

Phosphatidylcholine and Phosphatidylserine Uniquely Modify the Secondary Structure of Alpha-Synuclein Oligomers Formed in Their Presence at the Early Stages of Protein Aggregation

Tianyi Dou¹ and Dmitry Kurouski*^{1,3}

1. Department of Biochemistry and Biophysics, Texas A&M University, College Station, Texas 77843, United States

2. Department of Biomedical Engineering, Texas A&M University, College Station, Texas, 77843, United States

dkurouski@tamu.edu

Supporting Information

- S1. AFM images and height profile of α -Syn oligomers
- S2. Height profile of α -Syn oligomers formed in the presence of lipid LUVs
- S3. AFM image and AFM-IR map of α -Syn oligomers
- S4. Averaged AFM-IR spectra of α -Syn oligomers
- S5. Averaged AFM-IR spectra of α -Syn oligomers formed in the presence of lipid LUVs
- S6. Peak fitting for AFM-IR spectra
- S7. Bar plot of protein secondary structure of α -Syn, α -Syn:PC, α -Syn:PS oligomers
- S8. Mean and standard deviation of α -Syn:PC and α -Syn:PS AFM-IR spectra on D2, D8 and D15
- S9. CD spectra for α -Syn, α -Syn:PC and α -Syn:PS aggregates on D2, D8 and D15
- S10. FT-IR spectra of α -Syn, α -Syn:PC and α -Syn:PS aggregates on D2, D8 and D15

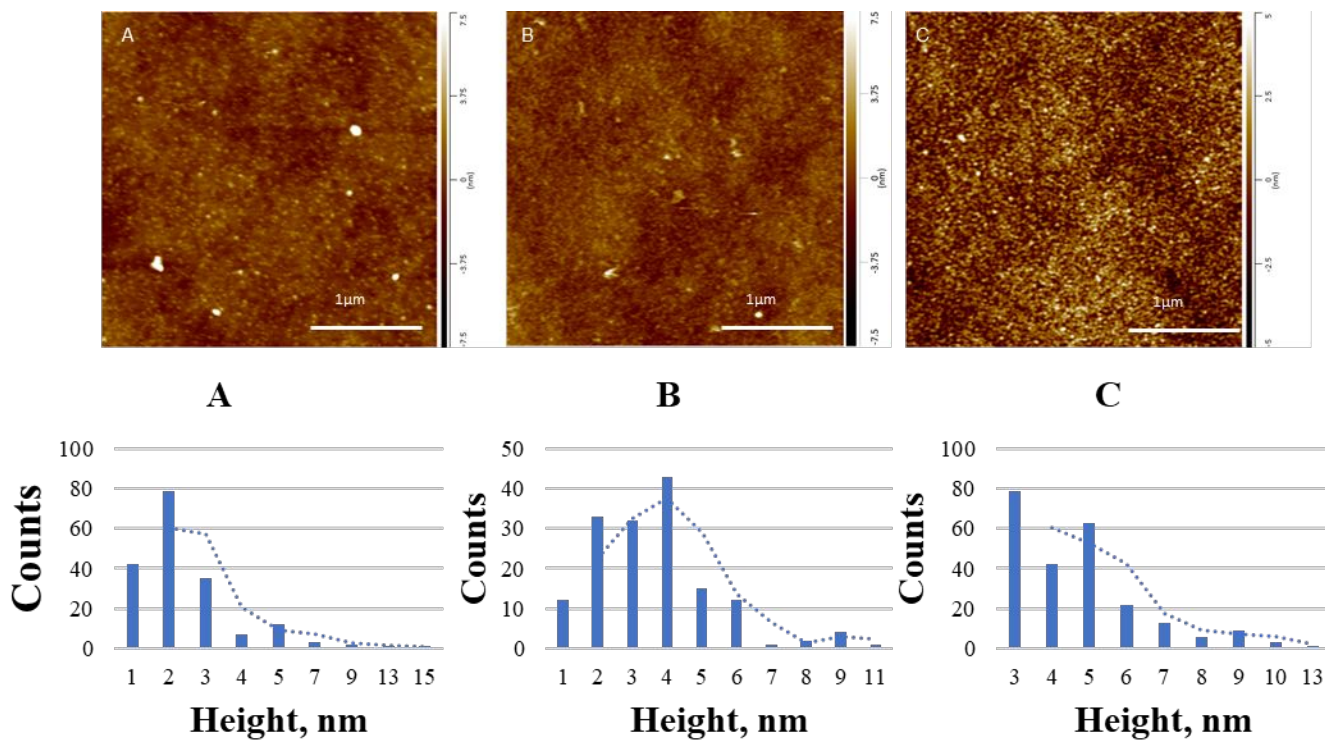


Figure S1. AFM images of α -Syn aggregates formed at day 2 (A), day8 (B) and day15 (C). Height profiles of α -Syn aggregates formed at day2 (D), day8 (E), and day 15 (F). Height profile of α -Syn aggregates formed at day 2 (A), day8 (B) and day15 (C).

