A Machine Learning Approach for Efficiently Predicting Polymer Aging from UV-Vis Spectra

Haishan Yu[1], DaDi Zhang[1], Lei Cui[1], Yuan Kong[2,*] Xuechen Jiao[1,*]

1. National Synchrotron Radiation Laboratory, University of Science and Technology of China, 42 Hezuohua Road, Hefei, Anhui 230029, China.

2. Hefei National Research Center for Physical Sciences at the Microscale and Department of Chemical Physics, University of Science and Technology of China, Hefei, Anhui 230026, China and Hefei National Laboratory, University of Science and Technology of China, Hefei, Anhui 230088, China.

Corresponding Author: kongyuan@ustc.edu.cn; xjiao@ustc.edu.cn

Contents

1. Experimental data: solution images and corresponding UV-Vis spectra

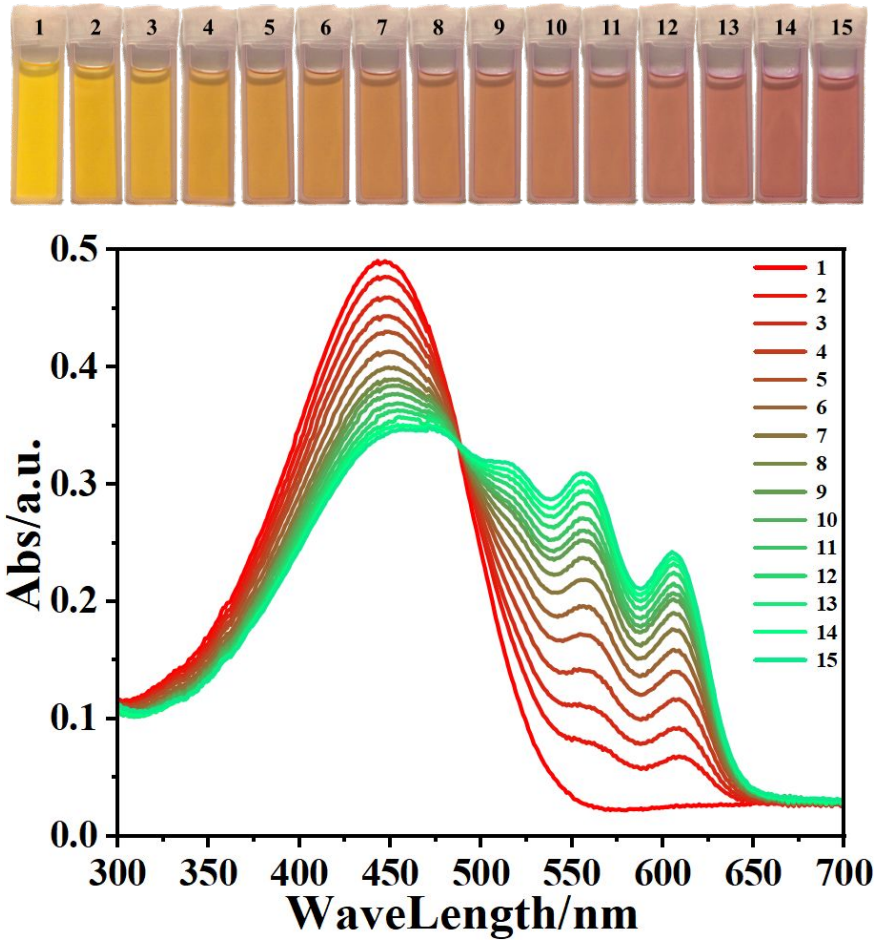

Figure S1. Solution images and corresponding UV-Vis spectra of P3HT-THF solution with a concentration of 0.05 mg/mL under aging effect. A total of 15 groups.

