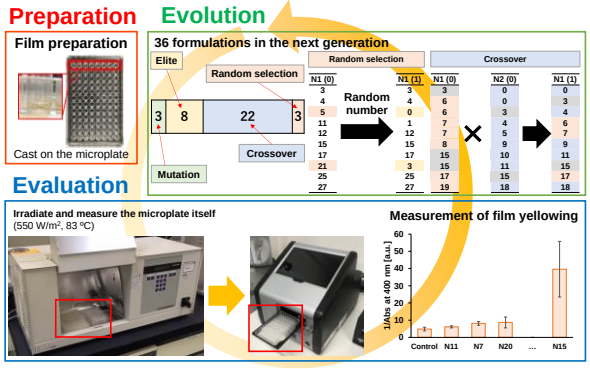
Design of Stabilizer Formulations for Yellowing Inhibition of Polymeric Materials based on High-Throughput Experiments and Genetic Algorithm

([1]*Graduate School of Japan Advanced Institute of Science and Technology*) ○Ken Takimoto,[1] Toshiaki Taniike[1]

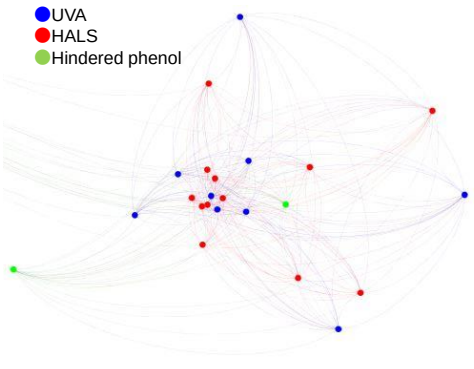
Keywords: Photo degradation; Synergism; Microplate method; Genetic algorithm; Combinatorial rules

Transparent plastics are used as alternatives to inorganic glass due to their advantages of transparency, processability, light weight, and low cost. On the other hand, their weaknesses are low scratch resistance and heat resistance, as well as their susceptibility to yellowing. In particular, yellowing due to outdoor exposure directly damages the high transparency, so its inhibition for a long term is highly desired. This problem is exclusively addressed by the addition of stabilizers. Although the basic strategy is to add a larger amount of stabilizers it with higher efficacy, there are limitations to increase the amount of the addition, so the development of synergistic formulations is essential.[1]

In this study, we developed a high-throughput experimental protocol, in order to efficiently explore stabilizer formulations regarding yellowing inhibition. By combining with a genetic algorithm, we conducted non-empirical exploration of stabilizer formulations that can inhibit yellowing of atactic polystyrene without increasing the addition amount. Cast films containing different formulations are prepared on 96 well-microplates, and the microplates were directly subjected to photo irradiation, which enabled simultaneous photo aging of 288 samples (3 microplates). Then, the yellowing of films was rapidly determined by subjecting the microplates after the irradiation to a microplate reader. Furthermore, the obtained big data corresponding to the 7 years of photo aging was analyzed in order to understand common features of high-performing formulations as well as rules of making synergistic combinations.



Stabilizer formulations exploration



Visualization of binary interactions

1) T. Taniike, T. Kitamura, K. Nakayama, K. Takimoto, N. Aratani, T. Wada, A. Thakur, P. Chammingkwan, *ACS Appl. Polym. Mater.*, **2020,** 2, 8, 3319–3326.