

Diversity Bread Analysis

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Research Manager Mass Spectrometry

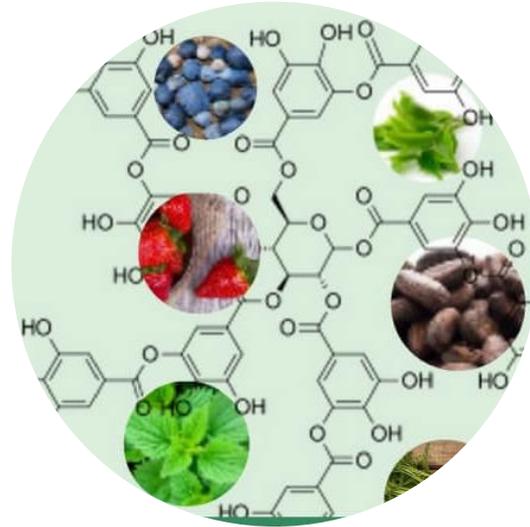
June 5th, 2023



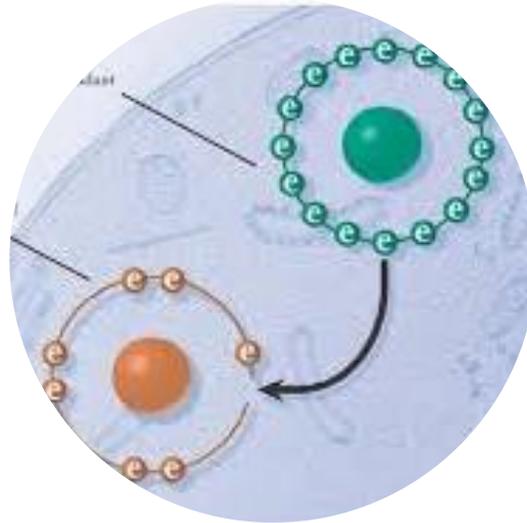
**FOOD
INNOVATION
FOR GOOD**



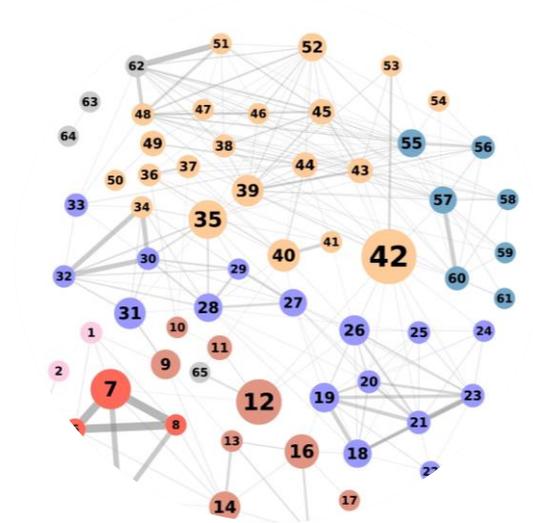
Overview of Analysis



**POLYPHENOL
CONTENT**

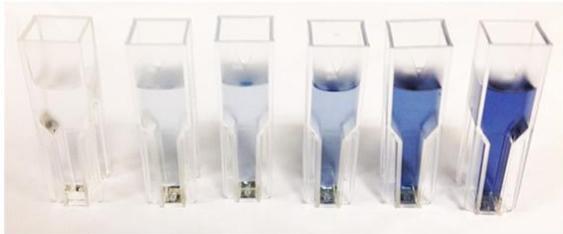
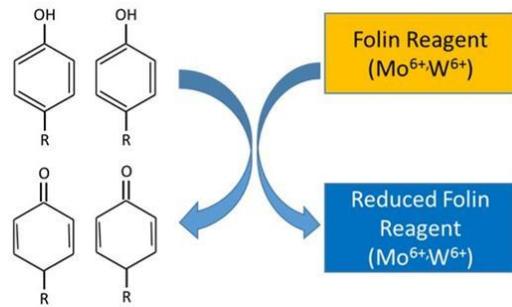


