Supporting Information

The nature of the DNA substrate influences pre-catalytic conformational changes of DNA polymerase β

Ji Huang[1#], Khadijeh S. Alnajjar[1], Mariam M. Mahmoud[1], Brian Eckenroth[3], Sylvie Doublié[3], Joann B. Sweasy[1,2*]

From the [1]Department of Therapeutic Radiology, Yale University School of Medicine, New Haven, CT 06520; [2]Department of Genetics, Yale University School of Medicine, New Haven, CT 06520; [3]Department of Microbiology and Molecular Genetics, University of Vermont, Burlington, Vermont 05405

[#]Present address: Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL 60208

[*]To whom correspondence should be addressed: Joann B. Sweasy: Department of Therapeutic Radiology, Yale University School of Medicine, New Haven, CT 06520; Department of Genetics, Yale University School of Medicine, New Haven, CT 06520; joann.sweasy@yale.edu; Tel. (203)737-2626; Fax. (203)785-6309.

Table of Contents

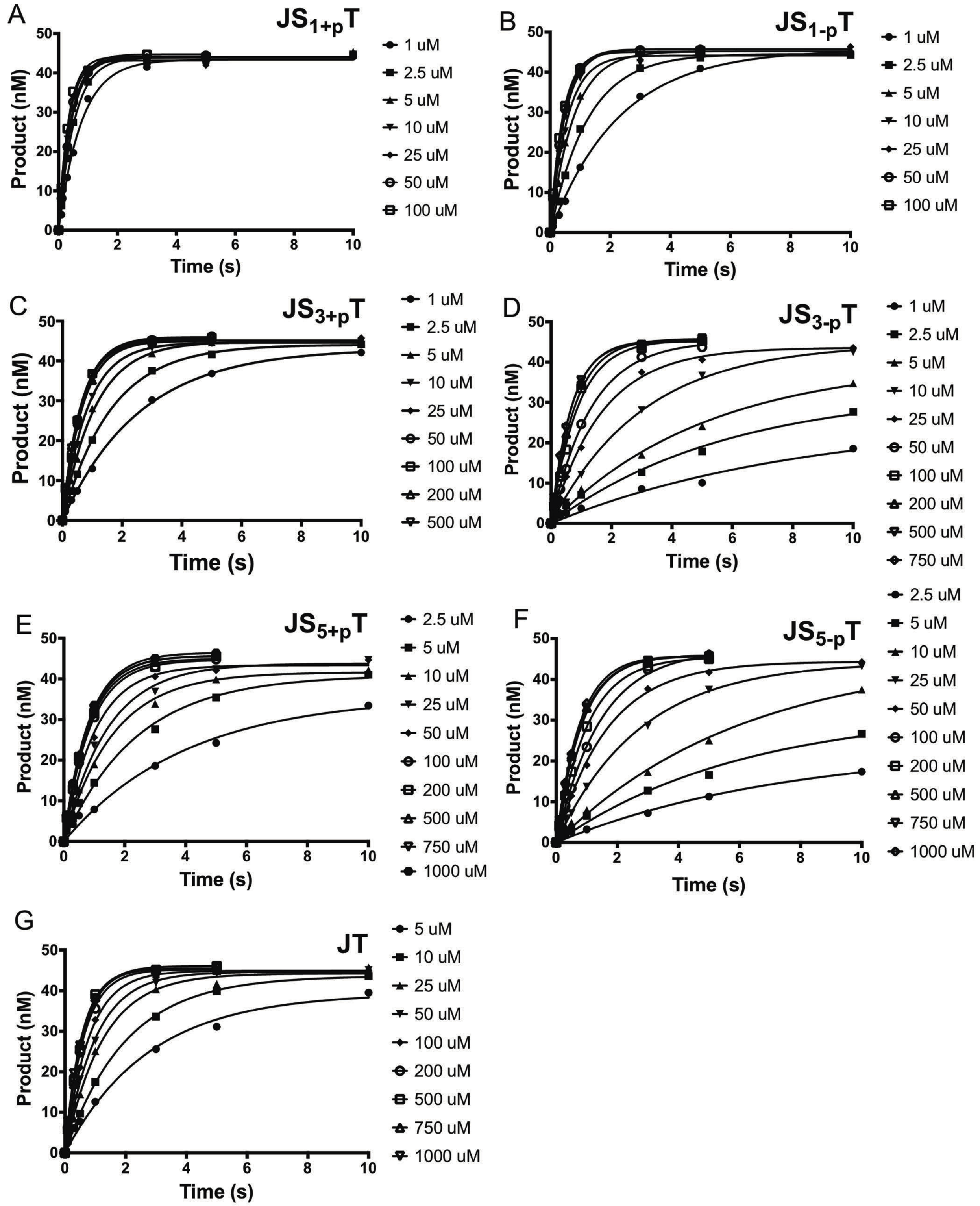

Figure S1. Single turnover kinetics of different DNA substrates. The DNA substrates are (A) JS$_{1+p}$T, (B) JS$_{1-p}$T, (C) JS$_{3+p}$T, (D) JS$_{3-p}$T, (E) JS$_{5+p}$T, (F) JS$_{5-p}$T, (G) JT DNA.

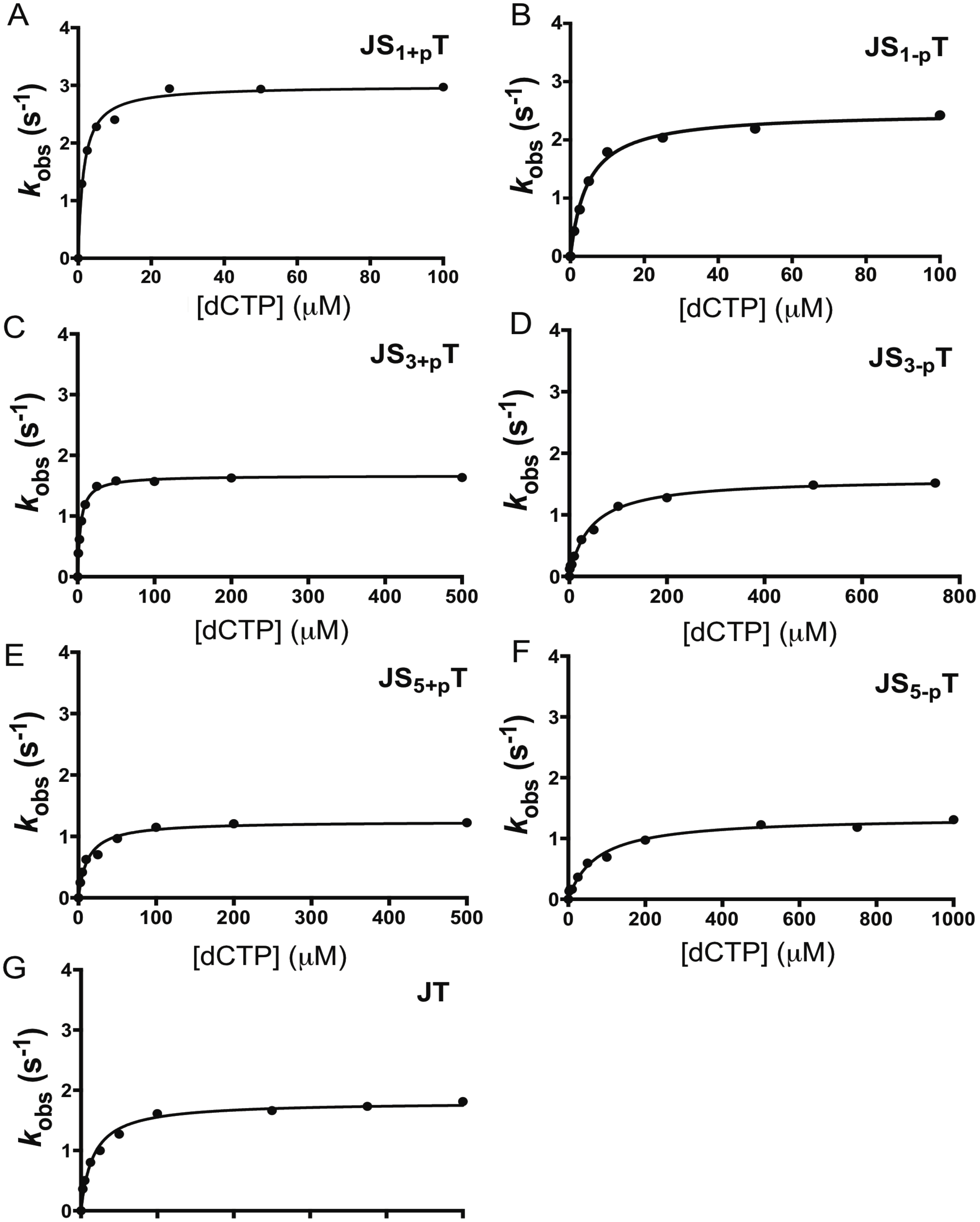

Figure S2. Determination of k_{pol} and $K_{d\ (dNTP)}$ from single turnover kinetics experiments. The DNA substrates are (A) $JS_{1+p}T$, (B) $JS_{1-p}T$, (C) $JS_{3+p}T$, (D) $JS_{3-p}T$, (E) $JS_{5+p}T$, (F) $JS_{5-p}T$, (G) JT DNA.

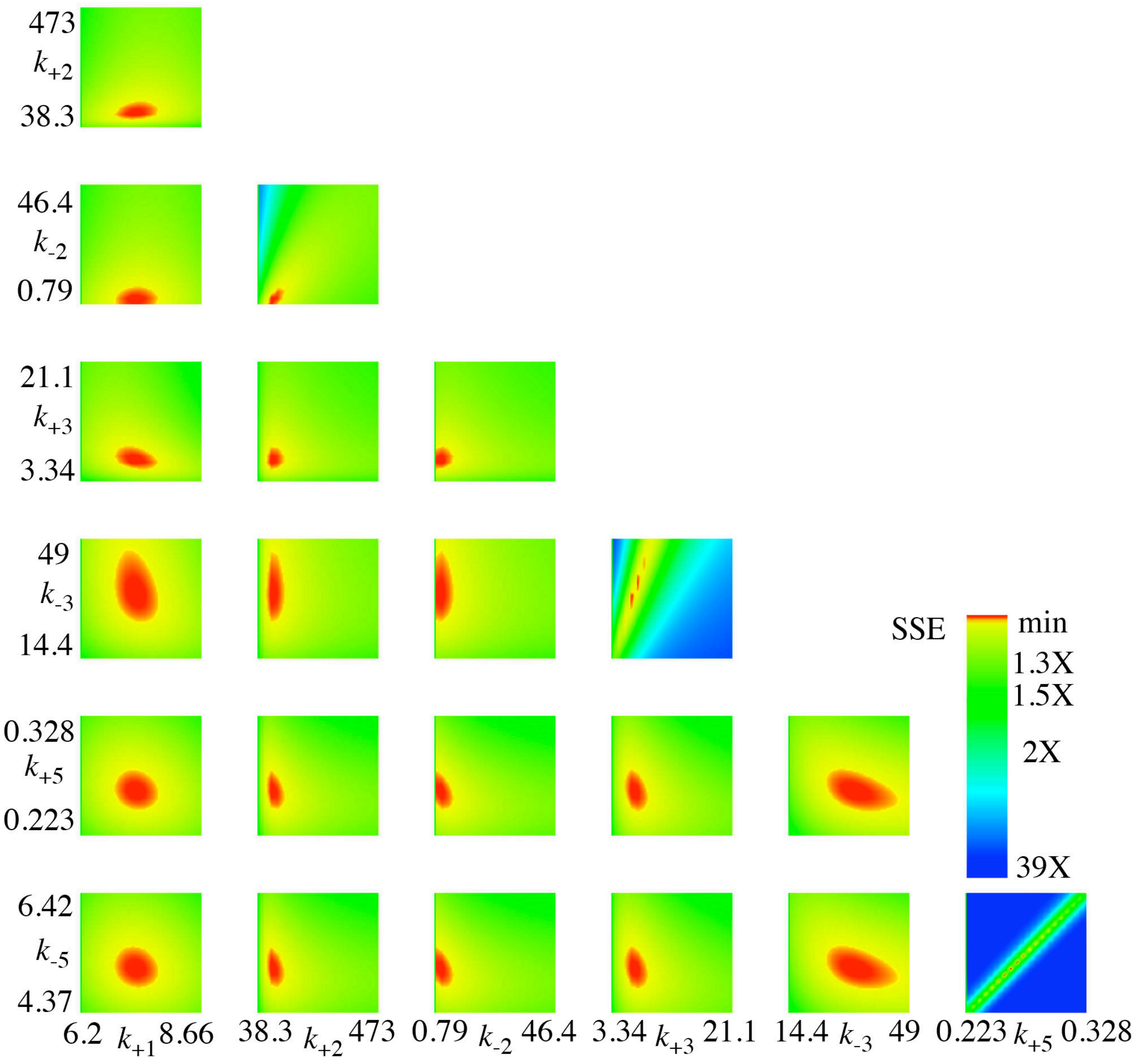

Figure S3. Confidence contours for the rate constants determined by KinTek Explorer for $JS_{1+p}T$ DNA with ***model containing the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

