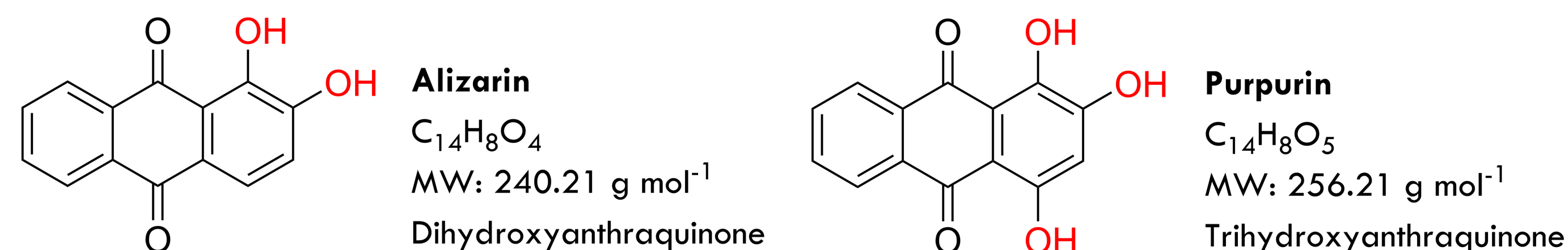


INTRODUCTION

- The Problem:** Ubiquitous discharge of toxic synthetic dyes (e.g., anthraquinone-based dyes like Alizarin and Purpurin) into aquatic ecosystems poses severe environmental and health risks.



Charge Profile: pH-dependent (Anionic at neutral/alkaline pH)

Fig. 1: The structures of alizarin and purpurin.

- The Components:**

MOFs: High surface area, porous, chemically tunable, but often difficult to process/recover as fine powders.

Biopolymers (CMC/PEG): Renewable, biodegradable, eco-compatible, providing excellent processable hydrogel matrices, prevent MOF leaching.

