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ABSTRACT SUBMISSION FORM

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Title

Building a Food Intake Biomarkers database for Mass Spectrometry based nutrimetabolomics profiling: A Novel Workflow to Enhanced Nutritional Assessment

Authors

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Summary: *Aging is a natural biological event that has some negative aspects, including the development of frailty. The crucial role of diet in frailty onset is recognized. In this scenario Food-Intake Biomarkers, molecules derived from food intake and metabolisms, may be able to provide objective information on the humans' nutritional status.*

Keywords: *Food-intake biomarkers, Mass spectrometry, Nutrimetabolomics*

Introduction

Frailty is a geriatric syndrome characterized by a decrease in the physiological reserves, leading to higher vulnerability to stressors. Food-intake biomarkers (FIBs) cast light on food metabolism, to establish the association between dietary habits and the risk of developing frailty [1]. The aim of this work is the construction of an *in-house* FIBs database to evaluate the interaction between diet, FIBs, and the development of frailty.

Methods

FIBs database was built by curating and integrating literature-known molecules with established associations to specific foods [1,2] also including phase I and II metabolites.

Monoisotopic masses of each FIBs were queried against three different databases: the Human Metabolome Database (HMDB), FoodDB and Phenol Explorer, obtaining more than 1500 possible FIBs. The database was cleaned and reduced by considering only FIBs with validated MS/MS spectra.

Results

Our *in-house developed* database included 976 FIBs. The database structure was designed to accommodate monoisotopic mass and the most common adducts (+Na, +K), the HMDB ID, the molecular classes, and food species. Table 1 shows the food categories and the number of analytes in each categories that are included in the database. To test the performance of the database we extracted and analysed metabolites from plasma samples of 130 elderly subjects using flow-injection analysis-mass spectrometry (FIA-MS). EASY-FIA [3] was used to pre-process and annotate the obtained data using the *in-house* FIBs database and MS/MS fragmentation patterns were used to confirm the FIBs identity.

Food categories	
Alcoholic beverages (N=39)	Heat-treated foods (N=11)
Artificial Sweeteners (N=12)	Legumes (N=59)
Cereals (N=125)	Meat (N=7)
Citrus fruits (N=38)	Olive oil (N=10)
Coffee, tea (N=21)	Plant foods (329)
Curcuma (N=15)	Preservatives (N=17)
Fish&Seafood (N=4)	Tuber or cereals (N=16)
Fruit (N=74)	Ultra-processed food (N=21)
Fruit&Vegetables (N=128)	Vegetables (N=50)

Table 1: Food categories included into the FIBs database

Conclusions

We developed an *in-house* FIBs database ready-to-use on our free software EASY-FIA, for FIA-MS pre-processing and annotation.

We tested our database on a small population without dietary intervention (130 elderly subjects, 65 Fit and 65 Frail) confirming the presence of 83 plasma FIBs that capture a picture of individual dietary habits.

The FIBs approach must be validated in further Italian Longitudinal cohorts to assess the role of diet in the development of frailty.

References

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