Supplementary Data

Phenolic Compound, Antioxidant, Antibacterial, and In Silico Studies of Extracts from the Aerial Parts of *Lactuca saligna* L.

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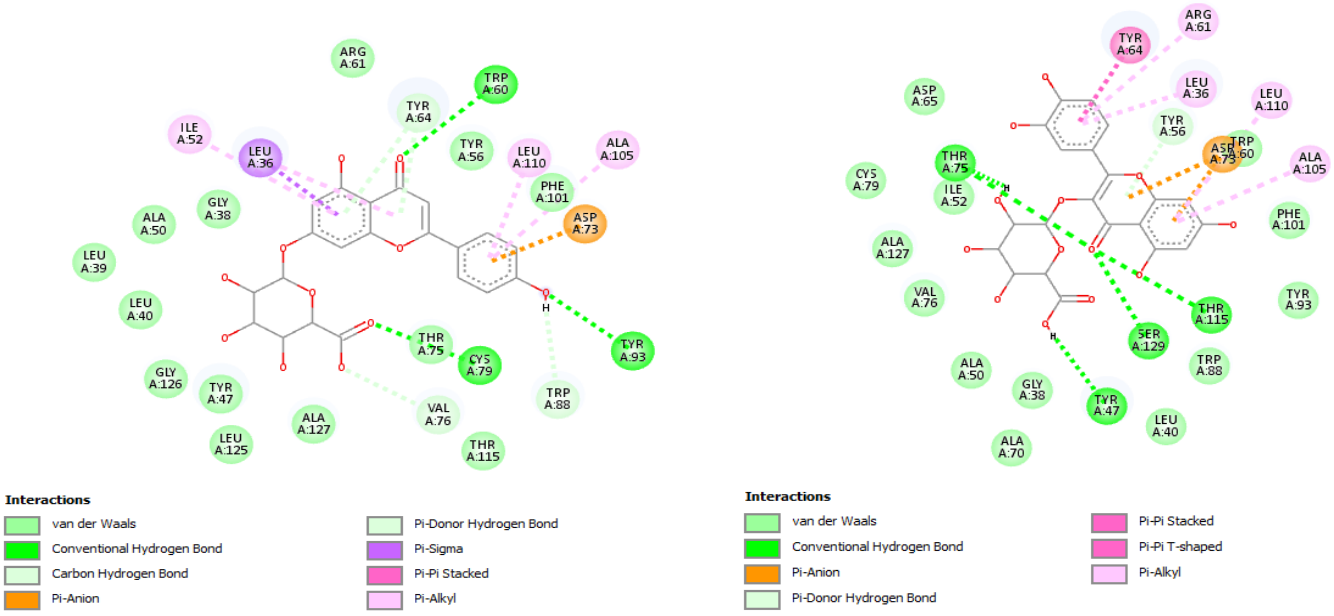
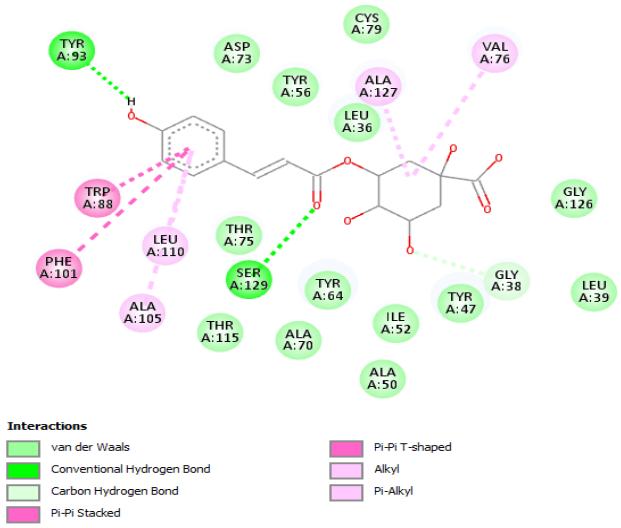
Abstract: Medicinal plants are considered a major source for discovering novel effective drugs. To our knowledge, no studies have reported the chemical composition and biological activities of Moroccan *Lactuca saligna* extracts. In this context, the study aims to characterize the polyphenolic compounds distributed in hydro-methanolic extract of *L. saligna* and evaluate its antioxidant and antibacterial activity; in addition, *in silico* analysis based on molecular docking and ADMET has been performed to predict the antibacterial activity of the identified phenolic compounds. Our results showed the identification of 29 among 30 detected phenolic compounds with the abundance of dicaffeoyltartaric acid, luteolin 7-glucoronide, 3,5-di-O-caffeoylquinic acid, and 5-caffeoylquinic acid with 472.77, 224.30, 196.79, and 171.74 mg/Kg of dried extract, respectively. Additionally, antioxidant activity assessed by DPPH scavenging activity, ferric reducing antioxidant power (FRAP) assay, and ferrous ion-chelating (FIC) assay showed interesting antioxidant activity. Moreover, the results showed remarkable antibacterial activity against *Escherichia coli*, *Salmonella* Typhimurium, *Pseudomonas aeruginosa*, *Enterococcus faecalis*, *Staphylococcus aureus*, and *Listeria monocytogenes* with minimum inhibitory concentrations between 1.30±0.31 and 10.41±0.23 mg/mL. Furthermore, *in silico* analysis identified three compounds, including Apigenin 7-O-glucuronide, Quercetin-3-O-glucuronide, and 3-p-Coumaroylquinic acid as potent candidates for developing new antibacterial agents with acceptable pharmacokinetic properties. Hence, *L. saligna* can be considered a source for phytochemical compounds with remarkable activities, while further *in vitro* and *in vivo* studies are required to explore the main biological activities of this plant.

