Supplemental Material

Potassium phosphate catalyzed synthesis of substituted o-propargylsalicylaldehydes

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A. General:

Various substituted salicylaldehydes (Sigma Aldrich), Propargyl bromide (Sigma Aldrich) were used as received. Melting points (M.P) recorded were determined in open capillary and are uncorrected. IR spectra were recorded on ATR-IR-4600 spectrometer. NMR spectra were recorded on Bruker AMX-400 spectrometer (400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR) in $CDCl_3$ employing TMS as an internal standard and δ values are expressed in ppm.

B. Typical procedure:

Synthesis of o-propargyl salicylaldehydes:

In 25 mL round bottom flask containing salicylaldehyde (1 mmol), propargyl bromide (1.2 mmol) in DMF (5mL) was added anhydrous K_3PO_4 (1.1 mmol), and stirring was carried out till completion of reaction. Progress of reaction was monitored by TLC. Then ice was added to reaction mixture. Precipitated product formed was filtered and washed with water and dried.

Spectral data of o-propargyl salicylaldehyde derivatives

Entry 3a, Table 3: 2-(prop-2-ynyloxy)*benzaldehyde*

Brownish solid; Obs. m.p. 70 °C, Lit. m.p. 69.0-72.0 ^{o}C (CAS No.- 29978-83-4), IR (Figure 1): 3269, 2928, 2871, 2108, 1678, 1597, 1458, 1296, 1215, 1003, 744, 679 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) (Figure 2): δ 10.48 (s, 1H, -CHO), 2.57 (s, 1H, Propargyl-CH), 4.83 (d, 2H, -OCH_2), 7.07-7.13 (m, Ar-2H), 7.54-7.59 (m, Ar-1H), 7.84-7.87 (dd, Ar-1H, *J* 8 Hz, 1.6 Hz) ppm [25]; ^{13}C NMR (400 MHz, $CDCl_3$) (Figure 3, 4): δ 56.36, 113.16, 121.68, 125.46, 128.58, 135.72, 159.74, 189.57 ppm

Entry 3i, Table 3 : *3,5-dichloro-2-(prop-2-ynyloxy)benzaldehyde*

White solid; Obs. m.p. 82-84 ^{o}C, Lit. m.p. 84-86 °C (CAS No.-1126527-53-4); IR (Figure 5): 3268, 2975, 2869, 2113, 1683, 1598, 1479, 1457, 1400, 1286, 1218, 1193, 1103, 1043, 1012, 923, 831, 757, 698 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) (Figure 6): δ 10.39 (s, 1H, -CHO) ,2.55 (s, 1H, Propargyl-CH), 4.90 (d, 2H, -OCH_2), 7.64-7.65 (d, Ar-1H, *J* 2.4 Hz), 7.77-7.78 (d, Ar-1H, *J* 2.4 Hz) ppm [25]; ^{13}C NMR (400 MHz, $CDCl_3$) (Figure 7, 8): δ 61.84, 70.25, 77.21, 126.41, 129.75, 131.33, 132.79, 135.58, 188.18 ppm

IR, ^{1}H and ^{13}C NMR spectra of synthesized o-propargyl salicylaldehyde derivatives

Entry 3a, Table 3:

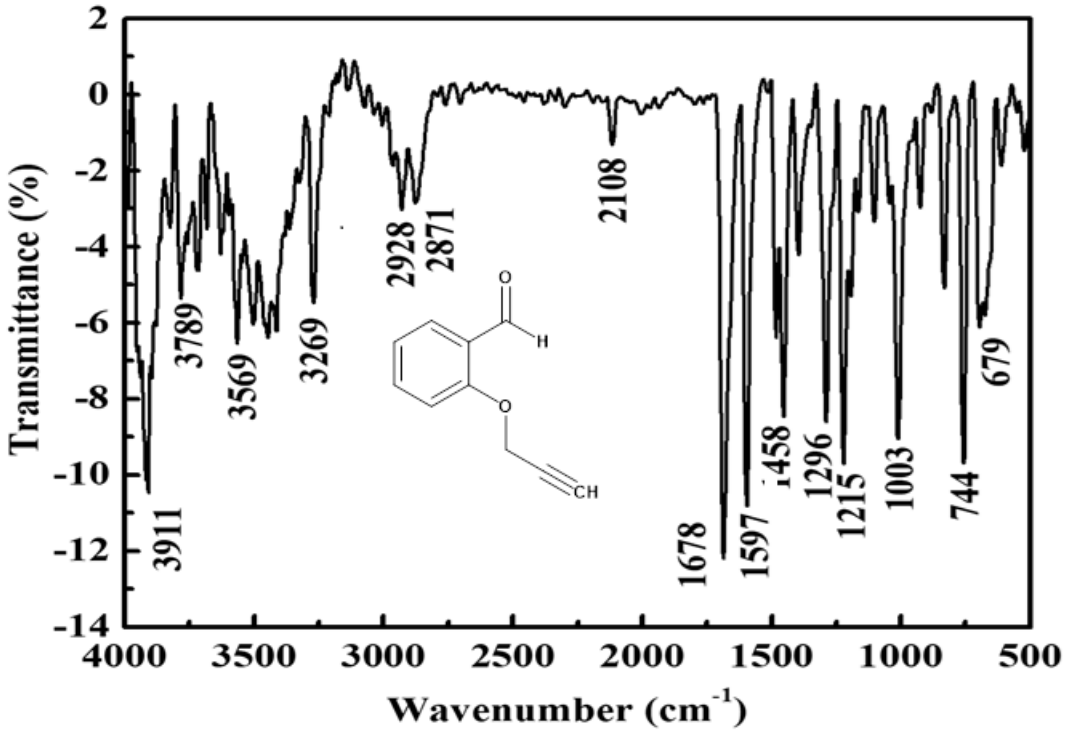

Figure 1

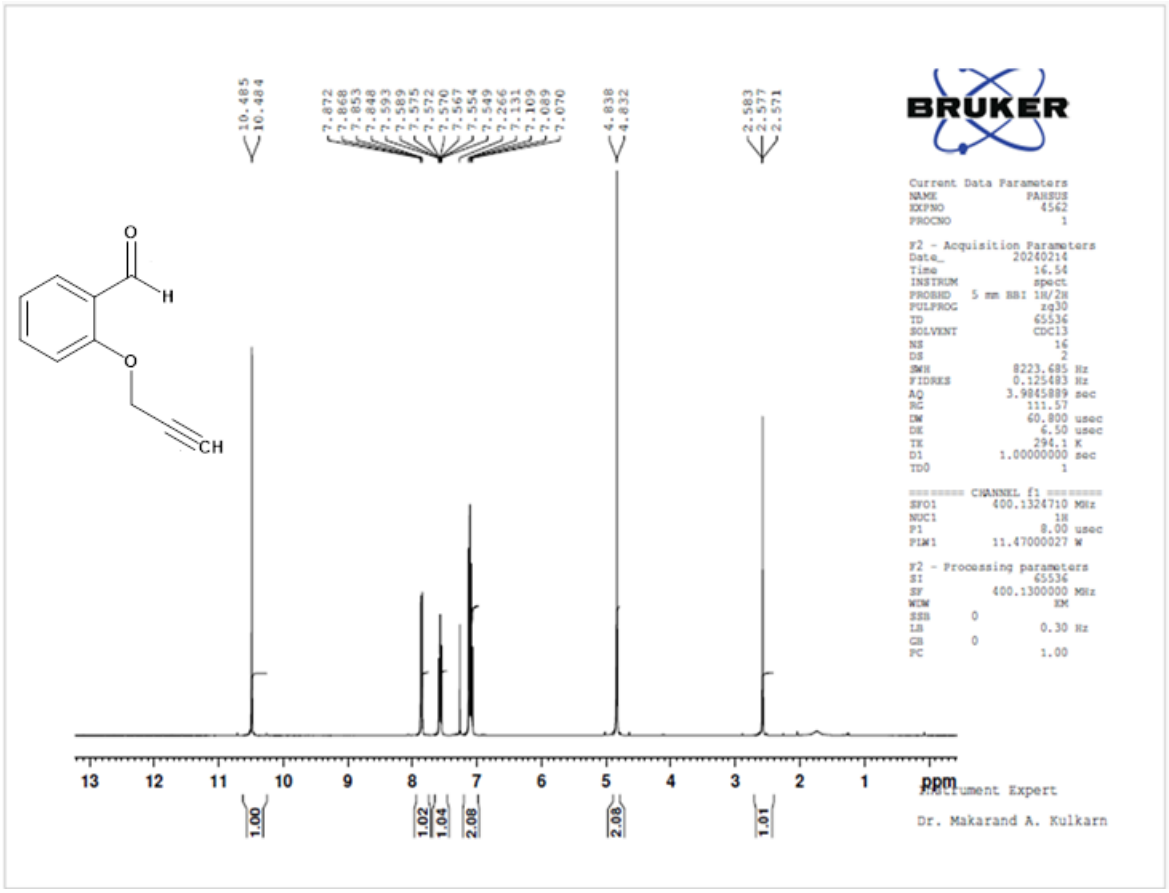

