Electronic Supplementary Information

Full list of all Descriptors

These Descriptors were used to describe the molecules to the models. The Radial Basis Function (RBF) models described below used the full set of 31 descriptors as model input. The MLP models described in the main article only used 10 of these as a starting point for the PCA. These 10 were selected by chemical expert judgment and screening model runs to assess descriptor performance.

Molecular Weight	# of hydroxyl groups	# of Fluorine atoms
# of functional groups (total)	# of carboxylic acid groups	# of isocyano groups
# of Oxygen atoms in keto and aldehyde groups	# of amine and amide groups	# of Triazine ring structures
	# of nitro groups	# of carbamate groups
# of Oxygen atoms not in keto and aldehyde groups	# of Chlorine atoms	# of sulfonic acid groups
	# of ether groups	# of non-aromatic C-C double bonds
# of Nitrogen atoms	# of esters and acid anhydrides	
# of halogen atoms	# of cyanide groups	# of heteroatoms in other, not listed functional groups
# of aromatic or aliphatic rings	# of keto groups	
# of ternary or quarternary Carbon atoms	# of aldehyde groups	# of aromatic Carbon atoms
	# of aromatic rings	# of aromatic heteroatoms
# of heteroatoms in rings		# of Oxygen atoms
# of unique substitutes on aromatic rings		

Table SI 1: Descriptors selected to describe the molecular structure to the models. The 10 descriptors selected for the MLPs are printed in bold.

To apply the models, the numerical descriptors have to be calculated. All descriptors that are not self-explanatory are defined here. Some of these rules are not completely intuitive to a chemist, they were chosen to best identify production-relevant molecular properties.

of functional groups (total):

A sum of the individual group-counting descriptors, meaning the sum of

# of hydroxyl groups +

# of carboxylic acid groups +

# of amine and amide groups +

# of nitro groups +

# of Chlorine atoms +

# of ether groups +

# of esters and acid anhydrides +

# of cyanide groups +

# of keto groups +

# of aldehyde groups +

# of aromatic rings +

# of Fluorine atoms +

# of isocyano groups +

# of Triazine ring structures +

# of carbamate groups +

# of sulfonic acid groups +

# of non-aromatic C-C double bonds +

# of heteroatoms in other, not listed functional groups

# of aromatic or aliphatic rings:
Fused rings count as individual rings (e.g. naphthalene counts as 2). Bridged rings count as 2 rings (e.g. camphor counts as 2). Dieldrin counts as 5 rings.

# of ternary or quarternary Carbon atoms
This counts all carbon atoms with bonds to 3 or 4 other carbon atoms. Note that double or triple bonds only count as one connected carbon, as this descriptor would otherwise be dominated by aromatic carbon atoms.

# of heteroatoms in rings

Only heteroatoms in the ring count. Heteroatoms bound to a ring but not part of the ring structure do not count (e.g. chlorobenzene counts as 0).

# of unique substitutes on aromatic rings

A substitute counts as unique if an identical group is not present in the molecule. Examples:

Chlorobenzene counts as 1

Dichlorobenzene counts as 1

Chlorotoluene counts as 2

Dichlorotoluene counts as 2

Chlorofluorotoluene counts as 3

Chlorophenylbenzene counts as 3 (Chlorine on ring A, phenyl substituent on ring A, chlorophenyl substituent on ring B)

# of non-aromatic C-C double bonds

This includes conjugated double bonds, even double bonds conjugated with an aromatic ring (e.g. Styrene counts as 1).

# of heteroatoms in other, not listed functional groups

All functional groups not represented by another functional group descriptor are accounted for in this descriptor. Each heteroatom in a group counts as 1.

# of aromatic Carbon atoms

Carbon atoms in aromatic rings.

# of aromatic heteroatoms

Heteroatoms in aromatic rings.

Additional Information on the error distribution

Figure 2 in the main article presents the relative error of the chemicals with the chemicals sorted by descending error. Additionally, it shows the CED inventory data for the chemicals as well as the model predictions for the CED.

The Figures S1 and S2 show similar plots for the molecular weight and the number of functional groups. As seen in Table 4 of the main article, there is a trend towards lower relative errors for increasing molecular weights and numbers of functional groups. The figures and the linear fits included in them agree with this conclusion. However, the figures reveal that this is only a trend and that specific chemicals unfortunately cannot be declared to have higher errors purely based on their input values. Nevertheless, the additional figures are helpful in assessing the error distribution of the models.

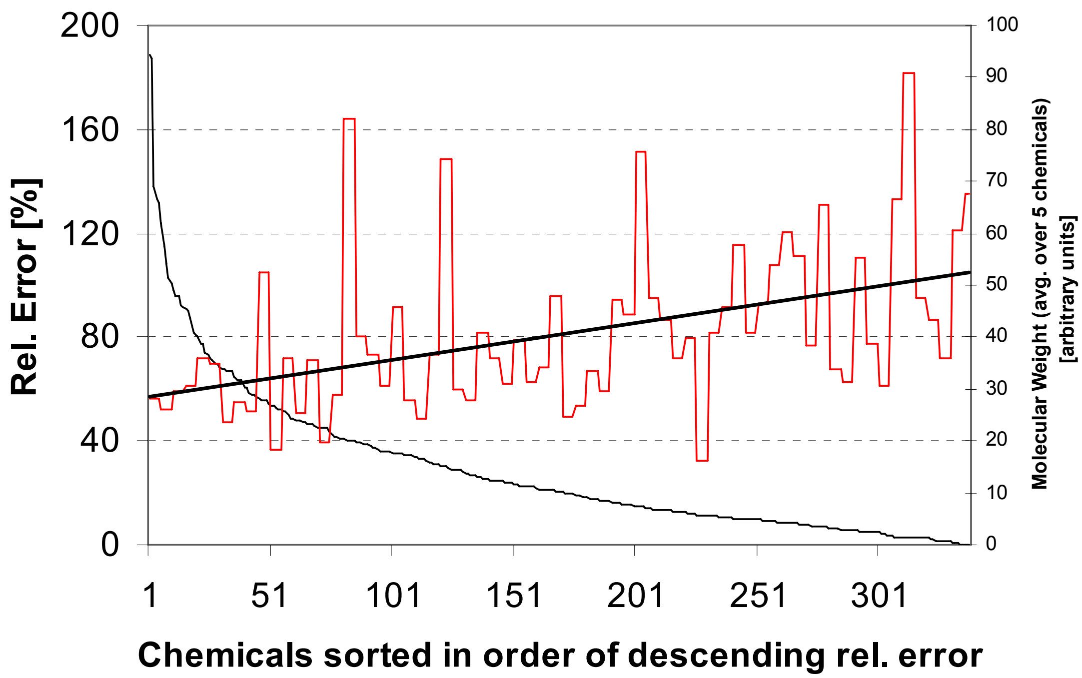

Figure S1: Chemicals sorted in order of descending rel. error, with the molecular weight on the secondary axis. The bold line is the result of a linear fit of the molecular weight function.

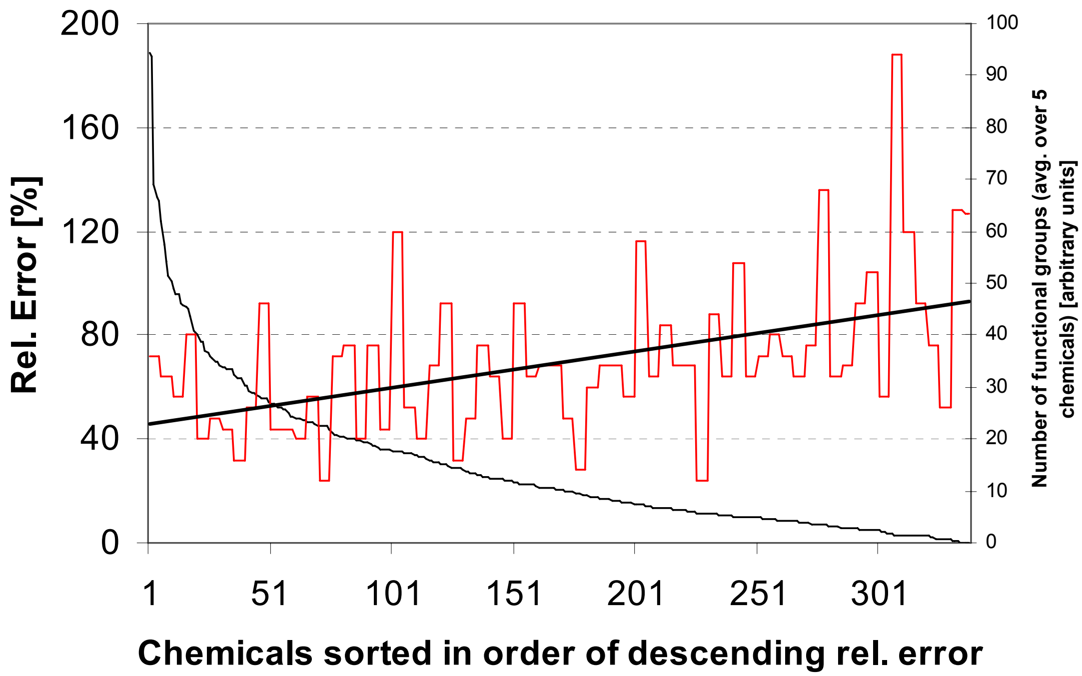

Figure S2: Chemicals sorted in order of descending rel. error, with the number of functional groups on the secondary axis. The bold line is the result of a linear fit of the molecular weight function.