Keywords: *Lactuca saligna* L.; Phenolic compounds; Willow leaf lettuce; HPLC-PDA/ESI-MS; Antioxidant activity; Antibacterial activity; ADMET; Molecular docking; Morocco

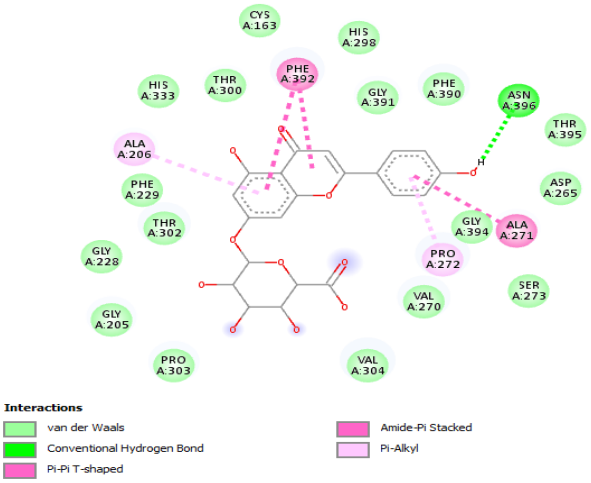


Apigenin 7-O-glucuronide **Quercetin-3-O-glucuronide**

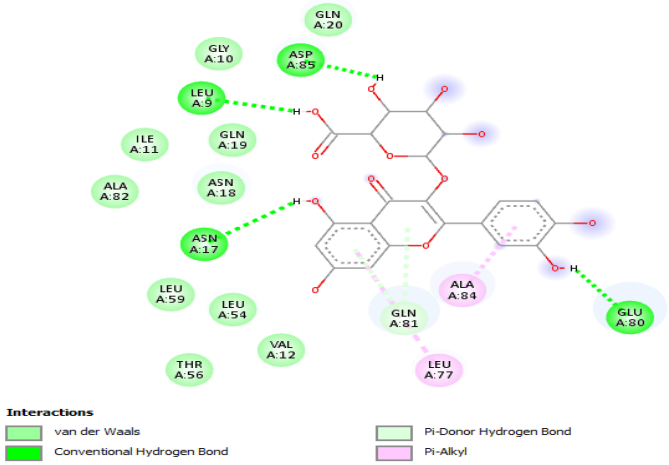


3-p-Coumaroylquinic acid

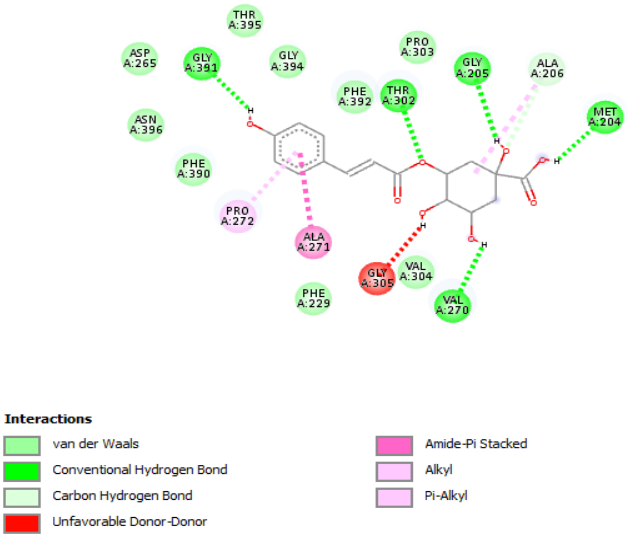
Figure S1. 2D view of the conformations of different interactions between the three inhibitors in the 1U1Z active site.



Apigenin 7-O-glucuronide

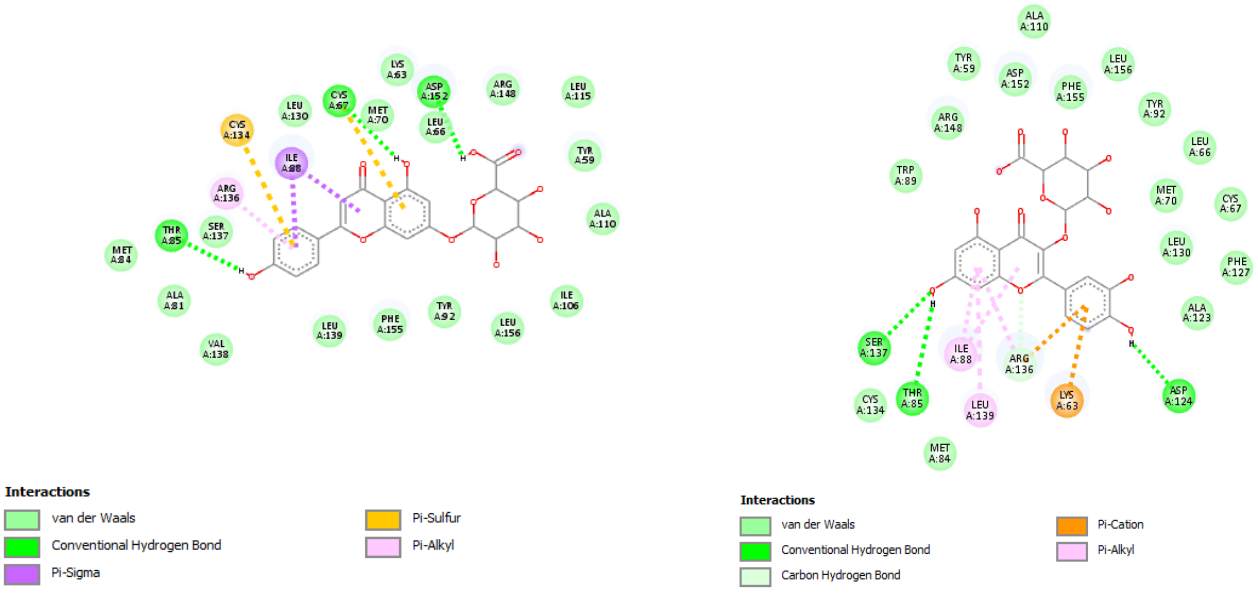


Quercetin-3-O-glucuronide

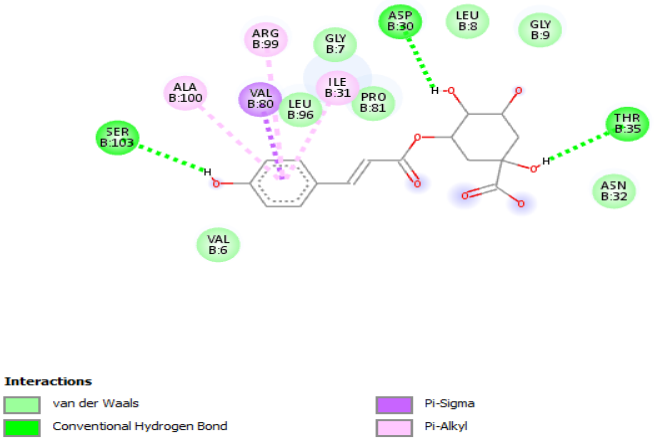


3-p-Coumaroylquinic acid

Figure S2. 2D view of the conformations of different interactions between the three inhibitors in the 1FJ4 active site.

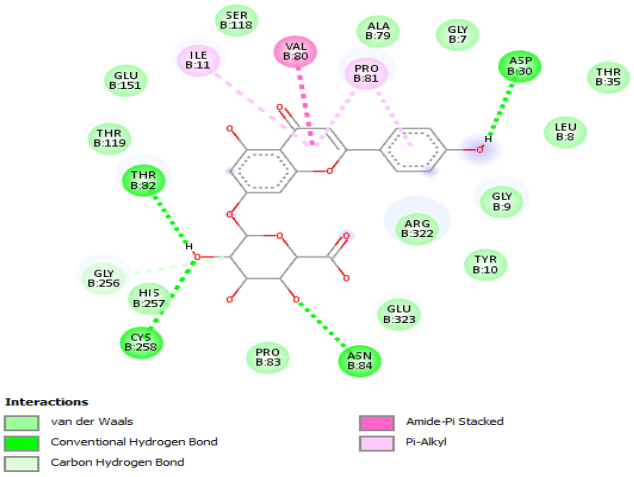


Apigenin 7-O-glucuronide **Quercetin-3-O-glucuronide**

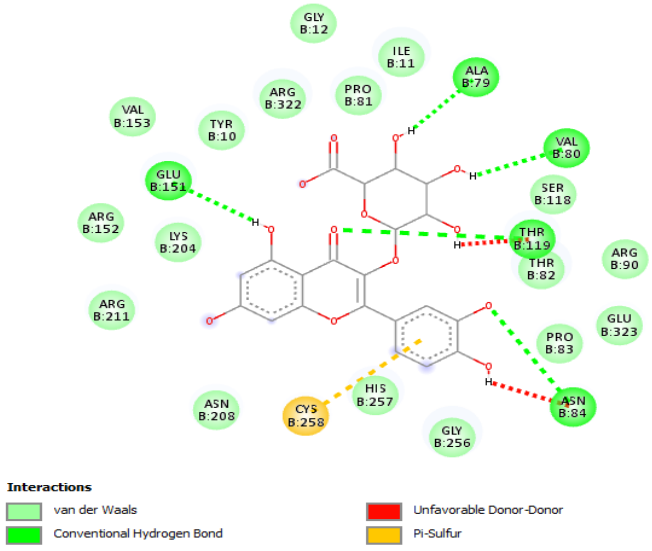


3-p-Coumaroylquinic acid

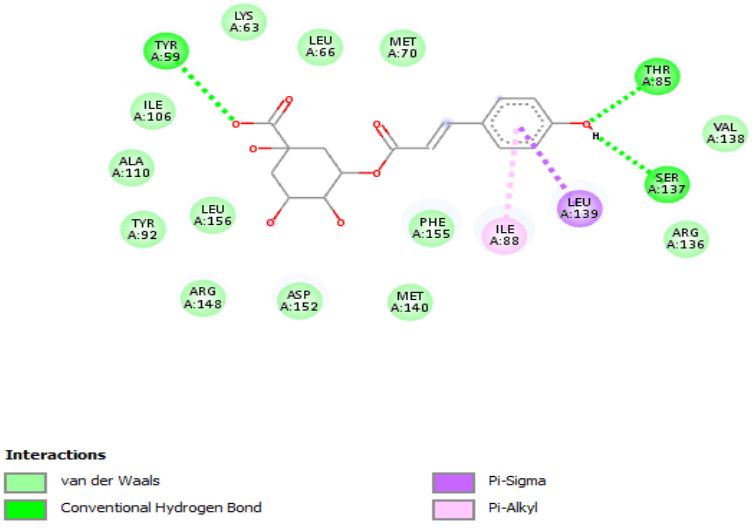
Figure S3. 2D view of the conformations of different interactions between the three inhibitors in the 6IE9 active site.



