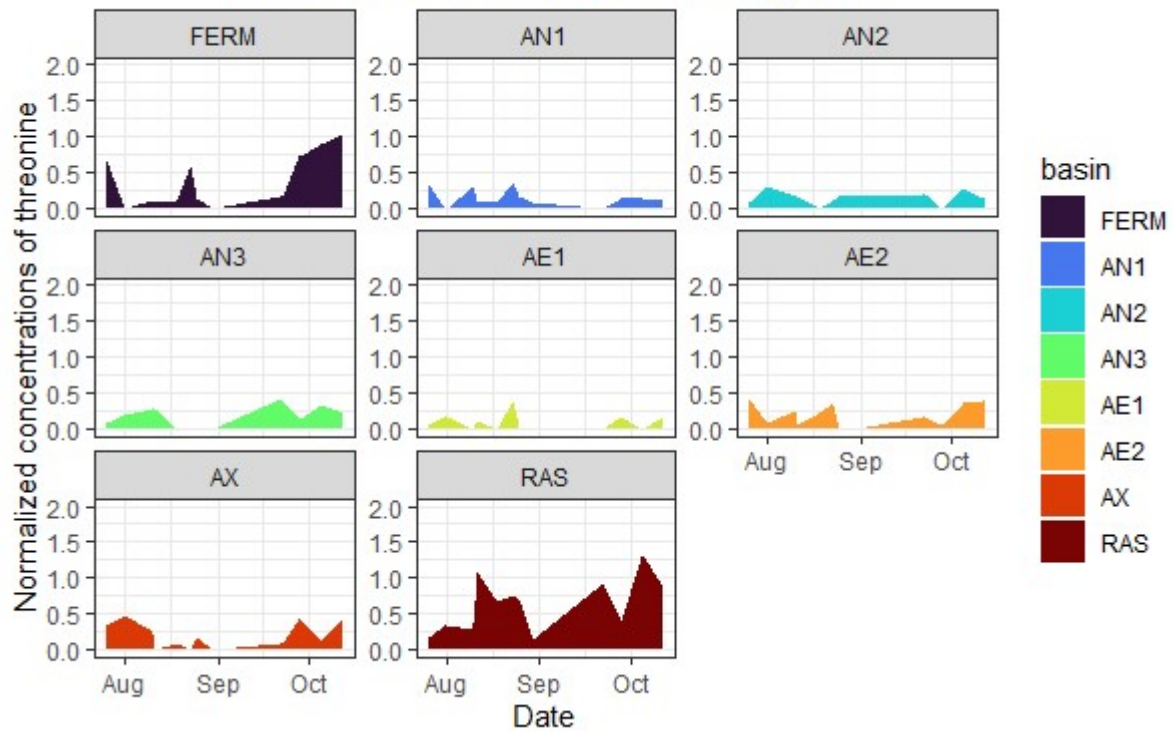
Serine concentration over time by basin



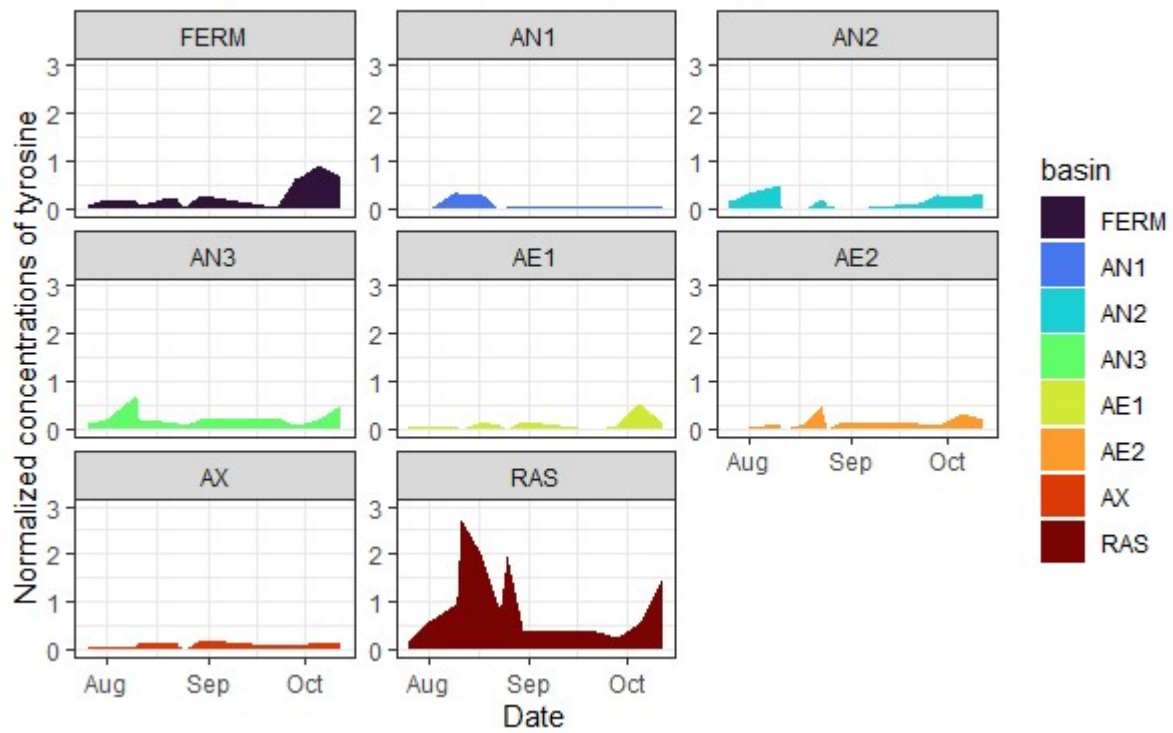
Succinic acid concentration over time by basin