**ANTI-OXIDANT
ACTIVITY**

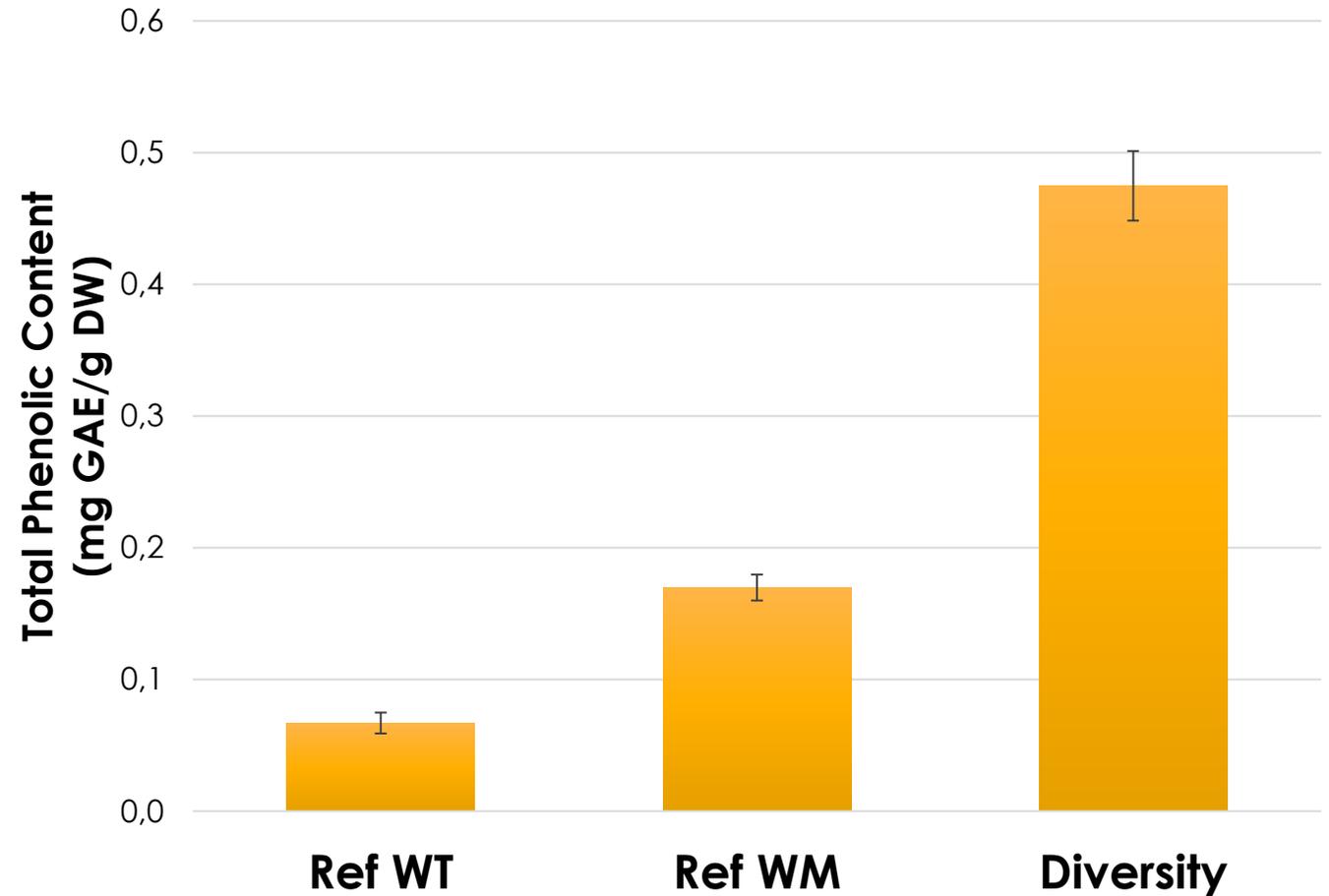


**FOOD
METABOLOME**

Total Poly Phenol Content



Based on Christopher et al., 2021, Applied Microbiology

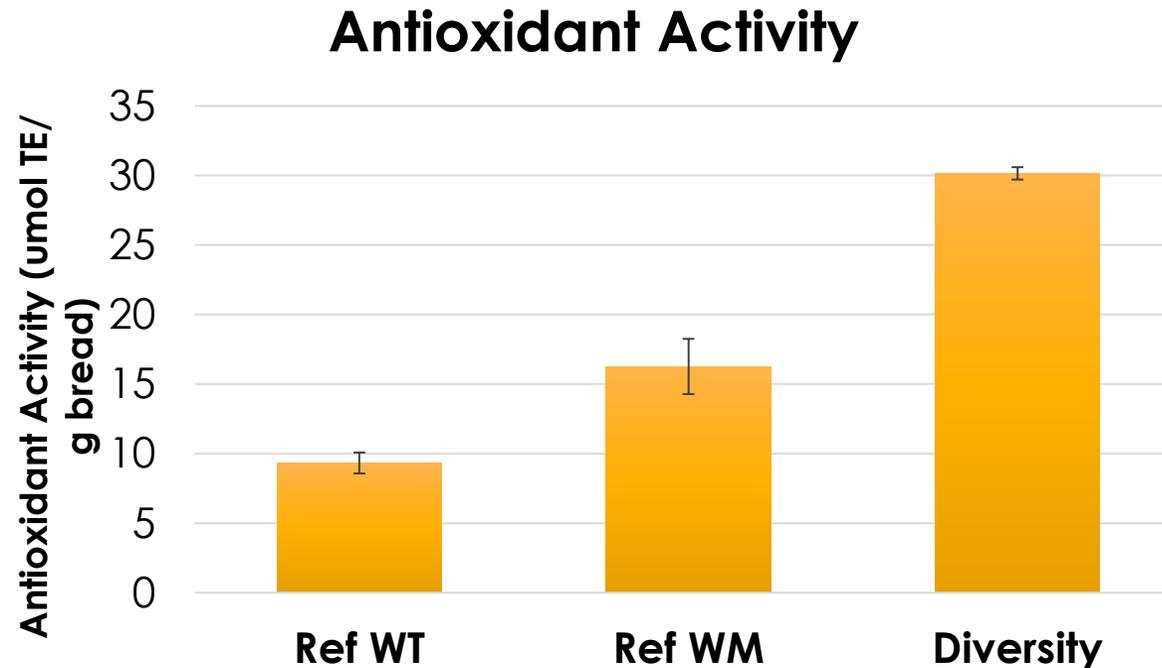


Diversity ~ x 2.8 **WM** (**W**hole **M**eal)

Diversity ~ x 8 **WT** (**W**hite)

