

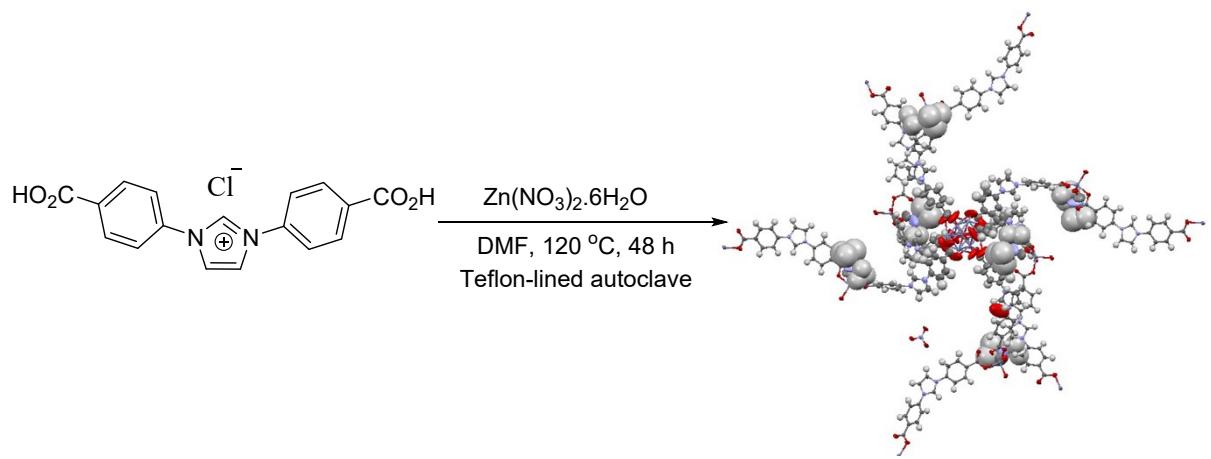
Supporting information

MOF-Zn-NHC as an efficient *N*-heterocyclic carbene catalyst for aerobic oxidation of aldehydes to their corresponding carboxylic acids *via* a cooperative geminal anomeric based oxidation

Saeed babae, Mahmoud Zarei,* Mohammad Ali Zolfigol*

Department of Organic Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan 6517838683, Tel: +988138282807, Fax: +988138380709 Iran. E-Mail: zolfi@basu.ac.ir & mzolfigol@yahoo.com, (M. A. Zolfigol) or mahmoud8103@yahoo.com (M. Zarei).
[Saeed.babai@yahoo.com.](mailto:Saeed.babai@yahoo.com)

Scheme S1: Preparation of MOF-Zn-NHC as <i>N</i> -Heterocyclic carbene.....	3
Figure S1: XRD diagram for the MOF-Zn-NHC (Blue line) in compare with MOF-Zn-NHC (Red line)	3
FT-IR spectrum of 4-methylbenzoic acid.....	4
¹ H NMR spectrum of 4-methylbenzoic acid	5
¹³ C NMR spectrum of 4-methylbenzoic acid	5
FT-IR spectrum of 4-methoxybenzoic acid	5
¹ H NMR spectrum of 4-methoxybenzoic acid.....	6
¹³ C NMR spectrum of 4-methoxybenzoic acid	6
FT-IR spectrum of 3-methylbenzoic acid.....	7
¹ H NMR spectrum of 3-methylbenzoic acid	7
FT-IR spectrum of 4-chlorobenzoic acid.....	8
¹ H NMR spectrum of 4-chlorobenzoic acid	8
¹³ C NMR spectrum of 4-chlorobenzoic acid	9
FT-IR spectrum of cinnamic acid	9
¹ H NMR spectrum of cinnamic acid.....	10
FT-IR spectrum of 2-chlorobenzoic acid.....	10
¹ H NMR spectrum of 2-chlorobenzoic acid	11
FT-IR spectrum of 4-fluorobenzoic acid	11
¹ H NMR spectrum of 4-fluorobenzoic acid	12
¹ H NMR spectrum of 4-nitrobenzoic acid	12
¹ H NMR spectrum of 4-nitrobenzoic acid	13
¹³ C NMR spectrum of 4-nitrobenzoic acid	13
FT-IR spectrum of 4-hydroxybenzoic acid.....	14
¹ H NMR spectrum of 4-hydroxybenzoic acid	14
¹³ C NMR spectrum of 4-hydroxybenzoic acid	15
FT-IR spectrum of Isophthalic acid.....	15
¹ H NMR spectrum of Isophthalic acid.....	16



Scheme S1: Preparation of MOF-Zn-NHC as *N*-Heterocyclic carbene

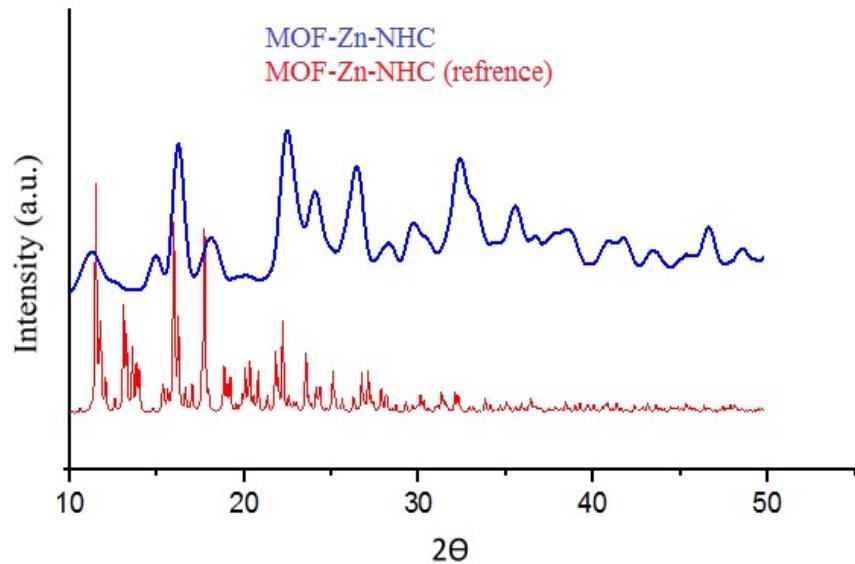
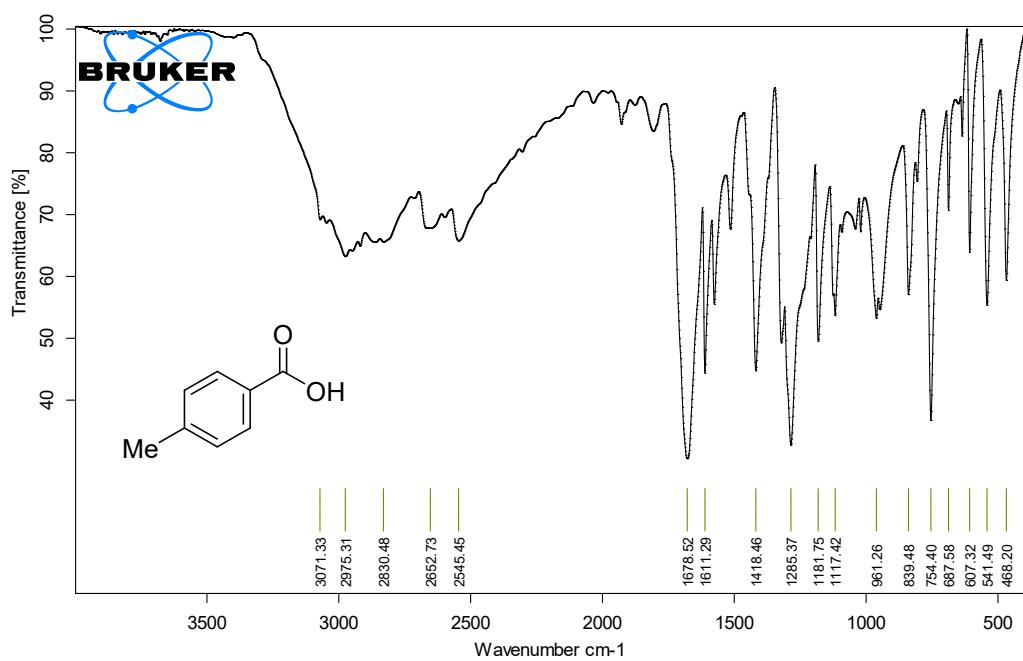
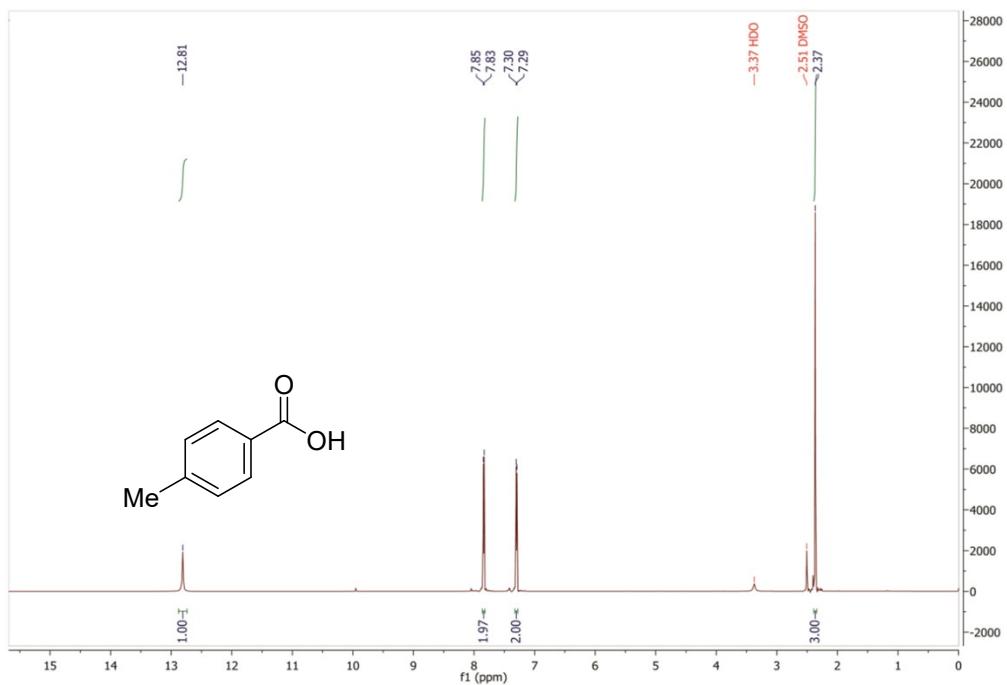


