Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2016

Supporting information for

A Novel Access to Carbonyl and Acetylated Compounds: the Role of *tetra-n*-Butylammonium Bromide/Sodium Nitrite Catalyst†

Mehdi Sheykhan,†Hadi Fallah Moafi,†Masoumeh Abbasnia‡*

†Chemistry Department, University of Guilan, P.O. Box 41335-1914, Rasht, Iran, Fax: +981333367262, Email: sheykhan@guilan.ac.ir

‡School of Chemistry, College of Science, University of Tehran, P.O. Box 14155-6455, Tehran, Iran.

Contents

1 General Remarks

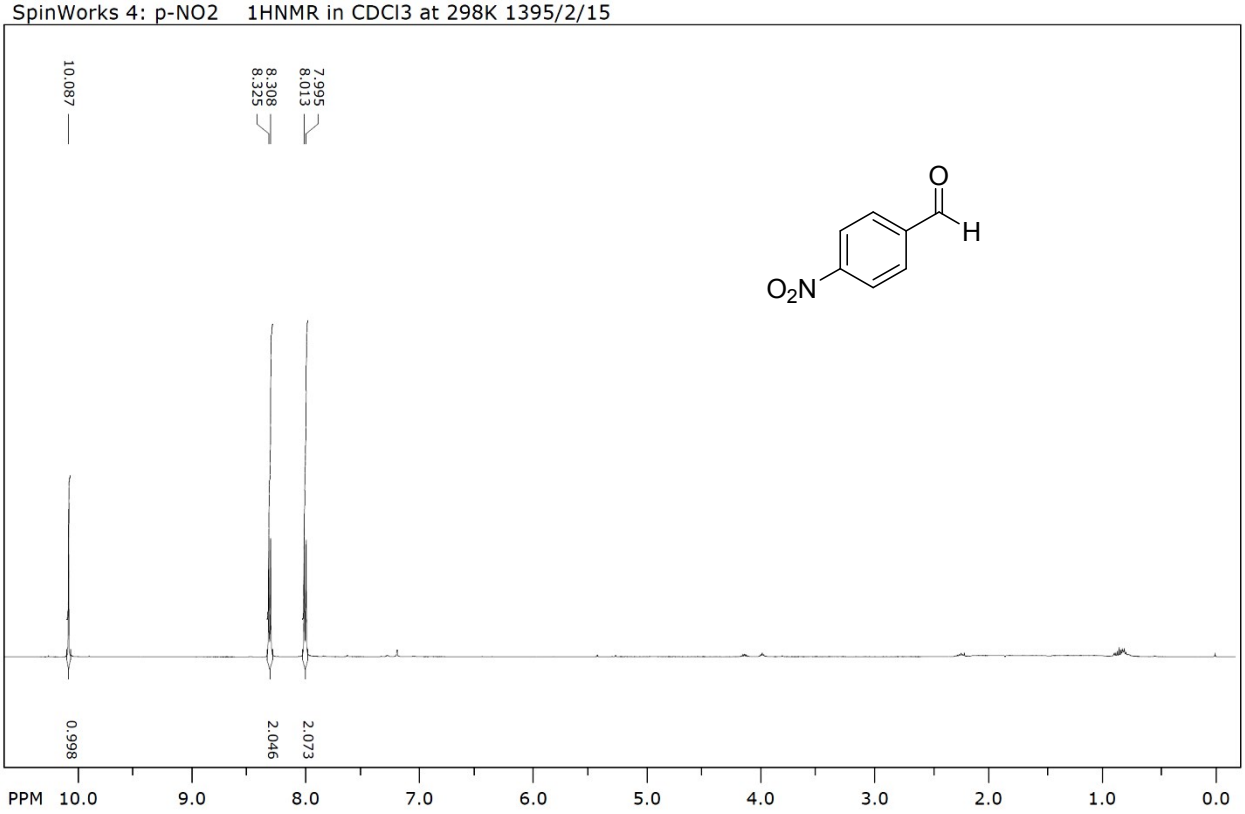
All commercially available reagents were used without further purification. TLC was conducted on silica gel 250 micron, F254 plates. Flash chromatography was carried out on silica gel. ^{1}H NMR spectra were recorded at room temperature on 500 MHz spectrometers, using $CDCl_3$ as the NMR solvent. Chemical shifts are reported in ppm with TMS as an internal standard (TMS: δ 0.0 ppm).

General Procedure for the aerobic oxidation of benzylic alcohols and acetylation of primary aliphatic alcohols

A mixture of alcohol (1 mmol), sodium nitrite (0.05 mmol, 5 mol%), tetra-n-butylammonium bromide (TBAB, 0.05 mmol, 5 mol%), and acetic acid (0.5 mL) was prepared in a two-necked flask and then the flask filled with air by use of a balloon. The reaction mixture stirred at 70 ^{o}C and the progress of the reaction was monitored by means of TLC. After completion of the reaction followed by addition of dichloromethane (5 mL) to the reaction flask, the mixture was centrifuged and the solute was separated and dried with sodium sulfate. After evaporation of dichloromethane and chromatographic purification, the structures of carbonyl/acetylated products were proved by the comparison of their $^{1}HNMR$ by related literatures.

3 Copies of some of ^{1}H NMR Spectra of the aerobic oxidized products

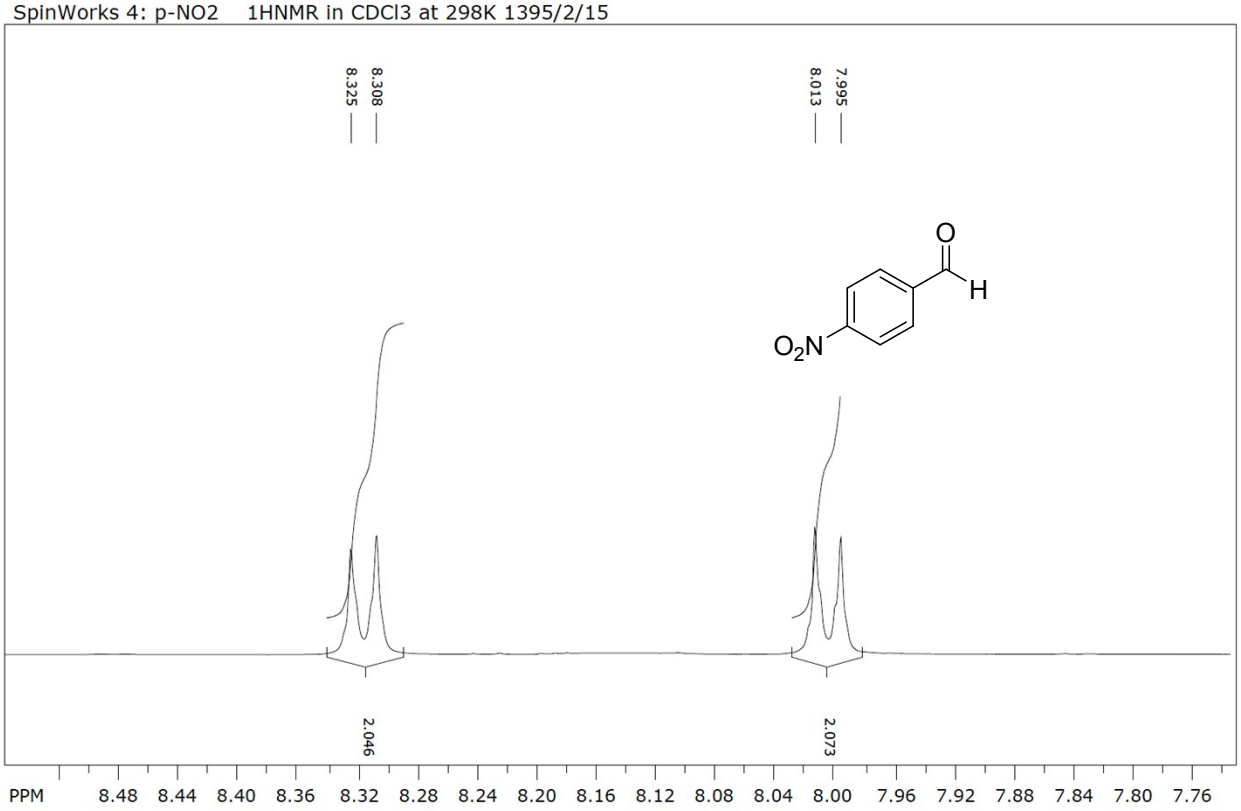
SpinWorks 4: p-NO2 1HNMR in CDCl3 at 298K 1395/2/15



file: ...:\catalysis\aerobic\Sheykhan\4\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt

freq. of 0 ppm: 500.130055 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 216.884 ppm/cm: 0.43365

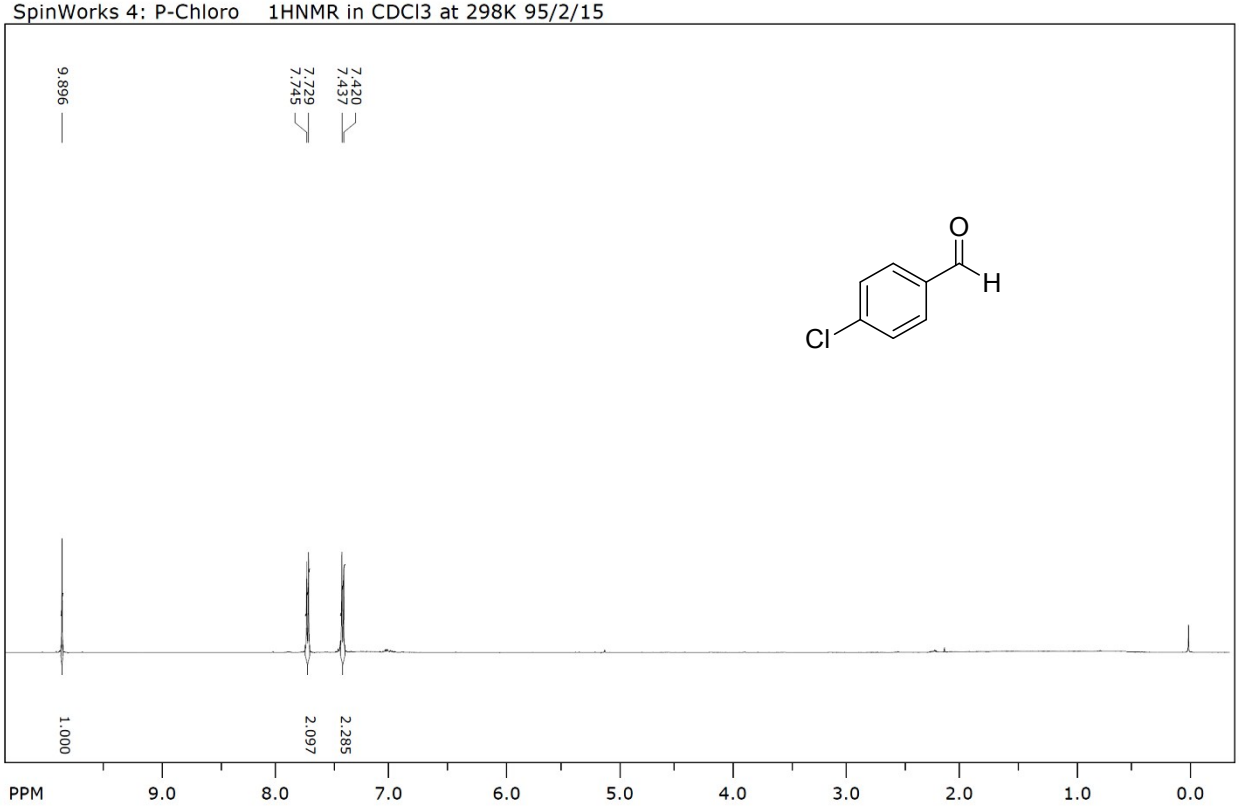
SpinWorks 4: p-NO2 1HNMR in CDCl3 at 298K 1395/2/15



