Click Chemistry

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Ethynylation Reagents
Azide Compounds
Organic Azides
PEG Azides
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Terminal Acetylenes
Hydrocarbons
Hydrocarbons having Benzene Ring
Carboxylic Acids & Their Derivatives
Alcohols
Other Functional Terminal Acetylenes
"Click Chemistry" is a term which was first described by K. B. Sharpless of the Scripps Research Institute in 2001 to describe reactions that afford products in high yields and in excellent selectivities by carbon-hetero bond formation reactions. The term "Click" means joining molecular pieces as easily as clicking together the two pieces of a seat belt buckle. In general, the definition of click chemistry is described as follows:

1. give very high chemical yields of desired products
2. combination of readily available simple building blocks
3. generate almost no byproducts
4. simple product isolation by non-chromatographic methods
5. reaction proceeds in water, as well as in organic solvents

While there are a number of reactions that fulfill this criteria, the Huisgen 1,3-dipolar [3 + 2] cycloaddition1) of azides and alkynes has emerged as the frontrunner. In general, the 1,2,3-triazole ring is not almost oxidized or reduced, which makes it possible to strongly connect two substrates.

This reaction system affords desired products in almost 100% yield with no need of repurification, such as recrystallization or column chromatography. Thus, this methodology is an eco-friendly reaction. Moreover, the combination of various alkynes and azides allows it to rapidly construct large compound libraries, and 1,2,3-triazole itself exhibits various kinds of biological activities, such as anti-allergic or anti-bacterial activities. In addition, the reaction proceeds even in water, and thus, click chemistry has been widely used in many research fields as below:

● Research of Various Pharmaceutical Lead Candidates

a) Application of Anti-HIV Agent Discovery 2)
Whiting and Sharpless et al. have reported the synthesis of a series of 1,4-disubstituted-1,2,3-triazoles as potential candidates for HIV protease inhibitors in a combination of azide-containing fragments with a diverse array of functionalized alkyne-containing building blocks by using click chemistry. After further optimization, it was revealed that 1 has the highest activity, exhibiting 8 nM of Ki value.

b) Research of Mycobacterium Tuberculosis Cell Wall Synthetase 3)
Dondoni et al. have reported the synthesis of a set of C-oligomannosides (2a-f) through click chemistry using a 1,2,3-triazole ring as the interglycosidic linker. The compounds 2a-f inhibit mannosyltransferases, which are involved in the biosynthesis of the cell envelope of Mycobacterium tuberculosis cell wall synthase. Among them, the hexamer (n = 4) 2c and octamer (n = 6) 2f show the highest activities IC50 = 0.14 and 0.22 mM, respectively.

● Synthesis of Functional Materials
Click chemistry have been also successfully applied into polymer synthesis or material science. For example, Kang and Jin et al. have reported the synthesis of side-chain liquid-crystal polymers 3 and 4 by using click chemistry. According to their results, the dye-sensitized solar-cell fabricated from 3 gives a power-conversion efficiency of 4.11%.

N3 + CuSO4, CuPh
CuSO4·5H2O, Et3N
Na-L-ascorbate

N3

CuSO4·5H2O

CuSO4·5H2O

Na-L-ascorbate

THF, 35°C, 48 h

CuSO4·5H2O, Et3N

Na-L-ascorbate

THF, 35°C, 48 h

R = OMe

R = CN
●Bioscience

Bioconjugation (example: surface modification of virus)

In general, viruses are made up of a number of protein subunits, and capsids, which enclose DNA or RNA, are formed as protein shells. In particular, in the case of spherical viruses, the capsids have an icosahedral symmetry form with sixty protein subunits. Finn and Sharpless et al. have reported the modification of the exterior surface of a spherical virus, cowpea mosaic virus by azides or alkynes, followed by the labeling of these species using fluorescein dye-azide or alkyne by click chemistry.

Thus, click chemistry has been widely used as a methodology of synthesizing novel molecules in a number of research fields. Other than these applications, click chemistry also has been applied in various fields, such as the synthesis of dendrimers, dendrons, calyxtrenes, rotaxanes, catenanes, the development of chemical sensors, and the labeling of DNA.

