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PTML Study of Dual Antibacterial Drug – Nanoparticle (DADNP) Systems

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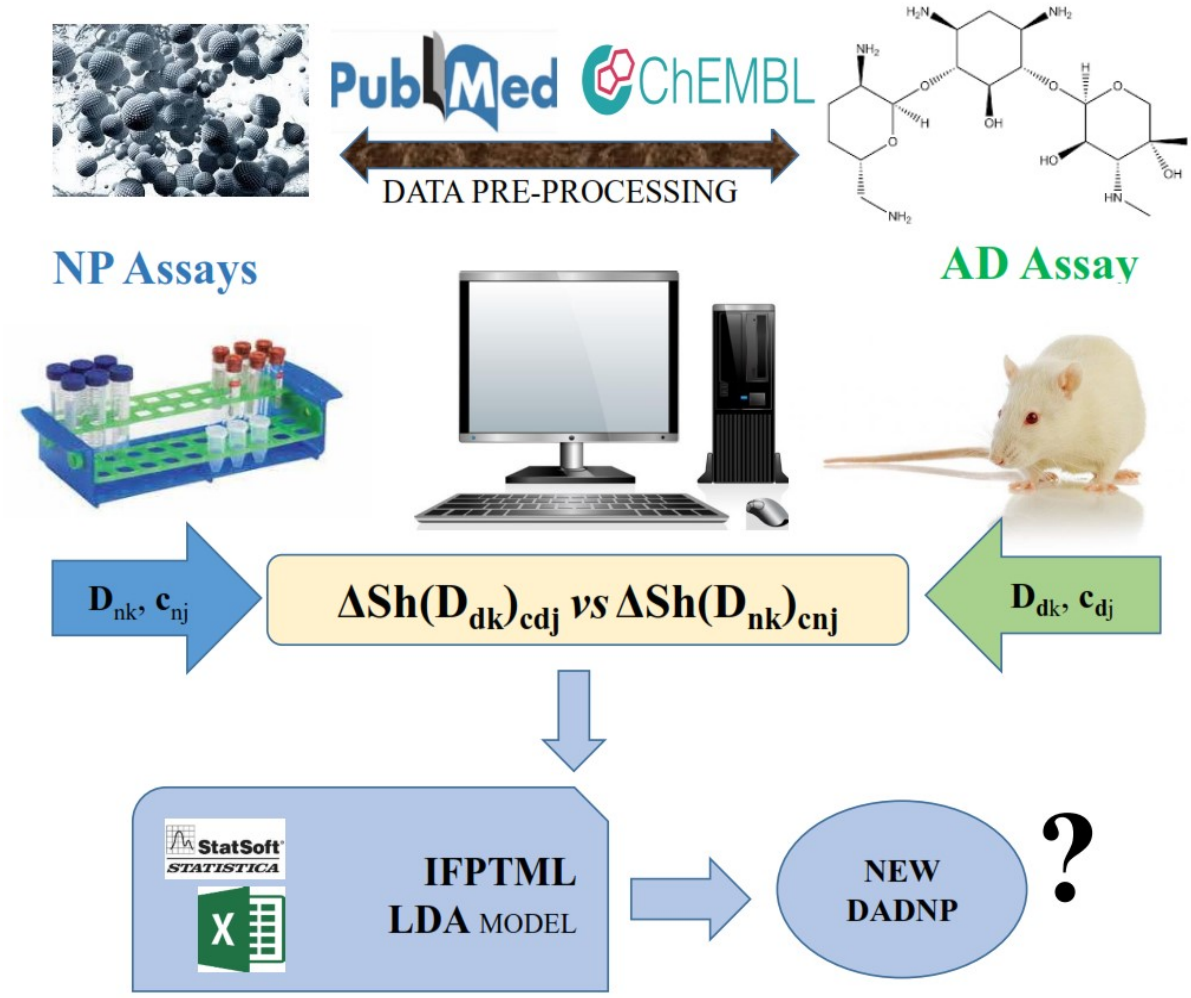
Graphical Abstract



Abstract. The emergence of Multidrug-Resistant (MDR) strains promotes the improvement of Antibacterial Drugs (AD). Some nanoparticles (NP) may be AD carriers, but some have antibacterial activity per se. This opens a window of opportunity for the design of Dual Antibacterial Drug-Nanoparticle (DADNP) systems. DADNP discovery is a slow process due to the high number of combinations of NP vs. AD compounds, assays, etc. Artificial Intelligence/Machine Learning (AI/ML) algorithms that anticipate which potential DADNP systems should be shortlisted for assay may speed up the process. Despite this, the low amount of DADNP activity indicates that AI/ML analysis is tough. To solve this problem in an additive manner, the IFPTML = Information Fusion (IF) + Perturbation-Theory (PT) + Machine Learning (ML) technique was applied. Two datasets were combined (>165000 ChEMBL AD experiments with 300 NP assays) against multiple bacteria species. Next, all vectors of AD and NP properties and experimental conditions (Ddk, Dnk, cdj, and cnj) were zipped into a few input PT Operators (PTOs). IFPTML-LDA models show an Accuracy ≈ 89%, Specificity ≈ 90% and Sensibility ≈ 74% in the training/validation series. The IFPTML models may become a useful tool in the design of DADNP systems for antibacterial therapy against multidrug-resistant microbial pathogens.

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