

Designing nano-systems for anticancer purposes by applying Perturbation Theory Machine Learning (PTML) models

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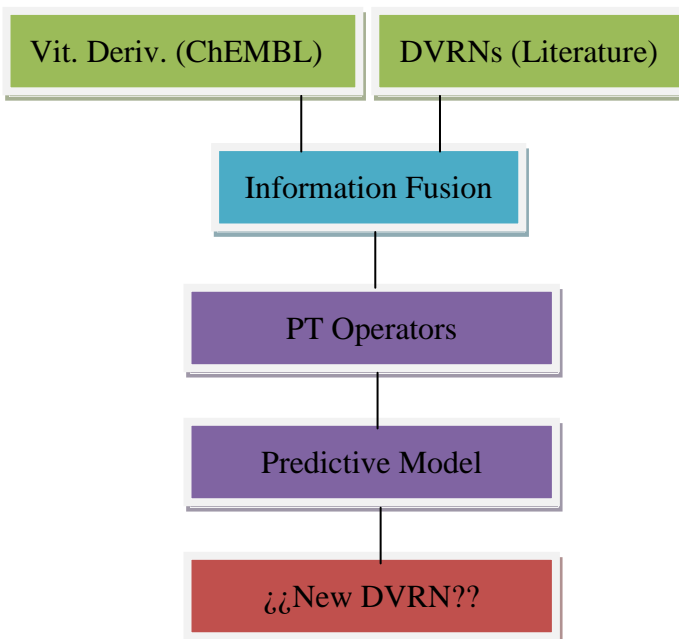
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Graphical Abstract



Abstract.

The number of possible designs of nano-systems is elevated. The design depends on the function we need to develop. Among these systems we highlight Nanoparticle Drug Delivery Systems (DDNS) of high interest not only for Nanotechnology but also for Biomaterials science.¹⁻³

In this work we fusion the following information: 1) Drug-vitamin release nano-systems (DVRNs). This data set was collected from literature. 2) Vitamin derivatives data set extracted from ChEMBL database. Both data sets contain different assay conditions and molecular descriptors. Once we fusion the information, we apply Perturbation Theory Machine Learning (PTML) method in order to build the model. Once built with Perturbation Theory Operators (PT Operators), it presents both Specificity and Sensibility higher than

	80%.
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Until the best of our knowledge, we developed the first multi-label PTML model useful to design DVRNs for optimal biological activity.

Keywords

Nanotechnology; Drug Delivery; Machine Learning; PTML

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