



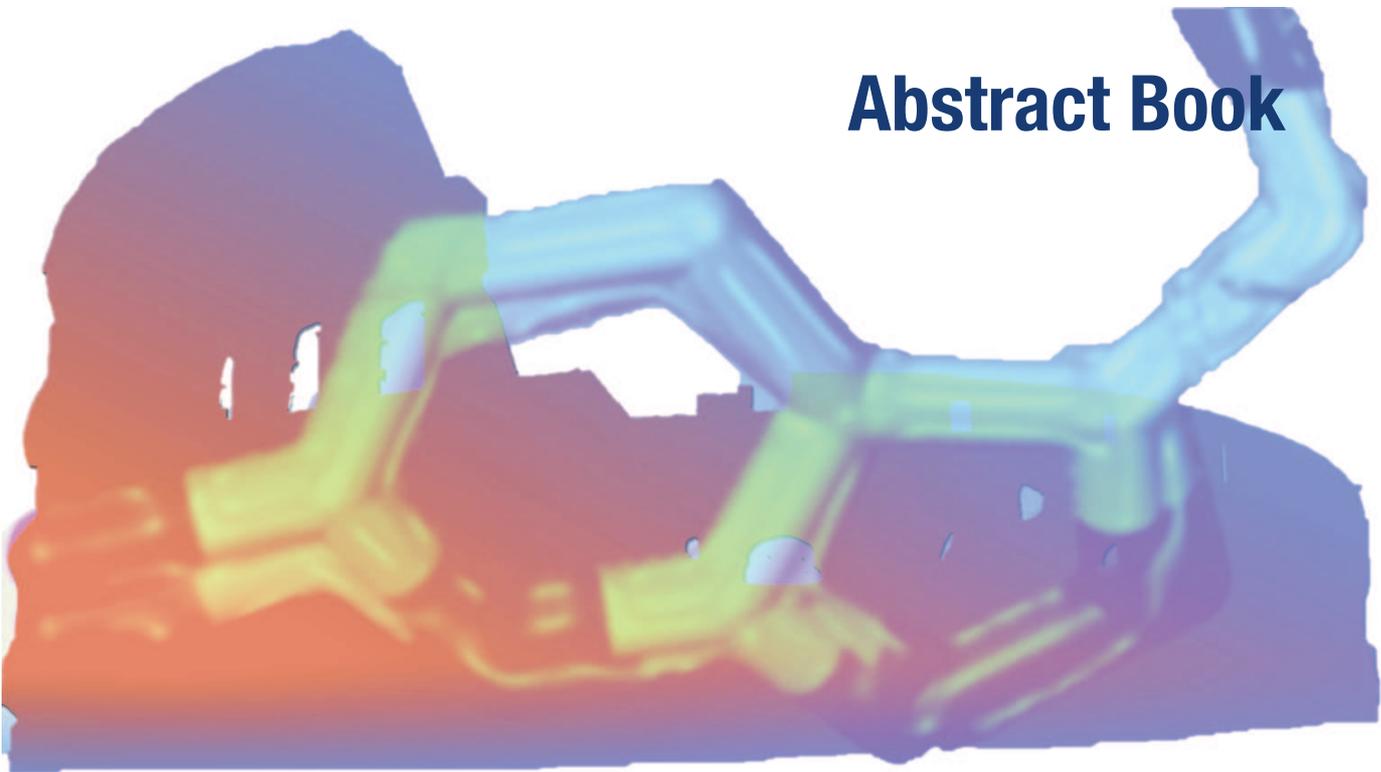
Italian Chemical Society
Division of Medicinal Chemistry

European Federation
for Medicinal Chemistry



XXII National Meeting on Medicinal Chemistry

September 10-13, Roma - Italy



Abstract Book

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APPLICATION OF METABOLOMICS IN THE INVESTIGATION OF THE FATE AND ROLE OF FOOD BIOACTIVE COMPOUNDS

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Mass spectrometry-based metabolomics provides an invaluable tool to identify, measure and interpret the complex time related concentration, activity and flux of exogenous and endogenous metabolites in cells, tissues, biofluids and organs.

One example of such application can be provided by the study of the metabolism and distribution of cyanidin 3-glucoside in mammals combining the results of both targeted and untargeted UPLC-MS experiments. In rats, cyanidin 3-glucoside is rapidly taken up from blood into tissues ($t_{1/2} = 0.36$ min), where they accumulate up to their bioactivity threshold.^[1] Methylation appears faster than other metabolic pathways. Both cyanidin 3-glucoside and its methylated form, peonidin 3-glucoside, can be detected in plasma, kidneys, and liver. Traces of other minor metabolites of cyanidin 3-glucoside (delphinidin 3-glucoside and its methylated forms petunidin and malvidin 3-glucoside) were also observed. The capacity of cyanidin 3-glucoside and their metabolites to affect mammalian metabolism was demonstrated in an investigation of the transient metabolomic changes in the brain and the plasma of adult rats after intravenously administration of cyanidin 3-glucoside. It was shown that cyanidin 3-glucoside alters certain important cellular metabolites, such as bile acids, glutathione, oxidized glutathione, and some lipids in the blood, kidneys, and liver of rats.^[2] Moreover, these results demonstrating the ultra-fast distribution and metabolism of IV-administered anthocyanins in rats suggest that in mammalian plasma the sink could largely exceed the capacity of the source. This raised the question if the fast-changing concentrations of anthocyanins measured in plasma can be at all wise indicators to estimate their putative bioefficacy.^[3]

In some case, the presence in food of a natural phyto-complex of oligomeric structures can be addressed with a combined approach requiring MS-based targeted metabolomics and NMR. We have indeed still a very partial understanding of the presence of some important bioactives in food, as in the case of berry ellagitannins.^[4-6] While the metabolic fate of the ellagitannins in the gut is expected to follow a common mechanism, the precise characterisation of their native structure is important for example in explaining their anti-inflammatory activity at gastric level, which has been only recently investigated.^[7]

References

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