

Appendix A

Title: Analysis of Protein Disorder Predictions in the light of Protein Structural Alphabet.

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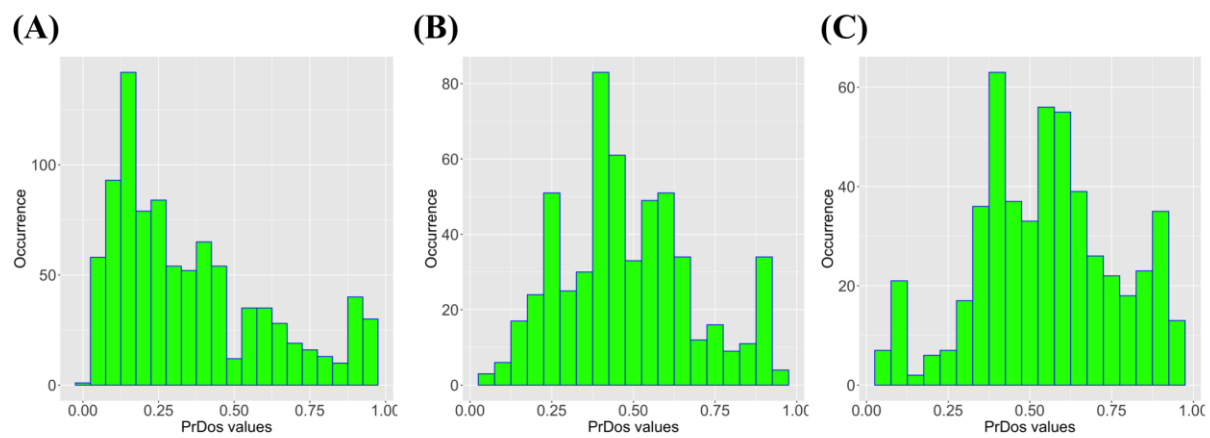


Figure A1. Prediction disorder results of PrDOS on PED³ dataset. For N_{eq} (A) lower than 4, (B) between 4 and 8 and (C) higher than 8.

