Supporting Information for:

Between Descriptors and Properties: Understanding the Ligand Efficiency Trends for GPCR and Kinase Structure Activity Data Sets

Jaroslaw Polanski[a]*, Aleksandra Tkocz[a]

[a]*Institute of Chemistry, University of Silesia, 9 Szkolna Street, 40-006 Katowice, Poland*

Corresponding Author

*polanski@us.edu.pl

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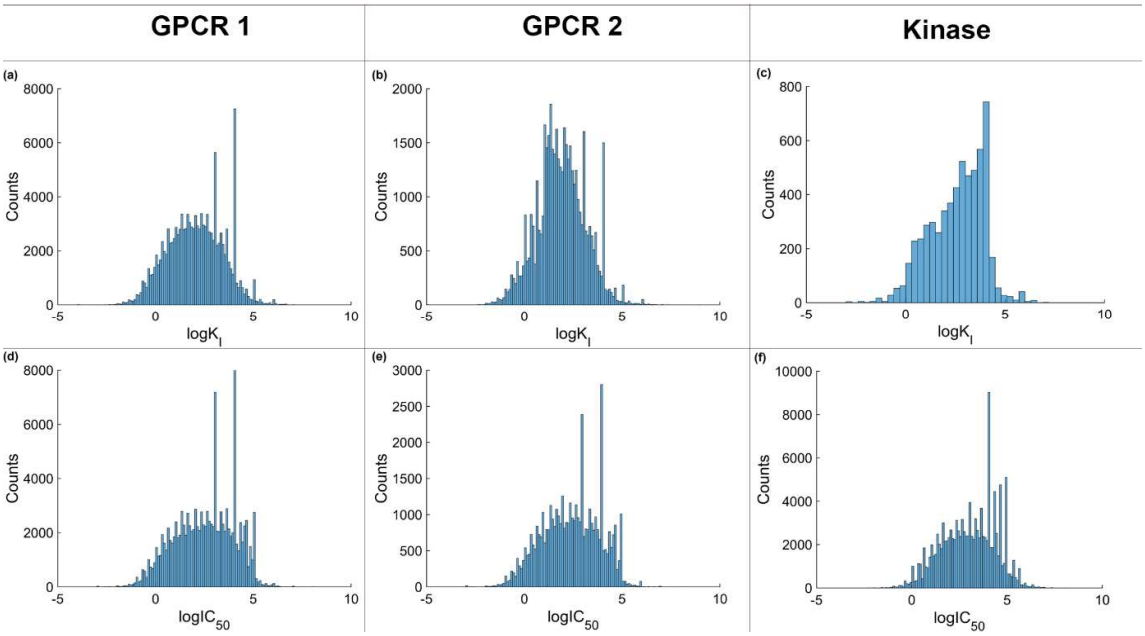


FIGURE S2. Distribution of MW for K_i **(a-c)** and IC_{50} **(d-f)** subdata.

