

谷胱甘肽分子伞的构象分析及VolSurf表征

胡桂香,商志才,邹建卫,李文静,俞庆森

浙江大学化学系

收稿日期 修回日期 网络版发布日期 接受日期

摘要 使用分子动力学模拟迟火和半经验AMI方法对谷胱甘肽分子伞进行了构象分析,结果表明,真空下屏蔽构象和暴露构象的最低能量值相差很小(26.00kJ/mol)。考虑溶剂效应后,屏蔽构象的能量值最高,暴露构象的能量值最低。屏蔽构象的能量最低值高于暴露构象的能量最低值89.24kJ/mol,从理论上解释了谷胱甘肽分子伞在水溶液中呈现暴露构象的原因。利用VolSurf参数分析了分子伞以屏蔽构象穿透磷脂双分子层的影响因素,结果表明屏蔽构象较小的两亲矩及较大的分子褶皱程度是其能够穿透细胞膜的主要影响因素,与构象的绝对疏水区域无关。

关键词 [谷胱甘肽\\$构象A药物设计](#) [疏水性](#)

分类号 [R914](#)

Conformational Analysis and VolSurf Characterization of Glutathione Molecular Umbrella

Hu Guixiang,Shang Zhicai,Zou Jianwei,Li Wenjing,Yu Qingsen

Department of Chemistry, Zhejiang University

Abstract Conformational analysis of glutathione molecular umbrella was performed with molecular dynamics simulated annealing and semi-empirical AMI methods. The results show that the difference of the lowest energy values in vacuum between exposed and shielded conformations is small (26.00 kJ/mol). When solvent effect is included, the energy of the shielded conformation is highest and the exposed conformation lowest. The lowest energy of the shielded conformation is higher than the lowest energy of the exposed conformation by 89.24 kJ/mol. This point accounts for why the exposed conformation of glutathione molecular umbrella exists in water. The influencing factors that glutathione molecular umbrella penetrates lipid bilayers with the shielded conformation were analyzed with VolSurf parameters. The results show that the major influencing factors are smaller amphiphilic moment and larger molecular rugosity of the shielded conformation, which are independent of definite hydrophobic regions of the conformation.

Key words [GLUTATHIONE](#) [CONFORMATION](#) [DRUGS DESIGN](#) [HYDROPHOBILITY](#)

DOI:

通讯作者

扩展功能

本文信息

▶ [Supporting info](#)

▶ [PDF\(0KB\)](#)

▶ [\[HTML全文\]\(0KB\)](#)

▶ [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](#)

▶ [复制索引](#)

▶ [Email Alert](#)

▶ [文章反馈](#)

▶ [浏览反馈信息](#)

相关信息

▶ [本刊中 包含“谷胱甘肽\\$构象A药物设计”的 相关文章](#)

▶ [本文作者相关文章](#)

- [胡桂香](#)
- [商志才](#)
- [邹建卫](#)
- [李文静](#)
- [俞庆森](#)