



# Genome-wide association analysis of seed color-related metabolites (mGWAS) in *Brassica napus* L.

Cunmin Qu

Southwest University

2023-09-27



# Cotents

**1** Backgrounds

**2** DMetFinder V1.0

**3** Metabolites in seed of U-triangle species

**4** mGWAS and Candidate genes selection

# 1. Backgrounds

## Yellow-seeded *Brassica*

Thinner seed coat, higher proportion of protein and/or oil in seed;

Lower anti-nutritive fiber, fewer condensed tannins and other pigments;

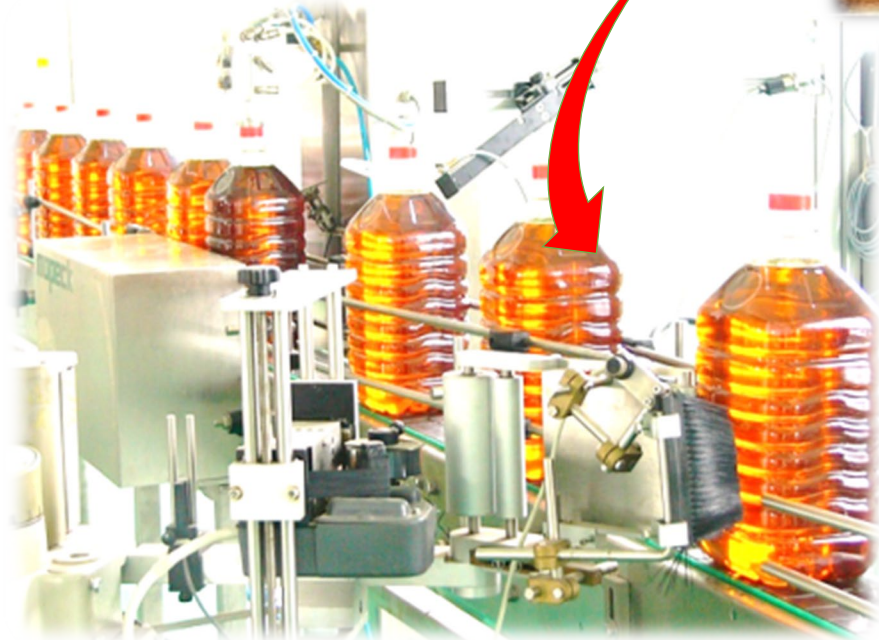
Source of edible oil, vegetable protein for feed and Rape oil-based Biodiesel.



# 1. Backgrounds

## High commercial application

The price of yellow-seeded press oil and meal is higher 10-20% than that of black seeded cultivars.

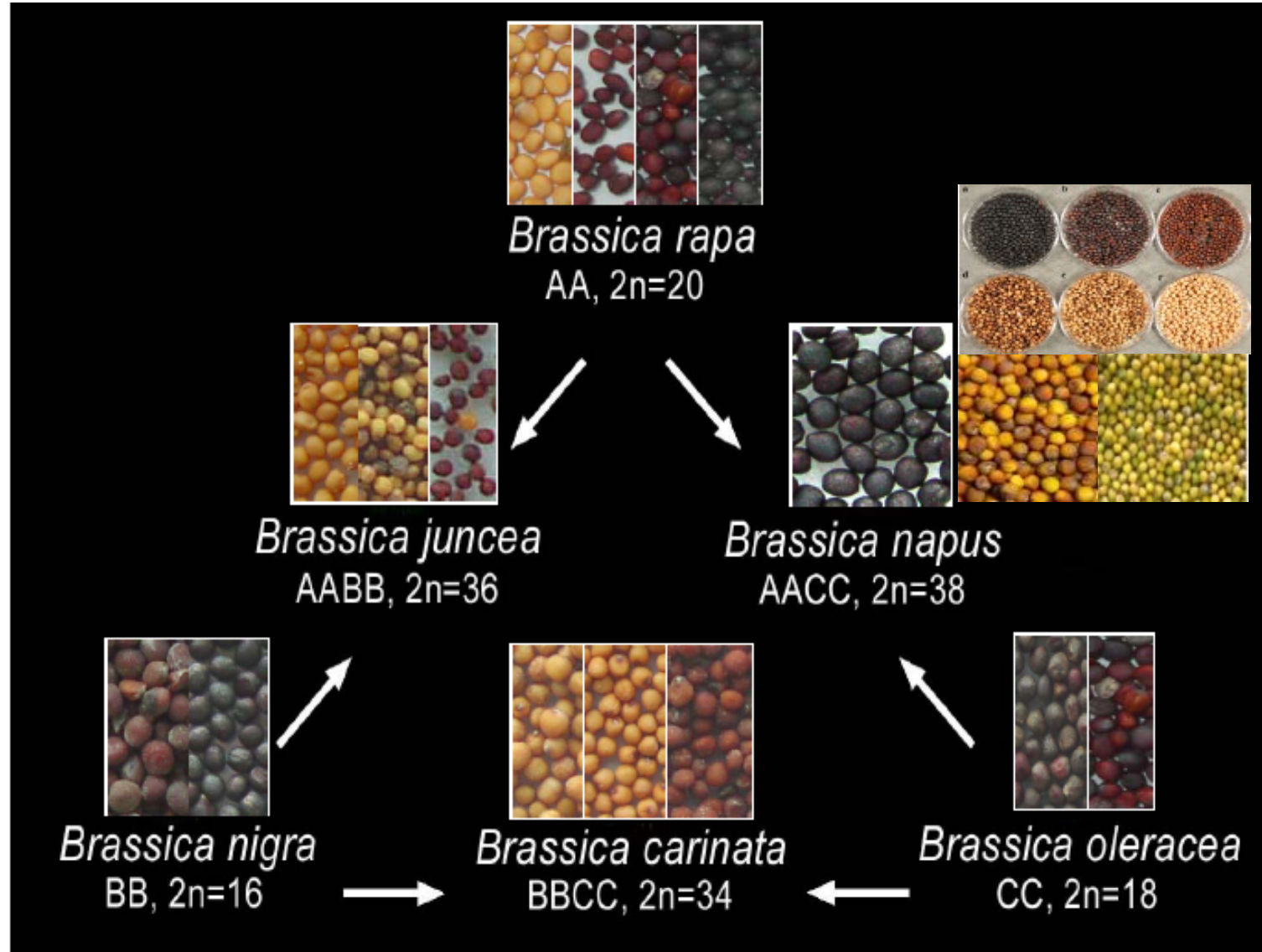


Press oil



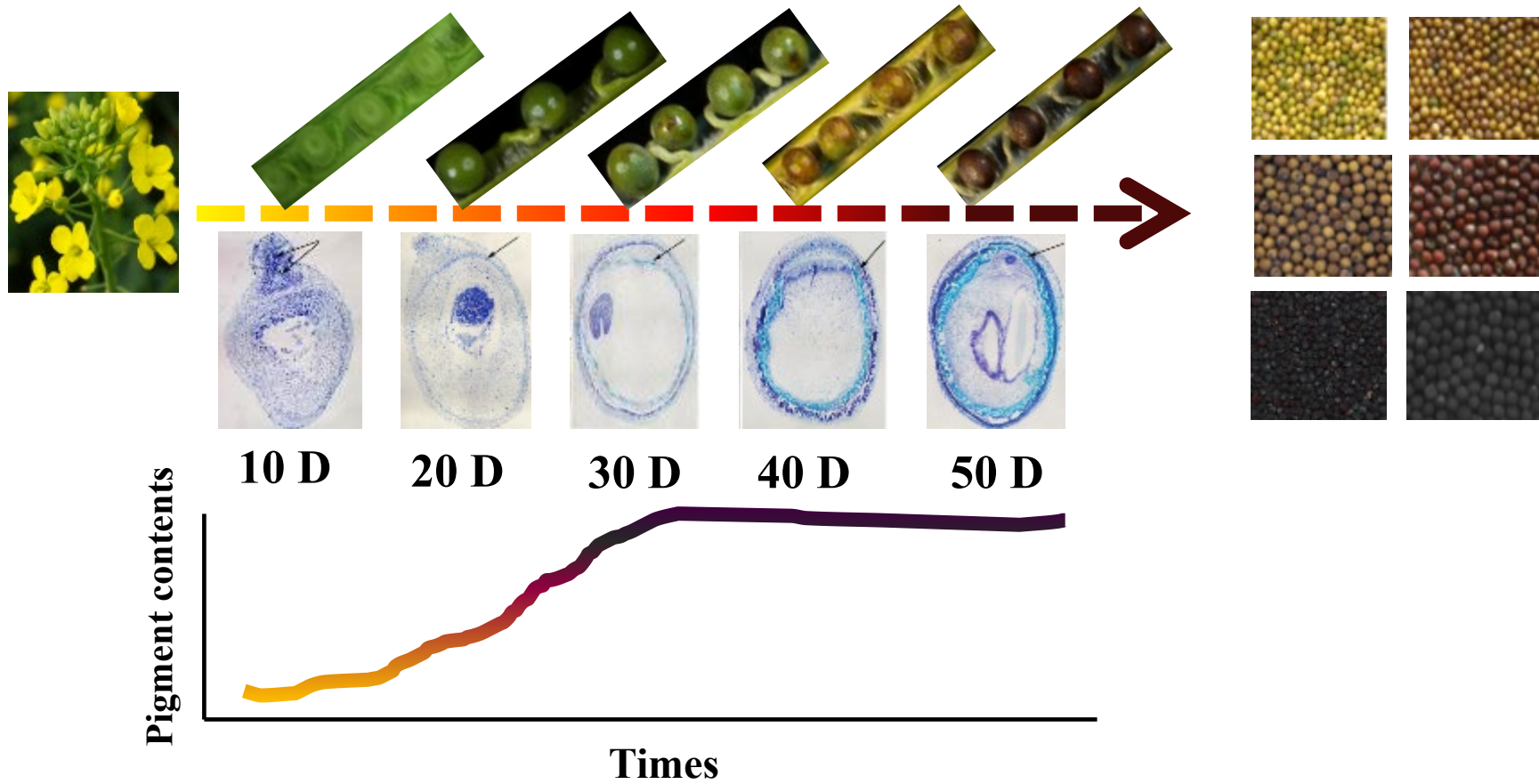
Yellow meal

# 1. Backgrounds



# 1. Backgrounds

## The pigments accumulation and seed coloration



Abundant accumulation of pigments during seed development may be lead to different color formation after maturation, regulated by many genes. (Qu et al., *JXB*, 2013)



