Supporting Information for:

Solid-Liquid Phase Transfer Catalyzed Selective Reduction of Bifunctional Moieties

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3.1 General procedure for chemoselective reduction of bifunctional carbonyl moieties with NaBH4/TBAI in Aqueous conditions :

Equimolar (0.009) mixture of aldehyde and ketone is mixed with 0.0009 moles of TBAI and 0.0036 moles of NaBH4 in 10 ml distilled water. The reaction mixture is stirred at room temperature. Quenching of reaction was done by using saturated solution of sodium chloride and extraction was done with chloroform. $Na_2SO_4$was used for drying organic layer. Evaporation of the organic solvent afforded the crude product which was further purified by column chromatography. Progress of reaction was observed with TLC and identification of product was done by IR and NMR.

3.2 General Procedure for Chemoselective Reduction of α, β–unsaturated carbonyl compound with NaBH4/TBAI:

Aqueous NaBH4 (3.95 mmol) and tetrabutylammonium iodide (0.87 g, 2.3 mmol, in one lot) were introduced to a stirred solution of α, β – unsaturated carbonyl compound (7.9 mmol) in ethanol (10 mL). The mixture was stirred at room temperature. Ethanol was removed by distillation. Extraction of aqueous layer was performed by diethyl ether (3.25mL) which was further dried (anhyd. Na_2SO_4), and concentrated. Column chromatography was used to purify the crude product by involving a solvent mixture of Ethyl acetate and hexane over silica gel. Reaction was examined with TLC and the product was recognized by IR and NMR. Spectroscopic data of all reduction product molecules are explained below.

IR and HNMR Data of newly synthesized compounds

Phenyl methanol (3a-3h): IR (υ, cm-1): 3363, 2873, 1953, 1874, 1652, 1604, 1495, 1452, 1206, 1016, 1010, 965, 848, 765.

1H NMR (400 MHz, CDCl3): 4.07 (s, 1H, OH), 4.40 (s, 2H, CH2), 7.15- 7.23 (m, 5H, ArH) ppm.

2- Nitro Phenyl methanol (3i): IR (υ, cm-1): 3287, 2961, 2420, 1610, 1522, 1338, 1186, 1035,856.

1H NMR (400 MHz, CDCl3): 3.41 (s, 1H, OH), 4.93 (s, 2H, CH2), 7.41-7.45 (t, 1H, ArH), 7.61-7.65 (t, 1H, ArH), 7.72-7.74 (d, 1H, ArH), 8.02-8.05 (d, 1H, ArH) ppm.

3 phenylprop-2-en-1-ol (3j): IR (υ, cm-1): 3345, 3030, 2873, 1952, 1873, 1646, 1495, 1453, 1206, 1015, 911, 738

1H NMR (400 MHz, CDCl3): 4.12 (s, 1H, OH), 4.31-4.33 (d, 2H, CH2), 6.33-6.40 (m, 1H, HC=CH), 6.60-6.64 (d, 1H, CH), 7.22-7.40 (m, 5H, ArH) ppm.

but-2-ene-2-ol (3k):1H NMR (400 MHz, CDCl3): 2.52 (d, 3H, CH3), 3.92 (s,1H, OH), 4.42 (d, 2H, CH2), 5.66-5.75 (m, 2H, HC=CH) ppm.

4-(4-chlorophenyl)but-3-en-2-ol (3l): IR (υ, cm-1): 3347, 2873, 1953, 1874, 1810, 1646, 1495, 1453, 1206, 1015, 911, 739, 595.

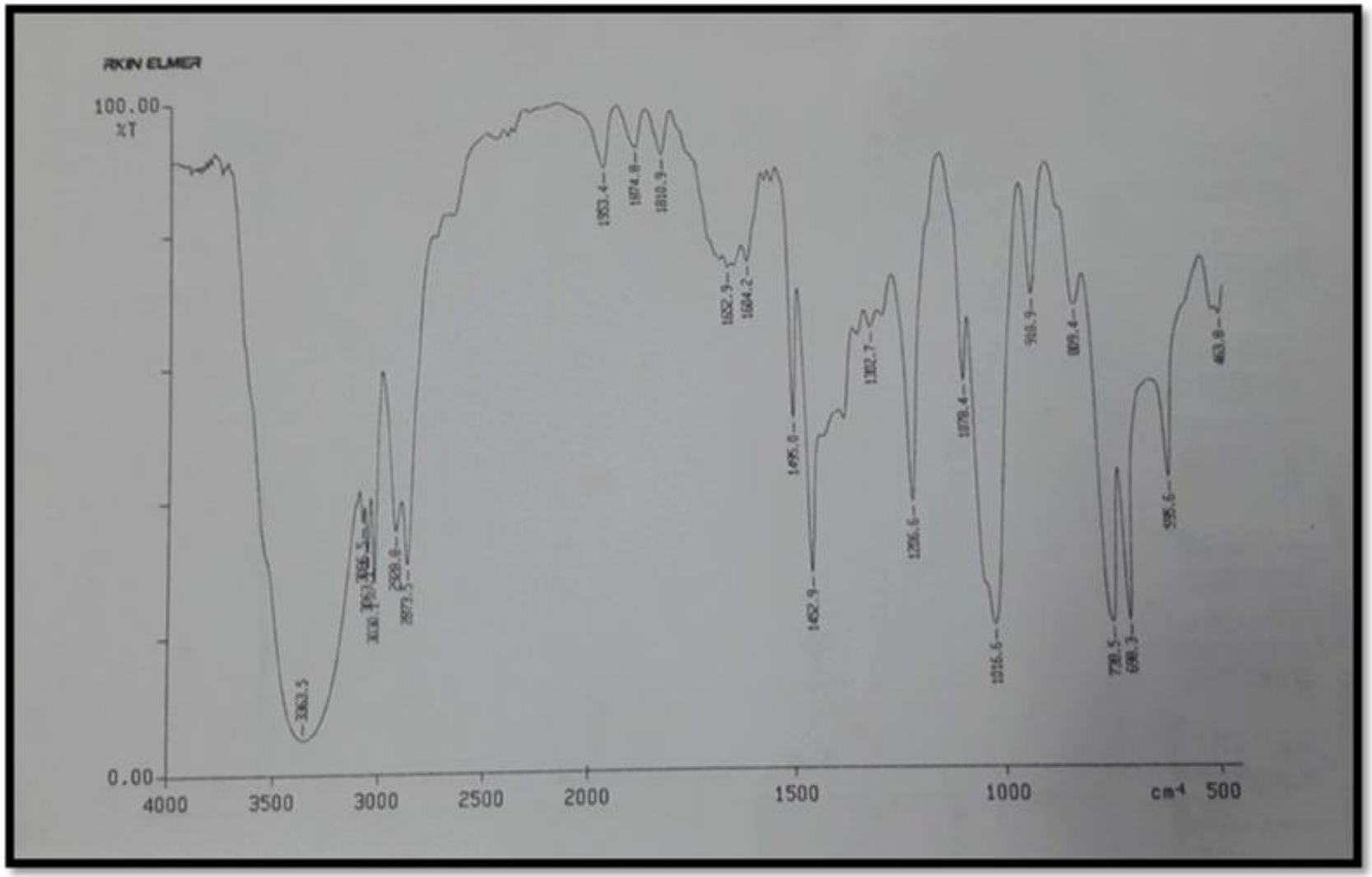
1H NMR (400 MHz, CDCl3): 2.45 (s, 1H, OH), 4.59 (d, 2H, CH2), 7.22 (s, 1H, HC=CH), 7.26-7.33(m, 5H, CH) ppm.

