

Supplementary Information

Essential Step toward Mining Big Polymer Data:

PolyName2Structure, Mapping Polymer Names to Structures

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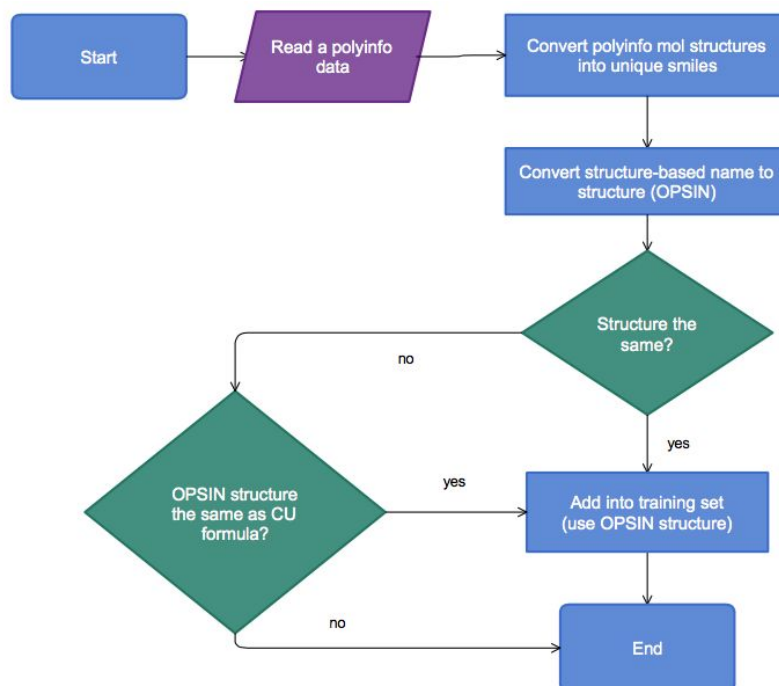
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S1. Data cleaning steps for data from the PoLyInfo database

The data cleaning steps performed in this study are illustrated in Figure S1. For each polymer data entry in the PoLyInfo database, the structure (MDL mol file) provided by the PoLyInfo database is first converted to SMILES format and then compared with the SMILES string generated by OPSIN¹ using the structure-based name of the same entry. If they are the same, this data entry will be assumed to be reliable. If they are not the same, we will further check whether the OPSIN structure is the same as the chemical formula of the constitutional unit (elements are in alphabetical order) provided by the PoLyInfo database. If the answer is yes, this data entry will be assumed to be reliable. It is assumed that this step can filter out some of the errors of polymer structures in the PoLyInfo database.



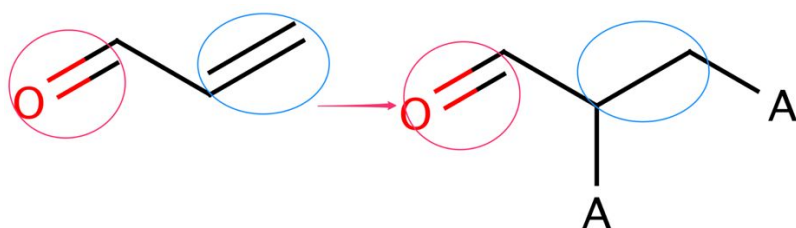
Supplementary Figure1. The data cleaning procedure of the PoLyInfo database.

S2. Descriptors used to build the models for the identification of the reaction group

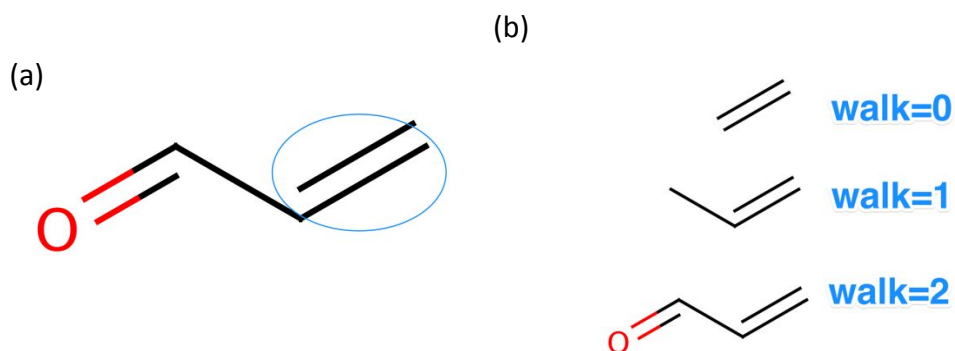
Since chemists usually take observation of neighborhood conditions of important functional groups to determine if one reaction will happen or not. It is straightforward to use the sub-graph of the monomer to model the neighborhood conditions. In this study, we used the sub-graph with distance $\leq N$ to the bond (where N is an arbitrary integer) and we chose $N=5$ in this study. Several supplementary figures and tables are provided below to make reader get the idea. Supplementary figure 2, 3 and supplementary Table 1 illustrate an example of addition reaction. Supplementary figure 4, 5 and supplementary Table 2 illustrate an example of ring opening reaction. Similarly, supplementary figure 6 and supplementary Table 3 illustrate an example of ring opening reaction. The final descriptor sets used in the study are provided in supplementary Table 4, 5, 6.

Descriptors used to build the models for each reaction type are summarized in following sections.

An example of addition reaction:



Supplementary Figure 2. A simple case of addition reaction. The left part is the monomer structure, the right part is the polymer structure. There are two double bonds in the monomer structure, and only the right double will open. Therefore, the left double bond can be marked as “not open” and the right double bond as “open” in training set.

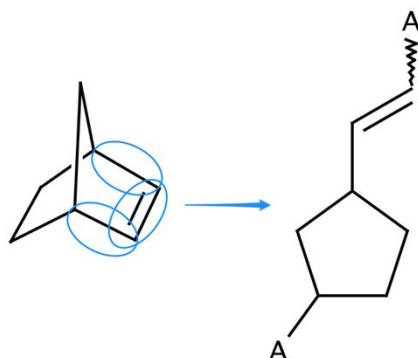


Supplementary Figure 3. The figure shows how to employ the neighborhood condition of each double/triple bond. This is a $N \leq 2$ condition. (a) The “C=C” bond to be calculated the neighborhood condition. (b) The neighborhood conditions of walk=0,1,2 respectively.

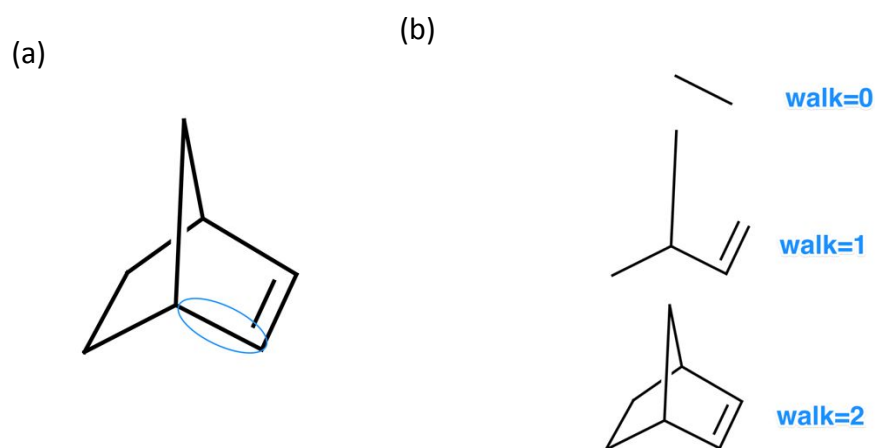
Supplementary Table 1. The training set and the descriptor set of Supplementary Figure 1 and Supplementary Figure 2 with $N=0$.

Data\Des	Des1 (O=C)	Des2(C=C)	Answer (bond open)
O=C	1	0	0
C=C	0	1	1

An example of ring opening reaction:



Supplementary Figure 4. a simple case of ring opening reaction. If one of the three bonds in the left monomer structure is open, then the right polymer structure provided by PoLyInfo database can be obtained. These three ring bonds will be marked as “open”, and other ring bonds will be marked as “not open”.



Supplementary Figure 5. a simple case of generating neighborhood condition of a bond. (a) The bond selected to calculate the neighborhood condition. (b) The neighborhood conditions with walk ≤ 2 .

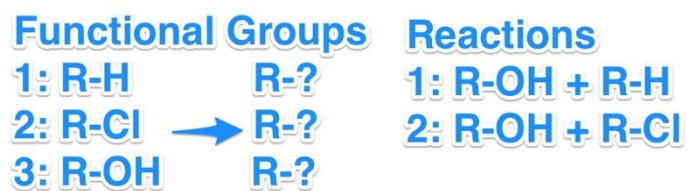
Supplementary Table 2. The training set and the descriptor set with walk ≤ 1 of the simple case.

Data\Des	Des1 (CC)	Des2 (C=C)	Des3 (CC(C)C=C)	Des4 (CC=CC)	Des5 (CC(C)CC)	Des6 (CCCC)	Answer
CC(C)C=C	1	0	1	0	0	0	1
CC=CC	0	1	0	1	0	0	1

C=CC(C)C	1	0	1	0	0	0	1
CC(C)CC	1	0	0	0	1	1	0

An example of ring opening reaction:

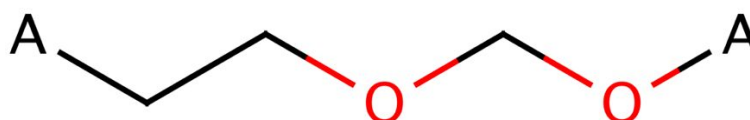
(a)



(b)



(c)



Supplementary Figure 6. This figure shows the case is reaction #2. (a) A simple database of functional groups and reactions. (b) The monomer structures. (c) The polymer structures.

Supplementary Table 3. The training set and descriptor set of the above case.

Case\Des	Des1_m1 (R-H)	Des2_m1 (R-Cl)	Des3_m1 (R-OH)	Des4_m2 (R-H)	Des5_m2 (R-Cl)	Des6_m2 (R-OH)	Answer
Case1 OCCO(m1) + ClCCl(m2)	6	0	2	2	2	0	2

Descriptors used to build the models for each reaction type are summarized below.

A. Addition: Double/Triple Bond Opening Descriptors (SMILES Format)

Walk 0 Descriptors

C=C	N=O	P=S	C#N	O=S	N=N	C=N
[NH2+]=O	C=O	O=P	C=S	C#C	O=[PH3]	

Walk 1 Descriptors

OC=O	CC(S)=O	CS(F)(=O)=O	NS(O)(=O)=O
CC(N)=S	CS(Cl)(=O)=O	N=C=O	CC1=C(C)CC1
CN=C=O	CC=CO	O=S(=O)=O	N=C=S
CN=C=S	NC=O	CC(N)=C	CC=NC
CS(O)(=O)=O	CC=C(C)N	CC(C)=NO	CC=NN
CN(=O)=O	CS(C)=O	CS(N)(=O)=O	CC(C)=C(O)[O-]
CN=C(N)N	C=C=O	CC(C)=O	CC=O
OC(O)=C	CC(C)=C=O	CC=C	OC=C
CC(C)=C(C)C	CC=C(C)C	S=C=S	CC(C)=C
CC#C[SiH3]	CC=CC	FC=C	C1CC=C1
CC(N)=O	CC(O)=O	CC#N	CC(F)=C(F)F
CC=CF	C[N+](=[O-])=O	CC=C[NH3+]	NC=C
[2H]C([2H])=C([2H]) C	O[N+](=[O-])=O	CC(O)=C	OC=CO
SC=C	OC(F)=C(F)F	OC(O)=C(F)F	OC=C(F)F
OC(F)=CF	CC(F)=C	NC(O)=O	CN=C(C)O
[GeH3]C=C	CC#C	[SiH3]C=C	PC=C
CP(C)(C)=O	CC#CC	CC([SnH3])=C	CS(C)(=O)=O
CC(Cl)=C	CC(Br)=C	CC=CCl	CN=NC
ClC=C	FC(F)=C	ClC(Cl)=C	FC=C(F)F
FC(F)=C(F)F	FC(F)=C(F)Cl	FC=CF	BrC=C
FC(F)=C=C	BrC(Br)=C	FC=C(Cl)Cl	FC(Cl)=C(F)Cl
CC(Cl)=C(Cl)Cl	ClC=C(Cl)Cl	C=C=C	OC(F)=C(O)F
OC=C(O)F	FC(F)=S	OC(O)=O	CP(N)(N)=O
OC=CCl	CC#CCl	SC#CS	BC=C
CC#Cl	IC#Cl	BrC#CBr	CC#CS
CP(O)(O)=O	CC(P)=C	CC#C[GeH3]	NC(N)=O

[2H]C([2H])=C(C)C	CN=NS	CS([O-])(=O)=O	CIC=CCI
FC(Cl)=C	[2H]C#C[2H]	CC=C(C)O	CP(N)(O)=O
CC([O-])=O	CC=C[SiH3]	CC(C)=C[PH4]	C[PH2]=O
CP(C)(C)=S	OP(O)([O-])=O	CN=O	FC(F)=C(F)Br
FC(F)=C(F)S	CC=C(C)Cl	CN=C(C)C	

Walk 2 Descriptors

CC(=O)C=Cc(:c):c	CCC(=C)C(O)=O	CC(C)(C)N=C=O
CC(C)(O)C=C	c:c(:c)C=Cc(:c):c	CNC=C
OC(=O)C(=Cc(:c):s)C#N	CCC(=O)C=C	CC1(C)CCCC1=O
CC(N)C(C)=O	OC(=O)C(=Cc(:c):c)C#N	CCC(=C)CC
OCC#C	OC(=O)C=C	c:c(:s)C(=O)c(:c):s
CCC(=C)C=C	CCC=CCC	c:c(:c)C=O
CC(=O)c(:c):c	CC(=C)C(=C(C#N)C#N)c(:c):s	CC=C1CCCC1C
C[Si](C)(C)C#Cc(:c):c	CC(=C)C(=C(C#N)C#N)c(:c):c	c:c1cOC(=O)C=C1
CC(=C)C=Cc(:c):c	c:c(:s)C#N	CCC#N
c:c(:c)C#N	CCC(C)=O	NC(=O)C=C
CC(C)C=C(C)C	C=CN=C	C#CC#N
COC(C)=O	COC(=O)C(C)=C	c:c(:c)C=CC=C
OCC#N	CC(C)C#N	CC(C)C=C
SCC#N	c:c(:c)C#Cc(:c):c	CCC=O
C=CC#N	CCC=CC=C	NCC=C
C1CC=CC1	FC(F)(F)N=O	FC(F)(F)C(=O)C(F)(F)F
CC(F)(F)N=O	CC(=C)C=C	ClCC=O
CC(=O)C=C	CCC(C)=C	SC(=O)C=C
CCC#CC#C	C=CC=O	c:c(:c)C=C
CCC=C	C=CC=C	OC(=N)C=C
OC(=O)C=CC(O)=O	C=CC1CC1	CC(C)(C)C=C
C1CCC=CC1	CC(C)C(=C)C=C	CC(C)C=CC=C
CC(C)(C)C(=C)C=C	CNC(=O)c(:c):c	CN(C)C(=O)c(:c):c
OC(=O)c(:c):c	COC(=O)c(:c):c	CC(=NO)c(:c):c
CCC(=O)c(:c):c	c:c(:c)C(=O)c(:c):c	COS(=O)(=O)c(:c):c
CC(=C)c(:c):c	FC(F)=C(F)c(:c):c	CCC(=NO)c(:c):c
OC(=O)C(=C)c(:c):c	FC=Cc(:c):c	c:c(:c)C(=C(c(:c):c)c(:c):c)c(:c):c
[O-][N+](=O)C=C	FC(F)(F)C(=O)c(:c):c	c:c(:[nH2])C=C
c:n(:[nH2])C=C	[2H]C([2H])=C([2H])c(:c):c	CCC(=O)OC

COC=C	CC(C)C(=O)C=C	CC(=C)C(C)=O
CC(=C)C#N	CCC(=C)C#N	CC(C)C(=C)C#N
c:n(:c)C=C	[SiH3]CC=C	CC(=C)C(O)=O
CO[N+](=[O-])=O	[NH3+]OC=C	COC(=O)C=C
OC(=O)C=CC=C	COC=O	COC=CC
COC(C)=C	COC(=O)C(F)(F)F	COC=CC=C
COC=COC	CC(C)(C)C(=O)C=C	c:c(:c)C(=O)C=C
CSC=C	COC(F)=C(F)F	COC(OC)=C(F)F
COC=C(F)F	COC(F)=CF	CC(=O)C(F)=C
COC(=C)C#N	OC(=C)C#N	COC(=O)C(C)C
COC(=O)C(C)(C)C	COC(=O)C(C)(F)F	COC(=O)C(C)(C)F
CNC(=O)OC	[O-][N+](=O)c(:c):c	CN(C)C=C
CN1Ccc(:c)C1=O	CC1(C)COC(C=C)=N1	CC1(C)N=COC1=O
CC(=C)C(O)=N	CC(=C)C1=NC(C)(C)CO1	C[Ge](C)(C)C=C
c:c(:c)C#C	COC(=C)C(O)=O	COC(=O)C(O)=C
COC(=O)CCl	CC(O)C=C	c:c(:s)C=C
C[SiH2]C=C	CP(C)(=O)C=C	[nH2]:c(:[nH2])C=C
C1CC2CC1C=C2	c:c1cCC=C1	CC#Cc(:c):c
c:c(:o)C=C	CC#C[Si](C)(C)C	C[Sn](C)(C)C(=C)C=C
[SnH3]C(=C)C=C	CN1CCCC1=O	OCC=C
CN(C)S(=O)(=O)C(C)(F)F	CCS(=O)(=O)c(:c):c	CC(C)(C)[N+](=[O-])=O
COC(=O)C(Cl)=C	OC(=O)C(Cl)=C	COC(=O)C(Br)=C
OC(=O)C(Br)=C	CSC(=O)C(C)=C	CC(=C)C(S)=O
CNC(=O)C=C	CN(C)C(=O)C=C	CNC(=O)C(C)=C
CC(=C)C(N)=O	OC(=O)C(=C)C#N	CC[N+](=[O-])=O
CCS(=O)CC	COC(=O)C(F)=C	OC(=O)C(F)=C
OC(=O)C(=C)CF	OC(=O)C=CCl	CC(C)(C)C#N
CN1CC=CC1=O	O=C1NC(=O)C=C1	OC(=O)C(=C)C(O)=O
CC(C)C(=O)C(C)=C	c:c(:c)N=Nc(:c):c	c:c(:c)S(=O)(=O)c(:c):c
CCC(O)=O	OCC(=C)C(O)=O	O=C1OCC=C1
ClC(=C)C=C	FC(=C)C(F)(F)F	FC(F)=C(F)C(F)(F)F
FC(F)(F)C=C	CC(F)(F)C=C	FC(F)=C=C(F)F
ClC(=C)C(Cl)=C	BrC(=C)C=C	FC(F)=C(F)C(Cl)=C
FC(=C)C(Cl)=C	FC(F)=C(F)C=C	FC(=C)C=C
CC(F)(F)C(F)=C(F)F	ClC(Cl)=C(Cl)C(Cl)=C	FC(F)(F)C(=CC=C)C(F)(F)F
CC(=C)C(C)=C	CC(C)(C)C=CC=C	C1CC=CC=C1
CC=CC(C)=C	ClC(Cl)(Cl)C=O	CC(C)C=O

FC1=C(F)OCO1	FC1=COCO1	CCN=C=O
COC(=O)CN	C=C1CCNC1=O	CN1CCC(=C)C1=O
NCC#CC#C	OCC#CC#C	C#CC#CC#C
c:c1C=Cc(:c)c1	CC(=C)c(:[nH2]):[nH2]	OOC(=O)c(:c):c
CC(=C)c(:c):[nH2]	CNC(C)=O	OS(=O)(=O)c(:c):c
CCC#C[Si](C)(C)C	CCC#C	[Na]OS(=O)(=O)c(:c):c
COC(=C)c(:c):c	COC(=O)OC	[Li]OS(=O)(=O)c(:c):c
COC(=O)CO	COC(=O)C(Cl)(Cl)Cl	CN(C)P(=O)(C=C)N(C)C
NP(N)(=O)C=C	CC(=O)n(:c):[nH2]	COC(=O)c(:c):[nH2]
C[Si](C)(C)C=C	NCC=CC=C	COC=CCl
[nH2]:c(:[nH2])C#C	CNC=O	CCC#Cc(:c):c
ClC#Cc(:c):c	CC([SiH3])C#C	ClS(=O)(=O)C=C
CN1CCCC1=S	CN1Scc(:c)C1=O	CS(=O)C=C
NCC#C	c:c(:[nH2])C#C	O[Si](O)(O)C=C
CC1CCN(C)C1=O	CSC#CSC	NB(N)C=C
c:c(:c)S(=O)C=C	C=C(C#N)C#N	ClC(=C)C#N
IC#Cc(:c):c	OC1CC=CC=C1	CSC#CC
c:c(:s)C#C	COP(=O)(OC)C(C)=C	OP(O)(=O)C(=C)C(P)=C
C#CC#C	CC1=CCOC1=O	CC(=C)C=C(C)C(O)=O
CC(=CC=C)C(O)=O	CC(=C)C(Cl)=C	CCC=C(C)C
CC(=C)C(=C)c(:c):c	NC(N)C=C	CC#C[Ge](C)(C)C
FS(=O)(=O)C=C	CC(C)(O)C#C	CSC(=O)C=C
c:c(:c)C=Nc(:c):c	CNC(=O)N(C)C	CN1CNC(=O)C=C1C#N
NC(=C)C#N	c:c(:c)C(C#N)=C(C#N)C#N	c:c(:c)N=Nc(:c):s
COC(=O)C(C)Cl	CCS(=O)(=O)OC	CCS(N)(=O)=O
CC(=Cc(:c):c)c(:c):c	COC(=O)C(C)O	CN(O)C(=O)C=C
[2H]C([2H])=C(C(O)=O)C([2H])([2H])[2H]	CNC(=O)CN	CCS(=O)(=O)O[Na]
CC(=O)ON	ON1CCCC1=O	COC(=O)C(C)N
NOC(=O)C(F)(F)F	CNN=Cc(:c):c	NCP(O)(O)=O
CCS(O)(=O)=O	c:c(:c)C=Cc(:c):[nH2]	C=CC1=CC(=C)CCC1
CCC(C=C)=C(C#N)C#N	c:c(:c)P(=O)(c(:c):c)c(:c):c	CCP(=O)(OC)OC
NC(=O)C1=Cc(:c)cOC1=O	CCC(=O)N(C)C	OCC(=O)c(:c):c
[Li]OS(=O)(=O)CC	[Li]OC(=O)CC	OC(=O)C1=Cc(:c)cOC1=O
CNS(=O)(=O)c(:c):c	CC1=C(CO)C2(C)C=CC12C	CC1=C(C)C2(C)C=CC12C
[Na]OS(=O)(=O)N=N	OS(=O)(=O)N=Nc(:c):c	CCS(=O)(=O)N(C)C
c:c(:c)C=C(C#N)c(:c):c	O=C1OCCO1	CNC(=O)NC

CNC1=NC(=O)C=CN1	C=CC(=O)N=C	CC1=CC(=O)N=CN1
CCS([O-])(=O)=O	CNC(=O)CO	OC(=O)C(=C)C(F)(F)F
CN(C)C(=O)CO	c:c(:c)N=Nc(:[nH2]):s	CS(=O)(=O)c(:c):c
CCC#CC	CC(C)(C)C#C	CC(C)=C1C=CC=C1
C=C1C=CC=C1	CC1=CCC=C1	CC1CC=CC1=C(C)C
CC1CC(=C)C=C1	c:c1cCCC=C1	CC=C(C)C=C
CCC=CC	CC1CCC=C1	C=CC=CC=C
CC#CC(C)C	C1CC=CO1	CC1=CCCO1
ClC(Cl)C=O	C=C1OCCO1	FC(F)=C1OCCO1
CCN=C=S	CC(C)N=C=O	O=C1NCC=C1
NC(P)P(O)(O)=O	FC(=C)C#N	CC(F)(F)S(O)(=O)=O
CC(F)(F)P(O)(O)=O	FC(F)=C(F)C(F)(F)P	CC(F)(F)S(F)(=O)=O
CC(C)C(C)=C	COP(=O)(C=C)N(C)C	NP(O)(=O)C=C
c:c(:[cH2-])C=C	[O-]C(=O)C=C	C[Si](C)(O)C=Cc(:c):c
C[Si](O)(O)C=Cc(:c):c	O[Si](O)(O)C=Cc(:c):c	CCC(CC)=C[PH2]=O
C=C[PH2]=O	CP(C)(=S)C=C	c:c(:[cH2-])C#C
NCC([O-])=O	COC([O-])=C(C#N)C#N	COP([O-])(=O)OC
c:c(:c)N(=O)=O	ClCC=Cc(:c):c	c:c(:o)C=O
CSC(F)=C(F)F	C1COC=CC1	ClC1=CC(=O)NC1=O
CN1CC=C(Cl)C1=O	COC(=O)N=C	CCC(C=C)=NC(O)=O
CN(C)C1=CCCC=C1	NC1=CCC(=N)C=C1	CC(=C)N=C
CNC(C)=C	CC1=C(C)C(=O)OC1=O	

Walk 3 Descriptors

CC1(C)CC2CC1C=C2	c:c(:c)C(=C)C=C	Cc1csc(N)c1C#N
CC(=O)CC(O)=O	CC(=O)CC(C)(C)N	c:c:c(C=C(C#N)C#N):c:c
COC(=O)C=CC=CC	CCCC=O	CCC(CC)C=C
CC=CCC=C	CCCC#CC#CC	CN=NS(=O)(=O)O[Na]
CCCC=C	CC=CC#N	OC([O-])=C(C#N)C#N
c:c(:c)CC#N	C=CCN=C	CCCC#CC#C
CCOC(=O)CC(C)=C	COC(=O)C(C)=CC=CC	CCCC=C(C)C
CC1CCC=CC1	C=CN=C=O	CC(=C)N=C=O
C[Si](C)(C)CC=C	c:c:c(:c:c)C#C	COC(=O)C=Cc(:c:c):c:c
CC(C)=CC=C	CCCC=CCCC	CC(C)CC=C
c:c(:c)CC=C	CCC(C)(O[SiH3])C=C	CCCC(C)=C
CC=CC(O)=O	CC=CC=CC	c:c(:c)N=C=O
C=CC1CCC1	C=CC1CCCC1	CC(C=C)c(:c):c

<chem>CCC(C)C=C</chem>	<chem>CC(C)(C)CC=C</chem>	<chem>C=C1CCCCC1</chem>
<chem>CCCC(=C)C=C</chem>	<chem>CCC(C)C=CC=C</chem>	<chem>CC=CC=C</chem>
<chem>c:c:c(C=C):c:c</chem>	<chem>Cc(:c):c(C=C):c:c</chem>	<chem>CNC(=O)c(:c:c):c(C):c</chem>
<chem>CN(C)C(=O)c(:c:c):c(C):c</chem>	<chem>Cc(:c):c(:c:c)C(=O)Nc(:c):c</chem>	<chem>Cc(:c):c(:c:c)C(O)=O</chem>
<chem>COC(=O)c(:c:c):c(C):c</chem>	<chem>CCOC(=O)c(:c:c):c(C):c</chem>	<chem>CC(C)OC(=O)c(:c:c):c(C):c</chem>
<chem>Cc(:c):c(:c:c)C(=O)Oc(:c):c</chem>	<chem>CCOC(=O)c(:c:c):c:c</chem>	<chem>Oc(:c):c(C=C):c:c</chem>
<chem>Clc(:c):c(C=C):c:c</chem>	<chem>Fc(:c):c(C=C):c:c</chem>	<chem>c:c:c(:c:c)C#N</chem>
<chem>CC(=NO)c(:c:c):c:c</chem>	<chem>CN(C)C(=O)c(:c:c):c:c</chem>	<chem>CCN(CC)C(=O)c(:c:c):c:c</chem>
<chem>NCCC(=O)c(:c:c):c:c</chem>	<chem>OC(=O)c(:c:c):c:c</chem>	<chem>COC(=O)c(:c:c):c:c</chem>
<chem>CC(C)OC(=O)c(:c:c):c:c</chem>	<chem>CCC(=O)c(:c:c):c:c</chem>	<chem>CCCC(=O)c(:c:c):c:c</chem>
<chem>c:c:c(:c:c)C(=O)Cc(:c):c</chem>	<chem>c:c:c(:c:c)C(=O)c(:c:c):c:c</chem>	<chem>CCOS(=O)(=O)c(:c:c):c:c</chem>
<chem>Clc(:c):c(C=C):c(Cl):c</chem>	<chem>BrC(:c):c(C=C):c:c</chem>	<chem>Cc(:c):c(C=C):c(C):c</chem>
<chem>Fc(:c):c(C=C):c(F):c</chem>	<chem>CC(=C)c(:c:c):c:c</chem>	<chem>FC(F)=C(F)c(:c:c):c:c</chem>
<chem>FC(F)=C(F)c(:c(F):c):c(F):c</chem>	<chem>ON=C(Cc(:c):c)c(:c:c):c:c</chem>	<chem>c:c:c(C=C):c(:c):c</chem>
<chem>CC(=O)c(:c:c):c:c</chem>	<chem>COC(=O)C(=C)c(:c):c</chem>	<chem>FC=Cc(:c:c):c:c</chem>
<chem>c:c:c(:c:c)C(=C(c(:c:c):c:c)c(:c:c):c:c)c(:c:c):c:c</chem>	<chem>CC=C[N+](=[O-])=O</chem>	<chem>[O-][N+](=O)C=Cc(:c:c):c:c</chem>
<chem>FC(F)(F)C(=O)c(:c:c):c:c</chem>	<chem>c:c:c(C=C):n:c</chem>	<chem>c:c:c(C=C):c:[nH2]</chem>
<chem>C=Cn1cccn1</chem>	<chem>CC(=O)Oc(:c):c</chem>	<chem>[2H]C([2H])=C([2H])c(:c([2H])):c(:c([2H])):c</chem>
<chem>CCCC(=O)OC=C</chem>	<chem>CC(=O)OC=C</chem>	<chem>CCCC(=O)C#N</chem>
<chem>C=CN1C(=C)C=CC1=C</chem>	<chem>CCOC=C</chem>	<chem>c:c:c(:c:c)C(=O)OC=C</chem>
<chem>CCOC(=O)C(C)=C</chem>	<chem>NCCC=C</chem>	<chem>[O-][N+](=O)OC=C</chem>
<chem>COC(=O)C=CC</chem>	<chem>[SiH3]CCC=C</chem>	<chem>C=COC=O</chem>
<chem>CC(C)OC=C</chem>	<chem>CC(C)(C)OC=C</chem>	<chem>CCOC=CC</chem>
<chem>FC(F)(F)C(=O)OC=C</chem>	<chem>OC=CC=C</chem>	<chem>CC=COC(C)(C)C</chem>
<chem>CC=COC(C)C</chem>	<chem>CCOC=COC</chem>	<chem>Oc(:c):c(:c:c)C(=O)C=C</chem>
<chem>CCSC=C</chem>	<chem>CC(F)(F)OC(F)=C(F)F</chem>	<chem>FC(F)=C(OC(F)(F)F)OC(F)(F)F</chem>
<chem>FC(F)=COC(F)(F)F</chem>	<chem>FC=C(F)OC(F)(F)F</chem>	<chem>CC(F)(F)OC=C</chem>
<chem>CC(=C)OC(C)=O</chem>	<chem>Oc(:c):c(:c:c)C(=O)OC=C</chem>	<chem>CCCC(=O)Oc(:c):c</chem>
<chem>Clc(:c):c(:c:c)C(=O)OC=C</chem>	<chem>CCC(CC)C(=O)OC=C</chem>	<chem>CC(C)CC(=O)OC=C</chem>
<chem>CCC(C)(C(=O)OC=C)C(C)(C)C</chem>	<chem>CC(F)(F)C(F)(F)C(=O)OC=C</chem>	<chem>CC(F)(F)C(F)(C(=O)OC=C)C(C)(F)F</chem>
<chem>CC(C)(C)OC(=O)NC=C</chem>	<chem>OC(=O)NC=C</chem>	<chem>FC(F)(F)C(F)(F)C(=O)OC=C</chem>
<chem>Cc(:c):c(:c:c)C(=O)OC=C</chem>	<chem>CC(C)(C)CC(=O)OC=C</chem>	<chem>CCC(C)(C)C(=O)OC=C</chem>
<chem>CC(C)(C)C(C)(C)C(=O)OC=C</chem>	<chem>CC(C)C(C)(C)C(=O)OC=C</chem>	<chem>c:c:c(:c:[nH2])C(=O)OC=C</chem>
<chem>[O-][N+](=O)c(:c:c):c:c</chem>	<chem>CCC(=O)Oc(:c):c</chem>	<chem>C=CN1C(=O)C=CC1=O</chem>

c:c:c1C(=O)N(C=C)C(=O)c1: c	C=CN1CCCC1	CC1(C)N=C(OC1=O)C=C
CC1=NC(C)(C)C(=O)O1	C=CC1=NCCO1	CC(=C)C1=NCCO1
CC(C)(F)OC=C	CC=COC(C)(C)F	CCOC(=C)C(=O)OC
COC(=C)C(=O)OC(C)C	ClCC(=O)OC=C	C=CC1CCCCO1
C=Cc1cccs1	CC[SiH2]C=C	COC(=O)C(=C)CC(O)=O
CCOC(=O)C(=C)CC	C=COC(=O)C1CCCC1	CCC(C)(CC)C(=O)OC=C
c:c(:c)P(=O)(C=C)c(:c):c	c:n:c(C=C):n:c	CC1CC2CC1C=C2
c:c:c1C=CCc1:c	CC#Cc(:c):c:c	C=Cc1ccco1
CC[Si](C)(C)C#CC	CC#C[Si](C)(C)C(C)C	CC#C[Si](C)(C)c(:c):c
[O-][N+](=O)c(:c:c):c:[nH2]	CNCC=C	Cc(:c):c(:c:c)[N+](O)=O
Nc(:c):c(:c:c)[N+](O)=O	COC(C=C)C(C)O	CCCC(=O)OC(C)C
CC(O)CC=C	CCC(OC)C=C	C=Cn1ccnc1
CC[Sn](CC)(CC)C(=C)C=C	CC(F)OC(F)=C(F)F	C=CN1CCCC1=O
CCOC(=O)C=C	CC(C)OC(=O)C=C	CC(C)(C)OC(=O)C=C
COCC=C	CC(C)(F)OC(=O)C=C	CCN(CC)S(=O)(=O)C(F)(F)C(C)(F)F
CC(C)OC(=O)C(C)=C	OCCS(=O)(=O)c(:c:c):c:c	CC(C)(CO)[N+](O)=O
CCOC(=O)C(Cl)=C	CC(C)OC(=O)C(Cl)=C	CC(C)OC(=O)C(Br)=C
CCSC(=O)C(C)=C	CC(C)NC(=O)C=C	CCN(CC)C(=O)C=C
CCNC(=O)C=C	CCNC(=O)C(C)=C	COC(=O)C(=C)C#N
COCC#N	OCCC#N	CCCC#N
FCOC(=O)C=C	CSCC#N	SCCC#N
COC(=O)c(:c:c):c(O):c	CCOC(=O)c(:c:c):c(O):c	CN(C(=O)C=C)c(:c):c
CC(C)(C)NC(=O)C=C	CC(C)N(C(C)C)C(=O)C=C	OCC[N+](O)=O
CCS(=O)CCO	CC(=C)C(=O)O[SiH3]	CCC(=C)C(=O)OC
CCOC(=O)C(=C)C#N	COC(=O)C(=C)CF	CCOC(=O)C(=C)CF
CC(C)OC(=O)CC(C)=C	CCC(=C)C(=O)OC(C)C	CC(=C)CC(=O)Oc(:c):c
CCC(=C)C(=O)Oc(:c):c	COC(=O)C=CCl	CC(C)(CO)C#N
CCC(CO)C#N	CC(O)CC#N	COC(=O)CC(C)=C
CCOC(=O)C=CC	COC(=O)C=CC(=O)OC	CC(C)N1C(=O)C=CC1=O
CN1C(=O)C=CC1=O	CCOC(=O)C(=C)C(O)=O	COC(=O)C(=C)C(=O)OC
CN(C)C(=O)C(C)=C	c:c(:c)N1C(=O)C=CC1=O	CCN(C)S(=O)(=O)C(F)(F)C(C)(F)F
CCC(C)C(=O)C(C)=C	c:c:c(:c:c)N=Nc(:c:c):c:c	CC(=O)NC(=O)Oc(:c):c
c:c:c(:c:c)S(=O)(=O)c(:c:c):c: c	CCOC(=O)NC(C)=O	CC(C)OC(=O)NC(C)=O

