



Estrogen receptor molecular docking of iridoids from *Villara odorata* (Blanco) Merr. (butong manok)

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Sir,

Villarata odorata (Blanco) Merr is an endemic Rubiaceae of the Philippines commonly known as *butong manok*. It contains the iridoids morandolide, hydrophylin A, and hydrophylin B (Tan et al., 2014). We employed molecular docking to examine their binding affinity to the estrogen receptor α expressed by MCF-7 cell line (Algarni et al., 2022). All three iridoids docked better than tamoxifen with morindolide (binding affinity = -6.17 kcal/mol; binding energy, K_i = 30.14 nM) (Table 1). The results suggest that morindolide should undergo further *in-vivo* investigation.

Table 1. Binding Affinity and Inhibition Constants of Iridoids in Estrogen Receptor Alpha of MCF-7 Cells

Ligand	Binding Energy (G, kcal/mol)	Final Intermolecular Energy (kcal/mol)	Inhibition Constant
Tamoxifen	- 5.23	- 5.53	146.72
Morindolide	- 6.17	- 6.79	30.14
Hydrophylin A	- 5.73	- 6.62	62.73
Hydrophylin B	- 5.84	- 6.73	52.76

DECLARATIONS OF INTEREST

None

DECLARATION OF HONOUR

We declare in our honor that our results are not fake and made up.

REFERENCES

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