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How does an Amorphous Surface Influence Molecular Binding? - Ovocleidin-17 and Amorphous Calcium Carbonate

1 Supplementary Information

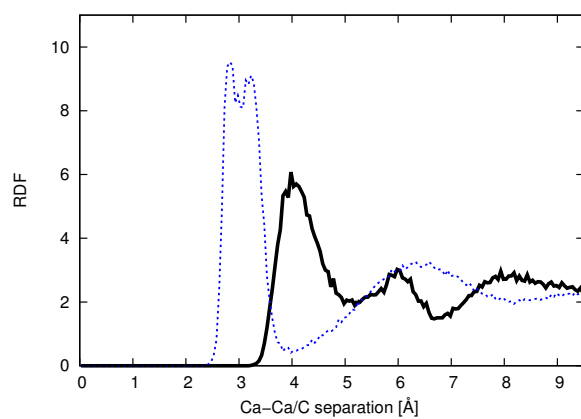


Figure 1 Radial Distribution of Ca-Ca (solid black) and Ca-C (dotted blue) for amorphous calcium carbonate slab.

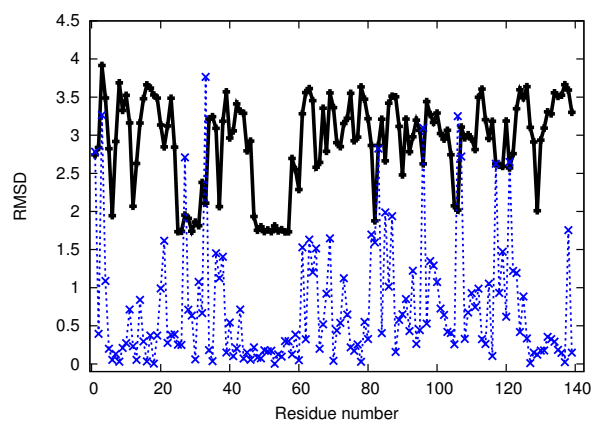


Figure 2 1-4 Root-mean Square Deviation of the OC-17 protein plotted to 2 standard deviations when solvated in water (solid black) and on the amorphous calcium carbonate surface (dotted blue).

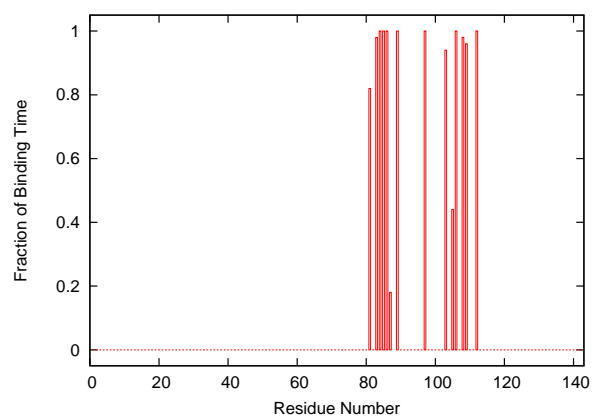


Figure 3 Fraction of simulation time residue spends bound to the amorphous calcium carbonate surface.

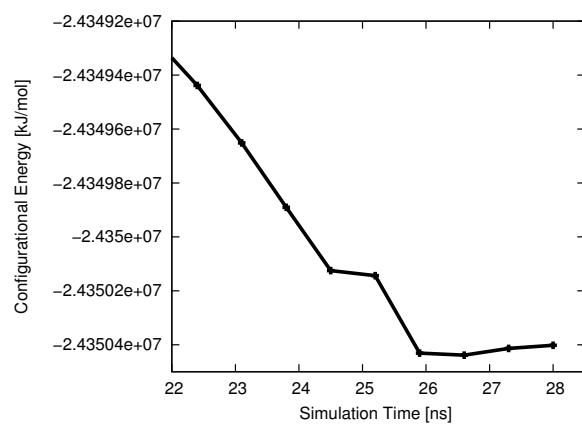


Figure 4 Configuration Energy of OC-17 bound to amorphous calcium carbonate over simulation.

