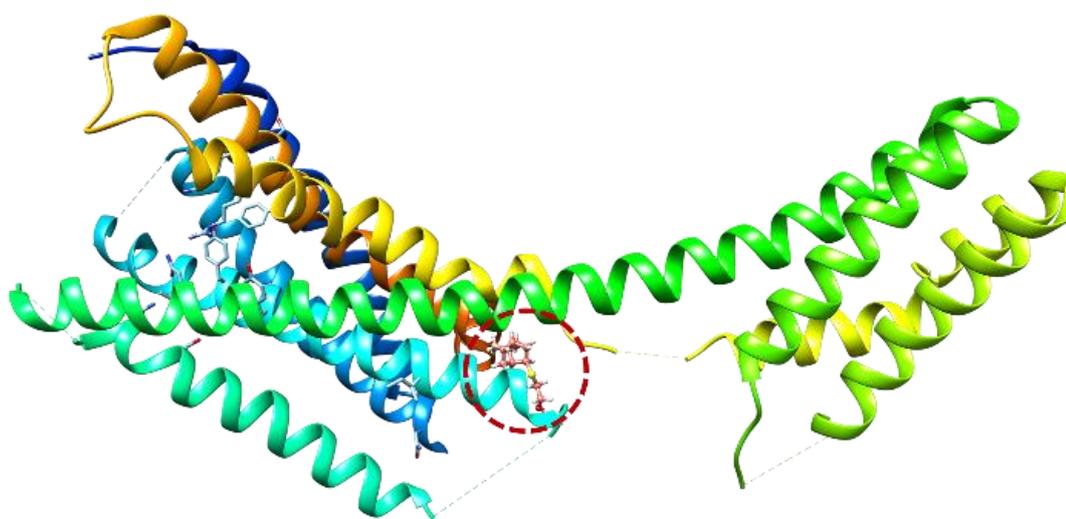
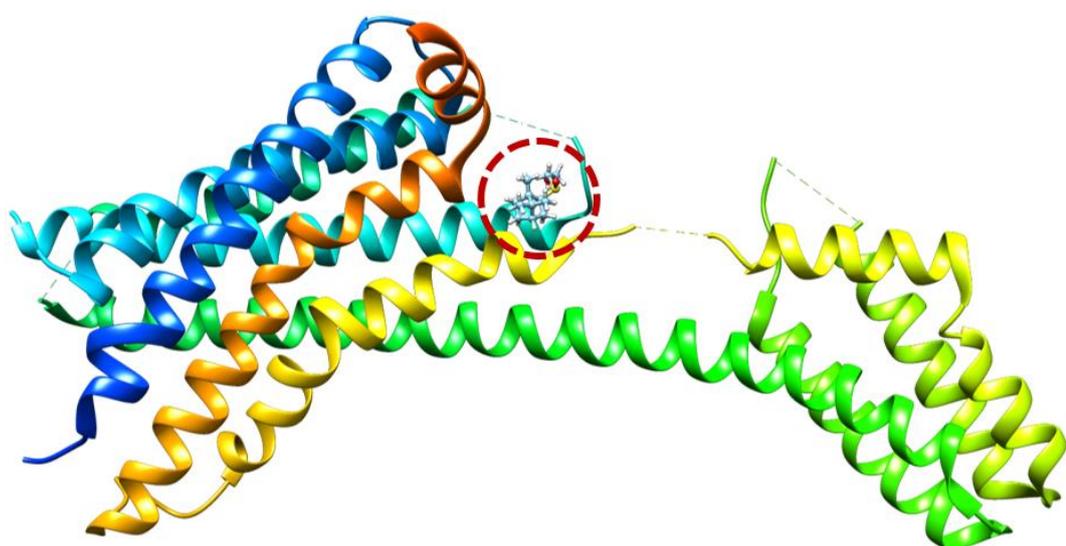


