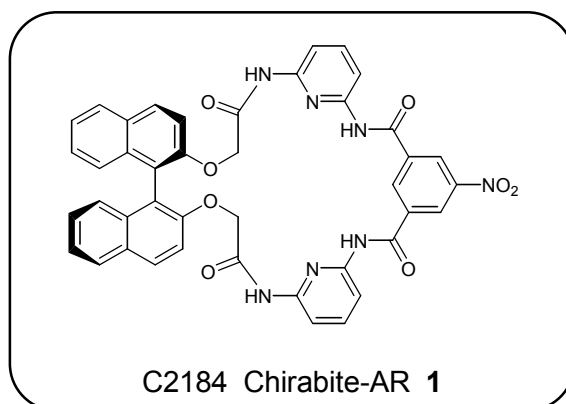


e.e. Determination of Wide Range of Chiral Compounds



Chirabite-AR (**1**) is a macrocyclic compound developed by Ema *et al.*, and has been shown to be a highly versatile chiral shift reagent. **1** has a very unique cavity where the hydrogen-bond donor and acceptor sites are well organized to enable the binding of a wide range of compounds as guest molecules. The incorporated guest molecules experience a strong anisotropic ring-current effect arising from the BINOL moiety, which is a chiral source, resulting in the chemical-shift nonequivalence between the two enantiomers.

Chart 1.

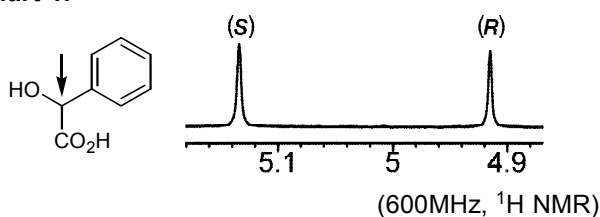
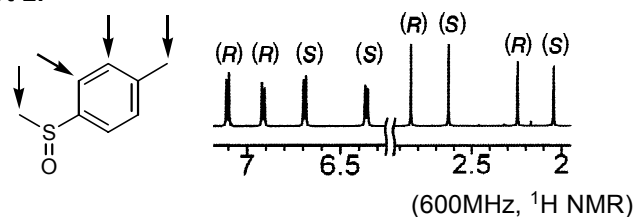


Chart 2.



Chirabite-AR (7mg) in CDCl₃ at 22°C

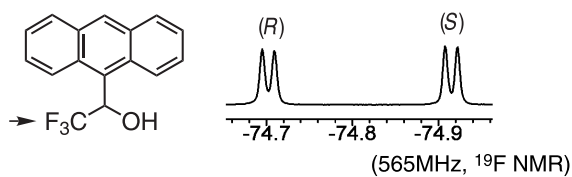
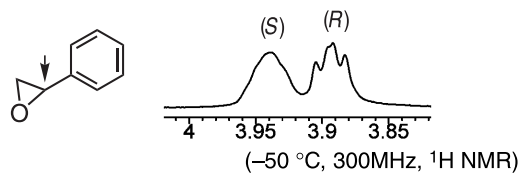
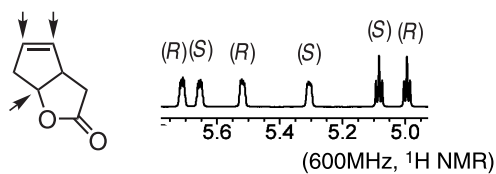
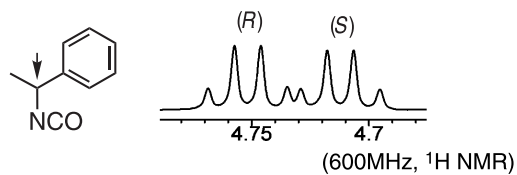
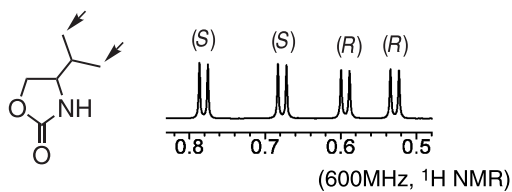
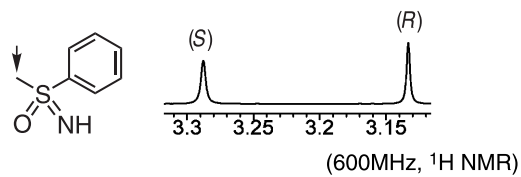
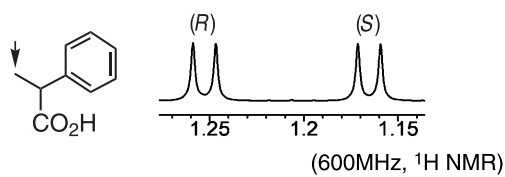
When conventional Eu-complexes are used on high-field NMR spectrometers, which are widely spread nowadays, signal broadening occurs, and as a result, satisfactory NMR spectra cannot be obtained. Because **1** contains no paramagnetic metals, which cause signal broadening, it can be used for both high- and low-field NMR spectrometers. Using **1**, therefore, the enantiomeric purities of various compounds such as carboxylic acids, lactones, oxazolidinones, alcohols, sulfoxides, sulfoximines, isocyanates and epoxides can be determined. Moreover, a protocol for its determination is extremely easy; NMR spectra showing chemical-shift nonequivalences can be obtained just by adding **1** to the NMR tube containing a target sample in CDCl₃.

The reagent **1** is characterized by its facile use, versatility, and applicability to the low- and high-field NMR spectrometers. Thus, **1** has been shown to possess a highly effective capacity superior to that of the conventional chiral shift reagents.

Keywords : Chirabite-AR, chiral shift reagent, high-field NMR

2007. Mar., A-1095E

Other applications



C2184 Chirabite-AR

[(*R*)-2,2'-[5-Nitroisophthalamidobis(2,6-pyridylenecarbonylmethoxy)]-1,1'-binaphthyl]

(**1**) 100mg

Reference

Versatile and practical chiral shift reagent with hydrogen-bond donor / acceptor sites in a macrocyclic cavity

T. Ema, D. Tanida, T. Sakai, *Org. Lett.*, **2006**, *8*, 3773.