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Sustainable Lithium Recovery: Overcoming Brine Complexity with Regenerable Biological Binders Designed via Deep Learning

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Lithium demand continues to accelerate, yet much of the remaining resource is hosted in geothermal and produced brines where high salinity, competing ions, variable pH, dissolved organics, and H_2S degrade the selectivity and longevity of conventional sorbents (1). We are developing an end-to-end platform that couples machine learning (ML)-guided protein binder design with experimental evolution to create regenerable binders optimized for brine-relevant chemistries. Candidate scaffolds and sequences are generated computationally and prioritized using structure prediction and confidence metrics, with the highest-confidence "parent" designs then expanded into focused mutational libraries that target predicted binding-site residues and are expressed via yeast surface display. To select binders that function under realistic matrices, we use a lithium-responsive readout integrated with cell sorting, iterating directed evolution (mutation/recombination) between sorting rounds. Selection stringency increases from simple electrolytes to synthetic brines spanning ionic strength and major-ion ratios, and finally to representative, field-collected Li-bearing sedimentary brines. Down-selected variants are evaluated for lithium selectivity against competing ions, robustness across pH and salinity ranges, and lithium recovery efficiency across regeneration cycles, yielding both brine-tolerant lithium-binding candidates and transferable design rules for the selective capture of ions like lithium in industrial geofluids.

(1) Seip, A. *et al.* (2021) Chemical Engineering Journal 426: 130713