Electronic Supplementary Information (ESI)

γ-Fe_2O_3@Cu_3Al-LDH-*N*-amidinoglycine: A new amphoteric and reusable magnetic nanocatalyst for synthesis of new pyrimidonaphthyridine derivatives and their antioxidant and antifungal evaluation

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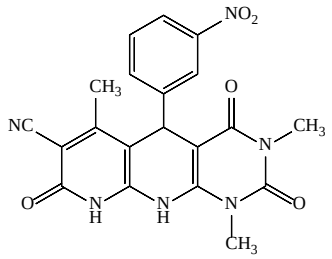
Table of Contents	Page number

1,3,6-trimethyl-2,4,8-trioxo-5-(3NO_2-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_1)

White solid, mp 255-258 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.51 (s, 9H, 3CH_3), 5.67 (s, 1H, CH), 7.51-8.01 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.91, 28.04, 35.28, 120.24, 121.35, 129.13, 133.69, 142.46, 147.84, 150.39 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3347, 3138, 2934, 2206, 1703, 1603, 1607; MS *m/z* = 420.1 (M^+).



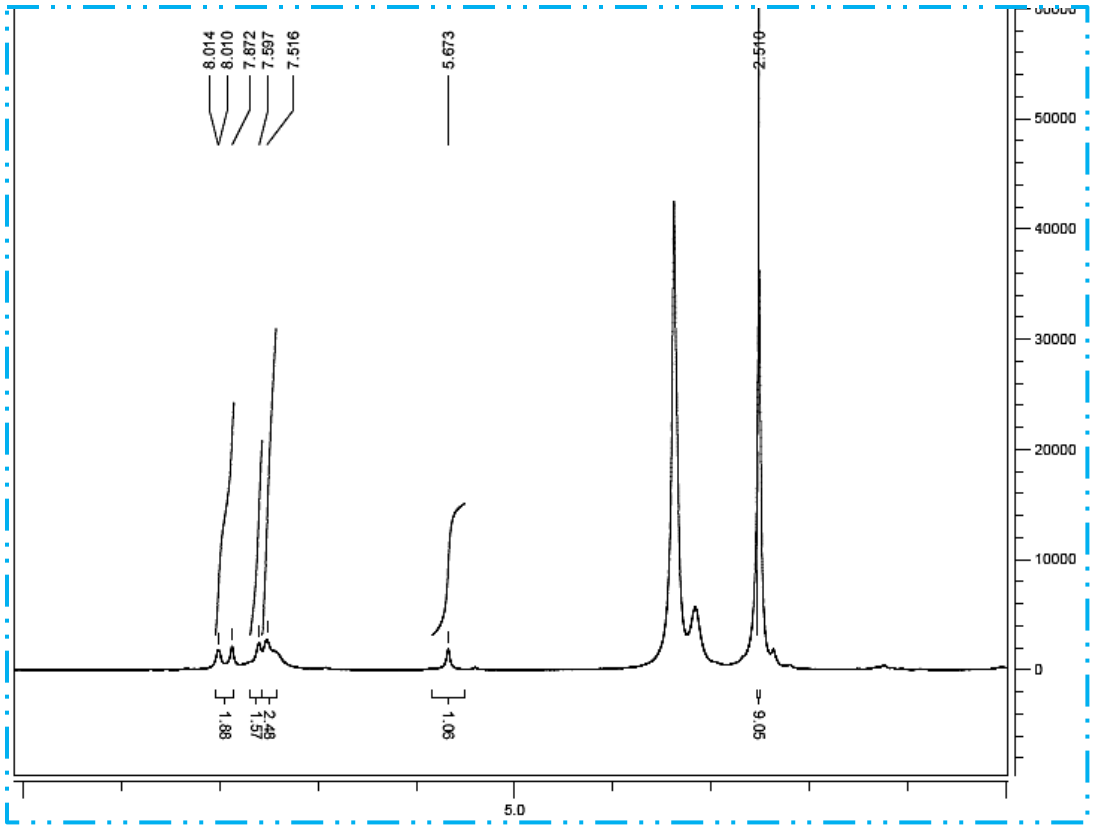


Fig. 1 The ^{1}H NMR spectrum of product (**C_1**)

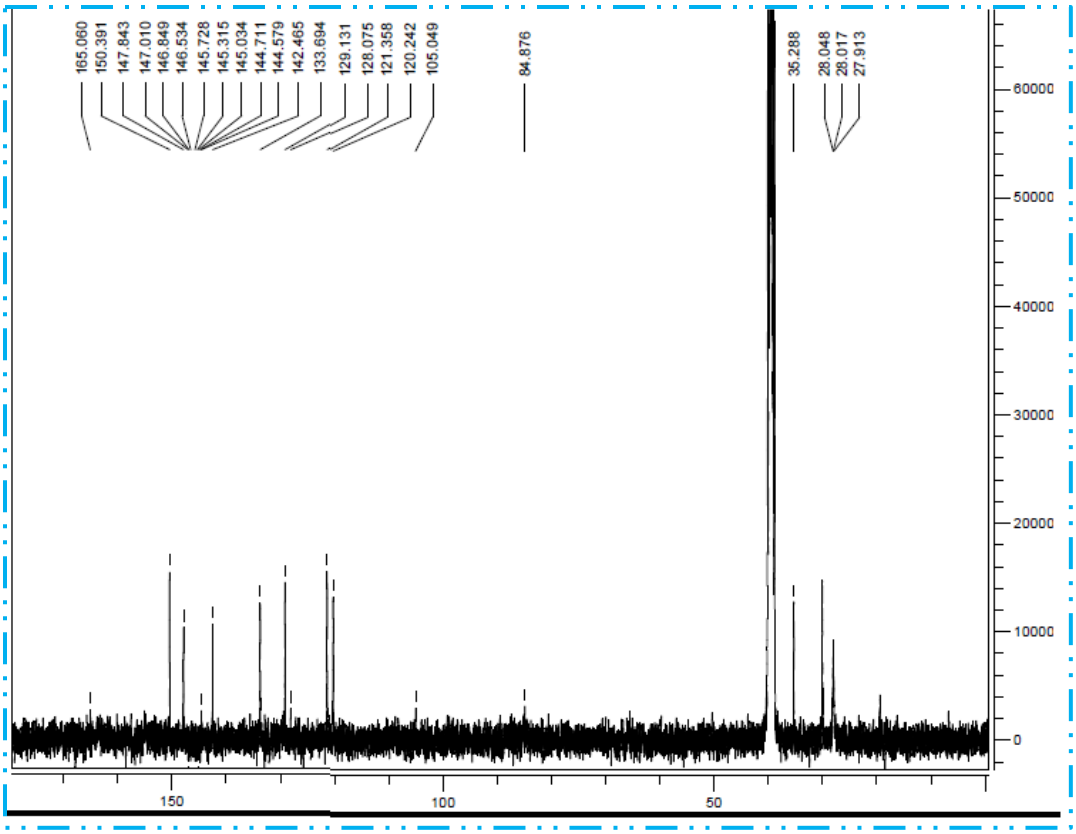


Fig. 2 The ^{13}C NMR spectrum of product (**C_1**)

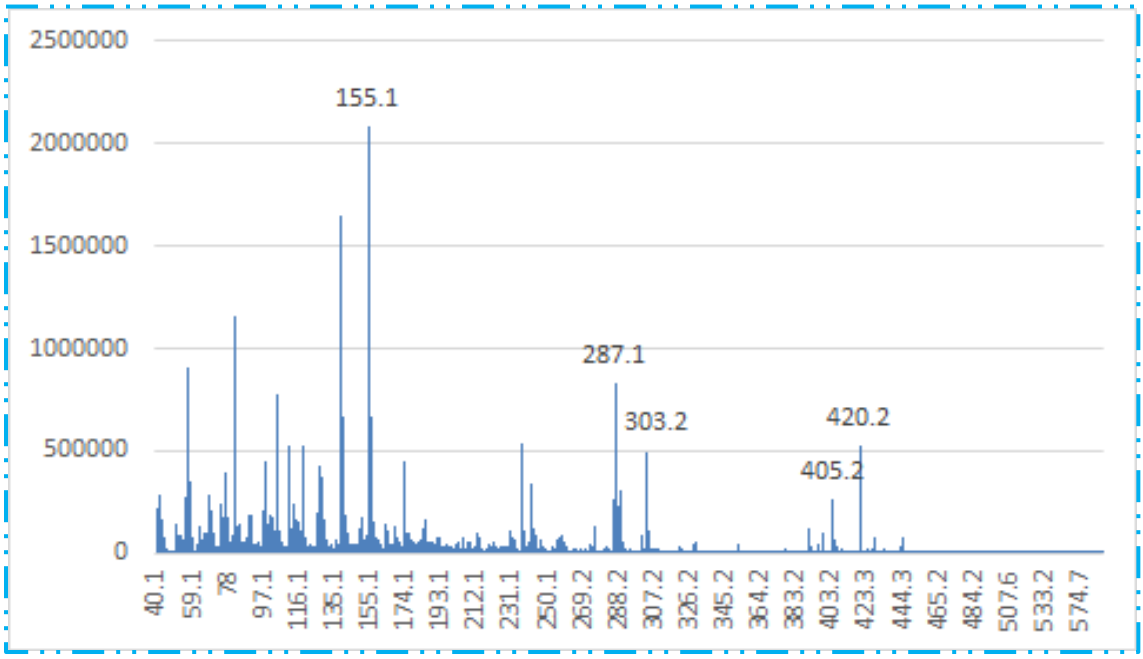


Fig. 3 The MASS spectrum of product (**C_1**)

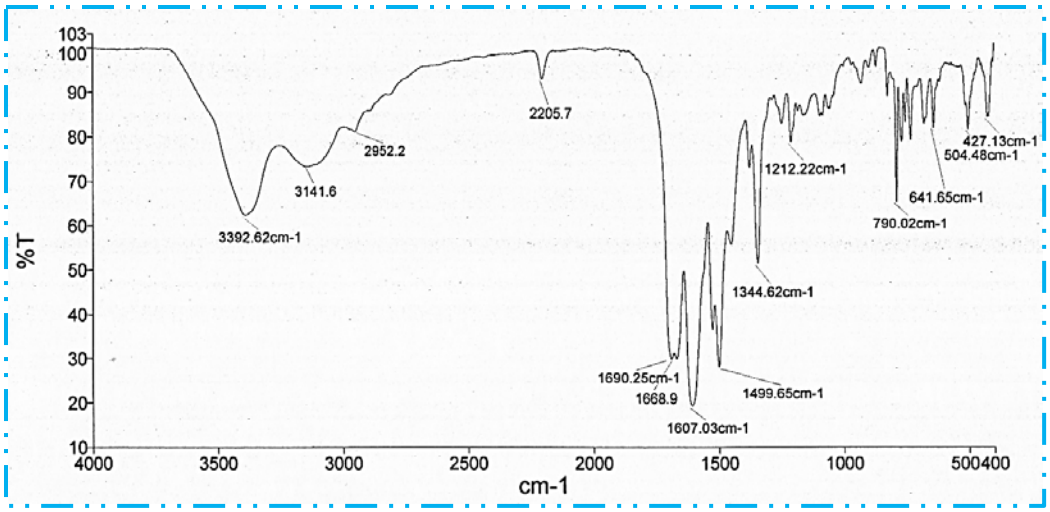
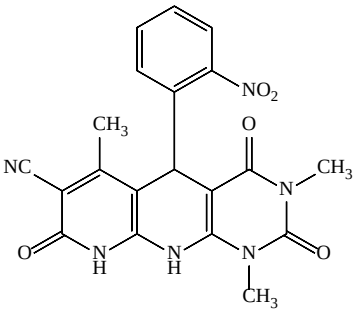


Fig. 4 The IR spectrum of product (C_1)

1,3,6-trimethyl-2,4,8-trioxo-5-(2NO_2-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_2)

White solid, mp 289-290 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.59 (s, 9H, 3CH_3), 6.17 (s, 1H, CH), 7.28-7.67 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.56, 28.27, 29.88, 30.19, 123.46, 126.70, 128.65, 131.41, 133.30, 149.60, 150.23 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3436, 3101, 2952, 2197, 1693, 1656, 1598 ; MS *m/z* = 420.1 (M^+).



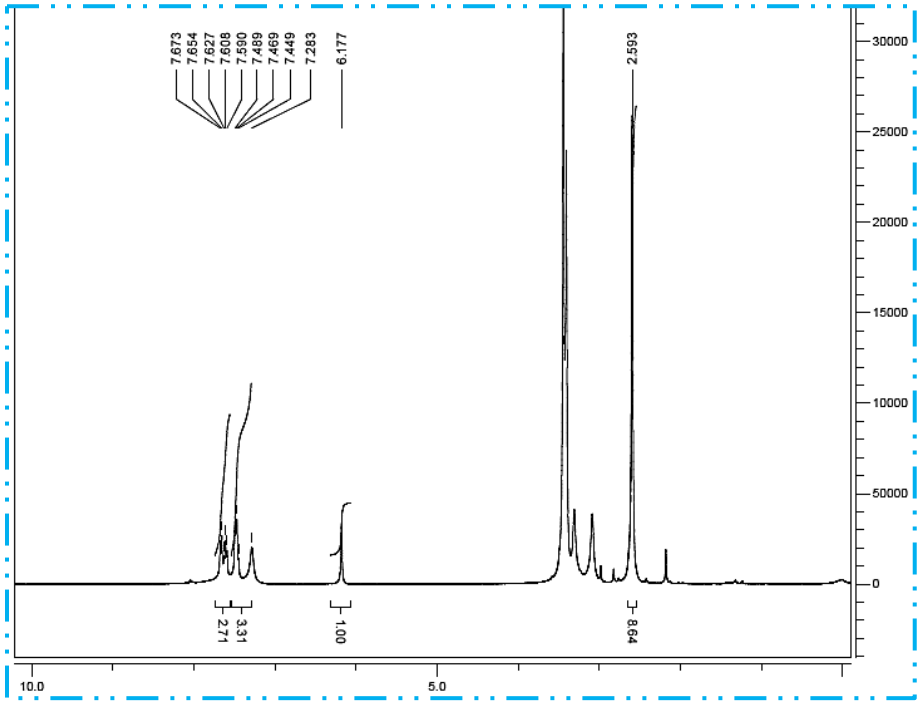


Fig. 5 The ^{1}H NMR spectrum of product (**C_2**)

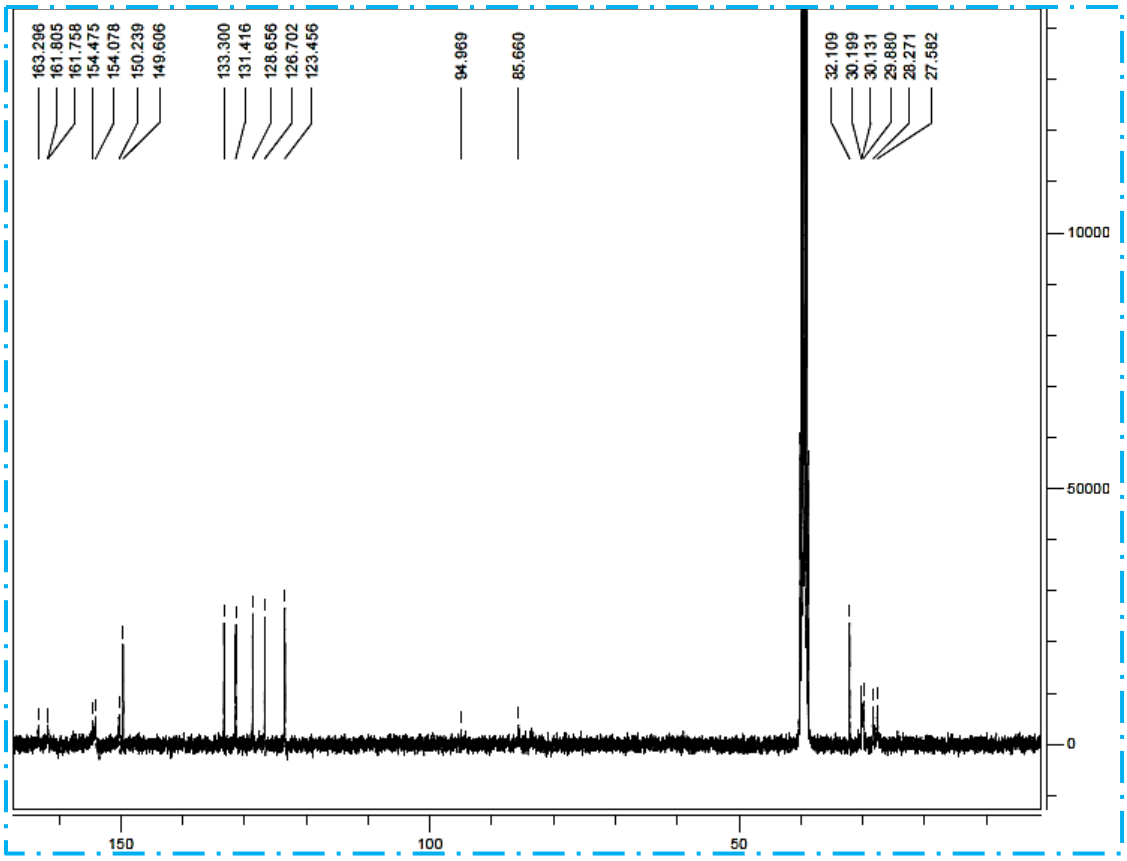


Fig. 6 The ^{13}C NMR spectrum of product (**C_2**)

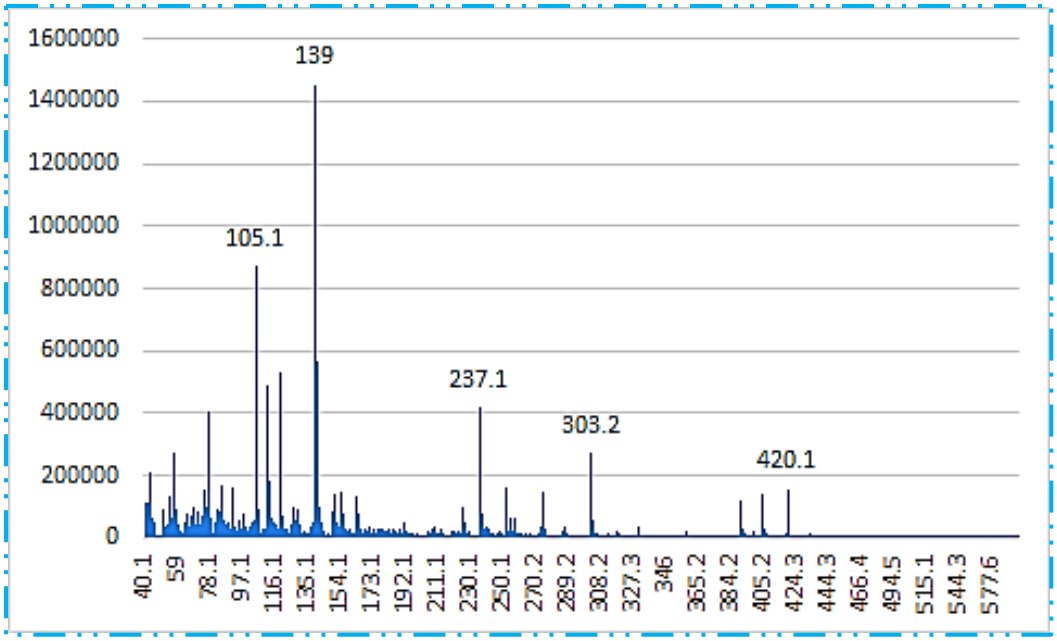


Fig. 7 The MASS spectrum of product (**C_2**)

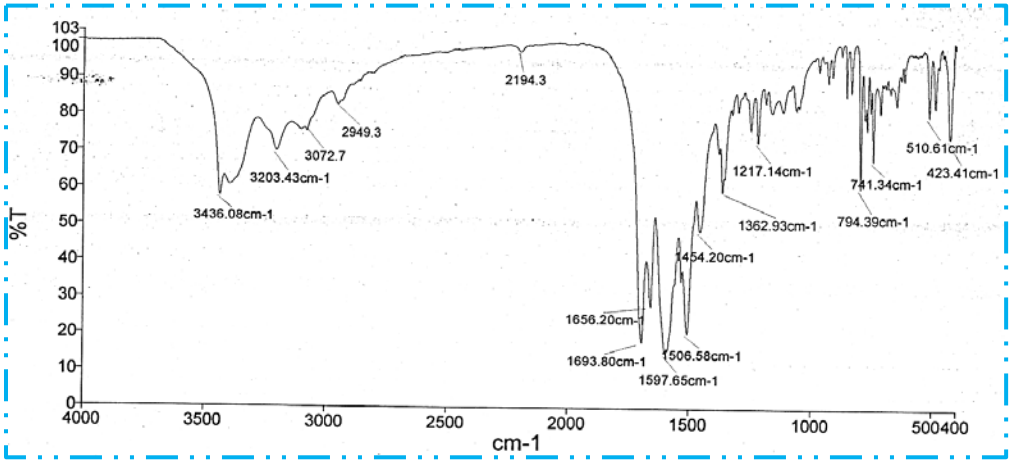


Fig. 8 The IR spectrum of product (**C_2**)

1,3,6-trimethyl-2,4,8-trioxo-5-(4NO_2-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_3)

White solid, mp 289-290 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.56 (s, 9H, 3CH_3), 5.74 (s, 1H, CH), 7.46-8.15 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.76, 28.07, 35.80, 122.84, 127.95, 145.18, 148.88, 150.37 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3456, 3106, 2934, 3194, 1686, 1667; MS *m/z* = 420.1 (M^+).

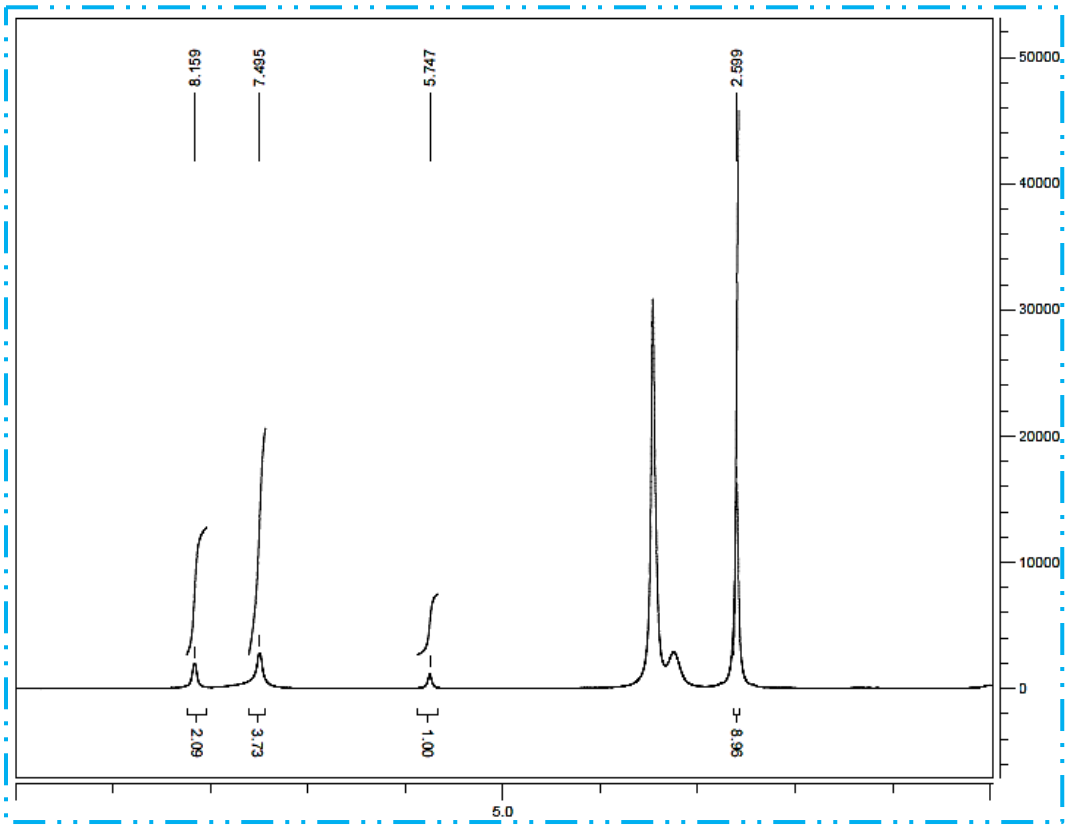


Fig. 9 The ^{1}H NMR spectrum of product (**C_3**)

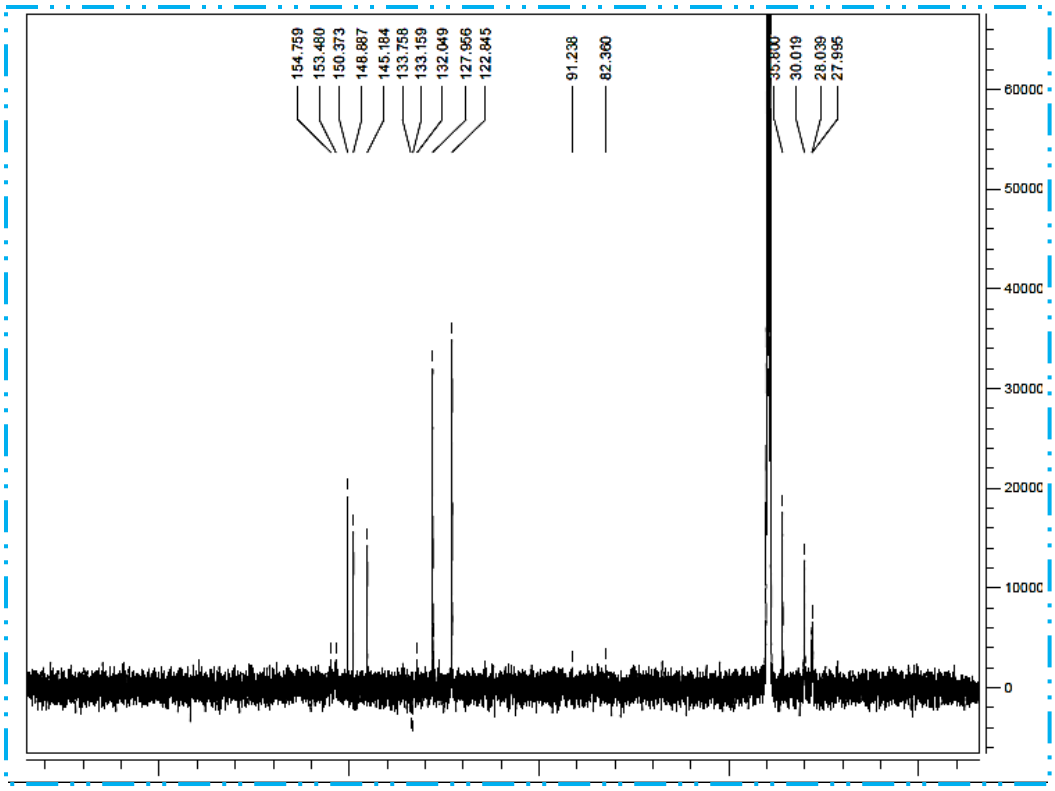


Fig. 10 The ^{13}C NMR spectrum of product (**C_3**)

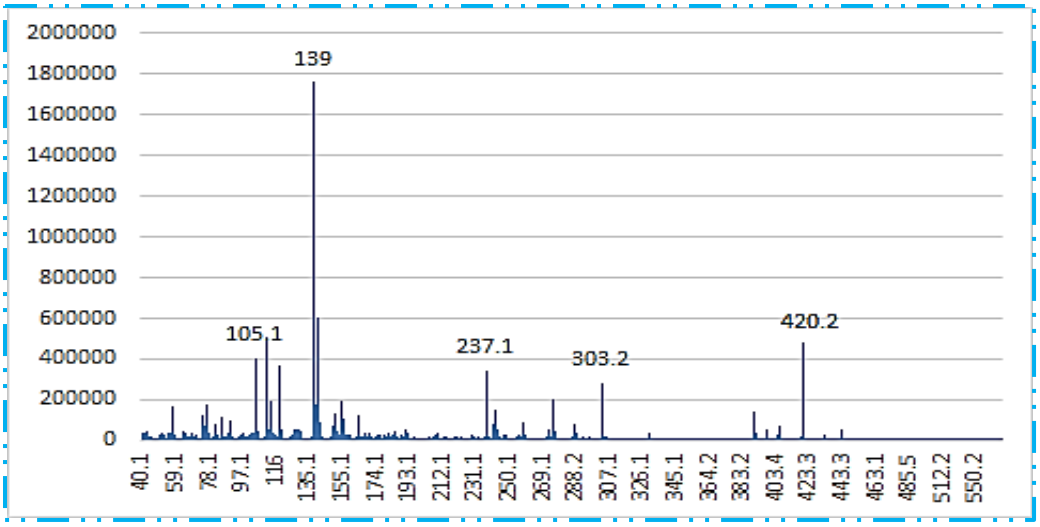


Fig. 11 The MASS spectrum of product (**C_3**)

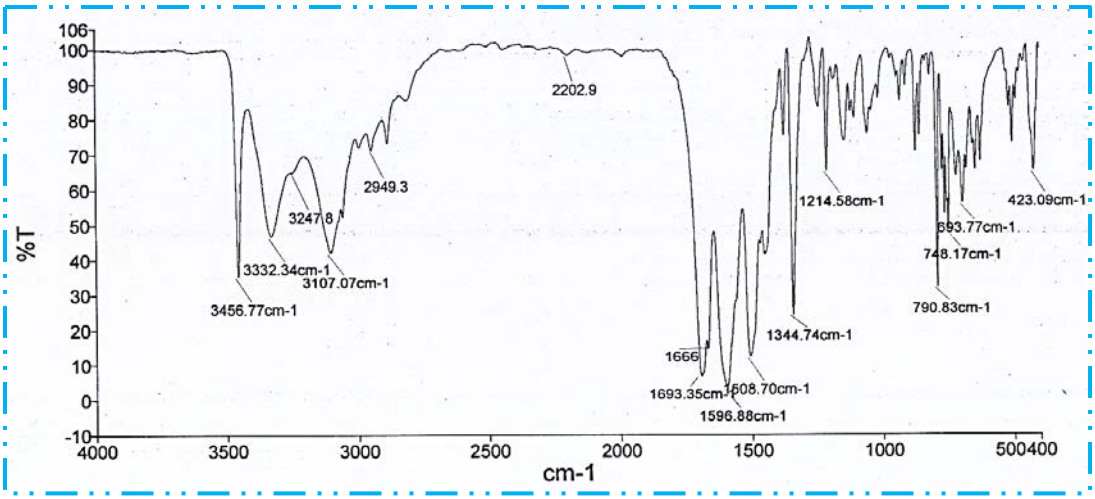


Fig. 12 The IR spectrum of product (**C_3**)

1,3,6-trimethyl-2,4,8-trioxo-5-(4-Cl-3NO_2-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_4)

White solid, mp 230-232 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.57 (s, 9H, 3CH_3), 5.57 (s, 1H, CH), 7.05-7.56 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.57, 29.92, 34.36, 126.41, 128.70, 130.65, 133.19, 137.64, 150.28 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3352 3118, 2955, 2202, 1698, 1680, 1560 ; MS *m/z* = 454.07 (M^+).

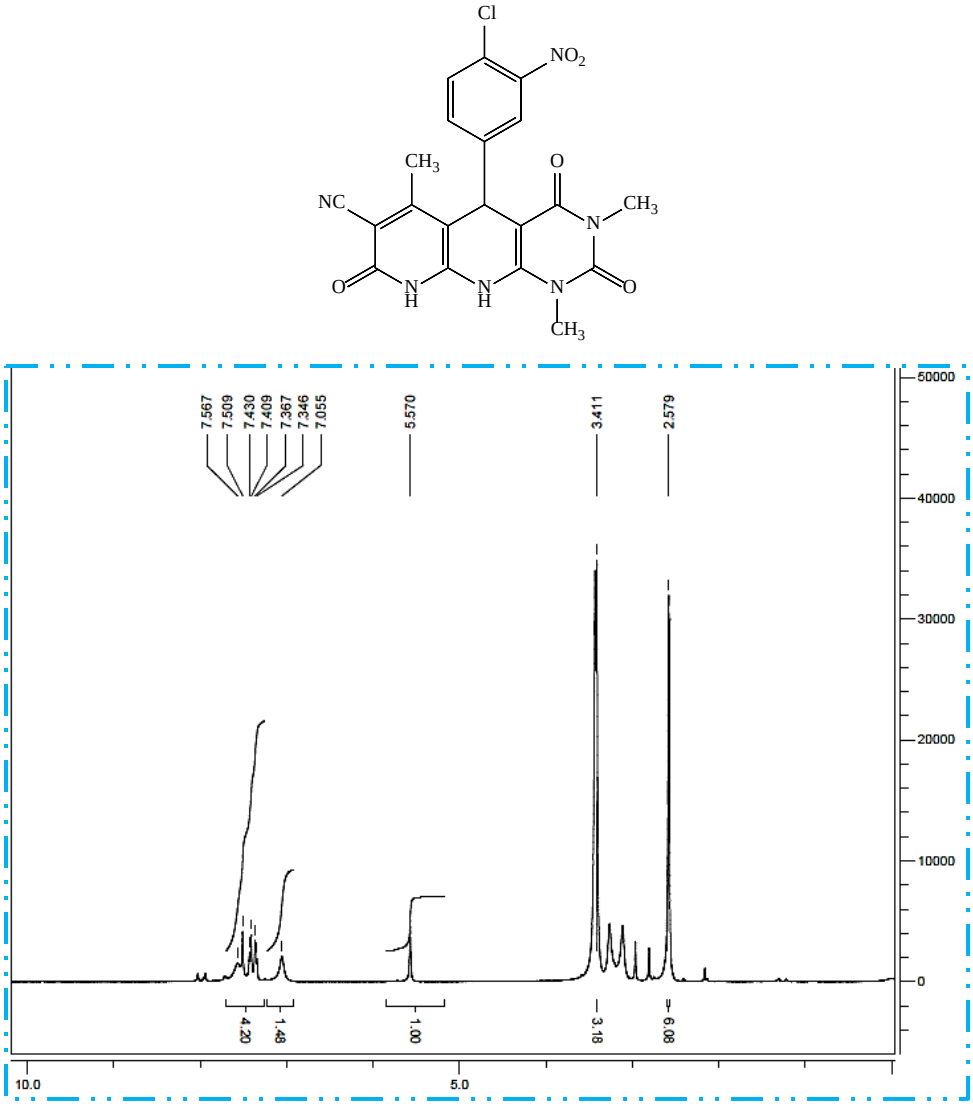


Fig. 13 The ^{1}H NMR spectrum of product (**C_4**)

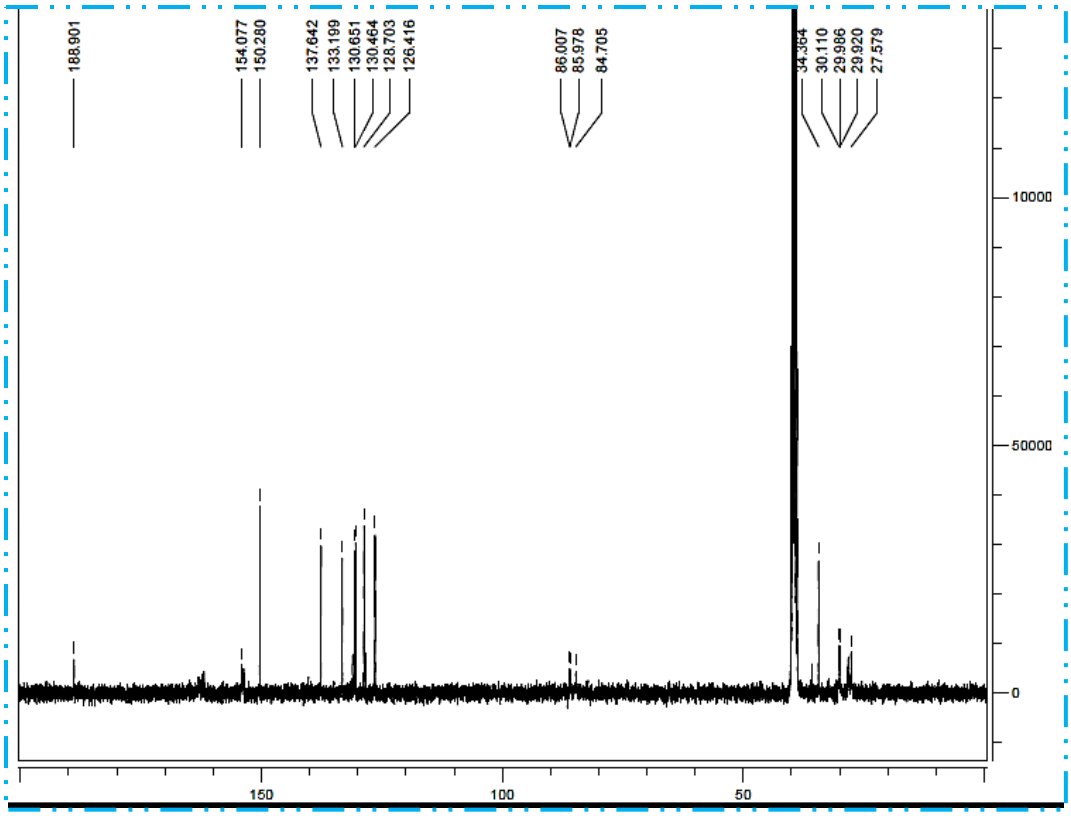


Fig. 14 The ^{13}C NMR spectrum of product (**C_4**)

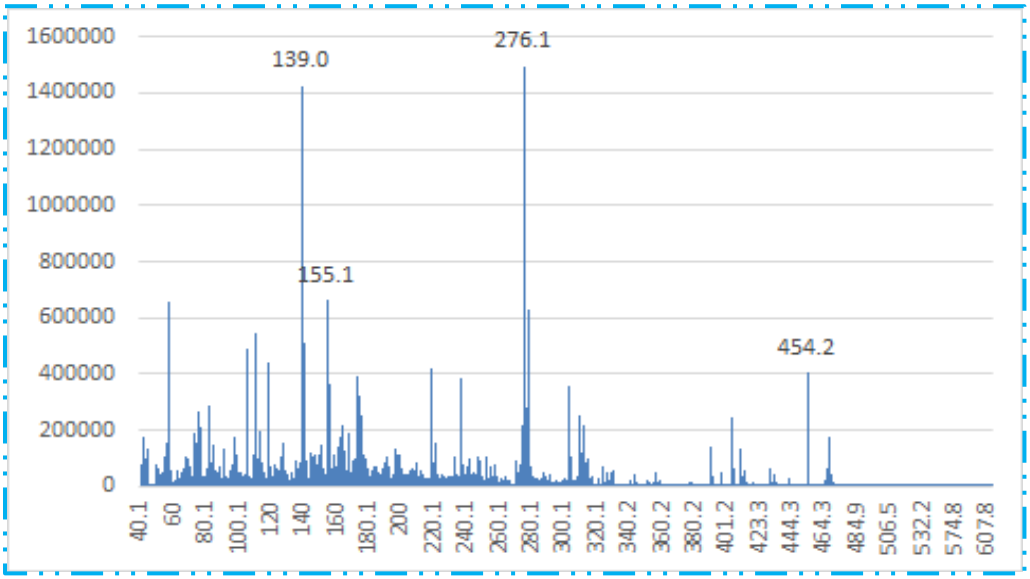


Fig. 15 The MASS spectrum of product (**C_4**)

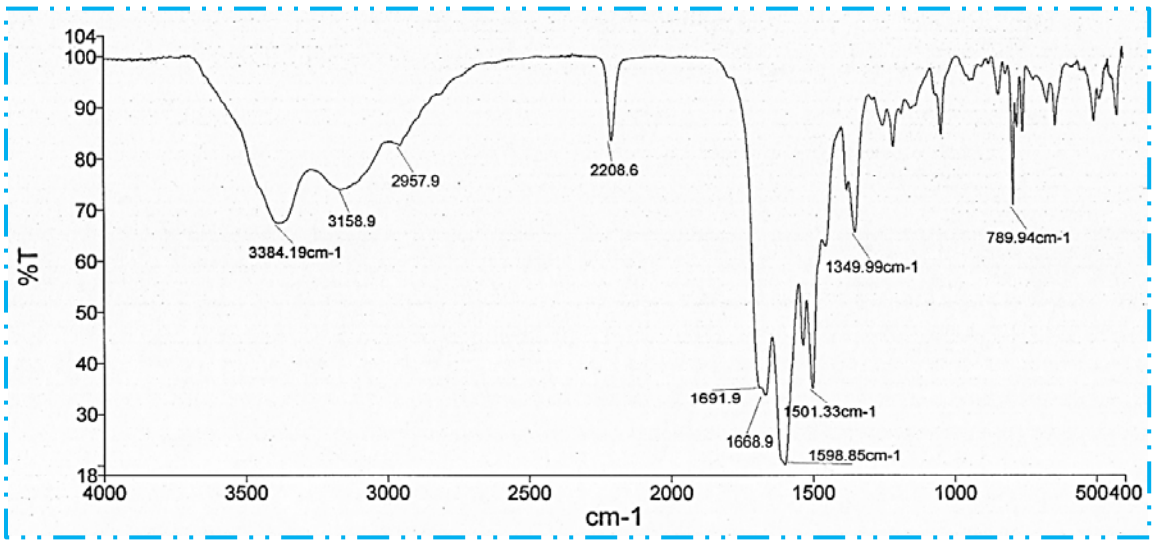
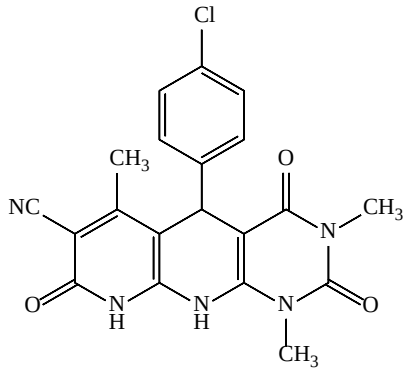


Fig. 16 The IR spectrum of product (**C_4**)

1,3,6-trimethyl-2,4,8-trioxo-5-(4-Cl-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_5)

White solid, mp 256 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.55 (s, 9H, 3CH_3), 5.60 (s, 1H, CH), 7.15-7.29 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.96, 28.09, 34.88, 127.50, 128.55, 129.39, 138.75, 150.38 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3349, 3158, 2955, 2205, 1700, 1678, 1595 ; MS *m/z* = 409.09 (M^+).



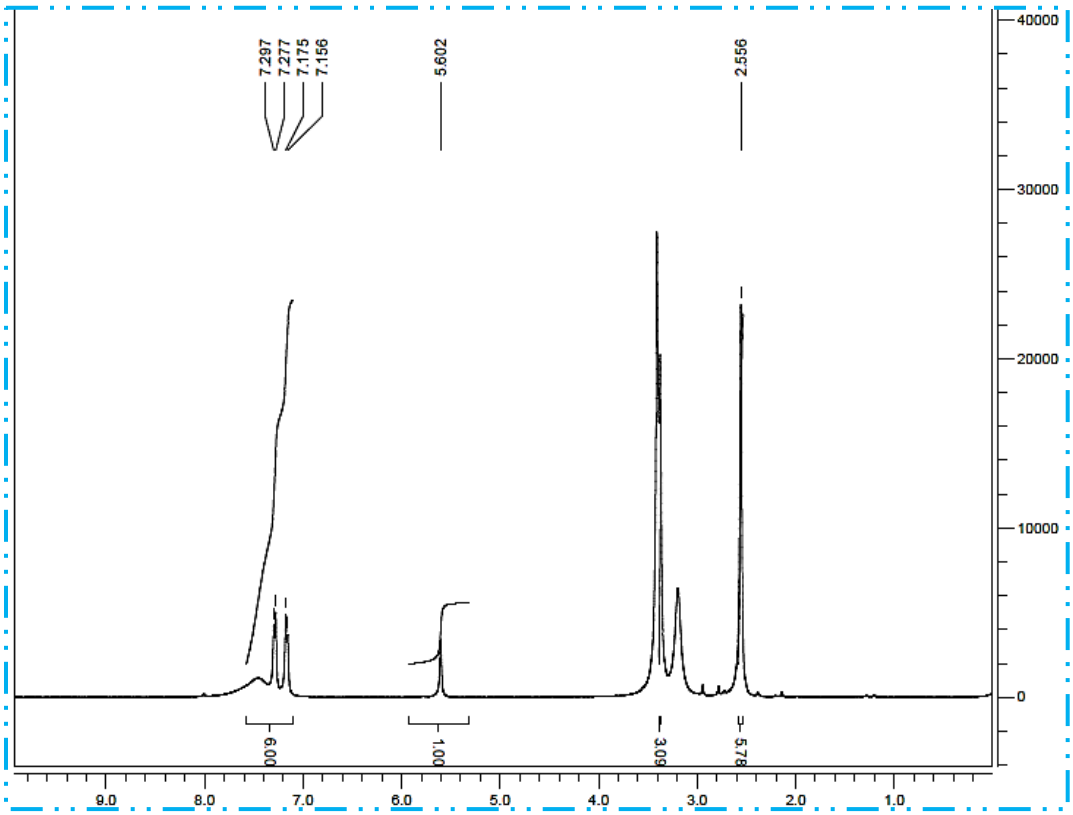


Fig. 17 The ^{1}H NMR spectrum of product (**C_5**)

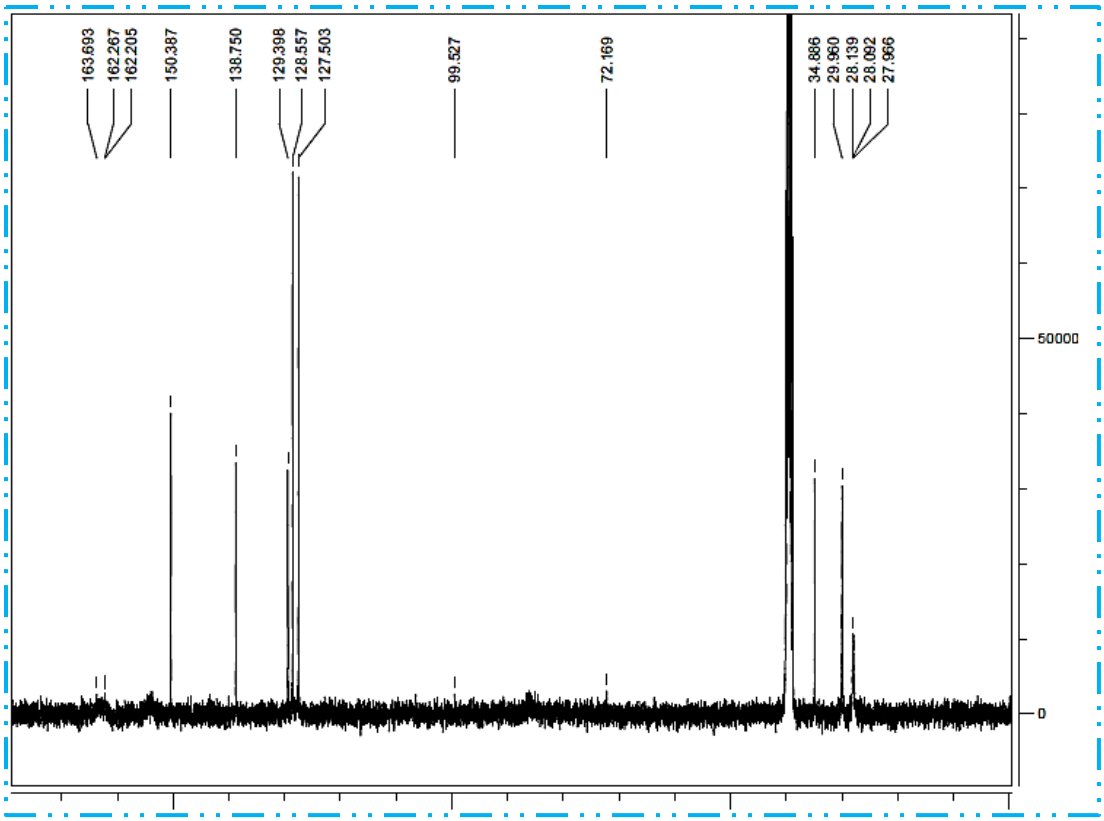


Fig. 18 The ^{13}C NMR spectrum of product (**C5**)

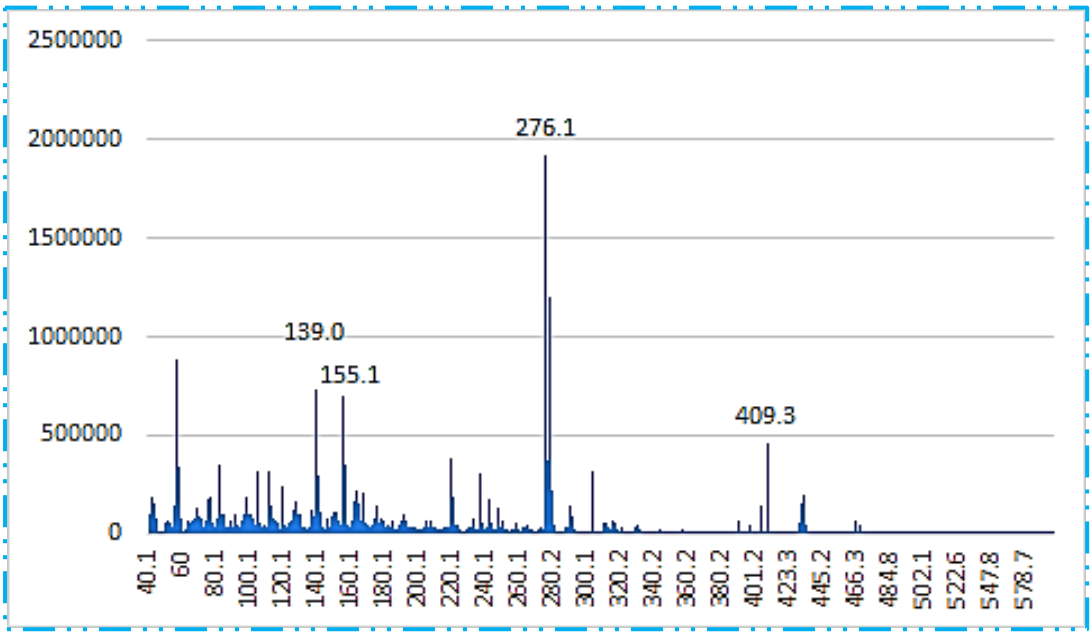


Fig. 19 The MASS spectrum of product (**C5**)

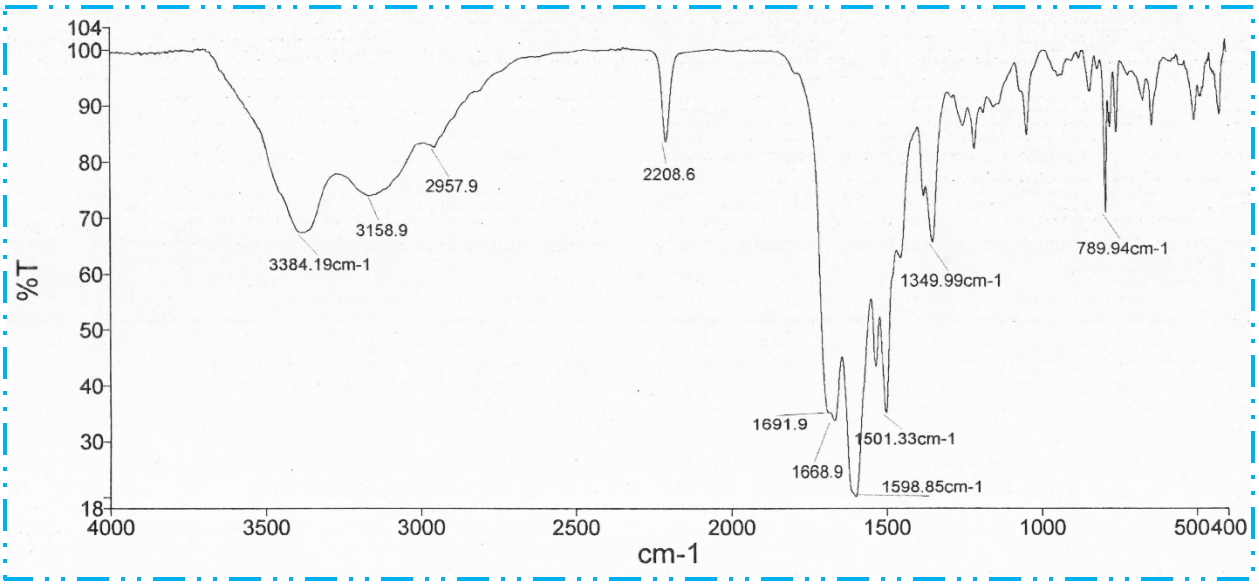


Fig. 20 The IR spectrum of product (**C_5**)

1,3,6-trimethyl-2,4,8-trioxo-5-(2, 4-Cl_2-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_6)

White solid, mp 259 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.59 (s, 9H, 3CH_3), 5.70 (s, 1H, CH), 7.53-7.83 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.98, 28.04, 35.03, 120.82, 123.42, 130.30, 132.24, 141.74, 147.76, 150.41, 162.28, 162.38 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3388, 3156, 2955, 2200, 1690, 1671, 1610 ; MS *m/z* = 443.06 (M^+).

