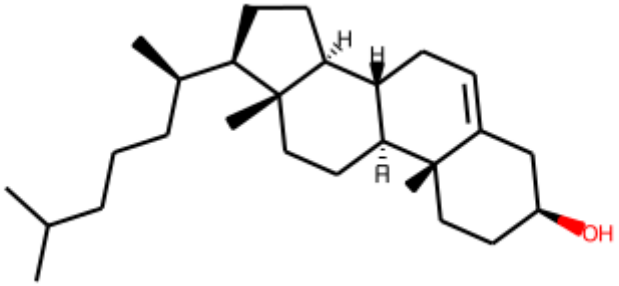
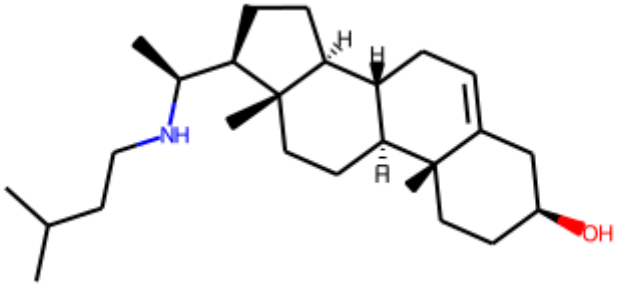
In [1]:
```
from rdkit.Chem import MolFromSmiles


chol_smiles = ("C[C@H](CCCC(C)C)[C@H]1CC[C@@H]2[C@@]1(CC"
               "[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C")
chol = MolFromSmiles(chol_smiles)
chol
```

Out[1]:



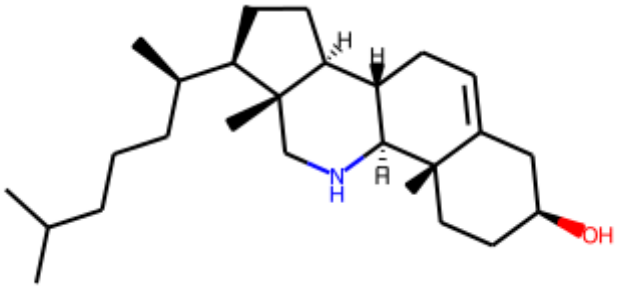
In [2]:
```
from copy import deepcopy


chol_2isN = deepcopy(chol)
chol_2isN.GetAtomWithIdx(2).SetAtomicNum(7)
chol_2isN
```

Out[2]:



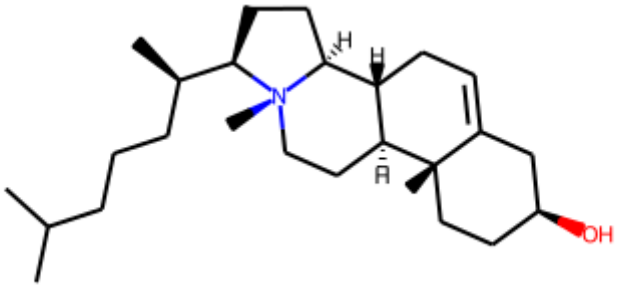
In [3]:
```
from copy import deepcopy


chol_14isN = deepcopy(chol)
chol_14isN.GetAtomWithIdx(14).SetAtomicNum(7)
chol_14isN
```

Out[3]:



In [4]:
```
chol_12isN = deepcopy(chol)
chol_12isN.GetAtomWithIdx(12).SetAtomicNum(7)
chol_12isN
```

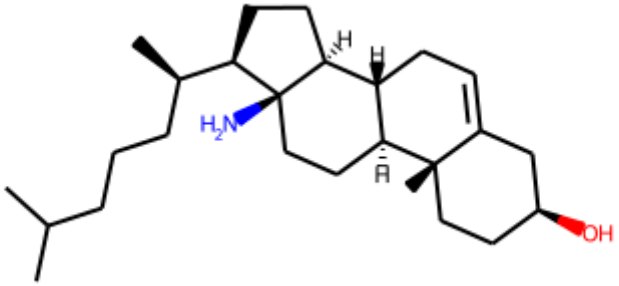
Out[4]:



In [5]:

```
chol_27isN = deepcopy(chol)
chol_27isN.GetAtomWithIdx(27).SetAtomicNum(7)
chol_27isN
```

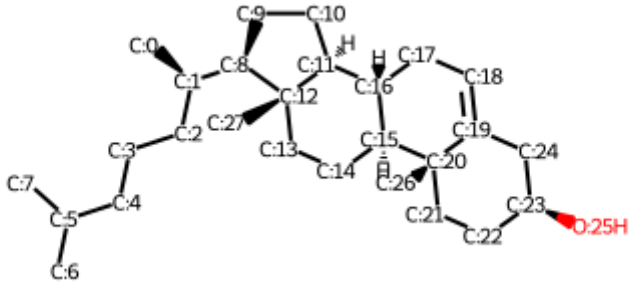
Out[5]:



In [9]:

```
chol_num = deepcopy(chol)
for atom in chol_num.GetAtoms():
    atom.SetProp('molAtomMapNumber', str(atom.GetIdx()))

chol_num
```

Out[9]:



In [2]:

```
from rdkit.Chem import MolFromSmiles


q_smiles = "N12CCC(CC1)CC2"
q_mol = MolFromSmiles(q_smiles)
for atom in q_mol.GetAtoms():
    atom.SetProp('molAtomMapNumber', str(atom.GetIdx()))

q_mol
```

Out[2]: