

Supporting Information

Near-IR MCD of the Non-Heme Ferrous Active Site in Naphthalene 1,2-Dioxygenase: Correlation to Crystallography and Structural Insight into the Mechanism of Rieske Dioxygenases

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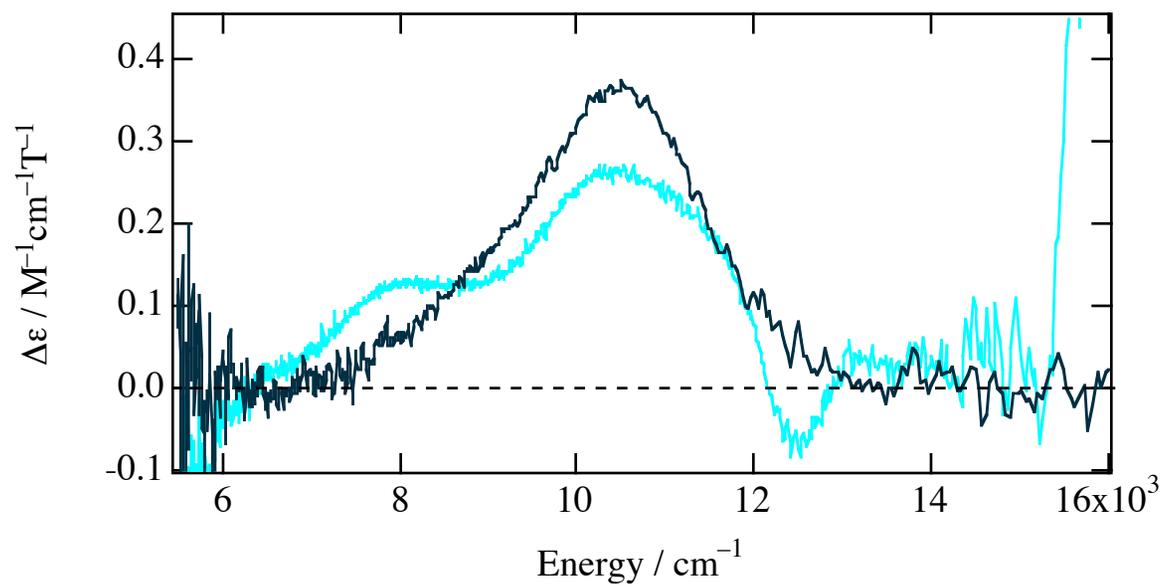


Figure S1. The overlay plot of the MCD spectra of NDOox-Naph (navy) and NDOred-Naph (aqua)

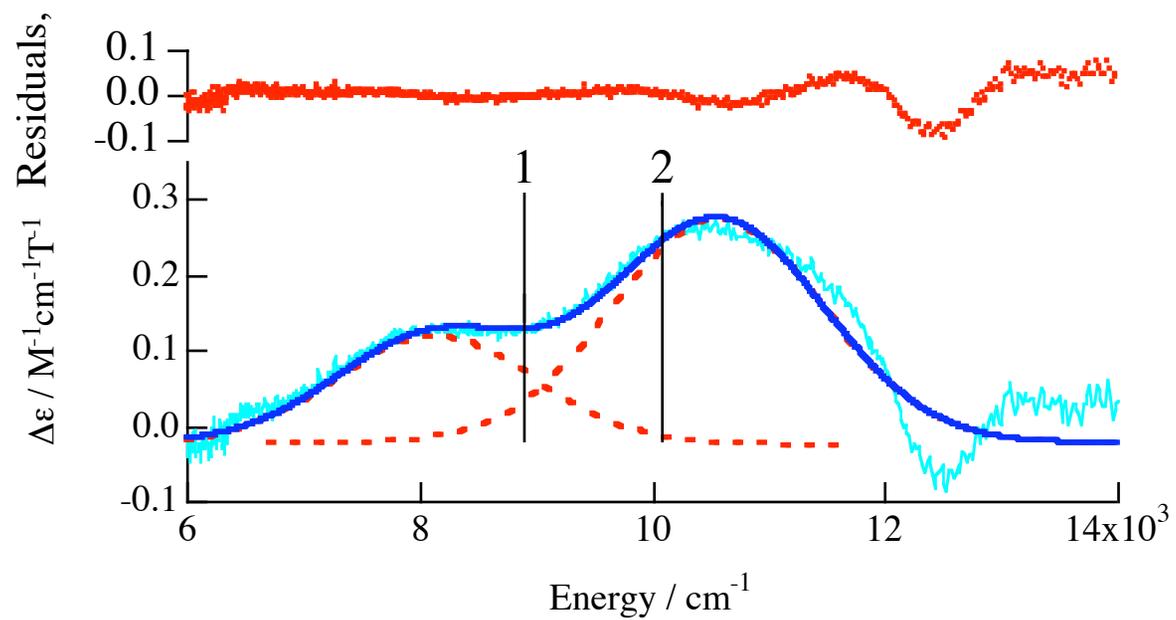


Figure S2. Deconvolution of the MCD spectrum of NDOred-Naph:
1 and **2** are 8890 and 10010 cm^{-1} , respectively.