4-(p- tolyl)but-3ene-2ol (3m): 1H NMR (400 MHz, CDCl3): 2.75 (d, 3H, CH_3), 3.76 (s, 1H, OH), 4.44 (d, 2H, CH_2), 6.4 (d, 1H, CH), 6.6 (1H, CH), 7.17 – 7.24 (m, 4H, ArH) ppm.

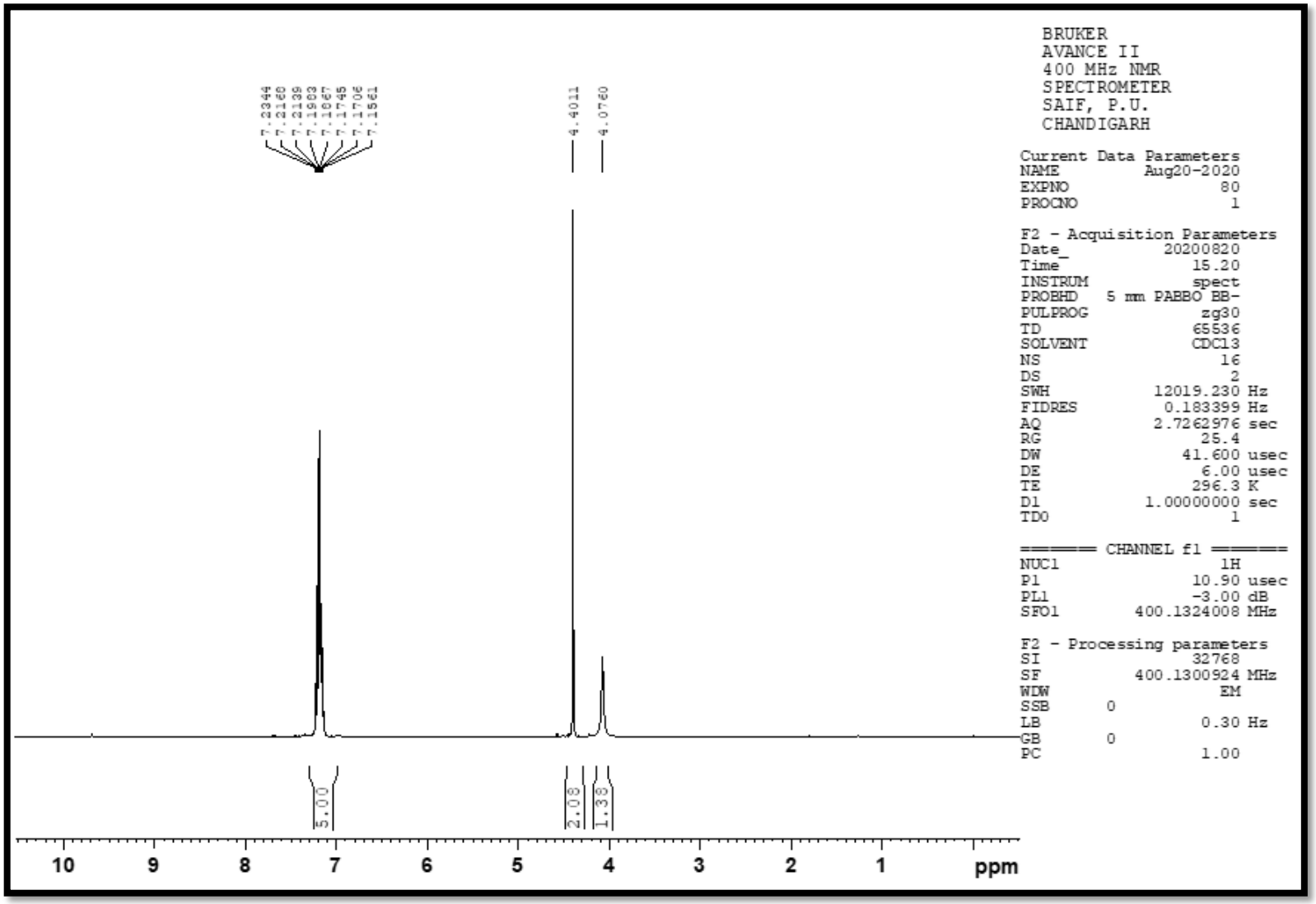
1,3 phenylprop-2-en-1-ol (3n): 1H NMR (400 MHz, CDCl3): 3.46 (s, 1H, OH), 5.78 (s,1H, CH), 6.73-6.89 (m, 2H, HC=CH), 7.30-7.89(m, 10H, ArH) ppm.

