In [1]:
```python
import pickle
from rdkit import Chem
from rdkit.Chem import Draw
from rdkit.Chem.Draw import IPythonConsole
from IPython.display import display
import matplotlib.pyplot as plt
from IPython.display import HTML
import pandas as pd

IPythonConsole.ipython_useSVG=True
```

In [2]:
```python
with open('predictions/w_tie_embedding_logs.pkl', 'rb') as file: w_te_data =
with open('predictions/wo_tie_embedding_logs.pkl', 'rb') as file: wo_te_data
original = pd.read_csv('predictions/chem_departm_output_wo_tie_embedding/outp
```

In [3]:
```python
def mol_with_atom_index(mol, indices=[]):
    new_idx = []
    for atom in mol.GetAtoms():
        #print(atom.GetIdx(), indices)
        idx = atom.GetIdx()
        if idx in indices:
            atom.SetAtomMapNum(idx)
        new_idx.append(idx)
    return mol, new_idx
```

Generation

In [16]:
```python
for i, sample in enumerate(w_te_data):
    if i > 12:
        break
    elif i < 12:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------', HTML
    num_atom = len(list(Chem.MolFromSmiles(step_f0['partial-graph']).GetAtoms
    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        else:
            print('Skip, current fragment has not next fragment to be attache
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]

            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                    list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            num_atom = len(list(Chem.MolFromSmiles(step_f['partial-graph']).G
            display('------------------------------------------------
        else:
            print("Skip, the best next fragment to be attached to the current
```
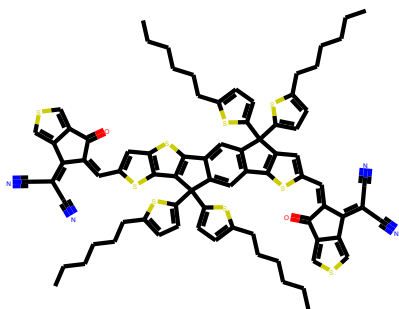
```
'Original: CCCCCCC1=CC=C(S1)C2(C(S3)=CC=C3CCCCCC)C(C(SC(/C=C(C4=O)/C(C5=CSC=C4
5)=C(C#N)\\C#N)=C6)=C6S7)=C7C8=CC9=C(C(SC(/C=C(C%10=O)/C(C%11=CSC=C%10%11)=C(C
#N)\\C#N)=C%12)=C%12C9(C(S%13)=CC=C%13CCCCCC)C(S%14)=CC=C%14CCCCCC)C=C28'
```

```
'***************Sample 12th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([590, 670, 653, 675, 663]),
 'super-root-idx': tensor(590),
 'top-5-root-fragment-cands': [('O=C([O-:1])[CH3:2]', tensor(13.9317)),
  ('O=C([O-])[CH3:1]', tensor(-12.5431)),
  ('CC(=O)[O-:1]', tensor(-16.1744)),
  ('[O:1]=[CH2:2]', tensor(-980.1329)),
  ('C(#C[CH3:2])[CH3:1]', tensor(-980.1487))],
 'Attaching Fragment': 'O=C([O-:1])[CH3:2]',
 'partial-graph': 'CC(=O)[O-]'}
'Displaying partial graph (aka molecule): CC(=O)[O-]'
```
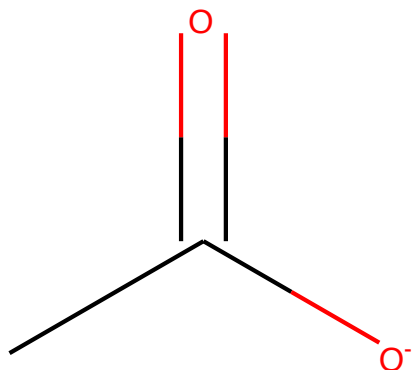


```
'--------------------------------------------------------'

'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.07073831
55822754'
```
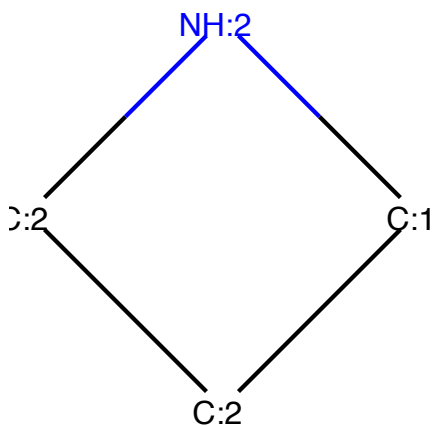
'--'

'Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][NH:2][CH2:2]1 w/ prob
ability -1.16451895236969'

C:2

H:2   C:1

C:2

'--'
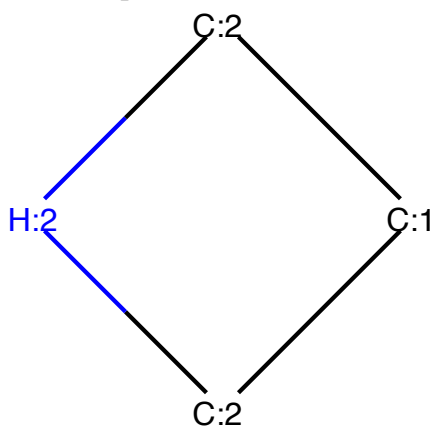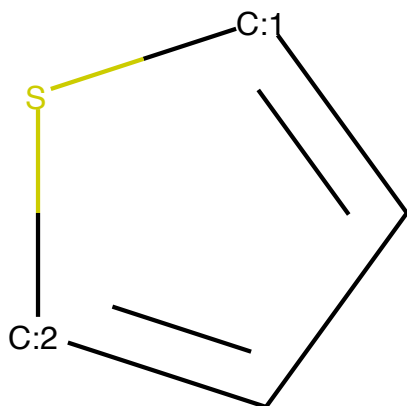
'Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2]1 w/ prob
ability -1.808347225189209'

