Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

TiO_2/porous carbon as a new nanocomposite and catalyst for the preparation of 4H-pyrimido[2,1-*b*]benzimidazoles

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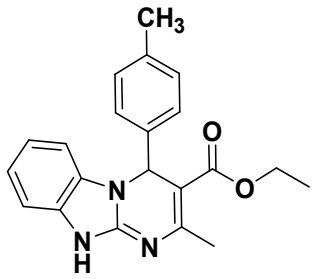
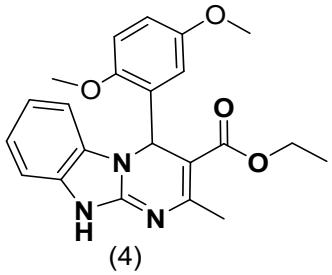
Ethyl 2-methyl-4-(p-tolyl)-4,10-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carboxylate (2)



(2)

Yellow Solid; M.p: 258-260 ºC; Yield: 92%; IR (KBr, cm^{-1}): 3238, 3162,3106,2934, 1698, 1659, 1621, 852, 474; ^{1}H-NMR: (250 MHz, DMSO-d_6): δ (ppm) 1.12 (t, *J*=7.50 Hz ,3H), 2.43 (s, 3H), 3.62(s, 3H), 3.98 (q, *J*=7.50 Hz, 2H), 6.35 (s, 1H), 6.77 (d, *J*=7.50 Hz, 2H), 6.88-7.04 (m, 2H), 7.20-7.33 (m, 4H), 10.77, (s, 1H); ^{13}CNMR: (62.5 MHz, DMSO-d_6): δ (ppm); 14.50, 19.01, 55.37, 55.77, 59.74, 98.61, 110. 31, 114.07, 117.15, 120.50, 122.10, 128.72, 131.98, 134.60, 142.76, 146.06, 146.55, 159.07, 165.67

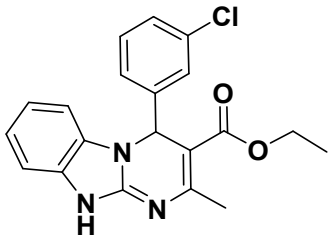
Ethyl 4-(2,5-dimethoxyphenyl)-2-methyl-4,10-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carboxylate (4)



(4)

Yellow Solid; M.p: 255-258 ºC; Yield: 90 %; IR (KBr, cm^{-1}): 3231, 3100,3170,2974,2839, 1658, 1617, 1575, 828,701; ^{1}H-NMR: (250 MHz, DMSO-d_6): δ (ppm) 1.07 (t, *J*=7.50 Hz ,3H), 2.43(s, 3H), 3.61 (s, 3H), 3.70 (s, 3H), 3.94 (q, *J*=7.50 Hz, 2H), 6.58 (s, 1H), 6.72 (d, *J* = 7.50 Hz, 1H), 6.83 (d, *J* = 7.50 Hz, 2H), 6.91-7.02 (m, 2H), 7.29 (d, *J*=7.50, 1H), 10.74 (s, 1H); ^{13}CNMR: (62.5 MHz, DMSO-d_6): δ (ppm); 14.39, 18.99, 51.76, 55.65, 56.44, 59.55, 96.84, 109.76, 112.88, 113.51, 115.55, 117.04, 120.46, 121.99, 130.90, 132.26, 142.61, 146.30, 147.45, 151.14, 153.34, 165.68

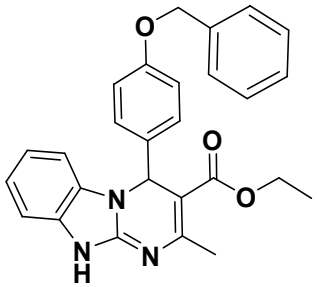
Ethyl 4-(3-chlorophenyl)-2-methyl-4,10-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carboxylate (10)



(10)

Yellow Solid; M.p: 245-247 ºC; Yield: 97 %; IR (KBr, cm^{-1}): **:**3275, 3258,32,19,3090,2955, 1661, 1642, 1606, 844, 529; ^{1}H-NMR: (250 MHz, DMSO-d_6): δ (ppm) δ (ppm) 1.12 (t, *J*=7.50 Hz ,3H), 2.44 (s, 3H),4.00 (t, *J*=7.5 Hz, 2H), 6.43 (s, 1H), 9.91-7.06 (m, 2H), 7.24-7.35 (m, 5H), 7.44(s, 1H), 10.89 (s, 1H); ^{13}CNMR: (62.5 MHz, DMSO-d_6): δ (ppm); 14.42,19.10, 55.77, 59.88, 97.74, 110.29, 117.31, 120.79, 122.38, 126.09, 127.54, 128.21, 130.86, 131.83, 133.28, 142.65, 144.83, 145.83, 147.49, 165.45

Ethyl 4-(4-(benzyloxy)phenyl)-2-methyl-4,10-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carboxylate



(12)

Yellow Solid; M.p: 261-263 ºC; Yield: 95%; IR (KBr, cm^{-1}): 3238, 3106,3034, ,2980, 1697, 1617, 1510, 830, 696; ^{1}H-NMR: (250 MHz, DMSO-d_6): δ (ppm) 1.11 (t, *J*=7.50 Hz ,3H), 2.43 (s, 3H), 3.98 (q, *J*=7.50 Hz, 2H), 4.95 (s, 2H), 6.35 (s, 1H), 6.84-7.04 (m, 5H), 7.21-7.34 (m, 8H), 10.79 (s, NH); ^{13}CNMR: (62.5 MHz, DMSO-d_6): δ (ppm); 14.51, 19.01, 55.74, 59.78, 69.63, 98.59, 110.34, 114.89, 117.17, 120.54, 122.14, 128.16, 128.28, 128.74, 128.83, 131.97, 134.84, 137.35, 142.74, 146.05, 146.62, 158.26, 165.69

