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

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Progesterone: How does it look like??



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Today applicatio

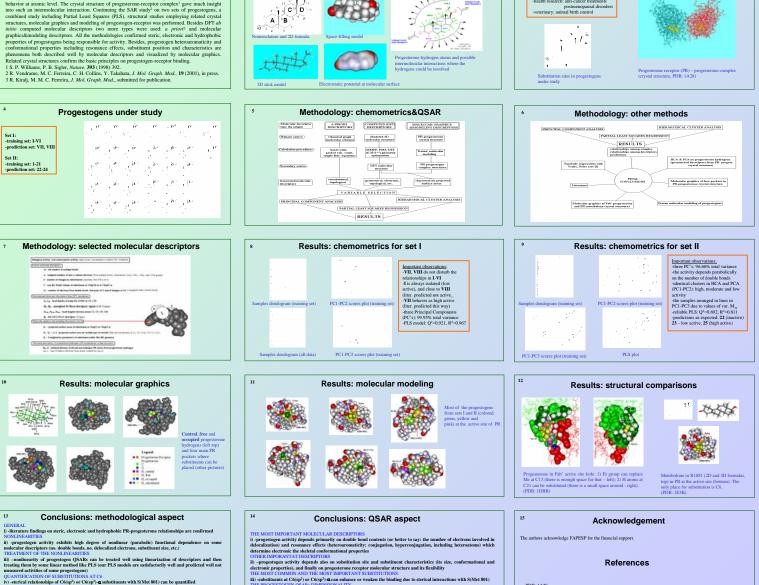
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Progestogens – progesterone derivatives

Abstract

E-mails:

erone and proges ns are known not only as contraceptives but also as potential drugs for Frogestories and progesogeist encloses in an only a commargencies. The last has for farger number and homomodi, anti-access and other threngies, as an investment predices. The last has for larger number and homogenicity of biological activity data makes it difficult to have a clear picture of the progestogens, behavior at atomic level. The crystal miterix the of progestomers are used in singht into such an intermolecular interaction. Continuing the SAR structural studies endoying ended crystal southeast study and an anticelevent structure of the structural studies endoying ended crystal models and an intermolecular interaction. Continuing the SAR structural studies endoying related crystal Related crystal structures confirm the basic principles on progestogen-receptor binding.



AN INFOCATION OF SOLIS IT O HOARS AT CO sterical relationships of  $C6(sp^2)$  or  $C6(sp^3)$ - $\alpha$  substituents with S(Met 801) can be quantified C = C = A DIADLAND MOLECUL AD (DAPH(CSEMODELING DESCEPTORS)

vi) - chemometric study combined with molecular graphics&modeling and structural studies is an excellent choice, which enables to treat well small data sets (like set I) and helps to interpret the 3D nature of molecular descriptors

THE PROGESTOGEN QSARs DIMENSIONALITY iv) -QSARs of progestogens are three-dimensional phen

THE FINAL GOAL OF THE GOAL OF THE RESEARCH

PDB: 1A28 PDB: 1A28 Williams, S. P., Sigler, P. B., *Nature*, **393** (1998) 1392. PDB: IE3K Matias, P. M., Donner et al., J. Biol. Chem., **275** (2000) 26164. PDB: IDBB Arevalo, J. H. et al., J. Mol. Biol., 1993 **231** (1993) 103.