



Table S4 ANOVA and Bonferroni results for SRD-CRRN data of non-titratable residues in  $\alpha$ -synuclein at pH=4.21, BMRB 18857.

$p$ (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6
<math>10^{-7}</math>	Potenci	24.41	****					
	Prosecco neutral	24.44	****					
	Prosecco acidic	25.07	****					
	ncIDP	26.59			****			
	Wishart	27.79				****		
	Kjaergaard	33.18		****				
	Camcoil pH=6.1	33.79		****				
	Camcoil pH=2.0	34.06		****				
	Wang	36.07					****	
Schwarzinger	40.26						****	

Table S5 ANOVA and Bonferroni results for SRD-CRRN data of titratable residues in  $\alpha$ -synuclein at pH=7.51, BMRB 18857.

$p$ (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4
<math>10^{-7}</math>	Potenci	16.81		****		
	Wishart	16.85		****		
	ncIDP	18.99	****			
	Prosecco	19.44	****			
	Kjaergaard	20.34	****			
	Wang	22.49			****	
	Camcoil	32.10				****

Table S6 ANOVA and Bonferroni results for SRD-CRRN data of non-titratable residues in  $\alpha$ -synuclein at pH=7.51, BMRB 18857.

$p$ (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6	G7
<math>10^{-7}</math>	ncIDP	18.96	****						
	Potenci	20.08		****					
	Wishart	22.02			****				
	Prosecco	24.82				****			
	Kjaergaard	26.53					****		
	Wang	33.03						****	
	Camcoil	40.28							****

Tables containing ANOVA and Bonferroni test results for the SRD-CRRN data of  $\alpha$ -synuclein at different temperatures and pH= 5.87 (BMRB 18857). These data augment Fig. 11 of the main text.

Table S7 ANOVA and Bonferroni results for SRD-CRRN data of  $\alpha$ -synuclein at pH=5.87, and T=278 K, BMRB 18857.

$p$ (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6
<math>10^{-7}</math>	ncIDP	17.69		****				
	Wishart	24.63			****			
	Prosecco	26.93	****					
	Potenci	27.48	****					
	Wang	29.87				****		
	Kjaergaard	31.27					****	
	Camcoil	41.64						****

Table S8 ANOVA and Bonferroni results for SRD-CRRN data of  $\alpha$ -synuclein at pH=5.87, and T=288 K, BMRB 18857.

<i>p</i> (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6
<10 <sup>-7</sup>	nclDP	20.35		****				
	Potenci	26.31			****			
	Wishart	28.67				****		
	Prosecco	31.21					****	
	Kjaergaard	32.65	****					
	Wang	33.64	****					
	Camcoil	49.07						****

Table S9 ANOVA and Bonferroni results for SRD-CRRN data of  $\alpha$ -synuclein at pH=5.87, and T=293 K, BMRB 18857.

<i>p</i> (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6
<10 <sup>-7</sup>	nclDP	21.02		****				
	Potenci	24.64			****			
	Wishart	28.42	****					
	Prosecco	28.58	****					
	Kjaergaard	32.37				****		
	Wang	35.01					****	
	Camcoil	49.93						****

Table S10 ANOVA and Bonferroni results for SRD-CRRN data of  $\alpha$ -synuclein at pH=5.87, and T=298 K, BMRB 18857.

<i>p</i> (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6
<10 <sup>-7</sup>	nclDP	22.26		****				
	Potenci	24.63			****			
	Prosecco	29.62	****					
	Wishart	30.82	****					
	Kjaergaard	33.43				****		
	Wang	36.28					****	
	Camcoil	51.02						****

Table S11 ANOVA and Bonferroni results for SRD-CRRN data of  $\alpha$ -synuclein at pH=5.87, and T=303 K, BMRB 18857.

<i>p</i> (ANOVA)	Method	Mean SRD score	G1	G2	G3	G4	G5	G6
<10 <sup>-7</sup>	nclDP	22.93	****					
	Potenci	23.67	****					
	Wishart	29.20		****				
	Prosecco	30.70			****			
	Kjaergaard	33.03				****		
	Wang	37.44					****	
	Camcoil	51.08						****