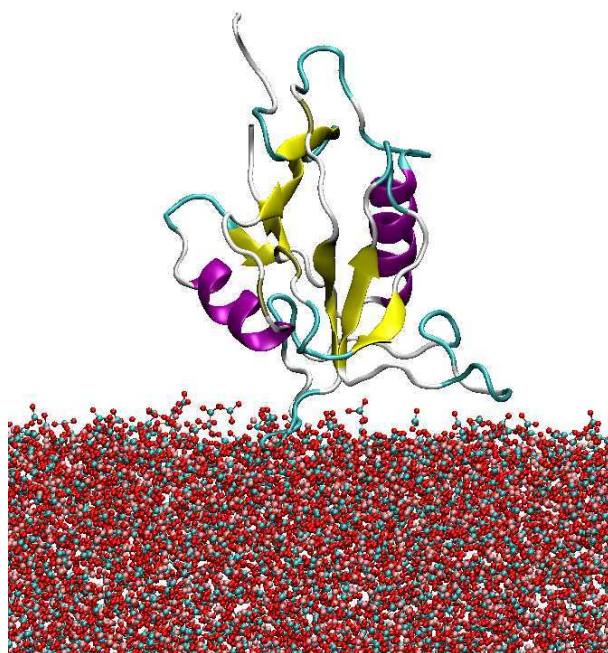


Figure 5 OC-17 binding to ACC highlighting backbone only.

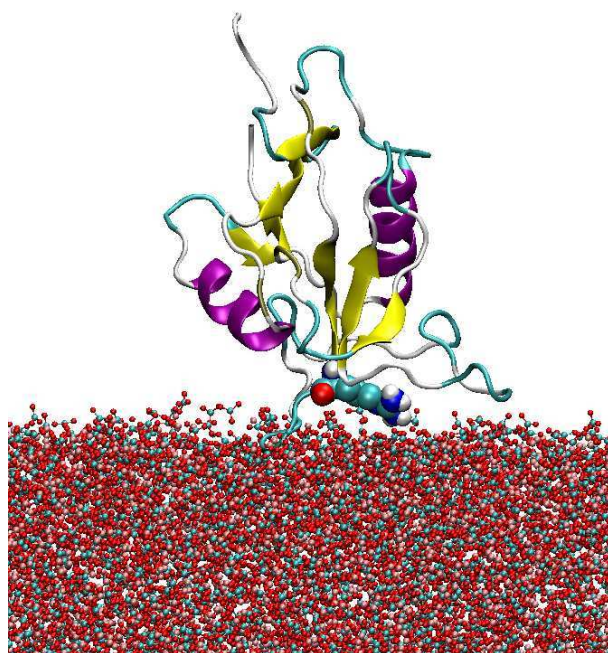


Figure 6 OC-17 binding to ACC highlighting residue 81 (arginine).

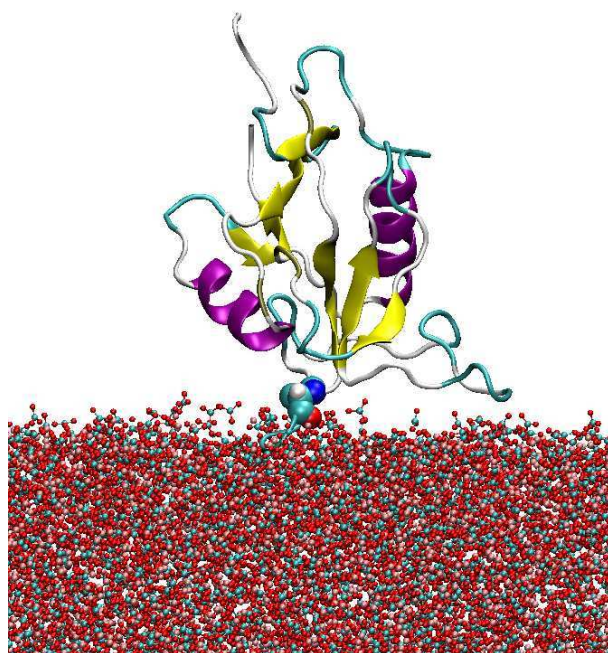


Figure 7 OC-17 binding to ACC highlighting residue 82 (proline).

