Supplementary Materials

How precise are our QSAR derived predictions for new query chemicals?

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Table S1 Automated weighting analysis for CDK data set (Model Dataset 1).

Model	Division method	Best weighting combinations			% Correct predictions (Test set)	Training set range
1	Sorted response	0.5	0	0.5	87.84%	2.3968
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
2		0.5	0	0.5	86.49%	
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
3		0	0.5	0.5	85.14%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.5	0	0.5		
4		0	0.5	0.5	85.14%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		

		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.5	0	0.5		
5		0	0.5	0.5	83.78%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
6	Kennard-Stone	0	0.5	0.5	88.24%	2.3424
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		

		0.2	0.7	0.1		
		0.2	0.8	0		
7		0	0.5	0.5	85.29%	
8		0	0.5	0.5	91.17%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
9		0	0.5	0.5	89.71%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
10		0.3	0.2	0.5	89.10%	
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		

		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
11	Modified-k-medoids	0	0.5	0.5	89.33%	2.3968
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
12		0.3	0.2	0.5	89.33%	
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
13		0	0.5	0.5	88%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		

		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
14		0.3	0.2	0.5	92%	
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		

		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
15		0	0.5	0.5	88%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		

Table S2 Automated weighting analysis for AChE data set (Model Dataset 2).

Model	Division method	Best weighting combinations			% Correct predictions (Test set)	Training set range
1	Sorted response	0.5	0	0.5	87.32%	7.8195
2		0.5	0	0.5	85.92%	
3		0	0.1	0.9	86.62%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
4		0	0.1	0.9	88.03%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
5		0	0.1	0.9	86.62%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.5	0	0.5		
6	Kennard-Stone	0	0.1	0.9	84.38%	7.8195
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
7		0	0.1	0.9	91.41%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		

		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
8		0	0.1	0.9	91.41%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
9		0	0.1	0.9	86.72%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
10		0	0.1	0.9	88.28%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.5	0	0.5		

11	Modified-k-medoids	0	0.1	0.9	86.62%	7.7558
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
12		0.5	0	0.5	87.32%	
13		0.5	0	0.5	85.92%	
14		0.5	0	0.5	85.21%	
15		0.5	0	0.5	87.32%	

Table S3 Automated weighting analysis for C60 solubility in organic solvents data set (Model Dataset 3).

Model	Division method	Best weighting combinations			% Correct predictions (Test set)	Training set range
1	Sorted response	0.3	0.2	0.5	97.87%	6.97
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
2		0.5	0	0.5	95.75%	
3		0	0.5	0.5	93.62%	
		0	0.6	0.4		
		0	0.7	0.3		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
4		0.3	0.2	0.5	95.74%	
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		

		0.5	0.2	0.3		
5		0.3	0.2	0.5	95.74%	
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
6	Kennard-Stone	0.4	0	0.6	100%	6.97
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
7		0.5	0	0.5	97.87%	
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
8		0.4	0	0.6	95.74%	
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
9		0.5	0	0.5	95.74%	
		0.5	0.1	0.4		
		0.5	0.2	0.3		

		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
10		0.5	0	0.5	95.74%	
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
11	Modified-k-medoids	0	0.5	0.5	95.74%	6.97
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0.5	0		
12		0	0.1	0.9	93.62%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.4	0.1	0.5		
		0.4	0.2	0.4		

		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
13		0	0.5	0.5	91.49%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0.5	0		
14		0.5	0	0.5	95.74%	
15		0	0.5	0.5	91.49%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.8	0		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.5	0.1		
		0.4	0.6	0		

		0.5	0.5	0		

Table S4 Automated weighting analysis for bioluminescent repression of the bacterium genus *Pseudomonas* data set (Model Dataset 4)

Model	Division method	Best weighting combinations			% Correct predictions (Test set)	Training set range
1	Sorted response	0	0.1	0.9	80.65%	4.0604
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		

		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
2		0	0.1	0.9	80.65%	
		0	0.2	0.8		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.6	0		
		0.5	0	0.5		
3		0	0.1	0.9	87.10%	
		0	0.2	0.8		
		0	0.3	0.7		

		0	0.4	0.6		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
4		0	0.1	0.9	83.87%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		

		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
5		0	0.3	0.7	87.10%	
		0	0.4	0.6		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.4	0.1	0.5		
		0.4	0.2	0.4		

		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
6	Kennard-Stone	0	0.1	0.9	81.25%	4.0604
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		

		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
7		0	0.1	0.9	84.38%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		

		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
8		0	0.1	0.9	78.13%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		

		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
9		0	0.1	0.9	81.25%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		

		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
10		0	0.1	0.9	78.13%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		

		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
11	Modified-k-medoids	0	0.1	0.9	80.65%	4.0604

		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		

		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
12		0.3	0	0.7	83.87%	
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
13		0	0.1	0.9	80.65%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.9	0		

		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.3	0.5		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
14		0	0.1	0.9	80.65%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
15		0	0.1	0.9	87.10%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		

Table S5 Automated weighting analysis for Persistent, bioaccumulative and toxic (PBT) index of chemicals (Model Dataset 5)

Model	Division method	Best weighting combinations			% Correct predictions (Test set)	Training set range
1	Sorted response	0	0.5	0.5	100%	8.1
		0.1	0.5	0.4		
		0.2	0.5	0.3		
		0.3	0.5	0.2		
		0.4	0.5	0.1		
		0.5	0.5	0		
2		0.5	0	0.5	100%	
3		0.5	0	0.5	100%	
4		0	0.5	0.5	97.22%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0.5	0		
5		0	0.1	0.9	88.89%	
		0	0.2	0.8		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		

		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.2	0.5		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.5	0		
6	Kennard-Stone	0.3	0.2	0.5	95.56%	8.1
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
7		0	0.5	0.5	95.56%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		

		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
8		0	0.5	0.5	95.56%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		

		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
9		0	0.5	0.5	95.56%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		

		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
10		0	0.5	0.5	95.56%	
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0.4	0.5		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0.3	0.5		
		0.2	0.4	0.4		
		0.2	0.5	0.3		
		0.2	0.6	0.2		
		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0.2	0.5		
		0.3	0.3	0.4		
		0.3	0.4	0.3		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0.1	0.5		
		0.4	0.2	0.4		
		0.4	0.3	0.3		
		0.4	0.4	0.2		

		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
		0.5	0.3	0.2		
		0.5	0.4	0.1		
		0.5	0.5	0		
11	Modified-k-medoids	0	0.1	0.9	93.18%	7.24
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
12		0	0.1	0.9	86.36%	
		0	0.2	0.8		
		0	0.3	0.7		
		0	0.4	0.6		
		0	0.5	0.5		
		0	0.6	0.4		
		0	0.7	0.3		
		0	0.8	0.2		
		0	0.9	0.1		
		0	1	0		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.1	0.3	0.6		
		0.1	0.5	0.4		
		0.1	0.6	0.3		
		0.1	0.7	0.2		
		0.1	0.8	0.1		
		0.1	0.9	0		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.2	0.5	0.3		
		0.2	0.6	0.2		

		0.2	0.7	0.1		
		0.2	0.8	0		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.3	0.5	0.2		
		0.3	0.6	0.1		
		0.3	0.7	0		
		0.4	0	0.6		
		0.4	0.5	0.1		
		0.4	0.6	0		
		0.5	0	0.5		
		0.5	0.5	0		
13		0	0.1	0.9	93.18%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
		0.5	0.1	0.4		
		0.5	0.2	0.3		
14		0	0.5	0.5	95.45%	
		0.1	0.5	0.4		
		0.2	0.5	0.3		
		0.3	0.5	0.2		
		0.4	0.5	0.1		
		0.5	0.5	0		
15		0	0.1	0.9	93.18%	
		0	0.2	0.8		
		0.1	0	0.9		
		0.1	0.1	0.8		
		0.1	0.2	0.7		
		0.2	0	0.8		
		0.2	0.1	0.7		
		0.2	0.2	0.6		
		0.3	0	0.7		
		0.3	0.1	0.6		
		0.4	0	0.6		
		0.5	0	0.5		
		0.5	0.1	0.4		

		0.5	0.2	0.3		

Table S6 Automated weighting analysis for refractive index of polymers dataset (True external dataset 1)

Model	Combination found with model			% Correct predictions (Test set)	% Correct predictions (True external set)
1	0.5	0	0.5	98.51%	94.90%
2	0	0.5	0.5	97.01%	89.80%
	0.5	0	0.5		91.84%
3	0.5	0	0.5	97.01%	94.90%
4	0.5	0	0.5	97.01%	94.90%
5	0.5	0	0.5	98.51%	98.51%

Table S7 Automated weighting analysis for BACE1 dataset (True external dataset 2)

Model	Combination found with model			% Correct predictions (Test set)	% Correct predictions (True external set)
1	0	0.1	0.9	86.36%	82.35%
	0	0.2	0.8		82.35%
	0	0.3	0.7		76.47%
	0	0.4	0.6		76.47%
	0	0.5	0.5		76.47%
	0.1	0	0.9		82.35%
	0.1	0.1	0.8		82.35%
	0.1	0.2	0.7		76.47%
	0.1	0.3	0.6		76.47%
	0.1	0.4	0.5		76.47%
	0.2	0	0.8		82.35%
	0.2	0.1	0.7		82.35%
	0.2	0.2	0.6		76.47%
	0.2	0.3	0.5		76.47%
	0.3	0	0.7		82.35%
	0.3	0.1	0.6		82.35%
	0.3	0.2	0.5		76.47%
	0.4	0	0.6		82.35%
	0.4	0.1	0.5		76.47%
	0.5	0	0.5		82.35%
2	0	0.1	0.9	91.30%	88.24%

	0	0.2	0.8		88.24%
	0.1	0	0.9		88.24%
	0.1	0.1	0.8		88.24%
	0.2	0	0.8		88.24%
	0.2	0.1	0.7		88.24%
	0.3	0	0.7		88.24%
	0.3	0.1	0.6		88.24%
	0.4	0	0.6		88.24%
	0.5	0	0.5		88.24%
3	0	0.1	0.9	95.65%	88.24%
	0	0.2	0.8		88.24%
	0	0.3	0.7		88.24%
	0	0.4	0.6		88.24%
	0	0.5	0.5		88.24%
	0.1	0	0.9		88.24%
	0.1	0.1	0.8		88.24%
	0.1	0.2	0.7		88.24%
	0.1	0.3	0.6		88.24%
	0.1	0.4	0.5		88.24%
	0.2	0	0.8		88.24%
	0.2	0.1	0.7		88.24%
	0.2	0.2	0.6		88.24%
	0.2	0.3	0.5		88.24%
	0.3	0	0.7		88.24%
	0.3	0.1	0.6		88.24%
	0.3	0.2	0.5		88.24%
	0.4	0	0.6		88.24%
	0.4	0.1	0.5		88.24%
	0.5	0	0.5		88.24%
4	0	0.1	0.9	91.30%	88.24%
	0	0.2	0.8		88.24%
	0	0.3	0.7		88.24%
	0	0.4	0.6		88.24%
	0	0.5	0.5		88.24%
	0	0.6	0.4		88.24%
	0	0.7	0.3		88.24%
	0	0.8	0.2		88.24%
	0	0.9	0.1		82.35%
	0	1	0		82.35%
	0.1	0	0.9		82.35%
	0.1	0.1	0.8		82.35%
	0.1	0.2	0.7		82.35%
	0.1	0.3	0.6		82.35%

	0.1	0.4	0.5		82.35%
	0.1	0.5	0.4		82.35%
	0.1	0.6	0.3		82.35%
	0.1	0.7	0.2		82.35%
	0.1	0.8	0.1		82.35%
	0.1	0.9	0		82.35%
	0.2	0	0.8		82.35%
	0.2	0.1	0.7		82.35%
	0.2	0.2	0.6		82.35%
	0.2	0.3	0.5		82.35%
	0.2	0.4	0.4		82.35%
	0.2	0.5	0.3		82.35%
	0.2	0.6	0.2		82.35%
	0.2	0.7	0.1		82.35%
	0.2	0.8	0		82.35%
	0.3	0	0.7		88.24%
	0.3	0.1	0.6		88.24%
	0.3	0.2	0.5		88.24%
	0.3	0.3	0.4		88.24%
	0.3	0.4	0.3		88.24%
	0.3	0.5	0.2		88.24%
	0.3	0.6	0.1		88.24%
	0.3	0.7	0		88.24%
	0.4	0	0.6		88.24%
	0.4	0.1	0.5		88.24%
	0.4	0.2	0.4		88.24%
	0.4	0.3	0.3		88.24%
	0.4	0.4	0.2		88.24%
	0.4	0.5	0.1		88.24%
	0.4	0.6	0		88.24%
	0.5	0	0.5		88.24%
	0.5	0.1	0.4		88.24%
	0.5	0.2	0.3		88.24%
	0.5	0.3	0.2		88.24%
	0.5	0.4	0.1		82.35%
	0.5	0.5	0		82.35%
5	0	0.1	0.9	91.30%	82.35%
	0	0.2	0.8		82.35%
	0	0.3	0.7		82.35%
	0	0.4	0.6		82.35%
	0	0.5	0.5		82.35%
	0.1	0	0.9		82.35%
	0.1	0.1	0.8		82.35%

	0.1	0.2	0.7		82.35%
	0.1	0.3	0.6		82.35%
	0.1	0.4	0.5		82.35%
	0.2	0	0.8		82.35%
	0.2	0.1	0.7		82.35%
	0.2	0.2	0.6		82.35%
	0.2	0.3	0.5		82.35%
	0.3	0	0.7		82.35%
	0.3	0.1	0.6		82.35%
	0.3	0.2	0.5		82.35%
	0.4	0	0.6		82.35%
	0.4	0.1	0.5		82.35%
	0.5	0	0.5		82.35%

Table S8 Automated weighting analysis for glass transition temperature of polymers dataset (True external dataset 3)

Model	**Combination found with model**			**% Correct predictions (Test set)**	**% Correct predictions (True external set)**
1	0	0.1	0.9	86.54%	68.42%
	0	0.2	0.8		68.42%
	0.1	0	0.9		68.42%
	0.1	0.1	0.8		68.42%
	0.2	0	0.8		68.42%
	0.2	0.1	0.7		68.42%
	0.3	0	0.7		68.42%
	0.3	0.1	0.6		68.42%
	0.4	0	0.6		68.42%
	0.5	0	0.5		68.42%
2	0	0.1	0.9	88.46%	84.21%
	0	0.2	0.8		84.21%
	0.1	0	0.9		84.21%
	0.1	0.1	0.8		84.21%
	0.2	0	0.8		84.21%
	0.2	0.1	0.7		84.21%
	0.3	0	0.7		84.21%
	0.3	0.1	0.6		84.21%
	0.4	0	0.6		84.21%
	0.5	0	0.5		84.21%

3	0	0.1	0.9	92.31%	86.84%
	0	0.2	0.8		86.84%
	0.1	0	0.9		86.84%
	0.1	0.1	0.8		86.84%
	0.2	0	0.8		86.84%
	0.2	0.1	0.7		86.84%
4	0	0.1	0.9	94.23%	78.95%
	0	0.2	0.8		78.95%
	0.1	0	0.9		78.95%
	0.1	0.1	0.8		78.95%
	0.2	0	0.8		78.95%
5	0	0.1	0.9	86.54%	78.95%
	0	0.2	0.8		78.95%
	0.1	0	0.9		78.95%
	0.1	0.1	0.8		78.95%
	0.2	0	0.8		78.95%
	0.2	0.1	0.7		81.58%

Table S9 Automated weighting analysis for sweetness potency of organic molecules (True external dataset 4)

Model	Combination found with model			% Correct predictions (Test set)	% Correct predictions (True external set)
1	0	0.5	0.5	95%	80.00%
	0	0.6	0.4		80.00%
	0	0.7	0.3		80.00%
	0	0.8	0.2		80.00%
	0	0.9	0.1		80.00%
	0	1	0		80.00%
	0.1	0.4	0.5		80.00%
	0.1	0.5	0.4		80.00%
	0.1	0.6	0.3		80.00%
	0.1	0.7	0.2		80.00%
	0.1	0.8	0.1		80.00%
	0.1	0.9	0		80.00%
	0.2	0.3	0.5		80.00%
	0.2	0.4	0.4		80.00%
	0.2	0.5	0.3		80.00%
	0.2	0.6	0.2		80.00%
	0.2	0.7	0.1		80.00%
	0.2	0.8	0		80.00%
2	0	0.1	0.9	95%	83.33%
	0	0.2	0.8		83.33%
	0.1	0	0.9		83.33%
	0.1	0.1	0.8		83.33%
	0.2	0	0.8		83.33%
	0.2	0.1	0.7		83.33%
	0.3	0	0.7		83.33%
	0.3	0.1	0.6		83.33%
	0.4	0	0.6		83.33%
	0.5	0	0.5		83.33%
3	0	0.5	0.5	80%	75%
	0.1	0.5	0.4		75%
	0.2	0.5	0.3		75%
4	0	0.5	0.5	93.75%	73.33%
	0	0.6	0.4		73.33%
	0	0.7	0.3		73.33%
	0	0.8	0.2		73.33%
	0	0.9	0.1		73.33%

	0	1	0		73.33%
	0.1	0.4	0.5		73.33%
	0.1	0.5	0.4		73.33%
	0.1	0.6	0.3		73.33%
	0.1	0.7	0.2		73.33%
	0.1	0.8	0.1		73.33%
	0.1	0.9	0		73.33%
	0.2	0.3	0.5		73.33%
	0.2	0.4	0.4		73.33%
	0.2	0.5	0.3		73.33%
	0.2	0.6	0.2		73.33%
	0.2	0.7	0.1		73.33%
	0.2	0.8	0		73.33%
	0.3	0.2	0.5		73.33%
	0.3	0.3	0.4		73.33%
	0.3	0.4	0.3		73.33%
	0.3	0.5	0.2		73.33%
	0.3	0.6	0.1		73.33%
	0.3	0.7	0		73.33%
	0.4	0.1	0.5		73.33%
	0.4	0.2	0.4		73.33%
	0.4	0.3	0.3		73.33%
	0.4	0.4	0.2		73.33%
	0.4	0.5	0.1		73.33%
	0.4	0.6	0		73.33%
	0.5	0	0.5		73.33%
	0.5	0.1	0.4		73.33%
	0.5	0.2	0.3		73.33%
	0.5	0.3	0.2		73.33%
	0.5	0.4	0.1		73.33%
	0.5	0.5	0		73.33%
5	0	0.1	0.9	92.5%	86.67%
	0	0.2	0.8		86.67%
	0	0.3	0.7		86.67%
	0	0.4	0.6		86.67%
	0	0.5	0.5		86.67%
	0	0.6	0.4		86.67%
	0	0.7	0.3		86.67%
	0	0.8	0.2		86.67%
	0	0.9	0.1		86.67%
	0	1	0		86.67%
	0.1	0	0.9		86.67%
	0.1	0.1	0.8		86.67%

	0.1	0.2	0.7		86.67%
	0.1	0.3	0.6		86.67%
	0.1	0.4	0.5		86.67%
	0.1	0.5	0.4		86.67%
	0.1	0.6	0.3		86.67%
	0.1	0.7	0.2		86.67%
	0.1	0.8	0.1		86.67%
	0.1	0.9	0		86.67%
	0.2	0	0.8		86.67%
	0.2	0.1	0.7		86.67%
	0.2	0.2	0.6		86.67%
	0.2	0.3	0.5		86.67%
	0.2	0.4	0.4		86.67%
	0.2	0.5	0.3		86.67%
	0.2	0.6	0.2		86.67%
	0.2	0.7	0.1		86.67%
	0.2	0.8	0		86.67%
	0.3	0	0.7		86.67%
	0.3	0.1	0.6		86.67%
	0.3	0.2	0.5		86.67%
	0.3	0.3	0.4		86.67%
	0.3	0.4	0.3		86.67%
	0.3	0.5	0.2		86.67%
	0.3	0.6	0.1		86.67%
	0.3	0.7	0		86.67%
	0.4	0	0.6		86.67%
	0.4	0.1	0.5		86.67%
	0.4	0.2	0.4		86.67%
	0.4	0.3	0.3		86.67%
	0.4	0.4	0.2		86.67%
	0.4	0.5	0.1		86.67%
	0.4	0.6	0		86.67%
	0.5	0	0.5		86.67%
	0.5	0.1	0.4		86.67%
	0.5	0.2	0.3		86.67%
	0.5	0.3	0.2		86.67%
	0.5	0.4	0.1		86.67%
	0.5	0.5	0		86.67%