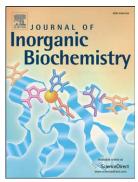
## Accepted Manuscript

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## Nanosized mesoporous metal–organic framework MIL-101 as a nanocarrier for photoactive hexamolybdenum cluster compounds

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*Keywords*: Molybdenum clusters / MIL-101 / Luminescence / Singlet oxygen / Hep-2 cells / Phototoxicity

## ABSTRACT

Inclusion compounds of photoluminescent hexamolybdenum cluster complexes in the chromium terephthalate metal-organic framework, MIL-101 (MIL, Matérial Institut Lavoisier) were successfully synthesized in two different ways and characterized by means of powder X-Ray diffraction, chemical analysis and nitrogen sorption. Some important functional properties of hexamolybdenum cluster complexes for biological and medical applications, in particular singlet oxygen generation ability, luminescence properties, cellular uptake behavior and cytotoxicity were studied. It was revealed that the inclusion compounds possessed significant singlet oxygen generation activity. The materials obtained showed a low cytotoxicity, thus allowing them to be used in living cells. Confocal microscopy of human larynx carcinoma (Hep-2) cells incubated with the inclusion compounds showed that MIL-101 performed as a nanocarrier adhering to the external cell membrane surface and releasing the cluster complexes which that penetrated into the cells. Moreover, photoinduced generation of reactive oxygen species (ROS) in Hep-2 cells incubated with inclusion compounds was demonstrated. The cluster supported on MIL-101 was shown to possess *in vivo* phototoxicity.

## 1 Introduction

Octahedral molybdenum cluster complexes with the general formula  $[{Mo_6X_8}L_6]^{2-}$  (X – Cl, Br or I; L – an organic or inorganic ligand) (see Fig. S1 for structure details) are gaining a lot of

† Equally contributed to the work reported.

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