■ Electronic Suplimentary Information (ESI)

Probabilistic Diagram for Designing Chemicals with Reduced Potency to Incur Cytotoxicity

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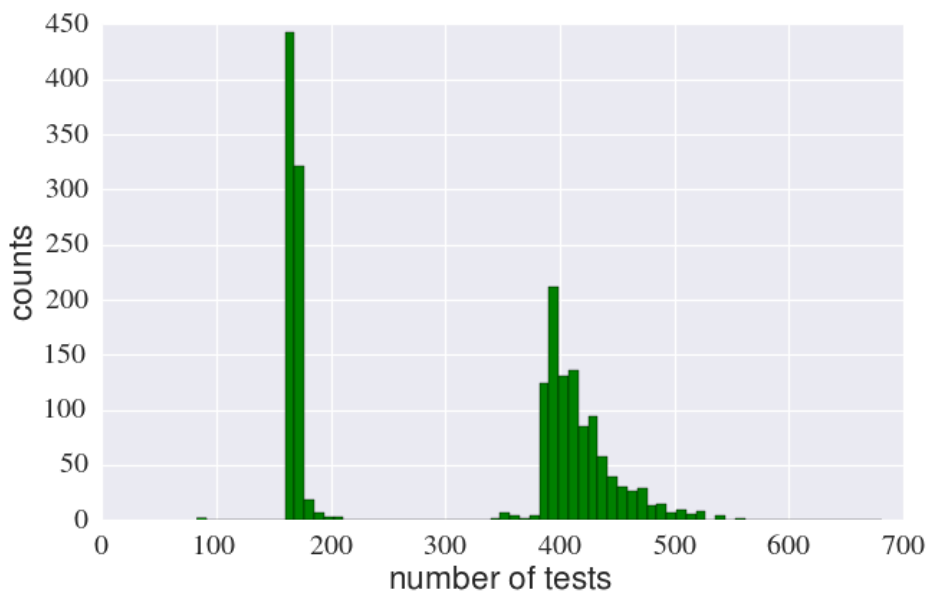
1   Distribution for the Number of Tests

Figure S 1: Distribution for the number of tests for chemicals in ToxCast data set

The chemicals that have been tested more than 300 assays were chosen for this study.
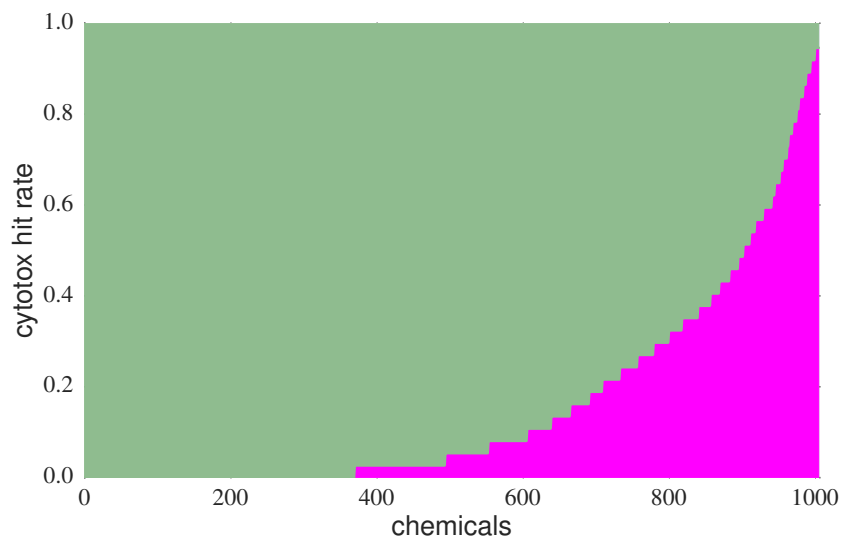
2   Cytotoxicity Hitrate Plot

Figure S 2: Hit rate plot for cytotoxity assays. Green zone represents negative test outcomes and pink zone represents positive test outcomes.

