

Supporting Information

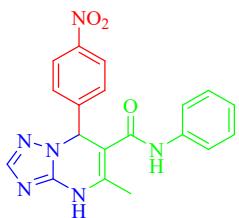
The preparation of [1,2,4]Triazolo[1,5-*a*]pyrimidines catalyzed by Schiff base zinc (II) complex supported on magnetite nanoparticles under mild condition

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Iran .

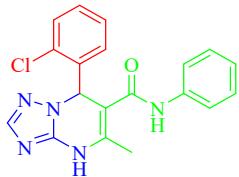
*E-mail: moosavizare@yahoo.com

Spectral data of compounds:



5-methyl-7-(4-nitrophenyl)-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

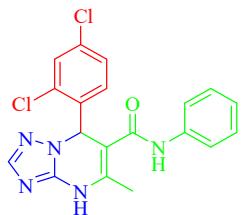
White Solid; M.p: 259-261 °C; IR (KBr, cm⁻¹): 3255, 3101, 2915, 1667, 1621, 1596, 1247, 825, 749, 545; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.17 (s, 3H, CH₃), 6.66 (s, 1H, H-benzylic), 6.99 (s, 1H), 7.22 (s, 2H, ArH), 7.47 (d, *J* = 6.25 Hz, 4H, ArH), 7.67 (s, 1H, ArH), 8.16 (d, *J* = 6.75 Hz, 2H, ArH), 9.78 (s, 1H, NH), 10.39 (s, 1H, NH); ¹³C-NMR (DMSO-*d*₆, 62.5 MHz): δ 25.4, 60.0, 103.0, 120.1, 123.8, 124.2, 129.0, 130.0, 137.8, 138.4, 139.2, 147.6, 148.0, 148.3, 149.2, 150.7, 165.0.



7-(2-chlorophenyl)-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

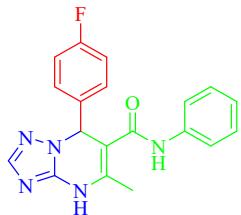
White Solid; M.p: 252-254 °C; IR (KBr, cm⁻¹): 3414, 3299, 3098, 3037, 2866, 1670, 1636, 1595, 1499, 1328, 1262, 975, 872, 750, 546; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.14 (s, 3H, CH₃), 6.92 (s, 1H), 6.97 (s, 1H), 7.27 (s, 5H, ArH), 7.44 (s, 3H, ArH), 7.60 (s, 1H, ArH), 9.81 (s, 1H, NH),

10.28 (s, 1H, NH); ^{13}C -NMR (DMSO- d_6 , 62.5 MHz): δ 17.5, 58.2, 103.2, 119.9, 123.7, 128.0, 129.0, 130.3, 130.5, 132.5, 137.2, 138.1, 139.3, 148.3, 150.4, 165.0.



7-(2,4-dichlorophenyl)-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

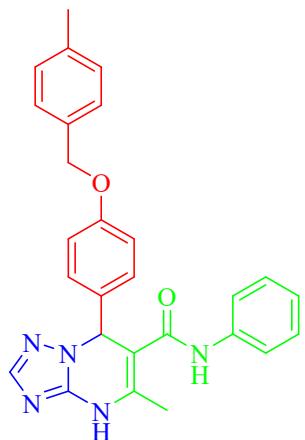
White Solid; M.p: 248-250 °C; IR (KBr, cm⁻¹): 3414, 3304, 3095, 3027, 1739, 1670, 1533, 1491, 1332, 1260, 857, 759, 547; ^1H NMR (250 MHz, DMSO- d_6): 2.13 (s, 3H, CH3), 6.88 (s, 1H, H-benzylic), 6.98 (s, 1H, ArH), 7.21 (s, 2H, ArH), 7.30 (d, $J = 7.30$ Hz, 1H, ArH), 7.36 (s, 1H, ArH), 7.45 (s, 3H, ArH), 7.52 (s, 1H, ArH), 7.61 (s, 1H, ArH), 9.82 (s, 1H, NH), 10.33 (s, 1H, NH); ^{13}C NMR (DMSO- d_6 , 62.5 MHz): δ 17.6, 57.8, 59.1, 102.7, 119.9, 123.8, 128.3, 129.0, 129.5, 131.9, 133.6, 134.0, 137.5, 139.3, 148.3, 150.6, 164.9.



7-(4-fluorophenyl)-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

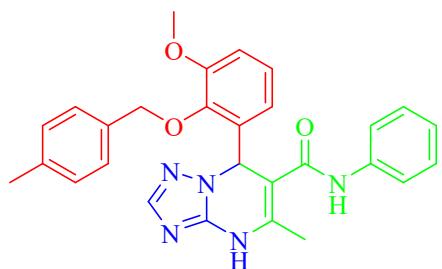
White Solid; M.p: 276-278 °C; IR (KBr, cm⁻¹): 3270, 3102, 2977, 1663, 1627, 1595, 1509, 1325, 1231, 977, 839, 747, 516; ^1H NMR (250 MHz, DMSO- d_6): δ 2.16 (s, 3H, CH3), 6.53 (s, 1H), 6.95-7.01 (m, 1H), 7.10 (d, $J = 8.00$ Hz, 2H, ArH), 7.15 (s, 1H), 7.24 (d, $J = 6.75$ Hz, 3H, ArH), 7.48 (d, $J = 7.5$ Hz, 2H, ArH), 7.63 (s, 1H, ArH), 9.73 (s, 1H, NH), 10.24 (s, 1H, NH); ^{13}C -NMR

(DMSO-*d*₆, 62.5 MHz): δ 17.7, 60.0, 103.8, 115.5, 115.9, 120.0, 123.7, 129.0, 129.7, 137.1, 137.4, 139.3, 148.2, 150.4, 165.2.



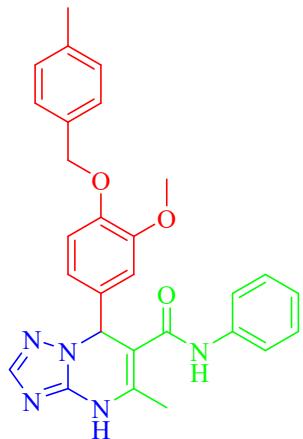
5-methyl-7-(4-((4-methylbenzyl)oxy)phenyl)-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

White Solid; M.p: 232-234°C; IR (KBr, cm⁻¹): 3445, 3271, 3101, 3027, 2920, 2869, 1667, 1626, 1596, 1510, 1441, 1330, 1243, 1010, 750, 728, 691 ; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.16 (s, 3H, CH₃), 2.26 (s, 3H, CH₃), 4.95 (s, 2H), 6.47 (s, 1H), 6.89 (d, *J* = 7.00 Hz, 2H, ArH), 7.00 (d, *J* = 6.50 Hz, 2H, ArH), 7.14 (d, *J* = 5.75 Hz, 2H, ArH), 7.19 (s, 1H, ArH), 7.24 (s, 3H, ArH), 7.49 (d, *J* = 6.75 Hz, 3H, ArH), 7.60 (s, 1H, ArH), 9.70 (s, 1H, NH), 10.15 (s, 1H, NH); ¹³C-NMR (DMSO-*d*₆, 62.5 MHz): δ 17.7, 21.1, 60.1, 69.5, 104.1, 115.0, 120.0, 123.7, 128.2, 128.8, 129.0, 129.3, 133.4, 134.3, 136.8, 137.5, 139.4, 150.2, 158.6, 165.4; MS: m/z = 451.



7-(3-methoxy-2-((4-methylbenzyl)oxy)phenyl)-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

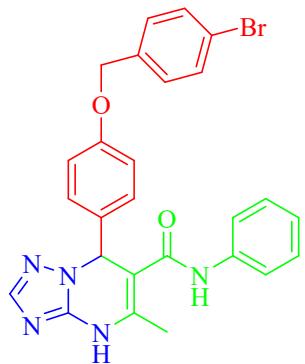
White Solid; M.p: 241-243°C;IR (KBr, cm⁻¹): 3407, 3274, 3134, 3055, 2890, 1595, 1670, 1589, 1529, 1481, 1314, 1224, 1070, 766 ; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.12 (s, 3H, CH₃), 2.30 (s, 3H, CH₃), 3.76 (s, 3H, CH₃), 4.73 (d, *J* = 10.25 Hz, 1H, ArH), 5.01 (d, *J* = 10.25 Hz, 1H), 6.78-6.84 (m, 2H, ArH), 6.95 (s, 2H, ArH), 7.00 (s, 1H, ArH), 7.18 (s, 3H, ArH), 7.38 (d, *J* = 7.00 Hz, 2H, ArH), 7.46 (d, *J* = 7.50 Hz, 2H, ArH), 7.56 (s, 1H, ArH), 9.72 (s, 1H, NH), 10.09 (s, 1H, NH); ¹³C-NMR (DMSO-*d*₆, 62.5 MHz): δ 17.6, 21.2, 56.1, 74.4, 104.2, 112.9, 119.8, 120.6, 123.6, 124.7, 128.5, 128.9, 129.1, 134.7, 135.3, 136.5, 137.3, 139.4, 150.1, 152.7. MS: m/z = 481.5.



7-(3-methoxy-4-((4-methylbenzyl)oxy)phenyl)-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

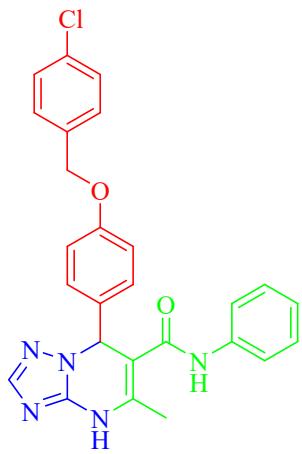
White Solid; M. p: 246-248°C;IR (KBr, cm⁻¹): 3277, 3098, 3027, 2918, 1673, 1628, 1596, 1515, 1441, 1262, 1003, 754 ; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.15 (s, 3H, CH₃), 2.26 (s, 3H, CH₃), 3.62 (s, 3H, CH₃), 4.93 (s, 2H), 6.45 (s, 1H), 6.68 (d, *J* = 8.00 Hz, 1H, ArH), 6.81 (s, 1H, ArH), 6.90-7.02 (m, 2H, ArH), 7.13 (d, *J* = 7.50 Hz, 2H, ArH), 7.20 (s, 1H, ArH), 7.25 (d, *J* = 7.50 Hz,

2H, ArH), 7.34 (s, 1H, ArH), 7.50 (d, $J = 7.75$ Hz, 2H, ArH), 7.62 (s, 1H, ArH), 9.70 (s, 1H, NH), 10.15 (s, 1H, NH); ^{13}C -NMR (DMSO- d_6 , 62.5 MHz): δ 17.7, 21.2, 56.0, 60.3, 70.2, 104.0, 111.6, 113.7, 120.0, 123.7, 128.3, 129.0, 129.3, 133.8, 134.4, 136.8, 137.5, 139.4, 148.1, 149.2, 150.2, 165.4; MS: m/z = 481.6.



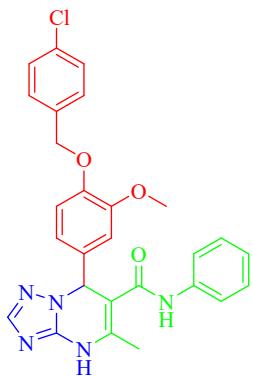
7-((4-bromobenzyl)oxy)phenyl-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

White Solid; M.p: 237-239°C; IR (KBr, cm⁻¹): 3406, 3262, 3103, 2925, 1754, 1665, 1626, 1595, 1509, 1440, 1321, 1242, 1011, 752 ; ^1H NMR (250 MHz, DMSO- d_6): δ 2.15 (s, 3H, CH₃), 4.99 (s, 2H), 6.47 (s, 1H), 6.91 (s, 2H, ArH), 6.98 (s, 2H, ArH), 7.14 (d, $J = 7.00$ Hz, 2H, ArH), 7.22 (s, 2H, ArH), 7.35 (s, 3H, ArH), 7.51-7.59 (m, 4H, ArH), 9.69 (s, 1H, NH), 10.15 (s, 1H, NH); ^{13}C -NMR (DMSO- d_6 , 62.5 MHz): δ 17.7, 60.1, 68.8, 104.1, 115.0, 120.0, 121.3, 123.7, 129.0, 130.2, 131.7, 133.6, 136.8, 139.4, 158.3, 165.4.