file: ...:\catalysis\aerobic\Sheykhan\4\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt

freq. of 0 ppm: 500.130055 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 16.518 ppm/cm: 0.03303

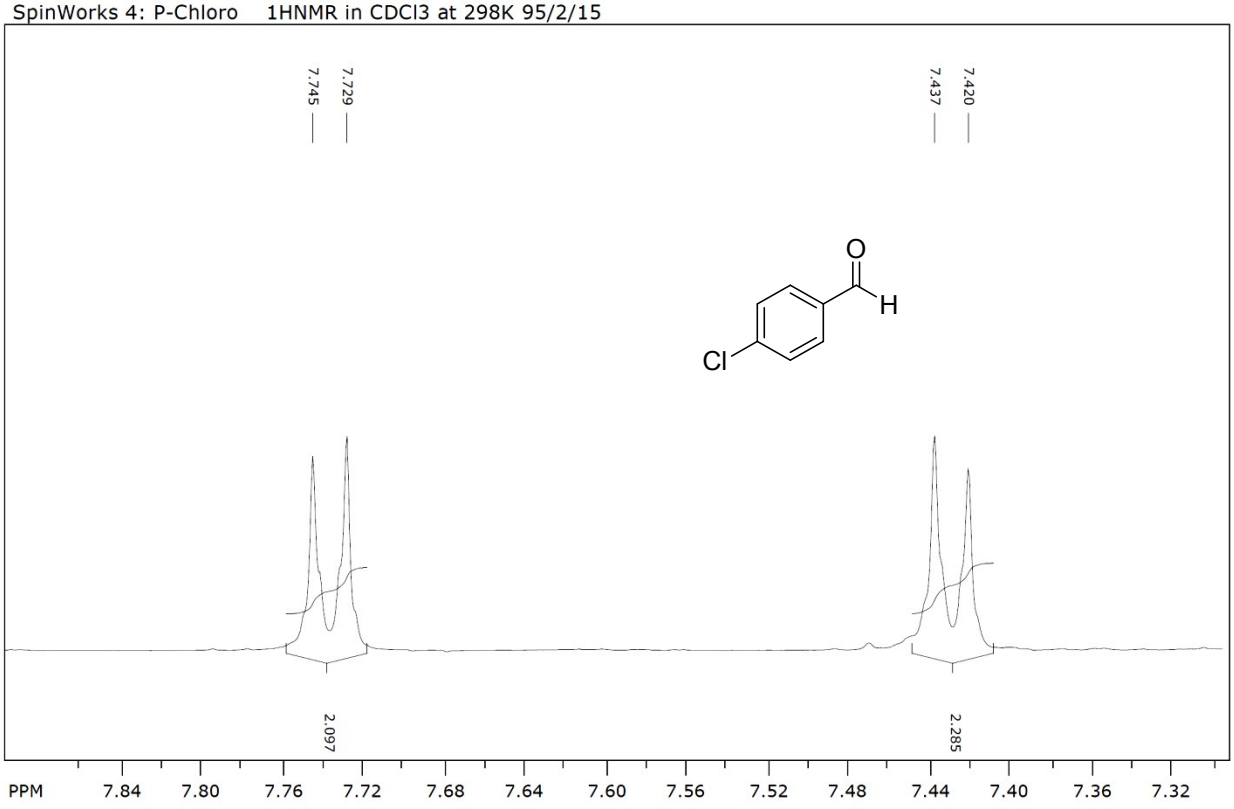
SpinWorks 4: P-Chloro 1HNMR in CDCl3 at 298K 95/2/15



file: ...:\catalysis\aerobic\Sheykhan\8\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

freq. of 0 ppm: 500.130063 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 215.409 ppm/cm: 0.43070

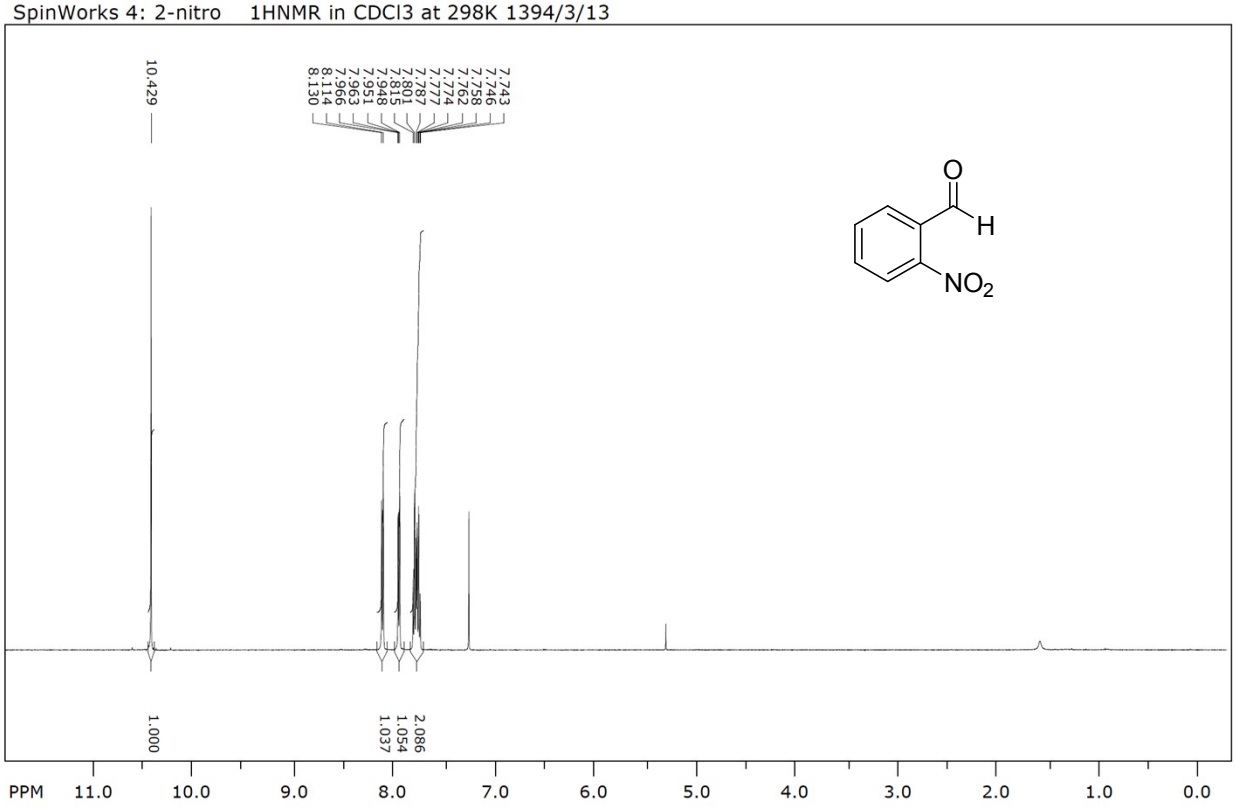
SpinWorks 4: P-Chloro 1HNMR in CDCl3 at 298K 95/2/15



file: ...:\catalysis\aerobic\Sheykhan\8\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

freq. of 0 ppm: 500.130063 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 12.114 ppm/cm: 0.02422

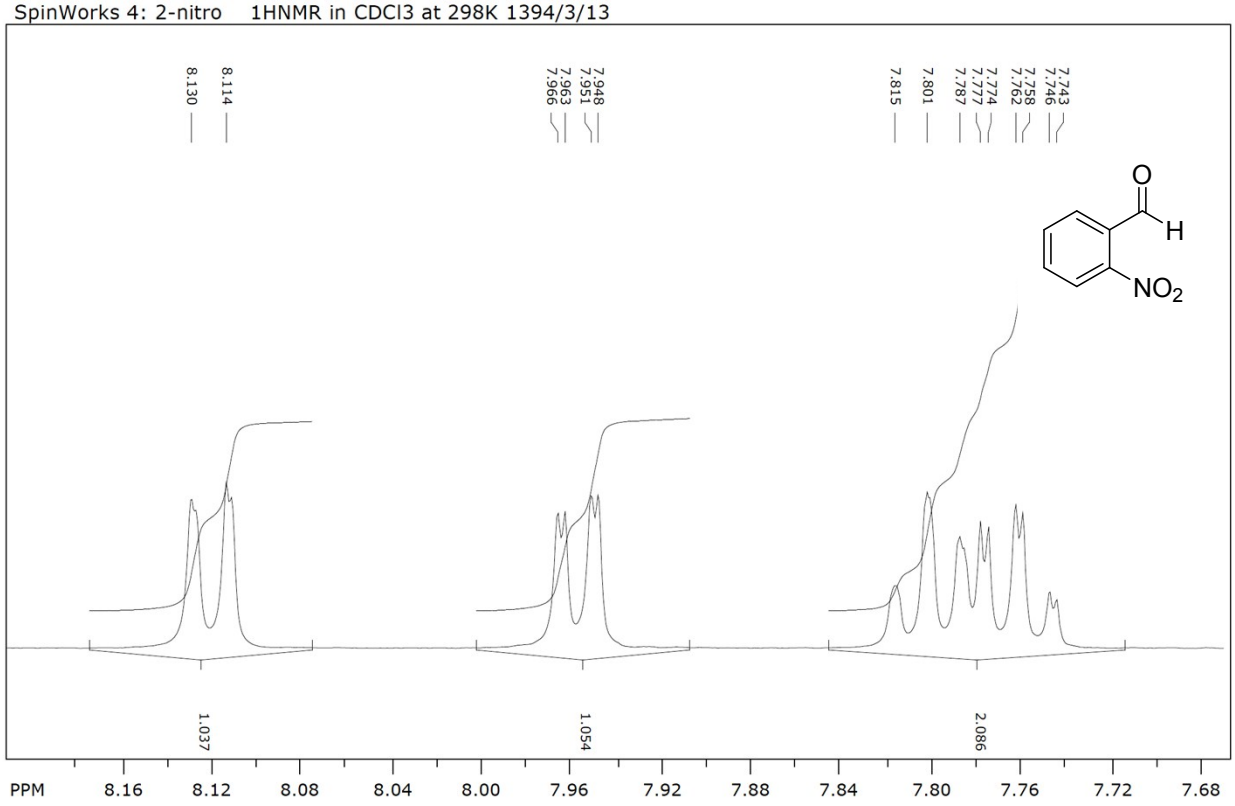
SpinWorks 4: 2-nitro 1HNMR in CDCl3 at 298K 1394/3/13



