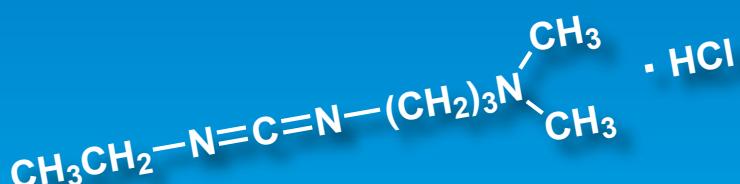
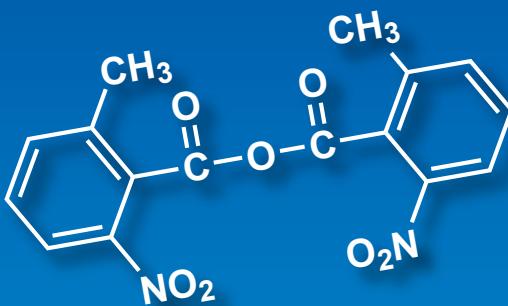


Condensing Agents



Active Esters, Additives

Carbodiimides

Carbonyldiimidazoles

Phosgene Derivatives

Phosphonium Salts, Uronium Salts, Formamidinium Salts

Condensation Organocatalysts

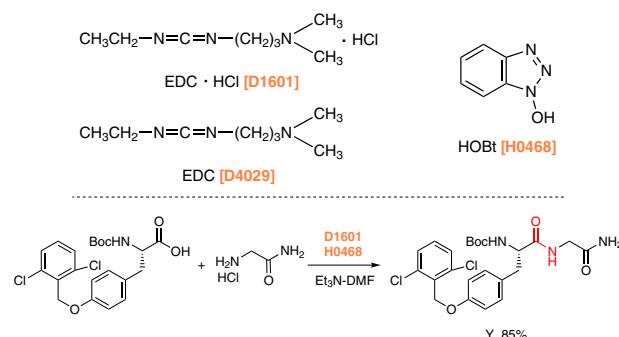
Others

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 a-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 + HOBr

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.

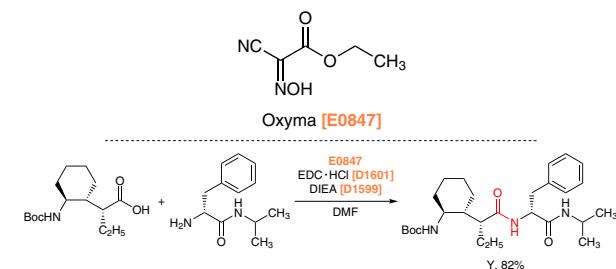


PS-DCC

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⁾

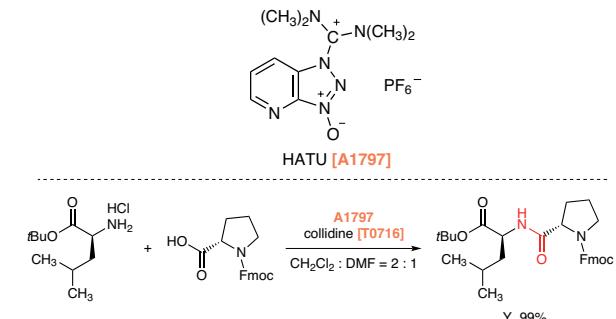
Oxyma

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.⁶⁻⁸⁾



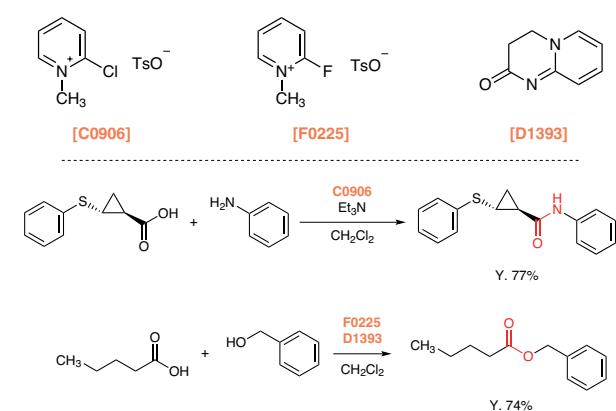
 HATU

Uranium salts represented by HATU [A1797] have been known as condensing agents with both high reactivity and suppressed epimerization.^{9,10}



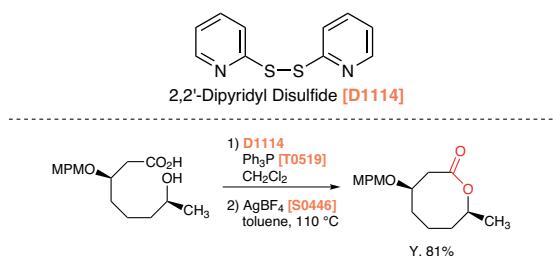
● Mukaiyama Condensing Agents

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.^{11,12)} In this reaction, either conventional organic bases such as triethylamine or acid captor H [D1393] can be used as an acid sequestrant.



