**Supplementary Materials**

**Novel Sono-synthesized Triazole Derivatives Conjugated with Selenium Nanoparticles for Cancer Treatment**

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**S1. Conventional method for the synthesis of compound 5**

A mixture of compound **4a** (2.87 g, 0.01 mol) and formamide (0.45g, 0.01mol) was heated under reflux for 6 h. The reaction mixture was allowed to cool to room temperature and poured onto water (100 mL). The solid formed was collected by filtration, dried, and crystallized from ethanol. Yield 67%; mp 260-262 °C.

**S2. Ultrasonic radiation method for the synthesis of compound 5**

A mixture of compound **4a** (2.87 g, 0.01 mol) and formamide (0.45g, 0.01 mol) in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 3 hr. at 25 oC. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization. Yield 73%. mp 260-262 °C.

**Ethyl 7-amino-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate 4a**

Yellow powder,IR (KBr, ν, cm-1); 3420 (NH2), 1714 (C=O), 1H-NMR (DMSO-*d6*, δ ppm): 1.27-1.30 (t, 3H, *J* = 5.3 Hz, -CH2CH3), 2.51 (s, 3H, *-*CH3), 3.35 (br s, 2H, -NH2, D2O exchangeable), 4.24-4.30 (q, 2H, *J* = 5.3 Hz, -CH2CH3), 6.55-6.56 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.45-7.46 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 8.01 (s, 1H, *-*CH, triazole ring); MS (*m/z*, %) (287.30, 31.23%); *Anal*; Calcd; for, C13H13N5O3 (287.28): C, 54.35; H, 4.56; N, 24.38; Found: C, 54.25; H, 4.40; N, 24.60%.

**7-amino-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4b**

Brown crystals, IR (KBr, ν, cm-1); 3418 (NH2), 1645 (C=O), 1064 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.31 (s, 3H,CH3), 4.60 (br s, 2H, NH2, D2O exchangeable), 5.52 (br s, 2H, NH2, D2O exchangeable), 6.45-6.47(d, 1H, *J*=2.5Hz, CH, furan ring), 7.32-7.34(d, 1H, *J*=2.5Hz, CH, furan ring), 8.07 (s, 1H,CH, triazole ring); MS (*m/z*, %) (258, 41%); *Anal.* Calcd. For C11H10N6O2 (258.24): C, 51.16; H, 3.90; N, 32.54; Found: C, 51.10; H, 3.80; N, 32.69%.

**7-amino-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidine-6-carbonitrile 4c**

Brown crystals, IR (KBr, ν, cm-1); 3428 (NH2), 2218 (C=N), 1060 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.47 (s, 3H,CH3), 5.02 (br s, 2H, NH2, D2O exchangeable), 6.50-6.52 (d, 1H, *J* = 2.5Hz, CH, furan ring), 7.45-7.49(d, 1H, *J* = 2.5Hz, CH, furan ring), 8.03 (s, 1H,CH); MS (*m/z*, %) (240, 15%); *Anal*. Calcd; for C11H8N6O (240.23): C, 55.00; H, 3.36; N, 34.98; O, 6.66; Found: C, 55.15; H, 3.26; N, 34.91%.

**5-(5-methylfuran-2-yl)pyrimido[5,4-e][1,2,4]triazolo[1,5-*a*]pyrimidin-6(7*H*)-one 5**

Brown crystals; IR (KBr, ν, cm-1); 3428 (NH), 1659 (C=O), 1059 (C=C); 1H-NMR (DMSO-*d6*, δ ppm), 2.50 (s, 3H, -CH3), 6.46-6.49 (d, 1H, *J* = 2.5 Hz, -CH, furan ring), 7.40-7.41 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 8.07 (s, 1H, *-*CH, triazole ring), 9.01 (s, 1H, *-*CH), 10.76 (br s, 1H, -NH exchangeable with D2O);MS (*m/z*, %) (268, 51%); *Anal*; Calcd; for, C12H8N6O2 (268.24): C, 53.73; H, 3.01; N, 31.33; Found: C, 53.75; H, 3.00; N, 31.30%.

**S3. Conventional method for the synthesis of compound 6**

A mixture of compound **4a** (2.87 g, 0.01 mol) and acetic anhydride (10 mL) was heated under reflux for 4 h. The reaction mixture was allowed to cool to room temperature and poured onto water (100 mL). The solid formed was collected by filtration, dried, and crystallized from ethanol. Yield 60 %; mp 120-122 °C.

