Table S1. Organisation of criteria from Cronin et al. (2019) scheme into hallmarks, or key characteristics, of in silico models and / or predictions.

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| Criterion Number | Description |
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| Hallmark 1: *Data* | |
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| 1.2a | Quality of individual studies in the data set |
| 1.2b | Consistency of the data set including comparability of data, homogeneity of protocols etc. |
| 1.2c | Checking of toxicological data |
| 1.2d | Error associated with biological data |
| 1.2e | (if required) Units of concentration known, stated and appropriate for use |
| 1.2f | (If appropriate) Nominal or measured concentrations |
| 1.2g | Taking internal exposure into account |
| 1.4a | Data set is complete e.g. structures, descriptors, properties etc. |
| 1.4b | Data set has appropriate variation in potency (quantitative) or balance of actives vs inactives (qualitative) |
| 1.4c | Selection of training set data for modelling |
| 1.4d | Training set homogeneity across chemical space |
| 1.4e | Suitable training and test sets defined and utilised |
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| Hallmark 2: *Structures* | |
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| 1.1a | Accuracy of chemical structure |
| 1.1b | Assessment of significant impurities or mixtures |
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| Hallmark 3: *Descriptors* | |
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| 1.3a | Measurement of physico-chemical properties |
| 1.3b | Calculation of properties and 2-D descriptors |
| 1.3c | Calculation of 3-D descriptors |
| 1.3d | Software utilised |
| 1.3e | Definition of molecular fragments |
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| Hallmark 4: *Modelling* | |
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| 1.5a | How appropriate is the modelling approach for the endpoint and to deal with the complexity / non-linearity of the data |
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| Hallmark 5: *Performance* | |
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| 2.2a | Statement of statistical fit, performance and predictivity of model |
| 2.2b | Interpretation of statistical fit etc with respect to biological error (see Criterion 1.2d) |
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| Hallmark 6: *Mechanisms* | |
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| 2.3a | Chemical applicability domain of model |
| 2.3b | Mechanistic applicability domain of model |
| 2.3c | Biological applicability domain of model |
| 2.4a | Mechanistic justification |
| 2.4b | Presence / availability of other and supporting information |
| 2.4c | Relevance to descriptors to mechanism of action / AOP |
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| Hallmark 7: *Toxicokinetics* | |
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| 2.5a | Metabolism and / or effect of significant metabolites have been considered |
| 2.5b | Toxicokinetics have been addressed in the model |
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| Hallmark 8: *Description* | |
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| 2.1a | Documentation and reporting of the model and / or prediction |
| 2.1b | Data set is complete and described for the training / test sets |
| 2.1c | Transparency of the model |
| 3.1a | Reproducibility of the models |
| 3.1b | Reproducibility of the prediction |
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| Hallmark 9: *Usability* | |
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| 3.2a | Implementation of the model into software or a tool |
| 3.2b | Software accessibility |
| 3.2c | Software transparency |
| 3.2d | Relative cost |
| 3.2e | Sustainability |
| 3.2f | Maintenance and support |
| 3.2g | Intellectual Property |
| 3.2h | Ownership |
| 3.2i | Ethics |
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| Hallmark 10: *Relevance* | |
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| 3.3a | Heterogeneity and density of chemical space |
| 3.3b | Relevance of the predicted endpoint for the regulatory risk assessment purpose/protection goal |
| 3.3c | Adequacy of the prediction for stated purpose |
| 3.3d | Extrapolation and relevance to humans |
| 3.3.e | Extrapolation and relevance to environmental biota |