Electronic Supplementary Material (ESI) for New Journal of Chemistry.

This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2021

Novel 1,3,5-triazine based pyrazole derivatives as potential antitumor agents and EFGR kinase inhibitors: Synthesis, cytotoxicity, DNA binding, molecular docking and DFT studies

M. S. Raghu,^a C. B. Pradeep Kumar,^b M. K. Prashanth,^c K. Yogesh Kumar,^d B. S. Prathibha,^c G. Kanthimathi,^e Siham Abdulrahman Alissa,^f Hanan Abdulrahman Alghulikah,^f Sameh M. Osman,^g

^aDepartment of Chemistry, New Horizon College of Engineering, Bengaluru 560 103, India

^bDepartment of Chemistry, Malnad College of Engineering, Hassan 573 202, India

^cDepartment of Chemistry, B N M Institute of Technology, Bengaluru 560 070, India

^dDepartment of Chemistry, School of Engineering and Technology, Jain University, Ramanagara, 562 112, India

^eDepartment of Chemistry, Ramco Institute of Technology, Rajapalayam, Tamilnadu, 626117, India

^fDepartment of Chemistry, College of Science, Princess Nourabbint Abdulrahman University. Riyadh 11671, Saudi Arabia

^gDepartment of Chemistry, College of Science, King Saud University, Riyadh, 11451, Saudi Arabia

Supporting information

^{*}Corresponding author e-mail address: *prashanthmk87@gmail.com*

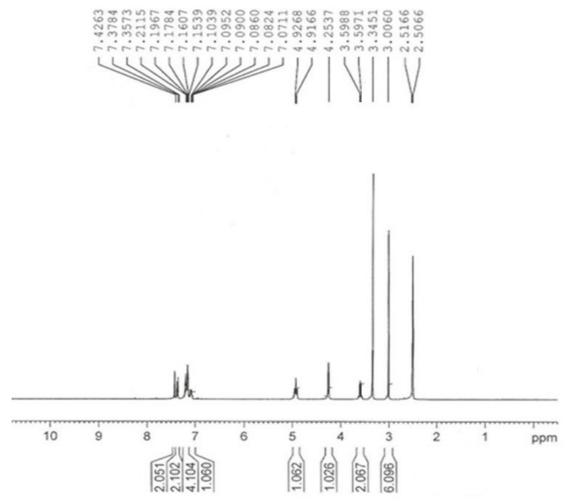
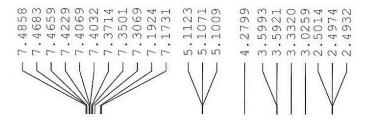


Figure S1: ¹H NMR spectrum 6-chloro-N²,N²-dimethyl-N⁴-(1-phenyl-5-(4-(trifluoro methyl)phenyl)-4,5-dihydro-1H -pyrazol-3-yl)-1,3,5-triazine-2,4-diamine (5a).



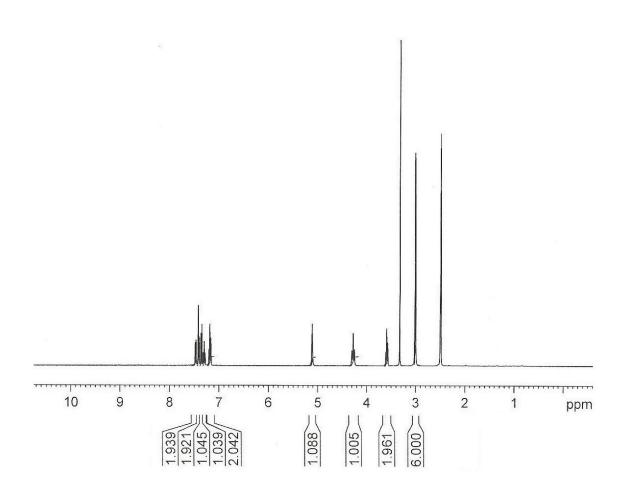


Figure S2: 1 H NMR spectrum of N^{2} -(1,5-bis(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-6-chloro- N^{4} , N^{4} -dimethyl-1,3,5-triazine-2,4-diamine (5h).