## **Supplementary Materials**

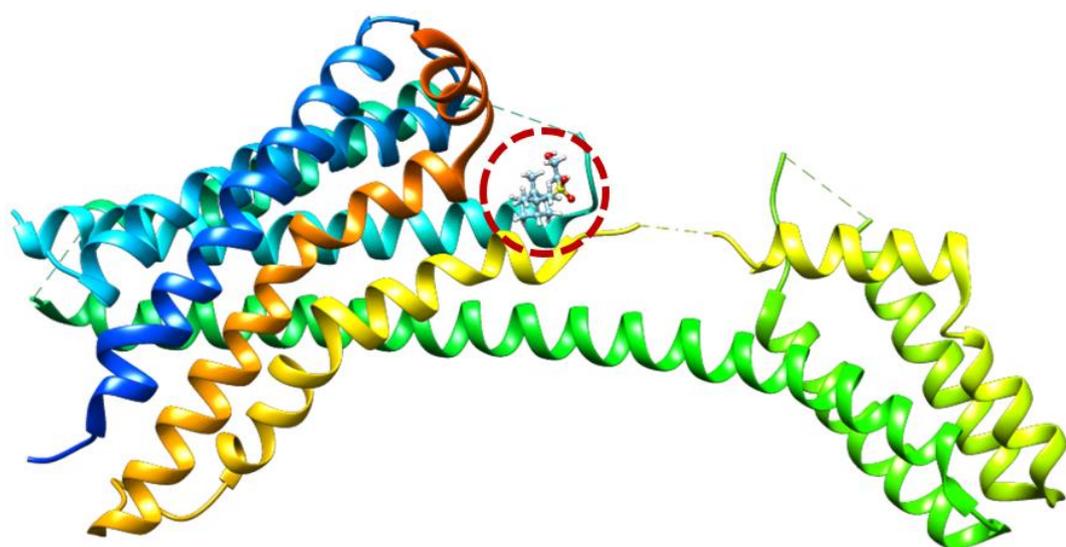
**Thioterpenoids as Potential Antithrombotic Drugs: Molecular Docking, Antiaggregant, Anticoagulant and Antioxidant activities**



