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Artificial neural network (ANN) in drug delivery and pharmaceutical research

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Artificial Neural Networks (ANNs) technology models the pattern recognition capabilities of the neural networks of the brain. Similarly, to a single neuron in the brain, artificial neuron unit receives inputs from many external sources, processes them, and makes decisions. Interestingly, ANN simulates the biological nervous system and draws on analogues of adaptive biological neurons. ANNs do not require rigidly structured experimental designs and can map functions using historical or incomplete data, which makes them a powerful tool for simulation of various non-linear systems. ANNs have many applications in various fields, including engineering, psychology, medicinal chemistry and pharmaceutical research. Because of their capacity for making predictions, pattern recognition, and modeling, ANNs have been very useful in many aspects of pharmaceutical research including modeling of the brain neural network, analytical data analysis, drug modeling, protein structure and function, dosage optimization and manufacturing, pharmacokinetics and pharmacodynamics modeling, and *in vitro-in vivo* correlations. This presentation will discusse the applications of ANNs in drug delivery and pharmacological research.

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Influence of structural factors in the modulation of cytotoxic activity

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The development of new drugs to fight cancer is of upmost importance since this disease is responsible for millions of deaths each year. The drugs in clinical use, mainly based on platinum, only treat a limited range of cancers and own a lack of selectivity towards malignant cells, resulting in serious side effects. Ruthenium is a promising alternative due its unique chemistry. Two very well-known examples of this class of compounds, that entered Phase II clinical trials, are NAMI-A and KP1019. During the last decade other structuraly different ruthenium compounds have been synthesized with auspicious results. Our research group has been engaged in the synthesis of new ruthenium compounds based on the $[Ru^{II}(\eta^5\text{-}C_5H_5)(PP)(L)]+$ structure (PP=monodentate or bidentate phosphane; L=monodentate or bidentate heteroaromatic ligand) that proved to have, in most cases, lower IC_{50} than cisplatin. There are many factors that modulate the cytotoxic activity of Ru-based drugs and seem to be dependent on the family compounds under scrutiny. We are interested in pinpointing/understanding whether (and how) structural factors control and potentiate the anti-tumor activity of ruthenium-cyclopentadienyl complexes. In this frame, the structure–activity performance of a new family of complexes of general formula $[Ru^{II}(\eta^5\text{-}C_5H_5)(bipy)(L)][PF_6]$ (bipy=2,2'-bipyridine; L=imidazole; 1-benzyl-1-imidazole; 4-(1H-imidazol-1-yl)phenol; 1-(4-methoxyphenol)-1H-imidazole; dimethyl sulfoxide; carbon monoxide and triphenylphosphane) was designed using TM34, $[Ru^{II}(\eta^5\text{-}C_5H_5)(bipy)(PPh_3)][CF^3SO_3]^{[6]}$, as a model. Thus, the introduction of coligand diversity was achieved by σ-coordination of different atoms, namely N, S, C and P. In addition, the precursor of these compounds, $[Ru^{II}(\eta^5\text{-}C_5H_5)(bipy)(NCCH_3)][PF_6]$ was isolated and characterized for comparison and better understanding of the spectroscopic and electrochemical data.

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