**Table 7.1 Overview of Currently Used Programs for Protein–Ligand Docking**

| Class of Docking Method[a] | Name of Program | Year Published | Original References | Selected References to Further Developments and Applications |
|---|---|---|---|---|
| **Geometric/combinatorial** | | | | |
| **Shape/descriptor** matching | DOCK | 1982 | (106) | (11, 127, 143, 371) |
| | FLOG | 1994 | (121) | (366) |
| | ADAM | 1994 | (135) | (386) |
| | LIGIN | 1996 | (387) | (234) |
| | SANDOCK | 1998 | (105) | (13) |
| | QSDOCK | 2000 | (136) | |
| | SLIDE | 2000 | (111) | |
| | FRED | 2001 | (123) | |
| | (Diller & Merz) | 2001 | (112) | |
| Incremental construction | FlexX | 1996 | (110) | (130, 138, 139, 216, 233) |
| | Hammerhead | 1996 | (388) | |
| | DOCK4.0 | 1998 | (328) | (131) |
| Systematic search (transl. + rot.) | EUDOC | 2001 | (125) | (389) |
| **Energy-driven/stochastic** | | | | |
| Monte Carlo simulated annealing | AutoDock | 1990 | (113) | (95, 115, 390) |
| | RESEARCH | 1992 | (146) | (145) |
| | MCDOCK | 1999 | (147) | |
| Monte Carlo minimization | ICM | 1994 | (116) | (82, 117, 201) |
| | (Caflisch et al.) | 1997 | (150) | (151) |
| | QXP | 1997 | (152) | |
| | PRODOCK | 1998 | (119) | (118) |
| Molecular dynamics (MD) | MDD | 1994 | (164) | (165) |
| | (Luty et al.) | 1995 | (169) | |
| | (Vieth et al.) | 1998 | (166) | |
| | q-jumping MD | 2000 | (167) | (168) |
| Genetic algorithm | GOLD | 1995 | (176) | (177) |
| | AutoDock3.0 | 1998 | (115) | (208, 228, 391) |
| | GAMBLER | 1999 | (86) | |
| | DARWIN | 2000 | (178) | |
| Tabu search | PRO_LEADS | 1998 | (188) | (189, 360) |
| Tabu search + genetic algorithm | SFDock | 1999 | (392) | |
| Eigenvector following | Low Mode Search | 1999 | (211) | |
| Mining Minima algorithm | Mining Minima | 2001 | (190) | |

[a]The classification provided in the first column can only be approximate for programs that offer a variety of different functionalities or follow multistep strategies.

tion of protein structures. The general principle of this approach is that the protein is represented by a set of affinity grids or maps that cover the entire search region. These regularly spaced, orthogonal grids are calculated before the actual docking process. At every grid point, some sort of scoring value or interaction energy of a probe atom with the entire