Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

La-Mg mixed oxide as highly basic water resistant catalyst for utilization of CO_2 in synthesis of quinazoline-2,4(1*H*,3*H*)-dione

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1. La-Mg MO characterization

The catalyst was fully characterized by different techniques like XRD, FTIR, TGA, SEM, TPD and BET surface area and porosity. The powder XRD were recorded using a Bruker AXS, D8 discover instrument (USA) with Cu-Kα (1.54Å) radiation over a range of 10-70° 2θ value. FT-IR spectra were recorded using Perkin-Elmer instrument spectrum 100 series, using KBr pallet technique over a range of 400-4000 cm^{-1}. The TGA were recorded using NETZSCH STA 449 F-3, the sample was heated up to 750°C at the rate 20°C/min. The SEM images were obtained on a JEOL JSM 6380 LA instrument. The SEM image shows the nano composite formation. The CO_2 temperature programmed desorption analysis were performed to evaluate the total basicity of catalyst using Micromeritics (USA), equipped with TCD detector. The N_2 adsorption/desorption isotherm was obtained by using Tri-Star-II 2020 (Micromeritics, USA) instrument, initially sample was degassed for 2 h at 350°C and calculate the surface area pore size distribution.

2. IR of catalysts

a. Pure La_2O_3

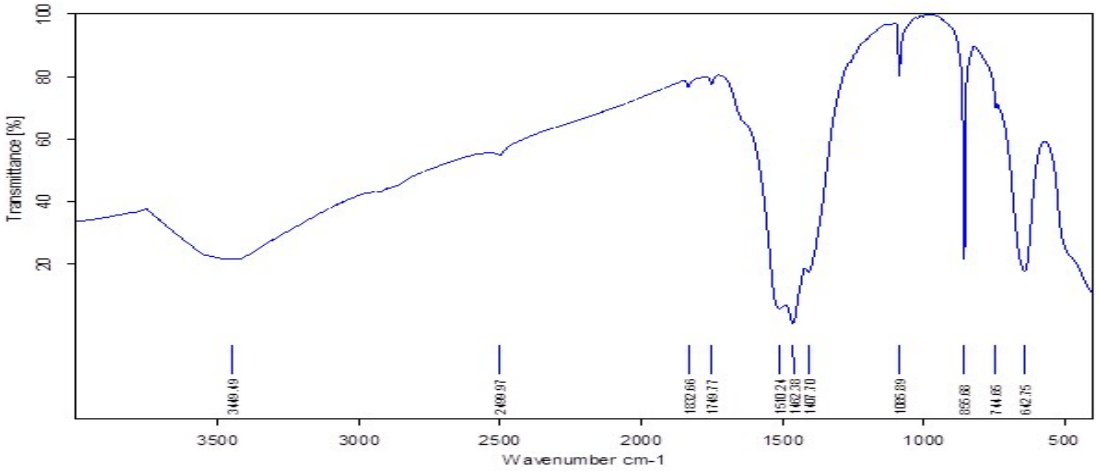


Figure S1: IR spectrum of La_2O_3

b. Pure MgO

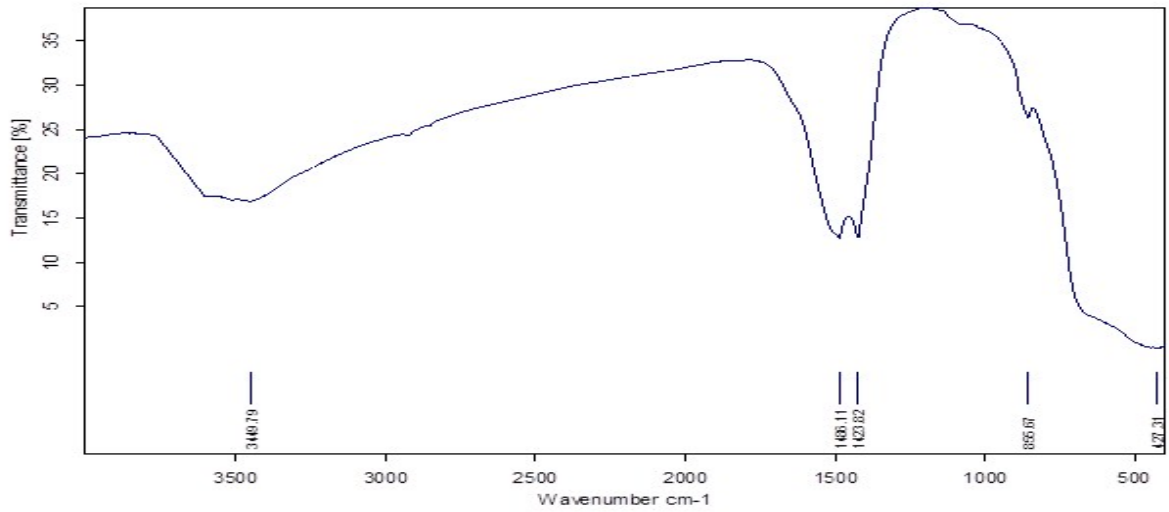


Figure S2: IR spectra of pure MgO

3. *XRD of reused catalyst*

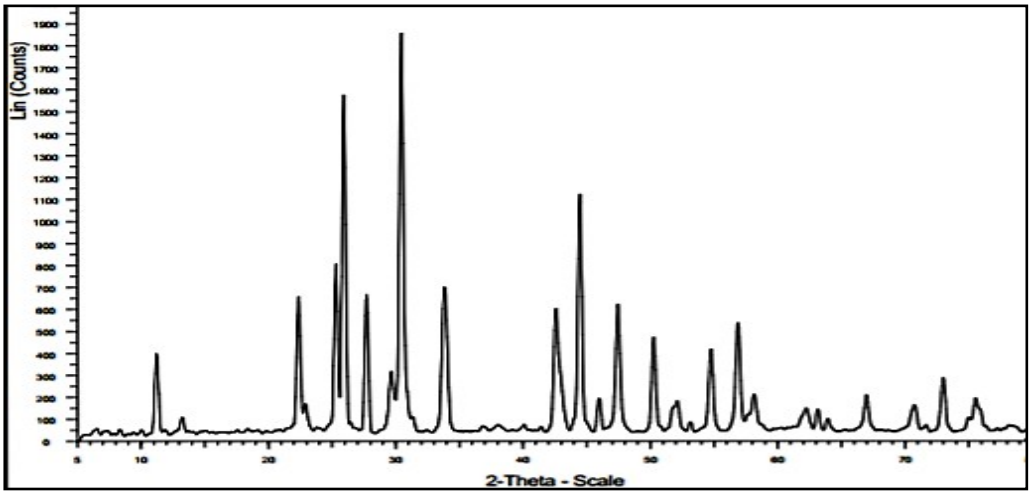


Figure S3: XRD of reused La-Mg MO

4. *HPLC method forquinazoline-2,4(1H,3H)-dione*

The reaction progress as well as purity of quinazolinedione was analyzed by following HPLC method;

Mobile phase A	**:**	Acetonitrile
Mobile phase B	:	0.1%Trifluoroacetic acid (TFA) in deionized water
Column used	:	Zorbax C18 [4.6 mm (id) x 250 mm (length) x 5µm (particle size)]
Gradient program		Time / Mobile phase A / Mobile phase B 0 / 20 / 80 5 / 20 / 80 10 / 90 / 10 15 / 90 / 10 18 / 20 / 80 20 / 20 / 80
Wavelength (λ_{max})	:	243nm
flow rate	:	1.0 mL/min
Diluent	:	Methanol
sample preparation	:	Calculated amount of sample + add minimum quantity of DMF to solubilize sample, then dilute up to mark with methanol (2000 ppm)
retention time	:	2-aminobenzonitrile 4.2 min and quinazolinedione 10.7 min

