**Supporting information:**

**Benchmarks for interpretation of QSAR models**

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Table S1. Correlations between count of patterns of interest for molecules of each regression data set and counts of the most common chemical elements.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Dataset | Pattern 1 (SMARTS) | Pattern 2 (SMARTS) | | | | | |
| [C,c] | [O,o] | [S,s] | [N,n] | Cl | Br |
| N | [N,n] | 0.09 | -0.13 | 0.07 | 1 | -0.02 | -0.04 |
| N-O | [N,n] | 0.09 | 0.02 | 0.02 | 1 | -0.04 | -0.07 |
| [O,o] | 0.06 | 1 | 0.07 | 0.02 | -0.1 | -0.04 |
| N+O | [N,n] | 0.23 | 1 | 0.1 | 1 | -0.11 | 0.0 |
| Amide | NC=O | 0.09 | 0.3 | 0.11 | 0.25 | 0.04 | 0.02 |

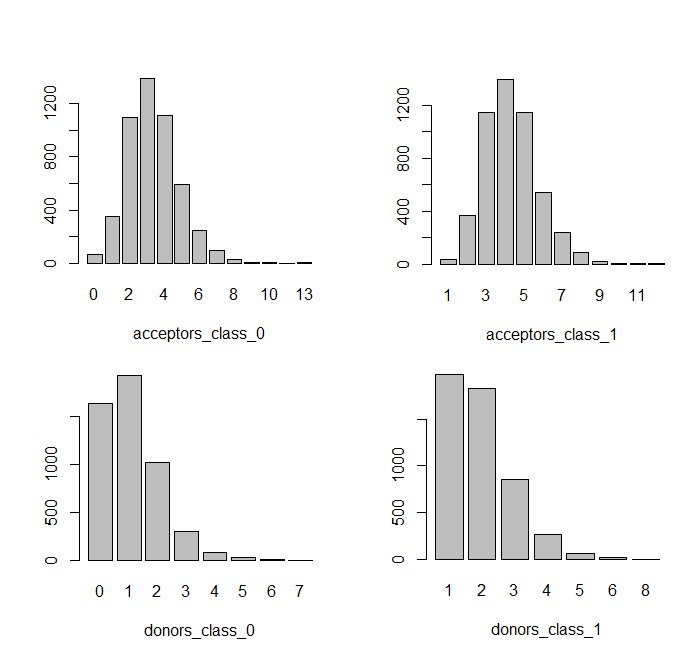


Figure S1. Class-wise distributions of hydrogen bond donors and acceptors for the pharmacophore data set

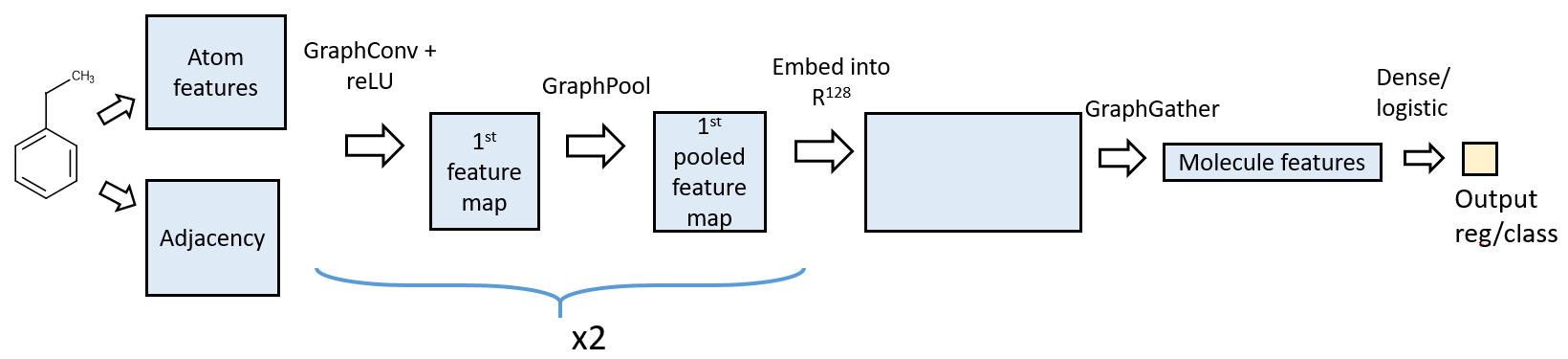


Figure S2. Architecture of Graph convolutional network

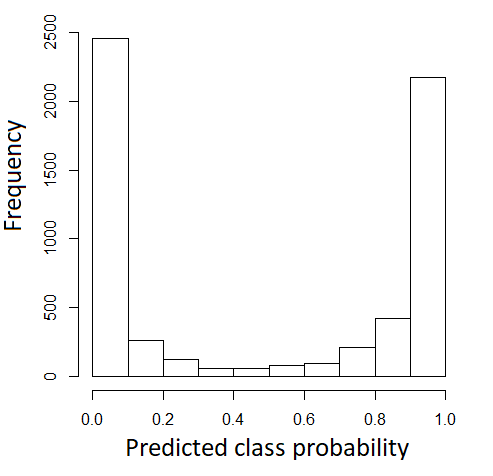


Figure S3. Distribution of predicted class probabilities by GC model for the pharmacophore data set