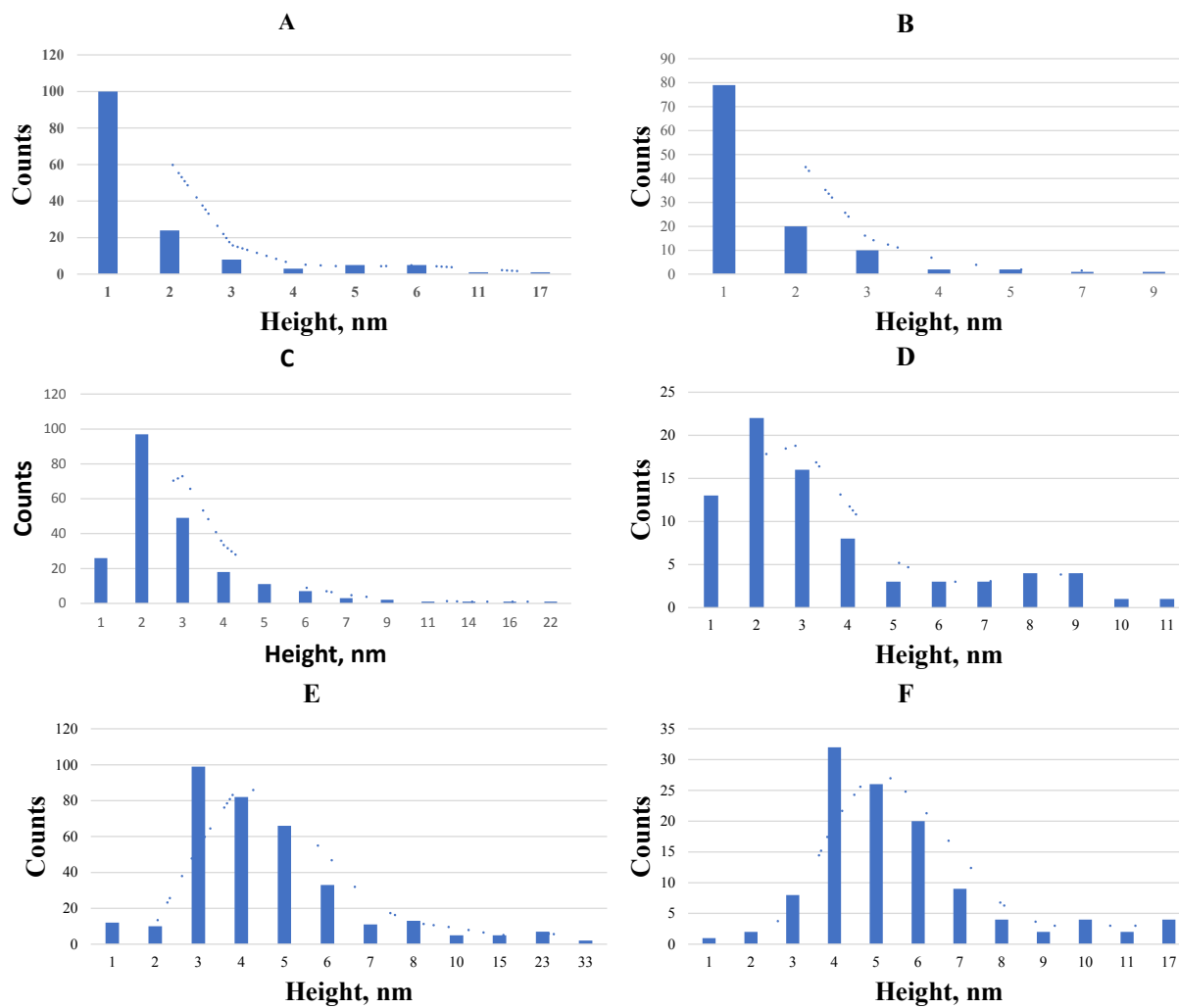


Figure S2. Height profiles of α -Syn:PC (A, C and E) and α -Syn:PS (B, D and F) oligomers observed at D2 (A-B), D8 (C-D) and D15 (E-F).