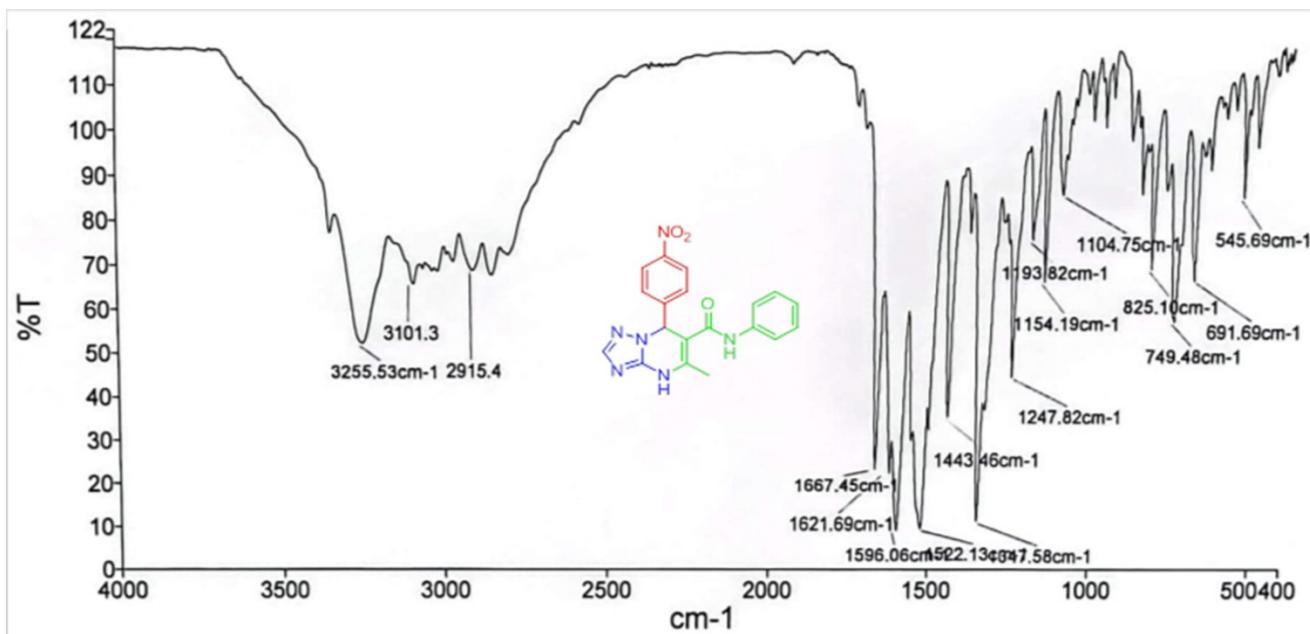
7-((4-chlorobenzyl)oxy)phenyl-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

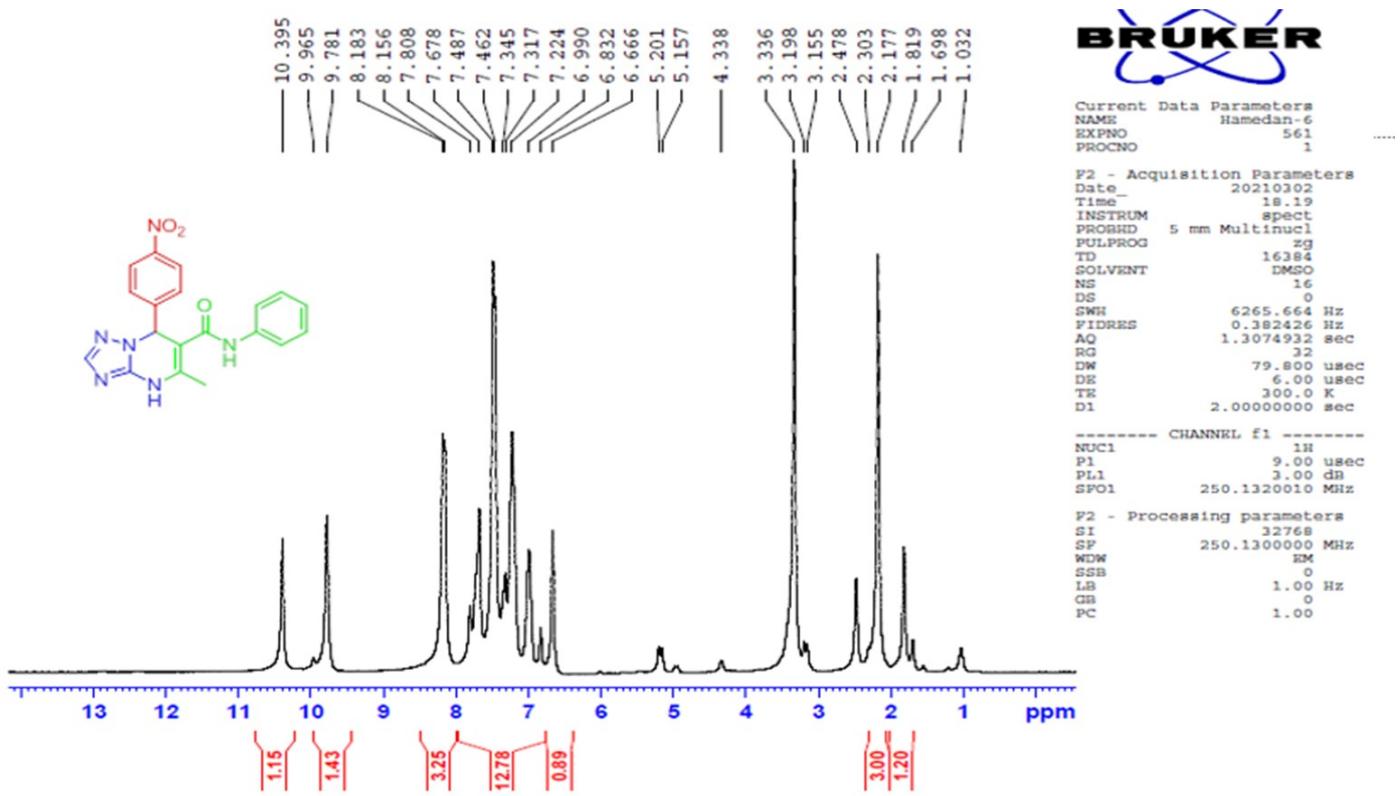
White Solid; M.p: 237-239 °C; IR (KBr, cm⁻¹): 3263, 3101, 3032, 2925, 1665, 1626, 1595, 1510, 1440, 1329, 1249, 1014, 752; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.15 (s, 3H, CH₃), 5.01 (s, 2H), 6.47 (s, 1H), 6.91 (d, *J* = 7.50 Hz, 2H, ArH), 6.98 (s, 1H, ArH), 7.15 (d, *J* = 7.75 Hz, 2H, ArH), 7.21 (d, *J* = 7.25 Hz, 2H, ArH), 7.40 (s, 4H, ArH), 7.49 (d, *J* = 7.25 Hz, 2H, ArH), 7.60 (s, 1H, ArH), 9.69 (s, 1H, NH), 10.15 (s, 1H, NH); ¹³C-NMR (DMSO-*d*₆, 62.5 MHz): δ 17.7, 60.0, 68.7, 115.0, 119.9, 123.7, 128.8, 129.9, 133.6, 139.4, 150.2, 158.4, 165.4; MS: m/z = 477.4.

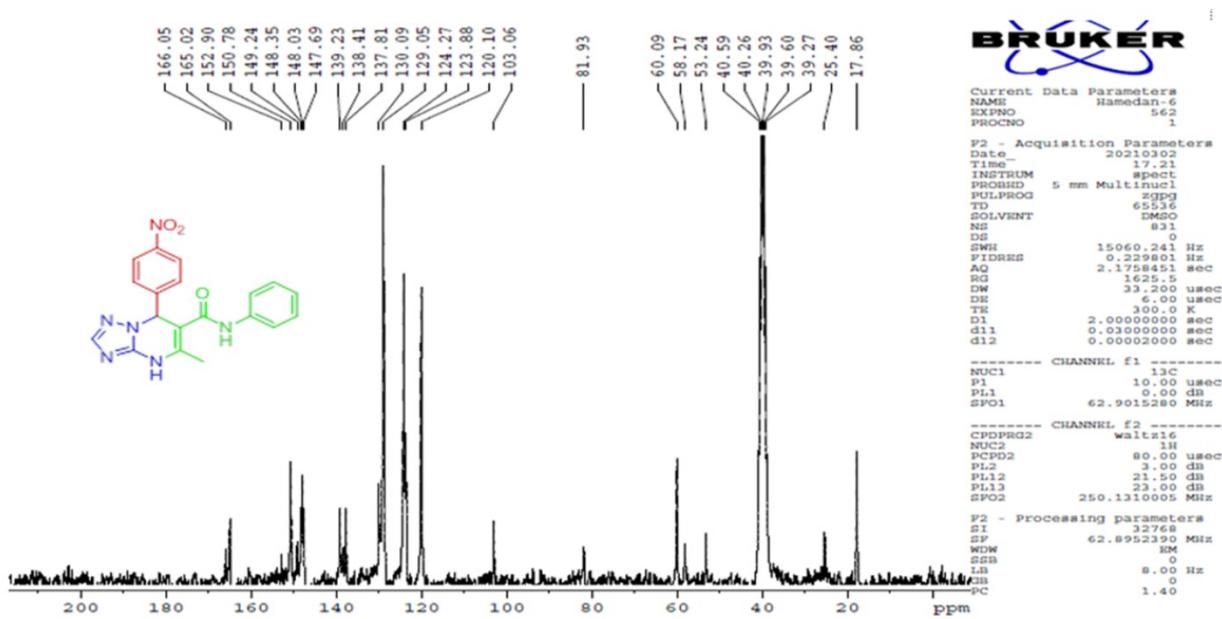


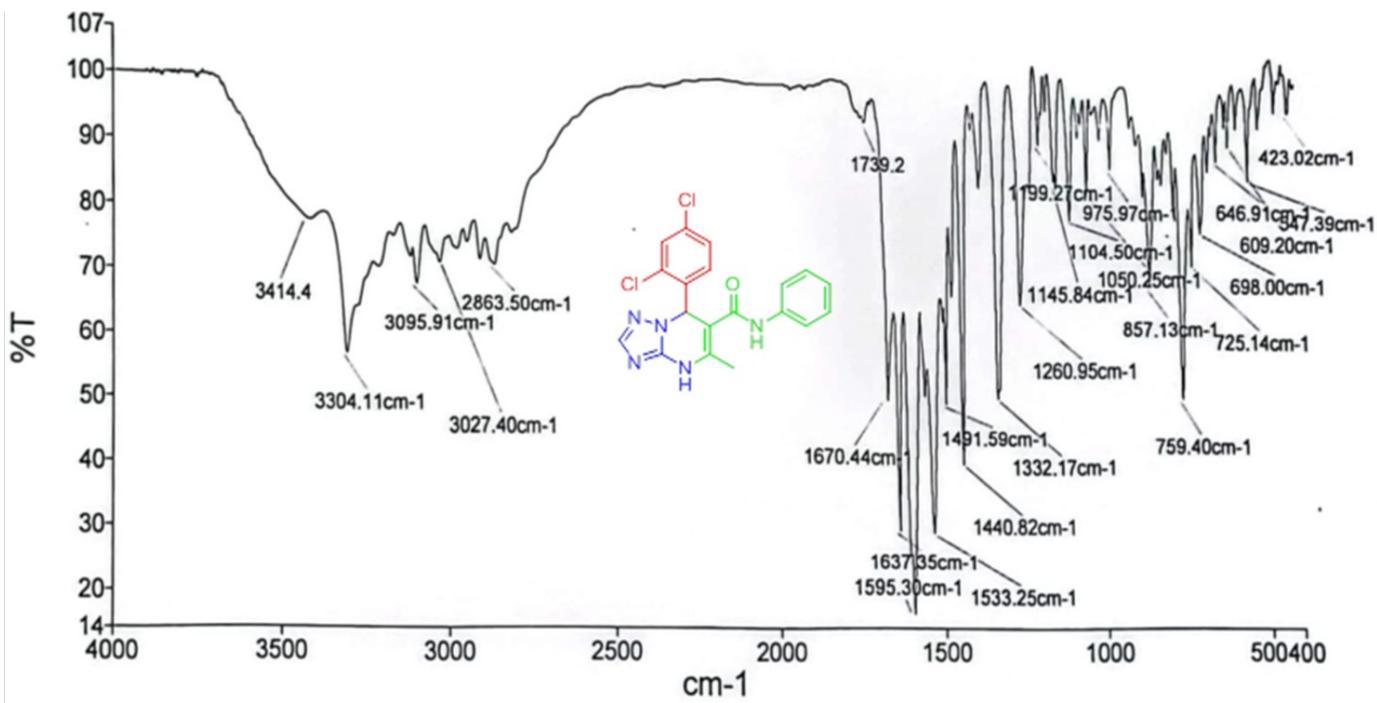
7-((4-chlorobenzyl)oxy)-3-methoxyphenyl-5-methyl-N-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide

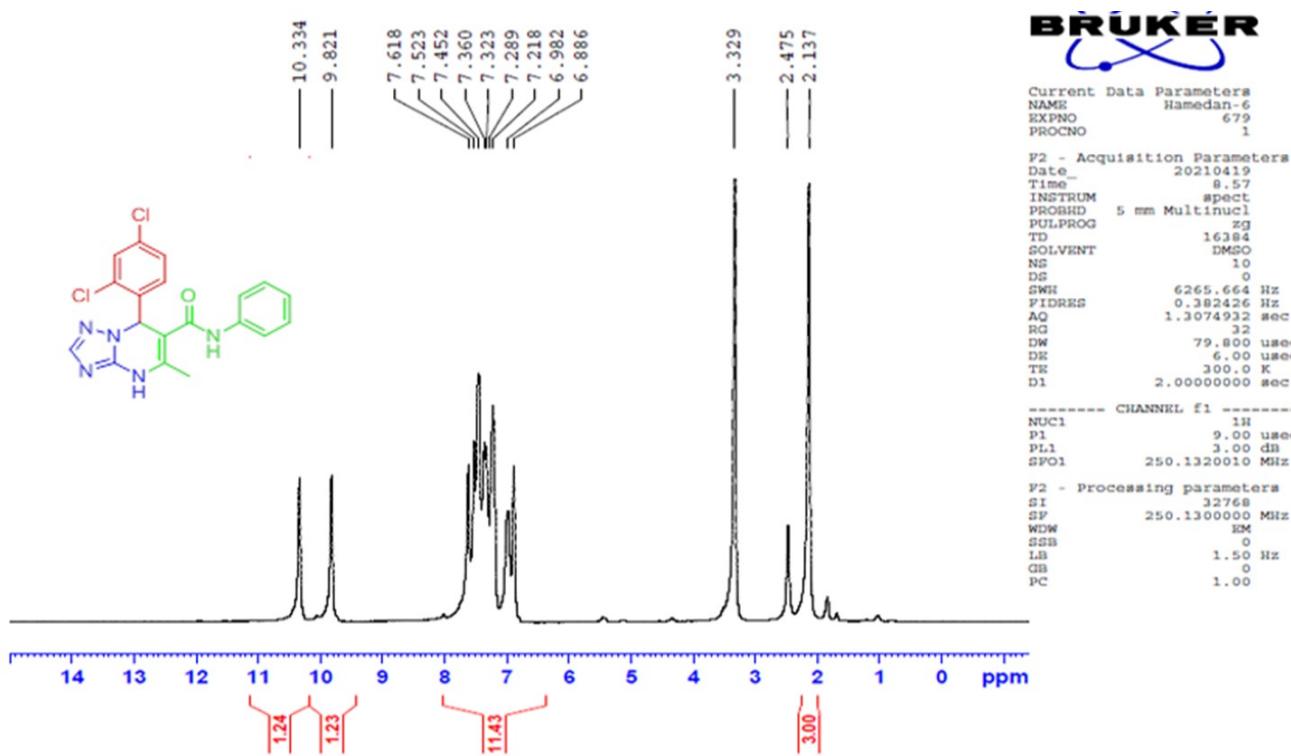
White Solid; M.p: 256-258 °C; IR (KBr, cm⁻¹): 3263, 3103, 2917, 2865, 1667, 1626, 1509, 1596, 1515, 1440, 1330, 1228, 1031, 874, 753, 541; ¹H NMR (250 MHz, DMSO-*d*₆): δ 2.15 (s, 3H, CH₃), 3.63 (s, 3H, CH₃), 4.98 (s, 2H), 6.46 (s, 1H), 6.69 (d, *J* = 7.00 Hz, 1H, ArH), 6.82 (s, 1H, ArH), 6.90-6.98 (m, 2H, ArH), 7.23 (s, 2H, ArH), 7.39 (s, 4H, ArH), 7.50 (d, *J* = 6.75 Hz, 2H, ArH), 7.62 (s, 1H, ArH), 9.70 (s, 1H, NH), 10.15 (s, 1H, NH); ¹³C-NMR (DMSO-*d*₆, 62.5 MHz): δ 17.7, 56.0, 60.3, 69.5, 104.0, 111.7, 113.9, 119.9, 123.7, 128.8, 129.0, 129.9, 132.8, 134.1, 136.5, 136.8, 139.4, 147.9, 149.2, 150.2, 165.4; MS: m/z = 507.5.