Total Anti-Oxidant Capacity Assay Kit

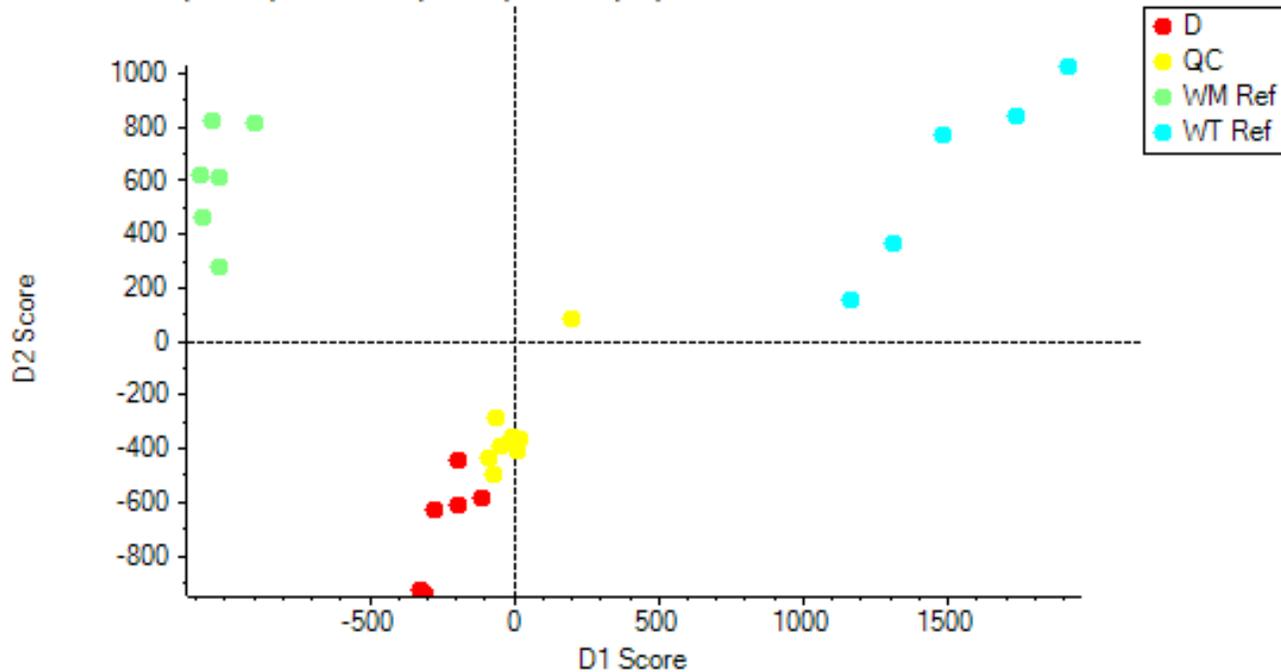
- Based on Cu^{2+} to Cu^{+} conversion (Sigma, MAK187)
- Diversity Bread ~ x2 WM Breads ~x3 WT Bread



LC-MS Metabolomics Analysis: PCA

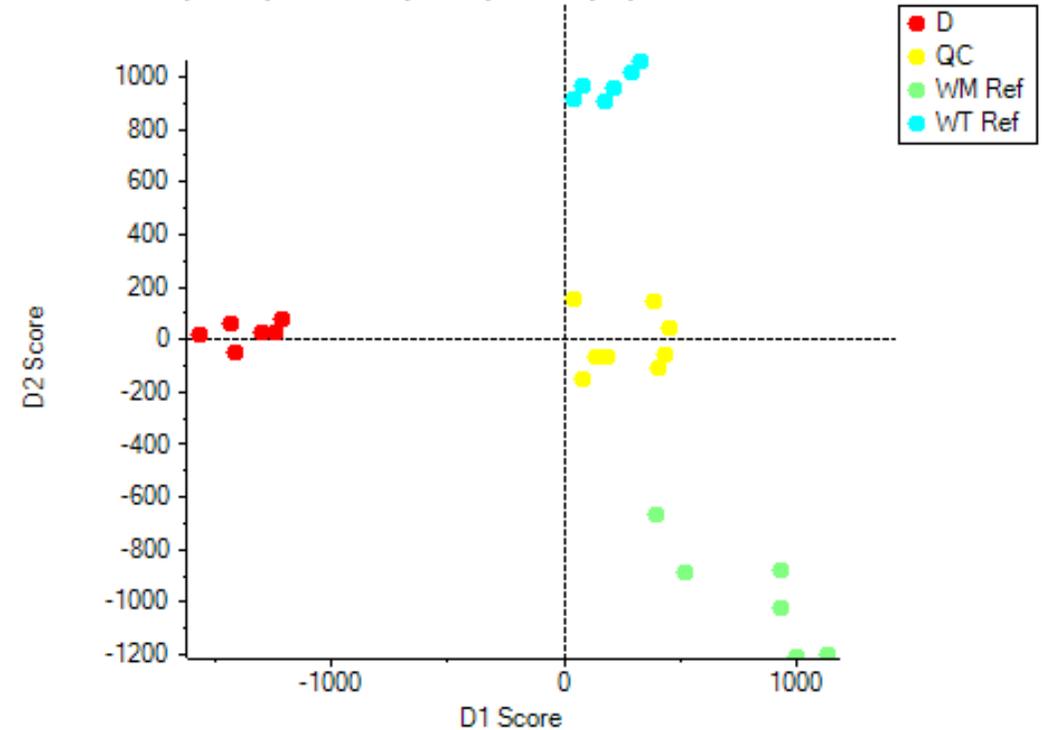
Pos Mode

Scores for D1 (30.4 %) versus D2 (30.2 %), Pareto (DA)



Neg Mode

Scores for D1 (28.9 %) versus D2 (28.6 %), Pareto (DA)