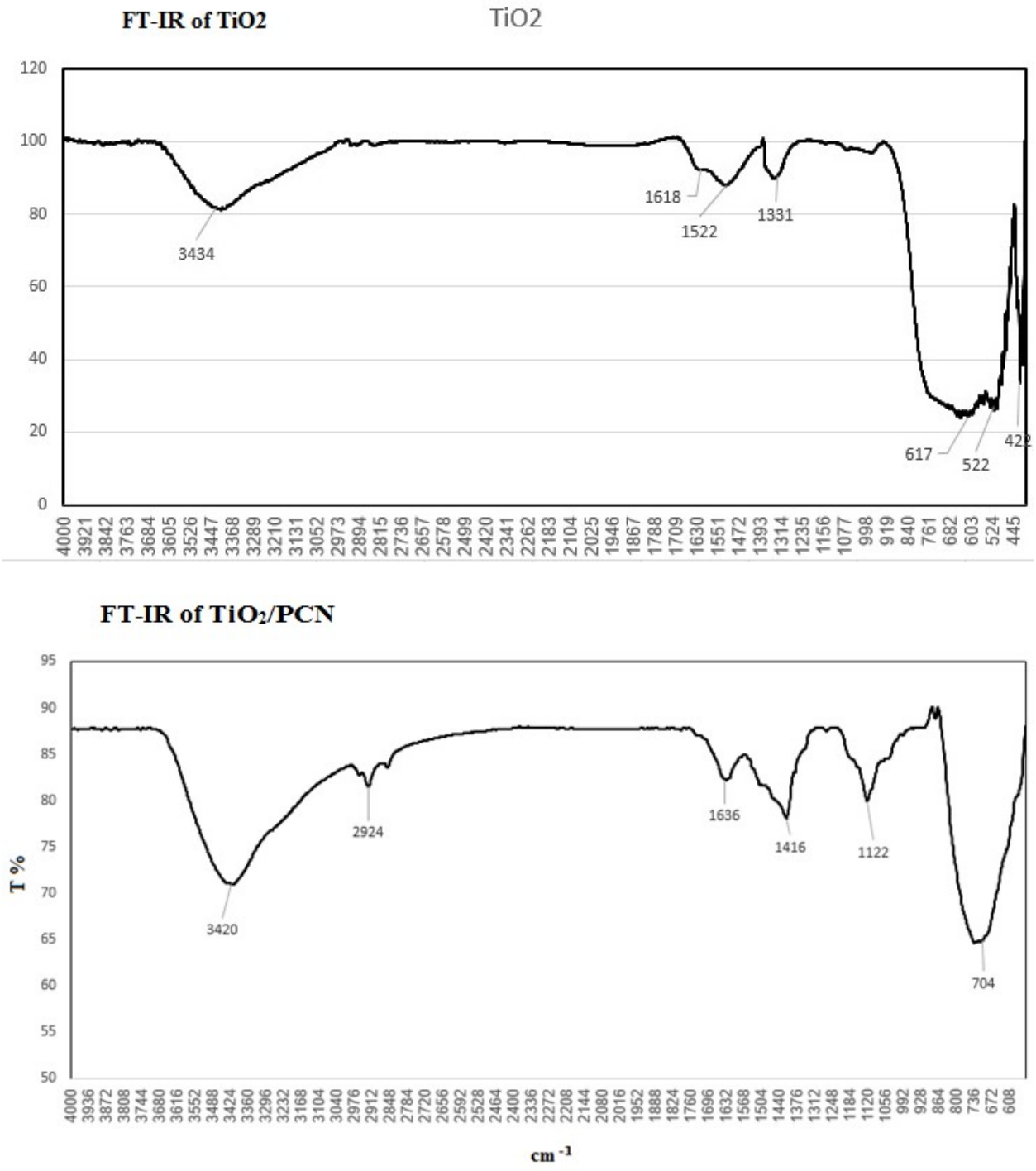


Figure S1. FT-IR spectrum of TiO_2/PCN in comparison with TiO_2.

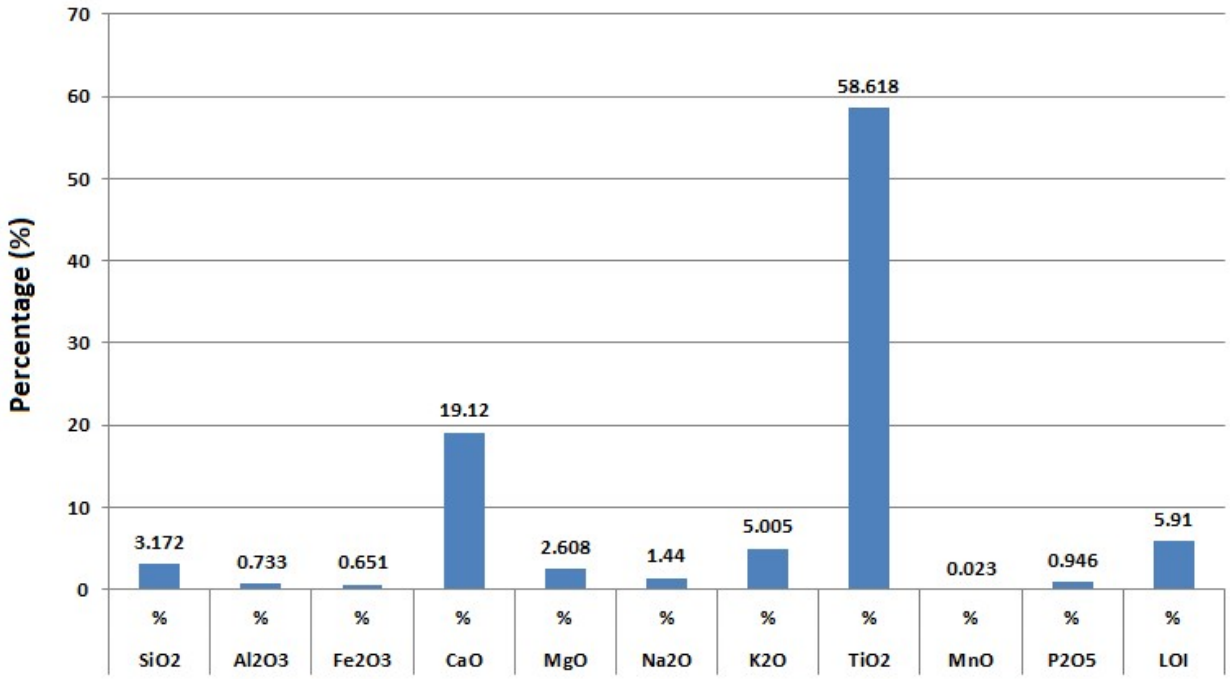


Figure S2. Types of elemental oxides in the nanocomposite structure determined by X-ray fluorescence (XRF) analysis.