Training of the MLP models and PCA

The optimal number of factors for the MLP models was selected by performing model training for a series of factors ranging from 3 or 4 factors to 10. 10 Factors contain 100% of the variance of the original 10 descriptors. Depending on the output, the optimal number of factors varied. While 8 factors proved to be ideal for most outputs (resulting in networks using 7 hidden neurons and therefore with 71 weights), the Eco-indicator 99 models used 6 factors and 5 hidden neurons, resulting in 41 weights. As the training data for the Eco-indicator 99 models were fewer than for the other models, these models were more likely to be affected by overfitting. Therefore, a smaller number of weights resulted in better performance.

All networks followed the standard design of a multi-layer perceptron (MLP). Each neuron had a linear output function. Inputs and outputs were normalized to increase network performance. The training algorithm was the Broyden-Fletcher-Goldfarb-Shanno

(BFGS) algorithm (Venables & Ripley, 2002). A weight decay parameter of 0.0006 was used in training. All of these parameters were determined to be optimal in a series of experiments with varying parameter selections. All training was terminated after a maximum of 200 iterations or if the relative improvement in respect to the squared errors (SSE) of the output dropped below a certain level:

$$f = tol_{rel} * SSE + tol_{rel} \quad \text{(S1)}$$

The parameter for the relative tolerance tol_{rel} was 1.5e-08. The basic step size of the gradient approximation was 0.001. To ensure that the global error minimum was reached or at least closely approximated, all networks were trained 100 times with different initializations and the best network was selected based on the q^2 results of the training set.

MLP Training set coefficients of determination

The training results can be of value to assess the quality of the models and to determine the likelihood of overfitting. A large discrepancy in the coefficients of determination of the training and test sets indicates that the models are overfitted. As seen in the table, some overfitting is indeed occurring. Model tests with various input sizes nevertheless showed that the more chosen models were best among the alternative model designs.

	CED	GWP	Eco-indicator '99	Electricity Use	Heat Use
MLP models	0.84 (0.03)	0.77 (0.07)	0.89 (0.04)	0.86 (0.02)	0.88 (0.03)

Table SI 2: Coefficients of determination for the structure-based MLP models. All values are means over the 30 training sets, standard deviations in parentheses.

Final Results - RBF models

In a second approach, the input dimensionality reduction is achieved in two steps using pure data-mining procedures without taking into account any prior knowledge about the suitability of the descriptors. In the end, these models ended up not offering comparable predictive capabilities to the MLP models. They are therefore not presented in the main article. Nevertheless, the results may be of interest to practitioners familiar with different neural network structures and are therefore presented here.

In this approach, PCA is performed in the first step using the whole set of 31 descriptors (Table SI 1) and dimensionality reduction is achieved by applying the "latent root criterion" or a threshold value for an acceptable loss of information (e.g. 10%) in order to select a certain number of principal components. This first step is very important because the second step of this approach involves simultaneous optimization of the network size and the input variables (i.e. without pre-assigning importance for the selected principal components), which may result in "combinatorial explosion", if dimensionality reduction was not performed. In this approach Radial Basis Functions neural networks (RBFs) were used instead of MLPs, because they do not involve a non-linear optimization algorithm for their training (unsupervised training), and therefore respond faster to the optimization algorithm for the inference of the variables and network size selection, while being also universal approximators (Liao et al., 2003, Wu et al., 2008).

RBFs were trained with a "fuzzy input space partition algorithm" for the unsupervised training of the hidden layer (Sarimveis et al., 2002). The RBFs were trained on the basis of the results of PCA applied to the whole set of the 31 molecular descriptors. The dimensionality reduction according to the "latent root criterion" resulted in 10 factors, covering 75% of the variance of the 31 descriptors. Using a threshold value of 90% variance to be covered by the PCA solution, a set of 15 factors would be necessary. Having these 10 factors (or 15 depending on the criterion used for the selection of the factors) as starting point, the step of simultaneous variable and network size selection was implemented for each one of the thirty training/test set couples. For this task, the "direct global optimization algorithm" was used (Jones, 2008), as applied in TOMLAB v7.0 optimization software. As decision variables for the factors selection 10 (or 15) binary variables were used. Depending on the values of these binary variables the size of the input layer of the network is determined. Additionally, one integer variable ranging from 4 to 10 is used, which represents the number of the fuzzy sets in which each input variable is partitioned for the unsupervised training of the hidden layer. The weights of the output layer are fitted with a typical linear least-squares algorithm. The performance criterion of the resulting models was the same like in the first approach, namely the maximization of the coefficient of determination (q^2) for the predictions of the test data. Two different modes were used for the optimization algorithm: the maximization of q^2 for each one of the the test sets separetely (mode-1) and the optimization of the average q^2 overall the thirty training/test couples (mode-2). Altogether this approach differs from the first one (i.e. MLP models) in the following two aspects: the neural network type and the parallel variable/network size selection which results in a thorough search of the solution space.

From the overall performance of the combined models (Table SI 3) over the 338 data points for the CED prediction, it is obvious that despite the thorough search of the solution space a better performance compared to the MLP models has not been achieved. In fact, even for mode-1, which resulted in smaller values than mode-2 for all the error indicators, the performance is still somewhat inferior to the MLP models (see Table 4 of the main text).

Conclusively, the approaches presented in this paragraph demonstrate that neither a more thorough optimization of the input variables and the network size, nor another type of neural network would result in significantly better results than those proposed in the present study (i.e. the MLP models of the main text).

RBF models	Mode-1 (10 fac.)	Mode-1 (15 fac.)	Mode-2 (10 fac.)	Mode-2 (15 fac.)
Mean absolute error (MJ-eq/kg)	65	65	77	68
Median absolute error (MJ-eq/kg)	41	41	45	36
Mean relative error [%]	48	48	54	49
Median relative error [%]	35	36	38	36
Mean error in standard deviations	1.7	1.9	5.3	3.9
Median error in	1.3	1.4	3.7	2.5

standard deviations				

Table SI 3: Predictive measures for the final RBF models.

Application of the models. MLPs – CED:

To use the models, the following information can be used to recreate the neural networks independently. The models are also available for free to download at the authors' homepage (see main article for link).

All models have 8 input neurons, 7 hidden neurons and 1 output. The neurons have a logistic activation function, only the connection weights are affected by training. The models can therefore be described by the 71 weights in the model. They are given in the following order: Bias for hidden neuron 1, followed by the weights from input 1 to input 8, bias and input connections for hidden neurons 2 to 7 in the same order, then the bias for the output and the 7 connecting weights for the output.