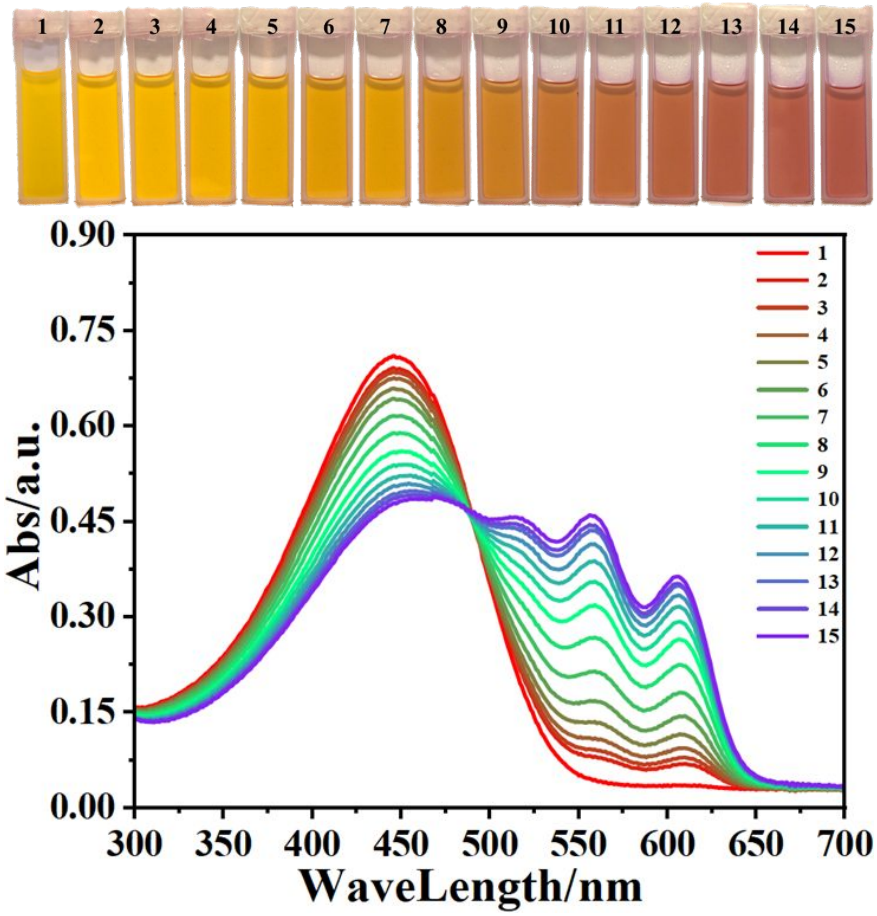

Figure S2. Solution images and corresponding UV-Vis spectra of P3HT-THF solution with a concentration of 0.10 mg/mL under aging effect. A total of 15 groups.

