Supplementary Data

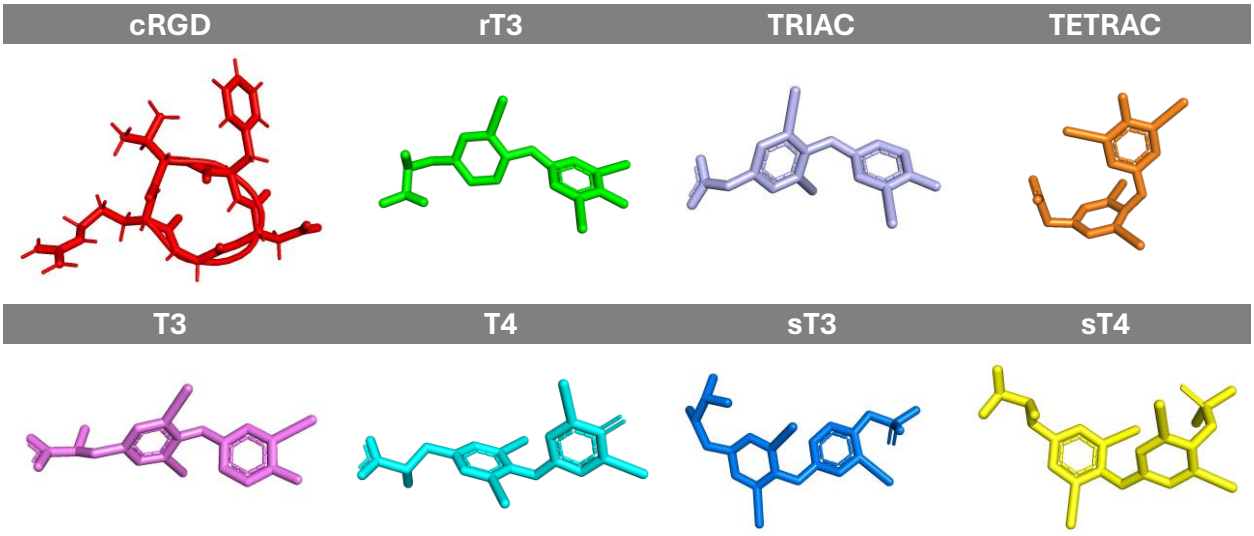
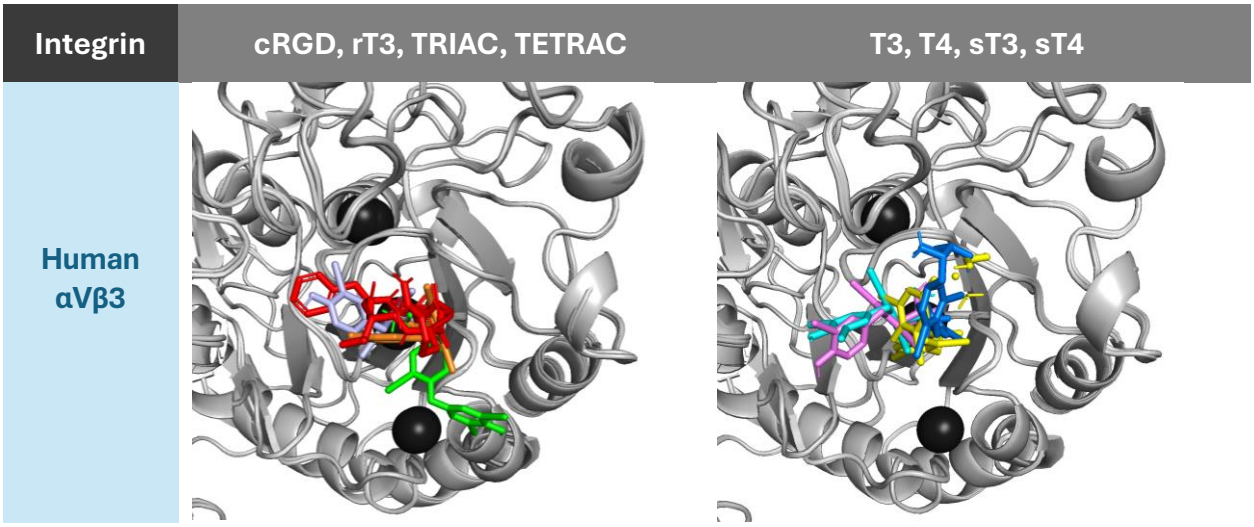
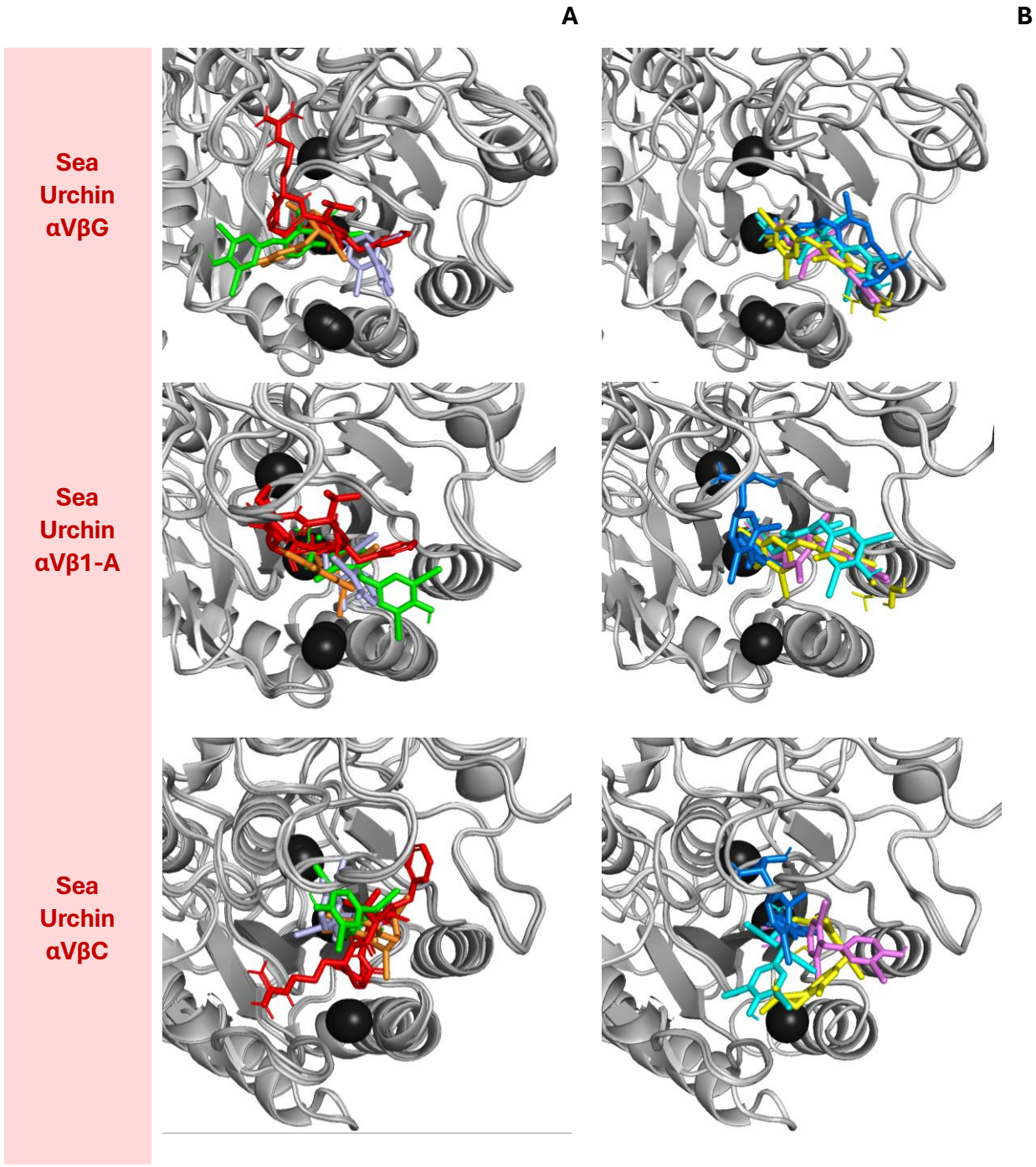


