

ELN: Chemical AI Agent

The Chemical AI Agent (colloquial name TBD) in the ELN is a retrieval-augmented generative large language model. It is trained on over 10,000 research papers in the domains of chemistry and materials science. Only approved BioPACIFIC MIP users can ask questions to the agent.

The agent can be found in the bottom-right corner of any given ELN page. When expanded (Fig 1), users can submit their query to the agent. Upon receiving a response, users can submit a star rating, from 1-5 (5 being the best), evaluating the response (Fig 2). The agent will also return the top three paper titles and abstracts relevant in formulating the response. User evaluations and agent responses are stored in the BioPACIFIC MIP LIMS and are used to improve the model.



Fig 1. Expanded Chemical ChatBot window. Users write their queries in the text field and click "Submit". Once the query is processed, the AI agent response is populated.



Fig 2. Evaluating AI Agent Responses. Users can rate, on a scale of 1-5, the usefulness/relevance of the response returned by the AI agent. Additionally, users can view the top three relevant paper titles and abstracts involved in generating the AI agent's response.

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