

Program	Scoring Function	Function componet	Component ID
Dock 6.8	Grid	Grid_Score	D6Grid
		Grid_vdw_energy	D6GridVDW
		Grid_es_energy	D6GridES
		Internal_energy_repulsive	D6GridInt
	Contact	Contact_Score	D6Contact
	Continuous	Continuous_Score	D6Continuous
		Continuous_vdw_energy	D6ContinuousVDW
		Continuous_es_energy	D6ContinuousES
	Hawkins	Hawkins_GBSA_Score	D6Hawkins
		Hawkins_GBSA_vdw_energy	D6HawkinsVDW
		Hawkins_GBSA_es_energy	D6HawkinsES
		Hawkins_GBSA_gb_energy	D6HawkinsGB
		Hawkins_GBSA_sa_energy	D6HawkinsSA
	D6Pbsa	PBSA_Score	D6Pbsa
		PBSA_vdw_energy	D6PbsaVDW
		PBSA_pb_energy	D6PbsaPB
		PBSA_sa_energy	D6PbsaSA
	SASA	SASA_Score	D6SASA
		SASA_com_lig_sasa_tot	D6SASAComLigTot
		SASA_lig_sasa_tot	D6SASALigTot
		SASA_%_phobic_lig_exposed	D6SASAPercPhobicExpo
		SASA_com_lig_sasa_phobic	D6SASAComPhobic
		SASA_lig_sasa_phobic	D6SASAPhobic
		SASA_%_philic_lig_exposed	D6SASAPercPhilicExpo
		SASA_com_lig_sasa_philic	D6SASAComPhilic
		SASA_lig_sasa_philic	D6SASAPhilic
		SASA_%_other_lig_exposed	D6SASAPercOtherExpo
		SASA_com_lig_sasa_other	D6SASAComOther
		SASA_lig_sasa_other	D6SASAOther
		OEDocking	ChemGauss 3
CG3:Steric	OECCG3Steric		
CG3:Clash	OECCG3Clash		
CG3:ProDesolv	OECCG3ProDesolv		
CG3:LigDesolv	OECCG3LigDesolv		
CG3:LigDesolvHB	OECCG3LigDesolvHB		
CG3:Acc	OECCG3ACC		
CG3:Don	OECCG3Don		
CG3:Metal	OECCG3Metal		
ChemGauss 4	Chemgauss4		OEChemgauss4
	CG3:Steric		OECCG4Steric
	CG3:Clash		OECCG4Clash
	CG3:ProDesolv		OECCG4ProDesolv
	CG3:LigDesolv		OECCG4LigDesolv
	CG3:LigDesolvHB		OECCG4LigDesolvHB
	CG4:HB		OECCG4HB
ChemScore	Chemscore		OEChemScore
	CS:RB		OECSRB
	CS:Clash		OECSClash
	CS:LIPO		OECSLipo
	CS:METAL		OECSMetal
PLP	CS:HB		OECSHB
	PLP		OEPLP
	PLP:NonPolar		OEPLPNonPolar
	PLP:HB		OEPLPHB
Shapegauss	PLP:Metal		OEPLPMetal
	PLP:Sulphur		OEPLPSulphur
	Shapegauss		OEShapegauss
Gold	ASP		Score
		NoSimplexScore	GASPNoSimpler
		ASP	GASPASP
		S(Map)	GASPS
		DE(clash)	GASPDEClash
		DE(int)	GASPDeInt
	ChemScore	Score	GChemscore
		NoSimplexScore	GCSNoSimplex
		DG	GCSDG
		S(hbond)	GCSSHB
		S(metal)	GCSSMetal
		S(lipo)	GCSSLipo
		H(rot)	GCSHRot
		DE(clash)	GCSDeClash
		DE(int)	GCSDeInt
	GoldScore	Fitness	GGoldscore
		NoSimplexScore	GGSNoSimpler
		S(hb_ext)	GGSSHBExt
		S(vdw_ext)	GGSSVDWExt
		S(hb_int)	GGSSHBInt
		S(int)	GGSSInt
	PLP	Score	GPLP
		NoSimplexScore	GPLPNoSimpler
		S(PLP)	GPLPSPLP
		S(hbond)	GPLPSHB
		S(cho)	GPLPSCO
		S(metal)	GPLPSMetal
		DE(clash)	GPLPDEClash
DE(tors)		GPLPDETors	
Dock 3.6	Dock 3.6 (From .eel1 file)	energy	Dock35