

Supplementary data

Use of Network Model to explore dynamic and allosteric properties of three GPCR homodimers

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Table S1 Indexes of residues in the ligand-binding region and the G-protein binding one, which are severed as the two extremities to search PSN paths.

	CXCR4	β1AR	κ-OR
Extracellular side	93-94, 96-97, 112-113, 116, 199-200, 262, 281, 284-285, 288, 187, 181	101, 102, 117-118, 121- 122, 125, 207-208, 211, 215, 303, 306-307, 310, 325-326, 329-330, 333	108, 111, 115, 134, 138- 139, 142, 227,230, A:287, 290-291, 294, 312, 316, 319-320
Intracellular side	73, 134, 137, 138, 139, 222, 225, 226, 233, 236, 237, 240, 241, 244, 298- 302	76, 139, 142, 143, 144, 230, 233, 234, 284, 287, 288, 291, 292, 295, 346, 339-343	94, 156, 159, 160, 161, 249, 252, 253, 265, 268, 271, 272, 275, 276, 279, 334, 326-330

Table S2 Positions located in the meta-paths revealed by the work and simultaneously belonged to 36 positions in one conserved interaction network reported by Venkatakrishnan [64].

	monomer	protomer
CXCR4	7.39, 7.46, 7.45, 6.48, 6.44, 6.41, 3.51	7.39, 7.46, 6.48, 6.51, 6.44, 7.45, 6.41
Beta1AR	7.39, 6.48, 6.44, 2.50 1.50 7.50 1.53, 1.57, 7.53, 2.43, 3.46, 7.45	7.39, 6.48, 6.44, 2.50 1.50 7.50 1.53, 1.57, 7.53, 3.46, 2.43, 2.42
κ -OR	6.51, 7.39, 6.48, 6.44, 3.40, 2.42, 3.46, 7.45, 7.53, 2.43	6.51, 7.39, 6.48, 6.44, 3.40, 3.44, 6.41, 5.54, 3.47, 5.57, 3.51, 5.54, 7.45, 7.53, 2.43

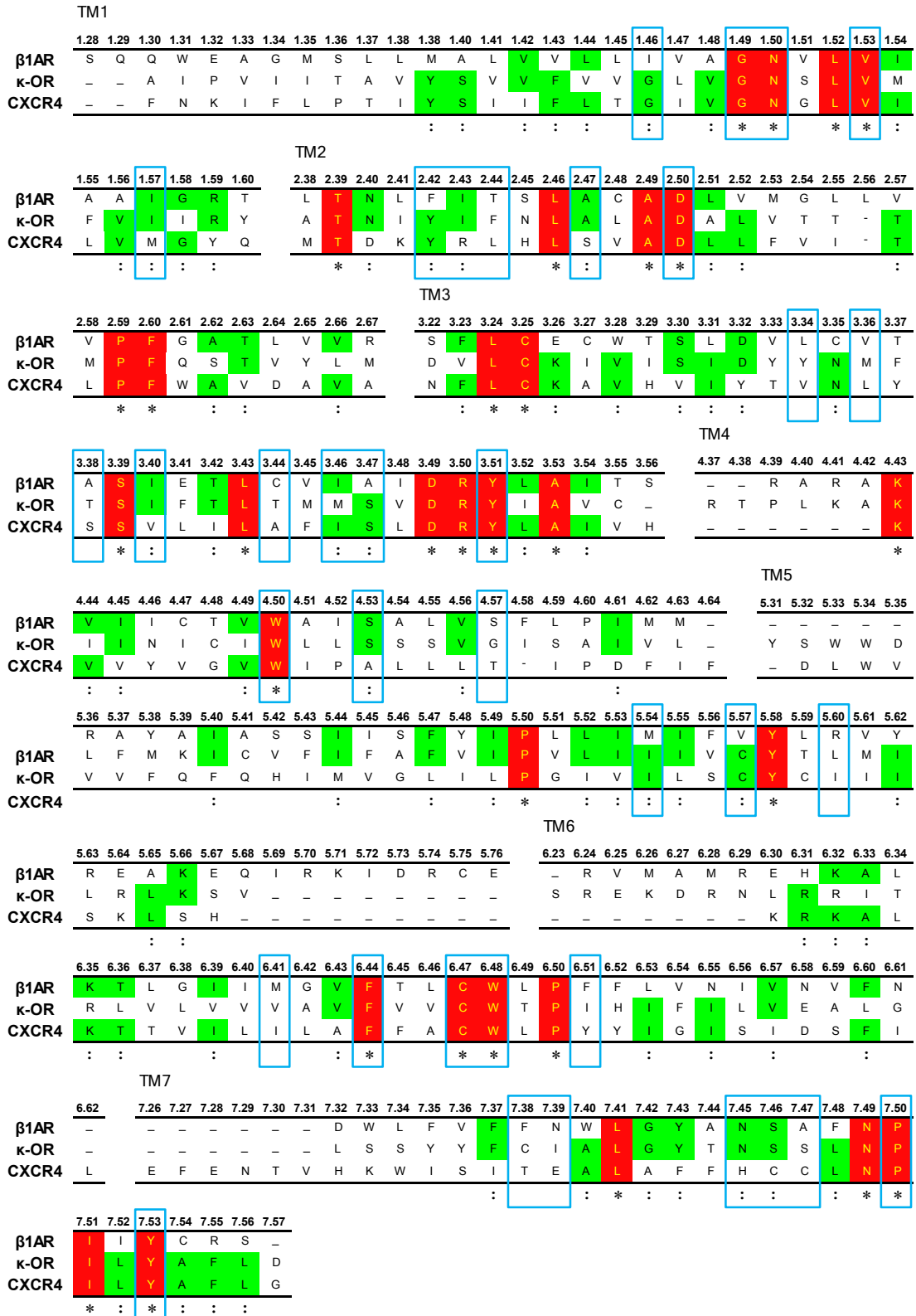


Fig.S1 Sequence alignment for the three GPCRs. Decimals are Ballesteros-Weinstein numbering. ‘*’ and ‘:’ indicate identity and conservation, respectively. Positions located in the conserved interaction network reported⁶⁴ are highlighted by blue rectangles.