Connecting molecules – made easy

High-end reagents, building blocks
and additives for R&D and production.

EMD Millipore Corp. is a subsidiary of Merck KGaA, Darmstadt, Germany

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Your partner for …
High-end reagents, building blocks and additives for R&D and production

Are you satisfied with the cost-efficiency of your synthesis? Do you need support in finding suitable and more cost-efficient reagents and building blocks for your synthesis? Would you like higher yields and to use less hazardous and more environment-friendly starting materials? Are you looking for innovative additives to improve your products?

EMD Millipore now offers a range of selected, innovative and highly-efficient reagents, building blocks and additives for R&D, scale-up and production processes.

These unique products provide an outstanding asset for developing new products or improving your existing manufacturing processes.

And if you need a customized solution – we can supply these products in amounts ranging from single grams to several tons either as catalog pack or in tailor-made volumes.

Index

T3P®

The coupling performance leader

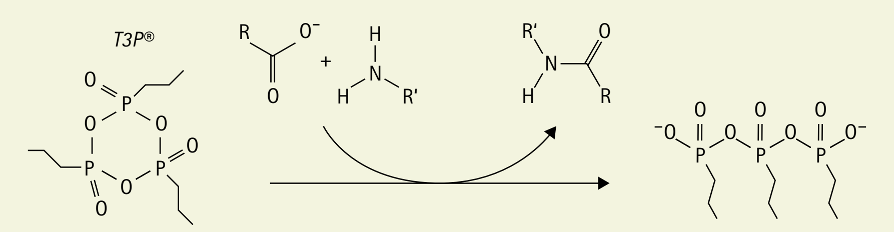
n-Propanephosphonic acid anhydride (T3P®) is a highly-efficient reagent for amide/peptide bond formation and other condensation and dehydration reactions.

It provides high selectivity, coupled with low epimerization and high yields, without the need for hazardous additives such as the explosive 1-Hydroxybenzotriazole (HOBt).

Additionally, T3P® is really green: it is non-toxic, non-allergenic, non-sensitizing, and because the only waste products are phosphate salts, products isolation can be achieved by simple extraction.

High selectivities and minor product losses in the purification steps result in great yields that makes T3P® particularly attractive for high-value synthesis involving expensive reacting agents.

Reaction mechanism



T3P® Coupling: easy purification (only water soluble by-products)

Due to its viscous nature, we offer T3P® as 50 % solution for your convenience:

- T3P® in Ethyl acetate (EtOAc)
- T3P® in 2-Methyl-tetrahydrofuran (MeTHF)
- T3P® in Dimethylformamide (DMF)

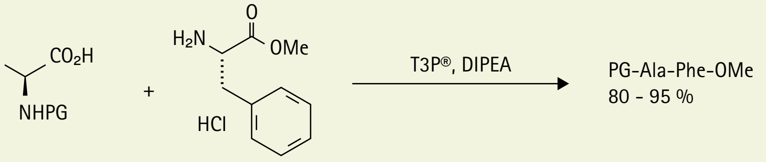
Advantages

- Significantly higher yields compared to Dicyclohexylcarbodiimide (DCC)/HOBt coupling
- Safe handling, non-toxic, no CMR properties, no allergenic nor sensitizing properties
- Minimal epimerization during coupling, no additives required
- Mild reaction conditions – lower total cost
- Couplings can be performed in many different solvents
- Mediates condensation reactions on a wide variety of substrates

T3P® works in a broad variety of applications:

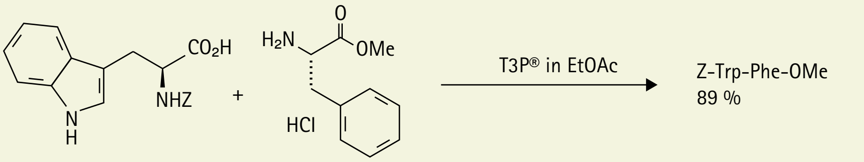
Peptide couplings and amide formations

1) Peptide coupling with common protecting groups (PG)

