S1. Bioprivileged Starting Molecules (SMILES)

C=C(C(=C)C(=O)O)C(=O)O
C=C(C(=O)O)C(=O)CCC
C=C(C(=O)O)C(C)C(=O)O
C=C(C)C(=O)C(C)CO
C=C(C)C(=O)CO
C=C(C)C(=O)OC(C)(O)CO
C=C(C)C(=O)OC=CC(=O)O
C=C(C)C(O)CO
C=C(C)C=C(C)CO
C=C(C=O)COC
C=C(CC(=O)O)C(=O)O
C=C(CC(=O)O)C(C)=O
C=C(CC(C)C(=O)O)C(=O)O
C=C(CCC(=O)O)CC(=O)O
C=C(CCC=CO)C(=O)O
C=C(CO)C(C)=O
C=C(CO)CCO
C=C(CO)OCOC
C=C(COC)C(=O)O
C=C(O)CC=C(C)C(=O)O
C=C(O)CCC(=C)C(=O)O
C=C1C(=O)OCC1C(=O)O
C=C1C(=O)OCC1O
C=C1CC(CO)OC1=O
C=C1CC(O)CC(=O)O1
C=CC(=O)C(=O)CCC
C=CC(=O)C(C)=O
C=CC(=O)C(C)O
C=CC(=O)C(CC)C(=O)O
C=CC(=O)CC(=O)O
C=CC(=O)CCO
C=CC(=O)CCOC=O
C=CC(=O)COC
C=CC(C)(O)C(=O)O
C=CC(C)(O)C=O
C=CC(C)(O)CO
C=CC(CCC(=O)O)C(=O)O
C=CC(O)C(C)O
C=CC(O)C1CO1
C=CC(O)CCO
C=CC(O)COC
C=CCC(=O)C(=O)O
C=CCC(C(=O)O)=C(C)O
C=CCC(C=O)C=O
C=CCC(O)=C(C)C(=O)O
C=CCC(O)C1CO1
C=CCC(O)CO
CC(=CC(=O)O)C(=O)O
CC(=CC(=O)O)CC(=O)O
CC(=CCC=CO)C(=O)O
CC(=CCCC(=O)O)C(=O)O
CC(=CCO)C(=O)O
CC(=CCO)C(C)C(=O)O
CC(=CCO)CCC(=O)O
CC(=CCO)CO
CC(=O)C(C(=O)O)C(C)C(=O)O
CC(=O)C(C)(O)CO
CC(=O)C(C)C(=O)O
CC(=O)C(C)C=O
CC(=O)C(CCC(=O)O)C(=O)O
CC(=O)C1(O)CCOC1=O
CC(=O)C1C(=O)OC1C
CC(=O)C1CC(=O)OC1=O
CC(=O)C=C(C)C(=O)O
CC(=O)C=CCC(=O)O
CC(=O)C=CCO
CC(=O)CCC(=O)O
CC(C(=O)O)=C(C)C(=O)C(=O)O
CC(C(=O)O)C(=O)C(=O)O
CC(C(=O)O)C(C)(O)C(=O)O
CC(C(=O)O)C(C)C(=O)C(=O)O
CC(C=CC(=O)O)C(=O)O
CC(C=CCC(=O)O)C(=O)O
CC(C=O)CC(=O)O
CC(C=O)CCO
CC(CC(=O)C(=O)O)C(=O)O
CC(CC(=O)O)=C(C)C(=O)O
CC(CC(=O)O)C(=O)C(=O)O
CC(CCC(=O)O)C(=O)C(=O)O
CC(CO)C(=O)C(=O)O
CC(CO)CC=O
CC(O)(CO)CCO
CC(O)C(C)(O)CO
CC(O)C(C)C(=O)O
CC(O)C(C)C=O
CC(O)C=CCO
CC(O)CC1OC1CO
CC(O)CCC(=O)O
CC(O)c1ocCC(=O)c1O
CC1(C(=O)O)CCC(O)CO1
CC1(O)C(=O)COC1=O
CC1(O)C(=O)OCC1O
CC1(O)COC(=O)C1O
CC1=C(C(=O)O)COC1=O
CC1=C(O)OC(=O)C1(C)O
CC1OC1CC(O)CO
CC1OC=CC(=O)C1=O
CC=C(CC=CO)C(=O)O
CC=C(CCC(=O)O)C(=O)O
CC=C(CO)C(=O)O
CC=C(COC=O)C(=O)O
CC=CC(=O)C(=O)O
CC=CC(C)(O)C(=O)O
CC=CC(CC(=O)O)C(=O)O
CC=CC(O)C(=O)O
CC=CC(O)CO
CCC(=CCO)C(=O)O
CCC(=O)C(=O)CO

CCC(=O)C(OC)C(=O)O
CCC(=O)C=C(C)C(=O)O
CCC(=O)C=CC(C)=O
CCC(=O)C=CCO
CCC(=O)C=CCOC
CCC(=O)CC(=O)O
CCC(C(=O)O)C(=O)C(=O)O
CCC(C(=O)O)C(=O)CC(=O)O
CCC(C(=O)O)C(O)C(=O)O
CCC(C)(O)C=O
CCC(C)=C(CO)C(=O)O
CCC(C)C(=O)C(=O)C(=O)O
CCC(C)C(O)C(=O)CO
CCC(C=CCO)C(=O)O
CCC(C=O)(CO)COC
CCC(C=O)CO
CCC(CC(=O)C(=O)O)OC
CCC(CC(=O)O)C(=O)C(=O)O
CCC(CC(O)C(=O)O)OC
CCC(CO)(CC(=O)O)OC
CCC(CO)(OC)C(=O)O
CCC(O)(CC(=O)O)OC
CCC(O)(COC=O)C(=O)O
CCC(O)C(=O)CO
CCC(O)CC=O
CCC=C(CC(=O)O)C(=O)O
CCCC(=CC(=O)O)C(=O)O
CCCC(C(=O)O)C(=O)C(=O)O
CCCC(C(=O)O)C(O)C(=O)O
CCCC(C=O)C(C)=O
CCCC(O)C=O
CCCC=C(CO)C(=O)O
CCCC=CC(=O)C=O
COC(=O)C(=O)C(C)O
COC(=O)C(C)(O)C=O
COC(=O)C(C)(O)CC(=O)O
COC(=O)C(C)=CC=O
COC(=O)C(C)C(=O)CC(=O)O
COC(=O)C(C)CC=O
COC(=O)C(C=O)OC
COC(=O)C(O)C(C)CC(=O)O
COC(=O)C(O)CCO
COC(=O)C=CCCC=O
COC(=O)C=CCO
COC(=O)CC(=O)C(=O)C(=O)OC
COC(=O)CC(=O)CO
COC(=O)CC(O)CC(=O)O
COC(=O)CC(O)CCC(=O)O
COC(=O)CCC(=O)CO
COC(=O)CCC(O)CC(=O)O
COC(=O)c1cc(C=O)co1
COC(=O)c1ccc(C(=O)O)o1
COC(=O)c1ccoc1C=O
COC(=O)c1coc(C=O)c1
COC(=O)c1cocc1C=O
COC(C(=O)O)=C(C)C(=O)O
COC(C)(CO)C(=O)O
COC(C)=C(C(C)=O)C(=O)O
COC(C)C(C(C)=O)C(=O)O
COC(CC(=O)O)C(C)=O
COC(CO)C(C)O
COC(CO)c1ccco1
COC1(C)OCC(C=O)O1
COC1C(C)OC(CO)C1O
COC1C(CO)OC(C)C1O
COC1CC(O)C(CO)O1
COC1COC(C)C(O)C1O
COC1COC(C=O)C1OC
COC1OC(CO)C2OC12
COCC(=O)c1ccco1
COCC(C)(O)C(=O)O
COCC(C=O)OC
COCC(O)C(C)O
COCC1OC(C)C(O)C1O
COCC1OC(O)CC1O
COCC1OCC2OC2C1O
COCC=CC=O
COCCC(=O)C(=O)O
COCCC(=O)C(C)C(=O)O
COCCC(=O)CO
COCCC(C)(O)C(=O)O
COCCCCC(O)C(=O)O
COCc1cc(=O)c(O)co1
COCc1ccc(C(=O)O)o1
COCc1ccc(C=O)o1
COCc1ccc(CO)o1
COCc1ccoc1C(=O)O
COCc1ccoc1C=O
COCc1ccoc1CO
COCc1cocc1C(=O)O
COCc1occc(=O)c1O
COc1c(C(=O)O)occc1=O
COc1cc(CO)oc(=O)c1
COc1ccc(CO)o1
COc1coc(C(=O)O)cc1=O
COc1coc(C=O)cc1=O
COc1coc(CO)cc1=O
Cc1cc(C(=O)O)c(C(=O)O)o1
Cc1cc(O)cc(=O)o1
Cc1cc(O)oc(=O)c1
Cc1ccc(C(O)C(=O)O)o1
Cc1oc(=O)cc(O)c1O
Cc1oc(CO)cc1C(=O)O
Cc1occ(C(=O)O)c1C(=O)O
O=C(CCO)CCC1CO1
O=C(O)C(=O)Cc1ccco1
O=C(O)C(O)C1CCCO1
O=C(O)C(O)CCCC(O)C(=O)O
O=C(O)C(O)c1ccco1
O=C(O)C(O)c1ccoc1
O=C(O)C1=CC=COC1
O=C(O)C1=CCOC=C1
O=C(O)C1=COC=CO1
O=C(O)C1=COCC=C1

