Table 1. Algorithms for Docking Small Molecules or Fragments against a Target					
	Program	Flexible Protein?	Flexible Ligand?	Description	Reference
Virtual screening	DOCK	no	yes	docks either small molecules or fragments, includes solvent effects	[46‑49]
	FlexX	no	yes	incremental construction	[51]
	FlexE	yes	yes	incremental construction; samples ensembles of receptor structures	[52]
	SLIDE	yes	yes	anchor fragments placed, remainder of ligand added; backbone flexibility	[50]
	Flo98	no	yes	can rapidly dock a large number of ligand molecules, graphically view results	[76]
	ADAM	no	yes	fragments aligned based on hydrogen bonding	[77]
	Hammerhead	no	yes	genetic algorithms to link tail fragments to anchor fragments	[78]
	MCSA-PCR	yes	yes	uses simulated annealing to generate conformations of target	[64]
	AUTODOCK	yes	yes	uses averaged interaction energy grid to account for receptor conformations and simulated annealing for ligand conformations	[79]
	MCDOCK	no	yes	Monte Carlo to sample ligand placement	[80]
	ProDOCK	yes	yes	Monte Carlo minimization for flexible ligand, flexible site	[81]
	ICM	yes	yes	Monte Carlo minimization for proteinligand docking	[82]
	DockVision	no	no	Monte Carlo minimization	[83]
De novo generation of ligands	LUDI	no	yes	docks and scores fragments	[54]
	GRID	no	yes	calculates binding energies for functional groups	[55]
	MCSS	no	yes	exhaustive search of binding site for functional group minima	[56]
	SMoG	no	yes	knowledge-based scoring function;molecules built by joining rigid fragments	[58]
	CONCERTS	no	yes	fills active site with molecular fragments,links fragments	[57]
	Legend	no	yes	grows molecule atom by atom	[84]
	DLD	no	yes	saturates binding site with sp3 carbons,later linked	[85]
	GrowMol	no	yes	builds ligands from a library of atom types	[86]
	GenStar	no	yes	builds ligands from sp3 carbons	[87]
	GROW	no	yes	constructs a peptide by residue addition	[88]
	GroupBuild	no	yes	builds ligand from a predefined library of fragments	[89]
	HOOK	no	yes	searches database of molecular skeletons for fit to binding site; hooks two MCSS functional groups to skeleton	[90]
	SPROUT	no	yes	generates skeletons that fit site, substitutes atoms into skeleton to give molecule with correct properties	[91]
	CAVEAT	no	yes	searches database of small molecules to connect fragments	[92]