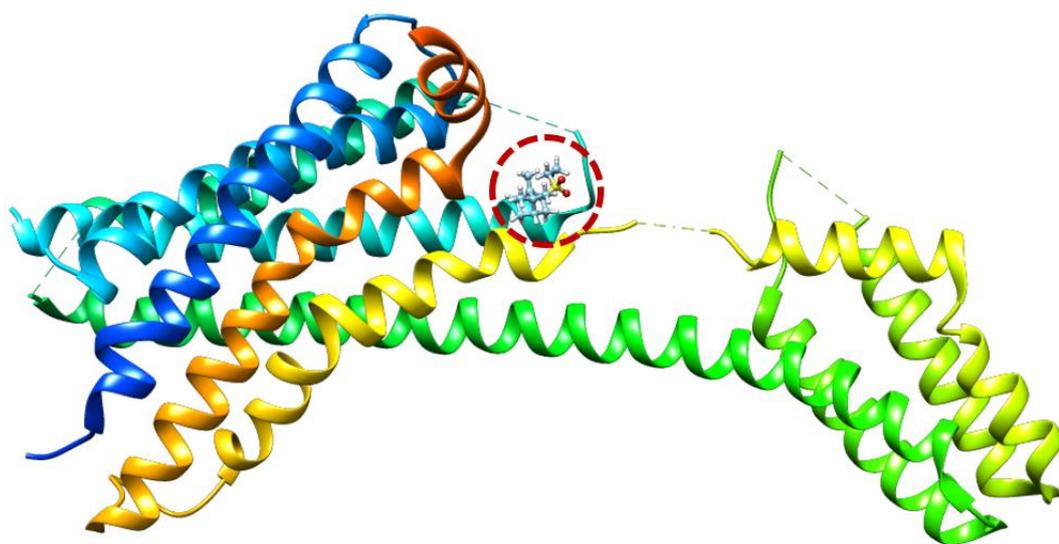
*a*



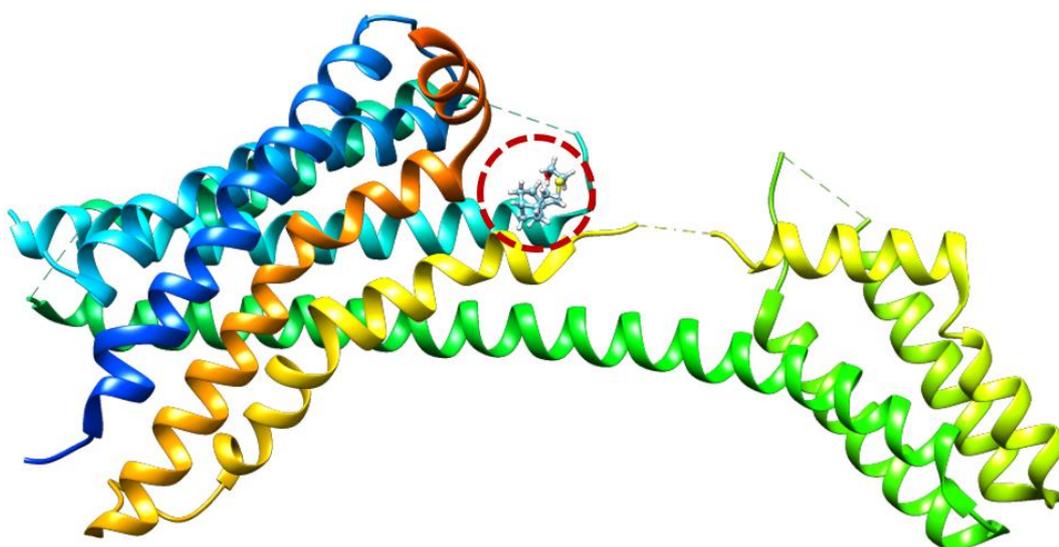
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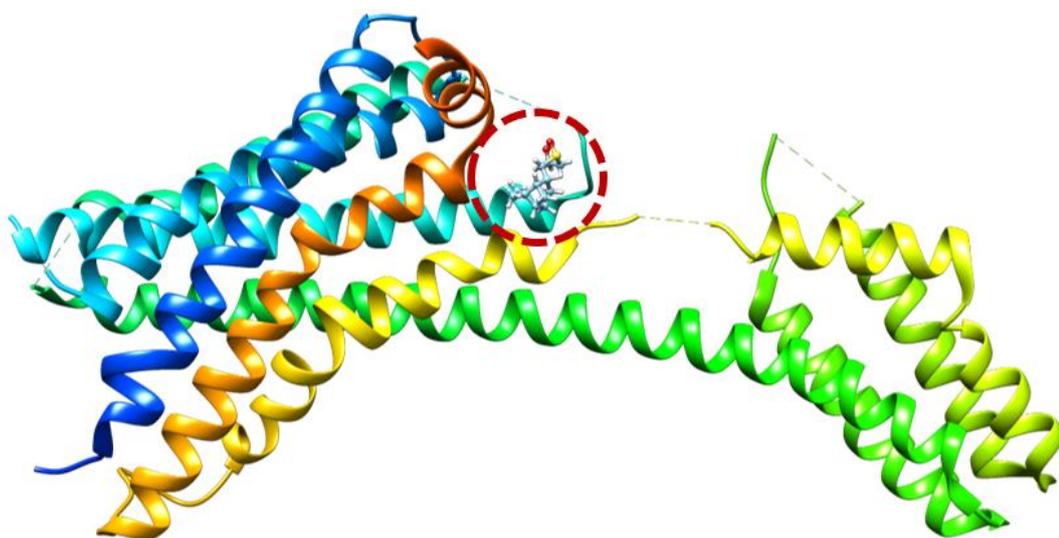
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*d*

