

Spectroscopic fingerprints of a water-bridged twisted retinal structure in the bacteriorhodopsin proton pump

Supporting Information

Tino Wolter, Kai Welke, Prasad Phatak, Ana-Nicoleta Bondar and Marcus Elstner

Here we show the dihedral angles along the retinal polyene chain for each used crystal structure and its QM/MM optimized structure for the L state and the bR resting state.

Table 1: Dihedrals of the retinal within different L structures and the bR resting state (1C3W)

	1C3W-opt	1UCQ-xray	1UCQ-opt	L-bridged	1VJM-xray	1VJM-opt	2NTW-xray	2NTW-opt
CD-CE-NZ=C15	-102.5	113.2	133.9	123.8	139.0	120.6	-126.6	-100.3
CE-NZ=C15-C14	-164.5	-148.7	-164.3	-169.4	-179.2	-159.9	146.4	-165.9
NZ=C15-C14=C13	171.5	-162.4	-163.0	-169.9	-179.3	-155.6	175.8	171.2
C15-C14=C13-C12	-151.4	10.3	22.6	21.4	-1.0	20.9	-107.9	-150.7
C14=C13-C12=C11	175.1	177.3	164.4	175.1	176.6	162.9	174.4	174.8
C13-C12=C11-C10	-172.4	176.4	-174.7	-168.9	179.9	170.3	-171.1	-172.5
C12=C11-C10=C9	-171.7	-178.4	-179.5	-178.4	177.9	-179.6	-170.1	-172.3
C11-C10=C9-C8	175.5	171.0	173.8	-175.7	177.3	175.3	-173.5	175.9
C10=C9-C8=C7	-166.9	-173.9	-171.0	-175.9	179.6	-168.7	-173.0	-168.4
C9-C8=C7-C6	172.3	172.7	173.5	178.2	177.1	172.9	169.3	172.6
C8=C7-C6=C5	169.0	177.3	172.5	173.5	179.5	175.2	172.1	172.6
C7-C6=C5-C4	179.6	174.6	179.8	-178.9	176.2	-179.7	166.9	179.4