

# UV-vis experiments

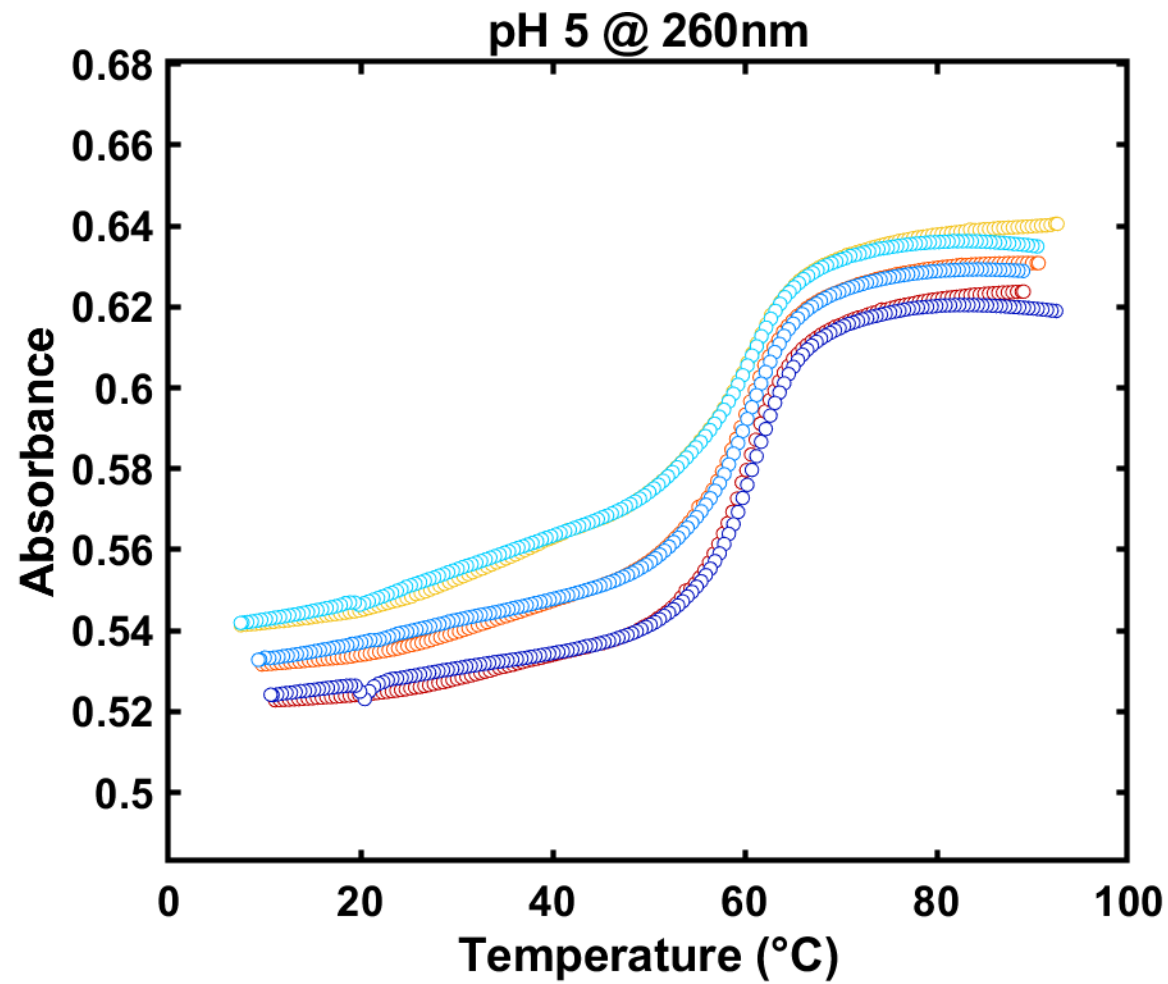
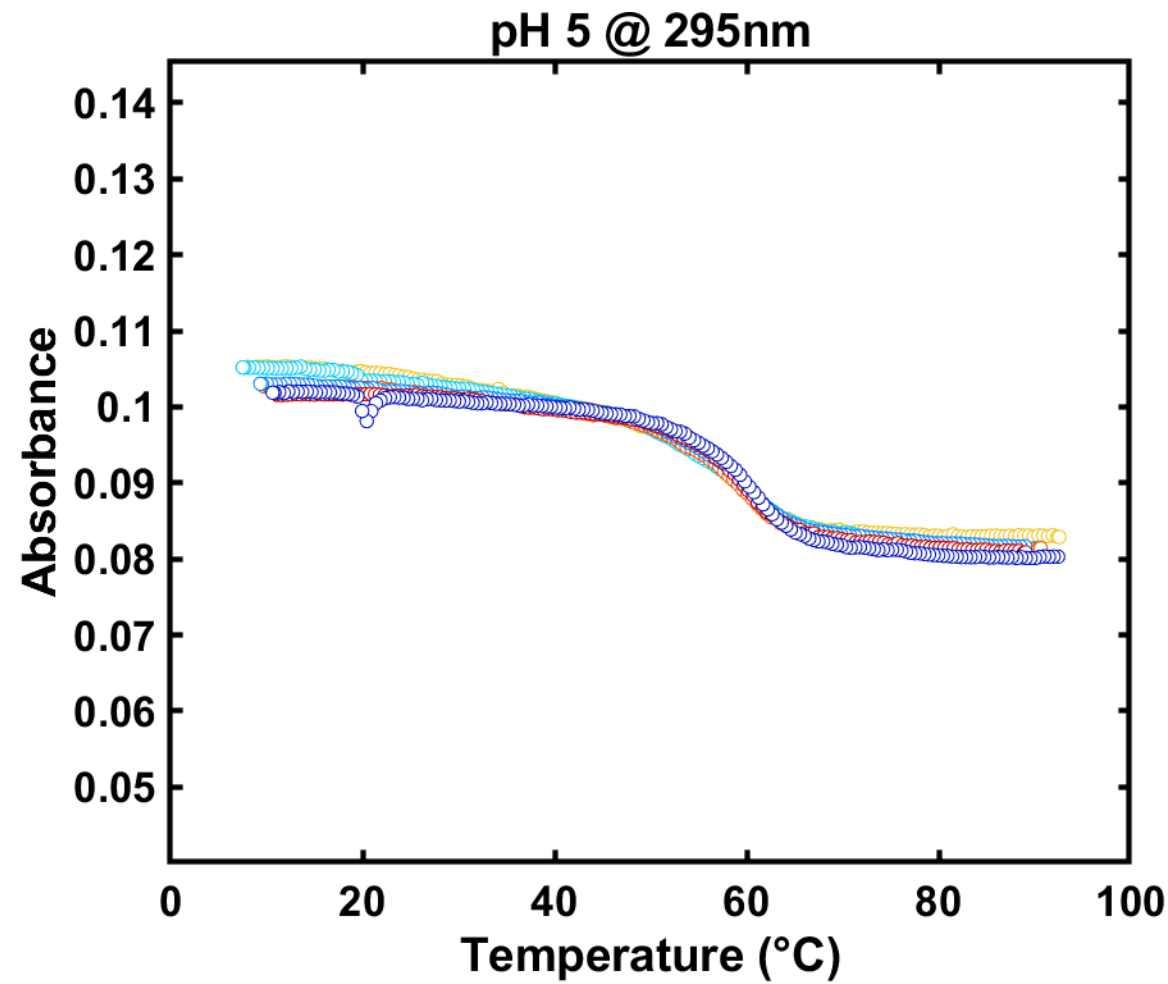
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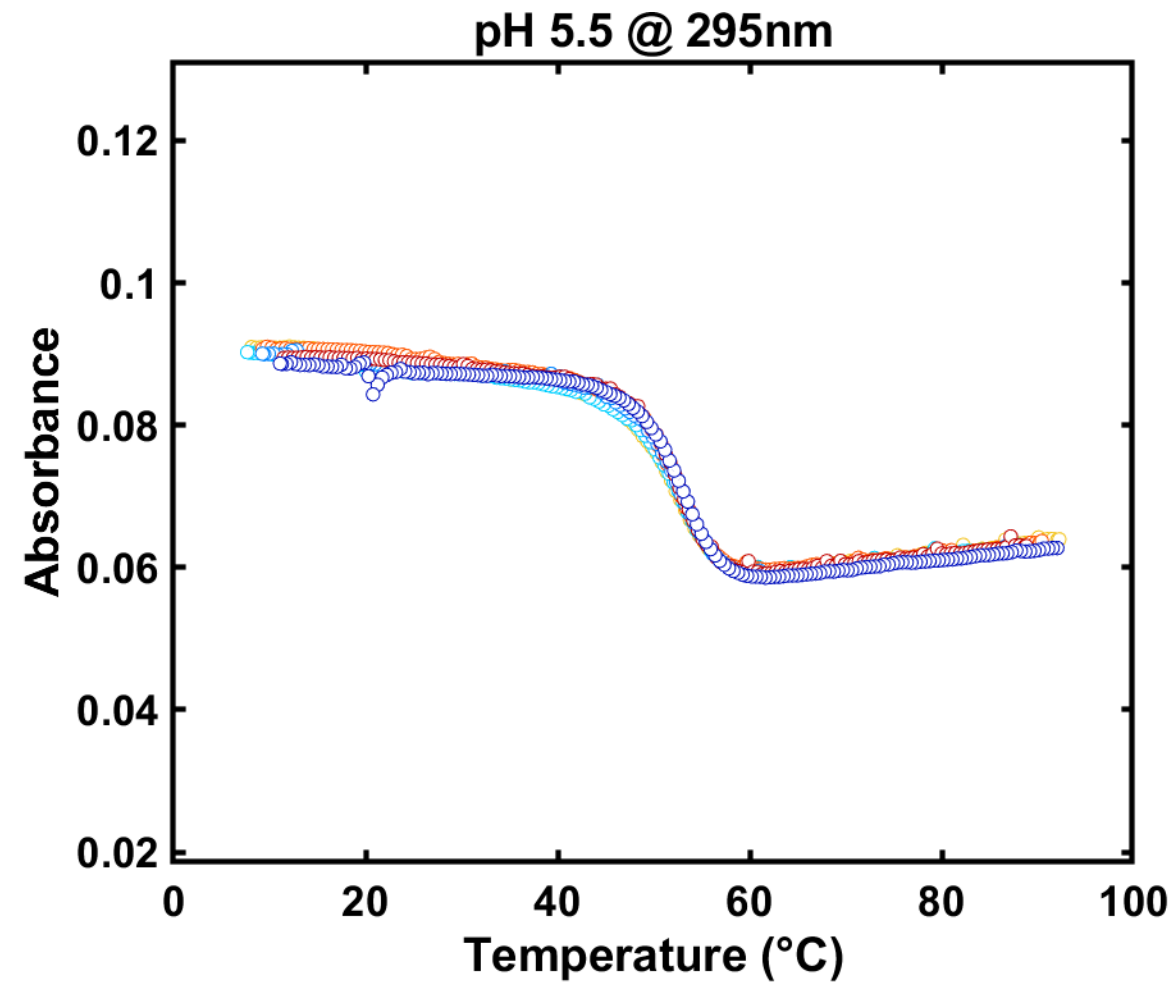
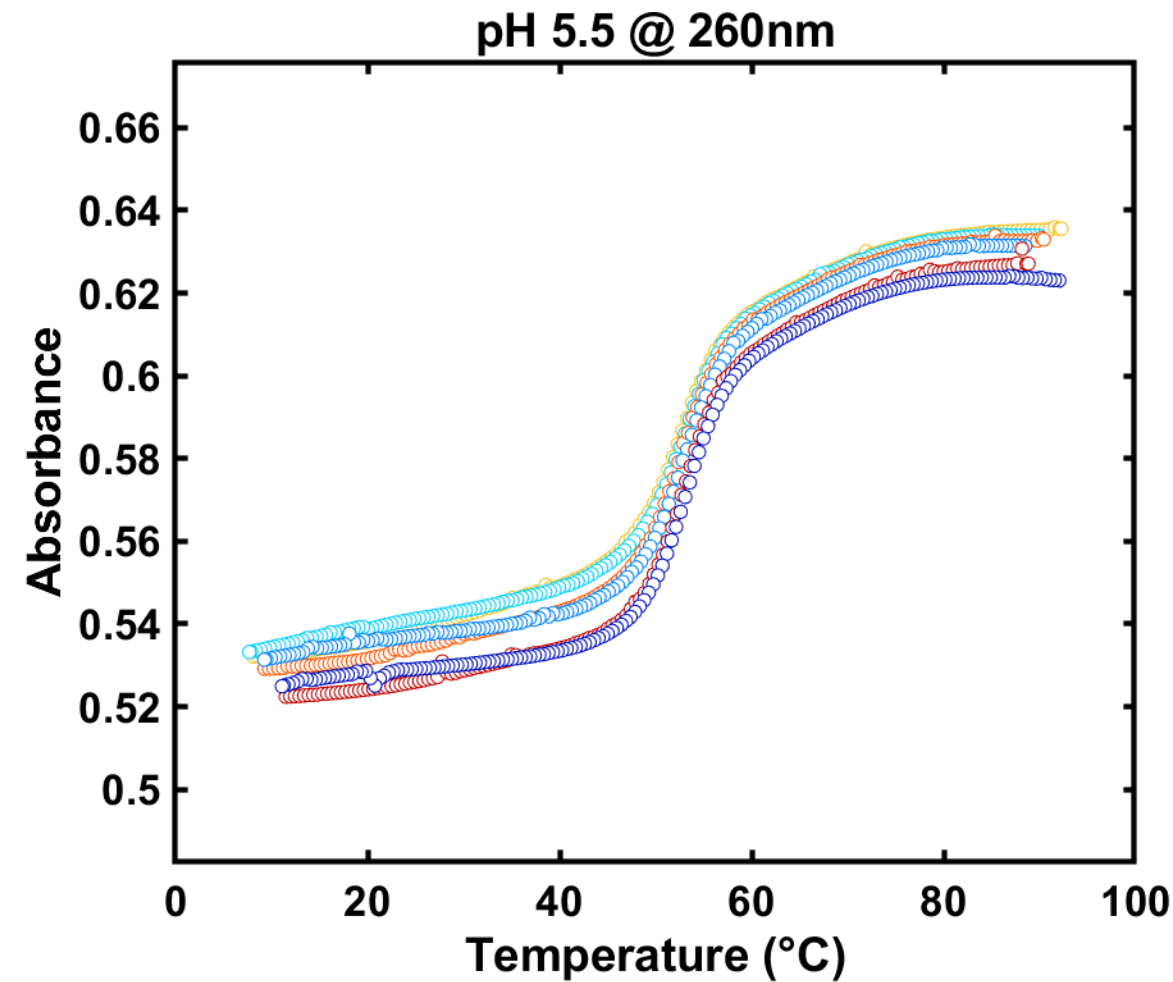
# Sample: IDJ1