Threonine concentration over time by basin



Tyrosine concentration over time by basin



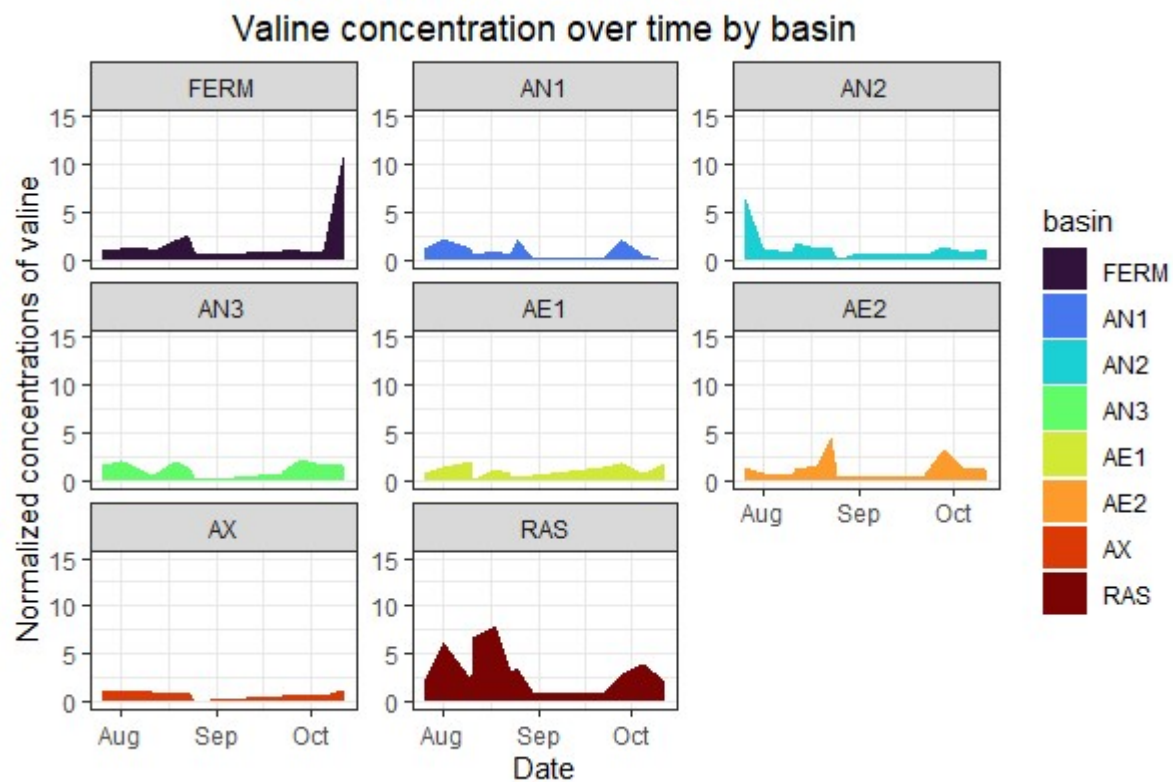


Figure S2: Temporal metabolome trends by basin, normalized to warfarin. Data up to and including Aug. 1st was pre-ROC; Aug. 2-Sept. 28 represents data for a ROC augmented WRRF; Sept. 29-Oct. 13 represents post-ROC loading.

