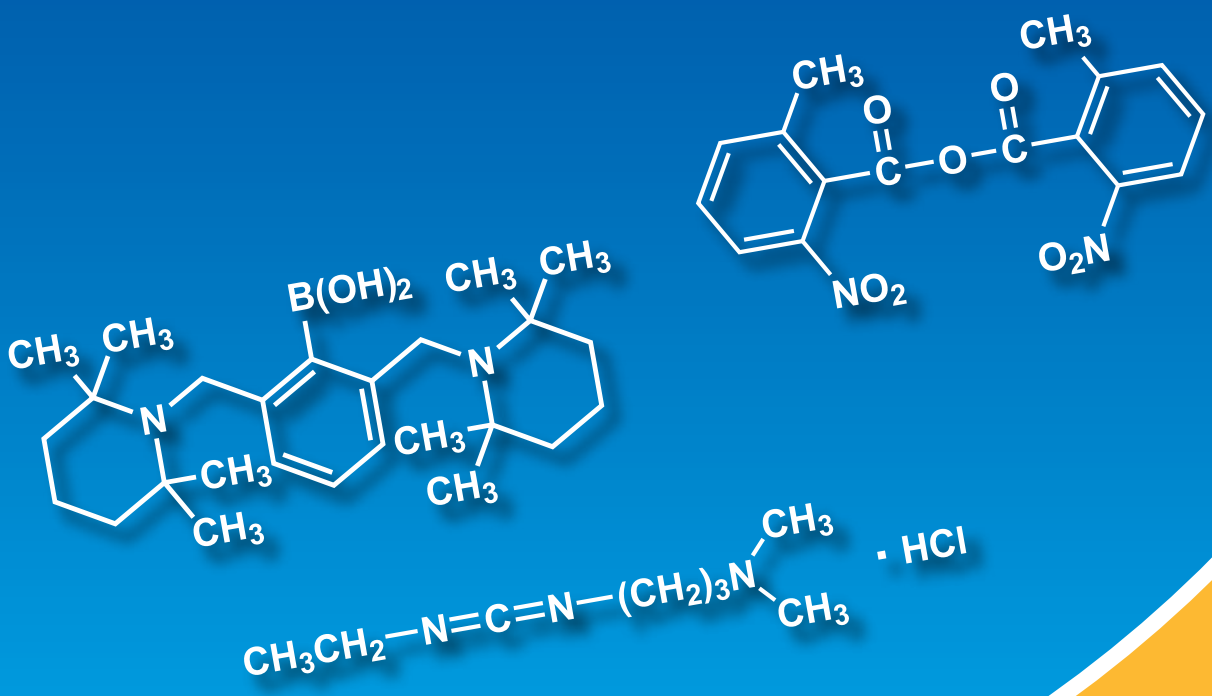
CHEMISTRY

TCI

Condensing Agents



Active Esters, Additives

Carbodiimides

Carbonyldiimidazoles

Phosgene Derivatives

Phosphonium Salts, Uronium Salts, Formamidinium Salts

Condensation Organocatalysts

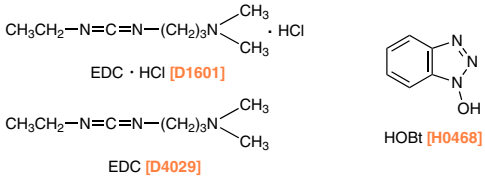
Others

Condensing Agents

Esterification and amidation have been regarded as one of the most basic reactions in organic chemistry. Among them, esterification under an acidic conditions has been known for more than 100 years,[1] the conditions of which being dependent on Le Chatelier's principle. To drive the reaction to completion, water is removed as the reaction progresses, usually via a Dean-Stark trap or a dehydrating reagent. However, this method is often ineffective when applied to thermally unstable materials. Milder conditions and condensing agents have been developed to surmount this problem. For amidation, the activation of a carboxylic acid is key with the amide bond formed through the nucleophilic addition of amines to an activated carboxylic acid. However, if the reactivity of the activated carboxy group is too high, epimerization at α-position can occur. Reagents that do not impart epimerization have since been developed to avoid this potential issue. With significant research into esterification and amidation having been conducted for many years, many condensing agents which have both high reactivity and control of epimerization are readily available. Furthermore, many reviews of these methods and reagents have been reported.[2] Applications and references for these varied methods are available on each of TCI's product pages.

