SUPPLEMENTARY INFORMATION

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One Step Synthesis of a Fused Four-Ring Heterocycle

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Fig. S1. ^{1}H NMR of yellow IDQQ crystals dissolved in DMSO-d_6.

Fig. S2. Predicted 1H-NMR chemical shifts for IDQQ Tautomers **I-IV**.

Fig. S3. TGA of IDQQ crystals.

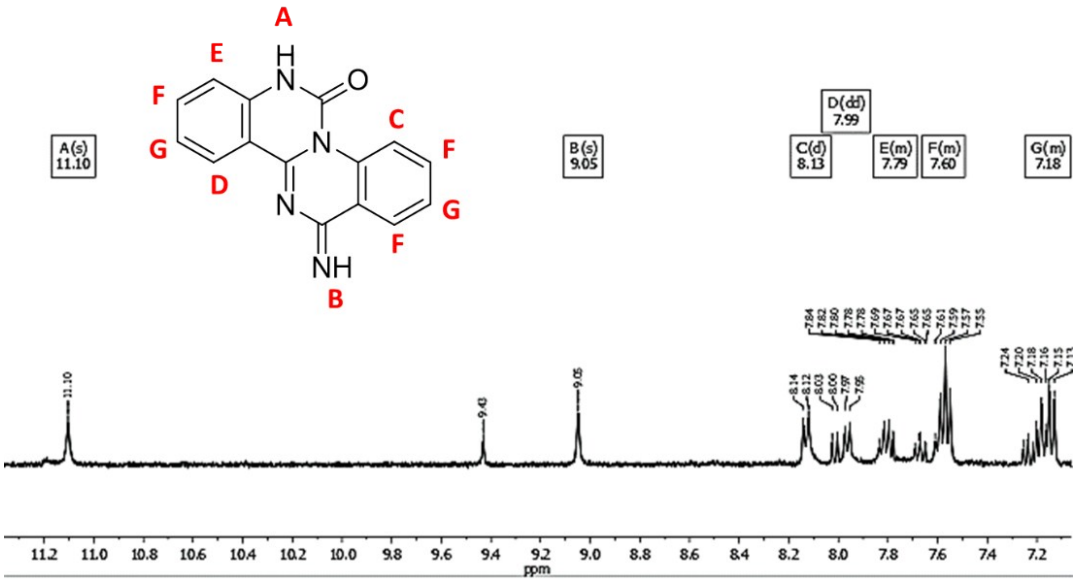
Fig. S4. DSC of IDQQ crystals. The broad transition beginning at ~113°C likely correlates to solvent loss. IDQQ decomposes at 272.42°C.

Fig. S5. Raman spectra of single crystals of **3** and IDQQ, and crystals of **3** heated to 170, 180 and 190°C. The Raman spectra quality was greatly affected by multiple factors, including thin crystals that were destroyed by low laser intensity coupled with background fluorescence. Background corrections were applied.

Fig. S6. Solvent mediated transformation of **3** to IDQQ over time monitored as a function of concentration. Concentrations are based on UV-Vis absorbance data and an experimentally determined extinction coefficient (ε = 5323.3 L mol^{-1} cm^{-1}).

Fig. S7. Three degassed ethanol solutions of **3** (left) before and (right) after storage in the dark for 6 hours. The vial on the left was purged for 30 min with O_2 before **3** was added; the center vial was purged for 30 min with O_2 before **3** was added, then saturated with O_2 for another 30 min; the vial on the right was purged with Ar before **3** was added.

Fig. S8. Proposed mechanism for cyclization of **3** to IDQQ in ethanol.



