Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Steric Hindrance Dependence on the Spin and Morphology Properties of Highly Oriented Self-Doped Organic Small Molecule Thin Films

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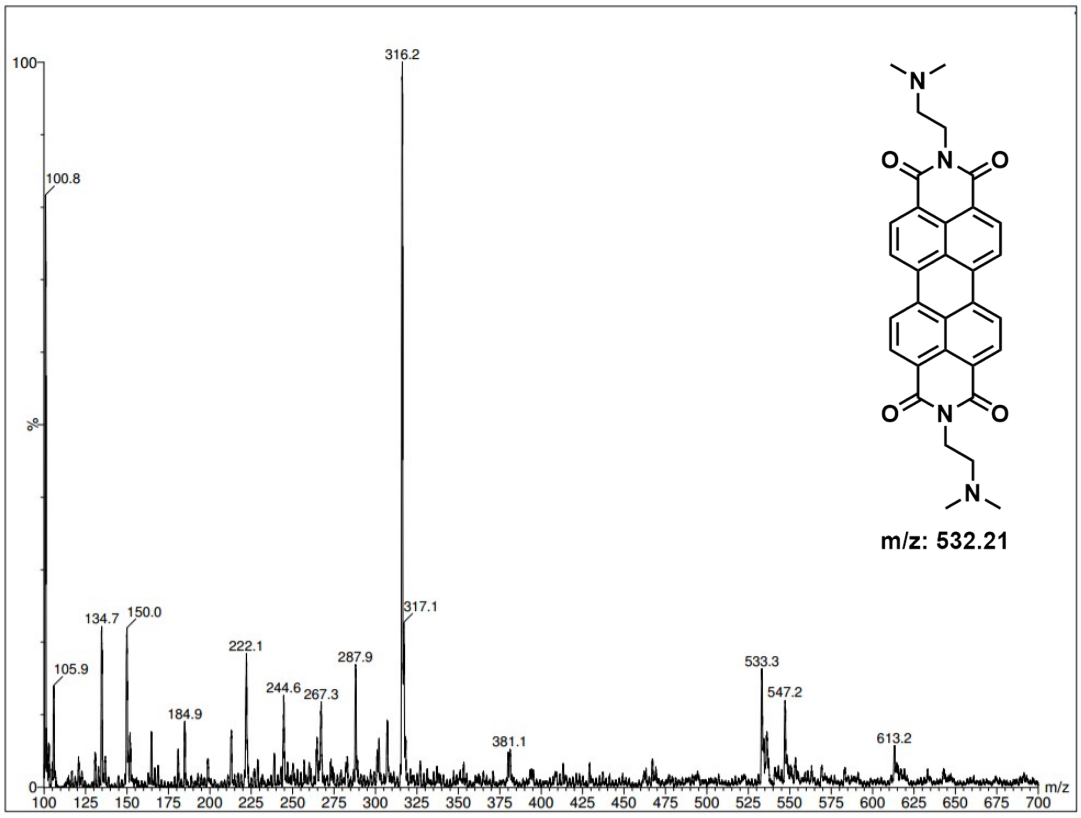

Figure S1. MALDI mass spectrum for self-doped PDI (compound #1). Exact mass and structure provided as an inset. The expected m/z is 532.21 and the observed peak at 533.3 is likely due to protonated species.

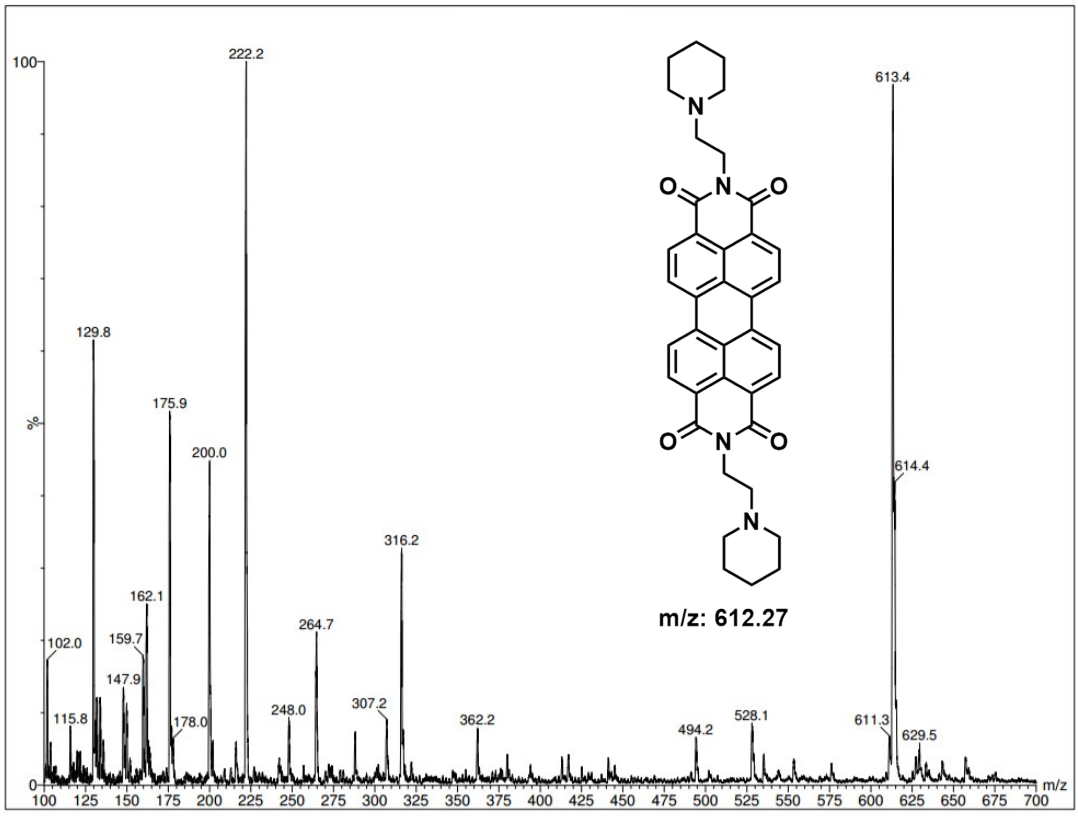

Figure S2. MALDI mass spectrum for self-doped PDI (compound #2). Exact mass and structure provided as an inset.