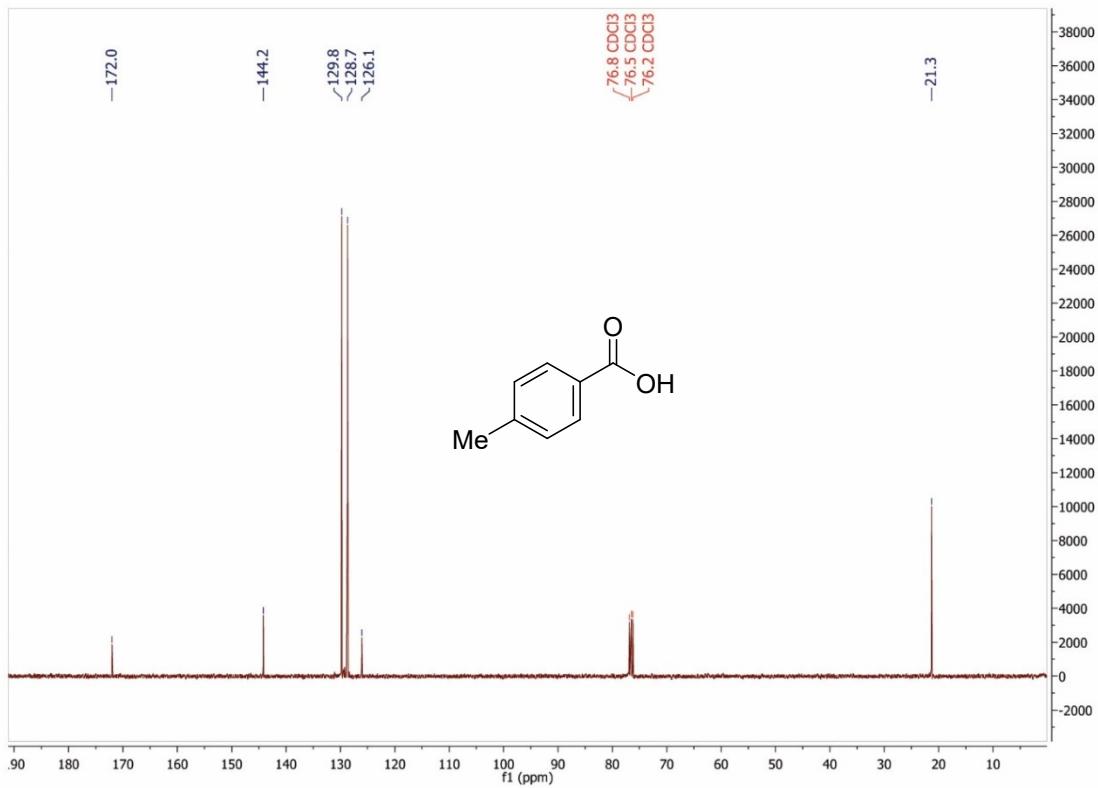
Figure S1: XRD diagram for the MOF-Zn-NHC (Blue line) in compare with MOF-Zn-NHC (Red line)



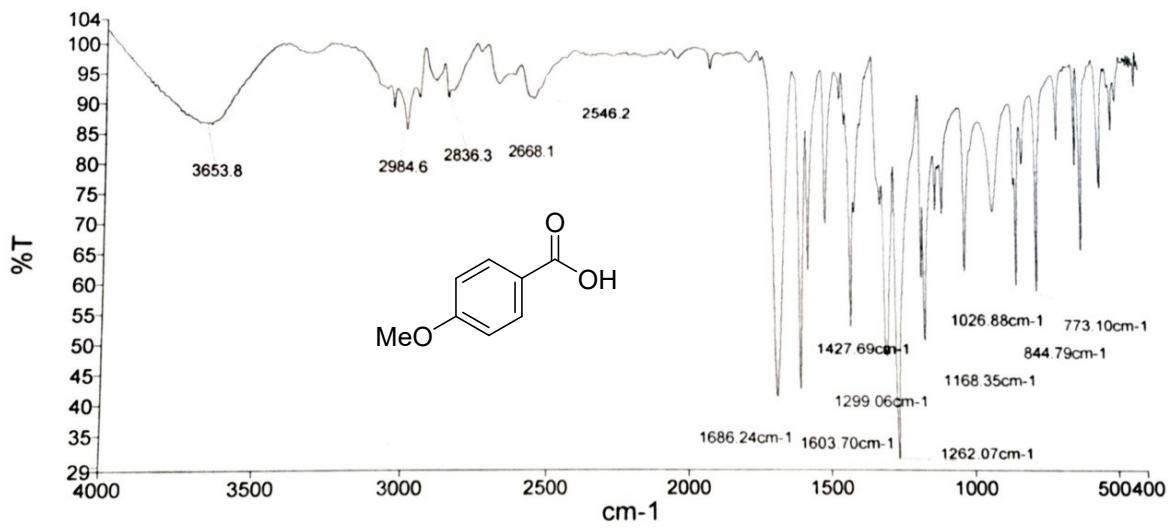
FT-IR spectrum of 4-methylbenzoic acid



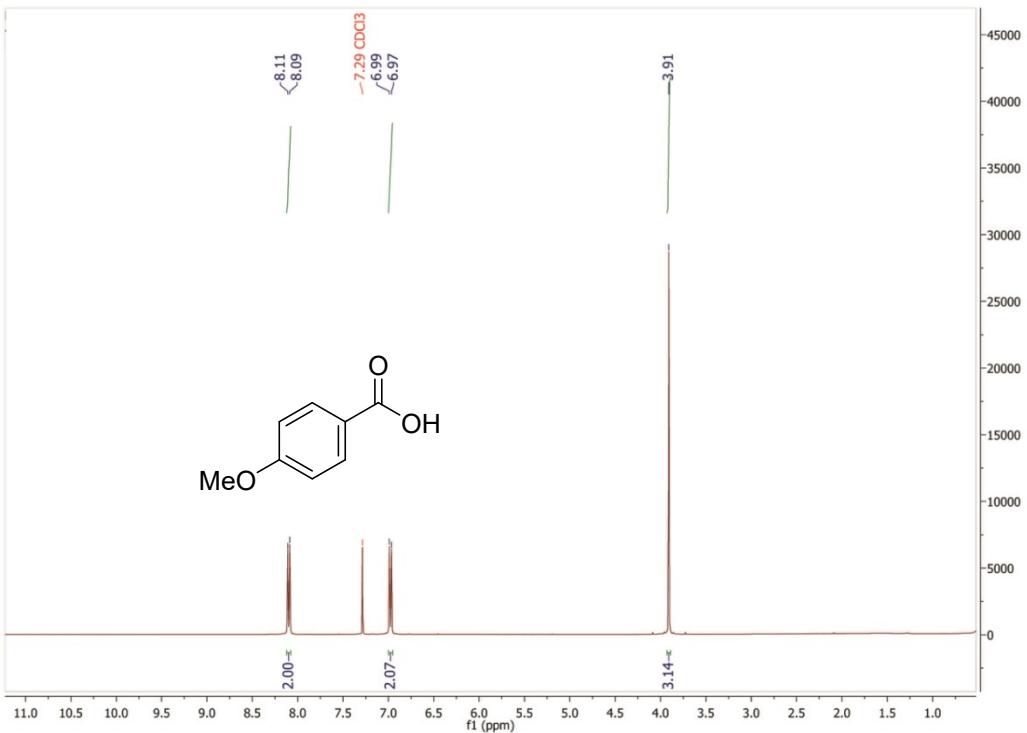
^1H NMR spectrum of 4-methylbenzoic acid