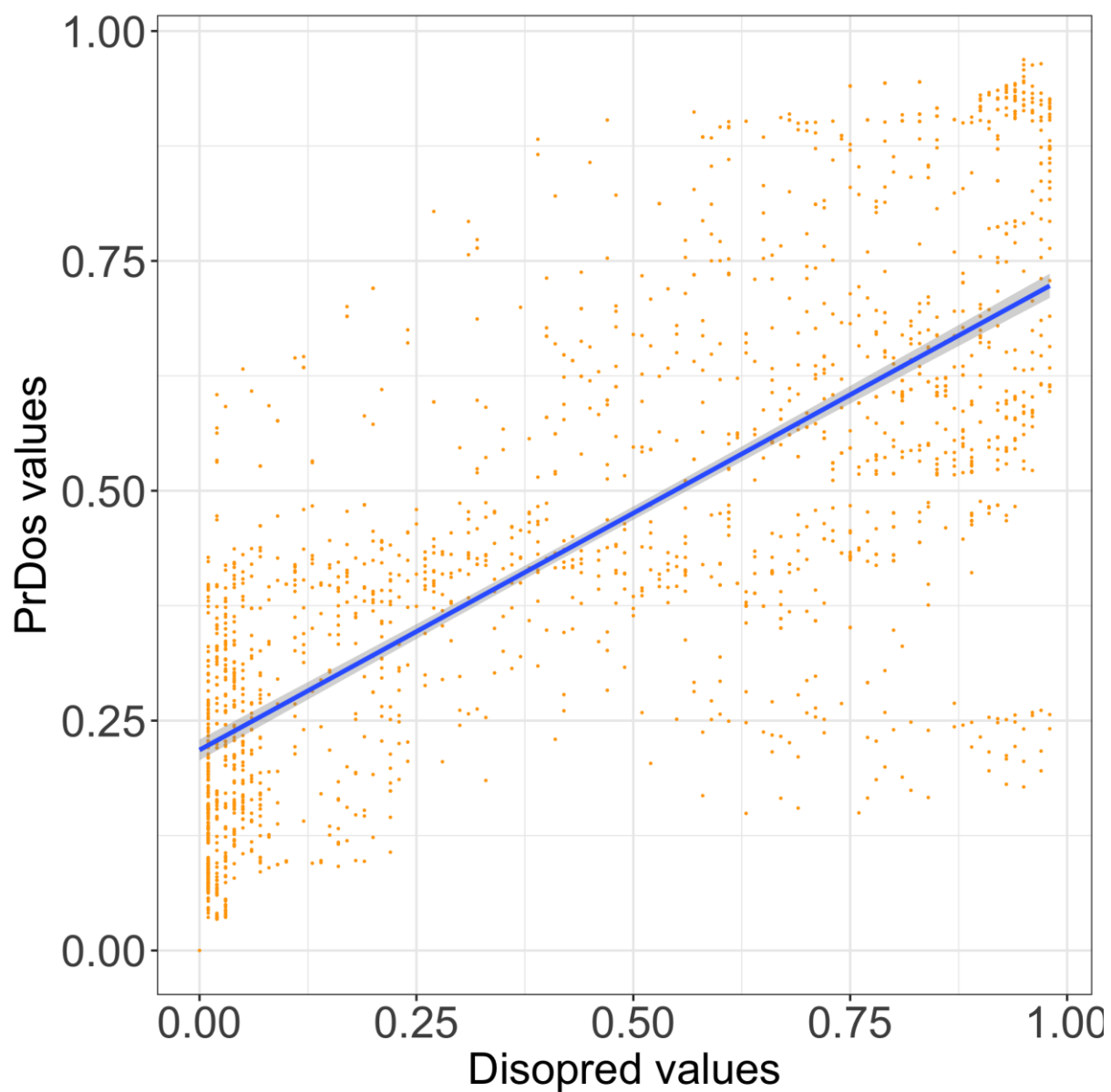


Figure A2. Prediction disorder results on PED³ dataset. (A) DisoPred3 values (x-axis) against PrDOS values (y-axis) for N_{eq} values higher than 8 (correlation is of 0.76).

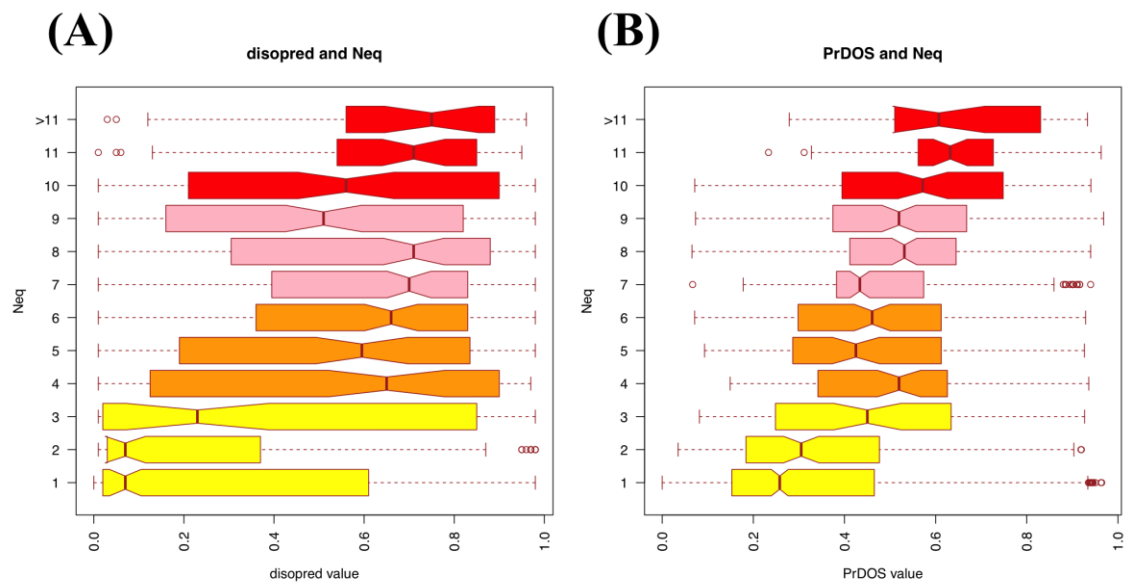


Figure A3. Analyses of prediction disorder results on PED³ dataset per class of N_{eq} . (A) DisoPred3 values (x-axis) and N_{eq} classes (y-axis). (B) PrDOS values (x-axis) and N_{eq} classes (y-axis).