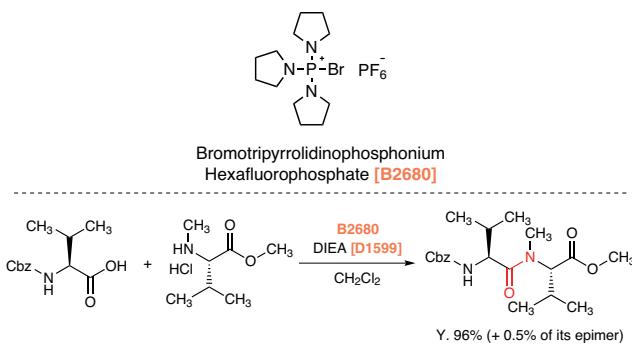
Corey-Nicolaou macrolactonization

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.^{13,14)}



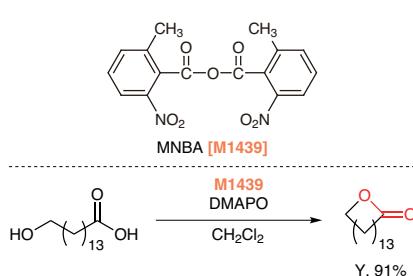
Bromotripyrrolidinophosphonium Hexafluorophosphate

Phosphonium salts such as bromotripyrrolidinophosphonium hexafluorophosphate [B2680] also have utility in condensation reactions.¹⁵⁾ 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.



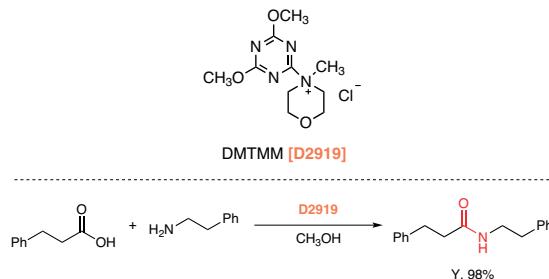
Shiina Macrolactonization

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.^{16,17)} This method is also utilized in macrolactonizations.



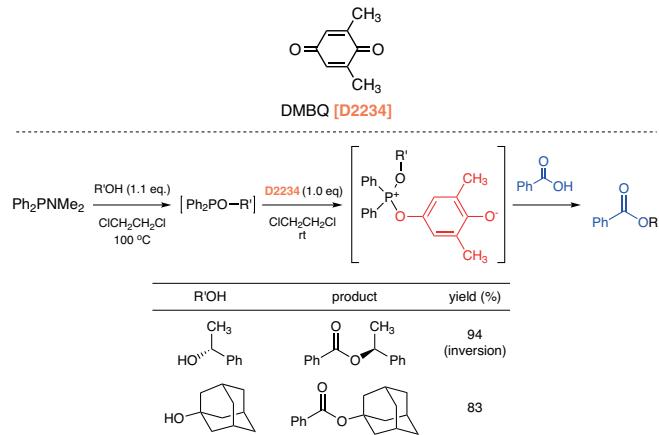
DMTMM

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.^{18,19)} This reagent has some advantages: amidation proceeds selectively even in alcohol solvent and the byproducts are easy to remove. D2919 can be used as a powerful condensing reagent.²⁰⁾



Mukaiyama Redox Condensation

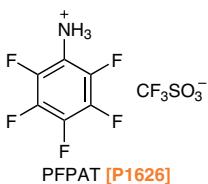
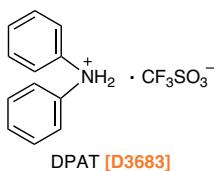
Mukaiyama *et al.* have reported a redox condensation reaction using dihydroquinone derivatives such as 2,6-dimethyl-1,4-benzoquinone (DMBQ) [D2234].^{21,22)} In this reaction, tertiary alcohols with high steric hindrance can react and afford products with stereoinversion. Furthermore, this reaction is even applicable to 1-adamantananol, the structure of which being highly resistant to stereoinversion.



