In [1]:
```
import pickle
from rdkit import Chem
from rdkit.Chem import Draw
from rdkit.Chem.Draw import IPythonConsole
from rdkit.Chem import rdFMCS
from rdkit.Chem.Draw import rdDepictor

from IPython.display import display
import matplotlib.pyplot as plt
from IPython.display import HTML
import pandas as pd

IPythonConsole.ipython_useSVG=True
rdDepictor.SetPreferCoordGen(True)
#IPythonConsole.drawOptions.minFontSize=20
```

In [2]:
```
with open('predictions/w_logs.pkl', 'rb') as file: w_te_data = pickle.load(fi
with open('predictions/wo_logs.pkl', 'rb') as file: wo_te_data = pickle.load(
original = pd.read_csv('predictions/chem_departm_output_wo_tie_embedding/outp
```

In [3]:
```
def view_difference(mol1, mol2):
    mcs = rdFMCS.FindMCS([mol1,mol2])
    mcs_mol = Chem.MolFromSmarts(mcs.smartsString)
    match1 = mol1.GetSubstructMatch(mcs_mol)
    target_atm1 = []
    for atom in mol1.GetAtoms():
        if atom.GetIdx() not in match1:
            target_atm1.append(atom.GetIdx())
    match2 = mol2.GetSubstructMatch(mcs_mol)
    target_atm2 = []
    for atom in mol2.GetAtoms():
        if atom.GetIdx() not in match2:
            target_atm2.append(atom.GetIdx())
    return Draw.MolsToGridImage([mol1, mol2],highlightAtomLists=[target_atm1,
```

Generation

Notes:

- Predict the next fragment when probability p > 0.5
- The logic takes top-5 attachments from combinations of top-5 motifs and its possible configs. E.g., motif C1=CC=CC=C1 has 2 possible configs, C1=[CH:1]C=C[CH:2]=C1 or C1=[CH:1]C=CC=C1. The first config could be connected to other motifs that the connections are marked by *:X*, X is a number. The second config is the end motif that couldn't connected to other motifs. Atoms marked by different mark numbers are connected together. No two atoms with same mark numbers are used for connection.
- For every attachment, it's checked for validity:
  - If the to-connect motif and to-be-connected (aka predicted motif) share common atoms for connections.
  - No self-loop.
  - If all atoms in the to-be-connected motif exist in the to-connect motif, no need to attach them.
- To view prediction logs of other molecules, subtract 2 from the molecule's index in Excel file.

In [4]:

```
def view(data, i, _original):
    print('Original: {}'.format(_original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(_original[i])]))

    sample = data[i]
    # step 0
    step_f0 = sample[0]
    print('***************Sample {}th***************'.format(i))
    print('-----Step-0-----')
    print('Root motif: {}'.format(step_f0['root']))
    print('Top 5 root motif configs:', '\n'.join([str(x) for x in step_f0['to

    # display
    mol = Chem.MolFromSmiles(step_f0['top-5-root-attachments'][0][0])
    print('Displaying partial graph (aka molecule): {}'.format(step_f0['parti
    display(Draw.MolsToGridImage([mol]))
    print('------------------------------------------------------------')


    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        print('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            print('Generate next fragment p = {}'.format(step_f['Generate fra
        else:
            print('Skip, current fragment has no next fragment to be attached
            continue

        if 'top-5-inter-cands' in step_f:
            print('Top 5 next motifs to attach:')
            for fragment in step_f['top-5-inter-cands']:
                print('Molecule {} and its specific config {} w/ p={}'.format
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                print('------------------------------------------------------
            if 'Attaching Fragment' in step_f:
                frag = step_f['Attaching Fragment']

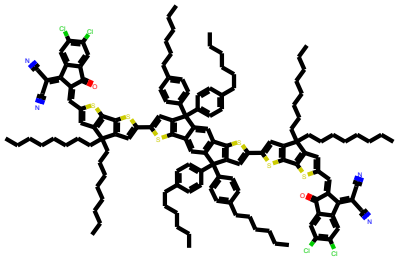
                sub_mol = Chem.MolFromSmiles(step_f['partial-graph'])
                print('Attaching fragment {} of config {}'.format(frag[0], fr
                print('Latest partial graph: {}'.format(step_f['partial-graph
                print('Lastest graph (left) vs graph in last step (right)')
                display(view_difference(sub_mol, mol))
                mol = sub_mol
                print('------------------------------------------------------
            else:
                print("Skip, the best next fragment to be attached to the cur
```

