Structure	Name	CAS#	SMILES
H ₃ C Br	2-Acetoxy-2-methyl-propionyl bromide	40635-67-4	BrC(C(C)(OC(C)=O)C)=O
HO N N N N N N N N N N N N N N N N N N N	9-(2'-O-Acetyl-3'-bromo-3'-deoxy-β-D- xylofuranosyl)adenine	42867-78-7	Br[COH]1[COOH](CO)0[COOH](N2C(N=C N=C3N)=C3N=C2)[COOH]1OC(C)=O
сно	Benzo(b)thiophene-3-carboxaldehyde	5381-20-4	O=CC1=CSC2=C1C=CC=C2
CHO CF ₃	3,5-Bis(trifluoromethyl)-benzaldehyde	401-95-6	FC(C1=CC(C=O)=CC(C(F)(F)F)=C1)(F)F
CF ₃ CH ₂ Br	Bis(trifluoromethyl)-benzyl bromide	140690-56-8	FC(C1=CC(C(F)(F)F)=CC=C1CBr)(F)F
F ₃ C NHNH ₂ HCI	3,5-Bis(trifluoromethyl)phenylhydrazine hydrochloride	502496-23-3	NNC1=CC(C(F)(F)F)=CC(C(F)(F)F)=C1.Cl
O CH ₂ Br	2-Bromoacetophenone	186402-62-0	O=C(C1=CC=CC=C1)CBr
O CH ₃ CH ₃ Br	1-(2-Bromoacetyl)-5,5- dimethylpyrrolidin-2-one	NA	O=C1CCC(C)(C)N1C(CBr)=O

СНО	2-Bromo-6-chlorobenzaldehyde	64622-16-8	BrC1=C(C=O)C(CI)=CC=C1
CI F F Br	2-Bromo-2,2-difluoroacetyl chloride	3832-48-2	CIC(C(Br)(F)F)=O
OH F Br	2-Bromo-2,2-difluoro-N-{2-hydroxy-5- nitrophenyl)acetamide	NA	OC1=C(NC(C(F)(F)Br)=O)C=C([N+]([O-])=O)C=C1
Br F	α-Bromo-2,3-difluorotoluene	113211-94-2	FC1=C(CBr)C=CC=C1F
Br N CI	5-Bromo-2-chloropyrimidine	32779-36-5	CIC1=NC=C(Br)C=N1
HO N NH2	9-(3'-Bromo-3'-deoxy-β-D- xylofuranosyl)adenine	37731-73-0	Br[COH]1[COOH](CO)0[COOH](N2C(N=C N=C3N)=C3N=C2)[COOH]10
CHO Br F	2-Bromo-6-fluorobenzaldehyde	360575-28-6	FC1=CC=CC(Br)=C1C=O
F O CH ₂ Br	2-Bromo-1-(2-fluorophenyl)ethanone	655-15-2	FC1=CC=CC=C1C(CBr)=O

СНО	2-Bromo-3-hydroxybenzaldehyde	196081-71-7	OC1=CC=CC(C=O)=C1Br
СНО Вг	2-Bromo-3-methoxybenzaldehyde	10401-18-0	BrC1=C(C=O)C=CC=C1OC
Br OOH2	2-(2-(Bromomethyl)-3-(2- (bromomethyl)-6-methoxypyridin-3- yl)phenyl)-8-fluorophthalazin-1(2H)-one	NA	FC1=CC=CC2=C1C(N(C3=C(CBr)C(C4=CC=C (OC)N=C4CBr)=CC=C3)N=C2)=O
HO N Br	2-(Bromomethyl)-6-(hydroxymethyl)- pyridine	40054-0101	BrCC1=NC(CO)=CC=C1
F G Br	2-(Bromomethyl)-5- (trifluoromethyl)furan	17515-77	BrCC1=CC=C(C(F)(F)F)O1
CH ₂ Br	2-Bromo-4'- (trifluoromethoxy)acetophenone	103962-10-3	O=C(CBr)C1=CC=C(C(F)(F)F)C=C1
H ₃ C NH NH ₂ CIH	2-Butoxyethanimidamide hydrochloride	NA	OC1=NC(OCCCC)=NC(O)=C1
H ₃ C CH ₃ O CH ₂ Br	t-Butyl bromoacetate	5292-43-3	O=C(CBr)OC(C)(C)C