NH:2

C:2   C:1

C:2

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-2.6687560081481934'

'——'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -3.12031841
27807617'

'——'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCC(=O)[O-]'
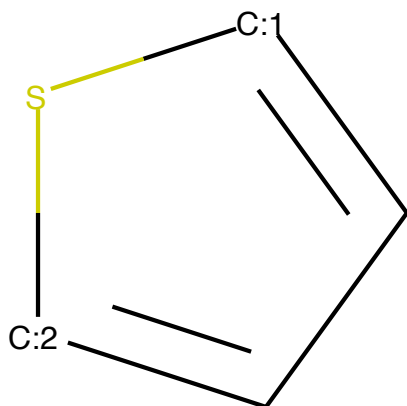

'——'
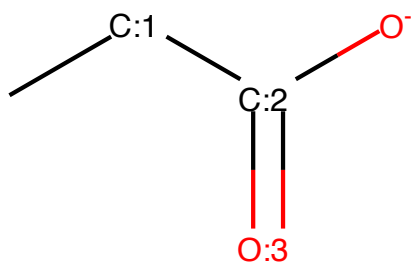
'-----Step-2-----'
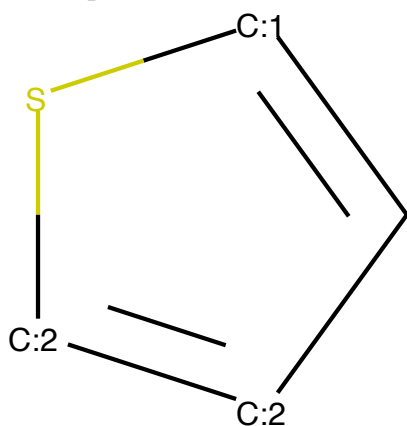'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
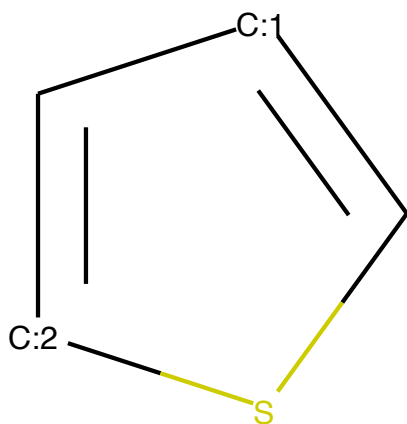-0.015211270190775394'

'_____'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -4.913881301879883'

'_____'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]C=[CH:2]S1 w/ probability
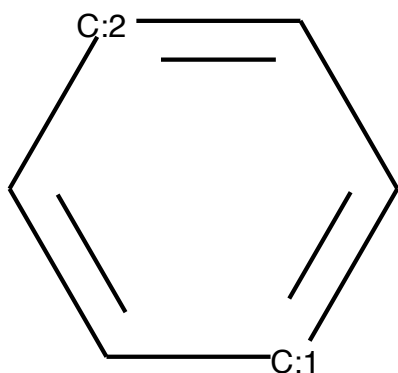-5.474489212036133'

'_____'

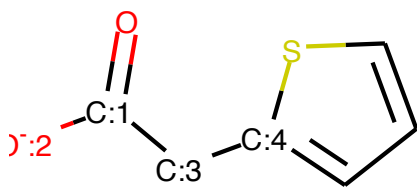'Molecule C and its specific config C w/ probability -5.725157260894775'

'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -8.778680801391602'

'--'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1cccs1'

'--'
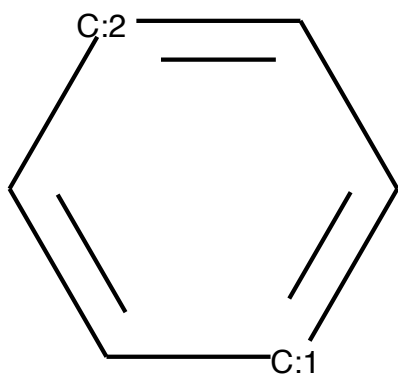
'-----Step-3-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.81196483
0267243e-05'

'---'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -11.434046745300293'

'---'

'Molecule C and its specific config C w/ probability -11.994294166564941'

'---'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -13.705684661865234'

