

Session: Ames Mutagenicity, Model: AMG_Ames Mutagenicity_Model_DT14

Fri May 13 2011, 12:01

Modeled property: Tox

Modeling technique: Decision Tree

Model Statistics:

	Number	Kappa	Accuracy
TRN	4594	0.8084	0.9051
VAL	1149	0.5846	0.7946

Parameters used:

Descriptor pre-selection:

- Threshold for minimum occurrence: 4%
- Threshold for minimum standard deviation: 0.0005
- Threshold for maximum correlation between descriptors: 0.95

Descriptors remaining after pre-selection: 154

Descriptors used in the model: 108

Model details:

Data was classified into 2 classes

- class Non-mutagenic
- class Mutagenic

Confusion Matrices

Training set

		Predicted	
		Non-mutagenic	Mutagenic
Observed	Non-mutagenic	1857	211
	Mutagenic	225	2301

Sensitivity for Non-mutagenic: 0.898

Specificity for Non-mutagenic: 0.892

Sensitivity for Mutagenic: 0.911

Specificity for Mutagenic: 0.916

Validation set

		Predicted	
		Non-mutagenic	Mutagenic
Observed	Non-mutagenic	396	116
	Mutagenic	120	517

Sensitivity for Non-mutagenic: 0.773

Specificity for Non-mutagenic: 0.767

Sensitivity for Mutagenic: 0.812
Specificity for Mutagenic: 0.817

Descriptors

logP
Vx
NegativeCharge
PositiveCharge
Flex
ERTLNotPSA
HBA-prof
HBD-lip
HBD-prof
CH1Aa
CH2Aa
CH2hetero
CH2link
CH3Aa
CH3hetero
Ester
HaloC
NO
NRB
allylic-oxyd-t10
aminoethanol1
anycarbonyl
aromCl
aromO
arylNHCO
benzylicOH
branchedCnotRing
est-lact-latm-carbm-t7
ether
intraHbond5
intraHbond6
lipovolume
nonring-at
p-hetero-or-halo
phenolic-tautomer
pyridine
ring-join
ringOdouble
ringat
t-16-1
nC(sp2)
nC(sp3)
nOH
nCO
nX
ssCH2
dsCH
aaCH
sssCH
dssC
aasC
aaaC

ssssC
sNH2
dsN
aaN
sOH
ssO
dS
sCl
nNneutral
PRX-time-1
UB
HAN
HAT
HAO
AliRingAttachment
C4
C6
C3
C1
C11
N8
N2
H3
BasicGroup
H4
O3
O5
O9
O10
HydrophobicGroup
H1a
C5
C21
C23
ed70
ed40
ew10
f004
f007
f244
f245
f407
f440
f441
q017
q039
q137
q192
q257
q300
q358
q453
q457
q458
q481
frg-8

