**Supplementary information**

**Investigation of sphingosine kinase 1 inhibitory potential cinchonine and colcemid targeting anticancer therapy**

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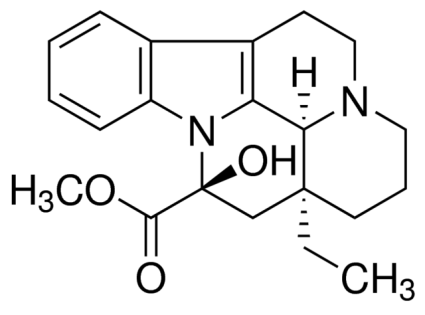
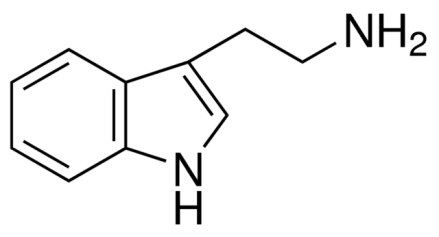
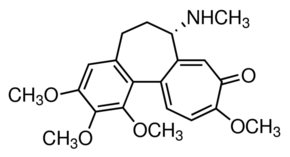
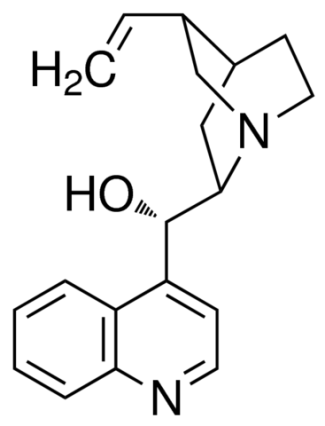
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**A**

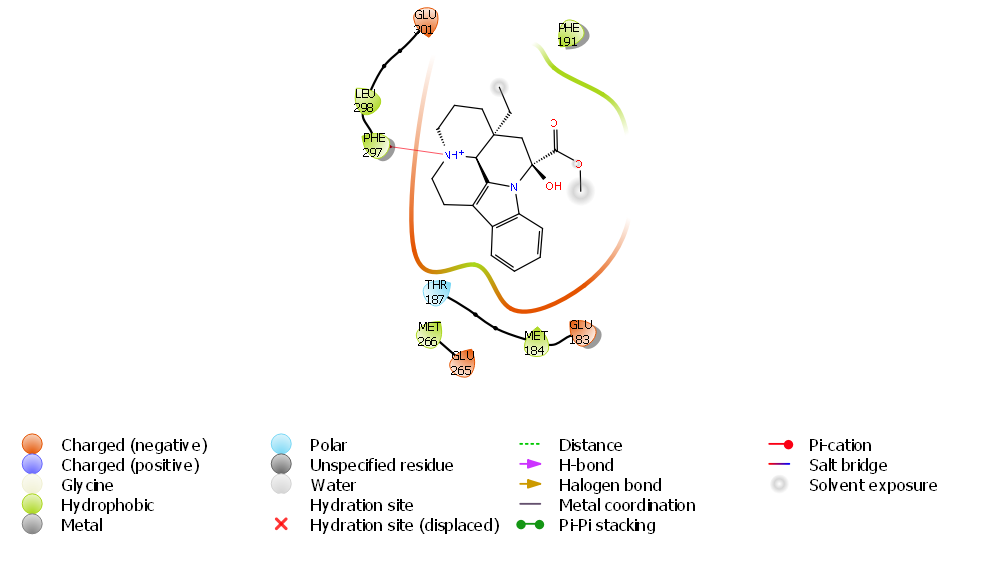
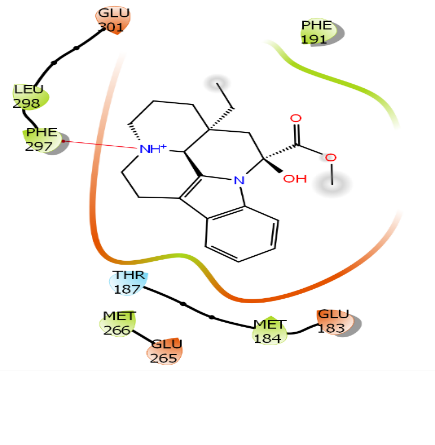
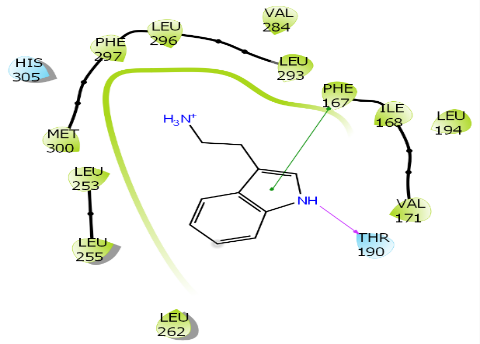
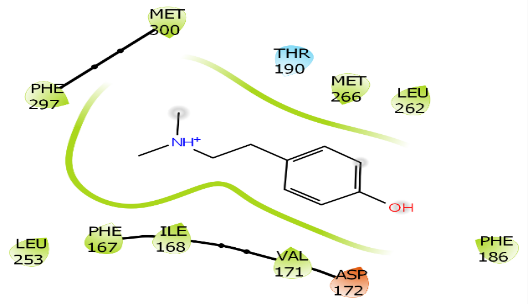
**B**