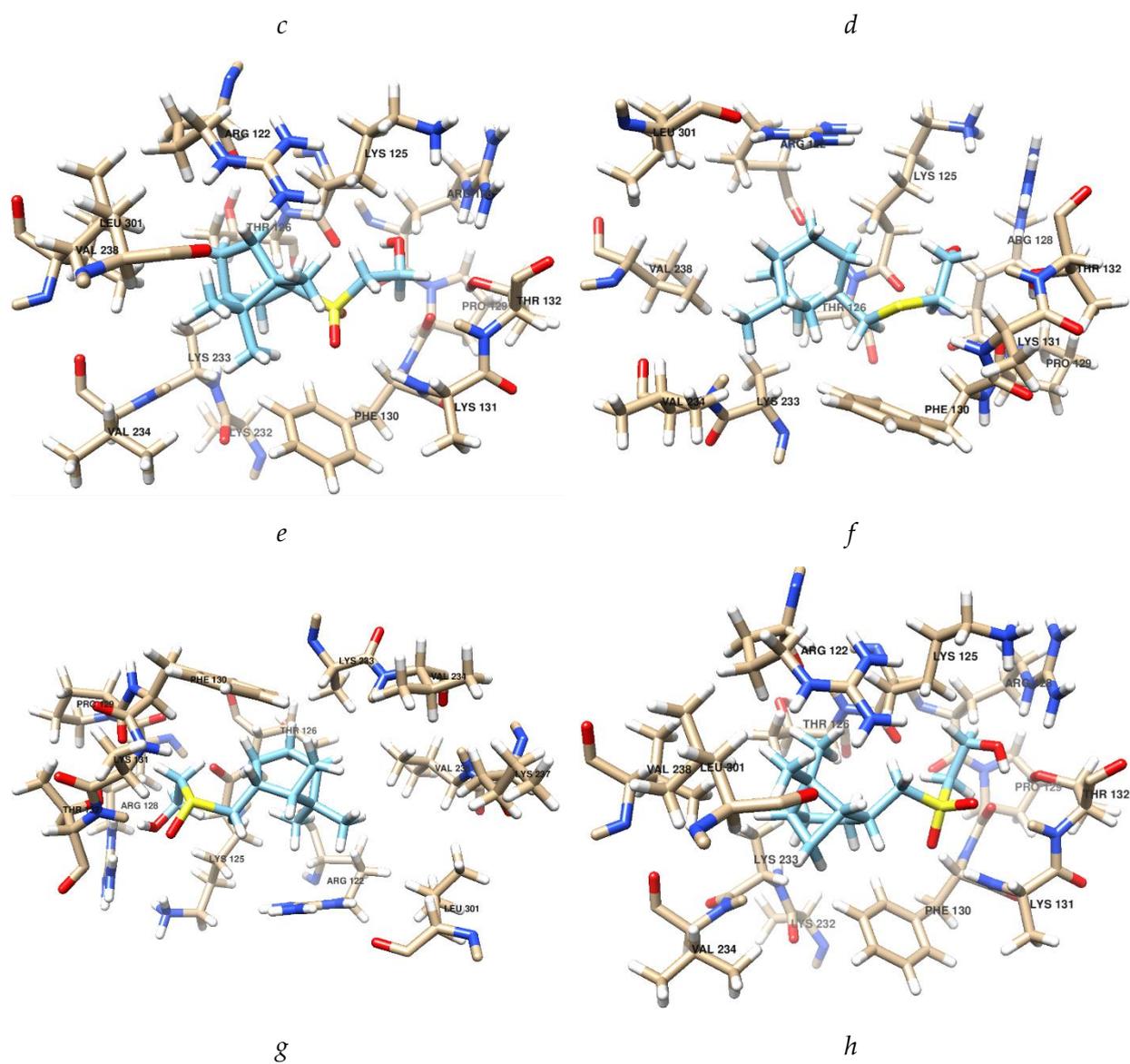


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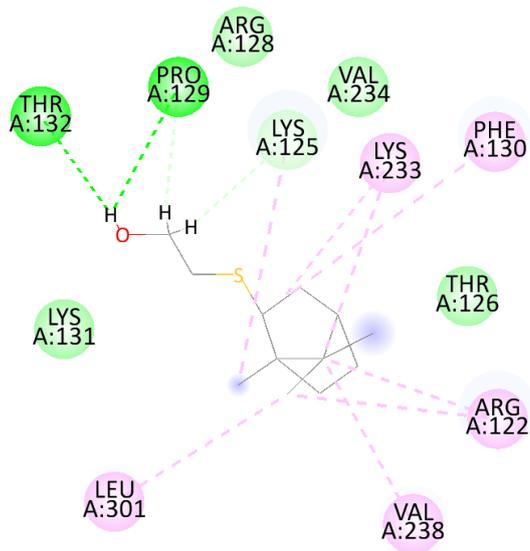