**S4. Ultrasonic radiation method for the synthesis of compound 6**

A mixture of compound **4a** (2.87 g, 0.01 mol) and acetic anhydride (10 mL) in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 3 hrs. at room temperature. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization. Yield 63 %; mp 120-122 °C.

**Ethyl7-acetamido-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate6**

Brown crystals; IR (KBr, ν, cm-1); 3436 (NH), 1711, 1659 (C=O), 1054 (C=C); 1H-NMR (DMSO-*d6*, δ ppm), 1.20-1.28 (t, 3H, *J*=5.4Hz, CH3), 2.47 (s, 3H, OCH3), 2.55 (s, 3H,CH3), 4.22-4.28 (q, 2H, *J* = 5.4Hz, CH2), 6.50-6.55 (d, 1H, *J* = 2.5 Hz, -CH, furan ring), 7.43-7.45 (d, 1H, *J* = 2.5 Hz, -CH, furan ring), 7.99 (s, 1H,CH), 10.75 (br s, 1H, NH, D2O exchangeable); 13C-NMR (DMSO-*d6*, δ ppm), 21.46, 22.62, 23.88, 62.40, 95.04, 112.03, 116.05, 138.96, 144.79, 147.51, 157.84, 161.21, 163.05, 168.01, 172.49; MS (*m/z*, %) (329, 21%); *Anal*. Calcd.for C15H15N5O4 (329.32), C, 54.71; H, 4.59; N, 21.27; Found: C, 54.60; H, 4.66; N, 21.19%.

**S5. Conventional method for the synthesis of compounds 7a-d**

Equimolar amounts of compound **6** (3.29, 0.01 mol) and the appropriate amine [hydrazine hydrate, m-Anisidine, 2-Chloroaniline,2-Bromoaniline] (10 mmol) in ethanol (20 mL) was reflux for (6 h). The precipitate formed was filtered off, washed with cold ethanol, dried and recrystallized from ethanol.**7a,** yield 60 %; mp 220-222 °C.**7b,** yield68 %; mp 200-202 °C; **7c,** yield72 %; mp 211-213 oC,**7d,** yield 68 %; mp 215-217 °C.

**S6. Ultrasonic radiation method for the synthesis of 7a-d**

Equimolar amounts of compound **6** (3.29, 0.01 mol) and the appropriate amine [hydrazine hydrate, m-Anisidine,2-Chloroaniline and 2-Bromoanilin, respectively] in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 2 hrs; at room temperature. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization. **7a,** yield 63 %; mp 220-222 °C.**7b,** yield 70 %; mp 200-202 °C, **7c**, yield74 %; mp 211-213 °C, **7d,** yield 70 %; mp 215-217 °C.

**7-amino-8-methyl-5-(5-methylfuran-2-yl)pyrimido[5,4-*e*][1,2,4]triazolo[1,5-*a*]pyrimidin-6 (7*H*)-one 7a.**

Brown crystals, IR (KBr, ν, cm-1); 3430 (NH2), 1669 (C=O), 1054 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 1.21 (s, 3H, *-*CH3), 2.33 (s, 3H, -CH3), 3.63 (br s, 2H, -NH2 exchangeable with D2O), 6.31-6.37 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.38-7.43 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 8.35 (s, 1H, *-*CH, triazole ring); MS (*m/z*, %) (297, 58); 13C-NMR (DMSO-*d6*, δ ppm), 21.17, 21.73, 111.53, 116.89, 136.91, 139.78, 142.89, 143.20, 152.96, 153.57, 155.03, 155.72, 168.29; *Anal*; Calcd; for, C13H11N7O2 (297, 28%): C, 52.52; H, 3.73; N, 32.98; Found: C, 52.40; H, 3.90; N, 32.90%.

**7-(3-methoxyphenyl)-8-methyl-5-(5-methylfuran-2-yl)pyrimido[5,4-*e*][1,2,4]triazolo[1,5-*a*]pyrimidin-6(7*H*)-one 7b**

Brown crystals, IR (KBr, ν, cm-1);1709 (C=O), 1066 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.34 (s, 3H, *-*CH3), 2.37 (s, 3H, -CH3), 3.58 (s, 3H, *-*OCH3), 6.50-6.53 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.55-7.58 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.92-8.03 (m, 4H, aromatic protons), 8.07 (s, 1H, *-*CH, triazole ring); MS (*m/z*, %) (388, 46%); *Anal*; Calcd; for, C20H16N6O3 (388.39): C, 61.85; H, 4.15; N, 21.64; Found: C, 61.70; H, 4.02; N, 21.88%.