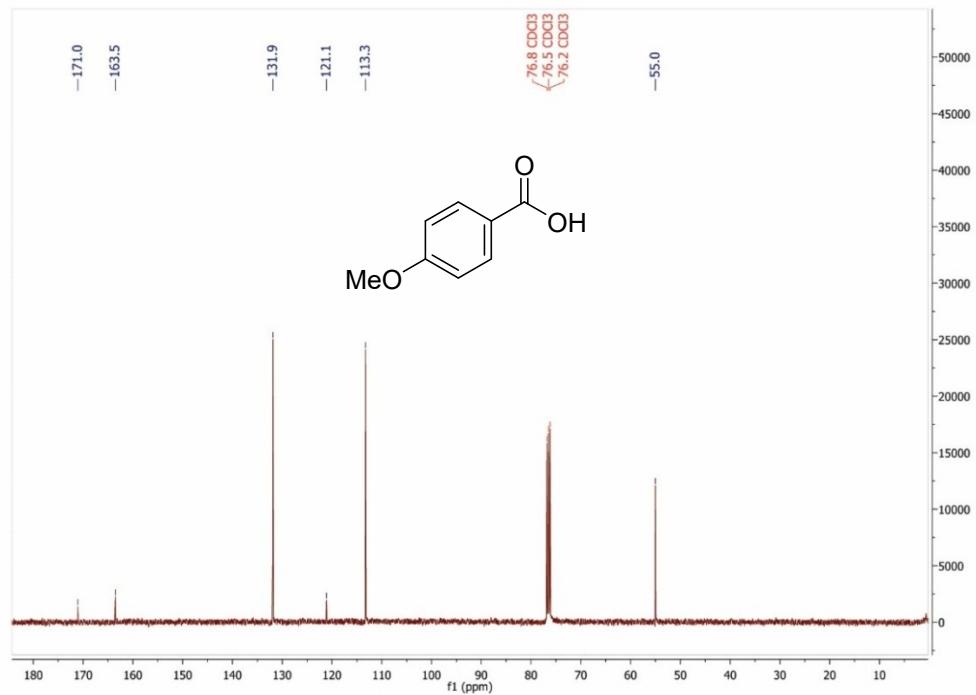
^{13}C NMR spectrum of 4-methylbenzoic acid



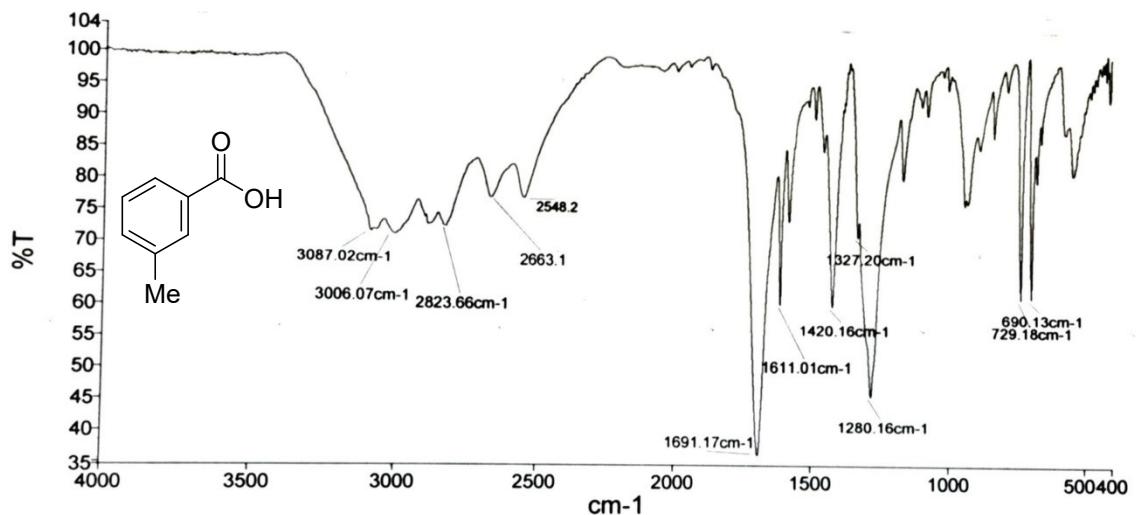
FT-IR spectrum of 4-methoxybenzoic acid



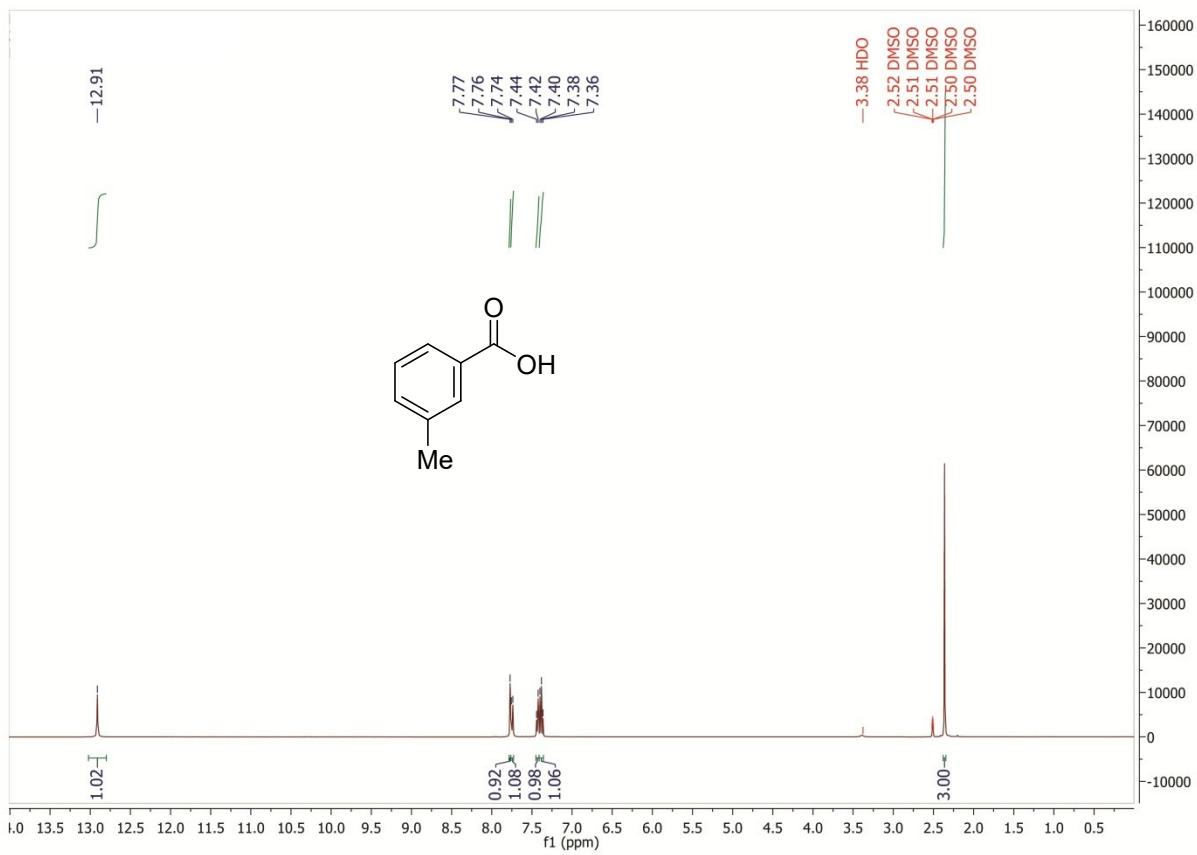
¹H NMR spectrum of 4-methoxybenzoic acid