file: ...:\catalysis\aerobic\Sheykhan\2\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

freq. of 0 ppm: 500.130023 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 243.750 ppm/cm: 0.48737

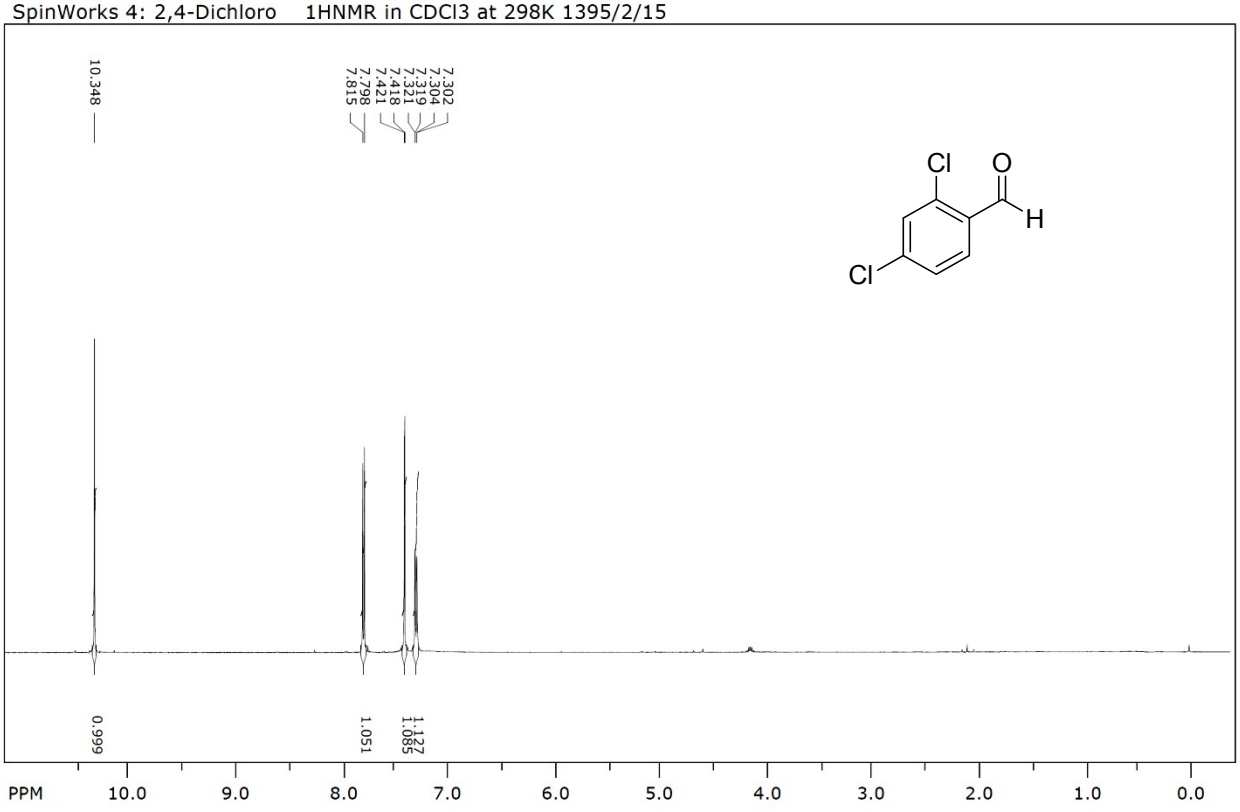
SpinWorks 4: 2-nitro 1HNMR in CDCl3 at 298K 1394/3/13



file: ...:\catalysis\aerobic\Sheykhan\2\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

freq. of 0 ppm: 500.130023 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 10.895 ppm/cm: 0.02178

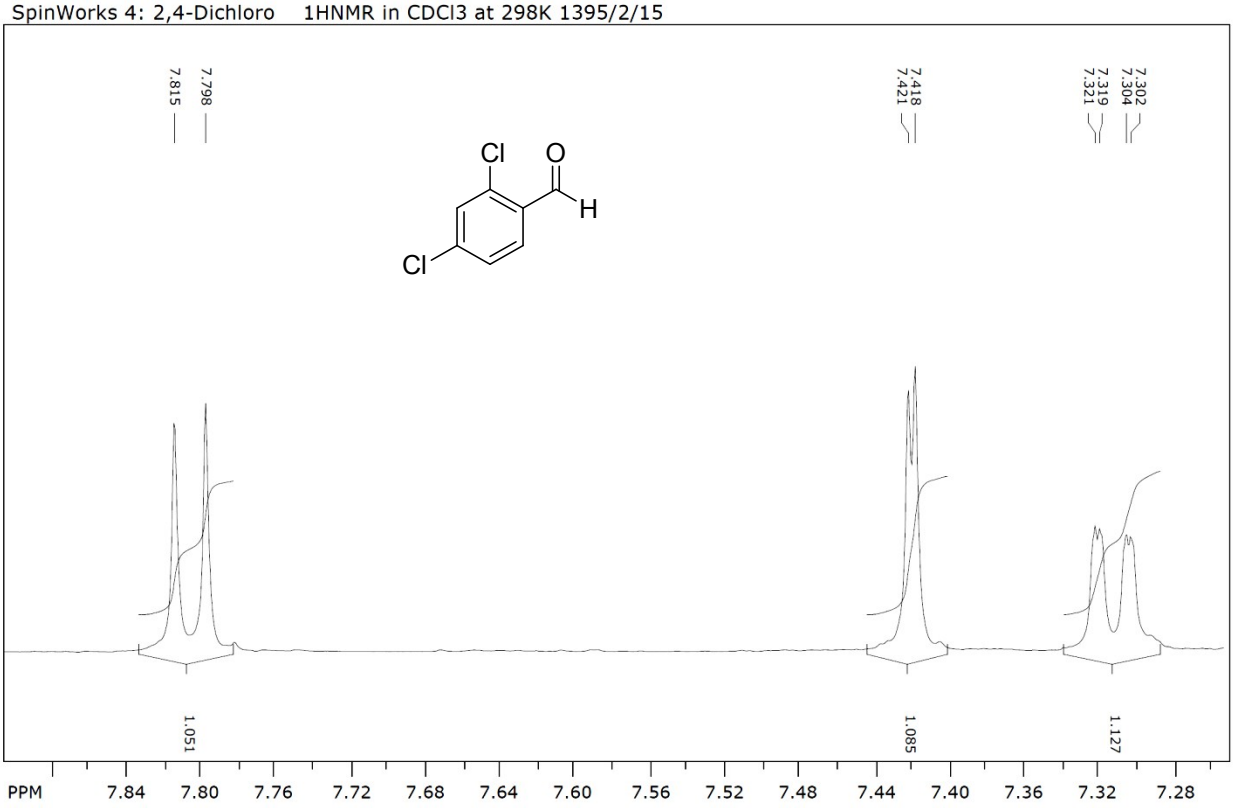
SpinWorks 4: 2,4-Dichloro 1HNMR in CDCl3 at 298K 1395/2/15



file: ...:\catalysis\aerobic\Sheykhan\3\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130055 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 231.782 ppm/cm: 0.46344

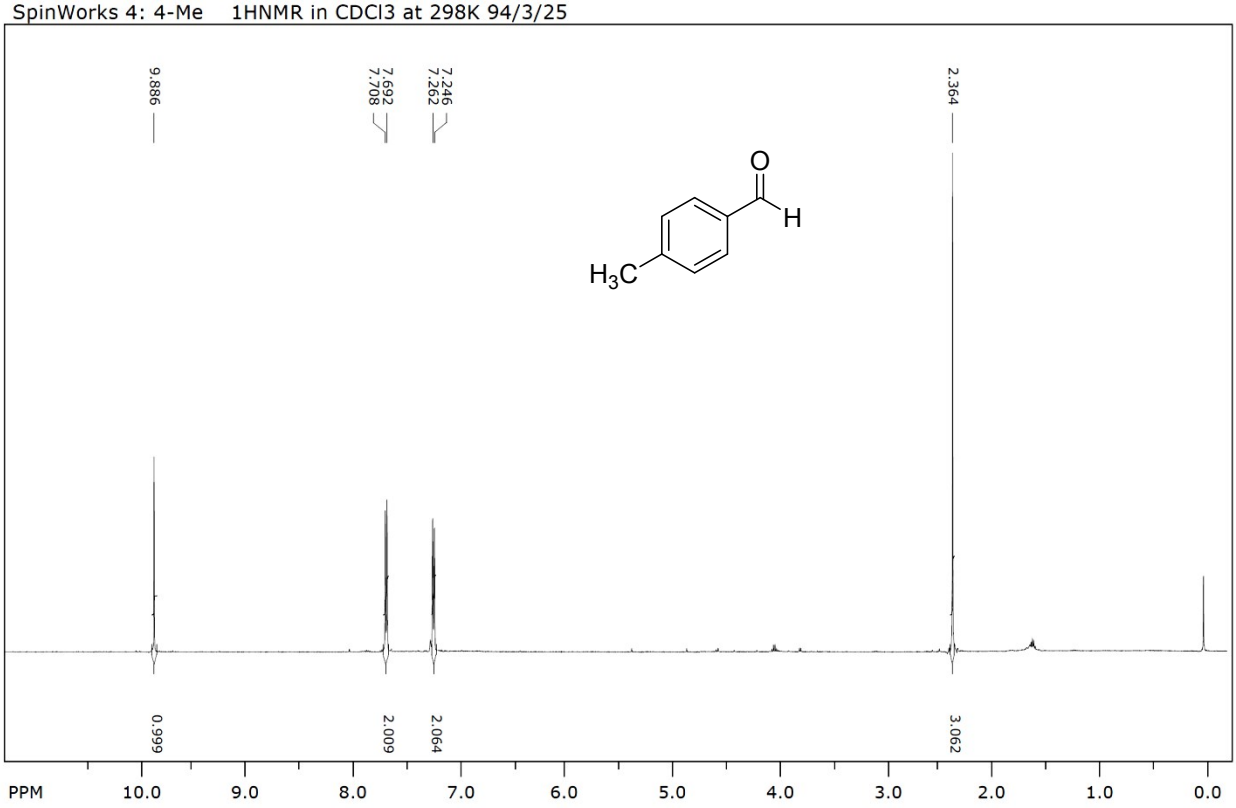
SpinWorks 4: 2,4-Dichloro 1HNMR in CDCl3 at 298K 1395/2/15



