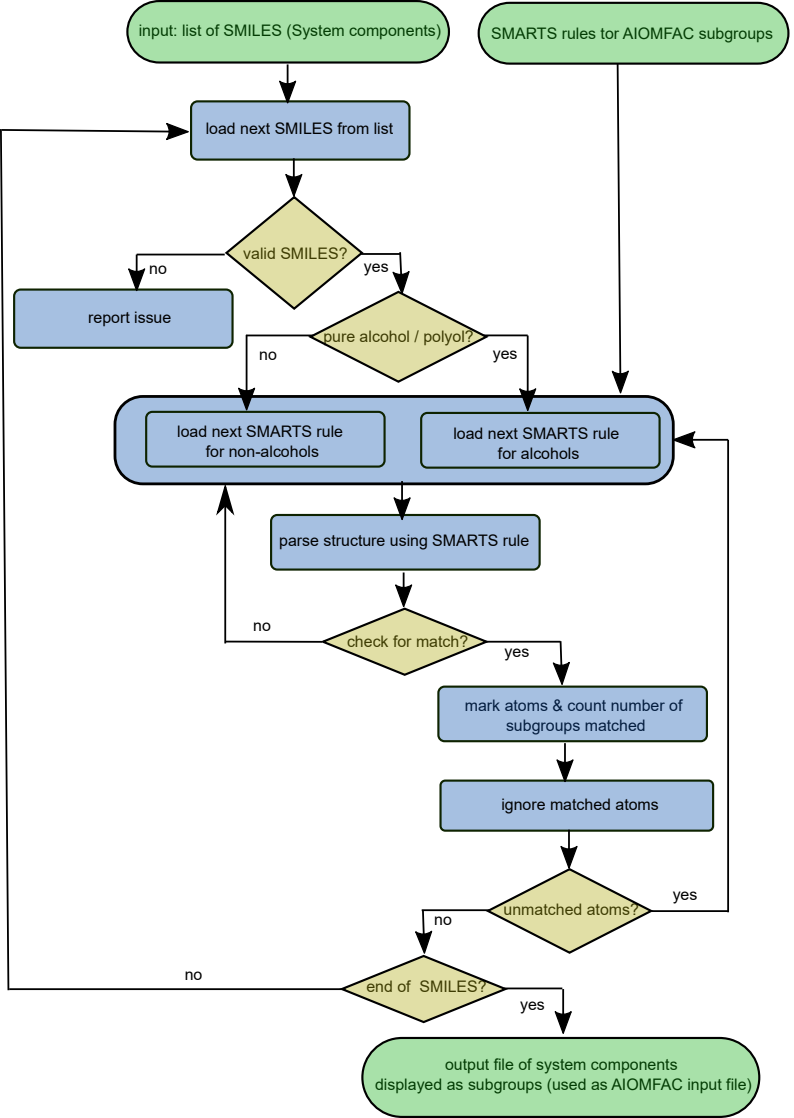
input: list of SMILES (System components)
SMARTS rules tor AIOMFAC subgroups
load next SMILES from list
valid SMILES?
no
yes
report issue
pure alcohol / polyol?
no
yes
load next SMARTS rule for non-alcohols
load next SMARTS rule for alcohols
parse structure using SMARTS rule
no
check for match?
yes
mark atoms & count number of subgroups matched
ignore matched atoms
unmatched atoms?
yes
no
no
end of SMILES?
yes
output file of system components displayed as subgroups (used as AIOMFAC input file)