O=C(O)C1CC(O)CCO1
O=C(O)C1CC(O)CO1
O=C(O)C1CCC(O)CO1
O=C(O)C1COCC(O)C1
O=C(O)C1COCC1=O
O=C(O)C1COCCC1=O
O=C(O)C=CC1CO1
O=C(O)C=CC=CC(=O)O
O=C(O)CC1C=CC(=O)O1
O=C(O)CC1OC(=O)CC1O
O=C(O)CC=CCO
O=C(O)CCC1CC1=O
O=C(O)CCCC(O)C(=O)O
O=C(O)CCCCC(O)C(=O)O
O=C(O)CCCOCO
O=C(O)Cc1ccc(C(=O)O)o1
O=C(O)Cc1occc1C(=O)O
O=C(O)c1cc(=O)cco1
O=C(O)c1ccc(=O)oc1
O=C(O)c1ccoc(=O)c1
O=C(O)c1coccc1=O
O=C1C=C(C(=O)O)CO1
O=C1C=C(CCO)O1
O=C1C=C(CO)CO1
O=C1C=C(CO)OC1
O=C1C=CC(CCO)O1
O=C1C=CCC(CO)O1
O=C1C=CCOC1O
O=C1C=COC1CO
O=C1C=COCC1=O
O=C1CC(O)(CO)CO1
O=C1CC(O)CC(CO)O1
O=C1CC=C(CCO)O1
O=C1CCC(C(O)CO)O1
O=C1CCOC(C(=O)O)C1
O=C1CCOCC1O
O=C1COC(CO)C1
O=C1COCCC1O
O=C1OC(CO)CC1O
O=C1OC=CC1CO
O=C1OCC=C1CO
O=C1OCCC1(O)CO
O=CC1(C(=O)O)CCCO1
O=CC1=CC=COC1
O=CC1=CCOC=C1
O=CC1=CCOCC1
O=CC1=COC=CO1
O=CC1=COCC=C1
O=CC1=COCCC1=O
O=CC1C=CCCO1
O=CC1CC=CCO1
O=CC1OCCC1C(=O)O
O=CC=CC1CO1
O=CCc1ccco1
O=COCC(=O)CC(=O)O
O=COCCCC=CC(=O)O
O=Cc1ccc(CO)o1
O=Cc1ccco1
O=c1cc(O)cc(CO)o1
OC1C2COC(O2)C1O
OC1C=CC2OCC1O2
OC1COC(C2CO2)C1O
OC1COC2COC1C2O
OCC(O)C1CCCCO1
OCC(O)CC1CO1
OCC(O)CCC1CO1
OCC1C=CC(O)O1
OCC1OC(O)C2OC12
OCC1OC1C(O)C1CO1
OCC1OC=CC1O
OCC1OCC=CC1O
OCC1OCCC1O
OCC=CCCO
OCCC1(CO)CO1
OCc1ccoc1CO

S2. Corrosion Inhibitors Produced with Limited Reactions and Complex Helper Molecules (SMILES)

O=C(O)CCCCCO
O=C(Br)CCCCCO
CCOCC1CCCO1
COC(=O)C(C)C(C)C(=O)O
O=C(O)c1ccoc1
CCC(C)C(O)C(C)=O
CCC(C)CC(C)=O
CC(O)(CO)C(O)CO
CCC(C)CO
CCC(CO)(CO)CO
CCC(CO)(CO)OC
CCOC(C)CC
CC(=O)OCC(C)C
NC1C2COC1C(O)CO2
O=C1C2COC1C(O)CO2
OC1COC2COC1C2
OC1COC2COC1C2O
CCC(CO)(OC)C(=O)O
CCC(CO)C(C)=O
CCCCC(=O)O
Cc1cc(Sc2ncn[nH]2)cc(=O)o1
Cc1cc(Sc2ncns2)cc(=O)o1
CC(=O)C(C(=O)O)C(C)O
O=C(O)CCCCO
CC(O)CCCN
CC(N)CCC(C)O
COCCCCC(=O)O
CC(=O)OC1CCCC1=O
O=C(O)CCCO
COCCCC(=O)O
CCC(O)CC(C)=O
O=C(O)c1ccco1
CCC(O)C(C)O
CC(C(=O)O)C(O)C(=O)O
CC(=O)C1CCOC1O
CC(O)C1CCOC1=O
CC(C(=O)O)C(C)C(O)CO
CC(O)C(C)C(C)C(=O)O
CCC(C)CCO
O=C1CCC(=O)OC1
CC(C)(O)CC(C)(O)CO
O=C(CO)C(O)C(O)CO
COc1cc(CSc2nc3ccccc3[nH]2)oc(=O)c1
CC(N)CC1CC(=O)OC1=O
CC(O)CC1CC(=O)OC1=O
COCCC(C)(O)C(C)(O)O
CCCC(C)C(C)=O
CC=CC=CCCCOC
CC(CO)C(C)C(=O)O
COc1ccc(CSc2nc3ccccc3[nH]2)o1
CC1CCCC(=O)OC1=O
C=CC=CCCC
C=CCCCCC
COC(C)(CO)C(=O)O
COC(C)(CO)CO
CCOCC1CCOC1=O
CC(=O)C1CCOC1
CC(N)C(O)C(C)C(=O)O
CC=CC(O)C(CO)OCC
CC(=O)C1CC(=O)O1
NCC1CCCCO1
C=C(C)C(=O)OCC
CCOC(C)COC
COc1coc(CSc2ncn[nH]2)cc1=O

S3. Expanded Reaction Family List with Operator SMARTS

Operator Name	Operator SMARTS
Hydrogenation of Alkene	[C+0:1]=[C+0:2].[H][H]>>[*:1][*:2]
Oxidative Cleavage of Alkenes	[C+0:1]=!@[C+0:2].[O+0:4]=[O+0:5]>>[*:1]=[*:4].[*:2]=[*:5]
Oxidative Cleavage of Alkenes, Intramolecular	[C+0:1]=@[C+0:2].[O+0:4]=[O+0:5]>>([*:1]=[*:4].[*:2]=[*:5])
Olefin Cross Metathesis (CM)	[C+0:1]=!@[C+0:2].[C+0:3]=!@[C+0:4]>>[*:1]=[*:3].[*:2]=[*:4]
Olefin Ring-Opening Metathesis (ROM) 1	[C+0:1]=@[C+0:2].[C+0:3]=!@[C+0:4]>>([*:1]=[*:3].[*:2]=[*:4])
Olefin Ring-Opening Metathesis (ROM) 2	[C+0:1]=@[C+0:2].[C+0:3]=!@[C+0:4]>>([*:1]=[*:3].[*:2]=[*:3]).([*:1]=[*:4].[*:2]=[*:4])
Olefin Ring-Closing Metathesis (RCM)	([C+0:1]=!@[C+0:3].[C+0:2]=!@[C+0:4])>>[*:1]=[*:2].[*:3]=[*:4]
Reductive Cross-Coupling of Alkenes	[C+0:1]=[C+0:2].[C+0:3]=[C+0:4].[H][H]>>[*:1][*:2][*:3][*:4]
Epoxidation of Alkene	[C+0:1]=[C+0:2].[O+0:3]=[O+0]>>[*:1]1[*:2][*:3]1
Hydration of Alkene, Ethers from Addition of Alcohols to Alkenes	[C+0:1]=[C+0:2].[O+0!H0;!$(*C=O):3]>>[*:1][*:2][*:3]
Ethers from Addition of Alcohols to Alkenes, Intramolecular	([C+0:1]=[C+0:2].[O+0H:3][C!$(*=O)+0:4])>>[*:1][*:2][*:3][*:4]
Hydrohalogenation of Alkenes	[C+0:1]=[C+0:2].[F,Cl,Br,I;+0H:3]>>[*:1][*:2][*:3]
Halogenation of Alkenes	[C+0:1]=[C+0:2].[F,Cl,Br,I;+0:3][F,Cl,Br,I;+0:4]>>[*:1]([*:3])[*:2][*:4]
Diels-Alder Reaction with Alkenes	[C+0:1]=[C+0:2][C+0:3]=[C+0:4].[C+0:5]=[C+0:6]>>[*:1]1[*:2]=[*:3][*:4][*:6][*:5]1
Diels-Alder Reaction with Alkenes, Intramolecular	([C+0:1]=[C+0:2][C+0:3]=[C+0:4].[C+0:5]=[C+0:6])>>[*:1]1[*:2]=[*:3][*:4][*:6][*:5]1
Diels-Alder Reaction with Alkynes	[C+0:1]=[C+0:2][C+0:3]=[C+0:4].[C+0:5]#[C+0:6]>>[*:1]1[*:2]=[*:3][*:4][*:6]=[*:5]1
Diels-Alder Reaction with Alkynes, Intramolecular	([C+0:1]=[C+0:2][C+0:3]=[C+0:4].[C+0:5]#[C+0:6])>>[*:1]1[*:2]=[*:3][*:4][*:6]=[*:5]1
Halohydrin Formation	[C+0:1]=[C+0:2].[F,Cl,Br,I;+0:3][F,Cl,Br,I;+0:4].[O+0H2:5]>>[*:1]([*:5])[*:2][*:3].[*:4]
Diol Formation by Oxidation	[C+0:1]=[C+0:2].[O+0:3]=[O+0].[O+0H2:4]>>[*:1]([*:3])[*:2][*:4]
Conjugated Dienes 1,4	[C+0:1]=[C+0:2][C+0:3]=[C+0:4].[F,Cl,Br,I;+0

Addition with Hydrogen Halide	H:5]>>[*:5][*:1][*:2]=[*:3][*:4]
Conjugated Dienes 1,4 Addition with Halogens	[C+0:1]=[C+0:2][C+0:3]=[C+0:4].[F,Cl,Br,I;+0:5][F,Cl,Br,I;+0:6]>>[*:5][*:1][*:2]=[*:3][*:4][*:6]
Claisen Rearrangement, Cope Rearrangements	[C+0:1]=[C+0:2][O,C;+0:3][C+0:4][C+0:5]=[C+0:6]>>[*:3]=[*:2][*:1][*:6][*:5]=[*:4]
Aromatic Claisen Rearrangement 1	[c+0H:1]1:[c+0:2]:[c+0:3]:[c+0:4]:[c+0:5]:[c+0:6]:1[O+0:7][C+0:8][C+0:9]=[C+0:10]>>[*:1]1([*:10][*:9]=[*:8]):[*:2]:[*:3]:[*:4]:[*:5]:[*:6]:1-[*:7]
Aromatic Claisen Rearrangement with Ortho Substituents	[c+0H0:1]1:[c+0:2]:[c+0:3]:[c+0:4]:[c+0H0:5]:[c+0:6]:1[O+0:7][C+0:8][C+0:9]=[C+0:10]>>[*:1]1:[*:2]:[*:3]([*:8][*:9]=[*:10]):[*:4]:[*:5]:[*:6]:1-[*:7]
Tsuji–Trost Reaction, Nu = Active Methylenes	[C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]-!@[F,Cl,Br,I,O$(*C=O);+0:4].[C+0:5](=[O+0:6])[C+0!H0:7][C+0:8]=[O+0:9]>>[*:1]=[*:2][*:3][*:7]([*:5]=[*:6])[*:8]=[*:9].[*:4]
Tsuji–Trost Reaction, Nu = Enolates	[C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]!@[F,Cl,Br,I,O$(*C=O);+0:4].[C+0:5][C+0!H0:7][C+0;!$(*CC=O):8]=[O+0:9]>>[*:1]=[*:2][*:3][*:7]([*:5])[*:8]=[*:9].[*:4]
Tsuji–Trost Reaction, Nu = Amines	[C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]!@[F,Cl,Br,I,O$(*C=O);+0:4].[N+0!H0:7][C,c;+0:8]>>[*:1]=[*:2][*:3][*:7][*:8].[*:4]
Tsuji–Trost Reaction, Nu = Phenols	[C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]@[F,Cl,Br,I,O$(*C=O);+0:4].[O+0H:7][c+0:8]>>[*:1]=[*:2][*:3][*:7][*:8].[*:4]
Intramolecular Tsuji-Trost Reaction, Nu = Active Methylenes	([C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]!@[F,Cl,Br,I,O$(*C=O);+0:4].[C+0:5](=[O+0:6])[C+0!H0:7][C+0:8]=[O+0:9])>>[*:1]=[*:2][*:3][*:7]([*:5]=[*:6])[*:8]=[*:9].[*:4]
Intramolecular Tsuji-Trost Reaction, Nu = Enolates	([C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]!@[F,Cl,Br,I,O$(*C=O);+0:4].[C+0:5][C+0!H0:7][C+0;!$(*CC=O):8]=[O+0:9])>>[*:1]=[*:2][*:3][*:7]([*:5])[*:8]=[*:9].[*:4]
Intramolecular Tsuji-Trost Reaction, Nu = Amines	([C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]!@[F,Cl,Br,I,O$(*C=O);+0:4].[N+0!H0:7][C,c;+0:8])>>[*:1]=[*:2][*:3][*:7][*:8].[*:4]
Intramolecular Tsuji-Trost Reaction, Nu = Phenols	([C+0:1]=[C+0:2][C+0;!$(*[OH]);!$(*=O):3]!@[F,Cl,Br,I,O$(*C=O);+0:4].[O+0H:7][c+0:8])>>[*:1]=[*:2][*:3][*:7][*:8].[*:4]
Alcohols React with Hydrogen Halides to form	[C+0:1][O+0H:2].[F,Cl,Br,I;+0H:3]>>[*:1][*:3].[*:2]

