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Synthesis of diversely substituted 5-methylpyrazolo[1,5-*a*]pyrimidines assisted by ultrasound in aqueous media: Molecular docking for potential antiviral, anticancer activities

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5-Methylpyrazolo[1,5-*a*]pyrimidine derivatives have been synthesized with starting materials that are either commercially or easily available. This is achieved by the ultrasonication of 3-amino-1*H*-pyrazoles (**3-7**) and enaminones (**2**) assisted by $KHSO_4$ in aqueous medium. The structures are established by spectral and analytical techniques. An X-ray crystallographic study of compound *N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)-7-(4-methoxyphenyl)-5-methylpyrazolo[1,5-a]pyrimidine-3-carboxamide (**8b**) confirms the structural orientation and eliminates any ambiguity pertaining to its regioselectivity. Its space group is P21/n with the following unit cell parameters: a = 17.5775 (8), b = 7.1707 (4), c = 18.113 (1) Å, β = 91.449 (2) and Z = 4. Crystal structure is solved to a final R value of 0.062 and to a GOOF value of 1.09. Molecular docking of the compounds has been executed to identify the potential antiviral and anticancer agents. Moreover, molecular dynamics simulation study of the ligand **9c** in a complex with 3pp0, reveals the stability of the potential ligand candidate **9c**.

Keywords: Pyrazolo[1,5-*a*]pyrimidines, X-ray crystallography, Molecular docking, Ultrasonication