**Table S1: Docking Summary of HSA with different coumarin derivatives generated different ligand conformers by the AutoDock program using the Lamarkian Genetic Algorithm. (1) Docking Summary of HSA with CD enamide. (2) Docking Summary of HSA with CD enoate. (3) Docking Summary of HSA with CDM enamide.\***

1. **CD enamide**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Rank** | **Sub-Rank** | **Run** | **Binding Energy [Kcal M-1]** | **Inhibitory Constant Ki** | **Ka [M-1]** |
| **1** | **1** | **7** | **-6.80** | **10.45µM** | **9.56×104** |
| 2 | 1 | 12 | -5.33 | 123.97µM | 8.06×103 |
| 3 | 1 | 11 | -5.22 | 148.09µM | 6.75×103 |
| 4 | 1 | 18 | -5.17 | 161.06µM | 6.21×103 |
| 5 | 1 | 15 | -5.16 | 164.88µM | 6.06×103 |
| 6 | 1 | 4 | -5.09 | 185.00µM | 5.41×103 |
| 7 | 1 | 26 | -5.02 | 209.83µM | 4.76×103 |
| 8 | 1 | 24 | -5.01 | 214.42µM | 4.66×103 |
| 9 | 1 | 5 | -4.73 | 338.25µM | 2.95×103 |
| 10 | 1 | 28 | -4.69 | 362.20µM | 2.76×103 |
| 11 | 1 | 8 | -4.47 | 526.33µM | 1.90×103 |
| 12 | 1 | 25 | -4.36 | 638.33µM | 1.56×103 |
| 12 | 2 | 13 | -4.27 | 737.21µM | 1.36×103 |
| 13 | 1 | 14 | -4.29 | 720.25µM | 1.38×103 |
| 14 | 1 | 17 | -4.19 | 851.30µM | 1.17×103 |
| 15 | 1 | 10 | -4.16 | 897.90µM | 1.11×103 |
| 16 | 1 | 20 | -4.11 | 975.36µM | 1.02×103 |
| 17 | 1 | 9 | -4.10 | 988.98µM | 1.01×103 |
| 18 | 1 | 30 | -4.08 | 1.02mM | 9.80×102 |
| 18 | 2 | 19 | -3.99 | 1.20mM | 8.33×102 |
| 18 | 3 | 16 | -3.91 | 1.37mM | 7.29×102 |
| 19 | 1 | 1 | -3.64 | 2.16mM | 4.63×102 |
| 20 | 1 | 29 | -3.56 | 2.44mM | 4.09×102 |
| 21 | 1 | 22 | -3.51 | 2.69mM | 3.72×102 |
| 22 | 1 | 23 | -3.50 | 2.72mM | 3.67×102 |
| 23 | 1 | 3 | -3.34 | 3.56mM | 2.81×102 |
| 24 | 1 | 2 | -3.32 | 3.70mM | 2.70×102 |
| 25 | 1 | 6 | -2.97 | 6.66mM | 1.50×102 |
| 26 | 1 | 27 | -2.93 | 7.15mM | 1.39×102 |
| 27 | 1 | 21 | -2.35 | 18.95mM | 5.27×101 |

