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Sex, Drugs and Engineering

Determination and Remediation of Bioactive Chemicals in Wastewater Treatment

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Sex, Drugs and Engineering

Remediation of bioactive chemicals using enzyme-based water treatment

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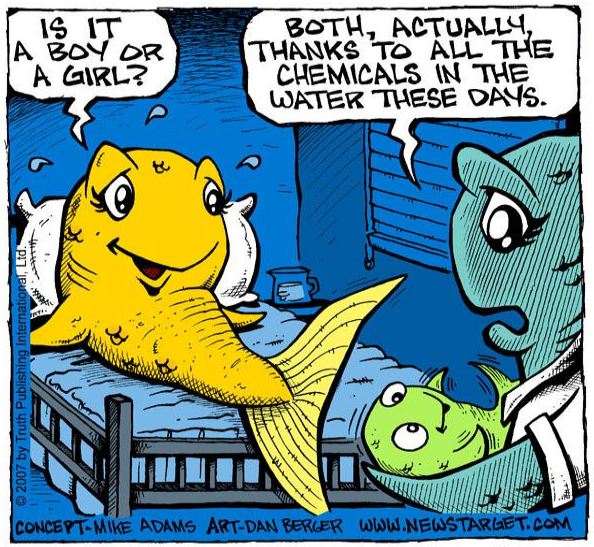
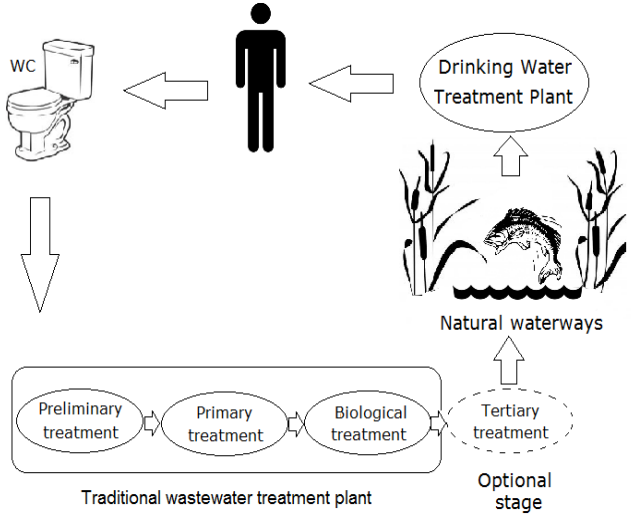
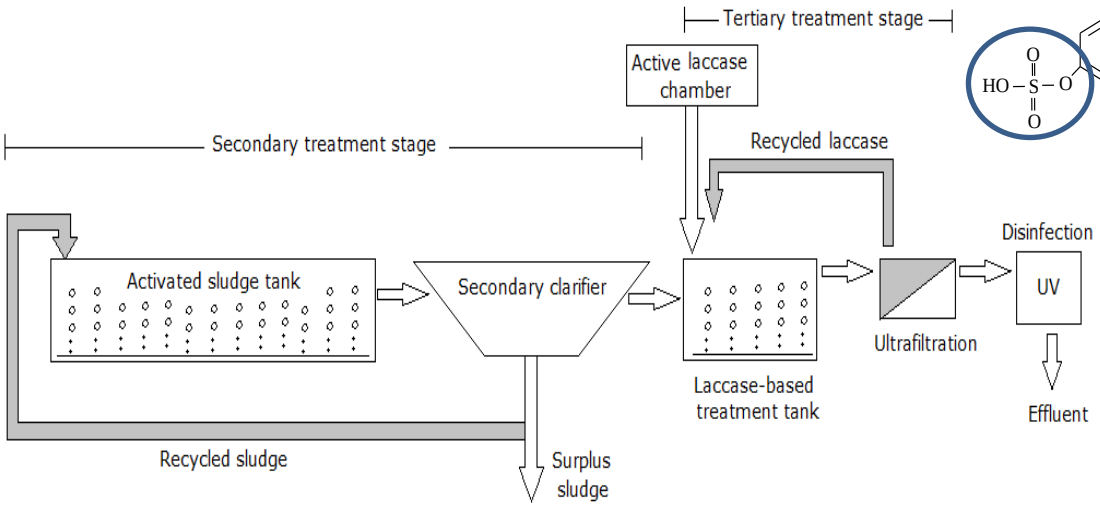
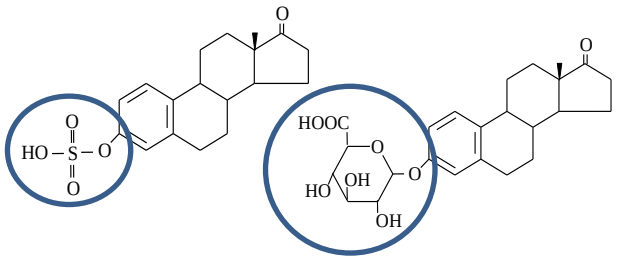
Research need

