OpenTox: Questions for Use Cases: Summary of Responses

1a. What type of institution do you represent?

Industry	☐	7
Government	☐	0
Academia	☐	0
Name of Institution *(optional)*		

1b. What is the institution's main business?

Food industry	☐	0
Pharma industry	☐	2
Suppliers of industrial chemicals	☐	1
Other…		4

(type in the gray box)

2. For what purpose do you need to predict/estimate toxicity of chemicals?
(check all that apply)

early candidate screening	☐	5
high throughput screening	☐	1
regulatory submissions,	☐	5
research (toxicological mechanisms...),	☐	5
risk assessment,	☐	3
prioritisation of biological tests	☐	5
Other…		1

(type in the gray box)

3. Who does the prediction measurement/estimation?

trained toxicologist	☐	5
bioinformatician	☐	0
lab technician	☐	1
computational chemist/modeler	☐	3
Other…		

(type in the gray box)

4. How are toxicity data obtained currently?

experimental animal tests	☐	5
QSAR	☐	4
read across	☐	4
Other…		3

(type in the gray box)

5. What methods does your institution use?

Experimental testing	☐	5
TopKat	☐	1
Derek	☐	3
ADAPT	☐	1
Codessa	☐	0
Other…		4

(type in the gray box)

6. What level of detail do you need for individual predictions?

just active/inactive predictions   ☐   3
detailed information how the prediction was obtained,   ☐   5
   please explain…   5
      (type in the gray box)

7. For which types of compounds would you use a program such as OpenTox?

pharmaceuticals   ☐   2
industrial chemicals   ☐   4
cosmetics   ☐   2
food additives   ☐   1
Other…   3
      (type in the gray box)

8. What are the most important endpoints?

please describe the purpose e.g. a regulatory endpoint (please specify which one), human adverse effects (which one, do you have human data, what would be suitable animal/in vitro models) for general risk assessment, ecotoxicological effects

      (type in the gray box)   (6) see details

9. Quantitative predictions?

Yes/No decisions are sufficient   ☐   3
Quantitative predictions are needed   ☐   6

Comments: 5
      (type in the gray box)

10. Types of end-points needed

Single endpoints   ☐   4
Activity profiles   ☐   4

Comments: 4
      (type in the gray box)

11. Do you need to be able to create your own prediction models

Yes ☐   7   No ☐   0

If yes, do you have a preference for certain methods or algorithms?   4
      (type in the gray box)

12. Maximum number of compounds processed per day/week/month

         per   *(type in the gray box)*   3 per month - 1 million per week

Typical number of compounds processed: per   *(type in the gray box)*

13. Preferred computer platform(s) for (Q)SAR etc. (if applicable)

Linux	☐	2
Windows desktop	☐	5
Macintosh desktop	☐	0
Windows laptop	☐	3
Macintosh laptop	☐	0
Other…		0

(type in the gray box)

14. Any restrictions from corporate IT policies

No corporate IT restrictions	☐	2
Must be via client-server on corporate intranet	☐	4
Must be standalone and not send data over the internet	☐	2
Other…		3

(type in the gray box)

15. What level of in-house experience in the use and application of QSAR tools is available?

none	☐	0
limited	☐	0
moderate	☐	5
expert	☐	4

Please explain with examples... 4
(type in the gray box)

16. What level of in-house experience in the development of QSAR models is available?

none	☐	0
limited	☐	2
moderate	☐	1
expert	☐	3

Please explain with examples... 3
(type in the gray box)

17. What do see as the benefits and disadvantages of QSAR methods for toxicity assessment (please list)

Benefits/advantages....   5
(type in the gray box)

Disadvantages....   5
(type in the gray box)

18. What do see as the benefits and disadvantages of other non-testing methods for toxicity assessment (please list)

Benefits/advantages....   2
(type in the gray box)

Disadvantages....   1
(type in the gray box)

19. What do see as the benefits and disadvantages of experimental testing methods for toxicity assessment (please list)

Benefits/advantages....   4
(type in the gray box)

Disadvantages....   4
(type in the gray box)

20. What features/functionality/culture would be necessary to encourage wider use of QSAR for toxicity assessment

please list and explain...
(type in the gray box)   5

21. Which workflow systems do you currently use (if any)?

None   ☐   0
Pipeline Pilot   ☐   1
Other…   *(type in the gray box)*   2

22. Which workflow systems would you wish to use with OpenTox?

None   ☐
Pipeline Pilot   ☐   2
Other…   *(type in the gray box)*   1

23. Which QSAR models and formats would you want to import into OpenTox?

Models: *(type in the gray box)*

Formats: 1

24. What features and capabilities in OpenTox (assuming you could specify them) would make you want to use OpenTox over your existing methods, or in conjunction with them?

Please specify: *(type in the gray box)*   0

Thank you very much for your help with this OpenTox questionnaire!