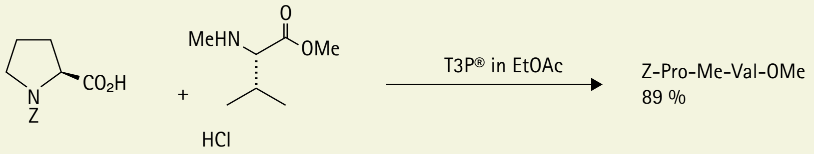


PG=Z, Boc, Fmoc. Solvents, e.g. EtOAc, BuOAc, DMF, Toluene, THF, DMC, ACN, MeTHF

2) Peptide coupling with side-chain unprotected amino acids

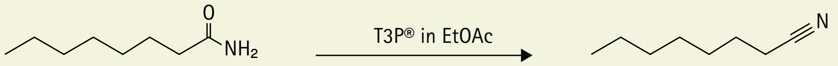


3) Peptide coupling with sterically demanding amino acids



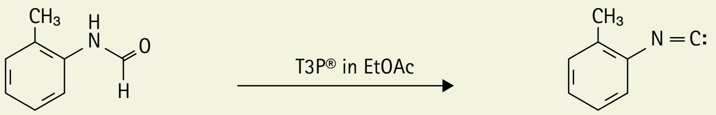
Nitrile formations with T3P®

Synthesis of Octanenitrile



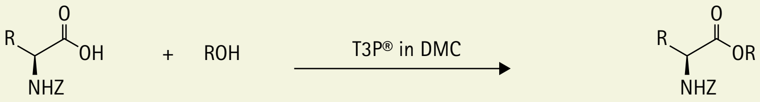
Isonitrile formation with T3P®

Synthesis of 2-Methylphenylisocyanide



Ester formation with T3P®

Synthesis of Amino Acid Esters

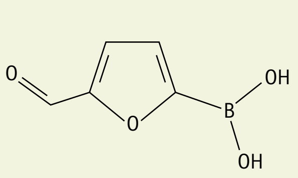


Bifunctional boronic acids

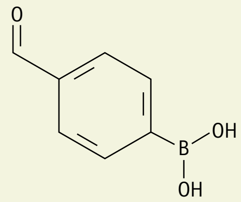
Efficient C-C coupling reagents

Boronates are valuable tools for organic synthesis as they undergo Pd-mediated carbon-carbon cross-coupling (Suzuki reaction) with aryl halides, enabling the preparation of complex substituted aryl scaffolds quickly under mild conditions. EMD Millipore's bifunctional boronic acids are particularly useful as they contain aldehyde and alcohol functionalities which facilitate further synthetic elaboration.

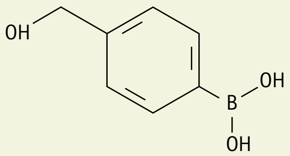
Boronic acids are also capable of forming reversible covalent complexes with sugars, amino acids, hydroxyamic acids and other Lewis bases, making them potentially useful as temporary scaffolds and protecting groups for these groups.



5-Formylfurane-2-boronic acid



4-Formylphenyl boronic acid



4-Hydroxymethylphenyl boronic acid

Advantages

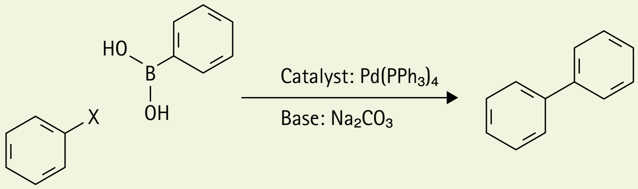
- Bifunctional compounds for various chemical applications
- Perfectly suitable for Suzuki and other carbon-carbon bond couplings under mild conditions
- Ideal for further chemical modification due to second chemical function
- Use as catalysts or temporary scaffolds in regio-, stereo- and enantioselective synthesis

Suzuki coupling reaction

The first step of this Pd catalyzed reaction is the oxidative addition of palladium to the aryl(Ar) or vinyl(Vin) halide to form an Ar/Vin-Pd-X complex. This reacts with the R-B$(OH)_4$ – form of the boronate to form a R-Pd-Ar/Vin complex which then goes by reductive elimination to give R-Ar/Vin. The original palladium catalyst is restored. This coupling reaction is widely used to synthesize polyolefine, styrenes, substituted biphenyls and to incorporate alkyl bromides.

