Supplementary Materials

Identification and biological evaluation of CK2 allosteric fragments through structure-based virtual screening

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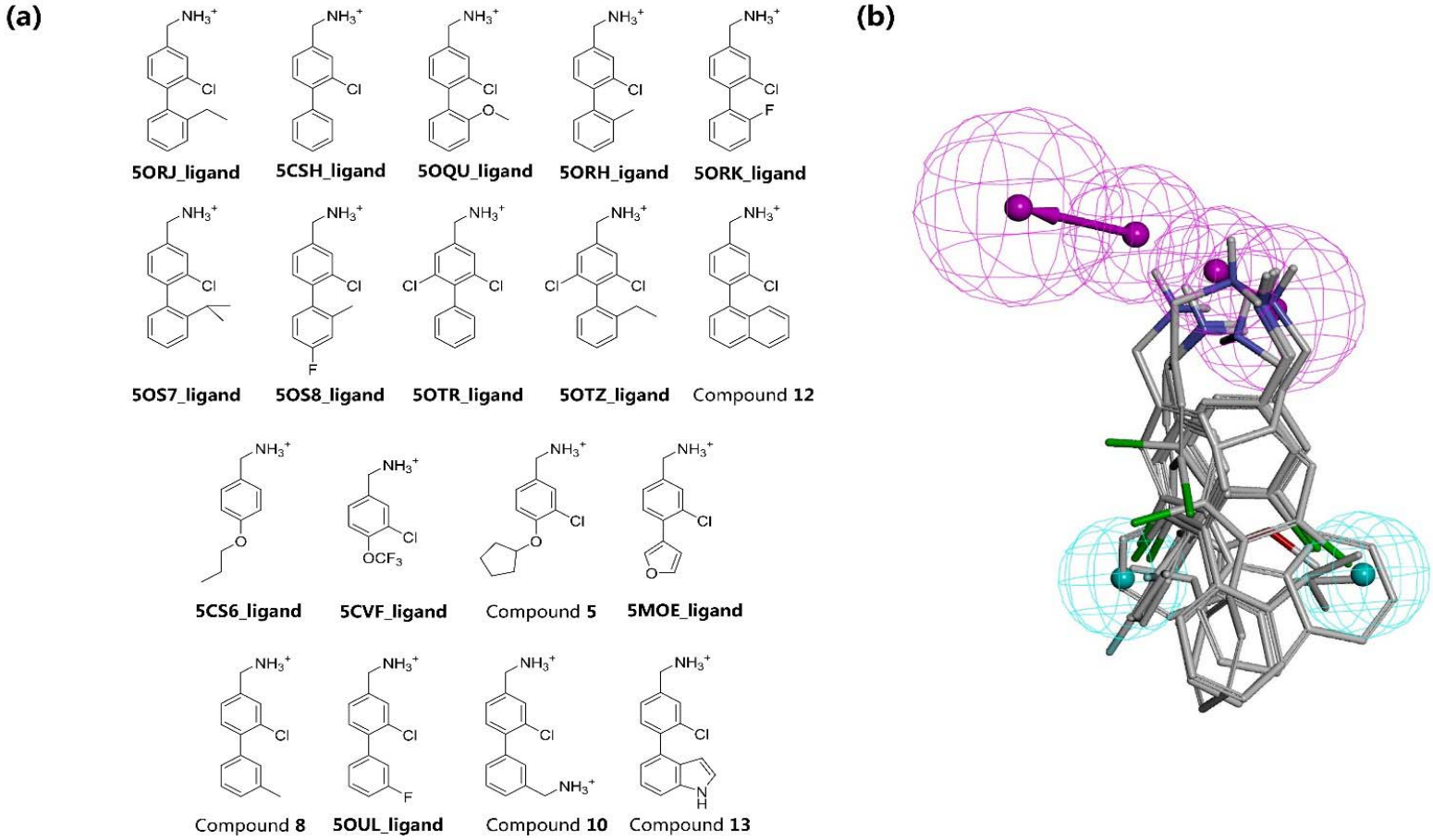

Figure S1. (a) Structures of ten active compounds and eight inactive compounds;

(b) Superimposition of four pharmacophoric features on the ten active compounds.