*f*





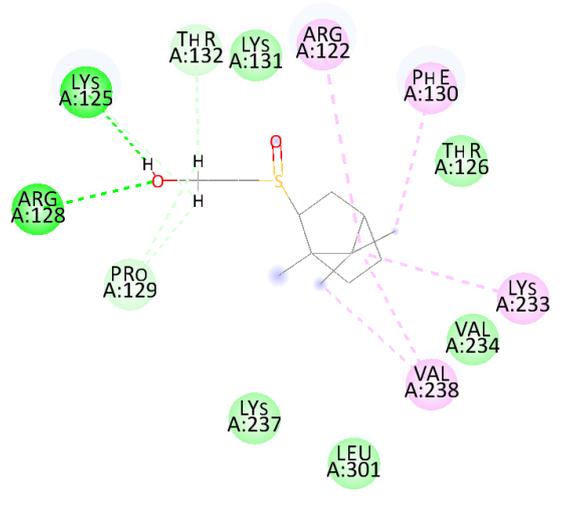
**Figure S2.** Amino acid composition of P2Y<sub>12</sub> binding sites with **1** [10.1016/j.saa.2021.120638] (a), **2** (conformer A) (b), **2** (conformer B) (c), **3** (monomer A) (d), **3** (monomer B) (e), **4** (f), **5** (g), and **6** (h).



**Interactions**

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Alkyl
- Pi-Alkyl

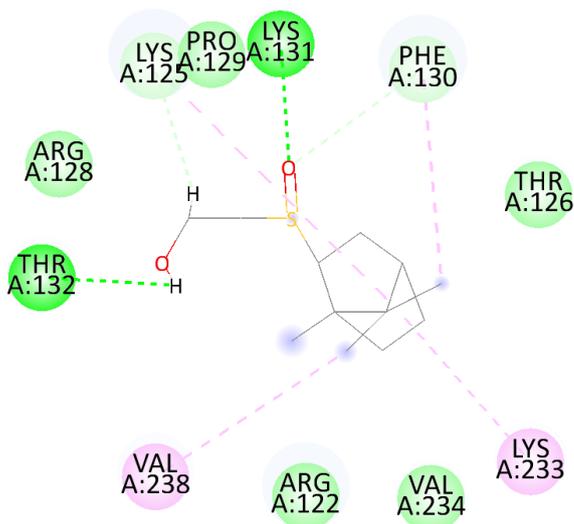
*a*



**Interactions**

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Alkyl
- Pi-Alkyl

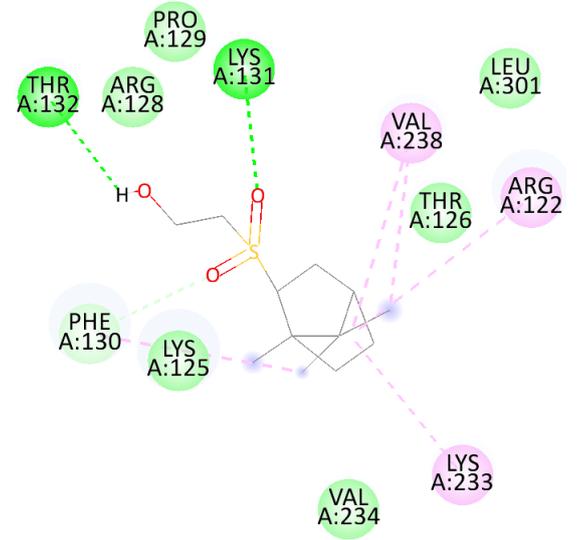
*b*



**Interactions**

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Donor-Donor
- Alkyl
- Pi-Alkyl

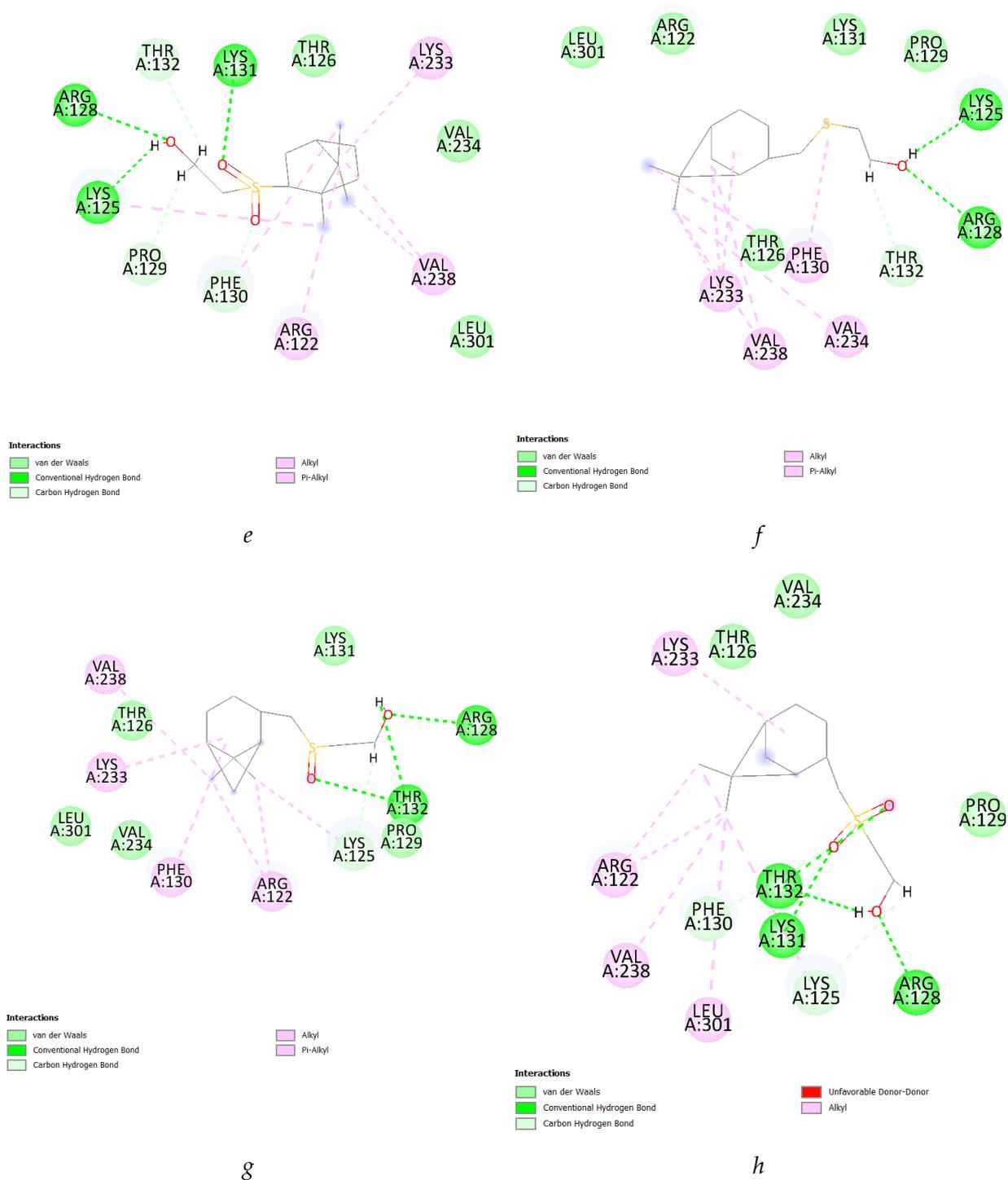
*c*



**Interactions**

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Alkyl
- Pi-Alkyl

*d*



**Figure S3.** 2D diagram of **1** (a), **2** (conformer A) (b), **2** (conformer B) (c), **3** (monomer A) (d), **3** (monomer B) (e), **4** (f), **5** (g), and **6** (h) and P2Y<sub>12</sub> interaction generated by Discovery Studio.

**Table S1.** Amino acid composition of binding sites of compounds **1 - 6** with P2Y<sub>12</sub>

<b>Compound</b>	<b>Amino acid residues</b>
<b>1</b> [10.1016/j.saa.2021.120638]	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS233, VAL234, VAL238, LEU301
<b>2 (conformer A)</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS233, VAL234, LYS237, VAL238, LEU301
<b>2 (conformer B)</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS233, VAL234, VAL238, LEU301
<b>3 (monomer A)</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS233, VAL234, VAL238, LEU301
<b>3 (monomer B)</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS232, LYS233, VAL234, VAL238, LEU301
<b>4</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS233, VAL234, VAL238, LEU301
<b>5</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS233, VAL234, LYS237, VAL238, LEU301
<b>6</b>	ARG122, LYS125, THR126, ARG128, PRO129, PHE130, LYS131, THR132, LYS232, LYS233, VAL234, VAL238, LEU301