**Quantum DNA (qDNA) Research Group Metadata**

**Dye Synthesis and DNA Construct Synthesis Teams**

**For public disclosure of publication data through Albertsons Library and ScholarWorks**

1. **DESCRIPTIVE METADATA**

**A. TITLE**

Dataset for Exciton Delocalization and Scaffold Stability in Bridged Nucleotide-Substituted, DNA Duplex-Templated Cyanine Aggregates

**B. IDENTIFIER**

<https://doi.org/>10.18122/quantum\_data.1.boisestate

**C. SUMMARY**

Molecular excitons play a foundational role in chromophore aggregates found in light-harvesting systems and offer potential applications in engineered excitonic systems. Controlled aggregation of chromophores to promote exciton delocalization has been achieved by covalently tethering chromophores to deoxyribonucleic acid (DNA) scaffolds. Although many studies have documented changes in the optical properties of chromophores upon aggregation using DNA scaffolds, more limited work has investigated how structural modifications of DNA via bridged nucleotides and chromophore covalent attachment impact scaffold stability as well as the configuration and optical behavior of attached aggregates. Here we investigated the impact of two types of bridged nucleotides, LNA and BNA, as a structural modification of duplex DNA-templated cyanine (Cy5) aggregates. The bridged nucleotides were incorporated in the domain of one to four Cy5 chromophores attached between adjacent bases of a DNA duplex. We found that bridged nucleotides increase the stability of DNA scaffolds carrying Cy5 aggregates in comparison with natural nucleotides in analogous constructs. Exciton coupling strength and delocalization in Cy5 aggregates were evaluated via steady-state absorption, circular dichroism, and theoretical modeling. Replacing natural nucleotides with bridged nucleotides resulted in a noticeable increase in the coupling strength (≥10 meV) between chromophores and increased H-like stacking behavior (i.e., more face-to-face stacking). Our results suggest that bridged nucleotides may be useful for increasing scaffold stability and coupling between DNA templated chromophores.

**D. CREATOR(S)**

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**E. DATE(S)**

Dataset Release Date: 20230328

Time Period Covered by Data: 2018-2021

**F. LIST OF data and README files RELATED TO THE STUDY**

* **Data files (.csv)**
  + **Roy2021\_Figure­\_2\_Melting\_Summary**
  + **Roy2021\_Figure\_4\_Abs\_and\_CD**
  + **Roy2021\_Figure\_S1–S5\_Melting\_Data**
  + **Roy2021\_Figure\_S6–S13\_Hysteresis**
  + **Roy2021\_Figure\_S27\_H-R\_Study**
  + **Roy2021\_Figure\_S28\_H-R\_Study\_2**
  + **Roy2021\_Figure\_S29\_A-form\_vs\_B-form\_CD**
  + **Roy2021\_Figure\_S30\_UV\_CD\_Comparison**
  + **Roy2021\_Figure\_S31\_SS\_Fluorescence**
  + **Roy2021\_Table\_S6**
  + **Roy2021\_Table\_S7**
  + **Roy2021\_Table\_S8**
  + **Roy2021\_Table\_S9**
  + **Roy2021\_Table\_S10**
  + **Roy2021\_Table\_S11**
  + **Roy2021\_Table\_S12**
  + **Roy2021\_Table\_S13**
  + **Roy2021\_Table\_S14**
* **README files (.txt)**
  + **Data\_Attribute\_README\_Absorption**
  + **Data\_Attribute\_README\_Circular\_Dichroism**
  + **Data\_Attribute\_README\_Fluorescence\_Emission**
  + **Data\_Attribute\_README\_KRM\_Modeling**
  + **Data\_Attribute\_README\_Melting\_Profiles**
  + **Data\_Attribute\_README\_PAGE**

**G. FILE FORMATS**

\*.csv, \*.xlsx, \*.docx, \*.txt

**H. LANGUAGE**

English

**I. RIGHTS OR LICENSING INFORMATION**

Users are free to share, copy, distribute and use the dataset; to create or produce works from the dataset; to adapt, modify, transform and build upon the dataset as long as the user attributes any public use of the dataset, or works produced from the dataset, referencing the author(s) and DOI link. For any use or redistribution of the dataset, or works produced from it, the user must make clear to others the license of the dataset and keep intact any notices on the original dataset.

**J. FUNDER CITATION**

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**I. RELATED PUBLICATIONS**

Roy, Simon K.; Mass, Olga A.; Kellis, Donald L.; Wilson, Christopher K.; Hall, John A.; Yurke, Bernard; and Knowlton, William B. (2021). Exciton Delocalization and Scaffold Stability in Bridged Nucleotide-Substituted, DNA Duplex-Templated Cyanine Aggregates. The Journal of Physical Chemistry B, 125(50), 13670-13684. <https://doi.org/10.1021/acs.jpcb.1c07602>

1. **FIGURE/TABLE FILE CORRESPONDENCE**

The Figure/Table File Correspondence file provides a mapping to understand how underlying data and DATA ATTRIBUTE README files correspond to the figures/tables that are shown in the published text and Supplemental Information.