5. *Characterization of Quinazoline-2,4(1H,3H)-dione derivatives*

a) Quinazoline-2,4(1*H*,3*H*)-dione

i. IR spectra

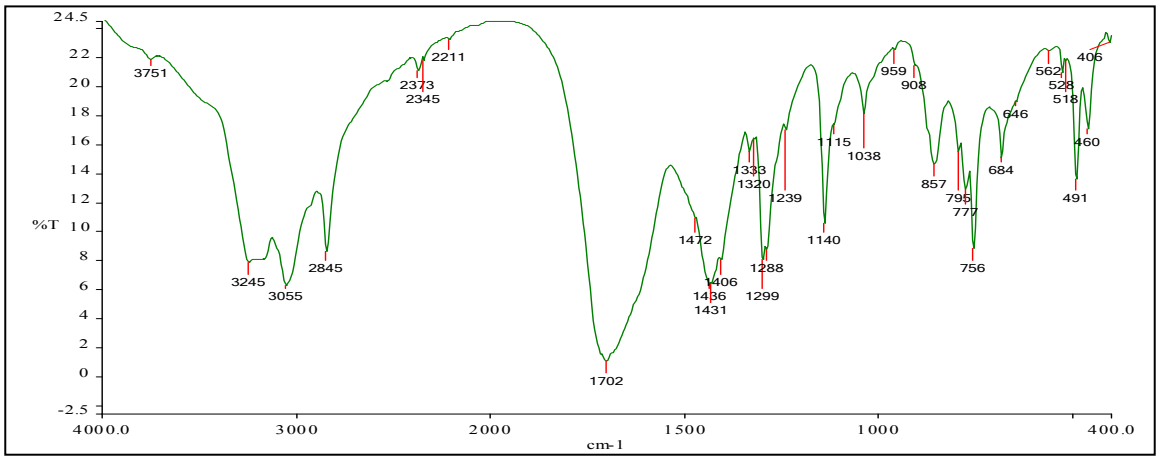


Figure S4: FT-IR of Quinazoline-2,4(1*H*,3*H*)-dione

ii. GC-Mass spectra quinazoline-2,4(1*H*,3*H*)-diones

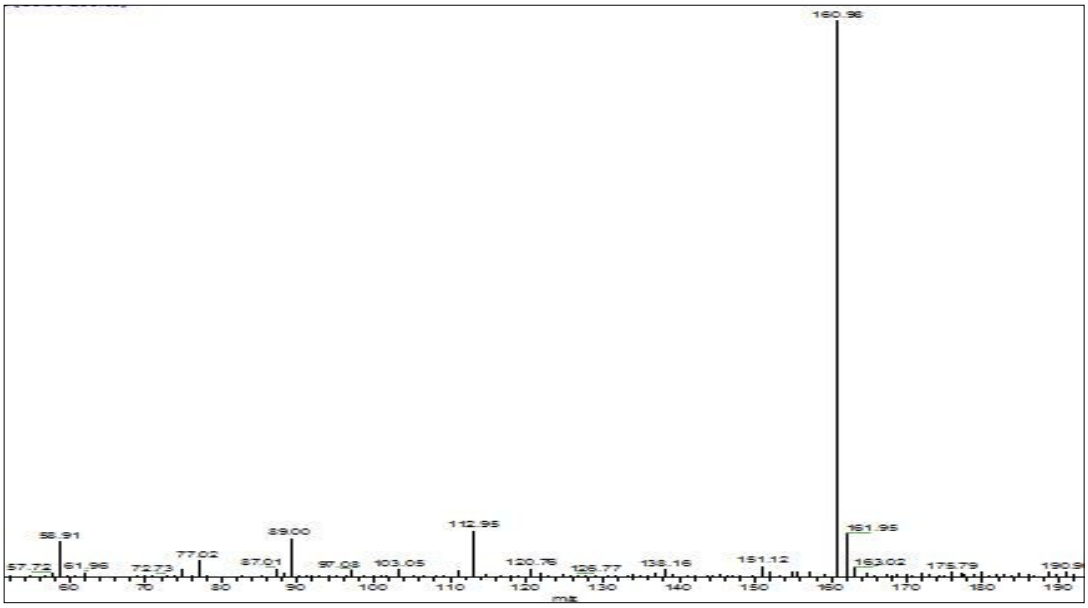
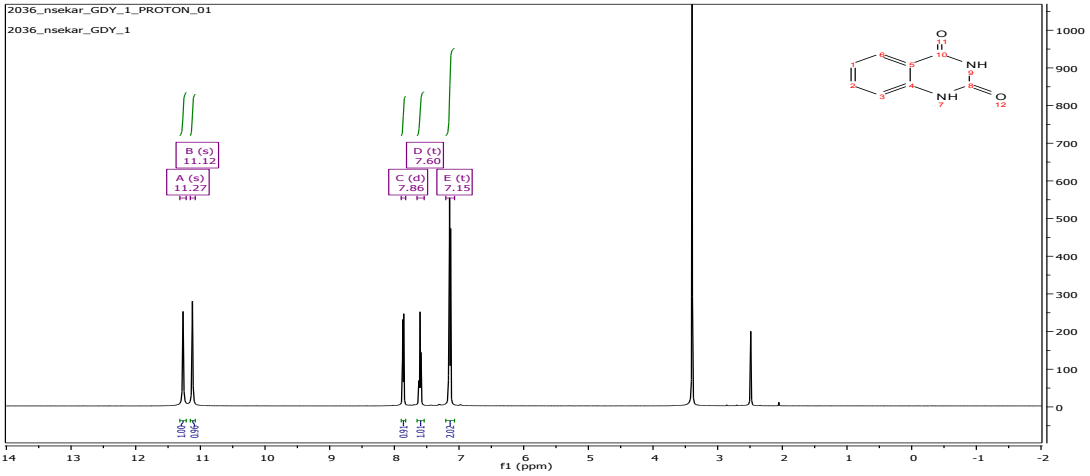
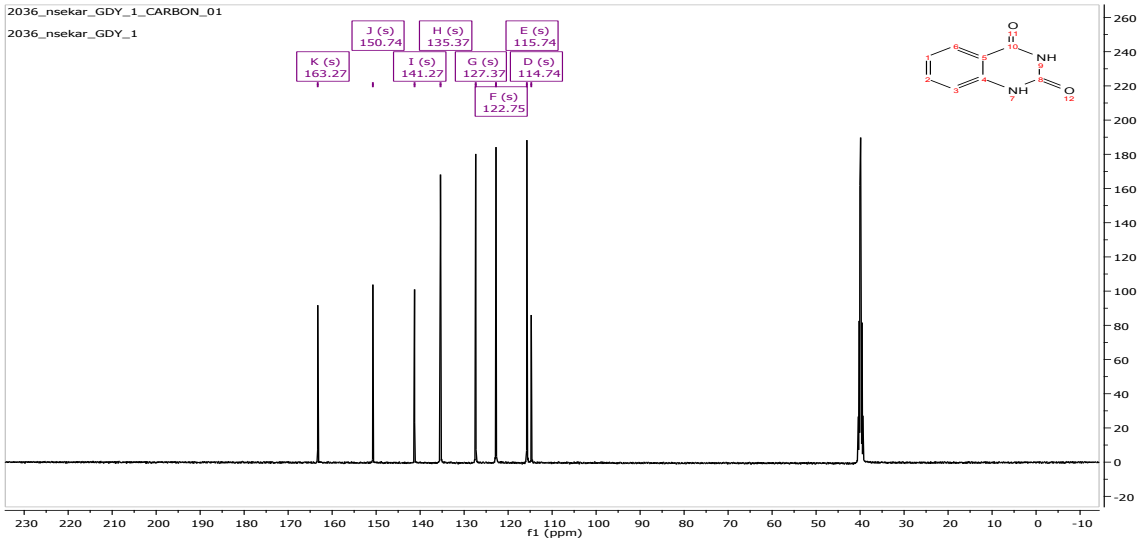


Figure S5: GC-MS of Quinazoline-2,4(1*H*,3*H*)-dione

H-NMR Spectra: (a) quinazoline-2,4(1*H*,3*H*)-diones

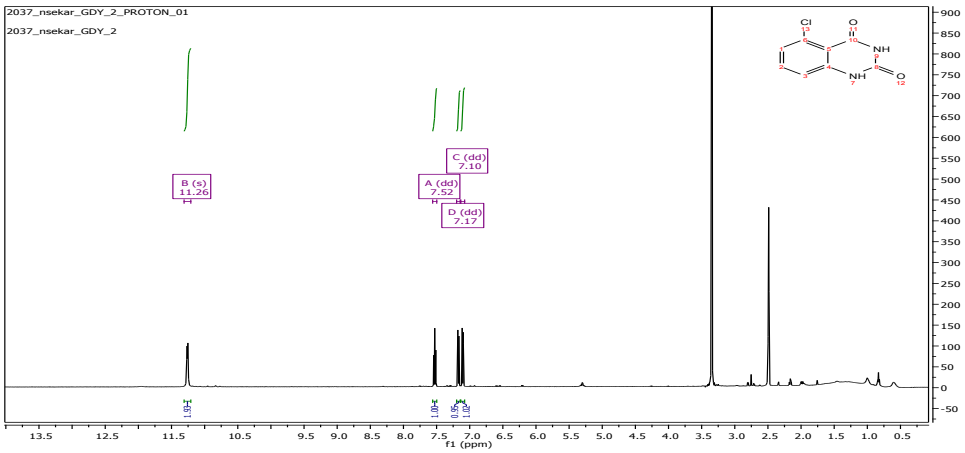


C^{13}-NMR spectra: quinazoline-2,4(1*H*,3*H*)-diones

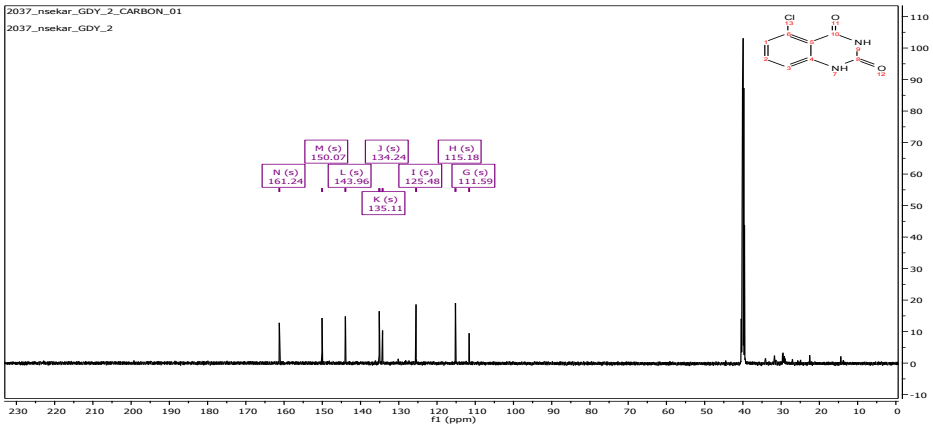


b) 5-chloro quinazoline-2,4(1*H,*3*H*)-dione

^{1}H-NMR

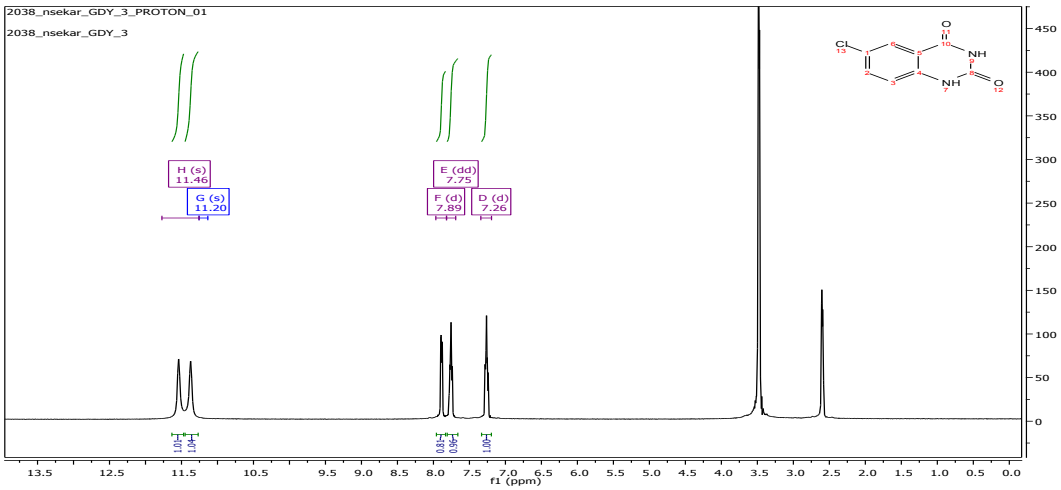


^{13}C-NMR

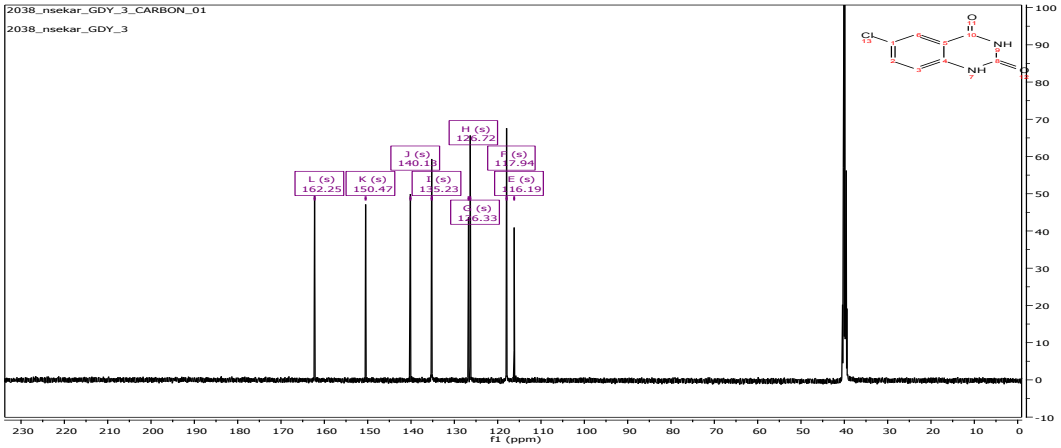


c) 6-chloro quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR

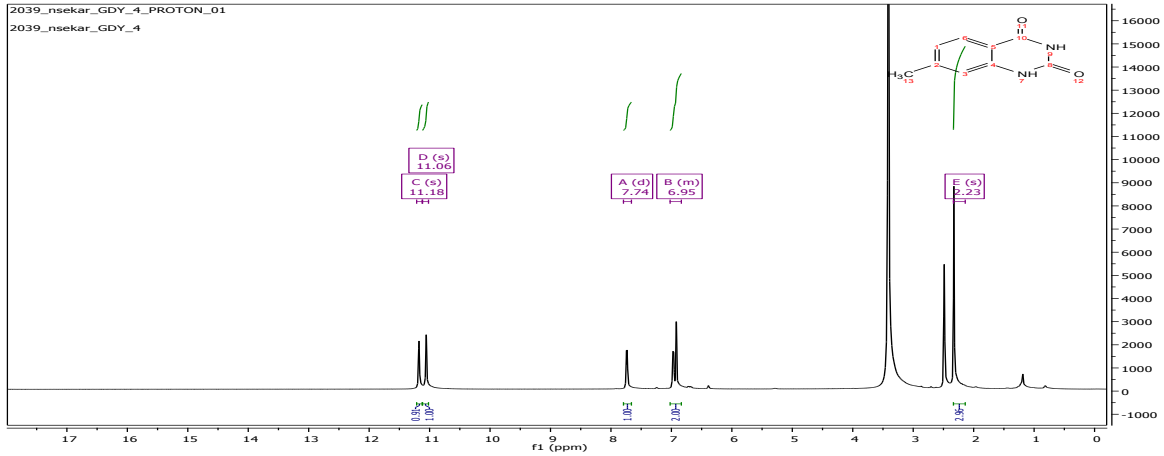


^{13}C NMR

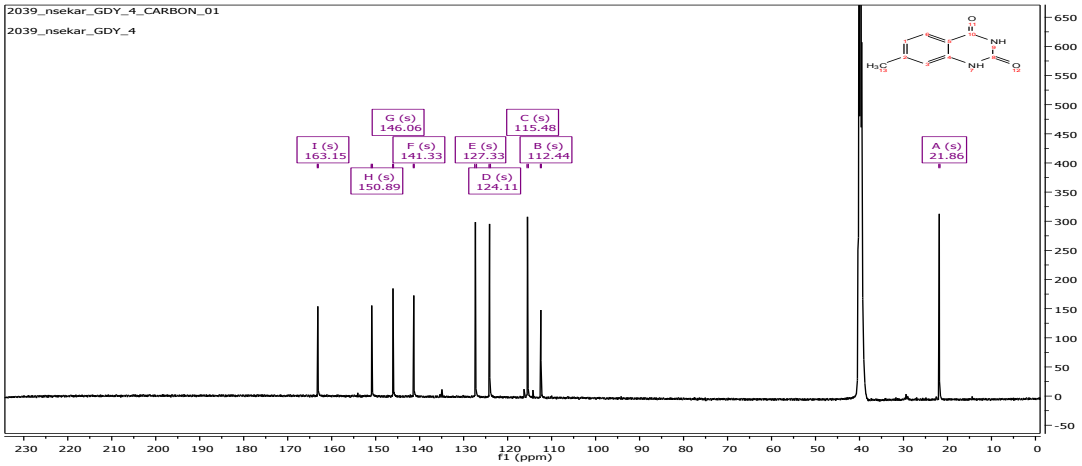


