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Mechanism for the SNAr reaction of atrazine with endogenous thiols: experimental and theoretical study.

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Abstract

Reaction mechanism in aromatic nucleophilic substitution reactions is discussed using kinetic study complemented with quantum chemical calculations. The model system is the reaction of a series of biothiols toward atrazine (ATZ) in aqueous media. The proposed reaction mechanism discloses a non-catalyzed pathway and the presence of a deprotonated (thiolate) nucleophile in water suggests that the reaction mechanism is borderline between a stepwise route and a concerted process. The full analysis of the potential energy surface reinforces the addition/elimination mechanism. Despite of numerous attempts to locate transition structures associated with the leaving group departure were unsuccessful, presumably because this step is extremely fast.