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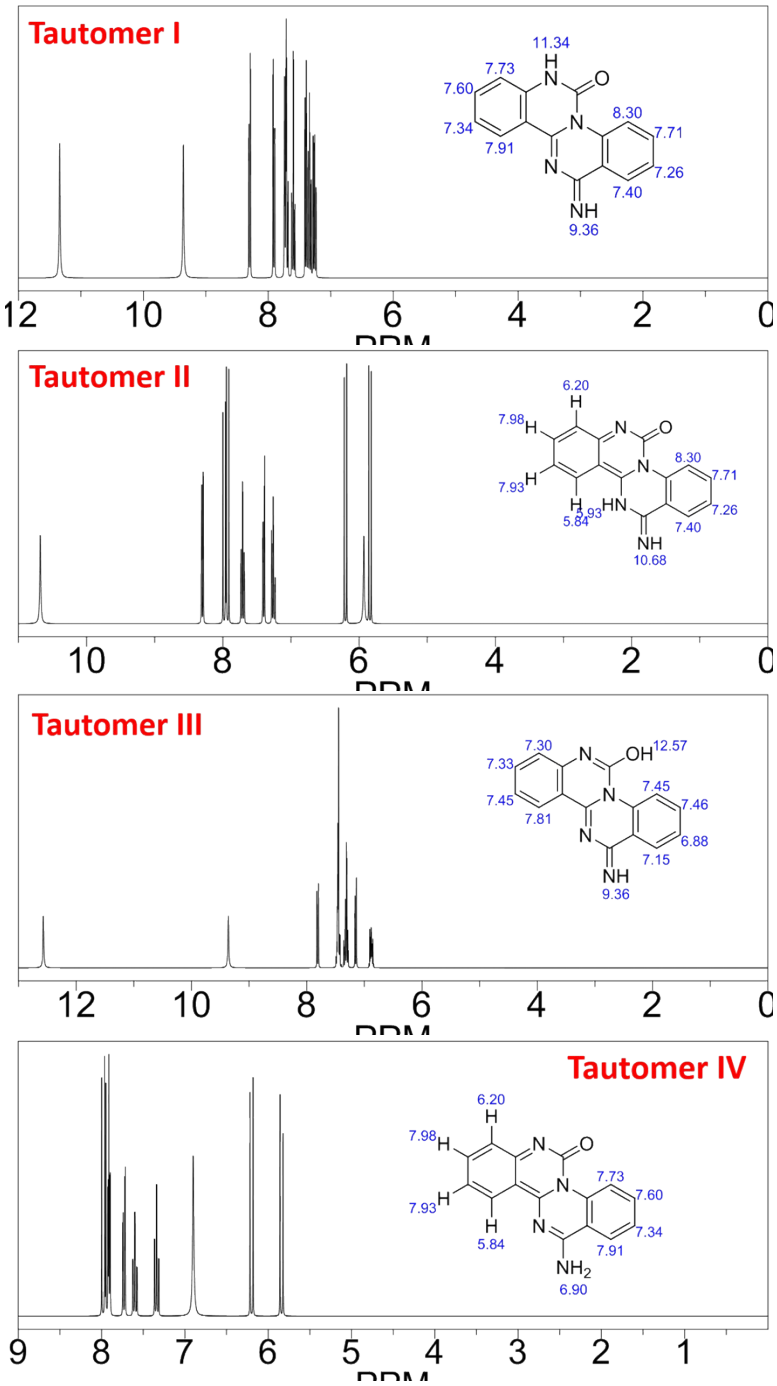

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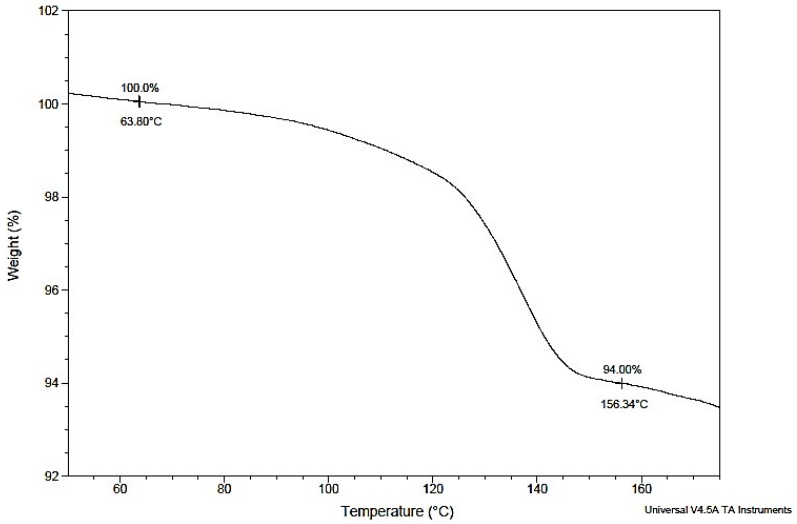


Fig. S3. TGA of IDQQ crystals.