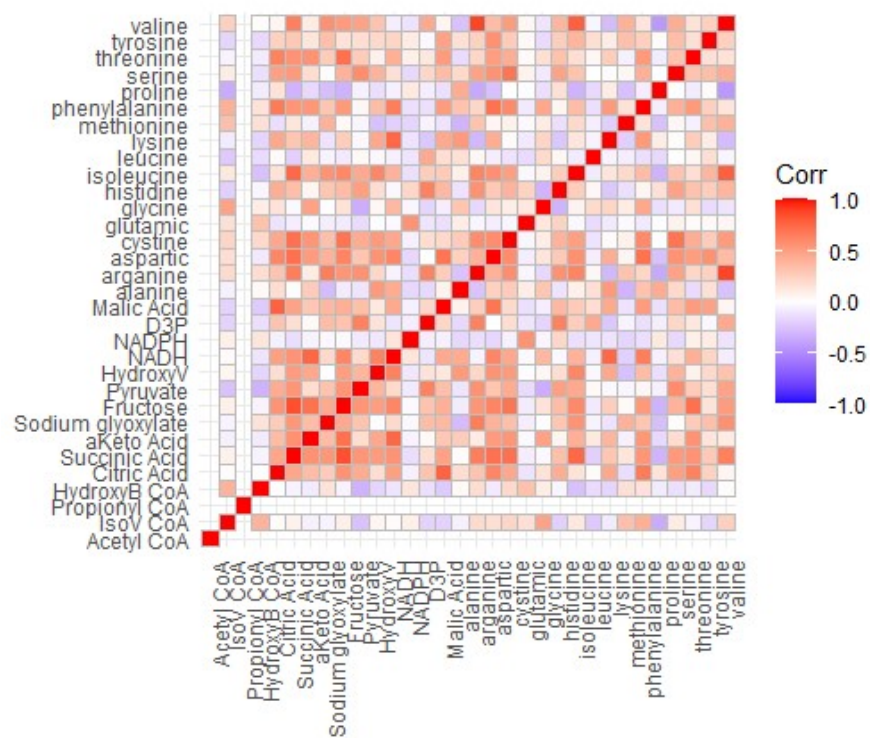


Figure S3: Heatmap for Metabolites and Amino Acids, Scale Model Anaerobic Zone with ROC

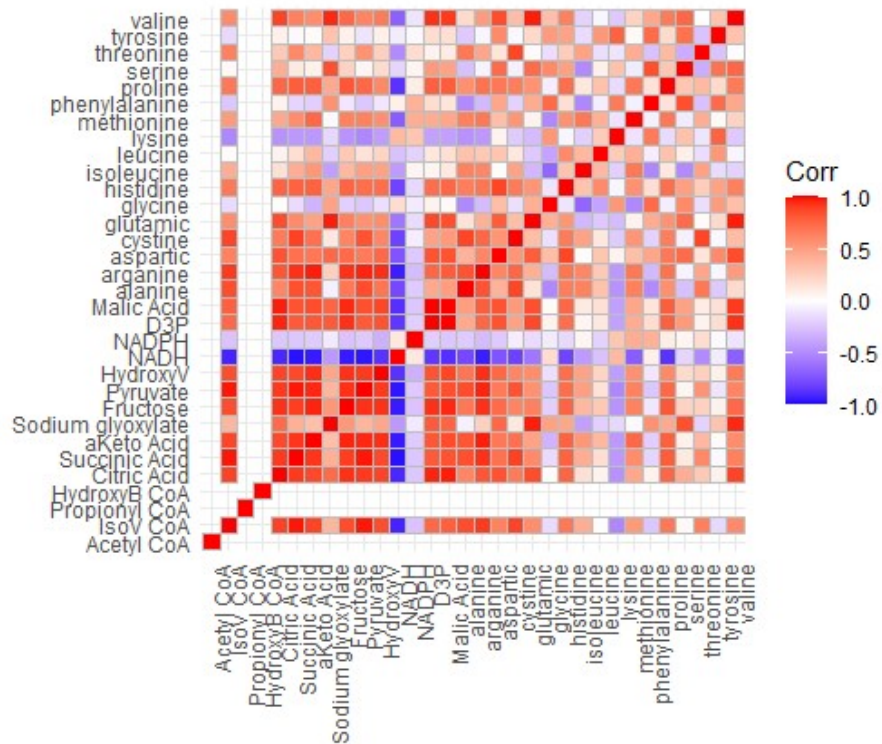


Figure S4: Heatmap for Metabolites and Amino Acids, Scale Model Anaerobic Zone without ROC

