

Supplementary Information

Water extract of pomegranate ash (WEPA) catalyzed, green and efficient, one-pot multicomponent synthesis of 5-aminopyrazole-4-carbonitrile

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1.0 Data and values:

1. Physical and spectral data of all synthesized 5-aminopyrazole-4-carbonitrile

Structures of all the compounds were established on the basis of ^1H NMR, ^{13}C NMR, Physical data of all the compounds were found to be consistent to the structures assigned to these molecules.

Spectral Analysis of synthesized compounds

5-Amino-1,3-diphenyl-1H-pyrazole-4-carbonitrile (KNP 150)

Pale yellow solid; Yield: 92%; M.P.: 158-160°C. ^1H -NMR(DMSO- d_6 , 400MHz, δ ppm.): δ 7.87 (d, 2H); 7.39 (t, 2H); 7.10 (t, 1H); 7.36 (d, 2H); 7.27 (t, 2H); 6.90 (t, 1H), 10.29 (s, 2H). ^{13}C -NMR (101 MHz, DMSO- d_6) δ 145.9, 137.0, 136.4, 129.6, 129.2, 128.4, 126.1, 119.3, 112.6, 40.7, 40.5, 40.3, 40.1, 39.9, 39.7, 39.5

5-Amino-3-(4-bromo-phenyl)-1-(3,5-dinitro-phenyl)-1H-pyrazole-4-carbonitrile(KNP151)

Yellow solid; Yield: 92%; M.P.:152-155°C. ^1H -NMR(DMSO- d_6 , 400MHz, δ ppm.): 7.81(d, 2H); 7.57 (t, 2H); 7.55 (t, 1H); 7.20 (d,2H); 7.51 (d, 2H); 10.39 (s, 2H) ^{13}C -NMR (101 MHz, DMSO- d_6) δ 145.6, 135.7, 135.6, 132.1, 129.6, 128.0, 121.2, 119.5, 112.6, 40.7, 40.5, 40.3, 40.1, 39.9, 39.7, 39.5

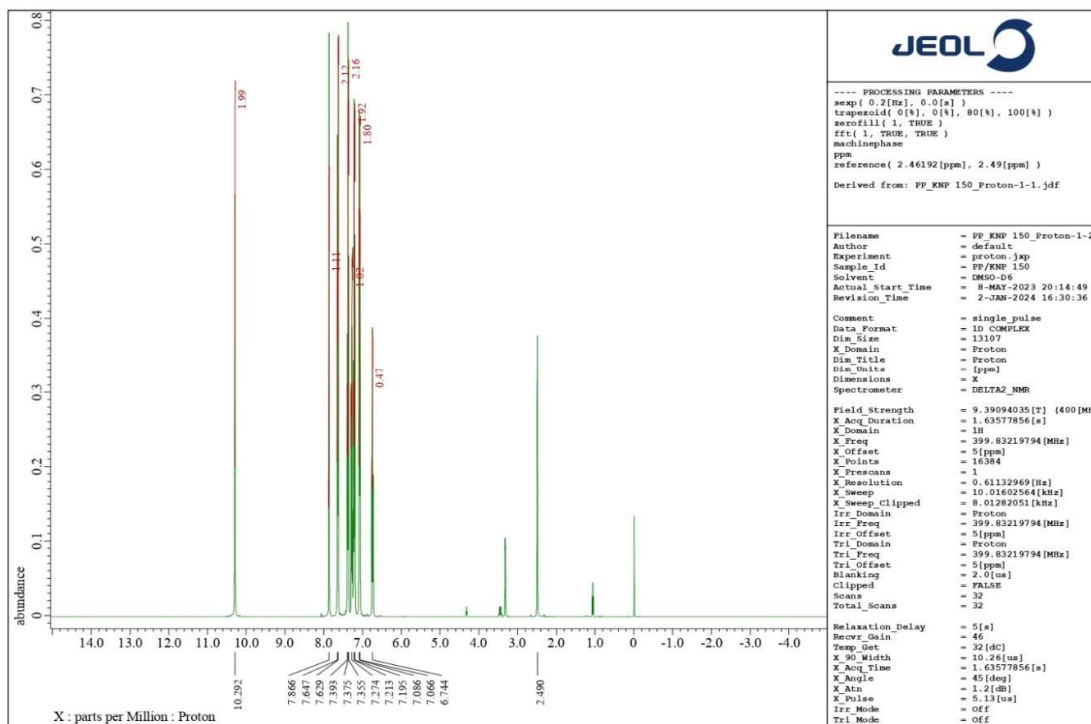
5-Amino-3-(4-chloro-phenyl)-1-phenyl-1H-pyrazole-4-carbonitrile(KNP 152) :Chrome

