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Supporting Information

Designing a New Method for Growing of Metal-Organic Framework (MOF) on MOF: Synthesis, Characterization and Catalytic Application

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Experimental

General

All reagents used in this work were consumed without more purification and were obtained from Sigma-Aldrich and Merck chemical companies. The progress of the reaction and the purity determination of the products was accomplished by thin-layer chromatography (TLC) upon silica gel polygram STL G/UV 254 polyester sheets. Using an Electrothermal Type 9100 melting point apparatus the melting points of the synthesized products were determined. The spectra of FT-IR in transmission method 4000-400 cm^{-1} were collected on an AVATAR 370 FT-IR Thermo Nicolet spectrometer at room temperature. The NMR spectra were measured with a Bruker Avance 300 and 400 MHz instruments in DMSO-d_6. Mass spectra were exported with a CH7A Varianmat Bremem instrument at 70 eV electron impact ionization, in *m/z* (rel %). The crystal structure of the catalyst was characterized by PANalytical Company X'Pert Pro MPD diffractometer with Cu K_α (λ = 0.154 nm) radiation. BET surface area and pore size distributions (PSD) were calculated from their nitrogen adsorption isotherms using a Quantachrome instrument version 2.2 at -196

˚C. Transmission electron microscopy (TEM) was also employed in order to obtain the size and structure of the particles using an EM10C-100 KV microscope (Zeiss, Germany). FE-SEM images, EDX, and EDX mapping were assessed using a TESCAN (model: Sigma VP) scanning electron microscope operating at an acceleration voltage of 15.00 kV and resolution of about 500 nm (Zeiss, Germany). Thermogravimetric analysis (TGA) was carried out using a Shimadzu Thermogravimetric Analyzer (TG-50) in the temperature range of 25–900 °C at a heating rate of 10 °C min-1 under an Argon atmosphere. The magnetic properties of the catalyst were deliberated using a vibrating sample magnetometer (VSM, Magnetic Danesh Pajoh Inst.). Inductively coupled plasma optical emission spectroscopy (ICP-OES) was determined by 76004555 SPECTRO ARCOS ICP-OES analyzer. The reported yields are attributed to pure products isolated after purification by a thin layer or column chromatography.

2-Phenylquinazolin-4(*3H*)-one (1a)

(219 mg, 99%); White solid; mp 234–236 °C[1]; FT-IR (KBr): vmax/cm^{-1} 3195-3061 (N-H, C-H Ar), 2953, 1669 (C=O), 1560, 1481 (C=C), 1296 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm]= 12.33 (s, 1H), 7.94 (t, *J* = 6.0 Hz, 3H), 7.62 (t, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 9.6 Hz, 1H), 7.38 – 7.21 (m, 4H).; ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm]= 163.67, 152.4, 148.9, 134.6, 133.2, 130.3, 129.0, 128.3, 127.1, 126.9, 126.3, 121.2; MS, m/z 224 (M+2, 2.5%), 221 (M-1, 75%), 118 (C_7H_5NO, 100%), 76 (C_6H_5, 80%), 28 (CO, 97%).

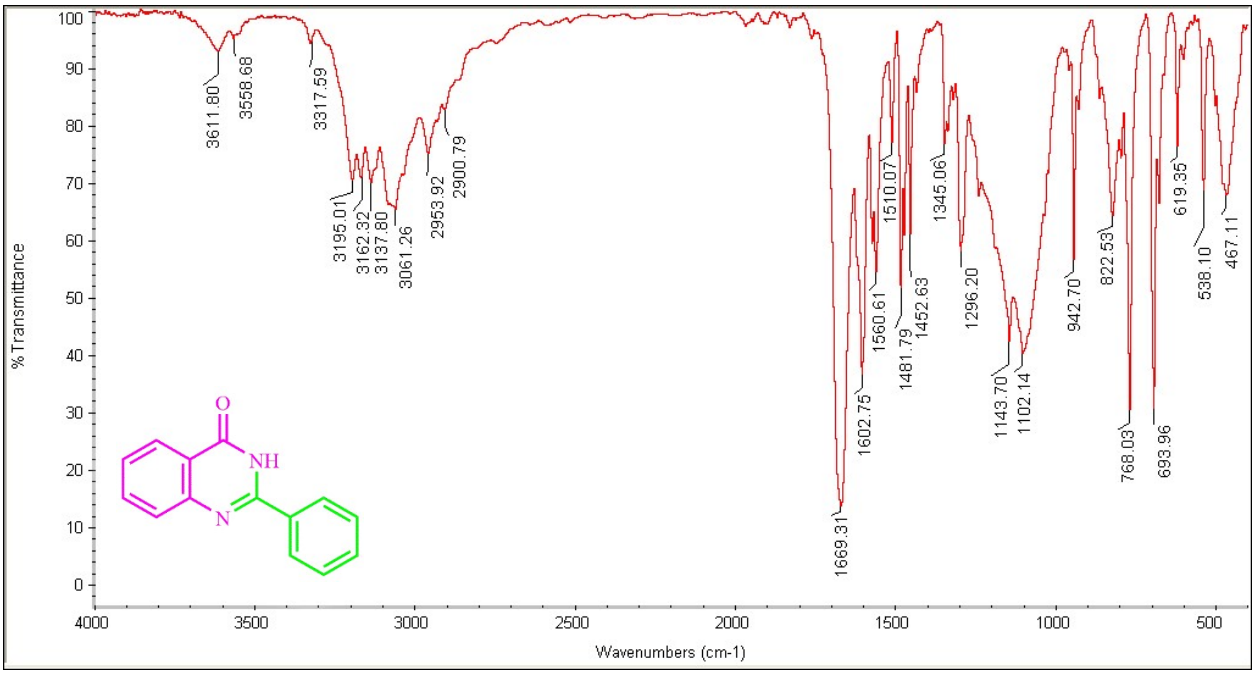

Fig. 1 FT-IR (KBr) of 2-Phenylquinazolin-4(*3H*)-one.