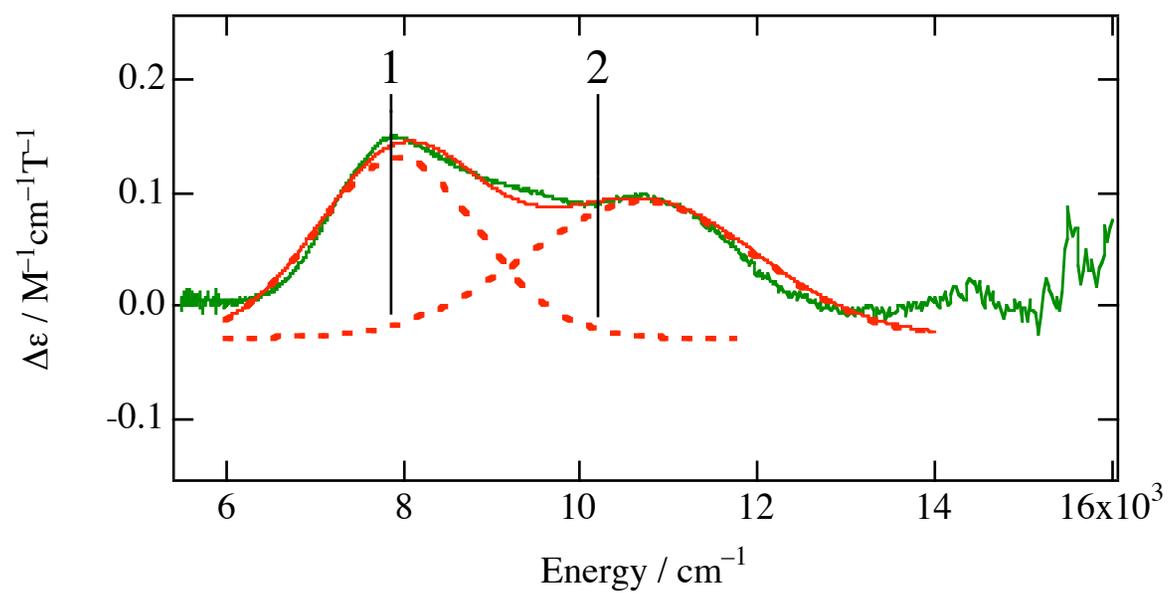


Figure S3. Deconvolution of the MCD spectrum of NDOox located two bands at 7950 cm^{-1} and 10700 cm^{-1} : **1** and **2** are 7810 and 10200 cm^{-1} , respectively.

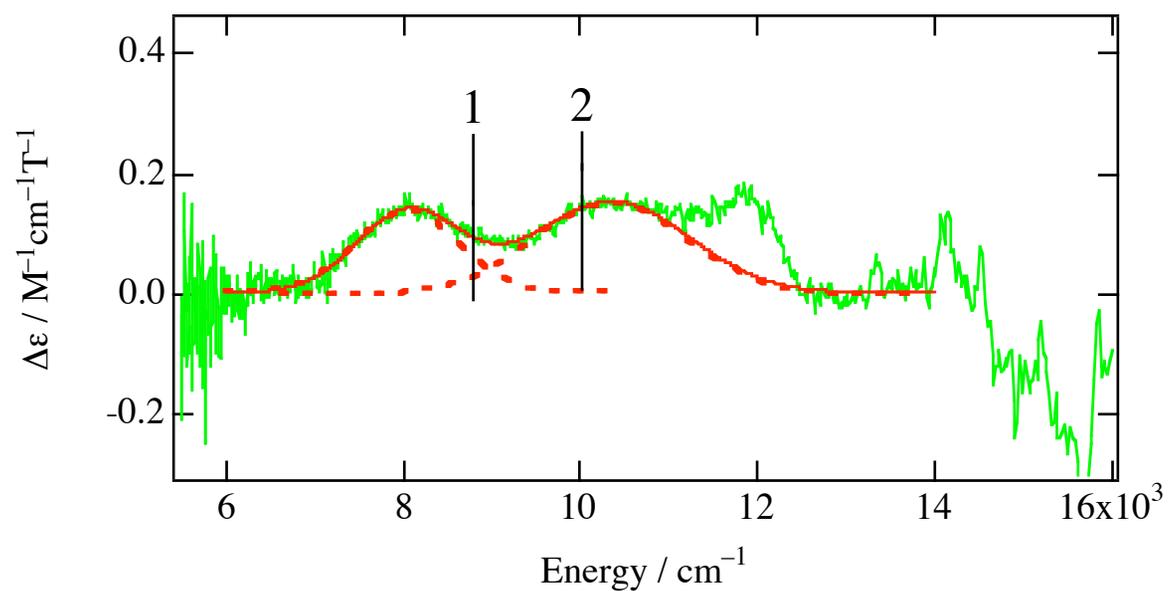


Figure S4. Deconvolution of the MCD spectrum of NDOox located two bands at 8060 cm^{-1} and 10350 cm^{-1} : **1** and **2** are 8810 and 10010 cm^{-1} , respectively. At 8810 cm^{-1} , the contribution from the 8060 cm^{-1} and 10010 cm^{-1} bands are 75 % and 25%, respectively.

