



**Drug Code:** **sm7v1v4**

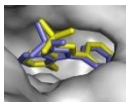
**Drug Family:** small organic molecule (<500 Da)

**Drug Category:** MOA-B antagonist, reversible

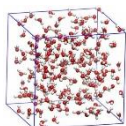


**Disease Category:** Parkinson's Disease treatment: click [HERE](#) to learn more about PD

**Drug Design Approach:** fragment-based, docking, VLS, MD simulations, ADMET predictions



**Docking Results:** Candidate "**sm7v1v4**" exhibited superior docking performance compared to 15 known experimental and FDA-approved MAO-B inhibitors. Docking (AutoDock VINA) carried out against three MAO-B high-resolution x-ray crystallographic models, including 5MRL, 3PO7 and 1OJ9 (**Figure 1**).



**MD Results:** Docked drug stable over ns-time scales at 310°K in physiological saline, pH7.4 (NPT).



**ADMET Profile:** Compared to current FDA-approved MAO-B inhibitors, candidate **sm7v1v4** exhibited a moderate to satisfactory ADMET profile, suggesting it as a promising candidate for PD treatment (Figure 2).

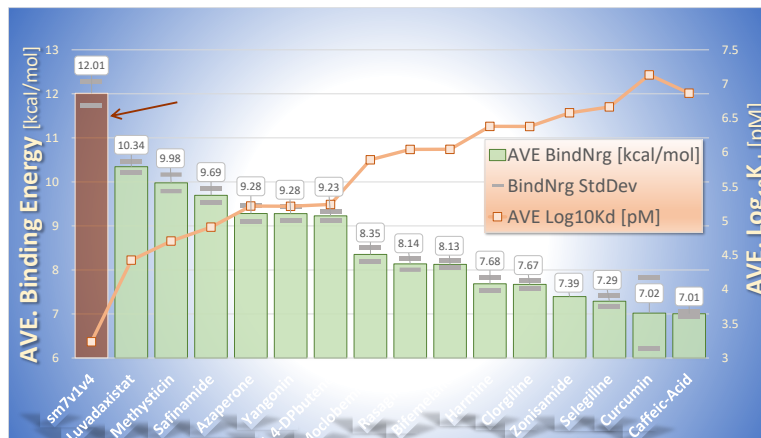
## SUMMARY

Candidate **sm7v1v4** **binds non-covalently in the catalytic pocket of MAO-B**, which degrades L-dopamine in the central and peripheral nervous systems. Thus, MAO-B inhibition

alleviates Parkinson's symptoms by augmenting the level of L-dopamine in the brain. *In-silico* docking and MD indicate **sm7v1v4** **has a superior target binding and stability profile compared to FDA-approved MAO-B antagonists. Candidate drug sm7v1v4 exhibits a favorable ADMET profile** with good drug-like properties (QED, MCE/18), ease of synthesis (Synth), good membrane transport (BBB, Caco2), low toxicity (SkinSen, Respira, LC50 DM, hERG), low carcinogenicity (Carcino), and acceptable minimum daily dose profile (FDAMDD) (**Figure 2**).

**DATA CONVEYANCE**  
All raw and supporting research data shall convey with purchase.

**Figure 1:** Molecular Docking Performance of sm7v1v4 Compared to Known MAO-B Antagonists [Large View](#)



**Figure 2:** Comparison of ADMET Profiles for sm7v1v4 and Three FDA-Approved MAO-B Antagonists [Large View](#)