Figure 3. Chemical structures of the ligands used in the HADDOCK docking simulations. Ligands include the reference cyclic RGD peptide (cRGD), known for its high-affinity binding to αVβ3 integrin, and seven thyroid hormone metabolites: reverse triiodothyronine (rT3), triiodothyroacetic acid (TRIAC), tetraiodothyroacetic acid (TETRAC), triiodothyronine (T3), thyroxine (T4), sulfated triiodothyronine (sT3), and sulfated thyroxine (sT4).




A
B
Sea Urchin αVβG
Sea Urchin αVβ1-A
Sea Urchin αVβC

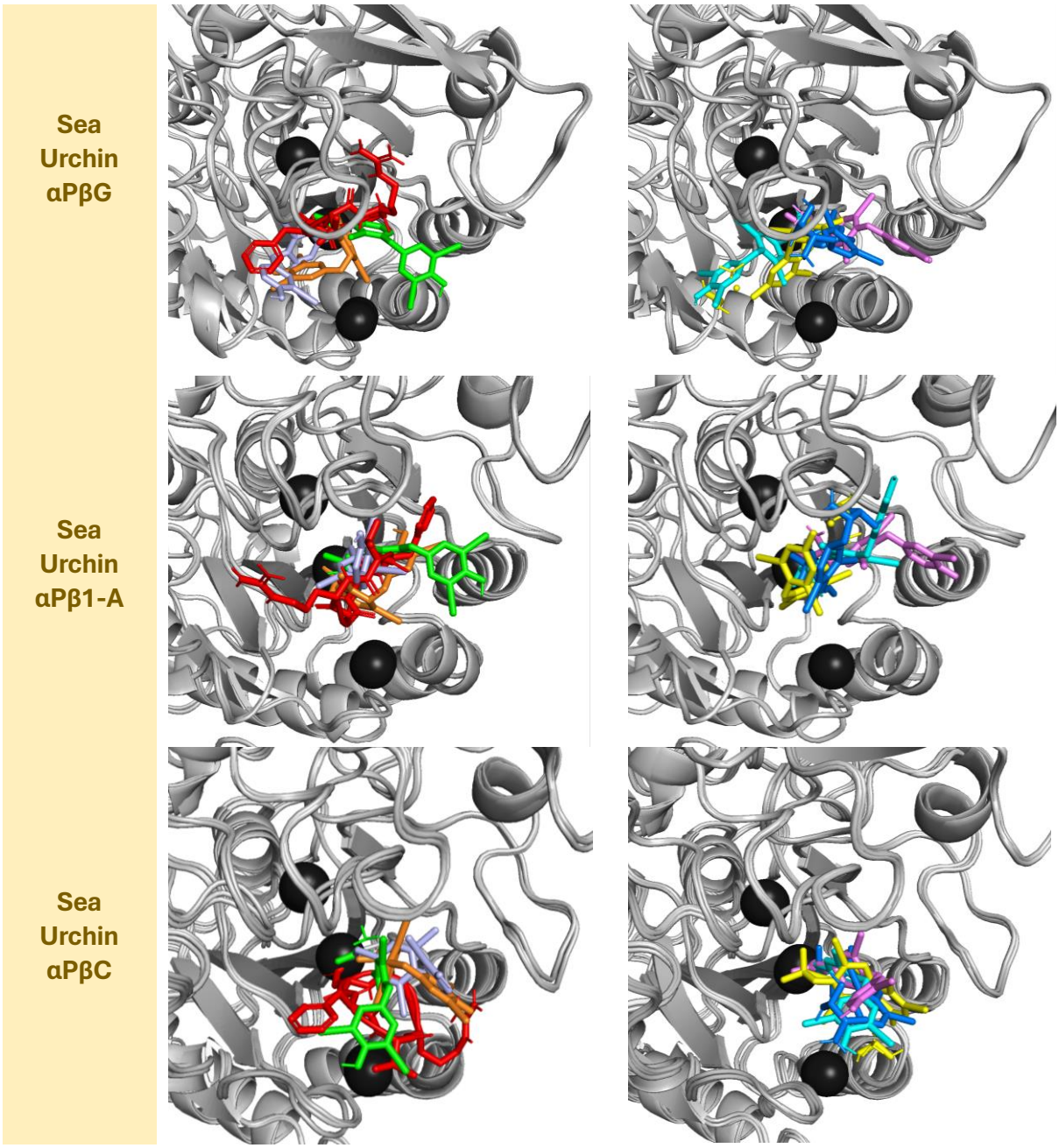


Figure 4. *Docking of cRGD, rT3, TRIAC, TETRAC, and thyroid hormones (T3, T4, sT3, sT4) to human αVβ3 and predicted sea urchin integrin heterodimers.* Left panels: cRGD (red), rT3 (green), TRIAC (light purple), and TETRAC (orange) bound at the RGD-binding site. Right panels: T3 (pink), T4 (cyan), sT3 (blue), and sT4 (yellow) bound at the thyroid hormone-binding site. Integrin dimers are shown as grey ribbons, with Mn^{2+} ions as black spheres.