

Supplementary Information

Jujube fruit metabolomic profiles reveal cultivar differences and function as cultivar fingerprints

Shengrui Yao ^{1,3*}, Dikshya Sapkota¹, Jordan Hungerford², and Roland Kersten²

1. Department of Plant and Environmental Sciences, New Mexico State University, Las Cruces, NM 88003, USA;
2. Department of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor, MI, 48109, USA;
3. Sustainable Agriculture Sciences Center, New Mexico State University, Alcalde, NM 87511, USA.

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Table S1 | Significant differential metabolites and corresponding metabolic pathways between cultivars. A vs B, if down-regulated, A has more metabolite than B; if up-regulated, B has more metabolite than A. Abbreviations: MP – multipurpose.

Cultivar groups (fruit types)	All significant differential metabolites	Up-regulated metabolites	Down-regulated metabolites	Up-regulated metabolic pathways	Down-regulated metabolic pathways	Differential secondary metabolites [%]
Alcalde1/ Dongzao	475	246	229	Stilbenoid, Flavone & Flavonol, Glutathione, Sulfur	Arginine, Linoleic acid, Alanine/ Aspartate/ Glutamate, Proline, Porphyrin, Nitrogen, Cyanoamino acid, Valine/ Leucine/ Isoleucine, D- amino acid, Pyrimidine, Glyoxylate and decarboxylate, Butanoate, Propanoate	41.4
Alcalde1/ Jinsi	375	192	183	Arginine & Proline, Purine alkaloids, Phenylpropanoid, Pyrimidine, Nucleotides, Tropane/piperidine/pyridine alkaloids, Betalain, Fatty acid, alpha-linoleic acid, glutathione, Purine, Stilbenoid	Sphingolipid, Flavonoid	40.5
Alcalde1/ Jixin	415	173	242	Flavonoid, Phenylpropanoid, Tryptophan, Arginine & Proline	Nucleotide, Pyrimidine, Purine, Arginine, D-amino acid, Linoleic acid	41.1
Alcalde1/ JKW	422	171	251	Phenylpropanoid, Arginine & Proline, Flavonoid, Flavone & Flavonol	Pyrimidine, Nucleotide	40.5
Alcalde1/ KFC	483	365	118	Flavonoid, Flavone & flavonol, Phenylpropanoid, Stilbenoid	Tryptophan	53.7
Alcalde1/ Lang	330	212	118	Flavonoid, Phenylpropanoid, Tryptophan, Phenylalanine, Glutathione		38.5
Alcalde1/ Li	336	206	130	Flavonoid, Sphingolipid, Quinone	Tyrosine, Isoquinoline alkaloids, Nucleotide	42.6
Alcalde1/ Maya	489	368	121	Phenylalanine, Phenylpropanoid, Flavonoid, Arginine & Proline	Flavone & Flavonol	42.5
Alcalde1/ Shanxi Li	378	103	275	Flavonoid, Quinone, Flavone & Flavonol, Purine, Nucleotide	Tyrosine, Isoquinoline alkaloids	55.6
Alcalde1/ ZCW	404	203	201	Arginine & Proline, Phenylpropanoid	Nucleotide	43.7
Dongzao/ Jinsi	544	278	266	Linoleic acid, Cyanoamino acid, Amino acid, Tropane/piperidine/pyridine alkaloid, Quinone, 2-oxocarboxylic acid, glucosinolate	Sphingolipid	45.8
Dongzao/ Jixin	511	230	281	Arginine & Proline, Nucleotide, Purine	Glutathione, Flavone & Flavonol	42.6
Dongzao/ JKW	564	316	248	Linoleic acid, Nucleotide, Purine, Arginine & Proline, Phenylalanine, D-amino acid,	Flavone & Flavonol	39.4
Dongzao/ KFC	531	403	128	Arginine & Proline, Flavonoid, Isoquinoline alkaloid, Linoleic acid, Flavone & flavonol, Tyrosine, Phenylalanine	Glutathione	42.4
Dongzao/ Lang	520	209	311	Amino acid, Cyanoamino acid, D-amino acid, Glutathione, Nucleotide	Phenylpropanoid	48.2
Dongzao/ Li	487	260	227	Amino acid, Flavonoid, Linoleic acid, Sphingolipid	Phenylpropanoid, Flavone & flavonol, Sulfur	50
Dongzao/ Maya	575	400	175	Linoleic acid, Quinone, Tyrosine, Arginine & proline, Tropane/piperidine/pyridine alkaloid, Isoquinoline alkaloid, Cyanoamino acid, Purine, Pyrimidine, Alanine/ Aspartate/ Glutamate, Nucleotide		42.4
Dongzao/ Shanxi Li	528	188	340	Amino acids, Linoleic acid, Flavonoid, Isoquinoline alkaloid, Phenylalanine, Nucleotide	Phenylpropanoid	46.7
Dongzao/ ZCW	571	302	269	Linoleic acid, Purine, Nucleotide, Pyrimidine, Arginine & proline		35.3
Jinsi/ Jixin	473	195	278	Vitamin B6	Linoleic acid, Amino acids, Betalain, Phenylpropanoid, Glutathione	50.7
Jinsi/ JKW	47	36	11		Amino acid, Tropane/piperidine/pyridine alkaloid, glucosinolate, 2- oxocarboxylic acid	62.5
Jinsi/ KFC	494	379	115	Sphingolipid, Flavonoid, Flavone & Flavonol	Cyanoamino acid, Thiamine, Amino acids, Nucleotide, Pantothenate & CoA, Purine	46.8
Jinsi/ Lang	420	270	150	Fructose & Mannose, Nucleotide,	Linoleic acid, Phenylpropanoid, D-amino acid	43.5
Jinsi/ Li	403	195	208	Sphingolipid, Flavonoid, Flavone & Flavonol, Lysine	Linoleic acid, Tropane/piperidine/pyridine alkaloid, zeatin, phenylpropanoid, arginine & proline, glutathione, Nucleotide	39.8
Jinsi/ Maya	533	394	139	Phenylalanine, Tyrosine, Arginine & proline	Purine, Nucleotide, Glutathione	39.2
Jinsi/ Shanxi Li	473	178	295	Flavonoid, Flavone & flavonol	Linoleic acid, Tropane/piperidine/pyridine alkaloid, phenylpropanoid	40.2
Jinsi/ ZCW	339	158	181		Tropane/ Piperidine/ Pyridine alkaloid, Glucosinolate, Amino acids, 2- oxocarboxylic acid	45.5
Jixin/ JKW	498	267	231	Linoleic acid, Phenylpropanoid	Flavonoid	43.9
Jixin/ KFC	531	377	154	Flavone & flavonol, Flavonoid, Phenylpropanoid, Tropane/piperidine/pyridine alkaloid, phenylalanine	Tryptophan, Purine	56.7
Jixin/ Lang	466	215	251	Nicotinate/ Nicotinamide, Glutathione, Nucleotide, Pyrimidine, Linoleic acid	Phenylpropanoid	40.9
Jixin/ Li	481	256	225	Flavonoid, Sphingolipid, Arginine, Flavone & Flavonol	Tyrosine, Phenylpropanoid	44.8
Jixin/ Maya	574	192	382	Phenylalanine, Tryptophan, Arginine & proline, Tropane/piperidine/pyridine alkaloid, linoleic acid,	Sulfur, flavonoid	45.2
Jixin/ Shanxi Li	553	245	308	Flavonoid, Sphingolipid, Flavone & flavonol, Linoleic acid, Glutathione	Phenylpropanoid	39.7
Jixin/ ZCW	510	286	224	Glutathione, Pantothenate and CoA, Linoleic acid, Flavone & flavonol, Nucleotide,	Purine	37.1
JKW/ KFC	517	132	385	Flavonoid, Flavone & flavonol, Sphingolipid, phenylpropanoid, arginine, phenylalanine	Nucleotide, Purine	49.2
JKW/ Lang	436	177	259	Flavonoid	Purine	40
JKW/ Li	452	207	245	Flavonoid, Flavone & flavonol	Linoleic acid	44.3
JKW/ Maya	561	392	169	Phenylalanine, Sphingolipid, Tyrosine, Tryptophan, Arginine & proline	Purine, Phenylpropanoid	40
JKW/ Shanxi Li	510	232	278	Flavonoid, Flavone & Flavonols, Sphingolipid	Linoleic acid, unsaturated fatty acids, tropane/piperidine/pyridine alkaloids, phenylalanine	43.1
JKW/ ZCW	384	160	224	Sphingolipid, Flavonoid, Flavone & flavonol	Phenylalanine, Purine	37
KFC/ Lang	498	178	320	Glutathione	Phenylpropanoid, Flavone & flavonol, Tyrosine	45.5
KFC/ Li	492	154	338	Glutathione, D-amino acid,	Phenylpropanoid, Flavonoid, Tropane/piperidine/pyridine alkaloid, Flavone & flavonol	50.8
KFC/ Maya	474	222	252	Linoleic acid, Tryptophan	Purine, Nucleotide, Flavonoid, Flavone & flavonol	52.2
KFC/ Shanxi Li	504	293	211	D-amino acid, glutathione, cofactors, tryptophan, sucrose, cyanoamino acid, cysteine & methionine, purine	phenylpropanoid, linoleic acid, betalain	51.7
KFC/ ZCW	498	381	117	arginine & proline	flavonoid, flavone & flavonol, purine, phenylpropanoid, stilbenoid, nucleotide	49.2
Lang/ Li	355	149	206	Purine, Nucleotide	Flavonoid, Isoquinoline alkaloid, Phenylpropanoid, Tyrosine, Phenylalanine	50
Lang/ Maya	437	265	172	Tyrosine, Phenylpropanoid, Linoleic acid, Arginine & proline	Phenylalanine, Glutathione, Purine, Flavonoid, Nucleotide	41.8
Lang/ Shanxi Li	392	193	199	Purine, Nucleotide	Phenylalanine, Flavonoid, Phenylalanine, Phenylpropanoid, Cysteine & methionine, Pyrimidine	50
Lang/ ZCW	445	181	264	Arginine & proline, Tyrosine, Glutathione, Tropane/piperidine/pyridine alkaloid, phenylpropanoid	Nucleotide, Purine, D-amino acid, Flavonoid	42.2
Li/ Maya	486	337	149	Linoleic acid, Tryptophan, Phenylpropanoid	Purine, Glutathione, Nucleotide	44.6
Li/ Shanxi Li	42	36	6		Glucosinolate, Amino acids, Phenylpropanoid, 2-oxocarboxylic acid	75
Li/ ZCW	436	198	238		Glucosinolate, Amino acids, 2-Oxocarboxylic acid	42
Maya/ Shanxi Li	500	297	203	Purine, Nucleotide, Glutathione, Sulfur	Tryptophan, Linoleic acid, Quinones, Tyrosine, Phenylalanine, Isoquinoline alkaloid	42.9
Maya/ ZCW	519	130	389	Tropane/piperidine/pyridine alkaloids	Phenylalanine, Tryptophan, Arginine & proline, Flavonoid	53.1
Shanxi Li/ ZCW	494	312	182	Phenylpropanoid, Arginine & Proline, Linoleic acid	Flavonoid, Purine, D-amino acid, Pyrimidine, Nucleotide	47.8

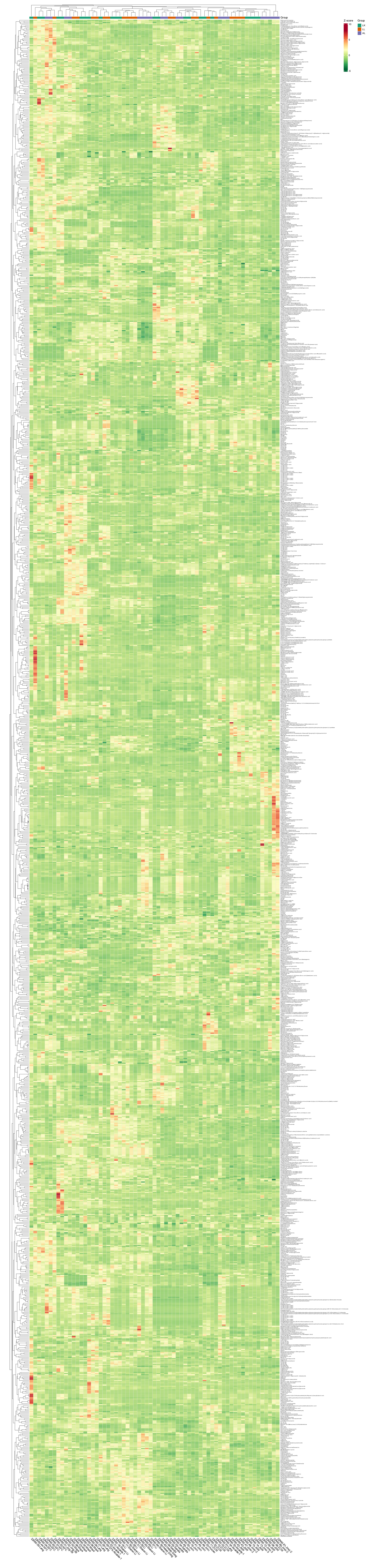


Figure S1. Heatmap of all cultivars, locations and metabolites with clustering for both locations (top) and metabolites (left).

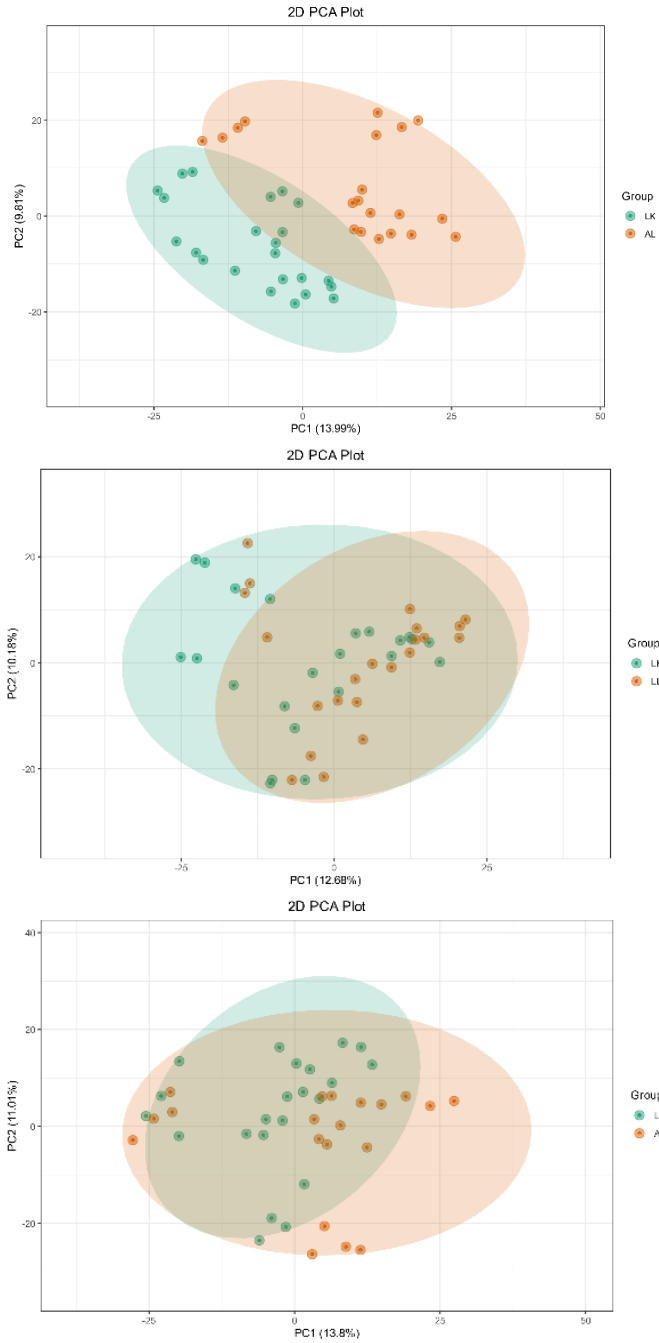


Figure S2. PCA eclipse figures of 11 jujube cultivars at three locations: left: LK vs AL (a), middle: LK vs LL, and right: LL vs AL. AL: Alcalde, NM; LK: Leyendecker/Las Cruces, NM, and LL-Los Lunas, NM.



Figure S3. All cultivars and all metabolites heatmap. The X axis indicates cultivar names and Y axis is metabolite classes.

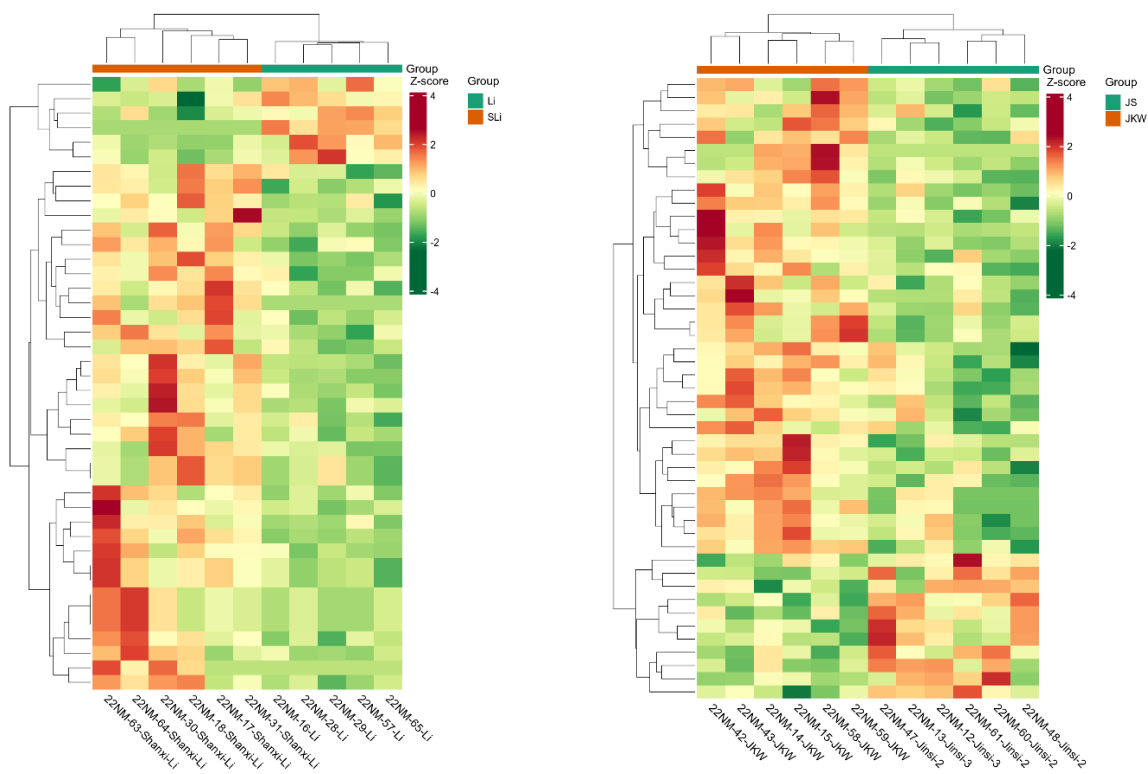
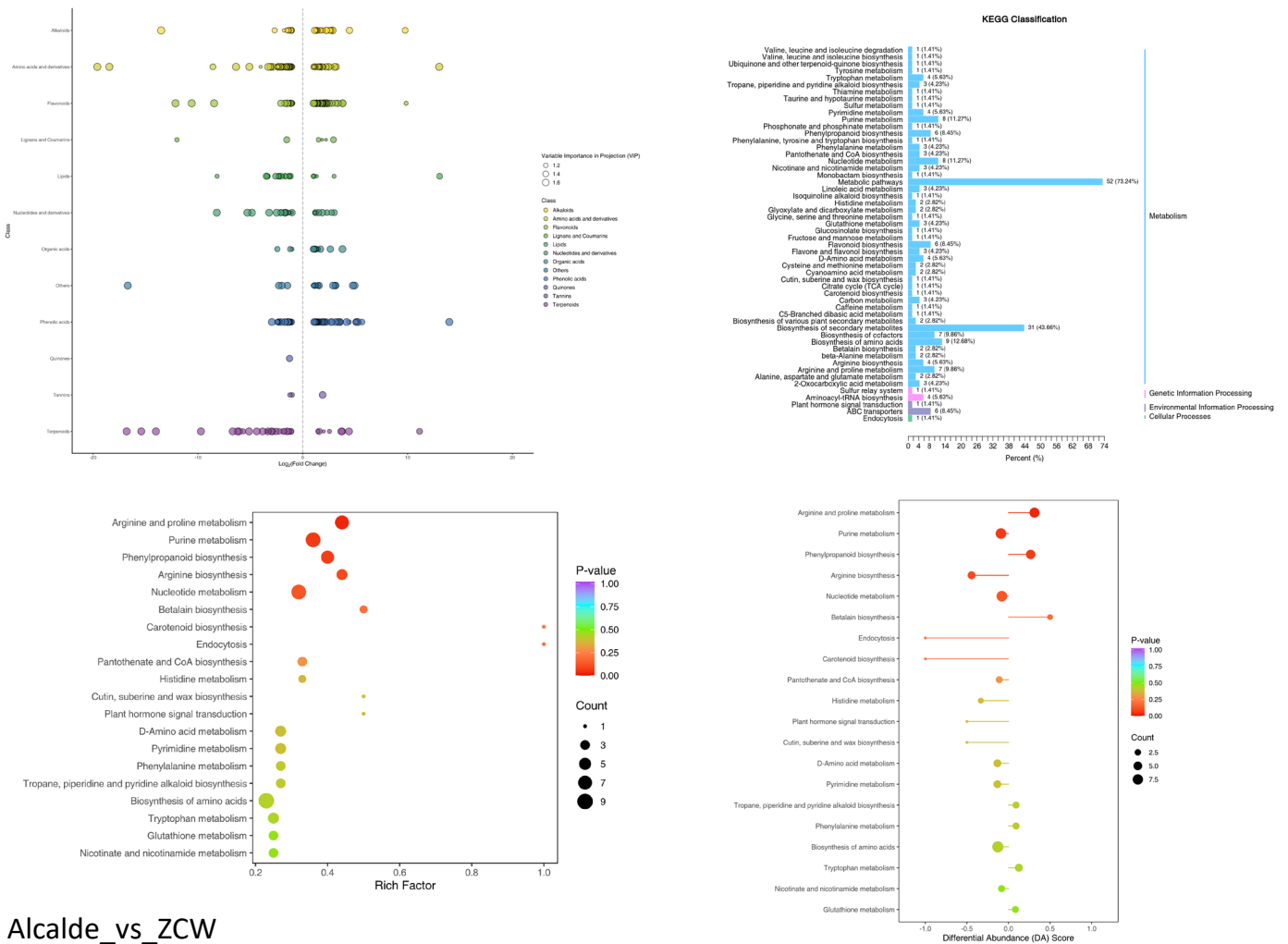
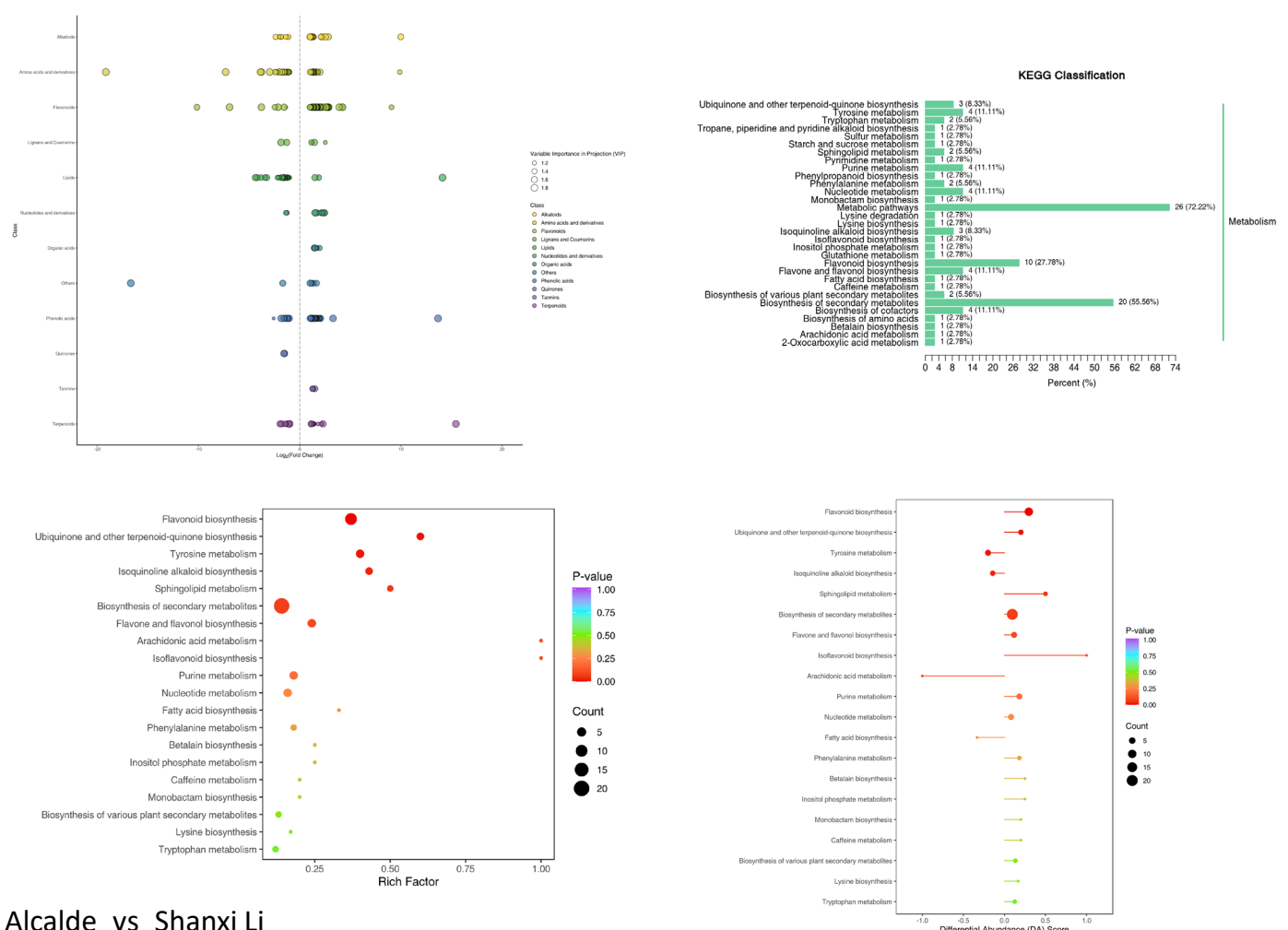


Figure S4. Heatmaps of differential metabolites of Li vs Shanxi Li and JS vs JKW.



