

Direct, Rapid and Convenient Synthesis of Esters and Thioesters Using PPh_3/N -Chlorobenzotriazole System

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General

The products were purified by column chromatography. The purity determinations of the products were accomplished by TLC on silica gel polygram STL G/UV 254 plates. The melting points of products were determined with an Electrothermal Type 9100 melting point apparatus. The FTIR spectra were recorded on an Avatar 370 FT-IR Thermo

Nicolet spectrometer. The NMR spectra were provided on Bruker Ultrashield Avance III 400 MHz instruments in CDCl_3 . All of the products were known compounds and characterized by the IR, ^1H NMR spectra and comparison of their melting points with known compounds. Mass spectra were recorded with a CH7A Varianmat Bremem instrument at 70 eV, in m/z (rel%).

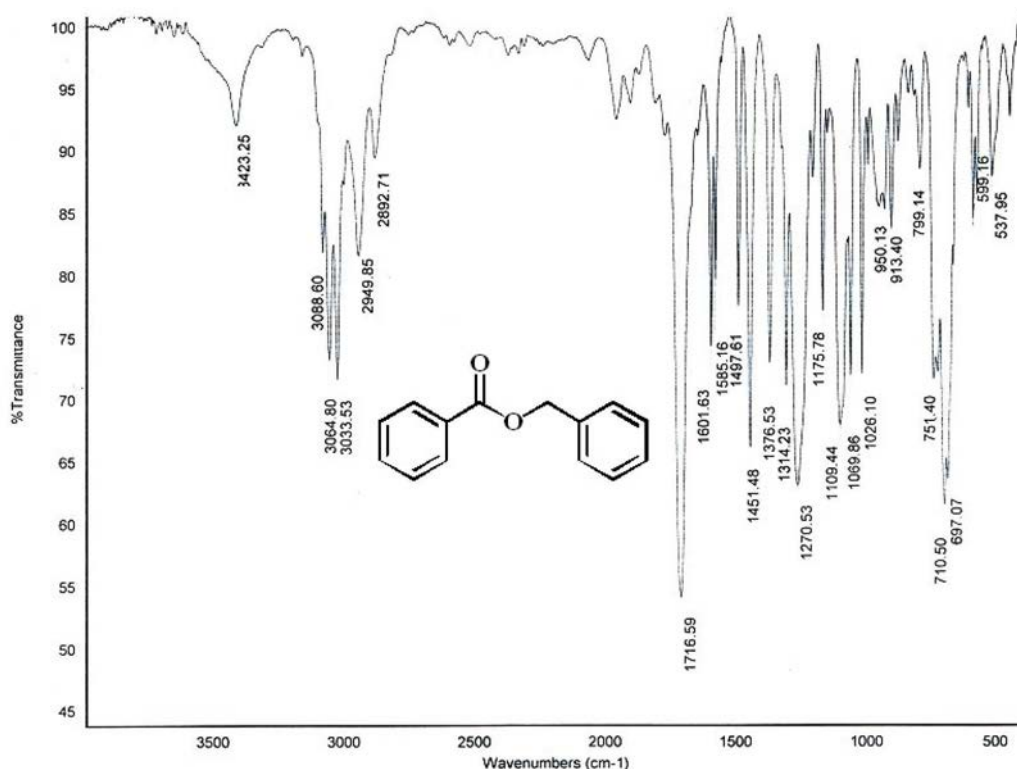


Figure S1. FTIR (neat) spectrum of benzyl benzoate (Table 3, entry 1).

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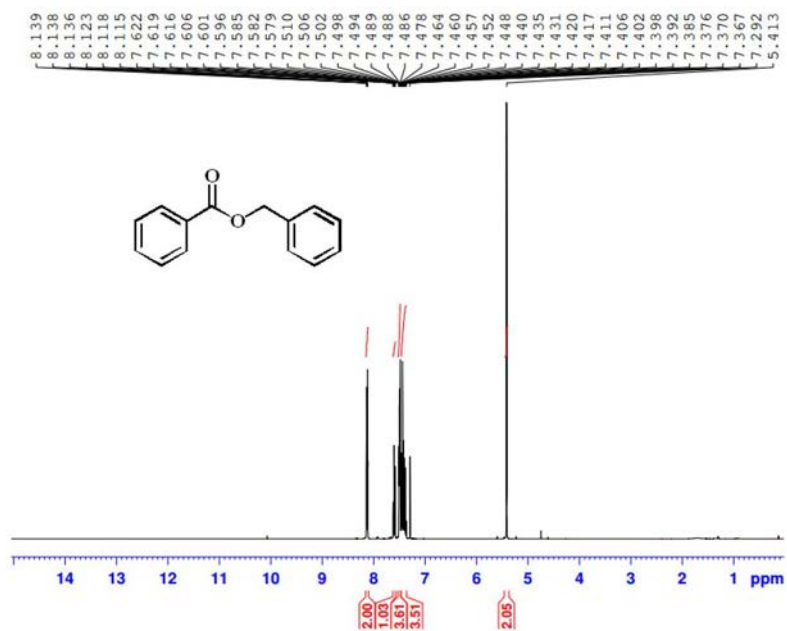


Figure S2. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl benzoate (Table 3, entry 1).

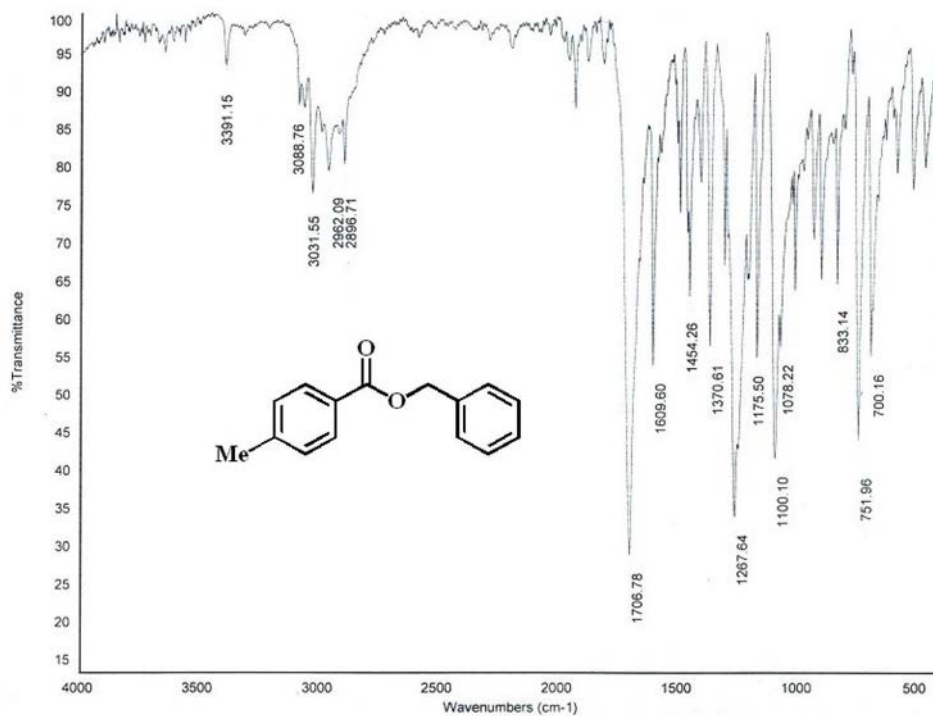


Figure S3. FTIR (KBr) spectrum of benzyl 4-methylbenzoate (Table 3, entry 2).

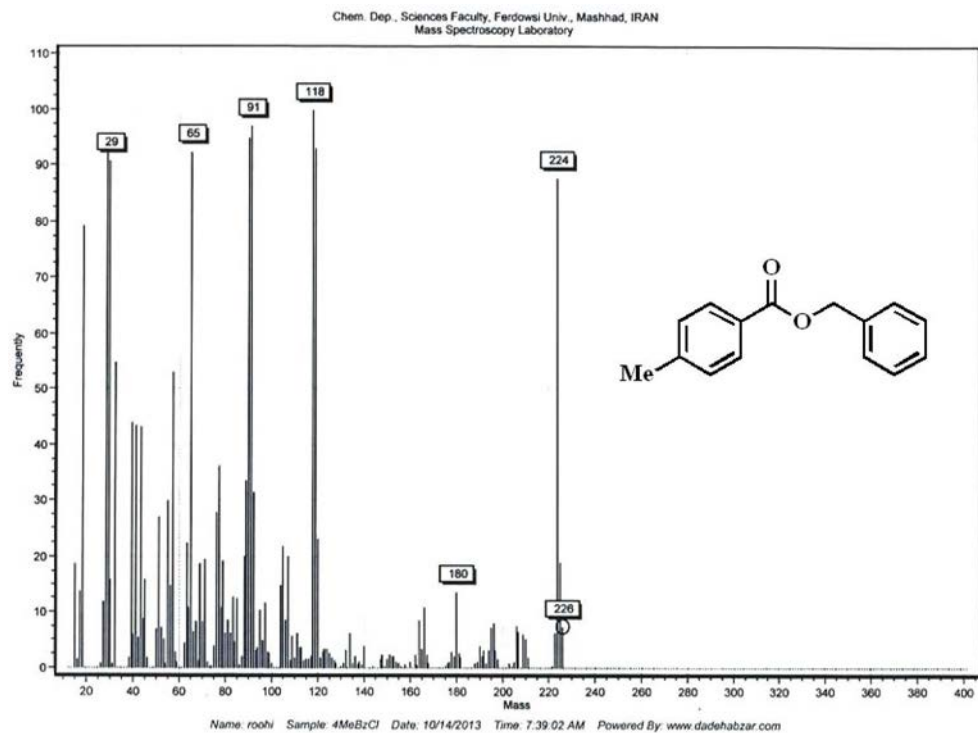


Figure S4. Mass spectrum of benzyl 4-methylbenzoate (Table 3, entry 2).

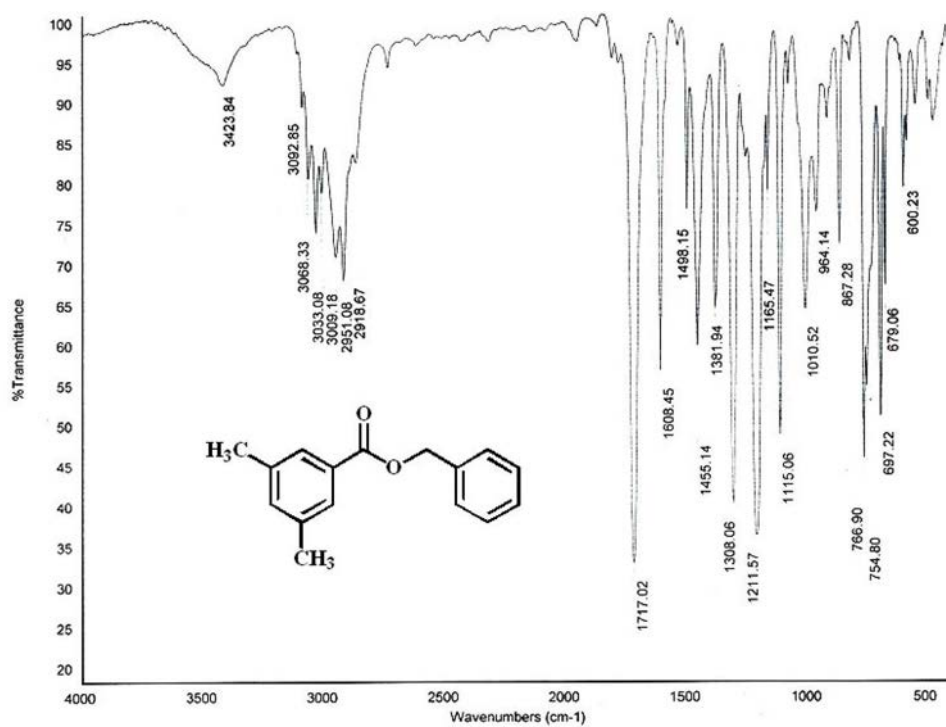


Figure S5. FTIR (KBr) spectrum of benzyl 3,5-dimethylbenzoate (Table 3, entry 3).

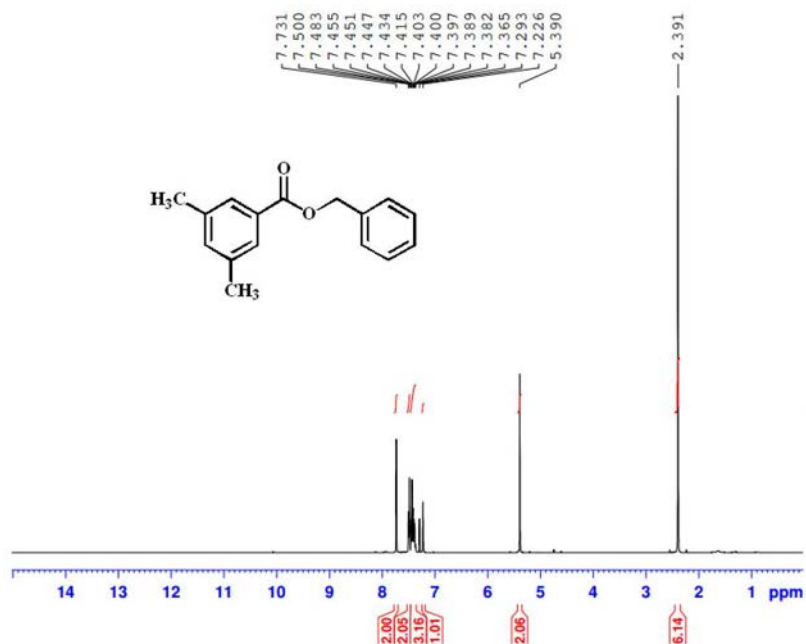


Figure S6. ^1H NMR (400 MHz, CDCl_3) spectrum of benzyl 3,5-dimethylbenzoate (Table 3, entry 3).

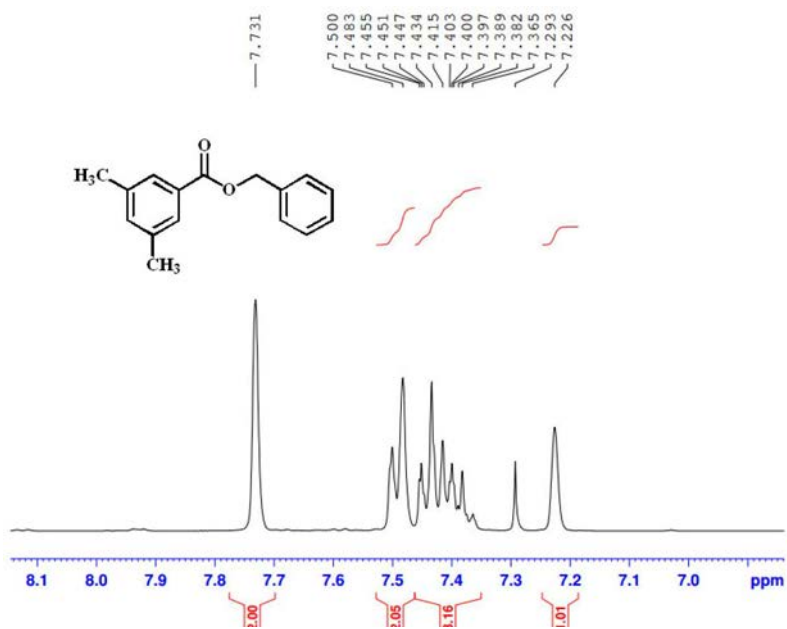


Figure S7. ^1H NMR (400 MHz, CDCl_3) spectrum of benzyl 3,5-dimethylbenzoate (Table 3, entry 3).

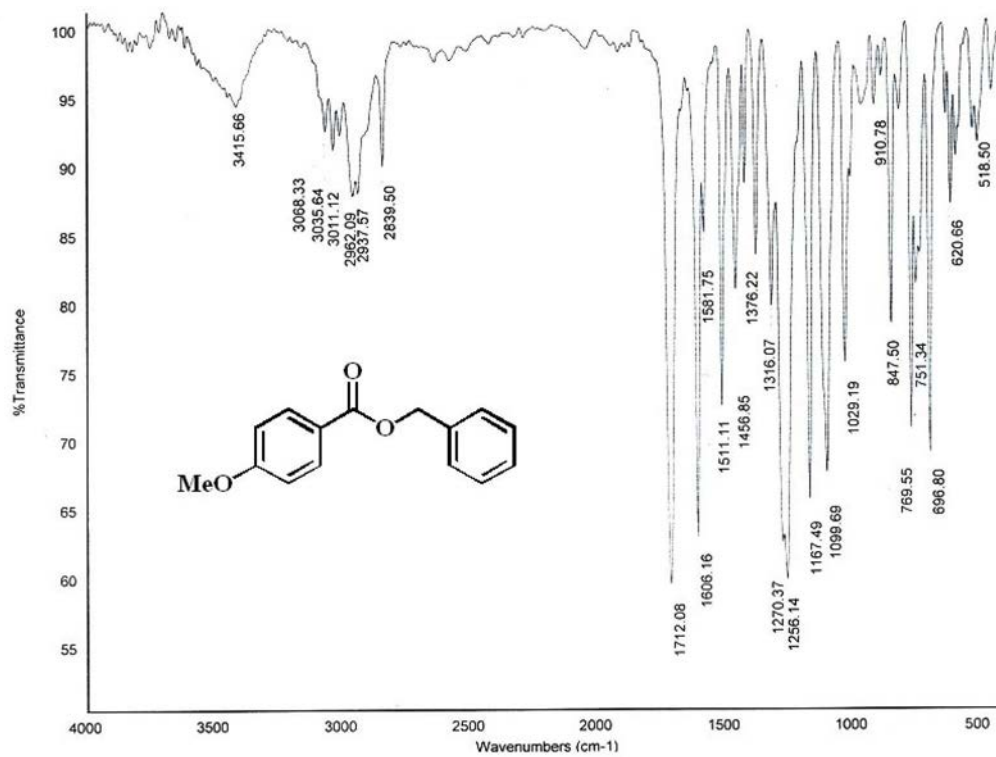


Figure S8. FTIR (neat) spectrum of benzyl 4-methoxybenzoate (Table 3, entry 4).

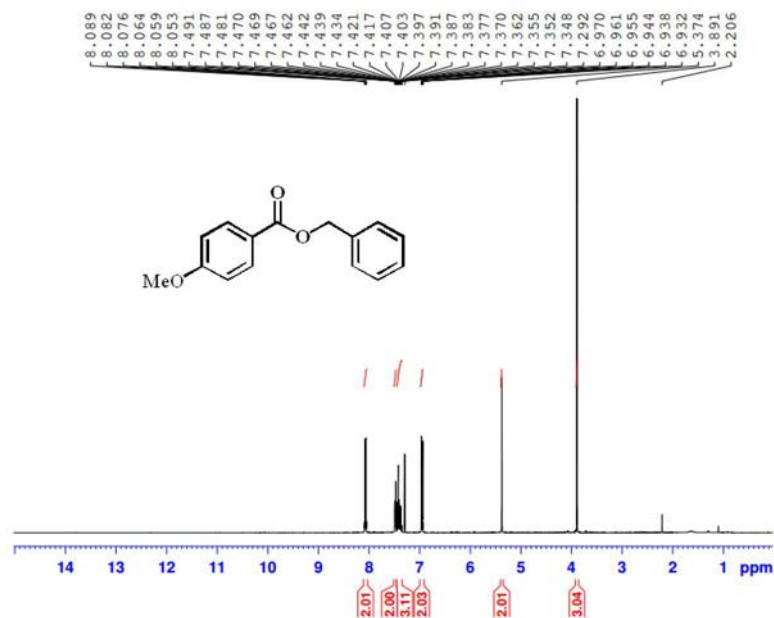


Figure S9. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 4-methoxybenzoate (Table 3, entry 4).

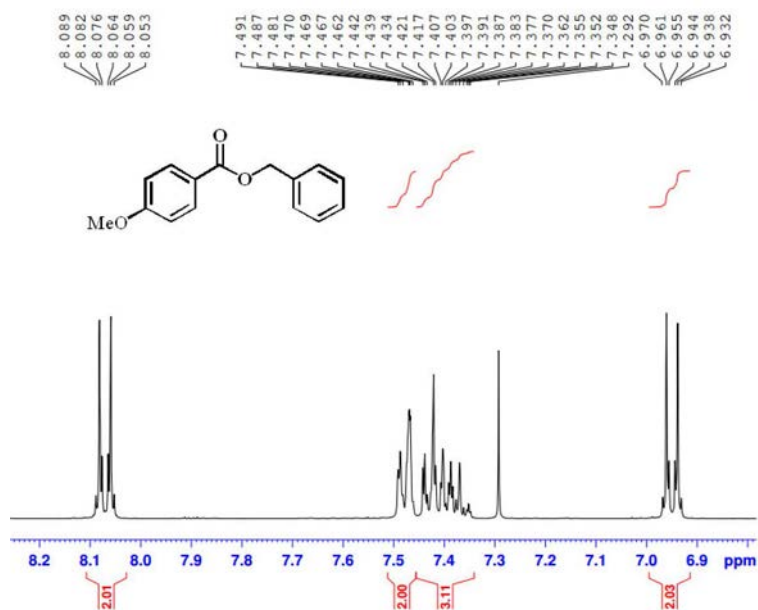


Figure S10. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 4-methoxybenzoate (Table 3, entry 4).

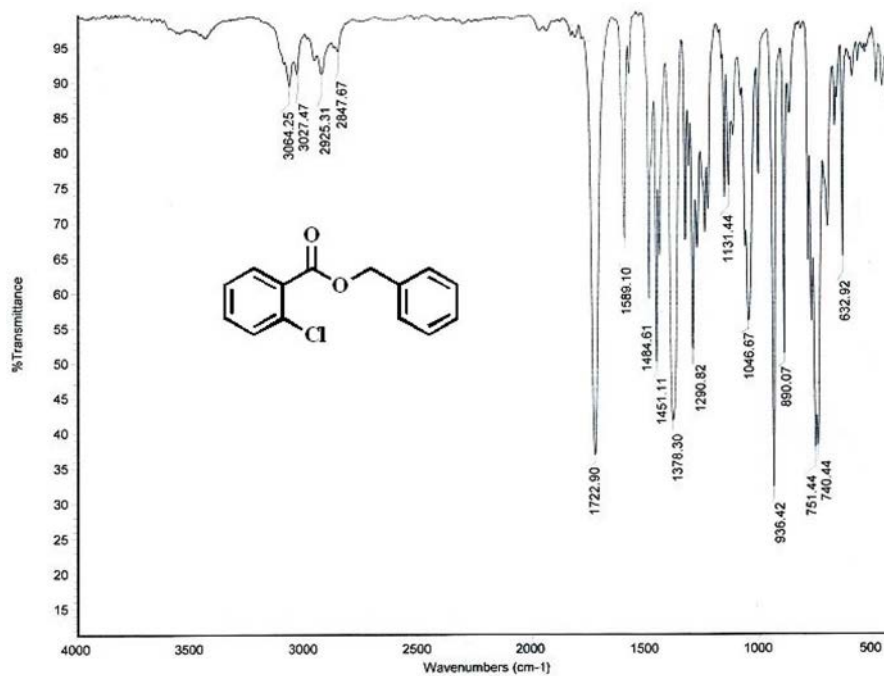


Figure S11. FTIR (neat) spectrum of benzyl 2-chlorobenzoate (Table 3, entry 5).

