

SUPPLEMENTARY ONLINE DATA

Insights into the molecular evolution of oxytocin receptor ligand binding

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Table S1 | Insights into the molecular evolution of OTR ligand binding

N/OFG, nociceptin/orphanin FQ.

Receptor	PDB code	Residue number ^a																									
		88	91	95	98	99	103	116	119	123	124	188	200	204	205	208	209	288	291	292	295	298	308	311	315		
Human																											
β_2 -adrenergic	2RH1								x	x			x	x	x	x		x	x	x	x					x	
	3D45								x	x			x	x		x		x	x	x	x					x	
	35N6	x						x	x	x		x	x	x		x		x	x	x	x				x	x	
	3P0G							x	x	x		x	x	x		x		x	x	x	x		x		x	x	
	3PDS				x		x	x	x	x		x	x	x		x		x	x	x	x				x	x	
Turkey																											
β_1 -adrenergic	2Y00								x	x				x		x		x	x	x	x					x	
	2Y04								x	x				x		x		x	x	x	x					x	
	2VT4								x	x		x	x	x		x		x	x	x					x	x	
Human A_{2A} adenosine	3EML								x	x				x		x		x	x	x	x					x	
	3PWH								x			x				x		x	x	x	x		x	x		x	
Bovine rhodopsin	3OAX								x	x				x		x		x	x	x	x		x	x		x	
CXCR4 chemokine	3OE6	x	x	x	x	x			x			x							x		x				x	x	
Human dopamine D_3	3PBL								x	x				x		x		x	x	x	x					x	
Human M_2 muscarinic acetylcholine	3U0N			x	x	x					x	x				x	x	x	x	x	x						
Sphingosine 1-phosphate	3V2Y								x	x				x		x		x	x	x	x					x	x
	3V2W	x	x	x	x				x	x				x		x		x	x		x					x	x
M_3 muscarinic acetylcholine	4DAJ	x	x	x	x				x	x	x			x		x	x	x	x	x	x						
Human κ -opioid	4DJH							x	x	x			x	x	x	x	x	x	x	x	x					x	
Mouse μ -opioid	4DKL								x	x				x	x			x	x	x	x		x			x	x
Human N/OFG opioid	4EA3	x	x	x					x	x				x		x		x	x	x	x					x	x
Human δ -opioid	4EJ4								x	x			x	x	x	x		x	x	x	x		x			x	x
Human histamine H_1	3RZE	x	x	x	x				x										x	x	x					x	x

^aResidue numbers are listed for the human OTR receptor sequence SwissProt P30559 and correspond to equivalent positions (by alignment) of other receptors.Received 26 September 2012
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