

البحث السادس (رقم 39 في قائمة البحوث الكلية)

Title	Design, Sonosynthesis, Quantum-Chemical Calculations, and Evaluation of New Mono- and Bis-pyridine Dicarbonitriles as Antiproliferative Agents
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A highly efficient, simple, and clean single-step sonosynthetic procedure has been sophisticated for assembling new series of mono- and bis-pyridine dicarbonitriles from ketones, HCl, and tetracyanoethylene. The presented protocol is applicable for the preparation of a broad range of uniquely substituted pyridine dicarbonitriles and seems to be superior in comparison with other previously reported methods. The antiproliferative impact of the newly synthesized derivatives was screened towards three representative cancer cell lines (MCF-7, A549, and HCT116). Most of the evaluated derivatives showed a moderate to excellent anti-proliferative activity towards the selected cell lines. Of these, compounds 4h, 4k, 10, 12a, and 12b showed both potent anticancer activity ($IC_{50} < 10 \mu M$) and lower cytotoxic effect ($IC_{50} > 58 \mu M$) on non-tumorigenic cells (MCF-10A and NCM460), suggesting their promising potential to be lead molecules for future antitumor drug discovery. The structure-activity relationships have been also discussed. Moreover, quantum chemical studies based on Density Functional Theory (DFT) of the synthesized compounds were investigated and found to be consistent with the in vitro inhibitory activities.