<chem>c:c:c(:c:c)C(=O)Oc(:c):c</chem>	<chem>CCCC(O)=O</chem>	<chem>CCC(C)C(=O)OC</chem>
<chem>CCCC(=C)C(=O)OC</chem>	<chem>COCC#C</chem>	<chem>CC(C)OC(=O)C(=C)C#N</chem>
<chem>CCOC(=O)C(=C)CO</chem>	<chem>COC(=O)C(=C)CO</chem>	<chem>O=C1OC(=O)C=C1</chem>
<chem>FC(F)(F)C(F)(F)C=C</chem>	<chem>CC(F)(F)C(F)(F)C=C</chem>	<chem>FC(F)(F)CC=C</chem>
<chem>FC(F)(F)C(C=C)C(F)(F)F</chem>	<chem>CC(F)(F)C(F)(F)C(F)=C(F)F</chem>	<chem>ICCC=C</chem>
<chem>ClC(Cl)=C(Cl)C(Cl)=C(Cl)Cl</chem>	<chem>CCCC=CC=C</chem>	<chem>CC(C)CC=CC=C</chem>
<chem>CC(C)=CC=C(C)C</chem>	<chem>CC=CC(=O)OC(C)C</chem>	<chem>O=CCC#N</chem>
<chem>CC(C)CC=O</chem>	<chem>CCCC(=O)OC</chem>	<chem>CC1(C)OC(F)=C(F)O1</chem>
<chem>FC1=C(F)OC(F)(F)O1</chem>	<chem>CC1(F)OC(F)=C(F)O1</chem>	<chem>CC1(C)OC=C(F)O1</chem>
<chem>CCCN=C=O</chem>	<chem>CC(C)CN=C=O</chem>	<chem>CCOC(=O)CNC</chem>
<chem>CCNC(=O)OCC</chem>	<chem>COC(=O)c(:c:c):c(N):c</chem>	<chem>CCOC(=O)c(:c:c):c(N):c</chem>
<chem>CN1C(=O)CC(=C)C1=O</chem>	<chem>c:c(:c)N(C=C)c(:c):c</chem>	<chem>CC#CC#CCn(:c):c</chem>
<chem>COCC#CC#CC</chem>	<chem>CC#CC#CCO</chem>	<chem>CC#CC#CC#CC</chem>
<chem>CCOC(=O)Nc(:c):c</chem>	<chem>c:c:c1C=Cc(:c:c)c1:c</chem>	<chem>C1CC=CCCC=C1</chem>
<chem>CC(=C)c(:n:c):n:c</chem>	<chem>c:c:c(C=O):c:c</chem>	<chem>COOC(=O)c(:c:c):c:c</chem>
<chem>CC(=C)c(:c:c):n:c</chem>	<chem>CC(=O)Nc(:c):c</chem>	<chem>OS(=O)(=O)c(:c:c):c:c</chem>
<chem>[2H]c(:c):c(C=C):c([2H]):c</chem>	<chem>C[Si](C)(C)C#Cc(:c:c):c:c</chem>	<chem>Cc(:c):c(:c:c)C#C[Si](C)(C)C</chem>
<chem>CCCC#C[Si](C)(C)C</chem>	<chem>CCCC#C</chem>	<chem>[Na]OS(=O)(=O)c(:c:c):c:c</chem>
<chem>CC=C(C#N)C#N</chem>	<chem>CCOC(=O)C(=CC)C#N</chem>	<chem>COC(=O)C(=Cc(:c:c):c:c)C#N</chem>
<chem>CC=C(C#N)C(O)=O</chem>	<chem>c:c:c(C=CC#N):c:c</chem>	<chem>CC(=O)OC(=C)c(:c:c):c:c</chem>
<chem>COC(=O)Oc(:c):c</chem>	<chem>[Li]OS(=O)(=O)c(:c:c):c:c</chem>	<chem>c:c:c(:c:c)S(=O)(=O)c(:c:c):c(:c):c</chem>
<chem>[O-][N+](=O)c(:c:c):c(Cl):c</chem>	<chem>c:c:c(C=Cc(:c:c):c:c):c:c</chem>	<chem>CC(C)=C(C(=C(C#N)C#N)c1ccc1)c(:c):c</chem>
<chem>CC(C)=C(C#N)C#N</chem>	<chem>CC(C)=C(C(=C(C#N)C#N)c(:c):c):c:c)c(:c):s</chem>	<chem>Cc(:c):c(:c:c)C#Cc(:c:c):c:c</chem>
<chem>c:c:c(:c:c)C#Cc(:c:c):c:c</chem>	<chem>CCOC(=O)NC(C)(C)C</chem>	<chem>CC(C)(C)OC(=O)Nc(:c):c</chem>
<chem>OC(=O)C=Cc(:c:c):c:c</chem>	<chem>CCCC(=O)OCC</chem>	<chem>c:c:c(:c:c)C(=O)c(:c:c):c(:c):c</chem>
<chem>CCNC(=O)c(:c:c):c(O):[nH2]</chem>	<chem>CCOC(C)=O</chem>	<chem>CC(C)OC(C)=O</chem>
<chem>CC(C)(C)OC(=O)OC(C)(C)C</chem>	<chem>COCC(=O)OC(C)(C)C</chem>	<chem>ClC(Cl)(Cl)C(=O)OC=C</chem>
<chem>CC(=O)n1cccc1:c</chem>	<chem>c:c1c[nH]nc1C(=O)OC=C</chem>	<chem>c:n(:[nH2])CC=C</chem>
<chem>CC=CC=CCN</chem>	<chem>CCOC=C(Cl)</chem>	<chem>CC=CC=Cc(:c:c):c:c</chem>
<chem>CC#CC#CCCO</chem>	<chem>CC#CC#CCOS</chem>	<chem>c:c:c(C#C):c(:c):c</chem>
<chem>Cn1ccnc1C#C</chem>	<chem>C#Cc1ncc[nH]1</chem>	<chem>c:c(:c)NC=O</chem>
<chem>CC#CC#N</chem>	<chem>c:c:c(:c:c)C#CC#N</chem>	<chem>CCOC(=O)OC=C</chem>
<chem>OC(=O)OC=C</chem>	<chem>CCC#Cc(:c:c):c:c</chem>	<chem>CCCC#Cc(:c:c):c:c</chem>
<chem>ClC#Cc(:c:c):c:c</chem>	<chem>CC#C[Si](C)(C)C[SiH3]</chem>	<chem>CCC(C#C)[Si](C)(C)C</chem>

<chem>CC(=C)CC(O)=O</chem>	<chem>COCC(=O)OC</chem>	<chem>C=CN1CCCC1=S</chem>
<chem>CN(S)C(=O)C=C</chem>	<chem>CC(=O)N1Sc(:c)c(:c:c)C1=O</chem>	<chem>C[Si](C)(C=C)c(:c):c</chem>
<chem>CC[Si](C)(C)C=C</chem>	<chem>CCOC(=O)NC(C)C</chem>	<chem>CNCC#C</chem>
<chem>c:c:c(:n:c)C#C</chem>	<chem>CO[Si](OC)(OC)C=C</chem>	<chem>CC(=O)CC(=O)OC=C</chem>
<chem>c:c:c1C(=O)N(c(:c):c)C(=O)c1:c</chem>	<chem>C[Si](C=C)(c(:c):c)c(:c):c</chem>	<chem>CC(C)C1CCN(C=C)C1=O</chem>
<chem>CC=CC(=O)OC(C)(C)C</chem>	<chem>CCC(CC)(CC)C(=O)OC=C</chem>	<chem>CCSC#CSCC</chem>
<chem>BNB(NB)C=C</chem>	<chem>C=CNC=O</chem>	<chem>c:c:c(:c:c)S(=O)C=C</chem>
<chem>c:c(:c)OC=C</chem>	<chem>IC#Cc(:c:c):c:c</chem>	<chem>COC1C=CC=CC1O</chem>
<chem>Cc(:c):c(:c:c)C#C</chem>	<chem>[SiH3]c(:c):c(:c:c)C#C</chem>	<chem>Cc(:c):c(C#C):c(C):c</chem>
<chem>[GeH3]c(:c):c(:c:c)C#C</chem>	<chem>Fc(:c):c(C#C):c(F):c</chem>	<chem>CCSC#CC</chem>
<chem>CC=CC(=O)OC=C</chem>	<chem>Cc1occc1C#C</chem>	<chem>C#Cc1ccsc1</chem>
<chem>C#Cc1cccs1</chem>	<chem>Cc1sccc1C#C</chem>	<chem>CCOP(=O)(OCC)C(=C)C(P)=C</chem>
<chem>COP(=O)(OC)C(=C)C(=C)P(O)(O)=O</chem>	<chem>PC(=C)C(=C)P(=O)(Oc(:c):c)Oc(:c):c</chem>	<chem>CC#CC#C</chem>
<chem>COC(=O)C(=CC)C#N</chem>	<chem>CCOC(=O)NC(O)=O</chem>	<chem>CC(=C)C1=CCOC1=O</chem>
<chem>CC1=CC(=O)OC1=O</chem>	<chem>COC(=O)C(C)=CC</chem>	<chem>CC(C)=CC(C)=C</chem>
<chem>CC=CC=C(C)C</chem>	<chem>C=Cn1cncn1</chem>	<chem>c:c:c(:c:c)C(=C)C(=C)c(:c):c</chem>
<chem>CN(C)C(C=C)N(C)C</chem>	<chem>CCNC(=O)OC=C</chem>	<chem>NC(=O)OC=C</chem>
<chem>CCOC(=O)CC</chem>	<chem>OC1(C#C)c(:c)c-cc1:c</chem>	<chem>CCSC(=O)C=C</chem>
<chem>CC(C)SC(=O)C=C</chem>	<chem>c:c:c(C=Nc(:c:c):c:c):c:c</chem>	<chem>CC(F)(F)OC(=O)C=C</chem>
<chem>c:n(:c)C(=O)C=C</chem>	<chem>CCN1C(C)=CC(=O)NC1=O</chem>	<chem>CC1=CC(=O)NC(=O)N1</chem>
<chem>CCN1C(=O)NC(=O)C=C1C#N</chem>	<chem>CC=C(C#N)N(C)C</chem>	<chem>Oc(:c):c(:c:c)[N+][[O-]]=O</chem>
<chem>CC(C)NC(=O)C(C)=C</chem>	<chem>CCN(C)C(=O)C=C</chem>	<chem>CC(O)OC(=O)C=C</chem>
<chem>CC(O)OC(=O)C(C)=C</chem>	<chem>c:c:c1C(=O)c(:c:c)c(:c)Cc1:c</chem>	<chem>CC(C)=C(C#N)c(:c):c</chem>
<chem>CC(=C)CC(=O)OC(C)(C)C</chem>	<chem>CCC(=C)C(=O)OC(C)(C)C</chem>	<chem>CN(C)CC=C</chem>
<chem>CCN(C(=O)C=C)c(:c):c</chem>	<chem>Cc1ccsc1N=Nc(:c:c):c:c</chem>	<chem>Cc1ccsc1C#N</chem>
<chem>CCOC(=O)C(C)Cl</chem>	<chem>CCOS(=O)(=O)CC(C)(C)C</chem>	<chem>CC1(C)C2CCC1(CS)C(=O)C2</chem>
<chem>CC(C)(C)OC(=O)Oc(:c):c</chem>	<chem>OCNC(=O)C=C</chem>	<chem>CC(=O)NC(C)=O</chem>
<chem>CC(C)(N)CS(N)(=O)=O</chem>	<chem>CC(C)NC(=O)c(:c:c):c:c</chem>	<chem>CCNC(=O)N(CC)CC</chem>
<chem>CC(=Cc(:c:c):c:c)c(:c:c):c:c</chem>	<chem>c:c(:c)OC(=O)C1COCO1</chem>	<chem>ON(C(=O)C=C)c(:c):c</chem>
<chem>[2H]C([2H])=C(C(=O)OC)C([2H])([2H])[2H]</chem>	<chem>CN(C)CC(=O)NC(C)(C)C</chem>	<chem>CCCS(=O)(=O)O[Na]</chem>
<chem>OCCS(=O)(=O)O[Na]</chem>	<chem>Nc(:c):c(:c:c)C(O)=O</chem>	<chem>CCN1CCCC1=O</chem>
<chem>CC(=O)N1CCCC1=O</chem>	<chem>CN(C)OC(C)=O</chem>	<chem>CON1C(C)CCC1=O</chem>
<chem>CCOC(=O)C1CCCN1O</chem>	<chem>CN(C)OC(=O)C(F)(F)F</chem>	<chem>CC(=O)c(:c:c):c(O):c</chem>
<chem>COC(=O)C(=Cc1cccs1)C#N</chem>	<chem>O=C(c1cccs1)c1cccs1</chem>	<chem>CC(Cl)OC(=O)C=C</chem>

<chem>Oc(:c):c(C=Nc(:c:c):c:c):c:c</chem>	<chem>c:c:c(C=CC(=O)c(:c):c):c:c</chem>	<chem>CC=CC(=O)c(:c:c):c:c</chem>
<chem>c:c:c(C=NNc(:c):c):c:c</chem>	<chem>CNCP(O)(O)=O</chem>	<chem>PCNC(=O)C=C</chem>
<chem>CC1(O)CCOC(=O)C1</chem>	<chem>NCCC(O)=O</chem>	<chem>CC(C)(N)CS(O)(=O)=O</chem>
<chem>c:c:c(C=Cc(:c:c):n:c):c:c</chem>	<chem>Clc(:c):c(:c:c)N=Nc(:c:c):c:c</chem>	<chem>[NH3+]c(:c):c(C=Cc(:c:c):c:c):c:c</chem>
<chem>CCC(=CC)C=Cc(:c:c):c:c</chem>	<chem>CC=CC1=CC(CC(C)(C)C1)=C(C)C</chem>	<chem>CC1=CC(CC(C)(C)C1)=C(C#N)C#N</chem>
<chem>c:c:c(:c:c)P(=O)(c(:c:c):c:c)c(:c:c):c:c</chem>	<chem>CCOP(=O)(CC(O)O)OCC</chem>	<chem>CNC(=O)C1=Cc(:c:c)c(:c)OC1=O</chem>
<chem>CCNC(=O)C(=CC)C(O)=O</chem>	<chem>NC(=O)C1=Ccc(:c)OC1=O</chem>	<chem>CCN(C(C)=O)C(=O)NC(C)C</chem>
<chem>NC(=O)N1CCCCC1=O</chem>	<chem>COCC(=O)c(:c:c):c:c</chem>	<chem>Cc(:c):c(:c:c)N=Nc(:c:c):c:c</chem>
<chem>Nc(:c):c(:c:c)C#N</chem>	<chem>[Li]OS(=O)(=O)CCC</chem>	<chem>[Li]OC(=O)CCC</chem>
<chem>COC(=O)C1=Cc(:c:c)c(:c)OC1=O</chem>	<chem>CCOC(=O)C(=CC)C(O)=O</chem>	<chem>OC(=O)C1=Ccc(:c)OC1=O</chem>
<chem>CC=CC(=O)Oc(:c):c</chem>	<chem>CC(C)C(=O)C=Cc(:c:c):c:c</chem>	<chem>CC=CC(=O)C(c(:c):c)c(:c):c</chem>
<chem>c:c1OC(=O)C=Cc1</chem>	<chem>c:c:c1C=CC(=O)Oc1:c</chem>	<chem>CC(C)(N)CS(=O)(=O)O[Na]</chem>
<chem>CC(=C)C(=O)OCS</chem>	<chem>CCN1C(=O)c(:c)c(:c:c)C1=O</chem>	<chem>c:c:c(:c:c)S(=O)(=O)Nc(:c):[nH2]</chem>
<chem>COCC1=C(C)C2(C)C(C)=C(C)C12C</chem>	<chem>CC1=C(C)C2(C)C(C)=C(C)C12C</chem>	<chem>[Na]OS(=O)(=O)N=Nc(:c:c):c:c</chem>
<chem>CCOC(=O)C(F)(F)C(C)(F)F</chem>	<chem>CCCS(=O)(=O)N(C)CC</chem>	<chem>c:c:c(C=C(C#N)c(:c:c):c:c):c:c</chem>
<chem>CC=C(C#N)c(:c):c</chem>	<chem>Oc(:c):c(:c:c)C(=O)c(:c:c):c:c</chem>	<chem>CC1COC(=O)O1</chem>
<chem>Oc(:c):c(C=NNc(:[nH2]):s):c:c</chem>	<chem>CCNC(=O)NC(N)=N</chem>	<chem>CC1=CC(=O)N=C(NC(N)=O)N1</chem>
<chem>CC1=CC(=O)N=C(N)N1</chem>	<chem>CCCS([O-])(=O)=O</chem>	<chem>CCOC(=O)CCN</chem>
<chem>COCC(=O)Nc(:c):[nH2]</chem>	<chem>COCC(=O)Nc(:c):c</chem>	<chem>CC(C)(C)OC(=O)C(=C)C(F)(F)F</chem>
<chem>COC(=O)C(=C)C(F)(F)F</chem>	<chem>CCN(CC)C(=O)COC</chem>	<chem>COCC(=O)N1CCCC1</chem>
<chem>c:c:c(:c:c)N=Nc1nccs1</chem>	<chem>CS(=O)(=O)c(:c:c):c:c</chem>	<chem>CC(C=C)C(F)(F)F</chem>
<chem>CCCC#CC</chem>	<chem>CCC(C)C=C(C)C</chem>	<chem>CCC1C(C)C=CC1=C(C)C</chem>
<chem>CCC1C=CC(C1C)=C(C)C</chem>	<chem>CC1CC=CCC1C</chem>	<chem>c:c:c1C=CCCc1:c</chem>
<chem>CCC(CC)(CC)C#C</chem>	<chem>CCC(C)(C)C#C</chem>	<chem>C=CCC=C</chem>
<chem>CC=C1CC2CC1C=C2</chem>	<chem>C=C1CC2CC1C=C2</chem>	<chem>CC1CCC2CC=CC12</chem>
<chem>CC1C(C)C2CC1C=C2</chem>	<chem>C1=CC=CC=CC=C1</chem>	<chem>CC1(C)CC=CO1</chem>
<chem>CCC(C=O)C(C)C</chem>	<chem>CC1COC(=C)O1</chem>	<chem>OC(F)(F)C(F)(F)C(F)=C(F)F</chem>
<chem>OCOC=C(F)F</chem>	<chem>CC1(F)OC(OC1(F)F)=C(F)F</chem>	<chem>CCN(C(=O)C=C)C(C)(C)C</chem>

CCCN=C=S	c:c(:c)N=C=S	CC(N=C=O)C(C)=O
CC(N=C)C(C)=O	CC(C)(C)N1C(=O)C=CC1=O	CCN1C(=O)C=CC1=O
c:c:c(:c:[nH2])C#N	CN(C)CP(O)(O)=O	CN(C)C(P(O)(O)=O)P(O)(O)=O
CCOC(F)=C(F)F	OC(F)(F)C(F)(F)S(O)(=O)=O	OP(O)(=O)C(F)(F)C(F)=C
CC(C)(F)OC(F)=C(F)F	OC(F)(F)C(F)(F)S(F)(=O)=O	FC(F)=C(F)OC(F)(F)F
CCOP(=O)(C=C)N(C)C	CN(C)P(=O)(Oc(:c):c)C=C	[Fe++][c-]1cccc1C=C
C[Si](C)(O[SiH3])C=Cc(:c:c):c:c	C[Si](O[SiH3])(O[SiH3])C=Cc(:c:c):c:c	[SiH3]O[Si](O[SiH3])(O[SiH3])C=Cc(:c:c):c:c
CC(C)=C[PH2]=O	[2H]C([2H])([2H])OC(=O)OC=C	c:c(:c)P(=S)(C=C)c(:c):c
[Fe++][c-]1cccc1C#C	c:c1cnnn1C=C	COC(C)C(=O)Oc(:c):c
CC(C)(N=C=O)c(:c):c	CCC(=O)C(C)=C	CN(C)CC([O-])=O
CCOC([O-])=C(C#N)C#N	CCOP([O-])(=O)OCC	c:c:c(:c:c)N(=O)=O
ClCC=Cc(:c:c):c:c	FC(F)(Br)C(F)(F)N=O	O=Cc1ccco1
CCC(C)(O)C=C	FC(F)=C(F)SC(F)(F)F	CN1C(=O)C=C(Cl)C1=O
CCOC(=O)N=C(C)C	COC(=O)N=C1CC=CC=C1	N=C1CC=C(C=C1)N1C(=O)C=CC1=O
CN=C1CC=C(C=C1)N(C)C	CC(=C)N1C(=O)C=CC1=O	CCOC(=O)NC(C)=C
CC(=C)NC(O)=O		

Walk 4 Descriptors

c:c(:c)CCC#C	CC1(C)CC(C=C)=CC(C1)=C(C#N)C#N
c:c(:c)OC(=O)C=C	c:c1cccc(C=O)c1
C1C=CC2C3CC(C=C3)C12	C=Cc1cccc1C#C
C=COC(=O)C=C	CC(=O)OCC=C
c:c1cccc(C=Cc2ccccc2)n1	Cc1cccc(c1)C#Cc1ccccc1
Cc1ccccc1C#C	C=CCCC=C
[O-][N+](=O)c1ccccc1	CCC(C)(C)CC=C
N#Cc1ccccc1	CC(=O)OCC#C
C=Cc1ccccc1C#Cc1ccccc1	c:c(:c)C=CC(=O)OC=C
c:c(:c)OC(=O)C=Cc1ccccc1	C[Si](C)(CC=C)C=C
CCCC=CCCC	COC(=O)C(=Cc(:c):s)C#N
CN(CC=C)C(C)=O	CN(CC=C)C(=O)C=C
C=CC1CCC=CC1	C=CCN=C=O
C=CCN=C=S	CC(=O)N(CC=C)c(:c):c
CC(=O)N(CC=C)C(C)(C)C	CCC1CC2CC1C=C2

<chem>C=C1C=CC2CC=CCC12</chem>	<chem>CC(C)=CCCC(C)(C)O</chem>
<chem>CC(=O)OC(=O)C=C</chem>	<chem>CCCC=CC=C</chem>
<chem>NCCN=C=O</chem>	<chem>CCC(CC)CC=C</chem>
<chem>CCCC=C</chem>	<chem>CCOC(=O)C(=Cc(:c):c)C#N</chem>
<chem>N#CC(C#N)=C(C#N)C#N</chem>	<chem>c:c(:c)CN=C=O</chem>
<chem>CC(C)CCC=C</chem>	<chem>C=CCC1CCCC1</chem>
<chem>C=CC1CCCCC1</chem>	<chem>c:c:c(CC=C):c:c</chem>
<chem>c:c(:c)CCC=C</chem>	<chem>CC(C=C)c(:c:c):c:c</chem>
<chem>CCC(C)CC=C</chem>	<chem>CCCC(C)C=C</chem>
<chem>CC1CCC(=C)CC1</chem>	<chem>CC1CCCC(C1)C=C</chem>
<chem>CCCC(=C)C=C</chem>	<chem>CC(C)(C)CCC=C</chem>
<chem>C=Cc1ccccc1</chem>	<chem>Cc1ccccc1C=C</chem>
<chem>CCc1ccccc1C=C</chem>	<chem>OCc1ccccc1C=C</chem>
<chem>CNC(=O)c1ccccc1C=C</chem>	<chem>NC(=O)c1ccccc1C=C</chem>
<chem>CN(C)C(=O)c1ccccc1C=C</chem>	<chem>c:c:c(NC(=O)c1ccccc1C=C):c:c</chem>
<chem>OC(=O)c1ccccc1C=C</chem>	<chem>COC(=O)c1ccccc1C=C</chem>
<chem>CCOC(=O)c1ccccc1C=C</chem>	<chem>CCCOC(=O)c1ccccc1C=C</chem>
<chem>CC(C)OC(=O)c1ccccc1C=C</chem>	<chem>CC(C)COC(=O)c1ccccc1C=C</chem>
<chem>c:c:c(OC(=O)c1ccccc1C=C):c:c</chem>	<chem>NCCOC(=O)c1ccccc1C=C</chem>
<chem>NCCOC(=O)c1ccccc1</chem>	<chem>COc1ccccc1C=C</chem>
<chem>Clc1ccccc1C=C</chem>	<chem>Fc1ccccc1C=C</chem>
<chem>Cc1cccc(C=C)c1</chem>	<chem>Clc1cccc(C=C)c1</chem>
<chem>Fc1cccc(C=C)c1</chem>	<chem>CC(=NO)c1ccccc1</chem>
<chem>CN(C)C(=O)c1ccccc1</chem>	<chem>CCN(CC)C(=O)c1ccccc1</chem>
<chem>O=C(N1CCCCC1)c1ccccc1</chem>	<chem>CN(C)CCC(=O)c1ccccc1</chem>
<chem>O=C(N1CCOCC1)c1ccccc1</chem>	<chem>OC(=O)c1ccccc1</chem>
<chem>COC(=O)c1ccccc1</chem>	<chem>CCOC(=O)c1ccccc1</chem>
<chem>CCCOC(=O)c1ccccc1</chem>	<chem>CC(C)OC(=O)c1ccccc1</chem>
<chem>CC(C)COC(=O)c1ccccc1</chem>	<chem>CCC(=O)c1ccccc1</chem>
<chem>CCCC(=O)c1ccccc1</chem>	<chem>CCCCC(=O)c1ccccc1</chem>
<chem>c:c:c(CC(=O)c1ccccc1):c:c</chem>	<chem>O=C(c1ccccc1)c1ccccc1</chem>
<chem>CCCOS(=O)(=O)c1ccccc1</chem>	<chem>Clc1cccc(Cl)c1C=C</chem>
<chem>CC(C)c1ccccc1C=C</chem>	<chem>BrC1CCCC1C=C</chem>
<chem>FC(F)(F)c1ccccc1C=C</chem>	<chem>Cc1ccc(C)c(C=C)c1</chem>
<chem>CC(C)c1ccc(C)cc1C=C</chem>	<chem>Clc1ccc(Cl)c(C=C)c1</chem>
<chem>Fc1ccc(F)c(C=C)c1</chem>	<chem>Cc1ccc(F)c(C=C)c1</chem>
<chem>COc1ccc(Br)cc1C=C</chem>	<chem>Cc1cc(C)cc(C=C)c1</chem>

<chem>Cc1cccc(C)c1C=C</chem>	<chem>Fc1cc(F)c(F)c(C=C)c1F</chem>
<chem>CC(=C)c1cccc1</chem>	<chem>FC(F)=C(F)c1cccc1</chem>
<chem>FC(F)=C(F)c1c(F)c(F)cc(F)c1F</chem>	<chem>ON=C(Cc(:c:c):c:c)c1cccc1</chem>
<chem>c:c:c1c(C=C)cccc1:c</chem>	<chem>CC(=O)c1cccc1</chem>
<chem>COC(=O)C(=C)c(:c:c):c:c</chem>	<chem>COC(=O)C(=C)c1cccc1</chem>
<chem>FC=Cc1cccc1</chem>	<chem>c1ccc(cc1)C(=C(c1cccc1)c1cccc1)c1cccc1</chem>
<chem>[O-][N+](=O)C=Cc(:c):c</chem>	<chem>[O-][N+](=O)C=Cc1cccc1</chem>
<chem>FC(F)(F)C(=O)c1cccc1</chem>	<chem>Bc1cccc(C=C)c1</chem>
<chem>c:c1cccc(C=C)c1</chem>	<chem>C=Cc1ccncc1</chem>
<chem>Cc1cccc(C=C)n1</chem>	<chem>C=Cc1cccnc1</chem>
<chem>c:c1cn(C=C)nc1:c</chem>	<chem>Nc1cccc(C=C)c1</chem>
<chem>CC(=O)Oc(:c:c):c:c</chem>	<chem>OC(=O)c1cccc1C(O)=O</chem>
<chem>Cc1ccc(C(O)=O)c(c1)C(O)=O</chem>	<chem>[2H]C([2H])=C([2H])c1c([2H])c([2H])cc([2H])c1[2H]</chem>
<chem>CCCCC(=O)OC=C</chem>	<chem>CCC(=O)OC=C</chem>
<chem>C=Cc1ccccn1</chem>	<chem>c:c:c1n(C=C)c(:c:c)c(:c)c1:c</chem>
<chem>CCCOC=C</chem>	<chem>c:c(:c)C(=O)OC=C</chem>
<chem>C=COC(=O)c1cccc1</chem>	<chem>CC(C)COC=C</chem>
<chem>CCCOC(=O)C(C)=C</chem>	<chem>CN(C)CCC=C</chem>
<chem>NCCCC=C</chem>	<chem>COC(=O)C=CC=C</chem>
<chem>CC=CC=CC(O)=O</chem>	<chem>C[Si](C)(C)CCC=C</chem>
<chem>[SiH3]CCCC=C</chem>	<chem>c:c(:c)COC=C</chem>
<chem>CCC(C)OC=C</chem>	<chem>CC=COCC(C)C</chem>
<chem>CC(C)(C)COC=C</chem>	<chem>CCCOC=CC</chem>
<chem>Cc(:c):c(CC=C):c:c</chem>	<chem>CCC(CC)C(=O)C=C</chem>
<chem>C=CC(=O)C1CCCCC1</chem>	<chem>Oc1cccc1C(=O)C=C</chem>
<chem>c:c:d(:c:c)C(=C)C=C</chem>	<chem>C=CC(=C)c1cccc1</chem>
<chem>CCCSC=C</chem>	<chem>CCC(CC)OC=C</chem>
<chem>CC(F)(F)C(F)(F)OC(F)=C(F)F</chem>	<chem>FC(F)=C(F)OC(F)(F)C(F)(F)F</chem>
<chem>CC(F)(F)C(F)(F)OC=C</chem>	<chem>c:c:c(:c:c)C(=O)C=C</chem>
<chem>C=CC(=O)c1cccc1</chem>	<chem>Oc1cccc(c1)C(=O)C=C</chem>
<chem>Cc1cccc(c1)C(=O)C=C</chem>	<chem>CC(=O)OC(=C)C#N</chem>
<chem>CC(=O)Oc(:c:c):c(C):c</chem>	<chem>COc1cccc1C(=O)OC=C</chem>
<chem>CCCC(=O)Oc(:c:c):c:c</chem>	<chem>Clc1cccc1C(=O)OC=C</chem>
<chem>Clc1cccc(c1)C(=O)OC=C</chem>	<chem>CC(C)C(=O)OC=C</chem>
<chem>C=COC(=O)C1CCCCC1</chem>	<chem>CCC(CC)CC(=O)OC=C</chem>

CC(C)CCC(=O)OC=C	CC(C)(C)C(=O)OC=C
FC(F)(F)C(F)(F)C(F)(F)C(=O)OC=C	CC(F)(F)C(=O)OC=C
FC1(F)CC(F)(F)C(F)(F)C(F)(C(=O)OC=C)C1(F)F	CC(C)(F)C(=O)OC=C
COC(=O)NC=C	CC(F)(F)C(F)(F)C(F)(F)C(=O)OC=C
C=COC(=O)c1ccncc1	Oc1cccc(c1)C(=O)OC=C
Cc1ccccc1C(=O)OC=C	Cc1cccc(c1)C(=O)OC=C
CC(C)(CC(=O)OC=C)c(:c):c	[SiH3]c1cccc(c1)C(=O)OC=C
CCCC(C)(C)C(=O)OC=C	CCC(C)(C)C(C)(C)C(=O)OC=C
CC(C)C(C)C(C)(C)C(=O)OC=C	CC(C)(C)CC(C)(C)C(=O)OC=C
C=COC(=O)c1cccnc1	Cc1cccc(c1)[N+](=[O-])=O
[NH3+]c1cccc(c1)C(=O)OC=C	CCC(=O)Oc(:c):c:c
C=CN1C(=O)C(=C)C(=C)C1=O	C=CN1C(=O)c2ccccc2C1=O
CC(=C)C1=NC(C)(C)C(=O)O1	C#Cc1ccccc1
FC(F)(F)C(F)(OC=C)C(F)(F)F	CC=COC(F)(C(F)(F)F)C(F)(F)F
CCOC(=C)C(=O)OC(C)C	CCOC(=C)C(=O)OC(CC)CC
ClCCOC=C	OCCOC=C
FC(F)(F)COC=C	CCCOC(=O)CC(=C)C(O)=O
CCOC(=O)C(=C)CC(=O)OC	CCCOC(=O)C(=C)CC(O)=O
CC1(CCCCC1)C(=O)OC=C	c:c:c(:c:c)P(=O)(C=C)c(:c:c):c:c
C=CP(=O)(c1ccccc1)c1ccccc1	Cc1nc(C)nc(C=C)n1
OCC1CC2CC1C=C2	C1C=Cc2ccccc12
CC#Cc1ccccc1	CCC[Si](C)(C)C#CC
CC#C[Si](C)(C)c(:c):c:c	[O-][N+](=O)c1cccnc1
c:c(:[nH2])NCC=C	c:c(:c)NCC=C
[O-][N+](=O)c1ccccc1C(F)(F)F	[NH3+]c1cccc(c1)[N+](=[O-])=O
CNc1ccc([NH3+])cc1[N+](=[O-])=O	COC(C=C)C(OC(C)=O)C=C
CCCCC(=O)OC(C=C)C(C)O	COC(CC=C)C=C
CCCCC(=O)OC(CC)C=C	CC(=O)OC(CC=C)C=C
CCC(CC=C)OC	CCCCC(=O)OC(CC)CC
CCC[Sn](CCC)(CCC)C(=C)C=C	FC(F)C(F)OC(F)=C(F)F
CCCOC(=O)C=C	CC(C)COC(=O)C=C
CCC(C)OC(=O)C=C	C=CCOC(=O)C=C
FC(F)(F)COC(=O)C=C	CC(F)(F)COC(=O)C=C
FC(F)(F)C(OC(=O)C=C)C(F)(F)F	FC(F)(F)C(F)(OC(=O)C=C)C(F)(F)F
FC(F)(F)C(F)(OC(=O)C=C)C(F)(F)Cl	FC(F)(Cl)C(F)(OC(=O)C=C)C(F)(F)Cl
OCCOC(=O)C=C	NCCOC(=O)C=C

