# Extending the Scope of Dynamic Chromatography to Integrate Catalysis and Separations: Fast and Precise Determination of Reaction Rate Constants with the Unified Equation

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Stereoselective chromatographic and electrophoretic separation techniques permit the fast and precise investigation of enantiomerization, epimerization and isomerization barriers of stereolabile molecules [1]. For data analysis straightforward calculation methods to evaluate elution profiles in enantioselective dynamic chromatography are of great interest because the commonly used iterative computer simulations are time-consuming and computationally expensive despite of recent improvements [2]. For diastereomers this ratio usually differs from one and is thermodynamically controlled. Therefore the elution profile is a more complex convolution of the forward and backward reaction and makes the derivation of a direct calculation method more complicated.

The here presented *unified equation* [3] allows the direct and precise calculation of enantiomerization, epimerization and isomerization barriers in capillary electrophoresis [4,5] and chromatography. In contrast to the classical evaluation approach by iterative computer simulation the here presented novel unified equation allows the direct and precise calculation of enantiomerization, epimerization and isomerization barriers in electrophoresis and chromatography without any simulation step. The rate constant of the stereoisomerization process is directly obtained as a function of the experimental chromatographic parameters. One of the major advantages is that this equation can be used for the evaluation of elution profiles of equilibrated as well as non-equilibrated stereoisomeric mixtures. Because of the calculation minimization, real-time data analysis is now possible even in high-throughput separation setups.[6,7]

Finding highly efficient reagents and catalysts, screening of potential drugs and lead structures or disease markers in medical diagnostics is of considerable scientific and economical interest. Parallelized high-throughput assays in combination with sophisticated analytical techniques are currently used to quickly identify and quantify target structures and reaction kinetics. Depending on the sample complexity sample preparation, involving labelling steps, chromatography and electrophoresis in combination with spectroscopy or mass spectrometry are required to analyse the composition.

Our research goal is to integrate chemical reactions and chromatographic analysis in an on-column reaction chromatographic (ocRC) setup. Here we are focussing on the development of stationary phases for gas chromatographic and electrophoretic separations combining separation selectivity and catalytic activity. This includes modification of selector/catalysts with spacers and binding to suitable polymers and solid materials. Currently we are investigating first-order and pseudo-first-order reactions namely hydrogenations, ring closure metathesis and cyclizations to obtain kinetic data and from temperature dependent measurements activation parameters. For the kinetic analysis in-house software packages are written in Delphi based on novel algorithms and implementing the recently derived Unified Equation.


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