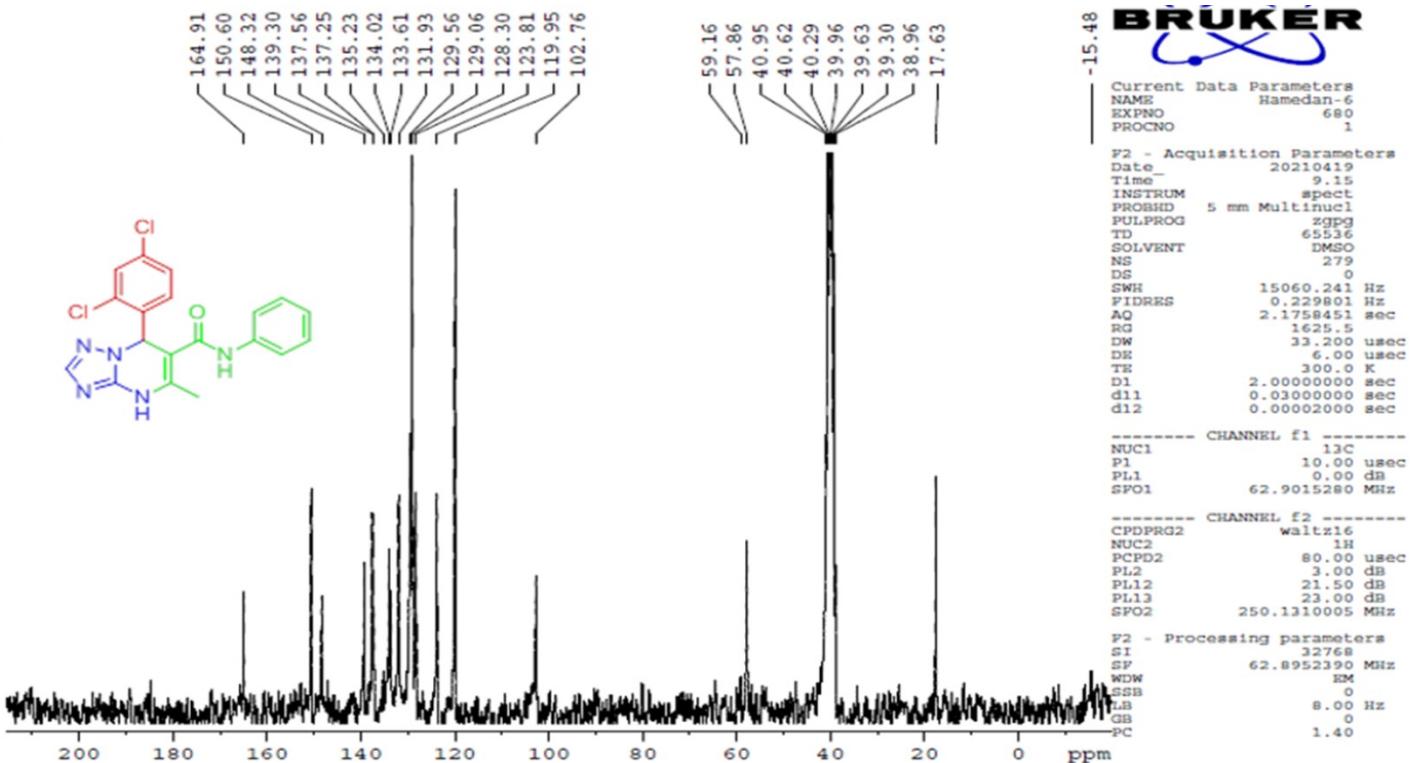


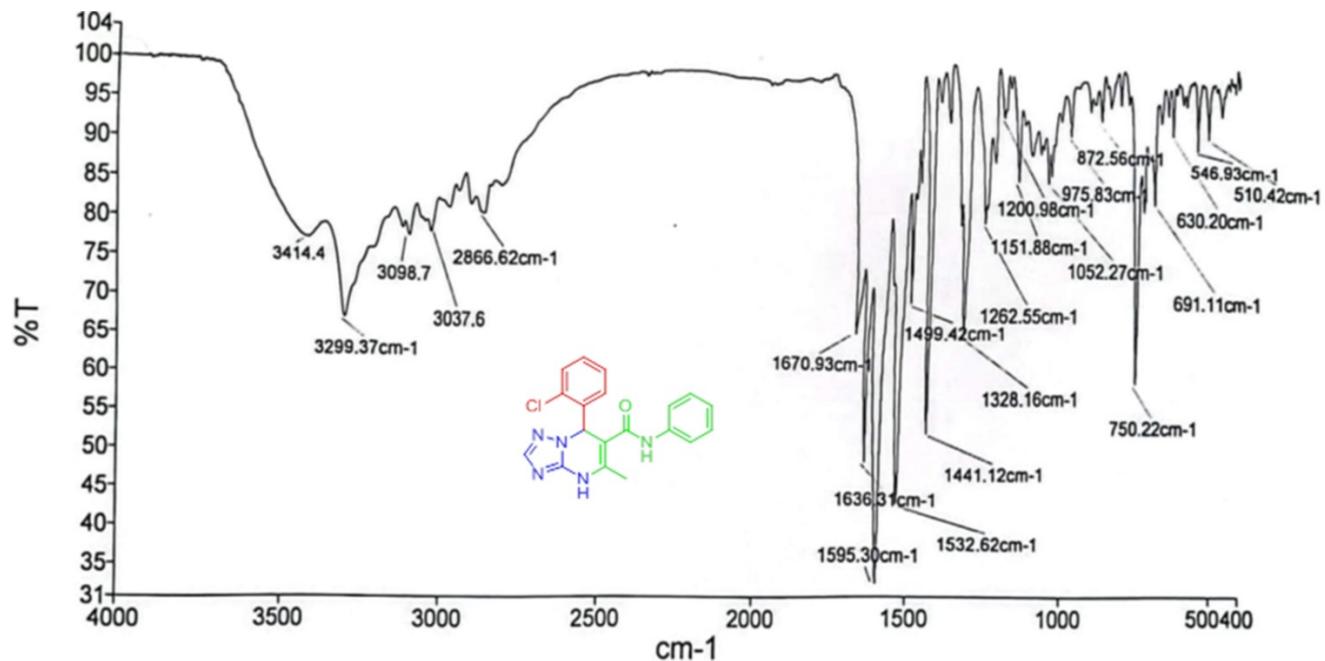


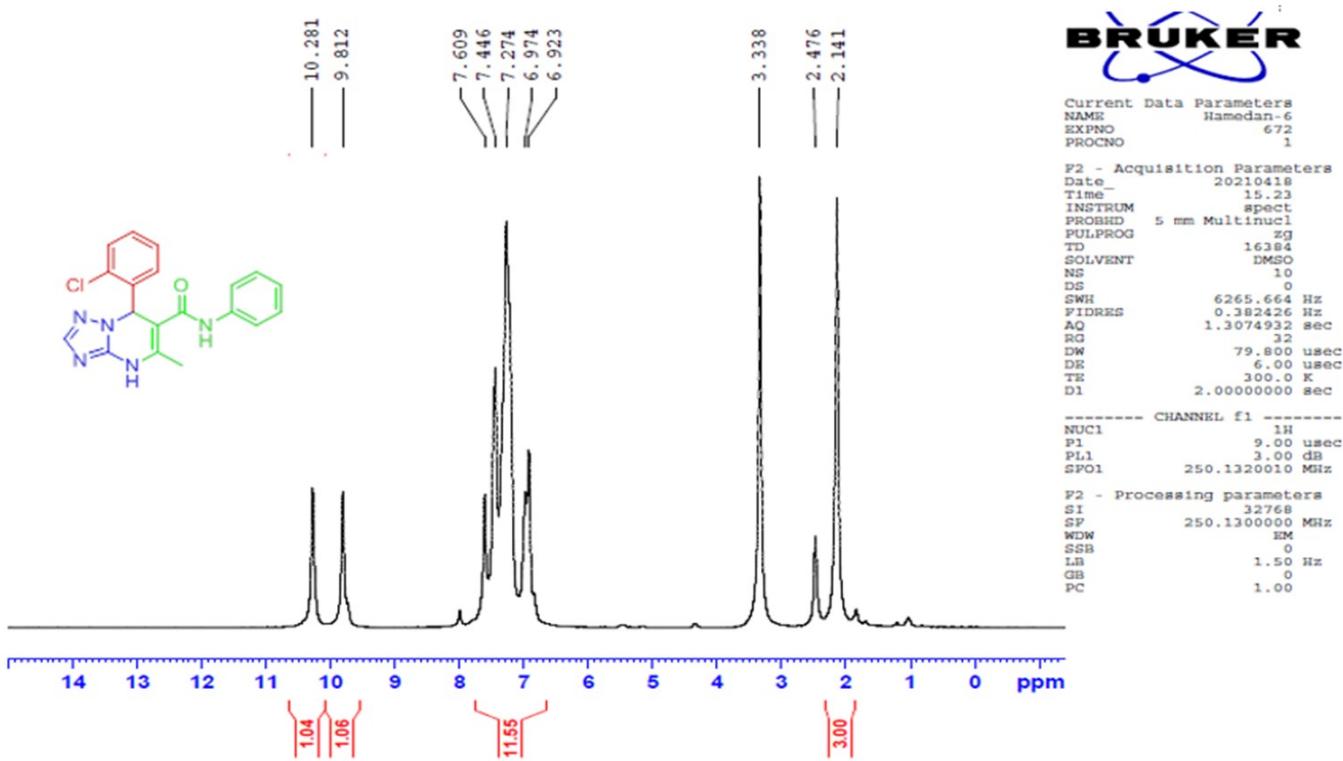


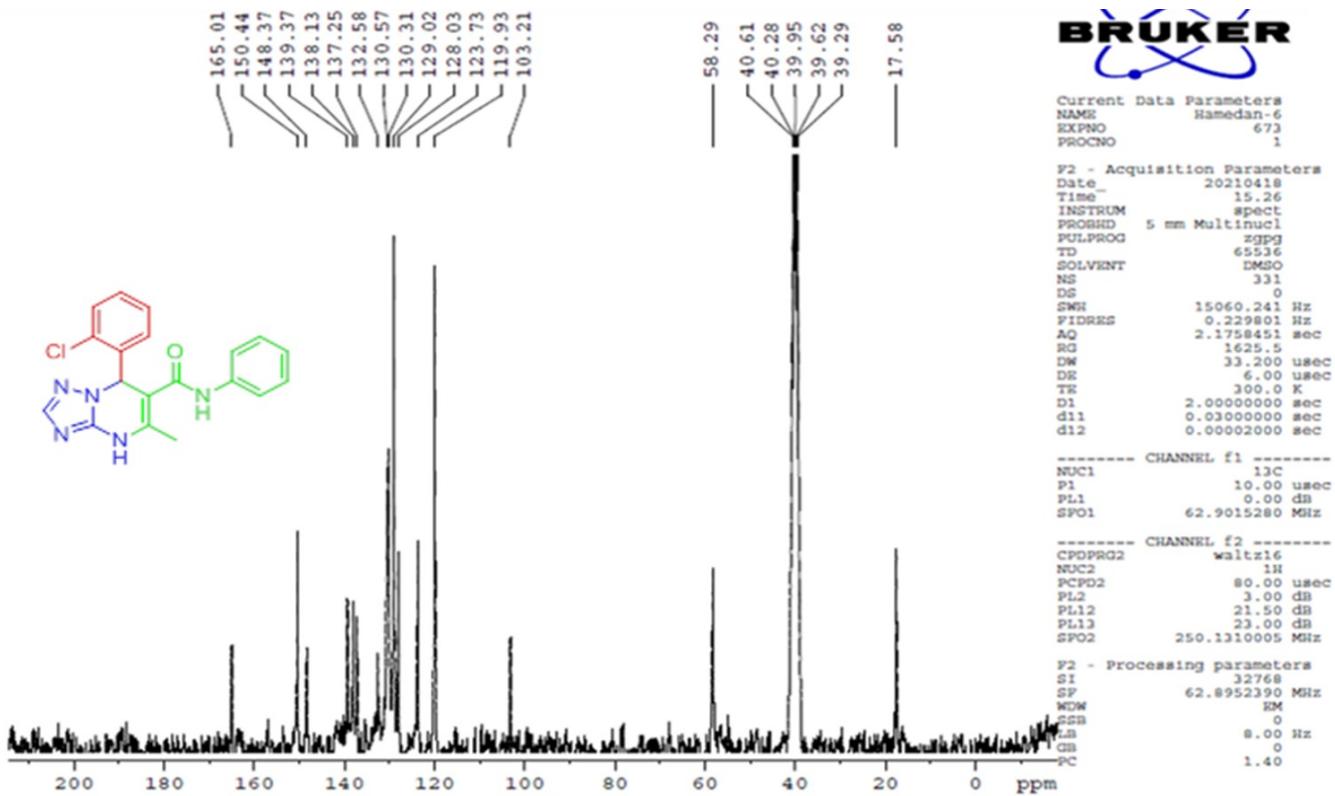


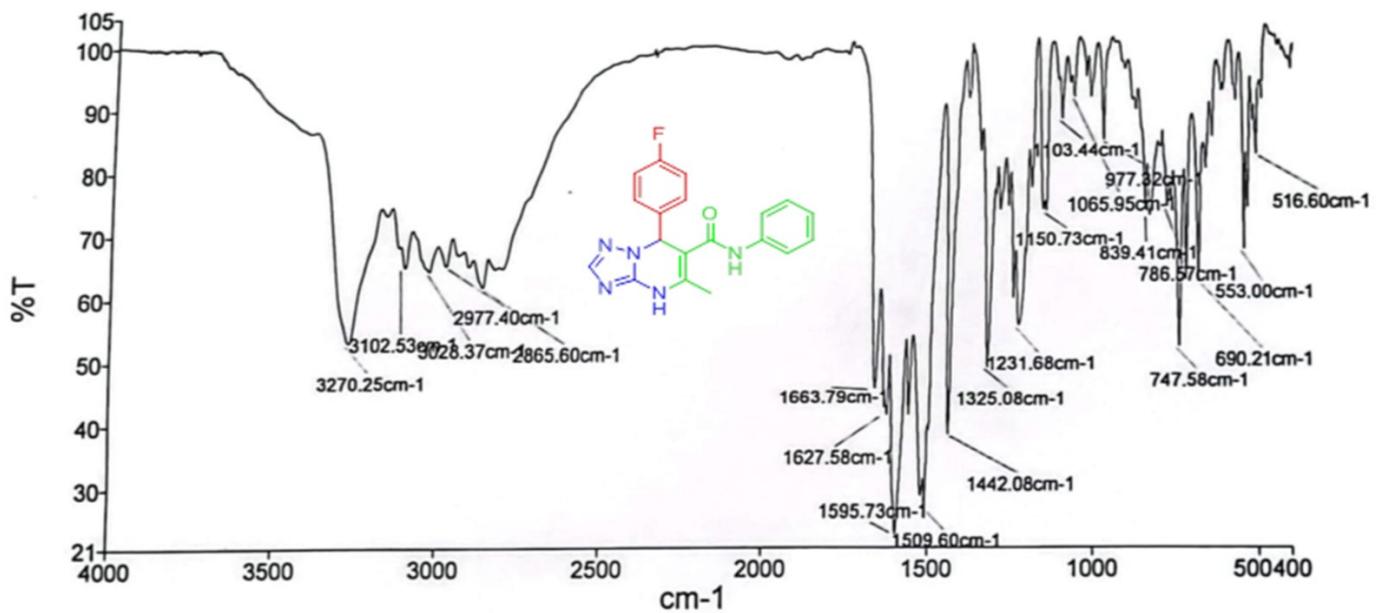