3   Histograms for the Training Set of the Chemicals

(a) eletron affinity

(b) electrophilicity

(c) polarizability

(d) softness

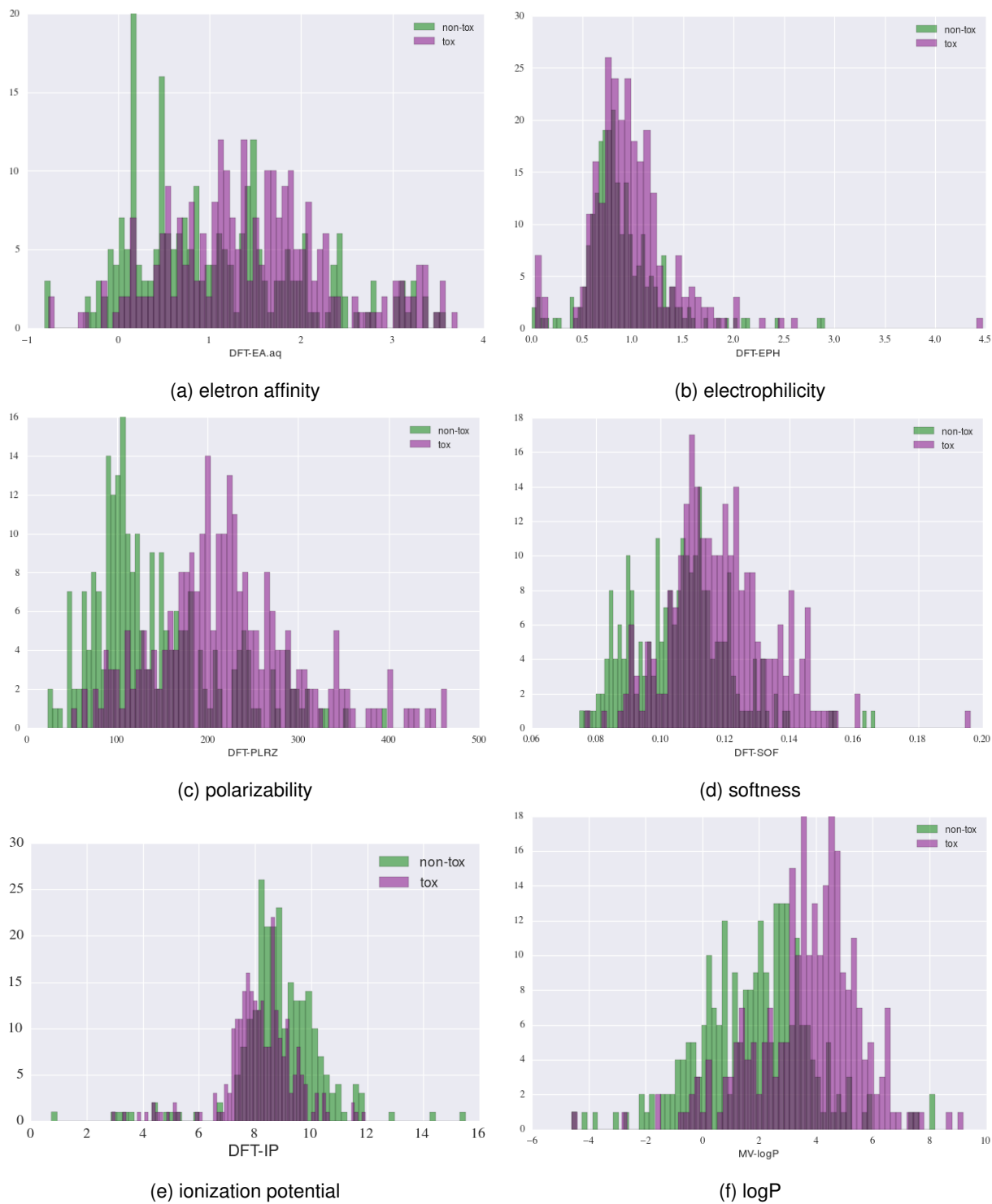(e) ionization potential

(f) logP

Figure S 3: Histograms for the training set (50% of the total chemicals). Color coding : green – non-toxic (inactive) chemicals. purple – toxic (active) chemicals.