**C**

**D**

**E**

**Figure S1.** 2D structure of studied compounds. (A) Cinchonine (B) Colcemid (C) Hordenine (D) Tryptamine and (E) Vincamine.

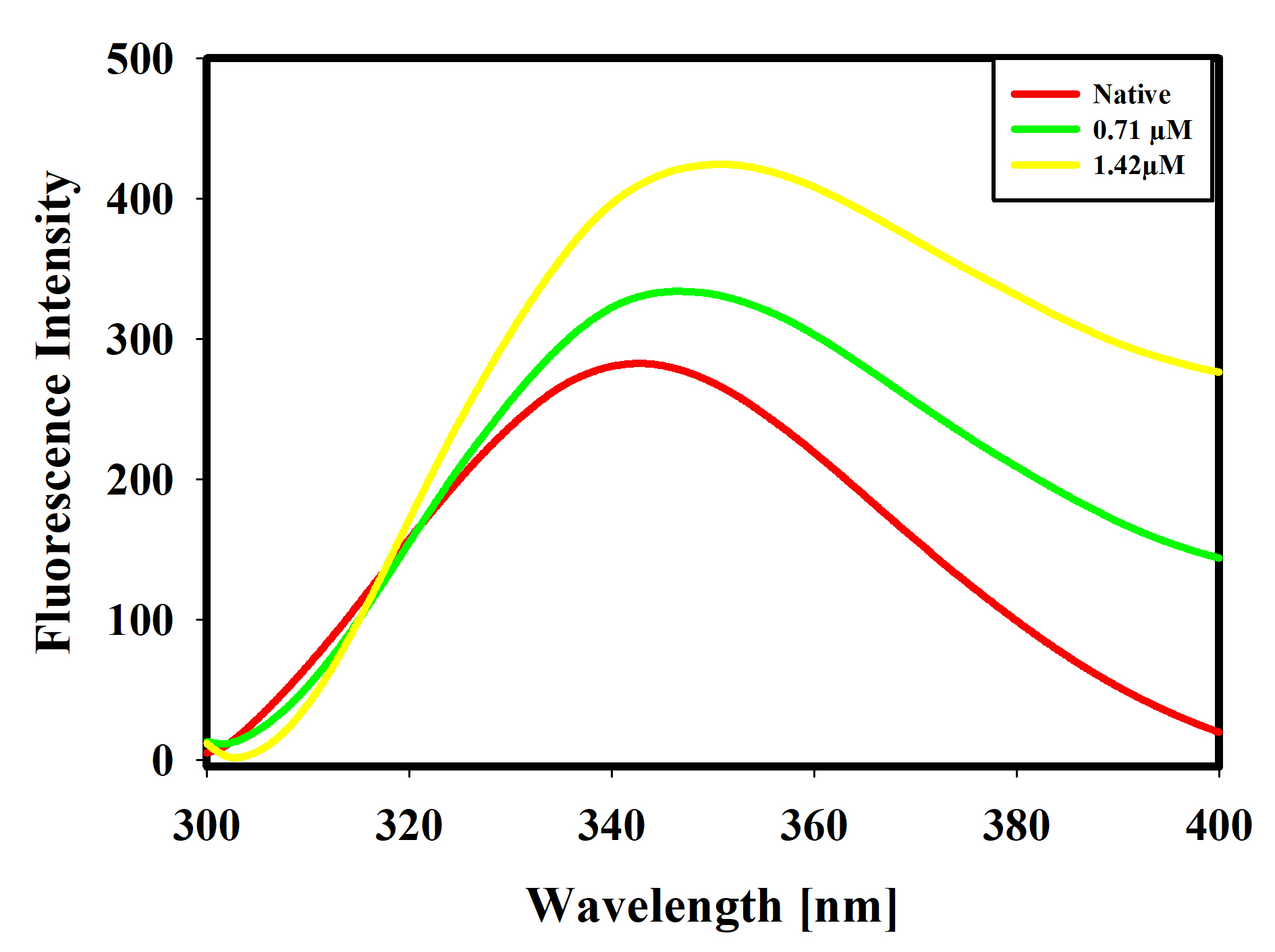
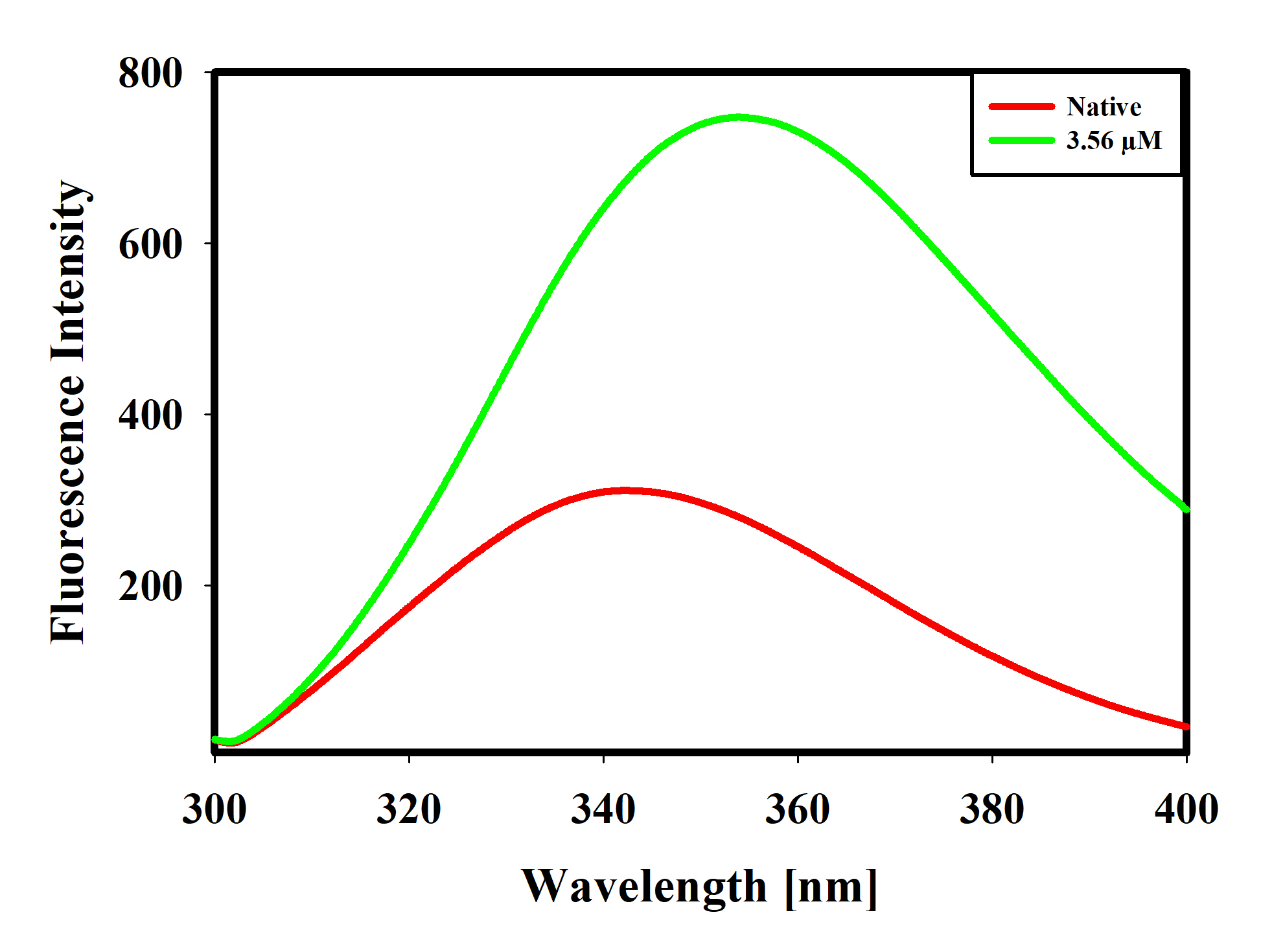
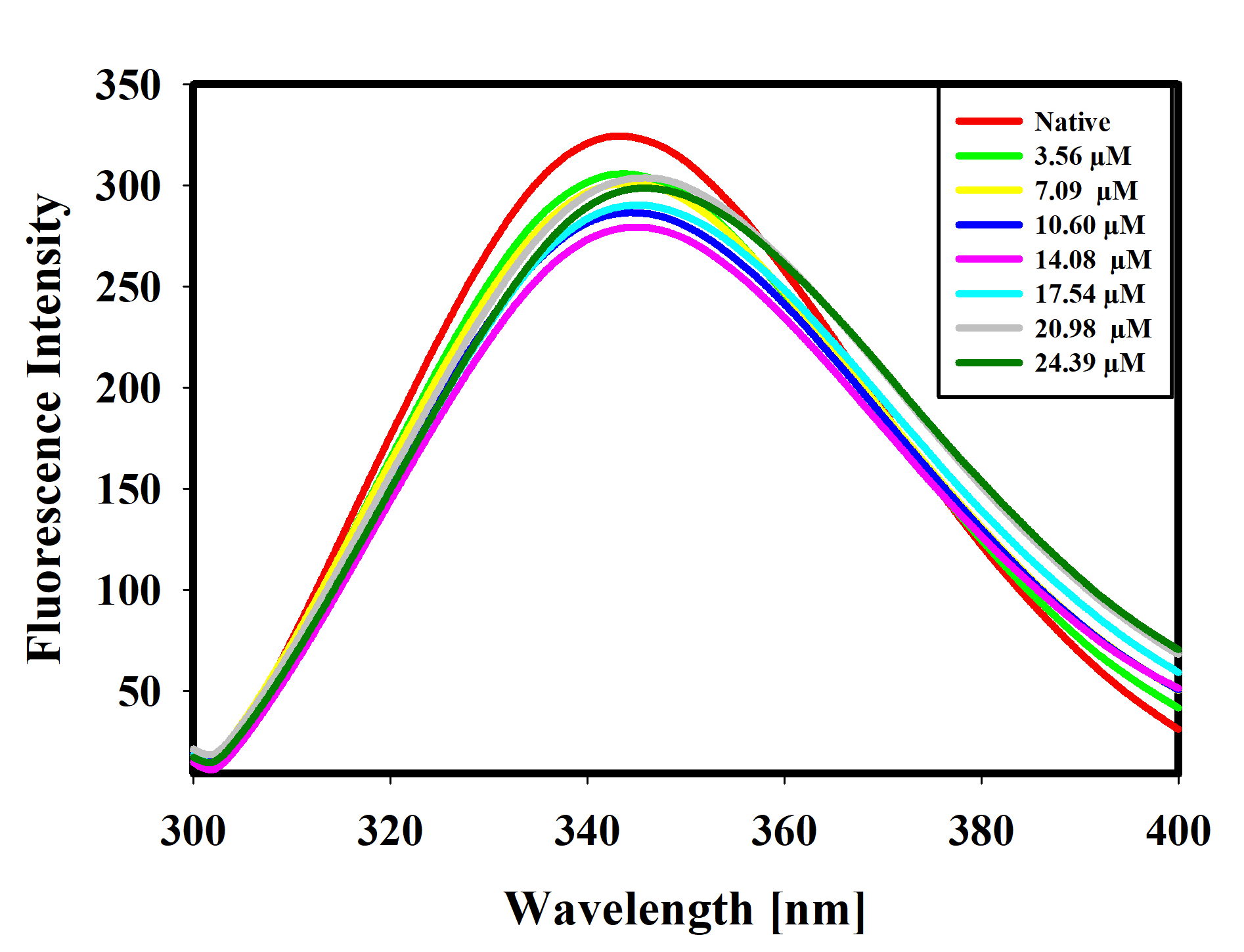