1-(4-chlorophenyl)-3-phenylprop-2-ene-1-ol (3o):1H NMR (400 MHz, CDCl3): 3.36 (s, 1H, OH), 5.19 (s,1H, CH), 6.06-6.29 (m, 2H, HC=CH), 7.30-7.75 (m, 9H, ArH) ppm.

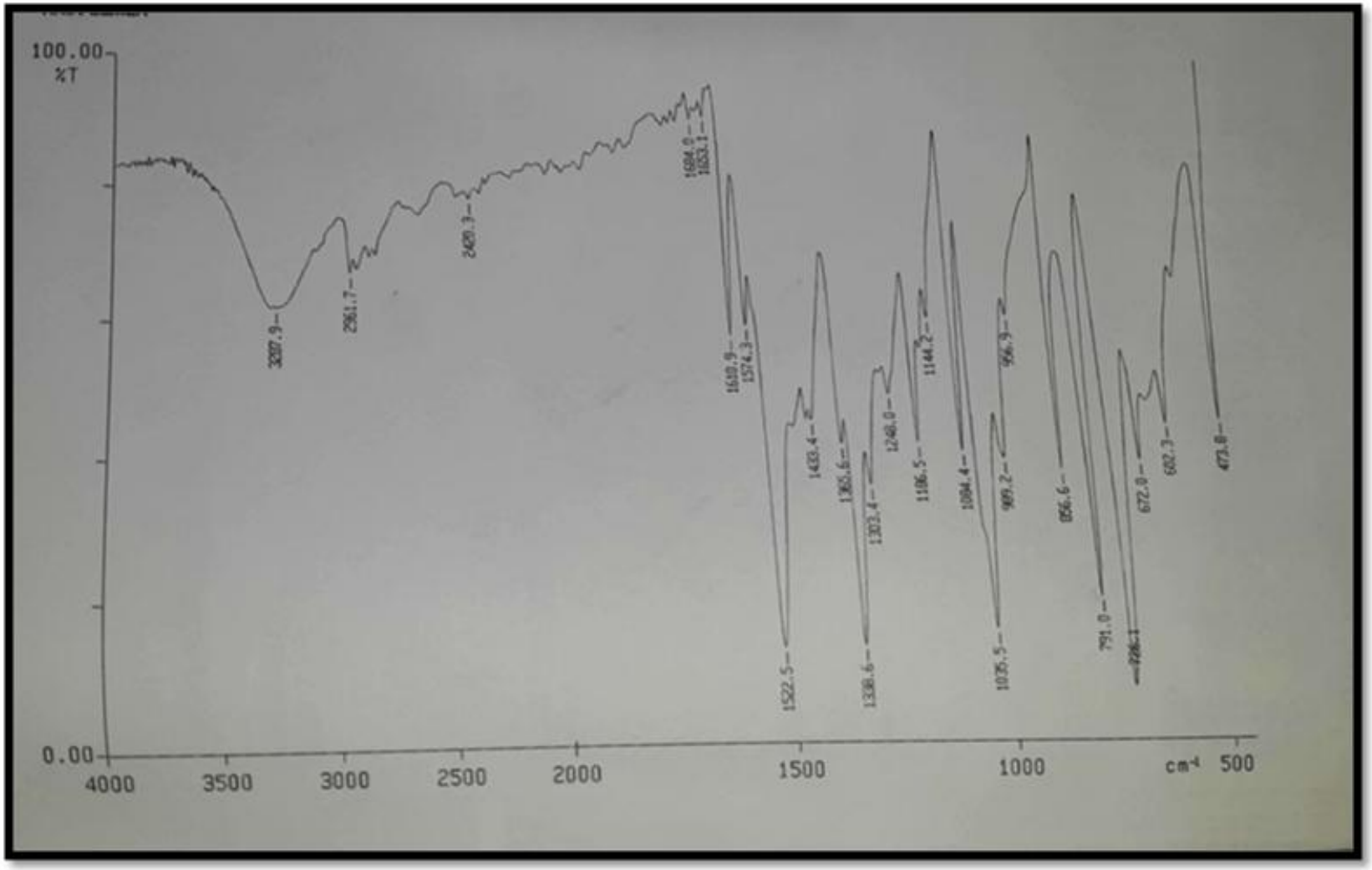
IR Spectra of Phenyl methanol (3a-3h)



