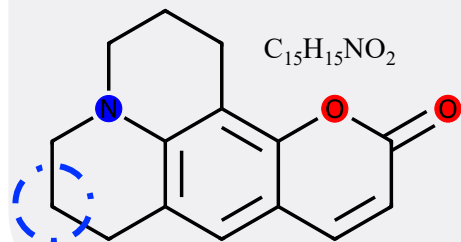




Toxicity Type: Mutagenicity

Molecular Image: IMG_i



Prompt Scheduler: \mathcal{F}_{prompt}

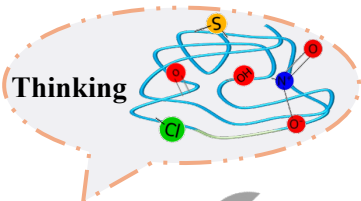
Task Prompt: I_{task}

Basic Template:

\mathcal{P}_{base}

O=c1ccc2cc3c4c(c2o1)CCCN4CCC3

$SMILES_i$ & Task Name: $\mathcal{T}(AMES)$



Multimodal Large Language Model

Modified SMILES: \mathcal{R} & $\mathcal{T}(AMES)$

- 1 : O=c1ccc2cc3c4c(c2o1)CCCN4CCCC3=O
- 2 : CN4CCc3cc2oc(=O)cc2c3CCCN4
- 3 : O=c1ccc2cc3c4c(c2o1)CCCN4CC(O)C3



Structure
Validity Check

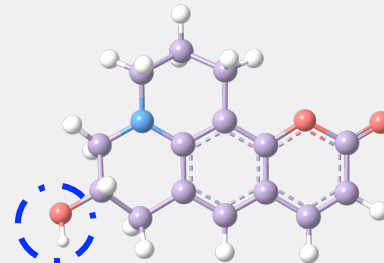
2



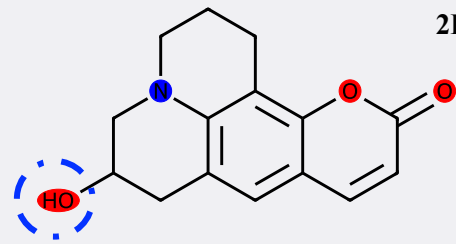
\mathcal{S}_{soft}	1	
\mathcal{Q}	3	
ν_{ro5}	3	
\mathcal{S}_{sas}	3	
\mathcal{S}_{sim}	3	



Repair Successful



O=c1ccc2cc3c4c(c2o1)CCCN4CC(O)C3



Molecular Toxicity Repair Tasks

ToxiEval: A Multi-Criteria Evaluation Chain