Scientia Pharmaceutica

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MDPI

Supplementary Materials

Multiple Virtual Screening Strategies for the Discovery of Novel Compounds Active Against Dengue Virus: A Hit Identification Study

Kowit Hengphasatporn [1,4], Arthur Garon[2], Peter Wolschann[2,3], Thierry Langer[3], Shigeta Yasuteru[4], Thao N.T. Huynh [5], Warinthorn Chavasiri[5], Thanaphon Saelee[6], Siwaporn Boonyasuppayakorn[6], Thanyada Rungrotmongkol[1,7,*]

[1] Ph.D. Program in Bioinformatics and Computational Biology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.
[2] Department of Pharmaceutical Chemistry, Faculty of Life Sciences, University of Vienna, Althanstraße 14, 1090 Vienna, Austria
[3] Institute of Theoretical Chemistry, University of Vienna, Vienna 1090, Austria
[4] Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577, Japan
[5] Center of Excellence in Natural Products Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
[6] Applied Medical Virology Research Unit, Department of Microbiology, Faculty of Medicine, Chulalongkorn University, Bangkok, 10330, Thailand
[7] Biocatalyst and Environmental Biotechnology Research Unit, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

* Correspondence: T.rungrotmongkol@gmail.com; Tel.: +66-2218-5426; Fax: +66-2218-5418.

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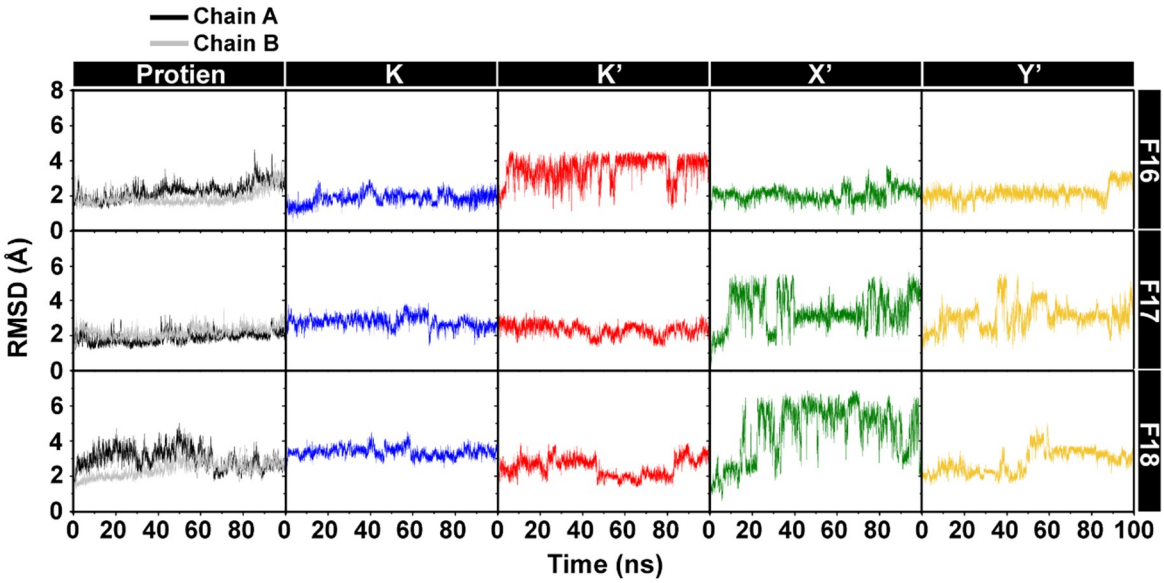

Figure S1. RMSD plot for the protein backbone and all ligand atoms of flavones/E protein complexes along 100-ns simulations.