Decision Tree

```
O5 > 0
-->
aaaC > 0
--> Result: Mutagenic(Trn: 373/23 Val:82/7 Test:0/0) Leaf 1
aaaC <= 0
-->
HAT > 2
-->
HBD-lip > 3
-->
N8 > 0
--> Result: Mutagenic(Trn: 5/0 Val:1/0 Test:0/0) Leaf 2
N8 <= 0
-->
nOH > 0
--> Result: Non-mutagenic(Trn: 11/1 Val:8/5 Test:0/0) Leaf 3
nOH <= 0
--> Result: Mutagenic(Trn: 5/1 Val:1/0 Test:0/0) Leaf 4
HBD-lip <= 3
-->
q481 > 3
-->
nCO > 0
-->
f441 > 3
-->
C3 > 2
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 5
C3 <= 2
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 6
f441 <= 3
--> Result: Mutagenic(Trn: 54/0 Val:17/6 Test:0/0) Leaf 7
nCO <= 0
-->
lipovolume > 5
--> Result: Non-mutagenic(Trn: 3/0 Val:2/0 Test:0/0) Leaf 8
lipovolume <= 5
-->
q457 > 2
--> Result: Mutagenic(Trn: 13/0 Val:1/0 Test:0/0) Leaf 9
q457 <= 2
-->
HBD-lip > 1
--> Result: Non-mutagenic(Trn: 6/1 Val:1/0 Test:0/0) Leaf 10
HBD-lip <= 1
--> Result: Mutagenic(Trn: 18/5 Val:5/2 Test:0/0) Leaf 11
q481 <= 3
--> Result: Mutagenic(Trn: 163/3 Val:44/3 Test:0/0) Leaf 12
HAT <= 2
-->
nOH > 0
-->
f007 > 1
--> Result: Non-mutagenic(Trn: 8/0 Val:2/2 Test:0/0) Leaf 13
f007 <= 1
-->
q453 > 5
--> Result: Mutagenic(Trn: 10/2 Val:2/0 Test:0/0) Leaf 14
q453 <= 5
-->
CH2link > 0
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 15
CH2link <= 0
--> Result: Non-mutagenic(Trn: 12/1 Val:3/2 Test:0/0) Leaf 16
nOH <= 0
-->
logP > 2.37313
-->
frg-8 > 0
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--> Result: Mutagenic(Trn: 28/3 Val:11/0 Test:0/0) Leaf 17
frg-8 <= 0
-->
ringat > 12
--> Result: Mutagenic(Trn: 9/0 Val:2/2 Test:0/0) Leaf 18
ringat <= 12
-->
aasC > 4
--> Result: Non-mutagenic(Trn: 12/0 Val:1/0 Test:0/0) Leaf 19
aasC <= 4
-->
HBD-lip > 0
-->
f004 > 0
--> Result: Mutagenic(Trn: 13/4 Val:5/1 Test:0/0) Leaf 20
f004 <= 0
--> Result: Non-mutagenic(Trn: 22/4 Val:6/4 Test:0/0) Leaf 21
HBD-lip <= 0
--> Result: Mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 22
logP <= 2.37313
-->
q137 > 10
--> Result: Mutagenic(Trn: 48/0 Val:4/0 Test:0/0) Leaf 23
q137 <= 10
-->
NRB > 3
--> Result: Mutagenic(Trn: 86/14 Val:27/3 Test:0/0) Leaf 24
NRB <= 3
-->
q453 > 0
--> Result: Mutagenic(Trn: 17/5 Val:5/2 Test:0/0) Leaf 25
q453 <= 0
--> Result: Non-mutagenic(Trn: 8/1 Val:1/1 Test:0/0) Leaf 26
O5 <= 0
-->
ring-join > 2
-->
HBA-prof > 4
-->
phenolic-tautomer > 0
-->
aromO > 1
--> Result: Non-mutagenic(Trn: 6/0 Val:0/0 Test:0/0) Leaf 27
aromO <= 1
-->
CH1Aa > 0
--> Result: Non-mutagenic(Trn: 6/1 Val:2/1 Test:0/0) Leaf 28
CH1Aa <= 0
--> Result: Mutagenic(Trn: 22/2 Val:4/2 Test:0/0) Leaf 29
phenolic-tautomer <= 0
--> Result: Non-mutagenic(Trn: 19/2 Val:7/3 Test:0/0) Leaf 30
HBA-prof <= 4
-->
branchedCnotRing > 0
--> Result: Non-mutagenic(Trn: 4/0 Val:1/1 Test:0/0) Leaf 31
branchedCnotRing <= 0
-->
Vx > 209.45
-->
sCl > 1
--> Result: Non-mutagenic(Trn: 3/0 Val:1/0 Test:0/0) Leaf 32
sCl <= 1
-->
ringOdouble > 0
-->
O10 > 1
--> Result: Mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 33
O10 <= 1
-->
q192 > 9
--> Result: Non-mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 34
q192 <= 9

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-->
C1 > 1
--> Result: Non-mutagenic(Trn: 3/0 Val:1/0 Test:0/0) Leaf 35
C1 <= 1
--> Result: Mutagenic(Trn: 3/0 Val:1/1 Test:0/0) Leaf 36
ringOdouable <= 0
-->
q458 > 12
-->
N2 > 0
--> Result: Non-mutagenic(Trn: 2/0 Val:1/1 Test:0/0) Leaf 37
N2 <= 0
-->
f004 > 0
--> Result: Mutagenic(Trn: 81/9 Val:26/8 Test:0/0) Leaf 38
f004 <= 0
-->
HBD-lip > 0
-->
aasC > 3
--> Result: Non-mutagenic(Trn: 4/0 Val:2/1 Test:0/0) Leaf 39
aasC <= 3
-->
q458 > 18
--> Result: Mutagenic(Trn: 22/4 Val:7/1 Test:0/0) Leaf 40
q458 <= 18
-->
q458 > 15
--> Result: Non-mutagenic(Trn: 18/7 Val:3/1 Test:0/0) Leaf 41
q458 <= 15
--> Result: Mutagenic(Trn: 3/0 Val:1/0 Test:0/0) Leaf 42
HBD-lip <= 0
--> Result: Mutagenic(Trn: 40/4 Val:13/3 Test:0/0) Leaf 43
q458 <= 12
--> Result: Mutagenic(Trn: 15/0 Val:2/0 Test:0/0) Leaf 44
Vx <= 209.45
--> Result: Mutagenic(Trn: 344/34 Val:98/14 Test:0/0) Leaf 45
ring-join <= 2
-->
HydrophobicGroup > 1
-->
NO > 0
--> Result: Mutagenic(Trn: 11/0 Val:4/1 Test:0/0) Leaf 46
NO <= 0
-->
nC(sp2) > 7
-->
ERTLNotPSA > 9.23
-->
H1a > 0
-->
Vx > 285.56
-->
f407 > 4
-->
lipovolume > 7
--> Result: Non-mutagenic(Trn: 4/1 Val:1/0 Test:0/0) Leaf 47
lipovolume <= 7
--> Result: Mutagenic(Trn: 4/0 Val:0/0 Test:0/0) Leaf 48
f407 <= 4
--> Result: Non-mutagenic(Trn: 21/0 Val:4/0 Test:0/0) Leaf 49
Vx <= 285.56
-->
C3 > 0
--> Result: Mutagenic(Trn: 8/1 Val:1/0 Test:0/0) Leaf 50
C3 <= 0
--> Result: Non-mutagenic(Trn: 12/4 Val:2/1 Test:0/0) Leaf 51
H1a <= 0
--> Result: Non-mutagenic(Trn: 12/0 Val:3/1 Test:0/0) Leaf 52
ERTLNotPSA <= 9.23
--> Result: Mutagenic(Trn: 10/1 Val:4/1 Test:0/0) Leaf 53
nC(sp2) <= 7

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-->
ERTLNotPSA > 29.1
-->
Ester > 2
-->
anycarbonyl > 3
--> Result: Non-mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 54
