Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


**Supporting Information**

# Development of antithrombotic peptides based on the molecular interactions between von Willebrand factor and GPIbα

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**Table S1. Screening of inhibitor by docking and binding conformation**

| candidate | label | $E_{vina}$(kcal/mol) | RMSD(nm) |
|---|---|---|---|
| EWEYWDPD | I1 | -7.5 | 0.341763 |
| EPEGFDWD | I2 | -7.5 | 0.357641 |
| ESEYWDYD | I3 | -7.5 | 0.362230 |
| EPEGPDWD | I4 | -7.5 | 0.365492 |
| EAEYWDFD | I5 | -7.6 | 0.366498 |
| EGEYWDFD | I6 | -7.5 | 0.374358 |
| EGEPWDGD | I7 | -7.7 | 0.377362 |
| EPEWWDVD | I8 | -8.2 | 0.379835 |
| ESEYWDFD | I9 | -7.5 | 0.380284 |
| EPEWLDYD | I10 | -7.7 | 0.381267 |
| EPEPWDPD | I11 | -7.9 | 0.385159 |
| EPEWFDWD | I12 | -7.8 | 0.385899 |
| EDECGDWD | I13 | -7.5 | 0.390631 |
| EAEPFDCD | I14 | -7.5 | 0.392722 |
| EGEPWDLD | I15 | -7.8 | 0.393510 |
| EWEYWDDD | I16 | -7.6 | 0.396083 |
| EAEPWDPD | I17 | -7.6 | 0.398703 |
| EPEWWDED | I18 | -7.9 | 0.399933 |

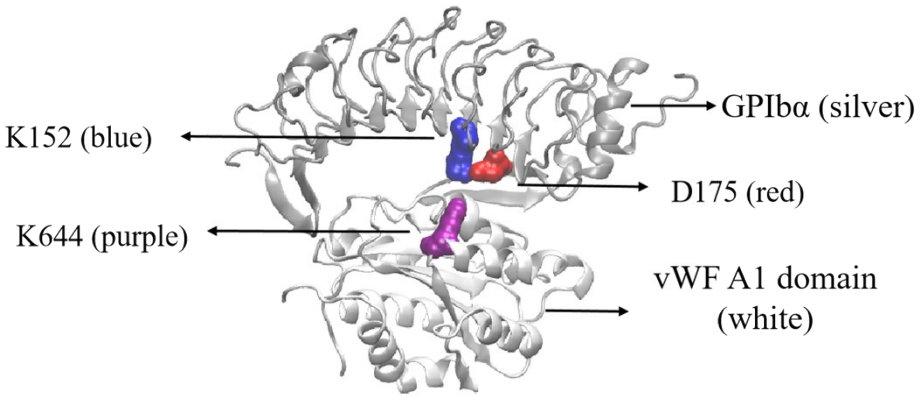


Figure S1. Molecular interface around K644.

