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Untargeted Metabolomic Profiling Reveals Variation in Metabolites Associated with Nutritional Values in Tef Accessions

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Supplementary data

Table.S1: Details of teff accessions used for the study. Teff seeds were obtained from NPGS-GRIN germplasm. Table represents the accession details, name, region of origin, seed color, plant height, panicle type., group. Each genotype is assigned a group number from 1-4 based on tentatively identified metabotypes.

Serial No:	Accession number	Genotype/ Cultivar name	Area/Altitude	Seed colour	Plant height	Panicle type	Groups
1	PI 524438	Dabbi	Gojam, Ethiopia	red	55-58 cm	very loose	2
2	PI 524440	Gea-lamie	Wellega, Ethiopia	red	20-50 cm	very loose	2
3	PI 524442	Karadebi	Wellega, Ethiopia	red	40-80 cm	very loose	4
4	PI 557457	Red dabi	Ethiopia	brown	91 cm	very loose	4
5	PI 524433	Ada	Shewa, Ethiopia	white	50-100 cm	semi compact	1
6	PI 524434	Addisie	Shewa, Ethiopia	white	65-90 cm	very compact	2
7	PI 524435	Alba	Shewa,Ethiopia /1700- 2500m	white	60-135 cm	fairly loose	4
8	PI 524437	Beten	Shewa, Ethiopia	white	40-85 cm	very loose	4
9	PI 524439	Enatite	Shewa,Ethiopia/2000m	white	45-85 cm	very loose	4
10	PI 524443	Manyi	Shewa, Ethiopia	white	40-100 cm	fairly loose	3
11	PI 524444	Rosea	Shewa, Ethiopia	white	50-95 cm	fairly loose	4
12	PI 524445	Tullu Nasy	Wellega, Ethiopia	white	30-50 cm	very loose	4
13	PI 557456	DZ-01-354	Ethiopia	white	125 cm	fairly loose	4
14	PI 243908	Magna	Ethiopia	white	110 cm	fairly loose	4

Table S2: Significant metabolite features associated with flavone and flavonol biosynthesis within 14 teff genotypes. Query mass denotes the masses identified from the untargeted metabolomics datasets. The annotations are made based on the rice reference metabolome, masses, compound ID's and formula are derived from KEGG library

No	Query.Mass	Matched. Compound (KEGG ID)	Matched. Form	Hit	Exact mass (KEGG)	Mol. weight (KEGG)	Formula (KEGG)
1	285.04156	C05903/ C01477/ C01514	M-H[-]	Kaempferol/Luteolin/ Apigenin	286.0477	286.2363	C15H10O6
2	413.08948	C16911	M-H2O- H[-]	Afzelin	432.1056	432.3775	C21H20O10
3	429.08463	C01750/ C12249	M-H2O- H[-]	Quercitrin/Kaempferol -3-O-glucoside	448.1006	448.3769	C21H20O11
4	431.10034	C16911	M-H[-]	Quercetin 3-glucoside	432.1056	432.3775	C21H20O10
5	432.10315	C16911	M(C13)- H[-]	Afzelin	432.1056	432.3775	C21H20O10
6	447.09537	C01750/ C12249	M-H[-]	Kaempferol 3-O- rhamnoside-7-O- glucoside/Kaempferol- 3-O-glucoside	448.1006	448.3769	C21H20O11
7	448.09863	C01750/ C12249	M(C13)- H[-]	Quercitrin/Kaempferol -3-O-glucoside	448.1006	448.3769	C21H20O11
8	485.06958	C05623	M+Na- 2H[-]	Quercetin 3-O- glucoside	464.0955	464.3763	C21H20O12
9	513.02112	C16911	M+Br81[-]	Afzelin	432.1056	432.3775	C21H20O10
10	523.10883	C05623	M+CH3C OO[-]	Quercetin 3-O- glucoside	464.0955	464.3763	C21H20O12
11	593.15399	C21833/ C21854	M-H[-]	Kaempferol-3-O- rutinoside/Kaempferol 3-O-rhamnoside-7-O- glucoside	594.1585	594.5181	C27H30O15
12	647.11829	C05625/ C19796	M+Cl37[-]	Rutin/Quercetin 3-O- rhamnoside 7-O- glucoside	610.1534	610.5175	C27H30O16