*Figures and tables that are self-contained and not reliant on an underlying data file are noted as such.*

**Data are provided as a single workbook with sheets corresponding to each figure/table, or as individual worksheet files (folder named: Roy2021\_Data). Data are available as .xlsx workbook files or in .csv format. Data attribute README files are provided with .txt extensions**

**Main Text**

* Figure 1 – Sequences and schematics
  + No underlying data. Figures created using Chemdraw, Inkscape, and Powerpoint
* Figure 2 – Melting profiles summary
  + **Roy2021\_Figure­\_2\_Melting\_Summary**
    - Data\_Attribute\_README\_Melting\_Profiles
* Figure 3 – PAGE image
  + No underlying data
    - Data\_Attribute\_README\_PAGE
* Figure 4 – Absorption and Circular Dichroism
  + **Roy2021\_Figure\_4\_Abs\_and\_CD**
    - Data\_Attribute\_README\_Absorption
    - Data\_Attribute\_README\_Circular\_Dichoism
* Figure 5 – Image of dimer orientation parameters
  + No underlying data
* Figure 6 – Example KRM result for DNA:DNA dimer
  + Example modeling result from Table S6 and Figure S23
* Table 1 – Predicted melting temperatures
  + Theoretical melting temperatures were obtained by using an online software program provided by European Molecular Biology Laboratory77 (Cambridgeshire, UK) using the nearest-neighbor method “Allawi et al. 1997”, 15 mM MgCl2, and 89 mM TRIS. Salt correction was included by using the “SantaLucia et al. 1998” option.
* Table 2 – KRM summary
  + Summary of key KRM modeling parameters reported in Tables S6-S14

**Supplementary Info**

* Figure S1–S5 – Melting profiles
  + **Roy2021\_Figure\_S1–S5\_Melting\_Data**
    - Data\_Attribute\_README\_Melting\_Profiles
* Figure S6–S13 – Hysteresis Plots: Unlabeled DNA:DNA
  + **Roy2021\_Figure\_S6–S13\_Hysteresis**
    - Data\_Attribute\_README\_Melting\_Profiles
* Figure S14-S18 – PAGE gel images and design schematics
  + No underlying data
* Figure S19—S22 — KRM model images to describe parameters
  + No underlying data
* Figure S23—S25 – 3D plots of transition dipole moments
  + Coordinates are listed in Tables S6—S14
  + Molecular images created with Avogadro and Chimera using the coordinates in Tables S6—S14, assuming the transition dipole lies on the long axis of the Cy5 dye.
* Figure S26 – Example orientation from Figure S23 for further discussion
  + Coordinates given in Table S4
* Figure S27 – KRM Absorption and CD prediction for varying Huang-Rhys factors
  + **Roy2021\_Figure\_S27\_H-R\_Study**
    - Data\_Attribute\_README\_KRM\_Modeling
* Figure S28 – Select curves from Figure S27 with vibronic/electronic cross sections
  + **Roy2021\_Figure\_S28\_H-R\_Study\_2**
    - Data\_Attribute\_README\_KRM\_Modeling
* Figure S29 – A vs B form DNA
  + **Roy2021\_Figure\_S29\_A-form\_vs\_B-form\_CD**
* Figure S30 – A vs B form content estimate plots
  + **Roy2021\_Figure\_S30\_UV\_CD\_Comparison**
    - Data\_Attribute\_README\_Circular\_Dichoism
    - Data\_Attribute\_README\_KRM\_Modeling
* Figure S31 – Steady-state relative fluorescence
  + **Roy2021\_Figure\_S31\_SS\_Fluorescence**
    - Data\_Attribute\_README\_Fluorescence\_Emission
* Table S1 – Summary of melting transitions in Figures S1-S5
  + See Figures S1—S5
* Table S2 – Typo, there is no such table
  + References to Table S2 in the Supplemental Information should refer to Table S3 ; Previous Table S2 was labeled as Table S3 in the final version of the SI.
* Table S3—S5 – Descriptions of KRM parameters
  + No underlying data
* Table S6-S14 – KRM model results tables: Model results derived from absorption and circular dichroism data in Figure 4 (**Roy2021\_Figure\_4\_Abs\_and\_CD**)
  + **Roy2021\_Table\_S6**
  + **Roy2021\_Table\_S7**
  + **Roy2021\_Table\_S8**
  + **Roy2021\_Table\_S9**
  + **Roy2021\_Table\_S10**
  + **Roy2021\_Table\_S11**
  + **Roy2021\_Table\_S12**
  + **Roy2021\_Table\_S13**
  + **Roy2021\_Table\_S14**
    - **Data\_Attribute\_README\_Absorption**
    - **Data\_Attribute\_README\_Circular\_Dichoism**
    - **Data\_Attribute\_README\_KRM**
* Table S15 – Summary of data from Figure S28
  + See Figure S28

1. **STRUCTURAL METADATA: General format**

Each DATA ATTRIBUTE README file describes the data (e.g., how collected, measurements metrics and conditions, data column definitions) specific to each data type**.** The following are the sections included in each README file.

**A. TITLE**

The title matches a dataset listed in the “LIST OF DATA and README FILES RELATED TO THE STUDY” section of the DESCRIPTIVE METADATA.

**B. DATA DESCRIPTION**

Provides a generic description of what the data are and how they were collected.

**C. LIST OF FILES**

Lists the names of the data files associated with each README file.

**D. FILE FORMATS**

Lists file formats used for data files.

**E. SOFTWARE & VERSION**

States the name(s) and specific version(s) of any commercial software that may be needed to work with the data.

**F. DATA DICTONARY**

Provides a brief description of each unit of measurement used in Column headings of the associated data files or of any other key term otherwise mentioned in the DATA ATTRIBUTE README file.