Generating bioactive molecules *de novo*

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The computer-assisted generation of new chemical entities (NCEs) has matured into solid technology supporting early drug discovery. Both ligand- and receptor-based methods are increasingly used for designing small lead- and druglike molecules with anticipated multi-target activities. Advanced "polypharmacology" prediction tools are essential pillars of these endeavors. In addition, it has been realized that iterative design-synthesis-test cycles facilitate the rapid identification of NCEs with the desired activity profile. Lab-on-a-chip platforms integrating synthesis, analytics and bioactivity determination and controlled by adaptive, chemistry-driven *de novo* design software will play a decisive role for future drug discovery.