Haloalkanes, Carboxylic Acids Conversion to Acid Chlorides	
Haloalkane Hydrolysis, Acid Chlorides Hydrolysis, Haloarenes Hydrolysis	[C,c;+0:1][F,Cl,Br,I;+0:2].[O+0H2:3]>>[*:1][*:3].[*:2]
Wurtz Reaction, Coupling of Halides with Gilman Reagent	[C,c;+0:1][F,Cl,Br,I;+0:2].[C,c;+0:3][F,Cl,Br,I;+0:4]>>[*:1][*:3].[*:2][*:4]
Wurtz Reaction, Coupling of Halides with Gilman Reagent, Intramolecular	([C,c;+0:1][F,Cl,Br,I;+0:2].[C,c;+0:3][F,Cl,Br,I;+0:4])>>[*:1][*:3].[*:2][*:4]
Dehydrohalogenation	[C+0:1]([F,Cl,Br,I;+0:2])[C+0!H0:3]>>[*:1]=[*:3].[*:2]
Aromatic Halogenation	[c+0H:1].[F,Cl,Br,I;+0:2][F,Cl,Br,I;+0:3]>>[*:1][*:2].[*:3]
Friedel–Crafts Reaction	[c+0H:1].[CX4,C$(*=O);+0:2][F,Cl,Br,I;+0:3]>>[*:1][*:2].[*:3]
Friedel–Crafts Reaction, Intramolecular	([c+0H:1].[CX4,C$(*=O);+0:2][F,Cl,Br,I;+0:3])>>[*:1][*:2].[*:3]
Friedel–Crafts Acylation with Carboxylic Acids	[c+0H:1].[C$(*=O)+0:2][O+0H:3]>>[*:1][*:2].[*:3]
Friedel–Crafts Acylation with Carboxylic Acids, Intramolecular	([c+0H:1].[C$(*=O)+0:2][O+0H:3])>>[*:1][*:2].[*:3]
Friedel–Crafts Acylation with Acid Anhydrides	[c+0H:1].[C$(*=O)+0:2][O+0:3]!@[C$(*=O)+0:4]>>[*:1][*:2].[*:3][*:4]
Friedel–Crafts Reaction with Alkenes	[c+0H:1].[C+0:2]=[C+0:3]>>[*:1][*:2][*:3]
Friedel–Crafts Reaction with Alkenes, Intramolecular	([c+0H:1].[C+0:2]=[C+0:3])>>[*:1][*:2][*:3]
Heck Reaction	[C+0:1]=[C+0!H0:2].[C,c;+0:3][F,Cl,Br,I;+0:4]>>[*:1]=[*:2][*:3].[*:4]
Heck Reaction, Intramolecular	([C+0:1]=[C+0!H0:2].[C,c;+0:3][F,Cl,Br,I;+0:4])>>[*:1]=[*:2][*:3].[*:4]
Suzuki Coupling with Boranes from Alkyl, Alkenyl, or Aryl Halides	[c,C!$(*~O);!$(*#*);+0:1][F,Cl,Br,I;+0].[c,C$(*=,#C);+0:2][F,Cl,Br,I;+0]>>[*:1][*:2]
Suzuki Coupling with Boranes from Alkenes	[C+0:1]=[C+0:2].[c,C$(*=,#C);+0:3][F,Cl,Br,I;+0]>>[*:1]-[*:2][*:3]
Suzuki Coupling with Boranes from Alkynes	[C+0:1]#[C+0:2].[c,C$(*=,#C);+0:3][F,Cl,Br,I;+0]>>[*:1]=[*:2][*:3]
Reduction of Haloalkanes	[CX4,c;+0:1][F,Cl,Br,I;+0:2].[H][H]>>[*:1].[

	*:2]
Grignard Reagent with Oxiranes	[c,C!$(*~O);!$(*#*);+0:1][F,Cl,Br,I;+0].[C+0:2]1[C+0:3][O+0:4]1>>[*:1][*:2][*:3][*:4]
Dichlorocarbene with Alkenes	[C+0H:1]([F,Cl,Br,I;+0:2])([F,Cl,Br,I;+0:3])[F,Cl,Br,I;+0:4].[C+0:5]=[C+0:6]>>[*:1]1([*:2])([*:3])[*:5][*:6]1.[*:4]
Simmons-Smith Reaction	[C+0H2:1]([F,Cl,Br,I;+0:2])[F,Cl,Br,I;+0:3].[C+0:5]=[C+0:6]>>[*:1]1[*:5][*:6]1.[*:2].[*:3]
Esterification with Alkyl and Aryl Halides	[C+0:2](=[O+0:3])[O+0H:4].[CX4,c;+0:5][F,Cl,Br,I;+0:6]>>[*:2](=[*:3])[*:4][*:5].[*:6]
Esterification with Alkyl and Aryl Halides, Intramolecular	([C+0:2](=[O+0:3])[O+0H:4].[CX4,c;+0:5][F,Cl,Br,I;+0:6])>>[*:2](=[*:3])[*:4][*:5].[*:6]
Glycol Cleavage by Oxidation	[C+0:1]([O+0H:5])!@[C+0:2][O+0H:6].[O+0:3]=[O+0]>>[*:1]=[*:5].[*:2]=[*:6].[*:3]
Glycol Cleavage by Oxidation Intramolecular	[C+0:1]([O+0H:5])@[C+0:2][O+0H:6].[O+0:3]=[O+0]>>([*:1]=[*:5].[*:2]=[*:6]).[*:3]
Hydrodeoxygenation of Alcohol, Classic Synthesis of Aldehydes from Carboxylic Acids	[C,c;+0:1][O+0H:2].[H][H]>>[*:1].[*:2]
Dehydration of Alcohol	[C+0!H0:1][C+0:2][O+0H:3]>>[*:1]=[*:2].[*:3]
Dehydration of Alcohol, 2-step	([C+0!H0:1][C+0:2][O+0H:3].[C+0!H0:4][C+0:5][O+0H])>>([*:1]=[*:2].[*:4]=[*:5]).[*:3]
Selective Oxidation of Alcohols	[C+0!H0:1][O+0H:2].[O+0:3]=[O+0]>>[*:1]=[*:2].[*:3]
Diol Carboxylation	[O+0H:1][C+0:2][C+0:3][O+0H:4].[O+0:5]=[C+0:6]=[O+0:7]>>[*:1].[*:2]1[*:3][*:4][*:6](=[*:7])[*:5]1
Diol Carboxylation 2	[O+0H:1][C+0:2][C+0:8][C+0:3][O+0H:4].[O+0:5]=[C+0:6]=[O+0:7]>>[*:1].[*:2]1[*:8][*:3][*:4][*:6](=[*:7])[*:5]1
Hydrogenolysis of Primary Alcohol	[C+0:1][C+0H2:3][O+0H:2].[H][H]>>[*:1].[*:3].[*:2]
Pinacol Rearrangement, no H on Carbon#2	[C+0:1][C+0:2]([C+0:3])([O+0H:4])[C+0X4:5][O+0H:8]>>[*:1][*:2](=[*:4])[*:5]([*:3]).[*:8]
Pinacol Rearrangement, 1 H on Carbon#2	[C+0H:2]([C+0:3])([O+0H:4])[C+0X4:5][O+0H:8]>>[*:2](=[*:4])([*:3])[*:5].[*:8]
Pinacol Rearrangement, 2 Hs on Carbon#2	[C+0H2:2]([O+0H:4])[C+0X4:5][O+0H:8]>>[*:2](=[*:4])[*:5].[*:8]
Dehydration of Geminal Diol	[C+0:1]([O+0H:2])[O+0H:3]>>[*:1]=[*:2].[*:3]
Formation of Acetals from	[C+0X4:1]([O+0H0X2:2])[O+0H:3].[O+0H:4][C+0X