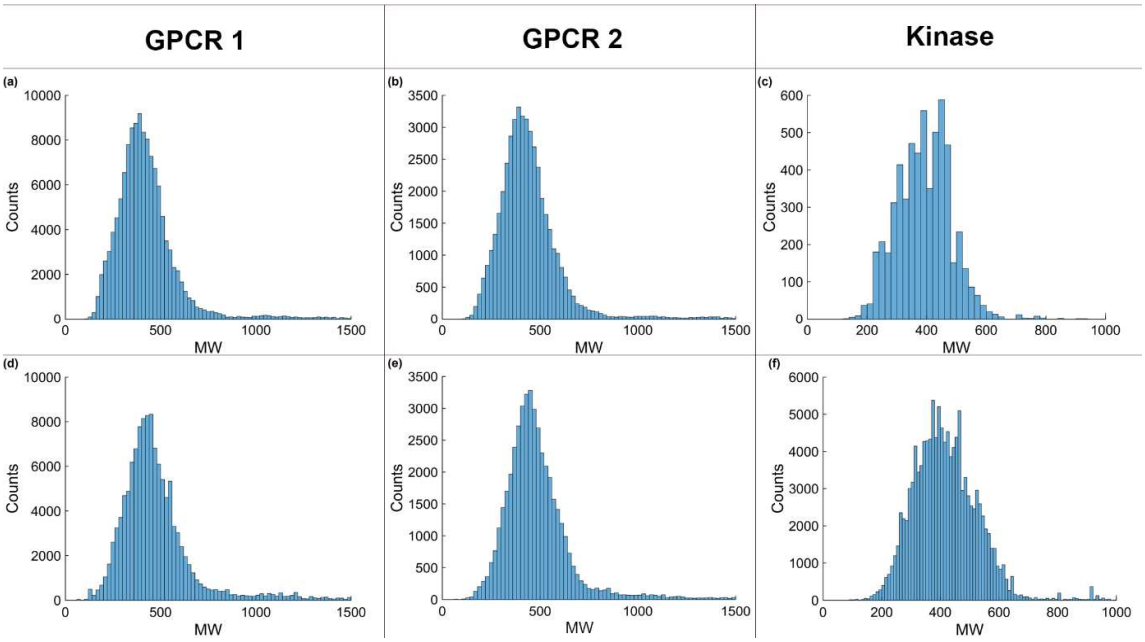


FIGURE S3. Distribution of HAC for K_i **(a-c)** and IC_{50} **(d-f)** subdata.

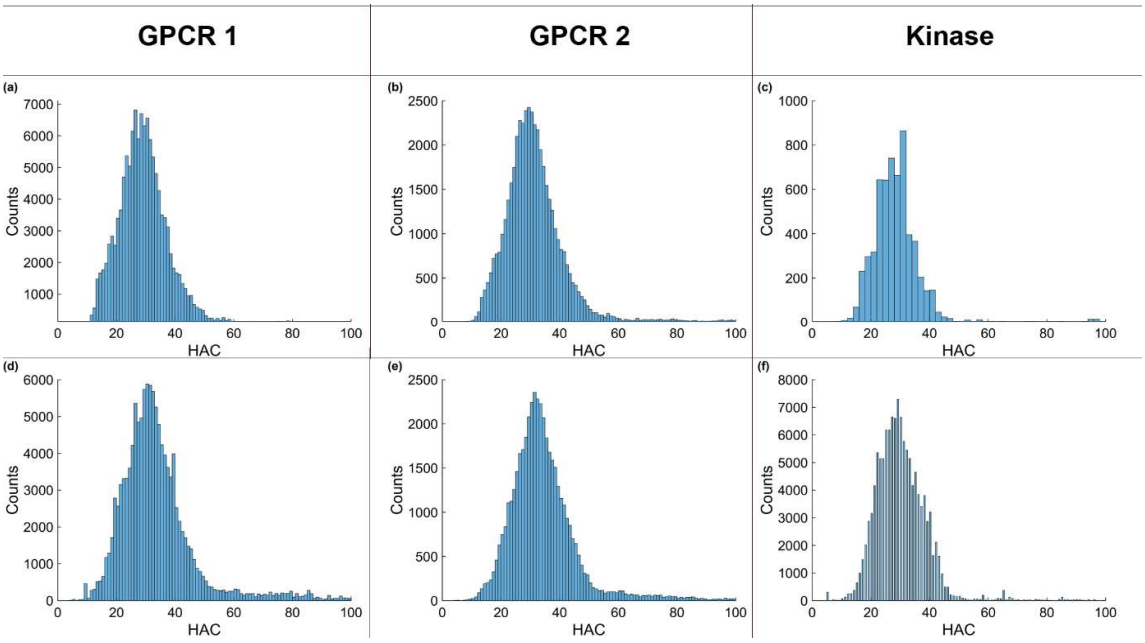


FIGURE S4. Variable distribution for 5HT2A subdata: **a)** $\log K_i$ (GPCR 1) , **b)** MW (GPCR 1), **c)** HAC (GPCR 1), **d)** $\log K_i$ (GPCR 2), **e)** MW (GPCR 2), **f)** HAC (GPCR 2), **g)** $\log IC_{50}$ (GPCR 1), **h)** MW (GPCR 1), **i)** HAC (GPCR 1), **j)** $\log IC_{50}$ (GPCR 2), **k)** MW (GPCR 2), **l)** HAC (GPCR 2).

