

# **A Rapid Screen of Potential i-Motif Forming Sequences in DNA Repair Gene Promoters**

R. Aaron Rogers\*, Aaron M. Fleming\*, Cynthia J. Burrows\*

\*Dept. of Chemistry, Univ. of Utah, 315 South 1400 East, Salt Lake City, Utah 84112,

USA

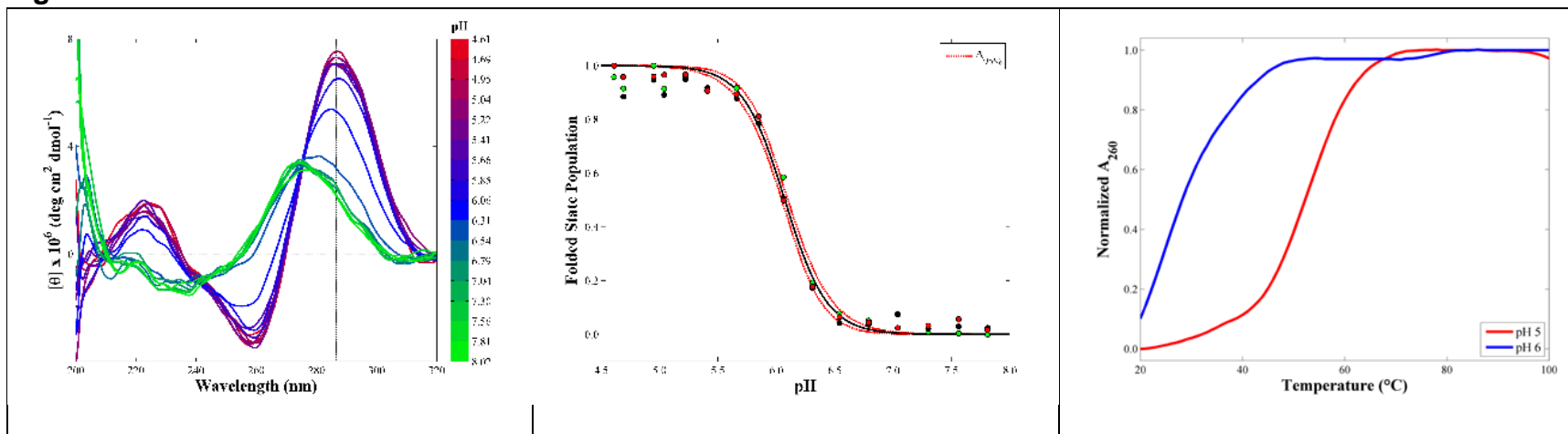
**Supporting Information**

**Table S1:** Tabulated results for all oligodeoxynucleotides studied; Low pH CD maxima; IDS  $\lambda_{\max}$  pHT values ( $\pm$  std. error);  $T_M$  values ( $\pm$  std. error); calculated UV molar absorptivity values at 260 nm ( $\epsilon_{260}$ ).

Sequence Name	CD $\lambda_{\max}$ (nm)	IDS $\lambda_{\max}$ (nm)	IDS $\lambda_{\min}$ (nm)	pHT ( $\pm$ std. error)	$T_M$ at pH 5 ( $\pm$ std. error) in °C	$T_M$ at pH 6 ( $\pm$ std. error) in °C	$\epsilon_{260}$ (L $\mu\text{mol}^{-1}$ $\text{cm}^{-1}$ )
<i>APE1</i> – 4 track	286.6	243.7	292.4	6.07 (0.01)	55.6 (0.1)	24.0 (1.2)	0.1827
<i>APE1</i> – 5 track	285.9	241.1	291.5	6.15 (0.02)	56.1 (0.1)	37.1 (2.4)	0.2935
<i>FEN1</i>	284.8	240.8	292.2	6.36 (0.03)	58.0 (0.1)	37.1 (0.1)	0.4249
<i>MGMT</i>	286.0	243.2	293.9	6.67 (0.03)	72.6 (0.1)	47.7 (0.3)	0.3611
<i>NEIL1</i>	286.9	241.6	293.4	6.48 (0.01)	63.3 (0.1)	37.5 (0.3)	0.2232
<i>NEIL2</i> – 4 track	286.5	242.2	292.8	5.68 (0.02)	57.6 (0.7)	ND	0.1802
<i>NEIL2</i> – 5 track	286.7	243.6	293.1	6.09 (0.02)	39.8 (1.8)	ND	0.2659
<i>NEIL2</i> – 6 track	286.7	243.5	294.0	6.30 (0.03)	55.8 (0.9)	32.2 (1.2)	0.3046
<i>NEIL3</i> – 4 track	287.5	240.3	291.1	5.14 (0.02)	ND	ND	0.2086
<i>NEIL3</i> – 5 track	286.0	240.9	291.1	5.79 (0.01)	55.7 (1.2)	ND	0.3023
<i>NTHL1</i> – 4 track	285.3	240.6	291.5	5.34 (0.01)	59.5 (1.4)	ND	0.2099
<i>NTHL1</i> – 5 track	286.1	249.5	294.3	5.65 (0.02)	57.7 (0.2)	ND	0.3044
<i>PCNA</i> – Sequence 1	285.9	242.2	292.8	5.91 (0.02)	59.7 (0.1)	45.1 (1.9)	0.3017
<i>PCNA</i> – Sequence 2	287.3	240.1	292.5	6.63 (0.02)	68.0 (0.1)	45.4 (0.4)	0.2647
<i>Poi<math>\beta</math></i>	286.5	240.8	293.5	6.46 (0.01)	61.2 (0.4)	37.4 (0.2)	0.2519
<i>Poi<math>\eta</math></i>	287.1	239.9	291.2	6.19 (0.01)	56.4 (0.1)	31.3 (0.7)	0.2255
<i>RAD17</i> – Sequence 1	287.4	240.3	293.5	6.24 (0.01)	56.3 (0.1)	33.3 (0.1)	0.2835
<i>RAD17</i> – Sequence 2	288.5	239.9	293.9	6.90 (0.02)	74.5 (0.1)	63.2 (0.3)	0.2005
<i>RAD21</i>	286.0	240.2	293.5	6.53 (0.04)	64.7 (0.1)	40.7 (0.1)	0.3017
<i>RAD54L</i>	287.6	239.7	295.0	6.51 (0.04)	71.3 (0.1)	45.0 (0.2)	0.3649
<i>UDG</i> – 4 track	286.9	241.4	292.8	6.69 (0.02)	60.1 (0.1)	35.0 (0.4)	0.2196
<i>UDG</i> – 5 track	285.6	244.2	293.0	6.26 (0.03)	58.6 (0.1)	38.7 (0.3)	0.4926
<i>XRCC2</i>	285.1	241.1	292.7	5.99 (0.08)	48.6 (0.1)	31.4 (0.6)	0.4162
<i>XRCC3</i>	287.0	241.3	293.4	5.78 (0.05)	61.3 (0.3)	45.0 (1.0)	0.2522
<i>XRCC5</i>	284.6	240.6	293.2	6.44 (0.02)	56.1 (0.2)	34.3 (0.1)	0.2475

**Figures S1 – S25;** Example pH-dependent CD spectra from a single replicate experiment (left); pH<sub>T</sub> regression curves using data extracted from pH-dependent CD spectra at the CD maximum wavelength *circa* 285 nm; representative normalized T<sub>M</sub> curves at pH 5 and 6.

