Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

The shuttling mechanism of foldaxanes: More than just the translocation and rotation

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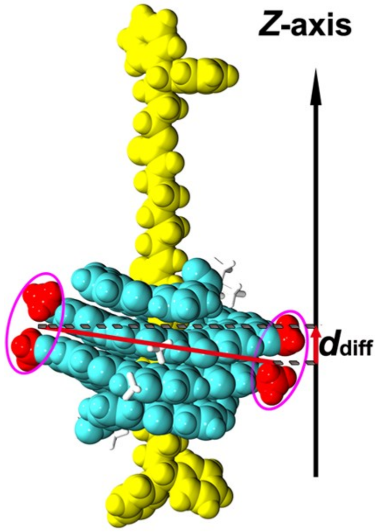

Figure S1. Detailed definition of the collective variable d_{diff}.

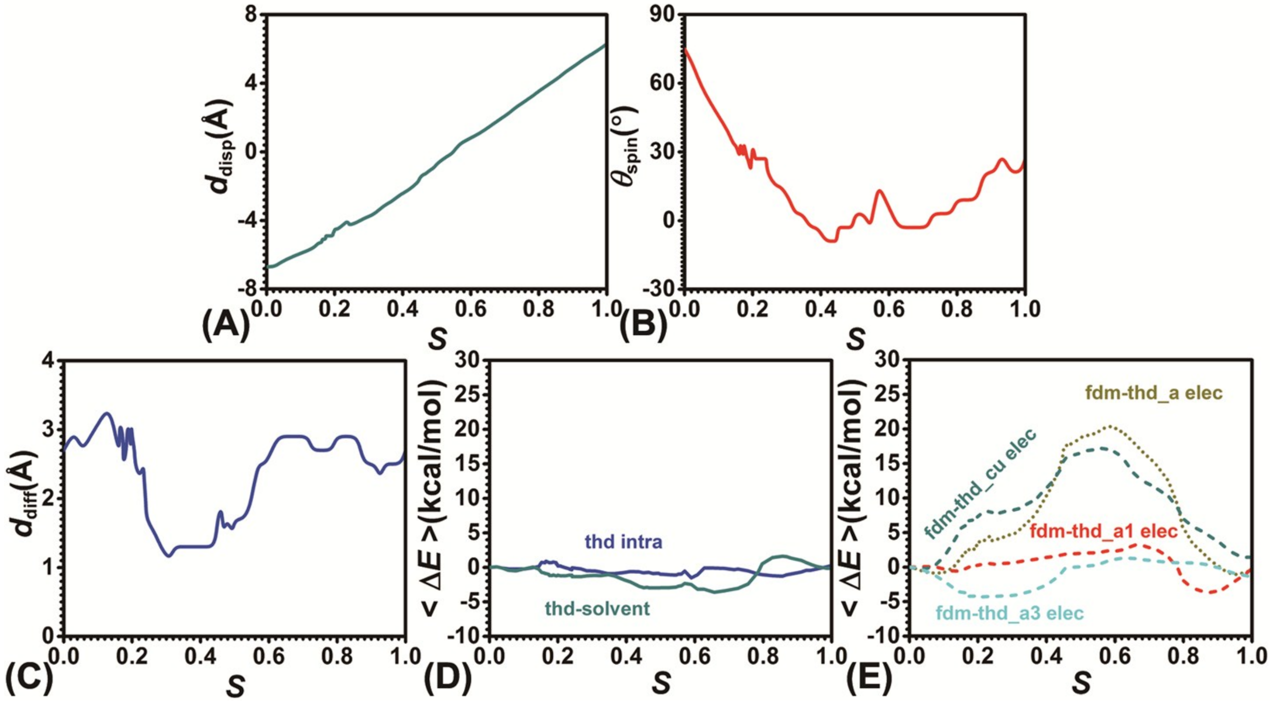

Figure S2. Evolution of reaction coordinates (A) d_{disp}, (B) θ_{spin}, and (C) d_{diff} along the least free–energy pathway. (D) Thread intramolecular interaction term and thread–solvent interaction term. (E) Decomposition of foldamer–thread amides electrostatic interaction into foldamer–thread amide1, foldamer–thread central urea, and foldamer–thread amide3 terms.