file: ...:\catalysis\aerobic\Sheykhan\3\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130055 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 13.109 ppm/cm: 0.02621

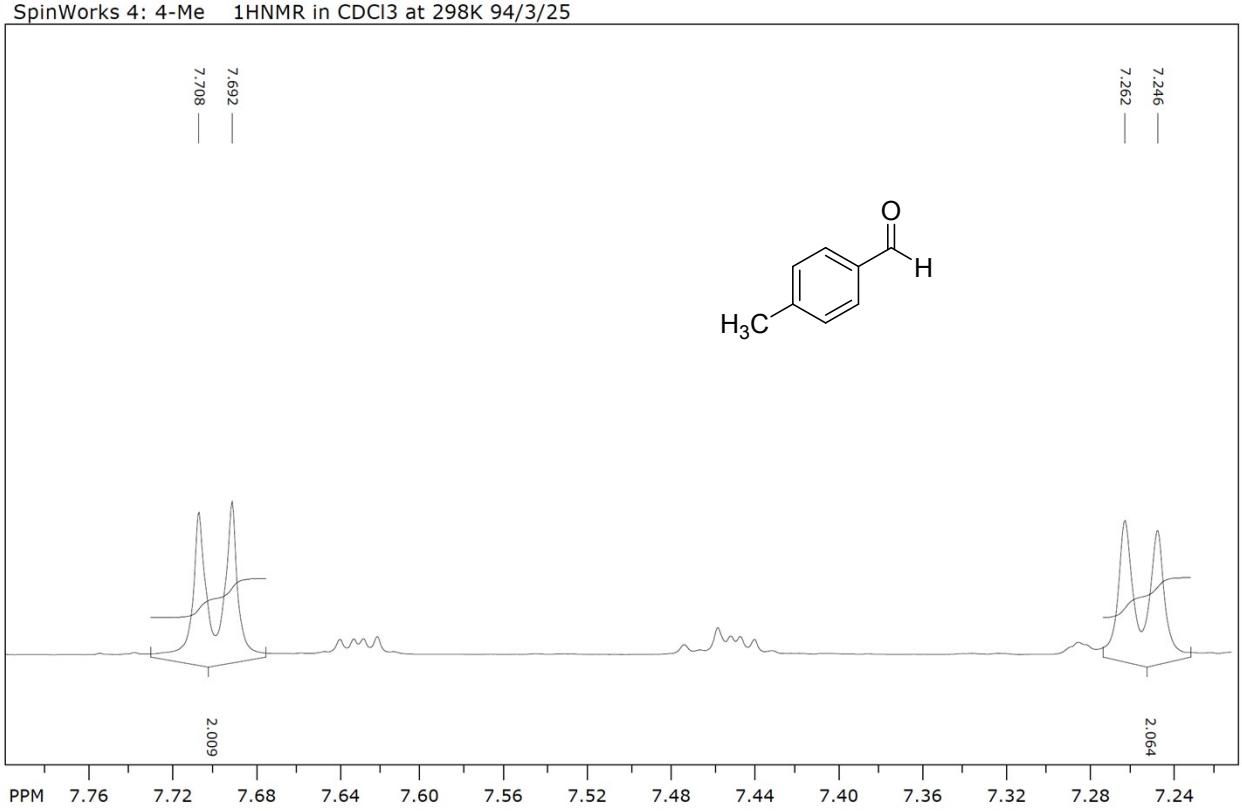
SpinWorks 4: 4-Me 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\12\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

freq. of 0 ppm: 500.130063 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 230.498 ppm/cm: 0.46087

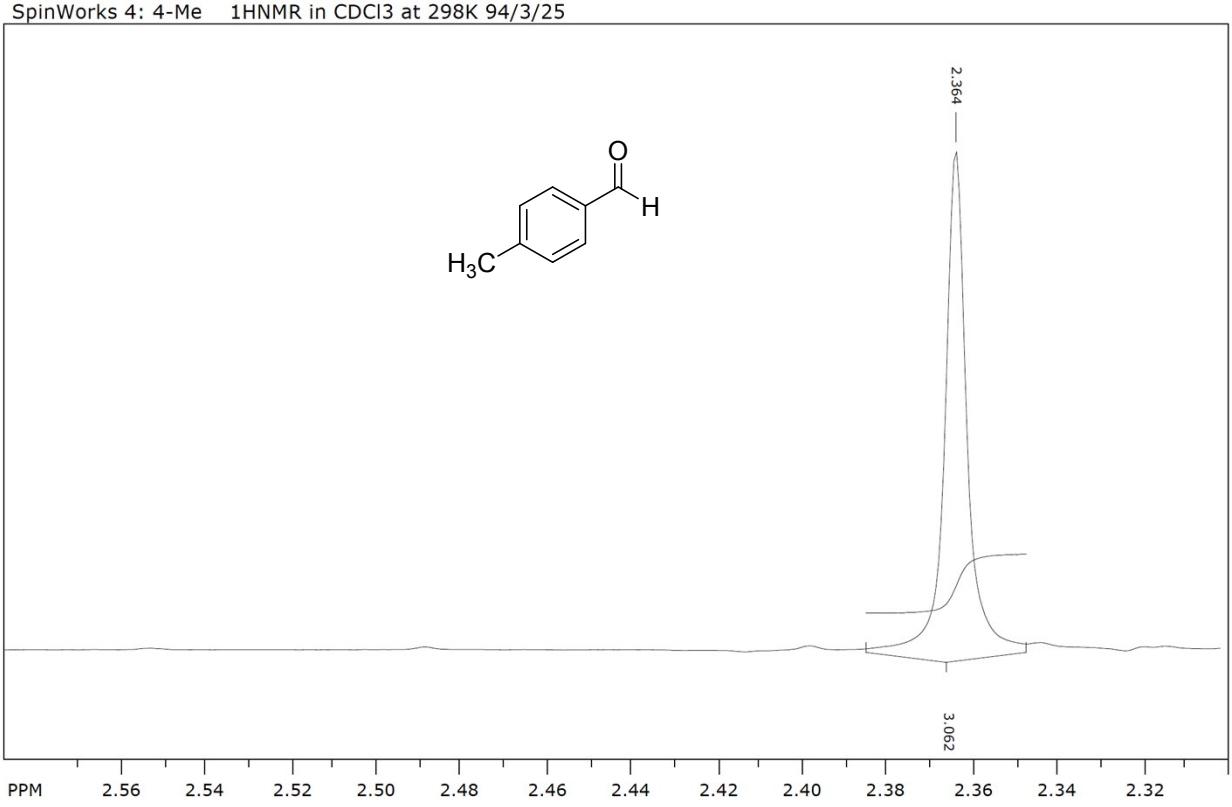
SpinWorks 4: 4-Me 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\12\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

freq. of 0 ppm: 500.130063 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 11.839 ppm/cm: 0.02367

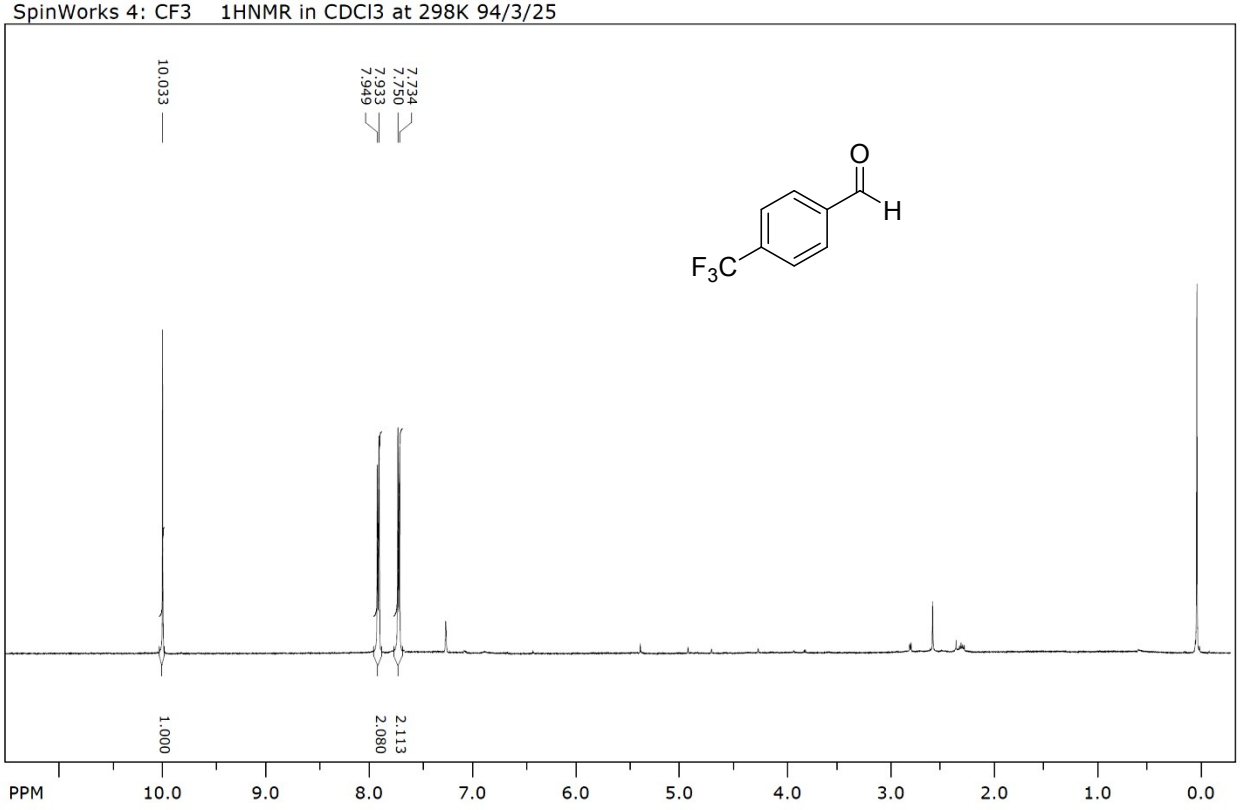
SpinWorks 4: 4-Me 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\12\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 8