<chem>CCCN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(C)(F)F</chem>	<chem>CCC(C)OC(=O)C(C)=C</chem>
<chem>CC(C)COC(=O)C(C)=C</chem>	<chem>CC(=C)C(=O)OC(C)(C)C</chem>
<chem>CCC(CC)(CC)OC(=O)C(C)=C</chem>	<chem>CCC(CC)OC(=O)C(C)=C</chem>
<chem>CCC(C)(CC)OC(=O)C(C)=C</chem>	<chem>CCC(OC(=O)C(C)=C)C(C)C</chem>
<chem>CC(=C)C(=O)Oc(:c):c</chem>	<chem>CC(=C)C(=O)Oc(:c:c):c:c</chem>
<chem>CC(=C)C(=O)Oc(:c:c):c(C):c</chem>	<chem>CC(=C)C(=O)OCc(:c):c</chem>
<chem>CC(OC(=O)C(C)=C)c(:c):c</chem>	<chem>CC(=C)C(=O)OC(c(:c):c)c(:c):c</chem>
<chem>CCC(CC)(OC(=O)C(C)=C)c(:c):c</chem>	<chem>CC(=C)C(=O)OCCF</chem>
<chem>CC(=C)C(=O)OCCCl</chem>	<chem>CC(=C)C(=O)OCCBr</chem>
<chem>CC(=C)C(=O)OCC(F)(F)F</chem>	<chem>CC(=C)C(=O)OCC(C)(F)F</chem>
<chem>CC(Cl)OC(=O)C(C)=C</chem>	<chem>CCC(Cl)OC(=O)C(C)=C</chem>
<chem>CC(OC(=O)C(C)=C)C(F)(F)F</chem>	<chem>CC(=C)C(=O)OC(C(F)(F)F)C(F)(F)F</chem>
<chem>CC(=C)C(=O)OC(CCl)CCl</chem>	<chem>CC(Br)COC(=O)C(C)=C</chem>
<chem>CC(=C)C(=O)OC(C)(C)F</chem>	<chem>CC(=C)C(=O)OC(F)(C(F)(F)F)C(F)(F)F</chem>
<chem>CC(=C)C(=O)OC(F)(C(F)(F)F)C(F)(F)Cl</chem>	<chem>CC(=C)C(=O)Oc(:c:c):c(Cl):c</chem>
<chem>CC(=C)C(=O)Oc(:c(Cl):c):c(Cl):c</chem>	<chem>CC(=C)C(=O)Oc(:c(Br):c):c(Br):c</chem>
<chem>CC(=C)C(=O)OCCO</chem>	<chem>CC(=C)C(=O)Oc(:c:c):c(O):c</chem>
<chem>CC(O)COC(=O)C(C)=C</chem>	<chem>CC(=C)C(=O)OCc(:c):o</chem>
<chem>CC(=C)C(=O)OCCS</chem>	<chem>COCCS(=O)(=O)c1ccccc1</chem>
<chem>CC(=C)C(=O)OCCN</chem>	<chem>CC(=C)C(=O)OCC(C)(C)[NH3+]</chem>
<chem>COCC(C)(C)[N+][[O-]]=O</chem>	<chem>CCC(C)OC(=O)C(Cl)=C</chem>
<chem>ClCCOC(=O)C(Cl)=C</chem>	<chem>CCC(C)OC(=O)C(Br)=C</chem>
<chem>CCC(CC)OC(=O)C(Br)=C</chem>	<chem>CCC(CC)OC(=O)C(Cl)=C</chem>
<chem>BrC(=C)C(=O)Oc(:c):c</chem>	<chem>BrC(=C)C(=O)Oc(:c:c):c:c</chem>
<chem>CCCSC(=O)C(C)=C</chem>	<chem>CCCN(CCC)C(=O)C=C</chem>
<chem>CCCNC(=O)C=C</chem>	<chem>CCCNC(=O)C(C)=C</chem>
<chem>CC(=C)C(=O)NCc(:c):c</chem>	<chem>CC(=C)C(=O)NCCO</chem>
<chem>CCC(CC)OC(=O)C=C</chem>	<chem>CCC(OC(=O)C(C)=C)c(:c):c</chem>
<chem>CCCOC(=O)C(Cl)=C</chem>	<chem>CC(C)(C)COC(=O)C=C</chem>
<chem>C=CC(=O)OCC#N</chem>	<chem>CC(=O)OCC#N</chem>
<chem>COCCC#N</chem>	<chem>CCCCC#N</chem>
<chem>CC(O)COC(=O)C=C</chem>	<chem>SCCOC(=O)C=C</chem>
<chem>CCSCC#N</chem>	<chem>CSCCC#N</chem>
<chem>SCCCC#N</chem>	<chem>CCC(CC)(CC)OC(=O)C=C</chem>
<chem>c:c:c(OC(=O)C=C):c:c</chem>	<chem>Cc(:c):c(OC(=O)C=C):c:c</chem>
<chem>COC(=O)c1ccccc1OC</chem>	<chem>CCOC(=O)c1ccccc1OC</chem>

<chem>COC(=O)c1cccc(O)c1</chem>	<chem>CCOC(=O)c1cccc(O)c1</chem>
<chem>c:c(:c)COC(=O)C=C</chem>	<chem>CN(C(=O)C=C)c(:c:c):c:c</chem>
<chem>Clc(:c):c(OC(=O)C=C):c:c</chem>	<chem>Clc(:c):c(OC(=O)C=C):c(Cl):c</chem>
<chem>c:c:c(OC(=O)C=C):c(:c):c</chem>	<chem>CCC(C)NC(=O)C=C</chem>
<chem>CC(OC(=O)C(C)=C)C(C)(C)C</chem>	<chem>CC(=C)C(=O)NC(C)(C)C</chem>
<chem>CC(=C)C(=O)OCC[NH3+]</chem>	<chem>COCC[N+](O-)=O</chem>
<chem>CC(=C)C(=O)OC(C)(F)F</chem>	<chem>CC(=C)C(=O)OC(F)(F)C(C)(F)F</chem>
<chem>CCS(=O)CCOC</chem>	<chem>CC(=C)C(=O)O[Si](C)(C)C</chem>
<chem>CC(=C)C(=O)OCC(C)(C)C</chem>	<chem>c:c:c(CC#N):c:c</chem>
<chem>CC(=C)C(=O)Nc(:c):c</chem>	<chem>CC(=C)C(=O)Nc(:c:c):c:c</chem>
<chem>CCOC(=O)CC(=C)C(O)=O</chem>	<chem>CCOC(=O)C(=C)CC(O)=O</chem>
<chem>CCCOC(=O)C(=C)C#N</chem>	<chem>COC(=O)CC(=C)C(=O)OC(C)C</chem>
<chem>CCC(CC)OC(=O)CC(=C)C(O)=O</chem>	<chem>CCC(CC)OC(=O)C(=C)CC(O)=O</chem>
<chem>CC(C)COC(=O)CC(=C)C(O)=O</chem>	<chem>CC(C)COC(=O)C(=C)CC(O)=O</chem>
<chem>COC(=O)CC(=C)C(=O)Oc(:c):c</chem>	<chem>OC(=O)C(=C)CC(=O)Oc(:c:c):c:c</chem>
<chem>OC(=O)CC(=C)C(=O)Oc(:c:c):c:c</chem>	<chem>OC(=O)C(=C)CC(=O)OCc(:c):c</chem>
<chem>OC(=O)CC(=C)C(=O)OCc(:c):c</chem>	<chem>CC(C)COC(=O)C(Cl)=C</chem>
<chem>COCC(C)(C)C#N</chem>	<chem>CCCC(COC)C#N</chem>
<chem>COC(C)CC#N</chem>	<chem>COC(=O)CC(=C)C(O)=O</chem>
<chem>COC(=O)CC(=C)C(=O)OC</chem>	<chem>CCOC(=O)C=CC(O)=O</chem>
<chem>CCOC(=O)C=CC(=O)OCC</chem>	<chem>COC(=O)C=CC(O)=O</chem>
<chem>CCCOC(=O)C=CC(O)=O</chem>	<chem>CCC(COC)C#N</chem>
<chem>CC(=C)C(=O)Oc(:c:c):c(:c):c</chem>	<chem>CCC(CC)N1C(=O)C=CC1=O</chem>
<chem>CCCOC(=O)C(=C)C(=O)OC</chem>	<chem>CCOC(=O)C(=C)C(=O)OCC</chem>
<chem>Cc(:c):c(OC(=O)CC(=C)C(O)=O):c:c</chem>	<chem>Cc(:c):c(OC(=O)C(=C)CC(O)=O):c:c</chem>
<chem>CCN(CC)C(=O)C(C)=C</chem>	<chem>CC(=C)C(=O)N1CCCCC1</chem>
<chem>c:c:c(N1C(=O)C=CC1=O):c(:c):c</chem>	<chem>c:c:c(:c:c)N1C(=O)C=CC1=O</chem>
<chem>CCN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(C)(F)F</chem>	<chem>CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(C)(F)F</chem>
<chem>CC(=C)C(=O)OCC1CO1</chem>	<chem>CC(C)CC(C)C(=O)C(C)=C</chem>
<chem>c1ccc(cc1)N=Nc1ccccc1</chem>	<chem>CC(=C)C(=O)NC(O)=O</chem>
<chem>COC(=O)NC(=O)C(C)=C</chem>	<chem>CC(=C)C(=O)NC(=O)Oc(:c:c):c:c</chem>
<chem>O=S(=O)(c1ccccc1)c1ccccc1</chem>	<chem>CC(=C)C(=O)NC(=O)OCCO</chem>
<chem>CC(CO)OC(=O)NC(=O)C(C)=C</chem>	<chem>CC(=C)C(=O)NC(=O)Oc(:c(Br):c):c(Br):c</chem>
<chem>Brcc1cc(Br)cc(c1)S(=O)(=O)c1cc(Br)cc(Br)c1</chem>	<chem>[NH3+]c1cc([NH3+])cc(c1)C(=O)OCCO</chem>
<chem>Cc1cc([NH3+])cc(c1)[N+](O-)=O</chem>	<chem>c:c:c(OC(=O)c1ccccc1):c:c</chem>
<chem>c:c:c(OC(=O)C=C):c(:c):[nH2]</chem>	<chem>CC(=C)C(=O)Oc(:c:c):c(:c):[nH2]</chem>

CCCC(O)=O	CCCC(C)C(=O)OC
COC(=O)C(=C)CCC(C)C	CC(=C)C(=O)OCC#C
CC(C)COC(=O)C(=C)C#N	FC(F)(F)C(F)(F)C(F)(F)C=C
FC(F)(F)CCC=C	CC(F)(F)C(F)(F)C(F)(F)C(F)=C(F)F
ICCCC=C	CC(CC=C)C(F)(F)F
CC(C)OC(=O)C=CC=C	CC(C)OC(=O)C=CC=CC(O)=O
CCCOC(=O)C=CC=C	CCCOC(=O)C=CC=CC
O=CCCC#N	CCCCC=O
COC(=O)CCC=O	OC(=O)CCC=O
FC1=C(F)OC(O1)(C(F)(F)F)C(F)(F)F	FC1=C(F)OC(F)(O1)C(F)(F)F
CC(F)(F)C1(F)OC(F)=C(F)O1	CC(F)(F)C1(OC(F)=C(F)O1)C(F)(F)F
FC1=COC(O1)(C(F)(F)F)C(F)(F)F	CCCCN=C=O
CCC(C)CN=C=O	c:c:c(:c:c)N=C=O
O=C=Nc1ccccc1	CCCOC(=O)CNC(O)=O
CCCOC(=O)NCC(O)=O	CCCCC#CC#CCC
Cc(:c):c(N1C(=O)C=CC1=O):c(C):c	Cc(:c):c(:c:c)N1C(=O)C=CC1=O
COC(=O)c1ccccc1N(C)C	CCCOC(=O)c1ccccc1N(C)C
CCCOC(=O)c1ccccc1N(C)C	c:c(:c)N1C(=O)CC(=C)C1=O
c:c:c(:c:c)N1C(=O)CC(=C)C1=O	CC(=O)OC(=O)C(C)=C
CC(=C)C(=O)OC(=O)C(C)=C	C=CC(=O)OC(=O)C=C
c:c:c(:c:c)N(C=C)c(:c:c):c:c	NCC#CC#CCN1C(=C)C=CC1=C
CCNC(=O)OCC#C	NC(=O)OCC#CC#CCO
OCC#CC#CC#C	OCC#CC#CC#CCO
c:c:c(NC(=O)OCC#C):c:c	NC(=O)OCC#CC#CC#C
CCCOC(=O)NCC	CCCOC(=O)Nc(:c:c):c:c
C1=Cc2ccccc3ccccc1c23	C=CC1CCCCC1
CC(=C)c1ncncn1	COc1ccc(O)cc1C=C
O=Cc1ccccc1	CC(C)(C)OOC(=O)c1ccccc1
CC(=C)c1cccc(:c)n1	Oc1cccc(C=C)c1
CC(=O)Nc(:c:c):c:c	CC(=C)c1cccc(:c)c1
OS(=O)(=O)c1ccccc1	[2H]c1cc([2H])c([2H])c(C=C)c1[2H]
C[Si](C)(C)C#Cc1ccccc1	Cc1cccc(c1)C#C[Si](C)(C)C
C[Si](C)(C)C#Cc1ccccc1C=C	C[Si](C)(C)C#CCCc(:c):c
[Na]OS(=O)(=O)c1ccccc1	c:c(:c)C=C(C#N)C#N
N#CC(=Cc1ccccc1)C#N	CCCOC(=O)C(=Cc1ccccc1)C#N
COC(=O)C(=Cc(:c):c)C#N	c:c(:c)C=CC#N
N#CC=Cc1ccccc1	Nc1nc(N)nc(C=C)n1

CC(=O)OC(=C)c(:c):c	CC(=O)OC(=C)c1ccccc1
COC(=O)Oc(:c:c):c:c	[Li]OS(=O)(=O)c1ccccc1
Oc1ccccc1C=C	Oc1cc(O)cc(C=C)c1
CC(=O)Oc(:c(O):c):c(O):c	c:c:c1c(cccc1:c)S(=O)(=O)c1ccccc1
Cc1ccc(Cl)c(c1)[N+][[O-]]=O	[NH3+]c1cccc(C=C)c1
C(=Cc1ccccc1)c1ccccc1	Cc1ccc(s1)C(=C(C#N)C#N)C(=C(C#N)C#N)c (:c:c):c:c
N#CC(C#N)=C(C(=C(C#N)C#N)c1ccccc1)c1 cccs1	BrC1cccc(C=C)c1
CC(=O)Oc(:c:c):c(O):c	c1ccc(cc1)C#Cc1ccccc1
CC(=C)c1cccc(C)c1	CC(C)(NC(=O)OCCN)c(:c):c
CC(C)(C)OC(=O)Nc(:c:c):c:c	OC(=O)C=Cc(:c):c
OC(=O)C=Cc1ccccc1	OCCCC(=O)OCc(:c):c
Cc(:c):c(OC(=O)c1ccccc1):c:c	c:c1cccc(c1)C(=O)c1ccccc1
c:c:c1c(cccc1:c)C(=O)c1ccccc1	COc1ncccc1C(=O)NCc(:c):c
Cc1cccc(c1)C(=O)Oc(:c:c):c:c	Cc1ccc(C(O)=O)c(C=C)c1
CC(O)COC(C)=O	CC(O)C(OC(C)=O)C(O)O
CC(O)C(OC(C)=O)C(C)O	CC(C)(C)OC(=O)OC(c(:c):c)(C(F)(F)F)C(F)(F) F
CC(C)(C)OCC(=O)OC(C)(C)C	CC(=O)OCCO
CC(=C)c1nc(N)nc(N)n1	OCCCC=C
CC(=O)n1nc(C)c(:c)c1:c:c	Cn1nc(C(=O)OC=C)c(:c:c)c1:c
c:c:[nH2]C(=O)OC=C	c:c1ccnn1CC=C
C=CC=CC#N	CCOC(=O)C=CC=C
CC=CC=CC(=O)OC(C)C	CC(C)COC(=O)C=CC=C
NCC=CC=CC(O)=O	CCCOC=CCl
CCOC(=O)C=CC=Cc(:c):c	OC(=O)C=CC=Cc1ccccc1
COC(=O)C=CC=Cc(:c):c	CCC#CC#CCCOS
O=S(=O)(OCC#C)c1ccccc1	CS(=O)(=O)OCC#CC#CCO
c:c1cccc(c1)C#C	c:c:c1c(cccc1:c)C#C
CN1C(=C)C(=C)N=C1C#C	C=C1NC(=NC1=C)C#C
c:c:c(NC=O):c:c	c:c(:c)C#CC#N
N#CC#Cc1ccccc1	ClC(Cl)(Cl)COC(=O)OC=C
COC(=O)OC=C	FC(F)(F)COC(=O)OC=C
CCCOC(=O)OC=C	CCC#Cc1ccccc1
CCCC#Cc1ccccc1	ClC#Cc1ccccc1
CC#C[Si](C)(C)C[Si](C)(C)C	CC#C[Si](C)(C)CC[SiH3]

CCCC(C#C)[Si](C)(C)C	OC(=O)CC(=C)C(O)=O
COC(=O)COC=C	OC(=O)COC=C
C=CC(=O)N1SC=CC1=O	C=CC(=O)N1SC(=C)C(=C)C1=O
C=CC(=O)N1Sc2cccc2C1=O	C[Si](C)(C=C)c(:c:c):c:c
C[Si](C)(Cc(:c):c)C=C	CCCOC(=O)NC(C)C
CCNCC#C	Cc1cccc(c1)C#C
Cc1cccc(n1)C#C	CCO[Si](OCC)(OCC)C=C
BrC1cccc(c1)C#C	Clc1cccc(c1)C#C
[SiH3]c1cccc(c1)C#C	[SnH3]c1cccc(c1)C#C
COC(=O)CC(C)=O	Cc1ccc2C(=O)N(c(:c:c):c:c)C(=O)c2c1
C[Si](C=C)(c(:c:c):c:c)c(:c:c):c(:c):c	CC1CCN(C=C)C1=O
CC(C)C(C)C1CCN(C=C)C1=O	CC=CC=CC(=O)OC(C)(C)C
CCC(CC)(CC)OC(=O)C=CC=C	CCCC(CCC)(CCC)C(=O)OC=C
CCC(CC)(CC)OC=C	C=CB1NBNBN1
C=Cc1cccc2OCOC12	C=CS(=O)c1cccc1
c:c:c(OC=C):c:c	IC#Cc1cccc1
CC(O)C(OC(C)=O)C=C	COC1C=CC=CC1OC(C)=O
FC(F)(F)c1cccc1C#C	C[Si](C)(C)c1cccc1C#C
OCCCC#C	Cc1cccc(C)c1C#C
C[Ge](C)(C)c1cccc1C#C	[SiH3]Cc1cccc1C#C
Fc1cc(F)c(F)c(C#C)c1F	[SiH3]c1cccc(c1)C#Cc1cccc1
[GeH3]c1cccc(c1)C#Cc1cccc1	CCCC(C#C)[Si](C)(C)CC
CCCC(C#C)[Si](C)(C)c(:c):c	CCCSC#CC
C=COC(=O)C=Cc1cccc1	Cc1cc(C#C)c(o1)C(F)(F)F
Cc1cc(C#C)c(C)s1	Cc1cc(C#C)c(s1)C(F)(F)F
CCOP(=O)(OCC)C(=C)C(=C)P(O)(O)=O	CCOP(=O)(OCC)C(=C)C(=C)P(=O)(OC)OC
COP(=O)(OC)C(=C)C(=C)P(=O)(Oc(:c):c)Oc(:c):c	OP(O)(=O)C(=C)C(=C)P(=O)(Oc(:c:c):c:c)Oc(:c:c):c:c
CCCCC#C	CCCCC#CC#C
COC(=O)C(=Cc1cccc1)C#N	CCCOC(=O)NC(=O)OC
CC(=C)C1=CC(=O)OC1=O	COC(=O)C(C)=CC(C)=C
COC(=O)C(C)=CC=C	CC=CC=C(C)C(O)=O
CCCC(C)(O[Si](C)(C)C)C=C	c:c:c(:c:c)C(=C)C(=C)c1cccc1
CC(O)OCC=C	CCN(CC)C(C=C)N(CC)CC
CCCNC(=O)OC=C	CNC(=O)OC=C
CCC(=O)OCC=C	OC1(C#C)c(:c:c)c(:c)-c(:c)c1:c:c
c:c(:c)COC(=O)C=CC=C	CCCOC(=O)C=CC=CC(O)=O

<chem>c:c:c(OC(=O)c1ccccc1C#C):c:c</chem>	<chem>Cc1ccc(C(O)=O)c(c1)C#C</chem>
<chem>CCCSC(=O)C=C</chem>	<chem>CCC(C)SC(=O)C=C</chem>
<chem>CC(C)CSC(=O)C=C</chem>	<chem>C(=Nc1ccccc1)c1ccccc1</chem>
<chem>CC(=C)C(=O)OC1CCCC1</chem>	<chem>CC(F)(F)C(F)(F)OC(=O)C=C</chem>
<chem>C=CC(=O)N1C(=C)C=CC1=C</chem>	<chem>c:c:c1n(C(=O)C=C)c(:c:c)c(:c)c1:c</chem>
<chem>CNC(C)(C)CC(C)=O</chem>	<chem>CCC(C)(C)NC(=O)C=C</chem>
<chem>CCN(CC(C)O)C(=O)C=C</chem>	<chem>CC(=C)C(=O)OCC#N</chem>
<chem>OCCN1C(=O)NC(=O)C=C1C#N</chem>	<chem>CN1C(=O)NC(=O)C=C1C#N</chem>
<chem>CC(C)(C)OC(=O)C=CC(O)=O</chem>	<chem>CC(C)(C)OC(=O)C=CC(=O)OC(C)(C)C</chem>
<chem>CCC(C)(C)OC(=O)C=CC(O)=O</chem>	<chem>CC(=C)C(=O)Oc(:c:c):c([NH3+]):c</chem>
<chem>COc1ccccc1[N+](=[O-])=O</chem>	<chem>C=CC(=O)NC1CC1</chem>
<chem>CC(=C)C(=O)NC1CC1</chem>	<chem>C=CC(=O)N1CCCC1</chem>
<chem>COC(OC(=O)C=C)C(F)(F)F</chem>	<chem>COC(OC(=O)C(C)=C)C(F)(F)F</chem>
<chem>CC(=C)C(=O)OCc(:c):[se]</chem>	<chem>OCCOC(=O)CC(=C)C(O)=O</chem>
<chem>OCCOC(=O)C(=C)CC(O)=O</chem>	<chem>BrC(:c):c(OC(=O)C=C):c(Br):c</chem>
<chem>c:c(:o)COC(=O)C=C</chem>	<chem>c:c(:c)NC(=O)C=C</chem>
<chem>c:c:c(NC(=O)C=C):c:c</chem>	<chem>O=C1c2ccccc2C(=O)c2ccccc12</chem>
<chem>Nc1ccc2C(=O)c3ccccc3C(=O)c2c1</chem>	<chem>CC(=C)C(=O)Oc(:c(C):c):c(C):c</chem>
<chem>c:c:c(:c:c)C(C#N)=C(C#N)C#N</chem>	<chem>N#CC(C#N)=C(C#N)c1ccccc1</chem>
<chem>CCC(CC)(CC)OC(=O)C=CC(O)=O</chem>	<chem>CC(C)OC(=O)C=CC(O)=O</chem>
<chem>CC(C)OC(=O)C=CC(=O)OC(C)(C)C</chem>	<chem>COC(=O)CC(=C)C(=O)OC(C)(C)C</chem>
<chem>CCC(CC)(CC)OC(=O)CC(=C)C(O)=O</chem>	<chem>CCC(CC)(CC)OC(=O)C(=C)CC(O)=O</chem>
<chem>CC(C)OC(=O)CC(=C)C(O)=O</chem>	<chem>CC(C)OC(=O)C(=C)CC(O)=O</chem>
<chem>CCC(C)(C)OC(=O)C=CC</chem>	<chem>CC1CCCC1OC(=O)C(C)=C</chem>
<chem>CC(=C)C(=O)OC1CCCC1</chem>	<chem>CCC(CC)(CC)OC(=O)C=CC</chem>
<chem>Cc(:c):c(N(CC=C)C(=O)C=C):c(C):c</chem>	<chem>CCN(CC=C)C(C)=O</chem>
<chem>C=CCN(CC=C)C(=O)C=C</chem>	<chem>Cc1sc(N=Nc2ccccc2)c(C#N)c1C</chem>
<chem>Cc1c(C)c(sc1N)C#N</chem>	<chem>Cc1sc(N=N)c(C#N)c1C</chem>
<chem>CCCOC(=O)C(C)Cl</chem>	<chem>CCCOS(=O)(=O)CC12CCC(CC1=O)C2(C)C</chem>
<chem>CC1(C)C2CCC1(CS(O)(=O)=O)C(=O)C2</chem>	<chem>CCC(OC(=O)C(C)=C)C(C)Cl</chem>
<chem>CC(C)(C)OC(=O)Oc(:c:c):c:c</chem>	<chem>CC(C)CNC(=O)C=C</chem>
<chem>FC(F)(F)CNC(=O)C=C</chem>	<chem>CC(=O)NC(=O)C=C</chem>
<chem>OCCNC(=O)C=C</chem>	<chem>CNC(C)(C)CS(N)(=O)=O</chem>
<chem>CC(C)(CS)NC(=O)C=C</chem>	<chem>CC(NC(=O)c1ccccc1)c(:c):c</chem>
<chem>ClCCOC(=O)C=C</chem>	<chem>BrCCOC(=O)C=C</chem>
<chem>CCCN(CCO)C(=O)NCC(C)O</chem>	<chem>CCCN(C(=O)N(CCO)CC(C)O</chem>
<chem>CC(=Cc1ccccc1)c1ccccc1</chem>	<chem>Cc(:c):c(NC(=O)C=C):c:c</chem>

<chem>CC(=C)C(=O)OCC=C</chem>	<chem>CC1(C)OCC(O1)C(=O)Oc(:c:c):c:c</chem>
<chem>ON(C(=O)C=C)c(:c:c):c:c</chem>	<chem>Cc(:c):c(:c:c)N(O)C(=O)C=C</chem>
<chem>[2H]C([2H])=C(C(=O)OC([2H])([2H])[2H])C([2H])([2H])[2H]</chem>	<chem>OCC(CO)(CO)NC(=O)C=C</chem>
<chem>CCN(CC(=O)NC(CO)(CO)CO)C(C)=O</chem>	<chem>NC(=O)CN(CC(N)=O)C(=O)C=C</chem>
<chem>C=CC(=O)N1CCNCC1</chem>	<chem>Oc1cccc(c1)C(=O)Oc(:c:c):c:c</chem>
<chem>COc1ccc(O)cc1[N+](=[O-])=O</chem>	<chem>Oc1cccc(c1)C(=O)c1ccccc1</chem>
<chem>CCCCS(=O)(=O)O[Na]</chem>	<chem>COCCS(=O)(=O)O[Na]</chem>
<chem>CC(C)(C)COC(=O)c1ccccc1</chem>	<chem>CNc1ccccc1C(O)=O</chem>
<chem>OCCN1CCCC1=O</chem>	<chem>CCCN1CCCC1=O</chem>
<chem>CC(=C)C(=O)N1CCCC1=O</chem>	<chem>CC1CCC(=O)N1OC(C)=O</chem>
<chem>CC(=O)ON1C(CCC1=O)C(O)=O</chem>	<chem>CON1C(CCC1=O)C(=O)OCCO</chem>
<chem>CC1CCC(=O)N1OC(=O)C(F)(F)F</chem>	<chem>CC(=O)c1ccccc1O</chem>
<chem>CCOC(=O)C(=Cc(:c):s)C#N</chem>	<chem>CCOC(=O)C(=Cc1ccc(C)s1)C#N</chem>
<chem>Cc1ccc(s1)C(=O)c1ccc(N)s1</chem>	<chem>Brc1cccc(c1)C(=O)Oc(:c:c):c:c</chem>
<chem>c:c:c(OC(=O)c1cccc(:c)c1):c:c</chem>	<chem>ClC(OC(=O)C=C)C(Cl)(Cl)Cl</chem>
<chem>Fc(:c):c(OC(=O)C=C):c(F):c</chem>	<chem>CC(=C)C(=O)Oc(:c(F):c):c(F):c</chem>
<chem>Oc1ccccc1C=Nc1ccccc1</chem>	<chem>c:c:c(:c:c)C(=O)C=Cc1ccccc1</chem>
<chem>c:c(:c)C=CC(=O)c1ccccc1</chem>	<chem>[NH3+]c(:c):c(NN=Cc1cccc(:c)c1):c:c</chem>
<chem>NNc1ccc([NH3+])cc1[N+](=[O-])=O</chem>	<chem>CCCCC(=C)C(=O)OC</chem>
<chem>CC(=O)NCP(O)(O)=O</chem>	<chem>OP(O)(=O)CNC(=O)C=C</chem>
<chem>COC1(C)CCOC(=O)C1</chem>	<chem>CNCCC(O)=O</chem>
<chem>CNC(C)(C)CS(O)(=O)=O</chem>	<chem>CCC(CC)OC(=O)C=CC(O)=O</chem>
<chem>CC(C)OC(=O)C=CC(=O)OC(C)C</chem>	<chem>[O-][N+](=O)c1cccc(:c)c1</chem>
<chem>c:c1cccc(C=Cc2cccc(:c)n2)c1</chem>	<chem>[O-][N+](=O)c1cccc(:o)c1</chem>
<chem>Cc1cccc(c1)N=Nc1ccccc1</chem>	<chem>CC(F)(F)CNC(=O)C=C</chem>
<chem>Clc1ccc(Cl)c(c1)N=Nc1ccccc1</chem>	<chem>CC(=C)C(=O)OCC(Cl)(Cl)Cl</chem>
<chem>[O-][N+](=O)c1ccccc1C=Cc1ccccc1</chem>	<chem>[NH3+]c1ccc(C=C)c(c1)[N+](=[O-])=O</chem>
<chem>CC1(C)CC(=C)C=C(C1)C=Cc1ccccc1</chem>	<chem>CC1(C)CC(C=Cc(:c):c)=CC(C1)=C(C#N)C#N</chem>
<chem>O=P(c1ccccc1)(c1ccccc1)c1ccccc1</chem>	<chem>CC(C)C(C)(OC(=O)C(C)=C)C(C)C</chem>
<chem>CCOP(=O)(CC1OCCO1)OCC</chem>	<chem>CCOP(=O)(CC(OC)OC)OCC</chem>
<chem>CC(=C)C(=O)OC(CO)CO</chem>	<chem>CCNC(=O)C1=Cc2ccccc2OC1=O</chem>
<chem>OCCNC(=O)C1=Cc(:c)cOC1=O</chem>	<chem>CNC(=O)C1=Cc(:c)c(OC1=O):c:c</chem>
<chem>CC(C)(C)CNC(=O)OCCO</chem>	<chem>CCC(CC)NC(=O)N1CCCCC1=O</chem>
<chem>CNC(=O)N1CCCCC1=O</chem>	<chem>CC(=O)COC(=O)C(C)=C</chem>
<chem>CC(=O)OCC(=O)c1ccccc1</chem>	<chem>COC(C)OC(=O)C(C)=C</chem>
<chem>CCC(OC)OC(=O)C(C)=C</chem>	<chem>N#Cc1ccccc1N=Nc1ccccc1</chem>

<chem>Cc1ccc(N=N)c(c1)C#N</chem>	<chem>Cc1cccc(c1)C#N</chem>
<chem>[Li]OS(=O)(=O)CCCC</chem>	<chem>[Li]OC(=O)CCCO</chem>
<chem>CC(=C)C(=O)Oc(:c(:c):c):c(:c):c</chem>	<chem>CCOC(=O)C1=Cc2cccc2OC1=O</chem>
<chem>OCCOC(=O)C1=Cc(:c)cOC1=O</chem>	<chem>COC(=O)C1=Cc(:c)c(OC1=O):c:c</chem>
<chem>c:c:c(OC(=O)C=Cc(:c):c):c:c</chem>	<chem>c:c(:c)C(C(=O)C=Cc1cccc1)c(:c):c</chem>
<chem>c:c:c1C(C(=O)C=Cc(:c):c)c(:c:c)c(:c)Cc1:c</chem>	<chem>CC1c2cccc2C(=O)c2cccc12</chem>
<chem>c:c:c1OC(=O)C=Cc1:c</chem>	<chem>Oc1ccc2OC(=O)C=Cc2c1</chem>
<chem>CNC(C)(C)CS(=O)(=O)O[Na]</chem>	<chem>CSCOC(=O)C(C)=C</chem>
<chem>CC(O)CN1C(=O)c2cccc2C1=O</chem>	<chem>c:c:c(NS(=O)(=O)c1cccc1):n:c</chem>
<chem>CC(=C)COC(=O)C(C)=C</chem>	<chem>CC(=O)OCC1=C(C)C2(C)C(C)=C(C)C12C</chem>
<chem>CC1=C(C)C2(C)C(CO)=C(C)C12C</chem>	<chem>[Na]OS(=O)(=O)N=Nc(:c):c</chem>
<chem>[Na]OS(=O)(=O)N=Nc1cccc1</chem>	<chem>CC(F)(F)C(F)(F)C(F)(F)C(=O)OCCO</chem>
<chem>CN(CCO)S(=O)(=O)CCC(C)(F)F</chem>	<chem>c:c1cccc(C=C(C#N)c2cccc2)c1</chem>
<chem>c:c:c(:c:c)C(=Cc(:c):c)C#N</chem>	<chem>c:c1cccc(c1)N=Nc1cccc1</chem>
<chem>Oc1cccc(C=CC(=O)c(:c):c):c1</chem>	<chem>COc1ccc(C)cc1C(=O)c1cccc1</chem>
<chem>Cc1cccc(C=C(C#N)c2cccc2)c1</chem>	<chem>CCCCC(=O)Oc(:c):c:c</chem>
<chem>OCC1COC(=O)O1</chem>	<chem>c:c(:c)COC(=O)c1cccc1</chem>
<chem>CC(=C)C(=O)OCc(:c):[nH2]</chem>	<chem>Oc1cccc1C=NNc1nccs1</chem>
<chem>CNC(NC(=O)NCCO)=NC</chem>	<chem>CNC(=O)NC1=NC(=O)C=C(C)N1</chem>
<chem>CNC1=NC(=O)C=C(C)N1</chem>	<chem>Clc(:c):c(NC(=O)C=C):c:c</chem>
<chem>[NH3+]CCCS([O-])(=O)=O</chem>	<chem>OCCOC(=O)CCn(:c):c</chem>
<chem>CC(=C)C(=O)OCC(N)=O</chem>	<chem>CC(=O)OCC(=O)Nc1ccon1</chem>
<chem>c1ccc(cc1)N=Nc1ccncc1</chem>	<chem>OC(=O)C(=C)CC(=O)OCCCl</chem>
<chem>OC(=O)CC(=C)C(=O)OCCCl</chem>	<chem>CC(=O)OCC(=O)Nc(:c):c:c</chem>
<chem>CC(=C)C(=O)OC[SiH3]</chem>	<chem>CC(=C)C(=O)OC[Si](C)(C)C</chem>
<chem>CC(=O)OCC(=O)N1CCOCC1</chem>	<chem>CC(=O)OCC(=O)N1CCCC1</chem>
<chem>CCC(CC)(CC)NC(=O)C=C</chem>	<chem>Brc1cccc(C=CC(=O)c(:c):c):c1</chem>
<chem>Cc1cccc1N=Nc1cccc1</chem>	<chem>C=C1SC(N=Nc2cccc2)=NC1=C</chem>
<chem>[O-][N+](=O)c1cccc(:s)c1</chem>	<chem>CS(=O)(=O)c1cccc1</chem>
<chem>CCCCS([O-])(=O)=O</chem>	<chem>CCCCC#CC</chem>
<chem>CCCC(C)C=C(C)C</chem>	<chem>CC(C)=C1C=CC2CC=CCC12</chem>
<chem>C1Cc2cccc2C=C1</chem>	<chem>C#CC12CC3CC(CC(C3)C1)C2</chem>
<chem>CCCC(C)(C)C#C</chem>	<chem>O=CC1CCCCC1C=O</chem>
<chem>CCC(C)CC=O</chem>	<chem>CCC(CC=O)c(:c):c</chem>
<chem>c:c(:c)C1COC(=C)O1</chem>	<chem>COCC(=C)C(O)=O</chem>
<chem>CCOCC(=C)C(O)=O</chem>	<chem>COC(F)(F)C(F)(F)C(F)=C(F)F</chem>
<chem>COCOC=C(F)F</chem>	<chem>FC(F)=C1OC(F)(F)C(F)(O1)C(F)(F)F</chem>

