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EVALUTION OF PROPORTIES FROM QUANTUM MECHANICAL CALCULATIONS FOR AZULENIC COMPOUNDS

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The BIBLIOGRAPHY RESEARCH part (chapters 1 - 3) presents some fields of application of chemoinformatics tools, notions of molecular docking used in the rational design of drugs, as well as the presentation of molecular descriptors for the evaluation of properties from quantum mechanics calculations and molecular docking simulation for 3 recognized therapeutic organic compounds.

The part of ORIGINAL CONTRIBUTIONS (chapters 4 - 7) contains *in silico* characterizations for the evaluation of properties by quantum mechanical calculations and the realization of molecular docking simulations for azulene derivatives: 5 compounds 1,3,4-thiadiazole, 3 derivatives of (Z) -5- (azulen-1-ylmethylene) -2-thioxothiazolidin-4-one, 6 azulene substituted with thiophene-vinyl-pyridine or furan-vinyl-pyridine. The evaluated compounds have future uses for the creation of new analytical tools based on modified electrodes or for use in therapy.