**2 DMetFinder V1.0**

## 2. DMetFinder V1.0

Business



**MarkerView**

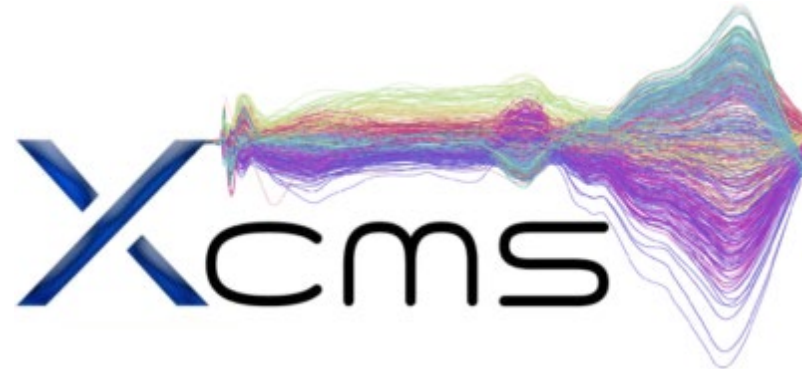


**Compound Discoverer**

Free



MS-DIAL

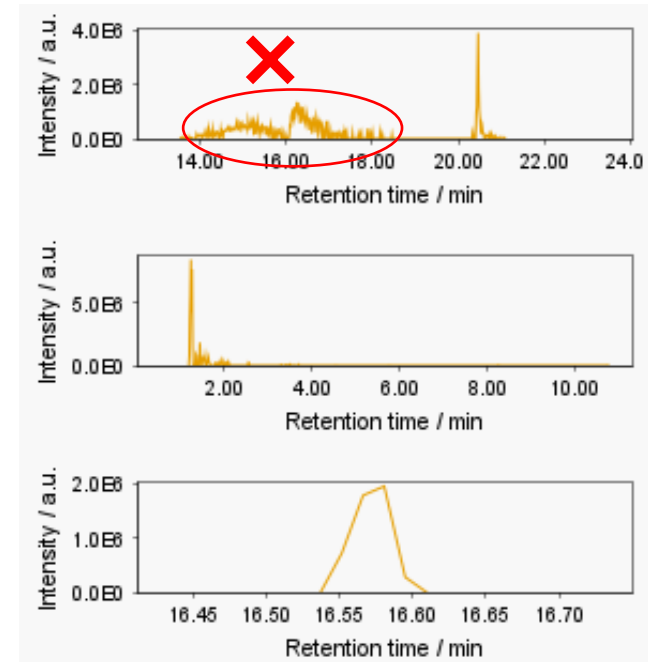


**MZmine 2**

## 2. DMetFinder V1.0

### Disadvantages of MS data analysis

- Not full Covering
- Un-sensitivity for the low-abundance metabolites
- False positive and negative
- No identification standards based on ion chromatographic peak



Comprehensive evaluation of untargeted metabolomics data processing software in feature detection, quantification and discriminating marker selection

Zhucui Li<sup>a, b, c</sup>, Yan Lu<sup>a, b, d</sup>, Yufeng Guo<sup>c</sup>, Haijie Cao<sup>e</sup>, Qinrong Wang<sup>c</sup>, Wenqing Shui<sup>b, d, \*</sup>



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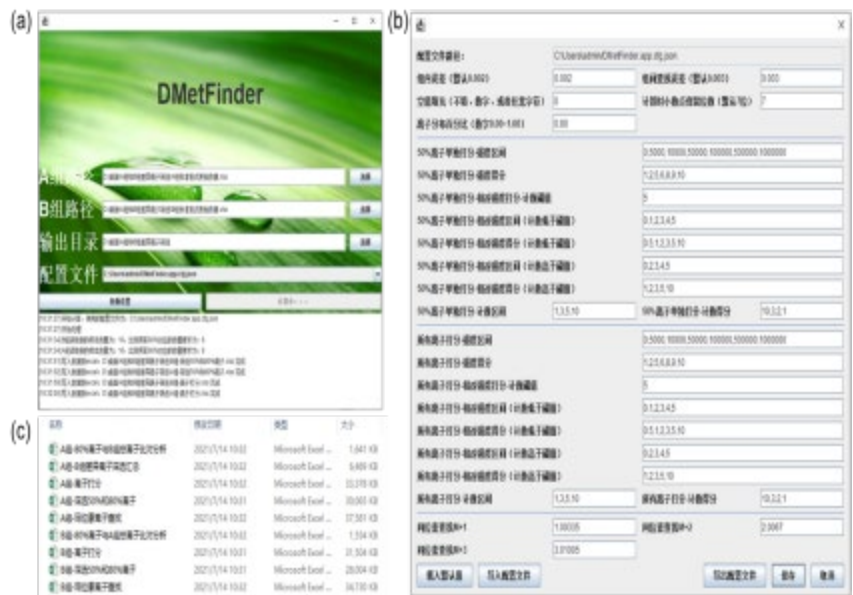
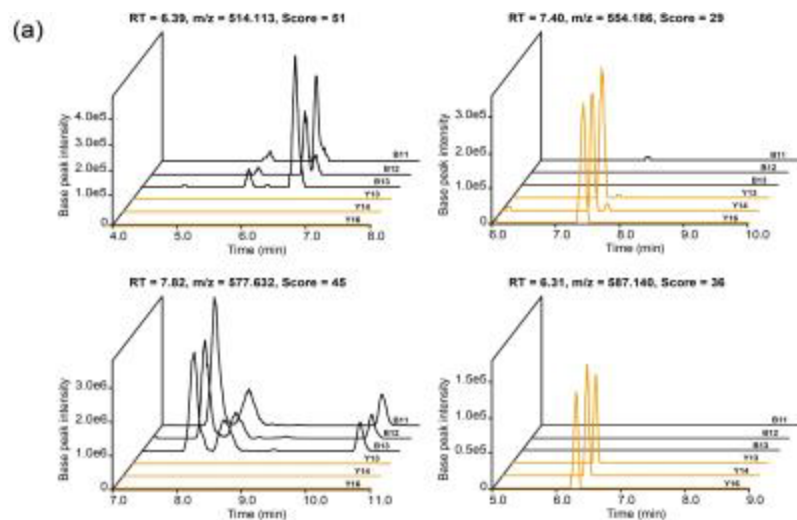
### Enhancing Metabolome Coverage in Data-Dependent LC–MS/MS Analysis through an Integrated Feature Extraction Strategy

Yaxi Hu,<sup>†,‡</sup> Betty Cai,<sup>†</sup> and Tao Huan<sup>\*,†</sup>

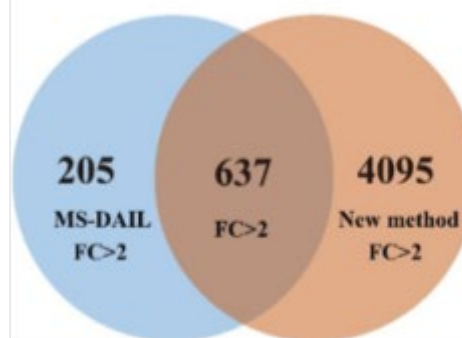
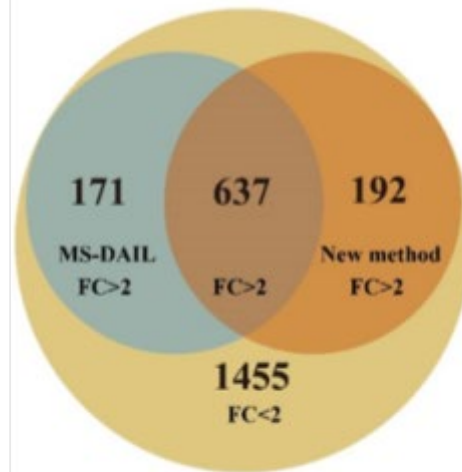
<sup>†</sup>Department of Chemistry, Faculty of Science, University of British Columbia, 2036 Main Mall, Vancouver V6T 1Z1, British Columbia, Canada

<sup>‡</sup>Food, Nutrition and Health Program, Faculty of Land and Food Systems, University of British Columbia, Vancouver V6T 1Z4, British Columbia, Canada

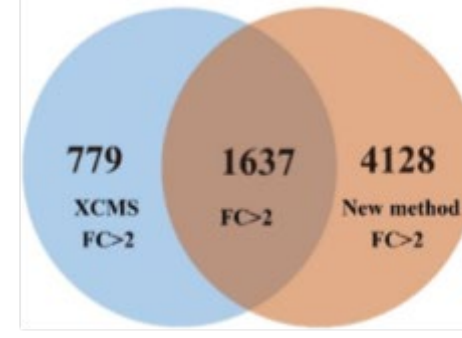
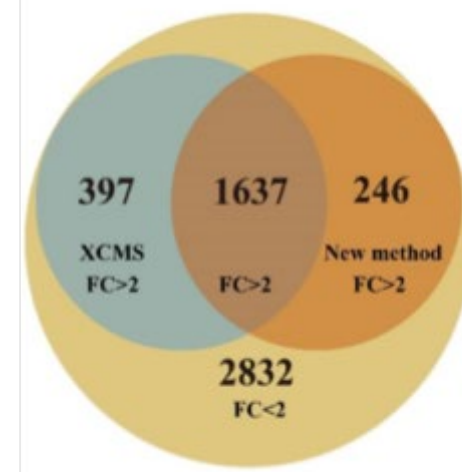
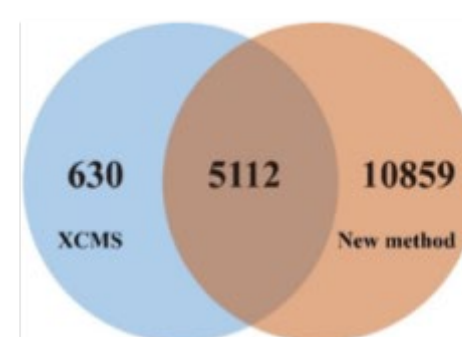
# 2. DMetFinder V1.0