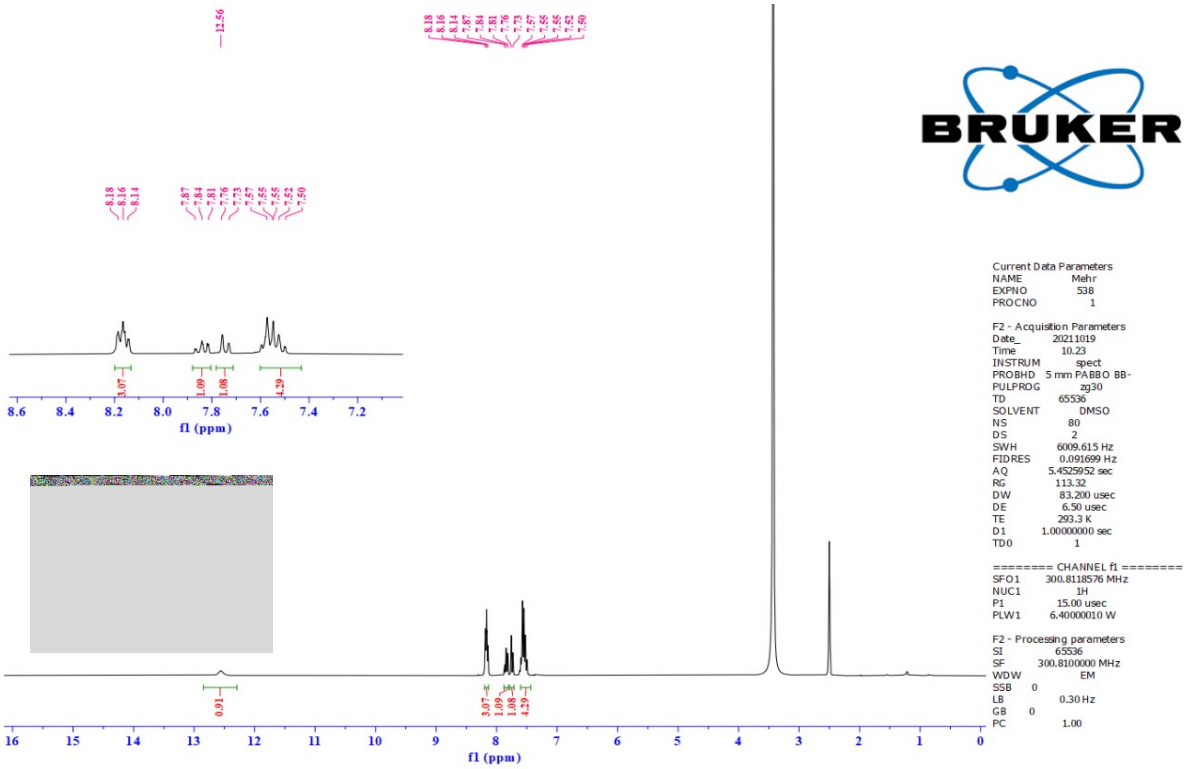

Fig. 2 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-Phenylquinazolin-4(*3H*)-one.

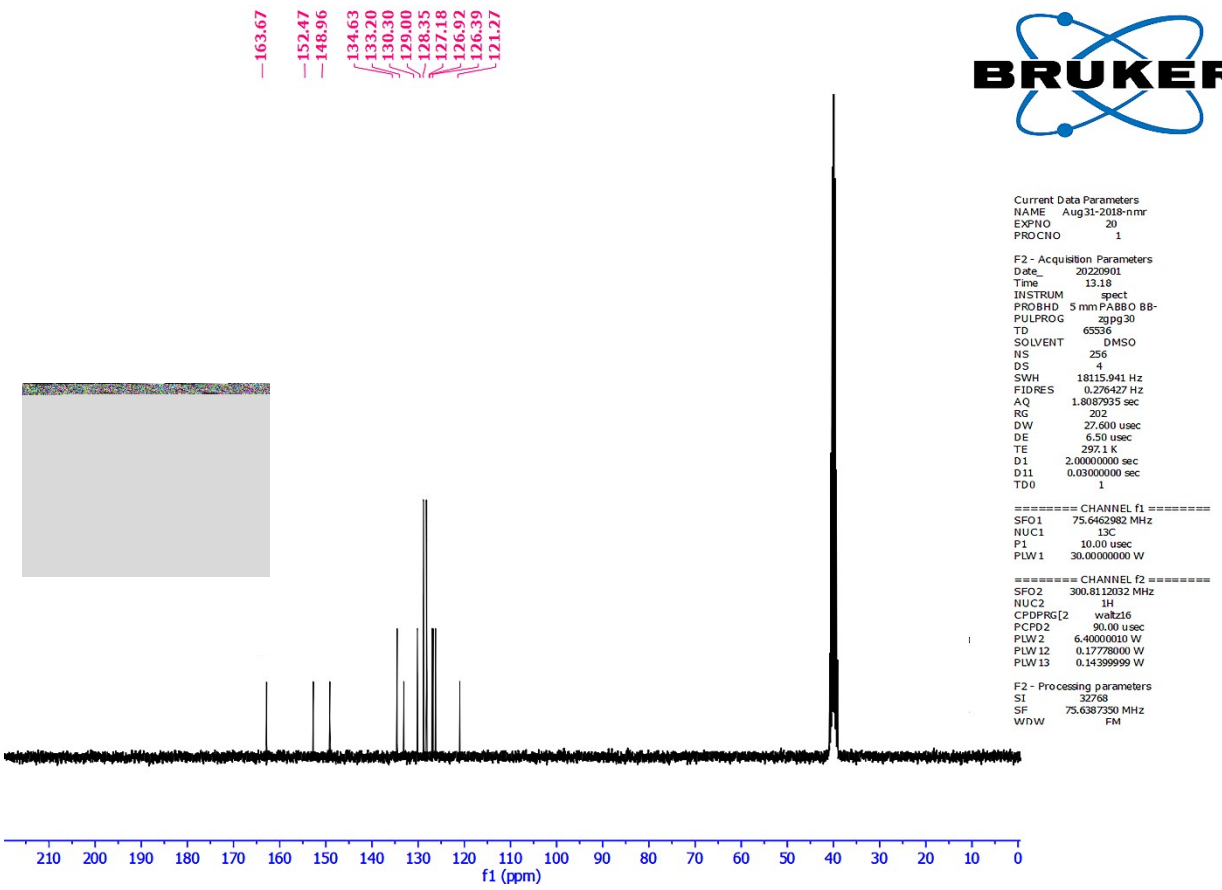

Fig. 3 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-Phenylquinazolin-4(3*H*)-one.

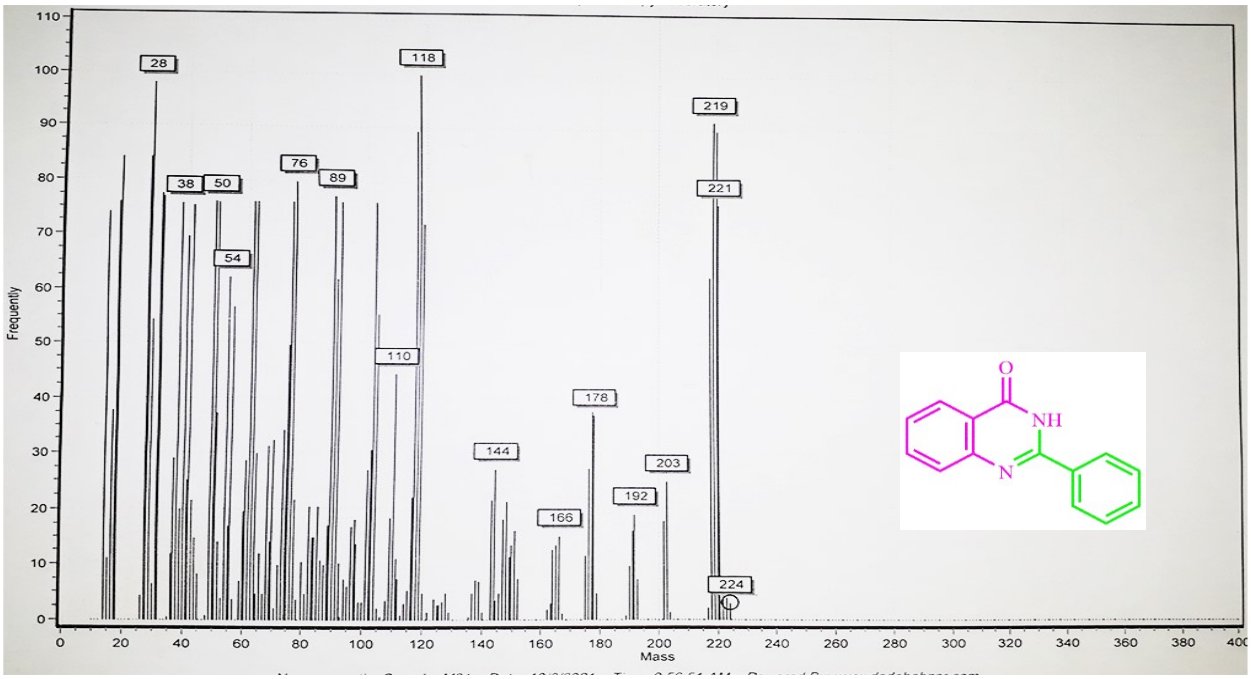

Fig. 4 Mass spectrum of 2-Phenylquinazolin-4(*3H*)-one.