Figure.S1: Fresh shoot weight of teff seedlings. 15- day old Teff seedlings (14 genotypes/accessions) harvested and used for metabolite extraction. The data represented as average fresh weight (mg) \pm standard deviation (SD) of three to four biological replicates. Independent seedling is taken as each biological replicate. Statistically significant changes (Tukey- Kramer HSD test, $p \leq 0.05$) between genotypes are identified by different letters.

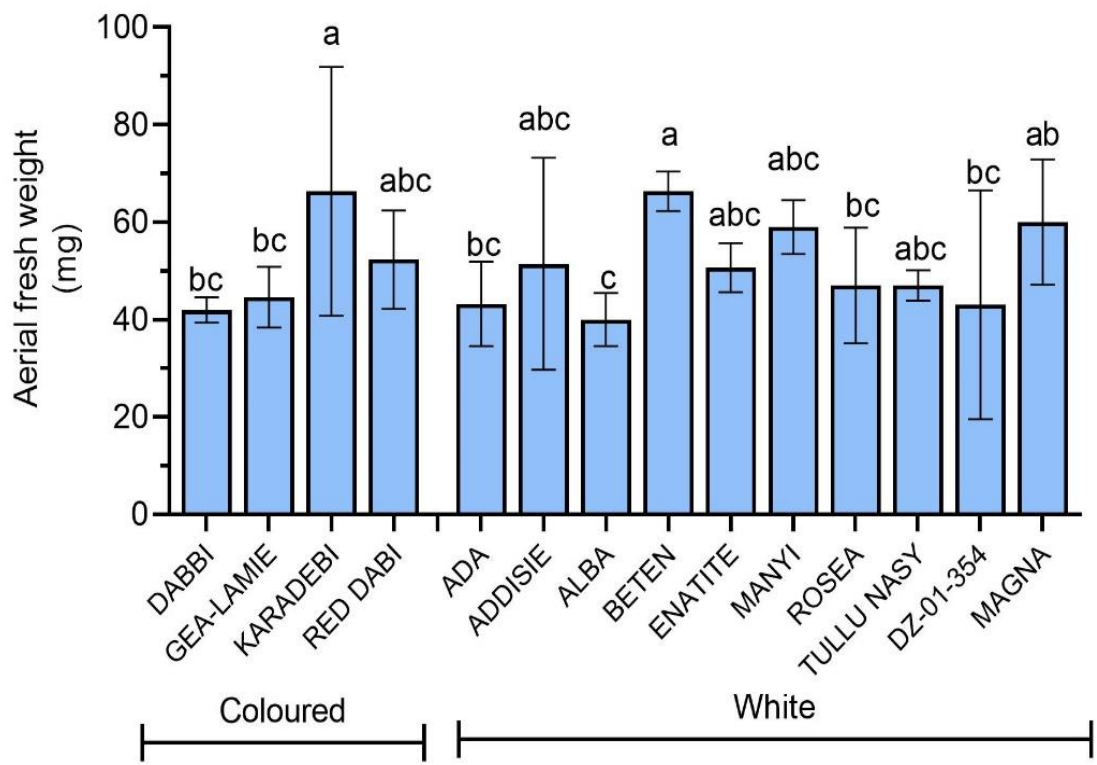


Figure S2. Initial mapping of teff seedling metabolome (a) Principal component analysis (b) Dendrogram showing clustering of 14 teff genotypes based on the metabolite features. Four groups, ‘metabotypes’ were identified based on the m/z features on negative mode.

