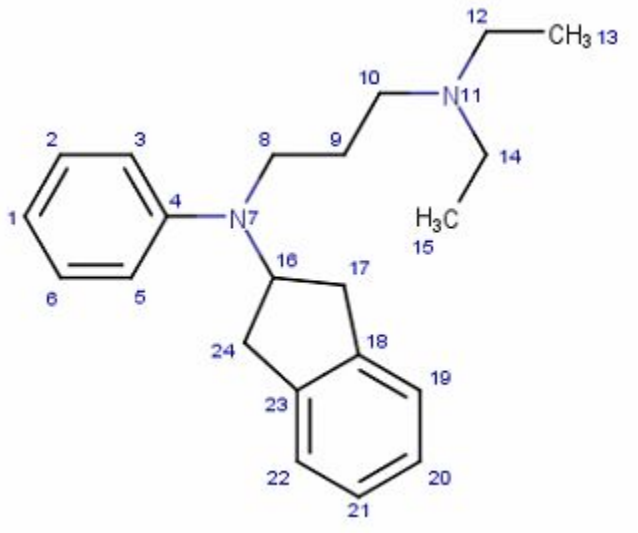
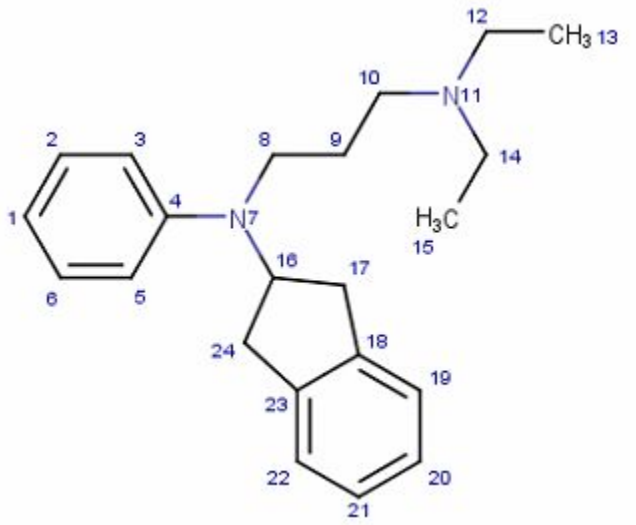
NZLBHDRPUJLHCE-UHFFFAOYSA-N (Aprindine)



True BoMs	Converted True SoMs
<12,11;Cleavage;R1> <12,H;Oxidation;R1>	12
<14,11;Cleavage;R2> <14,H;Oxidation;R2>	14
<21,H;Hydroxylation;R3>	21
<20,H;Hydroxylation;R3>	20
<1,H;Hydroxylation;R3>	1

FAME2 Predicted Result (Aprindine)



FAME2 Predicted SoMs

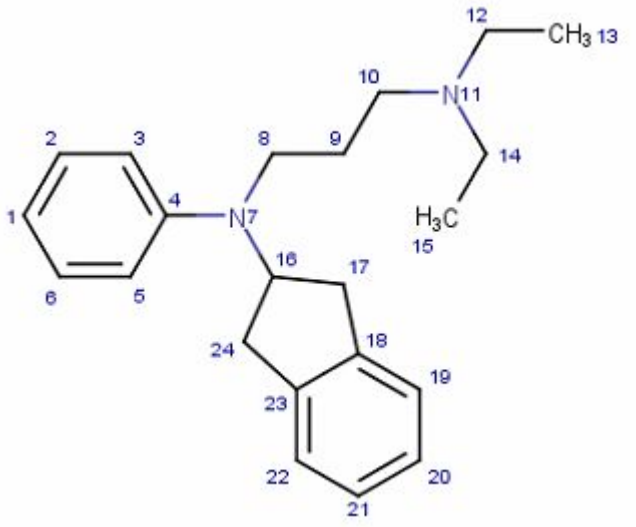
Model: circCDK_ATF_1

Molecule Aprindine

Atom	Probability
C.14	**0.954**
C.12	**0.954**
C.21	**0.586**
C.20	**0.586**
C.1	0.37
C.24	0.216
C.17	0.216