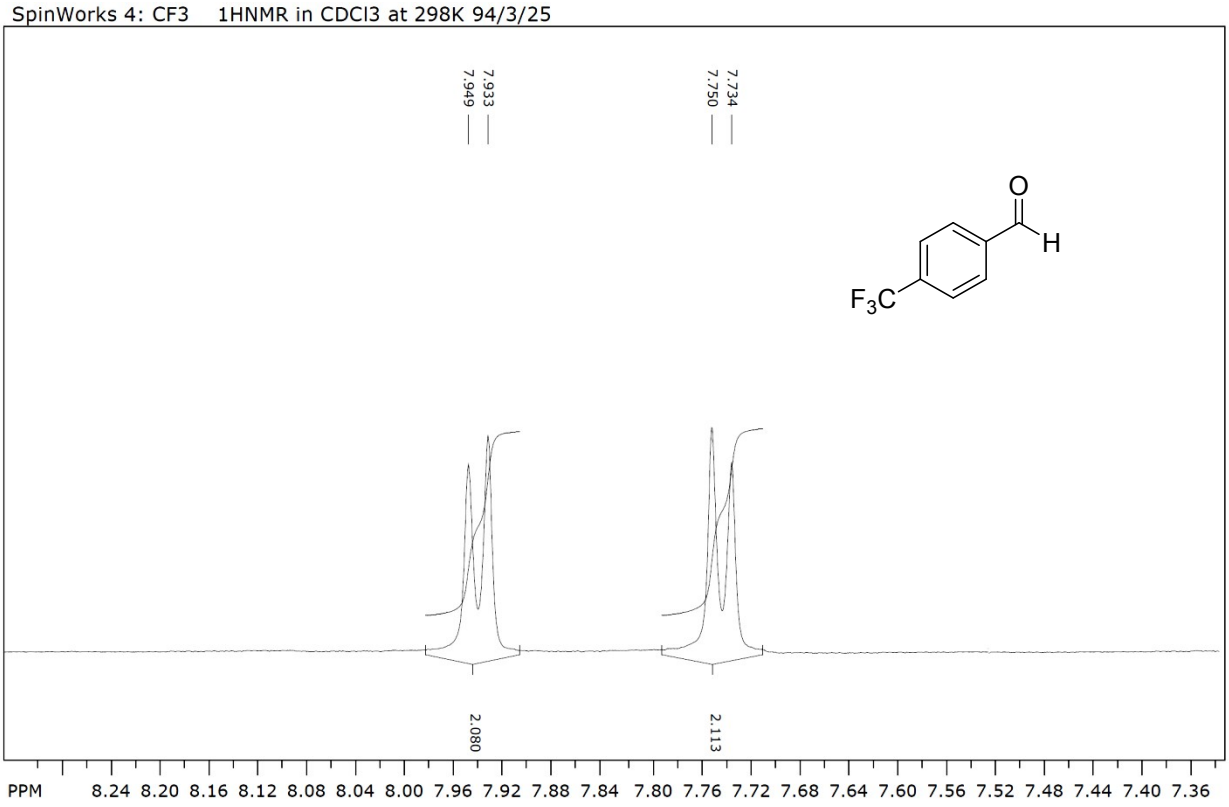
freq. of 0 ppm: 500.130063 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 5.752 ppm/cm: 0.01150

SpinWorks 4: CF3 1HNMR in CDCl3 at 298K 94/3/25



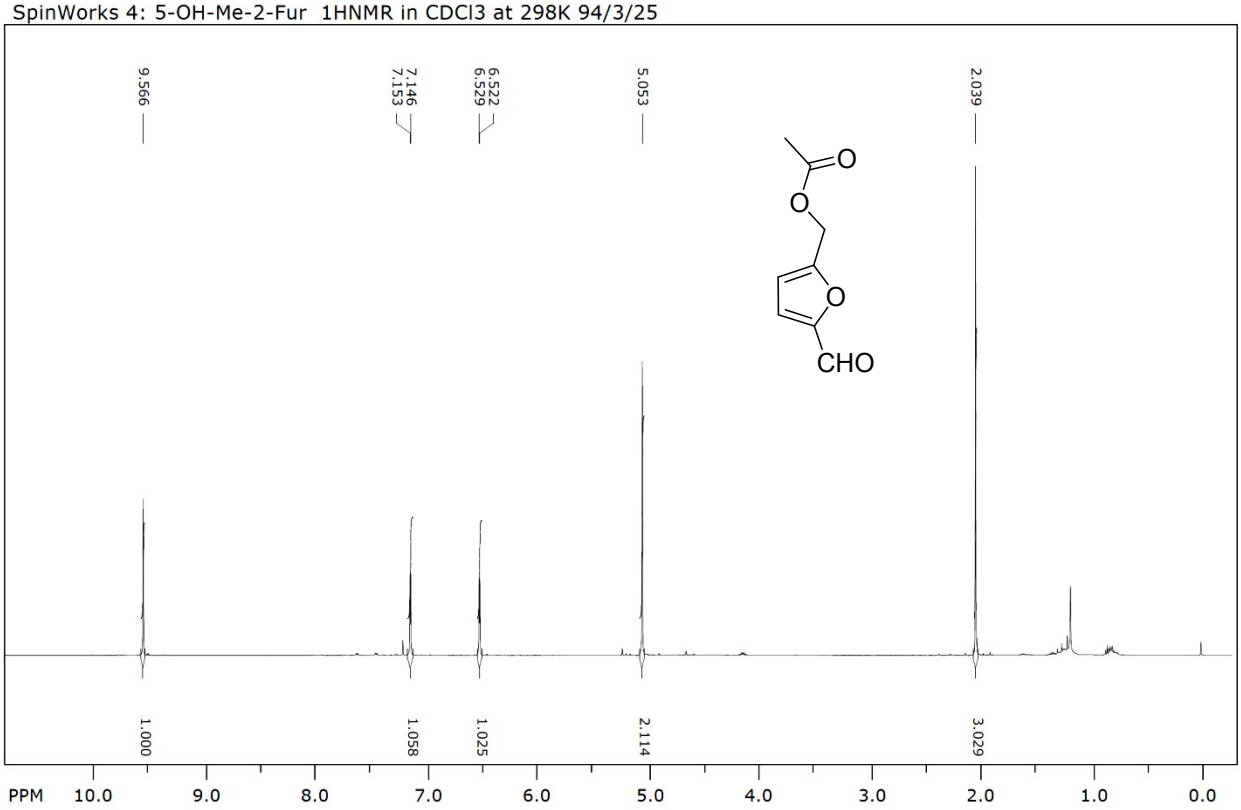
file: ...\catalysis\aerobic\Sheykhan\13\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130058 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 237.881 ppm/cm: 0.47564



4 [1]HNMR of some of the acetylated products

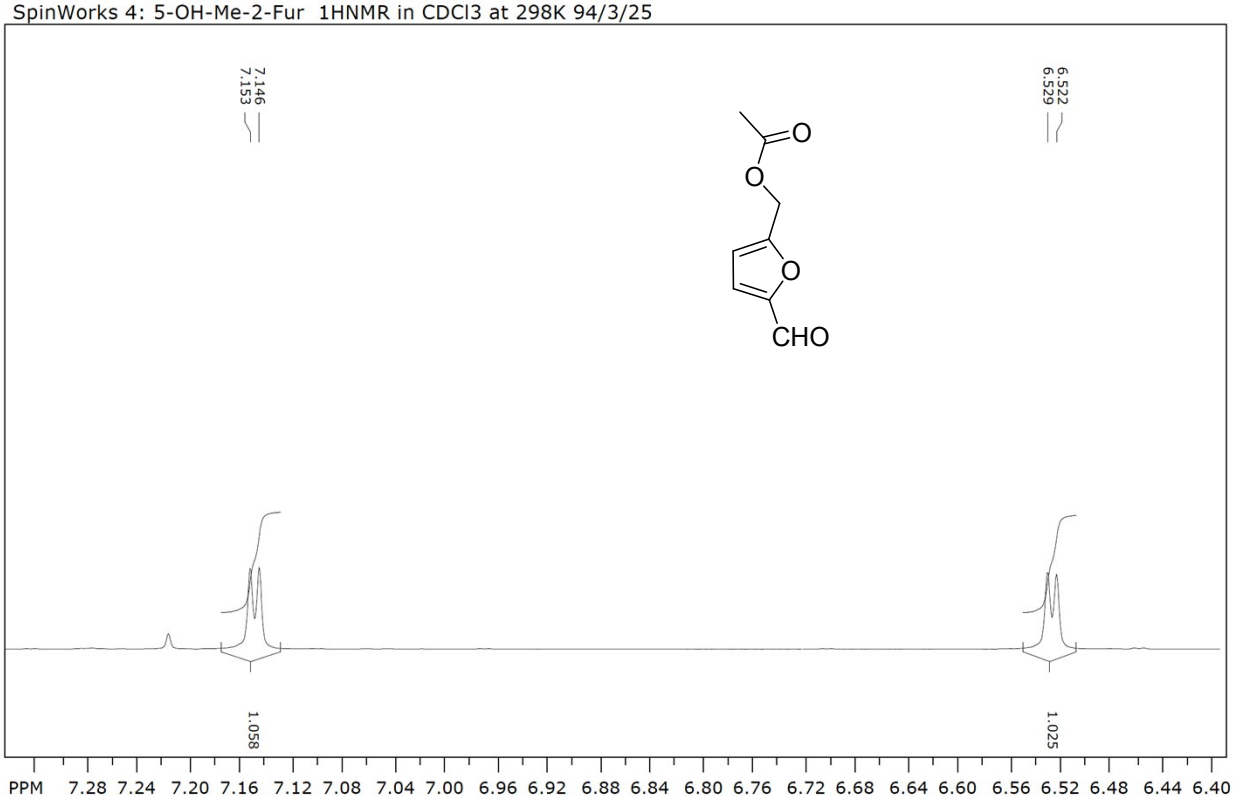
SpinWorks 4: 5-OH-Me-2-Fur 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\10\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130044 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 222.151 ppm/cm: 0.44418