Hemiacetals	4;!$(*OC):5]>>[*:1]([*:2])[*:4][*:5].[*:3]
Oxidation Of Primary Alcohols to Carboxylic Acids	[C+0;H3,H2:1][O+0H:2].[O+0:3]=[O+0:4]>>[*:1](=[*:3])[*:2].[*:4]
Oxidation Of Primary Alcohols to Carboxylic Acids, 2-step	([C+0;H3,H2:1][O+0H:2].[C+0;H3,H2:5][O+0H:6]).[O+0:3]=[O+0:4]>>([*:1](=[*:3])[*:2].[*:5](=[*:6])[O]).[*:4]
Formation of Cyclic Acetals from Ketones/Aldehydes with Diols	[C+0X3!$(*O):1]=[O+0:2].[O+0H:3][C+0X4:4][C+0X4:5][O+0H:6]>>[*:1]1[*:3][*:4][*:5][*:6]1.[*:2]
Hydrolysis of Ethers, Esters, Anhydrides	[C,c;+0:1][O+0:2]!@[C,c;+0:3].[O+0H2:4]>>[*:1][*:2].[*:3][*:4]
Hydrolysis of Ethers, Esters, Anhydrides, Intramolecular	[C,c;+0:1][O+0:2]@[C,c;+0:3].[O+0H2:4]>>([*:1][*:2].[*:3][*:4])
Hydrogenolysis of Ethers	[C,c;+0;!$(*=O):1]!@[O+0:2][C,c;+0;!$(*=O):3].[H][H]>>[*:1].[*:2][*:3]
Hydrogenolysis of Ethers Intramolecular	[C,c;+0;!$(*=O):1]@[O+0:2][C,c;+0;!$(*=O):3].[H][H]>>([*:1].[*:2][*:3])
Williamson Ether Synthesis, Ullmann Condensation	[C,c;!$(*=O);+0:1][O+0H:2].[CX4!H0,c;+0:3][F,Cl,Br,I;+0:4]>>[*:1][*:2][*:3].[*:4]
Williamson Ether Synthesis, Ullmann Condensation, Intramolecular	([C,c;!$(*=O);+0:1][O+0H:2].[CX4!H0,c;+0:3][F,Cl,Br,I;+0:4])>>[*:1][*:2][*:3].[*:4]
Ether Cleavage	[C,c;+0;!$(*=O):1][O+0:2]!@[C;+0;!$(*=O):3].[F,Cl,Br,I;+0H:4]>>[*:1][*:2].[*:3][*:4]
Ether Cleavage, Intramolecular	[C,c;+0;!$(*=O):1][O+0:2]@[C;+0;!$(*=O):3].[F,Cl,Br,I;+0H:4]>>([*:1][*:2].[*:3][*:4])
Ether Synthesis by Dehydration	[C,c;!$(*=O);+0:1][O+0H:2].[C,c;!$(*=O);+0:3][O+0H:4]>>[*:1][*:2][*:3].[*:4]
Ether Synthesis by Dehydration, Intramolecular	([C,c;!$(*=O);+0:1][O+0H:2].[C,c;!$(*=O);+0:3][O+0H:4])>>[*:1][*:2][*:3].[*:4]
Epoxides Ring Opening	[C+0:1]1[C+0:2][O+0:3]1.[O+0!H0;!$(*C=O):4]>>[*:4][*:1][*:2][*:3]
Aldehyde Oxidation	[C+0!H0:1]=[O+0:2].[O+0:3]=[O+0]>>[*:1](=[*:2])[*:3]
Aldehyde Oxidation, 2-step	([C+0!H0:1]=[O+0:2].[C+0!H0:5]=[O+0:6]).[O+0:3]=[O+0:4]>>([*:1](=[*:2])[*:3].[*:5](=[*:6])[*:4])
Aldehyde & Alcohol	([C+0!H0:1]=[O+0:2].[C+0;H3,H2:5][O+0H:6]).[

Oxidation, 2-step	O+0:3]=[O+0:4]>>([*:1](=[*:2])[*:3].[*:5](=[*:6])[O]).[*:4]
Ketone Oxidation	[C,c;+0:1][C+0:2](=[O+0:3])!@[C+0H2:4][C,c;+0:5].[O+0:6]=[O+0:7]>>[*:1][*:2](=[*:3])[*:6].[*:5][*:4](=[*:7])[O]
Ketone Oxidation, Intramolecular	[C,c;+0:1][C+0:2](=[O+0:3])@[C+0H2:4][C,c;+0:5].[O+0:6]=[O+0:7]>>([*:1][*:2](=[*:3])[*:6].[*:5][*:4](=[*:7])[O])
Baeyer-Villiger Oxidation (Ketones)	[C,c;+0:5][C+0:1](=[O+0:2])[C,c;+0:3].[O+0:4]=[O+0]>>[*:5][*:1](=[*:2])[*:4][*:3]
Baeyer-Villiger Oxidation (Aldehydes)	[C+0H:1](=[O+0:2])[C$(*(C)(C)C),C$(*=*),C$(*c),c;+0:3].[O+0:4]=[O+0]>>[*:1](=[*:2])[*:4][*:3]
Hydrogenation of Ketones	[C+0!$(*-O):1]=[O+0:2].[H][H]>>[*:1][*:2]
Keto-enol Tautomerization	[C,N;+0!H0:1][C+0:2]=[O,N;+0:3]>>[*:1]=[*:2][*:3]
Keto-enol Tautomerization Reverse	[C,N;+0:1]=[C+0:2][O,N;+0!H0:3]>>[*:1][*:2]=[*:3]
Decarbonylation of Aldehydes	[*+0:1][C+0H:2]=[O+0:3]>>[*:1].[*-:2]#[*+:3]
Ketonization	[*+0:1][C+0:2](=[O+0:3])[O+0H:4].[*+0:5][C+0:6](=[O+0:7])[O+0H:8]>>[*:1][*:2](=[*:3])[*:5].[*:4]=[*:6]=[*:7].[*:8]
Ketonization, Intramolecular	([*+0:1][C+0:2](=[O+0:3])[O+0H:4].[*+0:5][C+0:6](=[O+0:7])[O+0H:8])>>[*:1][*:2](=[*:3])[*:5].[*:4]=[*:6]=[*:7].[*:8]
Oxidative Esterification of Aldehydes and Alcohols	[C+0;!$(*=O):5][O+0H:1].[O+0:2]=[C+0!H0:3].[O+0:4]=[O+0]>>[*:5][*:1][*:3]=[*:2].[*:4]
Oxidative Esterification of Aldehydes and Alcohols, Intramolecular	([C+0;!$(*=O):5][O+0H:1].[O+0:2]=[C+0!H0:3]).[O+0:4]=[O+0]>>[*:5][*:1][*:3]=[*:2].[*:4]
McMurry Reaction	[*+0:1][C+0;!$(*O):2](=[O+0:3]).[*+0:5][C+0;!$(*O):6](=[O+0:7]).[H][H]>>[*:1][*:2]=[*:6][*:5].[*:3].[*:7]
McMurry Reaction, Intramolecular	([*+0:1][C+0;!$(*O):2](=[O+0:3]).[*+0:5][C+0;!$(*O):6](=[O+0:7])).[H][H]>>[*:1][*:2]=[*:6][*:5].[*:3].[*:7]
Hydration of Ketone and Aldehyde	[C+0;!$(*O):2]=[O+0:3].[O+0H2:4]>>[*:2]([*:3])[*:4]
Hemiacetal Dissociation, Addition of Alcohols to Carbonyl Groups Reverse	[C;!$(*=O):1]([O+0H:2])!@[O+0:3][C;!$(*=O):4]>>[*:1]=[*:2].[*:3][*:4]
Hemiacetal Dissociation, Addition of Alcohols to Carbonyl Groups Reverse,	[C;!$(*=O):1]([O+0H:2])@[O+0:3][C;!$(*=O):4]>>([*:1]=[*:2].[*:3][*:4])

Intramolecular	
Hemiacetal Formation, Addition of Alcohols to Carbonyl Groups	[CX3;!$(*O):1]=[O+0:2].[O+0H:3][C;!$(*=O):4]>>[*:1]([*:2])[*:3][*:4]
Hemiacetal Formation, Addition of Alcohols to Carbonyl Groups	([C;!$(*O):1]=[O+0:2].[O+0H:3][C;!$(*=O):4])>>[*:1]([*:2])[*:3][*:4]
Reduction of Carbonyl Groups	[C,c,N;+0:1][C+0:2]=[O+0:3].[H][H]>>[*:1][*:2].[*:3]
a-Halogenation	[C+0:2](=[O+0:3])[C+0!H0:4].[F,Cl,Br,I;+0:5][F,Cl,Br,I;+0:6]>>[*:2](=[*:3])[*:4][*:5].[*:6]
Wittig Reaction (Combined with Ylide Formation)	[C+0!H0;!$(*~[O,S,N]):1][F,Cl,Br,I;+0].[C,c;+0:3][C+0;!$(*O):4]=[O+0]>>[*:1]=[*:4][*:3]
Wittig Reaction, Intramolecular (Combined with Ylide Formation)	([C+0!H0;!$(*~[O,S,N]):1][F,Cl,Br,I;+0].[C,c;+0:3][C+0;!$(*O):4]=[O+0])>>[*:1]=[*:4][*:3]
Carboxylic Acids Decarboxylation	[*+0:1][C+0:2](=[O+0:3])[O+0H:4]>>[*:1].[*:3]=[*:2]=[*:4]
Acid Anhydrides React with Alcohols to Form Esters	[C+0;!$(*[OH]):1](=[O+0:2])[O+0!R:3][C+0;!$(*[OH]):4](=[O+0:5]).[C,c;+0;!$(*=O):6][O+0H:7]>>[*:1](=[*:2])[*:3][*:6].[*:4](=[*:5])[*:7]
Acid Anhydrides React with Alcohols to Form Esters, Intramolecular	[C+0;!$(*[OH]):1](=[O+0:2])[O+0R:3][C+0;!$(*[OH]):4](=[O+0:5]).[C,c;+0;!$(*=O):6][O+0H:7]>>([*:1](=[*:2])[*:3][*:6].[*:4](=[*:5])[*:7])
Aldol Condensation	[C+0:2](=[O+0:3])[C+0!H0:4].[O+0:5]=[C+0X3:6]>>[*:2](=[*:3])[*:4][*:6]([*:5])
Aldol Condensation, Intramolecular	([C+0:2](=[O+0:3])[C+0!H0:4].[O+0:5]=[C+0X3:6])>>[*:2](=[*:3])[*:4][*:6]([*:5])
Aldol Condensation (2H)	[C+0:2](=[O+0:3])[C+0;H3,H2:4].[O+0:5]=[C+0X3:6]>>[*:2](=[*:3])[*:4]=[*:6].[*:5]
Aldol Condensation (2H), Intramolecular	([C+0:2](=[O+0:3])[C+0;H3,H2:4].[O+0:5]=[C+0X3:6])>>[*:2](=[*:3])[*:4]=[*:6].[*:5]
Claisen Condensation	[C+0:2](=[O+0:3])!@[O+0:7][C+0:4].[O+0:5]=[C+0:6][C+0!H0:8]>>[*:2](=[*:3])[*:8][*:6]=[*:5].[*:7][*:4]
Dieckmann Condensation	([C+0:2](=[O+0:3])!@[O+0:7][C+0:4].[O+0:5]=[C+0:6][C+0!H0:8])>>[*:2](=[*:3])[*:8][*:6]=[*:5].[*:7][*:4]
Michael Reaction	[C+0:1](=[O+0:2])[C+0!H0:3][C+0:4]=[O+0:5].[C+0:6]=[C+0:7][C+0:8]=[O+0:9]>>[*:1](=[*:2])[*:3]([*:6][*:7][*:8]=[*:9])[*:4]=[*:5]