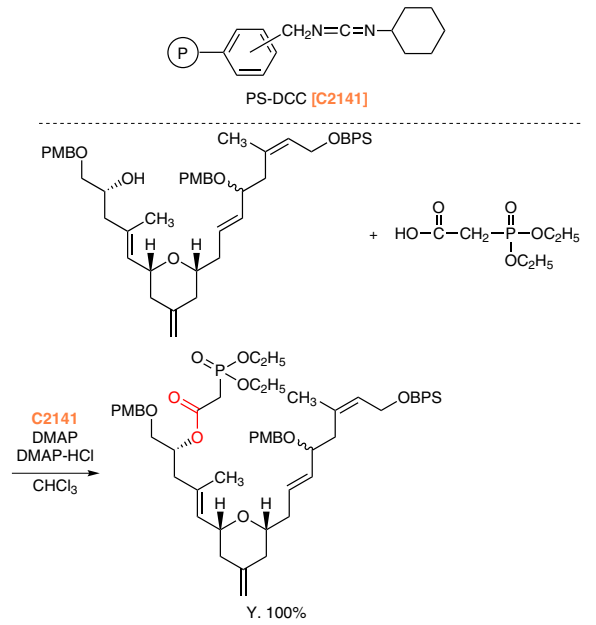
● EDC + HOBt

Since the first report of a condensation reaction utilizing *N*,*N*'-dicyclohexylcarbodiimide (DCC) **[D0436]** in 1950's,[3] many carbodiimide reagents have been developed. Among them, 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide (EDC) **[D1601]**, and **[D4029]** are favored as the byproducts are easily removed by partition. EDC can be used together with 1-hydroxybenzotriazole (HOBt)[4] **[H0468]** which is one of the most used conditions for condensations.



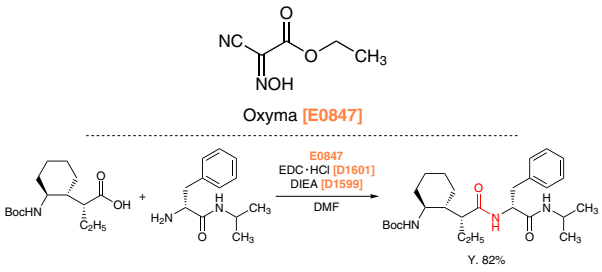
● PS-DCC

It often becomes troublesome to remove byproducts when applying to condensing agents. Removal of byproducts from condensation reactions is one of the more troublesome aspects of the reactions. Dicyclohexylurea, a byproduct from DCC, is notoriously difficult to remove. However, polymer supported PS-DCC **[C2141]** has the advantage of easily removal by simple filtration and is often employed in the total synthesis of natural products.[5]



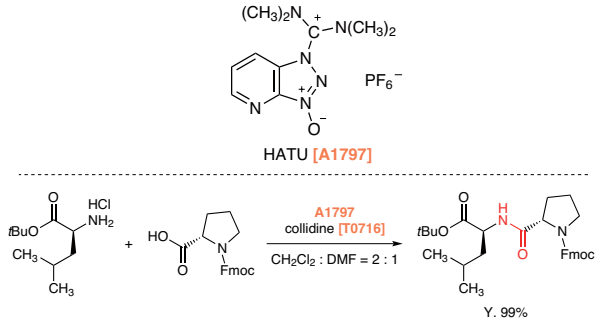
● Oxyma

1,2,3-Triazol derivatives are utilized in the synthesis of active esters and are frequently used with carbodiimides, but are potentially explosive if dried. The reagent oxyma **[E0847]** bears the same reactivity to that of triazoles with a minimized explosion risk.[6-9]



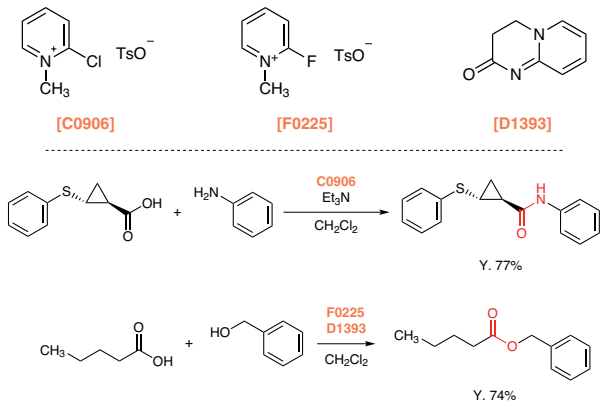
● HATU

Uronium salts represented by HATU **[A1797]** have been known as condensing agents with both high reactivity and suppressed epimerization.[10,11]



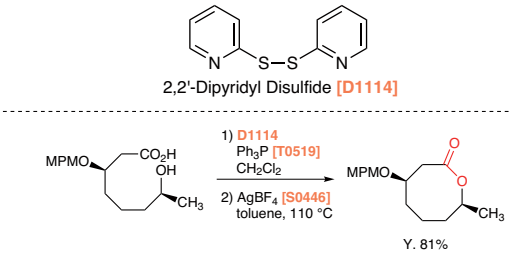
Mukaiyama Condensing Agents

Mukaiyama *et al*. reported 2-chloro-1-methylpyridinium *p*-toluenesulfonate **[C0906]** and 2-fluoro-1-methylpyridinium *p*-toluenesulfonate **[F0225]** which were utilized in condensation reactions.[12,13] In this reaction, either conventional organic bases such as triethylamine or acid captor H **[D1393]** can be used as an acid sequestrant.



