

## SUPPLEMENTARY DATA

### Potent and selective inhibition of CYP1A2 enzyme by obtusifolin and its chemopreventive effects

Eun-Ji Park <sup>1,†</sup>, Keunwan Park <sup>2,†</sup>, Prasannavenkatesh Durai <sup>2</sup>, Ki-Young Kim <sup>1</sup>, So-Young Park <sup>1</sup>, Jaeyoung Kwon <sup>2</sup>, Hee Ju Lee <sup>2</sup>, Cheol-Ho Pan <sup>2,\*</sup> and Kwang-Hyeon Liu <sup>1,3,\*</sup>

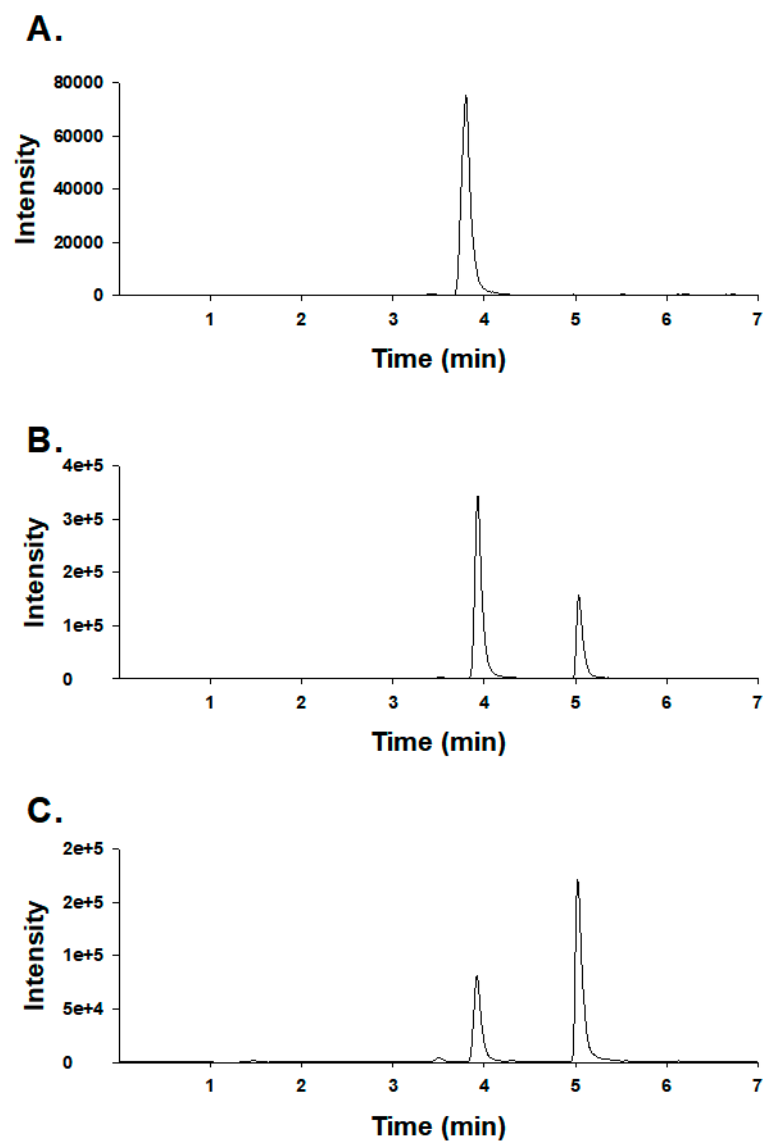
<sup>1</sup> BK21 FOUR KNU Community-Based Intelligent Novel Drug Discovery Education Unit, College of Pharmacy and Research Institute of Pharmaceutical Sciences, Kyungpook National University, Daegu 41566, Republic of Korea

<sup>2</sup> Mass Spectrometry Based Convergence Research Institute, Kyungpook National University, Daegu 41566, Republic of Korea