**7-(2-chlorophenyl)-8-methyl-5-(5-methylfuran-2-yl)pyrimido[5,4-*e*][1,2,4]triazolo[1,5-*a*]pyrimidin-6(7*H*)-one 7c**

Brown crystals, IR (KBr, ν, cm-1) 1669 (C=O), 1066 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.33 (s, 3H, CH3), 2.40 (s, 3H, -CH3), 6.47-6.50 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.49-7.53(d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.59-7.89 (m, 4H, aromatic protons), 8.02 (s, 1H, CH, triazole ring);MS (*m/z*, %) (392, 58%); *Anal*; Calcd; for, C19H13ClN6O2 (392.80): C, 58.10; H, 3.34; Cl, 9.02; N, 21.40; Found: C, 58.22; H, 3.28; Cl, 9.21; N, 21.30%.

**7-(2-bromophenyl)-8-methyl-5-(5-methylfuran-2-yl)pyrimido[5,4-*e*][1,2,4]triazolo[1,5-*a*]pyrimidin-6(7*H*)-one 7d**

Brown crystals, IR (KBr, ν, cm-1)1675 (C=O), 1062 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.40 (s, 3H, *-*CH3), 2.38(s, 3H, *-*CH3), 6.69-7.00 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.40-7.42(d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.60-7.90 (m, 4H, aromatic protons), 8.12 (s, 1H, *-*CH, triazole ring); MS (*m/z*, %) (437, 62%); *Anal*; Calcd; for, C19H13BrN6O2 (437.26): C, 52.19; H, 3.00; Br, 18.27; N, 19.22;; Found: C, 52.20; H, 3.15; Br, 18.00; N, 19.17%.

**S7. Conventional method for the synthesis of compound 8**

A mixture of compound **4a** (2.87 g, 0.01 mol) and formic acid (10mL) was heated under reflux for 5 h. The excess of formic acid was removed under reduced pressure. The resulting residue was crystallized from ethanol. Yield 65 %; mp 162-164oC.

**S8. Ultrasonic radiation method for the synthesis of compound 8**

A mixture of compound Yield 69 %; mp 162-164 °C **4a** (2.87g, 0.01 mol) and formic acid (0.46g, 0.01 mol) in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 3 hrs. at room temperature. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization.

**Ethyl 7-formamido-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate 8**

Brown crystals, IR (KBr, ν, cm-1);3443 (NH), 1710, 1659, (C=O), 1060 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 1.20-1.23 (t, 3H, *J* = 5.4Hz, -CH2CH3), 2.41 (s, 3H, -CH3), 4.26-4.28 (q, 2H, *J* = 5.4Hz, CH2CH3), 6.42-6.45 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.43-7.44 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 8.01 (s, 1H, *-*CH, triazole ring), 8.11 (s, 1H, *-*CH), 10.73 (br s, 1H, -NH exchangeable with D2O); MS (*m/z*, %) (315, 67%); *Anal*; Calcd; for, C14H13N5O4 (315.29): C, 53.33; H, 4.16; N, 22.21; Found: C, 53.23; H, 4.36; N, 22.08%.

**S9. Conventional method for the synthesis of compounds (9, 11)**

A mixture of **8** (3.15g, 0.01 mol) or **10** (3.29g, 0.01mol) and hydrazine hydrate (10 mL) in ethanol (30 mL) was heated under reflux for 4 h. The reaction mixture was allowed to cool to room temperature and poured into water (100 mL). The solid formed was collected by filtration, dried and crystallized from ethanol. **9,** yield 68 %; mp170-172 °C and 11 yield 64 %; mp 205-207 °C.

**S10. Ultrasonic radiation method for the synthesis of compounds (9, 11)**

A mixture of compound **8** (3.15g,0.01 mol) or **10** (3.29g, 0.01mol) and hydrazine hydrate (10 mL) in ethanol (30 mL) in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 3 hrs; at room temperature. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization.