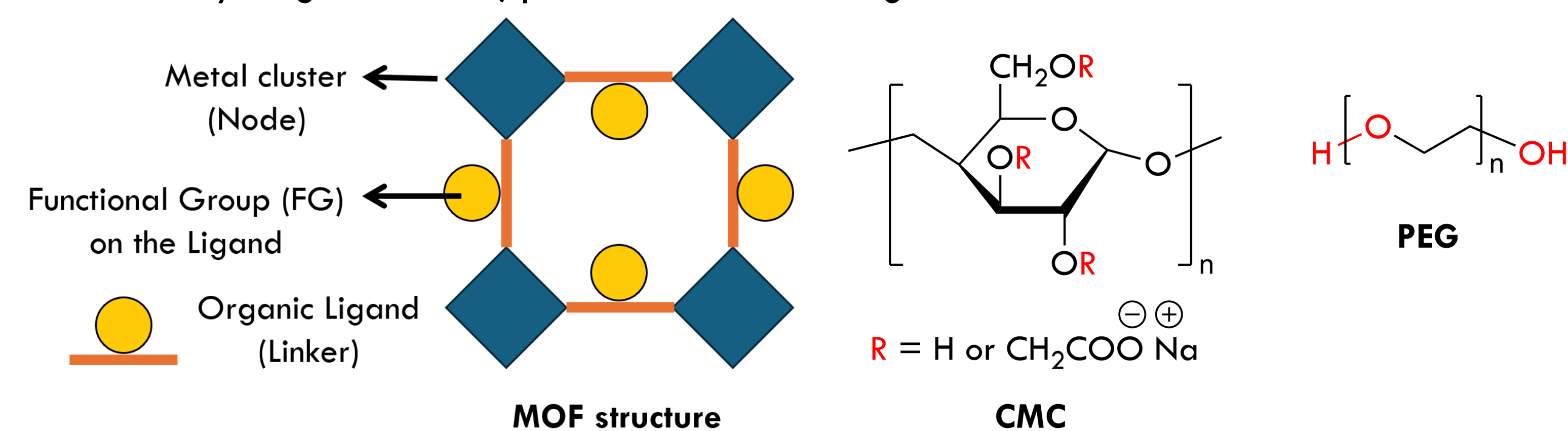


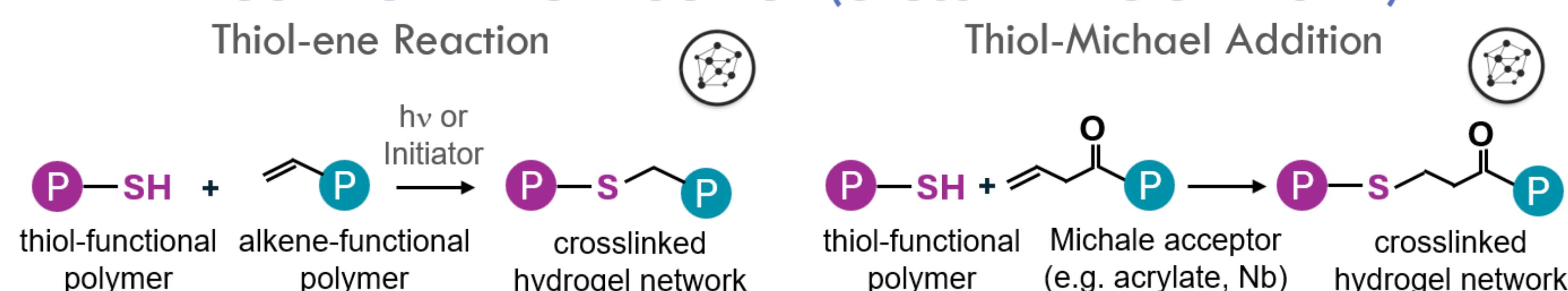
Fig. 2: The structures of MOF, CMC, and PEG.

- The Solution (The "Click" Approach):** Utilizing atom-economical, highly chemoselective click chemistry (Thiol–Maleimide and Thiol–Norbornene) to covalently link functionalized MOFs with polymer networks without toxic byproducts, aligning with green chemistry principles.

- Objectives:**

- **Phase 1 (Achieved):** Synthesize and characterize thiolated and ene-functionalized polymer backbones (CMC–Thiol, PEG–Mal, CMC–Nb).
- **Phase 2 (Current/Upcoming):** Covalently integrate water-stable, functionalized MOFs into the hydrogel matrix via orthogonal click reactions.
- **Phase 3 (Future):** Evaluate the composite hydrogels for the systematic batch adsorption and remediation of hazardous organic dyes.

HYDROGEL FORMATION TOOLBOX (CROSSLINKING CHEMISTRY)



(a)

