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Task 3.6 Development of multi-model approaches (Deliverable 3.6)

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Corresponding authors of document: Paola Gramatica[1], Ester Papa[1], Simona Kovarich[1], Willie Peijnenburg[2], Magnus Ramberg[3], Tomas Öberg [4], Ullrika Sahlin[4], Igor Tetko[5], Nina Jeliazkova[6]

1. QSAR Research Unit in Environmental Chemistry and Ecotoxicology, University of Insubria, Via J.H. Dunant 3 - 21100 Varese, Italy (paola.gramatica@uninsubria.it)
2. RIVM Laboratory for Ecological Risk Assessment - P.O. Box 1 3720 BA Bilthoven, The Netherlands (marga.deventer@rivm.nl, willie.peijnenburg@rivm.nl)
3. IVL Swedish Environmental Research Institute, Box 210 60, SE- 100 31 Stockholm, Sweden
4. Linnaeus University, School of Natural Sciences, 391 82 Kalmar, Sweden.
5. Helmholtz Zentrum Muenchen - German Research Center for Environmental Health, Ingolstaedter Landstrasse 1, D-85764 Neuherberg, Germany
6. IdeaConsult Ltd., 4 A.Kanchev str. Sofia 1000, Bulgaria

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Work package 3. Development and validation of QSARs

Work Package Leader: Paola Gramatica (Partner 3: University of Insubria)

Partners involved in WP3:

- Partner 3 (WP Leader): University of Insubria (UI): Paola Gramatica, Ester Papa, Simona Kovarich, Barun Bhhatarai, Partha Pratim Roy, Stefano Cassani.
- Partner 4: IVL Swedish Environmental Research Institute: Magnus Rahmberg, Sara Nilsson, Håkan Fridén
- Partner 5: Linnaeus University (LnU): Tomas Öberg, Tao Liu, Ullrika Sahlin
- Partner 6: Helmholtz Zentrum Muenchen (HMGU): Igor V. Tetko, Stefan Brandmaier, Wolfram Teetz, Iurii Sushko, Pantelis Sopasakis
- Partner 7: Ideaconsult Ltd.: Nina Jeliazkova, Nikolay Kochev, Ognyan Pukalov

Task 3.6 Development of multi-model approaches

Summary

The aim of this task was to develop multi-model approaches and consensus models in order to expand the chemical domain of QSAR models while keeping the higher accuracy of more specific models. An investigation of several different approaches (such as robustness, individual model's domain, chemical space diversity and analysis in the property-based space) was planned for selecting and/or weighting the individual models to create a final consensus model.

The present report provides a summary of all the consensus models developed within the CADASTER Project, as a collaborative activity between WP3 project partners, i.e University of Insubria (UI), Swedish Environmental Research Institute (IVL), Linnaeus University (LnU), Helmholtz Zentrum Muenchen (HMGU), and Ideaconsult Ltd (IDEA).

An overview of the new QSAR models specifically developed within the Project for the chemicals of the 4 CADASTER classes (i.e. Polybrominated diphenyl ethers (PBDEs) (extended to other Brominated Flame retardants (BFRs)), Perfluoroalkylated substances (PFCs) (extended to Poly-fluorinated compounds), Substitued musks/Fragrances, Triazoles/Benzo-triazoles (B)-TAZs)) is reported in Deliverable 3.5.

In brief, local models for several SIDS and non SIDS endpoints related to physico-chemical properties, toxicological and eco-toxicological effects were individually developed by different WP3 Partners for the

four chemical classes studied within CADASTER. The models were developed taking into account the OECD principles for validation and acceptability of QSARs for regulation purposes, paying particular attention to external validation and check of applicability domain.

The QSARs developed in the Project, have been documented in publications in international peer reviewed (ISI) journals and in meeting presentations. All QSARs are also uploaded in the CADASTER database (qspr-thesaurus) and the CADASTER website (http://www.cadaster.eu).

Different approaches and methodologies were applied by different WP3 Partners for the development and validation of the models. Finally, the consensus approach was used to combine the individual models developed for the same endpoint and chemical class, i.e. Melting Point and Boiling Point for PFCs, aquatic toxicity of (B)TAZs and biodegradation of fragrances. This procedure allowed arriving at better and, potentially, more reliable QSAR predictions.

The present report presents the consensus models developed for the melting and the boiling point of PFCs and the aquatic toxicity of (B)TAZs. These models were chosen for the consensus analysis because they are the only QSA(P)Rs developed on SIDS endpoints among the models created within the CADASTER project by all the WP3 Partners. An additional consensus model for biodegradability of fragrances will be part of deliverable 3.7. As it was discussed in the last CADASTER Meeting in Madrid, experimental data for the biodegradation of fragrances became available after the start of the modelling activity (task 3.5). This prevented the WP3 Partners to develop QSAR models for this endpoint for the scheduled deadline (month 36). At the moment classification models for ready biodegradability of fragrances are under development by several WP3 Partners and will be reported in Deliverable 3.7, together with Consensus predictions and external validation.

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Deliverable 3.6 Multi-model approaches for better QSAR predictions (models and report)

Paola Gramatica[1], Ester Papa[1], Simona Kovarich[1], Stefano Cassani[1], Magnus Rahmberg[2], Sara Nilsson[2], Tomas Öberg [3], Ullrika Sahlin[3], Igor Tetko[4], Stefan Brandmaier[4], Nina Jeliazkova[5], Nikolay Kochev [6], Ognyan Pukalov[6]

1. QSAR Research Unit in Environmental Chemistry and Ecotoxicology, University of Insubria, Via J.H. Dunant 3 - 21100 Varese, Italy
2. IVL Swedish Environmental Research Institute, Box 210 60, SE- 100 31 Stockholm, Sweden
3. Linnaeus University, School of Natural Sciences, 391 82 Kalmar, Sweden.
4. Helmholtz Zentrum Muenchen - German Research Center for Environmental Health, Ingolstaedter Landstrasse 1, D-85764 Neuherberg, Germany
5. IdeaConsult Ltd., 4 A.Kanchev str. Sofia 1000, Bulgaria
6. University of Plovdiv, Department of Analytical Chemistry and Computer Chemistry Plovdiv, Bulgaria

1 Consensus models for Perfluorinated compounds (PFCs): physico-chemical properties

Per- and polyfluorinated compounds (PFCs) are a class of synthetic substances widely used in different materials as waterproof fabrics, food packaging, non-adhesives, fire-fighting foams, paints, etc.. The amphiphylic nature of some PFCs, characterized by a hydrophobic fluorinated alkyl chain and a polar terminal group (such as carboxylic and sulfonic acids), gives them a great stability, thermal and stress resistance, and excellent surfactant properties.

PFCs studied under the CADASTER Project include 382 chemicals, both linear and aromatic chemicals, with different carbon chain length, fluorination degree (per- and polyfluorinated compounds) and functional groups (carboxylates, sulfonates, sulfonamides, alcohols, etc.).

The majority of these compounds were included in the ECHA pre-registration list. This highlights the importance of providing QSAR predictions for key endpoints that could be useful for the registration of chemicals under REACH.

Within the CADASTER Project, WP3 Partners developed local QSPR models for the prediction of Melting Point (MP) and Boiling Point (BP) of per- and poly-fluorinated chemicals (PFCs). MP and BP are important physicochemical properties that indirectly affect the solubility, and hence the transport, distribution and environmental fate of these compounds.

Individual models based on various molecular descriptors (0D-2D Dragon descriptors, E-state descriptors and fragment based descriptors) were developed by the WP3 Partners UI, LnU, IDEA and HMGU by applying different modelling approaches, namely Multiple Linear Regression (MLR), Partial Least Squares Regression (PLSR) and Neural Network (NN). Consensus models were then derived by averaging the predictions obtained by all the models.

Details regarding data collection, modelling descriptors, model development, validation, and applicability domain are reported in the joint publication of Bhhatarai *et al.* 2011 [1] and will be summarized in the following paragraphs.

1.1 Melting Point

Experimental Dataset and splitting

Experimental data on the MP of 94 poly- and perfluorinated compounds were collected from the SRC-PhysProp database and literature (Trepka et al., Gajewski et al., Platonov et al.). The datasets were split (~50%), by applying two different splitting methods (self organizing maps (SOM) and random selection of compounds by arranging them in terms of increasing activity), into a training set, used for the development of the model, and a prediction set, used for model external validation.

An additional blind external validation set of 15 PFCs was then collected from the PERFORCE dataset ("EV-set") [2], which was used to assess the models' performance in prediction.

Modeling approaches, molecular descriptors and applicability domain

A summary of the modeling approaches and molecular descriptors used by the different partners is provided in Table 1.

Table 1. Modelling approaches applied by WP3 Partners for the MP QSPR model of PFCs.

	UI	LnU	IDEA	HMGU
Molecular Descriptors	0D-2D Dragon descriptors	0D-2D Dragon descriptors	Fragment based descriptors	E-state descriptors
Descriptor selection	Genetic Algorithm	variable influence on projection (VIP)	Exhaustive isomorphism search of fragment against structure	Pearson Pairwise Correlation
Modelling Descriptors	4 descriptors: AAC, F02[C-F], C-013, RBF	37 descriptors at 3 components	3 descriptors: In^2W, W_{rel}^F, N_{HBDON}	87 indices

Algorithm	Multiple Linear Regression (MLR) using ordinary-least-squares (OLS)	Partial least squares regression (PLSR)	Multiple Linear Regression (MLR) using ordinary-least-squares (OLS)	Associative Neural Network (ASNN) Architecture: 10x3x1
Applicability Domain	Williams plot for response outliers Leverage approach (H matrix) for structural chemical domain	residual standard deviation (Euclidean distance) and leverage (Mahalanobis distance)	Williams plot for response outliers Leverage approach (H matrix) for structural chemical domain	Distance to model (DM) on standard deviation of ensemble prediction, 5xcross-validation

WP3 QSPR models for MP and Consensus model

All the models developed by WP3 Partners are statistically robust, internally and externally validated, and with a verified applicability domain. Models have been applied to predict MP data for 303 PFCs for which experimental measurements are unknown, always verifying the degree of interpolation/extrapolation of predictions. Model equations, statistical performances, predictions and information on applicability domain (interpolated/extrapolated predictions) are provided in the publication of Bhhatarai et al. 2011 [1]. Individual WP3 models have been uploaded in the CADASTER database and are freely available on-line. Their application for the prediction of MP data for new chemicals is recommended for perfluorinated or similar compounds included in their structural applicability domain. Consensus predictions were derived by averaging the predictions obtained by individual models. The coefficient of determination (R^2) and the root mean square of errors (RMSE) in the training set were calculated also for the consensus model.

The statistical parameters of the individual WP3 Full Models (i.e. models developed on all 94 experimental data) and consensus models are summarized in Table 2. External validation parameters refer to the validation on the blind evaluation set (EV set = 15 PFCs).

Table 2. Statistical performances of WP3 QSPR models for MP of PFCs (Individual Full Models) and of the Consensus Model.

WP3 Partner	R^2	Q_{LOO}^2	$RMSE_{TR}$	$RMSE_{EXT}$	Q_{EXT}^2 (range)	R_{YS}^2
UI	0.80	0.78	40.24	27.19	0.83-0.91	0.04
LnU	0.82	0.76	38.64	25.96	nc	nc
IDEA	0.79	0.77	40.67	38.82	0.65-0.81	0.03
HMGU	0.85	nc	37.00	34.00	nc	nc
Consensus	0.88	nc	31.81	nc	nc	nc

nc= not calculated

As it is reported in Table 2, the highest accuracy in prediction was obtained when the consensus approach was applied. Indeed, the Consensus Model is characterized by the highest R^2 values and the lowest value of RMSE.

The plot of experimental vs. predicted MP data for the full models developed by WP3 Partners and for the Consensus model is shown in Figure 1. The compounds are tagged with different labels representing the predictions calculated by the models developed by the different WP3 partners and the predictions by consensus. One compound (#28: CAS 75-73-0) was particularly outlier for the response in the IDEA model and is tagged in the plot.

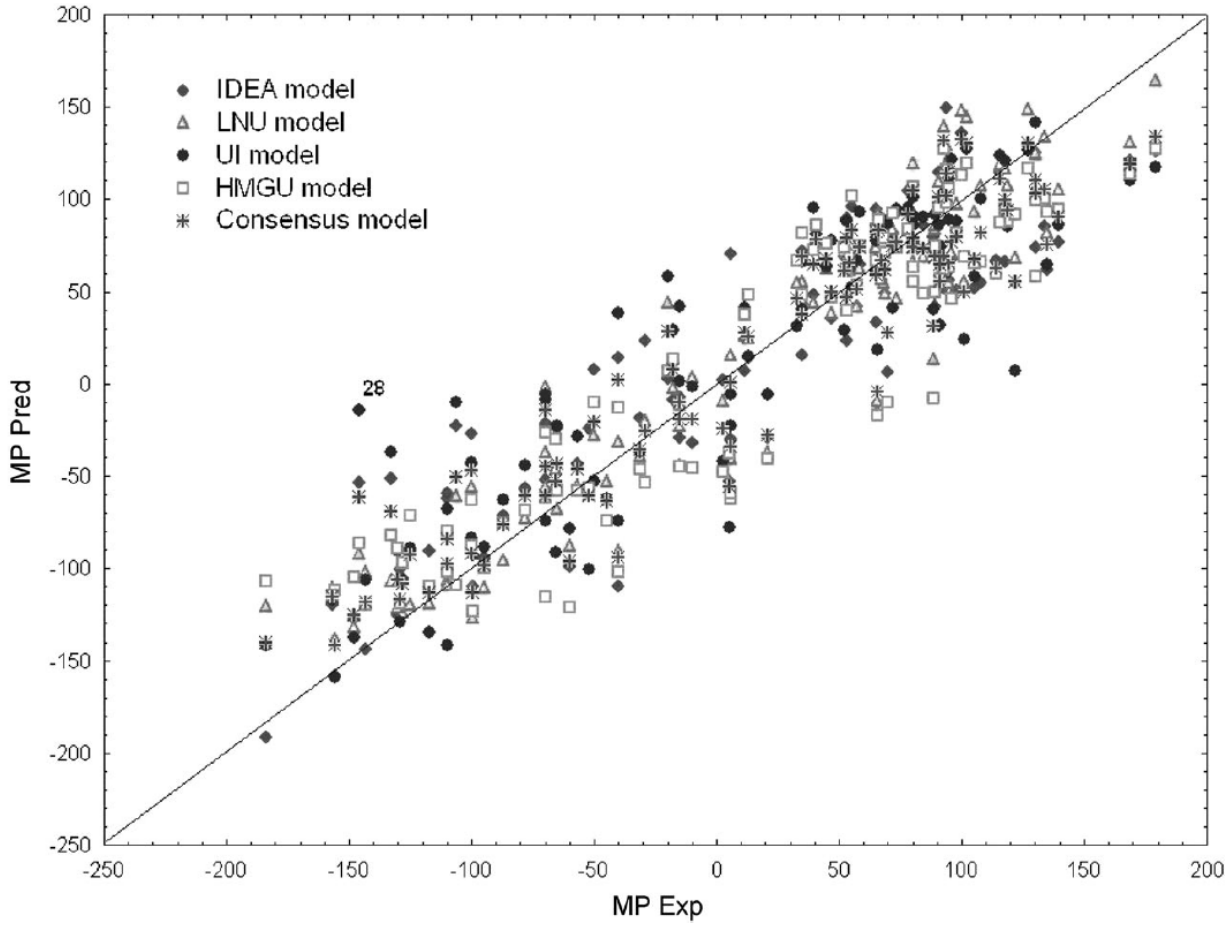

Figure 1. Combined experimental vs. prediction plot for MP data of the WP3 full models and Consensus Model.

Finally, the WP3 individual models and the consensus model were compared with the EPI Suite model for the prediction of MP, by calculating the value of the RMSE (Root Mean Square of Errors). As expected, the accuracy in prediction of the local models (WP3 models) and the consensus model, which

are specific for PFCs, was higher than the accuracy in prediction obtained by applying the general EPI Suite model ($RMSE_{EPI}$ for training set chemicals = 47.97 Vs. $RMSE_{Consensus}$= 31.81).

The results obtained by the application of the consensus approach for the prediction of MP of PFCs shows that in the reported study the consensus by predictions calculated by independently developed models using different descriptors and using different algorithms, delivers the best prediction results.

In this specific case study, simple statistical algorithms (like MLR and PLS) applied to complex descriptors perform about as good as complex algorithms (like NN) applied to simple descriptors. In fact, the combination of different modeling approaches helps to increase the prediction power as the different approaches complement each other.

1.2 Boiling Point

Experimental Dataset and splitting

Experimental data of BP for 93 poly- and perfluorinated compounds were collected from the SRC-PhysProp database and literature (Hendriks, 1953). The datasets were split (~50%), by applying two different splitting methods, into a training set, used for the development of the model, and a prediction set, used for the external validation of the models.

An additional blind external validation set of 25 PFCs was then collected from PERFORCE dataset ("EV-set"), which helps to assess the models' performance in prediction.

Modeling approaches, molecular descriptors and applicability domain

A summary of the modeling approaches and molecular descriptors used by the different partners is provided in Table 3.

Table 3. Modelling approaches applied by WP3 Partners for developing QSPR models for predicting the BP of PFCs.

	UI	LnU	IDEA	HMGU
Molecular Descriptors	0D-2D Dragon descriptors	0D-2D Dragon descriptors	Fragment based descriptors	E-state descriptors
Descriptor selection	Genetic Algorithm	variable influence on projection (VIP)	Exhaustive isomorphism search of fragment against structure	Pearson Pairwise Correlation

Modelling Descriptors	4 descriptors: ATS1m, Ms, nROH, AMW	149 descriptors at 4 components	8 descriptors: $MW^{1/4}$, W_{rel}^{F}, N_{HBDON}, $N_{[Cl,Br,I]}$, N_{COC}, $N_{C(=O)([!O])[!O]}$, N_N	66 indices
Algorithm	Multiple Linear Regression (MLR) using ordinary-least-squares (OLS)	Partial least squares regression (PLSR)	Multiple Linear Regression (MLR) using ordinary-least-squares (OLS)	Associative Neural Network (ASNN) Architecture: 10x3x1
Applicability Domain	Williams plot for response outliers Leverage approach (H matrix) for structural chemical domain	residual standard deviation (Euclidean distance) and leverage (Mahalanobis distance)	Williams plot for response outliers Leverage approach (H matrix) for structural chemical domain	Distance to model (DM) on standard deviation of ensemble prediction, 5xcross-validation

WP3 QSPR models for BP and Consensus model

Also for this endpoint, all the models developed by the WP3 Partners are characterized by high robustness and predictivity, and were checked for their applicability domain. Models have been applied to predict BP data for 271 PFCs for which experimental measurements are unknown, always verifying the degree of interpolation/extrapolation of predictions. Model equations, statistical performances, predictions and information on the applicability domain (interpolated/extrapolated predictions) are provided in the publication of Bhhatarai *et al.* 2011 [1]. All the individual WP3 models have been uploaded in the CADASTER database and are freely available. Their application for the prediction of BP data for new chemicals is recommended for perfluorinated or similar compounds included in their structural applicability domain. As it was done for the MP models, consensus predictions were derived by averaging the predictions obtained by individual models. The coefficient of determination (R^2) and the root mean square of errors (RMSE) in the training set were calculated also for the consensus model.

The statistical parameters of the individual WP3 Full Models (i.e. models developed on all 93 experimental data) and consensus models are summarized in Table 4. External validation parameters are referred to the validation on the blind evaluation set (EV set = 25 PFCs).

Table 4. Statistical performances of the WP3 QSPR models for BP of PFCs (Individual Full Models) and of the Consensus Model.

WP3 Partner	R^2	Q_{LOO}^2	$RMSE_{TR}$	$RMSE_{EXT}$	Q_{EXT}^2 (range)	R_{YS}^2
UI	0.94	0.93	19.73	30.32	0.86-0.93	0.04
LnU	0.97	0.94	14.11	21.92	nc	nc
IDEA	0.95	0.94	17.25	22.56	0.92-0.96	0.07
HMGU	0.85	nc	32.00	22.00	nc	nc
Consensus	0.96	nc	14.92	nc	nc	nc

nc = not calculated

The plot of experimental vs. predicted BP data calculated by the full models developed by WP3 Partners and by the Consensus model is shown in Figure 2. The compounds are tagged with different labels representing the predictions obtained by project partners and consensus predictions. Compounds particularly outlier for the response in the HMGU model are tagged in the plot (#1: CAS 75-73-0; #33: CAS 354-65-4; #9: CAS 98-16-8; #72: CAS 773-82-0).

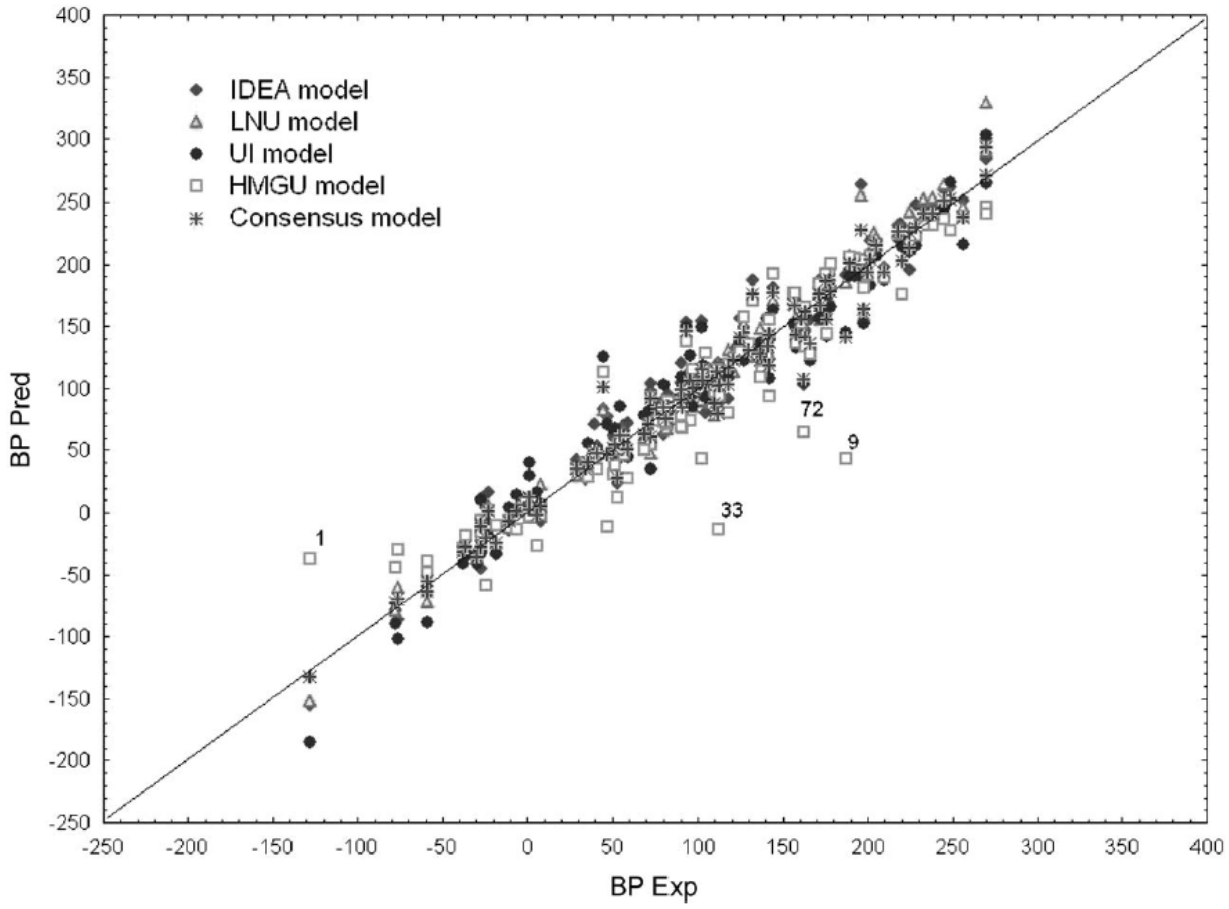

Figure 2. Combined experimental vs. prediction plot for BP data of the WP3 full models and Consensus Model.

The comparison of WP3 local models (Individual Full Models and Consensus Model) with EPI Suite estimations of BP data highlighted again the higher prediction accuracy obtained by applying local models specifically developed for PFCs than general models ($RMSE_{EPI}$ for training set chemicals = 24.8 Vs. $RMSE_{Consensus}$= 14.92).

2 Consensus models for Triazoles and Benzotriazoles (BTAZs): aquatic toxicity

Triazoles and benzotriazoles (B-TAZs) are a class of synthetic molecules characterized by the presence of a simple or condensed aromatic heterocyclic ring (2C + 3N atoms). (B)TAZs find a wide application in many fields; they are used as components of many pesticides, pharmaceuticals (e.g. painkillers, antimycotic and antidepressants medicines), UV stabilizer for plastics, but also they are abundantly used as components of liquid de-icing agents for aircraft and airport runways.

(B)TAZs studied under the CADASTER Project include 386 compounds, included also in the ECHA pre-registration list, they are structurally highly heterogeneous, and are characterized by different use pattern and different mechanism of actions.

Within the CADASTER project, several QSAR models have been developed by WP3 Partners UI, LnU, IVL, IDEA and HMGU for the prediction of aquatic toxicity of (B)TAZs. The QSARs were realized by different modeling approaches (e.g. MLR-OLS, PLSR, Kohonen Neural Network) starting from theoretical molecular descriptors calculated by commercial and freely available software (DRAGON, PaDEL-Descriptor, QSPR-THESAURUS web). The considered end-points were:

- EC50 (72h) in *Pseudokirchneriella subcapitata*
- EC50 (48h) in *Daphnia magna*
- LC50 (96h) in *Onchorhynchus mykiss*

Experimental data for algae, zooplankton and fish are among the key data required for risk assessment of chemicals.

Experimental data were collected from the FOOTPRINT Pesticide Properties Database (PPDB), a database of physiochemical and (eco)toxicological data on pesticides developed in the context of the EU-FP6 research project FOOTPRINT. In the database, each data point is associated to a score related to data quality which varies between 1 (worst quality data) and 5 (best quality data). In particular, 1 stands for “estimated data with little or no verification”, 2 for “unverified data of unknown source”, 3 for “unverified data of known source”, 4 for “verified data, and 5 for “verified data used for regulatory purposes”. Due to the fundamental relevance of the quality of the input data to the performance of QSAR models, and in order to limit the effects of experimental variability, only data corresponding to the highest quality-scores (4 and 5) were used for QSAR modeling. Data were collected for various (B)TAZs,

and also for other azo-aromatic compounds, including diazines, triazines and similar compounds, to enlarge the response and structural domain of the dataset.

QSARs were checked for their goodness-of-fit, robustness, predictivity and applicability domain, in agreement with OECD principles for the validation of QSARs for regulatory purposes.

Predictions by consensus were obtained by combining predictions from different models and approaches, taking into account statistical performances and applicability domains of individual models.

Models were also applied for the screening of more than 300 (B)TAZs without experimental data, many of them included in the European Chemicals Agency (ECHA) pre-registration list. This screening allowed for the identification of the compounds potentially most problematic in the aquatic environment.

A summary of the modeling approaches and molecular descriptors used by different partners is provided in Table 5.

Table 5. Modelling approaches applied by WP3 Partners for the QSAR models on aquatic toxicity of (B)TAZs.

	UI	LnU	IVL	IDEA	HMGU
Modelled Endpoint	EC50 algae EC50 Daphnia LC50 fish	EC50 algae EC50 Daphnia LC50 fish	EC50 algae EC50 Daphnia LC50 fish	EC50 Daphnia LC50 fish	EC50 algae EC50 Daphnia LC50 fish
Input format of chemical structures	HIN files for DRAGON, MOL for PaDEL, SMILES for CADASTER	SMILES	HIN files	SMILES	3D SDF files prepared by Corina
Molecular Descriptors	0D-2D Dragon v.5.5 "pruned"*, PaDEL, CADASTER	0D-3D Dragon v.6	0D-3D Dragon v.6	0D-2D Dragon v.5.5	0D-3D CADASTER
Descriptor selection	Genetic Algorithm in QSARINS [3]	Latent variables	Descriptors with VIP>1. Four latent variables	Genetic Algorithm in MobyDigs	Only highly cross-correlated (R>0.95) and almost constant descriptors (less than 3 unique values) were eliminated
Algorithm	Multiple Linear Regression (MLR) using ordinary-least-squares (OLS)	Partial least squares regression (PLSR) and Bayesian Lasso on PLS latent variables (BLASSO-PLS)	Partial least squares regression (PLSR)	Multiple Linear Regression (MLR) using ordinary-least-squares (OLS)	kNN, ASNN, FSMLR, PLS, MLRA, SVM
Applicability Domain	Leverage	Leverage distance to the model on PLS latent variables	DModX	Leverage	STD of ASNN

* Molecular descriptors no more available or with different values in Dragon 6 were deleted. Semi-constant descriptors (molecular descriptors that have value only for less 20% of chemicals, or less) were also deleted.

Details regarding datasets, modelling descriptors, modelling methodologies (model development, validation and applicability domain) will be discussed in the following paragraphs. A joint publication on these models, as proceedings of the final CADASTER Workshop of October 2012, is under preparation.

2.1 Acute toxicity in algae

2.1.1 Experimental datasets and Methods

Partner 3: University of Insubria (UI)

Experimental data for EC50 72h in *Pseudokirchneriella subcapitata* were collected for 17 (B)TAZs and 18 additional azo-aromatic compounds, for a total of 35 training set chemicals from the FOOTPRINT database and from other sources. Only data corresponding to quality scores 4 and 5 in the FOOTPRINT database were included in the dataset.

To verify the predictive capability of the models the dataset was split, before model development, into a training set and a prediction set, used for the external validation. Two different splitting techniques were applied: a) by ordered response (N_{TR} = 24, N_P = 11), and b) by structural similarity using Kohonen Artificial Neural Networks (K-ANN) (N_{TR} = 22, N_P = 13).

Three different programs were used to generate molecular descriptors (i.e. the commercial software Dragon ver. 5.5 ("Pruned"), the CADASTER on-line platform "QSPR-THESAURUS", and the freely available software PaDEL v. 2.12). For each group of descriptors separate MLR-OLS models were developed (i.e. "Dragon Model", "CADASTER Model" and "Padel Model").

The selection of modeling descriptors (by Genetic Algorithm), model's validation and AD analysis were performed by the QSARINS software [3].

Several validation techniques were applied in order to evaluate model robustness (e.g. LOO, LMO, Bootstrap). Different external validation parameters (Q^2_{ext}-F1 (*Shi et al., 2001*, in OECD guidance [4]), F2 (*Schüürmann et al., 2008* [5]), F3 (*Consonni et al., 2010* [6]) and the Concordance Correlation Coefficient (*Chirico and Gramatica, 2011* [7])) were calculated and compared, in order to select only models that are recognized as externally predictive by all the validation criteria. The Y-scrambling procedure has been applied to verify the absence of chance correlation in each model. Williams graph was always verified to highlight outliers for the response and high leverage chemicals. The Insubria graph (Plot of hat values Vs. Predictions) was analyzed in order to verify the structural applicability domain (AD) of the models for (B)TAZs without experimental data (N = 369) (Figure 3).

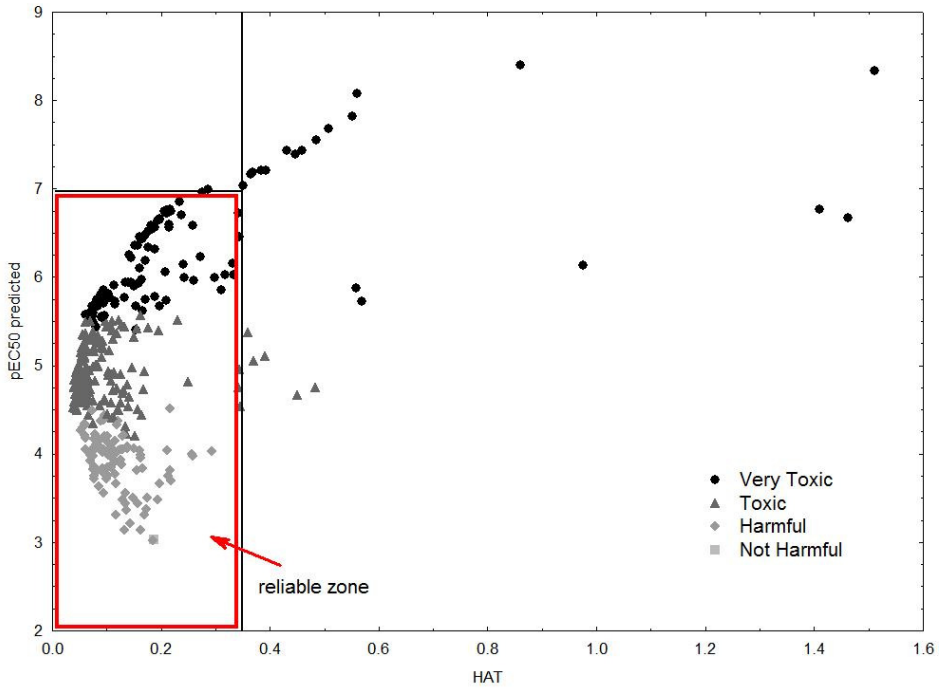

Figure 3. Insubria plot (hat values vs. predictions). In this example the "reliable" zone of the plot is defined by the hat cut-off line (separating interpolated vs. extrapolated predictions) and an horizontal arbitrary cut off defined on the basis of both predicted values and hat values (pEC50 >7 are mainly extrapolated)

Partner 4: IVL Swedish Environmental Research Institute (IVL)

The training set was selected from the FOOTPRINT database with the same criteria as used by UI. However, only experimental data available for (B)TAZs were used by IVL for the development of the models (differently to other WP3 partners, data for additional azo-aromatic compounds were not considered). During the modelling phase several substances were classified as outliers in the training set which resulted in 15 substances used for model development. Hence no validation set was created. Descriptors used in the modelling were calculated by the Dragon software, version 6.0.

PLS regression is used as modelling method. Two measures can be considered to determine if a new substance is in the model domain, i.e. applicability domain. The first is the distance to the model plane (also called residual magnitude) and the second is the distance between the model centre and the projection in the model plane. In the SIMCA software, used for PLS, the distance to the model plane of a prediction is known as DModXPS (Distance to Model in X space for the Prediction Set), while also considering the distance in the model plane leads to the statistic DModXPS+. From these distances and

the corresponding distances in the training set, it is possible to calculate a probability that a (new) substance is in the applicability domain.

Partner 5: Linneaus University , Sweden (LnU)

A QSAR for acute algae toxicity (EC50) was developed using literature data collected in WP2. We used descriptors derived by Dragon 6.0, and descriptors with less than 0.01 in std and with only two values different from the others (seen over the training data set) were removed according to the recommendations on the CADASTER web site.

LC50 values were transformed into pLC50 by taking the negative natural logarithm of the values.

With the aim to build a QSAR model that delivers predictions with associated uncertainty a Bayesian approach was used. In order to simplify the fitting and address the large descriptor space, a Bayesian model was fitted in two steps, first Latent Variables were generated from the PLS-components. The number of Latent Variables was set to the smallest number for which the cross-validated predictive error lied within 10% of the distance from the smallest to the largest error. Second, uncertainty in predictions was estimated by the use of Markov Chain Monte Carlo sampling using the Bayesian Lasso as model algorithm.

Predictive performance of the Bayesian lasso on PLS Latent Variables were similar to PLS since the PLS point predictions to a high extent were similar to posterior mean or mode. Thus, the gain of BLASSO on PLS was to get a way to assess predictive uncertainty in terms of a probability distribution. Due to the small data sets it was not possible to fit Bayesian lasso directly on the raw descriptors. How to solve these issues is currently being dealt with and a manuscript is in preparation. Models predictions were derived using the monomvr package in R.

Partner 6: Helmholtz Zentrum Muenchen (HMGU)

31 molecules were used for model development. Several sets of descriptors were used:

ADRIANA.Code (3D) comprises 211 molecular descriptors based on a sound geometric and physicochemical basis. The classes of descriptors cover global molecular descriptors, shape and size descriptors, topological and 3D property-weighted autocorrelation descriptors [8].

CDK (3D) included topological, geometrical, constitutional, electronic and hybrid descriptors [9]. In total 204 descriptors were calculated.

ChemAxon descriptors (3D) included elemental analysis, charge, geometry, partitioning, protonation, isomers and "other" descriptors [10].

Dragon6 (3D) represented the largest pool, which included 4885 descriptors grouped in 29 different blocks [11].

E-state indices [12-13] (2D) were calculated using E-state program, which was used to predict logP and water solubility in the ALOGPS program [14].

ISIDA Fragmentor (2D) [15] was used to calculate augmented atoms of length 3 to 5.

GSFRAG (2D) included descriptors based on fragments that contain a labeled vertex, allowing one to capture the effect of heteroatoms [16].

Inductive descriptors (3D), which are based on LFER (Linear Free Energy Relationships) equations for inductive and steric substituent constants, were implemented according to ref [17].

Mera (3D) included geometrical, energy characteristics and physicochemical descriptors [18]. In this set we also included MERSY, which estimates molecular symmetry and chirality.

Shape Signatures (3D) encoded spatial shape characteristics of molecules using ray tracing, which explores volume enclosed by the solvent accessible surface of a molecule [19].

Spectrophores fingerprints (3D) are calculated as one-dimensional compression of molecular properties fields surrounding molecules.

Models were developed with each set of descriptors individually. No descriptor selection was performed. However, descriptors that were highly correlated one with another in the training set ($R>0.95$) or had almost constant values (less than 2 unique values) were excluded. Models were developed using several machine learning methods, namely

k Nearest Neighbors (kNN) predicts a property for a compound using the consensus voting of k compounds from the training set that are nearest to it according to some distance metric. We used the Euclidean distance calculated using normalized descriptors (mean 0 and standard deviation 1). The number of nearest neighbors that provided the highest accuracy of classification was calculated following a systematic search in range (0, 100).

ASsociative Neural Network (ASNN) uses the correlation between ensemble responses as a measure of distance amid the analyzed cases for the nearest neighbor technique [20-21]. Thus ASNN performs kNN in the space of ensemble predictions. This provides an improved prediction by the bias correction of the neural network ensemble. The configurable options are: the number of neurons in the

hidden layer, the number of iterations, the size of the model ensemble and the method of neural network training. The default values provided at the OCHEM web site were used.

Fast Stagewise Multivariate Linear Regression (FSMLR) is a procedure for stage-wise building of linear regression models by means of greedy descriptor selection [22].

Partial Least Squares (PLS). The number of latent variables was optimized automatically using 5-fold cross-validation on the training set.

Multiple Linear Regression Analysis (MLRA) uses step-wise variable selection. The method eliminates on each step one variable that has a regression coefficient non-significantly different from zero (according to the *t*-test). Thus MLRA has only one parameter, ALPHA, which corresponds to the *p*-value of variables to be kept for the regression. ALPHA=0.05 was used.

Support Vector Machine (SVM) uses the LibSVM program [23]. The SVM method has two important configurable options: the SVM type (ε-SVR and μ-SVR) and the kernel type (linear, polynomial, radial basis function and sigmoid). Classic ε-SVR and radial basis function kernel were used. The other SVM parameters, namely cost *C* and width of the RBF kernel were optimized using default grid search, which was performed according to the LibSVM manual.

We used the 5-fold cross-validation procedure to identify the most predictive combinations of models and descriptors. On each cross-validation step we calculated a new model, which was then used to predict the activity of compounds from the respective validation set. This method, as shown in our earlier publications [24-25], provides a correct estimation of the prediction accuracy of models.

The analysis of all 3 sets considered in this chapter (see Tables 6) indicated that Associative Neural Networks [20-21, 26] provided models with the lowest RMSE. Therefore, models calculated with this method were used for all studies. The best cross-validation results for the Algae dataset were calculated using Dragon descriptors.

Table 6. RMSE of HMGU models developed with different combinations of methods and descriptors for the Algae dataset.

Descriptors/method	ASNN	MLRA	LibSVM	FSMLR	KNN	PLS
CDK	0.572	1.12	0.646	0.6	0.94	0.619
Dragon6 (blocks: 1-29)	***0.484***	1.04	1.1	0.809	0.677	0.813
Fragmentor (Length 2 - 4)	1.09	1.46	1.38	1.01	0.973	0.809
GSFrag	0.791	1.08	1.11	0.623	0.876	0.649
Mera, Mersy	0.651	1.59	0.931	0.73	0.791	0.802

ChemaxonDescriptors (7.4)	0.718	0.947	1.03	0.758	0.795	0.673
InductiveDescriptors	0.706	1.19	0.584	0.647	0.719	0.596
Adriana	0.511	1.74	0.908	0.68	0.636	0.682
Spectrophores	0.697	0.733	0.838	0.658	0.756	0.663
Estate	0.78	1.21	0.848	1.19	1.07	0.628

2.1.2 Individual WP3 models used for Consensus

Partner 3: University of Insubria (UI)

Several MLR models, based on DRAGON, PaDEL and CADASTER descriptors, were developed for the endpoint EC_{50} in *Pseudokirchneriella subcapitata*. In particular, QSAR models based on 3 molecular descriptors were reported in Deliverable 3.5 and presented in several meetings (SETAC-Europe 2011, CMTPI 2011, SETAC 2012, QSAR 2012) as well as in a publication now in preparation.

The new models developed for the consensus study (with performances comparable to the other WP3 models) are based on 4 molecular descriptors (DRAGON and PaDEL only) and summarized in Table 7.

Table 7. UI models selected for the prediction of EC_{50} in *Pseudokirchneriella subcapitata* (72h).