<chem>c:c:c(CN=C=O):c:c</chem>	<chem>Cc1cccc(c1)N=C=O</chem>
<chem>CC(C)(C)N(CC=C)C(=O)C=C</chem>	<chem>c:c:c(:c:c)N=C=S</chem>
<chem>S=C=Nc1ccccc1</chem>	<chem>C=NCCN=C=O</chem>
<chem>OCCN1C(=O)C=CC1=O</chem>	<chem>CCCN1C(=O)C=CC1=O</chem>
<chem>CC(=C)C(=O)OC(=O)C=C</chem>	<chem>N#Cc1ccncc1</chem>
<chem>N#Cc1ccncc1</chem>	<chem>CCN(CC)CP(O)(O)=O</chem>
<chem>CCN(CP)CC=C</chem>	<chem>CCN(CC)C(P(O)(O)=O)P(O)(O)=O</chem>
<chem>CCN(CC=C)C(P)P</chem>	<chem>CCOC(=O)C(F)=C</chem>
<chem>FC(=C)C(=O)OCC(F)(F)F</chem>	<chem>CC(F)(F)COC(=O)C(F)=C</chem>
<chem>CCCOC(=O)C(F)=C</chem>	<chem>FC(F)=C(F)OCC(F)(F)F</chem>
<chem>COC(F)(F)C(F)(F)S(O)(=O)=O</chem>	<chem>FC(F)=C(F)OC(F)(F)C(F)(F)S</chem>
<chem>OP(O)(=O)C(F)(F)C(F)=C(F)F</chem>	<chem>C#Cc1ccccc1C#Cc1ccccc1</chem>
<chem>Cc1ccc(C#C)c(c1)C#Cc1ccccc1</chem>	<chem>Oc1ccc(C#C)c(c1)C#Cc1ccccc1</chem>
<chem>CC(C)OC(=O)C(F)=C</chem>	<chem>FC(=C)C(=O)OC(C(F)(F)F)C(F)(F)F</chem>
<chem>FC(F)=C(F)OC(F)(C(F)(F)F)C(F)(F)F</chem>	<chem>CC(O)(F)C(F)(F)OC(F)=C(F)F</chem>
<chem>COC(F)(F)C(F)(F)S(F)(=O)=O</chem>	<chem>CN(C)P(=O)(Oc(:c:c):c:c)C=C</chem>
<chem>[CH2-][Fe++][c-]1cccc1C=C</chem>	<chem>c:c(:[cH2-])COC(=O)C=C</chem>
<chem>CC(=C)C(=O)OCc(:c):[cH2-]</chem>	<chem>C1CC2C3CC(C=C3)C2C1</chem>
<chem>C1CC2CC1C1C3CC(C=C3)C21</chem>	<chem>C[Si](C)(O)O[Si](C)(C)C=Cc1ccccc1</chem>
<chem>C[Si](C)(C)O[Si](C)(O[Si](C)(C)C)C=Cc1cccc c1</chem>	<chem>C[Si](C)(C)O[Si](O[Si](C)(C)C)O[Si](C)(C)C C=Cc1ccccc1</chem>
<chem>C=CCn1cccn1</chem>	<chem>c:c:c(:c:c)P(=S)(C=C)c(:c:c):c:c</chem>
<chem>C=CP(=S)(c1ccccc1)c1ccccc1</chem>	<chem>[CH2-][Fe++][c-]1cccc1C#C</chem>
<chem>C=COC(=O)C12CC3CC(CC(C3)C1)C2</chem>	<chem>CCC(CC=C)O[SiH3]</chem>
<chem>c:c:c1n(C=C)nnc1:c</chem>	<chem>FC(F)(F)C(OC(=O)C=C)(C(F)(F)F)C(F)(F)F</chem>
<chem>CC(OC(=O)C(C)=C)C(O)=O</chem>	<chem>CC(OC(C)=O)C(=O)Oc(:c:c):c:c</chem>
<chem>OCC1(CO)CC2CC1C=C2</chem>	<chem>CC(C)(N=C=O)c(:c:c):c:c</chem>
<chem>OC(=O)C(=C)CC(=O)OC1CCC1</chem>	<chem>OC(=O)CC(=C)C(=O)OC1CCC1</chem>
<chem>CC(O)CC(=O)C(C)=C</chem>	<chem>CC(=C)C(=O)CC(O)CN</chem>
<chem>CCN(CC)CC([O-])=O</chem>	<chem>[NH3+]CCOC(=O)C=C</chem>
<chem>[NH3+]CCOC([O-])=C(C#N)C#N</chem>	<chem>[NH3+]CCOP([O-])(=O)OCCO</chem>
<chem>CCCCC(=O)OCCC</chem>	<chem>CCCOP([O-])(=O)OCC[NH3+]</chem>
<chem>O=N(=O)c1ccccc1</chem>	<chem>ClCC=Cc1ccccc1</chem>
<chem>C1CC2CC1C1CC=CC21</chem>	<chem>C(=Cc1ccccc1)c1ccccc1</chem>
<chem>COC(=O)C(=C)CC#N</chem>	<chem>CCCC(C)(O)C=C</chem>
<chem>NCCN1C(=O)C=CC1=O</chem>	<chem>Nc1cccc(c1)C(O)=O</chem>
<chem>ClC1=CC(=O)N(c(:c):c)C1=O</chem>	<chem>ClC1=CC(=O)N(c(:c:c):c:c)C1=O</chem>

<chem>Clc(:c):c(:c:c)N1C(=O)C=CC1=O</chem>	<chem>CCC(C=C)=NC(=O)OCC(C)N</chem>
<chem>CCOC(=O)N=C1CC=C(N)C=C1</chem>	<chem>CN=C1CC=C(C=C1)N1C(=O)C=CC1=O</chem>
<chem>OC(=O)N=C1CC=C(C=C1)N1C(=O)C=CC1=O</chem>	<chem>CC=C(C=C)N1C(=O)C=CC1=O</chem>
<chem>CC(=C)NC(=O)OCCN</chem>	<chem>COC(=O)NC(C)=C</chem>
<chem>[O-][N+](=O)c1cccc(:[nH2])c1</chem>	

B. Ring Opening: Ring Bond Opening Descriptors (SMILES Format)

Walk 0 Descriptors

<chem>C=N</chem>	<chem>c:s</chem>	<chem>PS</chem>	<chem>CP</chem>	<chem>CO</chem>
<chem>CS</chem>	<chem>CC</chem>	<chem>C=C</chem>	<chem>SS</chem>	<chem>N=S</chem>
<chem>NP</chem>	<chem>N=P</chem>	<chem>NS</chem>	<chem>C#C</chem>	<chem>CN</chem>
<chem>C[SiH3]</chem>	<chem>O[SiH3]</chem>	<chem>[SiH3][SiH3]</chem>	<chem>OS</chem>	<chem>C=O</chem>
<chem>OP</chem>	<chem>c:[nH2]</chem>	<chem>N[SiH3]</chem>	<chem>C[SiH2]</chem>	<chem>C[GeH3]</chem>

Walk 1 Descriptors

<chem>C1C2CC12</chem>	<chem>CN(C)C(C)=O</chem>	<chem>CCN=C</chem>	<chem>COC=N</chem>
<chem>c:c:c:s</chem>	<chem>CN(C)C(N)=O</chem>	<chem>COC(C)(C)O</chem>	<chem>NCCO</chem>
<chem>CN(C)CO</chem>	<chem>CC(C)N(C)C</chem>	<chem>CCCP</chem>	<chem>COC(N)=O</chem>
<chem>CCOC</chem>	<chem>CN(C)C(C)(C)C</chem>	<chem>CC(C)(N)C(N)=O</chem>	<chem>NCCN</chem>
<chem>CCC(C)C</chem>	<chem>CCN(C)C</chem>	<chem>C1COC1</chem>	<chem>CC(N)C(N)=O</chem>
<chem>COC(C)O</chem>	<chem>CCc(:c):c</chem>	<chem>CC(C)=C(C)C</chem>	<chem>CNC(N)=O</chem>
<chem>CCCS</chem>	<chem>CCCO</chem>	<chem>COC(C)C</chem>	<chem>CCC=C</chem>
<chem>CCCC</chem>	<chem>CC=CC</chem>	<chem>CCNC</chem>	<chem>CCC(C)O</chem>
<chem>CC(O)CN</chem>	<chem>C1CC=C1</chem>	<chem>CC(O)CO</chem>	<chem>CCCN</chem>
<chem>C1CNC1</chem>	<chem>NC(=O)CO</chem>	<chem>NCC(O)=O</chem>	<chem>CCC(O)=O</chem>
<chem>CNC(O)=O</chem>	<chem>OCCO</chem>	<chem>CN(C)C(O)=S</chem>	<chem>CCC(N)=O</chem>
<chem>CC1(C)CC1</chem>	<chem>CC1CC=C1</chem>	<chem>CC(C)C=C</chem>	<chem>CC1(C)CC1(C)C</chem>
<chem>CC1CC1</chem>	<chem>CC12CC1C2</chem>	<chem>OC(=C)C=C</chem>	<chem>C=CC=C</chem>
<chem>CC(=C)C=C</chem>	<chem>CC=C(C)C</chem>	<chem>CCC(C)=C</chem>	<chem>ClC(=C)C=C</chem>
<chem>C1CO1</chem>	<chem>CC1CO1</chem>	<chem>CC1(C)CO1</chem>	<chem>CC(=C)C(O)=C</chem>
<chem>OC(=C)C(Cl)=C</chem>	<chem>c:c:c(:c):c</chem>	<chem>Oc(:c):c(:c):c</chem>	<chem>c:c(:c):c(:c):c</chem>
<chem>FC(=C)C(F)=C</chem>	<chem>CC(=C)C(F)=C</chem>	<chem>FC1(F)CO1</chem>	<chem>CC1(C)COC1</chem>
<chem>CCC(C)(C)C</chem>	<chem>C=C1OC=C1</chem>	<chem>COc(:c):c</chem>	<chem>COCO</chem>

OCCS	CCSS	CSSC	COC(C)=O
OC(=O)c(:c):c	OCC(O)=O	OC(=C)C(O)=C	OC(=O)C(O)=O
CC(C)C(O)=O	CC1CCO1	CC1COC1	OCc(:c):c
CCS(C)(=O)=O	CCSC	OC1COC1	CCC(O)O
CC(C)(C)CO	C1CS1	C1CSS1	SCCS
CSSS	SSSS	CC1CS1	C1CSC1
CC1(C)CSC1	CC1(C)CS1	CC1CCS1	OC(=O)CS
SCc(:c):c	CSc(:c):c	SC(=C)C=C	CCc(:c):s
Cc(:s):c:c	Cc(:c):s:c	NS(Cl)=NP	CIP(Cl)(=N)N=S
NP(Cl)(Cl)=NP	CIP(Cl)(=N)N=P	NP(Cl)(Cl)=NS	CIS(=N)N=P
OCC=C	OCC#C	CC#CC	CC(=C)C(C)=C
OC(=O)C=C	CC(C)CO	CC(C)C(C)C	c:c(:c)-c(:c):c
O=C1CCO1	CNC(C)=O	CNc(:c):c	NC(=C)C=C
CS(=O)(=O)c(:c):c	NC(=O)c(:c):c	CSC(C)=O	CCC(S)=O
C=C1CCO1	CC1(C)COC1=C	O=C1CCN1	CC1(C)CNC1
CNC(C)C	CC(N)C(O)=O	CCC(N)=S	CNC(C)=S
CNC(C)O	CCC(N)O	CC(O)C(N)=O	COC(C)N
CCC(C)N	CN(C)C(O)=O	CC(C)(C)c(:c):c	COC(S)=O
CSC(O)=O	COC(O)=O	C1CN1	CN1CC1
CN=C(C)O	COC(C)=N	C[Si]1(C)C[SiH2]C1	C[Si]1(C)CCC1
C1C[SiH2]C1	[SiH3]C(=C)C=C	C[Si](C)(O)O[SiH3]	C[Si](O)(O)O[SiH3]
C[Si]1(C)[SiH2][SiH2] [Si]1(C)C	CC[Si](C)(C)C	[SiH3]CC=C	SOc(:c):c
COS(C)(=O)=O	OS(=O)(=O)c(:c):c	O=S1(=O)CCC1	O=S1(=O)CC1
CC(=C)C(Cl)=C	BrC(=C)C=C	CC(=C)C(Br)=C	CC(F)(F)c(:c):c
CC(F)(F)C(C)(F)F	CCC1(C)CC1	CC(C)C(C)=C	CC(C)C(C)(C)C
CC(C)C(C)(F)F	CC(C)(C)C(C)(F)F	CC(C)C(C)(O)F	CC(O)(F)C(C)(F)F
CCC(C)(C)[SiH3]	CC(C)C(C)(C)[SiH3]	C=C1CC=C1	CC(C)(C)C=C
CC1(F)CO1	CC(=O)C=C	C=CC=O	c:c:o:c
Cc(:c):o:c	CCC(C)(O)O	CC(C)C(N)=O	COP(O)(O)=O
CCOP	CC=CO	COC=C	CC(=C)C(O)=O
CC(C)=C(C)N	CCC(N)=C	CC1(C)CCN1	CC1CCN1
CC1NCC1(C)C	CC1(C)CNC1(C)C	CCC(C)(Cl)Cl	CC(Cl)(Cl)C(N)=O
CC(=C)C(N)=C	COC(C)(C)Cl	CC(O)(Cl)C(C)(O)Cl	CC(C)C(C)(O)Cl
CN=CO	Cn(:c):c(:c):c	c:c:c(:c):[nH2]	c:c(:c):c(:c):[nH2]
CN1[SiH2]N[Si]1(C)C	CN1[SiH2]C[Si]1(C)C	C[Si]1(C)C[SiH2]N1	c:c:s:c
Cc(:c):c:s	COCN	NCc(:c):c	C1[SiH2]C[SiH2]1

C[Si]1C[SiH]C1	C[Si](C)([SiH3])O[SiH3]	C[Si](C)(O)[Si](C)(C)O	C[Si]1(C)CC=C1
c:c1C[SiH2]c1	C[Si]1(C)Ccc1:c	C=C1C[SiH2]C1=C	[SiH3]Cc(:c):c
CCC[SiH3]	CC(=C)C[SiH3]	C[Si](C)([SiH3])C#C	[SiH3]C#C[SiH3]
C[Si](C)(C)[Si](C)(C)C	CC1C[SiH2]C1	Cc(:c):c(:c):c	CC[Si](C)(O)O
[SiH3]CC[SiH3]	CC[Si](C)(C)O	C[Si](C)(C)O[SiH3]	CCC(C)[SiH3]
[SiH3]c(:c):c(:c):c	CCSP	CSP(C)C	CCP(C)S
PC(=C)C=C	CC[Ge](C)(C)C	[GeH3]CC=C	COC(N)=S
C[Si]1(Cl)C[SiH2]C1	C[Si]1(O)CCC1	CC(C)c(:c):c	NSN=S
SN=S=N			

Walk 2 Descriptors

Cc1ccccc1	c1ccccc1	C1CCCCC1
CCN1CCNCC1	CC(O)C1CO1	CC=C(C(O)=O)C(=C(C)N)C(O)=O
CN1COcc(:c)C1	CC1CCCCO1	CCCCC(N)=C
CN1CCN(C)CC1	C1COC=NC1	c:c:c1C2C=CC(C=C2)c1:c
CC1CC=CC1	CC1OCC(C)(C)CO1	CC1(Cl)COC(=O)O1
c1ccoc1	C1COC=CC1	CCC1NCO1=O
CCC1OCCCO1	OC(=O)N1CCNCC1	CC1=C(C2C=CC1C=C2)C(O)=O
OCC1(CO)COCOC1	CCCC(C)O	CCCC=C(C)C
NC1CCCCO1	C1CCNC1	CC1CCC(C)O1
CNCCC(C)C	Cc1ccc(C)s1	C1CN=CO1
O=C1CNC(=O)O1	CCC1OC1CC	CC(C)C1CCC=CC1
CCCC1OC1C	Cc1ccsc1	CC12CCCC(CCC1)C2
C1CC2OC2C1	C1CCC=CC1	[SiH3]C1CCCCC1
CCC1NC(=O)OC1=O	C1CC2CCC1CC2	C1CC2CCC1C2
C1COCO1	C1C2CC3CC12CCC3	COc1ccccc1
[SiH3]c1ccccc1	COC1(F)C2CC(C=C2)C1(F)F	CCC=C(C(C)=C)C(O)=O
C1OCC11COCOC1	Nc1ccccc1	CN1CCCC1
Sc1ccccc1	ClC12OCOC1(Cl)C1CC2C=C1	C1CC2C=CC1C=C2
Oc1ccc(O)cc1	OC(=N)c1ccsc1	FC1(F)CC2CC1C=C2
CC=CCC(O)=O	CC1(C)OCCO1	C1CCSPC1
Pc1ccccc1	C1OCC11CCC=CC1	CC12CCC(C1)C=C2
Clc1ccccc1	CC1(C)CC2CC1C=C2	Cc1cccs1
CCC=CCC	C1CPSC1	CCCC=C

OCC1CC2CC1C=C2	COCCCCO	CCC1=NCCO1
CCNC(=O)OC	OCC1(CO)COC1	CCC1CCCO1
c1ccsc1	C1CC2CC1C=C2	CCCCNC
CCCCOC	O=C1CCCN1	COCCN(C)C
C1CNCOC1	CN(C)CCC(O)=O	CN1CCOC1
COCCc(:c):c	CC1=CCCC1	C1CCOC1
OCCCCO	CCCC=CC	CC1CC1(C)C
CCCCc(:c):c	CCCCCN	CCCCCS
CCCCCO	c:c(:c)CCc(:c):c	CCCCCC
CCCCC(C)C	C1CC=CC1	CCCC(C)C=C
CCC=CC(C)C	CCC(C)C=CC	N#CC12CC1C2
Cc1ccc(O)cc1	CC(=C)c1ccccc1	c:c(:c)C1=CCCC1
CCC1OCOC(C)O1	ClCC1CO1	BrCC1CO1
FCC1CO1	CCC1CO1	C=CC1CO1
CC1(CCl)CO1	CC(C)(C)C1CO1	OCC1CO1
Oc1ccccc1	Cc1ccccc1O	Oc1ccccc1Cl
Clc1ccc(Cl)c1	Oc1ccc(Cl)cc1Cl	COc1c(Cl)cccc1Cl
COc1ccccc1:c	c:c1ccccc1	c:c:c1ccccc1:c
COc1cccc(:c)c1:c:c	Oc1ccc(:c)cc1	Oc1ccc(:c)c(:c)c:c1
COc1cccc(:c)c1	CC(C)c1ccccc1O	OCC1(CO1)c(:c):c
CC1(CO1)c1ccccc1	FC(F)(F)c1ccccc1	Fc1ccc(F)c(F)c1F
Cc1ccc(F)c(F)c1F	CC1(CO1)c1c(F)ccc(F)c1F	CC1OC1C
CC1OC1(C)C	CC1(C)OC1(C)C	FC1(F)OC1(F)F
ClCC1(CCl)COC1	FCC1(CF)COC1	lCC1(Cl)COC1
BrCC1(CBr)COC1	CCCOCC	CC1CCCCC1
C1OCC11CCCCC1	CCC1(CC)COC1	O1c2cc1ccc2
CCCOc(:c):c	CCOc(:c:c):c:c	CCCOCO
CCOCOC	COCCSS	CSSCCO
CCSSCC	CCOCCS	CCCC(=O)OC
CCCCC(O)=O	CCOC(=O)CC	CC(=O)OCCO
COCCOC	CCOCCO	CCOC(=O)c(:c):c
COC(=O)c(:c:c):c:c	OC(=O)c1ccccc1	c:c:c(Oc(:c):c):c:c
OCCOc(:c):c	CCCOC(C)=O	CC(O)CCC(O)=O
CCCC1CCCO1	CCC(=O)OC(C)=O	CCC1CCC(C)O1
COCC(=O)OC	OC(=O)COc(:c):c	CC(=O)OC(=O)CO
CC(=O)OC(=O)c(:c):c	OCOc(:c:c):c:c	COCOc(:c):c
COc1cc(C)ccc1O	COc1ccccc1O	COc1ccccc1OC

CCOc(:c:c):c(O):c	CCOC(=O)C(O)=O	COC(=O)C(=O)OC
COC(=O)CC(O)=O	COC(=O)C(C)C(O)=O	CCOC(=O)C(C)C
CCC(C(O)=O)C(=O)OC	OC(=O)CCC(O)=O	CCC1(CCl)COC1
CCC1OC1C	CC(C)C1CO1	CCOCC(O)=O
CCOC(=O)CO	Cc1ccc(C)cc1	OCc1ccccc1
COCc(:c:c):c:c	CCOCc(:c):c	ClCC1(CCl)CO1
CC1OC1CCl	CCCCS(C)(=O)=O	CCCS(=O)(=O)CC
CCCCSC	CCCSCC	CCc1ccccc1
CCCc(:c:c):c:c	c:c:c(Cc(:c):c):c:c	COC(C)CCO
COCCC(C)O	CC(C)OC(=O)CO	CCC(C)OC(C)=O
CCCC(O)O	CCCC(OC)OC	CC(C)(C)C1COC1
CCC1(C)COC1	CC1(CO)COC1	NCC1CO1
C1CSSSS1	CC(C)(C)C1CS1	CC1SC1C
CCC1CS1	OCC1CS1	C1CSSC1
CCC1(C)CSC1	C1CCSC1	C1CCSSC1
CCCCSS	CCSSC	SCCCCS
CCSCCS	CSCCSC	CCSSS
CCSSSS	CSSSSC	COC(=O)CCS
CSCCC(O)=O	COC(=O)CSC	CCSCC(O)=O
CC(=O)OC(=O)CS	CSSCc(:c):c	SSCc(:c:c):c:c
SCc1ccccc1	CCCSc(:c):c	CCSc(:c:c):c:c
CSc1ccccc1	Sc1ccc(S)cc1	CCSCc(:c):c
CSCc(:c:c):c:c	Cc1ccc(S)cc1	c:c:c(Sc(:c):c):c:c
SCCSc(:c):c	OC(=O)CCc(:c):s	CCCc1cccs1
CCc1cccs1	CCc1ccc(C)s1	CC(C)C1CS1
COCC(C)OC	CC(O)COC(C)=O	CCC(=O)OC(C)C
CC(CO)OC(C)=O	ClS1=NP(Cl)(Cl)=NP=N1	ClP1(Cl)=NP(Cl)(Cl)=N[S]=N1
ClS1=NP=NP(Cl)(Cl)=N1	O=C1OCCOC1=O	O=C1COCCO1
C1COCCO1	Cc1ccc(:c)cc1	Cc1ccc(:c)c(:c:c)c1
OC(=O)c1cccc(:c)c1	CC(=O)OCC=C	COCC=CC
OCC=CCO	CC(=O)OCC#C	COCC#CC
OCC#CCO	COC(=O)c(:c:c):c(C):c	Cc1ccccc1C(O)=O
c:c(:c)OC(=O)c(:c):c	CC(=O)Oc(:c:c):c:c	O=C1CCCO1
O=C1CCCCO1	C1CCOCC1	CCOC(=O)C=C
COC(=O)C=CC	OC(=O)C=CC(O)=O	COCC(C)C(C)C
CC(C)COC(C)=O	CC(CO)C(C)CO	CCC(COC)C(C)C

CCC(CO)C(CC)CO	COCC(C(C)C)C(C)C	CC(C)C(CO)C(CO)C(C)C
Cc1cc(O)ccc1O	c:c(:c)-c1ccccc1	c:c:c(:c:c)-c(:c:c):c:c
CC(=O)Oc(:c:c):c(C):c	CC1(C)COC1=O	CC1COC1=O
CCC(=O)Oc(:c):c	CCCC(C)CC	CC(C)CCC(O)=O
COC(=O)CC(C)C	CCC(C)CC(O)=O	CCCC(=O)NC
CCCCC(N)=O	CCNC(=O)CC	CCCNC(C)=O
CCC(=O)Nc(:c):c	CC(=O)Nc(:c:c):c:c	CNc1ccccc1
Cc1ccc(N)cc1	COC(=O)Cc(:c):c	OC(=O)Cc(:c:c):c:c
CS(=O)(=O)c1ccccc1	CCS(=O)(=O)c(:c:c):c:c	CCCS(=O)(=O)c(:c):c
c:c:c(:c:c)S(=O)(=O)c(:c):c	CS(=O)(=O)Cc(:c:c):c:c	CCS(=O)(=O)Cc(:c):c
CCNC(=O)c(:c):c	CNC(=O)c(:c:c):c:c	NC(=O)c1ccccc1
OC(=O)CCCS	ClCC1(CCl)COC1=O	CCC1(CC)COC1=O
CC(Cl)(Cl)C1CC(=O)O1	CC1CC(=O)O1	CCC(C)CCS
CSCCC(C)C	CCCSC(C)=O	CCSC(=O)CC
CCCC(=O)SC	CC(C)CCC(S)=O	OC(=O)CCc(:c):c
OCCc(:c:c):c:c	COC(=O)CCN	CCCN(CC)CC
CC1COCCO1	CC1COC(=O)CO1	CC1COCC(=O)O1
COCC(C)(C)CO	CC(=O)OCC(C)(C)C	CC(C)OC(=O)c(:c):c
COCC(CO)(CCl)CCl	CC(=O)OCc(:c):c	CCC(C)CCO
COCCC(C)C	CCCC(C)OC	CCCC(C)C(O)=O
CCC(C)C(=O)OC	CC(C)OC(=O)C(C)C	CC(C)=C1OC(=O)C1(C)C
CC1(C)C(=C)OC1=O	Cc1ccc(C)c(C)c1	Cc1ccccc1-c(:c):c
Cc(:c):c(:c:c)-c(:c:c):c(C):c	CC1(C)CNC1=O	CC1COC(=O)N1
CCCC(=S)NC	CCCCC(N)=S	CCCNC(C)=S
CCNC(=S)CC	CNCC(C)OC	CC(O)CNC(C)=O
CNC(=O)CC(C)O	COC(C)CC(N)=O	CCC(C)OC(C)C
CC(C)OC(C)CN	CC(C)C1NC(=O)OC1=O	CC(C)C1NCOC1=O
CC1NC(=O)C(C)O1	CCC1NC(=O)CO1	C1NC2CCCC1O2
CCC1OCNC1=O	CCCC(C)NC	CCCCC(C)N
CCC(=O)NC(C)C	CCC(C)NC(C)=O	CCOC(=O)N(C)C
NC(=O)OCCO	CCN(CC)C(=O)OC	O=C1NCCN1
C1CNCN1	CCN1C(=O)NC(=O)C1(C)C	CC1(C)CNC(=O)N1CCO
CC(=O)OCCN	OCCN1C(=O)CNC1=O	CCN1C(=O)CN(C)C1=O
CCN1C(=O)N(C)CC1(C)C	CCN1C(=O)NC(C)(C)C1=O	CN1CN(C)C(C)(C)C1=O
CC(C)C1N(C)CN(C)C1=O	CC(N)C1CCCCC1	CCN1C(C(C)C)C(=O)NC1=O
CC1CNC(=O)N1CCO	CCN1C(=O)NC(C)C1=O	CCN1C(C)CN(C)C1=O

CCN1C(=O)NC(=O)C1(c(:c):c)c(:c):c	CN1CN(C)C(c(:c):c)(c(:c):c)C1=O	CC(C)(N)c1cccc1
CC(C)(c(:c):c)c(:c:c):c:c	CC(C)(C)c1cccc1	C=C1C=CC(=O)OC1=O
c:c:c1ccCOC1=O	CCOC(=O)SC	CCCOC(S)=O
COC(=O)SC(O)=O	CCOC(=O)OC	CCCOC(O)=O
OC(=O)OCc(:c):c	CC(=O)N1CC1	CC1=NCCO1
CCC1=NCCCO1	CC1=NCCCO1	OC(=N)C1CCCCC1
OC(=N)c1cccc1	CC(F)(F)C1=NCCCO1	CC(C)(C)C1=NCCCO1
ClC(Cl)C1=NCCO1	ClC(Cl)(Cl)C1=NCCO1	C[Si]1(C)C[Si](C)(C)C1
C[Si](C)(C)c1cccc1	c:c(:c)[Si]1(CCC1)c(:c):c	C[Si](C)(O)O[Si](C)(C)O[SiH3]
C[Si]1(C)O[SiH2]O[Si](C)(C)O1	C[Si]1(C)O[SiH2]O[Si](C)(O1)c(:c):c	C[Si](O)(O)c1cccc1
C[Si](C)(O)O[Si](C)(O[SiH3])c(:c):c	C[Si](C)(O)O[Si](C)(O[SiH3])O[SiH3]	C[Si](O)(O)O[Si](C)(C)O[SiH3]
CC[Si](C)(O[SiH3])O[Si](C)(C)O	C[Si]1(C)[Si](C)(C)[Si](c(:c):c)(c(:c):c)[Si]1(c(:c):c)c(:c):c	CC[Si]1(C)O[SiH2]O[Si](C)(C)O1
C[Si]1(C)CC=CC1	C1[SiH2]CC=C1	CC[Si]1(CC)C[Si](C)(C)C1
SOc1cccc1	CS(=O)(=O)Oc(:c):c:c	c:c(:c)OS(=O)(=O)c(:c):c
COS(=O)(=O)c(:c):c:c	OS(=O)(=O)c1cccc1	O=S1(=O)CCCC1
CCC1(CC)CS(=O)(=O)C1	CC1(C)CS(=O)(=O)C1	CC1CS1(=O)=O
CCc1cccc(C)c1	CCCc(:c):c(C):c	CCc1cccc1C
CCc1cc(C)ccc1C	CCc1cccc1CC	Cc1ccc(C)c(Cl)c1
CCc1cccc(Cl)c1	CCCc(:c):c(Cl):c	CCc1cccc1Cl
Cc1ccc(C)c(Br)c1	CCc1cccc(Br)c1	CCCc(:c):c(Br):c
CCc1cccc1Br	CC(F)(F)C(F)(F)c(:c):c:c	CC(F)(F)c1cccc1
FC(F)(c(:c):c)C(F)(F)c(:c):c	CCC12CC3CC3(C1)CCC2	CC12CC34CC3(CC(C4)C1)C2
C1C23CCCC12CCC3	C1C23CC4CC12CC(C3)C4	CC12CC3CC(CC3C1)C2
CCC12CC3CC(CC3C1)C2	OC(=O)C1=C(C2C=CC1C=C2)C(O)=O	CC1=CC2C=CC1C=C2
C1=CC2C=CC1C=C2	FC(F)(F)C1(C2CC(C=C2)C1(F)F)C(F)(F)F	FC(F)(F)C1=C(C2CCC1C=C2)C(F)(F)F
CC1CC2C=CC1C(=C2C)C(F)(F)F	CC1CC2C=CC1C(C)=C2	CC1=CC2C=CC1C1=CC21
CC(C)C1C=CC1C	CC1C=CC1C	OC(=O)C1CC2CC1C=C2
CC1CC2CC1C=C2	OC1(F)CC2CC1C=C2	N#Cc1cccc1
CC1C2CC(C=C2)C1C(O)=O	N#CC1CC2CC1C=C2	CCC1(CC2CC1C=C2)C#N

C[Si](C)(C)C1(CC2CC1C=C2)C#N	CC1([SiH3])CC2CC1C=C2	C[Si](C)(O)C1(CC2CC1C=C2)C#N
[SiH3]CC1(CC2CC1C=C2)C#N	C[Si](C)([SiH3])C1(CC2CC1C=C2)C#N	CCN1C(=O)cc(:c)C1=O
NCC1CC2CC1C=C2	CN1Cc(:c)c(:c:c)C1=O	O=C1NCc2ccccc12
CC(C)=C1C=CC1=C	C=C1C=CC1=C	CC1CCC=C1
CC1CCC=CC1	COC(CC(N)=O)c(:c):c	CCC(OC(C)C)c(:c):c
CC(C)OC(CN)c(:c):c	CNCC(OC)c(:c):c	CC(O)c1ccccc1
OCC1(CCl)COC1	CC1(C)CC2CCC1C2	CC1(C)OCCCCO1
CC1(C)CC2CCC1CC2	FC(F)(F)C1(F)OC1(F)F	CC1(F)OC1(F)F
CC1COCO1	CC1CCOC1	Cc1ccco1
CCC1(CO)COC1	COC(=O)CCO	COCCC(O)=O
CC(O)(O)CCC(O)=O	CCCC1(CC)OCCO1	CCC1(CCO)OCCO1
COCCC(C)(O)O	CCC1(CC)OCCO1	COC(C)CC(O)=O
COC(=O)CC(C)O	CC(C)OCCO	CCOC(C)CC
CC1CCC2CN(C)C(=O)C12	O=C1NCC2C3CC(C=C3)C12	CCN1C(=O)CC(C)C1=O
CN(C)c1ccccc1	CC1CC(=O)N(c(:c):c)C1=O	CC1OC1CO
OCC1OC1CO	COP1(=O)OCCO1	OP1(=O)OCCO1
C1COPO1	CCC1(CC)CSC1	O=C1CCCCS1
C1CCSCC1	CC(C)(C)C1CC(=O)O1	CCC1(COC1=O)c(:c):c
CCc1cc(O)ccc1O	CCc1ccccc1OC	C=CC1CC(=O)O1
CC(O)C1CCC=CO1	CC1CCC=CO1	CC1CCCCO1
CC1CCOCC1	COC(=O)CC=C	CC1NC(=O)COC1=O
CC1COCC(=O)N1	O=C1COCCN1	O=C1COC(=O)CN1
CC1NCCOC1=O	CC1COC(C)C(=O)N1	CC1OCCNC1=O
CC1OC(=O)CNC1=O	CC1CNC(C)C(=O)O1	CCOC(=O)C(C)=C
COC(=O)C(=C(C)N)C(C)=C	CCC(N(C)C)=C(C(C)=C)C(O)=O	CCCC(N(C)C)=C(C)C
COC(=O)C(=CC)C(C)=C	CC(=C)N1CCCC1	O=C1CNCCO1
OC(=O)C1CC(=O)O1	CCC(CCO)C(O)=O	CCCC(CC)C(O)=O
CCC1(C)CC(=O)N1	CC1(C)CC(=O)N1	CC1NC(=O)C1(C)C
CCC(C)CCN	CC(C)CCC(N)=O	CC(C)C1CC(=O)N1
CC1CC(=O)N1	CC(N)c1ccccc1	CC(C)C1NC(=O)C1(C)C
CC1(C)C(NC1=O)c(:c):c	CC1(C)NC(=O)C1(C)C	C=CC1CC(=O)N1
CCC1CC(=O)N1	CCCC(Cl)(Cl)C(N)=O	CCCCC(C)(Cl)Cl
CCNC(=O)C(C)(Cl)Cl	CCC(Cl)(Cl)C(=O)NC	OC(=O)C1CC(=O)N1
O=C1NCCCCO1	CCCNC(O)=O	NCCCCO