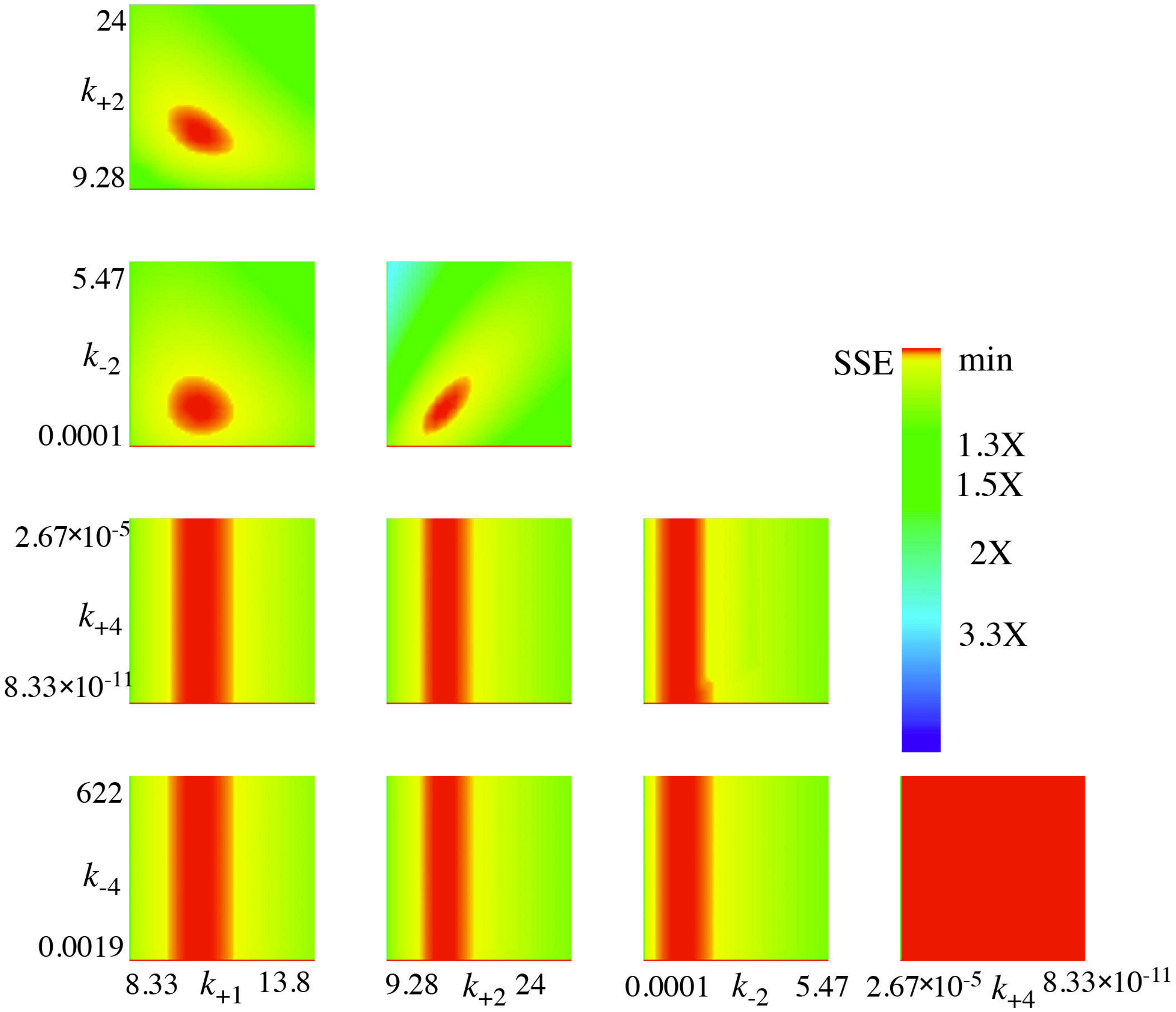

Figure S4. Confidence contours for the rate constants determined by KinTek Explorer for $JS_{1+p}T$ DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

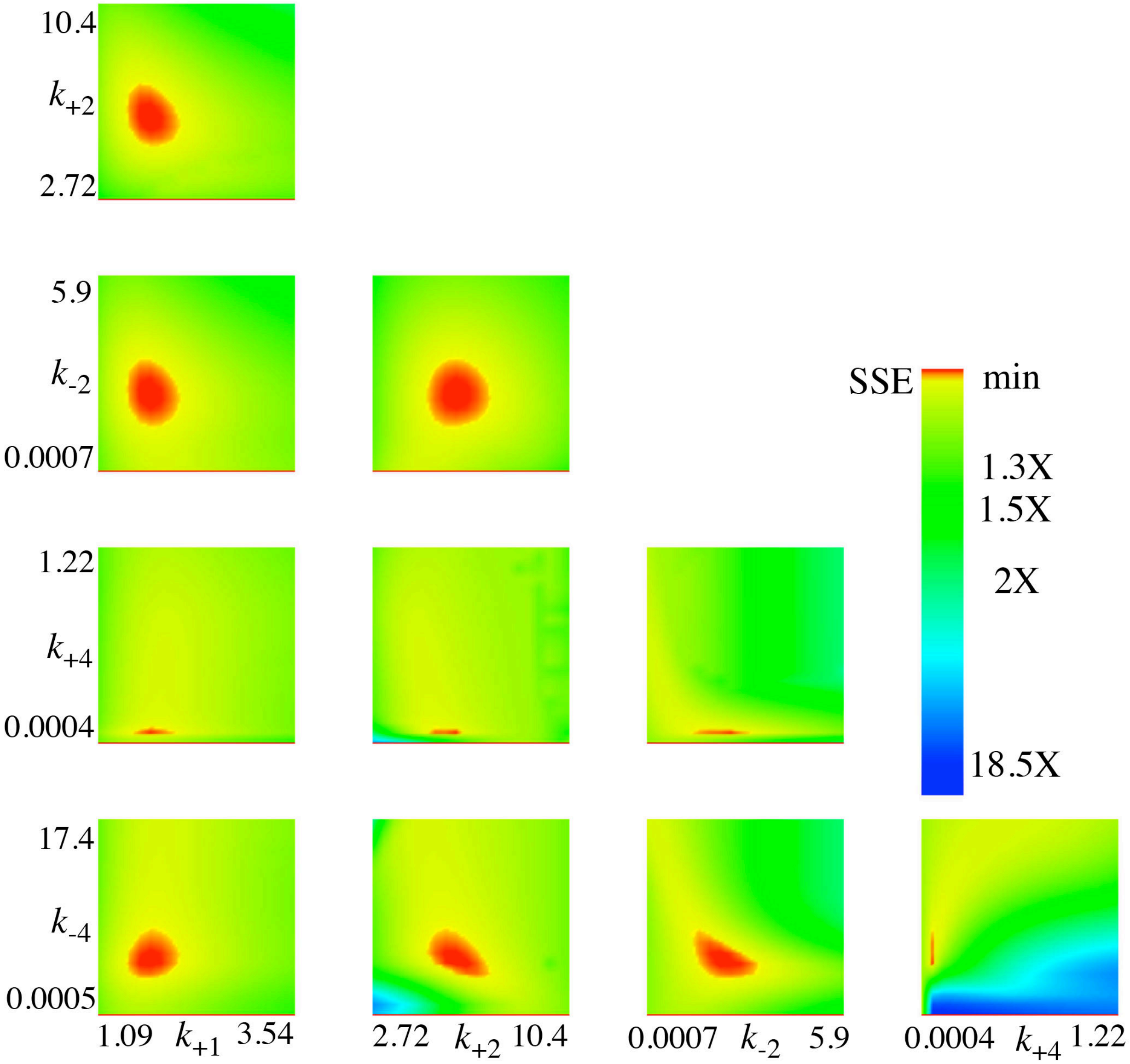

Figure S5. Confidence contours for the rate constants determined by KinTek Explorer for $JS_{1\text{-}p}T$ DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