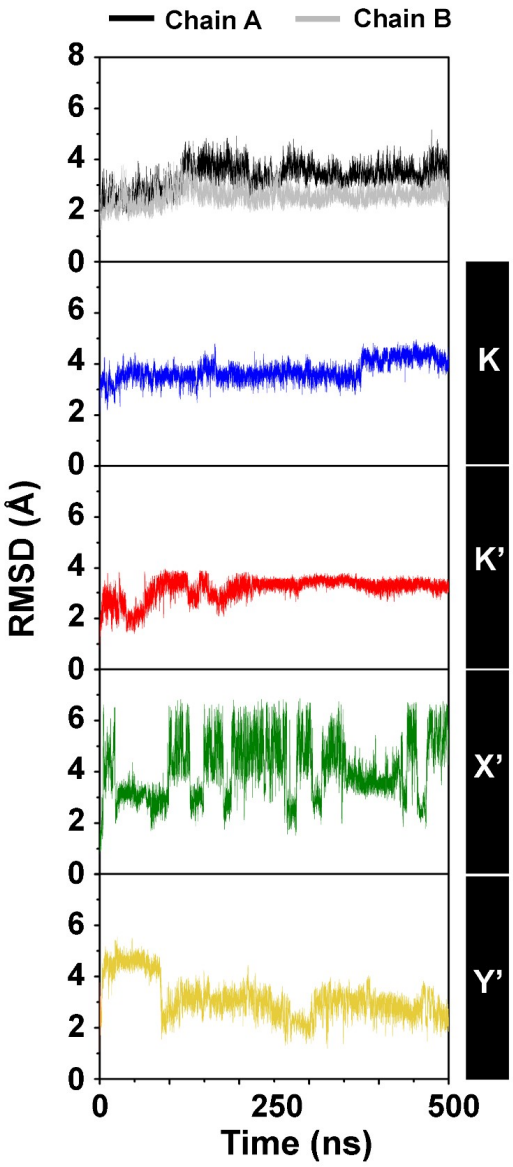

Figure S2. RMSD plot for the protein backbone and all ligand atoms of F18/E protein complexes along 500-ns simulations.

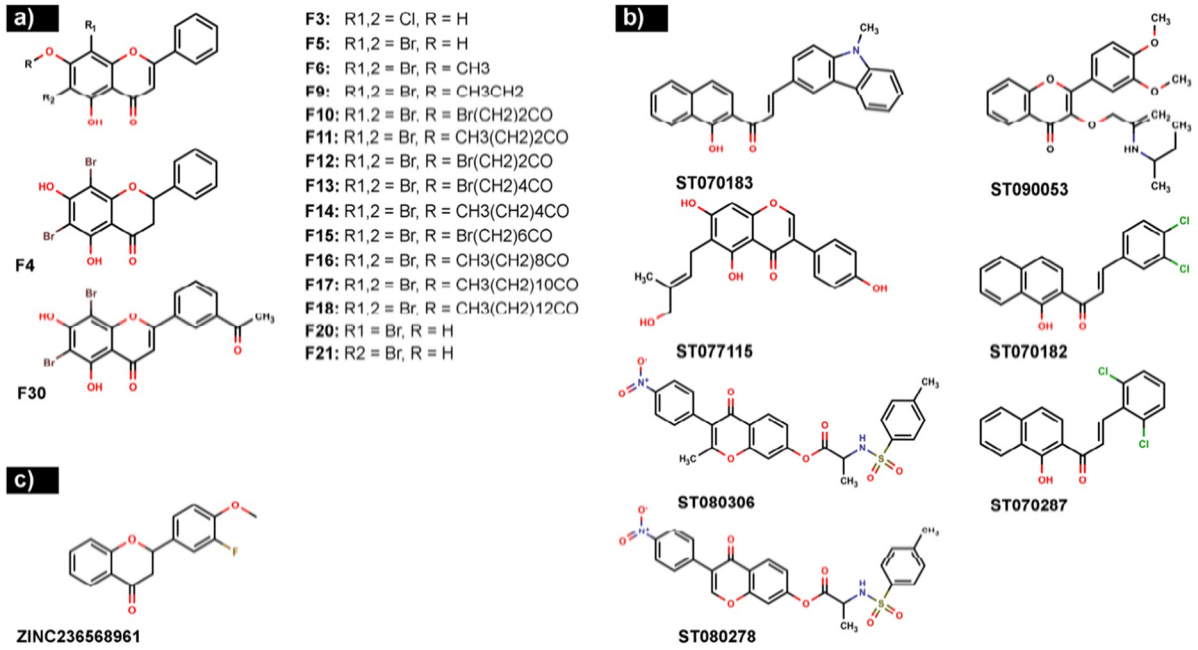

Figure S3. 2D structures of the 26 hit compounds from a) in-house database, b) TimTec and c) Zinc database.