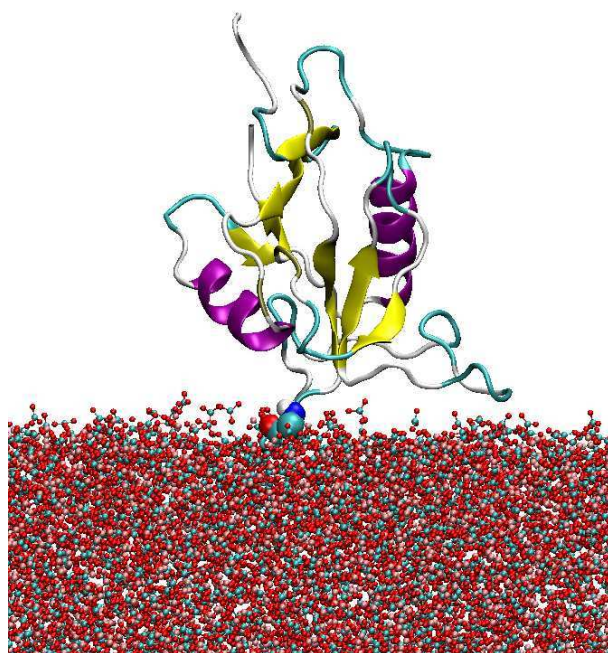


Figure 8 OC-17 binding to ACC highlighting residue 83 (alanine).

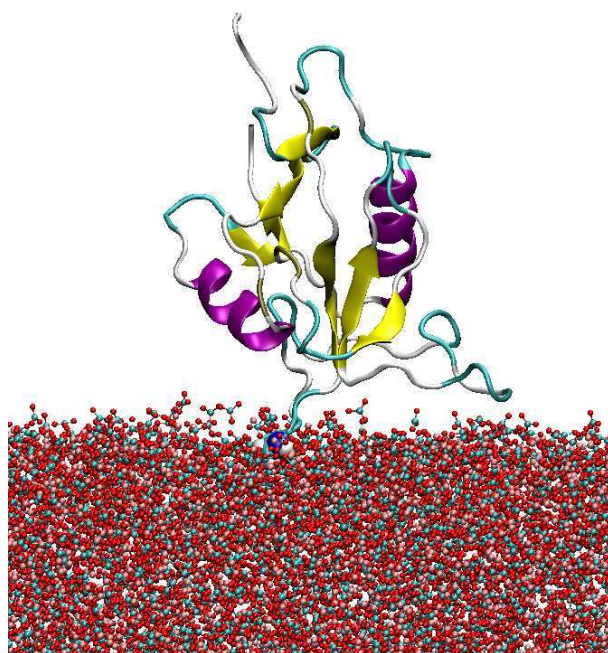


Figure 9 OC-17 binding to ACC highlighting residue 84 (glycine).

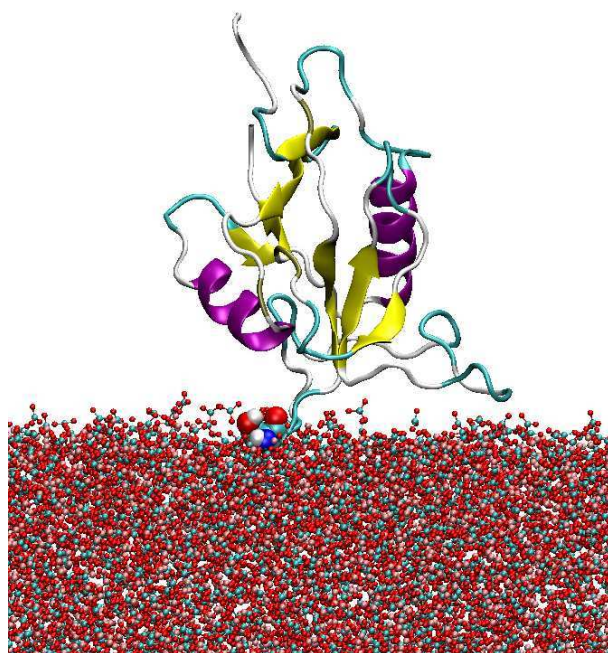


Figure 10 OC-17 binding to ACC highlighting residue 85 (serine).

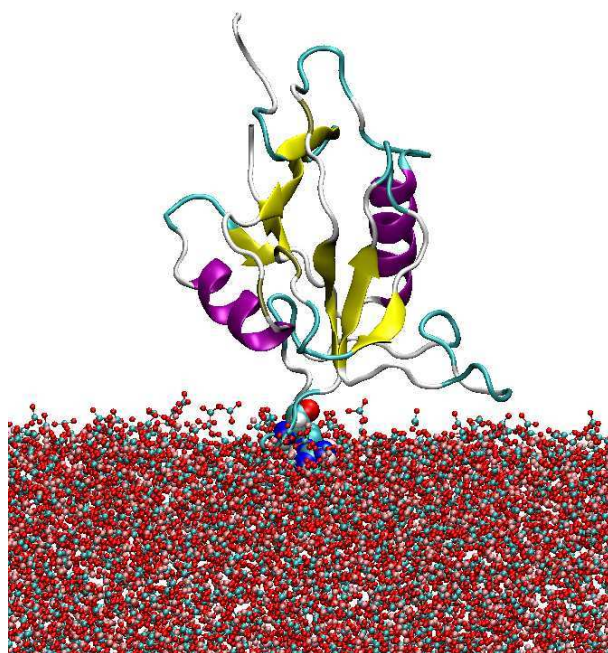


Figure 11 OC-17 binding to ACC highlighting residue 86 (arginine).