'_____'
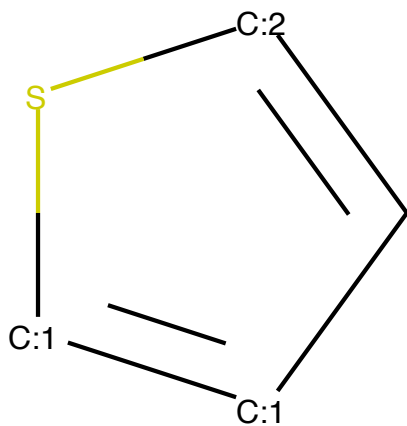
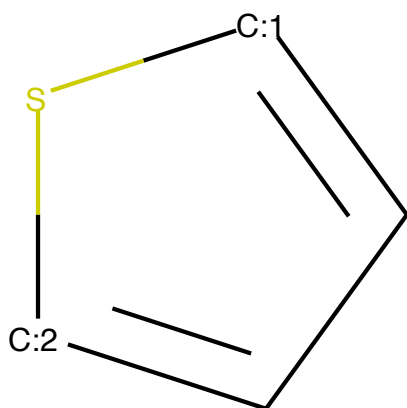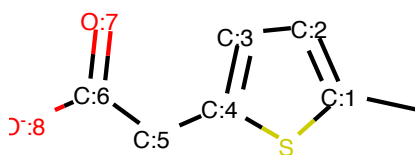'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -17.18779754638672'

'_____'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(CC(=O)[O-])s1'

'_____'
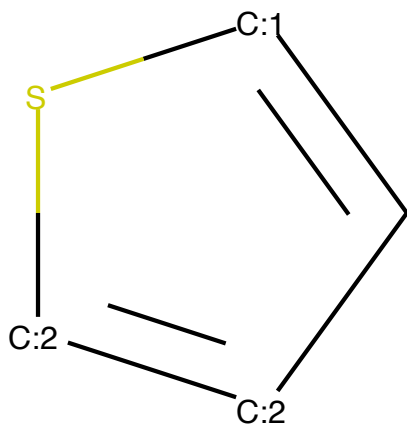
'-----Step-4-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probability -0.009146904572844505'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability −4.787027835845947'

'--'
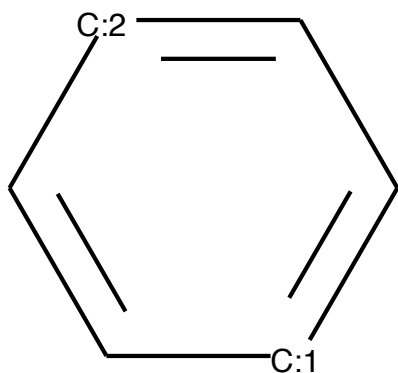
'Molecule C and its specific config C w/ probability −7.912520408630371'

'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probability −8.354876518249512'

'_____'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -8.9
74496841430664'

'_____'
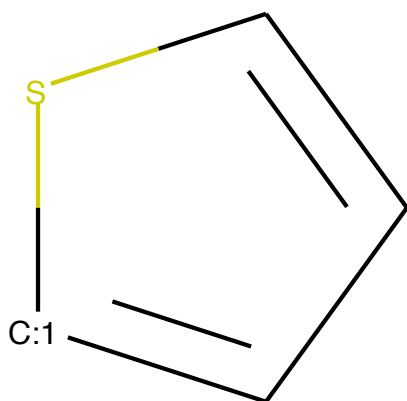
'Attaching fragment C1=[CH:1]S[CH:2]=[CH:2]1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2cccs2)s1'

'_____'
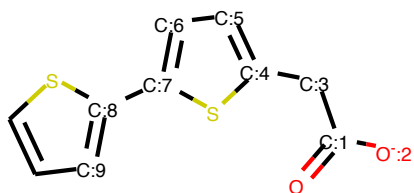
'-----Step-5-----'
'Generate next fragment: 0.9997887015342712'
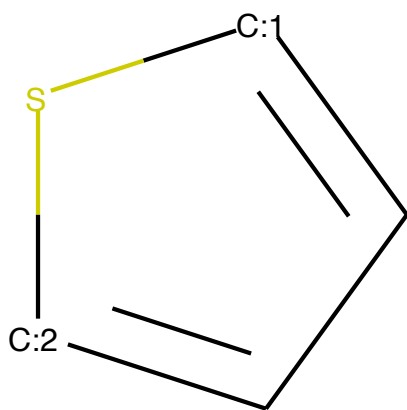'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.56950706
24351501'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.1753448247909546'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -2.7043516635894775'

'--'

'Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ probability
-3.261600971221924'

'_____'
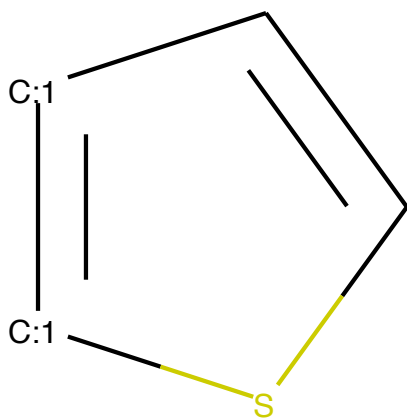
'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -4.33
6895942687988'

'_____'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(CC(=O)[O-])s2)s1'

'_____'
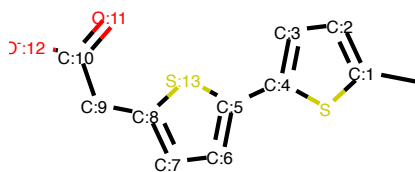
'-----Step-6-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.010365660302340984'

'——'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]SC=C1 w/ probability -4
.703817367553711'

'——'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -6.875165939331055'

'——'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:2]=[CH:1]S1 w/ probab
ility -9.226217269897461'