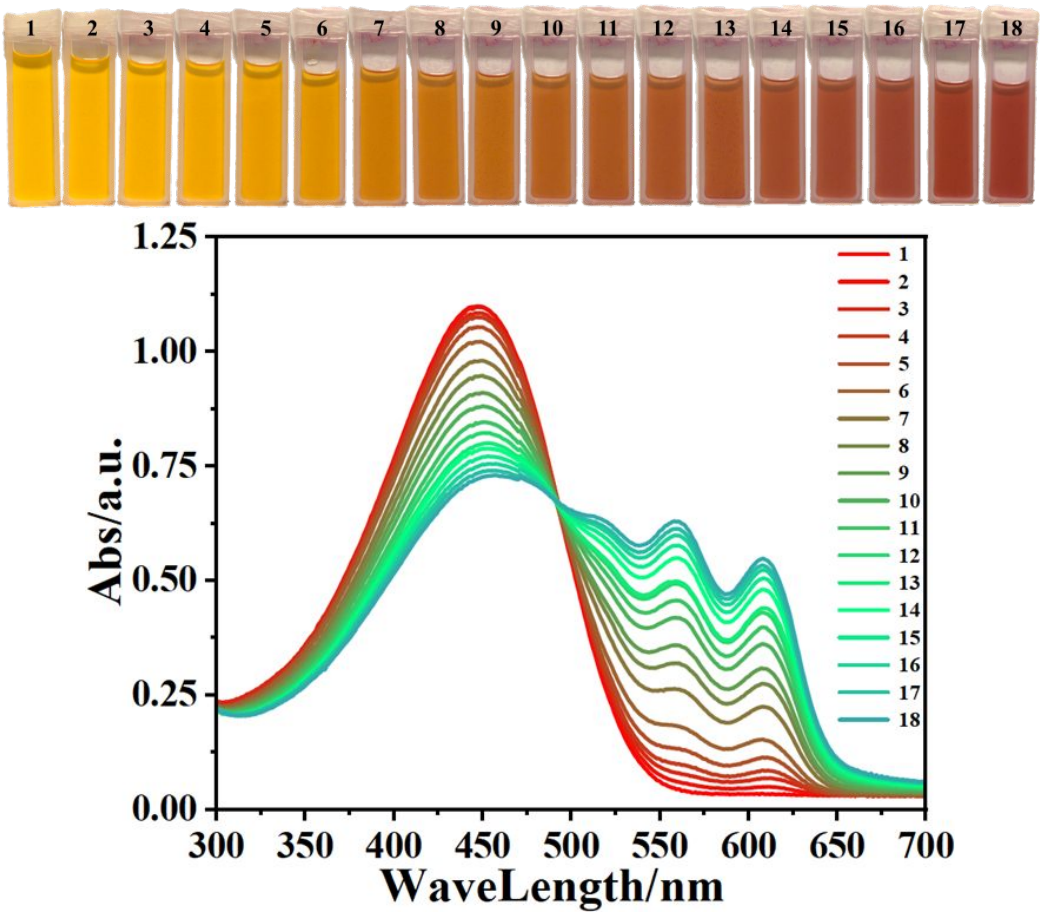

Figure S3. Solution images and corresponding UV-Vis spectra of P3HT-THF solution with a concentration of 0.15 mg/mL under aging effect. A total of 18 groups.

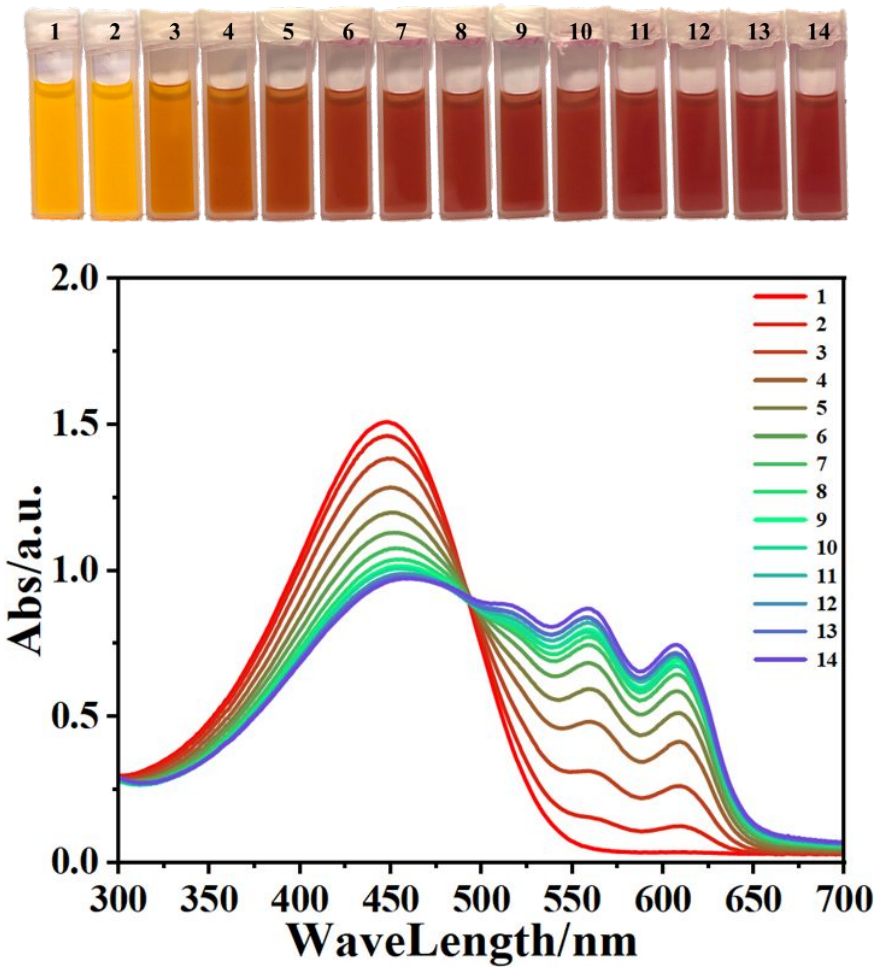

Figure S4. Solution images and corresponding UV-Vis spectra of P3HT-THF solution with a concentration of 0.20 mg/mL under aging effect. A total of 14 groups.

