Message

From: Brennan, Amanda [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=BRENNAN, AMANDA]
Sent: 1/26/2022 5:31:27 PM
To: Stevens, Caroline [Stevens.Caroline@epa.gov]
Subject: RE: Chemical Transformation Simulator

Hi Caroline,

That's great news! I'm more than happy to chat further. I am available Friday, but maybe we can set something up for next week? We're meeting with researchers from the University of Nebraska to discuss sampling efforts and proposals early next week, and I think I would have more specifics after that meeting. If your calendar is up to date, I can schedule something for Tuesday or Wednesday?

Thanks,
Amanda

From: Stevens, Caroline <Stevens.Caroline@epa.gov>
Sent: Tuesday, January 25, 2022 5:22 PM
To: Brennan, Amanda <brennan.amanda@epa.gov>
Subject: RE: Chemical Transformation Simulator

Hi Amanda,

I'd definitely be interested in joining this effort. We've previously proposed that CTS could be used to help with chemical identification in NTA, so we'd welcome the opportunity to work on a case study application. The CTS web application offers a batch prediction mode, but it's limited to 10 chemicals right now. I could run longer chemical lists outside of the application, so that would probably work better for your purposes. It would be good to hear more about the project over a Teams meeting. My calendar is open Thursday after 1 pm or all day Friday—would you be available then?

Thanks,
Caroline

From: Brennan, Amanda <brennan.amanda@epa.gov>
Sent: Monday, January 24, 2022 9:56 AM
To: Stevens, Caroline <Stevens.Caroline@epa.gov>
Subject: Chemical Transformation Simulator

Hi Caroline,

Some work is being proposed for Ex. 5 Deliberative Process (DP) (Jon Sobus's Output) to use some of the transformation prediction tools you developed (CTS) to compare to non-targeted analysis results. We would use the tools to create suspect screening lists to help with identification of transformation products from parent pesticides in contaminated soils. We would be collaborating with researchers from the University of Nebraska who are currently monitoring contamination of pesticides and select transformation products in various matrices from a closed ethanol plant in Mead, Nebraska (AltEn). Jon Sobus suggested you would be a great contact for this proposed research. Do you have any suggestions on using these tools for the proposed research, or would you or anyone else involved in CTS be interested in joining this effort? I'm more than happy to chat more details via Teams.

Thanks,
Amanda

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