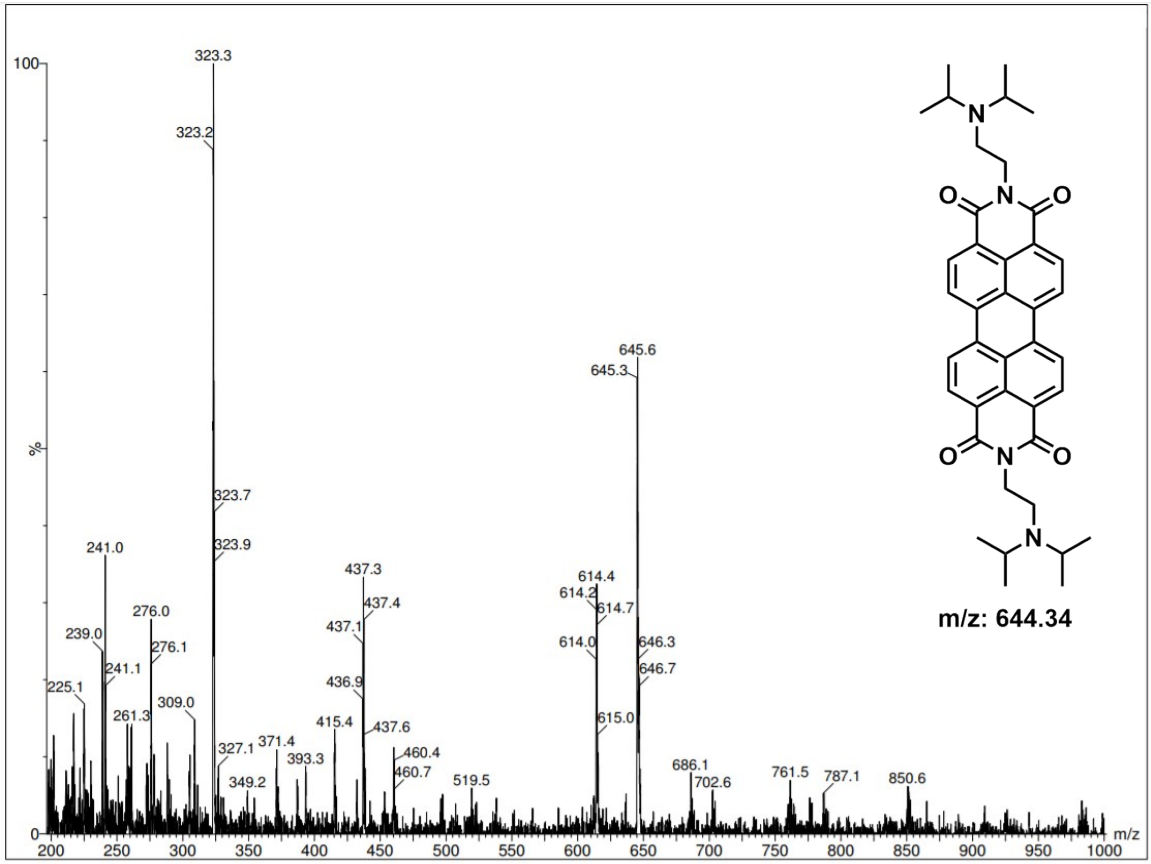

Figure S3. MALDI mass spectrum for self-doped PDI (compound #3). Exact mass and structure provided as an inset.

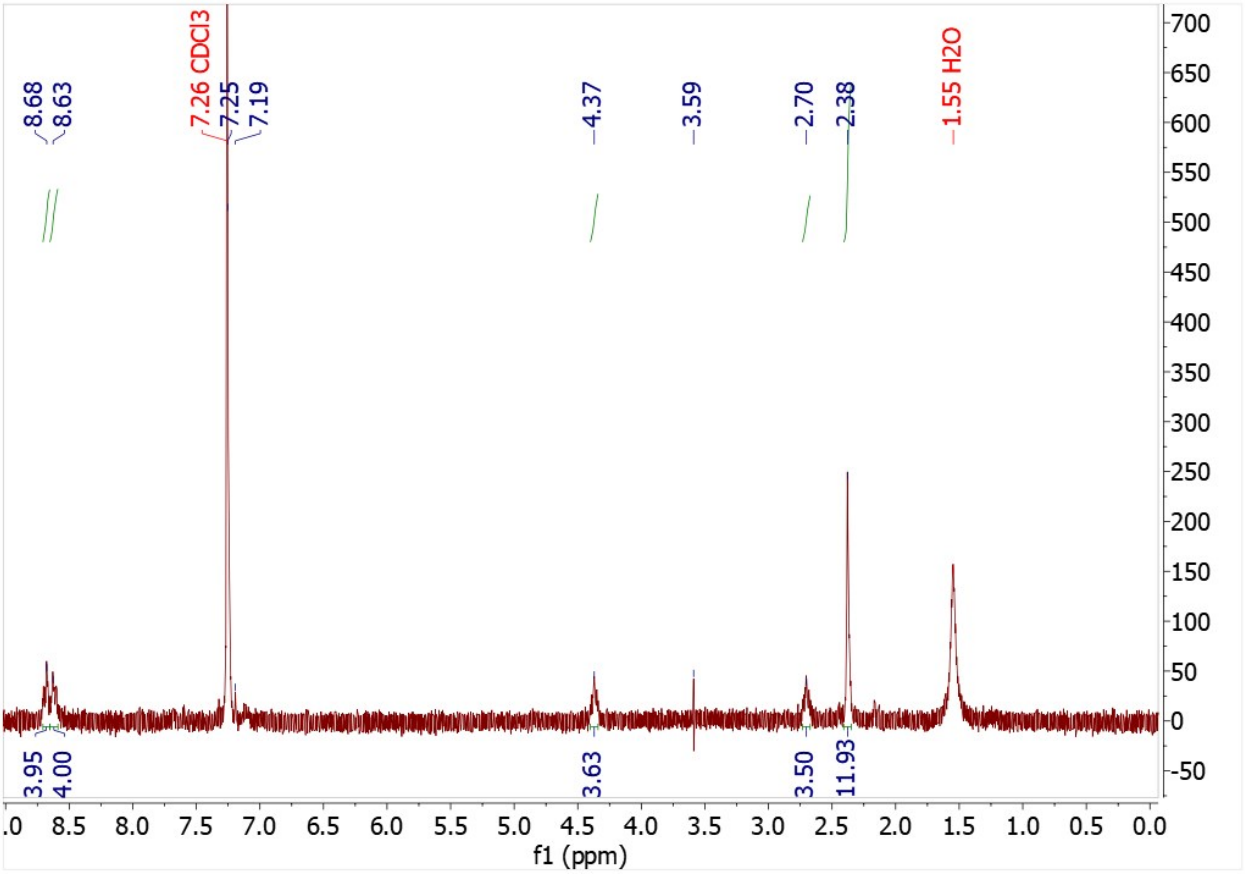

Figure S4. HNMR spectrum of compound #1.

