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Activity and stability of feruloyl esterase A from *Aspergillus niger* in ionic liquid systems

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Feruloyl esterases (FAEs; EC 3.1.1.73) are accessory plant cell wall-degrading enzymes, which catalyse the hydrolysis of the ester bond between ferulic acid and the monosaccharide to which it is covalently linked. FAEs can however also be brought to catalyse the (trans)esterification reaction in solvents that favour synthesis over hydrolysis, i.e. systems with low water content such as organic solvents or ionic liquids (ILs). The esterification of sinapic acid with glycerol catalysed by FAE A from *Aspergillus niger* (AnFaeA) in a series of ILs containing 15% (v/v) buffer showed that AnFaeA stability – and hence activity – was highly dependent on the anion nature: AnFaeA was stable and active for more than 2 hours in [PF₆]⁻-based ILs, but rapidly lost activity in [BF₄]⁻-based systems. This effect can be explained in terms of hydrogen bonding capacity of the two anions: As predicted by the quantum chemistry-based COSMO-RS method, [BF₄]⁻ has a tendency to form hydrogen bonds and thus interfere with the secondary structure of the enzyme, while [PF₆]⁻ is unlikely to form hydrogen bonds and therefore does not cause denaturation of the enzyme. Similar results have been obtained for lipases [1], but this is the first report on FAE stability in ILs [2]. COSMO-RS, which is now widely used for solvent screening in the complex IL systems [3], may be a valuable tool for fast enzyme stability predictions and/or solvent screening in the future.

References:

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[3]: Klamt, A., Eckert, F., and Arlt, W. *Annu. Rev. Chem. Biomol. Eng.*, **2010**, 1, 101-122.