Final Program

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831 Session 47, Growth Regulators and Hormones

THE prediction of herbicidal activity and toxicity of chemicals using descriptors which have an active hydrogen atom, unsaturated structures, and quaternary nitrogen. Kurchii, Bogdan A. Institute of Plant Physiology and Genetics, Vasyilivska 31/17, 252022 Kiev, Ukraine

This report is a continuation of our work to extend the predictive capability of structure/activity relationships (SAR) model for the biological activity of chemicals and have primarily concerned pure design of novel bioregulators. Some our conclusions from the SAR studies of plant growth regulators and herbicides were published earlier (Kurchii, 1996). The milestone of these studies is the determination of descriptors (D) as unsuspected. We have proposed that the presence of an "active (mobile) hydrogen atom" in D is an essential factor determining biological activity of any chemical. General conclusions: (1) The primary role of proposed Descriptors in the designing of novel bioregulators is to detect leads without performing experiments. (2) Using of Descriptors with NH-groups may be preferable in the designing of novel bioregulators with desirable prompt biological effects. In order to achieve prolonged and more strong biological effects using of Descriptors with CH-groups may be more suitable. (3) Substances bearing flanking substitute such as -COOH, -OH, -COR and -COOR possess strong biological activity for plants and microbes whereas their toxicity for mammals is moderately or slightly. (4) Only substituents which have small sizes in alpha-position to active hydrogen atom are suitable for their introduction to basic formula of the designing bioregulator with potent strong biological activity. (5) In order to design potent bioregulators with strong biological effects it is needed to introduce to their formula cis isomers. (6) Selection of D, FRG and flanking groups are main conditions that must be carry out in the designing of novel bioregulators.