The study of the brain is one of the most exciting frontiers in science and medicine today. Although neuroscience is by nature a multi-disciplinary effort, chemistry has played many critical roles in the development of modern neuroscience, neuropharmacology, and brain imaging. Chemistry, and the chemical probes it generates, such as molecular modulators, therapeutics, imaging agents, sensors, or actuators, will continue to impact neuroscience on both preclinical and clinical levels. In this course, two major themes will be discussed. In the first one, titled “Imaging brain function with chemical tools,” we will discuss molecular designs and functional parameters of widely used fluorescent sensors in neuroscience (calcium, voltage, and neurotransmitter sensors), their impact on neuroscience, pros and cons of genetically encoded sensors versus chemical probes, and translatability of these approaches to the human brain. In the second major theme, titled “Perturbation of the brain function with chemical tools,” we will examine psychoactive substances, the basics of medicinal chemistry, brain receptor activation mechanisms and coupled signaling pathways, and their effects on circuit and brain function. We will also discuss recent approaches, failures and successes in the treatment of neurodegenerative and psychiatric disorders. Recent advances in precise brain function perturbation by light (optogenetics and photopharmacology) will also be introduced. In the context of both themes we will discuss the current and future possibilities for the design of novel functional materials, drawing on the wide molecular structural space (small molecules, proteins, polymers, nanomaterials), aimed at monitoring, modulating, and repairing human brain function. This course is intended for students (undergraduate and graduate) with diverse majors/specializations (e.g., science, engineering, and medical majors/departments).