Figure 2

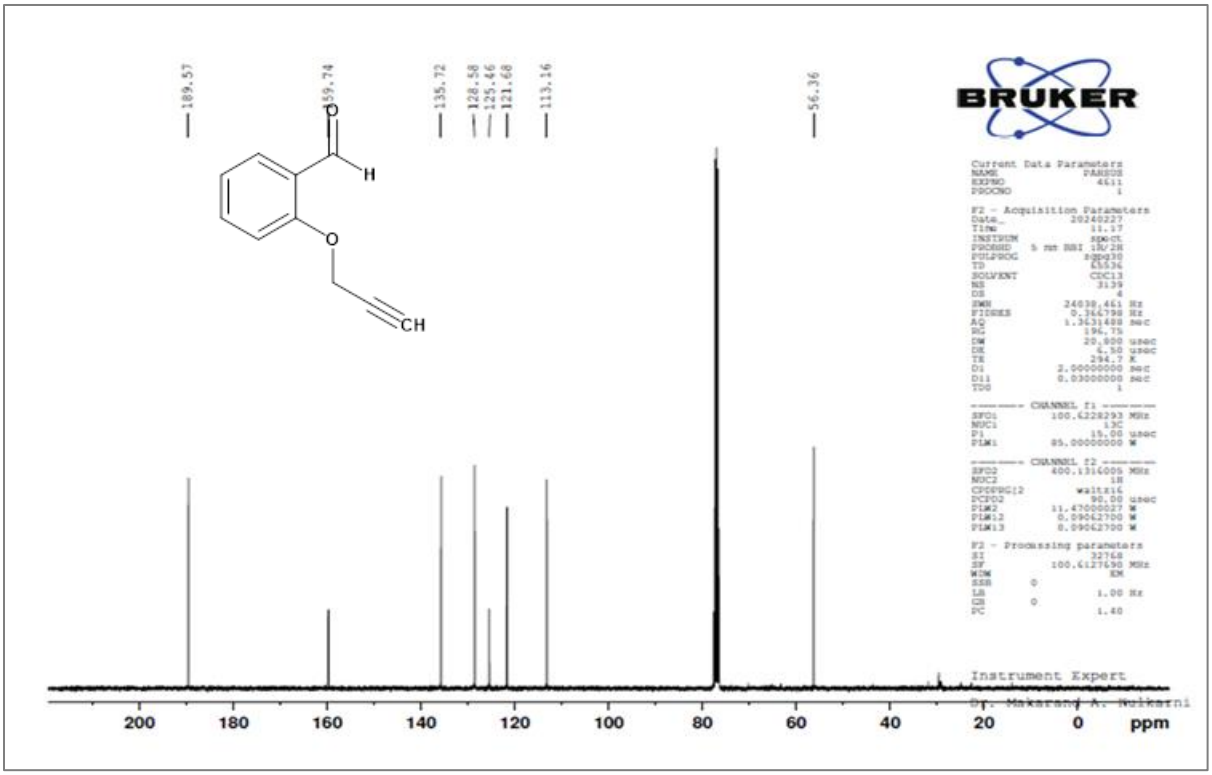

Figure 3