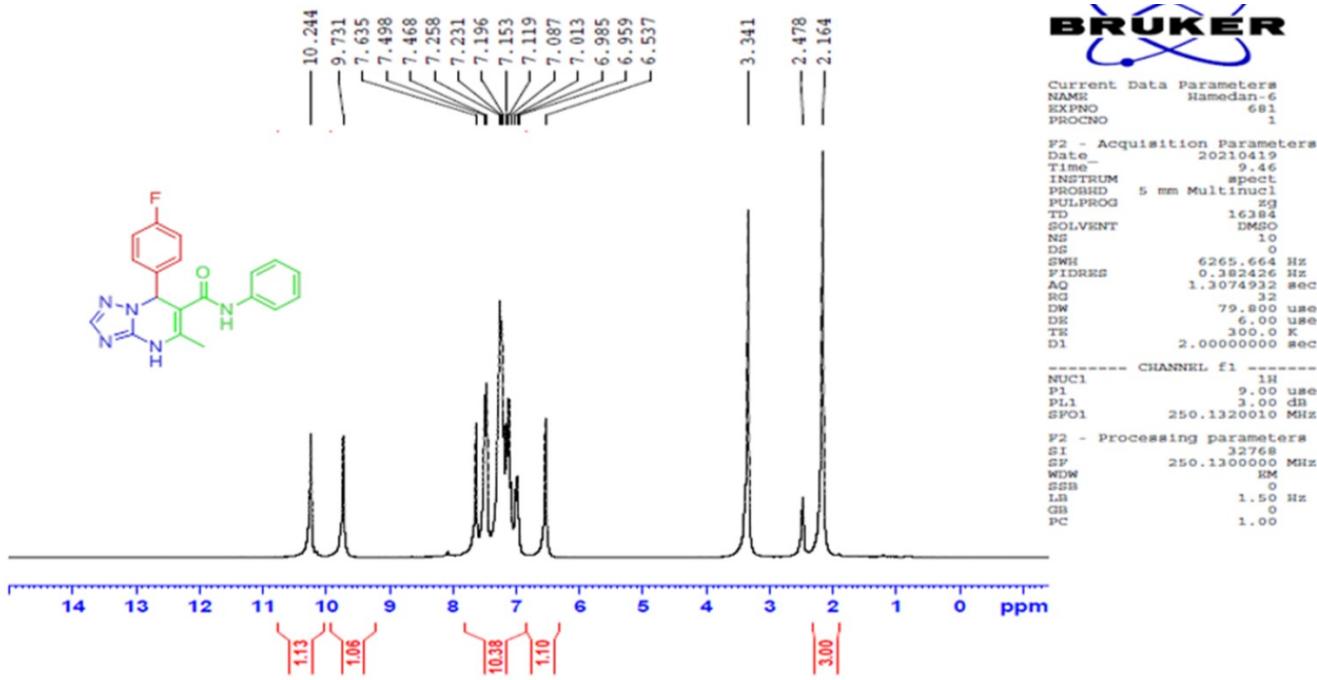


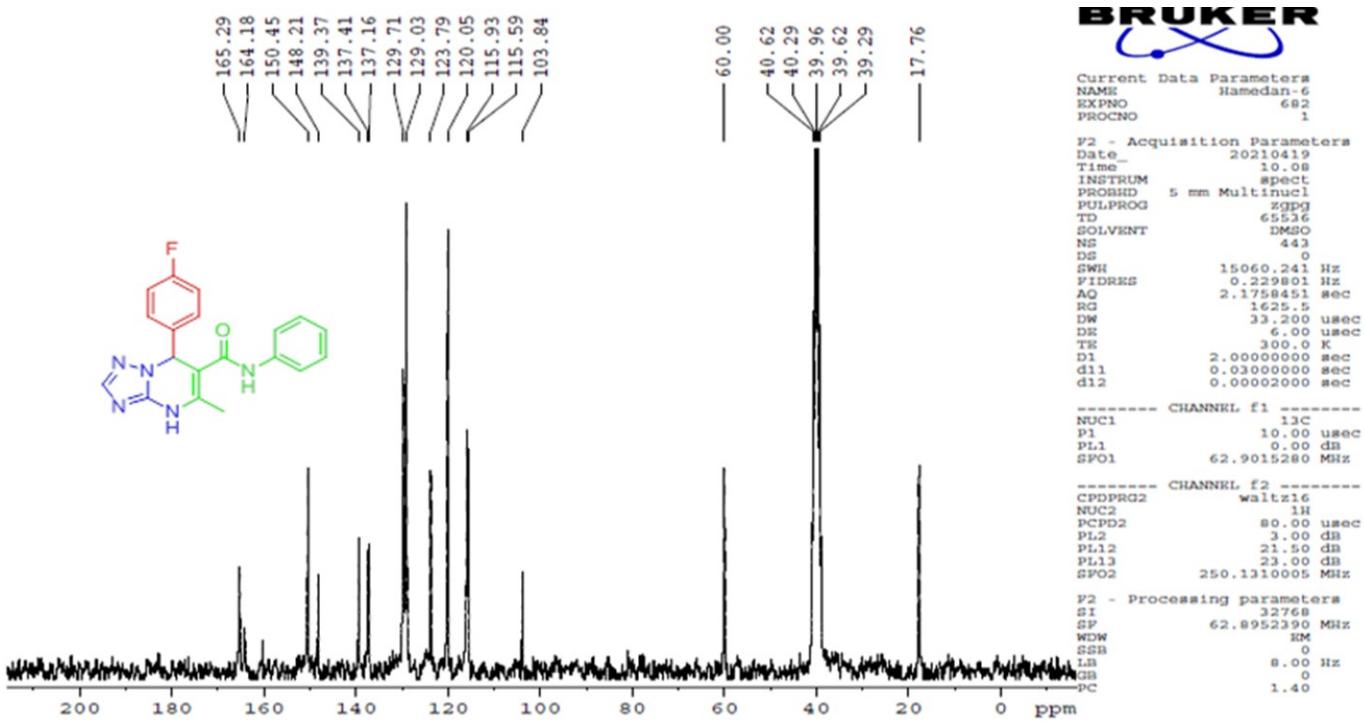


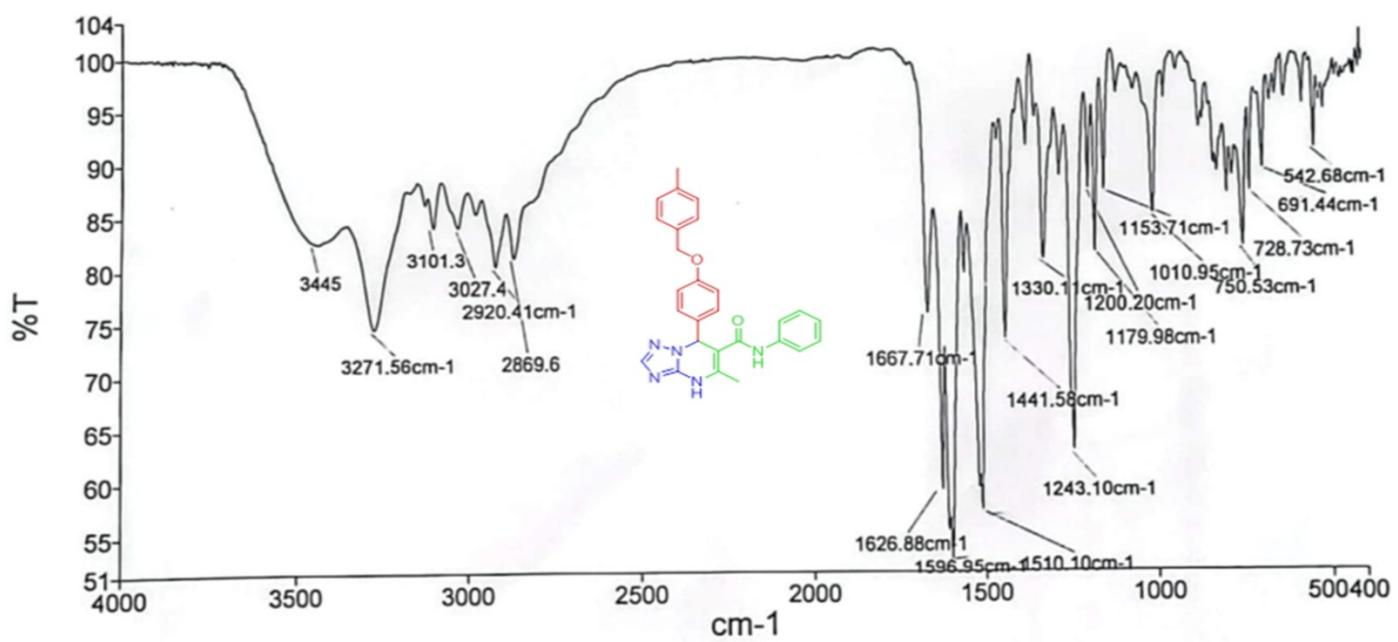




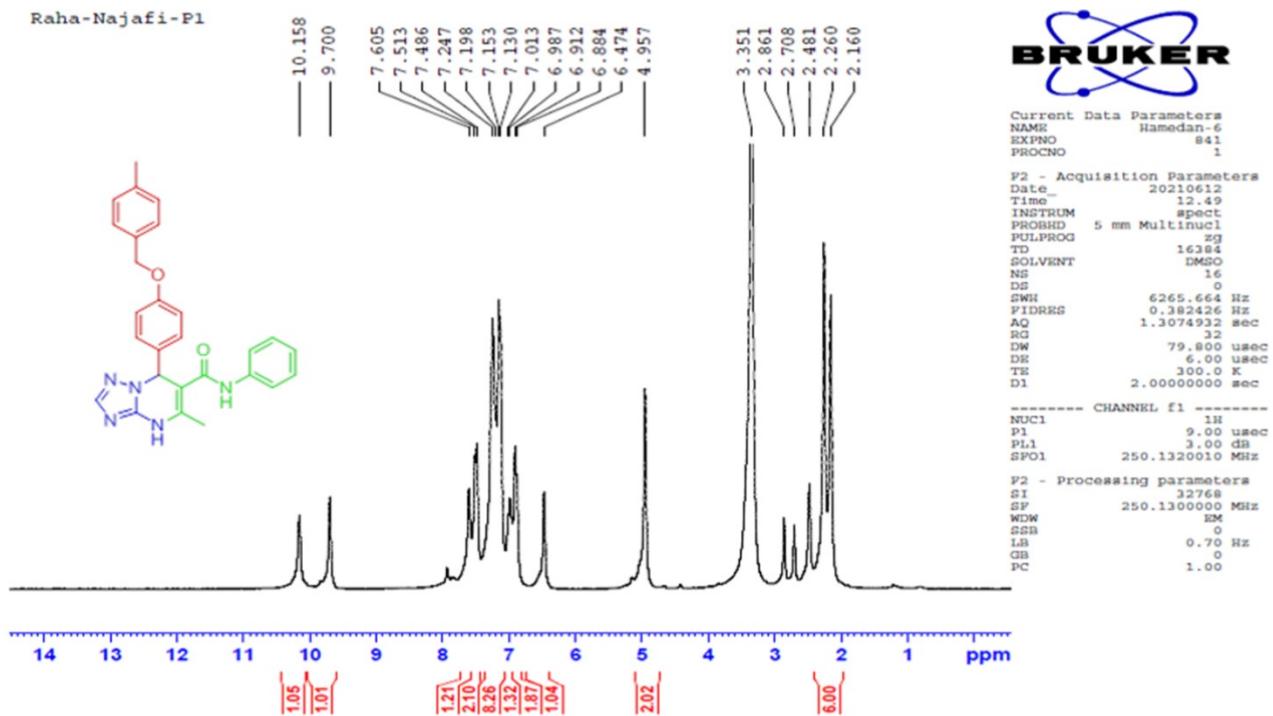


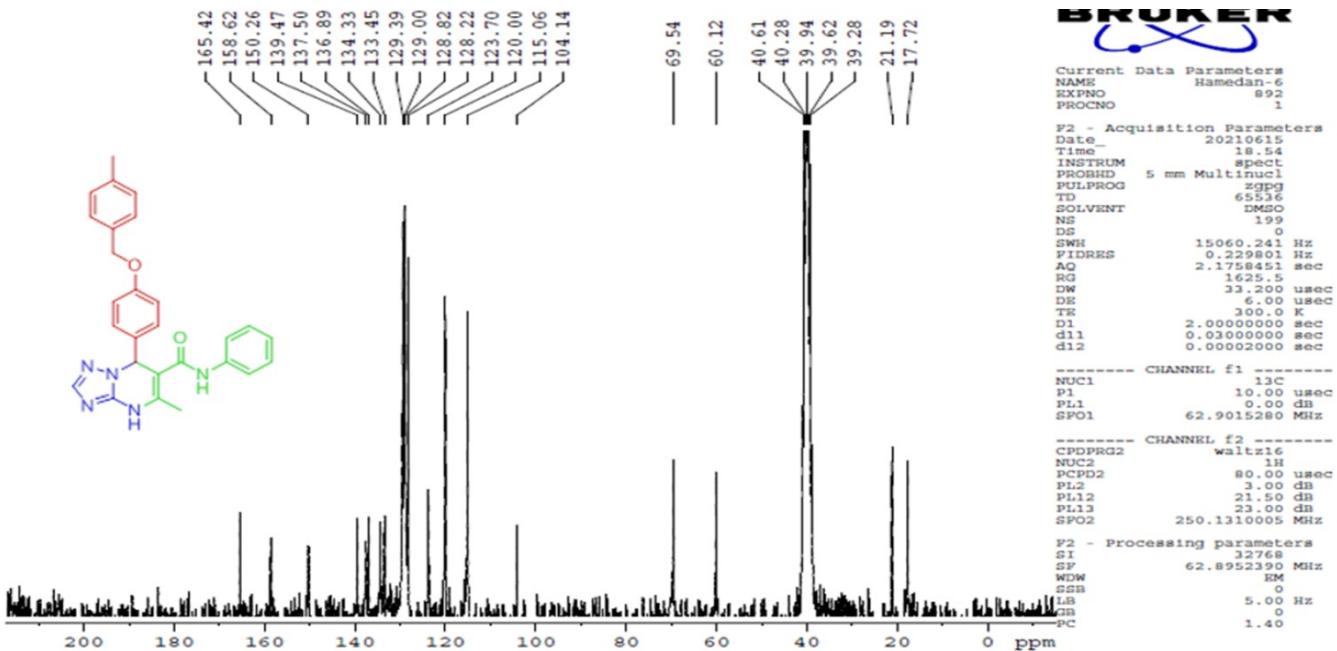


