Supporting Information

High-Throughput Screening to Identify Chemical Cardiotoxic Potential

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Supplementary File 1:

Supplementary File 2 (xlsx):

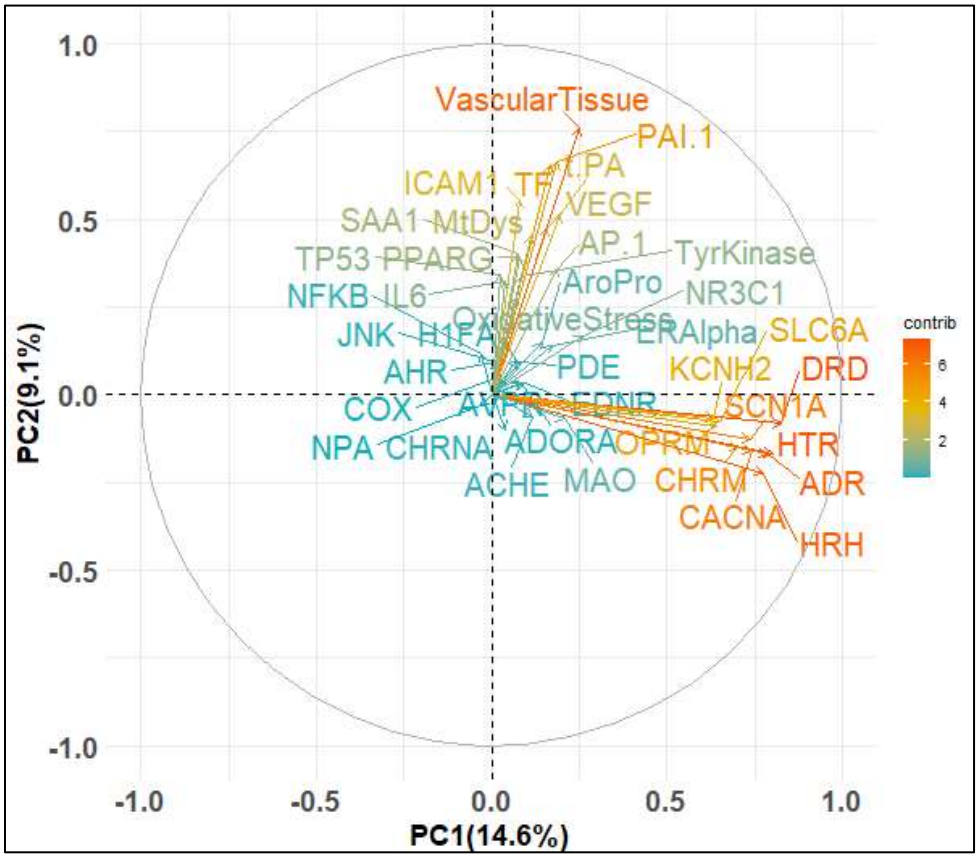

Figure S1. Vectors on the PCA plot indicate the relative influence of each slice on the plot of PC1 vs PC2.