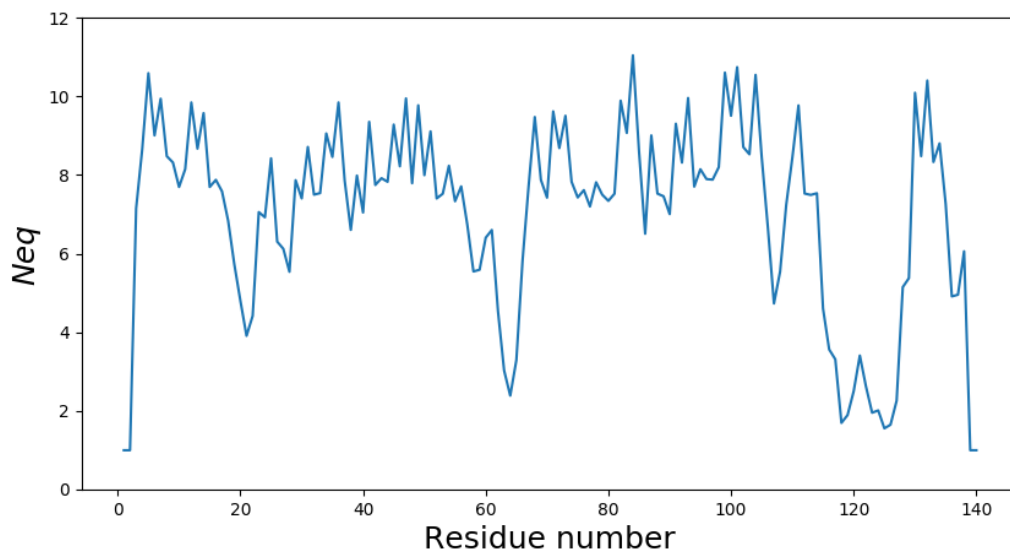


Figure A4. N_{eq} values for the alpha-synuclein, a solution-state ensemble from PRE-NMR ensemble-restrained MD simulations (PED³ 9AAC entry). Computation done with PBxplore software.

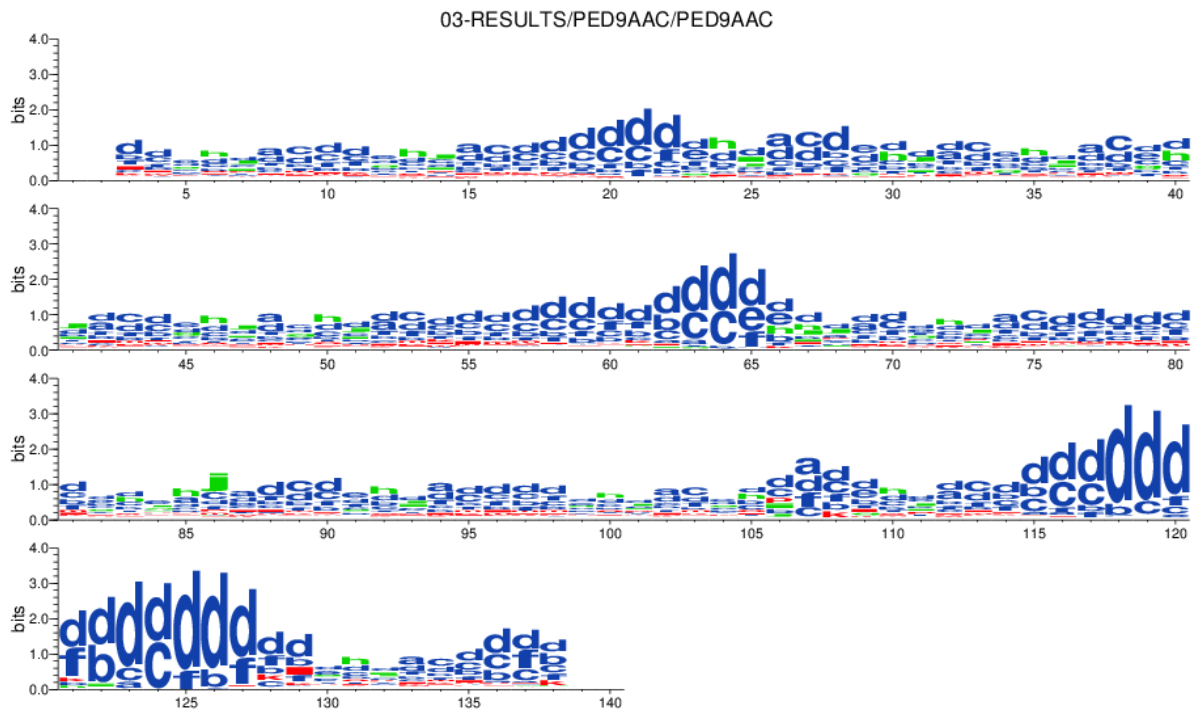


Figure A5. PB distribution for the alpha-synuclein, a solution-state ensemble from PRE-NMR ensemble- restrained MD simulations (PED³ 9AAC entry). Computation done with PBxplore software and represented with WebLogo.