'_____'
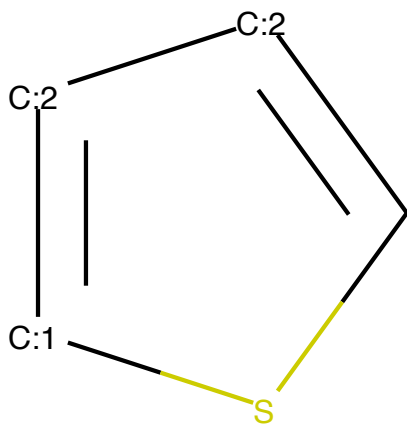
'Molecule C and its specific config C w/ probability -9.870923042297363'

'_____'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3cccs3)s2)s1'
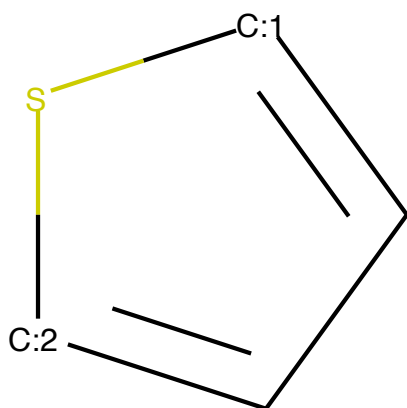

'_____'
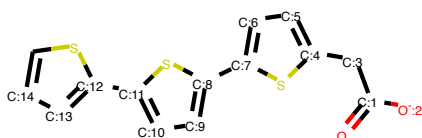
'-----Step-7-----'
'Generate next fragment: 0.9998983144760132'
'Top 5 next fragments to attach (current and potential graph)'
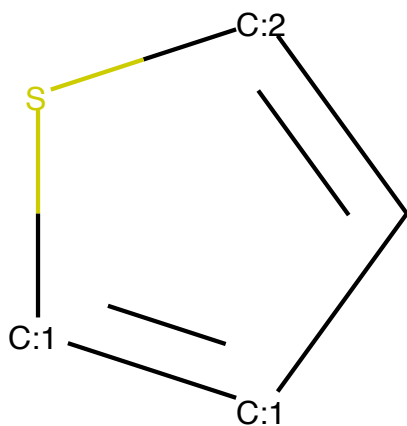'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00630442
42560863495'

'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -5.35567331314086
9'

'--'

'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][CH2:2][NH:2][CH2:2]1
w/ probability -7.019346714019775'

'--'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -7.966949939727783'

'_____'
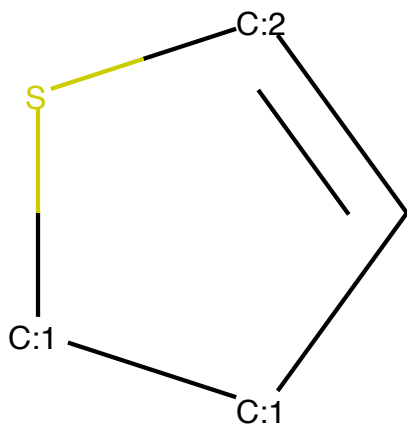
'Molecule C=O and its specific config O=[CH2:1] w/ probability -9.378978729248
047'

'_____'

'Attaching fragment [CH3:1][CH3:2]'
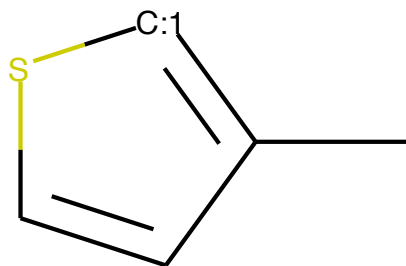'Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(CC(=O)[O-])s3)s2)s1'

'_____'
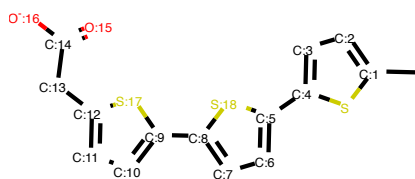
'-----Step-8-----'
'Generate next fragment: 0.9967923760414124'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
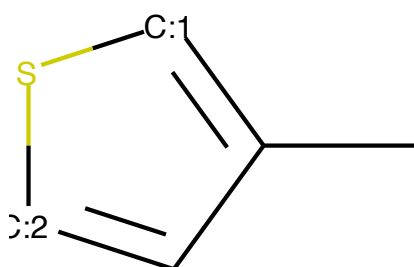-0.12386856973171234'

'_____'

'Molecule C and its specific config C w/ probability -2.2312333583831787'

'_____'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -5.375985622406006'

'_____'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -6.157557010650635'

'_____'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -6.570703983306885'

'_____'
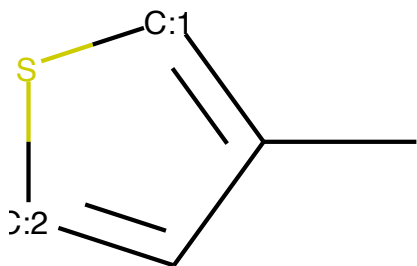
'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4cccs4)s3)s2)s1'

'_____'
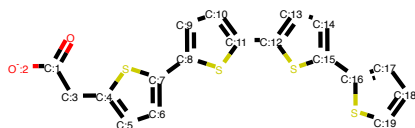
'-----Step-9-----'
'Generate next fragment: 0.9993383288383484'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00063137
20368780196'

'--'