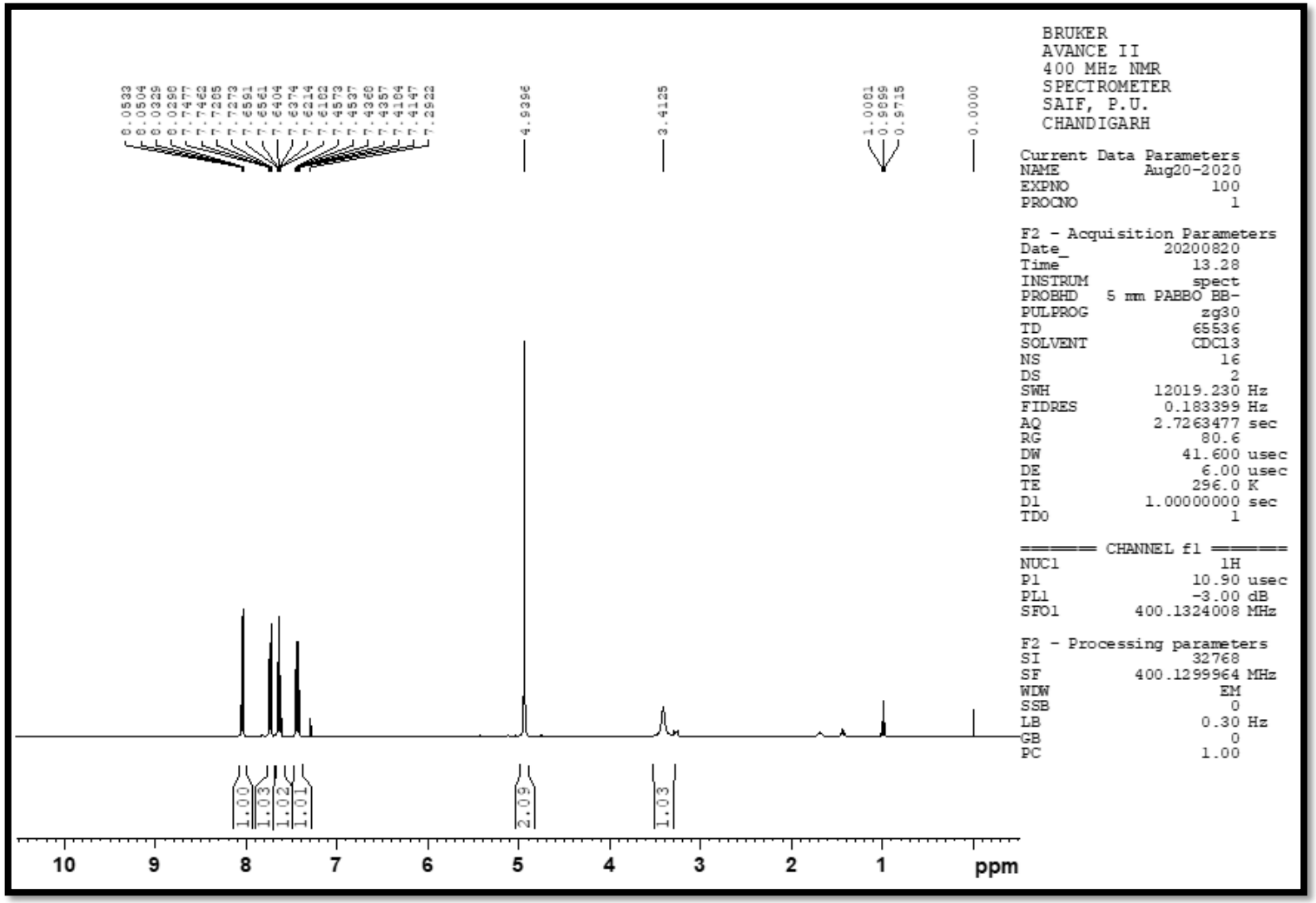
[1]HNMR Spectra of Phenyl methanol (3a-3h)



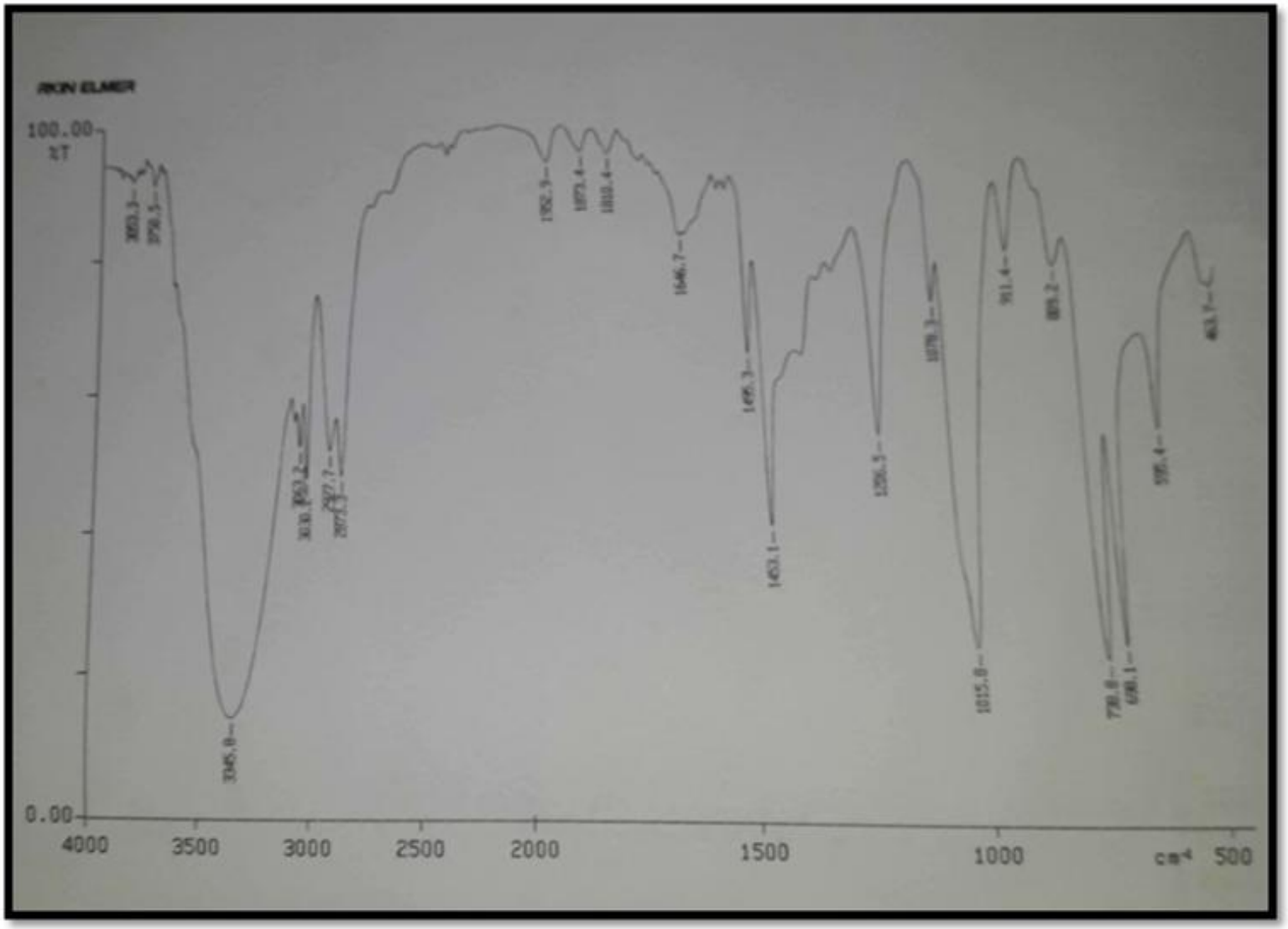
IRSpectra of 2- Nitro Phenyl methanol (3i)



