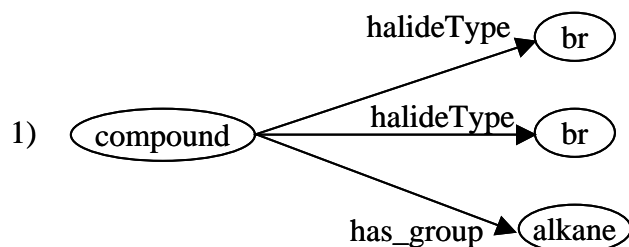


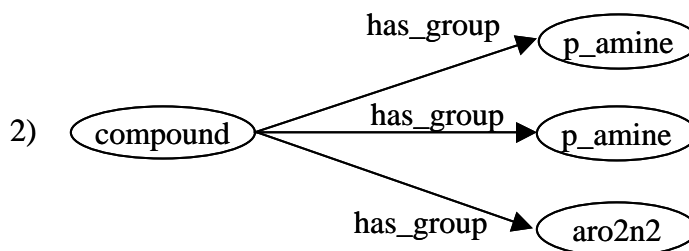
**PREDICTIVETOXICOLOGYCHALLENGE:  
ModelofToxicologyPredictionforMaleRats**

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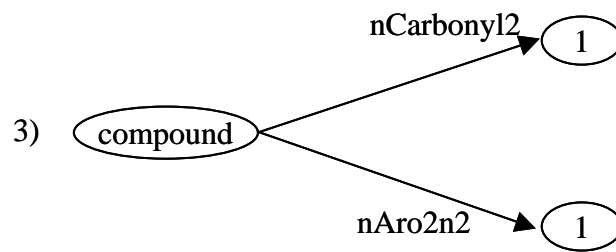
ThefollowinghypothesiswasgeneratedbytheSubdueCLsystemtopredictifachemical compoundwillcausecancerinmalerats.Thehypothesisstatesatachemical compoundthatcontainsoneormoreofthe24substructure spresentedbelowwillcause cancerinmalerats.Ifnoneofthesubstructuresarepresent,thenthecompoundwillnot causecancerinmalerats.BothagraphicalandEnglishdescriptionaregivenbelowfor eachsubstructure.



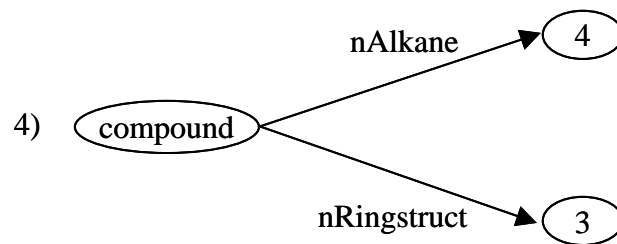
Acompoundthatcontains an *alkane*groupandtwo *halide* groupsoftype *bromine*willcausecancerinmalerats.



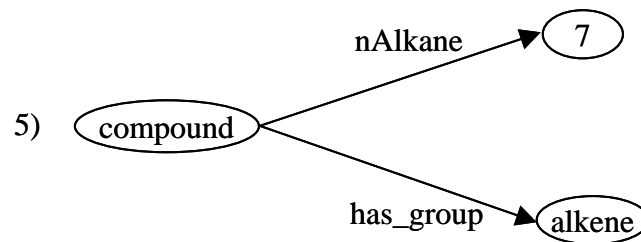
Acompoundthatcontainstwo *p\_amine*groupsandone *aro2n2*groupwillcausecancerinmalerats.



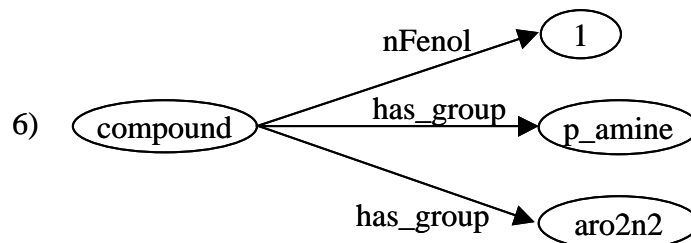
A compound that contains one *carbonyl2* group and one *aro2n2* group will cause cancer in male rats.



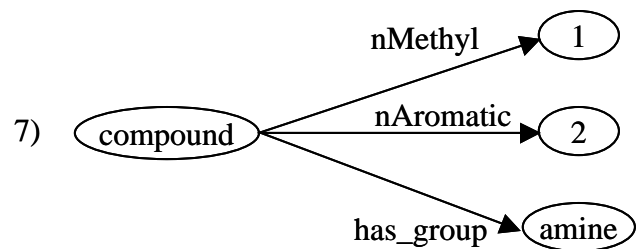
A compound that contains four *alkane* groups and three *ringstructures* will cause cancer in male rats.