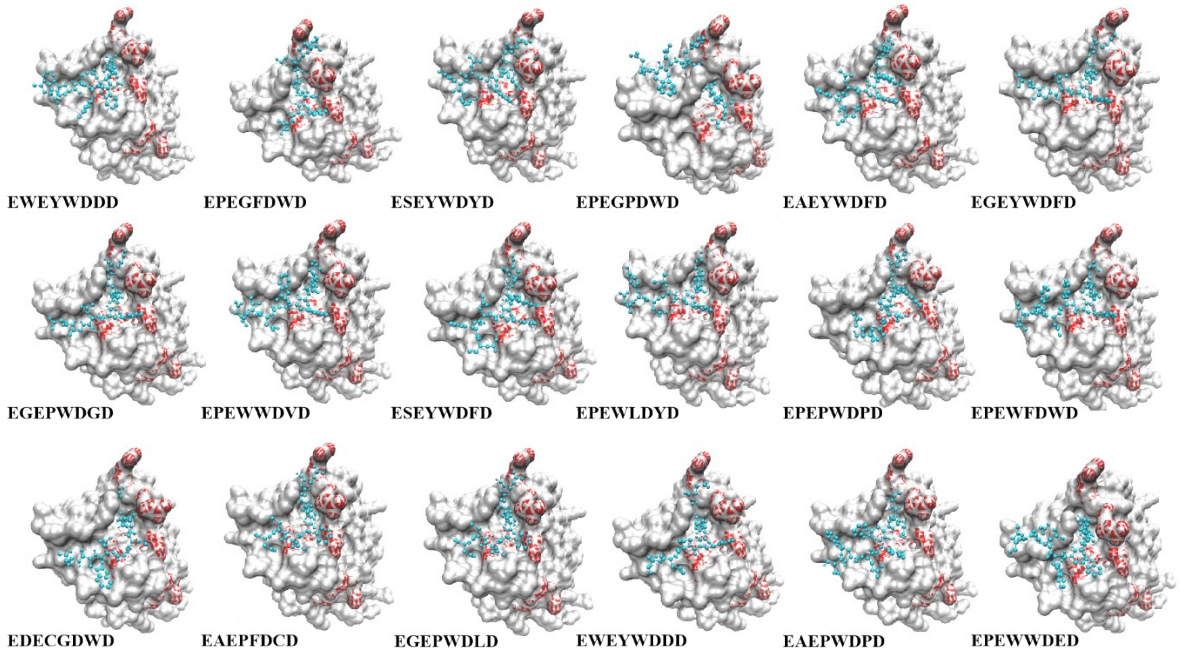


Figure S2. Binding conformation of inhibitors. vWF A1domain is shown as a Surf structure and the key amino acid residues are in red. The inhibitors are shown as a CPK structure in cyan.

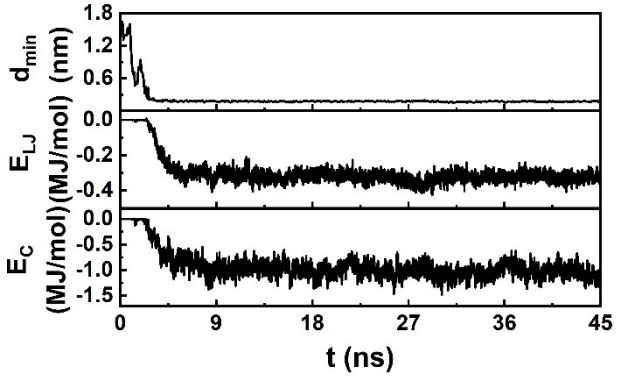


Figure S3. Time courses of $d_{min}$, $E_C$ and $E_{LJ}$ between vWF A1 domain and GPIbα.