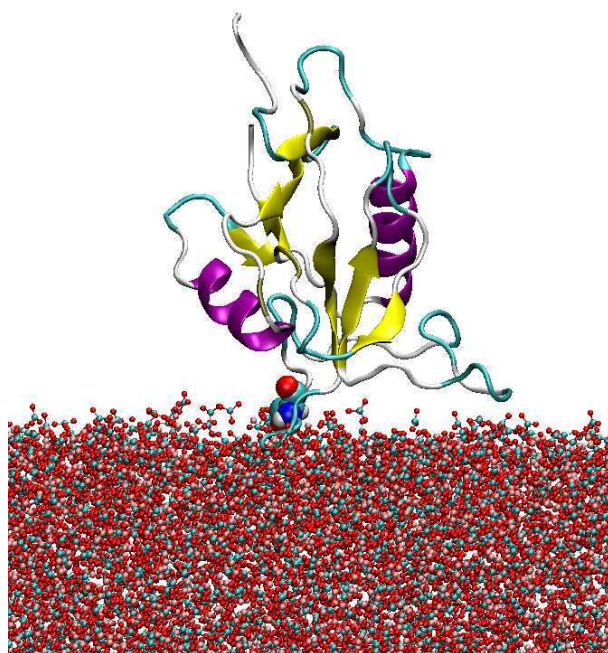


Figure 12 OC-17 binding to ACC highlighting residue 87 (serine).

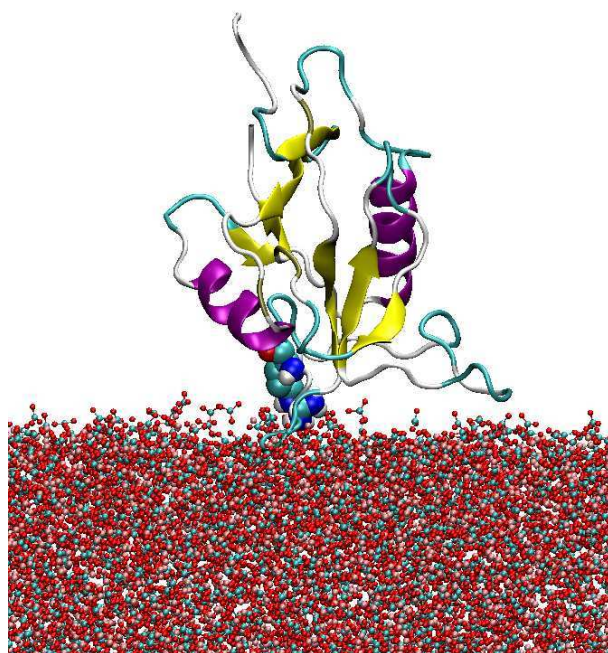


Figure 13 OC-17 binding to ACC highlighting residue 89 (arginine).

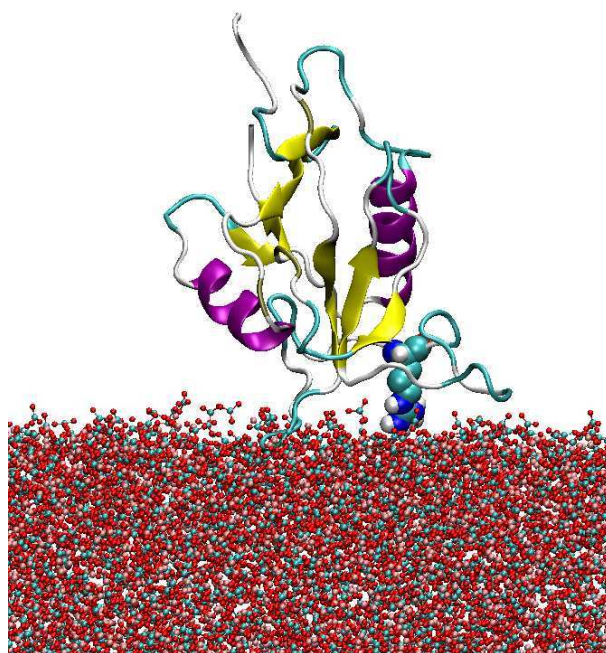


Figure 14 OC-17 binding to ACC highlighting residue 97 (arginine).