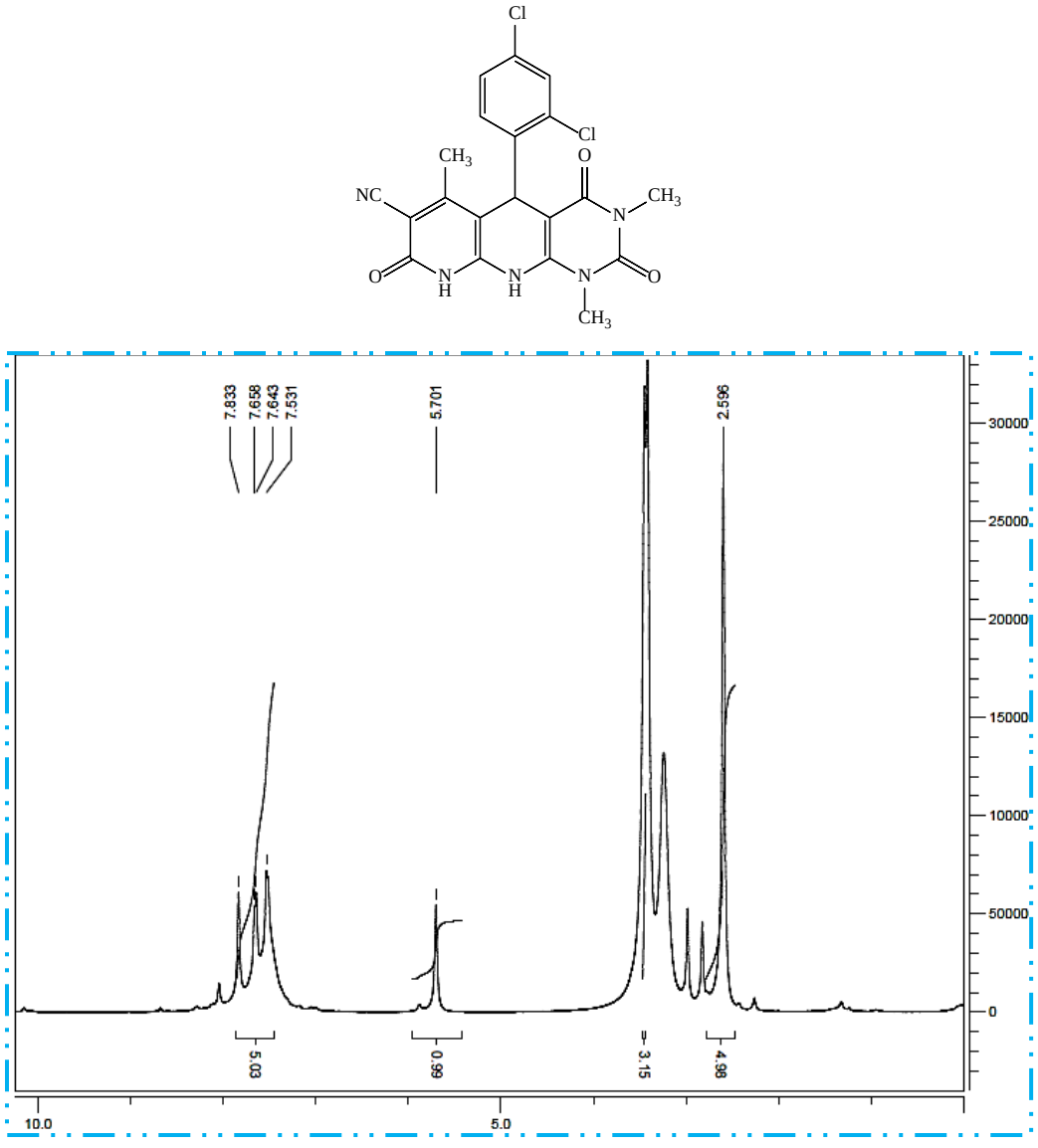


Fig. 21 The ^{1}H NMR spectrum of product (**C_6**)

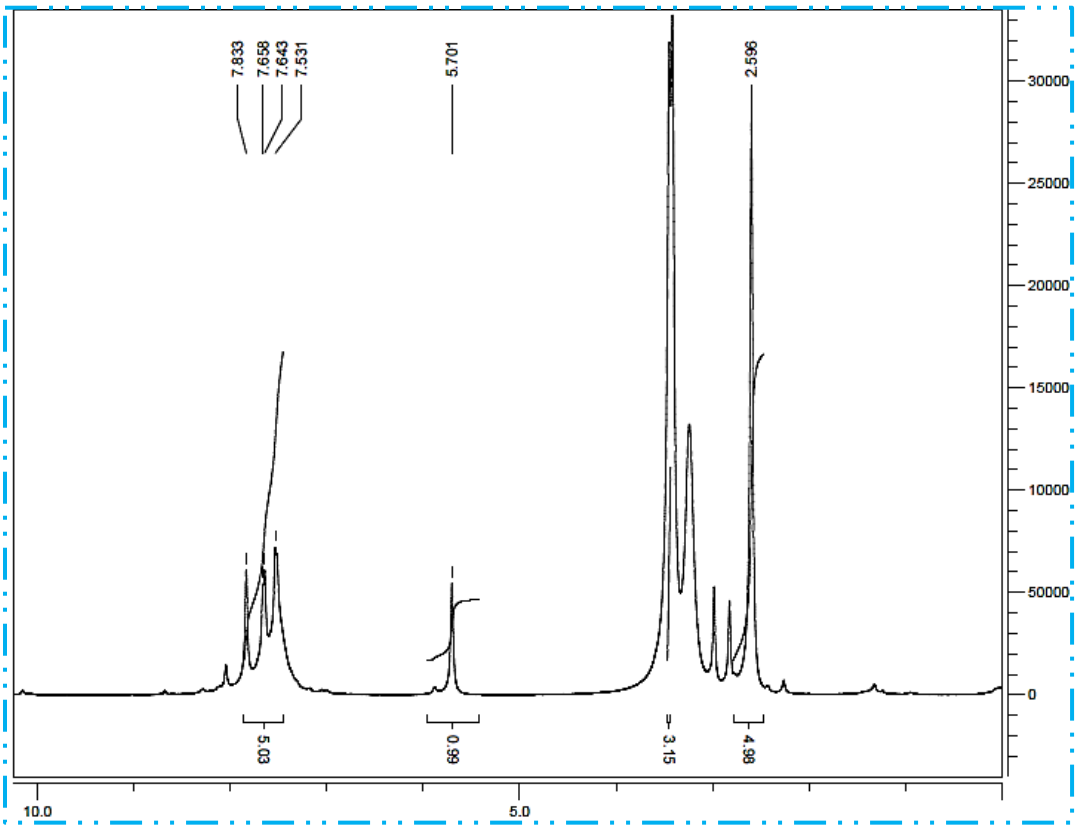


Fig. 22 The ^{13}C NMR spectrum of product (**C_6**)

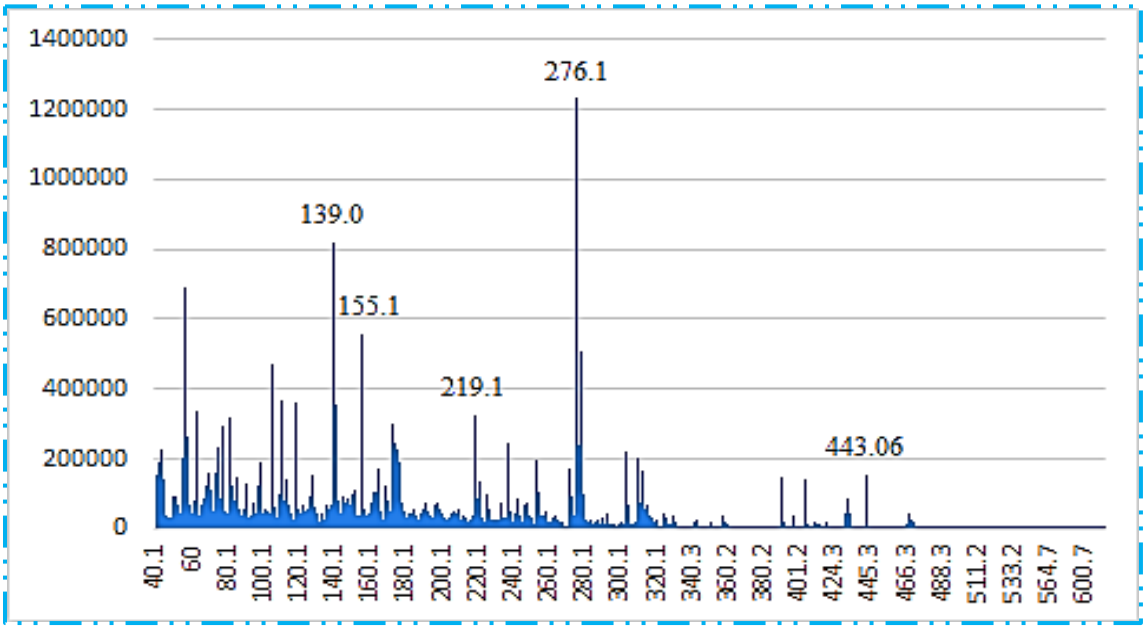


Fig. 23 The MASS spectrum of product (**C_6**)

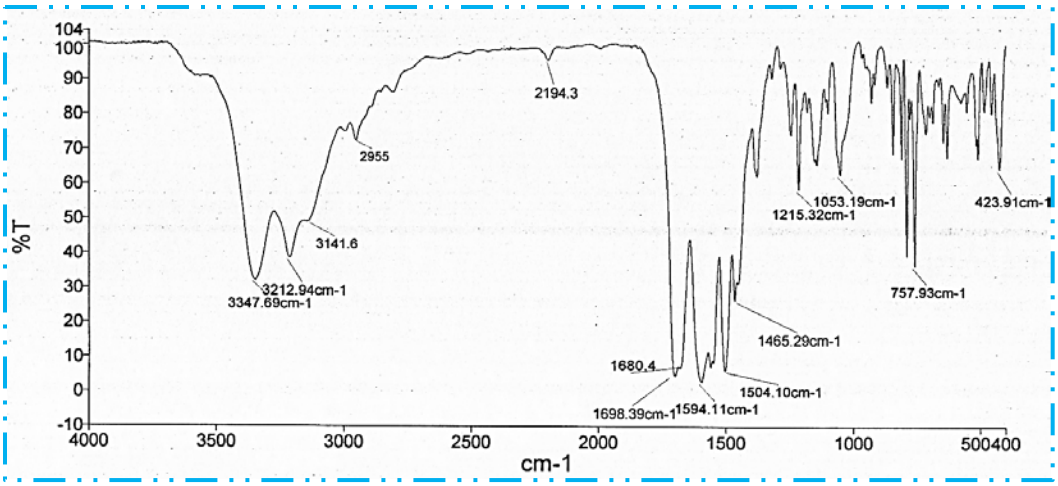


Fig. 24 The IR spectrum of product (C_6)

1,3,6-trimethyl-2,4,8-trioxo-5-(4-Br-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_7)

White solid, mp 255-258 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.59 (s, 9H, 3CH_3), 5.61 (s, 1H, CH), 7.15-7.45 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.95, 29.96, 34.94, 117.85, 129.01, 130.41, 139.23, 150.38 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3345, 3164, 2949, 2208, 1699, 1676, 1595; MS *m/z* = 453.04 (M^+).

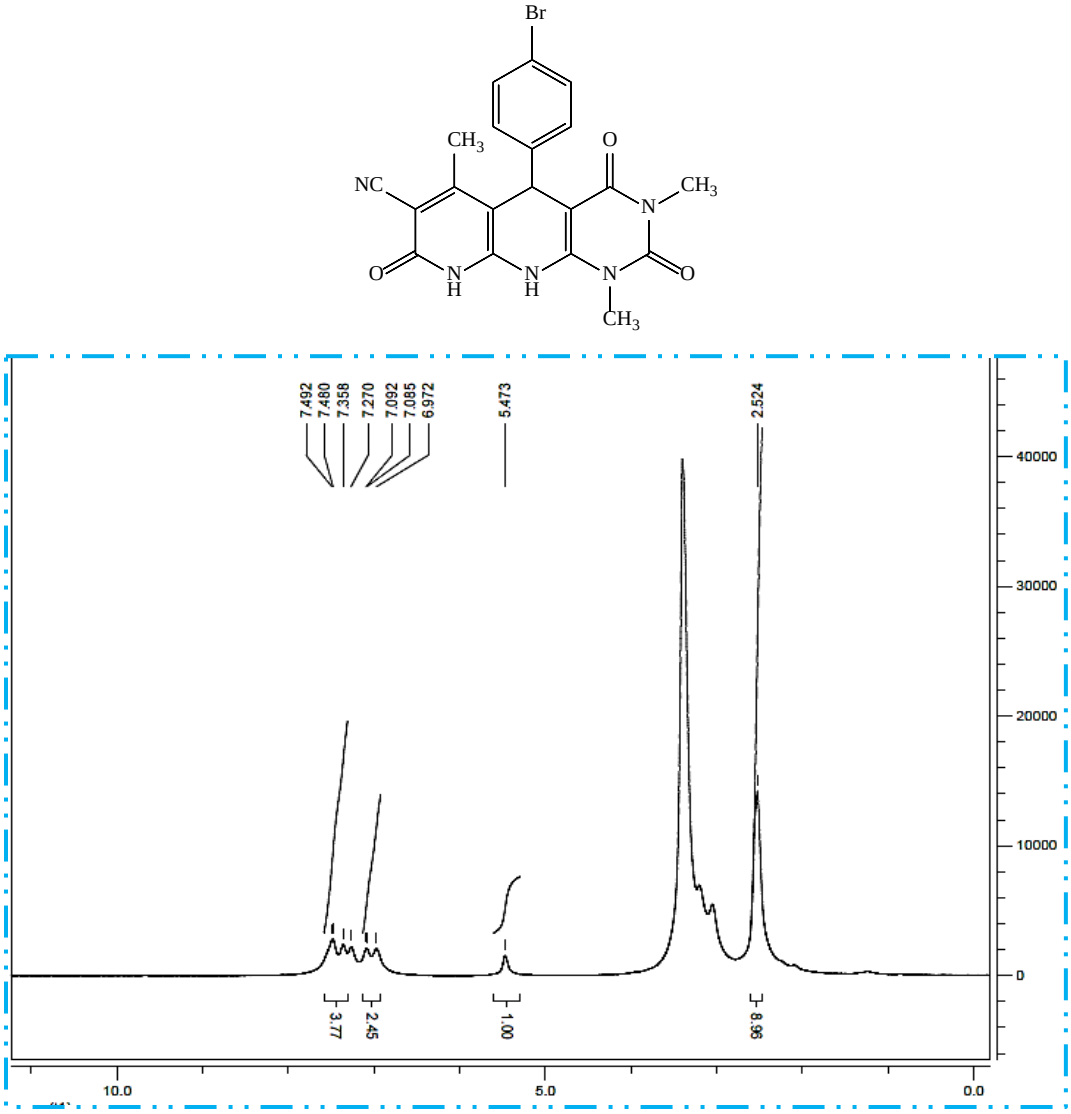


Fig. 25 The ^{1}H NMR spectrum of product (**C_7**)

