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生命科学

角鲨烯合成酶抑制剂的高通量虚拟筛选

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摘要:

以SQS抑制剂CP 320473为先导物, 在60%结构相似性的基础上, 先通过AutoDock Vina软件进行分子对接, 再选取结合能量最低的新化合物进行分
子对接研究. 结果表明: zinc_8442249比先导化合物CP 320473的抑制效果更好; SQS活性位点的Lys52通过与氢键与抑制剂结合, 在抑制过程中具有重要作用.

关键词: 角鲨烯合成酶; 高通量虚拟筛选; 分子对接; 抑制剂

High Throughout Screening with Computer of a New Inhibitor of Human Squalene Synthase

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Abstract:

On the basis of a structural similarity of 60%, we took the SQS inhibitor CP 320473 as a lead compound to perform molecular docking by
AutoDock Vina. In the end, the new compound with the lowest binding energy with SQS was selected for further investigation. The docking results show that the new compound (named zinc_8442249) is a better inhibitor than CP 320473. Lys52 is important in inhibition as it forms a hydrogen bond.

Keywords: squalene synthase high throughout screening; docking inhibitor

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