

Supporting Information

High-Throughput Screening to Identify Chemical Cardiotoxic Potential

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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.

Supplementary File 2 (xlsx):

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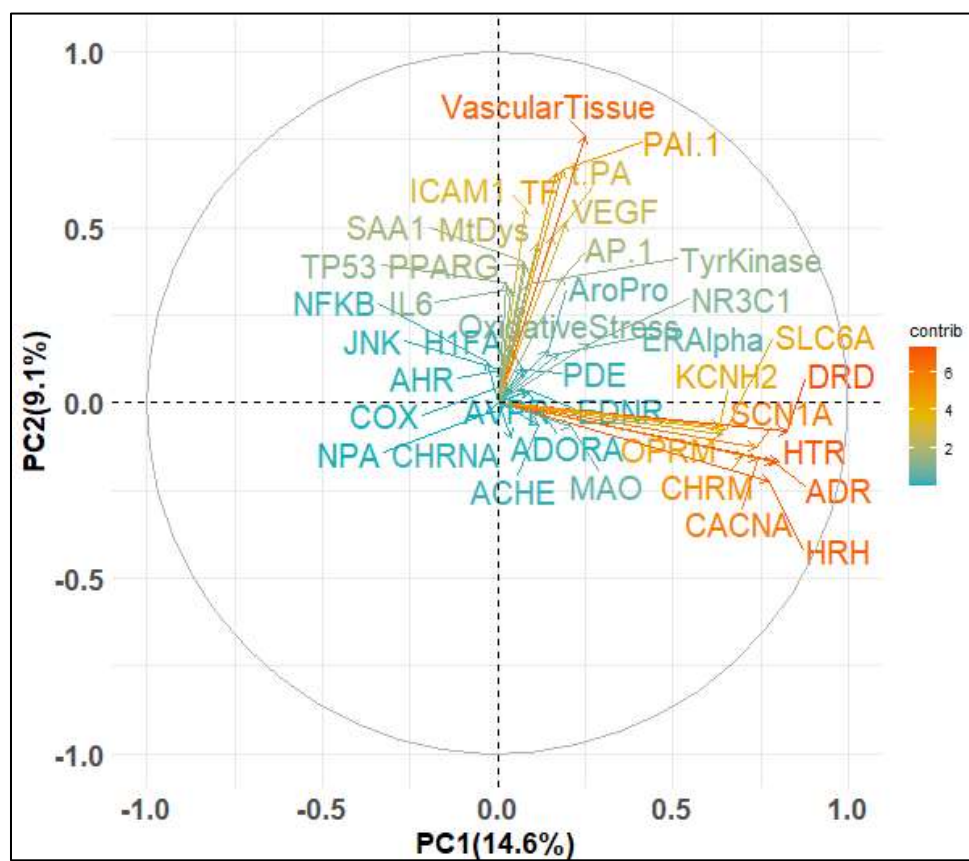