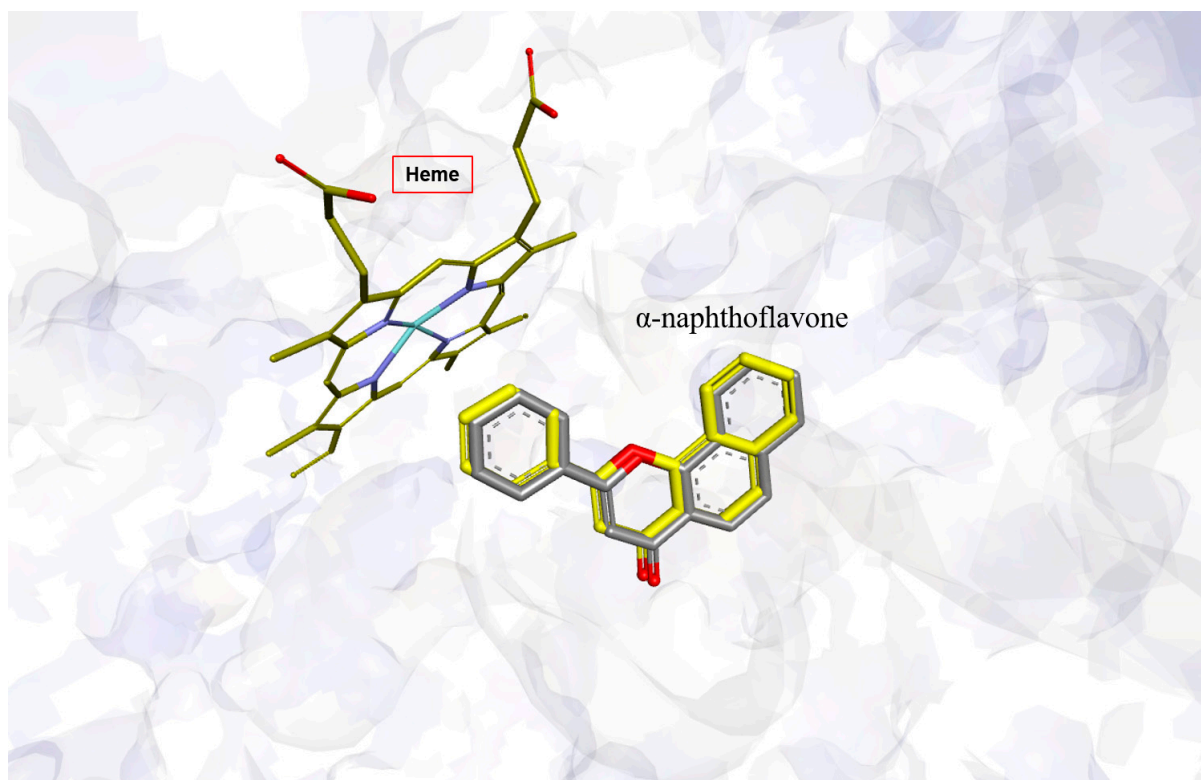
<sup>3</sup> Natural Product Informatics Research Center, KIST Gangneung Institute of Natural Products, Gangneung 25451, Republic of Korea

\* Correspondence: panc@kist.re.kr (C.-H.P); dstlkh@knu.ac.kr (K.-H.L.); Tel.: +82-33-650-3652 (C.-H.P.); +82-53-950-8567 (K.-H.L.); Fax: +82-33-650-3419 (C.-H.P.); +82-53-950-8557 (K.-H.L.);

