A COMBINED CHEMOMETRIC, STRUCTURAL, MOLECULAR GRAPHICS AND MODELING STUDY OF PROGESTOGENS

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Abtract

Progestogens and progestogens are known not only as contraceptives but also as potential drugs for hormonal, anti-cancer and other therapies, and in veterinary practice. The lack of logical method and homogeneous of biological activity data make it difficult to have a clear picture of the progestogens behavior at atomic level. The crystal structure of progestogens-receptor complex give much insight into such intermolecular interactions. Combining the SAR study on two sets of progestogens, a combined study including Partial Least Squares (PLS), structural studies employing related crystal structures, molecular graphics and modeling to study the interactions between hormones and hormone receptors could be used.

Methodology: chemometrics&QSAR

Methodology: other methods

Progestogens = progestosterone derivatives

Methodology: selected molecular descriptors

Methodology: molecular graphics

Methodology: molecular modeling

Methodology: structural comparisons

Results: chemometrics for set I

Results: chemometrics for set II

Results: molecular graphics

Results: molecular modeling

Results: structural comparisons

Progestogens under study

Progestogen: How does it look like??

Progestogens – progestosterone derivatives

Conclusions: methodological aspect

Conclusions: QSAR aspect

Acknowledgement

References