$$R_1{-}By_2 + R_2{-}X \xrightarrow[\text{Base}]{\text{Pd catalyst}} R_1{-}R_2$$

Using phenylboronic acids leads to biphenyl derivatives:



Oxa acids

Bifunctional PEG-like modifiers

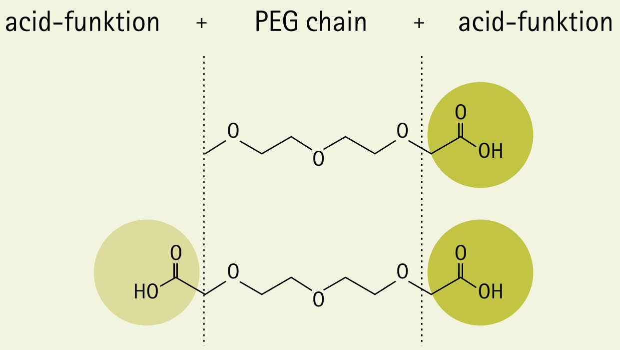
Oxa acids are versatile materials which are used in pharmaceutical and cosmetic industry, as well as nano-technology and other high-tech applications. By varying chain length and controlling the number of ionization functionalities, their properties can be exactly tailored for a given application.

Due to low melting and high boiling points oxa acids remain liquid over a broad range of temperatures. The unique combination of lipophilic $[(CH_2CH_2O)n]$ and hydrophilic [COOH] functions makes these clear and colorless substances “multifunctional”, useful in various chemical and physical applications.

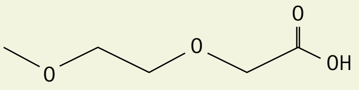
Advantages

- No salts formed, high yields
- Water soluble and biologically degradable
- Non-toxic and non-irritating
- Excellent heat stability
- Outstanding complexation properties

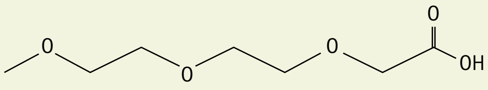
Fine tuning of properties



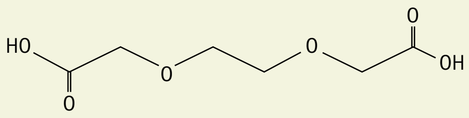
Choose from a portfolio of oxa acids with one or two acid functions and a wide variety of different chain lengths for exactly tailored properties. Due to their biodegradability oxa acids are a new generation of environment-friendly products.



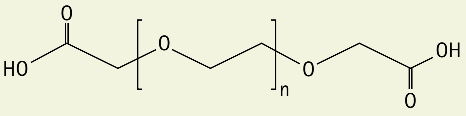
3,6-Dioxaheptanoic acid



[2-(2-Methoxyethoxy)ethoxy] acetic acid



2,2'-[Ethylenebis(oxy)] bisacetic acid



Polyglycol diacid (n=10-12)

Pharmaceutical applications

- Surfactants in lipid emulsion systems
- Linkers for chemical fixing of organic compounds
  - Complexing agents in organometallic chemistry
  - Phase transfer catalysts
  - Polar high boiling solvents and distillation additives
  - Additives in electroplating processes

Vinylphosphonic acids (VPA)

Metal surface modifiers

VPA and dimethylvinyl phosphonate (DMVPA) are monomers for radical homo- or co-polymerization. Polymers containing VPA and DMVPA exhibit remarkable properties due to the presence of both lipophilic and hydrophilic functionalities in one molecule. VPA-polymers may be used to promote adhesion between metals, pigments, glass and plastics, and incorporation of these monomers can help improve the properties of coatings, corrosion inhibitors and additives for dispersions.

VPA is able to form complexes with a broad range of metal ions, offering the potential for applications in metal-binding polymers.

Polymers containing VPA have enhanced flame-retardant properties due to the presence of phosphorous. Incorporation of the flame-retardant directly into the polymers eliminates problems with volatility associated with traditional flame-retardant additives.