yellow solid; Yield: 90%; M.P.:128-130°C. ^1H -NMR(DMSO- d_6 , 400MHz, δ ppm.): 7.87

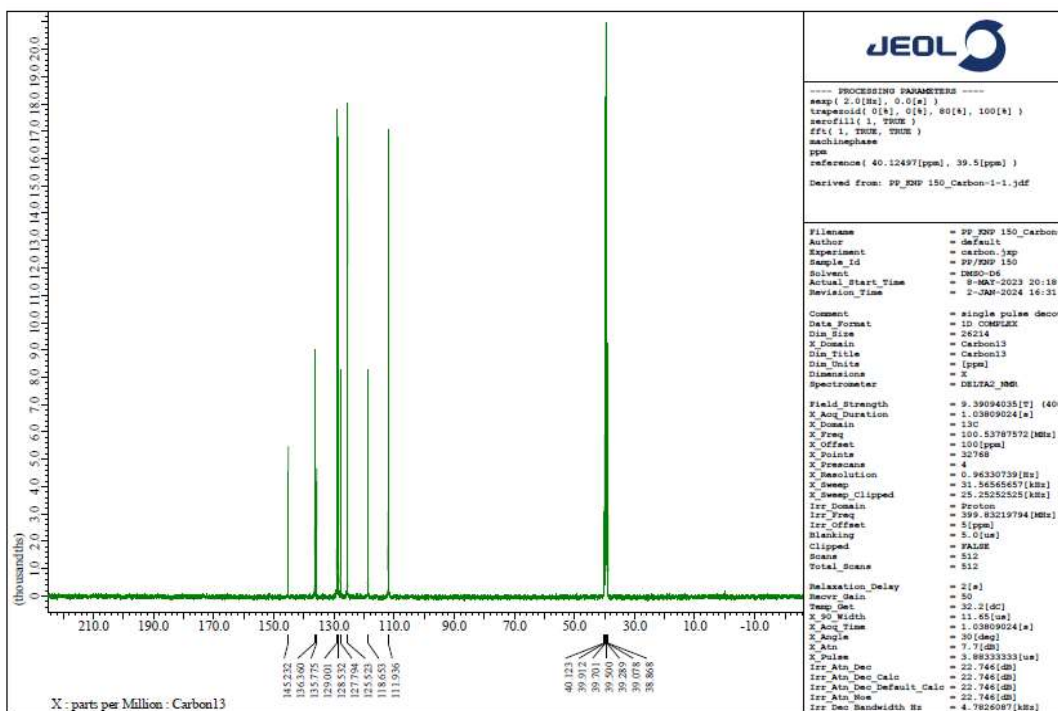
(d, 2H); 7.66 (t, 2H); 7.64 (t, 1H); 7.42 (d, 2H); 7.23 (d, 2H); 10.38 (s, 2H).¹³C-NMR (101 MHz, DMSO-*d*₆) δ 145.6, 135.6, 135.4, 132.6, 129.6, 129.2, 127.7, 119.5, 112.6, 40.7, 40.5, 40.3, 40.1, 39.9, 39.7, 39.5