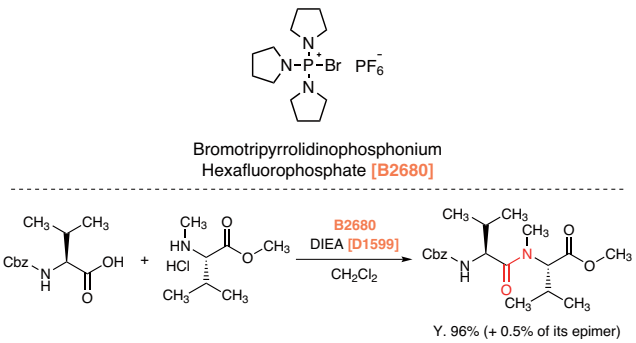
Corey-Nicolaou macrolactonization

2,2'-Dipyridyl disulfide **[D1114]** is useful for the lactonization and is conducted under mild conditions. Corey and Nicolaou have reported this method in several total syntheses making use of this reagent.[14,15]



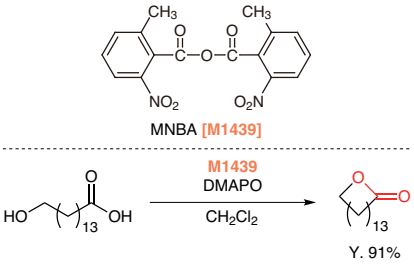
Bromotripyrrolidinophosphonium Hexafluorophosphate

Phosphonium salts such as bromotripyrrolidinophosphonium hexafluorophosphate **[B2680]** also have utility in condensation reactions.[16] When using these salts, additives like HOBt are not necessary. Furthermore, the rate of epimerization is low and N-methyl amino acid derivatives, which are difficult to impart reactivity on, are applicable. In this way, these salts are anticipated to be used more frequently in further research.



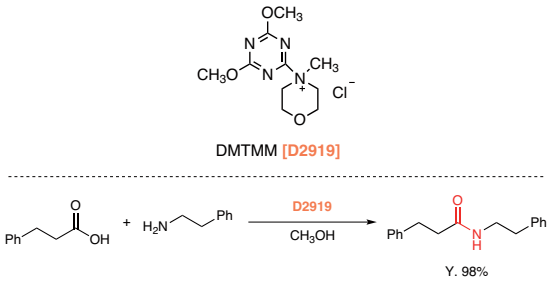
Shiina Macrolactonization

Shiina *et al*. have reported that 2-methyl-6-nitrobenzoic anhydride (MNBA) **[M1439]** affords esters or amides in high yields from mostly equimolar carboxylic acid and alcohols or amines under basic conditions.[17,18] This method is also utilized in macrolactonizations.



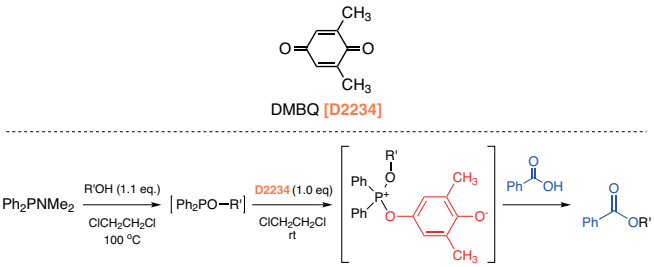
DMTMM

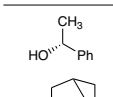
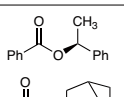
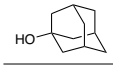
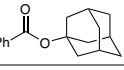
Kunishima *et al*. have reported the utility of 4-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-methylmorpholinium chloride (DMTMM) **[D2919]** as a condensing reagent.[19,20] This reagent has some advantages: amidation proceeds selectively even in alcohol solvent and the byproducts are easy to remove. **D2919** can be used used as a powerful condensing reagent.[21]



Mukaiyama Redox Condensation

Mukaiyama *et al*. have reported a redox condensation reaction using dihydroquinone derivatives such as 2,6-dimethyl-1,4-benzoquinone (DMBQ) **[D2234]**.[22,23] In this reaction, tertiary alcohols with high steric hindrance can react and afford products with stereoinversion. Furthermore, this reaction is even applicable to 1-adamantanol, the structure of which being highly resistant to stereoinversion.

