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Duality based direct resolution of unique profiles using zero concentration region information

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ABSTRACT

Self Modeling Curve Resolution (SMCR) is a class of techniques concerned with estimating pure profiles underlying a set of measurements on chemical systems. In general, the estimated profiles are ambiguous (non-unique) except if some special conditions fulfilled. Implementing the adequate information can reduce the so-called rotational ambiguity effectively, and in the most desirable cases lead to the unique solution. Therefore, studies on circumstances resulting in unique solution are of particular importance. The conditions of unique solution can particularly be studied based on duality principle. In bilinear chemical (e.g., spectroscopic) data matrix, there is a natural duality between its row and column vector spaces using minimal constraints (non-negativity of concentrations and absorbances). In this article, the conditions of the unique solution according to duality concept and using zero concentration region information is intended to show. A simulated dataset of three components and an experimental system with synthetic mixtures containing three amino acids tyrosine, phenylalanine and tryptophan are analyzed. It is shown that in the presence of sufficient information, the

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