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.^{23,24)} 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.²⁵⁾

PFPAT [P1626] shows higher activity than DPAT and it can be applied widely to esterification and lactonization.²⁴⁾ Furthermore, PFPAT can be removed after work-up; washing with NaOH aqueous solution removed CF₃SO₃H, followed by distillation of C₆F₅NH₂.



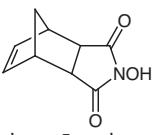
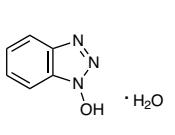
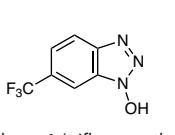
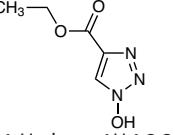
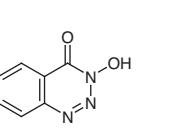
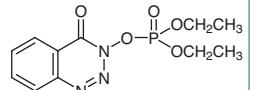
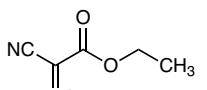
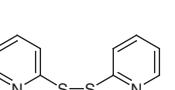
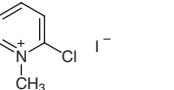
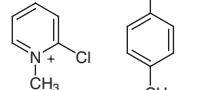
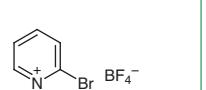
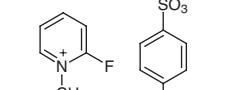
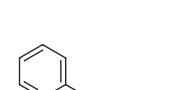
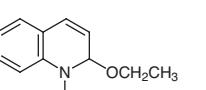
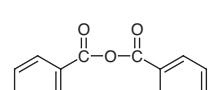
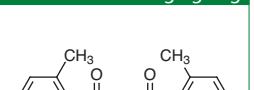
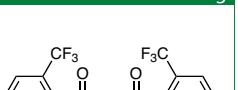
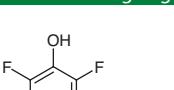
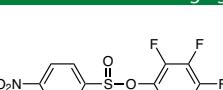
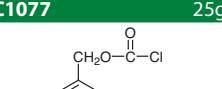
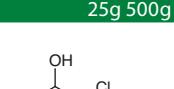
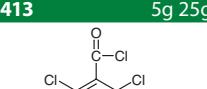
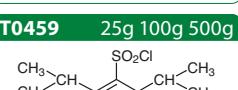
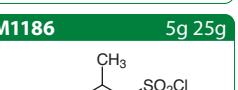
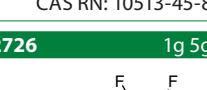
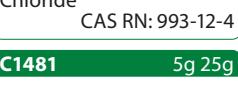
R ¹	R ²	catalyst	time (h)	Y. (%)
PhCH ₂ CH ₂ -	CH ₂ =CH(CH ₂) ₈ -	D3683	8	96
PhCH ₂ CH ₂ -	CH ₂ =CH(CH ₂) ₈ -	P1626	3	96
'Bu-	CH ₃ (CH ₂) ₇ -	D3683	24	92
'Bu-	CH ₃ (CH ₂) ₇ -	P1626	6	90

References

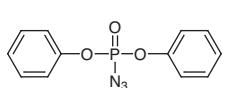
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Active Esters, Additives

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M3571	1g 5g		M3572	1g 5g		H1765	1g 5g				
		4-Methyl-N-hydroxyphthalimide CAS RN: 173962-59-9			4-Methoxy-N-hydroxyphthalimide CAS RN: 214754-50-4			TCNHPI CAS RN: 85342-65-0			

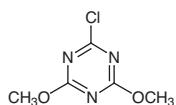
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D3262 5g  DEPBT CAS RN: 165534-43-0	E0847 25g 100g  Oxyma CAS RN: 3849-21-6	D1114 5g 25g 250g  2,2'-Dithiodipyridine CAS RN: 2127-03-9	C0903 25g  2-Chloro-1-methylpyridinium Iodide CAS RN: 14338-32-0	C0906 25g  2-Chloro-1-methylpyridinium p-Toluenesulfonate CAS RN: 7403-46-5
B1036 5g 25g  2-Bromo-1-ethylpyridinium Tetrafluoroborate CAS RN: 878-23-9	F0225 5g 25g  2-Fluoro-1-methylpyridinium p-Toluenesulfonate CAS RN: 58086-67-2	H0672 25g  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
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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

