# Molecular Dynamics Study of the Hapten-Binding Antibody B1-8

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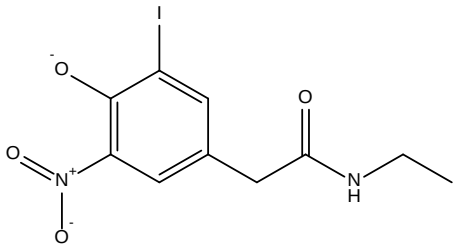
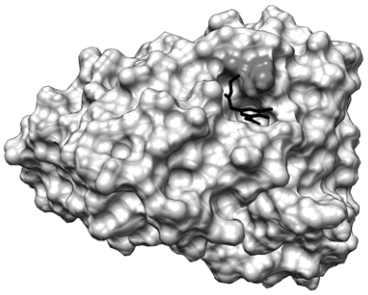



4-(2-(ethylamino)-2-oxoethyl)-2-iodo-6-nitrophenolate



Left: Structure of NIP. Right: B1-8 FV-Fragment (light grey) with NIP (black) and $Y101_H$ highlighted in dark grey.

Antibodies are vital to humoral immunity. With recurring exposures to the same antigen, the affinity of serum antibodies for this specific antigen will increase. This process is referred to as affinity maturation and can yield antibodies in a secondary response that have an affinity several orders of magnitude higher than in the primary response. The hapten-binding antibody B1-8 represents a model system to investigate affinity maturation. The mutation W33L in the heavy chain ($W33_HL$) is especially interesting since it always occurs in the secondary response and increases affinity approximately by one order of magnitude. This study uses MD-simulations of wildtype B1-8 and $W33_HL$ B1-8 in an unliganded state and bound to 4-(2-(ethylamino)-2-oxoethyl)-2-iodo-6-nitrophenolate (NIP) to assess the molecular basis for this increase in affinity. Initial results indicate that the $W33_HL$ mutation alters the dynamics of $Y101_H$, which in turn facilitates the access of ligands to the hapten binding pocket.