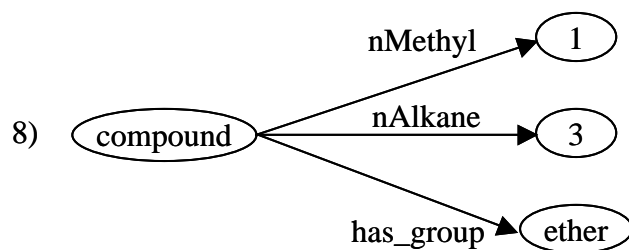
A compound that contains seven *alkane* groups and one *alkene* group will cause cancer in male rats.



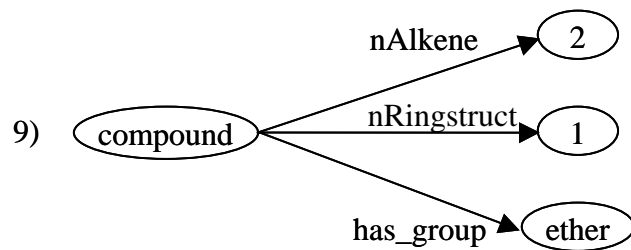
A compound that contains one *fenol* group, one *p\_amine* group, and one *aro2n2* group will cause cancer in male rats.



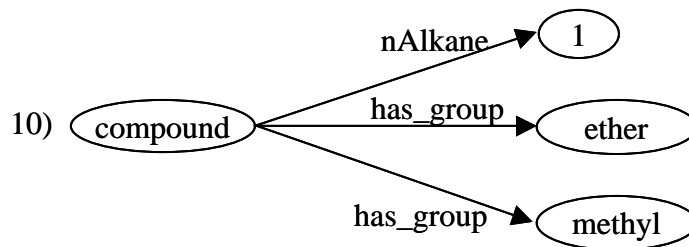
A compound that contains one *methyl* group, two *aromatic* groups, and one *amine* group will cause cancer in male rats.



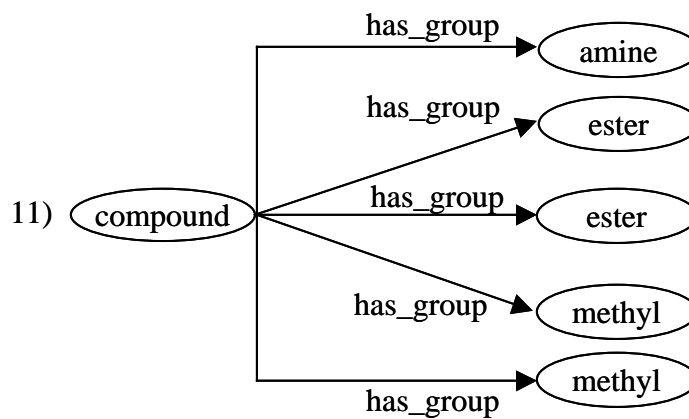
A compound that contains one *methyl* group, three *alkane* groups, and one *ether* group will cause cancer in male rats.



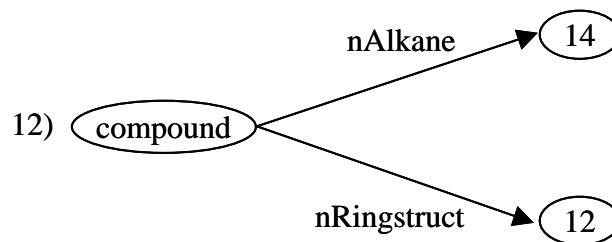
A compound that contains two *alkene* groups, one *ring structure*, and one *ether* group will cause cancer in male rats.



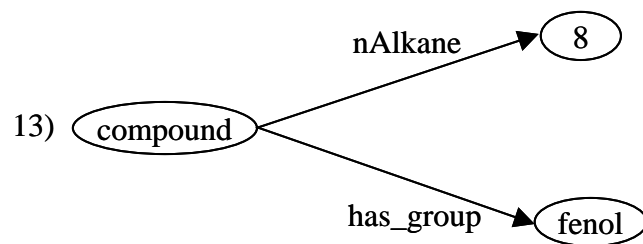
A compound that contains one *alkane* group, one *ether* group, and one *methyl* group will cause cancer in male rats.



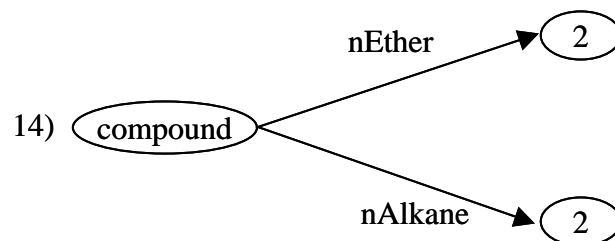
A compound that contains one *amine* group, two *ester* groups, and two *methyl* groups will cause cancer in male rats.



