البحث الأول

رقم البحث فى قائمة الأبحاث الكلية (22)

عنوان البحث باللغة الإنجليزية:

Title:

Novel 4-Heteroaryl-antipyrines: Synthesis, Molecular Docking, and Evaluation as Potential Anti-breast Cancer Agents

اسم المجلة المنشور بها البحث وسنة النشر

J. Heterocyclic Chem., 55, 2408 (2018).

Abstract:

Reaction of 1-[4-(1,2-dihydro-1,5-dimethyl-2-phenyl-3-oxo-3H-pyrazol-4-yl)-2-phenylsulfonyl-1- ethanone (1) with phenyl isothiocyanate afforded the 4-(3-mercapto-3-(phenylamino)-2-(phenylsulfonyl) acryloyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one (2). Treatment of compound 2 with hydrazonoyl chlorides 3a–h afforded the corresponding1,3,4-thiadiazole derivatives 5a–h. Cyclocondensation reaction of compound 2 with the appropriate α-halo-compounds 6, 8, 10, 12a,b or 14 (ethyl 2-chloroacetate, chloroacetonitrile, 1-chloropropan-2-one, 2-bromo-1-phenylethanone, 2-bromo-1-p-tolylethanone, and 2- bromoacetyl-3H-benzo [f]chromen-3-one) afforded the 1,3-thiazole derivatives 7, 9, 11, 13a,b, and 15, respectively. Coupling of the ketosulphone 1 with the appropriate diazotized 4H-1,2,4-triazol-3-amine 16 and 2-aminobenzimidazole 19 afforded triazolo[5,1-c][1, 2, 4]triazine 18 and benzo[4,5]imidazo[2,1-c][1, 2, 4]triazine 21, respectively. The structures of the synthesized compounds were confirmed on the basis of their elemental analysis and spectral data and evaluated as potential anti-breast cancer agents. Moreover, the computational studies

using MOE 2014.09 software are confirming the results in biological activity.

أسماء المشاركون:

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