- pH: 5 to 8 in 0.5 increments
- Wavelengths: 260nm, 295nm
- Salt/buffer:  $\text{KH}_2\text{PO}_4/\text{NaOAc}$ (25mM) &  $\text{KCl}$ (75mM)
- Temperature range: 5°C to 95°C
- Scan rates: 3,2,1 °C/min

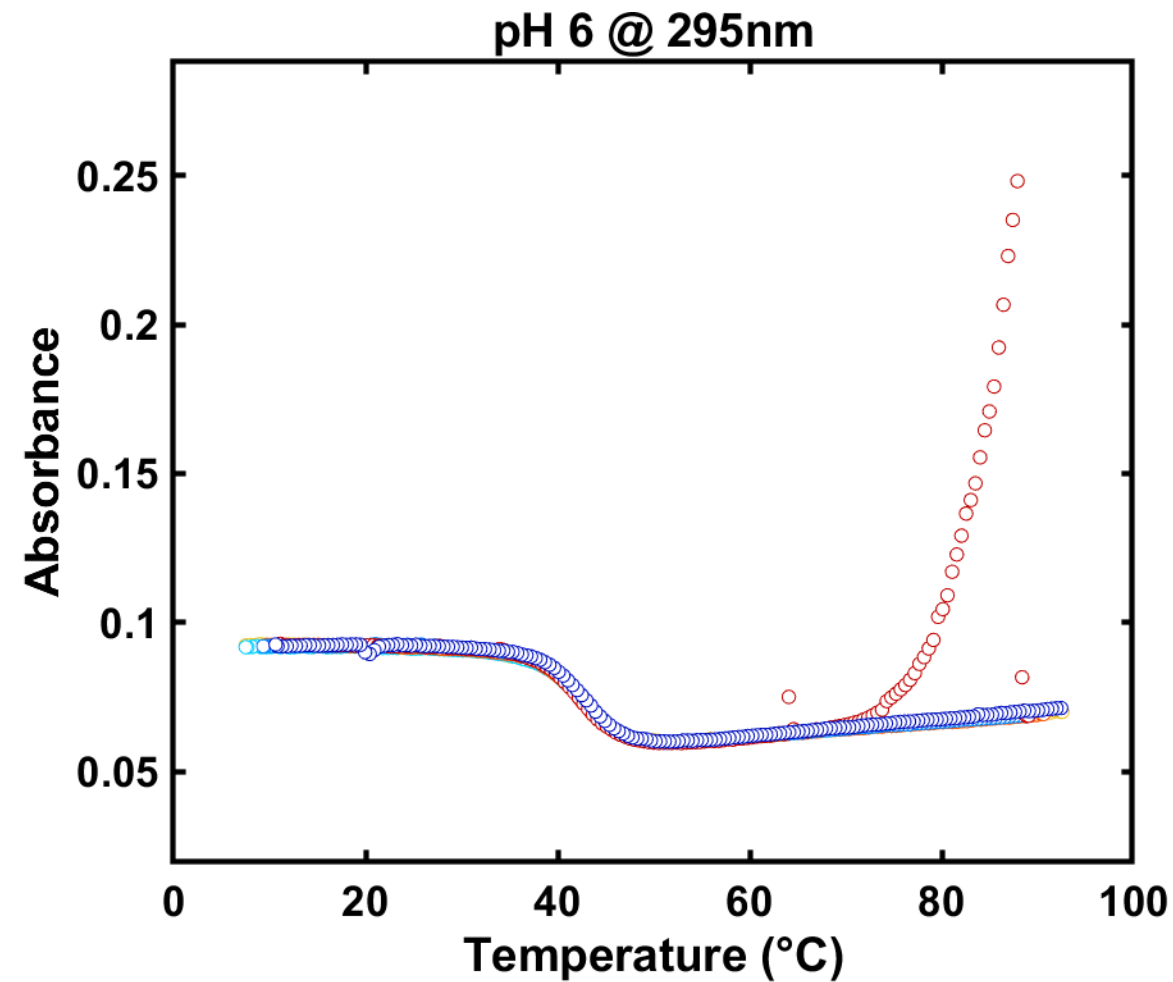
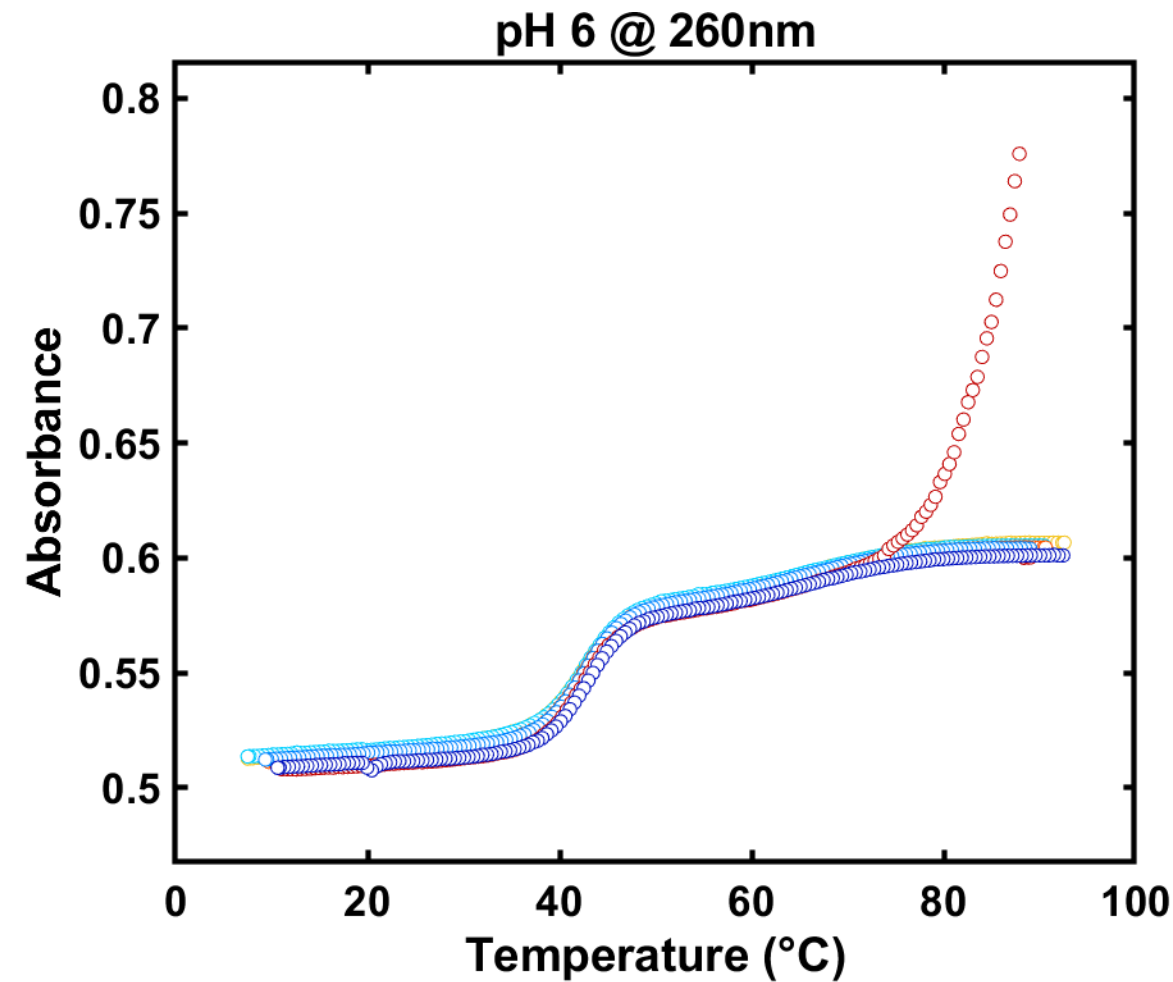
IDJ1 raw data – pH 5