**Figure S1: APE1 – 4 track**



**Figure S2: APE1 – 5 track**

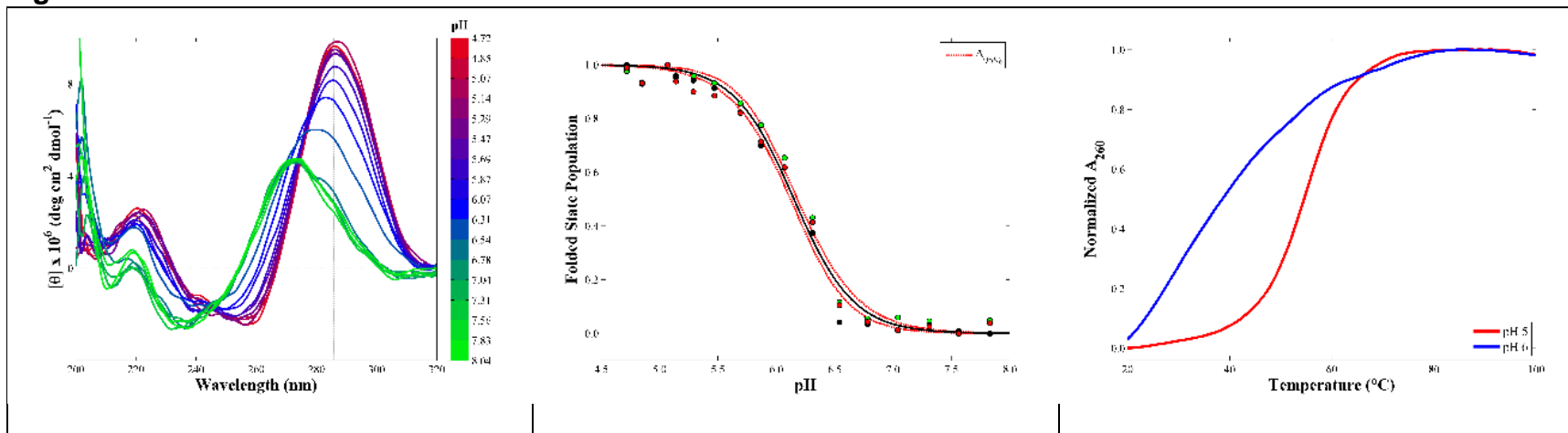


Figure S3: *FEN1*

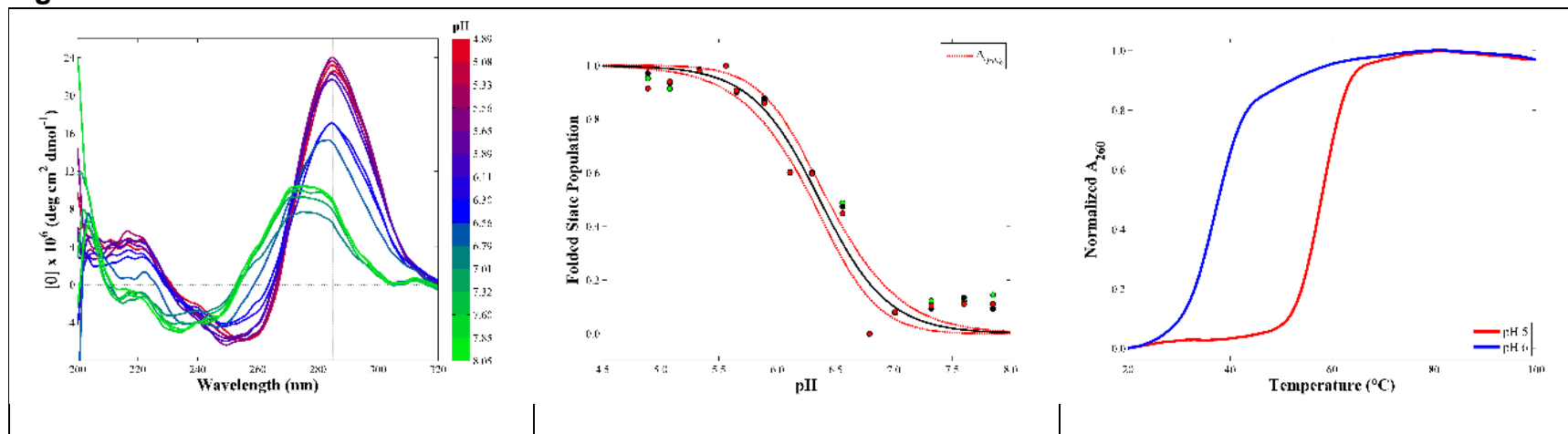


Figure S4: *MGMT*

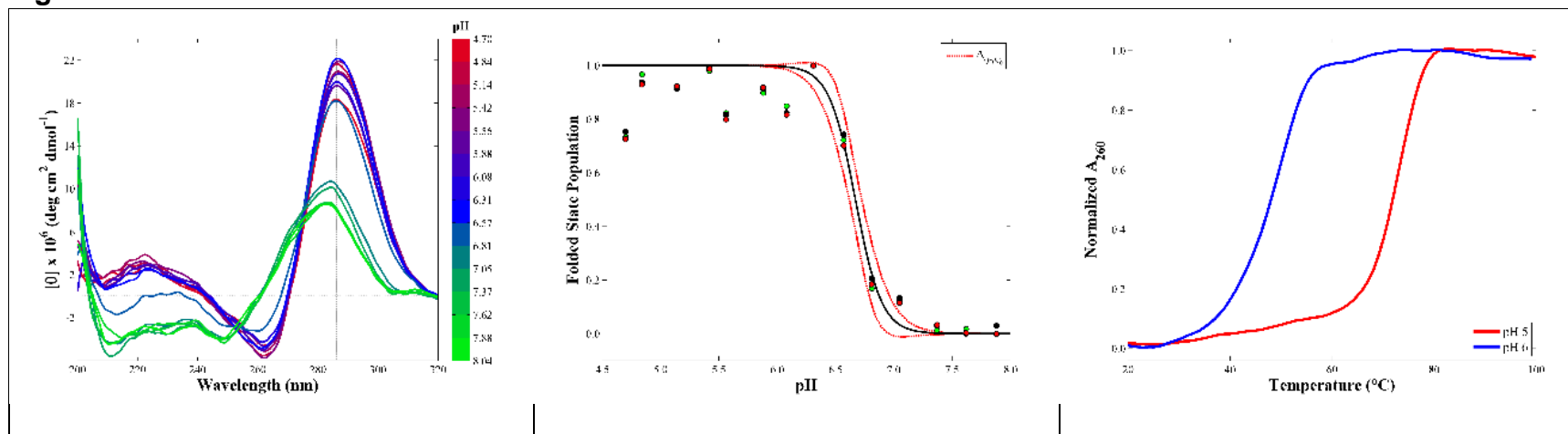


Figure S5: NEIL1