In [14]:

```
view(wo_te_data, 7, original)
```

```
Original: CCCCCCC1=CC=C(C2(C3=CC=C(CCCCCC)C=C3)C4=CC(C(SC(C5=CC(C6(CCCCCCCC)CC
```

```
CCCCCC)=C(C7=C6C=C(/C=C(C8=O)/C(C9=CC(Cl)=C(Cl)C=C89)=C(C#N)/C#N)S7)S5)=C%10)=
C%10C%11(C%12=CC=C(CCCCCC)C=C%12)C%13=CC=C(CCCCCC)C=C%13)=C%11C=C4C%14=C2C=C(C
%15=CC(C%16(CCCCCCCC)CCCCCCCC)=C(C%17=C%16C=C(/C=C(C%18=O)/C(C%19=CC(Cl)=C(Cl)
C=C%18%19)=C(C#N)\C#N)S%17)S%15)S%14)C=C1
```



```
***************Sample 7th***************
-----Step-0-----
Root motif: CN
Top 5 root motif configs: ('[NH2:1][CH3:2]', tensor(4.3962))
('[CH3:1][NH2:2]', tensor(-3.9628))
('C[NH2:1]', tensor(-15.1147))
('N[CH3:1]', tensor(-19.5112))
('C([OH:1])[CH3:2]', tensor(-975.5828))
Displaying partial graph (aka molecule): CN
```

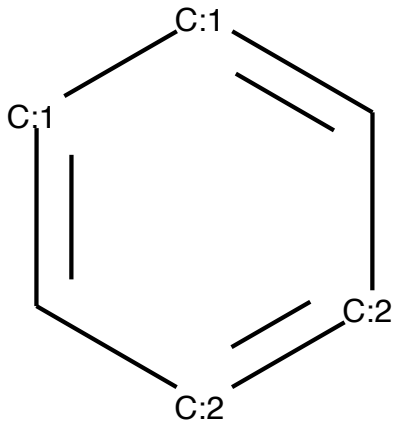
```
------------------------------------------------------------
-----Step-1-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.018248876556754112
```

```
------------------------------------------------------------
Molecule C=O and its specific config [O:1]=[CH2:2] w/ p=-4.561677932739258
```

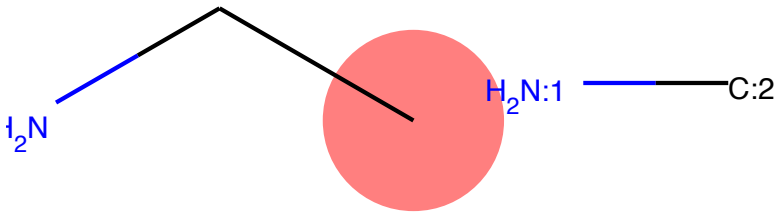
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-5.438595294952393
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-5.8340559005737305
```

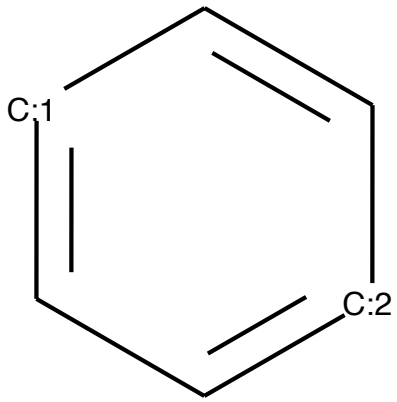
```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1 w
/ p=-8.586238861083984
```