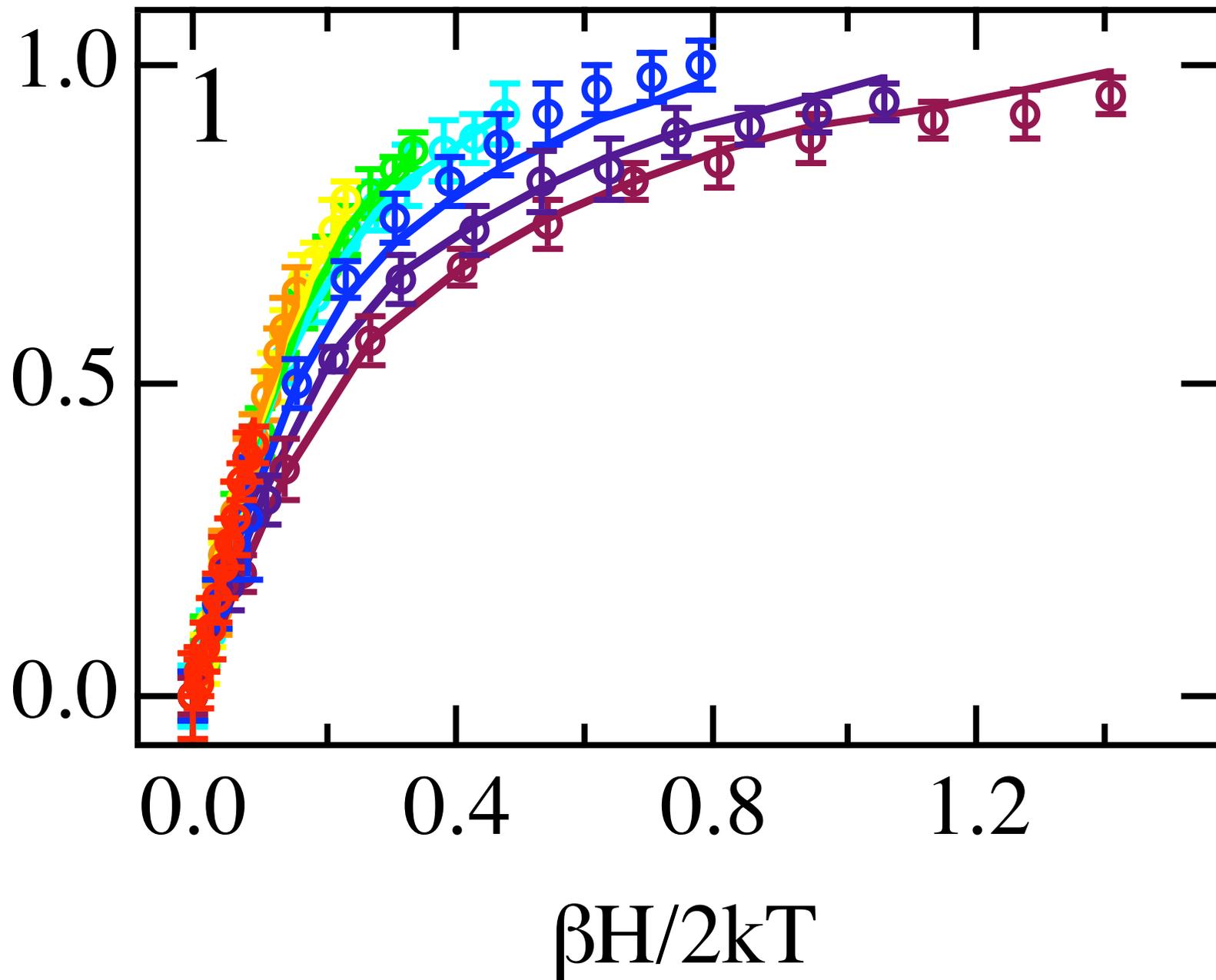


Figure S5. 3-fold expanded Figure 2B-1

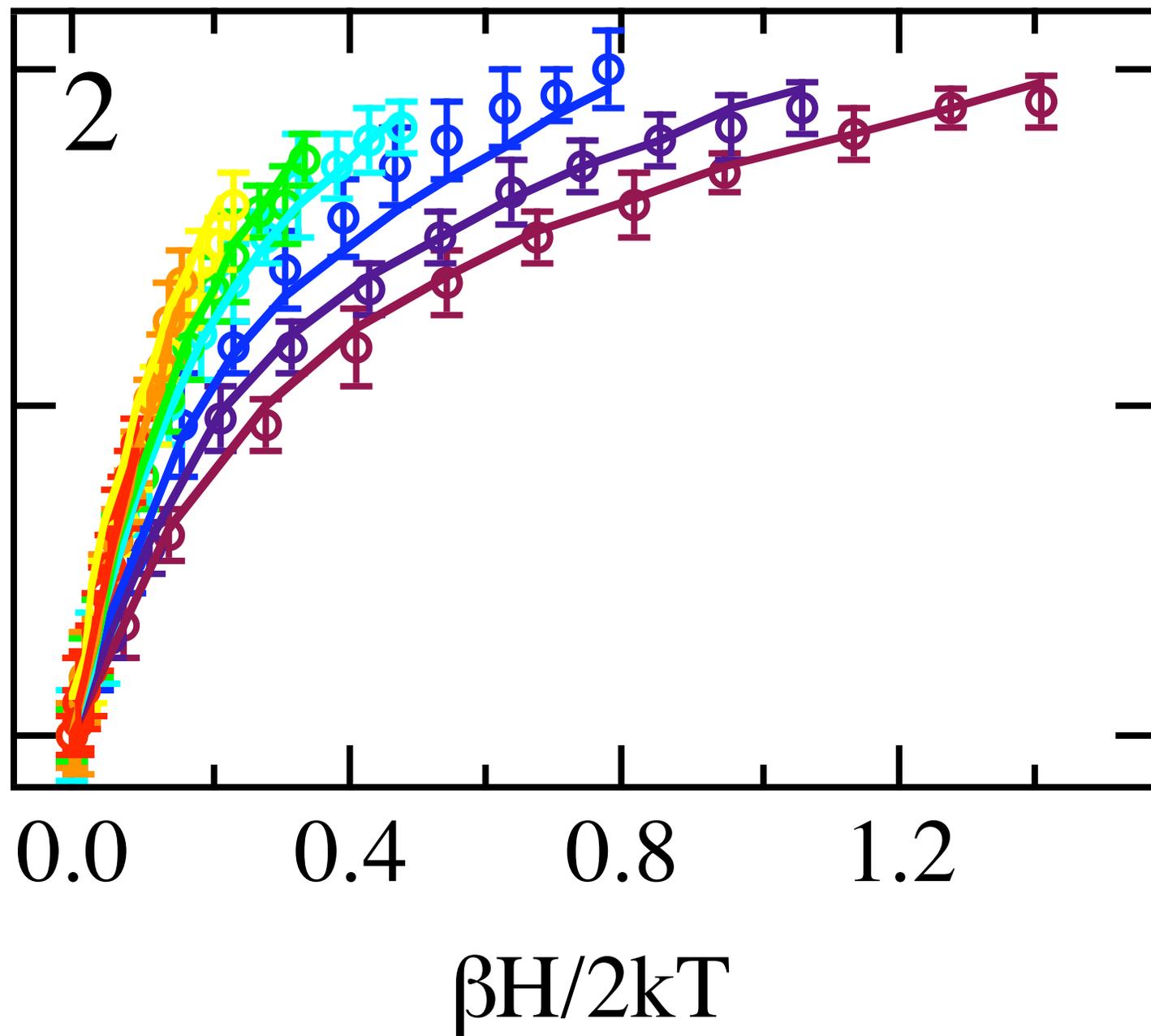


