

Abstract

This bachelor thesis deals with the preparation of chiral shift reagents sodium [(R)- and (S)-1,2-diaminopropane-N,N,N',N'-tetraacetate]samarate, for short Sm-(R)-pdta and Sm-(S)-pdta. These reagents have the ability to differentiate NMR signals of enantiomers of amino acids in an aqueous environment. The main aim of this work was to develop a new, efficient and cheap method of the preparation of these reagents which would enable their routine use in laboratory practice, because these reagents are commercially available only in limited quantities and at high price.

This work describes simplified method of separation of racemic 1,2-diaminopropane to its enantiomers from easily available starting substances, L-tartaric acid and racemic 1,2-diaminopropane.

We also developed and optimized a new process of synthesis of the key intermediate, (R)- and (S)-1,2-diaminopropane-N,N,N',N'-tetraacetic acid from (R)- and (S)-1,2-diaminopropane dihydrochloride, with a new synthetic step involving tetrabenzylester of this acid and its deprotection by hydrogenolysis without contamination by extraneous ions. This process affords very pure anhydrous acid in high yield.

Finally, the target complexes Sm-(R)-pdta and Sm-(S)-pdta were successfully prepared from (R)- and (S)-1,2-diaminopropane-N,N,N',N'-tetraacetic acid in high yield and purity.

Keywords: chiral recognition, NMR spectroscopy, samarium, 1,2-diaminopropane, amino acids.