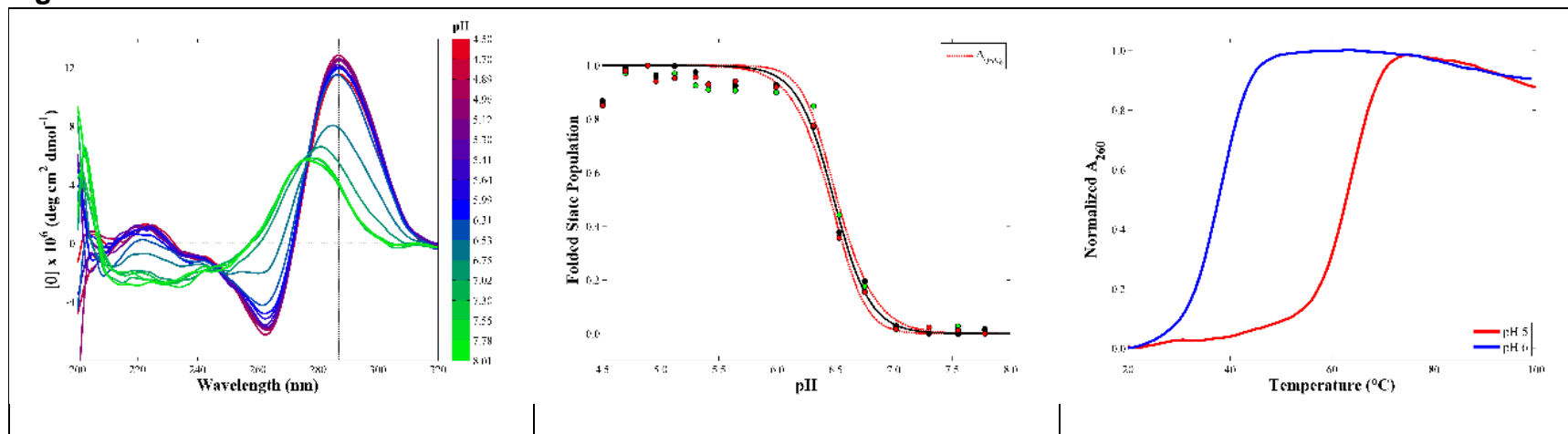


Figure S6: NEIL2 – 4 track

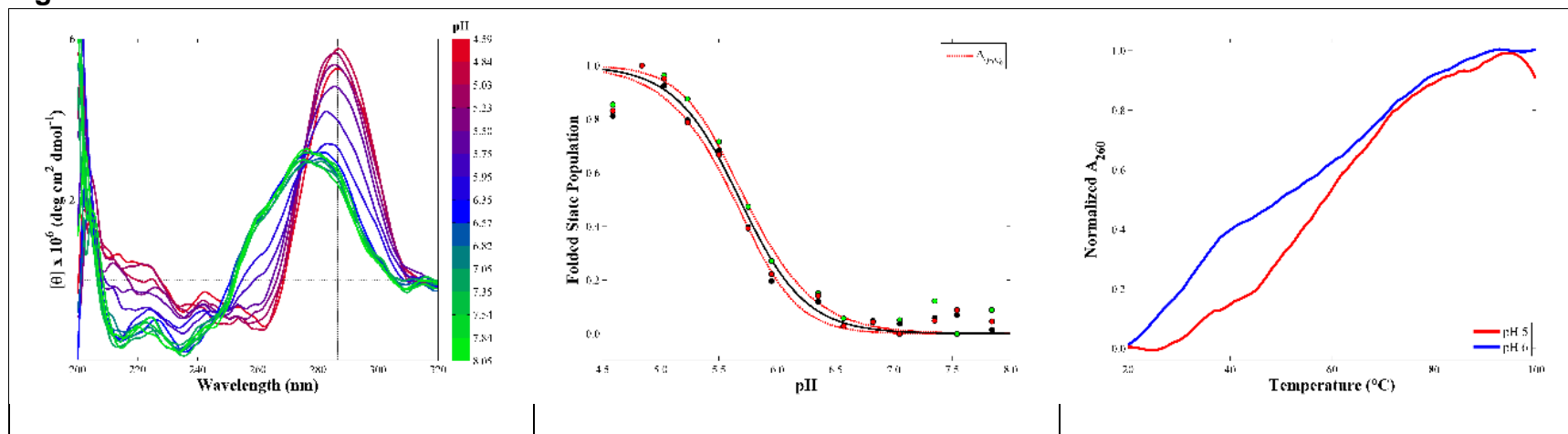


Figure S7: NEIL2 – 5 track

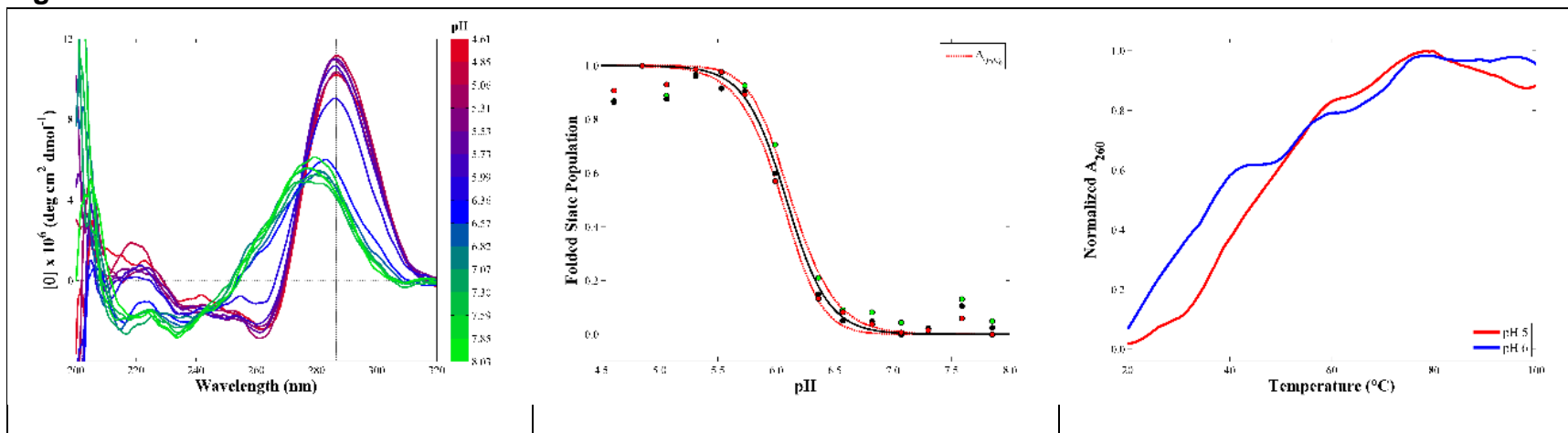


Figure S8: NEIL2 – 6 track

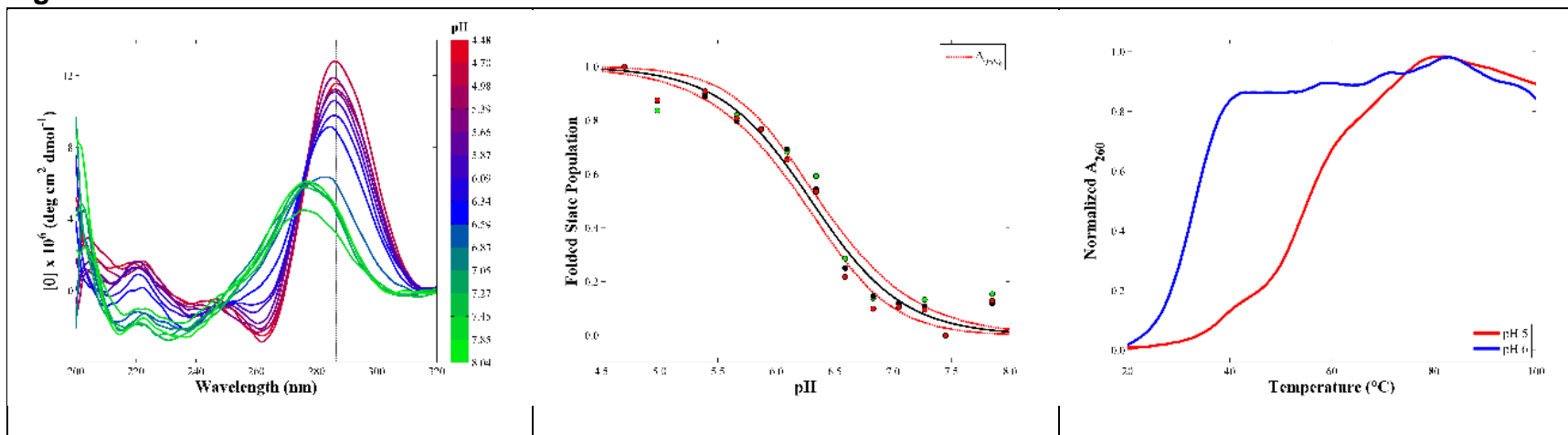


