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## **Fundamentals of isoelectric focusing elucidated by computer simulation and experimental validation**

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For more than 30 years, dynamic computer simulation together with experimental validation was employed to elucidate the fundamentals of isoelectric focusing [1-3]. This presentation will comprise an overview on the efforts conducted and provide a summary of the achievements together with an outlook of possible future investigations. Configurations with closed columns and those featuring the pH gradient bracketed between an anolyte and a catholyte will be compared. Attention will be focused on pH gradient formation, gradient shift, decay processes at gradient edges, gradient mobilization, sampling strategy and separation of analytes, including proteins. For these aspects, the impact of the properties of carrier and sample components (pKa, pI and mobility) as well as those of anolyte and catholyte (particularly their compositions) on the focusing configuration will be discussed. Furthermore, in relation to capillary isoelectric focusing, the generation and role of the electroosmotic flow and the impact of imposed hydrodynamic flow will be mentioned. Detailed descriptions of selected topics can be found in the literature [4].

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