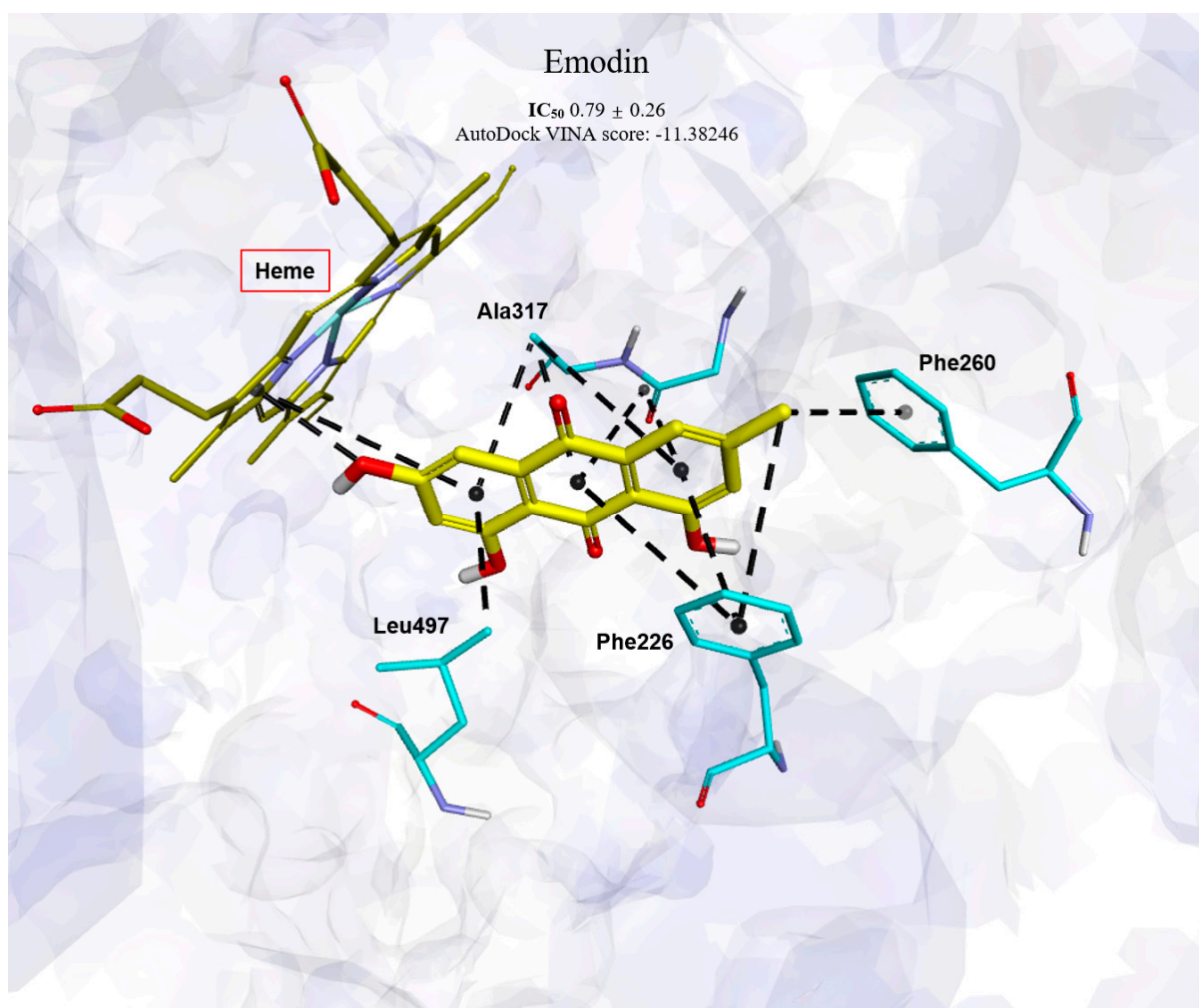
† These authors contributed equally to this work.