anycarbonyl <= 3
--> Result: Mutagenic(Trn: 6/0 Val:0/0 Test:0/0) Leaf 55
Ester <= 2
-->
q017 > 15
--> Result: Non-mutagenic(Trn: 56/0 Val:10/0 Test:0/0) Leaf 56
q017 <= 15
-->
UB > 10
--> Result: Non-mutagenic(Trn: 17/0 Val:4/1 Test:0/0) Leaf 57
UB <= 10
-->
ssCH2 > 3
-->
N8 > 0
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 58
N8 <= 0
-->
branchedCnotRing > 1
-->
f244 > 5
--> Result: Mutagenic(Trn: 5/0 Val:2/1 Test:0/0) Leaf 59
f244 <= 5
--> Result: Non-mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 60
branchedCnotRing <= 1
-->
Vx > 96.09
-->
f441 > 11
--> Result: Non-mutagenic(Trn: 22/0 Val:0/0 Test:0/0) Leaf 61
f441 <= 11
-->
CH1Aa > 0
-->
CH1Aa > 2
--> Result: Non-mutagenic(Trn: 21/1 Val:5/1 Test:0/0) Leaf 62
CH1Aa <= 2
-->
UB > 0
-->
Vx > 257.54
-->
nC(sp3) > 16
--> Result: Non-mutagenic(Trn: 7/2 Val:1/0 Test:0/0) Leaf 63
nC(sp3) <= 16
--> Result: Mutagenic(Trn: 4/0 Val:1/0 Test:0/0) Leaf 64
Vx <= 257.54
--> Result: Non-mutagenic(Trn: 11/1 Val:5/2 Test:0/0) Leaf 65
UB <= 0
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 66
CH1Aa <= 0
--> Result: Non-mutagenic(Trn: 47/2 Val:13/1 Test:0/0) Leaf 67
Vx <= 96.09
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 68
ssCH2 <= 3
-->
ssCH2 > 0
-->
q257 > 1
-->
ERTLNotPSA > 72.83
--> Result: Mutagenic(Trn: 6/0 Val:1/0 Test:0/0) Leaf 69
ERTLNotPSA <= 72.83
-->
CH2Aa > 2

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--> Result: Mutagenic(Trn: 3/0 Val:2/1 Test:0/0) Leaf 70
CH2Aa <= 2
--> Result: Non-mutagenic(Trn: 15/1 Val:10/3 Test:0/0) Leaf 71
q257 <= 1
--> Result: Mutagenic(Trn: 7/0 Val:3/1 Test:0/0) Leaf 72
ssCH2 <= 0
--> Result: Non-mutagenic(Trn: 6/0 Val:3/2 Test:0/0) Leaf 73
ERTLNotPSA <= 29.1
--> Result: Non-mutagenic(Trn: 151/7 Val:42/3 Test:0/0) Leaf 74
HydrophobicGroup <= 1
-->
nC(sp2) > 9
-->
Flex > 0.121212
-->
NO > 0
-->
f007 > 1
--> Result: Non-mutagenic(Trn: 7/1 Val:1/0 Test:0/0) Leaf 75
f007 <= 1
--> Result: Mutagenic(Trn: 45/3 Val:8/0 Test:0/0) Leaf 76
NO <= 0
-->
intraHbond6 > 1
-->
ringOdouble > 0
--> Result: Mutagenic(Trn: 16/0 Val:3/1 Test:0/0) Leaf 77
ringOdouble <= 0
-->
CH2Aa > 1
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 78
CH2Aa <= 1
--> Result: Non-mutagenic(Trn: 4/0 Val:3/1 Test:0/0) Leaf 79
intraHbond6 <= 1
-->
q039 > 10
--> Result: Non-mutagenic(Trn: 39/3 Val:15/2 Test:0/0) Leaf 80
q039 <= 10
-->
ERTLNotPSA > 83.83
-->
ringOdouble > 1
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 81
ringOdouble <= 1
-->
CH3hetero > 0
-->
O3 > 1
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 82
O3 <= 1
--> Result: Non-mutagenic(Trn: 11/1 Val:4/2 Test:0/0) Leaf 83
CH3hetero <= 0
--> Result: Non-mutagenic(Trn: 34/0 Val:8/2 Test:0/0) Leaf 84
ERTLNotPSA <= 83.83
-->
q300 > 0
-->
pyridine > 0
-->
N2 > 0
--> Result: Mutagenic(Trn: 2/0 Val:1/1 Test:0/0) Leaf 85
N2 <= 0
--> Result: Non-mutagenic(Trn: 19/0 Val:6/1 Test:0/0) Leaf 86
pyridine <= 0
-->
q300 > 5
--> Result: Non-mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 87
q300 <= 5
-->
dsN > 1
--> Result: Mutagenic(Trn: 32/4 Val:9/2 Test:0/0) Leaf 88
dsN <= 1

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-->
ether > 0
-->
NegativeCharge > 0
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 89
NegativeCharge <= 0
-->
HAN > 0
-->
aasC > 3
--> Result: Mutagenic(Trn: 22/0 Val:8/3 Test:0/0) Leaf 90
aasC <= 3
-->
frg-8 > 0
--> Result: Mutagenic(Trn: 4/0 Val:1/0 Test:0/0) Leaf 91
frg-8 <= 0
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 92
HAN <= 0
--> Result: Non-mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 93
ether <= 0
-->
q300 > 3
--> Result: Mutagenic(Trn: 10/1 Val:3/2 Test:0/0) Leaf 94
q300 <= 3
-->
q453 > 8
--> Result: Non-mutagenic(Trn: 7/0 Val:4/1 Test:0/0) Leaf 95
q453 <= 8
-->
f440 > 4
--> Result: Non-mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 96
f440 <= 4
-->
q453 > 1
-->
p-hetero-or-halo > 0
--> Result: Non-mutagenic(Trn: 4/0 Val:0/0 Test:0/0) Leaf 97
p-hetero-or-halo <= 0
-->
q481 > 4
-->
logP > 1.71515
-->
aaCH > 7
-->
f440 > 0
--> Result: Non-mutagenic(Trn: 4/0 Val:1/1 Test:0/0) Leaf 98
f440 <= 0
--> Result: Mutagenic(Trn: 10/2 Val:1/0 Test:0/0) Leaf 99
aaCH <= 7
--> Result: Mutagenic(Trn: 5/0 Val:1/1 Test:0/0) Leaf 100
logP <= 1.71515
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 101
q481 <= 4
--> Result: Mutagenic(Trn: 9/0 Val:6/1 Test:0/0) Leaf 102
q453 <= 1
--> Result: Non-mutagenic(Trn: 15/3 Val:2/0 Test:0/0) Leaf 103
q300 <= 0
-->
CH2hetero > 0
-->
sssCH > 0
--> Result: Mutagenic(Trn: 13/1 Val:4/0 Test:0/0) Leaf 104
sssCH <= 0
-->
ringOdouble > 0
--> Result: Mutagenic(Trn: 3/0 Val:1/1 Test:0/0) Leaf 105
ringOdouble <= 0
-->
Flex > 0.266667
-->
est-lact-latm-carbm-t7 > 0

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--> Result: Non-mutagenic(Trn: 4/1 Val:0/0 Test:0/0) Leaf 106
est-lact-latm-carbm-t7 <= 0
