

**Table S1. Restraints applied to the metal bridges and the four transmembrane helices (secondary structure; S1: residues 170–184, S2: residues 224–238, S3: residues 260–275, S4: residues 284–305) were gradually changed.**

	Metal-ligand bonds (kcal/mol/Å <sup>2</sup> )	Backbone atoms bonds (kcal/mol/Å <sup>2</sup> )	Angles (kcal/mol/rad <sup>2</sup> )	Dihedrals (kcal/mol/rad <sup>2</sup> )	Improper torsions (kcal/mol/rad <sup>2</sup> )	Secondary structure (kcal/mol/rad <sup>2</sup> )	Dummy Delta (Å)	Time (ns)
1	1.0	0.2	1.0	1.0	1.0	500.0	2	2
2	2.0	0.5	2.0	2.0	2.0	500.0	2	2
3	5.0	1.0	5.0	5.0	5.0	500.0	2	2
4	10.0	2.0	10.0	10.0	10.0	500.0	2	2
5	10.0	5.0	10.0	10.0	10.0	500.0	2	2
6	10.0	10.0	10.0	10.0	10.0	500.0	2	2
7	10.0	20.0	10.0	10.0	10.0	500.0	2	2
8	10.0	50.0	10.0	10.0	10.0	400.0	2	2
9	10.0	50.0	10.0	10.0	10.0	300.0	2	2
10	10.0	50.0	10.0	10.0	10.0	200.0	2	2
11	10.0	50.0	10.0	10.0	10.0	100.0	1	80