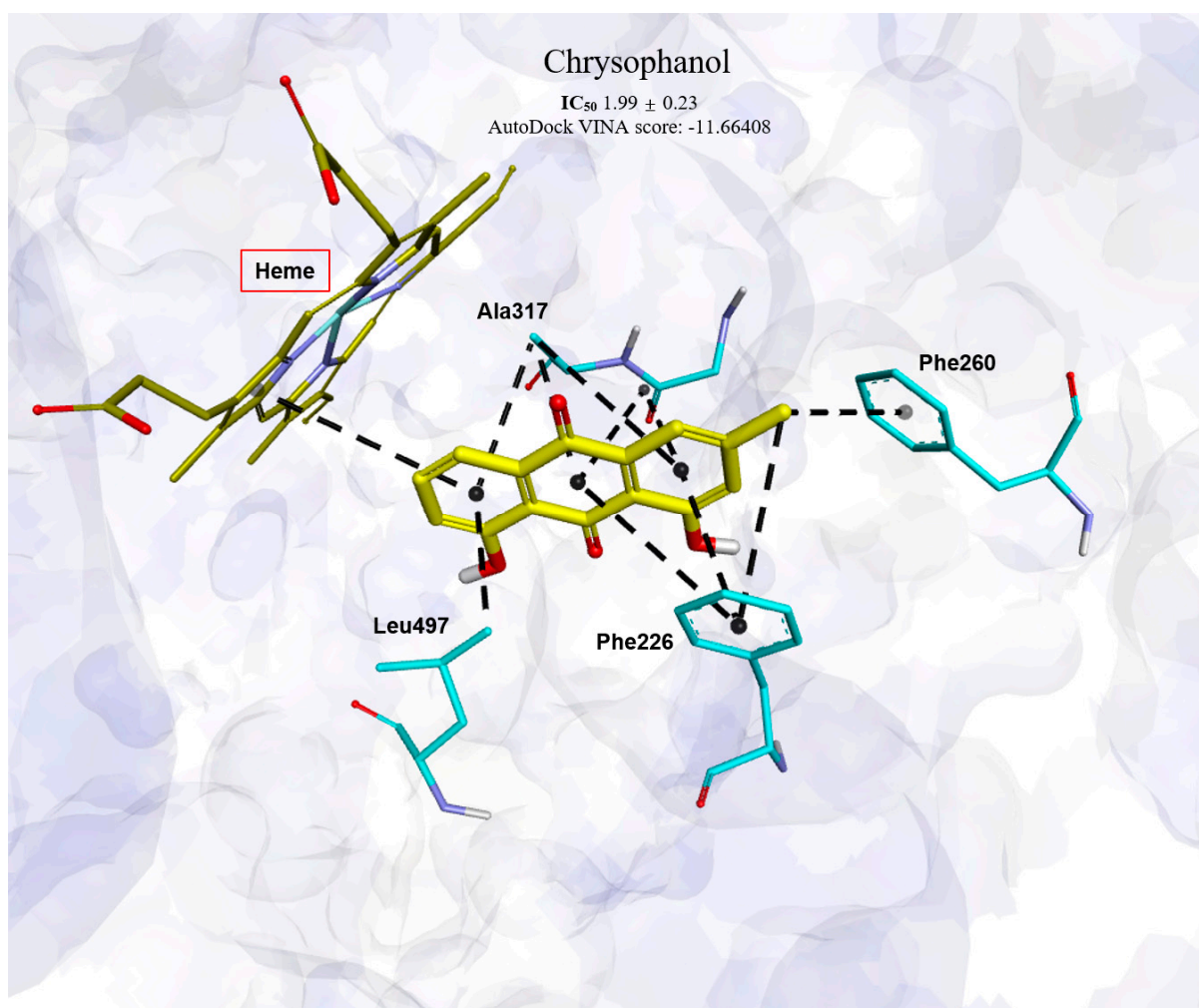
**Figure S1.** Selected reaction chromatograms for acetaminophen obtained from an acetaminophen standard (A) 200  $\mu$ M and an incubation study in human liver microsomes (B) 0  $\mu$ M obtusifolin; (C) 0.5  $\mu$ M obtusifolin.



