analysis. Recovery of both Compound X and the internal standard was monitored, along with matrix effects, using the UHPLC-DAD-MS. Recovery of Compound X was achieved with minimal matrix effects allowing quantitative measurements of the molecule extracted from rat plasma. Issues including solubility, stock stability and suitable internal standard were overcome. The developed bioanalysis method was an in–house first and will underpin further development to support preclinical pharmacokinetics and toxicokinetics in efficacy and safety studies, and subsequent clinical studies.

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O14

Determination of DQ-798 in rat plasma by UHPLC-MS/MS and its application to a pharmacokinetic study

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DQ-798 is a more druggable derivative of astragaloside IV prepared by TEMPO-mediated oxidation, which possess significant pharmacological activities. In this study, an ultra-high performance liquid chromatographic method combined with a tandem mass spectrometry for the determination of DQ-798 in rat plasma was developed. After simple protein precipitation with acetonitrile including digoxin (internal standard, IS), the analyte were analyzed by multiple reaction monitoring in positive ESI mode at *m*/*z* transitions of $[M + Na]^+821 \rightarrow 627$ for DQ-798 and $803 \rightarrow 387$ for the IS. The mobile phase is the distilled water and acetonitrile (66:34). The flow rate for the mobile phase was set at 0.35 mL/min. The lower limit of quantification of DQ-798 was obtained as 2 ng/mL. The calibration curve was linear at a range of 2–2000 ng/mL ($R^2 > 0.999$). The validation parameters investigated, which were specificity, precision, accuracy, matrix effect, recovery, and stability, were well within acceptable limits. This analytical method was successfully applied to monitor the plasma concentrations of DQ-798 following oral administration in rats.

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O15

Bioaccessibility of organosulphur compounds from *Allium sativum*

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Garlic (*Allium sativum*), apart from its use as food, has been used as a medicinal plant for over 4000 years. Several investigations suggest that the biological and medical functions of garlic are due to the high content of organosulphur compounds. The bioaccessibility of the organosulphur compounds is an important factor for the evaluation of the functional activity of the garlic. In the present study, a Dynamic Gastrointestinal Digester (DGD) was used to determine the bioaccessibility after digestion of two extracts containing the organosulphur compounds; ajoene and allicin. The DGD is a multi-compartmental, dynamic and computer-controlled system, which reproduces the gastrointestinal digestion process including the chewing, the gastric digestion and the digestion of the small intestine phases. The study showed that after an *in vitro* gastrointestinal digestion process, ajoene is seven times more bioaccessible when encapsulated than in unencapsulated doses, recovering approximately 51% of the compound administered. Allicin recovered after digestion, administered as a combination of alliin and alliinase, showed no significant difference in bioaccessibility when comparing unencapsulated and encapsulated doses. The allicin recovered after the gastrointestinal digestion in both cases exceeded 40%. The results show significant bioaccessibility of the two organosulphur compounds after *in vitro* gastrointestinal digestion, which enables the prediction of their behaviour in the gastrointestinal tract. The stability of the unencapsulated allicin-potential formulation is also promising for whole gut availability. Future work is recommended to understand the absorption of the compounds for a better understanding of their possible beneficial effects in human health.

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Session 6: Novel sources of bioactives IV

O16

Phyto-oestrogenic property of mimosine: A phenylalanine alkaloid

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Hormone replacement therapy (HRT) has been generally used in postmenopausal symptoms in women caused by a lack of endogenous oestrogen. However, due to the increased concern around the potential associated risks of breast and endometrial cancer there is an increased demand for natural oestrogenic agents with lesser side effects. Mimosine is a phenylalanine class of alkaloid. It has been reported that, another phenylalanine alkaloid capsaicine and its analogues possess oestrogenic activity. Therefore, this study was designed to investigate the oestrogen like activity of mimosine by using *in vitro* assays with the ER positive MCF-7 cell line and *in silico* models. Cell viability by cellular count and MTT cell proliferation assays were performed using the oestrogen-dependent MCF-7 breast cancer cells. The regulation of oestrogen marker TFF1 and PGR gene expression were also studied. The binding ability of mimosine to ERα was predicted by *in silico* docking method. The results indicated that mimosine caused significant cell proliferation ($P < 0.05$) and increased cellular viability at 0.1 μM concentration. It also increased the expression of both TFF1 ($P < 0.01$) and PGR mRNA levels ($P < 0.05$), while co-treatment with anti-oestrogenic tamoxifen significantly decreased MCF-7 cell proliferation ($P < 0.001$) indicating an ER mediated effect of mimosine. The docking result showed moderate interaction with the ERα binding site as compared to estradiol. The results indicate the oestrogenicity of mimosine for the first time and suggest that, it can be further studied and developed as an alternative to HRT for postmenopausal women.

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