MS-DAIL vs DMetFinder

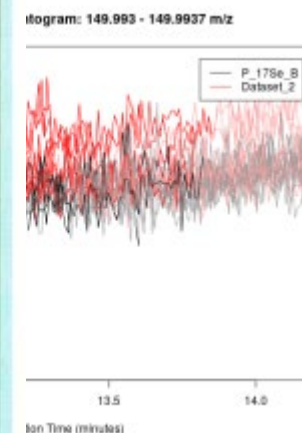
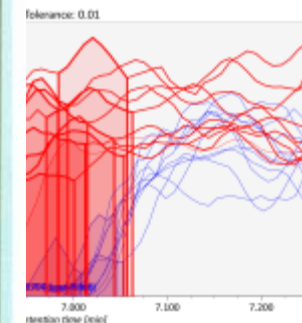


XCS vs DMetFinder



## 2. DMetFinder V1.0

ID	RT	m/z	MS-DIAL	XCMS	Changin
3112	5.97	649.14496	0.33	1.73	1.61
1158	6.35	298.13018	0.20	1.65	0.57
46	6.86	121.02811	0.26	1.74	1.47
2664	10.60	547.10713	3.96	/	1.60
2534	14.69	518.2544	3.21	1.89	1.38
3194	14.07	693.3356	0.32	0.81	0.68
2345	14.66	474.26331	4.53	1.84	1.93
2650	15.03	544.26683	4.63	0.75	1.30
667	13.59	223.09704	4.31	0.22	1.37
977	16.40	271.22835	3.69	/	1.58



=589.21049, Score=50

NL: 8.03E5

NL: 2.05E5

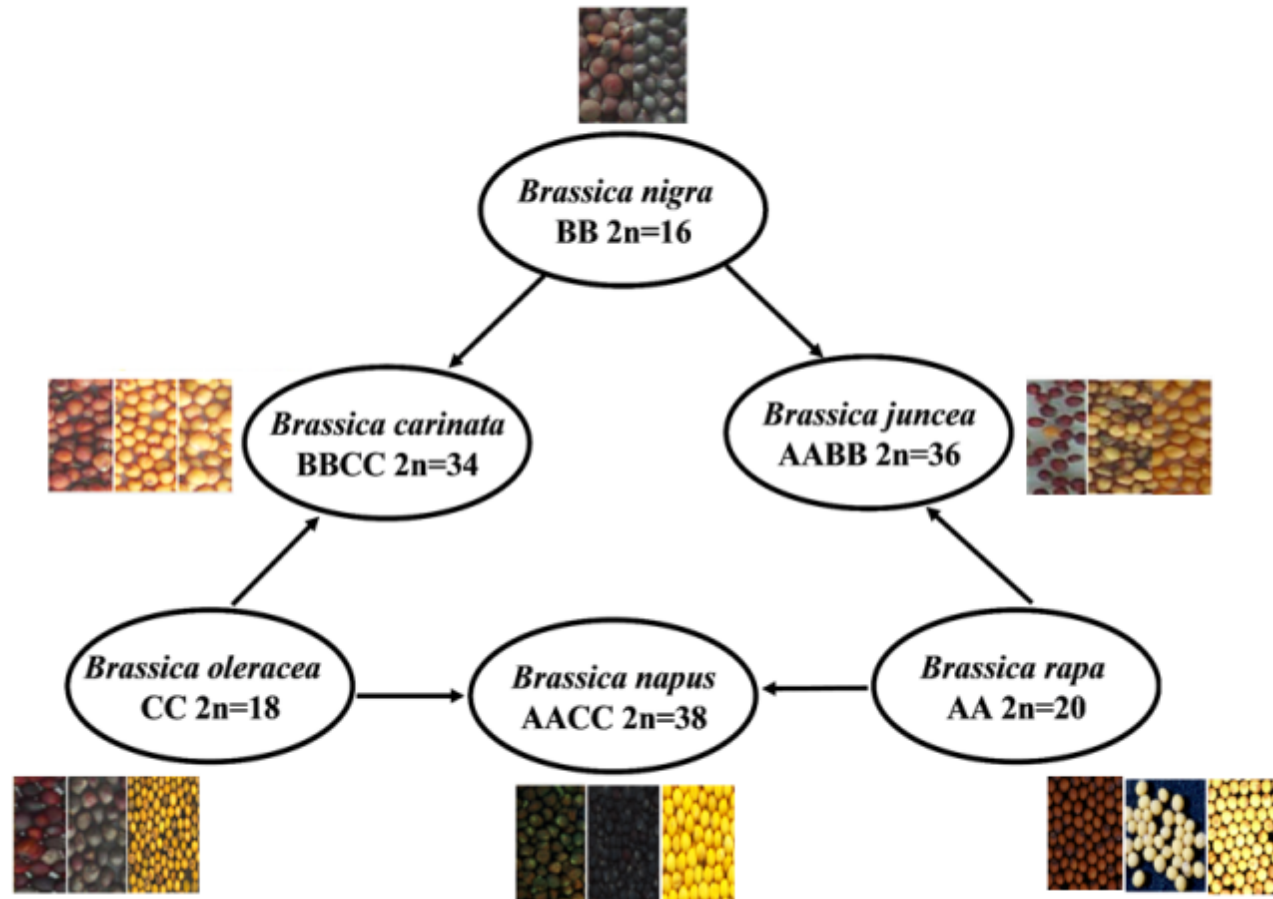
NL: 2.33E5



**3**

**Metabolites in seeds of U-triangle species**

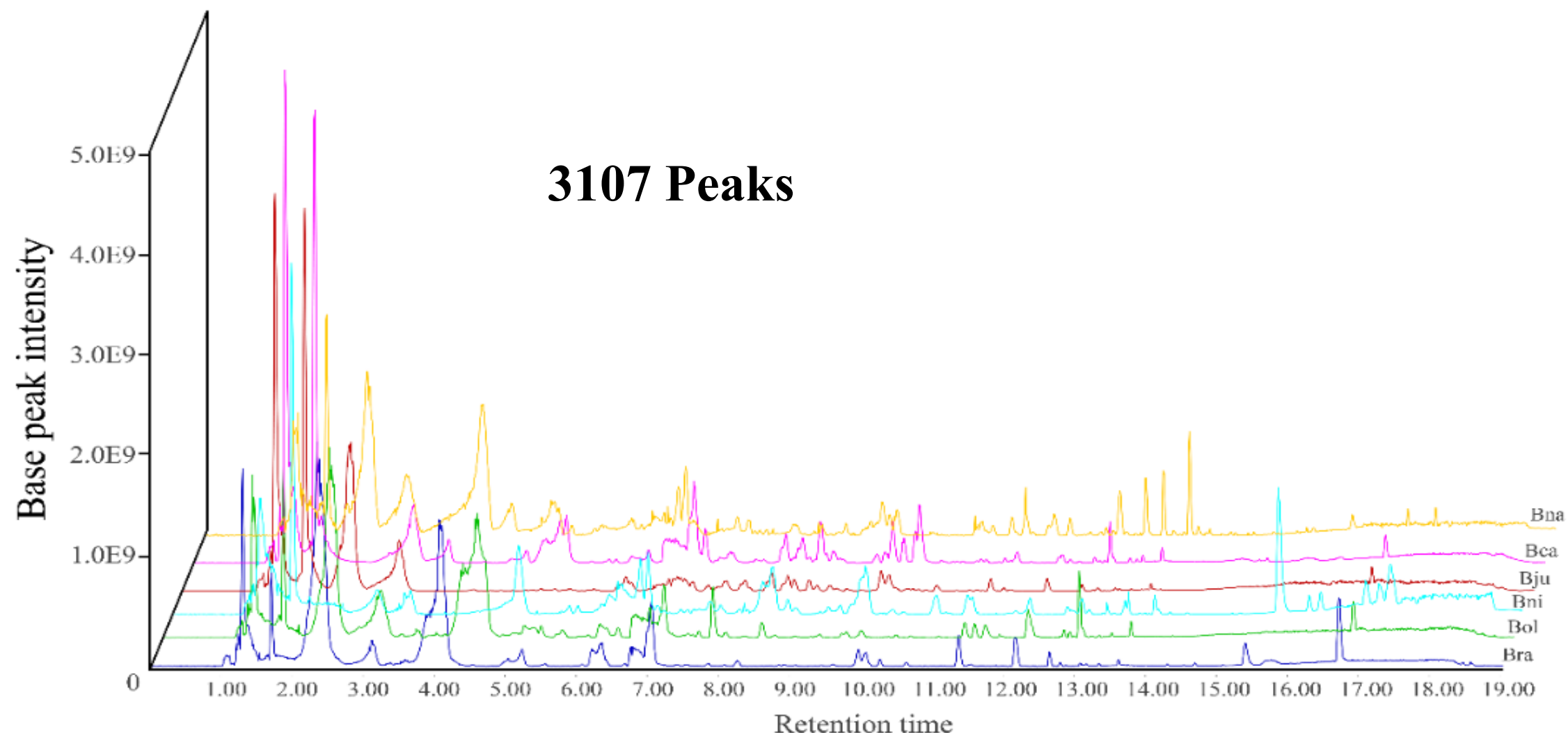
### 3. Metabolites in seed of U-triangle species



