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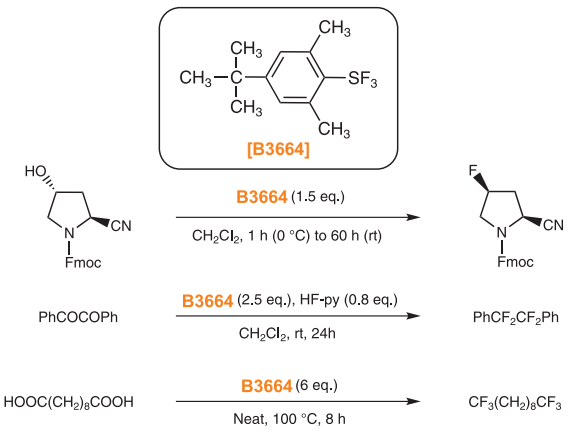
# Halogenation Reagents

Halogenation is a basic and fundamental transformation in organic chemistry, and halogenated compounds are of extreme importance as building blocks in organic synthesis.

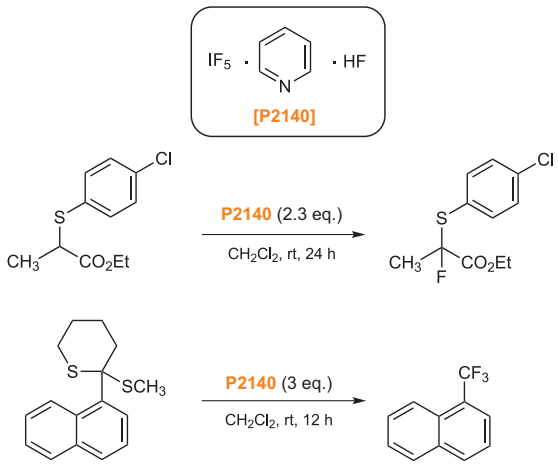
The development of modern coupling reactions, such as the Suzuki-Miyaura and Mizoroki-Heck reactions, have greatly increased the demand for halogenated compounds as starting materials.

On the other hand, introduction of fluorine into a certain position of bioactive compound such as a pharmaceutical and an agricultural chemical may remarkably reduce the toxicity of the compound, or improve the efficiency of medicine. This is due to the structurally mimic and blocking effect characterized by fluorine. In response to this situation, a number of novel halogenation reagents have been developed.

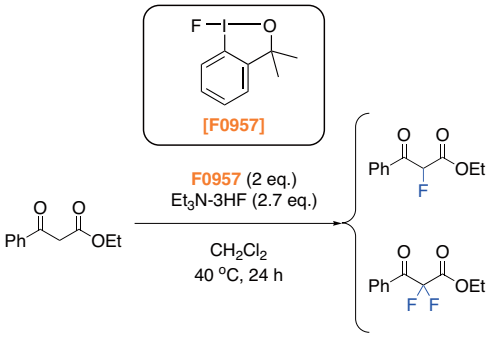
4-*tert*-Butyl-2,6-dimethylphenylsulfur trifluoride (FLUOLEAD™) **[B3664]** is introduced as below: **B3664** is a novel nucleophilic fluorinating agent which was first reported by Umemoto *et al.*[1] Differing from other existing fluorinating agents, such as DAST, **B3664** is a crystalline solid with high thermal stability and less fuming character, which makes it easier to handle. **B3664** fluorinates a hydroxyl or carbonyl group to afford the corresponding fluorinated compounds in good yields.[1]




$IF_5$-Pyridine-HF (Hara Reagent) **[P2140]** is also a novel fluorinating agent which was first reported by Hara *et al.*[2] **P2140** is a crystalline solid reagent with air stability and non-hygroscopicity, and can be used as an alternative reagent to $IF_5$ which is a unstable liquid in air. **P2140** can be applied to various fluorination reactions of sulfides as follows.




1-Fluoro-3,3-dimethyl-1,2-benziodoxole **[F0957]** is a hypervalent iodine derivative developed by Stuart *et al.*[3] **F0957** is stable to air and moisture and used as an electrophilic fluorinating reagent for a α-monofluorination of β-ketoesters in the presence of triethylamine trihydrofluoride.




