Figure 6: The occupancy of ligands on predicted pocket sites. Grey: the whole pocket sites, Red: mass center of pocket sites and Magenta: ligand.  

**a**). Carbonic anhydrase II (2cba), a perfect prediction. 

**b**). Acetylchitotriose (1hel) good prediction but only a small part of ligand atoms occupy the pocket sites. 

**c**). Purine nucleoside phosphorylase (1ula), the pocket sites cover all atoms of the ligand. The minimal distance is 5.10 Å since ligand is very small and it is not counted as a hit.