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drug design

Drug design includes not only ligand design, but also pharmacokinetics and toxicity, which are mostly beyond the possibilities of structure- and/or computer-aided design. Nevertheless, appropriate chemometric tools, including experimental design and multivariate statistics, can be of value in the planning and evaluation of pharmacokinetic and toxicological experiments and results. Drug design is most often used instead of the correct term 'Ligand Design'.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1142

