Supporting Information

Annotation of Allosteric Compounds to Enhance Bioactivity Modeling for Class A GPCRs

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Figure S1: Physicochemical properties of orthosteric and allosteric compounds in ChEMBL per protein family (png)

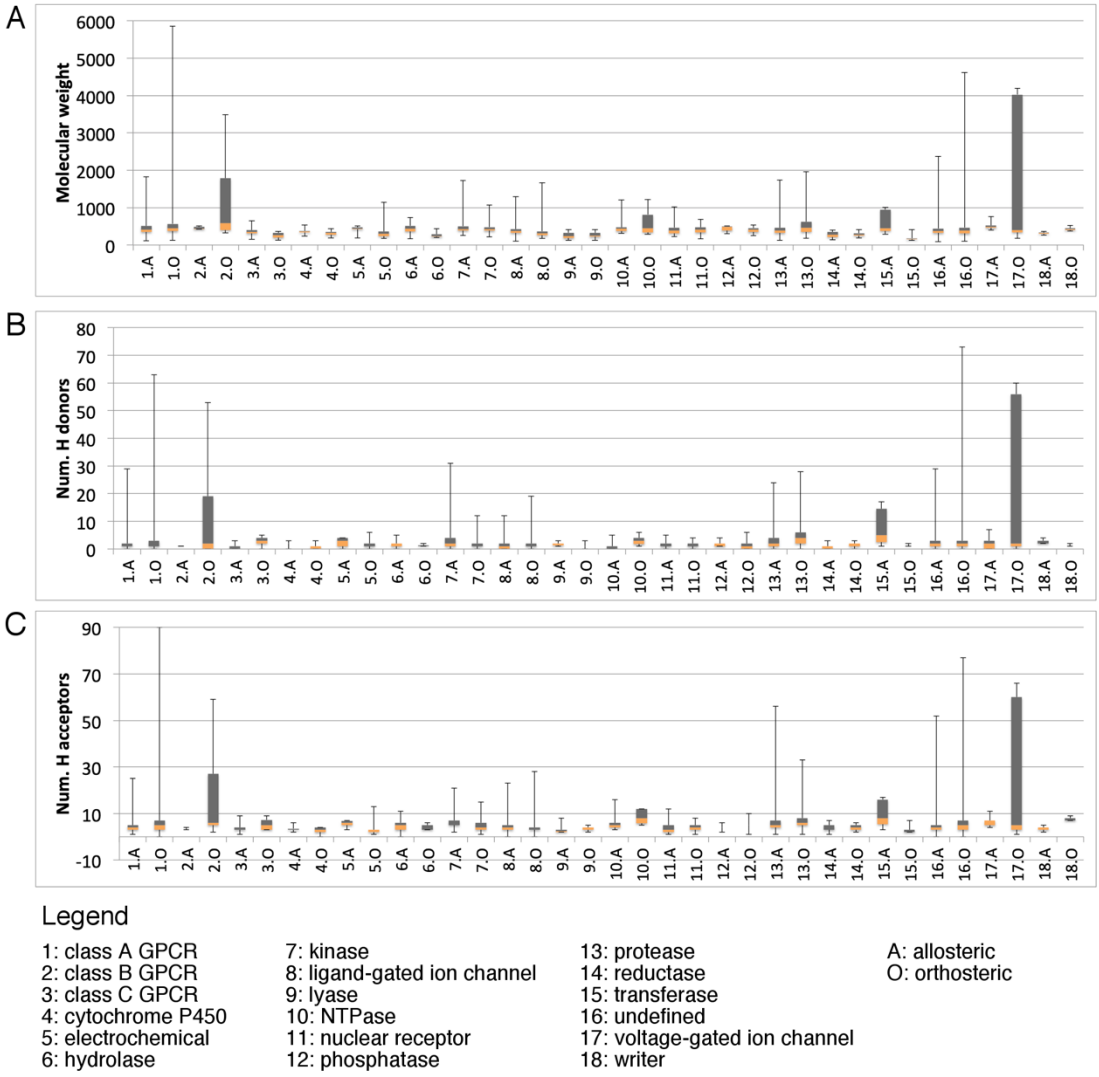

Table S2: Performance of bioactivity models for orthosteric compounds (xlsx)

Table S3: Keywords used in text mining (xlsx)

Protocol S4: Pipeline Pilot protocol for text mining (ppxml)

Dataset S5: Compound dataset, including binding type annotation (tsv)

Available at DOI: http://dx.doi.org/10.4121/uuid:de9e9805-916f-47e5-8e72-323f675d5d5a

Data S6: Compound descriptors (tsv)

Available at DOI: http://dx.doi.org/10.4121/uuid:5738caea-2390-4dc7-9830-8d9644232144

Script S7: Python script to run Convolutional Deep Neural Networks and Random Forest models (py)