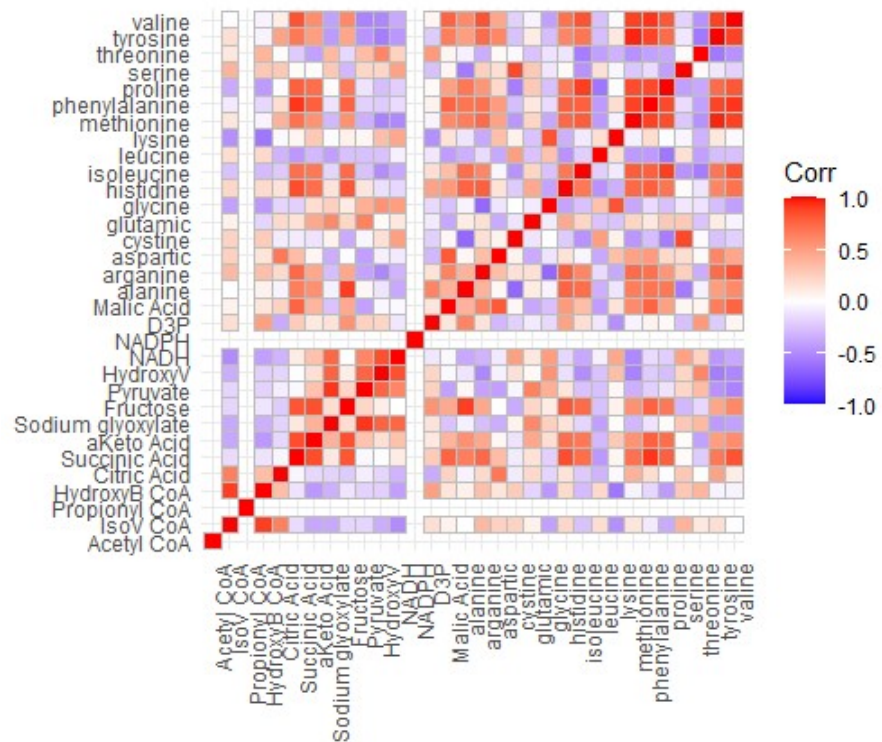


Figure S5: Heatmap for Metabolites and Amino Acids, Scale Model Anoxic Zone with ROC