Apigenin 7-O-glucuronide

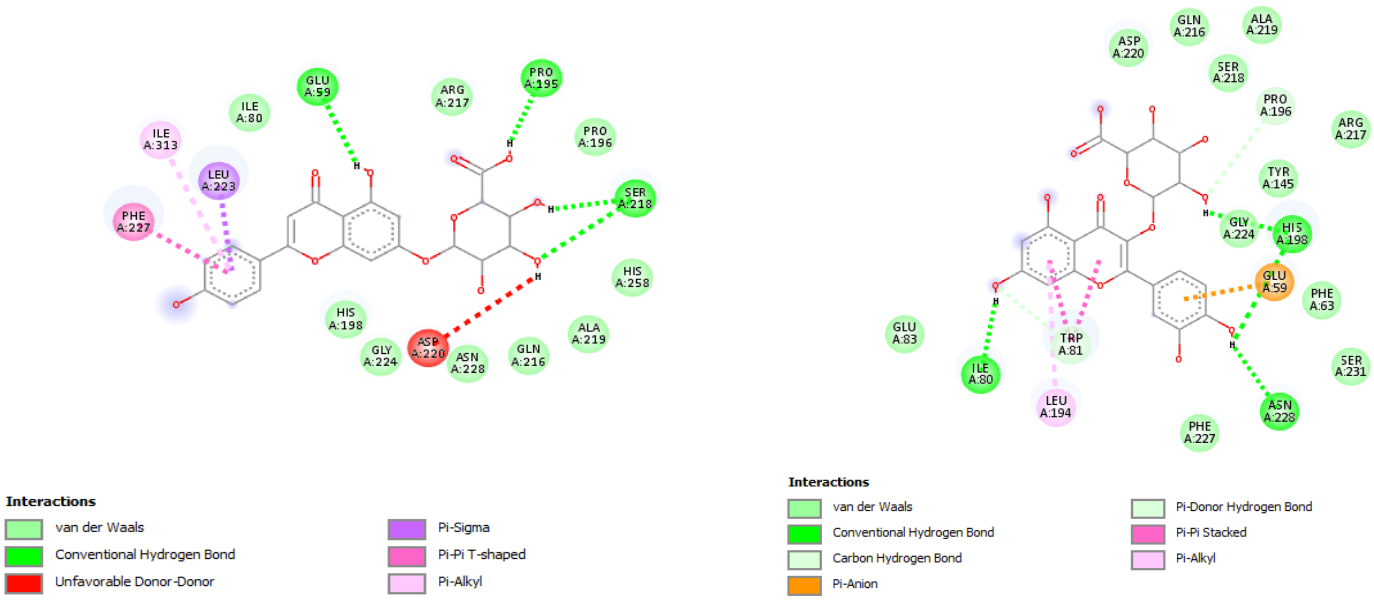


Quercetin-3-O-glucuronide



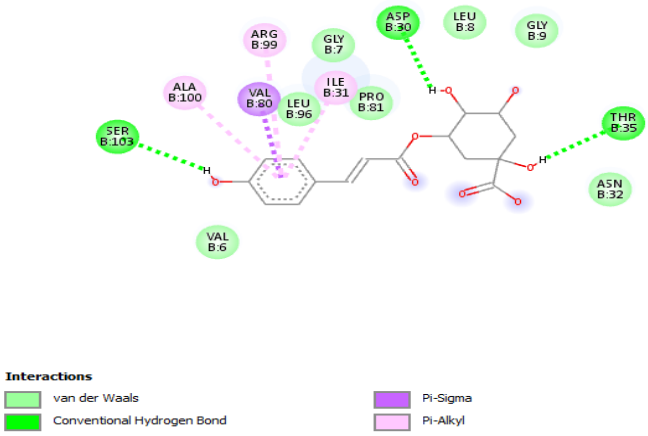
3-p-Coumaroylquinic acid

Figure S4. 2D view of the conformations of different interactions between the three inhibitors in the 3JOL active site.



