

# NEWSLETTER Nº 08

# ACE

## European Association of Chemistry and the Environment

<http://www.research.plymouth.ac.uk/ace/>

November 2006

### 1. EDITORIAL

Dear ACE members,

In a few weeks the 7th European Meeting on Environmental Chemistry (EMEC7) will be underway in Brno. We are looking forward to an inspiring conference in an impressive city. Traditionally, this is also the moment to look back on the events and progress related to the *Association of Chemistry and the Environment*. In 2006 further planning of EMEC meetings has meant that venues until 2009 have been confirmed. In EMEC tradition, these are planned for various cities and regions in the northern and western part of Europe. The transfer of the ACE location from France to Luxembourg is nearly completed. This will allow for more efficient work on the administrative issues of ACE.

Suggestions and recommendations for the future direction, concepts and activities of ACE are always welcome and an annual general meeting (AGM) is planned to coincide with the EMEC meeting in future years. The meeting in Brno will be a good opportunity for the exchange of ideas and suggestions for the development of the ACE.

Jan Schwarzbauer

### 2. MEETINGS

#### 7<sup>th</sup> European Meeting of Environmental Chemistry



Dear colleagues,

It is my great pleasure to invite you to participate at the 7th European Meeting on Environmental Chemistry, which will take place in Brno, Czech Republic from 6-9th December, 2006. The conference will be hosted by the Faculty of Chemistry of the Brno University of

Technology under the auspices of the Rector of the University, Professor Karel Rais.



The Brno City

With almost 400,000 residents, Brno (<http://www.brno.cz/>) is the second largest city in the Czech Republic. Brno is the educational centre of the Moravian part of the Czech Republic. Former residents include many great scientists, such as Johan Gregor Mendel, who discovered the basic laws of genetics in 1865, or Viktor Kaplan who invented the water turbine with adjustable rotor blades in 1912. Brno was also home to the composer Leoš Janáček. Today, there are 6 state universities with a total enrolment of almost 50,000 students, and 5 private universities.

Brno is situated right in the centre of the Europe and is easily accessed from many destinations. There are 4 daily flights from Brno airport to the International Airport in Prague, which has direct connections to London and other major cities. There are also direct buses from Prague Airport to Brno, operated either by Czech Airlines or by the Student Agency Company (SAC). The SAC also operates direct buses from Vienna Airport (Schwechat) to Brno. Brno is also easily accessible by train (including the velocity express train Pendolino) or by car, using the D1 or D2 motorways.

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Brno University of Technology (BUT, <http://www.vutbr.cz>) is the oldest university in the town and the second oldest in the Czech Republic, having been founded in 1849. The Faculty of Chemistry of BUT (<http://www.fch.vutbr.cz>) celebrates the 95<sup>th</sup> anniversary of its establishment in 2006, and it is a pleasure and an honour to host EMEC7 during this special year.

The modern and comfortable facilities of the Faculty of Chemistry will serve as the conference base. The university college will offer inexpensive but comfortable accommodation for participants. Of course, many hotels ranging from luxury five-star to economical private pensions will also be available for conference participants. The conference will take place in the Brno Congress Centre.

The conference web site is live, and contains information on the academic and social aspects of the meeting. The address is <http://www.fch.vutbr.cz/EMEC7>. A dedicated e-mail address is also available for expressions of interest and for communication of participants with the conference organisers. The e-mail address is [emec7@fch.vutbr.cz](mailto:emec7@fch.vutbr.cz).

We warmly invite you to join us and enjoy the stimulating programme of EMEC7 as well as the cultural and architectural heritage of Brno.



