Glu 106 targeted inhibitors of ORAI1 as potential Ca²⁺ release-activated Ca²⁺ (CRAC) channel blockers- Molecular modeling and docking studies

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Table S1: Recommended range for the predicted physicochemical descriptors

S.No	Descriptor	Description	Recommended range
1	Qplogpw	Predicted water/gas partition coefficient.	4.0–45.0
2	Qp log kp	Predicted skin permeability	−8.0 to −1.0
3	% of Human oral absorption	Prediction of human oral absorption on 0 to 100% scale. This property correlates well with the human oral absorption.	>80% is high and < 25% is poor.
4	Q Plog Khsa	Prediction of human serum albumin	−1.5 to 1.5
5	Q Plog HERG	Predicted IC ₅₀ value for blockage of HERG K ⁺ channels	< -5
6	Lipinski's rule of five	Molecular weight of the molecule	<500
		Hbond Donors	≤5
		Hbond Acceptors	≤10
		Compounds satisfy these rule considered to be drug like.	

Table S2: Comparison docking score of hit compounds and reported ORAI1 inhibitors

Reported compounds	Docking Score (kcal mol ⁻¹)	Insilico based novel hit compounds	Docking Score (kcal mol ⁻¹)
2-APB	-2.697	KM06293	-5.992
Synta66	-3.818	SB01990	-5.335
Btp2	-2.806	SPB06836	-5.106

Supplementary Figures:

Figure S1: Structure validation of modeled ORAI1 protein.

Figure S2: Representation of Global Structure Assessment.

Figure S3: Graphical representation of ANOLEA, QMEAN and GROMOS analysis of modeled ORAI1 protein.

Figure S4: Secondary structure of modeled ORAI1 protein.

Figure S5: Average RMSD C-alpha atoms of modeled ORAI1 with 5ns interval.

Figure S6: A time line representation of Secondary structure elements of modeled ORAI1 throughout the 30ns simulation trajectory.

Figure S7: RMSF plot represents the fluctuating amino acids in modeled ORAI1 for throughout the 30 ns stimulation.

Figure S8: Two dimensional conformations of 'Hit' compounds. (A- SB01990, B- SPB06836, C- KM06293, D- RHO1882).

Figure S9: A schematic representation of ligand atom interactions with the protein residues (calcium-Blue color). (A- SB01990, B- SPB06836, C- KM06293, D- RHO1882).

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