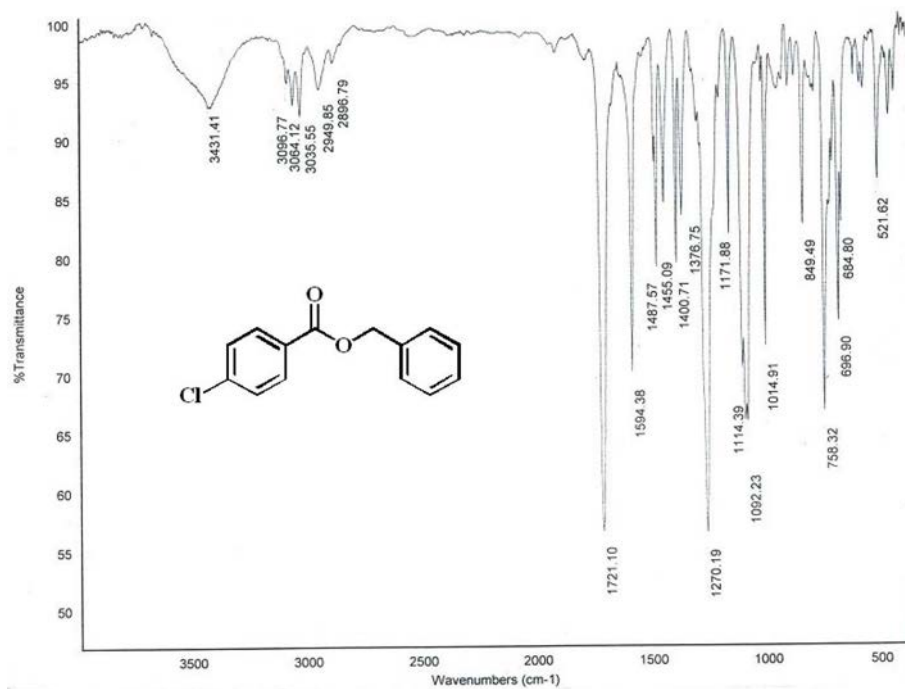


Figure S12. FTIR (neat) spectrum of benzyl 4-chlorobenzoate (Table 3, entry 6).

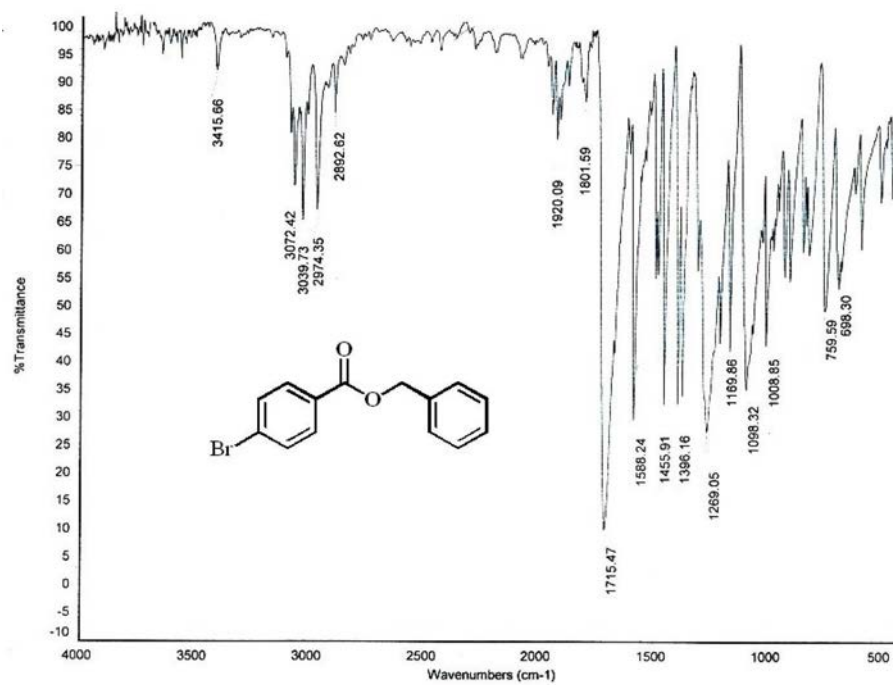


Figure S13. FTIR (KBr) spectrum of benzyl 4-bromobenzoate (Table 3, entry 7).

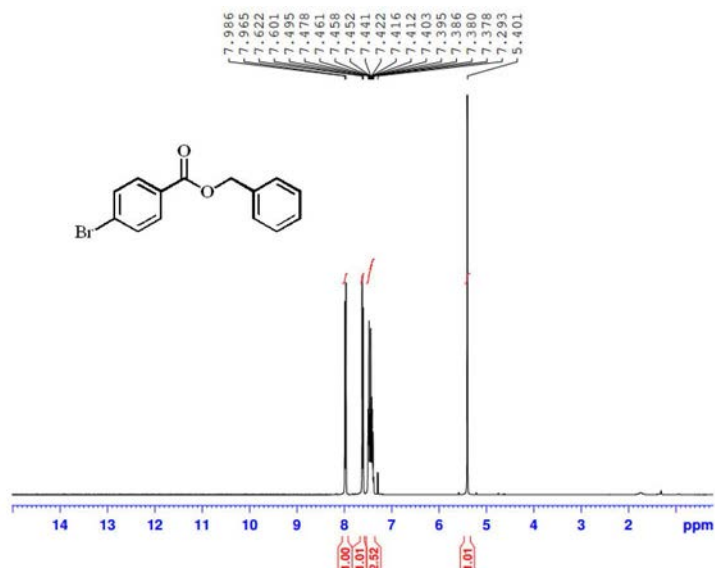


Figure S14. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 4-bromobenzoate (Table 3, entry 7).

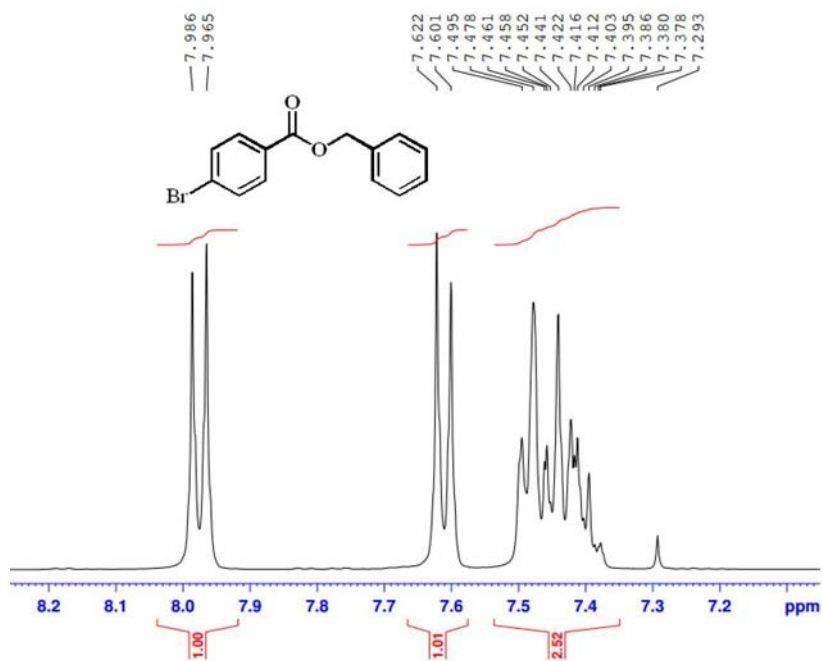


Figure S15. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 4-bromobenzoate (Table 3, entry 7).

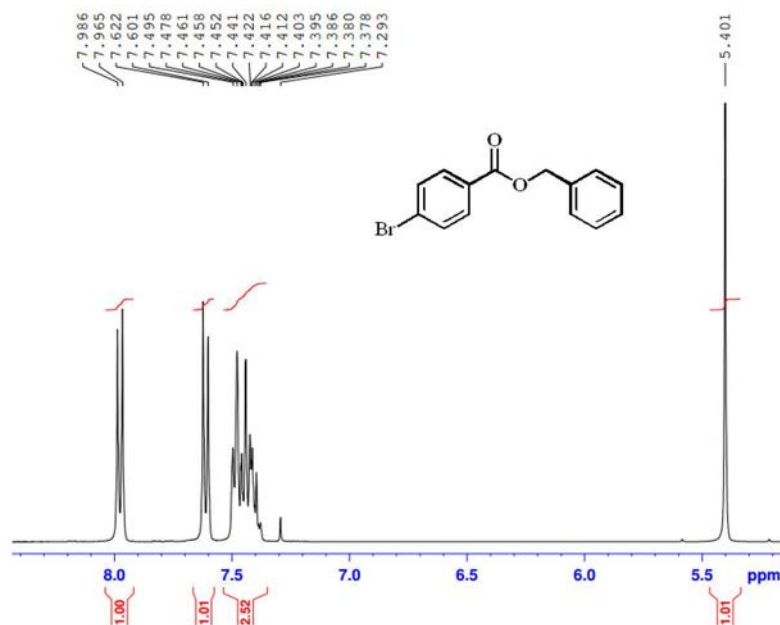


Figure S16. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 4-bromobenzoate (Table 3, entry 7).

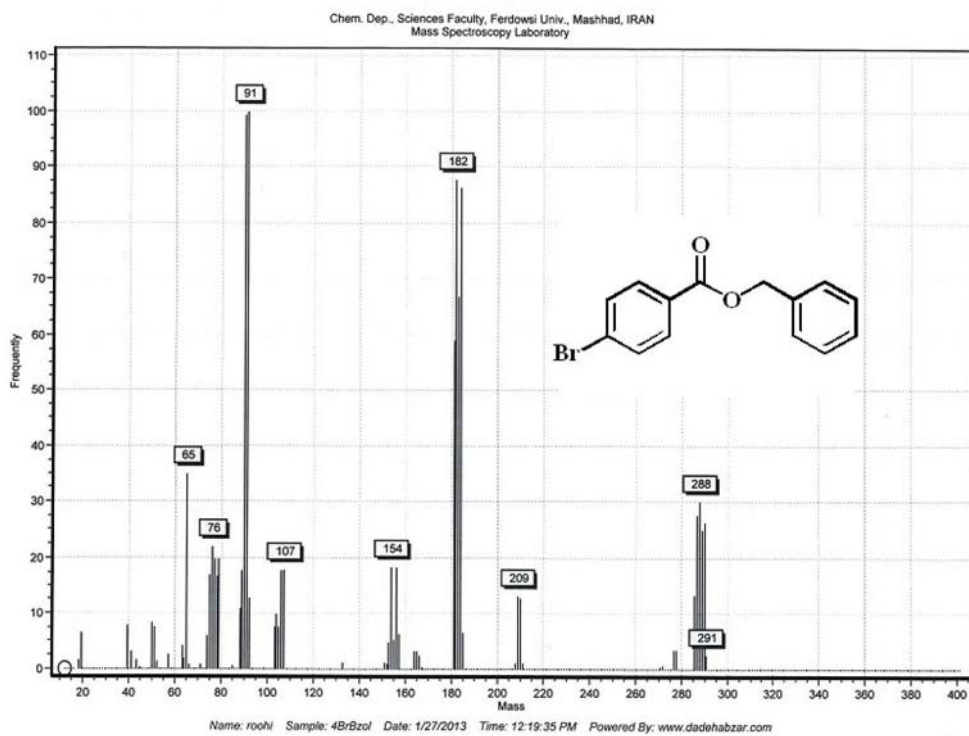


Figure S17. Mass spectrum of benzyl 4-bromobenzoate (Table 3, entry 7).

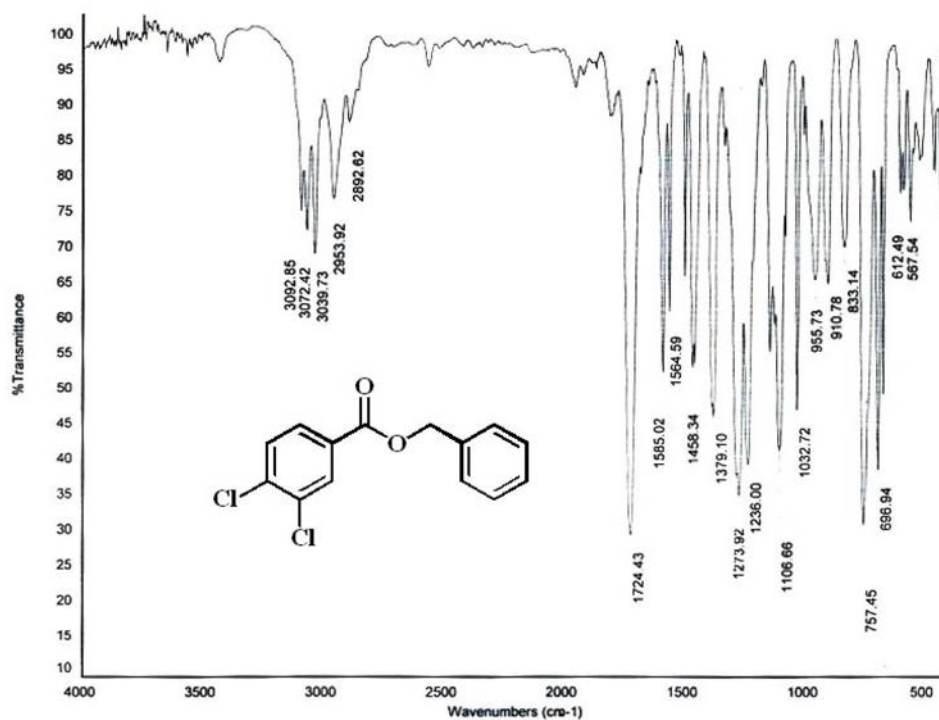


Figure S18. FTIR (KBr) spectrum of benzyl 3,4-dichlorobenzoate (Table 3, entry 8).

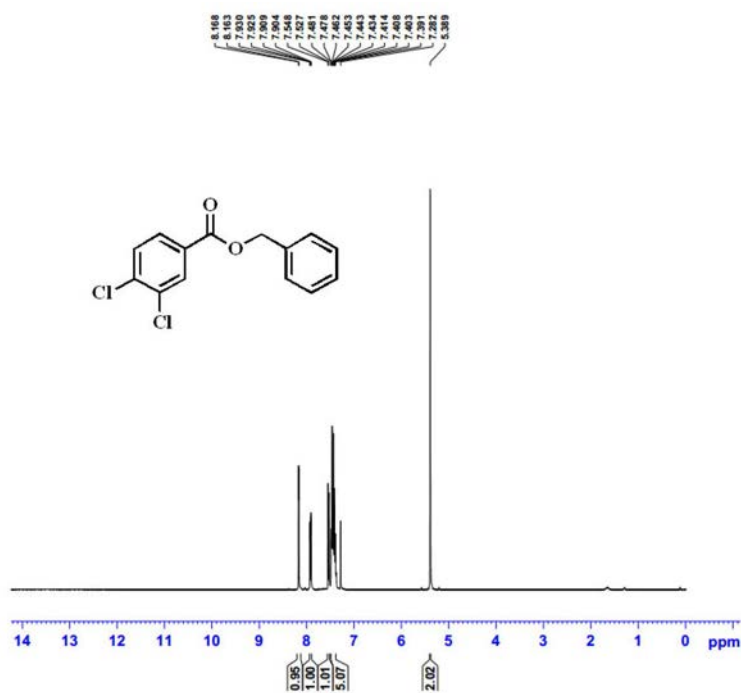


Figure S19. ^1H NMR (400 MHz, CDCl_3) spectrum of 3,4-dichlorobenzoate (Table 3, entry 8).

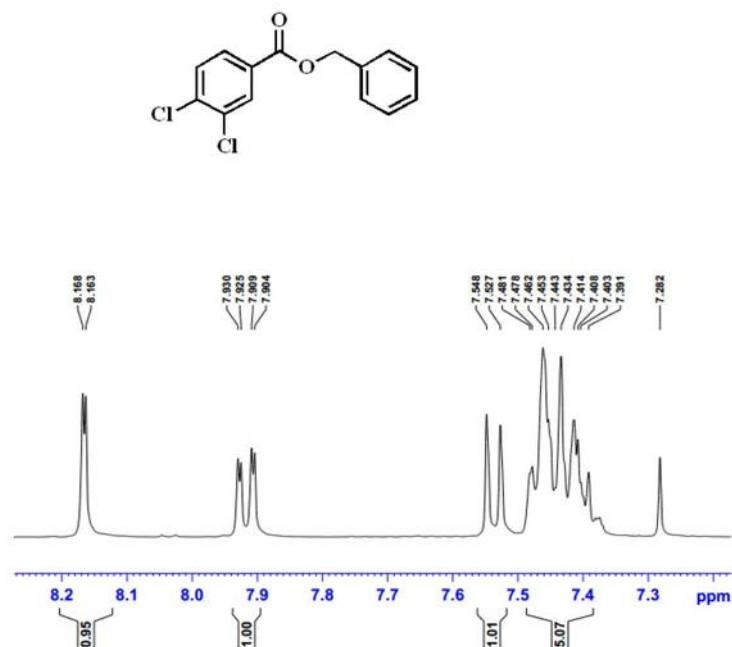


Figure S20. ¹H NMR (400 MHz, CDCl₃) spectrum of 3,4-dichlorobenzoate (Table 3, entry 8).

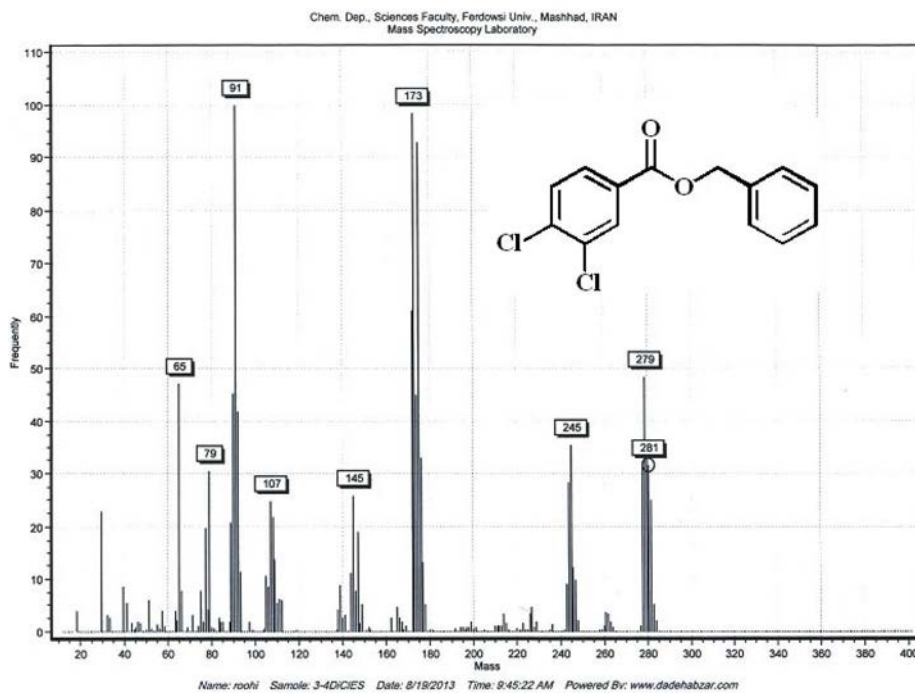


Figure S21. Mass spectrum of benzyl 3,4-dichlorobenzoate (Table 3, entry 8).

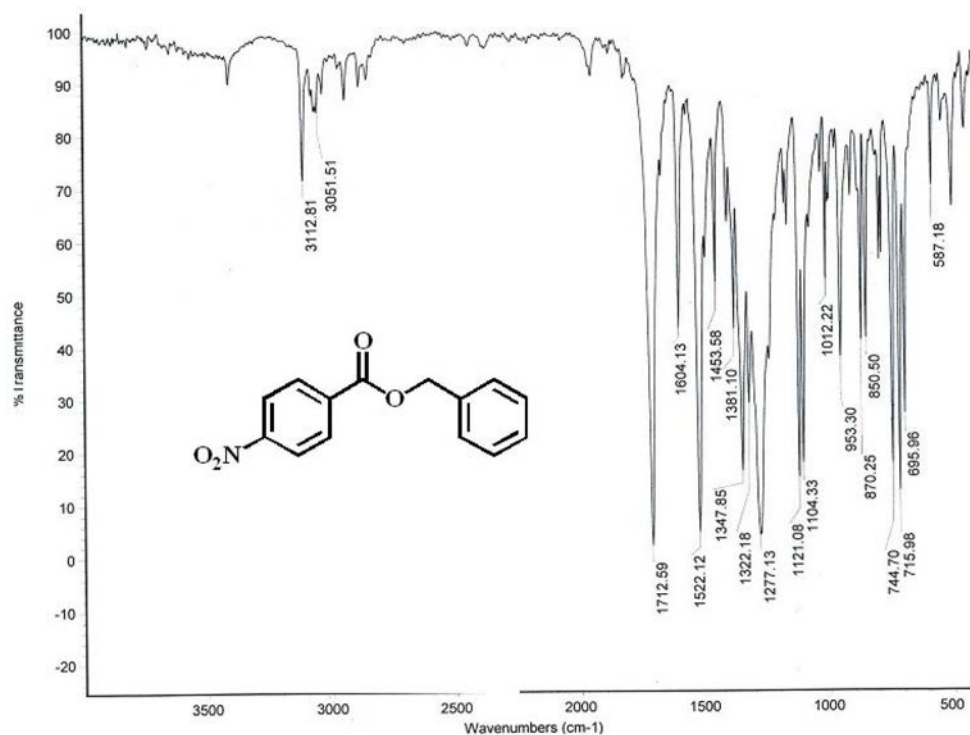


Figure S22. FTIR (KBr) spectrum of benzyl 4-nitrobenzoate (Table 3, entry 9).

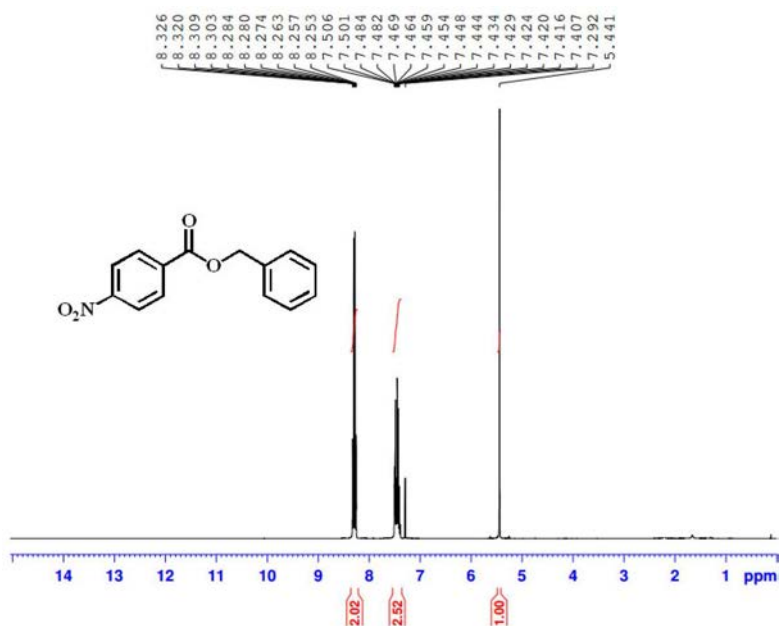


Figure S23. ^1H NMR (400 MHz, CDCl_3) spectrum of benzyl 4-nitrobenzoate (Table 3, entry 9).