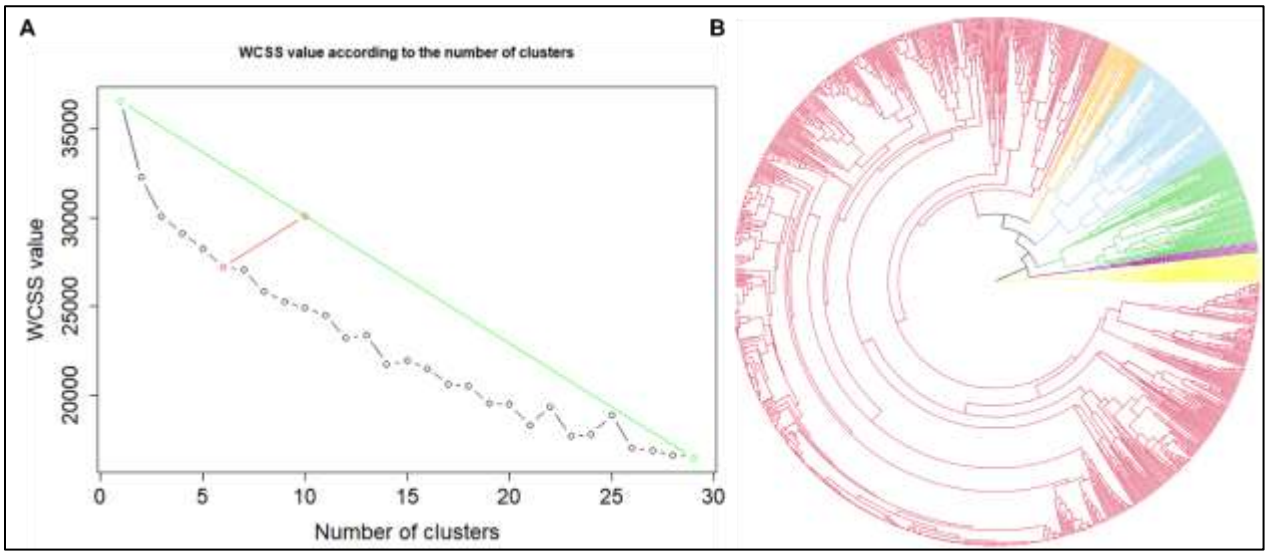

Figure S2. (A) Optimum number of clusters as obtained by Elbow method. (B) Overview of the cluster structure obtained by hierarchical clustering of the compounds.

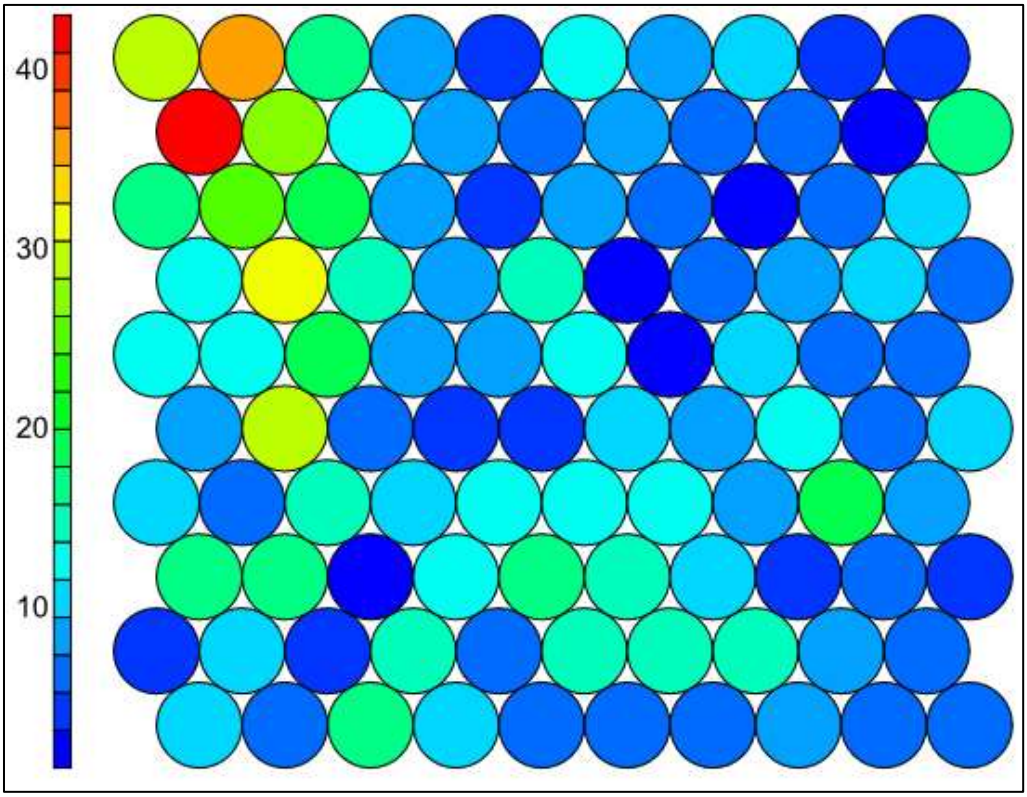

Figure S3. Structure based SOM on 1095 chemicals obtained from CardioToxPi analysis, color represents the chemical count by cluster (scale on left). 100 clusters are included in total.