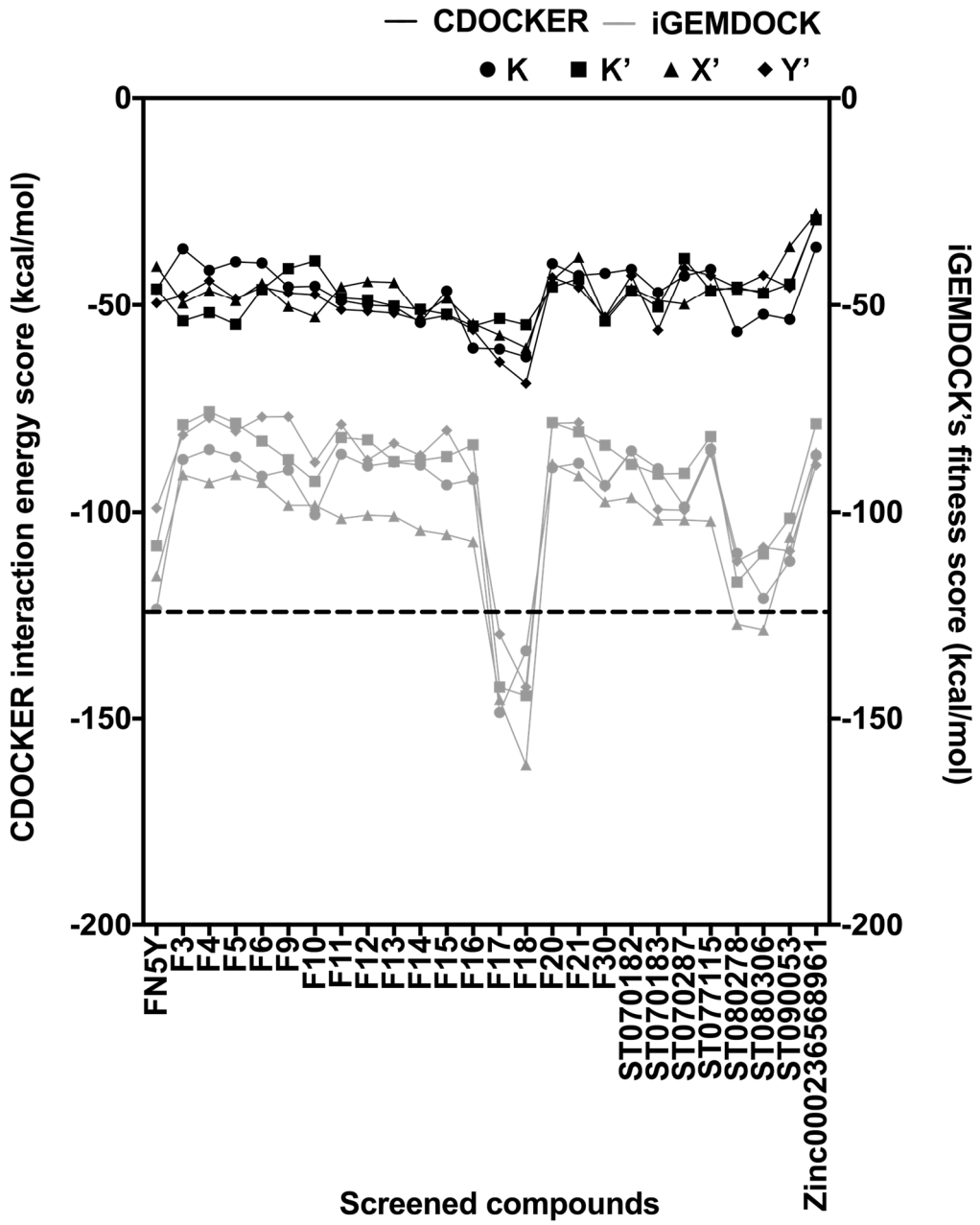

Figure S4. CDOCKER interaction energies (black) and iGEMDOCK's fitness scores (grey) of the 26 hit compounds docking to DENV E protein at the four sites K, K′, *X*′ and Y′.