Model ID	Descriptors	Set	N_{TR}	N_P	R^2	Q^2_{LOO}	Q^2_{EXT} (range)*	AD% on 386
DRAGON	T(N..S), AEigZ, Seigv, Lop	Split R	24	11	0.86	0.76	0.80 - 0.85	
		Split K	22	13	0.83	0.72	0.75 - 0.85	
		FULL	35	--	0.85	0.80	--	93
PaDEL	AMR, maxwHBa, MDEN-22, maxaasN	Split R	24	11	0.87	0.79	0.69 - 0.76	
		Split K	22	13	0.84	0.74	0.69 - 0.82	
		FULL	35	--	0.83	0.76	--	94

*Range of values calculated using different Q^2_{EXT} parameters (Q^2_{EXT-F1}, Q^2_{EXT-F2}, Q^2_{EXT-F3} and CCC).

Partner 4: IVL Swedish Environmental Research Institute (IVL)

The statistical parameters for the final PLS model developed by IVL for *Pseudokirchneriella subcapitata* are presented in Table 8.

Table 8. Summarised statistics of the IVL PLS model for *Pseudokirchneriella subcapitata* (72h).

NTR	Descriptors	N Descriptors	R^2	Q^2_{LOO}	RMSEE
15	DRAGON 6.0	2440	0.97	0.56	0.15

Partner 5: Linneaus University (LnU)

Performances of LnU models developed for algae acute pEC50 are summarized in Table 9.

Table 9. Predictive performances of LnU models generated by Partial Least Squares (PLS) regression and Bayesian Lasso applied on PLS Latent Variables (BLASSO-PLS).

		Supervised learning algorithm				
		PLS		BLASSO.PLS		
Dataset	N	R2 (Q2)	MSE (MSEP)	R2 (Q2)	MSE (MSEP)	in AD
Training	27	0.73	0.58	0.77	0.51	0.93
External	18	0.11	0.89	0.07	1.07	0.83

Neither of the models developed by LnU was regarded as good enough to qualify for the consensus modelling.

Partner 6: Helmholtz Zentrum Muenchen (HMGU)

The model selected for the consensus study is based on neural networks. The statistical parameters as calculated for the training set are summarised in Table 10.

Table 10. HMGU model selected for the prediction of EC_{50} in *Pseudokirchneriella subcapitata* (72h).

Statistical parameters	Training set (n=31)
RMSE	0.48
MAE	0.39
R2	0.77
Q2	0.77

After the unsupervised filtering procedure, the model included 1144 descriptors.

INDIVIDUAL WP3 MODELS SELECTED FOR THE CONSENSUS MODEL

Individual models selected by different WP3 partners for the consensus study are summarized in Table 11. Statistical performances reported in the table are related to the individual training and validation sets used by different partners.

Table 11. Statistical performances of individual WP3 models selected for the Consensus model for EC_{50} in *Pseudokirchneriella subcapitata* (72h).

WP3 Partner	N_{TR}	R^2	Q^2	$RMSE_{TR}$	$RMSE_{EXT}$	Ext. Validation	AD 386
UI-Dragon	35	0.85	0.80 [a]	0.45	0.40-0.41	Yes (Q^2_{ext}>0.75)	93%
UI-PaDEL	35	0.83	0.76 [a]	0.48	0.46-0.50	Yes (Q^2_{ext}>0.69)	94%
IVL	15	0.97	0.56	0.15 [b]	nc	No	37.8%
HMGU	31	0.77	0.77	0.48	0.61	Yes [c]	97.4%

[a] Q^2_{LOO}; [b] RMSE calculated in fitting; [c] the external validation was performed on additional data measured by PHI (Partner 2 in the CADASTER Project), and are not reported in this Deliverable since they will be included in Deliverable 3.7.

As it can be concluded from table 10, the IVL model is characterized by a limited applicability domain toward the 386 (B)TAZs. This is due to the limited training set (15 chemicals).

2.1.3 Consensus predictions for 386 (B)TAZs

Individual WP3 models reported in Table 10 (UI-Dragon, UI-Padel, IVL, HMGU) were applied to predict acute toxicity in the algae *Pseudokirchneriella subcapitata* for 386 (B)TAZs with and without experimental data. Consensus predictions were then derived by averaging (arithmetic mean) the predictions obtained by individual models.

For each chemical, the absolute deviation between individual model prediction ($\hat{y}_{UI\text{-}D}$ / $\hat{y}_{UI\text{-}P}$ / $\hat{y}_{IVL}$ / $\hat{y}_{HMGU}$) and the consensus prediction ($\hat{y}_C$) was calculated ("ID"). Additionally, to verify the agreement among predictions obtained by different WP3 models for single (B)TAZs, the median deviation ("MD") of individual models predictions from the consensus prediction was calculated:

$$MD = \frac{\sum |\hat{y} - \hat{y}_C|}{n}$$

The higher the MD value is, the higher is the disagreement among WP3 model predictions. This analysis was performed taking into account:

a) predictions for 386 (B)TAZs (into and out the AD of the individual models); and
b) predictions only for (B)TAZs included in the AD of all the individual models (i.e. 143 (B)TAZs).

As expected, the highest MD values (MD > 1) were mainly obtained for compounds outside the AD of the models. In particular, a marked disagreement in prediction was observed for 6 (B)TAZs outside the AD of the UI-Dragon model, whose pEC50 predictions are 4 to 10 log unit higher than predictions generated by other models. However, it is to note that these compounds are very far from the structural domain of the UI-Dragon model and the predictions have to be considered as pure extrapolations of the model.

When the same analysis was performed only on (B)TAZs included in the AD of all the WP3 models (143 BTAZs), comparable predictions were obtained for all the compounds (0.06 < MD < 0.64). In this case, the highest deviation from consensus predictions was observed for IVL predictions. However, consensus predictions were not particularly affected by IVL values.

The fact that different models, based on different descriptors and modeling approaches, lead to similar predictions adds confidence and reliability to QSAR predictions obtained by the Consensus approach.

Individual WP3 predictions and applicability domain, consensus predictions, individual model deviations and MD are reported in Appendix II.

In Figure 4, individual model and consensus predictions for 386 (B)TAZs are reported.

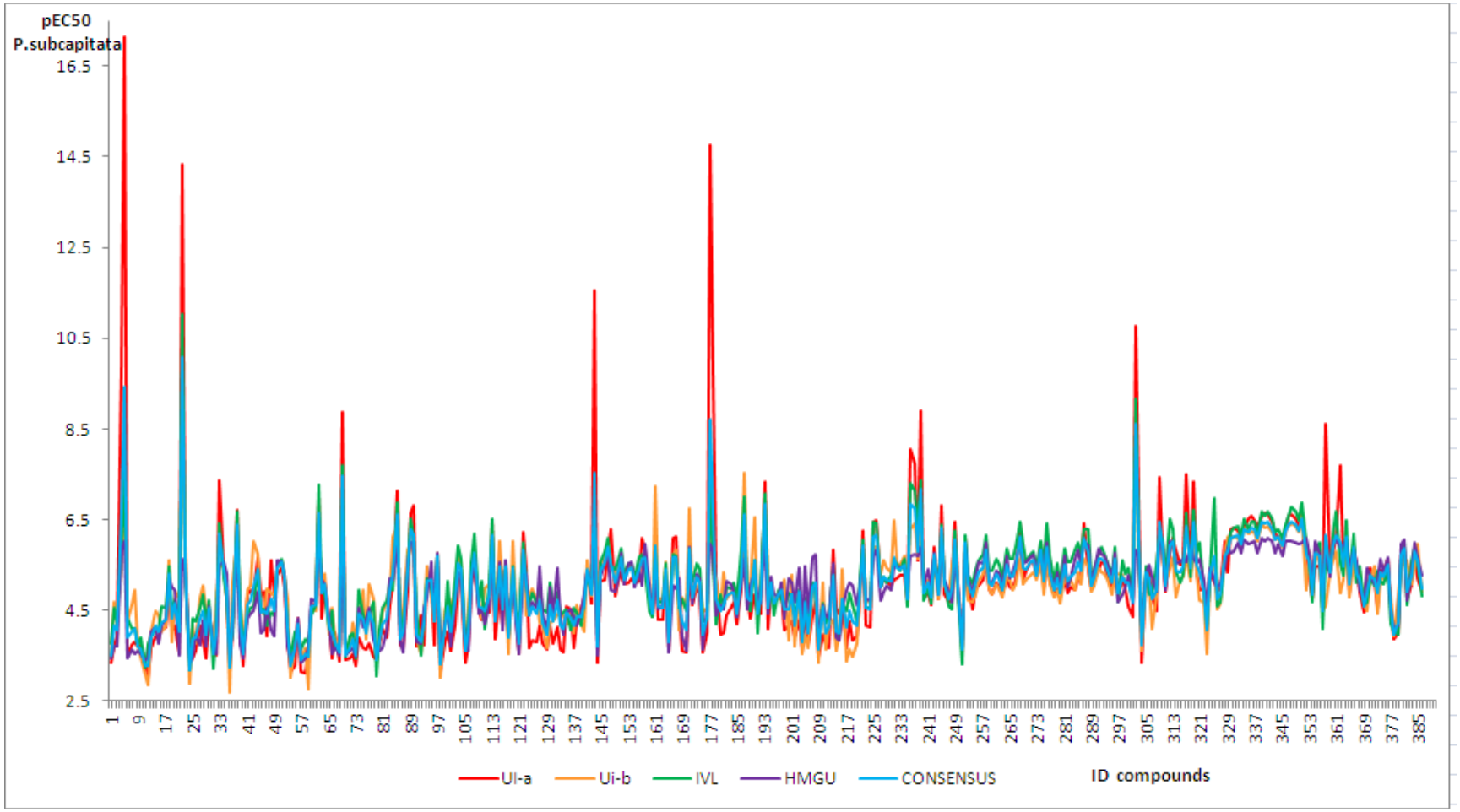

Figure 4. Prediction for 386 (B)TAZs obtained by individual WP3 models and consensus model for acute toxicity in *Pseudokirchneriella subcapitata*. UI-a = UI-Dragon model; UI-b = UI-PaDEL model.

2.2 Acute toxicity in Daphnia

2.2.1 Experimental datasets and Methods

Partner 3: University of Insubria (UI)

Experimental data for EC50 48h in *Daphnia magna* were collected for 46 (B)TAZs and 51 additional azo-aromatic compounds, for a total of 97 training set chemicals. Only data corresponding to quality score 4 and 5 of the FOOTPRINT database were included in the dataset.

The dataset was split (by response and by structure) into a training set (N_{TR}=65), used for model development, and a prediction set (N_P=32), used for external validation. A Full model based on all 97 compounds was then derived.

MLR-OLS models were developed using Dragon, PaDEL and CADASTER descriptors. Models were validated for internal robustness and external predictivity by applying several validation techniques and statistical parameters (e.g. Q^2_{LOO}, Q^2_{LMO}, Q^2_{Boot}, R^2_{YS}, Q^2_{EXT}F1/F2/F3, CCC). Williams graph has been verified to highlight outliers for the response and high leverage chemicals. The Insubria graph (Plot of hat values Vs. Predictions) was analyzed in order to verify the structural AD of the model for (B)TAZs without experimental data (N = 340).

Partner 4: IVL Swedish Environmental Research Institute (IVL)

The model development for Daphnia was almost performed in the same way as for Algae. The main difference was however that the Daphnia data could be split into one training set (29 compounds) and one validation set (8 compounds).

Partner 5: Linneaus University (LnU)

The same approach was used as for Daphnia (see above).

Partner 6: Helmholtz Zentrum Muenchen (HMGU)

The same procedure as for the Algae dataset was used. The training set included 97 molecules. Table 12 shows the performance of the different methods and descriptors. The lowest RMSE using 5-fold cross-validation protocol was calculated using Adriana descriptors. This model was used to predict the EC50 value of the test set compounds.

Table 12. RMSE of HMGU models developed with different combinations of methods and descriptors for the Daphnia dataset.

	ASNN	LibSVM	MLRA	FSMLR	PLS	KNN
CDK	0.574	0.483	0.586	0.479	0.561	0.64
Dragon6 (blocks: 1-29)	0.502	0.47	0.67	0.549	0.523	0.546
Fragmentor (Length 2 - 4)	0.608	0.557	0.578	0.616	0.54	0.715
GSFrag	0.53	0.581	0.623	0.607	0.552	0.621
Mera, Mersy	0.551	0.61	0.56	0.638	0.885	0.673
ChemaxonDescriptors (7.4)	0.5	0.472	0.501	0.528	0.519	0.582
InductiveDescriptors	0.624	0.696	0.657	9.03	0.705	0.666
Adriana	***0.448***	0.534	0.529	0.561	0.601	0.565
Spectrophores	0.592	0.565	0.62	0.611	0.555	0.62
EState	0.682	0.607	0.631	0.647	0.546	0.699

Partner 7: Ideaconsult Ltd. (IDEA)

The training set consisted of 97 chemicals: 46 (B)TAZs and 51 additional azo-aromatic compounds.

Linear regression QSAR models for Triazoles and Benzo-triazoles (B-TAZ) have been developed. We used 2D molecular structures encoded in SMILES, and calculated descriptors by DRAGON 5.4 2006 software. Several feature selection procedures have been explored, starting from preliminary variable elimination, removing correlated descriptors and following by genetic algorithm by Mobydigs[1] version 1.0 / 2004 software and expert selection. A set of 20 models with different complexity (5,6,7 and 10 variables) is generated and model selection performed, by analysing the trade-off between the model accuracy and over-fitting. Additional models were created by selecting descriptors by expert knowledge. The expert variable selection is guided by the genetic algorithm, and additionally includes functions of the descriptors variables (e.g. logarithm, square root, power of two, etc.). Model performance is further checked by y-scrambling procedure and leave one out validation, as well as against two external dataset, selected for validation by project partners.

2.2.2 Individual WP3 models used for Consensus

Partner 3: University of Insubria (UI)

Among the models developed by UI for the prediction of acute toxicity on *Daphnia magna*, only the models based on Dragon and CADASTER descriptors gave satisfying results. Among the best models (with similar performances), those based on logP were not selected for the consensus, in order to guarantee the highest diversity in the description of the structural space (e.g. IDEA models are based also on Dragon descriptors, including logP). A model based on 5 Dragon descriptors and a model based on 3 CADASTER descriptors were previously reported in Deliverable 3.5 and presented in several meetings (SETAC-Europe 2011, CMTPI 2011, SETAC 2012, QSAR 2012). Additionally, the Dragon model was also proposed for publication (the paper is now under revision).

The new model developed for the consensus study is based on 6 DRAGON descriptors. Statistical parameters of both the Split and Full model are reported in Table 13.

Table 13. Details on the UI model selected for the prediction of EC_{50} in *Daphnia magna* (48h).

Model ID	Descriptors	Set	N_{TR}	N_P	R^2	Q^2_{LOO}	Q^2_{EXT} (range)*	AD% on 386
DRAGON	TPSA (NO), Aeigm,nCar, nHDon, H-052, X5A	Split R	65	32	0.79	0.74	0.74 - 0.75	
		Split K	65	32	0.78	0.72	0.79 – 0.83	
		FULL	97		0.79	0.76		90.2

*Range of values calculated using different Q^2_{EXT} parameters (Q^2_{EXT-F1}, Q^2_{EXT-F2}, Q^2_{EXT-F3} and CCC).

Partner 4: IVL Swedish Environmental Research Institute (IVL)

The statistical parameters for the final PLS model developed by IVL for *Daphnia magna* are presented in Table 14.

Table 14. Summarised statistics for IVL the PLS model for *Daphnia magna.*

N_{TR}	Descriptors	N Descriptors	R^2	Q^2_{LOO}	RMSEE	RMSEP
29	DRAGON 6.0	1715	0.97	0.88	0.18	0.37

Partner 5: Linneaus University (LnU)

Performances of LnU models developed for daphnia acute pEC50 are summarized in Table 15.

Table 15. Predictive performances of LnU models generated by Partial Least Squares (PLS) regression and Bayesian Lasso applied on PLS Latent Variables (BLASSO-PLS).

		Supervised learning algorithm				
		PLS		BLASSO.PLS		
Dataset	N	R2 (Q2)	MSE (MSEP)	R2 (Q2)	MSE (MSEP)	in AD
Training	80	0.76	0.42	0.76	0.42	0.95
External	15	0.34	0.61	0.33	0.62	1

The models developed by LnU for Daphnia were not good enough to qualify for the consensus modelling.

Partner 6: Helmholtz Zentrum Muenchen (HMGU)

The statistical parameters of the model selected for the consensus study are summarised in Table 16.

Table 16. Statistical parameters calculated for the Daphnia dataset using ASNN method and Adriana descriptors.

Statistical parameters	Training set (n=97)
RMSE	0.45
MAE	0.35
R2	0.70
Q2	0.70

The model was based on 136 descriptors, which were left after the unsupervised filtering.

Partner 7: Ideaconsult Ltd. (IDEA)

The statistical parameters for the model selected for the consensus study are summarised in Table 17.

Table 17. IDEA model selected for the prediction of EC_{50} in *Daphnia magna* (48h).

Descriptors	N_{TR}	R^2	Q^2_{LOO}
ATS4m, nCar, N-072, ALOGP, nR09^2	97	0.85	0.83

INDIVIDUAL WP3 MODELS SELECTED FOR CONSENSUS MODEL

Individual models selected by different WP3 partners for the consensus study are summarized in Table 18. Statistical performances reported in the table are related to the individual training and validation sets used by different partners.

Table 18. Statistical performances of individual WP3 models selected for the Consensus model for EC_{50} in *Daphnia magna* (48h).

WP3 Partner	N_{TR}	R^2	Q^2	$RMSE_{TR}$	$RMSE_{EXT}$	Ext. Validation	AD 386
UI	97	0.79	0.76 [a]	0.40	0.34-0.41	Yes (Q^2_{ext}>0.74)	90.2%
IVL	29	0.97	0.88	0.18	0.37	Yes [b]	13.2%
HMGU	97	0.70	0.70	0.45	nc	Yes [b]	63.7%
IDEA	97	0.85	0.83 [a]	0.34	0.31	Yes [b]	88%

[a] Q_{LOO}^2; [b] the external validation was performed on additional data measured by PHI (Partner 2 in the CADASTER Project), and are not reported in this Deliverable since they will be included in Deliverable 3.7.

2.2.3 Consensus predictions for 386 (B)TAZs

Individual WP3 models reported in Table 16 (UI, IVL, HMGU, IDEA) were applied to predict acute toxicity in *Daphnia magna* for 386 (B)TAZs with and without experimental data. Consensus predictions were then derived by averaging the predictions obtained by individual models.

As it was done for algae, individual model predictions deviation and median deviation (MD) from consensus predictions were calculated for each chemical.

Again, the highest MD values (MD > 1) were mainly obtained for compounds outside the AD of all (or most of) the models. In this case, the most discordant predictions were those generated by the IVL model. It should be noted that the training set used by IVL, which is based only on (B)TAZs, is limited in comparison with the other models. In fact, the majority of (B)TAZs (87%) fell outside the structural applicability domain of this model. The high discordance in prediction could be due to the fact that most of the predictions are actually extrapolations.

When the same analysis was performed only on (B)TAZs included in the AD of all the WP3 models (45 (B)TAZs), comparable predictions were obtained for all the compounds (0.04 < MD < 0.42).

Individual WP3 predictions and applicability domain, consensus predictions, individual model deviations ("ID") and median deviations ("MD") are reported in Appendix III.

In Figure 5, individual model and consensus predictions for 386 (B)TAZs are reported.

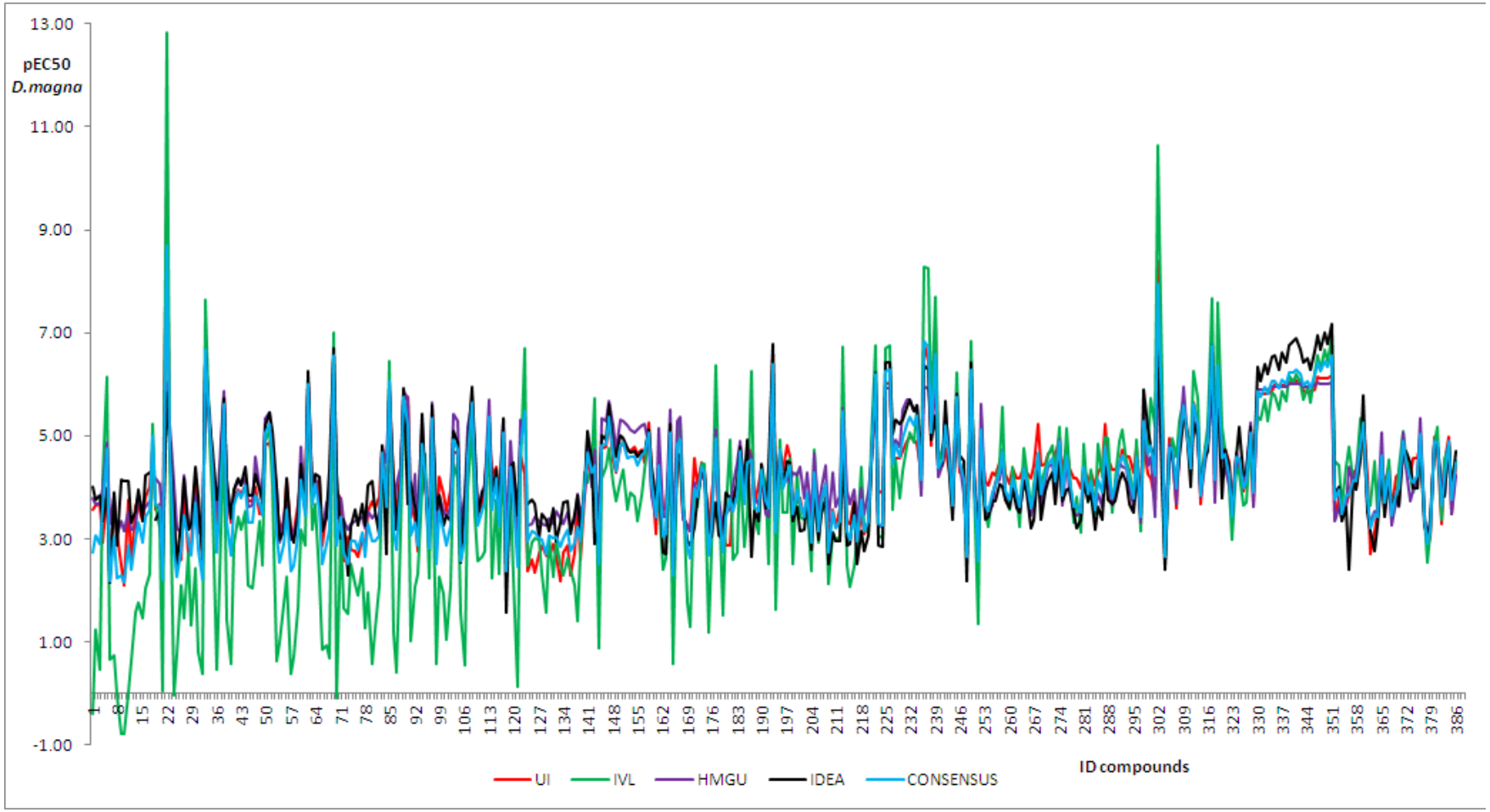

Figure 5. Prediction for 386 (B)TAZs obtained by individual WP3 models and consensus model for acute toxicity in *Daphnia magna*.

2.3 Acute toxicity in Fish

2.3.1 Experimental datasets and Methods

Partner 3: University of Insubria (UI)

Experimental data for LC50 96h in *Oncorhynchus mykiss* were collected for 28 (B)TAZs and 48 additional azo-aromatic compounds, for a total of 76 training set chemicals. As a relatively limited amount of data on fish toxicity were available, data of quality-score 3 (in addition to data of scores 4 and 5 of the FOOTPRINT database), were also included in the dataset in order to obtain a sufficiently large dataset for QSAR modeling.

The dataset was split (by response and by structure) into a training set (N_{TR}=53), used for model development, and a prediction set (N_P=23), used for external validation. An additional set of experimental data, composed of 18 (B)TAZs, was used by all the WP3 Partners as a blind evaluation set (EV).

Two different pools of molecular descriptors (DRAGON and PaDEL descriptors) were separately used for model development.

Models were validated for internal robustness and external predictivity by applying several validation techniques and statistical parameters (e.g. Q^2_{LOO}, Q^2_{LMO}, Q^2_{Boot}, R^2_{YS}, Q^2_{EXT}F1/F2/F3, CCC). Williams graph has been a verified to highlight outliers for the response and high leverage chemicals. The Insubria graph (Plot of hat values Vs. Predictions) was analyzed in order to verify the structural AD of the model for (B)TAZs without experimental data (N = 340).

Partner 4: IVL Swedish Environmental Research Institute (IVL)

Regarding models for acute fish toxicity the method was the same as for the two previous species.

The training set consists of 19 compounds.

Partner 5: Linneaus University (LnU)

A QSAR for acute fish toxicity (LD50) was developed using literature data collected in WP2. This data set is heterogeneous, representing several modes of action, and an initial attempt to extend it with narcosis acting compounds was therefore not successful. Instead a general PLSR model was fitted and validated using the same data as UI (a calibration set of 76 triazoles and triazines and a validation set of 18 triazoles).

Partner 6: Helmholtz Zentrum Muenchen (HMGU)

The same procedure as for the previous two datasets was used. The training set included 76 molecules. We excluded Azocyclotin (CAS RN 41083-11-8), as this was the only one compound containing [Sn]. Table 19 shows the performance of the different methods and the descriptors used. The lowest RMSE using 5-fold cross-validation protocol was calculated using ChemAxon descriptors. This model was used to predict the toxicity of test set compounds.

Table 19. RMSE of HMGU models developed with different combinations of methods and descriptors for the Fish dataset.

Descriptors/Method	ANN	LibSVM	MLRA	PLS	FSMLR	KNN
CDK	0.791	0.712	0.995	0.889	0.915	0.731
Dragon6 (blocks: 1-29)	0.793	0.739	1.1	0.784	0.905	0.771
Fragmentor (Length 2 - 4)	0.941	1.15	1.05	0.871	1.08	0.991
GSFrag	0.937	0.857	0.936	1.09	0.952	0.922
Mera, Mersy	0.785	0.882	0.915	1.04	0.819	0.846
ChemaxonDescriptors (7.4)	***0.683***	0.703	0.878	0.843	0.787	0.708
InductiveDescriptors	0.929	0.919	1.05	0.914	1.04	0.933
Adriana	0.811	0.867	1.13	0.882	0.854	0.905
Spectrophores	0.899	0.944	0.998	0.943	0.924	0.974
ShapeSignatures	0.883	0.896	0.975	0.881	1.76	0.95
Estate	0.876	0.833	1.1	0.826	1.04	0.915

Partner 7: Ideaconsult Ltd. (IDEA)

Molecular structures encoded in SMILES notation were used. Calculation of molecular descriptors was performed using DRAGON 5.4 software. The final number of calculated descriptors was 929. Two filtering criteria were then applied as preliminary variable selection procedure. The first filter is pairwise correlation which removes one of each pair of highly correlated ($R > 0.9$) descriptors. The second criteria removes constant and near constant descriptors. The final set of molecular descriptors (n=721) was

used as input variables for MobyDigs program which performs a more elaborate variable selection procedure by applying genetic algorithm.

The genetic algorithm was carried out by using the following *tabu* list criteria:

- R2(x,y) > 0.01
- Correlation between x/x < 0,95
- Standardized entropy > 0.05

If any descriptor violates one of the above conditions it was send to a t*abu* list, i.e. it was not used in the model developing process. Q2 (LOO cross-validation correlation coefficient) was used as fitness function and a maximum of six variables were allowed in the models developed.

The best 10 models (with 5 and 6 variables) were selected and their performance further checked by y-scrambling procedure and bootstrap validation (both were set up to 1000 iterations) as well as their performance against the validation test dataset. Models with 7 and 10 variables were generated by a similar procedure. Additionally, several models were created by choosing the descriptors by expert selection. This selection was based on the variables obtained by means of genetic algorithm, including also the modified versions of these variables (i.e. descriptors or functions of these descriptors).

2.3.2 Individual WP3 models used for Consensus

Partner 3: University of Insubria (UI)

Two MLR models, based respectively on 4 Dragon descriptors and 3 PaDEL descriptors, have been proposed for publication (paper under revision). These models were also reported in Deliverable 3.5 and presented in several meetings, e.g. SETAC-Europe 2011, CMTPI 2011, SETAC 2012, QSAR 2012, (in some cases a PaDEL models based on 4 variables was also proposed).

For the consensus study, two new models, based respectively on 5 DRAGON and PaDEL descriptors, were developed. Statistical parameters of the models (Split and Full) are reported in Table 20.

Table 20. UI models selected for the prediction of EC_{50} in *Oncorhynchus mykiss* (96h).

Model ID	Descriptors		N_{TR}	N_P	R^2	Q^2_{LOO}	Q^2_{EXT} (range)*	AD% on 386
DRAGON	MP, CIC1, JGI4, H-052, TPSA(Tot)	Split R	53	23	0.81	0.76	0.83 - 0.88	
		Split K	53	23	0.83	0.79	0.76 - 0.86	
		FULL	76	18#	0.82	0.79	0.87-0.88	93.8
PaDEL	VP-1, SHBint-2, minHBd, maxHaaCH, PubchemFP293	Split R	53	23	0.82	0.77	0.77-0.83	
		Split K	53	23	0.82	0.77	0.77-0.86	
		FULL	76	18#	0.81	0.78	0.83.0.84	97.7

*Range of values calculated using different Q^2_{EXT} parameters (Q^2_{EXT-F1}, Q^2_{EXT-F2}, Q^2_{EXT-F3} and CCC). #Evaluation set (EV)

Partner 4: IVL Swedish Environmental Research Institute (IVL)

The statistical parameters for the final PLS model developed by IVL for *Oncorhynchus mykiss* is presented in Table 21.

Table 21. Summarised statistics for IVL - PLS model for *Oncorhynchus mykiss* (96h).

N_{TR}	N_{EV}	Descriptors	N Descriptors	R^2	Q^2_{LOO}	RMSEE	RMSEP
19	18	DRAGON 6.0	2275	0.98	0.79	0.18	0.54

Partner 5: Linneaus University (LnU)

The PLS model selected for consensus is based on DRAGON descriptors (Dragon 6) projected down to four latent variables selected by cross-validation. These latent variables can be considered as new meta-descriptors. The performance of this model can be summarised as follows: RMSEC 0.285 (log units), R2cal 0.935, RMSEP 0.478 (log units), and Q2ext 0.814. One organotin compound and two organophosphorous compounds were slightly out of the applicability domain.

Partner 6: Helmholtz Zentrum Muenchen (HMGU)

The statistical parameters for model selected for the consensus study are summarised in Table 22.

Table 22. Statistical parameters calculated for Fish dataset using ASNN method and ChemAxon descriptors.

Statistical parameters	Training set (n=76)	Test set (n=18)
RMSE	0.68	0.58
MAE	0.51	0.38
R2	0.63	0.72
Q2	0.63	0.70

The model was based on 90 descriptors that were left after the unsupervised filtering.

Partner 7: Ideaconsult Ltd. (IDEA)

Three MLR models were selected by IDEA for the consensus study. The statistical parameters of the models are reported in Table 23.

Table 23. IDEA models selected for the prediction of EC_{50} in *Oncorhynchus mykiss* (96h).

Model ID	N_{TR}	N_{EV}	R^2	Q_{LOO}^2	$RMSE_{TR}$	$RMSE_{EXT}$	Ext. Validation	AD 386
IDEA-A	79	18	0.83	0.79	0.536	0.46	Yes (Q^2_{ext}>0.77)	97.4%
IDEA-B	79	18	0.85	0.81	0.512	0.46	Yes (Q^2_{ext}>0.79)	94.6%
IDEA-C	79	18	0.85	0.81	0.546	0.29	Yes (Q^2_{ext}>0.78)	91.7%

IDEA model A: Mp, nN, SIC1, EEig07d, O-058
IDEA model B: Mp, nN, SIC1, EEig07d, C-024, O-058
IDEA model C: Num(P), Mp, nN, SIC1, EEig07d, O-058

INDIVIDUAL WP3 MODELS SELECTED FOR THE CONSENSUS MODEL

The individual models selected by the different WP3 partners for the consensus study are summarized in Table 24. Statistical performances reported in the table are related to the individual training and validation sets used by different partners.

Table 24. Statistical performances of individual WP3 models selected for the Consensus model for LC_{50} in *Oncorhynchus mykiss* (96h).

WP3 Partner	N_{TR}	N_{EV}	R^2	Q^2_{LOO}	$RMSE_{TR}$	$RMSE_{EXT}$	Ext. Validation	AD 386
UI-Dragon	76	18	0.82	0.79	0.51	0.39*	YES (Q^2_{ext}>0.87)	94%
UI-PaDEL	76	18	0.81	0.78	0.53	0.45*	YES (Q^2_{ext}>0.83)	98%
IVL	19	18	0.98	0.79	0.18	0.54	Yes	40.2%
LnU	76	18	0.94	0.81	0.29	0.48	Yes (Q^2_{ext}=0.81)	Not verified
HMGU	76	18	0.63	0.63	0.68	0.58	Yes	84%
IDEA-A	79	18	0.83	0.79	0.536	0.46	Yes (Q^2_{ext}>0.77)	97.4%
IDEA-B	79	18	0.85	0.81	0.512	0.46	Yes (Q^2_{ext}>0.79)	94.6%
IDEA-C	79	18	0.85	0.81	0.546	0.29	Yes (Q^2_{ext}>0.78)	91.7%

2.3.3 Consensus predictions for 386 (B)TAZs

Individual WP3 models reported in Table 22, except the LnU model, were applied to predict acute toxicity in *Oncorhynchus mykiss* for 386 (B)TAZs with and without experimental data. Consensus predictions were then derived by averaging the predictions obtained by individual models.

As was done for algae and daphnia, individual model predictions deviation ("ID") and median deviation ("MD") from consensus predictions were calculated for each chemical.

As a general comment, high MD values (MD > 1) were observed for few (B)TAZs. In particular the highest MD was obtained for compound ID 22 (1325-58-2) (MD=2.16), which fell outside the applicability domain of the majority of WP3 models.

When the same analysis was performed only on (B)TAZs included in the AD of all the WP3 models (85 (B)TAZs), comparable predictions were obtained for all the compounds (0.06 < MD < 0.86). It is important to note that consensus predictions obtained for fish are highly influenced by the three IDEA models, which are based on very similar descriptors and the same training set, giving the same information.

Individual WP3 predictions and applicability domain, consensus predictions, individual model deviations ("ID") and median deviations ("MD") are reported in Appendix IV.

In Figure 6, individual model and consensus predictions for 386 (B)TAZs are reported.

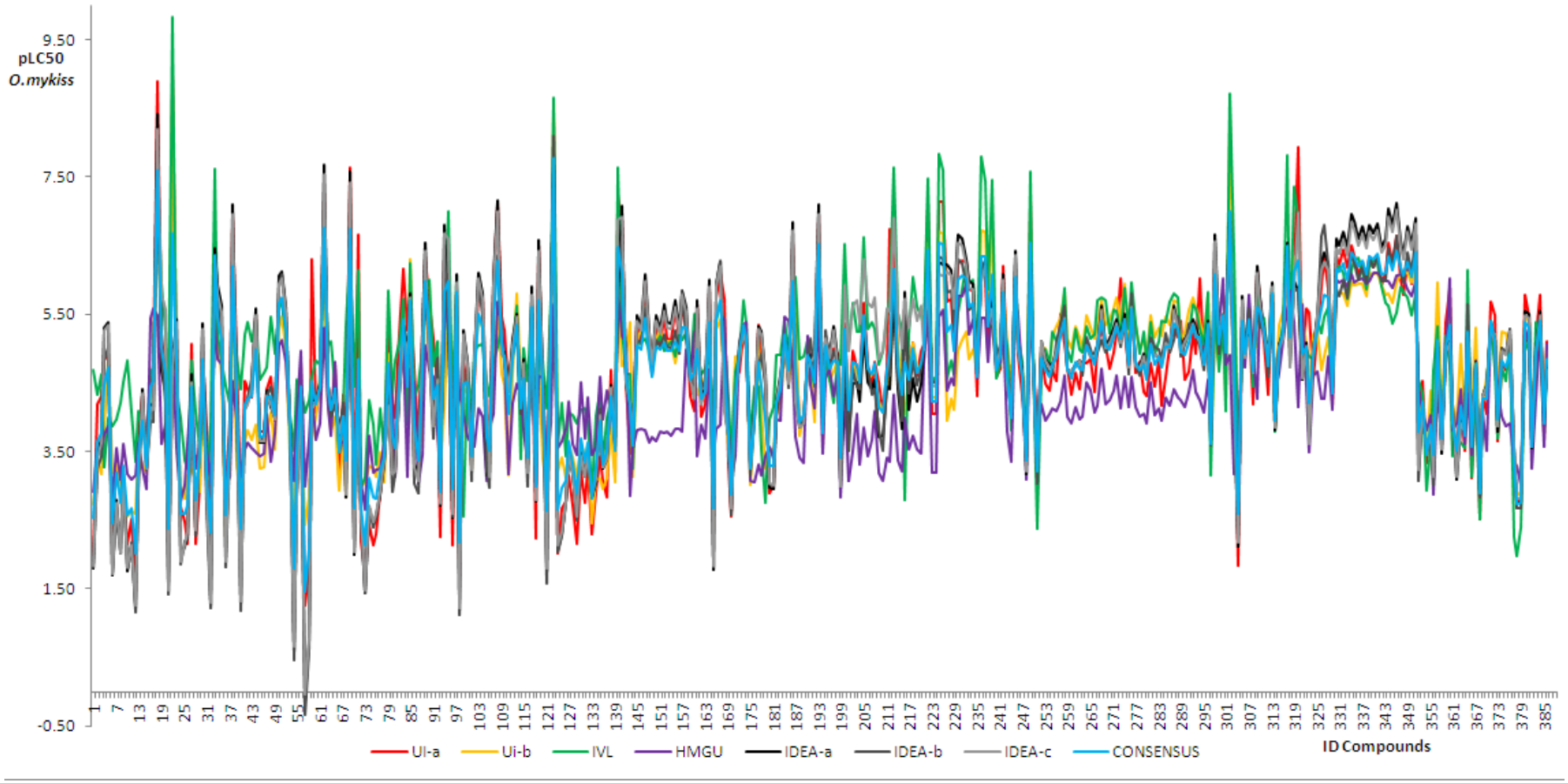

Figure 6. Prediction for 386 (B)TAZs obtained by individual WP3 models and consensus model for acute toxicity in *Oncorhynchus mykiss.*

UI-a = UI-Dragon model; UI-b = UI-PaDEL model.

2.4 Final considerations on Consensus models for aquatic toxicity

As an output of the CADASTER project, consensus predictions were proposed for more than 386 (B)TAZs, many of them included in the ECHA pre-registration list. Since the experimental data were not available for the majority of the considered chemicals, particular attention was given to the analysis of the applicability domain of the models used to derive consensus predictions. As expected, higher disagreement in prediction among different models was observed for compounds falling outside the domains of individual QSARs. Predicted values for these chemicals are considered as less reliable since model extrapolations, and should be used carefully.

Comparable predictions were obtained when only (B)TAZs included in the AD of all the WP3 models were considered. The fact that different models, based on different descriptors and/or modeling approaches, lead to similar predictions adds confidence and reliability to QSAR predictions obtained by Consensus approach. As it was commented for the Consensus models for MP/BP of PFCs, the combination of different modeling approaches helps to complement the deficiencies of one model with the support of another.

Consensus predictions of algae, daphnia and fish acute toxicity obtained for (B)TAZs included in the AD of the models were analyzed by PCA (Principal Component Analysis) in order to characterize the toxicological profile of BTAZs and to identify the most active compounds in the aquatic environment.

Since the models developed by IVL had a very limited AD when they were applied to the 386 (B)TAZs (AD_{algae}=38%, $AD_{daphnia}$=13%, AD_{fish}=40%) a PCA analysis based only on predictions into the AD of all the models could be performed only on a limited number of (B)TAZs (36 compounds). The results of this analysis are shown in Appendix V.

The analysis of (B)TAZs in PCA was also performed after exclusion of IVL predictions. In this way it was possible to characterize the aquatic toxicity of 120 (B)TAZs (Figure 7).

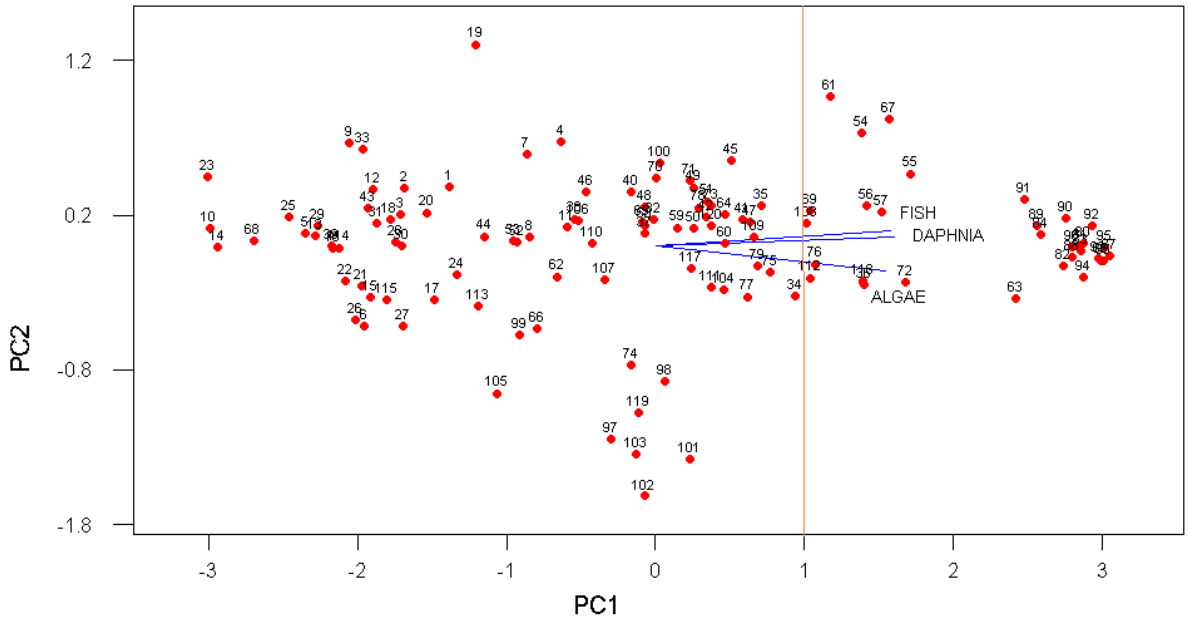

Figure 7. PCA analysis of consensus predictions obtained for algae (pEC50 *Pseudokirchneriella subcapitata*), daphnia (pEC50 *Daphnia magna*) and fish (pLC50 *Onchorhynchus mykiss*).