Figure S9: NEIL3 – 4 track

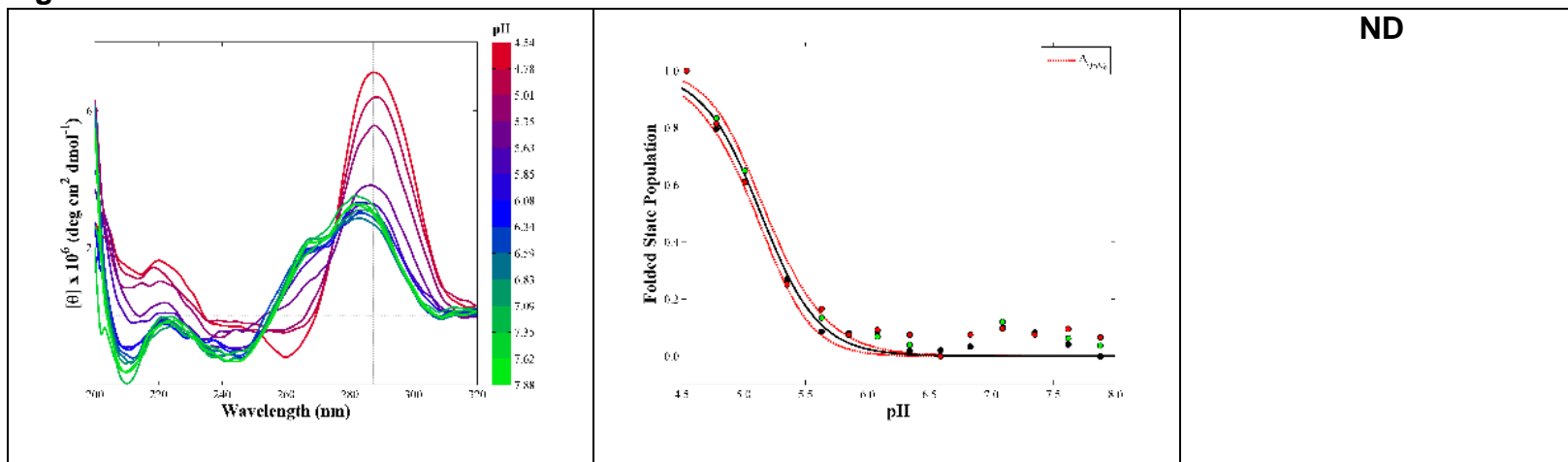


Figure S10: NEIL3 – 5 track

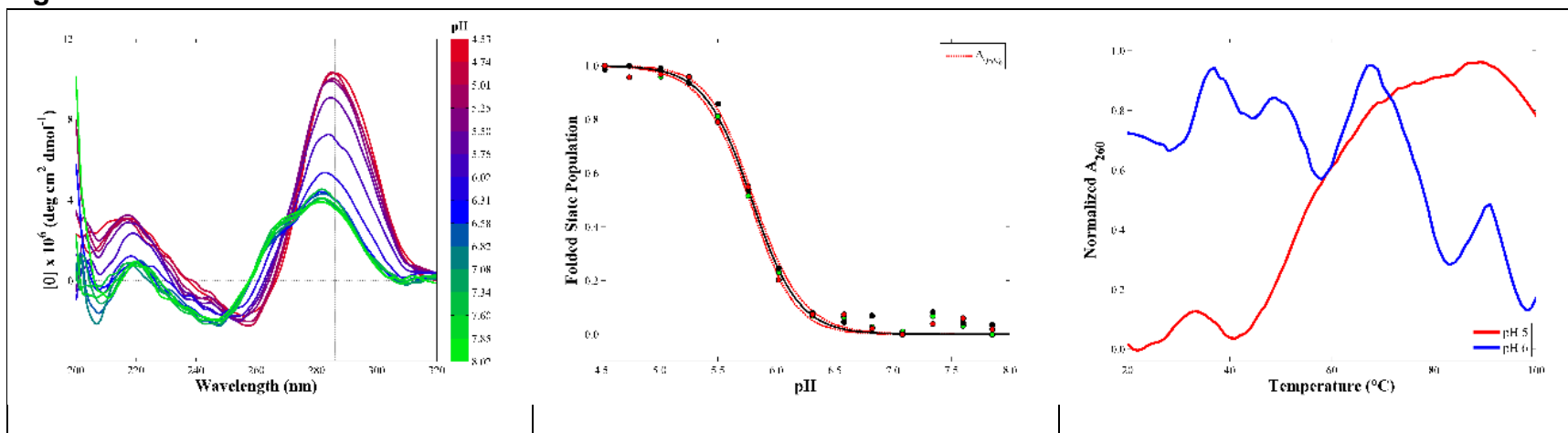


Figure S11: *NTHL1* – 4 track

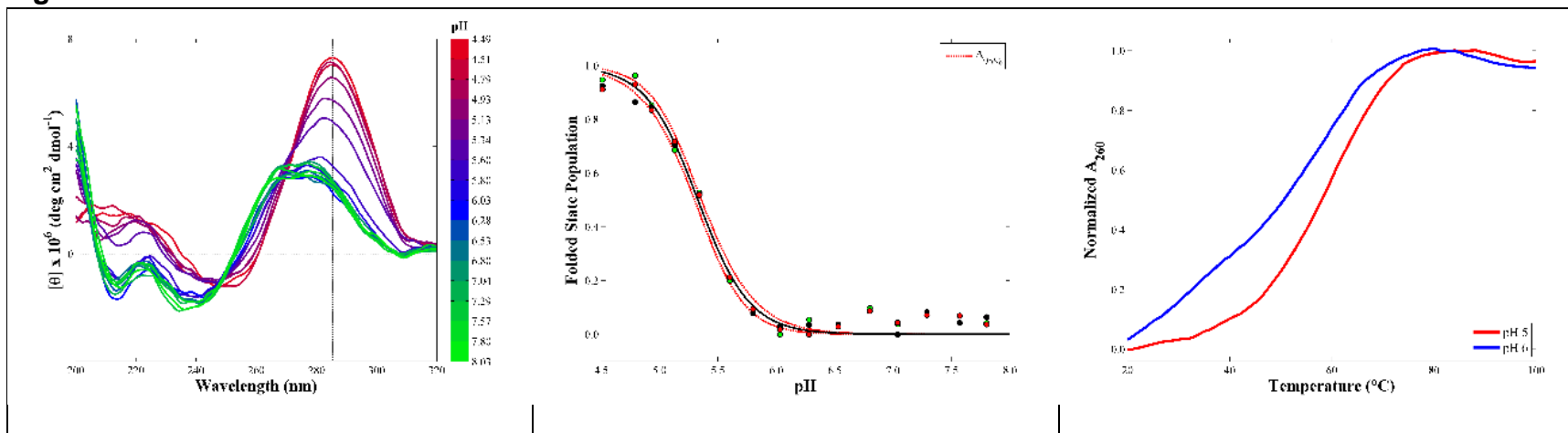


Figure S12: *NTHL1* – 5 track