```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CCN
Lastest graph (left) vs graph in last step (right)
```

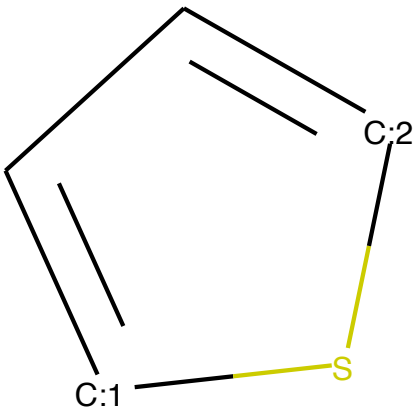



```
------------------------------------------------------------
-----Step-2-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.515
5307054519653
```



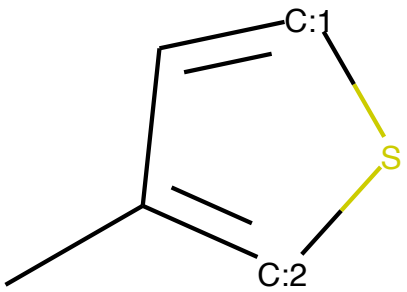
Molecule C#N and its specific config N#[CH:1] w/ p=-1.1474868059158325

Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-2.9674770832061768

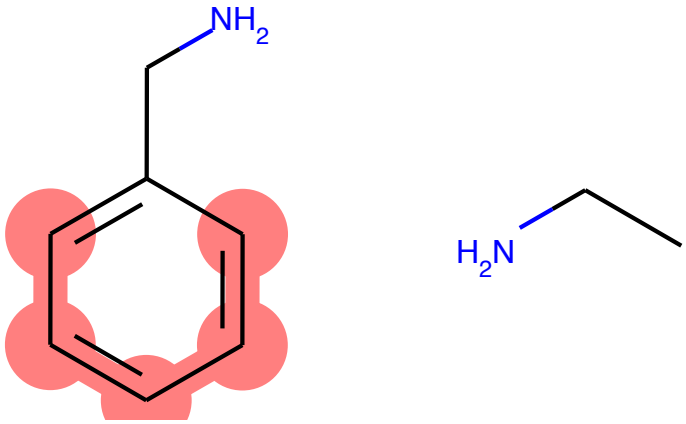


Molecule C=O and its specific config O=[CH2:1] w/ p=-3.7076351642608643

```
------------------------------------------------------------
Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ p=-5.48992
8245544434
```

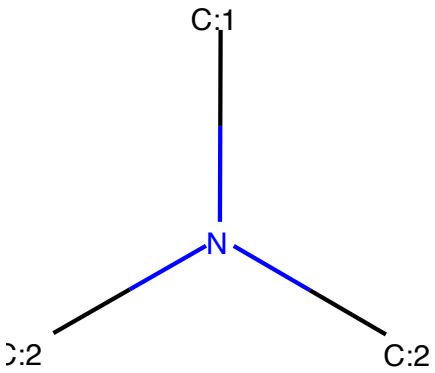



```
------------------------------------------------------------
Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: NCc1ccccc1
Lastest graph (left) vs graph in last step (right)
```

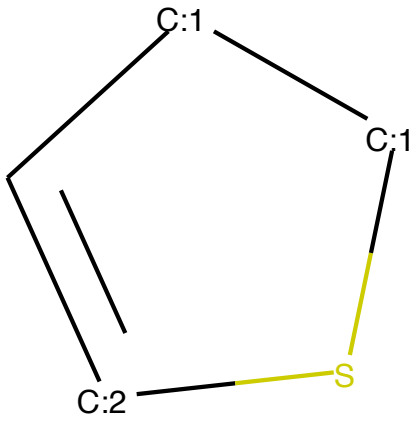