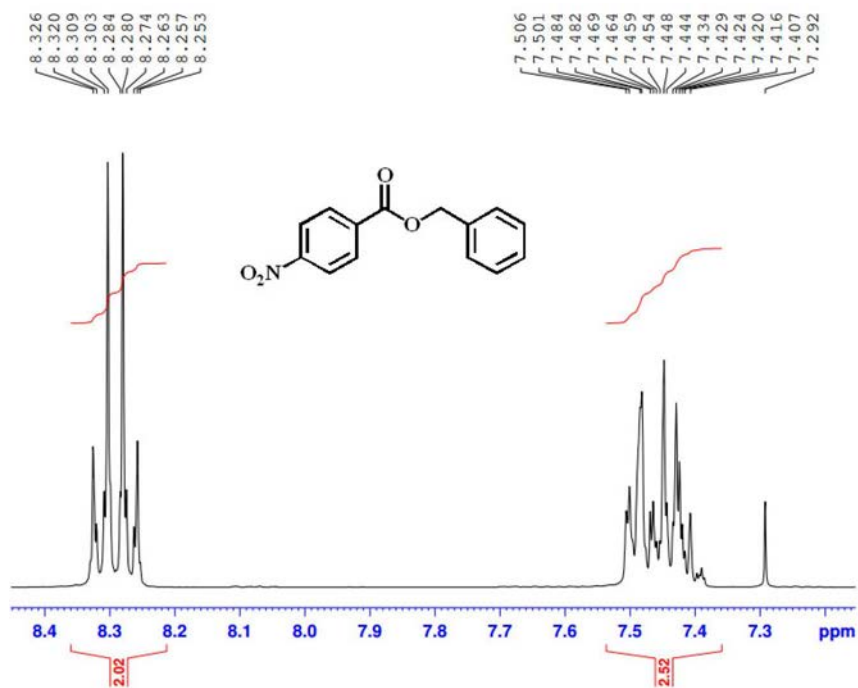


Figure S24. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 4-nitrobenzoate (Table 3, entry 9).

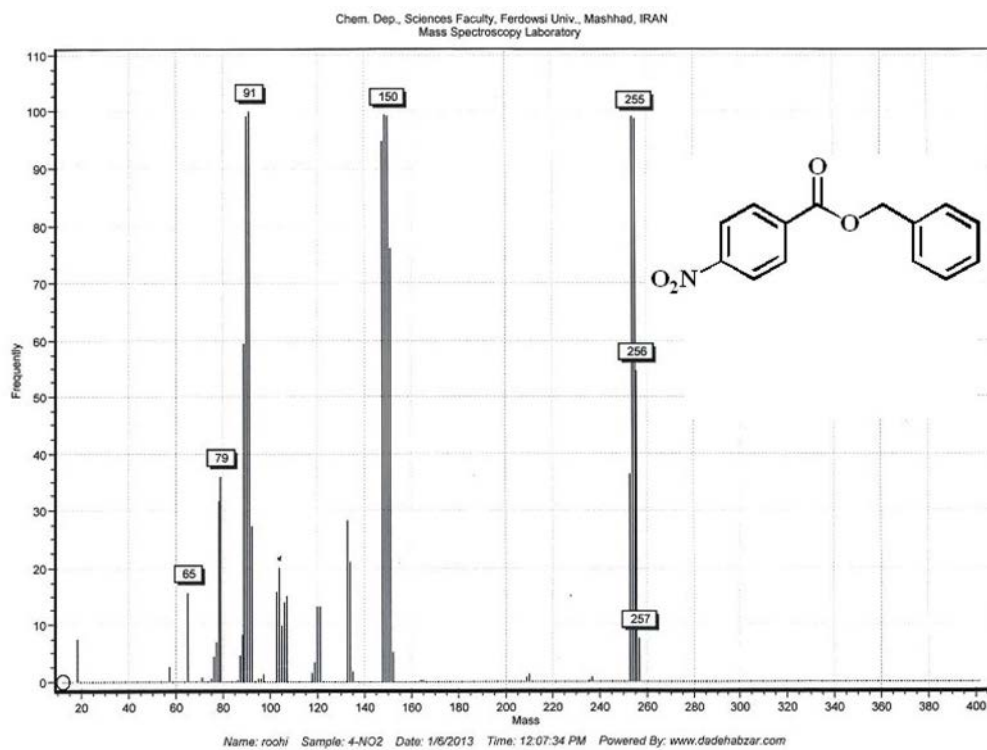


Figure S25. Mass spectrum of benzyl 4-nitrobenzoate (Table 3, entry 9).

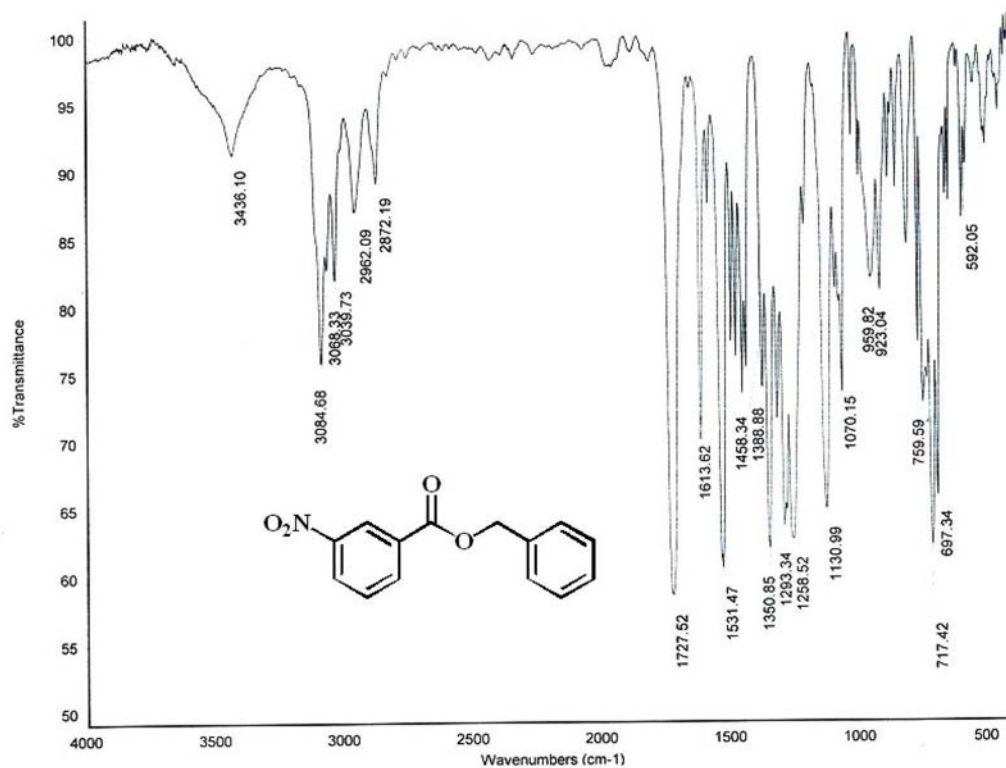


Figure S26. FTIR (KBr) spectrum of benzyl 3-nitrobenzoate (Table 3, entry 10).

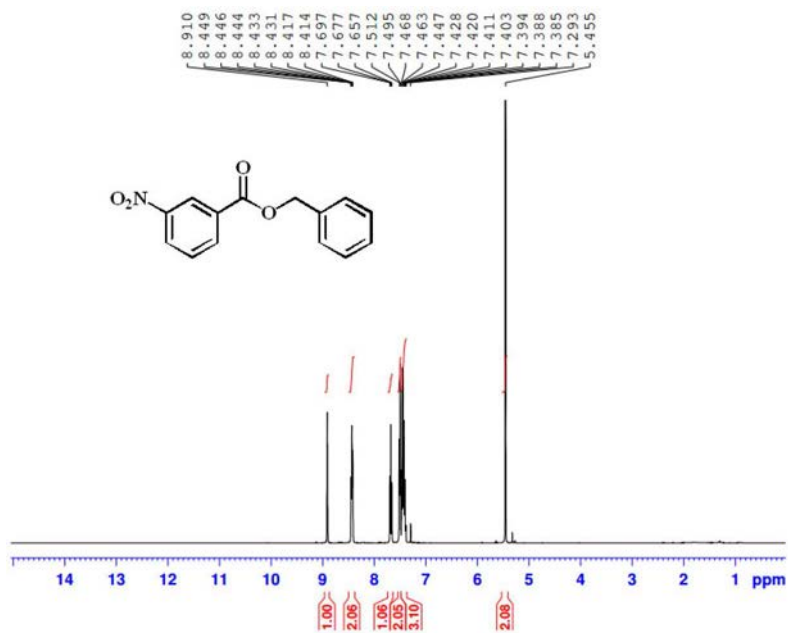


Figure S27. ^1H NMR (400 MHz, CDCl_3) spectrum of benzyl 3-nitrobenzoate (Table 3, entry 10).

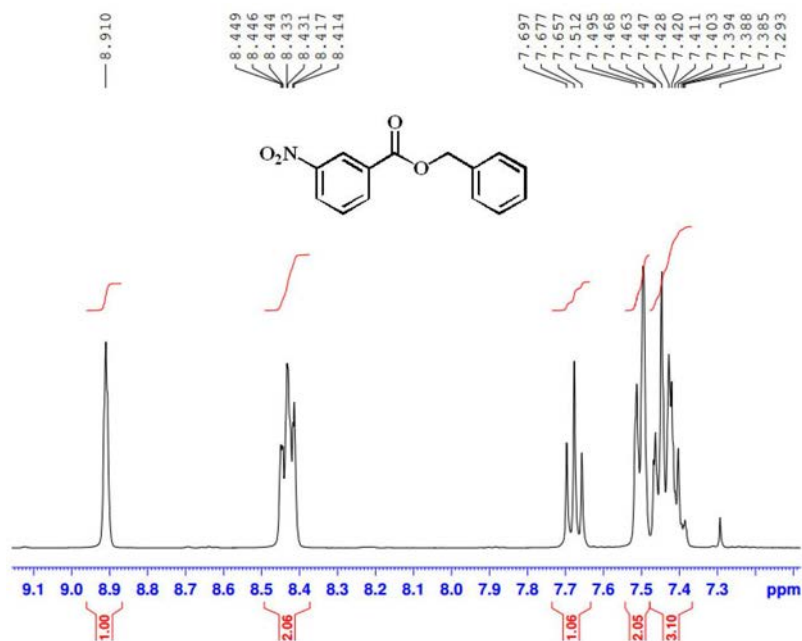


Figure S28. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 3-nitrobenzoate (Table 3, entry 10).

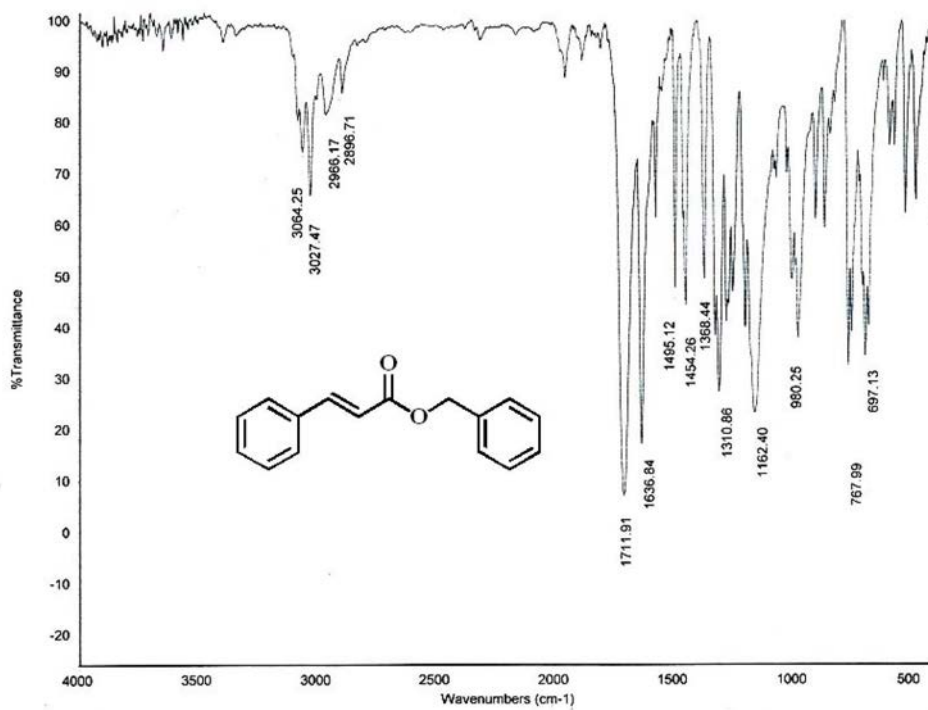


Figure S29. FTIR (KBr) spectrum of benzyl cinnamate (Table 3, entry 11).

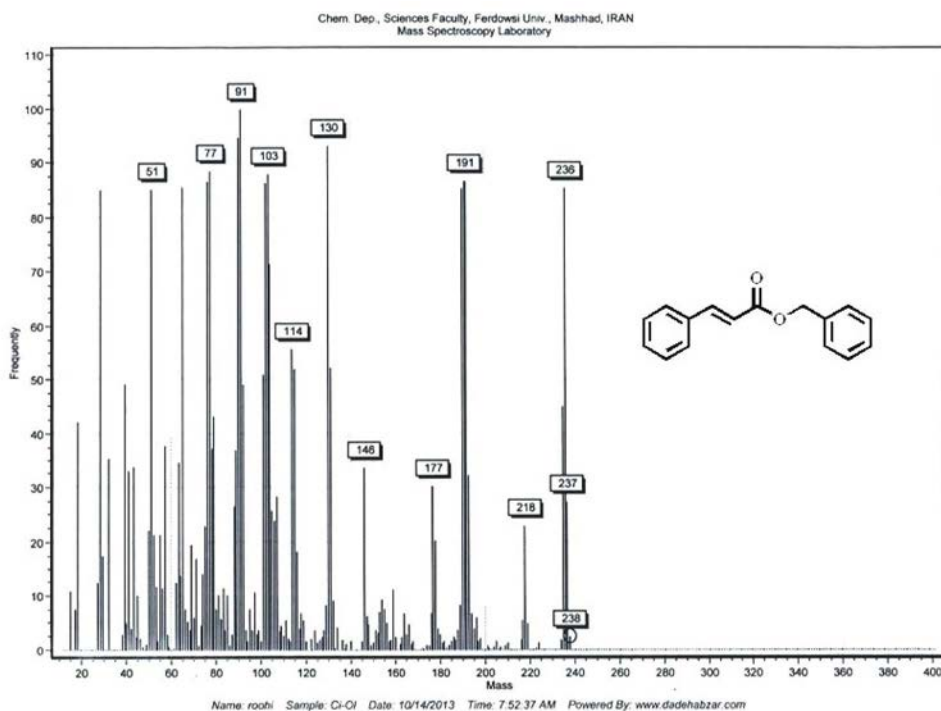


Figure S30. Mass spectrum of benzyl cinnamate (Table 3, entry 11).

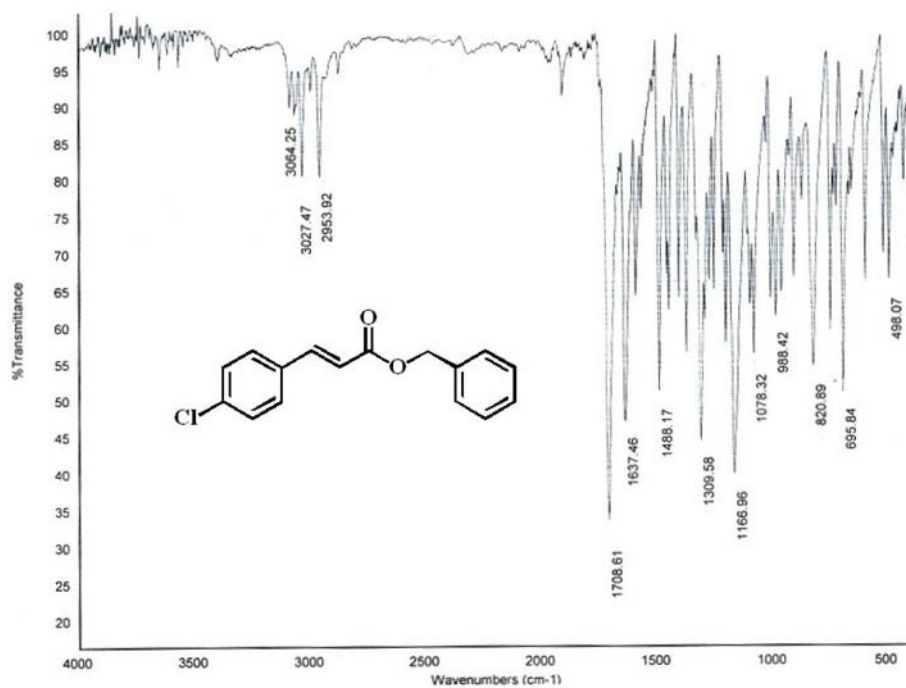


Figure S31. FTIR (KBr) spectrum of (*E*)-benzyl 3-(4-chlorophenyl)acrylate (Table 3, entry 12).

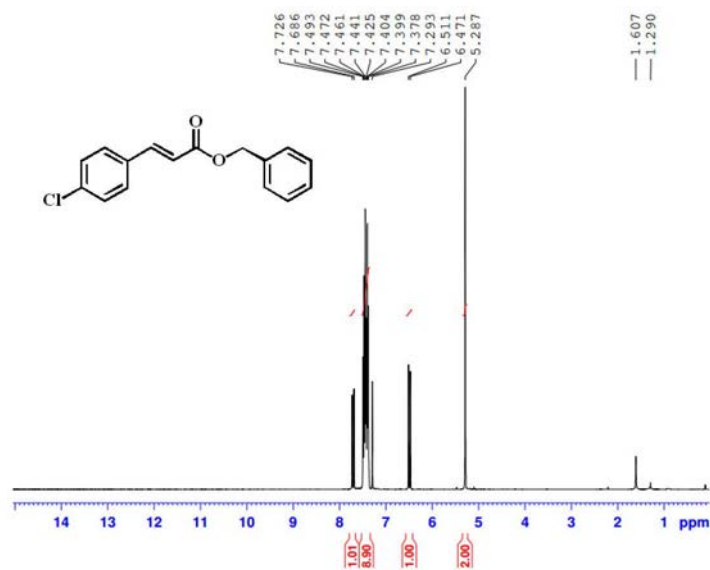


Figure S32. ^1H NMR (400 MHz, CDCl_3) spectrum of (*E*)-benzyl 3-(4-chlorophenyl)acrylate (Table 3, entry 12).

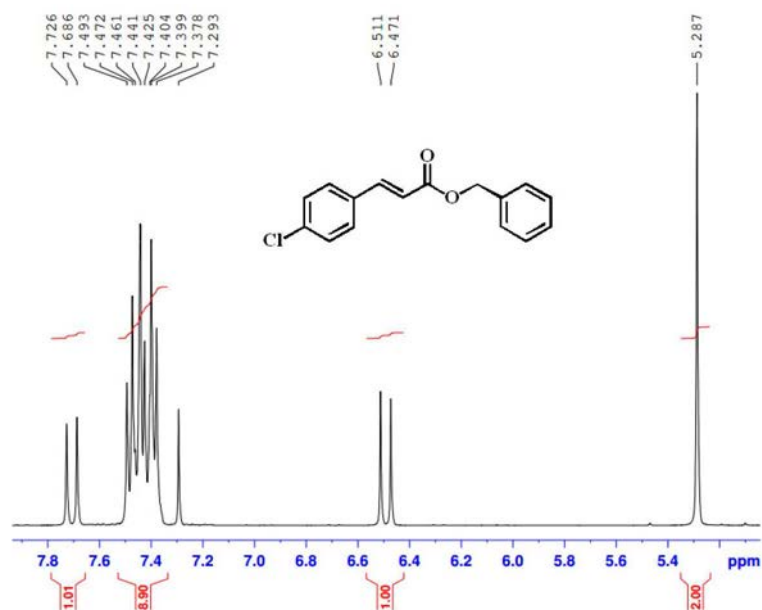


Figure S33. ^1H NMR (400 MHz, CDCl_3) spectrum of (*E*)-Benzyl 3-(4-chlorophenyl)acrylate (Table 3, entry 12).

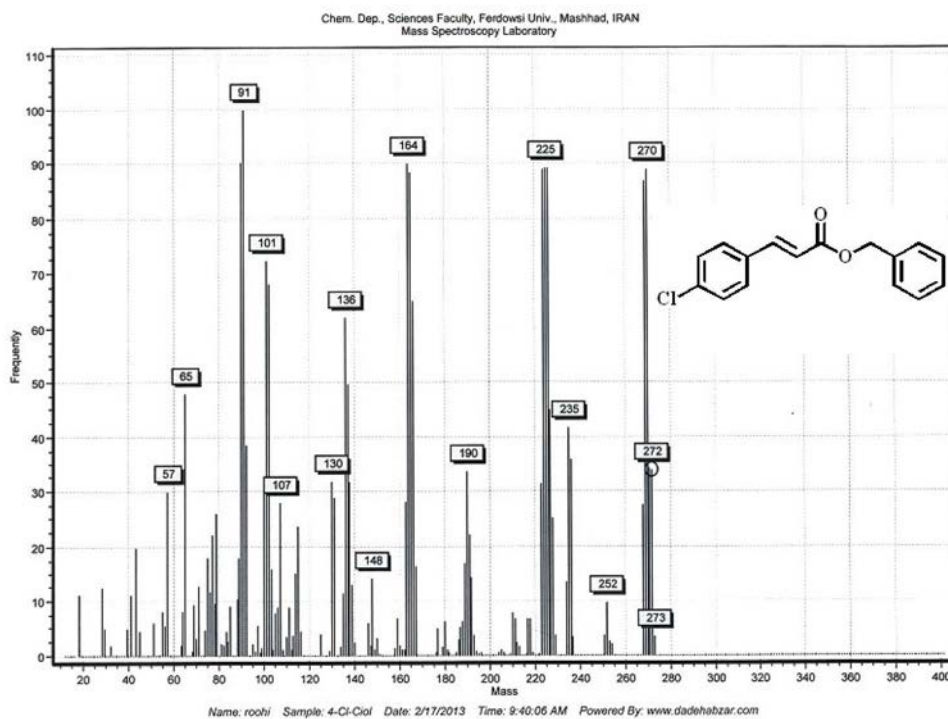


Figure S34. Mass spectrum of (*E*)-benzyl 3-(4-chlorophenyl)acrylate (Table 3, entry 12).