TCI offers a variety of azide and terminal acetylene compounds readily available in the field of click chemistry as below. In addition, azidation and ethynylation reagents are also listed in this brochure.

● Azidation Reagent

Organic azide compounds can be synthesized in a simple manner by the reaction of sodium azide with halogenated alkyl compounds, or the reaction with trifluoromethanesulfonfnyl azide and primary amines, however, these azide sources potentially have highly explosive character, which makes it difficult to handle. 2-Azido-1,3-dimethylimidazolinium hexafluorophosphate (A2457) (9), which was developed by Kitamura et al., is a crystalline diazotransfer reagent having high thermal stability and low explosibility. The differential scanning calorimetry (DSC) experiment of 9 has revealed that the exothermic decomposition temperature was approximately 200 °C. Moreover, 9 has tested negative for the impact and friction-sensitivity tests.

Under basic conditions, 9 reacts with several kinds of primary amines in a short time to afford the corresponding diazo compounds in high yields. In these reactions, the by-products can be removed by conventional extraction procedures due to their high solubility in water.

● Ethynylation Reagents

A number of ethynylation reagents have been developed for the synthesis of terminal acetylenes. For example, ethynyl(phenyl)iodonium tetrafluoroborate (EO467) (10) is an electrophilic ethynylation reagent developed by Ohira et al., which reacts with active methylene compounds to afford the corresponding α-ethynlated products in high yields under mild conditions. As for other existing electrophilic ethynylation reagents, ethyl lead triacetate has been exploited, which is prepared from ethynyl(trimethyl)stannane and lead tetraacetate. However, preparation of this reagent requires the use of heavy metal compounds, which make it an unattractive procedure. The ethynylation procedure using this reagent requires careful control of the reaction conditions. The ethynylation method using 10 has been at the center of attention in many fields, as this method does not use highly toxic heavy metal compounds, and the reaction proceeds under mild conditions.

Additionally, (1-diazo-2-oxopropyl)phosphonate (D3546) (11) is a reagent for the synthesis of terminal alkynes, which was developed by Ohira and Bestmann et al. 11 reacts with aldehydes in the presence of potassium carbonate and methanol to give the one homologated terminal alkynes in high yields. 11 is widely known as the "Ohira-Bestmann reagent" after its discoverers, and the reaction proceeds in mild conditions without using strong bases.
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**References**


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**Metal Catalysts**

- **T2665** 5g
  - (CH₂CN)₄ CuPF₆
  - Tetraakis(acetonitrile) copper(I) Hexafluorophosphate [64443-05-6]

- **A1540** 5g
  - CH₃ O COCu
  - Copper(I) Acetate [598-54-9]

- **C2346** 25g
  - (CH₃CHOH)₂ Cu⁺ · H₂O
  - Copper(I) Acetate Monohydrate [6046-93-1]

- **T1442** 1g
  - CP₂ CuPF₆ · Hexafluorophosphate
  - Copper(II) Trifluoromethanesulfonate Benzene Complex [42152-46-5]

**Azidation Reagents**

- **T0920** 5g
  - CH₃ N₃
  - Tetrabutylammonium Azide [993-22-6]

- **A2457** 5g
  - 2-Azido-1,3-dimethyl-imidazolinium Hexafluorophosphate [1266134-54-6]

- **D1672** 5g
  - Diphenylphosphoryl Azide [26386-88-9]

- **T0801** 25g
  - CH₃ N₃
  - Trimethylsilyl Azide [4648-54-8]

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Ethynylation Reagents

D3546 1g 5g
Dimethyl[1-Diazo-2-oxopropyl]phosphonate
(Ohira-Bestmann Reagent)
[90965-06-3]

E0467 1g
Ethynyl(phenyl)iodonium Tetrafluoroborate
[Ethynylation Reagent]
[127783-34-0]

M0180 25mL 500mL
2-Methyl-3-buten-2-ol
[115-19-5]

T1239 5mL 25mL 250mL
Trimethylsilylacetylene
[1066-54-2]

Azide Compounds

Ethynylation Reagents

A0930 5g 25g
4-Azidobenzoic Acid
[6427-66-3]

A0971 5g
N-Succinimidyl 5-Azido-2-nitrobenzoate
[60117-35-3]