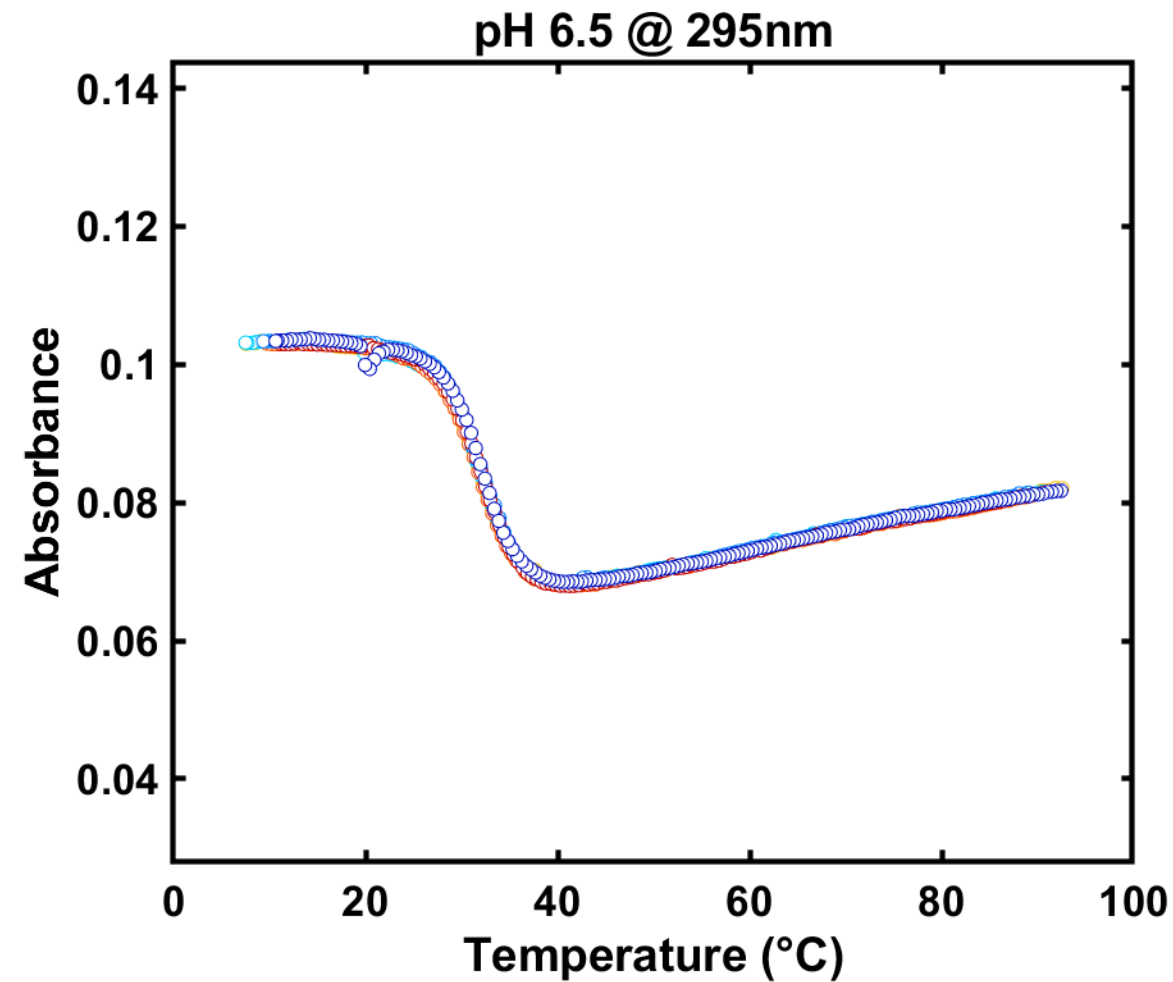
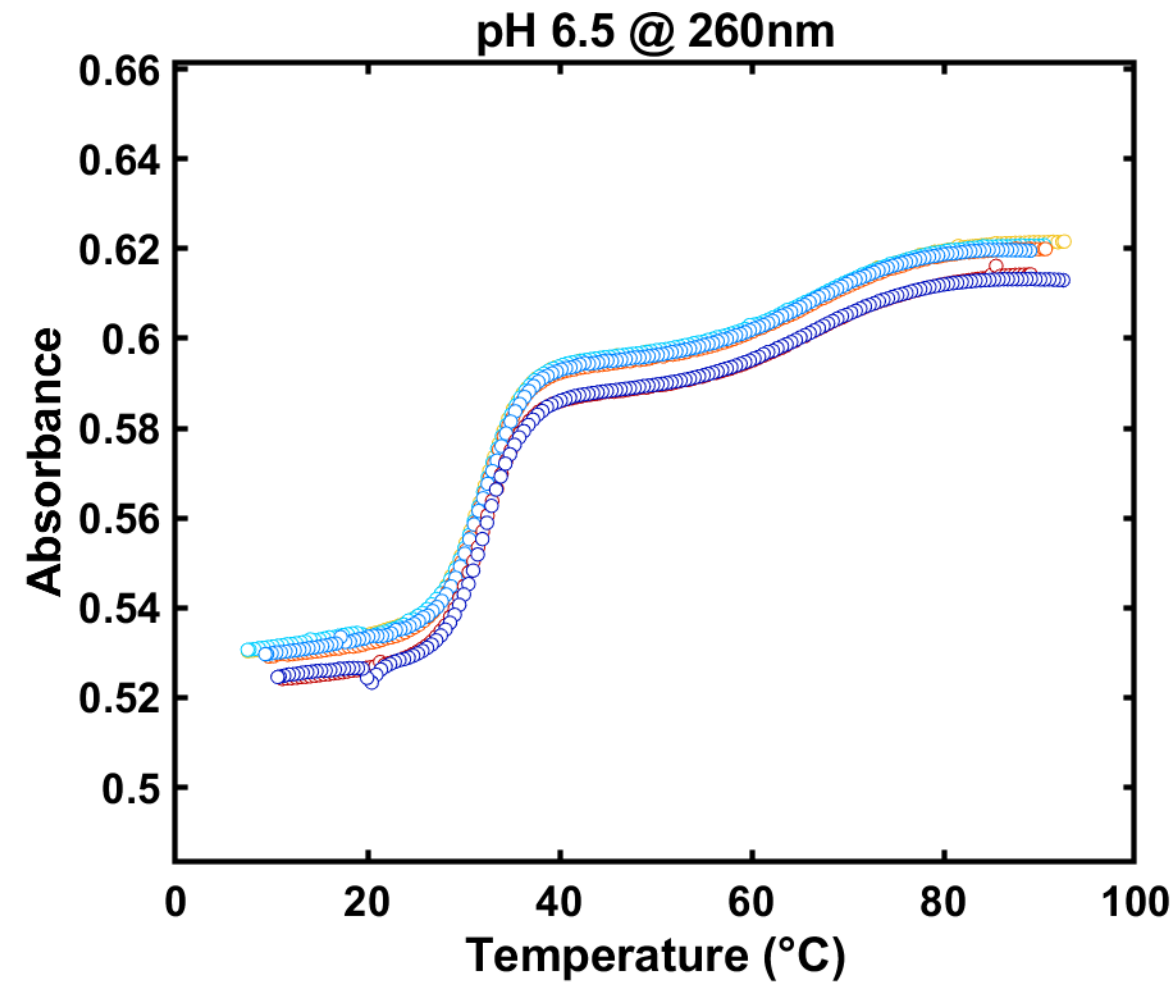
IDJ1 raw data – pH 5.5