1. **CD enoate**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Rank** | **Sub-Rank** | **Run** | **Binding Energy [Kcal M-1]** | **Inhibitory Constant Ki** | **Ka [M-1]** |
| **1** | **1** | **27** | **-6.69** | **12.57µM** | **7.95×104** |
| 2 | 1 | 1 | -5.32 | 125.63µM | 7.96×103 |
| 3 | 1 | 11 | -5.22 | 149.00µM | 6.71×103 |
| 4 | 1 | 9 | -5.04 | 201.91µM | 4.95×103 |
| 5 | 1 | 23 | -5.00 | 216.92µM | 4.61×103 |
| 6 | 1 | 12 | -4.93 | 243.47µM | 4.11×103 |
| 7 | 1 | 22 | -4.91 | 253.39µM | 3.94×103 |
| 8 | 1 | 26 | -4.91 | 253.63µM | 3.94×103 |
| 9 | 1 | 21 | -4.77 | 319.30µM | 3.13×103 |
| 10 | 1 | 4 | -4.76 | 322.68µM | 3.09×103 |
| 10 | 2 | 13 | -4.63 | 404.35µM | 2.47×103 |
| 11 | 1 | 14 | -4.73 | 339.01µM | 2.95×103 |
| 12 | 1 | 19 | -4.67 | 380.55µM | 2.61×103 |
| 12 | 2 | 25 | -4.61 | 414.42µM | 2.41×103 |
| 13 | 1 | 5 | -4.61 | 416.22µM | 2.40×103 |
| 14 | 1 | 10 | -4.56 | 457.52µM | 2.18×103 |
| 15 | 1 | 18 | -4.45 | 548.46µM | 1.82×103 |
| 16 | 1 | 16 | -4.37 | 624.39µM | 1.60×103 |
| 17 | 1 | 20 | -4.24 | 779.65µM | 1.28×103 |
| 18 | 1 | 28 | -4.23 | 799.74µM | 1.25×103 |
| 19 | 1 | 24 | -4.19 | 855.31µM | 1.17×103 |
| 20 | 1 | 8 | -4.11 | 968.47µM | 1.03×103 |
| 21 | 1 | 7 | -4.09 | 999.68µM | 1.00×103 |
| 22 | 1 | 15 | -4.04 | 1.10mM | 9.09×102 |
| 23 | 1 | 6 | -4.04 | 1.20mM | 8.33×102 |
| 24 | 1 | 3 | -3.74 | 1.80mM | 5.56×102 |
| 25 | 1 | 17 | -3.64 | 2.13mM | 4.69×102 |
| 26 | 1 | 29 | -3.59 | 2.34mM | 4.27×102 |
| 27 | 1 | 2 | -3.56 | 2.46mM | 4.06×102 |
| 28 | 1 | 30 | -3.45 | 2.97mM | 3.36×102 |

1. **CDM enamide**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Rank** | **Sub-Rank** | **Run** | **Binding Energy [Kcal M-1]** | **Inhibitory Constant Ki** | **Ka [M-1]** |
| **1** | **1** | **5** | **-6.37** | **21.50µM** | **4.65×104** |
| 2 | 1 | 12 | -6.18 | 29.47µM | 3.39×104 |
| 3 | 1 | 2 | -6.15 | 30.91µM | 3.24×104 |
| 4 | 1 | 23 | -5.68 | 68.55µM | 1.46×104 |
| 5 | 1 | 26 | -5.67 | 70.02µM | 1.43×104 |
| 6 | 1 | 8 | -5.54 | 87.48µM | 1.14×104 |
| 6 | 2 | 29 | -5.13 | 172.27µM | 5.80×103 |
| 7 | 1 | 17 | -5.36 | 117.30µM | 8.52×103 |
| 8 | 1 | 18 | -5.33 | 123.86µM | 8.07×103 |
| 9 | 1 | 27 | -5.18 | 160.03µM | 6.25×103 |
| 10 | 1 | 22 | -5.12 | 176.27µM | 5.67×103 |
| 11 | 1 | 30 | -5.12 | 177.73µM | 5.63×103 |
| 12 | 1 | 21 | -5.01 | 214.18µM | 4.67×103 |
| 13 | 1 | 24 | -4.67 | 376.69µM | 2.65×103 |
| 14 | 1 | 11 | -4.67 | 377.37µM | 2.65×103 |
| 15 | 1 | 7 | -4.64 | 395.62µM | 2.53×103 |
| 16 | 1 | 16 | -4.58 | 437.68µM | 2.28×103 |
| 17 | 1 | 28 | -4.57 | 450.04µM | 2.22×103 |
| 18 | 1 | 3 | -4.43 | 567.94µM | 1.76×103 |
| 19 | 1 | 10 | -4.39 | 606.45µM | 1.65×103 |
| 20 | 1 | 15 | -4.36 | 642.03µM | 1.56×103 |
| 21 | 1 | 13 | -4.18 | 861.64µM | 1.16×103 |
| 22 | 1 | 4 | -4.17 | 872.25µM | 1.15×103 |
| 23 | 1 | 20 | -4.12 | 961.87µM | 1.04×103 |
| 24 | 1 | 1 | -4.03 | 1.11mM | 9.01×102 |
| 25 | 1 | 14 | -3.93 | 1.32mM | 7.57×102 |
| 26 | 1 | 6 | -3.80 | 1.64mM | 6.09×102 |
| 27 | 1 | 9 | -3.68 | 2.02mM | 4.95×102 |
| 28 | 1 | 25 | -3.37 | 3.36mM | 2.98×102 |
| 29 | 1 | 19 | -2.75 | 9.71mM | 1.03×102 |

\* The lowest free energy conformations are shown by the bold font which are the most stable conformations matching with the fluorescence spectrometry experiments.