Bitter taste detection has an important role in preventing the accidental ingestion of potentially toxic substances, though not all bitter tastants are toxic. Bitter tastant molecules span a diverse chemical structure space and are detected by more than 25 human bitter taste receptors (hTAS2Rs), all of which belong to the seven-helical transmembrane superfamily of G-Protein Coupled Receptors (GPCRs). About one-third of the hTAS2Rs have been deorphanized and are known to be activated by one or more bitter tastants. Little is known about the structure-function relationships of these receptors and how they can be activated by structurally diverse bitter tastant molecules. We have predicted the detailed atomic structure of hTAS2R47 using the methodology developed in our group for GPCR structure prediction (MembStruk). We have used the predicted structure of hTAS2R47 to identify the binding sites for several bitter tastant molecules (using our docking program MSCDock) to understand the selectivity and in some cases the specificity of hTAS2Rs for some of these bitter tastants. We will present the results of these studies and compare with available experimental data. The results will include key residues predicted to be involved in binding to bitter tastant molecules, which suggest mutagenesis experiments that can be used to validate the predicted binding sites and shed light on the selectivity of bitter receptors.