1	[1] -1.94491556 -0.07178381 2.19795349 1.36389921 1.67844955 -1.11864995 1.98464354 0.73380938 0.78463777 -0.93570175 [11] -0.58893227 -0.08141622 -0.38817009 0.94651264 0.14475422 -1.99617583 -0.15784622 -1.14798811 -1.22301399 0.15039748 [21] 0.63678142 0.48416729 0.55226879 -0.55485372 1.31628888 0.38893654 0.63898330 0.92697338 -0.94185619 -1.29208894 [31] -1.33145763 0.74651285 -0.92165275 0.06383962 0.40957031 -0.51616330 1.25636579 -1.11860893 -1.39282823 -1.78534110 [41] 0.80201034 -1.41205056 0.65641424 0.49856142 -0.16266809 -0.96010875 1.26590398 2.09880738 1.90112786 -0.73137519 [51] 0.71012063 0.52422021 -0.45346607 1.19195190 -3.08005417 5.37395017 17.28733206 20.06283020 5.10138206 -3.48855661 [61] 3.40482742 0.40853745 8.56520775 6.35788716 -3.34727264 1.99997781 6.80074066 -17.09245880 7.70018748 -7.49944425 [71] 1.08131048
2	[1] 2.52894540 2.48753087 -0.07053184 0.11268304 1.20908276 -3.02964314 0.08136141 -0.01656575 -1.88342855 0.18676380 [11] -20.90469486 -1.79271159 -7.76819687 -4.71882859 10.33319550 12.89580977 -4.24757366 10.48290336 -4.70963812 2.24789301 [21] -1.15851422 2.48873680 1.15525316 0.53911798 4.14017302 -2.47568799 2.39715201 -3.52500950 -1.14685634 -1.77598190 [31] -0.36514735 1.71965458 -1.18361557 0.66446890 -1.49701755 -1.78067174 7.62951344 -5.56103530 -1.83696270 -7.51822559 [41] 2.27097924 2.88819483 -12.12278511 -2.89671664 -0.37602610 2.12340812 2.36672603 0.10010712 0.57588654 1.06089915 [51] -2.49743519 0.10286804 0.10680337 -1.41521107 15.59680959 7.72670109 5.20658968 14.10823792 -0.93348445 -5.90552729 [61] 8.46915201 5.35523708 5.65689800 -3.41935663 -12.20407623 1.33024314 3.13630637 -2.05403333 2.04244709 15.33971556 [71] -1.55340148
3	[1] -25.68002041 2.21803085 4.59916366 1.78947412 -0.54097661 0.88265075 4.83926532 1.17028958 6.64418726 9.07549429 [11] -21.25839926 3.21593299 4.50777612 -5.28173033 -12.10616334 -6.79228232 0.04837884 -9.76984091 18.68368089 0.90232947 [21] -8.57295183 -10.98281735 6.64300394 -1.88440882 -9.75236028 5.33777507 13.21352759 19.08823403 -13.31855172 -7.69908342 [31] -7.09048075 -6.15379155 -1.44270593 -21.67246200 -3.41754230 -10.90669170 -0.96663746 -1.99218158 0.31194277 -20.44440850 [41] 1.57777738 -2.70904312 -3.47802410 -4.64353205 0.87693036 7.54850540 -9.60685316 -4.08422499 14.46332403 -3.75632797 [51] -7.91410337 -5.85338571 -3.99892611 -5.22317395 -1.27430435 -2.11947263 -1.44201976 -13.84630699 1.78275933 -3.45956844 [61] -2.92774032 -2.42368284 0.01245434 1.70881042 6.06184903 -0.87893695 -0.78505781 -0.86254214 -5.91420668 0.37815346 [71] 5.93062749
4	[1] 0.36214696 -3.22340487 -2.23038797 0.25599172 0.76914394 -6.31616157 -0.29885351 2.17561353 1.44811352 12.38595739 [11] 16.47402953 -1.04462854 8.66877596 10.23457876 -22.61324013 -14.98062638 4.89387978 -16.04299213 -12.77689214 -6.63149015 [21] -2.36611691 -0.12648746 -1.40968633 16.73006323 0.01242635 -8.67994721 8.52435145 13.27974490 3.87406090 -2.95405889 [31] -10.73019976 0.71155127 11.85587954 -9.66903246 -0.43118517 -10.46787855 10.53664832 -2.52795436 -2.11899525 -4.35789554 [41] 3.95248126 -2.72209154 -8.01515717 -0.92369589 -4.46067905 16.75158270 -4.42194854 -5.28536831 -5.65805563 9.81235874 [51] -3.95030154 -14.62013438 -3.45613832 -5.70975899 -12.52683252 -13.93459279 -1.97420727 -5.19835343 -4.91842599 10.46208196 [61] 4.89416968 -16.85396370 5.98058309 3.90911227 -0.63933907 -2.14089018 0.56088890 -1.05148070 -3.73519203 3.13717780 [71] -3.02043271
5	[1] 4.32101290 -4.02554499 -8.02293114 -6.00655931 -0.79641268 -6.60234442 -1.46970107 -5.01592224 -1.00126292 3.14795422 [11] -2.12474565 2.26003079 -4.90754150 -0.05637182 1.58360084 -5.87064104 1.23199435 -2.90414716 1.21126388 -2.20856042 [21] 0.16645807 -1.55539620 -0.79912282 -0.41899044 -2.51943244 -0.31721419 -1.44747612 4.23755734 -1.13239544 3.31241862 [31] -5.91757878 -0.25395329 2.22126133 -6.30626243 1.83647112 -3.50493218 2.24460932 -3.31628693 -9.95912721 -11.14510477

	[41] -2.59150104 -8.58527590 -8.27907402 -3.67207431 -4.70927688 -1.29006683 6.06289296 -0.25879283 0.11202338 2.63008853 [51] -0.79579874 6.01681789 0.37395672 5.06367402 11.41601634 -4.44846613 2.54571696 -3.56909310 -2.61061657 -1.53516544 [61] 1.71494016 -5.23647703 0.67651633 1.77341746 -2.64002123 7.41398605 -6.43372679 -5.77020232 2.33525166 -1.46772372 [71] 2.83267854
6	[1] -1.00687527 -1.08219881 0.27088184 -0.31589346 -0.16283363 0.21977747 -0.22456733 -0.06165590 0.26618575 0.94879544 [11] 0.68578828 -0.65334473 -0.40292235 0.36800549 0.46701750 -0.94878026 0.02440115 -0.94274673 0.19819269 -0.65744308 [21] 0.67648915 -0.99293089 -1.22894006 10.22545752 0.48383424 0.05432875 -3.26405001 -1.71573733 -1.04367040 0.25978290 [31] 0.09076040 0.15590161 0.61309604 -0.32607078 -0.23101044 -0.33482999 1.84838802 1.18474007 0.60931485 -0.74231706 [41] -0.64718434 0.24236692 -0.57117391 0.01313276 1.12897205 3.12798099 0.48720447 6.75873166 -2.80054390 -0.95743072 [51] 9.42405120 -3.61374331 -0.22692690 5.38865205 -0.62370515 -1.76221529 -0.02146145 -1.17014200 0.23302160 0.24998321 [61] -1.29085603 -0.01354465 0.58810196 1.97331817 -18.44224911 -7.05680235 1.40744279 10.08403027 5.12635205 -1.58856620 [71] 5.83227532
7	[1] 0.364282917 -0.672058737 0.025947335 -0.052141129 -0.356595300 -0.216745854 -0.442172371 -0.530699438 -0.276013814 0.207776979 [11] -0.109435993 0.394918157 0.086682315 -0.894134443 0.052214015 1.016349118 0.332811292 -0.247962345 0.268216468 - 0.713867987 [21] -0.754035050 0.238224336 0.669919521 -0.548774159 0.026648743 -0.048647795 -0.365984343 6.206324271 4.484842065 - 3.058158715 [31] -5.241249173 7.069357070 3.877578848 -7.831321264 1.621972276 -9.844164102 1.424200974 -0.838663320 -0.251092334 0.461039782 [41] 0.280618286 -0.278107514 0.539419249 0.003784784 -0.814608670 -0.353335064 -0.469750772 -0.483087079 0.152940690 - 0.543195270 [51] 0.102586581 -0.367012248 -0.308552354 -0.710812815 0.792004199 -0.395105486 0.495493526 -0.134804118 -0.520805845 - 0.397572125 [61] 0.876479877 -0.004141408 0.222433054 2.053144601 -11.479463556 -11.902041173 -8.389750591 -1.236128440 8.306754553 8.382471319 [71] 10.199546622
8	[1] -0.326671298 0.053851903 2.041097978 -1.120572160 -1.574709662 -2.881021660 1.297350317 -0.755960047 -0.657425228 - 2.398221866 [11] 5.006750792 1.130669476 -7.800143219 -10.987042539 7.695294309 0.021519701 4.154604747 -11.253034509 -0.282125788 0.133182930 [21] 2.534649664 -1.351915576 -1.659124567 -2.845483345 1.801859660 -0.856359099 -0.373197387 18.500844786 -3.308940250 14.937944405 [31] -7.363605550 4.968520894 23.677860470 -9.372317761 -0.260927307 -8.129762868 -0.101344215 -7.691581901 6.441936978 1.979552654 [41] -4.317239858 -10.514378851 7.329623234 -0.326985187 -3.296521776 21.031630707 -0.002918038 -3.724782426 -3.486569847 0.620189501 [51] 1.678835463 -4.649696397 -0.867844236 -6.066742838 -0.442187447 1.564100007 0.770377872 -0.240928868 0.040761907 - 1.052866465 [61] -0.788565728 -0.578275388 -0.467366970 2.878992986 -9.721416260 0.407679084 7.576475963 -0.934871824 1.180668057 - 2.641540834 [71] 1.727256371
9	[1] -2.06611252 0.14612370 -0.06230748 -0.10099360 -0.38676700 -0.17351728 0.16905109 0.35501907 0.18863993 -5.39440160 [11] 9.05954883 9.39759955 5.26080873 -0.06172506 0.50117456 3.61364017 1.40636810 4.45111943 3.73267636 -6.90308316 [21] -3.26326144 -17.51955795 -4.12336653 -5.55225607 -9.48234596 -0.91252566 -4.22908681 -0.81924268 -8.89491050 1.78761687 [31] -8.05822896 0.67158570 1.43793210 -10.42629175 2.33902357 0.88236582 1.67603752 -3.54827364 -1.35372980 -8.46790963 [41] -2.51927450 -1.48486913 -4.73801965 -0.76925165 -2.74124263 -0.91073289 1.25268501 -0.06983798 0.03854061 -0.28473952 [51] 0.20015438 -0.01259965 0.09242669 0.57730365 -0.82969554 1.34734948 0.25286812 0.32159522 -0.14072400 0.34006959 [61] 0.20133031 -0.15137878 0.50954151 -1.83204928 7.41975523 -1.62946783 6.98645368 0.98598246 -7.39680242 -10.83727308 [71] 13.47033843
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26	[1] -17.45355136 15.01145151 3.71336969 3.67711149 -4.68769978 5.89596847 9.79545490 3.77710725 8.20626935 19.69539957 [11] 13.58928427 -2.33184102 -14.41771057 0.35684877 3.15965608 1.88973738 -2.65059402 -12.95554747 19.60173872 -5.56175644 [21] -1.42663677 1.88378890 -0.56788238 -4.46822032 -0.25994820 -2.83573375 -7.86337617 5.29032870 0.47943705 1.15079152 [31] -1.60910744 -0.70596184 -3.18054935 1.48169970 0.17680249 1.62097503 -7.26383893 3.33611263 0.69933040 -9.06484324 [41] 2.03011934 16.19252827 -3.72129487 -1.20615054 9.58274788 -4.33732931 0.69734151 -0.35592467 0.79702112 0.69919518 [51] 5.33513222 -0.29448319 -1.17792237 -0.23737138 19.91489506 1.75889239 -2.60291285 -0.05842168 -2.79124608 6.41734354 [61] 2.26268517 -1.96260715 -5.60475889 5.25246567 1.99675419 -0.73406044 1.96352131 1.99952906 -0.67604198 2.76360718 [71] -8.91285322
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28	[1] -0.208597550 -1.657269374 -1.419893883 -5.354870755 1.012915994 0.173047516 -4.368257440 -0.136546810 -0.012161094 0.079159322 [11] -0.032374107 -0.879828813 0.796229897 1.348368520 -1.382614255 -0.004114986 0.346642413 -1.297718143 1.342589226 2.867263784 [21] 3.084449926 7.402993780 -1.058456980 0.250440339 5.638582711 -0.142638338 1.579502270 0.688631104 -2.076952842 - 4.163697380 [31] 0.558659771 -2.724052288 -1.398798725 -2.196456203 -0.474087525 -4.195774287 0.475395950 0.229737971 -0.501325379 1.140788247 [41] 1.810280538 -1.686058966 0.445934374 0.179609832 -1.501570920 -1.160828251 -2.360672707 3.586140841 -2.066336035 9.098034467 [51] -14.576591523 2.443310267 -4.380614520 7.361525972 1.218012355 -0.487136780 -0.110511765 -0.627082568 -0.570254460 0.283180200 [61] -0.495758672 -0.368116887 -0.688205858 -3.899207772 7.911045211 -9.245952715 6.511809980 1.571230325 8.174596244 - 0.894324238 [71] -5.331455005
29	[1] -3.27718711 2.14784111 -2.85847317 -2.41108070 3.44176262 3.85174194 -8.56803566 3.48553793 -5.46824451 3.17941449 [11] 4.28177000 -0.71157410 -3.36128977 -0.72804005 4.14804128 15.17855802 -1.51338041 7.43913880 20.54159875 -11.77173968 [21] -3.87617329 -3.55223675 -5.54619255 -3.15970993 -6.15065827 -3.07043658 -2.92725524 0.96377871 -0.28340867 1.50128239 [31] -0.86637001 -0.54801085 -0.91461739 0.41668834 -1.73202982 -0.36008160 -1.41124966 0.24460595 -1.56173825 0.78564678 [41] 0.49503255 0.67791971 -0.65261197 1.88476647 -0.01098754 0.52741563 3.44871502 0.07696638 -0.62345443 1.76520752 [51] 2.11689069 -0.03276901 1.01100134 -0.90336006 0.06089416 2.18394148 -0.67912821 -0.71136750 1.52104483 1.88054018 [61] -1.33139454 0.82285826 -1.29732488 10.30536855 1.70851485 -0.91763629 -1.93598593 -8.22946699 -8.48914250 3.95593508 [71] -6.03183539
30	[1] -11.366463214 -13.121316573 1.139440459 8.950901559 -7.248620411 -12.824687682 7.372194331 0.367139144 7.551491501 6.000760075 [11] -6.640993276 -3.113290803 0.100303075 -2.196784809 21.006333552 -9.225824239 5.712097821 6.624713559 -5.875343129 - 5.502768453 [21] 1.638989557 4.875361011 -3.654477195 -6.957616581 5.457170471 0.000559665 4.983459434 6.936767664 -2.341239871 - 2.216003094 [31] 12.788800178 -3.841437933 6.649708830 -3.383910387 3.191382349 -3.920553581 -19.164839407 9.605912811 6.691936141 - 5.217599420 [41] -5.272338674 17.154278915 10.562168026 0.126928499 5.791265586 -2.275933123 2.367435661 -0.478878099 -1.863429542 1.364117491 [51] -1.981856068 -0.124159107 -2.232966460 -1.575390978 -31.859564900 4.446675111 4.753620201 6.236700054 -0.783105664 -