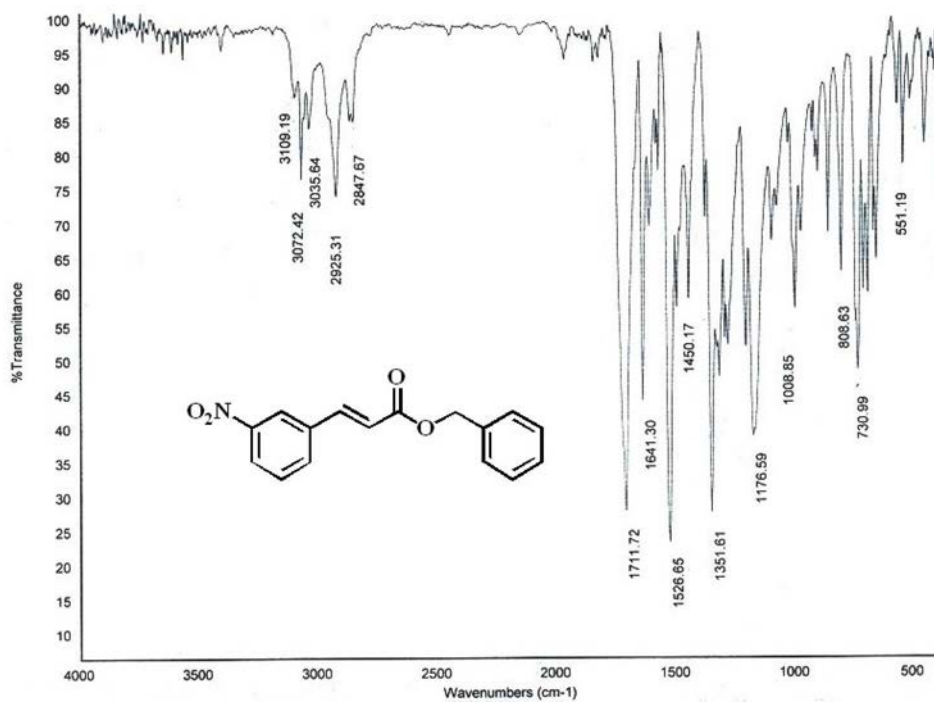


Figure S35. FTIR (KBr) spectrum of (*E*)-benzyl 3-(3-nitrophenyl)acrylate (Table 3, entry 13).

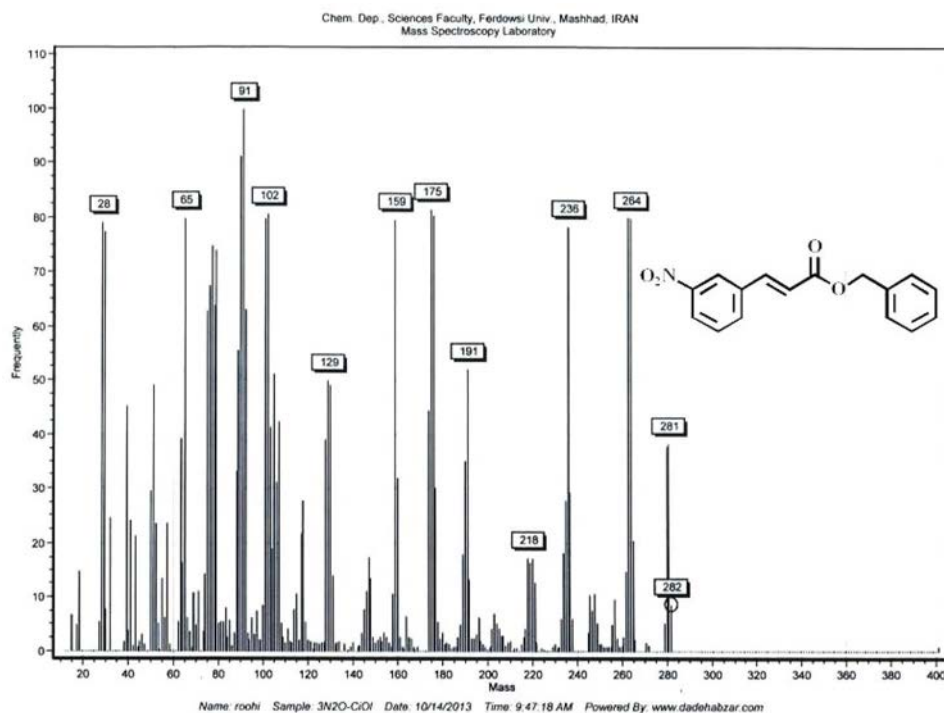


Figure S36. Mass spectrum of (*E*)-benzyl 3-(3-nitrophenyl)acrylate (Table 3, entry 13).

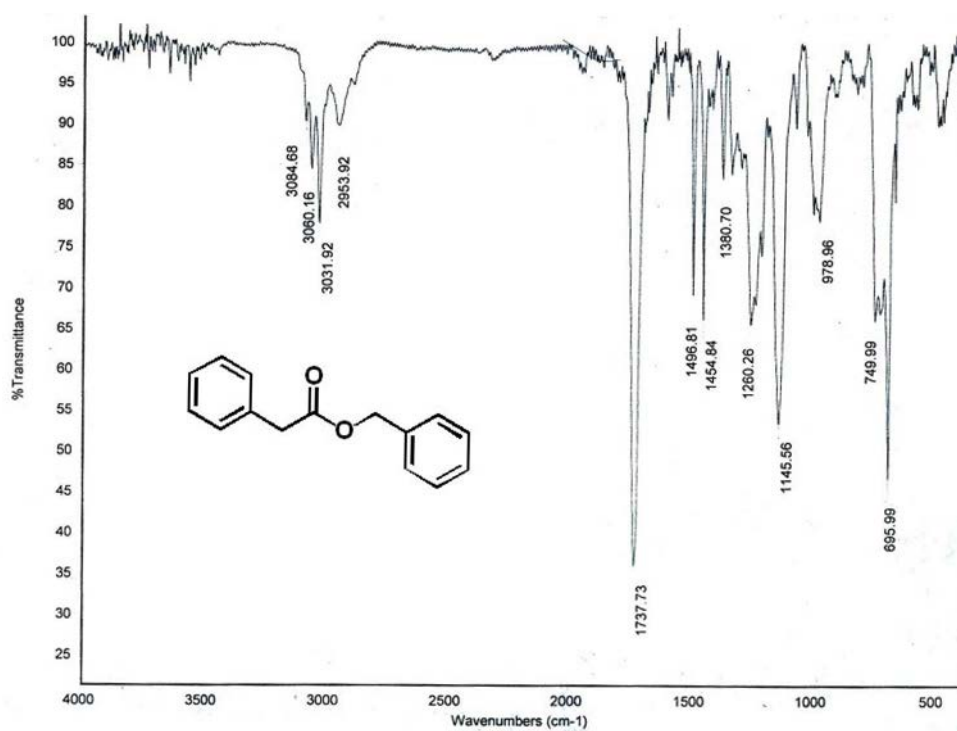


Figure S37. FTIR (KBr) spectrum of benzyl 2-phenylacetate (Table 3, entry 14).

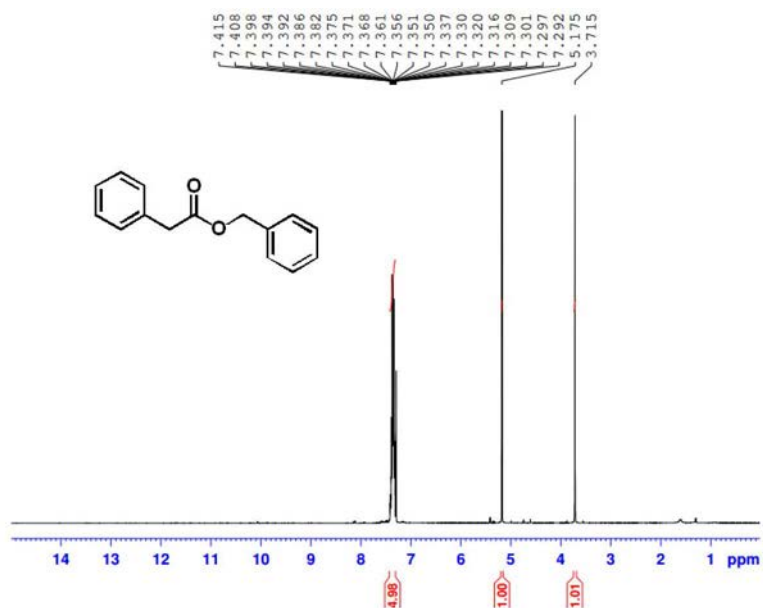


Figure S38. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 2-phenylacetate (Table 3, entry 14).

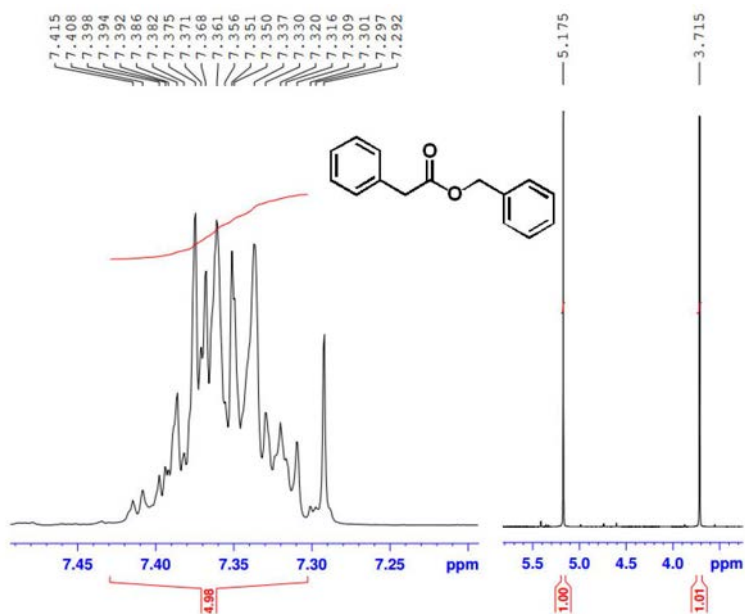


Figure S39. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl 2-phenylacetate (Table 3, entry 14).

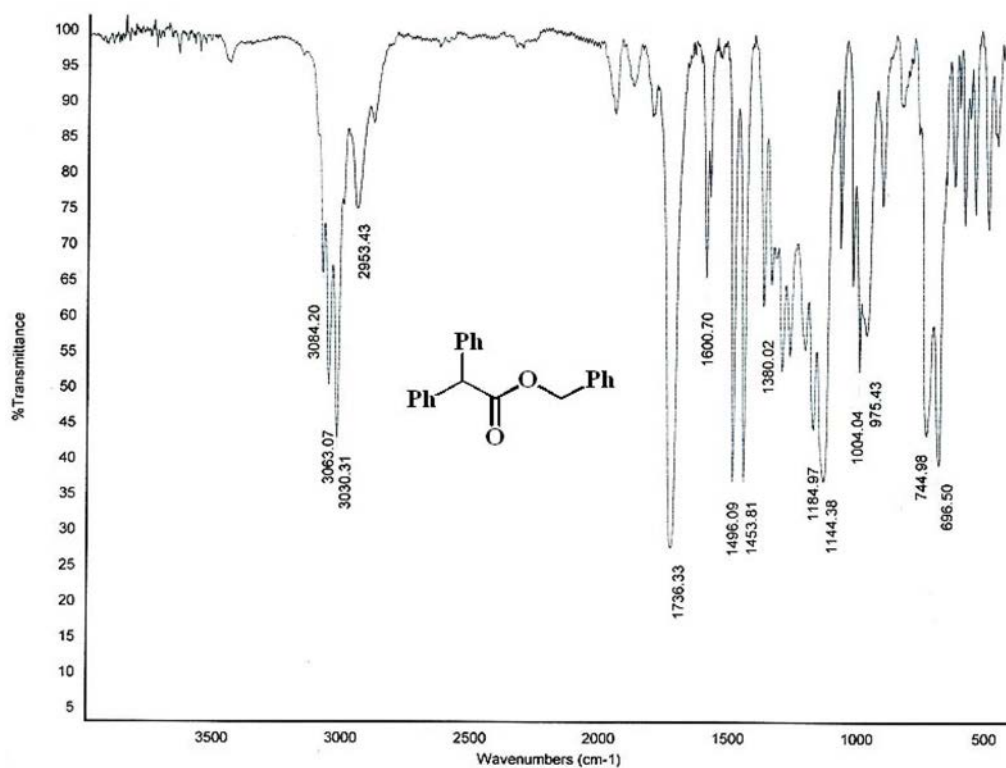


Figure S40. FTIR (neat) spectrum of benzyl 2,2-diphenylacetate (Table 3, entry 15).

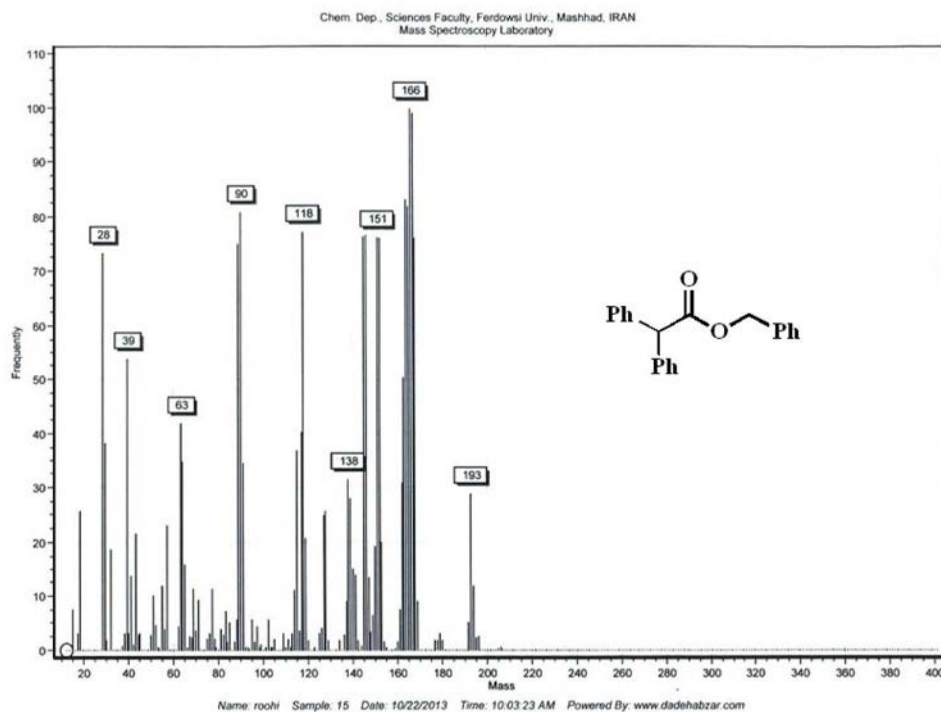


Figure S41. Mass spectrum of benzyl 2,2-diphenylacetate (Table 3, entry 15).

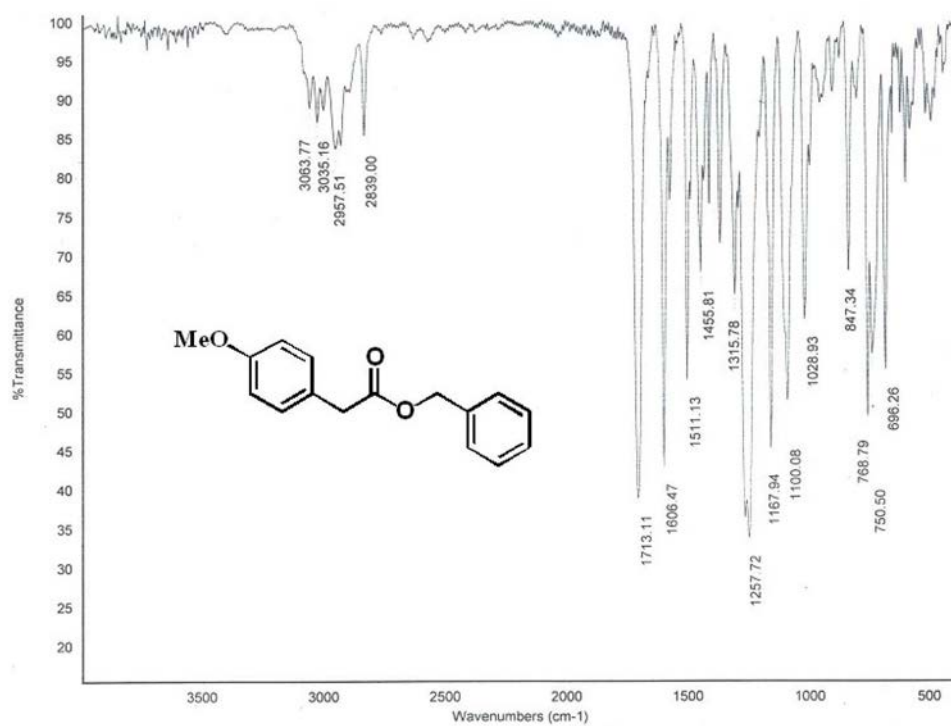


Figure S42. FTIR (KBr) spectrum of benzyl 2-(4-methoxyphenyl)acetate (Table 3, entry 16).

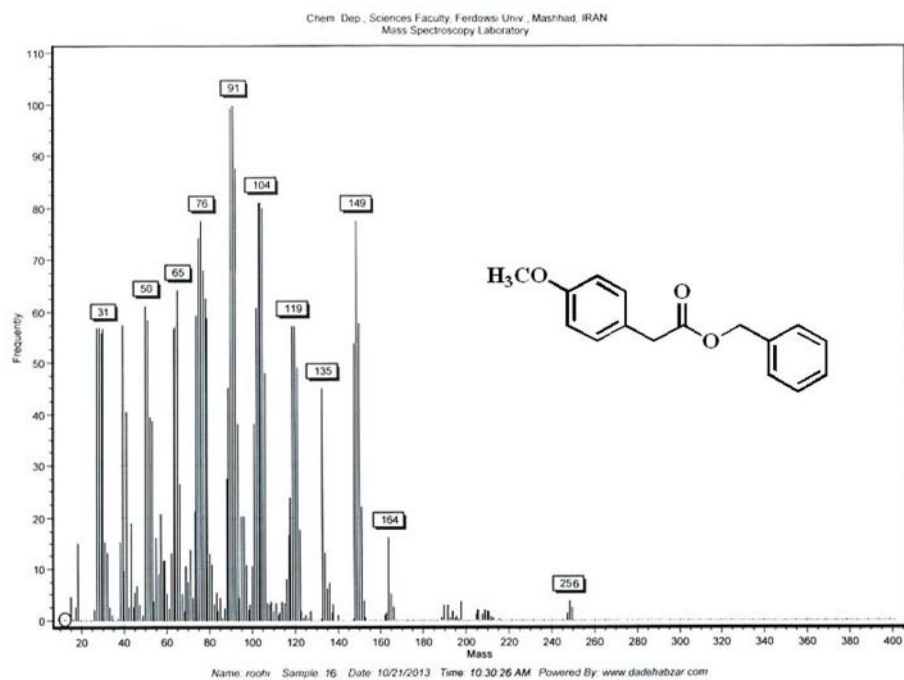


Figure S43. Mass spectrum of benzyl 2-(4-methoxyphenyl)acetate (Table 3, entry 16).

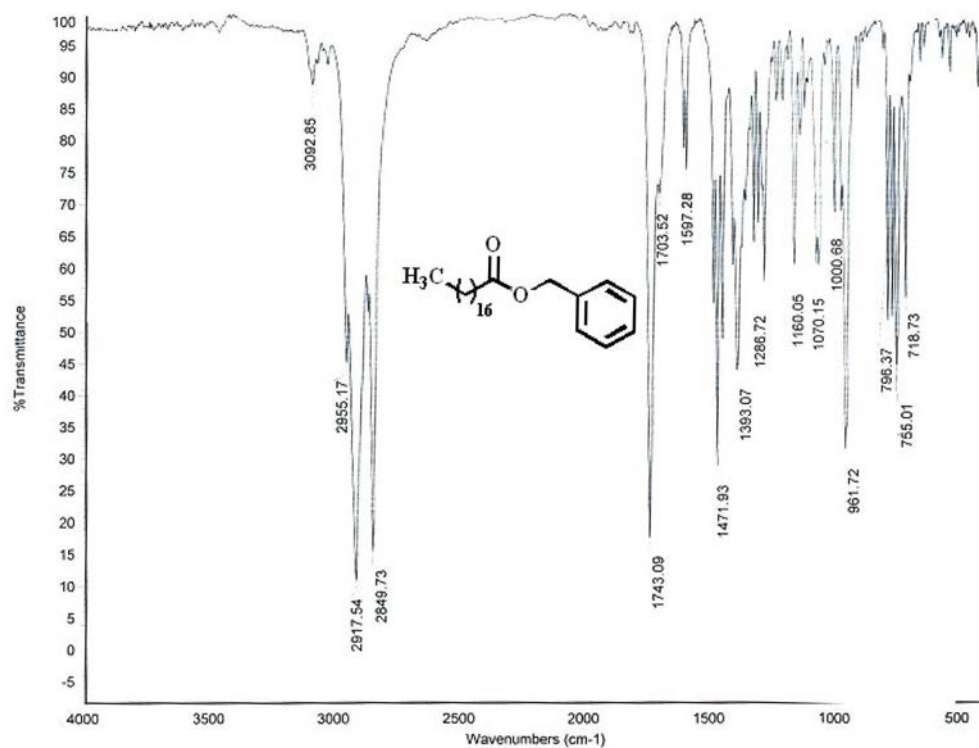


Figure S44. FTIR (KBr) spectrum of benzyl stearate (Table 3, entry 17).

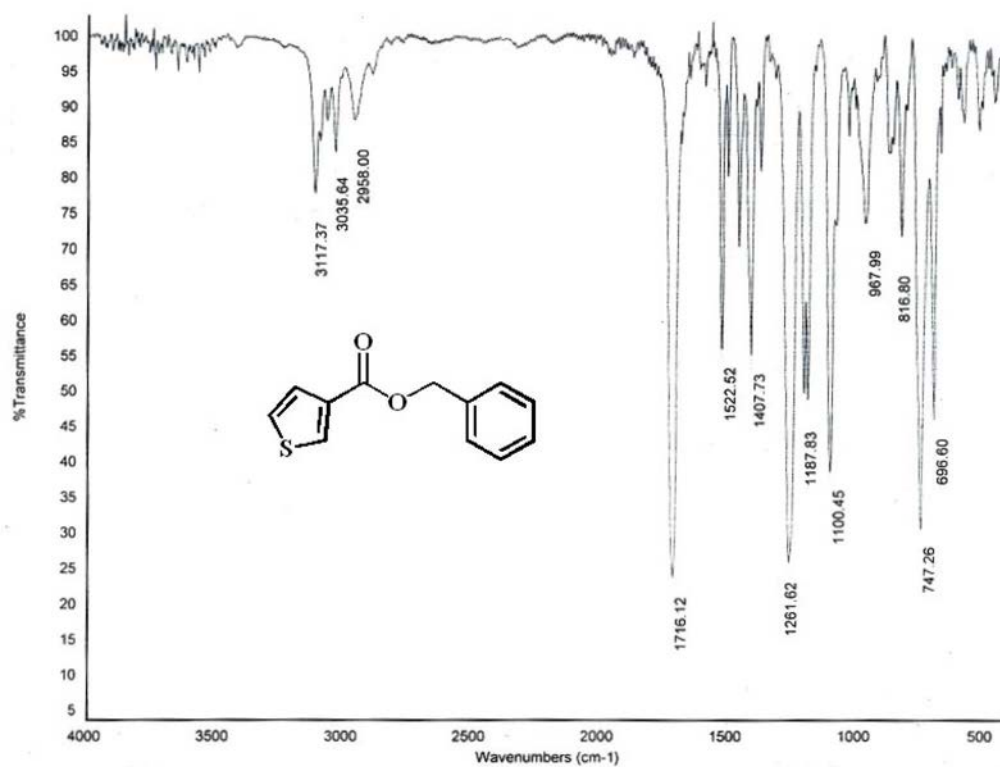


Figure S45. FTIR (KBr) spectrum of benzyl thiophene-3-carboxylate (Table 3, entry 18).