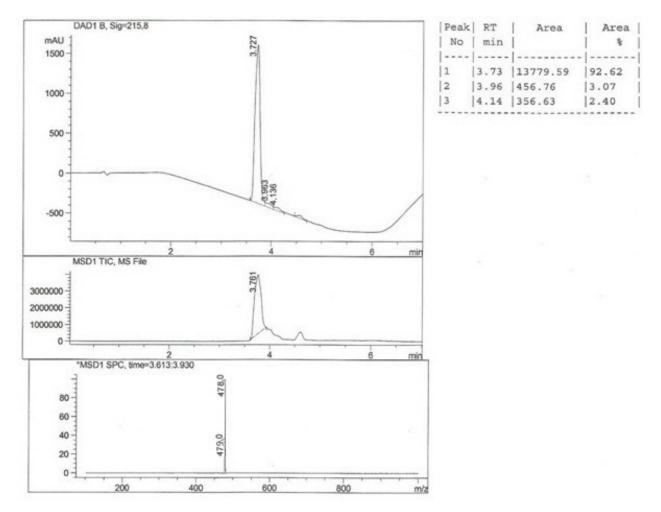


Figure S3: Mass spectrum of 4-(3-((4-chloro-6-(dimethylamino)-1,3,5-triazin-2-yl)amino)-5-(4-(trifluoromethyl) phenyl)-4,5-dihydro-1H-pyrazol-1-yl)phenol (5b).

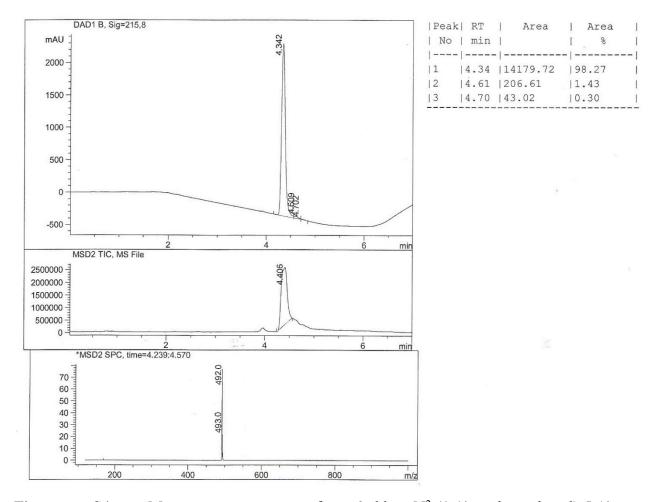


Figure S4: Mass spectrum of 6-chloro-N²-(1-(4-methoxyphenyl)-5-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-N⁴,N⁴-dimethyl-1,3,5-triazine-2,4-diamine (5d).

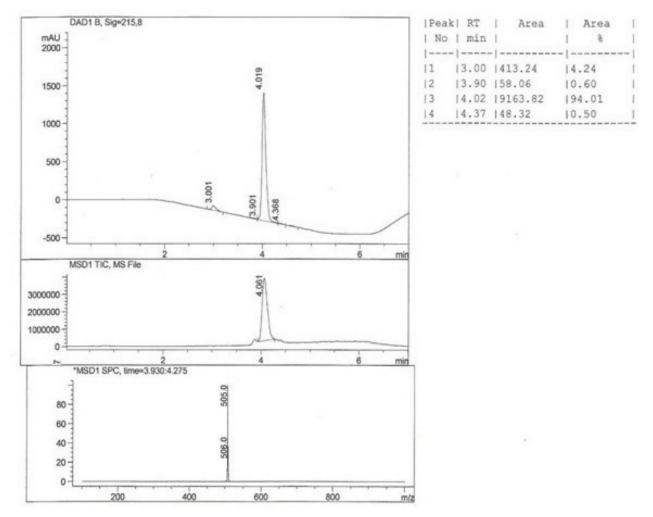


Figure S5: Mass spectrum of 6-chloro-N²-(1-(4-(dimethylamino)phenyl)-5-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-N⁴,N⁴-dimethyl-1,3,5-triazine-2,4-diamine (5i).