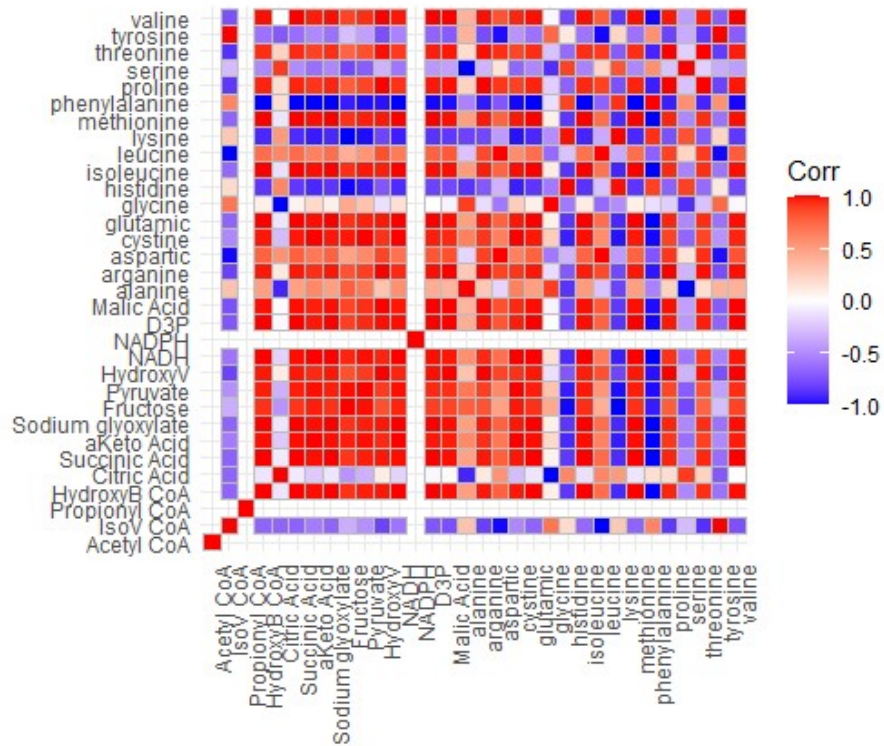
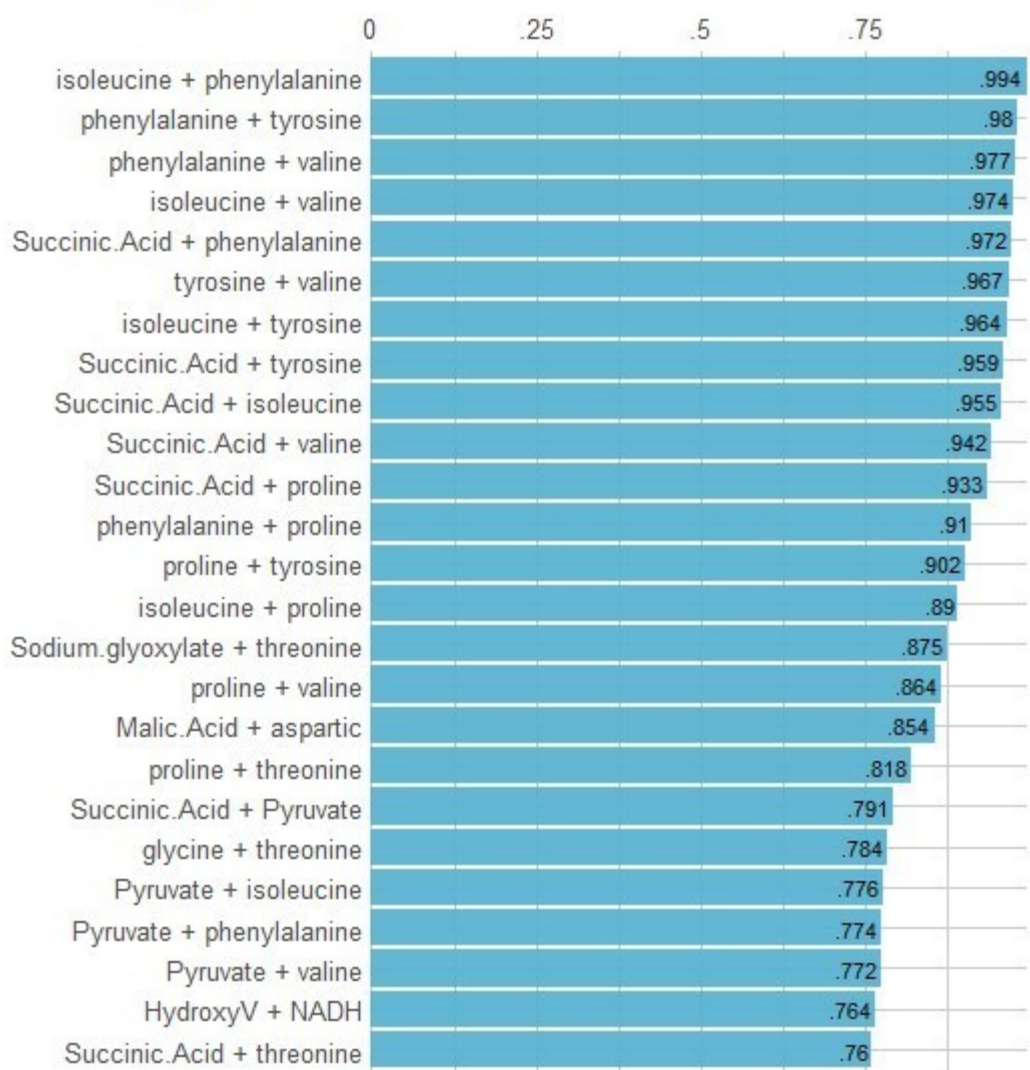