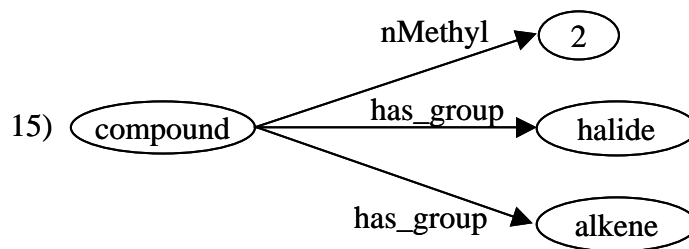
A compound that contains fourteen *alkane* groups and twelve *ringstructures* will cause cancer in male rats.



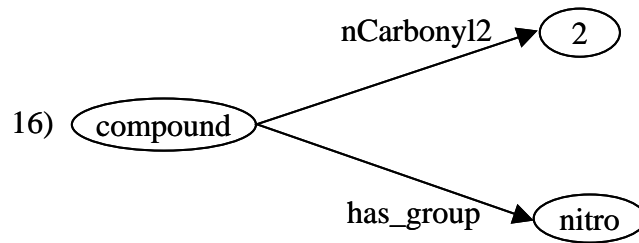
A compound that contains eight *alkane* groups and one *fenol* group will cause cancer in malarats.



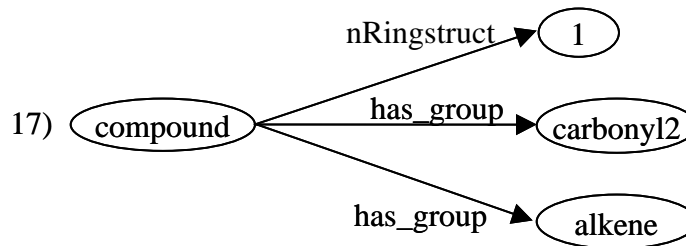
A compound that contains two *ether* groups and two *alkane* groups will cause cancer in malarats.



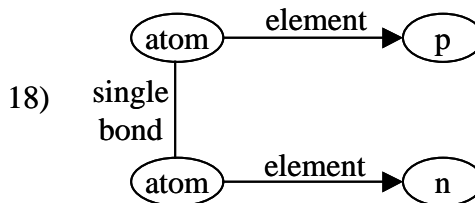
A compound that contains two *methyl* groups, one *halide* group, and one *alkene* group will cause cancer in malarats.



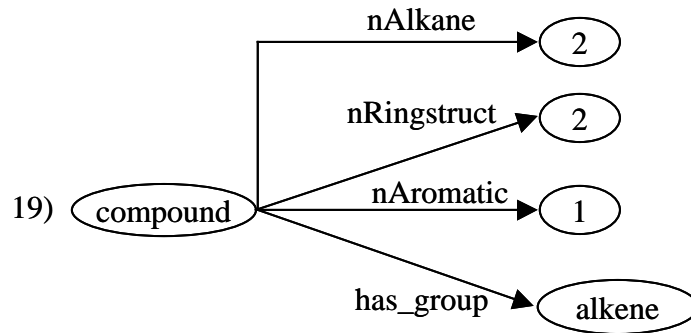
A compound that contains two *carbonyl2* groups and one *nitro* group will cause cancer in male rats.



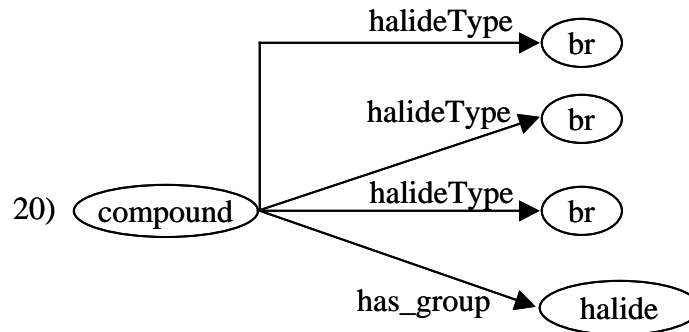
A compound that contains one *ringstructure*, one *carbonyl2* group and one *alkene* group will cause cancer in male rats.