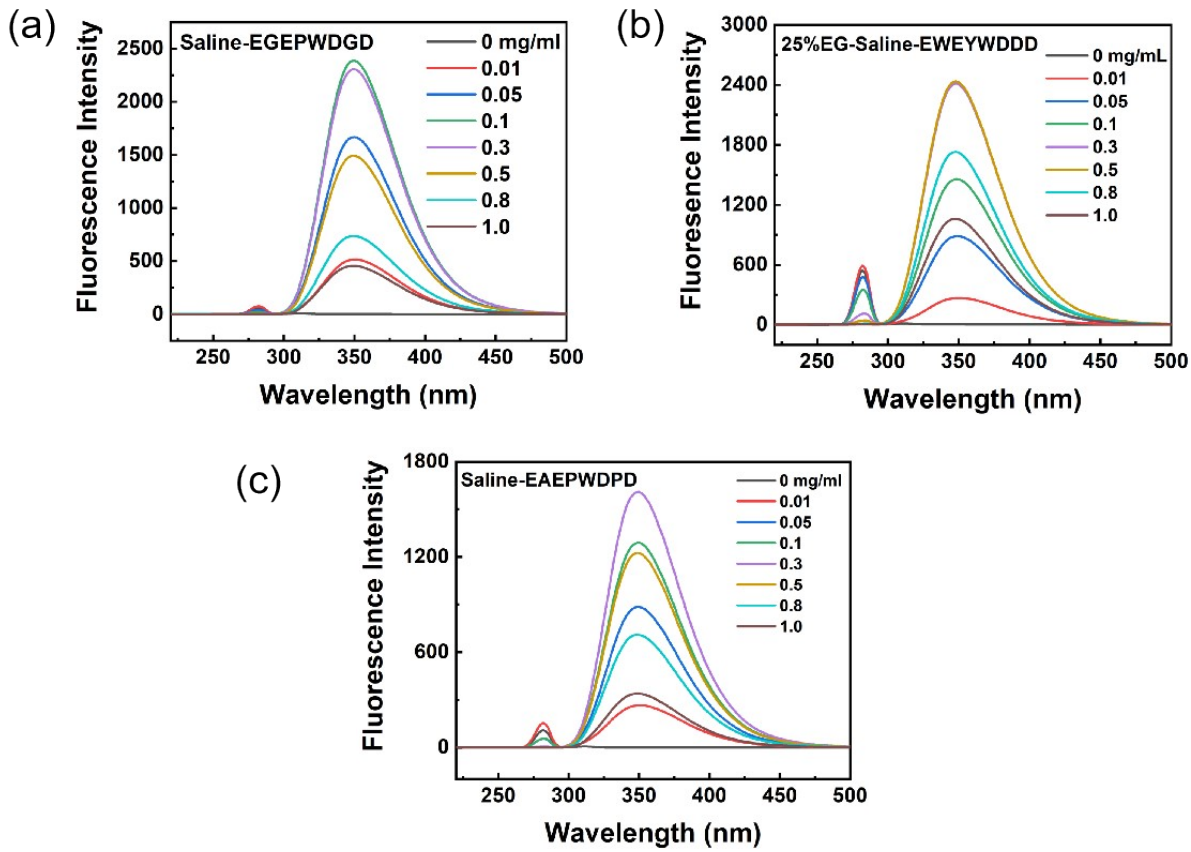


Figure S4. Fluorescence spectra of EGEPWDGD (a), EWEYWDDD (b), EAEPWDPD (c).

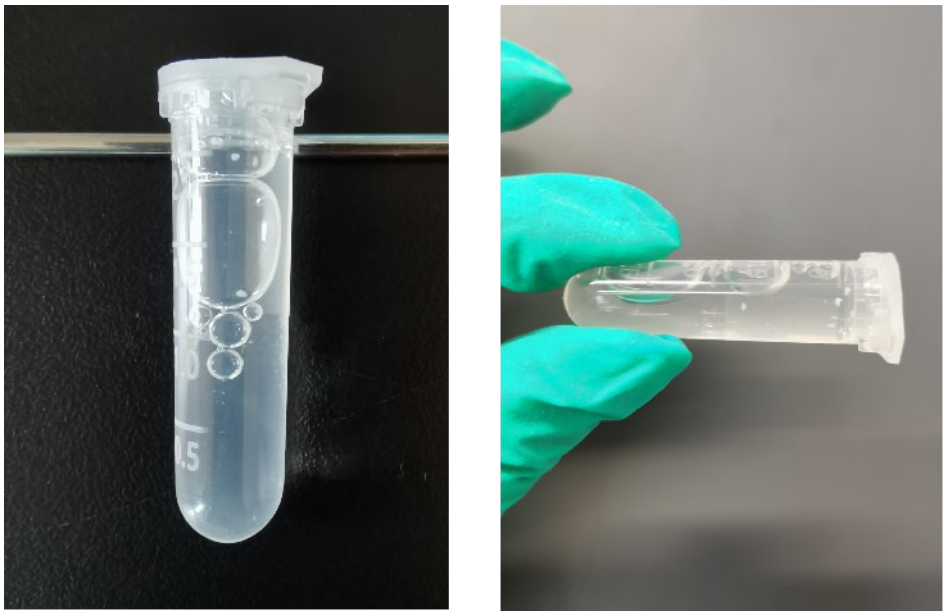

Figure S5. Dissolution of I16 in PRP.