As it can be observed in Figure 7, PC1 (EV=91%) provides a trend of aquatic toxicity, since it separates (B)TAZs predicted as globally "more toxic" (i.e. with an overall higher toxicity for the three key organisms in the analyzed aquatic scenario), from less hazardous ones. An arbitrary cut-off along the PC1 was defined and the most globally active (B)TAZs (PC1 scores >1), among more than 300 (B)TAZs considered in this study, were identified (Table 25). For these chemicals, the following ranges of toxicity were predicted for the three organisms:

- *Pseudokirchneriella subcapitata:* EC_{50}(72h) 0.18 - 4.62 mg/L
- *Daphnia magna:* EC_{50}(48h) 0.19 – 5.37 mg/L
- *Onchorhynchus mykiss:* LC50(96h) 0.12 – 4.65 mg/L

According to EU classification criteria, as described in Annex VI of Directive 67/548/EEC (EC (1991)), these prioritized (B)TAZs can be all classified as "very toxic" ($EC(LC)_{50} \leq 1$ mg/L) or "toxic" ($EC(LC)_{50} \leq 10$ mg/L), and are threfore highlighted for the necessary experimental tests.

Table 25. Consensus predictions (into AD) for the "globally" most hazardous (B)TAZs for the three considered aquatic species and relative EU toxicity classes.

ID PCA	ID	CAS	Algae *(P. Subcapitata)*		Daphnia *(D. Magna)*		Fish *(O. mykiss)*	
			EC_{50} mg/l	EU CLASS	EC_{50} mg/l	EU CLASS	EC_{50} mg/l	EU CLASS
92	346	141079-15-4	0.29	very toxic	0.30	very toxic	0.12	very toxic
80	334	141078-95-7	0.24	very toxic	0.32	very toxic	0.14	very toxic
90	344	141079-13-2	0.35	very toxic	0.33	very toxic	0.14	very toxic
81	335	141078-99-1	0.22	very toxic	0.25	very toxic	0.16	very toxic
87	341	141079-07-4	0.19	very toxic	0.20	very toxic	0.17	very toxic
85	339	141079-03-0	0.19	very toxic	0.23	very toxic	0.18	very toxic
83	337	141079-01-8	0.22	very toxic	0.26	very toxic	0.19	very toxic
86	340	141079-06-3	0.18	very toxic	0.20	very toxic	0.20	very toxic
95	349	141079-18-7	0.24	very toxic	0.20	very toxic	0.20	very toxic
91	345	141079-14-3	0.55	very toxic	0.37	very toxic	0.22	very toxic
67	298	099793-38-1	2.56	toxic	1.36	very toxic	0.22	very toxic
54	230	081518-29-8	2.38	toxic	2.04	toxic	0.25	very toxic
82	336	141079-00-7	0.21	very toxic	0.33	very toxic	0.25	very toxic
93	347	141079-16-5	0.21	very toxic	0.19	very toxic	0.26	very toxic
89	343	141079-12-1	0.40	very toxic	0.32	very toxic	0.27	very toxic
84	338	141079-02-9	0.34	very toxic	0.29	very toxic	0.29	very toxic
88	342	141079-08-5	0.24	very toxic	0.23	very toxic	0.31	very toxic
96	350	141079-19-8	0.29	very toxic	0.22	very toxic	0.33	very toxic
55	232	081518-32-3	1.28	toxic	1.15	very toxic	0.35	very toxic
94	348	141079-17-6	0.20	very toxic	0.25	very toxic	0.37	very toxic
63	245	086598-92-7	0.22	very toxic	1.02	very toxic	0.39	very toxic
61	242	085509-19-9	4.62	toxic	1.63	toxic	0.40	very toxic
72	310	114369-43-6	0.46	very toxic	2.32	toxic	0.87	very toxic
56	233	081518-37-8	1.28	toxic	1.63	toxic	0.91	very toxic
57	234	081518-41-4	1.30	toxic	1.78	toxic	0.95	very toxic
69	305	106325-08-0	1.74	toxic	4.79	toxic	1.06	very toxic
118	384	XXX021	0.64	very toxic	4.25	toxic	1.23	very toxic
116	380	XXX017	0.65	very toxic	4.25	toxic	1.24	very toxic
108	371	XXX008	1.73	toxic	5.37	toxic	1.44	very toxic
36	158	055179-31-2	0.60	very toxic	2.95	toxic	1.66	toxic
76	316	125225-28-7	1.01	very toxic	5.22	toxic	1.87	toxic
112	376	XXX013	1.08	toxic	3.54	toxic	4.65	toxic

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APPENDIX I

Presentations of CADASTER Consensus models in Meetings.

QSPR Models for Predictions and Data Quality Assurances: Melting Point and Boiling Point of Perfluorinated Chemicals
Bhhatarai B., Teetz W., Öberg T., Liu T., Jeliazkova N., Kochev N., Pukalov O., Tetko I., Gramatica P.

- 2nd international workshop on new developments of fluorinated surfactants. Idstein, Germany, Jun 17-19, 2010.
- 18th European Symposium on QSARs (EuroQSAR2010) Rhodes (Greece) 19-24 Sept 2010.

QSAR prediction of aquatic and mammalian toxicity of triazoles and benzo-triazoles
Ester Papa, Stefano Cassani, Elisa D'Onofrio, Simona Kovarich, Partha Pratim Roy, Magnus Rahmberg, Sara Nilsson, Paola Gramatica

- 21th Annual Meeting SETAC-Europe, Milan, Italy, 15-19 May 2011.

QSAR prediction of aquatic toxicity of triazoles and benzo-triazoles
S. Cassani, E. D'Onofrio, S. Kovarich, E. Papa, P.P. Roy and P. Gramatica

- 6th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI), Maribor, Slovenia, 3-7 September 2011.

QSAR models for aquatic toxicity of triazoles and benzo-triazoles: WP3 results within the FP7 European Project CADASTER

- 6th SETAC World Congress (SETAC-Europe 22nd Annual Meeting), Berlin, Germany, 20-24 May 2012.
- 15th International Workshop on Quantitative Structure-Activity Relationships (QSAR2012) in Environmental and Health Sciences, Tallinn, Estonia, 18-22 June, 2012.

Papers on CADASTER Consensus models.

Bhhatarai, B.; Teez, W.; Liu, T.; Öberg, T.; Jeliazkova, N.; Kochev, N.; Pukalov, O.; Tetko, I.V.; Kovarich, S.; Papa, E.; Gramatica, P. *CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals*. Molecular Informatics, 2011, 30, 189-203.

PAPERS SUBMITTED OR IN PREPARATION:

Stefano Cassani, Simona Kovarich, Ester Papa, Partha Pratim Roy, Elisa D'Onofrio, and Paola Gramatica. *Daphnia and fish toxicity of (benzo)triazoles: validated QSAR models, and interspecies quantitative activity-activity modelling*. Submitted to Water Research (under revision)

QSAR models for algae acute toxicity (in preparation)

WP3 models and Consensus models for the prediction of aquatic toxicity of Triazoles and Benzotriazoles. Proceedings of the Final CADASTER Workshop.

Appendix II

Consensus models for EC50 in *Pseudokirchneriella subcapitata*: predictions and applicability domain of individual WP3 models (i.e. UI-Dragon (UI-a), UI-PaDEL (UI-b), IVL and HMGU), consensus predictions, individual model deviations (ID) and median deviation (MD).

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
1	000061-82-5	3.36	0.11	in	3.47	0.25	in	3.76	out	3.43	0.31	in	3.50	0.15	0.04	0.26	0.07	0.13
2	000094-97-3	3.71	0.10	in	4.67	0.33	in	4.56	out	3.71	0.36	in	4.16	0.46	0.51	0.39	0.45	0.45
3	000095-14-7	3.93	0.26	in	4.46	0.31	in	4.21	out	3.69	0.39	in	4.07	0.14	0.39	0.14	0.38	0.26
4	000130-34-7	9.86	3.57	out	5.43	0.19	in	5.75	out	5.83	0.56	in	6.72	3.14	1.28	0.97	0.89	1.57
5	000131-43-1	17.13	15.78	out	6.99	0.57	out	7.55	out	6.02	0.61	out	9.42	7.71	2.43	1.87	3.40	3.85
6	000134-58-7	3.50	0.11	in	4.27	0.51	out	4.34	out	3.44	0.3	in	3.89	0.38	0.38	0.45	0.45	0.42
7	000136-85-6	3.75	0.10	in	4.62	0.30	in	4.10	out	3.63	0.31	in	4.03	0.27	0.60	0.07	0.40	0.34
8	000273-40-5	3.80	0.28	in	4.95	0.69	out	4.11	out	3.55	0.38	in	4.10	0.31	0.85	0.01	0.55	0.43
9	000288-36-8	3.71	0.29	in	3.75	0.34	in	3.69	out	3.61	0.48	in	3.69	0.02	0.06	0.00	0.08	0.04
10	000288-88-0	3.71	0.29	in	3.48	0.27	in	3.89	in	3.53	0.3	in	3.65	0.06	0.17	0.24	0.12	0.15
11	000584-13-4	3.35	0.11	in	3.07	0.29	in	3.24	out	3.41	0.3	in	3.27	0.08	0.20	0.02	0.14	0.11
12	000932-64-9	3.03	0.14	in	2.85	0.32	in	3.78	out	3.43	0.35	in	3.27	0.25	0.42	0.51	0.16	0.33
13	000938-56-7	3.66	0.08	in	4.02	0.21	in	3.94	in	4.03	0.37	in	3.91	0.25	0.11	0.03	0.12	0.13
14	000939-07-1	3.93	0.09	in	4.48	0.18	in	4.07	out	4.13	0.4	in	4.15	0.22	0.33	0.08	0.02	0.16
15	000939-08-2	3.87	0.10	in	4.38	0.19	in	4.07	out	3.76	0.32	in	4.02	0.15	0.36	0.05	0.26	0.21
16	000944-91-2	4.08	0.06	in	4.04	0.12	in	4.58	in	4.17	0.39	in	4.22	0.14	0.18	0.36	0.05	0.18
17	000947-85-3	4.12	0.05	in	4.17	0.11	in	4.55	in	4.33	0.4	in	4.29	0.17	0.13	0.26	0.04	0.15
18	000974-29-8	4.93	0.20	in	5.59	0.14	in	5.46	out	5.2	0.55	in	5.29	0.37	0.29	0.17	0.09	0.23
19	001028-08-6	4.08	0.24	in	3.81	0.33	in	4.47	out	5	0.51	in	4.34	0.26	0.53	0.13	0.66	0.40
20	001031-47-6	4.16	0.06	in	4.76	0.06	in	4.70	out	4.95	0.44	in	4.64	0.48	0.11	0.06	0.31	0.24
21	001123-54-2	3.54	0.11	in	4.94	0.58	out	4.18	out	3.52	0.39	in	4.05	0.51	0.89	0.14	0.53	0.52
22	001325-58-2	14.35	4.64	out	9.32	1.29	out	11.04	out	5.64	0.74	out	10.09	4.26	0.77	0.96	4.45	2.61
23	001326-66-5	5.64	0.07	in	5.89	0.12	in	5.33	in	5.35	0.56	in	5.55	0.09	0.34	0.22	0.20	0.21

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
24	001455-77-2	3.35	0.11	in	2.88	0.27	in	3.18	out	3.35	0.3	in	3.19	0.16	0.31	0.01	0.16	0.16
25	001468-26-4	3.45	0.12	in	4.17	0.53	out	4.33	out	3.48	0.29	in	3.86	0.41	0.31	0.47	0.38	0.39
26	001600-61-9	3.60	0.10	in	3.77	0.07	in	4.27	out	3.98	0.48	in	3.91	0.30	0.14	0.37	0.07	0.22
27	001680-44-0	4.18	0.24	in	4.77	0.26	in	4.56	out	3.74	0.32	in	4.31	0.14	0.46	0.25	0.57	0.36
28	001704-66-1	3.79	0.10	in	5.03	0.21	in	4.85	out	4.28	0.57	in	4.49	0.70	0.54	0.37	0.21	0.45
29	002338-12-7	3.46	0.09	in	4.51	0.19	in	4.23	out	3.7	0.35	in	3.97	0.52	0.54	0.26	0.27	0.40
30	002440-22-4	4.38	0.06	in	4.50	0.07	in	4.73	in	4.6	0.4	in	4.55	0.17	0.05	0.18	0.05	0.11
31	002592-95-2	3.60	0.11	in	3.82	0.15	in	3.22	out	3.59	0.36	in	3.56	0.04	0.26	0.34	0.03	0.17
32	002683-90-1	3.51	0.12	in	4.79	0.60	out	4.14	out	3.53	0.32	in	3.99	0.48	0.80	0.15	0.46	0.47
33	003142-42-5	7.37	1.12	out	5.51	0.10	in	6.40	out	5.51	0.55	in	6.20	1.17	0.69	0.21	0.69	0.69
34	003147-75-9	5.44	0.13	in	5.43	0.09	in	5.21	out	5.58	0.44	in	5.41	0.02	0.02	0.20	0.17	0.10
35	003147-76-0	4.75	0.04	in	4.89	0.07	in	4.80	in	5.31	0.35	in	4.94	0.19	0.05	0.14	0.37	0.19
36	003232-84-6	3.21	0.12	in	2.68	0.34	in	3.64	out	3.41	0.3	in	3.24	0.02	0.56	0.40	0.17	0.29
37	003310-68-7	4.09	0.08	in	5.14	0.35	in	3.99	out	4.2	0.39	in	4.36	0.27	0.79	0.36	0.16	0.39
38	003333-62-8	6.72	0.25	in	6.12	0.19	in	6.67	out	5.98	0.42	in	6.37	0.35	0.25	0.30	0.39	0.32
39	003357-42-4	4.17	0.24	in	4.53	0.20	in	4.59	out	3.73	0.32	in	4.26	0.09	0.27	0.34	0.53	0.31
40	003641-10-9	3.28	0.12	in	3.76	0.30	in	3.71	out	3.45	0.37	in	3.55	0.27	0.21	0.16	0.10	0.19
41	003652-22-0	4.84	0.21	in	4.93	0.15	in	4.41	in	4.32	0.51	in	4.62	0.21	0.31	0.22	0.30	0.26
42	003652-23-1	4.93	0.24	in	5.04	0.14	in	4.54	in	4.41	0.53	in	4.73	0.20	0.31	0.19	0.32	0.25
43	003652-25-3	4.89	0.24	in	6.01	1.05	out	4.58	in	4.5	0.53	in	5.00	0.10	1.02	0.42	0.50	0.51
44	003652-27-5	5.67	0.30	in	5.72	0.22	in	5.36	out	4.91	0.49	in	5.42	0.25	0.31	0.06	0.51	0.28
45	003652-31-1	4.83	0.17	in	4.50	0.11	in	4.52	in	4	0.32	in	4.46	0.37	0.04	0.06	0.46	0.23
46	003652-32-2	4.92	0.20	in	4.42	0.10	in	4.51	in	4.06	0.31	in	4.48	0.44	0.06	0.03	0.42	0.24
47	003663-24-9	3.94	0.13	in	4.99	0.27	in	4.17	in	4.57	0.49	in	4.42	0.48	0.57	0.24	0.15	0.36
48	003683-95-2	5.60	0.58	out	4.88	0.11	in	4.45	out	4.05	0.49	in	4.75	0.85	0.14	0.30	0.70	0.50
49	003770-47-6	4.80	0.20	in	4.80	0.16	in	4.39	in	3.93	0.44	in	4.48	0.32	0.32	0.09	0.55	0.32
50	003846-71-7	5.29	0.07	in	5.47	0.08	in	5.42	out	5.61	0.48	in	5.45	0.16	0.02	0.02	0.16	0.09

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		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
51	003864-99-1	5.43	0.09	in	5.60	0.10	in	5.63	out	5.57	0.48	in	5.56	0.13	0.05	0.07	0.01	0.06
52	003896-11-5	4.97	0.05	in	5.21	0.07	in	5.28	out	5.28	0.42	in	5.19	0.21	0.03	0.09	0.09	0.11
53	004184-79-6	3.81	0.09	in	4.75	0.28	in	4.10	out	3.71	0.49	in	4.09	0.29	0.66	0.01	0.38	0.33
54	004314-22-1	3.16	0.16	in	3.01	0.23	in	3.47	out	3.44	0.29	in	3.27	0.11	0.26	0.20	0.17	0.19
55	004343-73-1	3.27	0.20	in	3.76	0.17	in	4.03	out	3.59	0.34	in	3.66	0.39	0.10	0.36	0.07	0.23
56	004368-68-7	4.34	0.22	in	4.13	0.23	in	4.06	in	4.31	0.39	in	4.21	0.13	0.08	0.15	0.10	0.12
57	004928-87-4	3.15	0.12	in	3.45	0.18	in	3.64	out	3.36	0.29	in	3.40	0.25	0.05	0.24	0.04	0.14
58	004928-88-5	3.13	0.16	in	3.67	0.17	in	3.86	out	3.45	0.35	in	3.53	0.40	0.14	0.33	0.08	0.24
59	005302-27-2	3.64	0.08	in	2.75	0.48	out	3.76	out	3.7	0.5	in	3.46	0.18	0.71	0.30	0.24	0.36
60	005369-84-6	4.62	0.05	in	4.62	0.13	in	4.40	in	4.76	0.44	in	4.60	0.02	0.02	0.20	0.16	0.10
61	005472-71-9	4.66	0.22	in	4.49	0.18	in	4.61	in	4.69	0.47	in	4.61	0.04	0.12	0.00	0.08	0.06
62	005516-20-1	6.98	0.29	in	6.39	0.20	in	7.27	out	5.98	0.43	in	6.66	0.32	0.26	0.62	0.68	0.47
63	005873-30-3	4.33	0.04	in	5.03	0.11	in	4.93	in	5.16	0.54	in	4.87	0.53	0.17	0.07	0.29	0.27
64	006054-53-1	5.09	0.08	in	5.30	0.14	in	4.84	out	5.09	0.46	in	5.08	0.01	0.22	0.24	0.01	0.12
65	006085-94-5	4.34	0.22	in	3.96	0.20	in	4.10	in	4.28	0.41	in	4.17	0.17	0.21	0.07	0.11	0.14
66	006299-39-4	3.43	0.09	in	4.55	0.20	in	4.49	out	3.55	0.34	in	4.00	0.58	0.55	0.48	0.45	0.52
67	006789-99-7	4.01	0.25	in	3.90	0.19	in	3.64	out	3.7	0.52	in	3.81	0.20	0.09	0.18	0.11	0.14
68	006818-99-1	3.38	0.12	in	3.66	0.25	in	3.77	out	3.52	0.3	in	3.58	0.20	0.08	0.19	0.06	0.13
69	006994-51-0	8.86	0.67	out	7.10	0.50	out	7.68	out	6.16	0.44	in	7.45	1.41	0.35	0.23	1.29	0.82
70	007170-01-6	3.42	0.11	in	3.58	0.24	in	3.47	out	3.52	0.32	in	3.50	0.08	0.08	0.03	0.02	0.05
71	007411-23-6	3.45	0.12	in	3.71	0.14	in	3.95	out	3.59	0.49	in	3.67	0.22	0.04	0.27	0.08	0.15
72	007532-52-7	3.55	0.10	in	4.24	0.11	in	3.99	out	3.68	0.47	in	3.87	0.31	0.37	0.13	0.19	0.25
73	010109-05-4	3.27	0.19	in	3.92	0.14	in	3.43	out	3.46	0.33	in	3.52	0.25	0.40	0.09	0.06	0.20
74	010187-79-8	3.89	0.09	in	4.28	0.12	in	4.95	out	4.57	0.61	out	4.42	0.53	0.14	0.53	0.15	0.34
75	010187-84-5	3.67	0.08	in	4.94	0.25	in	4.38	out	4.14	0.54	in	4.28	0.61	0.66	0.10	0.14	0.38
76	010187-86-7	3.64	0.09	in	3.88	0.16	in	4.22	out	4.29	0.52	in	4.01	0.36	0.13	0.21	0.28	0.25
77	010187-89-0	3.78	0.08	in	5.07	0.23	in	4.38	out	4.57	0.6	in	4.45	0.67	0.62	0.07	0.12	0.37

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		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
78	013091-80-0	3.47	0.09	in	4.76	0.21	in	4.67	out	3.82	0.35	in	4.18	0.71	0.58	0.49	0.36	0.54
79	013257-88-0	3.39	0.13	in	3.56	0.40	in	3.06	out	3.67	0.43	in	3.42	0.03	0.14	0.36	0.25	0.19
80	013351-73-0	3.73	0.10	in	3.87	0.27	in	4.09	out	3.62	0.33	in	3.83	0.10	0.04	0.26	0.21	0.15
81	014803-99-7	4.11	0.24	in	4.44	0.21	in	4.55	in	3.67	0.38	in	4.19	0.09	0.25	0.36	0.52	0.30
82	015421-84-8	3.89	0.10	in	4.68	0.12	in	4.70	in	4.07	0.45	in	4.34	0.45	0.35	0.37	0.27	0.36
83	015497-45-7	4.63	0.36	in	4.85	0.15	in	5.12	out	5.22	0.47	in	4.96	0.33	0.11	0.17	0.26	0.22
84	015805-10-4	5.09	0.20	in	6.12	0.38	in	4.96	out	5.17	0.48	in	5.33	0.24	0.78	0.37	0.16	0.39
85	016515-58-5	7.15	0.36	in	6.39	0.20	in	6.89	out	5.98	0.46	in	6.60	0.55	0.21	0.29	0.62	0.42
86	016584-05-7	3.74	0.08	in	3.99	0.27	in	3.99	out	3.79	0.35	in	3.88	0.14	0.11	0.12	0.09	0.11
87	018076-61-4	3.67	0.10	in	4.52	0.25	in	4.31	out	3.57	0.34	in	4.02	0.34	0.50	0.29	0.45	0.39
88	018811-70-6	4.93	0.08	in	5.84	0.24	in	5.41	out	5.49	0.45	in	5.42	0.49	0.42	0.01	0.07	0.25
89	019683-09-1	6.66	0.23	in	5.99	0.17	in	6.53	out	5.98	0.42	in	6.29	0.37	0.30	0.24	0.31	0.30
90	019794-93-5	6.81	0.25	in	5.67	0.25	in	6.13	out	6	0.45	in	6.15	0.66	0.49	0.02	0.15	0.33
91	021050-95-3	3.69	0.10	in	3.88	0.30	in	4.53	out	3.79	0.42	in	3.97	0.28	0.09	0.56	0.18	0.28
92	021532-04-7	4.40	0.33	in	3.53	0.28	in	3.50	out	3.78	0.43	in	3.80	0.60	0.27	0.31	0.02	0.30
93	023633-05-8	3.73	0.10	in	4.33	0.18	in	4.35	out	4.54	0.56	in	4.24	0.51	0.09	0.12	0.30	0.25
94	023711-34-4	5.12	0.09	in	5.47	0.12	in	5.22	in	4.79	0.48	in	5.15	0.03	0.32	0.07	0.36	0.20
95	024017-47-8	5.22	0.34	in	4.85	0.08	in	4.99	out	5.58	0.48	in	5.16	0.06	0.31	0.17	0.42	0.24
96	024054-57-7	3.73	0.10	in	4.27	0.15	in	4.66	out	4.36	0.55	in	4.26	0.52	0.02	0.40	0.10	0.26
97	025973-55-1	5.58	0.14	in	5.77	0.11	in	5.74	out	5.76	0.42	in	5.71	0.13	0.06	0.03	0.05	0.07
98	026621-45-4	3.14	0.12	in	3.00	0.25	in	3.65	out	3.44	0.37	in	3.31	0.16	0.31	0.34	0.13	0.24
99	027022-50-0	3.76	0.10	in	4.45	0.07	in	4.09	out	4.2	0.5	in	4.13	0.37	0.32	0.03	0.07	0.20
100	027210-18-0	4.05	0.05	in	4.77	0.09	in	5.14	in	4.45	0.45	in	4.60	0.56	0.17	0.54	0.15	0.35
101	027799-91-3	3.61	0.08	in	4.60	0.24	in	4.24	out	3.69	0.33	in	4.04	0.43	0.57	0.21	0.35	0.39
102	028401-89-0	4.16	0.04	in	4.90	0.09	in	5.16	out	4.67	0.46	in	4.72	0.56	0.18	0.44	0.05	0.31
103	028911-01-5	5.21	0.07	in	5.71	0.16	in	5.94	in	5.34	0.45	in	5.55	0.34	0.16	0.39	0.21	0.28
104	028981-97-7	5.14	0.08	in	5.57	0.16	in	5.64	in	5.27	0.42	in	5.40	0.27	0.16	0.24	0.13	0.20

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
105	029440-31-1	3.33	0.13	in	3.65	0.15	in	3.82	out	3.68	0.37	in	3.62	0.29	0.03	0.20	0.06	0.14
106	029878-31-7	3.74	0.10	in	4.62	0.30	in	4.15	in	3.59	0.35	in	4.02	0.29	0.60	0.12	0.43	0.36
107	029975-16-4	5.03	0.09	in	5.45	0.15	in	5.57	in	5.07	0.46	in	5.28	0.25	0.17	0.29	0.21	0.23
108	031251-03-3	5.51	0.11	in	5.63	0.14	in	6.18	out	5.74	0.48	in	5.76	0.25	0.14	0.42	0.02	0.21
109	031409-18-4	4.48	0.09	in	4.76	0.22	in	4.64	in	4.43	0.42	in	4.58	0.09	0.18	0.06	0.15	0.12
110	031701-42-5	4.29	0.07	in	4.33	0.06	in	5.15	out	4.51	0.58	in	4.57	0.28	0.24	0.58	0.06	0.29
111	032362-89-3	4.67	0.16	in	4.96	0.26	in	4.09	out	4.19	0.47	in	4.48	0.19	0.48	0.38	0.29	0.34
112	032723-50-5	4.46	0.06	in	5.09	0.10	in	5.07	in	4.63	0.49	in	4.81	0.35	0.28	0.26	0.18	0.27
113	034771-66-9	6.41	0.19	in	5.89	0.15	in	6.51	out	5.81	0.46	in	6.15	0.25	0.27	0.36	0.34	0.31
114	035515-45-8	3.86	0.10	in	4.35	0.09	in	4.45	out	4.36	0.54	in	4.26	0.39	0.10	0.20	0.10	0.20
115	036325-69-6	4.90	0.07	in	6.03	0.47	out	5.36	out	5.57	0.39	in	5.46	0.57	0.57	0.10	0.11	0.34
116	036411-52-6	4.12	0.08	in	5.13	0.25	in	4.76	out	4.05	0.35	in	4.52	0.40	0.61	0.25	0.47	0.43
117	036437-37-3	5.28	0.10	in	5.43	0.08	in	5.52	out	5.59	0.41	in	5.46	0.18	0.02	0.07	0.13	0.10
118	036791-04-5	3.86	0.11	in	3.53	0.14	in	3.98	out	4.22	0.54	in	3.90	0.04	0.37	0.08	0.32	0.20
119	037160-06-8	5.16	0.20	in	6.03	0.18	in	5.48	out	5.13	0.53	in	5.45	0.29	0.58	0.03	0.32	0.30
120	038942-51-7	4.37	0.08	in	4.59	0.11	in	4.50	in	4.22	0.36	in	4.42	0.05	0.17	0.08	0.20	0.12
121	039968-33-7	3.53	0.12	in	3.84	0.18	in	4.22	out	3.55	0.35	in	3.78	0.26	0.05	0.44	0.23	0.25
122	040054-69-1	6.23	0.28	in	5.75	0.19	in	5.98	in	5.39	0.39	in	5.84	0.39	0.08	0.14	0.45	0.27
123	041083-11-8	5.41	0.20	in	4.39	0.29	in	5.09	out	5.26	0.62	out	5.04	0.37	0.65	0.05	0.22	0.32
124	041735-28-8	3.66	0.12	in	4.85	0.14	in	4.62	out	4.4	0.57	in	4.38	0.72	0.47	0.23	0.02	0.36
125	041735-29-9	3.82	0.11	in	4.98	0.13	in	4.89	out	4.67	0.56	in	4.59	0.77	0.39	0.30	0.08	0.39
126	041735-30-2	3.81	0.14	in	4.71	0.06	in	4.64	out	4.57	0.57	in	4.43	0.62	0.28	0.21	0.14	0.31
127	041735-38-0	4.15	0.11	in	4.22	0.09	in	5.04	out	5.47	0.51	in	4.72	0.57	0.50	0.32	0.75	0.54
128	041735-41-5	3.77	0.08	in	4.17	0.16	in	4.52	out	4.41	0.55	in	4.22	0.45	0.05	0.30	0.19	0.25
129	041735-42-6	3.65	0.09	in	3.68	0.14	in	4.45	out	4.05	0.49	in	3.95	0.31	0.28	0.49	0.10	0.29
130	041735-44-8	4.15	0.11	in	4.23	0.10	in	5.10	out	5	0.54	in	4.62	0.47	0.39	0.48	0.38	0.43
131	041735-45-9	3.76	0.08	in	4.26	0.16	in	4.61	out	4.43	0.55	in	4.27	0.50	0.01	0.35	0.16	0.25

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
132	041735-50-6	4.14	0.11	in	4.43	0.10	in	4.91	out	5.44	0.55	in	4.73	0.59	0.30	0.18	0.71	0.44
133	041735-51-7	3.63	0.15	in	4.35	0.14	in	4.38	out	4.32	0.61	out	4.17	0.54	0.18	0.21	0.15	0.27
134	041735-54-0	3.57	0.09	in	4.38	0.11	in	4.47	out	3.97	0.5	in	4.10	0.53	0.28	0.37	0.13	0.33
135	041735-55-1	4.60	0.12	in	4.19	0.18	in	4.51	out	4.47	0.5	in	4.44	0.16	0.25	0.07	0.03	0.13
136	041735-56-2	4.52	0.11	in	4.18	0.10	in	4.07	out	4.52	0.57	in	4.32	0.20	0.14	0.25	0.20	0.20
137	041735-57-3	3.67	0.09	in	4.01	0.15	in	4.56	out	4.37	0.54	in	4.15	0.48	0.15	0.41	0.22	0.31
138	041814-78-2	4.21	0.11	in	4.64	0.16	in	4.47	in	4.16	0.43	in	4.37	0.16	0.26	0.10	0.21	0.18
139	041834-21-3	4.56	0.11	in	4.21	0.13	in	4.16	in	4.46	0.5	in	4.35	0.21	0.14	0.19	0.11	0.16
140	042509-80-8	4.79	0.45	out	4.04	0.30	in	4.73	out	4.89	0.5	in	4.61	0.18	0.58	0.12	0.28	0.29
141	043029-44-3	5.42	0.20	in	5.61	0.12	in	5.27	out	5.36	0.48	in	5.41	0.00	0.19	0.14	0.05	0.10
142	043121-43-3	4.65	0.05	in	4.80	0.06	in	4.92	in	5.03	0.41	in	4.85	0.20	0.05	0.07	0.18	0.12
143	051627-14-6	11.54	4.12	out	6.32	0.20	in	6.32	out	5.96	0.48	in	7.54	4.01	1.22	1.21	1.58	2.00
144	053817-16-6	3.33	0.12	in	4.11	0.29	in	3.83	out	3.5	0.46	in	3.69	0.36	0.41	0.14	0.19	0.27
145	054028-81-8	5.13	0.08	in	5.51	0.16	in	5.56	in	5.23	0.42	in	5.36	0.23	0.15	0.20	0.13	0.18
146	054028-83-0	5.19	0.05	in	5.69	0.15	in	5.81	in	5.57	0.38	in	5.57	0.37	0.12	0.25	0.00	0.19
147	054028-84-1	5.80	0.12	in	6.02	0.17	in	6.08	out	5.7	0.4	in	5.90	0.10	0.12	0.18	0.20	0.15
148	054028-85-2	6.30	0.43	in	5.48	0.18	in	5.47	in	4.94	0.46	in	5.55	0.75	0.07	0.08	0.61	0.38
149	054028-86-3	4.81	0.07	in	5.25	0.15	in	5.41	in	4.93	0.51	in	5.10	0.29	0.15	0.31	0.17	0.23
150	054028-89-6	5.15	0.08	in	5.51	0.15	in	5.62	in	5.16	0.42	in	5.36	0.21	0.15	0.26	0.20	0.20
151	054028-90-9	5.33	0.06	in	5.69	0.15	in	5.86	in	5.75	0.36	in	5.66	0.33	0.03	0.20	0.09	0.16
152	054028-91-0	5.07	0.09	in	5.30	0.15	in	5.28	in	5.09	0.43	in	5.18	0.12	0.11	0.10	0.09	0.11
153	054028-92-1	5.11	0.05	in	5.48	0.14	in	5.55	in	5.54	0.37	in	5.42	0.31	0.06	0.13	0.12	0.16
154	054028-93-2	5.22	0.06	in	5.48	0.15	in	5.54	in	5.56	0.37	in	5.45	0.23	0.03	0.09	0.11	0.12
155	054028-94-3	5.10	0.20	in	5.16	0.16	in	5.22	in	5	0.42	in	5.12	0.02	0.04	0.10	0.12	0.07
156	054028-95-4	5.13	0.05	in	5.46	0.15	in	5.67	in	5.37	0.38	in	5.41	0.27	0.05	0.26	0.04	0.16
157	054123-06-7	6.08	0.27	in	5.65	0.20	in	5.73	out	5.06	0.43	in	5.63	0.45	0.02	0.10	0.57	0.28
158	055179-31-2	5.79	0.11	in	5.50	0.09	in	5.41	out	5.95	0.34	in	5.66	0.13	0.16	0.26	0.29	0.21

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
159	055219-65-3	4.67	0.05	in	4.82	0.07	in	4.50	in	5.08	0.41	in	4.77	0.10	0.06	0.27	0.31	0.18
160	055375-40-1	4.55	0.45	out	4.35	0.12	in	4.37	out	4.47	0.57	in	4.44	0.12	0.08	0.07	0.03	0.08
161	055425-38-2	5.44	0.21	in	7.23	0.80	out	5.76	out	5.28	0.5	in	5.93	0.49	1.30	0.16	0.65	0.65
162	056383-06-3	4.28	0.09	in	4.77	0.13	in	4.72	in	4.52	0.48	in	4.57	0.29	0.20	0.15	0.05	0.17
163	056383-11-0	4.28	0.09	in	4.73	0.11	in	4.65	in	4.61	0.47	in	4.57	0.28	0.16	0.08	0.04	0.14
164	056396-43-1	5.30	0.07	in	5.57	0.09	in	5.55	in	5.2	0.46	in	5.40	0.11	0.17	0.14	0.20	0.16
165	056881-36-8	3.60	0.09	in	3.91	0.14	in	4.14	out	3.56	0.29	in	3.80	0.20	0.11	0.34	0.24	0.22
166	057801-81-7	6.11	0.28	in	5.74	0.20	in	5.75	out	5.05	0.48	in	5.66	0.45	0.08	0.09	0.61	0.30
167	057801-94-2	6.14	0.30	in	5.82	0.20	in	5.71	out	4.98	0.57	in	5.66	0.48	0.16	0.05	0.68	0.34
168	059026-08-3	4.62	0.32	in	4.07	0.11	in	4.56	out	5.21	0.45	in	4.61	0.00	0.55	0.05	0.60	0.30
169	059338-86-2	3.62	0.09	in	4.78	0.14	in	4.76	out	3.92	0.43	in	4.27	0.65	0.51	0.49	0.35	0.50
170	059338-92-0	3.58	0.08	in	4.60	0.14	in	4.49	out	3.6	0.3	in	4.07	0.49	0.53	0.43	0.47	0.48
171	059338-93-1	5.41	0.08	in	6.76	1.00	out	5.43	out	5.89	0.34	in	5.87	0.46	0.89	0.44	0.02	0.45
172	060207-31-0	4.62	0.07	in	4.76	0.11	in	5.14	in	4.64	0.45	in	4.79	0.17	0.03	0.35	0.15	0.18
173	060207-90-1	5.03	0.05	in	5.06	0.09	in	5.53	in	5.29	0.4	in	5.23	0.20	0.17	0.30	0.06	0.18
174	060207-93-4	4.86	0.04	in	4.97	0.10	in	5.42	in	5.17	0.4	in	5.11	0.25	0.13	0.31	0.06	0.19
175	060932-58-3	3.56	0.08	in	4.45	0.18	in	4.26	out	3.64	0.31	in	3.98	0.42	0.48	0.28	0.34	0.38
176	061691-97-2	4.00	0.18	in	4.55	0.13	in	4.30	in	4.63	0.49	in	4.37	0.38	0.18	0.07	0.26	0.22
177	063216-86-4	14.77	9.61	out	6.81	0.55	out	7.28	out	5.95	0.61	out	8.70	6.07	1.89	1.42	2.75	3.03
178	063251-40-1	9.70	3.77	out	5.42	0.14	in	5.55	out	5.81	0.55	in	6.62	3.08	1.20	1.07	0.81	1.54
179	063870-37-1	5.23	0.34	in	5.16	0.13	in	4.18	out	4.38	0.5	in	4.74	0.49	0.42	0.56	0.36	0.46
180	064057-50-7	3.96	0.11	in	4.56	0.15	in	4.84	out	4.63	0.56	in	4.50	0.54	0.06	0.34	0.13	0.27
181	064082-38-8	4.01	0.11	in	5.33	0.19	in	4.57	out	4.53	0.59	in	4.61	0.60	0.72	0.04	0.08	0.36
182	066104-34-5	4.40	0.04	in	4.77	0.10	in	5.00	out	5.15	0.49	in	4.83	0.43	0.06	0.17	0.32	0.25
183	066104-44-7	4.55	0.05	in	4.91	0.11	in	4.98	out	5.07	0.44	in	4.88	0.33	0.03	0.11	0.19	0.16
184	066246-88-6	4.69	0.08	in	4.83	0.14	in	5.10	in	4.89	0.4	in	4.88	0.19	0.04	0.22	0.01	0.12
185	066492-64-6	4.20	0.05	in	4.38	0.08	in	4.76	in	4.35	0.51	in	4.42	0.22	0.04	0.34	0.07	0.17

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		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
186	066535-86-2	4.97	0.09	in	5.20	0.13	in	5.86	out	5.09	0.51	in	5.28	0.31	0.08	0.58	0.19	0.29
187	066975-54-0	6.34	0.51	out	7.52	0.54	out	7.00	out	5.64	0.66	out	6.62	0.29	0.89	0.38	0.98	0.64
188	067465-03-6	4.89	0.21	in	5.05	0.13	in	4.67	in	4.52	0.48	in	4.78	0.11	0.27	0.12	0.26	0.19
189	067465-05-8	4.32	0.09	in	5.08	0.13	in	4.48	in	5.03	0.46	in	4.73	0.41	0.35	0.25	0.30	0.33
190	068049-83-2	4.86	0.07	in	6.56	2.05	out	5.60	in	5.34	0.41	in	5.59	0.73	0.97	0.01	0.25	0.49
191	069141-50-0	4.43	0.23	in	4.35	0.11	in	4.00	out	4.84	0.5	in	4.41	0.02	0.05	0.40	0.43	0.23
192	070292-10-3	4.43	0.04	in	4.88	0.08	in	5.00	in	4.65	0.48	in	4.74	0.31	0.14	0.26	0.09	0.20
193	070321-86-7	7.33	0.36	in	6.85	0.36	in	7.09	out	6.12	0.43	in	6.85	0.48	0.01	0.24	0.73	0.36
194	075020-35-8	4.10	0.06	in	5.07	0.16	in	4.65	out	4.43	0.43	in	4.56	0.46	0.50	0.09	0.13	0.30
195	075736-33-3	5.01	0.07	in	5.16	0.09	in	5.02	in	5.23	0.44	in	5.10	0.09	0.05	0.09	0.13	0.09
196	076608-88-3	4.65	0.06	in	4.78	0.08	in	4.37	in	4.84	0.4	in	4.66	0.01	0.12	0.29	0.18	0.15
197	076674-21-0	4.86	0.09	in	4.75	0.09	in	4.96	in	4.82	0.4	in	4.85	0.01	0.10	0.11	0.03	0.06
198	076738-62-0	4.92	0.07	in	4.95	0.09	in	4.76	in	5.1	0.41	in	4.93	0.01	0.01	0.17	0.17	0.09
199	077314-77-3	4.05	0.06	in	5.17	0.28	in	4.52	out	4.31	0.49	in	4.51	0.46	0.65	0.01	0.20	0.33
200	078149-96-9	4.16	0.32	in	3.83	0.33	in	4.87	out	5.21	0.44	in	4.52	0.35	0.69	0.35	0.69	0.52
201	078150-00-2	4.26	0.06	in	5.27	0.15	in	4.82	out	5.1	0.44	in	4.86	0.60	0.40	0.05	0.24	0.32
202	078150-02-4	3.89	0.17	in	3.72	0.33	in	4.35	out	4.67	0.48	in	4.16	0.26	0.44	0.19	0.51	0.35
203	078218-51-6	4.31	0.06	in	4.96	0.06	in	4.95	out	5.43	0.43	in	4.91	0.60	0.05	0.04	0.52	0.30
204	078218-52-7	3.59	0.11	in	3.53	0.34	in	4.08	out	4.07	0.49	in	3.82	0.23	0.29	0.26	0.25	0.26
205	078218-53-8	4.54	0.44	out	3.97	0.34	in	4.79	out	5.47	0.59	in	4.69	0.15	0.72	0.10	0.78	0.44
206	078218-54-9	3.74	0.09	in	3.66	0.34	in	4.08	out	4.44	0.51	in	3.98	0.24	0.32	0.10	0.46	0.28
207	078218-55-0	4.41	0.06	in	4.90	0.07	in	5.11	out	5.68	0.41	in	5.02	0.62	0.12	0.08	0.66	0.37
208	078218-56-1	4.68	0.06	in	5.08	0.06	in	4.99	out	5.72	0.45	in	5.12	0.44	0.04	0.12	0.60	0.30
209	078218-57-2	3.46	0.11	in	3.35	0.37	in	3.95	out	3.81	0.43	in	3.64	0.18	0.29	0.31	0.17	0.24
210	078218-58-3	3.97	0.07	in	5.10	0.15	in	4.66	out	4.62	0.43	in	4.59	0.62	0.51	0.07	0.03	0.31
211	078218-59-4	3.75	0.12	in	3.63	0.33	in	4.21	out	4.39	0.52	in	4.00	0.25	0.37	0.22	0.39	0.31
212	078218-60-7	3.67	0.19	in	4.15	0.13	in	4.35	out	4.33	0.57	in	4.12	0.45	0.02	0.23	0.21	0.23