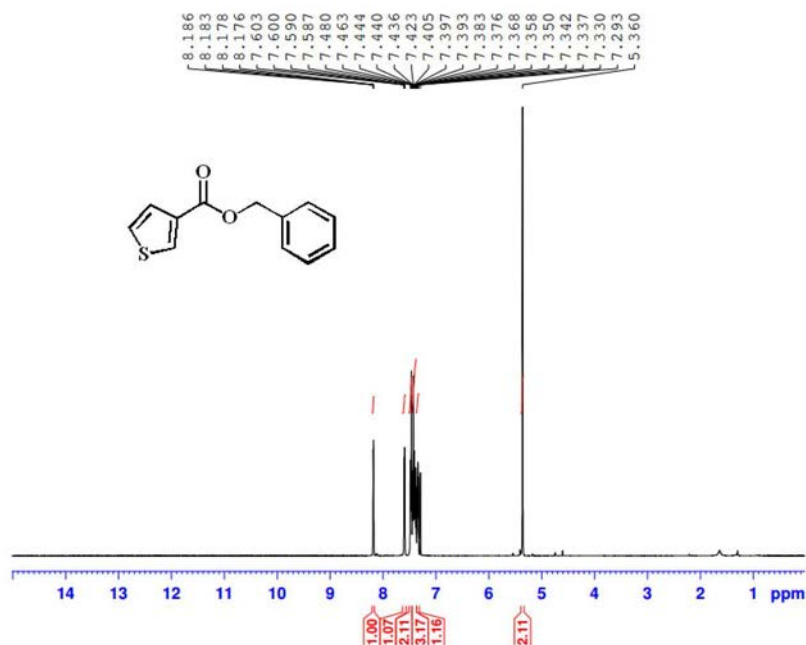


Figure S46. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl thiophene-3-carboxylate (Table 3, entry 18).

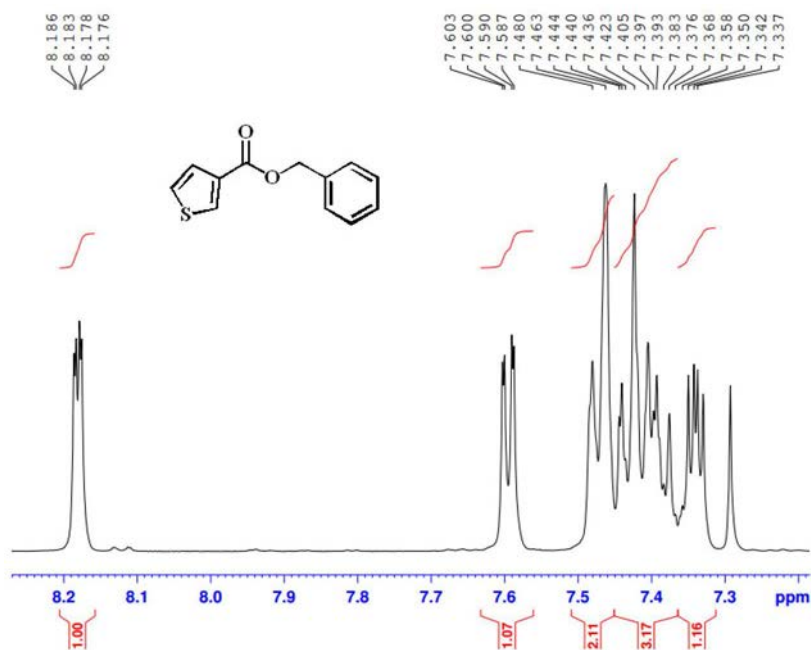


Figure S47. ¹H NMR (400 MHz, CDCl₃) spectrum of benzyl thiophene-3-carboxylate (Table 3, entry 18).

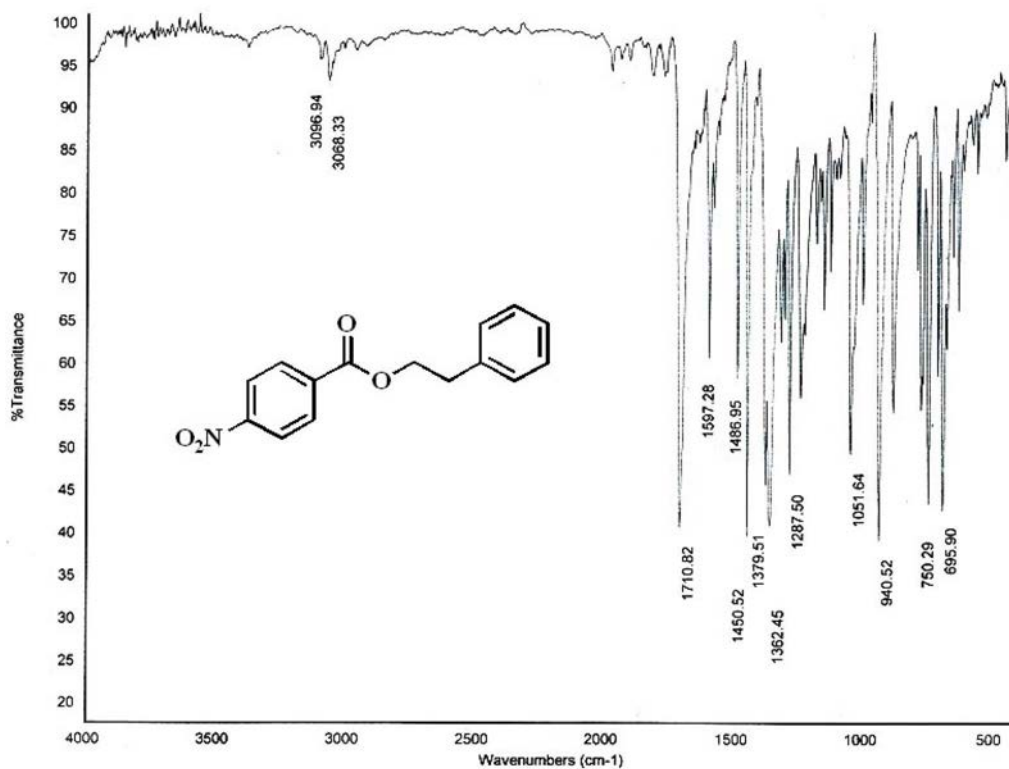


Figure S48. FTIR (KBr) spectrum of phenethyl 4-nitrobenzoate (Table 3, entry 19).

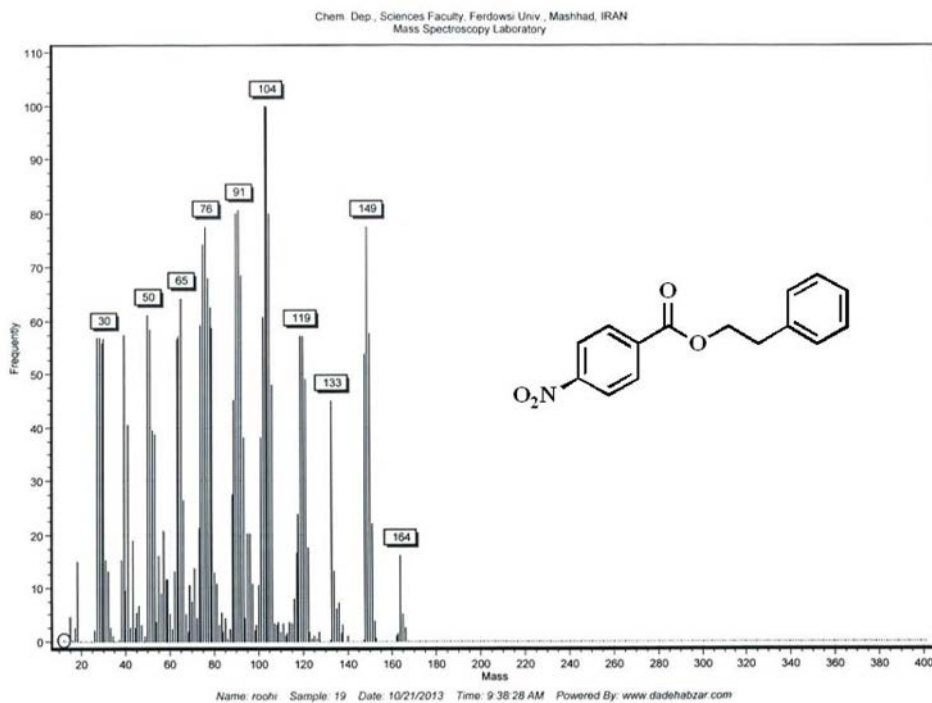


Figure S49. Mass spectrum of phenethyl 4-nitrobenzoate (Table 3, entry 19).

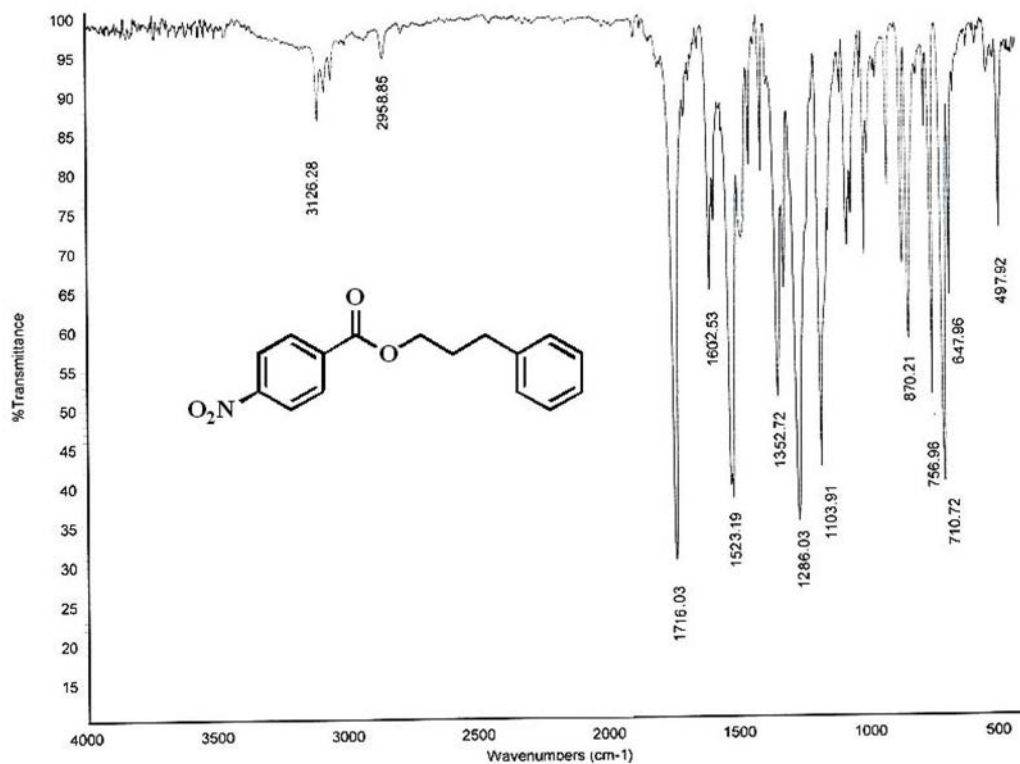


Figure S50. FTIR (KBr) spectrum of 3-phenylpropyl 4-nitrobenzoate (Table 3, entry 20).

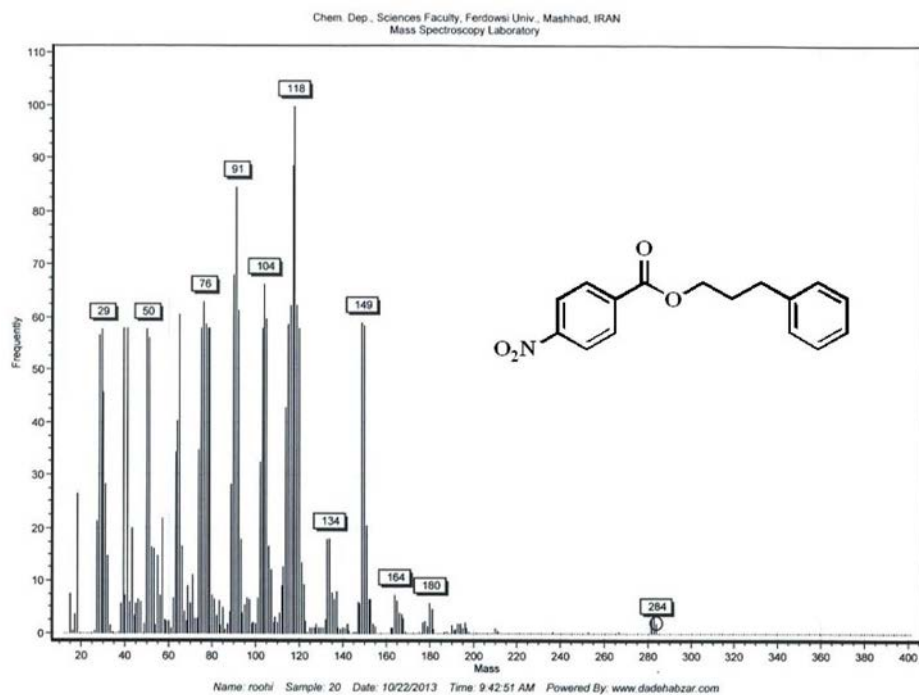


Figure S51. Mass spectrum of 3-phenylpropyl 4-nitrobenzoate (Table 3, entry 20).

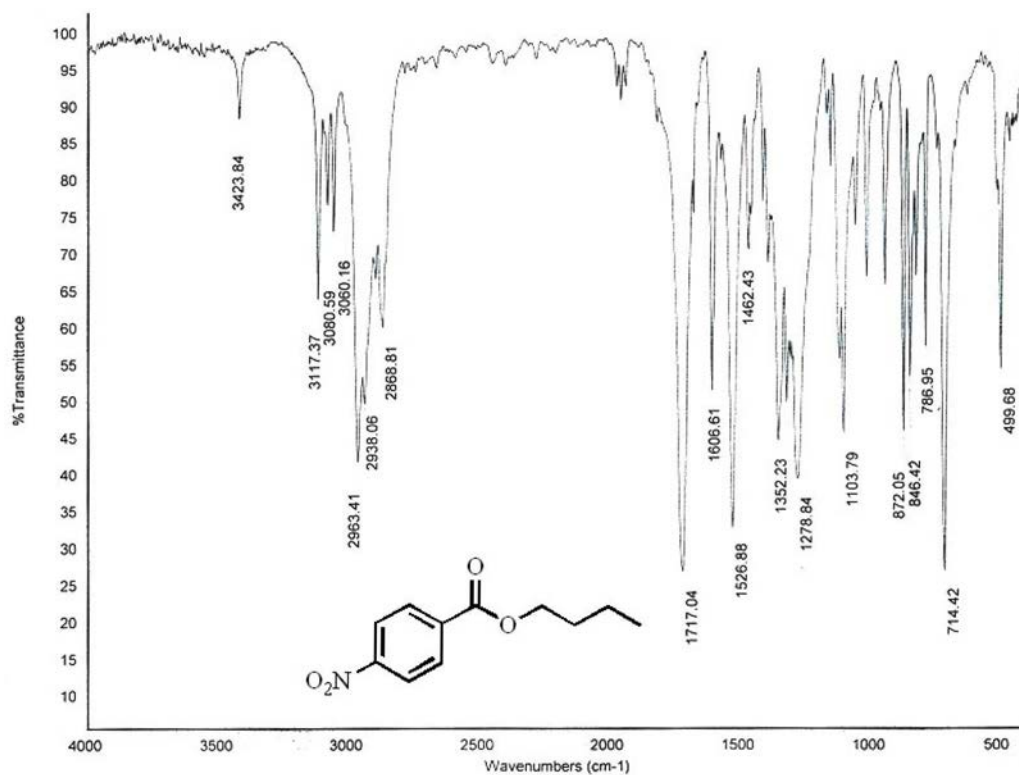


Figure S52. FTIR (neat) spectrum of butyl 4-nitrobenzoate (Table 3, entry 21).

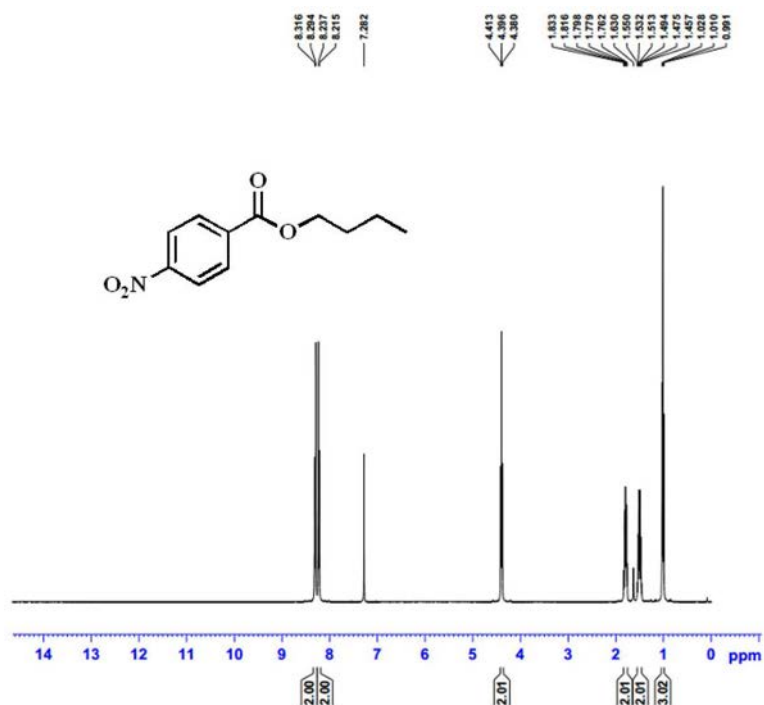


Figure S53. ¹H NMR (400 MHz, CDCl₃) spectrum of butyl 4-nitrobenzoate (Table 3, entry 21).

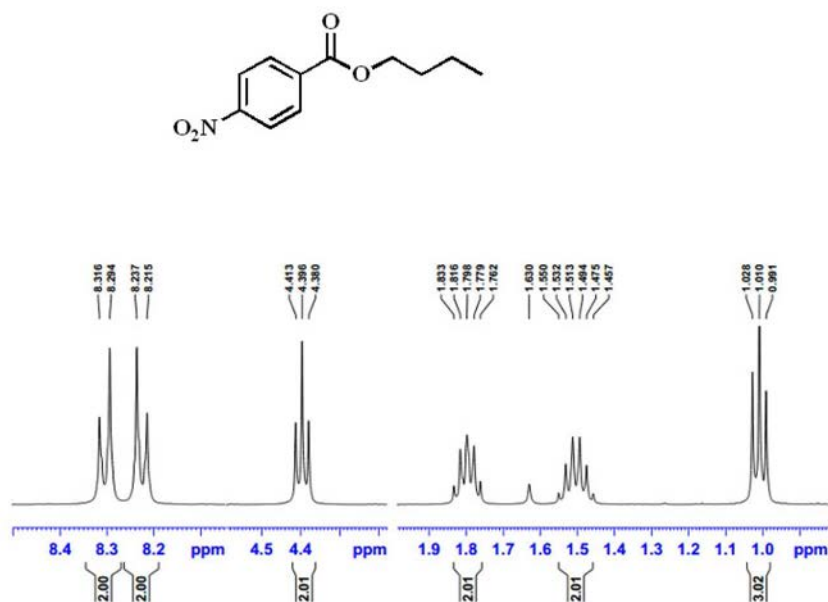


Figure S54. ¹H NMR (400 MHz, CDCl₃) spectrum of butyl 4-nitrobenzoate (Table 3, entry 21).

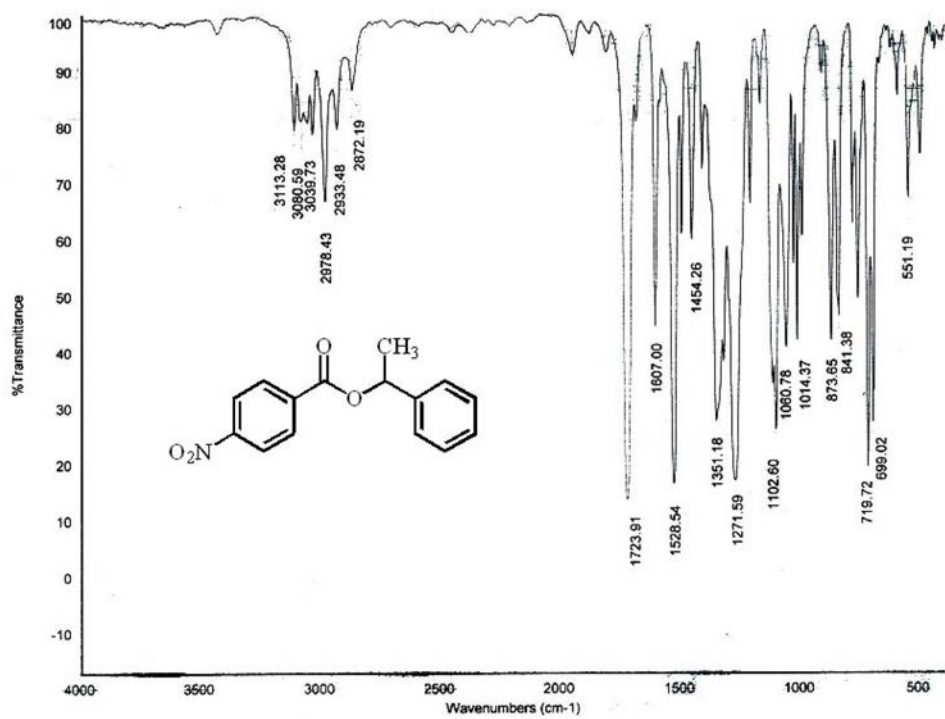


Figure S55. FTIR (KBr) spectrum of 1-phenylethyl 4-nitrobenzoate (Table 3, entry 22).