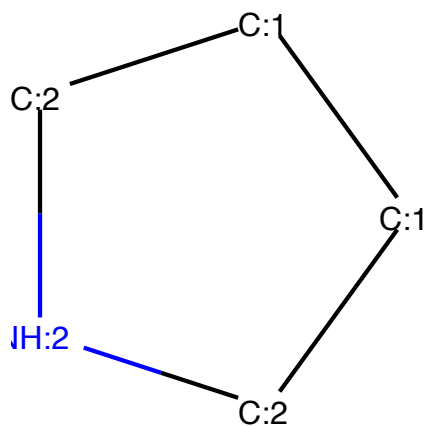'Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:1]=[CH:1]S1 w/ probability -7.514693737030029'

'--'

'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -11.040324211120605'

'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -11.106101036071777'

'--'

'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -11.327986
717224121'

'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(-c4ccc(CC(=O)[O-])s4)s3)s2)s1'

'--'
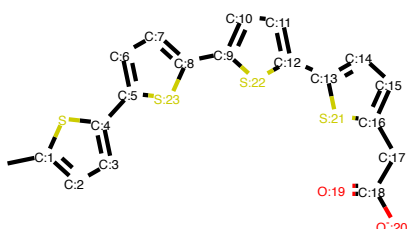
'-----Step-10-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.09625552594661713'

'_____'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.943636894226074'

'_____'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -3.4
166290760040283'

'_____'

'Molecule C and its specific config C w/ probability -5.316184997558594'

'_____'

'Molecule [SiH4] and its specific config [SiH4] w/ probability -6.750178337097
168'

'_____'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
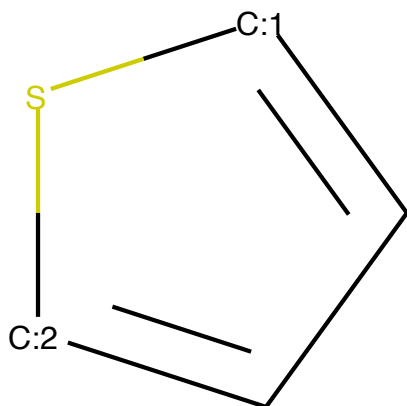'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5cccs5)s4)s3)s2)
s1'

'_____'

'-----Step-11-----'
'Generate next fragment: 0.8303309679031372'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.04151012
0034217834'

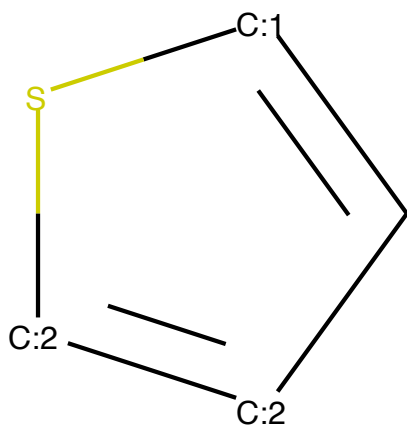'--'
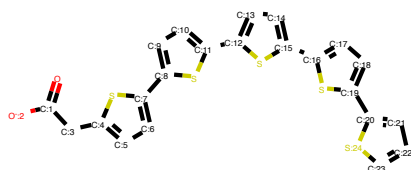
'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -3.214354038
2385254'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:1]=[CH:1]S1 w/ probab
ility -7.846226692199707'

'--'
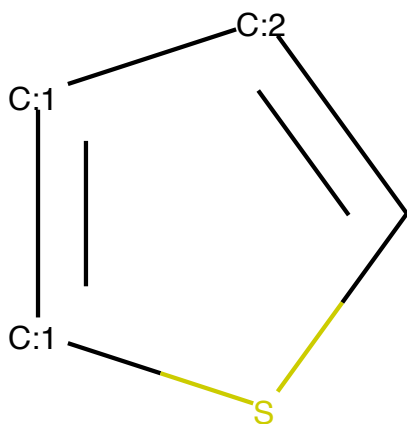
'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -10.278705
596923828'

'―――'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -10.48699951171
875'

'―――'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)
s2)s1'

'―――'
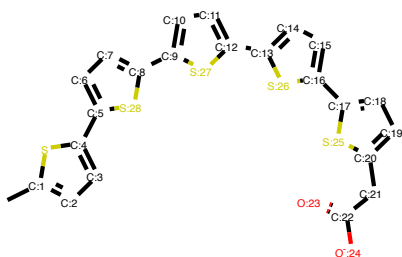
'-----Step-12-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.5011690258979797'

'_____'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -1.3
847014904022217'

'_____'
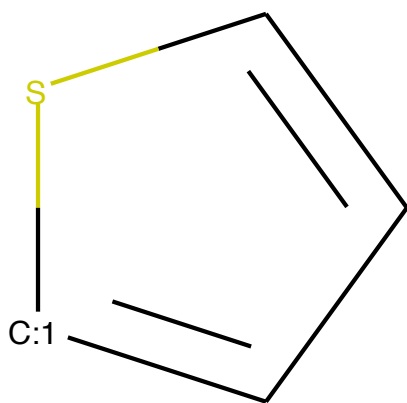
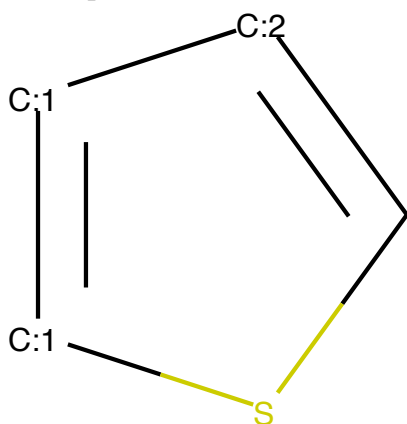'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.0013294219970703'