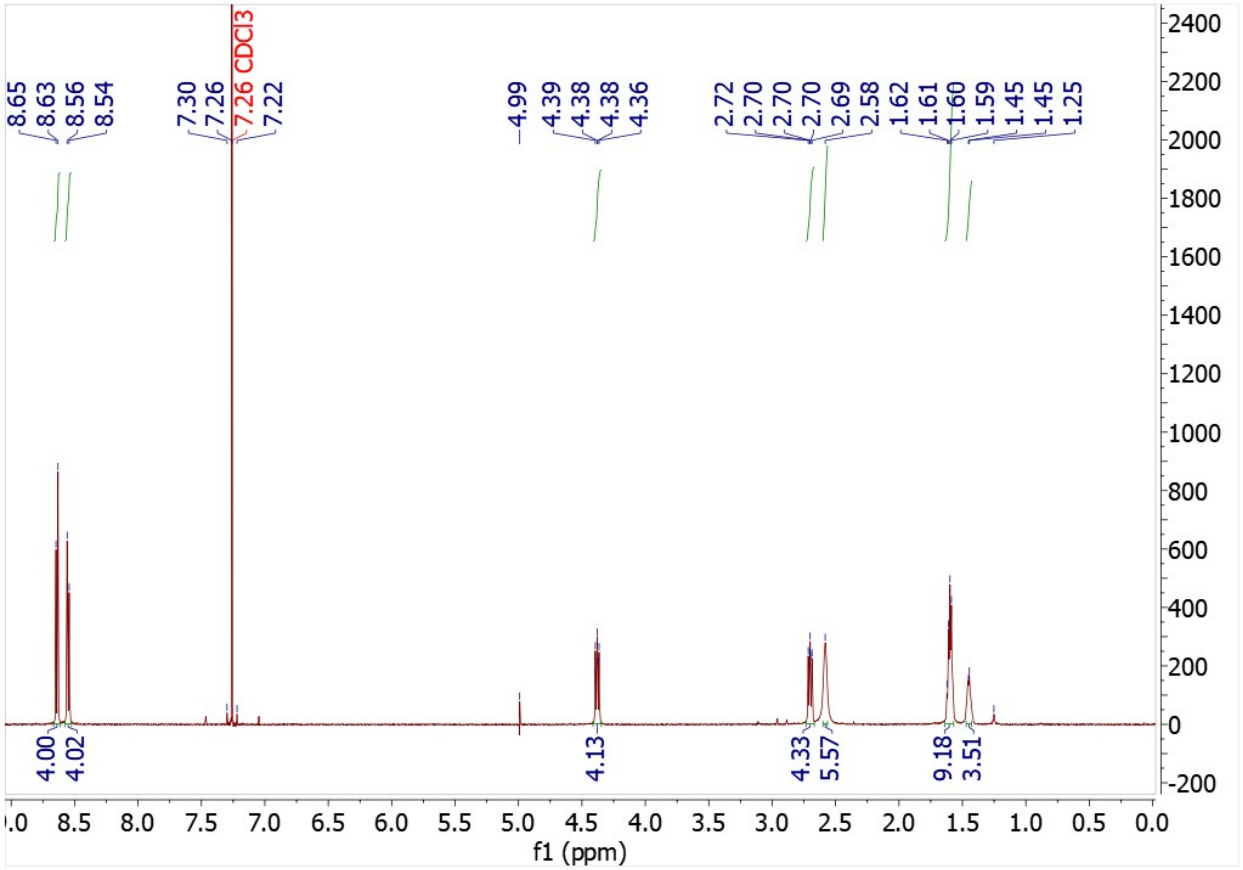

Figure S5. HNMR spectrum of compound #2.