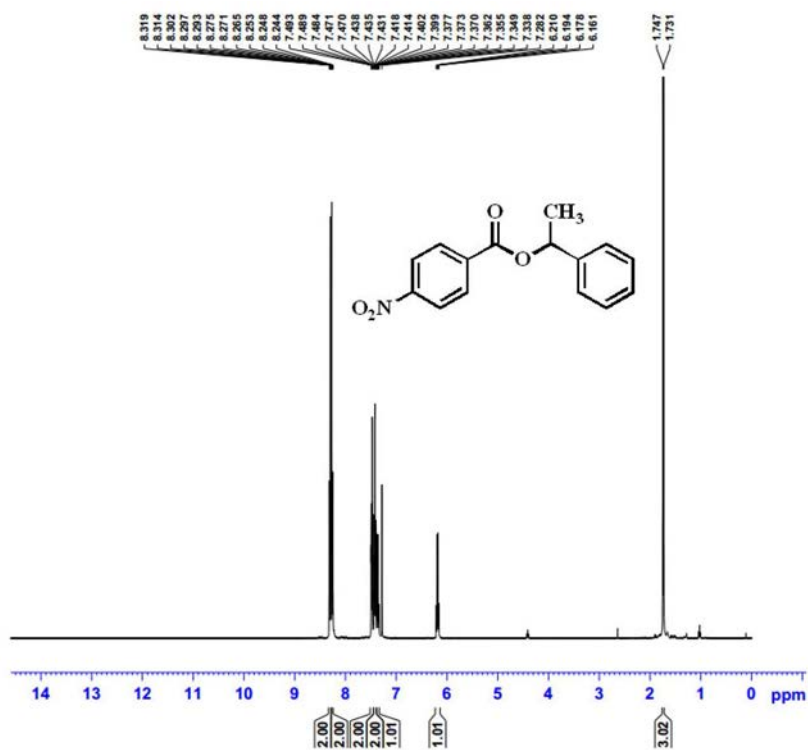


Figure S56. ¹H NMR (400 MHz, CDCl₃) spectrum of 1-phenylethyl 4-nitrobenzoate (Table 3, entry 22).

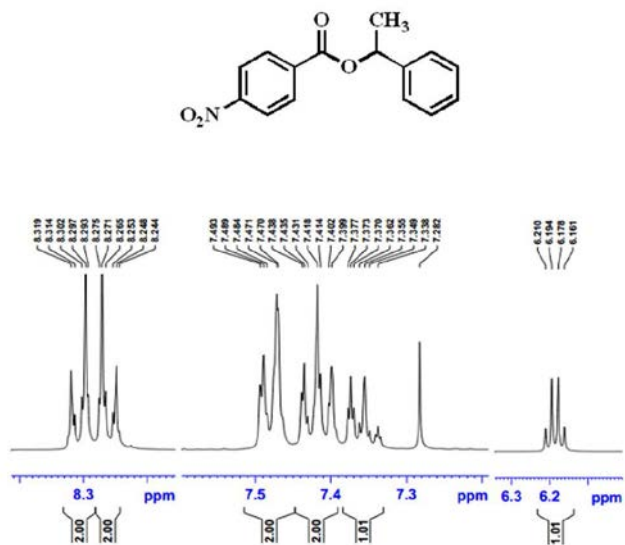


Figure S57. ¹H NMR (400 MHz, CDCl₃) spectrum of 1-phenylethyl 4-nitrobenzoate (Table 3, entry 22).

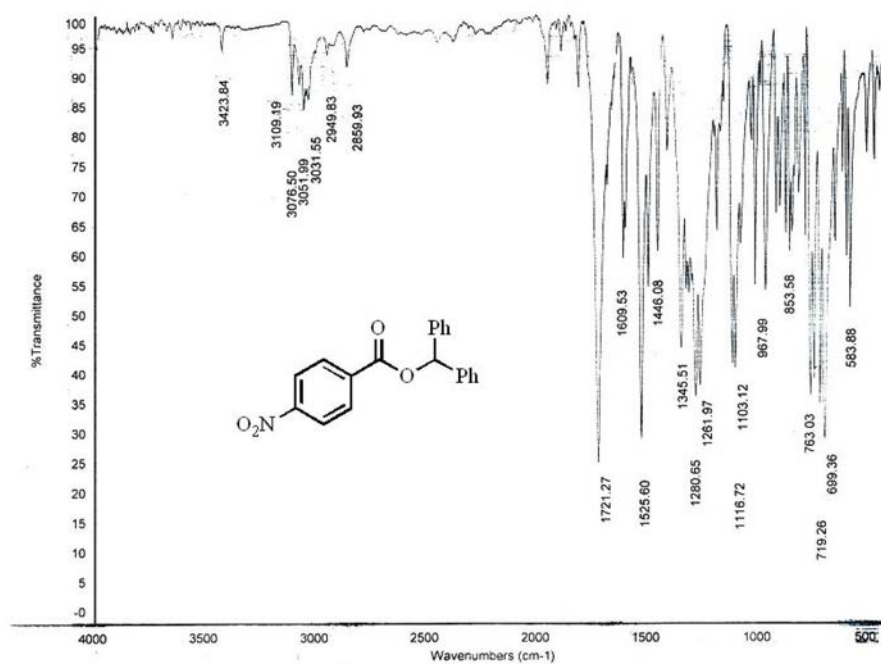


Figure S58. FTIR (KBr) spectrum of benzhydryl 4-nitrobenzoate (Table 3, entry 23).

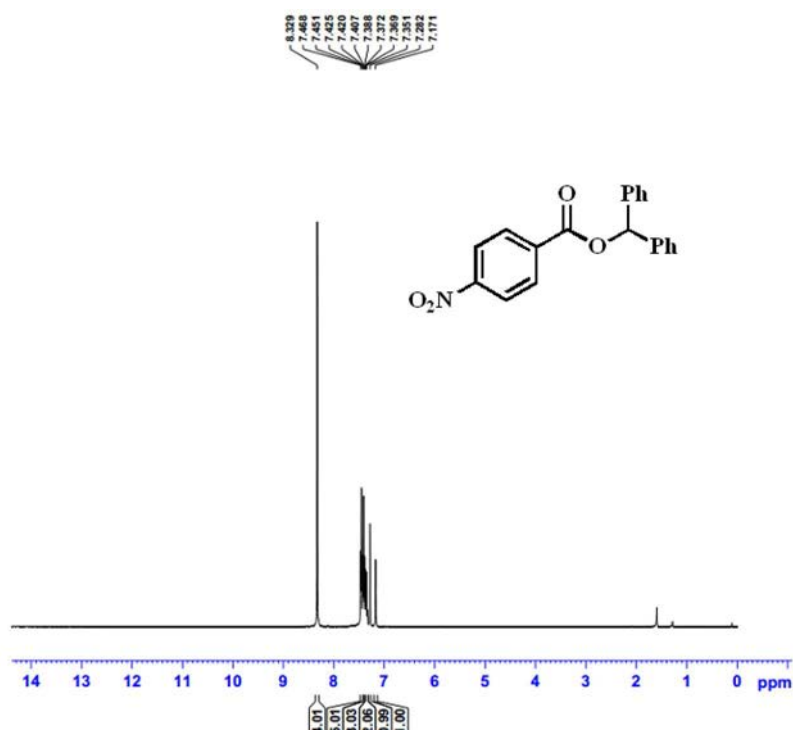


Figure S59. ¹H NMR (400 MHz, CDCl₃) spectrum of benzhydryl 4-nitrobenzoate (Table 3, entry 23).

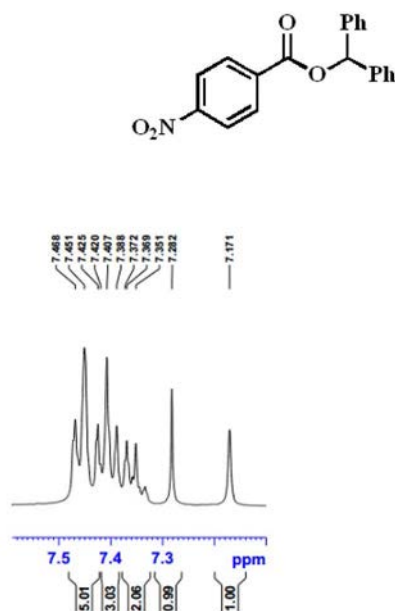


Figure S60. ¹H NMR (400 MHz, CDCl₃) spectrum of benzhydryl 4-nitrobenzoate (Table 3, entry 23).

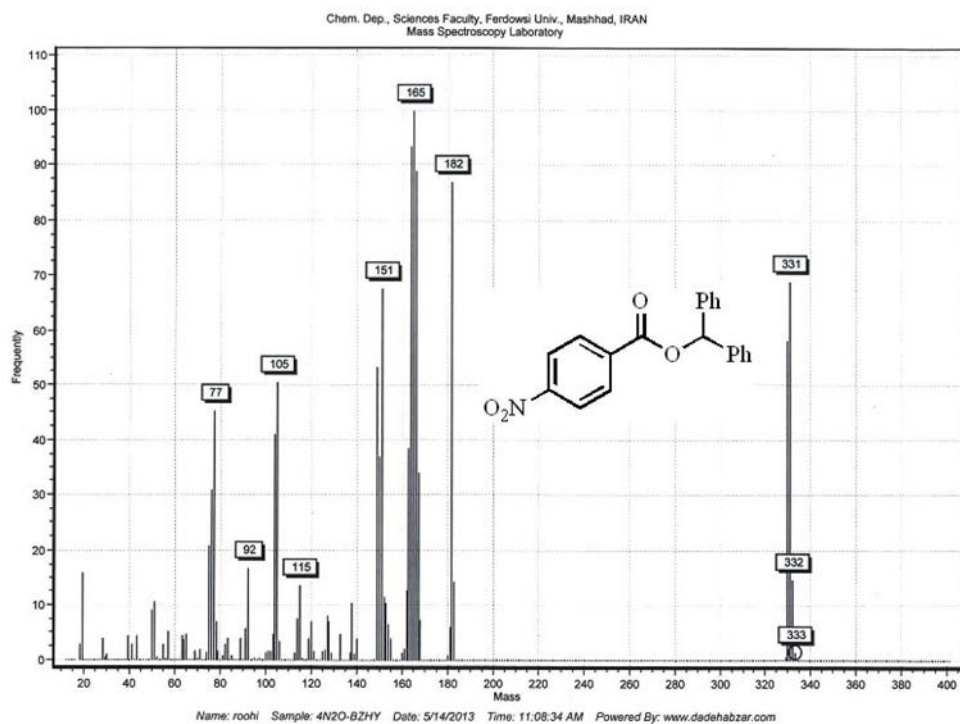


Figure S61. Mass spectrum of benzhydryl 4-nitrobenzoate (Table 3, entry 23).

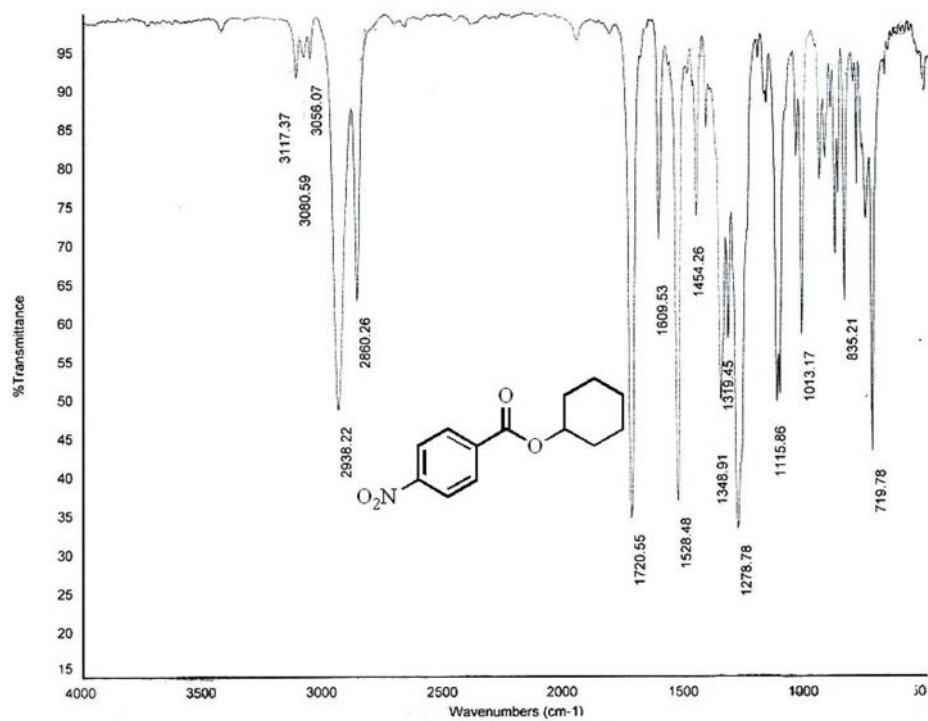


Figure S62. FTIR (KBr) spectrum of cyclohexyl 4-nitrobenzoate (Table 3, entry 24).

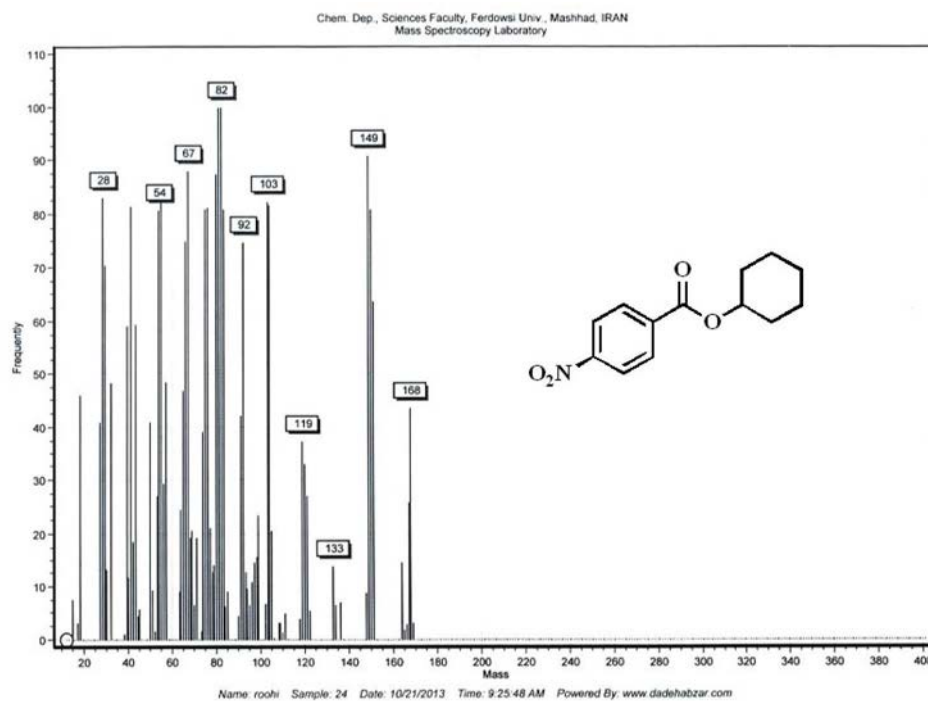


Figure S63. Mass spectrum of cyclohexyl 4-nitrobenzoate (Table 3, entry 24).

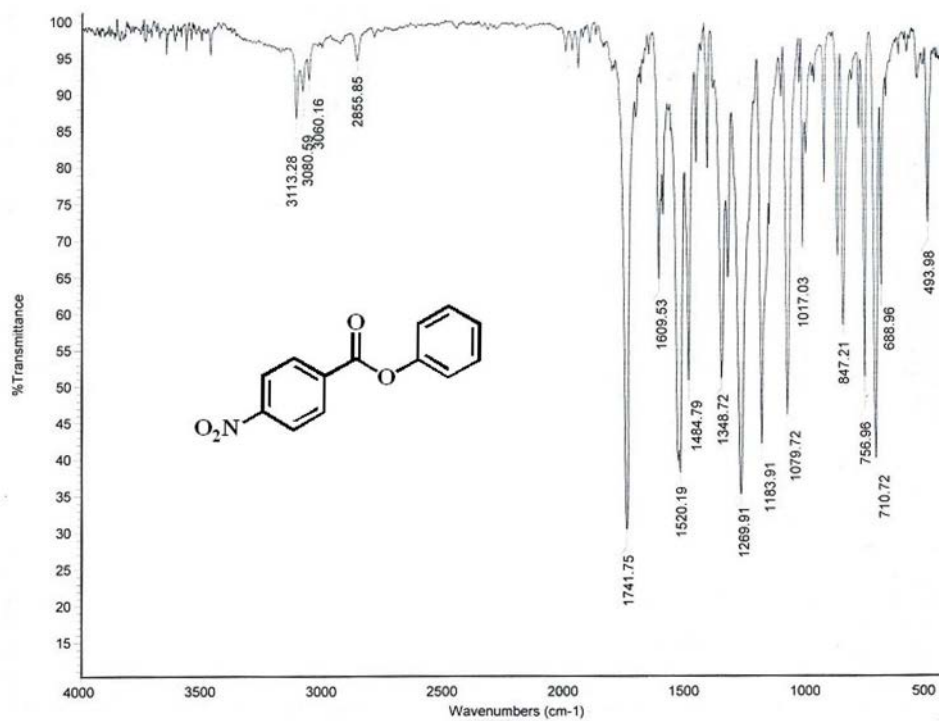


Figure S64. FTIR (KBr) spectrum of phenyl 4-nitrobenzoate (Table 3, entry 26).

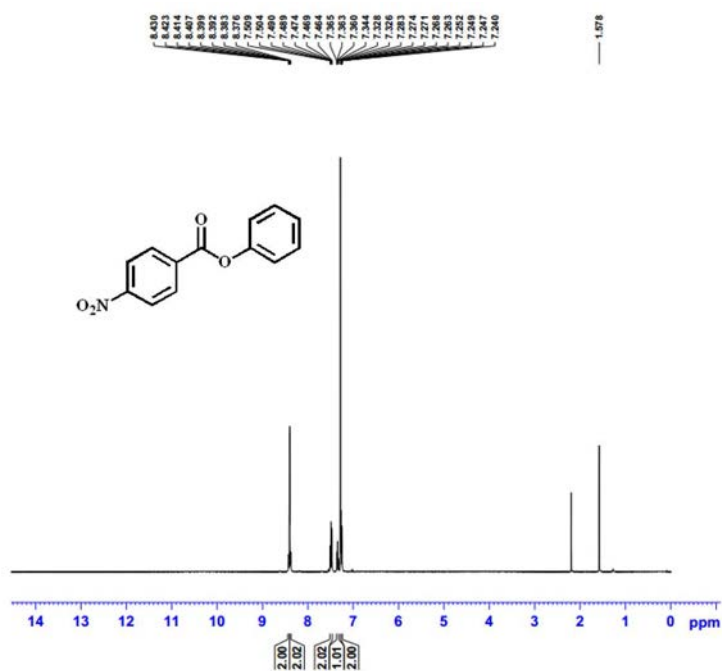


Figure S65. ¹H NMR (400 MHz, CDCl₃) spectrum of phenyl 4-nitrobenzoate (Table 3, entry 26).

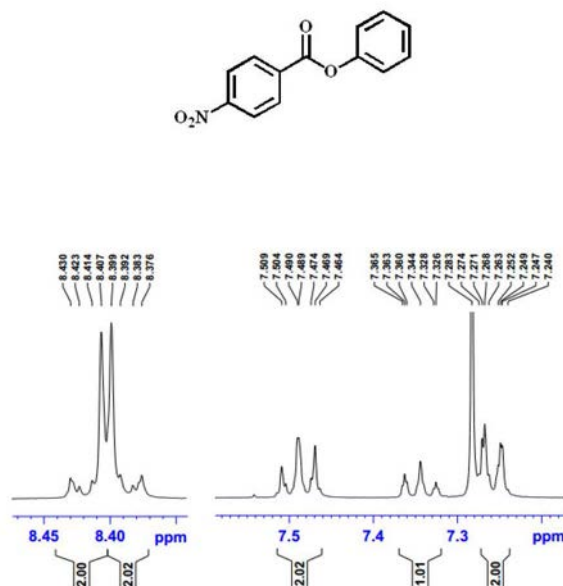


Figure S66. ¹H NMR (400 MHz, CDCl₃) spectrum of phenyl 4-nitrobenzoate (Table 3, entry 26).

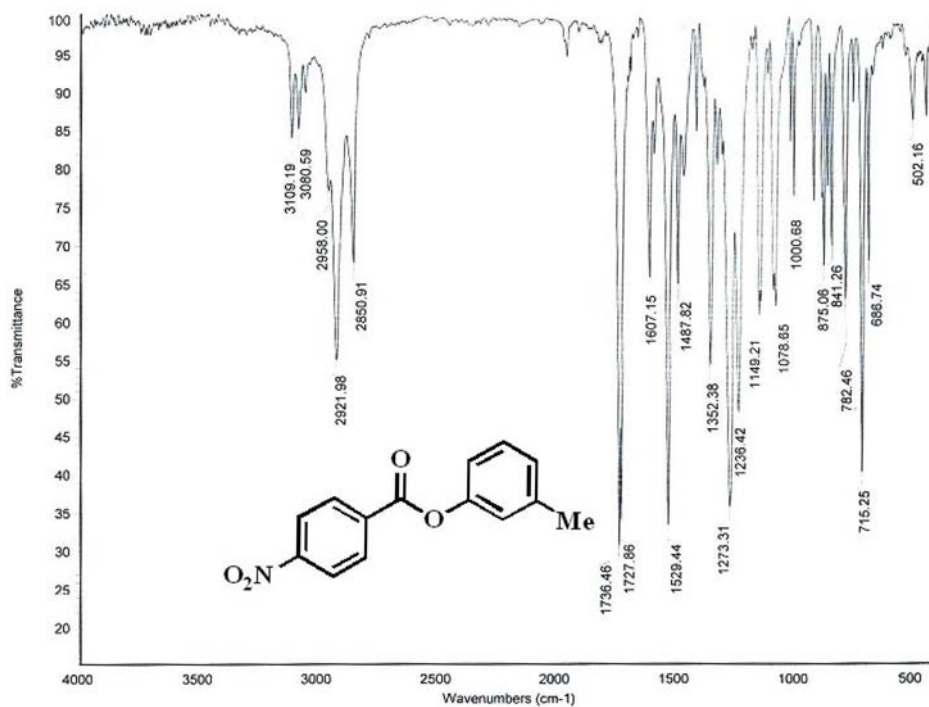


Figure S67. FTIR (KBr) spectrum of *m*-tolyl 4-nitrobenzoate (Table 3, entry 27).

