Designing safer aminopyrazoles through simple quantum mechanical predictions for Ames activity

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

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