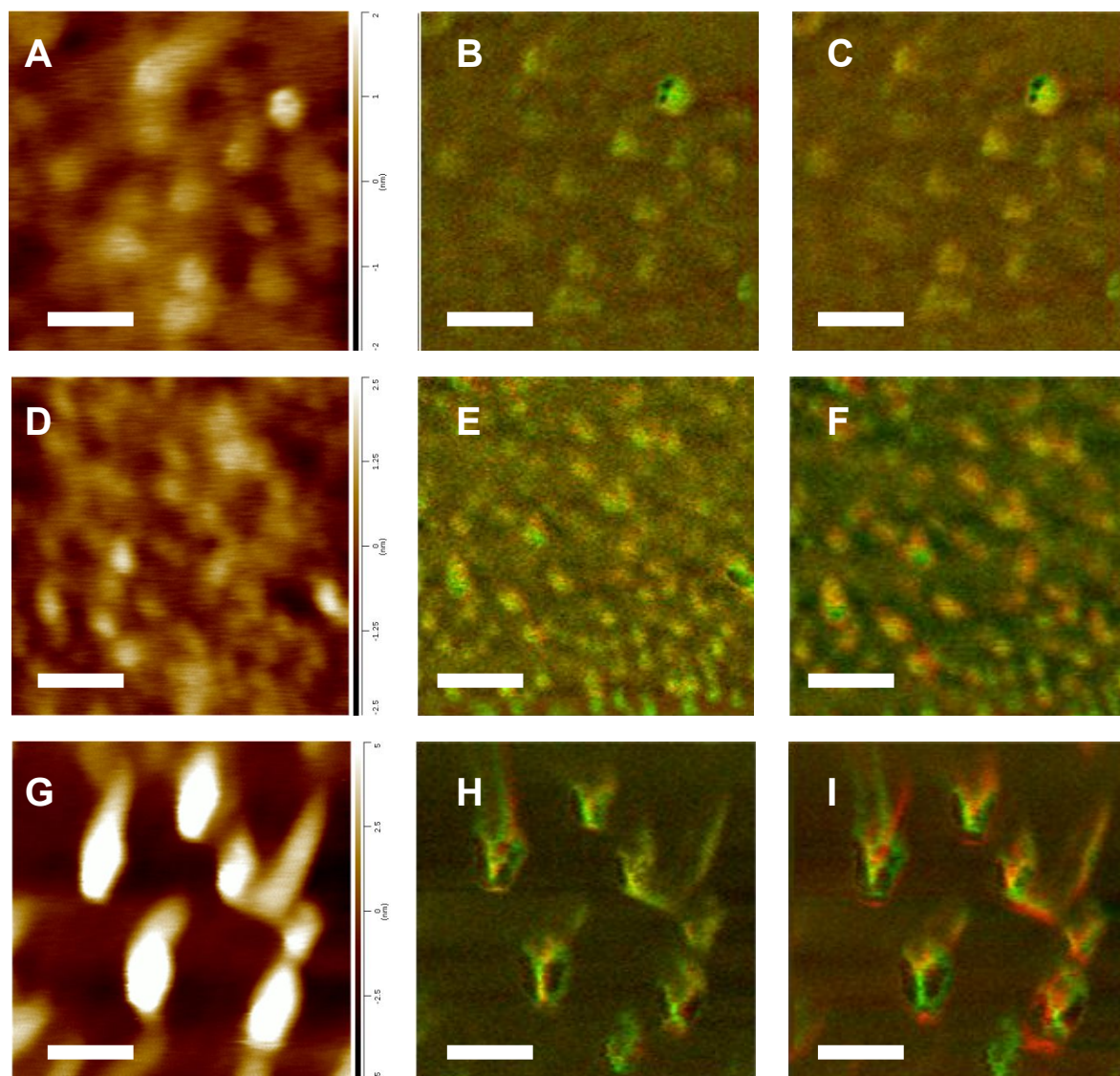


Figure S3. AFM-IR maps of α -Syn oligomers formed at D2 (A-C), D8 (D-F) and D15 G-I) in the lipid-free environment. AFM height images (A, D, G), IR ratio overlaying map of 1624 cm^{-1} (parallel β -sheet) (green) and 1655 cm^{-1} (α -helix/unordered protein secondary structure) (red) (B, E, H), and overlaying map of 1624 (parallel β -sheet) and 1694 cm^{-1} (antiparallel β -sheet) (C, F, I). Scale bar, 100nm.

