CHEMISTRY

HPMC Capsule Reagents

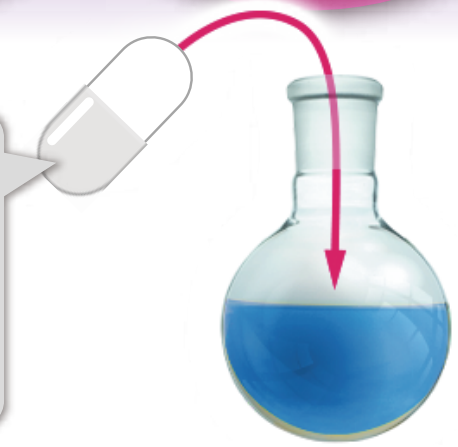
— No Need for Weighing Scales —

Condensation Reactions

Photoredox Reactions

Cross-Coupling Reactions

- Condensing agents
- Photoredox catalysts
- Palladium complexes
- Copper salts
- Phosphine ligands
- Nitrogen-donor ligands



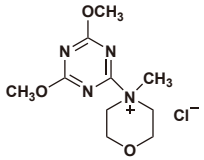
No weighing required supports your rapid organic synthesis experiments.

- Encapsulates a precise amount of chemicals, eliminating the need for weighing and enabling efficient coupling reactions.
- Hydroxypropyl methylcellulose (HPMC) capsule dissolves in polar solvents, making it simple to carry out reactions.
- The formation of the reactive site in the hydrophobic pockets of HPMC in water allows chemical reactions to proceed very rapidly.
- Dissolved HPMC can be removed easily after reaction.

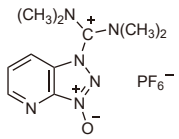
Solubility of HPMC Capsules in Solvents

Solvent	Solubility	Solvent	Solubility	Solvent	Solubility
Water	Soluble	Dioxane	Soluble with heat	THF/Water(1:1)	Soluble
DMSO	Soluble	Acetonitrile	Insoluble	THF/Water(4:1)	Soluble
DMF	Soluble	Dichloromethane	Insoluble	Dioxane/Water(1:1)	Soluble
NMP	Soluble	THF	Insoluble	Ethanol/Water(1:1)	Soluble
Methanol	Soluble	Ethanol	Insoluble	IPA/Water(1:1)	Soluble
DMAc	Soluble	IPA	Insoluble		

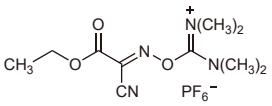
Capsule Reagents Encapsulating a Condensing Agent



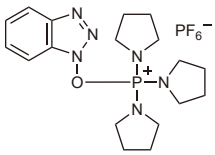
DMT-MM
ca. 0.30 mmol
[R0294]



HATU
ca. 0.45 mmol
[R0295]

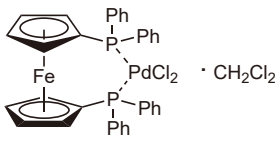


HOTU
ca. 0.25 mmol
[R0297]

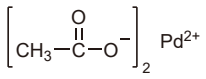


1*H*-Benzotriazol-1-yloxytripyrrolidino-phosphonium Hexafluorophosphate
ca. 0.25 mmol
[R0296]

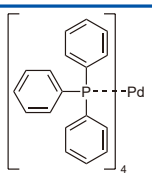
Capsule Reagents Encapsulating a Palladium Complex



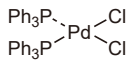
$PdCl_2(dppf)\cdot CH_2Cl_2$
ca. 0.09 mmol
[R0307]



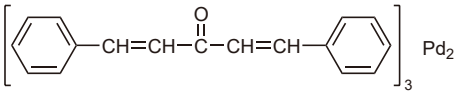
$Pd(OAc)_2$
ca. 0.50 mmol
[R0303]



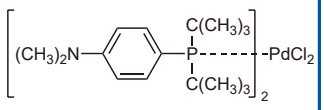
$Pd(PPh_3)_4$
ca. 0.06 mmol
[R0304]



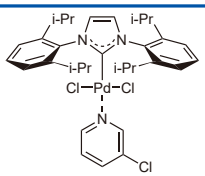
$PdCl_2(PPh_3)_2$
ca. 0.09 mmol
[R0308]



