**Supplementary information for**

***In silico* evaluation of pharmacokinetic parameters, delivery, distribution, and anticoagulative effects of new 4,7-dihydroxycoumarin derivative**

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**Figure S1.** Fluorescence emission spectra of **HSA** with the presence of different concentrations of **L** (T = 303 K, pH = 7.4). The initial concentration was [**HSA**] = 2 µM; The concentration of **L** was in the range of [**L**]= 0–5 µM. Inset: Graph dependence of (F0-F)/F on [Q] – Stern-Volmer plots of the fluorescence quenching of **HSA-L** at 303 K with error bars estimated from at three individual measurements.



**Figure S2.** Fluorescence emission spectra of **HSA** with the presence of different concentrations of **L** (T = 310 K, pH = 7.4). The initial concentration was [**HSA**] = 2 µM; The concentration of **L** was in the range of [**L**]= 0–5 µM. Inset: Graph dependence of (F0-F)/F on [Q] – Stern-Volmer plots of the fluorescence quenching of **HSA-L** at 310 K with error bars estimated from at three individual measurements.







**Figure S3.** Graphs of the dependence of log[(F0-F)/F] on log[Q] at different temperatures 296 (up), 303 (middle), and 310 (down) K with error bars estimated from at three individual measurements.

**Table S1.** Binding energies (ΔG*bind*) obtained through the molecular dynamic simulations (kJ mol–1)

|  |  |  |
| --- | --- | --- |
| Compound/Protein | **HSA** | **VKOR** |
| **WF** | -136.4 | -166.8 |
| **L** | -108.2 | -179.8 |