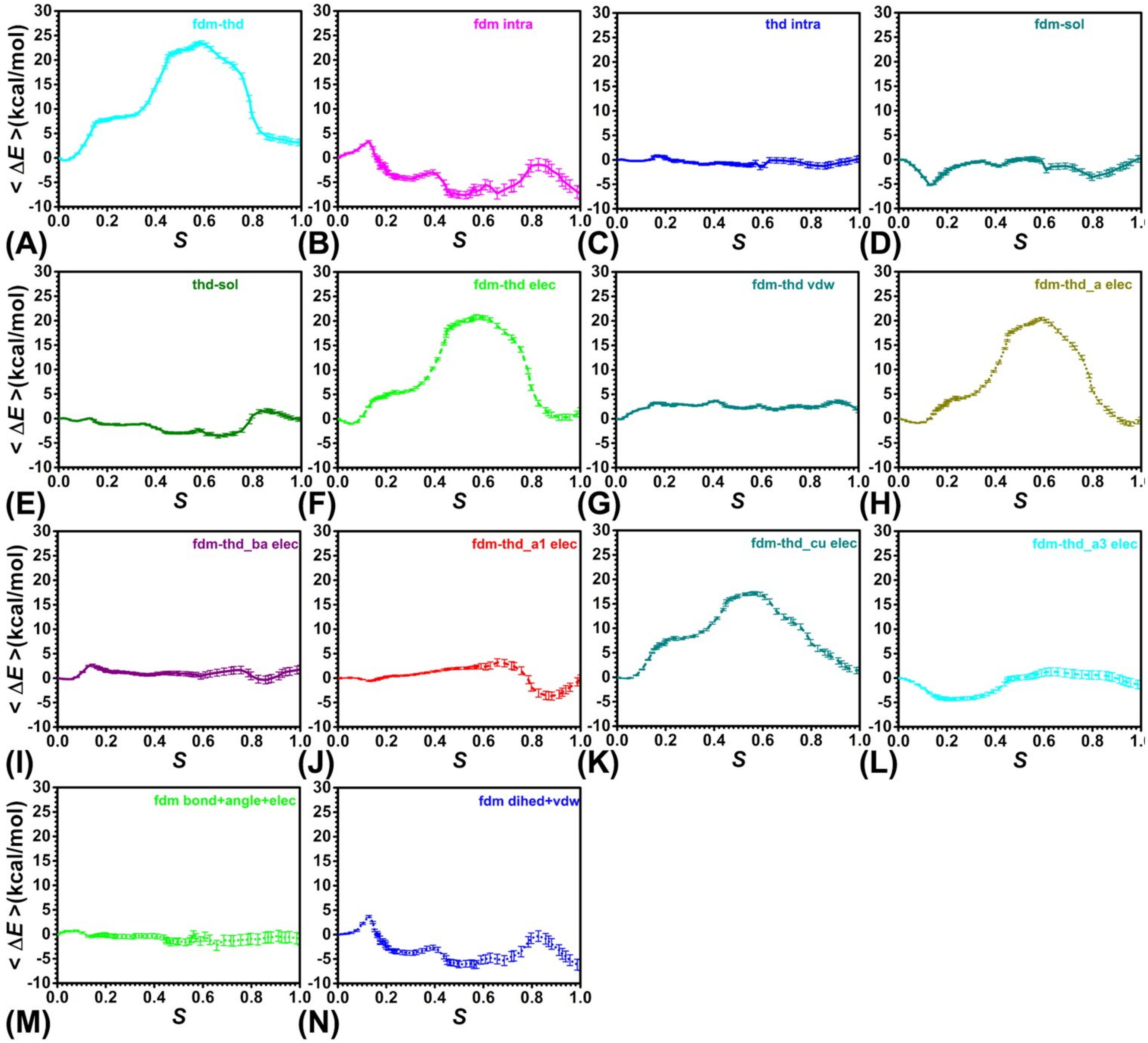

Figure S3. The standard error associated with interaction components.

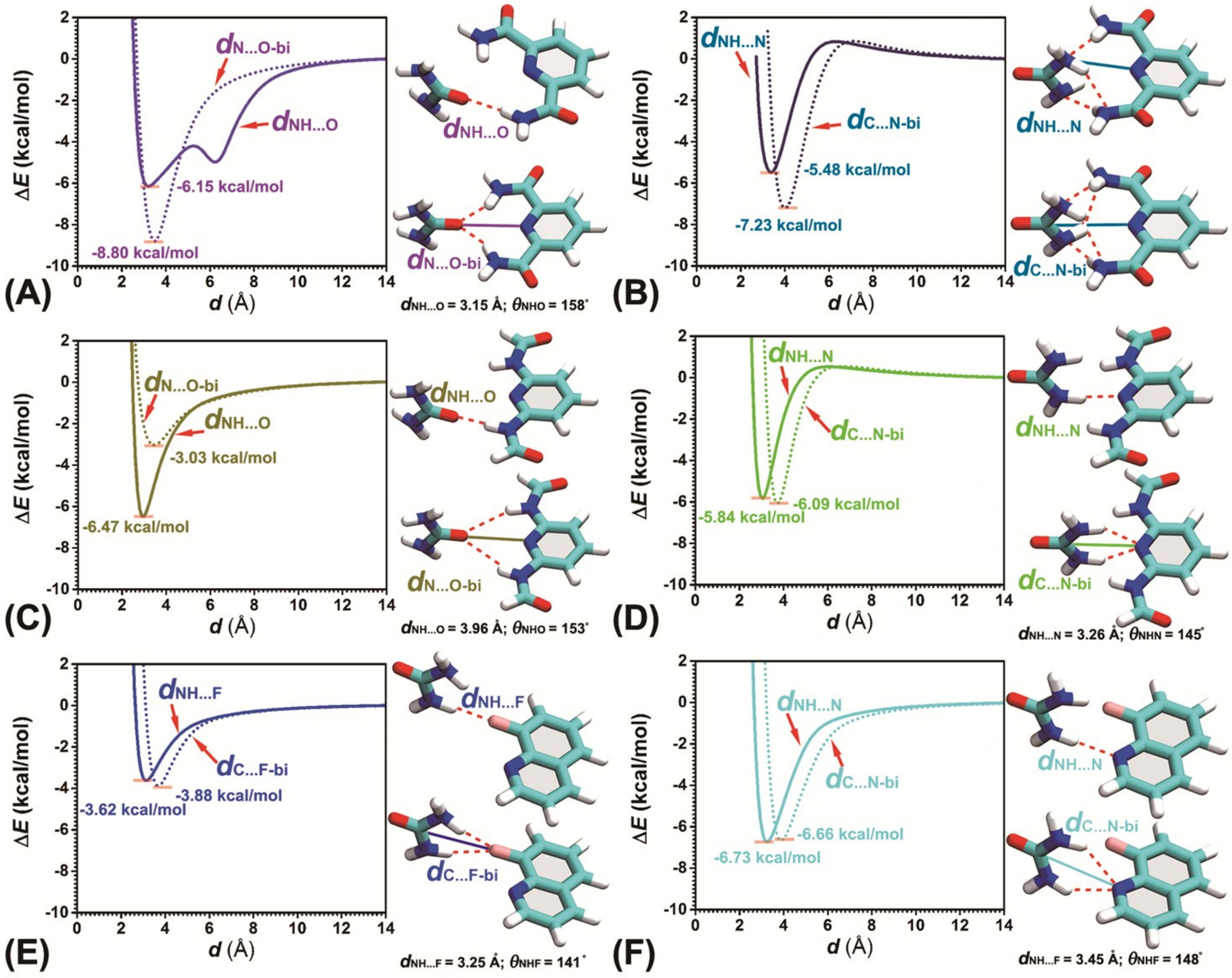

Figure S4. Potential energy profiles for the formation processes of normal hydrogen bonds and bifurcated hydrogen bonds between (A) **O** in urea and **NH** in pyridine-2,6-dicarboxamide, (B) **NH** in urea and **N** in pyridine-2,6-dicarboxamide, (C) **O** in urea and **NH** in *N*,*N*'-(pyridine-2,6-diyl)diacetamide, (D) **NH** in urea and **N** in *N*,*N*'-(pyridine-2,6-diyl)diacetamide, (E) **NH** in urea and **F** in 8-fluoroquinoline, and (F) **NH** in urea and **N** in 8-fluoroquinoline. Calculated at the B3LYP/6-311g(d,p) level of theory.