(d) 7-Methyl quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR

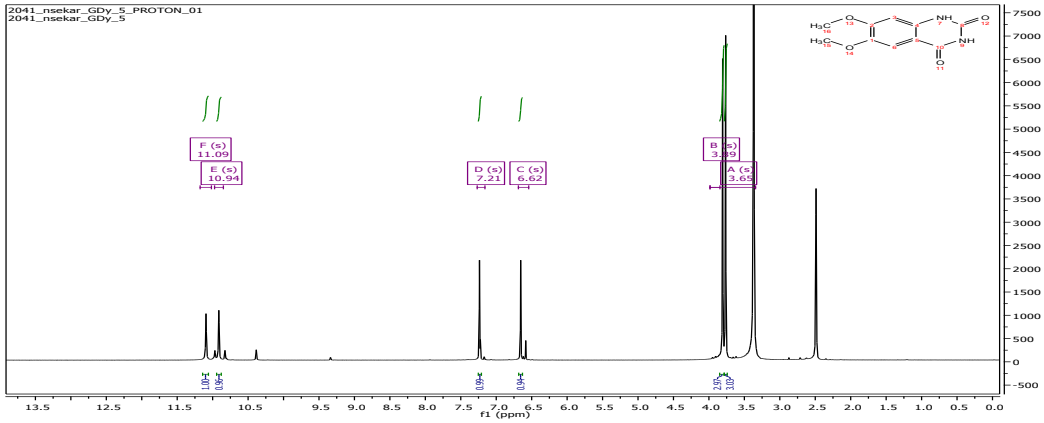


^{13}C-NMR

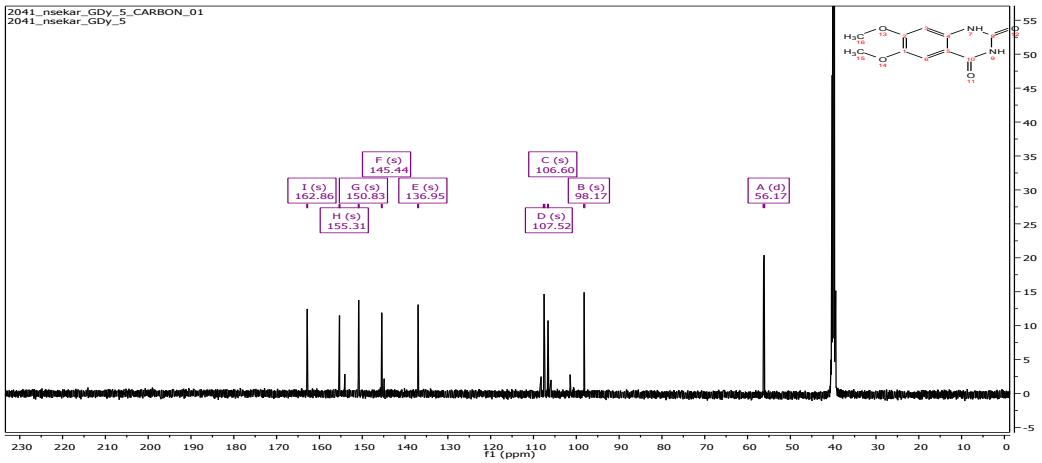


e) 6,7-Dimethoxy quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR

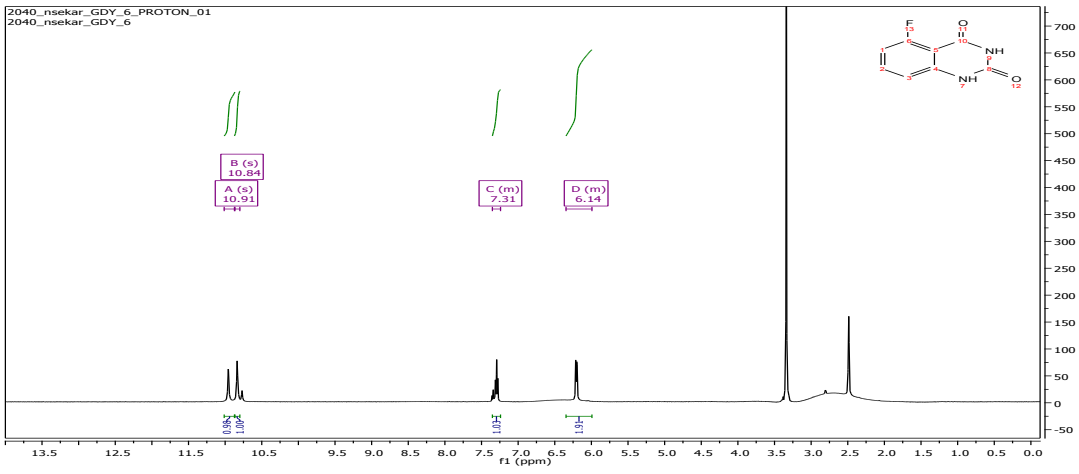


^{13}C-NMR

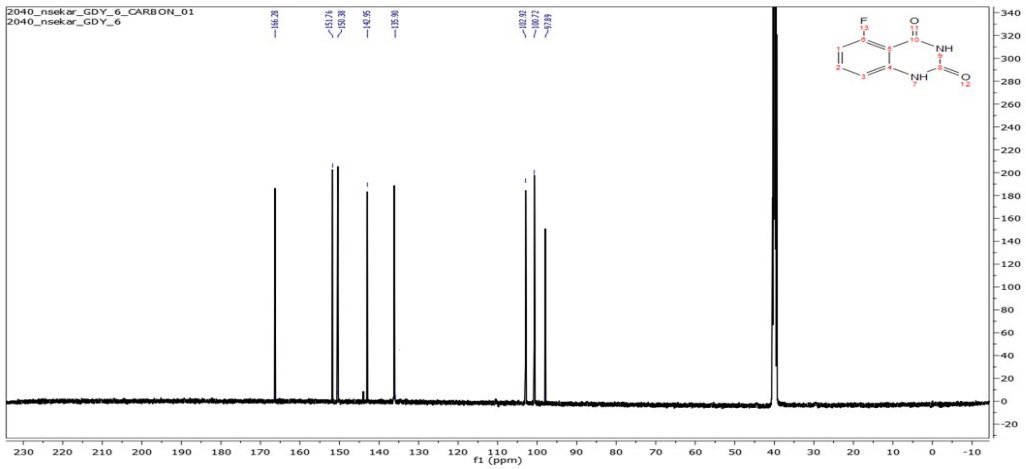


