

# Some 1,3,5-trisubstituted pyrazoline derivatives targeting breast cancer: Design, synthesis, cytotoxic activity, EGFR inhibition and molecular docking

*Dina Yousry , F. George , Manal Kandeel , Dina Y. El-Ansary , Ahmed M. El Kerdawy "*

## Abstract

Different 1,3,5-trisubstituted pyrazoline derivatives 2a-c, 3-c, 4a-f, 6a-c, 7a-f and 8a-d were prepared via condensation reaction of the appropriate chalcone 1a-c or 5a-c with various hydrazine derivatives. All compounds were screened for their cytotoxicity against breast MCF-7 cancer cell line and the normal fibroblasts WI38. Thirteen compounds 2a, 3a, 3c, 4a-d, 6c, 7d, 7e, 8b, 8d and 8f revealed promising cytotoxicity against MCF7 compared to the reference standard staurosporine and they were safe to the normal fibroblasts WI-38. In addition, compounds 3c, 6c, 7d, 8b and 8d elicited higher cytotoxicity than erlotinib and exhibited promising EGFR inhibitory activity at submicromolar level comparable to that of erlotinib except for compound 8b that may exert its cytotoxicity via another mechanism besides EGFR inhibition. Molecular docking of 3c, 6c, 7d, 8b and 8d in the active site of EGFR confirmed the obtained results.

*Bioorganic Chemistry 2020, March*