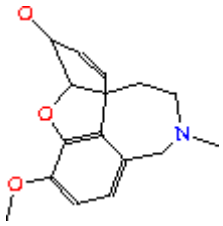
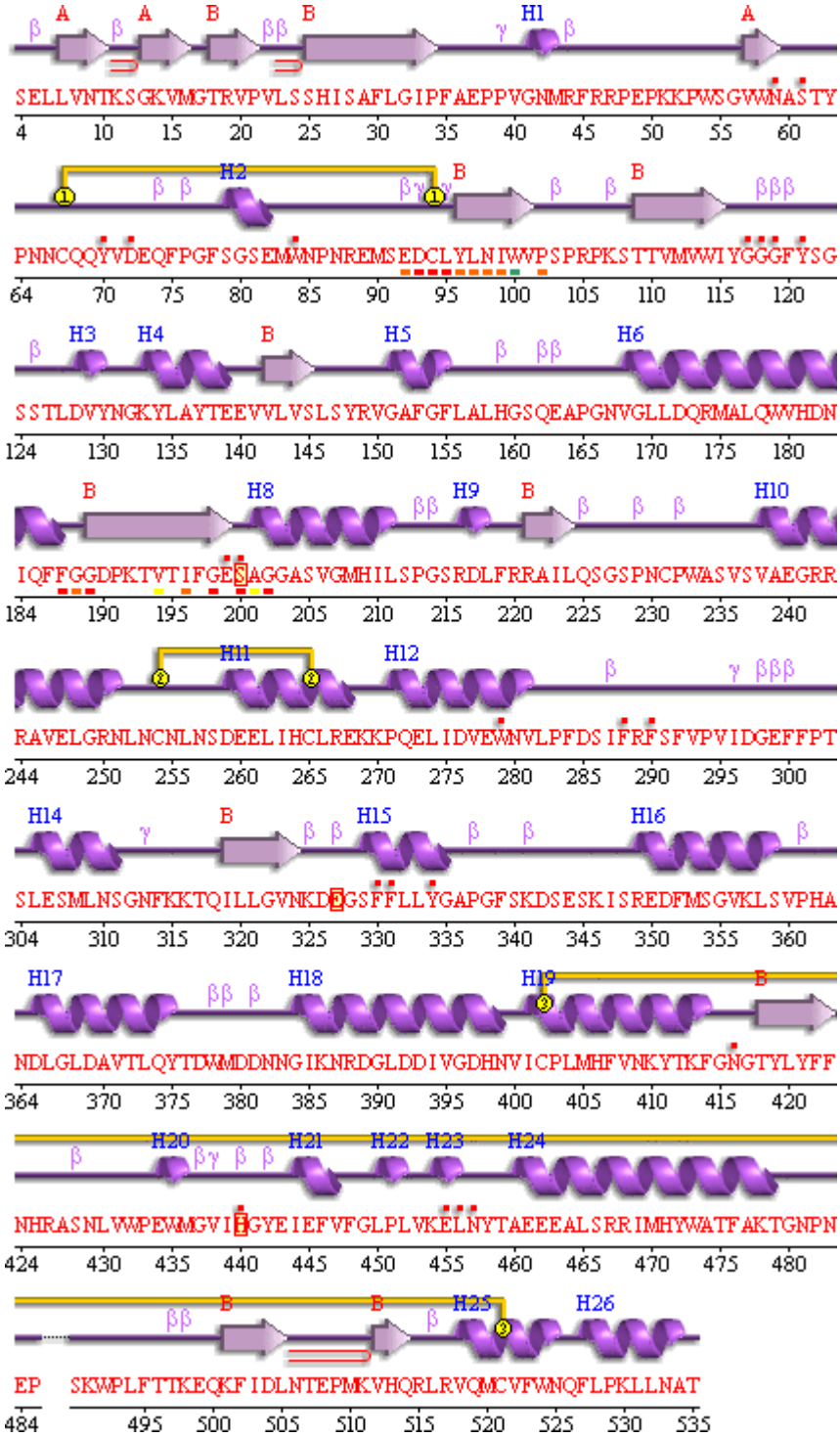
Information from PDBSum

