# Annex II – (Q)SAR prediction reporting format (QPRF) v.2.0

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| --- | --- | --- |
|  | **Element** | **Explanation** |
| 1. | **General information** | *Information about the compilation of the current QPRF is provided in this section.* |
| 1.1. | **Date of QPRF** | {{ general.date\_QPRF }} |
| 1.2. | **QPRF author and contact details** | {%p **if** general.authors %}  {%for i in general.authors %}  {{ i }}  {%endfor%}  {%p endif %} |
| 2. | **Substance** | *Information about the substance under analysis. Some substances might be associated to more than one structure. The information on the structure(s) used as input is expected in Section 5.1.* |
| 2.1. | **CAS number** | {{ substance.CAS }} |
| 2.2. | ***EC number*** | {{ substance.EC }} |
| 2.3. | **Other regulatory numerical identifiers** | {{ substance.other\_identifiers }} |
| 2.4. | **Chemical name** | {{ substance.IUPAC }} |
| 2.5. | **Structural formula** | {{ substance.structural\_formula }} |
| 2.6. | **Structural and composition information**     1. **SMILES** | {{ substance.SMILES }} |
|  | 1. **InChI** | {{ substance.InChI }} |
|  | 1. **Other structural representation** | {{ substance.other\_representation }} |
|  | 1. **Stereochemical features** | {{ substance.stereochemical }} |
|  | 1. **Composition information** | {{ substance.composition }} |
|  | **Comments on substance information** | {{ substance.comments }} |
| 3. | **Model and software** | *Information about the model and software used to make the prediction* |
| 3.1 | **Model**  **a. Model or submodel name** | {{ model.identifier }} |
|  | **b. Model version** | {{ model.version }} |
|  | 1. **Reference to QMRF** | {{ model.QMRF }} |
|  | **Comments on model** | {{ model.comments }} |
| 3.2 | **Software**  **a. Software name** | {{ model.software }} |
|  | **b. Software version** | {{ model.version }} |
|  | **c. Software reference** | {%p **if** model.reference %}  {%for i in model.reference %}  {{ i }}  {%endfor%}  {%p endif %} |
|  | **d.****Software availability** | {{ model.availability }} |
|  | **Comments on software** | {{ model.comments\_softwaremode }} |
| 4. | **Prediction** | *Information about the prediction of the model* |
| 4.1 | **a. Predicted Property** | 1. {{ prediction.property }} |
|  | **b. Test guideline covered** | 1. {{ prediction.test\_guidelines }} |
|  | **c. Dependent variable** | 1. {{ prediction.dependent\_variable }} |
|  | 1. **Comments on the predicted property** | {{ prediction.comments\_property }} |
| 4.2 | 1. **a. Predicted value** | 1. {{ prediction.value }} |
|  | 1. **b. Predicted value (comments)** | 1. {{ prediction.comments\_value }} |
|  | 1. **c. Unit** | 1. {{ prediction.unit }} |
|  | 1. **Comments on the predicted value** | 1. {{ prediction.comments }} |
| 5 | **Input** | *Information about the input used to generate the prediction. It should be detailed enough to allow reproducibility of the prediction by others when using the same model and software.* |
| 5.1 | 1. **Input structure** | {{ input.structure }} |
|  | 1. **Stereochemical features** | {{ input.stereochemistry }} |
|  | 1. **Tautomerism** | {{ input.tautomerism }} |
|  | **Comments on the input structure** | {{ input.comments }} |
| 5.2 | **Descriptors** | {{ input.descriptors }} |
|  | **Comments on descriptors** | {{ input.comment\_descriptors }} |
| 5.3 | **Model and/or software settings** | {{ input.model }} |
