

Assessment and quantification of new metabolites in quinoa (*Chenopodium quinoa* Willd.) using UHPLC-Q-Orbitrap mass spectrometer

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INTRODUCTION

- Quinoa (*Chenopodium quinoa* Willd.) is a pseudo-cereal from the Chenopodiaceae family originating in the Andean Mountains of the South America region [1].
- Quinoa possesses excellent nutritional quality and contains numerous secondary metabolites [2].
- The two principal groups of secondary metabolites in quinoa are flavonoids and phenolic acids, both showing many biological activities and health benefits [2].
- The main goal of the study was to analyze the metabolomic profile of selected quinoa genotypes cultivated in the Czech Republic.

METHODOLOGY

- A total of 56 quinoa samples of different seed colors were involved in the study.
- All genotypes were cultivated under the climatic conditions of the Czech Republic at the Crop Research Institute v.v.i., in the year 2021.
- Metabolites were analysed using a UHPLC-Q-Orbitrap high-resolution tandem mass spectrometer [3].
- Obtained data were processed in Xcalibur Quan Browser (Thermo Fisher Scientific).



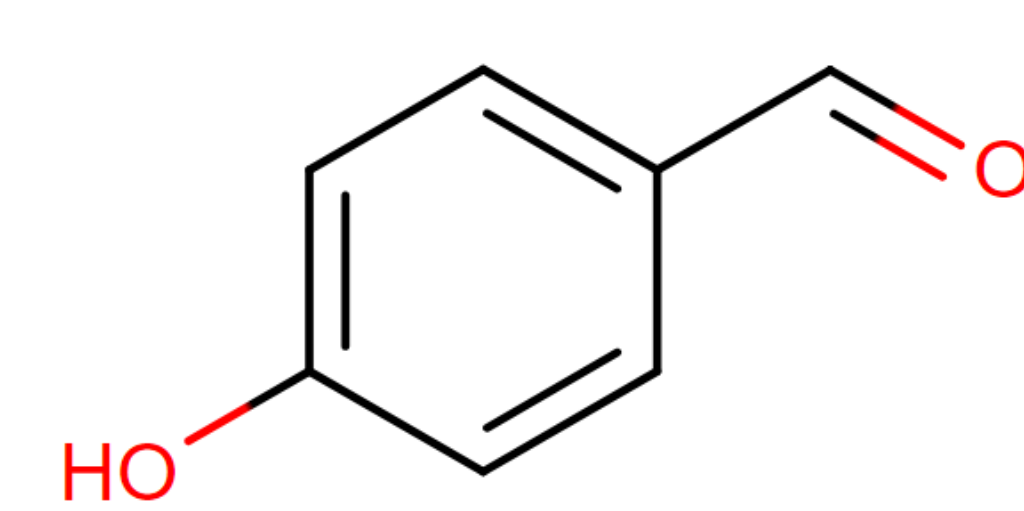
RESULTS

Metabolomic spectrum detected in samples:

- 8 flavonoids: isoquercetin, naringenin, pinocembrin, emodin, isorhamnetin, quercitrin, taxifolin, and vitexin
- 1 phenolic acid: salicylic acid
- 1 phenolic amid: N-feruloyloctopamine
- 1 organooxygen compounds: 4-hydroxybenzaldehyde

2 detected compounds (4-hydroxybenzaldehyde, N-feruloyl octopamine) have not been identified in quinoa, genus *Chenopodium* or family Chenopodiaceae so far.