```
------------------------------------------------------------
-----Step-3-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.7866892218589783
```

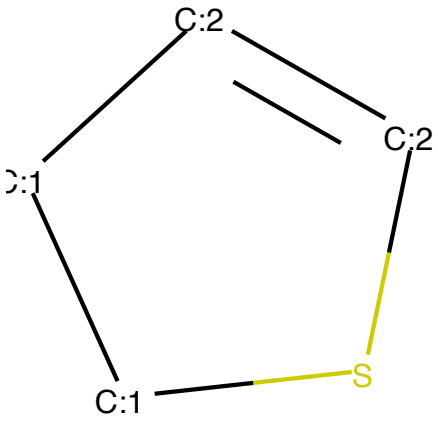
```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-1.003
0741691589355
```



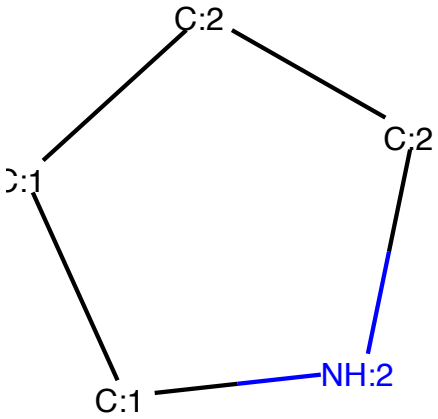

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-2.74
15366172790527
```



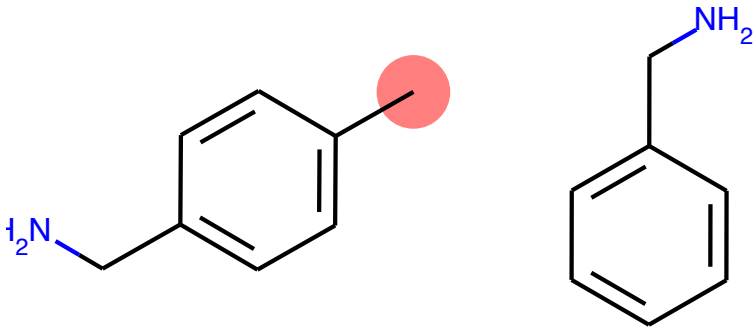

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config S1[CH2:1][CH2:1][CH:2]=[CH:2]1 w/ p=
-2.939915180206299
```




```
------------------------------------------------------------
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ p=-3.278656482696533
```

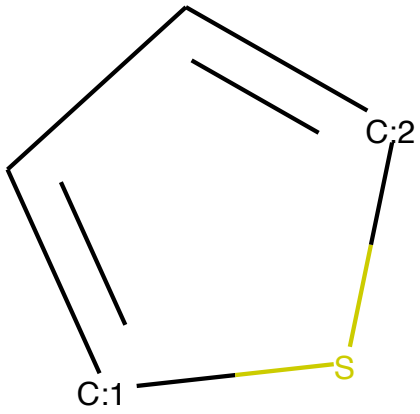



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```



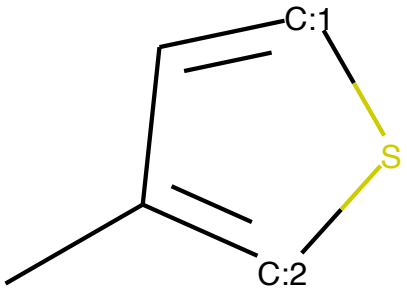

```
------------------------------------------------------------
-----Step-4-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-0.5388051867485046
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-1.7531983
852386475
```

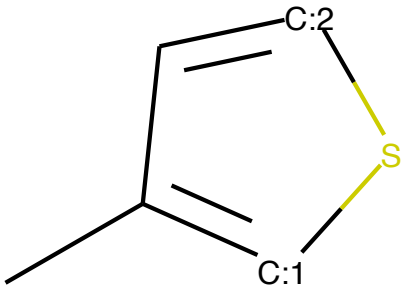