**N-(6-(hydrazinecarbonyl)-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-yl)formamide 9**

Brown crystals, Yield 71 %; mp 170-172 °C, IR (KBr, ν, cm-1); 3419 (NH2), 1640 (C=O), 1051 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.37 (s, 3H, *-*CH3), 3.59 (br s, 2H, NH2, D2O exchangeable), 6.31-6.34 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.40-7.45 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 8.00 (s, 1H, *-*CH), 8.35 (s, 1H, *-*CH, triazole ring), 9.50 (br s, 1H, -NH, D2O exchangeable), 10.51 (br s, 1H, -NH, D2O exchangeable),MS (*m/z*, %) (301, 70%); *Anal*; Calcd; for, C12H11N7O3 (301.27): C, 47.84; H, 3.68; N, 32.55; Found: C, 47.82; H, 3.66; N, 32.60%.

**S11. Conventional method for the synthesis of compound 10**

A mixture of compound **4a** (2.87 g, 0.01 mol) and trimethylorthoformate (10 mL) was heated under reflux with stirring for 4 h. The reaction mixture was filtered off and the filtrate was left to cool to room temperature. The solid formed was filtered off, dried and crystallized from ethanol. Yield 67 %; mp 172-174 °C.

**S12. Ultrasonic radiation method for the synthesis of compound 10**

A mixture of compound **4a** (2.87 g, 0.01 mol) and trimethylorthoformate (10 mL) in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 4hrs. at room temperature. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization.

**Ethyl -7-((methoxymethylene)amino)-5-(5-methylfuran-2-yl)-[1,2,4]triazolo[1,5-*a*]pyramid-ine-6-carboxylate 10**

Light brown crystals, Yield 70 %; mp 172-174 °C, IR (KBr, ν, cm-1); 1673 (C=O), 1058 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 1.26-1.29 (t, 3H, *J*=5.4Hz, -CH2CH3), 2.42 (s, 3H, -CH3), 3.83 (s, 3H, *-*OCH3), 4.25-4.27 (q, 2H, *J* = 5.4Hz, -CH2CH3), 6.36-6.37 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.45-7.46 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 8.10 (s, 1H, *-*CH, triazole ring), 8.41 (s, 1H, *-*N=CH); MS (*m/z*, %) (329, 72%); *Anal*; Calcd; for, C15H15N5O4 (329.32): C, 54.71; H, 4.59; N, 21.27; Found: C, 54.90; H, 4.33; N, 21.25%.

**7-amino-5-(5-methylfuran-2-yl)pyrimido[5,4-*e*][1,2,4]triazolo[1,5-*a*]pyrimidin-6(7*H*)-one (11).**

Brown crystals, Yield 69 %; mp 205-207 oC, IR (KBr, υ, cm-1);3423 (NH2), 1676 (C=O), 1067 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.39 (s, 3H,CH3), 3.58 (br s, 2H, NH2 D2O exchangeable), 6.37-6.40 (d, 1H, *J* = 2.4Hz, CH), 7.40-7.46 (d, 1H, *J* = 2.7Hz, CH), 8.00 (s, 1H,CH), 8.19 (s, 1H,CH);MS (*m/z*, %) (282, 80); 13C-NMR (DMSO-*d6*, δ ppm), 22.82, 111.53, 115.81, 135.70, 138.93, 141.33, 144.10, 154. 69, 155.07, 155.53, 156.11, 167.98; *Anal*; *Anal*. Calcd. for C12H9N7O2 (283.25): C, 50.88; H, 3.20; N, 34.62; Found: C, 50.85; H, 3.25; N, 34.61%.

**S13. Conventional method for the synthesis of compounds 12a,b,c,d &13a,b**

An equimolar mixture of compound **7a** and**11** (10 mmol) and respective monosaccharides or 2,3,4-trimethoxybenzaldehyde (10 mmol) was dissolved in ethanol (10 ml) and a catalytic amounts of acetic acid and refluxed for eight hours. The reaction mixture was allowed to cool to room temperature. The precipitate so-formed was filtered-off, washed with cold ethanol (1 ml) and recrystallized from ethanol. **12a,** yield 68 %; mp 180-182 °C**, 12b**, yield 66 %; mp 185-187 °C; **12c,** yield 64 %; mp 165-167 °C. **12d**, yield 62 %; mp 168-170 °C, **13a,** yield 70 %; mp 210-211 °C, **13b**, yield 74 %; mp 201-203 °C.

