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Preliminary Market Research – Questionnaire for cheminformatics providers

Introduction

European Chemicals Agency, ECHA, is inviting you to reply to this questionnaire by **18/07/2022 by 18.00 Helsinki time (EET)**, via e-mail addressed to the functional mailbox procurement@echa.europa.eu with the subject reference: Questionnaire for cheminformatics providers.

This questionnaire is meant for market consultation conducted by the Agency in order to better appreciate the current market offering on cheminformatics.

In accordance with the principles of non-discrimination, equal treatment and transparency, a Prior Information Notice for this contract has been published in the Official Journal of European Union including the invitation to participate in this market consultation.

Important: Before answering the questions, please read carefully the background information provided below.

ECHA will preserve the confidentiality of the information provided in response to this questionnaire. Your data will be processed in accordance with [ECHA's privacy rules](#).

1. General Information

- The information included in this questionnaire is only indicative; it is meant to give context for the respondents to provide their answers, but does not commit or bind ECHA, i.e. with regard to any procurement launched by the Agency in the future.
- The responses do not bind the respondents in any way. The information to be collected through this questionnaire will not be considered by ECHA in the evaluation of request to participate or tenders submitted during an eventual procurement procedure launched by the Agency.
- The identity of the companies that will respond to this questionnaire will not be disclosed to any third party except the European Court of Auditors, the European Anti-Fraud Office or, for the processing of personal data, the European Data Protection Supervisor if requested for the performance of audits and checks.
- The responses to be provided in the free text fields of this questionnaire should be clear and standalone, i.e. without web links to documents or websites.
- No further interviews are planned to take place with the respondents. Therefore we kindly invite you to provide as many information as you feel is relevant for ECHA to assess best the market situation.

2. Background Information

To support our regulatory activities, ECHA relies on extensive cheminformatics capabilities. This entails the use of a cheminformatics library. Some examples are:

- to convert a chemical name into a chemical structure
- to check molecular structures for errors
- to correct molecular structures errors

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- to standardise molecular structures
- to persist molecular structures in a database
- to generate structural images
- to draw and edit structural images
- to perform substructure and other chemical structure pattern searching
- to search for structurally similar substances and cluster substances based on similarity

As ECHA wants to ensure it makes the best use of the products and services available on the market, ECHA is reviewing its current cheminformatics capabilities.

The aims of this market survey are to:

- Validate the availability of offerings on the market for any of the cheminformatics functionalities
- Investigate both proprietary software and open-source offerings that can cover some or all functionality listed above (solutions that include customisation and extensions to cover ECHA's use cases are also considered.)
- Ensure that a potential call for tender is sufficiently attractive to the market players
- More specifically help ECHA in
 - Identifying the types of offerings that could cover ECHA needs
 - Choosing an approach to cheminformatics product and services implementations
 - Budgeting for the procurement of cheminformatics services

3. Questions

1. What exactly is the service offering of your organisation related to cheminformatics (e.g., provision of products or services, product or service support, consultancy services)? Please provide a detailed description of the products, services and capabilities offered.
2. What is the pricing of this offering? Please provide more details regarding the cost structure (e.g., price for 100 – 1000 licenses; full assignment of IPR).
3. What previous experience do you have with
 - a. Providing cheminformatics products/services
 - b. Working with public entities
 - c. Ability to offer customised or completely tailored solutions/deliverables
 - d. Different types of intellectual property rights (IPR) arrangements (e.g., IPR licencing; full or partial assignment of IPR to customer in the deliverable/product or customisation)
4. What timeline should be considered for your organisation to provide some or all of the products/services mentioned in the previous section? Are there any prerequisites before you can start providing products/services (e.g., software, system and connectivity requirements)?
5. What is your level of interest in submitting an offer should ECHA decide to send out a call for tenders for some cheminformatics products/services?
6. Please explain your roadmap and future plans for your cheminformatics product or service offering, i.e., how long do you intend to maintain it, how might it evolve

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(e.g. products/services at their end of life or under major upgrades), and how many staff do you expect to have allocated to it in the coming years?

7. Any other feedback/remarks