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
213	078218-61-8	5.82	1.05	out	4.30	0.37	in	5.51	out	5.53	0.69	out	5.29	0.53	0.99	0.22	0.24	0.49
214	078218-65-2	4.54	0.27	in	3.62	0.42	in	4.00	out	3.91	0.43	in	4.02	0.52	0.40	0.02	0.11	0.26
215	078218-66-3	4.41	0.28	in	3.92	0.21	in	3.89	out	3.82	0.4	in	4.01	0.40	0.09	0.12	0.19	0.20
216	078324-76-2	4.49	0.07	in	5.39	0.12	in	4.67	out	4.51	0.71	out	4.76	0.27	0.63	0.10	0.25	0.31
217	078371-72-9	3.67	0.16	in	3.39	0.62	out	4.49	out	4.94	0.49	in	4.12	0.45	0.73	0.37	0.82	0.59
218	078371-73-0	4.27	0.35	in	3.65	0.66	out	4.88	out	5.11	0.57	in	4.48	0.21	0.83	0.40	0.63	0.52
219	078371-74-1	3.83	0.20	in	3.49	0.63	out	4.62	out	5.05	0.48	in	4.25	0.42	0.76	0.37	0.80	0.59
220	078592-90-2	3.93	0.11	in	3.78	0.34	in	4.28	out	4.63	0.51	in	4.15	0.22	0.37	0.12	0.48	0.30
221	079983-71-4	4.78	0.09	in	4.92	0.09	in	5.21	in	5.05	0.44	in	4.99	0.21	0.07	0.22	0.06	0.14
222	080301-64-0	6.24	0.92	out	5.76	0.14	in	6.06	out	5.65	0.4	in	5.93	0.32	0.16	0.13	0.28	0.22
223	080584-88-9	4.16	0.19	in	4.71	0.12	in	4.57	out	4.74	0.5	in	4.54	0.39	0.17	0.02	0.20	0.19
224	080584-89-0	4.13	0.19	in	4.70	0.12	in	4.57	out	4.72	0.51	in	4.53	0.40	0.17	0.04	0.19	0.20
225	080584-90-3	6.44	0.96	out	5.89	0.15	in	6.45	out	5.71	0.42	in	6.12	0.32	0.23	0.32	0.41	0.32
226	080595-74-0	6.48	0.97	out	5.90	0.15	in	6.41	out	5.84	0.44	in	6.16	0.32	0.26	0.25	0.32	0.29
227	081518-26-5	5.03	0.07	in	5.30	0.10	in	5.00	in	4.72	0.43	in	5.01	0.01	0.29	0.01	0.29	0.15
228	081518-27-6	5.17	0.07	in	5.59	0.13	in	5.25	out	4.91	0.46	in	5.23	0.06	0.36	0.02	0.32	0.19
229	081518-28-7	5.13	0.06	in	5.45	0.11	in	5.11	in	5.04	0.45	in	5.18	0.05	0.26	0.07	0.14	0.13
230	081518-29-8	5.03	0.08	in	5.33	0.16	in	5.27	in	4.95	0.42	in	5.15	0.12	0.18	0.13	0.20	0.16
231	081518-31-2	5.18	0.11	in	6.47	0.56	out	5.53	in	5.47	0.39	in	5.66	0.49	0.81	0.13	0.19	0.40
232	081518-32-3	5.21	0.11	in	5.55	0.17	in	5.54	in	5.47	0.37	in	5.44	0.23	0.11	0.10	0.03	0.12
233	081518-37-8	5.29	0.12	in	5.49	0.14	in	5.39	in	5.43	0.4	in	5.40	0.11	0.10	0.01	0.03	0.06
234	081518-41-4	5.27	0.10	in	5.69	0.14	in	5.64	out	5.47	0.41	in	5.52	0.25	0.17	0.12	0.05	0.15
235	082200-72-4	4.67	0.05	in	4.82	0.07	in	4.58	in	4.97	0.45	in	4.76	0.09	0.06	0.18	0.21	0.14
236	083044-89-7	8.07	1.31	out	6.28	0.22	in	7.30	out	5.69	0.53	in	6.83	1.23	0.55	0.46	1.14	0.85
237	083044-90-0	7.71	1.01	out	6.40	0.25	in	7.13	out	5.72	0.51	in	6.74	0.97	0.34	0.39	1.02	0.68
238	083044-91-1	5.60	0.17	in	5.65	0.11	in	6.30	out	5.7	0.37	in	5.81	0.22	0.16	0.49	0.11	0.24
239	083366-66-9	8.92	0.83	out	6.56	0.48	out	7.36	out	5.91	0.51	in	7.19	1.73	0.62	0.17	1.28	0.95

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
240	083657-17-4	4.79	0.06	in	4.98	0.07	in	4.72	in	5.03	0.41	in	4.88	0.09	0.10	0.16	0.15	0.12
241	083657-24-3	4.87	0.07	in	5.19	0.08	in	4.99	in	5.39	0.42	in	5.11	0.24	0.08	0.12	0.28	0.18
242	085509-19-9	4.63	0.07	in	4.86	0.11	in	4.65	in	5.02	0.35	in	4.79	0.16	0.07	0.14	0.23	0.15
243	085634-51-1	5.89	0.12	in	5.53	0.10	in	5.71	out	5.77	0.44	in	5.72	0.16	0.19	0.02	0.05	0.11
244	086386-73-4	4.74	0.14	in	4.75	0.10	in	5.02	in	4.86	0.46	in	4.84	0.10	0.09	0.18	0.02	0.10
245	086598-92-7	6.80	0.33	in	6.01	0.13	in	6.39	out	6.02	0.39	in	6.31	0.50	0.30	0.09	0.29	0.29
246	088671-89-0	4.85	0.13	in	5.06	0.12	in	5.17	in	5.19	0.42	in	5.07	0.22	0.01	0.10	0.12	0.11
247	089482-17-7	4.67	0.05	in	4.82	0.07	in	4.57	in	4.91	0.46	in	4.74	0.07	0.08	0.17	0.17	0.12
248	089786-04-9	5.25	0.13	in	5.51	0.71	out	4.51	out	4.68	0.56	in	4.99	0.26	0.52	0.47	0.31	0.39
249	094270-86-7	6.44	0.96	out	5.89	0.15	in	6.26	out	5.66	0.42	in	6.06	0.38	0.17	0.20	0.40	0.29
250	094361-06-5	5.04	0.06	in	4.83	0.09	in	4.91	in	5.09	0.44	in	4.97	0.07	0.14	0.06	0.12	0.10
251	094667-47-7	3.59	0.09	in	4.00	0.08	in	3.30	out	3.7	0.31	in	3.64	0.06	0.35	0.35	0.06	0.20
252	097232-75-2	6.08	0.13	in	5.78	0.09	in	6.16	out	5.91	0.43	in	5.98	0.10	0.20	0.18	0.07	0.14
253	098518-95-7	5.04	0.24	in	4.73	0.08	in	5.28	in	5.19	0.47	in	5.06	0.02	0.33	0.22	0.13	0.17
254	098518-96-8	4.53	0.04	in	4.70	0.08	in	5.07	in	4.9	0.48	in	4.80	0.27	0.10	0.27	0.10	0.19
255	098518-99-1	4.99	0.07	in	4.86	0.08	in	5.39	in	5.24	0.46	in	5.12	0.13	0.26	0.27	0.12	0.19
256	098519-00-7	5.06	0.09	in	5.13	0.08	in	5.61	in	5.58	0.39	in	5.34	0.29	0.22	0.27	0.24	0.25
257	098519-01-8	5.16	0.07	in	5.30	0.08	in	5.72	in	5.54	0.45	in	5.43	0.27	0.13	0.29	0.11	0.20
258	098519-02-9	5.62	0.12	in	5.56	0.09	in	6.17	out	6	0.36	in	5.84	0.22	0.28	0.33	0.16	0.25
259	098519-04-1	4.96	0.08	in	4.99	0.08	in	5.36	in	5.18	0.44	in	5.12	0.16	0.13	0.23	0.06	0.15
260	098519-05-2	4.85	0.11	in	4.86	0.08	in	5.39	in	5.07	0.47	in	5.04	0.19	0.18	0.35	0.03	0.19
261	098519-06-3	5.09	0.06	in	5.08	0.08	in	5.63	in	5.36	0.38	in	5.29	0.20	0.22	0.34	0.07	0.21
262	098519-07-4	5.01	0.11	in	4.95	0.08	in	5.51	in	5.3	0.39	in	5.19	0.18	0.24	0.32	0.11	0.21
263	098519-24-5	4.87	0.10	in	4.78	0.08	in	5.20	in	5	0.53	in	4.96	0.09	0.18	0.24	0.04	0.14
264	098519-25-6	5.16	0.06	in	5.26	0.08	in	5.85	in	5.71	0.41	in	5.49	0.33	0.24	0.35	0.22	0.28
265	098519-26-7	5.03	0.07	in	5.17	0.08	in	5.64	in	5.21	0.48	in	5.26	0.23	0.09	0.38	0.05	0.19
266	098519-28-9	4.99	0.07	in	4.95	0.08	in	5.63	in	5.33	0.4	in	5.23	0.23	0.28	0.41	0.10	0.26

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
267	098519-29-0	5.18	0.06	in	5.07	0.08	in	5.91	in	5.57	0.36	in	5.43	0.25	0.36	0.48	0.14	0.31
268	098519-30-3	6.42	0.33	in	5.64	0.13	in	6.45	out	6.03	0.37	in	6.13	0.28	0.50	0.31	0.10	0.30
269	098519-31-4	5.18	0.06	in	5.07	0.08	in	5.95	out	5.53	0.39	in	5.43	0.25	0.36	0.52	0.10	0.31
270	098519-32-5	5.36	0.07	in	5.17	0.09	in	5.57	in	5.58	0.43	in	5.42	0.06	0.25	0.15	0.16	0.15
271	098519-33-6	5.56	0.08	in	5.27	0.09	in	5.73	out	5.68	0.43	in	5.56	0.00	0.29	0.17	0.12	0.15
272	098519-34-7	5.58	0.08	in	5.33	0.10	in	5.78	out	5.74	0.41	in	5.61	0.03	0.27	0.17	0.13	0.15
273	098519-35-8	5.23	0.08	in	5.16	0.09	in	5.43	in	5.34	0.44	in	5.29	0.06	0.13	0.14	0.05	0.10
274	098519-37-0	5.96	0.14	in	5.49	0.11	in	6.03	out	5.83	0.39	in	5.83	0.13	0.34	0.21	0.00	0.17
275	098519-39-2	4.99	0.07	in	4.86	0.08	in	5.50	in	5.22	0.47	in	5.14	0.15	0.28	0.35	0.08	0.22
276	098519-41-6	5.60	0.10	in	5.61	0.10	in	6.41	out	5.98	0.35	in	5.90	0.30	0.29	0.51	0.08	0.29
277	098519-43-8	5.09	0.06	in	5.08	0.08	in	5.69	in	5.34	0.4	in	5.30	0.21	0.22	0.39	0.04	0.21
278	098519-49-4	4.87	0.10	in	4.78	0.08	in	5.13	in	5	0.52	in	4.95	0.08	0.17	0.19	0.05	0.12
279	098532-64-0	4.99	0.07	in	4.95	0.08	in	5.52	in	5.33	0.39	in	5.20	0.21	0.25	0.32	0.13	0.23
280	098532-65-1	4.89	0.24	in	4.65	0.09	in	5.09	in	4.95	0.52	in	4.90	0.00	0.25	0.20	0.05	0.13
281	098532-66-2	5.16	0.06	in	5.26	0.08	in	5.86	in	5.7	0.37	in	5.50	0.33	0.24	0.37	0.20	0.29
282	098532-67-3	4.89	0.08	in	5.04	0.08	in	5.57	in	5	0.47	in	5.13	0.23	0.08	0.44	0.13	0.22
283	098532-68-4	5.03	0.07	in	5.17	0.08	in	5.58	in	5.22	0.46	in	5.25	0.22	0.08	0.33	0.03	0.16
284	098532-69-5	4.94	0.09	in	4.96	0.09	in	5.84	out	5.63	0.37	in	5.34	0.40	0.38	0.50	0.29	0.39
285	098532-70-8	5.18	0.06	in	5.34	0.08	in	5.98	in	5.82	0.35	in	5.58	0.40	0.24	0.40	0.24	0.32
286	098532-71-9	5.18	0.06	in	5.07	0.08	in	5.74	out	5.5	0.39	in	5.37	0.19	0.30	0.37	0.13	0.25
287	098532-72-0	6.42	0.33	in	5.64	0.13	in	6.29	out	6.01	0.37	in	6.09	0.33	0.45	0.21	0.08	0.27
288	098532-73-1	5.38	0.08	in	5.46	0.09	in	6.30	in	5.93	0.37	in	5.77	0.39	0.30	0.53	0.16	0.35
289	098532-74-2	4.97	0.08	in	4.91	0.08	in	5.25	in	5.11	0.51	in	5.06	0.09	0.15	0.19	0.05	0.12
290	098532-75-3	5.21	0.09	in	5.04	0.08	in	5.38	in	5.36	0.47	in	5.24	0.04	0.21	0.13	0.12	0.12
291	098532-77-5	5.40	0.08	in	5.43	0.09	in	5.78	in	5.87	0.4	in	5.62	0.22	0.19	0.16	0.25	0.20
292	098532-80-0	5.58	0.08	in	5.33	0.10	in	5.89	out	5.72	0.44	in	5.63	0.06	0.30	0.26	0.09	0.18
293	098532-81-1	5.53	0.08	in	5.31	0.09	in	5.74	out	5.7	0.43	in	5.57	0.04	0.26	0.17	0.13	0.15

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		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
294	098532-82-2	5.23	0.08	in	5.16	0.09	in	5.54	in	5.5	0.43	in	5.36	0.13	0.20	0.18	0.14	0.16
295	098532-83-3	5.02	0.11	in	4.86	0.08	in	5.32	in	5.28	0.43	in	5.12	0.10	0.26	0.20	0.16	0.18
296	098532-85-5	5.62	0.09	in	5.28	0.09	in	5.89	out	5.76	0.38	in	5.64	0.01	0.36	0.25	0.12	0.19
297	098967-40-9	4.80	0.11	in	5.32	0.08	in	4.69	in	4.7	0.46	in	4.88	0.07	0.44	0.19	0.18	0.22
298	099793-38-1	5.21	0.08	in	5.28	0.11	in	5.60	in	4.86	0.45	in	5.24	0.03	0.05	0.36	0.38	0.20
299	099793-75-6	4.96	0.03	in	5.12	0.07	in	5.30	in	5.02	0.41	in	5.10	0.14	0.02	0.20	0.08	0.11
300	103112-35-2	4.58	0.09	in	5.16	0.10	in	5.43	out	5.28	0.54	in	5.11	0.53	0.05	0.31	0.17	0.27
301	103112-36-3	4.35	0.04	in	4.90	0.10	in	4.81	out	4.64	0.64	out	4.67	0.33	0.23	0.14	0.03	0.18
302	103597-45-1	10.77	1.87	out	8.68	1.11	out	9.16	out	5.82	0.53	in	8.61	2.16	0.07	0.56	2.79	1.39
303	103922-48-1	6.94	0.28	in	5.65	0.09	in	6.01	out	5.7	0.59	in	6.08	0.86	0.42	0.07	0.38	0.43
304	104958-85-2	3.35	0.33	in	3.60	0.14	in	4.00	out	4.06	0.53	in	3.75	0.41	0.15	0.25	0.31	0.28
305	106325-08-0	5.36	0.09	in	5.17	0.09	in	5.47	in	5.3	0.39	in	5.33	0.04	0.15	0.14	0.03	0.09
306	107534-96-3	5.34	0.07	in	5.09	0.08	in	4.85	in	5.5	0.43	in	5.20	0.14	0.10	0.34	0.30	0.22
307	112143-82-5	4.83	0.32	in	4.10	0.33	in	4.89	out	5.23	0.43	in	4.76	0.07	0.66	0.13	0.47	0.33
308	112281-77-3	4.49	0.15	in	4.80	0.06	in	5.51	out	4.93	0.47	in	4.93	0.44	0.13	0.58	0.00	0.29
309	113518-46-0	7.45	0.39	in	6.19	0.19	in	6.22	out	6	0.36	in	6.46	0.98	0.27	0.24	0.46	0.49
310	114369-43-6	5.89	0.12	in	5.71	0.11	in	6.06	in	6	0.3	in	5.92	0.02	0.20	0.14	0.08	0.11
311	116255-48-2	4.90	0.06	in	5.08	0.11	in	5.29	out	4.94	0.49	in	5.05	0.15	0.03	0.24	0.11	0.13
312	119126-15-7	5.78	0.38	in	5.43	0.12	in	6.53	out	6.02	0.36	in	5.94	0.16	0.51	0.59	0.08	0.34
313	119446-68-3	6.09	0.15	in	5.67	0.12	in	6.28	in	6	0.32	in	6.01	0.08	0.34	0.27	0.01	0.17
314	122836-35-5	5.83	0.29	in	4.78	0.11	in	5.37	out	5.55	0.57	in	5.38	0.45	0.60	0.01	0.17	0.31
315	125116-23-6	5.51	0.08	in	5.16	0.08	in	5.13	in	5.57	0.37	in	5.34	0.17	0.18	0.22	0.23	0.20
316	125225-28-7	5.67	0.09	in	5.25	0.09	in	5.31	in	5.64	0.38	in	5.47	0.20	0.22	0.16	0.17	0.19
317	125304-04-3	7.51	1.18	out	5.66	0.11	in	6.66	out	5.56	0.5	in	6.35	1.16	0.68	0.31	0.79	0.74
318	125306-83-4	5.40	0.12	in	5.14	0.06	in	5.24	out	5.93	0.35	in	5.43	0.03	0.29	0.19	0.50	0.25
319	127519-17-9	7.32	0.87	out	6.14	0.21	in	6.71	out	5.62	0.6	in	6.45	0.88	0.31	0.26	0.83	0.57
320	128625-52-5	5.32	0.22	in	5.32	0.09	in	5.75	out	5.55	0.52	in	5.49	0.16	0.17	0.27	0.06	0.17

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
321	128639-02-1	4.96	0.23	in	4.72	0.19	in	6.01	out	5.62	0.52	in	5.33	0.37	0.61	0.68	0.29	0.49
322	129586-32-9	4.98	0.07	in	4.67	0.11	in	4.94	in	5.13	0.42	in	4.93	0.05	0.26	0.01	0.20	0.13
323	129909-90-6	4.02	0.11	in	3.52	0.31	in	4.14	out	4.58	0.55	in	4.07	0.05	0.54	0.08	0.51	0.29
324	131983-72-7	5.37	0.07	in	5.20	0.08	in	5.25	in	5.45	0.41	in	5.32	0.05	0.12	0.07	0.13	0.09
325	136426-54-5	5.10	0.08	in	5.59	0.07	in	6.98	in	5.14	0.44	in	5.70	0.60	0.11	1.28	0.56	0.64
326	139158-24-0	4.92	0.08	in	4.51	0.05	in	4.59	out	5	0.59	in	4.76	0.17	0.25	0.16	0.24	0.20
327	139158-25-1	4.99	0.07	in	4.65	0.05	in	4.68	out	5.08	0.6	in	4.85	0.14	0.20	0.17	0.23	0.18
328	139158-26-2	6.01	0.15	in	5.77	0.15	in	5.57	out	5.43	0.49	in	5.70	0.32	0.07	0.13	0.27	0.20
329	139528-85-1	5.34	0.05	in	6.12	0.15	in	5.88	in	5.91	0.41	in	5.81	0.47	0.31	0.07	0.10	0.24
330	141078-91-3	6.30	0.17	in	6.05	0.17	in	6.24	out	5.78	0.39	in	6.09	0.21	0.04	0.15	0.31	0.18
331	141078-92-4	6.33	0.17	in	6.11	0.17	in	6.32	out	5.79	0.34	in	6.14	0.19	0.02	0.18	0.35	0.19
332	141078-93-5	6.25	0.17	in	6.10	0.17	in	6.34	out	5.98	0.37	in	6.17	0.08	0.07	0.17	0.19	0.13
333	141078-94-6	6.10	0.15	in	5.92	0.15	in	6.12	out	5.76	0.37	in	5.97	0.12	0.05	0.14	0.21	0.13
334	141078-95-7	6.33	0.17	in	6.31	0.18	in	6.51	in	6.07	0.34	in	6.30	0.02	0.00	0.20	0.23	0.12
335	141078-99-1	6.53	0.20	in	6.17	0.18	in	6.27	out	5.97	0.4	in	6.24	0.29	0.06	0.04	0.27	0.16
336	141079-00-7	6.57	0.20	in	6.24	0.19	in	6.45	out	5.98	0.36	in	6.31	0.26	0.07	0.14	0.33	0.20
337	141079-01-8	6.48	0.20	in	6.22	0.18	in	6.45	out	6.04	0.35	in	6.30	0.18	0.08	0.15	0.26	0.17
338	141079-02-9	6.33	0.17	in	6.04	0.16	in	6.20	out	5.77	0.37	in	6.08	0.24	0.04	0.11	0.31	0.18
339	141079-03-0	6.57	0.21	in	6.43	0.19	in	6.68	out	6.08	0.35	in	6.44	0.13	0.01	0.24	0.36	0.19
340	141079-06-3	6.66	0.22	in	6.33	0.20	in	6.59	out	6.03	0.38	in	6.40	0.26	0.07	0.19	0.37	0.22
341	141079-07-4	6.61	0.22	in	6.35	0.20	in	6.69	out	6.09	0.36	in	6.44	0.17	0.08	0.26	0.35	0.22
342	141079-08-5	6.46	0.19	in	6.21	0.17	in	6.50	out	6.04	0.33	in	6.30	0.16	0.09	0.20	0.26	0.18
343	141079-12-1	6.19	0.16	in	6.05	0.16	in	6.22	out	5.75	0.38	in	6.05	0.14	0.00	0.17	0.30	0.15
344	141079-13-2	6.14	0.15	in	6.10	0.16	in	6.29	in	5.97	0.37	in	6.13	0.01	0.02	0.17	0.16	0.09
345	141079-14-3	5.98	0.16	in	5.88	0.15	in	6.09	in	5.7	0.38	in	5.91	0.07	0.03	0.18	0.21	0.12
346	141079-15-4	6.22	0.16	in	6.31	0.17	in	6.39	out	6.03	0.33	in	6.24	0.01	0.07	0.15	0.21	0.11
347	141079-16-5	6.57	0.20	in	6.34	0.20	in	6.58	out	6.04	0.38	in	6.38	0.19	0.04	0.19	0.34	0.19

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
348	141079-17-6	6.62	0.22	in	6.41	0.21	in	6.77	out	6.04	0.39	in	6.46	0.16	0.05	0.31	0.42	0.24
349	141079-18-7	6.52	0.20	in	6.36	0.20	in	6.69	out	6	0.37	in	6.39	0.13	0.03	0.30	0.39	0.21
350	141079-19-8	6.37	0.19	in	6.22	0.17	in	6.48	out	5.97	0.37	in	6.26	0.11	0.04	0.22	0.29	0.16
351	141079-20-1	6.62	0.21	in	6.57	0.21	in	6.88	out	6	0.38	in	6.52	0.11	0.05	0.36	0.52	0.26
352	145026-81-9	5.93	0.17	in	4.95	0.16	in	5.99	out	6.08	0.38	in	5.74	0.19	0.79	0.25	0.34	0.39
353	145701-21-9	5.20	0.06	in	5.78	0.11	in	5.60	in	5.74	0.44	in	5.58	0.38	0.20	0.02	0.16	0.19
354	145701-23-1	4.74	0.16	in	4.96	0.08	in	4.69	in	5.04	0.46	in	4.86	0.12	0.10	0.16	0.18	0.14
355	147150-35-4	5.45	0.10	in	5.84	0.11	in	5.75	out	6.03	0.39	in	5.77	0.32	0.07	0.02	0.26	0.17
356	147993-59-7	5.51	0.18	in	5.53	0.09	in	5.99	out	5.72	0.57	in	5.69	0.18	0.15	0.30	0.03	0.17
357	149508-90-7	4.54	0.04	in	4.50	0.10	in	4.10	out	4.83	0.54	in	4.49	0.05	0.01	0.39	0.34	0.19
358	173980-17-1	8.60	2.43	out	4.60	0.29	in	5.56	out	5.9	0.45	in	6.16	2.43	1.56	0.61	0.26	1.22
359	178928-70-6	5.47	0.07	in	5.34	0.14	in	5.29	in	5.25	0.42	in	5.34	0.13	0.00	0.04	0.09	0.06
360	212201-70-2	5.76	0.14	in	5.59	0.25	in	6.16	out	6.04	0.36	in	5.88	0.13	0.30	0.27	0.16	0.21
361	219714-96-2	6.08	0.39	in	5.80	0.15	in	6.67	out	6.06	0.42	in	6.15	0.07	0.35	0.52	0.09	0.26
362	317815-83-1	7.69	1.44	out	4.87	0.12	in	5.54	out	5.91	0.49	in	6.00	1.69	1.13	0.46	0.09	0.84
363	348635-87-0	5.55	0.22	in	5.17	0.12	in	5.27	out	5.92	0.41	in	5.48	0.08	0.31	0.21	0.44	0.26
364	422556-08-9	6.05	0.32	in	5.92	0.15	in	6.47	in	6.07	0.49	in	6.13	0.08	0.20	0.34	0.06	0.17
365	865318-97-4	4.89	0.50	out	4.78	0.05	in	5.21	out	5.4	0.5	in	5.07	0.18	0.29	0.14	0.33	0.24
366	XXX002	5.92	0.39	in	5.58	0.15	in	6.18	out	5.84	0.43	in	5.88	0.04	0.30	0.30	0.04	0.17
367	XXX003	5.46	0.07	in	5.11	0.08	in	5.12	in	5.52	0.36	in	5.30	0.16	0.20	0.18	0.22	0.19
368	XXX004	4.87	0.35	in	5.37	0.18	in	5.49	out	4.95	0.57	in	5.17	0.30	0.20	0.32	0.22	0.26
369	XXX006	4.45	0.04	in	4.62	0.12	in	4.61	in	4.72	0.38	in	4.60	0.15	0.02	0.01	0.12	0.08
370	XXX007	4.90	0.06	in	4.51	0.13	in	4.70	in	5.44	0.37	in	4.88	0.01	0.38	0.19	0.56	0.28
371	XXX008	5.45	0.07	in	5.22	0.11	in	5.21	in	5.28	0.32	in	5.29	0.16	0.07	0.08	0.01	0.08
372	XXX009	5.11	0.06	in	5.48	0.16	in	5.04	in	5.09	0.45	in	5.18	0.07	0.30	0.14	0.09	0.15
373	XXX010	4.56	0.16	in	4.42	0.16	in	5.38	out	5.16	0.6	in	4.88	0.32	0.46	0.50	0.28	0.39
374	XXX011	5.38	0.07	in	5.16	0.07	in	5.16	in	5.63	0.41	in	5.33	0.04	0.17	0.17	0.30	0.17

ID	CAS	UI Models						IVL Model		HMGU Model			Consensus pred	ID Ula	ID Uib	ID IVL	ID IDEA	MD
		pred UI-a	*hat* UI-a	AD UI-a	pred UI-b	*hat* UI-b	AD UI-b	pred	AD	pred	STD	AD						
375	XXX012	5.37	0.07	in	5.21	0.07	in	5.07	in	5.34	0.38	in	5.25	0.12	0.04	0.18	0.09	0.11
376	XXX013	5.65	0.10	in	5.26	0.09	in	5.38	in	5.68	0.3	in	5.49	0.15	0.23	0.11	0.19	0.17
377	XXX014	4.66	0.21	in	4.81	0.07	in	4.20	in	4.49	0.55	in	4.54	0.12	0.27	0.34	0.05	0.20
378	XXX015	3.85	0.16	in	3.93	0.10	in	4.02	out	4.11	0.57	in	3.98	0.12	0.05	0.04	0.13	0.09
379	XXX016	3.98	0.17	in	4.84	0.11	in	3.96	in	4.15	0.52	in	4.23	0.25	0.61	0.28	0.08	0.31
380	XXX017	5.82	0.12	in	5.44	0.09	in	5.77	in	5.96	0.3	in	5.75	0.07	0.31	0.03	0.21	0.15
381	XXX018	5.83	0.10	in	5.63	0.09	in	5.99	in	6.05	0.31	in	5.88	0.04	0.24	0.11	0.17	0.14
382	XXX019	4.74	0.07	in	5.60	0.21	in	4.63	in	4.72	0.52	in	4.92	0.18	0.68	0.29	0.20	0.34
383	XXX020	5.09	0.06	in	5.08	0.09	in	5.60	in	5.36	0.34	in	5.28	0.19	0.20	0.32	0.08	0.20
384	XXX021	5.82	0.12	in	5.44	0.09	in	5.91	in	5.98	0.3	in	5.79	0.03	0.35	0.12	0.19	0.17
385	XXX022	5.22	0.05	in	5.96	0.14	in	5.55	in	5.68	0.49	in	5.60	0.38	0.36	0.05	0.08	0.22
386	XXX023	4.90	0.07	in	4.92	0.08	in	4.83	in	5.26	0.35	in	4.98	0.08	0.06	0.15	0.28	0.14

Appendix III

Consensus models for EC50 in *Daphnia magna*: predictions and applicability domain of individual WP3 models (UI, IVL, HMGU and IDEA), consensus predictions, individual model deviations (ID) and median deviation (MD).

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
1	000061-82-5	3.57	0.28	out	-0.41	out	3.80	0.26	in	4.01	0.33	out	2.74	0.83	3.15	1.06	1.27	1.58
2	000094-97-3	3.66	0.05	in	1.23	out	3.68	0.38	in	3.75	0.19	in	3.08	0.58	1.85	0.60	0.67	0.92
3	000095-14-7	3.68	0.05	in	0.46	out	3.68	0.29	in	3.83	0.27	out	2.91	0.77	2.45	0.77	0.92	1.23
4	000130-34-7	2.94	0.24	out	4.18	out	3.99	0.75	out	3.33	0.24	out	3.61	0.67	0.57	0.38	0.28	0.48
5	000131-43-1	3.99	0.38	out	6.13	out	4.88	1.00	out	3.99	0.37	out	4.75	0.75	1.38	0.13	0.76	0.76
6	000134-58-7	2.58	0.15	in	0.66	out	3.28	0.26	in	2.14	0.22	out	2.17	0.41	1.50	1.11	0.02	0.76
7	000136-85-6	3.69	0.05	in	0.73	out	3.85	0.31	in	3.89	0.24	out	3.04	0.65	2.31	0.81	0.85	1.16
8	000273-40-5	3.08	0.07	in	-0.05	out	3.08	0.23	in	2.88	0.24	out	2.25	0.84	2.30	0.83	0.63	1.15
9	000288-36-8	2.48	0.52	out	-0.77	out	3.34	0.31	in	4.13	0.34	out	2.30	0.19	3.07	1.04	1.84	1.54
10	000288-88-0	2.10	0.52	out	-0.80	out	3.15	0.27	in	4.12	0.33	out	2.14	0.04	2.94	1.01	1.98	1.49
11	000584-13-4	3.77	0.27	out	0.02	out	3.54	0.28	in	4.12	0.34	out	2.86	0.90	2.84	0.68	1.26	1.42
12	000932-64-9	2.47	0.11	in	0.64	out	3.17	0.23	in	3.31	0.11	in	2.40	0.08	1.76	0.77	0.91	0.88
13	000938-56-7	3.66	0.04	in	1.56	out	3.20	0.30	in	3.55	0.17	in	2.99	0.67	1.43	0.21	0.55	0.72
14	000939-07-1	3.65	0.04	in	1.76	out	3.87	0.44	out	3.96	0.06	in	3.31	0.34	1.55	0.56	0.65	0.78
15	000939-08-2	3.35	0.04	in	1.46	out	3.54	0.37	in	3.33	0.06	in	2.92	0.43	1.46	0.62	0.41	0.73
16	000944-91-2	3.82	0.06	in	2.03	out	3.62	0.42	out	4.24	0.03	in	3.43	0.39	1.40	0.19	0.81	0.70
17	000947-85-3	4.00	0.06	in	2.31	out	3.74	0.38	in	4.27	0.02	in	3.58	0.42	1.27	0.16	0.69	0.64
18	000974-29-8	4.81	0.31	out	5.22	out							5.02	0.21	0.21			0.21
19	001028-08-6	3.56	0.08	in	3.65	out	4.17	0.36	in	3.38	0.07	in	3.69	0.13	0.04	0.48	0.31	0.24
20	001031-47-6	3.68	0.03	in	3.21	out	4.07	0.42	out	3.54	0.04	in	3.63	0.05	0.41	0.44	0.08	0.25
21	001123-54-2	2.88	0.08	in	0.05	out	3.38	0.25	in	2.52	0.20	in	2.21	0.67	2.16	1.17	0.31	1.08

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
22	001325-58-2	10.11	2.73	out	12.83	out	6.03	0.36	in	5.85	0.43	out	8.71	1.40	4.13	2.68	2.85	2.76
23	001326-66-5	4.53	0.12	in	4.65	out	5.19	0.56	out	4.89	0.08	in	4.82	0.29	0.16	0.37	0.08	0.23
24	001455-77-2	3.43	0.33	out	-0.03	out	4.07	0.49	out	3.45	0.19	in	2.73	0.70	2.76	1.34	0.72	1.38
25	001468-26-4	2.58	0.09	in	0.76	out	3.21	0.24	in	2.45	0.31	out	2.25	0.33	1.49	0.96	0.20	0.75
26	001600-61-9	2.60	0.09	in	2.10	out	3.11	0.26	in	3.39	0.04	in	2.80	0.20	0.70	0.31	0.59	0.45
27	001680-44-0	3.90	0.05	in	1.46	out	4.22	0.44	out	4.19	0.06	in	3.44	0.46	1.99	0.78	0.75	0.99
28	001704-66-1	2.69	0.06	in	2.73	out	3.35	0.34	in	3.18	0.05	in	2.99	0.30	0.26	0.36	0.19	0.28
29	002338-12-7	2.87	0.08	in	1.31	out	3.21	0.31	in	3.29	0.17	in	2.67	0.20	1.36	0.54	0.62	0.68
30	002440-22-4	4.17	0.07	in	2.44	out	3.86	0.44	out	4.40	0.17	in	3.72	0.46	1.28	0.14	0.68	0.64
31	002592-95-2	3.50	0.05	in	0.79	out	3.12	0.26	in	3.80	0.22	out	2.80	0.70	2.01	0.32	1.00	1.01
32	002683-90-1	2.73	0.06	in	0.39	out	3.14	0.22	in	2.52	0.25	out	2.20	0.54	1.81	0.94	0.32	0.90
33	003142-42-5	6.64	0.35	out	7.66	out	5.82	0.32	in	6.59	0.43	out	6.68	0.03	0.98	0.86	0.08	0.49
34	003147-75-9	5.01	0.04	in	4.92	out	5.45	0.38	in	5.22	0.19	in	5.15	0.14	0.23	0.30	0.07	0.18
35	003147-76-0	4.47	0.05	in	3.74	out	4.41	0.44	out	4.72	0.17	in	4.33	0.13	0.59	0.08	0.38	0.30
36	003232-84-6	3.28	0.20	in	0.45	out	3.50	0.24	in	3.76	0.52	out	2.75	0.54	2.30	0.75	1.01	1.15
37	003310-68-7	3.87	0.18	in	2.27	out	4.41	0.52	out	4.07	0.06	in	3.65	0.21	1.38	0.76	0.42	0.69
38	003333-62-8	5.79	0.18	in	5.05	out	5.86	0.33	in	5.72	0.32	out	5.60	0.19	0.55	0.26	0.11	0.28
39	003357-42-4	3.90	0.05	in	1.43	out	3.82	0.40	in	4.16	0.06	in	3.33	0.57	1.89	0.49	0.83	0.95
40	003641-10-9	3.31	0.18	in	0.57	out	3.45	0.24	in	3.39	0.14	in	2.68	0.63	2.11	0.77	0.71	1.06
41	003652-22-0	3.86	0.05	in	2.90	out	3.93	0.49	out	3.95	0.03	in	3.66	0.20	0.76	0.27	0.29	0.38
42	003652-23-1	3.95	0.03	in	3.42	out	4.14	0.53	out	4.17	0.03	in	3.92	0.03	0.50	0.22	0.25	0.25
43	003652-25-3	3.87	0.03	in	3.18	out	4.05	0.53	out	4.05	0.03	in	3.79	0.08	0.61	0.26	0.26	0.30
44	003652-27-5	4.04	0.07	in	3.54	out	4.18	0.57	out	4.39	0.07	in	4.04	0.00	0.49	0.14	0.35	0.25
45	003652-31-1	3.74	0.03	in	2.10	out	3.62	0.41	out	3.83	0.04	in	3.32	0.41	1.22	0.30	0.51	0.61
46	003652-32-2	3.74	0.03	in	2.05	out	3.64	0.41	out	3.84	0.04	in	3.32	0.42	1.27	0.32	0.52	0.64
47	003663-24-9	4.01	0.03	in	2.54	out	4.59	0.41	out	4.27	0.22	out	3.85	0.16	1.31	0.74	0.42	0.66
48	003683-95-2	3.47	0.04	in	3.33	out	4.00	0.32	in	3.96	0.02	in	3.69	0.22	0.36	0.31	0.27	0.29

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
49	003770-47-6	3.70	0.04	in	2.50	out	3.93	0.21	in	3.71	0.05	in	3.46	0.24	0.96	0.47	0.25	0.48
50	003846-71-7	4.80	0.04	in	4.89	out	5.33	0.32	in	5.20	0.19	in	5.05	0.25	0.17	0.28	0.15	0.21
51	003864-99-1	4.86	0.05	in	5.11	out	5.46	0.35	in	5.45	0.22	in	5.22	0.36	0.11	0.24	0.23	0.24
52	003896-11-5	4.60	0.04	in	4.04	out	4.70	0.48	out	5.08	0.18	in	4.60	0.01	0.57	0.10	0.47	0.29
53	004184-79-6	3.69	0.04	in	0.61	out	3.97	0.38	in	3.98	0.22	in	3.06	0.63	2.45	0.91	0.91	1.22
54	004314-22-1	3.21	0.10	in	0.99	out	2.92	0.21	in	2.99	0.08	in	2.53	0.69	1.54	0.39	0.46	0.77
55	004343-73-1	3.32	0.07	in	1.74	out	3.39	0.31	in	3.15	0.06	in	2.90	0.42	1.16	0.49	0.25	0.58
56	004368-68-7	4.12	0.08	in	2.27	out	3.68	0.41	out	4.17	0.05	in	3.56	0.56	1.29	0.12	0.61	0.65
57	004928-87-4	3.09	0.08	in	0.37	out	2.98	0.21	in	3.10	0.09	in	2.38	0.70	2.01	0.60	0.71	1.01
58	004928-88-5	3.16	0.09	in	0.72	out	3.16	0.19	in	2.91	0.09	in	2.49	0.67	1.77	0.67	0.42	0.88
59	005302-27-2	3.68	0.24	out	1.69	out	3.42	0.27	in	3.49	0.08	in	3.07	0.61	1.38	0.35	0.42	0.69
60	005369-84-6	4.21	0.04	in	3.17	out	4.79	0.52	out	4.45	0.03	in	4.16	0.06	0.99	0.63	0.30	0.49
61	005472-71-9	3.99	0.05	in	2.86	out	3.48	0.40	in	3.53	0.15	in	3.47	0.53	0.61	0.01	0.06	0.30
62	005516-20-1	6.07	0.17	in	5.75	out	5.96	0.29	in	6.25	0.35	out	6.01	0.07	0.26	0.05	0.24	0.15
63	005873-30-3	3.97	0.02	in	3.18	out	3.82	0.52	out	3.79	0.14	in	3.69	0.28	0.51	0.13	0.10	0.26
64	006054-53-1	4.10	0.03	in	3.67	out	4.20	0.51	out	4.27	0.03	in	4.06	0.04	0.39	0.14	0.21	0.19
65	006085-94-5	4.12	0.08	in	2.24	out	3.66	0.41	out	4.20	0.05	in	3.56	0.56	1.31	0.10	0.65	0.66
66	006299-39-4	2.87	0.09	in	0.84	out	3.16	0.25	in	3.14	0.15	in	2.50	0.37	1.66	0.66	0.64	0.83
67	006789-99-7	3.54	0.06	in	0.94	out	3.71	0.32	in	3.43	0.28	out	2.91	0.64	1.96	0.80	0.52	0.98
68	006818-99-1	3.90	0.30	out	0.68	out	3.77	0.29	in	4.35	0.35	out	3.17	0.72	2.50	0.60	1.18	1.25
69	006994-51-0	6.55	0.34	out	7.02	out	5.98	0.34	in	6.69	0.51	out	6.56	0.01	0.46	0.58	0.13	0.29
70	007170-01-6	3.92	0.29	out	-0.09	out	3.41	0.29	in	4.24	0.34	out	2.87	1.05	2.96	0.54	1.37	1.48
71	007411-23-6	3.76	0.19	in	3.16	out	3.79	0.27	in	3.02	0.08	in	3.43	0.32	0.27	0.36	0.41	0.34
72	007532-52-7	2.57	0.09	in	1.64	out	3.35	0.33	in	3.36	0.06	in	2.73	0.16	1.09	0.62	0.63	0.62
73	010109-05-4	3.04	0.15	in	1.54	out	3.17	0.27	in	2.28	0.14	in	2.51	0.53	0.97	0.66	0.23	0.60
74	010187-79-8	2.78	0.08	in	2.51	out	3.30	0.31	in	3.24	0.04	in	2.96	0.18	0.45	0.34	0.28	0.31
75	010187-84-5	2.77	0.06	in	2.11	out	3.33	0.35	in	3.57	0.04	in	2.95	0.17	0.83	0.38	0.62	0.50

