EuroSciCon

8th Edition of International Conference on

Mass Spectrometry

March 12-13, 2018
London, UK

Int J Drug Dev & Res 2018, Volume 10

WHERE IS THE CHARGE LOCATED IN IONS GENERATED FROM PHARMACEUTICALS? A SURVEY BY ION MOBILITY MASS SPECTROMETRY

Athula Attygalle
Stevens Institute of Technology, USA

Same drug molecule sometimes generates entirely different mass spectra depending on the instrumental parameters and sample preparation methods used. We demonstrate that this is primarily due to the co-existence of different protonated forms (protomers) or deprotonated forms (deprotomers) of the same molecule. The co-existence of protomers or deprotomers can be demonstrated by ion-mobility mass spectrometry. By this method, millisecond difference in arrival times of different protomers to the detector can be measured. The separated protomers can be fragmented individually and a unique spectrum can be obtained for each protomer. For example, difloxacin, a fluoroquinolone antibiotic was shown to exist as a mixture of two protomers: an O-protomer, due to pronation at the carbonyl group, and an N-protomer due to protonation on the N atom. Upon fragmentation, the O-protomer undergoes the loss of a water molecule exhibiting two signals at m/z 400 and m/z 382, whereas the N-protomer fragments by a loss of a CO_2 molecule. The commonly published spectrum in mass spectrometric databases for this antibiotic is actually a composite of two overlapping spectra. Data obtained from many similar examples will be presented.

aattygal@stevens.edu