Electronic Supplementary Material (ESI) for RSC Advances.

GLY67ARG substitution in RSPO4 disrupts WNT signaling pathway due to abnormal binding pattern with LGRs leading to anonychia

Supplementary Information

Table S1 Molecular docking scores for LGR4-6 with normal and mutated RSPO4.

Complexes		No. of Clusters	Score	RMSD (Å)	Van-der Waals energy (kcal/mol)	Electrostatic Energy (kcal/mol)	Z-score
LGR4-RSPO4	**Normal**	11	-131	14.6	-48.8	-349.7	-2.2
	Mutated	9	-122	4.6	-52.0	-492.9	-1.1
LGR5-RSPO4	**Normal**	8	-156	0.9	-52.4	-530.4	-2.0
	Mutated	7	-132	1.5	-48.7	-498.6	-1.0
LGR6-RSPO4	**Normal**	8	-163	1.2	-50.6	-599.1	-2.1
	Mutated	8	-163	1.4	-57.6	-630.6	-1.7

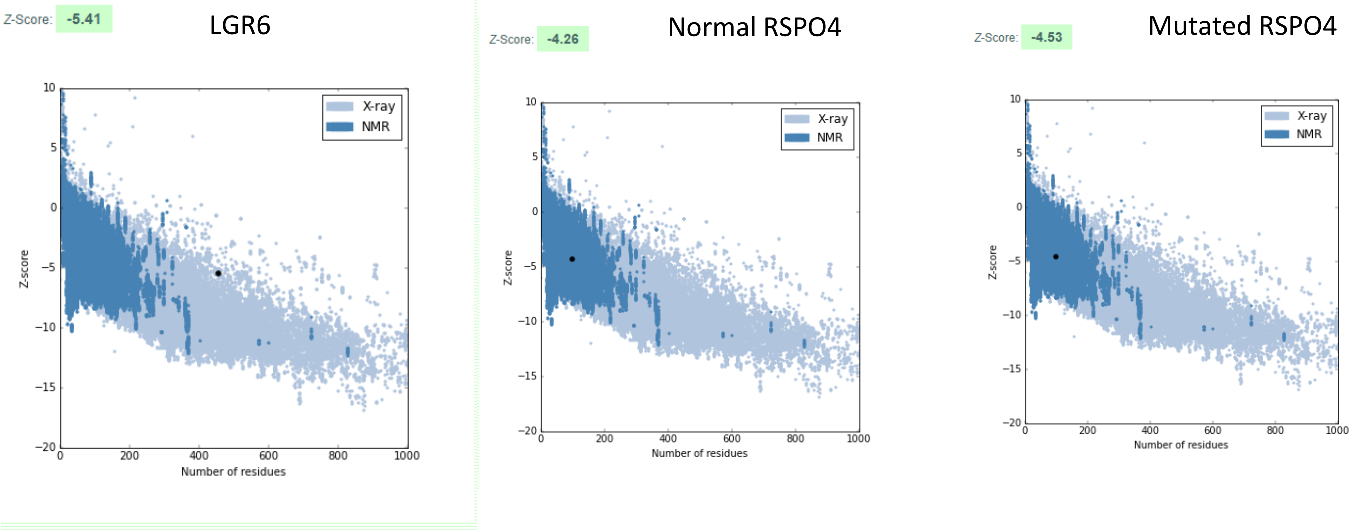

Fig. S1 Structural evaluation (Z-score) of LGR6, normal RSPO4 and mutated RSPO4.

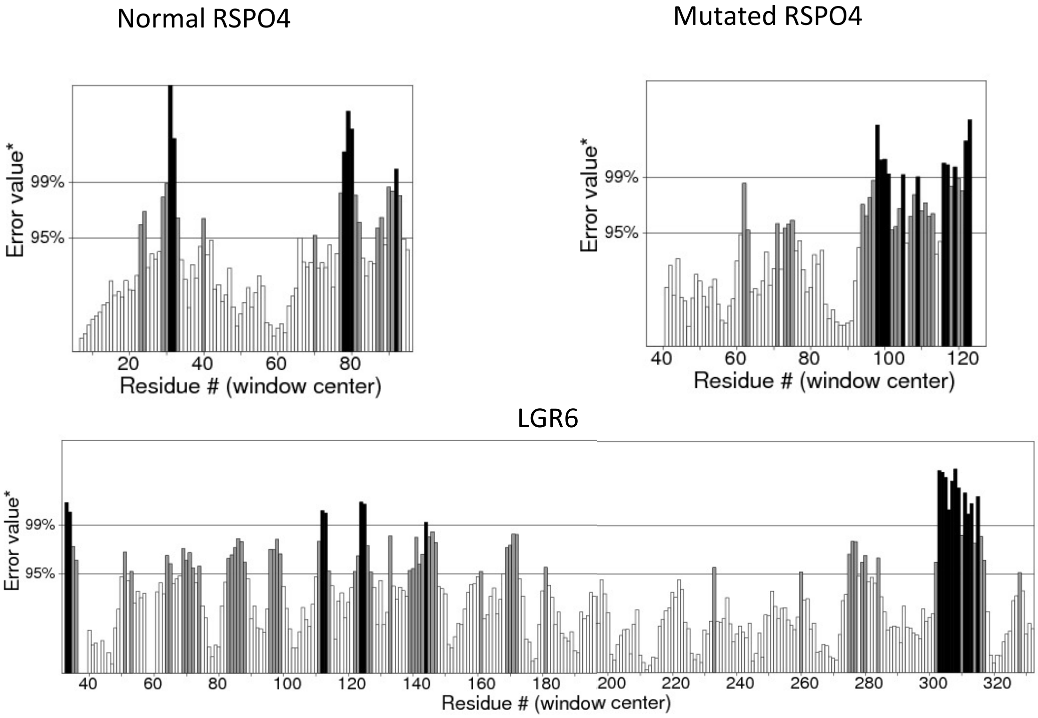

Fig. S2 Structural evaluation (Errat) of LGR6, normal RSPO4 and mutated RSPO4.

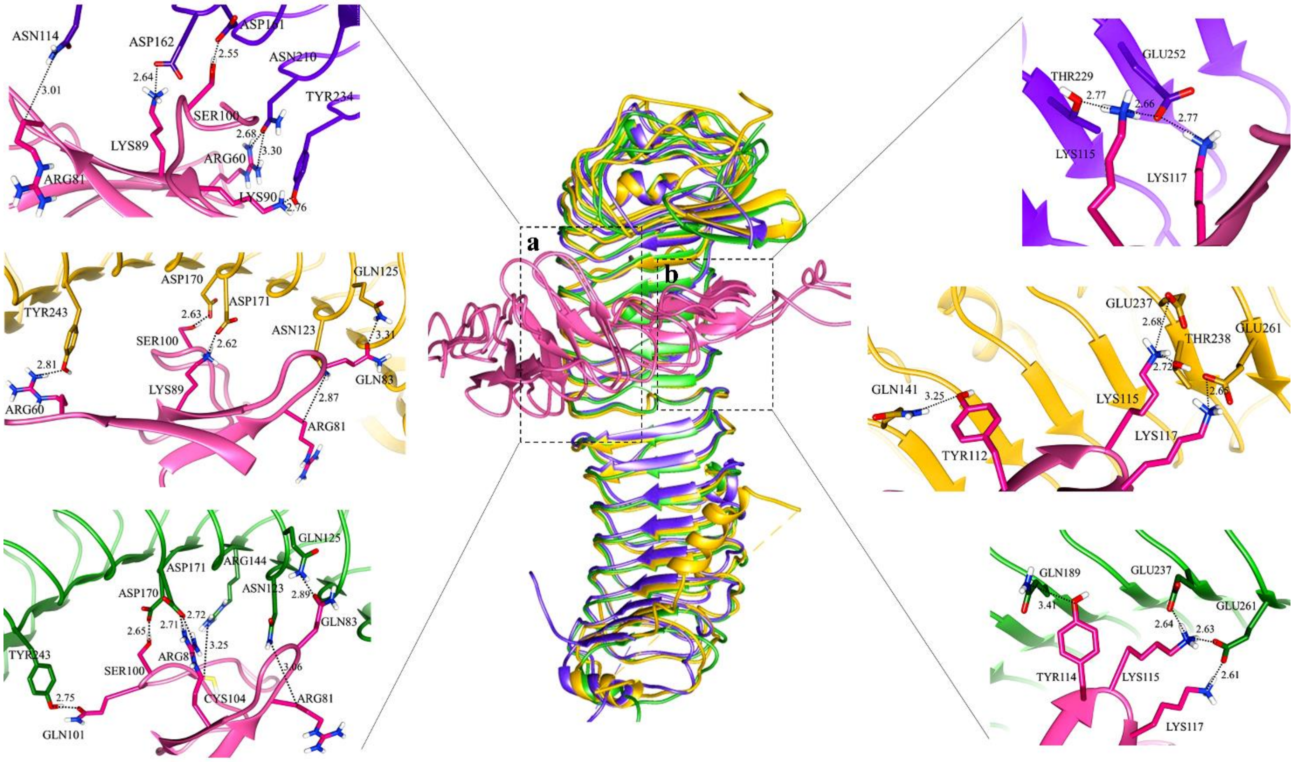

Fig. S3 Comparative binding analysis of LGR4-6 and RSPO4. LGR4-6 are shown in purple, yellow and green colors, respectively. RSPO4 is shown in pink. Box ‘a’ and ‘b’ represent LGRs binding sites ‘a’ and ‘b’, respectively. Site 'a' of the complexes is comparatively larger as compared to site 'b'.

