



Niche Wittig Reagents

Wittig reagents are among the most powerful and versatile tools in small-molecule synthesis. They enable the formation of carbon-carbon double bonds (alkenes) with remarkable precision, giving chemists excellent control over both the position and geometry (E/Z selectivity) of the newly formed double bond. The reaction proceeds by transforming a carbonyl group—typically an aldehyde or ketone—into an alkene through the intermediacy of a phosphonium ylide.

A key advantage of the Wittig reaction lies in its mild, relatively neutral operating conditions. These gentle conditions make it compatible with a wide range of functional groups that are often sensitive to strong acids, bases, or oxidizing/reducing agents. This combination of mildness and predictability has made the Wittig reaction a cornerstone of modern synthetic organic chemistry.

Beyond academic research, Wittig chemistry plays a central role in industrial and applied synthesis. It is widely used in the production of pharmaceuticals, agrochemicals, fragrances, and flavors, as well as in total synthesis of complex natural products where precise double-bond placement determines biological activity. Modified versions of the reaction—such as the Horner–Wadsworth–Emmons reaction and the Schlosser modification—further expand its stereoselectivity and substrate scope.

The development of Wittig reagents revolutionized carbon–carbon bond formation, providing chemists with a robust, flexible, and reliable method for alkene construction. Even decades after its discovery, the Wittig reaction remains an indispensable technique in synthetic chemistry

Benzyltriphenylphosphonium chloride

Molecular Formula: C25H22PCI

Molecular Weight: 388.87 g/mol

• CAS Number: 1100-88-5

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Applications

1. Wittig Reaction: Key reagent for the generation of ylides (benzylidene ylides); Used in olefination reactions to convert aldehydes/ketones into alkenes

2. Phase Transfer Catalyst (PTC): Acts as a quaternary phosphonium salt for facilitating reactions between immiscible phases (aqueous/organic).

3. Pharmaceutical & Fine Chemicals: Intermediate in organic synthesis; Applied in synthesis of specialty molecules requiring phosphonium intermediates.

3-Carboxypropyltriphenylphosphonium

Molecular Formula: C22H22BrO2P

Molecular Weight: 429.29 g/mol

• CAS Number: 17857-14-6

Applications

1. Mitochondrial Targeting: The triphenylphosphonium (TPP) cation preferentially accumulates in mitochondria due to the negative membrane potential

2. Drug Delivery & Conjugation: Used in synthesizing targeted therapeutic agents for oxidative stress, cancer, and neurodegenerative diseases.

3. Biological Probes & Imaging: Facilitates structure—activity relationship (SAR) studies of mitochondria-directed molecules.

4. Research Tool in Biomedicine: Helps in studying mitochondrial dysfunction, apoptosis, and metabolic diseases.

4-Carboxybutyltriphenylphosphonium bromide

Molecular Formula: C23H24BrO2P

Molecular Weight: 427.3 g/molCAS Number: 17814-85-6

O PHO Br

Applications

1. Mitochondrial Targeting: The triphenylphosphonium (TPP) cation preferentially accumulates in mitochondria due to the negative membrane potential

2. Bioconjugation & Synthetic Intermediate: Used in peptide/drug conjugation research as a mitochondrial anchor; Also applied in synthetic chemistry as a precursor for more complex phosphonium-based probes and drug candidates.

(2-Hydroxybenzyl)triphenylphosphonium

Molecular Formula: C₂₅H₂₂BrOP

Molecular Weight: 449.32 g/mol

• CAS No. 70340-04-4

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Applications

1. Antioxidant Research: The 2-hydroxybenzyl moiety resembles phenolic antioxidants; Investigated for reactive oxygen species (ROS) scavenging when localized in mitochondria.

2. Chemical Biology & Probe Development: Can serve as a starting point in synthesizing Mito-analogues of known drugs (e.g., MitoQ-like structures).

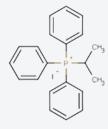
3. Biological Studies: Explored in models of neurodegeneration, cardiovascular damage, and cancer.

(2-Propyl)triphenylphosphonium iodide

Molecular Formula: C21H22IP

Molecular Weight: 432.28 g/mol

• CAS No. 24470-78-8



Applications

1. Mitochondrial Targeting: PTPPI is used as a delivery vehicle to target drugs, imaging agents, and probes to mitochondria.

2. Drug Conjugation Intermediate: The propyl group acts as a tether for attaching bioactive molecules; Precursor for developing mitochondria-targeted antioxidants, cytotoxic agents, and metabolic modulators.

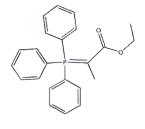
3. Anticancer Research: Conjugates of TPP with chemotherapeutics are being explored for selective delivery to tumor mitochondria, enhancing efficacy and reducing systemic toxicity

4. Neurodegenerative & Metabolic Disorders: Applied in the development of mitochondriatargeted antioxidants or Parkinson's, Alzheimer's, and other oxidative stress-driven conditions.

Ethyl 2-(triphenylphosphoranylidene)

Molecular formula: C₂₃H₂₁O₂P

Molecular weight: ~360.39 g/mol



Applications

1. As a Stabilized Wittig Reagent: Used to convert aldehydes (and some ketones) into α,β -unsaturated esters with high selectivity; Typically gives predominantly E-alkenes due to resonance stabilization of the ylide.

2. Synthesis of Conjugated Esters: Plays a key role in constructing trans-α,β-unsaturated esters for pharmacueicals: Trichostatin A, Transcrocetinate, Sacubitril, gamma-Tocotrienol, etc.



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