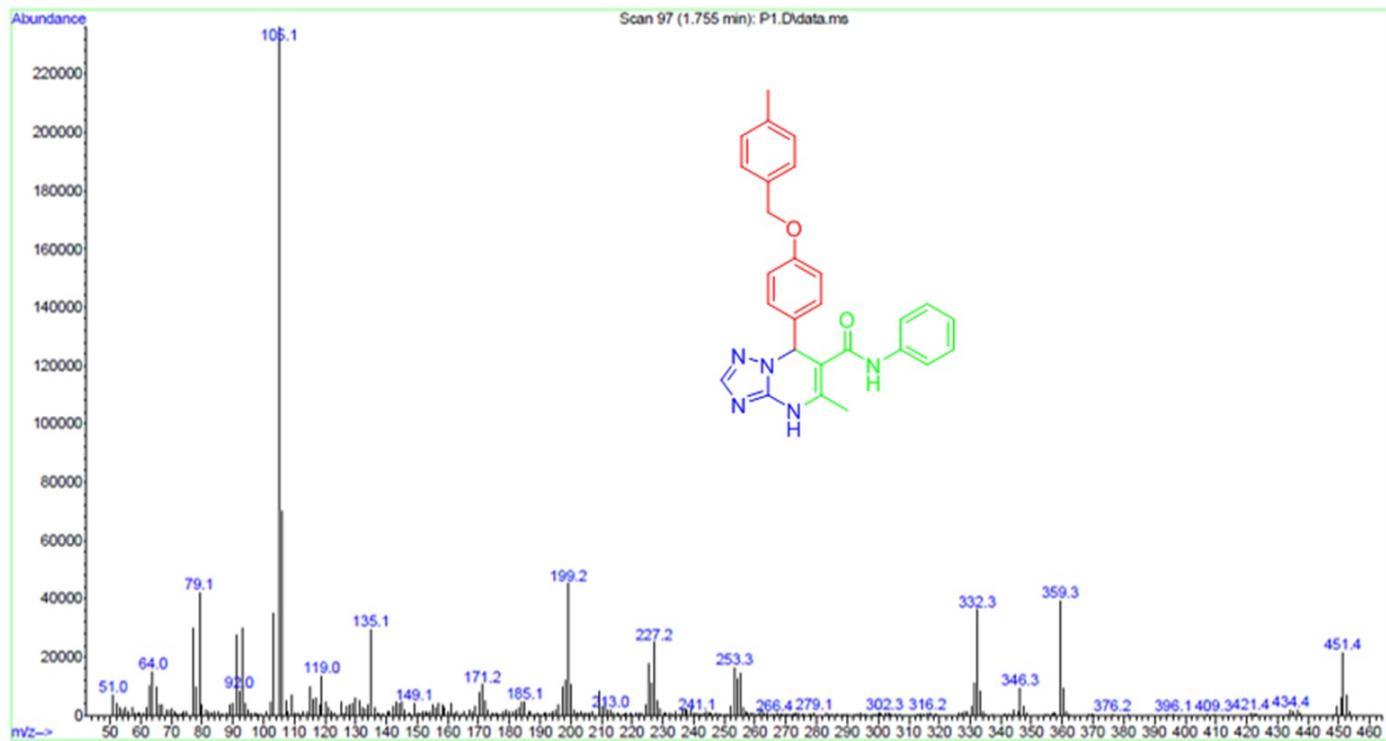


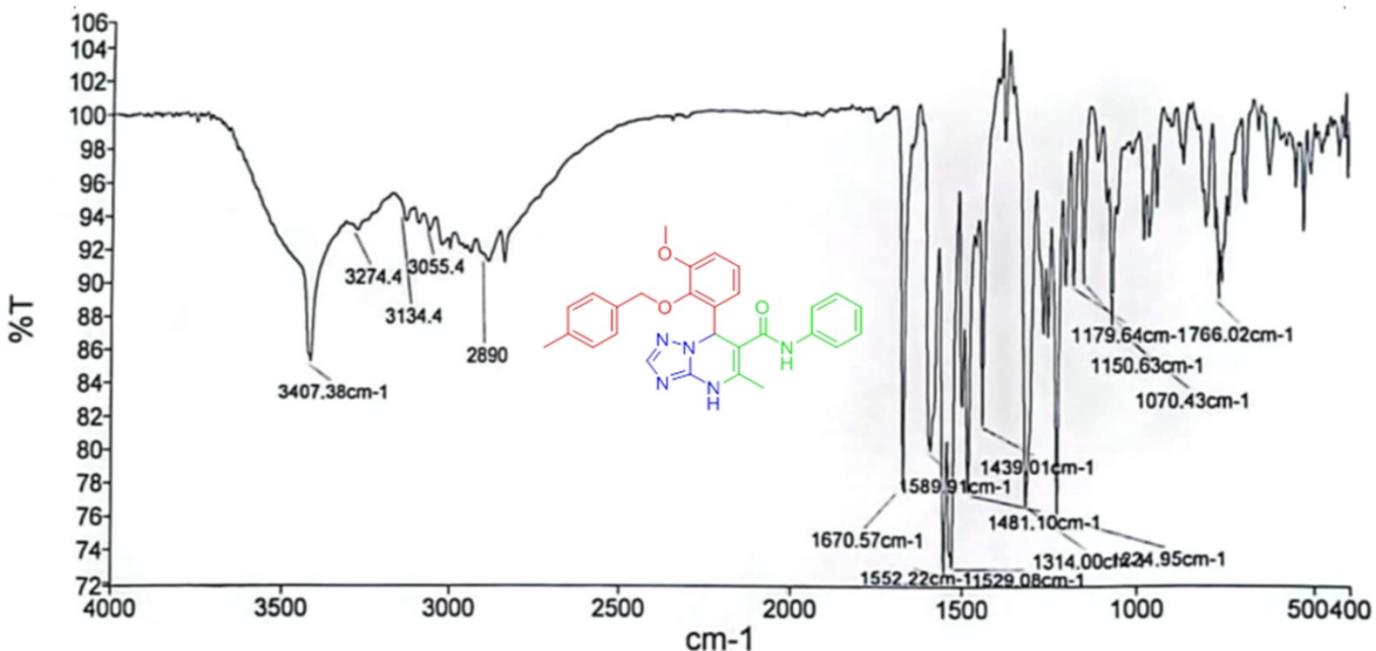


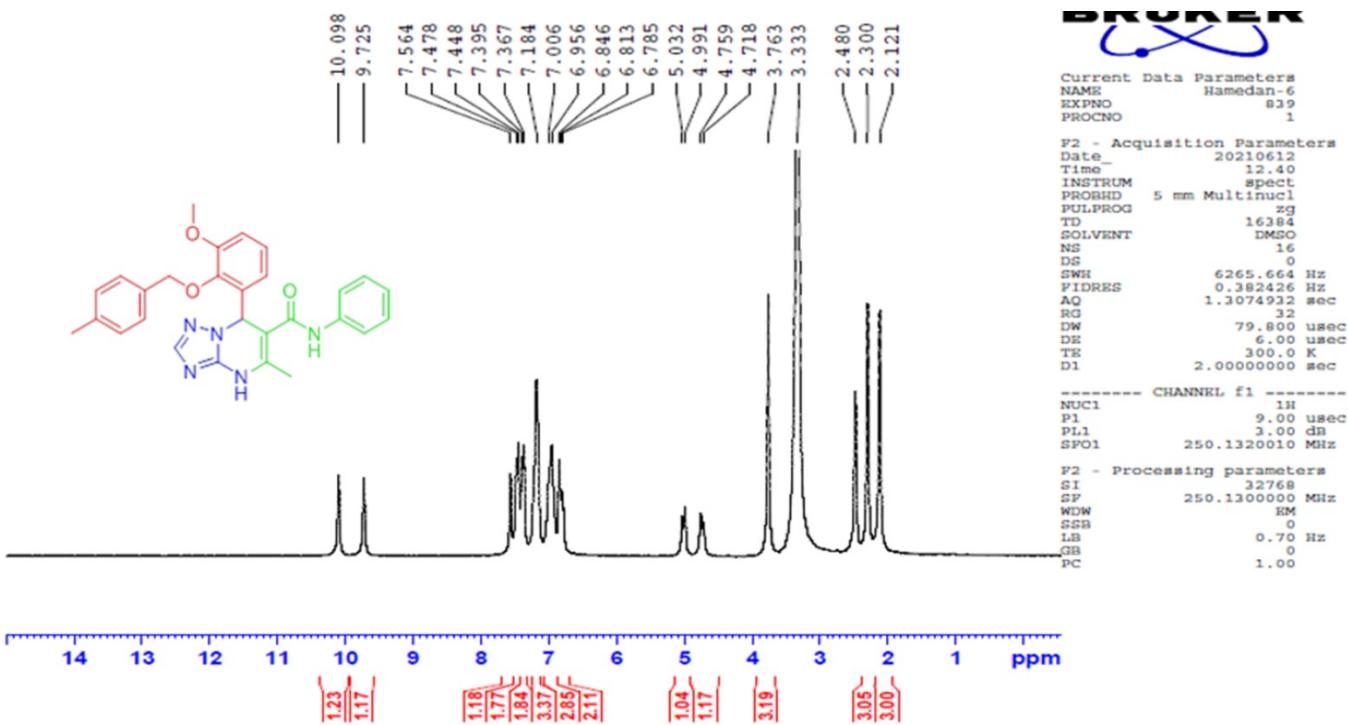
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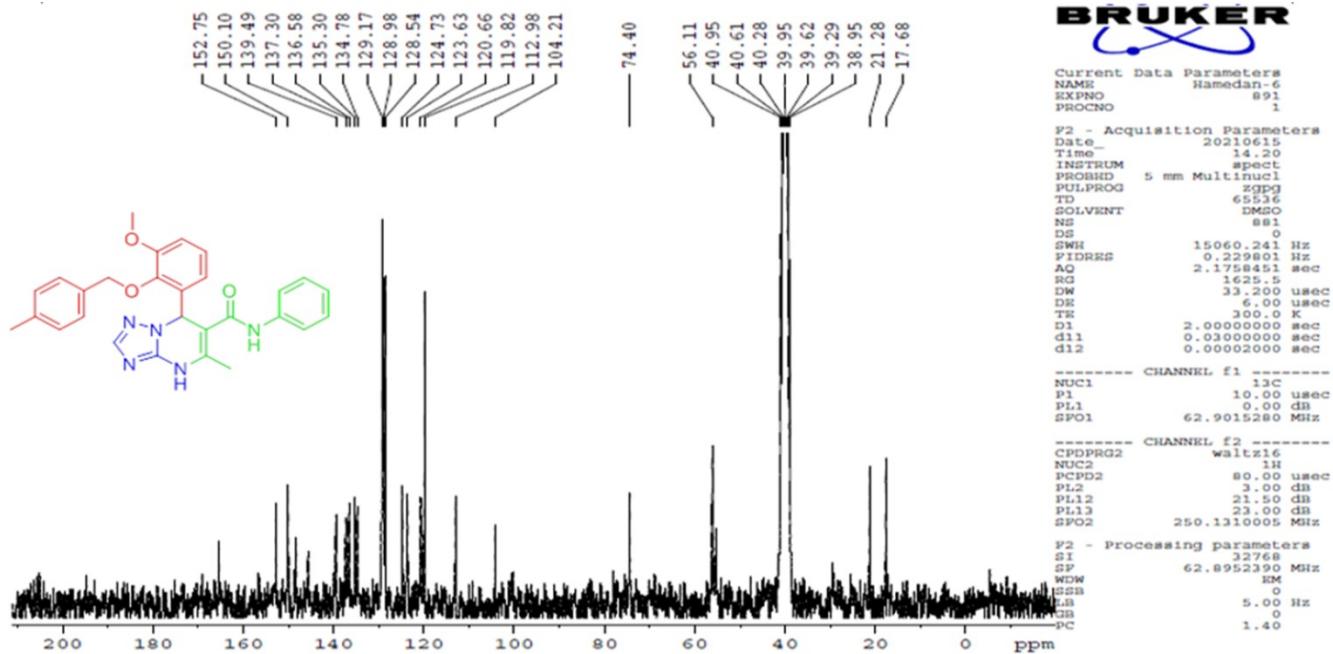