--> Result: Mutagenic(Trn: 3/0 Val:2/1 Test:0/0) Leaf 107
Flex <= 0.266667
--> Result: Non-mutagenic(Trn: 12/0 Val:2/1 Test:0/0) Leaf 108
CH2hetero <= 0
--> Result: Non-mutagenic(Trn: 51/6 Val:17/4 Test:0/0) Leaf 109
Flex <= 0.121212
-->
sNH2 > 0
--> Result: Mutagenic(Trn: 93/11 Val:13/0 Test:0/0) Leaf 110
sNH2 <= 0
-->
C11 > 0
-->
benzylicOH > 1
--> Result: Non-mutagenic(Trn: 8/2 Val:1/1 Test:0/0) Leaf 111
benzylicOH <= 1
-->
nC(sp2) > 15
--> Result: Mutagenic(Trn: 27/0 Val:6/0 Test:0/0) Leaf 112
nC(sp2) <= 15
-->
C23 > 3
--> Result: Non-mutagenic(Trn: 6/1 Val:5/2 Test:0/0) Leaf 113
C23 <= 3
-->
NRB > 10
--> Result: Mutagenic(Trn: 23/0 Val:8/1 Test:0/0) Leaf 114
NRB <= 10
-->
Vx > 194.46
--> Result: Non-mutagenic(Trn: 4/0 Val:2/1 Test:0/0) Leaf 115
Vx <= 194.46
--> Result: Mutagenic(Trn: 26/5 Val:1/0 Test:0/0) Leaf 116
C11 <= 0
-->
ew10 > 0
--> Result: Non-mutagenic(Trn: 37/9 Val:8/1 Test:0/0) Leaf 117
ew10 <= 0
-->
f245 > 1
--> Result: Non-mutagenic(Trn: 13/1 Val:0/0 Test:0/0) Leaf 118
f245 <= 1
-->
f007 > 0
-->
ed70 > 1
--> Result: Non-mutagenic(Trn: 14/4 Val:4/1 Test:0/0) Leaf 119
ed70 <= 1
--> Result: Mutagenic(Trn: 81/17 Val:30/10 Test:0/0) Leaf 120
f007 <= 0
-->
aaN > 1
--> Result: Mutagenic(Trn: 5/0 Val:1/0 Test:0/0) Leaf 121
aaN <= 1
-->
O3 > 0
--> Result: Mutagenic(Trn: 3/0 Val:2/2 Test:0/0) Leaf 122
O3 <= 0
-->
nonring-at > 1
-->
Vx > 124.39
-->
logP > 3.05964
-->
q192 > 0
--> Result: Mutagenic(Trn: 13/4 Val:1/0 Test:0/0) Leaf 123
q192 <= 0
--> Result: Non-mutagenic(Trn: 3/0 Val:1/0 Test:0/0) Leaf 124
logP <= 3.05964

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--> Result: Non-mutagenic(Trn: 8/0 Val:3/0 Test:0/0) Leaf 125
Vx <= 124.39
--> Result: Mutagenic(Trn: 4/0 Val:0/0 Test:0/0) Leaf 126
nonring-at <= 1
--> Result: Non-mutagenic(Trn: 19/3 Val:5/1 Test:0/0) Leaf 127
nC(sp2) <= 9
-->
logP > 3.24756
-->
nC(sp3) > 0
-->
nNneutral > 2
--> Result: Mutagenic(Trn: 3/0 Val:1/0 Test:0/0) Leaf 128
nNneutral <= 2
-->
ssCH2 > 5
--> Result: Mutagenic(Trn: 7/2 Val:1/1 Test:0/0) Leaf 129
ssCH2 <= 5
-->
nX > 1
-->
ssssC > 2
--> Result: Non-mutagenic(Trn: 11/0 Val:2/0 Test:0/0) Leaf 130
ssssC <= 2
-->
q458 > 2
-->
sCl > 3
-->
nonring-at > 10
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 131
nonring-at <= 10
--> Result: Mutagenic(Trn: 5/0 Val:1/1 Test:0/0) Leaf 132
sCl <= 3
--> Result: Non-mutagenic(Trn: 28/4 Val:10/1 Test:0/0) Leaf 133
q458 <= 2
--> Result: Mutagenic(Trn: 7/1 Val:2/0 Test:0/0) Leaf 134
nX <= 1
--> Result: Non-mutagenic(Trn: 47/2 Val:11/2 Test:0/0) Leaf 135
nC(sp3) <= 0
--> Result: Non-mutagenic(Trn: 44/0 Val:5/0 Test:0/0) Leaf 136
logP <= 3.24756
-->
nX > 0
-->
aromCl > 0
-->
HAO > 1
--> Result: Non-mutagenic(Trn: 56/4 Val:14/1 Test:0/0) Leaf 137
HAO <= 1
-->
Vx > 113.44
-->
aaCH > 0
-->
q453 > 2
-->
aminoethanol1 > 0
--> Result: Non-mutagenic(Trn: 2/0 Val:1/0 Test:0/0) Leaf 138
aminoethanol1 <= 0
-->
C21 > 0
--> Result: Mutagenic(Trn: 6/0 Val:3/2 Test:0/0) Leaf 139
C21 <= 0
-->
aaCH > 3
--> Result: Non-mutagenic(Trn: 6/1 Val:1/0 Test:0/0) Leaf 140
aaCH <= 3
--> Result: Mutagenic(Trn: 13/3 Val:3/0 Test:0/0) Leaf 141
q453 <= 2
--> Result: Mutagenic(Trn: 7/0 Val:2/1 Test:0/0) Leaf 142
aaCH <= 0

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--> Result: Non-mutagenic(Trn: 5/0 Val:1/0 Test:0/0) Leaf 143
Vx <= 113.44
--> Result: Non-mutagenic(Trn: 48/8 Val:8/3 Test:0/0) Leaf 144
aromCl <= 0
-->
allylic-oxyd-t10 > 0
-->
HAT > 3
-->
C3 > 0
--> Result: Non-mutagenic(Trn: 3/0 Val:2/2 Test:0/0) Leaf 145
C3 <= 0
--> Result: Mutagenic(Trn: 2/0 Val:1/1 Test:0/0) Leaf 146
HAT <= 3
--> Result: Mutagenic(Trn: 38/0 Val:9/0 Test:0/0) Leaf 147
allylic-oxyd-t10 <= 0
-->
C3 > 3
-->
sCl > 2
-->
q453 > 0
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 148
q453 <= 0
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 149
sCl <= 2
--> Result: Mutagenic(Trn: 32/0 Val:4/1 Test:0/0) Leaf 150
C3 <= 3
-->
ssssC > 0
-->
dsCH > 0
--> Result: Mutagenic(Trn: 4/0 Val:0/0 Test:0/0) Leaf 151
dsCH <= 0
-->
sCl > 2
-->
HBA-prof > 0
-->
Vx > 169.24
--> Result: Non-mutagenic(Trn: 2/0 Val:1/1 Test:0/0) Leaf 152
Vx <= 169.24
--> Result: Mutagenic(Trn: 8/1 Val:1/0 Test:0/0) Leaf 153
HBA-prof <= 0
--> Result: Non-mutagenic(Trn: 3/0 Val:5/2 Test:0/0) Leaf 154
sCl <= 2
--> Result: Non-mutagenic(Trn: 43/8 Val:7/1 Test:0/0) Leaf 155
ssssC <= 0
-->
nX > 1
-->
logP > 2.55413
--> Result: Non-mutagenic(Trn: 21/8 Val:3/3 Test:0/0) Leaf 156
logP <= 2.55413
--> Result: Mutagenic(Trn: 59/10 Val:12/1 Test:0/0) Leaf 157
nX <= 1
-->
C11 > 0
--> Result: Non-mutagenic(Trn: 11/1 Val:2/0 Test:0/0) Leaf 158
C11 <= 0
-->
HaloC > 0
-->
logP > 1.77374
-->
HBD-lip > 0
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 159
HBD-lip <= 0
--> Result: Non-mutagenic(Trn: 12/4 Val:3/3 Test:0/0) Leaf 160
logP <= 1.77374
--> Result: Mutagenic(Trn: 22/2 Val:8/0 Test:0/0) Leaf 161
HaloC <= 0