Organic Azides

A2523 100mg
N-[2-[2-[2-Azidoethoxy]ethoxy]ethyl]-biotinamide
[875770-34-6]

Sugar Azides

A1678 1g 5g
2-Acetamido-3,4,6-tri-O-benzyl-2-deoxy-β-D-glucopyranosyl Azide
[188397-31-1]

A1812 1g
2-Acetamido-3-O-allyl-4,6-O-benzylidene-2-deoxy-β-D-glucopyranosyl Azide

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**Terminal Acetylenes**

- **A1813** 1g
  - 2-Acetamido-3-0-benzyl-4,6-O-benzylidene-2-deoxy-β-D-glucopyranosyl Azide [80887-27-0]
- **A1832** 100mg
- **A1833** 100mg
- **A2172** 500mg
  - 2-Azidoethyl 2-Acetamido-2-azido-2-deoxy-β-D-glucopyranoside [142072-12-6]
- **A2267** 1g
  - 2-Azidoethyl β-D-Glucopyranoside [165331-08-8]
- **A2377** 1g 5g
  - 2-Azidoethyl 2-Acetamido-2-azido-2-deoxy-β-D-glucopyranoside [140428-81-5]
- **G0330** 1g 5g
  - Gal[2346Ac][1-3]Gal[b(46Bzd)]-β-MP
- **G0337** 100mg
  - GlcNAc β(1-2)Man α-1-Ethylazide
- **G0372** Price on request
  - GlcA[53][β(1-3)Gal β(1-4)GlcNAc β(1-2)Man α-1-Ethylazide
- **G0373** Price on request
  - GalNAc β(1-3)GlcNAc β-Ethylazide
- **M1617** 1g
  - 4-Methoxyphenyl 2-Azido-3,6-di-O-benzyl-2-deoxy-β-D-glucopyranoside [1272755-25-5]
- **M1637** 1g 5g
  - 4-Methoxyphenyl 2-Azido-4,6-O-benzylidene-2-deoxy-β-D-glucopyranoside [889453-78-5]
- **M1638** 1g
  - 4-Methoxyphenyl 3-0- Allyl-2-azido-4,6-O-benzylidene-2-deoxy-β-D-glucopyranoside [889453-83-2]
- **T1732** 100mg
  - 1,3,4,6-Tetra-0-acetyl-2-azido-2-deoxy-α-D-glucopyranoside [56883-33-1]
- **T1733** 100mg
  - 1,3,4,6-Tetra-0-acetyl-2-azido-2-deoxy-α-D-mannopyranoside [68733-20-0]
- **T2196** 200mg 1g
  - 1,3,4,6-Tetra-0-acetyl-2-azido-2-deoxy-β-D-glucopyranoside [80321-89-7]

**Hydrocarbons**

- **B1114** 10mL 100mL
  - 3,3-Dimethyl-1-butylene [917-92-0]
- **D0037** 5mL 25mL
  - 1-Decyne [764-93-2]
- **D0997** 5mL
  - 1-Dodecyne [766-03-7]
- **D1326** 5mL
  - 1,9-Decadiyne [1720-38-3]
- **D1723** 5g
  - 1,4-Decadiyne (50% in Hexane, ca. 2.7mol/L) [929-53-3]
- **D1724** 1mL 5mL
  - 1,5-Decadiyne [53963-03-4]
- **H0048** 25mL
  - 1-Heptyne [628-71-7]
- **H0140** 25mL 250mL
  - 1-Hexyne [693-02-7]
- **H0433** 5mL
  - 1-Hexadecyne [629-74-3]
- **H0440** 1g
  - 1-Heptadecyne [26186-00-5]
- **H0483** 5mL
  - 1,6-Heptadiyne [2396-63-6]
- **H0485** 5mL
  - 4-Methyl-1-pentyne [7154-75-8]

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**Alcohols**

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<th>Volume</th>
<th>Description</th>
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<td>3-Butyn-2-ol (85% in Water, ca. 7.5 mol/L) [2028-63-9]</td>
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<td>3-Butyn-1-ol [927-74-2]</td>
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**Other Functional Terminal Acetylenes**

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<td>3-Butyn-2-one [1423-60-5]</td>
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