$Pd_2(dba)_3$
ca. 0.06 mmol
[R0305]

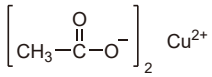


$PdCl_2(amphos)_2$
ca. 0.06 mmol
[R0306]



Organ's Catalyst
ca. 0.06 mmol
[R0321]

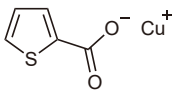
Capsule Reagents Encapsulating a Copper Salt



$Cu(OAc)_2$
ca. 0.60 mmol
[R0312]

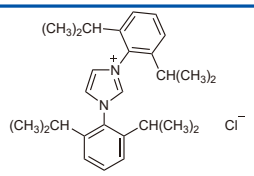
CuI

CuI
ca. 0.80 mmol
[R0314]



CuTC
ca. 0.65 mmol
[R0315]

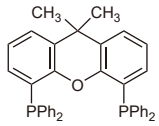
Capsule Reagent Encapsulating a *N*-Heterocyclic Carbene (NHC) Ligand Precursor



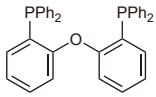
IPr·HCl
ca. 0.125 mmol
[R0316]

HPMC Capsule Reagents — No Need for Weighing Scales —

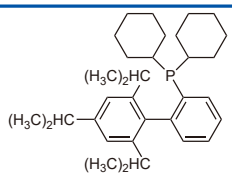
Capsule Reagents Encapsulating a Phosphine Ligand



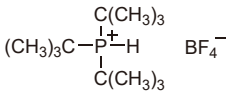
Xantphos
ca. 0.125 mmol
[R0300]



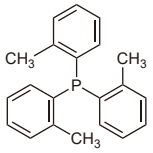
DPEphos
ca. 0.15 mmol
[R0301]



Xphos
ca. 0.125 mmol
[R0302]

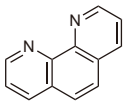


P(*t*Bu)$_3$·HBF$_4$
ca. 0.27 mmol
[R0318]

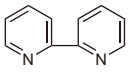


Tri(*o*-tolyl)phosphine
ca. 0.25 mmol
[R0319]

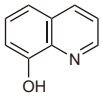
Capsule Reagents Encapsulating a Nitrogen Donor



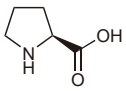
1,10-Phenanthroline
ca. 0.35 mmol
[R0309]



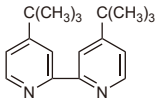
2,2'-Bipyridyl
ca. 0.50 mmol
[R0310]



8-Quinolinol
ca. 0.45 mmol
[R0311]



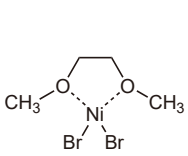
L-Proline
ca. 0.50 mmol
[R0313]



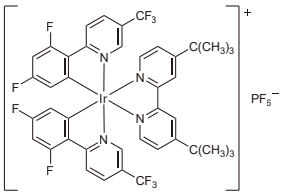
4,4'-Di-*tert*-butyl-2,2'-bipyridyl
ca. 0.20 mmol
[R0320]

Capsule Reagents Encapsulating Multiple Components

These reagents encapsulate multiple components, allowing the reaction to be performed simply by adding the substrate and solvent.



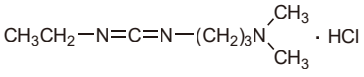
NiBr$_2$(dme)
ca. 0.03 mmol



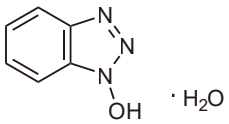
[Ir[dF(CF$_3$)ppy]$_2$(dtbbpy)]PF$_6$
ca. 0.12 mmol

DABCO
ca. 1.10 mmol

[R0273]

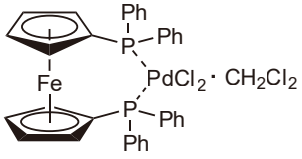


EDCI·HCl
ca. 0.25 mmol

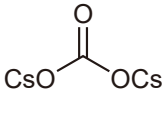


HOBt·H$_2$O
ca. 0.04 mmol

[R0274]