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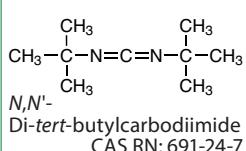
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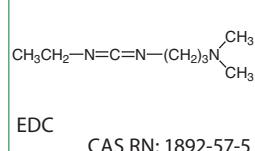
Carbodiimides

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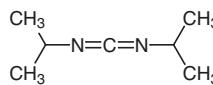
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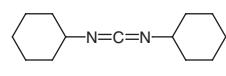
EDC
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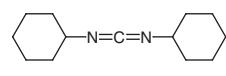
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D0436 25g 400g



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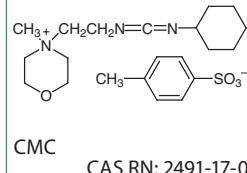
D0437 100mL



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

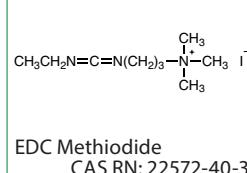
C0793 5g 25g

D1601 5g 25g 100g 250g



CMC
CAS RN: 2491-17-0

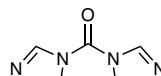
D5334 5g



EDC Methiodide
CAS RN: 22572-40-3

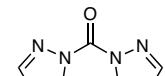
Carbonyldiimidazoles

C0119 5g 25g 250g



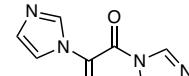
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CAS RN: 530-62-1

C2325 5g 25g



CDT
CAS RN: 41864-22-6

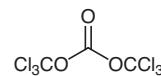
O0200 1g 5g



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

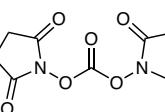
Phosgene Derivatives

T1467 25g 250g



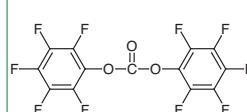
Triphosgene
CAS RN: 32315-10-9

D1662 5g 25g



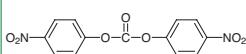
DSC
CAS RN: 74124-79-1

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



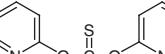
Di-2-pyridyl Carbonate
CAS RN: 1659-31-0

T1320 25g 100g



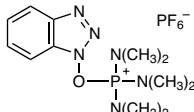
Thiophosgene
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T1906 1g



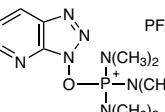
O,O'-Di-2-pyridyl
Thiocarbonate
CAS RN: 96989-50-3

B1651 5g 25g 100g



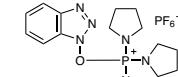
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CAS RN: 56602-33-6

A2782 1g 5g



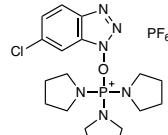
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CAS RN: 156311-85-2

B1774 5g 25g



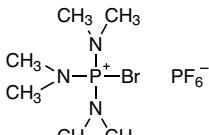
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yl-oxytripyrrolidinophosphonium
Hexafluorophosphate
CAS RN: 128625-52-5

C3461 5g 25g



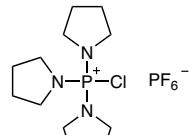
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CAS RN: 893413-42-8

B3838 1g 5g



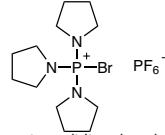
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CAS RN: 50296-37-2