```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-2.007772922515869
```

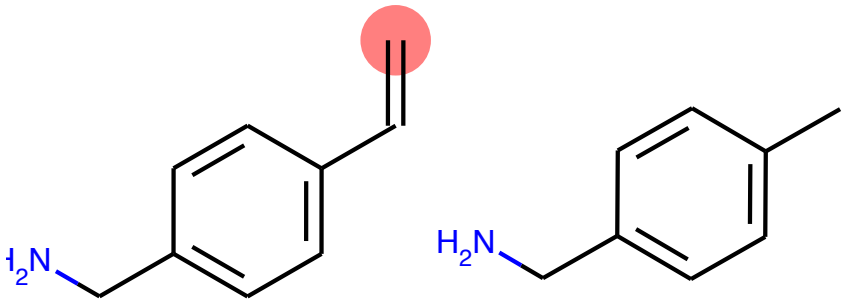
```
------------------------------------------------------------
Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ p=-2.70720
6964492798
```




```
------------------------------------------------------------
Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ p=-3.88095
21198272705
```



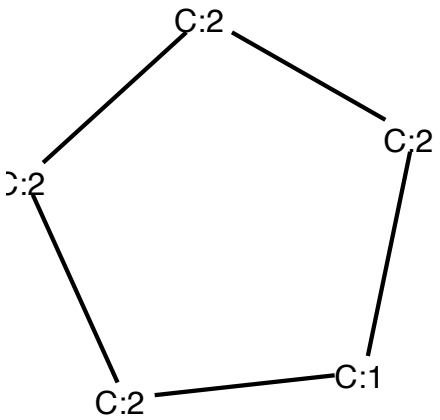

```
------------------------------------------------------------
Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```



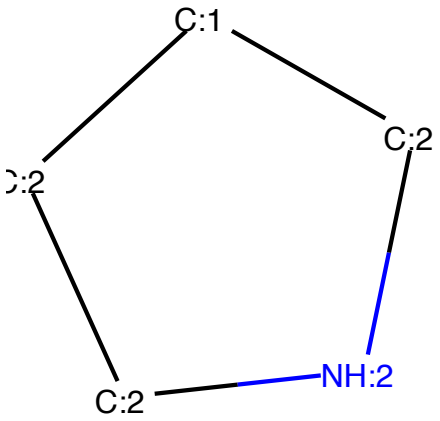

```
------------------------------------------------------------
-----Step-5-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.023258958011865616
```

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-3.813816785812378
```

```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1
w/ p=-7.317326545715332
```

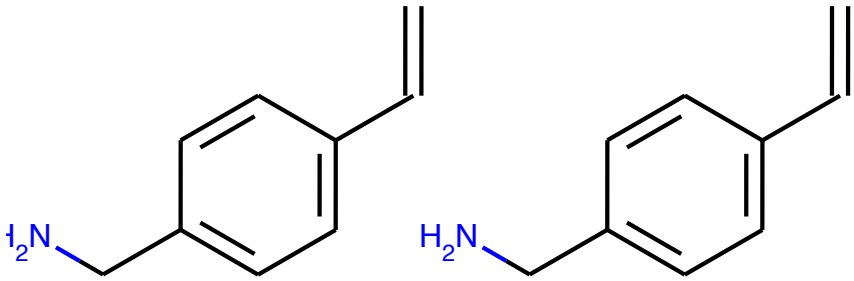



```
------------------------------------------------------------
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2]1
w/ p=-8.82868766784668
```




```
------------------------------------------------------------
Molecule [CH3-] and its specific config [CH3-] w/ p=-9.969855308532715
```

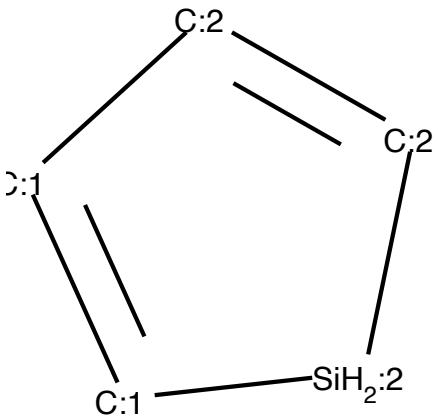
```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```