CHO H ₃ C CH ₃	3-t-Butyl-5-fluoro-benzaldehyde	1123172-37-1	CC(C)(C)C1=CC(C=O)=CC(F)=C1
CHO CF ₃	4-t-Butyl-2-fluoro-6-formylphenyl trifluoromethanesulfonate	NA	FC1=CC(C(C)(C)C)=CC(C=O)=C1OS(=O)(C(F)(F)F)=O
Н ₃ С СН ₃ СНО	5-t-Butyl-3-fluoro-2- hydroxybenzaldehyde	NA	FC1=C(O)C(C=O)=CC(C(C)(C)C)=C1
CI F CI F	2-Chloro-2,2-difluoroacetic anhydride	[2834-23-3]	O=C(OC(C(F)(Cl)F)=O)C(F)(Cl)F
СНО	5-Chloro-2,4-difluorobenzaldehyde	695187-29-2	FC1=C(Cl)C=C(C(F)=C1)C=O
СНО	3-Chloro-2-fluorobenzaldehyde	85070-48-0	CIC1=C(F)C(C=O)=CC=C1
СНО	Chloro-2-fluorobenzaldehyde	61072-56-8	FC1=CC(CI)=CC=C1C=O
СНО	5-Chloro-2-fluorobenzaldehyde	96515-79-6	CIC1=CC=C(F)C(C=O)=C1

NHNH ₂ HCI	3-Chloro-2-fluorophenylhydrazine hydrochloride	517920-75-1	FC1=C(CI)C=CC=C1NN.CI
CHO CI	4-Chloro-3-fluorobenzaldehyde	5527-95-7	CIC1=C(F)C=C(C=C1)C=O
CHO CI F	3-Chloro-4-fluorobenzaldehyde	34328-61-5	CIC1=CC(C=O)=CC=C1F
B(OH) ₂	3-Chloro-5-fluoroboronic acid	328956-61-2	FC1=CC(B(O)O)=CC(Cl)=C1
F——NHNH ₂ HCI	2-Chloro-4-fluorophenylhydrazine hydrochloride	119452-65-2	CIC1=CC(F)=CC=C1NN.Cl
НО СНО	3-Chloro-4-hydroxbenzaldehyde	2420-16-8	OC1=C(Cl)C=C(C=O)C=C1
СНО	2-Chloro-5-fluorobenzaldehyde	84194-30-9	CIC1=CC=C(F)C=C1C=O
F O CI CI	2-Chloro-6-(8-fluoro-1-oxophthalazin- 2(1H)-yl)benzaldehyde	NA	FC1=CC=CC2=C1C(N(C3=C(C=O)C(CI)=CC= C3)N=C2)=O

СНО	2-Chloro-6-fluorobenzaldehyde	387-45-1	FC1=CC=CC(Cl)=C1C=O
OCH ₂ CH ₃	2-Chlorobenzyl diethylphosphonate	29074-98-4	ClC1=CC=CC=C1CP(OCC)(OCC)=O
B(OH) ₂	3-Chlorophenylboronic acid	63503-60-6	CIC1=CC(B(O)O)=CC=C1
СІСНО	4-Chloropyridine-3-carboxaldehyde	114077-82-6	ClC1=C(C=O)C=NC=C1
СІСНО	5-Chloro-salicylaldehyde	635-93-8	ClC1=CC=C(O)C(C=O)=C1
O N C O	Chlorosulfonyl Isocyanate	1189-71-5	O=C=NS(=O)(CI)=O
CI SO ₂ CI	5-Chloro-2-thiophenesulfonyl chloride	2766-74-7	CIC1=CC=C(S(=O)(CI)=O)S1
CHO CI	2-Chloro-3- (trifluoromethyl)benzaldehyde	93118-03-7	CIC1=C(C(F)(F)F)C=CC=C1C=O