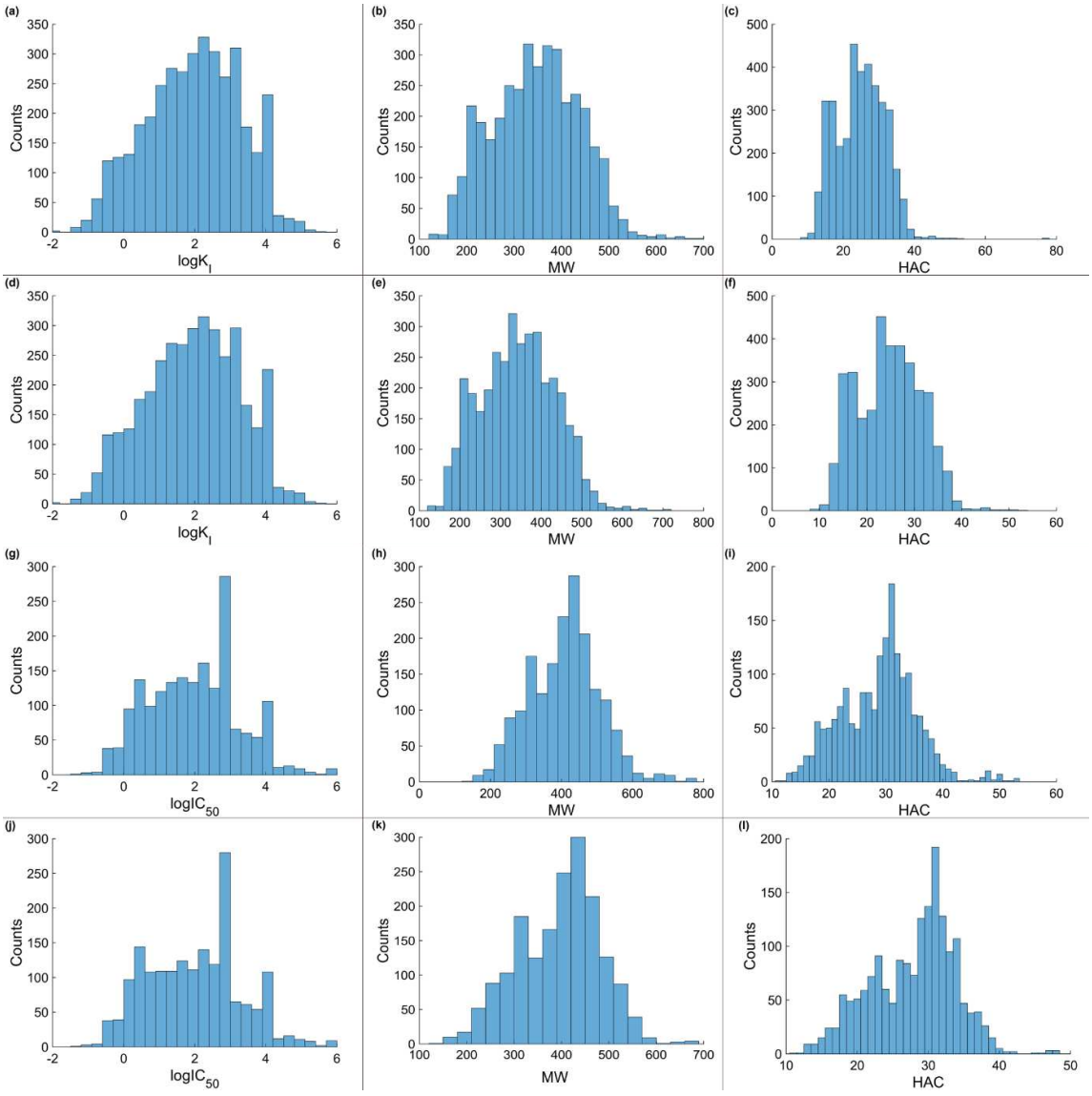


FIGURE S5. Variable distribution for 5HT2B K_i (a-f) and IC_{50} (g-l) subdata **a)** $logK_i$ (GPCR 1), **b)** MW (GPCR 1), **c)** HAC (GPCR 1), **d)** $logK_i$ (GPCR 2), **e)** MW (GPCR 2), **f)** HAC (GPCR 2), **g)** $logIC_{50}$ (GPCR 1), **h)** MW (GPCR 1), **i)** HAC (GPCR 1), **j)** $logIC_{50}$ (GPCR 2) , **k)** MW (GPCR 2), **l)** HAC (GPCR 2).