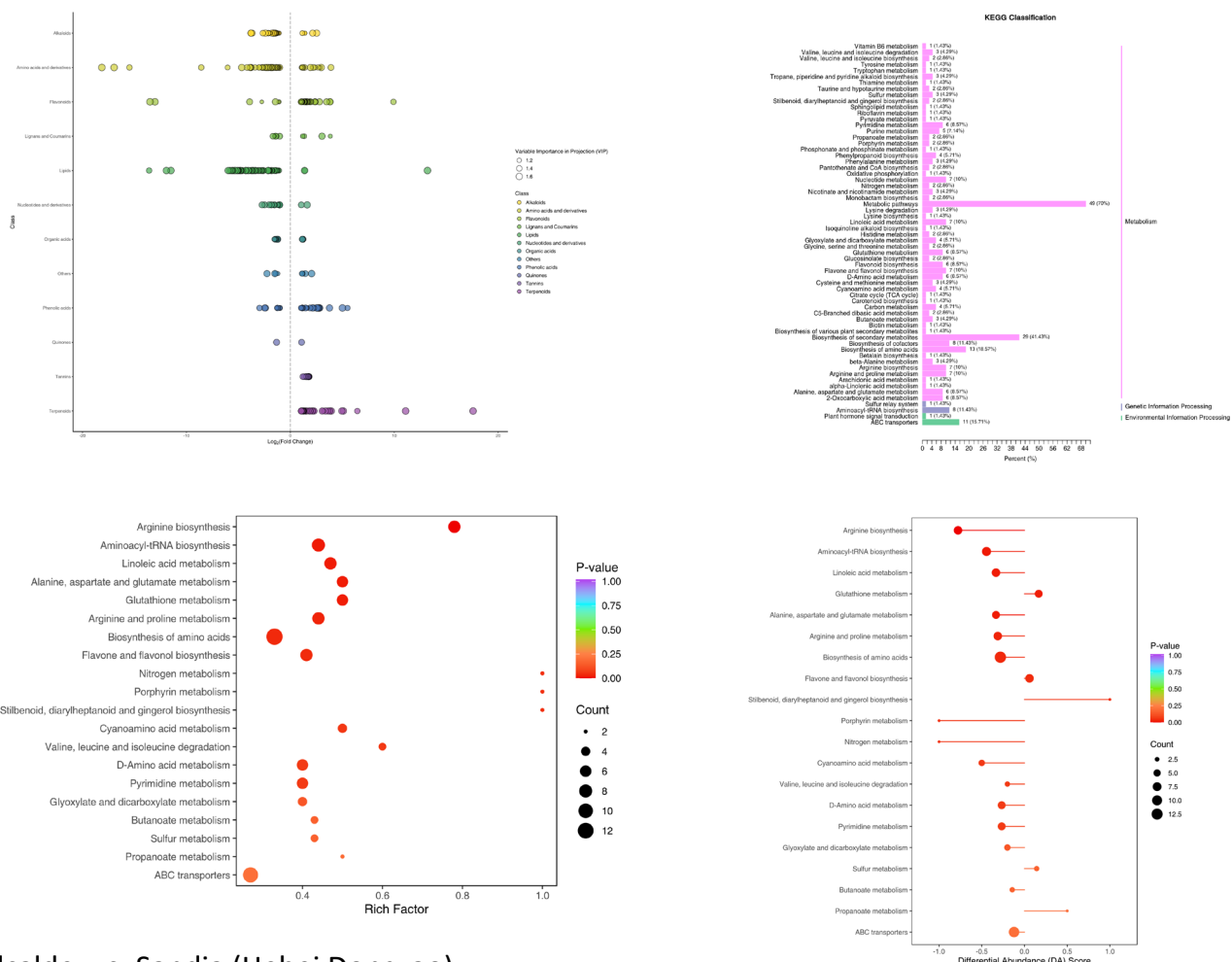
Alcalde_vs_ZCW

Figure S5 | Pairwise differential metabolite analysis between *Ziziphus jujuba* cultivars. Scatter plot of differential metabolites shown on top, left. Each dot in the graph indicates a metabolite, and different colors indicate different metabolite subclasses; the horizontal coordinate indicates the logarithmic value of the multiplicative difference in the content of a substance in two groups of samples ($\log_2\text{FC}$), the larger the absolute value of the horizontal coordinate, the greater the difference in the content of the substance between the two groups of samples, and the size of the dot represents the VIP value. **KEGG classification of differential metabolites on the top right.** The Y-axis shows the name of the KEGG pathway. The number of significant differential metabolites and the proportion of the total significant differential metabolites are shown next to the bar plot. **KEGG enrichment diagram of differential metabolites on bottom left.** The X-axis represents the Rich Factor and the Y-axis represents the pathway. The color of points reflects the p-value. The darker the red, the more significant the enrichment. The size of the dot represents the number of enriched differential metabolites. **Analysis of overall changes in KEGG metabolic pathway on bottom right.** The Y-axis represents the name of differential pathway, and the X-axis represents DA Score. DA Score reflects the overall change of all metabolites in the metabolic pathway. A Score of 1 indicates that the expression trend of all identified metabolites in this pathway is up-regulated, and -1 indicates that the expression trend of all identified metabolites in this pathway is down-regulated. The length of the line represent the absolute value of DA-score while the size of the dot at the end of the line represent the number of differential metabolites. A dot on the left of the line represent the pathway is down-regulated; a dot on the right of the line represents the pathway is up-regulated. The color of the line and dot represent the p-value. The darker the red, the smaller the p-value and the darker the purple, the larger the p-value.



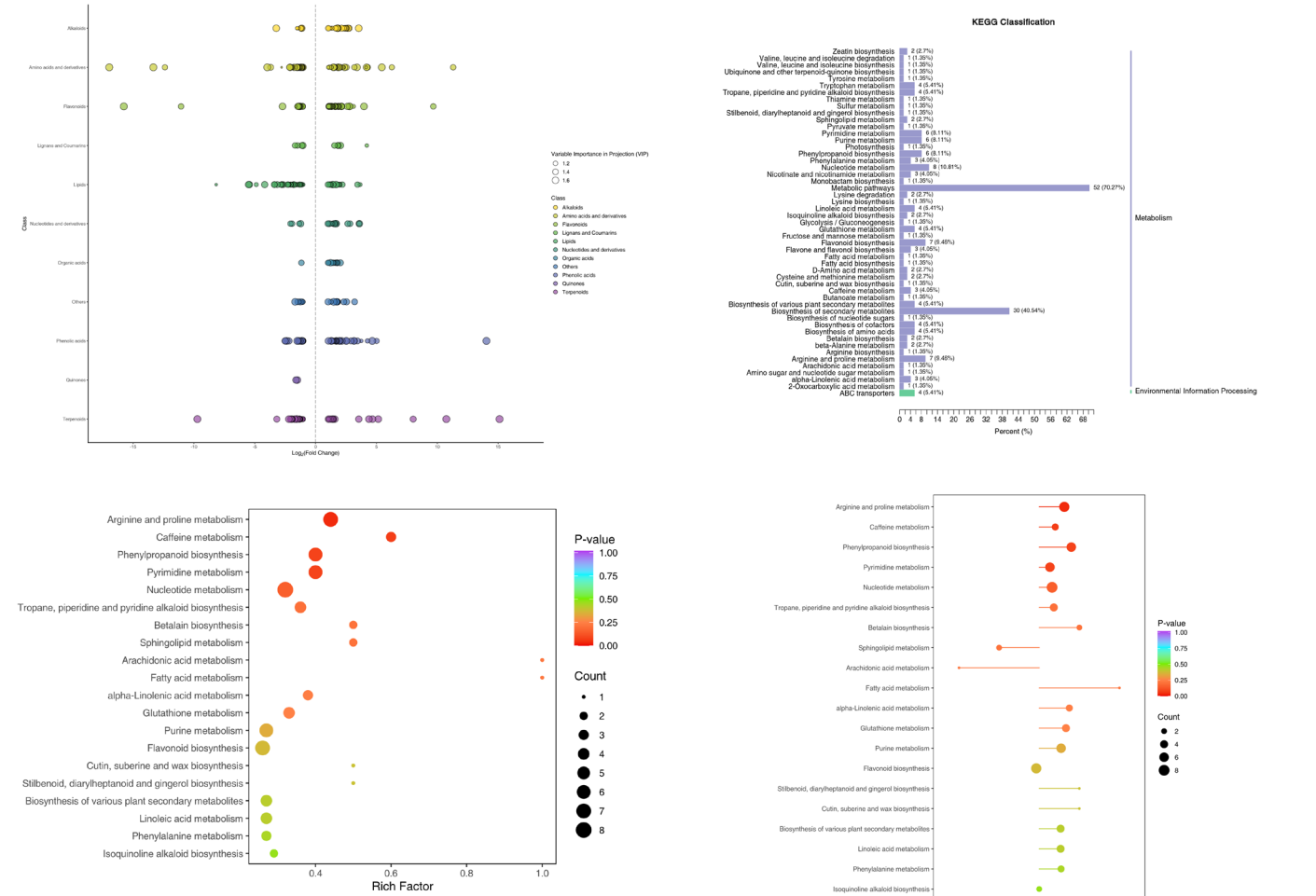
Alcalde_vs_Shanxi Li

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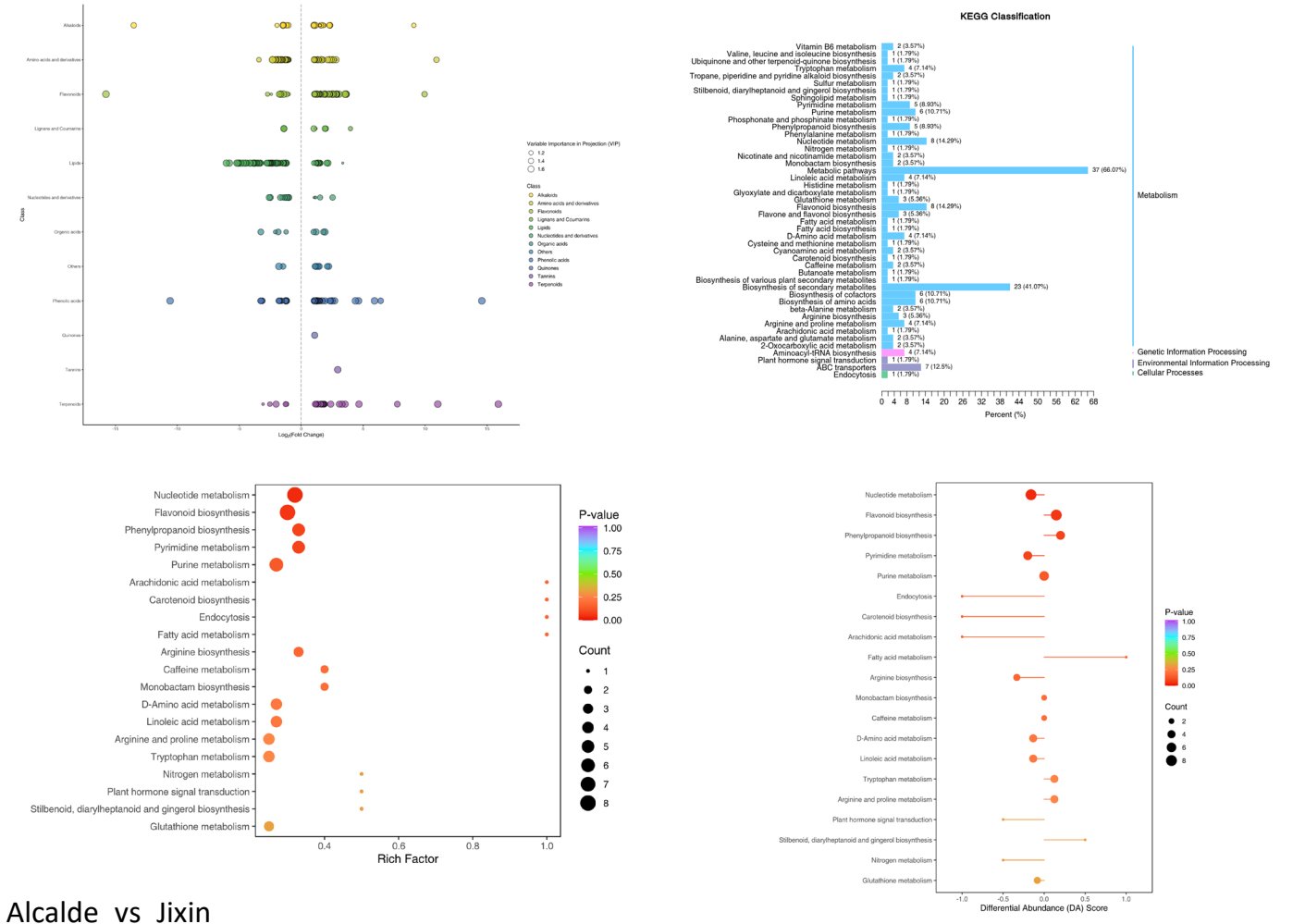
Alcalde_vs_Sandia (Hebei Dongzao)

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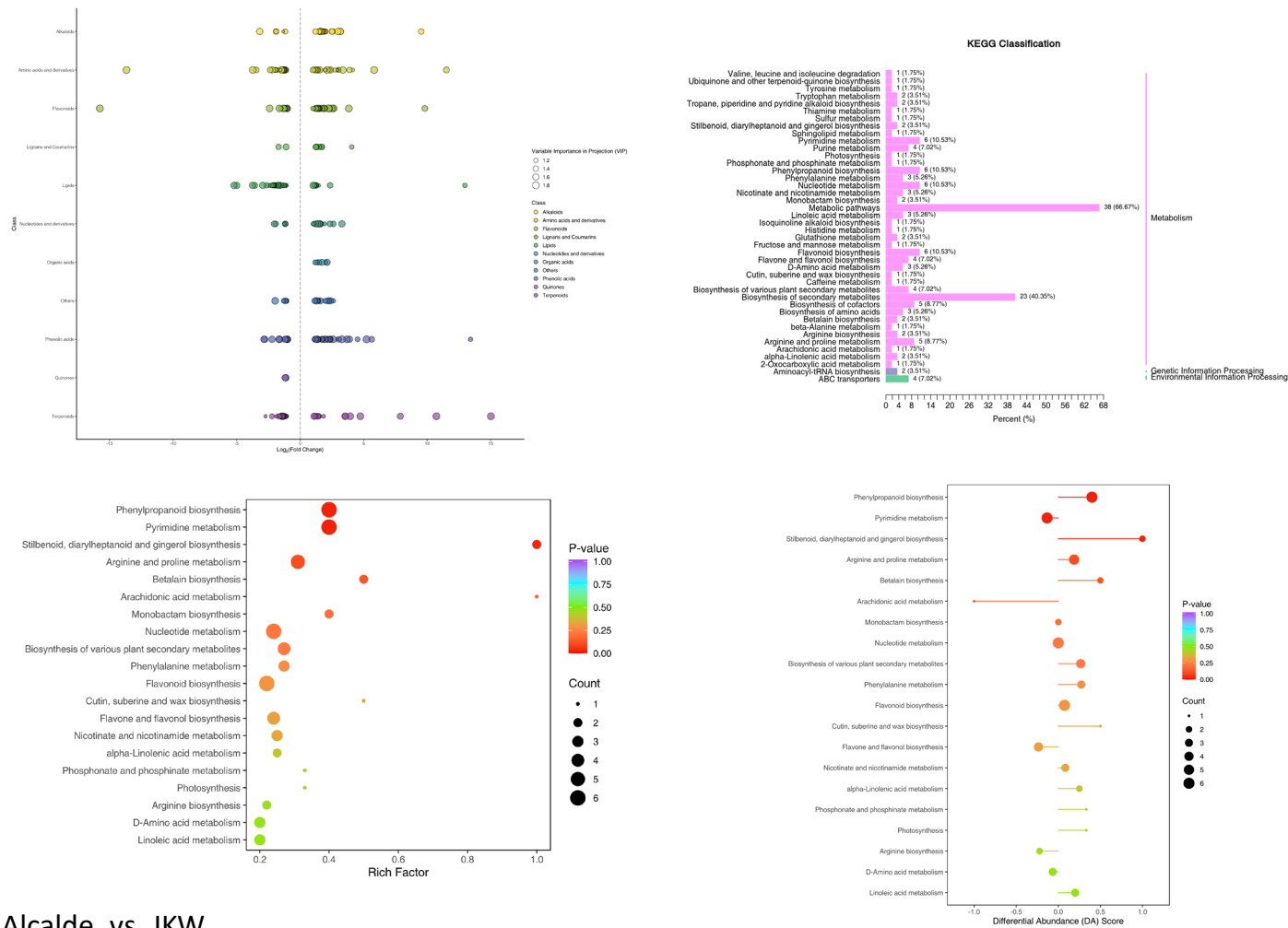


Alcalde_vs_Jinsi

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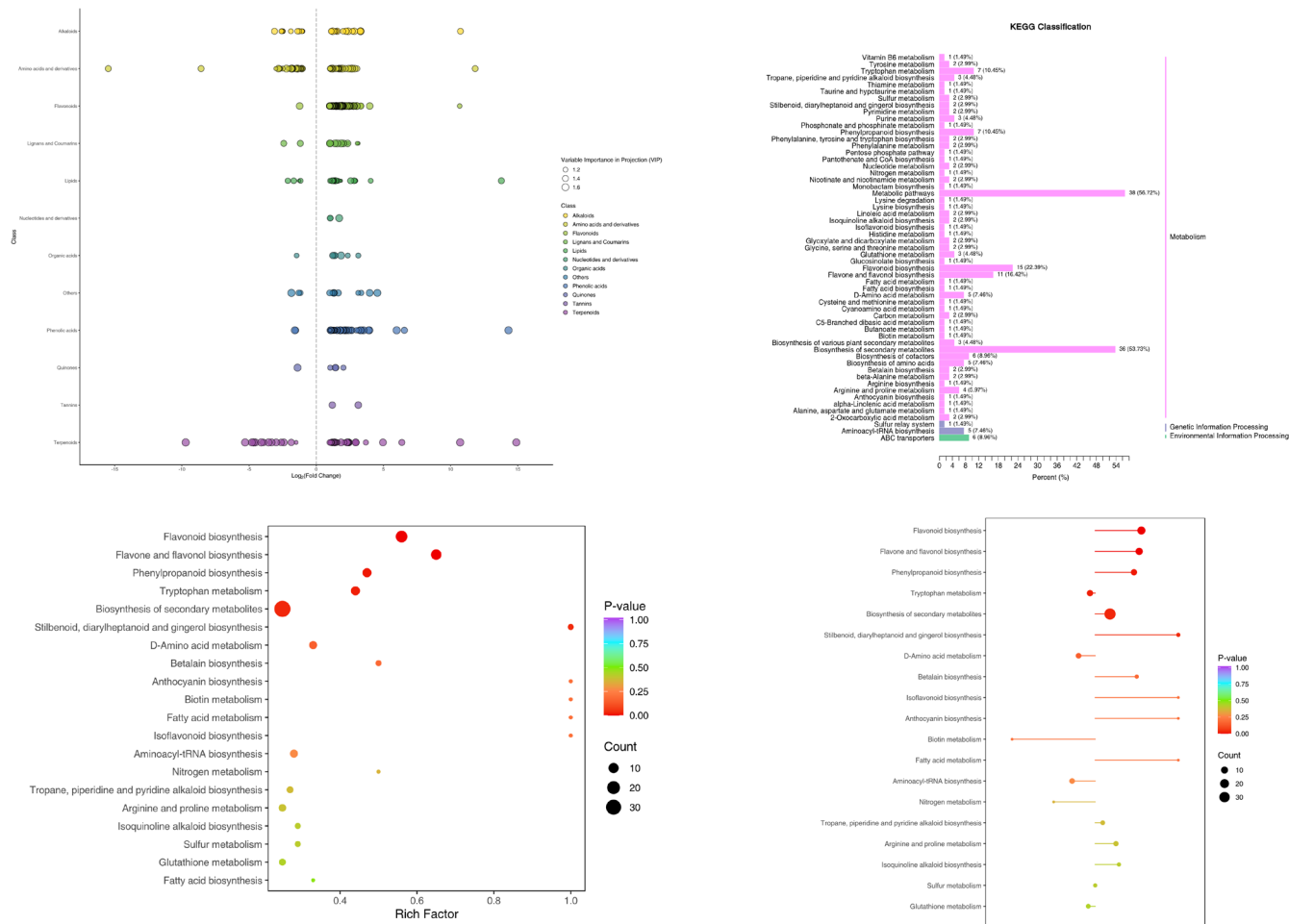


Alcalde_vs_Jixin



Alcalde_vs_JKW

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Alcalde_vs_KFC

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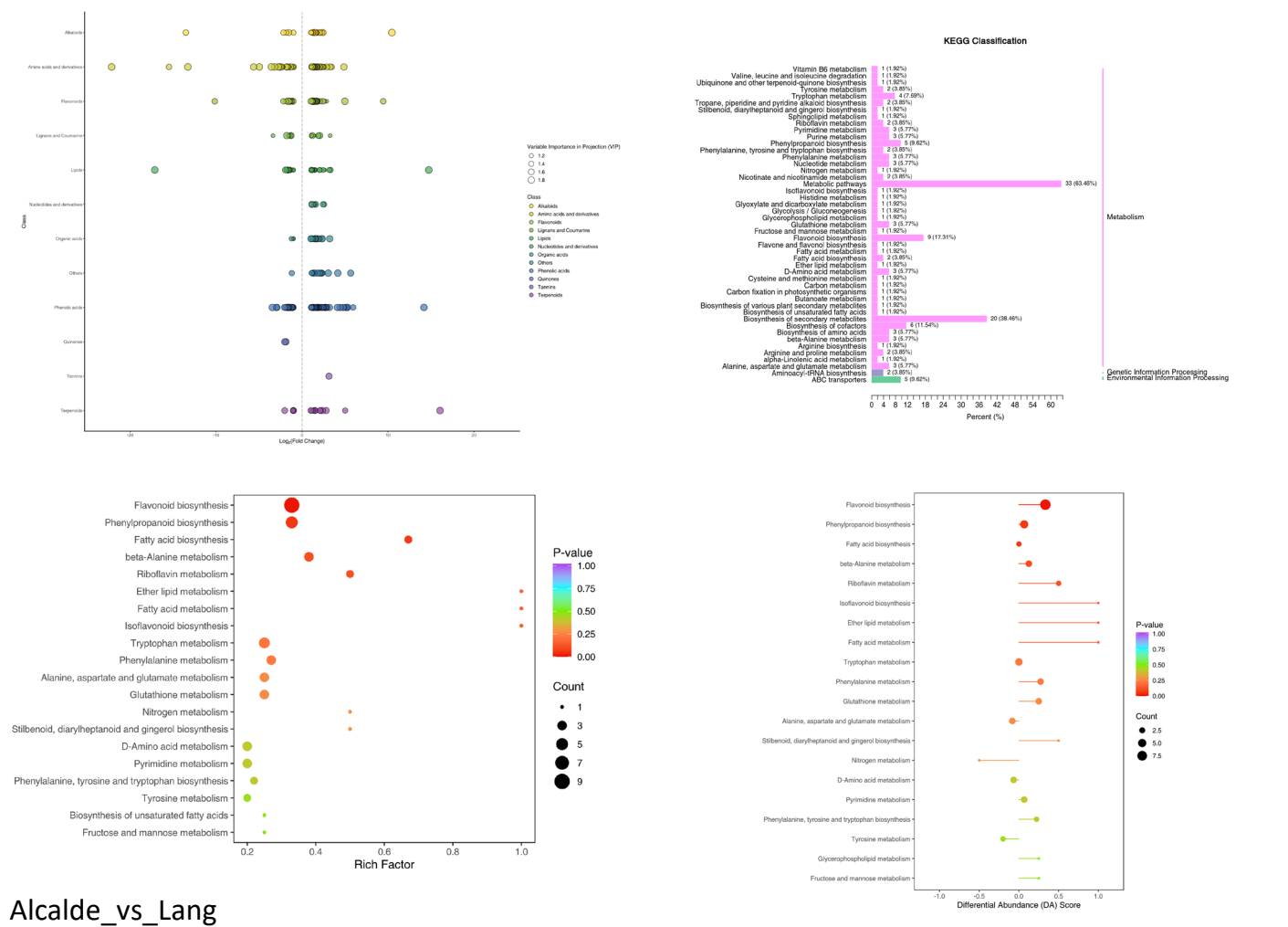
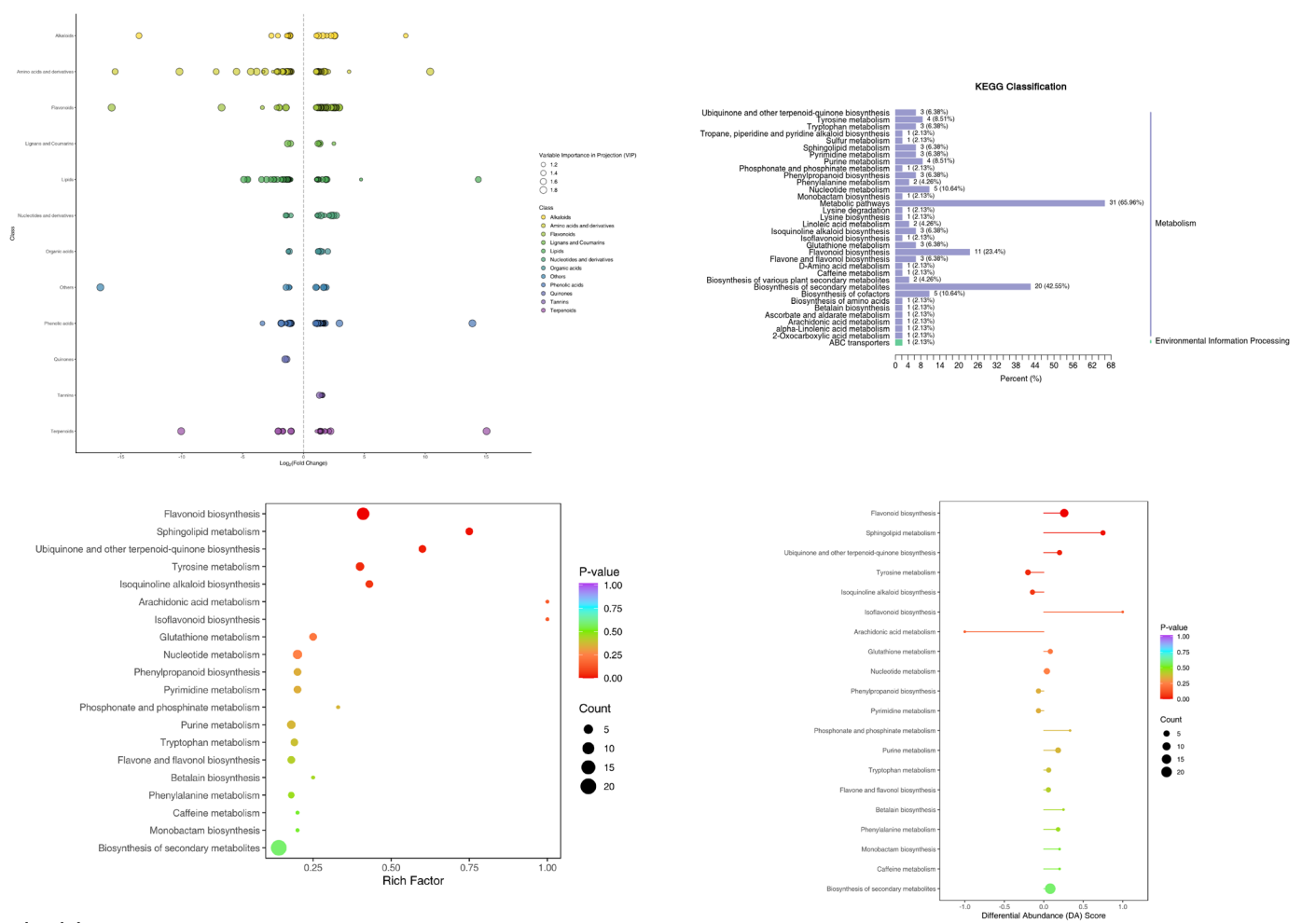
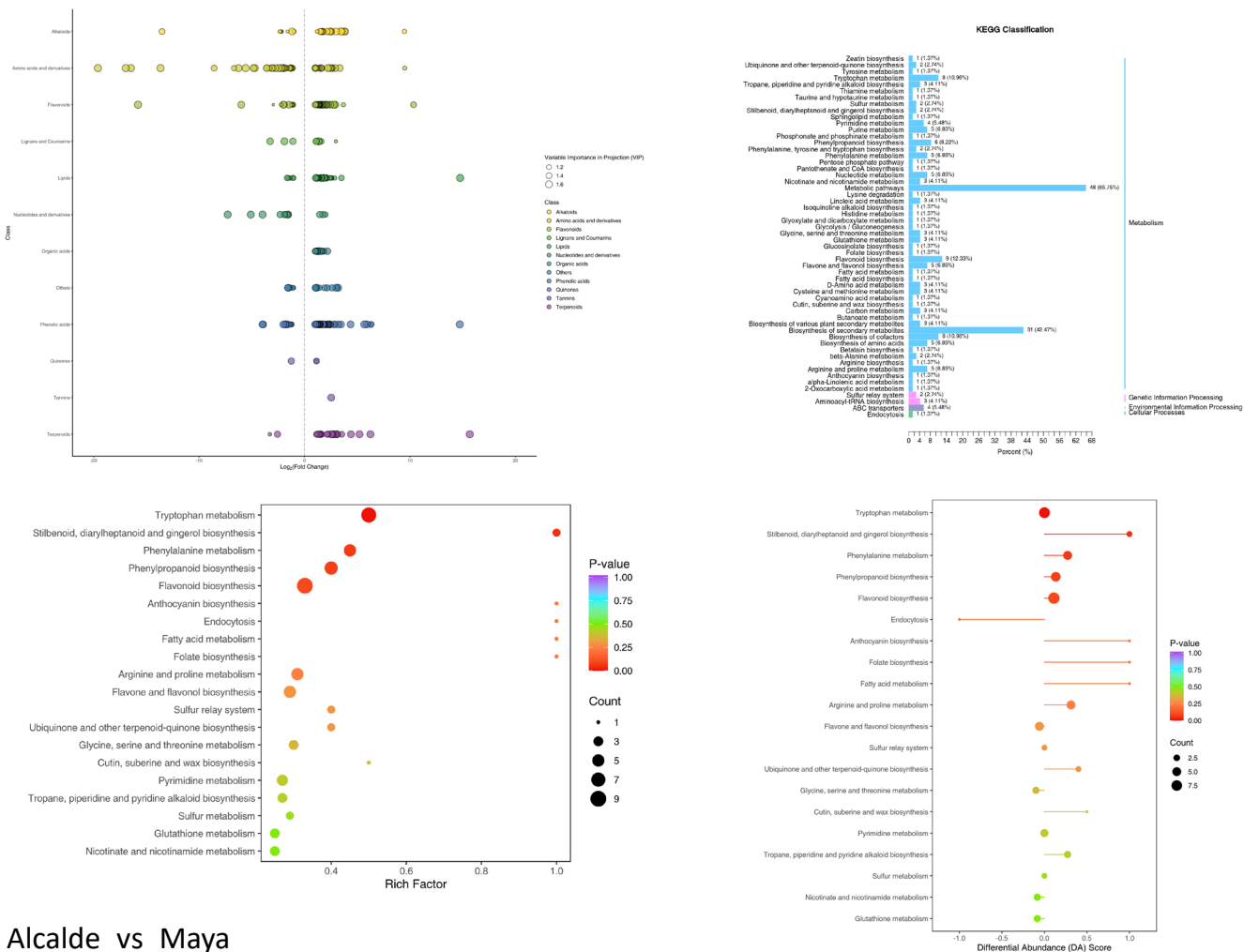