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
76	010187-86-7	2.65	0.07	in	1.90	out	3.38	0.34	in	3.27	0.05	in	2.80	0.15	0.90	0.58	0.47	0.53
77	010187-89-0	3.00	0.06	in	2.43	out	3.42	0.39	in	3.68	0.03	in	3.13	0.13	0.70	0.29	0.55	0.42
78	013091-80-0	2.88	0.08	in	1.27	out	3.20	0.23	in	3.25	0.13	in	2.65	0.23	1.38	0.55	0.60	0.69
79	013257-88-0	3.55	0.11	in	1.96	out	3.55	0.31	in	4.04	0.10	in	3.28	0.27	1.31	0.27	0.77	0.66
80	013351-73-0	3.74	0.08	in	0.58	out	3.39	0.30	in	4.12	0.25	out	2.96	0.78	2.38	0.43	1.16	1.19
81	014803-99-7	3.60	0.05	in	1.22	out	3.49	0.37	in	3.53	0.08	in	2.96	0.64	1.74	0.53	0.57	0.87
82	015421-84-8	3.82	0.12	in	2.10	out	3.27	0.34	in	3.06	0.13	in	3.06	0.76	0.97	0.21	0.00	0.48
83	015497-45-7	4.78	0.06	in	4.35	out	4.75	0.32	in	4.82	0.24	out	4.68	0.10	0.33	0.07	0.15	0.16
84	015805-10-4	3.86	0.10	in	3.42	out	4.48	0.57	out	2.70	2.268 **	out	3.62	0.24	0.19	0.86	0.91	0.55
85	016515-58-5	6.06	0.13	in	6.45	out	5.88	0.31	in	5.87	0.25	out	6.06	0.00	0.38	0.18	0.20	0.19
86	016584-05-7	3.89	0.09	in	1.17	out	3.48	0.36	in	4.10	0.22	out	3.16	0.73	1.99	0.32	0.94	1.00
87	018076-61-4	3.48	0.10	in	0.40	out	4.07	0.42	out	3.17	0.20	in	2.78	0.70	2.38	1.29	0.39	1.19
88	018811-70-6	4.38	0.11	in	3.17	out	4.40	0.57	out	4.18	0.29	out	4.03	0.35	0.86	0.37	0.15	0.43
89	019683-09-1	5.71	0.13	in	5.53	out	5.88	0.29	in	5.92	0.19	in	5.76	0.05	0.23	0.12	0.16	0.14
90	019794-93-5	5.76	0.12	in	5.60	out	5.74	0.38	in	3.68	0.18	in	5.20	0.57	0.40	0.54	1.52	0.76
91	021050-95-3	3.71	0.08	in	1.01	out	3.42	0.37	in	4.09	0.21	in	3.06	0.66	2.05	0.36	1.03	1.02
92	021532-04-7	3.36	0.06	in	2.06	out	4.26	0.42	out	3.61	0.06	in	3.32	0.04	1.26	0.94	0.29	0.63
93	023633-05-8	2.76	0.06	in	2.31	out	3.31	0.32	in	3.07	0.06	in	2.86	0.10	0.55	0.45	0.21	0.33
94	023711-34-4	4.71	0.05	in	3.97	out	5.24	0.45	out	5.42	0.13	in	4.84	0.13	0.86	0.40	0.59	0.50
95	024017-47-8	4.18	0.12	in	4.65	out	4.11	0.48	out	4.17	0.03	in	4.28	0.10	0.38	0.17	0.11	0.19
96	024054-57-7	2.76	0.05	in	2.23	out	3.19	0.30	in	3.07	0.06	in	2.81	0.05	0.58	0.38	0.25	0.32
97	025973-55-1	5.05	0.05	in	5.05	out	5.64	0.29	in	5.60	0.24	out	5.33	0.28	0.28	0.31	0.26	0.28
98	026621-45-4	2.79	0.19	in	0.56	out	3.08	0.26	in	3.57	0.08	in	2.50	0.29	1.94	0.58	1.07	0.97
99	027022-50-0	4.19	0.07	in	2.26	out	3.84	0.46	out	3.84	0.13	in	3.53	0.66	1.27	0.31	0.31	0.64
100	027210-18-0	3.86	0.08	in	1.94	out	3.53	0.46	out	3.26	0.15	in	3.15	0.72	1.21	0.38	0.11	0.60
101	027799-91-3	3.55	0.04	in	1.05	out	3.44	0.36	in	3.47	0.19	in	2.88	0.67	1.83	0.56	0.59	0.91
102	028401-89-0	3.94	0.07	in	2.11	out	3.63	0.48	out	3.35	0.14	in	3.26	0.69	1.15	0.37	0.09	0.57

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
103	028911-01-5	4.71	0.07	in	4.45	out	5.41	0.31	in	5.09	0.07	in	4.92	0.20	0.46	0.49	0.17	0.33
104	028981-97-7	4.65	0.08	in	4.16	out	5.29	0.27	in	4.87	0.07	in	4.74	0.09	0.58	0.55	0.13	0.34
105	029440-31-1	2.98	0.05	in	1.56	out	3.22	0.23	in	2.55	0.10	in	2.58	0.40	1.02	0.64	0.03	0.52
106	029878-31-7	3.67	0.05	in	0.54	out	3.86	0.32	in	3.80	0.22	in	2.97	0.71	2.43	0.89	0.83	1.21
107	029975-16-4	4.55	0.09	in	3.95	out	5.17	0.29	in	4.78	0.08	in	4.61	0.07	0.66	0.56	0.17	0.36
108	031251-03-3	5.76	0.16	in	5.18	out	5.64	0.26	in	5.96	0.13	in	5.63	0.12	0.46	0.01	0.33	0.23
109	031409-18-4	4.29	0.06	in	3.46	out	4.64	0.52	out	4.72	0.03	in	4.28	0.01	0.81	0.36	0.44	0.41
110	031701-42-5	3.51	0.07	in	2.56	out	3.51	0.43	out	3.42	0.13	in	3.25	0.26	0.69	0.26	0.17	0.35
111	032362-89-3	3.66	0.04	in	2.65	out	3.93	0.53	out	3.91	0.05	in	3.54	0.12	0.89	0.39	0.37	0.44
112	032723-50-5	4.12	0.08	in	2.76	out	4.04	0.41	out	3.99	0.15	in	3.72	0.39	0.97	0.32	0.26	0.48
113	034771-66-9	5.15	0.09	in	5.40	out	5.71	0.37	in	5.26	0.12	in	5.38	0.23	0.02	0.33	0.12	0.18
114	035515-45-8	4.23	0.05	in	2.22	out	3.94	0.47	out	3.87	0.14	in	3.56	0.66	1.34	0.38	0.31	0.67
115	036325-69-6	4.39	0.05	in	3.75	out	4.27	0.56	out	4.33	0.19	in	4.18	0.20	0.44	0.09	0.15	0.22
116	036411-52-6	3.61	0.07	in	2.33	out	3.48	0.30	in	3.60	0.05	in	3.25	0.35	0.92	0.23	0.34	0.46
117	036437-37-3	4.84	0.04	in	4.72	out	5.30	0.34	in	5.34	0.21	in	5.05	0.21	0.33	0.25	0.29	0.27
118	036791-04-5	2.66	0.27	out	2.22	out	3.03	0.23	in	1.55	0.18	in	2.37	0.30	0.14	0.66	0.81	0.48
119	037160-06-8	4.43	0.15	in	3.87	out	4.90	0.36	in	4.38	0.20	in	4.40	0.04	0.53	0.50	0.01	0.27
120	038942-51-7	4.04	0.03	in	2.28	out	4.07	0.44	out	4.47	0.06	in	3.71	0.33	1.44	0.36	0.76	0.72
121	039968-33-7	3.20	0.06	in	0.14	out	3.07	0.26	in	3.44	0.21	in	2.46	0.74	2.32	0.61	0.98	1.16
122	040054-69-1	4.63	0.05	in	4.34	out	5.30	0.28	in	4.86	0.05	in	4.78	0.15	0.44	0.52	0.08	0.30
123	041083-11-8	4.25	0.13	in	6.71	out							5.48	1.23	1.23			1.23
124	041735-28-8	2.38	0.13	in	2.49	out	3.26	0.38	in	3.66	0.03	in	2.95	0.57	0.46	0.31	0.71	0.51
125	041735-29-9	2.59	0.15	in	2.92	out	3.30	0.36	in	3.76	0.02	in	3.14	0.55	0.22	0.16	0.62	0.39
126	041735-30-2	2.34	0.19	in	3.00	out	3.42	0.53	out	3.68	0.03	in	3.11	0.77	0.11	0.31	0.57	0.44
127	041735-38-0	2.69	0.17	in	2.99	out	3.33	0.38	in	3.02	0.05	in	3.01	0.32	0.02	0.32	0.01	0.17
128	041735-41-5	2.87	0.07	in	2.32	out	3.29	0.28	in	3.48	0.04	in	2.99	0.12	0.67	0.30	0.49	0.39
129	041735-42-6	2.67	0.07	in	1.57	out	3.27	0.31	in	3.37	0.05	in	2.72	0.05	1.15	0.55	0.65	0.60

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
130	041735-44-8	2.66	0.17	in	3.03	out	3.41	0.46	out	3.15	0.04	in	3.06	0.40	0.03	0.35	0.09	0.22
131	041735-45-9	2.89	0.07	in	2.26	out	3.28	0.35	in	3.58	0.04	in	3.00	0.12	0.74	0.28	0.58	0.43
132	041735-50-6	2.69	0.17	in	2.95	out	3.55	0.49	out	2.96	0.06	in	3.04	0.35	0.08	0.51	0.08	0.26
133	041735-51-7	2.18	0.17	in	2.48	out	3.40	0.47	out	3.32	0.06	in	2.84	0.67	0.36	0.56	0.47	0.52
134	041735-54-0	2.74	0.09	in	2.30	out	3.29	0.32	in	3.70	0.03	in	3.01	0.27	0.71	0.28	0.69	0.49
135	041735-55-1	2.87	0.13	in	2.64	out	3.51	0.45	out	3.73	0.03	in	3.19	0.31	0.55	0.32	0.54	0.43
136	041735-56-2	2.29	0.22	out	2.41	out	3.27	0.34	in	3.08	0.08	in	2.76	0.47	0.35	0.51	0.32	0.41
137	041735-57-3	2.74	0.15	in	2.08	out	3.35	0.39	in	3.49	0.04	in	2.92	0.17	0.83	0.43	0.57	0.50
138	041814-78-2	3.78	0.09	in	1.41	out	3.86	0.42	out	3.85	0.15	in	3.22	0.55	1.81	0.64	0.62	0.91
139	041834-21-3	2.58	0.17	in	2.72	out	3.44	0.61	out	3.11	0.07	in	2.96	0.38	0.24	0.48	0.14	0.31
140	042509-80-8	3.86	0.30	out	4.28	out	3.88	0.46	out	4.01	0.11	in	4.01	0.15	0.27	0.13	0.00	0.14
141	043029-44-3	4.58	0.11	in	4.08	out	4.98	0.39	in	5.09	0.09	in	4.68	0.11	0.60	0.30	0.41	0.35
142	043121-43-3	4.14	0.04	in	4.50	in	4.00	0.27	in	4.52	0.02	in	4.29	0.15	0.21	0.29	0.23	0.22
143	051627-14-6	4.34	0.64	out	5.73	out	4.74	0.70	out	2.90	0.09	in	4.43	0.09	1.30	0.31	1.53	0.81
144	053817-16-6	2.87	0.16	in	0.86	out	3.03	0.27	in	3.27	0.07	in	2.51	0.37	1.65	0.52	0.76	0.82
145	054028-81-8	4.77	0.07	in	4.18	out	5.33	0.37	in	5.00	0.07	in	4.82	0.05	0.64	0.51	0.18	0.35
146	054028-83-0	4.77	0.06	in	4.39	out	5.28	0.37	in	4.92	0.07	in	4.84	0.07	0.45	0.44	0.08	0.26
147	054028-84-1	5.39	0.13	in	4.76	out	5.68	0.36	in	5.63	0.14	in	5.37	0.03	0.61	0.31	0.27	0.30
148	054028-85-2	4.51	0.06	in	4.05	out	5.19	0.37	in	4.80	0.05	in	4.64	0.13	0.59	0.55	0.16	0.36
149	054028-86-3	4.28	0.05	in	3.74	out	4.71	0.42	out	4.58	0.05	in	4.33	0.04	0.59	0.38	0.25	0.32
150	054028-89-6	4.78	0.07	in	4.12	out	5.32	0.39	in	5.00	0.07	in	4.81	0.02	0.69	0.51	0.20	0.35
151	054028-90-9	4.87	0.06	in	4.35	out	5.29	0.42	out	4.96	0.07	in	4.87	0.00	0.52	0.42	0.09	0.26
152	054028-91-0	4.71	0.08	in	3.57	out	5.19	0.37	in	4.76	0.08	in	4.56	0.16	0.99	0.63	0.20	0.50
153	054028-92-1	4.71	0.06	in	3.88	out	5.12	0.36	in	4.66	0.08	in	4.59	0.12	0.71	0.53	0.07	0.35
154	054028-93-2	4.79	0.06	in	3.82	out	5.07	0.43	out	4.71	0.08	in	4.60	0.19	0.78	0.47	0.11	0.39
155	054028-94-3	4.64	0.08	in	3.33	out	5.12	0.37	in	4.60	0.09	in	4.42	0.22	1.09	0.70	0.17	0.54
156	054028-95-4	4.72	0.06	in	3.84	out	5.19	0.35	in	4.69	0.08	in	4.61	0.11	0.77	0.58	0.08	0.39

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
157	054123-06-7	4.47	0.06	in	4.33	out	5.22	0.28	in	4.67	0.05	in	4.67	0.20	0.34	0.55	0.00	0.27
158	055179-31-2	5.26	0.05	in	5.07	in	4.81	0.39	in	5.10	0.07	in	5.06	0.20	0.01	0.25	0.04	0.13
159	055219-65-3	4.27	0.02	in	3.86	in	3.85	0.29	in	4.40	0.02	in	4.09	0.17	0.24	0.24	0.31	0.24
160	055375-40-1	3.09	0.11	in	3.50	out	3.41	0.26	in	3.73	0.07	in	3.43	0.35	0.07	0.02	0.30	0.18
161	055425-38-2	4.46	0.08	in	3.87	out	5.14	0.42	out	4.23	0.17	in	4.42	0.03	0.56	0.72	0.19	0.37
162	056383-06-3	3.56	0.06	in	2.39	out	3.42	0.42	out	2.74	0.14	in	3.03	0.54	0.64	0.39	0.29	0.46
163	056383-11-0	3.59	0.06	in	2.62	out	3.43	0.43	out	2.69	0.15	in	3.08	0.51	0.47	0.35	0.39	0.43
164	056396-43-1	4.71	0.08	in	4.79	out	5.50	0.47	out	5.22	0.07	in	5.05	0.35	0.27	0.45	0.17	0.31
165	056881-36-8	3.07	0.06	in	0.56	out	3.11	0.23	in	2.39	0.25	out	2.28	0.79	1.72	0.83	0.11	0.86
166	057801-81-7	4.47	0.06	in	4.95	out	5.29	0.28	in	4.66	0.06	in	4.84	0.37	0.11	0.45	0.18	0.28
167	057801-94-2	4.46	0.06	in	5.25	out	5.36	0.28	in	4.62	0.06	in	4.92	0.46	0.32	0.44	0.30	0.38
168	059026-08-3	3.44	0.18	in	4.04	out	3.36	0.30	in	3.60	0.10	in	3.61	0.17	0.43	0.25	0.01	0.22
169	059338-86-2	3.27	0.04	in	1.76	out	3.27	0.27	in	2.94	0.13	in	2.81	0.46	1.06	0.46	0.13	0.53
170	059338-92-0	3.14	0.04	in	1.28	out	3.16	0.22	in	2.87	0.14	in	2.61	0.53	1.33	0.55	0.26	0.67
171	059338-93-1	4.55	0.06	in	4.06	out	4.09	0.41	out	3.22	0.15	in	3.98	0.57	0.08	0.11	0.76	0.38
172	060207-31-0	4.08	0.04	in	3.62	in	3.84	0.28	in	3.76	0.05	in	3.82	0.25	0.21	0.02	0.06	0.13
173	060207-90-1	4.48	0.04	in	4.46	in	4.30	0.25	in	4.36	0.03	in	4.40	0.08	0.06	0.10	0.04	0.07
174	060207-93-4	4.32	0.04	in	4.45	in	4.12	0.27	in	4.26	0.03	in	4.29	0.04	0.16	0.17	0.03	0.10
175	060932-58-3	3.21	0.05	in	1.17	out	3.22	0.21	in	3.17	0.17	in	2.69	0.52	1.52	0.53	0.47	0.76
176	061691-97-2	3.86	0.03	in	2.81	out	3.19	0.28	in	3.04	0.13	in	3.22	0.63	0.42	0.03	0.19	0.32
177	063216-86-4	4.64	0.49	out	6.38	out	5.12	0.90	out	3.70	0.42	out	4.96	0.32	1.42	0.16	1.26	0.79
178	063251-40-1	3.35	0.26	out	4.05	out	3.76	0.59	out	3.06	0.27	out	3.56	0.21	0.50	0.20	0.50	0.35
179	063870-37-1	3.17	0.10	in	1.50	out	3.23	0.29	in	3.01	0.15	in	2.73	0.44	1.23	0.50	0.29	0.61
180	064057-50-7	2.87	0.07	in	3.47	out	3.49	0.44	out	3.89	0.04	in	3.43	0.56	0.04	0.06	0.46	0.28
181	064082-38-8	2.86	0.05	in	4.93	out	3.59	0.46	out	3.79	0.02	in	3.79	0.93	1.14	0.20	0.01	0.57
182	066104-34-5	3.87	0.06	in	2.61	out	4.04	0.52	out	3.67	0.16	in	3.55	0.32	0.94	0.49	0.12	0.47
183	066104-44-7	4.01	0.06	in	2.75	out	4.47	0.53	out	4.15	0.16	in	3.84	0.17	1.10	0.63	0.31	0.55

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
184	066246-88-6	4.56	0.03	in	4.51	in	4.91	0.32	in	4.79	0.03	in	4.69	0.14	0.18	0.22	0.10	0.16
185	066492-64-6	3.88	0.05	in	2.84	out	3.94	0.54	out	4.05	0.03	in	3.68	0.20	0.84	0.26	0.37	0.42
186	066535-86-2	4.81	0.14	in	3.44	out	4.77	0.52	out	4.91	0.21	in	4.48	0.33	1.04	0.29	0.43	0.52
187	066975-54-0	4.65	0.24	out	6.25	out	4.59	0.83	out	2.66	0.13	in	4.54	0.11	1.72	0.05	1.88	0.94
188	067465-03-6	3.64	0.03	in	3.45	out	3.80	0.49	out	3.55	0.05	in	3.61	0.03	0.16	0.19	0.06	0.11
189	067465-05-8	4.06	0.02	in	3.11	out	3.67	0.43	out	3.35	0.07	in	3.55	0.52	0.44	0.12	0.20	0.32
190	068049-83-2	4.35	0.05	in	4.41	in	4.16	0.41	out	4.47	0.26	out	4.35	0.00	0.07	0.19	0.12	0.09
191	069141-50-0	3.81	0.09	in	4.01	out	3.49	0.31	in	3.58	0.07	in	3.72	0.09	0.29	0.23	0.14	0.19
192	070292-10-3	3.98	0.06	in	2.52	out	3.44	0.37	in	4.39	0.06	in	3.58	0.40	1.06	0.14	0.81	0.60
193	070321-86-7	6.60	0.25	out	6.22	out	5.99	0.28	in	6.77	0.41	out	6.40	0.20	0.18	0.41	0.38	0.29
194	075020-35-8	3.45	0.05	in	1.64	out	3.66	0.39	in	3.75	0.13	in	3.13	0.32	1.49	0.53	0.63	0.74
195	075736-33-3	4.60	0.02	in	4.93	in	4.66	0.15	in	4.70	0.04	in	4.72	0.12	0.21	0.06	0.02	0.10
196	076608-88-3	4.34	0.02	in	3.51	in	4.00	0.27	in	4.05	0.02	in	3.98	0.36	0.46	0.02	0.08	0.23
197	076674-21-0	4.80	0.06	in	3.52	in	4.19	0.29	in	4.51	0.06	in	4.26	0.55	0.74	0.07	0.26	0.40
198	076738-62-0	4.59	0.02	in	4.57	in	4.08	0.36	in	4.48	0.02	in	4.43	0.16	0.14	0.35	0.05	0.18
199	077314-77-3	3.73	0.14	in	2.52	out	4.30	0.50	out	3.34	0.07	in	3.47	0.25	0.95	0.83	0.13	0.54
200	078149-96-9	3.70	0.07	in	4.28	out	4.24	0.49	out	3.63	0.08	in	3.96	0.26	0.32	0.28	0.33	0.30
201	078150-00-2	3.80	0.16	in	3.43	out	4.41	0.54	out	3.15	0.07	in	3.70	0.10	0.27	0.71	0.54	0.41
202	078150-02-4	3.39	0.07	in	3.37	out	3.78	0.39	in	3.17	0.08	in	3.43	0.04	0.06	0.35	0.26	0.18
203	078218-51-6	3.76	0.03	in	3.69	out	4.29	0.54	out	3.83	0.03	in	3.89	0.13	0.21	0.40	0.06	0.20
204	078218-52-7	3.10	0.06	in	2.38	out	3.43	0.25	in	2.78	0.09	in	2.92	0.18	0.54	0.51	0.14	0.34
205	078218-53-8	3.98	0.13	in	4.73	out	4.66	0.50	out	3.79	0.08	in	4.29	0.31	0.44	0.37	0.50	0.40
206	078218-54-9	3.16	0.06	in	2.93	out	3.57	0.31	in	2.97	0.08	in	3.16	0.00	0.23	0.41	0.19	0.21
207	078218-55-0	3.73	0.03	in	3.81	out	3.97	0.53	out	3.49	0.05	in	3.75	0.02	0.06	0.22	0.26	0.14
208	078218-56-1	4.06	0.03	in	4.01	out	4.42	0.52	out	3.78	0.03	in	4.07	0.01	0.06	0.35	0.29	0.18
209	078218-57-2	3.02	0.06	in	2.12	out	3.33	0.24	in	2.50	0.10	in	2.74	0.28	0.62	0.59	0.24	0.43
210	078218-58-3	3.55	0.17	in	3.11	out	4.30	0.53	out	3.14	0.07	in	3.52	0.03	0.42	0.78	0.39	0.40

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
211	078218-59-4	3.22	0.06	in	2.97	out	3.63	0.32	in	2.97	0.08	in	3.20	0.02	0.22	0.43	0.23	0.23
212	078218-60-7	3.60	0.22	out	3.03	out	3.83	0.40	in	2.96	0.09	in	3.36	0.24	0.32	0.47	0.40	0.36
213	078218-61-8	5.01	0.40	out	6.74	out	5.54	0.41	out	4.62	0.15	in	5.48	0.46	1.26	0.06	0.86	0.66
214	078218-65-2	3.34	0.06	in	2.48	out	3.93	0.32	in	2.86	0.08	in	3.15	0.19	0.67	0.78	0.29	0.48
215	078218-66-3	3.30	0.06	in	2.07	out	3.67	0.26	in	2.90	0.08	in	2.98	0.32	0.92	0.69	0.08	0.50
216	078324-76-2	3.77	0.08	in	2.46	out	3.94	0.49	out	3.70	0.15	in	3.47	0.30	1.01	0.47	0.23	0.50
217	078371-72-9	2.95	0.05	in	2.99	out	3.34	0.31	in	2.51	0.11	in	2.95	0.00	0.05	0.39	0.44	0.22
218	078371-73-0	3.48	0.08	in	4.41	out	3.97	0.57	out	3.16	0.09	in	3.76	0.27	0.65	0.21	0.60	0.43
219	078371-74-1	3.10	0.05	in	3.24	out	3.48	0.40	in	2.75	0.10	in	3.14	0.04	0.10	0.34	0.40	0.22
220	078592-90-2	3.31	0.07	in	3.12	out	3.93	0.31	in	3.05	0.08	in	3.35	0.04	0.23	0.58	0.30	0.29
221	079983-71-4	4.51	0.02	in	4.83	in	4.47	0.25	in	4.45	0.03	in	4.56	0.06	0.27	0.09	0.11	0.13
222	080301-64-0	5.90	0.25	out	6.77	out	5.89	0.28	in	6.22	0.53	out	6.19	0.29	0.57	0.30	0.02	0.30
223	080584-88-9	3.93	0.04	in	3.07	out	3.26	0.29	in	2.87	0.13	in	3.28	0.64	0.21	0.02	0.41	0.32
224	080584-89-0	3.91	0.04	in	3.00	out	3.24	0.29	in	2.85	0.13	in	3.25	0.66	0.25	0.01	0.40	0.33
225	080584-90-3	6.00	0.29	out	6.71	out	5.92	0.27	in	6.41	0.58	out	6.26	0.26	0.45	0.34	0.15	0.30
226	080595-74-0	6.02	0.30	out	6.75	out	5.91	0.27	in	6.42	0.58	out	6.28	0.25	0.47	0.37	0.15	0.31
227	081518-26-5	4.49	0.08	in	3.57	out	4.68	0.41	out	5.05	0.10	in	4.45	0.05	0.88	0.23	0.60	0.44
228	081518-27-6	4.57	0.07	in	4.54	out	4.93	0.45	out	5.32	0.12	in	4.84	0.27	0.30	0.09	0.48	0.29
229	081518-28-7	4.57	0.07	in	3.79	in	4.79	0.39	in	5.24	0.11	in	4.60	0.03	0.80	0.19	0.64	0.42
230	081518-29-8	4.70	0.09	in	4.31	out	5.51	0.35	in	5.31	0.07	in	4.96	0.26	0.64	0.55	0.35	0.45
231	081518-31-2	4.89	0.07	in	4.81	out	5.70	0.29	in	5.57	0.07	in	5.24	0.35	0.43	0.46	0.33	0.39
232	081518-32-3	4.97	0.09	in	5.07	out	5.71	0.30	in	5.69	0.07	in	5.36	0.39	0.30	0.35	0.33	0.34
233	081518-37-8	4.92	0.06	in	4.86	out	5.49	0.34	in	5.49	0.07	in	5.19	0.27	0.33	0.30	0.30	0.30
234	081518-41-4	4.84	0.07	in	5.55	out	5.59	0.33	in	5.59	0.07	in	5.39	0.55	0.16	0.20	0.20	0.28
235	082200-72-4	4.26	0.02	in	3.96	in	3.84	0.28	in	4.50	0.02	in	4.14	0.12	0.18	0.30	0.36	0.24
236	083044-89-7	6.77	0.45	out	8.29	out	5.94	0.29	in	6.37	0.37	out	6.84	0.07	1.45	0.90	0.48	0.72
237	083044-90-0	6.45	0.35	out	8.24	out	5.92	0.31	in	6.28	0.35	out	6.72	0.27	1.52	0.80	0.44	0.76

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
238	083044-91-1	4.81	0.04	in	5.39	out	5.09	0.41	out	4.92	0.16	in	5.05	0.24	0.33	0.04	0.13	0.19
239	083366-66-9	7.18	0.55	out	7.70	out	6.01	0.30	in	5.41	0.05	in	6.57	0.61	1.12	0.56	1.17	0.87
240	083657-17-4	4.41	0.02	in	4.45	in	4.21	0.36	in	4.36	0.02	in	4.36	0.05	0.09	0.15	0.00	0.07
241	083657-24-3	4.42	0.02	in	4.78	in	4.46	0.32	in	4.48	0.02	in	4.53	0.11	0.24	0.07	0.06	0.12
242	085509-19-9	4.76	0.09	in	4.97	out	5.42	0.24	in	5.68	0.06	in	5.21	0.45	0.24	0.21	0.47	0.34
243	085634-51-1	4.26	0.07	in	4.64	out	4.67	0.61	out	4.18	0.22	out	4.44	0.17	0.20	0.23	0.26	0.22
244	086386-73-4	4.06	0.02	in	3.63	in	3.52	0.34	in	3.38	0.06	in	3.65	0.41	0.01	0.13	0.27	0.21
245	086598-92-7	5.21	0.06	in	6.22	out	5.80	0.29	in	5.80	0.07	in	5.76	0.54	0.46	0.04	0.04	0.27
246	088671-89-0	4.30	0.04	in	4.49	in	4.47	0.30	in	4.62	0.02	in	4.47	0.17	0.02	0.00	0.15	0.09
247	089482-17-7	4.26	0.02	in	4.00	in	3.84	0.28	in	4.50	0.02	in	4.15	0.11	0.15	0.31	0.35	0.23
248	089786-04-9	2.86	0.10	in	2.48	out	3.05	0.21	in	2.17	0.16	in	2.64	0.22	0.16	0.41	0.47	0.32
249	094270-86-7	6.00	0.29	out	6.83	out	5.93	0.27	in	6.41	0.58	out	6.29	0.29	0.54	0.36	0.11	0.33
250	094361-06-5	4.41	0.02	in	4.15	in	4.07	0.41	out	4.20	0.02	in	4.21	0.21	0.06	0.14	0.01	0.10
251	094667-47-7	2.84	0.09	in	1.35	out	3.03	0.21	in	3.04	0.13	in	2.56	0.27	1.21	0.47	0.47	0.61
252	097232-75-2	4.80	0.24	out	5.41	out	5.61	0.51	out	4.62	0.04	in	5.11	0.31	0.30	0.50	0.49	0.40
253	098518-95-7	4.11	0.05	in	3.54	out	3.62	0.46	out	3.36	0.12	in	3.66	0.45	0.12	0.04	0.30	0.23
254	098518-96-8	4.02	0.05	in	3.22	out	3.49	0.37	in	3.43	0.12	in	3.54	0.48	0.32	0.05	0.11	0.24
255	098518-99-1	4.27	0.05	in	3.88	out	3.66	0.43	out	3.73	0.12	in	3.89	0.39	0.01	0.23	0.15	0.19
256	098519-00-7	4.22	0.04	in	4.07	out	4.09	0.52	out	3.74	0.11	in	4.03	0.19	0.04	0.06	0.29	0.15
257	098519-01-8	4.48	0.11	in	4.45	out	4.16	0.41	out	4.06	0.12	in	4.29	0.19	0.16	0.13	0.23	0.18
258	098519-02-9	4.74	0.05	in	5.55	out	4.53	0.46	out	4.02	0.12	in	4.71	0.03	0.84	0.18	0.69	0.44
259	098519-04-1	4.26	0.06	in	3.89	out	3.76	0.53	out	3.75	0.12	in	3.92	0.34	0.02	0.16	0.16	0.17
260	098519-05-2	4.07	0.05	in	3.57	out	3.75	0.54	out	3.60	0.11	in	3.75	0.33	0.18	0.00	0.15	0.16
261	098519-06-3	4.36	0.04	in	4.39	out	3.93	0.54	out	3.98	0.12	in	4.16	0.20	0.22	0.23	0.18	0.21
262	098519-07-4	4.19	0.04	in	3.84	out	3.88	0.54	out	3.60	0.11	in	3.88	0.31	0.04	0.00	0.27	0.16
263	098519-24-5	4.18	0.07	in	3.24	out	3.51	0.41	out	3.51	0.12	in	3.61	0.57	0.37	0.10	0.10	0.28
264	098519-25-6	4.40	0.04	in	4.76	out	4.15	0.51	out	4.12	0.13	in	4.36	0.04	0.40	0.21	0.23	0.22

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
265	098519-26-7	4.30	0.06	in	4.33	out	4.00	0.44	out	3.89	0.12	in	4.13	0.17	0.20	0.13	0.24	0.18
266	098519-28-9	4.16	0.04	in	3.57	out	3.46	0.44	out	3.21	0.12	in	3.60	0.56	0.03	0.14	0.39	0.28
267	098519-29-0	4.43	0.05	in	4.06	out	3.65	0.50	out	3.36	0.11	in	3.88	0.56	0.19	0.23	0.51	0.37
268	098519-30-3	5.22	0.07	in	4.61	out	4.50	0.56	out	4.39	0.15	in	4.68	0.54	0.07	0.18	0.29	0.27
269	098519-31-4	4.43	0.05	in	4.05	out	3.65	0.50	out	3.36	0.11	in	3.87	0.56	0.17	0.22	0.51	0.37
270	098519-32-5	4.46	0.04	in	4.38	out	4.12	0.45	out	3.93	0.12	in	4.22	0.24	0.16	0.10	0.29	0.20
271	098519-33-6	4.65	0.04	in	4.61	out	4.40	0.39	in	4.11	0.13	in	4.44	0.20	0.17	0.04	0.33	0.19
272	098519-34-7	4.74	0.04	in	4.82	out	4.44	0.38	in	4.28	0.14	in	4.57	0.16	0.25	0.13	0.29	0.21
273	098519-35-8	4.60	0.19	in	4.28	out	3.97	0.40	in	3.67	0.11	in	4.13	0.47	0.15	0.16	0.46	0.31
274	098519-37-0	4.98	0.06	in	5.18	out	4.92	0.34	in	4.50	0.16	in	4.90	0.09	0.29	0.02	0.40	0.20
275	098519-39-2	4.27	0.05	in	3.74	out	3.66	0.43	out	3.73	0.12	in	3.85	0.42	0.11	0.19	0.12	0.21
276	098519-41-6	4.82	0.09	in	5.15	out	4.54	0.45	out	3.95	0.12	in	4.61	0.20	0.54	0.07	0.67	0.37
277	098519-43-8	4.36	0.04	in	4.32	out	3.93	0.54	out	3.98	0.12	in	4.15	0.21	0.17	0.22	0.17	0.19
278	098519-49-4	4.18	0.07	in	3.31	out	3.51	0.41	out	3.51	0.12	in	3.63	0.55	0.32	0.12	0.12	0.28
279	098532-64-0	4.16	0.04	in	3.82	out	3.46	0.44	out	3.21	0.12	in	3.66	0.50	0.16	0.20	0.45	0.33
280	098532-65-1	3.99	0.06	in	3.12	out	3.52	0.46	out	3.36	0.12	in	3.50	0.49	0.37	0.02	0.14	0.26
281	098532-66-2	4.40	0.04	in	4.84	out	4.24	0.44	out	4.12	0.13	in	4.40	0.01	0.44	0.16	0.28	0.22
282	098532-67-3	4.10	0.05	in	3.70	out	3.92	0.53	out	3.73	0.11	in	3.86	0.24	0.16	0.06	0.14	0.15
283	098532-68-4	4.30	0.06	in	4.33	out	4.00	0.44	out	3.89	0.12	in	4.13	0.17	0.20	0.13	0.24	0.18
284	098532-69-5	4.03	0.05	in	3.48	out	3.63	0.55	out	3.17	0.12	in	3.58	0.45	0.09	0.05	0.41	0.25
285	098532-70-8	4.29	0.04	in	4.84	out	3.88	0.53	out	3.61	0.11	in	4.16	0.14	0.68	0.28	0.54	0.41
286	098532-71-9	4.43	0.05	in	4.20	out	3.61	0.47	out	3.36	0.11	in	3.90	0.53	0.30	0.29	0.54	0.41
287	098532-72-0	5.22	0.07	in	4.98	out	4.50	0.56	out	4.39	0.15	in	4.77	0.44	0.21	0.27	0.38	0.33
288	098532-73-1	4.57	0.05	in	4.95	out	4.11	0.52	out	3.77	0.11	in	4.35	0.22	0.60	0.24	0.58	0.41
289	098532-74-2	4.35	0.12	in	3.51	out	3.65	0.40	in	3.67	0.12	in	3.79	0.55	0.28	0.14	0.13	0.28
290	098532-75-3	4.33	0.04	in	4.14	out	3.91	0.46	out	3.75	0.12	in	4.03	0.30	0.10	0.12	0.29	0.20
291	098532-77-5	4.46	0.04	in	4.89	out	4.48	0.45	out	4.13	0.13	in	4.49	0.03	0.40	0.01	0.36	0.20

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
292	098532-80-0	4.74	0.04	in	5.11	out	4.40	0.40	in	4.28	0.14	in	4.63	0.10	0.48	0.23	0.35	0.29
293	098532-81-1	4.59	0.04	in	4.48	out	4.38	0.40	in	4.10	0.13	in	4.39	0.20	0.09	0.01	0.28	0.15
294	098532-82-2	4.60	0.19	in	4.35	out	3.97	0.40	in	3.67	0.11	in	4.15	0.45	0.20	0.18	0.48	0.33
295	098532-83-3	4.28	0.06	in	3.75	out	3.63	0.46	out	3.50	0.11	in	3.79	0.49	0.03	0.16	0.29	0.24
296	098532-85-5	4.78	0.04	in	4.92	out	4.36	0.40	in	4.29	0.14	in	4.59	0.19	0.33	0.23	0.30	0.26
297	098967-40-9	3.70	0.06	in	3.15	in	3.32	0.28	in	3.49	0.13	in	3.41	0.28	0.27	0.09	0.08	0.18
298	099793-38-1	4.83	0.08	in	4.99	out	5.44	0.32	in	5.91	0.08	in	5.29	0.46	0.30	0.15	0.62	0.38
299	099793-75-6	4.27	0.10	in	4.81	out	4.43	0.42	out	5.14	0.07	in	4.66	0.39	0.15	0.23	0.47	0.31
300	103112-35-2	4.16	0.05	in	5.72	out	4.59	0.42	out	4.80	0.05	in	4.82	0.65	0.90	0.23	0.02	0.45
301	103112-36-3	3.75	0.03	in	5.18	out	3.43	0.28	in	4.54	0.04	in	4.22	0.48	0.95	0.79	0.32	0.64
302	103597-45-1	8.39	0.89	out	10.64	out	6.00	0.34	in	6.81	2.914 **	out	7.96	0.43	2.68	1.96	1.15	1.55
303	103922-48-1	5.49	0.28	out	6.01	out	5.23	0.56	out	4.05	0.02	in	5.19	0.30	0.81	0.04	1.14	0.57
304	104958-85-2	2.66	0.08	in	2.52	out	3.05	0.23	in	2.40	0.09	in	2.66	0.00	0.13	0.39	0.26	0.20
305	106325-08-0	4.94	0.06	in	4.56	in	4.84	0.22	in	4.73	0.08	in	4.77	0.17	0.21	0.07	0.04	0.12
306	107534-96-3	4.82	0.03	in	4.95	in	4.59	0.46	out	4.66	0.02	in	4.75	0.07	0.19	0.16	0.10	0.13
307	112143-82-5	3.61	0.11	in	4.59	out	3.68	0.35	in	4.04	0.13	in	3.98	0.37	0.61	0.30	0.06	0.34
308	112281-77-3	4.82	0.05	in	5.29	in	4.76	0.39	in	4.58	0.03	in	4.86	0.04	0.42	0.10	0.28	0.21
309	113518-46-0	5.40	0.12	in	5.70	out	5.96	0.28	in	5.32	0.15	in	5.59	0.20	0.11	0.37	0.28	0.24
310	114369-43-6	5.09	0.05	in	5.15	in	5.16	0.27	in	5.24	0.07	in	5.16	0.07	0.01	0.00	0.08	0.04
311	116255-48-2	4.31	0.04	in	4.72	out	4.46	0.20	in	4.02	0.04	in	4.38	0.07	0.34	0.08	0.36	0.21
312	119126-15-7	5.64	0.16	in	6.24	out	5.37	0.60	out	5.26	0.06	in	5.63	0.01	0.62	0.26	0.37	0.31
313	119446-68-3	5.29	0.07	in	5.72	in	4.93	0.42	out	5.02	0.07	in	5.24	0.05	0.48	0.31	0.22	0.26
314	122836-35-5	3.67	0.03	in	3.95	out	3.81	0.28	in	3.99	0.04	in	3.85	0.19	0.10	0.04	0.14	0.12
315	125116-23-6	4.75	0.04	in	4.75	in	4.46	0.29	in	4.58	0.02	in	4.63	0.11	0.12	0.17	0.06	0.12
316	125225-28-7	4.92	0.05	in	5.21	in	4.81	0.30	in	4.69	0.02	in	4.91	0.01	0.30	0.10	0.22	0.16
317	125304-04-3	6.73	0.39	out	7.66	out	5.89	0.29	in	6.77	0.47	out	6.76	0.03	0.90	0.87	0.01	0.45
318	125306-83-4	3.91	0.13	in	4.29	out	3.71	0.40	in	4.69	0.06	in	4.15	0.24	0.14	0.44	0.54	0.34

