

Αξιοποίηση Φυσικών Αντιοξειδωτικών στην Εκτροφή των Αγροτικών Ζώων για Παραγωγή Προϊόντων Ποιότητας

Γεωπονικό Πανεπιστήμιο Αθηνών

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A comparison study in the processing procedure of data from untargeted metabolomic approaches by UPLC-ESI(-)-HRMS

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ABSTRACT

A comparison study in the processing procedure of data from untargeted metabolomic approaches by UPLC-ESI(-)-HRMS

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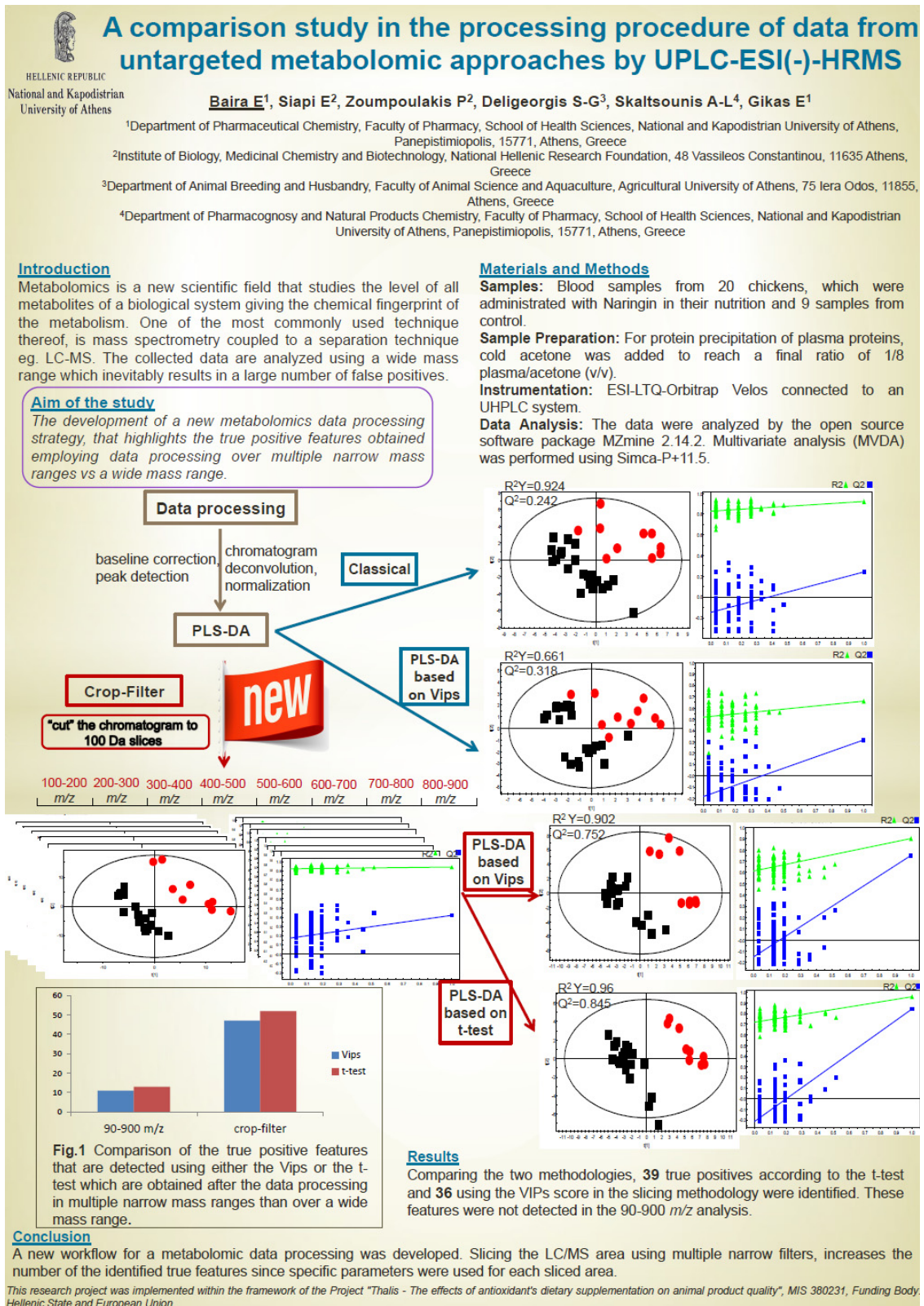
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In the case of the MS-based metabolomics a fundamental problem is the large number of false positives. The aim of this study is to develop a new strategy, which highlights true positives by applying data processing in multiple narrow mass ranges instead over a wide mass range.

Blood samples from 20 chickens, which were administrated with Naringin in their nutrition and 9 samples from control, were analyzed by UPLC-HRMS (Orbitrap Velos).

Two methodologies have been applied for data processing. In the first one (classical approach), all data i.e in the 90-900 m/z were included in the data processing procedure. To the newly developed methodology, the data were shred in 100 Da slices generating 8 datasets, which has been subjected to the downstream MS data processing. Each dataset was treated as separate and mz/t_R features obtained by either the VIP's or the t-test values were used as input for the construction of the general model. Comparing the two methodologies, 34 true positives according to the t-test and 36 using the VIPs score in the slicing methodology were identified. These features were not detected in the 90-900 m/z analysis.

A new workflow for a metabolomic data processing was developed. Slicing the LC/MS area using multiple narrow filters, increases the number of the identified true features since specific parameters were used is for each sliced area.



Η Επιτροπή Πιστοποίησης Παραδοτέων

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