2-(*p*-tolyl) quinazolin-4(*3H*)-one (1b)

(233 mg, 99%); White solid; mp 245-247 °C[1]. ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm]= 12.50(s, 1H), 8.84 (d, *J* = 2.7 Hz, 1H), 8.56(d, *J* = 6.3 Hz, 2H), 8.16 (dd, *J* = 9, 7.9 Hz, 1H), 7.91(d, *J* = 9 Hz, 1H), 7.31 (t, *J* = 9 Hz, 1H), 7.41 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6): δ (ppm) = 163.6, 154.9, 148.9, 140.8, 134.6, 130.7, 129.4, 128.7, 127.8, 126.9, 126.3, 121.2, 21.3.

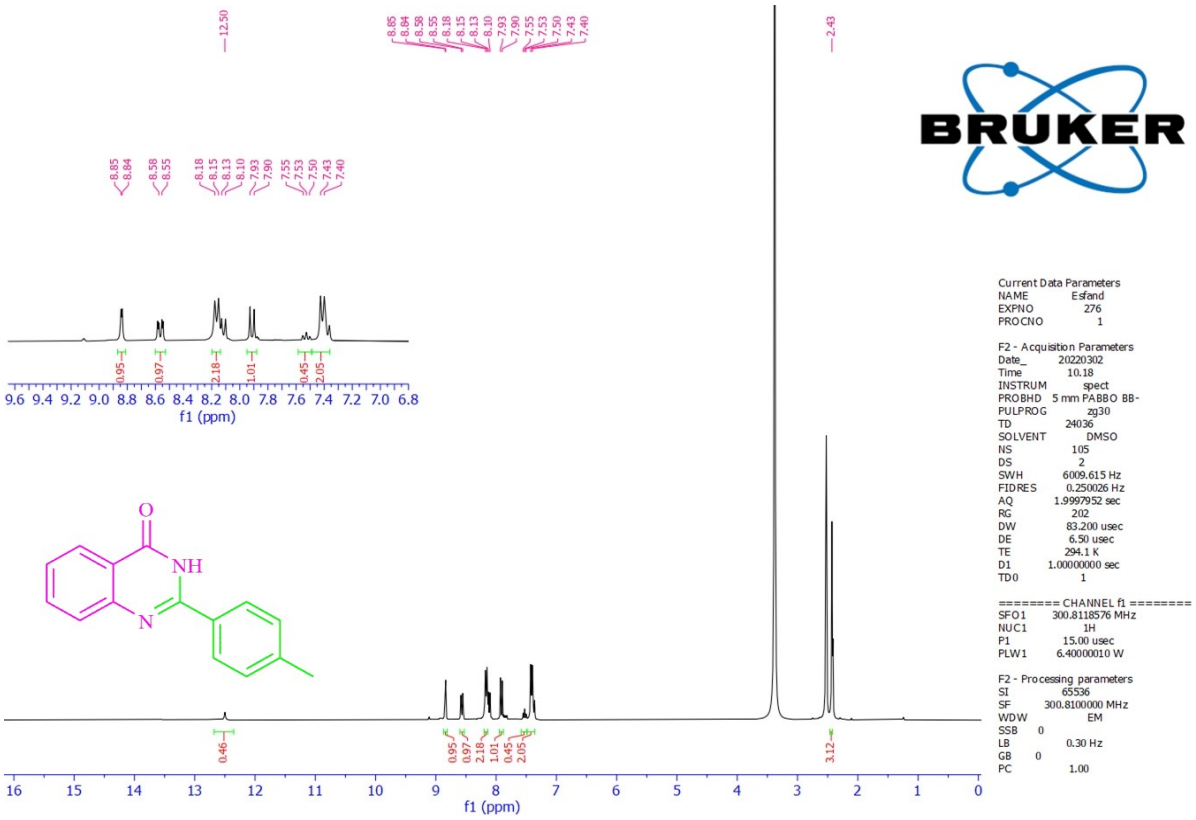

Fig. 5 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-(p-tolyl) quinazolin-4(*3H*)-one.

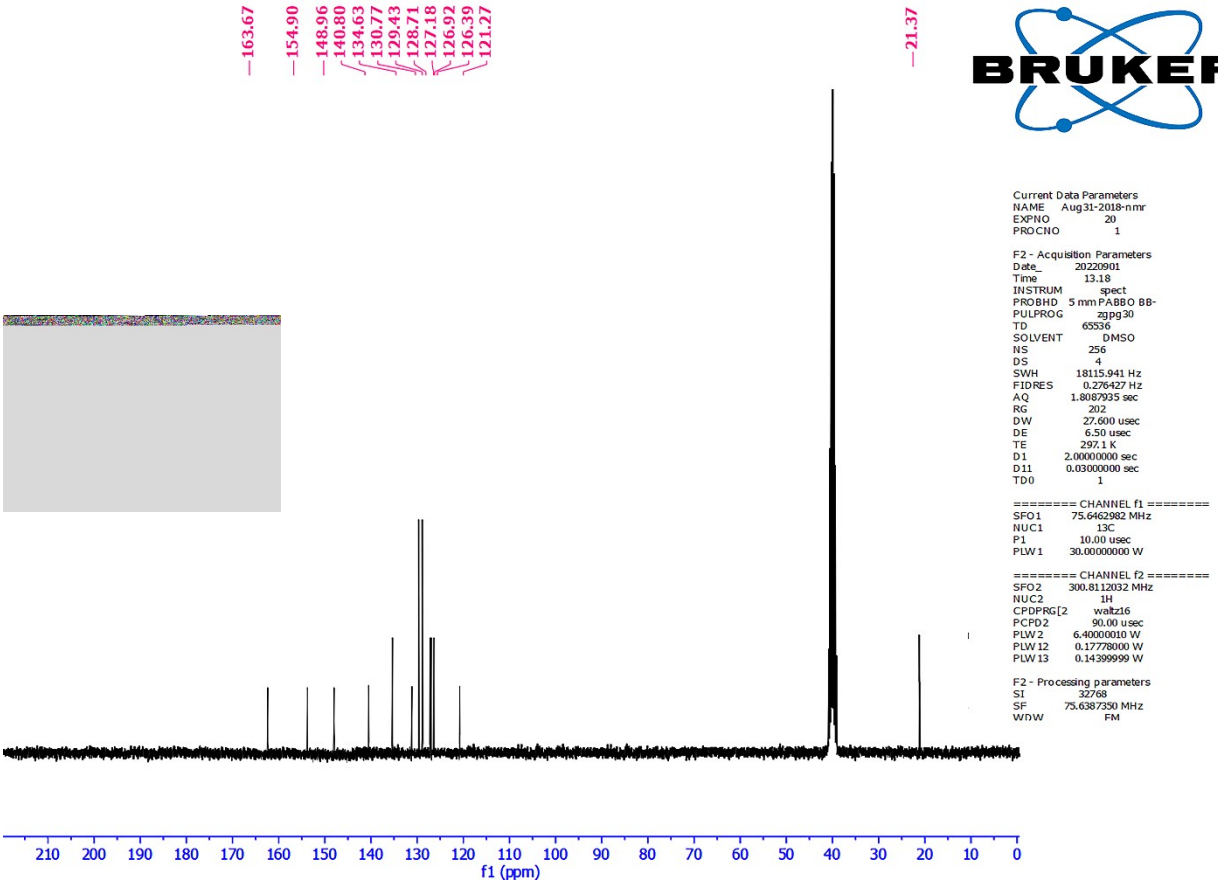

Fig. 6 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-(p-tolyl) quinazolin-4(*3H)*-one.