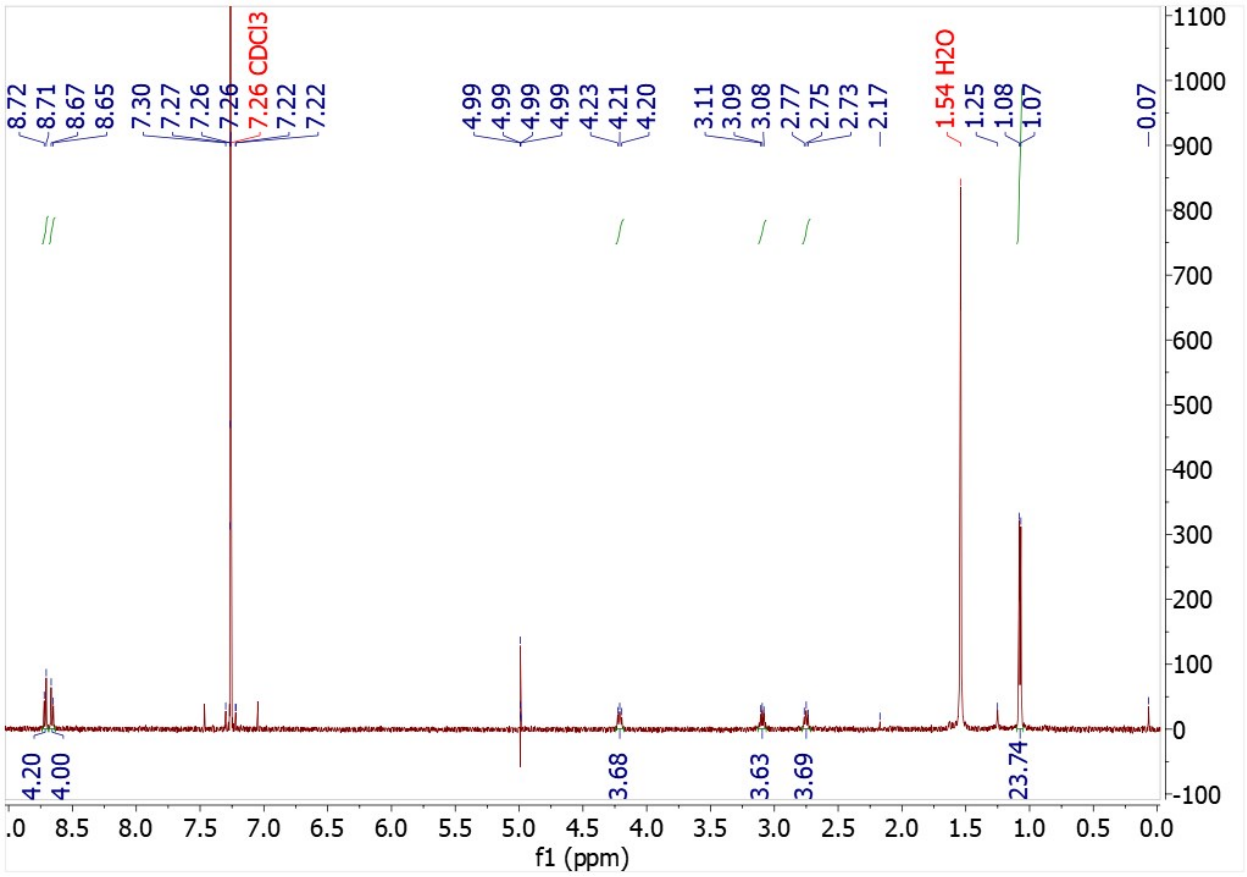

Figure S6. HNMR spectrum of compound #3.

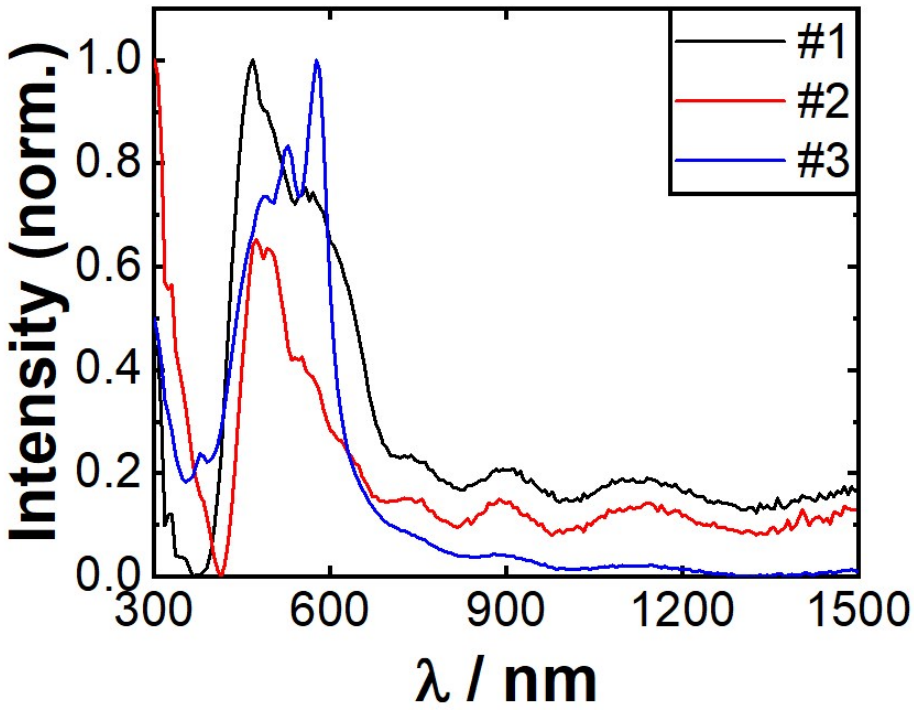

Figure S7. Solid-state absorption spectra for compounds #1-3. The peaks centered at ≈ 750 nm, ≈ 900 nm, and ≈ 1000 nm are consistent with the absorption of the PDI radical anion $[PDI]^-$.

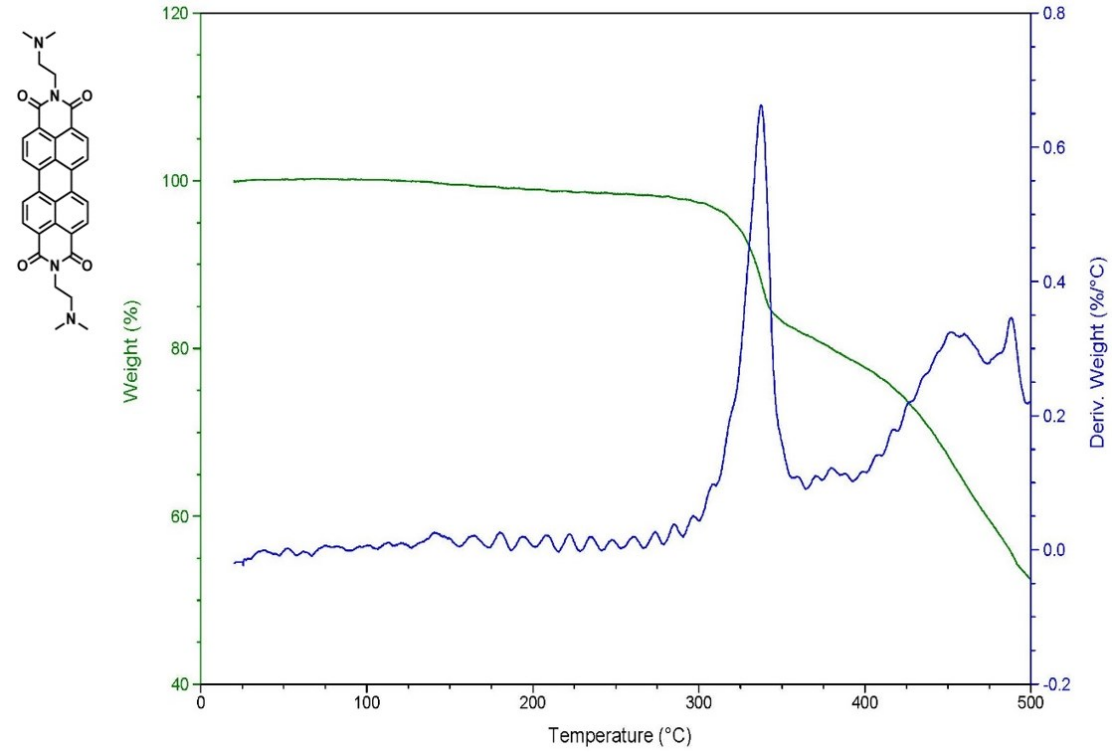

Figure S8. TGA spectra for self-doped PDI (compound #1).