Michael Reaction, Intramolecular	([C+0:1](=[O+0:2])[C+0!H0:3][C+0:4]=[O+0:5].[C+0:6]=[C+0:7][C+0:8]=[O+0:9])>>[*:1](=[*:2])[*:3]([*:6][*:7][*:8]=[*:9])[*:4]=[*:5]
Michael Reaction with Cyclic Ketones	[C+0:1]1(=[O+0:2])[C+0!H0:3][C+0:10][C+0:11][C+0:12][C+0:13]1.[C+0:6]=[C+0:7][C+0:8]=[O+0:9]>>[*:1]1(=[*:2])[*:3]([*:10][*:11][*:12][*:13]1)[*:6][*:7][*:8]=[*:9]
Michael Reaction with Cyclic Ketones, Intramolecular	([C+0:1]1(=[O+0:2])[C+0!H0:3][C+0:10][C+0:11][C+0:12][C+0:13]1.[C+0:6]=[C+0:7][C+0:8]=[O+0:9])>>[*:1]1(=[*:2])[*:3]([*:10][*:11][*:12][*:13]1)[*:6][*:7][*:8]=[*:9]
Robinson Annulation	[C+0:1]1(=[O+0:2])[C+0!H0:3][C+0:14][C+0:15][C+0:16][C+0:17]1.[C+0:8]=[C+0:9][C+0:10](=[O+0:11])[C+0;H2,H3:12]>>[*:1]12[*:3]([*:8][*:9][*:10](=[*:11])[*:12]=2)[*:14][*:15][*:16][*:17]1.[*:2]
Esterification, Acid Anhydride Formation	[C+0:2](=[O+0:3])[O+0H:4].[C,c;+0:5][O+0H:6]>>[*:2](=[*:3])[*:6][*:5].[*:4]
Esterification, Acid Anhydride Formation, Intramolecular	([C+0:2](=[O+0:3])[O+0H:4].[C,c;+0:5][O+0H:6])>>[*:2](=[*:3])[*:6][*:5].[*:4]
Esterification of Acid Halides	[C+0:1](=[O+0:2])[F,Cl,Br,I;+0:3].[C,c;!$(*=O);+0:4][O+0H:5]>>[*:1](=[*:2])[*:5][*:4].[*:3]
Esterification of Acid Halides, Intramolecular	([C+0:1](=[O+0:2])[F,Cl,Br,I;+0:3].[C,c;!$(*=O);+0:4][O+0H:5])>>[*:1](=[*:2])[*:5][*:4].[*:3]
Ester Reduction to Aldehydes and Alcohols	[O+0H0!R:1][C+0:2]=[O+0:3].[H][H]>>[*:1].[*:2]=[*:3]
Ester Reduction to Aldehydes and Alcohols, Intramolecular	[O+0H0R:1][C+0:2]=[O+0:3].[H][H]>>([*:1].[*:2]=[*:3])
Ester Reduction to Alcohols	[O+0H0!R:1][C+0:2]=[O+0:3].[H][H]>>[*:1].[*:2][*:3]
Ester Reduction to Alcohols, Intramolecular	[O+0H0R:1][C+0:2]=[O+0:3].[H][H]>>([*:1].[*:2][*:3])
Transesterification	[C+0:1](=[O+0:2])!@[O+0:3][*+0:4].[*+0:6][O+0H;!$(*C=O):5]>>[*:1](=[*:2])[*:5][*:6].[*:4][*:3]
Transesterification, Intramolecular	([C+0:1](=[O+0:2])!@[O+0:3][*+0:4].[*+0:6][O+0H;!$(*C=O):5])>>[*:1](=[*:2])[*:5][*:6].[*:4][*:3]
Kolbe Carboxylation	[c+0:1]1:[c+0:2]([O+0H:7]):[c+0H:3]:[c+0:4]:[c+0:5]:[c+0:6]:1.[O+0:8]=[C+0:9]=[O+0:10]>>[*:1]1:[*:2]([*:7]):[*:3]([*:9](=[*:8])[*:10

	]):[*:4]:[*:5]:[*:6]:1
Phenols Oxidation to Quinones 1	[c+0;!$(*~O):1]1:[c+0:2]([O+0H:7]):[c+0;!$(*~O):3]:[c+0;!$(*~O):4]:[c+0H:5]:[c+0;!$(*~O):6]:1.[O+0:8]=[O+0:9]>>[*:1]1[*:2](=[*:7])[*:3]=[*:4][*:5](=[*:8])[*:6]=1.[*:9]
Phenols Oxidation to Quinones 2	[c+0;!$(*~O):1]1:[c+0:2]([O+0H:7]):[c+0H;!$(*~O):3]:[c+0;!$(*~O):4]:[c+0:5]([*;!O+0:10]):[c+0;!$(*~O):6]:1.[O+0:8]=[O+0:9]>>[*:1]1[*:2](=[*:7])[*:3](=[*:8])[*:4]=[*:5]([*:10])[*:6]=1.[*:9]
Phenols Oxidation to Quinones 3	[c+0;!$(*~O):1]1:[c+0:2]([O+0H:7]):[c+0:3]([O+0H:8]):[c+0;!$(*~O):4]:[c+0;!$(*~O):5]:[c+0;!$(*~O):6]:1.[O+0:9]=[O+0]>>[*:1]1[*:2](=[*:7])[*:3](=[*:8])[*:4]=[*:5][*:6]=1.[*:9]
Phenols Oxidation to Quinones 3 Reverse	[C+0:1]1[C+0:2](=[O+0:7])[C+0:3](=[O+0:8])[C+0:4]=[C+0:5][C+0:6]=1.[H][H]>>[*:1]1:[*:2]([*:7]):[*:3]([*:8]):[*:4]:[*:5]:[*:6]:1
Phenols Oxidation to Quinones 4	[c+0;!$(*~O):1]1:[c+0:2]([O+0H:7]):[c+0;!$(*~O):3]:[c+0;!$(*~O):4]:[c+0:5]([O+0H:8]):[c+0;!$(*~O):6]:1.[O+0:9]=[O+0]>>[*:1]1[*:2](=[*:7])[*:3]=[*:4][*:5](=[*:8])[*:6]=1.[*:9]
Phenols Oxidation to Quinones 4 Reverse	[C+0:1]1[C+0:2](=[O+0:7])[C+0:3]=[C+0:4][C+0:5](=[O+0:8])[C+0:6]=1.[H][H]>>[*:1]1:[*:2]([*:7]):[*:3]:[*:4]:[*:5]([*:8]):[*:6]:1
Quinones Addition	[C+0:1]1[C+0:2](=[O+0:7])[C+0:3]=[C+0H:4][C+0:5](=[O+0:8])[C+0:6]=1.[F,Cl,Br,I;+0H:9]>>[*:1]1:[*:2]([*:7]):[*:3]:[*:4]([*:9]):[*:5]([*:8]):[*:6]:1
Naphthalene Oxidation with CrO3	[c+0:1]1:[c+0H:2]:[c+0:3]([c+0:9][c+0:10][c+0:11][c+0:12]2):[c+0:4]2:[c+0H:5]:[c+0:6]:1.[O+0:7]=[O+0:8]>>[*:1]1[*:2](=[*:7])[*:3](:[*:9]:[*:10]:[*:11]:[*:12]:2)=[*:4]2[*:5](=[O])[*:6]=1.[*:8]
Naphthalene Oxidation with V2O5 Catalyst	[c+0:1]1:[c+0:2]:[c+0:3]([c+0H:9][c+0H:10][c+0H][c+0H:12]2):[c+0:4]2:[c+0:5]:[c+0:6]:1.[O+0:7]=[O+0:8]>>[*:1]1:[*:2]:[*:3]([C:9](=[O])[O]):[*:4]([C:12](=[O])[O]):[*:5]:[*:6]:1.[*:7]=[C:10]=[O].[*:8]
Oxidation of Aromatic Alkanes Ar-CH3	[c+0:1][C+0H3:2].[O+0:3]=[O+0:4]>>[*:1][*:2](=[*:3])[O].[*:4]
Oxidation of Aromatic Alkanes Ar-CH2CH3	[c+0:1][C+0H2:2][C+0H3:3].[O+0:4]=[O+0:5]>>[*:1][*:2](=[*:4])[O].[O]=[*:3]=[O].[*:5]
Oxidation of Aromatic Alkanes Ar-(CH3)CH3	[c+0:1][C+0H:2]([C+0H3:3])[C+0H3].[O+0:4]=[O+0:5]>>[*:1][*:2](=[*:4])[O].[O]=[*:3]=[O].[*:5]
Oxidation of Aromatic	[c+0:1][C+0H2:2]!@[C+0H2:3][C+0!H3:4].[O+0:5

