Indian Journal of Biochemistry & Biophysics
Vol. 62, August 2025, pp. 919-928
DOI: 10.56042/ijbb.v62i8.16065

Antagonists binding at 5-HT_3R_{AA}, 5-HT_3R_{AB} and 5-HT_3R_{AC} can potentially counteract nicotine binding

Kok Wai Lam[1], Malina Jasamai[1], Nor Azlan Nor Muhammad[2]& Nor Syafinaz Yaakob[1]*

[1]Centre for Drug and Herbal Development, Faculty of Pharmacy, Universiti Kebangsaan Malaysia, Jalan Raja Muda Abdul Aziz, Kuala Lumpur-50300, Malaysia

[2]Institute of Systems Biology, Universiti Kebangsaan Malaysia, Bangi, Selangor-43600, Malaysia

Received 03 January 2025; *revised 17 January 2025*

Supplementary Data

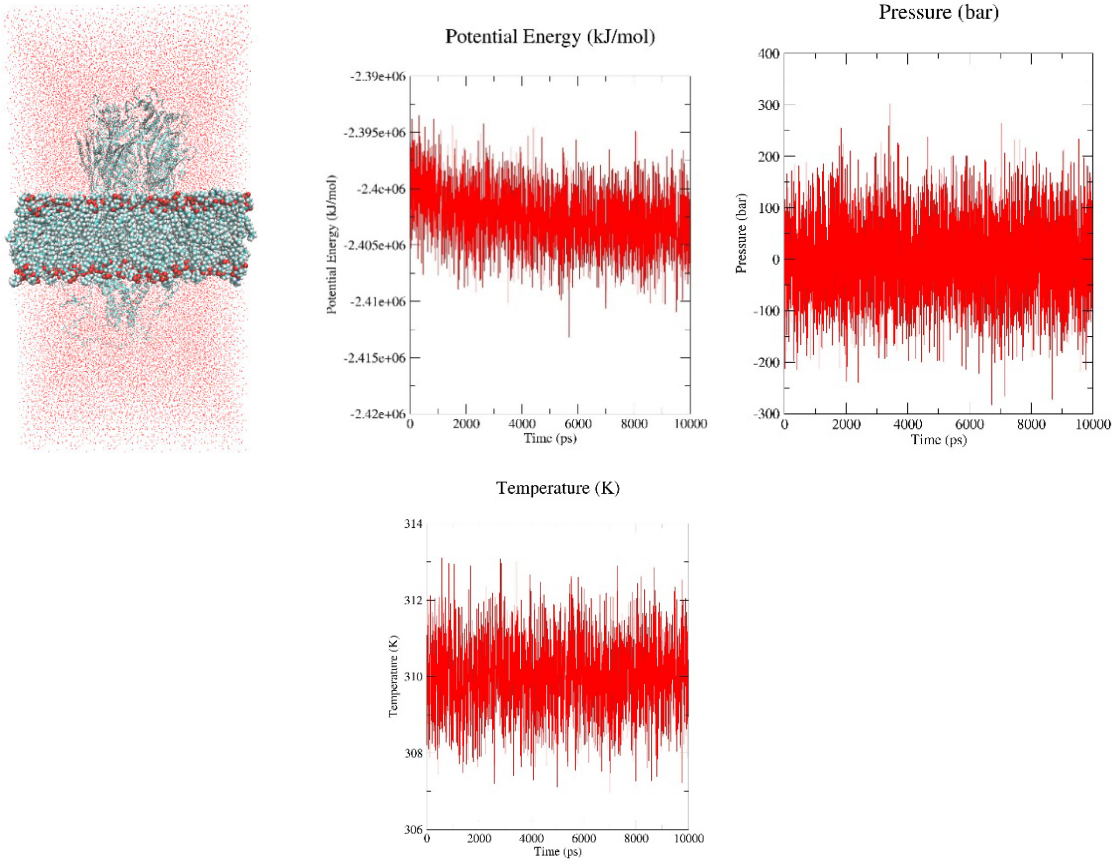

Fig. S1 — (A) Homology models prepared with POPC lipids, ions, and water molecules; (B) Potential energy of the system throughout 10 ns molecular dynamic simulation; (C) Pressure of the system throughout 10 ns molecular dynamic simulation; and (D) Temperature of the system throughout 10 ns molecular dynamic simulation