PdCl$_2$(dppf)·CH$_2$Cl$_2$
ca. 0.03 mmol

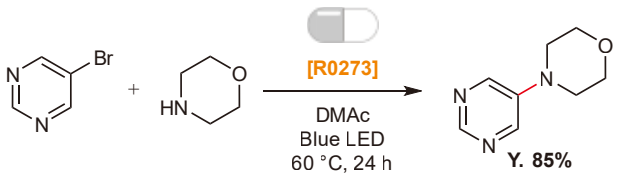


Cs$_2$CO$_3$
ca. 0.70 mmol

[R0275]

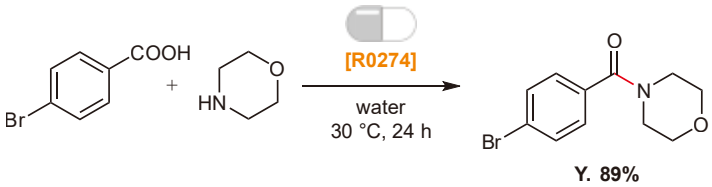
[Application 1]

Metallophotoredox Cross-Coupling Reaction with R0273



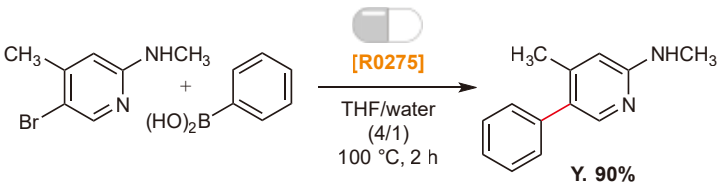
[Application 2]

Condensation Reaction with R0274



[Application 3]

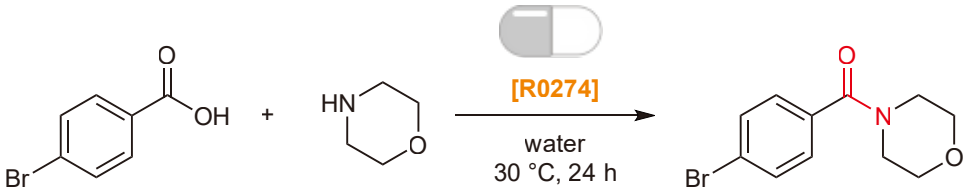
Suzuki-Miyaura Cross-Coupling Reaction with R0275



HPMC Capsule Reagents — No Need for Weighing Scales —

Application

TCI Practical Example: Condensation Reaction with R0274



Y. 89%

Procedure

Reagents for condensation capsule **[R0274]** (one capsule) were added to a solution of 4-bromobenzoic acid (40 mg, 0.20 mmol, 1.0 eq.), morpholine (17 µL, 0.20 mmol, 1.0 eq.) in water (1 mL) at room temperature. The mixture was stirred at 30 °C for 24 hours. The reaction solution was diluted with sat. Na_2SO_4 aq. (15 mL) and extracted with ethyl acetate (15 mL x 2), and the organic layer (*) was washed with 2 mol/L HCl aq. (15 mL), sat. $NaHCO_3$ aq. (15 mL) and brine (15 mL). The organic layer was dried over sodium sulfate, concentrated under reduced pressure, and the crude product was purified by silica gel chromatography (ethyl acetate:hexane = 2:1 to 1:1) to afford (4-bromophenyl)(morpholino)methanone (48 mg, 89% yield) as a white solid.

*If precipitates were present in the organic layer during separation, they were filtered through Celite.

See the "Applications" tab on TCI website page for more information. ▶▶▶ TCI HPMC

References N. Borlinghaus, A. Jolit, *et al.*, *J. Org. Chem.* **2021**, *86*, 1357. https://doi.org/10.1021/acs.joc.0c02576
S. Sharma, S. Handa, *et al.*, *ACS Sustain. Chem. Eng.* **2021**, *9*, 12719. https://doi.org/10.1021/acssuschemeng.1c04607
D. Petkova, S. Handa, *et al.*, *ACS Sustain. Chem. Eng.* **2020**, *8*, 12612. https://doi.org/10.1021/acssuschemeng.0c03975

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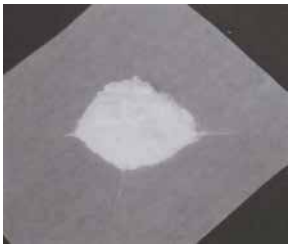

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