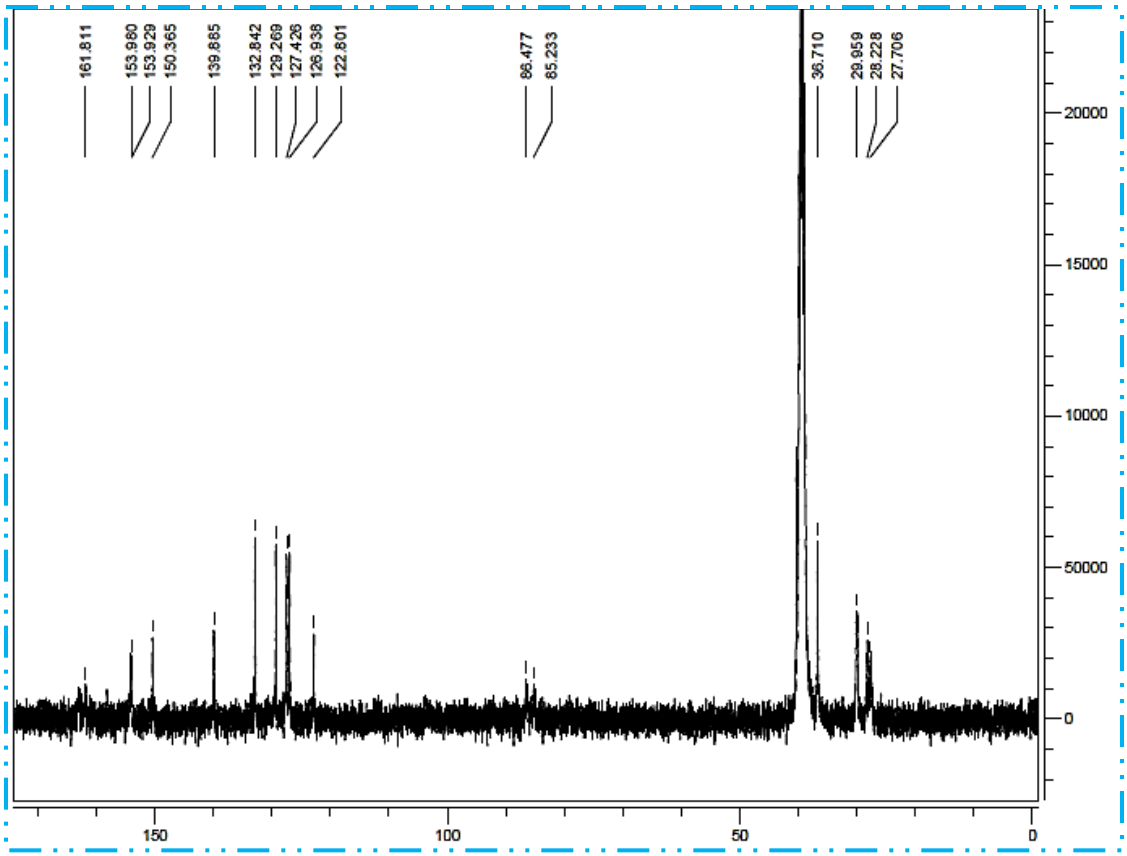


Fig. 26 The ^{13}C NMR spectrum of product (**C_7**)

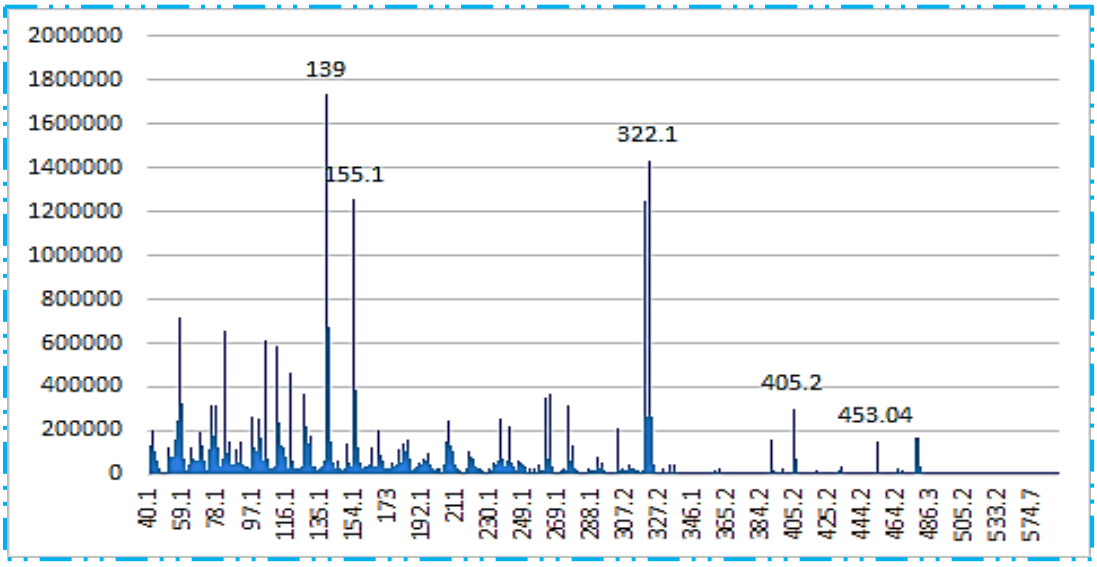


Fig. 27 The MASS spectrum of product (**C_7**)

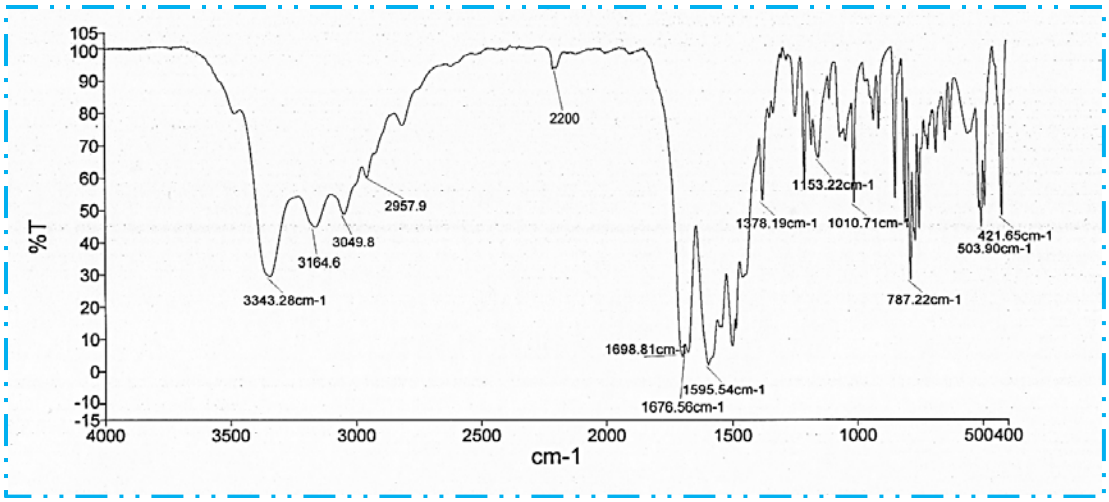
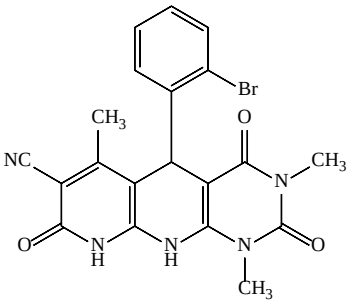


Fig. 28 The IR spectrum of product (**C_7**)

1,3,6-trimethyl-2,4,8-trioxo-5-(2Br-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_8)

White solid, mp 253-255 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.52 (s, 9H, 3CH_3), 5.47 (s, 1H, CH), 6.97-7.49 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.70, 28.22, 36.71, 122.80, 126.93, 129.26, 139.88, 153.98, 161.81 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3363, 3209, 3058, 2948, 2200, 1688, 1603; MS *m/z* = 453.04 (M^+).



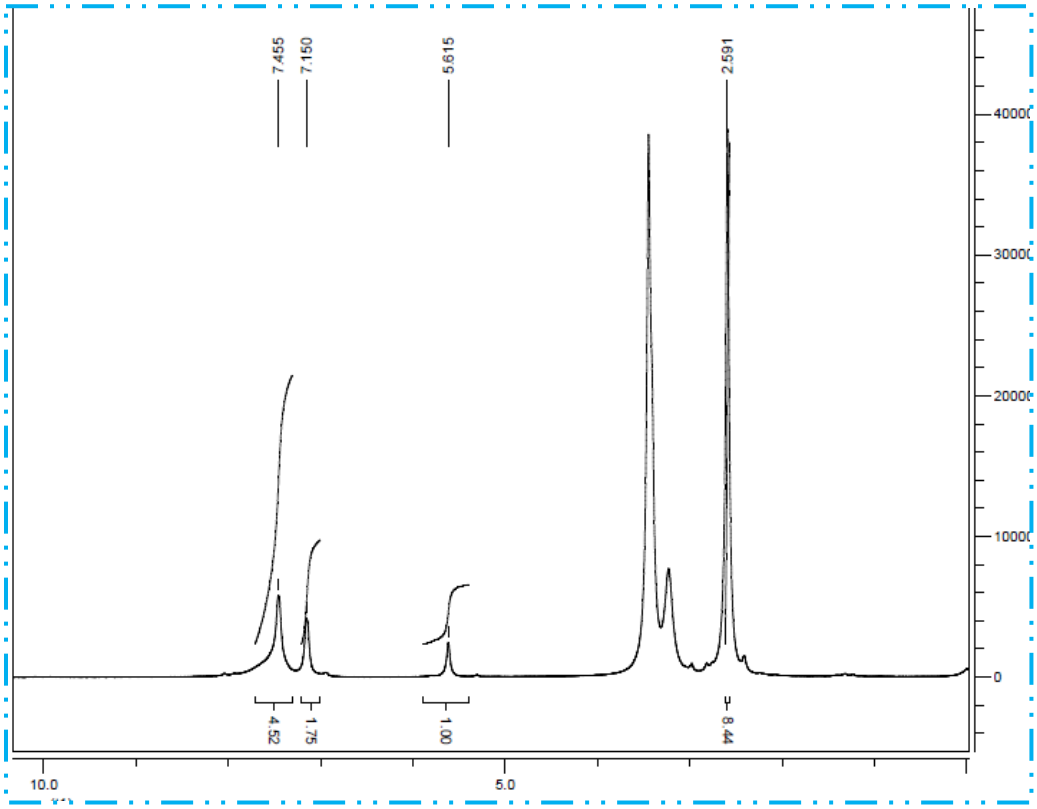


Fig. 29 The ^{1}H NMR spectrum of product (**C_8**)

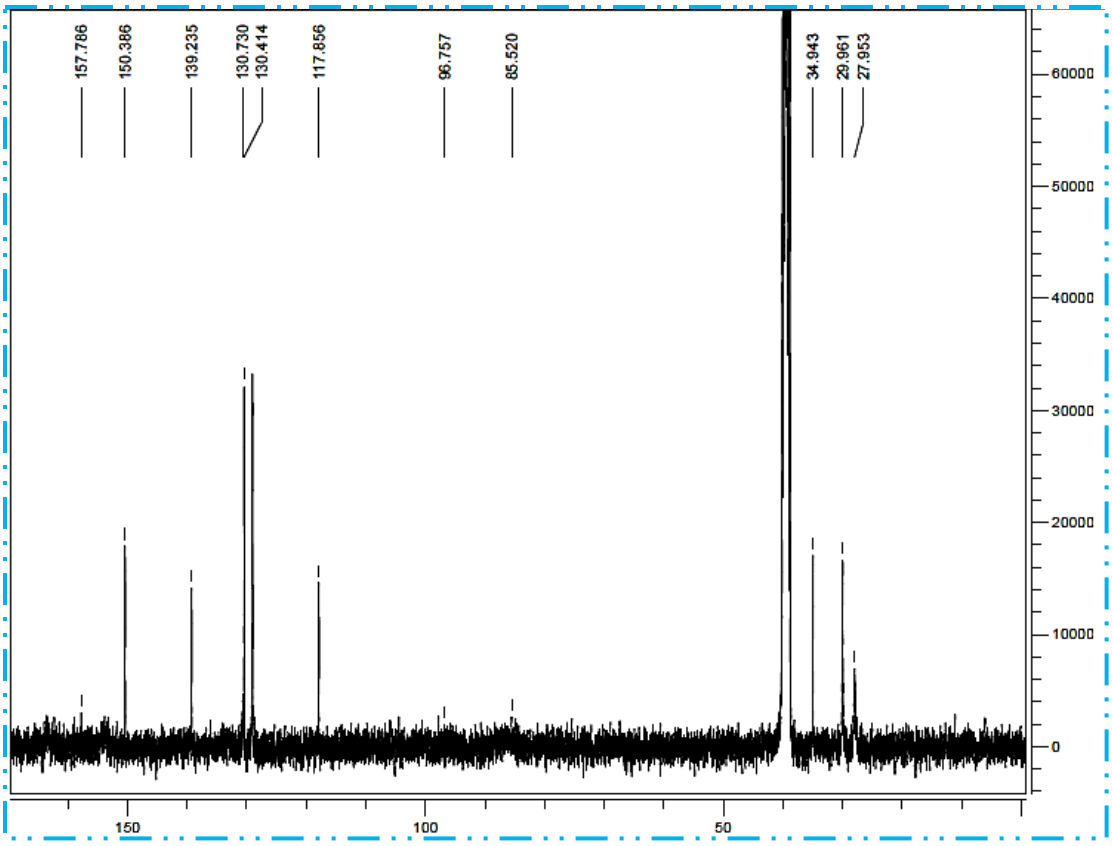


Fig. 30 The ^{13}C NMR spectrum of product (C_8)