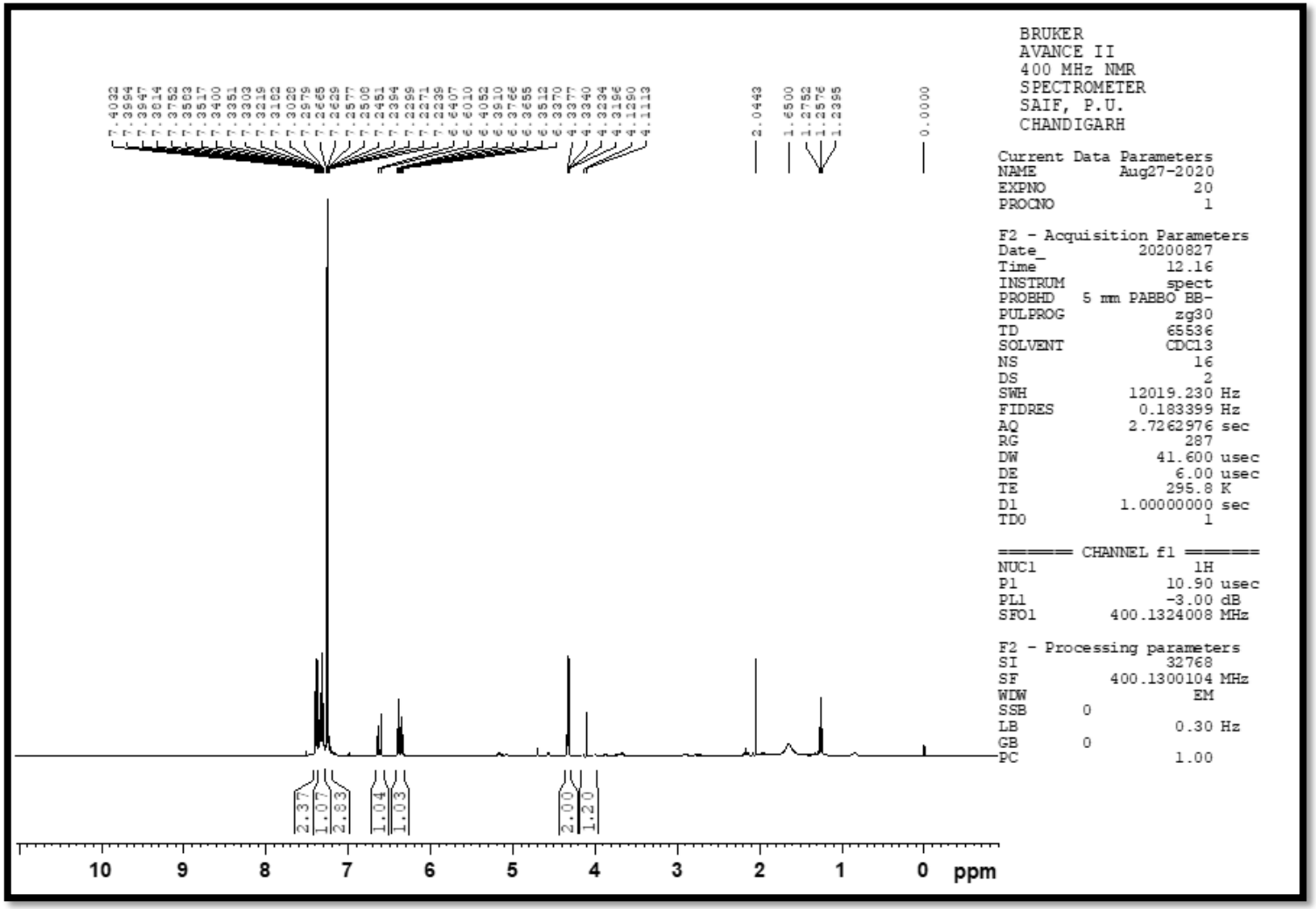
[1]HNMR Spectra of 2- Nitro Phenyl methanol (3i)