**S14. Ultrasonic radiation method for the synthesis of compounds 12a,b,c,d & 13a,b**

An equimolar mixture of compound **7a** and **11**(10 mmol) and respective monosaccharides or 2,3,4-trimethoxybenzaldehyde (10 mmol) was dissolved in ethanol (10 ml) and 2-3 drops of lemon juice in conical flask The mixture was introduced under ultrasonic waves using an ultrasonic bath (operating at 230 V generating 33 KHz output frequencies) for 8hrs. at room temperature. The product started to separate out during the course of reaction. The crystalline solid was filtered and found pure on TLC with no need of further recrystallization. **12a,** yield 71 %; mp 180-182 °C**; 12b**, yield 70 %; mp 185-187 °C; **12c,** yield 68 %; mp 165-167 °C. **12d**, yield 65 %; mp 168-170 °C, **13a,** yield 74 %; mp 210-211 °C, **13b**, yield 77 %; mp 201-203 °C.

**7-((Glucosylidene))amino)-8-methyl-5-(5-methylfuran-2-yl)pyrimido[5,4-e][1,2,4]triazolo-[1,5-a]pyrimidin-6(7H)-one 12a**

Pale brown solid, IR (KBr, υ, cm-1); 3455 (OH), 1675 (C=O), 1060 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 1.88 (s, 3H, CH3), 2.47 (s, 3H, CH3), 3.42-3.49 (m, 2H, H-6`, H-6``), 3.66-3.70 (m, 1H, H-5`), 3.76-3.92 (m, 2H, H-3`, H-4`), 4.38-4.42 (m, 1H, H-2`), 4.76-4.77 (m, 1H, OH), 4.83-4.88 (m, 1H, OH), 4.92-4.99 (m, 1H, OH), 5.01-5.31 (m, 1H, OH), 5.32-5.36 (m, 1H, OH), 6.41-6.47 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 6.81-6.89(d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.33-7.34 (d, 1H, *J* = 5.4Hz, H-1'), 8.11 (s, 1H, -CH, triazole ring); 13C-NMR (DMSO-*d6*, δ ppm): 21.13, 21.53, 61.64, 70.97, 72.46, 75.30, 77.27, 111.53, 116.89, 136.91, 139.78, 148.89, 152.20, 153.969, 156.57, 160.03, 163.72, 168.29, 172.68; *Anal*. Calcd; for C19H21N7O7 (459.42): C, 49.67; H, 4.61; N, 21.34; Found: C, 49.80; H, 4.55; N, 21.49 %.

**7-((Xylosylidene)amino))-8-methyl-5-(5-methylfuran-2-yl)pyrimido[5,4-*e*][1,2,**4**]triazolo-[1,5-a]pyrimidin-6(7*H*)-one 12b:**

Pale brown solid, IR (KBr, υ, cm-1); 3440 (OH), 1671 (C=O), 1067(C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.91(s, 3H, CH3), 2.45 (s, 3H, CH3), 3.65-3.73 (m, 2H, H-5`, H-5``), 3.75-3.90 (m, 2H, H-3`, H-4`), 4.35-4.40 (m, 1H, H-2`), 4.80-4.85 (m, 1H, -OH), 4.88-4.90 (m, 1H, -OH), 4.93-4.99 (m, 1H, OH), 5.32-5.40 (m, 1H,-OH), 6.39-6.40 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.42-7.43 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.31-7.34 (d, 1H, *J* = 5.4Hz, H-1'), 8.04 (s, 1H,-CH,triazole ring); *Anal*. Calcd. for C18H19N7O6 (429.39): C, 50.35; H, 4.46; N, 22.83; Found: C, 50.48; H, 4.68; N, 22.60%.

**7-((Glucosylidene))amino)-5-(5-methylfuran-2-yl)pyrimido[5,4-e][1,2,4]triazolo[1,5-a]pyrimidin-6(7H)-one 12c**

Pale brown solid, IR (KBr, ν, cm-1);3440(OH), 1670(C=O), 1061 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.48 (s, 3H,CH3), 3.49-3.57 (m, 2H, H-6`, H-6``), 3.62-3.70 (m, 1H, H-5`), 4.22-4.27 (m, 2H, H-3`, H-4`), 4.33-4.54 (m, 1H, H-2`), 4.47 (m, 1H, OH), 4.70 (m, 1H, -OH), 4.85 (m, 1H, -OH), 5.00 (m, 1H, -OH), 5.32 (m, 1H, -OH), 6.28-6.31, (d, 1H, *J* = 2.5Hz, -CH, furan ring), 6.95-7.00 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.23-7.24 (d, 1H, *J* = 5.4Hz, H-1'), 8.00 (s, 1H, *-*CH, triazole ring), 8.37 (s, 1H, *-*CH); 13C-NMR (DMSO-*d6*, δ ppm): 21.49, 61.63, 70.76, 72.67, 75.30, 77.28, 109.52, 119.28, 122.97, 148.07, 149.79, 154.39, 156.35, 158.90 , 161.99, 165.68, 167.65, 172.46*; Anal*; Calcd; for, C18H19N7O7 (445.39): C, 48.54; H, 4.30; N, 22.01; Found: C, 48.65; H, 4.21; N, 22.20%.