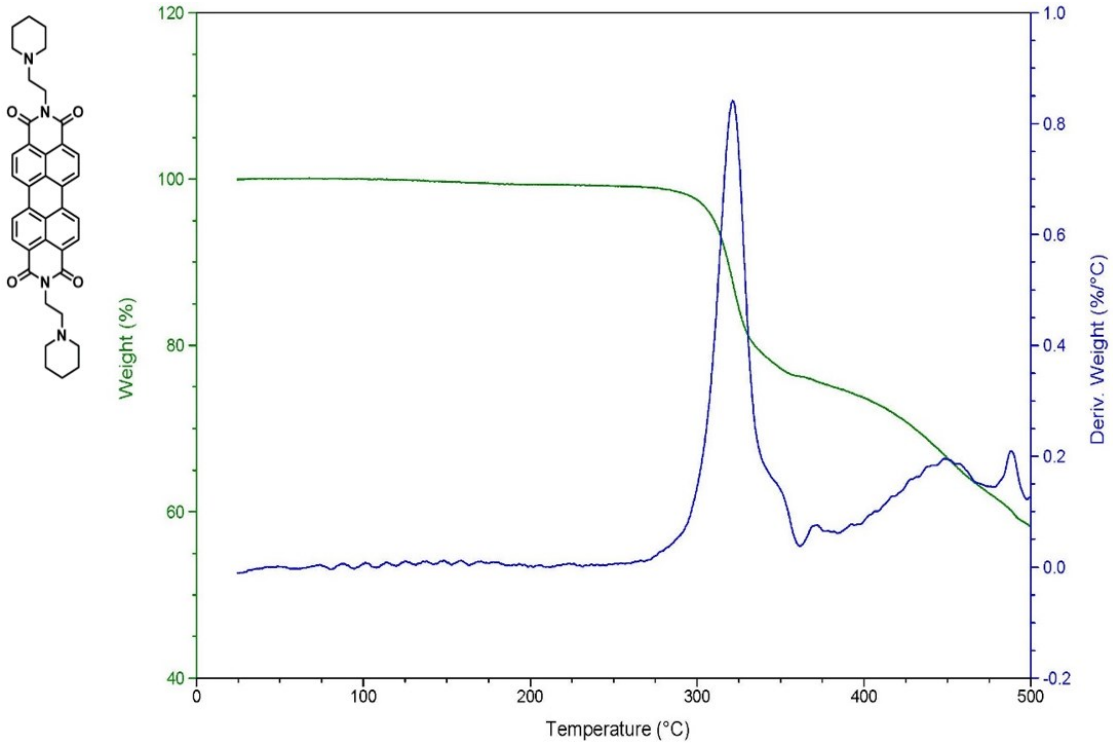

Figure S9. TGA spectra for self-doped PDI (compound #2).

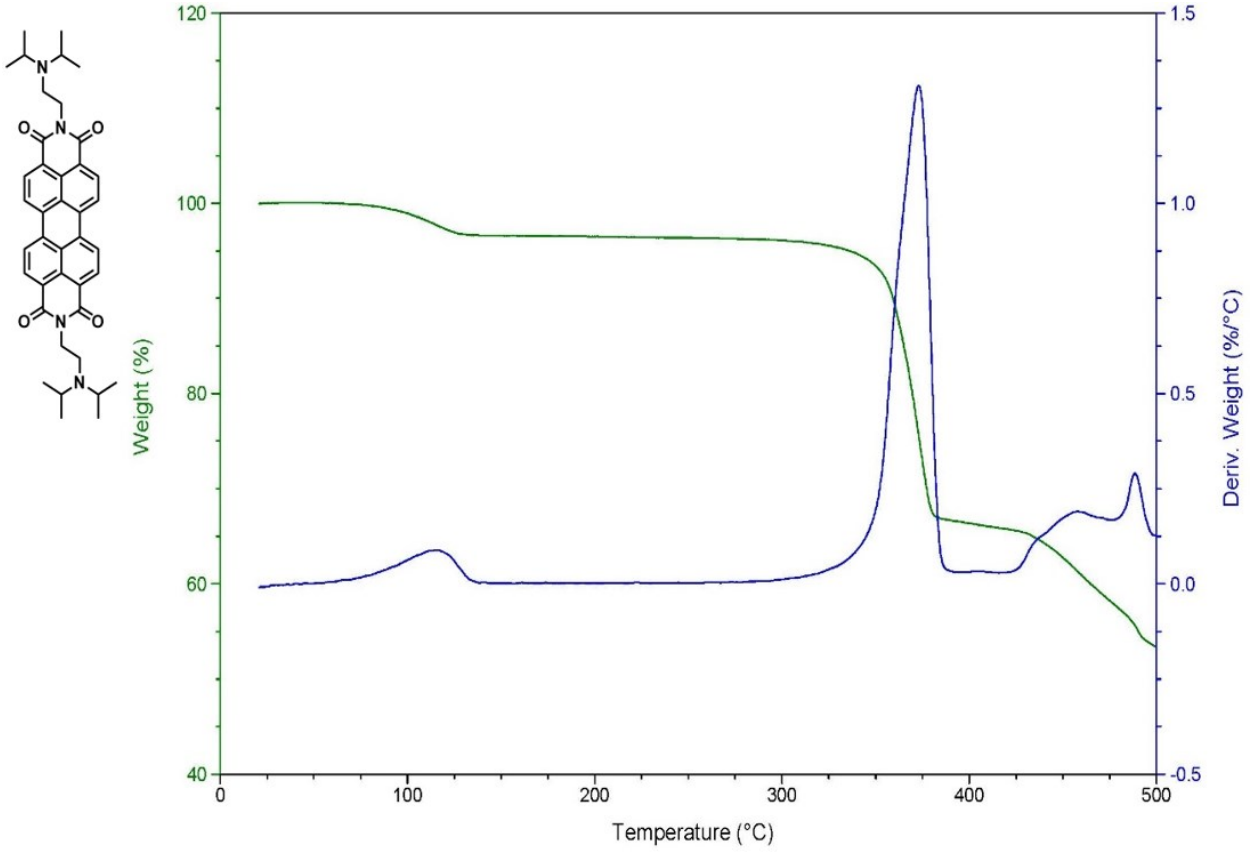

Figure S10. TGA spectra for self-doped PDI (compound #3). The small mass loss at ≈110 °C is attributed to the loss of water from the purification process, which is further supported by SSNMR studies.