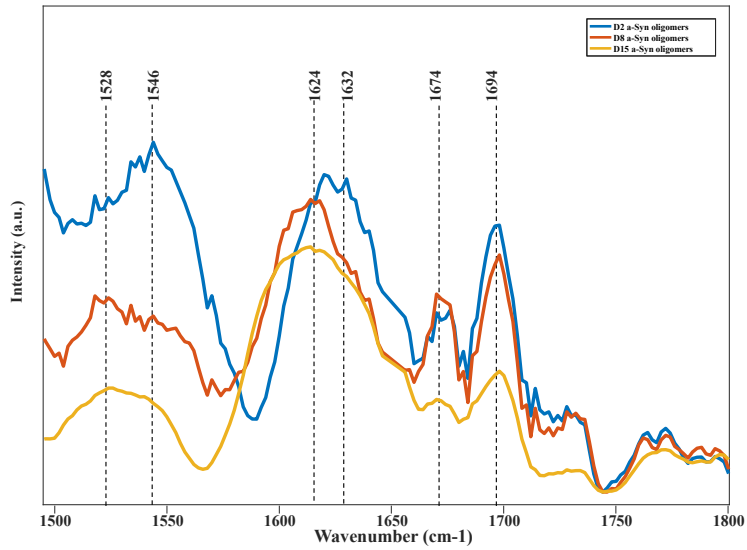


Figure S4. Averaged AFM-IR spectra collected from α -Syn oligomers at D2, D8 and D15 htau were grown in the lipid-free environment.

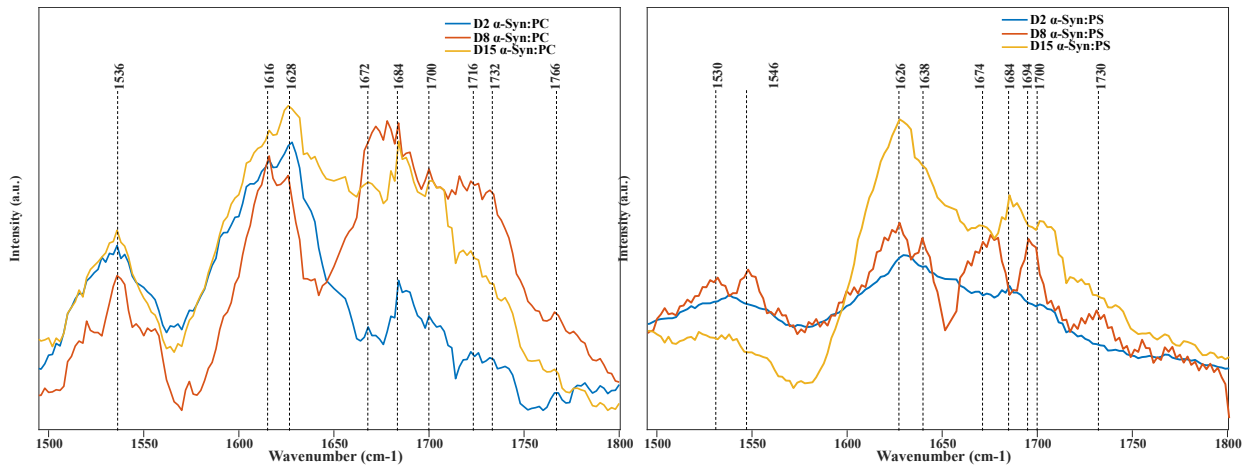


Figure S5. Averaged AFM-IR spectra collected from α -Syn:PC and α -Syn:PS oligomers at D2, D8 and D15.