Figure S6. 3-fold expanded Figure 2B-2

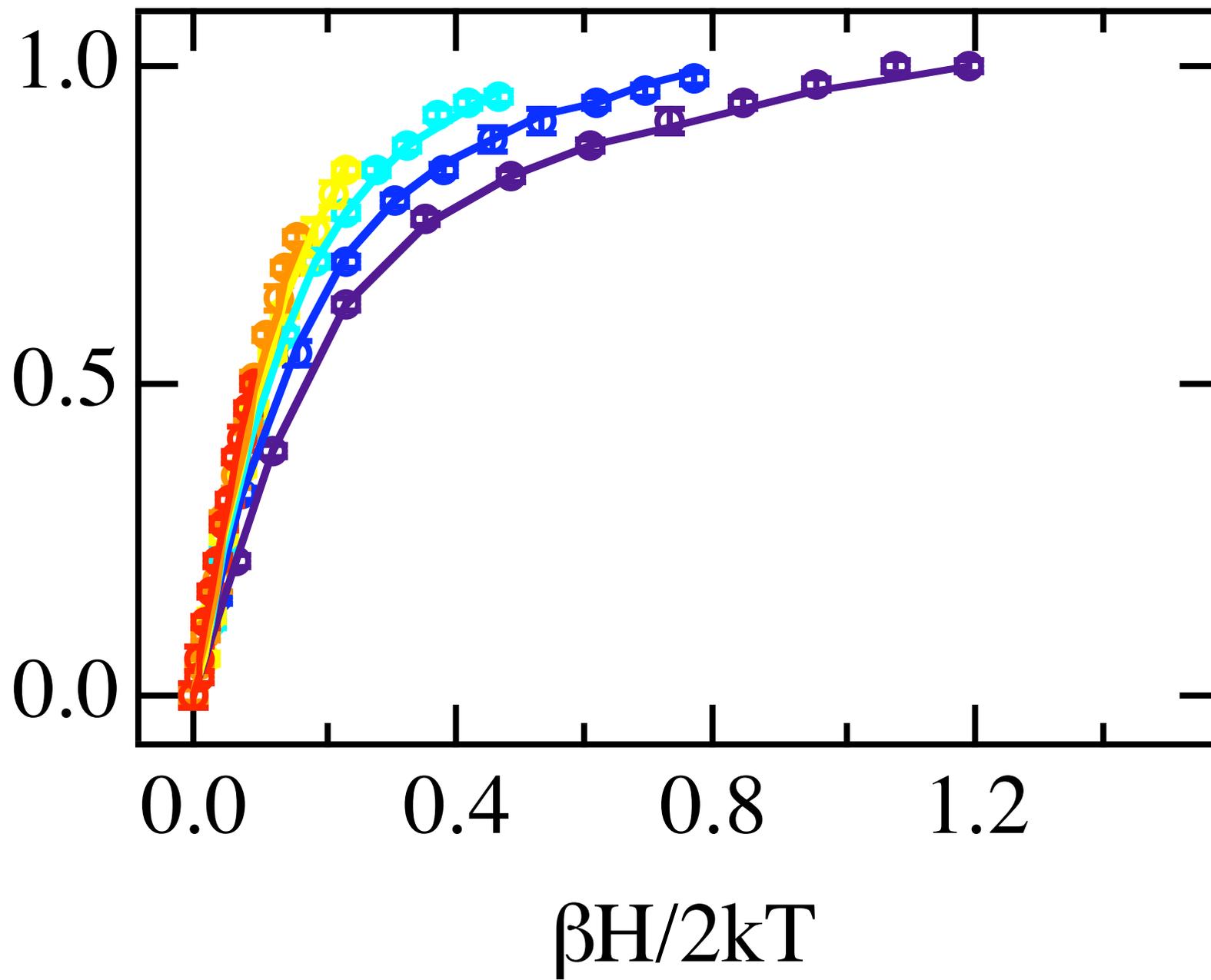