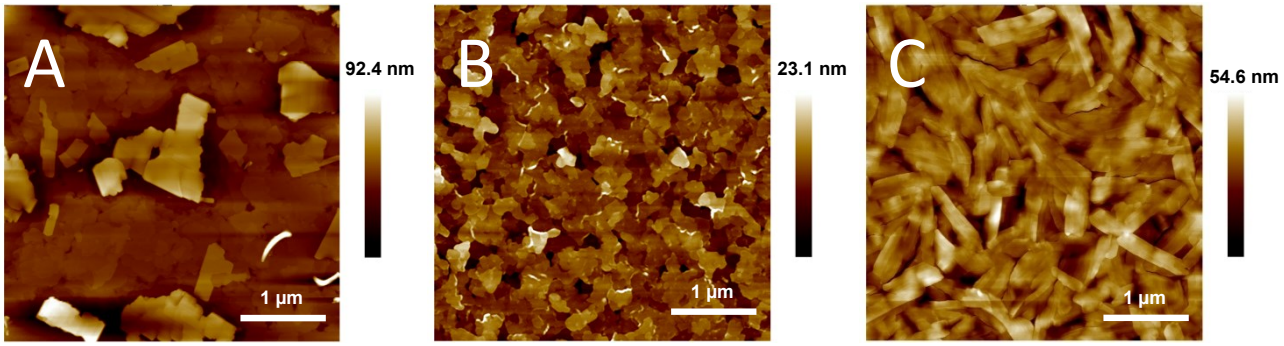

Figure S11. AFM images of **(A)** compound #1 **(B)** compound #2, and **(C)** compound #3.

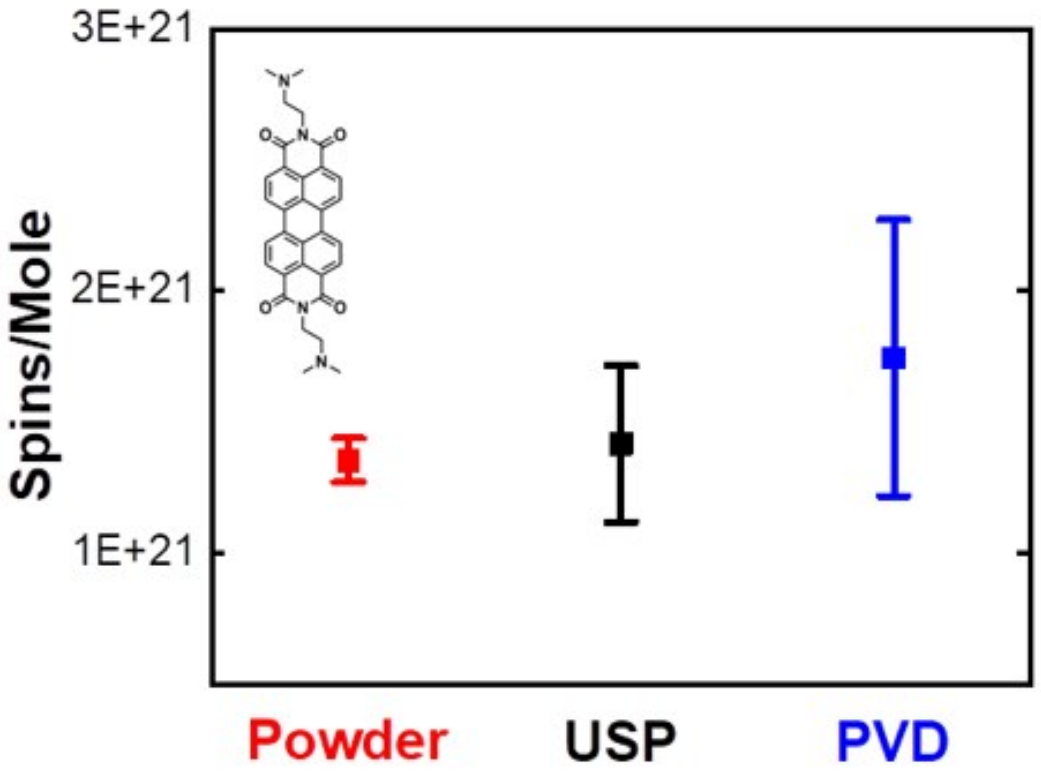

Figure S12. Spin concentration via EPR measurements of powder, ultrasonic spray coated, and physical vapor deposited thin films for a self-doped PDI. Structure provided as an inset.