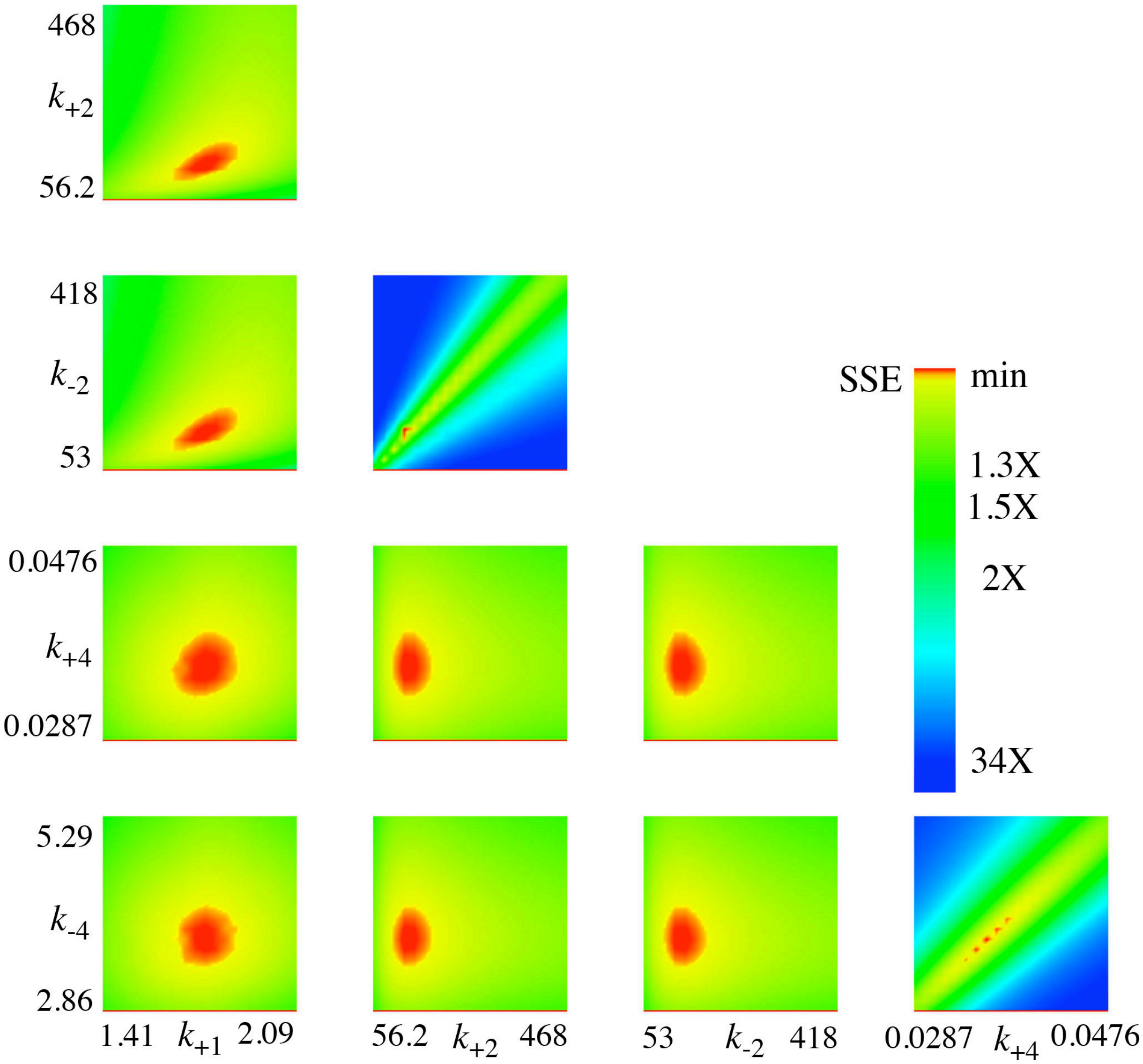

Figure S6. Confidence contours for the rate constants determined by KinTek Explorer for $JS_{3+p}T$ DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

