

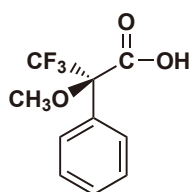
# Reagents for the Determination of Optical Purity by NMR

## Mosher's Acids and Derivatives

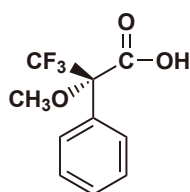
MTPA esters or amides, which are afforded by the condensation of Mosher's acid (MTPA) and alcohols or amines are frequently used to spectroscopically ( $^1\text{H-NMR}$ ) estimate the optical purity of a compound. Through the synthesis of diastereomers of (+) and (-)-MTPA and subsequent chemical shift analysis, absolute stereochemistry of chiral compounds can be readily determined.

1) J. A. Dale, H. S. Mosher, *J. Am. Chem. Soc.* **1973**, *95*, 512.

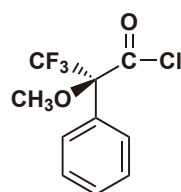
2) I. Ohtani, T. Kusumi, Y. Kashman, H. Kakisawa, *J. Am. Chem. Soc.* **1991**, *113*, 4092.



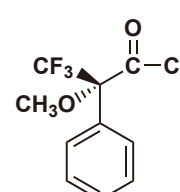
(+)-MTPA  
1g / 5g [M0831]



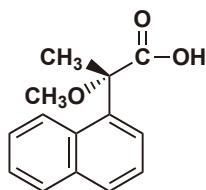
(-)-MTPA  
1g / 5g [M0832]



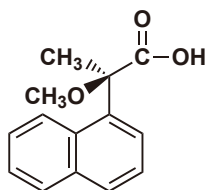
(S)-(+)-MTPA-Cl  
100mg / 1g [M1103]  
(ca. 18% in Dichloromethane)  
5g [M2214]



(R)-(-)-MTPA-Cl  
100mg / 1g [M1104]  
(ca. 18% in Dichloromethane)  
5g [M2215]



(S)-(+)-M  $\alpha$  NP Acid  
100mg [M1367]

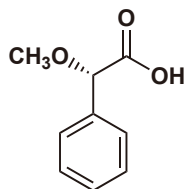


(R)-(-)-M  $\alpha$  NP Acid  
100mg [M1366]

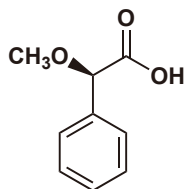
## Mandelic Acid Derivatives

The determination of absolute chemistry by using  $\alpha$ -methoxyphenyl acetic acids is referred to as The Trost method. Absolute stereochemistry of a secondary alcohol can be determined from the corresponding esters.

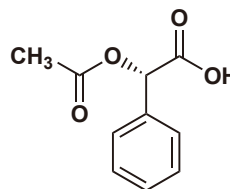
B. M. Trost, J. L. Belletire, S. Godleski, P. G. McDougal, J. M. Balkovec, J. J. Baldwin, M. E. Christy, G. S. Ponticello, S. L. Varga, J. P. Springer, *J. Org. Chem.* **1986**, *51*, 2370.



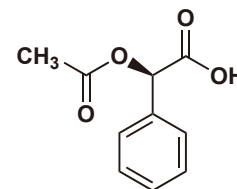
(S)-(+)- $\alpha$ -Methoxyphenylacetic Acid  
1g / 5g [M0829]



(R)-(-)- $\alpha$ -Methoxyphenylacetic Acid  
100mg / 1g / 5g [M0830]

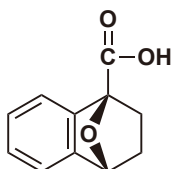


(+)-O-Acetyl-L-mandelic Acid  
5g / 25g [A1454]

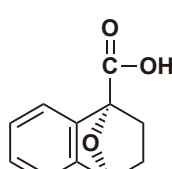


(-)-O-Acetyl-D-mandelic Acid  
100mg / 25g [A1453]

## THENA



(S)-THENA  
100mg [T3002]



(R)-THENA  
100mg [T3001]

The absolute chemistry of alcohols can be determined by NMR of esters from the alcohol and THENA. THENA is effective for alcohols which don't readily react with MTPA.