Table S1. SIE Binding free energy (ΔG_{bind}) in kcal/mol for each flavone bound to DENV E protein at the 4 sites, where its energy components, van de Waals interaction (ΔE_{vdW}), electrostatic interaction (ΔE_{elec}), the change of reaction energy (ΔG^R), the charge of molecular surface upon binding ($\gamma \bullet \Delta MSA$) are given. Note that conformational upon binding (α) is 0.104758, constant (c) value is -2.89 and molecular surface area coefficient (γ) is 0.012894.

		ΔE_{vdW}	ΔE_{elec}	ΔG^R	$\gamma \bullet \Delta MSA$	ΔG_{bind} (kcal/mol)
FN5Y	K	-27.33±0.1	6.14±0.1	6.3±0.4	1.48±0.2	-4.30±0.0
	K′	-23.36±0.2	5.95±0.2	6.07±0.4	1.14±0.2	-3.96±0.0
	X′	-5.09±0.4	-7.19±0.1	5.88±0.4	1.20±0.2	-3.43±0.1
	Y′	-13.06±1.0	-8.75±0.3	5.93±0.4	1.98±0.2	-4.35±0.1
F16	K	-46.28±0.3	-13.71±0.7	-27.46±1.1	-9.61±0.1	-13.06±0.9
	K′	-33.72±0.3	-21.37±0.4	-27.53±1.1	-9.52 ±0.1	-12.54±0.1
	X′	-33.98±0.4	-1.31±0.7	-27.52±1.1	-9.64±0.1	-10.48±0.1
	Y′	-41.98±0.3	-12.20±0.5	-20.56±0.6	-7.91±0.1	-11.55±0.1
F17	K	-48.82±0.2	-12.95±0.4	9.80±0.1	-9.89±0.1	-9.37±0.1
	K′	-53.24±0.2	-22.25±0.3	9.72±0.6	-9.86±0.1	-6.28±0.1
	X′	-32.53±0.2	-37.01±0.3	9.59±0.7	-10.35±0.1	-7.34±0.1
	Y′	-37.80±0.5	-16.16±0.5	9.72±0.6	-9.83±0.1	-8.56±0.1
F18	K	-51.91±0.2	-7.73±0.4	-39.92±0.7	-10.53±0.1	-14.42±0.1
	K′	-47.90±0.2	-15.00±0.4	-35.74±0.7	-10.73±0.1	-14.35±0.1
	X′	-28.72±0.3	-3.41±0.7	-35.74±0.7	-10.62±0.1	-11.11±0.1
	Y′	-46.94±0.2	-7.53±0.4	-35.78±0.7	-10.73±0.1	-13.47±0.1