CI——NHNH ₂ HCI CF ₃	4-Chloro-2-(trifluoromethyl) phenylhydrazine hydrochloride	502496-20-0	ClC1=CC=C(NN)C(C(F)(F)F)=C1.Cl
MeO OMe Br Br	1,3-Dibromoacetone Dimethyl Ketal	22094-18-4	BrCC(OC)(OC)CBr
СІ СНО	3,5-Dichlorobenzaldehyde	10203-08-4	ClC1=CC(Cl)=CC(C=O)=C1
CICOCI	3,5-Dichlorobenzoyl chloride	2905-62-6	CIC1=CC(CI)=CC(C(CI)=O)=C1
CHO CI CI F	2,4-Dichloro-3- (difluoromethoxy)benzaldehyde	NA	FC(F)OC1=C(CI)C=CC(C=O)=C1CI
но сно	2,6-Dichloro-4-hydroxybenzaldehyde	60964-09-2	ClC1=C(C=O)C(Cl)=CC(O)=C1
CI——NHNH ₂ HCI	2,4-Dichlorophenylhydrazine hydrochloride	5446-18-4	ClC1=CC(Cl)=CC=C1NN.Cl
CHO F O F	2,4-Difluoro-3- (difluoromethoxy)benzaldehyde	NA	FC(F)OC1=C(F)C=CC(C=O)=C1F

Р СНО	2,3-Difluorobenzaldehyde	2646-91-5	FC1=C(C=O)C=CC=C1F
CHO F	2,4-Difluorobenzaldehyde	1550-35-2	FC1=CC(F)=CC=C1C=O
CHO	2,5-Difluorobenzaldehyde	2646-90-4	FC1=CC=C(F)C=C1C=O
СНО F	2,6-Difluorobenzaldehyde	437-81-0	FC1=CC=CC(F)=C1C=O
СНО	3,5-3,4-Difluorobenzaldehyde	34036-07-2	FC1=CC(C=O)=CC=C1F
СНО	3,5-Difluorobenzaldehyde	32085-88-4	FC1=CC(C=O)=CC(F)=C1
so ₂ Cl	3,4-Difluorobenzenesulfonyl chloride	145758-05-0	FC1=C(F)C=C(S(=O)(Cl)=O)C=C1
COCI	2,4-Difluorobenzoyl chloride	72482-64-5	FC1=CC(F)=CC=C1C(CI)=O

COCI	3,4-Difluorobenzoyl chloride	76903-88-3	FC1=CC(C(Cl)=O)=CC=C1F
COCI	3,5-Difluorobenzoyl chloride	129714-97-2	FC1=CC(C(Cl)=O)=CC(F)=C1
F N C S	3,5-Difluorobenzoyl isothiocyanate	NA	O=C(N=C=S)C1=CC(F)=CC(F)=C1
N=c=s	3,5-Difluorobenzoyl isothiocyanate	926227-83-0	O=C(N=C=S)C1=CC(F)=CC(F)=C1
F Br	2,6-Difluorobenzyl bromide	85118-00-9	BrCC1=C(F)C=CC=C1F
F CI F CI	Difluorochloroacetic anhydride	2834-23-3	FC(F)(CI)C(OC(C(F)(CI)F)=O)=O
F F N=c=o	2,4-Difluorophenyl isocyanate	59025-55-7	FC1=CC(F)=CC=C1N=C=O
NHNH ₂ HCI	3,5-Difluorophenylhydrazine hydrochloride	134993-88-7	FC1=CC(F)=CC(NN)=C1.Cl

F F N=C=S	2,4-Difluorophenylisothiocyanate	141106-52-7	FC1=CC(F)=CC=C1N=C=S
H _{CO} OCH ₃	Dimethyl 2-((2S,4R,5R)-5-(6- (benzylamino)-9H-purin-9-yl)- tetrahydro-4-hydroxyfuran-2- yl)ethylphosphonate	NA	O=P(OC)(OC)CC[C@H]10[C@@H](N2C3= C(C(NCC4=CC=CC=C4)=NC=N3)N=C2)[C@ H](O)C1
H ₃ C H ₃ C—N ⁺ —O ⁻ H ₃ CH ₂ C	Dimethylethylamine-N-oxide	31820-06-1	C[N+](C)([O-])CC
H ₃ C CH ₃ N=C=S	2,6-Dimethylphenylisothiocyanate	19241-16-8	CC1=CC(C)=CC=C1N=C=S
O Na+	Ethane sulfinic acid sodium salt	20035-08-9	O=S(CC)[O-].[Na+]
о осң сң осң сң осң сң	2,4-Ethyl 2-(diethoxyphosphoryl)-2- fluoroacetate	2356-16-3	O=P(C(F)C(OCC)=O)(OCC)OCC
СНО	3-Fluorobenzaldehyde	456-48-4	FC1=CC=CC(C=O)=C1
SH	2-Fluorobenzenethiol	2557-78-0	SC1=CC=CC=C1F