Figure S6: Heatmap for Metabolites and Amino Acids, Scale Model Anoxic Zone without ROC

Ranked Cross-Correlations

25 most relevant



Correlations with p-value < 0.05

Figure S7: Ranked correlations for metabolomic heat maps for aerobic pilot scale data, with ROC

Ranked Cross-Correlations

25 most relevant

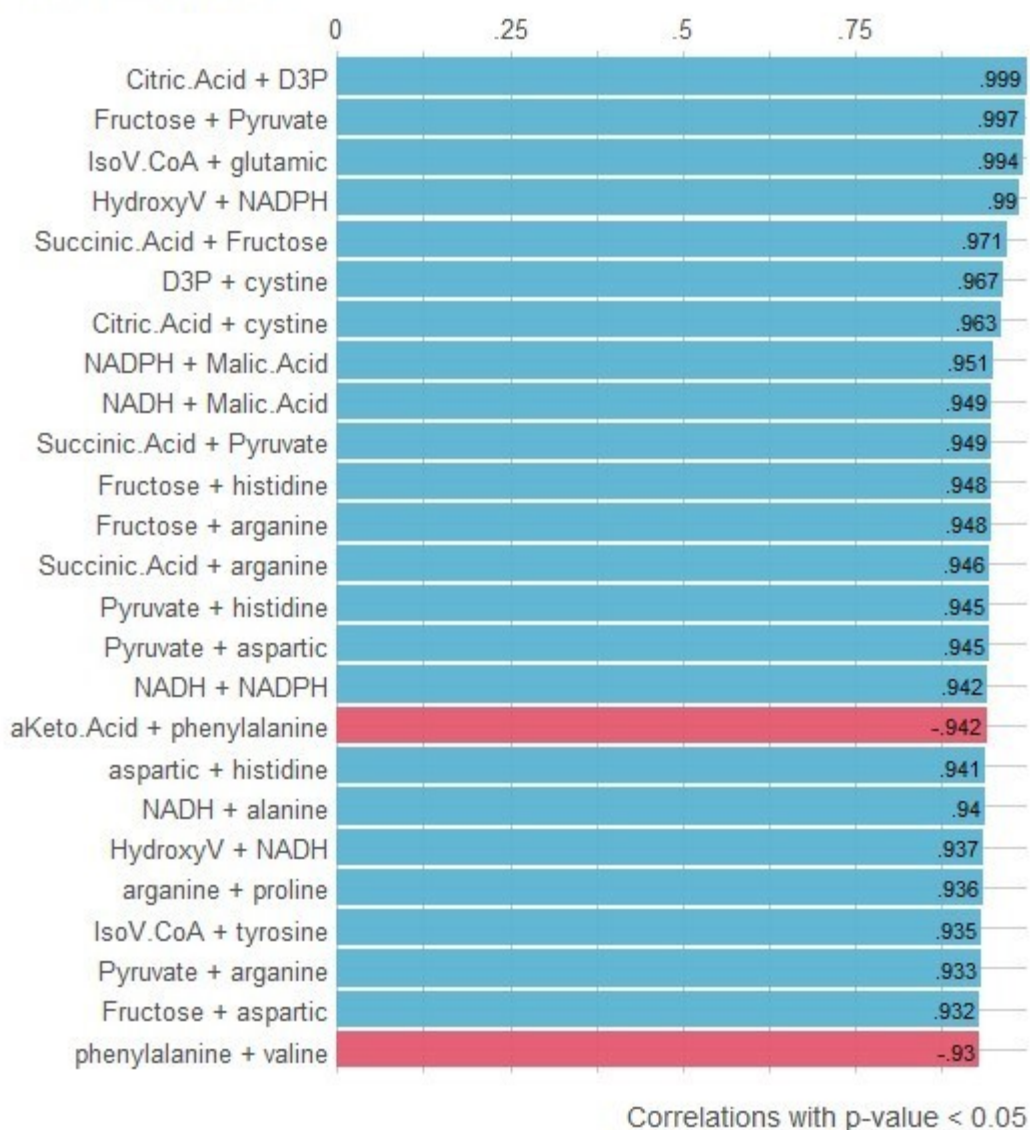


Figure S8: Ranked correlations for metabolomic heat maps for aerobic pilot scale data, without ROC

References.

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