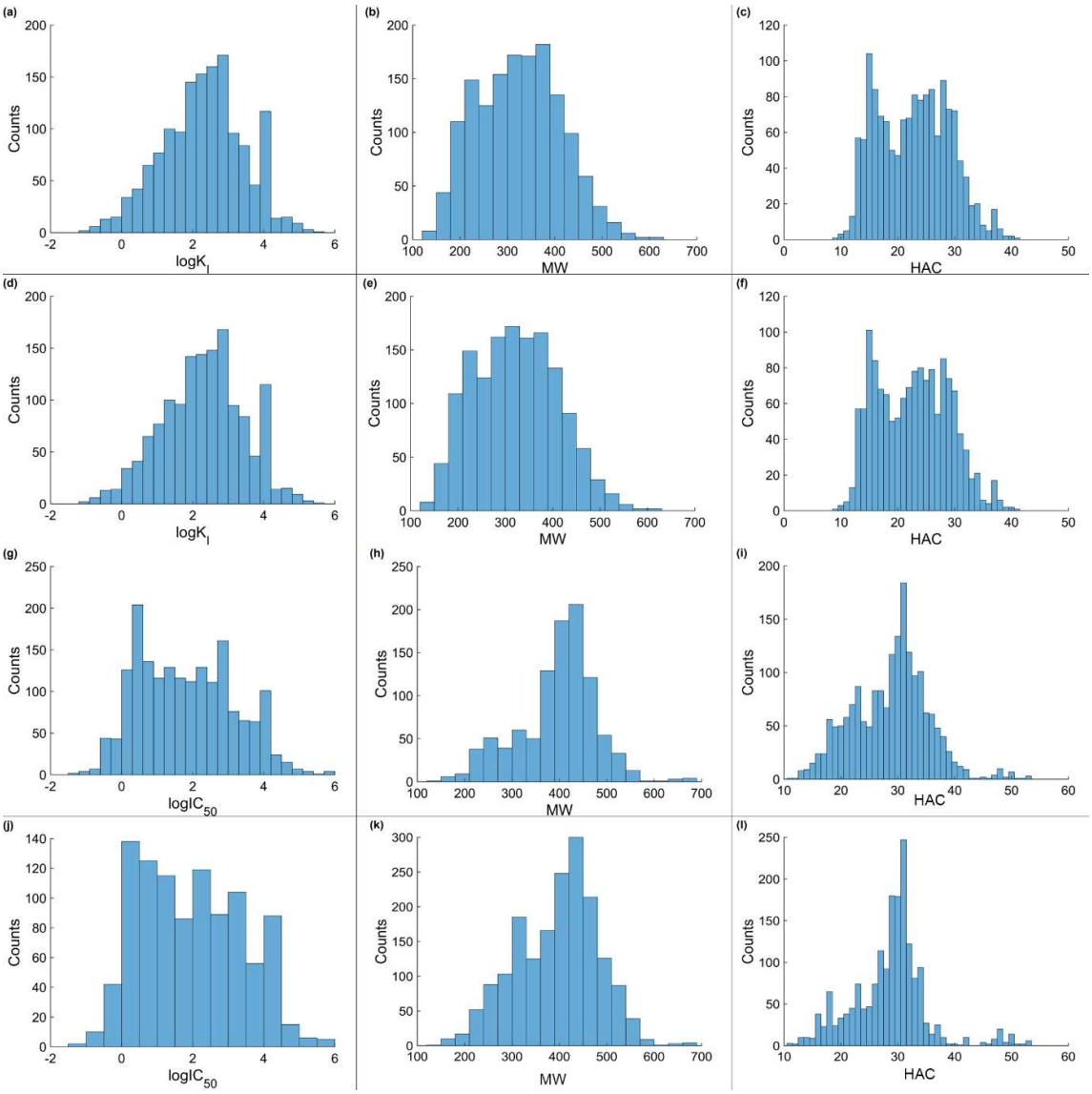
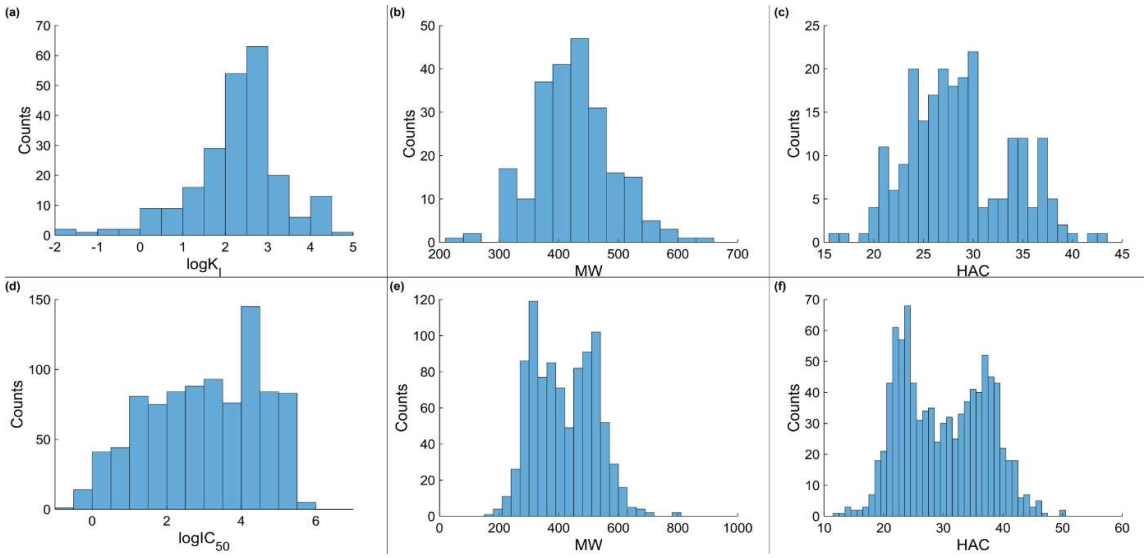