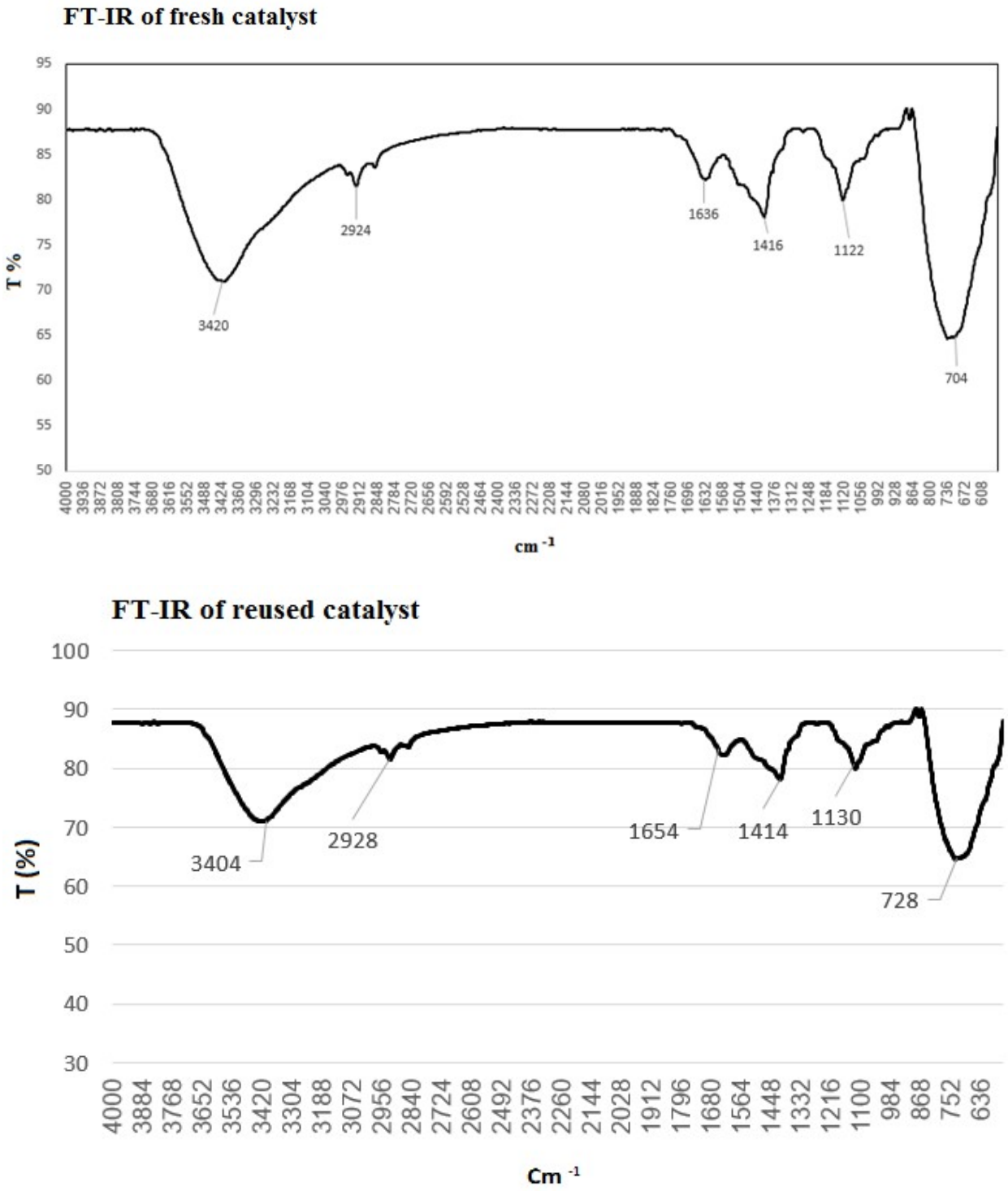
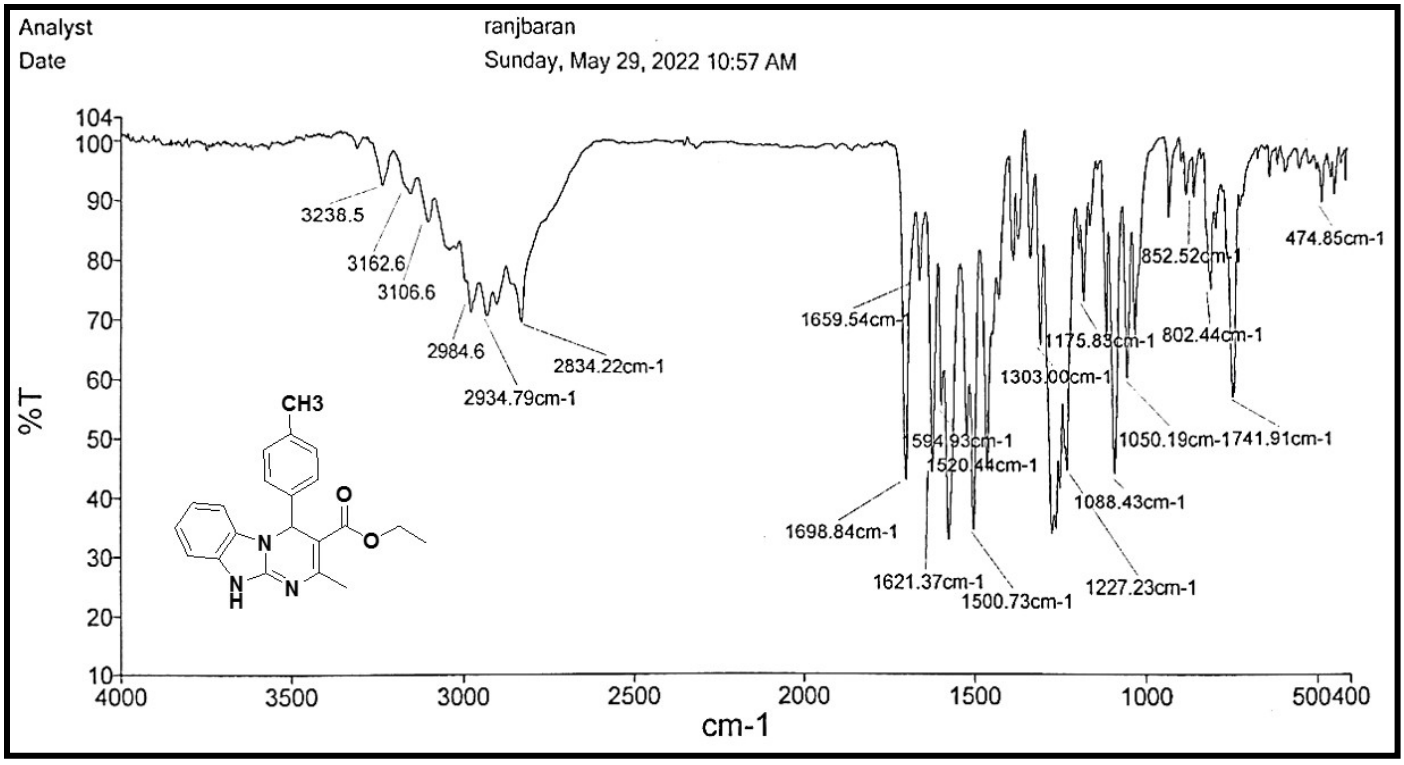