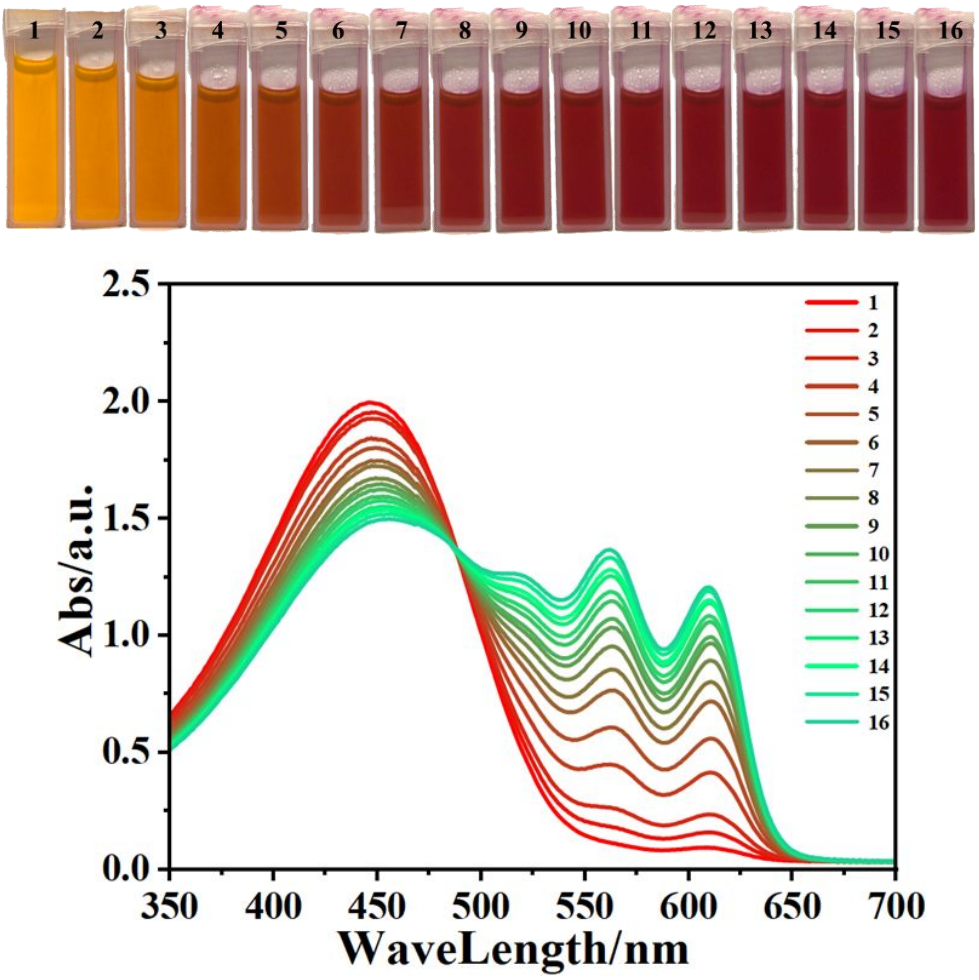

Figure S5. Solution images and corresponding UV-Vis spectra of P3HT-THF solution with a concentration of 0.25 mg/mL under aging effect. A total of 16 groups.