<chem>CCOC(N)=O</chem>	<chem>CCOC(=O)NC</chem>	<chem>Cc1ccccc1N</chem>
<chem>Nc1cccc(c1)C(F)(F)F</chem>	<chem>CC1CCC2(Cl)OC(=O)OC12Cl</chem>	<chem>OC1(Cl)CC2CC1C=C2</chem>
<chem>O=C1OCCO1</chem>	<chem>O=C1OCCCCO1</chem>	<chem>C1COCOC1</chem>
<chem>CC1(C)COCOC1</chem>	<chem>CC1(COCOC1)C(O)=O</chem>	<chem>OCC1=NCCO1</chem>
<chem>Oc1ccc(S)cc1</chem>	<chem>CCN1CC1</chem>	<chem>CCn1c(:c)cc(:c)c1:c:c</chem>
<chem>Cn1ccc2ccccc12</chem>	<chem>[nH2]:c1ccccc1</chem>	<chem>C=CC1=C(C=C)C(=C)NC1=C</chem>
<chem>CN1[Si](C)(C)N(C)[Si]1(C)C</chem>	<chem>CCN1[Si](C)(C)C[Si]1(C)C</chem>	<chem>CN1[Si](C)(C)C[Si]1(C)C</chem>
<chem>NC(=O)C12CCCC(CCC1)C2</chem>	<chem>C1CC2CCCC(C1)C2</chem>	<chem>CCC12CCCC(CCC1)C2</chem>
<chem>OC(=N)c1cccs1</chem>	<chem>CN1COc(:c)cC1</chem>	<chem>c:c:c1OCNCc1:c</chem>
<chem>CN1COc(:c)c(C1):c:c</chem>	<chem>c:c(:c)N1COcc(:c)C1</chem>	<chem>c:c(:c)N1COC=CC1</chem>
<chem>Cc1cccc(c1)C(C)(C)C</chem>	<chem>Cc1ccc(O)c(CN)c1</chem>	<chem>c:c(:c)C12CCCC(CCC1)C2</chem>
<chem>CN1COC=CC1</chem>	<chem>C[Si](C)(O)O[Si](C)(CCl)O[SiH3]</chem>	<chem>C[Si]1(C)C[Si](C1)(c(:c):c)c(:c):c</chem>
<chem>C[Si](C)(O)O[Si](C)(O[SiH3])C=C</chem>	<chem>C[Si]1(C)C[Si](C)(C1)c(:c):c</chem>	<chem>C[Si]1C[Si](C)C1</chem>
<chem>C[Si]1(C)O[Si](C)(C)[Si](C)(C)O[SiH2]1</chem>	<chem>C[Si]1(C)O[SiH2][SiH2]O[Si]1(C)C</chem>	<chem>C[Si]1(C)CC(=C)C1=C</chem>
<chem>C[Si]1(C)Cc(:c:c)c1:c</chem>	<chem>C1[SiH2]c2ccccc12</chem>	<chem>C[Si]1(C)Cc(:c)c1:c:c</chem>
<chem>C[Si]1(C)Ccc(:c)C1</chem>	<chem>C1[SiH2]Cc2ccccc12</chem>	<chem>C=C[Si]1(CC=CC1)C=C</chem>
<chem>C[Si]1(CCC=CC1)c(:c):c</chem>	<chem>C[Si]1(C)CCC=CC1</chem>	<chem>C1CC=CC[SiH2]1</chem>
<chem>CC1=CC[SiH2]C1</chem>	<chem>CC[Si](CC)(C#[SiH3])[Si](C)(C)C</chem>	<chem>C[Si](C)([SiH3])C#[Si](C)(C)[SiH3]</chem>
<chem>CC[Si](CC)(C#[SiH3])[Si](C)(C)C#C</chem>	<chem>C[Si](C)(C)[Si](C)(C#[SiH3])c(:c):c</chem>	<chem>C[Si](C)([SiH3])c1ccccc1</chem>
<chem>C[Si](C#C)(c(:c):c)[Si](C)(C#C)c(:c):c</chem>	<chem>CC1C[Si](C)(C)C1</chem>	<chem>CCc1ccccc1:c</chem>
<chem>CCc1cccc(:c)c1:c:c</chem>	<chem>CC(C)c1ccccc1:c</chem>	<chem>CC(C)c1cccc(:c)c1:c:c</chem>
<chem>C[Si]1(CC[SiH2]O1)O[SiH3]</chem>	<chem>C[Si]1(C)CC[Si](C)(O)O1</chem>	<chem>C[Si]1(C)CC[SiH2]O1</chem>
<chem>[SiH3]C[Si]1(C[SiH3])CCC1</chem>	<chem>C[Si]1(C[SiH3])CCC1</chem>	<chem>CC[Si]1(C)CCC1</chem>
<chem>C[Si](C)(C)C1CCCC1</chem>	<chem>C[Si](C)(C)c1ccccc1:c</chem>	<chem>C[Si](C)(C)c1cccc(:c)c1:c:c</chem>
<chem>CP(S)c1ccccc1</chem>	<chem>C[Ge]1(C)CC=CC1</chem>	<chem>C1[GeH2]CC=C1</chem>
<chem>CC1=CCCC1</chem>	<chem>Nc1ccc([SiH3])cc1</chem>	<chem>C[Si]1(CCC1)c(:c):c</chem>
<chem>C[Si]1(CC=CC1)c(:c):c</chem>	<chem>CC[Si]1(CC=CC1)c(:c):c</chem>	<chem>ClC(Cl)(Cl)C1CC(=O)O1</chem>
<chem>CCN(CCO)C(O)=O</chem>	<chem>CCCN(CC)C(O)=O</chem>	<chem>CN1CCOC1=S</chem>
<chem>S=C1NCCO1</chem>	<chem>NCc1ccccc1</chem>	<chem>CN1CCCOC1=S</chem>
<chem>S=C1NCCCO1</chem>	<chem>CN1CCCOC1</chem>	<chem>CC[Si]1(C)N(C)[Si](C)(C)N1C</chem>
<chem>CC(C)[Si]1(C)C[Si](C)(C)C1</chem>	<chem>CC(C)[Si]1(Cl)C[Si](C)(Cl)C1</chem>	<chem>C[Si](C)(Cl)C1CCCC1</chem>

C[Si]1(CC(=C)C1=C)c(:c):c	C[Si]1(Cc(:c)c1:c:c)c(:c):c	c:c:c1c(:c)C[Si]1(c(:c):c)c(:c):c
c:c(:c)[Si]1(CC(=C)C1=C)c(:c):c	C[Si]1(CCC1)O[SiH3]	CC(C)c1ccccc1
CC(C)c1ccccc1C	c:c1cC2C=CC1C=C2	CC(C)c1cc(C)ccc1C
N=S=NSN=S	NSN=S=NS	

Walk 3 Descriptors

CCN1CCOC1=S	CC1=C(C2C=CC1C1C=CC21)C(F)(F)F	CN(C)C1=C(C)C=CCCC1
CCCC1CCC(C)O1	CCN1C(=C)C(=C)c2ccccc12	CC1CCC2C=CCC12
Cc1cc(cc(c1)C(F)(F)F)C(F)(F)F	C1CCC2OC2CC1	CC1CCCC11COC1
CCC1(COC1)C(C)C	CCN1C(=O)N(CC)C(C)(C)C1=O	CC1CCC(C)(C)CC1
CC(C)CN1C(=O)c(:c)c(:c:c)C1=O	CC1(C)COC(=O)OC1	CCCOC(=O)OCC
COC(=O)C1=C(CCCC=C1C(O)=O)N1CCCC1	CCOCCCCO	Nc1cc(cc(c1)C(F)(F)F)C(F)(F)F
CC1=CCCC(N)=C1	COCC1CO1	C1CCCOCCCC1
CCCC1CO1	CCCCCOCC	CC(C)=C1C=CC1=C(C)C
C1CCCNCC1	CC1COC(=O)O1	O=C1CCOCCO1
COCCCOc(:c):c	S=C1CCCCCN1	O=C1NCCCCO1
C1CCC=CCC1	OCCCCCO	CCCCCCCC
CCOCCOCC	CCCCC=CC	COC(=O)C1=C(C2C=CC1C=C2)C(O)=O
COCCOC(C)=O	CN1C(=O)c2ccccc2C1=O	CCCC=CCCC
CCCCCCC=C	CCCCC=CCC	C1CCCC=CCC1
CC1CCCCC=C1	COc1ccc(C)cc1	Oc1ccc(cc1)C1=CCCC1
c:c:c(:c:c)C1=CCCC1	Cc1ccc(Cl)cc1	CCC1OC(C)OC(CC#N)O1
CC(C)(C)CC1CO1	c:c(:c)C1CO1	CCOc1ccccc1
COc1ccccc1C	Cc1ccc(O)c1	COc1ccccc1Cl
Oc1ccc(Cl)cc1	Oc1c(Cl)cc(Cl)cc1Cl	CCOc1cccc(:c)c1:c:c
COC1=CC=CC(=C)C1=C	Oc1cccc(:c:c)c1:c	Oc1cccc2ccccc12
C=C1C=CC=CC1=C	Oc(:c):c1ccccc1:c	CCOC1=CC(=C)C(=C)C=C1
COc1ccc(:c:c)c(:c)c1	Oc1ccc2ccccc2c1	c1ccc2ccccc2c1
CCOc1ccc(:c)c(:c:c)c1	COc1ccccc1C(C)C	COCC1(CO1)c(:c:c):c:c

OCC1(CO1)c1cccc1	Oc1cccc(c1)C(F)(F)F	Cc1cccc(c1)C1(CO)CO1
Cc1cccc(c1)C1(C)CO1	Cc1cccc(c1)C(F)(F)F	Cc1c(F)c(F)c(F)c(F)c1F
COCC1(CO1)c(:c(F):c):c(F):c	COCC1(COC)COC1	C1CCCOCC1
CCCCCCCO	CCCCCCOC	CCCCOCCC
OCCCOc(:c:c):c:c	CCCOc1cccc1	CCOc1ccc(O)cc1
COc1ccc(OC)cc1	C1CCOCOC1	C1CCOCOCC1
CCCCCOCO	CCCCOCOC	CCCCOCCC
COCCCCOC	COCCCCCO	C1CSSCCO1
CCCCC(=O)OCC	CCCCC(=O)OC	CCCCCCC(O)=O
CCCC(=O)OCCO	CCC(=O)OCCOC	CCOCCOC(C)=O
COCCOCCO	OCCOC(=O)c(:c:c):c:c	COCCOC(=O)c(:c):c
CCOC(=O)c1cccc(C)c1	COC(=O)c1cccc(C)c1	Cc1cccc(c1)C(O)=O
CC(=O)OCCOC(C)=O	CCOC(=O)c1cccc1	COC(=O)c1ccc(O)cc1
COc1ccc(cc1)C(O)=O	Cc1ccc(Oc(:c):c)cc1	c:c:c(Oc1cccc1):c:c
OCCOc1cccc1	COCCOc(:c:c):c:c	c:c(:c)OCCOc(:c):c
CCOC(=O)c1cccc(O)c1	COC(=O)c1cccc(O)c1	OC(=O)c1cccc(O)c1
Cc1cccc(OCCO)c1	CCCCOc(:c:c):c:c	CCCCCOc(:c):c
CCOC(=O)c(:c:c):c:c	CCCCOC(=O)c(:c):c	CCCCCOC(C)=O
CC(O)CCC(=O)OC(C)=O	COC(=O)CCC1CCCO1	CC1CCC(CCC(O)=O)O1
CCC1CCC(CC)O1	CCCC(=O)OC(=O)CC	CCCC1CCC(CC)O1
CC(=O)OC(=O)COc(:c):c	COC(=O)COc(:c:c):c:c	OC(=O)COc1cccc(O)c1
CCOc1cccc(O)c1	COc1cccc(O)c1	COCC(=O)OC(=O)CO
OC(=O)COc1cccc1	c:c:c(:c:c)C(=O)OC(=O)c(:c):c	CC(=O)OC(=O)c1cccc1
Cc1ccc(OCO)cc1	COCOc1cccc1	c:c:c(OCOc(:c):c):c:c
CC(=O)OC(=O)c1cccc(O)c1	CCOCCOc(:c):c	COc1ccc(cc1OC)C(O)=O
COC(=O)c1ccc(O)c(OC)c1	COC(=O)c1ccc(O)c(O)c1	COc1ccc(cc1O)C(O)=O
CCOc1ccc(C)cc1OC	CCCOc1cccc1OC	CCCCOc(:c:c):c(O):c
OCCCCOc(:c):c	COC(=O)C(=O)OCCO	COCCOC(=O)C(O)=O
CCOC(=O)C(=O)OCC	CCOC(=O)CC(=O)OC	OCCOC(=O)CC(O)=O
CCOC(=O)C(C)C(=O)OC	CC(C(O)=O)C(=O)OCCO	COCCOC(=O)C(C)C
CCCC(C(=O)OC)C(=O)OCC	CCC(C(O)=O)C(=O)OCCO	CCOC(=O)CCC(O)=O
COC(=O)CCC(=O)OC	COC(=O)CCCC(O)=O	OC(=O)CCCC(O)=O
ClC(Cl)(Cl)CC1CO1	C1CCC2OC2C1	OCCCOc(=O)c(:c):c
CC(=O)OCCCCO	CCOCC(=O)OCC	COC(=O)COCC(O)=O
CCCOc(=O)COC	CCCCOC(=O)CO	COC(=O)c1ccc(C)cc1
OC(=O)c1ccc(cc1)C(O)=O	OCc1ccc(cc1)C(O)=O	COCC1ccc(C)cc1

CCOCc1ccccc1	OCCOCc(:c:c):c:c	COCCOCc(:c):c
ClCC1OC1Cl	COCC(=O)OCCO	COCCOC(=O)CO
COC(=O)CCCCS	CS(=O)(=O)CCCC(O)=O	CCCCCS(=O)(=O)CC
CCCCS(=O)(=O)CCC	CSCCCCC(O)=O	CCCCSCC
CCCCSCCC	CCc1ccc(cc1)C(O)=O	CCc1ccc(C)cc1
c:c(:c)CCc1ccccc1	c:c:c(CCc(:c:c):c:c):c:c	Cc1ccc(Cc(:c):c)cc1
c:c:c(Cc1ccccc1):c:c	OCCOC(=O)CO	COCC(C)OC(C)=O
COC(C)CCOC(C)=O	CC(O)CCOC(=O)CO	CCOCC(=O)OC(C)C
CCC(C)OC(=O)COC	CC(CCO)OC(=O)CO	CCCCCCC(O)O
CCCCC(OC)OC	CCCCC1OCCCO1	CCCC1OCC(C)(C)CO1
CCC1OCC(CO)(CO)CO1	CC1OCC2(COCOC2)CO1	COc1c(C)cccc1C
Cc1cccc(C)c1O	[NH2+]=NCC1CO1	COCC1CS1
C1CCSSCC1	C1CCSSCC1	C1CCSSCC1
C1CCSCCSC1	CCCCCCCS	CCCCCCSS
CCCCSSC	CCCCSSCC	CCCSSCCC
SCCCCCCS	CCCCCCSC	CCCCSCCS
CCCSCCSC	CCSCCSCC	CCCCSSSS
CCCCSSSS	CCCCSSSC	CCSSSSCC
O=C1CCSCCC(=O)O1	O=C1CCSCCCO1	CCSCC(=O)OC(C)=O
COC(=O)CSCCS	CSCCSCC(O)=O	CSCC(=O)OC(=O)CS
CSCCC(=O)OC(C)=O	CCSCCC(=O)OC	OC(=O)CCSCCS
CCC(=O)OC(=O)CCS	C1SSCc2ccc1cc2	c:c(:c)C1CS1
COC(=O)CCSc(:c):c	OC(=O)CCSc(:c:c):c:c	CCCSc1ccccc1
CCSc1ccc(S)cc1	CSc1ccc(SC)cc1	COC(=O)CSCc(:c):c
OC(=O)CSCc(:c:c):c:c	CCSCc1ccccc1	CSCc1ccc(C)cc1
SCc1ccc(CS)cc1	OC(=O)CCSCc(:c):c	CCCSCc(:c:c):c:c
COC(=O)c1ccc(S)cc1	CSc1ccc(cc1)C(O)=O	Cc1ccc(Sc(:c):c)cc1
c:c:c(Sc1ccccc1):c:c	CCSc1ccc(C)cc1	CCCCSc(:c:c):c:c
SCCCSc(:c):c	CSCCCSC	SCCSc1ccccc1
CSCCSc(:c:c):c:c	c:c(:c)SCCSc(:c):c	CC(=O)OC(=O)CCc(:c):s
COC(=O)CCc1cccs1	Cc1ccc(CCC(O)=O)s1	CCc1ccc(C)s1
CCc1ccc(CC)s1	CCCc1ccc(CC)s1	CCOC(=O)CCC
CCCCOC(=O)CC	CCC(=O)OCCCO	CC(COC(C)=O)OC(C)=O
CCC(=O)OCC(C)OC	CCCC(=O)OCC(C)O	CCCCC(=O)OC(C)C
CCCC(=O)OC(C)CO	CCC(=O)OC(C)COC	CCC(=O)OCCC(C)O
CCCC(=O)OC(C)CC	CCC(=O)OC(C)CCO	ClS1=NP(Cl)(Cl)=NP(Cl)(Cl)=N1

<chem>CCCOC(=O)C(=O)OC</chem>	<chem>CCCCOC(=O)C(O)=O</chem>	<chem>O=C1CCC(=O)OCCO1</chem>
<chem>O=C1CCC(O)CCO1</chem>	<chem>CCOC(=O)c1cccc(:c)c1</chem>	<chem>COC(=O)C1=CC(=C)C(=C)C=C1</chem>
<chem>OC(=O)c1ccc(:c:c)c(:c)c1</chem>	<chem>Cc1ccc2cc(C)ccc2c1</chem>	<chem>OC(=O)c1ccc2cccc2c1</chem>
<chem>COC(=O)c1ccc(:c)c(:c:c)c1</chem>	<chem>CCCC(=O)OCC=C</chem>	<chem>CCC(=O)OCC=CC</chem>
<chem>CC(=O)OCC=CCO</chem>	<chem>COCC=CCOC</chem>	<chem>CCCC(=O)OCC#C</chem>
<chem>CCC(=O)OCC#CC</chem>	<chem>CC(=O)OCC#CCO</chem>	<chem>COCC#CCOC</chem>
<chem>c:c:c1C(=O)OCCOCc1:c</chem>	<chem>c:c1cCOCCOC1=O</chem>	<chem>O=C1OCCOC(=O)C=C1</chem>
<chem>COC(=O)c1cccc1C(O)=O</chem>	<chem>Cc1cccc1C</chem>	<chem>c:c:c(OC(=O)c(:c:c):c:c):c:c</chem>
<chem>Oc1cccc(OC(=O)c(:c):c)c1</chem>	<chem>CC(=O)Oc1cccc(O)c1</chem>	<chem>Cc1cccc(c1)C(=O)Oc(:c):c</chem>
<chem>O=C1CCCCCO1</chem>	<chem>O=C1CCCCCO1</chem>	<chem>O=C1OCCOCC=C1</chem>
<chem>CC(CO)C(C)COC(C)=O</chem>	<chem>CC(C)C(C)COC(=O)c(:c):c</chem>	<chem>CC(C)COC(=O)c(:c:c):c:c</chem>
<chem>COCC(C)C(C)COC</chem>	<chem>CCC(CO)C(CC)COC(C)=O</chem>	<chem>CCC(COC(=O)c(:c):c)C(C)C</chem>
<chem>CCC(COC)C(CC)COC</chem>	<chem>CCCC(COC(C)=O)C(CC)CO</chem>	<chem>CCCC(COC)C(CCC)COC</chem>
<chem>CC(C)C(CO)C(COC(C)=O)C(C)C</chem>	<chem>CC(C)C(COC(=O)c(:c):c)C(C)C</chem>	<chem>COCC(C(C)C)C(COC)C(C)C</chem>
<chem>COc1ccc(OC)c(C)c1</chem>	<chem>CC(=O)Oc1ccc(O)c(C)c1</chem>	<chem>Cc1cccc(OC(=O)c(:c):c)c1</chem>
<chem>c:c(:c)OC(=O)c1cccc1</chem>	<chem>OC(=O)c1ccc(cc1)-c(:c):c</chem>	<chem>Cc1ccc(cc1)-c(:c:c):c:c</chem>
<chem>c1ccc(cc1)-c1cccc1</chem>	<chem>Cc(:c):c(OC(=O)c(:c:c):c:c):c:c</chem>	<chem>Cc1cccc1OC(=O)c(:c):c</chem>
<chem>CC(=O)Oc1ccc(O)cc1C</chem>	<chem>CCCCC(=O)Oc(:c):c</chem>	<chem>CCCC(=O)Oc(:c:c):c:c</chem>
<chem>CCC(=O)Oc1cccc1</chem>	<chem>CC(=O)Oc1ccc(O)cc1</chem>	<chem>CC(CCC(O)=O)CC(O)=O</chem>
<chem>CCC(C)CCC(=O)OC</chem>	<chem>CCOC(=O)CCC(C)C</chem>	<chem>CCOC(=O)CC(C)C</chem>
<chem>CCOC(=O)CC(C)CC</chem>	<chem>CCCC(C)CC(=O)OC</chem>	<chem>CCCCC(=O)NCC</chem>
<chem>CCCCCC(=O)NC</chem>	<chem>NC(=O)CCCCC(N)=O</chem>	<chem>CCCNC(=O)CCC</chem>
<chem>CCCCNC(=O)CC</chem>	<chem>CCCCCNC(C)=O</chem>	<chem>CCCCCNC</chem>
<chem>NCCCCC(O)=O</chem>	<chem>CCCOC(=O)CC(O)=O</chem>	<chem>CCCCC(=O)Nc(:c):c</chem>
<chem>CCCCCC(N)=O</chem>	<chem>CCCC(=O)Nc(:c:c):c:c</chem>	<chem>CCC(=O)Nc1cccc1</chem>
<chem>CC(=O)Nc1ccc(C)cc1</chem>	<chem>CNc1ccc(cc1)C(O)=O</chem>	<chem>COC(=O)c1ccc(N)cc1</chem>
<chem>CCOC(=O)Cc(:c:c):c:c</chem>	<chem>COC(=O)Cc1cccc1</chem>	<chem>Cc1ccc(CC(O)=O)cc1</chem>
<chem>CCc1ccc(CC)cc1</chem>	<chem>OCCOC(=O)Cc(:c):c</chem>	<chem>CS(=O)(=O)c1ccc(cc1)C(O)=O</chem>
<chem>CCS(=O)(=O)c1ccc(C)cc1</chem>	<chem>CCCS(=O)(=O)c1cccc1</chem>	<chem>CCCS(=O)(=O)c(:c:c):c:c</chem>
<chem>CCCCCS(=O)(=O)c(:c):c</chem>	<chem>CCCCCS(C)(=O)=O</chem>	<chem>CCOC(=O)c(:c:c):c(C):c</chem>
<chem>CCOC(=O)c1cccc1C(O)=O</chem>	<chem>COC(=O)c1cccc1C(=O)OC</chem>	<chem>Cc1ccc(cc1)S(=O)(=O)c(:c):c</chem>
<chem>c:c:c(:c:c)S(=O)(=O)c1cccc1</chem>	<chem>OC(=O)c1ccc(CS)cc1</chem>	<chem>Cc1ccc(CS(C)(=O)=O)cc1</chem>

<chem>CCS(=O)(=O)Cc1cccc1</chem>	<chem>c:c:c(CS(=O)(=O)Cc(:c):c):c:c</chem>	<chem>CCCCNC(=O)c(:c):c</chem>
<chem>CCCNC(=O)c(:c):c:c</chem>	<chem>CCNC(=O)c1cccc1</chem>	<chem>CNC(=O)c1ccc(C)cc1</chem>
<chem>NC(=O)c1ccc(cc1)C(N)=O</chem>	<chem>CCOC(=O)CCCS</chem>	<chem>COC(=O)CCCS(C)(=O)=O</chem>
<chem>CCS(=O)(=O)CCCC(O)=O</chem>	<chem>CCCS(=O)(=O)Cc(:c):c</chem>	<chem>CCCS(=O)(=O)Cc(:c):c:c</chem>
<chem>CCCC1(CCC)COC1=O</chem>	<chem>CC1CCCSCC1</chem>	<chem>O=C1CCCCCS1</chem>
<chem>CCOC(=O)CCc(:c):c</chem>	<chem>COC(=O)CCc(:c):c:c</chem>	<chem>OC(=O)CCc1cccc1</chem>
<chem>CCC(=O)OCCc(:c):c</chem>	<chem>CC(=O)OCCc(:c):c:c</chem>	<chem>COCCc1cccc1</chem>
<chem>Cc1ccc(CCO)cc1</chem>	<chem>c:c(:c)CCOC(=O)c(:c):c</chem>	<chem>COC(=O)CC(=O)Oc(:c):c</chem>
<chem>OC(=O)CC(=O)Oc(:c):c:c</chem>	<chem>OC(=O)CCC(=O)Oc(:c):c</chem>	<chem>CCC(=O)Oc1cccc(O)c1</chem>
<chem>c:c(:c)C(=O)Oc1cccc1</chem>	<chem>CN(C)CCC(=O)Oc(:c):c</chem>	<chem>CCN(CC)CCC(=O)OC</chem>
<chem>OC(=O)CCN1CCNCC1</chem>	<chem>CCCN1CCN(C)CC1</chem>	<chem>CCN1CCN(CC)CC1</chem>
<chem>NCCC(=O)Oc(:c):c:c</chem>	<chem>CC1COC(=O)C(=O)O1</chem>	<chem>O=C1OCCCCOC1=O</chem>
<chem>O=C1COCCCCO1</chem>	<chem>C1CCOCCOC1</chem>	<chem>COCC(C)(C)COC(C)=O</chem>
<chem>CCC(=O)OCC(C)(C)CO</chem>	<chem>CCCC(=O)OCC(C)(C)C</chem>	<chem>CC(O)CCOC(=O)c(:c):c</chem>
<chem>CC(C)OC(=O)c1cccc(C)c1</chem>	<chem>CCC(C)OC(=O)c(:c):c:c</chem>	<chem>CC(CCO)OC(=O)c(:c):c</chem>
<chem>O=C1CC(=O)OCCCCO1</chem>	<chem>O=C1CCOCCCCO1</chem>	<chem>O=C1OCCCCOC1=O</chem>
<chem>O=C1COCCCCO1</chem>	<chem>C1CC1(CCl)COCC(=O)OC1</chem>	<chem>CC1(C)COC(=O)C(=O)OC1</chem>
<chem>CC1(C)COCC(=O)OC1</chem>	<chem>CC(C)OC(=O)c1cccc1C(O)=O</chem>	<chem>CCC(C)OC(=O)c(:c):c(C):c</chem>
<chem>CC(C)OC(=O)c1cccc1</chem>	<chem>CCCC(=O)OCc(:c):c</chem>	<chem>CCC(=O)OCc(:c):c:c</chem>
<chem>CC(=O)OCc1cccc1</chem>	<chem>OCc1ccc(CO)cc1</chem>	<chem>c:c:c(:c:c)C(=O)OCc(:c):c</chem>
<chem>c:c:c(COC(=O)c(:c):c):c:c</chem>	<chem>CC1(C)COCCCC(=O)OC1</chem>	<chem>CC1CCCOC1</chem>
<chem>CC1CCCCC(=O)O1</chem>	<chem>CC1CCCC(C)OC1</chem>	<chem>CC1CCCCOC1=O</chem>
<chem>CC1COC(=O)C=CC(=O)O1</chem>	<chem>CC1COC(=O)c(:c)cCO1</chem>	<chem>CC1COC(=O)c(:c:c)c(:c)CO1</chem>
<chem>CC1COCc(:c)c(:c:c)C(=O)O1</chem>	<chem>CC1COCc(:c)C(=O)O1</chem>	<chem>CCOC(=O)CCN(C)C</chem>
<chem>NCCC(=O)OCCO</chem>	<chem>CC1COC(=O)CCC(=O)O1</chem>	<chem>CC1COC(=O)CCCO1</chem>
<chem>CC1COCCCC(=O)O1</chem>	<chem>COC(C)COC(=O)c(:c):c</chem>	<chem>CC(O)COC(=O)c(:c):c:c</chem>
<chem>CC(CO)OC(=O)c(:c):c:c</chem>	<chem>COCC(C)OC(=O)c(:c):c</chem>	<chem>COC(=O)C(=O)OCc(:c):c</chem>
<chem>OC(=O)C(=O)OCc(:c):c:c</chem>	<chem>Cc1cc(ccc1-c(:c):c)C(O)=O</chem>	<chem>COC(=O)c1ccc(C)c(C)c1</chem>
<chem>Cc(:c):c(:c:c)-c1ccc(C)cc1C</chem>	<chem>Cc1cccc1-c1cccc1C</chem>	<chem>CC1CCCCO1</chem>
<chem>O=C1CCCCCN1</chem>	<chem>O=C1CCCCCN1</chem>	<chem>C1CCCNCCC1</chem>
<chem>CCCCCCCN</chem>	<chem>OC(=O)CC1NC(=O)OC1=O</chem>	<chem>CC1NC(=O)OC1=O</chem>
<chem>S=C1CCCCCN1</chem>	<chem>CC1CNC(=O)CC(C)O1</chem>	<chem>CC1CNC(=O)CCO1</chem>
<chem>CC1CC(=O)NCCO1</chem>	<chem>CC1CCNCC(C)O1</chem>	<chem>CCC(C)C1NC(=O)OC1=O</chem>
<chem>CC(C)CC1NC(=O)OC1=O</chem>	<chem>O=C1NC2CCCC1O2</chem>	<chem>CC1CCCCC(=O)N1</chem>
<chem>CC1CCCCCN1</chem>	<chem>CC(N)Cc1cccc1</chem>	<chem>CCN(CC)C(=O)OCCO</chem>
<chem>COCCOC(=O)N(C)C</chem>	<chem>NC(=O)OCCOC(N)=O</chem>	<chem>CCOC(=O)N1CCNCC1</chem>

<chem>COC(=O)N1CCN(C)CC1</chem>	<chem>OC(=O)N1CCN(CC1)C(O)=O</chem>	<chem>CN1C(=O)N(CCO)C(C)(C)C1=O</chem>
<chem>COCCN1C(=O)N(C)C(=O)C1(C)C</chem>	<chem>CC(=O)OCCN1C(=O)NCC1(C)C</chem>	<chem>CN(C)CCOC(=O)c(:c):c</chem>
<chem>NCCOC(=O)c(:c):c:c</chem>	<chem>CC(=O)OCCN1C(=O)CNC1=O</chem>	<chem>COCCN1C(=O)N(C)C(C)(C)C1=O</chem>
<chem>CCN1C(=O)N(CCO)C(=O)C1(C)C</chem>	<chem>CCN1C(=O)N(CCO)C(C)(C)C1=O</chem>	<chem>CN1C(=O)N(CCO)C(=O)C1(C)C</chem>
<chem>CCC(CC)C1N(CC)C(=O)N(CC)C1=O</chem>	<chem>CN1CNC(=O)C1C1CCCCC1</chem>	<chem>CCC(CC)C1N(CCO)C(=O)N(C)C1=O</chem>
<chem>COCCN1C(C(C)C)C(=O)N(C)C1=O</chem>	<chem>CC1CNC(=O)N1CCOC(C)=O</chem>	<chem>COCCN1C(=O)C(C)N(C)C1=O</chem>
<chem>CC(C)C1N(C)C(=O)N(CCO)C1=O</chem>	<chem>CCN1C(C)C(=O)N(CCO)C1=O</chem>	<chem>CCN1C(=O)C(C(C)C)N(CCO)C1=O</chem>
<chem>COCCN1C(=O)N(C)C(=O)C1(c(:c):c)c(:c):c</chem>	<chem>CCN1C(=O)N(CCO)C(c(:c):c)(c(:c):c)C1=O</chem>	<chem>CN1C(=O)N(CCO)C(c(:c):c:c(:c):c)c(:c):c)C1=O</chem>
<chem>CCN1C(=O)N(CC)C(c(:c):c)c(:c)(c(:c):c)c1=O</chem>	<chem>CN1C(=O)N(CCO)C(=O)C1(c(:c):c)c(:c):c</chem>	<chem>CN1CNC(=O)C1(c(:c):c)c1cccc1</chem>
<chem>O=C1CCCCC(=O)O1</chem>	<chem>CCCCC(=O)OC(C)=O</chem>	<chem>CCCCc1cccc1</chem>
<chem>CCCCCc(:c):c:c</chem>	<chem>CCCCCc(:c):c</chem>	<chem>CC(C)(c(:c):c)c1cccc1</chem>
<chem>Cc1ccc(cc1)C(C)(C)c(:c):c</chem>	<chem>CC(C)(C)c1ccc(cc1)C(O)=O</chem>	<chem>CC(=O)OC(=O)Cc(:c):c:c</chem>
<chem>CCC(=O)OC(=O)Cc(:c):c</chem>	<chem>CC(=O)OC(=O)CCc(:c):c</chem>	<chem>O=C1CCCCCC(=O)O1</chem>
<chem>O=C1OC(=O)c2ccc1cc2</chem>	<chem>O=C1OCc2ccc1cc2</chem>	<chem>c:c(:c)CCCCc(:c):c</chem>
<chem>c:c:c(CCCc(:c):c)c:c</chem>	<chem>O=C1OC(=O)c2cccc1c2</chem>	<chem>O=C1OCc2cccc1c2</chem>
<chem>CCOC(=O)SC(O)=O</chem>	<chem>CCCCOC(=O)SC</chem>	<chem>OCCCCOC(S)=O</chem>
<chem>CCOC(=O)SC(=O)OC</chem>	<chem>O=C1OCCCCO1</chem>	<chem>CCOC(=O)OCc(:c):c</chem>
<chem>COC(=O)OCc(:c):c:c</chem>	<chem>OC(=O)OCc1cccc1</chem>	<chem>CCCC1=NCCO1</chem>
<chem>CC(C)CC1=NCCO1</chem>	<chem>CCCC1=NCCO1</chem>	<chem>COC(=NC)c1cccc1</chem>
<chem>CC(F)(F)C(F)(F)C1=NCCCO1</chem>	<chem>Cc1ccc([SiH3])cc1</chem>	<chem>c:c:c(:c:c)[Si]1(CCC1)c(:c):c:c</chem>
<chem>C[Si]1(C)O[SiH2]O[Si](C)(C)O[Si](C)(C)O1</chem>	<chem>C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O1</chem>	<chem>C[Si]1(C)O[Si](C)(O[Si](C)(O1)c(:c):c)c(:c):c</chem>
<chem>C[Si](O[SiH3])(O[SiH3])c1cccc1</chem>	<chem>C[Si]1(C)O[SiH2]O[Si](C)(O[Si](C)(O1)c(:c):c)c(:c):c</chem>	<chem>C[Si](C)(C)O[Si]1(C)O[Si](C)(C)O[SiH2]O[Si](C)(C)O1</chem>
<chem>C[Si]1(C)O[SiH2]O[Si](C)(O[SiH3])O[Si](C)(C)O1</chem>	<chem>C[Si]1(C)O[SiH2]O[Si](C)(O[Si](C)(C)O1</chem>	<chem>CC[Si]1(C)O[SiH2]O[Si](C)(C)O[Si](C)(C)O1</chem>
<chem>CCC[Si]1(C)O[Si](C)(C)O[SiH2]O[Si](C)(C)O1</chem>	<chem>[SiH3]CCc1cccc1</chem>	<chem>C[Si]1(C)O[SiH2]O[Si](C)(O[Si](C)(C)O1)c(:c):c</chem>