MATERIALS DESIGN & SYNTHETIC STRATEGY

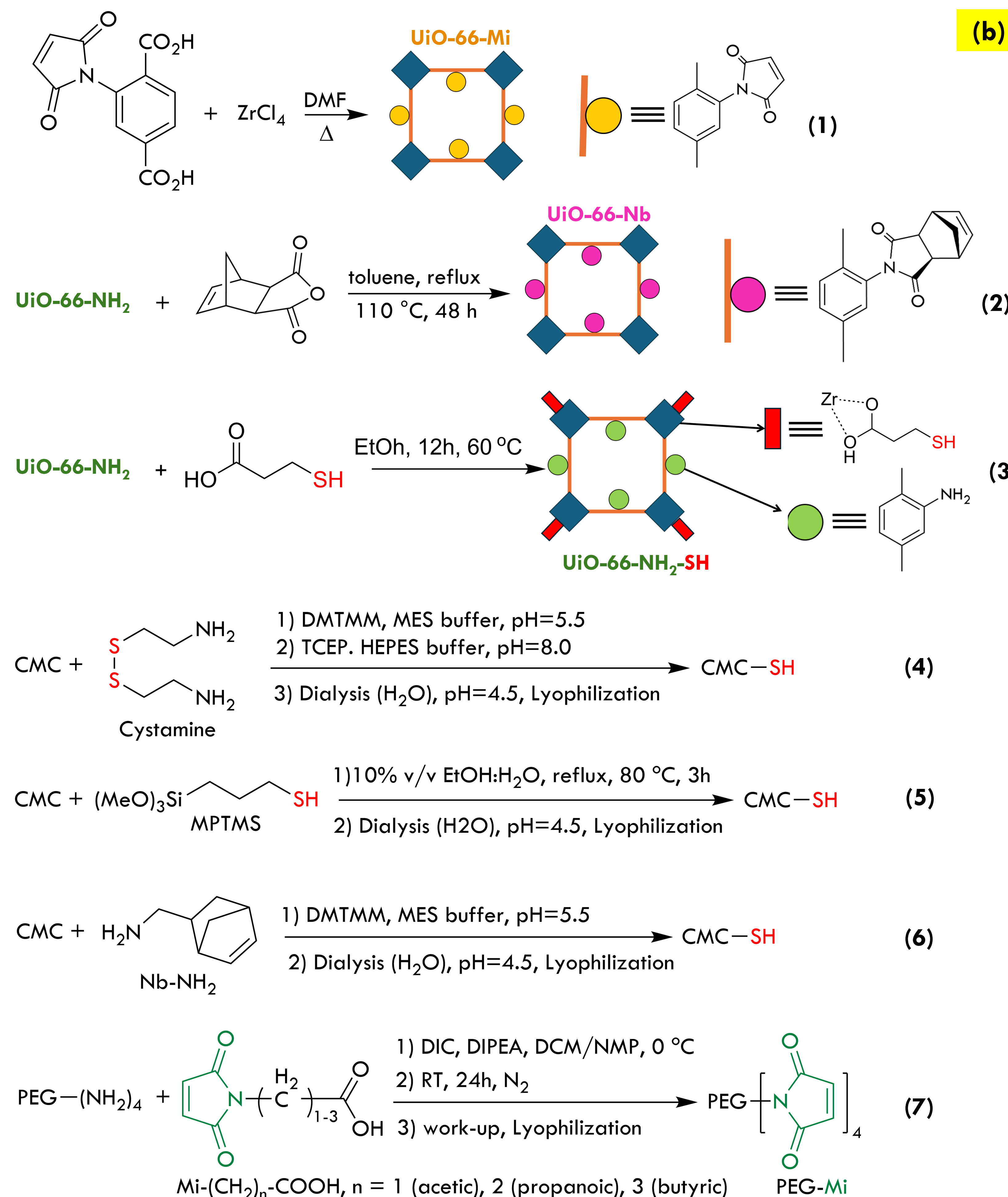
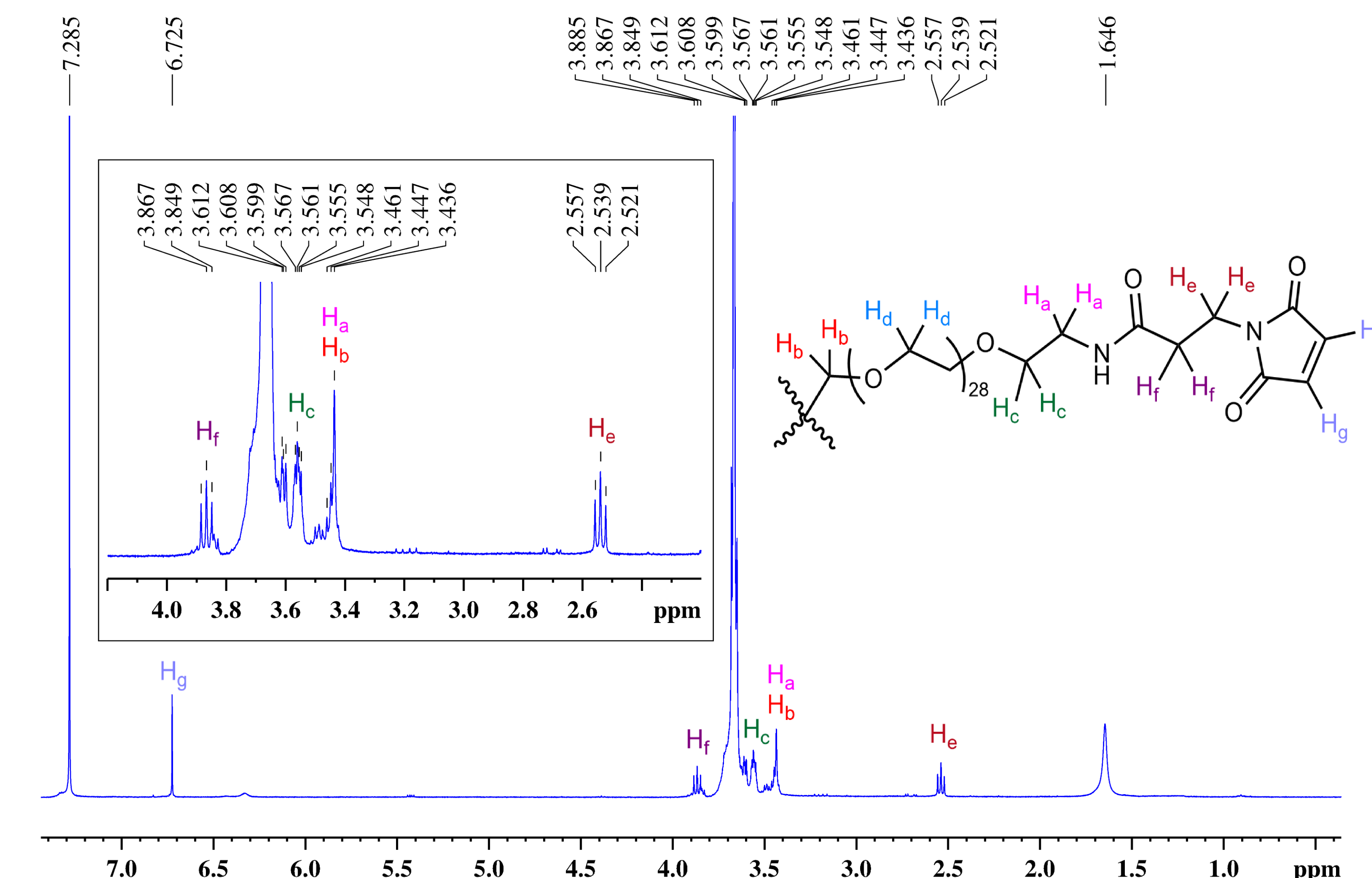