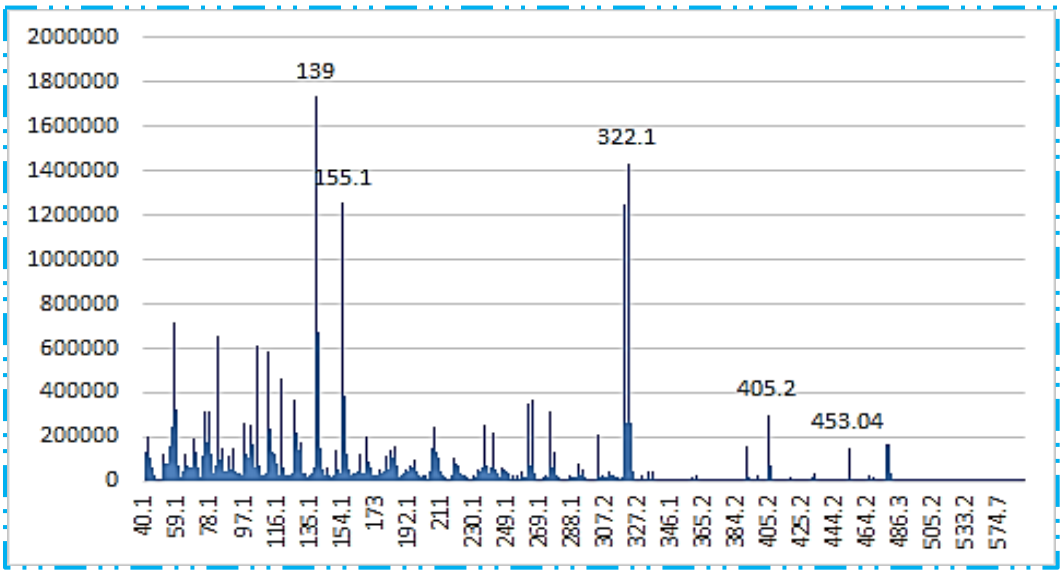


Fig. 31 The MASS spectrum of product (C_8)

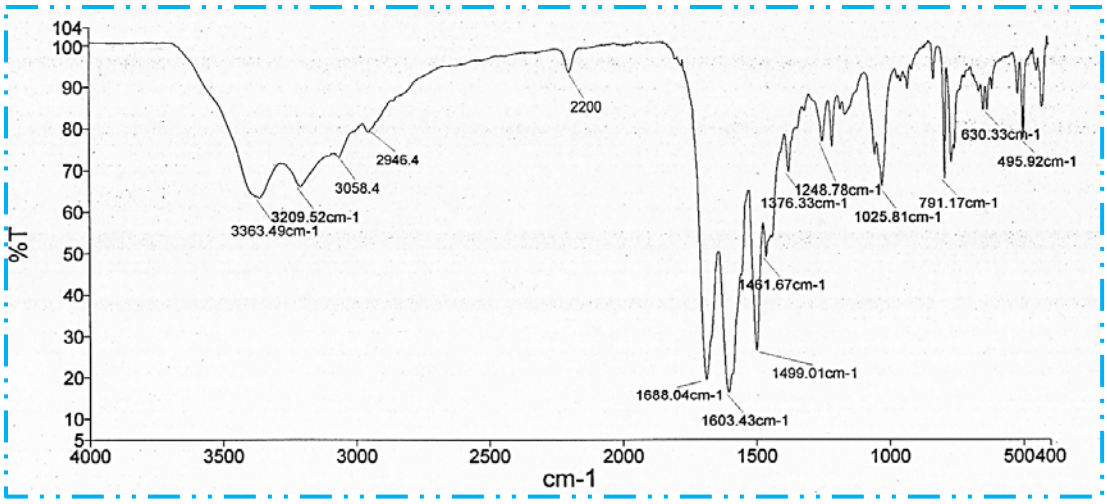
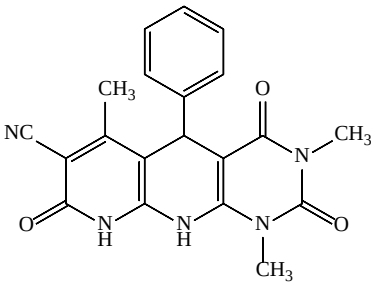


Fig. 32 The IR spectrum of product (**C_8**)

1,3,6-trimethyl-2,4,8-trioxo-5-(phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_9)

White solid, mp 280-282 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.55 (s, 9H, 3CH_3), 5.63 (s, 1H, CH), 7.15-5.51 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.93, 27.97, 29.94, 35.21, 124.83, 126.50, 127.66, 139.52, 150.41 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3458, 3200, 3003, 2200, 1693, 1654; MS *m/z* = 375.39 (M^+).



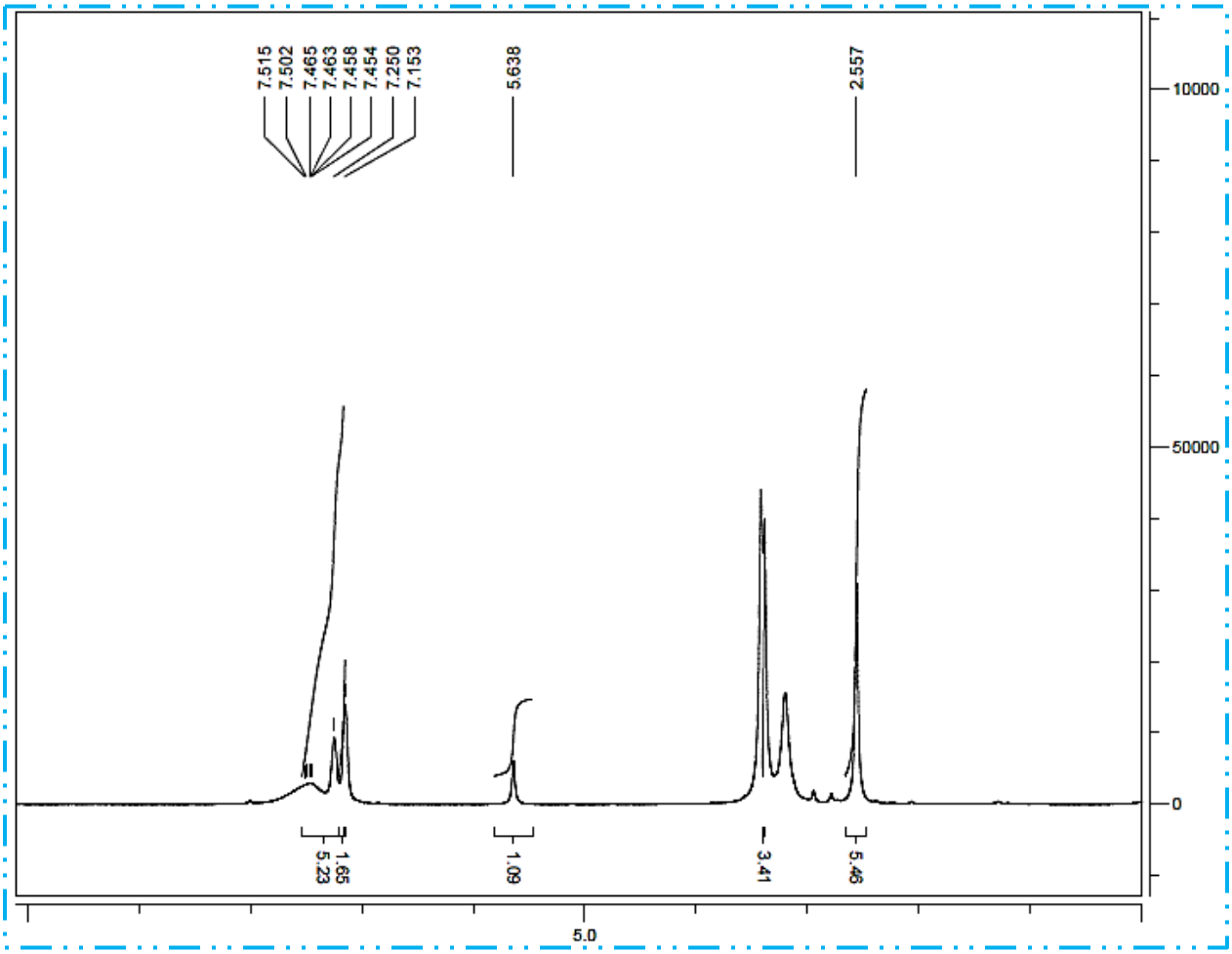


Fig. 33 The ^{1}H NMR spectrum of product (**C_9**)

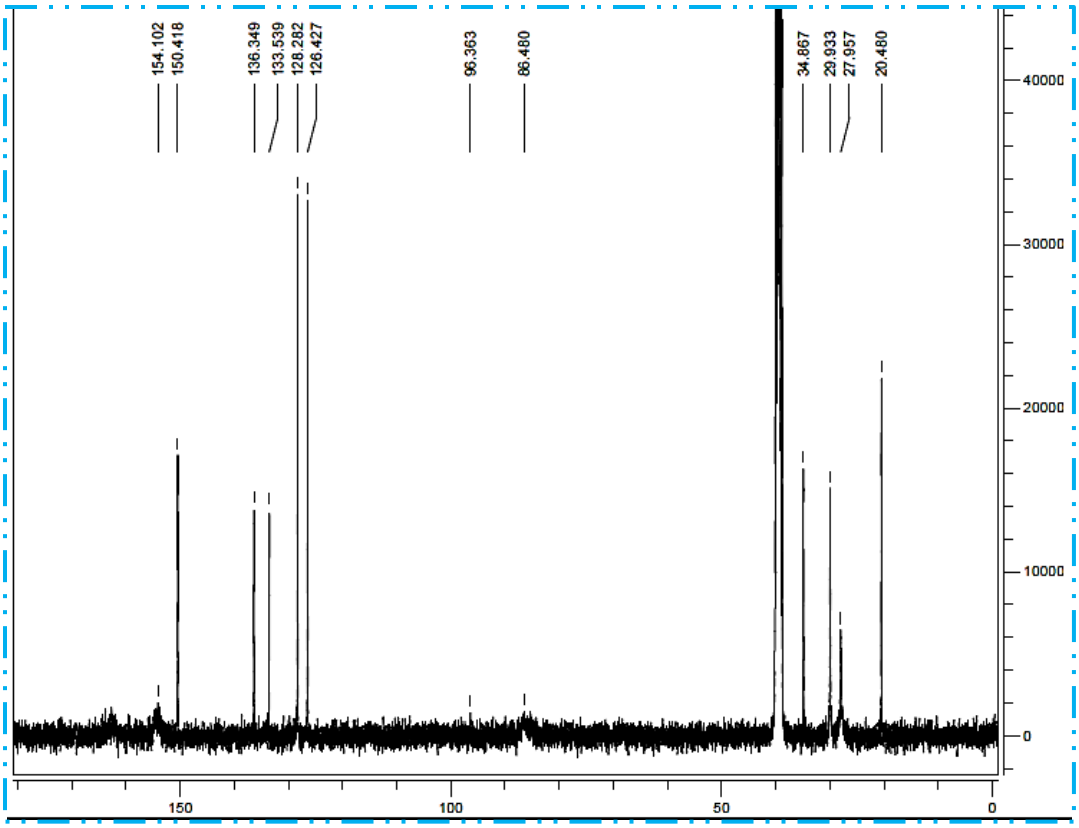


Fig. 34 The ^{13}C NMR spectrum of product (**C_9**)

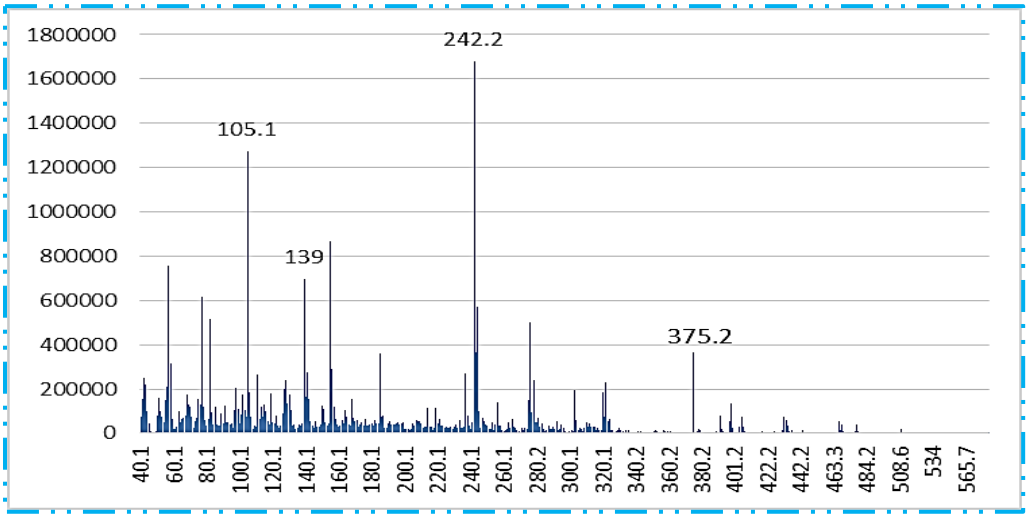


Fig. 35 The MASS spectrum of product (**C_9**)

