

Supplementary Information

We developed a web application that enables the user to calculate and fine-tune the model parameters in an interactive and visual fashion. Web application is accessible through the following link:

<http://ltpo2.fri1.uni-lj.si/dna/>

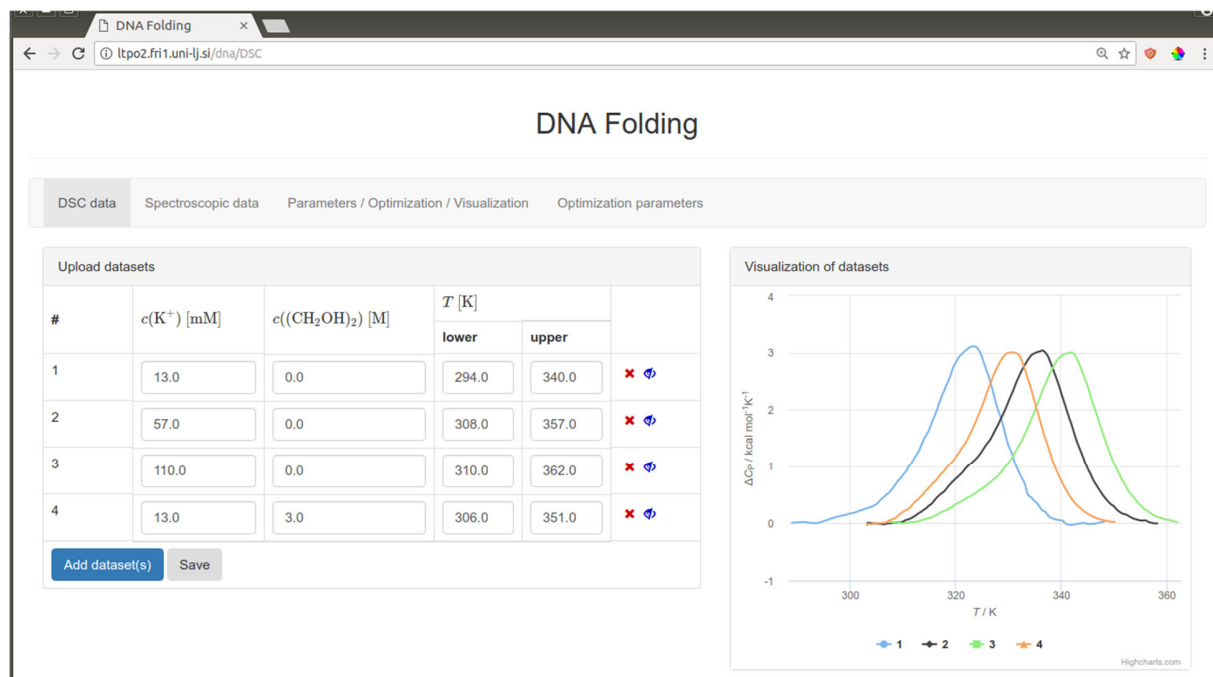


Fig. S1 User interface for the input of DSC data. The DSC curves are plotted in real time.