```

```

-->
ssO > 0
--> Result: Non-mutagenic(Trn: 15/2 Val:4/1 Test:0/0) Leaf 162
ssO <= 0
-->
C21 > 1
--> Result: Mutagenic(Trn: 5/0 Val:1/0 Test:0/0) Leaf 163
C21 <= 1
-->
logP > 2.10897
--> Result: Mutagenic(Trn: 13/3 Val:7/5 Test:0/0) Leaf 164
logP <= 2.10897
-->
H1a > 0
--> Result: Mutagenic(Trn: 7/1 Val:1/0 Test:0/0) Leaf 165
H1a <= 0
-->
Vx > 66.94
-->
t-16-1 > 0
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 166
t-16-1 <= 0
-->
C5 > 1
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 167
C5 <= 1
-->
q137 > 2
--> Result: Non-mutagenic(Trn: 12/1 Val:3/2 Test:0/0) Leaf 168
q137 <= 2
-->
HAT > 1
--> Result: Non-mutagenic(Trn: 8/2 Val:1/1 Test:0/0) Leaf 169
HAT <= 1
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 170
Vx <= 66.94
--> Result: Non-mutagenic(Trn: 7/0 Val:2/2 Test:0/0) Leaf 171

nX <= 0
-->
PositiveCharge > 2
-->
q300 > 5
--> Result: Non-mutagenic(Trn: 6/0 Val:1/0 Test:0/0) Leaf 172
q300 <= 5
-->
dsN > 0
--> Result: Mutagenic(Trn: 26/1 Val:9/0 Test:0/0) Leaf 173
dsN <= 0
-->
q137 > 12
-->
ERTLNotPSA > 106.18
-->
H3 > 1
--> Result: Mutagenic(Trn: 4/0 Val:1/1 Test:0/0) Leaf 174
H3 <= 1
--> Result: Non-mutagenic(Trn: 11/2 Val:2/2 Test:0/0) Leaf 175
ERTLNotPSA <= 106.18
--> Result: Mutagenic(Trn: 18/1 Val:4/1 Test:0/0) Leaf 176
q137 <= 12
-->
q137 > 8
--> Result: Non-mutagenic(Trn: 11/0 Val:4/0 Test:0/0) Leaf 177
q137 <= 8
-->
UB > 5
--> Result: Mutagenic(Trn: 6/0 Val:3/0 Test:0/0) Leaf 178
UB <= 5
-->
aminoethanol1 > 1
--> Result: Mutagenic(Trn: 2/0 Val:1/0 Test:0/0) Leaf 179
aminoethanol1 <= 1

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```

--> Result: Non-mutagenic(Trn: 6/0 Val:1/0 Test:0/0) Leaf 180
PositiveCharge <= 2
-->
t-16-1 > 0
-->
anycarbonyl > 0
-->
arylNHCO > 0
--> Result: Mutagenic(Trn: 3/0 Val:2/0 Test:0/0) Leaf 181
arylNHCO <= 0
--> Result: Non-mutagenic(Trn: 34/4 Val:11/2 Test:0/0) Leaf 182
anycarbonyl <= 0
--> Result: Mutagenic(Trn: 66/14 Val:17/5 Test:0/0) Leaf 183
t-16-1 <= 0
-->
O3 > 0
-->
ed40 > 0
-->
Vx > 186.72
--> Result: Non-mutagenic(Trn: 15/5 Val:5/1 Test:0/0) Leaf 184
Vx <= 186.72
-->
logP > 0.0110313
--> Result: Mutagenic(Trn: 33/1 Val:7/1 Test:0/0) Leaf 185
logP <= 0.0110313
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 186
ed40 <= 0
-->
dS > 0
--> Result: Mutagenic(Trn: 21/4 Val:5/1 Test:0/0) Leaf 187
dS <= 0
-->
q192 > 17
--> Result: Mutagenic(Trn: 5/0 Val:2/0 Test:0/0) Leaf 188
q192 <= 17
-->
est-lact-latm-carbm-t7 > 0
-->
PositiveCharge > 1
--> Result: Mutagenic(Trn: 2/0 Val:1/0 Test:0/0) Leaf 189
PositiveCharge <= 1
-->
BasicGroup > 0
--> Result: Mutagenic(Trn: 6/2 Val:5/2 Test:0/0) Leaf 190
BasicGroup <= 0
-->
CH2Aa > 0
--> Result: Non-mutagenic(Trn: 14/0 Val:3/1 Test:0/0) Leaf 191
CH2Aa <= 0
-->
HydrophobicGroup > 0
--> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 192
HydrophobicGroup <= 0
-->
ether > 0
-->
C6 > 0
--> Result: Non-mutagenic(Trn: 4/0 Val:1/0 Test:0/0) Leaf 193
C6 <= 0
--> Result: Mutagenic(Trn: 6/1 Val:1/0 Test:0/0) Leaf 194
ether <= 0
--> Result: Non-mutagenic(Trn: 47/5 Val:16/2 Test:0/0) Leaf 195
est-lact-latm-carbm-t7 <= 0
-->
NRB > 13
--> Result: Non-mutagenic(Trn: 11/0 Val:2/0 Test:0/0) Leaf 196
NRB <= 13
-->
C3 > 0
-->
lipovolume > 2