FIGURE S6. Variable distribution for Abl1 K_i (a-c) and IC_{50} (d-f) subdata **a)** $logK_i$, **b)** MW, **c)** HAC, **d)** $logIC_{50}$, **e)** MW, **f)** HAC.



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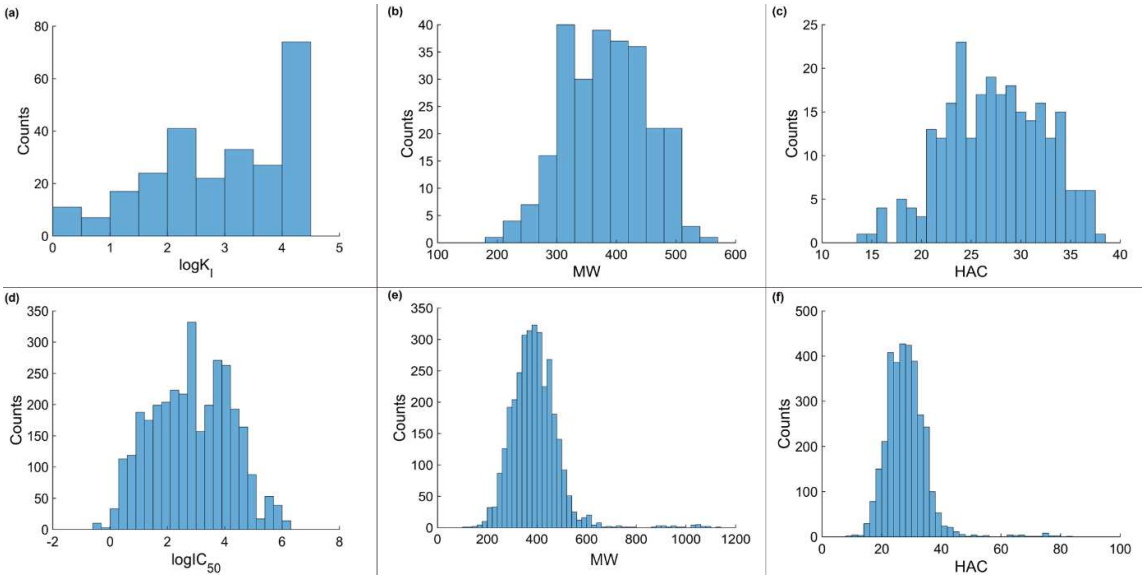