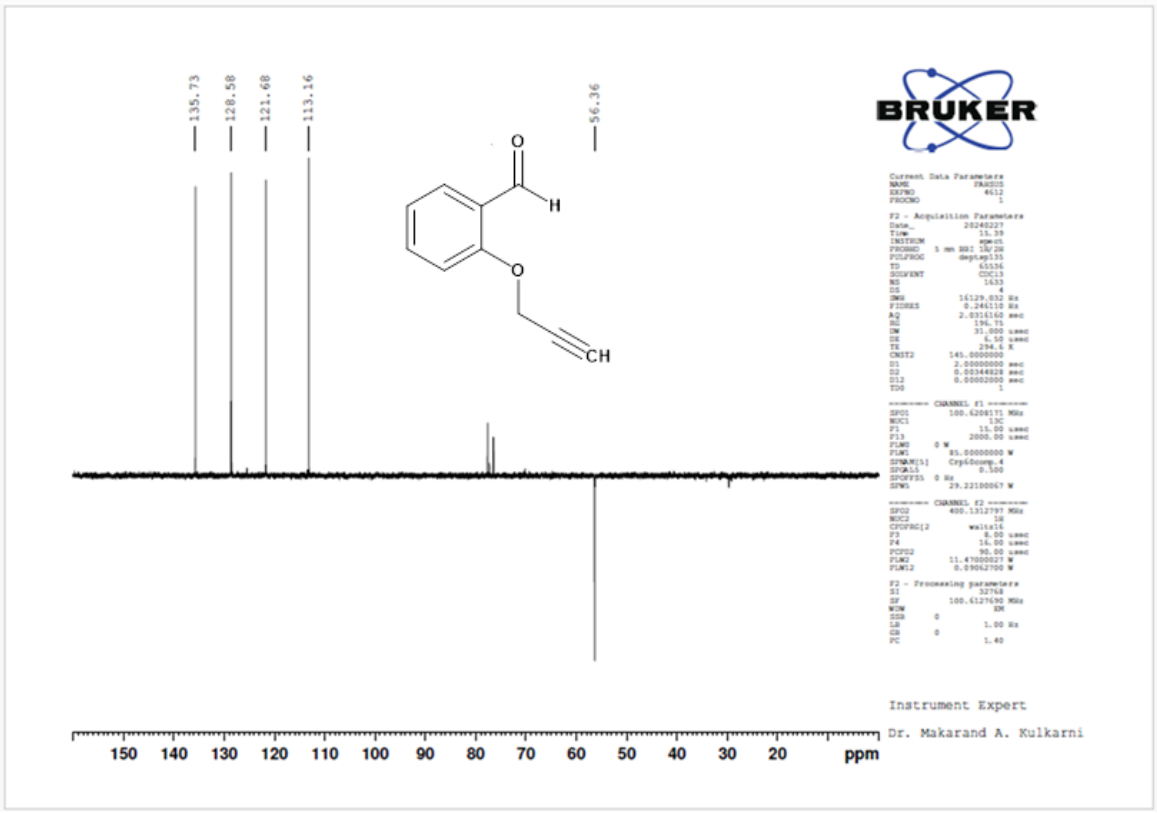

Figure 4

Entry 3i, Table 3:

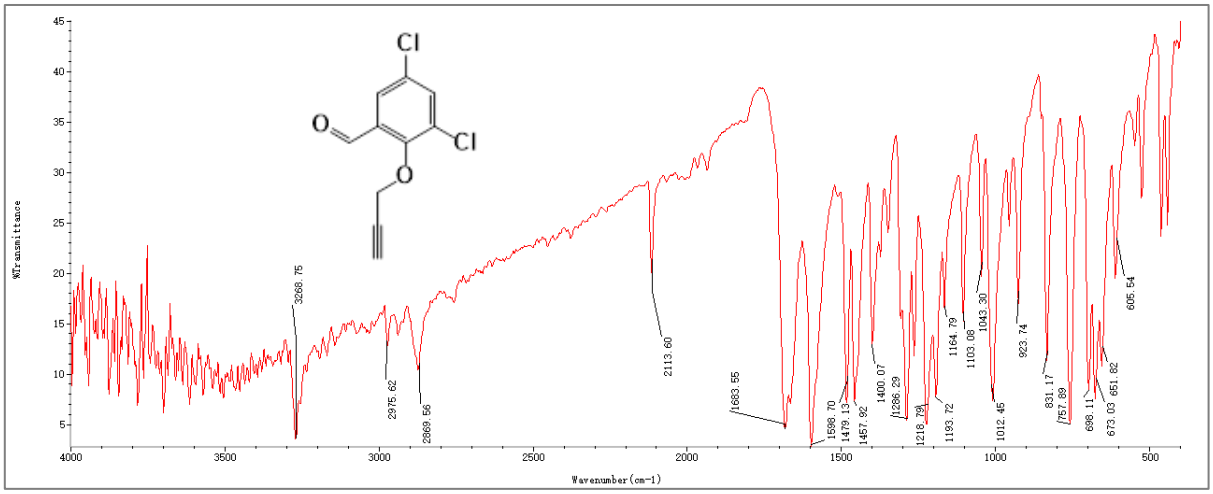

Figure 5