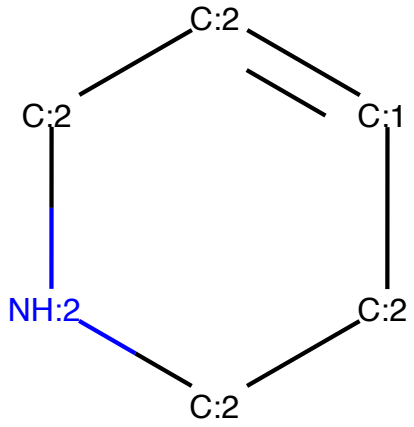

```
------------------------------------------------------------
-----Step-6-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-6.079655122448457e-06
```

Molecule C=O and its specific config O=[CH2:1] w/ p=-12.477263450622559

Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=[CH:2]1 w/ p=-13.782573699951172

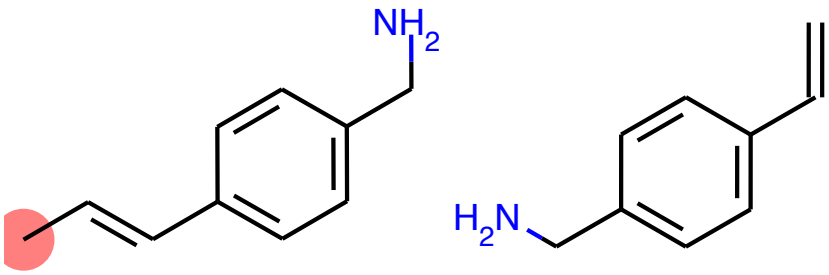


Molecule C1=CCNCC1 and its specific config [CH:1]1=[CH:2][CH2:2][NH:2][CH2:2][CH2:2]1 w/ p=-14.539703369140625



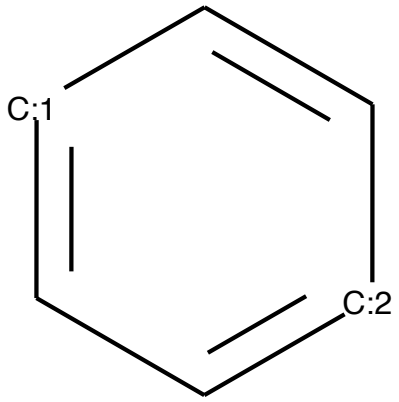

```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-14.90920639038086
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-7-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C#N and its specific config N#[CH:1] w/ p=-0.00034278715611435473
```

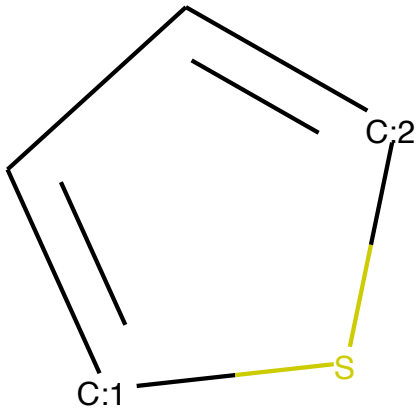
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-8.029106140136719



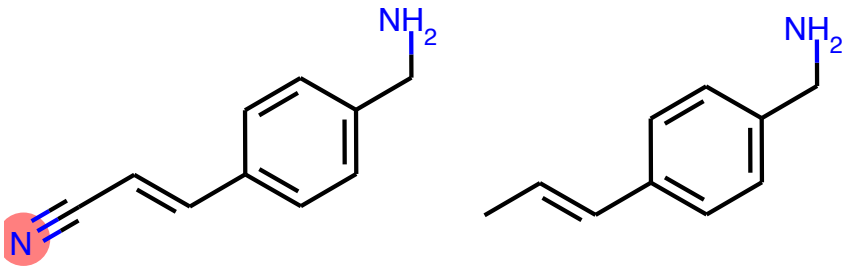
Molecule C=O and its specific config O=[CH2:1] w/ p=-11.653563499450684