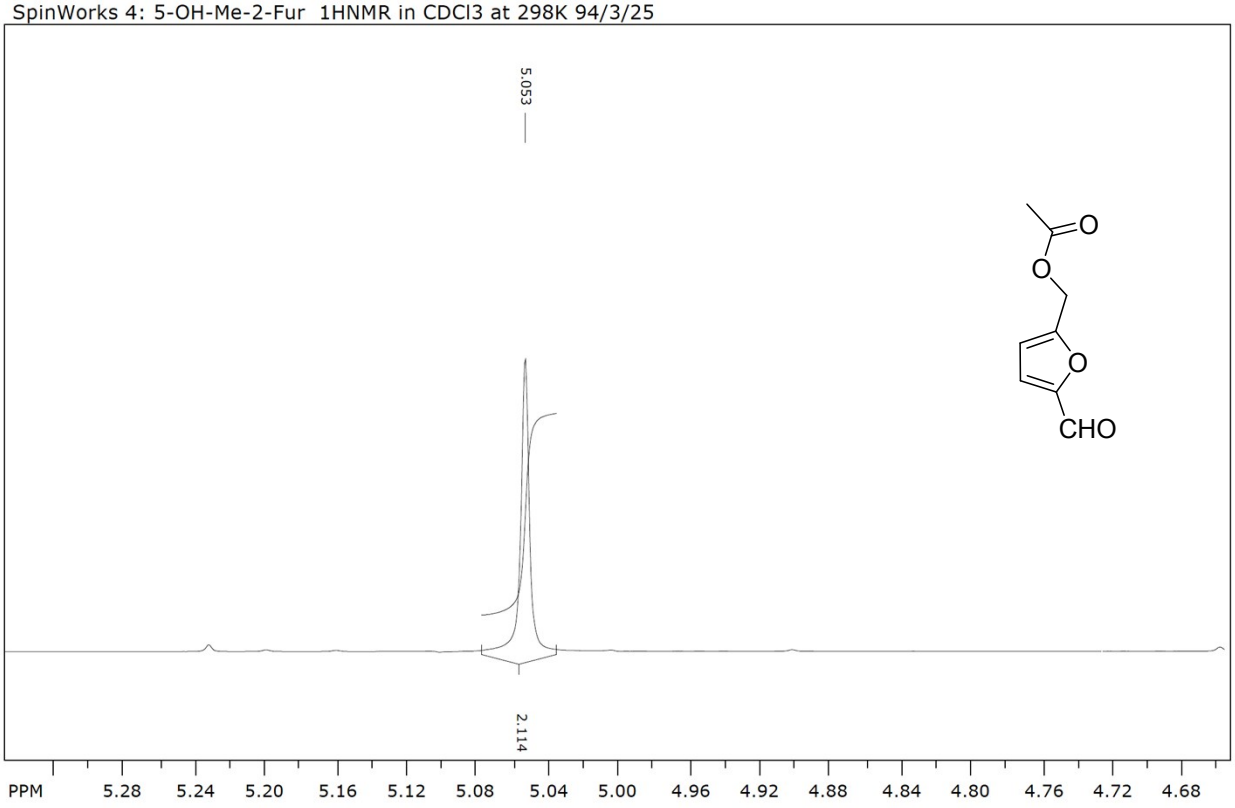
SpinWorks 4: 5-OH-Me-2-Fur 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\10\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130044 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 19.077 ppm/cm: 0.03814

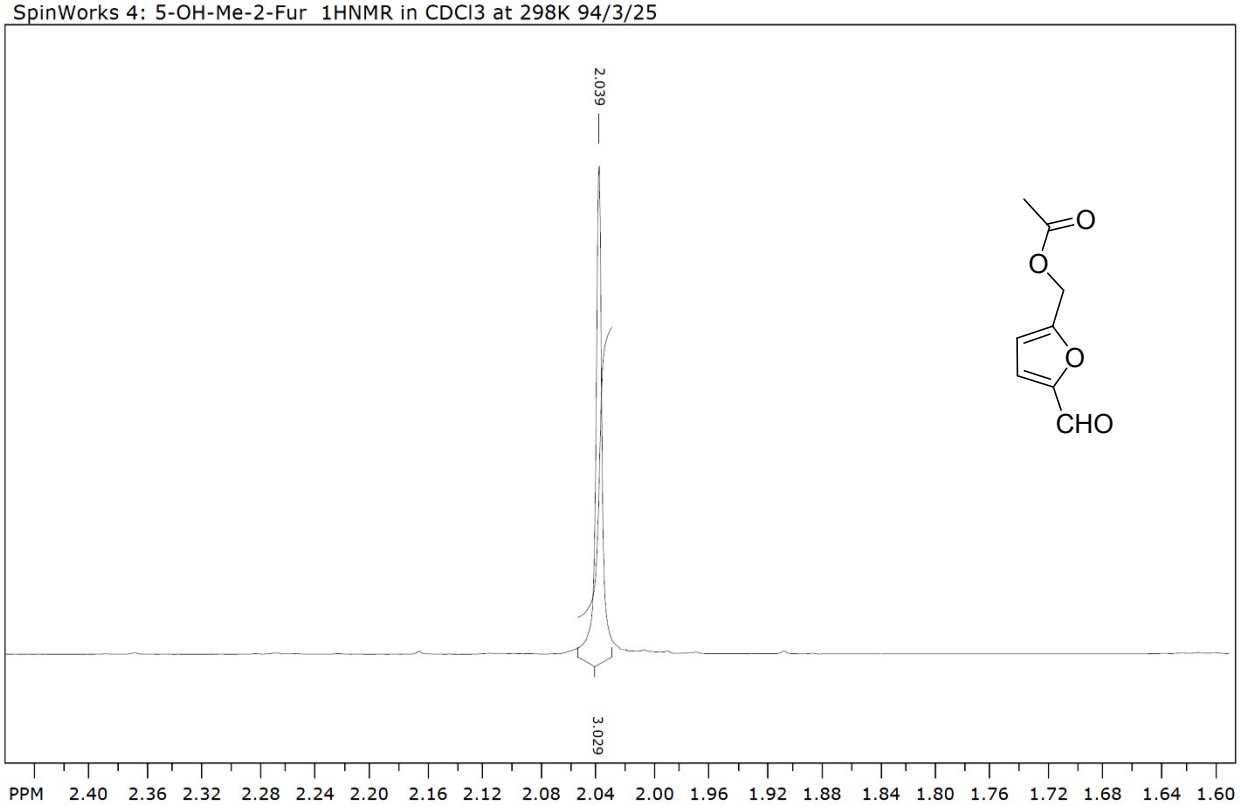
SpinWorks 4: 5-OH-Me-2-Fur 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\10\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130044 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 13.907 ppm/cm: 0.02781

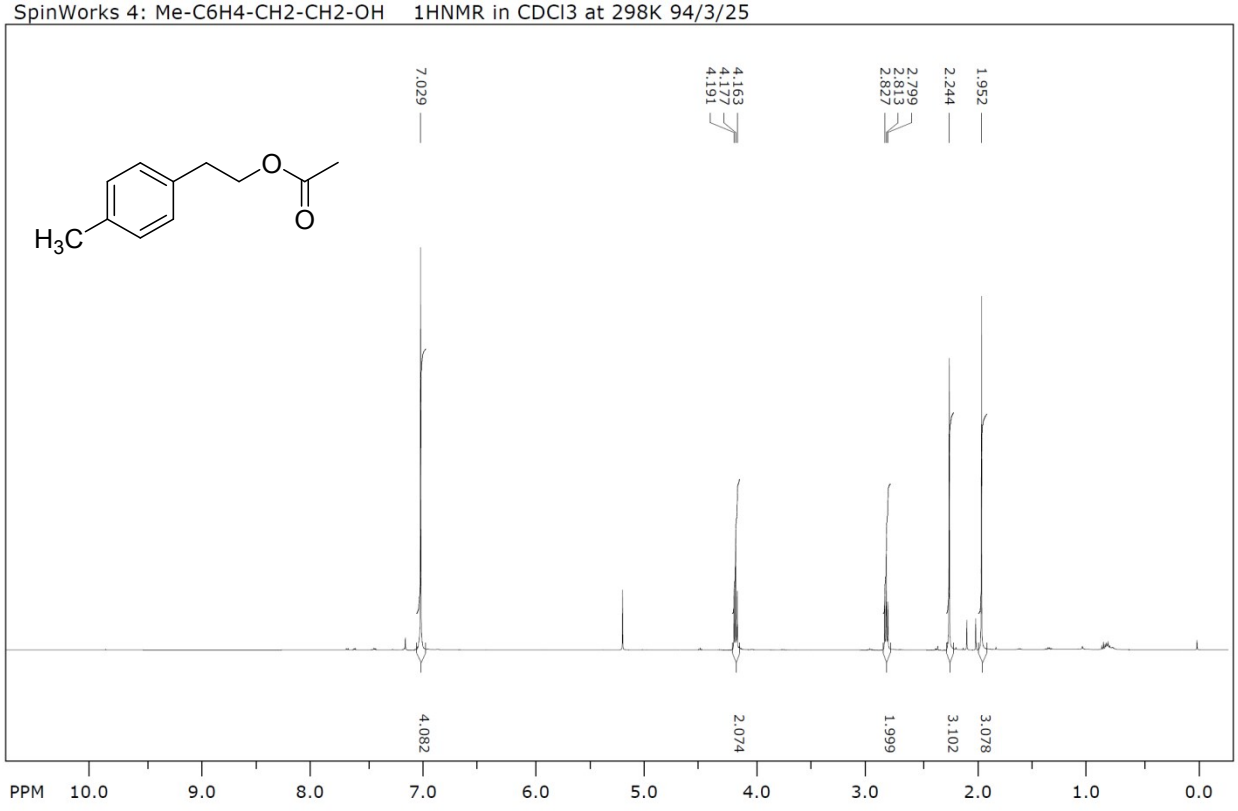
SpinWorks 4: 5-OH-Me-2-Fur 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\10\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130044 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 17.473 ppm/cm: 0.03494