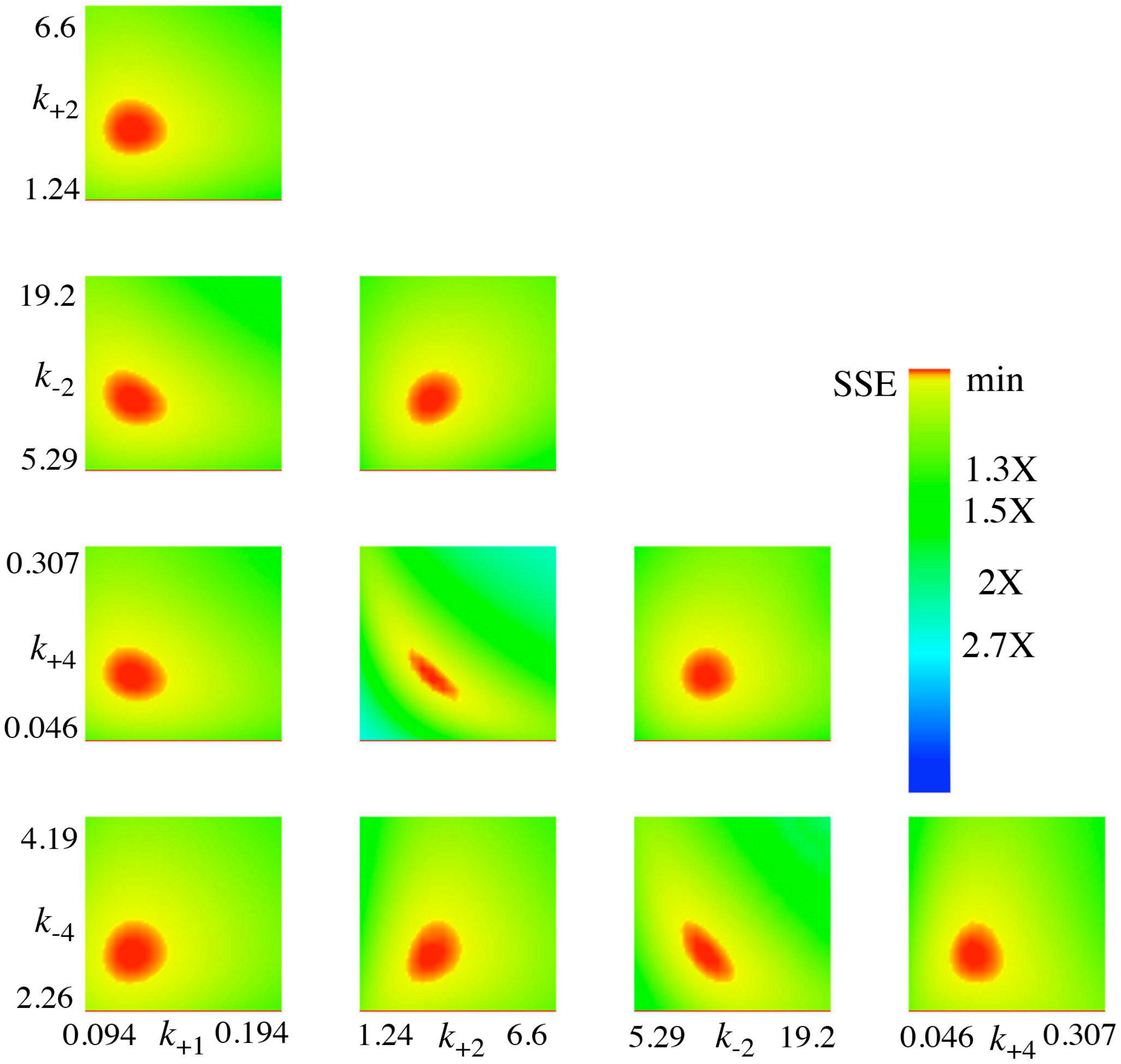

Figure S7. Confidence contours for the rate constants determined by KinTek Explorer for $JS_{3\text{-}p}T$ DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