2-(4-methoxyphenyl) quinazolin-4(*3H*)-one (1d)

(244 mg, 97%); White solid; mp 238-239 ^{o}C[2]; ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm]= 12.47 (s, 1H), 8.31 – 8.13 (m, 3H), 7.86 (t, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 7.1 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 8.9 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm]= 163.6, 161.1, 154.7, 148.9, 134.6, 129.9, 127.6, 127.1, 126.9, 126.3, 121.2, 114.3, 55.3.

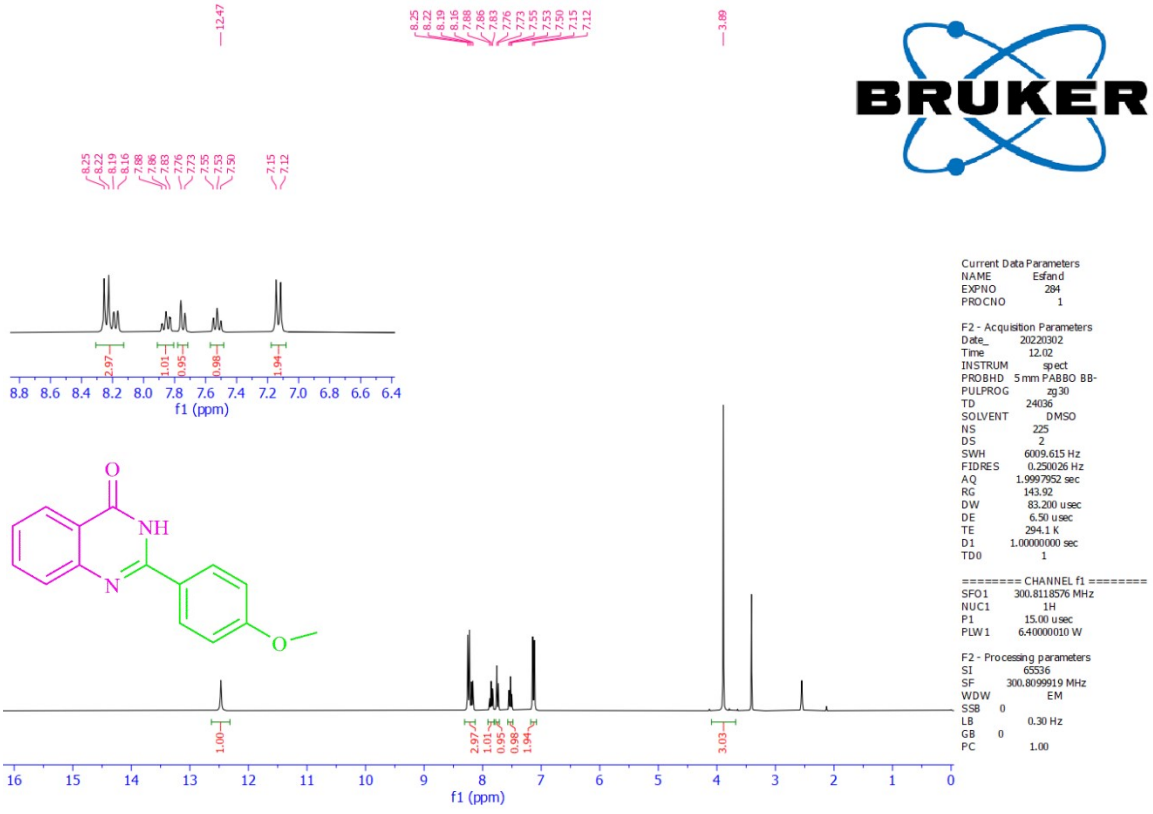

Fig. 7 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-(4-methoxyphenyl)quinazolin-4(*3H*)-one.

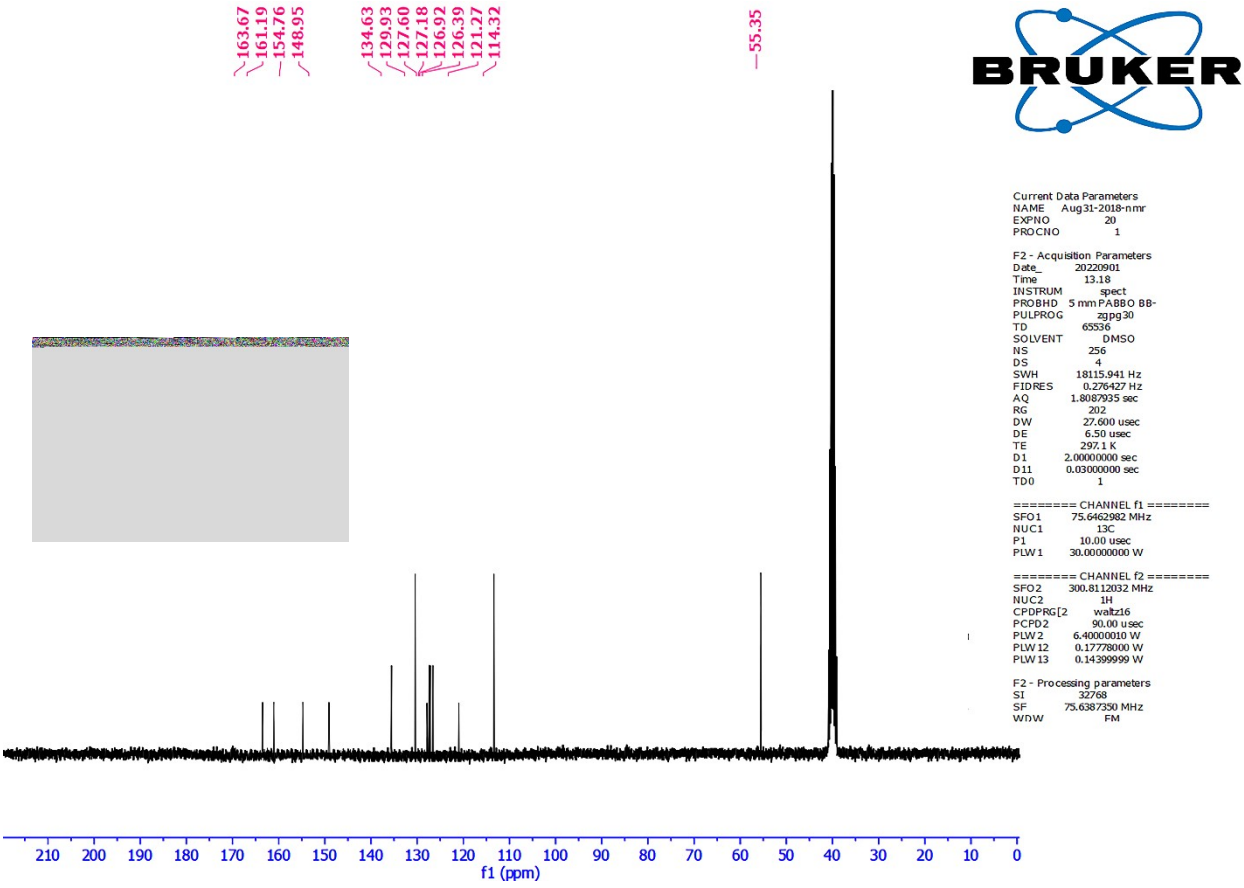

Fig. 8 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-(4-methoxyphenyl) quinazolin-4(3*H*)-one.