Fig. 3: (a) Thiol–ene and thiol–Michael addition reactions between thiol-containing molecules (–SH) and C=C-functionalized moieties such as norbornene (Nb) and maleimide (Mi). (b) Functionalized MOFs (1–3), modified CMC (4–6), and PEG (7) as precursors for click hydrogels.

RESULTS & DISCUSSION

Compounds **4–7** were successfully synthesized and confirmed by ¹H NMR, with compound **7** (PEG–Mi) shown here as a representative example. Also, **Ellman's test** confirmed ~15% and ~5% free –SH groups for compounds 5 and 4, respectively.


 Fig. 4: ¹H NMR of MOF–Mi (compound 1).

Future Work

- **Precursors and Hydrogels Synthesis:** Synthesis of MOFs (compounds 1–3). Execute the thiol–maleimide and thiol–norbornene click reactions to form the final MOF–hydrogel composite.
- **Characterization:** Confirm covalent network formation and MOF dispersion via FTIR and TEM.
- **Adsorption Optimization:** Conduct systematic batch studies for alizarin and purpurin removal, optimizing pH, adsorption time, dosage, and temperature.
- **Mechanistic Study:** Perform kinetic, isotherm, and thermodynamic analyses to elucidate binding energetics and process feasibility.
- **Sustainability Metrics:** Evaluate the reusability & recyclability of the adsorbent over multiple cycles.

Referecnes

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- He, Rui, et al. "Recent advances in multifaceted applications of MOF-based hydrogels." *Soft Sci.* 4.4 (2024): N-A.