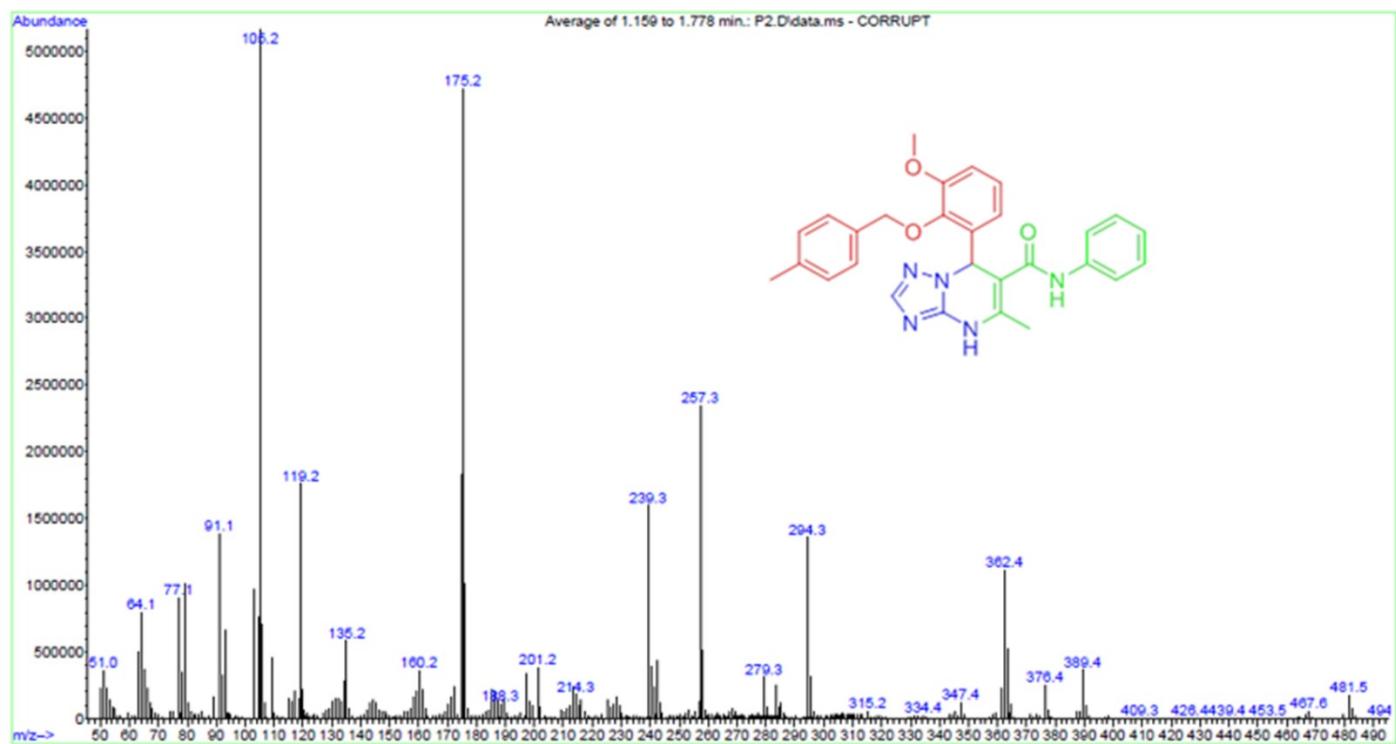


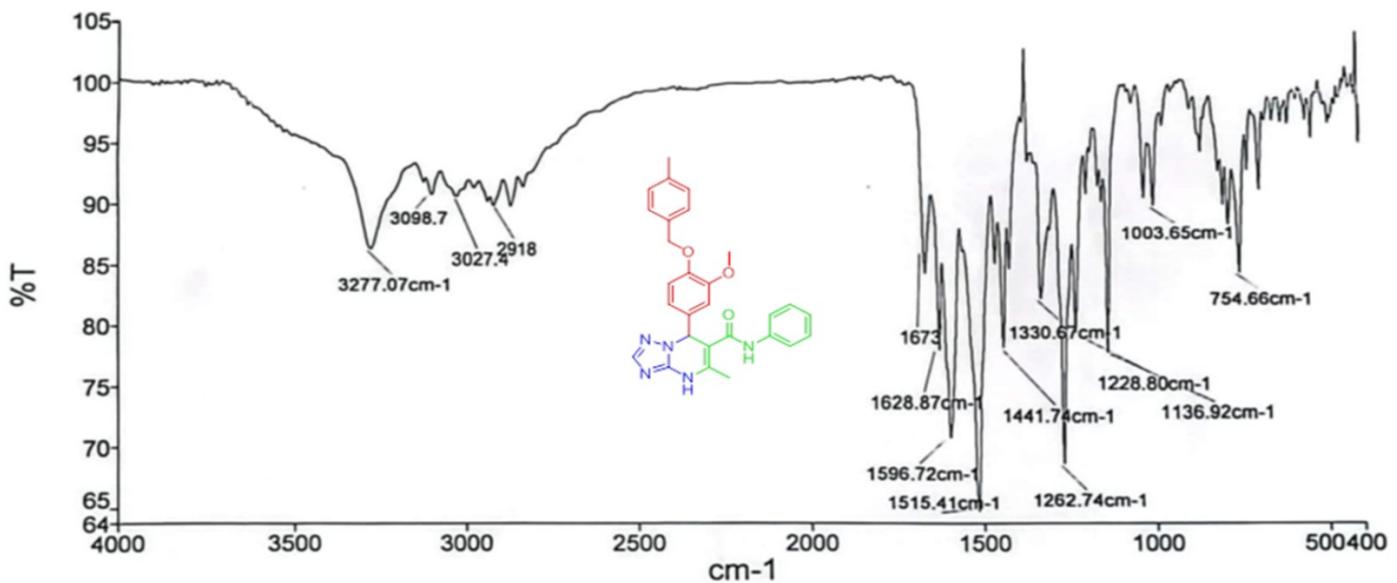


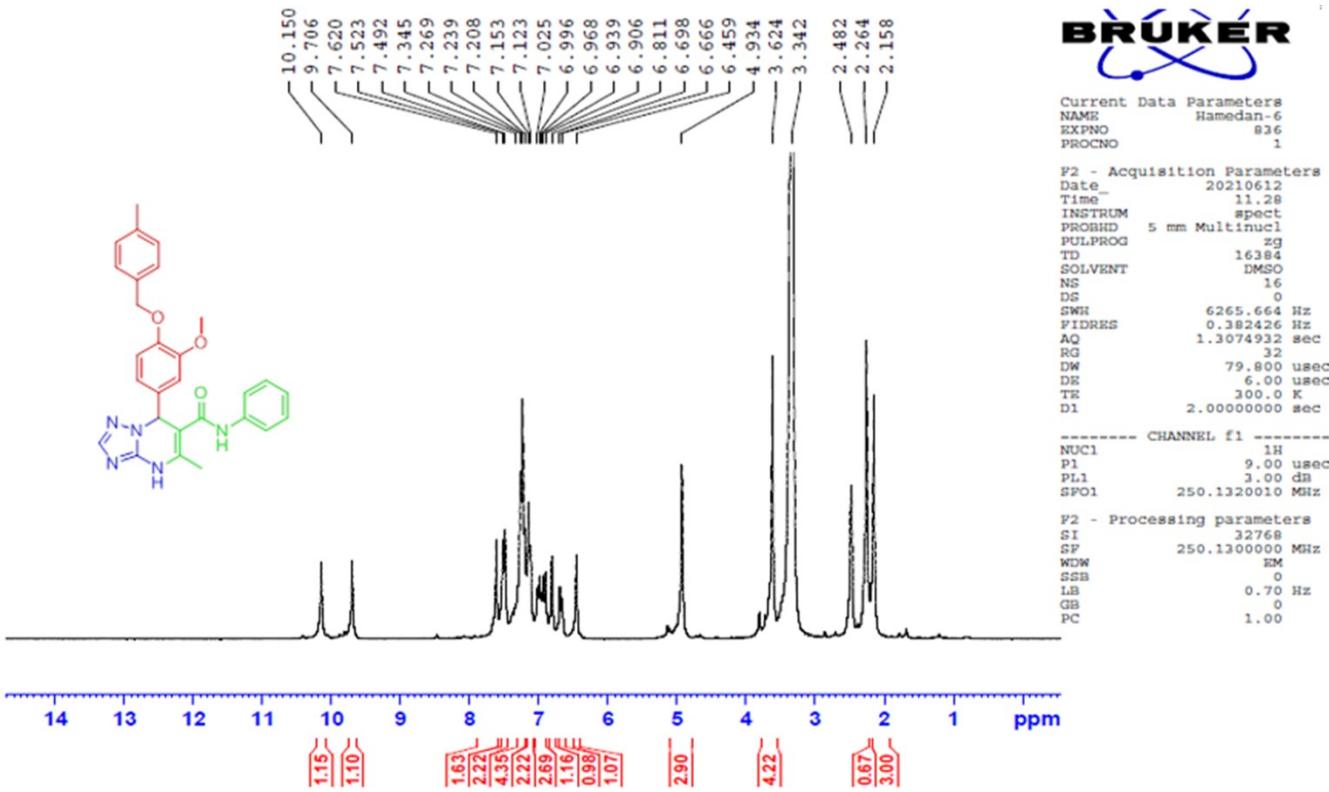


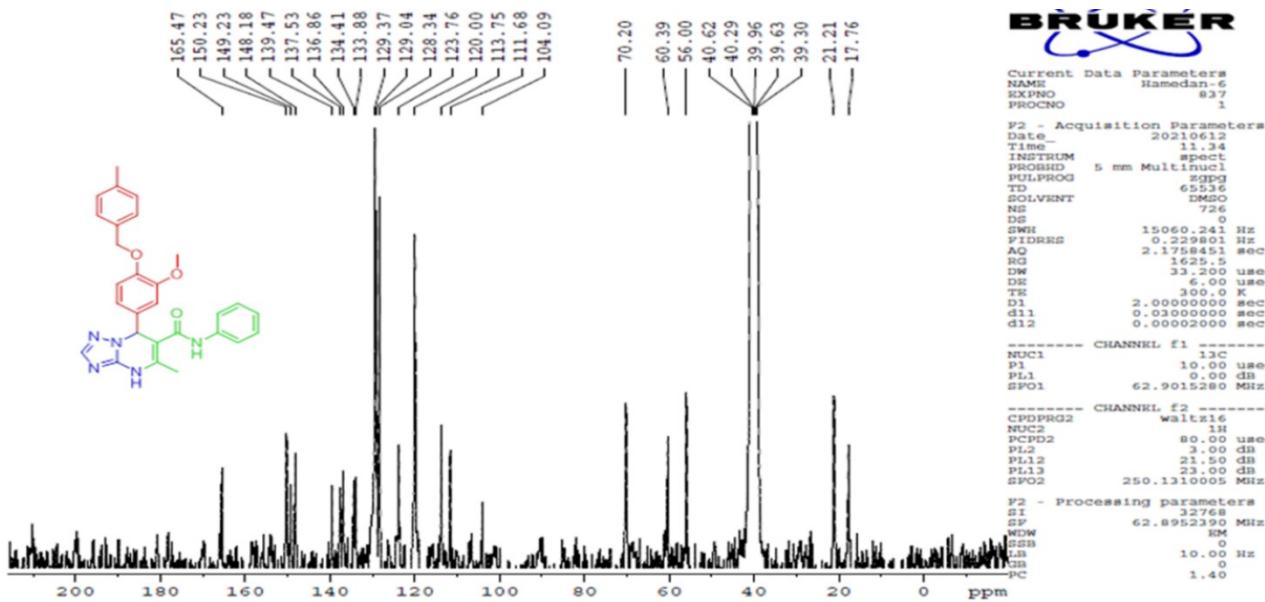


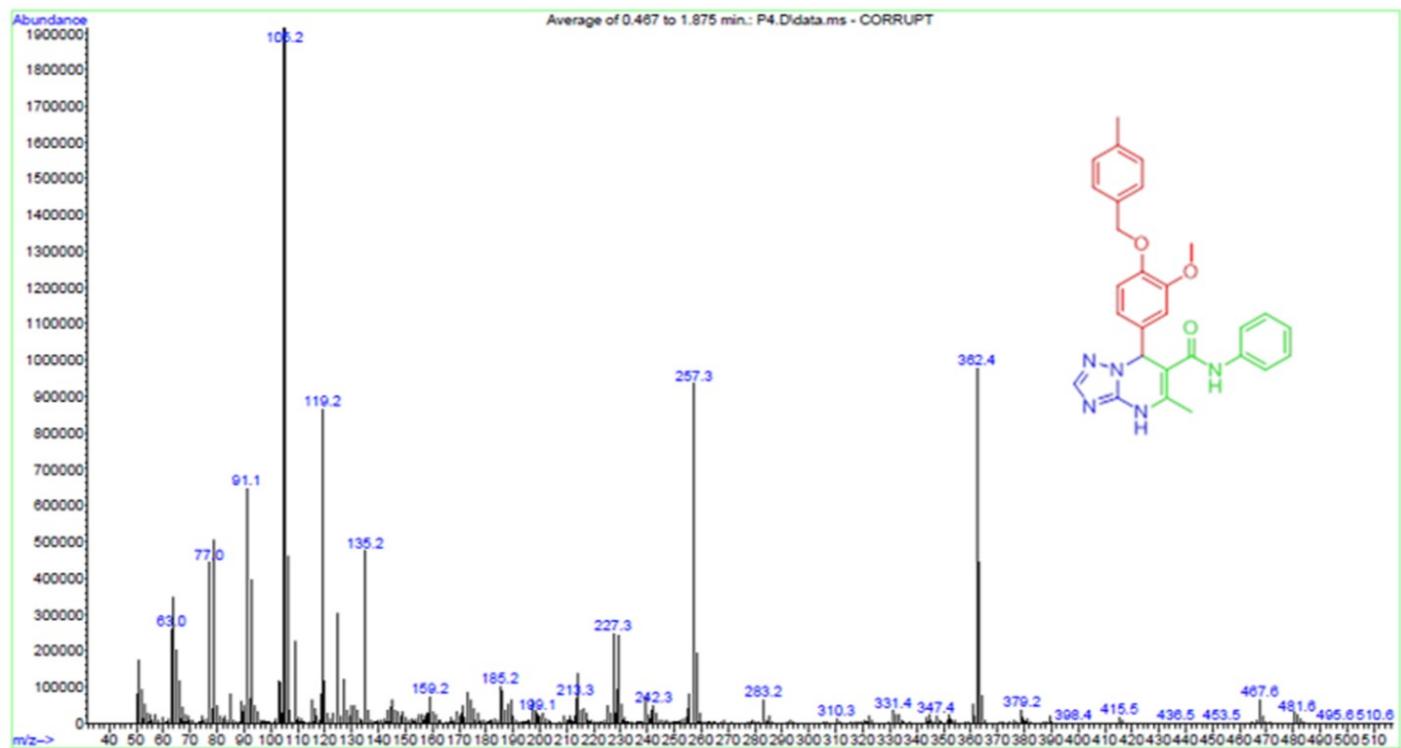