S. Sungsuwan, N. Ruangsapapichart, S. Prabpai, P. Kongsaree, T. Thongpanchang, *Tetrahedron Lett.* **2010**, *51*, 4965.

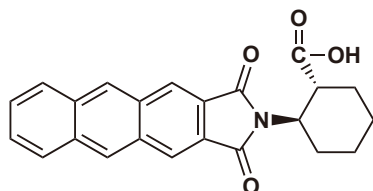
# Reagents for the Determination of Optical Purity by NMR

## Highly Potent Chiral Derivatizing Reagents

These acids, developed by Ohruí *et al.*, are particularly useful for alcohols whose chiral center is far away from the hydroxy group.<sup>1,2)</sup>

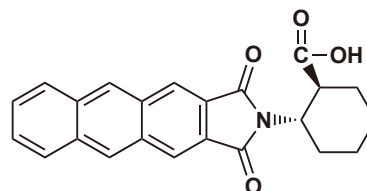
1) H. Ohruí, H. Terashima, K. Imaizumi, K. Akasaka, *Proc. Jpn. Acad., Ser. B: Phys. Biol. Sci.* **2002**, 78, 69.

2) K. Imaizumi, H. Terashima, K. Akasaka, H. Ohruí, *Anal. Sci.* **2003**, 19, 1243.



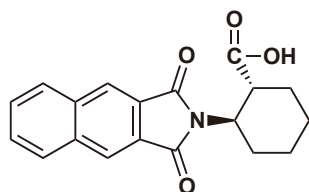
(1*R*,2*R*)-2-(Anthracene-2,3-dicarboximido)-cyclohexanecarboxylic Acid

100mg [A1657]



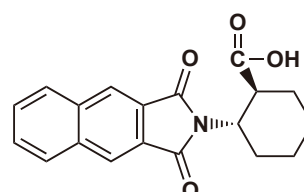
(1*S*,2*S*)-2-(Anthracene-2,3-dicarboximido)-cyclohexanecarboxylic Acid

100mg [A1658]



(1*R*,2*R*)-2-(Naphthalene-2,3-dicarboximido)-cyclohexanecarboxylic Acid

100mg [N0713]



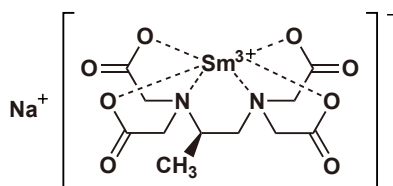
(1*S*,2*S*)-2-(Naphthalene-2,3-dicarboximido)-cyclohexanecarboxylic Acid

100mg [N0714]

## Water-soluble Chiral Shift Reagents

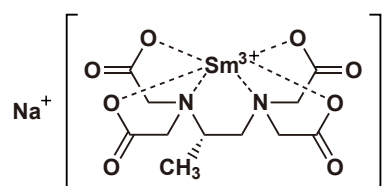
Samarium complexes developed by Kabuto *et al.* are used as chiral shift reagents for optical purity and absolute chemistry determination of  $\alpha$ -amino acids and  $\alpha$ -hydroxy acids.

K. Kabuto, Y. Sasaki, *J. Chem. Soc., Chem. Commun.* **1987**, 670.



Sodium [(*R*)-1,2-Diaminopropane-*N,N,N',N'*-tetraacetato]samarate(III)

100mg [S0473]



Sodium [(*S*)-1,2-Diaminopropane-*N,N,N',N'*-tetraacetato]samarate(III)

100mg [S0474]

For further information please refer to our website at [www.TCIchemicals.com](http://www.TCIchemicals.com).

optical purity



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