Figure S3. FT-IR spectrum of fresh catalyst in comparison with TiO_2.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H
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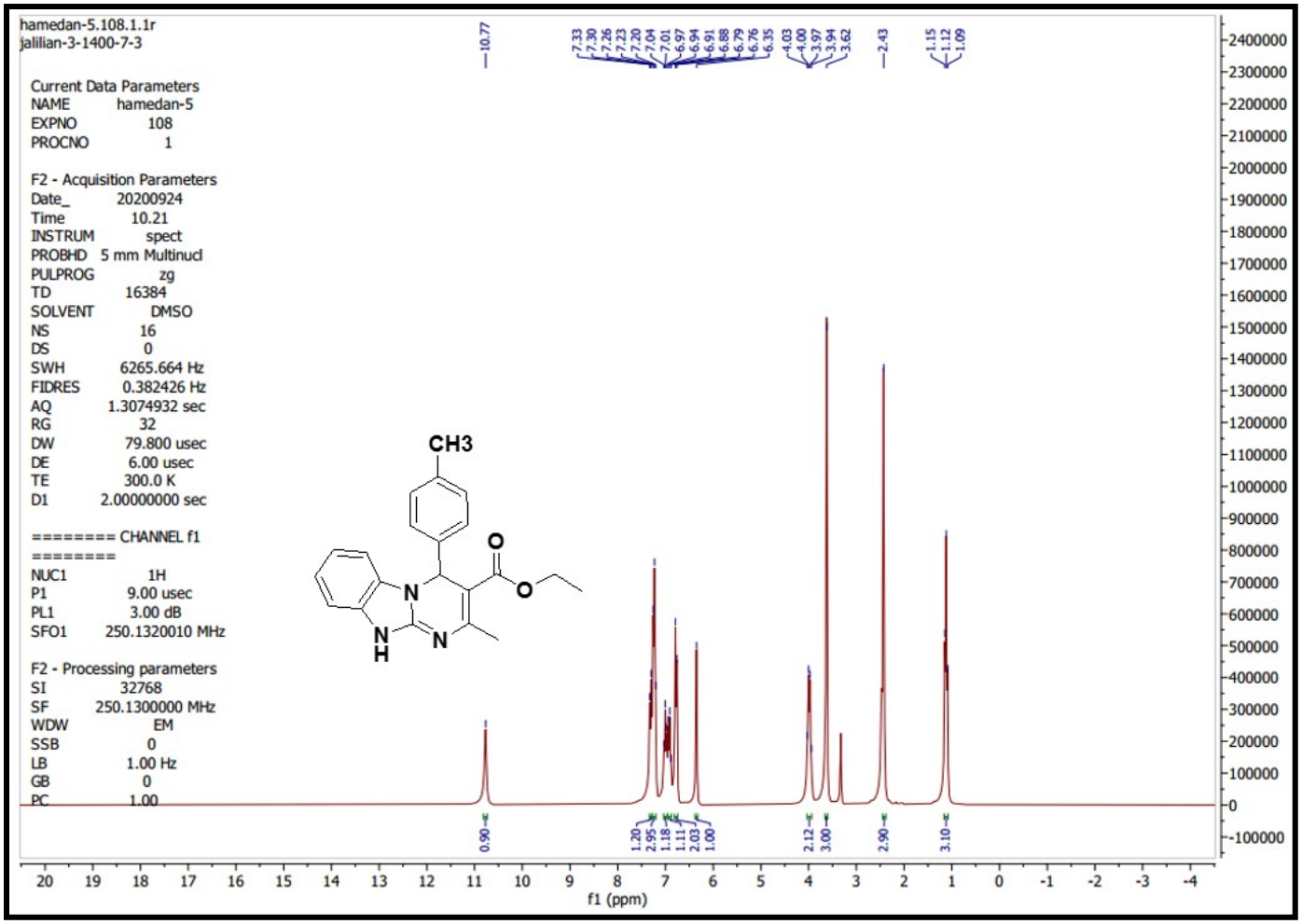
