

SAMPL8 Challenge

**MSKCC: Chodera, Isik
UCI: Mobley, Bergazin**

**GSK: Bahr, Graves, Kenna,
McQueen, Nandkeolyar, Nevins**

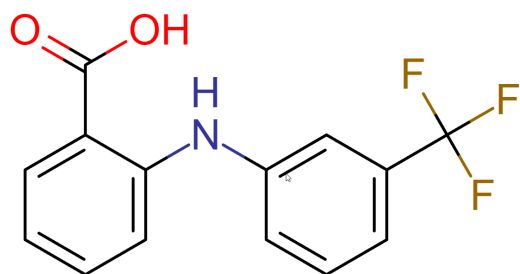
List of Completed pH Solubility Compounds

This is the completed list of compounds processed through Britton-Robinson pH solubility to determine pKa

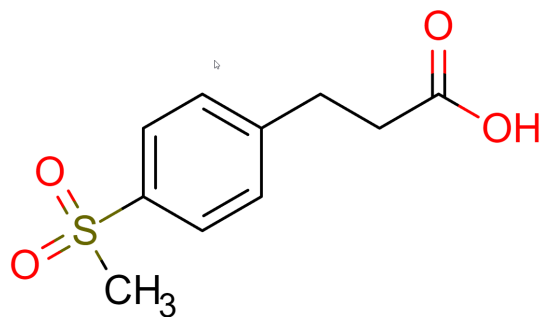


SAMPL Set 1	SAMPL Set 2	SAMPL Set 3	SAMPL Set 4
SAMPL8-1	SAMPL8-7	SAMPL8-13	SAMPL8-18
SAMPL8-2	SAMPL8-8	SAMPL8-14	SAMPL8-19
SAMPL8-3	SAMPL8-9	SAMPL8-15	SAMPL8-20
SAMPL8-4	SAMPL8-10	SAMPL8-16	SAMPL8-21
SAMPL8-5	SAMPL8-11	SAMPL8-17	SAMPL8-22
SAMPL8-6	SAMPL8-12		SAMPL8-23

