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Research Article

Docking and QSAR Studies of Aryl-valproic Acid Derivatives to Identify Antiproliferative Agents Targeting the HDAC8

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Abstract

Background: Histone deacetylase 8 (HDAC8) is a plausible target for the development of novel anticancer drugs using a metal-chelating group and hydrophobic moieties as pharmacophores. It is known that valproic acid (administered as its salt, sodium valproate; VPANa+) is an HDAC8 inhibitor characterized by its hydrophobic chains. Nevertheless, VPA is hepatotoxic and VPA analogues might be explored for less hepatotoxic antiproliferative compounds.