C[Si]1(C)O[SiH2]O[Si](C)(C)O[Si](C)(O1)c(:c):c:c	c:c:c(:c:c)[Si]1(c(:c):c:c)[Si](c(:c):c)(c(:c):c)[Si](c(:c):c)(c(:c):c)[Si]1(c(:c):c)c(:c):	:c:c
CCC[Si]1(C)O[Si](C)(C)O[Si](C)(CC)O1	CC[Si]1(C)O[Si](C)(C)O[Si](C)(CC)O1	CCC[Si]1(CCC)C[Si](CC)(CC)C1
CC(C)(c(:c):c)c1ccc(O)cc1	CC(C)(C)c1ccc(OS)cc1	Cc1ccc(OS(C)(=O)=O)cc1
c:c(:c)S(=O)(=O)Oc1cccc1	c:c:c(OS(=O)(=O)c(:c):c):c:c:c:c	Sc1cccc(c1)S(=O)(=O)Oc(:c):c
COS(=O)(=O)c1cccc(S)c1	OS(=O)(=O)c1cccc(S)c1	O=S1(=O)CCCCC1
CCCC1(CCC)CS(=O)(=O)C1	CCc1ccc(CC)c(C)c1	CCc1ccc(C)c(C)c1
Cc1cccc(CCc(:c):c)c1	Cc(:c):c(CCc(:c):c):c:c	Cc1cccc1CCc(:c):c
CCc1ccc(C)cc1C	CCc1ccc(CC)c(CC)c1	CCc1ccc(C)c(CC)c1
CCc1cccc1CCc(:c):c	CCc1ccc(C)cc1CC	CCc1ccc(CC)c(Cl)c1
CCc1ccc(C)c(Cl)c1	Clc1cccc(CCc(:c):c)c1	Clc(:c):c(CCc(:c):c):c:c
Clc1cccc1CCc(:c):c	CCc1ccc(C)cc1Cl	CCc1ccc(CC)c(Br)c1
CCc1ccc(C)c(Br)c1	Brc1cccc(CCc(:c):c)c1	Brc(:c):c(CCc(:c):c):c:c
Brc1cccc1CCc(:c):c	CCc1ccc(C)cc1Br	FC(F)(c(:c):c)C(F)(F)c1cccc1
Cc1ccc(cc1)C(F)(F)C(C)(F)F	CC(F)(F)c1ccc(cc1)C(C)(F)F	FC(F)(c(:c):c):c:c)C(F)(F)c(:c):c):c:c
CCCC12CC34CC3(CC(C4)C1)C2	CCC12CC34CC3(CC(C4)C1)C2	COC(=O)C1=C(C2C=CC1C=C2)C(=O)OC
CC1=C(C)C2C=CC1C=C2	CC1(C)C2CC(C=C2)C1(F)F	FC(F)(F)C1=C(C2C=CC1C=C2)C(F)(F)F
CC1=C(C)C2C=CC1C1C=CC21	C1=CC2C1C1C=CC2C=C1	COC(=O)C1CC2CC1C=C2
CC(F)(F)OC1(F)C2CC(C=C2)C1(F)F	OC1(F)C2CC(C=C2)C1(F)F	COc1ccc(cc1)-c(:c):c
Oc1ccc(cc1)-c(:c):c:c	c:c(:c)-c1ccc(cc1)C#N	Cc1ccc(cc1)C#N
COC(=O)C1C2CC(C=C2)C1C(O)=O	CC1C(C)C2CC1C=C2	COC(=O)C1C2CC(C=C2)C1C(=O)OC
CCCC1(CC2CC1C=C2)C#N	C[Si](C)(O[SiH3])C1(CC2CC1C=C2)C#N	C[Si](C)(C)CC1(CC2CC1C=C2)C#N
C[Si](C)(O)CC1(CC2CC1C=C2)C#N	C[Si](C)(C)[Si](C)(C)C1(CC2CC1C=C2)C#N	[SiH3]OCC1CC2CC1C=C2
CN(C)CC1CC2CC1C=C2	CCN1C(=O)c2cccc2C1=O	CCCC(C)C=CC
CCCCC(C)C=C	CCCCC(C)C	CCCC=CC(C)C
CCCC=CC(C)CC	CCCC(C)C=CCC	CC1CCC2CC=CC12

CC1CCCC1C1CCC=CC1	c:c(:c)C1CC(=O)NCCO1	c:c:c(:c:c)C1CC(=O)NCC(O1) c(:c):c
c:c:c(:c:c)C1CNCCC(O1)c(:c):c :c	CC1CC(=O)NCC(O1)c(:c:c):c c	c:c(:c)C1CNC(=O)CCO1
COC(CN)c1cccc1	CCC(OC)c1cccc1	COCC1(CCl)COC1
CC1(C)COC(C)(C)OC1	C1CCCCCCC1	CCCC1OC1CC
c:c(:o)C1CO1	C1COCCOC1	OC1(O)CCOC(=O)CC1
C1COC2(CCCOCC2)O1	CC1CC(=O)OCCO1	CC1CCOCCO1
CCN1C(=O)C2C3CC(C=C3)C 2C1=O	CN1C(=O)C2C3CC(C=C3)C2 C1=O	CC1CCC2C1C(=O)N(CC1CO1) C2=O
CN(C)CC1CO1	CCCN1C(=O)C2CCC(C)C2C1 =O	CN(C)c1ccc(cc1)C(O)=O
Cc1ccc(cc1)N1C(=O)CCC1=O	CC1CCC2C1C(=O)N(c(:c:c):c :c)C2=O	c:c(:c)N1C(=O)C2C3CC(C=C 3)C2C1=O
COCC1(C)COC1	COCC1OC1CO	COCC1OC1COC
CCC1(COC)COC1	CC(C)OP1(=O)OCCO1	CCOP1(=O)OCCO1
CCC1(COC1=O)c(:c:c):c:c	CCCc1cc(OC)ccc1OC	CCc1cc(OC(C)=O)ccc1O
CCc1cccc1OC(=O)c(:c):c	CCCc1cc(O)ccc1OC(C)=O	CCc1cc(O)ccc1OC(C)=O
CCCOC(=O)C=CC	CCCCOC(=O)C=C	CCOC(=O)C=CC(O)=O
COC(=O)C=CC(=O)OC	CC(O)C1CC(=O)O1	C1CC(O1)C1CCC=CO1
O=C1CC(O1)C1CO1	C1OC1C1CCO1	CC1CCC(=O)O1
CCC1CCC(=O)O1	CC1CCOC(=O)C1	CCOC(=O)CC=CC
CCC=CCC(=O)OC	OC(=O)CC=CCC(O)=O	CCCOC(=O)CC=C
CC1NC(=O)C(C)OC1=O	CC=C1C(=C)COCCOC1=O	C=C1CCOCCOC1=O
CC(N)=C1C(=C)COCCOC1=O	CC1=CCCC(N2CCCC2)=C1C (O)=O	CC1=CCCC=C1C(O)=O
CCC(N1CCCC1)=C(C)C	COCc1cccc1	COC(=O)C1CC(=O)O1
COC(=O)C1CCCOCC1	OC(=O)C1CCOC(=O)CC1	CCCC1(C)CC(=O)N1
CC1CCCNCC1	c:c(:c)C1CC(=O)N1	C1CC(N1)c1cccc1
CC1(C)C(NC1=O)c(:c:c):c:c	CC1(C)CNC1c1cccc1	ClC1(Cl)CCCCNC1=O
ClC1(Cl)CCCCNC1	COC(=O)C1CC(=O)N1	NC(=O)CC1NC(=O)OC1=O
C1CCOCNC1	CCCNC(=O)OCC	CCCCNC(=O)OC
CCCCNC(O)=O	NCCCCCO	CCCCOC(N)=O
CCCCOC(=O)NC	CCCOC(=O)NCC	O=C1CCC(=O)N1c1cccc1
CN(C)c1cccc1C	CC1CCC2C1C(=O)N(c(:c:c):c (C):c)C2=O	Cc1cccc(N)c1

<chem>CN(C)c1cc(C)cc(c1)C(F)(F)F</chem>	<chem>Cc1cc(cc(c1)C(F)(F)F)N1C(=O)CCC1=O</chem>	<chem>ClC12OC(=O)OC1(Cl)C1CC2C=C1</chem>
<chem>OC1(Cl)C2CC(C=C2)C1(O)Cl</chem>	<chem>CCCCOC(=O)OC</chem>	<chem>CCCCCOC(O)=O</chem>
<chem>COC(=O)C1(C)COC(=O)OC1</chem>	<chem>CC1(COC(=O)OC1)C(O)=O</chem>	<chem>COCC1=NCCO1</chem>
<chem>CSc1ccc(O)cc1</chem>	<chem>CCOc1ccc(S)cc1</chem>	<chem>[SiH3]CCN1CC1</chem>
<chem>NC(=O)Cn1c(:c:c)c(:c)c2cccc12</chem>	<chem>c:c1cccc1:[nH2]</chem>	<chem>c:c1c[nH]c2cccc12</chem>
<chem>CCn1c(:c)c(:c:c)c2cccc12</chem>	<chem>Cn1c2cccc2c2cccc12</chem>	<chem>NCC(=O)N1CC1</chem>
<chem>CCCN1[Si](C)(C)C[Si]1(C)C</chem>	<chem>CC(C)(C)C(=O)N1CC1</chem>	<chem>O=C(N1CC1)C12CC3CC(CC(C3)C1)C2</chem>
<chem>NC(=O)C12CC3CC(CC(C3)C1)C2</chem>	<chem>CC12CC3CC(CC(C3)C1)C2</chem>	<chem>NC(=O)CC12CC3CC(CC(C3)C1)C2</chem>
<chem>CCC12CC3CC(CC(C3)C1)C2</chem>	<chem>CCC(=O)N1CC1</chem>	<chem>COc1ccc(cc1)C(O)=N</chem>
<chem>Oc1ccc(cc1)C1=NCCO1</chem>	<chem>c:c:c1OCN(Cc1:c)c(:c):c</chem>	<chem>CN1COc2cccc2C1</chem>
<chem>C1NCc2cccc2O1</chem>	<chem>NCc1cccc1O</chem>	<chem>c:c:c(:c:c)N1COc(:c)c(C1):c:c</chem>
<chem>c:c:c(:c:c)N1COC(=C)C(=C)C1</chem>	<chem>CCN(CO)c1cccc1</chem>	<chem>Cc1ccc2OCNCc2c1</chem>
<chem>COc1ccc(cc1C)C(C)(C)C</chem>	<chem>CCC(CC)(CC)c1ccc(O)c(C)c1</chem>	<chem>CCC(CC)(CC)c1ccc(O)c(CN)c1</chem>
<chem>CN1COc2ccc(C)cc2C1</chem>	<chem>c:c:c(:c:c)C12CC3CC(CC(C3)C1)C2</chem>	<chem>c:c(:c)C12CC3CC(CC(C3)C1)C2</chem>
<chem>CN1COC(=C)C(=C)C1</chem>	<chem>CN1COc(:c:c)c(:c)c1</chem>	<chem>C[Si]1(C)O[SiH2]O[Si](C)(CC)O[Si](C)(C)O1</chem>
<chem>C[Si]1(C)O[SiH2]O[Si](C)(C)O[Si](C)(CC)O1</chem>	<chem>[SiH3]CCc1ccc(Cl)cc1</chem>	<chem>CCc1ccc(Cl)cc1</chem>
<chem>c:c(:c)[Si]1(CCC1)c1cccc1</chem>	<chem>c:c:c(:c:c)[Si]1(C[Si](C1)(c(:c):c)c(:c):c)c(:c):c:c</chem>	<chem>c:c(:c)[Si]1(C[SiH2]C1)c1cccc1</chem>
<chem>C[Si]1(C)O[SiH2]O[Si](C)(O[Si](C)(O1)C=C)C=C</chem>	<chem>C[Si]1(C[Si](C)(C1)c(:c:c):c:c)c(:c):c</chem>	<chem>C[Si]1(C[SiH2]C1)c1cccc1</chem>
<chem>C[Si]1(C)O[Si](C)(C)[Si](C)(C)O[Si]1(C)C</chem>	<chem>C[Si]1(C)Cc2cccc12</chem>	<chem>C[Si]1(C)Cc(:c)c(C1):c:c</chem>
<chem>C[Si]1(CCC=CC1)c(:c:c):c:c</chem>	<chem>CC[Si](C)(CC)c1cccc1</chem>	<chem>CC1=CC[Si](C)(C)C1</chem>
<chem>CCC[Si]1(CCC)C#C[Si](C)(C)[SiH2]C#C[Si]1(CC)CC</chem>	<chem>CC[Si]1(CC)C#C[Si](CC)(CC)[Si](C)(C)C#C[Si]1(C)C</chem>	<chem>CCC[Si]1(CCC)C#C[SiH2][SiH2]C#C[Si]1(CCC)CCC</chem>
<chem>C[Si]1(C)[SiH2]C#C[Si](C)(c(:c):c)[Si](C)(C#C1)c(:c):c:c</chem>	<chem>C[Si]1(C)C#C[Si](C)(C)[Si](C)(C#C[Si]1(C)c(:c):c)c(:c):c</chem>	<chem>C[Si](C)(C)[Si](C)(C#C)c1cccc1</chem>

<chem>C[Si]1(C#C[SiH2][SiH2]C#C[Si]1(C)c(:c:c):c:c)c(:c:c):c:c</chem>	<chem>CCC1C[Si](C)(C)C1</chem>	<chem>CC(C)Cc1cccc(:c)c1:c:c</chem>
<chem>CCC1=CC=CC(=C)C1=C</chem>	<chem>Cc1cccc(:c:c)c1:c</chem>	<chem>Cc1cccc2cccc12</chem>
<chem>Cc(:c):c1cccc1:c</chem>	<chem>CC(C)Cc1ccc(C)cc1</chem>	<chem>CCc1ccc(cc1)-c(:c):c</chem>
<chem>c:c:c(:c:c)-c1cccc1</chem>	<chem>C[Si]1(C)CC(C1)c(:c):c</chem>	<chem>c:c:c1c(cccc1:c)C1C[SiH2]C1</chem>
<chem>CC(C)C1=CC=CC(=C)C1=C</chem>	<chem>C[Si](C)(C)O[Si]1(C)CC[Si](C)(C)O1</chem>	<chem>C[Si]1(C)CC[Si](C)(O[SiH3])O1</chem>
<chem>C[Si](C)(C[SiH3])c1cccc1</chem>	<chem>C[Si](C)(C)C[Si]1(C[Si](C)(C)C)CCC1</chem>	<chem>C[Si](C)(C)C[Si]1(C)CCC1</chem>
<chem>CCC[Si]1(C)CCC1</chem>	<chem>CC(C)[Si]1(CCC1)c(:c):c</chem>	<chem>c:c(:c)[Si]1(CCC1)C1CCCC1</chem>
<chem>CC(C)[Si]1(CCC1)c1cccc(:c)c1:c:c</chem>	<chem>C[Si](C)(C)C1=CC=CC(=C)C1=C</chem>	<chem>[SiH3]c1cccc(:c:c)c1:c</chem>
<chem>[SiH3]c1cccc2cccc12</chem>	<chem>[SiH3]c(:c):c1cccc1:c</chem>	<chem>CCCc1cc(CC)ccc1CC</chem>
<chem>CCCc1ccc(C)cc1CCC</chem>	<chem>CP1CCCS1</chem>	<chem>CP1CCCS1</chem>
<chem>CCP(SC)c1cccc1</chem>	<chem>Cc1cc(cc(c1)C1(CO)CO1)C(F)(F)F</chem>	<chem>Cc1cc(cc(c1)C1(C)CO1)C(F)(F)F</chem>
<chem>CC1=CCC(C)(C)CC1</chem>	<chem>[SiH3]OCC1(CO[SiH3])COC1</chem>	<chem>CN(C)c1ccc([SiH3])cc1</chem>
<chem>C[Si]1(CCC1)c1ccc(N)cc1</chem>	<chem>C[Si]1(CCC1)c(:c:c):c:c</chem>	<chem>Nc1ccc(cc1)[Si]1(CCC1)c(:c):c</chem>
<chem>C[Si]1(CC=CC1)c(:c:c):c:c</chem>	<chem>CCC[Si]1(CC=CC1)c(:c:c):c:c</chem>	<chem>CC[Si]1(CC=CC1)c1cccc1</chem>
<chem>COC(=O)N1CCOCC1</chem>	<chem>OC(=O)N1CCOC(=O)CC1</chem>	<chem>CN1CCOC(=O)CC1</chem>
<chem>O=C1CCNCCO1</chem>	<chem>SCCC1NC(=O)OC1=O</chem>	<chem>CN(C)Cc1cccc1</chem>
<chem>CCN1CCCOC1=S</chem>	<chem>CN1[Si](C)(C)N(C)[Si]1(C)C=C</chem>	<chem>CCC(CC)[Si]1(C)C[Si](C)(C1)C(C)C</chem>
<chem>C[Si]1(C[SiH2]C1)C1CCCC1</chem>	<chem>CCC(CC)[Si]1(Cl)C[Si](Cl)(C1)C(C)C</chem>	<chem>Cl[Si]1(C[SiH2]C1)C1CCCC1</chem>
<chem>C[Si]1(Cc2cccc12)c(:c:c):c:c</chem>	<chem>C[Si]1(Cc2cccc12)c(:c):c</chem>	<chem>C[Si]1(Ccc1:c)c1cccc1</chem>
<chem>c:c(:c)[Si]1(Cc2cccc12)c(:c):c</chem>	<chem>c:c(:c)[Si]1(Ccc1:c)c1cccc1</chem>	<chem>COc1ccc(cc1)C#N</chem>
<chem>Oc1ccc(cc1)C#N</chem>	<chem>C[Si](C)(C)O[Si]1(C)CCC1</chem>	<chem>CC(=O)Oc1ccc(C)cc1</chem>
<chem>C1[SiH2]CC1c1cccc1</chem>	<chem>Cc1cccc([SiH3])c1</chem>	<chem>CCc1ccc(C(C)C)c(C)c1</chem>
<chem>Cc1ccc2C3C=CC(C=C3)c2c1</chem>	<chem>C1=CC2C=CC1c1cccc21</chem>	<chem>C=C1C2C=CC(C=C2)C1=C</chem>
<chem>CCCc1ccc(C)c(c1)C(C)C</chem>	<chem>S1N=S=NSN=S=N1</chem>	

Walk 4 Descriptors

<chem>O=C1C2C3CC(C=C3)C2C(=O)N1CC1CO1</chem>	<chem>CC1(C)OCC2(COC2)CO1</chem>
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<chem>CC(F)(F)CCC1=NCCO1</chem>	<chem>O=C1OCCOC(=O)C2=C(CCCC=C12)N1CCCC1</chem>
<chem>CCOCC1CO1</chem>	<chem>CC(C)C1=NCCO1</chem>
<chem>C1CSP(C1)c1cccc1</chem>	<chem>CCCCc1cc(CC)ccc1CCc(:c):c</chem>
<chem>CCN1C(C2CCCC2)C(=O)N(C)C1=O</chem>	<chem>CCCCC1=NCCO1</chem>
<chem>CCCCC1CO1</chem>	<chem>c:c(:c)N1COc2cccc2C1</chem>
<chem>c:c(:c)C1=NCCCO1</chem>	<chem>c:c(:c)C1=NCCO1</chem>
<chem>CCCCCCCC=CC</chem>	<chem>CCCCC=CCCC</chem>
<chem>CCCCCCCC=C</chem>	<chem>c:c(:c)OCC1(COc(:c):c)COC1</chem>
<chem>CCCCC=CCCC</chem>	<chem>CCCCCNC(=O)CC</chem>
<chem>CCCCCNC(=O)c(:c):c</chem>	<chem>C1CCCCNCCC1</chem>
<chem>CCCCCCCCOC</chem>	<chem>CCCCCCCCC</chem>
<chem>CCOC(=O)C1C2CC(C=C2)C1C(=O)OC</chem>	<chem>CCCC(C)C=CCCC</chem>
<chem>COCCCCCCCO</chem>	<chem>C1CCCCC=CCCC1</chem>
<chem>CCCCCCC=CCC</chem>	<chem>COc1ccc(cc1)C(C)=C</chem>
<chem>COc1ccc(cc1)C1=CCCC1</chem>	<chem>C1CC=C(C1)c1cccc1</chem>
<chem>CC(=C)c1ccc(Cl)cc1</chem>	<chem>Clc1ccc(cc1)C1=CCCC1</chem>
<chem>CCC1OC(CC#N)OC(CC#N)O1</chem>	<chem>c:c(:c(:c)c)C1CO1</chem>
<chem>C1OC1c1cccc1</chem>	<chem>C(Oc1cccc1)C1CO1</chem>
<chem>c:c(:c)OCC1CO1</chem>	<chem>CCOc1ccc(C)cc1</chem>
<chem>Cc1ccc(OCC2CO2)cc1</chem>	<chem>CCOc1cccc1C</chem>
<chem>Cc1cccc1OCC1CO1</chem>	<chem>COc1cccc(C)c1</chem>
<chem>CCOc1cccc(C)c1</chem>	<chem>Cc1cccc(OCC2CO2)c1</chem>
<chem>CCOc1cccc1Cl</chem>	<chem>Clc1cccc1OCC1CO1</chem>
<chem>COc1ccc(Cl)cc1</chem>	<chem>CCOc1ccc(Cl)cc1</chem>
<chem>Clc1ccc(OCC2CO2)cc1</chem>	<chem>COc1c(Cl)cc(Cl)cc1Cl</chem>
<chem>CCOc1c(Cl)cc(Cl)cc1Cl</chem>	<chem>Clc1cc(Cl)c(OCC2CO2)c(Cl)c1</chem>
<chem>C(Oc1cccc2cccc12)C1CO1</chem>	<chem>CCOc1cccc2cccc12</chem>
<chem>COc1cccc2cccc12</chem>	<chem>C(Oc1ccc2cccc2c1)C1CO1</chem>
<chem>CCOc1ccc2cccc2c1</chem>	<chem>COc1ccc2cccc2c1</chem>
<chem>CCOc1cccc1C(C)C</chem>	<chem>CC(C)c1cccc1OCC1CO1</chem>
<chem>CC(C)OCC1(CO1)c1cccc1</chem>	<chem>COCC1(CO1)c1cccc1</chem>
<chem>COc1cccc(c1)C(F)(F)F</chem>	<chem>CCOc1cccc(c1)C(F)(F)F</chem>
<chem>FC(F)(F)c1cccc(OCC2CO2)c1</chem>	<chem>CC(C)OCC1(CO1)c1cccc(C)c1</chem>
<chem>COCC1(CO1)c1cccc(c1)C(F)(F)F</chem>	<chem>OCC1(CO1)c1cccc(c1)C(F)(F)F</chem>
<chem>CC1(CO1)c1cccc(c1)C(F)(F)F</chem>	<chem>CC1(CO1)c1c(F)c(F)c(F)c(F)c1F</chem>
<chem>OCC1(CO1)c1c(F)c(F)c(F)c(F)c1F</chem>	<chem>COCC1(CO1)c1c(F)c(F)c(F)c(F)c1F</chem>

CC(C)OCC1(CO1)c1c(F)c(F)cc(F)c1F	CCOCC1(COCC)COC1
C1CCCCOCCC1	C1CCCCOCCC1
CCCCCCCCCO	CCCCCCCCOCC
CCCCCOCCC	CCCCOCCCC
CC1CCC2(COC2)CC1	C1COc2ccc(OC1)cc2
C1CCCOCOC1	COCCCCCOC
CCOCCCCCO	CCCOCCCCO
CCCOCCCCOC	CCOCCCCOCC
CCCOCCCCCO	CCOCCCCCOC
CCCCCC(=O)OCCO	CCCCCC(=O)OCC
CCCCCCCC(=O)OC	CCCCCCCC(O)=O
CCCCC(=O)OCCOC	CCCC(=O)OCCOCC
CCC(=O)OCCOCCO	COCCOCCOC(C)=O
CCOCCOCCOC	OCCOCCOCCO
COCCOC(=O)c1cccc(C)c1	CCOCCOC(=O)c(:c:c):c:c
OCCOCCOC(=O)c(:c):c	OCCOC(=O)c1cccc(c1)C(O)=O
CCOC(=O)c1cccc(c1)C(O)=O	COC(=O)c1cccc(c1)C(O)=O
CCOC(=O)c1cccc(c1)C(=O)OC	COCCOC(=O)c1cccc1
CC(=O)OCCOC(=O)c(:c:c):c:c	c:c(:c)C(=O)OCCOC(=O)c(:c):c
OCCOC(=O)c1ccc(O)cc1	CCOC(=O)c1ccc(OC)cc1
COC(=O)c1ccc(OC(:c):c)cc1	OC(=O)c1ccc(OC(:c):c):c:c)cc1
Cc1ccc(OC2CCCC2)cc1	CCOc1ccc(cc1)C(=O)OC
OCCOc1ccc(cc1)C(O)=O	COCCOc1ccc(C)cc1
c:c(:c)OCCOc1cccc1	c:c:c(OCCOc(:c):c):c:c
COCCOC(=O)c1cccc(O)c1	COc1cccc(c1)C(=O)OCCO
CCOC(=O)c1cccc(OC)c1	COC(=O)c1cccc(OC)c1
CCOc1cccc(c1)C(O)=O	OCCOc1cccc(c1)C(O)=O
COCCOc1cccc(c1)C(O)=O	Cc1cccc(OCCOc(:c):c)c1
CCOC(=O)c1cccc(OCC)c1	COC(=O)c1cccc(OCCO)c1
CCCOc1ccc(cc1)C(O)=O	Cc1ccc(OCCCO)cc1
COCCCOc1cccc1	c:c:c(OCCCOc(:c):c):c:c
CCCCOc1ccc(C)cc1	CCCCOc1cccc1
OCCCCCOc(:c:c):c:c	COCCCCCOc(:c):c
CCCCOC(=O)c1cccc1	CCCCOC(=O)c(:c:c):c:c
CCCCCOC(=O)c(:c):c	CC(=O)OCCCCCO
CCCOc(=O)c1ccc(O)cc1	O=C1CCC2CCC(CCC(=O)O1)O2
O=C1CCC2CCC(CCCO1)O2	CCC1CCC(CCC(O)=O)O1

CCCC1CCC(CCC)O1	CC1CCC(=O)OC(=O)CCCO1
c:c:c1OCC(=O)OC(=O)COcc1	O=C1COc2cccc(OCC(=O)O1)c2
O=C1COc2cccc(OCCO1)c2	COc1cccc(OCC(O)=O)c1
CCOc1cccc(OC)c1	C=C1OCC(=O)OC(=O)COC=C1
OCC(=O)OC(=O)COc(:c:c):c:c	CC(=O)OC(=O)COc1cccc1
COC(=O)COc1ccc(O)cc1	COc1ccc(OCC(O)=O)cc1
CCOc1ccc(OCC)cc1	COCC(=O)OC(=O)COc(:c):c
c:c:c(:c:c)C(=O)OC(=O)c1cccc1	Oc1ccc(cc1)C(=O)OC(=O)c(:c):c
COc1ccc(cc1)C(=O)OC(C)=O	COC(=O)c1ccc(OCO)cc1
COCOc1ccc(cc1)C(O)=O	Cc1ccc(OCOc(:c):c)cc1
c:c:c(OCOc1cccc1):c:c	Oc1cccc(c1)C(=O)OC(=O)c(:c:c):c:c
COc1cccc(c1)C(=O)OC(=O)c(:c):c	COc1cccc(c1)C(=O)OC(C)=O
CCOc1cccc(c1)C(=O)OC(C)=O	CCOCCOc1cccc1
OCCOCCOc(:c:c):c:c	COCCOCCOc(:c):c
CCOc1ccc(cc1OC)C(=O)OC	CCOC(=O)c1ccc(OC)c(OC)c1
CCCOc1ccc(cc1OC)C(O)=O	CCCCOc1ccc(C)cc1OC
COc1cccc1OCCCCO	COCCCCOc(:c:c):c(O):c
c:c(:c)OCCCCOc(:c):c	COc1cc(ccc1O)C(=O)OCCO
O=C1OCCOCCOC1=O	O=C1COCCOCCO1
O=C1CC(=O)OCCOCCO1	O=C1CCOCCOCCO1
CC1C(=O)OCCOCCOC1=O	CC1COCCOCCOC1=O
CCCCC1C(=O)OCCOCCOC1=O	CCCCC1C(=O)OCCOCCOC1=O
CCC1C(=O)OCCOCCOC1=O	COC(=O)CCC(=O)OCCO
CCOC(=O)CCC(=O)OCC	COCCOC(=O)CCC(O)=O
OCCOC(=O)CCCC(O)=O	CCOC(=O)CCCC(=O)OC
CCOC(=O)CCCCC(O)=O	COC(=O)CCCCC(=O)OC
COC(=O)CCCCCC(O)=O	OC(=O)CCCCCCC(O)=O
OCCCCOC(=O)c1cccc1	COCCCCOC(=O)c(:c:c):c:c
CC(=O)OCCCCOC(=O)c(:c):c	OCCCCOC(=O)c(:c:c):c:c
COCCCCOC(=O)c(:c):c	CC(=O)OCCCCOC(C)=O
CCCCCCCOC(C)=O	CCCOC(=O)COCC(O)=O
CCOC(=O)COCC(=O)OC	CCCCOC(=O)COCC
CCCCCOC(=O)COC	CCCCCOC(=O)CO
CCOC(=O)CC(=O)OCCO	COCCOC(=O)CC(=O)OC
CCOCCOC(=O)CC(O)=O	CCOC(=O)C(=O)OCCOC
CCOCCOC(=O)C(=O)OC	OCCOCCOC(=O)C(O)=O
OCCOC(=O)C(=O)OCCO	Cc1ccc(cc1)C(=O)OCCO

CCOC(=O)c1ccc(cc1)C(O)=O	COC(=O)c1ccc(cc1)C(=O)OC
CCOC(=O)c1ccc(CO)cc1	COc1ccc(cc1)C(=O)OC
CCOCc1ccc(cc1)C(O)=O	Cc1ccc(COCCO)cc1
COCCOCc1cccc1	COCCOCc(:c:c):c:c
c:c(:c)COCCOCc(:c):c	O=C1COCC(=O)OCCO1
OCCOC(=O)CCCCS	CCOC(=O)CCCCS(C)(=O)=O
CCS(=O)(=O)CCCC(=O)OC	CCCS(=O)(=O)CCCC(O)=O
CCCCCS(=O)(=O)CCCC	CCOC(=O)CCCCSC
CCSCCCCC(=O)OC	CCSCCCCC(O)=O
CCCCSCCCC	CCOC(=O)c1ccc(CC)cc1
CCCc1ccc(cc1)C(=O)OC	OC(=O)c1ccc(CCc(:c):c)cc1
Cc1ccc(CCc(:c):c:c)cc1	C(Cc1cccc1)c1cccc1
COC(=O)c1ccc(Cc(:c):c)cc1	OC(=O)c1ccc(Cc(:c):c:c)cc1
Cc1ccc(Cc2cccc2)cc1	OCCOC(=O)COCC(O)=O
COCC(=O)OCCOC	COCCOC(=O)COC
OCCOCCOC(=O)CO	OCCCCOC(=O)CO
COCCCCCOC(C)=O	O=C1COCC(=O)OCCCO1
O=C1COCCOCCCO1	CC1CCOC(=O)COCC(=O)O1
CC1CCOC(=O)COCCO1	CC1CCOCCOCC(=O)O1
CCCCCCCC(O)O	CCCCCCCC(OC)OC
CCCCCCC1OCCCO1	CCCCC1OCC(C)(C)CO1
CCCCC1OCC(CO)(CO)CO1	CCCC1OCC2(COCOC2)CO1
CCC1OCC2(COC(C)OC2)CO1	CCCC(=O)OCCOC(C)=O
CCC(=O)OCCOC(=O)CC	CCOc1c(C)cccc1C
Cc1cccc(C)c1OCC1CO1	[N-]=[N+]=NCC1CO1
COCC1CS1	C1CCCSSCCC1
C1CCCSCCSCC1	CCCCCCCCCS
CCCCCCCCSS	CCCCCCCCSSC
CCCCCSCC	CCCCSSCCC
CCCCSSCCC	CCCCCCCCSC
CCCCCCCCSCC	CCCCCSCCC
CCCCCCCCSSS	CCCCCSCSSS
CCCCSSSSC	CCCCSSSSCC
CCSSSSCCC	O=C1CSCCSCC(=O)O1
O=C1CSCCSCCO1	CCSCCC(=O)OC(=O)CC
CC(=O)OC(=O)CCSCC	COC(=O)CCSCCSC
CCSCCSCC(O)=O	CCSCCSCCC