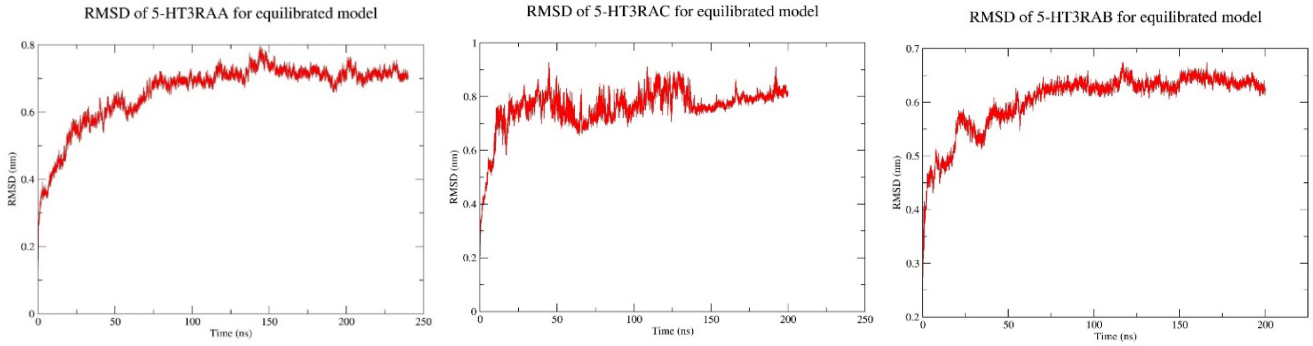

Fig. S2 — (A) RMSD of 5-HT$_3$R$_{AA}$ for equilibrated model; (B) RMSD of 5-HT$_3$R$_{AB}$ for equilibrated model; and (C) RMSD of 5-HT$_3$R$_{AC}$ for equilibrated model

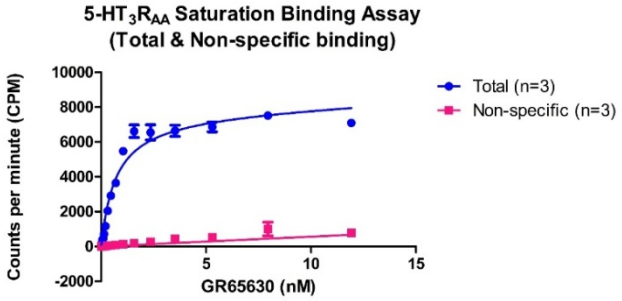

Fig. S3— 5-HT$_3$R$_{AA}$ Saturation Binding Assay (Total and Non-specific binding)

Table S1 — Validation scores for 5-HT3R homology models

Method/Software	Model	Ramachandran Plot		ERRAT	Verify3D
		Most favoured (%)	Additionally allowed (%)	Average score 3D-1D >0.2	Overall quality factor
	4PIR	87.7	10.9	90.58	46.90
MODELLER	5-HT$_3$R$_{AA}$	92.2	5.8	67.02	48.31
	5-HT$_3$R$_{AB}$	91.7	6.5	66.76	48.12
	5-HT$_3$R$_{AC}$	88.7	8.7	67.71	45.19
Swiss Model	5-HT$_3$R$_{AA}$	86.2	10.8	91.47	50.74
	5-HT$_3$R$_{AB}$	87.1	10.4	87.61	47.28
	5-HT$_3$R$_{AC}$	86.7	10.5	87.74	51.02
I-Tasser	5-HT$_3$R$_{AA}$	76.7	19.2	84.43	63.64
	5-HT$_3$R$_{AB}$	76.4	19.8	87.63	57.70
	5-HT$_3$R$_{AC}$	75.4	20.4	83.19	59.06

Table S2 — Validation scores for unequilibrated and equilibrated 5-HT3R homology models

Method	Model	Ramachandran Plot		ERRAT	Verify3D
		Most favoured (%)	Additionally allowed (%)	Average score 3D-1D >0.2	Overall quality factor
	4PIR	87.7	10.9	90.58	46.90
Swiss Model	5-HT$_3$R$_{AA}$	86.3	10.8	91.5	50.7
(unequilibrated)	5-HT$_3$R$_{AB}$	87.1	10.4	87.6	47.3
	5-HT$_3$R$_{AC}$	86.7	10.5	87.7	51.0
Swiss Model	5-HT$_3$R$_{AA}$	90.2	8.2	84.43	52.3
(equilibrated)	5-HT$_3$R$_{AB}$	89.5	9.3	87.63	48.1
	5-HT$_3$R$_{AC}$	89.3	8.9	83.19	53.2

Table S3 — Kd and Bmax value

Parameter	Value
K_d	0.69 nM
B_{max}	7695 CPM