Dibromoisocyanuric acid (DBI) **[D3753]** which was first reported by Gottardi, is a mild and highly effective brominating agent,[4a,b,c] and has superior brominating ability when compared with *N*-bromosuccinimide (NBS), which is frequently used in organic synthesis. For instance, nitrobenzene was converted to 3-bromonitrobenzene in 88% yield with **D3753** in conc. sulfuric acid in 5 min at 20 ºC,[4a] however, in only 70% yield with NBS in 50% sulfuric acid in 3 h at 85 ºC. Thus **D3753** has been widely used as an effective brominating agent.[4d,e]



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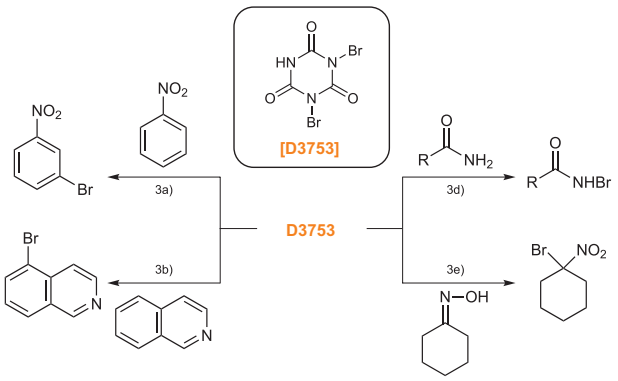
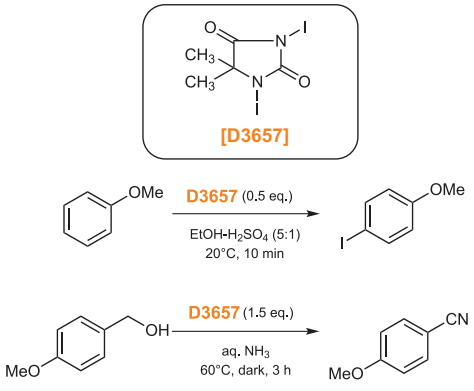



1,3-Diodo-5,5'-dimethylhidantoin (DIH) **[D3657]**, which was first reported by Orazi, is an useful iodinating agent.[5a] **D3657** has higher reactivity and selectivity than molecular iodine or *N*-iodosuccinimide (NIS), which are frequently used for iodination reactions. **D3657** reacts smoothly at room temperature with aromatic compounds in the presence of sulfuric acid to give the corresponding iodinate in a high regioselectivity and a high yield.[5b] And primary alcohols, and primary, secondary, and tertiary amines can be easily and efficiently converted into the corresponding nitriles in aqueous ammonia using **D3657**.[5c] In addition, dimethylhidantoin, which is formed after the reaction, can easily be removed by aqueous extraction.




TCI offers a variety of halogenation reagents other than the two items above. All the products are listed below.

## References


1) T. Umemoto, R. P. Singh, Y. Xu, N. Saito, *J. Am. Chem. Soc.* **2010**, *132*, 18199.
2) a) S. Hara, M. Monoi, R. Umemura, C. Fuse, *Tetrahedron* **2012**, *68*, 10145.
b) M. Kunigami, S. Hara, *J. Fluorine Chem.* **2014**, *167*, 101.
c) T. Inoue, C. Fuse, S. Hara, *J. Fluorine Chem.* **2015**, *179*, 48.
d) M. Kunigami, S. Hara, *Carbohydr. Res.* **2015**, *417*, 78.
3) G. C. Geary, E. G. Hope, K. Singh, A. M. Stuart, *Chem. Commun.* **2013**, *49*, 9263.
4) a) W. Gottardi, *Monatsh. Chem.* **1968**, *99*, 815.
b) W. D. Brown, A. H. Gouliaev, *Synthesis* **2002**, 83.
c) S. C. Virgil, in *Encyclopedia of Reagents for Organic Synthesis*, ed. by L. A. Paquette, John Wiley & Sons, Chichester, **2001**, pp. 1560-1561.
d) Z. P. Demko, M. Bartsch, K. B. Sharpless, *Org. Lett.* **2000**, *2*, 2221.
e) T. R. Walters, W. W. Zajac Jr., J. M. Woods, *J. Org. Chem.* **1991**, *56*, 316.
5) a) O. O. Orazi, R. A. Corral, H. E. Bertorello, *J. Org. Chem.* **1965**, *30*, 1101.
b) V. K. Chaikovskii, V. D. Filimonov, A. A. Funk, V. I. Skorokhodov, V. D. Ogorodnikov, Russ. *J. Org. Chem.* **2007**, *43*, 1291.
c) S. Iida, H. Togo, *Tetrahedron* **2007**, *63*, 8274.