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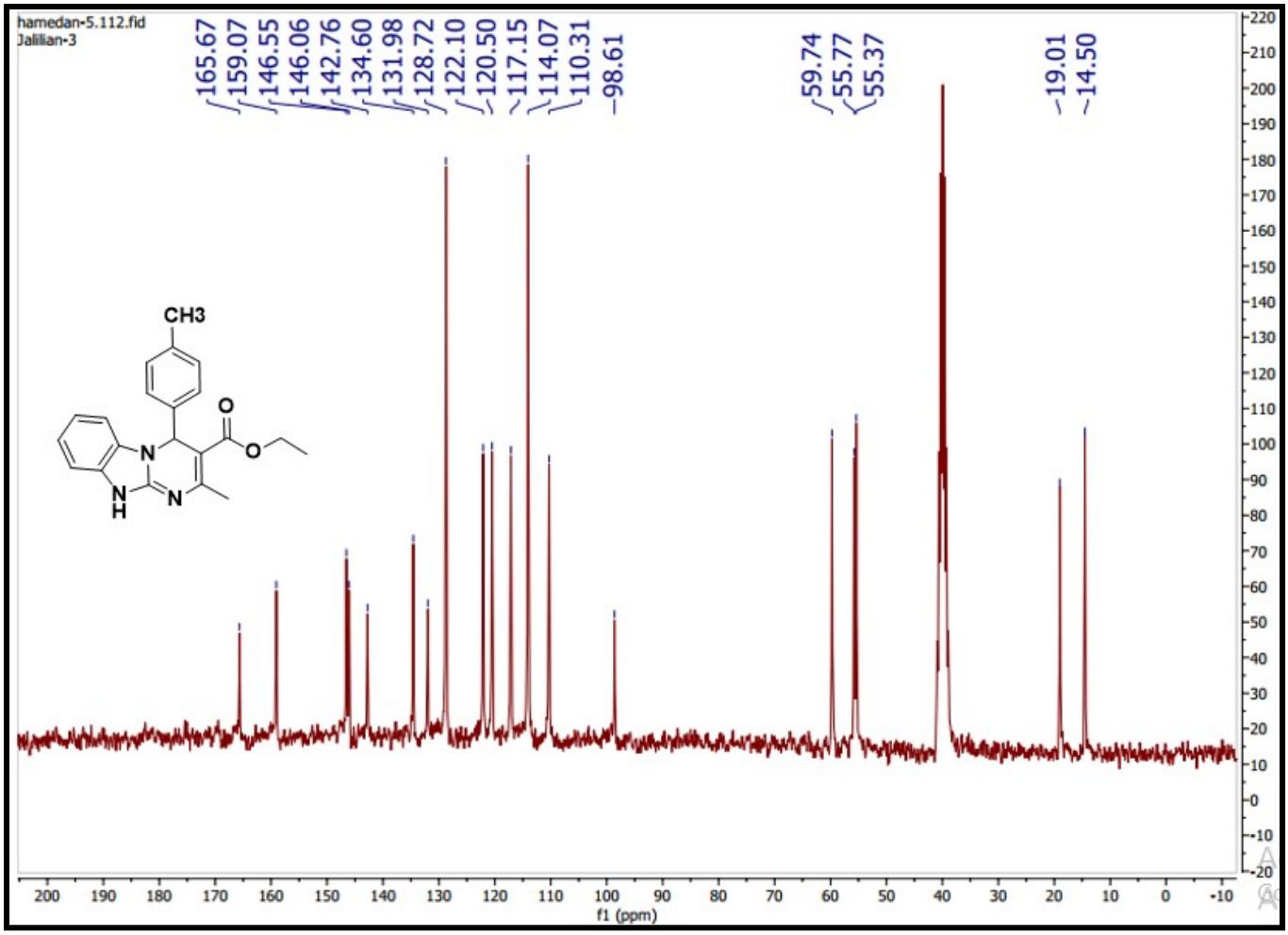
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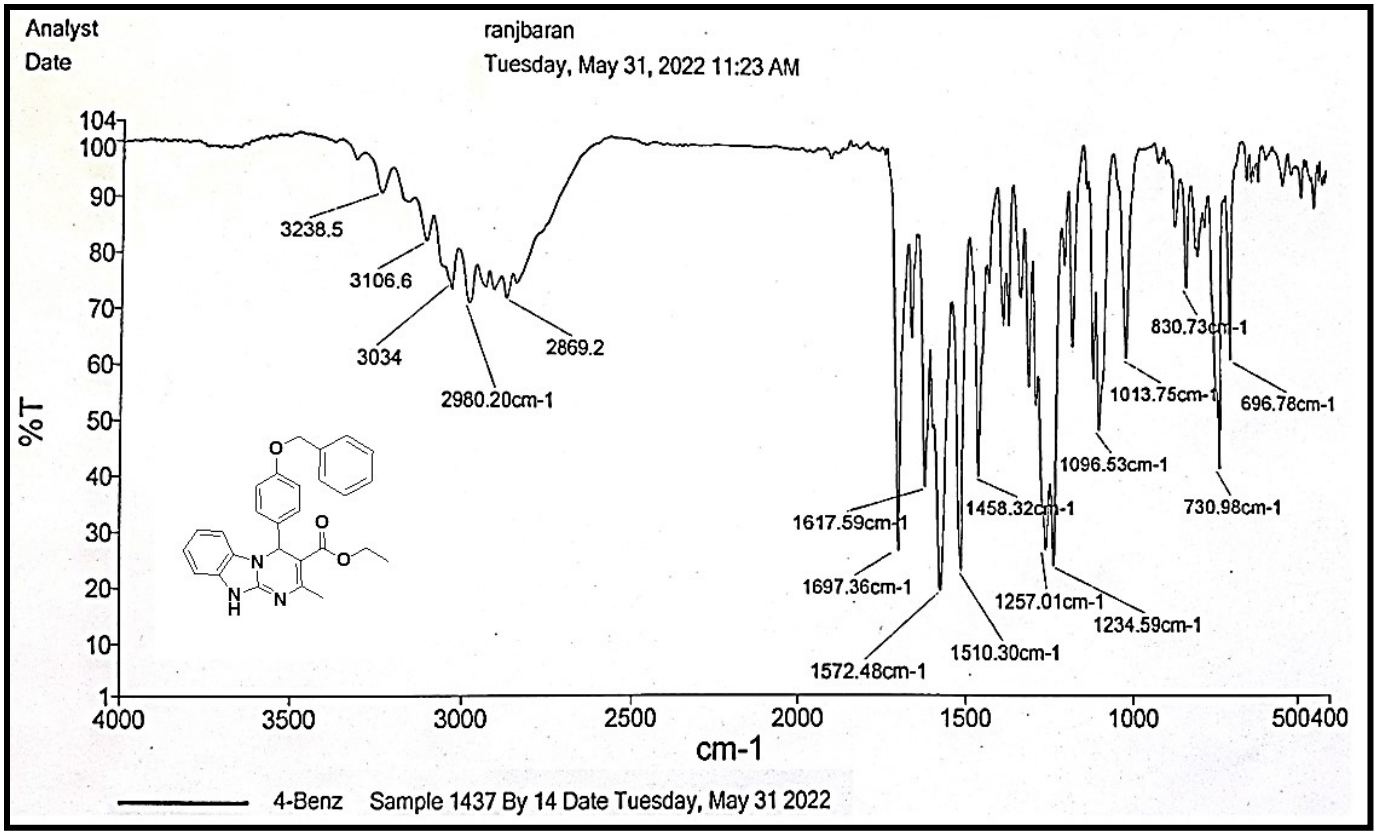
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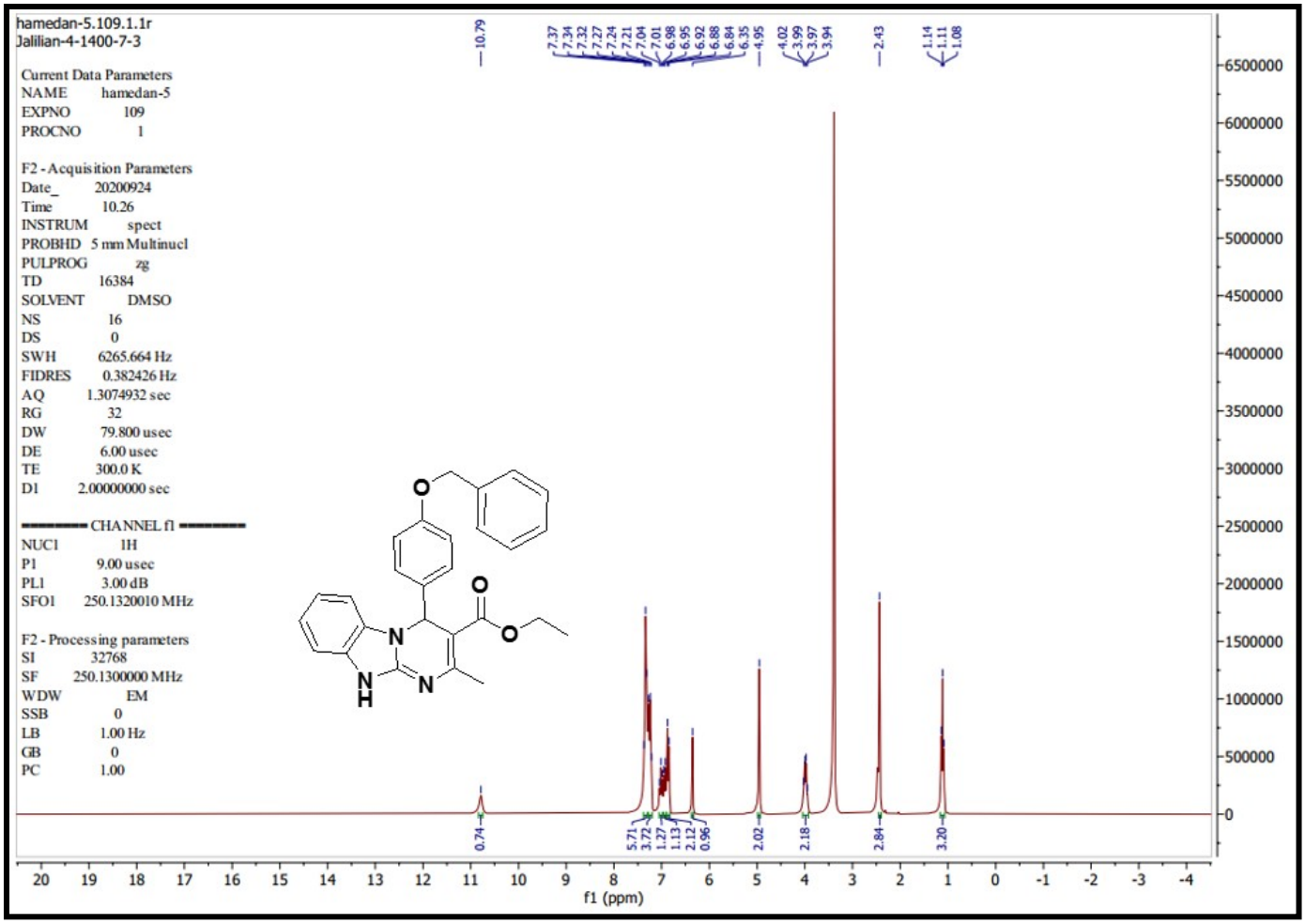