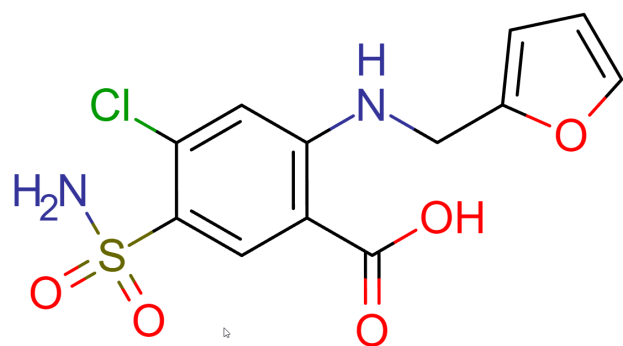
SAMPL8-1



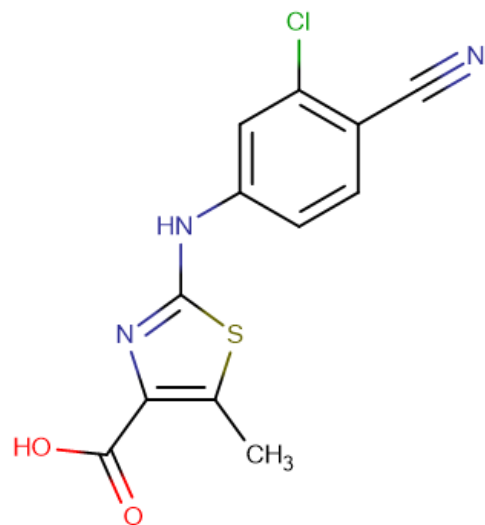
SAMPL8-2



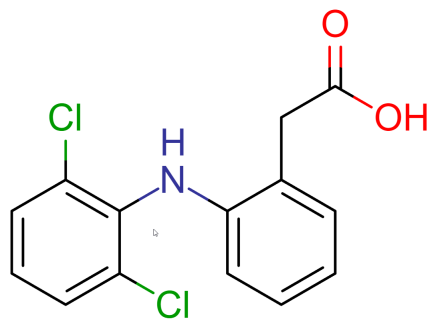
SAMPL8-3



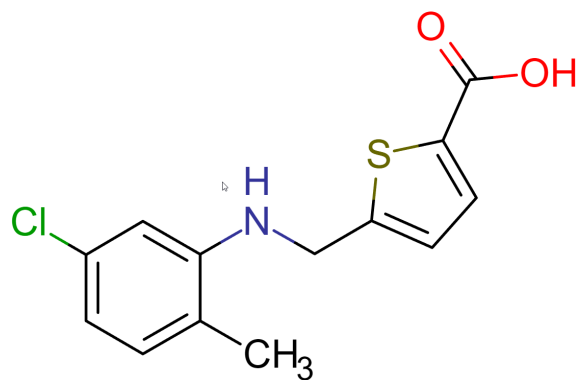
SAMPL8-4



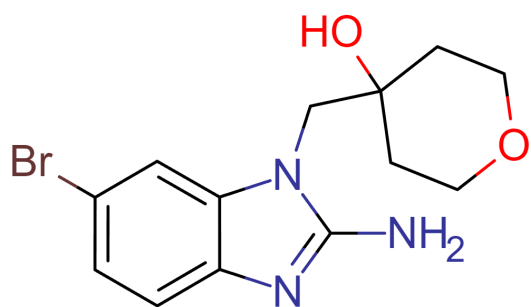
SAMPL8-5



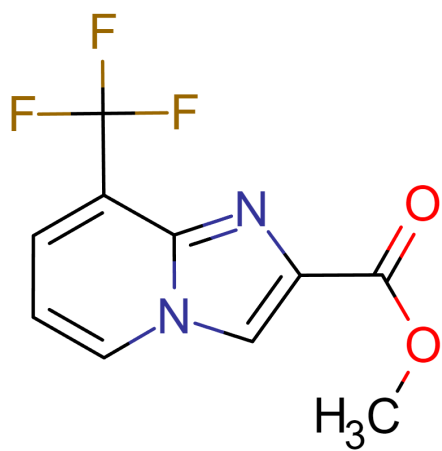
SAMPL8-6



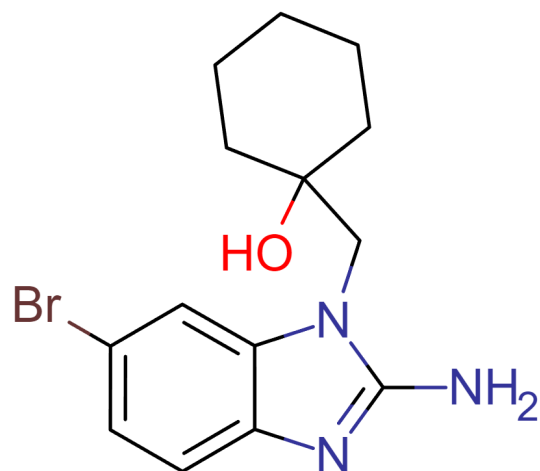
SAMPL8-7



