



Universidad
de Navarra

Facultad de Ciencias

Propuesta de Trabajo Fin de Máster

Año académico 2026-2027

MÁSTER EN CIENCIA DE DATOS PARA CIENCIAS EXPERIMENTALES

Proyecto Nº 2

Título: Surface Doping of Proteins to Program Substrate Selectivity While Preserving Core Packing

Departamento/ Laboratorio: Química

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Resumen:

This Master's thesis will develop a protein-engineering strategy to "surface-dope" a chosen protein scaffold with targeted tyrosine, lysine, and aspartic acid substitutions to program selective interactions with different substrates (e.g., charged, aromatic, or polar surfaces/ligands). The design approach will combine rational selection of surface positions with statistical/sequence analysis to identify mutation patterns that tune surface chemistry without destabilizing the fold. A central constraint of the project is to keep the internal packing unaffected—or even improved— by restricting substitutions to solvent-exposed sites and by using packing-aware filters during design.

To quantify structure–function relationships, the project will evaluate packing and structural integrity using spectroscopic readouts (e.g., fluorescence signatures, switching behavior if applicable, and activity assays), complemented by stability proxies that report on fold tightness. The resulting dataset will be used to build correlations between model-based packing metrics and experimental performance, testing the hypothesis that surface chemistry can be reprogrammed while maintaining (or enhancing) the packing environment that governs fluorescence, switching, and/or catalytic activity. The outcome will be a generalizable workflow for designing substrate-selective

OPTATIVAS RECOMENDADAS

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- 3.
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