The reporting of READ-ACROSS as a dossier and QSAR data must be set out in the format below, or the elements can be addressed in a different stylistic manner but the main points regarding any QSAR or READ across should fall into the categories below.

Note to Chemical suppliers:- Please fill in sections 1-3 as **fully** as possible, please ensure that the sections are filled in using the notes in italics as a guide. You can overtype the details in the boxes but please leave the subheadings in place. If you cannot enter data for a particular point this needs to be explained. Please also note that QSAR model is not the name of the platform but depends on the data chosen and the algorithms used. The algorithm should come with an explanation of why it was selected and the mechanisms that it uses.

1.	**Substance** *This section is aimed at defining the substance for which the (Q)SAR prediction is made.*
1.1	**CAS number** :- *Report the CAS number*
1.2	**EC number**: - *Report the EC number*
1.3	**Chemical name**: *report the chemical name (IUPAC and CAS names)*
1.4	**Structural formula**: *report the structural formula.*
1.5	a. **Structure codes:** *Report available structural information for the substance, including the structure code used to run the model. If you used a SMILES or InChII code, report the code in the corresponding field below. If you have used any other format (e.g. mol file), please include the corresponding structural representation as supporting information.* b. *SMILES: Report the SMILES of the substance (indicate if this is the one used for the model prediction* c. *InChI: report the InChi code of the substance (indicate if this is the one used for the model prediction).* d. *Other structural representation: Indicate if another structural representation was used to generate the prediction. Indicate whether this information is included as supporting information. Example: "mol file used and included in the supporting information* e. *Stereochemical features: Indicate whether the substance is a stereo isomer and consequently have properties that depend on the orientation of its atoms in space. Identify the stereochemical features that may affect the reliability of predictions for the substance, e.g. cis-trans isomerism, chiral centres. Are these features encoded in the structural representations mentioned above?*
2.	**General Information** *General information about the compilation of the current QPRF is provided in this section*
2.1	**Date of QPRF**: *report the date of the compilation of the current QPRF: example January 2007.*
2.2	**QPRF author and contact details**: *report the contact details of the author of the*

	QPRF.	
3.	**Prediction**	
	The information provided in this section will help to facilitate considerations on the scientific validity of the model (as defined in the OECD Principles for validation of (Q)SAR models) and the reliability of the prediction. Detailed information on the model are stored in the corresponding QMRF which is devised to reflect as much as possible the OECD principles. Remember that the QMRF and the QPRF are complementary, and a QPRF should always be associated with a defined QMRF.	
3.1	**Endpoint (OECD Principle 1)**	
	f.	**Endpoint**: *define the endpoint for which the model provides predictions (this information should correspond to the information provided in the QMRF under fields 3.2 and 3.3) Example: "Nitrate radical degradation rate constant KNO_3"*
	g.	**Dependent variable**: *Report the dependent variable for which the model provides predictions including any transformation introduced for modelling purposes (note that this information should correspond to the information provided in the QMRF under field 3.5). example "-log (KNO_3)".*
3.2	**Algorithm (OECD Principle 2)**	
	a.	**Model or submodel name**: *Identify the model used to make the prediction and possibly report its name as stored in the corresponding QMRF; in the QMRF the model name is reported in the field of the QSAR identifier. Examples: "BIOWIN for Biodegradation"; TOPKAT Skin irritation model". If applicable identify the specific submodel or algorithm applicable to the specific chemical examples "BIOWIN !"; TOPKAT Skin Irritation Acyclics (Acids, Amines, Esters) MOD v SEV Model"; "ECOSAR Esters model".*
	b.	**Model Version**: *Identify, where relevant, the version number and/ or date of the model and submodel.*
	c.	**Reference to QMRF**: *Provide relevant, information about the QMRF that stores information about the model used to make the prediction. Possible useful pieces of information are: availability, source, reference number (if any) of the QMRF. Examples: "The corresponding QMRF named BIOWIN 1 for Biodegradation has been downloaded from the JRC QSAR model Database"; "The corresponding QMRF named 'TOPKAT Skin Irritation Acyclics (Acids, amines, esters) MOD v SEV Model' has been newly compiled.*
	d.	**Predicted value (model result)**: *Report the predicted value (including units) obtained from the application of the model to the query chemical. For an expert system such as Derek for Windows, report the alert triggered together with the reasoning. Example: "aromatic amine – mutagenicity plausible".*
	e.	**Predicted value (comments):** *If the result is qualitative (e.g. yes/ no) or semi-quantitative (e.g. Low/ medium/ high), explain the cut-off values that were used as a basis for classification. In reporting the predicted value, pay attention to the transformations (e.g. if the prediction is made in log units, apply anti-logarithm function).*
	f.	**Input for prediction**: *Specify what kind of input was used to generate the prediction (SMILES, mol file, graphical interface etc). Please provide the structure code used to generate the prediction (unless already provided in section 1.5).*
	g.	**Descriptor values**: *Where appropriate, report the values (experimental or calculated data) for numerical descriptors and indicate which values were*

