Electronic Supplementary Information

S1: The training set, the test set, external test set and the deleted compound. The IC_{50} (LXRα), IC_{50} (LXRβ), SR, and classification values were given.

S2: The S-cluster results.

S3: The detailed results of Pearson correlation analysis for MOE descriptors.

S4: Table S1 Cross-validation results of 16 models derived from structural fingerprints.

Table S2 Statistics of the typical privileged fragments and unprivileged fragments.

Fig. S1 A: privileged fragments for selective LXRβ agonists (PS1~20). B: Unprivileged fragments for selective LXRβ agonists (NS1~20).

S5: The performance of the ensemble classifier, Adaboost, LibD3C, and random forest.

S6: The usage of LIBSVM for building SVM-PaDEL model.