High Throughput LogP Measurement Using Parallel LC/UV/MS and Sample-Pooling

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A novel approach to high throughput logP measurement based on LC/UV/MS has been proposed. The logP value is determined by correlation with the log*k* value, where *k* is the capacity factor $k=(t_r-t_0)/t_{0,}$ to the logP value using a defined set of standards. Since the analyte retention time (t_r) is determined from the appropriate extracted ion chromatogram (EIC), there are no interferences from impurities and this allows pooling multiple compounds into one injection. To ensure the accuracy and instrument robustness in a routine high throughput environment, a simple and MS-friendly mobile phase consisting of 20 mM ammonium carbonate (pH 8.0) for basic compounds or 20 mM ammonium formate (pH1.0) for acidic compounds, both in combination with methanol at a ratio of 45:55, is used. This approach has been successfully used on single as well as parallel multi-channel LC/UV/MS systems to screen small to large sets of lead compounds and their analogs. A high throughput capability to analyze over 1000 compounds per day has been achieved.