**Collision cross sections obtained with ion mobility mass spectrometry as new parameter for the prediction of blood-brain barrier permeation by drugs**

Armin Sebastian Guntner and Wolfgang Buchberger

Institute of Analytical Chemistry, Johannes Kepler University Linz,
Altenbergerstraße 69, 4040 Linz, Austria

Based on the structural complexity of the central nervous system, an evaluation of the ability of a substance to permeate the blood-brain barrier (BBB) is not a trivial task. However, it is important to determine such properties of a drug either to obtain an intended pharmacological effect within the brain or to impede undesirable side effects there. In the past various methods including *in vitro*, *in vivo* and *in silico* approaches have been developed in this context. However, these methods show systematic drawbacks and do not claim universal validity. Therefore, it seems reasonable to develop new methods in that field this allow a prediction of BBB permeation by small molecules [1-3].

Accordingly, in the framework of this research we introduced a new structure-derived parameter to forecast the blood-brain barrier permeation by pharmaceuticals based on ion mobility mass spectrometry experiments. Here, the collision cross section (CCS) was used to illustrate the branching and the molecular volume of a molecule. In detail, we utilized ion mobility quadrupole time-of-flight mass spectrometric data of 46 active small-molecule pharmaceuticals in addition to permeability and lipophilicity data derived from literature to constitute our model.

Based on the data we were able to identify for the first time a strong correlation between the CCS value of a molecule and its ability to pass the BBB.

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