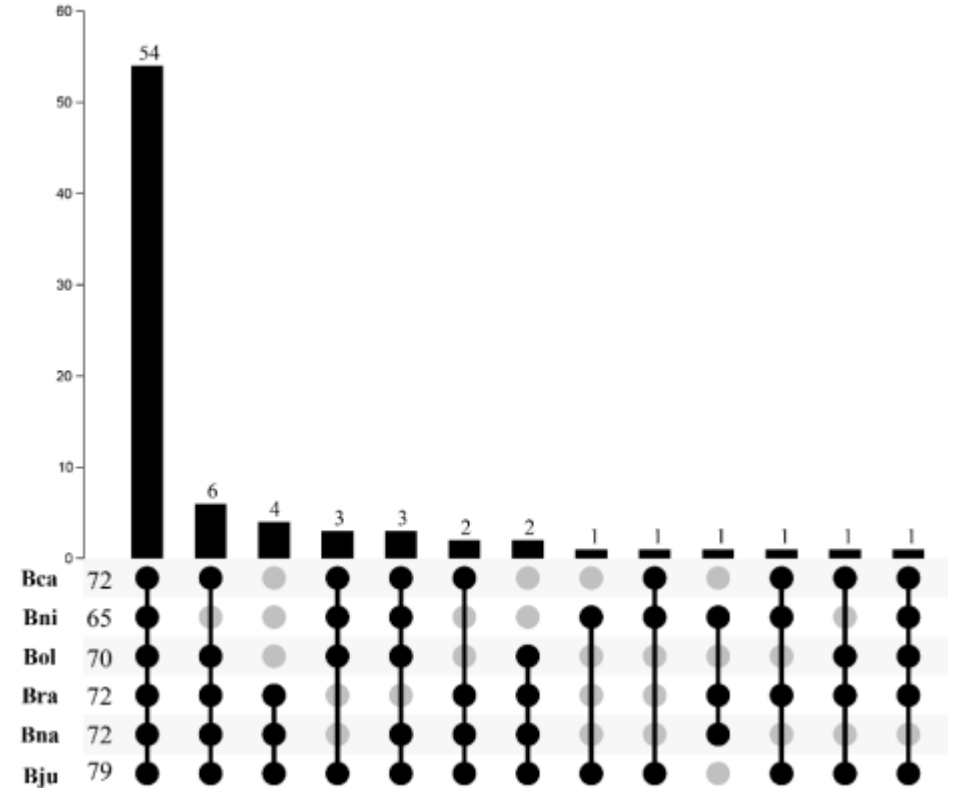
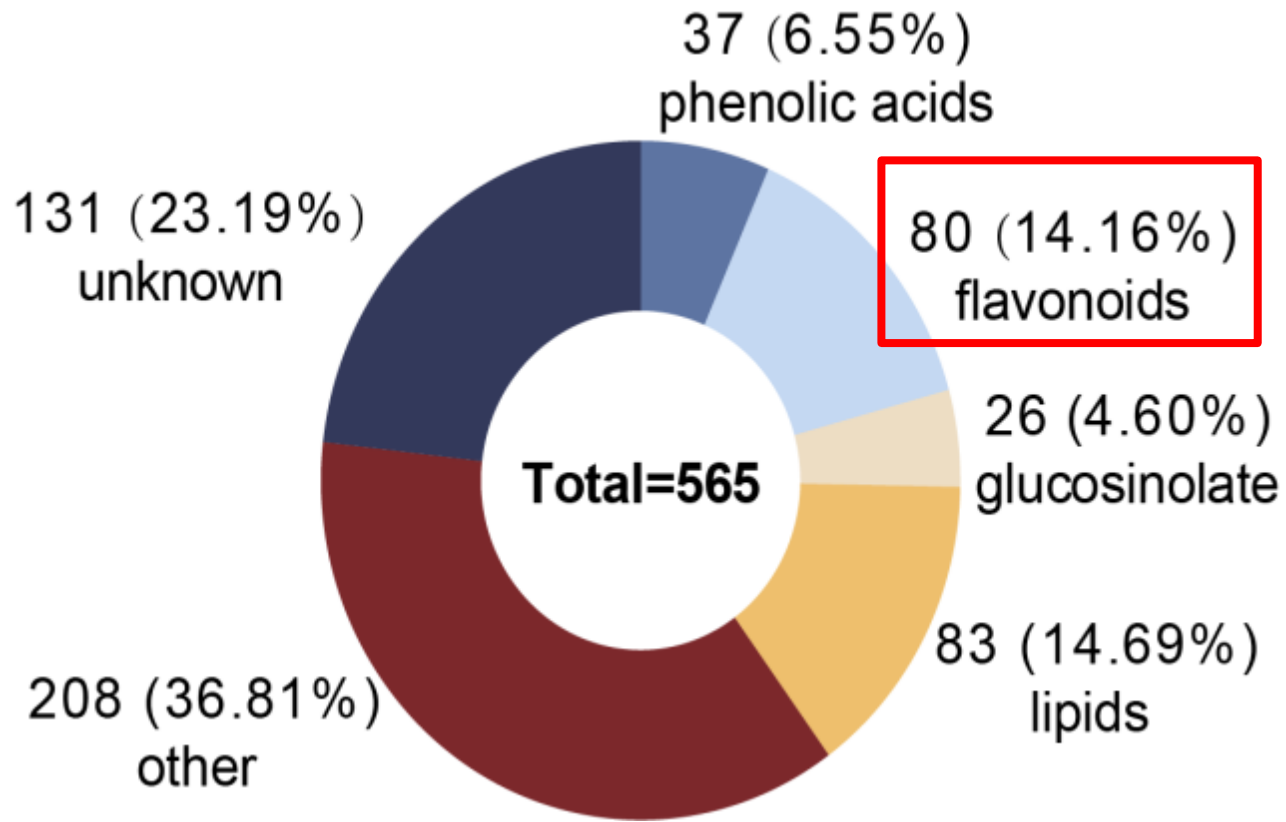
#### U's Triangle

(Nagaharu, The Journal of Japanese Botany, 1935)