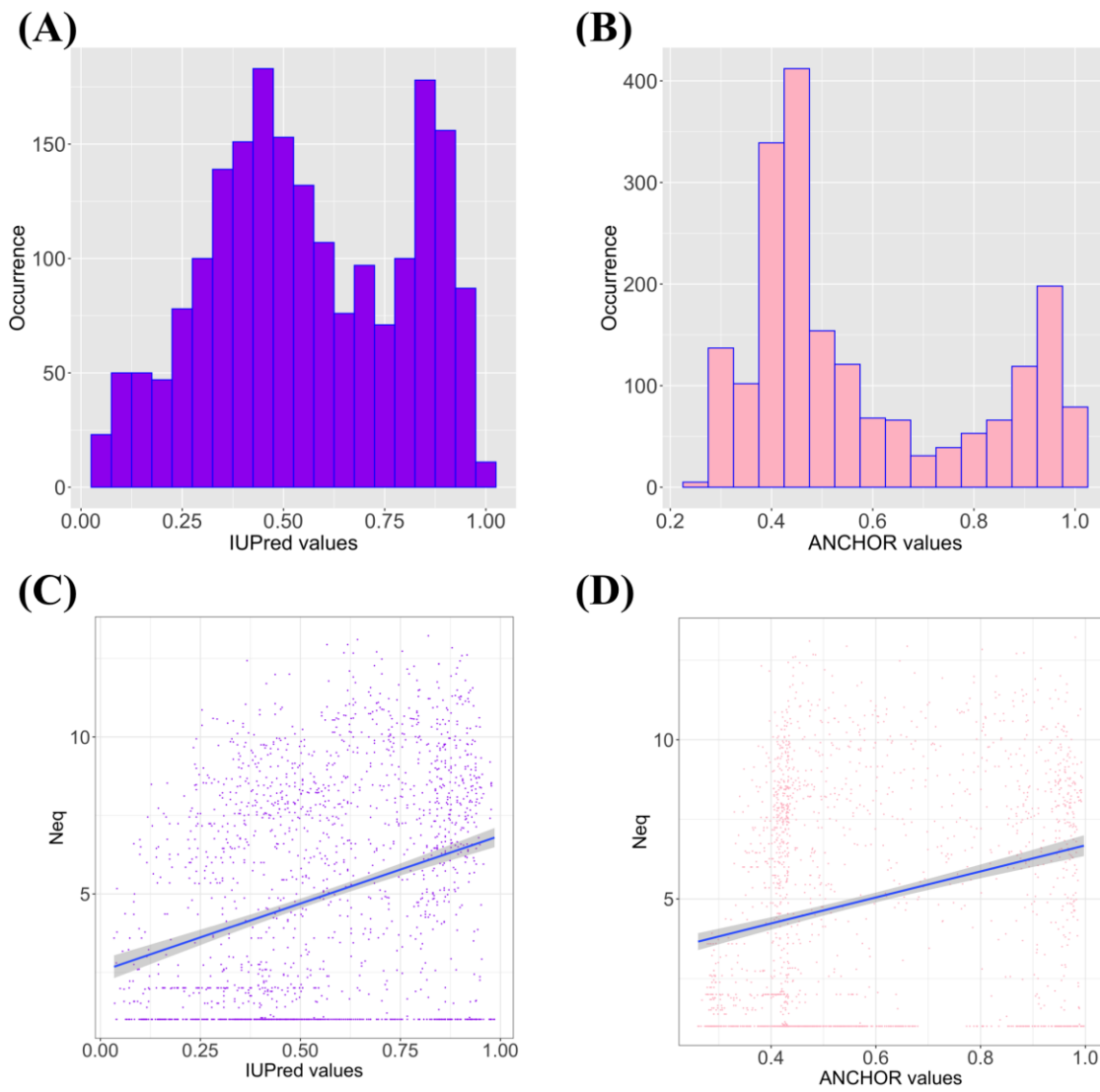


Figure A6. Distribution of N_{eq} and prediction disorder values & N_{eq} versus prediction disorder results. Distribution of (A) IUPred2A values (in purple), and (B) ANCHOR2 values (in pink), (C) N_{eq} values (x-axis) against IUPred2A values (y-axis) (correlation equals to 0.29). (D) N_{eq} values (x-axis) against ANCHOR2 values (y-axis) (correlation equals to 0.25).

	N_{eq}	DisoPred	PrDOS	IUPred2A	ANCHOR2
N_{eq}	--				
DisoPred	0.37	--			
PrDOS	0.34	0.75	--		
IUPred2A	0.29	0.56	0.65	--	
ANCHOR2	0.25	0.49	<u>0.44</u>	0.79	--

Table A1. Correlation between N_{eq} , Disopred3, PrDOS, IUPred2A and ANCHOR2 values on PED³ dataset.

Neq	1.0	>2.0	>3.0	>4.0	>5.0	>6.0	>7.0	>8.0	>9.0	>10.0	>11.0	>12.0
Prediction	61.39	42.43	38.71	38.36	38.51	37.31	36.65	34.39	34.99	35.14	36.40	37.96
<i>Order</i>	100.00	55.61	46.68	43.57	39.97	34.89	27.85	17.69	10.65	4.50	1.23	0.49
<i>Disorder</i>	0.00	21.48	26.04	30.08	36.20	41.15	50.65	60.94	73.70	83.85	92.32	97.53

Table A2. Evaluation of prediction rate according to N_{eq} values for Disopred3 approach.