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研究论文

拟南芥乙酰羟基酸合成酶与磺酰脲的相互作用以及CoMFA研究

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摘要 在分子水平上较为详尽地研究了85个磺酰脲类化合物与植物源野生型拟南芥AHAS酶的离体相互作用, 测定了这些化合物对AHAS酶的抑制常数K_i^{app}. 采用比较分子力场方法(CoMFA)对这些化合物与AHAS酶的相互作用进行了三维构效关系研究, 用此模型预测了检验组10个化合物的pK_i^{app}值, 模型的预测结果与测试结果一致.

关键词 乙酰羟基酸合成酶 拟南芥 磺酰脲 比较分子力场分析(CoMFA)

分类号 O641.3 O946.5

Interaction and CoMFA Studies on *A. thaliana* Acetohydroxyacid Synthase by Sulfonylureas

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Abstract Acetohydroxyacid synthase(AHAS) is the target for sulfonylurea, imidazolinone, triazolopymiding sulfonaniline and pyrimidin-2-yl salicylate herbicides. The interactions between wild type *A. thaliana* Acetohydroxyacid synthase(AHAS) and 85 synthesized sulfonylureas *in vitro* were studied, obtained K_i^{app} values of all compounds by the method of Westerfeld and Singh. The structure-activity relationship and 3D-QSAR was investigated by using comparative molecular fields analysis(CoMFA). The cross-validated q^2 and the relation coefficient r^2 for the model established by the study are 0.811 and 0.934 respectively, with a F value of 246.506 and a standard deviation(s) of 0.419. The obtained satisfied QSAR model was is consistent with those based on *in vivo* data and showed a high ability to predict the biological activity(-lgK_i^{app}) for ten test set compounds. These results will be useful for design and synthesis of highly active compounds.

Key words Acetohydroxyacid synthase *A. thaliana* Sulfonylureas CoMFA

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