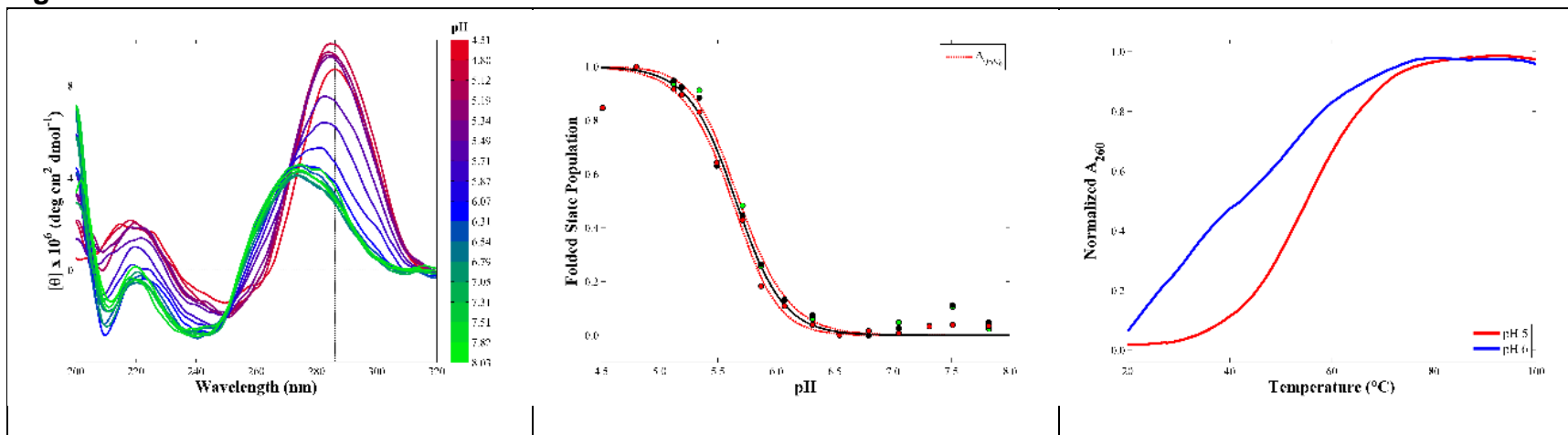




Figure S13: PCNA – Sequence 1

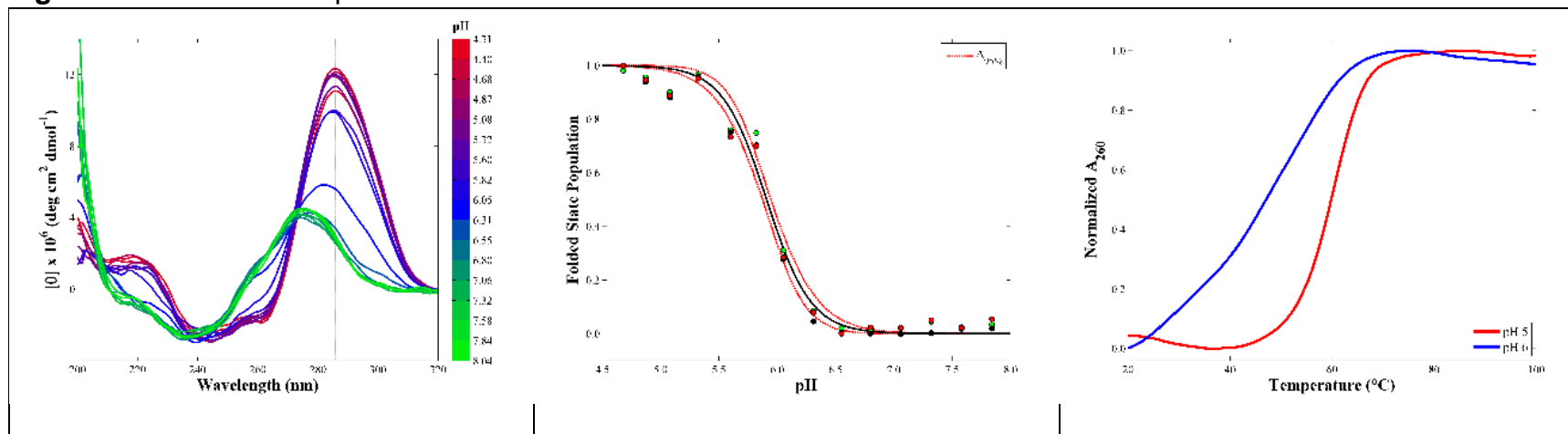


Figure S14: PCNA – Sequence 2

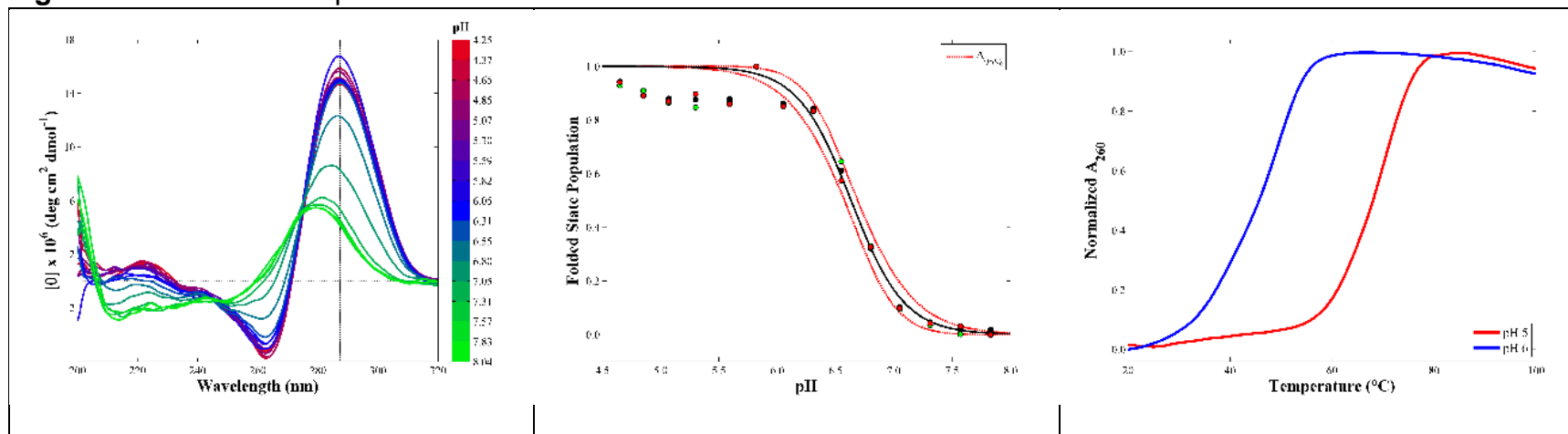


Figure S15: *Polβ*

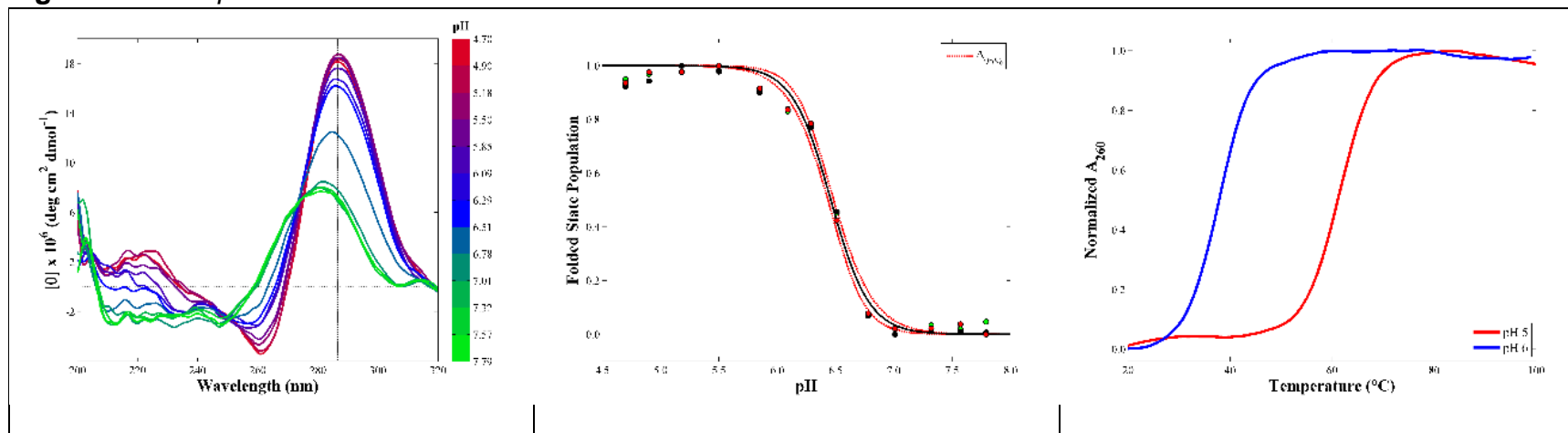


Figure S16: *Polη*