**7-((Xylosylidene)amino))-5-(5-methylfuran-2-yl)pyrimido[5,4-e][1,2,4]triazolo[1,5-a]pyrimidin-6(7H)-one 12d**

Pale brown solid, IR (KBr, ν, cm-1)3448 (OH), 1676 (C=O), 1066 (C=C); 1H-NMR (DMSO-*d6*, δ ppm): 2.45 (s, 3H,CH3), 3.84-3.86 (m, 2H, H-5`, H-5``), 4.22-4.25 (m, 2H, H-3`, H-4`), 4.32-4.35 (m, 1H, H-2`), 4.70-4.73 (m, 1H, -OH), 4.85-4.87 (m, 1H, -OH), 5.00-5.04 (m, 1H, -OH), 5.32-5.34 (m, 1H, -OH), 6.53-6.54, (d, 1H, *J*=2.5Hz, -CH, furan ring), 7.02-7.07 (d, 1H, *J*=2.5Hz, -CH, furan ring), 7.40-7.41 (d, 1H, *J*=5.4Hz, H-1'), 8.04 (s, 1H, *-*CH, triazole ring), 8.35 (s, 1H, *-*CH); *Anal*; Calcd; for, C17H17N7O6 (415.37): C, 49.16; H, 4.13; N, 23.61; Found: C, 49.27; H, 4.01; N, 23.70%.

**5-(5-methylfuran-2-yl)-7-((2,3,4-trimethoxybenzylidene)amino)pyrimido[5,4-e][1,2,4]triazolo[1,5-a]pyrimidin-6(7H)-one 13a**

Pale yellow crystals, IR (KBr, ν, cm-1) 1669 (C=O), 1054 (C=C); 1H-NMR (DMSO-*d6*, δ ppm):2.35 (s, 3H, CH3),3.36 (s, 3H, -OCH3), 3.38 (s, 3H, -OCH3), 3.40 (s, 3H, -OCH3), 6.44-6.46, (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.20-7.24 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.64-7.67 (d, 1H, *J* = 6.7Hz , aromatic proton), 8.13-8.24(d, 1H, *J* = 6.7Hz, aromatic proton), 7.99 (s, 1H, *-*CH), 8.29 (s, 1H, *-*CH), 9.14 (s, 1H, -CH=N); MS (*m/z*, %) (461, 72%); *Anal*; Calcd; for, C22H19N7O5 (461.44): C, 57.26; H, 4.15; N, 21.25; Found: C, 57.16; H, 4.00; N, 21.48;%.

**8-Methyl-5-(5-methylfuran-2-yl)-7-((2,3,4-trimethoxybenzylidene)amino)-pyrimido[5,4-e][1,2,4]triazolo[1,5-a]pyrimidin-6-one 13b**

Pale yellow crystals, IR (KBr, ν, cm-1); 1701(C=O), 1064 (C=C); 1H-NMR (DMSO-*d6*, δ ppm), 2.36 (s, 3H,CH3), 2.38 (s, 3H, CH3), 3.39 (s, 3H, -OCH3), 3.41 (s, 3H, -OCH3), 3.44 (s, 3H, -OCH3), 6.58-6.59 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.57-7.58 (d, 1H, *J* = 2.5Hz, -CH, furan ring), 7.73-7.78(d, 1H,  *J* = 6.7Hz , aromatic proton), 8.12-8.15(d, 1H, *J*=6.7Hz,,aromatic proton), 8.08 (s, 1H, CH), 9.02 (s, 1H, -CH=N); MS (*m/z*, %) (475, 68%); *Anal*. Calcd. for C23H21N7O5 (475.47): C, 58.10; H, 4.45; N, 20.62; Found: C, 58.22; H, 4.30; N, 20.88%.