2-(4-(dimethylamino) phenyl) quinazolin-4(*3H*)-one (1g)

(238 mg, 90%); White solid; mp 247-248 ˚C[1]; ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm]= 12.16 (s, 1H), 8.25 – 8.01 (m, 3H), 7.77 (t, *J* = 8.1 Hz, 1H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 8.1 Hz, 1H), 6.81 (d, *J* = 9.1 Hz, 2H), 3.04 (s, 6H); ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm]= 163.6, 155.0, 153.2, 148.9, 134.6, 129.7, 127.1, 126.9, 126.3, 125.3, 121.2, 112.7 , 40.3.

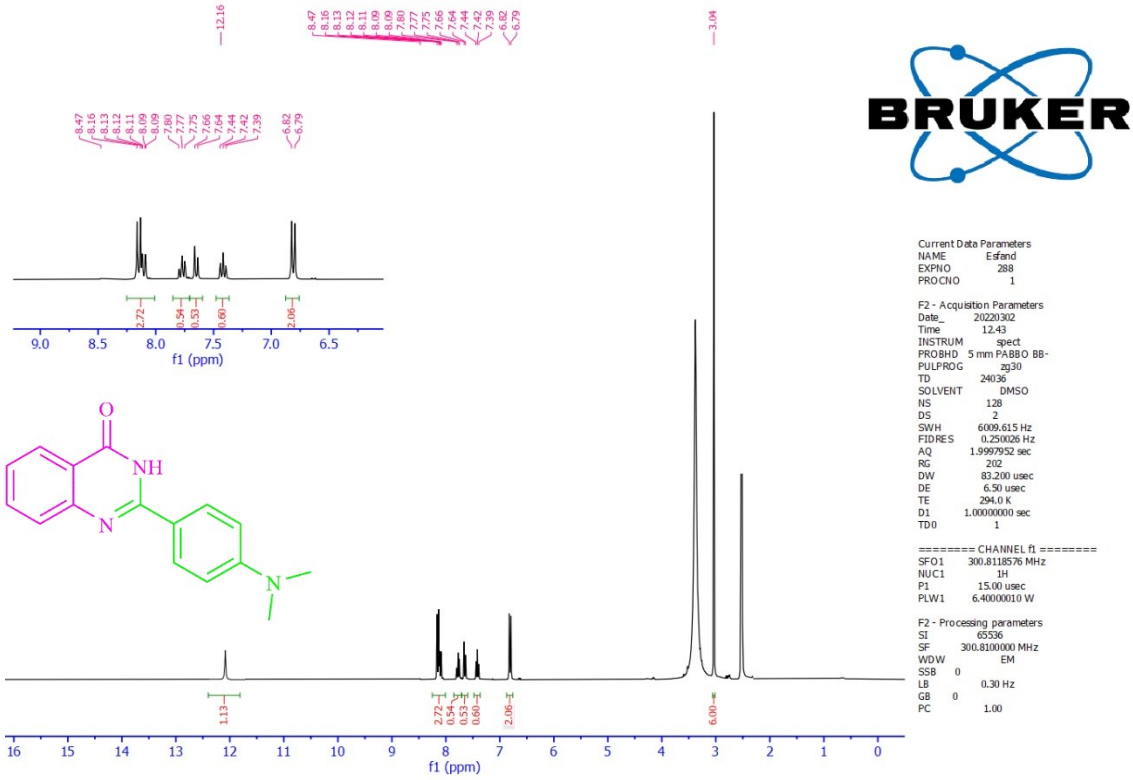

Fig. 9 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-(4-(dimethylamino) phenyl) quinazolin-4(3*H*)-one.

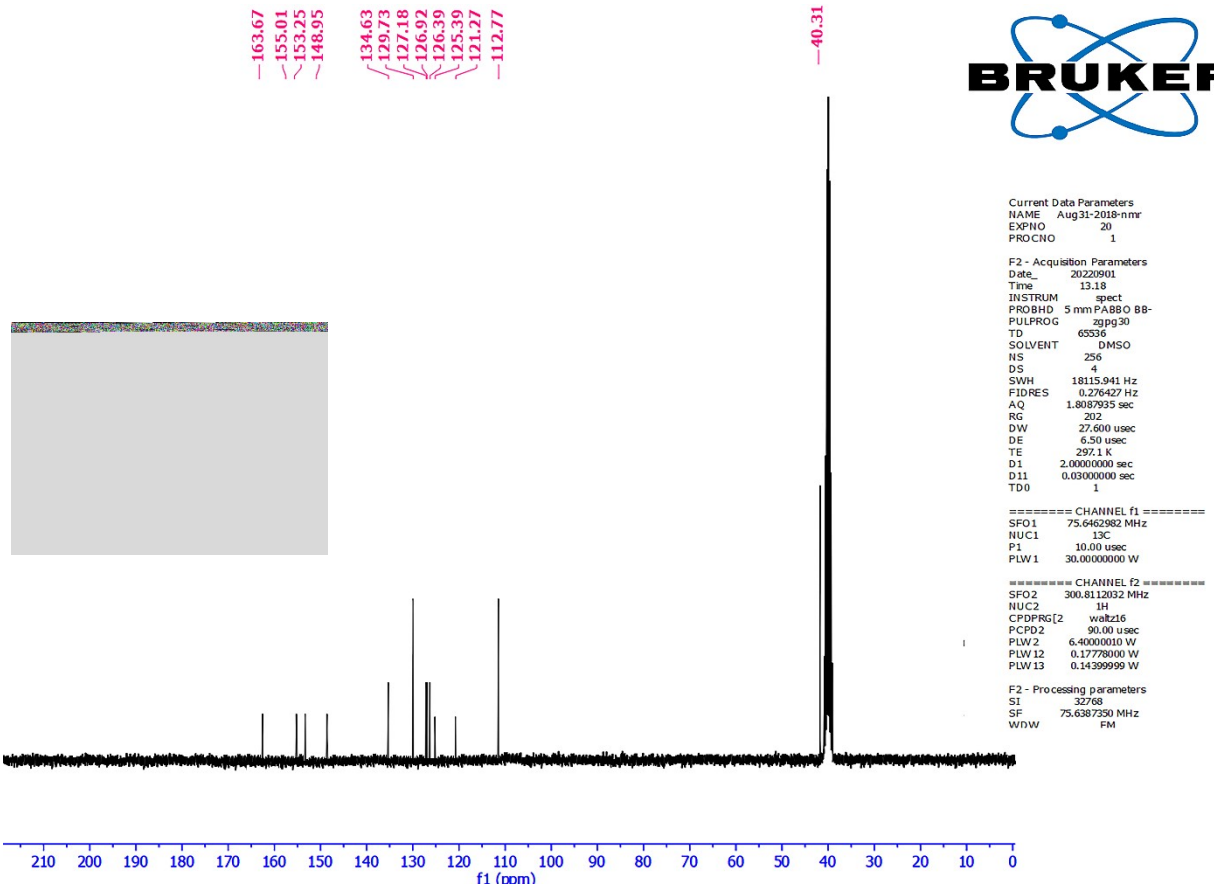

Fig. 10 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-(4-(dimethylamino) phenyl) quinazolin-4(3*H*)-one.

2-(4-chlorophenyl) quinazolin-4(*3H*)-one (1h)

(220 mg, 86%); White solid; mp 298−300 ^{o}C[3]; ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm]= 12.64 (s, 1H), 8.27 – 8.14 (m, 3H), 7.87 (t, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm]= 163.6, 154.5, 148.9, 136.3, 134.6, 132.1, 129.9, 129.6, 127.1, 126.9, 126.3, 121.2.