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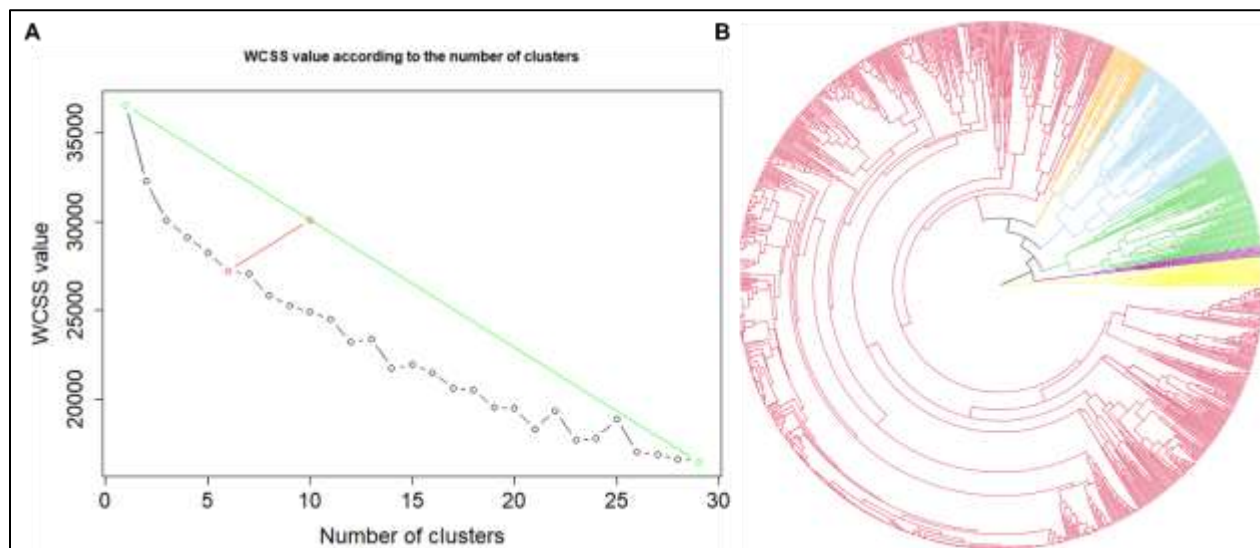


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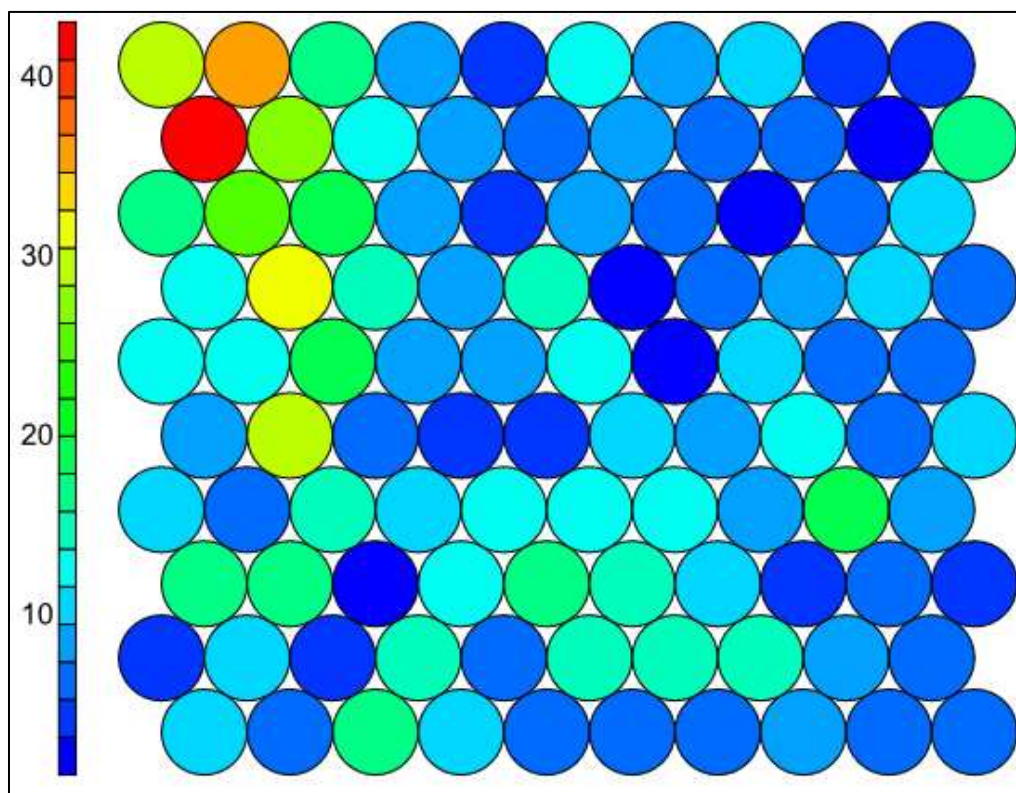