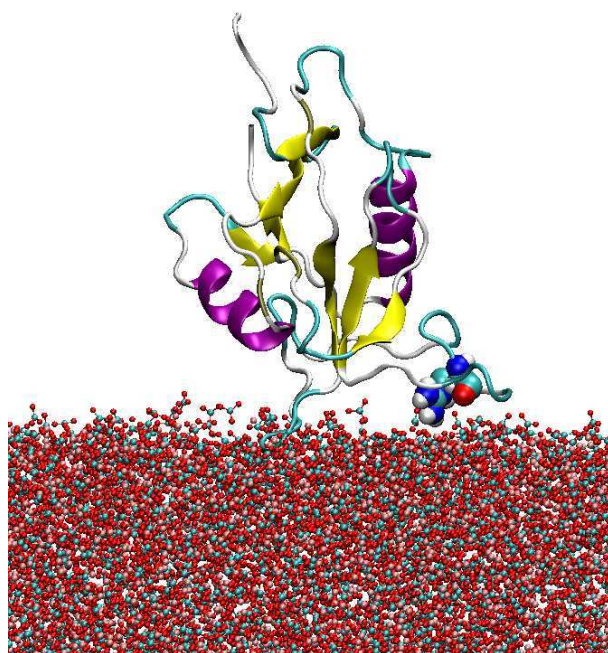


Figure 15 OC-17 binding to ACC highlighting residue 103 (arginine).

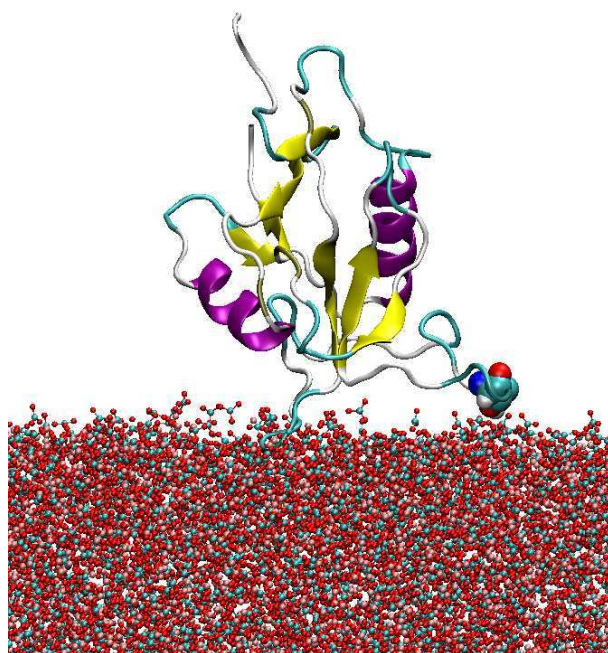


Figure 16 OC-17 binding to ACC highlighting residue 104 (threonine).

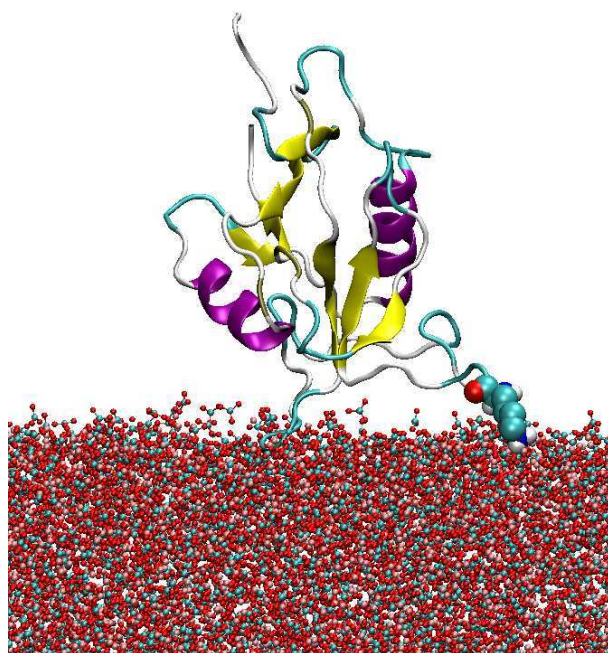


Figure 17 OC-17 binding to ACC highlighting residue 106 (lysine).