CSCCC(=O)OC(=O)CCS	c:c:c(:c:c)C1CS1
C1SC1c1ccccc1	CCC(=O)OC(=O)CCSc(:c):c
CC(=O)OC(=O)CCSc(:c:c):c:c	COC(=O)CCSc1ccccc1
OC(=O)CCSc1ccc(S)cc1	CCCS1ccc(SC)cc1
CCSc1ccc(SCC)cc1	SCC(=O)OC(=O)CSCc(:c):c
CC(=O)OC(=O)CSCc(:c:c):c:c	COC(=O)CSCc1ccccc1
Cc1ccc(CSCC(O)=O)cc1	CCSc1ccc(CS)cc1
CSCc1ccc(CSC)cc1	CCSCC(=O)OC(=O)CSC
CC(=O)OC(=O)CCSCc(:c):c	COC(=O)CCSCc(:c:c):c:c
OC(=O)CCSCc1ccccc1	CCCS1ccc(C)cc1
OCCOC(=O)c1ccc(S)cc1	CCOC(=O)c1ccc(SC)cc1
COC(=O)c1ccc(Sc(:c):c)cc1	OC(=O)c1ccc(Sc(:c:c):c:c)cc1
Cc1ccc(Sc2ccccc2)cc1	Sc1ccc(cc1)C(=O)OC(=O)c(:c):c
CSc1ccc(cc1)C(=O)OC(C)=O	CCSc1ccc(cc1)C(=O)OC
CCCS1ccc(cc1)C(O)=O	CCCS1ccc(C)cc1
SCCCSc1ccccc1	CSCCCSc(:c:c):c:c
c:c(:c)SCCCSc(:c):c	OC(=O)c1ccc(SCCS)cc1
CSCCSc1ccc(C)cc1	c:c(:c)SCCSc1ccccc1
c:c:c(SCCSc(:c:c):c:c):c:c	O=C1CCc2ccc(CCC(=O)O1)s2
O=C1CCc2ccc(CCCO1)s2	CCc1ccc(CCC(O)=O)s1
CCCc1ccc(CCC)s1	c:c1CCC(=O)OC(=O)CCc1
CCCOC(=O)CCCCS	CCCCOC(=O)CCCC
CCCCOC(=O)CCC	CCCCCOC(=O)CC
CCCC(=O)OCCCO	CCCC(=O)OCCCO
CCC(=O)OCCOC(C)=O	CCC(=O)OCC(C)OC(=O)CC
CCCC(=O)OCC(C)OC(C)=O	CCCC(=O)OCC(C)OC
CC(O)COC(=O)CCCCS	CSCCCCC(=O)OC(C)C
CC(CO)OC(=O)CCCCS	CCCC(=O)OC(C)COC
CCCC(=O)OC(C)COC(C)=O	CCC(=O)OC(C)CCOC(C)=O
CCC(=O)OCCC(C)OC(C)=O	CCCC(=O)OCCC(C)OC
CCCC(=O)OCCC(C)O	CCC(C)OC(=O)CCCCS
CCCC(=O)OC(C)CCO	CCCC(=O)OC(C)CCOC
CCCCOC(=O)C(=O)OCC	CCCCOC(=O)C(=O)OC
CCCCCOC(=O)C(O)=O	CCOC(=O)C(=O)OCCC
O=C1CCCCOCCO1	O=C1CCCCC(=O)OCCO1
CCCCC(=O)OCCC	O=C1OCCOCc2ccc1cc2
O=C1OCCOC(=O)c2ccc1cc2	O=C1OCCOCc2cccc1c2

c:c:c1ccC(=O)OCCOC1=O	c:c1cc(:c)C(=O)OCCOC1=O
O=C1OCCOC(=O)c2cccc1c2	OCCCCCOC(=O)c(:c):c
CCCOC(=O)c1ccc(C)cc1	COCCOC(=O)c1cccc(:c)c1
OCCOC(=O)c1ccc(:c)c(:c:c)c1	CCOC(=O)c1ccc2cccc2c1
COC(=O)c1ccc2cc(C)ccc2c1	OC(=O)c1ccc2cc(ccc2c1)C(O)=O
CCCOC(=O)CCC(=O)OC	CCCCOC(=O)CCC(O)=O
CCC(=O)OCCCCCO	CCCCC(=O)OCC=C
CCCCC(=O)OCC=CC	CCCC(=O)OCC=CCO
CCC(=O)OCC=CCOC	CC(=O)OCC=CCOC(C)=O
CCCCC(=O)OCC#C	CCCCC(=O)OCC#CC
CCCC(=O)OCC#CCO	CCC(=O)OCC#CCOC
CC(=O)OCC#CCOC(C)=O	O=C1OCCOC(=O)c2cccc12
c:c:c1C(=O)OCCOC(=O)c1:c	C=C1C(=C)C(=O)OCCOC1=O
OC(=O)c1cccc1C(O)=O	O=C1Oc2cccc(OCc3cccc1c3)c2
c:c:c1ccCOc2cccc(OC1=O)c2	COc1cccc(OC(=O)c(:c):c)c1
COc1cccc(OC(C)=O)c1	c:c:c1OC(=O)c2cccc(c2)C(=O)Occ1
OC(=O)c1cccc(c1)C(=O)Oc(:c):c	C=C1OC(=O)c2cccc(c2)C(=O)OC=C1
C=C1C=CC(=O)Oc2cccc(OC1=O)c2	O=C1CCCCCCCCO1
O=C1CCCCCCCCO1	CCCCOC(=O)c1cccc(C)c1
CCCOC(=O)c1cccc(c1)C(O)=O	COCC(C)C(C)COC(=O)c(:c):c
CC(CO)C(C)COC(=O)c(:c:c):c:c	CC(C)C(C)COC(=O)c1cccc1
CC(C)COC(=O)c1ccc(C)cc1	CC(COC(C)=O)C(C)COC(C)=O
CCC(COC)C(CC)COC(=O)c(:c):c	CCC(CO)C(CC)COC(=O)c(:c:c):c:c
CCC(COC(=O)c1cccc1)C(C)C	CCC(COC(C)=O)C(CC)COC(C)=O
CCCC(COC)C(CCC)COC(=O)c(:c):c	CCCC(COC(=O)c(:c:c):c:c)C(CC)CO
CCCC(COC(C)=O)C(CCC)COC(C)=O	CCCC(COC(=O)c(:c):c)C(CCC)COC
CCCC(COC(C)=O)C(CCCC)COC(C)=O	COCC(C(C)C)C(COC(=O)c(:c):c)C(C)C
CC(C)C(CO)C(COC(=O)c(:c:c):c:c)C(C)C	CC(C)C(COC(=O)c1cccc1)C(C)C
CC(C)C(COC(C)=O)C(COC(C)=O)C(C)C	CC(=O)Oc1ccc(OC(C)=O)c(C)c1
COc1ccc(OC(=O)c(:c):c)cc1C	Cc1cc(OC(=O)c(:c:c):c:c)ccc1O
Cc1cccc(OC(=O)c2cccc2)c1	Cc1ccc(cc1)C(=O)Oc(:c):c:c
c:c(:c)OC(=O)c1ccc(cc1)-c(:c):c	COC(=O)c1ccc(cc1)-c(:c:c):c:c
OC(=O)c1ccc(cc1)-c1cccc1	Cc1ccc(cc1)-c1ccc(C)cc1
Cc(:c):c(OC(=O)c1ccc(C)cc1):c:c	Cc1cccc1OC(=O)c1cccc1
Cc1cc(O)ccc1OC(=O)c(:c:c):c:c	COc1ccc(OC(=O)c(:c):c)c(C)c1
O=C1OCCCCCOC1=O	O=C1COCCCCCOC1
C1CCCOCOC1	OCCCCCCCCO

CCCCC(=O)Oc(:c:c):c:c	OC(=O)CCCCC(=O)Oc(:c):c
CCCCC(=O)Oc1ccccc1	CCCC(=O)Oc1ccc(O)cc1
CCC(=O)Oc1ccc(OC)cc1	CC(=O)Oc1ccc(OC(C)=O)cc1
COc(=O)CCC(C)CC(=O)OC	CCOC(=O)CCC(C)CC(O)=O
CCCOC(=O)CCC(C)CC	CCCOC(=O)CCC(C)C
CCCCCOC(=O)CC(C)C	CCCOC(=O)CC(C)CC
CCCOC(=O)CC(C)CCC	CCOC(=O)CC(C)CCC(O)=O
CCCCC(=O)NCCC	CCNC(=O)CCCC(N)=O
CNC(=O)CCCCC(=O)NC	CCCCNC(=O)CCCC
CCCCCNC(=O)CCC	CC(=O)NCCCCC(O)=O
CNCCCCC(=O)OC	CCOC(=O)CCCCCN
CCCOC(=O)CC(=O)OCC	CCCOC(=O)CC(=O)OC
CCCCCOC(=O)CC(O)=O	CCCCC(=O)Nc(:c:c):c:c
CCCCCCC(=O)Nc(:c):c	CCCCCCC(=O)NC
CCCCCCCC(N)=O	CCCCC(=O)Nc1ccccc1
CCCC(=O)Nc1ccc(C)cc1	CCC(=O)Nc1ccc(cc1)C(O)=O
COc(=O)c1ccc(NC(C)=O)cc1	CCOC(=O)c1ccc(NC)cc1
Nc1ccc(cc1)C(=O)OCCO	OCCOC(=O)Cc1ccccc1
CCOC(=O)Cc1ccc(C)cc1	CCc1ccc(CC(=O)OC)cc1
OC(=O)Cc1ccc(CC(O)=O)cc1	COCCOC(=O)Cc(:c:c):c:c
CC(=O)OCCOC(=O)Cc(:c):c	CCCOC(=O)c1ccc(N)cc1
CCCOC(=O)CCCC(O)=O	CCCOC(=O)c1ccc(S)cc1
CCOC(=O)c1ccc(cc1)S(C)(=O)=O	CCS(=O)(=O)c1ccc(cc1)C(=O)OC
CCCS(=O)(=O)c1ccc(cc1)C(O)=O	CCCS(=O)(=O)c1ccc(C)cc1
CCCCCS(=O)(=O)c1ccccc1	CCCCCS(=O)(=O)c(:c:c):c:c
SCCCCCS(=O)(=O)c(:c):c	CS(=O)(=O)CCCCCS(C)(=O)=O
CCCOC(=O)c1ccccc1C(O)=O	CCCOC(=O)c(:c:c):c(C):c
CCCOC(=O)c1ccccc1C(=O)OC	CCOC(=O)c1ccccc1C(=O)OC
CCOC(=O)c1ccccc1C(=O)OCC	NC(=O)CCCCCCC(N)=O
COc(=O)c1ccc(cc1)S(=O)(=O)c(:c):c	OC(=O)c1ccc(cc1)S(=O)(=O)c(:c:c):c:c
Cc1ccc(cc1)S(=O)(=O)c1ccccc1	CCOC(=O)c1ccc(CS)cc1
COc(=O)c1ccc(CS(C)(=O)=O)cc1	CCS(=O)(=O)Cc1ccc(cc1)C(O)=O
Cc1ccc(CS(=O)(=O)Cc(:c):c)cc1	c:c:c(CS(=O)(=O)Cc1ccccc1):c:c
CCCCCNC(=O)c(:c:c):c:c	CCCCNC(=O)c1ccccc1
CCNC(=O)c1ccc(C)cc1	CCNC(=O)c1ccc(cc1)C(N)=O
CNC(=O)c1ccc(cc1)C(=O)NC	CCCOC(=O)CCCS(C)(=O)=O
CCOC(=O)CCCS(=O)(=O)CC	COc(=O)CCCS(=O)(=O)Cc(:c):c

<chem>OC(=O)CCCS(=O)(=O)Cc(:c:c):c:c</chem>	<chem>CCCCS(=O)(=O)Cc1ccccc1</chem>
<chem>CCCS(=O)(=O)Cc1ccc(C)cc1</chem>	<chem>CCS(=O)(=O)Cc1ccc(CS)cc1</chem>
<chem>CS(=O)(=O)Cc1ccc(CS(C)(=O)=O)cc1</chem>	<chem>CCCCOC(=O)CCCS</chem>
<chem>CCCCC1(CCCC)COC1=O</chem>	<chem>CC1CCSC(=O)CC1</chem>
<chem>CCCCCCC(=O)Oc(:c):c</chem>	<chem>CCCOC(=O)CCC(:c:c):c:c</chem>
<chem>CCOC(=O)CCc1ccccc1</chem>	<chem>COC(=O)CCc1ccc(C)cc1</chem>
<chem>CCc1ccc(CCC(O)=O)cc1</chem>	<chem>CCc1ccc(CCC)cc1</chem>
<chem>c:c(:c)CCOC(=O)CCc(:c):c</chem>	<chem>CCCC(=O)OCCc(:c:c):c:c</chem>
<chem>CCC(=O)OCCc1ccccc1</chem>	<chem>CC(=O)OCCc1ccc(C)cc1</chem>
<chem>CCc1ccc(CCOC)cc1</chem>	<chem>OCCc1ccc(CCO)cc1</chem>
<chem>c:c(:c)CCOC(=O)c1ccccc1</chem>	<chem>c:c:c(CCOC(=O)c(:c:c):c:c):c:c</chem>
<chem>c:c(:c)C(=O)OCCc1ccccc1</chem>	<chem>O=C1CC(=O)Oc2ccc(O1)cc2</chem>
<chem>O=C1CCOc2ccc(O1)cc2</chem>	<chem>c:c:c1OC(=O)CCC(=O)Occ1</chem>
<chem>c:c1OC(=O)CCC(=O)Oc(:c)c1</chem>	<chem>O=C1CCC(=O)Oc2cccc(O1)c2</chem>
<chem>O=C1CCCOc2ccc(O1)c2</chem>	<chem>O=C1CCC(=O)Oc2ccc(O1)cc2</chem>
<chem>O=C1CCCOc2ccc(O1)cc2</chem>	<chem>O=C(Oc1ccccc1)c1ccccc1</chem>
<chem>Oc1ccc(OC(=O)c(:c:c):c:c)cc1</chem>	<chem>COc1ccc(OC(=O)c(:c):c)cc1</chem>
<chem>OC(=O)c1ccc(cc1)C(=O)Oc(:c):c</chem>	<chem>CCN(CC)CCC(=O)Oc(:c:c):c:c</chem>
<chem>c:c(:c)OC(=O)CCN1CCNCC1</chem>	<chem>COC(=O)CCN1CCN(C)CC1</chem>
<chem>CCN1CCN(CCC(O)=O)CC1</chem>	<chem>CCCN1CCN(CCC)CC1</chem>
<chem>CN(C)CCC(=O)Oc1ccccc1</chem>	<chem>NCCC(=O)Oc1ccc(O)cc1</chem>
<chem>CCCC(=O)OCCCCO</chem>	<chem>CCC(=O)OCCCCOC</chem>
<chem>O=C1CC(=O)OCCCCO1</chem>	<chem>O=C1CCOCCCCO1</chem>
<chem>COCC(=O)OCCCCO</chem>	<chem>COCCCCOC(=O)CO</chem>
<chem>O=C1OCCCCOC(=O)c2ccccc12</chem>	<chem>c:c:c1C(=O)OCCCCOCc1:c</chem>
<chem>c:c1cCOCCCCOC1=O</chem>	<chem>O=C1OCCCCOC(=O)C=C1</chem>
<chem>CCC(=O)OCC(C)(C)COC(C)=O</chem>	<chem>CCCC(=O)OCC(C)(C)COC</chem>
<chem>CCCCC(=O)OCC(C)(C)CO</chem>	<chem>CCCCC(=O)OCC(C)(C)C</chem>
<chem>O=C1OCCCOc2cccc1c2</chem>	<chem>c:c:c1ccCOCCCCOC1=O</chem>
<chem>C=C1C=CC(=O)OCCCOc1=O</chem>	<chem>O=C1OCCCOc(=O)c2cccc1c2</chem>
<chem>CC1CCOC(=O)C=CC(=C)C(=O)O1</chem>	<chem>CC1CCOC(=O)C(=C)C=CC(=O)O1</chem>
<chem>CC1CCOC(=O)c(:c:c)ccCO1</chem>	<chem>CC1CCOC(=O)c2cccc(CO1)c2</chem>
<chem>CC(C)OC(=O)c1cccc(c1)C(O)=O</chem>	<chem>CC1CCOC(=O)c2cccc(c2)C(=O)O1</chem>
<chem>CC1CCOCc2cccc(c2)C(=O)O1</chem>	<chem>CC1CCOCccc(:c:c)C(=O)O1</chem>
<chem>CC1(C)COC(=O)CCC(=O)OC1</chem>	<chem>CC1(C)COCCCC(=O)OC1</chem>
<chem>O=C1CCC(=O)OCCCCO1</chem>	<chem>ClCC1(CCl)COC(=O)C(=O)OC1</chem>
<chem>CC1CCOC(=O)cc(:c)C(=O)O1</chem>	<chem>CC1CCOC(=O)c(:c)cC(=O)O1</chem>

CC1CCOC(=O)c(:c:c)c(:c)CO1	CC1CCOC(=O)c2cccc2C(=O)O1
O=C1OCCOC(=O)c2cccc12	CC1CCOCc(:c)c(:c:c)C(=O)O1
CC(C)OC(=O)CCCCS(C)(=O)=O	CC(CCOC(C)=O)OC(=O)c(:c):c
CC(CCOC(=O)c(:c):c)OC(C)=O	COC(C)CCOC(=O)c(:c:c):c:c
CC(O)CCOC(=O)c1cccc1	CC(C)OC(=O)c1ccc(cc1)C(O)=O
CCC(C)OC(=O)c1ccc(C)cc1	CC(CCO)OC(=O)c1cccc1
COCCC(C)OC(=O)c(:c:c):c:c	OC(=O)CCCC(=O)OCc(:c):c
CCCCC(=O)OCc(:c:c):c:c	CCCC(=O)OCc1cccc1
CCC(=O)OCc1ccc(C)cc1	CC(=O)OCc1ccc(CO)cc1
COCc1ccc(COC)cc1	CCCCC(=O)OCc(:c):c
Cc1cccc(c1)C(=O)OCc(:c:c):c:c	c:c:c(:c:c)C(=O)OCc1cccc1
Cc1ccc(COC(=O)c(:c):c)cc1	OC(=O)c1cccc(c1)C(=O)OCc(:c):c
COC(=O)CCC(=O)OCc(:c):c	OC(=O)CCC(=O)OCc(:c:c):c:c
c:c:c(COC(=O)c1cccc1):c:c	Cc1ccc(cc1)C(=O)OCc(:c):c
CC1(C)COC(=O)CC(=O)OC1	CC1CCOC(=O)CC1
CC1CCCC(C)C(=O)O1	CCCCOC(=O)c1cccc(:c)c1
CCCOC(=O)c1ccc(:c)c(:c:c)c1	CC1COC(=O)C(=C)C(=C)C(=O)O1
CC1COC(=O)c(:c:c)c(:c)C(=O)O1	CC1COC(=O)c2cccc2C(=O)O1
CC1COC(=O)c(:c)c(:c:c)C(=O)O1	CCCCC(=O)OCC(C)O
CCCCCCC(=O)OC(C)C	CCCCC(=O)OC(C)CO
CCN(CC)CCC(=O)OCCO	CCOC(=O)CCN1CCNCC1
COCCOC(=O)CCN(C)C	CC(=O)OCCOC(=O)CCN
CC1COC(=O)c2ccc(cc2)C(=O)O1	CC1COC(=O)c2ccc(CO1)cc2
CC1COCc2ccc(cc2)C(=O)O1	O=C1OCc2ccc(COC1=O)cc2
O=C1COCc2ccc(CO1)cc2	C1COCc2ccc(CO1)cc2
COC(=O)c1ccc(-c(:c:c):c(C):c)c(C)c1	CCOC(=O)c1ccc(-c(:c):c)c(C)c1
Cc1cccc1-c1ccc(cc1C)C(O)=O	Cc1ccc(c(C)c1)-c1ccc(C)cc1C
Cc1ccc(cc1C)C(=O)OCCO	O=C1CCCCCCCN1
O=C1CCCCCCCN1	C1CCCCNCCCC1
CCCCCCC(=O)NCC	CCCCCCCCCN
CCCCCCCNC	CCCCCCCNC(C)=O
COC(=O)CC1NC(=O)OC1=O	c:c(:c)CC1NC(=O)OC1=O
c:c:c(CC1NC(=O)OC1=O):c:c	O=C1OCNC1Cc1cccc1
O=C1OCCOCN2CCN1CC2	O=C1OCCOC(=O)N2CCN1CC2
CCN1C(=O)N(CCOC)C(C)(C)C1=O	CCN1C(=O)N(CCOC(C)=O)C(C)(C)C1=O
CN1C(=O)N(CCOC(=O)c(:c):c)C(C)(C)C1=O	CC1(C)CNC(=O)N1CCOC(=O)c(:c:c):c:c
CN(C)CCOC(=O)c1cccc1	Cc1ccc(cc1)C(=O)OCCN

c:c:c(:c:c)C(=O)OCCN1C(=O)CNC1=O	CN1C(=O)N(CCOC(=O)c(:c):c)C(=O)C1(C)C
CCN1C(=O)N(CCOC(C)=O)C(=O)C1(C)C	COCCN1C(=O)N(CCOC(C)=O)C(=O)C1(C)C
COCCN1C(=O)N(CCO)C(=O)C1(C)C	CCN1C(=O)N(CCOC(C)=O)C(=O)C1(C)C
CC1(C)N(CCO)C(=O)N(CCO)C1=O	OCCN1C(C2CCCCC2)C(=O)N(CCO)C1=O
CCN1C(=O)C(C2CCCCC2)N(CCOC)C1=O	CCC(CC)C1N(CCOC(C)=O)C(=O)N(CC)C1=O
CC(C)C1N(CCOC(=O)c(:c):c)C(=O)N(C)C1=O	CC1CNC(=O)N1CCOC(=O)c(:c):c:c
CC1N(C)C(=O)N(CCOC(=O)c(:c):c)C1=O	CCN1C(C(C)C)C(=O)N(CCOC(C)=O)C1=O
CCC(CC)C1N(CC)C(=O)N(CCOC)C1=O	COCCN1C(=O)C(C(C)C)N(CCO)C1=O
CCC(CC)C1N(CCOC)C(=O)N(CCO)C1=O	COCCN1C(=O)N(CCO)C(c(:c):c)(c(:c):c)C1=O
CCN1C(=O)N(CCOC(C)=O)C(=O)C1(c(:c):c)c(:c):c	CN1C(=O)N(CCOC(=O)c(:c):c)C(c(:c):c)(c(:c):c)C1=O
CCN1C(=O)N(CCOC(C)=O)C(c(:c):c:c:c)(c(:c):c):c:c)C1=O	COCCN1C(=O)N(CCO)C(=O)C1(c(:c):c:c:c)c(:c):c:c
CCN1C(=O)N(CCOC)C(C1=O)(c1cccc1)c1cccc1	OCCN1C(=O)N(CCO)C(C1=O)(c1cccc1)c1cccc1
CCN1C(=O)N(CCOC)C(=O)C1(c(:c):c):c:c)c(:c):c:c	CCN1C(=O)N(C)C(=O)C1(c(:c):c):c:c)c1cccc1
O=C1CCCCCCCC(=O)O1	CCCCC(=O)OC(=O)CC
CCCCCCC(=O)OC(C)=O	CCCCC(=O)OC(=O)CCC
Cc1ccc(cc1)C(=O)OC(=O)c(:c):c	CCc1ccc(cc1)C(=O)OC(C)=O
CCCCc1ccc(cc1)C(O)=O	CCCCC1ccc(C)cc1
CCCCCCc1cccc1	CCCCCCCc(:c):c:c
c:c(:c)CCCCCc(:c):c	Cc1ccc(cc1)C(C)(C)c1cccc1
CC(C)(c(:c):c):c:c)c1ccc(cc1)C(O)=O	COC(=O)c1ccc(cc1)C(C)(C)c(:c):c
CC(=O)OC(=O)c1ccc(cc1)C(C)(C)C	c:c:c(CCCCCc(:c):c):c:c
O=C1Cc2ccc(CC(=O)O1)cc2	O=C1Cc2ccc(CCO1)cc2
CCC(=O)OC(=O)CCc(:c):c:c	CC(=O)OC(=O)CCc1cccc1
CCCC(=O)OC(=O)CCc(:c):c	O=C1CCCCCCCC(=O)O1
c:c(:c)CCCCc1cccc1	c:c:c(CCCCc(:c):c):c:c
Cc1ccc(CCCc(:c):c)cc1	c:c:c(CCCc1cccc1):c:c
O=C1OCCCCOC(=O)S1	O=C1OCCCCOCS1
O=C1OCc2ccc(CO1)cc2	C1OCc2ccc(CO1)cc2
CCCCC1=NCCCO1	CCC(CC)C1=NCCO1
C1CN=C(O1)C1CCCC1	c:c:c(:c:c)C1=NCCO1
C1CN=C(O1)c1cccc1	c:c:c(:c:c)C1=NCCCO1

C1COC(=NC1)c1ccccc1	Cc1ccc(cc1)C(O)=N
Cc1ccc(cc1)C1=NCCO1	CC(F)(F)C(F)(F)C(F)(F)C1=NCCCO1
Cc1ccc(cc1)[Si](C)(C)C	Cc1ccc(cc1)[Si]1(CCC1)c(:c):c
Cc1ccc(cc1)[Si]1(CCC1)c(:c):c:c	C1C[Si](C1)(c1ccccc1)c1ccccc1
C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	C[Si]1(O[Si](C)(O[Si](C)(O1)c1ccccc1)c(:c):c):c:c)c(:c):c
C[Si]1(C)O[Si](C)(C)O[Si](C)(O1)c1ccccc1	C[Si]1(C)O[Si](C)(O[Si](C)(O[Si](C)(O1)c(:c):c):c:c)c1ccccc1)c(:c):c
C[Si](C)(O)O[Si](C)(O[Si](C)(C)O)c1ccccc1	C[Si](C)(C)O[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
C[Si]1(C)O[Si](C)(C)O[Si](C)(O[SiH3])O[Si](C)(C)O1	C[Si]1(C)O[Si](C)(C)O[Si](C)(O)O[Si](C)(C)O1
CC[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	CCC[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
C[Si]1(C)O[Si](C)(C)O[Si](C)(CCc(:c):c)O[Si](C)(C)O1	C[Si](O)(O)CCc1ccccc1
C[Si]1(C)O[Si](C)(C)O[Si](C)(O[Si](C)(C)O1)c(:c):c	C[Si]1(C)O[Si](C)(C)O[Si](C)(O[Si](C)(C)O1)c(:c):c:c
C[Si]1(C)O[Si](C)(C)O[Si](C)(O[Si](C)(C)O1)c1ccccc1	C[Si]([SiH3])([SiH3])c1ccccc1
C[Si]1(C)[SiH2][Si](C)(C)[Si]1(c(:c):c)c1ccccc1	C[Si]1(C)[Si](c(:c):c)(c(:c):c)[Si](c(:c):c:c)(c2ccccc2)[Si]1(c(:c):c)c(:c):c
c(:c):c(:c):c[Si]1(c(:c):c:c:c)[Si](c(:c):c:c:c)(c(:c):c:c:c)[Si](c2ccccc2)(c2ccccc2)[Si]1(c1ccccc1)cc	c1ccccc1
CCC[Si]1(C)O[Si](C)(CC)O[Si](C)(CCC)O1	CC[Si]1(C)O[Si](C)(CC)O[Si](C)(CC)O1
CCCC[Si]1(C)O[Si](C)(CC)O[Si](C)(CCC)O1	CCC[Si]1(CCC)C[Si](CCC)(CCC)C1
CCCC[Si]1(CCCC)C[Si](CCC)(CCC)C1	CC(C)(c1ccccc1)c1ccc(O)cc1
CC(C)(c(:c):c)c1ccc(OS)cc1	CC(C)(c(:c):c)c1ccc(OS(C)(=O)=O)cc1
CC(C)(C)c1ccc(OS(=O)(=O)c(:c):c)cc1	Cc1ccc(OS(=O)(=O)c(:c):c:c)cc1
Sc1ccccc1)S(=O)(=O)Oc1ccccc1	OS(=O)(=O)c1cccc(c1)S(=O)(=O)Oc(:c):c:c
OS(=O)(=O)c1ccccc1)S(=O)(=O)Oc(:c):c	COS(=O)(=O)c1cccc(c1)S(O)(=O)=O
COS(=O)(=O)c1ccccc1)S(=O)(=O)Oc(:c):c	CCCCC1(CCCC)CS(=O)(=O)C1
CCCc1ccc(CCC)c(C)c1	CCc1ccc(CCC(:c):c)cc1C
Cc(:c):c(CCC1ccc(C)c(C)c1):c:c	Cc1ccccc1(CCC2ccccc2C)c1
Cc1ccc(CCC(:c):c)c(C)c1	CCc1ccc(CCC(:c):c)c(C)c1

<chem>CCCc1ccc(CCC)c(CC)c1</chem>	<chem>CCc1ccc(CCC(:c):c)cc1CC</chem>
<chem>CCc1cc(CCC(:c:c):c(C):c)ccc1C</chem>	<chem>CCc1cccc1CCc1cccc(C)c1</chem>
<chem>CCc1cc(C)ccc1CCc(:c:c):c:c</chem>	<chem>CCc1ccc(CCC(:c):c)c(CC)c1</chem>
<chem>CCCc1ccc(CCC)c(Cl)c1</chem>	<chem>CCc1ccc(CCC(:c):c)cc1Cl</chem>
<chem>Cc1ccc(CCC(:c:c):c(Cl):c)cc1Cl</chem>	<chem>Clc1cccc(CCC2cccc2Cl)c1</chem>
<chem>Cc1ccc(CCC(:c:c):c:c)c(Cl)c1</chem>	<chem>CCc1ccc(CCC(:c):c)c(Cl)c1</chem>
<chem>CCCc1ccc(CCC)c(Br)c1</chem>	<chem>CCc1ccc(CCC(:c):c)cc1Br</chem>
<chem>Cc1ccc(CCC(:c:c):c(Br):c)cc1Br</chem>	<chem>BrC1cccc(CCC2cccc2Br)c1</chem>
<chem>Cc1ccc(CCC(:c:c):c:c)c(Br)c1</chem>	<chem>CCc1ccc(CCC(:c):c)c(Br)c1</chem>
<chem>Cc1ccc(cc1)C(F)(F)C(F)(F)c(:c:c):c:c</chem>	<chem>CC(F)(F)c1ccc(cc1)C(F)(F)C(F)(F)c(:c):c</chem>
<chem>CC(F)(F)C(F)(F)c1ccc(cc1)C(F)(F)C(C)(F)F</chem>	<chem>FC(F)(c1cccc1)C(F)(F)c1cccc1</chem>
<chem>CCCCC12CC34CC3(CC(C4)C1)C2</chem>	<chem>CC(C)(C)OC(=O)C1=C(C2C=CC1C=C2)C(=O)OC(C)(C)C</chem>
<chem>COC(=O)C1=C(C2C=CC1C=C2)C(=O)OC(C)(C)C</chem>	<chem>CC(F)(F)C(F)(F)OC1(F)C2CC(C=C2)C1(F)F</chem>
<chem>CCCOc1ccc(cc1)-c(:c):c</chem>	<chem>CCOc1ccc(cc1)-c(:c:c):c:c</chem>
<chem>COc1ccc(cc1)-c1cccc1</chem>	<chem>N#Cc1ccc(cc1)-c1cccc1</chem>
<chem>c:c:c(:c:c)-c1ccc(cc1)C#N</chem>	<chem>OC(=O)C1C2CC(C=C2)C1C(O)=O</chem>
<chem>CCOC(=O)C1C2CC(C=C2)C1C(=O)OCC</chem>	<chem>OCCOc1ccc(cc1)-c(:c):c</chem>
<chem>CCCCC1(CC2CC1C=C2)C#N</chem>	<chem>C[Si](C)(C)O[Si](C)(C)C1(CC2CC1C=C2)C#N</chem>
<chem>C[Si](C)(O)O[Si](C)(C)C1(CC2CC1C=C2)C#N</chem>	<chem>C[Si](C)(CC1(CC2CC1C=C2)C#N)O[SiH3]</chem>
<chem>C[Si](C)(C)OCC1CC2CC1C=C2</chem>	<chem>CC1CCCC1CN1C(=O)c2cccc2C1=O</chem>
<chem>O=C1C=CC(=O)N1CC1CC2CC1C=C2</chem>	<chem>CC(C)CN1C(=O)c2cccc2C1=O</chem>
<chem>O=C1NC(=O)c2cccc12</chem>	<chem>CCCCC(C)C=CCC</chem>
<chem>CCCCCCC(C)C=CC</chem>	<chem>CCCCCCC(C)C=C</chem>
<chem>CCCCCCCCC(C)C</chem>	<chem>CCCCCCC=CC(C)C</chem>
<chem>CCCCCC=CC(C)CC</chem>	<chem>CCCCC=CC(C)CCC</chem>
<chem>C1C=CC2C3CC(C=C3)C12</chem>	<chem>CC(C)C1CC2CC1C=C2</chem>
<chem>CCC(CC)C1CC2CC1C=C2</chem>	<chem>C1C2CC(C1C=C2)C1CCC=CC1</chem>
<chem>CC1CNC(=O)CC(O1)c(:c:c):c:c</chem>	<chem>c:c(:c)C1CNC(=O)CC(O1)c1cccc1</chem>
<chem>c:c:c(:c:c)C1CNC(=O)CC(O1)c1cccc1</chem>	<chem>c:c:c(:c:c)C1CC(=O)NCC(O1)c1cccc1</chem>
<chem>c:c(:c)C1CC(=O)NCC(O1)c1cccc1</chem>	<chem>c:c(:c)C1CNC(=O)CC(O1)c(:c):c</chem>
<chem>CC1CCNCC(O1)c1cccc1</chem>	<chem>CC1CNC(=O)CC(O1)c1cccc1</chem>
<chem>CC(=O)OCC1(CCl)COC1</chem>	<chem>C1OCC11CC2CCC1C2</chem>
<chem>C1OCC11CC2CC1C=C2</chem>	<chem>C1OCC11CC2CCC1CC2</chem>
<chem>CC(C)(C)COc1cccc1</chem>	<chem>C1CCCC2OC2CC1</chem>
<chem>C1OC1c1ccco1</chem>	<chem>O=C1CCC2(CCO1)OCCO2</chem>