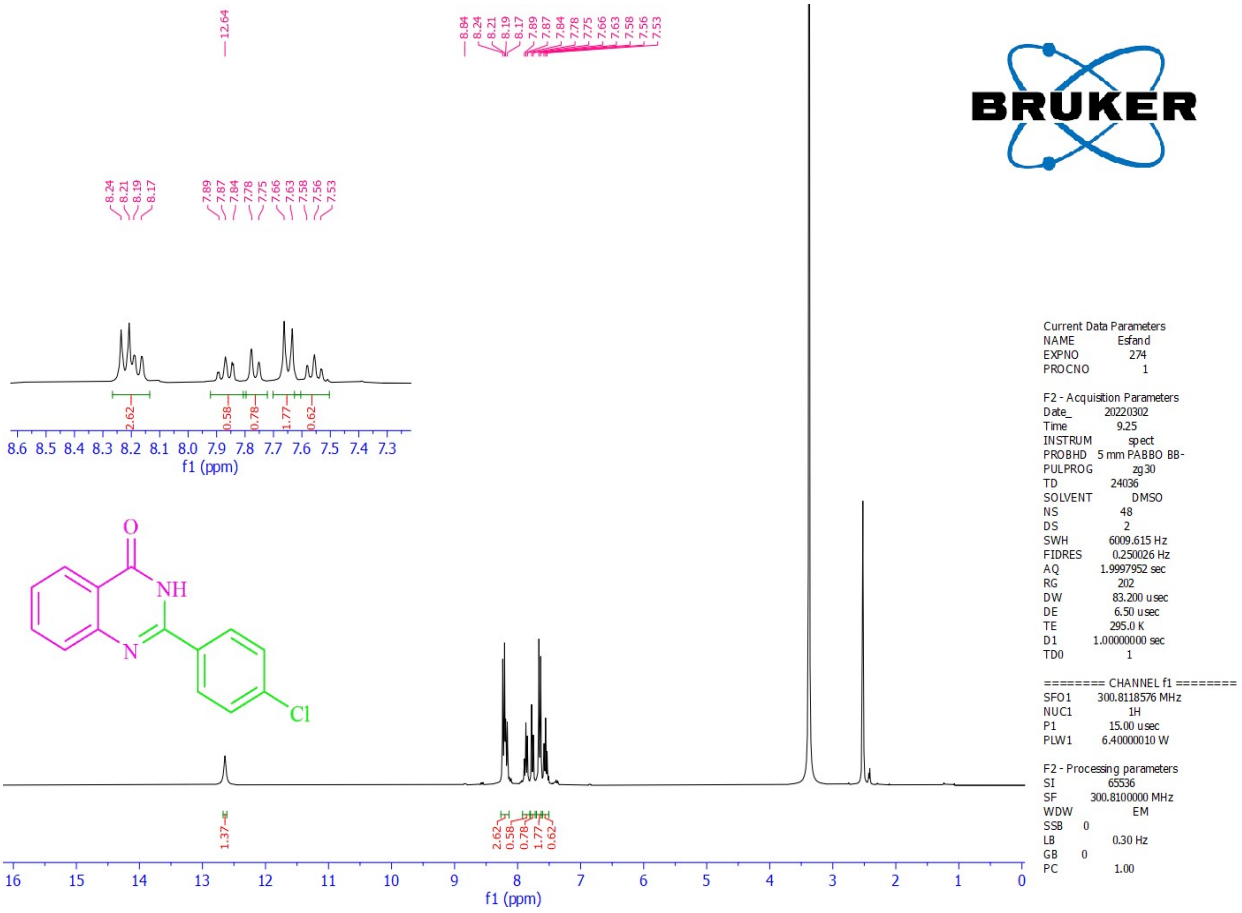

Fig. 11 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-(4-chlorophenyl) quinazolin-4(*3H*)-one.

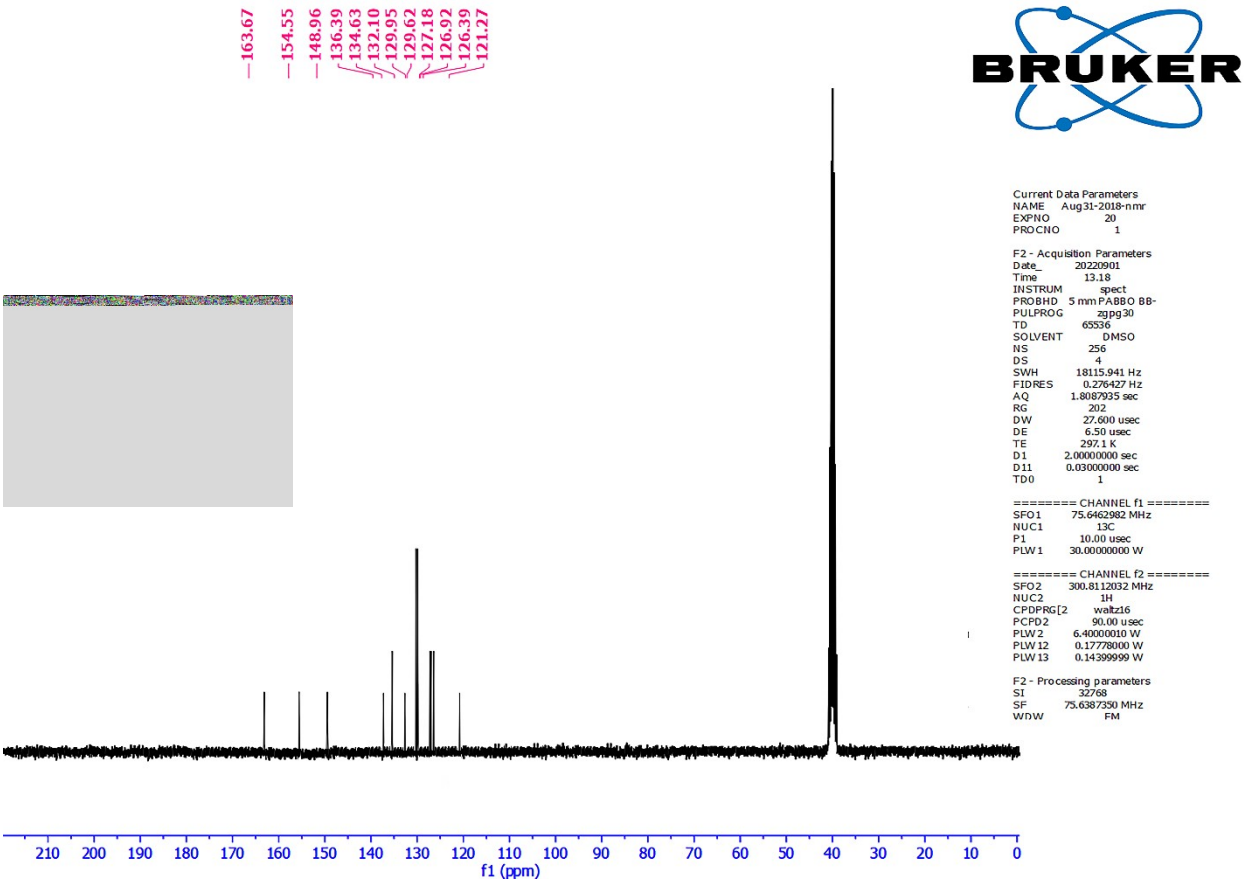

Fig. 12 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-(4-chlorophenyl) quinazolin-4(3*H*)-one.