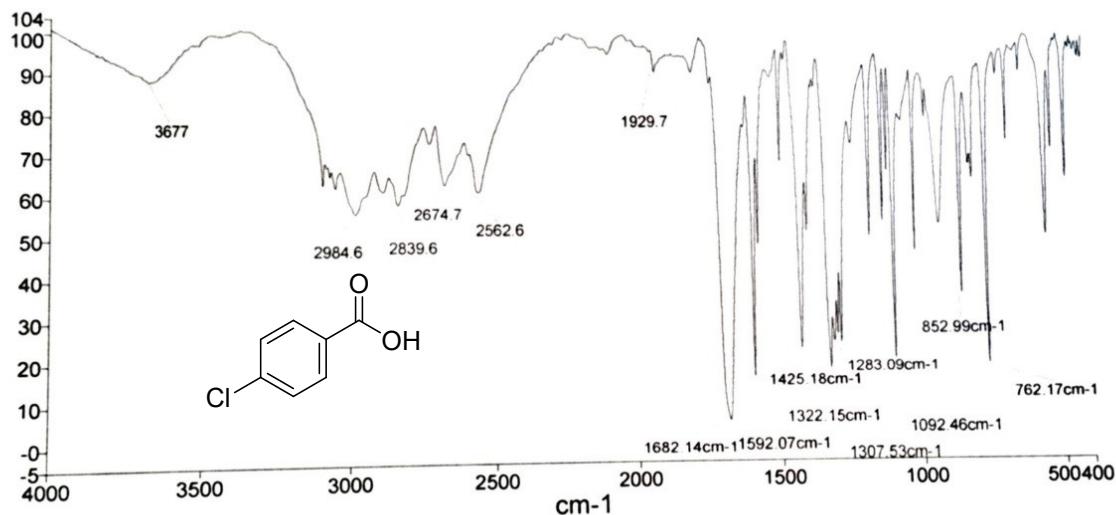
¹³C NMR spectrum of 4-methoxybenzoic acid