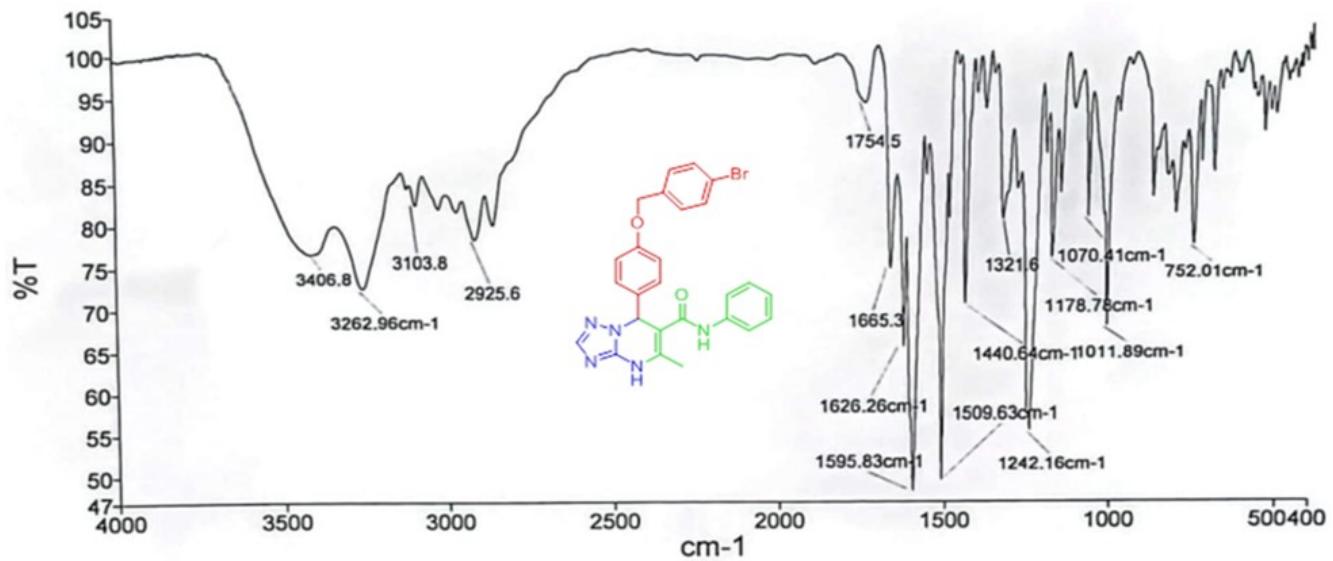


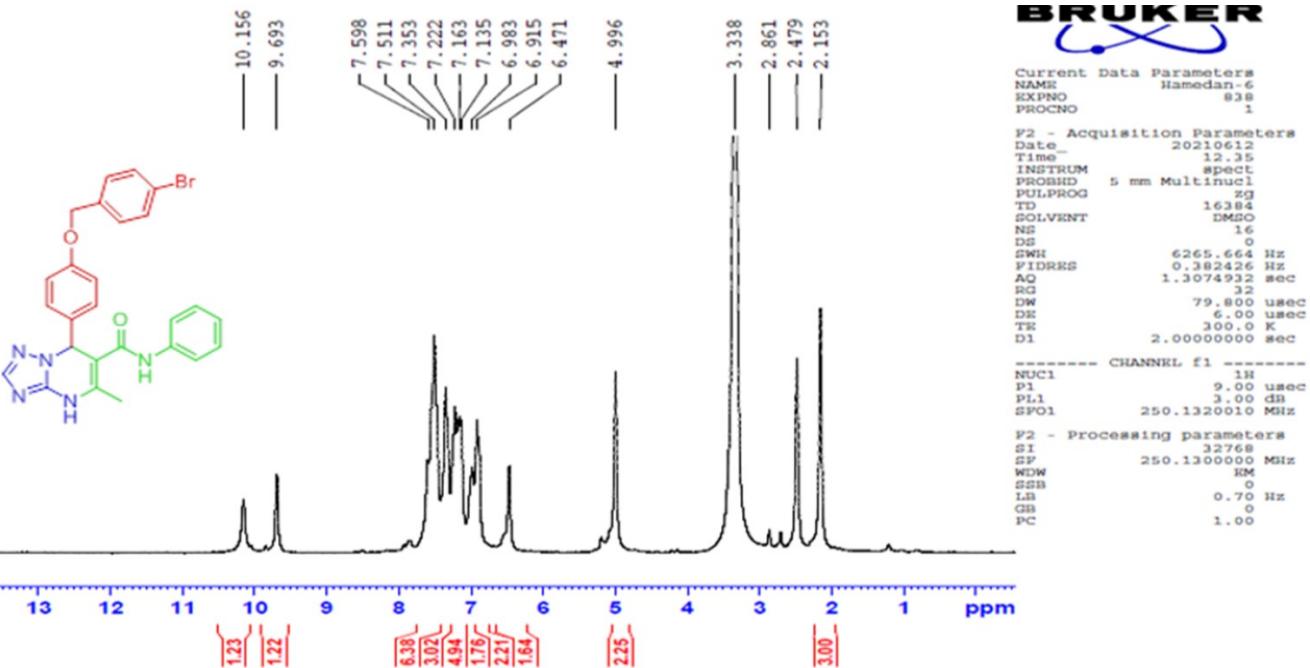


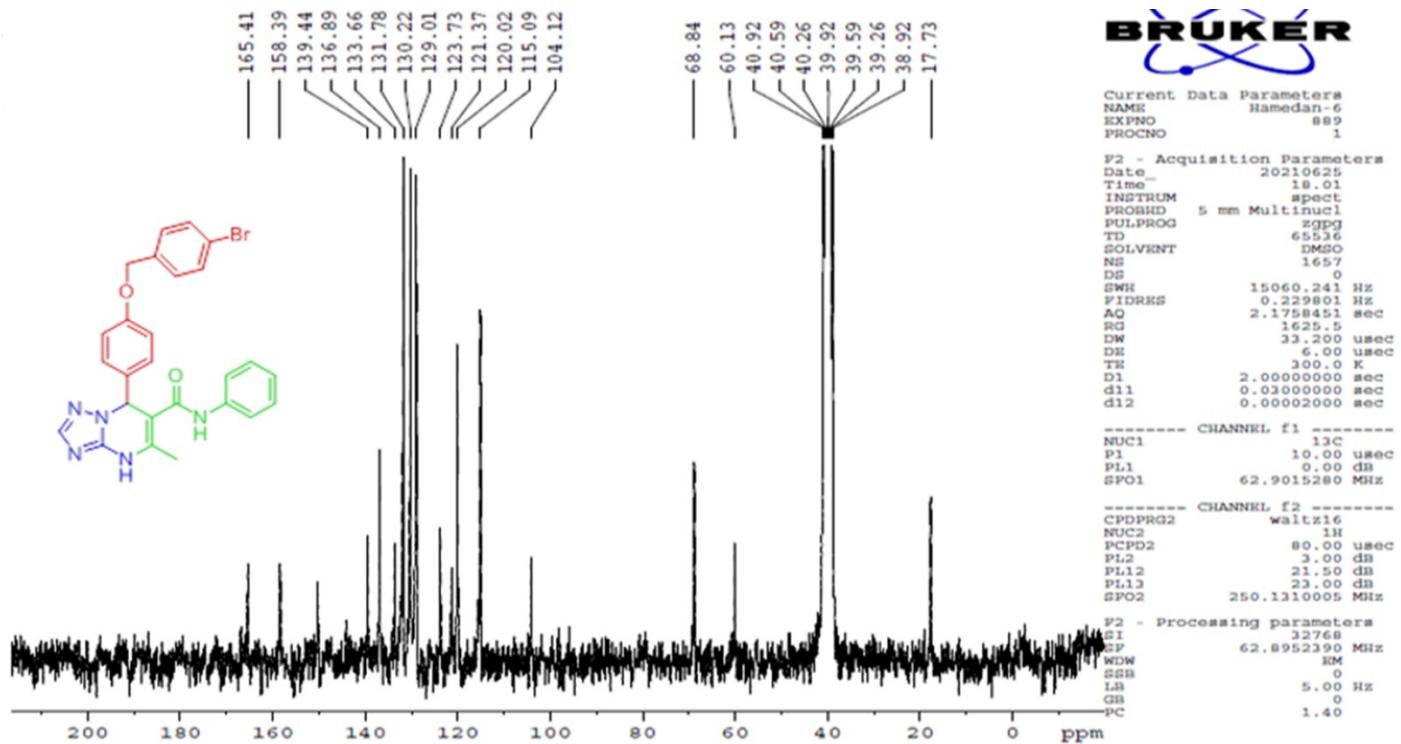


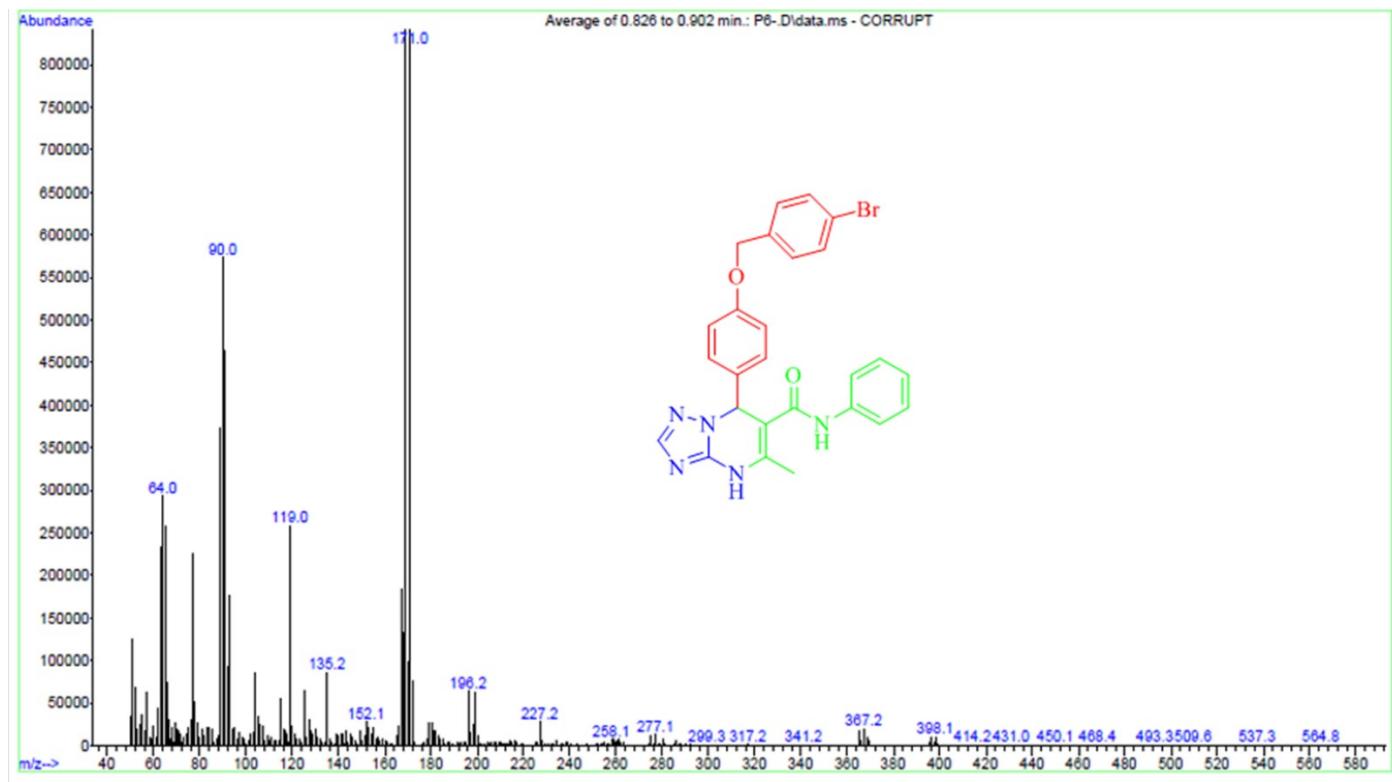


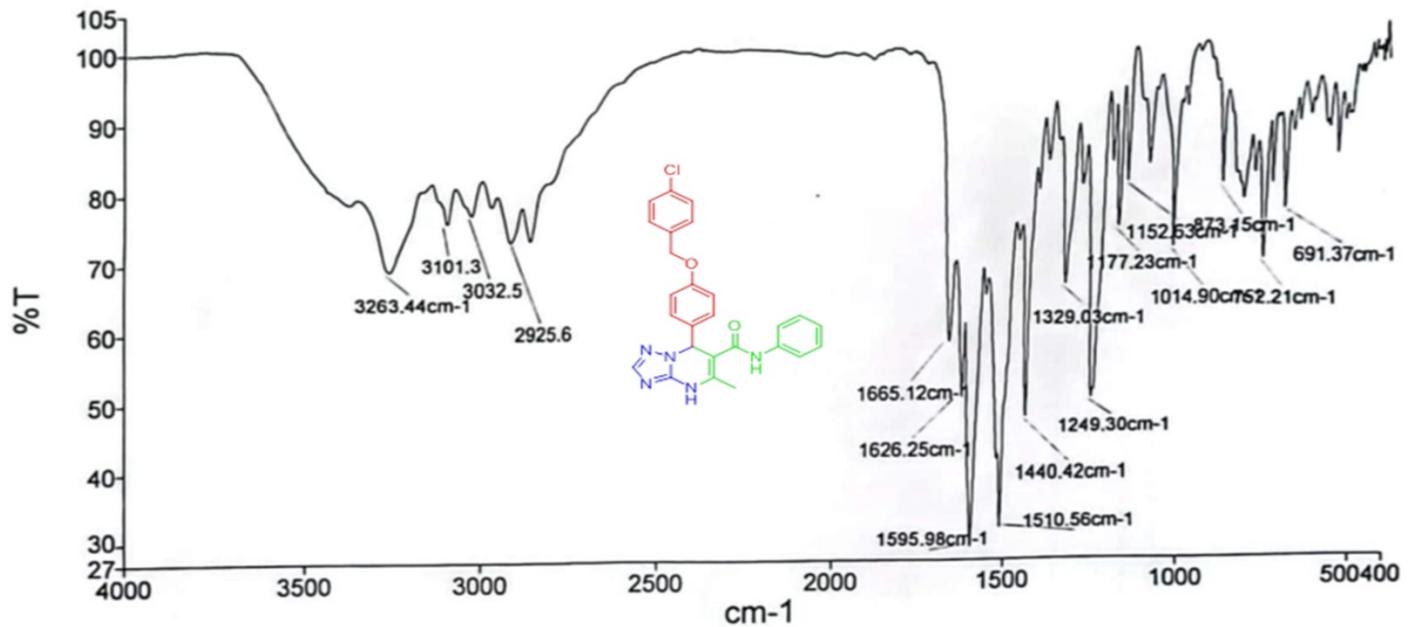