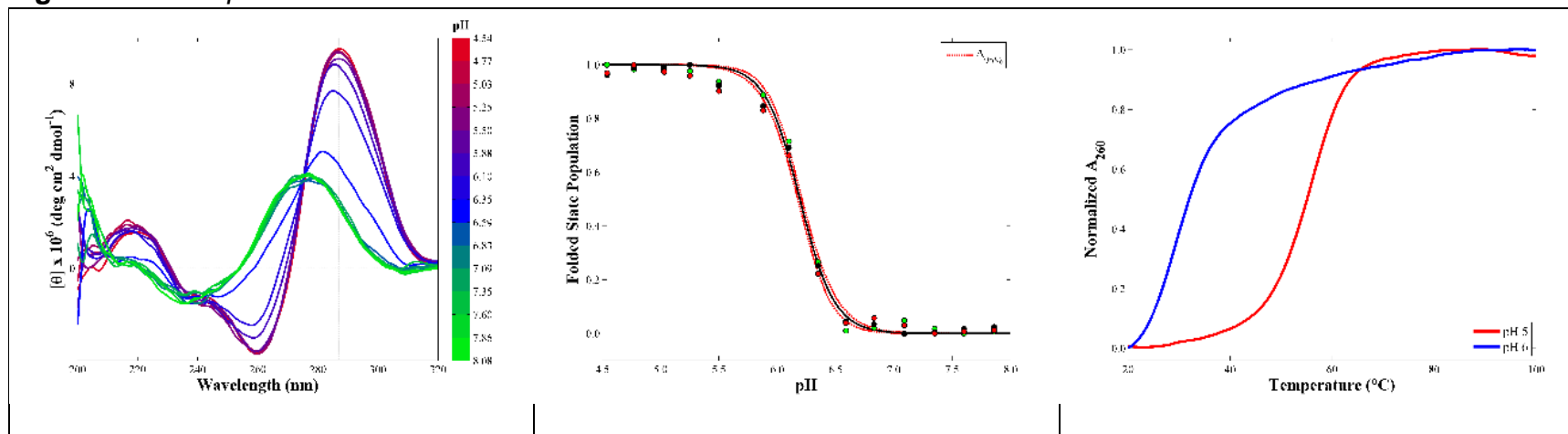


Figure S17: RAD17 – Sequence 1

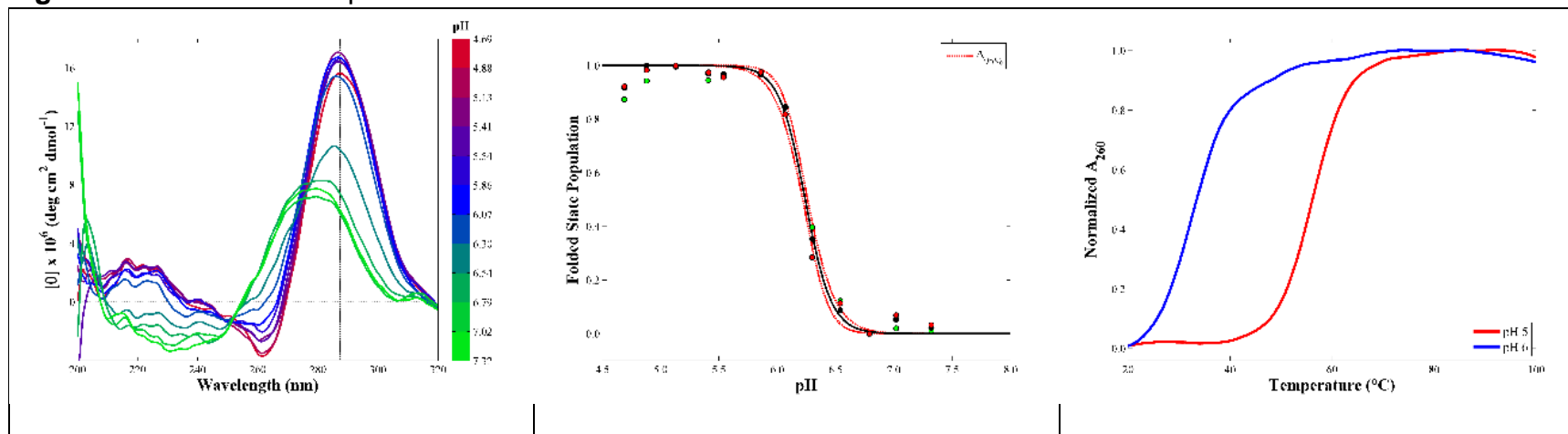


Figure S18: RAD17 – Sequence 2

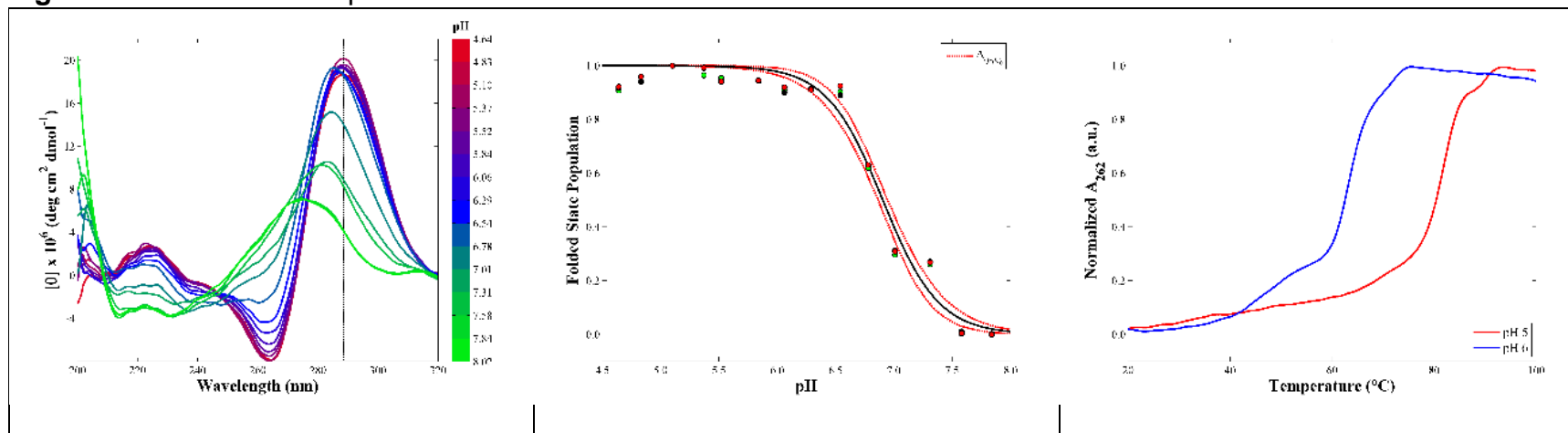


Figure S19: RAD21

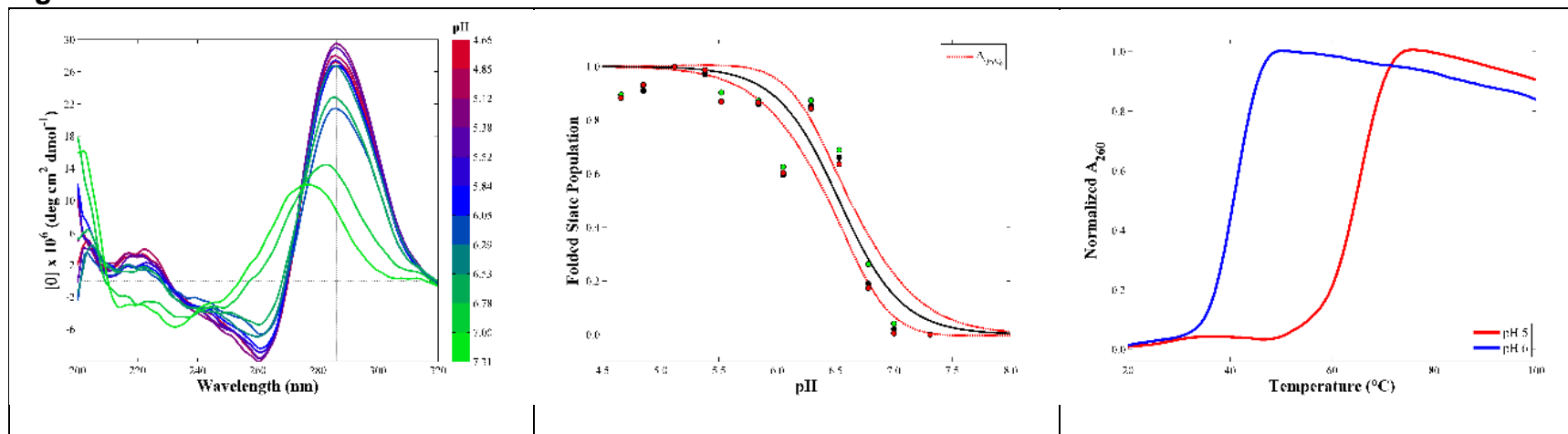