### 3. FORTHCOMING MEETINGS

December 2007 – 8th European Meeting on Environmental Chemistry

THURSO, UNITED KINGDOM

Dr. Stuart Gibb

December 2008 – 9th European Meeting on Environmental Chemistry

GIRONA, SPAIN

Dra. Isabel Villaescusa

December 2009 – 10th European Meeting on Environmental Chemistry

LIMOGES, FRANCE

Dr. Jean-Claude Bollinger

### 4. ACE MEMBERSHIP FOR 2007

Your ACE membership can now be extended for 2007. For the first time, a membership application or renewal can be made at the same time as registration for the EMEC meeting. The membership rate for the conference fee and the annual membership fee can now be transferred simultaneously. For all members who will not attending the EMEC conference, the established procedure for membership renewal is very straightforward:

1) Arrange for transfer of the membership fee of 50 € to the ACE bank account:

Cheques Postaux  
L-1090 Luxembourg  
Code BIC: CCPLULL  
IBAN: LU43 1111 0277 0964 0000

2) Add your name and the membership year to the transfer form so that we can update our records. Otherwise we cannot assign the fee received to your personal membership.

Please, don't forget to inform the ACE membership secretary, Mark Fitzsimons, about any changes of your contact details (postal address, e-mail, etc.). Mark can be contacted by e-mail at [m.fitzsimons@plymouth.ac.uk](mailto:m.fitzsimons@plymouth.ac.uk).

### 5. THESIS

**Author:** Dr Phillipa Curtis-Jackson, Petroleum and Environmental Geochemistry Group, University of Plymouth, UK

#### Thesis title:

Characterisation of Algal-Derived Organic Nitrogen



**Supervisor:** Dr. Mark Fitzsimons.

**Abstract:** The characterisation of compounds comprising the dissolved organic nitrogen (DON) pool is an important task for chemical oceanographers wishing to understand its role in the marine N cycle. Low DON concentrations, problems with saline matrices and a lack of pre-concentration methods have all contributed to DON being ignored and disregarded, until recently. Sub units of DON have been analysed as bulk parameters and the low molecular weight (< 1,500 Da) DON fraction has been proposed to drive *regenerated production* within the oceans. The largest producers of these compounds are

phytoplankton. Dissolved combined amino acids (DCAAs), specifically peptides, were chosen as the starting point for this study on DON characterisation. A method was developed for the characterisation of low molecular weight peptides, released either actively or passively from the axenically-cultured phytoplankton *Phaeodactylum tricornutum*.

Concentrations of DON in culture waters were determined through measurement of total dissolved nitrogen and total dissolved inorganic nitrogen. Methods for separation (HPLC), detection (MS), de-salination and pre-concentration (solid phase extraction; SPE), of the samples removed during the period of maximum DON concentration in water samples, were developed. Three chromatography columns were investigated for their separation capabilities with a mixed peptide standard solution. These were 1) Hypersil®PGC, 2) Waters® dC<sub>18</sub> columns in conjunction with mobile phases (acetonitrile, methanol and water) modified with ion pairing reagents, 3) A Phenomenex® Gemini C<sub>18</sub> column in conjunction with mobile phases (methanol, water) modified with formic acid. The third column produced the best chromatography. The SPE method was developed on a Hamilton PRP-1 column containing a polystyrene divinylbenzene (PS-DVB) stationary phase. During the extraction process the increased hydrophobicity of the PS-DVB phase was predicted to yield increased recoveries of peptides compared to a C<sub>18</sub> phase. The method was transferred to extraction cartridges (500 mg, StrataX). Further investigations were then carried out into the affects of salt and dissolved organic matter on the peptide-extraction process.

The extraction method was applied to 1 L culture water samples. Using the HPLC protocol developed on the Phenomenex® Gemini column, the mass analyser was set to acquire data in the full MS mode and then repeated for data acquisition in the data dependent mode (DDMS). The utilisation of both types of detection allowed manipulation of the instrumentation to ignore interfering ions. Mass spectra and chromatograms of ions unique to the cultured waters were identified. The DDMS allowed multistage mass spectrometry (collision induced dissociation) to be carried out on those ions that exceeded the threshold ion intensity of  $1 \times 10^5$ .

Unique ions identified in the axenic cultures included the amino acid TYR, and a modified structure directly related to TYR. Seven peptides were partially sequenced. These were H-(VAL, THR, Xxx)-OH, H-(GLU, Xxx)-OH, H-(ASN, ALA,

GLU, Xxx)-OH, H-(VAL, GLU, Xxx)-OH, H-(SER, HIS, Xxx)-OH, H-(PRO, XLE,HIS, GLN/LYS, GLY, Xxx)-OH and H-(Xxx, XLE, GLN/LYS, XLE, GLU)-OH. One peptide was identified and sequenced as H-TRP-PHE-OH. A significant loss of data was observed between the unique peptide ions identified in the MS analysis and the ions that underwent CID during the DDMS analysis. This was because they were present below the threshold ion count or co-eluted with a more dominant ion.