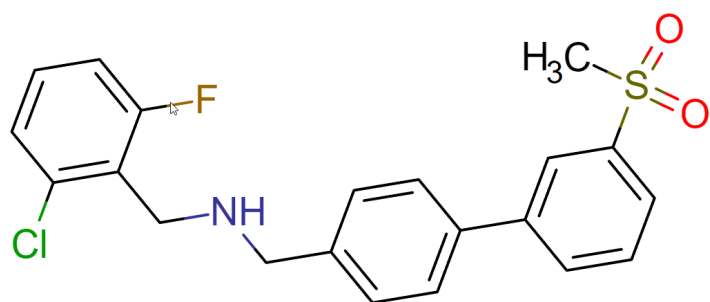
SAMPL8-8



SAMPL8-9



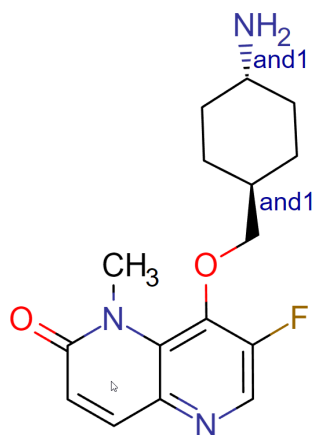
SAMPL8-10



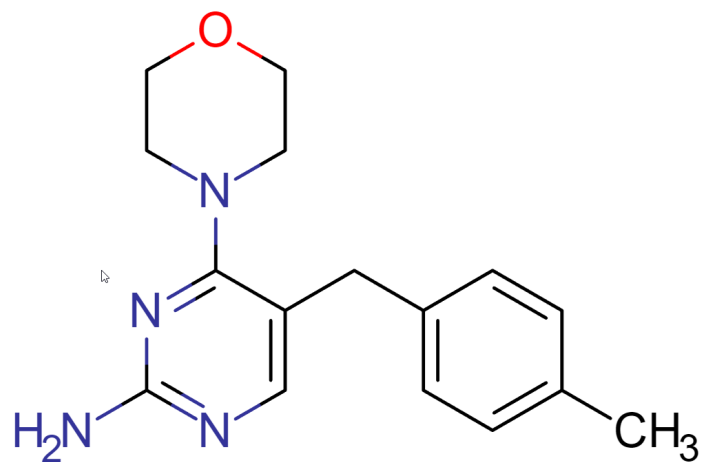
SAMPL8-11



– pKa not determined



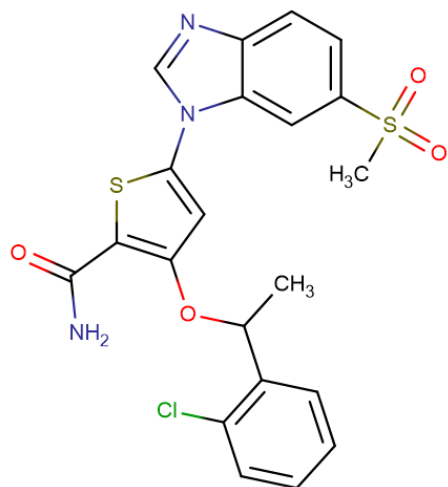
SAMPL8-12



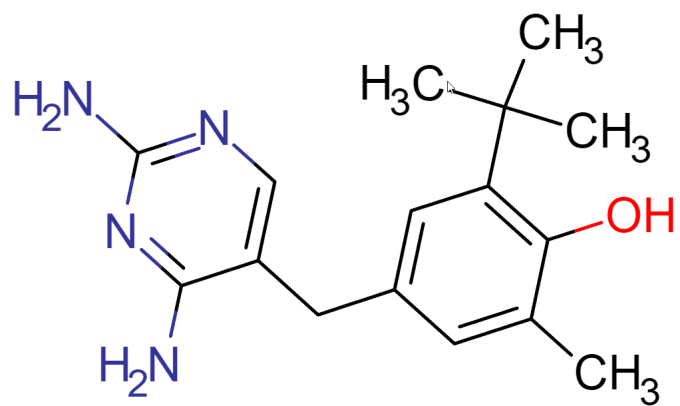
SAMPL8-13

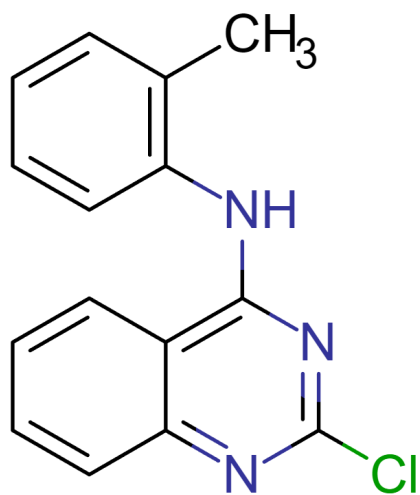


– pKa not determined

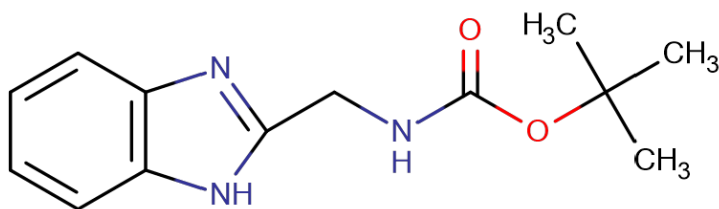


