Società Chimica Italiana
DIVISIONE DI SPETTROMETRIA DI MASSA
http://www.spettrometriadimassa.it

DSM Speciale GIOVANI:
lavori in corso ....

Posizioni aperte riguardanti la spettrometria di massa

1) PhD Studentship – Predicting MS/MS Fragmentation using Density Function Theory Calculations

Application Deadline: 15th June 2015

One of the BBSRC strategic priorities is “Data driven Biology”, focusing on research that will yield new ways of working through the initiation, or further development of, new computational technologies, methodologies and tools to extract value and generate new biological understanding from bioscience data now available. This proposal meets that challenge by applying minimum energy calculations (using Density Function Theory) to the identification of agrochemical metabolites in complex matrices.
The separation and identification of metabolites is performed by liquid chromatography-MS which produces protonated molecules, and then fragmentation of those ions and analysis of the fragments to deduce the original structure; termed tandem MS experiments. However, this process relies on expert spectrometrists to interpret these data and deduce what the original structures might have been. This is often a lengthy process and results in several potential structures being postulated. There is no automated means to speed up this process or to rank the postulated structures so that we can have high confidence in synthesising the correct molecule. The only route to improved certainty is to purify enough material for analysis by nuclear magnetic resonance spectroscopy (NMR), or to synthesise all the proposed structures, both of which can take weeks to months depending on complexity. Ideally what is required is a better tool to utilize the existing MS/MS data in predicting the most likely structure.

Density Functional Theory (DFT) is now widely used within chemical research. DFT calculations can help interpretation and understanding of MS/MS fragmentation by calculating the structures and electron

densities of species before and after protonation and fragmentation. However commercial software packages do not yet include such calculations (e.g. High Chem -Mass Frontier, ACD)

The application of DFT to aid prediction of tandem MS data has been successfully previously applied to several pharmaceutical standards and their MS/MS spectra. This project will apply these proven approaches to the identification of agrochemical metabolites. It will develop MS based tools to provide a novel means of more accurate elucidation of metabolite fragmentation (and therefore structure) by optimizing the prediction of that fragmentation using a combination of ab initio DFT methods and mechanistic insights from the fragmentation of the parent molecule.

In metabolism studies, the parent compound is available, so tandem MS data can be acquired. These data can then be interpreted using DFT computational data predicting sites of ionisation and likely fragment ions. In a second step, likely metabolites would be proposed (or predicted) and their MS/MS dissociations calculated using DFT. These predictions would then be compared with the recorded tandem mass spectra of metabolites to rank the candidate structures. This will focus the costly efforts of synthesis to confirm metabolite identification.

Syngenta has been interested in this area for some time and performed a limited study in 2010. DFT data was found to be promising for identifying major fragments and reduced the number of proposed structures. This shows that a computational rule-based DFT approach has potential to more rapidly identify the correct structure within a list of proposed metabolite structures. This studentship will build on the current literature knowledge and previous research by Langley and Pullen.

Applicants should have, or expect to have a good undergraduate degree in Chemistry or equivalent qualification in a relevant area of science.

Application Deadline: 15th June 2015. Interviews will be held in within two weeks of the closing date.

The position will be available from 1st October 2015.

This studentship

The BBSRC/Syngenta CASE conversion studentship is funded for 4 years and will offer the successful candidate experience of DFT software and calculations as well as practical skills in acquiring and interpreting MS/MS spectra on state-of-the-art high-resolution mass spectrometers. They will also obtain industrial experience through working at a Syngenta research site for at least 3 months.

We welcome applicants from the UK and EU who have or expect to obtain at least an upper second class degree in chemistry or allied subjects/relevant disciplines. A strong interest and experience of DFT is required and analytical chemistry knowledge is desirable.

Funding will cover fees and a stipend at current research council rates of £ 13,863 per annum.

Due to funding restrictions this position is only open to UK/EU applicants

Applications for an MPhil/PhD in Chemistry should be submitted online at https://studentrecords.soton.ac.uk/BNNRPROD/bzsksrch.P_Login?pos=4990&majr=4990&term=201516

General enquiries should be made to Dr John Langley at gjl@soton.ac.uk. Any queries on the application process should be made to pgafnes@soton.ac.uk

Applications will be considered in the order that they are received, and the position will be considered filled when a suitable candidate has been identified.

2) GSK Vaccines :

PhD Scholarship Open Day – Monday, May 25, 2015

The Open Day is planned to give the candidates the opportunity to get to know the Research Center of GSK Vaccines in Siena and to meet the scientists responsible for the projects.

For the Open Day organization, please send your contact details and the project title of your interest to academy.nvxit@novartis.com. The Vaccines Academy coordination will reply with necessary information and logistics.

http://www.novartisvaccines.it/ricerca/university-projects.shtml

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http://www.spettrometriadimassa.it/scuole_pratiche/scuole_pratiche_DSM.html

S.E.&O.