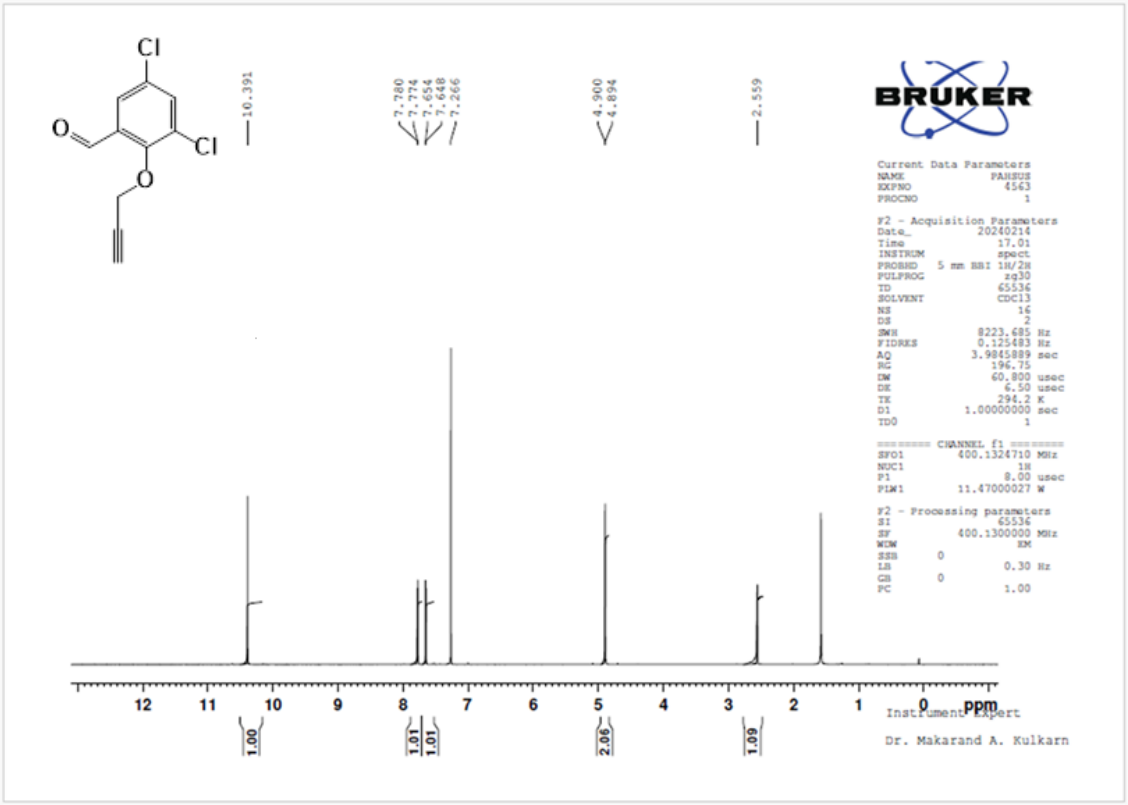

Figure 6

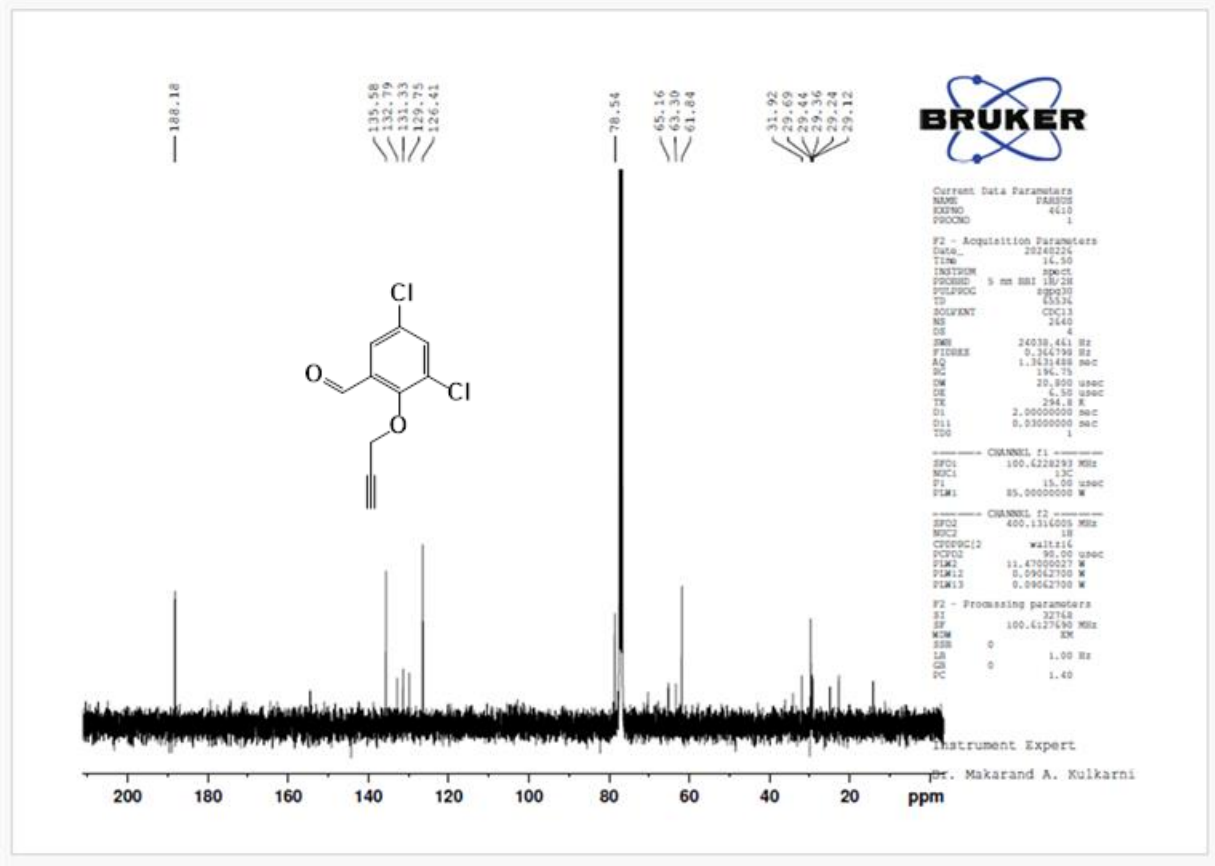