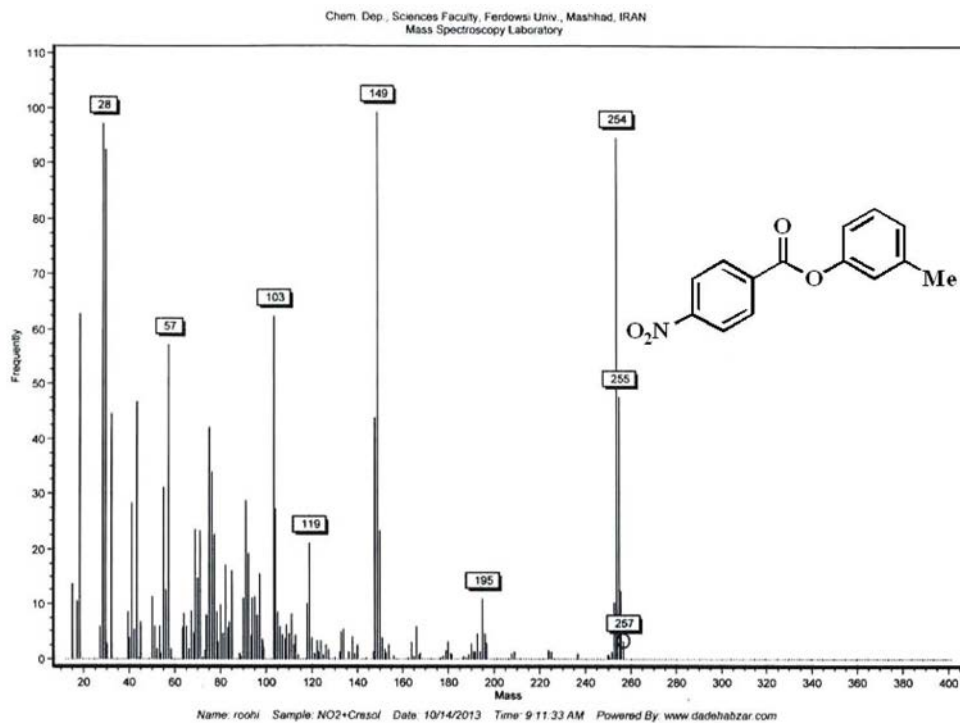


Figure S68. Mass spectrum of *m*-tolyl 4-nitrobenzoate (Table 3, entry 27).

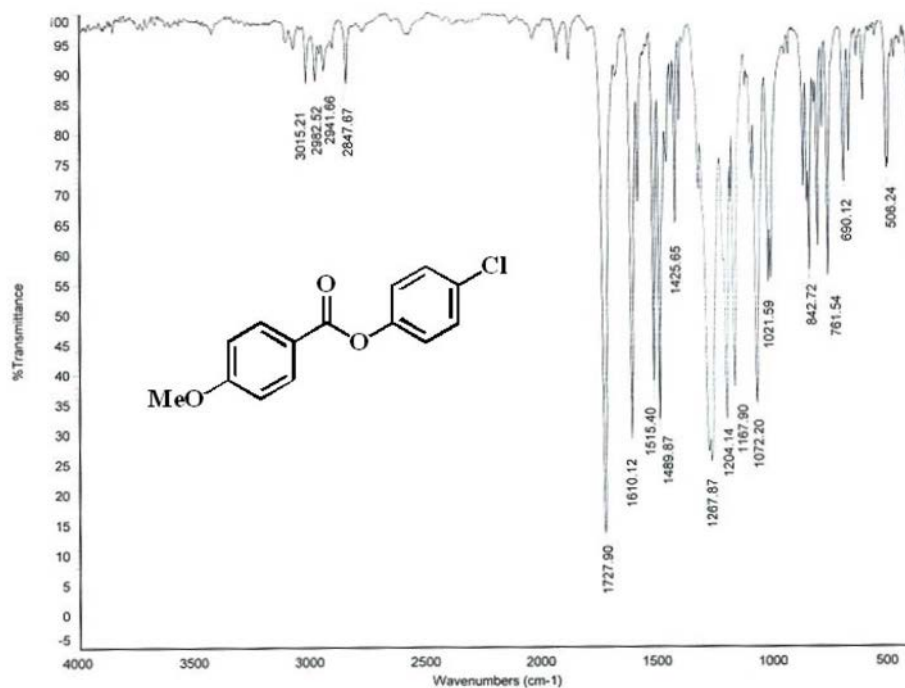


Figure S69. FTIR (KBr) spectrum of 4-chlorophenyl 4-methoxybenzoate (Table 3, entry 28).

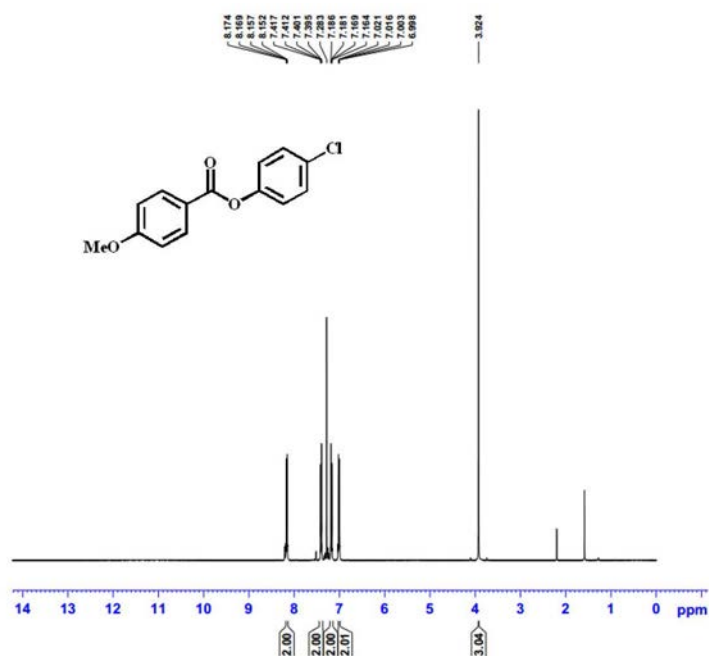


Figure S70. ¹H NMR (400 MHz, CDCl₃) spectrum of 4-chlorophenyl 4-methoxybenzoate (Table 3, entry 28).

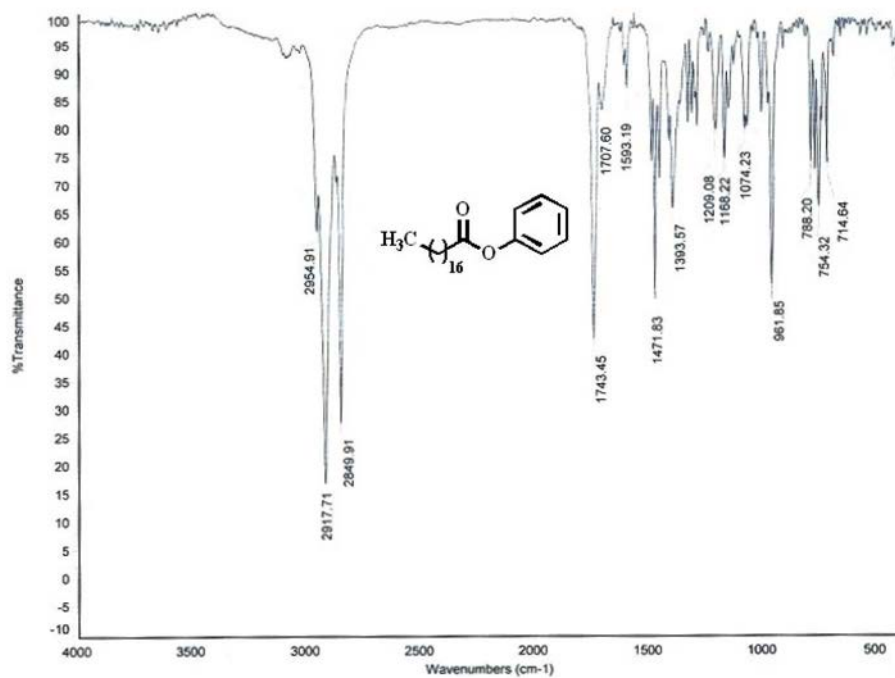


Figure S71. FTIR (KBr) spectrum of phenyl stearate (Table 3, entry 29).

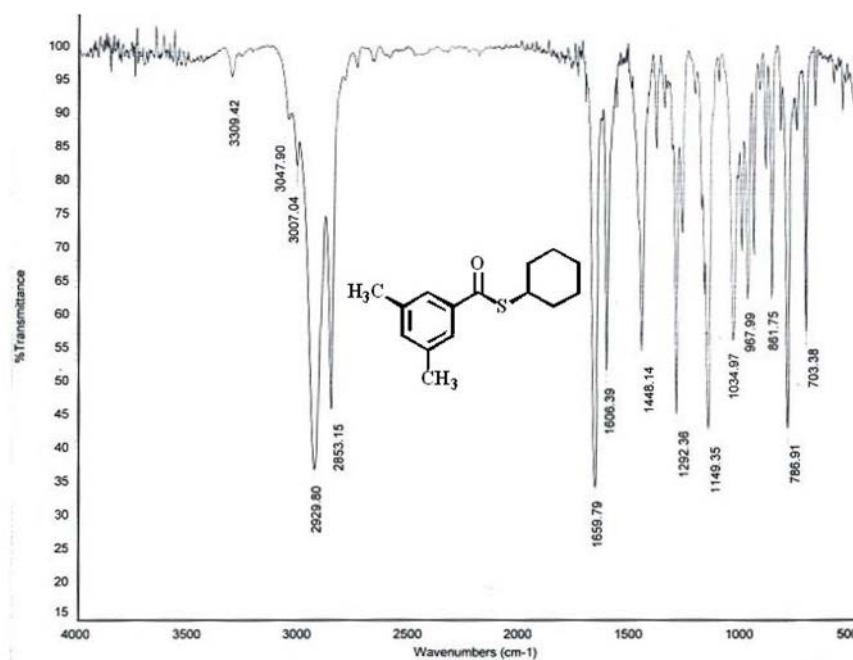


Figure S72. FTIR (KBr) spectrum of *S*-cyclohexyl 3,5-dimethylbenzothioate (Table 3, entry 30).

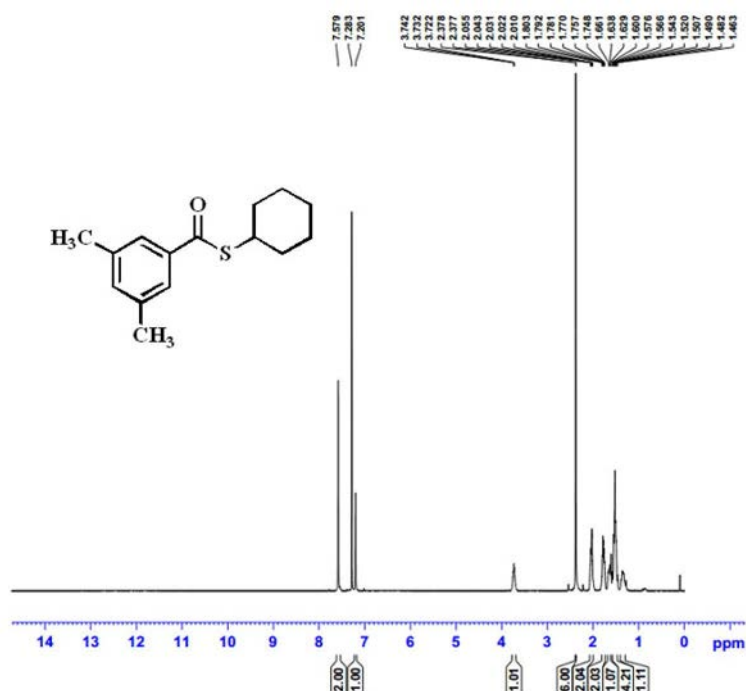


Figure S73. ¹H NMR (400 MHz, CDCl₃) spectrum of *S*-cyclohexyl 3,5-dimethylbenzothioate (Table 3, entry 30).

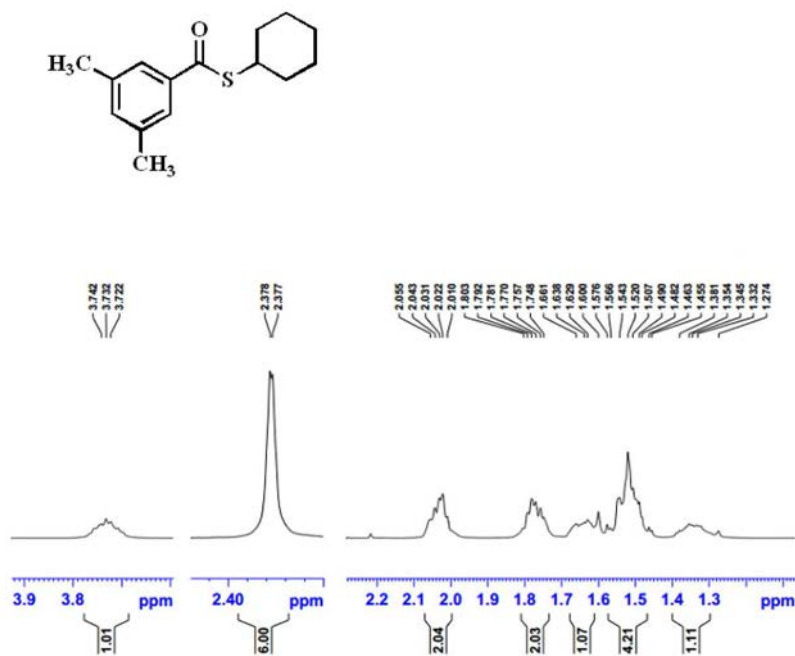


Figure S74. ¹H NMR (400 MHz, CDCl₃) spectrum of *S*-cyclohexyl 3,5-dimethylbenzothioate (Table 3, entry 30).

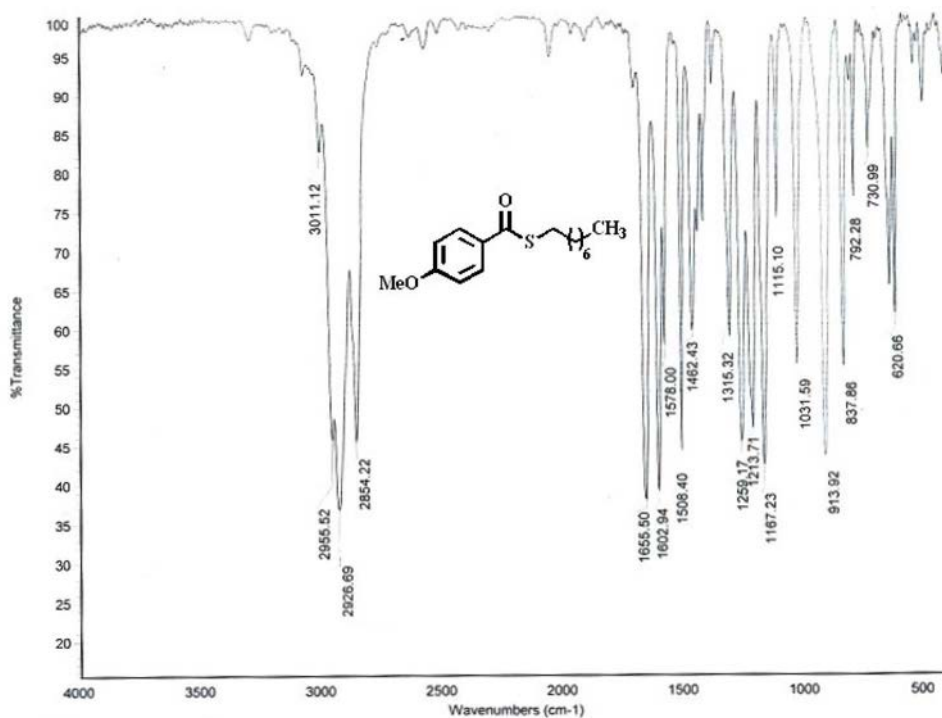


Figure S75. FTIR (neat) spectrum of *S*-octyl 4-methoxybenzothioate (Table 3, entry 31).

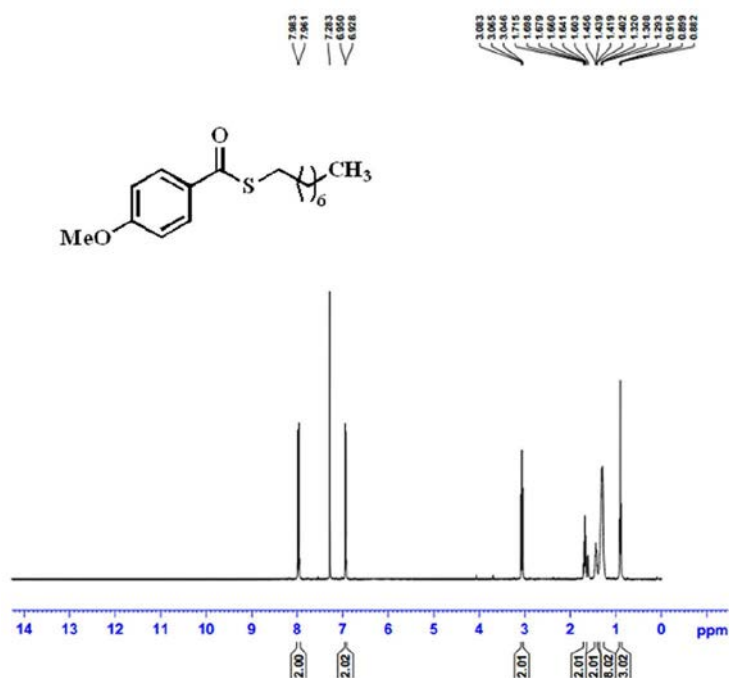


Figure S76. ¹H NMR (400 MHz, CDCl₃) spectrum of *S*-octyl 4-methoxybenzoate (Table 3, entry 31).

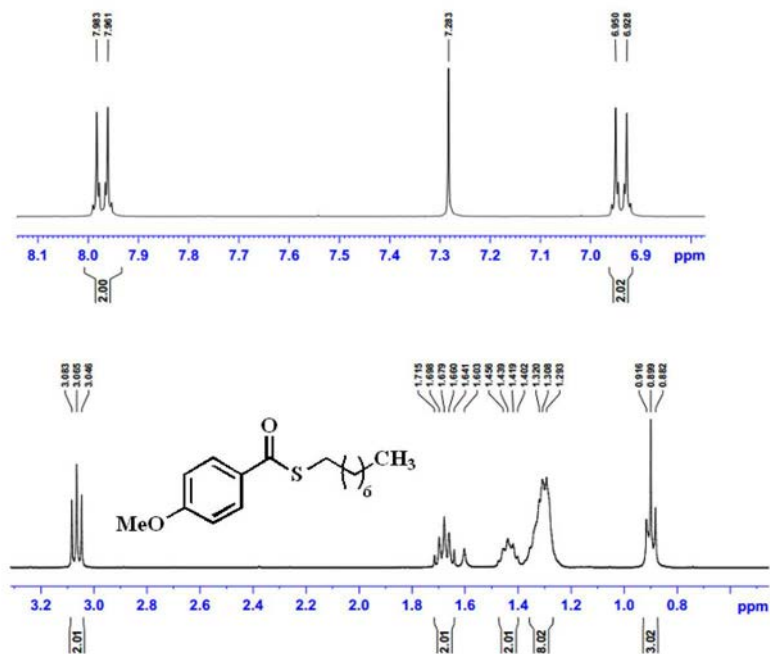


Figure S77. ¹H NMR (400 MHz, CDCl₃) spectrum of *S*-octyl 4-methoxybenzoate (Table 3, entry 31).

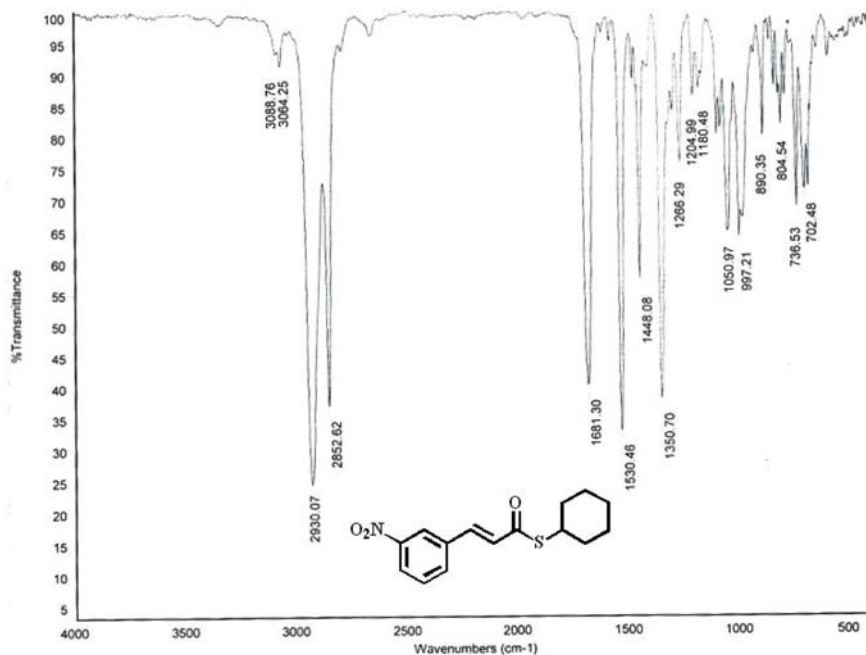


Figure S78. FTIR (KBr) spectrum of (E)-S-cyclohexyl 3-(3-nitrophenyl)prop-2-enoate (Table 3, entry 32).