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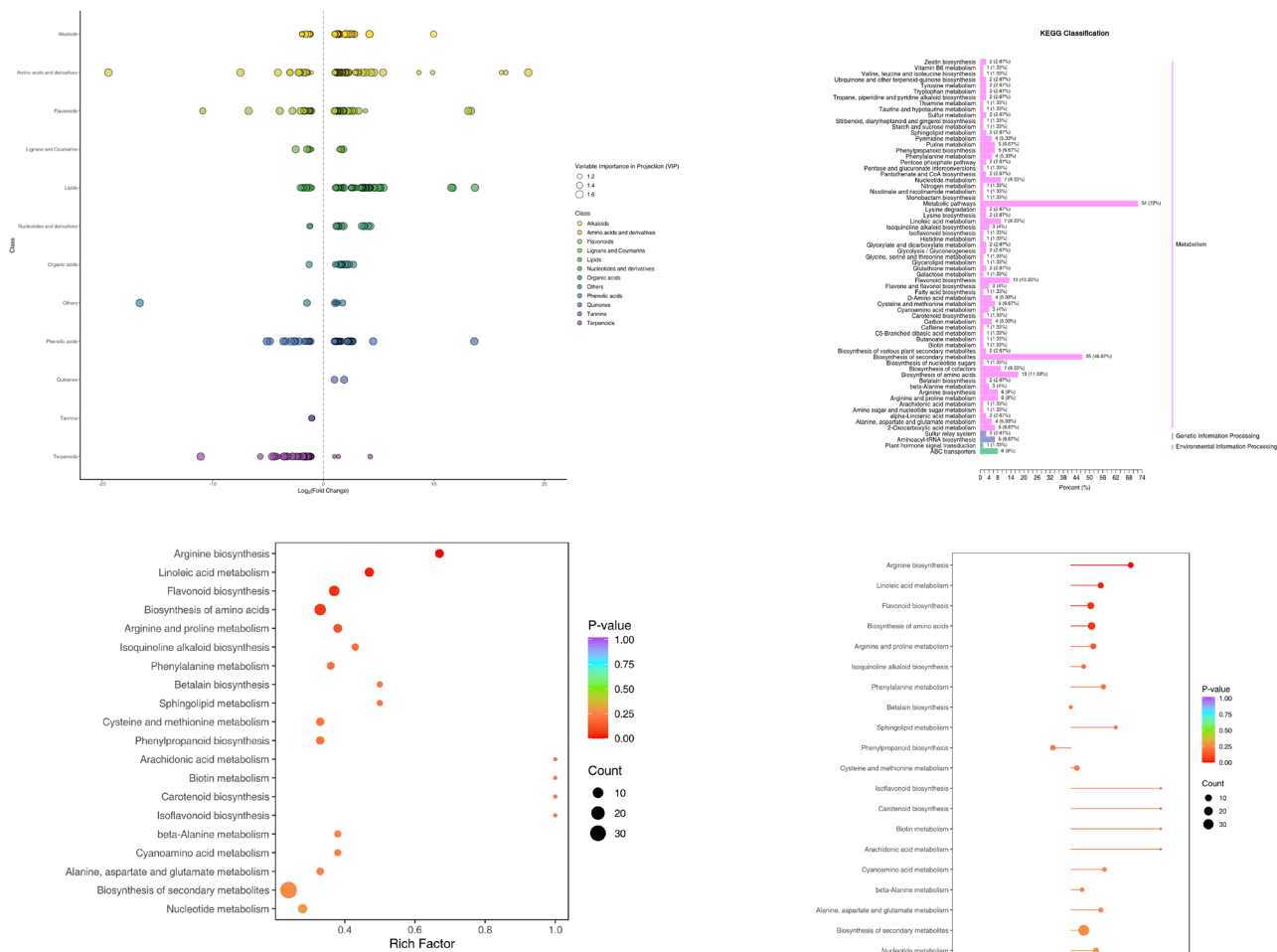
Alcalde_vs_Li

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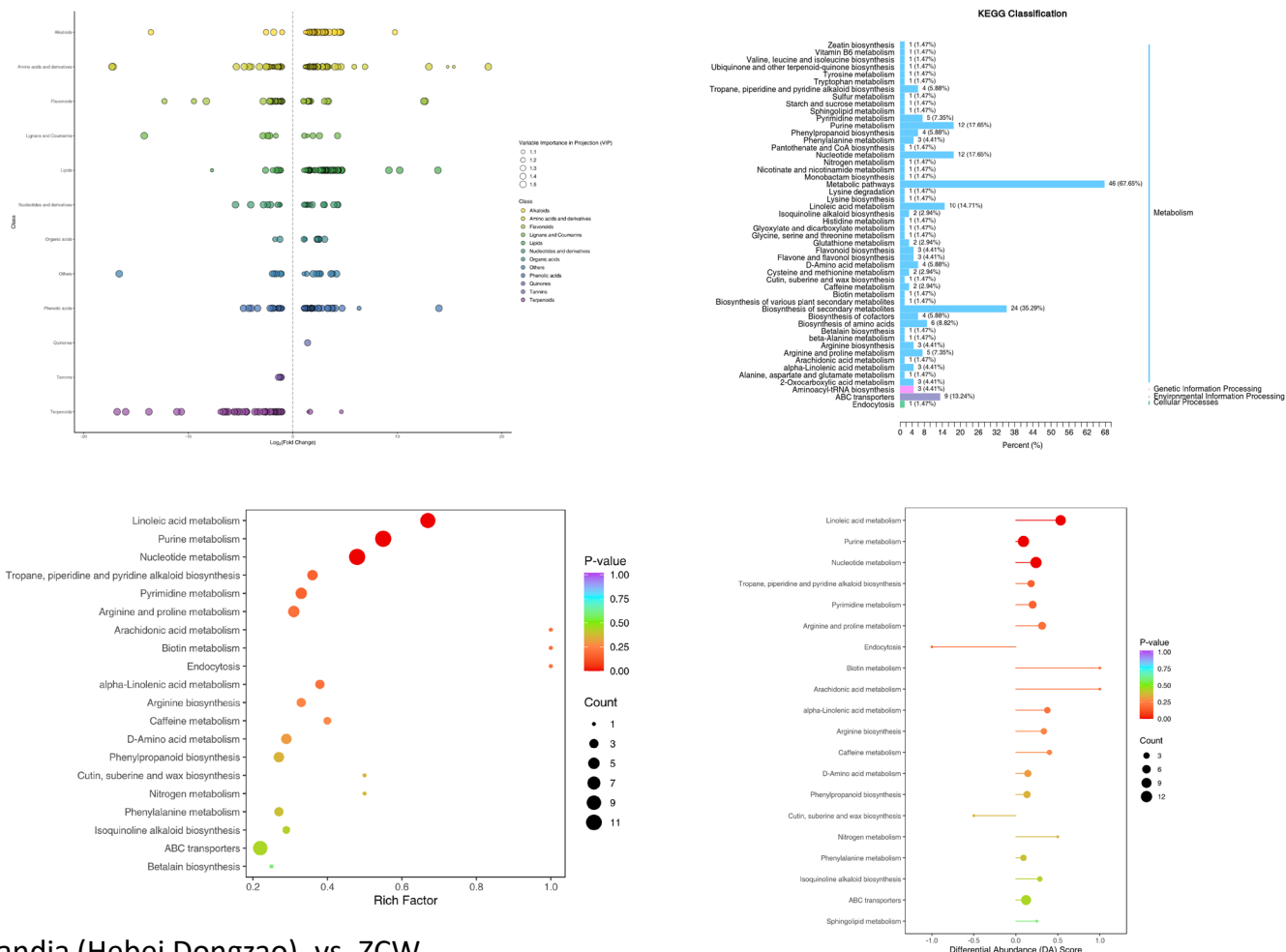
Alcalde_vs_Maya

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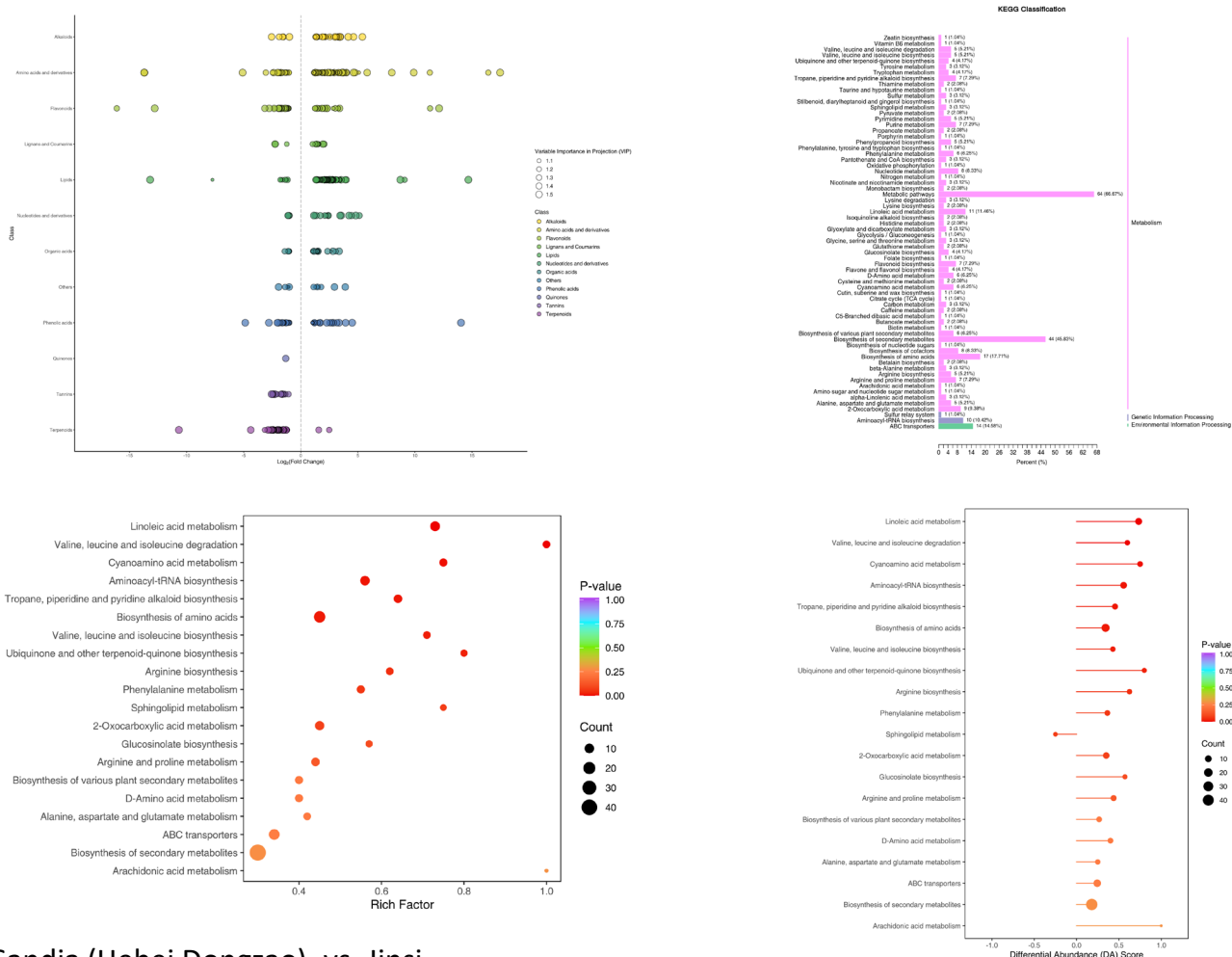
Sandia (Hebei Dongzao)_vs_Shanxi Li

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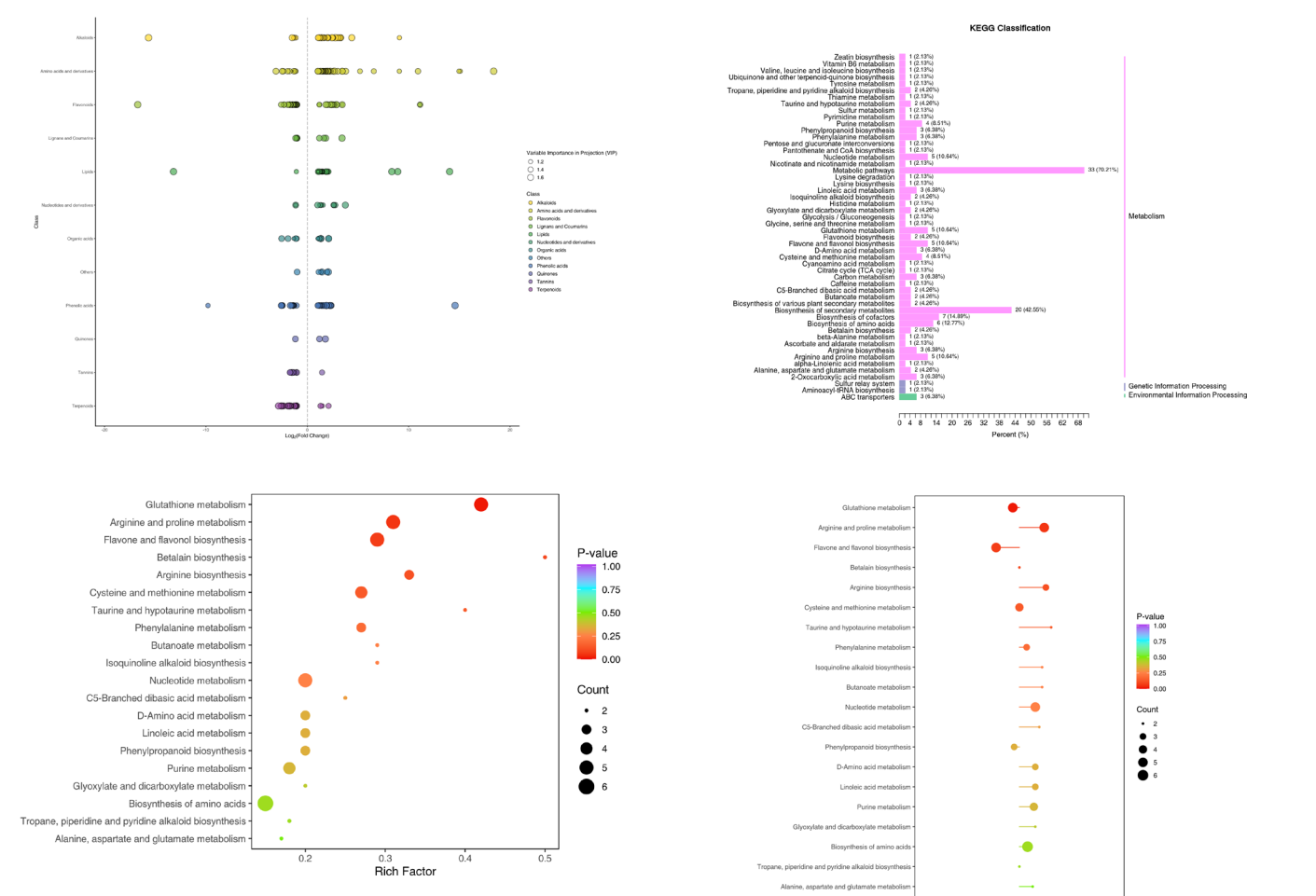
Sandia (Hebei Dongzao)_vs_ZCW

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Sandia (Hebei Dongzao)_vs_Jinsi

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Sandia (Hebei Dongzao)_vs_Jixin

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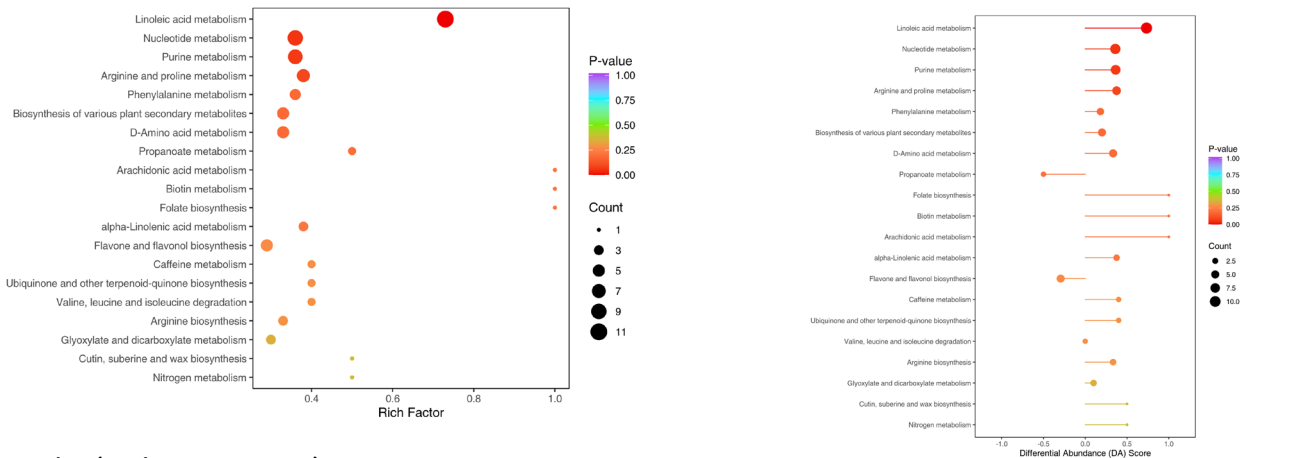
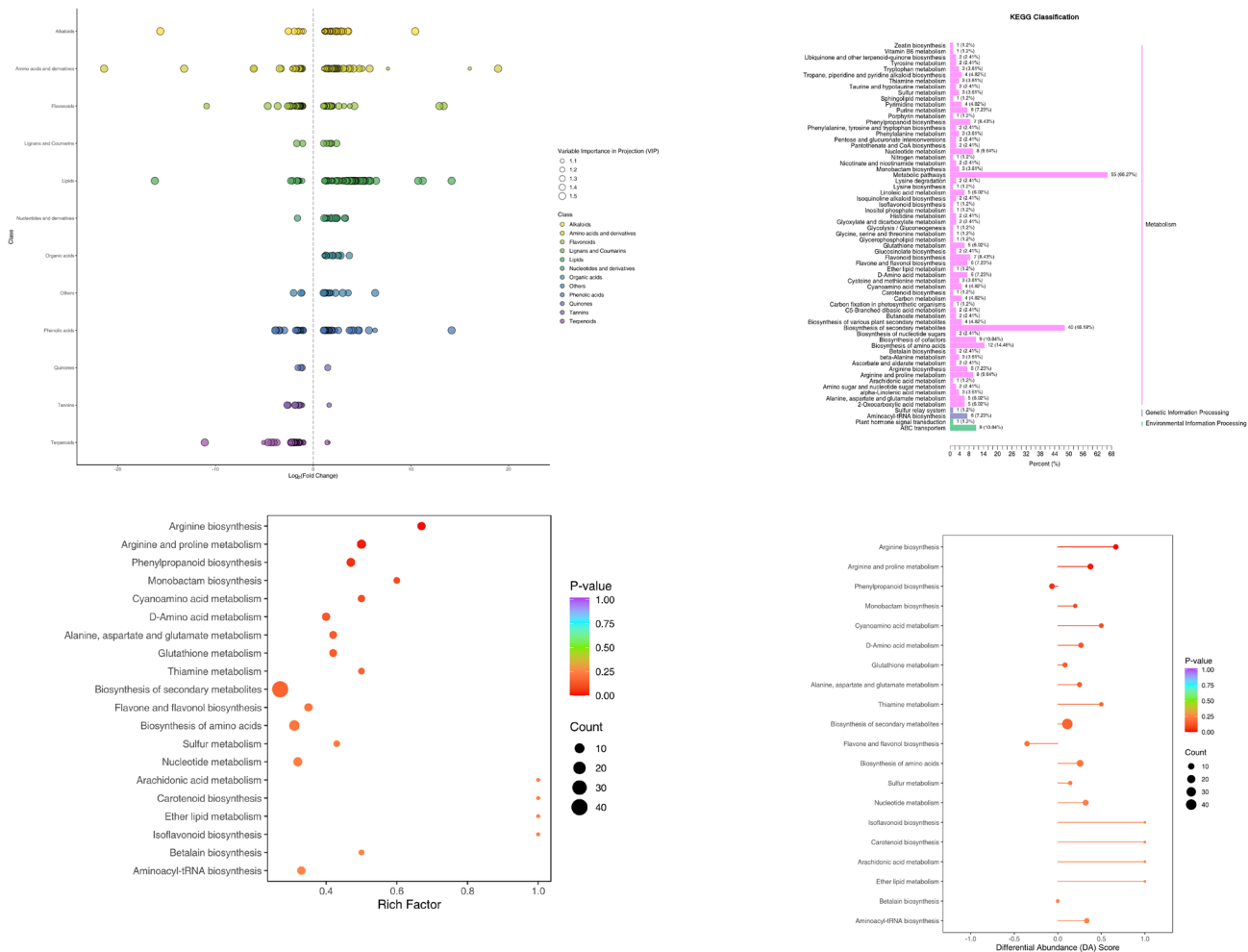


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Sandia (Hebei Dongzao)_vs_Lang

