# Tables

**Table 1. Geometric parameters for empirical terms**

| Term | X | $X_0$ | $\Delta X_{min}$ | $\Delta X_{max}$ | Description |
|---|---|---|---|---|---|
| $S_{polar}$ | $R_{12}$ | $\Sigma R + 0.05$Å | 0.25Å | 0.6Å | Distance between interaction centres |
| | $\alpha_{DON}$ | 180° | 30° | 80° | Angle around donor H |
| | $\alpha_{ACC}$ | 180° | 60° | 100° | Angle around acceptor |
| | $\alpha_{C+}$ | 180° | 60° | 100° | Angle between C+…ACC vector and normal to plane of guanidinium group |
| | $\phi_{ACC\_LP}$ | 45° | 15° | 30° | From ref [] Figure 2. |
| | $\theta_{ACC\_LP}$ | 0° | 20° | 60° | From ref [] Figure 2. |
| | $\phi_{ACC\_PLANE}$ | 0° | 60° | 75° | From ref [] Figure 2. |
| | $\theta_{ACC\_PLANE}$ | 0° | 20° | 60° | From ref [] Figure 2. |
| $S_{repul}$ | $R_{12}$ | $\Sigma R + 1.1$Å | 0.25Å | 0.6Å | Distance between interaction centres |
| | $\alpha_{DON}$ | 180° | 30° | 60° | Angle around donor H |
| | $\alpha_{ACC}$ | 180° | 30° | 60° | Angle around acceptor |
| $S_{arom}$ | $R_{perp}$ | 3.5Å | 0.25Å | 0.6Å | From ref [] Figure 3 |
| | $\alpha_{Slip}$ | 0° | 20° | 30° | From ref [] Figure 3 |

[a] Geometric variable; [b] Ideal value; [c] Tolerance on ideal value; [d] Deviation at which score is reduced to zero

**Table 2. Angular functions used to describe attractive and repulsive polar interactions**

| IC1[a] | $ANG_{IC1}$[b] | IC2[a] | $ANG_{IC2}$[b] |
|---|---|---|---|
| **Attractive ($S_{polar}$)** | | | |
| DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ | ACC_LP | $f_1(\lvert\Delta\phi_{ACC\_LP}\rvert).f_1(\lvert\Delta\theta_{ACC\_LP}\rvert)$ |
| DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ | ACC_PLANE | $f_1(\lvert\Delta\phi_{ACC\_PLANE}\rvert).f_1(\lvert\Delta\theta_{ACC\_PLANE}\rvert)$ |
| DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ | ACC | $f_1(\lvert\Delta\alpha_{ACC}\rvert)$ |
| M+ | 1 | ACC_LP | $f_1(\lvert\Delta\phi_{ACC\_LP}\rvert).f_1(\lvert\Delta\theta_{ACC\_LP}\rvert)$ |
| M+ | 1 | ACC_PLANE | $f_1(\lvert\Delta\phi_{ACC\_PLANE}\rvert).f_1(\lvert\Delta\theta_{ACC\_PLANE}\rvert)$ |
| M+ | 1 | ACC | $f_1(\lvert\Delta\alpha_{ACC}\rvert)$ |
| C+ | $f_1(\lvert\Delta\alpha_{C+}\rvert)$ | ACC_LP<br>ACC_PLANE<br>ACC | $f_1(\lvert\Delta\alpha_{ACC}\rvert)$ |
| **Repulsive ($S_{repul}$)** | | | |
| DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ | DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ |
| DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ | M+ | 1 |
| DON | $f_1(\lvert\Delta\alpha_{DON}\rvert)$ | C+ | 1 |
| M+ | 1 | C+ | 1 |
| C+ | 1 | C+ | 1 |
| ACC_LP<br>ACC_PLANE<br>ACC | $f_1(\lvert\Delta\alpha_{ACC}\rvert)$ | ACC_LP<br>ACC_PLANE<br>ACC | $f_1(\lvert\Delta\alpha_{ACC}\rvert)$ |

[a] Interaction centre types; [b]angular functions in **Error! Reference source not found.**

Table 3. Performance of WSAS model

| Solute class | Class size | RMS error (kcal/mol) | MAE (kcal/mol) |
|---|---|---|---|
| Hydrocarbons | 66 | 0.78 | 0.63 |
| Neutral | 382 | 0.74 | 0.56 |
| Ions | 13 | 2.52 | 1.82 |
| All | 395 | 0.86 | 0.60 |
| (Wang et al) | 401 | 0.79 | 0.54 |

**Table 4. Intermolecular scoring function weights under evaluation**

| SF | $W_{vdw}$ | $W_{polar}$ | $W_{solv}$ | $W_{repul}$[a] | $W_{arom}$ | $W_{rot}$[a] | $W_{const}$[a] | R[c] | RMSE[c] |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.400 | - | - | - | - | 0.000 | 0.000 | 0.62 | 10.9 |
| 1 | 1.126 | 2.360 | - | - | - | 0.217 | 0.000 | 0.64 | 10.2 |
| 2 | 1.192 | 2.087 | - | 2.984 | - | 0.000 | 0.000 | 0.63 | 10.4 |
| 3 | 1.000[b] | 3.400[b] | - | 5.000[b] | - | 0.000 | 0.000 | 0.59 | 10.9 |
| 4 | 1.317 | 3.560 | 0.449 | - | - | 0.000 | 0.000 | 0.67 | 9.6 |
| 5 | 1.500[b] | 5.000[b] | 0.500[b] | - | - | 0.568 | 4.782 | 0.62 | 10.7 |
| 6 | 1.314 | 4.447 | 0.500[b] | 5.000[b] | - | 0.000 | 0.000 | 0.62 | 10.4 |
| 7 | 1.500[b] | 5.000[b] | - | 5.000[b] | - | 0.986 | 12.046 | 0.55 | 12.9 |
| 8 | 1.000[b] | 3.400[b] | - | 5.000[b] | -1.6[b] | 0.000 | 0.000 | 0.53 | 11.8 |
| 9 | 1.500[b] | 5.000[b] | 0.500[b] | - | -1.6[b] | 0.647 | 5.056 | 0.58 | 11.5 |

[a] constrained to be > zero; [b] fixed values; [c] correlation coefficient (R), and root mean squared error (RMSE) between $S_{inter}$ and $\Delta G_{bind}$, for minimised experimental ligand poses, over binding affinity validation set (58 entries).