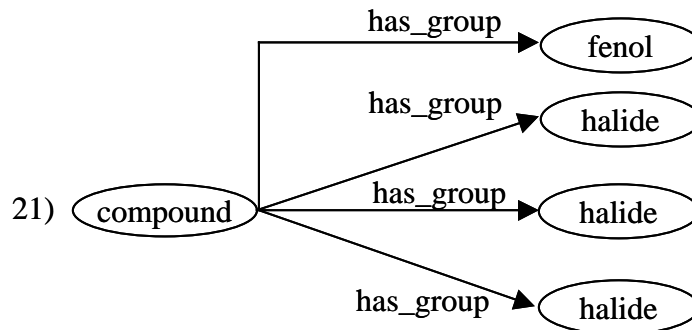
A compound that contains two *atoms* linked by a *single bond* and the element of one of the atoms is *phosphorus* and the element of the other atom is *nitrogen* will cause cancer in male rats.



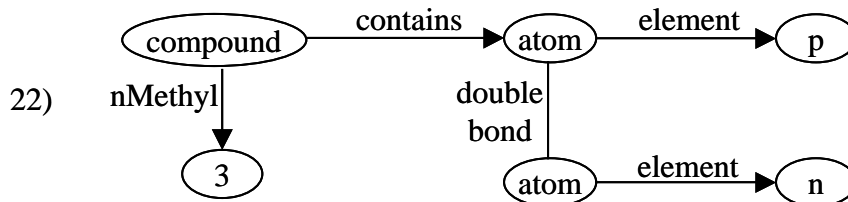
A compound that contains two *alkane* groups, two *ring structures*, one *aromatic* group and one *alkene* group will cause cancer in male rats.



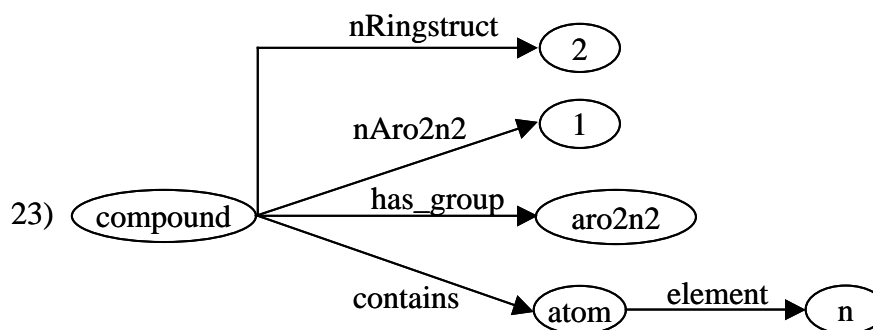
A compound that contains three *halide* groups of type *bromine* will cause cancer in male rats.



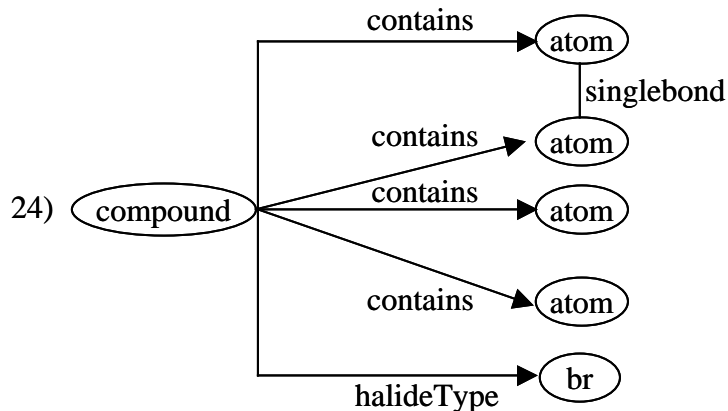
A compound that contains one *fenol* group and three *halide* groups will cause cancer in male rats.



A compound that contains three *methyl* groups and that also contains two *atoms* linked with a *double bond* and the *element* of one of the atoms is *phosphorus* and the *element* of the other atom is *nitrogen* will cause cancer in male rats.



A compound that contains two *ring structures*, one *aro2n2* group and that also contains one *atom* with *nitrogen* as its *element* will cause cancer in male rats.



A compound that contains one *halide* group of type *bromine* and also contains four *atoms*, and two of the atoms are linked by a *single bond* will cause cancer in male rats.



## PredictionDetails

When classifying the PTC test group compounds, the above substructures were applied in order. As soon as a substructure was found in a compound, that compound was classified as positive, and the remaining substructures were not checked. The following table shows the number of times the substructure was the first to be found in the compound. Of course, the compound may also contain occurrences of other higher-numbered substructures, but this was not checked. Note that only 7 of the 24 substructures were used to make the positive predictions for compounds in the PTC test group.

| Substructure# | Number of positive predictions |
|---------------|--------------------------------|
| 4             | 6                              |
| 5             | 3                              |
| 7             | 10                             |
| 8             | 1                              |
| 11            | 7                              |
| 15            | 2                              |
| 17            | 4                              |