f) 5-Fluoro quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR

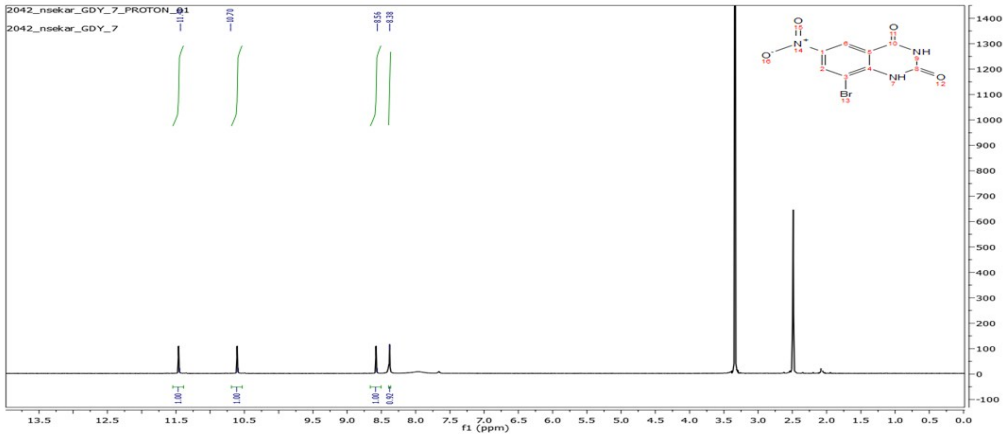


^{13}C-NMR

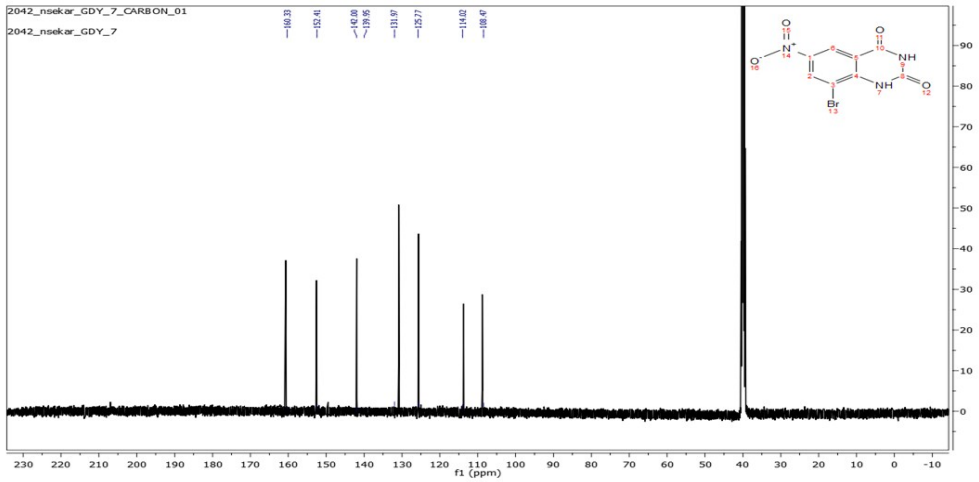


g) 8-Bromo-6-nitro quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR

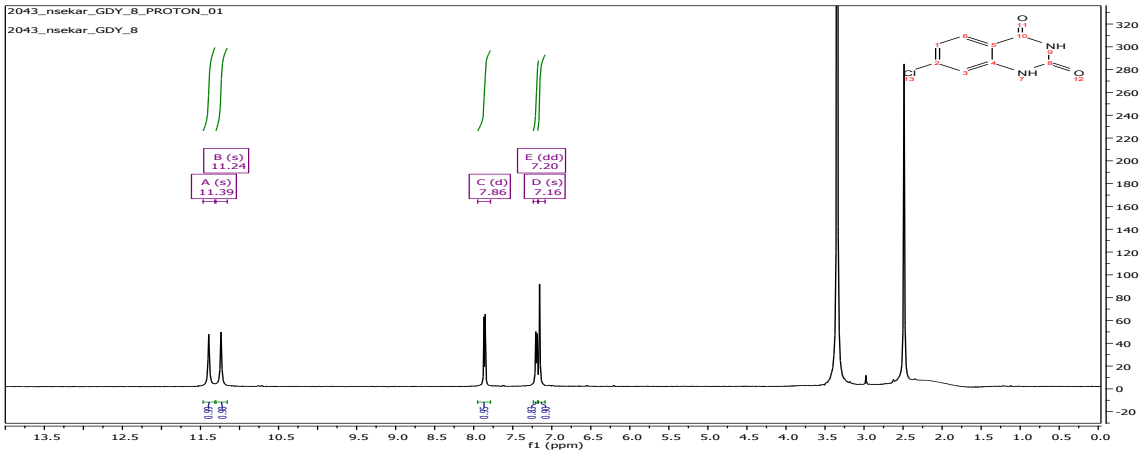