'_____'
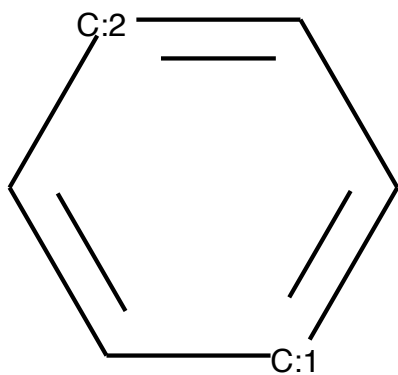
'Molecule C and its specific config C w/ probability -4.850032329559326'

'--'

'Molecule C#N and its specific config N#[CH:1] w/ probability -7.4061570167541
5'

'--'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(-c6cccs6)s5
)s4)s3)s2)s1'

'--'
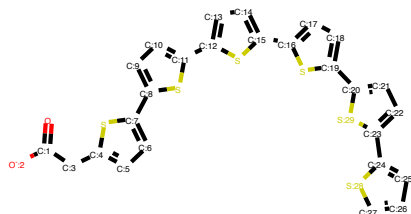
'-----Step-13-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.

```
'-----Step-14-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-15-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-16-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-17-----'
'Generate next fragment: 0.9976533055305481'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00015102
67611593008'
```
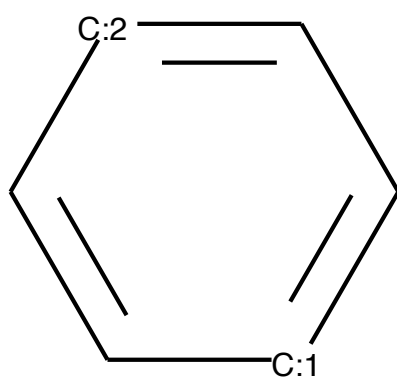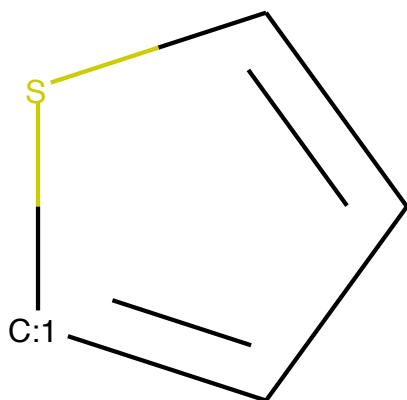
```
'----------------------------------------------------------'
```

```
'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -9.6594629
28771973'
```

```
'---------------------------------------------------------'
```

```
'Molecule S and its specific config S w/ probability -9.775293350219727'
```

'_____'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -10.877622604370117'

C:2

S

C:1

C:1

'_____'
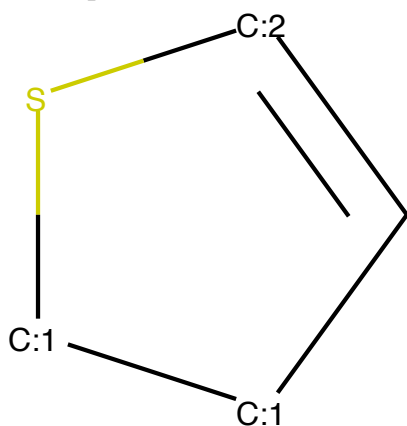
'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][CH2:2][NH:2][CH2:2]1
w/ probability -11.646870613098145'

C:1

C:2

C:1

NH:2

C:2

'_____'
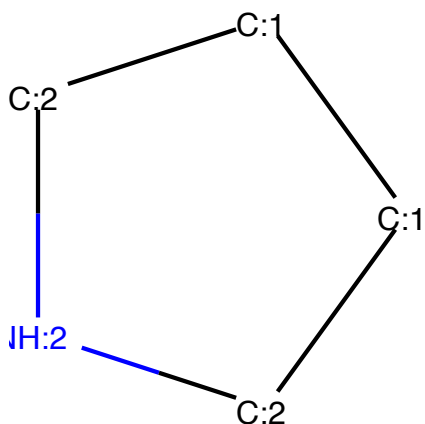
'Attaching fragment C1=[CH:2]S[CH2:1][CH2:1]1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)
c5sccc45)s3)s2)s1'
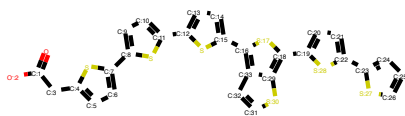
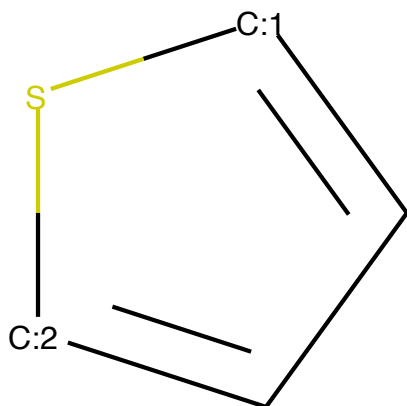'--'
'-----Step-18-----'
'Generate next fragment: 0.98321932554245'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -3.814624506
048858e-05'

'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -10.2314853
66821289'

'--'