N=C=S	4-Fluorobenzoyl isothiocyanate	78225-74-8	FC1=CC=C(C(N=C=S)=O)C=C1
СНО Б	2-Fluoro-4-methoxybenzaldehyde	331-64-6	FC1=CC(OC)=CC=C1C=O
сно	3-Fluoro-4-methoxybenzaldehyde	351-54-2	FC1=CC(C=O)=CC=C1OC
СНО ОСН3	4-Fluoro-2-methoxybenzaldehyde	450-83-9	FC1=CC=C(C(OC)=C1)C=O
F CHO	2-Fluoro-5-methoxybenzaldehyde	105728-90-3	FC1=CC=C(OC)C=C1C=O
СНО СН3	3-Fluoro-2-methylbenzaldehyde	147624-13-3	FC1=C(C)C(C=O)=CC=C1
NHNH ₂ HCI CH ₃	5-Fluoro-2-methylphenylhydrazine hydrochloride	325-50-8	CC1=CC=C(F)C=C1NN.Cl
CHO F CH ₃	2-Fluoro-3-methylbenzaldehyde	[348-27-6]	FC1=C(C)C=CC=C1C=O

O ₂ N CHO	3-Fluoro-4-nitrobenzaldehyde	160538-51-2	FC1=C([N+]([O-])=O)C=CC(C=O)=C1
F—CONHNH ₂	4-Fluorophenylacetic hydrazide	34547-28-9	FC1=CC=C(CC(NN)=O)C=C1
CHO CF ₃	4-Fluoro-3- (trifluoromethyl)benzaldehyde	67515-60-0	FC1=CC=C(C=C1C(F)(F)F)C=O
CHO CF3	4-Fluoro-2- (trifluoromethyl)benzaldehyde	90176-80-0	FC1=CC=C{C{C(F)(F)F}=C1}C=O
CHO F	2-Fluoro-4- (trifluoromethyl)benzaldehyde	89763-93-9	FC1=CC(C(F)(F)F)=CC=C1C=O
СНО	2-Formyl thiazole	10200-59-6	O=CC1=NC=CS1
он	4-Hydroxypyridine-3-carboxaldehyde	1849-54-3	OC1=C(C=O)C=NC=C1
H ₃ C CI	3-Methyl-4-fluorophenyl chloroformate	NA	O=C(Cl)OC1=CC=C(F)C(C)=C1

H ₃ COOC CHO	Methyl 5-formyl-2-methoxybenzoate	78515-16-9	O=CC1=CC(C(OC)=O)=C(OC)C=C1
CHO CH ₃	1-Methylindole-3-carboxaldehyde	19012-03-4	CN2C1=CC=CC=C1C(C=O)=C2
H ₃ C CH ₃ CH ₃ CH ₃	2-Methyl-5-(pinacolboryl)furan	338998-93-9	CC(O2)(C)C(C)(C)OB2C1=CC=C(C)O1
H ₂ N CH ₃ CH ₃	(R)-2-Methylpropane-2-sulfinamide	196929-78-9	N[\$@@]([C@@](C)(C)C)=O
N NOMD 2 C H ₃	(4-Methylpyridin-3-yl)boronic acid	148546-82-1	CC1=CC=NC=C1B(O)O
NH CIH	Methyl thiophene-2-carbimidate hydrochloride	54610-49-0	COC(C1=CC=CS1)=N.Cl
F ₃ C NHNH ₂ HCI NO ₂	2-Nitro-4- (trifluoromethyl)phenylhydrazine hydrochloride	1049748-69-7	NNC1=CC=C(C(F)(F)F)C=C1[N+]([O-])=O.Cl
ни мсно	1-Piperazinecarboxaldehyde	7755-92-2	O=CN1CCNCC1

