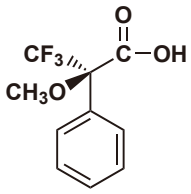
ANALYTICAL

Reagents for the Determination of Optical Purity by NMR

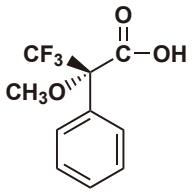
Mosher's Acids and Derivatives

MTPA esters or amides, which are afforded by the condensation of Mosher's acid (MTPA) and alcohols or amines are frequently used to spectroscopically (1H-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.

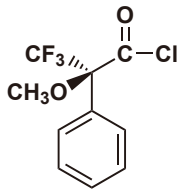
References 1) J. A. Dale, H. S. Mosher, *J. Am. Chem. Soc.* **1973**, *95*, 512. https://doi.org/10.1021/ja00783a034
2) I. Ohtani, T. Kusumi, Y. Kashman, H. Kakisawa, *J. Am. Chem. Soc.* **1991**, *113*, 4092. https://doi.org/10.1021/ja00011a006



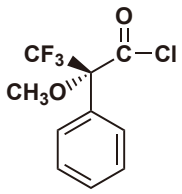
(+)-MTPA
1g / 5g [M0831]



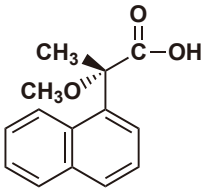
(-)-MTPA
1g / 5g [M0832]



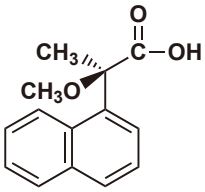
(*S*)-(+)-MTPA-Cl
100mg / 1g [M1103]
(*ca.* 18% in Dichloromethane)
5g [M2214]



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



(*S*)-(+)-MαNP Acid
100mg [M1367]

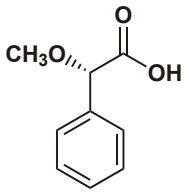


(*R*)-(-)-MαNP Acid
100mg [M1366]

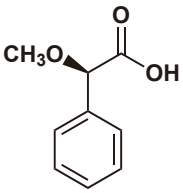
Mandelic Acid Derivatives

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

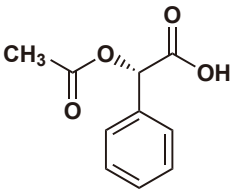
Reference B. M. Trost, J. P. Springer, *et al.*, *J. Org. Chem.* **1986**, *51*, 2370. https://doi.org/10.1021/jo00362a036



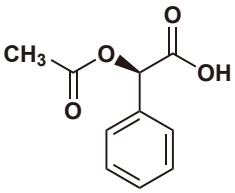
(*S*)-(+)-α-Methoxyphenylacetic Acid
1g / 5g [M0829]



(*R*)-(-)-α-Methoxyphenylacetic Acid
100mg / 1g / 5g [M0830]

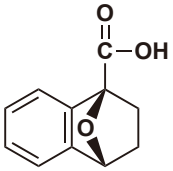


(+)-*O*-Acetyl-L-mandelic Acid
5g / 25g [A1454]

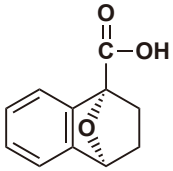


(-)-*O*-Acetyl-D-mandelic Acid
5g / 25g [A1453]

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.

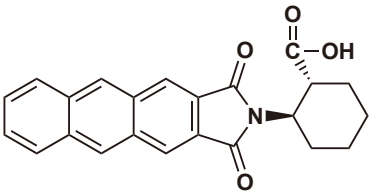
Reference S. Sungsuwan, T. Thongpanchang, *et al.*, *Tetrahedron Lett.* **2010**, *51*, 4965. https://doi.org/10.1016/j.tetlet.2010.07.062

Reagents for the Determination of Optical Purity by NMR

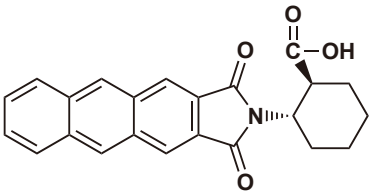
Highly Potent Chiral Derivatizing Reagents

These acids, developed by Ohrui *et al.*, are particularly useful for alcohols whose chiral center is far away from the hydroxy group.[1,2)]

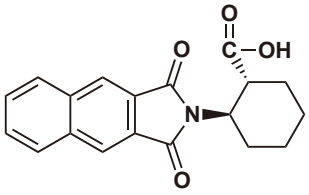
References 1) H. Ohrui, H. Terashima, K. Imaizumi, K. Akasaka, *Proc. Jpn. Acad., Ser. B* **2002**, *78*, 69. https://doi.org/10.2183/pjab.78.69
2) K. Imaizumi, H. Terasima, K. Akasaka, H. Ohrui, *Anal. Sci.* **2003**, *19*, 1243. https://doi.org/10.2116/analsci.19.1243



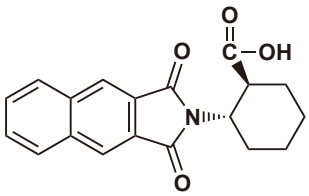
(1*R*,2*R*)-2-(Anthracene-2,3-dicarboximido)-cyclohexanecarboxylic Acid
100mg [A1657]



(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]

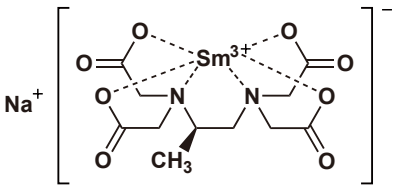


(1*S*,2*S*)-2-(Naphthalene-2,3-dicarboximido)-cyclohexanecarboxylic Acid
100mg [N0714]

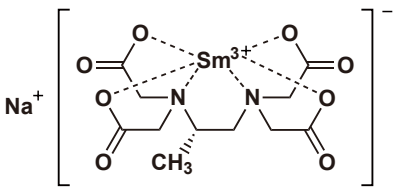
Water-soluble Chiral Shift Reagents

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

Reference K. Kabuto, Y. Sasaki, *J. Chem. Soc., Chem. Commun.***1987**, 670. https://doi.org/10.1039/C39870000670



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. ▶▶▶ TCI optical purity

Ordering and Customer Service

TCI AMERICA
Tel : 800-423-8616 / 503-283-1681
Fax : 888-520-1075 / 503-283-1987
E-mail : Sales-US@TCIchemicals.com

TCI EUROPE N.V.
Tel : +32 (0)3 735 07 00
Fax : +32 (0)3 735 07 01
E-mail : Sales-EU@TCIchemicals.com

TCI Deutschland GmbH
Tel : +49 (0)6196 64053-00
Fax : +49 (0)6196 64053-01
E-mail : Sales-DE@TCIchemicals.com

Tokyo Chemical Industry UK Ltd.
Tel : +44 (0)1865 78 45 60
E-mail : Sales-UK@TCIchemicals.com

TCI Chemicals (India) Pvt. Ltd.
Tel : 1800 425 7889 / 044-2262 0909
E-mail : Sales-IN@TCIchemicals.com

梯希爱(上海)化成工业发展有限公司
Tel : 800-988-0390 / 021-67121386
Fax : 021-6712-1385
E-mail : Sales-CN@TCIchemicals.com

TOKYO CHEMICAL INDUSTRY CO., LTD.
Tel : +81 (0)3-5640-8878
E-mail : globalbusiness@TCIchemicals.com