SAMPL8-14





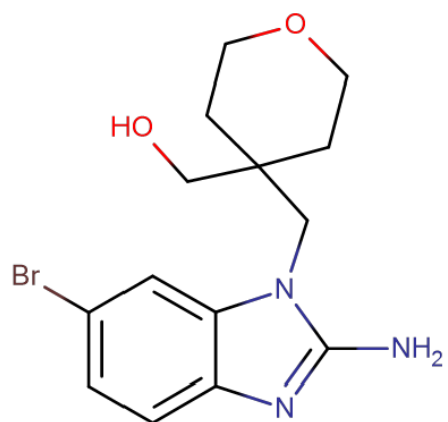
SAMPL8-16



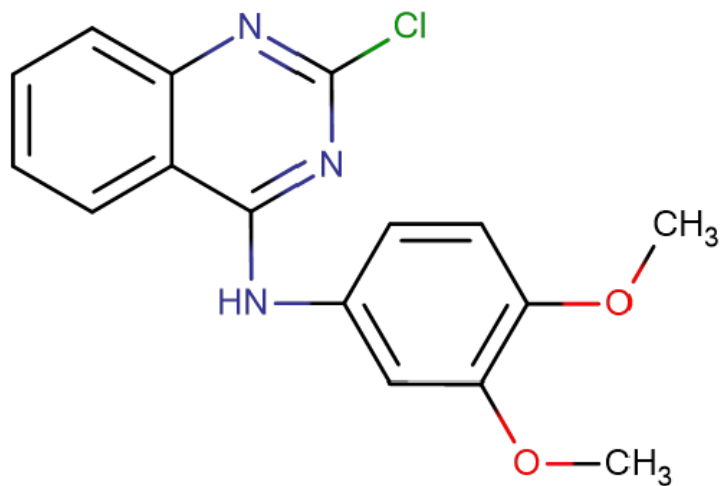
SAMPL8-17



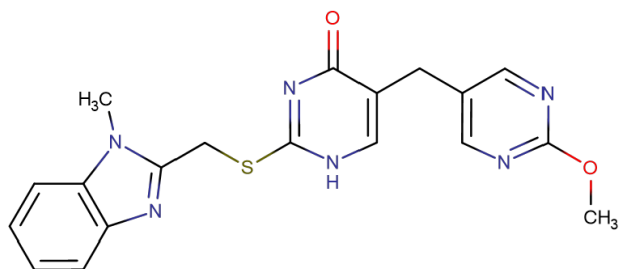
– pKa not determined

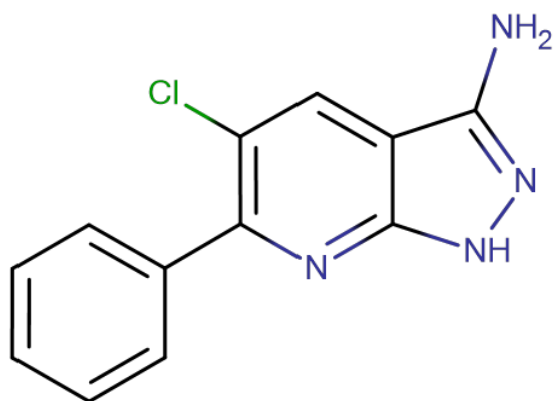


SAMPL8-18

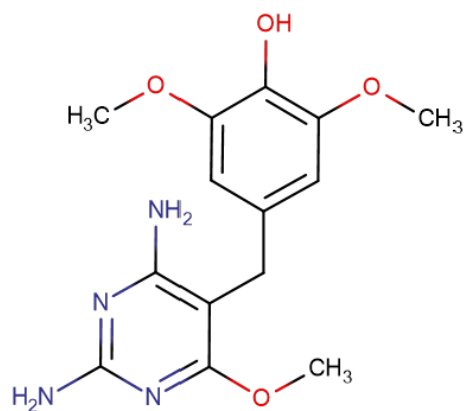


SAMPL8-19

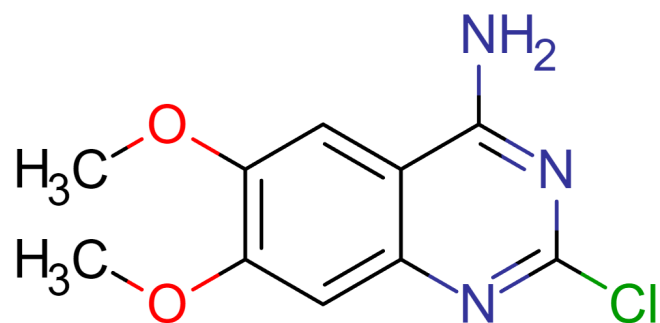




SAMPL8-21



SAMPL8-22



SAMPL8-23