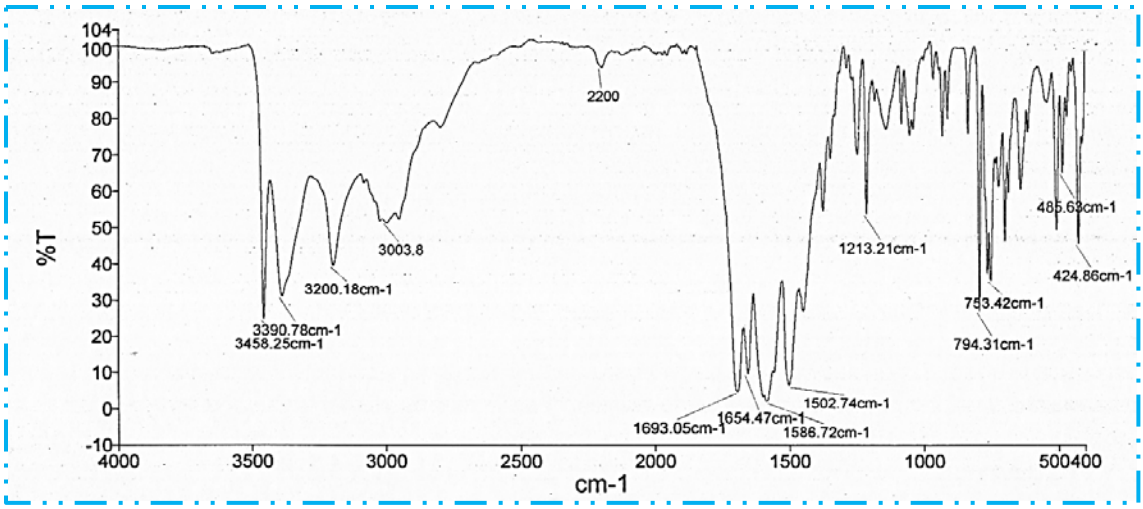


Fig. 36 The IR spectrum of product (**C_9**)

1,3,6-trimethyl-2,4,8-trioxo-5-(4-Me-phenyl)-1,2,3,4,5,8,9,10-octahydropyrimido[4,5 b][1,8]naphthyridine-7-carbonitrile(C_{10})

White solid, mp 263-265 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.33 (s, 3H, CH_3), 2.59 (s, 9H, $3CH_3$), 5.63 (s, 1H, CH), 7.06-7.49 (m, 4H, Ar-H and 2NH) ppm; ^{13}C NMR (100 MHz, DMSO): δ = 27.93, 27.97, 29.94, 35.21, 124.83, 126.56, 127.66, 139.52, 150.41 ppm; IR (KBr) (ν_{max}/cm^{-1}): 3366, 3158, 2957, 2205, 1698, 1677, 1594; MS *m/z* = 389.15 (M^+).

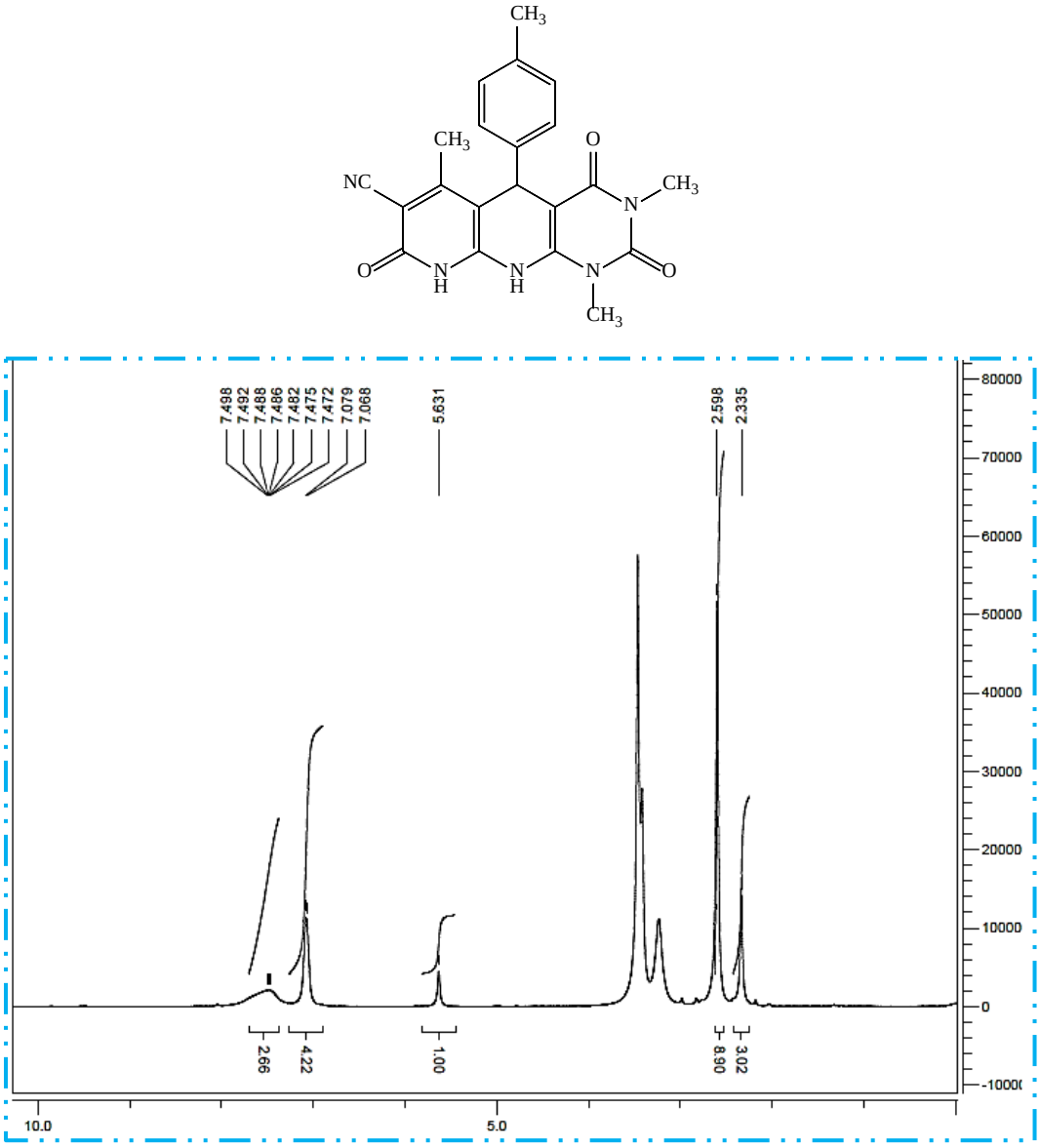


Fig. 37 The ^{1}H NMR spectrum of product (**C_{10}**)

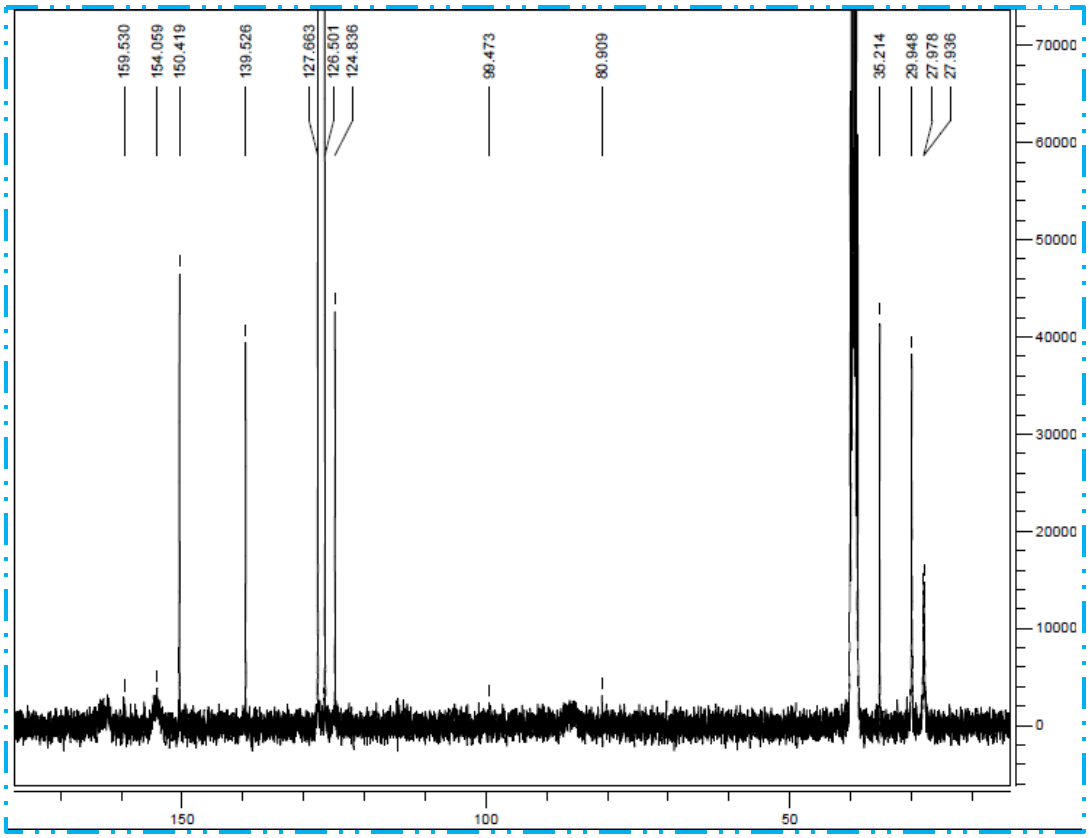


Fig. 38 The ^{13}C NMR spectrum of product (C_{10})

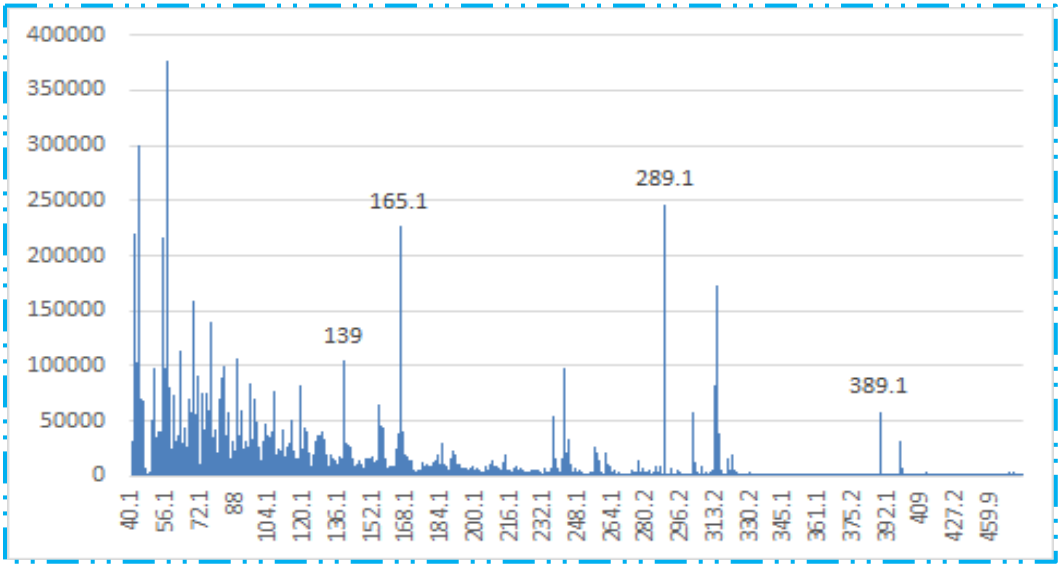


Fig. 39 The MASS spectrum of product (C_{10})

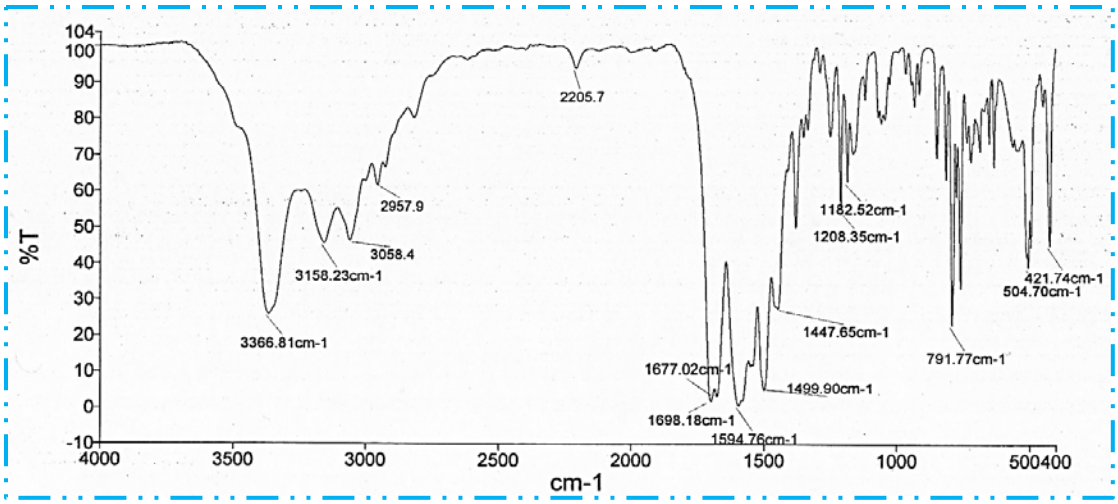


Fig. 40 The IR spectrum of product (C_{10})