

## BioISI - Biosystems & Integrative Sciences Institute

### VERÃO COM CIÊNCIA 2022 | BioISI Internship Projects

Project ID | VC22\_2

Project Title | An up-to-date C(pH,E)MD method for tackling heme-containing proteins

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Number of Fellowships available | 1 (one)

**Abstract** | Heme and heme-resembling groups are very common cofactors in proteins such as haemoglobin, myoglobin, cytochrome P450, cytochrome c/c3, and are essential for life. The use of in silico methods capable of accurately describing and studying the redox characteristics of these systems is very scarce. The first method developed to describe redox processes at constant-pH [C(pH,E)MD] was developed in 2009 suffering the last update in 2013. Therefore, an up-to-date and free-to-use implementation of the C(pH,E)MD method would be of great value to investigate the redox effects of porphyrinic systems in chemical and biochemical processes. In this project, we will start to update, calibrate, and benchmark a C(pH,E)MD method which, in the future, will be applied to increasingly complex porphyrinic systems.