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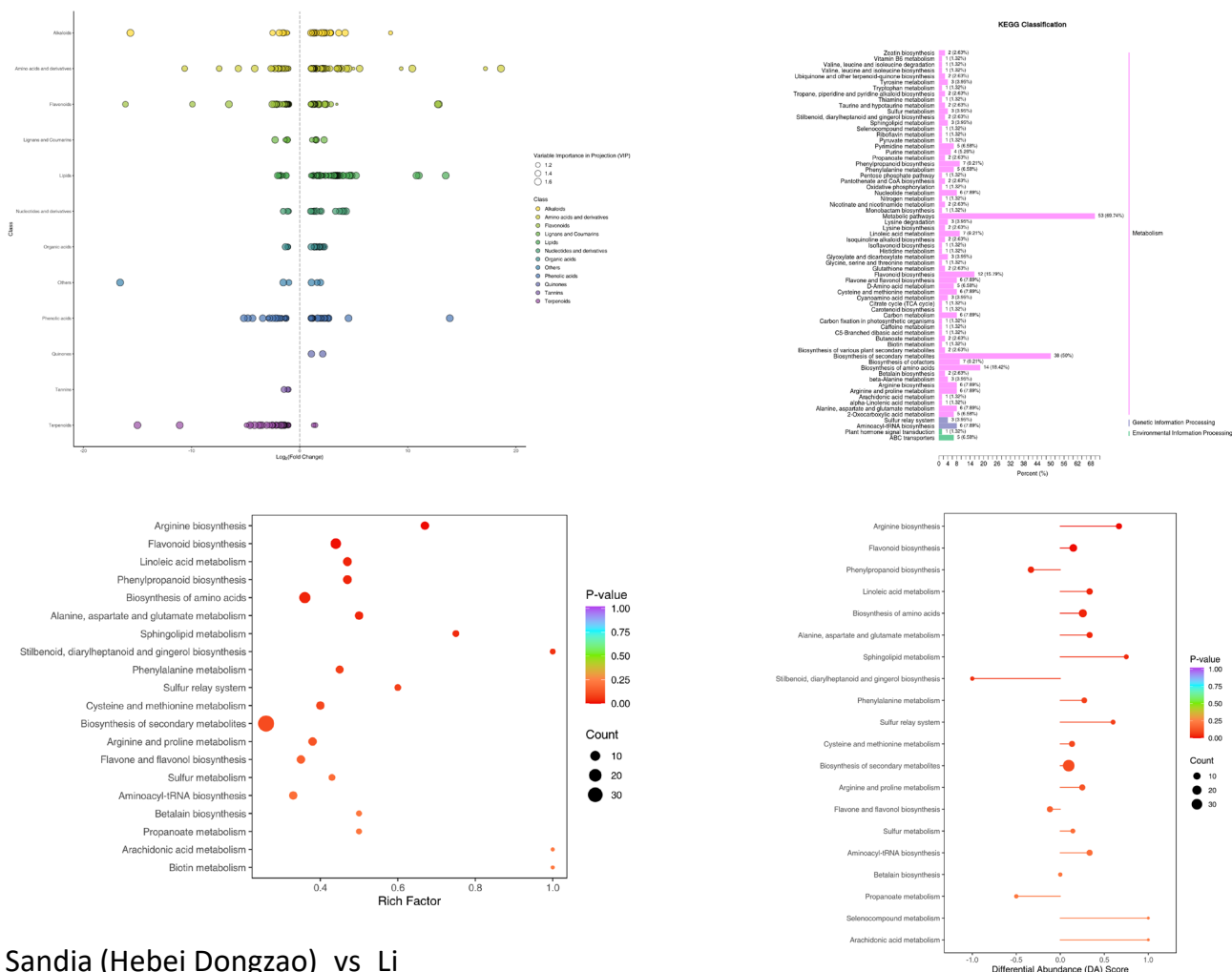
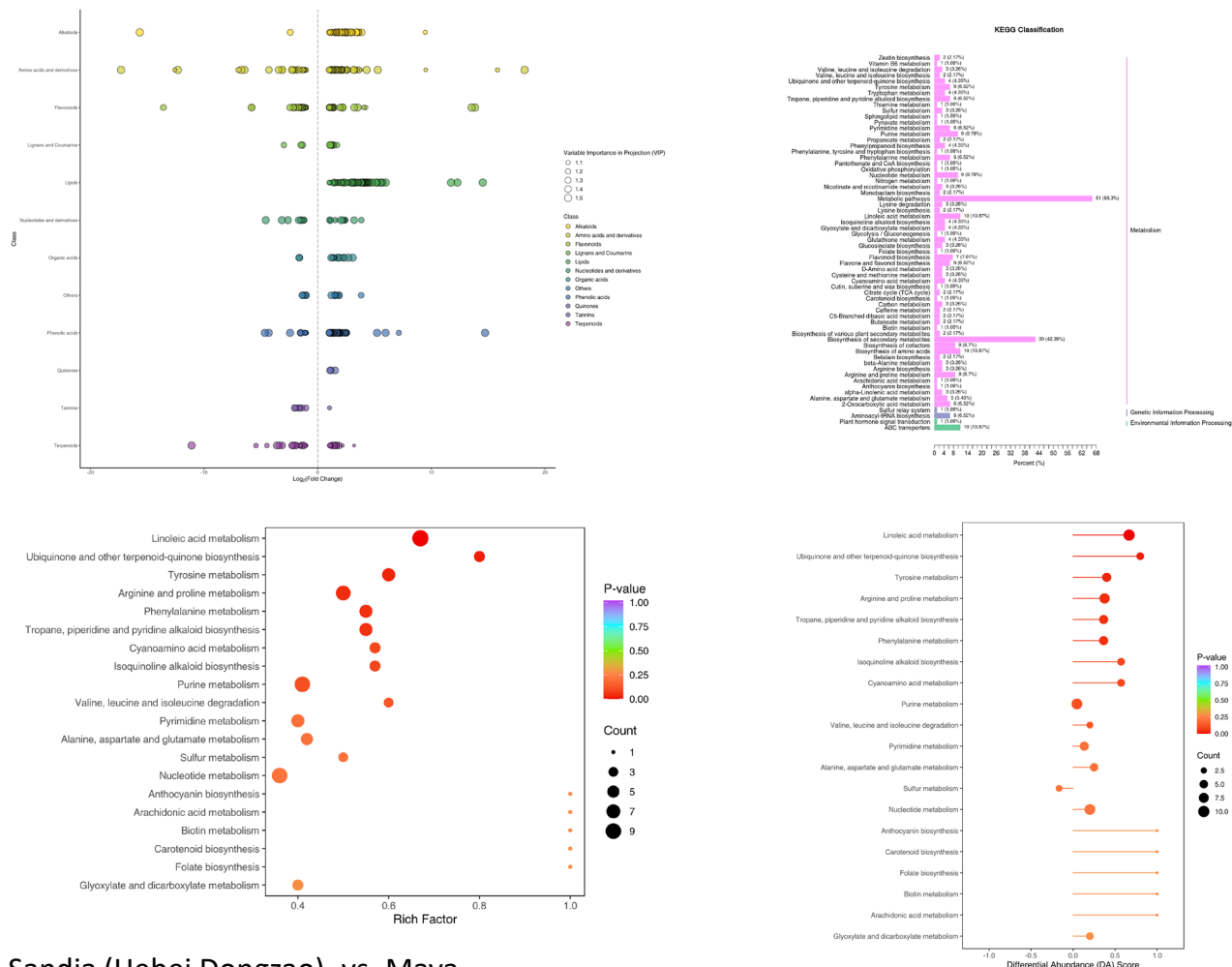
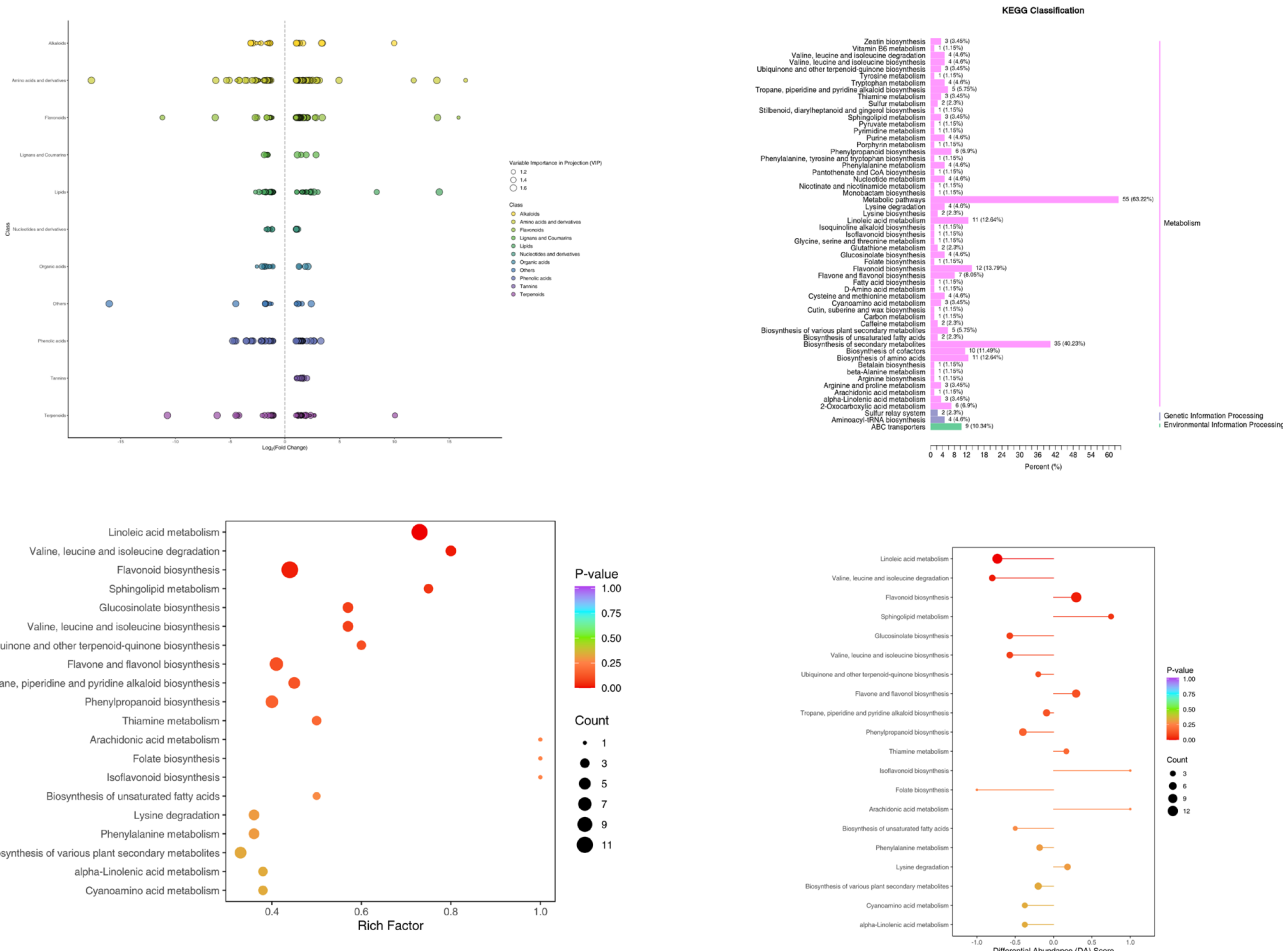


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Sandia (Hebei Dongzao)_vs_Maya

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Jinsi_vs_Shanxi Li

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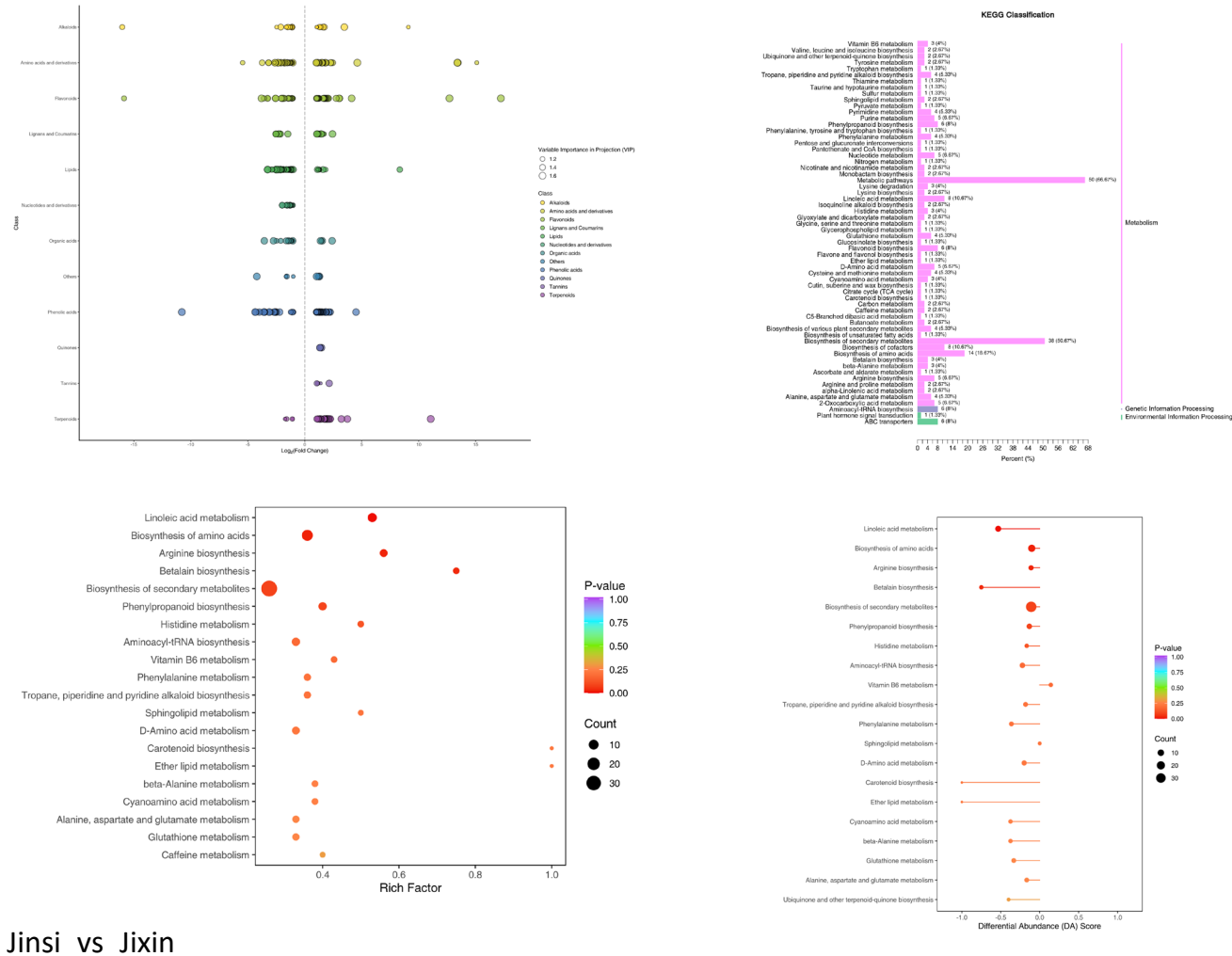


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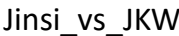
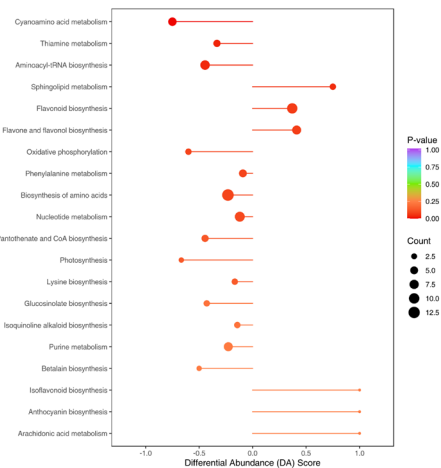
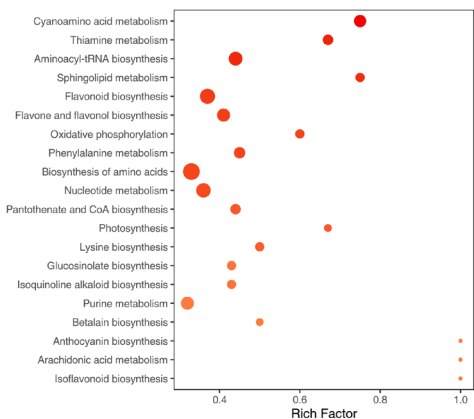
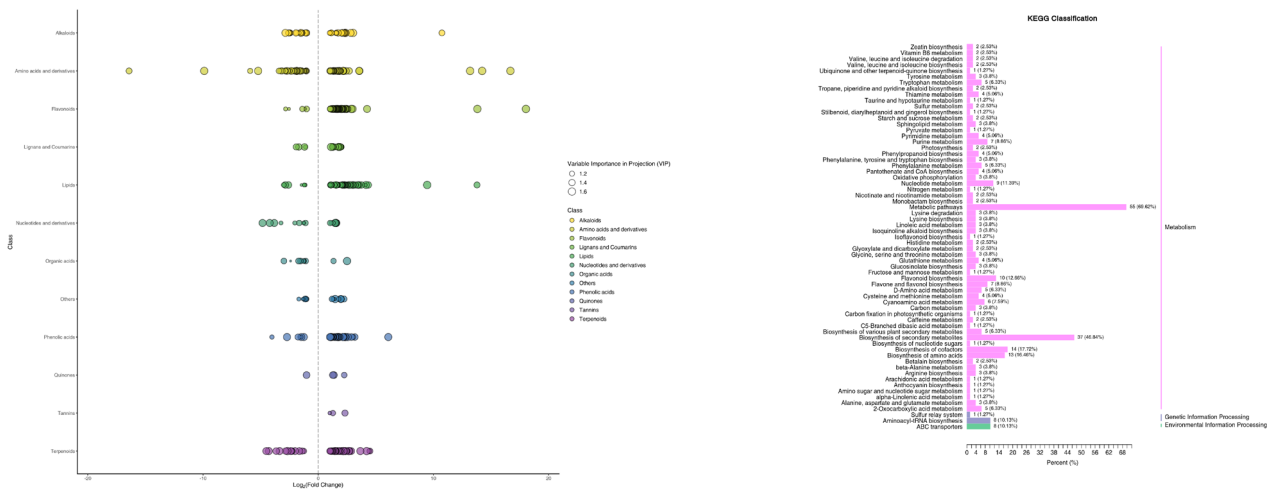
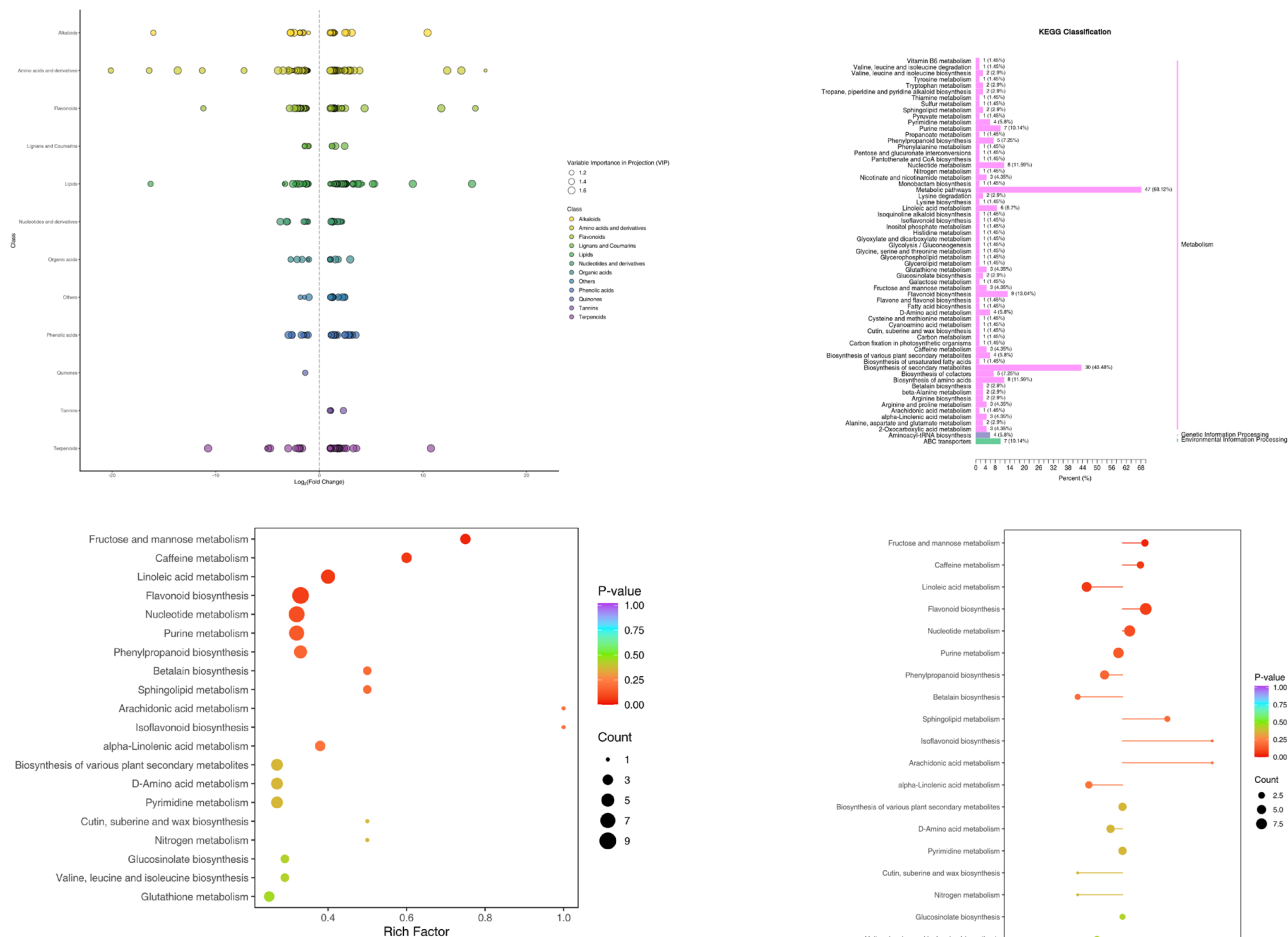


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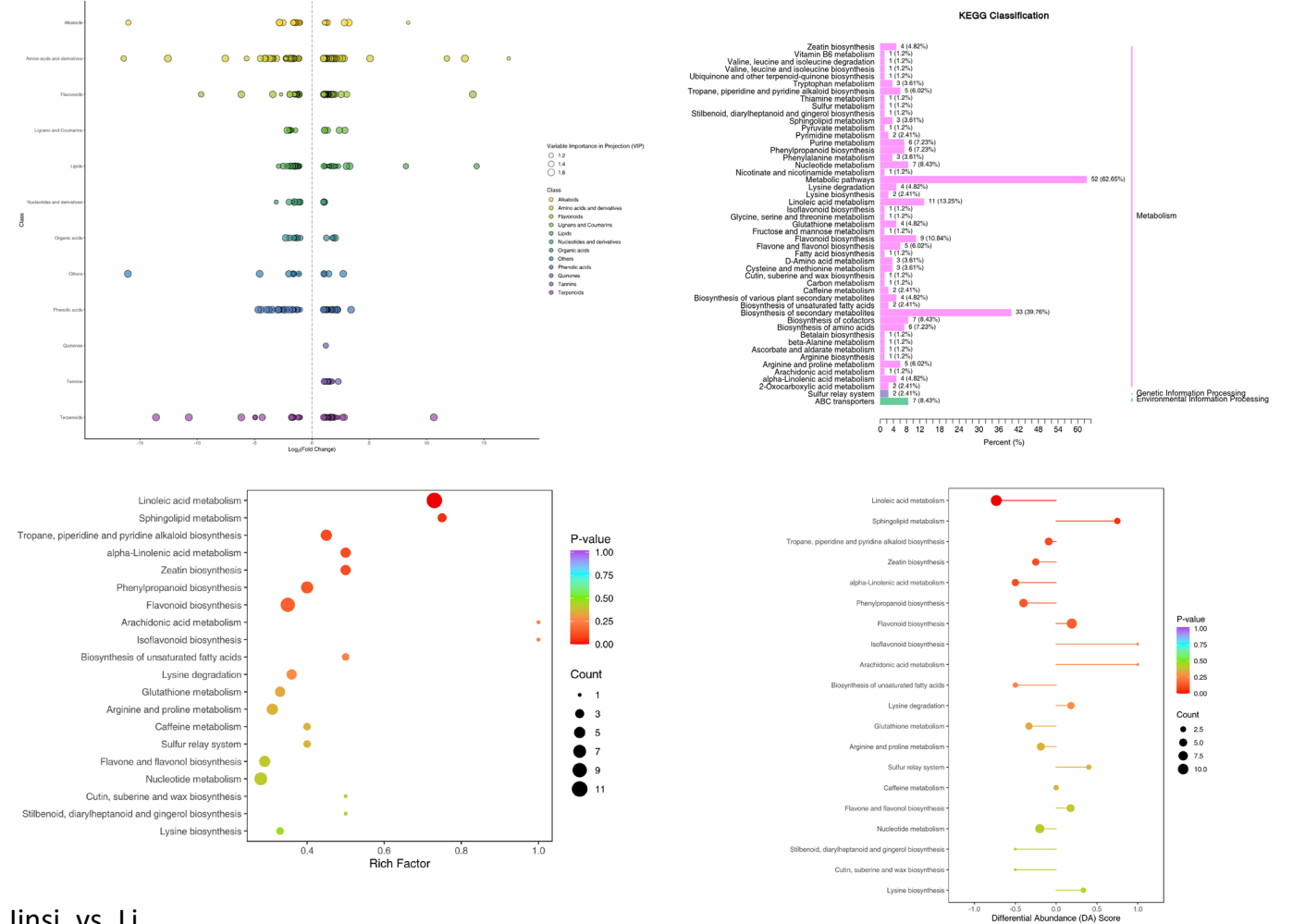
Jinsi_vs_KFC

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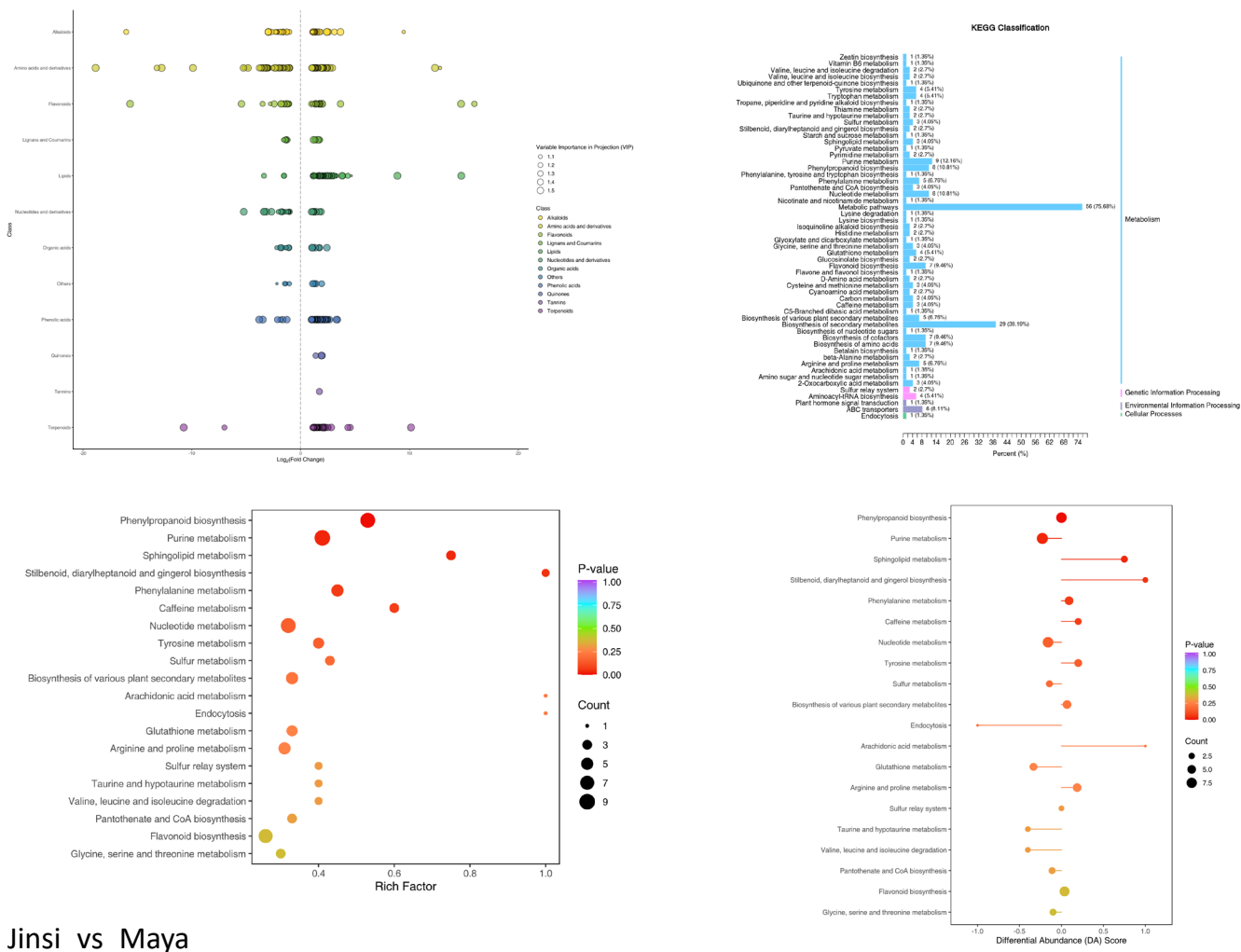
Jinsi_vs_Lang

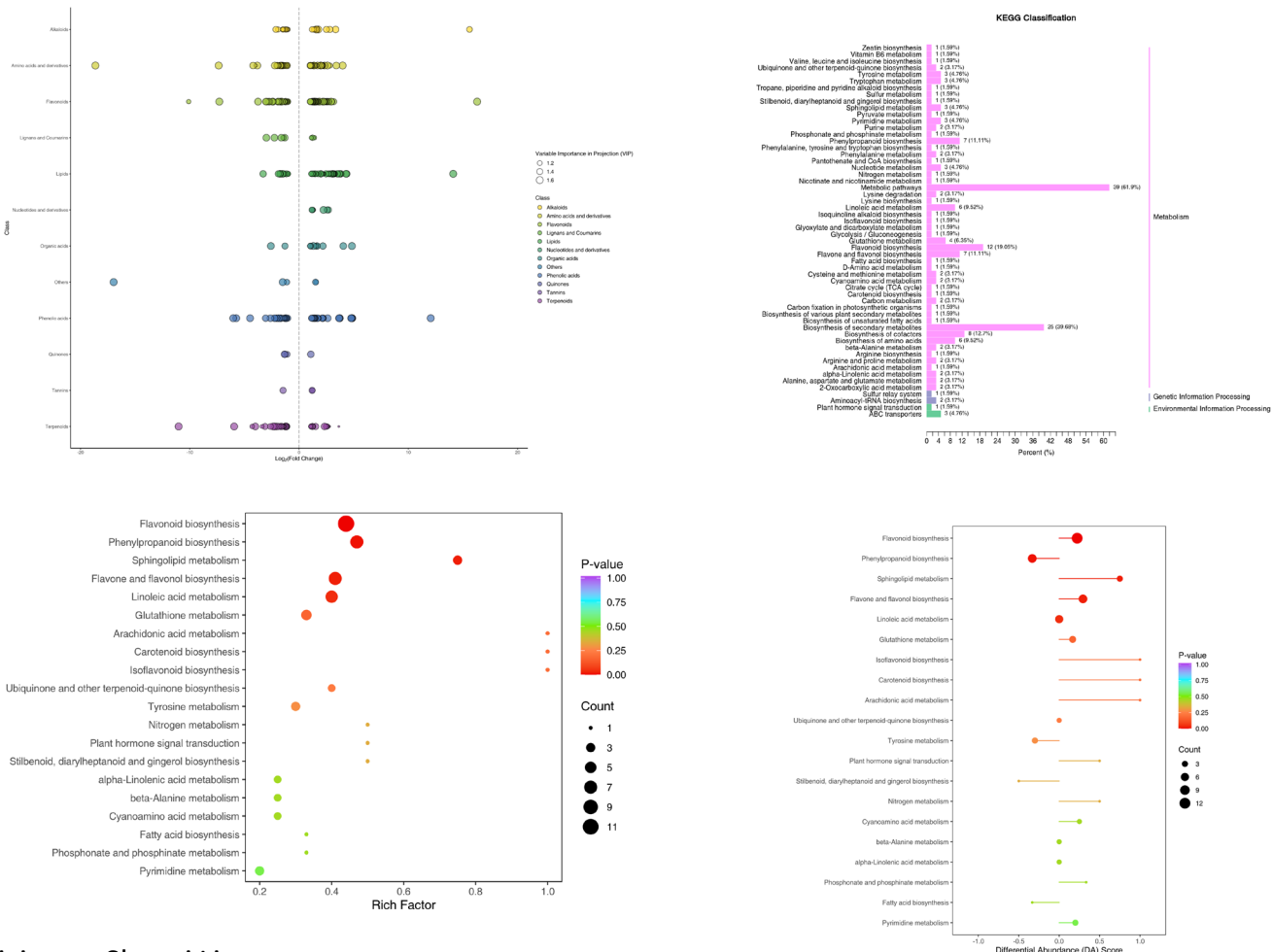
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Jinsi_vs_Li

