

Table S4. Summary of the PCA-analysis of the descriptors divided by the molecular weight, describing the eigenvalues of the covariance matrix, the total variance explained (cumulative R²) and the predictive ability (cumulative Q²).

Principal Component	Eigenvalue	Cumulative R ²	Cumulative Q ²
1	73.7	0.396	0.371
2	41.8	0.621	0.596
3	12.7	0.689	0.655
4	8.28	0.734	0.678
5	7.95	0.777	0.715
6	6.27	0.810	0.749
7	4.44	0.834	0.771
8	3.18	0.851	0.781
9	2.75	0.866	0.792
10	2.53	0.880	0.803
11	2.08	0.891	0.807
12	1.62	0.900	0.803
13	1.44	0.907	0.807