Alkanes Ar-long_chain	]=[O+0:6]>>[*:1][*:2](=[*:5])[O].[*:4][*:3](=[O])[O].[*:6]
Oxidation of Aromatic Alkanes Ring-opening 1	[c+0:1][C+0H2:2]@[C+0H2:3].[O+0:4]=[O+0:5]>>([*:1][*:2](=[*:4])[O].[*:3](=[O])[O]).[*:5]
Oxidation of Aromatic Alkanes Ring-opening 2	[c+0:1][C+0H:2]@=[C+0H:3].[O+0:4]=[O+0:5]>>([*:1][*:2](=[*:4])[O].[*:3](=[*:5])[O])
Oxidation of Aromatic Alkanes Ar-CH3, 2-step	([c+0:1][C+0H3:2].[c+0:5][C+0H3:6]).[O+0:3]=[O+0:4]>>([*:1][*:2](=[*:3])[O].[*:5][*:6](=[O])[O]).[*:4]
Oxidation of Aldehyde & Aromatic Alkanes, 2-step	([C+0!H0:1]=[O+0:2].[c+0:5][C+0H3:6]).[O+0:3]=[O+0:4]>>([*:1](=[*:2])[*:3].[*:5][*:6](=[O])[O]).[*:4]
Oxidation of Alcohol & Aromatic Alkanes, 2-step	([C+0;H3,H2:1][O+0H:2].[c+0:5][C+0H3:6]).[O+0:3]=[O+0:4]>>([*:1](=[*:2])[*:3].[*:5][*:6](=[O])[O]).[*:4]
Halogenation of Aromatic Alkanes	[c+0:1][C+0!H0:2].[F,Cl,Br,I;+0:3][F,Cl,Br,I;+0:4]>>[*:1][*:2][*:3].[*:4]
Electrophilic Aromatic Alkylation with Alkenes	[c+0H:1].[C+0:2]=[C+0:3]>>[*:1][*:2][*:3]
Electrophilic Aromatic Alkylation with Alkenes, Intramolecular	([c+0H:1].[C+0:2]=[C+0:3])>>[*:1][*:2][*:3]
Electrophilic Aromatic Alkylation with Alcohols	[c+0H:1].[C+0;!$(*=O):2][O+0H:3]>>[*:1][*:2].[*:3]
Electrophilic Aromatic Alkylation with Alcohols, Intramolecular	([c+0H:1].[C+0:2][O+0H:3])>>[*:1][*:2].[*:3]
Furan Carboxylation	[o+0:1]1:[c+0H:2]:[c+0:3]:[c+0:4]:[c+0:5]:1.[O+0:8]=[C+0:9]=[O+0:10]>>[*:1]1:[*:2]([*:9](=[*:8])[*:10]):[*:3]:[*:4]:[*:5]:1
Furan Carboxylation, 2-step	[o+0:1]1:[c+0H:2]:[c+0:3]:[c+0:4]:[c+0H:5]:1.[O+0:8]=[C+0:9]=[O+0:10]>>[*:1]1:[*:2]([*:9](=[*:8])[*:10]):[*:3]:[*:4]:[*:5]([C](=[O])[O]):1
Friedel-Crafts Hydroxyalkylation	[c+0H:1].[CX3!$(*O)+0:2]=[O+0:3]>>[*:1][*:2][*:3]
Friedel-Crafts Hydroxyalkylation, Intramolecular	([c+0H:1].[CX3!$(*O)+0:2]=[O+0:3])>>[*:1][*:2][*:3]
Friedel-Crafts Hydroxyalkylation(BPA Synthesis)	[c+0H:1].[c+0H:2].[CX3!$(*O)+0:3]=[O+0:4]>>[*:1][*:3][*:2].[*:4]
Hydroformylation	[C+0:1]=[C+0:2].[C1]#[O+1].[H][H]>>[*:1][*:2][C]=[O]
Cativa Process	[C!$(*=O)+0:1][O+0H:2].[C1]#[O+1]>>[*:1][C](

	=[O])[*:2]
Oxidative Carbonylation 1	[C!$(*=O)+0:1][O+0H:2].[C!$(*=O)+0:5][O+0H:6].[C1]#[O+1].[O+0:7]=[O+0]>>[*:1][*:2][C](=[O])[*:6][*:5].[*:7]
Oxidative Carbonylation 2	[C!$(*=O)+0:1][O+0H:2].[C!$(*=O)+0:5][O+0H:6].[C1]#[O+1].[O+0:7]=[O+0]>>[*:1][*:2][C](=[O])[C](=[O])[*:6][*:5].[*:7]
Hydrocarboxylation 1, Hydroesterification(Carboalkoxylation)	[C+0:1]=[C+0:2].[C1]#[O+1].[O+0!H0;!$(*C=O):5]>>[*:1][*:2][C](=[O])[*:5]
Hydrocarboxylation 2	[C+0:1]#[C+0:2].[C1]#[O+1].[O+0H2:5]>>[*:1]=[*:2][C](=[O])[*:5]
Dehydration of Amides	[C+0:1](=[O+0:2])[N+0H2:3]>>[*:1]#[*:3].[*:2]
Ketone Reductive Amination	[CX3!$(*[O,S,N])+0:2](=[O+0:3]).[N+0X3!H0:6].[H][H]>>[*:2][*:6].[*:3]
Ketone Reductive Amination, Intramolecular	([CX3!$(*[O,S,N])+0:2](=[O+0:3]).[N+0X3!H0:6]).[H][H]>>[*:2][*:6].[*:3]
Alkylation or Acylation of Amines	[C,c;+0:1][F,Cl,Br,I;+0:2].[NX3!H0,nH;+0:3]>>[*:1][*:3].[*:2]
Alkylation or Acylation of Amines, Intramolecular	([C,c;+0:1][F,Cl,Br,I;+0:2].[NX3!H0,nH;+0:3])>>[*:1][*:3].[*:2]
Alkylation of Tertiary Amines	[C,c;+0:1][F,Cl,Br,I;+0:2].[NX3H0+0:3]>>[*:1][*+1:3].[*-1:2]
Amine Alkylation with Alcohols or Primary Amines	[C,c;!$(*=O)+0:1][OH,NH2;+0:2].[NX3!H0,nH;+0:3]>>[*:1][*:3].[*:2]
Amine Alkylation with Alcohols or Primary Amines, Intramolecular	([C,c;!$(*=O)+0:1][OH,NH2;+0:2].[NX3!H0,nH;+0:3])>>[*:1][*:3].[*:2]
Synthesis of Amides with Carboxylic Acid	[CX3+0:2](=[O+0:3])[O+0H:4].[N+0X3!H0:5]>>[*:2](=[*:3])[*:5].[*:4]
Synthesis of Amides with Carboxylic Acid, Intramolecular	([CX3+0:2](=[O+0:3])[O+0H:4].[N+0X3!H0:5])>>[*:2](=[*:3])[*:5].[*:4]
Synthesis of Amides with Acid Anhydrides or Esters	[CX3+0:2](=[O+0:3])!@[O+0:4][C,c;+0:6].[N+0X3!H0:5]>>[*:2](=[*:3])[*:5].[*:4][*:6]
Synthesis of Amides with Acid Anhydrides or Esters, Intramolecular	([CX3+0:2](=[O+0:3])!@[O+0:4][C,c;+0:6].[N+0X3!H0:5])>>[*:2](=[*:3])[*:5].[*:4][*:6]
Hydrolysis of Amides	[CX3!$(*[OH,SH])+0:2](=[O+0:3])!@[N+0X3:5].[O+0H2:4]>>[*:2](=[*:3])[*:4].[*:5]
Hydrolysis of Amides,	[CX3!$(*[OH,SH])+0:2](=[O+0:3])@[N+0X3:5].[O

Intramolecular	+0H2:4]>>([*:2](=[*:3])[*:4].[*:5])
Hofmann Elimination R-NH2	[C+0X4!H0:1][CX4+0:2][N+0H2:3].[C+0:4][F,Cl,Br,I;+0:5]>>[*:1]=[*:2].[*:3]([*:4])([*:4])[*:4].[*:5]
Hofmann Elimination R-NHR	[C+0X4!H0:1][CX4+0:2]!@[N+0H:3].[C+0:4][F,Cl,Br,I;+0:5]>>[*:1]=[*:2].[*:3]([*:4])[*:4].[*:5]
Hofmann Elimination R-NHR Ringopening	[C+0X4!H0:1][CX4+0:2]@[N+0H:3].[C+0:4][F,Cl,Br,I;+0:5]>>([*:1]=[*:2].[*:3]([*:4])[*:4]).[*:5]
Hofmann Elimination R-NRR	[C+0X4!H0:1][CX4+0:2]!@[N+0X3H0:3].[C+0:4][F,Cl,Br,I;+0:5]>>[*:1]=[*:2].[*:3][*:4].[*:5]
Hofmann Elimination R-NRR Ringopening	[C+0X4!H0:1][CX4+0:2]@[N+0X3H0:3].[C+0:4][F,Cl,Br,I;+0:5]>>([*:1]=[*:2].[*:3][*:4]).[*:5]
Hofmann Rearrangement	[C,c;+0:1][C+0:2](=[O+0:3])[N+0H2:5].[F,Cl,Br,I;+0:6][F,Cl,Br,I;+0].[O+0H2:4]>>[*:1][*:5].[*:3]=[*:2]=[*:4].[*:6]
Hofmann Rearrangement with Alcohols	[C,c;+0:1][C+0:2](=[O+0:3])[N+0H2:5].[F,Cl,Br,I;+0:6][F,Cl,Br,I;+0].[C+0!$(*=[O,S]):7][O+0H:4]>>[*:1][*:5][*:2](=[*:3])[*:4][*:7].[*:6]
Hydroamination of Alkenes	[C+0:1]=[C+0:2].[N+0X3!H0:3]>>[*:1][*:2][*:3]
Hydroamination of Alkenes, Intramolecular	([C+0:1]=[C+0:2].[N+0X3!H0:3])>>[*:1][*:2][*:3]
Hydroamination of Alkynes	[C+0:1]#[C+0:2].[N+0X3!H0:3]>>[*:1]=[*:2][*:3]
Hydroamination of Alkynes, Intramolecular	([C+0:1]#[C+0:2].[N+0X3!H0:3])>>[*:1]=[*:2][*:3]
Hydroamination of Dienes	[C+0:1]=[C+0:2][C+0:3]=[C+0:4].[N+0X3!H0:5]>>[*:1][*:2]=[*:3][*:4][*:5]
Hydroamination of Dienes, Intramolecular	([C+0:1]=[C+0:2][C+0:3]=[C+0:4].[N+0X3!H0:5])>>[*:1][*:2]=[*:3][*:4][*:5]
Ring Opening of Epoxides by Amines	[C+0:1]1[C+0:2][O+0:3]1.[N+0X3!H0:4]>>[*:4][*:1][*:2][*:3]
Aromatic Nitrosation	[OH,N$(*([#6])([#6])[#6]);+0:10][c+0:1]1[c+0:2][c+0:3][c+0H:4][c+0:5][c+0:6]1.[O+0H:7][N+0:8]=[O+0:9]>>[*:10][*:1]1:[*:2]:[*:3]:[*:4]([*:8]=[*:9]):[*:5]:[*:6]:1.[*:7]
Secondary Amines with Nitrous Acid	[*+0:1][N+0H:2][*+0:3].[O+0H:4][N+0:5]=[O+0:6]>>[*:1][*:2]([*:5]=[*:6])[*:3].[*:4]
Primary Amines with Nitrous Acid to Alcohols	[C,c;+0:1][N+0H2:2].[O+0H:3][N+0:4]=[O+0:5]>>[*:1][*:3].[*:5].[*:2]#[*:4]