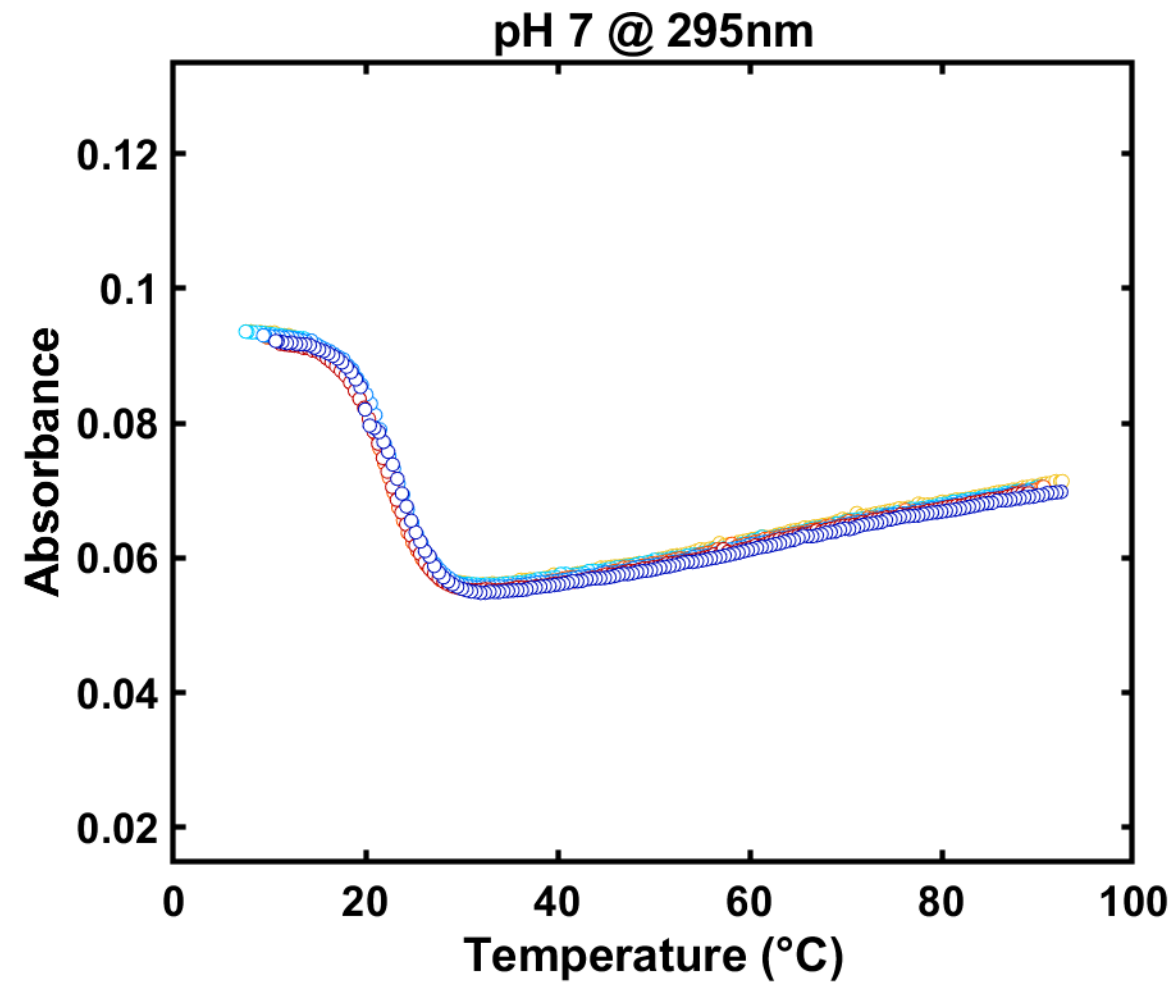
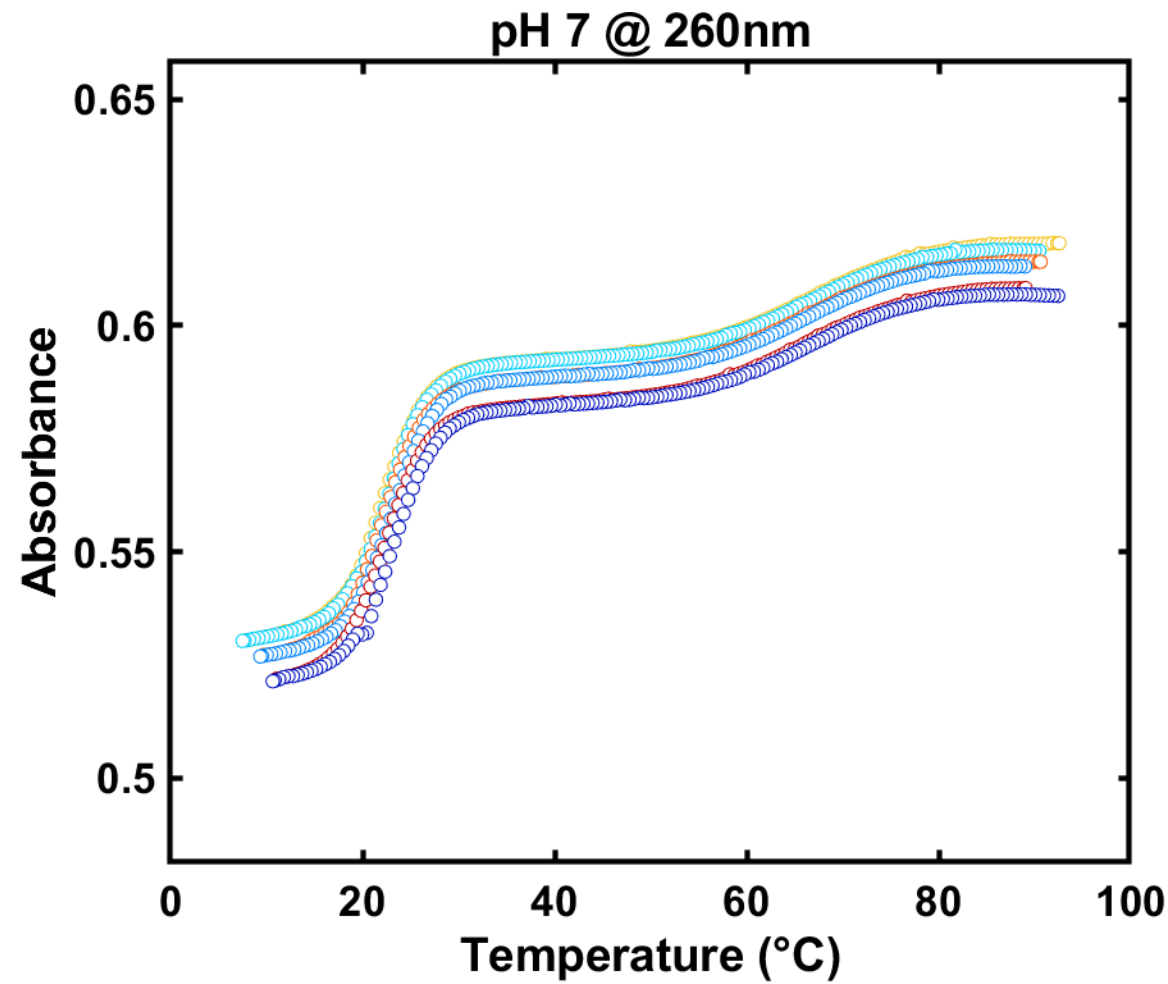
IDJ1 raw data – pH 6