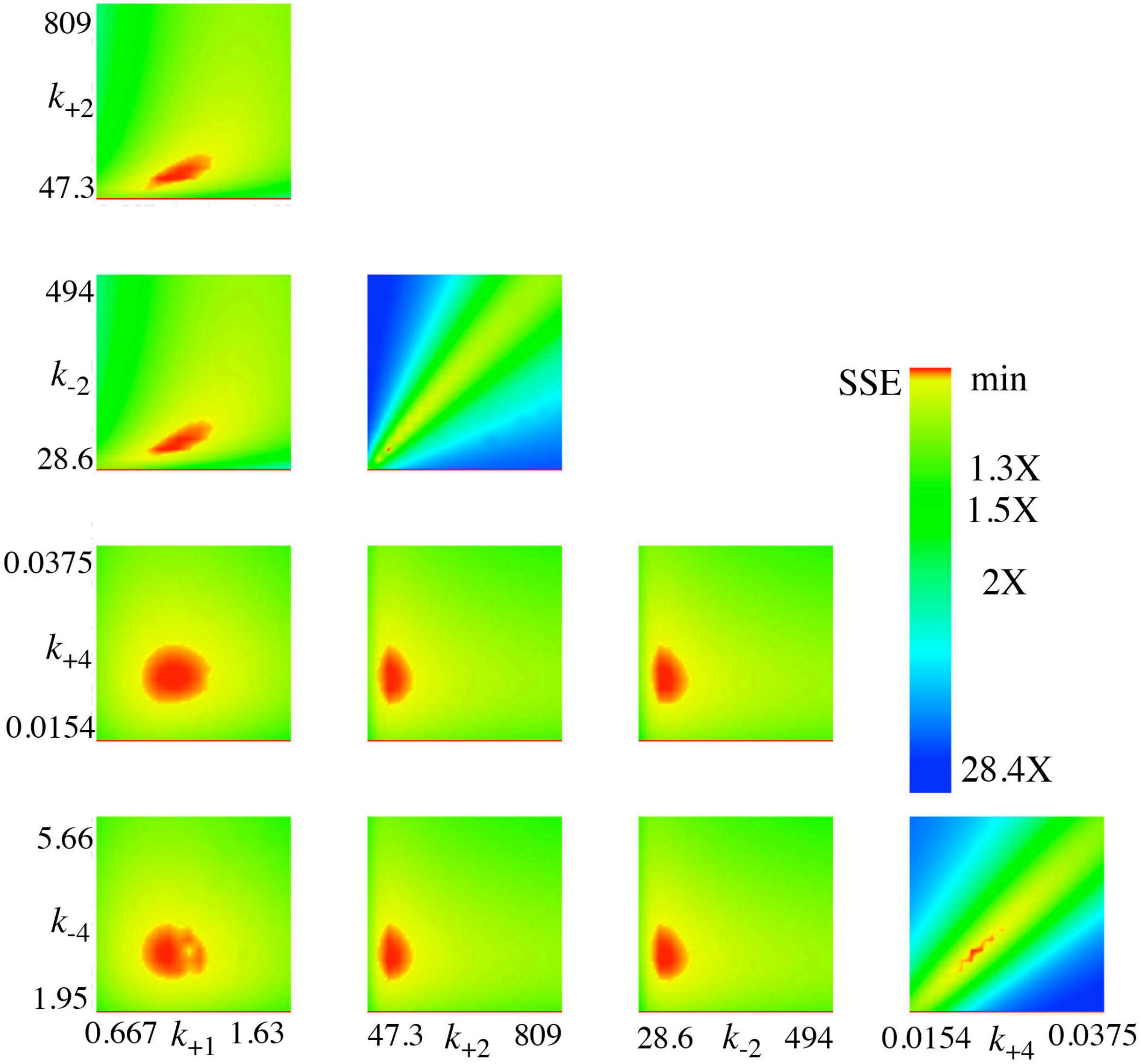

Figure S8. Confidence contours for the rate constants determined by KinTek Explorer for $JS_{5+p}T$ DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