# Fluorinating Agents

## Nucleophilic Fluorinating Agents

**P1888** 500g

$KHF_2$

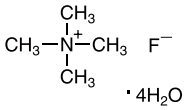
Potassium Hydrogenfluoride
CAS RN: 7789-29-9

**C2204** 25g 100g

CsF

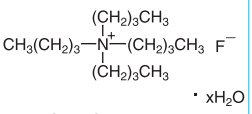
Cesium Fluoride
CAS RN: 13400-13-0

**T2754** 5g 25g



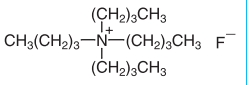
Tetramethylammonium Fluoride Tetrahydrate
CAS RN: 17787-40-5

**T1037** 25g 100g



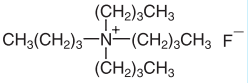
Tetrabutylammonium Fluoride Hydrate
CAS RN: 22206-57-1

**T1339** 25g 100g 500g



Tetrabutylammonium Fluoride (70-75% in Water)
CAS RN: 429-41-4

**T1338** 25mL 100mL 500mL



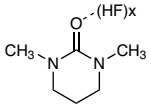
Tetrabutylammonium Fluoride (*ca.* 1mol/L in Tetrahydrofuran)
CAS RN: 429-41-4

**T2022** 10g

$(CH_3CH_2)_3N \cdot 3HF$

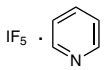
Triethylamine Trihydrofluoride
CAS RN: 73602-61-6

**D5272** 1g 5g



DMPU-HF Reagent
(HF 65%)
CAS RN: 287966-55-6

**P2140** 1g 5g



$IF_5$-Pyridine-HF
CAS RN: 2243786-10-7

**T2026** 10g

$(CH_3CH_2)_4NF \cdot 3HF$

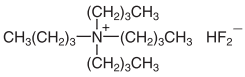
Tetraethylammonium Fluoride Trihydrofluoride
CAS RN: 42539-97-9

**T2027** 10g

$(CH_3CH_2)_4NF \cdot 4HF$

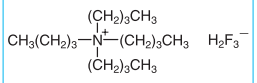
Tetraethylammonium Fluoride Tetrahydrofluoride
CAS RN: 145826-81-9

**T1295** 5g 25g



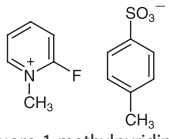
Tetrabutylammonium Bifluoride
CAS RN: 23868-34-0

**T1635** 5g 25g



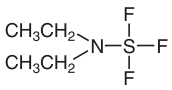
Tetrabutylammonium Dihydrogen Trifluoride
CAS RN: 99337-56-1

**F0225** 5g 25g



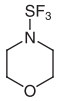
2-Fluoro-1-methylpyridinium *p*-Toluenesulfonate
CAS RN: 58086-67-2

**D1868** 5g 25g 100g



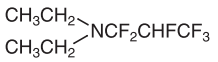
DAST
CAS RN: 38078-09-0

**M1573** 1g 5g



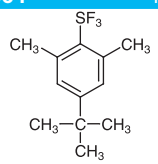
Morph-DAST
CAS RN: 51010-74-3

**H0598** 25g 100g 500g



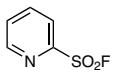
Ishikawa's Reagent
CAS RN: 309-88-6

**B3664** 1g 5g



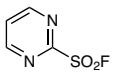
FLUOLEAD™
CAS RN: 947725-04-4

**P2398** 5g



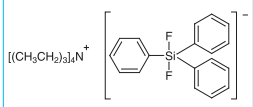
PyFluor
CAS RN: 878376-35-3

**P2465** 1g 5g



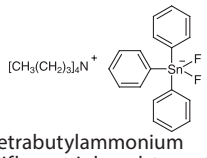
Pyrimidine-2-sulfonyl Fluoride
CAS RN: 35762-87-9