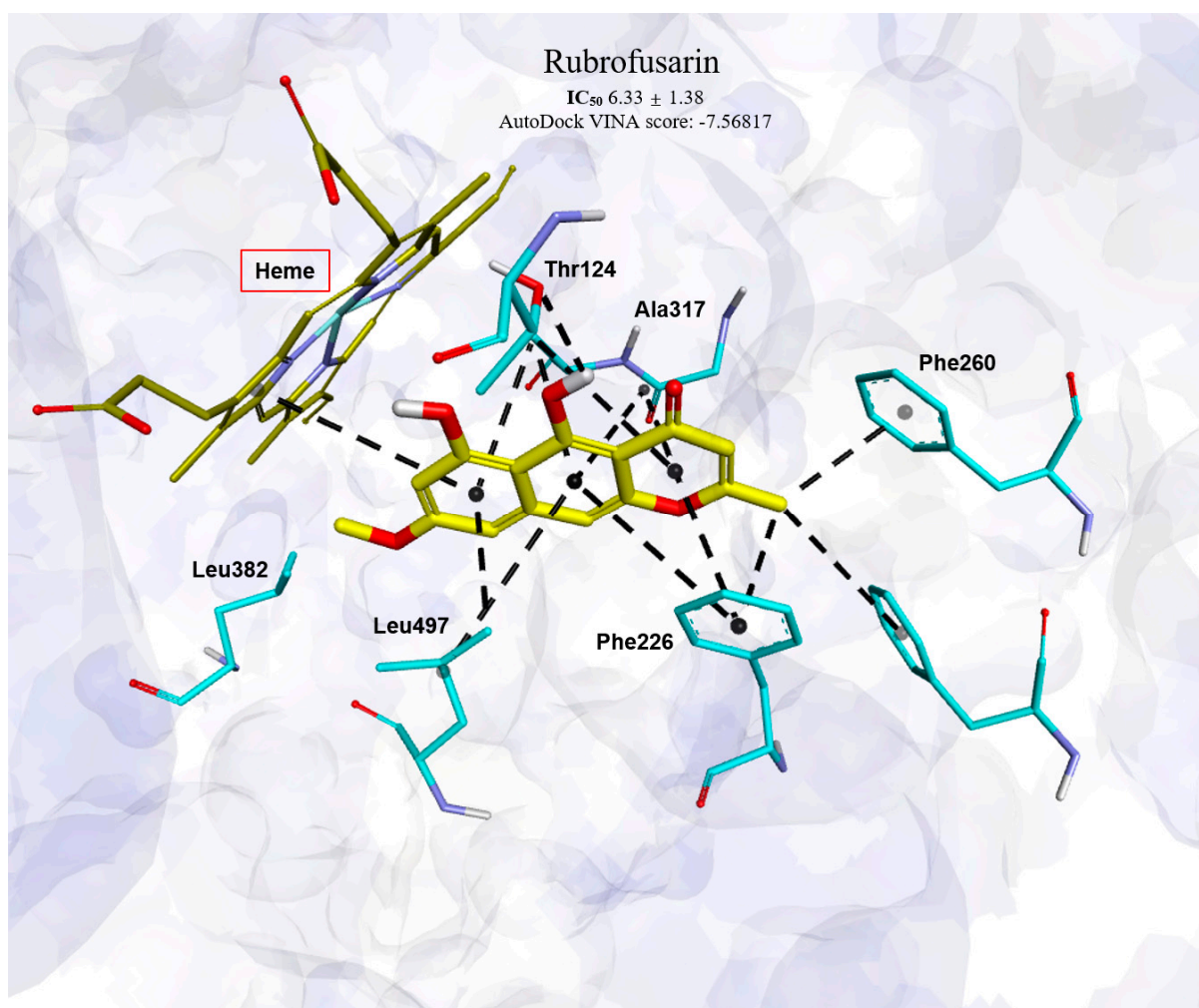
**Figure S2.** Molecular docking pose of  $\alpha$ -naphthoflavone in CYP1A2.