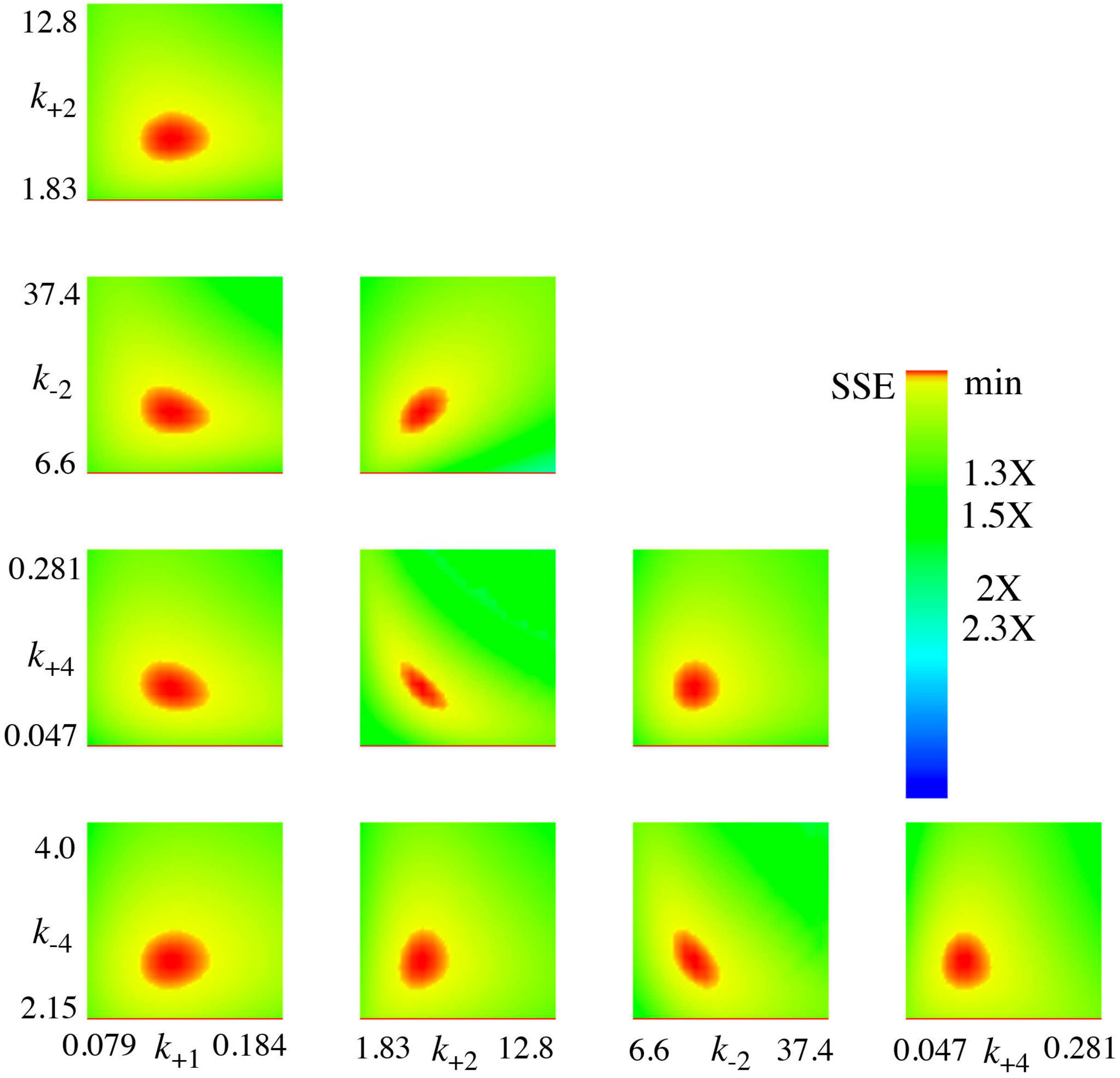

Figure S9. Confidence contours for the rate constants determined by KinTek Explorer for JS$_{5\text{-}p}$T DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.

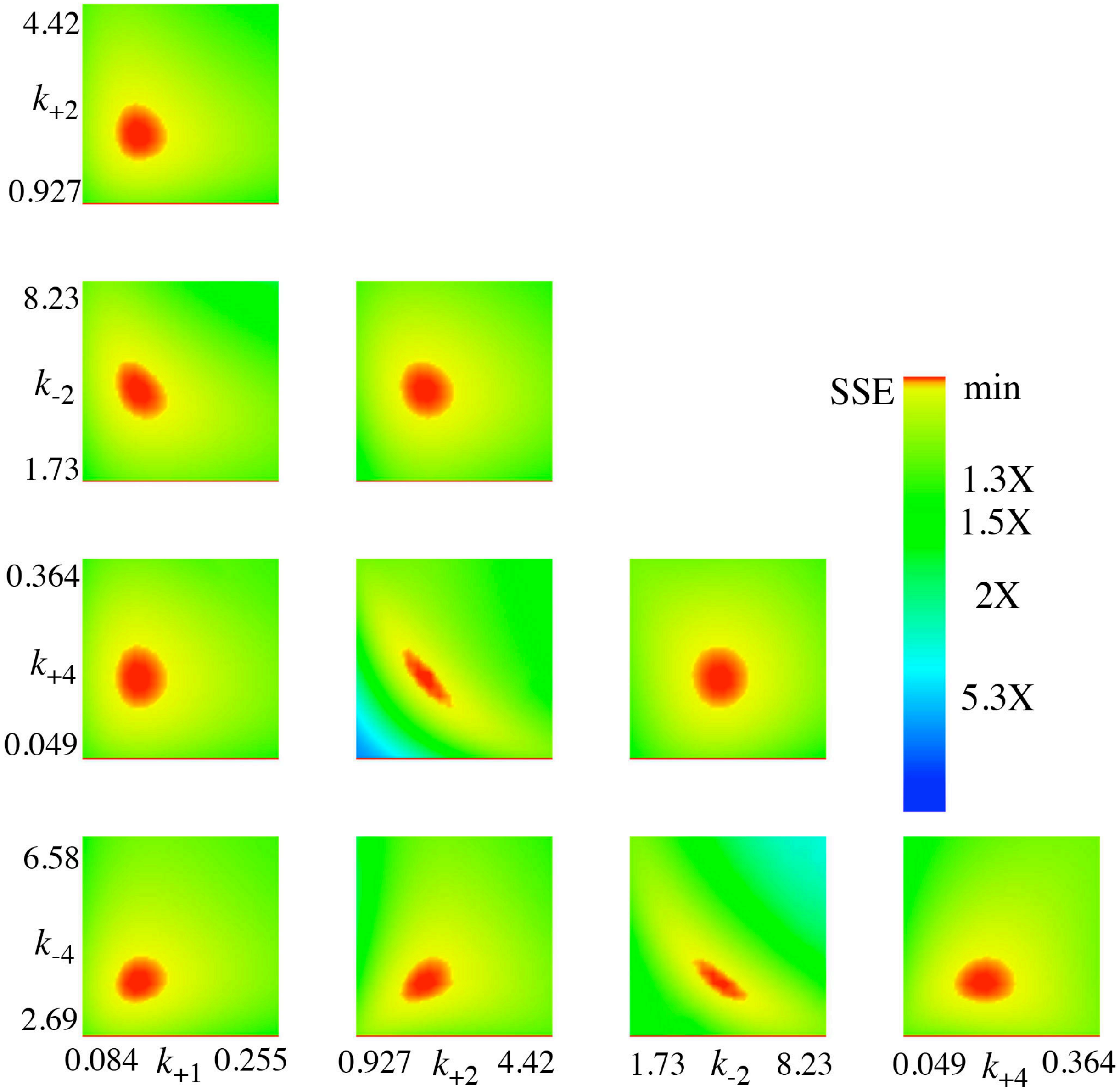

Figure S10. Confidence contours for the rate constants determined by KinTek Explorer for JT DNA with ***model that does not contain the non-covalent step***. For each case the search was carried out up to a sum of squares error (SSE) that is 2-fold higher than the minimum SSE. The upper and lower limits of each parameter were determined using an SSE threshold of 1.2. A red oval shape indicates the pairs of parameters are well constrained.