Ligand design software

1) Open Source software:

AutoClickChem; LigMerge (National Biomedical Computation Resource): produce large combinatorial libraries of compound models for use in virtual screens; systematically ‘swapping’ the chemical moieties of known ligands to generate novel ligands

CrystalDock (National Biomedical Computation Resource): use PDB database to identify molecular fragment and micro-environment for drug design.

AutoGrow, (Prof. J.A. McCammon, UCSD): Applying evolutionary algorithm that optimizes candidate ligands for predicted binding affinity and other druglike properties.

LigBuilder (Prof. Luhua Lai, PKU): multiple-purposed program for structure-based de novo drug design and optimization including ligand generation using fragments

LEA3D (Institut de Pharmacologie Moléculaire et Cellulaire) : Invent ideas of ligand (scaffold-hopping) by the de novo drug design. free program available for an academic use only. Also integrated with online service for drug design and screen.

GANDI (prof. Amedeo Caflisch, Zurich University): structure-based fragment-based ab initio (de novo) ligand design. Provide upon request.

Some algorithms such as LoFT, CoG, Flux were mainly described in research articles with access to the software.

2) Free Software:

ChemT (BioChemCore): building chemical compound libraries, based on a specific chemical template.

Legio; Indigo Toolkit (GGA software): explores the combinatorial chemistry.

3) Commercial software:

Discovery Studio (Accelrys): Enumerate reaction- or core-based libraries & CATALYST pharmacophore generation and virtual screening.

MOE (Chemical Computing Group): Ligand & Structure-Based Scaffold Replacement, Ligand & Structure-Based Query Editor, Pharmacophore Search, etc.

Core Hoping; Phase; CombiGlide (Schrodinger): ligand- and receptor-based scaffold exploration & pharmacophore modeling

SYBYL-X; Muse (Certata, formally Tripos): Ligand-based virtual screening; Uses a ligand-based scoring to generate ideas that optimize the shape and pharmacophoric similarity to a set of lead structures.

ReCore; FTrees-FS; LeadIT (BioSolveIT): 3D Scaffold Hopping; combinatorial fragment space extension, integrate other tools such as FlexNovo, CoLibri’s fragment library.

ACD/Structure Design Engine (ACDLabs): modification of a molecular scaffold and property-based structure optimization

SPROUT; (SimBioSys): structure-based fragment-based ab initio ligand design, based on growing and linking approaches.

AlleGrow; (Boston De Novo Design): based on growing and combinatorial approaches.

BOMB; (Cemcomco, LLC): De Novo Design; Molecule, Library and Model Building

ChIP (Eidogen-Sertanty, Inc.) exploration of synthetically feasible small molecule chemical space

NSisDesign & NSisNovo (Noesis Informatics): provide molecular library design tool and de novo molecular design tool

LeadGrow+ (vLife): Creating molecular library for effective scaffold hopping

INDDEx™ (Equinox Pharma): logic-based machine-learning technique for QSAR and virtual screening.

MED-SuMo/MED-Ligand (MEDIT): fragment-based drug design

MedChem Studio (Simulations Plus, Inc): Enumerate combinatorial chemistry libraries and synthetic; Perform R Group decomposition and scaffold hopping

Quasi; SkelGen; etc (De Novo Pharmaceuticals): de novo design of molecules to bind into its active site; Fragment-based drug design; ligand-based drug design

EMIL (CompuDrug): chemical modifications to hits

ilib diverse (inte:ligand): creating compounds by by combining user-defined fragments.

4) Commercial Service

GeometryLifeSci uses its proprietary GeometryFit & GLS-Fit technologies to help on drug design.