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Free Radicals: Properties, Targets, and Implication in Diseases

Oxidative stress (OS) is caused by an imbalance between the production of reactive radical species and a biological system's ability to detoxify the reactive intermediates or easily repair the resulting damage. Chronic exposure to stressors can lead to disturbances of the psychological balance, immunosuppression, and an increase in the likelihood of many diseases, such as cardiovascular, neurodegenerative, and inflammatory diseases, allergies, immune system dysfunctions, diabetes, aging, and cancer.

As most human diseases are very complex, multifactorial, and oxidative stress-related it is of high importance to create new types of biologically active compounds, which may be suitable for the treatment of different diseases or used as adjuvants with conventional therapeutic regimens.

Cancer is among the most prominent causes of death worldwide and nowadays there is an increased interest in new drug discovery, to adequately promote the survival rate against it. The innovative approach to the issue is reflected in a multidisciplinary, experimental, and theoretical, access to the problem that is solved by engaging scientists with qualifications and expertise in different scientific areas, and by applying many sophisticated and contemporary methods of analysis.

To overcome all potential problems with the application of leading chemotherapeutic agents, like platinum drugs, some naturally occurring phytochemicals (coumarins, flavonoids, vinca alkaloids ....), and their synthetic analogs with anticancer potential, are being widely explored. The incorporation of new pharmacophores in particular molecular scaffolds and the creation of new derivatives with multifunctional characteristics and improved antioxidant/therapeutic profiles is one of the priorities of contemporary research. Much attention has also been focused to transition metal complexes, other than platinum, which should be more effective and less toxic than the existing ones. Attention has been focused especially on metallopharmaceuticals based on Ru(II) and Ru(III) with the emphasis placed on two main classes: organometallic Ru(II)-arene complexes and Ru(II)-polypyridine complexes. The possibility of numerous structural modifications of these compounds represents a significant advance in the development of structurally different compounds with potential anticancer properties.

Besides scientifically sound experiments which provide a substantial amount of new information also a very important approach in modern drug design is based on theoretically optimized drug structures before the experimental tests themselves (Structure-Based Drug Design, SBDD). The SBDD is in expansion thanks to the rapid development of algorithms for complex theoretical calculations in an acceptable time frame that can give a realistic picture of biological systems and the processes within. Classical molecular dynamics simulations and related methods, such as molecular docking, allow the implementation of SBDD strategies that take into account the structural flexibility of the model drug-target system and the influence of the solvent, thus providing a unique insight into intermolecular interactions.

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