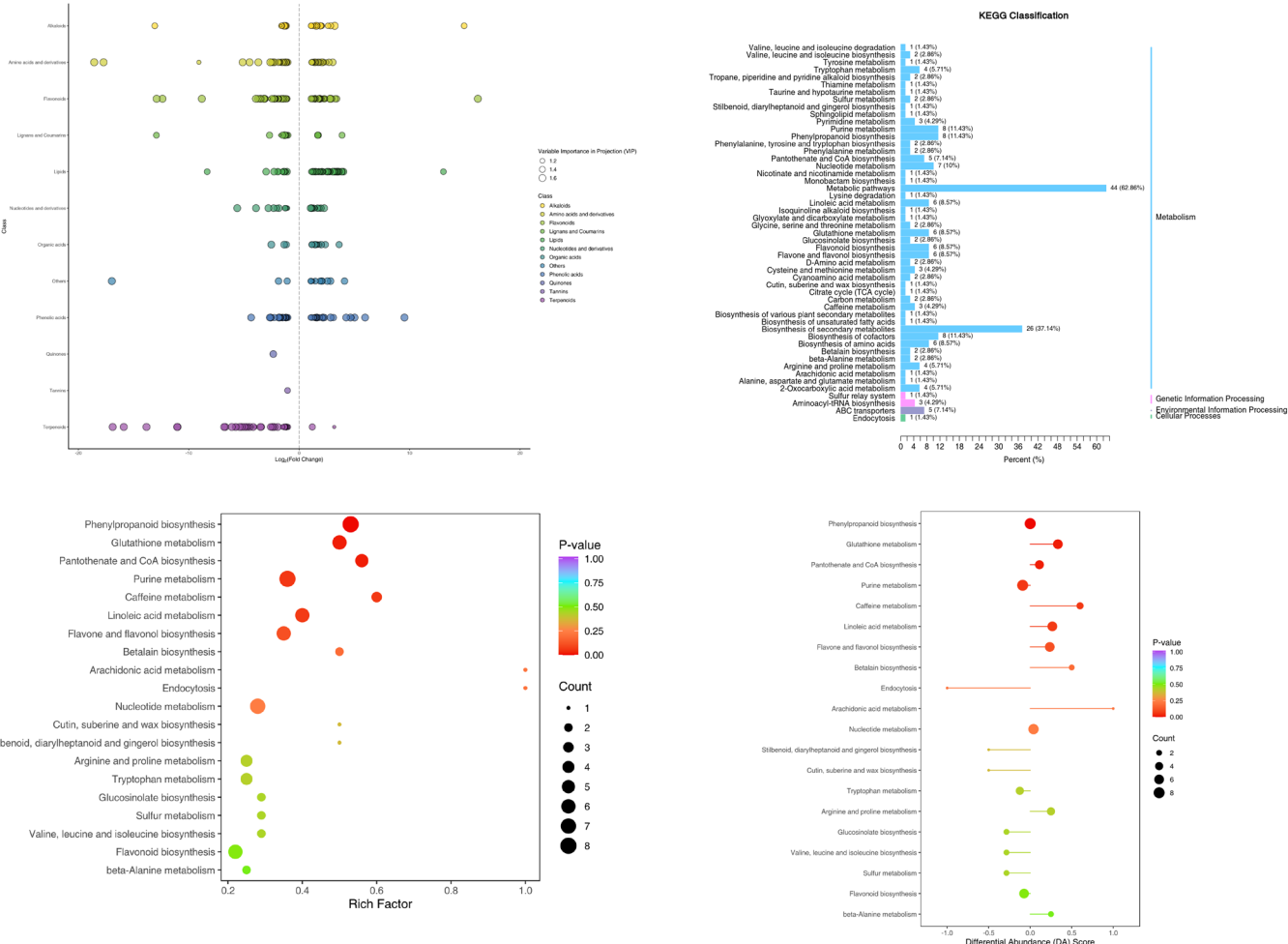
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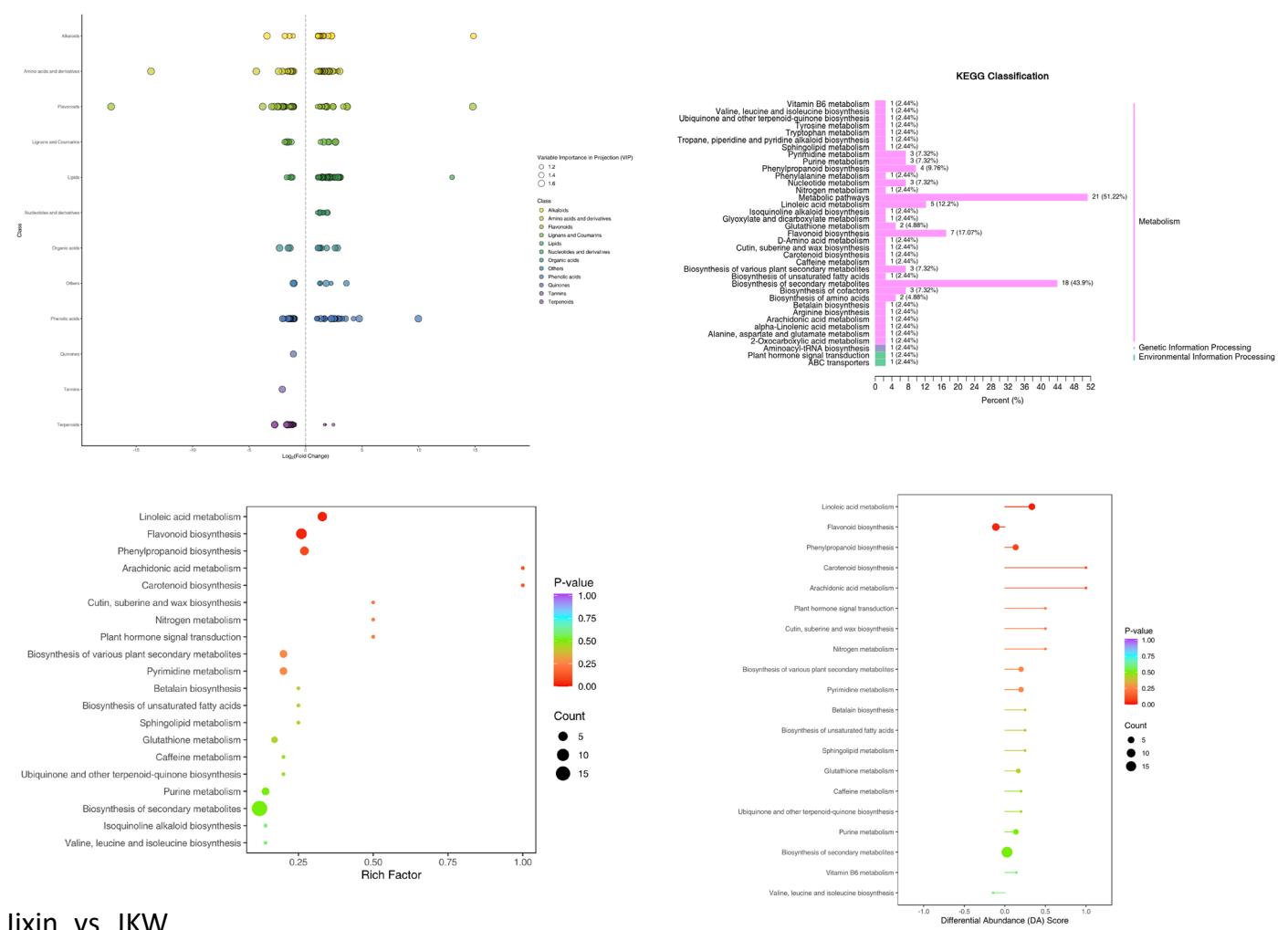
Jixin_vs_Shanxi Li

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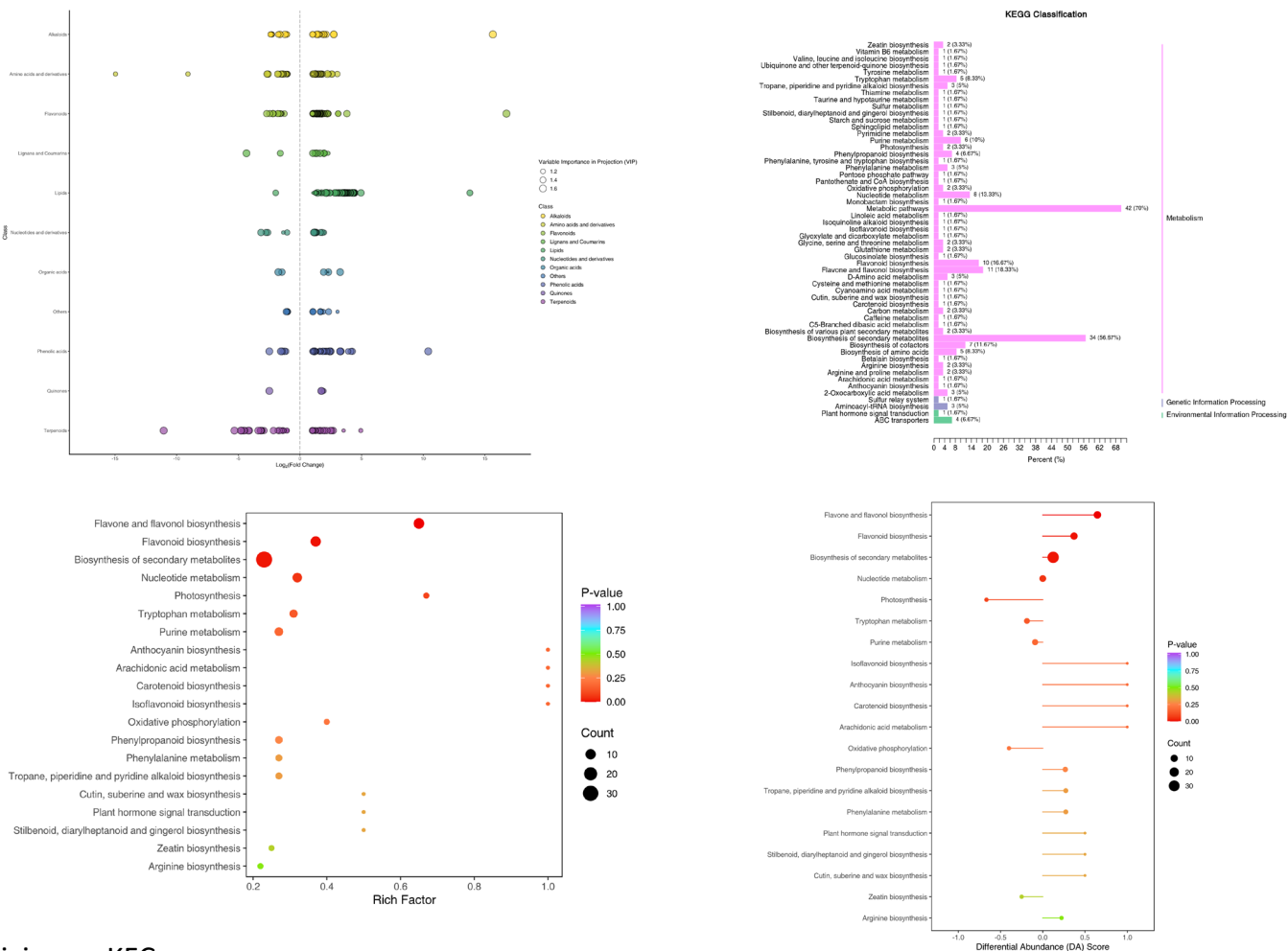
Jixin_vs_ZCW

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Jixin_vs_JKW

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Jixin_vs_KFC

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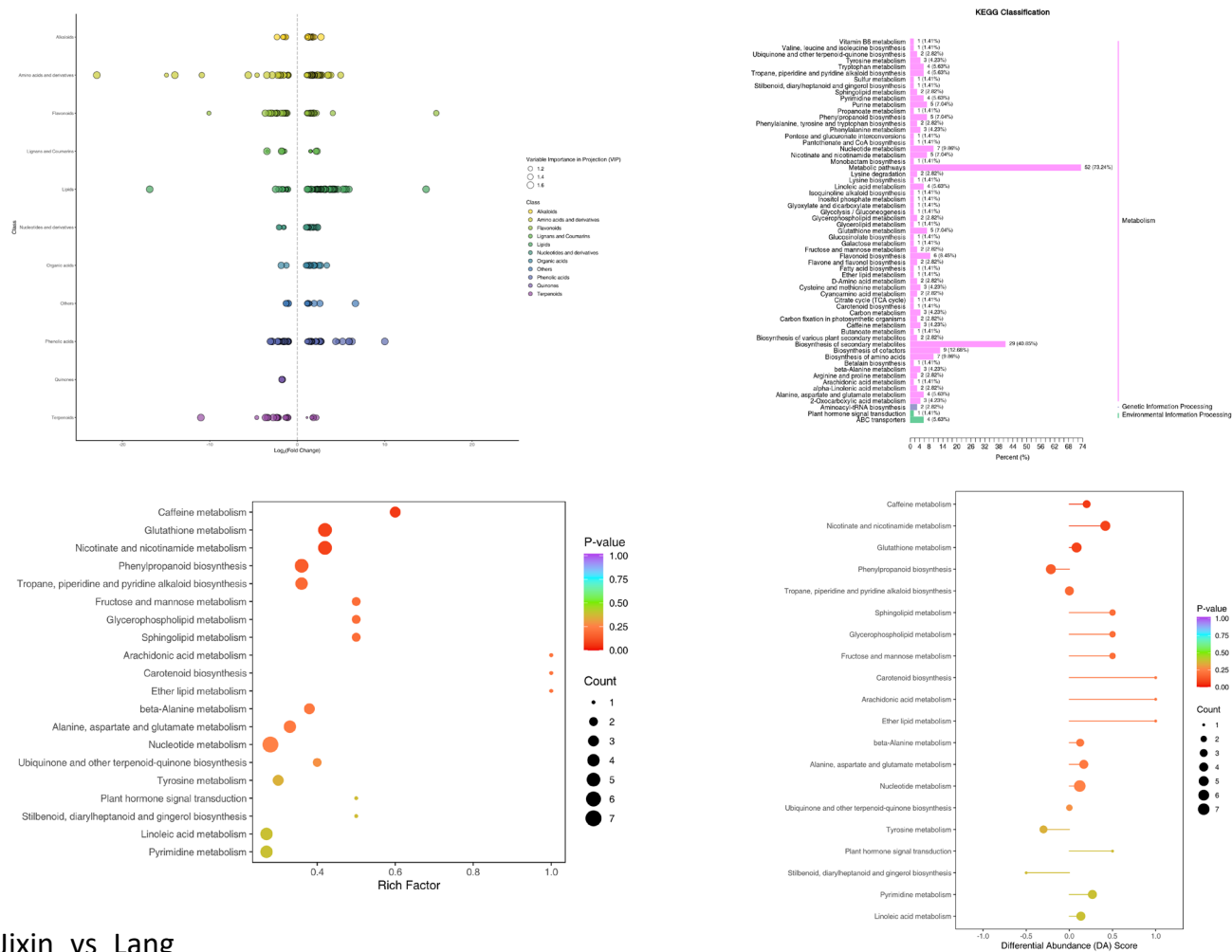
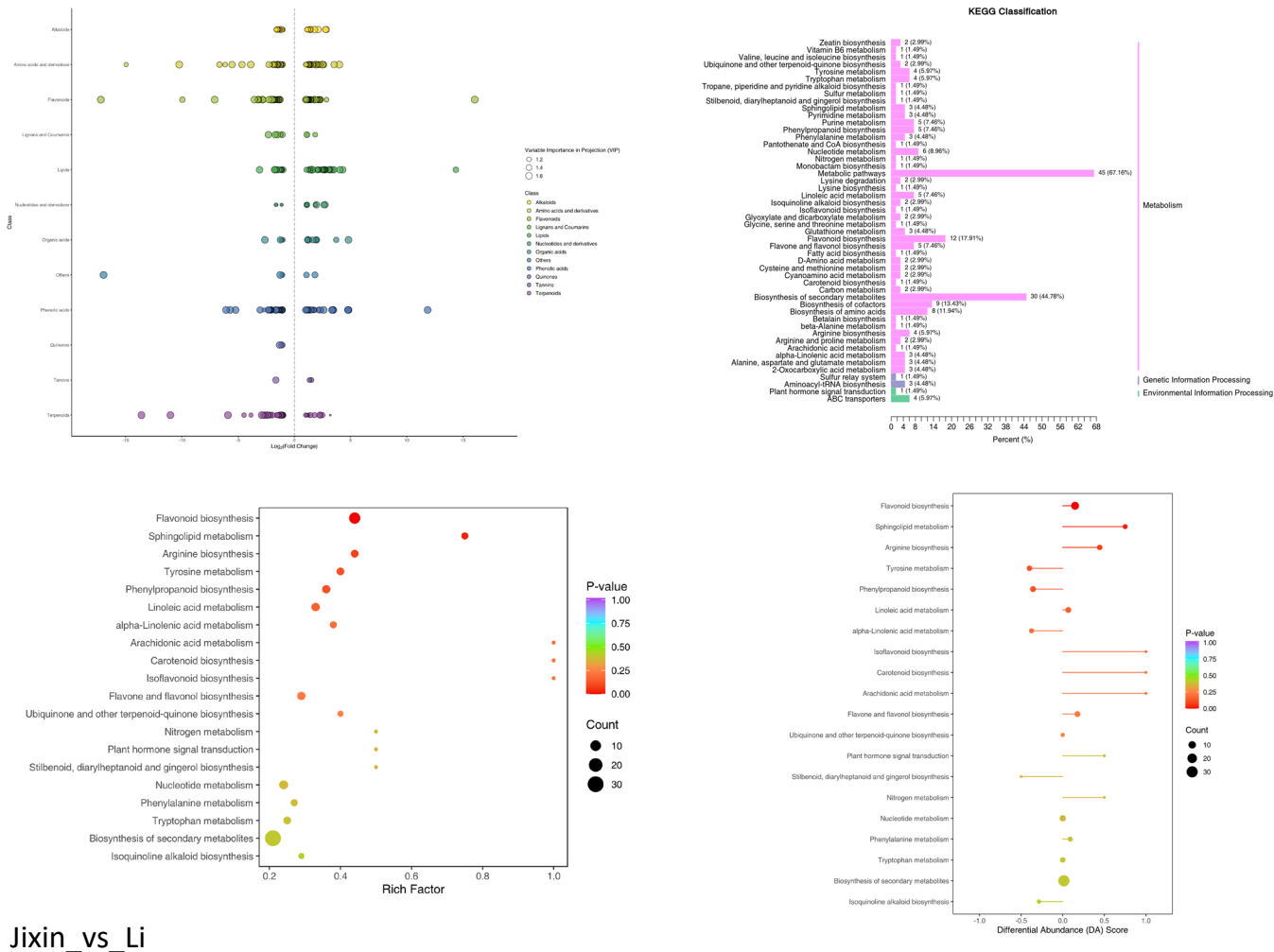
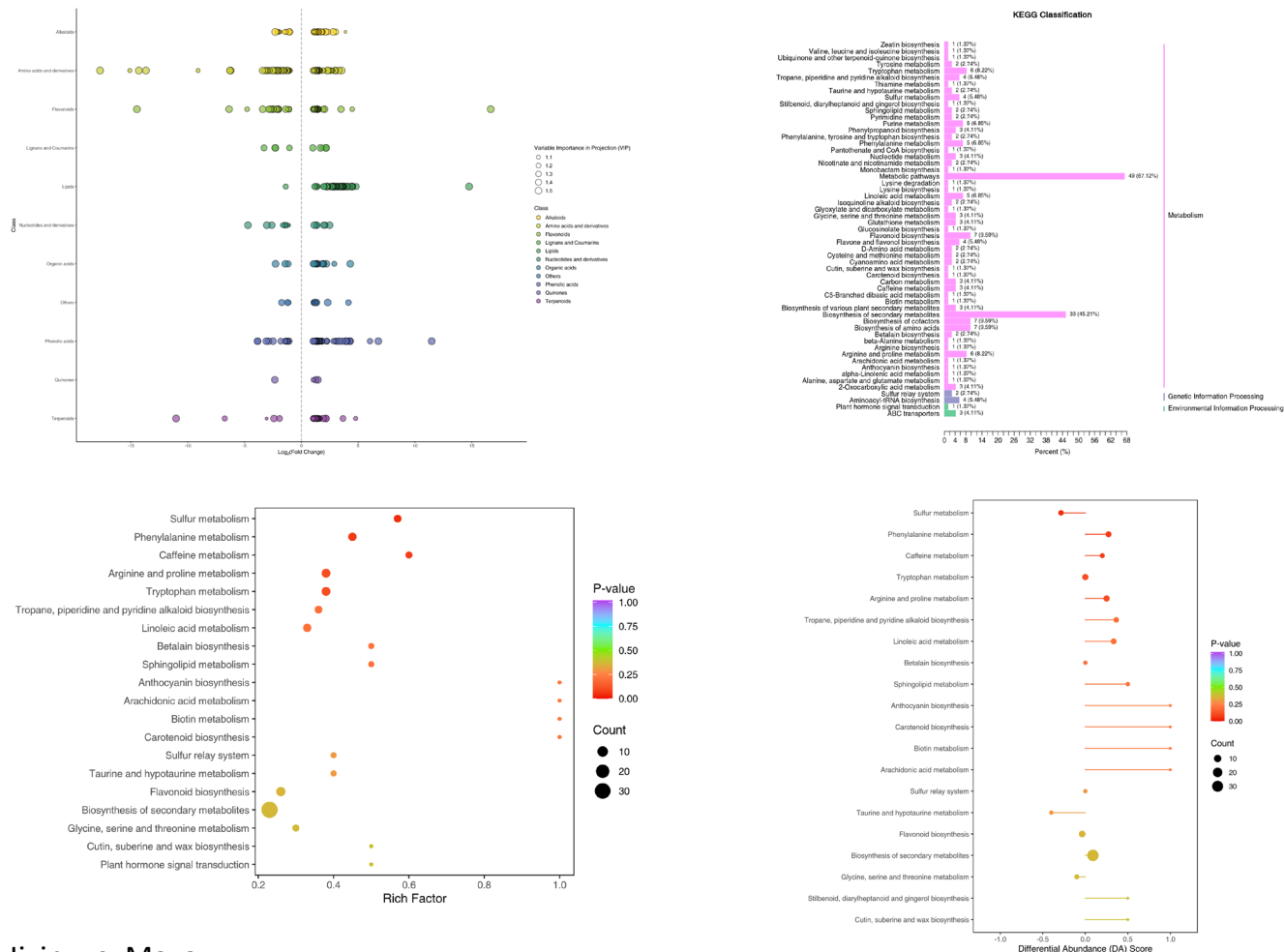


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Jixin_vs_Li

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Jixin_vs_Maya

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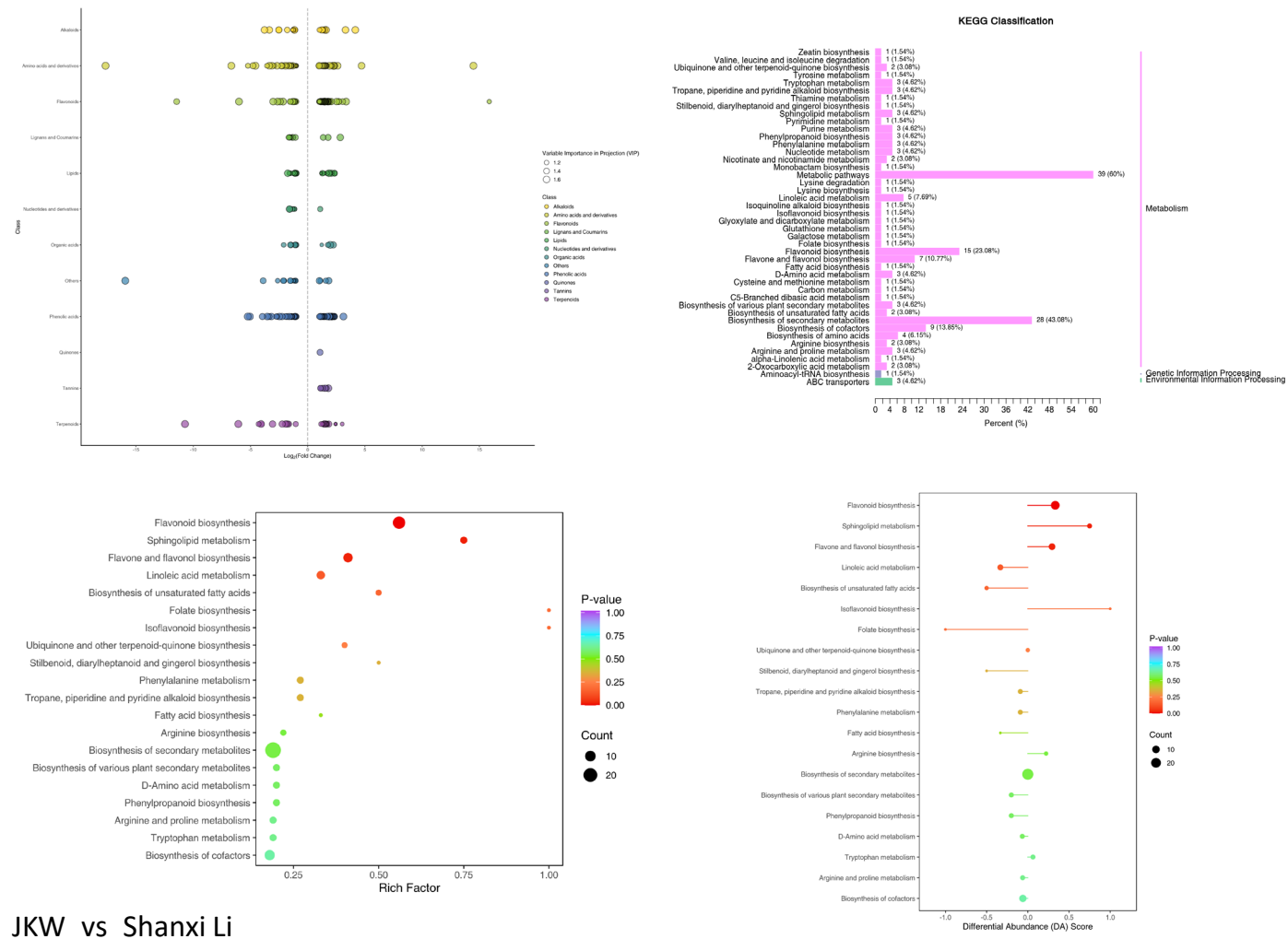


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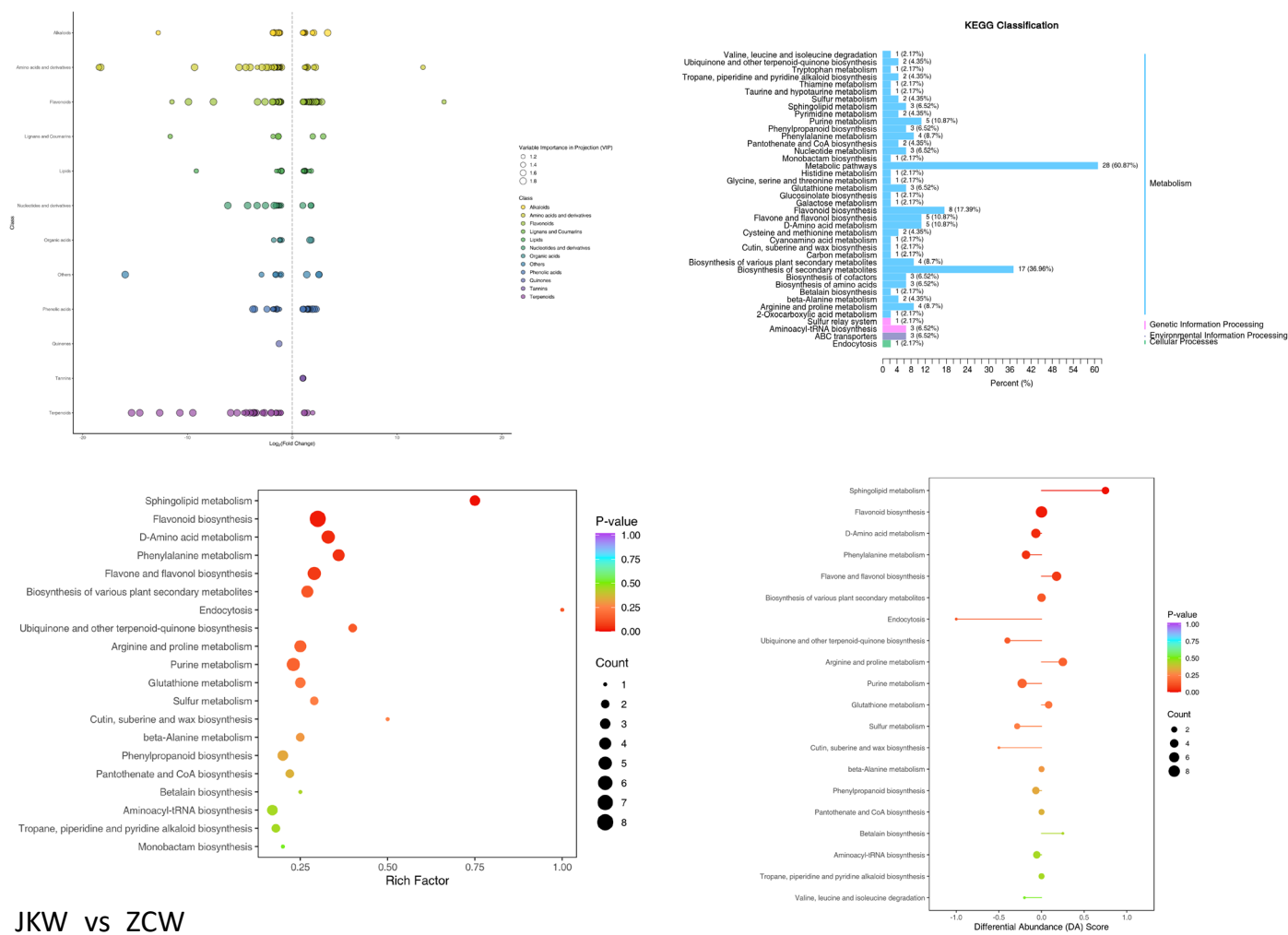