	2.567019597 [61] 6.739040237 -6.643590321 7.144602110 -2.016405210 -4.419577489 0.884932317 5.789212104 0.632115754 0.753322988 1.544745287 [71] 2.329118035

Table SI 4: CED model parameters.

To use the models, the input of 10 descriptors has to be transformed into 8 factors. This can be done using the following procedure. First, the input has to be normalized. To do this, the following formula is applied:

Normalized Input = (Input - A) / B

Descriptor	A	B
Molecular Weight	162.11	124.70
# of functional groups	3.49	2.99
# of Oxygen atoms in keto and aldehyde groups	0.38	0.76
# of Oxygen atoms not in keto and aldehyde groups	1.25	1.70
# of Nitrogen atoms	0.70	1.11
# of halogen atoms	0.28	0.83
# of aromatic or aliphatic rings	0.83	1.13
# of ternary or quarternary Carbon atoms	1.05	2.03
# of heteroatoms in rings	0.34	0.82
# of unique substitutes on aromatic rings	0.84	1.34

Table SI 5: CED & GWP input normalization.

Then, the factors can be calculated according to the following table.

Component Score Coefficient Matrix								
	Factor							
	1	2	3	4	5	6	7	8
Molecular Weight	.271	-.001	-.107	-.074	-.043	-.048	-.014	-.153
# of Nitrogen atoms	-.011	-.335	-.216	-.009	1.350	.080	.020	-.503
# of aromatic or aliphatic rings	-.024	-.071	-.079	.034	-.034	-.017	.024	-.390

# of ternary or quarternary Carbon atoms	1.033	.020	-.227	-.158	.022	-.075	.043	-.531
# of heteroatoms in rings	.006	1.245	-.010	.018	-.396	-.003	.038	-.543
# of unique substitutes on aromatic rings	-.235	-.010	1.309	-.061	-.217	-.036	-.144	.163
# of functional groups	-.102	-.102	.000	-.122	-.128	-.102	-.105	2.249
# of Oxygen atoms in keto and aldehyde groups	-.115	-.009	-.047	.176	.108	1.079	.091	-.455
# of Oxygen atoms not in keto and aldehyde groups	-.211	.015	-.071	1.157	-.013	.159	.121	-.484
# of halogen atoms	.048	.045	-.198	.137	.029	.093	1.070	-.524

Table SI 6: CED & GWP factor generation.

These values are then used as input. The model output is also normalized, to calculate the un-normalized CED, apply the following formula:

$$\text{CED} = \text{Model Output}*180.37\ \text{MJ-eq/kg} + 167.33\ \text{MJ-eq/kg}$$

The 30 results are then averaged and the model uncertainty for a given input is described by the standard deviation of the 30 results.

Other MLP models

The construction of the other models is identical in procedure to the CED models, only the parameters have to be exchanged.

Global Warming Potential models

The GWP models use the same input normalization and factor scores as the CED models. Only the models themselves and the output normalization change.

1	[1] 4.67819592 -14.60908955 -23.79417859 -29.71135033 5.16614346 -3.31447628 6.83939952 -11.27800364 -24.05357547 2.38582564 [11] -0.32538206 0.86642582 -0.74995948 -0.61339943 1.13706578 -1.38688483 -0.41639754 -0.90943457 -2.21229669 -0.77857222 [21] -2.35281191 0.53352683 0.13129978 -2.73583119 0.81669568 2.91856829 0.31855169 15.00375267 3.86658533 3.47223179 [31] -0.67225375 -14.06860362 10.42319428 3.37280169 -0.33565552 -5.15721528 1.67448668 -0.06051819 -1.33055462 -0.15441606 [41] -0.01367632 0.11605272 0.52038777 -2.88929634 -0.80139511 0.16662403 -0.90915209 -2.59646982 -0.65369314 -2.51480406 [51] -0.14646780 -0.81186572 -1.81883792 -2.41235841 -5.18087581 21.93482654 34.98553261 45.43321771 -9.08391594 5.96593351 [61] -10.55514648 20.04821301 36.20640413 -13.87945909 21.47238350 -4.92920578 -3.32236585 -1.06261662 -3.84961492 1.89102221

