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Screening therapeutics according to their uptake across the blood-brain barrier: A high throughput method based on immobilized artificial membrane liquid chromatography-diode-array-detection coupled to electrospray-time-of-flight mass spectrometry

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The blood-brain barrier (BBB) plays an essential role in protecting the brain tissues against possible injurious substances. In the present work, 79 neutral, basic, acidic and amphoteric structurally unrelated analytes were considered and their chromatographic retention coefficients on immobilized artificial membrane (IAM) stationary phase were determined employing a mass-friendly buffer based on ammonium acetate. Their BBB passage predictive strength was evaluated by developing statistical models based both on them and on *in silico* physico-chemical descriptors. Highly significant relationships were observed (r2 (n-1) = 0.78) and the predictive ability of the MS-friendly technique derived indexes was comparable to that achieved by the more "biomimetic" phosphate buffered saline, even if some differences in the elution order were observed. The method was transferred to the MS, employing a diode-array-detection coupled to electrospray-time-of-flight mass spectrometry. This setup allowed the simultaneous analysis of up to eight analytes yielding a remarkable acceleration of the analysis time.

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