Figure S7. 3-fold expanded Figure 3B

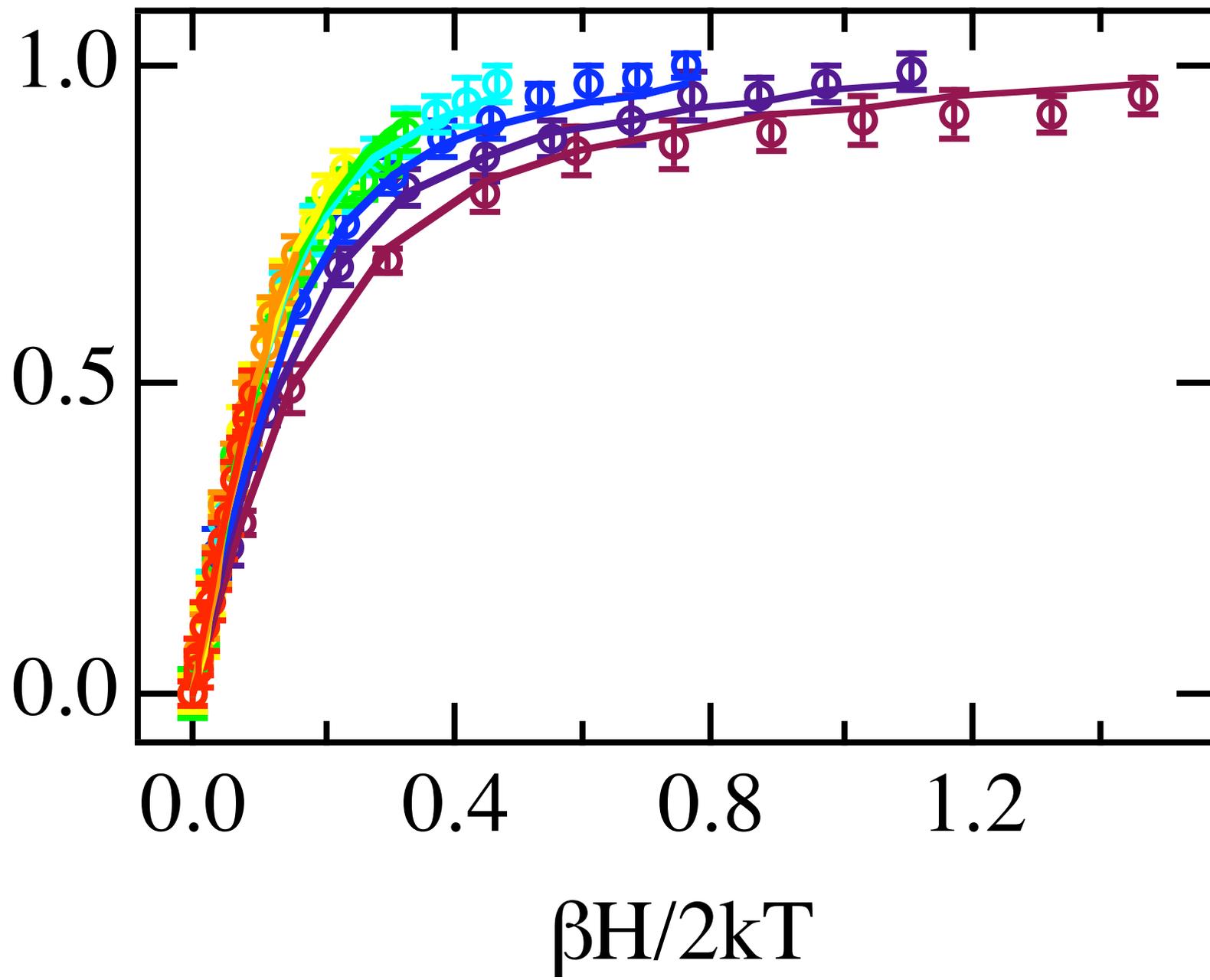


Figure S8. 3-fold expanded Figure 4B-1