Figure S20: RAD54L

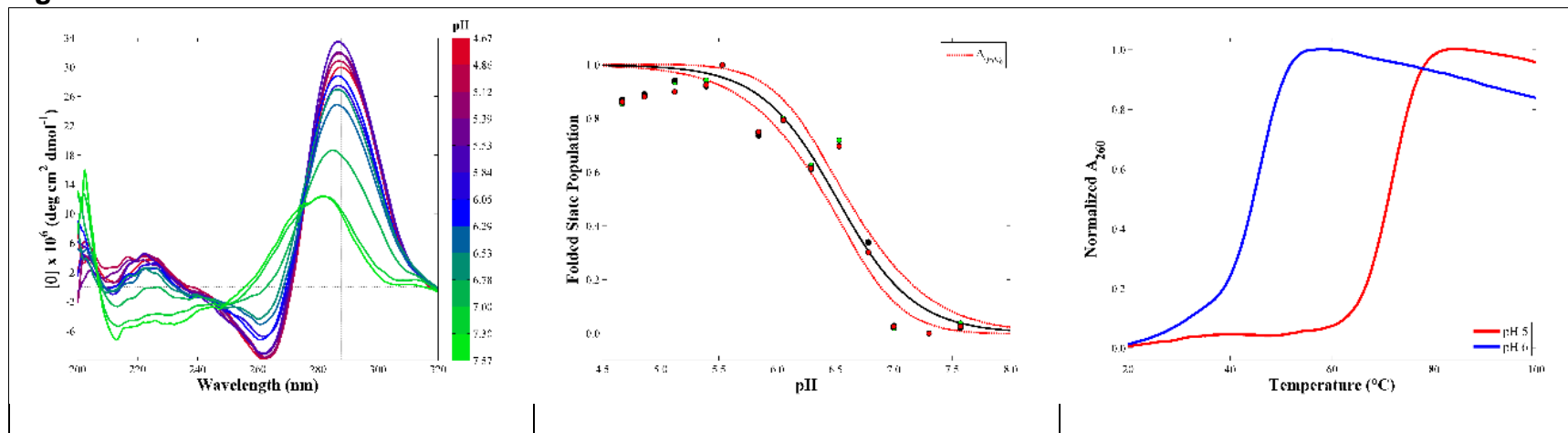


Figure S21: UDG – 4 track

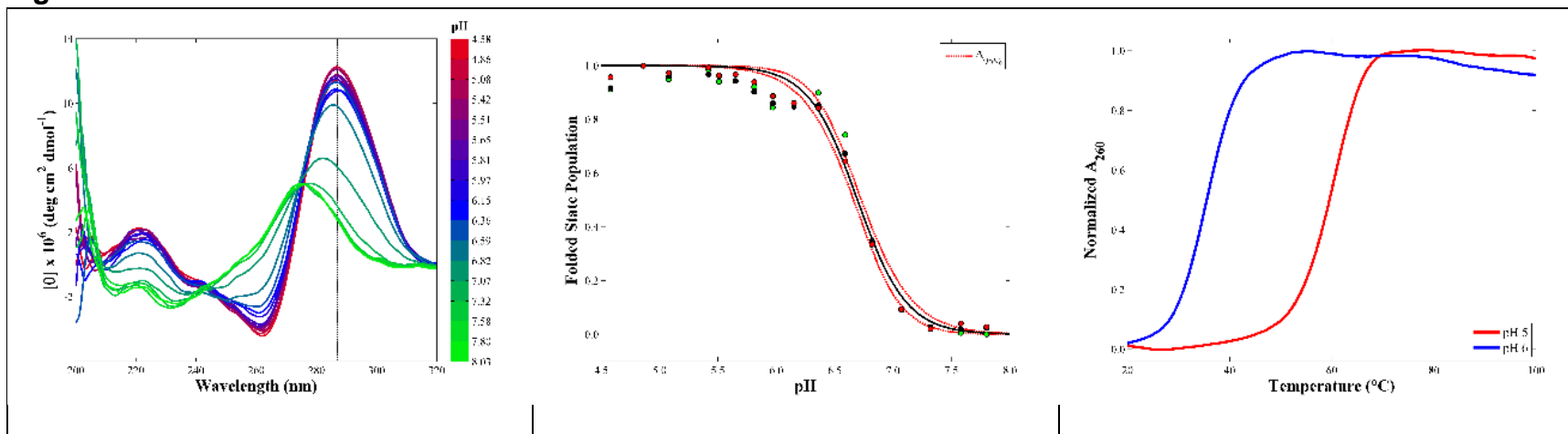


Figure S22: UDG – 5 track

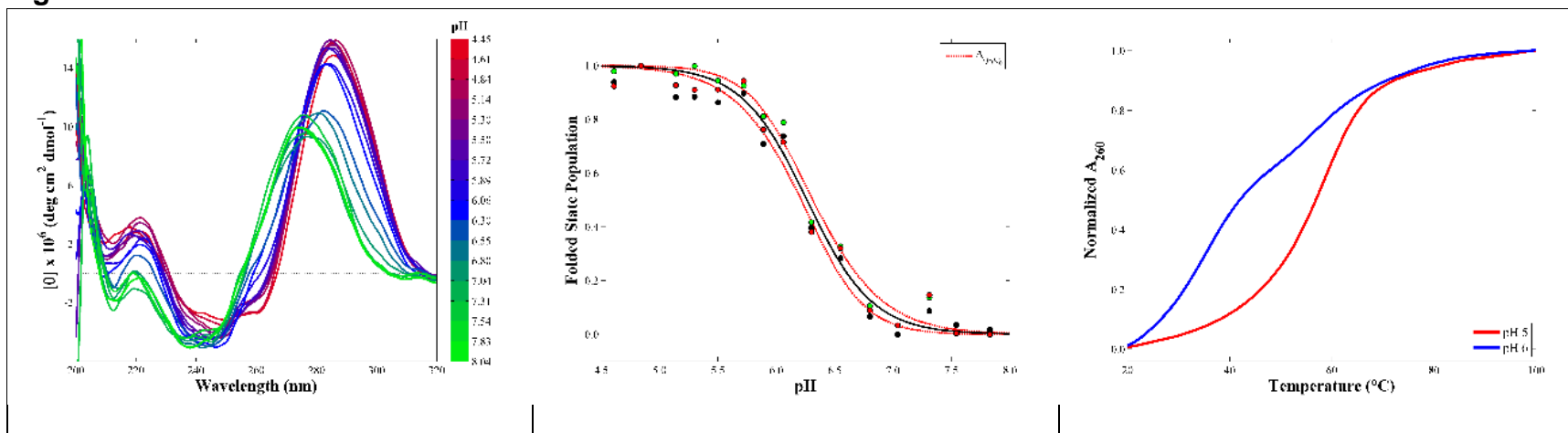


Figure S23: XRCC2

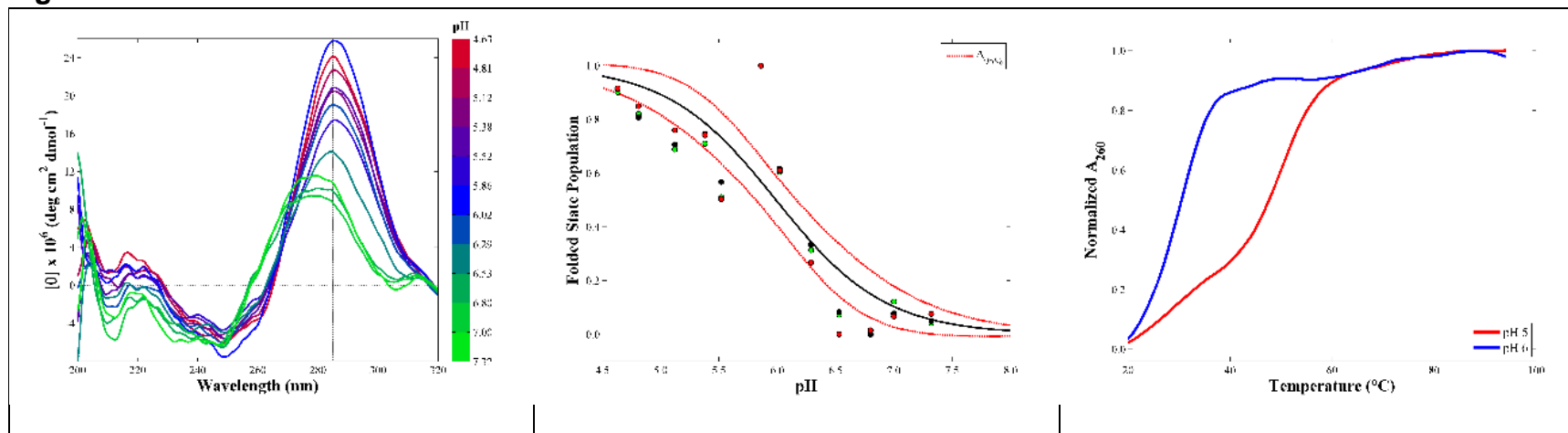