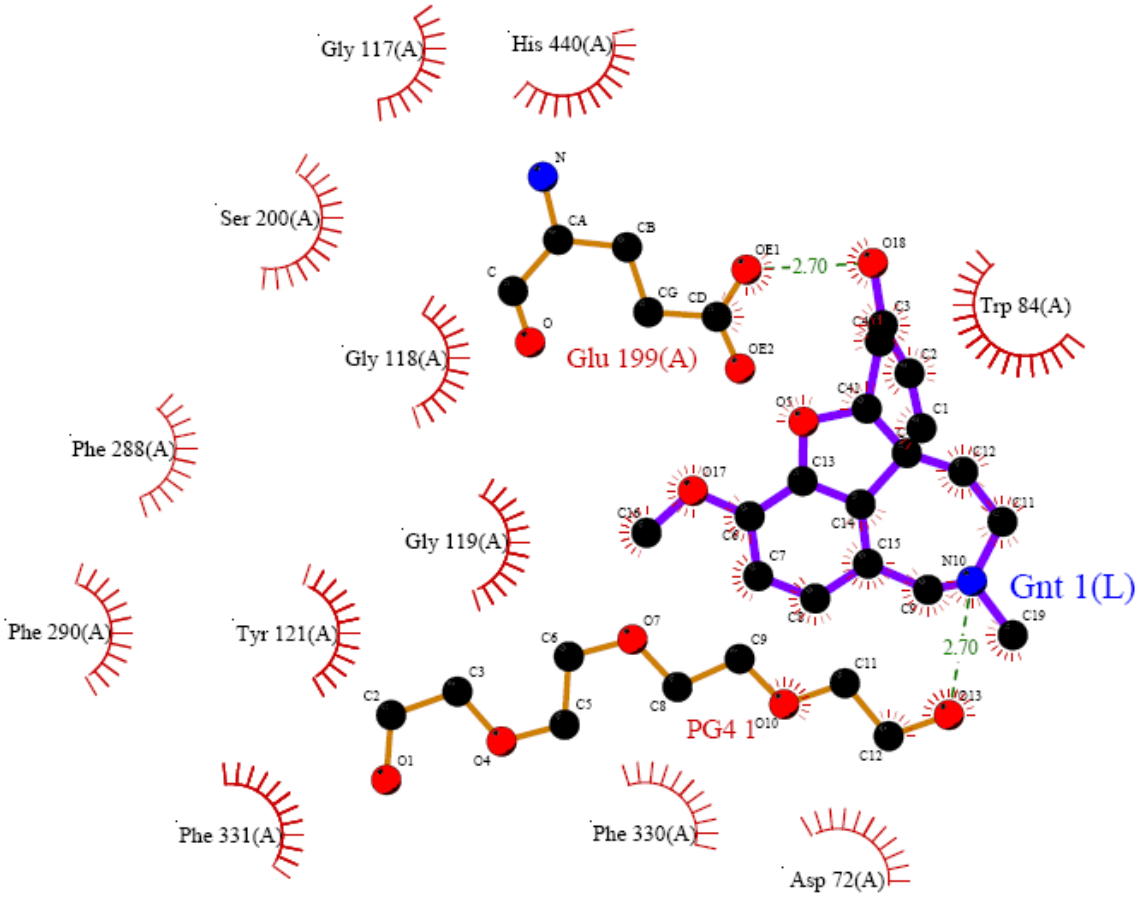


Here is an example using the acetylcholinesterase protein 1DX6 that complexes GNT1 (galanthamine). (-)-Galanthamine (there should be an H on the O at top)

This is the **wiring diagram**. Examples of amino acid residues that interact with the ligand are at positions 59 and 61 (the red dots); an example of a residue in the active site is at position 200.



This is the LIGPLOT for galanthamine.