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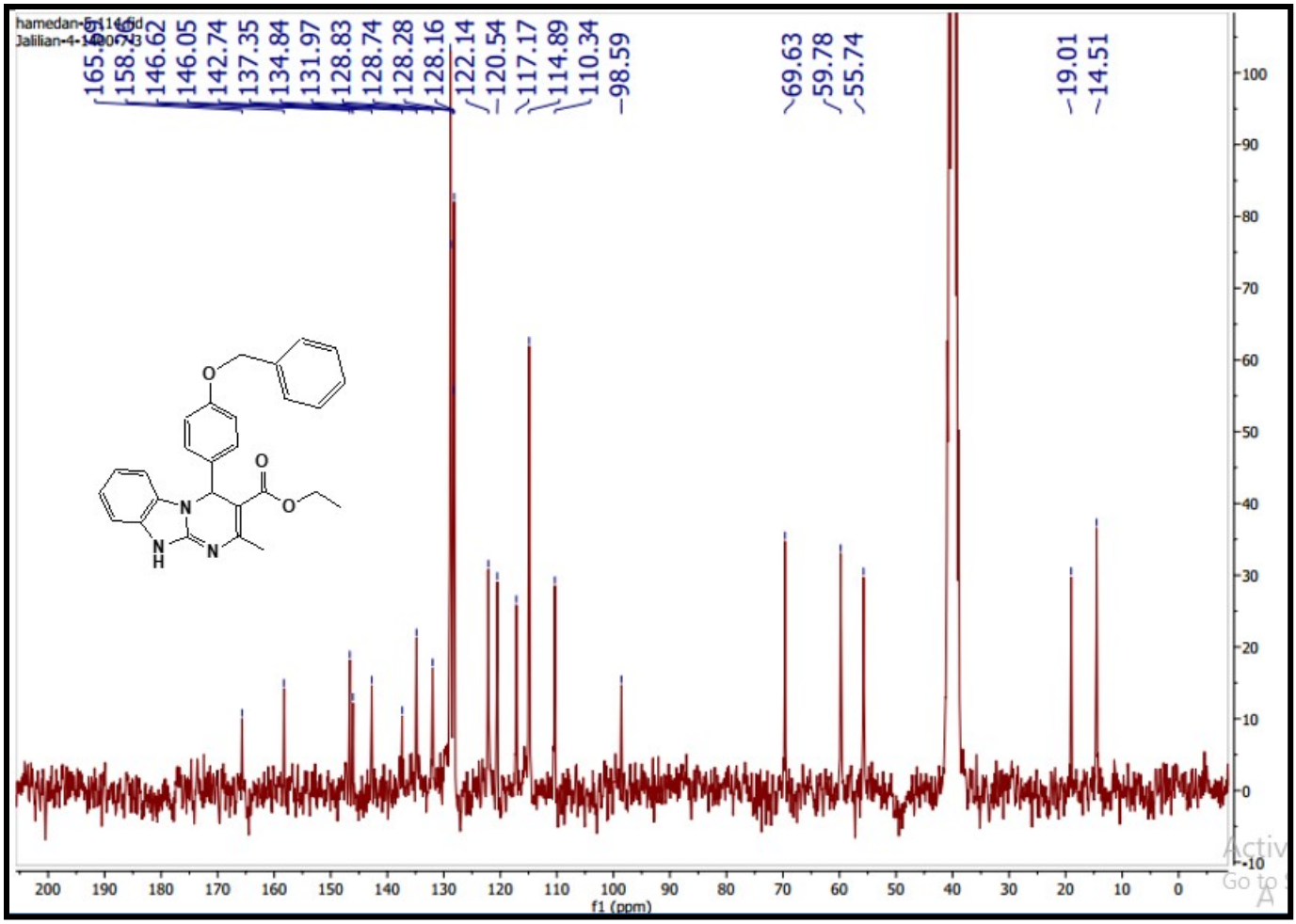
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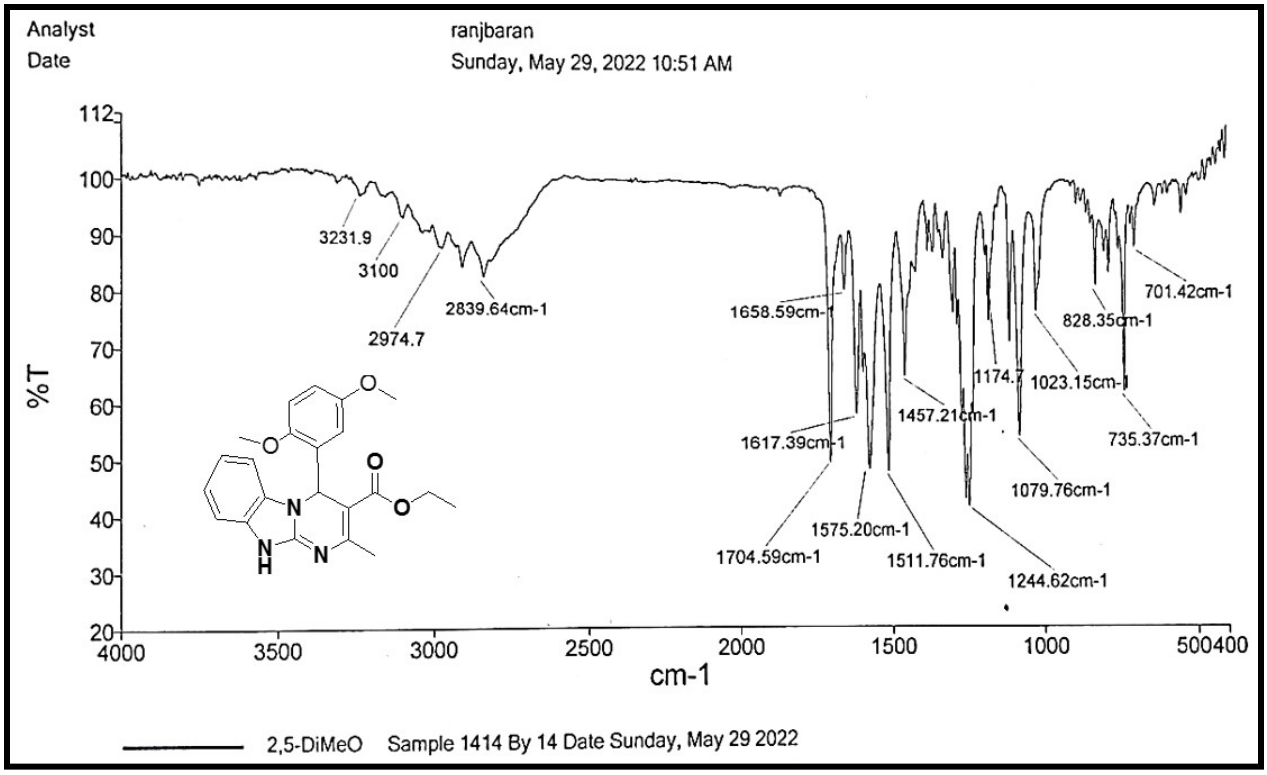
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