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
319	127519-17-9	6.22	0.25	out	7.59	out	5.86	0.29	in	5.79	0.27	out	6.37	0.14	1.22	0.51	0.57	0.61
320	128625-52-5	4.58	0.26	out	5.16	out	4.68	0.46	out	3.79	0.13	in	4.55	0.03	0.61	0.13	0.77	0.38
321	128639-02-1	4.74	0.10	in	4.76	out	4.36	0.51	out	4.72	0.14	in	4.65	0.10	0.11	0.29	0.08	0.14
322	129586-32-9	4.47	0.03	in	3.98	in	4.04	0.30	in	4.43	0.02	in	4.23	0.24	0.25	0.19	0.20	0.22
323	129909-90-6	3.51	0.16	in	2.99	out	3.68	0.34	in	3.48	0.09	in	3.42	0.09	0.42	0.26	0.07	0.21
324	131983-72-7	4.63	0.04	in	4.43	in	4.68	0.19	in	4.59	0.03	in	4.58	0.05	0.16	0.10	0.01	0.08
325	136426-54-5	4.39	0.08	in	4.27	out	4.46	0.50	out	5.16	0.06	in	4.57	0.18	0.30	0.11	0.59	0.30
326	139158-24-0	3.92	0.18	in	3.66	out	4.12	0.53	out	4.23	0.14	in	3.98	0.06	0.32	0.14	0.25	0.19
327	139158-25-1	4.12	0.15	in	3.71	out	4.35	0.56	out	4.29	0.15	in	4.12	0.00	0.41	0.23	0.17	0.20
328	139158-26-2	4.90	0.13	in	4.90	out	5.25	0.44	out	5.17	0.10	in	5.06	0.16	0.15	0.19	0.12	0.16
329	139528-85-1	3.64	0.05	in	4.27	out	3.62	0.34	in	4.09	0.12	in	3.91	0.27	0.37	0.29	0.19	0.28
330	141078-91-3	5.84	0.14	in	5.38	out	5.90	0.27	in	6.33	0.19	in	5.86	0.02	0.49	0.04	0.47	0.25
331	141078-92-4	5.80	0.13	in	5.31	out	5.90	0.26	in	6.06	0.19	in	5.77	0.03	0.46	0.13	0.29	0.23
332	141078-93-5	5.80	0.14	in	5.70	out	5.90	0.27	in	6.39	0.19	in	5.95	0.14	0.25	0.05	0.45	0.22
333	141078-94-6	5.82	0.14	in	5.29	out	5.90	0.26	in	6.19	0.19	in	5.80	0.02	0.51	0.10	0.39	0.26
334	141078-95-7	5.85	0.14	in	5.85	out	5.96	0.27	in	6.53	0.19	in	6.05	0.19	0.20	0.09	0.48	0.24
335	141078-99-1	6.01	0.14	in	5.77	out	5.95	0.26	in	6.56	0.20	in	6.07	0.06	0.30	0.12	0.48	0.24
336	141079-00-7	5.97	0.13	in	5.51	out	5.94	0.25	in	6.28	0.19	in	5.93	0.04	0.41	0.01	0.36	0.21
337	141079-01-8	5.97	0.14	in	5.86	out	5.95	0.26	in	6.62	0.20	in	6.10	0.13	0.24	0.15	0.52	0.26
338	141079-02-9	5.99	0.14	in	5.67	out	5.95	0.25	in	6.41	0.19	in	6.01	0.02	0.33	0.06	0.41	0.20
339	141079-03-0	6.02	0.13	in	6.16	out	6.00	0.26	in	6.75	0.20	in	6.23	0.21	0.07	0.23	0.52	0.26
340	141079-06-3	6.10	0.14	in	6.02	out	6.00	0.27	in	6.83	0.21	in	6.24	0.14	0.21	0.24	0.59	0.29
341	141079-07-4	6.06	0.14	in	6.21	out	6.00	0.27	in	6.89	0.21	in	6.29	0.23	0.08	0.29	0.60	0.30
342	141079-08-5	6.08	0.14	in	5.99	out	6.00	0.26	in	6.68	0.20	in	6.19	0.11	0.20	0.19	0.50	0.25
343	141079-12-1	5.88	0.14	in	5.71	out	5.94	0.27	in	6.44	0.19	in	5.99	0.11	0.28	0.05	0.44	0.22
344	141079-13-2	5.84	0.14	in	5.96	out	5.94	0.28	in	6.50	0.19	in	6.06	0.22	0.10	0.12	0.44	0.22
345	141079-14-3	5.86	0.14	in	5.65	out	5.94	0.28	in	6.29	0.19	in	5.94	0.08	0.28	0.00	0.36	0.18

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
346	141079-15-4	5.89	0.14	in	6.22	out	5.97	0.29	in	6.66	0.19	in	6.19	0.29	0.04	0.22	0.47	0.25
347	141079-16-5	6.14	0.13	in	6.57	out	6.02	0.27	in	6.94	0.21	in	6.42	0.28	0.15	0.40	0.52	0.34
348	141079-17-6	6.12	0.13	in	6.28	out	6.00	0.28	in	6.67	0.19	in	6.27	0.15	0.01	0.27	0.40	0.21
349	141079-18-7	6.10	0.13	in	6.67	out	6.00	0.27	in	7.00	0.22	in	6.44	0.34	0.22	0.44	0.56	0.39
350	141079-19-8	6.12	0.13	in	6.46	out	6.00	0.27	in	6.80	0.20	in	6.34	0.22	0.11	0.34	0.45	0.28
351	141079-20-1	6.16	0.14	in	6.93	out	6.03	0.28	in	7.17	0.23	out	6.57	0.41	0.36	0.54	0.60	0.48
352	145026-81-9	3.38	0.08	in	4.50	out	3.34	0.23	in	3.86	0.03	in	3.77	0.39	0.73	0.43	0.09	0.41
353	145701-21-9	3.82	0.07	in	4.41	in	3.62	0.38	in	4.01	0.12	in	3.96	0.15	0.45	0.34	0.04	0.25
354	145701-23-1	3.63	0.06	in	3.62	in	3.37	0.30	in	3.36	0.13	in	3.49	0.13	0.12	0.12	0.14	0.13
355	147150-35-4	3.69	0.09	in	4.41	out	3.61	0.41	out	3.63	0.12	in	3.83	0.15	0.57	0.22	0.20	0.29
356	147993-59-7	3.84	0.47	out	4.79	out	4.39	0.73	out	2.40	0.12	in	3.86	0.01	0.94	0.53	1.46	0.74
357	149508-90-7	4.30	0.02	in	4.12	out	4.08	0.25	in	4.14	0.02	in	4.16	0.14	0.04	0.08	0.02	0.07
358	173980-17-1	4.00	0.10	in	4.25	out	4.34	0.67	out	3.94	0.08	in	4.13	0.13	0.12	0.21	0.19	0.16
359	178928-70-6	4.61	0.08	in	5.34	in	4.81	0.43	out	4.55	0.04	in	4.83	0.22	0.51	0.02	0.28	0.26
360	212201-70-2	5.30	0.10	in	4.84	out	5.07	0.51	out	5.77	0.16	in	5.25	0.05	0.41	0.18	0.53	0.29
361	219714-96-2	4.21	0.04	in	3.76	in	3.66	0.32	in	3.52	0.13	in	3.79	0.42	0.03	0.13	0.27	0.21
362	317815-83-1	2.71	0.10	in	3.64	out	3.28	0.18	in	3.15	0.06	in	3.19	0.48	0.44	0.09	0.04	0.26
363	348635-87-0	3.14	0.14	in	4.51	out	3.54	0.36	in	2.77	0.14	in	3.49	0.35	1.02	0.05	0.72	0.54
364	422556-08-9	3.51	0.06	in	3.52	in	3.42	0.29	in	3.26	0.13	in	3.43	0.08	0.09	0.01	0.17	0.09
365	865318-97-4	4.49	0.11	in	4.63	out	5.06	0.44	out	4.29	0.19	in	4.62	0.13	0.02	0.44	0.33	0.23
366	XXX002	4.04	0.05	in	3.76	in	3.56	0.27	in	3.42	0.13	in	3.69	0.35	0.06	0.13	0.28	0.21
367	XXX003	4.41	0.03	in	4.53	in	4.14	0.36	in	4.21	0.02	in	4.32	0.09	0.21	0.18	0.11	0.15
368	XXX004	3.57	0.07	in	3.41	out	3.27	0.19	in	3.59	0.08	in	3.46	0.11	0.05	0.19	0.13	0.12
369	XXX006	4.20	0.02	in	3.66	in	3.75	0.20	in	3.87	0.03	in	3.87	0.33	0.21	0.12	0.00	0.16
370	XXX007	4.26	0.04	in	4.37	in	3.61	0.37	in	3.64	0.04	in	3.97	0.29	0.40	0.36	0.33	0.34
371	XXX008	4.71	0.05	in	5.10	in	5.05	0.28	in	4.71	0.04	in	4.89	0.18	0.20	0.16	0.18	0.18
372	XXX009	4.38	0.05	in	4.59	in	4.36	0.22	in	4.69	0.03	in	4.51	0.12	0.08	0.15	0.18	0.13

ID	CAS	UI Model			IVL Model		HMGU Model			IDEA Model			Consensus pred	ID UI	ID IVL	ID HMGU	ID IDEA	MD
		pred	*hat*	AD	pred	AD	pred	STD	AD	pred	*hat*	AD						
373	XXX010	4.25	0.04	in	4.29	out	3.74	0.39	in	4.47	0.05	in	4.19	0.06	0.10	0.45	0.28	0.22
374	XXX011	4.57	0.05	in	3.90	in	3.94	0.32	in	3.98	0.02	in	4.10	0.47	0.20	0.16	0.12	0.24
375	XXX012	4.57	0.05	in	4.20	in	4.11	0.31	in	3.99	0.02	in	4.22	0.35	0.02	0.11	0.23	0.18
376	XXX013	4.87	0.07	in	5.05	out	5.34	0.32	in	4.84	0.04	in	5.02	0.16	0.03	0.32	0.19	0.17
377	XXX014	3.44	0.06	in	3.46	in	3.35	0.20	in	3.26	0.14	in	3.38	0.06	0.08	0.03	0.12	0.07
378	XXX015	2.85	0.10	in	2.55	out	3.18	0.21	in	3.03	0.12	in	2.90	0.05	0.35	0.28	0.13	0.20
379	XXX016	3.04	0.07	in	3.11	in	3.15	0.19	in	3.36	0.08	in	3.16	0.13	0.05	0.01	0.19	0.10
380	XXX017	4.99	0.06	in	4.87	in	4.91	0.40	in	4.86	0.04	in	4.91	0.09	0.04	0.00	0.05	0.04
381	XXX018	4.80	0.06	in	5.18	in	4.78	0.43	out	4.77	0.05	in	4.88	0.08	0.30	0.10	0.11	0.15
382	XXX019	3.29	0.14	in	3.38	out	4.13	0.49	out	3.81	0.05	in	3.65	0.36	0.27	0.48	0.15	0.31
383	XXX020	4.49	0.03	in	4.54	in	3.82	0.31	in	3.85	0.04	in	4.18	0.31	0.36	0.36	0.32	0.34
384	XXX021	4.99	0.06	in	4.82	in	4.91	0.40	in	4.86	0.04	in	4.90	0.10	0.07	0.01	0.04	0.06
385	XXX022	3.48	0.05	in	4.05	out	3.49	0.29	in	3.99	0.12	in	3.75	0.27	0.29	0.26	0.24	0.27
386	XXX023	4.48	0.03	in	4.52	in	4.24	0.39	in	4.70	0.03	in	4.48	0.01	0.03	0.24	0.22	0.13

Appendix IV

Table 1. Consensus models for EC50 in *Oncorhynchus mykiss*: predictions and applicability domain of individual WP3 models (UI-Dragon (UI-a), UI-PaDEL (UI-b), IVL, HMGU, IDEA-A (A), IDEA-B (B), IDEA-C (C)) and consensus predictions.

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
1	000061-82-5	1.99	0.40	out	2.74	0.11	in	4.69	out	2.91	0.37	in	1.79	0.17	in	1.82	0.17	in	1.83	0.17	in	2.54
2	000094-97-3	4.20	0.09	in	3.36	0.06	in	4.33	out	3.57	0.49	in	3.43	0.16	in	3.26	0.17	in	3.41	0.16	in	3.65
3	000095-14-7	4.30	0.08	in	3.18	0.07	in	4.63	out	3.52	0.49	in	3.72	0.13	in	3.43	0.16	in	3.64	0.13	in	3.77
4	000130-34-7	4.84	0.20	in	3.86	0.09	in	3.28	out	3.76	0.66	out	5.31	0.13	in	5.01	0.17	in	5.27	0.13	in	4.48
5	000131-43-1	4.89	0.44	out	4.85	0.20	in	4.00	out	3.87	0.74	out	5.39	0.31	out	4.82	0.44	out	5.34	0.31	out	4.74
6	000134-58-7	2.17	0.09	in	3.18	0.18	in	3.86	out	2.84	0.43	in	1.69	0.14	in	1.73	0.14	in	1.72	0.14	in	2.46
7	000136-85-6	3.38	0.07	in	3.34	0.06	in	3.97	out	3.56	0.50	in	2.79	0.11	in	2.55	0.13	in	2.76	0.11	in	3.19
8	000273-40-5	3.07	0.14	in	2.84	0.13	in	4.21	out	3.10	0.41	in	2.01	0.16	in	2.01	0.16	in	2.02	0.16	in	2.75
9	000288-36-8	2.91	0.33	out	2.53	0.13	in	4.51	out	3.62	0.34	in	3.13	0.07	in	3.23	0.07	in	3.11	0.07	in	3.29
10	000288-88-0	2.15	0.43	out	2.55	0.13	in	4.82	out	3.17	0.35	in	1.75	0.17	in	1.79	0.17	in	1.82	0.17	in	2.58
11	000584-13-4	2.51	0.35	out	2.64	0.12	in	4.07	out	3.09	0.39	in	2.13	0.15	in	2.17	0.15	in	2.14	0.15	in	2.68
12	000932-64-9	1.45	0.23	in	2.60	0.27	out	3.36	out	3.16	0.33	in	1.22	0.17	in	1.15	0.17	in	1.25	0.17	in	2.03
13	000938-56-7	3.72	0.09	in	3.49	0.07	in	4.08	out	3.63	0.47	in	3.18	0.06	in	2.93	0.09	in	3.16	0.06	in	3.46
14	000939-07-1	4.35	0.05	in	3.31	0.04	in	3.84	out	3.25	0.30	in	4.41	0.04	in	4.17	0.06	in	4.34	0.04	in	3.95
15	000939-08-2	3.46	0.08	in	3.19	0.05	in	3.64	out	2.95	0.31	in	3.25	0.04	in	3.23	0.04	in	3.25	0.04	in	3.28
16	000944-91-2	4.41	0.04	in	4.29	0.12	in	4.67	in	5.45	0.34	in	4.19	0.03	in	3.95	0.05	in	4.14	0.03	in	4.44
17	000947-85-3	4.78	0.05	in	4.48	0.10	in	4.71	in	5.58	0.33	in	4.15	0.03	in	3.93	0.05	in	4.11	0.03	in	4.53
18	000974-29-8	8.89	0.37	out	7.17	0.15	in	7.39	out	5.49	0.39	in	8.42	0.36	out	7.60	0.63	out	8.20	0.37	out	7.59
19	001028-08-6	5.20	0.11	in	4.93	0.15	in	5.95	out	3.61	0.34	in	4.66	0.13	in	4.87	0.15	in	5.79	0.56	out	5.00
20	001031-47-6	4.62	0.03	in	4.48	0.06	in	5.23	in	3.91	0.34	in	4.37	0.07	in	4.19	0.08	in	5.56	0.55	out	4.62
21	001123-54-2	2.39	0.08	in	3.02	0.10	in	4.06	out	2.79	0.40	in	1.46	0.21	in	1.42	0.21	in	1.47	0.21	in	2.37
22	001325-58-2	8.97	2.41	out	8.80	0.87	out	9.84	out	5.02	0.87	out	4.82	0.25	out	4.60	0.27	out	4.74	0.25	in	6.68
23	001326-66-5	4.77	0.05	in	4.42	0.24	out	4.36	in	3.56	0.49	in	5.43	0.03	in	5.11	0.07	in	5.39	0.03	in	4.72
24	001455-77-2	2.70	0.29	out	3.00	0.16	in	3.98	out	2.77	0.42	in	1.97	0.22	in	1.85	0.23	in	1.89	0.23	in	2.60
25	001468-26-4	2.48	0.07	in	2.82	0.31	out	3.38	out	3.02	0.67	out	2.12	0.08	in	2.20	0.09	in	2.15	0.08	in	2.60
26	001600-61-9	2.16	0.09	in	3.16	0.05	in	3.25	out	3.64	0.41	in	2.27	0.11	in	2.24	0.12	in	2.34	0.12	in	2.72
27	001680-44-0	5.07	0.11	in	3.25	0.09	in	4.83	out	4.46	0.47	in	4.63	0.13	in	4.32	0.18	in	4.51	0.14	in	4.44
28	001704-66-1	2.16	0.09	in	3.07	0.09	in	4.06	out	3.26	0.44	in	2.30	0.11	in	2.28	0.11	in	2.36	0.11	in	2.79
29	002338-12-7	3.02	0.05	in	2.92	0.06	in	3.51	out	3.61	0.51	out	3.73	0.04	in	3.66	0.04	in	3.71	0.04	in	3.45
30	002440-22-4	4.98	0.04	in	4.10	0.05	in	4.72	in	4.49	0.62	out	5.36	0.03	in	5.05	0.07	in	5.28	0.03	in	4.85
31	002592-95-2	3.88	0.09	in	3.08	0.10	in	2.93	out	3.56	0.45	in	3.01	0.09	in	2.69	0.13	in	2.97	0.09	in	3.16
32	002683-90-1	2.28	0.09	in	3.24	0.15	in	3.91	out	3.03	0.49	in	1.25	0.17	in	1.22	0.17	in	1.30	0.17	in	2.32
33	003142-42-5	6.46	0.15	in	6.01	0.17	in	7.62	out	5.41	0.53	out	6.47	0.09	in	6.23	0.12	in	6.32	0.10	in	6.36
34	003147-75-9	5.61	0.08	in	5.18	0.07	in	5.21	out	4.85	0.59	out	5.92	0.05	in	5.66	0.08	in	5.80	0.06	in	5.46
35	003147-76-0	5.14	0.05	in	4.57	0.05	in	4.81	in	4.76	0.62	out	5.62	0.03	in	5.35	0.06	in	5.53	0.04	in	5.11
36	003232-84-6	2.68	0.30	out	2.16	0.49	out	4.45	out	3.02	0.39	in	1.95	0.25	out	1.82	0.26	in	1.89	0.25	in	2.57
37	003310-68-7	4.01	0.06	in	3.52	0.04	in	4.19	out	3.13	0.46	in	3.80	0.07	in	3.51	0.11	in	3.73	0.07	in	3.70

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
38	003333-62-8	6.93	0.15	in	5.93	0.04	in	5.61	out	4.52	0.92	out	7.10	0.14	in	6.32	0.38	out	6.96	0.14	in	6.20
39	003357-42-4	4.90	0.12	in	3.30	0.08	in	4.89	out	3.96	0.34	in	4.41	0.12	in	4.08	0.16	in	4.30	0.12	in	4.26
40	003641-10-9	2.58	0.10	in	2.71	0.11	in	4.41	out	3.14	0.35	in	1.28	0.24	out	1.18	0.24	in	1.31	0.24	in	2.37
41	003652-22-0	4.53	0.10	in	3.64	0.20	in	5.21	in	3.53	0.34	in	4.13	0.04	in	4.19	0.04	in	4.11	0.04	in	4.19
42	003652-23-1	4.40	0.07	in	3.82	0.20	in	5.38	in	3.63	0.33	in	4.21	0.03	in	4.28	0.04	in	4.18	0.03	in	4.27
43	003652-25-3	4.30	0.07	in	3.68	0.20	in	5.11	in	3.56	0.32	in	4.46	0.04	in	4.57	0.05	in	4.43	0.04	in	4.30
44	003652-27-5	5.51	0.10	in	3.89	0.22	in	5.42	out	3.49	0.39	in	5.59	0.11	in	5.49	0.12	in	5.49	0.12	in	4.98
45	003652-31-1	3.78	0.06	in	3.25	0.19	in	4.56	in	3.43	0.26	in	3.64	0.06	in	3.69	0.06	in	3.66	0.06	in	3.72
46	003652-32-2	3.78	0.06	in	3.27	0.18	in	4.64	out	3.47	0.27	in	3.64	0.06	in	3.69	0.06	in	3.66	0.06	in	3.74
47	003663-24-9	4.40	0.05	in	3.80	0.07	in	4.73	in	4.04	0.59	out	4.39	0.04	in	4.30	0.04	in	4.31	0.04	in	4.28
48	003683-95-2	4.58	0.29	out	4.07	0.18	in	5.46	out	3.35	0.44	in	4.15	0.27	out	4.44	0.30	out	4.18	0.27	out	4.32
49	003770-47-6	3.95	0.06	in	3.54	0.21	in	4.93	out	3.78	0.38	in	3.99	0.05	in	4.05	0.05	in	3.98	0.05	in	4.03
50	003846-71-7	5.72	0.11	in	5.28	0.04	in	5.61	out	5.04	0.56	out	6.07	0.06	in	5.91	0.07	in	5.95	0.07	in	5.66
51	003864-99-1	5.73	0.10	in	5.46	0.05	in	5.67	out	5.13	0.57	out	6.13	0.05	in	6.08	0.05	in	6.02	0.05	in	5.75
52	003896-11-5	5.13	0.06	in	4.99	0.03	in	5.22	out	4.81	0.60	out	5.60	0.03	in	5.52	0.03	in	5.53	0.03	in	5.26
53	004184-79-6	3.96	0.15	in	3.42	0.07	in	4.02	out	3.83	0.53	out	3.92	0.06	in	3.86	0.07	in	3.84	0.07	in	3.83
54	004314-22-1	1.76	0.19	in	2.54	0.10	in	3.52	out	3.08	0.41	in	0.58	0.25	out	0.47	0.25	in	0.66	0.25	in	1.80
55	004343-73-1	3.60	0.11	in	3.57	0.15	in	4.55	out	4.01	0.35	in	2.90	0.09	in	2.93	0.09	in	2.86	0.09	in	3.49
56	004368-68-7	4.77	0.09	in	4.05	0.13	in	4.43	out	4.97	0.50	in	4.42	0.04	in	4.17	0.06	in	4.35	0.04	in	4.45
57	004928-87-4	1.25	0.19	in	2.44	0.10	in	4.07	out	3.00	0.34	in	-0.14	0.33	out	-0.34	0.35	out	-0.04	0.33	out	1.46
58	004928-88-5	1.80	0.16	in	2.84	0.12	in	4.24	out	3.69	0.34	in	0.75	0.23	in	0.62	0.23	in	0.80	0.23	in	2.11
59	005302-27-2	6.31	0.62	out	3.68	0.19	in	4.59	out	4.35	0.35	in	4.24	0.14	in	4.36	0.15	in	4.12	0.15	in	4.52
60	005369-84-6	4.07	0.04	in	4.01	0.06	in	4.82	in	3.67	0.26	in	4.25	0.05	in	4.25	0.05	in	4.21	0.05	in	4.18
61	005472-71-9	4.46	0.08	in	4.66	0.08	in	4.77	in	3.91	0.48	in	4.50	0.05	in	4.41	0.05	in	4.44	0.05	in	4.45
62	005516-20-1	7.25	0.18	in	6.02	0.05	in	6.47	out	5.30	0.64	out	7.67	0.18	in	7.08	0.33	out	7.53	0.19	in	6.76
63	005873-30-3	4.17	0.04	in	4.15	0.07	in	5.05	in	4.12	0.58	out	4.44	0.04	in	4.45	0.04	in	4.41	0.04	in	4.40
64	006054-53-1	3.96	0.03	in	3.81	0.14	in	5.10	in	3.73	0.35	in	4.10	0.02	in	4.02	0.03	in	4.10	0.02	in	4.12
65	006085-94-5	4.77	0.09	in	4.00	0.14	in	4.43	out	4.80	0.25	in	4.43	0.04	in	4.18	0.06	in	4.36	0.04	in	4.42
66	006299-39-4	3.10	0.06	in	2.94	0.06	in	3.49	out	3.62	0.49	in	3.81	0.04	in	3.74	0.04	in	3.78	0.04	in	3.50
67	006789-99-7	4.33	0.09	in	3.66	0.14	in	4.13	out	3.65	0.54	out	4.14	0.12	in	4.20	0.13	in	4.01	0.13	in	4.02
68	006818-99-1	3.47	0.36	out	2.84	0.09	in	5.33	out	3.27	0.33	in	2.83	0.11	in	2.96	0.12	in	2.88	0.11	in	3.37
69	006994-51-0	7.64	0.24	out	6.30	0.16	in	6.41	out	5.53	0.56	out	7.57	0.22	in	6.39	0.78	out	7.41	0.23	in	6.75
70	007170-01-6	2.29	0.40	out	2.74	0.11	in	4.45	out	3.20	0.33	in	1.99	0.15	in	2.04	0.15	in	2.04	0.15	in	2.68
71	007411-23-6	6.65	0.86	out	3.64	0.13	in	6.13	out	4.02	0.38	in	4.44	0.87	out	4.59	0.88	out	4.40	0.87	out	4.84
72	007532-52-7	2.18	0.08	in	2.99	0.06	in	2.96	out	3.06	0.36	in	2.54	0.13	in	2.52	0.13	in	2.59	0.13	in	2.69
73	010109-05-4	1.75	0.14	in	3.05	0.06	in	3.14	out	2.66	0.40	in	1.44	0.15	in	1.43	0.15	in	1.48	0.15	in	2.14
74	010187-79-8	2.43	0.07	in	3.30	0.07	in	4.24	out	3.73	0.43	in	2.67	0.09	in	2.67	0.09	in	2.71	0.09	in	3.11
75	010187-84-5	2.13	0.09	in	3.25	0.05	in	3.89	out	3.19	0.37	in	2.43	0.14	in	2.40	0.15	in	2.48	0.15	in	2.82
76	010187-86-7	2.29	0.08	in	3.14	0.05	in	3.32	out	3.23	0.33	in	2.55	0.15	in	2.55	0.15	in	2.60	0.16	in	2.81
77	010187-89-0	2.91	0.10	in	3.49	0.05	in	4.13	out	3.25	0.38	in	2.88	0.12	in	2.89	0.12	in	2.91	0.12	in	3.21
78	013091-80-0	3.65	0.06	in	3.05	0.05	in	3.46	out	3.63	0.47	in	3.34	0.10	in	3.40	0.10	in	3.39	0.10	in	3.42
79	013257-88-0	5.22	0.09	in	4.92	0.06	in	5.85	out	4.76	0.40	in	4.29	0.16	in	4.37	0.16	in	4.16	0.16	in	4.80

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
80	013351-73-0	4.21	0.09	in	3.87	0.17	in	4.35	out	4.25	0.66	out	3.22	0.09	in	2.91	0.13	in	3.17	0.09	in	3.71
81	014803-99-7	3.99	0.14	in	3.24	0.08	in	4.82	out	3.13	0.26	in	3.27	0.10	in	3.17	0.10	in	3.22	0.10	in	3.55
82	015421-84-8	5.20	0.15	in	4.43	0.09	in	5.09	out	4.34	0.57	out	4.37	0.07	in	4.50	0.07	in	4.28	0.07	in	4.60
83	015497-45-7	6.16	0.14	in	5.27	0.05	in	5.72	out	5.04	0.49	in	5.34	0.08	in	5.27	0.08	in	5.21	0.08	in	5.43
84	015805-10-4	5.26	0.05	in	4.27	0.07	in	3.89	out	3.13	0.47	in	4.97	0.11	in	4.76	0.12	in	4.90	0.11	in	4.45
85	016515-58-5	5.78	0.04	in	6.30	0.06	in	6.24	out	4.71	0.80	out	5.80	0.03	in	5.33	0.12	in	5.74	0.03	in	5.70
86	016584-05-7	4.72	0.09	in	4.06	0.14	in	4.30	out	4.49	0.60	out	3.33	0.09	in	3.03	0.12	in	3.27	0.09	in	3.89
87	018076-61-4	3.65	0.03	in	3.29	0.06	in	4.47	out	3.04	0.35	in	3.14	0.12	in	2.90	0.14	in	3.07	0.12	in	3.37
88	018811-70-6	5.26	0.04	in	3.84	0.04	in	5.03	out	3.45	0.42	in	5.27	0.07	in	4.86	0.14	in	5.16	0.07	in	4.70
89	019683-09-1	6.35	0.09	in	5.83	0.04	in	5.91	out	5.04	0.56	out	6.54	0.08	in	5.82	0.29	out	6.43	0.08	in	5.99
90	019794-93-5	5.67	0.07	in	5.97	0.06	in	6.00	out	4.69	0.54	out	4.92	0.04	in	4.90	0.04	in	4.86	0.04	in	5.29
91	021050-95-3	5.15	0.12	in	3.89	0.16	in	4.74	out	4.58	0.62	out	3.94	0.13	in	3.69	0.16	in	3.87	0.13	in	4.27
92	021532-04-7	4.40	0.03	in	3.88	0.20	in	5.10	out	3.79	0.40	in	4.62	0.04	in	4.87	0.07	in	4.55	0.04	in	4.46
93	023633-05-8	2.26	0.08	in	3.24	0.08	in	3.46	out	3.22	0.37	in	2.71	0.17	in	2.73	0.17	in	2.76	0.17	in	2.91
94	023711-34-4	6.41	0.12	in	4.13	0.16	in	5.04	in	5.25	0.43	in	6.81	0.14	in	6.44	0.19	in	6.68	0.14	in	5.82
95	024017-47-8	5.93	0.21	in	5.61	0.04	in	7.00	in	5.95	0.33	in	5.43	0.03	in	5.31	0.03	in	6.61	0.51	out	5.98
96	024054-57-7	2.15	0.09	in	3.23	0.08	in	4.16	out	3.41	0.35	in	2.53	0.18	in	2.55	0.18	in	2.59	0.18	in	2.95
97	025973-55-1	5.86	0.13	in	5.69	0.06	in	6.06	out	5.22	0.56	out	6.09	0.07	in	5.92	0.08	in	5.96	0.07	in	5.83
98	026621-45-4	1.68	0.22	in	2.32	0.10	in	3.36	out	4.34	0.46	in	1.18	0.21	in	1.13	0.21	in	1.22	0.21	in	2.17
99	027022-50-0	4.84	0.05	in	4.35	0.10	in	2.56	out	4.05	0.61	out	5.27	0.03	in	5.14	0.03	in	5.20	0.03	in	4.49
100	027210-18-0	4.38	0.03	in	4.45	0.09	in	4.75	out	3.71	0.53	out	4.78	0.02	in	4.80	0.02	in	4.73	0.02	in	4.51
101	027799-91-3	3.52	0.05	in	3.23	0.09	in	4.08	out	3.61	0.51	out	3.26	0.07	in	3.08	0.08	in	3.23	0.07	in	3.43
102	028401-89-0	4.48	0.04	in	4.64	0.07	in	4.96	out	3.58	0.53	out	4.90	0.02	in	4.92	0.02	in	4.84	0.02	in	4.62
103	028911-01-5	5.91	0.08	in	5.46	0.05	in	5.05	in	4.12	0.66	out	6.10	0.09	in	5.92	0.10	in	6.03	0.09	in	5.51
104	028981-97-7	5.74	0.06	in	5.30	0.05	in	5.07	in	4.02	0.66	out	5.81	0.06	in	5.48	0.11	in	5.72	0.07	in	5.31
105	029440-31-1	4.06	0.05	in	3.64	0.06	in	4.53	out	3.08	0.31	in	3.15	0.13	in	3.21	0.13	in	4.32	0.60	out	3.71
106	029878-31-7	3.80	0.04	in	3.26	0.08	in	4.31	out	3.85	0.58	out	3.20	0.11	in	2.97	0.13	in	3.14	0.11	in	3.50
107	029975-16-4	5.95	0.08	in	5.05	0.05	in	4.81	in	4.05	0.67	out	6.03	0.09	in	5.72	0.13	in	5.93	0.09	in	5.36
108	031251-03-3	7.12	0.17	in	5.56	0.04	in	5.02	out	5.68	0.30	in	7.16	0.12	in	6.37	0.37	out	7.00	0.13	in	6.27
109	031409-18-4	5.46	0.05	in	4.62	0.11	in	5.34	in	5.35	0.30	in	4.98	0.03	in	4.93	0.03	in	4.93	0.03	in	5.09
110	031701-42-5	5.26	0.05	in	4.47	0.09	in	4.77	out	4.86	0.60	out	4.94	0.06	in	4.87	0.07	in	4.88	0.06	in	4.87
111	032362-89-3	4.38	0.09	in	3.16	0.20	in	4.53	out	3.18	0.30	in	4.40	0.07	in	4.39	0.07	in	4.37	0.07	in	4.06
112	032723-50-5	4.95	0.03	in	4.65	0.08	in	5.03	in	4.20	0.51	out	5.14	0.04	in	4.90	0.06	in	5.05	0.04	in	4.85
113	034771-66-9	5.26	0.04	in	5.80	0.04	in	5.62	out	4.49	0.64	out	5.51	0.07	in	5.24	0.10	in	5.47	0.07	in	5.34
114	035515-45-8	4.36	0.04	in	4.53	0.09	in	3.39	out	4.33	0.72	out	4.15	0.04	in	4.05	0.04	in	4.14	0.04	in	4.14
115	036325-69-6	4.64	0.02	in	4.40	0.03	in	5.00	out	3.82	0.48	in	4.84	0.02	in	4.54	0.05	in	4.79	0.02	in	4.58
116	036411-52-6	3.32	0.06	in	3.29	0.05	in	4.53	out	3.31	0.45	in	3.19	0.04	in	3.00	0.05	in	3.19	0.04	in	3.40
117	036437-37-3	5.53	0.10	in	5.35	0.05	in	5.71	out	5.20	0.61	out	5.90	0.05	in	5.73	0.06	in	5.79	0.06	in	5.60
118	036791-04-5	2.24	0.10	in	3.67	0.04	in	3.53	out	2.98	0.59	out	2.77	0.12	in	2.94	0.13	in	2.80	0.12	in	2.99
119	037160-06-8	6.49	0.10	in	4.87	0.06	in	4.90	out	4.61	0.52	out	6.59	0.16	in	6.10	0.26	in	6.43	0.17	in	5.71
120	038942-51-7	4.57	0.04	in	3.39	0.16	in	4.82	in	4.57	0.39	in	4.59	0.03	in	4.41	0.04	in	4.55	0.03	in	4.41
121	039968-33-7	2.93	0.15	in	2.96	0.12	in	4.14	out	3.24	0.39	in	1.75	0.15	in	1.57	0.16	in	1.79	0.15	in	2.63

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
122	040054-69-1	5.38	0.05	in	5.32	0.09	in	5.76	in	3.91	0.64	out	5.67	0.06	in	5.63	0.06	in	5.61	0.06	in	5.33
123	041083-11-8	8.29	0.32	out	8.57	0.38	out	8.65	out	5.65	0.37	in	7.68	0.22	in	8.10	0.29	out	7.45	0.24	in	7.77
124	041735-28-8	2.02	0.10	in	3.21	0.05	in	3.60	out	3.56	0.42	in	2.06	0.15	in	2.03	0.15	in	2.13	0.15	in	2.66
125	041735-29-9	2.68	0.14	in	3.41	0.04	in	4.20	out	3.66	0.42	in	2.29	0.13	in	2.27	0.13	in	2.34	0.13	in	2.98
126	041735-30-2	2.78	0.14	in	3.10	0.12	in	3.42	out	3.84	0.40	in	2.77	0.16	in	2.78	0.16	in	2.79	0.16	in	3.07
127	041735-38-0	3.15	0.05	in	3.60	0.07	in	4.08	out	4.23	0.56	out	3.47	0.04	in	3.54	0.05	in	3.48	0.04	in	3.65
128	041735-41-5	2.72	0.06	in	3.40	0.05	in	4.04	in	3.62	0.38	in	3.17	0.10	in	3.19	0.10	in	3.18	0.10	in	3.33
129	041735-42-6	2.17	0.09	in	3.14	0.05	in	3.92	out	3.46	0.37	in	2.51	0.15	in	2.50	0.15	in	2.56	0.15	in	2.89
130	041735-44-8	3.20	0.05	in	3.61	0.07	in	4.11	out	4.50	0.56	out	3.43	0.04	in	3.50	0.04	in	3.44	0.04	in	3.68
131	041735-45-9	2.75	0.06	in	3.41	0.05	in	4.13	out	3.70	0.37	in	3.13	0.10	in	3.15	0.10	in	3.14	0.10	in	3.34
132	041735-50-6	3.27	0.04	in	3.61	0.07	in	3.92	out	4.29	0.56	out	3.45	0.04	in	3.50	0.04	in	3.45	0.04	in	3.64
133	041735-51-7	2.30	0.09	in	2.45	0.34	out	2.87	out	3.46	0.36	in	2.84	0.16	in	2.86	0.16	in	2.87	0.16	in	2.81
134	041735-54-0	2.91	0.08	in	3.10	0.05	in	4.03	out	3.57	0.40	in	3.05	0.10	in	3.08	0.10	in	3.11	0.11	in	3.27
135	041735-55-1	3.43	0.04	in	3.11	0.16	in	4.37	in	4.59	0.49	in	4.03	0.05	in	4.13	0.05	in	4.03	0.05	in	3.96
136	041735-56-2	3.07	0.05	in	2.96	0.16	in	3.35	out	3.97	0.54	out	3.26	0.03	in	3.28	0.03	in	3.28	0.03	in	3.31
137	041735-57-3	2.84	0.05	in	3.11	0.06	in	4.00	out	4.39	0.52	out	3.39	0.07	in	3.42	0.07	in	3.40	0.07	in	3.51
138	041814-78-2	4.70	0.07	in	3.85	0.17	in	4.28	in	4.05	0.64	out	4.46	0.08	in	4.42	0.08	in	4.42	0.08	in	4.31
139	041834-21-3	3.19	0.04	in	3.04	0.16	in	3.70	in	3.92	0.55	out	3.57	0.03	in	3.63	0.03	in	3.59	0.03	in	3.52
140	042509-80-8	7.23	0.66	out	5.95	0.18	in	7.65	in	5.86	0.37	in	5.75	0.05	in	6.07	0.09	in	6.89	0.49	out	6.49
141	043029-44-3	6.88	0.15	in	4.74	0.10	in	5.28	out	5.19	0.50	in	7.08	0.20	in	6.62	0.29	out	6.92	0.21	in	6.10
142	043121-43-3	4.51	0.04	in	4.88	0.06	in	4.64	in	5.09	0.33	in	4.55	0.02	in	4.45	0.02	in	4.50	0.02	in	4.66
143	051627-14-6	3.47	0.19	in	5.39	0.14	in	4.62	out	2.86	0.46	in	4.15	0.08	in	4.20	0.08	in	4.19	0.08	in	4.13
144	053817-16-6	4.05	0.06	in	3.12	0.16	in	3.25	out	3.55	0.32	in	3.69	0.18	in	3.81	0.18	in	3.63	0.18	in	3.59
145	054028-81-8	5.36	0.04	in	5.13	0.03	in	5.07	in	3.81	0.52	out	5.48	0.04	in	5.13	0.09	in	5.40	0.05	in	5.05
146	054028-83-0	5.07	0.03	in	5.27	0.03	in	5.09	out	3.84	0.53	out	5.33	0.04	in	5.08	0.06	in	5.27	0.04	in	4.99
147	054028-84-1	5.94	0.07	in	5.60	0.05	in	5.14	out	3.81	0.67	out	6.08	0.07	in	5.60	0.16	in	5.98	0.07	in	5.45
148	054028-85-2	5.06	0.05	in	4.85	0.12	in	4.97	in	3.64	0.50	in	5.22	0.06	in	5.14	0.06	in	5.18	0.06	in	4.87
149	054028-86-3	4.60	0.03	in	4.85	0.02	in	4.75	in	3.71	0.48	in	4.79	0.04	in	4.67	0.04	in	4.76	0.04	in	4.59
150	054028-89-6	5.35	0.04	in	5.14	0.03	in	5.05	in	3.66	0.52	out	5.48	0.04	in	5.12	0.09	in	5.40	0.05	in	5.03
151	054028-90-9	5.04	0.03	in	5.28	0.03	in	5.19	in	3.79	0.56	out	5.29	0.04	in	5.03	0.06	in	5.23	0.04	in	4.98
152	054028-91-0	5.48	0.05	in	4.96	0.03	in	4.97	out	3.77	0.52	out	5.65	0.05	in	5.20	0.13	in	5.55	0.05	in	5.08
153	054028-92-1	5.15	0.04	in	5.10	0.03	in	5.02	out	3.80	0.53	out	5.39	0.04	in	5.03	0.09	in	5.31	0.04	in	4.97
154	054028-93-2	5.12	0.04	in	5.10	0.03	in	5.11	out	3.73	0.54	out	5.36	0.04	in	5.00	0.09	in	5.29	0.04	in	4.96
155	054028-94-3	5.59	0.05	in	4.79	0.02	in	4.89	out	3.84	0.50	in	5.71	0.05	in	5.26	0.13	in	5.60	0.06	in	5.10
156	054028-95-4	5.13	0.04	in	5.09	0.03	in	5.22	out	3.84	0.54	out	5.30	0.04	in	4.92	0.09	in	5.22	0.04	in	4.96
157	054123-06-7	5.58	0.11	in	5.16	0.09	in	5.13	in	3.80	0.60	out	5.84	0.11	in	5.83	0.11	in	5.79	0.11	in	5.30
158	055179-31-2	5.39	0.05	in	5.20	0.04	in	5.23	in	4.98	0.29	in	5.61	0.04	in	5.15	0.12	in	5.52	0.04	in	5.30
159	055219-65-3	4.30	0.04	in	4.66	0.03	in	4.63	in	4.55	0.23	in	4.62	0.03	in	4.52	0.03	in	4.56	0.03	in	4.55
160	055375-40-1	4.10	0.03	in	4.66	0.17	in	5.50	out	5.25	0.38	in	4.27	0.03	in	4.55	0.06	in	4.26	0.03	in	4.66
161	055425-38-2	5.64	0.06	in	4.33	0.08	in	4.99	out	3.43	0.48	in	5.70	0.13	in	5.28	0.21	in	5.59	0.14	in	5.00
162	056383-06-3	4.01	0.04	in	4.49	0.08	in	4.63	in	3.89	0.55	out	4.24	0.06	in	4.40	0.07	in	4.18	0.06	in	4.26
163	056383-11-0	4.20	0.06	in	4.58	0.08	in	4.71	in	3.69	0.49	in	4.45	0.06	in	4.54	0.07	in	4.39	0.07	in	4.37