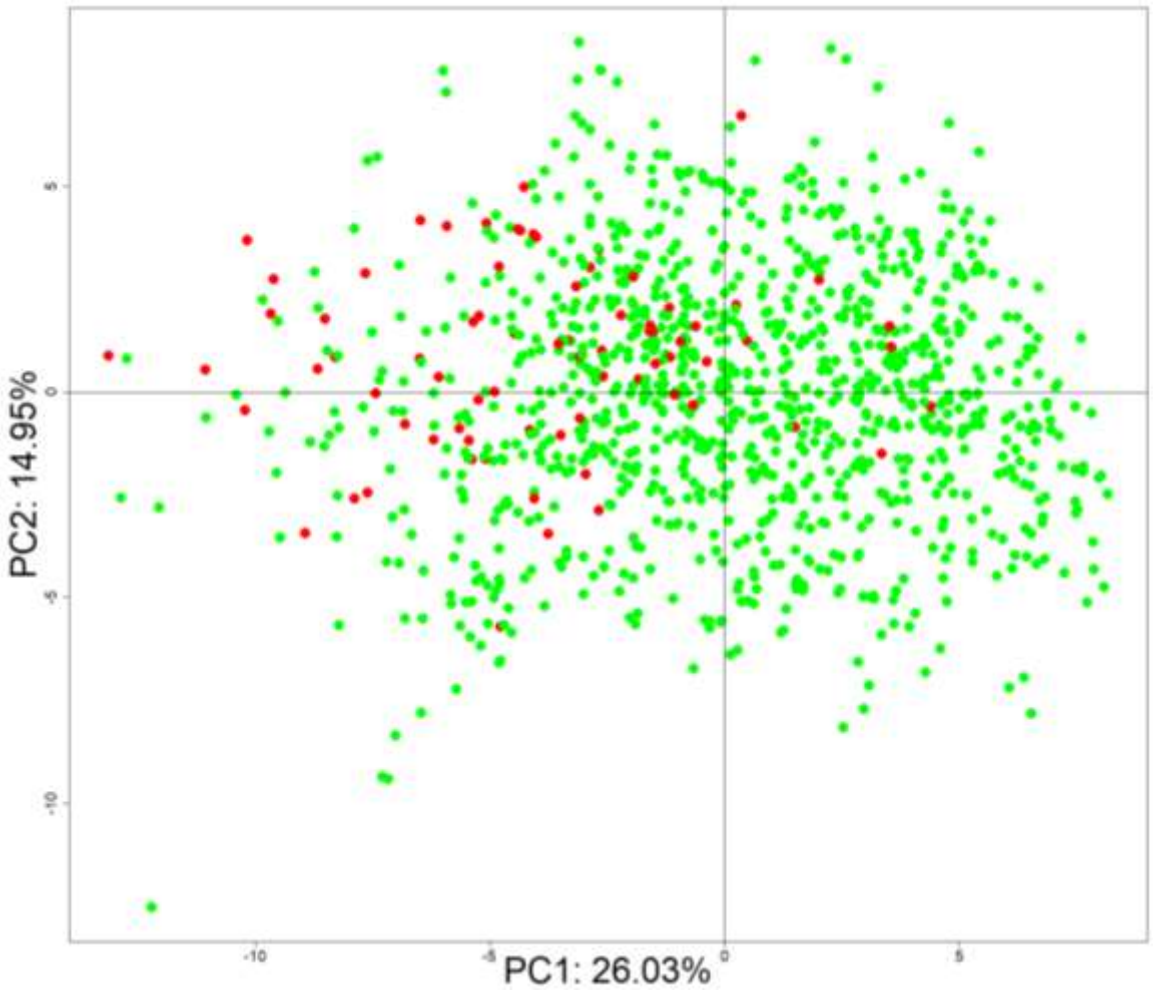

Figure S4. Principal component analysis of the 1111 chemicals obtained from CardioToxPi results, using the set of selected structural descriptors. The first component explains 26.03 % of the descriptor variability and the second 14.95 %. Chemicals are colored based on their activity in green for inactive chemicals, while red for active.

