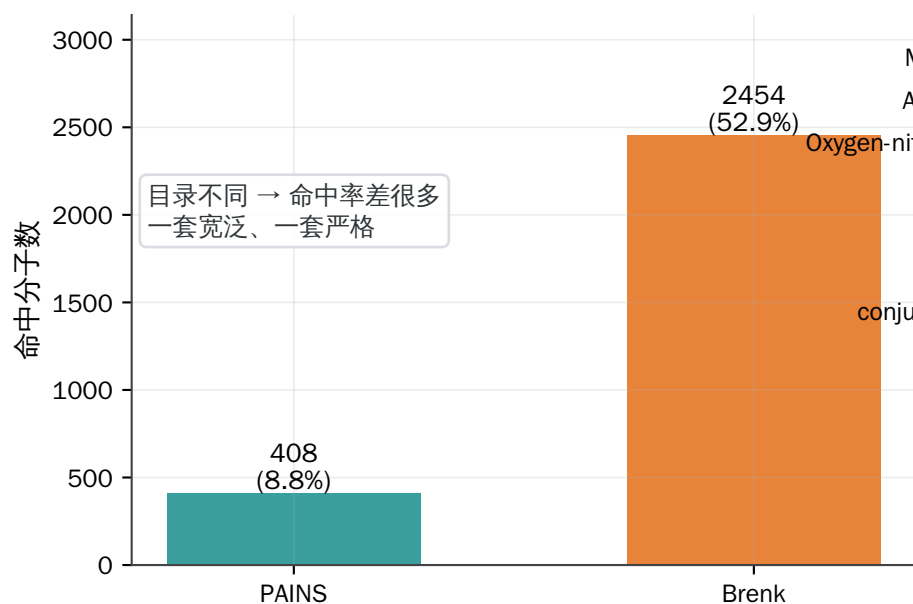


结构警示：同一批分子在两套目录下的命中

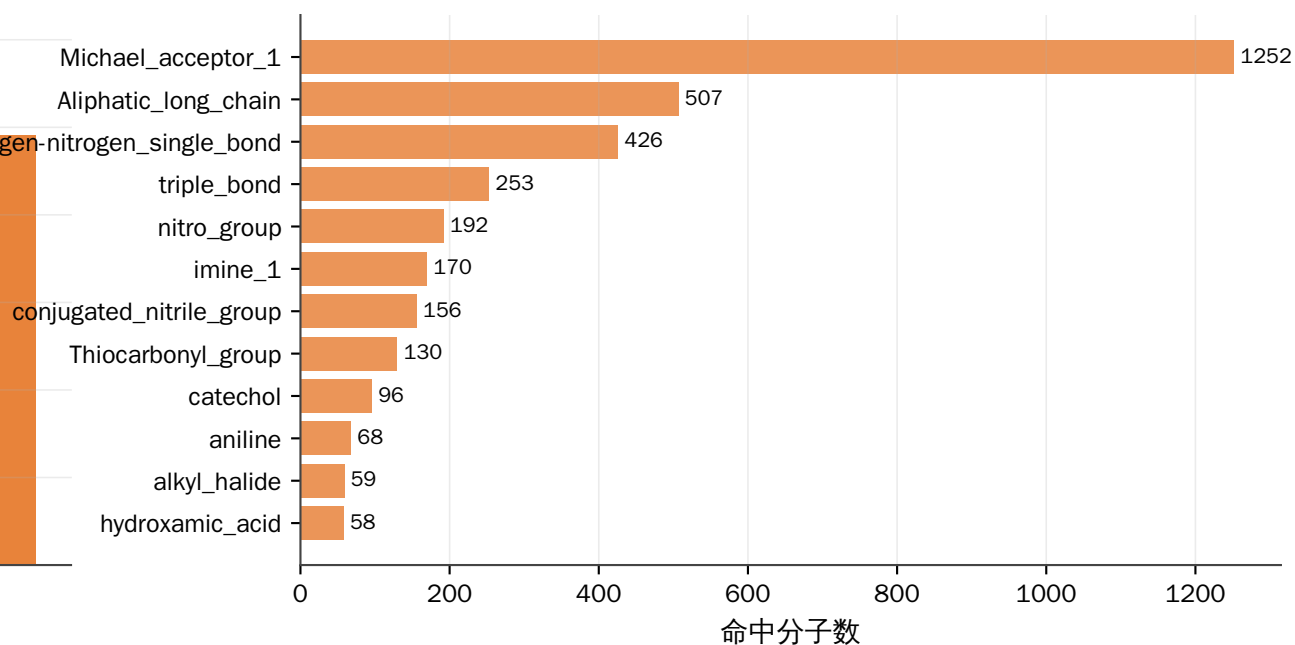
A

两套目录的命中率 (4635 个分子，按命中计数)



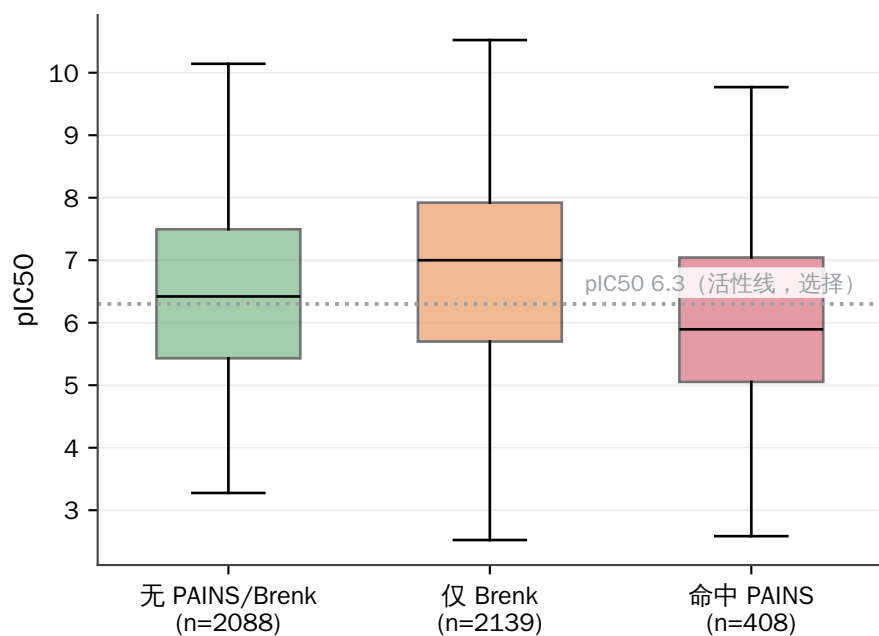
B

