CHAPTER V

CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

Seventy chiral alcohol analytes with closely related structure were enantioseparated with heptakis(2,3-di-*O*-methyl-6-*O*-*tert*-butyldimethylsilyl)-β-cyclodextrin (or BSiMe) and octakis(2,3-di-*O*-methyl-6-*O*-*tert*-butyldimethylsilyl)-γ-cyclodextrin (or GSiMe) columns. All analytes could be separated with either or both columns, except **35F** and **2oct**. Mostly, compounds could be resolved by BSiMe derivative and with higher degree of separation than by GSiMe derivative. The broader enantioselective property of BSiMe is probably due to the appropriate orientation of cyclodextrin derivative and analyte structure.

To derive more information about the influence of analyte structure on the enantioseparation on both of BSiMe and GSiMe phases systematically, various groups of analytes with closely related structure were selected and thermodynamic investigation was performed using van't Hoff approach. As expected, the interactions of analytes towards two chiral columns are greater than interactions towards polysiloxane column, as indicated by larger negative $-\Delta H$ and $-\Delta S$ values on chiral columns. The strength of interaction of alcohols on each stationary phase are quite similar, stating that major analyte contribution towards the interaction probably comes from the hydroxyl group. Nevertheless, the interaction strength does not necessarily correlate with the discrimination of enantiomers since some alcoholic compounds having the strong interaction with stationary phase do not display large enantioselectivity.

The degree of enantioseparation of the analytes studied involves several factors. Generally, on BSiMe, substitution at the *ortho*-position of aromatic ring of analytes tends to promote enantioresolution, while substitution at the side chain is likely to decrease enantioresolution. Type of substitution also plays a major role in enantioseparation. The most interesting substituent is trifluoromethyl group, which strongly shows both enhanced and decreased effect depending on the position of substitution. GSiMe, on the other hand, exhibits little enantioselectivity towards the

selected group of analytes. Among all analytes tested, the largest enantioseparation is obtained from 1-(2,4,5-trifluorophenyl)ethanol (**triF**) on BSiMe column.

Further study with larger group of analytes, including aliphatic alcohols, as well as identification of enantiomeric configuration should be explored. In addition, molecular modeling experiments should be performed to better understand the analyte-selector interaction that leads to separation mechanism.