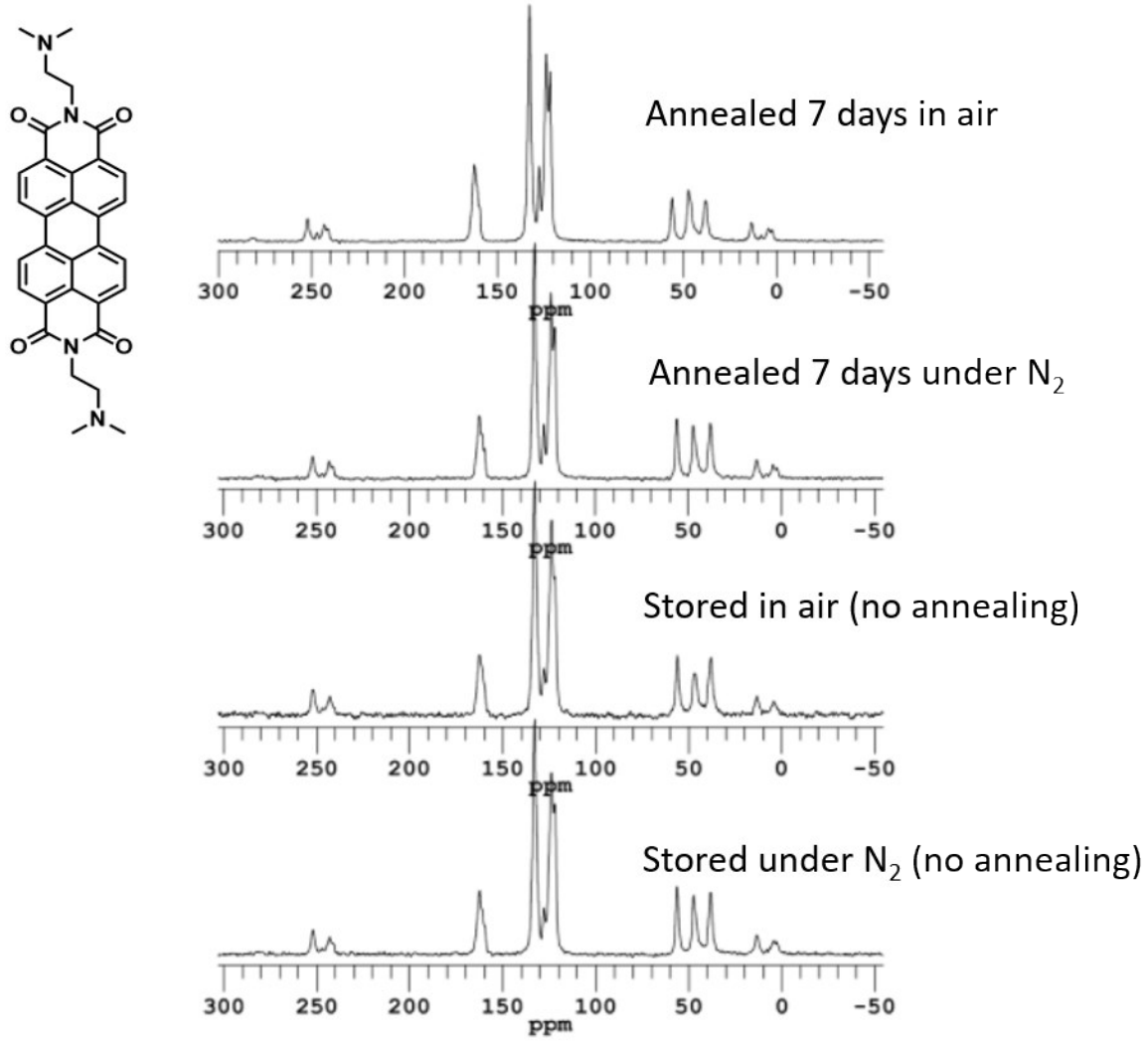

Figure S13. SSNMR spectra of compound #1 under different storing and annealing conditions.

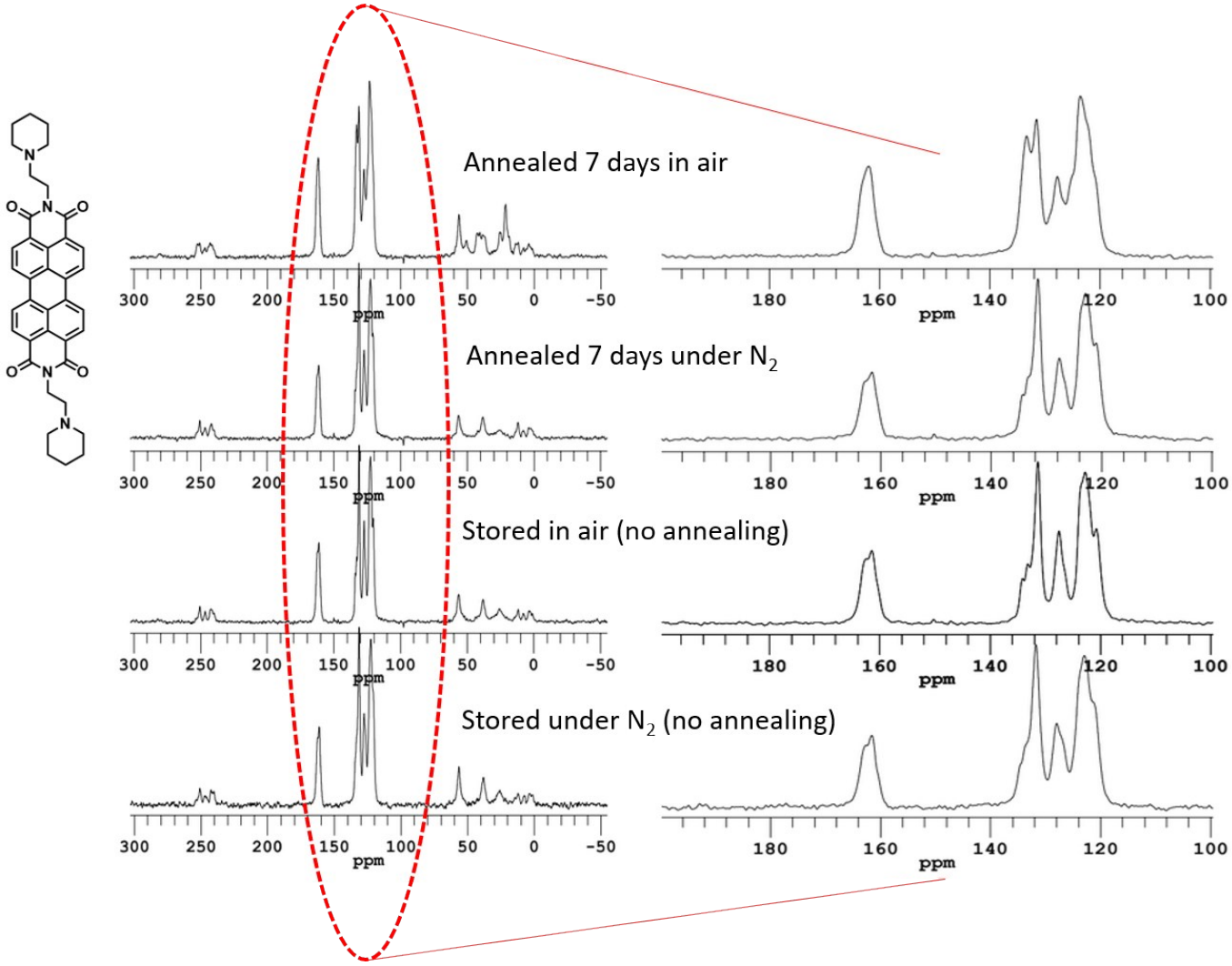

Figure S14. SSNMR spectra of compound #2 under different storing and annealing conditions. Spectral enlargement of the aromatic region from 120-140 ppm is shown on the right for clarity.