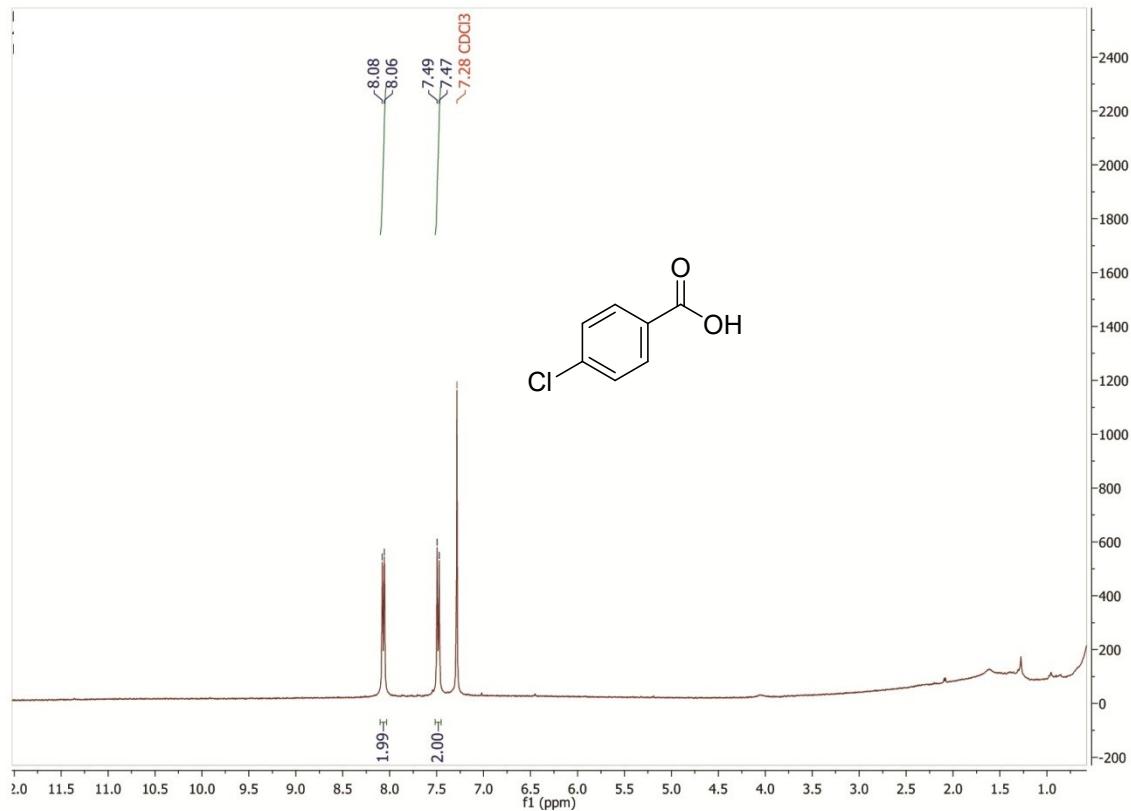
FT-IR spectrum of 3-methylbenzoic acid



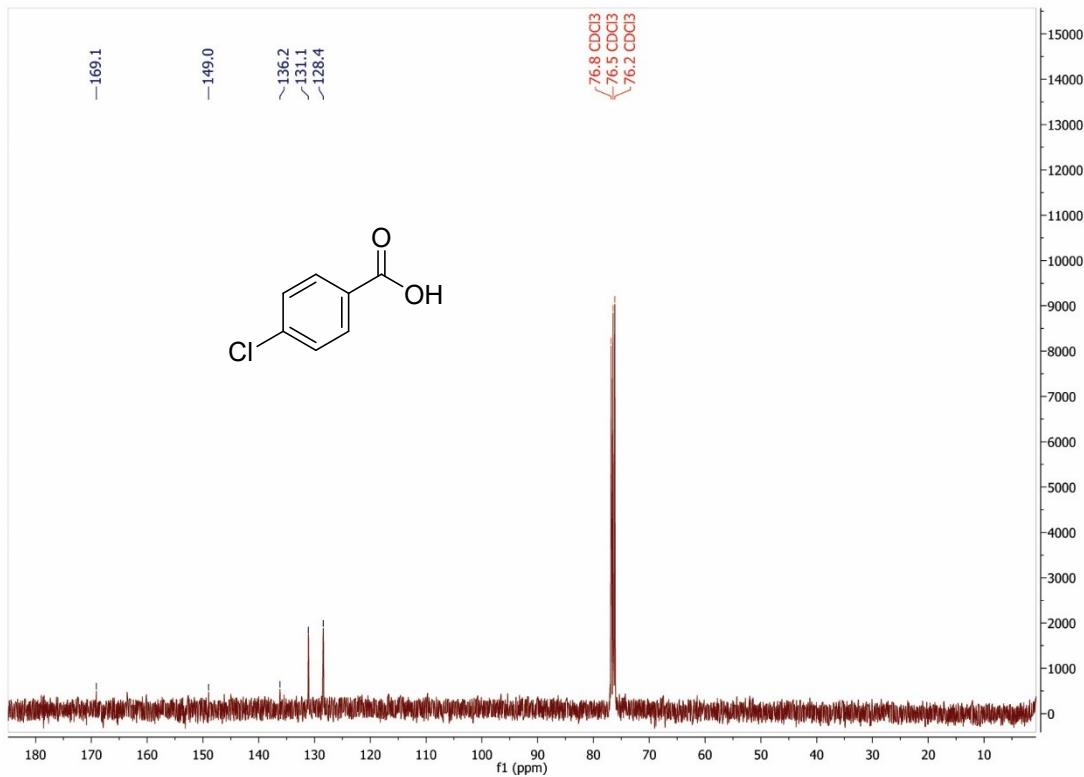
¹H NMR spectrum of 3-methylbenzoic acid



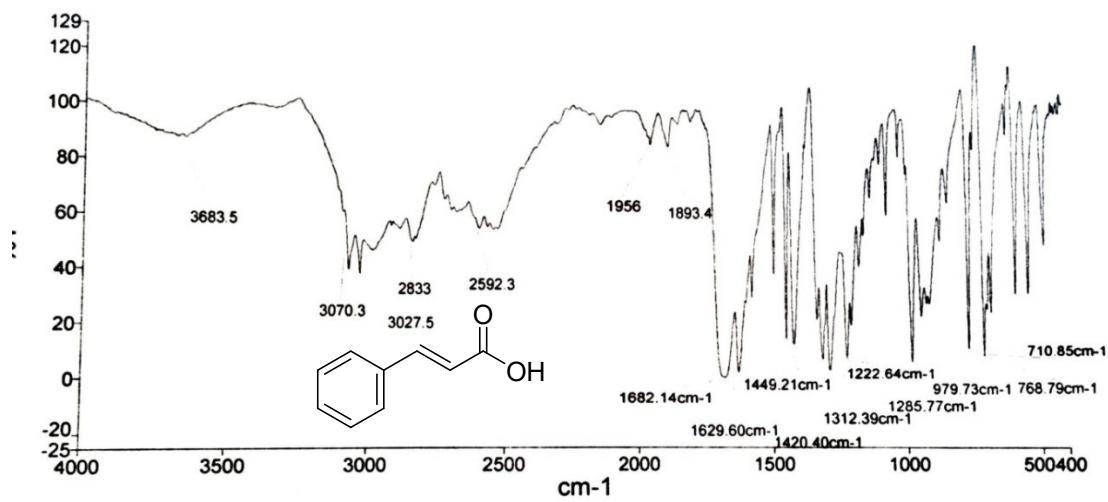
FT-IR spectrum of 4-chlorobenzoic acid



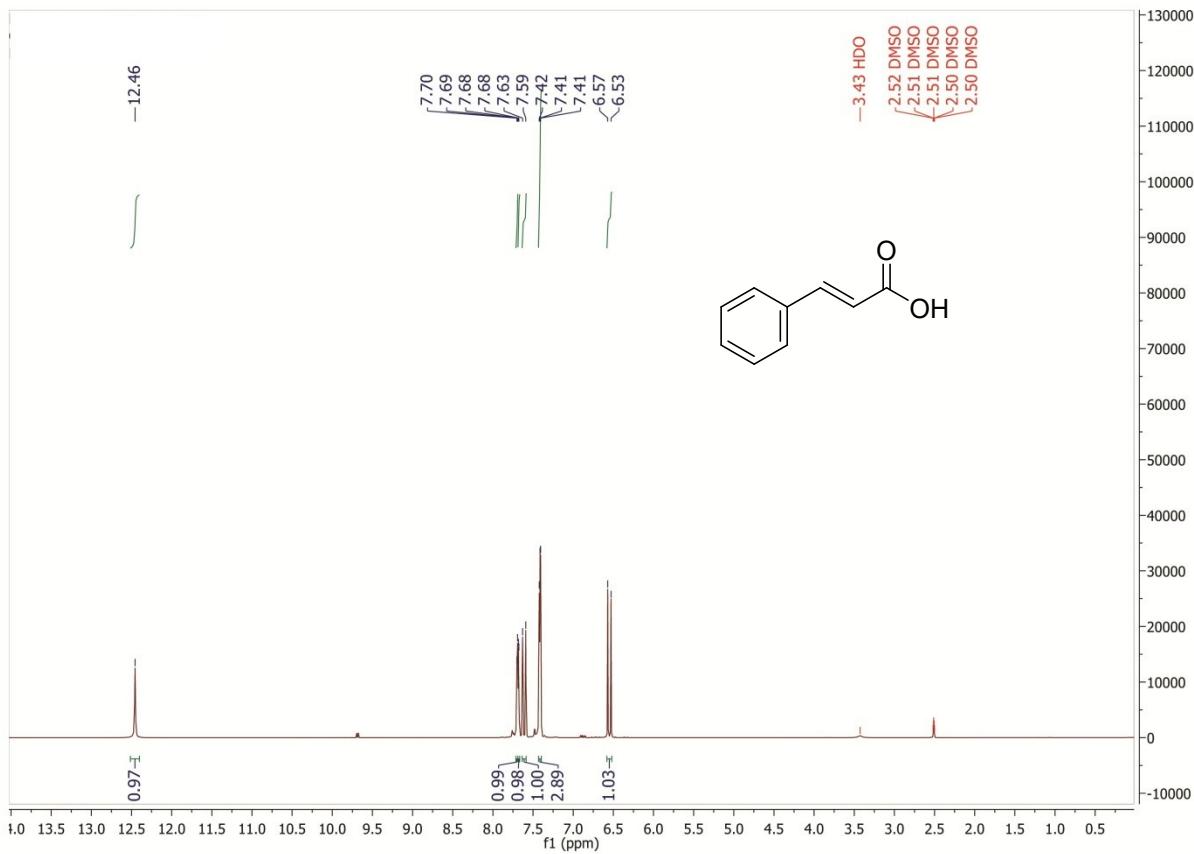
¹H NMR spectrum of 4-chlorobenzoic acid



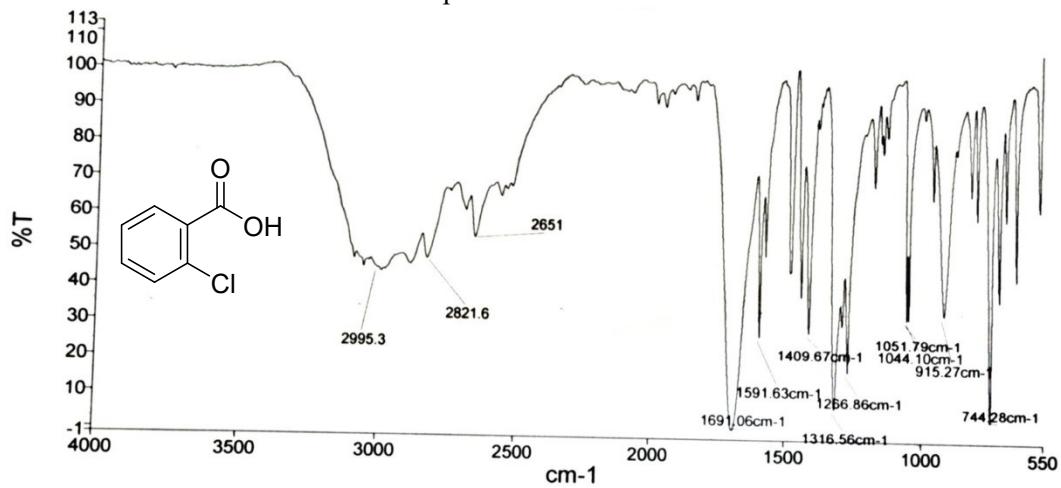
^{13}C NMR spectrum of 4-chlorobenzoic acid



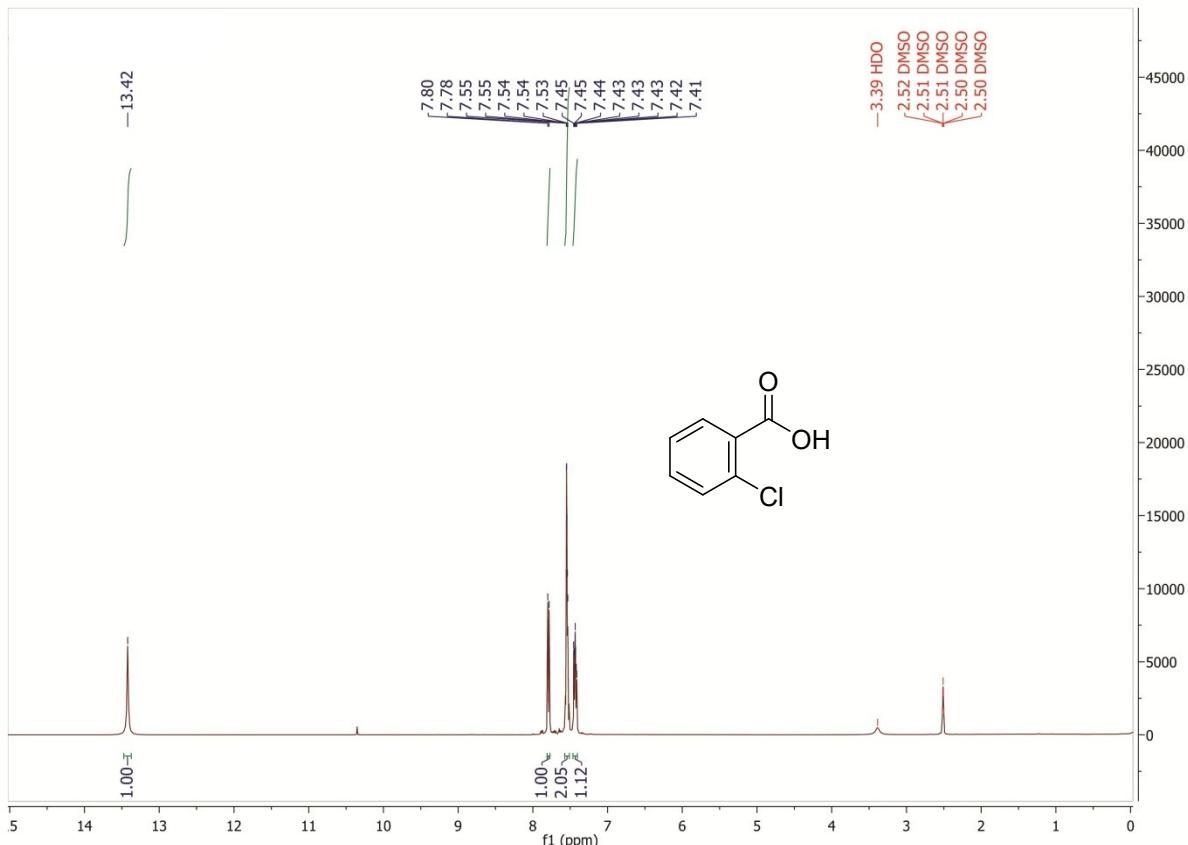
FT-IR spectrum of cinnamic acid



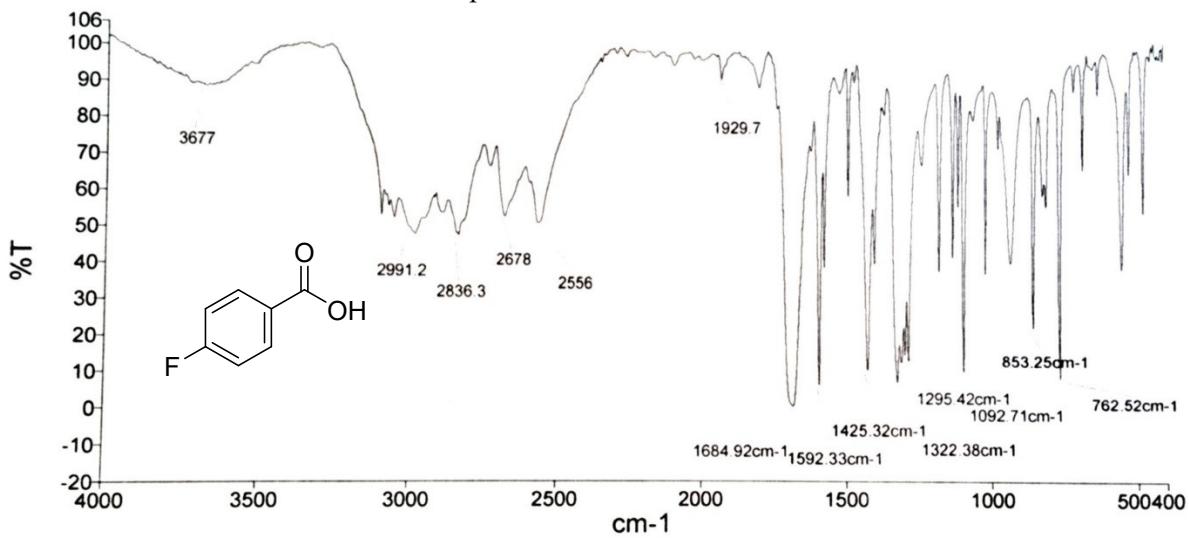
¹H NMR spectrum of cinnamic acid



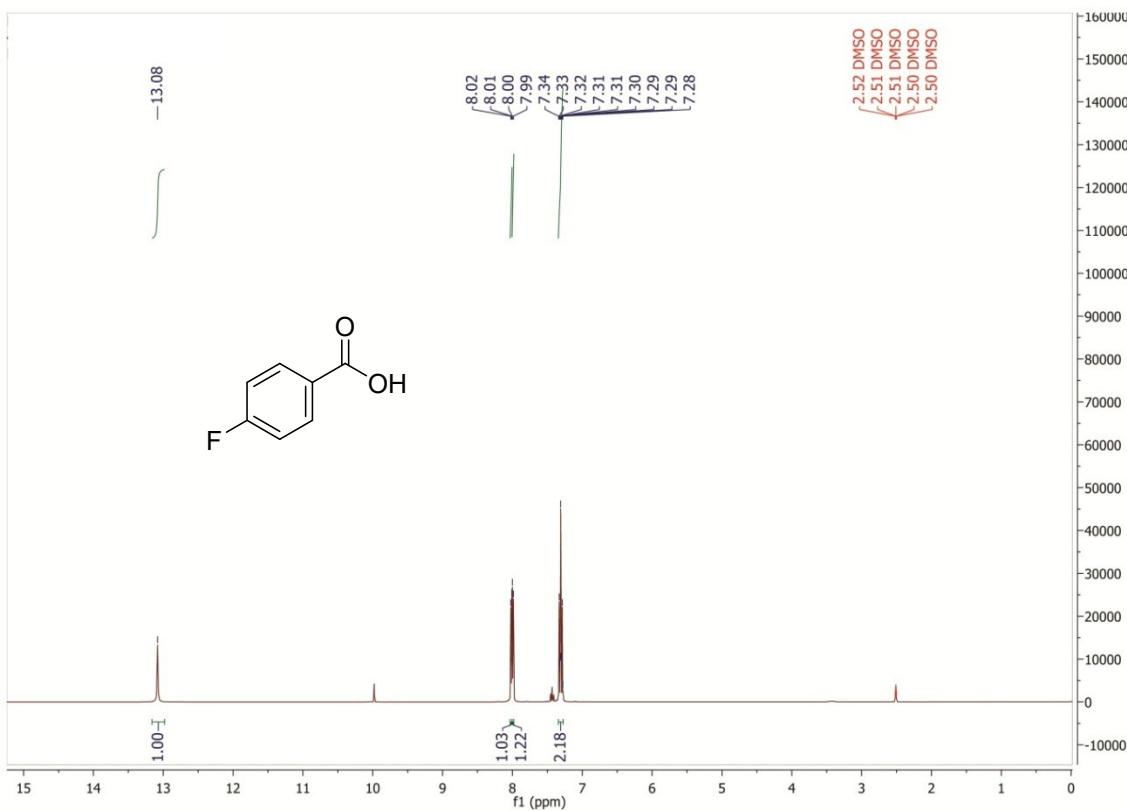
FT-IR spectrum of 2-chlorobenzoic acid



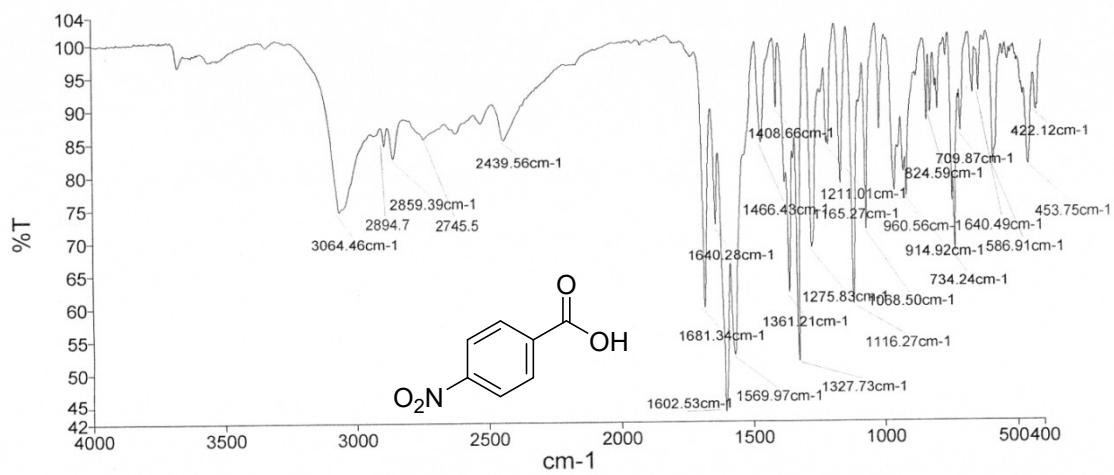
¹H NMR spectrum of 2-chlorobenzoic acid



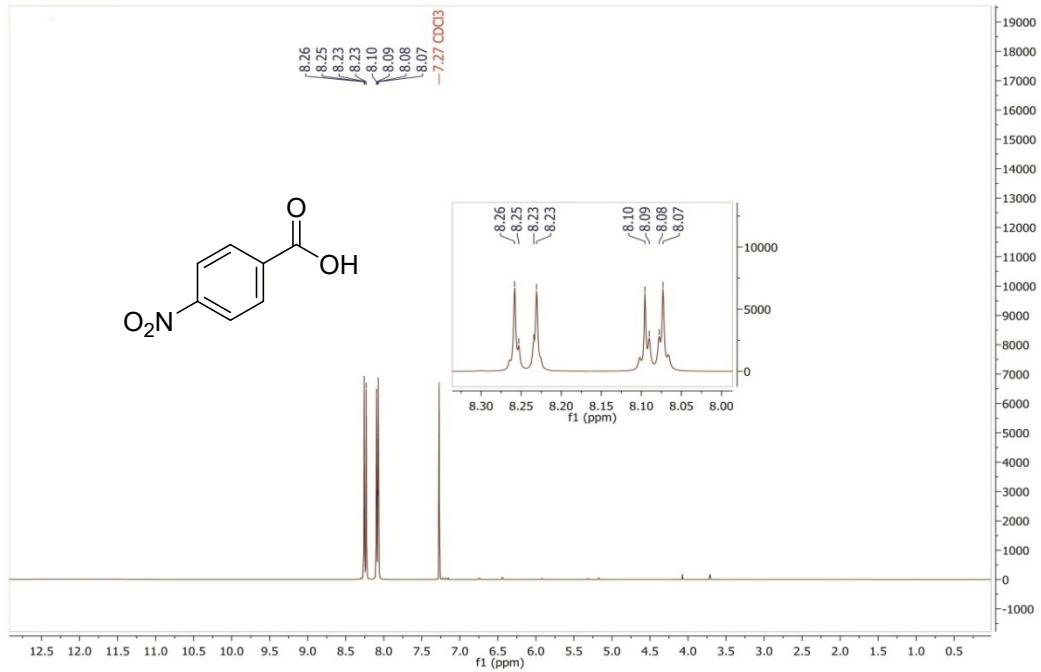