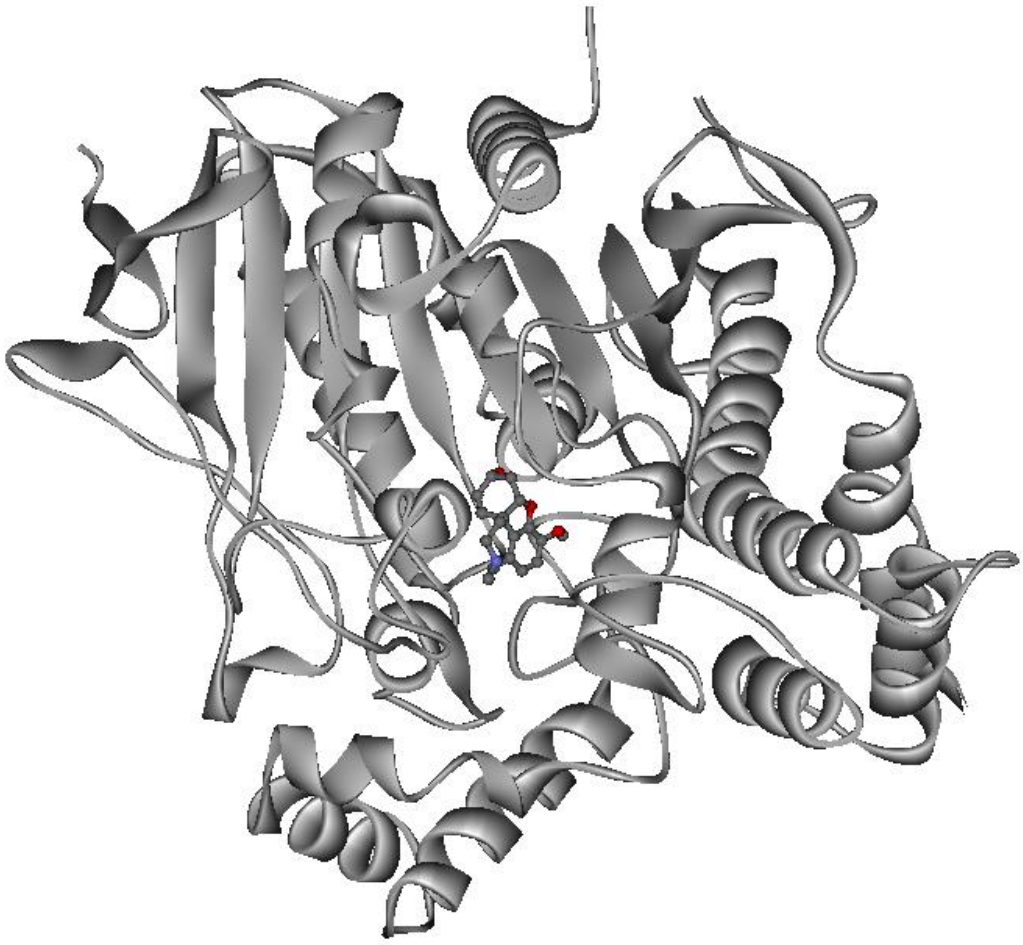


The ball-and-stick models are of galanthamine (Gnt) and a solvent molecule (PG4) that is complexed within the protein (PG4 1 is $HOCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2OH$). The Glu (or E) is an amino acid residue number 199 in the primary sequence and shown larger because of its important interaction with galanthamine.

