Constructing Negative Database: UV or IR Light Irradiation to Keratin with Sunscreens

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COLUMN ARTICLE

The sunscreen agent [1] accounts for 3% of the market value of cosmetics market in Japan (2015) and the shipment volume of 5,000 t is on the rise [2]. In addition to skin color correction and skin care, addition of safety, whitening and anti-aging is due to the effect of vitiligo problems. There is a demand for value. Normally, as a sunscreen agent, ultraviolet light scattering agent of titanium oxide or zinc oxide is used in combination with an organic ultraviolet ray absorbing agent. However, it reaches the dermal layer of the skin, and it is known skin aging, melanin pigmentation, active oxygen generation etc. There are few absorbents that can completely absorb light in the range of UVA (320 - 400 nm) wavelength area. So far, we have been aiming at practical application of ultraviolet absorption by a composite material of amino acid derivative Schiff base metal complex and titanium oxide [3,4]. In this way, we reported on a chiral Schiff base Zn(II) complex (ZnValH, Figure 1) absorb UVA light up to 400 nm and showed possibility of application of sunscreen cosmetics [3] and their less affinity to keratin protein by both experimental (Keratin from Wool purchased from TCI) and computational docking methods (with a GOLD program) [4].

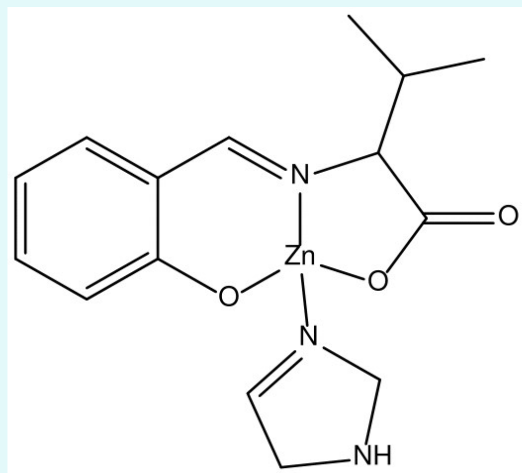

Figure 1: A chiral Schiff base Zn(II) complex (ZnValH) [1].

By the way, Infrared (IR) Free Electron Laser (FEL) Research Center at Tokyo University of Science (FEL-TUS) was established in 1998, where is the first facility in Japan for application researches utilizing free electron laser. The apparatus is a linac-type FEL, which was enabled to be downsized by adopting newly developed RF gun as an electron beam source. Irradiation of IR-FEL to a protein was reported to break 3-dimensional biomolecules selectively. As for hybrid materials of keratin protein with/without ZnValH, changes of molecular structures by irradiation of non-polarized UV light (Figure 2) and linearly polarized IR-FEL light (Figure 3) were observed for comparison.

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Figure 2 exhibits changes of IR spectra of keratin and ZnValH + keratin before and after non-polarized UV light (200 - 350 nm) irradiation for 10 minutes. As the cosmetic function stated, ZnValH could successfully protect damage of keratin due to UV light apparently, since little spectral changes concerning protein structural changes could be observed for ZnValH + keratin. On the other hand, Figure 3 exhibits changes of IR spectra of keratin and ZnValH + keratin before and after infrared free electron laser light (1652.7 cm^{-1}) irradiation for 80 min. Contrast to UV light, clearly spectral changes between before and after irradiation could not observed for both keratin and ZnValH + keratin samples. It should be noted that even only keratin sample had tolerance to strong IR-FEL light in this case. Under suitable conditions, dissociation of keratin aggregate could be done by IR-FEL light [5], therefore this case may be negative data in view of proving infrared light protection of ZnValH as well as dissociation of another keratin by IR-FEL light.

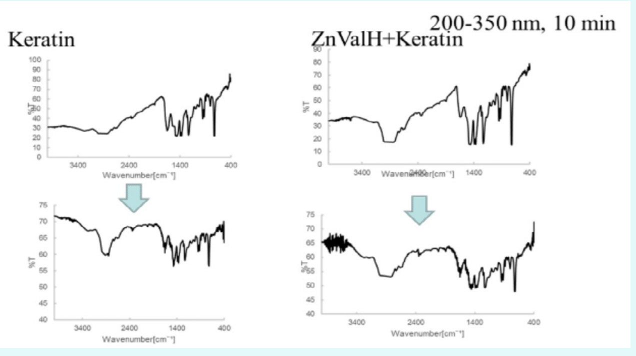

Figure 2: Changes of IR spectra of keratin (left) and ZnValH + keratin (right) before and after non-polarized UV light (200-350 nm) irradiation for 10 minutes.

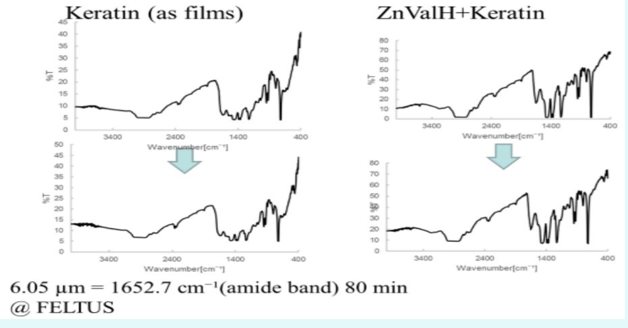

Figure 3: Changes of IR spectra of keratin (left) and ZnValH + keratin (right) before and after infrared free electron laser light (1652.7 cm^{-1}) irradiation for 80 min.

In the near future, AI in particular machine learning will be applied for drug design [6]. Big-data will be regarded as essential resources for molecular design, in which will only good data be useful surely? Database including negative data might be also constructed to prepare such a trend. However negative data (just like Figure 3) are not presented generally. Shall we construct such a negative database for AI in this journal?

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CONFLICT OF INTEREST

All authors declare that they have no conflict of interest.

BIBLIOGRAPHY

1. Baker LA., *et al*. "Photoprotection: extending lessons learned from studying natural sunscreens to the design of artificial sunscreen constituents". *Chemical Society Review* 46 (2017): 3770.
2. Akitsu T. "UVA absorbing materials of composite of chiral Schiff base Zn(II) complex and titanium(IV) oxide". *Chemical Economics* 63 (2016): 49.
3. Yoshida N., *et al*. "L-valine and salicylaldehyde derivative Schiff base Zn(II) complexes as UVA sunscreen". *Jacobs Journal of Inorganic Chemistry* 1 (2016): 6.
4. Akitsu T., *et al*. "Drug Design Based on Unfitted or Repulsive Metal Complexes". *EC Pharmacology and Toxicology* RCO.01 (2017): 01.
5. Kawasaki T., *et al*. "Irradiation Effect of Infrared Free Electron Laser on Dissociation of Keratin Aggregate". Memoirs of the SR Center Ritsumeikan University 17 (2015): 83.
6. Elazazy MS. "Factorial Design and Machine Learning Strategies: Impacts on Pharmaceutical Analysis". Spectroscopic Analyses - Developments and Applications (2017): 213.