



CHAPTER III

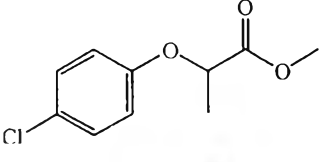
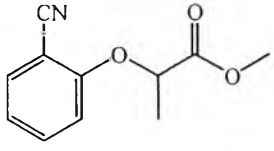
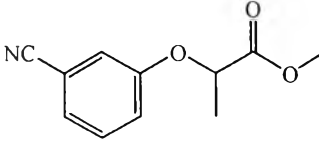
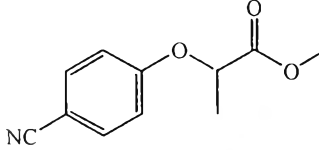
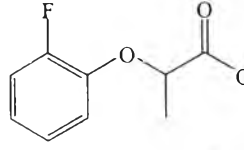
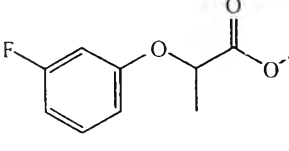
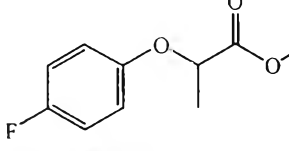
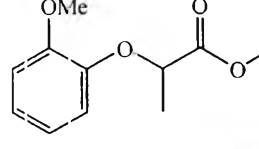
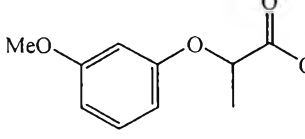
EXPERIMENTAL

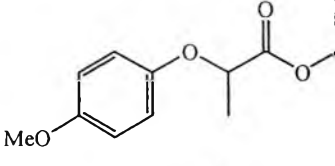
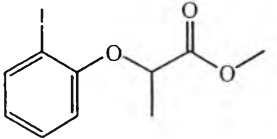
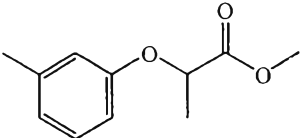
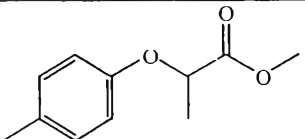
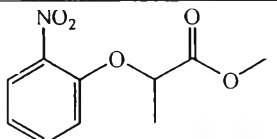
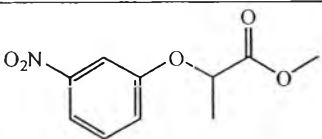
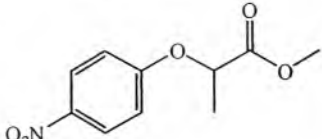
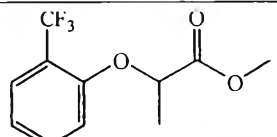
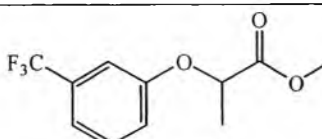
3.1 Phenoxy acid methyl esters

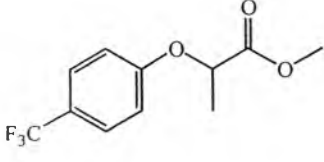
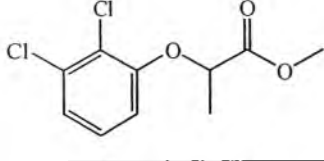
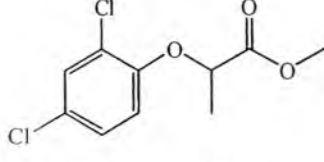
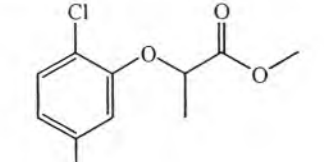
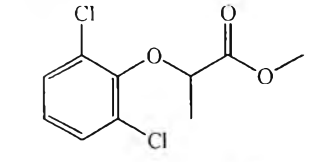
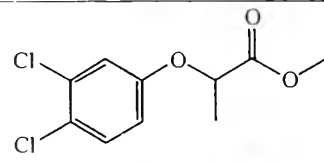
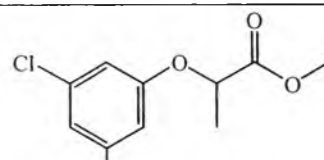
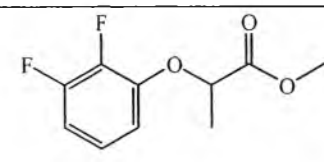
Forty-six phenoxy acid methyl esters used in this study were synthesized by Rodthongkum [23]. Chemical structure and abbreviation of all phenoxy acid methyl esters used in this study are shown in Table 3.1.