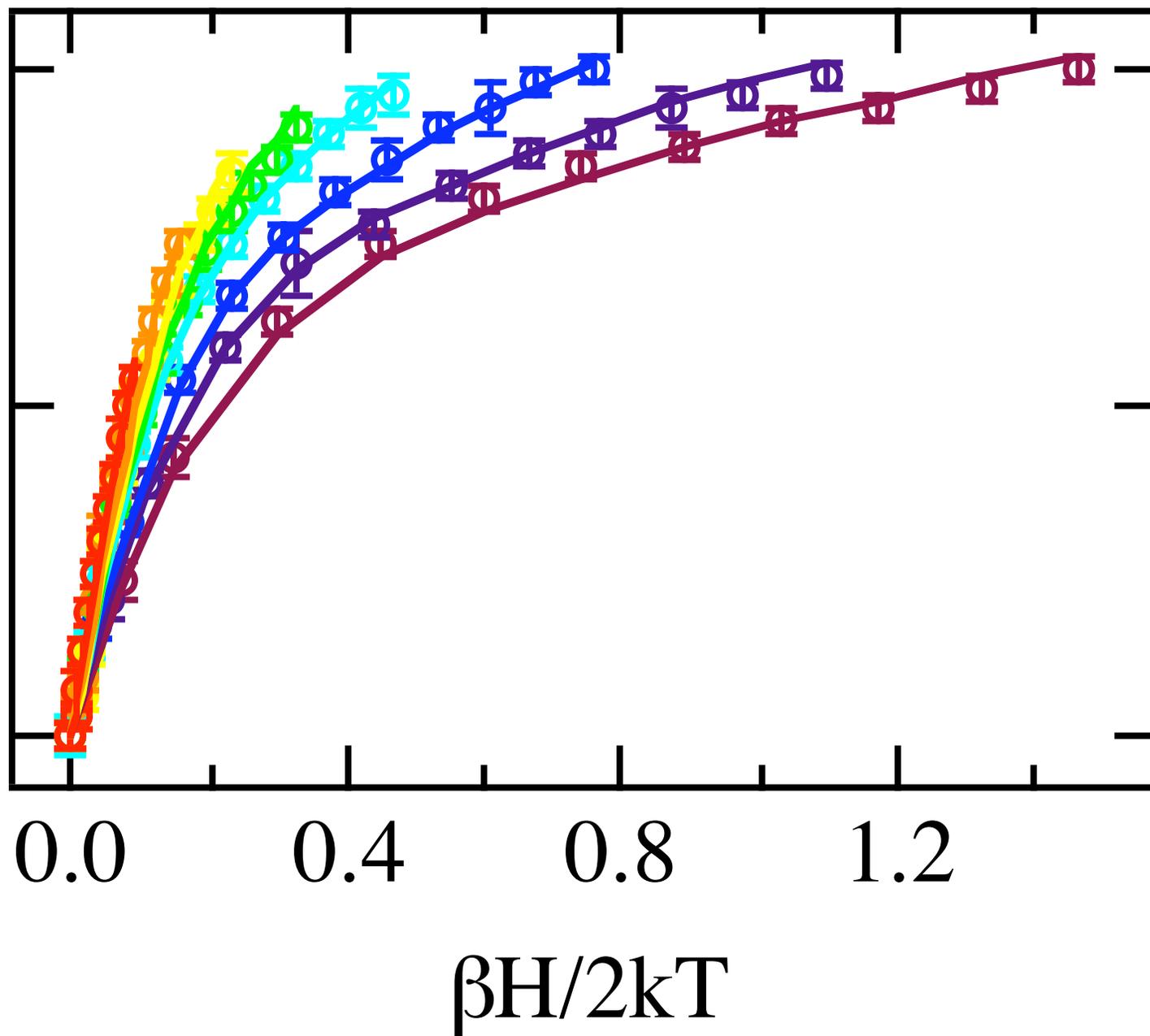


Figure S9. 3-fold expanded Figure 4B-2

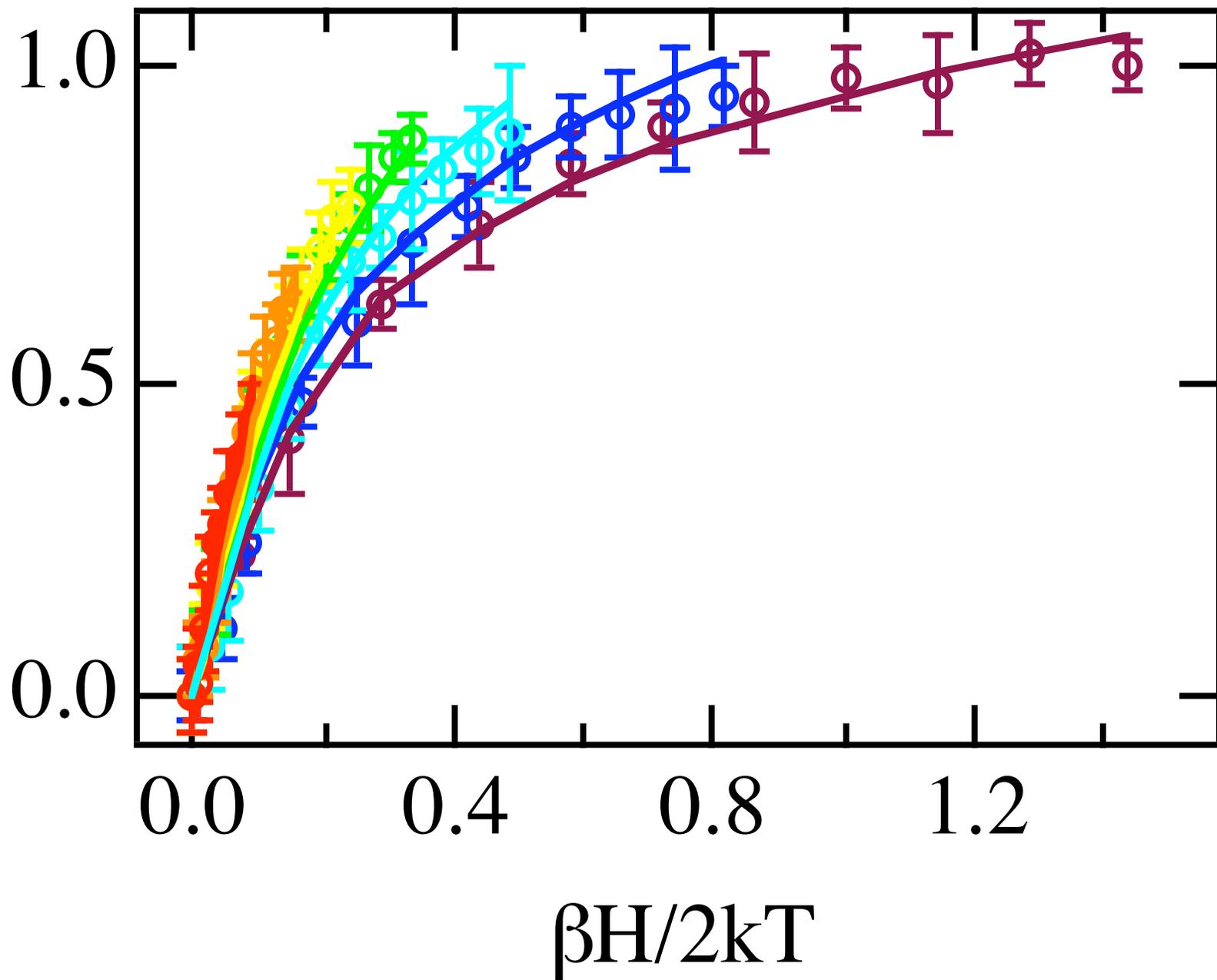


