

# 1 FireDock Scoring Parameters

Name	Enzyme/Inhibitor		Antibody/Antigen		Others	
	coarse	full	coarse	full	coarse	full
attrVdWWeight	1	1	1.5	1.5	1.5	1.5
repVdWWeight	0.95	0	0.6	0.1	0.8	0
ACEWeight	1.6	1.6	1.6	1.6	1.6	1.6
attrElWeight	0.07	0.07	0.21	0.21	0.21	0.21
repElWeight	0.12	0.12	0.21	0.21	0.21	0.21
l_attrElWeight	0	0	0.46	0.46	0	0
l_repElWeight	0.3	0.3	0.69	0.69	0.69	0.69
HBWeight	1.32	1.32	1.2	1.2	1.2	1.2
pipiWeight	1	1	1	1	1	1
catpiWeight	0.8	0.8	0.7	0.7	0.7	0.7
aliphWeight	0.5	0.5	2.5	2.5	2.5	2.5
insidenessWeight	1.55	1.55	0	0	0.7	0.7
confProbWeight	0	0	0	0	0	0

Table 1: Program parameters for score calculation for different complex types. Parameters are specified for the full and coarse refinement stages.

The parameters described in the table are weights of the following scoring terms:

- *attrVdWWeight* - softened attractive van der Waals interactions
- *repVdWWeight* - softened repulsive van der Waals interactions
- *attrElWeight* - attractive short-range Coulomb electrostatics
- *repElWeight* - repulsive short-range Coulomb electrostatics
- *l\_attrElWeight* - attractive long-range Coulomb electrostatics
- *l\_repElWeight* - repulsive long-range Coulomb electrostatics
- *ACEWeight* - Atomic Contact Energy (ACE) potential
- *HBWeight* - hydrogen and disulfide Bonds
- *catpiWeight* - cation- $\pi$  stacking
- *pipiWeight* -  $\pi$ - $\pi$  stacking
- *aliphWeight* - aliphatic interactions
- *insidenessWeight* - “insideness” measure
- *confProbWeight* - internal energy