^{13}C-NMR



h) 7-Chloro quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR



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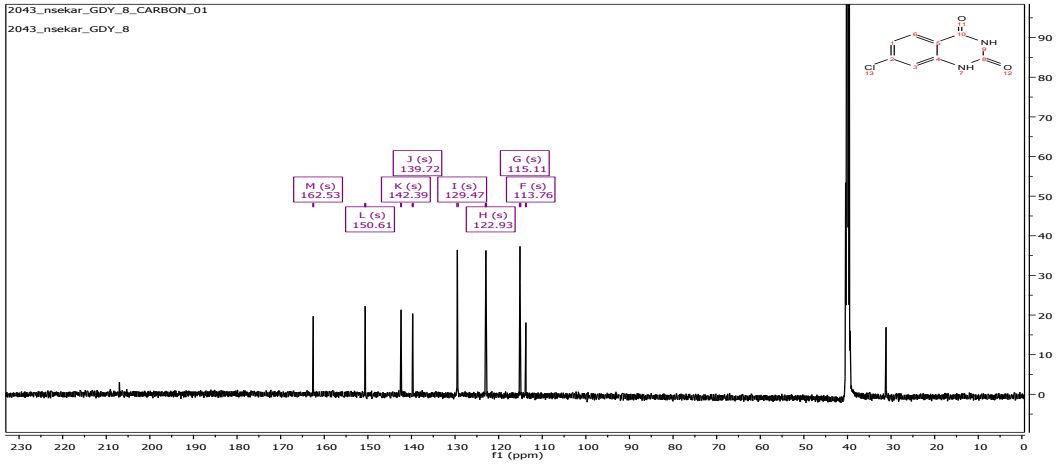
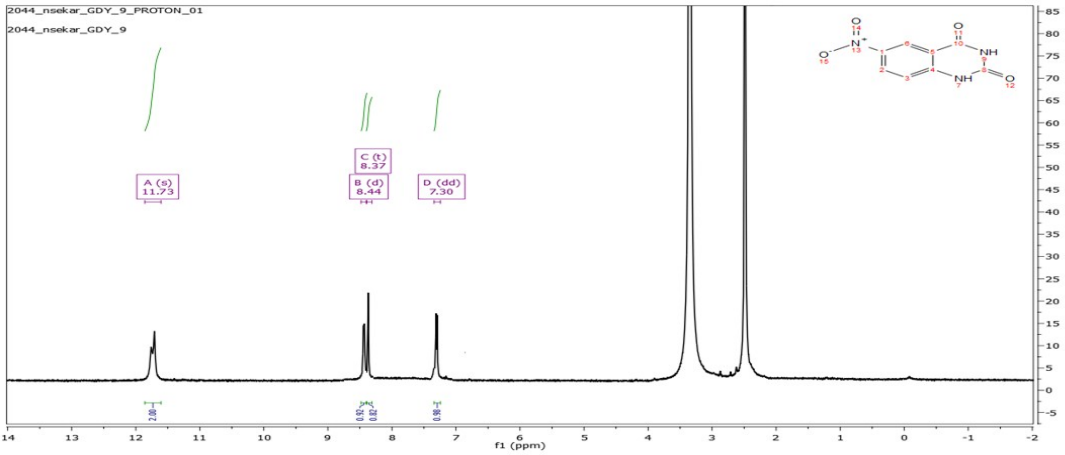


i) 6-Nitro quinazoline-2,4(1*H*,3*H*)-dione

^{1}H-NMR



^{13}C-NMR