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
164	056396-43-1	5.87	0.07	in	4.65	0.08	in	4.88	in	4.70	0.44	in	6.01	0.12	in	5.70	0.16	in	5.91	0.12	in	5.39
165	056881-36-8	2.35	0.10	in	3.61	0.13	in	3.91	out	3.41	0.43	in	1.77	0.12	in	1.81	0.12	in	1.83	0.12	in	2.67
166	057801-81-7	5.75	0.15	in	5.29	0.09	in	5.40	out	3.84	0.62	out	5.95	0.14	in	5.95	0.14	in	5.90	0.14	in	5.44
167	057801-94-2	6.11	0.19	in	5.43	0.10	in	5.69	out	3.89	0.63	out	6.26	0.18	in	6.29	0.18	in	6.21	0.18	in	5.70
168	059026-08-3	5.73	0.21	in	4.53	0.14	in	5.20	out	5.45	0.41	in	4.17	0.10	in	4.37	0.11	in	4.09	0.10	in	4.79
169	059338-86-2	3.31	0.04	in	3.50	0.10	in	4.25	in	3.80	0.53	out	3.71	0.03	in	3.75	0.03	in	3.71	0.03	in	3.72
170	059338-92-0	2.55	0.07	in	3.17	0.06	in	3.41	out	3.10	0.37	in	2.62	0.08	in	2.58	0.08	in	2.67	0.08	in	2.87
171	059338-93-1	4.57	0.07	in	4.88	0.03	in	4.68	in	3.44	0.46	in	4.17	0.04	in	4.26	0.05	in	4.13	0.04	in	4.30
172	060207-31-0	4.66	0.06	in	4.87	0.06	in	4.92	in	5.05	0.25	in	5.02	0.03	in	5.10	0.03	in	4.99	0.03	in	4.94
173	060207-90-1	5.25	0.04	in	5.35	0.04	in	5.70	in	5.34	0.16	in	5.27	0.02	in	5.35	0.03	in	5.22	0.03	in	5.36
174	060207-93-4	4.97	0.04	in	5.20	0.04	in	5.37	in	5.38	0.18	in	5.05	0.03	in	5.14	0.03	in	5.02	0.03	in	5.16
175	060932-58-3	3.30	0.04	in	3.01	0.06	in	3.70	out	3.08	0.38	in	3.27	0.05	in	3.15	0.05	in	3.27	0.05	in	3.26
176	061691-97-2	3.98	0.08	in	4.12	0.06	in	4.44	in	3.06	0.32	in	4.14	0.07	in	4.02	0.07	in	4.09	0.07	in	3.98
177	063216-86-4	5.35	0.36	out	5.13	0.12	in	4.44	out	3.31	0.59	out	5.33	0.32	out	4.75	0.45	out	5.28	0.32	out	4.80
178	063251-40-1	4.93	0.16	in	4.08	0.05	in	3.54	out	3.16	0.48	in	5.24	0.13	in	4.92	0.17	in	5.20	0.13	in	4.44
179	063870-37-1	4.52	0.04	in	3.26	0.09	in	2.75	out	3.43	0.51	out	4.62	0.06	in	4.46	0.07	in	4.59	0.06	in	3.95
180	064057-50-7	2.90	0.05	in	3.55	0.07	in	3.98	out	3.58	0.40	in	2.97	0.09	in	3.04	0.10	in	3.03	0.09	in	3.29
181	064082-38-8	3.02	0.08	in	3.51	0.08	in	4.16	out	3.40	0.42	in	2.95	0.10	in	3.00	0.10	in	3.01	0.10	in	3.29
182	066104-34-5	4.06	0.02	in	4.05	0.06	in	4.90	in	3.98	0.48	in	4.26	0.05	in	3.99	0.08	in	4.22	0.06	in	4.21
183	066104-44-7	4.25	0.04	in	4.17	0.06	in	4.91	out	3.95	0.48	in	4.61	0.06	in	4.47	0.06	in	4.56	0.06	in	4.42
184	066246-88-6	5.26	0.04	in	4.95	0.05	in	5.40	in	5.47	0.15	in	5.13	0.03	in	5.15	0.03	in	5.06	0.03	in	5.20
185	066492-64-6	4.48	0.03	in	4.55	0.09	in	4.98	in	5.41	0.42	in	4.52	0.02	in	4.43	0.03	in	4.49	0.02	in	4.70
186	066535-86-2	6.53	0.11	in	5.01	0.05	in	5.61	out	4.71	0.66	out	6.85	0.12	in	6.49	0.18	in	6.72	0.13	in	5.99
187	066975-54-0	5.22	0.36	out	5.75	0.15	in	6.04	out	3.71	0.88	out	4.22	0.07	in	4.30	0.07	in	4.20	0.07	in	4.78
188	067465-03-6	3.86	0.05	in	3.74	0.21	in	4.86	in	3.41	0.30	in	3.86	0.03	in	3.92	0.03	in	3.86	0.03	in	3.93
189	067465-05-8	4.03	0.05	in	4.02	0.05	in	4.89	in	3.33	0.33	in	3.96	0.06	in	3.99	0.06	in	3.91	0.06	in	4.02
190	068049-83-2	4.86	0.04	in	4.86	0.11	in	5.12	in	5.18	0.58	out	4.70	0.03	in	4.89	0.04	in	4.71	0.03	in	4.90
191	069141-50-0	4.93	0.14	in	4.68	0.02	in	4.70	out	4.46	0.41	in	4.90	0.08	in	5.14	0.10	in	4.80	0.08	in	4.80
192	070292-10-3	4.68	0.02	in	3.93	0.06	in	4.45	in	4.12	0.56	out	4.92	0.02	in	4.61	0.06	in	4.88	0.02	in	4.51
193	070321-86-7	6.95	0.15	in	6.47	0.12	in	6.50	out	5.55	0.55	out	7.10	0.10	in	6.14	0.47	out	6.95	0.11	in	6.52
194	075020-35-8	3.59	0.07	in	3.77	0.11	in	3.89	in	3.48	0.53	out	3.88	0.02	in	3.94	0.03	in	3.88	0.02	in	3.78
195	075736-33-3	5.19	0.03	in	5.03	0.02	in	4.98	in	4.57	0.23	in	5.19	0.03	in	5.27	0.03	in	5.14	0.03	in	5.05
196	076608-88-3	4.66	0.05	in	4.53	0.03	in	4.54	in	4.70	0.36	in	4.92	0.04	in	4.77	0.05	in	4.86	0.04	in	4.71
197	076674-21-0	5.01	0.03	in	4.68	0.03	in	4.21	in	4.31	0.29	in	5.32	0.03	in	4.97	0.08	in	5.26	0.03	in	4.82
198	076738-62-0	4.92	0.04	in	4.86	0.02	in	4.84	in	4.65	0.24	in	4.84	0.03	in	4.75	0.03	in	4.77	0.03	in	4.80
199	077314-77-3	3.47	0.09	in	3.83	0.03	in	4.77	out	2.84	0.39	in	3.00	0.12	in	2.99	0.12	in	2.99	0.12	in	3.41
200	078149-96-9	5.36	0.09	in	5.10	0.17	in	6.52	out	4.32	0.44	in	4.78	0.09	in	5.02	0.11	in	5.93	0.53	out	5.29
201	078150-00-2	4.13	0.03	in	4.27	0.06	in	5.06	out	3.08	0.42	in	3.75	0.07	in	3.52	0.09	in	4.97	0.57	out	4.11
202	078150-02-4	4.96	0.09	in	4.76	0.14	in	5.66	out	3.51	0.31	in	4.49	0.12	in	4.70	0.14	in	5.63	0.56	out	4.82
203	078218-51-6	4.71	0.03	in	4.65	0.06	in	5.25	in	4.05	0.34	in	4.50	0.07	in	4.45	0.07	in	5.71	0.56	out	4.76
204	078218-52-7	4.54	0.08	in	4.42	0.13	in	5.24	out	3.31	0.30	in	4.22	0.11	in	4.41	0.12	in	5.37	0.56	out	4.50
205	078218-53-8	5.66	0.14	in	5.26	0.18	in	6.62	out	3.85	0.40	in	5.19	0.14	in	5.46	0.17	in	6.30	0.57	out	5.48

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
206	078218-54-9	4.76	0.10	in	4.55	0.13	in	5.28	out	3.43	0.30	in	4.51	0.11	in	4.73	0.13	in	5.66	0.56	out	4.70
207	078218-55-0	4.43	0.04	in	4.63	0.07	in	5.39	out	3.67	0.29	in	4.40	0.07	in	4.33	0.07	in	5.60	0.57	out	4.64
208	078218-56-1	4.80	0.03	in	4.72	0.07	in	5.28	in	4.08	0.33	in	4.55	0.07	in	4.40	0.08	in	5.74	0.56	out	4.80
209	078218-57-2	4.50	0.06	in	4.22	0.13	in	4.77	out	3.20	0.29	in	3.71	0.13	in	3.81	0.13	in	4.85	0.58	out	4.15
210	078218-58-3	4.07	0.02	in	4.08	0.05	in	4.97	out	3.07	0.39	in	3.74	0.07	in	3.52	0.09	in	4.97	0.58	out	4.06
211	078218-59-4	4.72	0.08	in	4.59	0.14	in	5.48	out	3.42	0.31	in	4.44	0.11	in	4.65	0.12	in	5.59	0.56	out	4.70
212	078218-60-7	6.75	0.63	out	4.44	0.07	in	5.76	out	3.36	0.33	in	4.41	0.12	in	4.60	0.14	in	5.55	0.56	out	4.98
213	078218-61-8	6.32	0.22	in	5.92	0.26	out	7.63	out	4.33	0.52	out	5.82	0.18	in	6.15	0.22	in	6.91	0.59	out	6.16
214	078218-65-2	4.83	0.05	in	5.00	0.15	in	5.50	out	3.38	0.30	in	4.40	0.14	in	4.56	0.15	in	5.53	0.58	out	4.74
215	078218-66-3	4.51	0.03	in	4.45	0.06	in	5.29	out	3.22	0.29	in	3.84	0.13	in	3.96	0.14	in	5.00	0.59	out	4.33
216	078324-76-2	5.62	0.09	in	4.04	0.11	in	2.79	out	4.00	0.73	out	5.82	0.12	in	5.64	0.14	in	5.73	0.13	in	4.81
217	078371-72-9	4.70	0.07	in	4.58	0.15	in	5.23	out	3.54	0.40	in	4.10	0.08	in	4.35	0.10	in	5.30	0.56	out	4.54
218	078371-73-0	5.08	0.08	in	5.08	0.18	in	6.05	out	3.74	0.49	in	4.57	0.09	in	4.83	0.12	in	5.73	0.56	out	5.01
219	078371-74-1	4.60	0.07	in	4.74	0.16	in	5.60	out	3.53	0.42	in	4.22	0.08	in	4.47	0.11	in	5.41	0.56	out	4.65
220	078592-90-2	4.97	0.09	in	4.71	0.14	in	5.49	out	3.48	0.30	in	4.49	0.12	in	4.70	0.14	in	5.63	0.56	out	4.78
221	079983-71-4	5.07	0.03	in	4.99	0.02	in	5.30	in	4.78	0.30	in	5.04	0.02	in	5.08	0.02	in	4.98	0.02	in	5.03
222	080301-64-0	7.11	0.21	in	6.54	0.09	in	7.47	out	5.57	0.46	in	6.21	0.14	in	6.19	0.14	in	6.03	0.15	in	6.44
223	080584-88-9	4.06	0.05	in	4.28	0.07	in	4.55	in	3.19	0.35	in	4.53	0.06	in	4.53	0.06	in	4.47	0.06	in	4.23
224	080584-89-0	4.05	0.05	in	4.28	0.07	in	4.58	in	3.20	0.35	in	4.50	0.06	in	4.51	0.06	in	4.45	0.06	in	4.23
225	080584-90-3	7.13	0.21	in	6.69	0.10	in	7.84	out	5.47	0.59	out	6.26	0.14	in	6.34	0.14	in	6.08	0.15	in	6.54
226	080595-74-0	7.14	0.21	in	6.69	0.10	in	7.59	out	5.57	0.44	in	6.23	0.14	in	6.31	0.14	in	6.06	0.15	in	6.51
227	081518-26-5	5.69	0.07	in	3.96	0.17	in	4.57	in	4.38	0.50	in	6.23	0.07	in	5.83	0.14	in	6.13	0.07	in	5.26
228	081518-27-6	5.73	0.10	in	4.26	0.18	in	4.83	in	4.56	0.53	out	6.15	0.10	in	5.85	0.13	in	6.07	0.10	in	5.35
229	081518-28-7	5.07	0.04	in	4.11	0.17	in	4.63	in	4.47	0.51	out	5.63	0.04	in	5.31	0.08	in	5.58	0.04	in	4.97
230	081518-29-8	6.24	0.09	in	4.97	0.10	in	5.52	in	5.77	0.30	in	6.66	0.10	in	6.30	0.15	in	6.55	0.10	in	6.00
231	081518-31-2	6.28	0.09	in	5.12	0.09	in	5.86	in	5.76	0.29	in	6.61	0.09	in	6.25	0.14	in	6.50	0.09	in	6.05
232	081518-32-3	6.26	0.06	in	5.26	0.09	in	6.22	in	5.94	0.31	in	6.30	0.06	in	5.92	0.12	in	6.20	0.06	in	6.01
233	081518-37-8	5.86	0.05	in	4.85	0.22	in	5.97	in	5.20	0.32	in	5.98	0.04	in	5.56	0.11	in	5.88	0.04	in	5.61
234	081518-41-4	5.84	0.06	in	4.98	0.23	in	6.01	in	5.42	0.45	in	5.94	0.05	in	5.63	0.09	in	5.87	0.05	in	5.67
235	082200-72-4	4.30	0.04	in	4.65	0.03	in	4.78	in	4.56	0.23	in	4.65	0.03	in	4.58	0.03	in	4.61	0.03	in	4.59
236	083044-89-7	6.27	0.10	in	6.73	0.19	in	7.79	out	5.45	0.53	out	6.10	0.06	in	6.06	0.06	in	5.99	0.07	in	6.34
237	083044-90-0	6.03	0.10	in	6.71	0.19	in	7.44	out	5.45	0.53	out	6.29	0.07	in	6.30	0.07	in	6.20	0.07	in	6.35
238	083044-91-1	4.93	0.05	in	5.51	0.06	in	5.86	out	4.80	0.56	out	5.42	0.03	in	5.36	0.03	in	5.37	0.03	in	5.32
239	083366-66-9	6.02	0.10	in	6.81	0.11	in	7.45	out	5.80	0.38	in	5.68	0.07	in	5.30	0.14	in	5.59	0.08	in	6.09
240	083657-17-4	4.58	0.04	in	4.70	0.03	in	4.57	in	4.71	0.28	in	4.80	0.02	in	4.72	0.02	in	4.74	0.02	in	4.69
241	083657-24-3	4.70	0.03	in	4.87	0.03	in	4.78	in	4.81	0.24	in	5.04	0.02	in	5.09	0.02	in	4.99	0.02	in	4.90
242	085509-19-9	6.21	0.08	in	5.93	0.04	in	5.39	in	5.36	0.22	in	6.09	0.05	in	5.78	0.09	in	6.00	0.06	in	5.82
243	085634-51-1	4.78	0.04	in	5.05	0.10	in	5.08	out	3.79	0.57	out	4.54	0.04	in	4.58	0.04	in	4.49	0.04	in	4.62
244	086386-73-4	3.96	0.04	in	4.54	0.03	in	3.82	in	3.35	0.38	in	4.08	0.14	in	4.13	0.14	in	4.07	0.14	in	3.99
245	086598-92-7	6.05	0.10	in	5.37	0.12	in	6.13	out	5.66	0.30	in	6.42	0.10	in	6.30	0.11	in	6.36	0.11	in	6.04
246	088671-89-0	4.91	0.04	in	5.07	0.05	in	5.18	in	5.48	0.17	in	5.05	0.03	in	5.01	0.03	in	4.98	0.03	in	5.10
247	089482-17-7	4.30	0.04	in	4.65	0.03	in	4.81	in	4.54	0.23	in	4.65	0.03	in	4.58	0.03	in	4.61	0.03	in	4.59

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
248	089786-04-9	3.58	0.10	in	3.81	0.14	in	3.29	out	3.09	0.47	in	3.18	0.05	in	3.41	0.07	in	3.21	0.05	in	3.37
249	094270-86-7	7.13	0.21	in	6.69	0.10	in	7.58	out	5.64	0.45	in	6.26	0.14	in	6.34	0.14	in	6.08	0.15	in	6.53
250	094361-06-5	4.80	0.02	in	5.03	0.02	in	4.93	in	4.79	0.26	in	4.84	0.02	in	4.76	0.02	in	4.78	0.02	in	4.85
251	094667-47-7	3.80	0.03	in	3.06	0.06	in	2.37	out	3.70	0.54	out	3.25	0.07	in	3.03	0.09	in	3.24	0.07	in	3.21
252	097232-75-2	4.93	0.07	in	5.01	0.08	in	4.72	out	4.19	0.50	in	5.11	0.07	in	5.01	0.07	in	5.10	0.07	in	4.87
253	098518-95-7	4.48	0.03	in	5.01	0.05	in	4.99	in	3.96	0.59	out	4.85	0.04	in	4.74	0.04	in	4.82	0.04	in	4.69
254	098518-96-8	4.39	0.03	in	4.76	0.06	in	4.76	in	4.04	0.57	out	4.77	0.04	in	4.64	0.04	in	4.73	0.04	in	4.58
255	098518-99-1	4.69	0.02	in	5.16	0.04	in	5.24	in	4.13	0.64	out	4.76	0.04	in	4.63	0.05	in	4.72	0.04	in	4.76
256	098519-00-7	4.53	0.03	in	5.32	0.04	in	5.11	in	4.09	0.60	out	4.97	0.04	in	5.08	0.05	in	4.96	0.04	in	4.87
257	098519-01-8	5.50	0.14	in	5.45	0.04	in	5.28	in	4.23	0.65	out	5.24	0.04	in	5.36	0.04	in	5.21	0.04	in	5.18
258	098519-02-9	5.07	0.02	in	5.83	0.04	in	5.89	in	4.61	0.65	out	5.48	0.05	in	5.63	0.06	in	5.45	0.05	in	5.42
259	098519-04-1	4.72	0.04	in	5.14	0.05	in	4.99	in	4.02	0.65	out	4.69	0.04	in	4.68	0.04	in	4.68	0.04	in	4.70
260	098519-05-2	4.34	0.02	in	5.00	0.05	in	4.81	in	3.92	0.61	out	4.67	0.03	in	4.64	0.03	in	4.66	0.03	in	4.58
261	098519-06-3	4.64	0.02	in	5.32	0.04	in	5.29	in	4.14	0.65	out	4.76	0.04	in	4.74	0.04	in	4.74	0.04	in	4.80
262	098519-07-4	4.40	0.02	in	5.16	0.04	in	4.98	in	3.97	0.59	out	4.83	0.04	in	4.83	0.04	in	4.82	0.04	in	4.71
263	098519-24-5	4.80	0.03	in	4.98	0.05	in	4.95	in	4.02	0.64	out	4.74	0.04	in	4.61	0.04	in	4.71	0.04	in	4.69
264	098519-25-6	4.78	0.02	in	5.48	0.04	in	5.33	in	4.51	0.64	out	5.05	0.04	in	5.17	0.05	in	5.04	0.04	in	5.05
265	098519-26-7	4.85	0.04	in	5.30	0.04	in	5.15	in	4.38	0.64	out	4.89	0.05	in	4.99	0.05	in	4.88	0.05	in	4.92
266	098519-28-9	4.36	0.03	in	5.15	0.05	in	5.21	in	4.06	0.66	out	4.92	0.04	in	4.81	0.05	in	4.88	0.04	in	4.77
267	098519-29-0	5.05	0.04	in	5.35	0.04	in	5.70	in	4.17	0.66	out	5.05	0.05	in	4.95	0.05	in	5.00	0.05	in	5.04
268	098519-30-3	5.28	0.04	in	5.71	0.04	in	5.75	out	4.71	0.64	out	5.63	0.04	in	5.13	0.14	in	5.56	0.04	in	5.40
269	098519-31-4	5.05	0.04	in	5.35	0.04	in	5.70	in	4.18	0.66	out	5.05	0.05	in	4.95	0.05	in	5.00	0.05	in	5.04
270	098519-32-5	4.70	0.05	in	5.43	0.04	in	5.23	in	4.24	0.60	out	5.14	0.05	in	5.04	0.05	in	5.09	0.05	in	4.98
271	098519-33-6	4.94	0.05	in	5.59	0.04	in	5.56	in	4.39	0.60	out	5.30	0.05	in	5.21	0.05	in	5.23	0.05	in	5.17
272	098519-34-7	5.22	0.06	in	5.73	0.04	in	5.54	out	4.61	0.64	out	5.43	0.05	in	5.34	0.05	in	5.36	0.05	in	5.32
273	098519-35-8	6.03	0.32	out	5.41	0.04	in	5.21	in	4.12	0.84	out	5.13	0.05	in	5.03	0.05	in	5.08	0.05	in	5.14
274	098519-37-0	5.25	0.08	in	5.94	0.05	in	5.89	out	4.58	0.59	out	5.51	0.06	in	5.42	0.06	in	5.43	0.06	in	5.43
275	098519-39-2	4.69	0.02	in	5.16	0.04	in	5.29	in	4.14	0.65	out	4.76	0.04	in	4.63	0.05	in	4.72	0.04	in	4.77
276	098519-41-6	5.67	0.13	in	5.79	0.04	in	5.96	in	4.59	0.65	out	5.63	0.06	in	5.80	0.07	in	5.60	0.06	in	5.58
277	098519-43-8	4.64	0.02	in	5.32	0.04	in	5.37	in	4.15	0.65	out	4.76	0.04	in	4.74	0.04	in	4.74	0.04	in	4.82
278	098519-49-4	4.80	0.03	in	4.98	0.05	in	4.92	in	4.01	0.64	out	4.74	0.04	in	4.61	0.04	in	4.71	0.04	in	4.68
279	098532-64-0	4.36	0.03	in	5.15	0.05	in	5.25	in	4.04	0.65	out	4.92	0.04	in	4.81	0.05	in	4.88	0.04	in	4.77
280	098532-65-1	4.31	0.02	in	4.84	0.06	in	4.81	in	3.91	0.60	out	4.71	0.04	in	4.59	0.04	in	4.69	0.04	in	4.55
281	098532-66-2	4.78	0.02	in	5.48	0.04	in	5.39	in	4.51	0.64	out	5.05	0.04	in	5.17	0.05	in	5.04	0.04	in	5.06
282	098532-67-3	4.45	0.03	in	5.16	0.05	in	4.94	in	4.03	0.61	out	4.91	0.05	in	5.02	0.05	in	4.91	0.05	in	4.77
283	098532-68-4	4.85	0.04	in	5.30	0.04	in	5.10	in	4.13	0.65	out	4.89	0.05	in	4.99	0.05	in	4.88	0.05	in	4.88
284	098532-69-5	4.17	0.03	in	5.18	0.05	in	5.41	in	3.96	0.62	out	4.78	0.06	in	4.85	0.06	in	4.75	0.06	in	4.73
285	098532-70-8	4.58	0.02	in	5.47	0.04	in	5.39	in	4.29	0.67	out	5.10	0.04	in	5.22	0.05	in	5.08	0.04	in	5.02
286	098532-71-9	5.05	0.04	in	5.35	0.04	in	5.69	in	4.16	0.66	out	5.05	0.05	in	4.95	0.05	in	5.00	0.05	in	5.03
287	098532-72-0	5.28	0.04	in	5.71	0.04	in	5.81	out	4.41	0.66	out	5.63	0.04	in	5.13	0.14	in	5.56	0.04	in	5.36
288	098532-73-1	5.17	0.03	in	5.66	0.04	in	5.75	in	4.28	0.66	out	5.32	0.05	in	5.46	0.06	in	5.29	0.05	in	5.28
289	098532-74-2	5.41	0.13	in	5.13	0.05	in	5.08	in	4.24	0.66	out	5.00	0.04	in	4.89	0.05	in	4.95	0.04	in	4.96

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
290	098532-75-3	4.54	0.05	in	5.24	0.04	in	5.06	in	4.15	0.60	out	5.15	0.04	in	5.06	0.05	in	5.10	0.04	in	4.90
291	098532-77-5	4.66	0.04	in	5.56	0.04	in	5.20	in	4.36	0.61	out	5.25	0.04	in	5.36	0.04	in	5.21	0.04	in	5.09
292	098532-80-0	5.22	0.06	in	5.73	0.04	in	5.65	out	4.69	0.64	out	5.43	0.05	in	5.34	0.05	in	5.36	0.05	in	5.35
293	098532-81-1	4.93	0.05	in	5.61	0.04	in	5.59	in	4.36	0.60	out	5.30	0.05	in	5.21	0.05	in	5.23	0.05	in	5.18
294	098532-82-2	6.03	0.32	out	5.41	0.04	in	5.28	in	4.24	0.64	out	5.13	0.05	in	5.03	0.05	in	5.08	0.05	in	5.17
295	098532-83-3	4.84	0.04	in	5.15	0.05	in	5.07	in	4.06	0.62	out	4.80	0.04	in	4.68	0.05	in	4.77	0.04	in	4.77
296	098532-85-5	5.26	0.04	in	5.80	0.04	in	5.83	out	4.54	0.67	out	5.40	0.05	in	5.32	0.05	in	5.33	0.05	in	5.36
297	098967-40-9	3.67	0.08	in	3.58	0.10	in	3.15	in	3.88	0.46	in	3.67	0.04	in	3.59	0.04	in	3.69	0.04	in	3.60
298	099793-38-1	6.23	0.13	in	5.13	0.09	in	5.57	out	6.08	0.36	in	6.66	0.12	in	6.41	0.15	in	6.57	0.13	in	6.09
299	099793-75-6	5.20	0.06	in	4.78	0.11	in	4.66	in	5.33	0.35	in	5.29	0.07	in	4.93	0.12	in	5.24	0.07	in	5.06
300	103112-35-2	5.40	0.14	in	5.36	0.05	in	5.32	out	6.02	0.33	in	5.36	0.10	in	5.51	0.11	in	5.36	0.10	in	5.48
301	103112-36-3	5.36	0.22	in	4.31	0.07	in	4.10	out	4.76	0.36	in	5.34	0.20	in	5.48	0.21	in	5.34	0.20	in	4.96
302	103597-45-1	6.78	0.23	in	8.35	0.45	out	8.72	out	4.91	0.85	out	6.97	0.23	in	6.44	0.34	out	6.83	0.23	in	7.00
303	103922-48-1	5.02	0.11	in	5.36	0.09	in	6.40	out	3.17	0.29	in	4.32	0.18	in	4.44	0.19	in	4.26	0.18	in	4.71
304	104958-85-2	1.84	0.12	in	3.06	0.09	in	3.38	out	3.35	0.32	in	2.11	0.14	in	2.24	0.15	in	2.17	0.14	in	2.59
305	106325-08-0	5.39	0.05	in	5.22	0.04	in	4.88	in	5.43	0.26	in	5.77	0.04	in	5.45	0.08	in	5.70	0.04	in	5.41
306	107534-96-3	5.03	0.05	in	5.08	0.02	in	4.95	in	4.72	0.33	in	4.94	0.03	in	4.86	0.03	in	4.87	0.03	in	4.92
307	112143-82-5	5.43	0.11	in	5.11	0.15	in	5.66	in	5.79	0.37	in	5.25	0.07	in	5.58	0.11	in	5.16	0.07	in	5.43
308	112281-77-3	4.20	0.05	in	5.06	0.05	in	4.45	out	4.86	0.39	in	4.66	0.04	in	4.73	0.04	in	4.65	0.04	in	4.66
309	113518-46-0	6.15	0.10	in	5.03	0.17	in	5.88	out	4.26	0.38	in	6.21	0.10	in	5.57	0.27	out	6.10	0.11	in	5.60
310	114369-43-6	5.70	0.06	in	5.41	0.04	in	5.32	in	5.70	0.22	in	5.74	0.05	in	5.31	0.13	in	5.65	0.06	in	5.55
311	116255-48-2	5.08	0.08	in	5.32	0.04	in	5.44	in	5.17	0.19	in	5.23	0.05	in	5.33	0.05	in	5.21	0.05	in	5.25
312	119126-15-7	4.33	0.02	in	4.94	0.13	in	4.64	out	4.94	0.39	in	4.90	0.04	in	4.59	0.08	in	4.89	0.04	in	4.75
313	119446-68-3	5.78	0.06	in	5.75	0.04	in	5.95	in	5.52	0.20	in	5.96	0.05	in	5.78	0.06	in	5.90	0.05	in	5.80
314	122836-35-5	3.83	0.03	in	4.13	0.08	in	3.79	out	4.35	0.44	in	3.81	0.05	in	3.95	0.06	in	3.85	0.05	in	3.96
315	125116-23-6	4.93	0.04	in	5.34	0.03	in	4.97	in	4.65	0.25	in	5.07	0.03	in	5.02	0.03	in	5.01	0.03	in	5.00
316	125225-28-7	5.29	0.04	in	5.54	0.03	in	5.39	in	5.12	0.35	in	5.23	0.03	in	5.18	0.03	in	5.15	0.04	in	5.27
317	125304-04-3	6.48	0.17	in	6.26	0.15	in	7.82	out	5.59	0.51	out	6.55	0.10	in	6.41	0.10	in	6.40	0.10	in	6.50
318	125306-83-4	5.82	0.15	in	4.95	0.13	in	5.09	out	5.84	0.34	in	4.78	0.06	in	4.92	0.07	in	4.72	0.06	in	5.16
319	127519-17-9	6.06	0.09	in	6.35	0.14	in	7.37	out	5.38	0.53	out	5.99	0.06	in	5.85	0.07	in	5.89	0.07	in	6.13
320	128625-52-5	7.94	0.66	out	6.26	0.06	in	6.89	out	4.14	1.46	out	5.85	0.15	in	5.86	0.15	in	6.97	0.58	out	6.27
321	128639-02-1	4.63	0.11	in	5.48	0.04	in	4.83	out	5.65	0.22	in	4.54	0.05	in	4.74	0.07	in	4.56	0.05	in	4.92
322	129586-32-9	5.59	0.08	in	5.06	0.02	in	4.98	in	4.43	0.27	in	5.08	0.03	in	5.04	0.03	in	5.02	0.03	in	5.03
323	129909-90-6	5.52	0.37	out	4.43	0.14	in	4.90	out	3.50	0.32	in	3.71	0.09	in	3.85	0.10	in	3.62	0.10	in	4.22
324	131983-72-7	4.57	0.04	in	5.21	0.03	in	4.84	in	4.60	0.26	in	4.99	0.04	in	4.98	0.04	in	4.95	0.04	in	4.88
325	136426-54-5	5.21	0.08	in	5.27	0.04	in	5.42	in	4.66	0.58	out	5.48	0.10	in	5.40	0.10	in	5.46	0.10	in	5.27
326	139158-24-0	5.89	0.08	in	4.68	0.18	in	5.23	out	4.26	0.75	out	6.27	0.07	in	6.64	0.13	in	6.14	0.08	in	5.59
327	139158-25-1	6.33	0.08	in	4.89	0.19	in	5.46	out	4.26	0.72	out	6.41	0.08	in	6.80	0.14	in	6.27	0.08	in	5.77
328	139158-26-2	5.87	0.07	in	5.17	0.18	in	5.61	out	4.88	0.73	out	6.25	0.06	in	6.23	0.06	in	6.15	0.06	in	5.74
329	139528-85-1	4.18	0.08	in	4.39	0.10	in	4.34	in	4.10	0.52	out	4.45	0.04	in	4.54	0.05	in	4.45	0.04	in	4.35
330	141078-91-3	6.34	0.10	in	5.78	0.04	in	6.08	out	6.00	0.37	in	6.60	0.07	in	5.86	0.29	out	6.47	0.08	in	6.16
331	141078-92-4	6.22	0.09	in	5.80	0.04	in	6.20	out	5.96	0.37	in	6.51	0.06	in	5.77	0.28	out	6.38	0.07	in	6.12

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
332	141078-93-5	6.45	0.09	in	5.80	0.04	in	6.11	out	6.00	0.37	in	6.70	0.08	in	5.99	0.28	out	6.58	0.08	in	6.23
333	141078-94-6	6.18	0.08	in	5.62	0.04	in	5.73	out	5.91	0.36	in	6.49	0.06	in	5.75	0.28	out	6.37	0.07	in	6.01
334	141078-95-7	6.51	0.10	in	5.96	0.05	in	6.15	out	6.09	0.39	in	6.95	0.09	in	6.38	0.22	in	6.84	0.09	in	6.41
335	141078-99-1	6.36	0.11	in	5.92	0.05	in	6.29	out	5.96	0.36	in	6.86	0.08	in	6.27	0.22	in	6.74	0.08	in	6.34
336	141079-00-7	6.07	0.09	in	5.94	0.05	in	6.33	out	6.00	0.37	in	6.61	0.07	in	6.01	0.22	in	6.50	0.07	in	6.21
337	141079-01-8	6.26	0.09	in	5.94	0.05	in	6.11	out	6.03	0.37	in	6.78	0.07	in	6.19	0.21	in	6.67	0.08	in	6.28
338	141079-02-9	6.00	0.08	in	5.76	0.04	in	5.87	out	5.95	0.36	in	6.56	0.06	in	5.96	0.21	in	6.46	0.07	in	6.08
339	141079-03-0	6.34	0.09	in	6.10	0.06	in	6.17	out	5.98	0.36	in	6.81	0.08	in	6.33	0.17	in	6.71	0.08	in	6.35
340	141079-06-3	6.18	0.09	in	6.08	0.06	in	6.31	out	6.10	0.38	in	6.69	0.07	in	6.19	0.17	in	6.58	0.07	in	6.30
341	141079-07-4	6.32	0.09	in	6.11	0.06	in	6.24	out	6.10	0.38	in	6.82	0.08	in	6.34	0.17	in	6.72	0.08	in	6.38
342	141079-08-5	5.93	0.07	in	5.92	0.04	in	5.91	out	6.03	0.36	in	6.48	0.06	in	5.98	0.16	in	6.40	0.06	in	6.09
343	141079-12-1	6.10	0.07	in	5.79	0.04	in	5.66	out	5.98	0.36	in	6.60	0.06	in	6.01	0.21	in	6.51	0.07	in	6.09
344	141079-13-2	6.54	0.10	in	5.81	0.04	in	5.62	out	5.98	0.36	in	7.03	0.10	in	6.47	0.22	in	6.92	0.10	in	6.34
345	141079-14-3	6.27	0.08	in	5.67	0.04	in	5.37	out	5.88	0.34	in	6.81	0.08	in	6.23	0.21	in	6.71	0.08	in	6.13
346	141079-15-4	6.64	0.12	in	5.97	0.05	in	5.52	out	6.07	0.38	in	7.11	0.11	in	6.65	0.20	in	7.01	0.12	in	6.42
347	141079-16-5	6.01	0.08	in	6.08	0.05	in	5.89	out	6.08	0.36	in	6.56	0.07	in	6.17	0.13	in	6.49	0.07	in	6.18
348	141079-17-6	5.78	0.06	in	6.12	0.05	in	5.82	out	6.02	0.35	in	6.37	0.06	in	5.97	0.13	in	6.30	0.06	in	6.05
349	141079-18-7	6.26	0.10	in	6.11	0.05	in	5.75	out	5.87	0.32	in	6.78	0.09	in	6.41	0.15	in	6.70	0.09	in	6.27
350	141079-19-8	5.94	0.07	in	5.97	0.05	in	5.49	out	5.76	0.33	in	6.52	0.07	in	6.12	0.13	in	6.45	0.07	in	6.04
351	141079-20-1	6.43	0.12	in	6.27	0.06	in	5.79	out	5.99	0.35	in	6.91	0.11	in	6.64	0.14	in	6.83	0.11	in	6.41
352	145026-81-9	4.09	0.06	in	3.92	0.07	in	4.55	in	4.41	0.40	in	3.23	0.14	in	3.08	0.15	in	3.24	0.14	in	3.79
353	145701-21-9	4.53	0.10	in	4.24	0.11	in	4.34	in	4.08	0.50	in	4.12	0.06	in	4.09	0.06	in	4.14	0.06	in	4.22
354	145701-23-1	3.34	0.07	in	3.47	0.13	in	2.93	in	3.82	0.45	in	3.51	0.04	in	3.52	0.04	in	3.54	0.04	in	3.45
355	147150-35-4	4.10	0.09	in	4.39	0.12	in	3.61	in	4.03	0.51	out	3.73	0.05	in	3.68	0.05	in	3.76	0.05	in	3.90
356	147993-59-7	3.14	0.09	in	4.18	0.06	in	4.68	out	2.88	0.36	in	3.12	0.10	in	3.02	0.10	in	3.13	0.10	in	3.45
357	149508-90-7	5.06	0.03	in	5.97	0.06	in	5.32	out	4.44	0.21	in	5.08	0.02	in	5.02	0.02	in	5.01	0.02	in	5.13
358	173980-17-1	3.58	0.11	in	4.28	0.10	in	3.65	out	3.61	0.33	in	3.48	0.07	in	3.63	0.08	in	3.54	0.07	in	3.68
359	178928-70-6	5.38	0.18	in	4.92	0.09	in	5.19	in	4.88	0.46	in	4.95	0.04	in	4.96	0.04	in	4.94	0.04	in	5.03
360	212201-70-2	5.89	0.14	in	5.61	0.04	in	4.74	in	6.03	0.32	in	5.11	0.03	in	4.99	0.04	in	5.09	0.03	in	5.35
361	219714-96-2	3.51	0.04	in	4.20	0.15	in	3.44	out	3.82	0.48	in	4.08	0.06	in	4.17	0.06	in	4.10	0.06	in	3.90
362	317815-83-1	3.52	0.09	in	3.92	0.06	in	3.65	in	3.91	0.40	in	3.10	0.14	in	3.31	0.16	in	3.13	0.14	in	3.51
363	348635-87-0	4.27	0.05	in	5.07	0.13	in	3.62	out	4.41	0.63	out	3.90	0.08	in	3.95	0.08	in	3.92	0.08	in	4.16
364	422556-08-9	3.52	0.05	in	3.91	0.13	in	3.55	in	3.61	0.46	in	3.79	0.06	in	3.92	0.07	in	3.80	0.06	in	3.73
365	865318-97-4	5.21	0.12	in	4.85	0.07	in	6.14	out	4.35	0.55	out	5.35	0.11	in	5.64	0.14	in	5.21	0.11	in	5.25
366	XXX002	3.11	0.05	in	4.05	0.14	in	3.14	out	3.45	0.41	in	3.72	0.07	in	3.79	0.07	in	3.76	0.07	in	3.57
367	XXX003	4.54	0.04	in	5.30	0.03	in	4.50	in	4.83	0.30	in	4.80	0.02	in	4.78	0.02	in	4.77	0.02	in	4.79
368	XXX004	2.51	0.07	in	3.38	0.08	in	2.51	out	3.16	0.32	in	2.87	0.08	in	2.84	0.08	in	2.94	0.08	in	2.89
369	XXX006	4.31	0.04	in	4.22	0.05	in	4.31	in	4.06	0.26	in	4.31	0.03	in	4.31	0.03	in	4.30	0.03	in	4.26
370	XXX007	4.04	0.04	in	4.60	0.02	in	4.47	in	3.51	0.31	in	4.47	0.05	in	4.41	0.06	in	4.45	0.05	in	4.28
371	XXX008	5.68	0.16	in	5.23	0.12	in	5.41	in	5.36	0.32	in	5.36	0.04	in	5.41	0.04	in	5.33	0.04	in	5.40
372	XXX009	5.49	0.14	in	5.21	0.04	in	4.69	in	5.11	0.47	in	5.13	0.03	in	5.12	0.03	in	5.09	0.03	in	5.12
373	XXX010	3.65	0.05	in	4.42	0.07	in	3.70	out	4.41	0.34	in	3.80	0.09	in	3.97	0.10	in	3.88	0.09	in	3.97

ID	CAS	UI Models						IVL Mode		HMGU Model			IDEA Models									Consensus pred
		pred UI-a	*Hat* UI-a	AD UI-a	pred UI-b	*Hat* UI-b	AD UI-b	pred	AD	pred	STD	AD	pred A	*Hat* A	AD A	pred B	*Hat* B	AD B	pred C	*Hat* B	AD B	
374	XXX011	4.79	0.02	in	5.24	0.03	in	4.73	in	4.01	0.69	out	5.00	0.05	in	5.00	0.05	in	4.97	0.05	in	4.82
375	XXX012	4.69	0.02	in	5.23	0.03	in	4.53	in	3.88	0.43	in	4.93	0.05	in	4.93	0.05	in	4.90	0.05	in	4.73
376	XXX013	4.81	0.03	in	4.93	0.05	in	5.15	in	3.92	0.38	in	5.29	0.04	in	5.15	0.05	in	5.27	0.04	in	4.93
377	XXX014	3.30	0.10	in	3.33	0.13	in	2.25	out	3.36	0.42	in	3.54	0.04	in	3.55	0.04	in	3.57	0.04	in	3.27
378	XXX015	2.81	0.07	in	2.86	0.08	in	1.97	out	3.29	0.33	in	2.75	0.07	in	2.68	0.07	in	2.81	0.07	in	2.74
379	XXX016	2.76	0.10	in	2.91	0.08	in	2.40	out	3.01	0.38	in	2.75	0.07	in	2.68	0.07	in	2.81	0.07	in	2.76
380	XXX017	5.79	0.04	in	5.49	0.04	in	4.96	in	5.31	0.25	in	5.54	0.03	in	5.12	0.10	in	5.48	0.03	in	5.38
381	XXX018	5.46	0.05	in	5.38	0.04	in	5.12	in	5.07	0.31	in	5.50	0.03	in	5.10	0.10	in	5.45	0.03	in	5.30
382	XXX019	3.67	0.12	in	3.73	0.06	in	3.58	in	3.25	0.35	in	3.55	0.07	in	3.63	0.07	in	3.58	0.07	in	3.57
383	XXX020	5.15	0.09	in	4.87	0.12	in	5.38	in	4.27	0.31	in	4.95	0.04	in	5.03	0.04	in	4.92	0.04	in	4.94
384	XXX021	5.79	0.04	in	5.49	0.04	in	5.12	in	5.32	0.25	in	5.54	0.03	in	5.12	0.10	in	5.48	0.03	in	5.41
385	XXX022	3.68	0.10	in	4.25	0.10	in	3.77	in	3.57	0.46	in	4.00	0.06	in	4.08	0.06	in	4.04	0.06	in	3.91
386	XXX023	5.11	0.04	in	5.01	0.05	in	4.69	in	5.07	0.29	in	4.74	0.02	in	4.66	0.02	in	4.68	0.02	in	4.85

Table 2. Consensus models for EC50 in *Oncorhynchus mykiss*: individual model deviations (ID) of WP3 models (i.e., UI-Dragon (UI-a), UI-PaDEL (UI-b), IVL, HMGU, IDEA-A, IDEA-B, IDEA-C) and median deviation (MD).