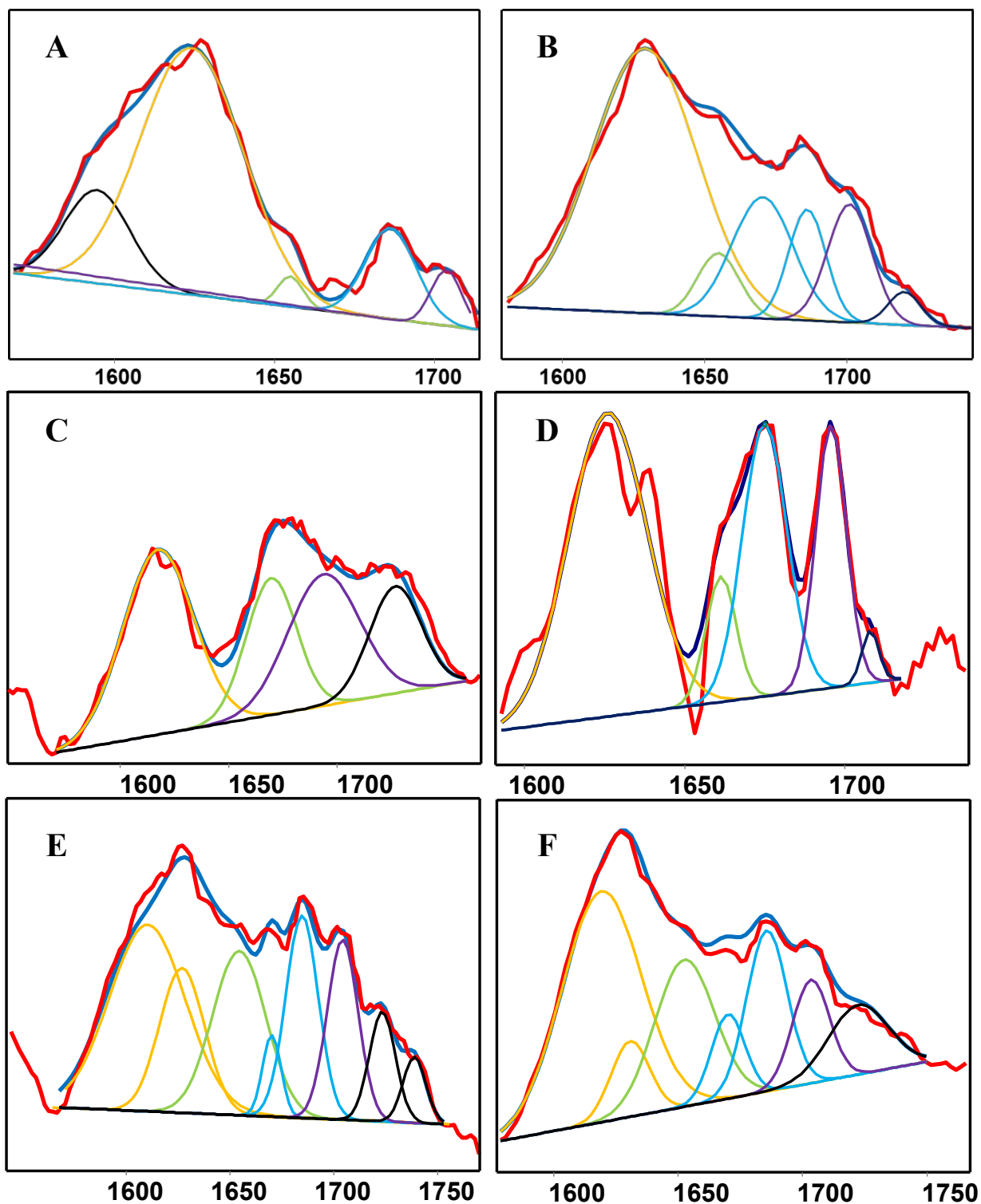


Figure S6. Averaged AFM-IR spectra and secondary structure deconvolution of amide I band of α -Syn:PC (A, C, E) and α -Syn:PS (B, D, F) oligomers formed at D2 (A,B), D8 (C,D) and D15 (E,F).