Primary Amines with Nitrous Acid to Halides	[C,c;+0:1][N+0H2:2].[F,Cl,Br,I;+0H:3].[O+0H][N+0:5]=[O+0:6]>>[*:1][*:3].[*:6].[*:2]#[*:5]
Primary Amines with Nitrous Acid to Alkenes	[C+0!H0:6][C+0:1][N+0H2:2].[O+0H][N+0:4]=[O+0:5]>>[*:6]=[*:1].[*:5].[*:2]#[*:4]
Tiffeneau–Demjanov Rearrangement	[O+0H:1][C+0:2]([C+0:3])([C+0:4])[C+0:5][N+0H2:6].[O+0H][N+0:7]=[O+0:8]>>[*:1]=[*:2]([*:3])[*:5][*:4].[*:8].[*:6]#[*:7]
Sandmeyer Cyanation	[c+0:1][N+0H2:2].[C+0H:3]#[N+0:4].[O+0H][N+0:5]=[O+0:6]>>[*:1][*:3]#[*:4].[*:6].[*:2]#[*:5]
Reduction of Primary Aromatic Amines	[c+0:1][N+0H2:2].[H][H].[O+0H][N+0:3]=[O+0:4]>>[*:1].[*:4].[*:2]#[*:3]
Cope Elimination	[C+0!H0:1][C+0:2]!@[N+0:3]([C+0:4])[C+0:5].[O+0]=[O+0:6]>>[*:1]=[*:2].[*:6][*:3]([*:4])[*:5]
Cope Elimination, Intramolecular	[C+0!H0:1][C+0:2]@[N+0:3]([C+0:4])[C+0:5].[O+0]=[O+0:6]>>([*:1]=[*:2].[*:6][*:3]([*:4])[*:5])
Hemiaminal Formation	[CX3!$(*O)+0:1]=[O+0:2].[N,n;+0X3!H0:3]>>[*:1]([*:2])[*:3]
Hemiaminal Formation, Reverse	[CX4!$(*(O)O)+0:1]([O+0H:2])!@[N+0X3:3]>>[*:1]=[*:2].[*:3]
Hemiaminal Dehydration	[C+0:1]([O+0H:2])[N+0X3!H0:3]>>[*:1]=[*:3].[*:2]
Hemiaminal Dehydration, Reverse	[C+0:1]=[N+0:3].[O+0H2:2]>>[*:1]([*:2])[*:3]
Reduction of Nitroso	[C,c;+0:1][N+0:2]=[O+0:3].[H][H]>>[*:1][*:2].[*:3]
Reduction of Nitro Compounds	[C,c;+0:1][N+1](=[O+0:3])[O1H0].[H][H]>>[*:1][N].[*:3]
Henry Reaction	[C+0!H0:1][N+1:2](=[O+0:3])[OX11:4].[CX3!$(*([OH])[OH])+0:5]=[O+0:6]>>[*:6][*:5][*:1][*:2](=[*:3])[*:4]
Henry Reaction, Intramolecular	([C+0!H0:1][N+1:2](=[O+0:3])[OX11:4].[CX3!$(*([OH])[OH])+0:5]=[O+0:6])>>[*:6][*:5][*:1][*:2](=[*:3])[*:4]
Benzene Nitration	[c+0H:1].[O+0H:2][N+1:3](=[O+0:4])[OX11:5]>>[*:1][*:3](=[*:4])[*:5].[*:2]
Oxidation of Nitroso	[*+0:1][N+0]=[O+0].[O+0]=[O+0]>>[*:1][N+1](=[O])[O-1]
Esterification, Acid Anhydride Formation with Nitric Acid	[C,c;+0:1][O+0H:2].[O+0H:3][N+1:4](=[O+0:5])[OX11:6]>>[*:1][*:2][*:4](=[*:5])[*:6].[*:3]
Nitrate Esters Hydrolysis	[C,c;+0:1][O+0:2][N+1:4](=[O+0:5])[OX11:6].[

	O+0H2:3]>>[*:1][*:2].[*:3][*:4](=[*:5])[*:6]
Imines from Aldehydes and Ketones	[CX3!$(*[OH])+0:1]=[O+0:2].[N+0X3;H2,H3:3]>>[*:1]=[*:3].[*:2]
Imines from Aldehydes and Ketones, Intramolecular	([CX3!$(*[OH])+0:1]=[O+0:2].[N+0X3;H2,H3:3])>>[*:1]=[*:3].[*:2]
Imines from Aldehydes and Ketones Reverse	[CX3!$(*[OH])+0:1]=!@[N+0:3].[O+0H2:2]>>[*:1]=[*:2].[*:3]
Imines from Aldehydes and Ketones, Intramolecular Reverse	[CX3!$(*[OH])+0:1]=@[N+0:3].[O+0H2:2]>>([*:1]=[*:2].[*:3])
Treatment of Aldehydes and Ketones with a Secondary Amine	[C,N;+0!H0:4][CX3!$(*[OH])+0:1]=[O+0:2].[N+0X3H:3]>>[*:4]=[*:1][*:3].[*:2]
Treatment of Aldehydes and Ketones with a Secondary Amine, Intramolecular	([C,N;+0!H0:4][CX3!$(*[OH])+0:1]=[O+0:2].[N+0X3H:3])>>[*:4]=[*:1][*:3].[*:2]
Treatment of Aldehydes and Ketones with a Secondary Amine Reverse	[C,N;+0:4]=[CX3!$(*[OH])+0:1]!@[NX3+0:3].[O+0H2:2]>>[*:4][*:1]=[*:2].[*:3]
Treatment of Aldehydes and Ketones with a Secondary Amine, Intramolecular Reverse	[C,N;+0:4]=[CX3!$(*[OH])+0:1]@[NX3+0:3].[O+0H2:2]>>([*:4][*:1]=[*:2].[*:3])
Oxime-Nitroso Tautomerization	[C+0:1]=[N+0:2][O+0H:3]>>[*:1][*:2]=[*:3]
Keto-enol Tautomerization Reverse	[C+0!H0:1][N+0:2]=[O+0:3]>>[*:1]=[*:2][*:3]
Reduction of Imines	[C+0:1]=[N+0:2].[H][H]>>[*:1][*:2]
Beckmann Rearrangement with Ketoximes	[C,c;+0:1][C+0:2](=[N+0:3][O+0H:4])[C,c;+0:5]>>[*:1][*:2](=[*:4])[*:3][*:5]
Beckmann Rearrangement with Aldoximes	[C,c;+0:1][C+0H:2](=[N+0:3][O+0H:4])>>[*:1][*:2]#[*:3].[*:4]
Beckmann Rearrangement from Ketones	[C,c;+0:1][C+0:2](=[O+0:3])[C,c;+0:4].[N+0H2:5][O+0H:6]>>[*:1][*:2](=[*:3])[*:5][*:4].[*:6]
Beckmann Rearrangement from Aldehydes	[C,c;+0:1][C+0H:2]=[O+0:3].[N+0H2:4][O+0H]>>[*:1][*:2]#[*:4].[*:3]
Beckmann Fragmentation	[C,c;+0:1][C+0:2](=[N+0:3][O+0H:4])!@[C+0:5]

	([C+0:6])([C+0:7])[*+0!H0:8]>>[*:1][*:2]#[*:3].[*:5]([*:6])([*:7])=[*:8].[*:4]
Beckmann Fragmentation, Intramolecular	[C,c;+0:1][C+0:2](=[N+0:3][O+0H:4])@[C+0:5]([C+0:6])([C+0:7])[*+0!H0:8]>>([*:1][*:2]#[*:3].[*:5]([*:6])([*:7])=[*:8]).[*:4]
Semmler–Wolff Reaction	[C+0!H0:1]1[C+0!H0:2][C+0!H0:3][C+0:4]=[C+0:5][C+0:6]1=[N+0:7][O+0H:8]>>[*:1]1[*:2]=[*:3][*:4]=[*:5][*:6]=1[*:7].[*:8]
Transimination	[C,c;+0:1]=!@[N!$(*[O,S])+0:2].[N!$(*[O,S]);H2,H3;+0:3]>>[*:1]=[*:3].[*:2]
Imine Metathesis	[C,c;+0:1]=!@[N!$(*[O,S])+0:2].[C,c;+0:3]=!@[N!$(*[O,S])+0:4]>>[*:1]=[*:4].[*:3]=[*:2]
Wolff–Kishner Reduction	[C,c;+0:1][C!$(*[O,S])+0:2](=[N+0:3][N+0H2:4])>>[*:1][*:2].[*:3]#[*:4]
Hydrosulfide Anion Substitution with Alkyl Halides	[C,c;+0:1][F,Cl,Br,I;+0:2].[S!H0X2+0:3]>>[*:1][*:3].[*:2]
Hydrosulfide Anion Substitution with Alkyl Halides, Intramolecular	([C,c;+0:1][F,Cl,Br,I;+0:2].[S!H0X2+0:3])>>[*:1][*:3].[*:2]

S4. Corrosion Inhibitors Produced with Many Reaction Families and Simple Helper Molecules (SMILES)

CC(O)(CO)C(O)CO
CCCC(C)C(C)=O
CCC(C)C(C)O
CCC(C)CO
CCC(C)CC(C)=O
CC(CO)C(C)C(=O)O
CC(CO)C(CO)C(=O)O
CC(CO)(CO)CCO
CCC(O)C(C)O
CC(=O)C(C)(CO)CO
CC(O)C(C)(CO)CO
CC(C)(O)C(C)(O)O
CC(O)(O)CCC(C)(O)CO
CC(C(=O)O)C(O)C(=O)O
C=C(C)C(O)COC(=O)CCO
CC(C)(CO)C(O)CO
CCOC(CO)C(C)=O
COC(=O)C(C)C(C)C(=O)O
CCCCC(C)(O)C(N)=O
CCC(C)CCO
O=C(O)CCCO
CC(=CCC(=O)O)C(N)=O
CCOC(C(=O)O)C(=O)O
O=C(O)CCCCCO
CCCC1COC(=O)O1
C=CC=CCCCO
C=CCC(=O)COC
C=CCC1COC(=O)O1
CC(O)CCCN
CCC(C)CC(C)O
CCC(C)CC(O)CN
CCOCC1CCCO1
O=C(O)CCCCO
CCCCC(=O)O
C=CC(=O)OCCOC(C)=O
C=CC(=O)OCCOCC
CC(C(=O)O)C(C)C(=O)OCCO
CCC(=O)CCCCCCCO
C=CC1CCOC1=O
CCCCCCCC(=O)O
C=CC1CC(=O)OC(=O)O1
C=CC=CCCC
C=CCOC(=O)C(CO)CCC
C=CC=CCCCCO
C=CC=CCCOCC
C=CCOC(=O)CCCCO
C=CC(=O)OCCCC
COCCCCC(=O)O
CC(=O)OC1CCCC1=O
COCCCC(=O)O
O=C(Br)CCCCCO
CCC(C)C
COC(C)(CO)C(=O)O
CCC(O)C(C)C
CC=CC1COC(=O)O1
CCC(CC)C(C)O
CCC(CO)(OC)C(=O)O
CCC(CO)C(C)=O
CCC(CC)(CO)CO
CCC(CO)(CO)C(=O)O
CCC(CO)(CO)C(=O)OC
CCC(CO)(CO)OC
CC=C(CO)C(=O)OCC
CCC(C)CC(=O)OC
CCCCC(C)CC
CCCCCCCC
C=C(C)COC(=O)CCCCO
CC(C(=O)O)C(C)C(O)CO
CC(O)C(C)C(C)C(=O)O
CCC(C)(C)OC(C)=O
CCOC(C)CC
CC(=O)OCC(C)C
CCC(C)COC(C)=O
CC(=O)C1CCOC1O
CC(=O)CC1COC1=O
COC(=O)OC(C)C(C)C(=O)O
CC(C(=O)O)C(C)C(N)O
CC(O)C1CCOC1=O
CC(O)CCCOCCCO
CC(C(N)=O)C(C)C(=O)O
CC(OC(=O)O)C(C)C(=O)O
CC(OC(N)=O)C(C)C(=O)O
COC(=O)NC(C)C(C)C(=O)O
C=C(C(C)=O)C(N)=O
CCC(CO)(CO)CO
CC(C)(O)CC(C)(O)CO
CC(O)(CO)CC(C)(O)CO
C=CC(F)C(=O)OC
CCC(F)C(=O)OC
C=CCOC(=O)C(CO)CCCC
CCC(=O)CCCCCO
CCC(C)C(O)C(C)=O
CCC(C)C(O)CN
CCC(C)CC(=O)CN
CCCC(C)OC(C)=O
CCC(O)CC(C)=O
C=C(C)C(=O)OCC
O=C(O)C(O)C(O)C(O)CO
CC1CCCC(=O)OC1=O
CC(=O)C1CC(=O)O1
CC=CC(=O)C(O)C(=O)O
O=C1CCC(=O)OC1
CCCCCCCCCC
CC(N)CCC(C)O
CCC(CC)OC(C)=O
O=C(O)CCCOCS