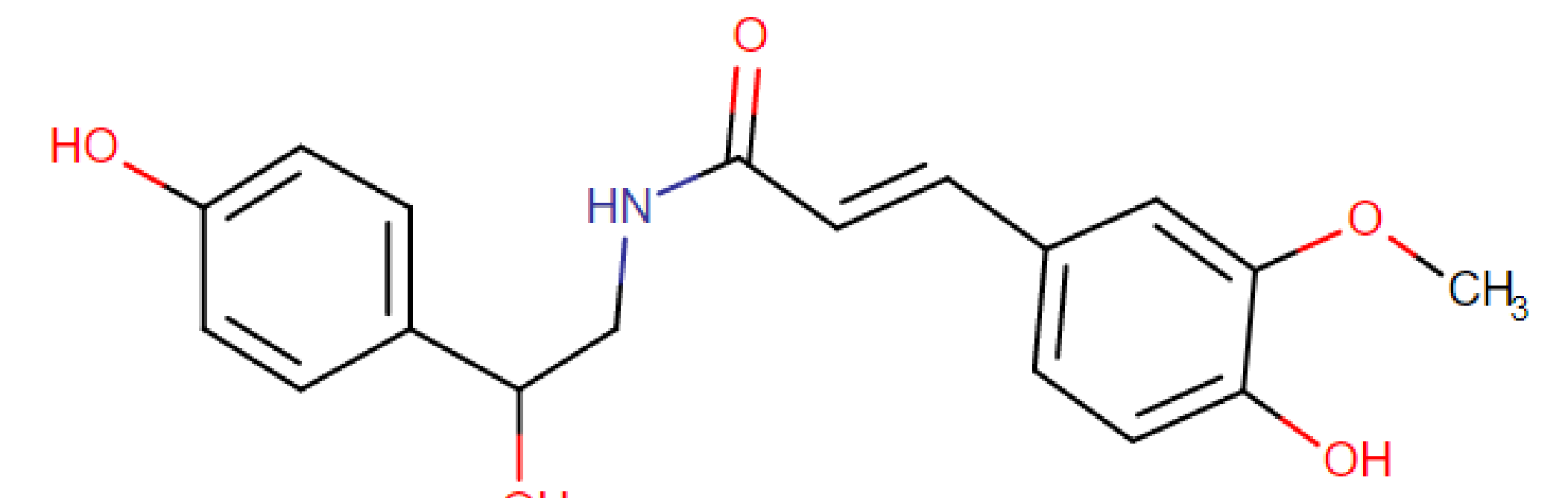
Compounds detected in quinoa for the first time:



4-hydroxybenzaldehyde

Bioactive functions [4–6]:

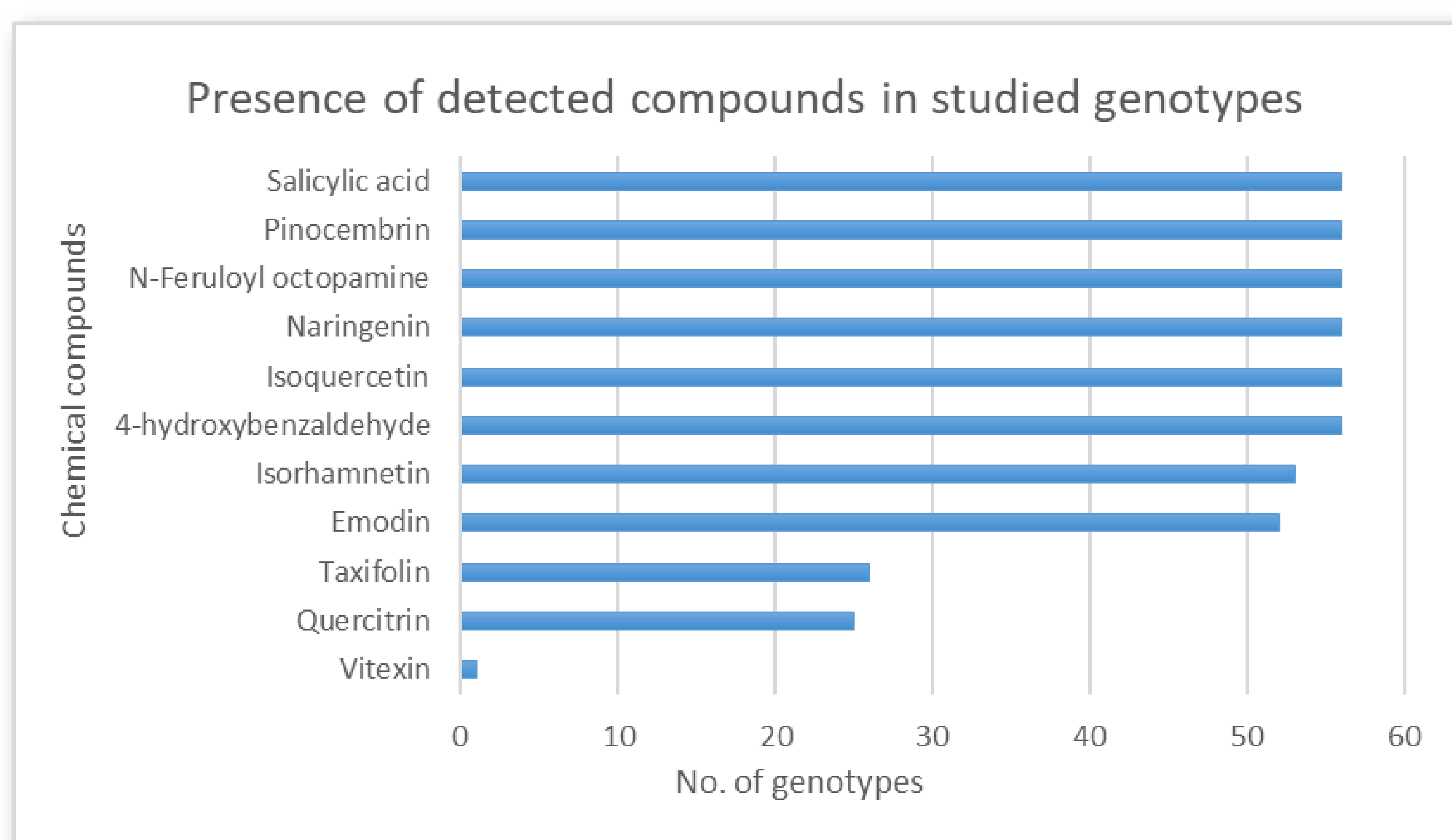
- anti-inflammatory
- anti-angiogenic
- anti-nociceptivem
- wound healing
- reducing insuline resistance



N-feruloyl octopamine

Bioactive functions [7–11]:

- hepatocellular carcinoma treatment
- antifungal activity
- alpha-glucosidase inhibition
- defence mechanisms in plants



Graph 1. Representation of the given chemical substances in the studied genotypes

HIGHLIGHTS

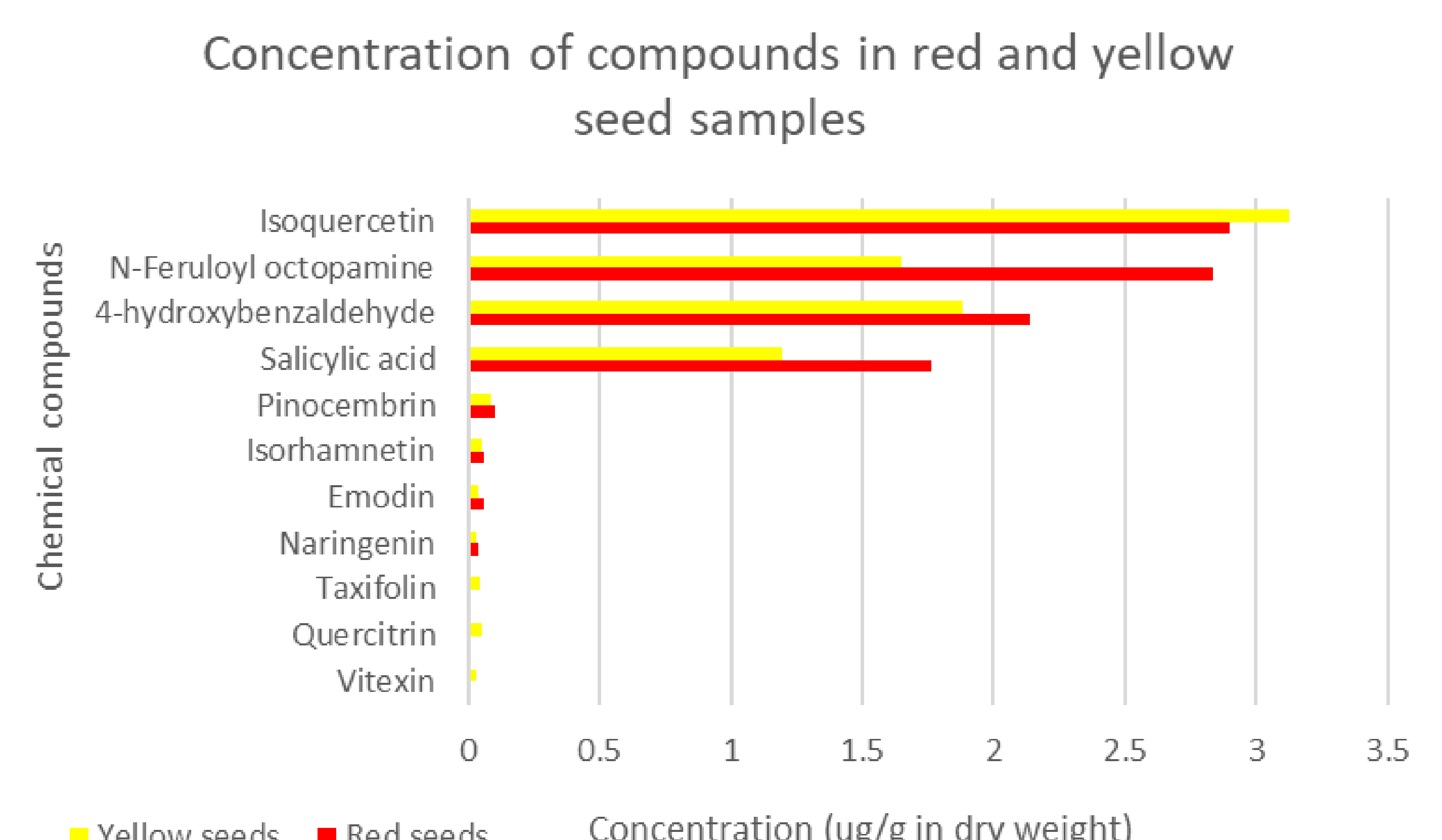
- New metabolites (4-hydroxybenzaldehyde, N-feruloyl octopamine) were identified in quinoa.
- More than half of analysed compounds had higher concentrations in red-seeded samples.
- Isorhamnetin showed the highest concentration among all analysed chemical compounds.
- Quinoa metabolomics is a potential area for further investigations of biologically active compounds.

ACKNOWLEDGEMENT

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RESULTS

- The majority of the studied chemical compounds were present in all analysed genotypes, except for emodin (48 samples), taxifolin (25 samples), quercitrin (25 samples) and vitexin (1 sample) (Graph 1).
- Red-seeded samples possessed higher concentration compared to yellow-seeded samples in following chemical compounds: N-feruloyl octopamine, 4-hydroxybenzaldehyde, salicylic acid, pinocembrin, isorhamnetin, emodin, naringenin (Graph 2).
- Taxifolin, quercitrin, and vitexin were found only in yellow samples.
- Compound with the highest concentration among tested samples:
 - isoquercetin (9.91 µg/g in dry weight, genotype QQ056)
- Compound with the lowest concentration among tested samples:
 - vitexin (0.03 µg/g in dry weight, genotype QQ63)



Graph 2. Comparison of compound concentrations in yellow and red-seeded samples

REFERENCES