Figure S10. 3-fold expanded Figure 5B-1

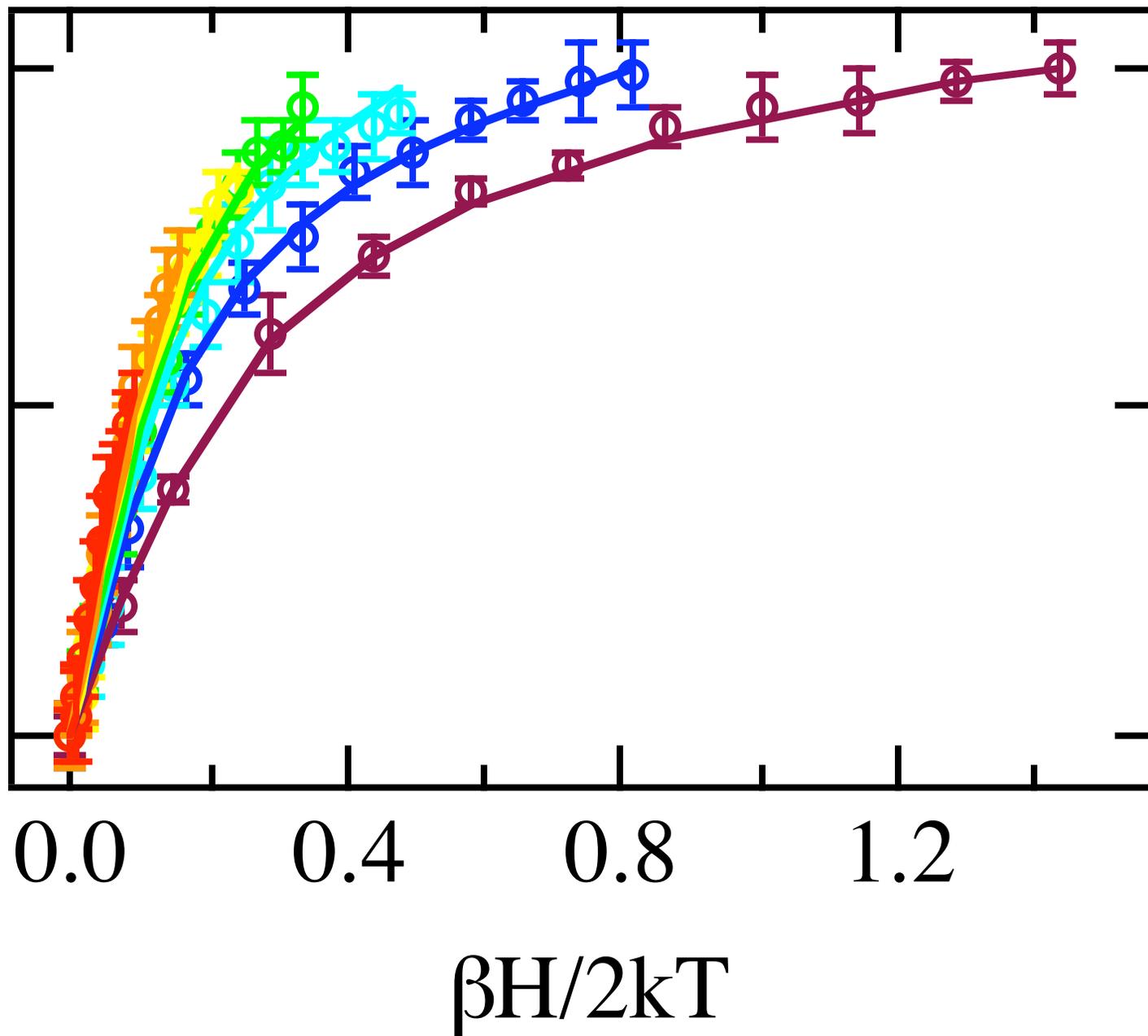


