In medicine, a classical treatment method for cancer is based on non-specific intravenous administration of chemotherapeutics resulting in various adverse effects on healthy tissues and organs (systemic toxicity) of the patient. Other than cancer, microbial infections and intoxications have also become a major threat to human health due to the presence of pathogenic bacteria and various organic/inorganic pollutants in waste and drinking water. In this case, nanotechnology supports the development of mesoporous nanocarriers as site-specific active drug delivery vehicles for curative cancer treatment as well as magnetic nanoadsorbents and nanoantimicrobials with useful surface chemistry for the adsorption and entrapment of pollutants in water and for its consequent disinfection. The research work described in this thesis is focused on (I) the design, synthesis, and surface engineering of magnetic iron oxide nanoaggregates and mesoporous silica nanoparticles followed by (II) the adsorption, loading, and conjugation of different ions, targeting moieties (folic acid, estrogen, surface-active ionic liquids/SAILs), anti-tumor and bactericidal drugs (doxorubicin, tetracycline, SAILs), and/or radiotracers (DOTA-^{68}Ga/^{177}Lu for theranostics) to the carriers. Mesoporous silica nanocarriers functionalized with target ligands were tested against hormone-sensitive and triple-negative breast cancer cell lines to verify the specific uptake and efficiency of the developed approach. The nanocarriers exhibited an outstanding radiochemical yield and purity of > 98 % and excellent stability in serum. In triple-negative breast cancer cell lines, mesoporous silica nanocarriers functionalized with targeting moiety revealed a significant time-dependent cell uptake after radiolabeling with ^{177}Lu tracer. The combined targeted delivery of ^{177}Lu radiations and doxorubicin induced a significant cell death to triple-negative breast cancer cell lines tested (dual therapeutic effect).