```

```

-->
q453 > 2
-->
  AliRingAttachment > 2
  --> Result: Mutagenic(Trn: 4/0 Val:0/0 Test:0/0) Leaf 197
  AliRingAttachment <= 2
  --> Result: Non-mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 198
q453 <= 2
  --> Result: Mutagenic(Trn: 13/0 Val:3/0 Test:0/0) Leaf 199
lipovolume <= 2
-->
  intraHbond5 > 0
  --> Result: Mutagenic(Trn: 5/0 Val:1/0 Test:0/0) Leaf 200
  intraHbond5 <= 0
  -->
  ether > 1
  -->
  C4 > 0
  --> Result: Mutagenic(Trn: 7/0 Val:1/0 Test:0/0) Leaf 201
  C4 <= 0
  -->
  q017 > 7
  --> Result: Mutagenic(Trn: 2/0 Val:1/1 Test:0/0) Leaf 202
  q017 <= 7
  -->
  ERTLNotPSA > 18.46
  --> Result: Non-mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 203
  ERTLNotPSA <= 18.46
  -->
  CH2link > 0
  --> Result: Mutagenic(Trn: 3/0 Val:2/2 Test:0/0) Leaf 204
  CH2link <= 0
  --> Result: Non-mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 205
ether <= 1
-->
  nC(sp3) > 2
  --> Result: Non-mutagenic(Trn: 53/14 Val:6/2 Test:0/0) Leaf 206
  nC(sp3) <= 2
  -->
  CH3hetero > 0
  -->
  lipovolume > 0
  --> Result: Mutagenic(Trn: 2/0 Val:0/0 Test:0/0) Leaf 207
  lipovolume <= 0
  --> Result: Non-mutagenic(Trn: 7/2 Val:4/1 Test:0/0) Leaf 208
  CH3hetero <= 0
  --> Result: Mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 209
C3 <= 0
-->
  nC(sp3) > 5
  --> Result: Non-mutagenic(Trn: 7/0 Val:0/0 Test:0/0) Leaf 210
  nC(sp3) <= 5
  -->
  CH3Aa > 1
  --> Result: Mutagenic(Trn: 7/2 Val:1/0 Test:0/0) Leaf 211
  CH3Aa <= 1
  -->
  Flex > 0
  --> Result: Non-mutagenic(Trn: 8/0 Val:1/0 Test:0/0) Leaf 212
  Flex <= 0
  -->
  ERTLNotPSA > 12.53
  --> Result: Non-mutagenic(Trn: 16/3 Val:2/1 Test:0/0) Leaf 213
  ERTLNotPSA <= 12.53
  --> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 214
O3 <= 0
-->
  H3 > 1
  -->
  HAN > 1
  -->
  q300 > 4