Figure S11. 3-fold expanded Figure 5B-2

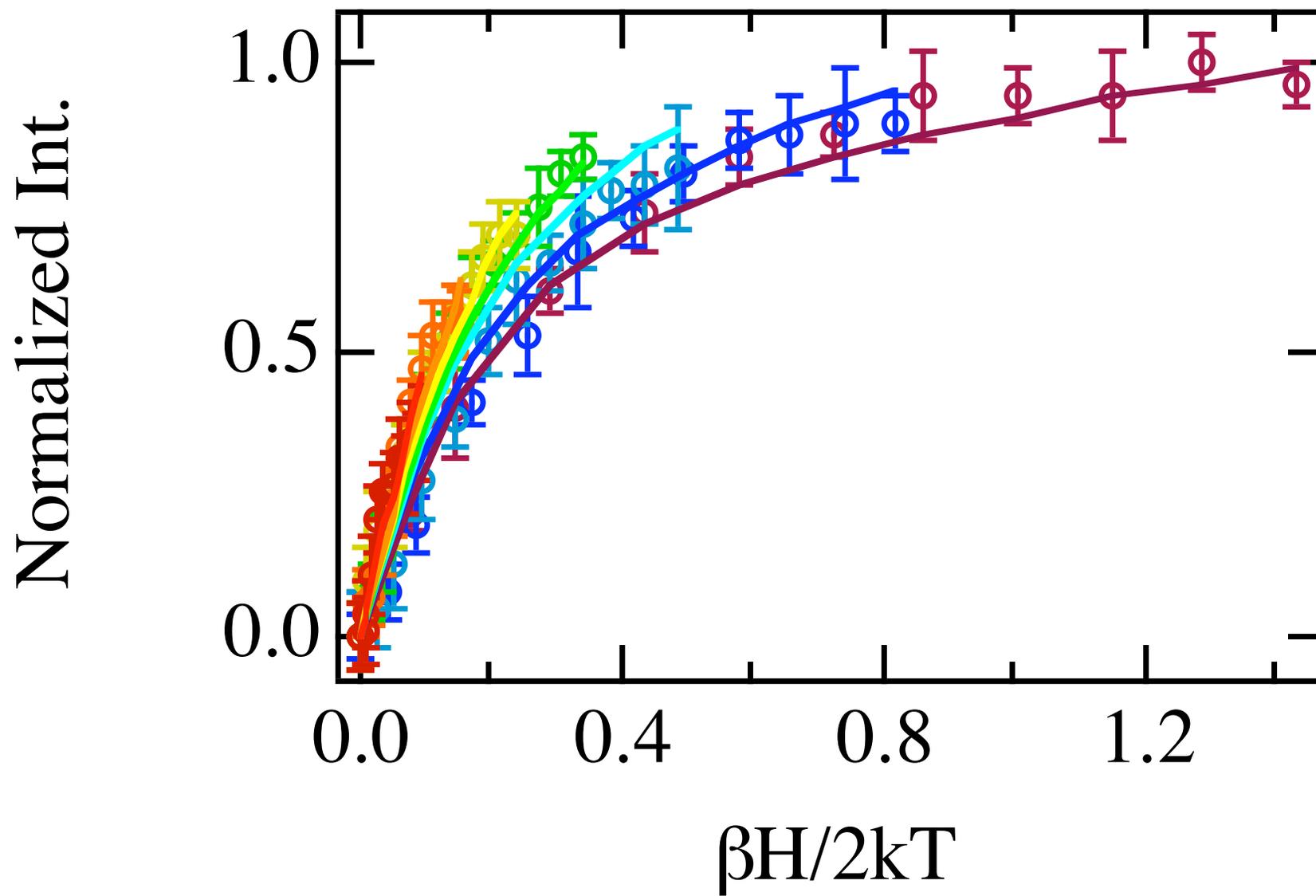


Figure S12. 3-fold expanded Figure 5C