CC(=O)C1CCOC1
CC(=O)C1CCOC1C
CC(C)(O)C(C)(C)O
CC(=O)C1CCC(=O)N1
CC(=O)CC1CC(=O)OC1=O
O=C1COC(=O)OC(=O)C1
CCOCC1CCOC1=O
CCC(CO)(CO)CCO
CC(O)(O)C(C)(O)Br
CCC(C)CCOC
COCCCCCCC(C)O
CCOC(C)COC
CC(O)C(=O)OC(C)C(=O)O
CC(N)C(O)C(C)C(=O)O
CC=CCCCC
CCC(C)OC(=O)C(C)=O
CC(=O)C(C(=O)O)C(C)O
CCOCC1COC(=O)CO1
O=C(O)c1ccoc1
O=C(O)c1ccco1
COCC(O)(CO)CO
C=CC=CCCCOC
CC=CC=CCCCOC
NCC1CCCCO1
CC(N)CC1CC(=O)OC1=O
CC(O)CC1CC(=O)OC1=O
COC(C)(CO)CO
CC(C)(O)COC(C)(O)CO
C=CC(=O)OCC(CO)CCC
COC(=O)C(F)c1ccco1
C=CCCCCC
C=CC(=O)C1CC(=O)OC1=O
CNC(C)C1CC(=O)OC1=O
CC=CC(O)C(CO)OCC
OC1COC2COC1C2O
COC(CO)C(O)C(O)C(O)CO
COC1COC2C(O)COC12
OC1COC2C(O)CNC12
NC1C2COC1C(O)CO2
O=C1C2COC1C(O)CO2
O=C1OC2OCC1OCC2O
OC1COC2COC1C2
O=C(CO)C(O)C(O)CO
COCCC(C)(O)C(C)(O)O
C=CC(=O)OC(CO)CCCCC
C=Cc1c(OC)cc(CO)oc1=O
CCc1cc(CO)oc(=O)c1
COc1cc(CO)oc(=O)c1Br
COc1cc(CO)oc(=O)c1C
COc1cc(CO)oc(=O)c1N
COc1cc(CO)oc(=O)c1O
COc1cc(CO)oc(=O)c1OC
O=C(CO)C(O)C(O)(Br)CO
C=CCCCC
O=C1CCCC(=O)O1
CCCCC(C(=O)OC)C(=O)OC

S5. Corrosion Inhibitors Produced with Many Reaction Families and More Complex Helper Molecules

CC(=O)C(C(=O)O)C(C)O
CCC(CO)C(C)=O
O=C1OCC(CO)O1
CCC(C)C
CCC(C)CC(C)=O
CCC(C)CC(C)O
CCC(CC)C(C)O
CCC(O)C(C)O
C=C(C(C)=O)C(N)=O
CC(C(=O)O)C(O)C(=O)O
CCC(C)CO
CCCC(C)C(C)=O
CC(=O)C(C)(CO)CO
C=CC(=O)C1CC(=O)OC1=O
CC(=O)C1CCOC1
CC(=O)C1CCOC1O
CC(O)C1CCOC1=O
O=C(O)CCCO
C=CCOC(=O)C(CO)CCC
CC(=O)CC1COC1=O
CCC(C)C(C)O
CC(O)CCCN
C=CC=CCCC
C=CC=CCCCCO
CC(O)CCCOCCCO
CCCCC(C(=O)OC)C(=O)OC
COC(=O)C(C)C(C)C(=O)O
CCCC1COC(=O)O1
CCCCC(=O)O
CCC(C)CCO
CC=CC1COC(=O)O1
CCC(C)CC(O)CN
O=C(O)CCCCCO
O=C(O)CCCCO
CCOCC1CCCO1
C=CC=CCCCO
C=CCC1COC(=O)O1
CC=CC(=O)C(O)C(=O)O
CCOC(C)CC
CC(=O)C1CC(=O)O1
C=CC(=O)OCCOCC
CC(C(=O)O)C(C)C(=O)OCCO
CCC(=O)CCCCCCCO
C=C(C)C(=O)OCC
C=C(C)C(=O)OCC(CO)OC(=O)C(C)C
C=C(C)C(=O)OCC(O)COC(=O)C(C)C
CC(=CCC(=O)O)C(N)=O
CCCCC(C)CC
CCCCCCCC
C=CC(=O)OCCCC
CCC(O)CC(C)=O
CCCCCCCCCC
C=CCOC(=O)CCCCO
O=C(Br)CCCCCO
CC1CCCC(=O)OC1=O
C=CC1CC(=O)OC(=O)O1
CCC(CC)(CO)CO
CCC(CO)(CO)C(=O)O
O=C(O)C(O)C(O)C(O)CO
CCC(CO)(OC)C(=O)O
COCCCC(=O)O
O=C1CCC(=O)OC1
CC(O)(CO)C(O)CO
O=C(CO)C(CO)C(O)CO
C=CC(=O)OC(CO)CCCCC
O=C(O)CCCOCS
CC=CC(O)C(CO)OCC
OC1COC2COC1C2O
CC(C(=O)O)C(C)C(O)CO
CC(CO)C(C)C(=O)O
CC(O)C(C)C(C)C(=O)O
C=C(C)C(O)C(O)C(O)CO
CC(C(O)CO)C(O)C(=O)CO
COCCCCC(=O)O
CCCCC(C)(O)C(N)=O
CC(C)(O)CC(C)(O)CO
CC(O)(CO)CC(C)(O)CO
CC(C(N)=O)C(C)C(=O)O
C=CC(=O)OCC(CO)CCC
CCC(CO)(CO)CCO
CCOC(C)COC
COC(C)(CO)C(=O)O
CCC(O)C(C)C
CC(C)(CO)C(O)CO
CC(CO)C(CO)C(=O)O
CCOC(CO)C(C)=O
O=C(CC(O)CO)C(O)CO
CC(O)C(C)(CO)CO
COC(C)(CO)CO
CCc1cc(CO)oc(=O)c1
O=C(CO)C(O)C(O)(Br)CO
O=C(CO)C(O)C(O)CO
O=C(O)c1ccoc1
O=C(O)c1ccco1
C=Cc1c(OC)cc(CO)oc1=O
COc1cc(CO)oc(=O)c1Br
COc1cc(CO)oc(=O)c1C
COc1cc(CO)oc(=O)c1N
COc1cc(CO)oc(=O)c1O
COc1cc(CO)oc(=O)c1OC
C=CC1CCOC1=O
CC(O)COC(C)C(O)CCO
NC1C2COC1C(O)CO2
O=C1C2COC1C(O)CO2

O=C1OC2OCC1OCC2O
OC1COC2COC1C2
C=C(C)COC(=O)CCCCO
CC(CO)(CO)CCO
CC(N)C(O)C(C)C(=O)O
CCC(C)C(O)C(C)=O
C=CC(F)C(=O)OC
CCC(C)CC(=O)OC
CCC(F)C(=O)OC
O=C(OCC(O)CO)C(O)C(O)CO
CCOCC1CCOC1=O
CC(C)(O)C(C)(C)O
CC=C(CO)C(=O)OCC
O=C1CCCC(=O)O1
CC(C)(O)C(C)(O)O
CC(OC(=O)O)C(C)C(=O)O
CC(OC(=O)OCCO)C(C)C(=O)O
CC(OC(N)=O)C(C)C(=O)O
COC(=O)OC(C)C(C)C(=O)O
C=CCOC(=O)C(CO)CCCC
CC(C)(O)COC(C)(O)CO
CC(O)(CO)OC(=O)O
OC1COC2C(O)CNC12
CCC(CO)(CO)C(=O)OC
CCC(CO)(CO)CO
CC(C(=O)O)C(C)C(N)O
C=CC=CCCOCC
CCC(C)C(O)CN
CCC(C)CC(=O)CN
CCC(CO)(CO)OC
CCC(=O)CCCCCO
NCC1CCCCO1
COCCC(C(=O)CO)C(O)CO
CC(O)(O)C(C)(O)Br
CCC(C)CCOC
COCCCCCCC(C)O
CCOCC1COC(=O)CO1
CC(O)(C(=O)CO)C(O)CO
CC(O)C(=O)OC(C)C(=O)O
O=C1COC(=O)OC(=O)C1
CCCCCCCC(=O)O
CCOC(C(=O)O)C(=O)O
CC(=O)C1CCC(=O)N1
CC(=O)CC1CC(=O)OC1=O
COCC(O)(CO)CO
C=CC=CCCCOC
CC=CC=CCCCOC
CC(N)CC1CC(=O)OC1=O
CC(O)CC1CC(=O)OC1=O
CCCC(C)OC(C)=O
CC=CCCCC
CCC(C)OC(=O)C(C)=O
C=CCCCC
CCOC(=O)Cc1ccco1
C=CCCCCC