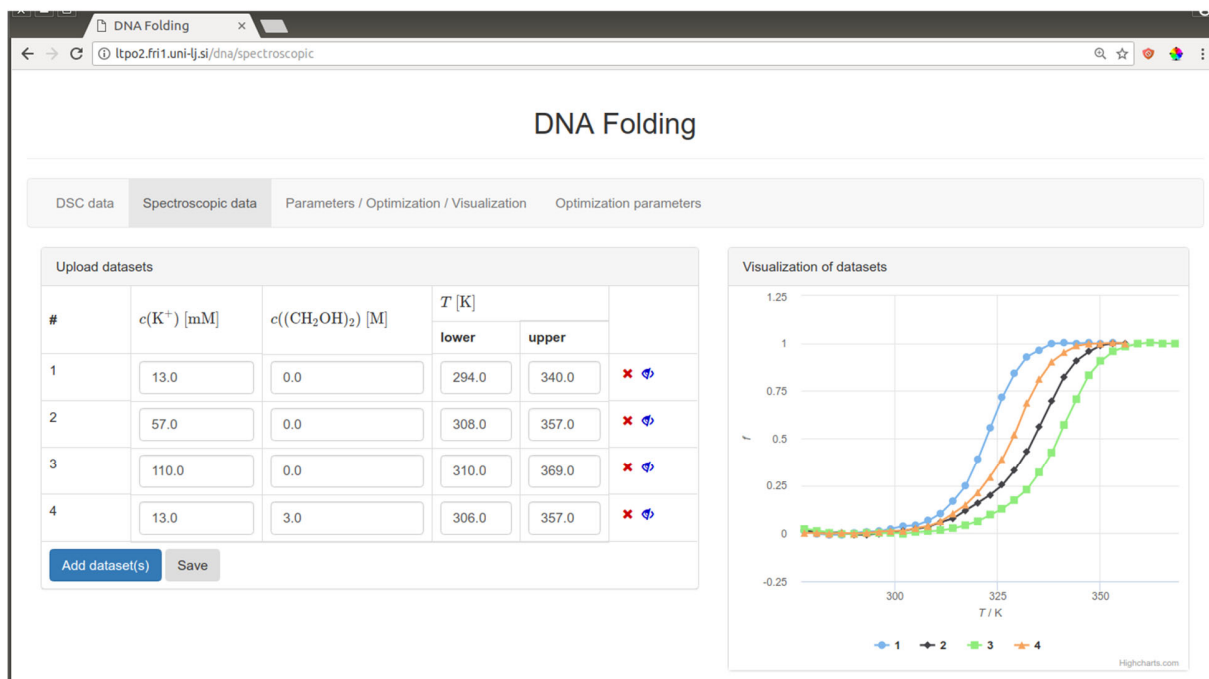


Fig. S2 User interface for the input of normalized CD melting curves. The normalized CD melting curves are plotted in real time.

DNA Folding

ltpo2.fri1.uni-lj.si/dna/parameters

DNA Folding

DSC data Spectroscopic data **Parameters / Optimization / Visualization** Optimization parameters

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	F → I	I → U	F → U	
$\Delta G_{ij}^o(T_0)$	4.19 <small>±0.057 3.1 ↻</small>	5.67 <small>±0.07 6.2 ↻</small>	9.86	kcal mol ⁻¹
$\Delta H_{ij}^o(T_0)$	36.84 <small>±0.76 19.3 ↻</small>	7.75 <small>±0.73 27.4 ↻</small>	44.59	kcal mol ⁻¹
$\Delta C_{P,ij}^o$	-204.11 <small>±12.0 92.8 ↻</small>	475.90 <small>±8.7 297.6 ↻</small>	271.79	cal mol ⁻¹ K ⁻¹
n_{ij}	0.48 <small>±0.0079 0.5 ↻</small>	1.91 <small>±0.011 1.7 ↻</small>	2.38	mol
m_{ij}	-9.34 <small>±0.38 -7.0 ↻</small>	-34.21 <small>±0.39 -33.0 ↻</small>	-43.55	mol
f_{ij}	0.61 <small>±0.022 0.55 ↻</small>			
T_0	298.15			K

Redraw Optimize Optimize & Errors Restore values before optimization Download ...

Fig. S3 User interface for the input of the parameters. The parameters can be uploaded from a file or typed/ increased/ decreased manually. The errors are displayed under the parameter values.



Fig. S4 Comparison of the fitting and experimental curves (left), and speciation diagram under the given conditions.

DNA Folding

DSC data Spectroscopic data Parameters / Optimization / Visualization **Optimization parameters**

Parameter		Current value	Fixed	Lower bound	Upper bound	
$\Delta G_{ij(T_0)}^o$	F → I	4.19	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	kcal mol ⁻¹
	I → U	5.67	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	kcal mol ⁻¹
$\Delta H_{ij(T_0)}^o$	F → I	36.84	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	kcal mol ⁻¹
	I → U	7.75	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	kcal mol ⁻¹
$\Delta C_{P,ij}^o$	F → I	-204.11	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	cal mol ⁻¹ K ⁻¹
	I → U	475.90	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	cal mol ⁻¹ K ⁻¹
n_{ij}	F → I	0.48	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	mol
	I → U	1.91	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	mol
m_{ij}	F → I	-9.34	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	mol
	I → U	-34.21	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	mol
f_{ij}	F → I	0.61	<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	

Optimization / error estimation

Number of function evaluations

Number of bootstrapping iterations

These values affect the duration of the optimization and error estimation processes.

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Fig. S5 User interface for the control of the parameters. The parameters can be fixed or limited by the upper and/or lower values, and the number of bootstrapping iterations can be set.