



eLife's transparent reporting form

We encourage authors to provide detailed information *within their submission* to facilitate the interpretation and replication of experiments. Authors can upload supporting documentation to indicate the use of appropriate reporting guidelines for health-related research (see [EQUATOR Network](#)), life science research (see the [BioSharing Information Resource](#)), or the [ARRIVE guidelines](#) for reporting work involving animal research. Where applicable, authors should refer to any relevant reporting standards documents in this form.

If you have any questions, please consult our Journal Policies and/or contact us: editorial@elifesciences.org.

Sample-size estimation

- You should state whether an appropriate sample size was computed when the study was being designed
- You should state the statistical method of sample size computation and any required assumptions
- If no explicit power analysis was used, you should describe how you decided what sample (replicate) size (number) to use

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn't apply to your submission:

This information does not apply to our submission because our study is based on computational modeling.

Replicates

- You should report how often each experiment was performed
- You should include a definition of biological versus technical replication
- The data obtained should be provided and sufficient information should be provided to indicate the number of independent biological and/or technical replicates
- If you encountered any outliers, you should describe how these were handled
- Criteria for exclusion/inclusion of data should be clearly stated
- High-throughput sequence data should be uploaded before submission, with a private link for reviewers provided (these are available from both GEO and ArrayExpress)

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn't apply to your submission:



The following information can be found in the figure captions:

Figure 2: The root mean square deviations in three different formin FH2 domains were reported as a function of time by including the exact data.

Figure 3: Two independent systems (FH2 domains interacting with actin-heptamer and actin-pentamer) were used for each formin FH2 domain for the measurements of steric clash (a total of three replicates).

Figures 4-5: Twist angles were measured as a function of time by using two independent systems (FH2 domains interacting with actin-heptamer (Figure 4) and actin-pentamer (Figure 5)). The probability distributions of twist angles were also given at various time intervals (a total of three replicates).

Figure 6: Two replicas of metabasin metadynamics simulations for each formin were run for 80 ns.

Figure 7: Average contacts were obtained by time-averaging number of contacts over last 20 ns of the 200 ns simulations.

Figures 8-9: The exact data was plotted as a function of time for three different systems (a total of three replicates).

Table 1: Two independent systems (FH2 domains interacting with actin-heptamer and actin-pentamer) were used for each formin FH2 domain (a total of three replicates). Measurements at two different time intervals were reported for actin-heptamer.

Table 2: The data from the last 20 ns of the 200 ns simulations were used for actin-heptamer.

Statistical reporting

- Statistical analysis methods should be described and justified
- Raw data should be presented in figures whenever informative to do so (typically when N per group is less than 10)
- For each experiment, you should identify the statistical tests used, exact values of N, definitions of center, methods of multiple test correction, and dispersion and precision measures (e.g., mean, median, SD, SEM, confidence intervals; and, for the major substantive results, a measure of effect size (e.g., Pearson's r, Cohen's d)
- Report exact p-values wherever possible alongside the summary statistics and 95% confidence intervals. These should be reported for all key questions and not only when the p-value is less than 0.05.

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn't apply to your submission:

Most of the plots show the exact data as a function of time without applying any statistical test or correction.
Mean and SD of the continuous numerical data were reported where appropriate in the text.
Mean and SD together with T-statistics for data shown in Figures 5 D,E,F were provided in Table S4.
Pearson correlation coefficients for the data shown in Figures S3 and S4 were provided in Table S3.

(For large datasets, or papers with a very large number of statistical tests, you may upload a single table file with tests, Ns, etc., with reference to sections in the manuscript.)



Group allocation

- Indicate how samples were allocated into experimental groups (in the case of clinical studies, please specify allocation to treatment method); if randomization was used, please also state if restricted randomization was applied
- Indicate if masking was used during group allocation, data collection and/or data analysis

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn't apply to your submission:

This information does not apply to our submission because this study is based on computational modeling and we do not have experimental groups.

Additional data files ("source data")

- We encourage you to upload relevant additional data files, such as numerical data that are represented as a graph in a figure, or as a summary table
- Where provided, these should be in the most useful format, and they can be uploaded as "Source data" files linked to a main figure or table
- Include model definition files including the full list of parameters used
- Include code used for data analysis (e.g., R, MatLab)
- Avoid stating that data files are "available upon request"

Please indicate the figures or tables for which source data files have been provided:

The model parameters required to set up the simulations were provided in the Methodology section.