Molecule C and its specific config C w/ p=-11.745807647705078

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-15.355421
06628418
```




```
------------------------------------------------------------
Attaching fragment N#[CH:1] of config ['N#[CH:1]']
Latest partial graph: N#CC=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-8-----
Generate next fragment p = 7.941371856083644e-23
-----Step-9-----
Generate next fragment p = 1.3385110247011046e-14
-----Step-10-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0013012760318815708
```

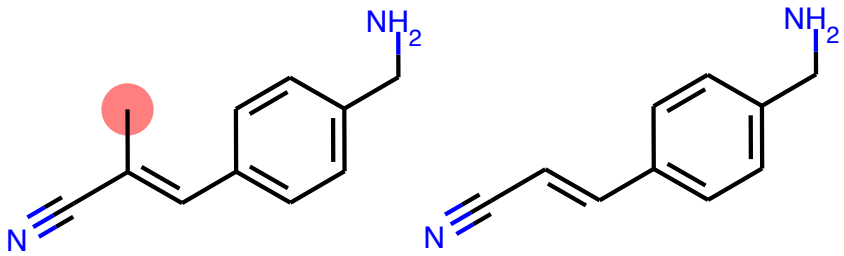
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-6.718320369720459
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-9.34375286102295
```

```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ p=-12.615152359008
789
```

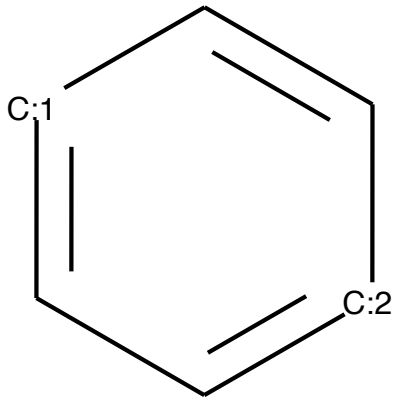
```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-14.469311714172363
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC(C#N)=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```



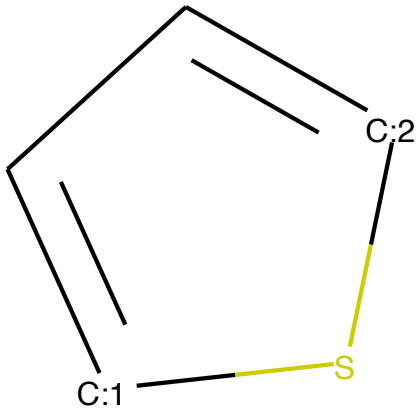

```
------------------------------------------------------------
-----Step-11-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.360306978225708
```

Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-1.380
9020519256592



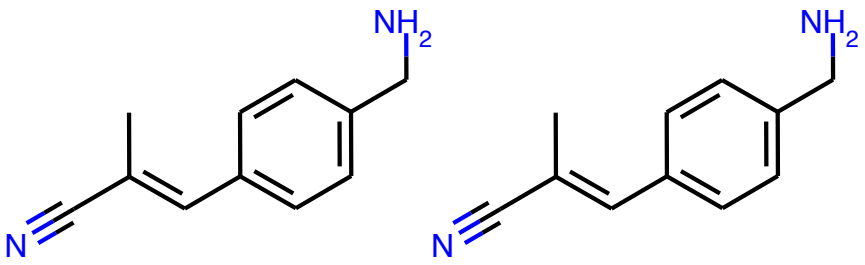
Molecule C#N and its specific config N#[CH:1] w/ p=-2.9761645793914795

Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-9.2919778
82385254