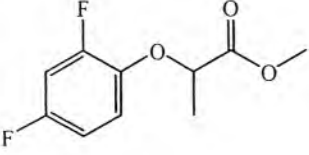
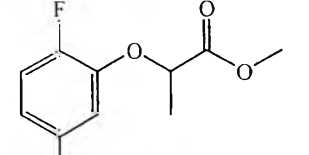
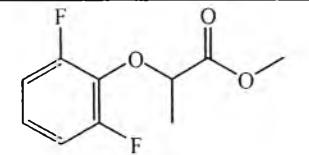
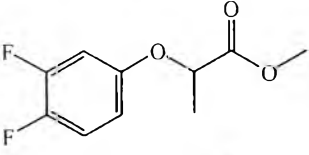
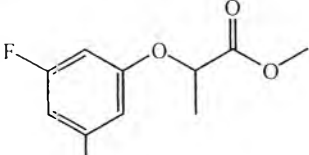
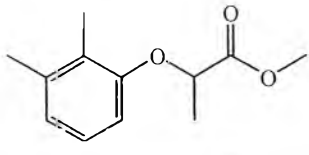
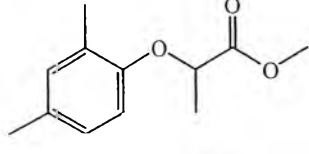
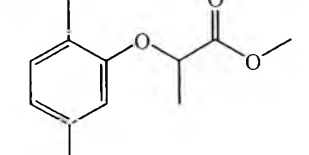
Table 3.1 Chemical structure and abbreviation of phenoxy acid methyl esters

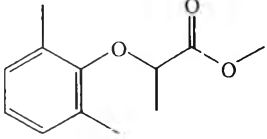
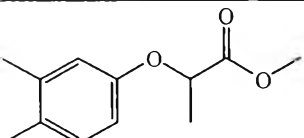
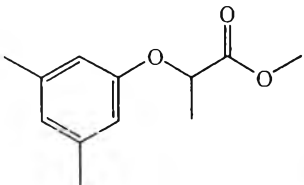
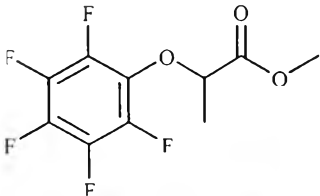
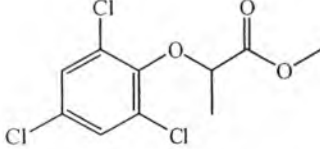
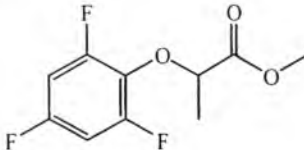
chemical structure	abbreviation	MW (g/mol)	compound name
	1	180.20	methyl 2-phenoxypropanoate
group 1: phenoxy acid methyl esters with mono-substitution on the aromatic ring			
	2Br	259.10	methyl 2-(2'-bromophenoxy)propanoate
	3Br	259.10	methyl 2-(3'-bromophenoxy)propanoate
	4Br	259.10	methyl 2-(4'-bromophenoxy)propanoate
	2Cl	214.65	methyl 2-(2'-chlorophenoxy)propanoate
	3Cl	214.65	methyl 2-(3'-chlorophenoxy)propanoate

chemical structure	abbreviation	MW (g/mol)	compound name
	4Cl	214.65	methyl 2-(4'-chlorophenoxy) propanoate
	2CN	205.21	methyl 2-(2'-cyanophenoxy) propanoate
	3CN	205.21	methyl 2-(3'-cyanophenoxy) propanoate
	4CN	205.21	methyl 2-(4'-cyanophenoxy) propanoate
	2F	198.19	methyl 2-(2'-fluorophenoxy) propanoate
	3F	198.19	methyl 2-(3'-fluorophenoxy) propanoate
	4F	198.19	methyl 2-(4'-fluorophenoxy) propanoate
	2OMe	210.23	methyl 2-(2'-methoxyphenoxy) propanoate
	3OMe	210.23	methyl 2-(3'-methoxyphenoxy) propanoate

