Supporting Information

The Role of Structured Water in Mediating General Anesthetic Action on α4β2 nAChR

Dan Willenbring,† Yan Xu,†‡§ and Pei Tang†‡¶*

Departments of †Anesthesiology, ‡Pharmacology and Chemical Biology, §Structural Biology, and ¶Computational Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA 15261

Figure S1: Number of partially occupied water sites, as measured by HOP analysis (see Methods Section), for closed- and open-channel α4β2 nAChR for each of the two time windows analyzed (10-15 ns and 15-20 ns). Open boxes indicate control systems and shaded boxes indicate systems with halothane.