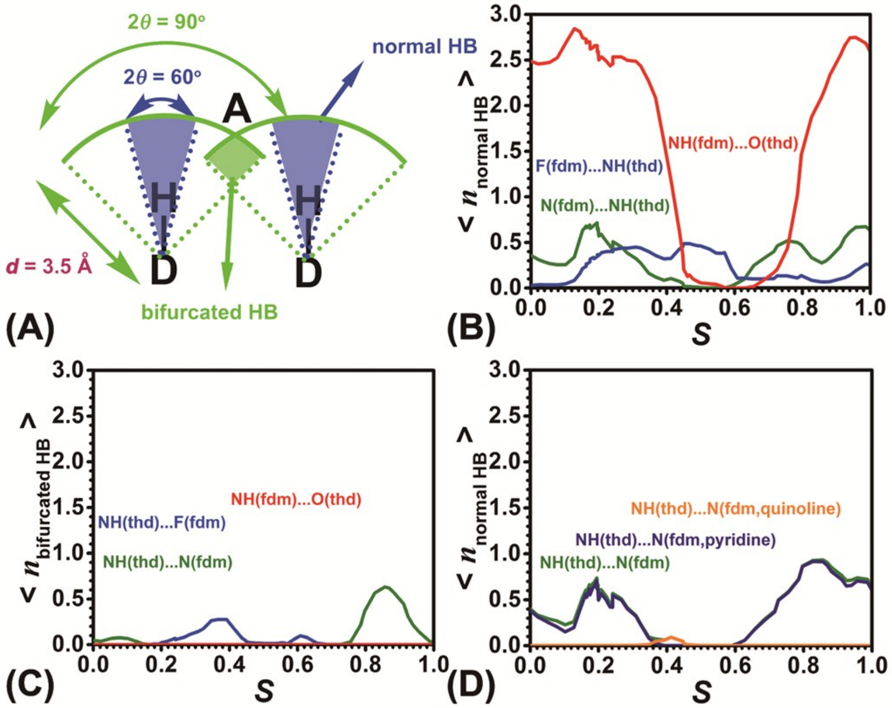

Figure S5. (A) Definition of normal hydrogen bonds and bifurcated hydrogen bonds. Evolution of the number of (B) normal hydrogen bonds and (C) bifurcated hydrogen bonds along the least free–energy pathway. (D) Evolution of the number of normal hydrogen bonds between amide moieties with aromatic nitrogen atoms (olive), pyridine nitrogen atoms (royal), and quinoline nitrogen atoms (orange).

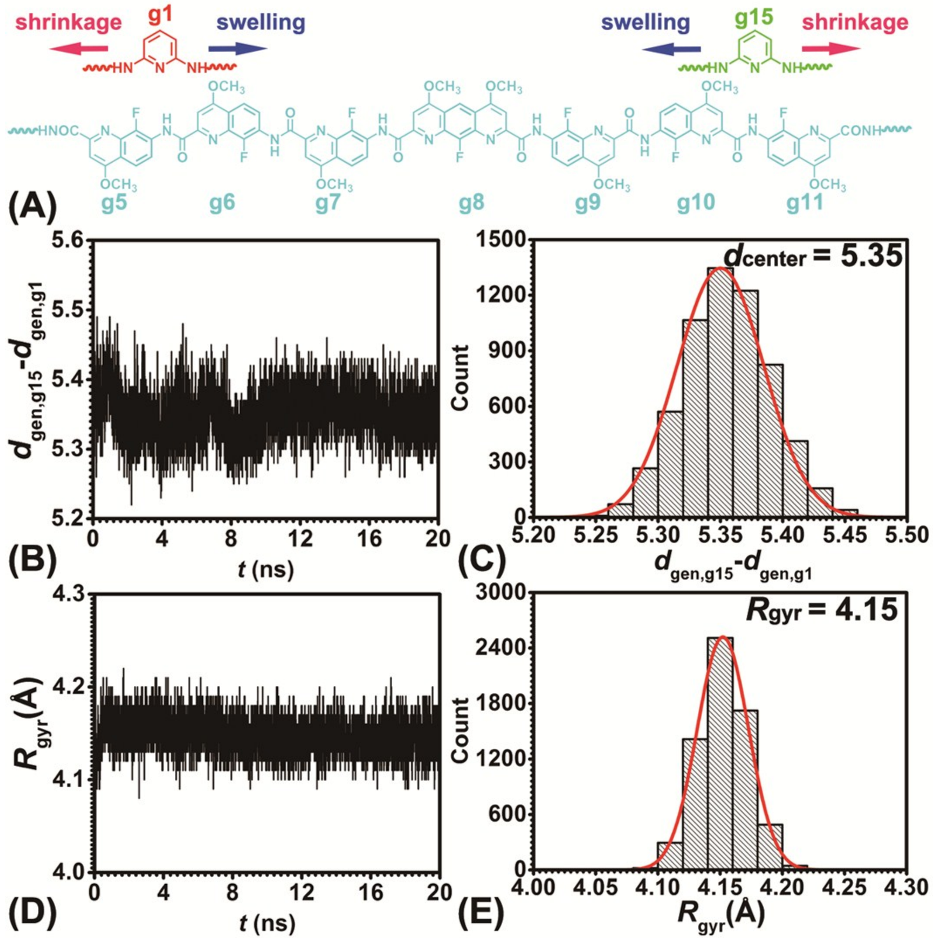

Figure S6. (A) Representation of the general distance for **g15** and **g1** on the chain **g5-g11**. (B) Evolution and (C) distribution of the difference between general distances, $\boldsymbol{d}_{\mathbf{gen,g15}} - \boldsymbol{d}_{\mathbf{gen,g1}}$, in the 20 ns equilibrium simulation. (D) Evolution and (E) distribution of the radius of gyration for fluorine atoms within the foldamer in the 20 ns equilibrium simulation.