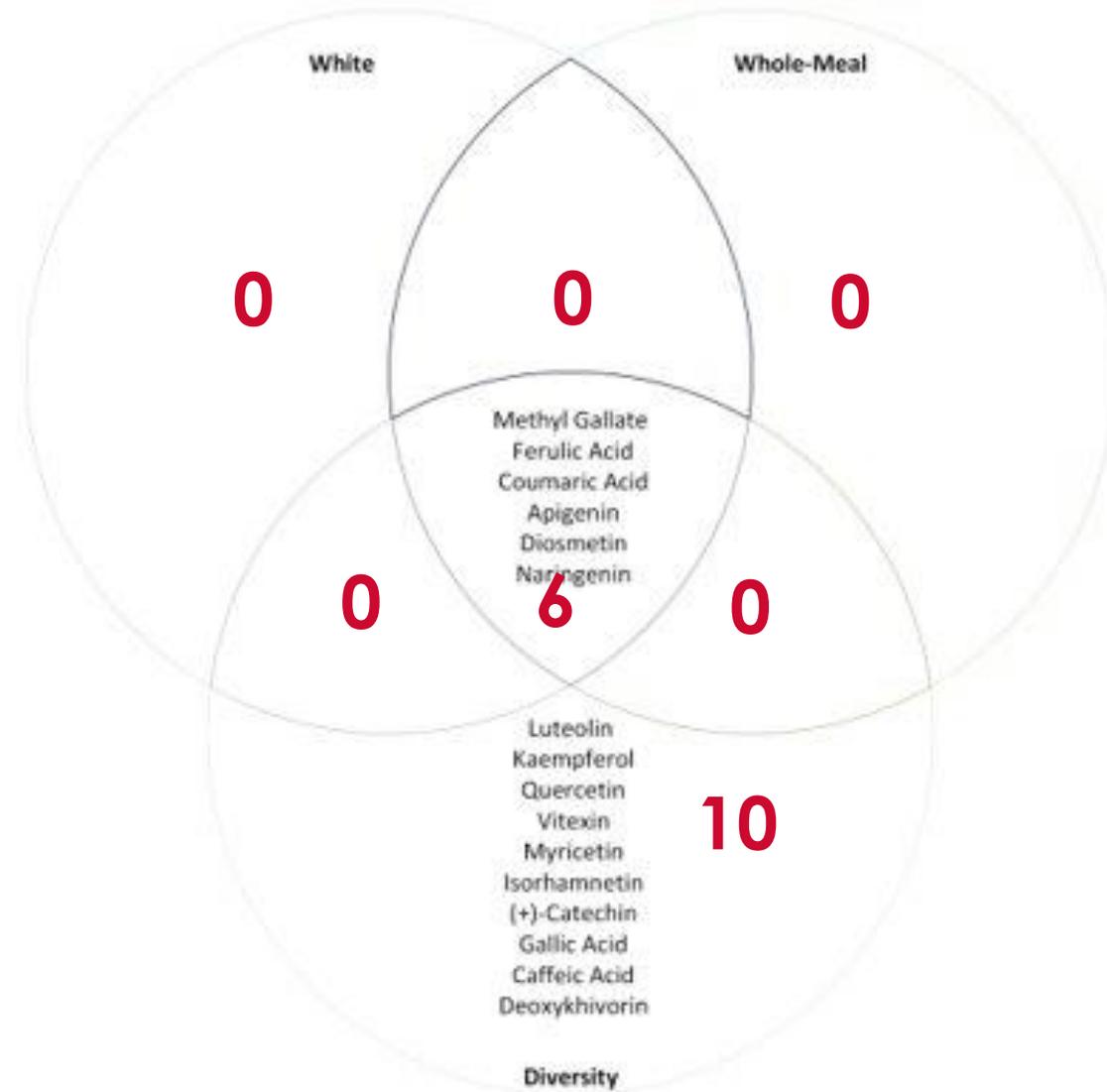


5

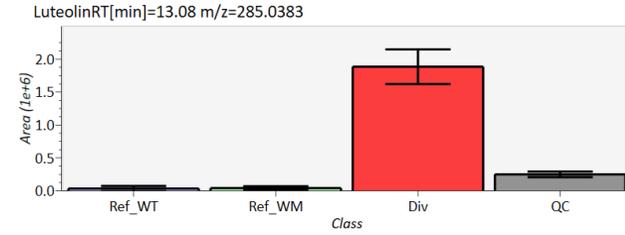
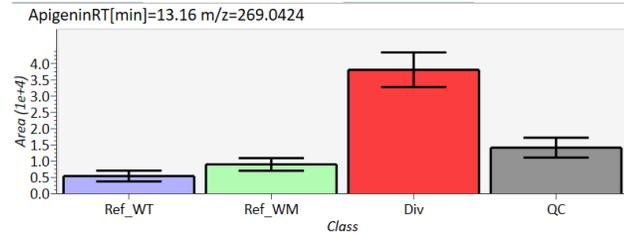
Diversity Bread is more similar to a WM (wholemeal) bread and less to WT (white).
Logic as 15% of Bran added to the recipe.

Metabolomics Analysis: Poly Phenols

LC- MS Analysis

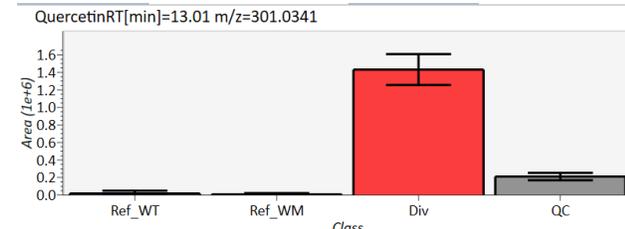
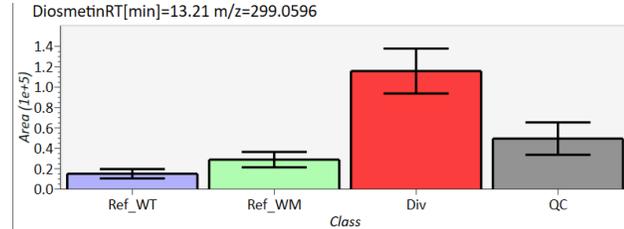


parsley, celery, basil,
chamomile, cilantro,
and oregano



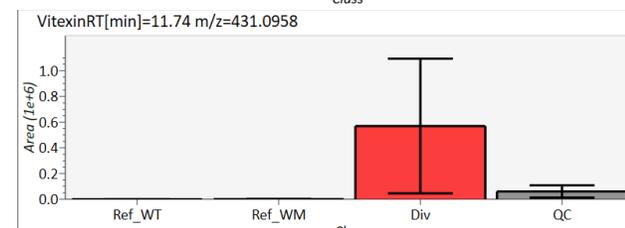
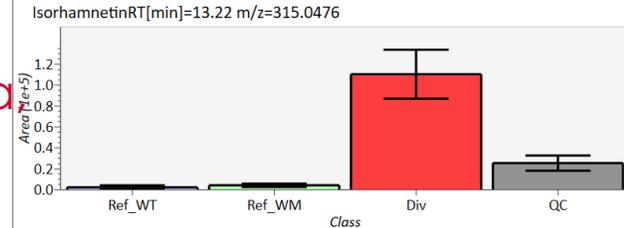
celery, parsley, broccoli,
onion leaves, carrots,
peppers, cabbages,
apple skins, and
chrysanthemum flowers

