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ELECTROSPRAY IONIZATION EFFICIENCY SCALE OF ORGANIC COMPOUNDS

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Ionization efficiency (IE) of different compounds in electrospray ionization (ESI) source differs widely, leading to widely differing sensitivities of ESI-MS to different analytes. An approach for quantifying ESI efficiencies (as log*IE* values) and setting up a self-consistent quantitative experimental ESI efficiency scale of organic compounds under predefined ionization conditions (ionization by monoprotonation) has been developed recently. Using this approach a log*IE* scale containing 62 compounds of different chemical nature and ranging for 6 orders of magnitude has been established. The scale is based on over 400 relative IE (Δlog*IE*) measurements between more than 250 different pairs of compounds.

To evaluate which molecular parameters contribute the most to the IE of a compound linear regression analysis log*IE* values and different molecular parameters were carried out. The two most influential parameters in predicting the IE in ESI source are the pK_a and the molecular volume of the compound. The standard deviation of the linear model in estimating log*IE* values is 0.8 log*IE* units. No measurement or compound, however deviating, has been excluded from the scale or the model. This, together with the high chemical diversity of the compounds, allows to rate the predictive power of the model as very realistic.

This scale and the whole approach can be a tool for practicing liquid chromatographists and mass spectrometrists. It can be used in any mass-spectrometry laboratory and we encourage practitioners to characterize their analytes with the log*IE* values so that a broad knowledge base on electrospray ionization efficiencies of compounds would eventually develop.

References

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