

## **Revolutionize Metabolite Identification with Cyclic IMS** Discover, Identify and Monitor more

#### WHY SELECT SERIES CYCLIC IMS?

SELECT SERIES<sup>™</sup> Cyclic<sup>™</sup> IMS adds benefit to pharma workflows. Ultra-high ion mobility resolution and novel multi-stage IMSn capability enables discovery of co-eluting, isomeric metabolites, rapid monitoring of metabolites in chemical reactions without the need for LC and improved spectral clarity. Importantly, more routine analysis is improved by the instruments superior TOF performance; high sensitivity, over 100,000 FWHM resolution, <1ppm mass accuracy and improved dynamic range.

#### **SEPARATION OF ISOMERS**



Increase in IMS resolution (# of cIMS passes)

In collaboration with Novartis - Christian Lanshoeft & Frédéric Lozach

#### **DISCOVER NEW CO-ELUTING METABOLITES**



Observation of additional +2x(+O) metabolite using cIMS improved resolution.

#### GAIN INFORMATION ON METABOLITE LOCALISATION

Increasing the number of passes in the cIMS mobility cell improves +O separation for the oxidized metabolites. Further localization information can be obtained from fragment ion shifts.







# WHY IS CCS IMPORTANT IN PHARMA?

- Collisional Cross Section (CCS) is a physiochemical property of an ion that provides confidence in metabolite confirmation/ identification and information about localisation of sites of metabolism.
- Unlike retention times (RT), CCS values are consistent across different instruments (facilities), sample matrices, LC methods and studies (CCS consistency - robust & routine).
- CCS provide potential for comparison with impurities.
- CCS prediction using CCSOnDemand (research grade software for modelling structures of potential metabolites) aids further understanding of metabolite structures.

#### NO NEED FOR LC - THE POWER OF IMS<sup>n</sup> & 'SLICING'



In collaboration with Imperial College London - Ian D. Wilson

### **REAL TIME MONITORING VIA INFUSION**



#### **CUSTOMER FEEDBACK**

"The Cyclic IMS can be used for routine analysis

- Straightforward familiarisation for routine operation
- Fast and fully automated calibration
- People in the lab like it very much."

RALF LAUX, Laboratory Supervisor, DMPK - Drug Metabolism Boehringer Ingelheim

- Investigation into acyl glucuronides via infusion
- Slicing enables further IMS separation of target metabolite (blue region) of interest and other ions can be ejected
- Increasing the IMS resolution reveals an additional 4-O acyl
- Real time monitoring of acyl migration via infusion
- Rapid study of acyl migration shows promise as potential screening approach
- Scope for any chemical reactions with isomeric species to be monitored

#### References

- Higton, D. Wilson, I. et al. (2021) The use of Cyclic Ion Mobility Spectrometry (cIM) Mass Spectrometry to Study the Intra Molecular Transacylation of Diclofenac Acyl. Glucuronide. Analytical Chemistry. https://doi.org/10.1021/acs. analchem.0c04487
- 2. Webinar Series link: The Innovation and Impact of IMS-MS
- 3. Webinar Series QR code:



#### **DISCOVER MORE**

https://ims.waters.com/the-cyclic/



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