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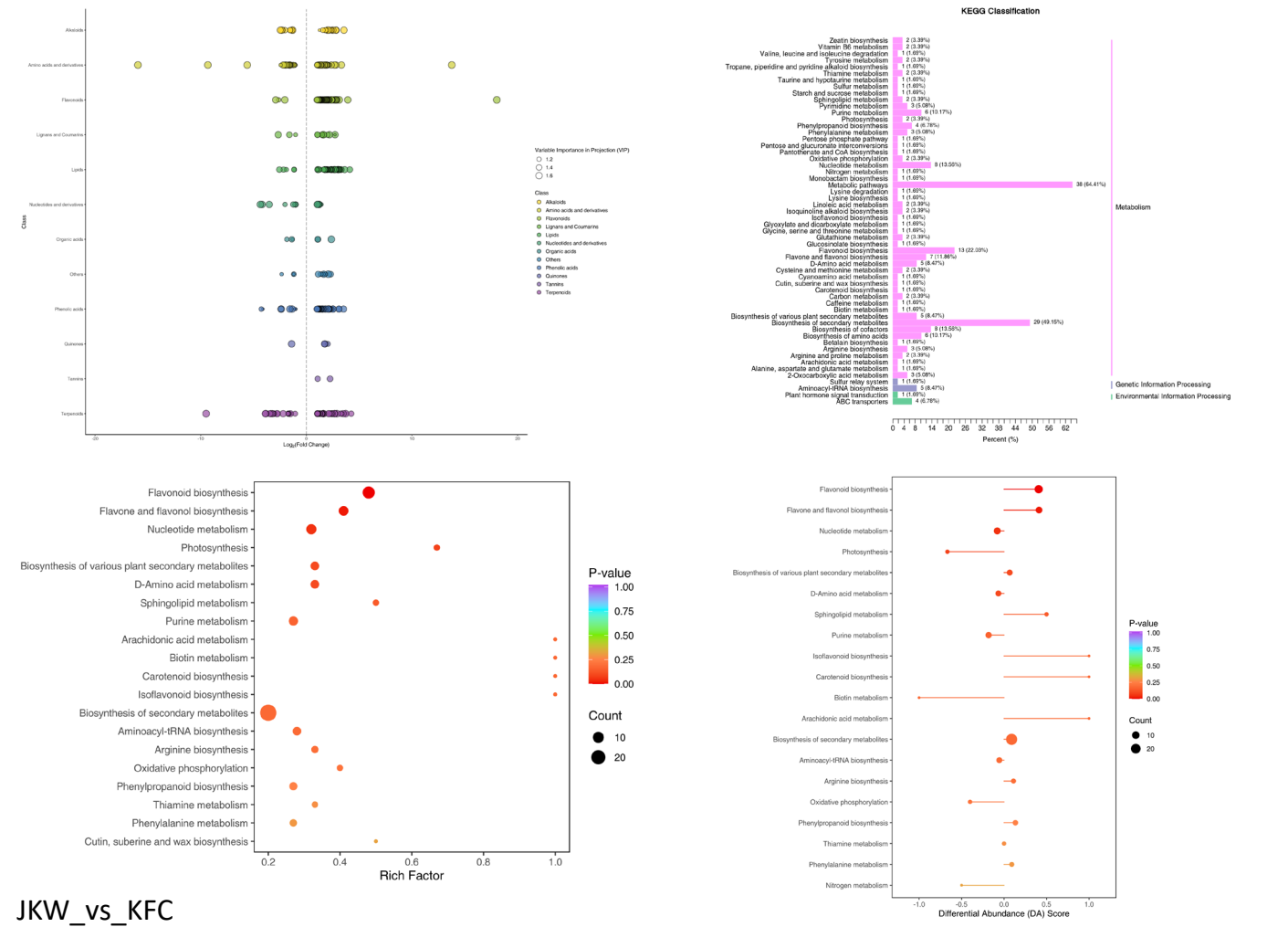


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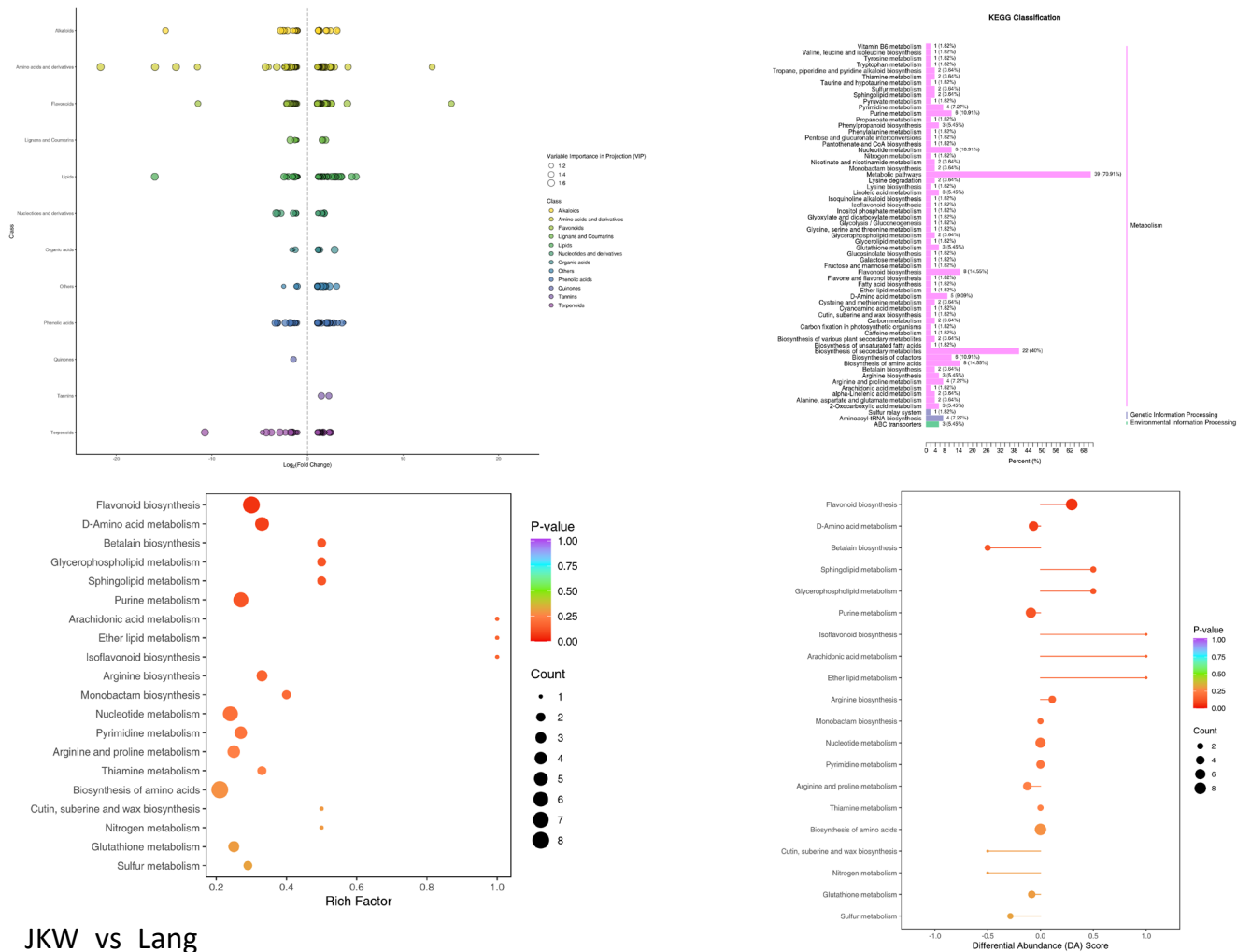
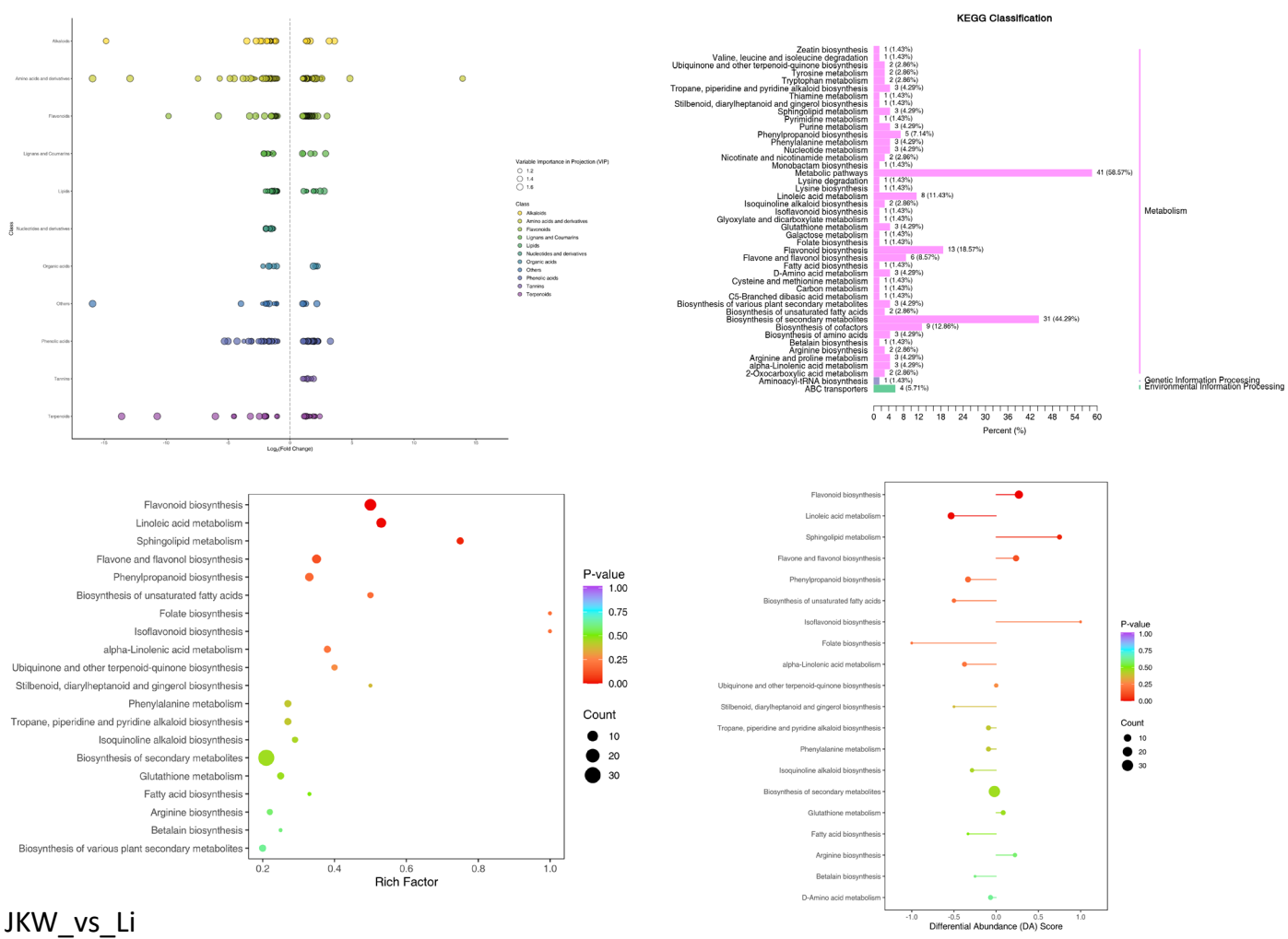


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JKW_vs_Li

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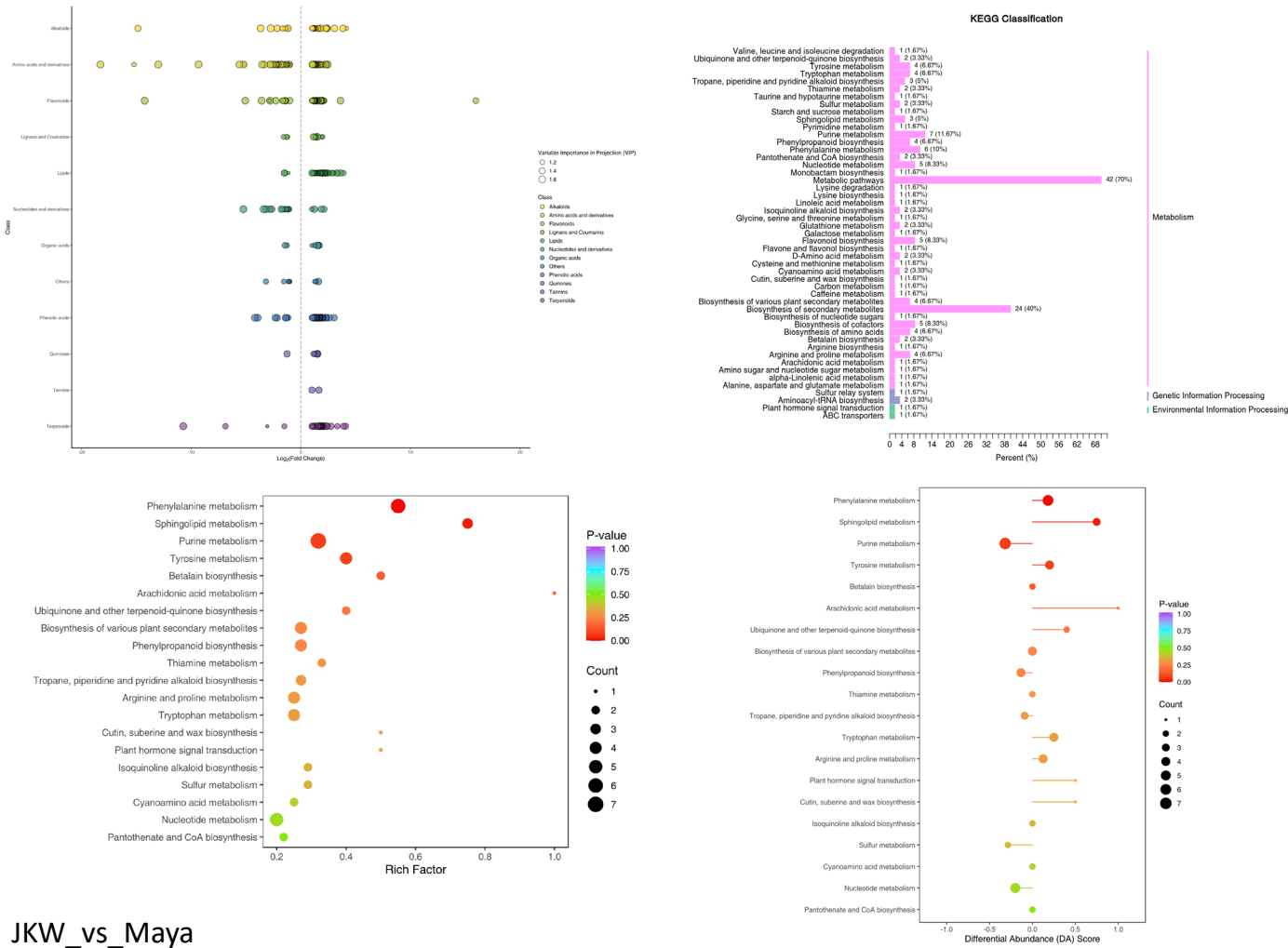
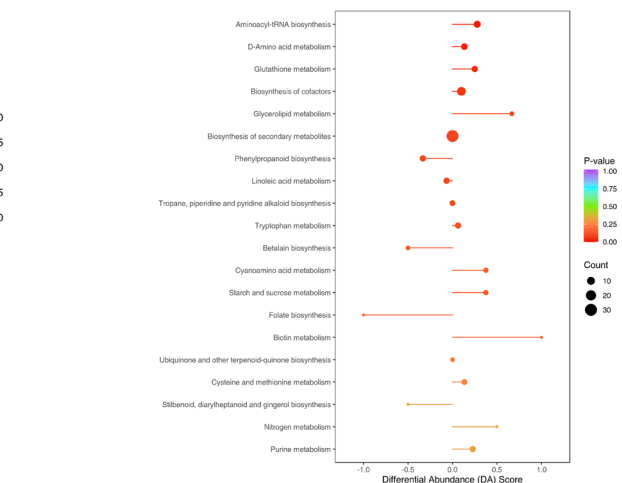
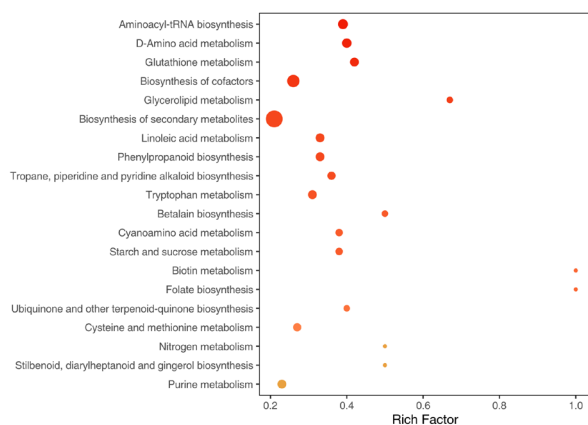
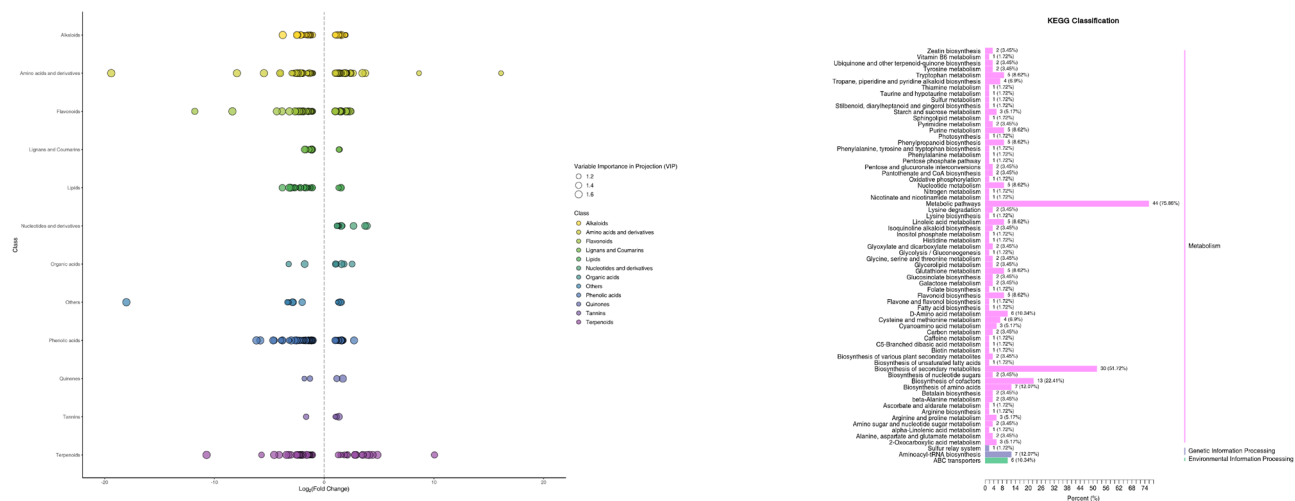


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KFC_vs_Shanxi Li

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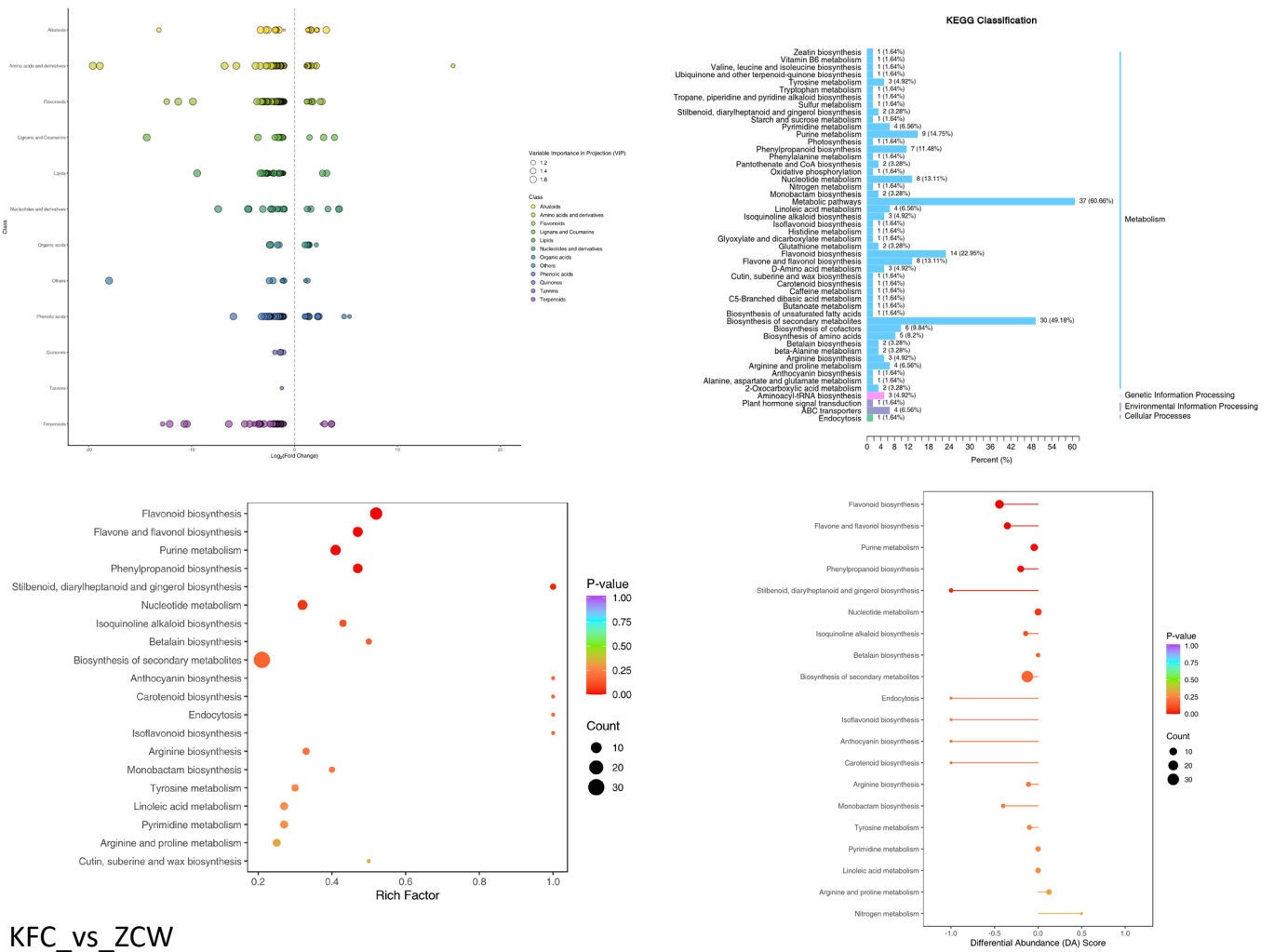
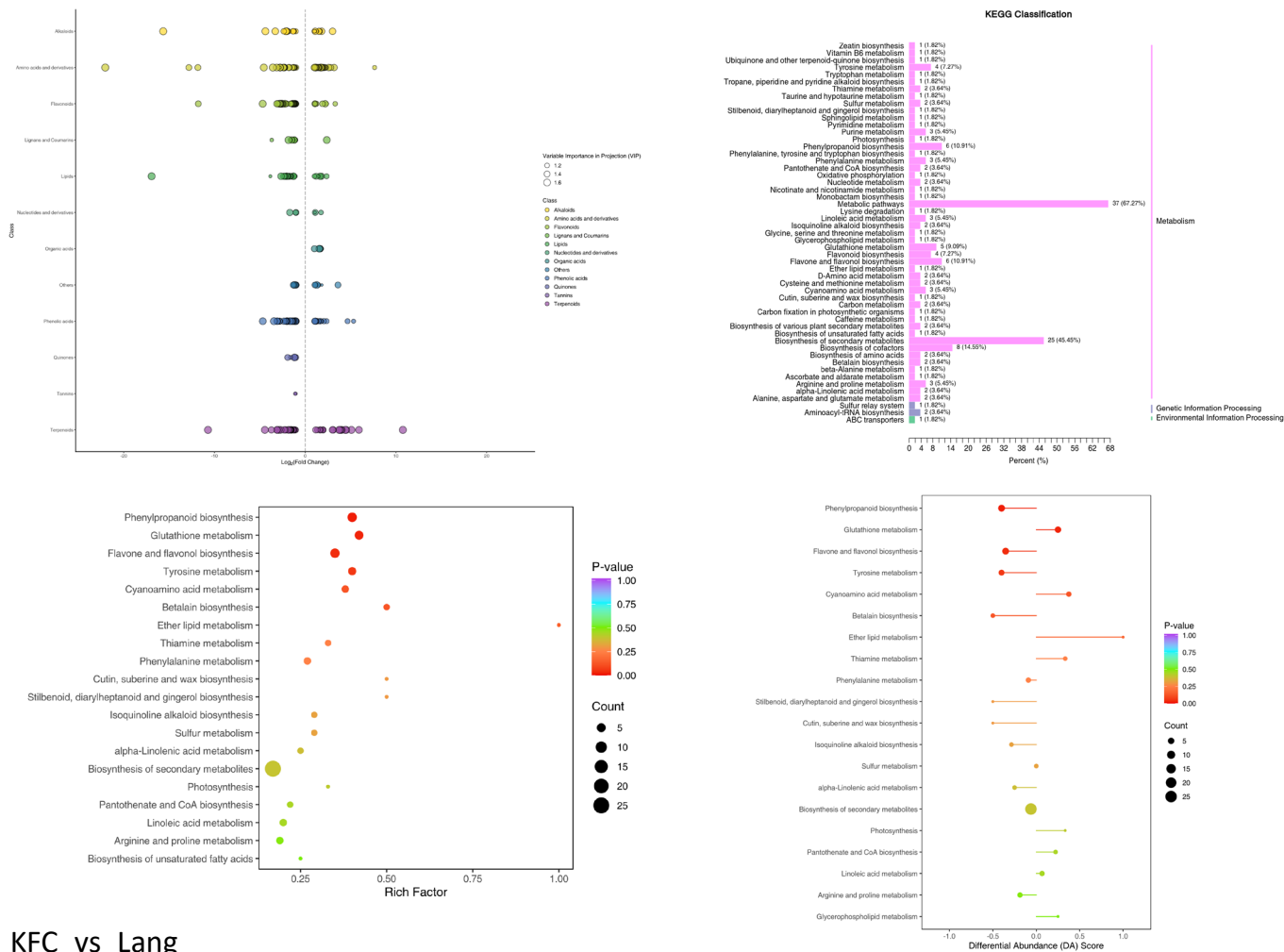


