

Table S4 Interactions of SHU9119 with MC1R.

SHU9119	MC1R	Interactions
Nle ^{U1}	V97 ^{2.63}	Hydrophobic interactions
	I98 ^{2.64}	
	D117 ^{3.25}	
Asp ^{U2}	E94 ^{2.60}	Van der Waals force
	I98 ^{2.64}	
His ^{U3}	F45 ^{1.39}	π - π interaction
	T95 ^{2.61}	Hydrogen bond
	E94 ^{2.60}	Hydrophobic interactions
	I98 ^{2.64}	
	F280 ^{7.35}	
L284 ^{7.39}		
D-Nal ^{U4}	E94 ^{2.60}	Hydrogen bond
	D121 ^{3.29}	Hydrophobic interactions
	C125 ^{3.33}	
	M128 ^{3.36}	
	F257 ^{6.51}	
L284 ^{7.39}		
Arg ^{U5}	D121 ^{3.29}	Hydrogen bond
	I180 ^{4.61}	Hydrophobic interactions
	Y183 ^{ECL2}	
	F280 ^{7.35}	
Trp ^{U6}	Y183 ^{ECL2}	Hydrogen bond
	V188 ^{5.39}	Hydrophobic interactions
	L189 ^{5.40}	
	L192 ^{5.43}	
	H26 ^{6.54}	
	L261 ^{6.55}	
I264 ^{6.58}		
Lys ^{U7}	F280 ^{7.35}	Hydrophobic interactions

Superscripts refer to the Ballesteros-Weinstein numbers and residues within 4 Å