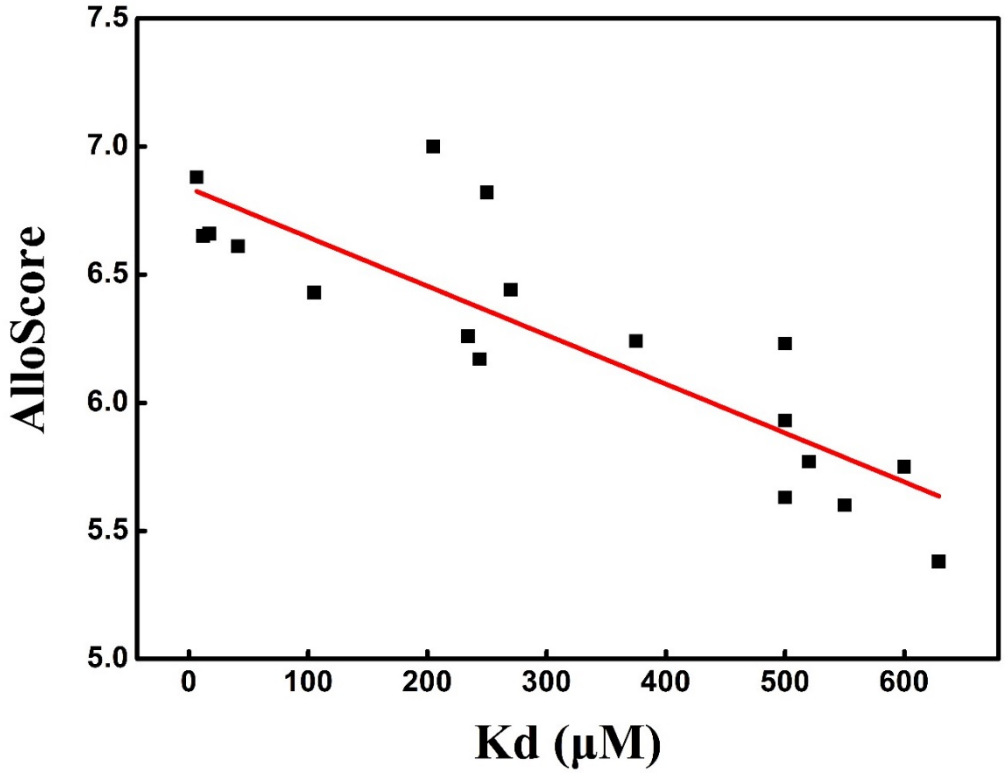

Figure S2. Correlation of AlloScore and experimental Kd values

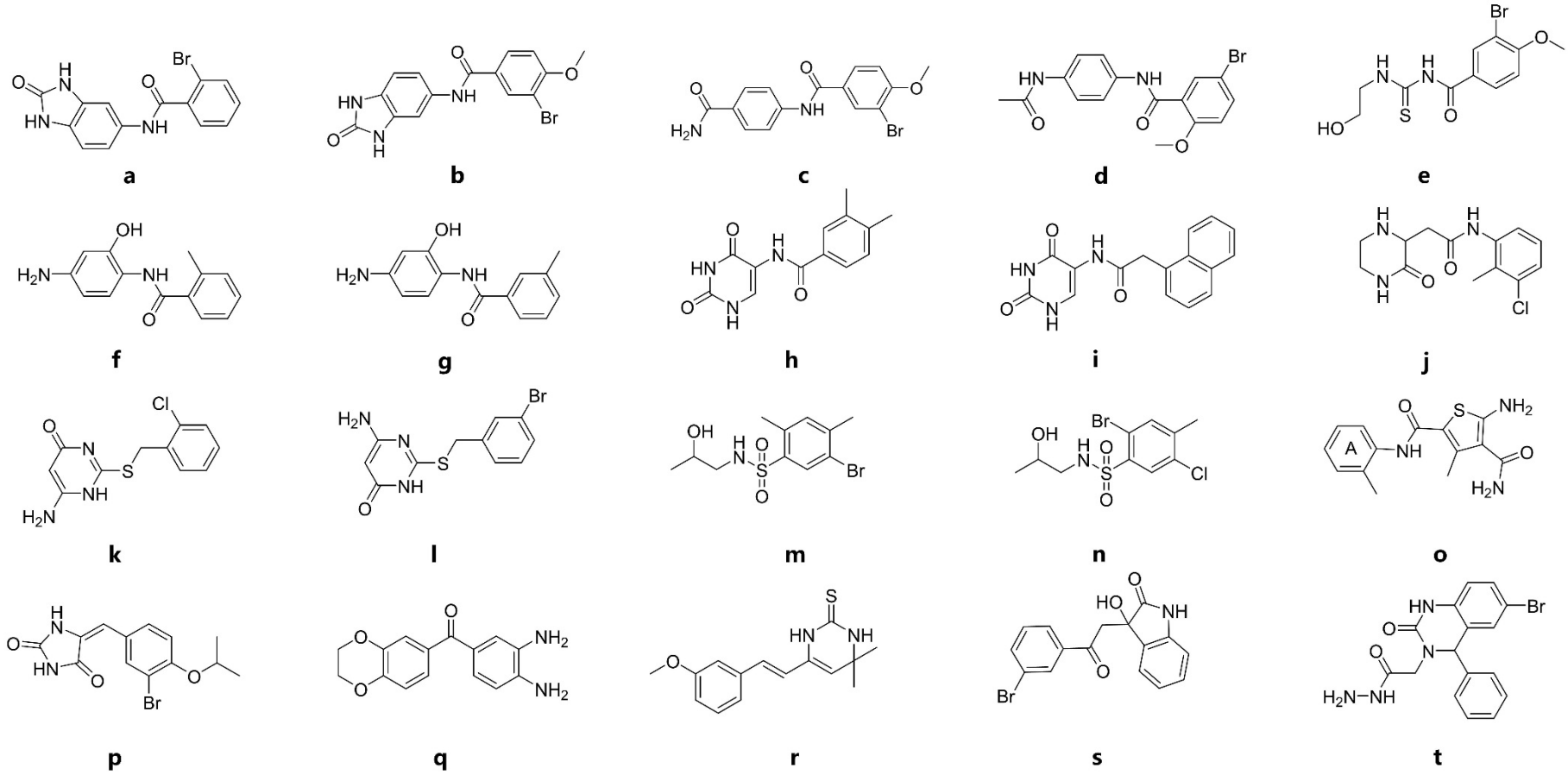

Figure S3. Structures of the selected 20 compounds with the AlloScore higher than 5.8.