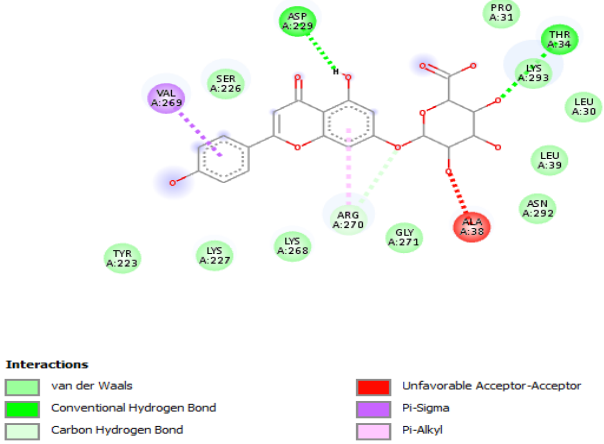
Apigenin 7-O-glucuronide

Quercetin-3-O-glucuronide

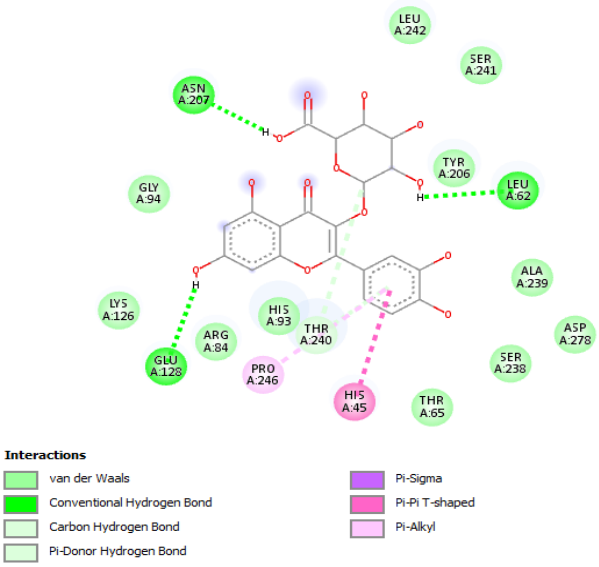


3-p-Coumaroylquinic acid

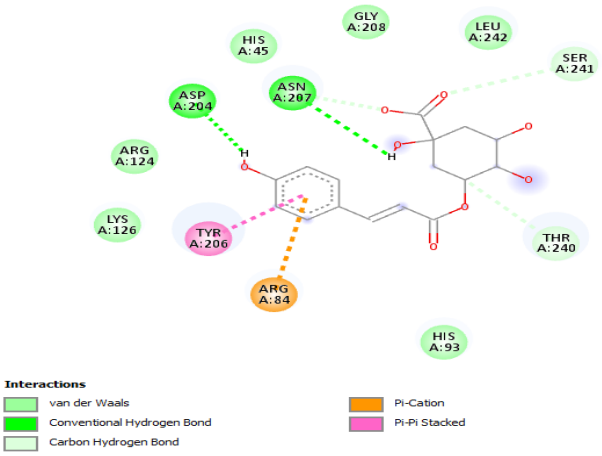
Figure S5. 2D view of the conformations of different interactions between the three inhibitors in the 6QXS active site.



Apigenin 7-O-glucuronide



Quercetin-3-O-glucuronide



3-p-Coumaroylquinic acid

Figure S6. 2D view of the conformations of different interactions between the three inhibitors in the 1AOD active site.