**A**

**B**

**C**

**Figure S2.** Docked poses of SphK1 with the studied inhibitors. Molecular interaction of (A) Hordenine (B) Tryptamine and (C) Vincamine with the active site of SphK1 enzyme.



**A**

**B**

**C**

**Hordenine**

**Tryptamine**

**Vincamine**

**Figure S3.** **Fluorescence binding study of SphK1 with selected alkaloids.** Fluorescence emission spectra of SphK1(4 µM) with increasing concentrations of selected alkaloids at pH 8.0. **A.** Hordenine **B.** Tryptamine **C.** Vincamine

**Table S1.** Docking score of selected and screened alkaloids with their binding site residues.

|  |  |  |
| --- | --- | --- |
| **Compounds** | **Docking score**  **(kcal/mol)** | **Interacting Binding Site Residues** |
| Cinchonine | -8.31 | Leu296, Leu257, Leu255, Leu262, Ala268, Ile168, Met300, Phe167, Thr190, Leu194, Leu293, Val284, Leu313, Cys310, Leu253, Phe282 |
| Colcemid | -7.36 | Ser162, Gly336, Asp335, Ala333, Leu255, Ala164, Ile168, Asp172, Met300, Phe297, Leu262, Met266, Val171, Phe186, Gly263, Thr187, Thr190, Glu183, Gly107, Asn108, Asp75, Ala109, Leu257, Leu161 |
| Hordenine | -5.90 | Met300, Phe297, Thr190, Met266, Leu262, Leu253, Phe167, Ile168, Val171, Asp172 |
| Tryptamine | -1.86 | Thr190, Phe167, Val171, Phe167, Ile168, Leu194, Leu293, Leu296, Val284, Phe297, Met300, His305, Leu253, Leu255, Leu262 |
| Vincamine | -2.99 | Phe297, Leu298, Glu301, Thr187, Met184, Glu183, Met266, Glu265. Phe191 |