chemical structure	abbreviation	MW (g/mol)	compound name
	4OMe	210.23	methyl 2-(4'-methoxyphenoxy)propanoate
	2Me	194.23	methyl 2-(2'-methylphenoxy)propanoate
	3Me	194.23	methyl 2-(3'-methylphenoxy)propanoate
	4Me	194.23	methyl 2-(4'-methylphenoxy)propanoate
	2NO ₂	225.20	methyl 2-(2'-nitrophenoxy)propanoate
	3NO ₂	225.20	methyl 2-(3'-nitrophenoxy)propanoate
	4NO ₂	225.20	methyl 2-(4'-nitrophenoxy)propanoate
	2CF ₃	248.20	methyl 2-(2'-trifluoromethylphenoxy)propanoate
	3CF ₃	248.20	methyl 2-(3'-trifluoromethylphenoxy)propanoate

chemical structure	abbreviation	MW (g/mol)	compound name
	4CF ₃	248.20	methyl 2-(4'-trifluoromethylphenoxy)propanoate
group 2: phenoxy acid methyl esters with di-substitution on the aromatic ring			
	2,3Cl	249.09	methyl 2-(2',3'-dichlorophenoxy)propanoate
	2,4Cl	249.09	methyl 2-(2',4'-dichlorophenoxy)propanoate
	2,5Cl	249.09	methyl 2-(2',5'-dichlorophenoxy)propanoate
	2,6Cl	249.09	methyl 2-(2',6'-dichlorophenoxy)propanoate
	3,4Cl	249.09	methyl 2-(3',4'-dichlorophenoxy)propanoate
	3,5Cl	249.09	methyl 2-(3',5'-dichlorophenoxy)propanoate
	2,3F	216.18	methyl 2-(2',3'-difluorophenoxy)propanoate

chemical structure	abbreviation	MW (g/mol)	compound name
	2,4F	216.18	methyl 2-(2',4'-difluorophenoxy) propanoate
	2,5F	216.18	methyl 2-(2',5'-difluorophenoxy) propanoate
	2,6F	216.18	methyl 2-(2',6'-difluorophenoxy) propanoate
	3,4F	216.18	methyl 2-(3',4'-difluorophenoxy) propanoate
	3,5F	216.18	methyl 2-(3',5'-difluorophenoxy) propanoate
	2,3Me	208.25	methyl 2-(2',3'-dimethylphenoxy) propanoate
	2,4Me	208.25	methyl 2-(2',4'-dimethylphenoxy) propanoate
	2,5Me	208.25	methyl 2-(2',5'-dimethylphenoxy) propanoate

chemical structure	abbreviation	MW (g/mol)	compound name
	2,6Me	208.25	methyl 2-(2',6'-dimethylphenoxy)propanoate
	3,4Me	208.25	methyl 2-(3',4'-dimethylphenoxy)propanoate
	3,5Me	208.25	methyl 2-(3',5'-dimethylphenoxy)propanoate
group 3: other phenoxy acid methyl esters with substitution on the aromatic ring			
	pentaF	270.15	methyl 2-(2',3',4',5',6'-pentafluorophenoxy)propanoate
	2,4,6Cl	283.54	methyl 2-(2',4',6'-trichlorophenoxy)propanoate
	2,4,6F	234.17	methyl 2-(2',4',6'-trifluorophenoxy)propanoate

3.2 Gas chromatographic analyses

All GC separations were performed on an Agilent 6890 series gas chromatograph equipped with a split injector and a flame ionization detector (FID). The injector and detector temperature were maintained at 250 °C. Hydrogen was used as a carrier gas with an average linear velocity of 50 cm/s. The separation was carried out on the 15 m × 0.25 mm i.d. capillary column coated with a 0.25 μm thick film of stationary phase. Two chiral columns were prepared to contain identical molality of

cyclodextrin derivatives in polysiloxane. Two types of stationary phases used in this research were:

- 26.8 % hexakis(2,3-di-*O*-methyl-6-*O*-*tert*-butyldimethylsilyl)cyclomaltohexaose (or ASiMe) diluted in polysiloxane OV-1701
- 32.8 % octakis(2,3-di-*O*-methyl-6-*O*-*tert*-butyldimethylsilyl)cyclomaltooctaose (or GSiMe) diluted in polysiloxane OV-1701

All columns were conditioned at 220 °C until a stable baseline was observed. Efficiency was determined at 140 °C with *n*-pentadecane which gave the plate number (*N*) above 3000 plates/m for both columns. Each phenoxy acid methyl ester was dissolved in dichloromethane. Approximately 0.2-0.8 μL of solution was injected at least in duplicate with a split ratio of 100:1. All thermodynamic studies were performed isothermally in the temperature range of 70-220 °C with 10 °C increments. Retention factors and enantioselectivities of all analytes were calculated from GC chromatograms and used for thermodynamic studies. Finally, the thermodynamic parameters were determined by means of van't Hoff approach.