'Molecule [SiH4] and its specific config [SiH4] w/ probability -14.02976989746
0938'

'---'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -14.39983177185
0586'

'---'

'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -14.9
18670654296875'

'---'

'Attaching fragment [CH3:1][SH:2]'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)
c5sc(S)cc45)s3)s2)s1'

'--'
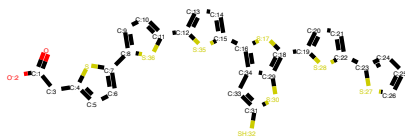
'-----Step-19-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule S and its specific config S w/ probability -0.9460978507995605'

'--'

'Molecule CS and its specific config C[SH:1] w/ probability -1.036858558654785
2'

'--'

'Molecule C and its specific config C w/ probability -1.455458164215088'

'_____'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -3.820958375930786'

'_____'
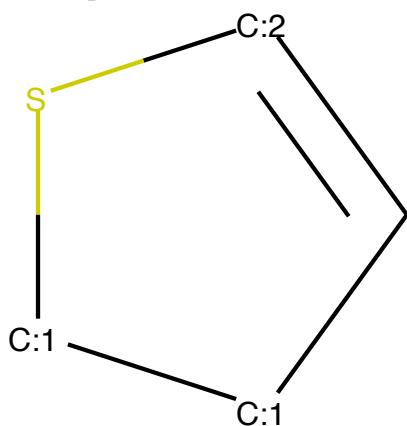
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-6.773167610168457'

'_____'
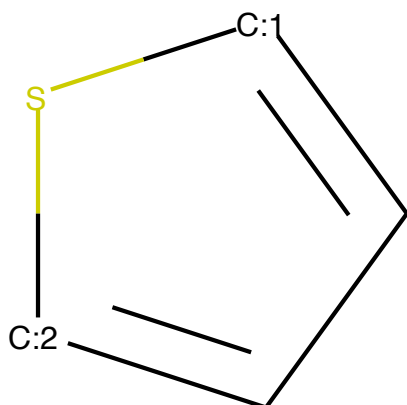
'Attaching fragment S'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)
c5sc(S)cc45)s3)s2)s1'

'---'

'-----Step-20-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CS and its specific config C[SH:1] w/ probability -2.765617318800650
5e-05'

'---'

'Molecule C[SiH3] and its specific config C[SiH3:1] w/ probability -10.8562269
21081543'

'---'

'Molecule CC#N and its specific config N#C[CH3:1] w/ probability -11.877511024
475098'

'———'

'Molecule O=S and its specific config O=[S:1] w/ probability -14.0730867385864
26'

'———'

'Molecule CC(F)(F)F and its specific config FC(F)(F)[CH3:1] w/ probability -14
.895258903503418'

F

F

C:1

F

'———'
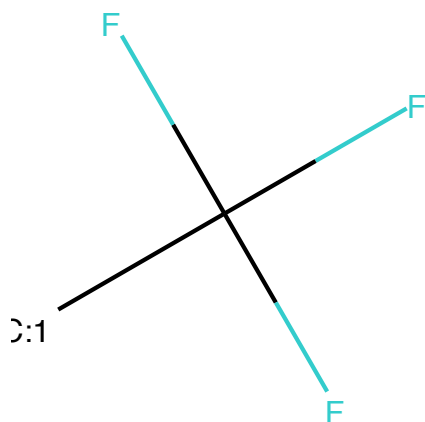
'Attaching fragment C[SH:1]'
'Latest partial graph: CSc1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)sc(-c
3ccc(-c4cccs4)s3)c2s1'
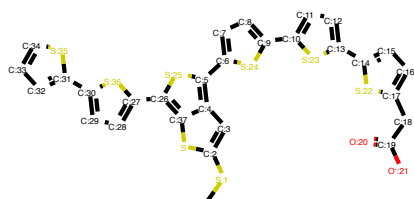
```
'--------------------------------------------------------'

'-----Step-21-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-22-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule O=S and its specific config O=[S:1] w/ probability -4.21991971961688
25e-05'
```

```
'--------------------------------------------------------'

'Molecule CS and its specific config C[SH:1] w/ probability -10.07938957214355
5'
```

'_____'

'Molecule C[SiH3] and its specific config C[SiH3:1] w/ probability -15.3585081
10046387'

'_____'

'Molecule [SiH4] and its specific config [SiH4] w/ probability -17.47427177429
1992'

'_____'

'Molecule CC(F)(F)F and its specific config FC(F)(F)[CH3:1] w/ probability -19
.046844482421875'

F

F

:1

F

'_____'
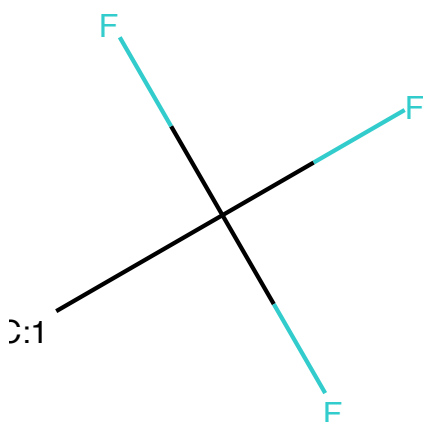
'Attaching fragment O=[S:1]'
'Latest partial graph: CS(=O)c1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)s
c(-c3ccc(-c4cccs4)s3)c2s1'
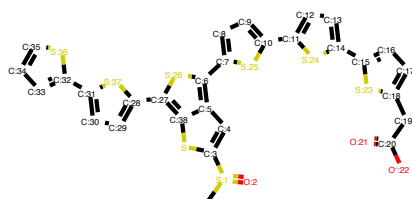
'--'