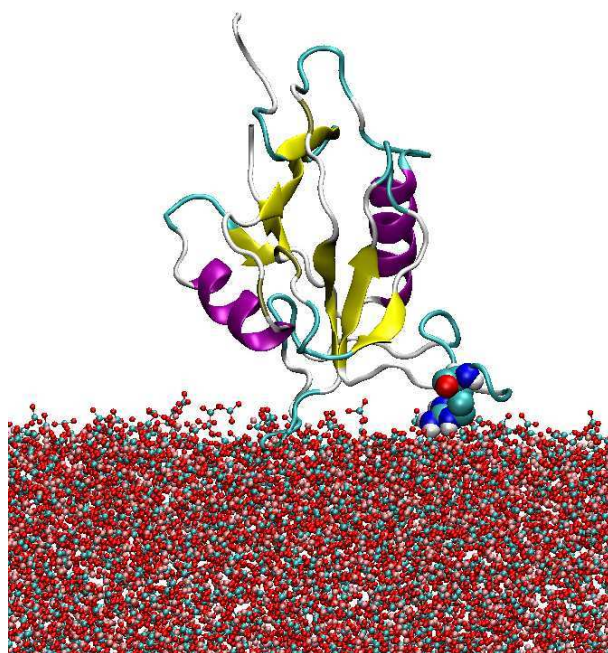


Figure 18 OC-17 binding to ACC highlighting residue 108 (arginine).

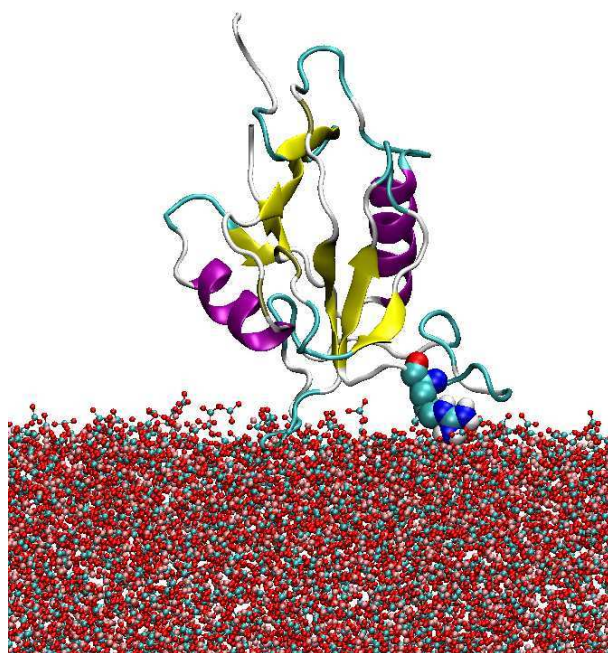


Figure 19 OC-17 binding to ACC highlighting residue 109 (arginine).

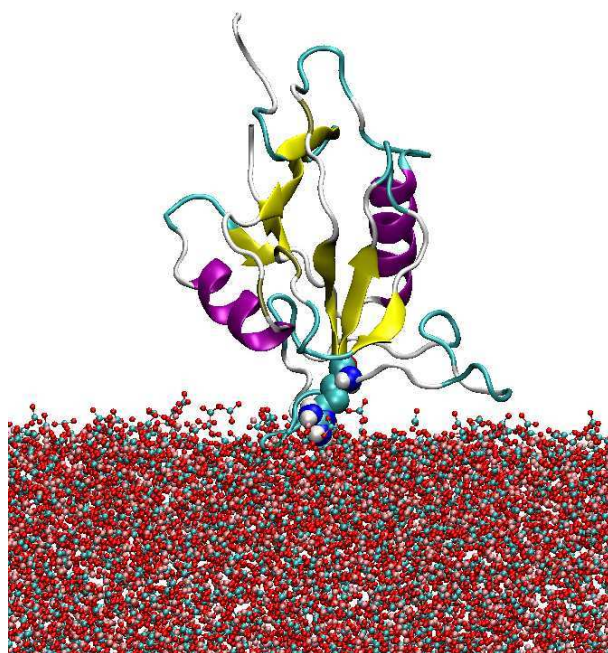


Figure 20 OC-17 binding to ACC highlighting residue 112 (arginine).