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Predicting preclinical activity values with PTML Model

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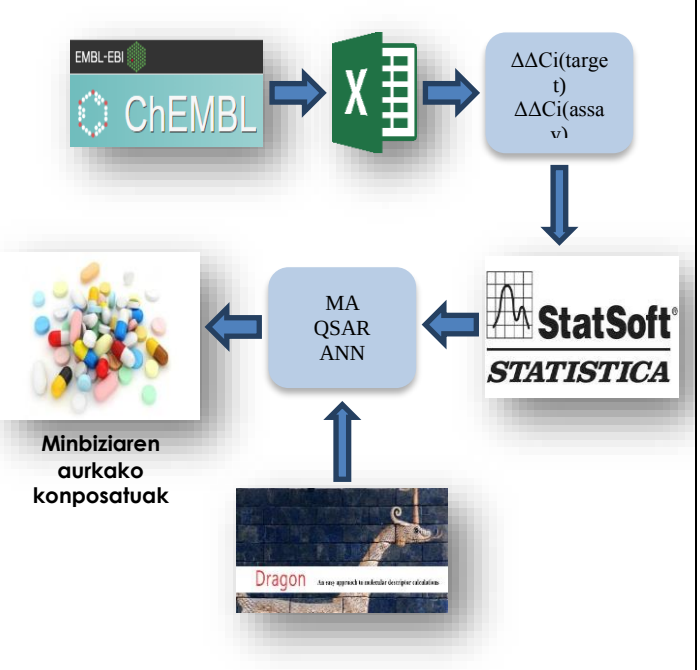
Graphical Abstract



Abstract.

ChEMBL-tik datu basea lortuta, perturbazio teoria (PT) eta Machine Learning (ML) teknikak erabilita PTML eredu bat eraiki da, zein perturbazioen efektua kuantifikatzeko erabili daitekeen konplexuak diren sistema biomolekularretan.
Eredua hau erabilita konposatu berri batek minbiziaren aurkako parametron klinikoen (k_i, LD_{50}, etab.) balioak aurresan ditzakegu.

After obtaining the database from ChEMBL to combine Perturbation Theory (PT) and Machine Learning (ML) we obtain PTML Model, it has been created to quantify the perturbations of complex biomolecular systems.
Using this model we can predict preclinical (k_i, LD_{50}, etc.) values of new compounds against cancer.

References

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