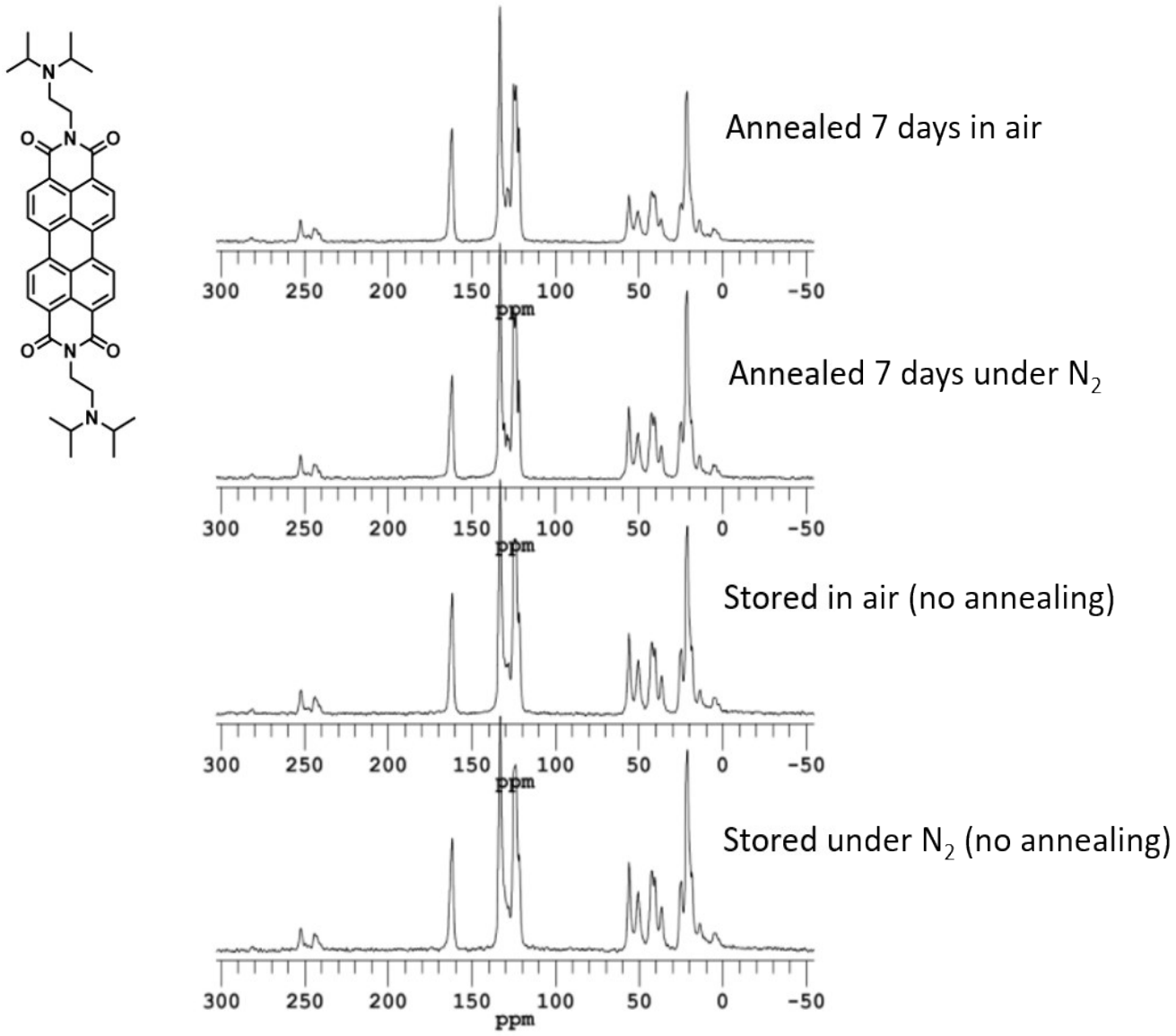

Figure S15. SSNMR spectra of compound #3 under different storing and annealing conditions.

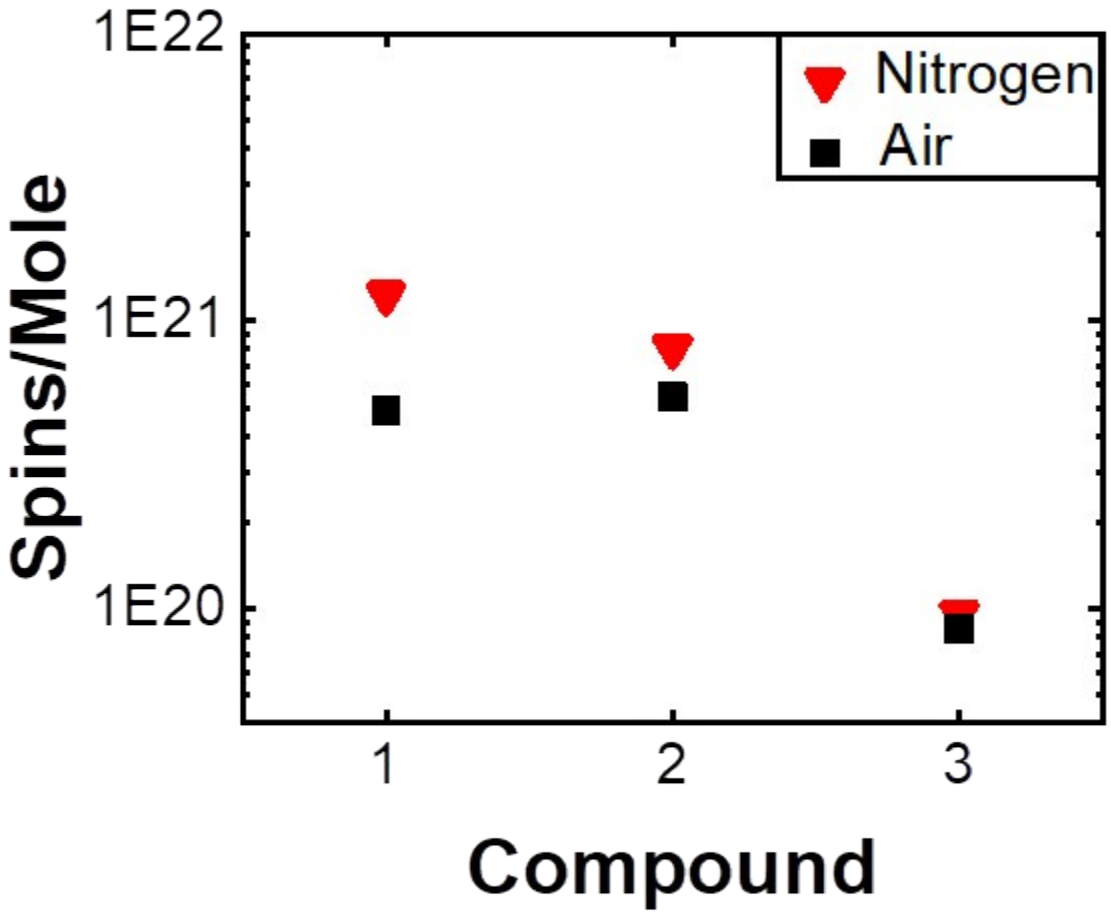

Figure S16. Spin concentration via EPR of compounds #1-3 measured under a nitrogen atmosphere and after 3 days of air exposure.