2-(3-Nitrophenyl) quinazolin-4(*3H*)-one (1m)

(213 mg, 80%); Yellow solid; mp 292-294[4] ˚C; ^{1}H NMR (300 MHz, DMSO-d_6): δ [ppm]= 12.91 (s, 1H), 8.18 (dd, *J* = 8.0, 2.2 Hz, 1H), 8.08 – 7.99 (m, 2H), 7.79 (t, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.61 – 7.46 (m, 2H), 7.44 (d, *J* = 4.7 Hz, 1H); ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm]= 163.3, 153.4, 147.9, 147.4, 134.6, 133.5, 132.4, 130.2, 127.1, 126.9, 126.3, 125.6, 123.7, 121.2.

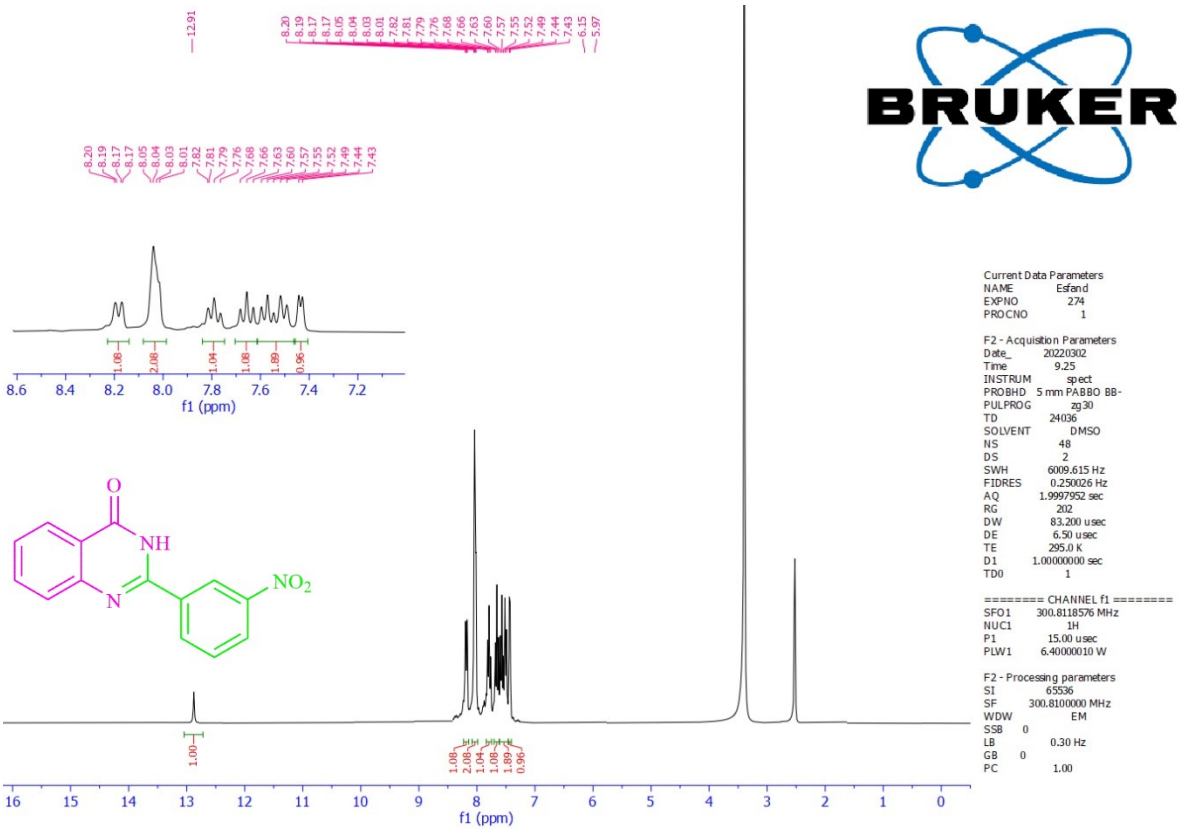

Fig. 13 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-(3-Nitrophenyl) quinazolin-4(*3H*)-one.

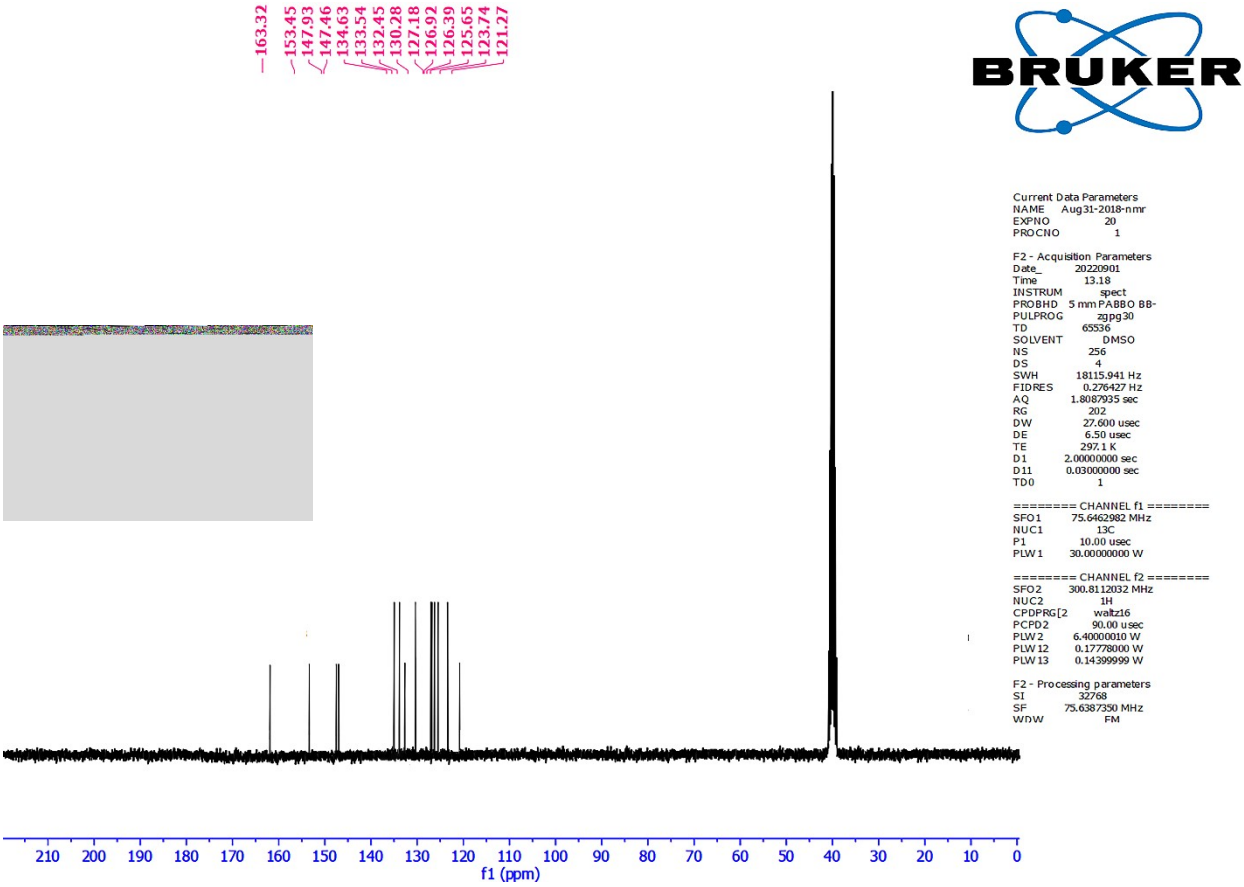

Fig. 14 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-(3-Nitrophenyl) quinazolin-4(3*H*)-one.