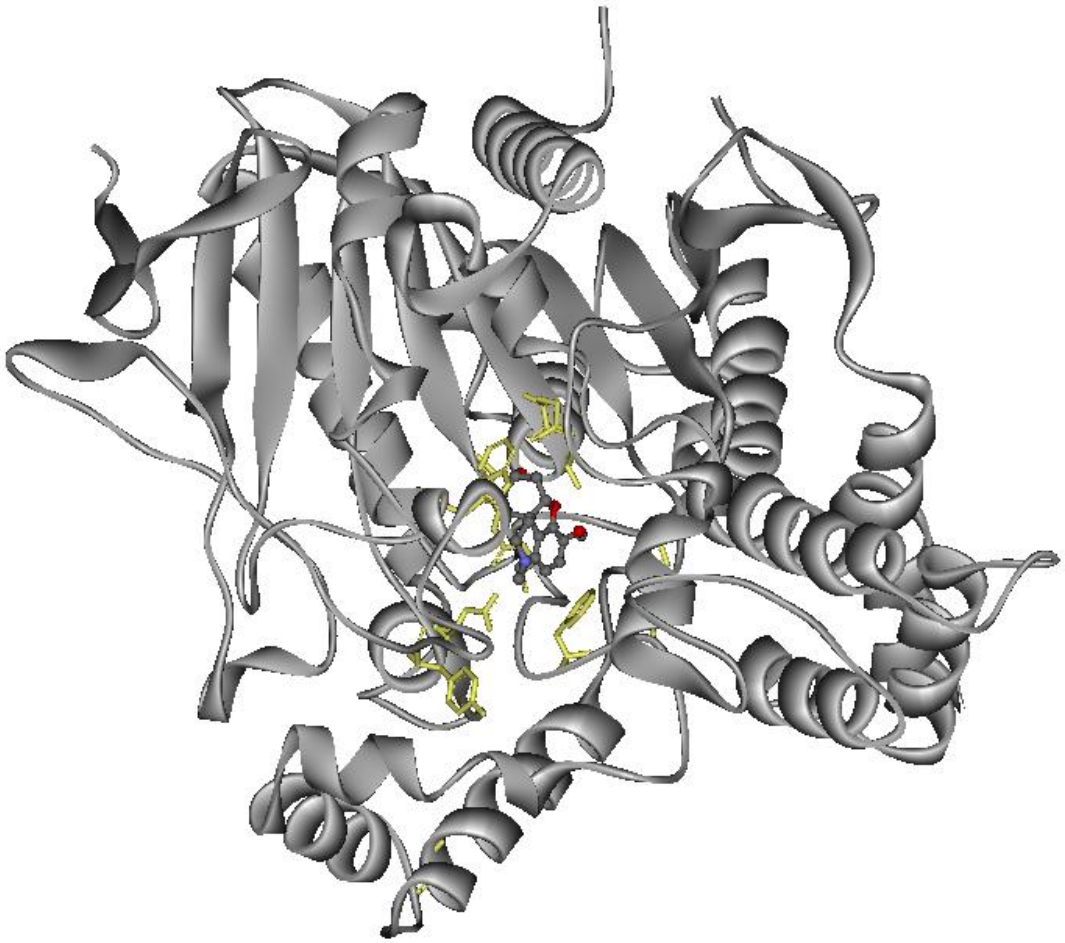
The dotted green lines denote hydrogen-bonding. However, hydrogens are not explicitly shown. For the hydrogen bond between PG4 and Gnt, there is a hydrogen on the O in PG4 that is the hydrogen-bond donor (HBD), while the lone pair of electrons on the nitrogen of Gnt is the hydrogen-bond acceptor (HBA) [there are no hydrogens on the tertiary amine N, so it cannot be an HBD]. The Glu is an anionic amino acid and the oxygens are not bonded to hydrogens and so an oxygen is the HBA. The hydroxyl hydrogen on Gnt (missing in the image at the top of the page) is the HBD. In some cases in LigPlots involving O and N, it is not always clear which is the HBD and which is the HBA.

The “eyelashes” denote other interactions, which were termed in an earlier version of LigPlot as “hydrophobic contacts” – but clearly were not as you could deduce by the interaction involving the -OH of Ser200 in the LigPlot above. The definition of the “eyelashes” is seemingly no longer on the webpage. You can assume they involve any of the interactions we have discussed for amino acid residues. There is another document linked to the assignment that gives more detail about these interactions.