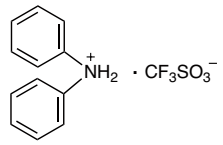


R'OH	product	yield (%)
		94 (inversion)
		83

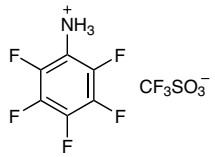
Organocatalysts for Condensation Reactions

DPAT **[D3683]** is a useful esterification catalyst developed by Tanabe *et al*. affording esters in high yields from equimolar amounts of carboxylic acids and alcohols under mild reaction condition.[24,25] In this case, desired esters can be obtained by simple operation without addition of dehydrating agent and azeotropic water removal. There is also a report using fluorous solvent, in which DPAT is useful for the substrate with high steric hindrance.[26]

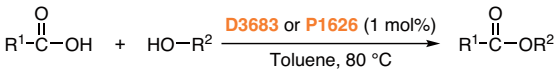
PFPAT **[P1626]** shows higher activity than DPAT and it can be applied widely to esterification and lactonization.[25] Furthermore, PFPAT can be removed after work-up; washing with NaOH aqueous solution removed CF_3SO_3H, followed by distillation of $C_6F_5NH_2$.



DPAT **[D3683]**



PFPAT **[P1626]**



R^1	R^2	catalyst	time (h)	Y. (%)
$PhCH_2CH_2$—	CH_2=$CH(CH_2)_8$—	D3683	8	96
$PhCH_2CH_2$—	CH_2=$CH(CH_2)_8$—	P1626	3	96
^{t}Bu—	$CH_3(CH_2)_7$—	D3683	24	92
^{t}Bu—	$CH_3(CH_2)_7$—	P1626	6	90

References

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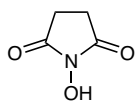
Active Esters, Additives

B0249 25g



N-Hydroxysuccinimide
[Coupling Reagent for Peptide]
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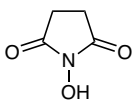
H0623 25g 100g 500g



N-Hydroxysuccinimide
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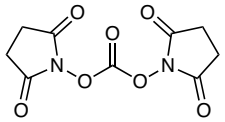
D1662 5g 25g



DSC
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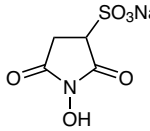

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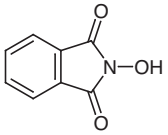

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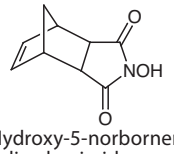

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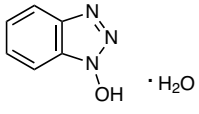

HOBt Monohydrate
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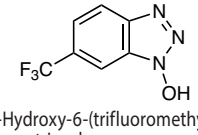
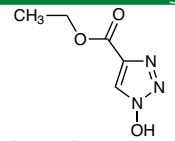
H1454 1g 5g



1-Hydroxy-6-(trifluoromethyl)-benzotriazole
CAS RN: 26198-21-0

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

E0901 1g 5g



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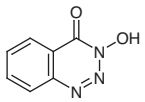

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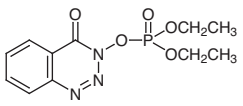

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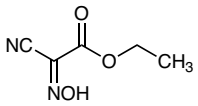

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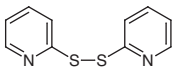

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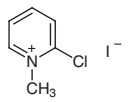

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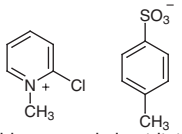

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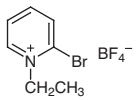
B1036 5g 25g



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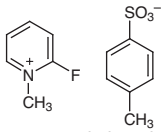
F0225 5g 25g



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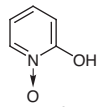
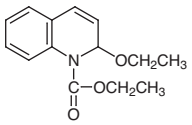


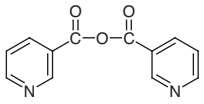
2-Hydroxypyridine *N*-Oxide
CAS RN: 13161-30-3

E0363 25g



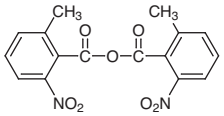
EEDQ
CAS RN: 16357-59-8

P1768 1g 5g



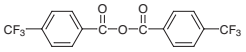
Nicotinic Anhydride
CAS RN: 16837-38-0

M1439 1g 5g 25g



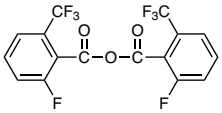
MNBA
CAS RN: 434935-69-0

T1593 10g



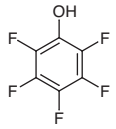
TFBA
CAS RN: 25753-16-6

F1184 1g



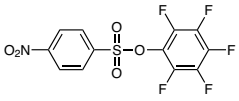
FTFBA
CAS RN: 2118332-08-2

P0919 10g 25g



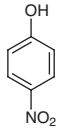
Pentafluorophenol
CAS RN: 771-61-9

P2231 1g 5g



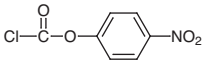
Pentafluorophenyl 4-Nitrobenzenesulfonate
CAS RN: 244633-31-6

N0220 5g 25g 100g 500g



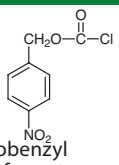
4-Nitrophenol
CAS RN: 100-02-7

C1400 25g 100g 250g



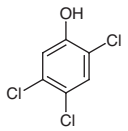
4-Nitrophenyl Chloroformate
CAS RN: 7693-46-1

