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Sanibel Abstract

“pH-dependence of NO-release in Nitrophorins 2 and 4”

Nitrophorins are a family of heme proteins that transport NO, binding and releasing it in a pH-dependent fashion. Because NO has many interesting physiological effects, acting as an anticoagulant and blood pressure elevator, several blood-sucking insects utilize these proteins to facilitate their feeding. We investigated the mechanism by which two members of the nitrophorin family, nitrophorin 2 (NP2) and nitrophorin 4 (NP4) work. These two proteins are members of different subsets of the nitrophorin family, having an overall sequence identity of about 39%. Our simulations, utilizing modern molecular dynamics methodologies, show underlying similarities between the mechanisms of the two proteins but also suggest differences corroborated by experimental evidence. Both proteins operate by a pH-induced conformational change that allows free diffusion of the bound NO into the bulk solvent at high pH but traps it inside the protein matrix at low pH.