C2551 5g 25g



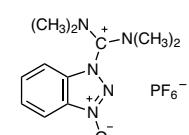
PyClop
CAS RN: 133894-48-1

B2680 5g 25g



Bromotripyrrolidinophosphonium
Hexafluorophosphate
CAS RN: 132705-51-2

B1657 5g 25g 100g

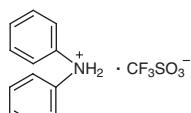
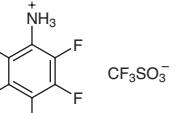
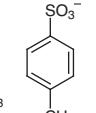
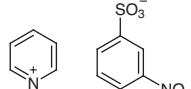
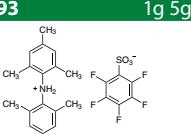
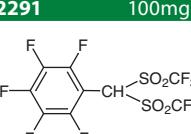
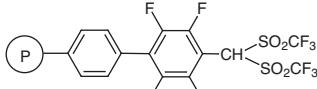
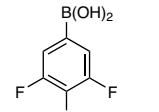
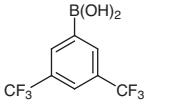
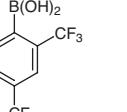
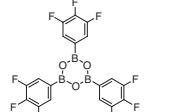
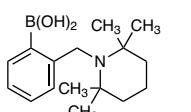
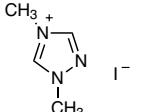
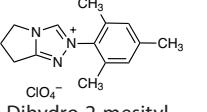
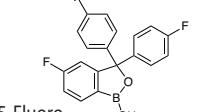
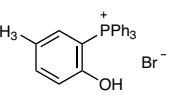
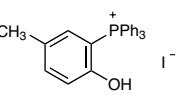
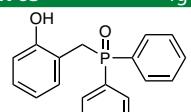
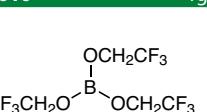
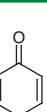
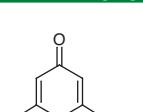
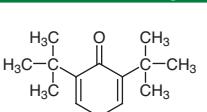
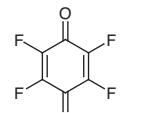
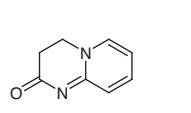
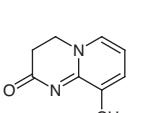
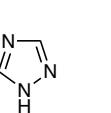
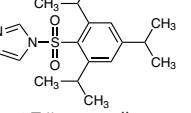


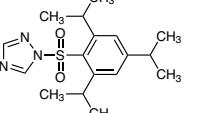
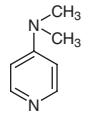
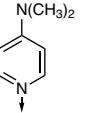
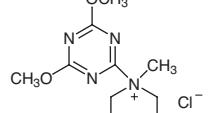
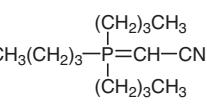
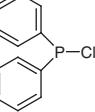
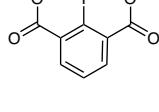
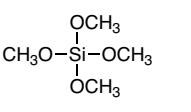
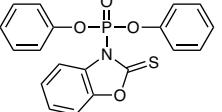
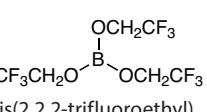
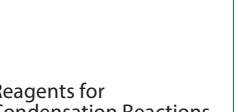
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B1658 TBTU CAS RN: 125700-67-6	A1797 HATU CAS RN: 148893-10-1	A1861 TATU CAS RN: 873798-09-5	C1926 TCTU CAS RN: 330641-16-2	C1988 HCTU CAS RN: 330645-87-9
 5g 25g	 5g 25g	 1g 5g	 5g 25g	 1g 5g
 TDBTU CAS RN: 125700-69-8	 HBPyU CAS RN: 105379-24-6	 HBPipU CAS RN: 206752-41-2	 TOTU CAS RN: 136849-72-4	 HOTU CAS RN: 333717-40-1
 5g 25g (1-Cyano-2-ethoxy-2-oxoethylideneaminoxy)-dimethylaminomorpholinocarbonium Hexafluorophosphate CAS RN: 1075198-30-9	 5g 25g (E)-[(1-Cyano-2-ethoxy-2-oxoethylideneaminoxy)-tri(pyrrolidin-1-yl)phosphonium Hexafluorophosphate(V) CAS RN: 153433-21-7			 1g 5g PTU CAS RN: 125700-71-2
 5g 25g TNTU CAS RN: 125700-73-4	 1g 5g TSTU CAS RN: 105832-38-0	 5g 25g HSTU CAS RN: 265651-18-1	 1g 5g HSPyU CAS RN: 207683-26-9	 5g 25g TOTT CAS RN: 255825-38-8
 5g HOTT CAS RN: 212333-72-7	 1g 5g TFFFH CAS RN: 164298-23-1	 1g 5g TCFH CAS RN: 94790-35-9	 5g 25g PyClU CAS RN: 135540-11-3	 5g 25g DMC CAS RN: 37091-73-9
 25g DMC (ca. 25% in Dichloromethane) CAS RN: 37091-73-9	 5g 25g CIP CAS RN: 101385-69-7	 1g 5g CIB CAS RN: 153433-26-2	 5g 25g N-(5-Chloro-2-pyridyl)-triflimide CAS RN: 145100-51-2	 5g N-(2-Pyridyl)bis(trifluoromethanesulfonimide) CAS RN: 145100-50-1
 5g 25g Phenyl Triflimide CAS RN: 37595-74-7	 10g 25g 250g Trifluoromethanesulfonic Anhydride CAS RN: 358-23-6	 1g 5g Trifluoromethanesulfonanilide CAS RN: 456-64-4	 1g 5g 1-(Trifluoromethanesulfonyl)-1H-benzotriazole CAS RN: 117632-84-5	 1g 5g 1-(Trifluoromethanesulfonyl)-imidazole CAS RN: 29540-81-6