Citrus fruit



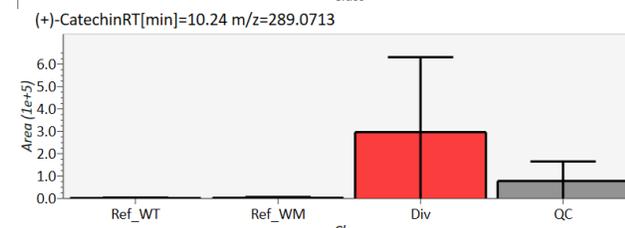
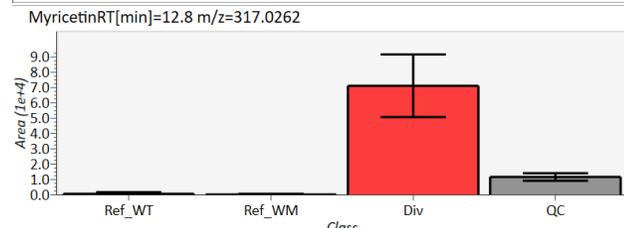
onions, grapes, berries,
cherries, broccoli, and
citrus fruits

Lotus ucrainicus,
Strychnos pseudoquina,
Quercetin 3'-methyl
ether



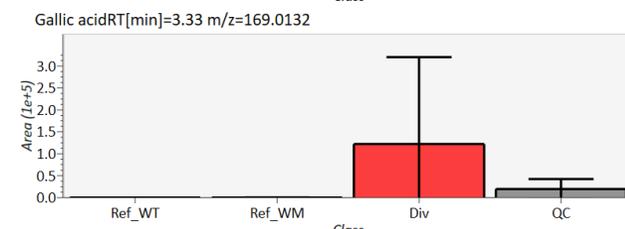
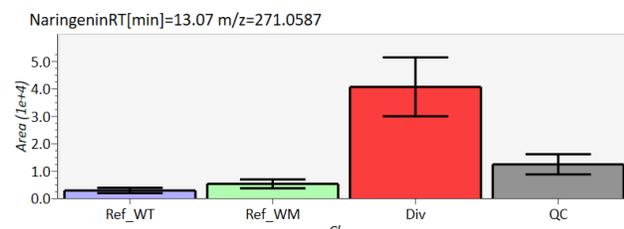
passion flower,
bamboo leaves and
pearl millet

Onion & Red Wine



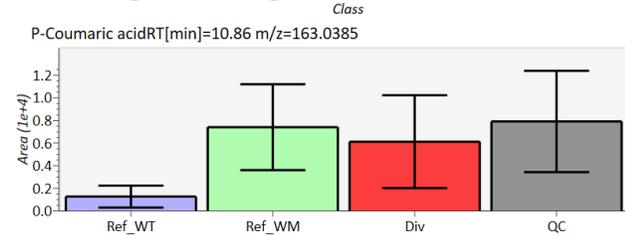
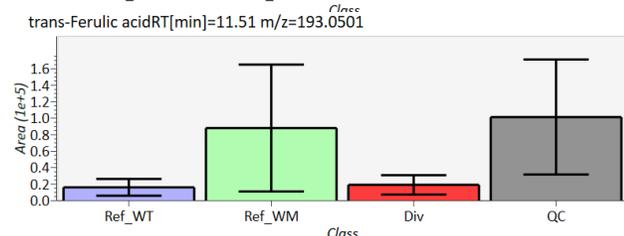
tea, apples,
persimmons, cacaos,
grapes, and berries

Citrus fruits,
bergamot, tomatoes
and other fruits



Most present Polyphenol
in fruits, berries

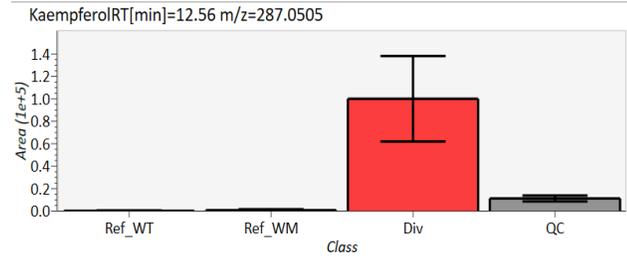
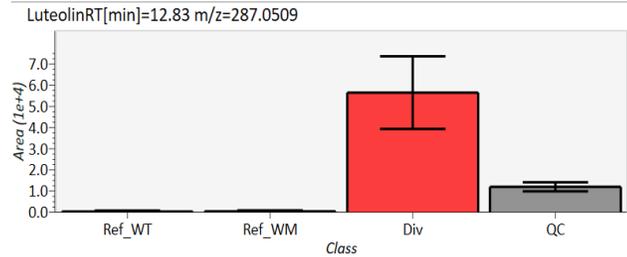
rice, wheat, oats,
and pineapple),
grasses, grains,
vegetables, flowers,



peanuts, navy beans,
tomatoes, carrots, basil
and garlic

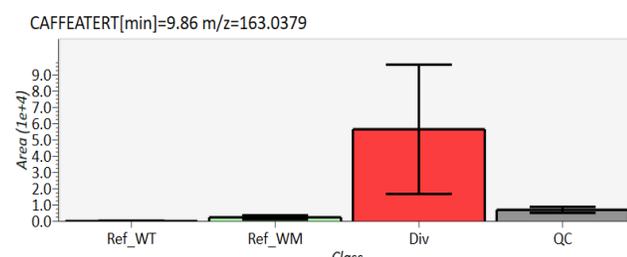
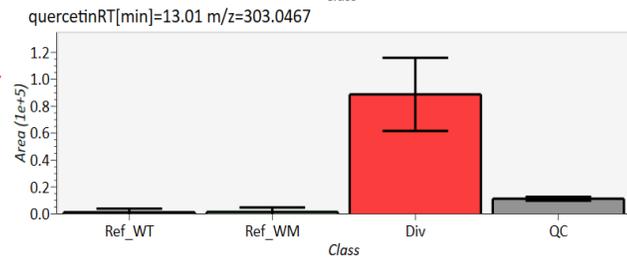


rinds, barks, clover blossom, and ragweed pollen



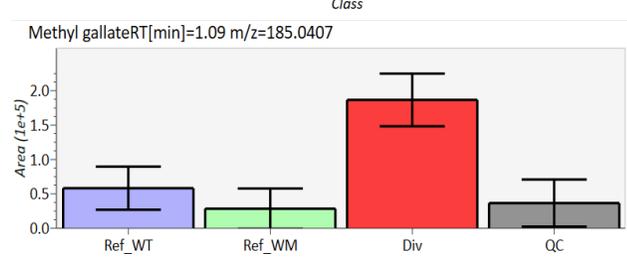
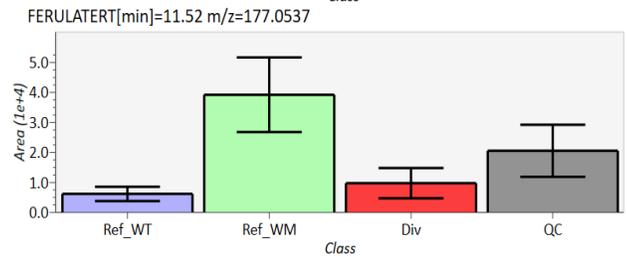
kale, beans, tea, spinach and broccoli.