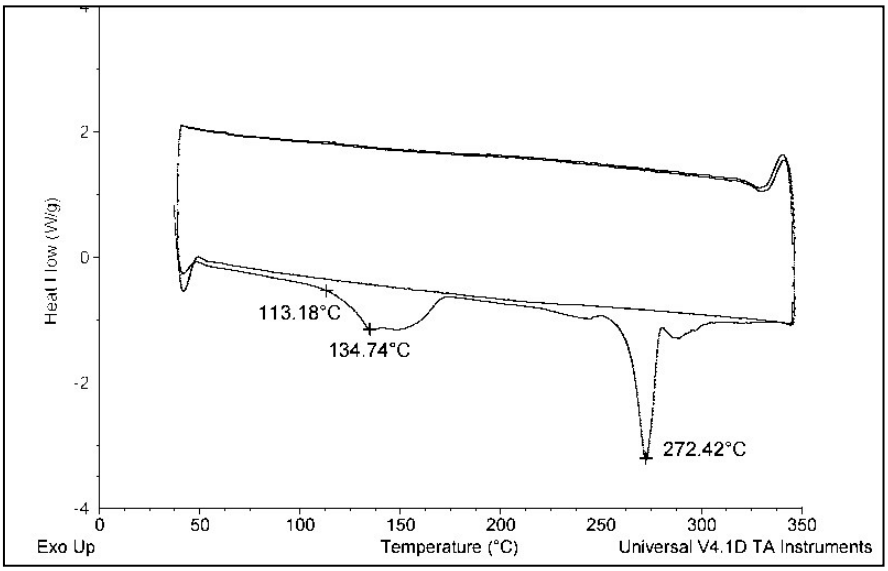
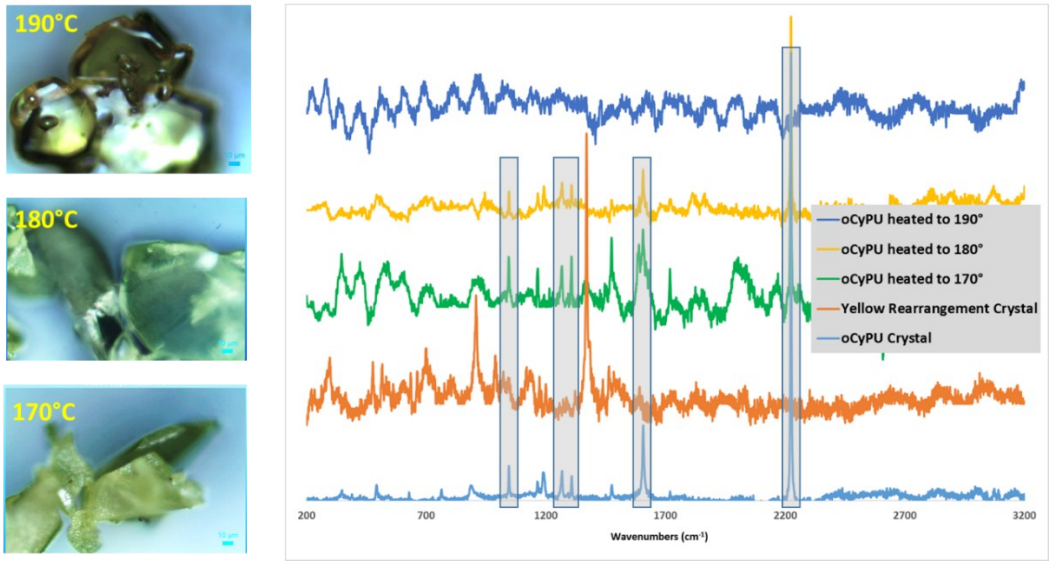


Fig. S4. DSC of IDQQ crystals. The broad transition beginning at ~113°C likely correlates to solvent loss. IDQQ decomposes at 272.42°C.