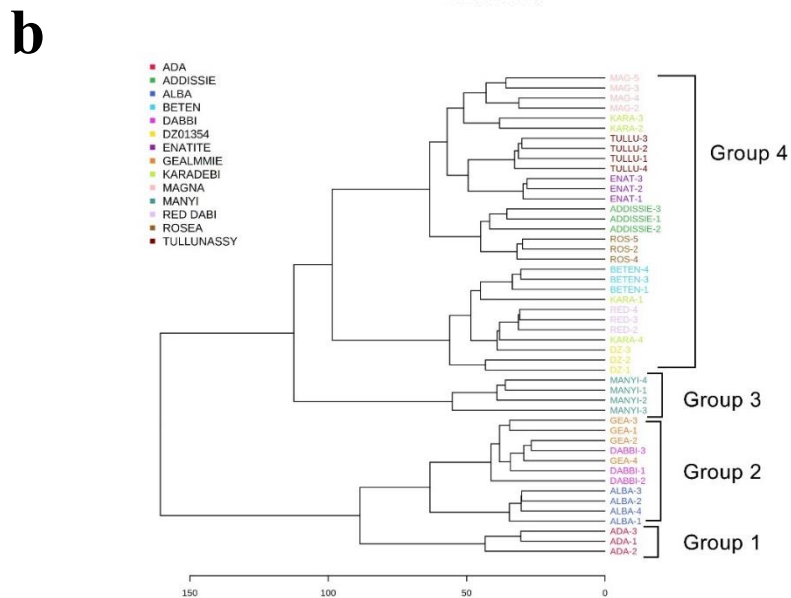
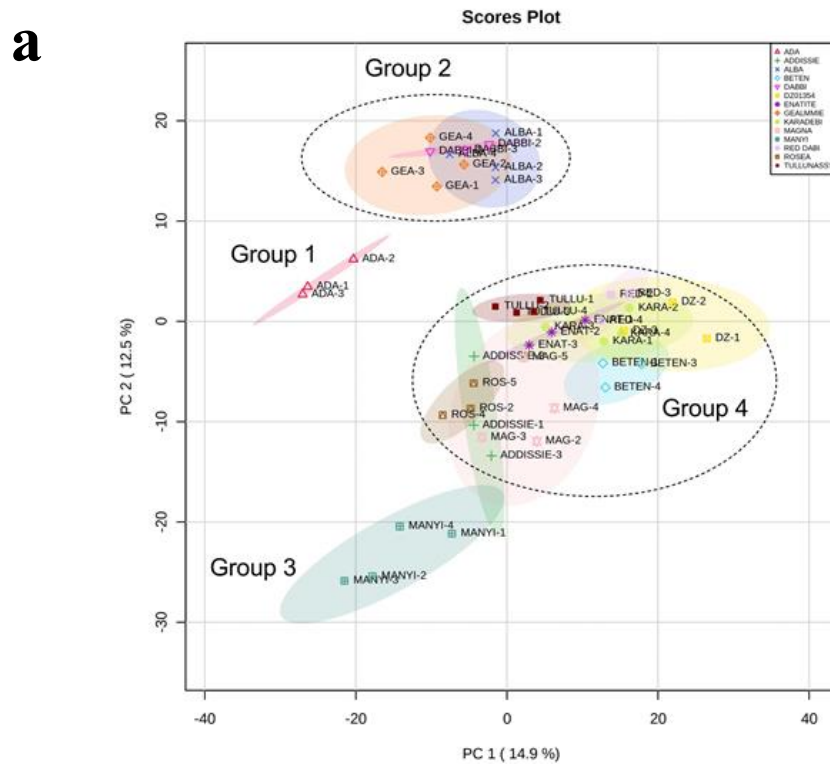


Figure S3. (a) Pathway enrichment analysis of metabolites **(b)**Heat map showing distribution of metabolites identified from flavone and flavonol biosynthesis within the teff genotypes. Seed groups are white = w and coloured (red/brown) = C. Group refers to the metabolomic group defined in Figure 1.