This study has shown the potential of LC-MS<sup>n</sup> for the identification of organic nitrogen compounds, both natural and anthropogenic, and its application to many fields of environmental science.

#### Publications :

Curtis-Jackson PK, G Masse, M Gledhill, MF Fitzsimons. A novel method for the pre-concentration and analysis of low molecular weight peptides in seawater. Submitted to *The Analyst*

Curtis-Jackson PK, G Masse, M Gledhill, MF Fitzsimons. Recovery and identification of peptides from saline waters by liquid chromatography-electrospray ionisation-tandem mass spectrometry. In prep.

#### 5. ACE PRIZES AWARDED AT EMECS

Since EMEC3 in 2002, the ACE has awarded two prizes at the EMEC meetings, one for the best poster and one for the best oral presentation. In 2005 during the EMEC5 in Bari the prizes were given to Anne-Marie Delort (France) and Charles West (UK)



The EMEC6 prizes were awarded as follows:

The award for the best oral presentation at EMEC6 was given to Polonca Trebse for the paper "A RELATION BETWEEN PHYSIOLOGICAL, BIOCHEMICAL AND ENERGETIC RESPONSES IN TERRESTRIAL ISOPODS *Porcellio scaber* AFTER EXPOSURE TO DIFFERENT PESTICIDES" by P. Trebse, M. Blazic & D. Drobne. (Laboratory for Environmental research, Nova Gorica Polytechnic, Vipavska 13, 5000 Nova Gorica, Slovenia; e-mail: [polonca.trebse@p-ng.si](mailto:polonca.trebse@p-ng.si))



The award of the best poster presentation at EMEC6 was given to Milada Vavrova for the paper "ECOTOXICOLOGICAL EVALUATION OF POLYURETHANE FOAMS" by M. Vavrova, K. Bednarik, L. Vojtova, J. David & J. Jancar. (Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology, Purkynova 118, 61200 Brno, Czech Republic; e-mail: [vavrova@fch.vutbr.cz](mailto:vavrova@fch.vutbr.cz))



## **7. CONTRIBUTIONS TO EMEC6 PUBLISHED IN ENVIRONMENTAL CHEMISTRY LETTERS**

In Belgrade the ACE Scientific Board invited authors of outstanding communications to submit manuscripts for publication in ECL. Based on the normal peer review process seven manuscripts

have been published (online first), or accepted. A further seven contributions are still under review. The following EMEC6 papers will be published in Issue 4/Vol. 4 of *Environmental Chemistry Letters*:

*Haley et al.*: A comparison of SEM-EDS with ICP-AES for the quantitative elemental determination of estuarine particles

*Escudero et al.*: Chromium sorption on grape stalks encapsulated in calcium alginate beads

*Rodriguez et al.*: Sources and features of atmospheric particulate matter in the Mediterranean - consequences for the air quality monitoring

*Mamba et al.*: Monofunctionalized cyclodextrin polymers for the removal of organic pollutants from water

*Turk et al.*: Determination of POPs in gaseous phase by active and passive sampling methods

*Fulladosa et al.*: Effects of arsenic compounds on *Vibrio fischeri* light emission and Butyrylcholinesterase activity

*Cafassi et al.*: Ultrasound enhanced chemical dechlorination of PCB in dielectric oils

## **8. ECL HAS BEEN CONSIDERED IN SCIENCE CITATION INDEX EXPANDED**

ECL, in its fourth year of publication, is now cited in the SCIE and also in Current Contents – Agriculture/Biology/ Environmental Sciences as well as Physical Chemistry/Earth Sciences. In the near future the first impact factors will be calculated and ECL will become a fully rated and (hopefully) highly ranked journal within the field of environmental publications.

## **CONTRIBUTORS TO THIS ISSUE**

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