### 3. Metabolites in seed of U-triangle species



### 3. Metabolites in seed of U-triangle species

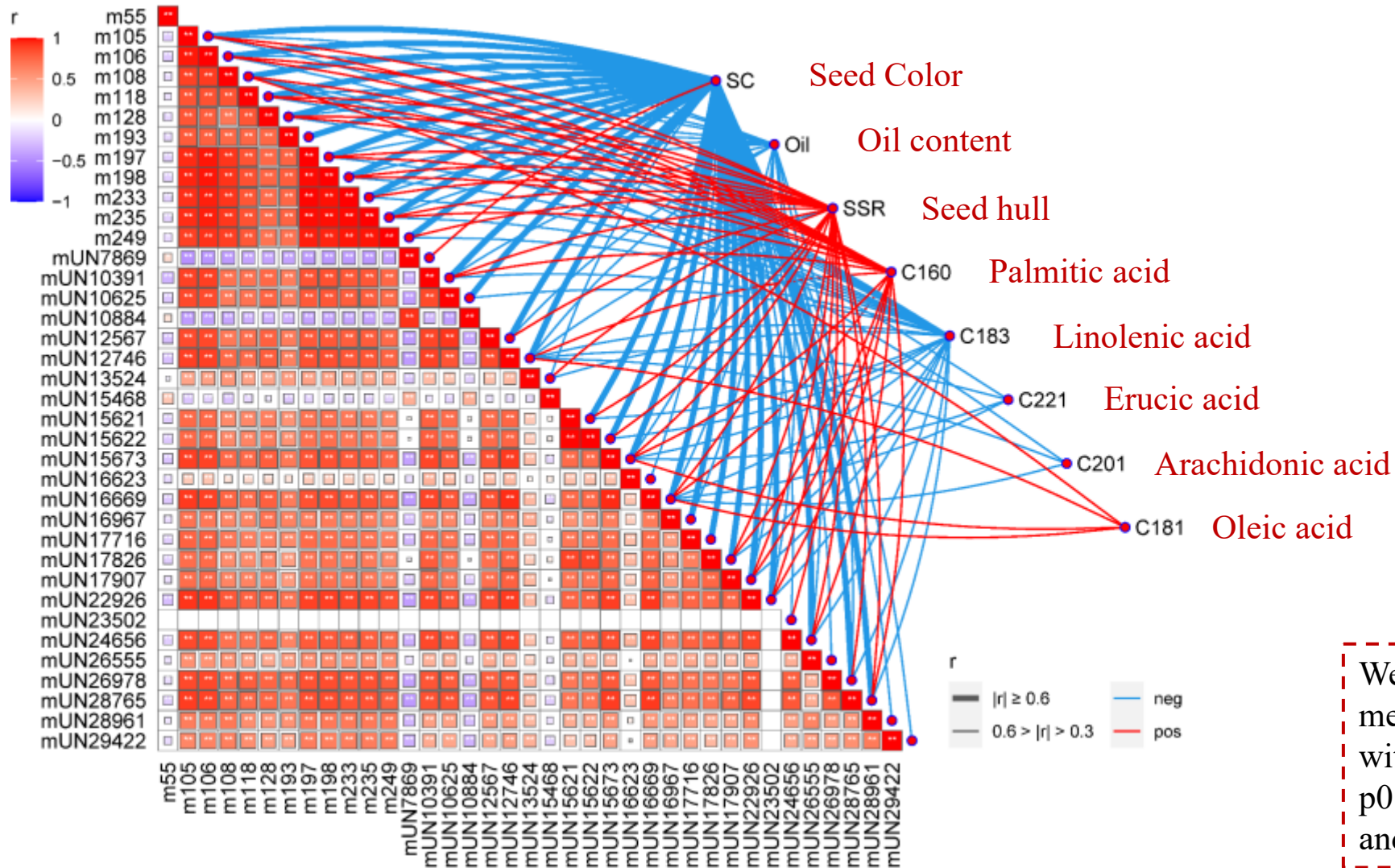


**Flavonoids distribution**

**565/3107, 18.18%**

# 3. Metabolites in seed of U-triangle species

## Analysis of differential metabolites with relative traits

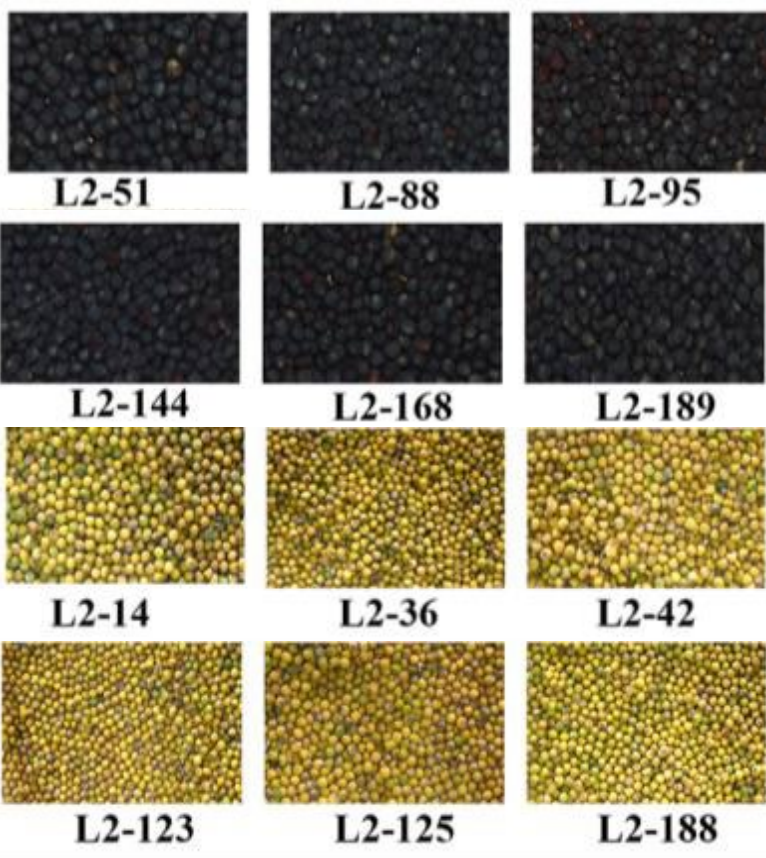


We obtained 27 differential metabolites ( $|r| > 0.6$ ,  $p < 0.001$ ) with high correlation ( $|r| \geq 0.6$ ,  $p < 0.001$ ) with different agronomy and quality traits.

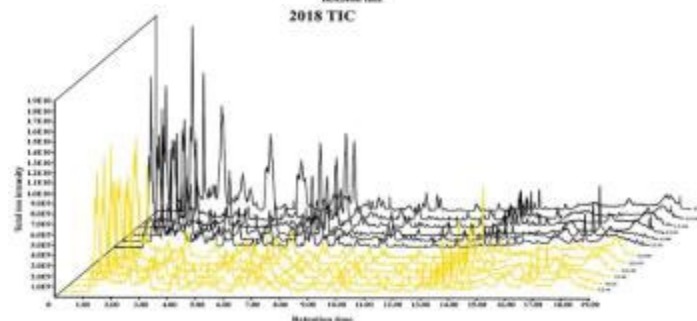
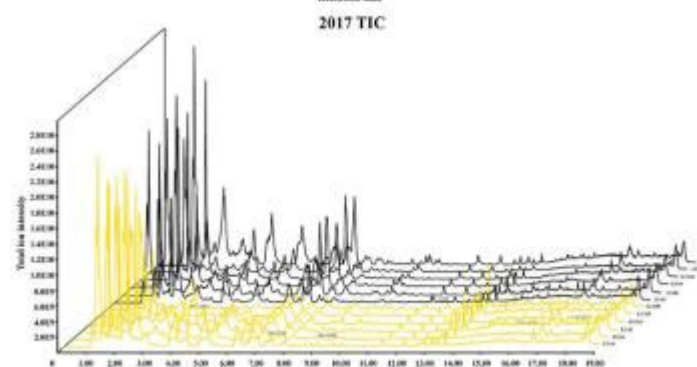
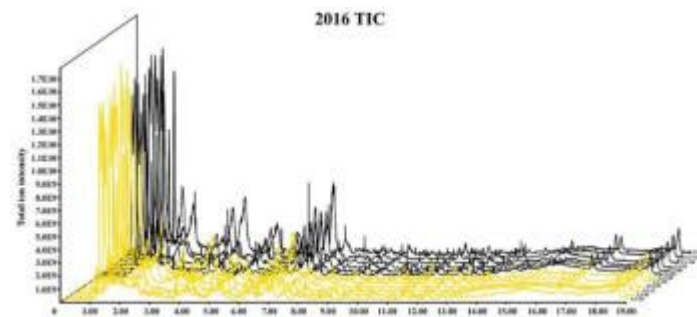
**4**

