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Anti-HIV Screening and Molecular Docking Studies of Benzothiazolyl Thioureas

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SUMMARY. A new series of 1-(substituted benzothiazol-2-yl)-3-aroylthioureas (7a-k) were synthesized by treating variously substituted benzothiazolamines with in situ prepared isothiocyanates. The synthesized compounds were screened for their in vitro anti-HIV-1 and HIV-2 activity. The compounds 7e, 7f and 7i were found to exhibit potent anti-HIV-1 and HIV-2 activity.

RESUMEN. Se sintetizó una nueva serie de 1- (benzotiazol-2-il) -3-aroiltioureas sustituidas (7a-k) tratando varias benzotiazolaminas sustituidas con isotiocianatos preparados in situ. Los compuestos sintetizados se seleccionaron para su actividad in vitro anti-HIV-1 y HIV-2. Se encontró que los compuestos 7e, 7f y 7i presentaban potente actividad anti-HIV-1 y HIV-2.

KEY WORDS: 2-aminobenzo-thiazoles, anti-HIV activity, 1-substituted (benzothiazol-2-yl)-3-aroylthioureas.

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