onions, grapes, berries, cherries, broccoli, and citrus fruits



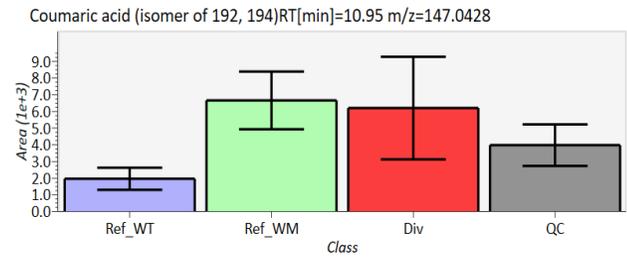
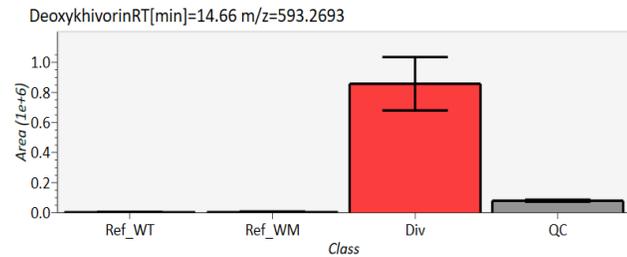
Coffee

Cereal bran and bran-enriched products



peach and pomegranate

Acalypha Indica Root

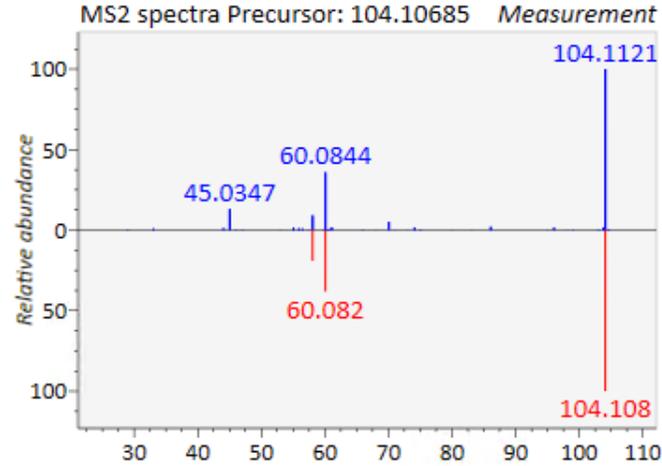
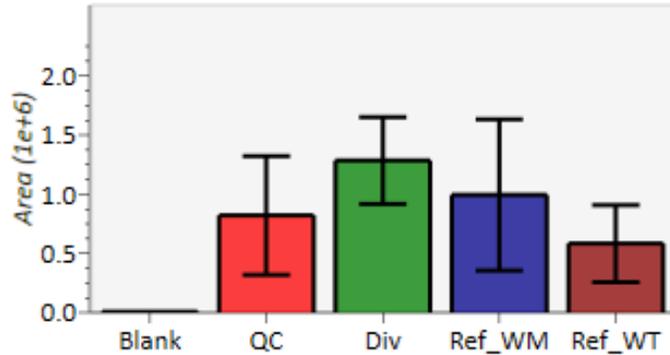


