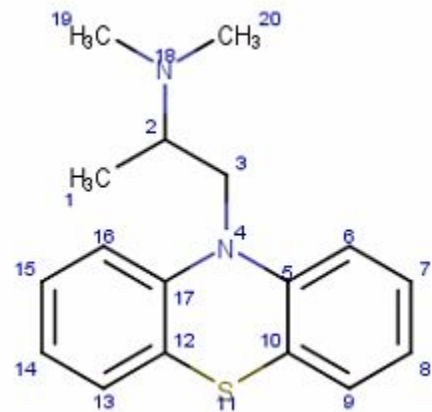


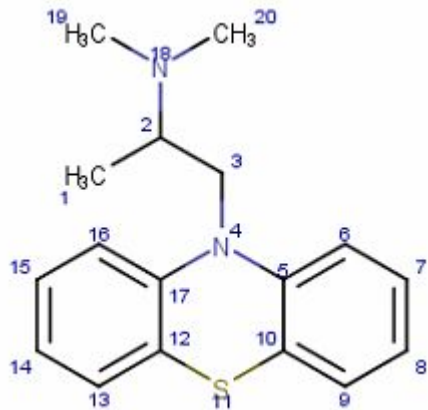
PWWVAXIEGOYWEE-UHFFFAOYSA-N

(Promethazine)



True BoMs		Converted True SoMs
<19,18;Cleavage;R1> <19,H;Oxidation;R1>	→	19
<20,18;Cleavage;R2> <20,H;Oxidation;R2>	→	20
<11,S;S-Oxidation;R3>	→	11
<14,H;Hydroxylation;R4>	→	14
<8,H;Hydroxylation;R5>	→	8

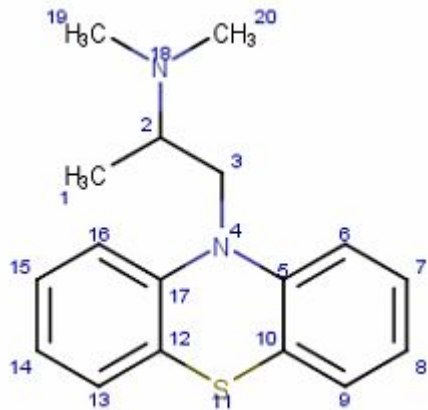
CypBoM-Tri predicted results (Promethazine)



CypBoM-Tri predicted BoMs	Converted True SoMs
<C.19;N.18> <C.19;H>	12
<C.20;N.18> <C.20;H>	14
<11;S>	11
<C.8;H>	8
<C.14;H>	14

True\Predicted	T	F
T	5	0
F	0	

FAME2 predicted results (Promethazine)



FAME2 Predicted SoMs

Molecule Promethazine

Atom Probability

C.20 0.998

C.19 0.998

S.11 0.984

C.14 0.576

C.8 0.576

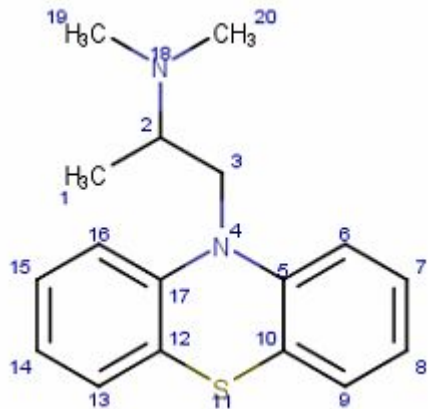
C.13 0.298

C.9 0.298

N.18 0.118

True\Predicted	T	F
T	5	0
F	0	

CypBoM-All predicted results (Promethazine)

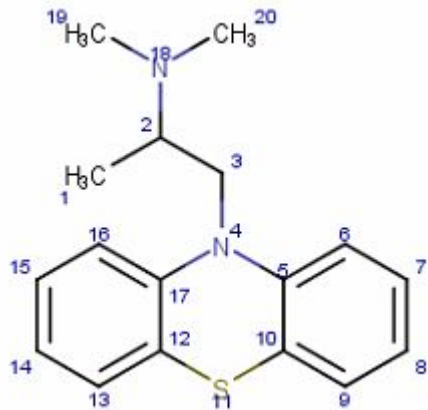


CypBoM-Tri predicted BoMs	Converted True SoMs
<C.19;N.18> <C.19;H>	12
<C.20;N.18> <C.20;H>	14
<11;S>	11
<C.8;H>	8
<C.14;H>	14

True\Predicted	T	F
T	5	0
F	0	

FAME3 predicted results

(Promethazine)



FAME2 Predicted SoMs		
Molecule mol_2		
Atom	Probability	FAMEscore
C.20	0.863	0.724
C.19	0.863	0.724
N.18	0.724	0.702
S.11	0.468	0.653
C.14	0.436	0.708
C.8	0.436	0.708
C.2	0.364	0.733
N.4	0.132	0.702
C.3	0.128	0.742
C.1	0.124	0.702
C.13	0.076	0.702
C.9	0.076	0.702
C.15	0.063	0.73
C.7	0.063	0.73
C.17	0.004	0.72
C.12	0.004	0.694
C.10	0.004	0.694
C.5	0.004	0.72
C.16	0.0	0.73
C.6	0.0	0.73

True\Predicted	T	F
T	5	0
F	1	