H————СН ₂ СІ	Propargyl chloride	624-65-7	[н]с#сссі
СНО	1H-Pyrrole-2-carboxaldehyde	1003-29-8	O=CC1=CC=CN1
Br Br CHO	2,2,3-Tribromo-3-methylbutanal	NA	CC(C)(Br)C(Br)(Br)C([H])=O
Br Br CHO	2,2,3-Tribromopropanal	26944-17-2	BrCC(Br)(Br)C=O
O COOCH ₂ CH ₃ H ₃ CH ₂ CO F	Triethyl-2-fluoro-2-phosphonoacetate	[2356-16-3]	O=P(C(C(OCC)=O)F)(OCC)OCC
H_3CH_2C H_3CH_2C N^+ $O^ H_3CH_2C$	Triethylamine-N-oxide	2687-45-8	[O-][N+](CC)(CC)CC
CHO F	2,4,6-Trifluorobenzaldehyde	58551-83-0	FC1=CC(F)=CC(F)=C1C=O
CHO F	2,3,5-Trifluorobenzaldehyde	126202-23-1	FC1=C(F)C=C(F)C=C1C=O

сно Б	2,3,6-Trilfuorobenzaldehyde	104451-70-9	FC1=C(F)C=CC(F)=C1C=O
CHO F	2,4,5-Trilfuorobenzaldehyde	165047-24-5	FC1=CC(F)=C(F)C=C1C=O
CHO	2,3,4-Trilfuorobenzaldehyde	161793-17-5	FC1=C(F)C(F)=CC=C1C=O
CHO	3,4,5-Trifluorobenzaldehyde	132123-54-7	FC1=C(F)C=C(C=O)C=C1F
F CHO	4-(2,2,2-Trifluoroethoxy)-2,3,5,6- tetrafluorobenzaldehyde	NA	FC1=C(C=O)C(F)=C(F)C(OCC(F)(F)F)=C1F
CHO CI CI F F	3-(2,2,2-Trifluoroethoxy)-2,4- dichlorobenzaldehyde	NA	CIC1=C(C=O)C=CC(CI)=C1OCC(F)(F)F
CHO F F	3-(2,2,2-Trifluoroethoxy)-2,4- difluorobenzaldehyde	NA	FC1=C(C=O)C=CC(F)=C1OCC(F)(F)F
CHO F	4-(2,2,2-Trifluoroethoxy)-2,6- difluorobenzaldehyde	NA	FC(F)(F)COC1=CC(F)=C(C=O)C(F)=C1

н _{со} Сно	3-(2,2,2-Trifluoroethoxy)-2-fluoro-4- methoxybenzaldehyde	NA	FC1=C(C=O)C=CC(OC)=C1OCC(F)(F)F
CI CHO	4-(2,2,2-Trifluoroethoxy)-3-chloro-2,5- difluorobenzaldehyde	NA	FC(F)(F)COC1=C(F)C=C(C=O)C(F)=C1Cl
CI CHO	4-(2,2,2-Trifluoroethoxy)-3- chlorobenzaldehyde	NA	CIC1=CC(C=O)=CC=C1OCC(F)(F)F
so ₂ cı	4-(Trifluoromethyl)benzenesulfonyl chloride	2991-42-6	O=S(C1=CC=C(C(F)(F)F)C=C1)(CI)=O
F ₃ C N=C=S	4-(Trifluoromethyl)phenyl- isothiocyanate	1645-65-4	S=C=NC(C=C1)=CC=C1C(F)(F)F
B(OH) ₂	4-(Trifluromethyl)phenyl boronic acid	128796-39-4	OB(C1=CC=C(C(F)(F)F)C=C1)O
NHNH ₂ HCI CF ₃	2-(Trifluromethyl)phenylhydrazine hydrochloride	3107-34-4	FC(C1=CC=CC=C1NN)(F)F.Cl
H ₃ C H ₃ C O O	Trimethylamine-N-oxide	1184-78-7	C[N+](C)([O-])C

CI N C O	3-Chloro-4-methylphenyl isocyanate	28479-22-3	O=C=NC1=CC(CI)=C(C)C=C1
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