	[71] 21.44802403
2	[1] -0.02208604 -30.82555290 -14.86839071 10.99721842 -17.24850023 -1.51433674 -2.12153110 -0.15285181 10.61343276 -17.33287913 [11] -20.63521923 -18.43060268 6.40001864 4.11742005 44.12303666 -9.29735122 13.91153356 20.30652858 -1.48608756 -0.92199674 [21] 0.14713189 0.43629042 -0.22209257 -0.02557721 1.22990069 -0.79232934 1.28012353 5.35440747 16.67061337 2.53079513 [31] -8.81611487 3.36154188 -4.01320823 -7.92088714 -12.05451735 11.22451891 -8.88195085 -10.82368254 -8.66438247 2.09656537 [41] 1.86220475 17.20171071 -3.67461603 0.71581522 6.24396795 -14.28898083 -16.82971476 2.84917652 -2.91240844 -4.06494389 [51] 0.33197250 4.61344650 1.78892788 9.10584260 4.48876518 3.16334206 3.86851836 -2.56288229 1.40772256 -3.94125424 [61] 1.31783060 -2.78732715 5.76370601 0.48144087 -0.87692309 3.46812274 3.48422373 0.68127592 -4.11698212 -1.63345838 [71] -1.56283206
3	[1] 0.4380996 -9.3885521 12.3037135 -18.5431989 -29.8469229 13.9630105 -16.7698476 16.5027053 14.8896666 9.6475692 [11] -1.2038174 -0.6557542 -1.6266931 -0.1404173 2.7769239 -1.4972397 -0.6976550 -2.3753872 17.9328076 -3.7337814 [21] -15.3856256 2.4438134 4.5939442 -3.5770079 -7.2119316 -5.5693955 12.6186599 -10.0504867 0.6153701 5.0950352 [31] -8.9643276 1.1275971 -4.7256921 13.0464555 1.3123924 -6.3563773 -6.3529649 17.8750038 -1.3800416 11.6919077 [41] 7.0526960 5.6809734 10.7481036 8.6931701 11.8062539 5.2556722 9.7692981 -4.5981063 2.1845557 12.5780577 [51] -3.6203058 12.8909403 4.0917218 -6.9946611 18.7553810 -0.4754751 -6.7099588 12.7306969 -0.1133904 6.2485042 [61] -13.0406947 16.0862723 8.9466480 1.5055786 -0.8407727 -3.2108286 -1.1214305 3.0923568 0.6460489 -0.9829067 [71] 3.2847541
4	[1] -3.29152145 -1.67914471 0.72473179 3.00064074 -1.19131005 -0.97608059 3.57428420 0.52162275 2.67540348 2.75539722 [11] -1.07331769 -1.35874785 -0.83357349 1.67559891 -0.39306860 -0.04241590 -1.13767697 -1.29930554 -0.70182189 24.85585663 [21] -1.70678456 2.44902608 -3.94833481 7.94299352 3.57117823 5.95790253 15.49705560 10.02571484 19.23501386 0.27012684 [31] 6.35150269 -2.95253039 7.04620566 17.55682885 1.46141385 14.98275301 4.31118984 2.63837605 -0.91956900 -3.97160850 [41] 1.60992450 0.77912403 -4.81358780 -1.02398350 -3.29092278 -2.80601071 1.67723205 0.80837581 0.09639678 -2.25411413 [51] -0.50315378 -0.89620548 0.45617013 2.22485115 3.84810170 -3.82287418 -18.72057239 -22.68248088 9.04653286 -3.13098991 [61] -14.44905358 -8.19639440 -14.71582341 -6.09511131 10.31378034 -3.88188490 1.53624775 -0.76468155 8.55513276 -3.24943183 [71] 1.07317986
5	[1] -1.45016178 9.53948030 -1.46534617 0.32888670 1.37345750 2.05535006 1.49580750 2.19433765 6.62418838 -5.87195323 [11] 14.31429316 -1.24785075 2.29741486 4.46515087 4.43451171 -4.15552701 2.74269961 11.09589808 -1.93631188 5.26374973 [21] 3.02353619 -0.19089997 4.44872283 1.50963662 0.93599754 1.83878894 5.52938508 -0.27821980 12.79000453 6.00710019 [31] -2.77566594 6.36655529 2.28182177 1.96445858 4.89812938 12.98152354 1.89118724 9.70372955 -4.82347677 6.89513633 [41] 10.98116714 8.61480107 -2.90853706 10.46321753 21.05575896 -5.94600149 0.45692708 0.74102298 0.41869928 -1.33512022 [51] -0.06802988 0.50118720 0.54449057 -0.02017876 9.66613896 0.53474692 0.52349703 -2.13324364 4.95857526 5.98879854 [61] 6.00008304 12.29938474 7.40050624 -0.35574952 3.04876887 -3.32398861 2.64496824 -2.20080099 0.60918186 15.46002185 [71] -0.28387049
6	[1] 4.0528682 -13.8941487 -2.8599507 -0.3521600 -12.0451677 -2.6446447 -4.8060429 -4.5307001 0.3926100 15.3560569 [11] -1.3913950 0.7795004 -3.0326710 4.2902192 1.8742789 -5.2581147 -0.9294493 -3.8915710 -10.8836276 -4.8157428 [21] 7.0785489 7.0305944 -0.4898035 -7.4204826 12.0098257 -13.7149907 6.6169334 -0.5685310 1.2965120 2.9589769 [31] -1.1982448 -0.9227171 -3.3366084 0.8478250 0.7520020 -1.2231089 5.1799047 -0.1536803 11.8977954 -3.3523016 [41] 0.9625161 -9.6404053 2.4042056 -0.2376914 4.9387830 -1.0136802 0.6934730 1.8160131 -0.6959498 0.7774592 [51] -1.6229247 0.7056220 -2.0958384 0.9540989 -0.6441243 1.2919727 2.6905336 -0.9950783 -0.5212223 -2.4187018 [61] 0.5736061 0.2024700 -0.6238464 2.3389465 -0.8277871 -1.8558598 1.0210062 -7.8109166 1.3736961 -3.0941022 [71] 8.5453247
7	[1] -22.041374543 23.759238787 -7.617621865 16.048573435 10.944458115 14.135610626 26.797435977 25.037608397 21.925257869 1.527350998 [11] 1.699803847 0.809154543 -1.180563551 0.992834534 0.364355901 0.246937656 0.004293338 -0.509175945 0.000829484 -5.943082413 [21] 6.636623506 -9.560345789 12.971627619 -11.975197080 17.875960798 -7.523626437 1.769909336 -30.726758631 17.770965506 -12.001244802 [31] 15.512615586 15.948205018 6.499845577 -9.354283772 14.009314368 38.142388249 -4.643737854 -8.316133555 -5.779646725 2.044366812 [41] -4.323117293 -1.152732449 -1.231103035 -0.188474400 -2.254164693 2.018471352 1.338342489 0.344578874 -1.390408497 0.665514941 [51] 0.398097321 0.344486574 0.057720008 -1.083982414 34.656630796 -23.843168956 21.743508377 -21.444076187 -18.693410094 -11.005284257 [61] -6.923692825 -26.884337979 -50.437494536 4.626877969 1.011103031 9.022250102 -0.247658741 -5.605580112 1.342875069 -8.664892009 [71] -4.786607708
8	[1] 0.415769103 0.758593440 -0.848107909 -1.320508644 0.447308084 -0.731940214 -1.105934089 -0.193151157 -0.612794750 -2.466382420 [11] 4.669565869 8.881528948 6.815120599 -2.742926265 6.747798078 3.718526476 3.875939876 8.603425407 5.452561651 4.711622442 [21] 0.641756141 4.422853406 -0.121583357 1.808146641 0.433036073 0.857124791 0.148389457 3.288918082 -0.919234354 -1.176502899