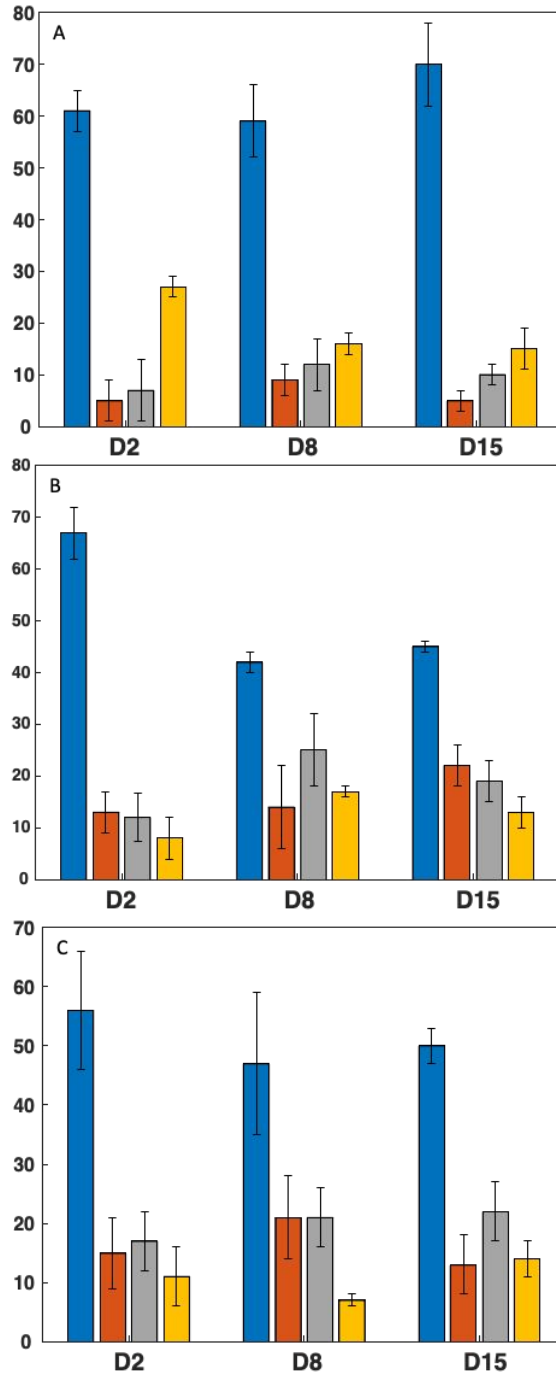


Figure S7. Bar plot of protein secondary structure of α -Syn (A), α -Syn:PC (B), α -Syn:PS (C) oligomers on day 2, day 8 and day 15. Parallel beta sheet (blue), alpha helix and random coil (red), beta-turn (grey) and antiparallel beta sheet (yellow) percentages were calculated based on peak fitting of 3-4 different oligomers.

