Research in the field of drug design has led to the development of algorithms for screening large numbers of compounds on the computer. In one common approach, molecular fragments are positioned within the protein active site and complete molecules are generated by covalently connecting them using linking fragments taken from a database. Although many potential applications exist in chemistry, software to allow the application of fragment-based design methods outside of proteins was lacking. To overcome this limitation we created HostDesigner, a code that builds and evaluates millions of 3D molecular structures in minutes on a laptop computer. This talk describes recent improvements to this software that enable the general application of structure-based design methods in supramolecular chemistry. Examples demonstrate how the software has been used to guide the design of ligands for metal ions, anion receptors, and molecular shapes that direct the formation of self-assembled polyhedra. HostDesigner is available at no cost from https://sourceforge.net/projects/hostdesigner/.