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研究论文

基于受体结构的AHAS抑制剂的设计、合成及生物活性

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摘要 在AHAS与磺酰脲类除草剂复合物的晶体结构基础上, 利用分子对接程序DOCK 4.0, 通过MDL/ACD三维数据库虚拟筛选, 得到了296个与AHAS结合能较低的小分子化合物结构信息, 从中选取了部分小分子进行化学合成, 并且测试了其生物活性. 部分化合物的体内和体外活性表现出一定的一致性.

关键词 乙酰乳酸合成酶(AHAS) 分子对接 有机合成 生物活性

分类号 0626

Molecular Design, Synthesis and Biological Activity Evaluation of Novel AHAS Inhibitors Basedon Receptor Structure

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Abstract Based on the crystal structure of AHAS/sulfonylurea complex, 296 molecules were obtained with low binding energy towards AHAS from MDL/ACD 3D database *via* virtual screening with program Dock 4.0, from which some compounds were synthesized. The biological activities of the synthesized compounds were measured *in vitro* and *in vivo*. The preliminary bioassay indicates some compounds displayed a good herbicidal activity on rape and barnygrass and had AHAS inhibition to some extent. These studies indicate the rationality of molecular design based on the crystal structure of AHAS complex.

Key words Acetohydroxyacid synthase(AHAS) Molecular docking Organic synthesis Biological activity

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