Figure S24: XRCC3

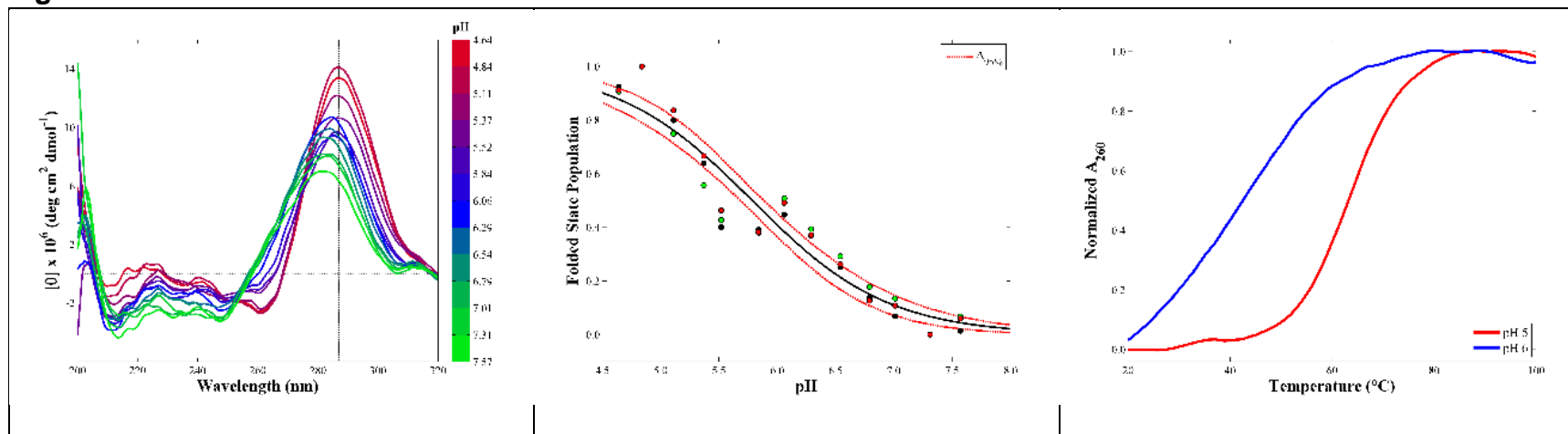
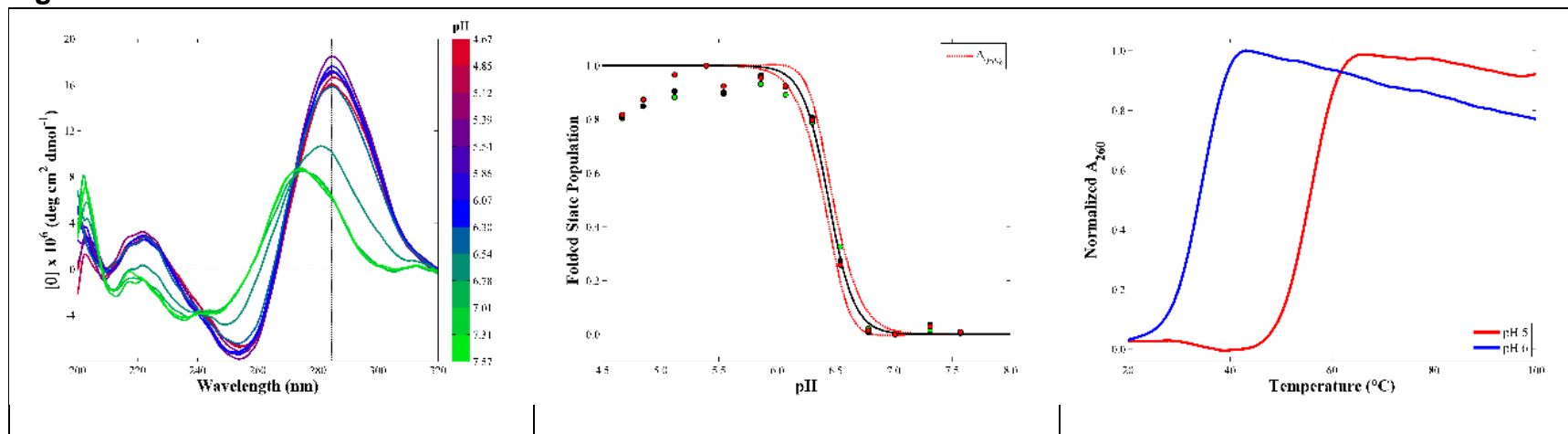


Figure S25: XRCC5



**Figure S26:** Top-to-bottom direct comparison of Figures 1 and 2 in the manuscript for ease of visual comparison of  $pH_T$  values.