FT-IR spectrum of 4-fluorobenzoic acid



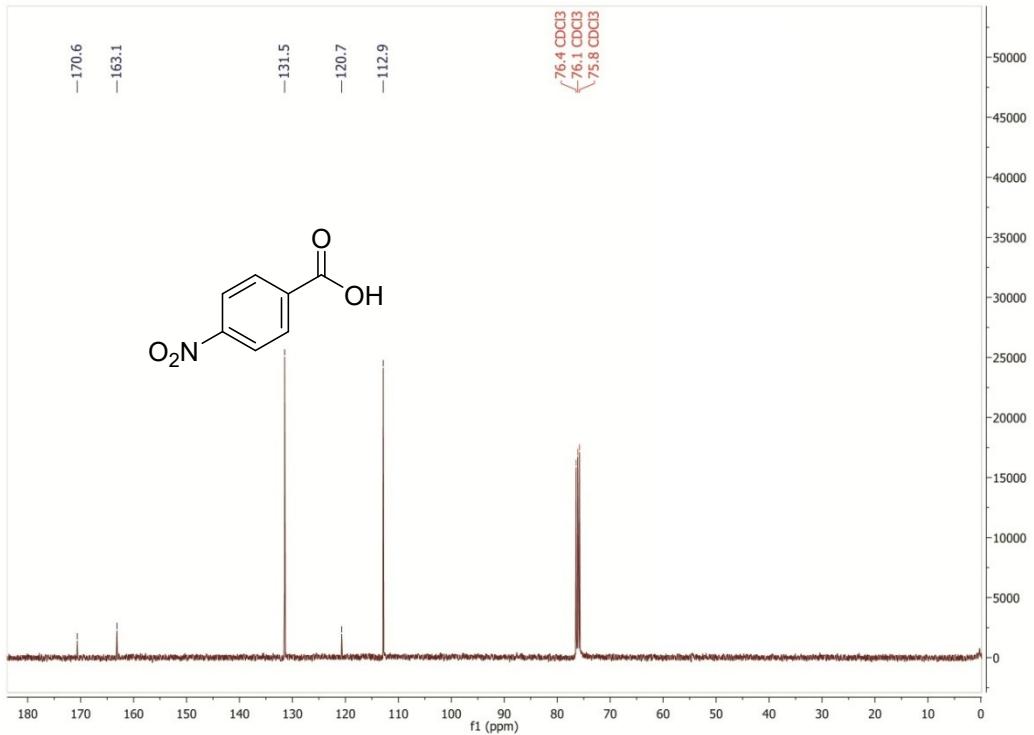
¹H NMR spectrum of 4-fluorobenzoic acid



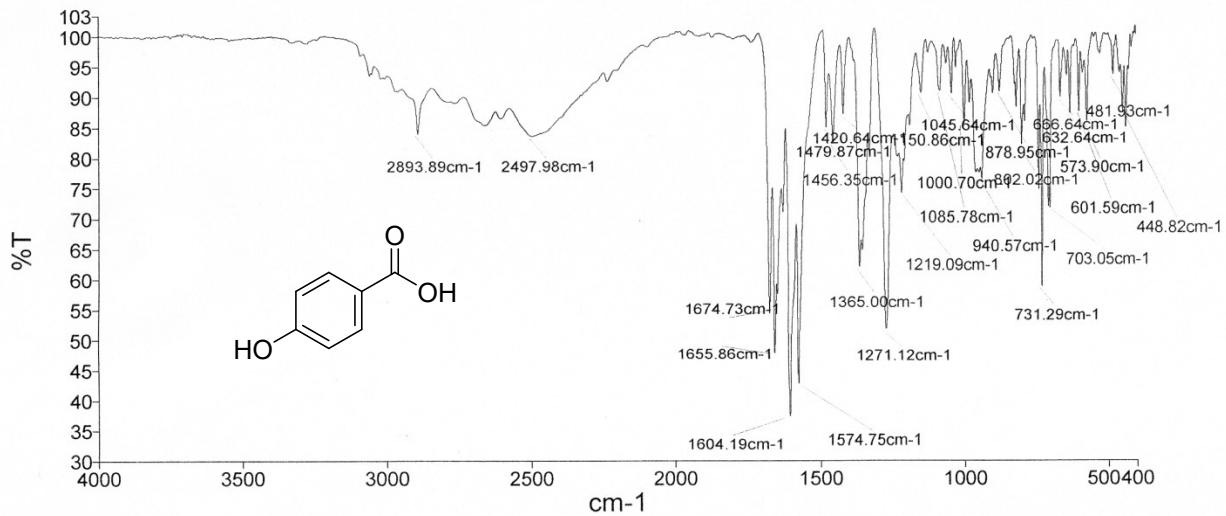
¹H NMR spectrum of 4-nitrobenzoic acid



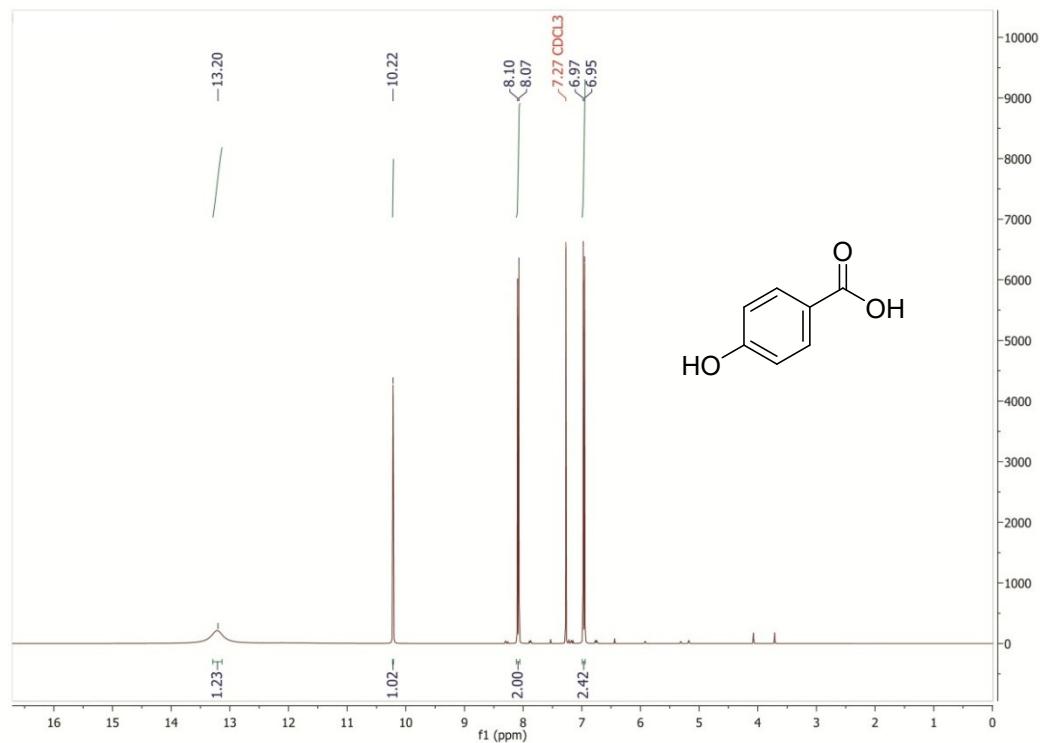
^1H NMR spectrum of 4-nitrobenzoic acid



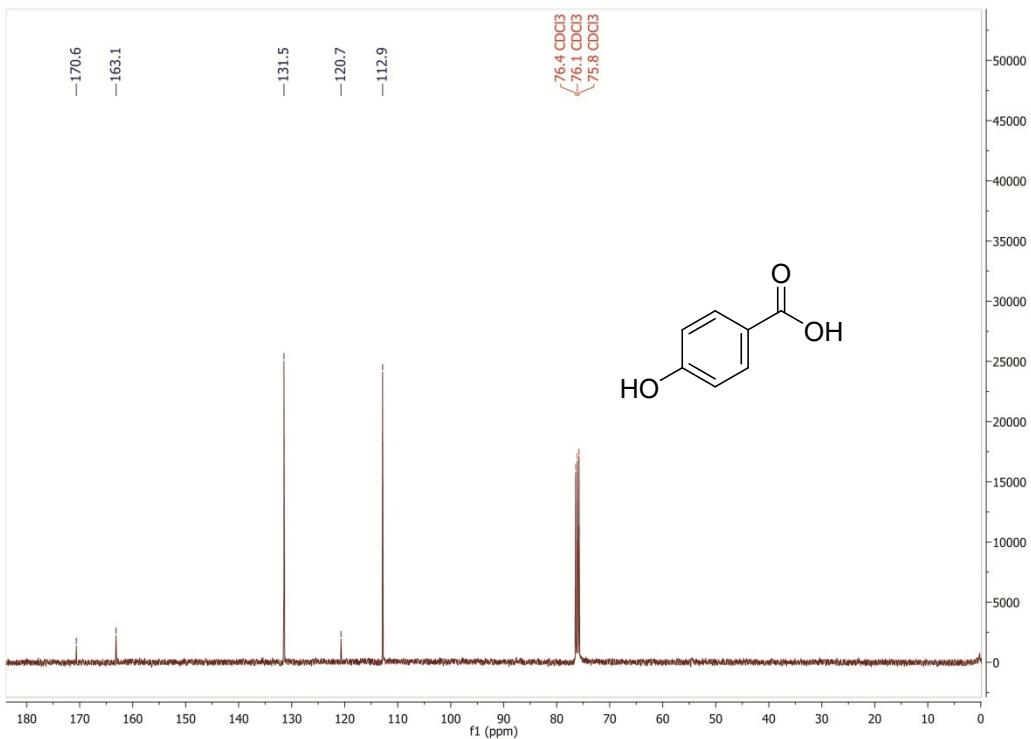