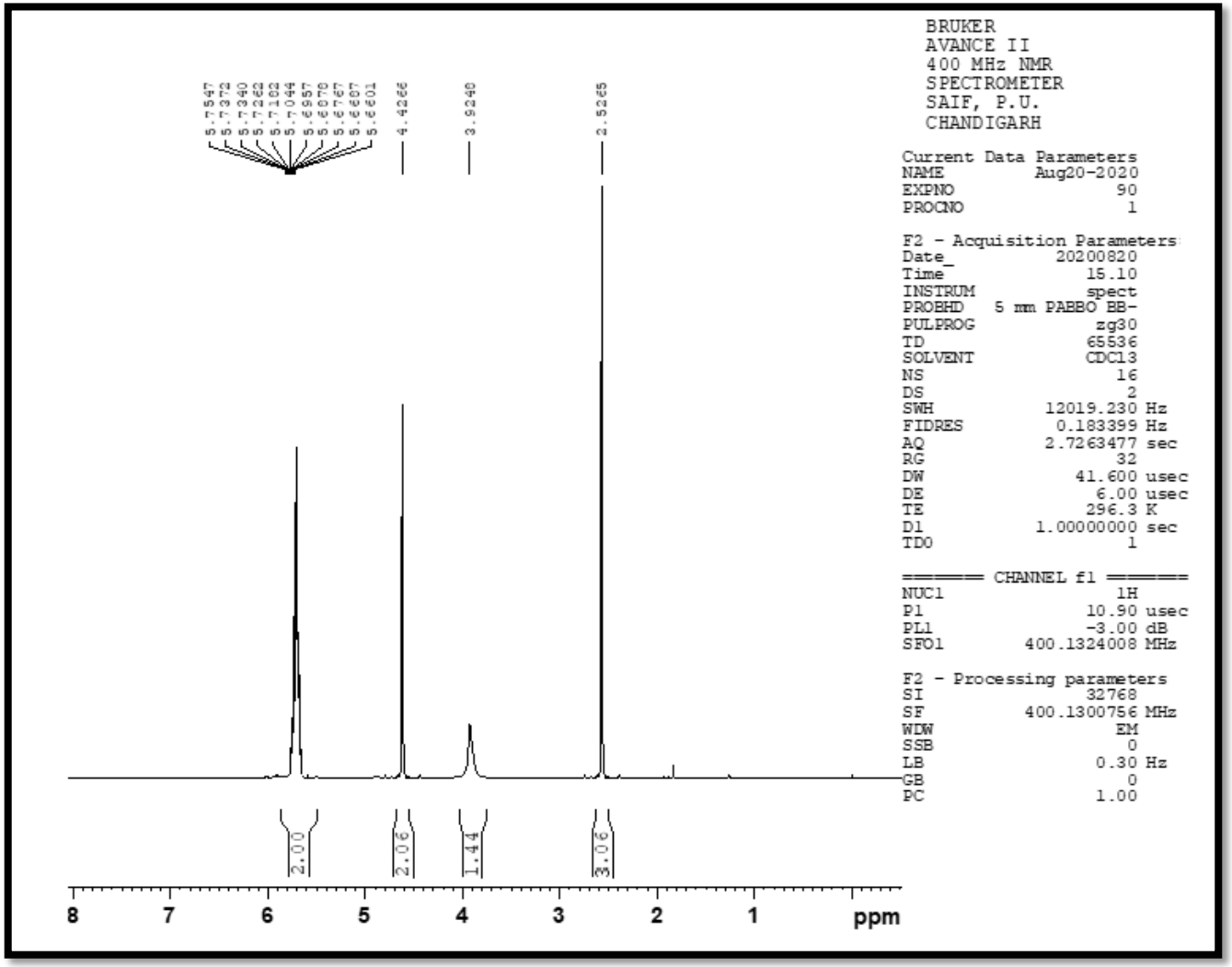
IR Spectra of 3-phenylprop-2-en-1-ol (3j)



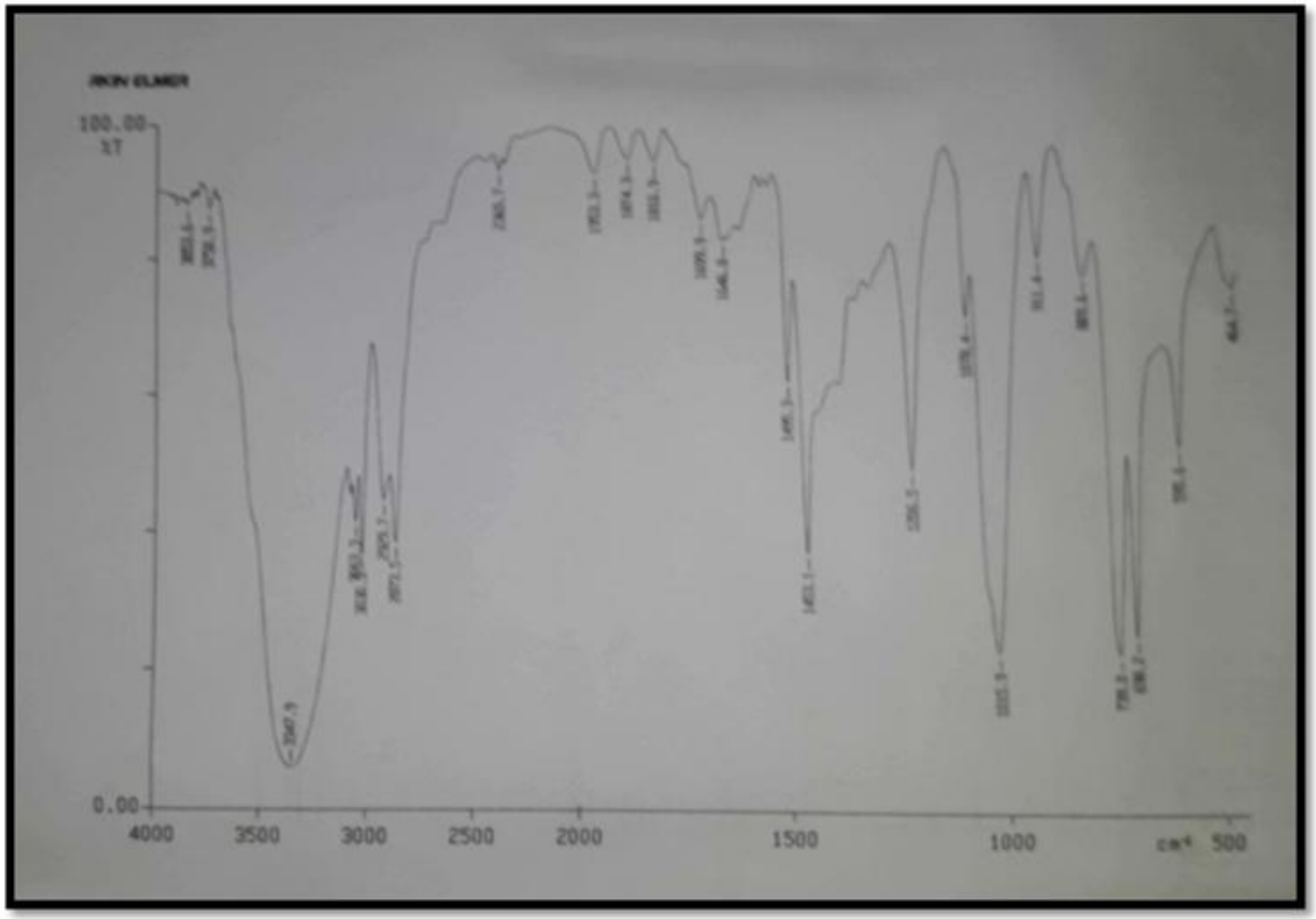
[1]HNMR Spectra of 3 phenylprop-2-en-1-ol (3j)



