

1

## Interactive Study between Two Types of 1-[2-(Hydroxyethoxy)methyl]-6-naphthylmethylthymines

MENG Ge(孟歌), CHEN Fen-er(陈芬儿), De Clercq Erik, et al.

1. Department of Chemistry, Fudan University, Shanghai 200433, China; 2. Rega Institute for Medical Research, Katholieke University Leuven, Leuven, Belgium

收稿日期 修回日期 网络版发布日期 接受日期

**摘要** Two different types of 1-[2-(hydroxyethoxy)methyl]-6-naphthylmethylthymines have been designed, synthesized and evaluated for their anti-HIV-1 activities in different cells lines. The binding free energy (DG) including steric and electrostatic between the two different ligands and reverse transcriptase Non-Nucleoside Binding Pocket (NNBP) have been docked and calculated to evaluate their accommodation circumstance on a SGI work station. The DG and anti-HIV-1 activity has been correlated in order to guide further drug design, which showed that the steric binding effect dominated in the whole binding action between the compounds and reverse transcriptase (RT). The results showed that more negative DG led to higher activity of compounds.

**关键词** [HIV-1 reverse transcriptase](#) [binding free energy](#) [6-naphthylmethyl HEPT analogs](#) [anti-HIV activity](#)

分类号 [O625.52+6](#) [TQ 463.54](#)

**DOI:**

对应的英文版文章: [2031-005](#)

通讯作者:

作者个人主页: MENG Ge(孟歌); CHEN Fen-er(陈芬儿); De Clercq Erik; et al.

### 扩展功能

本文信息

▶ [Supporting info](#)

▶ [PDF](#) (237KB)

▶ [\[HTML全文\]](#) (0KB)

▶ [参考文献\[PDF\]](#)

▶ [参考文献](#)

服务与反馈

▶ [把本文推荐给朋友](#)

▶ [加入我的书架](#)

▶ [加入引用管理器](#)

▶ [引用本文](#)

▶ [Email Alert](#)

相关信息

▶ [本刊中 包含“HIV-1 reverse transcriptase”的 相关文章](#)

▶ 本文作者相关文章

· [MENG Ge孟歌](#)

· [CHEN Fen-er陈芬儿](#)

· [De Clercq Erik](#)

· [et al](#)