peanuts, navy beans, tomatoes, carrots, basil and garlic

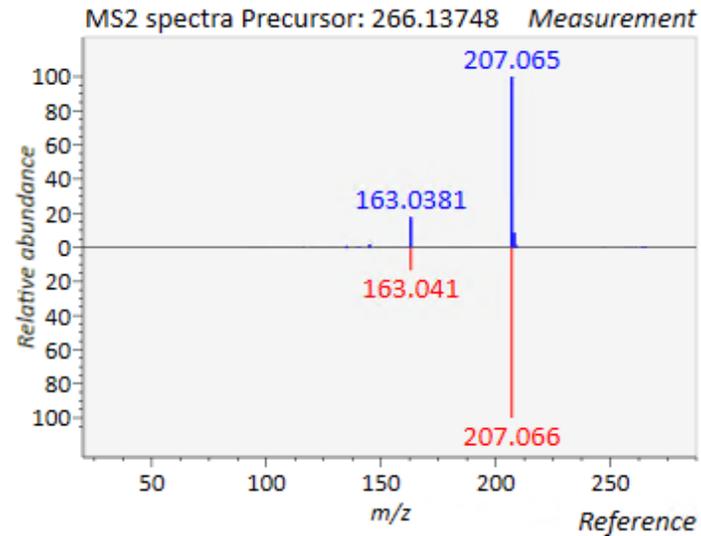
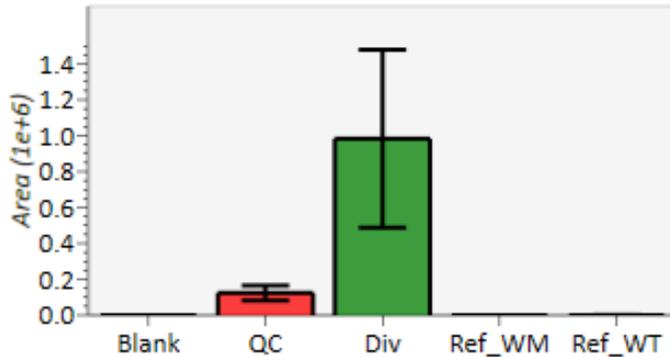
Class	Metabolite	Type of Ion	m/z	Retention Time/min	Potential Health Benefits
Positive Ionization					
Flavone	Luteolin	[M+H] ⁺	287.0509	12.83	Anti-oxidant
Flavonol	Kaempferol	[M+H] ⁺	287.0505	12.53	
	Quercetin	[M+H] ⁺	303.0467	13.01	
Phenolic Acids	Caffeic Acid	[M-H ₂ O+H] ⁺	163.0379	9.89	Anti-inflammatory & Anti-carcinogenic
	Ferulic Acid	[M-H ₂ O+H] ⁺	177.0537	11.53	Anti-oxidant
	Methyl Gallate	[M+H] ⁺	185.0407	1.07	Anti-platelet action
Anthocyanin	Deoxykhivorin	[M+Na] ⁺	593.2693	14.66	Reduce Localized Fat
Other	Coumaric Acid	[M+H-H ₂ O] ⁺	147.0428	10.96	Anti-inflammatory & Anti-microbial
Negative Ionization					
Flavone	Apigenin	[M-H] ⁻	269.0424	13.16	Anti-oxidant
	Luteolin	[M-H] ⁻	285.0383	13.16	
	Diosmetin	[M-H] ⁻	299.0596	13.21	
Flavonol	Quercetin	[M-H] ⁻	301.0341	13.01	Anti-inflammatory
	Isorhamnetin	[M-H] ⁻	315.0476	13.20	
	Myricetin	[M-H] ⁻	317.0262	12.79	Anti-oxidant
	Vitexin	[M-H] ⁻	431.0958	11.69	
Flavan-3-ol	(+)-Catechin	[M-H] ⁻	289.0713	10.24	Anti-oxidant
Flavanone	Narigenin	[M-H] ⁻	271.0587	13.09	
Phenolic Acids	Gallic Acid	[M-H] ⁻	169.0135	3.33	Anti-oxidant
	Ferulic Acid	[M-H] ⁻	193.0501	11.52	
Other	P-Coumaric Acid	[M-H] ⁻	163.0385	10.88	Anti-inflammatory & Anti-microbial

Other Metabolites

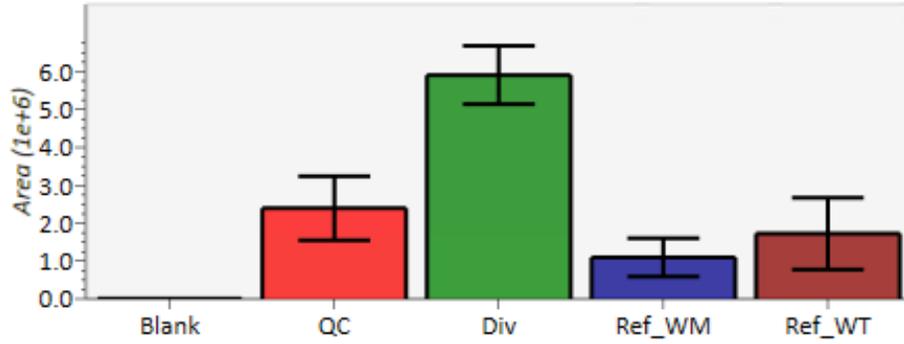
Choline RT[min]=1.16 m/z=104.1073



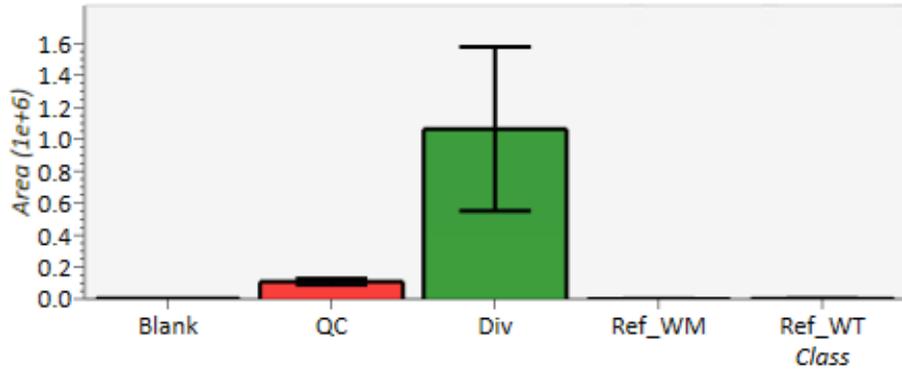
Caffeoylcholine RT[min]=9.46 m/z=266.1368