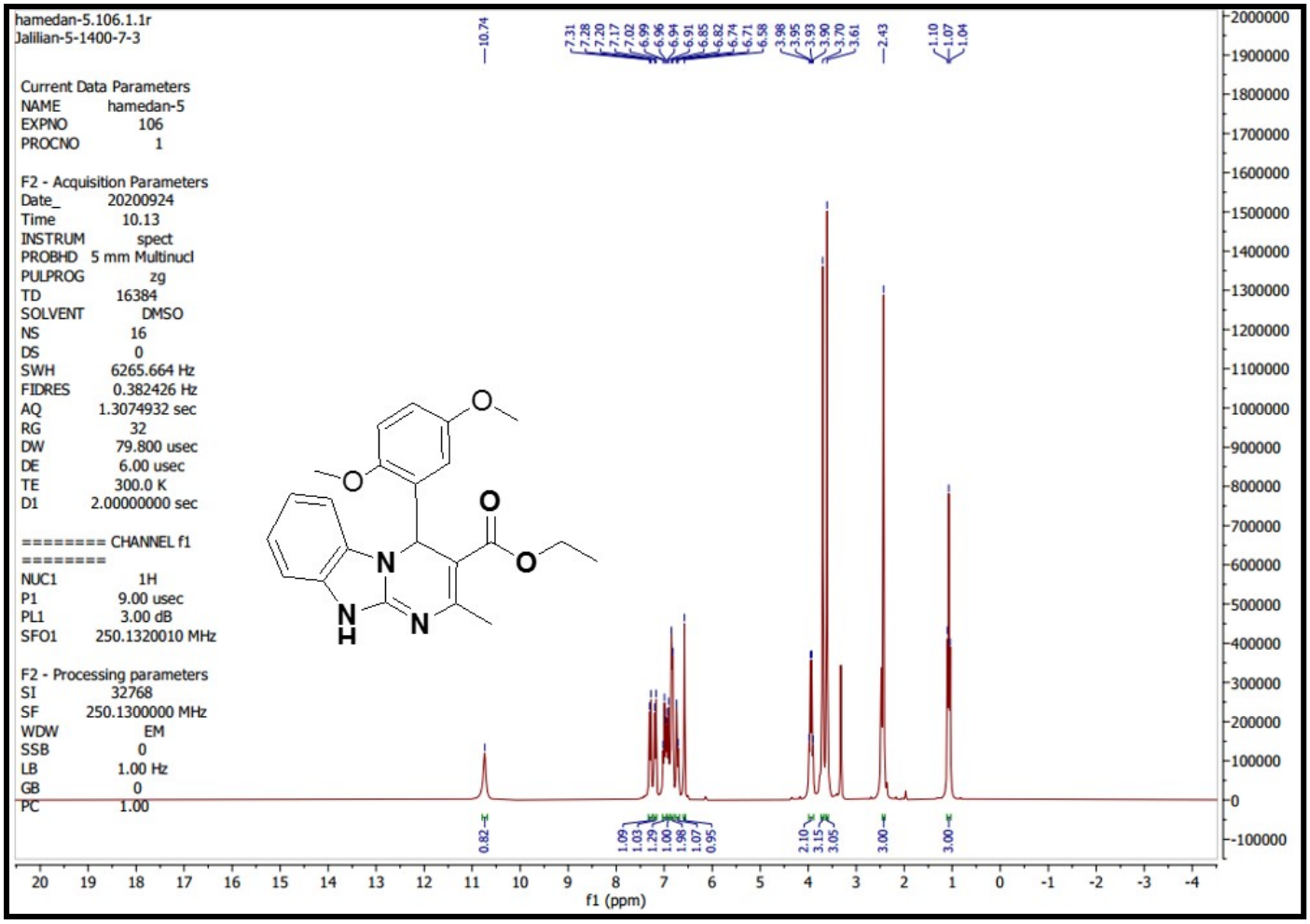
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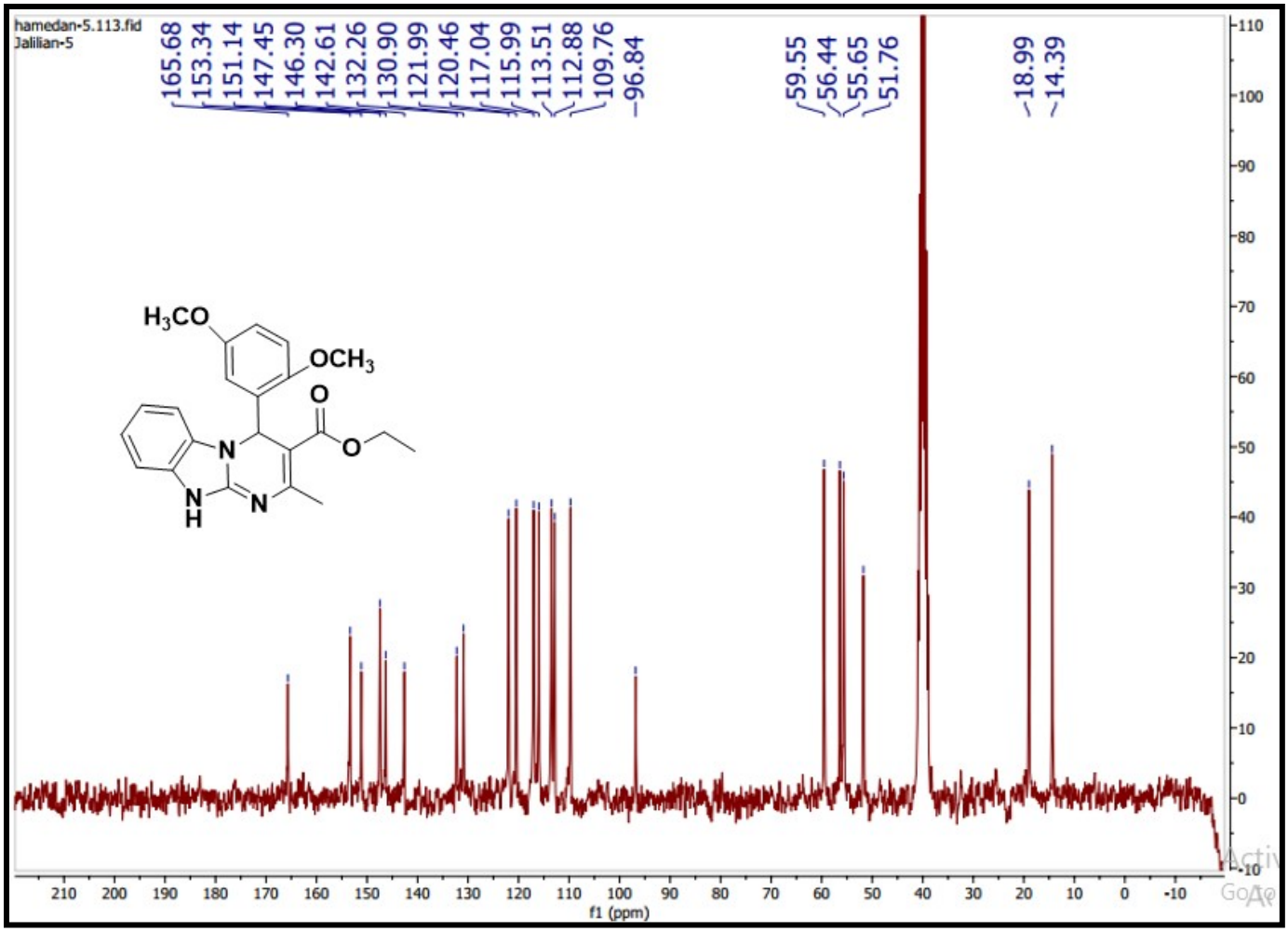
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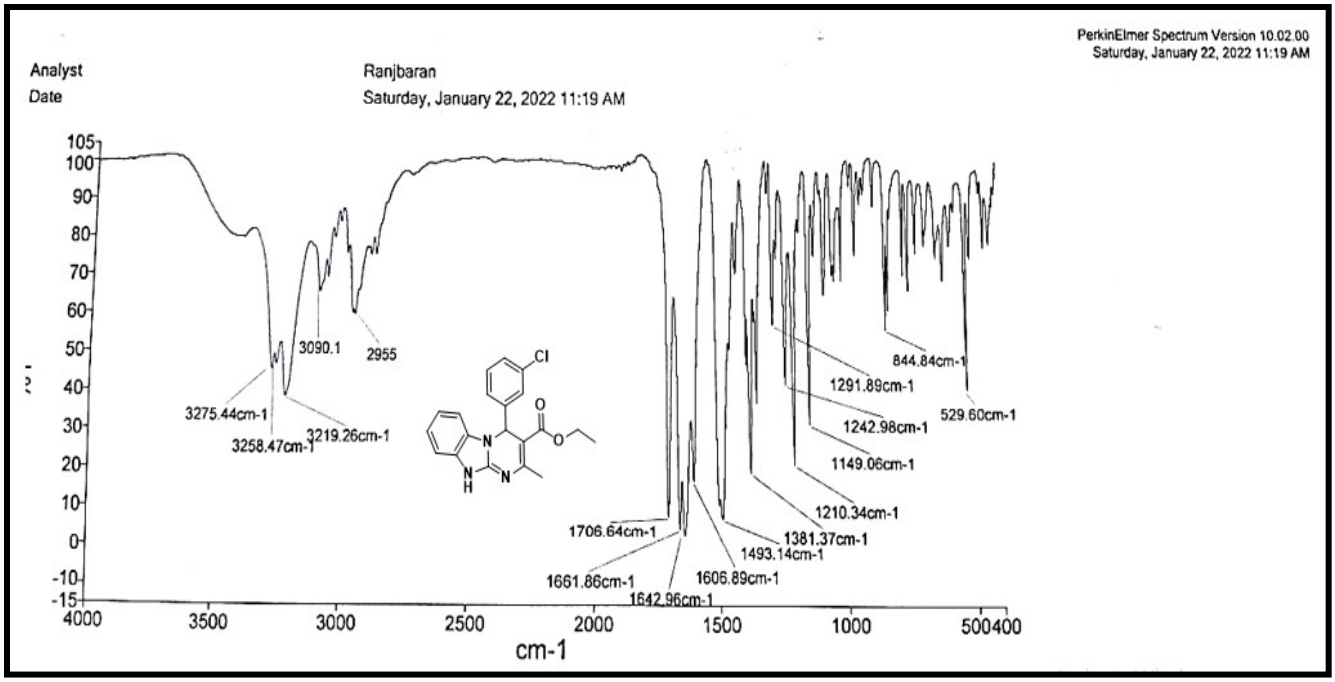