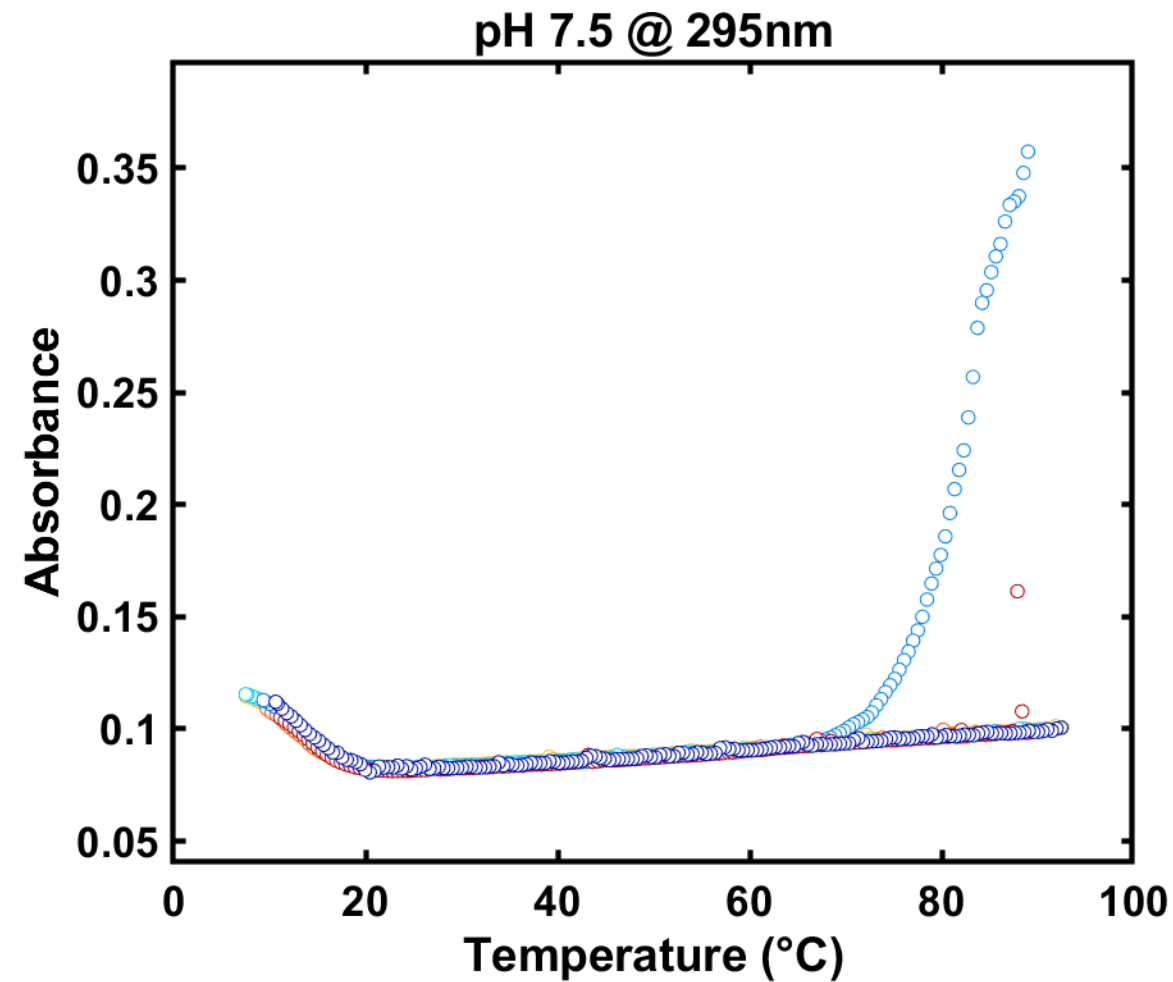
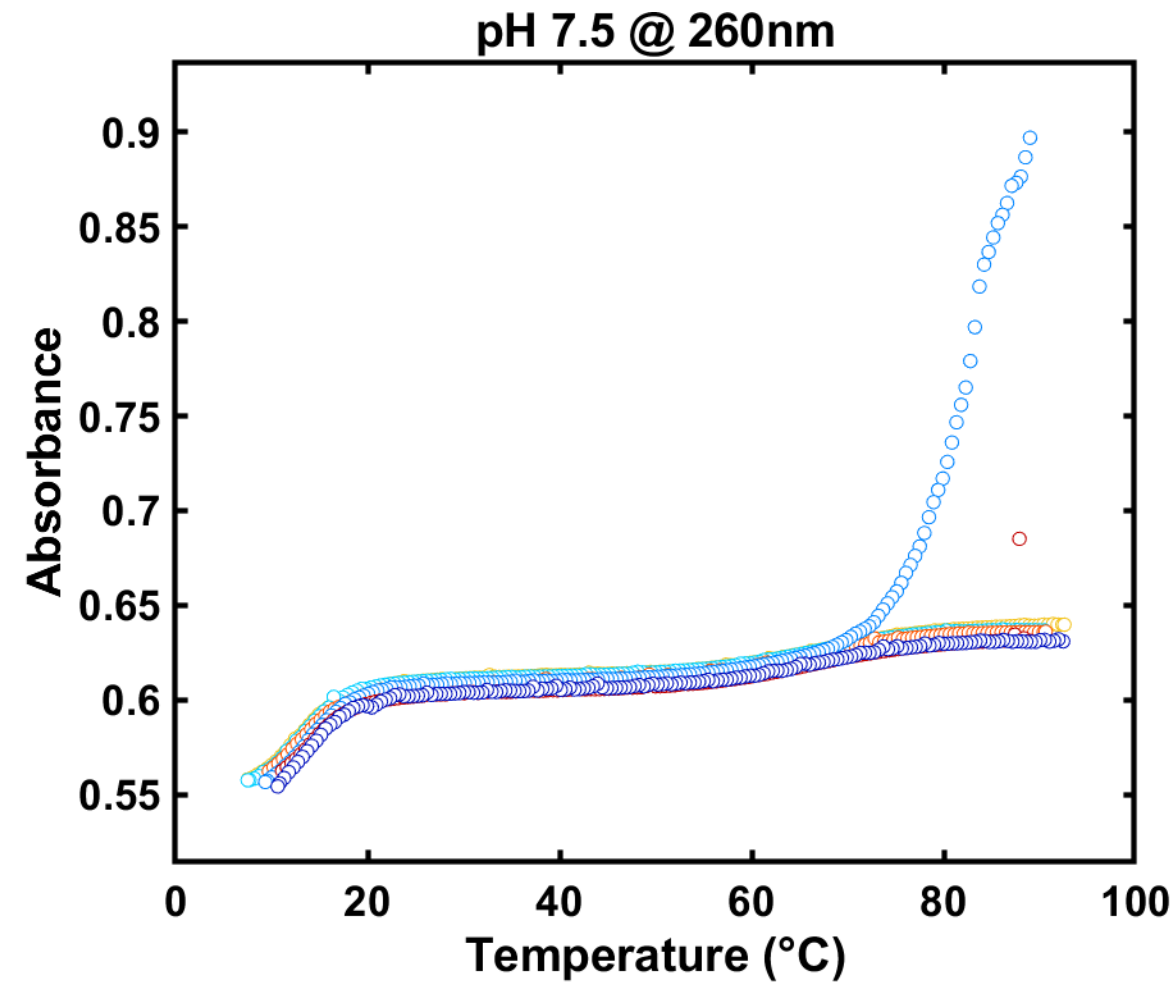
IDJ1 raw data – pH 6.5