**T1909** 5g 25g



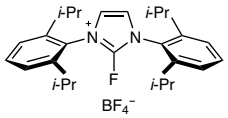
Tetrabutylammonium Difluorotriphenylsilicate
CAS RN: 163931-61-1

**T1592** 1g 5g



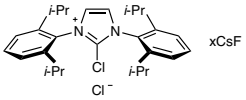
Tetrabutylammonium Difluorotriphenylstannate
CAS RN: 139353-88-1

**B5480** 200mg 1g



AlkylFluor™
CAS RN: 2043361-32-4

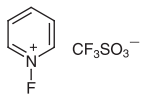
**P2420** 1g 5g



PhenoFluor™ Mix
CAS RN: 1648825-53-9

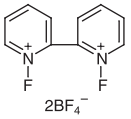
## Electrophilic Fluorinating Agents

**F0327** 5g 25g



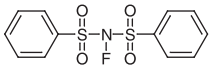
1-Fluoropyridinium Trifluoromethanesulfonate
CAS RN: 107263-95-6

**D3812** 1g 5g 25g 100g



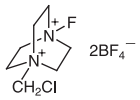
1,1'-Difluoro-2,2'-bipyridinium Bis(tetrafluoroborate)
CAS RN: 178439-26-4

**F0335** 1g 5g 25g



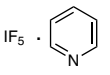
*N*-Fluorobenzenesulfonimide
CAS RN: 133745-75-2

**F0358** 5g 25g 100g



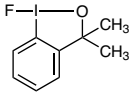
F-TEDA-$BF_4$
CAS RN: 140681-55-6

**P2140** 1g 5g



$IF_5$-Pyridine-HF
CAS RN: 2243786-10-7

**F0957** 1g



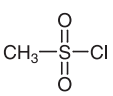
1-Fluoro-3,3-dimethyl-1,2-benziodoxole
CAS RN: 1391728-13-4

# Chlorinating Agents

**T2048** 500mL

Thionyl Chloride (*ca.* 1mol/L in Dichloromethane)
CAS RN: 7719-09-7

**M0094** 25g 500g



Methanesulfonyl Chloride
CAS RN: 124-63-0

**T0611** 5g 25g

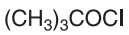
$CCl_3SO_2Cl$

Trichloromethanesulfonyl Chloride
CAS RN: 2547-61-7



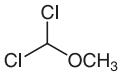
Please inquire for pricing and availability of listed products to our local sales representatives.

**H0362** 25g



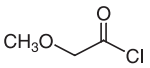
*tert*-Butyl Hypochlorite
CAS RN: 507-40-4

**D1645** 25g 100g 250g



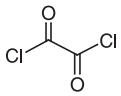
Dichloromethyl Methyl Ether
CAS RN: 4885-02-3

**M0970** 25g 100g 500g



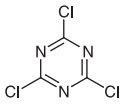
Methoxyacetyl Chloride
CAS RN: 38870-89-2

**O0082** 25g 100g 500g



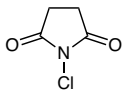
Oxalyl Chloride
CAS RN: 79-37-8

**C0460** 25g 500g



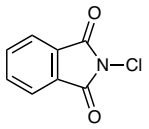
Cyanuric Chloride
CAS RN: 108-77-0

**C0291** 25g 100g 500g



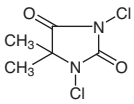
*N*-Chlorosuccinimide
(= NCS)
CAS RN: 128-09-6

**C0802** 25g 500g



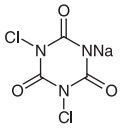
*N*-Chlorophthalimide
CAS RN: 3481-09-2

**D1783** 25g 100g 500g



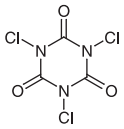
1,3-Dichloro-
5,5-dimethylhydantoin
CAS RN: 118-52-5

**D1003** 25g 500g



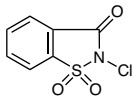
Sodium
Dichloroisocyanurate
CAS RN: 2893-78-9