## **mGWAS and Candidate genes selection**

# 4. mGWAS and Candidate genes selection

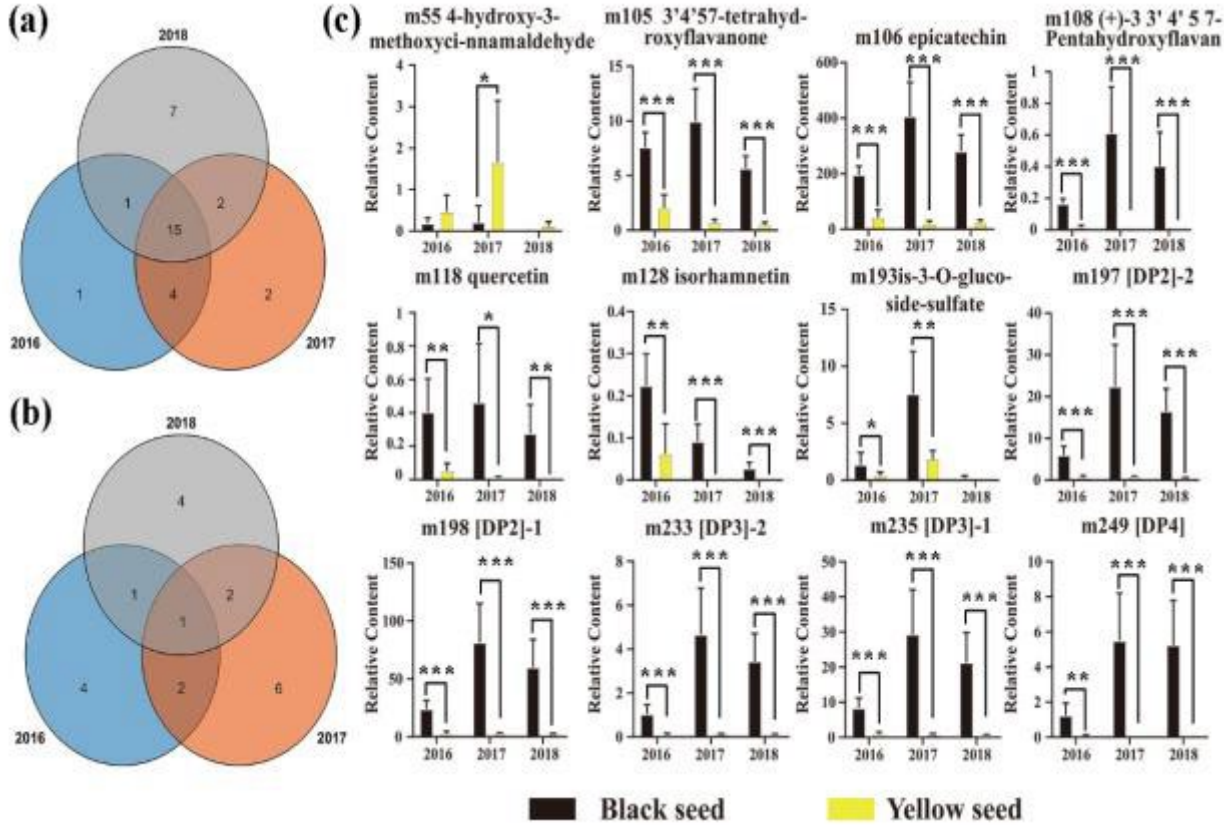


Yellow- and Black-seeded

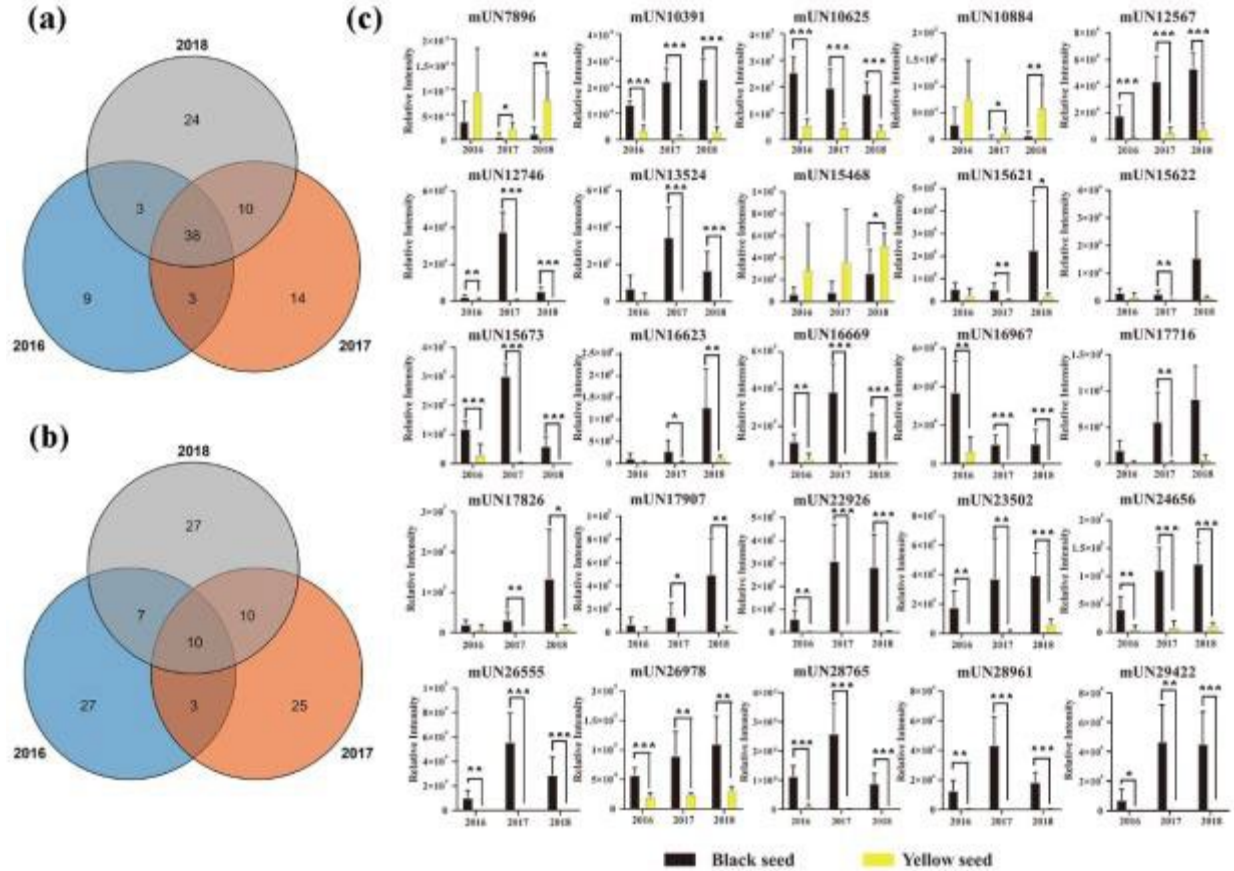


Category		NO.
Known (103)	Epicatechins	18
	Isorhamnetins	12
	Kaempferols	17
	Quercetins	5
	Caffeic acids	4
	p-Coumaric acids	4
	Ferulic acids	3
Phenolic acids (28)	Sinapic acids	17
Glucosinolates		23
Unknown		607
Total		710