IDJ1 raw data – pH 7

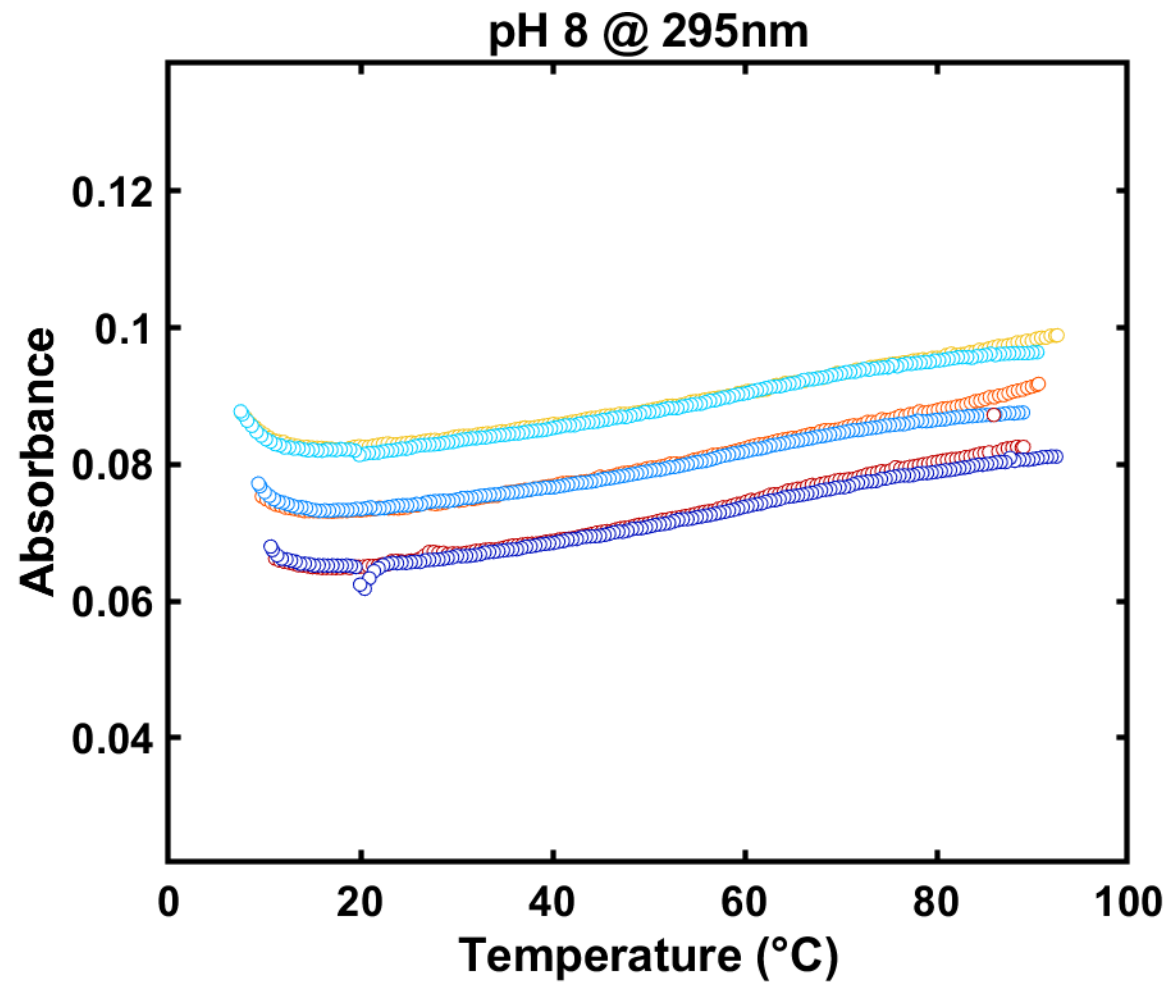
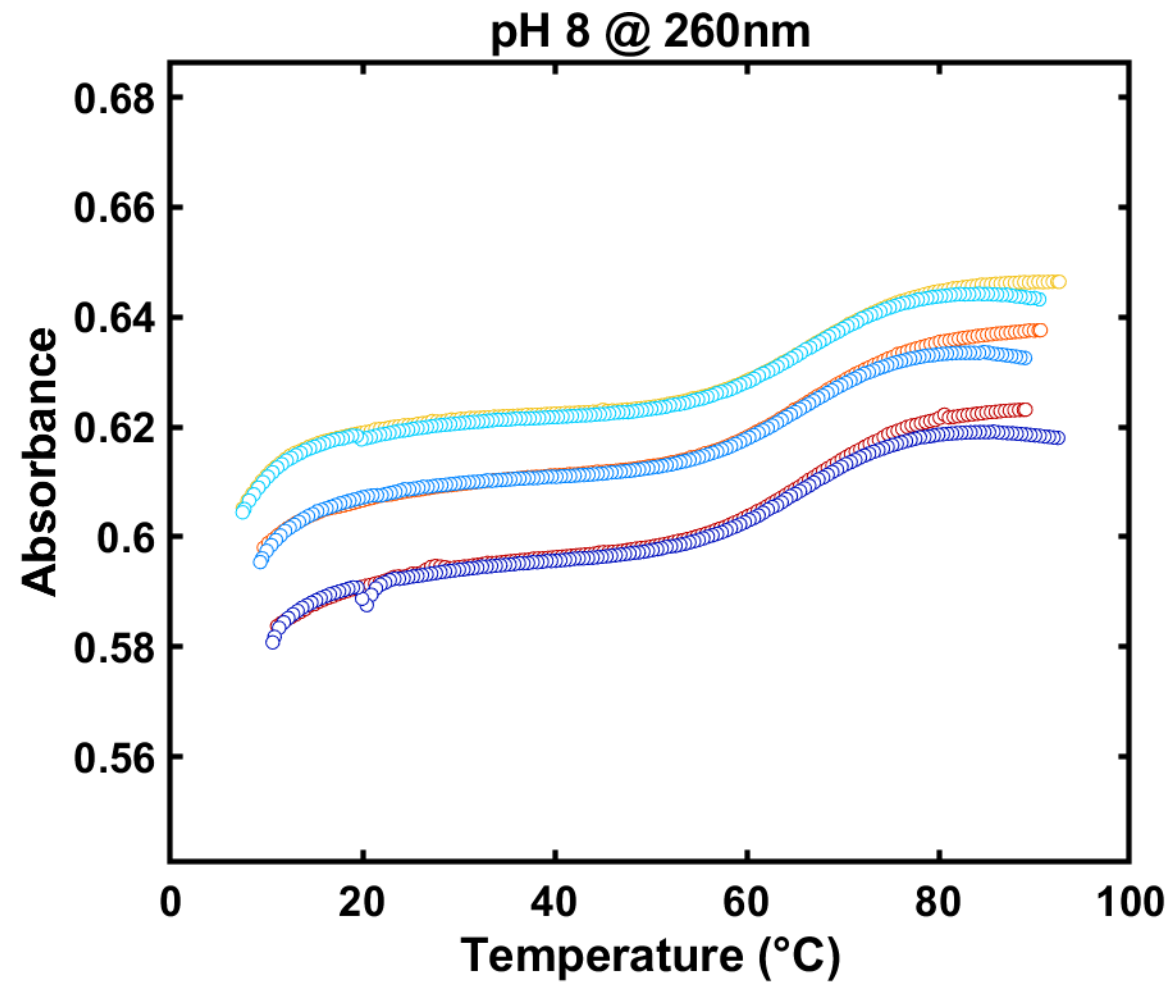