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KFC_vs_Lang

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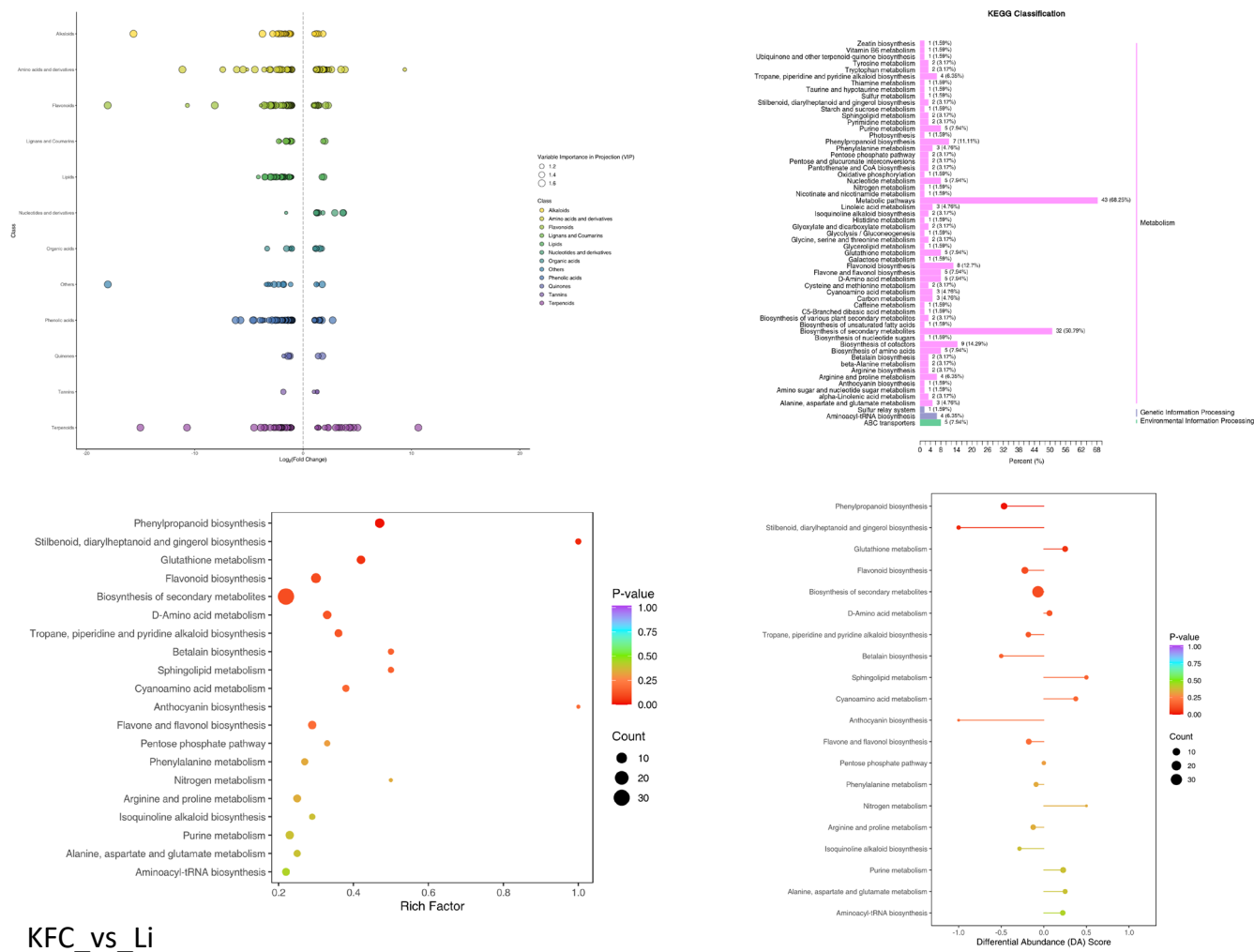


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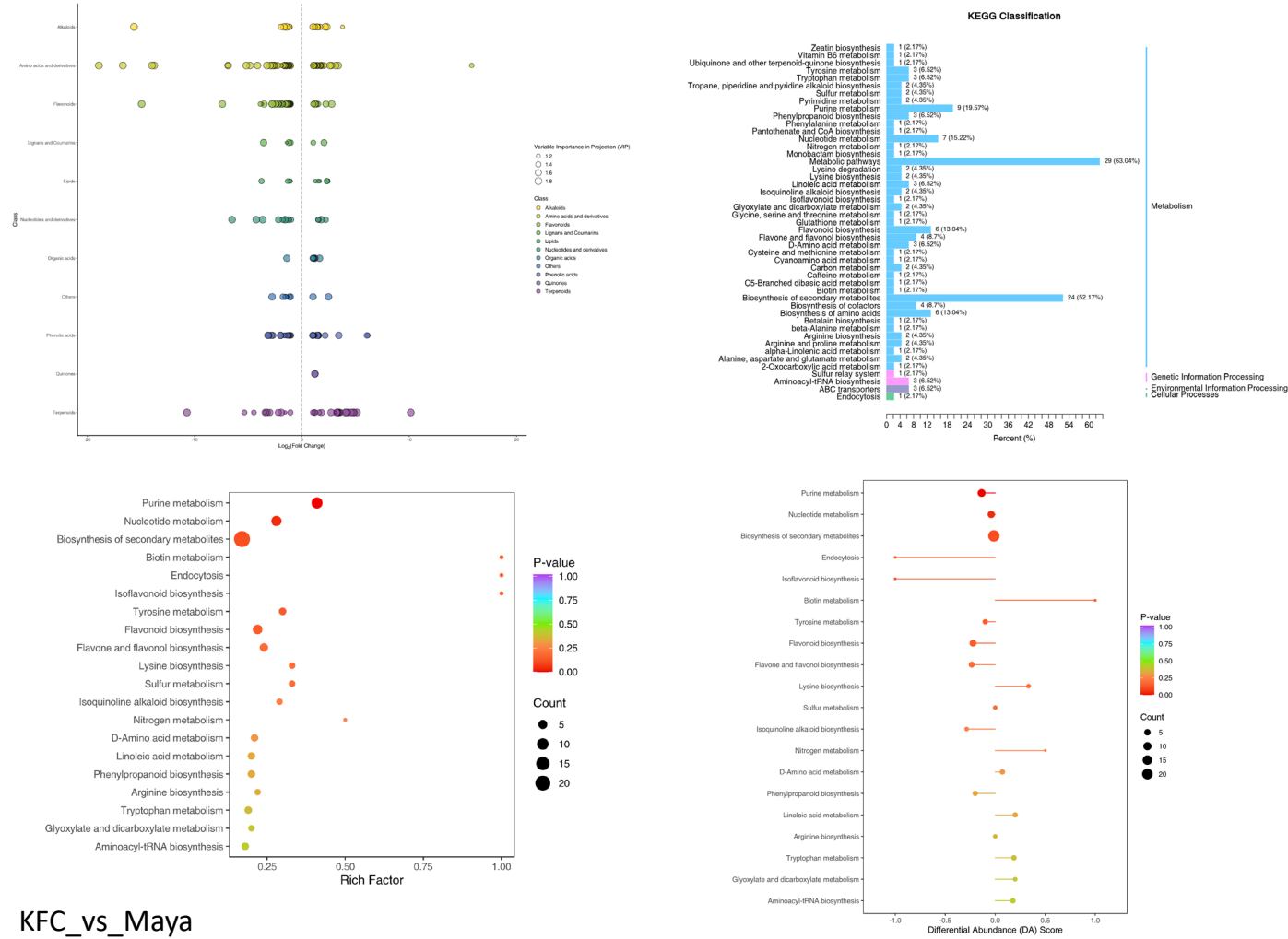


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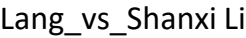
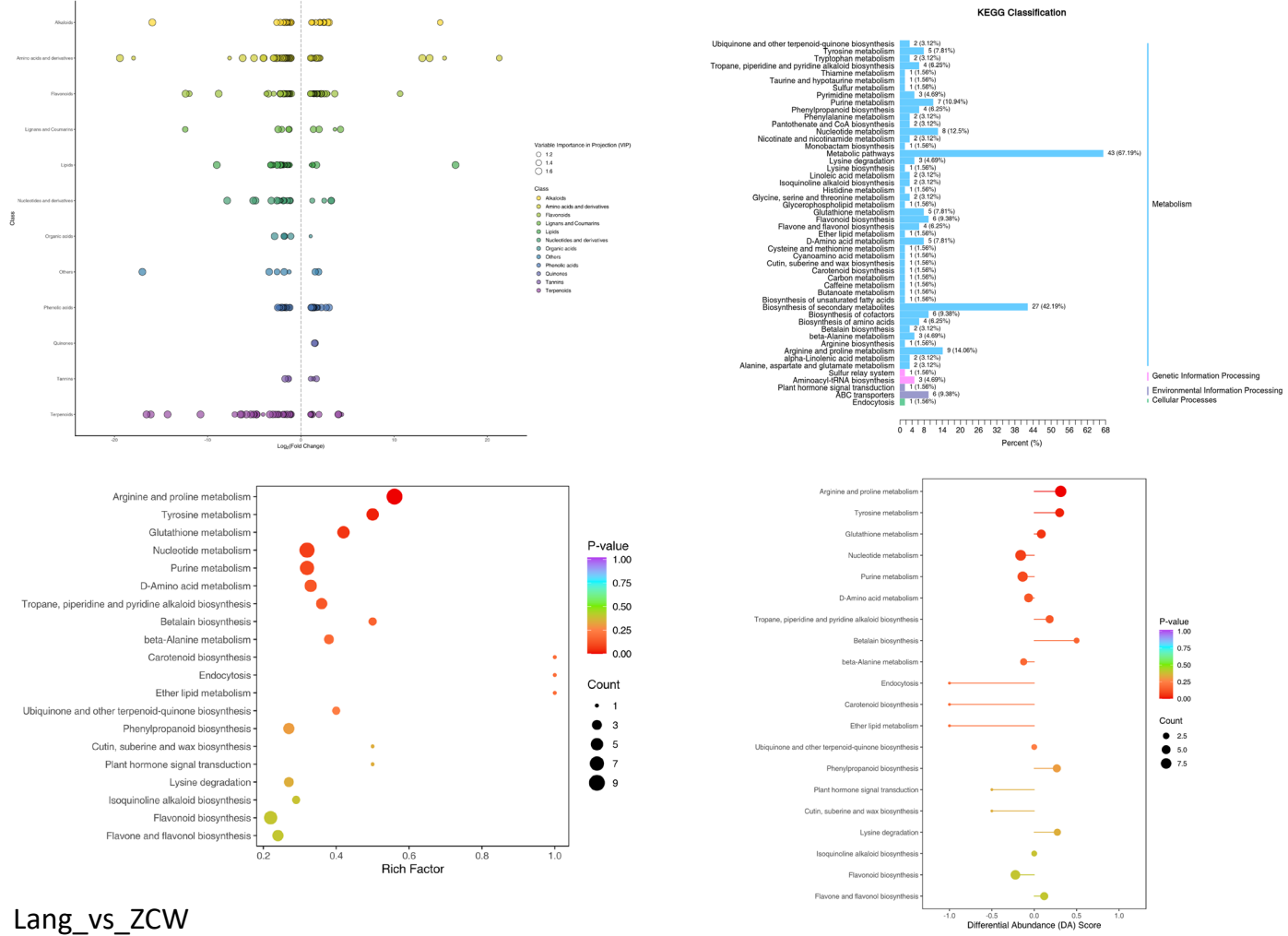
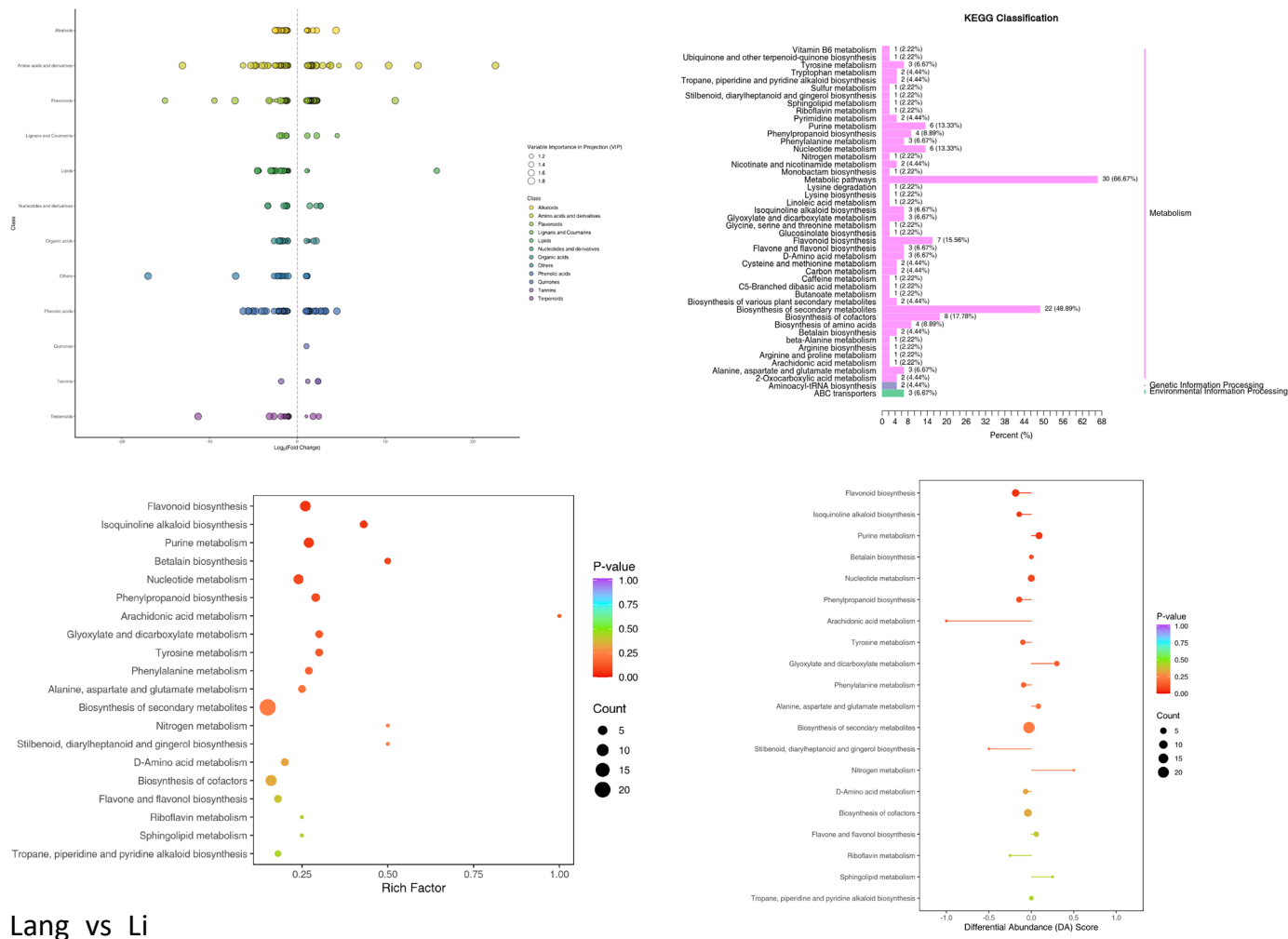


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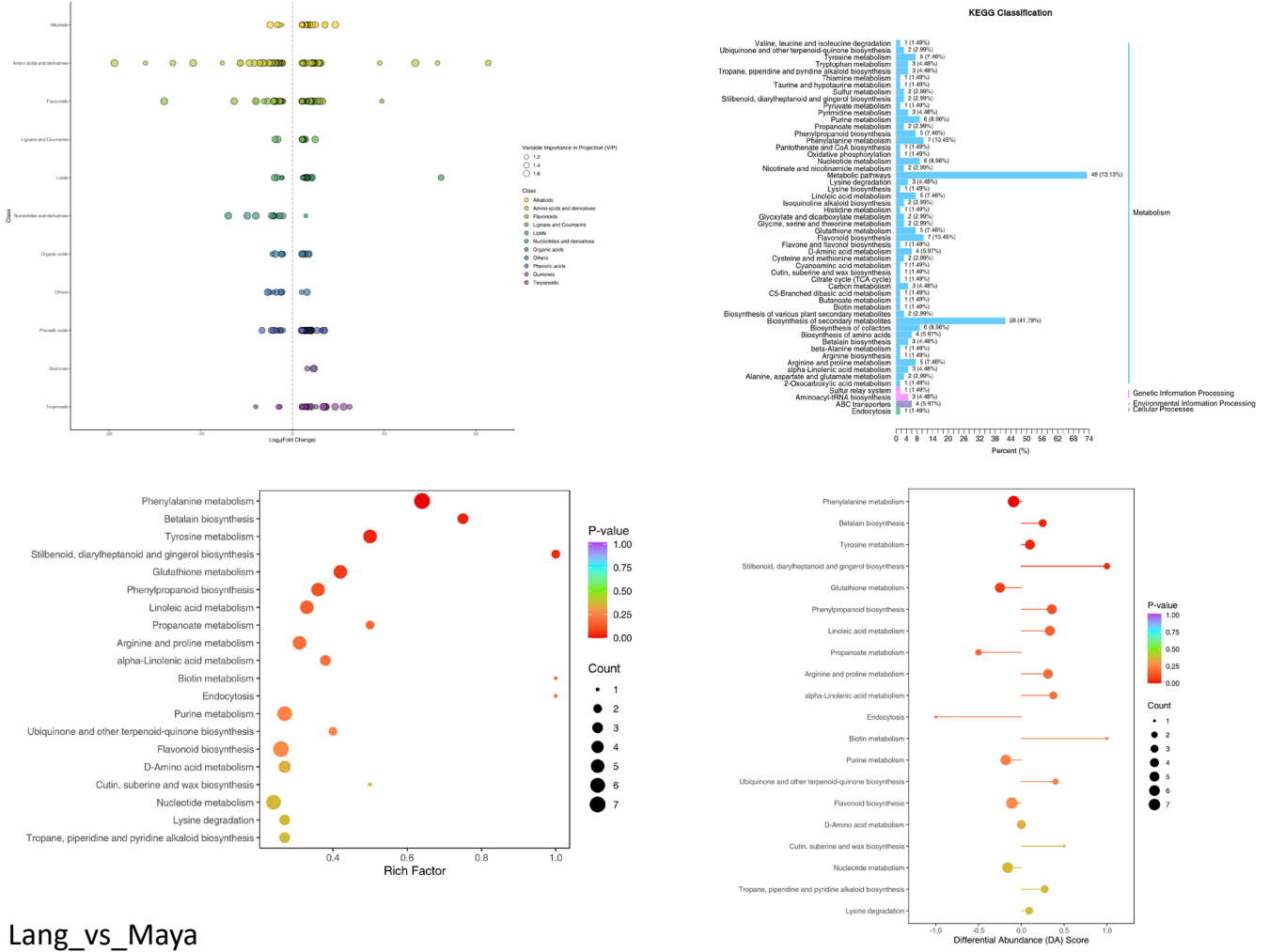
Lang_vs_ZCW

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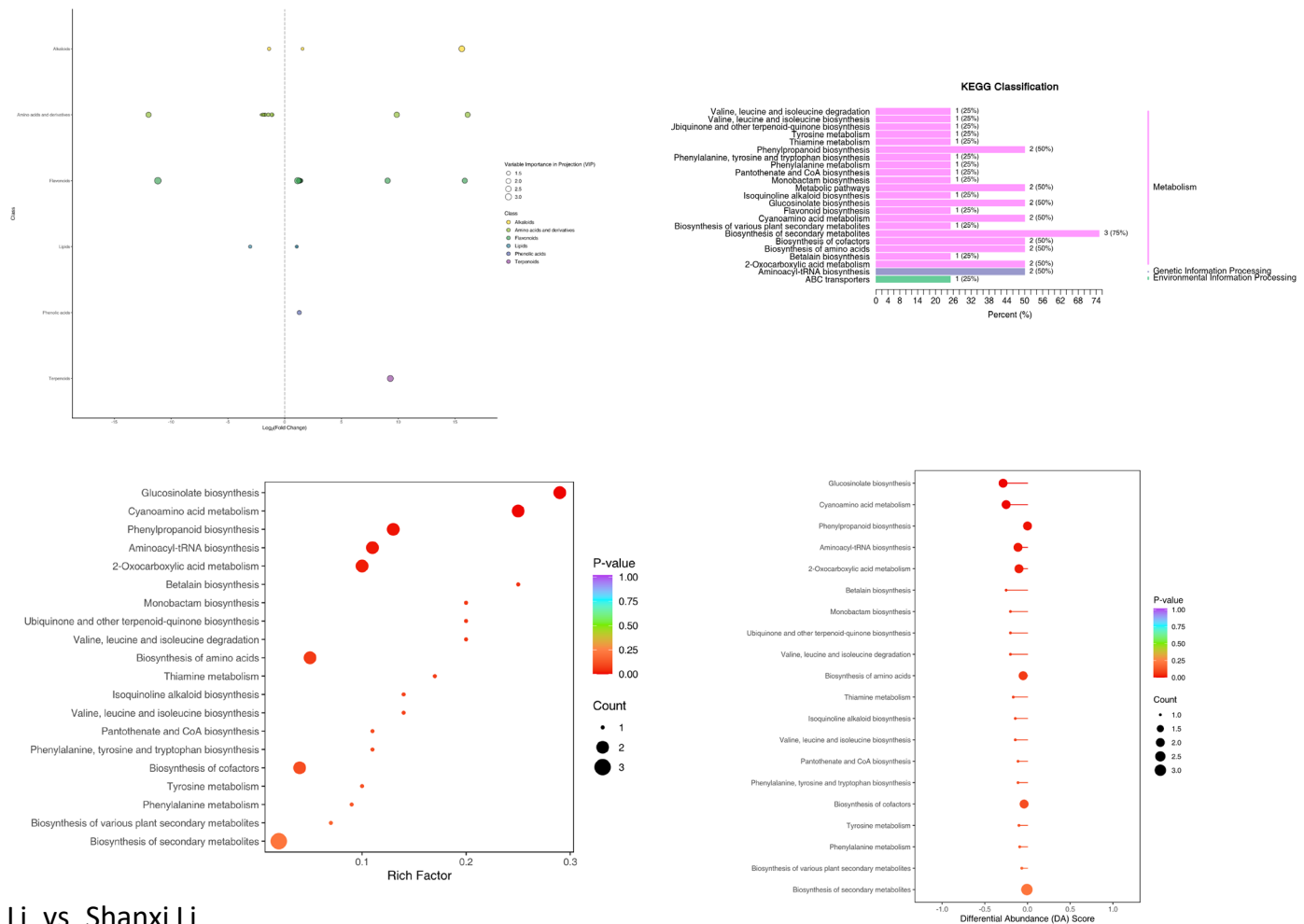
Lang_vs_Li

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Lang_vs_Maya

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Li_vs_Shanxi Li

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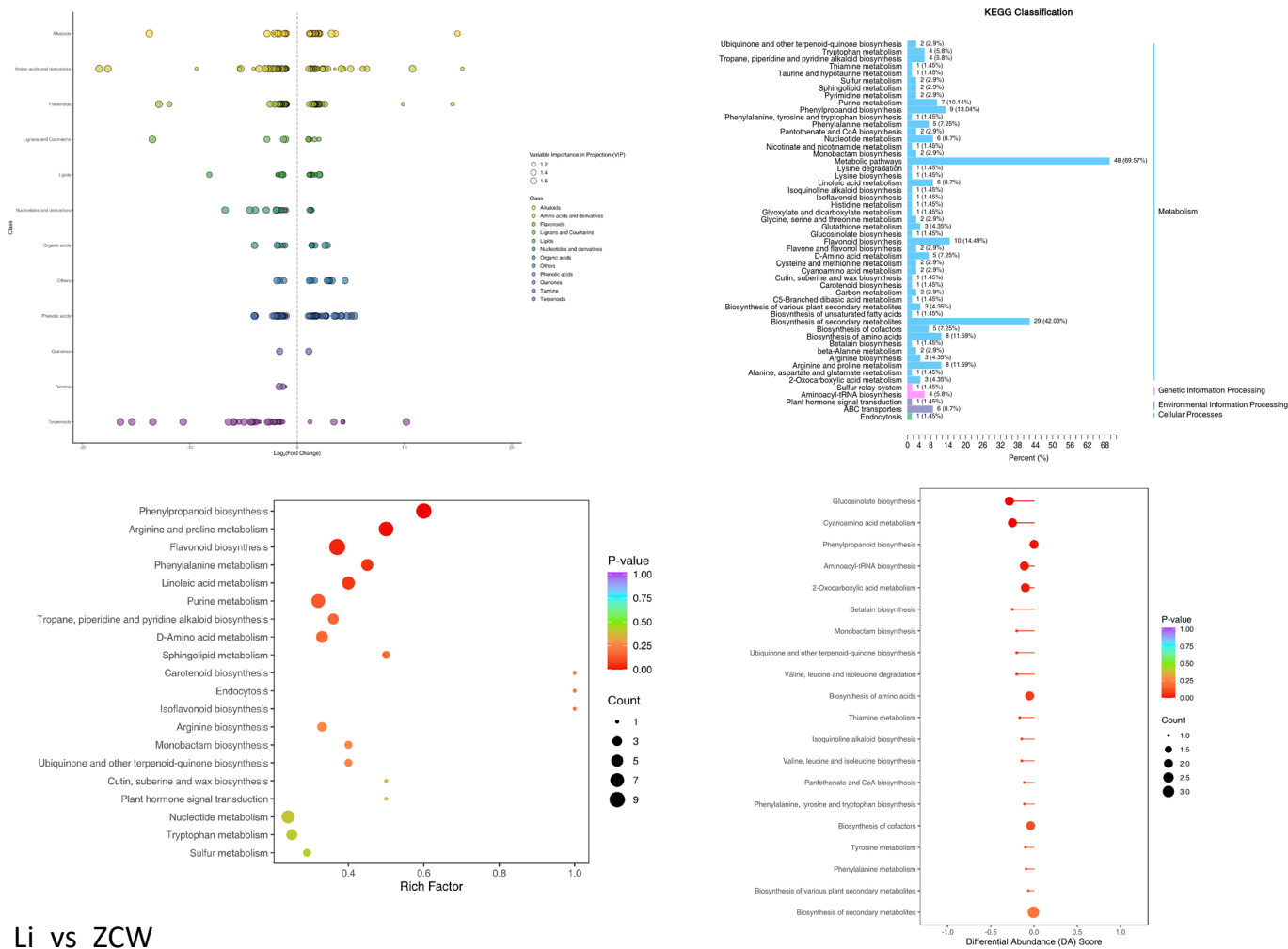