**Figure S3.** Molecular docking pose of emodin in CYP1A2.

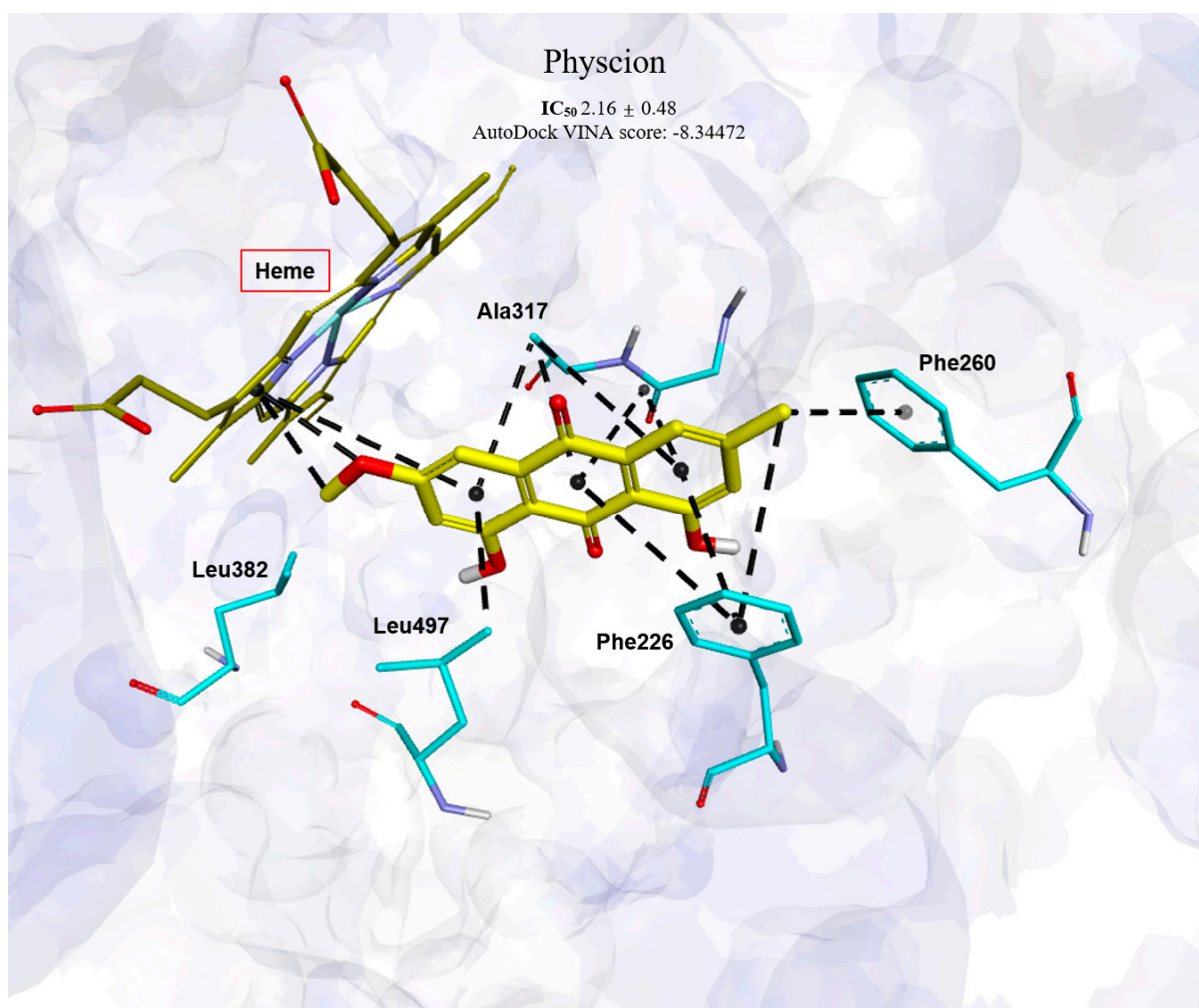


**Figure S4.** Molecular docking pose of chrysophanol in CYP1A2.



**Figure S5.** Molecular docking pose of rubrofusarin in CYP1A2.





**Figure S6.** Molecular docking pose of physcion in CYP1A2.