Triflating Reagent

Condensing Agents

T3592 CF ₃ SO ₂ Br Triflyl Bromide CAS RN: 15458-53-4	T1027 CF ₃ SO ₂ Cl Triflyl Chloride CAS RN: 421-83-0	D3683  DPAT CAS RN: 164411-06-7	P1626  PFPAT CAS RN: 912823-79-1	T1122  CPTS CAS RN: 59229-09-3
Condensation Organocatalysts				
P0941  Pyridinium 3-Nitrobenzenesulfonate CAS RN: 84752-61-4	D3293  Dimesitylammonium Pentafluorobenzenesulfonate CAS RN: 850629-65-1	B2291  a,a-Bis(trifluoromethanesulfonyl)- 2,3,4,5,6-pentafluorotoluene CAS RN: 405074-81-9	B2292  Bis(trifluoromethanesulfonyl)methyltetrafluorophenyl Polystyrene Resin cross-linked with 2% DVB (200- 400mesh) (0.9-1.2mmol/g)	
T2300  (3,4,5-Trifluorophenyl)- boronic Acid CAS RN: 143418-49-9	B1886  3,5-Bis(trifluoromethyl)- phenylboronic Acid CAS RN: 73852-19-4	B3022  2,4-Bis(trifluoromethyl)- phenylboronic Acid CAS RN: 153254-09-2	T1929  2,4,6-Tris(3,4,5- trifluorophenyl)boroxin CAS RN: 223440-94-6	T2908  2-[2,2,6,6-Tetramethyl-1-piperidyl]- methylphenylboronic Acid CAS RN: 815581-79-4
D3962  1,4-Dimethyl- 1,2,4-triazolium Iodide CAS RN: 120317-69-3	D3982  6,7-Dihydro-2-mesityl- 5H-pyrrolo[2,1-c]-1,2,4- triazolium Perchlorate CAS RN: 1334529-08-6	F1259  5-Fluoro- 3,3-bis(4-fluorophenyl)- benzo[c][1,2]oxaborol-1(3H)-ol CAS RN: 2366993-30-6	H1748  MeTAPS-Br CAS RN: 2005487-65-8	H1749  MeTAPS-I CAS RN: 2005487-70-5
H1763  2-[(Diphenylphosphoryl)- methyl]phenol CAS RN: 70127-50-3	T3010  Tris(2,2,2-trifluoroethyl) Borate CAS RN: 659-18-7	B0887  1,4-Benzoquinone CAS RN: 106-51-4	D2234  DMBQ CAS RN: 527-61-7	D2256  2,6-Di-tert-butyl-p-quinone CAS RN: 719-22-2
Others				
T0790  Fluoranil CAS RN: 527-21-9	D1393  Acid Captor H CAS RN: 5439-14-5	M0670  Acid Captor 9M CAS RN: 61751-44-8	T0340  1,2,4-Triazole CAS RN: 288-88-0	T1410  1-(2,4,6-Triisopropylbenzene- sulfonyl)imidazole CAS RN: 50257-40-4

T2951  1-(2,4,6-Triisopropylbenzenesulfonyl)-1,2,4-triazole CAS RN: 54230-60-3	P2822  1-Phenyl-1 <i>H</i> -imidazol-3-ium Triflate CAS RN: 361447-81-6	D1450  DMAP CAS RN: 1122-58-3	D3220  DMAPO CAS RN: 1005-31-8	D2919  DMTMM CAS RN: 3945-69-5
C2421  1-(Cyanomethyl)piperidinium Tetrafluoroborate CAS RN: 434937-12-9	C1500  Tsunoda Reagent CAS RN: 157141-27-0	C0597  Chlorodiphenylphosphine CAS RN: 1079-66-9	I0865  Iodosodilactone CAS RN: 2902-68-3	T0588  TMOS CAS RN: 681-84-5
D2038  DBOP CAS RN: 111160-56-6	T3010  Tris(2,2,2-trifluoroethyl) Borate CAS RN: 659-18-7	R0274  Reagents for Condensation Reactions (EDCI-HCl, HOBt-H ₂ O) (HPMC encapsulated)		

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