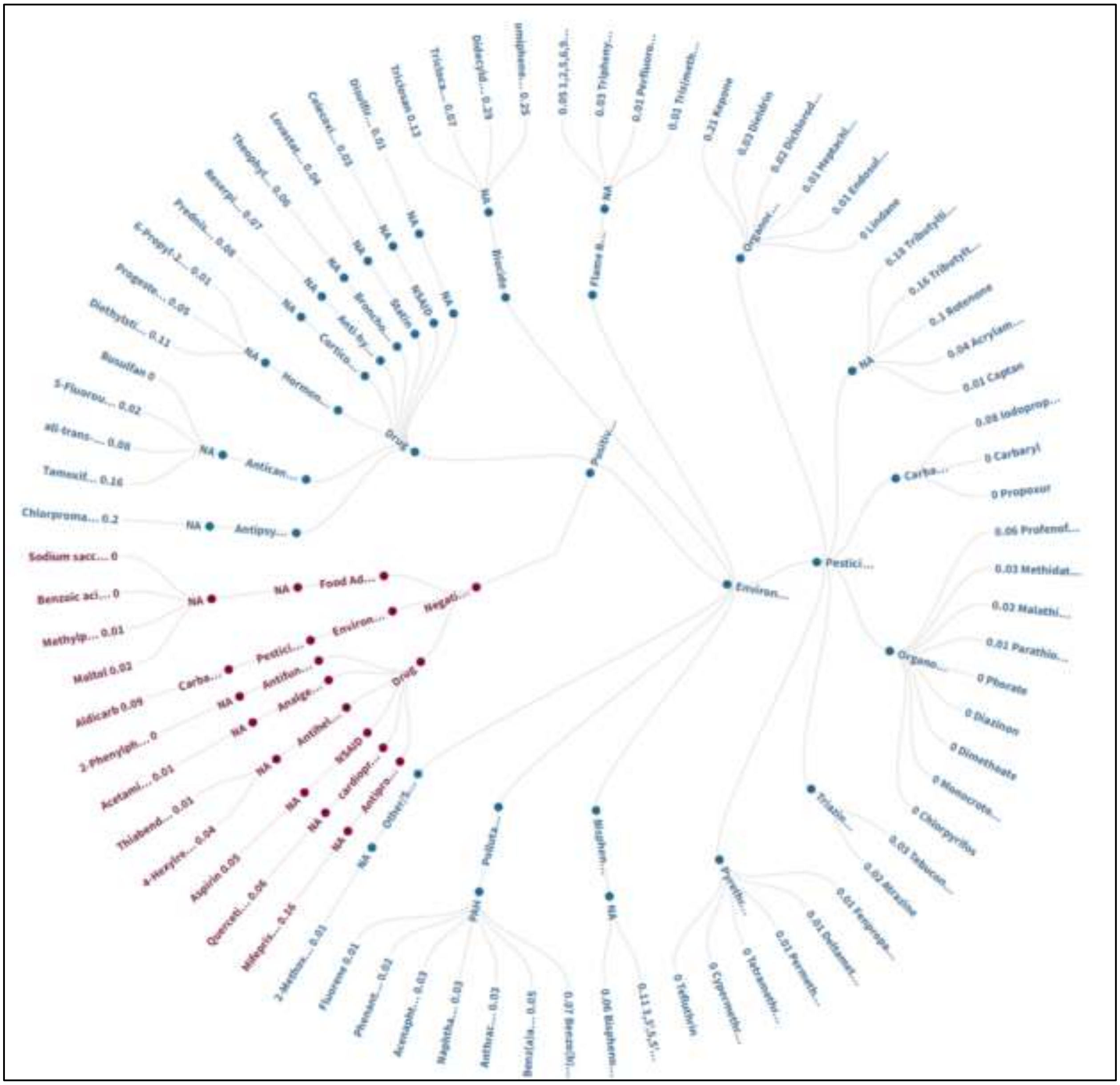

Figure S5: Drugs and environmental chemicals with reference literature data for positive and negative cardiotoxic effects, mapped to the CardioToxPi dataset. The number on the outer edges shows the individual CardioToxPi scores of the chemicals.