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EXTENDED ABSTRACTS

Use of Chemo-Informatics to Identify Molecular Descriptors of Auxins, Cytokinins and Gibberellins

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ABSTRACT

We have identified those molecular descriptors differentiating four auxins, four cytokinins and 4 gibberellins. DRAGON software (version 5.5, 2007) and CambridgeSoft ChemOffice (version 12, 2010) including ChemDraw and Chem3D were wont to calculate 212 molecular descriptors. Only 49 descriptors showed statistically significant differences among auxins, cytokinins and gibberellins. Of them, the foremost important differences are often described as follows. Gibberellins contain terminal tertiary C (sp3), terminal quaternary C (sp3), ring secondary C (sp3), ring tertiary C (sp3), and ring quaternary C (sp3) that aren't present either in cytokinins or auxins. Gibberellins also are relatively rich in terminal secondary C (sp3) and 10-membered rings which are absent in cytokinins. Cytokinins have 10 times more nitrogen atoms than auxins but this atom isn't present in gibberellins. Auxins have 10 times more substituted benzene C (sp2) and 5 times more benzene-like rings than cytokinins but these structures aren't in gibberellins. Regarding the numbers of unsubstituted benzene C (sp2), auxins average 4.50, cytokinins 1.25 but they're absent in gibberellins. A dendogram was generated using data of these molecular descriptors with statistical significant differences (49). The three groups of regulators were correctly classified in three independent branches. The procedure described here may help identify new chemical compounds with potential uses as plant growth regulators. DRAGON software and Cambridge Soft Chem Office including ChemDraw and Chem3D were wont to calculate 212 molecular descriptors. All data of this study were statistically evaluated using SPSS (Version 8.0 for Windows, SPSS Inc., New York, NY) to perform One - Way ANOVA and Tukey (p=0.05). the general coefficients of variation (OCV) were calculated as follows: (standard deviation/average) *100. during this formula, we considered the typical values of the three growth regulators compared (auxins, cytokinins, gibberellins) to calculate the quality deviation and average. Therefore, the upper the difference between the three groups of chemicals, the upper is that the OCV. A hierarchical cluster analysis using the molecular descriptors for auxins, cytokinins and gibberellins was performed. The dendogram was built using average linkage (between groups). Variables were standardized to vary from 0 to 1 consistent with Kantardzic . We have identified those molecular descriptors differentiating four auxins, four cytokinins and 4 gibberellins. DRAGON software and CambridgeSoft ChemOffice including ChemDraw and Chem3D were wont to calculate 212 molecular descriptors. Only 49 descriptors showed statistically significant differences among auxins, cytokinins and gibberellins. Of them, the foremost important differences are often described as follows. Gibberellins contain terminal tertiary C (sp3), terminal quaternary C (sp3), ring secondary C (sp3), ring tertiary C (sp3), and ring quaternary C (sp3) that aren't present either in cytokinins or auxins. Gibberellins also are relatively rich in terminal secondary C (sp3) and 10-membered rings which are absent in cytokinins. Cytokinins have 10 times more nitrogen atoms than auxins but this atom isn't present in gibberellins. Auxins have 10 times more substituted benzene C (sp2) and 5 times more benzene-like rings than cytokinins but these structures aren't in gibberellins. Regarding the numbers of unsubstituted benzene C (sp2), auxins average 4.50, cytokinins 1.25 but they're absent in gibberellins. A dendogram was generated using data of these molecular descriptors with statistical significant differences (49). The three groups of regulators were correctly classified in three independent branches. The procedure described here may help identify new chemical compounds with potential uses as plant growth regulators.

Keywords: Chemo-informatics; Plant growth regulators; Molecular descriptors

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