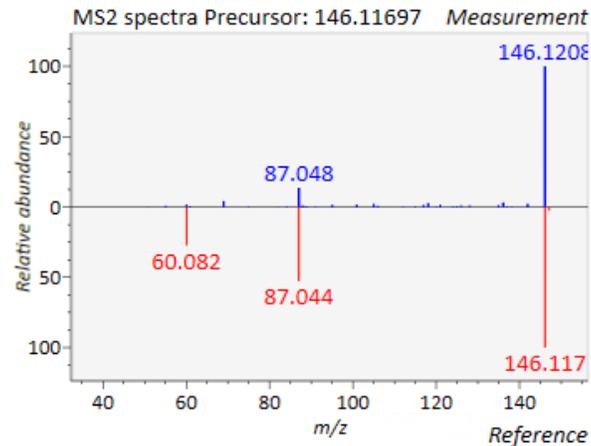
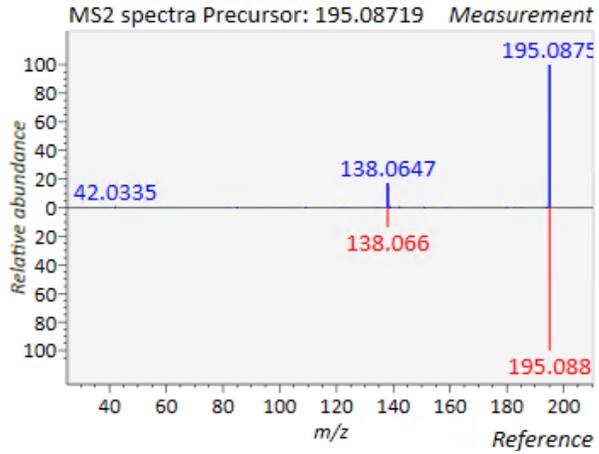
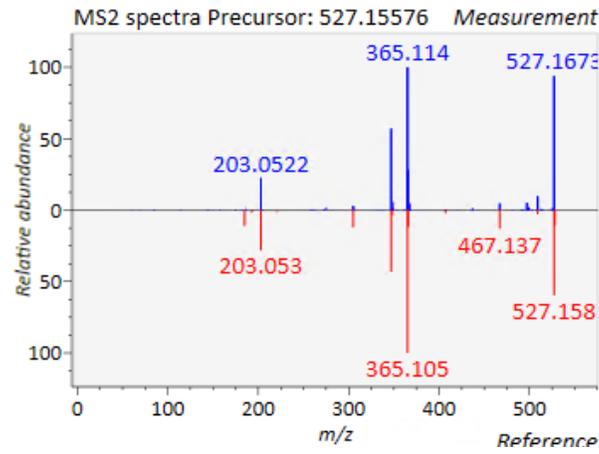
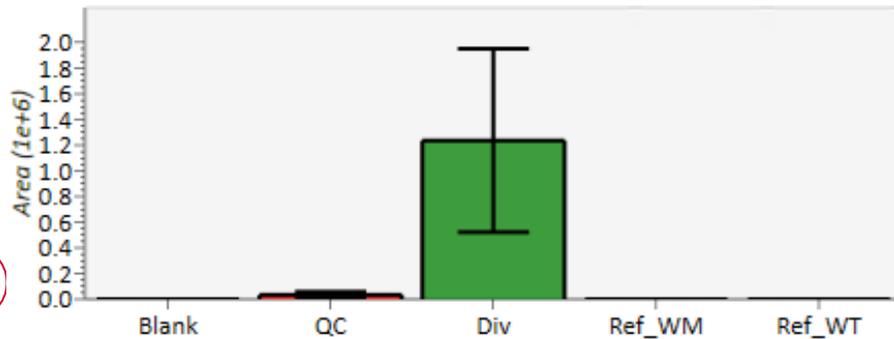
maltotriose RT [min]=1.13 m/z=527.1527



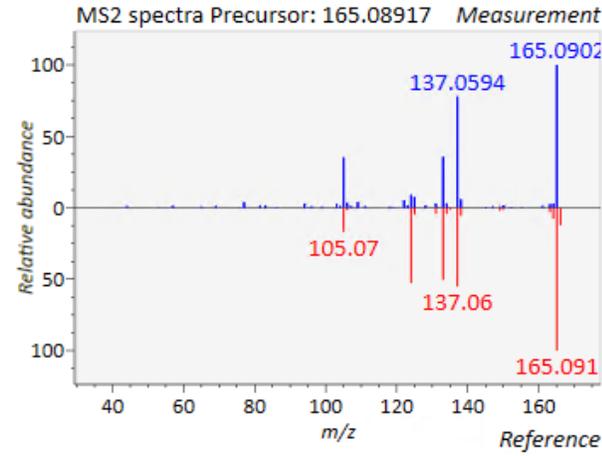
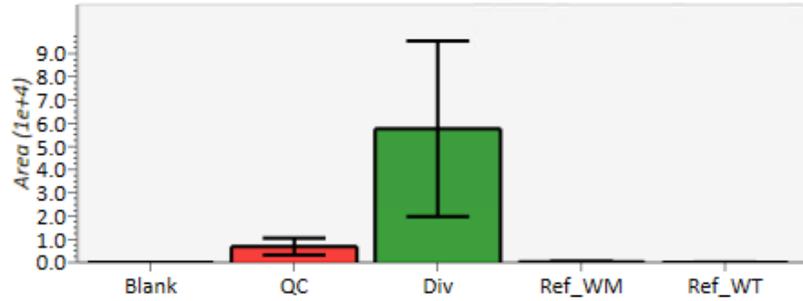
Caffeine RT [min]=10.06 m/z=195.0867



DEOXYCARNITIN RT [min]=2.14 m/z=146.1168

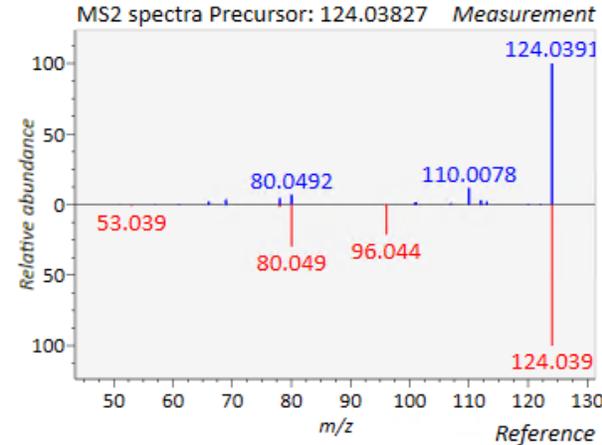
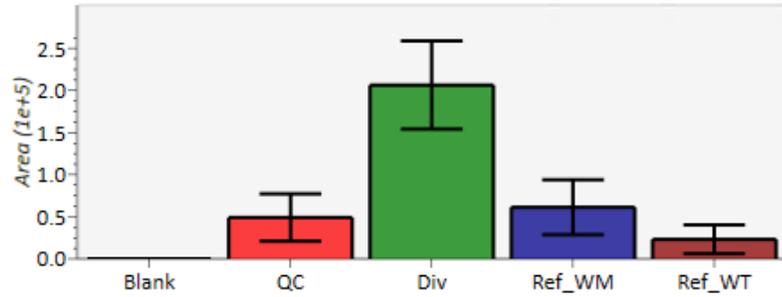


Eugenol RT[min]=13.25 m/z=165.0894



clove, nutmeg, cinnamon, basil and bay leaf. antibacterial, antifungal, antioxidant and antineoplastic activity

Nicotinic acid RT[min]=1.66 m/z=124.0387



Vitamine B3

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**THANK
YOU**

