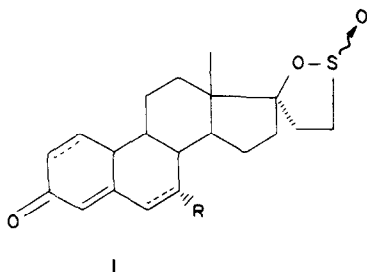
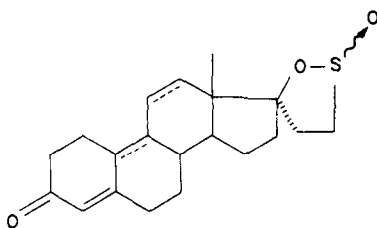


itions of the steroid nucleus. The 19-nor spirostulines of type 2 are mainly characterized by their strong affinity for the progestin receptor. In the Clauberg test, the trienic derivative appears to be a very potent progestomimetic agent with few other hormonal effects.



I



2

11. New 13-substituted gonenes

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13 β -formyl-gonenes generated from 18-iodo-19-norpregnene-20-one derivatives by a novel reaction sequence, served as precursors in the synthesis of a series of 13-substituted gonenes, consisting of 13-vinyl, 13-ethynyl and 13-difluoromethyl analogues of norethisterone and ethynylestradiol. The different steric requirements for the alkyl substituent on C(13) in these two groups are reflected by the biological activity of the individual compounds. On the whole, the biological profile of the new gestagens compares favourably with that of the corresponding mother compounds, whereas in the estrogenic group the activity is generally less pronounced.

12. A quantum mechanical study on hormonal steroids

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In the so-called hormonal steroids there are some phenomenological problems:

—chemical similarity, but different biological activity (sex steroids and their antagonists);

—a difference in the chemical structure (artificial sex steroids) but a similarity with the biological activity of natural sex steroids;

—a different quantitative scale in biological activity (oestradiol, oestrone, oestriol and others). The focus of the present study has been centered on methods allowing the evaluation of these kinds of bio-active molecules at the level of quantum mechanical parameters. For this purpose our modification and extension of the Hückel LCAO-MO method has been used. The parameters of a molecular diagram and the comparison between the energy in the initial and first excited state have been considered in the light

of the possibility that the receptors recognize quantum mechanical level parameters.

13. Molecular relaxation of methyl groups in hormonal steroids

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A theoretical expression for molecular relaxation due to methyl group rotation in some hormonal steroids has been worked out on the basis of quantum statistical mechanical methods. Special attention has been focused on quantum tunnelling in molecular processes underlying all double-minimum relaxation phenomena. The high temperature minimum is attributed to the classical reorientations of a group and the low temperature one to tunnelling disturbed by an interaction with the matrix. Our rate expression is of the form:

$$3\gamma^4 h^2 / 20nr^6 [J(w_0) + 4J(2w_0)]$$

with

$$J(w) = R_e \int_0^\infty dt f(t) \exp(-iwt)$$

and

$$f(t) = \langle \exp[2i\theta(0)] \exp[-2i\theta(t)] \rangle$$

The spectral density $J(w_0)$ is obtained from stochastic properties.

14. Phytoecdysones of the plants of Labiatae and Compositae families

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Phytoecdysones of some of the plants growing in Mid-Asia have been investigated. Along with the known ecdysones ecdysterone, cyasterone, ajugalactone and ajugasterone B new ecdysones turkesterone (I), $C_{27}H_{44}O_8$, and 22-acetylcysterone (VI), $C_{31}H_{46}O_9$, have been isolated from *Ajuga turkestanica* (Rgl) Brig. (Labiatae). Ecdysterone, viticosterone E and previously unknown phytoecdysone sogdisterone (II), $C_{27}H_{44}O_8$, have been found by studying *Serratula sogdiana* Bge. (Compositae). In addition to the ecdysterone, new phytoecdysones integristerone A (III), $C_{27}H_{44}O_8$, integristerone B (IV), $C_{27}H_{44}O_9$, and 24(28)-dehydromakisterone A (V), $C_{28}H_{44}O_7$, have been isolated from *Rhaponticum integrifolium* C. Winkl (Compositae). The isolated compounds offer MH-activity.

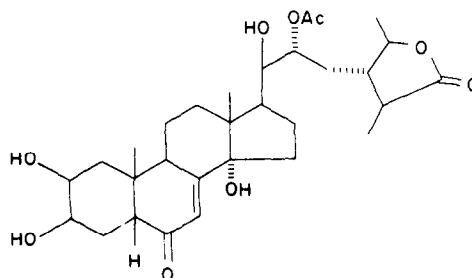
I $R=R^I=H$; $R^{II}=CH_3$; $R^{III}=OH$; $R^{IV}=H_2$

II $R=R^I=R^{III}=H$; $R^{II}=CH_2OH$; $R^{IV}=H_2$

III $R=R^{III}=H$; $R^{II}=CH_3$; $R^I=OH$; $R^{IV}=H_2$

IV $R=R^I=OH$; $R^{II}=CH_3$; $R^{III}=H$; $R^{IV}=H_2$

V $R=R^I=R^{III}=H$; $R^{II}=CH_3$; $R^{IV}=CH_2$



VI