5-Amino-3-(3-methoxy-phenyl)-1-phenyl-1*H*-pyrazole-4-carbonitrile (KNP 153) :Pale yellow solid; Yield: 91%; M.P.:162-164°C. ¹H-NMR(DMSO-*d*₆, 400MHz, δ ppm.): 7.85 (d, 2H); 7.66 (t, , 2H); 7.55 (t, 2H); 7.44(d, 1H); 7.84 (t, 1H); 6.66 (d, 1H); 6.65 (s, 1H); 5.2 (s, 2H); 10.3 (s, 2H).¹³C-NMR (101 MHz, DMSO-*d*₆) δ 159.9, 146.1, 137.2, 129.6, 129.1, 127.6, 118.9, 114.7, 112.4, 55.7, 40.7, 40.5, 40.3, 40.1, 39.9, 39.7, 39.5

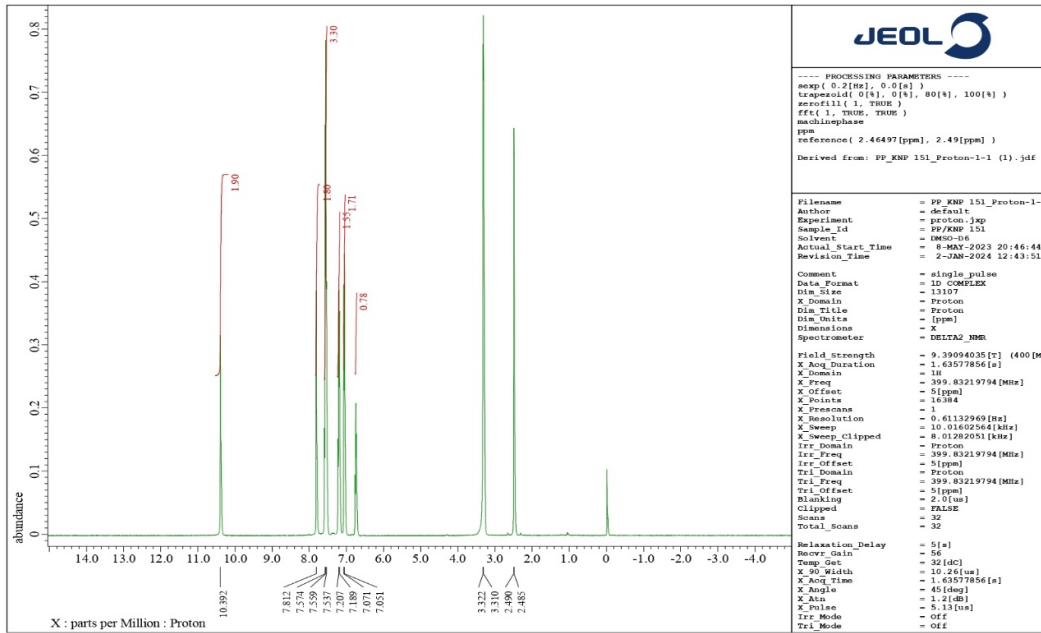
KNP 150 ¹H NMR



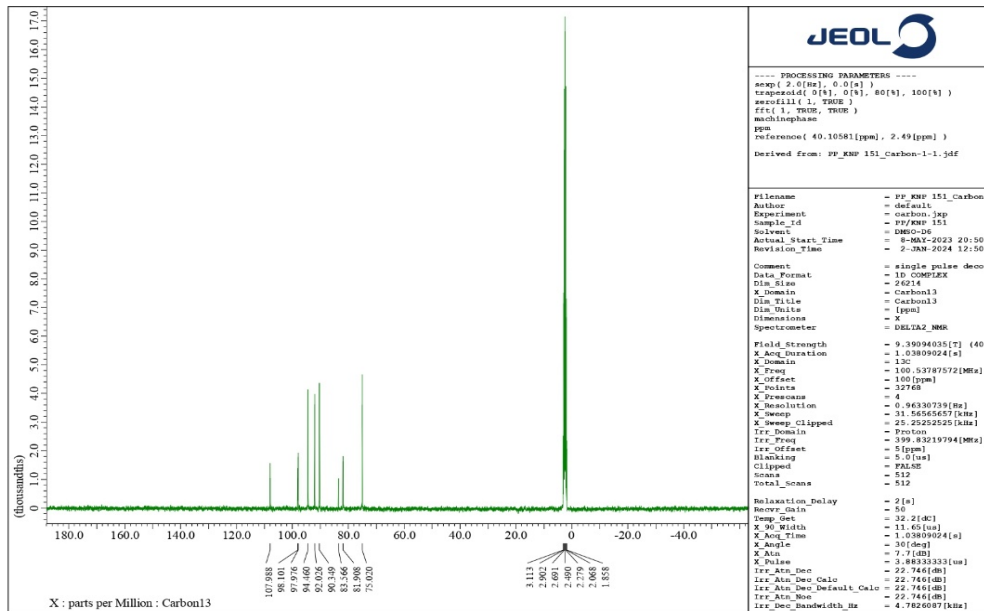
KNP 150 ¹³C NMR



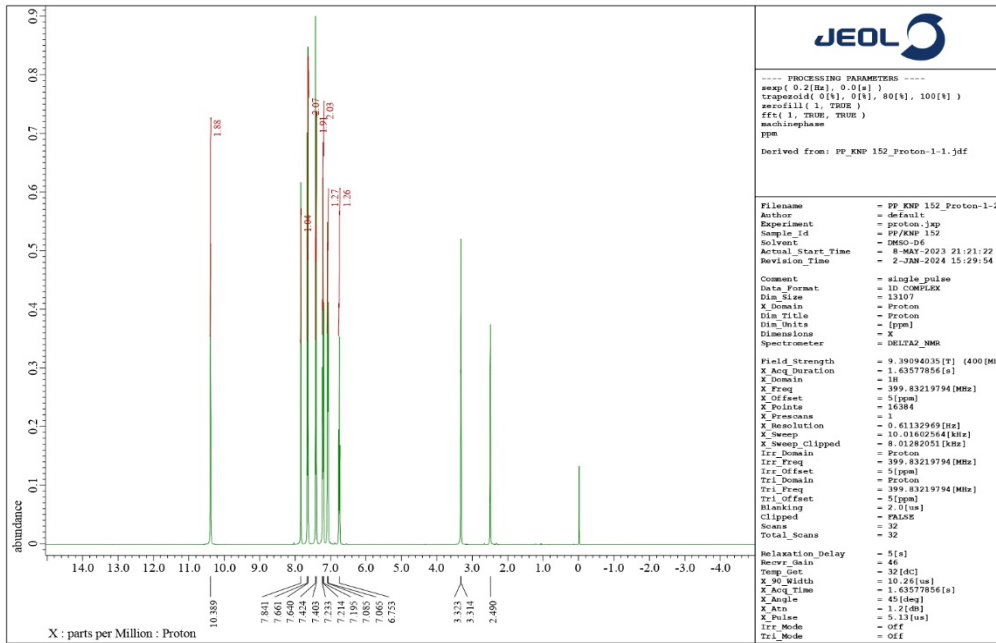
KNP 151 ¹H NMR



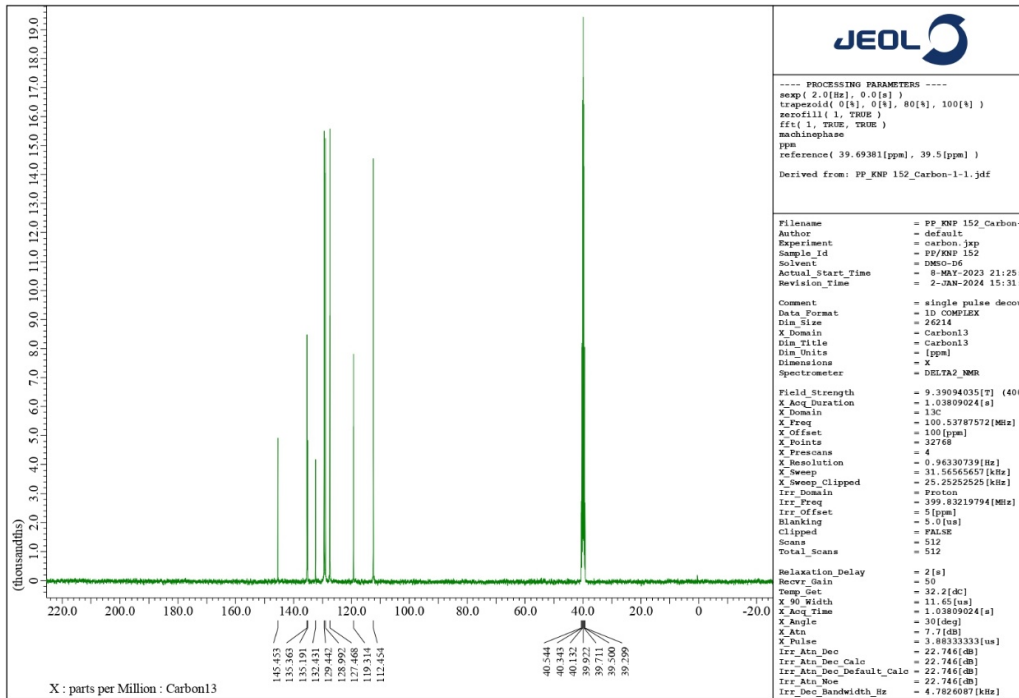
KNP 151 ¹³C NMR



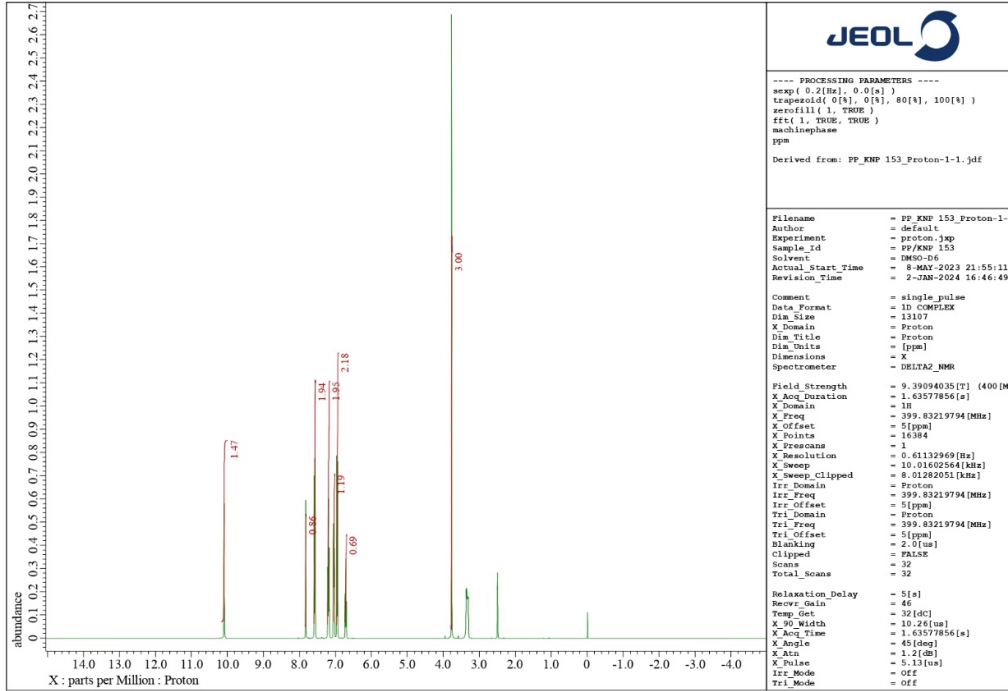
KNP 152 ¹H NMR



KNP 152 ¹³C NMR



KNP 153 ¹H NMR



KNP 153 ¹³C NMR

