

2 个文冠果新品种种皮颜色非靶向代谢组分析

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摘要:【目的】分析两个文冠果新品种“绯豆, feidou”(种皮绯红色)、“金珀, jinpo”(种皮橙黄色)种皮颜色产生明显差异原因。【方法】利用 GC-MS 以正离子模式和负离子模式(流动相 A: 0.1%甲酸水溶液; 流动相 B: 0.1%甲酸乙腈)分别对 2 个文冠果新品种和 1 个对照品种 ck(黑色种皮)进行种皮代谢组定性和相对定量分析, 使用 MassLynx V4.2 采集的原始数据在线 METLIN 数据库、公共数据库以及百迈客自建库进行鉴定, 对鉴定组分进行了主成分分析、差异组分分析、差异组分代谢通路分析和色素成分分析。【结论】分析共检测到了 22,427 个峰组分, 成功鉴定到 3910 种组分, 其中负离子模式鉴定到 1168 个组分, 正离子模式鉴定到 2742 个组分。对各样品中各组分进行主成分分析, 第一、二主成分特征值分别为 53.36%、35.95%, 累计贡献率 89.31%, 从第一主成分分量、第二主成分分量可以发现 feidou、jinpo 与 ck, 组间分离度极大, 说明个品种组分之间存在显著差异。对各差异组分进行代谢物注释分析, 其中 KEGG 数据库一级代谢通路 280 条, 包括次生代谢物的生物合成、外源生物物质生物降解和代谢、萜类和聚酮化合物代谢、碳水化合物代谢、信号转导等; Lipidmaps 数据库共注释到 35 条代谢通路, 包括脂肪酰基、甘油酯类、甘油磷脂、聚酮化合物、异戊烯醇脂质、鞘脂、甾醇类。基于多变量分析 OPLS-DA 模型的变量重要性投影(VIP, VIP≥1), 初步筛选出不同品种或组织间差异的代谢物, 同时结合单变量分析的 p-value (P value<0.05)、差异倍数(fold change, FC 阈值为 2)来进一步筛选出差异代谢物。其中 feidou 与 ck 比较上调组分 1289 种, 下调组分 1677 种; feidou 与 jinpo 比较上调组分 1152 种, 下调组分 1499 种; jinpo 与 ck 比较上调组分 1348 种, 下调组分 1603 种。对黄酮类相关组分进行分析共发现 140 种, 除银杏黄酮、山奈素、表没食子儿茶素没食子酸酯 EGCG、新补骨脂异黄酮、鸢尾苷在 3 个样品中的组分含量差异不明显外, 其他 135 种均表现出显著差异, 包括花青素类 5 种, 双黄酮和多黄酮 2 种, 查尔酮和二氢查尔酮 11 种, 香豆素类 4 种, 黄烷酮 11 种, 黄烷类、黄烷醇类和无色花青素 8 种, 黄酮和黄酮醇类化合物 71 种, 原花青素 4 种, 紫檀碱类 3 种, 鱼藤酮类 3 种, 异黄酮 13 种, 其他黄酮类 2 种, 各类黄酮类组分含量不一。对花青素类进一步分析发现共 5 种, 包括锦葵色素-3-(对-香豆酰基)-芸香糖苷-5-葡萄糖苷、龙胆翠雀花素、芍药素 3-O-葡萄糖苷、飞燕草素芸香糖苷、矢车菊苷。在各花青素成分中 feidou 和 jinpo 龙胆翠雀素的含量明显高于其它 4 种组分, 但显著低于 ck; 2 品种与 ck 相比, 含量降低, 其中, 锦葵素糖苷 feidou 略高于 jinpo, 而 jinpo 略高于 ck, 差异不显著。但芍药素糖苷 feidou 高于 jinpo 且显著高于 ck。而矢车菊苷 feidou 高于 jinpo 显著低于 ck。另外文冠果种皮种还含有大量红色色素包括苋菜红素、羟基茜草素、藻红素、辣椒红素; 黄色色素包括胆红素、6-脱氧巴西红厚壳素、叶黄素、姜黄素单葡萄糖苷、黄颜色素、全反式-4-氧代视黄酸、茶黄素等。推测这可能是 Jinpo 总体呈现橙黄色, 而 feidou 呈现出玫红的原因。

关键词: 文冠果; 种皮颜色; 代谢组学; 差异分析

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Non-targeted Metabolomics Analysis on Seed Coat Color of Two New Varieties of *Xanthoceras sorbifolia*

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Abstract: [Objective] The purpose was to analyze the reasons for the obvious differences in seed coat color between two new *Xanthoceras sorbifolia* varieties, Feidou (scarlet seed coat) and Jin Po (orange seed coat). [Methods] Qualitative and relative quantitative analysis of seed coat metabolome of two new varieties of *X. sorbifolia* and one control variety ck (black seed coat) were carried out by GC-MS in positive ion mode and negative ion mode, respectively (mobile phase A: 0.1% formic acid aqueous solution; The mobile phase B: 0.1% acetonitrile formate). and the original data collected by MassLynx V4.2 were used for online identification in METLIN database, public database and self-built database of Biomarker co.,ltd.. The identified components were analyzed by principal component analysis, differential component analysis, differential component metabolic pathway analysis and pigment component analysis.