[1]HNMR Spectra of but-2-ene-2-ol (3k)



IR Spectra of 4-(4-chlorophenyl)but-3-en-2-ol (3l)



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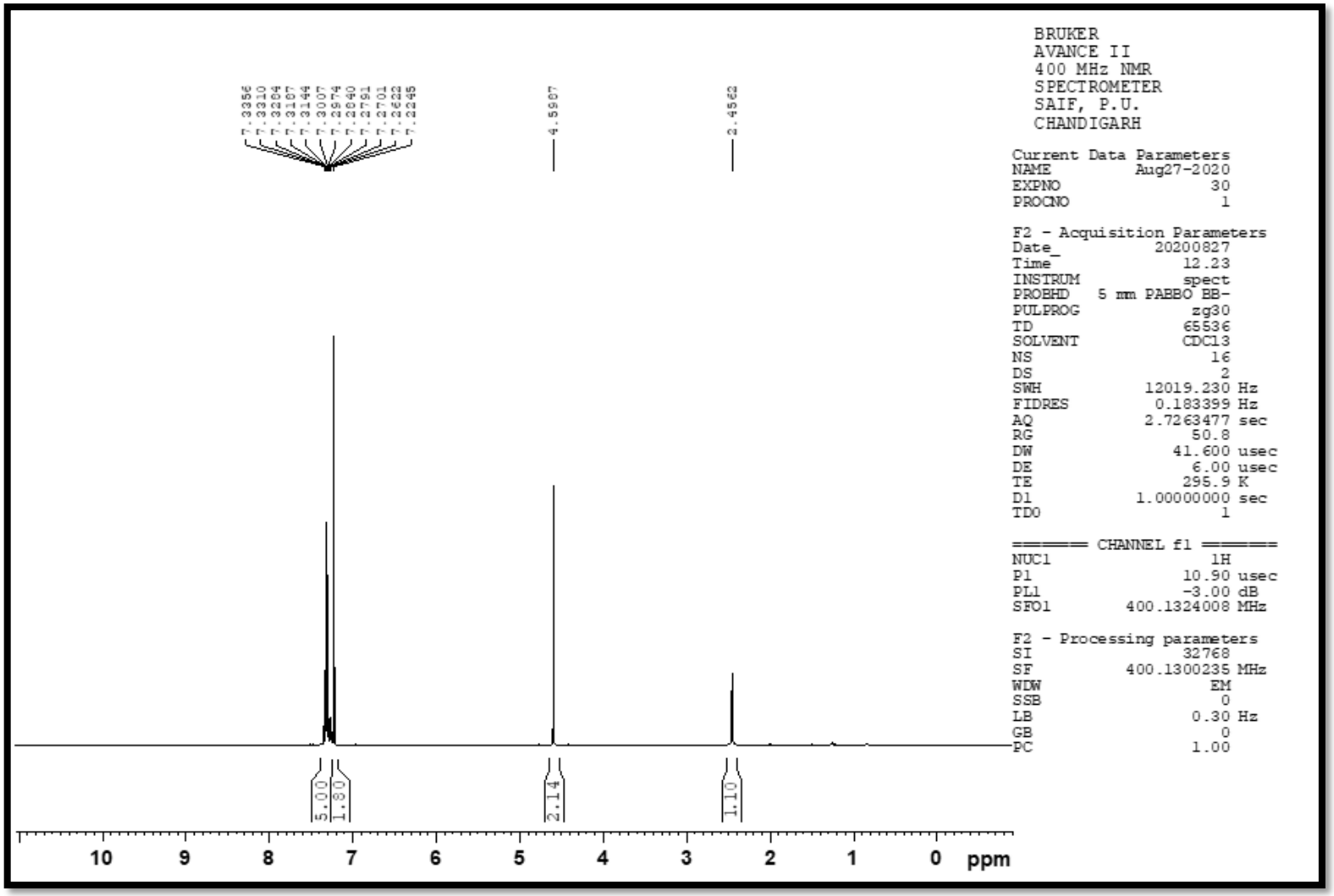
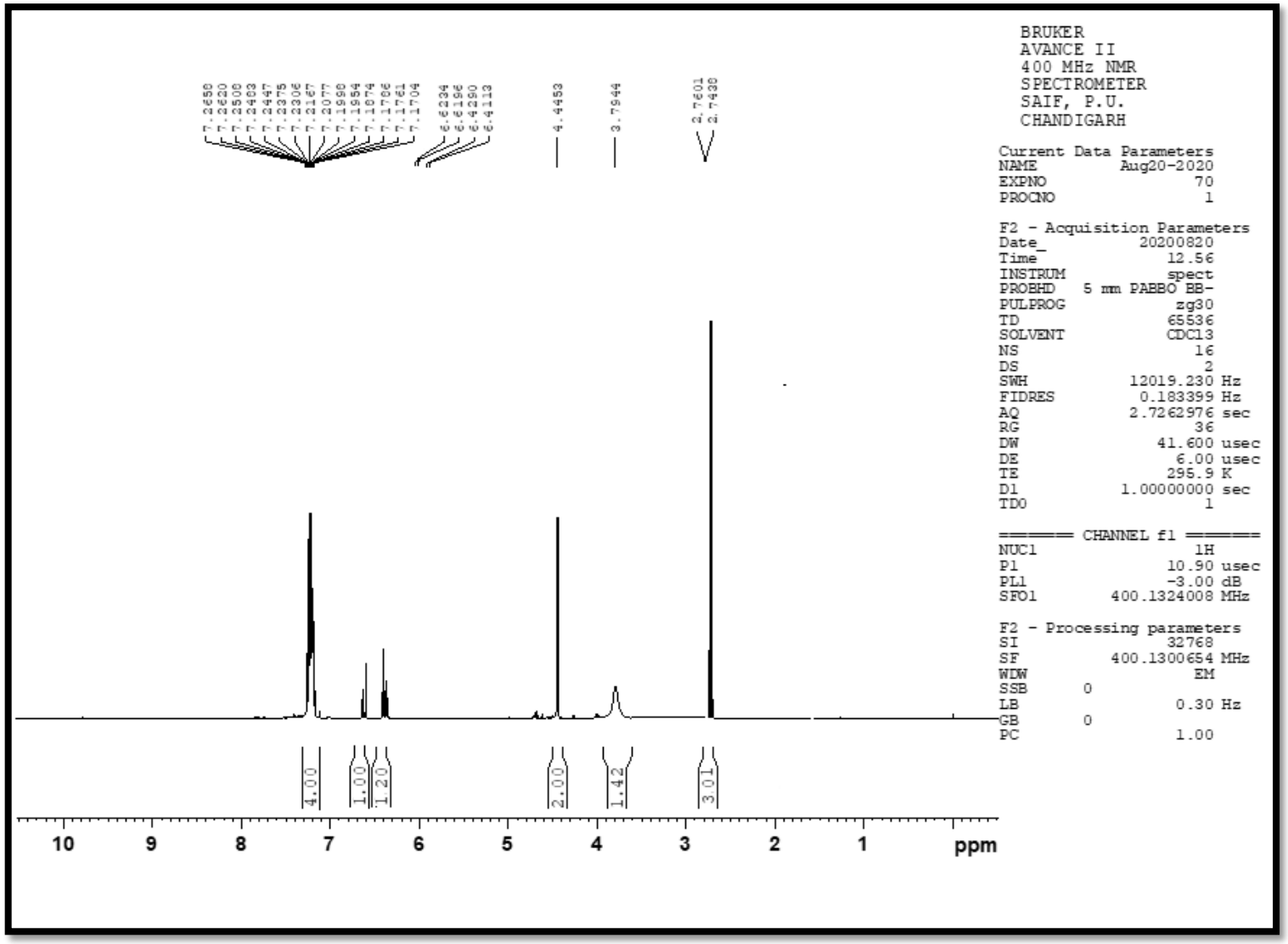
