SUPPLEMENTARY MATERIAL

Generation of errors for the synthetic SAXS curve

The *error-to-intensity ratio* (k_{exp}) was calculated by using the data points of a good quality experimental SAXS curve (measured from a sample having a concentration >10 mg/ml (Tobias Madl, personal communication)) (Figure S1). A second order Gaussian Error Function provided the best fit to k_{exp} (with R^2: 0.97 and RMSE: 0.01), which is used to simulate *error-to-intensity ratio*, k_{sim} for the s-range between 0.02 and 0.5, for the intensity range between -0.5 and 0.25:

$$k_{sim}\ s\ = a_1 exp\ \ -\frac{s-b_1}{c_1}\ ^2 + a_2 exp\ \ -\frac{s-b_2}{c_2}\ ^2 \quad (1)$$

The coefficients of k_{sim} and their confidence bounds (with 95% of confidence level) were determined to be:

a_1	b_1	c_1
0.2177 (0.2158, 0.2196)	0.4238 (0.419, 0.4286)	0.2044 (0.1984, 0.2104)

a_2	b_2	c_2
0.0642 (0.0574, 0.071)	0.2407 (0.238, 0.2437)	0.0861 (0.0794, 0.09285)

For a realistic error estimation, k_{sim} was randomly chosen within the confidence interval (95%) of the Gaussian Error Function (by using the *rand* function of MATLAB (2009)). An illustration of the randomly simulated k_{sim} is presented in Figure S1.

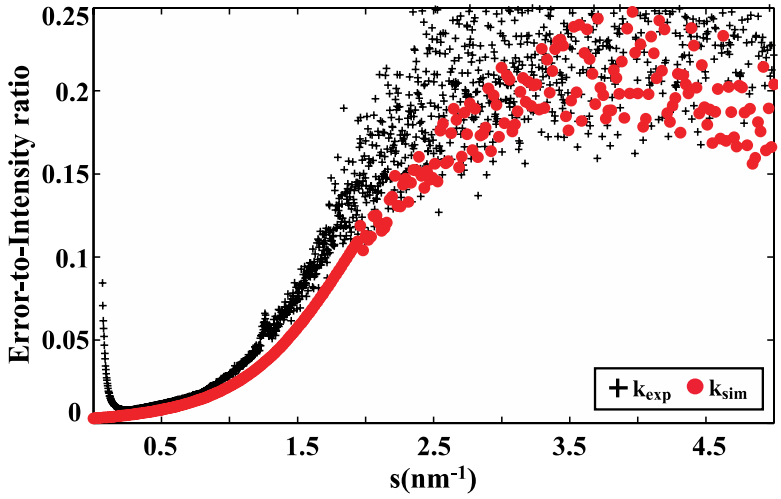

Figure S1. The evaluation of the real (k_{exp}) and simulated (k_{sim}) error-to-intensity ratio. The k_{exp} (black crosses) was calculated by using the data points of a good quality experimental SAXS curve, whereas k_{sim} (red dots) was randomly chosen within the confidence interval (95%) of the Gaussian Error Function (Eqn 1.), which was fit to k_{exp}.

Impact of flexible refinement on 138 successful cases of the Docking Benchmark 4.0

The overall performance after *water* refinement for the HADDOCK and HADDOCK$_{SAXS}$ scoring functions are presented in Figure S2.

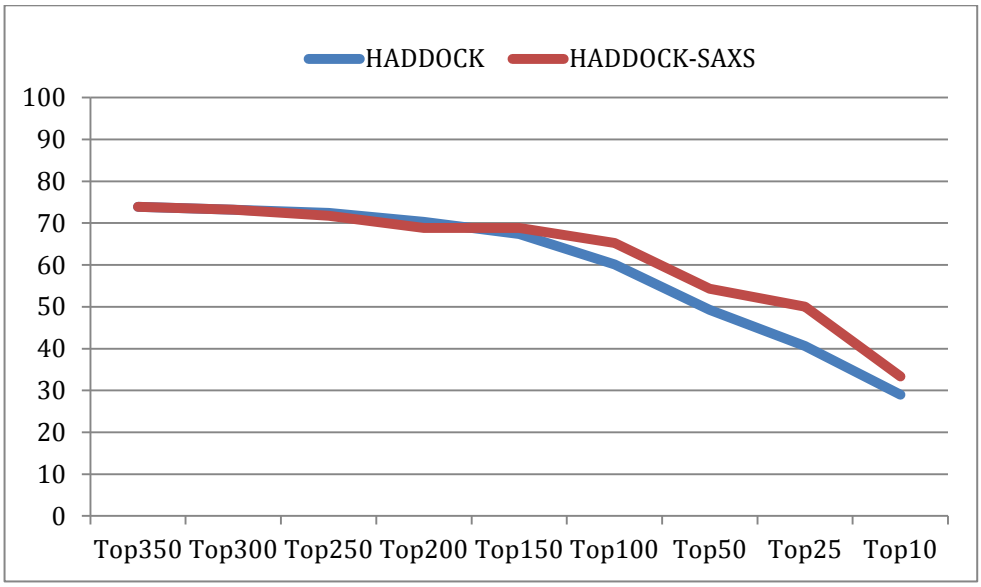

Figure S2. Performance comparison of HADDOCK (blue) and HADDOCK$_{SAXS}$ (red) at the end of the *water* refinement stage (calculated over 138 successful cases).