	[31] -1.020889306 -0.514886598 -0.750731667 -2.153323872 -1.601016897 -2.151059400 -6.529616058 1.241432719 2.438322544 2.379830562 [41] 0.988560113 1.637503132 3.507661885 2.548811281 4.373781165 1.173823315 -0.406723680 -1.576942880 -1.550966574 0.427043727 [51] -1.505973926 -0.524613868 -0.149831858 -1.271989083 -0.449336293 -2.284768320 0.260075223 0.458094588 -0.157051707 - 0.426202963 [61] 1.311217417 -0.001833786 0.131721457 8.934163395 7.355243612 -2.658919214 2.260357139 -10.644215168 -8.407744492 - 8.495814628 [71] 3.912432026
9	[1] 0.291157821 -0.870188068 0.855636406 0.042785466 -0.161821631 -1.079929038 1.352093341 -0.085897715 0.599569646 - 19.387307335 [11] -2.795675583 -4.350271725 -7.886370221 -2.084678435 -3.377170812 -6.672181627 1.512726329 -8.804756549 14.463362821 - 7.493751808 [21] 10.016003213 1.297454854 -2.938753123 -11.019363031 -12.309054227 -11.826193101 -12.793795885 -0.265851503 -0.578059588 - 0.372617829 [31] 0.231062129 1.057981055 -0.724318310 0.088620352 -0.329281169 -1.114945725 -1.593955066 0.290119913 0.658034000 0.111510036 [41] -0.639993346 0.027429135 0.220843429 0.642044780 0.452690183 -1.199525585 -0.227700261 0.890986755 0.197076904 - 1.132559798 [51] -0.031897393 1.584589412 1.246883706 0.009974618 0.603898777 -0.309404081 -0.270611878 0.372511541 0.789798005 - 0.237626703 [61] 0.505297970 -0.159995874 -0.992818805 -2.584157844 2.167186081 2.964643832 -1.137087432 -6.444878243 5.677033000 - 4.612709056 [71] 8.898167487
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28	[1] 40.57709447 17.51356277 -31.71184734 4.01443333 15.72802047 25.41503257 -31.30920386 -12.38088677 -25.50823175 16.45976269 [11] 12.51314014 -6.18092870 5.25114021 6.52423342 10.66941280 -8.90903583 -0.86503726 -5.92877300 -13.92405656 -1.43851293 [21] -6.05337162 3.73044328 -2.07784646 -7.72268531 11.85443727 -15.54482484 6.13516860 -1.20492354 7.18509057 15.66707866 [31] 21.45891594 -10.17126269 10.34706333 14.78572746 8.22054191 16.47196929 3.39572271 -1.91929495 -4.25800341 -2.90016204 [41] 3.59922905 -2.57263696 -0.58417202 -3.02519316 -2.25250715 23.71989370 -6.87720753 -0.03494244 8.43673873 13.79611844 [51] 12.28351064 -1.75810958 -6.93629467 -12.52521757 -2.28438827 -20.76934032 12.80231754 3.25975365 -6.64029096 -9.99408372 [61] 12.04357240 -0.73624612 0.26725221 1.50147965 -3.32861719 3.09737788 2.51307581 -2.20856854 -2.56640063 1.03179712 [71] -0.31664662
29	[1] -14.2103489 7.0641904 -9.4667361 12.5652694 3.1505495 -9.8125739 -1.4202510 1.5518229 -8.1193691 16.4886312 [11] -17.1591044 14.2932368 6.5122843 -9.2390277 -7.6414867 7.3041854 -6.0400462 -17.8197065 -3.9085413 23.9317057 [21] -3.8040033 11.8973543 9.5684569 -9.9505538 3.3174279 -5.8525128 7.7906278 6.7554848 -9.0804183 5.3108677 [31] -8.3410859 -9.0428510 -20.3666502 -3.5788729 -10.2742149 -11.9573378 29.3819864 28.0025859 -8.2084093 8.9198020 [41] 4.7113683 10.8680175 -13.1395859 -2.9909196 -12.8118871 -15.9291496 12.9376989 -2.5982702 8.3001749 3.8829469 [51] -0.2467490 3.8603588 11.6874491 1.4388870 -39.7622149 -28.2056672 21.9652548 -13.3755161 -3.4180809 -17.4883360 [61] 26.2623170 10.1955599 22.5579333 -5.6979389 -1.3539908 1.1638726 1.3468066 -0.8127375 4.9536208 0.8342879 [71] 4.9088949
30	[1] -1.38598843 -2.79533694 -1.43053371 -2.13786697 -0.64904375 1.15265944 -1.10336944 0.31189120 -1.28979345 40.83590674 [11] -0.46419092 -9.19326551 -2.17330014 -2.13039268 -8.28152454 -11.01066398 -17.05063334 -14.31829325 -1.67875613 -2.37500531 [21] -1.45219501 -2.01027892 -0.43102019 1.15593077 -1.23283760 0.09203021 -1.43796675 5.42528199 23.59681985 0.26091025 [31] 20.10245727 -3.36293194 8.78590481 0.95121362 4.61456096 8.86055293 -0.27673874 1.22042740 -0.07221046 0.63702915 [41] 0.67376412 2.00447458 -0.40006447 0.93747770 0.33348593 -19.15168377 -6.34228122 20.72626468 11.84060904 15.71997216 [51] -2.92606184 9.04036251 8.98035810 12.93514369 0.36464475 -1.02573115 0.29604875 -0.29442716 -0.63184859 -1.69058079 [61] 0.60666667 -0.57168729 0.04779237 -7.88167476 -10.93304032 -2.33967833 10.94835320 -0.93937358 10.76683562 -0.85602695 [71] 11.50799335

Table SI 7: GWP model parameters.

These values are then used as input. The model output is also normalized, to calculate the un-normalized GWP, apply the following formula:

$$GWP = \text{Model Output} * 10.03 \text{ kg } CO_2\text{-eq/kg} + 7.32 \text{ kg } CO_2\text{-eq/kg}$$

The 30 results are then averaged and the model uncertainty for a given input is described by the standard deviation of the 30 results.

Eco-indicator 99 models

1	[1] -0.8035842 4.4253968 8.4597299 17.2250709 -2.7631645 -6.4593315 -10.0897095 -0.3788919 -20.5919658 2.8433579 [11] -1.4378004 -2.9441559 -15.2347848 -2.5645071 -5.2030951 10.2330231 -0.3810514 1.0938733 4.1014850 0.7094444 [21] 4.2766684 2.9489599 4.3197838 4.6257525 9.8462754 -1.2118877 5.8800639 -5.5160365 0.4485134 -0.1185304 [31] 4.3699606 -1.6595934 -2.8089955 -2.3248477 -0.1775629 -4.9026483 -3.8375733 3.8588599 4.9343669 4.4346573 [41] 0.7532733
2	[1] 3.1155080 1.3721933 -13.1657715 -9.0762400 2.8967820 13.2887690 -20.8549486 -4.8321506 3.7571619 -4.2183017 [11] 3.5168252 4.1818468 1.5840504 2.0011630 7.7214584 -1.0565213 -9.4740876 -2.5633620 2.7957224 8.0800587 [21] -10.0619604 9.3003594 -2.0595528 14.4219912 0.8290236 -9.5531746 -0.1226655 -5.5428039 3.6125389 -7.6228658 [31] 4.2345378 -0.6981801 -6.8720446 -1.0393879 -3.7288046 0.7698890 -11.7717329 -0.7217205 11.5423222 4.8984396 [41] -5.8496594
3	[1] 8.58014499 -0.53577974 2.07757621 4.29347422 2.68407102 -2.25891442 0.03342915 -1.74563479 -1.61176417 7.26338506 [11] 0.42139577 -1.75699711 0.11469172 0.28594920 -0.74278626 2.54566567 7.90007466 -1.72572364 -1.96740892 2.81206520