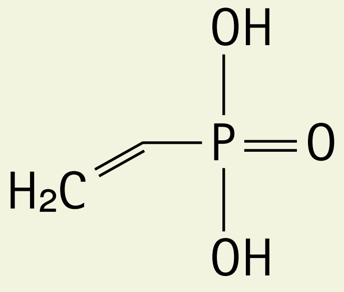
Polymers containing VPA are able to stabilize acid emulsions and dispersions. VPA is a highly polar monomer that has excellent solubility characteristics. It can be dissolved in many organic solvents.

Advantages

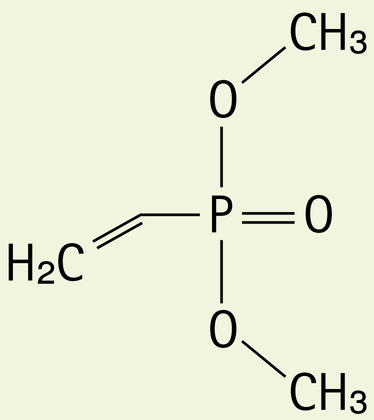
- Soluble in water and most organic solvents
- Flame-retardant properties
- Excellent heat and hydrolysis stability
- Dispersing benefits
- Strong metal complexation properties

Wide range of applications

- Lithography
- Coating
- Metal treatment
- Corrosion inhibitor
- Flame retardant



VPA



DMVPA

Chiral cyclopentenols

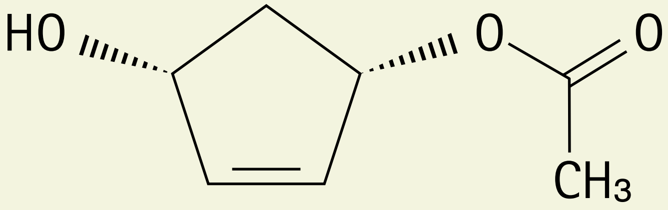
Stereospecific API precursors

Our chiral cyclopentenols have high enantiomeric purity and are therefore suitable as stereospecific API precursors and as reagents in enzymatic chemistry.

Advantages

- Perfectly suitable for enantioselective synthesis
- Funtional groups for further chemical modifications
- Both enantiomers available
- Purity > 99 %
- Safe synthesis of precursor

(1S,4R)-(+)-4-Acetoxy-2-cyclopentene-1-ol



(1R,4S)-(-)-4-Acetoxy-2-cyclopentene-1-ol

Classical heterocycles

Structure determining building blocks

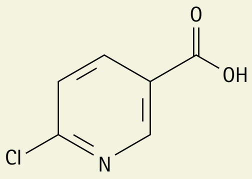
The vast majority of drugs on the market contain heterocyclic moieties. They can serve as isosteres for many functional groups and act as tools for modulating the hydrophobicity, polarity and hydrogen-bonding properties of molecules to enable pharmacological and physiochemical properties of drugs to be optimized.

We offer select products for the "classical" heterocyclic chemistry

- Nicotinic Acids and its derivatives
- Piperazine and its derivatives
- Multi-heteroatom heterocycles

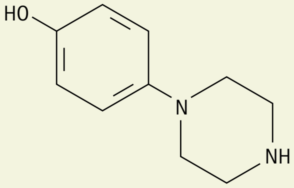
Examples:

Nicotinic acid and its derivatives



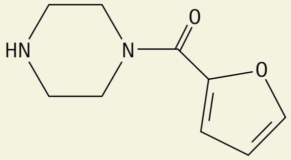
6-Chloro-3-pyridinecarboxylic acid

Piperazine and its derivatives



1-(4-Hydroxyphenyl) piperazine

Multiple heteroatom heterocycles



1-(Tetrahydro-2-furoyl) piperazine

Ordering information

Product	Description	CAS	VWR Cat. No.*
(1R, 4S)-(-)-4-Acetoxy-2-cyclopenten-1-ol	Chiral Cyclopentenoles	60176-77-4	**EM8.43918.0250**
(1S, 4R)-(+)-4-Acetoxy-2-cyclopenten-1-ol	Chiral Cyclopentenoles	60410-16-4	**EM8.43917.0001**
[2-(2-Methoxyethoxy)ethoxy] acetic acid	Oxa acid & derivatives	16024-57-1	**EM8.43910.0250**
1-(2,3-Dichlorophenyl) piperazine monohydrochloride	Heterocycles	119532-26-2	**EM8.43925.0025**
1-(4-Fluorophenyl) piperazine dihydrochloride	Heterocycles	64090-19-3	**EM8.43931.0005**
1-(4-Hydroxyphenyl) piperazine	Heterocycles	67914-60-7	**EM8.43929.0100**
1-(Tetrahydro-2-furoyl) piperazine	Heterocycles	63074-07-7	**EM8.43920.0005**
1-Methyl-1H-pyrazol-5-boronic acid pinacol ester	Bifunctional Boronic acid & derivatives	847818-74-0	**EM8.43927.0005**
1-Methylpyrazole-4-boronic acid pinacol ester	Bifunctional Boronic acid & derivatives	761446-44-0	**EM8.43919.0005**
1,2-Dihydro-2-oxonicotinic acid	Nicotinic Acids & derivatives	609-71-2	**EM8.43930.0100**
1,6-Dihydro-6-oxo-3-pyridinecarboxylic acid	Nicotinic Acids & derivatives	5006-66-6	**EM8.43932.0025**
2-Aminopyridin-3-carboxylic acid	Nicotinic Acids & derivatives	5345-47-1	**EM8.43936.0025**
2-Chloro-3-pyridylamine	Nicotinic Acids & derivatives	6298-19-7	**EM8.43940.0100**
2-Chloronicotinamide	Heterocycles	10366-35-5	**EM8.43939.0005**
2-Chloronicotinic acid	Nicotinic Acids & derivatives	2942-59-8	**EM8.43937.0025**
2,2'-[ethylenebis(oxy)] bisacetic acid	Oxa acid & derivatives	23243-68-7	**EM8.43913.0250**
2,2'-[Oxybis(2,1-ethanediyloxy)] bisacetic acid	Oxa acid & derivatives	13887-98-4	**EM8.43911.0250**
2(1H)-pyrimidinone monohydrochloride	Heterocycles	38353-09-2	**EM8.43938.0100**
4-Hydroxymethylphenyl boronic acid	Bifunctional Boronic acid & derivatives	59016-93-2	**EM8.43926.0005**
5-(4-Fluorophenyl)pyridine-3-carboxylic acid	Nicotinic Acids & derivatives	364064-17-5	**EM8.43818.0025**
5-Formylfurane-2-boronic acid	Bifunctional Boronic acid & derivatives	27329-70-0	**EM8.43928.0025**
6-Chloro-N-methyl nicotinamide	Nicotinic Acids & derivatives	54189-82-1	**EM8.43924.0005**
6-Methoxynicotinic acid methylester	Nicotinic Acids & derivatives	26218-80-4	**EM8.43923.0005**
Chloroiodomethane	Organohalogen	593-71-5	**EM8.43934.0025**
Dimethylvinyl phosphonate	VPA derivative	4645-32-3	**EM8.43916.0025**
N-tert-Butyl-6-chloronicotinamide	Heterocycles	115309-58-5	**EM8.43921.0005**
Neopentylamine	Aliphatic amine	5813-64-9	**EM8.43922.0025**
Polyglycoldiacid 600	Oxa acid & derivatives	39927-08-7	**EM8.43912.1000**
T3P® (50 % solution in 2-Methyl-THF)	T3P® coupling reagent	68957-94-8	**EM8.43943.0025**
T3P® (50 % solution in DMF)	T3P® coupling reagent	68957-94-8	**EM8.43944.0050**
T3P® (50 % solution in Ethylacetate)	T3P® coupling reagent	68957-94-8	**EM8.43942.0025**
Vinylphosphonic acid (80 % solution)	VPA	1746-03-8	**EM8.43915.0250**
Vinylphosphonic acid (90 % solution)	VPA	1746-03-8	**EM8.43914.1000**

*For Canadian customers, please substitute CA for EM in the Cat. No. when ordering.

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