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
1	000061-82-5	0.54	0.20	2.15	0.37	0.75	0.72	0.71	0.78
2	000094-97-3	0.55	0.29	0.68	0.08	0.22	0.39	0.24	0.35
3	000095-14-7	0.53	0.60	0.86	0.25	0.05	0.34	0.13	0.40
4	000130-34-7	0.37	0.62	1.19	0.72	0.83	0.53	0.79	0.72
5	000131-43-1	0.15	0.11	0.74	0.87	0.65	0.08	0.60	0.46
6	000134-58-7	0.28	0.73	1.41	0.38	0.77	0.73	0.74	0.72
7	000136-85-6	0.19	0.15	0.78	0.37	0.40	0.64	0.43	0.42
8	000273-40-5	0.32	0.09	1.46	0.35	0.74	0.74	0.73	0.63
9	000288-36-8	0.39	0.76	1.22	0.33	0.16	0.06	0.18	0.44
10	000288-88-0	0.43	0.03	2.24	0.59	0.83	0.79	0.76	0.81
11	000584-13-4	0.17	0.04	1.39	0.41	0.55	0.51	0.54	0.51
12	000932-64-9	0.58	0.57	1.33	1.13	0.81	0.88	0.78	0.87
13	000938-56-7	0.27	0.03	0.63	0.17	0.28	0.53	0.30	0.31
14	000939-07-1	0.40	0.64	0.12	0.70	0.46	0.22	0.39	0.42
15	000939-08-2	0.18	0.09	0.36	0.33	0.03	0.05	0.03	0.15
16	000944-91-2	0.04	0.15	0.23	1.01	0.25	0.49	0.30	0.35
17	000947-85-3	0.25	0.05	0.17	1.05	0.38	0.60	0.42	0.42
18	000974-29-8	1.29	0.43	0.20	2.10	0.83	0.01	0.61	0.78
19	001028-08-6	0.20	0.07	0.95	1.39	0.34	0.13	0.79	0.55
20	001031-47-6	0.01	0.14	0.60	0.71	0.25	0.43	0.94	0.44
21	001123-54-2	0.02	0.65	1.69	0.42	0.91	0.95	0.90	0.79
22	001325-58-2	2.28	2.12	3.15	1.66	1.86	2.08	1.94	2.16

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
23	001326-66-5	0.05	0.30	0.36	1.16	0.71	0.39	0.67	0.52
24	001455-77-2	0.11	0.41	1.39	0.17	0.63	0.75	0.71	0.59
25	001468-26-4	0.11	0.22	0.78	0.42	0.48	0.40	0.45	0.41
26	001600-61-9	0.56	0.43	0.53	0.92	0.45	0.48	0.38	0.54
27	001680-44-0	0.63	1.19	0.39	0.02	0.19	0.12	0.07	0.37
28	001704-66-1	0.62	0.29	1.28	0.47	0.49	0.51	0.43	0.58
29	002338-12-7	0.43	0.53	0.06	0.16	0.28	0.21	0.26	0.28
30	002440-22-4	0.12	0.76	0.14	0.36	0.51	0.20	0.43	0.36
31	002592-95-2	0.72	0.08	0.23	0.40	0.15	0.47	0.19	0.32
32	002683-90-1	0.04	0.92	1.59	0.71	1.07	1.10	1.02	0.92
33	003142-42-5	0.10	0.35	1.26	0.95	0.11	0.13	0.04	0.42
34	003147-75-9	0.15	0.28	0.25	0.61	0.46	0.20	0.34	0.33
35	003147-76-0	0.03	0.54	0.30	0.35	0.51	0.24	0.42	0.34
36	003232-84-6	0.11	0.41	1.88	0.45	0.62	0.75	0.68	0.70
37	003310-68-7	0.31	0.17	0.49	0.57	0.10	0.19	0.03	0.27
38	003333-62-8	0.73	0.26	0.58	1.68	0.90	0.12	0.76	0.72
39	003357-42-4	0.64	0.96	0.63	0.30	0.15	0.18	0.04	0.41
40	003641-10-9	0.21	0.33	2.04	0.77	1.09	1.19	1.06	0.96
41	003652-22-0	0.34	0.55	1.01	0.66	0.06	0.00	0.08	0.39
42	003652-23-1	0.13	0.45	1.11	0.64	0.06	0.01	0.09	0.36
43	003652-25-3	0.00	0.62	0.81	0.74	0.16	0.27	0.13	0.39
44	003652-27-5	0.53	1.09	0.44	1.49	0.61	0.51	0.51	0.74
45	003652-31-1	0.07	0.46	0.84	0.29	0.08	0.03	0.06	0.26
46	003652-32-2	0.05	0.47	0.91	0.27	0.10	0.05	0.08	0.27
47	003663-24-9	0.12	0.49	0.45	0.24	0.11	0.02	0.03	0.21
48	003683-95-2	0.26	0.25	1.14	0.97	0.17	0.12	0.14	0.44
49	003770-47-6	0.08	0.49	0.90	0.25	0.04	0.02	0.05	0.26
50	003846-71-7	0.07	0.37	0.04	0.62	0.41	0.25	0.29	0.29
51	003864-99-1	0.02	0.29	0.07	0.62	0.38	0.33	0.27	0.28
52	003896-11-5	0.13	0.26	0.03	0.45	0.34	0.26	0.27	0.25
53	004184-79-6	0.12	0.42	0.19	0.00	0.09	0.03	0.01	0.12
54	004314-22-1	0.04	0.74	1.72	1.28	1.22	1.33	1.14	1.07
55	004343-73-1	0.11	0.08	1.06	0.52	0.59	0.56	0.63	0.51
56	004368-68-7	0.32	0.40	0.02	0.52	0.03	0.28	0.10	0.24
57	004928-87-4	0.21	0.98	2.61	1.54	1.60	1.80	1.50	1.46
58	004928-88-5	0.30	0.73	2.14	1.58	1.36	1.49	1.31	1.27
59	005302-27-2	1.79	0.85	0.07	0.17	0.28	0.16	0.40	0.53
60	005369-84-6	0.12	0.17	0.64	0.51	0.07	0.07	0.03	0.23
61	005472-71-9	0.01	0.21	0.32	0.54	0.05	0.04	0.01	0.17
62	005516-20-1	0.49	0.74	0.29	1.46	0.91	0.32	0.77	0.71
63	005873-30-3	0.23	0.25	0.65	0.28	0.04	0.05	0.01	0.22
64	006054-53-1	0.16	0.31	0.98	0.39	0.02	0.10	0.02	0.28
65	006085-94-5	0.34	0.42	0.01	0.38	0.01	0.24	0.06	0.21
66	006299-39-4	0.40	0.56	0.01	0.12	0.31	0.24	0.28	0.28

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
67	006789-99-7	0.32	0.36	0.11	0.37	0.12	0.18	0.01	0.21
68	006818-99-1	0.10	0.53	1.96	0.10	0.54	0.41	0.49	0.59
69	006994-51-0	0.89	0.45	0.34	1.22	0.82	0.36	0.66	0.68
70	007170-01-6	0.39	0.06	1.77	0.52	0.69	0.64	0.64	0.67
71	007411-23-6	1.81	1.20	1.29	0.82	0.40	0.25	0.44	0.89
72	007532-52-7	0.51	0.29	0.27	0.37	0.15	0.17	0.10	0.27
73	010109-05-4	0.39	0.91	1.00	0.52	0.70	0.71	0.66	0.70
74	010187-79-8	0.68	0.19	1.13	0.62	0.44	0.44	0.40	0.56
75	010187-84-5	0.69	0.43	1.06	0.37	0.39	0.42	0.34	0.53
76	010187-86-7	0.52	0.33	0.51	0.42	0.26	0.26	0.21	0.36
77	010187-89-0	0.30	0.28	0.92	0.04	0.33	0.32	0.30	0.35
78	013091-80-0	0.23	0.37	0.04	0.21	0.08	0.02	0.03	0.14
79	013257-88-0	0.42	0.13	1.06	0.04	0.51	0.43	0.64	0.46
80	013351-73-0	0.50	0.16	0.64	0.54	0.49	0.80	0.54	0.52
81	014803-99-7	0.44	0.31	1.27	0.42	0.28	0.38	0.33	0.49
82	015421-84-8	0.60	0.17	0.48	0.26	0.23	0.10	0.32	0.31
83	015497-45-7	0.73	0.16	0.29	0.39	0.09	0.16	0.22	0.29
84	015805-10-4	0.81	0.19	0.56	1.32	0.52	0.31	0.45	0.59
85	016515-58-5	0.08	0.60	0.54	0.99	0.10	0.37	0.04	0.39
86	016584-05-7	0.83	0.18	0.41	0.60	0.56	0.86	0.62	0.58
87	018076-61-4	0.28	0.07	1.10	0.33	0.23	0.47	0.30	0.40
88	018811-70-6	0.56	0.86	0.34	1.25	0.57	0.16	0.46	0.60
89	019683-09-1	0.36	0.16	0.08	0.95	0.55	0.17	0.44	0.39
90	019794-93-5	0.38	0.68	0.71	0.60	0.37	0.39	0.43	0.51
91	021050-95-3	0.88	0.37	0.48	0.31	0.33	0.58	0.40	0.48
92	021532-04-7	0.06	0.58	0.64	0.67	0.16	0.41	0.09	0.37
93	023633-05-8	0.65	0.33	0.55	0.31	0.20	0.18	0.15	0.34
94	023711-34-4	0.59	1.70	0.78	0.57	0.99	0.62	0.86	0.87
95	024017-47-8	0.05	0.37	1.02	0.03	0.55	0.67	0.63	0.47
96	024054-57-7	0.80	0.29	1.22	0.46	0.42	0.40	0.36	0.56
97	025973-55-1	0.03	0.14	0.23	0.61	0.26	0.09	0.13	0.21
98	026621-45-4	0.50	0.14	1.18	2.17	0.99	1.04	0.95	1.00
99	027022-50-0	0.35	0.14	1.92	0.44	0.78	0.65	0.71	0.71
100	027210-18-0	0.13	0.07	0.24	0.80	0.27	0.29	0.22	0.29
101	027799-91-3	0.09	0.20	0.65	0.18	0.17	0.35	0.20	0.26
102	028401-89-0	0.14	0.02	0.34	1.04	0.28	0.30	0.22	0.34
103	028911-01-5	0.40	0.05	0.46	1.39	0.59	0.41	0.52	0.54
104	028981-97-7	0.44	0.01	0.23	1.29	0.50	0.17	0.41	0.44
105	029440-31-1	0.34	0.07	0.82	0.63	0.56	0.50	0.61	0.51
106	029878-31-7	0.30	0.25	0.81	0.35	0.30	0.53	0.36	0.41
107	029975-16-4	0.59	0.31	0.55	1.31	0.67	0.36	0.57	0.62
108	031251-03-3	0.85	0.71	1.25	0.59	0.89	0.10	0.73	0.73
109	031409-18-4	0.38	0.47	0.25	0.26	0.11	0.16	0.16	0.25
110	031701-42-5	0.40	0.39	0.09	0.01	0.07	0.00	0.01	0.14

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
111	032362-89-3	0.32	0.90	0.47	0.88	0.34	0.33	0.31	0.51
112	032723-50-5	0.11	0.19	0.18	0.65	0.29	0.05	0.20	0.24
113	034771-66-9	0.08	0.46	0.28	0.85	0.17	0.10	0.13	0.30
114	035515-45-8	0.23	0.39	0.75	0.19	0.01	0.09	0.00	0.24
115	036325-69-6	0.06	0.17	0.43	0.76	0.26	0.04	0.21	0.28
116	036411-52-6	0.09	0.12	1.13	0.09	0.21	0.40	0.21	0.32
117	036437-37-3	0.07	0.25	0.10	0.40	0.30	0.13	0.19	0.21
118	036791-04-5	0.75	0.68	0.54	0.01	0.22	0.05	0.19	0.35
119	037160-06-8	0.78	0.84	0.82	1.10	0.88	0.39	0.72	0.79
120	038942-51-7	0.15	1.03	0.41	0.16	0.18	0.00	0.14	0.29
121	039968-33-7	0.30	0.34	1.51	0.61	0.88	1.06	0.84	0.79
122	040054-69-1	0.06	0.00	0.43	1.42	0.34	0.30	0.28	0.41
123	041083-11-8	0.52	0.80	0.88	2.12	0.09	0.33	0.32	0.72
124	041735-28-8	0.64	0.55	0.94	0.90	0.60	0.63	0.53	0.68
125	041735-29-9	0.30	0.43	1.22	0.68	0.69	0.71	0.64	0.67
126	041735-30-2	0.29	0.03	0.36	0.77	0.30	0.29	0.28	0.33
127	041735-38-0	0.50	0.05	0.43	0.58	0.18	0.11	0.17	0.29
128	041735-41-5	0.61	0.07	0.71	0.29	0.16	0.14	0.15	0.30
129	041735-42-6	0.73	0.25	1.02	0.57	0.38	0.39	0.33	0.52
130	041735-44-8	0.48	0.08	0.42	0.82	0.25	0.18	0.24	0.35
131	041735-45-9	0.60	0.06	0.79	0.36	0.21	0.19	0.20	0.34
132	041735-50-6	0.37	0.03	0.28	0.65	0.19	0.14	0.19	0.27
133	041735-51-7	0.50	0.36	0.06	0.65	0.03	0.05	0.06	0.25
134	041735-54-0	0.35	0.16	0.77	0.30	0.22	0.19	0.16	0.31
135	041735-55-1	0.53	0.84	0.41	0.63	0.07	0.17	0.07	0.39
136	041735-56-2	0.24	0.35	0.04	0.66	0.05	0.03	0.03	0.20
137	041735-57-3	0.66	0.40	0.49	0.88	0.12	0.09	0.11	0.39
138	041814-78-2	0.39	0.46	0.03	0.26	0.15	0.11	0.11	0.21
139	041834-21-3	0.33	0.48	0.18	0.40	0.05	0.11	0.07	0.23
140	042509-80-8	0.74	0.53	1.16	0.63	0.74	0.42	0.40	0.66
141	043029-44-3	0.78	1.36	0.82	0.91	0.98	0.52	0.82	0.88
142	043121-43-3	0.15	0.22	0.02	0.43	0.11	0.21	0.16	0.19
143	051627-14-6	0.65	1.27	0.49	1.27	0.02	0.07	0.06	0.55
144	053817-16-6	0.46	0.46	0.34	0.04	0.10	0.22	0.04	0.24
145	054028-81-8	0.30	0.08	0.02	1.24	0.43	0.08	0.35	0.36
146	054028-83-0	0.08	0.28	0.10	1.15	0.34	0.09	0.28	0.33
147	054028-84-1	0.49	0.15	0.31	1.64	0.63	0.15	0.53	0.56
148	054028-85-2	0.19	0.02	0.10	1.23	0.35	0.27	0.31	0.36
149	054028-86-3	0.01	0.26	0.16	0.88	0.20	0.08	0.17	0.25
150	054028-89-6	0.32	0.11	0.02	1.37	0.45	0.09	0.37	0.39
151	054028-90-9	0.06	0.30	0.21	1.19	0.31	0.05	0.25	0.34
152	054028-91-0	0.39	0.12	0.11	1.31	0.57	0.12	0.47	0.44
153	054028-92-1	0.17	0.13	0.05	1.17	0.42	0.06	0.34	0.33
154	054028-93-2	0.16	0.14	0.15	1.23	0.40	0.04	0.33	0.35

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
155	054028-94-3	0.50	0.31	0.21	1.26	0.61	0.16	0.50	0.51
156	054028-95-4	0.17	0.13	0.26	1.12	0.34	0.04	0.26	0.33
157	054123-06-7	0.28	0.14	0.18	1.50	0.54	0.53	0.49	0.52
158	055179-31-2	0.09	0.10	0.06	0.32	0.31	0.15	0.22	0.18
159	055219-65-3	0.25	0.11	0.08	0.00	0.07	0.03	0.01	0.08
160	055375-40-1	0.56	0.01	0.85	0.59	0.39	0.11	0.40	0.41
161	055425-38-2	0.65	0.66	0.00	1.57	0.70	0.28	0.59	0.64
162	056383-06-3	0.25	0.23	0.37	0.37	0.02	0.14	0.08	0.21
163	056383-11-0	0.17	0.22	0.34	0.68	0.08	0.17	0.02	0.24
164	056396-43-1	0.48	0.74	0.51	0.69	0.62	0.31	0.52	0.55
165	056881-36-8	0.32	0.94	1.24	0.74	0.90	0.86	0.84	0.83
166	057801-81-7	0.31	0.15	0.04	1.60	0.51	0.51	0.46	0.51
167	057801-94-2	0.41	0.27	0.01	1.81	0.56	0.59	0.51	0.60
168	059026-08-3	0.94	0.26	0.41	0.66	0.62	0.42	0.70	0.57
169	059338-86-2	0.40	0.22	0.53	0.08	0.01	0.03	0.01	0.18
170	059338-92-0	0.33	0.30	0.54	0.23	0.25	0.29	0.20	0.31
171	059338-93-1	0.27	0.58	0.37	0.86	0.13	0.04	0.17	0.35
172	060207-31-0	0.28	0.07	0.03	0.11	0.08	0.16	0.05	0.11
173	060207-90-1	0.10	0.01	0.35	0.02	0.09	0.01	0.14	0.10
174	060207-93-4	0.19	0.04	0.21	0.22	0.11	0.02	0.14	0.13
175	060932-58-3	0.05	0.24	0.45	0.18	0.01	0.11	0.01	0.15
176	061691-97-2	0.00	0.14	0.46	0.92	0.16	0.04	0.11	0.26
177	063216-86-4	0.55	0.33	0.36	1.49	0.53	0.05	0.48	0.54
178	063251-40-1	0.49	0.36	0.90	1.28	0.80	0.48	0.76	0.72
179	063870-37-1	0.58	0.69	1.20	0.52	0.67	0.51	0.64	0.69
180	064057-50-7	0.39	0.26	0.68	0.29	0.32	0.25	0.26	0.35
181	064082-38-8	0.27	0.21	0.87	0.11	0.34	0.29	0.28	0.34
182	066104-34-5	0.15	0.16	0.69	0.23	0.05	0.22	0.01	0.22
183	066104-44-7	0.17	0.25	0.49	0.47	0.19	0.05	0.14	0.25
184	066246-88-6	0.06	0.25	0.19	0.27	0.07	0.05	0.14	0.15
185	066492-64-6	0.21	0.14	0.29	0.71	0.18	0.27	0.21	0.29
186	066535-86-2	0.54	0.98	0.37	1.28	0.86	0.50	0.73	0.75
187	066975-54-0	0.45	0.97	1.26	1.07	0.56	0.48	0.58	0.77
188	067465-03-6	0.07	0.19	0.93	0.52	0.07	0.01	0.07	0.26
189	067465-05-8	0.01	0.00	0.87	0.69	0.06	0.03	0.11	0.25
190	068049-83-2	0.05	0.04	0.22	0.28	0.20	0.01	0.19	0.14
191	069141-50-0	0.13	0.12	0.10	0.34	0.10	0.34	0.00	0.16
192	070292-10-3	0.17	0.59	0.06	0.39	0.41	0.10	0.37	0.30
193	070321-86-7	0.43	0.05	0.02	0.97	0.58	0.38	0.43	0.41
194	075020-35-8	0.18	0.01	0.11	0.30	0.10	0.16	0.10	0.14
195	075736-33-3	0.14	0.02	0.07	0.48	0.14	0.22	0.09	0.17
196	076608-88-3	0.05	0.18	0.17	0.01	0.21	0.06	0.15	0.12
197	076674-21-0	0.19	0.14	0.61	0.51	0.50	0.15	0.44	0.36
198	076738-62-0	0.12	0.05	0.04	0.15	0.04	0.05	0.03	0.07

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
199	077314-77-3	0.06	0.42	1.35	0.57	0.41	0.42	0.42	0.52
200	078149-96-9	0.07	0.19	1.23	0.97	0.51	0.27	0.64	0.56
201	078150-00-2	0.01	0.16	0.95	1.03	0.36	0.59	0.86	0.57
202	078150-02-4	0.14	0.06	0.85	1.31	0.33	0.12	0.81	0.52
203	078218-51-6	0.05	0.11	0.49	0.71	0.26	0.31	0.95	0.41
204	078218-52-7	0.03	0.08	0.74	1.19	0.28	0.09	0.87	0.47
205	078218-53-8	0.18	0.22	1.15	1.63	0.29	0.02	0.82	0.61
206	078218-54-9	0.06	0.15	0.58	1.27	0.19	0.03	0.96	0.46
207	078218-55-0	0.20	0.01	0.75	0.97	0.24	0.31	0.96	0.49
208	078218-56-1	0.01	0.08	0.48	0.72	0.25	0.40	0.94	0.41
209	078218-57-2	0.35	0.07	0.61	0.95	0.44	0.34	0.70	0.50
210	078218-58-3	0.01	0.02	0.91	0.99	0.32	0.54	0.91	0.53
211	078218-59-4	0.02	0.11	0.78	1.28	0.26	0.05	0.89	0.48
212	078218-60-7	1.76	0.54	0.78	1.62	0.57	0.38	0.57	0.89
213	078218-61-8	0.17	0.23	1.48	1.83	0.34	0.01	0.75	0.68
214	078218-65-2	0.09	0.26	0.75	1.36	0.34	0.18	0.79	0.54
215	078218-66-3	0.19	0.13	0.96	1.11	0.49	0.37	0.67	0.56
216	078324-76-2	0.81	0.76	2.02	0.81	1.01	0.83	0.92	1.02
217	078371-72-9	0.16	0.03	0.68	1.00	0.44	0.19	0.76	0.47
218	078371-73-0	0.07	0.07	1.04	1.27	0.44	0.18	0.72	0.54
219	078371-74-1	0.05	0.09	0.94	1.12	0.43	0.18	0.76	0.51
220	078592-90-2	0.18	0.07	0.71	1.30	0.29	0.08	0.85	0.50
221	079983-71-4	0.04	0.04	0.26	0.25	0.01	0.05	0.05	0.10
222	080301-64-0	0.66	0.09	1.02	0.87	0.23	0.25	0.41	0.51
223	080584-88-9	0.17	0.05	0.32	1.04	0.30	0.30	0.24	0.35
224	080584-89-0	0.17	0.06	0.36	1.03	0.27	0.28	0.22	0.34
225	080584-90-3	0.59	0.15	1.29	1.07	0.28	0.20	0.46	0.58
226	080595-74-0	0.63	0.17	1.08	0.94	0.28	0.20	0.45	0.54
227	081518-26-5	0.43	1.30	0.68	0.88	0.97	0.57	0.87	0.82
228	081518-27-6	0.38	1.09	0.52	0.79	0.80	0.50	0.72	0.69
229	081518-28-7	0.10	0.86	0.34	0.50	0.66	0.34	0.61	0.49
230	081518-29-8	0.23	1.03	0.48	0.23	0.66	0.30	0.55	0.50
231	081518-31-2	0.22	0.93	0.20	0.29	0.56	0.20	0.45	0.41
232	081518-32-3	0.25	0.76	0.20	0.07	0.29	0.09	0.19	0.26
233	081518-37-8	0.25	0.76	0.35	0.41	0.37	0.05	0.27	0.35
234	081518-41-4	0.17	0.69	0.34	0.25	0.27	0.04	0.20	0.28
235	082200-72-4	0.29	0.06	0.19	0.03	0.06	0.01	0.02	0.09
236	083044-89-7	0.07	0.39	1.45	0.89	0.24	0.28	0.35	0.52
237	083044-90-0	0.32	0.37	1.09	0.90	0.06	0.05	0.15	0.42
238	083044-91-1	0.39	0.19	0.54	0.52	0.10	0.04	0.05	0.26
239	083366-66-9	0.08	0.72	1.36	0.29	0.41	0.79	0.50	0.59
240	083657-17-4	0.11	0.01	0.11	0.02	0.11	0.03	0.05	0.06
241	083657-24-3	0.20	0.03	0.12	0.09	0.14	0.19	0.09	0.12
242	085509-19-9	0.38	0.10	0.43	0.46	0.27	0.04	0.18	0.27

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
243	085634-51-1	0.17	0.43	0.46	0.83	0.08	0.04	0.13	0.30
244	086386-73-4	0.03	0.55	0.17	0.64	0.09	0.14	0.08	0.24
245	086598-92-7	0.01	0.67	0.09	0.38	0.38	0.26	0.32	0.30
246	088671-89-0	0.19	0.03	0.08	0.38	0.05	0.09	0.12	0.13
247	089482-17-7	0.29	0.06	0.22	0.05	0.06	0.01	0.02	0.10
248	089786-04-9	0.21	0.45	0.08	0.28	0.19	0.04	0.16	0.20
249	094270-86-7	0.60	0.16	1.05	0.89	0.27	0.19	0.45	0.52
250	094361-06-5	0.04	0.19	0.08	0.06	0.01	0.09	0.07	0.08
251	094667-47-7	0.59	0.15	0.84	0.49	0.04	0.18	0.03	0.33
252	097232-75-2	0.07	0.14	0.15	0.68	0.24	0.14	0.23	0.24
253	098518-95-7	0.21	0.31	0.30	0.73	0.16	0.05	0.13	0.27
254	098518-96-8	0.20	0.17	0.18	0.54	0.19	0.06	0.15	0.21
255	098518-99-1	0.07	0.40	0.48	0.63	0.00	0.13	0.04	0.25
256	098519-00-7	0.34	0.46	0.24	0.78	0.10	0.21	0.09	0.32
257	098519-01-8	0.32	0.27	0.10	0.95	0.06	0.18	0.03	0.27
258	098519-02-9	0.35	0.40	0.47	0.81	0.06	0.21	0.03	0.33
259	098519-04-1	0.02	0.44	0.29	0.68	0.01	0.02	0.02	0.21
260	098519-05-2	0.24	0.42	0.24	0.66	0.09	0.06	0.08	0.26
261	098519-06-3	0.16	0.51	0.49	0.66	0.04	0.06	0.06	0.29
262	098519-07-4	0.32	0.45	0.27	0.74	0.12	0.12	0.11	0.30
263	098519-24-5	0.11	0.30	0.26	0.67	0.05	0.08	0.02	0.21
264	098519-25-6	0.27	0.43	0.28	0.54	0.00	0.12	0.01	0.24
265	098519-26-7	0.07	0.38	0.23	0.54	0.03	0.07	0.04	0.19
266	098519-28-9	0.41	0.38	0.44	0.71	0.15	0.04	0.11	0.32
267	098519-29-0	0.01	0.31	0.66	0.87	0.01	0.09	0.04	0.28
268	098519-30-3	0.11	0.31	0.36	0.69	0.23	0.27	0.16	0.30
269	098519-31-4	0.01	0.31	0.66	0.86	0.01	0.09	0.04	0.28
270	098519-32-5	0.28	0.44	0.25	0.74	0.16	0.06	0.11	0.29
271	098519-33-6	0.24	0.42	0.38	0.78	0.13	0.04	0.06	0.29
272	098519-34-7	0.10	0.42	0.22	0.71	0.11	0.02	0.04	0.23
273	098519-35-8	0.89	0.26	0.07	1.02	0.01	0.11	0.06	0.35
274	098519-37-0	0.18	0.51	0.46	0.85	0.08	0.01	0.00	0.30
275	098519-39-2	0.08	0.39	0.52	0.63	0.01	0.14	0.05	0.26
276	098519-41-6	0.09	0.21	0.38	0.99	0.05	0.22	0.02	0.28
277	098519-43-8	0.18	0.50	0.55	0.67	0.06	0.08	0.08	0.30
278	098519-49-4	0.12	0.30	0.24	0.67	0.06	0.07	0.03	0.21
279	098532-64-0	0.41	0.38	0.48	0.73	0.15	0.04	0.11	0.33
280	098532-65-1	0.24	0.29	0.26	0.64	0.16	0.04	0.14	0.25
281	098532-66-2	0.28	0.42	0.33	0.55	0.01	0.11	0.02	0.25
282	098532-67-3	0.33	0.38	0.16	0.74	0.14	0.25	0.14	0.31
283	098532-68-4	0.03	0.42	0.22	0.75	0.01	0.11	0.00	0.22
284	098532-69-5	0.56	0.45	0.68	0.77	0.05	0.12	0.02	0.38
285	098532-70-8	0.44	0.45	0.38	0.73	0.08	0.20	0.06	0.33
286	098532-71-9	0.02	0.31	0.65	0.87	0.02	0.08	0.03	0.28

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
287	098532-72-0	0.08	0.35	0.44	0.95	0.27	0.23	0.20	0.36
288	098532-73-1	0.11	0.39	0.47	1.00	0.04	0.18	0.01	0.32
289	098532-74-2	0.45	0.18	0.13	0.72	0.04	0.07	0.01	0.23
290	098532-75-3	0.36	0.34	0.16	0.75	0.25	0.16	0.20	0.32
291	098532-77-5	0.42	0.47	0.11	0.73	0.16	0.27	0.12	0.33
292	098532-80-0	0.13	0.39	0.30	0.66	0.08	0.01	0.01	0.23
293	098532-81-1	0.24	0.43	0.41	0.82	0.12	0.03	0.05	0.30
294	098532-82-2	0.86	0.23	0.11	0.93	0.04	0.14	0.09	0.34
295	098532-83-3	0.07	0.38	0.30	0.71	0.03	0.09	0.00	0.23
296	098532-85-5	0.09	0.45	0.48	0.82	0.04	0.04	0.03	0.28
297	098967-40-9	0.06	0.02	0.45	0.28	0.07	0.01	0.09	0.14
298	099793-38-1	0.14	0.97	0.52	0.01	0.57	0.32	0.48	0.43
299	099793-75-6	0.14	0.28	0.40	0.27	0.23	0.13	0.18	0.23
300	103112-35-2	0.08	0.11	0.16	0.54	0.12	0.03	0.12	0.17
301	103112-36-3	0.41	0.64	0.86	0.20	0.38	0.52	0.38	0.49
302	103597-45-1	0.22	1.35	1.72	2.09	0.03	0.56	0.17	0.88
303	103922-48-1	0.31	0.65	1.69	1.54	0.39	0.27	0.45	0.76
304	104958-85-2	0.76	0.47	0.79	0.76	0.48	0.35	0.42	0.58
305	106325-08-0	0.01	0.19	0.52	0.02	0.36	0.04	0.29	0.21
306	107534-96-3	0.11	0.16	0.02	0.20	0.02	0.06	0.05	0.09
307	112143-82-5	0.00	0.32	0.23	0.36	0.18	0.15	0.27	0.22
308	112281-77-3	0.46	0.40	0.21	0.20	0.00	0.07	0.01	0.19
309	113518-46-0	0.55	0.57	0.28	1.34	0.61	0.03	0.50	0.55
310	114369-43-6	0.16	0.14	0.23	0.15	0.19	0.24	0.10	0.17
311	116255-48-2	0.18	0.06	0.18	0.08	0.02	0.08	0.04	0.09
312	119126-15-7	0.42	0.20	0.10	0.19	0.15	0.16	0.14	0.19
313	119446-68-3	0.03	0.06	0.14	0.28	0.16	0.02	0.10	0.11
314	122836-35-5	0.13	0.17	0.17	0.39	0.15	0.01	0.11	0.16
315	125116-23-6	0.07	0.35	0.03	0.35	0.07	0.02	0.01	0.13
316	125225-28-7	0.02	0.27	0.12	0.15	0.04	0.09	0.12	0.12
317	125304-04-3	0.02	0.24	1.32	0.91	0.05	0.09	0.10	0.39
318	125306-83-4	0.66	0.21	0.07	0.68	0.38	0.24	0.44	0.38
319	127519-17-9	0.06	0.22	1.24	0.75	0.14	0.28	0.24	0.42
320	128625-52-5	1.67	0.02	0.62	2.13	0.42	0.41	0.70	0.85
321	128639-02-1	0.29	0.56	0.09	0.73	0.38	0.18	0.36	0.37
322	129586-32-9	0.56	0.03	0.05	0.60	0.05	0.01	0.01	0.19
323	129909-90-6	1.30	0.21	0.68	0.72	0.51	0.37	0.60	0.63
324	131983-72-7	0.31	0.33	0.03	0.28	0.11	0.10	0.07	0.18
325	136426-54-5	0.06	0.00	0.15	0.61	0.21	0.13	0.19	0.19
326	139158-24-0	0.31	0.90	0.36	1.33	0.68	1.05	0.55	0.74
327	139158-25-1	0.55	0.88	0.31	1.51	0.64	1.03	0.50	0.77
328	139158-26-2	0.13	0.56	0.13	0.86	0.51	0.49	0.41	0.44
329	139528-85-1	0.17	0.04	0.01	0.25	0.10	0.19	0.10	0.12
330	141078-91-3	0.18	0.38	0.08	0.16	0.44	0.30	0.31	0.26

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
331	141078-92-4	0.10	0.32	0.08	0.16	0.39	0.35	0.26	0.24
332	141078-93-5	0.22	0.43	0.12	0.23	0.47	0.24	0.35	0.29
333	141078-94-6	0.18	0.38	0.28	0.10	0.48	0.26	0.36	0.29
334	141078-95-7	0.10	0.45	0.26	0.32	0.54	0.03	0.43	0.30
335	141078-99-1	0.02	0.42	0.06	0.38	0.52	0.07	0.40	0.27
336	141079-00-7	0.14	0.27	0.12	0.21	0.40	0.20	0.29	0.23
337	141079-01-8	0.02	0.34	0.17	0.25	0.50	0.09	0.39	0.25
338	141079-02-9	0.08	0.32	0.21	0.13	0.48	0.12	0.38	0.25
339	141079-03-0	0.01	0.25	0.17	0.37	0.46	0.02	0.36	0.23
340	141079-06-3	0.12	0.22	0.00	0.20	0.39	0.11	0.28	0.19
341	141079-07-4	0.05	0.27	0.14	0.28	0.44	0.04	0.34	0.22
342	141079-08-5	0.16	0.17	0.19	0.06	0.39	0.11	0.31	0.20
343	141079-12-1	0.01	0.30	0.43	0.11	0.51	0.08	0.42	0.27
344	141079-13-2	0.20	0.53	0.72	0.36	0.69	0.13	0.58	0.46
345	141079-14-3	0.14	0.46	0.77	0.25	0.68	0.10	0.58	0.42
346	141079-15-4	0.22	0.45	0.91	0.35	0.69	0.23	0.59	0.49
347	141079-16-5	0.17	0.10	0.29	0.10	0.38	0.01	0.31	0.19
348	141079-17-6	0.27	0.06	0.24	0.03	0.32	0.08	0.25	0.18
349	141079-18-7	0.01	0.16	0.51	0.40	0.51	0.14	0.43	0.31
350	141079-19-8	0.10	0.07	0.54	0.28	0.48	0.08	0.41	0.28
351	141079-20-1	0.02	0.14	0.61	0.42	0.50	0.23	0.42	0.34
352	145026-81-9	0.30	0.14	0.76	0.62	0.56	0.71	0.55	0.52
353	145701-21-9	0.31	0.02	0.12	0.14	0.10	0.13	0.08	0.13
354	145701-23-1	0.11	0.02	0.51	0.37	0.06	0.07	0.09	0.18
355	147150-35-4	0.20	0.49	0.29	0.13	0.17	0.22	0.14	0.23
356	147993-59-7	0.31	0.73	1.23	0.57	0.33	0.43	0.32	0.56
357	149508-90-7	0.07	0.84	0.19	0.69	0.05	0.11	0.12	0.29
358	173980-17-1	0.10	0.60	0.03	0.07	0.20	0.05	0.14	0.17
359	178928-70-6	0.35	0.11	0.16	0.15	0.08	0.07	0.09	0.15
360	212201-70-2	0.54	0.26	0.61	0.68	0.24	0.36	0.26	0.42
361	219714-96-2	0.39	0.29	0.47	0.08	0.18	0.27	0.20	0.27
362	317815-83-1	0.02	0.41	0.15	0.40	0.41	0.20	0.38	0.28
363	348635-87-0	0.11	0.90	0.54	0.25	0.26	0.21	0.24	0.36
364	422556-08-9	0.21	0.18	0.18	0.12	0.06	0.19	0.07	0.15
365	865318-97-4	0.04	0.40	0.88	0.90	0.10	0.39	0.04	0.39
366	XXX002	0.47	0.48	0.43	0.12	0.15	0.22	0.19	0.29
367	XXX003	0.24	0.51	0.29	0.04	0.01	0.01	0.02	0.16
368	XXX004	0.37	0.50	0.38	0.27	0.02	0.05	0.05	0.23
369	XXX006	0.05	0.04	0.05	0.20	0.05	0.05	0.04	0.07
370	XXX007	0.24	0.32	0.19	0.77	0.19	0.13	0.17	0.29
371	XXX008	0.28	0.17	0.01	0.04	0.04	0.01	0.07	0.09
372	XXX009	0.37	0.09	0.43	0.01	0.01	0.00	0.03	0.13
373	XXX010	0.32	0.44	0.28	0.44	0.17	0.00	0.09	0.25
374	XXX011	0.03	0.42	0.09	0.81	0.18	0.18	0.15	0.27

ID	CAS	ID UIa	ID UIb	ID IVL	ID HMGU	ID IDEA-A	ID IDEA-B	ID IDEA-C	MD
375	XXX012	0.03	0.50	0.20	0.85	0.20	0.20	0.17	0.31
376	XXX013	0.12	0.00	0.22	1.01	0.36	0.22	0.34	0.32
377	XXX014	0.03	0.06	1.02	0.09	0.27	0.28	0.30	0.29
378	XXX015	0.07	0.12	0.77	0.55	0.01	0.06	0.07	0.24
379	XXX016	0.00	0.15	0.36	0.25	0.01	0.08	0.05	0.13
380	XXX017	0.41	0.11	0.43	0.07	0.16	0.26	0.10	0.22
381	XXX018	0.16	0.09	0.18	0.23	0.20	0.20	0.15	0.17
382	XXX019	0.10	0.16	0.01	0.32	0.02	0.06	0.01	0.10
383	XXX020	0.21	0.06	0.44	0.67	0.01	0.09	0.02	0.22
384	XXX021	0.38	0.08	0.29	0.09	0.13	0.29	0.07	0.19
385	XXX022	0.23	0.34	0.15	0.34	0.09	0.17	0.13	0.21
386	XXX023	0.26	0.16	0.16	0.22	0.11	0.19	0.17	0.18

Appendix V

PCA analysis of consensus predictions (considering IVL predictions also) obtained for algae (pEC50 *Pseudokirchneriella subcapitata*), daphnia (pEC50 *Daphnia magna*) and fish (pLC50 *Onchorhynchus mykiss*).