```

```

--> Result: Non-mutagenic(Trn: 10/0 Val:3/0 Test:0/0) Leaf 215
q300 <= 4
-->
q458 > 6
--> Result: Mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 216
q458 <= 6
-->
PRX-time-1 > 2
--> Result: Non-mutagenic(Trn: 4/0 Val:2/2 Test:0/0) Leaf 217
PRX-time-1 <= 2
-->
ERTLNotPSA > 95.5
--> Result: Mutagenic(Trn: 5/0 Val:0/0 Test:0/0) Leaf 218
ERTLNotPSA <= 95.5
-->
q453 > 3
--> Result: Non-mutagenic(Trn: 4/0 Val:1/1 Test:0/0) Leaf 219
q453 <= 3
-->
ERTLNotPSA > 71.09
--> Result: Mutagenic(Trn: 4/0 Val:0/0 Test:0/0) Leaf 220
ERTLNotPSA <= 71.09
-->
Vx > 76.32
-->
HBD-prof > 1
--> Result: Non-mutagenic(Trn: 6/2 Val:0/0 Test:0/0) Leaf 221
HBD-prof <= 1
--> Result: Mutagenic(Trn: 3/0 Val:0/0 Test:0/0) Leaf 222
Vx <= 76.32
--> Result: Non-mutagenic(Trn: 4/0 Val:1/1 Test:0/0) Leaf 223
HAN <= 1
--> Result: Mutagenic(Trn: 13/0 Val:7/0 Test:0/0) Leaf 224
H3 <= 1
-->
CH3Aa > 2
--> Result: Non-mutagenic(Trn: 24/0 Val:1/1 Test:0/0) Leaf 225
CH3Aa <= 2
-->
dsN > 1
--> Result: Mutagenic(Trn: 6/1 Val:5/0 Test:0/0) Leaf 226
dsN <= 1
-->
nC(sp2) > 7
-->
O10 > 1
--> Result: Mutagenic(Trn: 5/0 Val:2/0 Test:0/0) Leaf 227
O10 <= 1
-->
q358 > 0
--> Result: Non-mutagenic(Trn: 74/17 Val:26/4 Test:0/0) Leaf 228
q358 <= 0
--> Result: Mutagenic(Trn: 17/5 Val:3/2 Test:0/0) Leaf 229
nC(sp2) <= 7
-->
aaCH > 3
-->
nonring-at > 3
-->
nNneutral > 0
-->
UB > 6
--> Result: Non-mutagenic(Trn: 48/9 Val:12/2 Test:0/0) Leaf 230
UB <= 6
--> Result: Mutagenic(Trn: 7/1 Val:1/0 Test:0/0) Leaf 231
nNneutral <= 0
--> Result: Non-mutagenic(Trn: 21/0 Val:4/1 Test:0/0) Leaf 232
nonring-at <= 3
--> Result: Non-mutagenic(Trn: 76/1 Val:19/1 Test:0/0) Leaf 233
aaCH <= 3
-->
nonring-at > 0