|  | **Comments on settings** | {{ input.comment\_model }} |
| 6 | **Applicability domain (AD) and limitations** | *Information about how the substance relates to the AD as defined by the model developers and any other documented limitations. Any other reliability considerations can be reported in Section 7.* |
| 6.1 | **Applicability domain (AD) and limitations** | {{ ad.description }} |
|  | 1. **AD assessment** | {{ ad.assessment }} |
|  | 1. **AD assessment justification** | {{ ad.value }} |
|  | 1. **Any other limitation** | {{ ad.other }} |
|  | **Comments on AD** | {{ ad.comments }} |
| 7 | **Reliability assessment** | *Information about reliability of the prediction beyond the AD as defined by the model developers.* |
| 7.1 | **Reproducibility** | {{ reliability.reproducibility }} |
|  | **Comments on reproducibility** | {{ reliability.comments\_reproducibility }} |
| 7.2 | **Overall performance of the model** | {{ reliability.performance }} |
| 7.3 | **Additional reliability aspects based on the training set** | *Discuss whether the input structure is covered by the training set in terms of:* |
|  | 1. **Descriptor space** | {{ reliability.descriptor }} |
|  | 1. **Structural fragment space** | {{ reliability.fragment }} |
|  | 1. **Response space** | {{ reliability.response }} |
|  | 1. **Mechanism considerations** | {{ reliability.mechanism }} |
|  | 1. **Metabolic considerations** | {{ reliability.metabolism }} |
|  | **Comments on additional reliability aspects** | {{ reliability.comments }} |
| 7.4 | **Analogues** | *List the structural and/or mechanistic analogues with associated experimental data that can be used to support the reliability of the prediction. For each analogue indicate:* |
|  | 1. **Identifiers** | {{ analogues.smiles }} |
|  | 1. **Source of the analogue** | {{ analogues.source }} |
|  | 1. **Experimental value for the property of interest** | {{ "%0.2f" | format( analogues.value | float) }} |
|  | 1. **Reference for experimental value** | {{ analogues.reference }} |
|  | 1. **Predicted value for the property of interest** | {{ "%0.2f" | format( analogues.predicted\_value | float) }} |
|  | 1. **Accuracy of the prediction** | {{ analogues.accuracy }} |
|  | 1. **Comments on similarity** | {{ analogues.similarity }} |
|  | **Considerations on analogues** | {{ analogues.considerations }} |
|  | **Comments on analogues** | {{ analogues.comments }} |
| 7.5 | **Other reliable information on the property** | {{ reliability.property }} |
| 7.6 | **Conclusion on reliability** | {{ reliability.conclusion }} |
| 8 | **Purpose of use (for regulatory applications)** | *This information aims to facilitate considerations about the adequacy of the (Q)SAR prediction or the result derived from multiple predictions for a specific regulatory use* |
| 8.1. | **Regulatory purpose** | {{ purpose.purpose }} |
| 8.2. | **Approach for regulatory interpretation of the prediction or result derived from multiple predictions**: | {{ purpose.approach }} |
| 8.3. | **Regulatory interpretation of the result** | {{ purpose.interpretation }} |
| 8.4 | **Uncertainty** | {{ purpose.uncertainty }} |
| 8.5. | **Conclusion** | {{ purpose.conclusion }} |

Further, a mapping with between field numbers in QPRF v.2.0 and QPRF format v.1.1 in ECHA Guidance on information requirements and chemical safety assessment Chapter R6[[1]](#footnote-1) is provided.