True\Predicted	T	F
T	4	1
F	0	

CypBoM-Tri Predicted Result (Aprindine)



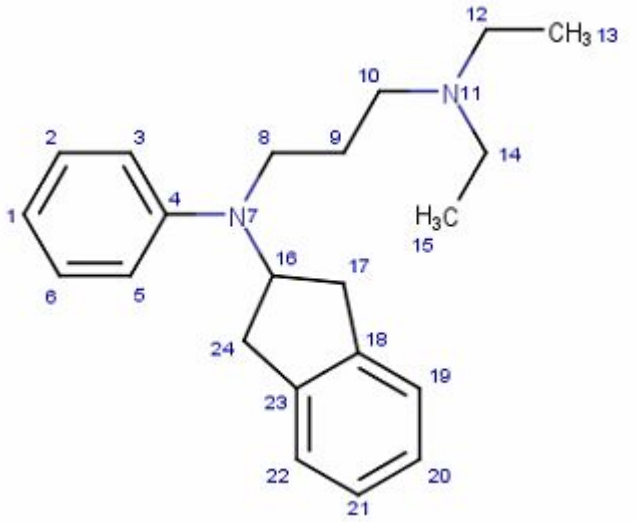
CypBoM-Tri predicted BoMs	Converted True SoMs
<12,11> <12,H>	12
<14,11> <14,H>	14
<10,11>	10

In the rules used to convert BoM to SoM:

- If the BoM_{X-Y} is a ⟨η-η⟩ bond ⟨i, j⟩
  - if atom i is C (Carbon) and atom j is N (Nitrogen), O (Oxygen) or S (Sulfur) and the reaction is dealkylation or deamination, then atom i is the SoM

True\Predicted	T	F
T	2	3
F	1	

FAME2 Predicted Result (Aprindine)



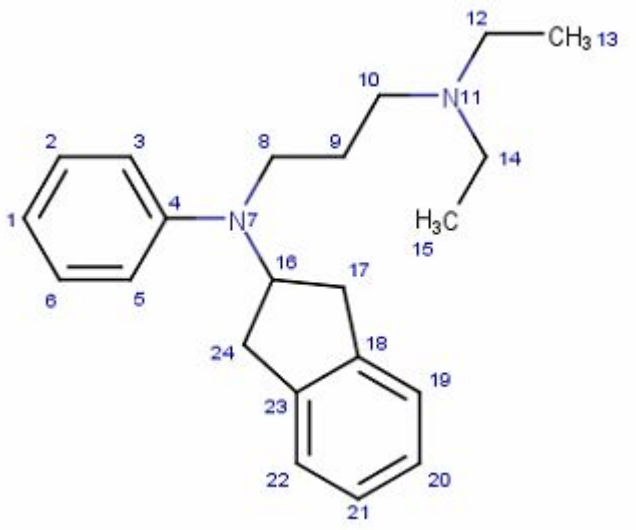
FAME3 Predicted SoMs

Molecule mol_17

Atom	Probability	FAMEscore
C.14	0.339	0.6
C.12	0.339	0.6
C.10	0.288	0.619
N.11	0.268	0.574
C.21	0.268	0.636
C.20	0.268	0.636
C.8	0.24	0.621
C.1	0.206	0.629
C.24	0.172	0.712

True\Predicted	T	F
T	0	5
F	0	

CypBoM-All Predicted Result (Aprindine)



CypBoM-Tri predicted BoMs	Converted True SoMs
<12,11> <12,H>	12
<14,11> <14,H>	14
<10,11>	10

In the rules used to convert BoM to SoM:

- If the BoM_{X-Y} is a ⟨η-η⟩ bond ⟨i, j⟩
  - if atom i is C (Carbon) and atom j is N (Nitrogen), O (Oxygen) or S (Sulfur) and the reaction is dealkylation or deamination, then atom i is the SoM

True\Predicted	T	F
T	2	3
F	1	