# 4. mGWAS and Candidate genes selection



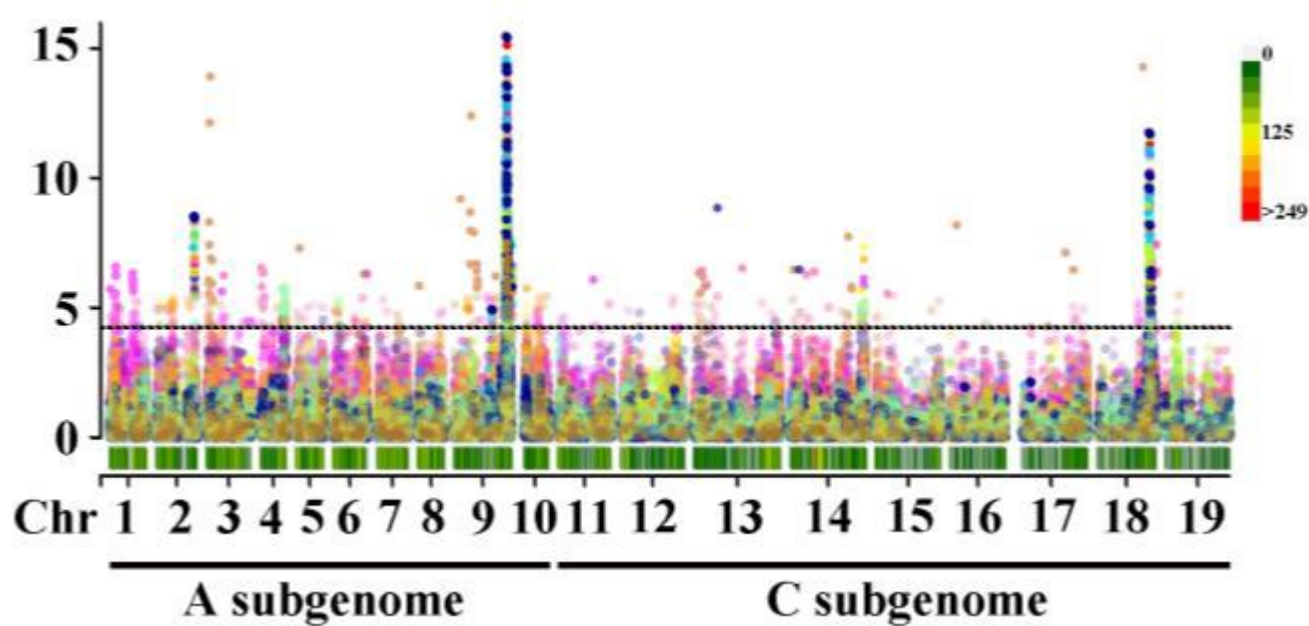
**Known (12)**



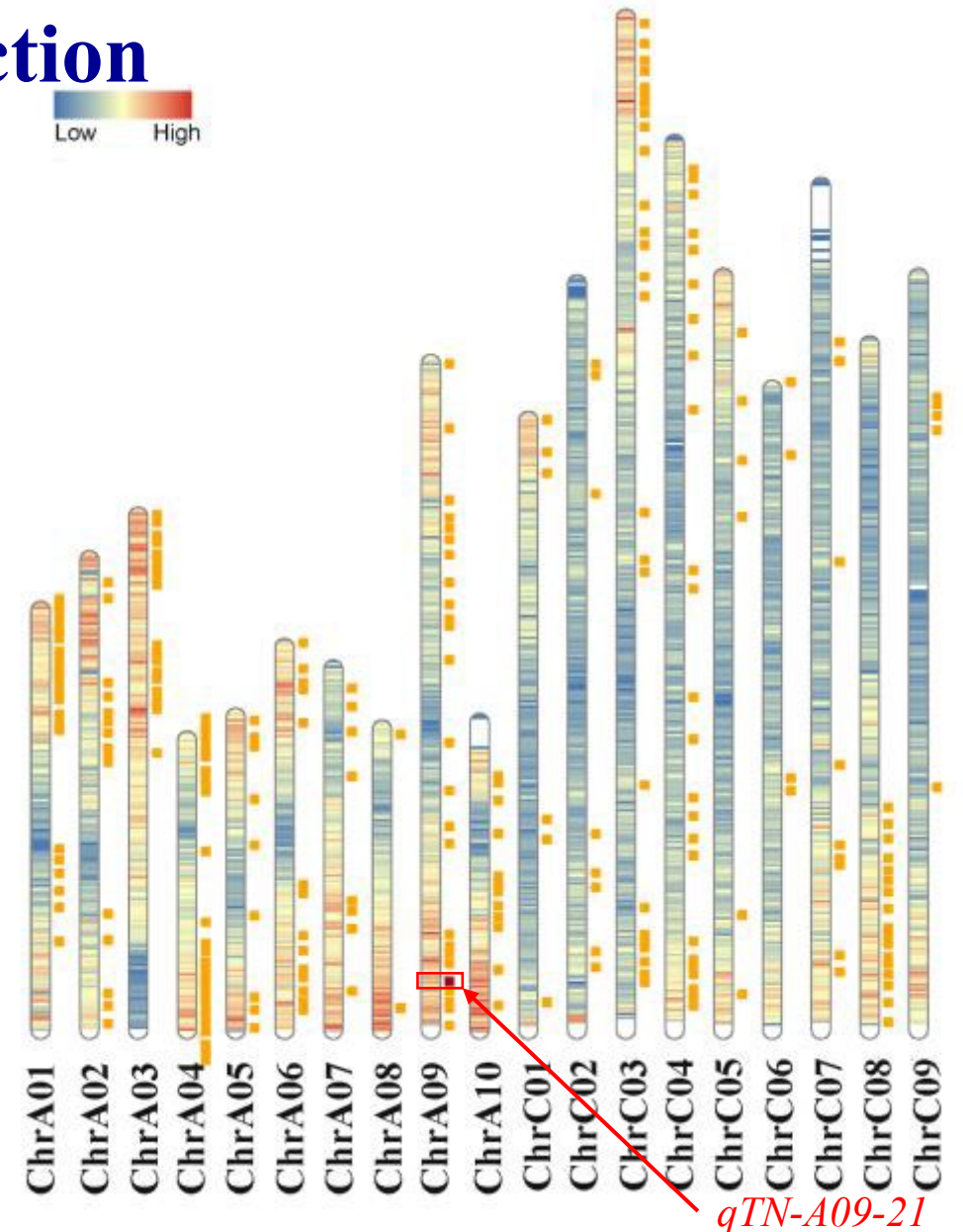
**Unknown (25)**

# 4. mGWAS and Candidate genes selection

mGWAS of the differential metabolites and seed color



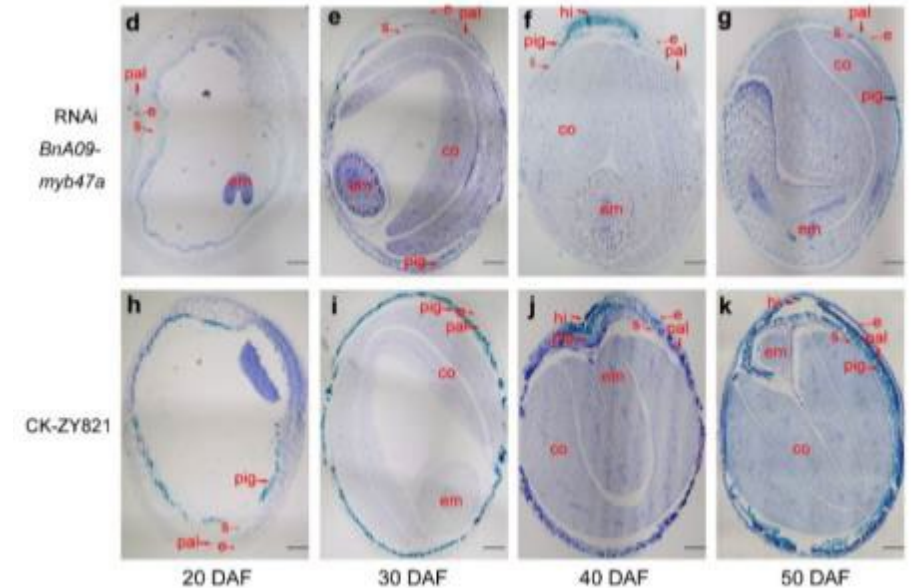
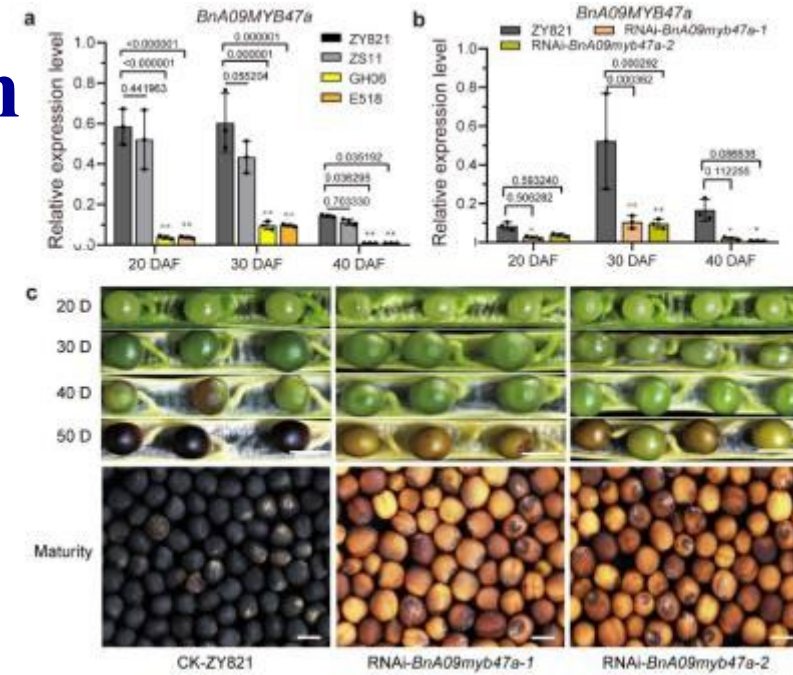
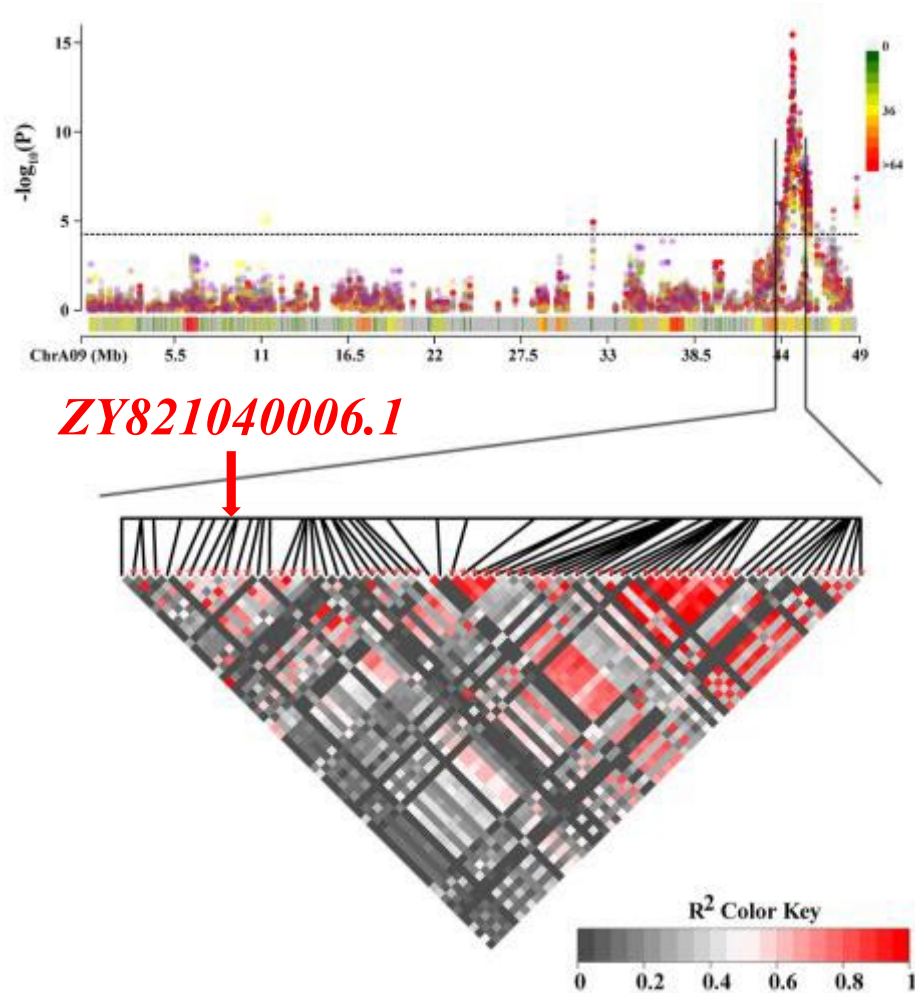
**Manhattan diagram of differential metabolites**



**Candidate intervals distribution diagram**

It was preliminarily determined that *qTN-A09-21* was an important candidate region for regulating the metabolism and synthesis of pigment differences, which was associated with the formation of color differences in *Brassica napus*.

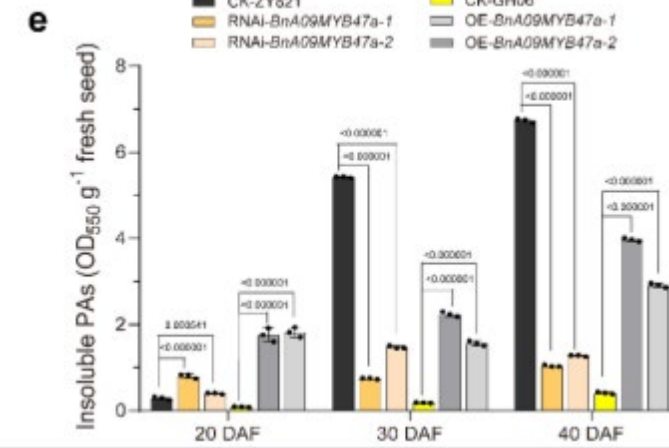
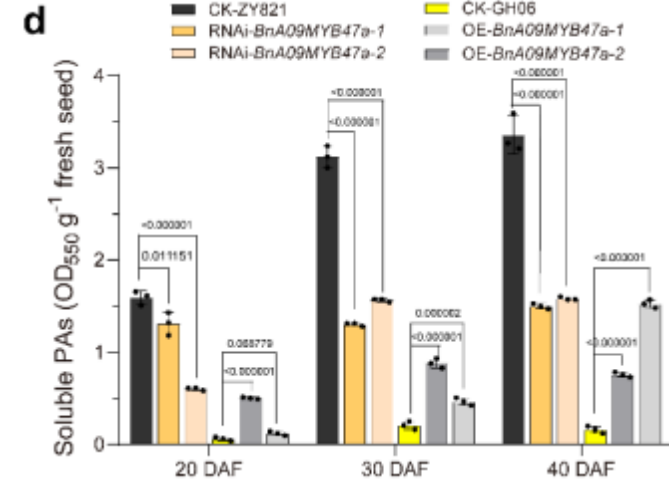
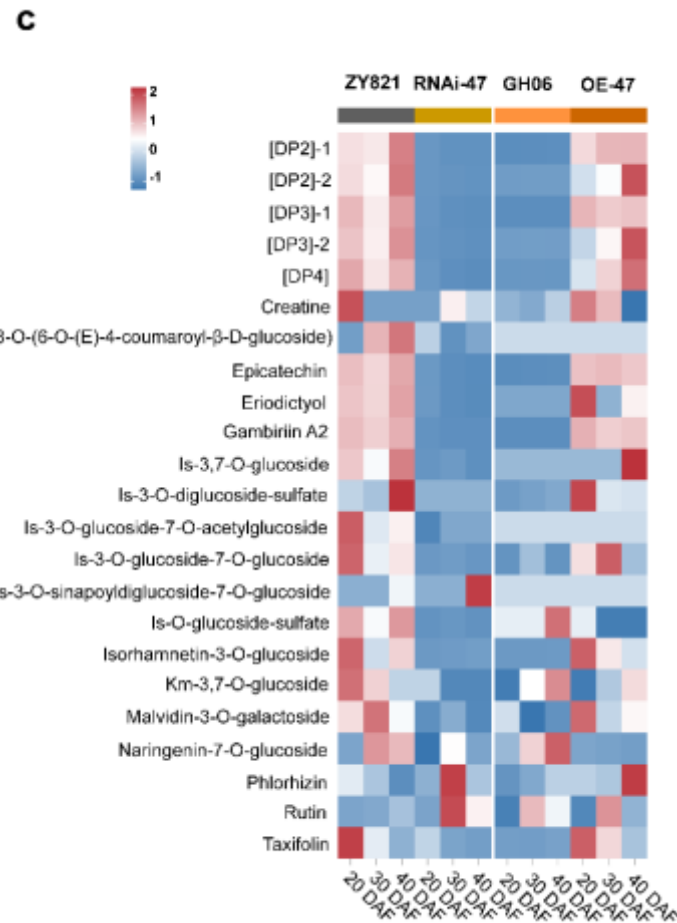
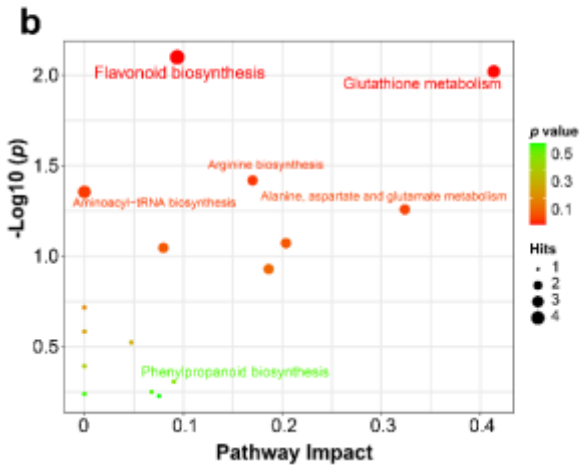
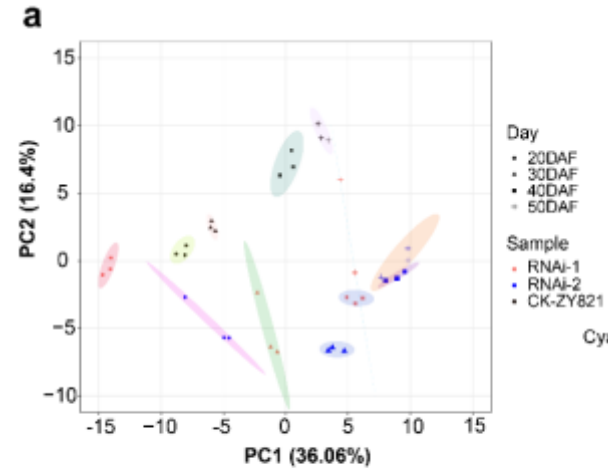
# 4. mGWAS and Candidate genes selection