```



```

-->
ether > 0
--> Result: Non-mutagenic(Trn: 26/1 Val:7/0 Test:0/0) Leaf 234
ether <= 0
-->
C5 > 0
-->
dssC > 1
--> Result: Non-mutagenic(Trn: 42/7 Val:11/2 Test:0/0) Leaf 235
dssC <= 1
-->
O9 > 1
--> Result: Mutagenic(Trn: 6/0 Val:1/0 Test:0/0) Leaf 236
O9 <= 1
-->
Vx > 46.48
-->
f407 > 0
--> Result: Non-mutagenic(Trn: 6/0 Val:3/0 Test:0/0) Leaf 237
f407 <= 0
-->
UB > 8
--> Result: Non-mutagenic(Trn: 6/0 Val:2/1 Test:0/0) Leaf 238
UB <= 8
-->
q453 > 2
--> Result: Mutagenic(Trn: 7/0 Val:3/3 Test:0/0) Leaf 239
q453 <= 2
-->
H4 > 0
-->
Vx > 108.62
--> Result: Mutagenic(Trn: 2/0 Val:1/0 Test:0/0) Leaf
240
Vx <= 108.62
--> Result: Non-mutagenic(Trn: 11/0 Val:2/0 Test:0/0)
Leaf 241
H4 <= 0
-->
CH2Aa > 0
--> Result: Non-mutagenic(Trn: 4/0 Val:0/0 Test:0/0)
Leaf 242
CH2Aa <= 0
-->
intraHbond6 > 0
--> Result: Non-mutagenic(Trn: 2/0 Val:0/0 Test:0/0)
Leaf 243
intraHbond6 <= 0
-->
sOH > 0
--> Result: Mutagenic(Trn: 5/0 Val:0/0 Test:0/0)
Leaf 244
sOH <= 0
-->
Vx > 88.37
--> Result: Non-mutagenic(Trn: 3/0 Val:0/0)
Test:0/0) Leaf 245
Vx <= 88.37
-->
UB > 2
--> Result: Mutagenic(Trn: 17/4 Val:2/1
Test:0/0) Leaf 246
UB <= 2
--> Result: Non-mutagenic(Trn: 6/1 Val:2/0)
Test:0/0) Leaf 247
Vx <= 46.48
--> Result: Non-mutagenic(Trn: 8/0 Val:1/1 Test:0/0) Leaf 248
C5 <= 0
--> Result: Non-mutagenic(Trn: 123/21 Val:33/3 Test:0/0) Leaf 249
nonring-at <= 0
--> Result: Mutagenic(Trn: 8/2 Val:1/1 Test:0/0) Leaf 250

```