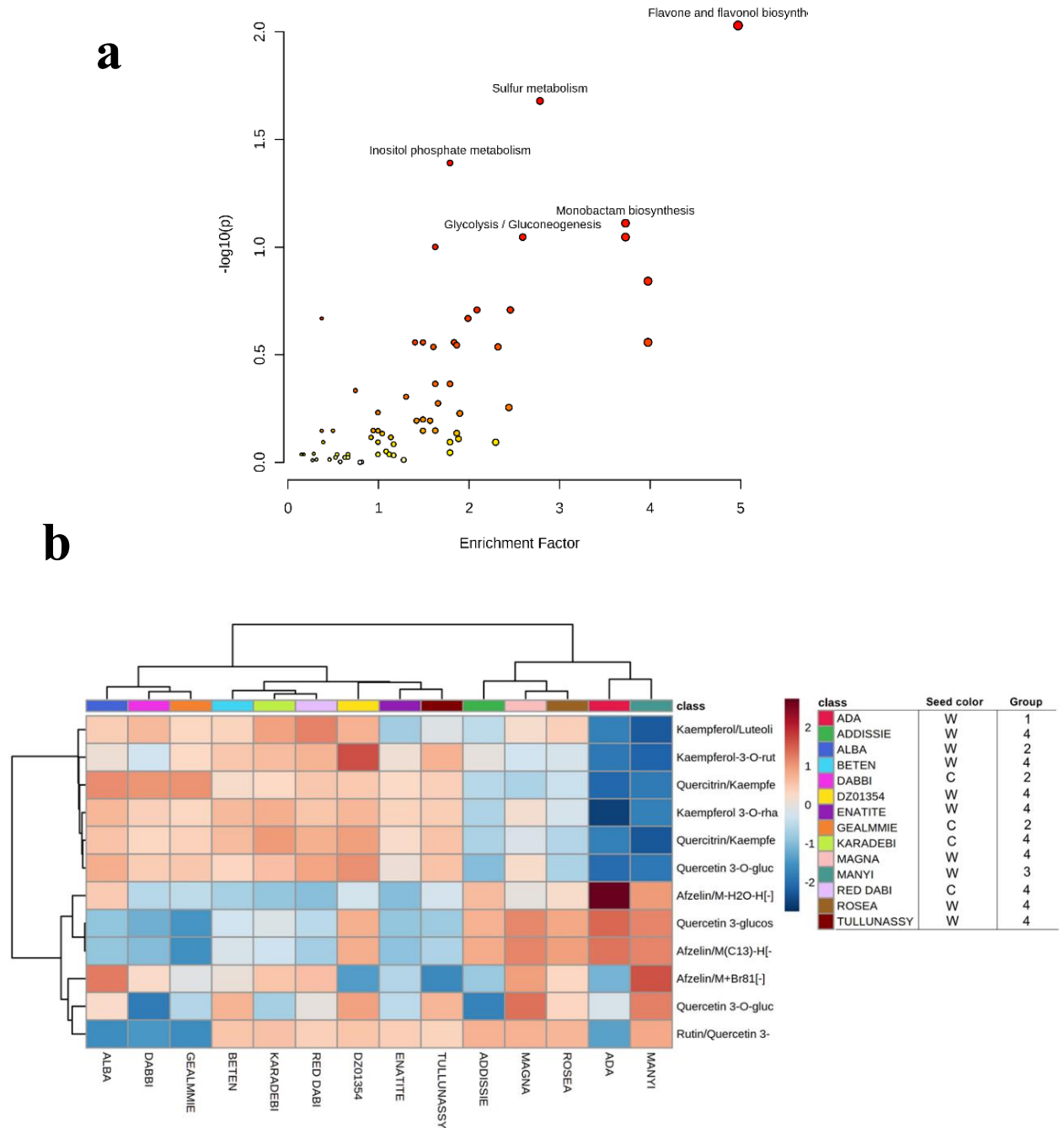


Fig S4: (a) PCA showing the metabolite variation between white and coloured seed accessions. **(b)** Heatmap showing 10 annotated significant metabolites within white and colored accessions

