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人类腺苷受体 A_3 亚型拮抗剂的构效关系分析

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QSAR Analysis of Human Adenosine A_3 Receptor Antagonists

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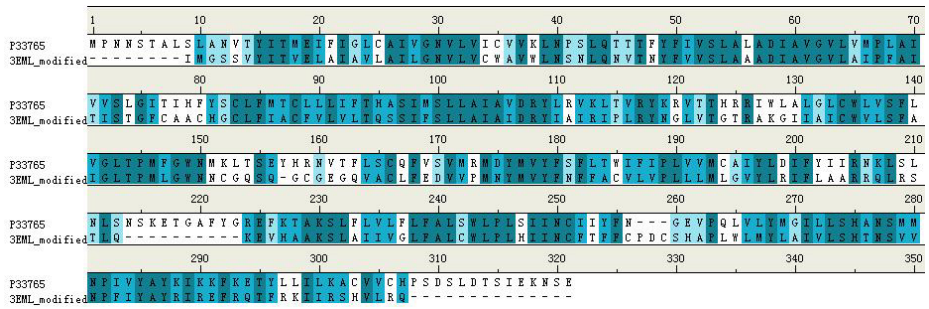

图 S1　A_3 腺苷受体与 A_{2A} 腺苷受体序列比对图

Fig.S1　Sequence alignment of adenosine A_3 receptor and adenosine A_{2A} receptor

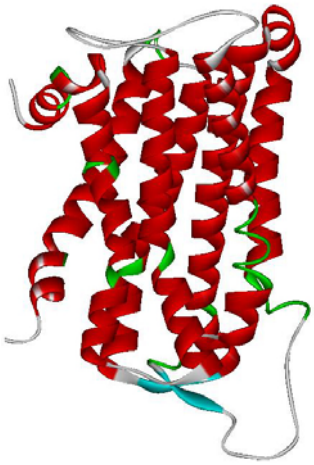

图 S2　A_3 受体蛋白的分子动力学模拟得到的稳定构象

Fig.S2　MD received stable conformation of adenosine A_3 receptor

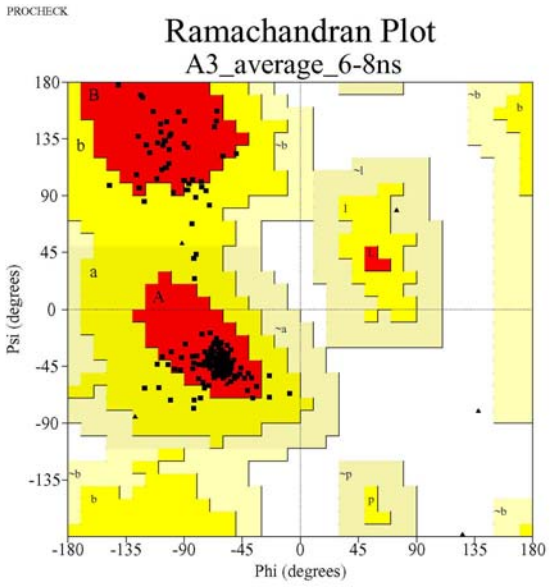

图 S3　A_3 受体模型的 Ramachandran 图

Fig.S3　Ramachandran plot of modeled adenosine A_3 receptor

A, B and L represent the residues in most favored regions; a, b, l and p represent the residues in additional allowed regions; ~a, ~b, ~l and ~p represent the residues in generously allowed regions.