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**EJIBCE**<sup>2019</sup>  
Encontro de Jovens Investigadores  
de Biologia Computacional Estrutural  
Faculdade de Ciências da Universidade de Lisboa

08:30

## \$ Registration



09:30

## \$ Welcome address



09:35

\K1 :: Ana Rita Colaço - Mining and Integration of Proteomics Data with Knowledge Graphs



10:05

O1 :: Bruno Calçada - In silico methodologies from an agrobusiness point of view



10:25

O2 :: Ana Sequeira - Building an automated platform for the classification of peptides/proteins using machine learning



10:45

## \$ Coffee break + Poster session



11:15

\K2 :: Ana Vila Verde - Molecular mechanisms behind protein halotolerance: a molecular dynamics study with optimised ion-ion force fields



11:45

O3 :: João Especial - Hydrophobic confinement modulates thermal stability and assists knotting in the folding of tangled proteins



12:05

O4 :: Ricardo Ferreira - Antibiotic uptake across gram-negative outer membranes: enabling targeted synthesis from optimized permeability predictions



12:25

## \$ Lunch + Poster session



14:30

\K3 :: Ana Sofia Oliveira - Understanding signal propagation in nicotinic acetylcholine receptors



15:00

\K4 :: Marta Perez - Addressing challenges in cancer immunotherapy with structural bioinformatics approaches



15:30

O5 :: Raquel Gouveia - Stargazin: CACNG2 Mutations in Neuropsychiatric Disorders



15:50

## \$ Coffee break + Poster session



16:30

\K5 :: Sara Campos - The effect of proton binding on dimer formation and other structural properties of  $\beta$ -lactoglobulin: a constant-pH MD study



17:00

O6 :: Carla Teixeira - Unraveling the chemistry beyond the catalytic activity of  $\omega$ -amidase



17:20

O7 :: Lucie da Rocha - Study of pH-dependent conformational changes on  $\beta$ -lactoglobulin using molecular modelling



17:40

## \$ Closing



18:00