In [27]:
```
pwd
```

Out[27]:
```
'C:\\Users\\L03121898\\Anaconda3\\envs\\Cadi22\\demo_chemi'
```

In [28]:
```
ls
```

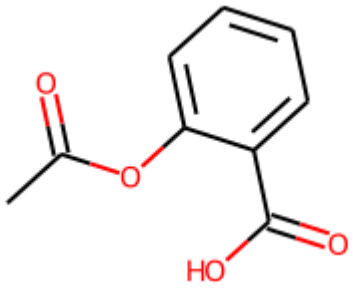
```
 El volumen de la unidad C no tiene etiqueta.
 El n£mero de serie del volumen es: C636-ABF1

 Directorio de C:\Users\L03121898\Anaconda3\envs\Cadi22\demo_chemi

10/01/2022  07:31 p.m.    <DIR>          .
10/01/2022  07:31 p.m.    <DIR>          ..
10/01/2022  04:11 p.m.    <DIR>          .ipynb_checkpoints
10/01/2022  12:17 p.m.             1,273 aspirin.mol
10/01/2022  12:17 p.m.             3,641 aspirin.sdf
10/01/2022  12:17 p.m.        15,740,199 erk2.csv
10/01/2022  12:17 p.m.            24,914 export.sdf
10/01/2022  12:17 p.m.               203 imatinib.smi
10/01/2022  12:17 p.m.             4,300 sample.csv
10/01/2022  12:17 p.m.             2,666 sample.mol
10/01/2022  07:31 p.m.            56,384 Untitled.ipynb
               8 archivos     15,833,580 bytes
               3 dirs  80,171,159,552 bytes libres
```

In [11]:
```
from rdkit import Chem
from rdkit.Chem import Draw
```

In [12]:
```
x=Chem.MolFromSmiles("CC(=O)OC1=CC=CC=C1C(=O)O")
```

In [13]:
```
x
```

Out[13]:



In [26]:
```
8(37)23-8-6-22(7-9-23)20-36-16-14-35(2)15-17-36;1-5(2,3)4/h3-13,18-19H,14-17,2
```

In [14]:
```
path="C:\\Users\\L03121898\\Anaconda3\\envs\\Cadi22\\demo_chemi\\"
```

x1

In [12]:
```
x1
```

Out[12]:

In [15]:
```
x2=Chem.SDMolSupplier(path+"aspirin.sdf")
x3=Chem.SmilesMolSupplier("imatinib.smi", delimiter="\t", titleLine=True)
x4= Chem.MolFromInchi("InChI=1S/C29H31N7O.CH4O3S/c1-21-5-10-25(18-27(21)34-29
```

In [24]:
```
x2=Chem.SmilesMolSupplier(path+"imatinib.smi",delimiter="\t", titleLine=True)
```

In [25]:
```
x2
```

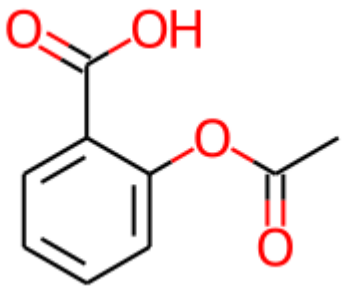
Out[25]: <rdkit.Chem.rdmolfiles.SmilesMolSupplier at 0x12ef0c663b0>

In [23]:
```
[mol.GetNumAtoms() for mol in x2 if mol is not None]
```

Out[23]: []

In [18]:
```
Chem.MolFromMolFile ("aspirin.mol")
```

Out[18]:



In [16]:
```
x1=Chem.MolFromSmiles("C1=CC=CC=C1")
x2=Chem.SDMolSupplier(path+"aspirin.sdf")
x3=Chem.SmilesMolSupplier(path+"imatinib.smi", delimiter="\t", titleLine=True
x4=Chem.MolFromInchi("InChI=1S/C29H31N7O.CH4O3S/c1-21-5-10-25(18-27(21)34-29-
```

In [17]:
```
x4
```

Out[17]: