

# The Fragment

Jan 2015

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On behalf of the committee of the IMSS I am very pleased to bring you the first edition of our newsletter 'The Fragment'. The objective of the IMSS is to provide a forum for practitioners of Mass Spectrometry. To do this, a meeting of the IMSS is held each year. This year's meeting will be held on Wednesday the 13<sup>th</sup> of May in the Moran Red Cow Hotel, Dublin.

The purpose of this newsletter is to highlight new developments or interesting applications of Mass Spectrometry to the membership of the IMSS. We also maintain an up to date website ([www.imss.ie](http://www.imss.ie)) which provides contact information of the IMSS, details on committee membership, meeting information and links to areas of interest for users of mass spectrometry. All of this takes a lot of effort and I would like to thank all those involved in the IMSS (past and present) who have kept and continue to keep the society and its activities going. I hope you enjoy the newsletter and if you would like to contribute please contact us at [contact@imss.ie](mailto:contact@imss.ie). We look forward to seeing you all in May.



Richie Maguire - IMSS Chairperson

## The Rosetta Mission and GC-MS Dr R. Maguire

On the 12<sup>th</sup> of November, 2014 a huge event occurred some 50 million miles from earth...a probe which had taken off from French Guyana in 2004 landed on comet 67P. While this event alone is fascinating, it is all the more intriguing to anyone with an interest in mass spectrometry as there was a GC-MS on-board.

The Rosetta mission, (named after the famous Rosetta Stone discovered and deciphered in part in 1799) concerns a robotic probe built and launched by the European Space Agency. Along with Philae, its lander module, Rosetta is performing a detailed study of comet 67P. The Philae lander is comprised of 9 separate experiments and one of these 'MODULUS Ptolemy' is concerned with the precise measurement of stable isotope ratios of light elements H, C, N and O in their various forms



Figure 1: The Philae Lander consisting of a baseplate, an instrument platform, and a polygonal sandwich construction. The lander carries ten instruments, with a total mass of about 21 kilograms.

## Dates for the Diary 2015

- Abstract close for IMSS annual meeting 2015, 28th Feb 2015. Email to [contact@imss.ie](mailto:contact@imss.ie)
- IMSS annual meeting 13th May 2015, Red Cow Moran's hotel, Dublin
- ASMS annual conference, 31st May - 4th June 2015, St. Louis, MO
- BSPR 2015 Meeting, 20th - 22nd July 2015, University of Reading, UK
- BMSS Annual meeting, 15th - 17th Sept 2015, University of Birmingham

## IMSS Committee 2015

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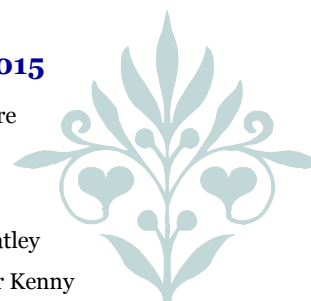
Communications - Brian Flatley

IMSF Representative - Peter Kenny

Committee Members

Stephen McClean, Steve Pennington, Gwen Manning, Patrick Ward, Mike Kinsella and Claire Tonry

Newsletter Editors: Brian Flatley and Richie Maguire



within material sampled from the comet subsurface, surface and near surface atmosphere.

The aim of the project is to determine the degree of isotopic enrichment (or depletion) of D (i.e., <sup>2</sup>H), <sup>13</sup>C, <sup>15</sup>N, <sup>17</sup>O and <sup>18</sup>O in cometary samples relative to specified standard reference materials. The idea for this experiment came from Prof Colin Pillinger and the project lead for Ptolemy is Prof. Ian Wright from the Open University.

The mass spectrometer is an ion trap; a type of analyser not normally associated with isotope ratio measurements but the reason for its inclusion is understandable given the size and weight limitations. This is no ordinary ion trap, as conventional systems were found to be unsuitable and so specific software and hardware had

to be developed and validated to ensure the mass accuracy and measurement precision required for the intended experiments. An advantage of mass spectrometry in space is that the working pressures required are ambient so there is no need for a vacuum system. In addition to the ion trap there are 3 GC columns, a Helium/Argon gas supply, a H<sub>2</sub> gas supply and also small bore chemical reactors pre-column with roles such as drying, protonation and fluoridation, necessary for the various experiments planned.

A drill (20cm depth) on board Philae will be used to take solid samples which will enter an oven, which is vented and then various temperature programmes will be executed before introduction of the gases into the GC-MS.

After 20 years of planning, building, launching and orbiting Philae made a soft landing on 67P, unfortunately it landed in

shadow and as result its batteries are not currently being charged by the solar panels incorporated into the system. It is hoped in 2015 that the lander will reawaken as the comet re-orientates relative to the sun. Please see references and links below for further information on this project.

### References

Chapter 9 'An Ion Trap too far? The Rosetta Mission to characterise a comet' from March, R.E.; Todd, J.F.J. 'Quadrupole Ion Trap Mass Spectrometry', 2<sup>nd</sup> Edition, Wiley, Hoboken, NJ, USA, 2005

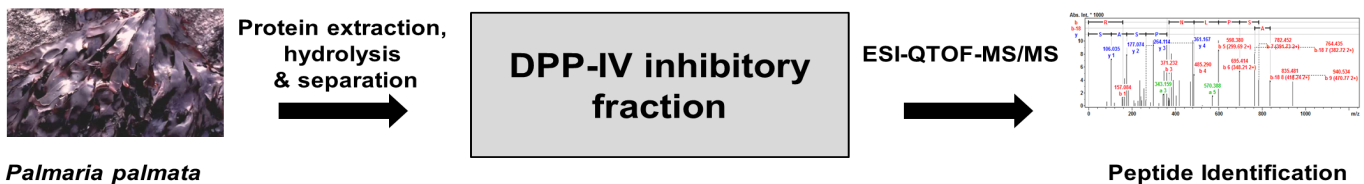
[www.bmss.org.uk/news2.shtml](http://www.bmss.org.uk/news2.shtml)

[http://en.wikipedia.org/wiki/Rosetta\\_%28spacecraft%29](http://en.wikipedia.org/wiki/Rosetta_%28spacecraft%29)

[http://www.esa.int/Our\\_Activities/Space\\_Science/Rosetta/](http://www.esa.int/Our_Activities/Space_Science/Rosetta/)

**Publication Focus: Dr M. O'Keeffe**

## Mass spectrometry identification of health promoting peptides



*Palmaria palmata*

Figure 2: Outline of the workflow approach taken by researchers in the Proteins and Peptides Research Group at the University of Limerick to identify novel DPP-IV inhibitory peptides from the macroalga, *Palmaria palmate*.

Diabetes mellitus is a leading public health problem in the industrialised world with approximately 347 million people affected worldwide currently. Potential strategies for the control of Type 2 diabetes (which accounts for ~ 90% of all diabetes cases) include diets rich in food-protein derived peptides, more specifically dipeptidyl peptidase (DPP)-IV inhibitory peptides.

A recent paper in *Food Chemistry* (Harnedy, O'Keeffe & FitzGerald, 2015) by researchers in the Proteins and Peptides Research Group at the University of Limerick has described the use of ESI-QTOF-MS combined with bioinformatic approaches to identify novel DPP-IV inhibitory peptides from the macroalga, *Palmaria palmata*. Limited sequence information is available for *P. palmata*, leading the team to take a *de novo* sequencing approach for peptide identification. PEAKS Studio 6.0 (Bioinformatics Solutions Inc., Waterloo, Canada) along with Data Analysis, Biotools and Sequence Editor software (Bruker Daltonics, Bremen, Germany) were used in combination with sequence homology with other macro- and micro-algal protein sequences to identify 13 peptides within a DPP-IV inhibitory fraction of a *P. palmata* enzymatic hydrolysate. These included 3 novel DPP-IV inhibitory peptide sequences.

The approach employed may be applied to the identification of peptides within complex mixtures where there is a deficit in knowledge of the primary sequence. The UL team have recently used similar approaches to identify bioactive peptides derived from milk (Norris *et al.*, 2014), Alaska Pollock skin collagen (Guo *et al.*, 2015), barley (Connolly *et al.*, accepted) and Thai

traditional fermented shrimp paste (Kleekayai *et al.*, accepted) samples.

### References:

Connolly, A., *et al.* (accepted). Generation and identification of angiotensin converting enzyme (ACE) inhibitory peptides from a brewers' spent grain protein isolate. *Food Chemistry*.

Guo, L., *et al.* (2015). Fractionation and identification of Alaska pollock skin collagen-derived mineral chelating peptides. *Food Chem*, 173, 536-542.

Harnedy, P. A., *et al.* (2015). Purification and identification of dipeptidyl peptidase (DPP) IV inhibitory peptides from the macroalga *Palmaria palmata*. *Food Chemistry*, 172(0), 400-406.

Kleekayai, T., *et al.* (accepted). Extraction of antioxidant and ACE inhibitory peptides from Thai traditional fermented shrimp pastes. *Food Chemistry*.

Norris, R., *et al.* (2014). Characterisation of the hydrolytic specificity of *Aspergillus niger* derived prolyl endoproteinase on bovine  $\beta$ -casein and determination of ACE inhibitory activity. *Food Chemistry*, 156, 29-36.

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