FIGURE S8. A comparison of BEI vs. MW and LE vs. HAC plots for kinase- Abl1 and GPCR-5HT2A data; **a-c)** BEI ($logK_i$/MW) vs. MW; **d-f)** BEI ($logIC_{50}$/MW) vs. MW; **g-i)** LE ($logK_i$/HAC) vs. HAC; **j-l)** LE ($logIC_{50}$/HAC) vs. HAC.

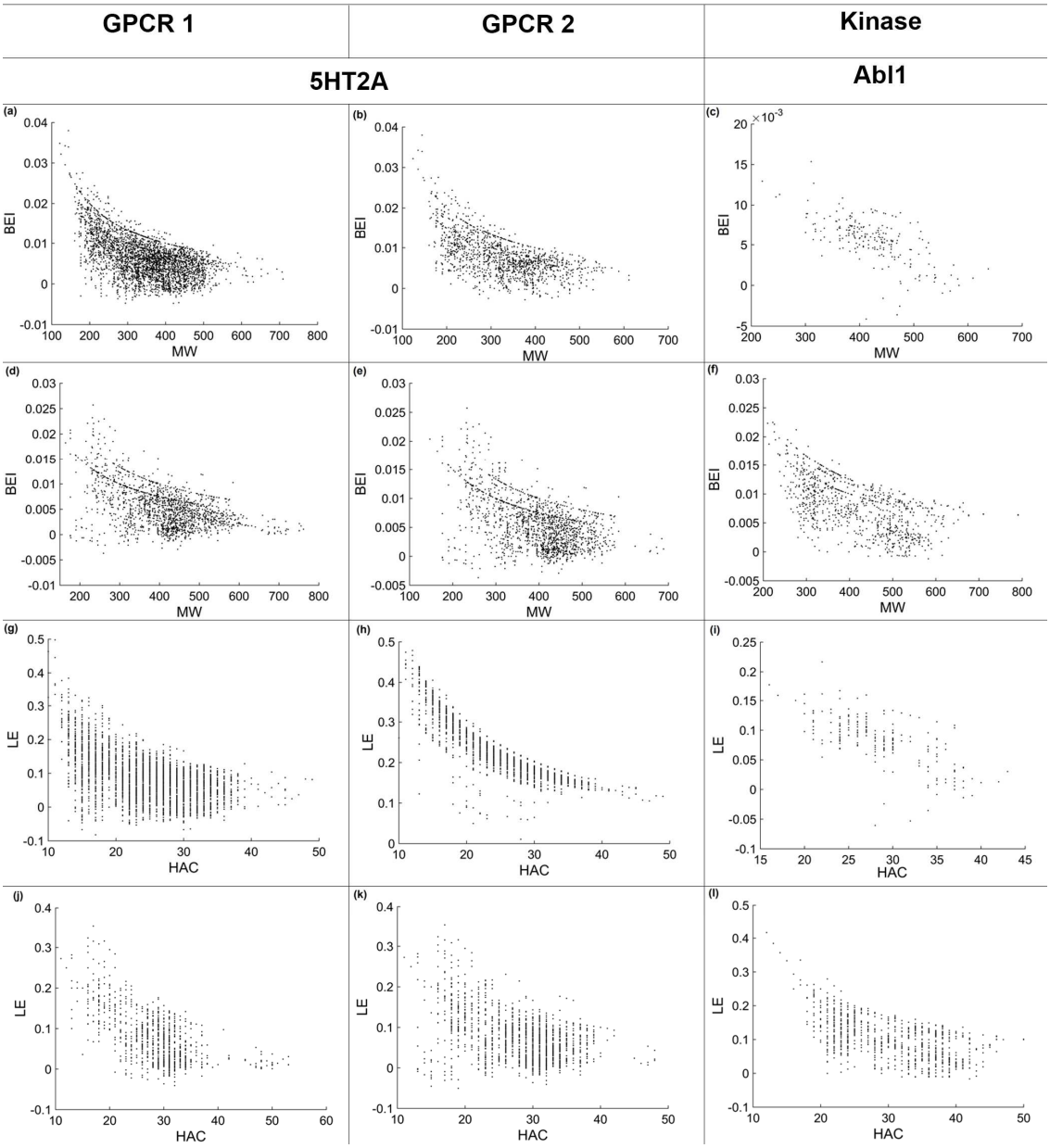

FIGURE S9. A comparison of BEI vs. MW and LE vs. HAC for kinase- CDK2 and GPCR- 5HT2B data; **a-c)** BEI ($logK_i$/MW) vs. MW; **d-f)** BEI ($logIC_{50}$/MW) vs. MW; **g-i)** LE ($logK_i$/HAC) vs. HAC; **j-l)** LE ($logIC_{50}$/HAC) vs. HAC.