2-isopropylquinazolin-4(*3H*)-one (1o)

(150 mg, 80%); White crystal; mp 234-236 ˚C[5]; ^{1}H NMR (500 MHz, DMSO-d_6): δ [ppm]= 12.47 (s, 1H), 8.04 (d, *J* = 1.5 Hz, 1H), 7.73 (t, *J* = 1.4 Hz, 1H), 7.60 (d, *J* = 1.5 Hz, 1H), 7.48 (t, 1H), 3.19 – 3.08 (m, 1H), 1.13 (d, *J* = 6.2 Hz, 6H). ^{13}C NMR (75 MHz, DMSO-d_6): δ [ppm]= 164.7, 162.7, 147.7, 135.0, 127.1, 126.5, 125.6, 121.9, 33.4, 20.0.

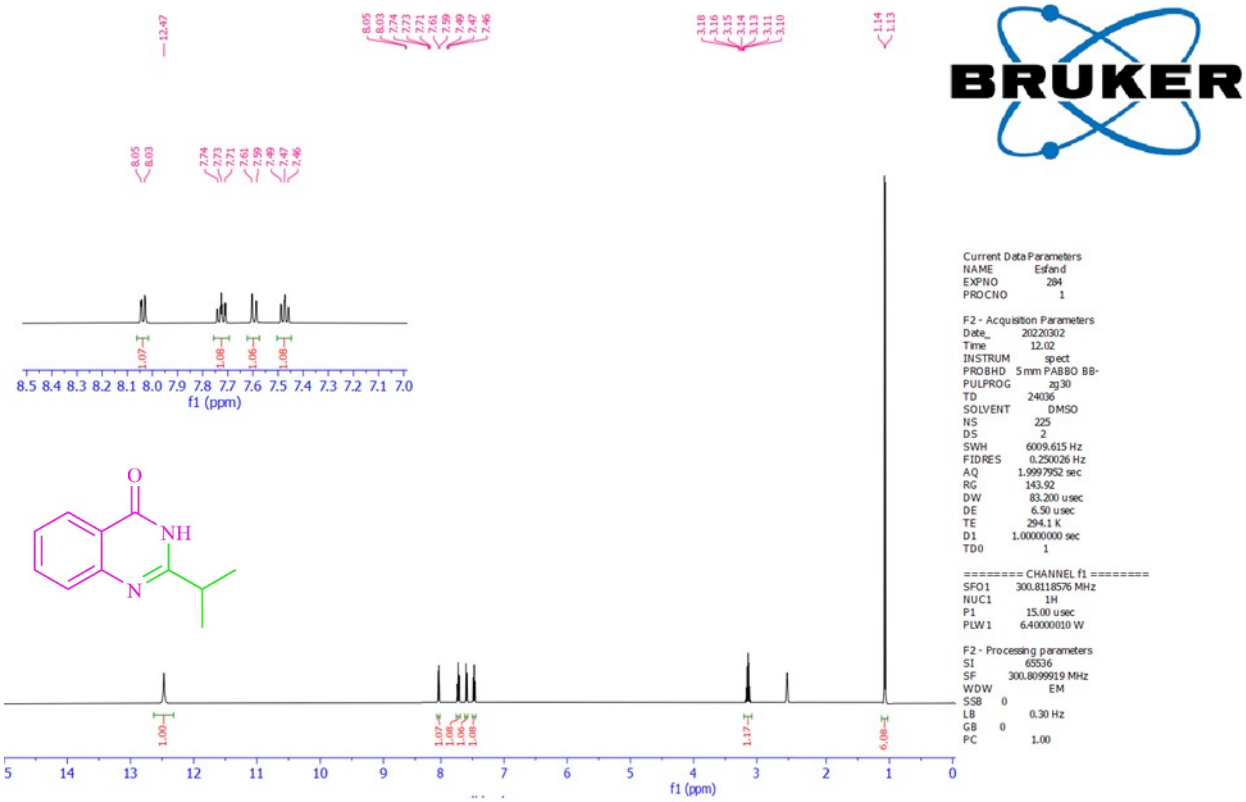

Fig. 15 ^{1}H NMR (300 MHz, DMSO-d_6) of 2-isopropylquinazolin-4(*3H*)-one.

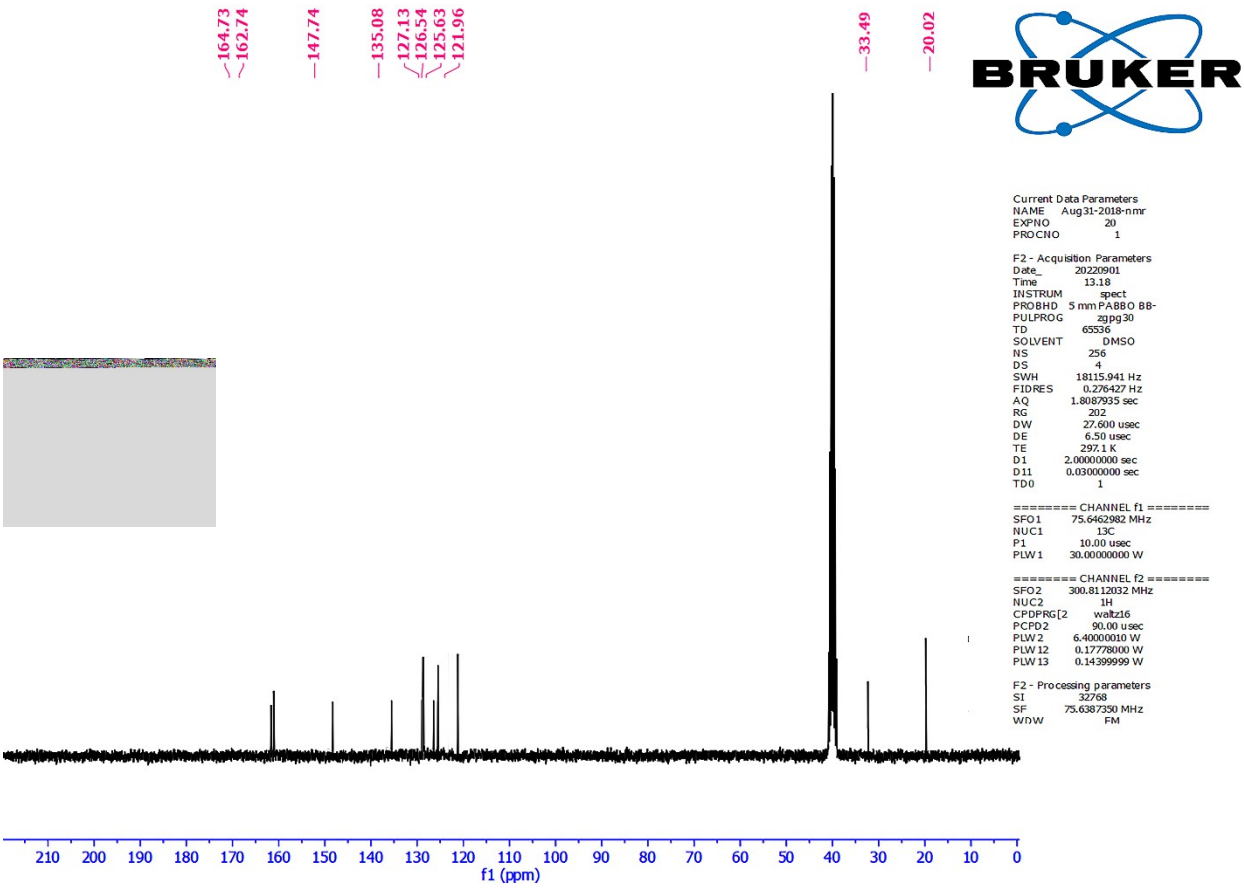

Fig. 16 ^{13}C NMR (75 MHz, DMSO-d_6) of 2-isopropylquinazolin-4(3*H*)-one.

references

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