Publications Template

#	Research Title	Field	Abstract	Year of Publication Publishing	Publishing Link "URL"
1	New 3-cyano-2-substituted pyridines induce apoptosis in MCF 7 breast cancer cells, Ahmed Malki, Mona Mohsen, Hassan Aziz, Ola Rizk, **Omaima Shaaban**, Mohamed El-Sayed, Zaki A. Sherif and Hayam Ashour, ***Molecule***s, **21(2), 230,** (**2016**).	Medicinal chemistry	The synthesis of new 3-cyano-2-substituted pyridines bearing various pharmacophores and functionalities at position 2 is described. The synthesized compounds were evaluated for their in vitro anti-cancer activities on five cancer cell lines using 5-FU as reference compound. The results revealed that the benzohydrazide derivative 9a induced growth inhibition in human breast cancer cell line MCF-7 with an IC50 value of 2 M and it showed lower cytotoxicity on MCF-12a normal breast epithelial cells. Additionally, 9a induced apoptotic morphological changes and induced apoptosis in MCF-7 in a dose and time-dependent manner according to an enzyme linked immunosorbent apoptosis assay which is further confirmed by a TUNEL assay. Flow cytometric analysis indicated that 9a arrested MCF-7 cells in the G1 phase, which was further confirmed by increased expression of p21 and p27 and reduced expression of CDK2 and CDK4. Western blot data revealed significant upregulation of the expression of p53, Bax, caspase-3 and down-regulation of Bcl-2, Mdm-2 and Akt. Additionally, 9a increased the release of cytochrome c from mitochondria to cytoplasm which provokes the mitochondrial apoptotic pathway while it showed no significant change on the expression of the death receptor proteins procaspase-8, caspase-8 and FAS. Furthermore, 9a reduced the expression of phospho	**2016**	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6274259/

			AKT and -catenin in dose dependent manner while inhibiting the expression of migration-related genes such as matrix metalloproteinase (MMP)-9 and vascular endothelial growth factor (VEGF). Our findings suggest that compound 9a could be considered as a lead structure for further development of more potent apoptosis inducing agents with anti-metastatic activities.		
2	Synthesis of some oxadiazolyl, pyrazolyl and thiazolyl derivatives of thiophene-2-carboxamide as antimicrobial and anti-HCV agents, Ola H. Rizk, **Omaima G. Shaaban**, Abeer E. Abdel Wahab, ***The Open Med Chem j*, 11, 38-53 (2017).**	Medicinal chemistry	Three series of pyrazole, thiazole and 1,3,4-oxadiazole, derivatives were synthesized starting from 5-amino-4-(hydrazinocarbonyl)-3-methylthiophene-2-carboxamide (2). Methods All compounds were investigated for their preliminary antimicrobial activity. They were proved to exhibit remarkable antimicrobial activity against Pseudomonas aeruginosa with insignificant activity towards Gram positive bacterial strains and fungi. Results In-vitro testing of the new compounds on hepatitis-C virus (HCV) replication in hepatocellular carcinoma cell line HepG2 infected with the virus utilizing the reverse transcription polymerase chain reaction technique (RT-PCR) generally showed inhibition of the replication of HCV RNA (–) strands at low concentration, while, eight compounds; 3a, 6, 7a, 7b, 9a, 9b, 10a and 11b proved to inhibit the replication of HCV RNA (+) and (–) strands at very low concentration range 0.08-0.36 µg/mL. Conclusion Compounds 7b and 11b displayed the highest anti-HCV and antimicrobial activities in this study	2017	https://pubmed.ncbi.nlm.nih.gov/28553409/
3	Design, synthesis, antibacterial evaluation and molecular docking studies of some new quinoxaline derivatives targeting dihyropteroate synthase enzyme, Maryam AZ El-Attar, Rasha Y Elbayaa, **Omaima G Shaaban**, Nargues S Habib, Abeer E Abdel Wahab, Ibrahim A Abdelwahab, Soad AM El-Hawash, ***Bio org. chem*. 76, 437-448, (2018)**	Medicinal chemistry	Development of new antimicrobial agents is a good solution to overcome drug-resistance problems. From this perspective, new quinoxaline derivatives bearing various bioactive heterocyclic moieties (thiadiazoles, oxadiazoles, pyrazoles and thiazoles) were designed and synthesized. The newly synthesized compounds were evaluated for their in vitro antibacterial activity against nine bacterial human pathogenic strains using the disc diffusion assay. In general, most of the synthesized compounds exhibited good antibacterial activities. The thiazolyl 11c displayed significant antibacterial activities against P. aeruginosa (MIC, 12.5 µg/mL vs levofloxacin 12.5 µg/mL). Molecular docking studies indicated that the synthesized	2018	https://pubmed.ncbi.nlm.nih.gov/29275262/

