

The influence of random-coil chemical shifts on the assessment of structural propensities in folded proteins and IDPs

Dániel Kovács^{a,b}, Andrea Bodor^a

^a ELTE, Eötvös Loránd University, Institute of Chemistry, Analytical and BioNMR Laboratory

^b Eötvös Loránd University, Hevesy György PhD School of Chemistry

Pázmány Péter sétány 1/A, Budapest 1117, Hungary

Electronic Supplementary Material (ESI)

Tables containing ANOVA and Bonferroni test results for the SRD-CRRN data of α -synuclein at different pH values and T=283 K (BMRB 18857). The results are also split base on the titrability of residues. These data augment Fig. 10 of the main text.

Table S1 ANOVA and Bonferroni results for SRD-CRRN data of titratable residues in α -synuclein at pH=2.16, BMRB 18857.

| p(ANOVA) | Method | Mean SRD score | G1 | G2 | G3 | G4 | G5 |
|-------------------|--------------|----------------|------|------|------|------|------|
| <10 ⁻⁷ | Kjaergaard | 10.37 | **** | | | | |
| | Potenci | 19.49 | | **** | | | |
| | Camcoil | 28.82 | | | **** | | |
| | Prosecco | 31.38 | | | | **** | |
| | Schwarzinger | 56.14 | | | | | **** |

Table S2 ANOVA and Bonferroni results for SRD-CRRN data of non-titratable residues in α -synuclein at pH=2.16, BMRB 18857.

| p(ANOVA) | Method | Mean SRD score | G1 | G2 | G3 | G4 | G5 |
|-------------------|--------------|----------------|------|------|------|------|------|
| <10 ⁻⁷ | Potenci | 18.13 | **** | | | | |
| | Kjaergaard | 25.22 | | **** | | | |
| | Prosecco | 27.42 | | | **** | | |
| | Schwarzinger | 36.47 | | | | **** | |
| | Camcoil | 37.74 | | | | | **** |

Table S3 ANOVA and Bonferroni results for SRD-CRRN data of titratable residues in α -synuclein at pH=4.21, BMRB 18857.

| p(ANOVA) | Method | Mean SRD score | G1 | G2 | G3 | G4 | G5 | G6 | G7 |
|-------------------|------------------|----------------|------|------|------|------|------|------|----|
| <10 ⁻⁷ | Camcoil pH=6.1 | 13.34 | | | | **** | | | |
| | Prosecco neutral | 23.83 | **** | | | | | | |
| | ncIDP | 25.90 | **** | **** | | | | | |
| | Kjaergaard | 25.97 | **** | **** | | | | | |
| | Wishart | 26.86 | | **** | | | | | |
| | Camcoil pH=2.0 | 31.72 | | | **** | | | | |
| | Wang | 31.76 | | | **** | | | | |
| | Potenci | 37.06 | | | | **** | | | |
| | Schwarzinger | 54.61 | | | | | **** | | |
| | Prosecco acidic | 58.70 | | | | | | **** | |

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

| <i>p</i> (ANOVA) | Method | Mean SRD score | G1 | G2 | G3 | G4 | G5 | G6 |
|------------------|------------------|----------------|------|------|------|------|------|----|
| $<10^{-7}$ | 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 α -synuclein at pH=7.51, BMRB 18857.

| <i>p</i> (ANOVA) | Method | Mean SRD score | G1 | G2 | G3 | G4 |
|------------------|------------|----------------|------|------|------|----|
| $<10^{-7}$ | 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 α -synuclein at pH=7.51, BMRB 18857.

| <i>p</i> (ANOVA) | Method | Mean SRD score | G1 | G2 | G3 | G4 | G5 | G6 | G7 |
|------------------|------------|----------------|------|------|------|------|------|------|------|
| $<10^{-7}$ | 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 α -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 α -synuclein at pH=5.87, and T=278 K, BMRB 18857.

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