IDJ1 raw data – pH 7.5





IDJ1 raw data – pH 8



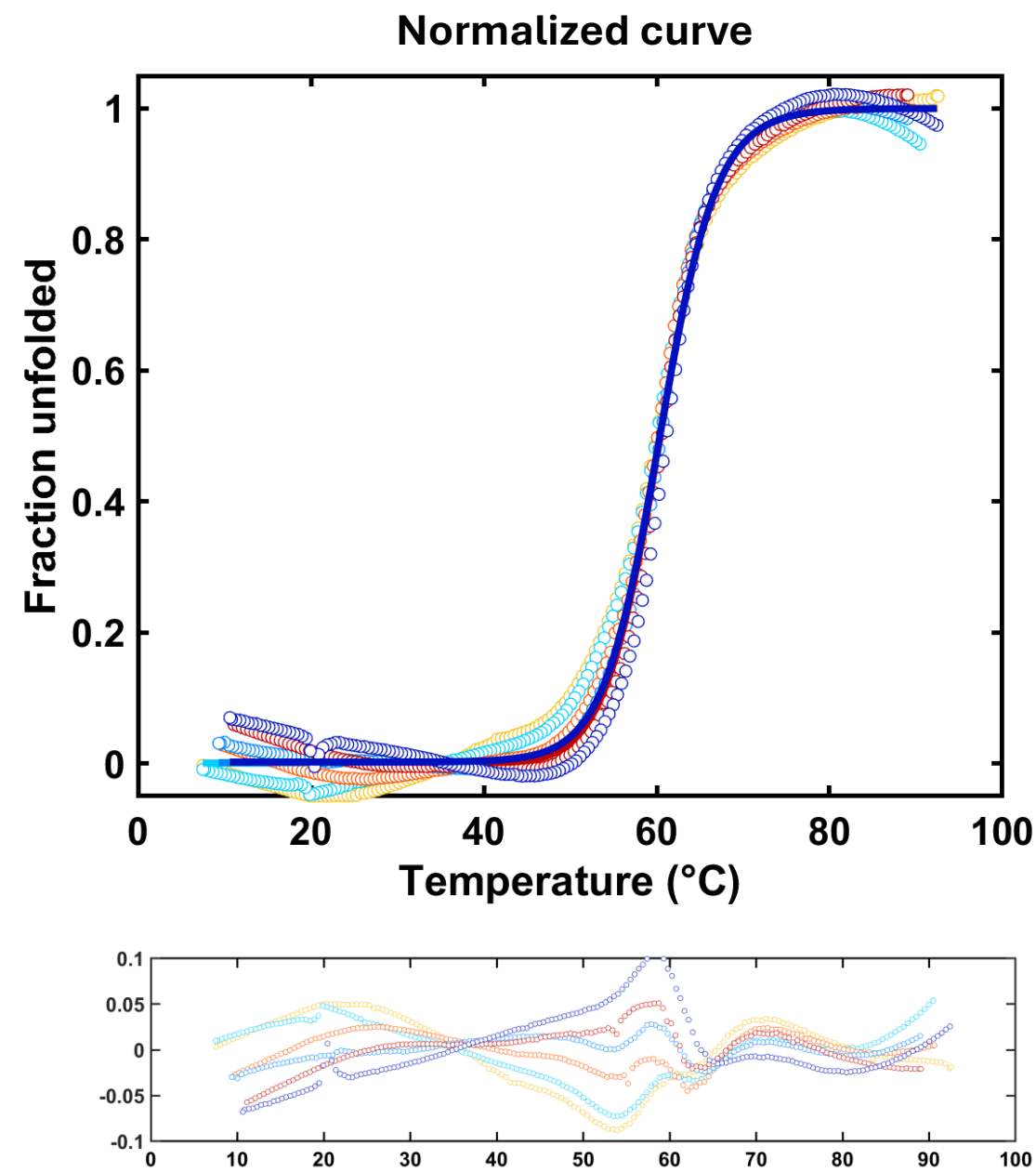
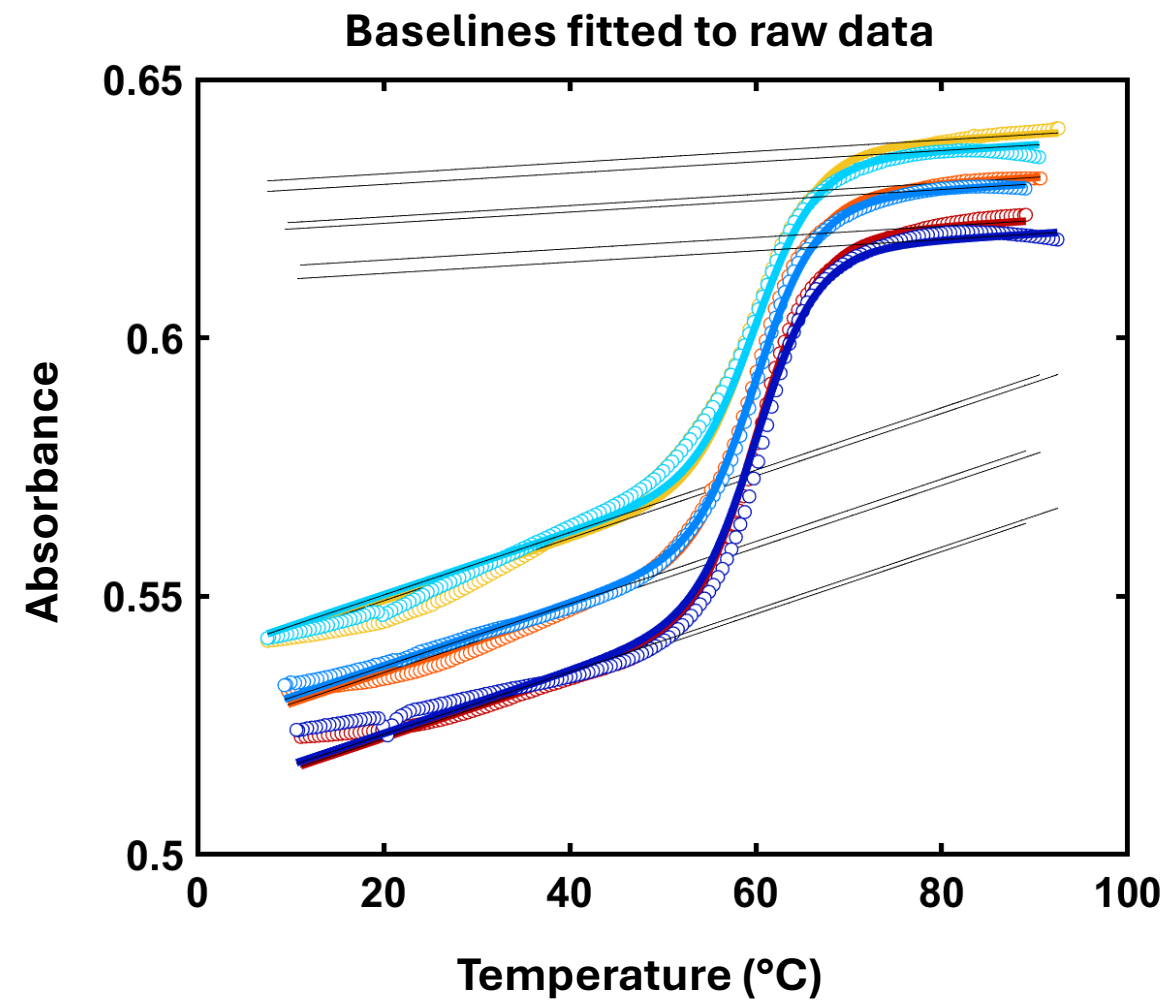
# Kinetic fitting