	[21] 2.55262940 -14.30551477 -0.89754212 1.57886279 0.68323672 2.88962240 -18.66806518 1.04470467 -1.98860579 -2.78441811 [31] 6.36276503 0.63465690 -0.47945346 -6.53008205 -2.22596572 7.97029634 -8.16827096 4.81772837 -3.62656575 3.75656842 [41] -1.20230061
4	[1] -3.19195448 2.20691439 -0.95408253 -1.89666015 4.74052506 2.19483835 4.72333664 -2.18553575 -15.31430686 1.73663958 [11] 3.11356462 -0.94093236 7.14246603 -2.95700304 -0.19205927 -1.79708621 -3.75098377 -0.17174727 0.86434110 0.93652691 [21] 1.30644213 -0.46464104 -13.00285550 -20.38606694 0.58242078 -7.49709967 -5.35119361 -1.09728189 -0.03893251 -10.80457932 [31] 1.68309381 3.44578536 -0.45527427 8.76621703 -2.59950816 -0.46026964 2.20993791 -7.18437780 -3.26346801 2.04410731 [41] 7.96245939
5	[1] -4.4999635 2.8294040 1.3976849 -0.7625016 3.2871084 2.6276319 3.7150364 -3.3025021 -8.6798829 -2.3600940 [11] 14.3930562 -8.2599503 -0.7731976 -11.4786537 4.5389782 -0.5222006 -0.9306464 0.8622449 -1.3443963 -1.2188591 [21] 1.3680932 -6.9080227 -4.0039233 -3.3607730 -0.6731097 -0.1310310 0.1191956 -1.0373432 8.0512969 -3.6539596 [31] -4.4165379 1.4842608 -6.7738694 -4.8653546 1.1490462 4.2761936 2.7637252 0.6354378 -7.4350608 -13.5954374 [41] 2.6796653
6	[1] -20.2327590 3.2443632 5.2740825 -4.9498728 1.6957854 4.0053609 -2.7422064 7.0426721 20.0647531 1.8257076 [11] -3.7164413 3.0413828 2.3033738 -11.3194478 -4.4413238 -6.3325302 -3.6978502 -12.9131057 5.0146690 -2.6132828 [21] -0.5863590 3.4975527 -11.2684351 0.4119986 4.6569326 3.5242654 -1.4308702 25.7377755 25.3612613 -1.8014504 [31] -5.6634002 -2.7934997 -8.0793879 1.3811176 0.7857874 2.8091917 7.9484427 1.0300035 -0.4283350 1.0236501 [41] -3.9692121
7	[1] 0.7542719 2.3859157 3.6729844 1.0515153 2.8481415 1.4634169 1.3137105 0.6247607 -1.3484565 0.9956405 [11] 1.4254328 -3.3375418 -0.3755390 -1.0202125 10.9266053 15.1719783 11.0759502 -6.7057822 10.1655324 7.0752921 [21] 7.2510162 8.2262325 0.6165362 -17.6893498 -5.0497783 1.4743344 -5.9473147 0.1400906 1.2078281 4.0991446 [31] 7.5389343 1.8643291 6.3339805 3.5755180 2.5925341 7.0930346 8.6155055 -4.1081397 -1.4050867 -4.0498190 [41] -9.9356848
8	[1] 6.4369667 -0.6374920 -2.6585420 -7.2877966 2.6498557 7.7332433 4.5998443 -4.5251039 -9.9763268 -5.1268494 [11] -1.7577668 4.1252892 3.2076944 3.4809393 -3.1329405 -7.6407711 -3.6347141 -4.2028593 8.3782169 4.9570216 [21] 7.5448332 -8.4016462 17.8128909 -3.8363988 2.3431433 8.0145669 1.0874540 9.1868896 6.6982632 -8.3293934 [31] 5.0027987 -3.1772970 -3.6586149 3.4444566 -4.4226332 -4.8671653 -0.6680238 -2.2939075 2.1113018 5.1165117 [41] 5.1570096
9	[1] 4.29555138 -0.54007543 -1.90468110 2.10436490 0.17244926 1.85724654 1.95305985 -3.43674397 -7.49661779 -1.69336901 [11] -2.09619299 4.97600620 -1.19191680 0.06893281 3.69385878 0.18916867 -1.84585394 1.27677391 -0.33519973 2.36506764 [21] 1.78569655 1.88626699 -3.82657154 -2.38075716 0.15380295 -5.86033310 -1.23005858 -2.88908528 7.03173900 -4.38264698 [31] -7.76196011 -0.14283334 -13.09866991 0.07459321 -5.16916261 0.83757470 9.40510309 -1.31392352 -9.37461595 -6.42285741 [41] 5.32103413
10	[1] -4.5174516 -12.1775947 7.7721339 20.0026162 -11.7370680 6.5523912 -11.7407214 12.1029527 1.3557682 7.3130350 [11] -8.2863030 -0.6315936 1.3003794 12.1730918 1.6076299 1.1323376 4.2489575 9.6584059 -0.4987284 4.0920779 [21] -3.0615196 4.6472285 -1.7122765 -2.2924107 2.9675162 -2.8956091 -0.8947928 -2.5013151 -2.4361489 4.2092993 [31] 11.6183036 -0.8589254 3.2895440 9.2150887 3.1968755 0.1843678 -2.0361513 2.3728461 4.3560798 -3.0644353 [41] -1.9593257
11	[1] 8.86624544 -0.68409378 -0.54418298 1.08072486 -0.71440760 16.01850656 -0.23094670 3.13003284 10.05638913 -2.66115631 [11] -0.92964545 -0.71679253 -7.95302375 0.66878496 4.37284897 10.66332726 -0.69728339 -1.09296519 -0.06068059 -5.35431144 [21] 0.11839052 9.83927987 7.44936068 9.70470337 -8.21403280 14.40821920 9.14673061 6.65392220 -7.63422155 3.72088094 [31] 1.25277127 -1.86129605 8.74345069 4.92611780 12.09381914 2.13728782 -1.52703310 -4.70625875 4.01713957 -1.24003327 [41] 1.21331536
12	[1] 0.50713991 -0.57546594 0.24544439 0.04823999 -2.80136887 -0.08562932 -0.71337546 -6.51817706 6.30230797 14.79822147 [11] 3.91323867 8.92752860 15.60958277 -6.59544554 1.44216408 -3.26215567 -3.41729241 -0.98968055 0.15282627 0.01907949 [21] -0.27592208 2.33934259 0.63799257 -9.76958983 -3.69280589 -0.18515590 -21.11422561 10.11979522 -1.51833164 -5.77068038 [31] -6.64780758 -2.29936212 -7.68544590 1.86461307 -1.81528721 10.20756159 -5.66233656 -4.70465316 -5.81835788 -4.21220446 [41] 3.95812022
13	[1] -6.365960685 -8.433660300 -8.776330452 -0.400545533 3.520258867 -3.418901789 3.610108995 -5.441001219 -7.260169985 -7.991145184 [11] -0.598287970 1.977449206 -2.480316955 3.208528787 0.857301018 -0.761616828 0.676499102 1.500354591 -1.258445635 -0.008173093 [21] -1.419071927 0.975320501 -0.472967216 1.090026939 1.392076039 -0.506691564 0.860644527 -1.180560318 -5.136343732 -7.438013259 [31] -3.482789159 -3.231340547 0.459753154 3.224052307 -0.949832935 0.502306742 -9.110545580 9.211101220 -9.135190681 8.736552247 [41] -2.107901353
14	[1] -8.9127734 8.5256420 -2.6899767 -7.4425393 4.0607421 1.1622374 3.7006273 3.5723152 8.0764670 -8.4143463 [11] -12.0043020 11.3577322 -9.3587758 25.2344493 5.4033470 4.6759053 12.2645552 2.8664932 -7.0508534 -2.9855499 [21] -1.4105129 2.7814175 -2.6514844 4.6464019 1.2289362 -6.1571601 -4.6208963 -4.8742646 -1.8996020 5.0315721 [31] -6.1370384 -8.7353149 2.9242173 -11.1072336 15.9611321 -0.2045755 0.9034007 4.0190104 1.8982805 -1.6098240 [41] -4.4314877
15	[1] 10.1069612 20.5244696 3.8707955 -3.2750617 13.4218376 -12.9010089 1.4017349 4.1178733 4.3265925 -4.2236477 [11] -5.0482709 5.2246938 1.6094294 -3.1885588 -8.2392771 3.7204603 -7.0115015 -1.8795073 4.4784307 1.0920855 [21] 4.1663427 -9.5266997 -17.9338441 -3.9068505 2.6181556 -21.3970986 20.3548750 -4.3403407 -3.5883085 4.3305589

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16	[1] 0.90934723 -13.42866143 -11.29529567 -1.34159095 1.21727999 -0.18229434 -2.17210814 5.59610083 0.77136563 11.00141908 [11] 1.77627168 6.21760199 -0.56527252 3.93167812 -5.34991397 -6.61694899 -7.57350739 1.24182175 2.76144921 -16.65114204 [21] -1.55099610 -1.68263613 2.10048909 1.18683934 -2.59873572 8.18985052 0.83231922 3.24056696 -6.33512775 -3.51704238 [31] -8.49418128 -0.08857417 3.32120942 -19.00064555 -1.64908911 3.87424141 -4.34229170 -3.89912787 11.87656263 3.91104950 [41] -11.61796009
17	[1] 1.410557 9.626284 -13.710515 14.863025 1.029362 -10.532986 -4.165718 0.984053 -19.473760 3.612698 [11] 2.977593 -4.528254 14.371761 7.381323 -6.399592 4.008820 4.736066 -1.122729 7.323955 3.461632 [21] 6.568929 -1.737310 -12.353980 18.804178 -11.549070 -2.489926 2.769894 1.745621 -3.589820 -22.107155 [31] 2.156851 2.651493 -4.929154 6.125111 6.562192 -4.092577 3.685279 4.245118 1.448608 3.667162 [41] -4.227170
18	[1] -0.85823633 -2.77911145 3.31364591 0.97976485 -4.90707857 0.49548808 -1.10119555 1.88600319 -0.02080510 4.59493218 [11] 1.36101860 -3.65112908 1.89778096 1.75144931 1.71262783 4.08335804 3.09937590 -0.15570672 -0.87606285 4.48969297 [21] 3.32509127 -0.01078589 -8.07002516 -10.12243018 -1.33314392 -4.21544026 -3.37453534 -7.24951991 -11.28664684 5.86176699 [31] -2.26231760 -1.88233286 9.76604997 15.81606901 8.49027375 2.40222353 -3.17584843 4.78338644 -4.18827989 -2.73411962 [41] 1.67520079
19	[1] -1.63998346 -0.94146217 -2.16160159 -2.27522392 0.98088138 -0.16004009 1.01698066 -1.85902043 0.67100059 -0.14583612 [11] -1.11806533 2.15486637 0.59192042 1.83445532 -1.44883617 2.17549284 10.30201035 -1.83516225 1.80983662 8.84134536 [21] -4.28625032 0.99298724 1.85967669 -3.90774151 1.53241362 -0.26460893 -1.64475437 2.19159981 -2.72375304 0.59335749 [31] -4.13162209 -2.04543016 -2.31413311 0.49815070 -0.08726604 3.30623408 -5.11273125 5.48765683 -3.43296135 -3.95525072 [41] 3.01565250
20	[1] -4.6957583 -18.2832580 -5.0781742 -3.3340140 5.7794556 4.8494603 8.0538898 -11.0693219 -7.8828045 31.8539812 [11] 2.0344986 -4.6532456 7.3960882 7.4401947 0.3537776 18.4094100 11.3189345 2.8420413 -10.4662458 -13.0989332 [21] -22.2071142 21.3408732 14.1834653 -23.0085735 3.8262254 19.8114282 -6.0720698 -0.5577644 1.1535126 -12.8074185 [31] 0.8480917 3.9586879 0.8056006 12.6667912 -7.2995632 -3.2059546 -1.5106187 4.3450393 -1.3712806 4.1287050 [41] 0.2101394
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22	[1] 6.8463046 13.6989242 8.5707832 -1.3431976 -3.2737859 0.6855081 -8.7512836 -5.9805989 4.2829225 2.6719736 [11] -0.3123574 1.8290886 3.1318526 3.2300073 4.7536908 12.4825123 18.0360792 -1.8317611 7.8392182 11.9524068 [21] 0.2046969 2.0291226 -0.5800140 5.6973805 1.2699657 -1.0166934 6.2210690 -2.4441820 -1.8556225 1.1395404 [31] -1.6256355 -0.5974527 2.3541017 -0.8779165 2.6922028 -3.4818321 2.3056619 2.3486308 -4.2236377 5.0991696 [41] 3.7566844
23	[1] 6.4390390 -5.1859367 0.2090743 -3.7679395 4.5991806 26.4131232 11.4601597 0.8640467 1.2640874 0.4476904 [11] -1.1187619 -0.7824801 3.2825548 3.1626919 23.1248374 -8.8614896 -7.9653404 11.5317295 -2.1212617 -4.4563226 [21] -2.3454046 10.8569509 -1.9738520 5.4671667 -8.6386564 11.0412903 -1.9052247 8.7928852 5.4289867 8.8958175 [31] 4.0492384 2.1552528 -2.8304338 1.3638899 0.2647955 2.2064631 2.6980006 -3.8358625 -3.5821450 0.8680423 [41] 1.4823921
24	[1] 0.2618426 1.8045009 -0.9062739 -2.7907268 -0.4109865 -2.7909582 1.2669405 0.1021304 -4.8500520 -1.1725598 [11] -10.9584229 -10.2883676 4.6962863 -4.1633738 8.2703253 18.7333372 5.7302620 -0.5033414 -1.6052257 -8.4987710 [21] 4.7936720 0.8586835 2.9481489 4.2630636 -0.8417804 1.8631032 7.6195240 0.2521578 -1.2525719 1.3733728 [31] 0.5282450 -0.6165731 1.1044054 -0.2363142 0.5825916 -0.5976267 -4.3537829 1.5589815 1.8206381 -1.5762962 [41] 5.3791776
25	[1] 3.56699824 4.94392406 1.83469561 1.10083904 -2.62046086 0.56358155 -0.56926033 -12.45201503 -2.96486866 13.44637464 [11] 12.13229033 1.39188226 -5.51100302 -3.83641430 -0.58379183 -6.48346530 -7.23204107 -5.59793859 -8.84082703 0.97605872 [21] -2.11119407 4.35922610 -5.16820933 -2.07352032 3.68079985 -15.42775756 -2.96867552 -9.24446590 10.84754493 0.74742392 [31] -4.29309511 2.23843296 -0.23448047 -3.18638256 -3.63317763 0.07444554 1.66319688 3.49918337 3.36624836 -4.50322415 [41] -0.82714189
26	[1] 4.10147946 -1.84891677 -1.87944157 1.39442322 -3.66720030 -2.88073710 -0.02474189 2.24569106 -1.06946039 -0.94529185 [11] 0.69873485 -1.67378501 -1.28362274 -1.09157594 -2.74251161 -1.08050434 -0.22287569 -0.57248742 0.71894439 0.54228267 [21] -0.30466324 1.52100645 4.26816438 3.70389574 -3.54513198 3.23748095 -2.77956721 11.70891409 4.99936125 0.20097784 [31] -0.62133858 1.35483222 -2.19369792 -1.94036955 2.00414827 8.64184241 6.75485553 -8.26684324 -9.40893912 -0.64171940 [41] -6.93534098

27	[1] -3.2370381 4.3673920 7.1309463 0.1465926 -6.6976891 14.4258656 -1.1468491 10.3340948 5.6040838 -2.2183856 [11] 6.5061354 -7.4108099 -14.6189558 -10.0060183 -15.4005499 23.8385783 1.3861300 0.3423062 5.9483935 -1.6165508 [21] -9.5021661 16.7669045 14.8964848 -9.5890684 -5.4886204 -0.9185915 13.2082345 2.7464173 -17.5343065 -2.6824465 [31] 7.5721527 -10.5384766 0.6665752 6.2139971 4.5371627 1.8603351 -1.0000061 -0.8134368 1.8324784 -1.4777515 [41] 1.5328706
28	[1] -1.36884859 -0.30895794 1.60558067 0.54259329 -0.21249850 1.21122859 -4.16315783 1.43583066 -0.05022668 -2.59202028 [11] -0.84815296 -0.23920695 -1.78456958 3.41270619 1.26333336 3.42969383 0.64562611 0.09764651 -2.42712240 -2.32391752 [21] 6.51878609 -0.61431009 2.38959477 0.70448994 0.40683074 0.36837903 0.24745721 0.28331202 -0.31453228 -4.26725009 [31] -3.75286380 -1.40170755 -2.78557681 -3.69685820 -0.14369981 9.07917324 -10.80240572 -11.05843184 -3.18960039 5.80635467 [41] 3.79436559
29	[1] 0.3291162 -5.3021649 7.1954911 4.0108867 -10.6200089 20.2036339 10.4029256 -0.7944971 1.7534948 -2.3464297 [11] -5.2048535 5.2926891 -4.4394089 -5.5285282 5.6565939 -3.6280700 -3.1442260 1.2494000 -5.7613110 -3.3714473 [21] -6.1722283 -4.7708516 -16.4757905 3.5805176 1.2927666 1.2885742 11.6621908 0.7320378 4.6166583 11.7444907 [31] -0.3190964 -2.8493908 -0.1587381 -7.0887391 -1.0808466 -1.2649561 -1.8669749 -2.0023739 -1.6181273 4.3924516 [41] 4.3814929
30	[1] -0.57039556 1.04861064 0.35944467 -0.35619056 2.75307811 0.28307590 1.36228400 -0.64364042 1.09294854 2.60102936 [11] 0.34519984 2.80259679 -0.19131566 0.77957813 0.90006255 0.72084911 -1.14038741 0.10418106 0.01632131 -0.22737246 [21] 0.80381565 -3.55536251 8.21314059 10.69197085 3.32988243 4.89718354 2.01305157 4.27032027 -1.45932587 -1.21650094 [31] -0.23033992 -0.61120776 -0.17375085 0.40559255 -0.27756504 4.68226763 5.42495867 -6.83655591 -5.25252819 2.35713032 [41] -5.28828238

Table SI 8: EI99 model parameters.

To use the models, the input of 10 descriptors has to be transformed into 6 factors. This can be done using the following procedure. First, the input has to be normalized. To do this, the following formula is applied:

$$\text{Normalized Input} = (\text{Input} - A) / B$$

Descriptor	A	B
Molecular Weight	148.2	138.3
# of functional groups	3.08	2.68
# of Oxygen atoms in keto and aldehyde groups	0.25	0.64
# of Oxygen atoms not in keto and aldehyde groups	1.49	1.99
# of Nitrogen atoms	0.48	0.87
# of halogen atoms	0.32	0.81
# of aromatic or aliphatic rings	0.82	1.15
# of ternary or quarternary Carbon atoms	1.01	2.53
# of heteroatoms in rings	0.28	0.68
# of unique substitutes on aromatic rings	0.77	1.19

Table SI 9: EI99 input normalization.

Then, the factors can be calculated according to the following table.

Component Score Coefficient Matrix						
	Factor					
	1	2	3	4	5	6
Molecular Weight	.412	-.118	-.072	-.018	-.059	-.008
# of Nitrogen atoms	.008	-.188	-.133	-.362	-.029	1.330
# of aromatic or aliphatic rings	.021	-.026	-.005	-.058	-.059	-.030
# of ternary or quarternary Carbon atoms	.874	-.182	-.293	-.035	-.123	.040
# of heteroatoms in rings	-.060	-.086	.156	1.251	.103	-.423
# of unique substitutes on aromatic rings	-.204	1.277	-.121	-.073	.006	-.180
# of functional groups	.013	-.044	-.114	-.062	-.064	-.051
# of Oxygen atoms in keto and aldehyde groups	-.185	.007	.221	.118	1.096	-.046
# of Oxygen atoms not in keto and aldehyde groups	-.325	-.131	1.308	.138	.167	-.146
# of halogen atoms	-.022	-.019	.204	.027	.086	.049

Table SI 10: EI99 factor generation.

These values are then used as input. The model output is also normalized, to calculate the un-normalized Eco-Indicator 99 (H/A) total scores, apply the following formula:

Eco-Indicator 99 Score = Model Output* 0.458+0.471 Pts

The 30 results are then averaged and the model uncertainty for a given input is described by the standard deviation of the 30 results.

Electricity use and Heat use models

Due to confidentiality issues, these models can unfortunately not be released at the present time. In case more data from other data sources become available, these models will be adapted and may then be provided to the public.

Range and scope limits of the models

The models used no training data of enantiomeric production data. Screening tests with data on chiral molecules revealed that the models are likely to underestimate the production efforts required and impacts caused by the synthesis of this type of chemicals. Furthermore, the models are valid only for petrochemical synthesis. In other words, they estimate the likely production impacts of a hypothetical petrochemical production of a molecule. If it is in fact easier to rely partially or fully on biochemical reactions to synthesize the chemical, the models results may not be accurate.

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