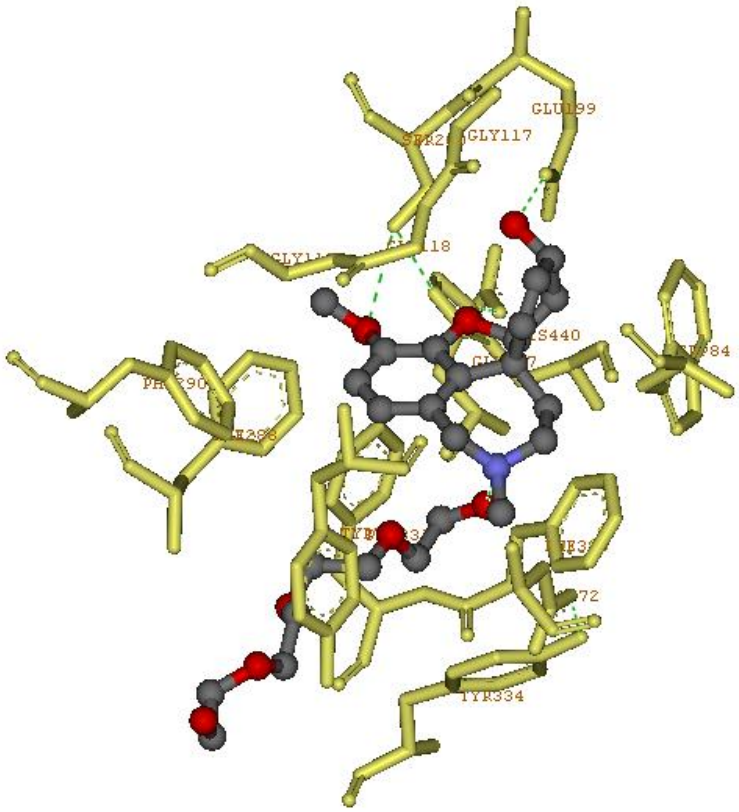
Sometimes the hydrogen-bonding interactions are with the amide groups of the protein backbone, not the side chains. The C=O of the peptide is the HBA and the NH of the peptide is the HBD.



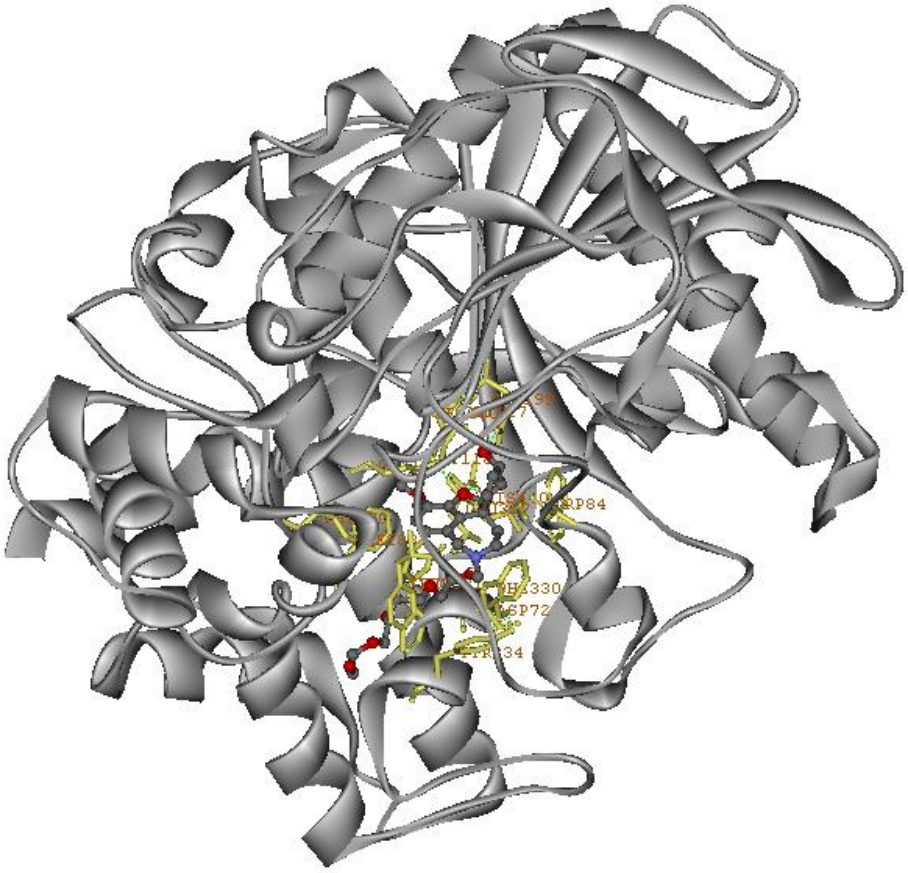
Galanthanine (ball and stick) within protein.



The interacting amino acid residues are shown in yellow.



Interactions between the amino acid residues and Gnt and PG4.
(Some of the interacting residues in the wiring diagram are interacting with other ligands, not galanthamine, and are not shown.)



Final rendering of the protein-heterocompound complex showing the interaction between the amino acid residues and the hetero compound.