

A virtual screening approach for identifying plants with anti H5N1 neuraminidase activity

ABSTRACT

Recent outbreaks of highly pathogenic and occasional drug-resistant influenza strains have highlighted the need to develop novel anti-influenza therapeutics. Here, we report computational and experimental efforts to identify influenza neuraminidase inhibitors from among the 3000 natural compounds in the Malaysian-Plants Natural-Product (NADI) database. These 3000 compounds were first docked into the neuraminidase active site. The five plants with the largest number of top predicted ligands were selected for experimental evaluation. Twelve specific compounds isolated from these five plants were shown to inhibit neuraminidase, including two compounds with IC₅₀ values less than 92 μ M. Furthermore, four of the 12 isolated compounds had also been identified in the top 100 compounds from the virtual screen. Together, these results suggest an effective new approach for identifying bioactive plant species that will further the identification of new pharmacologically active compounds from diverse natural-product resources.

Keyword: Influenza; Neuraminidase