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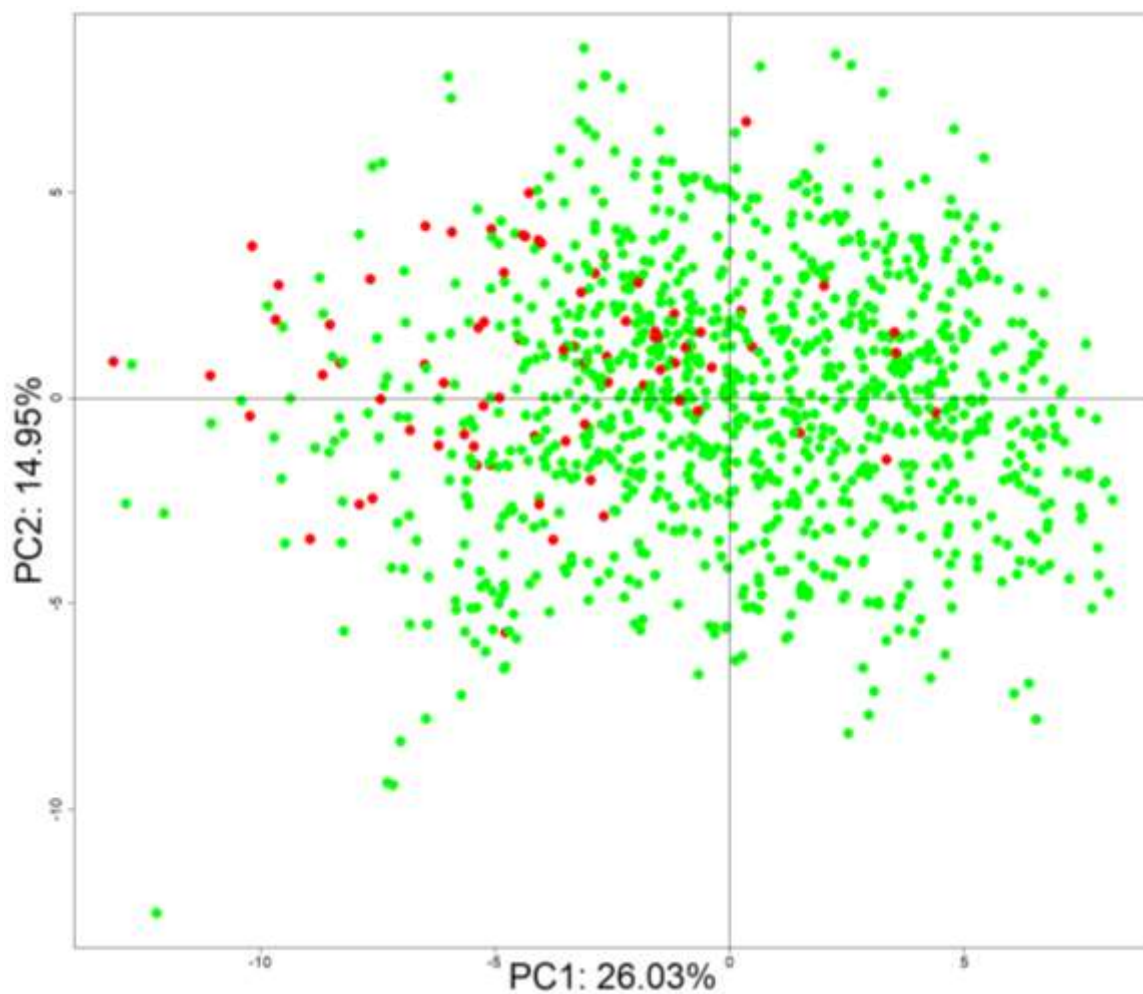


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