



Questions and Answers from the CRACK IT Challenge 43 Thyroid Tox

Launch webinar

- 1. The focus of the Challenge is on thyroid receptor mediated human endocrine disruption. Are tools for predicting disruption of thyroid hormone synthesis also in scope (e.g. by inhibiting key enzymes involved)?**

The proposal is looking specifically for chemicals interacting with the thyroid receptors (alpha and beta), but the tool could be flexible or adaptable for future use for other molecular initiating events (MIEs) that may occur in addition to a chemical binding to the alpha or beta receptors.

- 2. Is experimental data available for agrochemicals and petrochemicals and how do we get access to this data? Are there databases available?**

There is data for the validation of chemicals that are known to bind to the thyroid receptors available in the public domain that applicants could explore as a data mining exercise (e.g. data from literature, BindingDB, PDB, ECHA database and EPA databases). Sponsors may also be able to provide data for thyroid receptor-binding chemicals that could be used as a test set to validate the technology and/or as additional training data to build the models.

- 3. What applicability domains should be covered by the QSAR?**

The focus of applicability for the Challenge is for petrochemicals. However, the flexibility of the tool to be applied to other domains, such as agrochemicals, is desirable. This could include building a model with a broad applicability domain or it could simply entail providing a tool which enables users to re-train or update the model using their proprietary data.

- 4. Is the focus just on human or on other species too?**

The focus of this Challenge is for human thyroid receptor mediated toxicity.

- 5. Can you clarify the required access to the model, should the tool be made publicly available and different companies send their compounds to this resource?**

The tool should be made publicly accessible. Applicants should consider how the end-user would access the tool. For example, in the case of users generating novel and proprietary chemical structures, they may not be

able to use a tool that runs on an external server where chemical structures need to be submitted outside of a firewall.

6. Can PhD students be involved in the Challenge?

PhD students can be involved in the Challenge or contribute to the deliverables. However, CRACK IT funding cannot be used to support a PhD studentship.