

[Inicio](#) > CETEMMSA (Biotintes): conveni de col·laboració entre el BSC-CNS i CETEMMSA per a desenvolupar models computacionals de Bio-tintes

---

## **CETEMMSA (Biotintes): conveni de col·laboració entre el BSC-CNS i CETEMMSA per a desenvolupar models computacionals de Bio-tintes**

### **Description**

The objective of this project was to develop computational models of ink mixtures. Using different computational approaches, including atomistic and coarse-grain molecular dynamics, our in-house Protein Energy Landscape Exploration (PELE) technique and mixed quantum mechanics and molecular mechanics (QM/MM) methods, the stability of several ink mixtures in adverse conditions (such as high pressure, etc.) was evaluated. The goal was to understand which factors determine the ink decomposition and to develop a predictive model.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

---

**Source URL (retrieved on 23 Jul 2024 - 17:34):** <https://www.bsc.es/es/research-and-development/projects/cetemmsa-biotintes-conveni-de-col%C2%B7laboraci%C3%B3-entre-el-bsc-cns-i>