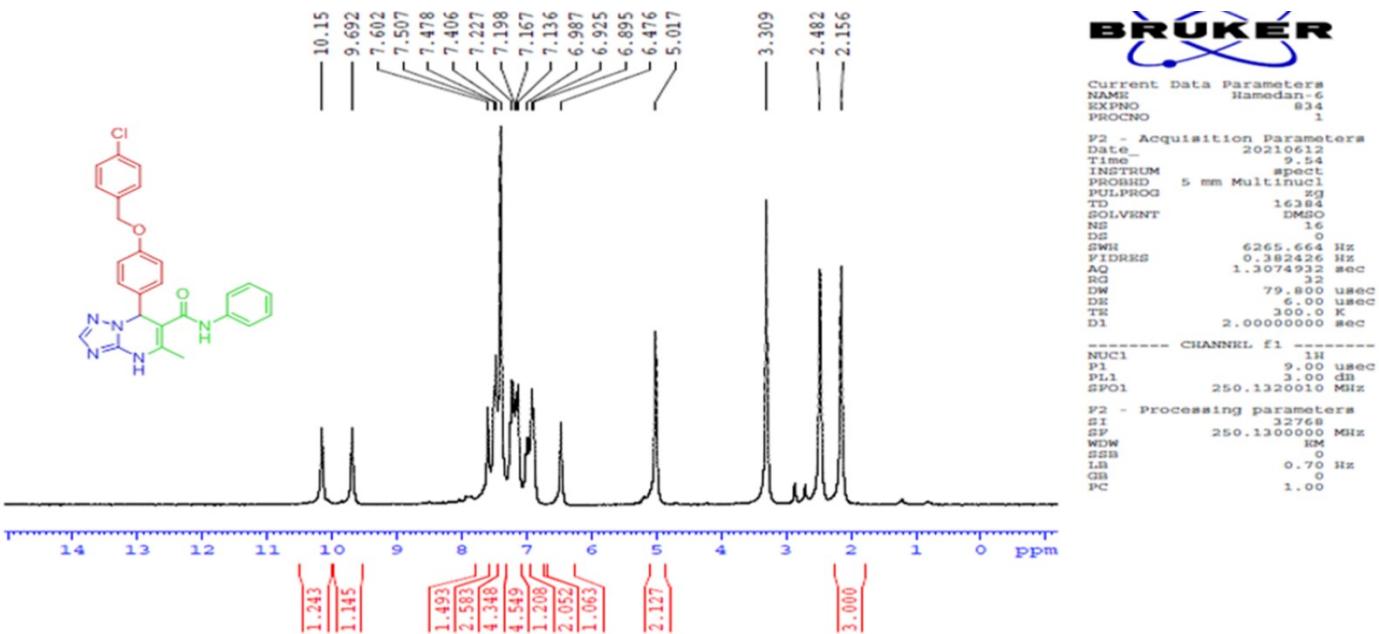


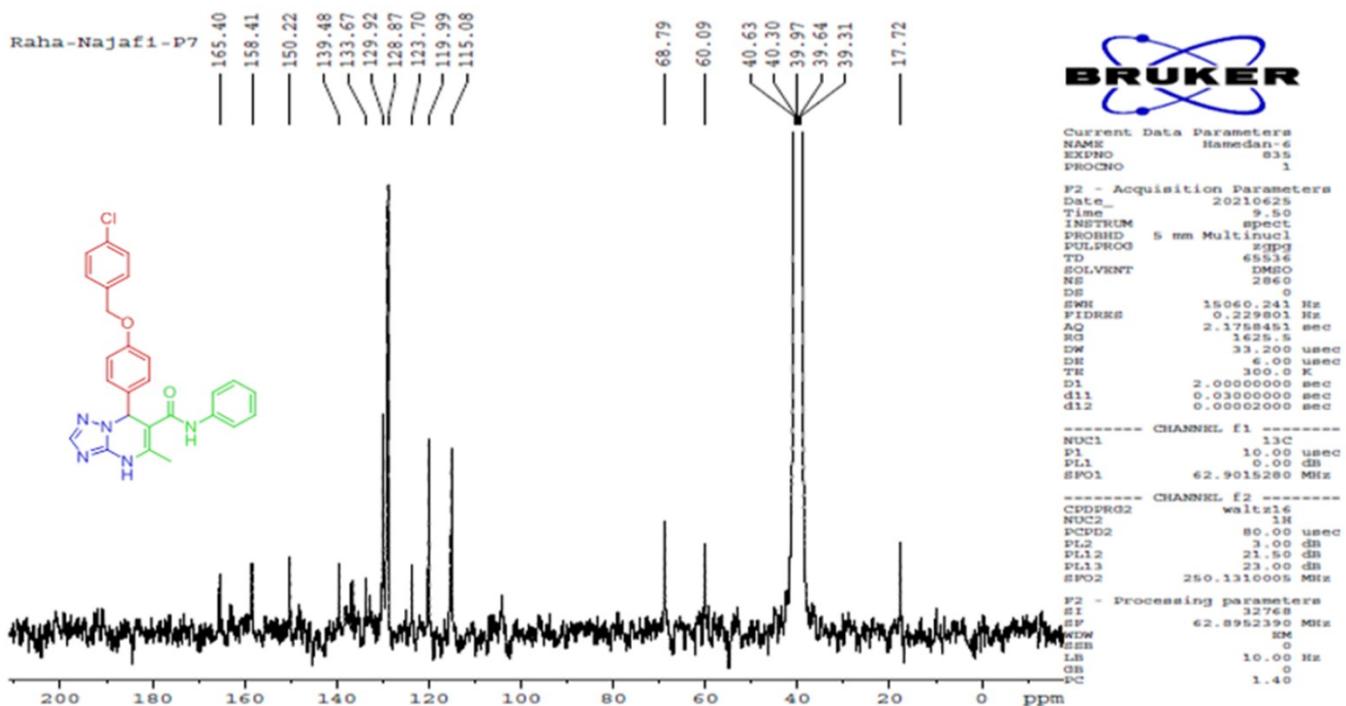


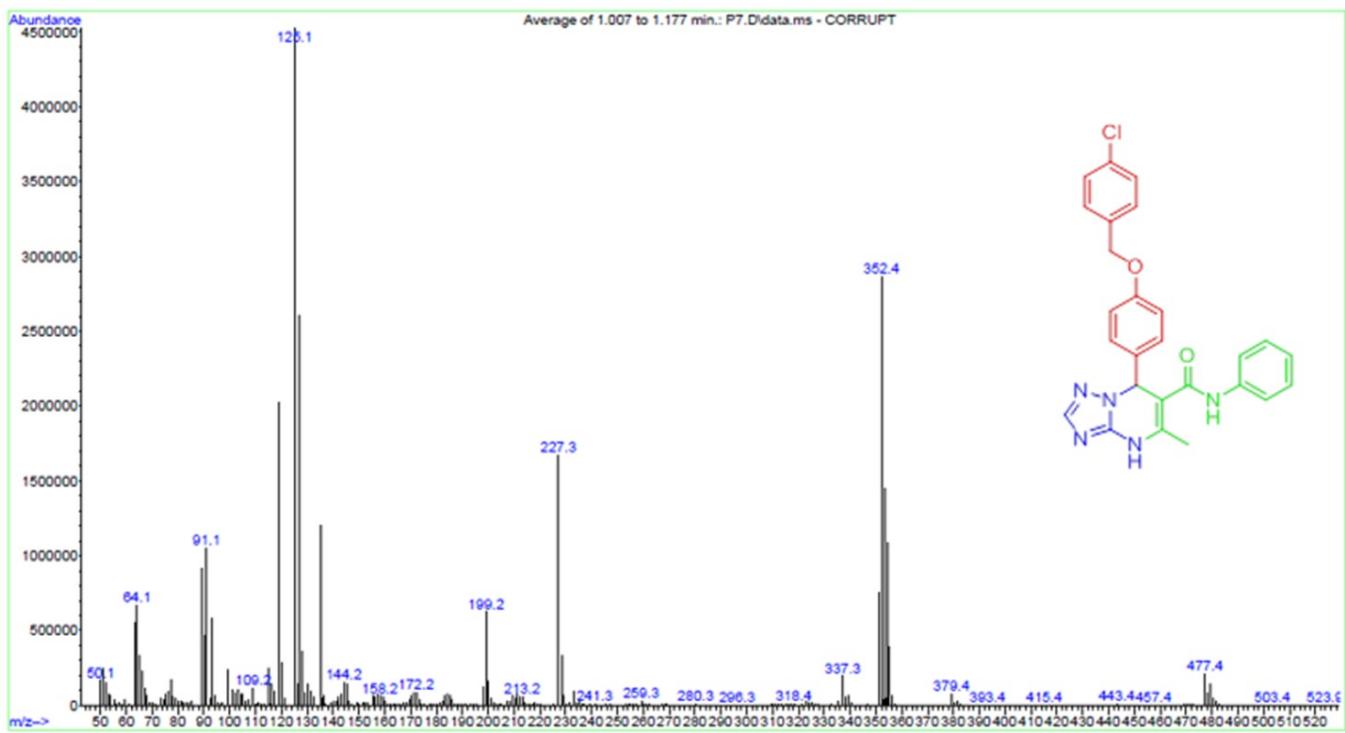


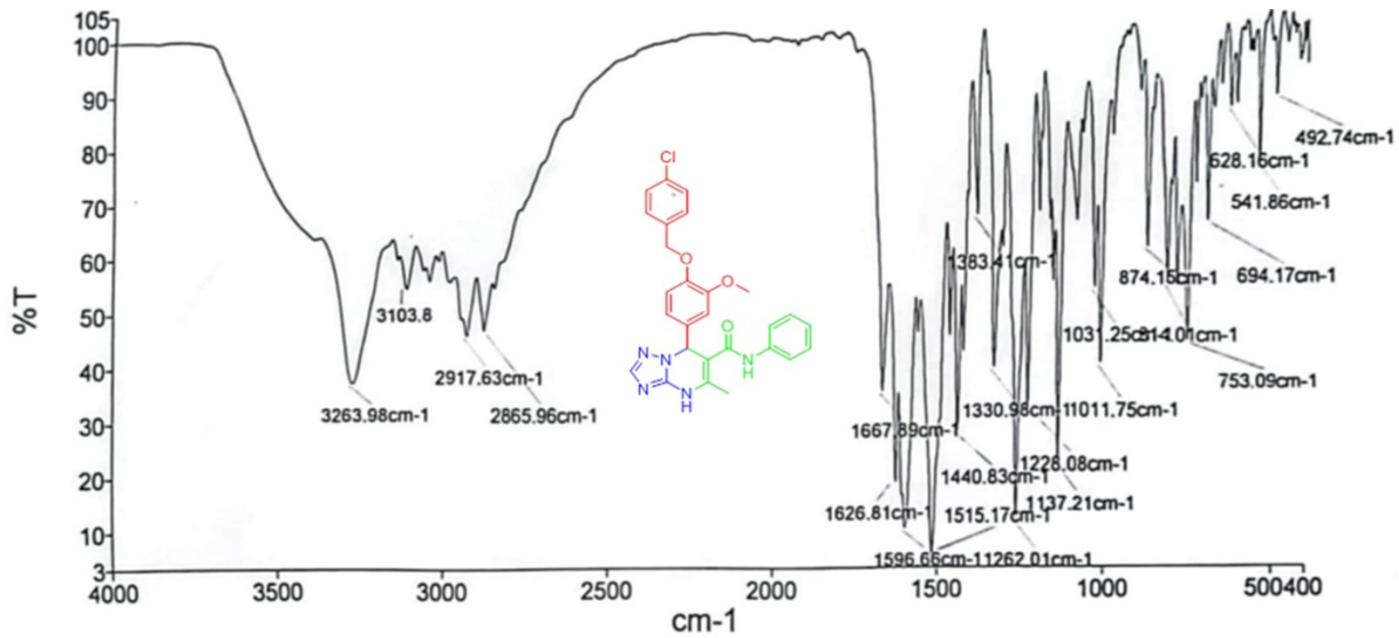












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