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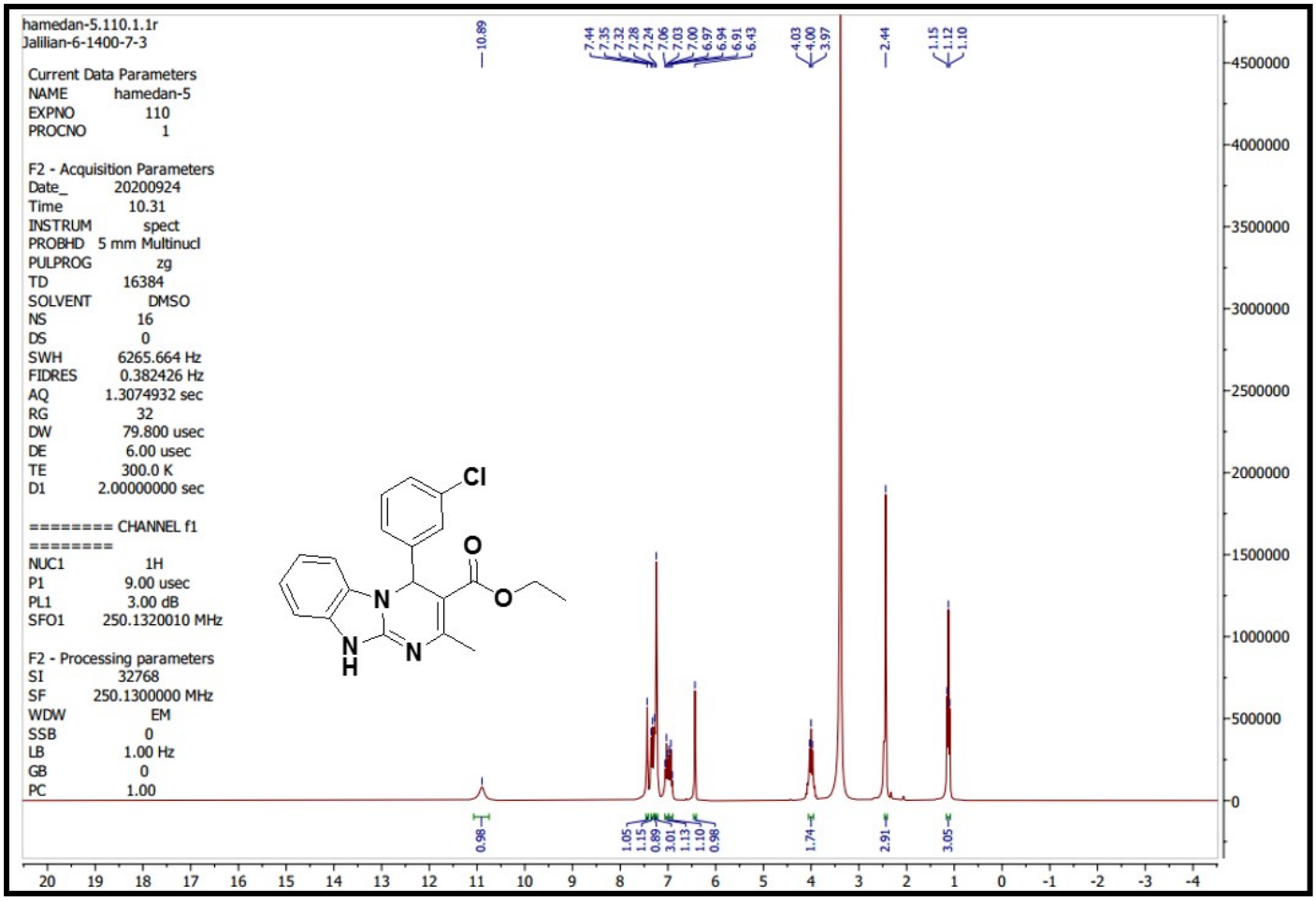
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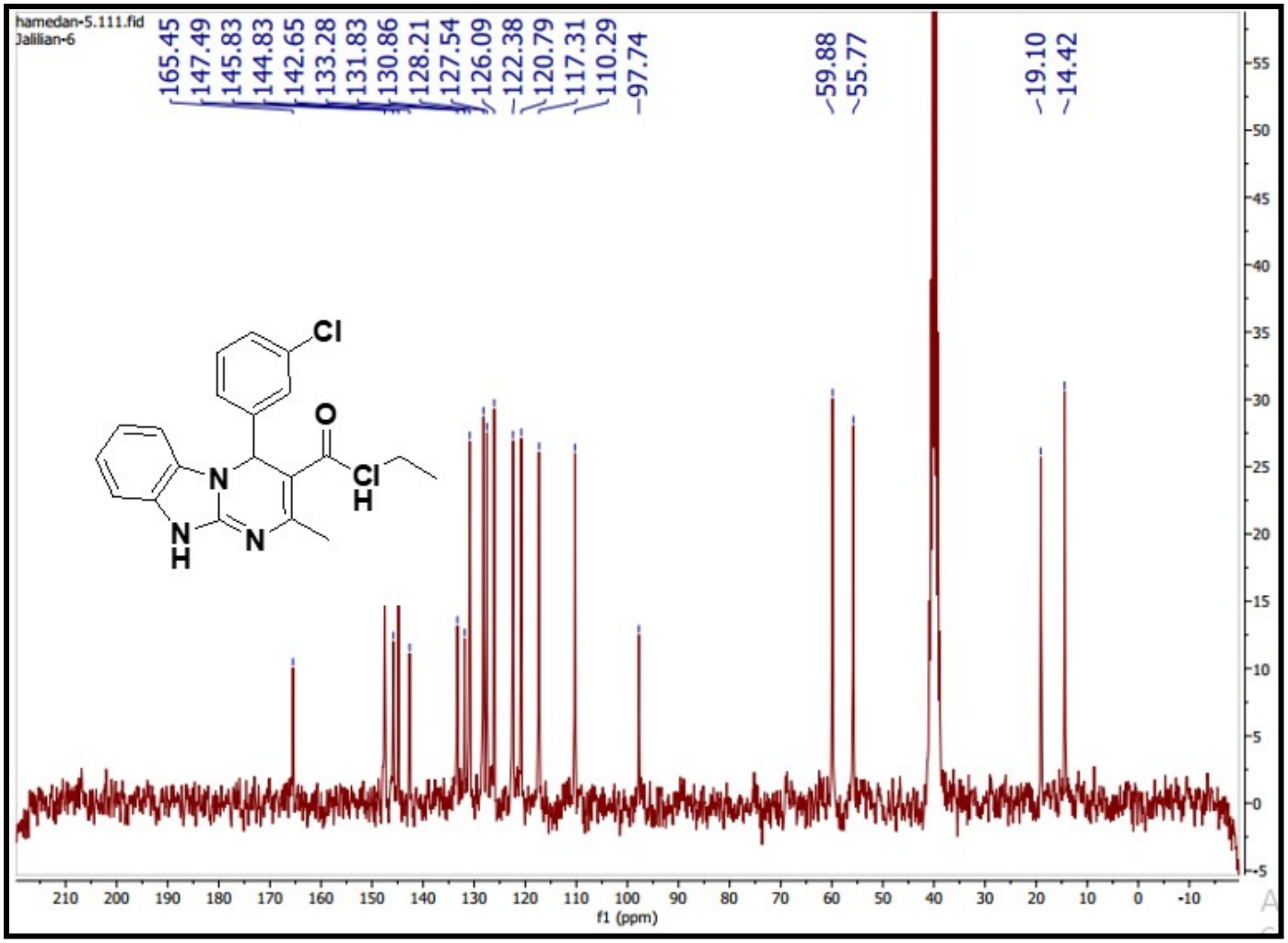
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f1 (ppm)