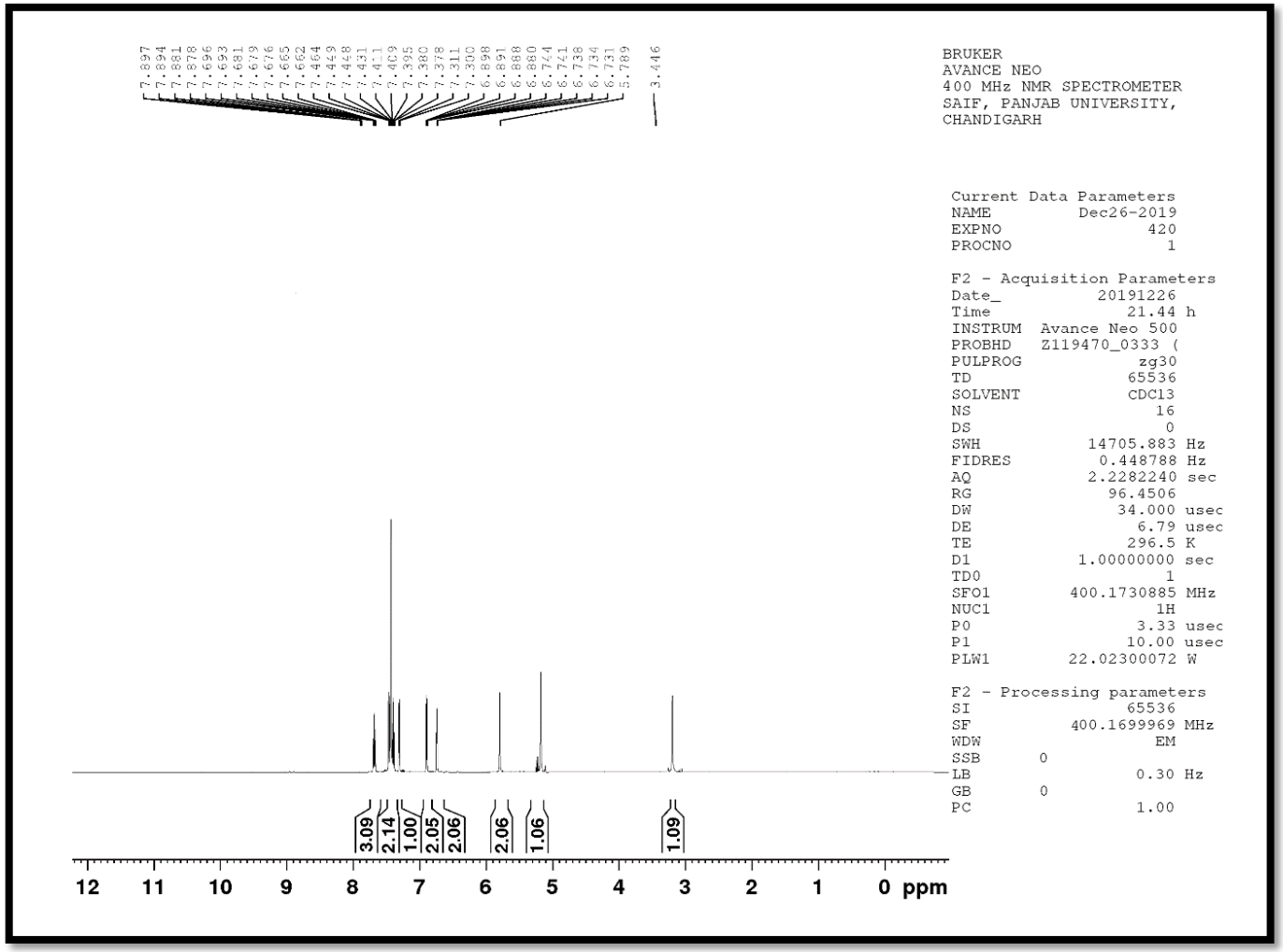


[1]HNMR spectra of 4-(p- tolyl)but-3ene-2ol (3m)



[1]HNMR Spectra 1,3 phenylprop-2-en-1-ol (3n)



[1]HNMR spectra of 1-(4-chlorophenyl)-3-phenylprop-2-ene-1-ol (3o)