- Initial parameters:  $k_{ref}, T_m, \Delta H$
- 2-state ODE:  $\frac{dF}{dT} = (-F \cdot k_u + U \cdot k_f) \cdot \frac{dt}{dT}$
- From Arrhenius equation,  $k = Ae^{-E_a/RT}$ , can obtain value of  $k$  at each temperature  $T$  by:

$$\frac{k(T)}{k_{ref}} = e^{\left(-\frac{E_a}{RT} + \frac{E_a}{RT_{ref}}\right)}$$

- Thus, given initial parameters, can simulate the corresponding melting curve. Obtain best fit by minimizing RSS between simulation and raw data.

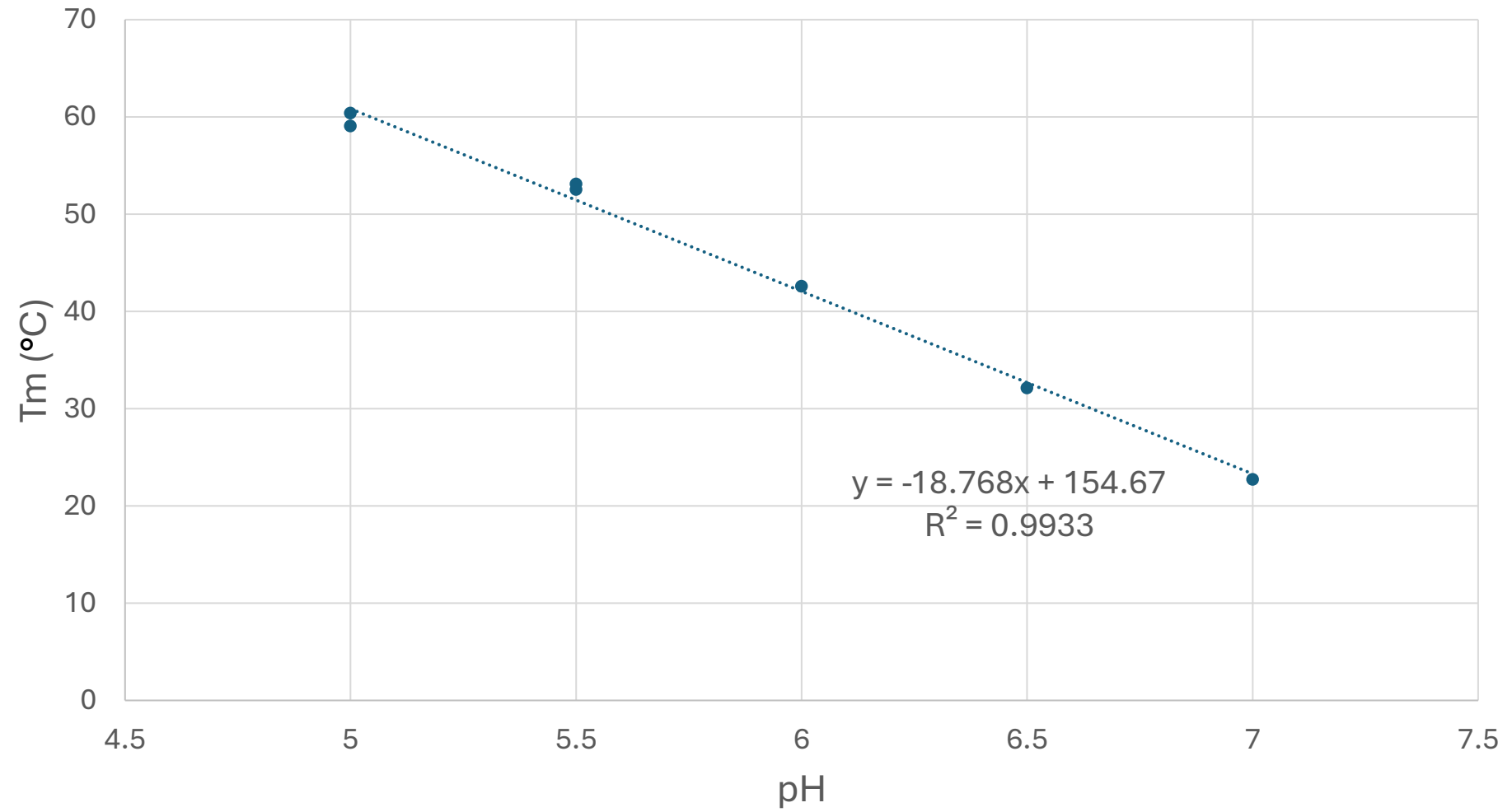
Kinetic fitting example:



# IDJ1 fit results

nm	pH	Tm (°C)	$\Delta G$ (kJ/mol)	$\Delta H$ (kJ/mol)	$\Delta S$ (kJ/mol/K)
260	5	60.39396	-283.81	-0.85089	-30.1164
295	5	59.07281	-250.516	-0.75406	-25.6929
260	5.5	53.10481	-311.656	-0.95525	-26.8472
295	5.5	52.54999	-393.512	-1.20821	-33.286
295	6	42.59998	-371.265	-1.17582	-20.6944
260	6.5	32.13573	-361.696	-1.18478	-8.45425
295	7	22.75022	-311.705	-1.05341	2.369943

## T<sub>m</sub> vs pH for IDJ1



# Folding rate constants

nm	pH	k1 (s <sup>-1</sup> )	k2 (s <sup>-1</sup> )
260	5	0.011629	6.15E-08
295	5	2.633137	8.30E-05
260	5.5	1.117284	2.21E-05
295	5.5	28.12226	4.14E-05
295	6	49.54645	0.01173
260	6.5	38.19638	1.261304
295	7	19.56203	50.89007