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Inhibition of PTP1B of phenolic compounds from the root bark of *Morus alba*

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As part of our continuing research to obtain pharmacologically active compounds from *Morus alba* L. (Moraceae), four new Diels-Alder type adducts (DAs) [morusalbins A–D], one new isoprenylated flavonoid [albanin T], together with twenty-one known phenolic compounds were isolated from its root bark. The chemical structures were established using NMR, MS, and ECD spectra. The DAs including morusalbins A–D, albasin B, macrourin G, yunanensin A, mulberrofuran G and K, and albanol B exhibited strong inhibitory activities against protein tyrosine phosphatase 1B (PTP1B) (IC_{50}, 1.90–9.67 μM). In the kinetic study, morusalbin D, albasin B, and macrourin G showed non-competitive PTP1B inhibition, with K_i values of 0.33, 1.00, and 1.09 μM, respectively. Furthermore, molecular docking studies revealed that these active DAs have high affinity and tight binding capacity towards the active site of PTP1B.

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