[Conclusion] A total of 22,427 peak components were detected and 3,910 components were successfully identified. Among them, 1168 components were identified by negative ion mode and 2742 components were identified by positive ion mode. Principal component analysis showed that the characteristic values of the first and second principal components were 53.36% and 35.95% respectively, and the cumulative contribution rate was 89.31%. Metabolite annotation analysis was carried out on the different components, including 280 primary metabolic pathways in KEGG database, including biosynthesis of secondary metabolites, biodegradation and metabolism of exogenous biomass, terpenoid and polyketone metabolism, carbohydrate metabolism, signal transduction, etc. Lipidmaps database annotated 35 metabolic pathways, including fatty acyls, glycerolipids, glycerolphospholipids, polyketone compound, isoprenol lipid, sphingolipids and sterols. **【Conclusion】** A total of 22,427 peak components were detected and 3,910 components were successfully identified, including 1,168 components identified by negative ion mode and 2,742 components identified by positive ion mode. Principal component analysis showed that the eigenvalues of the first and second principal components were 53.36% and 35.95%, respectively, and the cumulative contribution rate was 89.31%. The separation between groups of Feidou, Jinpo and ck could be found from first and the second principal component was great, indicating that there were significant differences among the components of the three varieties. Metabolite annotation analysis was carried out on the different components, including 280 primary metabolic pathways in KEGG database, including biosynthesis of secondary metabolites, biodegradation and metabolism of exogenous biomass, terpenoid and polyketone metabolism, carbohydrate metabolism, signal transduction, etc. Lipidmaps database annotated 35 metabolic pathways, including fatty acyls, glycerolipids, glycerolphospholipids, polyketone compound, isoprenol lipid, sphingolipids and sterols. Based on multivariate analysis of the variable importance projection (VIP, $VIP \geq 1$) of OPLS-DA model, the metabolites with differences among different varieties were preliminarily screened, and then, the metabolites with differences were further screened by combining the p-value ($P \text{ value} < 0.05$) and the fold change (FC threshold is 2) of univariate analysis. Compared with ck, feidou up-regulated 1289 components and down-regulated 1677 components. Compared with jinpo, feidou has 1152 up-regulated components and 1499 down-regulated components. Compared with ck, jinpo has 1348 up-regulated components and 1603 down-regulated components. A total of 140 kinds of flavonoids were found by analyzing the related components. Except for ginkgo

flavone, kaempferide, epigallocatechin gallate EGCG, neopsoralen isoflavone and tectoridin, the other 135 kinds showed significant differences, including 5 kinds of anthocyanins, 2 kinds of biflavonoids and multiflavonoids, 11 kinds of chalcones and dihydrochalcones, 4 kinds of coumarins and 11 kinds of flavanones. There are 8 kinds of flavans, flavanols and colorless anthocyanins, 71 kinds of flavonoids and flavonol compounds, 4 kinds of procyanidins, 3 kinds of pterostigmine, 3 kinds of rotenone, 13 kinds of isoflavones and 2 kinds of other flavonoids, All kinds of flavonoids have different contents. Further analysis showed that there were five kinds of anthocyanins, including mallow pigment -3- (p-coumaroyl)-rutinoside -5- glucoside, gentian delphinidin, paeoniflorin 3-O-glucoside, delphinidin rutinoside and cyanidin. The contents of feidou and jinpo gentiopicrin in each anthocyanin component were significantly higher than those in the other four components, but significantly lower than CK. Among other components, the mallow glycoside feidou was slightly higher than jinpo, while jinpo was slightly higher than ck, and the difference was not significant. However, the paeoniflorin glycoside feidou was higher than jinpo and significantly higher than ck. However, the cyanidin feidou was higher than jinpo but significantly lower than ck. In addition, *X. sorbifolia* seed coat also contains some red pigments and yellow pigment. The red pigments include amaranthin, purpurin, phycoerythrin and capsanthin. The yellow pigments include bilirubin, 6-Deoxyjacareubin, lutein, curcumin monoglucoside, fustin, all-trans -4- oxoretinoic acid and theaflavins. It is speculated that this may be the reason why Jinpo is orange and feidou is scarlet.

Key words: *Xanthoceras sorbifolia*; seed coat color; metabolomics; difference analysis