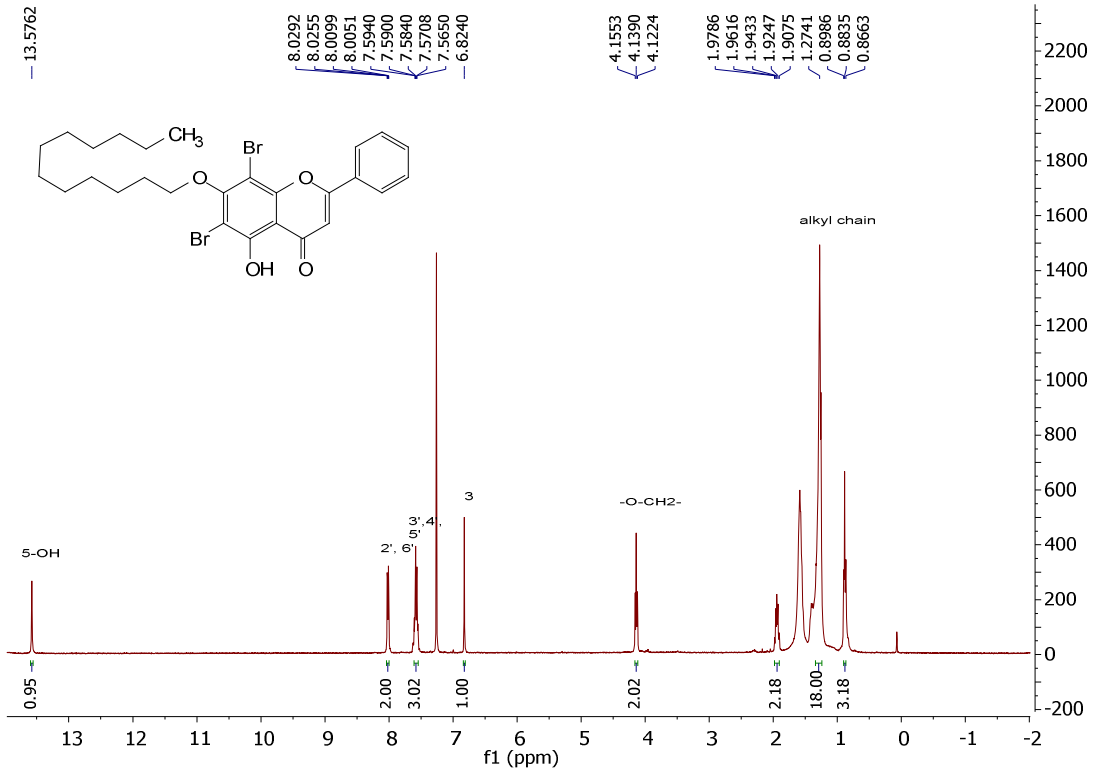

Figure S5. [1]H-NMR spectrum of 6,8-dibromo-5-hydroxy-7-dodecyloxyflavone (F18)

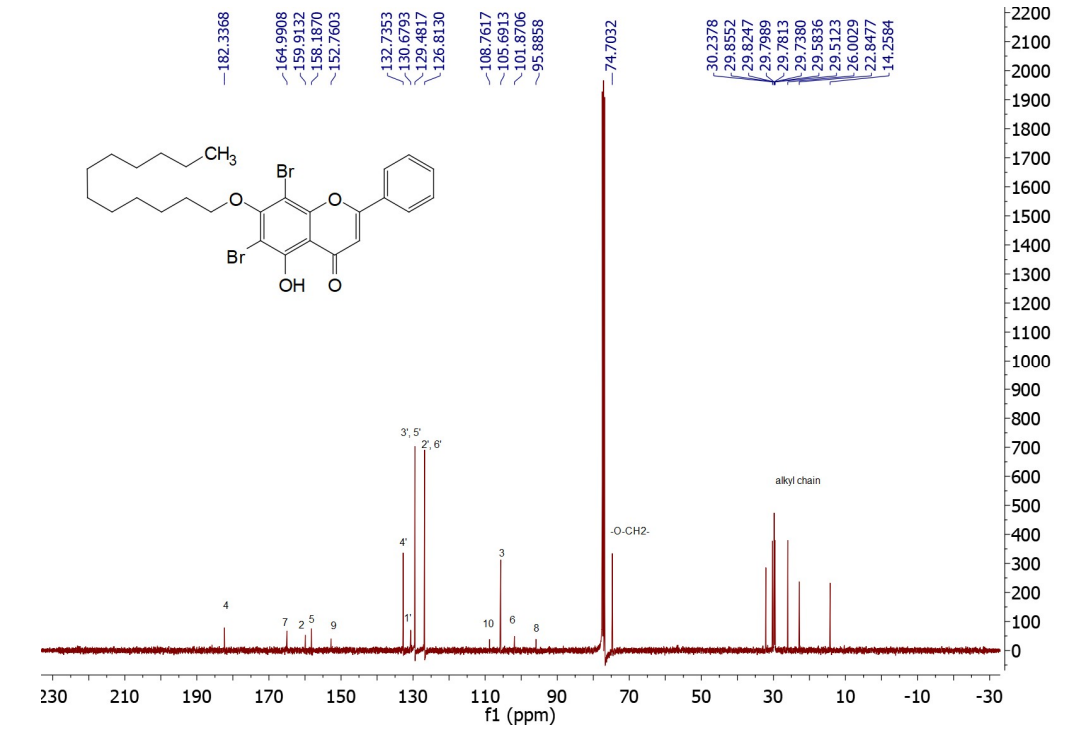

Figure S6. [13]C NMR spectrum of 6,8-dibromo-5-hydroxy-7-dodecyloxyflavone (F18)