

## QSAR AND CONFORMATIONAL STUDY OF 1H-INDOLE-3-ACETIC ACIDS WITH AUXIN ACTIVITY

**Rudolf Kiralj (PQ), Márcia M. C. Ferreira (PQ)**

[rudolf@iqm.unicamp.br](mailto:rudolf@iqm.unicamp.br)

*Instituto de Química - UNICAMP, Campinas SP, 13084-971 Brazil*

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1H-Indole-3-acetic acid (IAA) and its derivatives are among the most important plant-growth regulation hormones from auxin class. This work deals with QSAR and conformational properties of 22 IAAs, 11/15 of which has measured straight-growth promoting activities on *Avena Sativa L.* coleoptiles: the optimal coleoptile elongation, and the half-optimum and optimum concentrations. The geometry of conformers close to IAA in crystalline state was optimized at B3LYP 6-31G\*\* and MMFF94 level. Molecular descriptors were calculated and analyzed by means of chemometric methods. Regression models predicted the growth-promoting activities for 11/7 IAAs reasonable well. IAAs exhibit clustering with respect activity and molecular features. Remarkable differences in CH<sub>2</sub>CO<sub>2</sub>H side chain conformation are observed for IAAs in free state, crystals ABP1 (auxin binding protein 1) – IAA complexes, mostly related to biological activities and molecular properties at qualitative and even quantitative level.