**T0620** 25g 500g



Trichloroisocyanuric Acid
CAS RN: 87-90-1

**C1674** 5g 25g

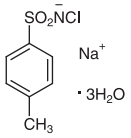


*N*-Chlorosaccharin
CAS RN: 14070-51-0

**C0075** 25g 100g 500g

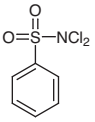
Chloramine B Hydrate
CAS RN: 304655-80-9

**C0076** 25g 500g



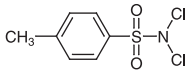
Chloramine T Trihydrate
CAS RN: 7080-50-4

**D0317** 5g 25g



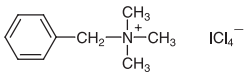
Dichloramine B
CAS RN: 473-29-0

**D0318** 25g 100g 500g



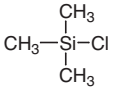
Dichloramine T
CAS RN: 473-34-7

**B1543** 5g



Benzyltrimethylammonium
Tetrachloroiodate
CAS RN: 121309-88-4

**C0306** 25mL 100mL 500mL



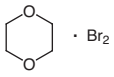
Trimethylsilyl Chloride
CAS RN: 75-77-4

# Brominating Agents

**B2414** 90g 500g

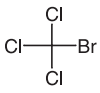
Bromine
CAS RN: 7726-95-6

**B2719** 5g 25g



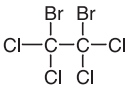
Bromine -
1,4-Dioxane Complex
CAS RN: 15481-39-7

**B0662** 25g 500g



Bromotrichloromethane
CAS RN: 75-62-7

**D1987** 25g

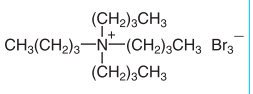


1,2-Dibromo-
1,1,2,2-tetrachloroethane
CAS RN: 630-25-1

**T0038** 5g 25g 100g 500g

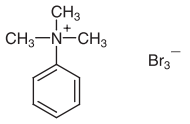
Carbon Tetrabromide
CAS RN: 558-13-4

**T1284** 25g 100g 500g



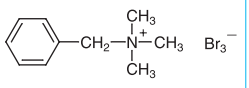
Tetrabutylammonium
Tribromide
CAS RN: 38932-80-8

**P0928** 25g 500g



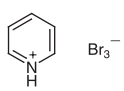
Trimethylphenylammonium
Tribromide
CAS RN: 4207-56-1

**T1382** 5g 25g



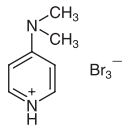
Benzyltrimethylammonium
Tribromide
CAS RN: 111865-47-5

**P0825** 25g 100g 500g



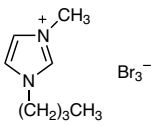
Pyridinium Bromide
Perbromide
CAS RN: 39416-48-3

**D1787** 5g 25g



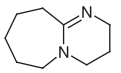
4-Dimethylaminopyridinium
Bromide Perbromide
CAS RN: 92976-81-3

**B3596** 5g



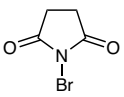
1-Butyl-3-methylimidazolium
Tribromide
CAS RN: 820965-08-0

**D3976** 5g



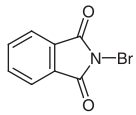
1,8-Diazabicyclo[5.4.0]-
7-undecene Hydrogen
Tribromide
CAS RN: 138666-59-8

**B0656** 25g 100g 500g



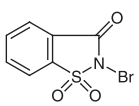
*N*-Bromosuccinimide
(= NBS)
CAS RN: 128-08-5

**B1697** 5g 25g



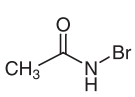
*N*-Bromophthalimide
CAS RN: 2439-85-2

**B2152** 5g 25g



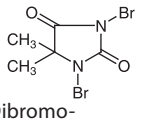
*N*-Bromosaccharin
CAS RN: 35812-01-2

**B0530** 5g 25g



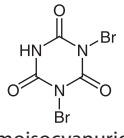
*N*-Bromoacetamide
CAS RN: 79-15-2

**D1265** 25g 500g



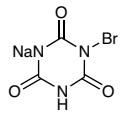
1,3-Dibromo-
5,5-dimethylhydantoin
CAS RN: 77-48-5