C1077 25g



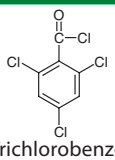
4-Nitrobenzyl Chloroformate
CAS RN: 4457-32-3

T0389 25g 500g



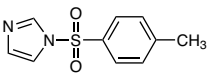
2,4,5-Trichlorophenol
CAS RN: 95-95-4

T1413 5g 25g



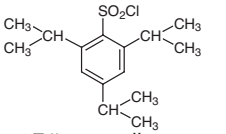
2,4,6-Trichlorobenzoyl Chloride
CAS RN: 4136-95-2

T1985 5g 25g



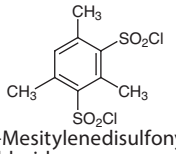
1-Tosylimidazole
CAS RN: 2232-08-8

T0459 25g 100g 500g



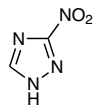
2,4,6-Triisopropylbenzene-sulfonyl Chloride
CAS RN: 6553-96-4

M1186 5g 25g



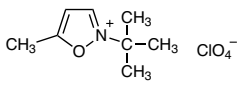
2,4-Mesitylenedisulfonyl Dichloride
CAS RN: 68985-08-0

N0477 1g 5g



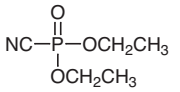
3-Nitro-1,2,4-triazole
CAS RN: 24807-55-4

B0832 1g 5g



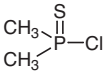
Woodward's Reagent L
CAS RN: 10513-45-8

C1242 5g 25g



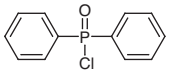
Diethyl Cyanophosphonate
CAS RN: 2942-58-7

D2159 1g 5g



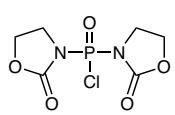
Dimethylthiophosphinoyl Chloride
CAS RN: 993-12-4

C1415 5g 10g 25g



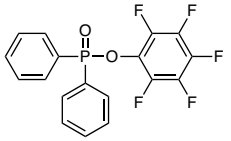
Diphenylphosphinic Chloride
CAS RN: 1499-21-4

B1213 5g 25g



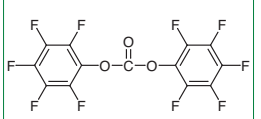
BOP-Cl
CAS RN: 68641-49-6

P2726 1g 5g



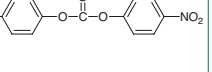
FDPP
CAS RN: 138687-69-1

B3604 5g



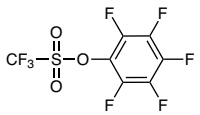
Bis(pentafluorophenyl)-Carbonate
CAS RN: 59483-84-0

C1481 5g 25g



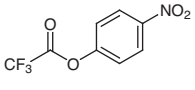
Bis(4-nitrophenyl) Carbonate
CAS RN: 5070-13-3

P2188 200mg 1g



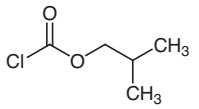
Pentafluorophenyl Triflate
CAS RN: 60129-85-3

T0681 5g 25g



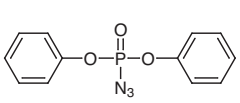
4-Nitrophenyl Trifluoroacetate
CAS RN: 658-78-6

C0178 25g 100g 500g



IBCF
CAS RN: 543-27-1

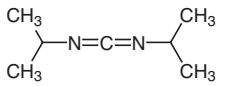
D1672 5g 25g 250g



DPPA
CAS RN: 26386-88-9

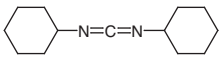
Carbodiimides

D0254 25g 250g



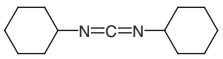
DIC
CAS RN: 693-13-0

D0436 25g 400g



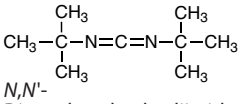
DCC
CAS RN: 538-75-0

D0437 100mL



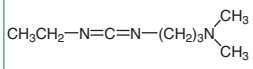
DCC
(25% in Pyridine, *ca.* 1.2mol/L)
CAS RN: 538-75-0

D5347 5mL 25mL



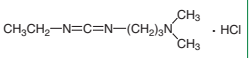
N,N'-
Di-*tert*-butylcarbodiimide
CAS RN: 691-24-7