最常见的 Brenk 警示 (Top 12)



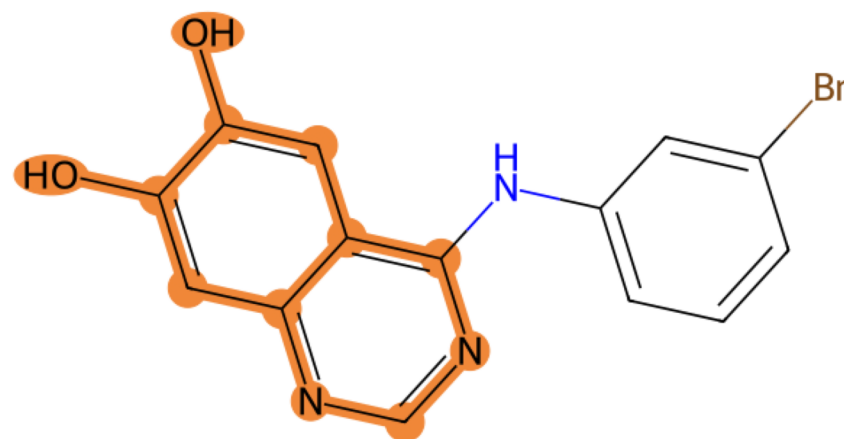
C

警示状态 vs 活性 (警示≠无效)



D

命中的子结构 (高亮) : catechol_A(92)



Oc1cc2ncnc(Nc3ccccc(Br)c3)c2cc1O

命中原子 12 个 (橙色高亮)

警示只说明“需要进一步核查”，不是毒性或无效的证据