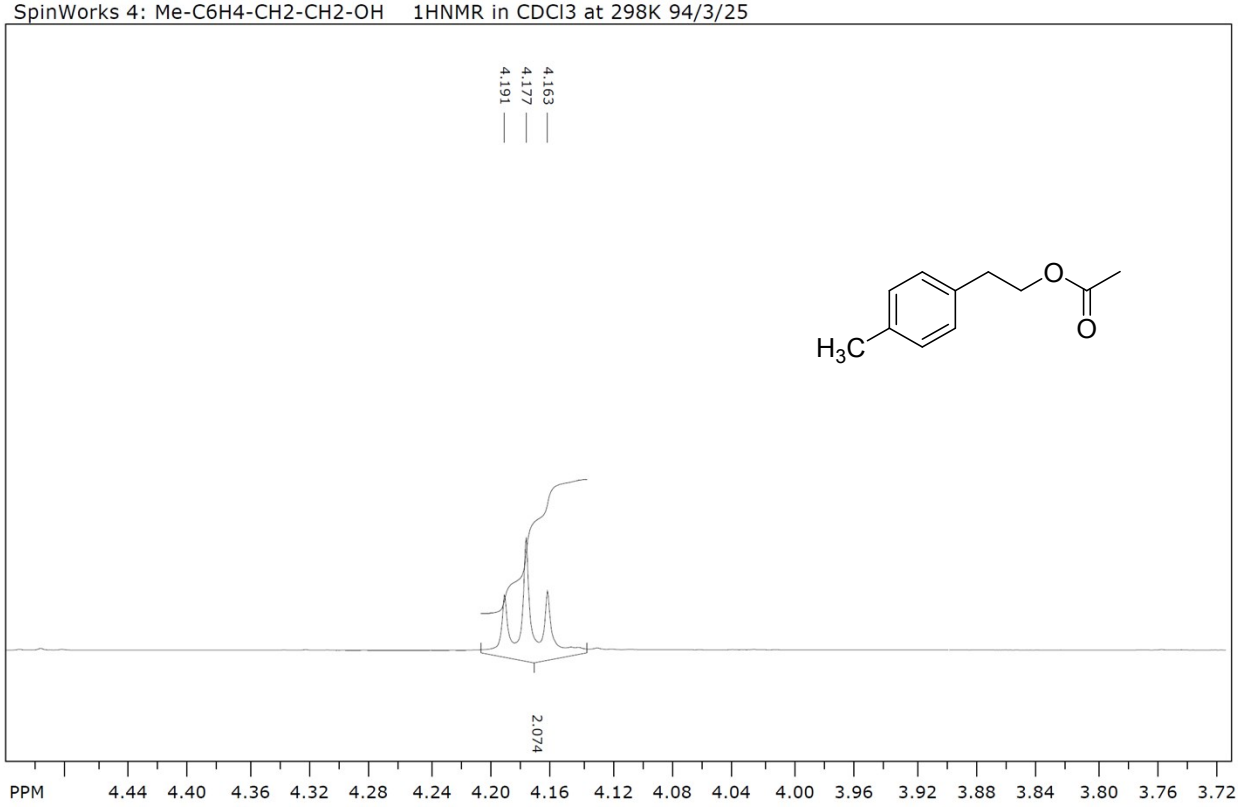
SpinWorks 4: Me-C6H4-CH2-CH2-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...:\catalysis\aerobic\Sheykhan\9\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130069 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 221.509 ppm/cm: 0.44290

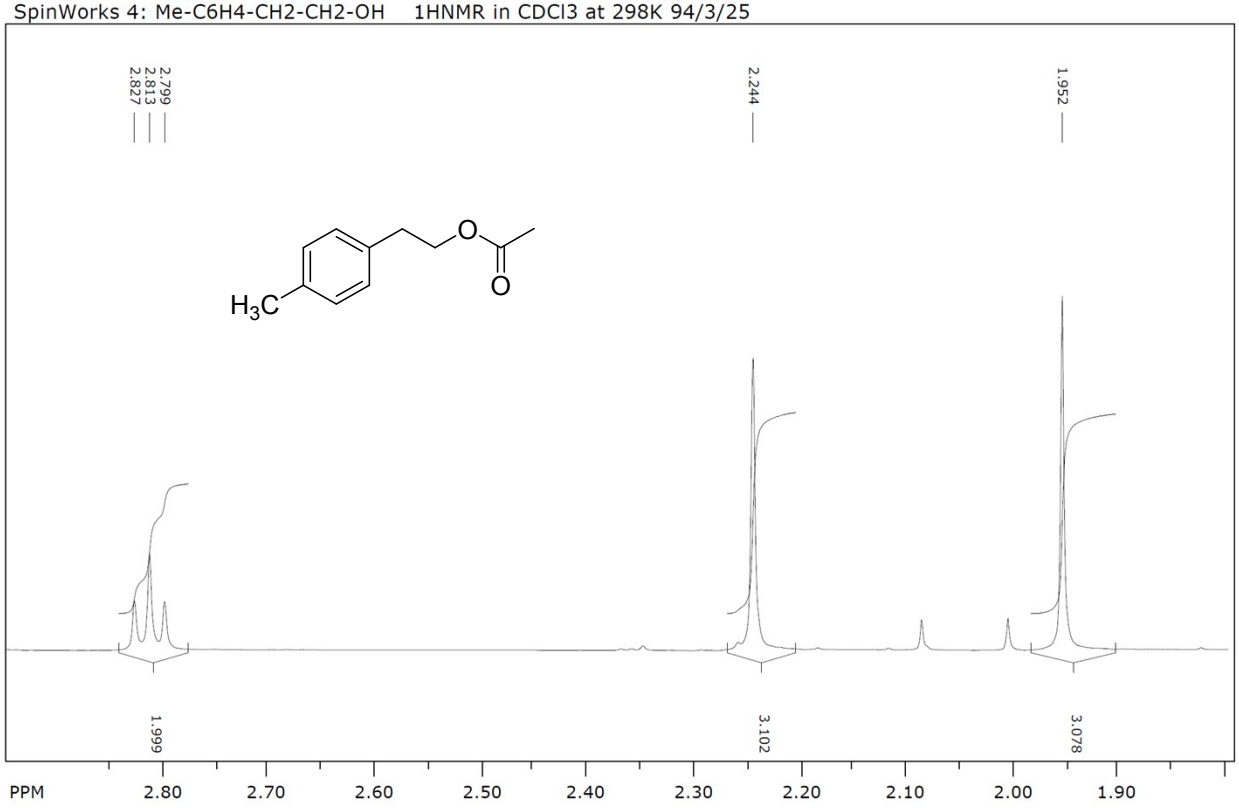
SpinWorks 4: Me-C6H4-CH2-CH2-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...:\catalysis\aerobic\Sheykhan\9\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130069 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 16.178 ppm/cm: 0.03235

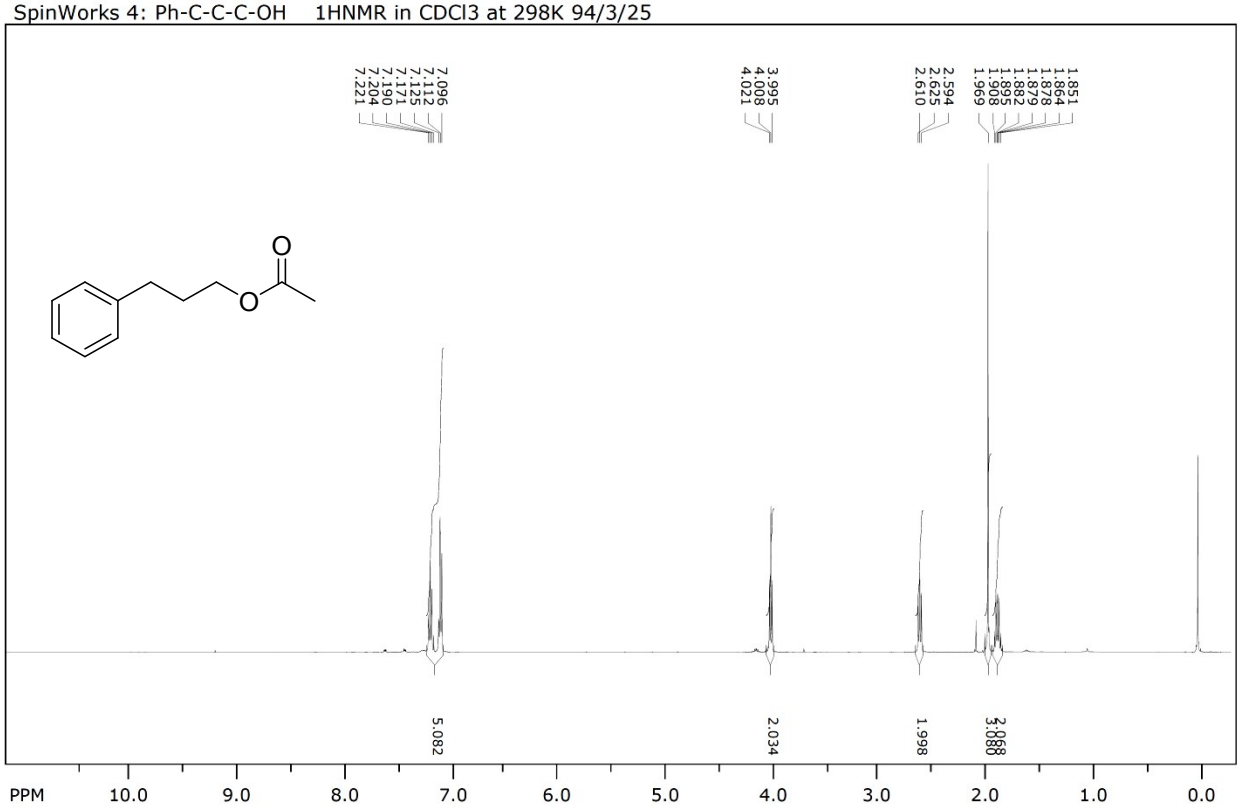
SpinWorks 4: Me-C6H4-CH2-CH2-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...:\catalysis\aerobic\Sheykhan\9\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130069 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 23.111 ppm/cm: 0.04621