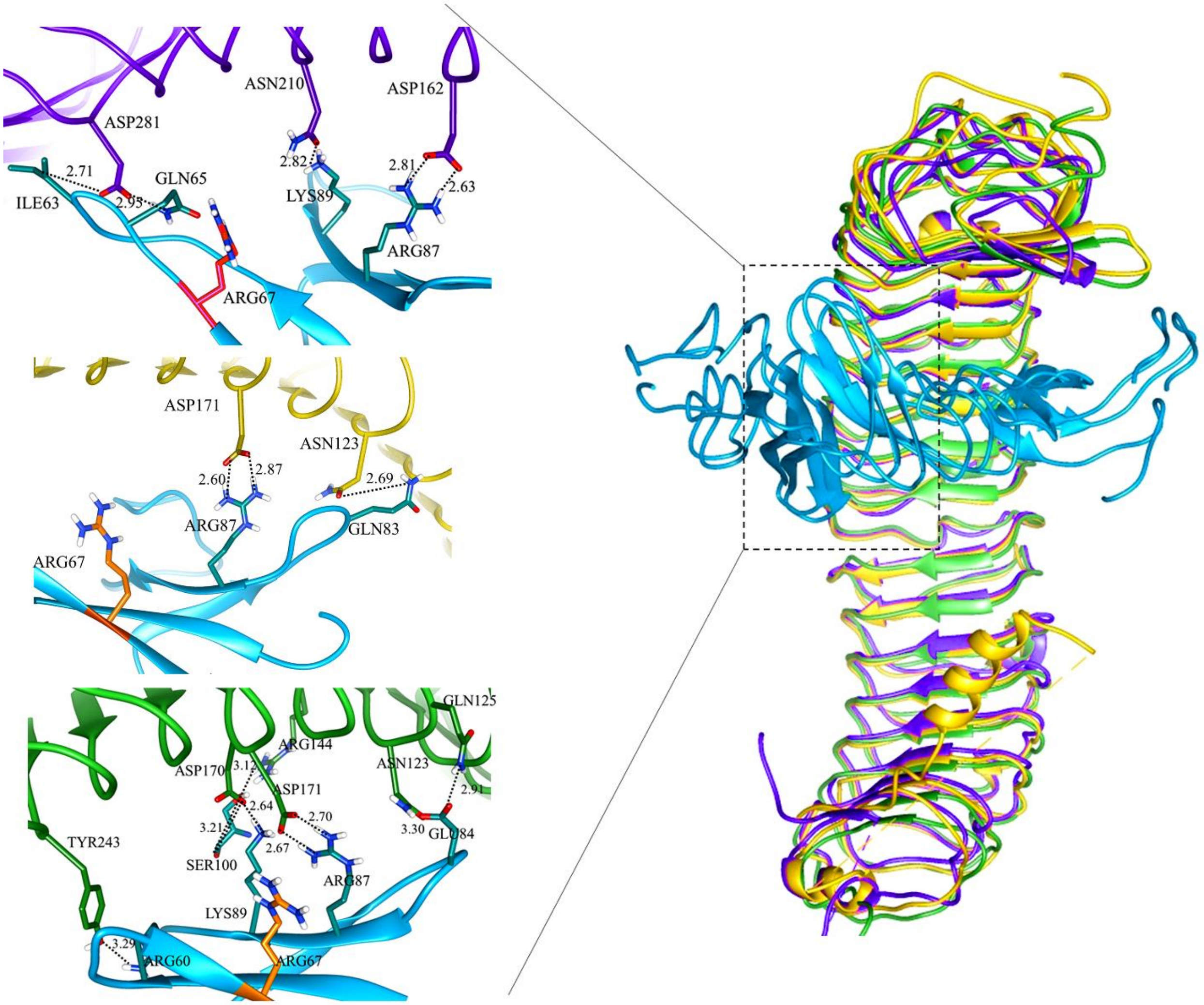

Fig. S4 Comparative binding analysis of LGR4-6 with mRSPO4. LGR4-6 are shown in purple, yellow and green, respectively; mRSPO4 is shown in blue. Dotted box represents the binding of mRSPO4 with LGRs at site 'a'. Mutated residue ARG67 is shown in orange in the vicinity of binding sites.