^{13}C NMR spectrum of 4-nitrobenzoic acid



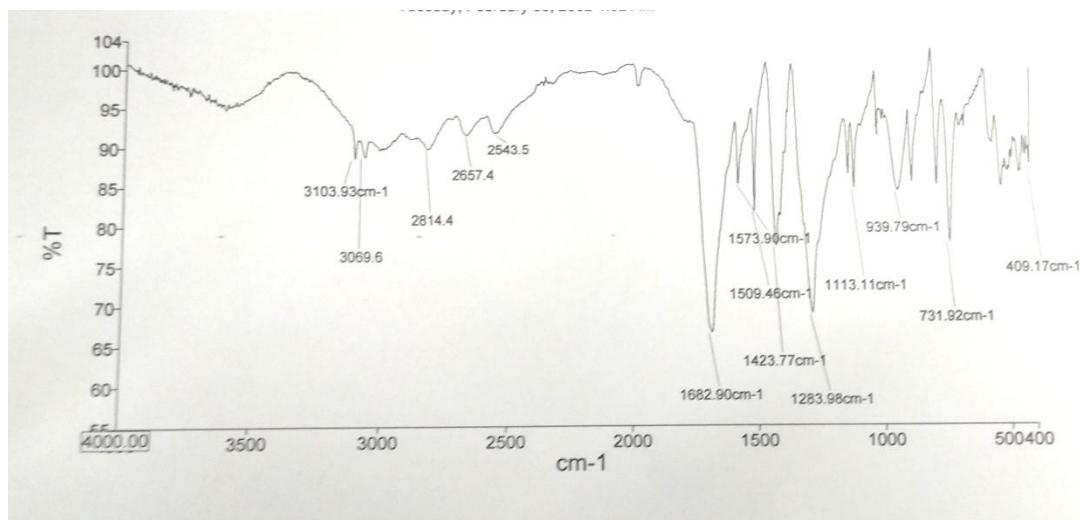
FT-IR spectrum of 4-hydroxybenzoic acid



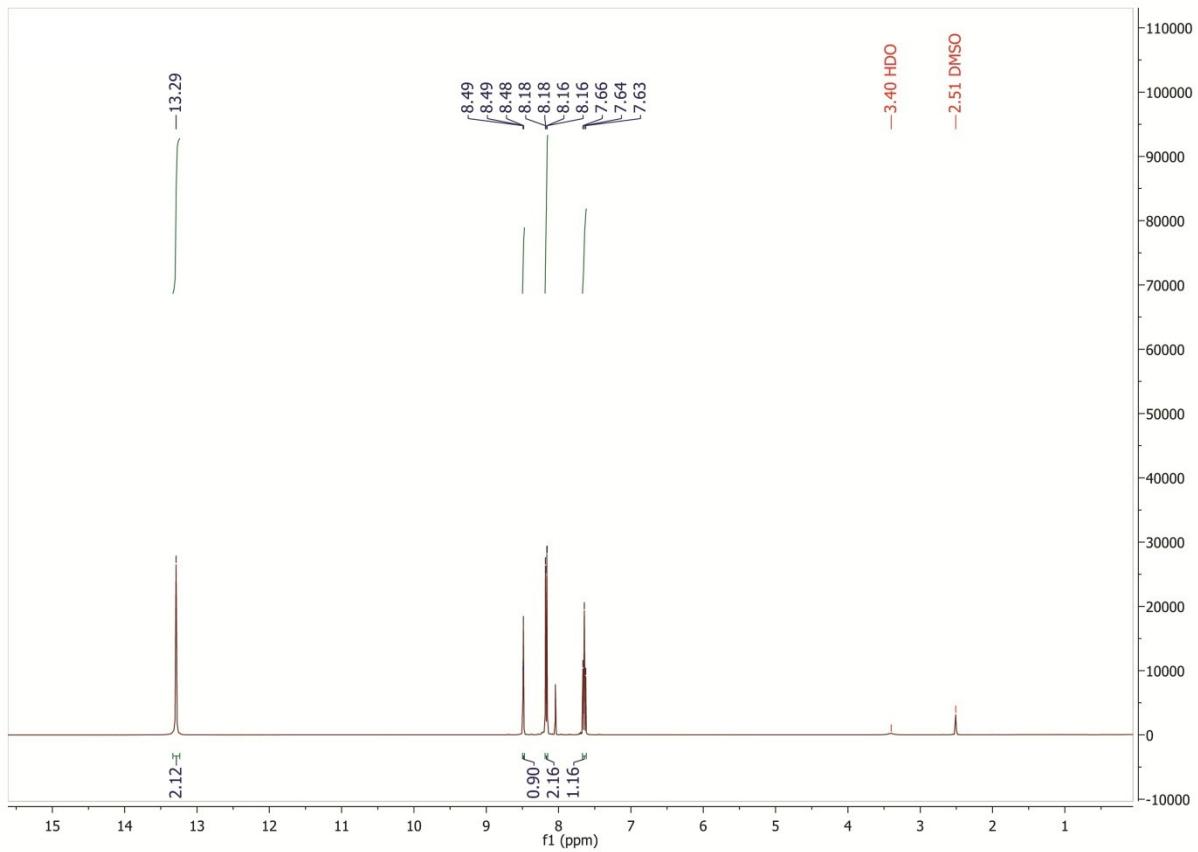
^1H NMR spectrum of 4-hydroxybenzoic acid



^{13}C NMR spectrum of 4-hydroxybenzoic acid



FT-IR spectrum of Isophthalic acid



¹H NMR spectrum of Isophthalic acid