			compounds could occupy both p-amino benzoic acid (PABA) and pterin binding pockets of the dihydropteroate synthase (DHPS), suggesting that the target compounds could act by the inhibition of bacterial DHPS enzyme. The results provide important information for the future design of more potent antibacterial agents.		
4	Purines and triazolo[4,3-e] purines containing pyrazole moiety as potential anticancer and antioxidant agents, **Omaima G Shaaban,** Heba A Abd El Razik, Shams El-Dine A Shams El-Dine, Fawzia A Ashour, Alaa A El-Tombary, Ola S Afifi & Marwa M Abu-Serie, ***Future Med. Chem.*** **10(12), 1449–1464 (2018)**	Medicinal chemistry	Targeting apoptosis regulators such as caspases aiming at inducing apoptosis is an attractive strategy in cancer therapy. **Materials & methods:** 8-substituted purine incorporating pyrazole moiety were designed, synthesized and evaluated for their anticancer and antioxidant activities. **Results:** Compounds **7a** and **8a** displayed potent and selective anticancer activity against lung cancer A549 cell line with low cytotoxicity on peripheral blood mononuclear normal cells. Compounds **7a** and **8a** induced caspase dependent apoptotic death and DNA damage in all cancer cell lines. In addition, compounds **2**, **5**, **6a**, **7a**, **8a**, **8c**, **11a, 11b** and **12b** showed good antioxidant activity higher than that of the standard ascorbic acid. **Conclusion:** Compounds **7a** and **8a** can be considered promising dual anticancer and antioxidant lead inducing caspase-dependent apoptotic death and DNA damage.	2018	https://pubmed.ncbi.nlm.nih.gov/29788781/
5	Synthesis of pyrazolo-1,2,4-triazolo[4,3-a]quinoxalines as antimicrobial agents with potential inhibition of DHPS enzyme. Maryam A.Z. El-Attar , Rasha Y. Elbayaa , **Omaima G. Shaaban** , Nargues S. Habib , Abeer E. Abdel Wahab , Ibrahim A. Abdelwahab , Soad A.M. El-Hawash. ***Future medicinal Chemistry***, **2018**. https://doi.org/10.4155/fmc-2018-0082	Medicinal chemistry	The development of a new class of antimicrobial agents is the optimal lifeline to scrap the escalating jeopardy of drug resistance. Experimental: This study aims to design and synthesize a series of pyrazolo-1,2,4-triazolo[4,3-a]quinoxalines, to develop agents having antimicrobial activity through potential inhibition of dihyropteroate synthase enzyme. The target compounds have been evaluated for their in-vitro antimicrobial activity. Results & discussion: Compounds 5b, 5c were equipotent (minimal inhibitory concentration= 12.5 µg/ml) to ampicillin. The docking patterns of 5b and 5c demonstrated that both fit into Bacillus Anthracis dihydropteroate synthase pterin and p-amino benzoic acid-binding pockets. Moreover, their physicochemical properties and pharmacokinetic profiles	2018	https://pubmed.ncbi.nlm.nih.gov/30088415/

			recommend that they can be considered drug-like candidates. The results highlight some significant information for the future design of lead compounds as antimicrobial agents.		
6	Synthesis and molecular docking study of Some 3,4-dihydrothieno[2,3-d] pyrimidine derivatives as potential antimicrobial agents. **Omaima G. Shaaban**, Doaa A. E. Issa , Alaa A. El-Tombary , Shrouk M. Abd El Wahab , Abeer E. Abdel Wahab, Ibrahim A. Abdelwahab. ***Bioorganic Chemistry***, 2019, doi.org/10.1016/j.bioorg.2019.102934	Medicinal chemistry	In continuation of our research program aiming at developing new potent antimicrobial agents, new series of substituted 3,4-dihydrothieno[2,3-d] pyrimidines was synthesized. The newly synthesized compounds were preliminary tested for their in vitro activity against six bacterial and three fungal strains using the agar diffusion technique. The results revealed that compounds 7, 8a, 10b, 10d and 11b exhibited half the potency of levofloxacine against the Gram-negative bacterium, Pseudomonas aeruginosa, while compounds 5a, 8b, 10c and 12 displayed half the potency of levofloxacine against Proteus Vulgaris. Whereas, compounds 7, 10b, 10d and 11b showed half the activity of ampicillin against the Gram-positive bacterium, B. subtilis. Most of the compounds showed high antifungal potency. Compounds 3, 6, 7, 9b, 10a, 11a, 11b, 15 and 16 exhibited double the potency of clotrimazole against A. fumigatus. While compounds 3, 4, 5a, 5b, 9b, 10a, 10b, 10c, 13, 15, 16 and 18 displayed double the activity of clotrimazole against R. oryazae. Molecular docking studies of the active compounds with the active site of the B. anthracis DHPS, showed good scoring for various interactions with the active site of the enzyme compared to the co-crystallized ligand.	2019	https://pubmed.ncbi.nlm.nih.gov/31026720/
7	Synthesis and biological evaluation of purine-pyrazole hybrids incorporating thiazole, thiazolidinone or rhodanine moiety as 15-LOX inhibitors endowed with anticancer and antioxidant potential. Ola S. Afifi, **Omaima G. Shaaban**, Heba A. Abd El Razik, Shams El-Dine A. Shams El-Dine, Fawzia A Ashour, Alaa A. El-Tombary, Marwa M. Abu-	Medicinal chemistry	Novel purine-pyrazole hybrids combining thiazoles, thiazolidinones and rhodanines, were designed and tested as 15-LOX inhibitors, potential anticancer and antioxidant agents. All tested compounds were found to be potent 15-LOX inhibitors with IC50 ranging from 1.76 to 6.12 μM. The prepared compounds were evaluated in vitro against five cancer cell lines: A549 (lung), Caco-2 (colon), PC3 (prostate), MCF-7 (breast) and HepG-2 (liver). Compounds 7b and 8b displayed broad spectrum anticancer activity against the five tested cell lines (IC50=18.5–95.39 μM). While, compound 7h demonstrated	2019	https://pubmed.ncbi.nlm.nih.gov/30999135/

