

Soggetto: proposta di tirocinio

<i>ID</i>	PTI_IT_Conti Nibali Valeria_12/05/2026 16.42.42
<i>Data</i>	12/05/2026 16.42.42

Supervisore del progetto

<i>Cognome</i>	Conti Nibali
<i>Nome</i>	Valeria
<i>Dipartimento</i>	MIFT
<i>Laboratorio</i>	Fisica Sperimentale e Computazionale dei Biosistemi
<i>E-mail</i>	vcontibali@unime.it
<i>Numero di telefono</i>	

Co-Supervisore del progetto

<i>Cognome</i>	Ciccolo
<i>Nome</i>	Andrea
<i>Posizione</i>	Dottorando di Ricerca in Fisica
<i>Dipartimento</i>	MIFT

<i>Laboratorio</i>	
<i>E-mail</i>	andrea.ciccolo@studenti.unime.it
<i>Numero di telefono</i>	

Dettagli del progetto

<i>Titolo</i>	Clustering Framework for Intrinsically Disordered Proteins	
<p><i>Descrizione dettagliata:</i> This internship aims to identify the dominant conformational families in intrinsically disordered proteins (IDPs) through an advanced computational protocol applied to the Amyloid-beta peptide. Using GROMACS, all-atom molecular dynamics simulations will be performed in explicit solvent with IDP-calibrated force fields, integrating enhanced sampling techniques and rigorous reweighting procedures to ensure exhaustive sampling. The project's core focus is the conformational clustering analysis, employing a strategy that combines density-based algorithms across multiple scales with hierarchical methods.</p> <p>The primary objective is to apply a rigorous methodology capable of extracting biologically relevant structural states from highly flexible molecular ensembles, while analyzing the impact of different solvents on the peptide's structural plasticity.</p>		
<i>Durata (mesi – max 12)</i>		6
<i>Durata (ore)</i>		75
<i>Numero di posizioni aperte</i>		2

Competenze richieste dal tirocinio

Requisiti tecnici:



<i>Altri requisiti</i>	