**BnA09MYB47a is involved in seed color and pigmentations accumulation**

Nature Communications, 2023

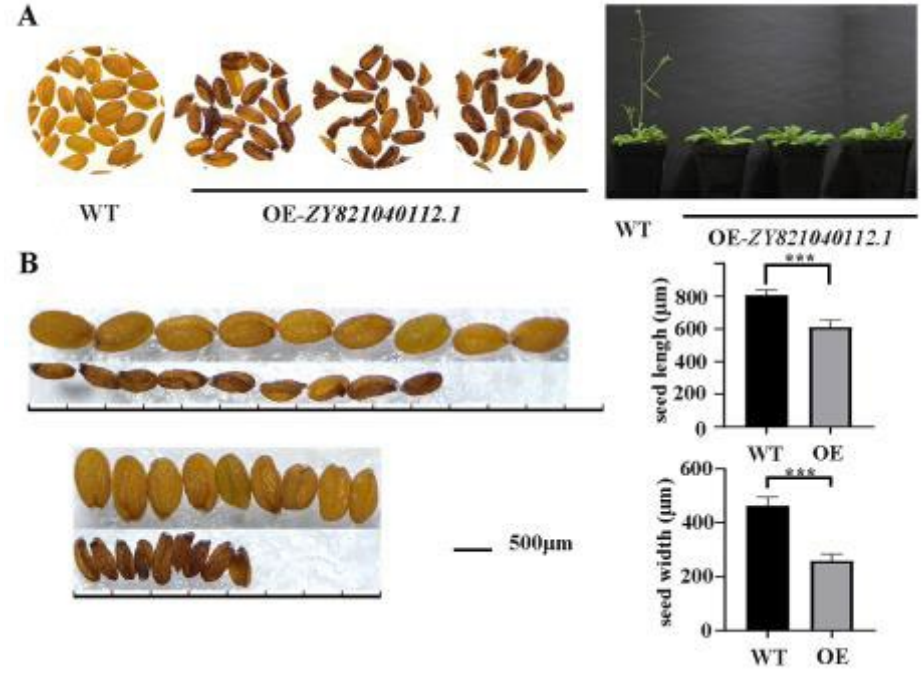
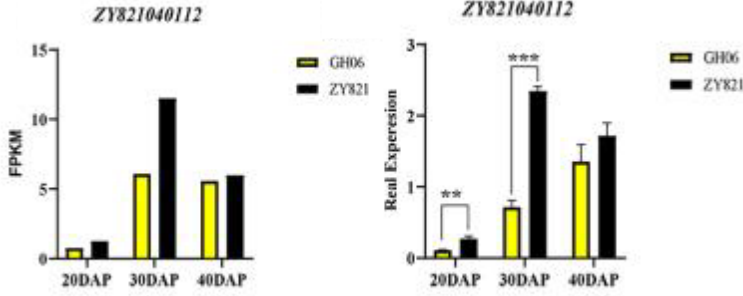
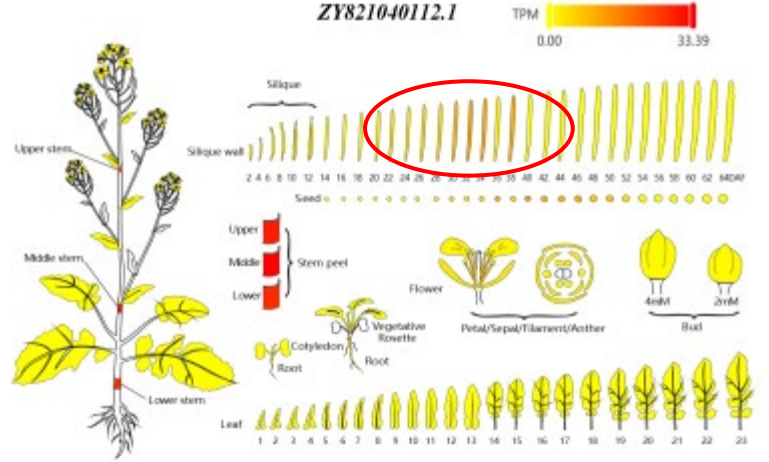
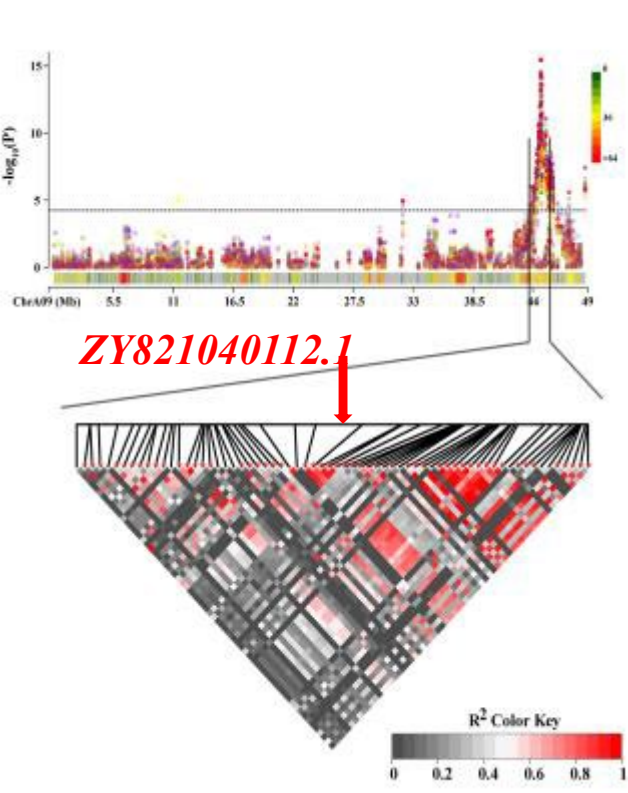
# 4. mGWAS and Candidate genes selection



**BnA09MYB47a affects the accumulation of flavonoid components**



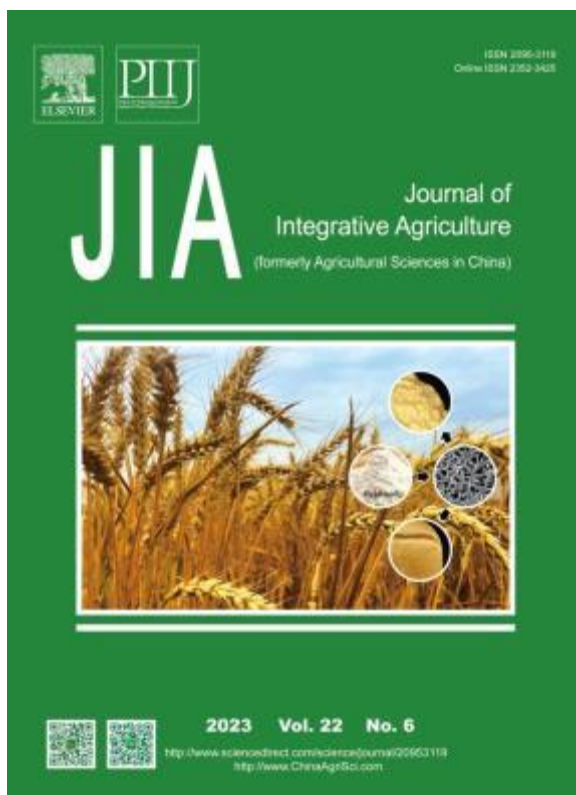
# 4. mGWAS and Candidate genes selection



**Biological functional identification of ZY821040112.1 in *A. thaliana***

# Conclusions

- Developed **DMetFinder V1.0** based on Base peak chromatograms
- Constructed the Metabolites database of seeds of U-triangle species, and identified the differentially metabolites between the yellow- and black-seeded rapeseed.
- Obtained the candidate interval *qTN-A09-21* for controlling seed coat color and pigmentations on chromosome A09, and fine-mapping the seed color genes *ZY821040006.1 (BnA09MYB47a)* and *ZY821040112.1*.



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