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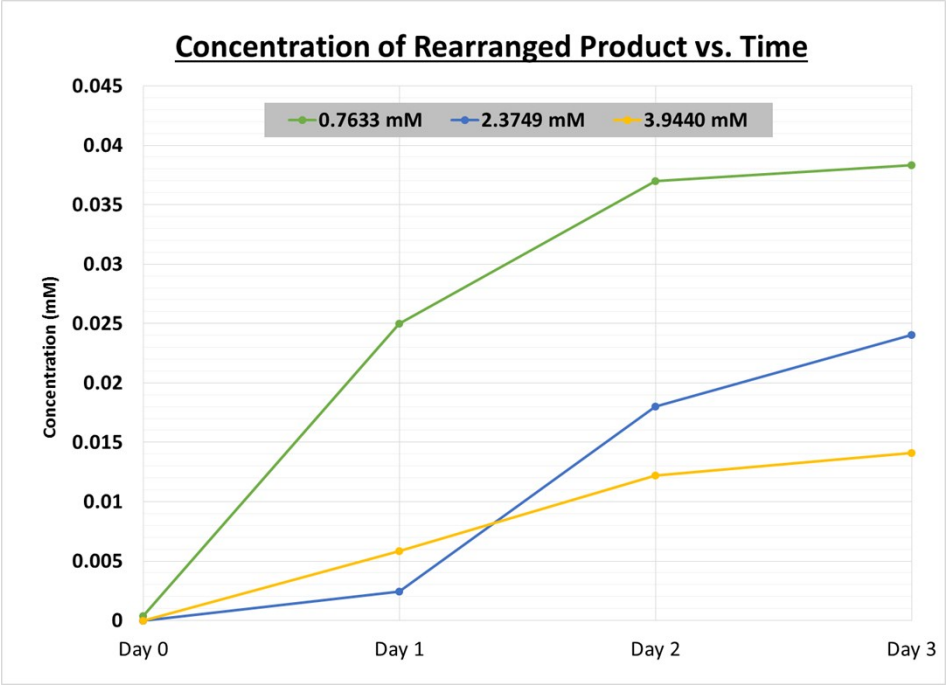

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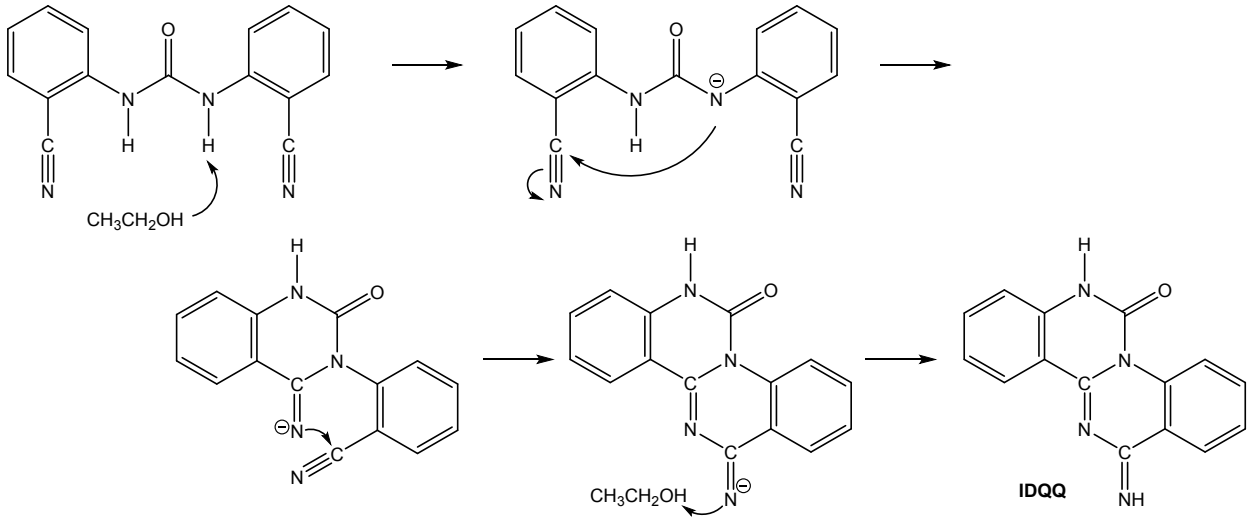

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