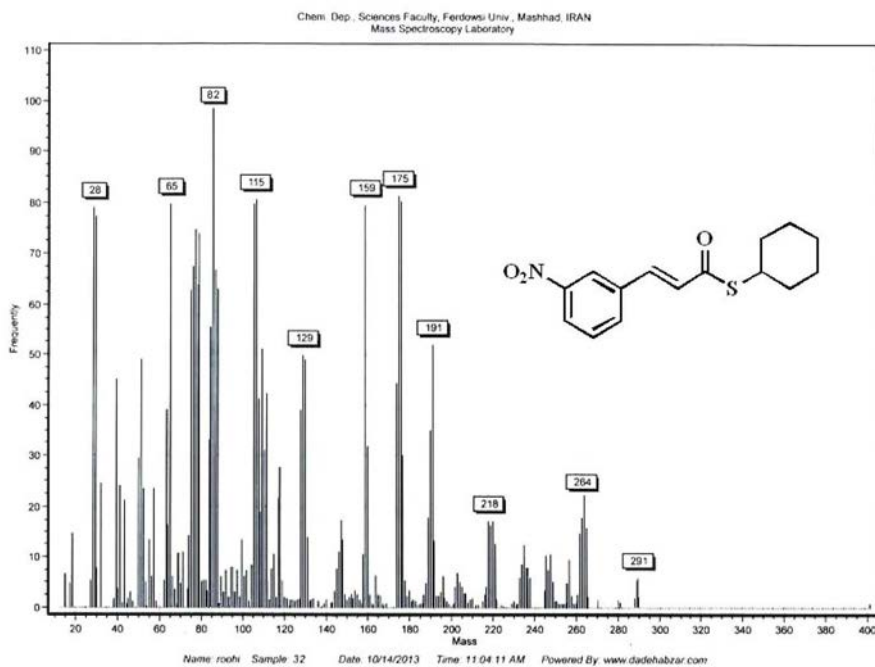


Figure S79. Mass spectrum of (E)-S-cyclohexyl 3-(3-nitrophenyl)prop-2-enoate (Table 3, entry 32)

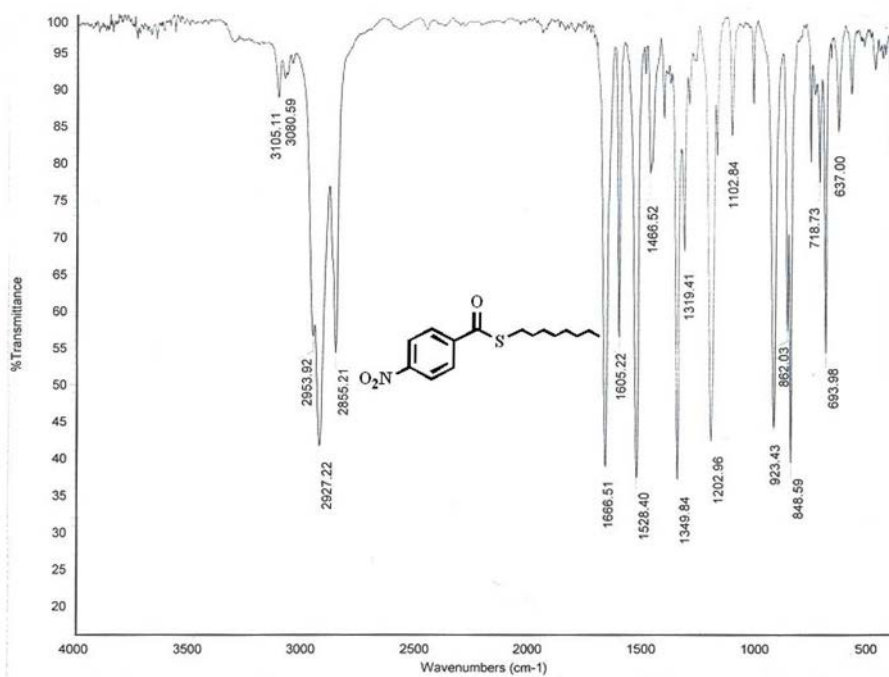


Figure S80. FTIR (neat) spectrum of *S*-octyl 4-nitrobenzothioate (Table 3, entry 33).

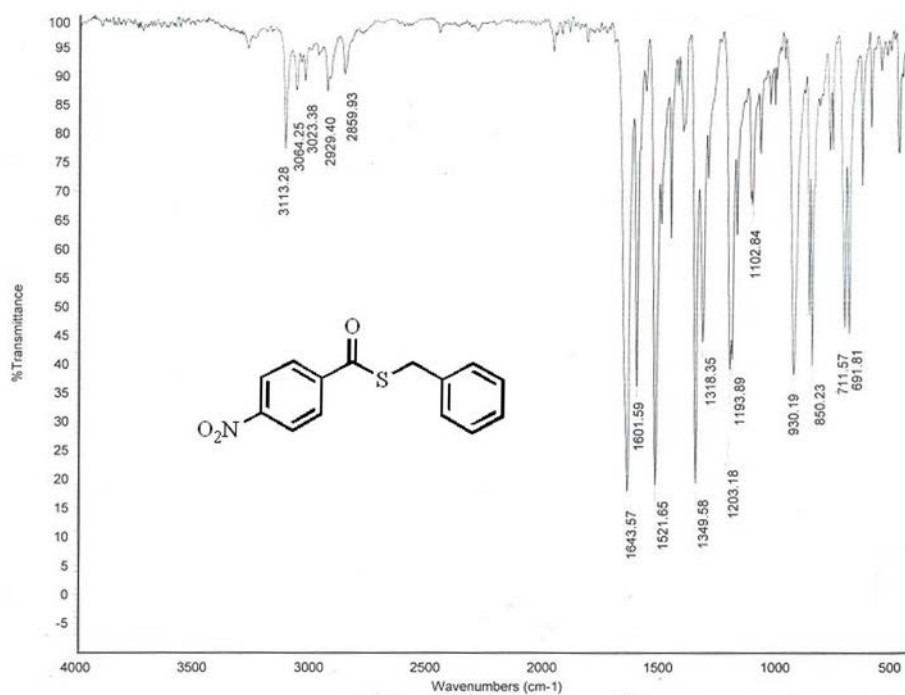


Figure S81. FTIR (KBr) spectrum of *S*-benzyl 4-nitrobenzothioate (Table 3, entry 34).

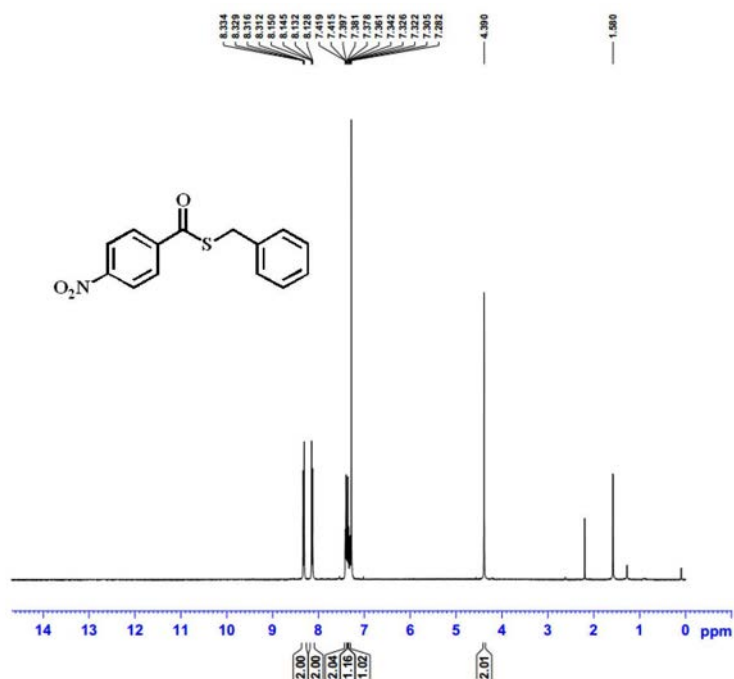


Figure S82. ¹H NMR (400 MHz, CDCl₃) spectrum of 4-nitrobenzothioate (Table 3, entry 34).

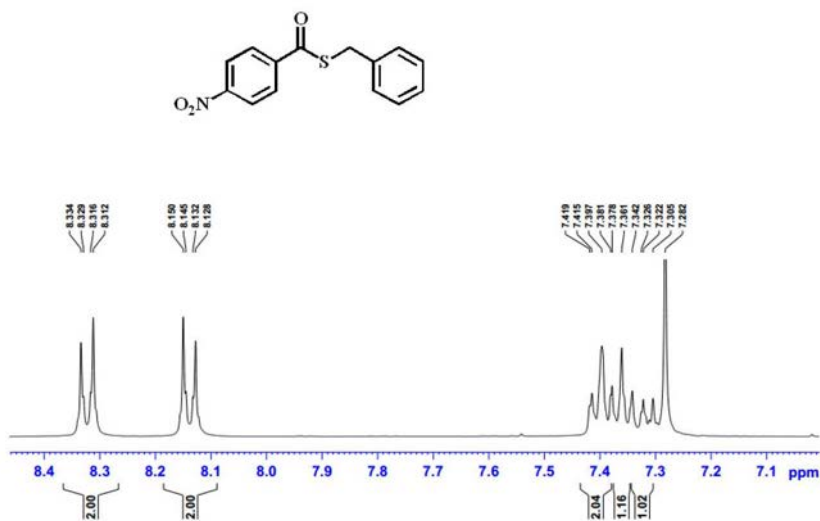


Figure S83. ¹H NMR (400 MHz, CDCl₃) spectrum of 4-nitrobenzothioate (Table 3, entry 34).

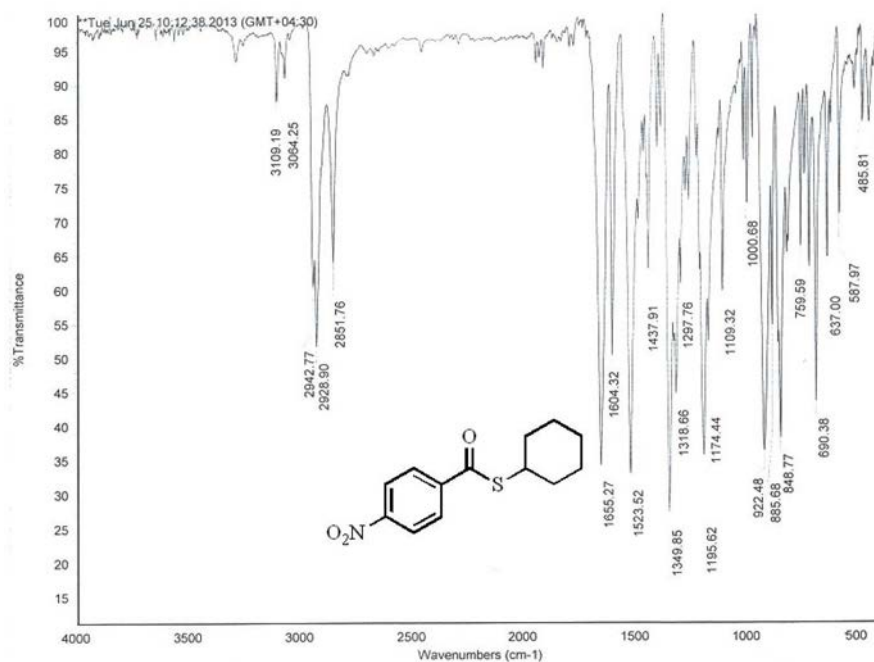


Figure S84. FTIR (KBr) spectrum of *S*-cyclohexyl 4-nitrobenzothioate (Table 3, entry 35).

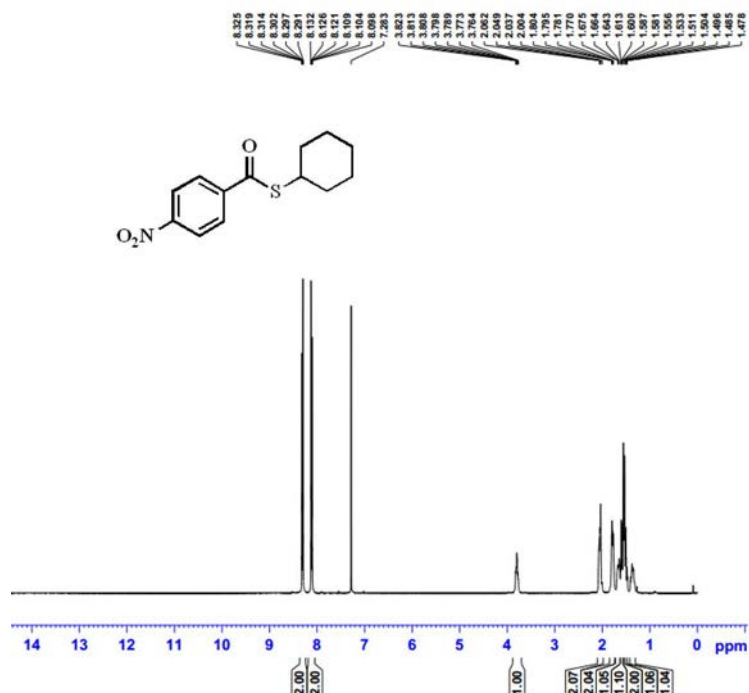


Figure S85. ¹H NMR (400 MHz, CDCl₃) spectrum of *S*-cyclohexyl 4-nitrobenzothioate (Table 3, entry 35).

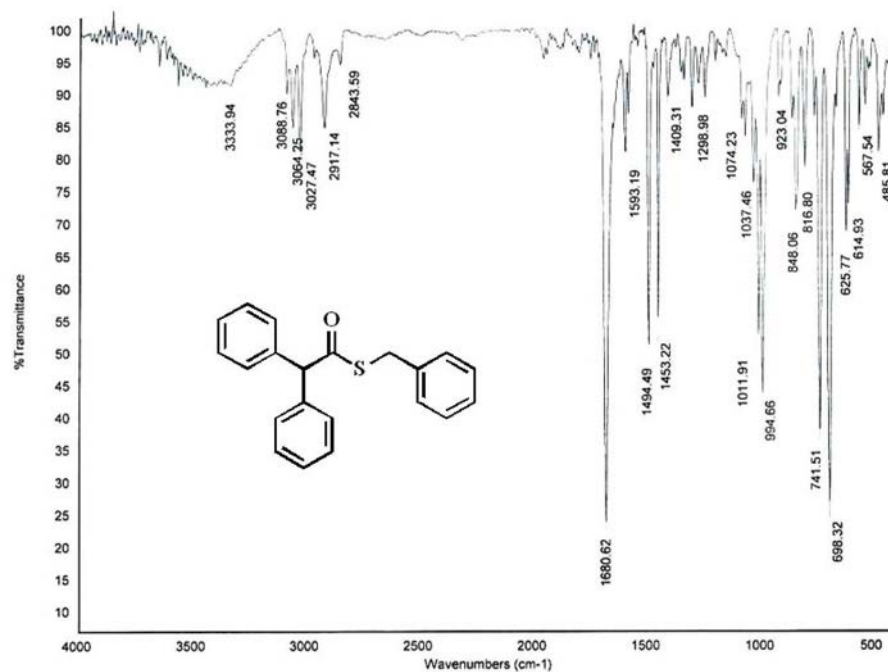


Figure S86. FTIR (KBr) spectrum of *S*-benzyl 2,2-diphenylethanethioate (Table 3, entry 36).

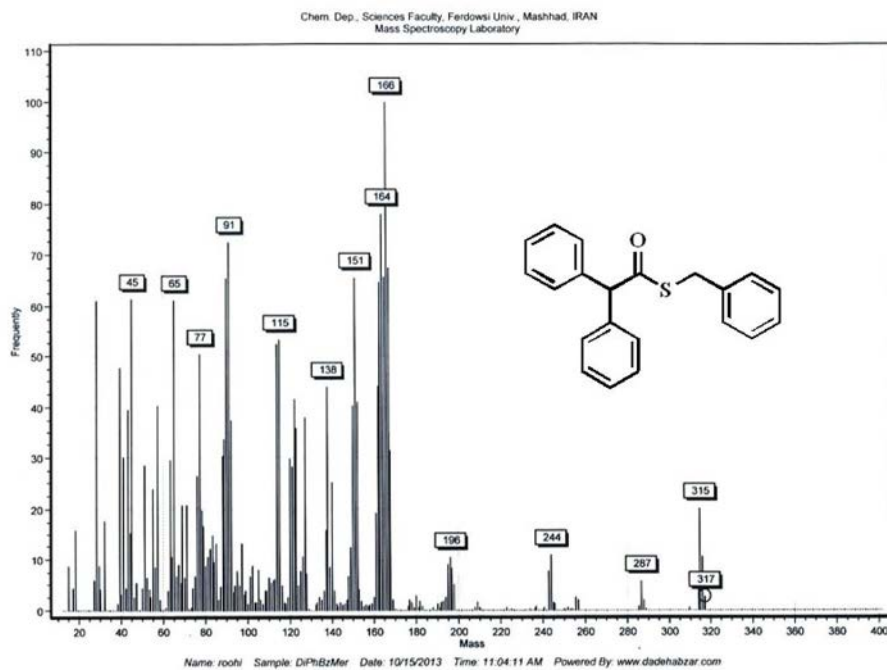


Figure S87. Mass spectrum of *S*-benzyl 2,2-diphenylethanethioate (Table 3, entry 36).

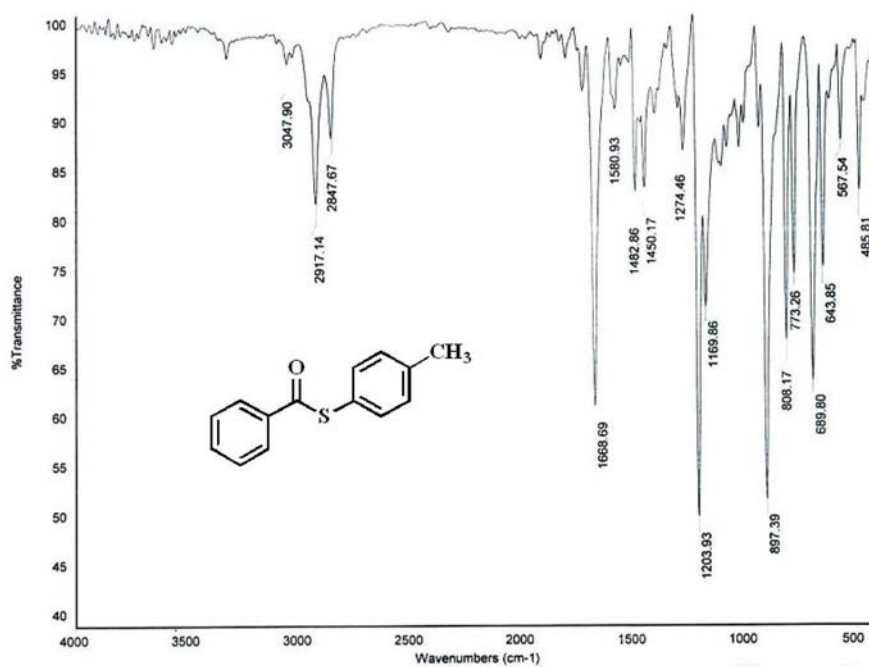


Figure S88. FTIR (KBr) spectrum of *S-p*-tolyl benzothioate (Table 3, entry 37).

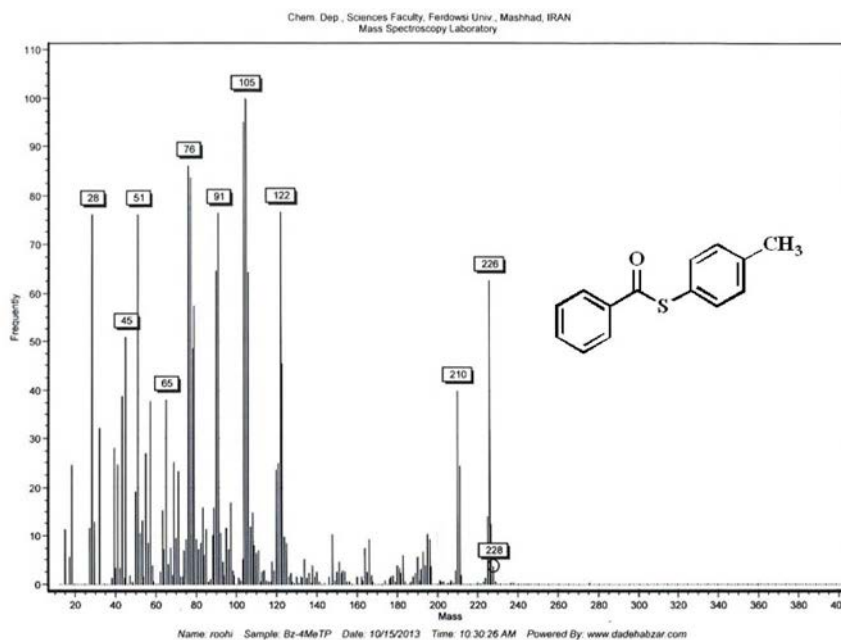


Figure S89. Mass spectrum of *S-p*-tolyl benzothioate (Table 3, entry 37).

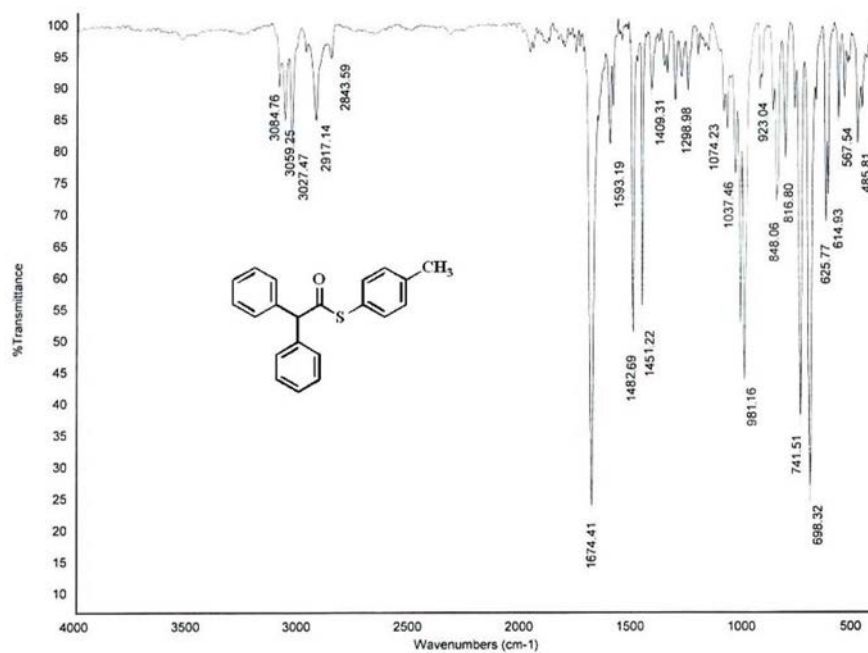


Figure S90. FTIR (KBr) spectrum of *S-p*-tolyl 2,2-diphenylethanethioate (Table 3, entry 38).

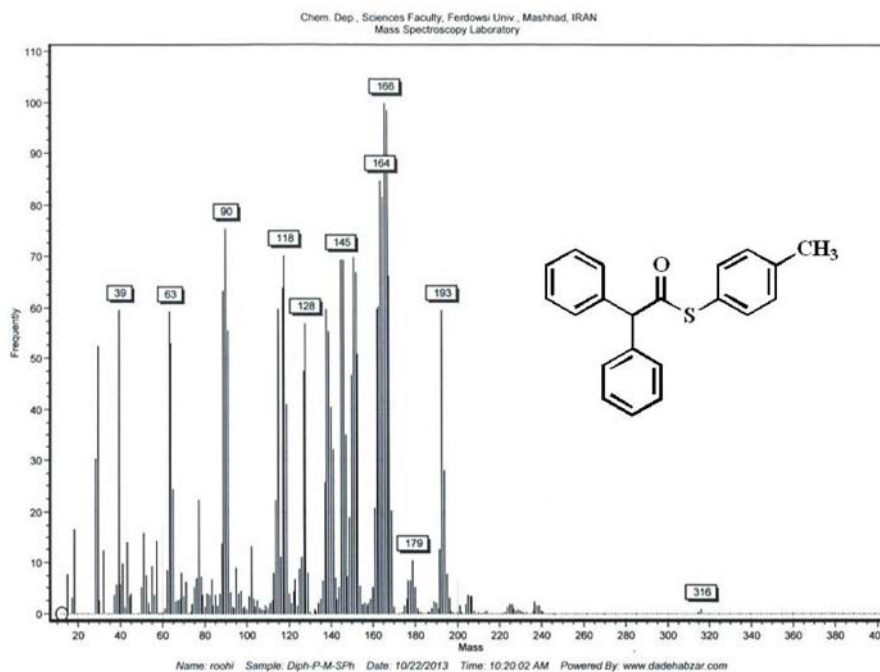


Figure S91. Mass spectrum of *S-p*-tolyl 2,2-diphenylethanethioate (Table 3, entry 38).