

Design and mechanistic study of new photo-activated carbon monoxide releasing molecules

Marina Russo,[†] Peter Štacko,[†] Lenka Štackova,[†] Petr Klán^{†,*}

[†]Department of Chemistry and RECETOX, Masaryk University, Kamenice 5, 625 00, Brno, Czech Republic

Carbon monoxide (CO) is an endogenous signaling molecule that controls several physiological processes. Studies of the effects of CO have demonstrated its potential to produce a variety of beneficial health outcomes, including anti-inflammatory, anti-bacterial effects, and antiproliferative effects on cancer.¹ To circumvent the inherent toxicity of CO, light-activated CO-releasing molecules (photoCORMs) have emerged as an alternative for its administration. A good photoCORM should be stable under ambient conditions and soluble in aerobic aqueous environments, it should release CO using light at wavelengths that do not have the potential to impart cellular damage.

Understanding the mechanism of CO photoreleasing is a key step for designing new derivatives with improved properties for biological applications.

Following this approach, the detailed mechanism of the photochemically induced CO release from 3-hydroxy-2-phenyl-benzo[*g*]chromen-4-one (flavonol) has been studied,² in addition, a more detailed structure and reactivity investigation of CO-liberating photoreactions from this family of compounds are still in progress.

Using our knowledge from the previous studies on flavonols and cyanines,³ we envisioned that fusing those two chromophores can lead to a novel CO-releasable hybrid system that could serve as a general strategy for designing new classes of photoCORMs. We found that such hybrids liberate in principle two molecules of CO in high chemical yields upon activation with NIR light up to 820 nm and exhibit excellent uncaging cross-sections, which surpass the cutting edges by two orders of magnitude.⁴

A comprehensive mechanistic study of those chromophores will be presented in the presentation with the aim to reveal the properties of the productive excited states and emphasize and specify the role of oxygen in the CO production.

¹ Vítek L., Gbelcová H., Muchová L., Koničková R., Šuk J., Zadinova M., Knejzlík Z., Ahmad S., Fujisawa T., Ahmed A., Ruml T., *Digestive and Liver Disease* **2014**, 46 369-375.

² Russo M., Štacko P., Nachtigallová D., Klán P. *J. Org. Chem.* 2020, 85, 3527-3537.

³ Štacková L., Muchová E., Russo M., Slavíček P., Štacko P., Klán P. *J. Org. Chem.* 2020, 85, 9776-9790.

⁴ Štacková L., Russo M., Muchová L., Orel V., Vítek L., Štacko P., Klán P. *Chem. Eur. J.* 2020, 26, 13184-13190.