D4029 5g 25g 100g



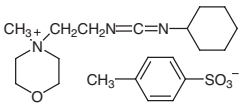
EDC
CAS RN: 1892-57-5

D1601 5g 25g 100g 250g



EDC·HCl
CAS RN: 25952-53-8

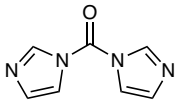
C0793 5g 25g



CMC
CAS RN: 2491-17-0

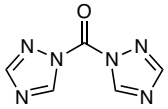
Carbonyldiimidazoles

C0119 5g 25g 250g



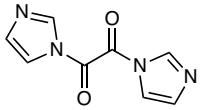
CDI
CAS RN: 530-62-1

C2325 5g 25g



CDT
CAS RN: 41864-22-6

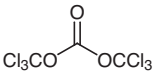
O0200 1g 5g



1,1'-Oxalyldiimidazole
CAS RN: 18637-83-7

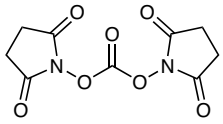
Phosgene Derivatives

T1467 25g 250g



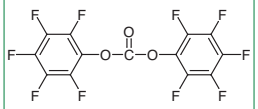
Triphosgene
CAS RN: 32315-10-9

D1662 5g 25g



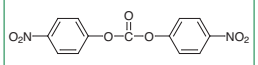
DSC
CAS RN: 74124-79-1

B3604 5g



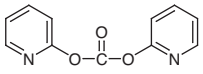
Bis(pentafluorophenyl)
Carbonate
CAS RN: 59483-84-0

C1481 5g 25g



Bis(4-nitrophenyl)
Carbonate
CAS RN: 5070-13-3

C1407 1g 5g

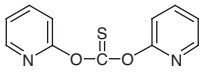


Di-2-pyridyl Carbonate
CAS RN: 1659-31-0

T1320 25g 100g

Thiophosgene
CAS RN: 463-71-8

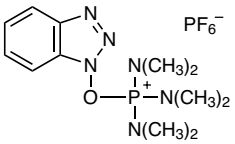
T1906 1g



O,O'-Di-2-pyridyl
Thiocarbonate
CAS RN: 96989-50-3

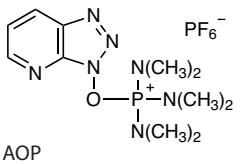
Phosphonium Salts, Uronium Salts, Formamidinium Salts

B1651 5g 25g 100g



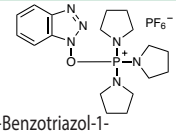
BOP
CAS RN: 56602-33-6

A2782 1g 5g



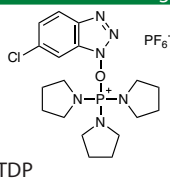
AOP
CAS RN: 156311-85-2

B1774 5g 25g



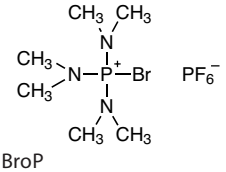
1*H*-Benzotriazol-1-
yloxytripyrrolidinophosphonium
Hexafluorophosphate
CAS RN: 128625-52-5

C3461 5g 25g



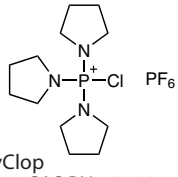
TPTDP
CAS RN: 893413-42-8

B3838 1g 5g



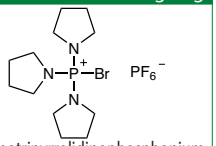
BroP
CAS RN: 50296-37-2

C2551 5g 25g



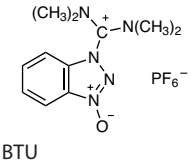
PyClop
CAS RN: 133894-48-1

B2680 5g 25g



Bromotripyrrolidinophosphonium
Hexafluorophosphate
CAS RN: 132705-51-2

B1657 5g 25g 100g



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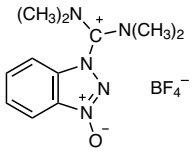
CAS RN: 94790-37-1

B1658 5g 25g



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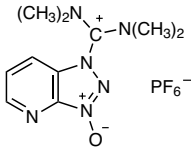
CAS RN: 125700-67-6

A1797 5g 25g



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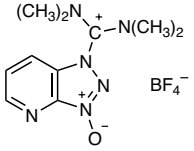
CAS RN: 148893-10-1

A1861 1g 5g



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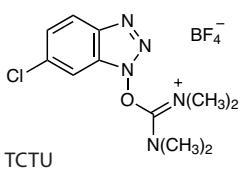
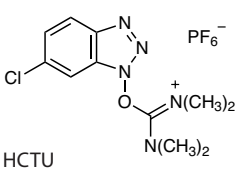
CAS RN: 873798-09-5

C1926 5g 25g



TCTU
CAS RN: 330641-16-2

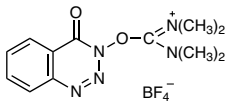
C1988 1g 5g



HCTU
CAS RN: 330645-87-9

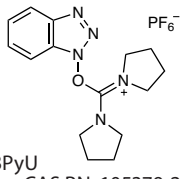
Please inquire for pricing and availability of listed products to our local sales representatives.