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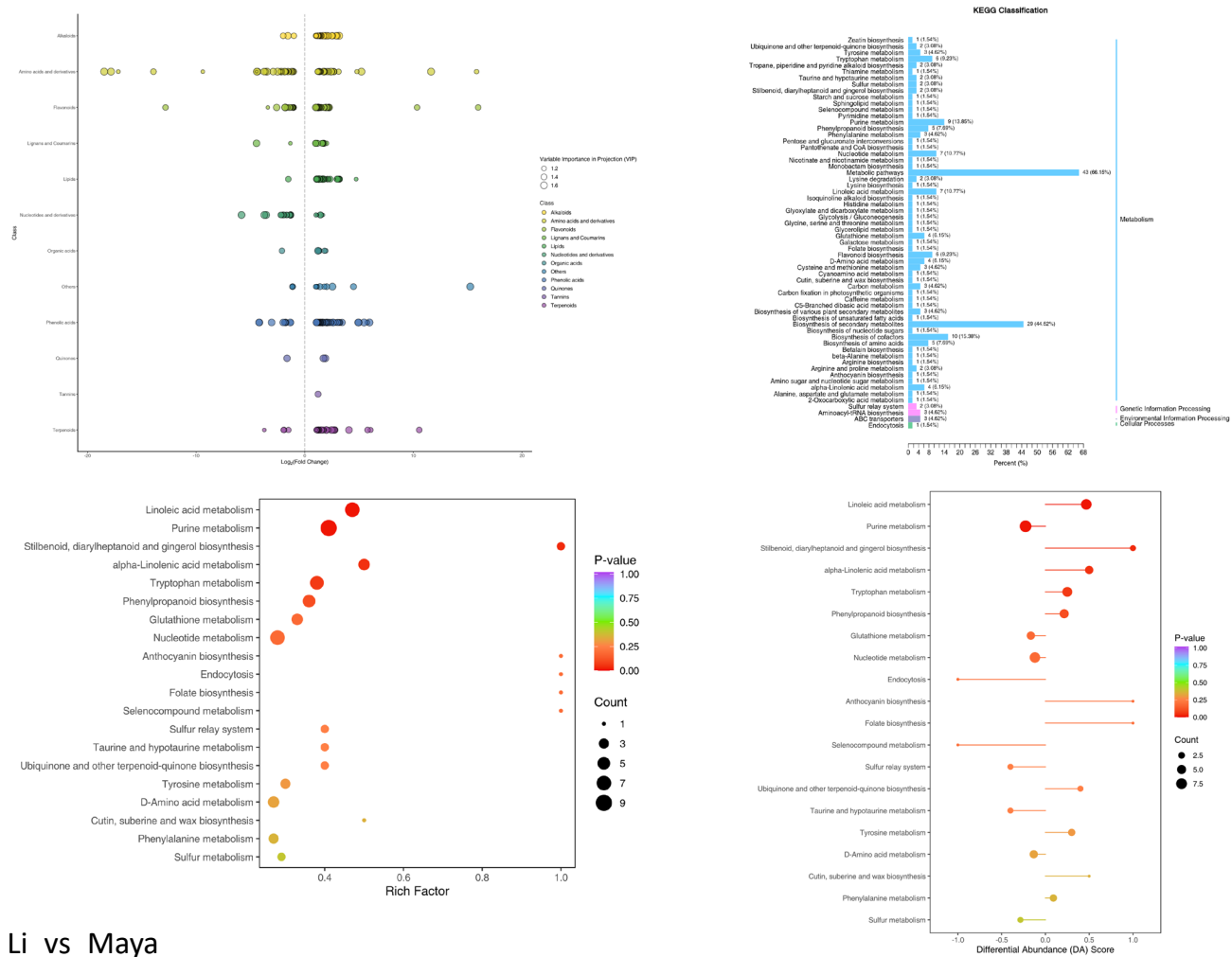
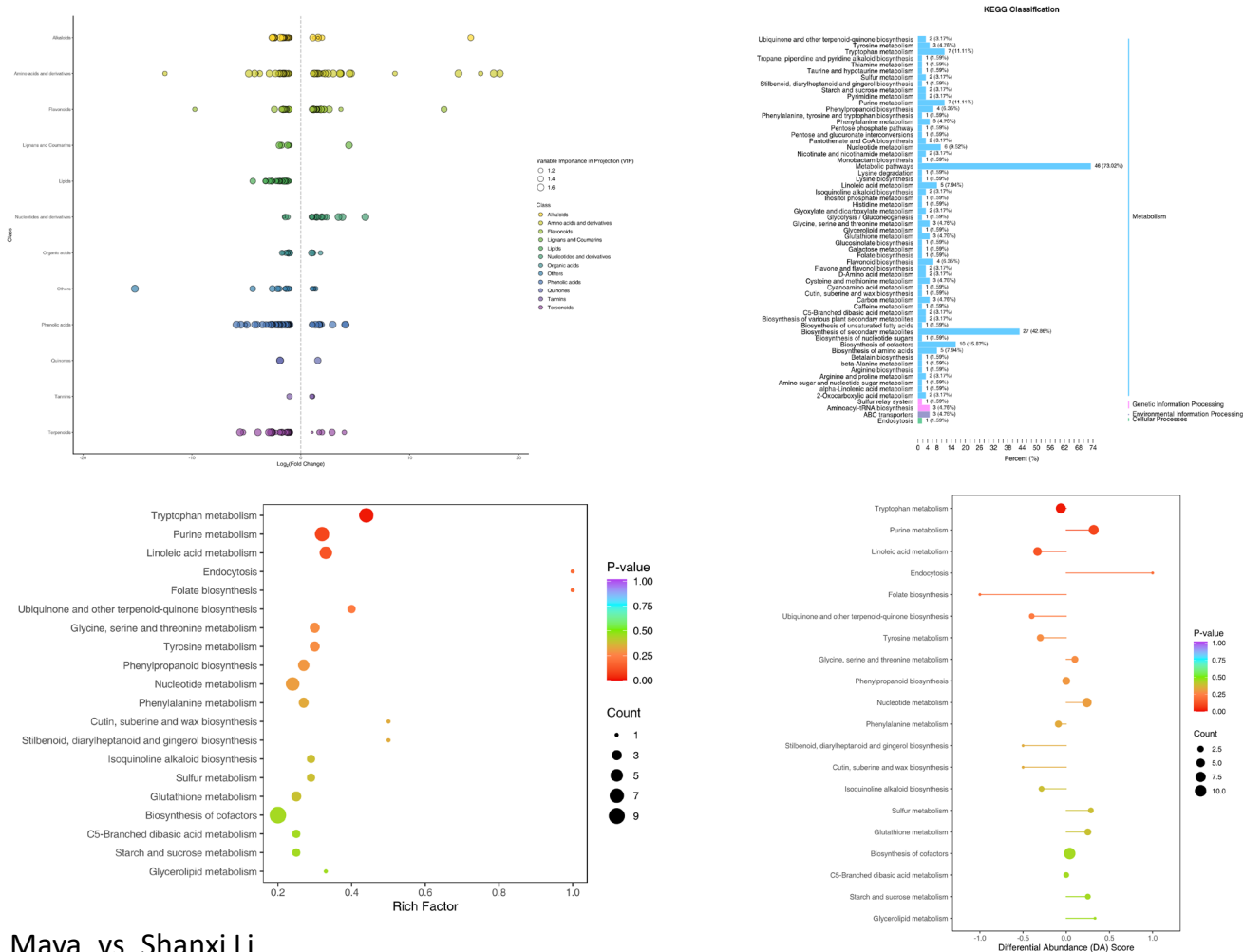
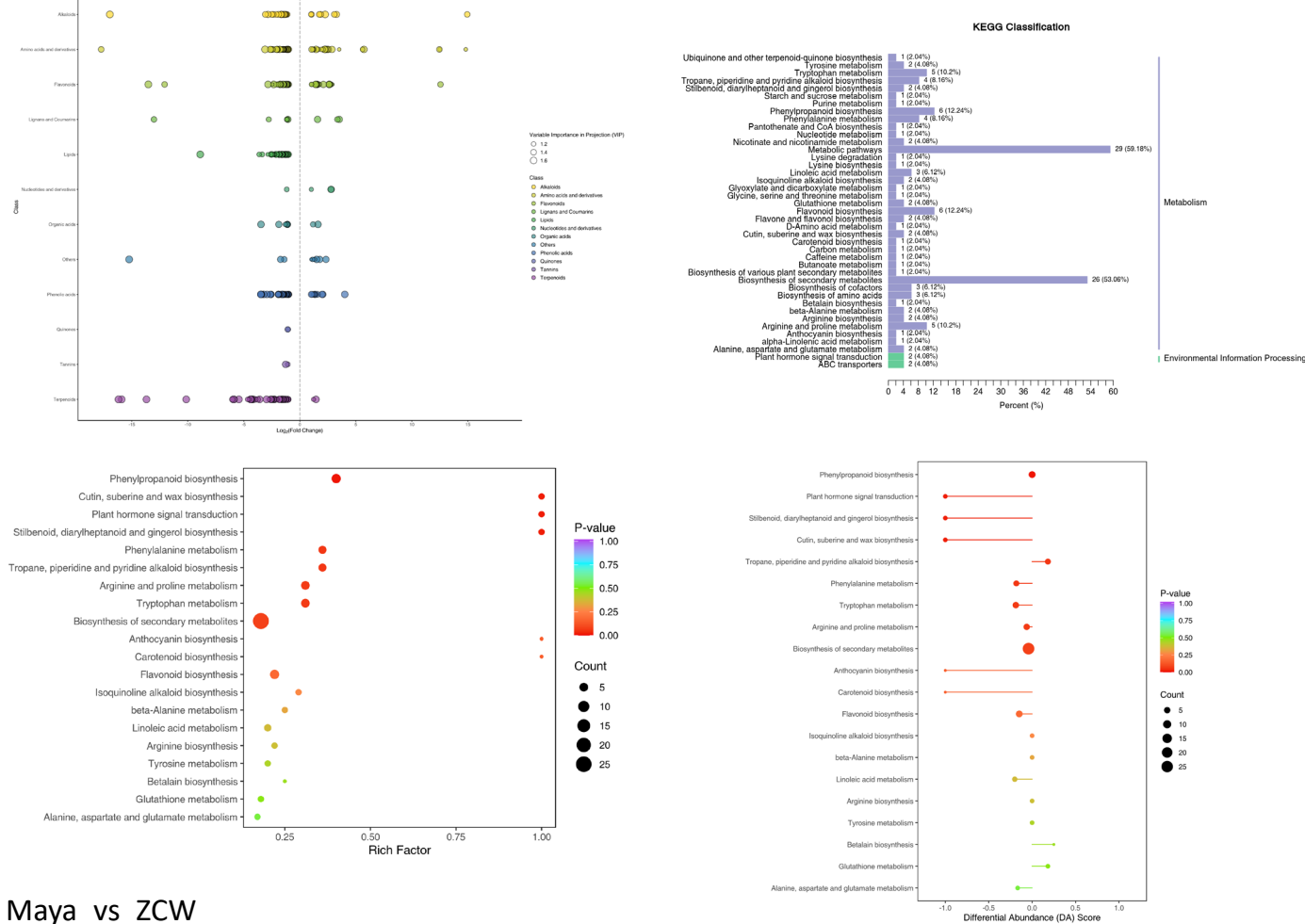


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Maya_vs_Shanxi Li

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Maya_vs_ZCW

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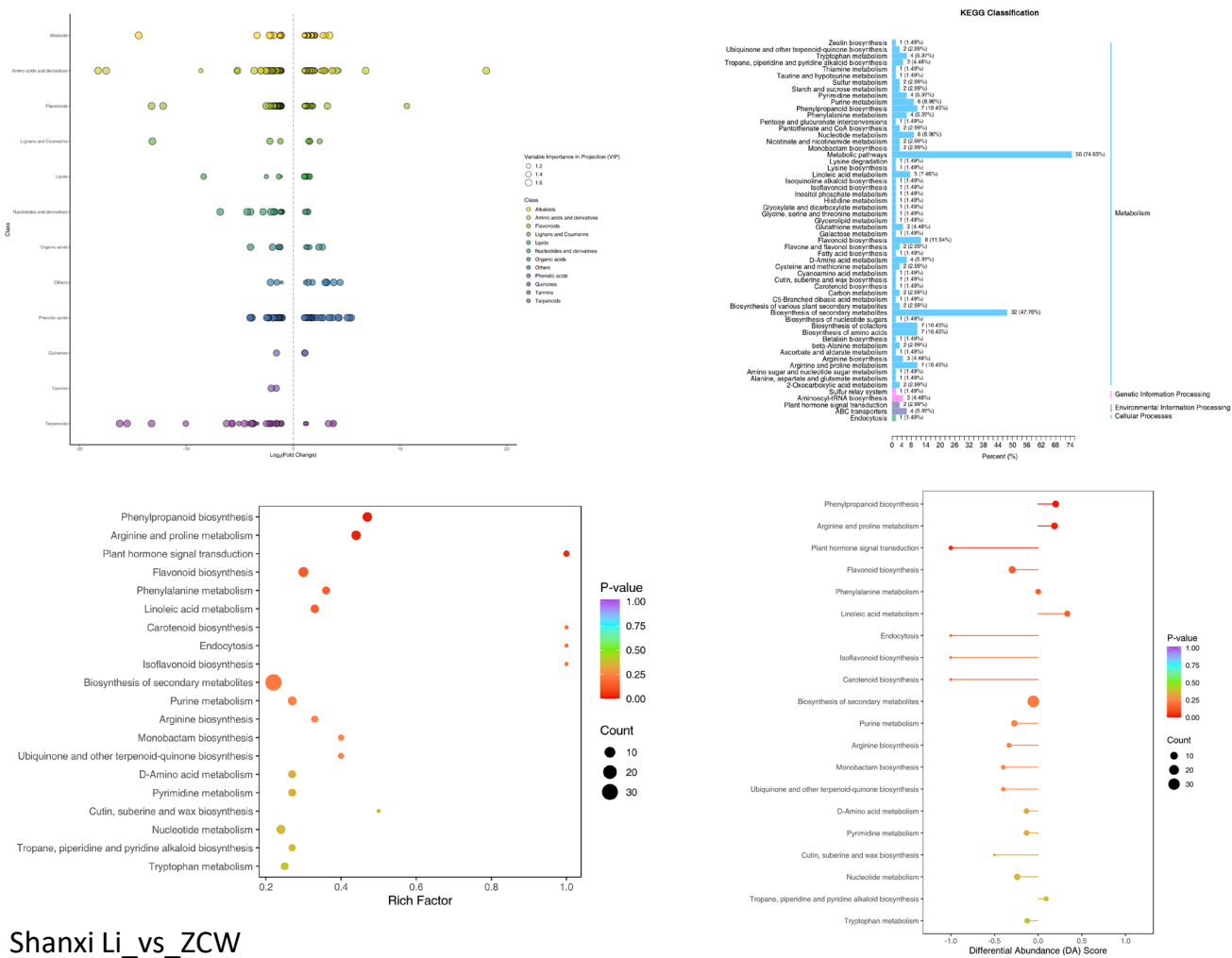
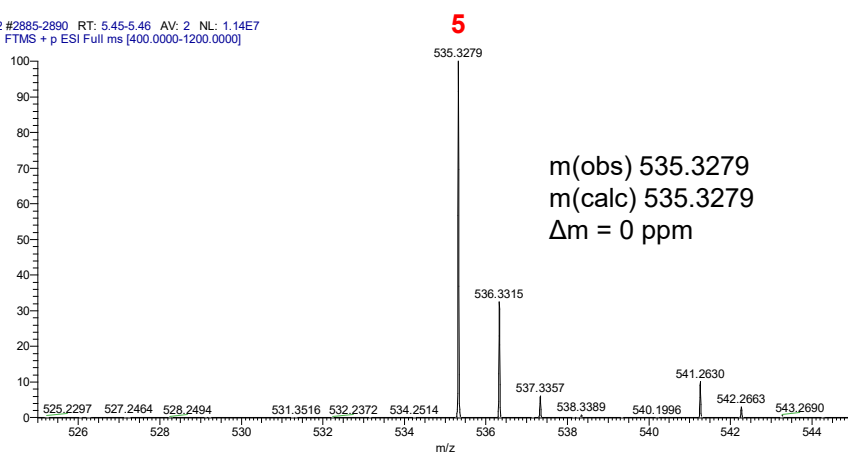
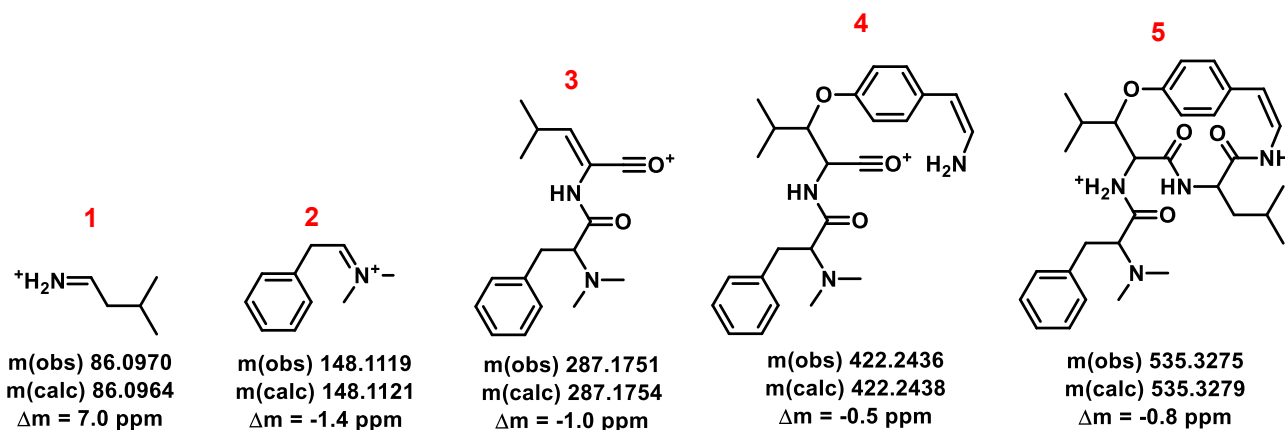


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A

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**B**

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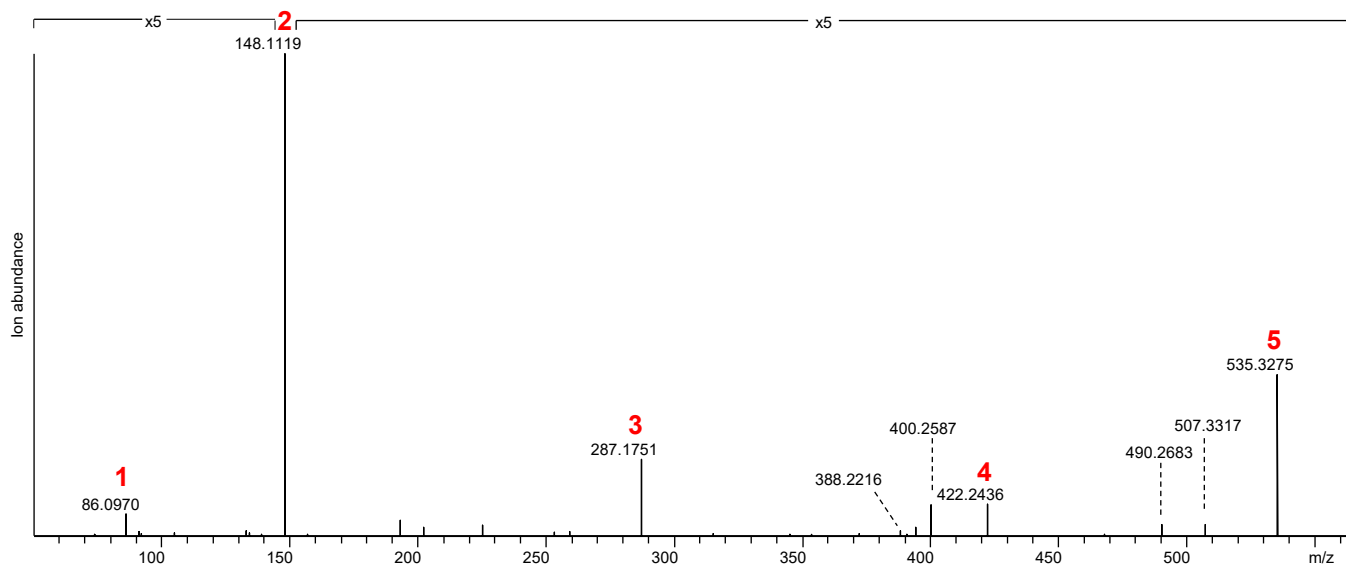
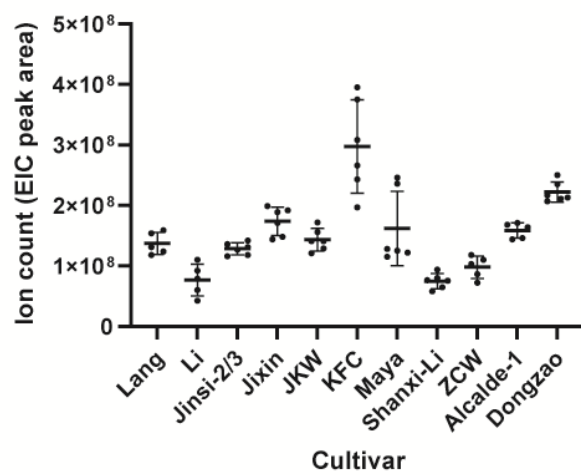
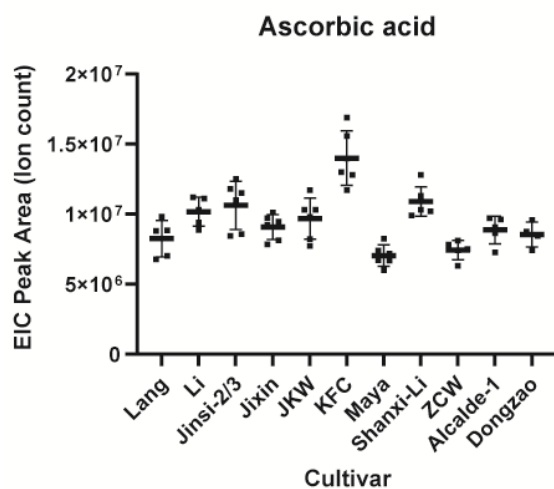
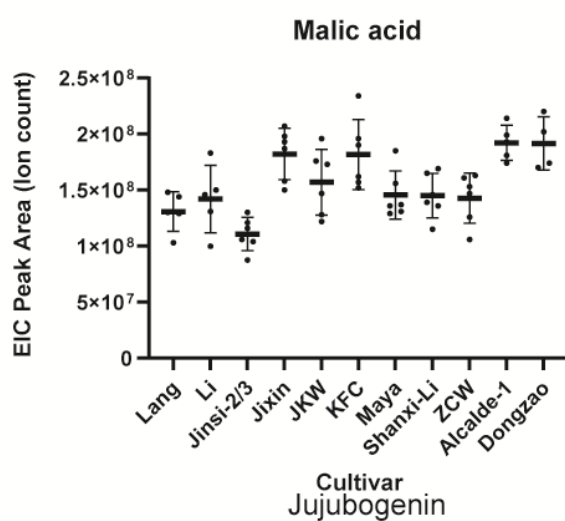
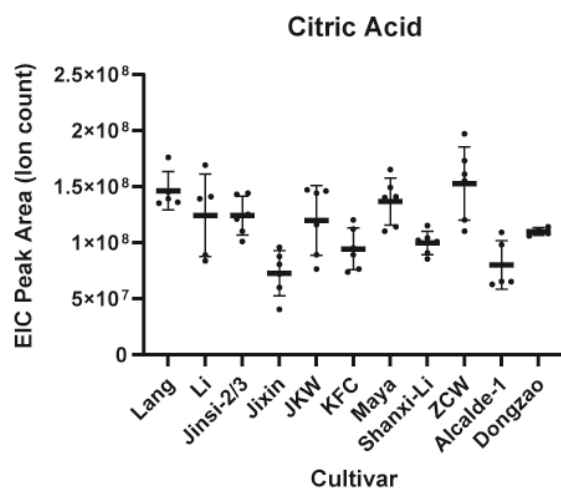
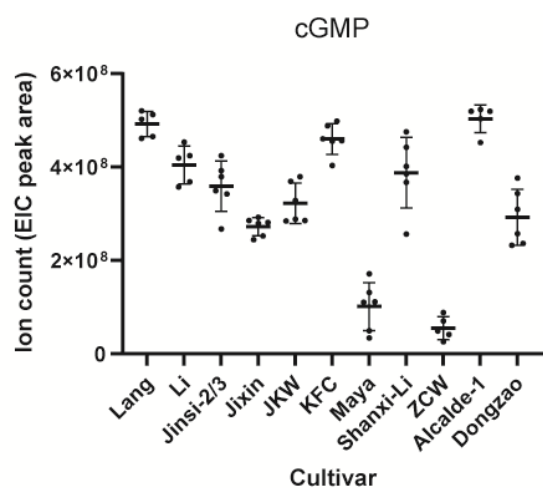
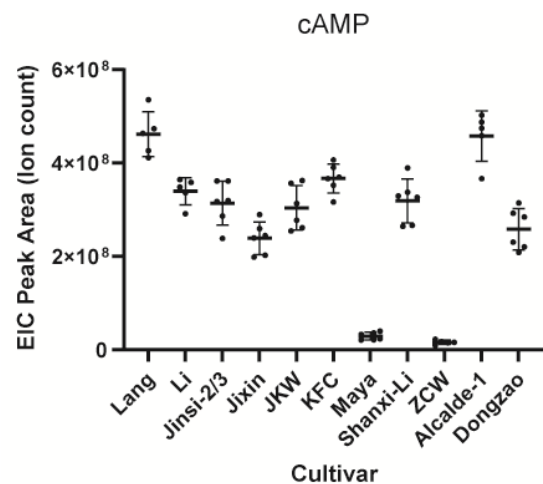


Figure S6 | MS analysis of a sanjoinine A. (A) MS1 analysis of sanjoinine A analyte and (B) MS/MS analysis of sanjoinine A analyte.

A



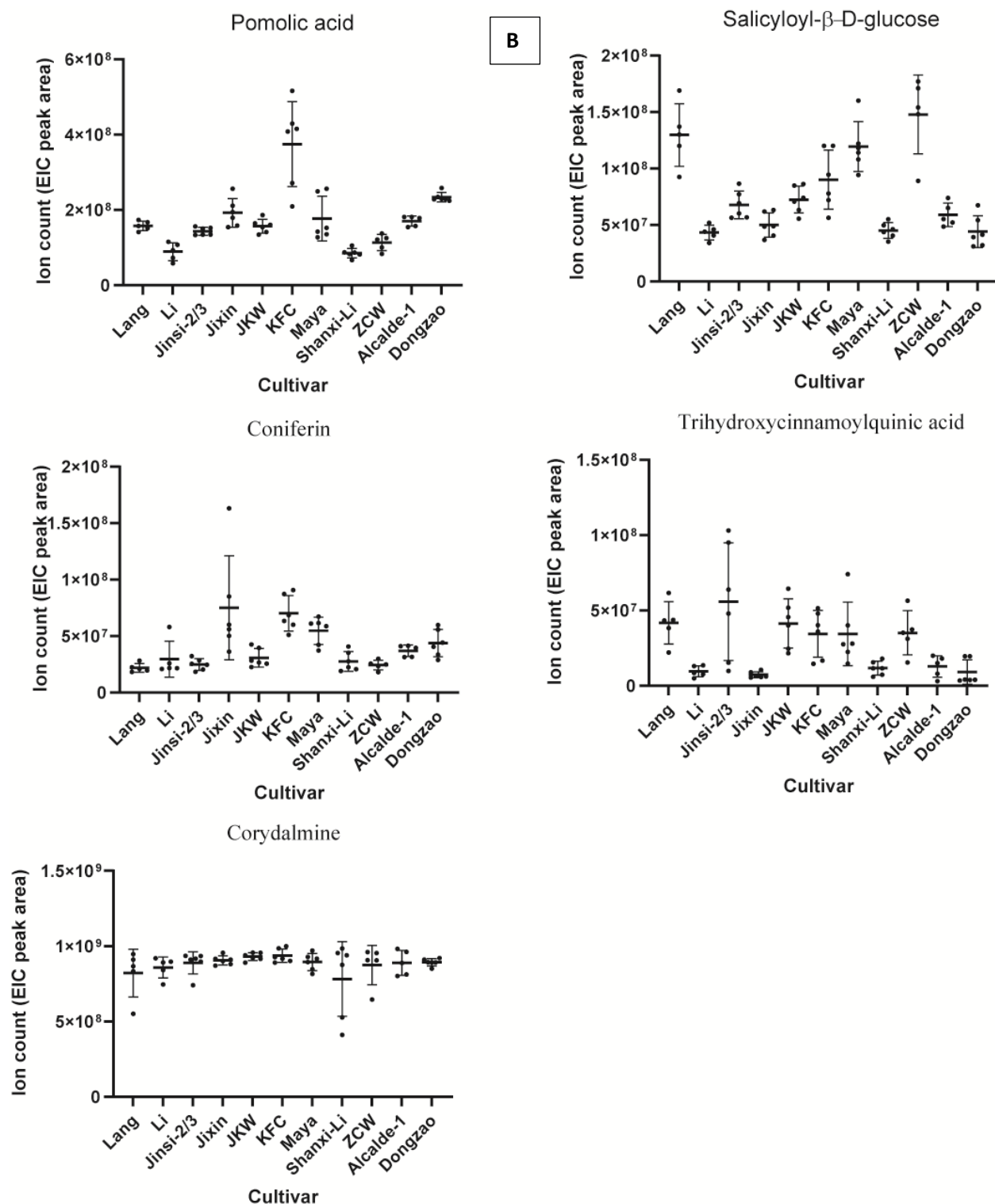


Figure S7. Significant metabolites of 11 jujube cultivars in different categories. A: cAMP, cGMP, citric acid, malic acid, ascorbic acid and jujubogenin, B: pomolic acid, salicyloyl-β-D-glucose, coniferin, trihydroxycinnamoylquinic acid, and corydalmine. The horizontal lines in cultivar plots represent the mean (n=5-6) and the error bars represent one standard deviation.