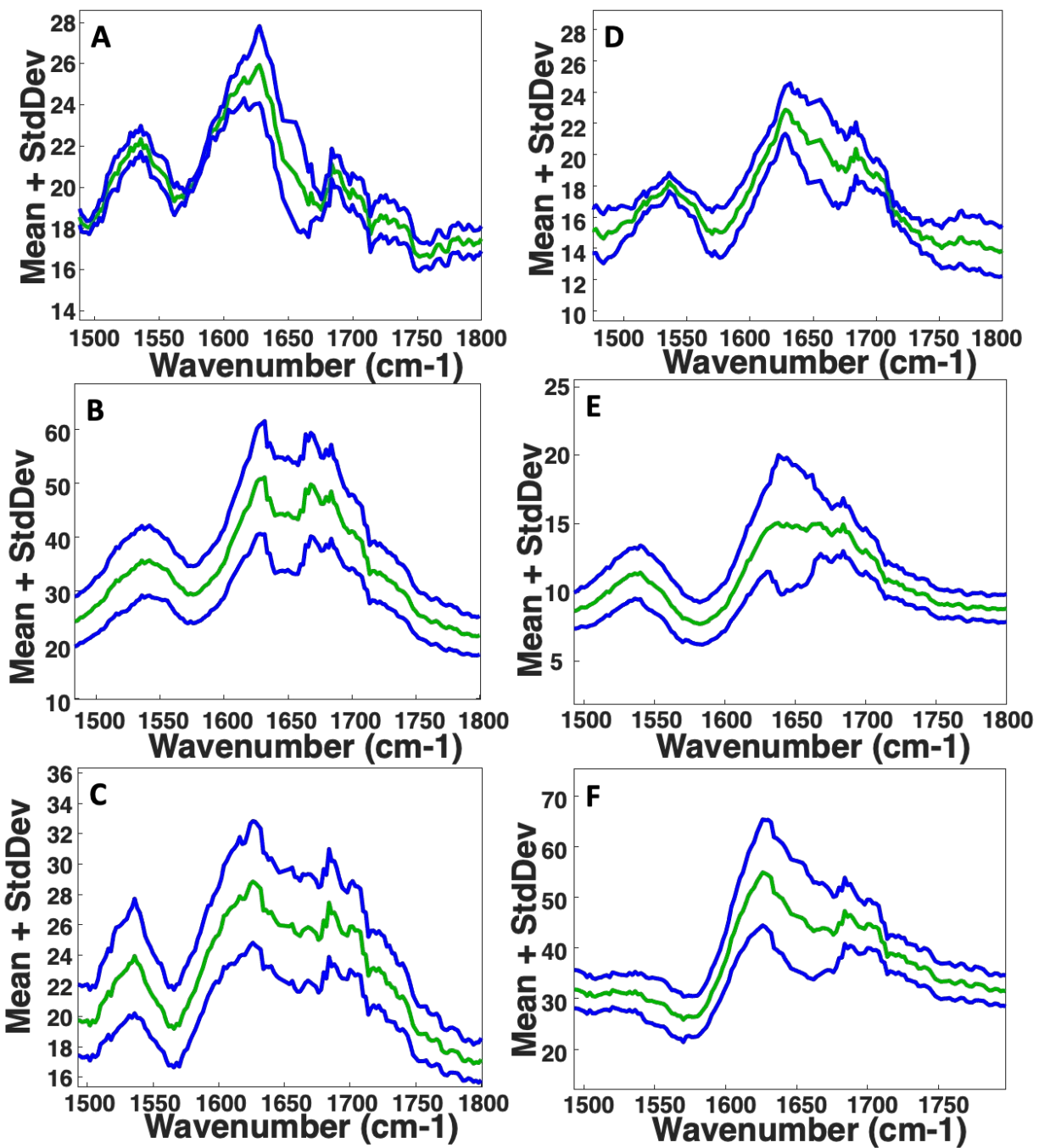


Figure S8. Mean (green) and standard deviation (blue) AFM-IR spectra of α -Syn:PC (A-C) and α -Syn:PS (D-F) oligomers on day 2 (A,D), day 8 (B,E) and day 15 (C, F).