'-----Step-23-----'
Skip, current fragment has not next fragment to be attached. Go back to the previous fragment.
Skip, the best next fragment to be attached to the current fragment does not yield a valid sub-molecule . Go back to the previous fragment.
'-----Step-24-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule O=S and its specific config O=[S:1] w/ probability 0.0'

'--'

'Molecule CC#N and its specific config N#C[CH3:1] w/ probability -19.532554626
464844'

'--'

'Molecule CS and its specific config C[SH:1] w/ probability -20.42498970031738
3'

'--'

'Molecule C[SiH3] and its specific config C[SiH3:1] w/ probability -21.0532894
1345215'

'--'

'Molecule CN and its specific config N[CH3:1] w/ probability -22.4043731689453
12'

'--'

'Attaching fragment O=[S:1]'
'Latest partial graph: CS(=O)(=O)c1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)
s3)sc(-c3ccc(-c4cccs4)s3)c2s1'

'--'
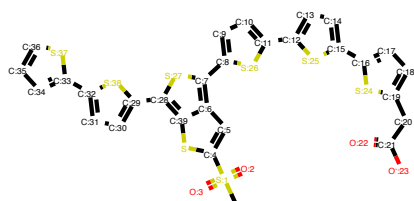
'-----Step-25-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-26-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-27-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-28-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-29-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-30-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-31-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-32-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-33-----'

Skip, current fragment has not next fragment to be attached. Go back to the previous fragment.
Skip, the best next fragment to be attached to the current fragment does not yield a valid sub-molecule . Go back to the previous fragment.
'-----Step-34-----'
Skip, current fragment has not next fragment to be attached. Go back to the previous fragment.
Skip, the best next fragment to be attached to the current fragment does not yield a valid sub-molecule . Go back to the previous fragment.
'-----Step-35-----'
Skip, current fragment has not next fragment to be attached. Go back to the previous fragment.
Skip, the best next fragment to be attached to the current fragment does not yield a valid sub-molecule . Go back to the previous fragment.
'-----Step-36-----'
Skip, current fragment has not next fragment to be attached. Go back to the previous fragment.
Skip, the best next fragment to be attached to the current fragment does not yield a valid sub-molecule . Go back to the previous fragment.
'-----Step-37-----'
'Generate next fragment: 0.9880258440971375'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00010168035078095272'

'--'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -9.30424690246582'

'--'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -11.4791316
98608398'

'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -15.40794467926
0254'

'--'

'Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][NH:2][CH2:2]1 w/ prob
ability -17.559106826782227'
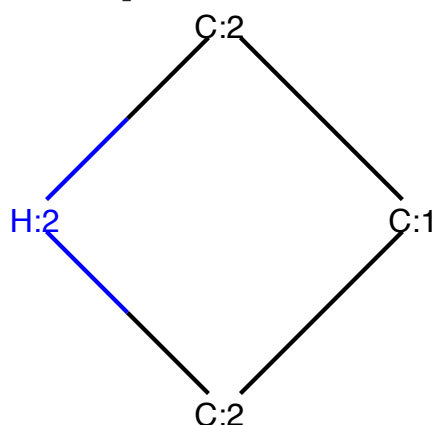
C:2

H:2

C:1

C:2

'--'

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-38-----'

Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-39-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-40-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-41-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-42-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-43-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-44-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-45-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-46-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-47-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-48-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-49-----'

Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-50-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-51-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-52-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-53-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-54-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-55-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-56-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-57-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-58-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-59-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-60-----'

Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-61-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-62-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-63-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-64-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-65-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-66-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-67-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-68-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-69-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-70-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-71-----'

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Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-72-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-73-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-74-----'
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evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-75-----'
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evious fragment.
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'-----Step-76-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-77-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-78-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-79-----'
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evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-80-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-81-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-82-----'
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Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-83-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-84-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-85-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-86-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-87-----'
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evious fragment.
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'-----Step-88-----'
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evious fragment.
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'-----Step-89-----'
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evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-90-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-91-----'
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evious fragment.
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'-----Step-92-----'
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evious fragment.
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ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-93-----'

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        Skip, current fragment has not next fragment to be attached. Go back to the pr
        evious fragment.
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        ield a valid sub-molecule . Go back to the previous fragment.
        '-----Step-94-----'
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        evious fragment.
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        ield a valid sub-molecule . Go back to the previous fragment.
        '-----Step-95-----'
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        evious fragment.
        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-96-----'
        Skip, current fragment has not next fragment to be attached. Go back to the pr
        evious fragment.
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        ield a valid sub-molecule . Go back to the previous fragment.
        '-----Step-97-----'
        Skip, current fragment has not next fragment to be attached. Go back to the pr
        evious fragment.
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        ield a valid sub-molecule . Go back to the previous fragment.
        '-----Step-98-----'
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        evious fragment.
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        ield a valid sub-molecule . Go back to the previous fragment.
        '-----Step-99-----'
        Skip, current fragment has not next fragment to be attached. Go back to the pr
        evious fragment.
        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-100-----'
        Skip, current fragment has not next fragment to be attached. Go back to the pr
        evious fragment.
        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.
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In [ ]: