Posters

Grains composition and nutrition online database

M Bellgard[1], H Williams[2], C Smith[1], A Macgregor[1], A Hunter[1], R Appels[1], T Griffiths[3]
[1]*Centre for Bioinformatics and Biological Computing, Murdoch University, Perth, WA 6150,*
[2]*School of Public Health, Curtin University of Technology, Perth WA,* [3]*BRI Australia, Sydney, NSW 2113*

Background - Data on the nutrient content and composition of grains, relevant to human nutrition, are scattered throughout the literature or in some cases may not exist at all. In other cases data may be found in databases compiled specifically for feed grain purposes and information that is relevant to human nutrition is difficult to identify. Scientists in this field do not have information integrated into an efficient/well authenticated web-based system and lack of accessibility significantly reduces the value of the publicly available information.[1]
Objectives - To compile, from public resources, a database profiling the composition and nutrient content of cereal grains and pulses for application to food production for human consumption. An essential part of this GrainFoods Cooperative Research Centre funded project is the presentation of the database in a "user-friendly" searchable interface that enables efficient web-based access to information and incorporates visualisation and analytic tools. In addition, the project will identify 'gaps' in the data and where the addition of information on grains, pulses or specific nutrients needs to be generated.
Design - An initial prototype database was established using information from a pilot study. Subsequently new prototype databases were generated with data sourced from a wide range of literature and datasets compiled in various formats. Archival information was scanned and edited for the electronic database. Tables of data were identified, critical summaries included and statistical analyses verified. A dictionary and language has been established for the database to allow meaningful queries and answers to be developed by industry users. A particular focus is to ensure the origins and descriptions of the data in the database are well defined. Prototype databases and interrogation systems are currently regularly updated and available for industry colleagues to test, criticise and send-back for revision.
Outcomes - A secure, web-based, fully searchable grains nutrition database has been developed. It has a web-based up-load facility, End-note based referencing system and graphical visualisation of nutrient/composition data.
Conclusion - The database allows immediate access to up-to-date nutrient data on grains and provides the ability to share confidential data in a secure environment.
References

1. Burlingame B. Fostering quality data in food composition databases: visions for the future. J Food Comp Analysis 2004; 17: 251-258.

A sensitive and selective method for quantification of natural folates in foods using electrospray tandem MS

S Vishnumohan[1], R Pickford[2], G Smythe[2], J Arcot[1]
[1]*Food Science and Technology, School of Chemical Engineering and Industrial Chemistry, University of New South Wales, Sydney 2052, Australia;*
[2] *Bioanalytical Mass Spectrometry Facility, University of New South Wales, Sydney 2052, Australia*

Background - In the present scenario of folate fortification there is an underestimation of the amounts actually present in foods and declared on labels, due to the lack of a robust analytical method to distinguish between the added and natural forms of folates. This is vital when the public derives its folate not only from the synthetic folic acid but also from the natural forms present in food as they have been proven to differ in stability and bioavailability.
Objective - The project aim was to develop and optimise a sensitive and robust method for quantifying folate vitamers in foods using electrospray ionization tandem MS and to evaluate MS compatible clean up procedures currently used in the purification of food samples.
Design - Liquid chromatography-tandem mass spectrometry (LC-MS/MS) was used as a sensitive and specific analytical tool capable of discriminating between the different vitamers and quantifying them accurately. LC was performed on a C18 reverse phase column with a binary gradient of aqueous formic acid and acetonitrile. The LC was interfaced to an ion trap mass spectrometer using positive mode electrospray ionisation. Folate vitamers are recognised by their individual *m/z* values, or specific fragment ions when using tandem mass spectrometry. Quantification of folates was performed using external and internal standards.
Outcome - Separation and identification of folate vitamers using a fast LC-MS method and confirmation on the specificity using Selected Reaction Monitoring (SRM) on MS/MS mode which identifies structurally diagnostic unique fragments were achieved. Ongoing validation of this method using commercially available folate standards and SPE-SAX purification, which has been proven effective for folate standards, helped to protect the mass spectrometer from the buffer ions which might otherwise contaminate the instrument and cause signal suppression. It was also found that ascorbic acid used as the main anti-oxidant in the sodium acetate buffer as the eluting solution, was capable of being fragmented and it interfered with the peak resolution. This is a major finding as ascorbic acid is the most commonly used anti-oxidant for folate analysis.
Conclusion - LC-MS/MS successfully separated and quantified folates in food samples.