	used for making the prediction.

3.3	**Applicability domain (OECD principle 3)**
	
	   a. **Domains**: *Discuss whether the query chemical falls in the applicability domain of the model as defined in the QMRF (Section 5 of the QMRF, defining the applicability domain – OECD principle 3). If additional software/methods were used to assess the applicability domain then they should also be documented in this section. Include a discussion about:*
	
	      i) *descriptor domain*
	
	      ii) *Structural fragment domain (e.g. discuss whether the chemical is known or considered to act according to the mechanism of action associated with the used model.*
	
	      iii) *Mechanism domain (discuss whether the chemical is known or considered to act according to the mechanism of action associated with the used model)*
	
	      iv) *Metabolic domain, if relevant*
	
	   b) **Structural analogues**: *List the structural analogues that are present in the training or test sets, or accessible from other sources (in this case you should explain how the structural analogue was retrieved and why they are considered analogues). For each analogue report the CAS number, the structural formula, the SMILES code, and the source (e.g. training set, test set or other source). For an expert system (like Derek for Windows or TOPKAT), the example compounds or structurally related analogues with their experimental data should be provided.*
	
	   c) **Considerations** *on the structural analogues: Discuss how predicted and experimental data for analogues support the prediction of the chemical under consideration.*

3.4	**The uncertainty of the prediction (OECD principle 4)** *If possible, comment on the uncertainty of the prediction for this chemical, taking into account relevant information (e.g. variability of the experimental results).*
3.5	**The chemical and biological mechanisms according to the model underpinning the predicted result (OECD principle 5).** *Discuss the mechanistic interpretation of the model predictions for this specific chemical. For an expert system based on structural alerts (e.g. Derek for Windows, Oncologic™) the rationale for the structural alert should be provided.*
FOLLOWING SECTIONS TO BE FILLED IN BY REGULATOR ONLY	
4.	**Adequacy** (optional in other cases of QSAR but not for regulator purposes) *The information provided in this section might be useful, depending on the reporting needs and formats of the regulatory framework of interest. This information aims to facilitate considerations about the adequacy of the (Q)SAR prediction (result). A (Q)SAR prediction may or may not be considered adequate ("fit for purpose") depending on whether the prediction is sufficiently reliable and relevant in relation to the particular regulatory purpose. The adequacy of the prediction also depends on the availability of the other information, and is determined in a weight-of-evidence assessment.*
4.1	**Regulatory purpose**: *Explain the regulatory purpose for which the prediction described in section 3 is being used.*
4.2	**Approach for regulatory interpretation of the model result**: *Describe how the*

	predicted result is going to be interpreted in the light of the specific regulatory purpose (e.g. by applying an algorithm or regulatory criteria). This may involve the need to convert the units of the dependent variable (e.g. from log molar units to mg/l). It may also involve the application of another algorithm, an assessment factor, or regulatory criteria, and the use or consideration of additional information in a weight-of-evidence assessment.
4.3	**Outcome**: *Report the interpretation of the model result in relation to the defined regulatory purpose.*
4.4	**Conclusion**: *Provide an assessment of whether the final result is considered adequate for a regulatory conclusion, or whether additional information is required (and, if so, what this additional information should be).* Please add any additional supporting data at this point.