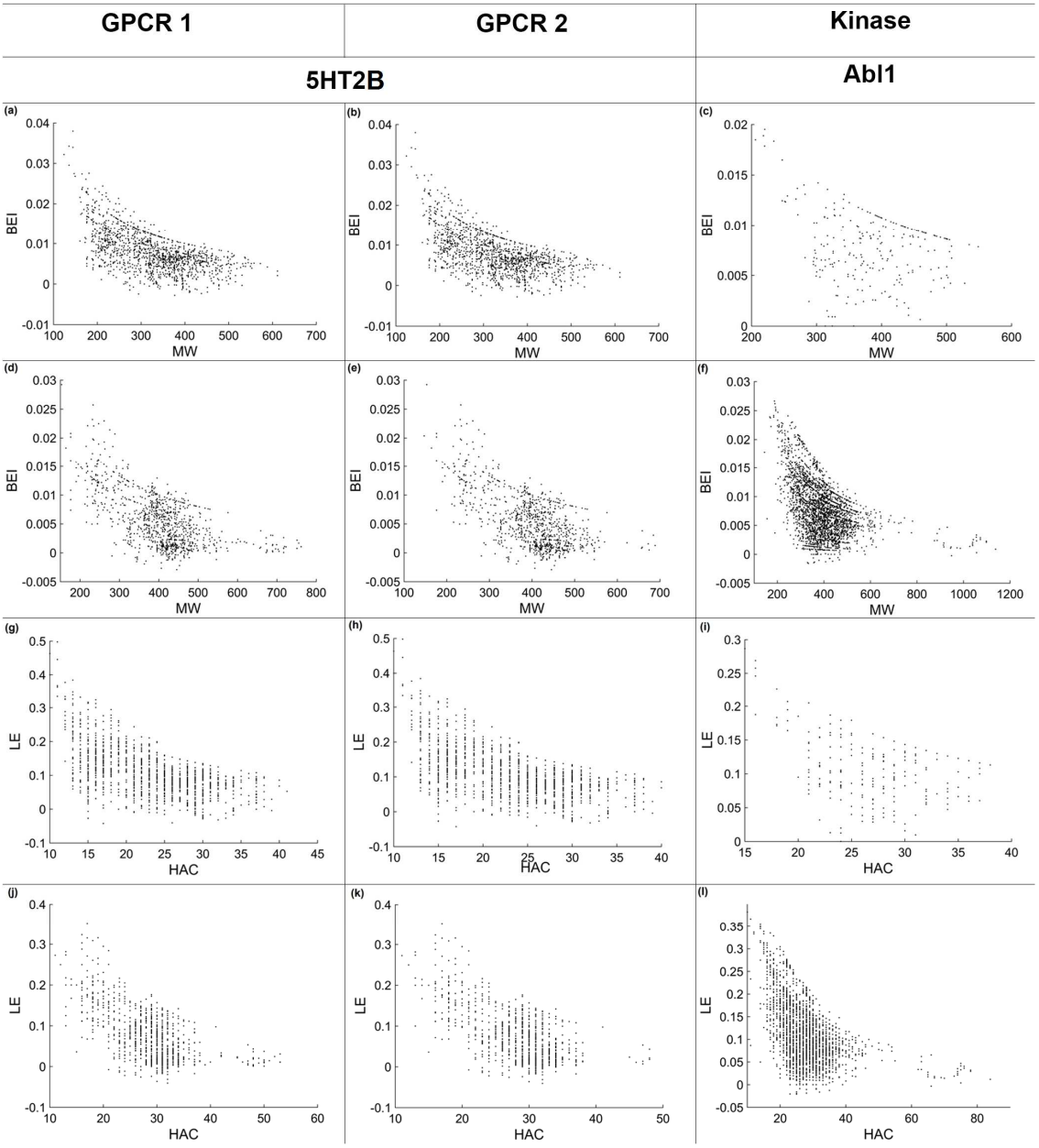

FIGURE S10. A relationship of BEI=logK_i/MW vs. 1/MW, correlation coefficient: R= 0,60; 0,58; 0,65 for **(a-c)**, respectively, and BEI=logIC_{50}/MW vs. 1/MW, correlation