**D3753** 1g 5g 25g



Dibromoisocyanuric Acid
(= DBI)
CAS RN: 15114-43-9

**B2148** 25g



Monosodium Bromoisocyanurate
CAS RN: 164918-61-0

**B2553** 25mL 100mL

$BBr_3$

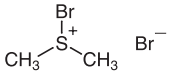
Boron Tribromide
(17% in Dichloromethane, *ca.* 1mol/L)
CAS RN: 10294-33-4

**P1743** 300g

$PBr_3$

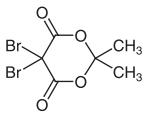
Phosphorus Tribromide
CAS RN: 7789-60-8

**B3311** 5g 25g



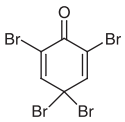
Bromodimethylsulfonium Bromide
CAS RN: 50450-21-0

**D1710** 5g 25g



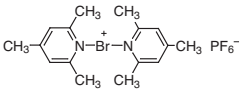
5,5-Dibromomeldrum's Acid
CAS RN: 66131-14-4

**T1235** 5g 25g



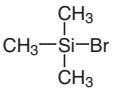
2,4,4,6-Tetrabromo-2,5-cyclohexadienone
CAS RN: 20244-61-5

**B2358** 1g 5g



Bis(2,4,6-trimethylpyridine)-bromonium Hexafluorophosphate
CAS RN: 188944-77-6

**B1087** 5mL 25mL 250mL



Trimethylsilyl Bromide
CAS RN: 2857-97-8

# Iodinating Agents

**I0604** 25g 500g

$I_2$

Iodine
CAS RN: 7553-56-2

**H1221** 300mL

HI

Hydriodic Acid (57%)
CAS RN: 10034-85-2

**C0936** 10g

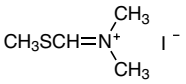
Carbon Tetraiodide
CAS RN: 507-25-5

**C1190** 1g 5g

$ICH_2CH_2Cl$

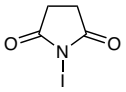
1-Chloro-2-iodoethane
CAS RN: 624-70-4

**D4340** 5g 25g



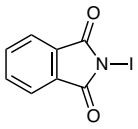
*N,N*-Dimethyl-*N*-(methylsulfanylmethylene)-ammonium Iodide
CAS RN: 29085-13-0

**I0074** 5g 25g 100g



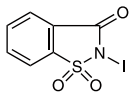
*N*-Iodosuccinimide
(= NIS)
CAS RN: 516-12-1

**I1052** 5g 25g



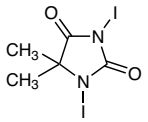
*N*-Iodophthalimide
CAS RN: 20919-42-0

**I0784** 5g



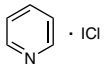
*N*-Iodosaccharin
CAS RN: 86340-94-5

**D3657** 5g 25g



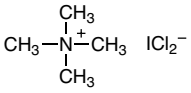
1,3-Diiodo-5,5-dimethylhydantoin (= DIH)
CAS RN: 2232-12-4

**P2086** 1g 5g



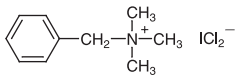
Pyridine Iodine Monochloride
CAS RN: 6443-90-9

**T2717** 5g



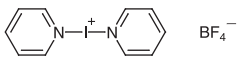
Tetramethylammonium Dichloroiodate
CAS RN: 1838-41-1

**B1604** 5g 25g



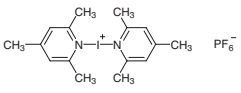
Benzyltrimethylammonium Dichloroiodate
CAS RN: 114971-52-7

**B2539** 1g



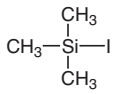
Bis(pyridine)iodonium Tetrafluoroborate
CAS RN: 15656-28-7

**B2359** 1g 5g



Bis(2,4,6-trimethylpyridine)-iodonium Hexafluorophosphate
CAS RN: 113119-46-3

**I0308** 5g 25g



Trimethylsilyl Iodide
CAS RN: 16029-98-4



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