D3263 5g 25g



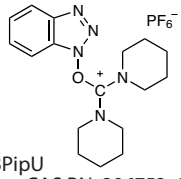
TDBTU
CAS RN: 125700-69-8

B4805 1g 5g



HBPyU
CAS RN: 105379-24-6

B3816 1g 5g



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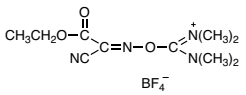
CAS RN: 206752-41-2

E0916 1g 5g



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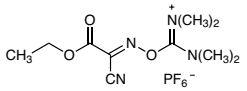
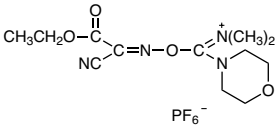
CAS RN: 136849-72-4

E1306 1g 5g



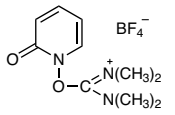
HOTU
CAS RN: 333717-40-1

C2733 5g 25g



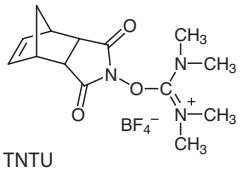
(1-Cyano-2-ethoxy-2-oxoethylidenaminooxy)-dimethylaminomorpholinocarbenium Hexafluorophosphate
CAS RN: 1075198-30-9

O0390 1g 5g



TPTU
CAS RN: 125700-71-2

N0634 5g 25g



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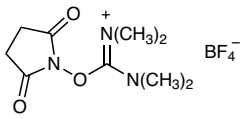
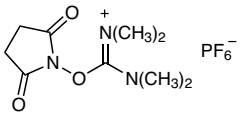
CAS RN: 125700-73-4

T2224 1g 5g



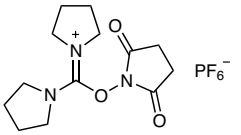
TSTU
CAS RN: 105832-38-0

T2929 5g 25g



HSTU
CAS RN: 265651-18-1

B3817 1g 5g



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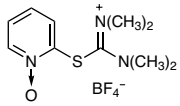
CAS RN: 207683-26-9

T3569 5g 25g



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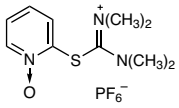
CAS RN: 255825-38-8

T2821 5g



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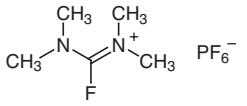
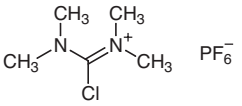
CAS RN: 212333-72-7

F0726 1g 5g



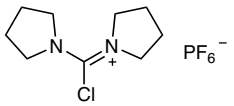
TFFH
CAS RN: 164298-23-1

C1957 1g 5g



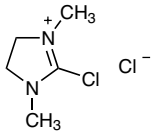
TCFH
CAS RN: 94790-35-9

C1379 5g 25g



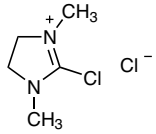
PyClU
CAS RN: 135540-11-3

C1408 5g 25g



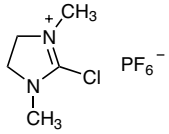
DMC
CAS RN: 37091-73-9

C1639 25g



DMC (*ca.* 25% in Dichloromethane)
CAS RN: 37091-73-9

C1651 5g 25g



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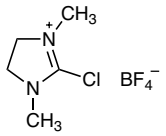
CAS RN: 101385-69-7

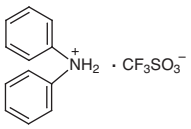
C3444 1g 5g



CIB
CAS RN: 153433-26-2

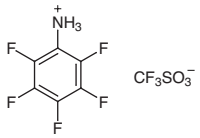
Condensation Organocatalysts

D3683 1g 5g 25g



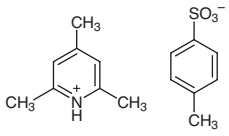
DPAT
CAS RN: 164411-06-7

P1626 1g 5g 25g



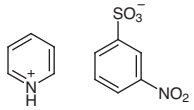
PFPAT
CAS RN: 912823-79-1

T1122 25g



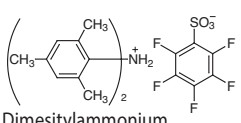
CPTS
CAS RN: 59229-09-3

P0941 5g 25g



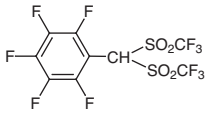
Pyridinium 3-Nitrobenzenesulfonate
CAS RN: 84752-61-4

D3293 1g 5g



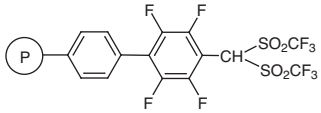
Dimesitylammonium Pentafluorobenzenesulfonate
CAS RN: 850629-65-1

B2291 100mg 1g



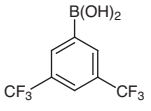
α,α-Bis(trifluoromethanesulfonyl)-2,3,4,5,6-pentafluorotoluene
CAS RN: 405074-81-9