coefficient: R= 0,73; 0,69; 0,68 for **(d-f)**, respectively.

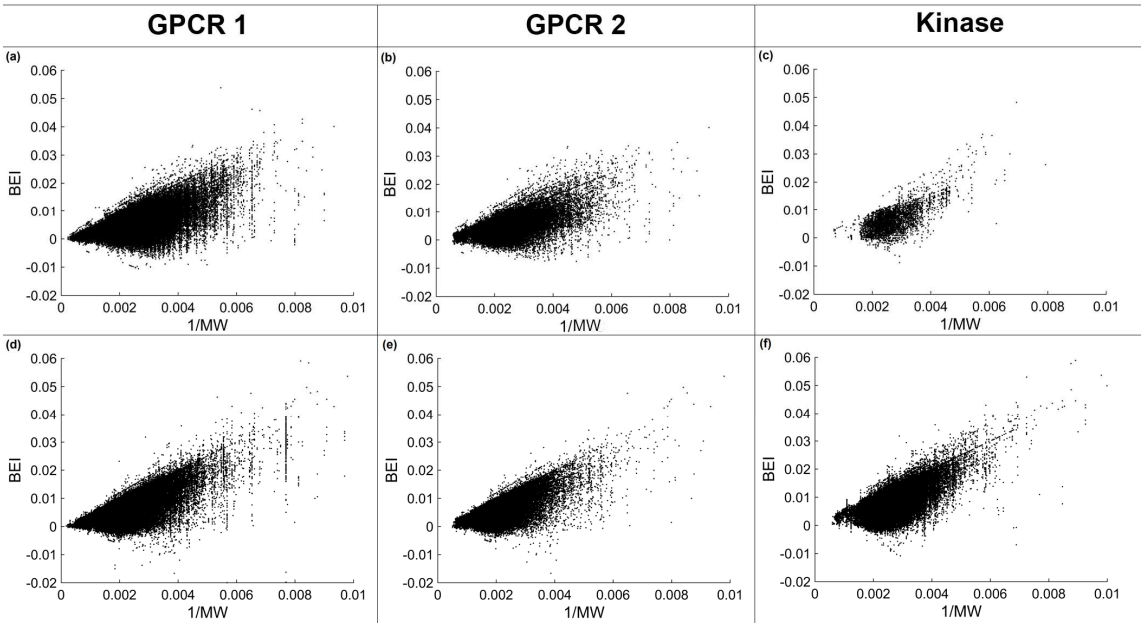

FIGURE S11. A relationship of LE=logK_i/HAC vs. 1/HAC, **(a-c)**, and logIC_{50}/HAC vs. 1/HAC, **(d-f)**, respectively.