- Bioactive chemicals e.g. sex steroids and pharmaceutical drugs are an emerging environmental and human health issue, arising from point sources such as the wastewater treatment process.
- There is a need to remediate bioactive chemicals during wastewater treatment to prevent entrance into rivers or drinking water supplies.
- Achieve by optimising current and utilising novel water treatment processes to maintain water resources that are fit for use.









Request for help

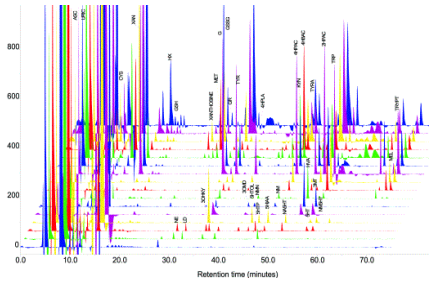
- Analytical facilities to determine target free and conjugated steroids and pharmaceuticals.
- Analytical capability to search for 'unknown' conjugated bioactive chemicals.
- Determining the bioactivity of these water-based contaminants.

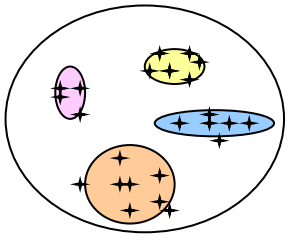
Dave Barrett- Centre for Analytical Bioscience, Pharmacy

- **Mass spectrometry** applied to life sciences and bioengineering (LC-MS/MS, LC-Orbitrap, LC-ion trap, surface MS analysis: 5 MS systems)
- Focus on **small biomolecules** (MWt 50-2000)

• Biomolecule profiling

('global profiling', metabolomics, lipidomics)

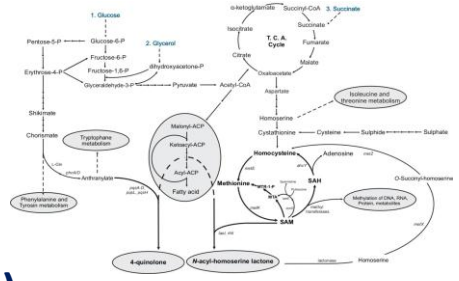


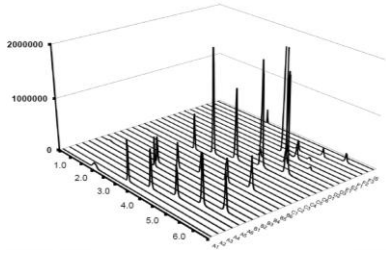


Charge	Exact m/z	Biomarker Database Search	
+	650.236	Tri-N-acetylchitotriose	"tri acetyl-hexosamine"
+	572.258	Quinagolide glucuronide	
+	276.144	Anabasamine	sn-glycero-3-Phosphocholine
+	684.221	Streptomycin 6-phosphate Na	
+	405.202	Glu Glu Lys	Glu Lys Glu