B2292 100mg



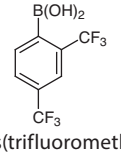
Bis(trifluoromethanesulfonyl)methyltetrafluorophenyl Polystyrene Resin cross-linked with 2% DVB (200-400mesh) (0.9-1.2mmol/g)

B1886 1g 5g 25g



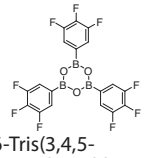
3,5-Bis(trifluoromethyl)-phenylboronic Acid
CAS RN: 73852-19-4

B3022 1g 5g



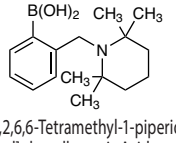
2,4-Bis(trifluoromethyl)-phenylboronic Acid
CAS RN: 153254-09-2

T1929 1g 5g



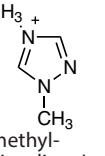
2,4,6-Tris(3,4,5-trifluorophenyl)boroxin
CAS RN: 223440-94-6

T2908 1g



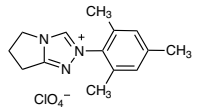
2-[(2,2,6,6-Tetramethyl-1-piperidyl)-methyl]phenylboronic Acid
CAS RN: 815581-79-4

D3962 1g 5g



1,4-Dimethyl-1,2,4-triazolium Iodide
CAS RN: 120317-69-3

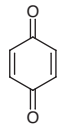
D3982 100mg



6,7-Dihydro-2-mesityl-5*H*-pyrrolo[2,1-*c*]-1,2,4-triazolium Perchlorate
CAS RN: 1334529-08-6

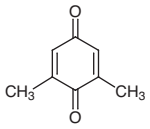
Others

B0887 25g 500g



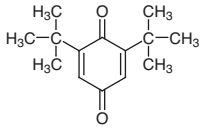
1,4-Benzoquinone
CAS RN: 106-51-4

D2234 1g 5g 25g



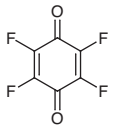
DMBQ
CAS RN: 527-61-7

D2256 5g 25g



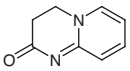
2,6-Di-*tert*-butyl-*p*-quinone
CAS RN: 719-22-2

T0790 1g 5g



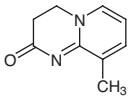
Fluoranil
CAS RN: 527-21-9

D1393 5g 25g



Acid Captor H
CAS RN: 5439-14-5

M0670 25g

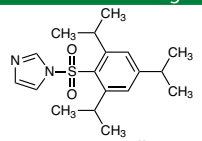


Acid Captor 9M
CAS RN: 61751-44-8

T0340 25g 100g 500g

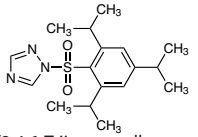
1,2,4-Triazole
CAS RN: 288-88-0

T1410 5g 25g



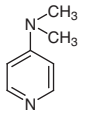
1-(2,4,6-Triisopropylbenzene-sulfonyl)imidazole
CAS RN: 50257-40-4

T2951 1g 5g



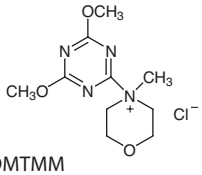
1-(2,4,6-Triisopropylbenzene-sulfonyl)-1,2,4-triazole
CAS RN: 54230-60-3

D1450 25g 100g 500g



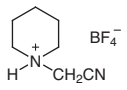
DMAP
CAS RN: 1122-58-3

D2919 5g 25g



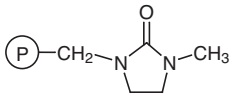
DMTMM
CAS RN: 3945-69-5

C2421 5g



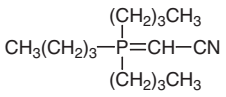
1-(Cyanomethyl)piperidinium Tetrafluoroborate
CAS RN: 434937-12-9

M1452 1g



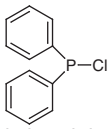
3-Methyl-2-oxoimidazolidin-1-ylmethyl Polystyrene Resin cross-linked with 1% DVB

C1500 1g 5g 25g



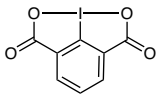
Tsunoda Reagent
CAS RN: 157141-27-0

C0597 25g 100g 500g



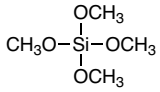
Chlorodiphenylphosphine
CAS RN: 1079-66-9

I0865 1g



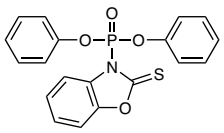
Iodosodilactone
CAS RN: 2902-68-3

T0588 25g 100g 500g



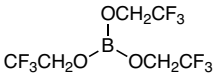
TMOS
CAS RN: 681-84-5

D2038 5g 25g



DBOP
CAS RN: 111160-56-6

T3010 1g



Tris(2,2,2-trifluoroethyl) Borate
CAS RN: 659-18-7

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