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| --- | --- | --- |
| **QPRF mapping** | **QPRF v2.0** | **QPRF v.1.1** |
| **Administrative information** | 1 | 2 |
| Date of QPRF | 1.1 | 2.1 |
| QPRF author and contact details | 1.2 | 2.2 |
|  |  |  |
| **Substance** | 2 | 1 |
| CAS number | 2.1 | 1.1 |
| EC number | 2.2 | 1.2 |
| Other numerical identifiers | 2.3 | **NA** |
| Chemical name | 2.4 | 1.3 |
| Structural formula | 2.5 | 1.4 |
| Structural and composition information | 2.6 | 1.5 |
| SMILES | 2.6.a | 1.6.a |
| InChI | 2.6.b | 1.6.b |
| Other structural representation | 2.6.c | 1.6.c |
| Stereochemical features | 2.6.d | 1.6.d |
| Composition information | 2.6.e | **NA** |
| Comments on substance information | - | **NA** |
|  |  |  |
| **Model and software** | **3** |  |
| Model name | 3.1.a | 3.2.a |
| Version | 3.1.b | 3.2.b |
| Reference to QMRF | 3.1.c | 3.2.c |
| Comments on model | - | **NA** |
| Software implementation | 3.2.a | **NA** |
| Software name | 3.2.b | **NA** |
| Software version | 3.2.c | **NA** |
| Software reference | 3.2.d | **NA** |
| Software availability | 3.2.e | **NA** |
| Comments on model and software | - | **NA** |
|  |  |  |
| **Prediction** | 4 |  |
| Property | 4.1.a | 3.1a |
| Test guideline(s) covered | 4.1.b | **NA** |
| Dependent variable | 4.1.c | 3.1b |
| Comments on predicted property | - | NA |
| Predicted value | 4.2.a | 3.2.d |
| Predicted value (comments) | 4.2.b | 3.2.e |
| Unit | 4.2.c | **NA** |
| Comments on predicted value | - | **NA** |
|  |  |  |
| **Input** | 5 |  |
| Input structure | 5.1 |  |
| Input structure | 5.1.a | 3.2.f |
| Stereochemical features | 5.1.b | 1.5.d |
| Tautomerism | 5.1.c | **NA** |
| Comments on the input structure | - | **NA** |
| Descriptor value and unit | 5.2.a | 3.2.g |
| Descriptor measured or calculated | 5.2.b | 3.2.g |
| Descriptor reference | 5.2.c | 3.2.g |
| Comments on descriptors | - | **NA** |
| User defined settings | 5.3 | **NA** |
| Comments on settings | - | **NA** |
|  |  |  |
| **Applicability domain and limitations** | 6 |  |
| AD assessment | 6.1.a | 3.3a |
| AD assessment methodology | 6.1.b | 3.3a |
| Any other limitations | 6.1.c | 3.3a |
| Comments on AD | - | 3.3a |
|  |  |  |
| **Reliability assessment** | 7 |  |
| Reproducibility | 7.1 | **NA** |
| Comments on reproducibility | - | **NA** |
| Overall performance of the model | 7.2 | **NA** |
| Descriptor space | 7.3.a | 3.3.a.i |
| Structural space | 7.3.b | 3.3.a.ii |
| Response space | 7.3.c | **NA** |
| Mechanistic considerations | 7.3.d | 3.3.a.iii - 3.5 |
| Metabolic considerations | 7.3.e | 3.3.a.iv |
| Comments on additional reliability | - | **NA** |
| Analogues: identifiers | 7.4.a | 3.3.b - c |
| Analogues: source | 7.4.b | 3.3.b - c |
| Analogues: Experimental value for the property of interest | 7.4.c | 3.3.b - c |
| Analogues: Reference for experimental value | 7.4.d | 3.3.b - c |
| Analogues: predicted value for the property of interest | 7.4.e | 3.3.b - c |
| Analogues: Accuracy of the prediction | 7.4.f | 3.3.b - c |
| Analogues: comments on similarity | 7.4.g | 3.3.b - c |
| Considerations on structural analogues | 7.4 | 3.3.b - c |
| Comments on analogues | - | 3.3.b - c |
| Other reliable information on the property | 7.5 | **NA** |
| Conclusion on reliability | 7.6 | **NA** |
|  |  |  |
| **Purpose of use (for regulatory applications)** | 8 |  |
| Regulatory purpose | 8.1 | 4.1 |
| Approach for regulatory interpretation of the prediction or result derived from multiple predictions | 8.2 | 4.2 |
| Regulatory outcome | 8.3 | 4.3 |
| Uncertainty | 8.4 | 3.4 |
| Conclusion | 8.5 | 4.4 |

1. https://echa.europa.eu/documents/10162/13632/information\_requirements\_r6\_en.pdf/77f49f81-b76d-40ab-8513-4f3a533b6ac9 [↑](#footnote-ref-1)