Correct clinical evaluation and diagnosis are crucial for effective treatment of cancer to develop and evolve cancer theranostics for personalized cancer therapy. Owing to the rapid advancement and development in the field of nanotechnology, various kinds of nanoparticles are explored for cancer therapy. Organic-inorganic hybrid nanoparticles have attracted vast interest due to their promising physicochemical properties, which make them suitable for biomedical applications. In this work, hybrid nanoparticles are prepared through different kinds of supramolecular interactions using self-assembly of small molecules or polymers with inorganic nanoparticles or salts. By combining both organic and inorganic components, we envisaged that we could circumvent the typical limitations of organic molecules such as low resistance to photobleaching and poor degradability of the inorganic nanoparticles. Utilizing the organic component scaffolds as the carrier or direct therapeutic agent and inorganic nanoparticles as the imaging agents or the direct therapeutic agents, we could attain hybrid nanostructures that are biocompatible, stable, and highly efficient. We employed strategies such as surface functionalization, one-pot synthesis, and wrapping techniques to bring all the components together.