<chem>O=C1NC(=O)C2C3CC(C=C3)C12</chem>	<chem>O=C1CCC(=O)N1CC1CO1</chem>
<chem>CCCCN1C(=O)C2C3CC(C=C3)C2C1=O</chem>	<chem>CCCN1C(=O)C2C3CC(C=C3)C2C1=O</chem>
<chem>CC(=O)OCC1CO1</chem>	<chem>CCOC(=O)c1ccc(cc1)N(C)C</chem>
<chem>COC(=O)c1ccc(cc1)N1C(=O)CCC1=O</chem>	<chem>CC1C(C)C(=O)N(C1=O)c1ccc(cc1)C(O)=O</chem>
<chem>O=C1C2C3CC(C=C3)C2C(=O)N1c1cccc1</chem>	<chem>c:c:c(:c:c)N1C(=O)C2C3CC(C=C3)C2C1=O</chem>
<chem>c:c(:c)-c1ccc(OCC2CO2)cc1</chem>	<chem>COc1ccc(cc1)-c(:c:c):c:c</chem>
<chem>CCOCC1(C)COC1</chem>	<chem>COCC1OC1COC(C)(C)F</chem>
<chem>CC(C)(F)OCC1OC1COC(C)(C)F</chem>	<chem>CCC1(COC(C)=O)COC1</chem>
<chem>OCCOP1(=O)OCCO1</chem>	<chem>CCC1(COC1=O)c1cccc1</chem>
<chem>CCCCc1cc(OC(C)=O)ccc1OC(C)=O</chem>	<chem>CCCCc1cc(OC(=O)c(:c):c)ccc1OC</chem>
<chem>CCc1cc(OC(=O)c(:c:c):c)c1ccc1O</chem>	<chem>CCc1cccc1OC(=O)c1cccc1</chem>
<chem>CCCCc1cc(O)ccc1OC(=O)c(:c:c):c:c</chem>	<chem>CCCCc1cc(OC)ccc1OC(=O)c(:c):c</chem>
<chem>CCCCc1cc(OC)ccc1OC(=O)c(:c):c</chem>	<chem>CCc1cc(OC(C)=O)ccc1OC(C)=O</chem>
<chem>CCc1cc(OC(=O)c(:c):c)ccc1OC</chem>	<chem>O=C1OCCCCOCC=C1</chem>
<chem>CCC(OC)C1CC(=O)O1</chem>	<chem>O=C1CC(O1)C1CCC=CO1</chem>
<chem>CCCOC(=O)CC=CCC</chem>	<chem>CCOC(=O)CC=CCC(O)=O</chem>
<chem>COC(=O)CC=CCC(=O)OC</chem>	<chem>CCCCOC(=O)CC=CC</chem>
<chem>CCCCCOC(=O)CC=C</chem>	<chem>NC1=C2C(=CCCC1)C(=O)OCCOC2=O</chem>
<chem>CC=C1C(=O)OCCOC(=O)C1=C</chem>	<chem>CC(N)=C1C(=O)OCCOC(=O)C1=C</chem>
<chem>CN(C)C1=C2C(=CCCC1)C(=O)OCCOC2=O</chem>	<chem>CN(C)C1=C(C)C(=CCCC1)C(O)=O</chem>
<chem>COC(=O)C1=CCCC(N)=C1C(O)=O</chem>	<chem>CCOC(=O)C1CC(=O)O1</chem>
<chem>CCOC(=O)C1CCOC(=O)CC1</chem>	<chem>COC(=O)C1CCOC(=O)CC1</chem>
<chem>CC1CCNC(=O)CC1</chem>	<chem>c:c:c(:c:c)C1CC(=O)N1</chem>
<chem>O=C1CC(N1)c1cccc1</chem>	<chem>CC1(C)C(NC1=O)c1cccc1</chem>
<chem>CCOC(=O)C1CC(=O)N1</chem>	<chem>CCc1ccc(O)cc1</chem>
<chem>CC(N)Cc1ccc(O)cc1</chem>	<chem>Oc1ccc(CC2NCOC2=O)cc1</chem>
<chem>O=C1NCCCCCO1</chem>	<chem>C1CCCOCNCC1</chem>
<chem>CC1C(C)C(=O)N(C1=O)c1cccc1</chem>	<chem>Cc1cccc1N1C(=O)CCC1=O</chem>
<chem>CC1C(C)C(=O)N(C1=O)c1cccc1C</chem>	<chem>Cc1cccc1N1C(=O)C2C3CC(C=C3)C2C1=O</chem>
<chem>Cc(:c):c(:c:c)N1C(=O)C2C3CC(C=C3)C2C1=O</chem>	<chem>CN(C)c1cccc(C)c1</chem>
<chem>O</chem>	
<chem>Cc1cccc(c1)N1C(=O)CCC1=O</chem>	<chem>CC1C(C)C(=O)N(C1=O)c1cccc(C)c1</chem>
<chem>Cc1cccc(c1)N1C(=O)C2C3CC(C=C3)C2C1=O</chem>	<chem>CN(C)c1ccc(C)cc1</chem>
<chem>O</chem>	
<chem>CC1C(C)C(=O)N(C1=O)c1ccc(C)cc1</chem>	<chem>FC(F)(F)c1cc(cc(c1)C(F)(F)F)N1C(=O)CCC1=O</chem>

CC1C(C)C(=O)N(C1=O)c1cc(cc(c1)C(F)(F)F)C(F)(F)F	CN(C)c1cc(cc(c1)C(F)(F)F)C(F)(F)F
Cc1cc(C)cc(c1)N1C(=O)C2C3CC(C=C3)C2C1=O	CCCCOC(=O)OCCC
CCCCCOC(=O)OCC	CCCCCOC(=O)OC
CCCCCCCOC(O)=O	CCOC(=O)C1(C)COC(=O)OC1
CC(=O)OCC1=NCCO1	COc1ccc(SC)cc1
CCOc1ccc(SC)cc1	CCCOc1ccc(SC)cc1
OCCCC1=NCCO1	C[Si](C)(C)CCN1CC1
O=C(Cn1c2cccc2c2cccc12)N1CC1	NC(=O)Cn1c2cccc2c2cccc12
Cn1cc(:c)c2cccc12	Cn1c(:c)c(:c:c)c2cccc12
CCn1c2cccc2c2cccc12	c:n(:c)CC(=O)N1CC1
CCC(CC)(CC)C(=O)N1CC1	O=C(CC12CC3CC(CC(C3)C1)C2)N1CC1
CC(C)(C)CC(=O)N1CC1	c:c(:s)C1=NCCO1
C1CN=C(O1)c1ccsc1	C1CN=C(O1)c1ccsc1
OC(=N)c1ccc(OCC=C)cc1	CCOc1ccc(cc1)C1=NCCO1
COc1ccc(cc1)C1=NCCO1	CCCOc1ccc(cc1)C(O)=N
c:c:c(:c:c)N1COc2cccc2C1	C1Oc2cccc2CN1c1cccc1
c:c1CN(COc1)c1cccc1	Cc1ccc2OCN(Cc2c1)c(:c):c
CN1COc2ccc(cc2C1)C(C)(C)C	CCC(CC)(CC)c1ccc2OCNCC2c1
C1NCc2cc(ccc2O1)C12CC3CC(CC(C3)C1)C2	CN1COc2ccc(cc2C1)C12CC3CC(CC(C3)C1)C2
CCC(CC)(CC)c1ccc2OCN(Cc2c1)c(:c):c	CC(C)(C)c1ccc2OCN(Cc2c1)c(:c):c
CC(C)(C)c1ccc2OCN(Cc2c1)c(:c:c):c:c	Cc1ccc2OCN(Cc2c1)c1cccc1
Cc1cccc(c1)C12CC3CC(CC(C3)C1)C2	CCC(CC)(CC)c1ccc2OCN(C)Cc2c1
C[Si]1(C)O[Si](C)(C)O[Si](C)(Cl)O[Si](C)(C)O1	C[Si](O)(O)CCc1ccc(Cl)cc1
CCc1ccc(C)cc1	Cc1ccc(CC[SiH3])cc1
Cc1ccc(CC[Si](C)(O)O)cc1	c:c:c(:c:c)[Si]1(CCC1)c1cccc1
c:c:c(:c:c)[Si]1(C[Si](C1)(c1cccc1)c1cccc1)c(:c:c):c:c	C[Si]1(C)C[Si](C1)(c(:c:c):c:c)c1cccc1
C[Si]1(C)O[Si](C)(O[Si](C)(O[Si](C)(O1)C=C)C=C)C=C	C[Si]1(C[Si](C)(C1)c1cccc1)c(:c:c):c:c
C[Si]1(C)C[Si](C)(C1)c1cccc1	CCC[Si]1(C)O[Si](C)(CC)O[Si](C)(CCC(C)(F)F)O1
C[Si]1(C)Cc2cccc2C1	C[Si]1(CCC=CC1)c1cccc1

CCCC[Si]1(CCCC)C#C[Si](CC)(CC)[Si](C)(C)C#C[Si]1(CCC)CCC	CCC[Si]1(CCC)C#C[Si](CCC)(CCC)[Si](CC)(C)C#C[Si]1(CC)CC
CCCC[Si]1(CCCC)C#C[Si](C)(C)[Si](C)(C)C#C[Si]1(CCCC)CCCC	C[Si]1(C)C#C[Si](C)(c(:c:c):c:c)[Si](C)(C#C[Si]1(C)c(:c):c)c1cccc1
C[Si]1(C#C[Si](C)(c(:c):c)[Si](C)(C#C[Si]1(C)c(:c:c):c)c(:c):c)c(:c):c	C[Si](C#C)(c(:c):c)[Si](C)(C#C[SiH3])c1cccc1
C[Si]1(C)C#C[Si](C)(c2cccc2)[Si](C)(C#C[Si]1(C)C)c1cccc1	C[Si]1(C)CC(Cc(:c):c)C1
C[Si]1(C)CC(Cc(:c):c)c(:c):c)C1	C(C1C[SiH2]C1)c1cccc2cccc12
CC(C)Cc1cccc2cccc12	CCc1cccc2cccc12
C[Si]1(C)CC(Cc(:c):c)c(:c):c)C1	c:c(:c)-c1ccc(CC2C[SiH2]C2)cc1
CC(C)Cc1ccc(cc1)-c(:c):c:c	CCc1ccc(cc1)-c1cccc1
C[Si]1(C)CC(C1)c(:c):c(:c):c	C[Si]1(C)CC(C1)c1cccc(:c)c1:c:c
C[Si]1(C)CC(C1)c1cccc2cccc12	C1[SiH2]CC1c1cccc2cccc12
CC(C)c1cccc2cccc12	C[Si](C)(C)C[Si](C)(C)c1cccc1
C[Si](C)(C[Si]1(C[Si](C)(C)c(:c):c)CCC1)c(:c):c	C[Si]1(CCC[SiH3])CCC1
CCC(CC)[Si]1(CCC1)c(:c):c(:c):c	c:c:c1c(cccc1:c)[Si]1(CCC1)C1CCCCC1
c:c:c(:c(:c):c)[Si]1(CCC1)C1CCCCC1	CCC(CC)[Si]1(CCC1)c1cccc2cccc12
CC(C)[Si]1(CCC1)c1cccc2cccc12	C[Si](C)(C)c1cccc2cccc12
CCCCc1cc(CCC)ccc1CCC	CCCc1cc(CCc(:c):c)ccc1CC
CCCc1cc(C)ccc1CCc(:c):c:c	CCCc1cc(CC)ccc1CCc(:c):c
c:c(:c)P1CCCS1	c:c:c(:c:c)P1CCCS1
c:c(:c)P1CCCCS1	c:c:c(:c:c)P1CCCCS1
C1CCP(SC1)c1cccc1	CC(C)OCC1(CO1)c1cc(C)cc(C)c1
COCC1(CO1)c1cc(cc(c1)C(F)(F)F)C(F)(F)F	OCC1(CO1)c1cc(cc(c1)C(F)(F)F)C(F)(F)F
CC1(CO1)c1cc(cc(c1)C(F)(F)F)C(F)(F)F	CC(C)(F)OCC1CO1
CC1=CCC2(COC2)CC1	C[Si](C)(C)OCC1(CO[Si](C)(C)C)COC1
CN(C)c1ccc(cc1)[Si](C)(C)C	CN(C)c1ccc(cc1)[Si]1(C)CCC1
C[Si]1(CCC1)c1cccc1	CN(C)c1ccc(cc1)[Si]1(CCC1)c(:c):c
CN(C)c1ccc(cc1)[Si]1(CCC1)c(:c):c:c	C[Si]1(CC=CC1)c1cccc1
[SiH3]CCCc1ccc(cc1)-c(:c):c	CCCc1ccc(cc1)-c(:c):c:c
CCCC[Si]1(CC=CC1)c1cccc1	CCC[Si]1(CC=CC1)c1cccc1
NC(=O)OCc1cccc1	CCOC(=O)N1CCOC(=O)CC1
COC(=O)N1CCOC(=O)CC1	CSCCC1NC(=O)OC1=O
c:c(:c)CN1CCOC1=S	c:c:c(CN1CCOC1=S):c:c
S=C1OCCN1Cc1cccc1	c:c(:c)CN1CCOC1=S

c:c:c(CN1CCCOC1=S):c:c	CCN(Cc1ccccc1)C(O)=S
CCC(CC)[Si]1(C)C[Si](C)(C1)C1CCCC1	C[Si]1(C)C[Si](C)(C1)C1CCCC1
CCC(CC)[Si]1(Cl)C[Si](Cl)(C1)C1CCCC1	C[Si]1(Cl)C[Si](Cl)(C1)C1CCCC1
C[Si]1(Cc2ccccc12)c1ccccc1	C[Si]1(Cc(:c)c1:c:c)c1ccccc1
c:c:c(:c:c)[Si]1(Cc2ccccc12)c(:c:c):c:c	C1c2ccccc2[Si]1(c1ccccc1)c1ccccc1
c:c:c(:c:c)[Si]1(Cc(:c)c1:c:c)c1ccccc1	CCOC1ccc(cc1)C#N
CCOC1ccc(cc1)C#N	CC[Si](C)(C)O[Si]1(C)CCC1
COc1ccc(cc1)C(=O)Oc(:c):c	c:c(:c)C(=O)Oc1ccc(cc1)C#N
CC(=O)Oc1ccc(cc1)C#N	c:c(:c)C(=O)Oc1ccc(cc1)-c(:c):c
CC(=O)Oc1ccc(cc1)-c(:c:c):c:c	C[Si]1(C)CC(C1)c(:c:c):c:c
C[Si]1(C)CC(C1)c1ccccc1	Cc1ccccc1)[Si](C)(C)C
Cc1ccccc1)[Si]1(C)CCC1	CCCCc1ccc2C3C=CC(C=C3)c2c1
CCCCc1ccc2C3C=CC(C=C3)c2c1	CCc1ccc2C3C=CC(C=C3)c2c1

C. Condensation: Functional Groups as Descriptor Set (SMARTS Format)

[#8]-*	[#6]-[#8]	[#8]-[#14]
[#6]- [#7]1[Si]([#6])([#6])[#8][Si]([#6]])([#6])[#7](-[#6])-*(-[#6])(- [#6])-[#8][Si]1([#6])[#6]	[#8]	[#6]=O
[#6]-[#8]-[#6](-[#6])=O	[#6]-[#8]-*	[#6]Cl
[#6]-[#8]-c1ccccc1	[#7]-*	O=*-1-[#8]-[#6]-[#6]-[#8]-1
-[#8]-c1ccccc1	[#6]-[#7]- 1[Si]([#6])([#6])[#8][Si]])([#6])([#6])[#8]--1(- [#6])-[#6]	[#6]-[#7]- 1[Si]([#6])([#6])[#8][Si]([#6])([#6])[#8][Si]([#6])([#6])[#8]- *-1(-[#6])-[#6]
[#16]Cl	[#6]-[#6]-[#7](-[#14])- [#6]-[#6]	[#6]Br
[#6]F	[#6]-[#7]	[#6]-[#8]-[#6]-[#6]-[#8]
[#6]-*	[#8]-[#6]-*	[#6]-[#6]-[#8]-[#6]
[#7]	*-[#6]=O	[#6]-[#6]-[#8]
[#16]-*	Cl*	[#6]-[#6]-[#6]-[#6][Sn]1([#6]- [#6]-[#6]-[#6])[#16]-[#6]- [#6]-*1

[#6]-[#6]-[#6]-[#6][Sn]1([#6]-[#6]-[#6]-[#6])[#16]-[#6]-[#6]-[#6]-*1	[#6]-[#6]-[#6]-[#6]-[#8]-[#6]	[#6]-[#6](-[#8])=O
S=C=S	[#6]-[#6](Cl)=O	[#7]-c1cccc1
C#*	[#14]Cl	[#6]-[#6]
[#8]-c(:c):c:c:c	[#6]=[N+]=[#7-]	[#8]-[#6]-[#6]-[#8]
[#6]-c1cccc(-[#6])c1	[#6]-[#6](=O)-[#8]-[#6]-[#6]-[#8]	[#6]I
[#8]-c1c(cccc1-c(:c):c)-c(:c):c	c1cccc1	[#8]-c1cccc2cccc12
[#8]-[#6]C([#6]-[#8])([#6]-[#8])[#6]-[#8]	[#6]-c1ccc(-[#6])o1	[#6]-[#8]-[#6](=O)-c1cccc1
[#16]	[#8]-c(:c):c	[#8]-[#6]-[#6](-[#8])=O
[#8]-[#6]-[#6]-[#6]-[#6](-[#8])=O	[#6]-[#6](-[#6])-[#8]	[#8]-[#6]-[#6]-[#6](-[#8])=O
[#6]C([#6])([#6]-[#8])[#6](-[#8])=O	[#6]-[#6]-[#8]-[#6](-[#6])=O	[#6]-[#6]-[#6]-[#8]-[#6](=O)-[#6]-[#6]-1-[#7]-[#6](=O)-[#8]-[#6]-1=O
[#6]-[#6](-[#7])-[#6](=O)-[#7](-[#6])-[#6]	[#6]-[#8]-[#7]-1-[#6](=O)-[#6]-[#6]-[#6]-1=O	[#6]-[#6](-[#6])-[#7]
[#6]-[#8]-c1ccc(cc1)-[#7+](-[#8-])=O	[#6]-[#6](-[#7])-[#6](-[#7])=O	[#6]-[#8]-c1cccc1-[#8]
[#6]-[#6](-[#6])-[#6](-[#7])-[#6](-[#7])=O	[#7]-[#6]-[#6](-[#7])=O	[#6]-[#8]-c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
[#6]-[#6]-[#6](-[#6])-[#6]-1-[#7]-[#6](=O)-[#8]-[#6]-1=O	[#6]-[#6](-[#6])-[#6]-[#6]-1-[#7]-[#6](=O)-[#8]-[#6]-1=O	[#6]-[#6](-[#6])-[#6]-1-[#7]-[#6](=O)-[#8]-[#6]-1=O
O=[#6]-1-[#7]-[#6](-[#6]-c2cccc2)-[#6](=O)-[#8]-1	[#7]=C=O	[#6][Si]([#6])(Cl)Cl
[#6][Si]([#6])([#6])[#7]	ClP(Cl)(Cl)=[#7]	FC(F)(F)[#6]-[#8]-[#15]
[#6]-c1cccc(c1)-[#6](-[#8])=O	[#6]-c(:c):c(:c:c)-[#6](-[#8])=O	Clc1ccc(Cl)cc1
[#6]-c(:c):c	[#6]-c1cccc1C#N	[#6]-[#6]Cl
BrC1cccc(Br)c1	[#6][S+]1[#6]-[#6]-[#6]-[#6]1	[#6]-[#6](Cl)Cl
[#6]C(F)(F)I	Ic(:c):c	[#8]-c1cccc1

[#6]-[#6](=O)-c1ccccc1-[#6]	[#6]C([#6])([#6]Br)C([#6])([#6])[#6]Br	[#6]-[#6](Br)-[#6]Br
[#6]-[#6](-[#6])Br	[#6]-[#6](-[#8])Br	[#8]-[#6](Br)-[#6]Br
C#C	[#6]C#C	[#6]C1([#6])[#6]=[#6]-c2ccccc12
[#6]-1-[#6]=[#6]-c2ccccc-12	[#8]-[#6]-[#6]-1-[#6]-[#8]-[#6]-[#8]-1	Clc1cc(Cl)cc(Cl)c1
Clc1cc(Cl)cc(Br)c1	Brc1cc(Br)cc(Br)c1	c1ccoc1
[#6]-c1ccc(-[#6])c(-[#8])c1	[#8]-[#6](=O)-c1cccc(-[#8])c1	[#6]-[#6]-1-[#6]-[#8]-c2csc2-[#8]-1
[#6]-1-[#6]-[#8]-c2csc2-[#8]-1	[#6]-[#8]-c1csc(-[#6])c1-[#8]	[#6]-c1ccco1
c1ccsc1	[#6]-c1cccs1	[#8]-[#6](=O)-c1ccc(-[#8])cc1-[#6](-[#8])=O
[#8]-[#6](=O)-c1ccccc1-[#6](-[#8])=O	[#6]=[#6]	[#6]-[#6]=[#6]
[#6]-c1cc(Br)sc1-[#6]	[#8]-c1ccsc1Br	[#6]-[#6]-[#6]=[#6]
[#6]-c1ccsc1	Brc(:c):s	Brc(:n):s
s:c1csc2ccsc12	c1cc2sccc2s1	c1ccnc1
Brc(:c):c	[#6]-c1cc(l)sc1l	[#6]-c1ccsc1l
[#6]-c1ccsc1-[#6]	[#6]-c1csc2ccsc12	[#6]-c1cc(Br)sc1Br
[#6]-c1ccsc1Br	c:c:s	[#8]-c1ccsc1
c1scc2ccccc12	[#16]-[#6]-[#16]	[#16]-c1cc(l)sc1l
[#16]-c1ccsc1l	[#6]-c1csc1-[#6]	[#6]-[#6]-c1csc1-[#6]
[#6]-[#8]-c1csc1-[#8]-[#6]	[#6]-[#6]-[#8]-c1csc1-[#8]-[#6]	[#16]C#N
[#6]-c1sccc1-[#8]	Brc1ccsc1	c:c(:n)-c1cccs1
c:c(:c)-c1cccs1	[#16]-c1ccsc1	[#6]-c1sccc1-[#16]
s:c1ccsc1	n:c1ccsc1	[#6]-[#6]-1=[#6]-[#6]-[#16]-[#6]-1=[#6]
[#8]-[#6](=O)-c(:c):c	[#6]-[#6]-[#6]-[#8]	[#6]-[#6]-[#6]-[#6]-[#6]-[#6](-[#8])=O
[#7]-[#7]	[#6]-[#7]-[#7]	[#6]-[#6](-[#7])=[#6]
[#6]-[#6](-[#7])=O	[#7]-c(:n):n	c:n:n:c(:c)=O
[#6][Si]([#6])([#8])c1ccccc1	[#6]-n1ccnc1	[#6]-n1ccccc1
[#6]-c1ccccc1-[#7]	[#6]-c1cccc(-[#7])c1	Clc1ccccc1
[#6]-c(:c):c(:c:c)-[#7]=C=O	[#6]-[#7]-[#6]	[#7]-c1nc(Cl)nc(Cl)n1

[#7]-c1cccc(-[#7])c1	[#6]-c(:c):c(-[#7]):c:c	[#6]-[#7]-c1cccc1
Brc(:c):n	[#7]-c1cccc1-c(:c):c	[#6]-[#6]-c1cccc1-[#7]
FC(F)(F)c1cccc1	[#6]-c1cccc1	[#6]-c1ccnc1
[#7]-c1cccc2cc(:c)ccc12	[#6]-c1cncc1-[#6](-[#8])=O	[#6]-c1cncc1-[#6]
c:c1cccc1	[#6]=[#6]-1-[#6]=[#7]-c2cccc-12	[#6]-[#8]-c1ccc(-[#8]-[#6])c(-[#7])c1
[#6]-[#6]-[#8]-c1ccc(-[#8]-[#6])c(-[#7])c1	[#8]-[#6](=O)-c1cccc1	[#6]-c1ccc(-[#6])c(-[#7])c1
[#6]-c1ccc(-[#8])cc1	[#6]-[#8]-c1cncc1-[#8]-[#6]	[#15]-[#8]-c1cccc1
Brc1cccc1	Clc1cccc1Cl	Clc(:c):c:c(Cl):c
Brc1ccc(Br)cc1	[#6]-[#16]-c1cccc1	[#7]-c1cccc2cccc12
[#7]-c1cccc1:c	c:c1cccc2cccc(:c)c12	c:c(:n)-c1ccc[se]1
c:c(:c)-c1ccc[se]1	[#6]-n1cccc1-c(:c):n	[#6]-n1cccc1-c(:c):c
[#6]-[#6]-[#5;a]1n[#5;a]n[#5;a]n1	[#6]-[#5;a]1n[#5;a]n[#5;a]n1	[#5;a]1n[#5;a]n[#5;a]n1
Fc1cccc1	[#6]-n1cc2cccc2c1	[#6]=[#6]-1-[#6]=[#6]-[#7]=[#6]-1
[#6]-[#8]-c1cccc(-[#7])c1	[#7]-c1ccc(-[#7])cc1	[#8]-c(:c):c:c(-[#8]):c
Fc1ccc(F)cc1	[#7]-c1ccc(F)cc1	Fc1cccc(F)c1
Fc(:c):c:c(F):c	c:c:c1cccc1:c	[#7]-c1ccc(-[#16])cc1
[#7]-c1ccc(cc1)S(=[#8])(=O)=O	[#6]-[#8]-c1cccc1-[#7]	n:c(:s)-c1cccc1
lc1cccc1	c:c:n	[#6]-1-[#6]-[#6]-c2cncc2-[#6]-1
[#6]-1-[#6]-c2cncc2-[#6]-1	[#6]-1-[#6]-[#6]-c2cncc2-[#6]-[#6]-1	[#6]-[#6]-n1cccc1-[#6]
c:c(:c)[Si](C#C)(C#C)c(:c):c	[#6]-[#6]-[#8][Si]([#8]-[#6]-[#6])([#8]-[#6]-[#6])[#8]-[#6]-[#6]	[#14]
[#6][Si]([#6])(Cl)[#6][Si]([#6])([#6])Cl	[#6][Si]([#14])(Cl)Cl	[#6][Si]([#6])(Cl)[Si]([#6])([#6])Cl
[#6][Si]([#6])(Cl)[Si]([#6])(Cl)c(:c):c	[#6]-[#6]-[#8][Si]([#8]-[#6]-[#6])([#8]-[#6]-[#6])c(:c):c	[#6]-[#6]-[#8][Si]([#8]-[#6]-[#6])(c(:c):c):c:c(:c):c:c

[#6]-[#6]-c1cccc1-[#6]	[#6][N+]#N	[#6][N+]([#6])([#6])[#6]
[#6]-[#6][S+]([#6]-[#6])[#6]-[#6]	[#6]-[#6][S+]([#6]-[#6])[#6]-c(:c):c	[#6]-c1cc(Cl)cc(Cl)c1
Clc1cccc(Cl)c1	[#6]-c(:c):c(Cl):c:c	[#8]-c1cccc(Cl)c1
[#8]-c(:c):c(Cl):c:c	[#6]-[#8]-c1ccc(-[#8])cc1	[#8]-c1ccc(-[#8])cc1
[#6]-[#7](-[#6])-c1cccc1	[#7]-c1cccc1-[#8]	[#6]-c1cccc(Cl)c1
[#8]-c1cc(Cl)cc(Cl)c1	[#6][Mg]Br	[#6]-[#6]-[#8]-c1ccc(-[#8]-[#6])cc1
[#6]-[#8]-c1ccc(-[#8]-[#6])cc1	[#6]-c1cccc(l)c1	[#6]-c(:c):c(l):c:c
[#6]-[#6]-1-[#6]-[#6]-[#6]-[#16+]-1	[#6]-c1cccc1-[#8]	[#7]-c1ccc(-[#8])cc1
[#8]-c1cccc(-[#6][S+]2[#6]-[#6]-[#6]-[#6]2)c1	[#8]-c(:c):c(-[#6][S+]1[#6]-[#6]-[#6]-[#6]1):c:c	[#6]-c(:c):c(-[#6][S+]1[#6]-[#6]-[#6]-[#6]1):c:c
[#6]-c1cccc(-[#6]Cl)c1	[#6]-c(:c):c(-[#6]Cl):c:c	[#8]-c1cccc(-[#6]Br)c1
[#8]-c(:c):c(-[#6]Br):c:c	[#8]-c1cccc1-[#6]=[#7]	Brc1cccc2c(Br)cccc12
c:c(:c)[Ge](C#C)(C#C)c(:c):c	Brc1ccc(Br)[se]1	c1cc2cccc2c1
c1cccc1	[#6][Sn]([#6])(Cl)Cl	[#6]-c1cc[se]c1
c1cc[se]c1	[Na][#16]	[#6]-[#8]-[#6]
c:c1coc2cccc12	[#6]-[#6]-c1cccc1-[#8]	[#6]-[#6]-[#6]-[#6][Sn]([#6])([#6]-[#6]-[#6]-[#6])[#6]-[#6]-[#6]-[#6]
[#8]-[#6](=O)-[#7]-c1cccc1	[#8]-[#6](=O)-c1cccc(-[#16])c1	[#6][Si]([#6])([#6])[#8]
[#6]-[#16]-[#6](-[#6])=S	[#6]-[#5]-1-[#8]C([#6])([#6])C([#6])([#6])[#8]-1	[#8][K]
[#6]-[#8]-c1c(F)c(F)nc(F)c1F	[#15]Cl	[#14]-[#7]-1-[#6]-[#6]-[#6]-[#6]-1
Fc1cc(F)c(F)c(F)c1F	[#6]N(=O)=O	[#8]-[#6]-1-[#6]-[#8]-[#6]-[#6]-1-[#8]
Fc(:c):c	O=[Se]	[#6]-[#6]-[#6]-[#6](-[#6])=O
[#6]-c1ccc2-[#6](=O)-[#8]-[#6](=O)-c2c1	O=[#6]-1-[#8]-[#6](=O)-c2cccc-12	[#6]-[#7]-[#6](=O)-[#6](-[#7])-[#6]-c(:c):c

[#8]-[#6]-c(:c):c	[#6]- c1ccc(cc1)S([#7])(=O)= O	[#6]-[#5]-1-[#8]-[#6]-[#6]- [#6]-[#8]-1
[#7]-[#6](=O)-[#6]C#N	[#6]C([#6])([#8])C#C	[#6][P+](c1ccccc1)(c1ccccc1) c1ccccc1
[#8]-[#6]-[#6]-c(:c):c	[#6]-[#6]-[#6]-[#7]- [#6](-[#16])=O	[#16][K]
[Li][#6]	[#6][Zn]Cl	[#6]-[#6]-[#6]
[#6]-[#6]-[#16]	FC(F)(F)S(=O)(=O)[#8]- [#14]	[#6]-[#6]- [#8]P([#6])(=O)[#8]-[#6]-[#6]
[#6]-c(:c):c(-[#8]):c(-[#6]):c	[#6]-n1nnc2ccccc12	[#8]-c(:c):c(-[#8]):c(-[#8]):c
[#8]-[#6](=O)-[#6]C#N	[#6]-[#6](-[#8])-[#6]- [#8]	[#6]-[#8]-c1ccc(-[#8])cc1- [#8]
[#7]-[#6](-[#7])=O	[#6]-[#7]-[#6]-[#7]	[#6]-[#6](-[#6])-[#6]-[#8]
[#7]-[#6]-[#6]-[#6]-[#7]	[#6]-[#6](=[#6])-[#6]- [#6](-[#7])=O	[#6]-c(:c):n
[#6]-[#5](-[#8])-[#8]	c:c(:c)-[#6]C#N	[#14]C#C
[#7]-c(:c):c:c:c	[Na][Se]	[#7]-[#6]-[#6]-[#8]
[#7]=S=O	*	c1cc2sccc2n1
c1cc2ccccc2n1	[#6]-[#6](=O)- c1ccc(F)cc1	[#6]-[#6](-[#6])=O
[#6]-[#14](-[#6])- [#8][Si]([#6])([#6])[#8]	[#6]-[#14](-[#6])- [#8][Si]([#6])([#6])[#8] [Si]([#6])([#6])[#8]	c:c:c
[#8][Na]	O=[#6]-1-[#6]=[#6]- [#6]=[#6]-1	[#7]-*
O=[#6]-[#8]-[#6]=O	[#7]-c1ccccc1-[#7]	[#6]-[#6](=O)-[#6]=O
Cl[#6]-[#6]-1-[#6]-[#8]-1	[#7]-c1ccccc1-[#16]- [*,#1]	[#14]-[#7]-c1ccccc1-[#8]- [#14]
[#6]-[#6](=O)-[#7]-[#7]	[#16]-[#6](Cl)=O	[#7]-[#7]-c1ccccc1
[#6]-[#6](=O)C#C	[#6]-[#7]-1-[#6]-[#6]-1	[#6]-[#16]
[#6][N]#N	[#8]-[#15](-[#8])=O	[#6]-[#6](-[#7])=S
Br[#6]-[#6]=O	[#8]-[#6]=O	c1nnnn1
[#7]-c1ccccc1-[#6]=O	[#6]-[#6](=O)- c1ccccc1	O=[#6]-1-[#6]-[#6]-[#6](=O)- [#6]-[#6]-1
[#7]-c1ccccc1-[#6](-[#8])=O	[#6]-[#6]-1-[#6]-[#8]-1	Cl[#6](-*)=O

[#7]-c1cccc(-[#8])c1	[#7]-[#6]-[#6]-[#6]-[#8]	[#7]-[#6]-[#6]-[#6]-[#6]-[#8]
[#7]-[#6]-c1cccc1-[#8]	[#7]-c1cccc2ccc(-[#8])cc12	[#16]-*
*-[#6]=C=[#6]	[#6]-[#6]-[#8]-[#6](-[#8]-[#6]-[#6])-[#8]-[#6]-[#6]	*C#C
-[#6]=[#6]	[,#1]C#C[*,#1]	[*,#1]-[#6]=[#6]-[*,#1]
*	C#N	[#6]-[#6](=O)-[#8]-*
[F,Cl,Br,I]-c1cccc1	[#8]-*	[#14]-[F,Cl,Br,I]
[F,Cl,Br,I,#1]-c1cccs1	[#7]-[#6](=O)-[#6]-[F,Cl,Br,I]	[#7]-[F,Cl,Br,I,#1]
*-[#8]-[F,Cl,Br,I,#1]	*-[F,Cl,Br,I]	[#8]-[#6](=O)-*~*-[#6](-[#8])=O

S3. Description of C5.0 algorithm

C5.0 classifier² is a data-mining tool designed to analyze substantial databases containing millions of records. It can be used to classify a given dataset into discrete classes depending on discrete- or continuous- valued descriptors. C5.0 is highly interpretable because C5.0 classifiers are expressed as decision trees or set of rules. C5.0 is selected as the machine-learning tool of PolyName2Structure system because chemical reactions are highly related to some specific patterns present in the chemical structures. If a rule-based training tool was used, then it will be easier to know which pattern plays an important role in chemical reactions by looking into the decision trees or the set of rules generated by C5.0.

C5.0 was developed as an improved version of its ancestor C4.5³. Compared to C4.5, C5.0 not only generates more accurate rules with less time and memory, but also includes several new techniques, such as boosting. The C5.0 classifier contains an easy-to-use command-line interface. Detailed description of C5.0 is in its published tutorial⁴.

C5.0 can generate classifiers based on decision trees or set of rules. In this study, however, the performance of these two kinds of classifiers shows no big difference. Besides, the classifiers based on set of rules can be much easier than decision trees to track the prediction process. Therefore, the set of rules is selected to generate classifiers as the prediction models of PolyName2Structure system.

Boosting is an innovative technique included in C5.0. It is based on the work, adaptive boosting, of Rob Schapire and Yoav Freund⁵. The idea is to generate multiple

classifiers rather than just one. Then, when a case needs to be classified, each classifier votes for its predicted class, and the class that has the most votes is the final class of the case.

To generate multiple classifiers for a single dataset, the first step is to generate a classifier as default setting. Then, the second step is to generate a classifier that focuses on the error cases of the first classifier. After that, the third classifier adopts the same principle: focusing on the error cases of the second classifier. The later classifiers will do the same procedure: focusing on the error cases of previous classifier. This process will continue until the pre-determined number of trials is reached, or the most recent classifier is either extremely accurate or inaccurate.

The default boosting option, specified by "-b" option, will generate 10 classifiers and vote to determine the class of any given case. In this study, every model uses the default "-b" option to generate 10 classifiers. The performances of models significantly increase with boosting options. Increasing the number of classifiers does not make explicit improvement in the performances of models when the number is at least 10. Therefore, the default "-b" option is used to train machine learning models.

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