Use of untargeted metabolomics for assessing soil quality and microbial function

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Table 1. General soil properties of the nine distinct soil types used in this study. Values represent means ± SEM ($n = 5$).

|	Saline alluvial gley soil 1	Saline alluvial gley soil 2	Gleyic sandy brown soil	Typical orthic brown soil	Stagno-orthic gley soil	Typical podzolic brown soil 1	Typical podzolic brown soil 2	Typical humic ranker soil	Non-calcaric lithosol
Altitude (m)	-1.0 ± 0.9	8.6 ± 0.9	10.4 ± 1.2	16.8 ± 2.8	37.0 ± 0.9	145.0 ± 4.4	311.2 ± 8.8	362.0 ± 6.9	367.2 ± 4.7
pH	8.03 ± 0.17	7.51 ± 0.16	5.62 ± 0.07	5.78 ± 0.29	5.68 ± 0.09	4.61 ± 0.10	5.89 ± 0.37	4.37 ± 0.13	4.27 ± 0.18
Electrical conductivity (μS cm^{-1})	1810 ± 217	1546 ± 240	35 ± 8	42 ± 10	30 ± 8	27 ± 3	30 ± 8	41 ± 8	39 ± 4
Total C (%)	2.89 ± 0.20	4.66 ± 0.37	2.64 ± 0.43	3.62 ± 0.21	9.98 ± 2.31	11.17 ± 1.67	11.32 ± 1.29	11.57 ± 1.42	29.14 ± 7.42
Total N (%)	0.17 ± 0.02	0.43 ± 0.03	0.28 ± 0.04	0.38 ± 0.01	0.89 ± 0.16	0.88 ± 0.11	0.91 ± 0.08	0.89 ± 0.09	1.16 ± 0.20
Moisture content (%)	28.8 ± 1.3	39.9 ± 2.0	26.4 ± 2.1	32.2 ± 2.6	60.6 ± 6.8	42.1 ± 2.1	47.2 ± 5.0	49.8 ± 2.9	64.9 ± 7.0
Nitrate (mg N kg^{-1})	3.45 ± 2.00	2.70 ± 1.4	5.95 ± 1.80	15.6 ± 6.9	2.70 ± 1.05	12.2 ± 4.0	3.75 ± 2.40	5.35 ± 2.25	0.80 ± 0.10
Ammonium (mg N kg^{-1})	3.05 ± 0.30	3.40 ± 0.60	3.0 ± 0.2	4.00 ± 0.65	5.30 ± 3.40	9.00 ± 2.20	7.55 ± 1.25	10.7 ± 1.7	3.45 ± 0.25
Free amino acids (mg N kg^{-1})	0.81 ± 0.12	0.20 ± 0.04	2.17 ± 0.35	0.89 ± 0.16	1.83 ± 0.22	6.48 ± 1.40	5.54 ± 1.24	6.82 ± 0.91	2.42 ± 0.57
K (mg kg^{-1})	213 ± 52	278 ± 15.5	26.9 ± 5.75	14.5 ± 2.4	44.0 ± 8.4	72.3 ± 7.9	62.0 ± 57.0	58.2 ± 6	52.9 ± 5.55
Ca (mg kg^{-1})	17600 ± 5200	1540 ± 675	33.5 ± 3.5	83.5 ± 43.0	35.5 ± 6.0	29 ± 9	268 ± 62	5.5 ± 1.0	25.0 ± 15.0
Na (mg kg^{-1})	1725 ± 470	1710 ± 70	1.95 ± 0.2	18.8 ± 3.9	27.9 ± 9.1	25.3 ± 8.8	30.8 ± 5.4	21.8 ± 3.2	32.2 ± 1.8
Phosphate (mg kg^{-1})	4.25 ± 0.60	5.25 ± 1.35	3.65 ± 1.60	8.30 ± 4.10	1.10 ± 0.25	1.65 ± 0.50	3.15 ± 1.70	2.25 ± 1.55	2.80 ± 1.15
Dissolved organic C (mg kg^{-1})	20.6 ± 1.2	12.4 ± 2.2	58.0 ± 4.0	40.5 ± 6.7	52.0 ± 13.0	219 ± 35	123 ± 12	250 ± 39	109 ± 9
Dissolved organic N (mg kg^{-1})	0.86 ± 0.91	< 0.01	9.94 ± 1.52	2.43 ± 1.68	4.96 ± 3.30	19.7 ± 3.9	8.60 ± 4.54	28.7 ± 6.2	7.55 ± 0.93
Labile C turnover (% h^{-1})	0.51 ± 0.12	1.35 ± 0.12	2.57 ± 0.58	2.69 ± 0.25	2.97 ± 0.54	3.14 ± 0.15	4.15 ± 0.54	3.22 ± 0.21	2.90 ± 0.32
Recalcitrant C turnover (% h^{-1})	0.29 ± 0.01	0.24 ± 0.02	0.31 ± 0.02	0.32 ± 0.01	0.24 ± 0.01	0.25 ± 0.01	0.25 ± 0.01	0.21 ± 0.02	0.18 ± 0.01
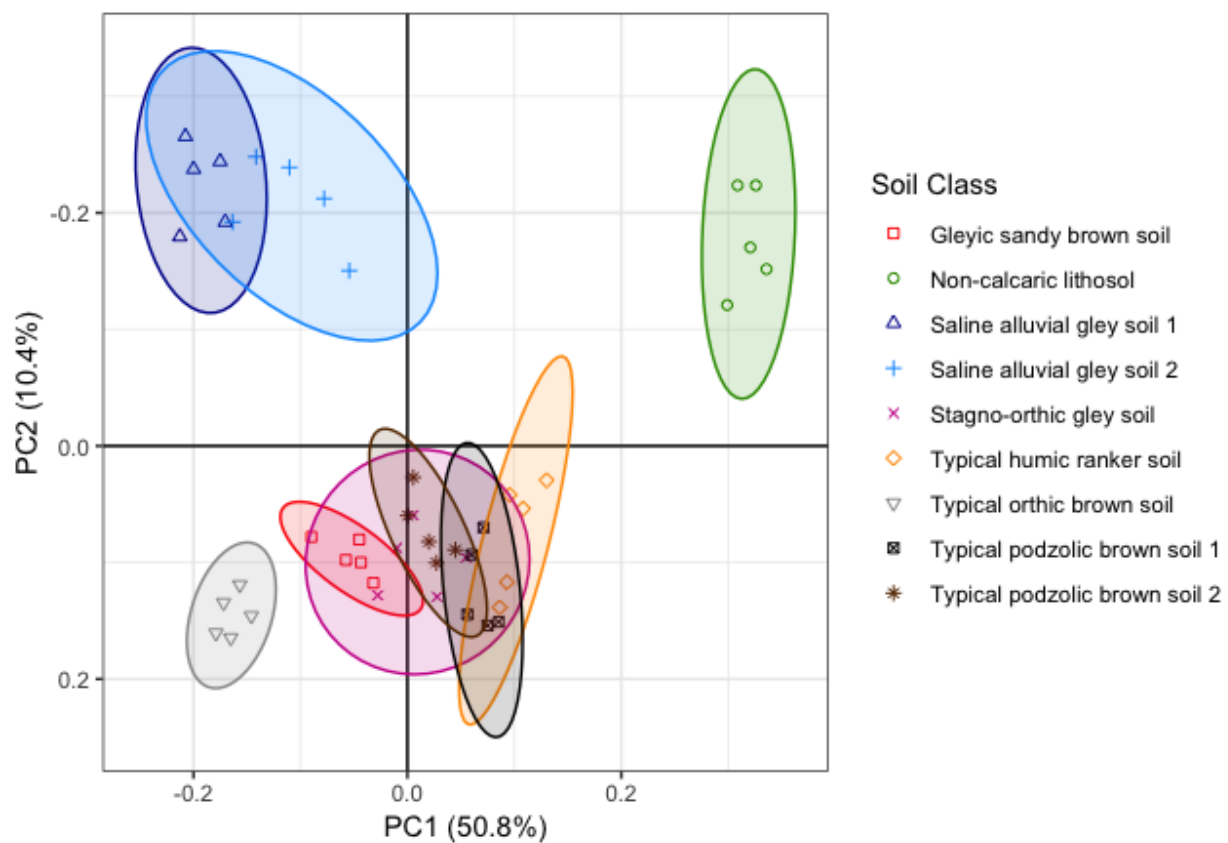
Fig. 1 2D principal component scores plot for all metabolites detected (n = 405). Each colour refers to an independent soil class, detailed in the key. Translucent ovals surrounding data points indicate 95% confidence intervals. Variance of each principal component is detailed on respective axes.
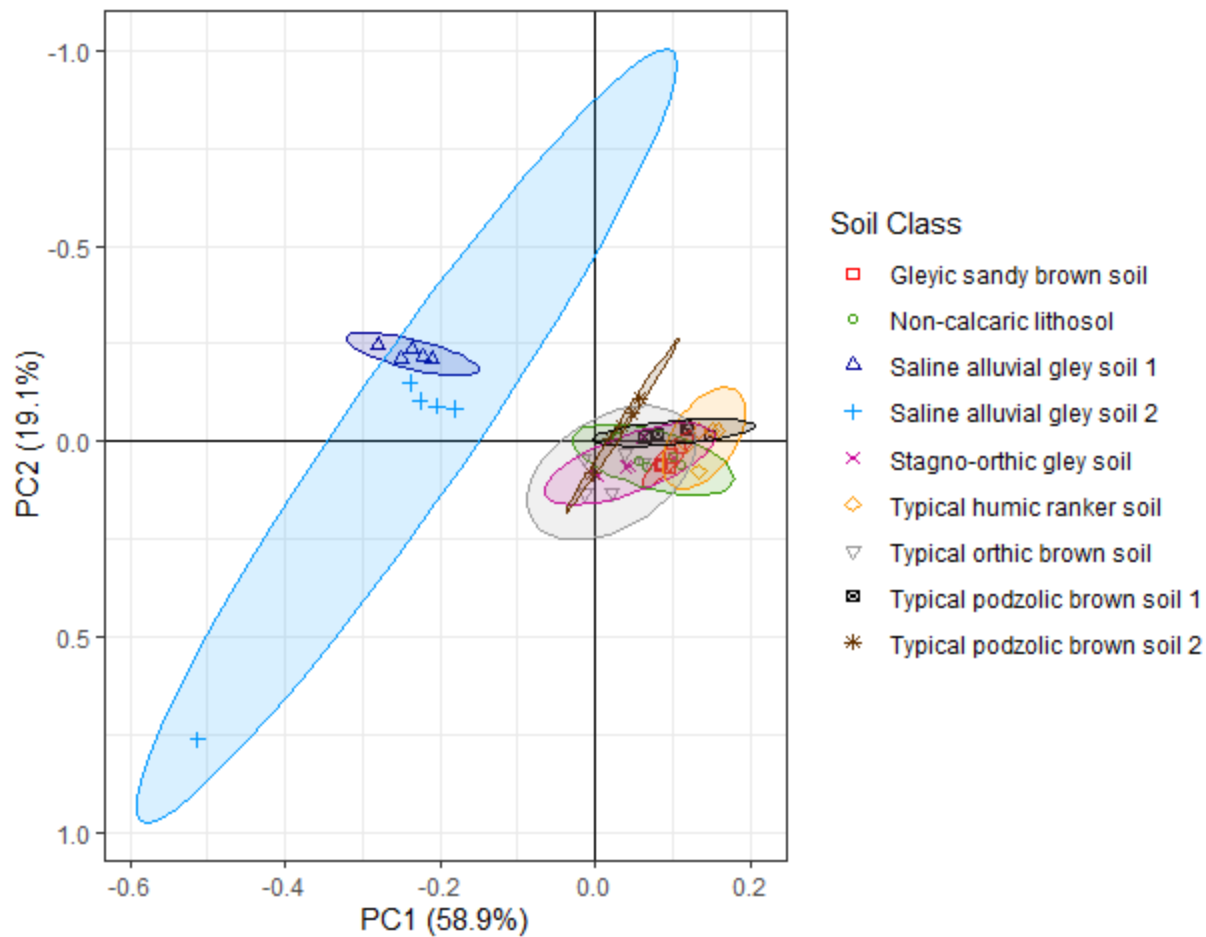
Fig. 2 2D principal components scores plot for general soil properties. Measured properties include pH, dissolved organic C and N, electrical conductivity, total C and N, available P, moisture content, total free amino acids, NH_4^+, NO_3^-, Na, Ca, K, labile C turnover and recalcitrant C turnover. Each colour refers to a distinct soil class, detailed in the key. Translucent ovals surrounding data points indicate 95% confidence intervals per soil class. Variance of each principal component is detailed on respective axes.
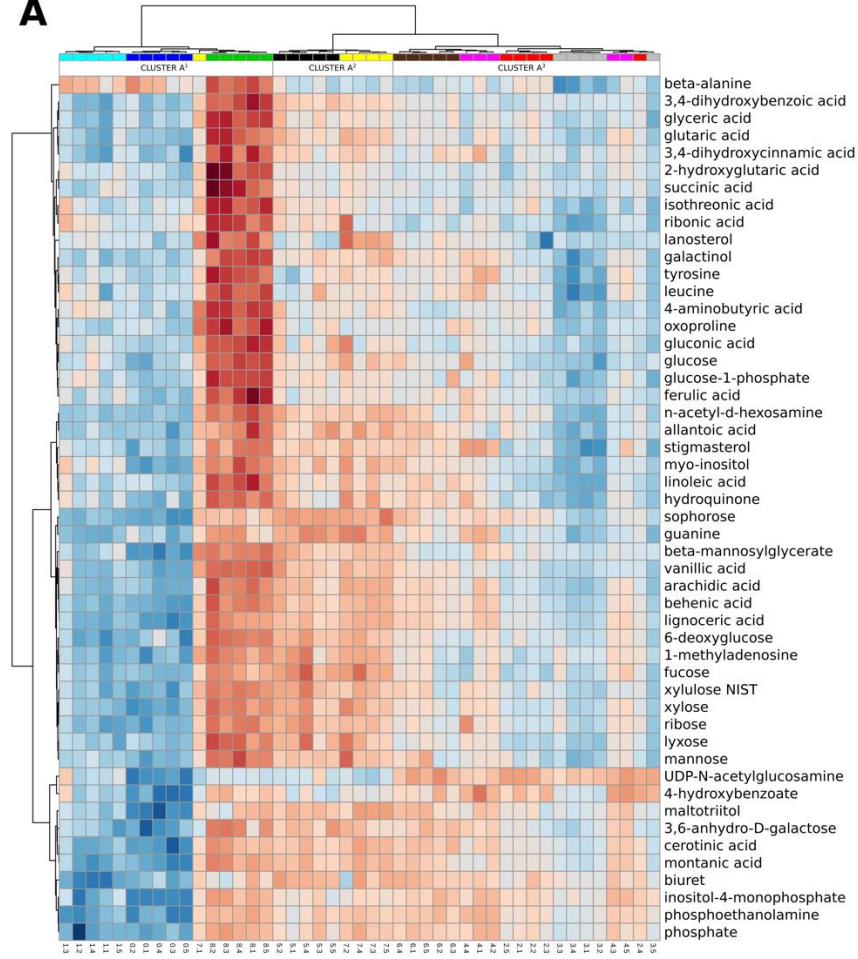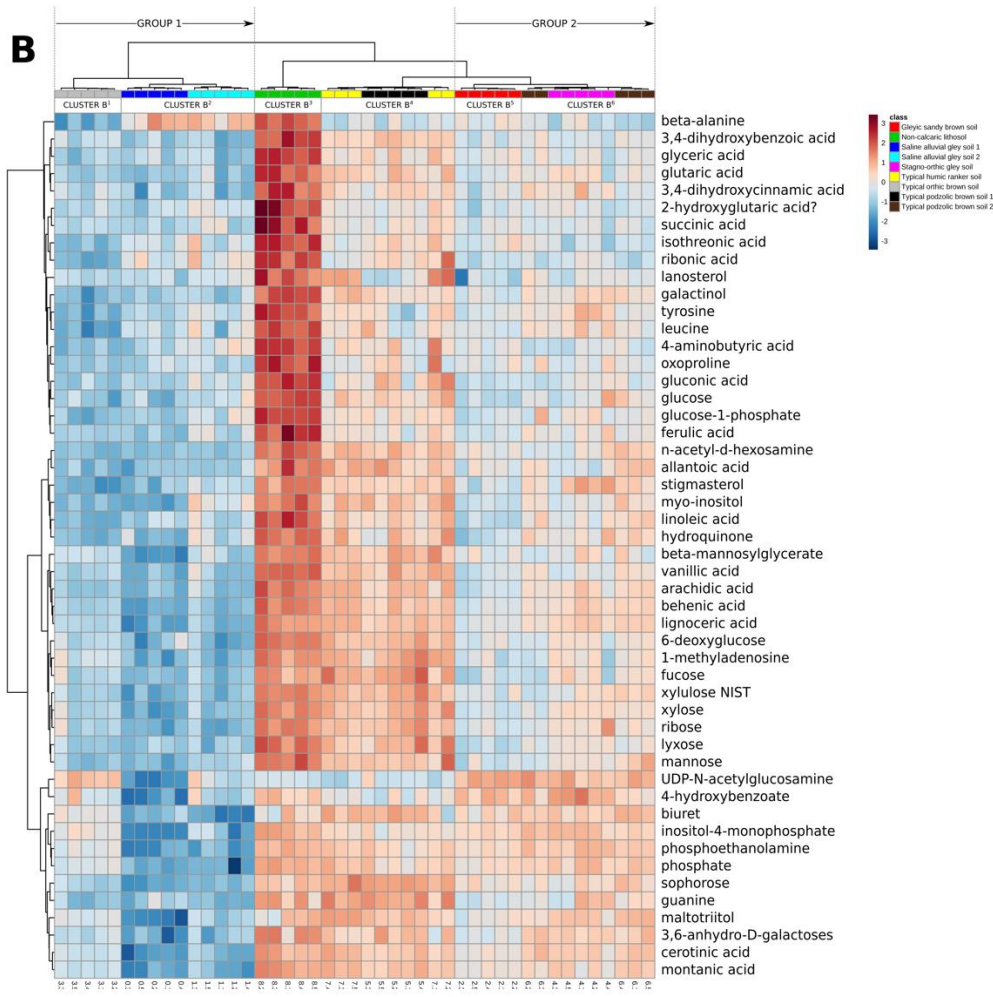
A

beta-alanine
3,4-dihydroxybenzoic acid
glyceric acid
glutaric acid
3,4-dihydroxycinnamic acid
2-hydroxyglutaric acid
succinic acid
isothreonic acid
ribonic acid
lanosterol
galactinol
tyrosine
leucine
4-aminobutyric acid
oxoproline
gluconic acid
glucose
glucose-1-phosphate
ferulic acid
n-acetyl-d-hexosamine
allantoic acid
stigmasterol
myo-inositol
linoleic acid
hydroquinone
sophorose
guanine
beta-mannosylglycerate
vanillic acid
arachidic acid
behenic acid
lignoceric acid
6-deoxyglucose
1-methyladenosine
fucose
xylulose NIST
xylose
ribose
lyxose
mannose
UDP-N-acetylglucosamine
4-hydroxybenzoate
maltotriitol
3,6-anhydro-D-galactose
cerotinic acid
montanic acid
biuret
inositol-4-monophosphate
phosphoethanolamine
phosphate

CLUSTER A¹   CLUSTER A²   CLUSTER A³

Fig. 3 Heatmap showing expression profiles of each soil sample based on the top 50 most significant known metabolites identified by ANOVA. Metabolites and classes are clustered by Pearson correlation and Ward's linkage (A), and by Euclidean distance and Ward's linkage (B). Clusters and Groups referred to in the text are indicated directly above the heatmap, and directly above the top dendrogram, respectively. Soil class is indicated by the coloured squares above cluster labels; each is defined in the key.

The colour of squares linking metabolites to samples ranges blue to red, indicating metabolite concentration z-score: numbers -3 to 3 on the scale bar indicate the number of standard deviations from the mean.