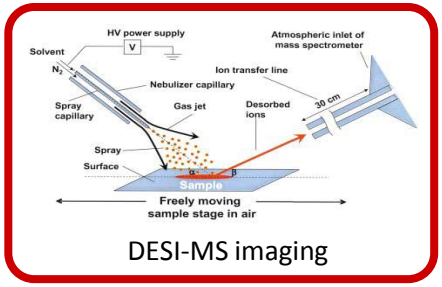
• Metabolites and metabolic pathway analysis

(targeted analysis of metabolites)

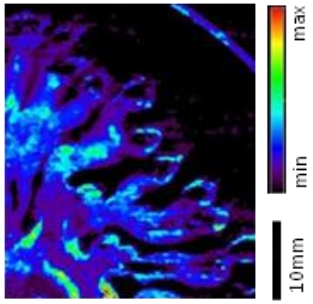




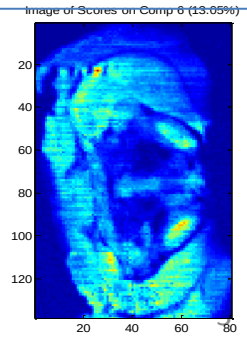
• Ambient imaging of surfaces by mass spectrometry



DESI-MS imaging



314.6 m/z



Project Aim and Objectives

- Aim to mitigate bioactive chemicals entering the water environment by improving the removal efficiency of the wastewater treatment plant

- Objectives were to
  - extrapolate biomolecule profiling and metabolite analysis developed for the life sciences into the field of chemical and environmental engineering
  - identify bioactive chemicals (free and conjugated) in environmental water matrices and potentially new bioactive chemicals of concern
  - inform on the development of a biocatalyst-based treatment technology to determine the removal efficiency of bioactive chemicals from environmental waters

Findings….and the future

- Focus was on identifying bioactive chemicals by targeted analysis and evaluating non-targeted analytical approaches
  - biomolecule profiling and metabolite analysis to the water environment identified new bioactive chemicals e.g. morphine glucuronide
  - validated the approach and original hypothesis of the need to be able to identify the precursor bioactive chemical metabolite when assessing the removal efficiency of wastewater treatment plants

- Improved treatment options are required to improve the removal efficiency of bioactive chemicals during wastewater treatment
  - bench scale studies using a biocatalyst-based treatment demonstrate that bioactive chemicals can be removed in water and modelled by artificial neural networks
  - application to wastewater highlights the inherent variability of the matrix and impact on degradation activity

Merits of our UNICAS collaboration

- Opportunity to undertake research which never would have been possible without the UNICAS Sandpit and funding
  - the new collaboration has enabled research in a direction that was not originally conceived by either Engineering nor Pharmacy
  - collaboration now established with research on-going including a PhD student co-supervised between Engineering and Pharmacy and a submitted EPSRC Grant

- Visits to US and Australia to discuss research including presenting conferences papers and meeting with UK and Australian Water Companies

- Clear direction for future research funding and publications
  - Contributed to successful £1M Leverhulme grant
  - £43k received from BBSRC
  - £125k in progress from EPSRC with reviewer comments received yesterday!
  - 1 publication reviewed (enzyme), 1 in progress (targeted method)
  - A wider University collaboration supported by pump priming that will apply the analytical knowledge and understanding derived from this UNICAS collaboration

UNICAS funding process

- It is quick!
  - may guide what you plan to do and then actually do
  - positives and negatives with the speed of the process

- Have back up plans to account for the short project duration
  - what if the identified postdoc/PhD breaks their leg and is out of action?!
  - inform finance in advance that speed is of the essence when ordering and processing invoices

- Valuable experience in
  - communicating your research in a short amount of time (1 min)
  - finding out what others do across the University and where your research / interests complement and add value
  - writing your research proposal to obtain funds
  - managing a project on a tight timescale and needing to deliver