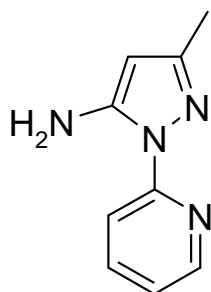


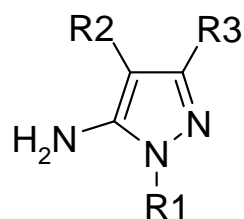
Poster
No. 19

Designing safer aminopyrazoles through simple quantum mechanical predictions for Ames activity

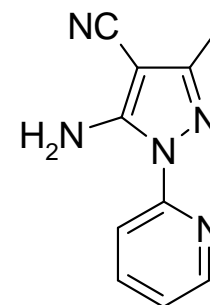
William McCoull, AstraZeneca



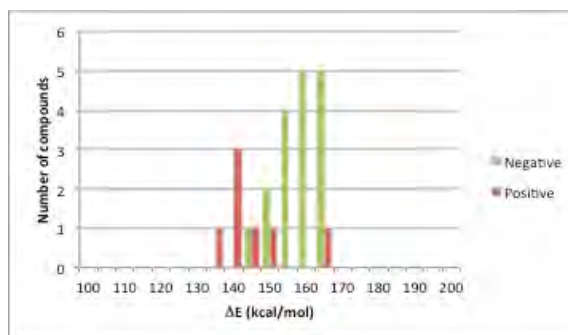
QM calculations to
predict Ames activity



Guidelines for
compound design



$\Delta E = 139$ kcal/mol
 $P(\text{active}) = 55\%$
Active in Ames test



$\Delta E = 153$ kcal/mol
 $P(\text{active}) = 36\%$
Inactive in Ames test