	Serie. **Bioorganic Chemistry**, 87, 821-837, 2019.		moderate anticancer activity against lung A549 and colon Caco-2 cell lines. Antioxidant screening revealed that six compounds (5a, 5b, 6b, 7b, 7h and 8b) with IC50 ranging from 0.93 to 14.43 µg/ml were found to be more potent scavengers of 2,2-diphenyl-picryl hydrazyl (DPPH) than the reference ascorbic acid with IC50 value of 15.34 µg/ml. Compounds 7b, 7h and 8b, when evaluated for their antioxidant activity, where found to be potent DPPH scavengers. Moreover, compound 7b displayed twice the potency of ascorbic acid as NO scavenger. Docking study was performed to elucidate the possible binding mode of the most active compounds with the active site of 15-LOX enzyme. Collectively, the purine-pyrazole hybrids having thiazoline or thizolidinone moieties (7b, 7h and 8b) constitute a promising scaffold in designing more potent 15- LOX inhibitors with anticancer and antioxidant potential.		
8	Dual VEGFR-2 / PIM-1kinase inhibition towards surmounting the resistance to antiangiogenic agents via hybrid pyridine and thienopyridine-based scaffolds: Design, synthesis and biological evaluation. Ola H. Rizk, Mohamed Teleb, Marwa M. Abu-Serie, **Omaima G. Shaaban**. ***Bio organic chemistry***, **2019**, **doi: https://doi.org/10.1016/j.bioorg.2019.103189**	Medicinal chemistry	Angiogenesis is a hallmark in cancer. Most antiangiogenic agents block the action of vascular endothelial growth factor (VEGF). In clinic, patients develop hypoxia-mediated resistance consistent with vascular responses to these agents. Recent studies underlying such resistance revealed hypoxia inducible PIM-1 kinase upregulation which promotes cancer progression. PIM-1 kinase expression is thus viewed as a new resistance mechanism to antiangiogenic agents. Hence, combining PIM kinase inhibitors with anti-VEGF therapies provides synergistic antitumor response. Inspired by these facts, the current study aims at designing novel dual VEGFR-2/PIM-1 kinase inhibitors via molecular hybridization and repositioning of their pharmacophoric features. Moreover, enhancing the cytotoxic potential of the designed compounds was considered via incorporating moieties mimicking caspase 3/7 activators. Accordingly, series of novel pyridine and thieno[2,3-b]pyridine derivatives were synthesized and screened via MTT assay for cytotoxic activities against normal fibroblasts and four cancer cell lines (HepG-2, Caco-2, MCF-7 and PC-3). Compounds 3a, 9e, 10b and 10c exhibited anticancer activities at nanomolar	2019	https://pubmed.ncbi.nlm.nih.gov/31473473/

			IC50 with promising safety, activated caspase 3/7 and induced apoptosis as well as DNA fragmentation more than doxorubicin in the four cancer cell lines. Furthermore, they exerted promising dual VEGFR-2/ PIM-1 kinase inhibition and significantly exhibited higher therapeutic potential to alter the expression levels of VEGF, p53 and cyclin D than doxorubicin. Interestingly, the most active anticancer compound 10b conferred the highest dual VEGFR-2/PIM-1 kinase inhibition. Finally, their in silico ligand efficiency metrics were acceptable.		