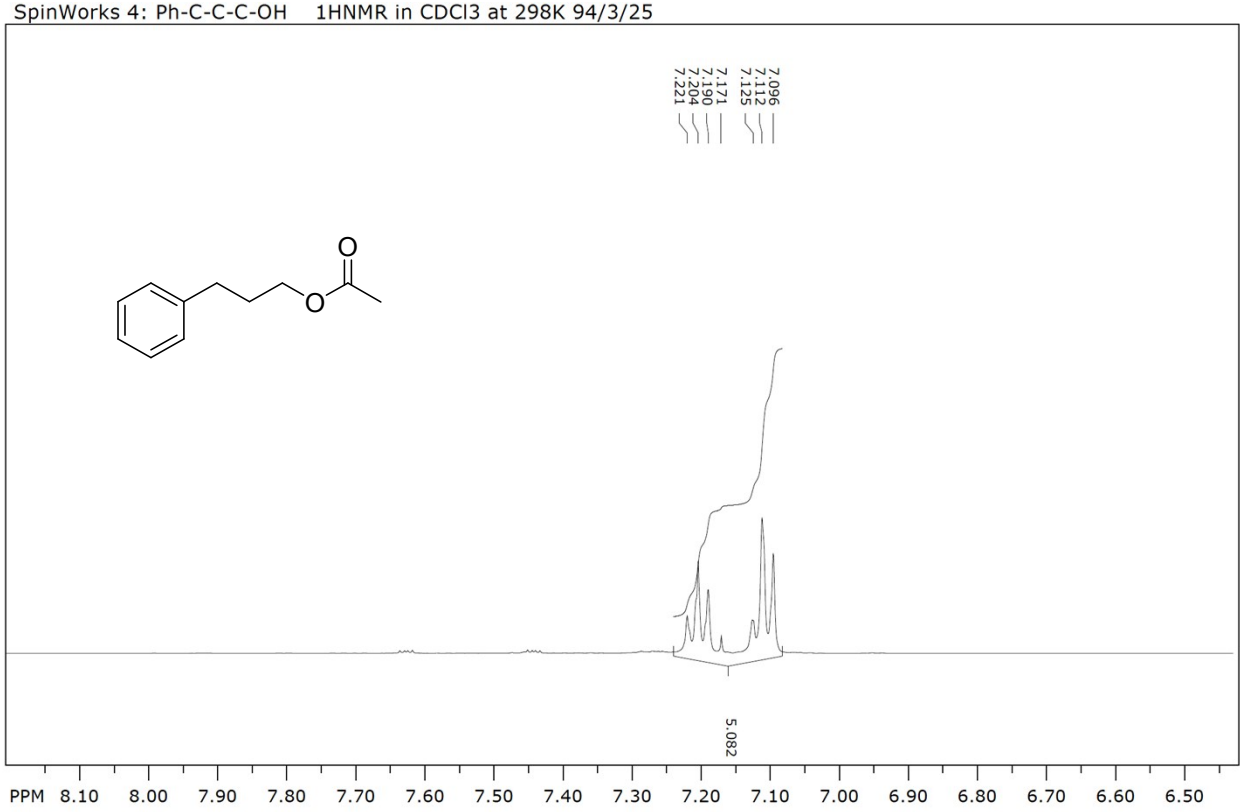
SpinWorks 4: Ph-C-C-C-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\14\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130067 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 230.177 ppm/cm: 0.46023

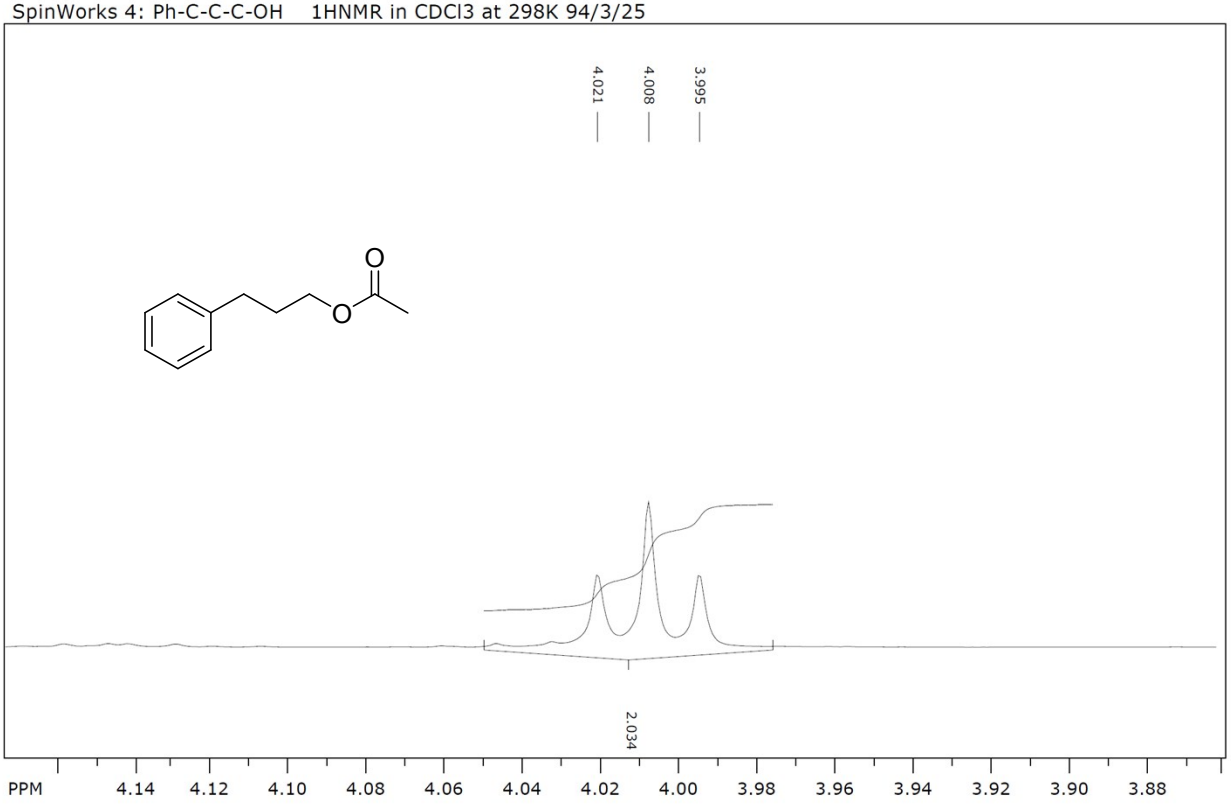
SpinWorks 4: Ph-C-C-C-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\14\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130067 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 35.653 ppm/cm: 0.07129

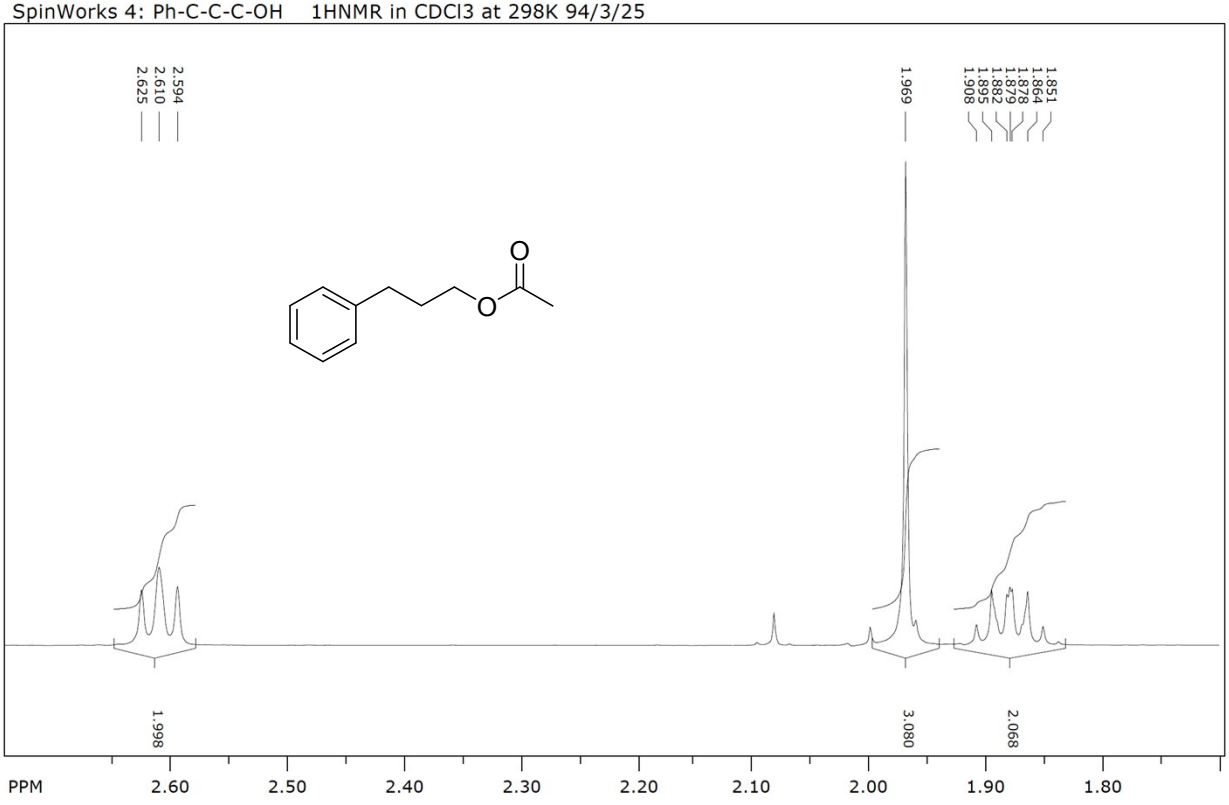
SpinWorks 4: Ph-C-C-C-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\14\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130067 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 6.281 ppm/cm: 0.01256

SpinWorks 4: Ph-C-C-C-OH 1HNMR in CDCl3 at 298K 94/3/25



file: ...\catalysis\aerobic\Sheykhan\14\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 32768 points
width: 10000.00 Hz = 19.9947 ppm = 0.305176 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130067 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 20.875 ppm/cm: 0.04174