Figure 7

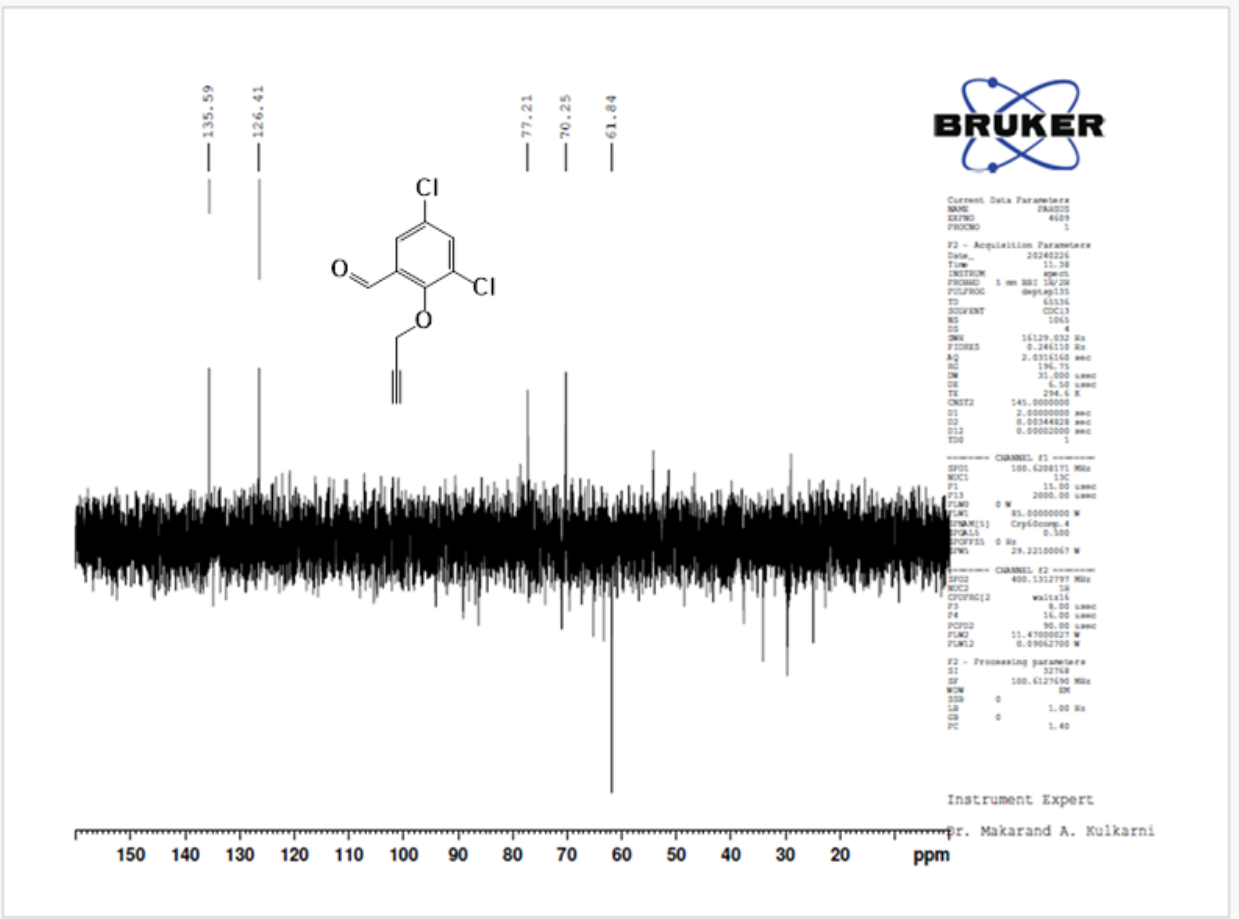

Figure 8