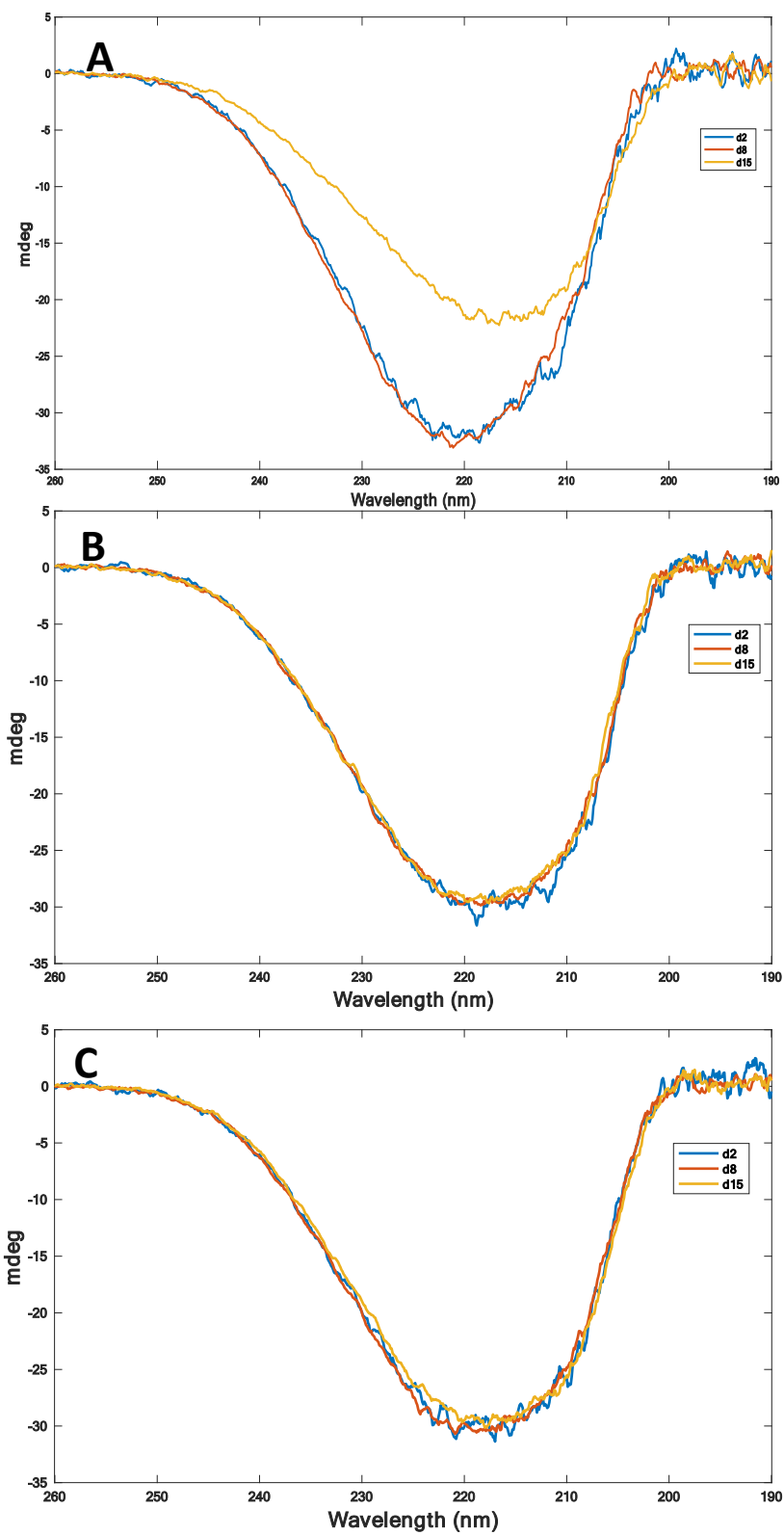


Figure S9. CD spectra of α -Syn (A), α -Syn:PC (B) and α -Syn:PS (C) on d2 (blue), d8 (orange) and d15 (yellow).

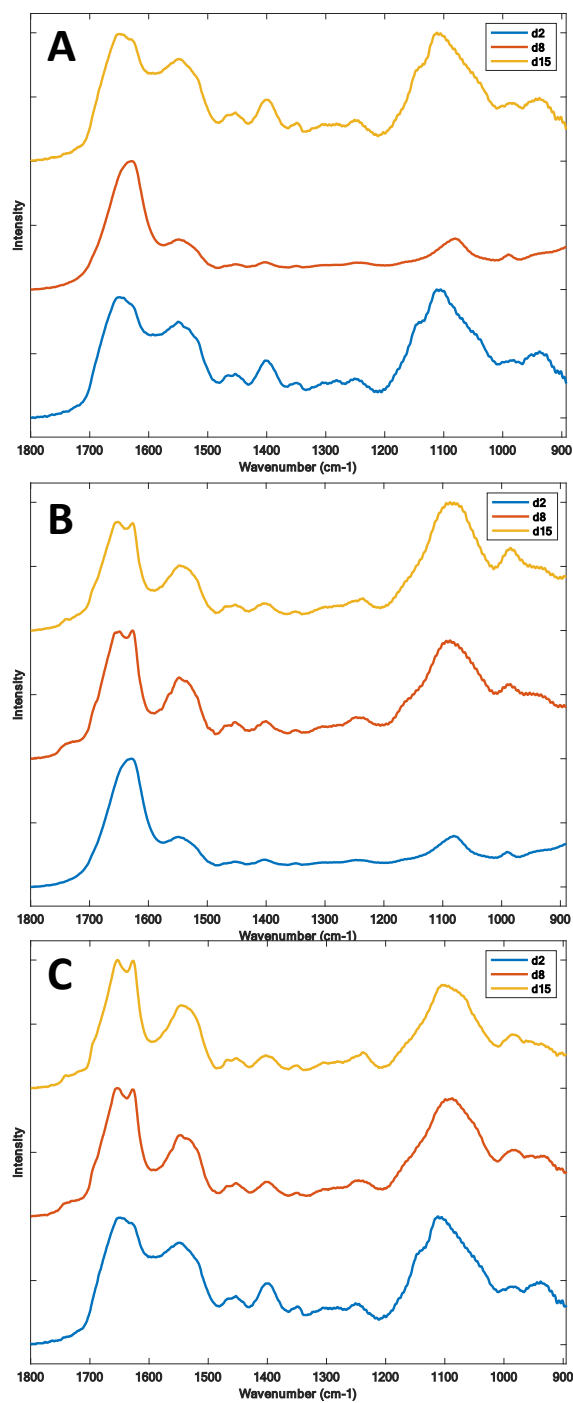


Figure S10. FT-IR spectra of α -Syn (A), α -Syn:PC (B) and α -Syn:PS (C) on d2 (blue), d8 (orange) and d15 (yellow).