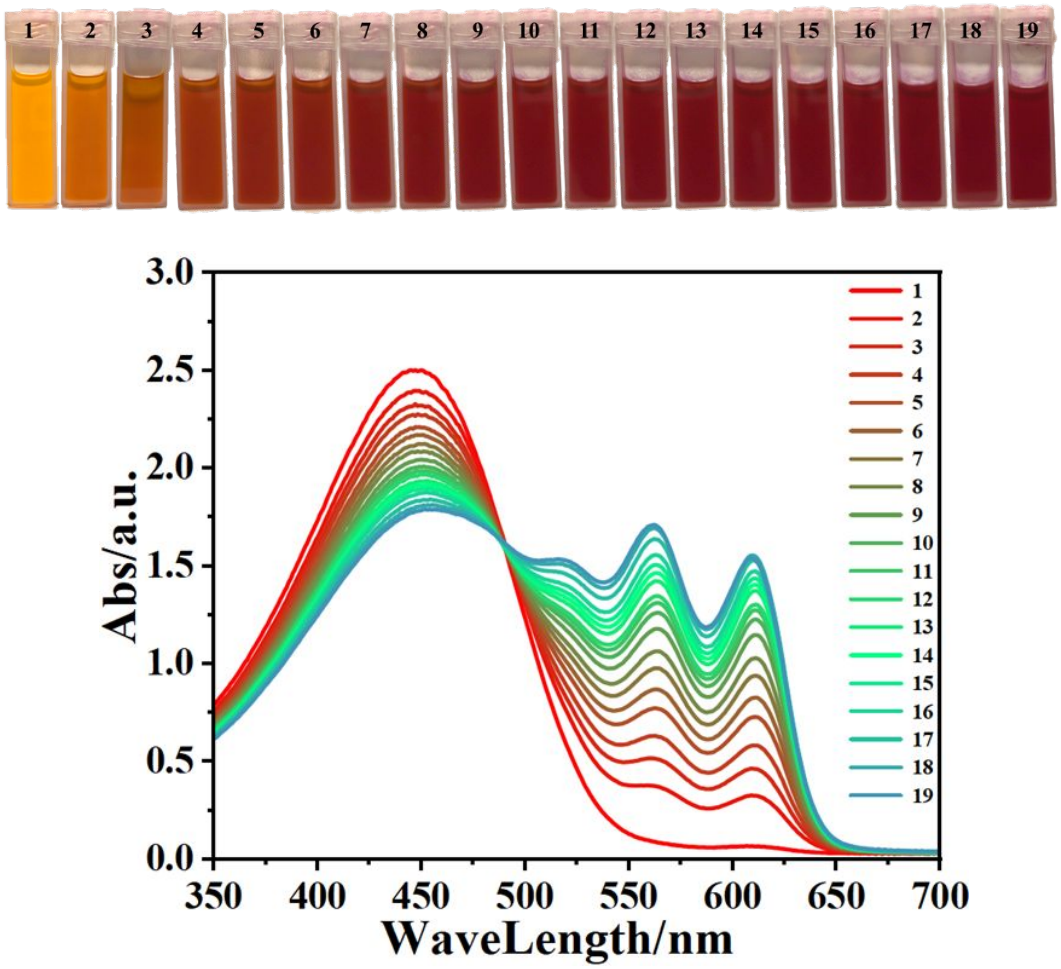

Figure S6. Solution images and corresponding UV-Vis spectra of P3HT-THF solution with a concentration of 0.30 mg/mL under aging effect. A total of 19 groups.

2. The calculation process of obtaining B, G, R values.

To eliminate the influence of background noise, we first select a specific color region of the solution in the bottle and calculate its mean BGR value, denoted as M_{S-X}. Next, we choose a specific region outside the bottle as background noise and obtain the mean BGR value for that area, denoted as M_{B-X}. Finally, we calculate the BGR difference between the solution color and the background color. The specific formula is defined as follows.

$$D_X = |M_{S-X} - (255 - M_{B-X})|$$

where X represents the three-color channels B (Blue), G (Green), and R (Red), respectively.

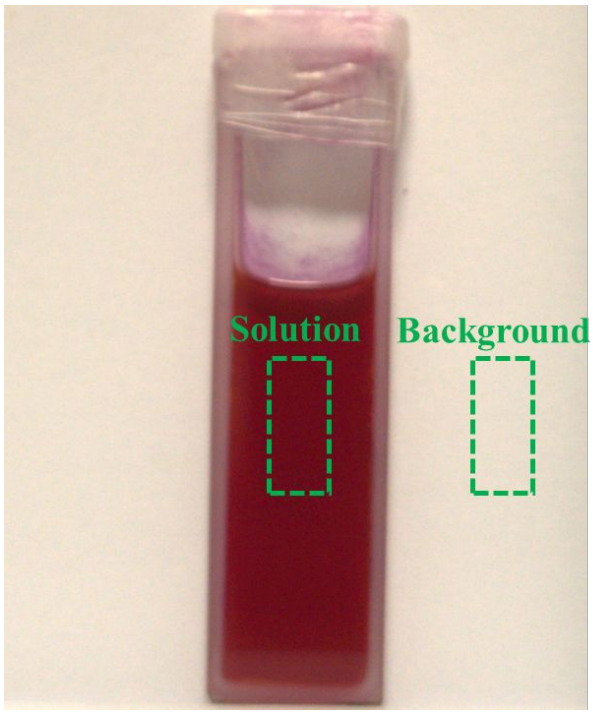

Figure S7. The region for the solution color and the background color.