```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-9.369268417358398
```

```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: CC(C#N)=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-12-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=O and its specific config O=[CH2:1] w/ p=-8.344646857949556e-07
```

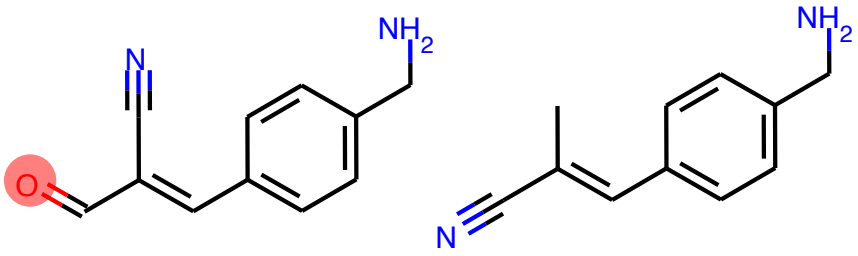
```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-14.197064399719238
```

```
------------------------------------------------------------
Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ p=-16.551809310913
086
```

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-17.004308700561523
```

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-17.063032150268555
```

```
------------------------------------------------------------
Attaching fragment O=[CH2:1] of config ['O=[CH2:1]']
Latest partial graph: N#CC(C=O)=Cc1ccc(CN)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-13-----
Generate next fragment p = 1.3058588372380847e-30
-----Step-14-----
Generate next fragment p = 0.9999996423721313
Top 5 next motifs to attach:
Molecule CO and its specific config O[CH3:1] w/ p=-0.05614574998617172
```

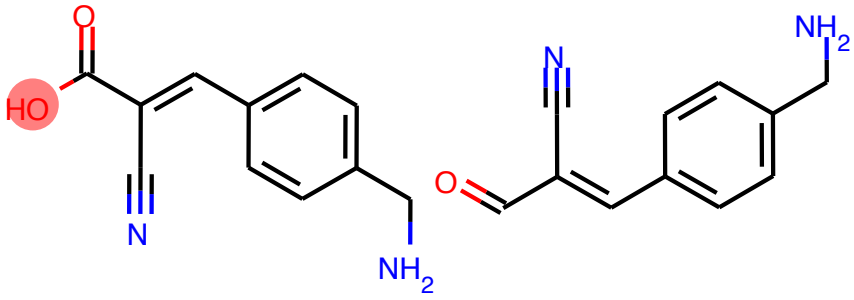
```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-3.5701329708099365
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-3.916741132736206
```

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.133025646209717
```

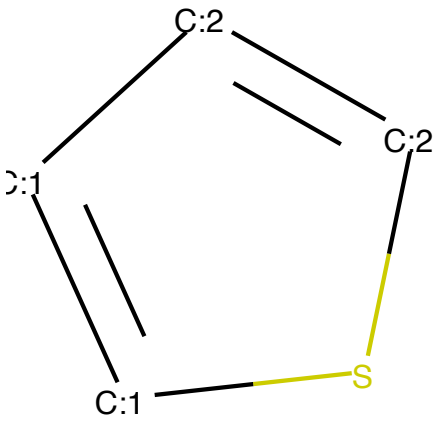
```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-7.986599445343018
```

```
------------------------------------------------------------
Attaching fragment O[CH3:1] of config ['O[CH3:1]']
Latest partial graph: N#CC(=Cc1ccc(CN)cc1)C(=O)O
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-15-----
Generate next fragment p = 5.937891955909436e-09
-----Step-16-----
Generate next fragment p = 1.972723200072135e-11
-----Step-17-----
Generate next fragment p = 1.0942924355290123e-13
-----Step-18-----
Generate next fragment p = 5.563708521671984e-11
-----Step-19-----
Generate next fragment p = 2.2453570764708252e-15
-----Step-20-----
Generate next fragment p = 2.1351219575431135e-19
-----Step-21-----
Generate next fragment p = 0.0028587025590240955
-----Step-22-----
Generate next fragment p = 5.627591465594398e-20
-----Step-23-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.019304610788822174
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=
-5.553902626037598
```

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------------------------------------------------------------
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-5.9536509513854
98
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-6.008213043212891
```

```
------------------------------------------------------------
Molecule CS and its specific config [CH3:1][SH:2] w/ p=-6.0181498527526855
```

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Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-24-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-25-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-26-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
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-----Step-27-----
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In [ ]: