

### S1. Top 50 Docking Results

| Rank | Ligand Name                | Docking Scores | xLogP | H-bond donors | H-bond acceptors | Molecular weight | Rotatable bonds | Rat Acute Toxicity LD50 mol/kg | Acute Oral Toxicity |
|------|----------------------------|----------------|-------|---------------|------------------|------------------|-----------------|--------------------------------|---------------------|
| 1    | Schizotenuin F             | 11.8           | 3.48  | 5             | 12               | 551.48           | 12              | 2.24                           | 3                   |
| 2    | Glucopyranoside            | 11.6           | -0.03 | 4             | 10               | 321.33           | 7               | 2.8831                         | 4                   |
| 3    | Emodin-8-beta-D-glucoside  | 11.5           | 0.96  | 6             | 10               | 432.381          | 3               | 2.5573                         | 4                   |
| 4    | Icaritin                   | 11.1           | 4.96  | 3             | 6                | 368.385          | 4               | 2.9476                         | 3                   |
| 5    | Isochlorogenic acid A      | 11             | 1.42  | 6             | 12               | 515.447          | 9               | 2.4467                         | 4                   |
| 6    | Nymphaeol A                | 10.9           | 5.52  | 4             | 6                | 424.493          | 6               | 3.1399                         | 4                   |
| 7    | Lonijaposides A            | 10.8           | -3.91 | 4             | 14               | 578.547          | 13              | 2.4583                         | 4                   |
| 8    | Salvianolic acid A         | 10.8           | 3.01  | 6             | 10               | 493.444          | 9               | 2.3482                         | 4                   |
| 9    | Trifolirhizin-6"-O-malonat | 10.7           | 0.51  | 3             | 13               | 531.446          | 7               | 2.5318                         | 4                   |
| 10   | (+)-Gallocatechin          | 10.6           | 1.08  | 6             | 7                | 306.27           | 1               | 1.87                           | 3                   |
| 11   | Cryptotanshinone           | 10.5           | 3.83  | 0             | 3                | 296.366          | 0               | 2.188                          | 3                   |
| 12   | Verbascoside               | 10.5           | -0.45 | 9             | 15               | 624.592          | 11              | 1.939                          | 3                   |
| 13   | Berbamine                  | 10.5           | 6.24  | 1             | 8                | 608.735          | 3               | 2.671                          | 3                   |
| 14   | 3-Galloylcatechin          | 10.4           | 2.54  | 7             | 10               | 442.376          | 4               | 2.6643                         | 4                   |
| 15   | Salvianolic acid B         | 10.4           | 1.62  | 7             | 16               | 716.604          | 14              | 3.2895                         | 3                   |
| 16   | Echinacoside               | 10.3           | -2.15 | 12            | 20               | 786.733          | 14              | 1.9237                         | 3                   |
| 17   | Indirubin                  | 10.2           | 2.18  | 1             | 4                | 262.268          | 1               | 2.2017                         | 3                   |
| 18   | Orientin                   | 10.2           | 0.003 | 8             | 11               | 448.38           | 3               | 2.3664                         | 4                   |
| 19   | Isocrenatoside             | 10.1           | 0.02  | 8             | 15               | 622.576          | 8               | 2.2693                         | 3                   |
| 20   | Gallotannin                | 10.1           | -     | -             | -                | 2073.541         | -               | 2.5311                         | 3                   |
| 21   | Delphinidin-3-O-glucoside  | 10.1           | -0.1  | 8             | 12               | 464.379          | 4               | 2.4148                         | 3                   |
| 22   | Pulmatin                   | 10             | 1.3   | 5             | 9                | 416.382          | 3               | 2.5573                         | 3                   |
| 23   | Eriocitrin                 | 10             | -1.4  | 9             | 15               | 596.538          | 6               | 2.4984                         | 3                   |

|    |                           |     |       |    |    |         |    |        |   |
|----|---------------------------|-----|-------|----|----|---------|----|--------|---|
| 24 | Ginkgolide B              | 10  | -2.38 | 3  | 10 | 424.402 | 1  | 2.497  | 3 |
| 25 | Isorhoifolin              | 10  | -0.02 | 8  | 14 | 578.523 | 6  | 2.4367 | 3 |
| 26 | Forsythoside A            | 10  | -0.23 | 9  | 15 | 624.592 | 11 | 2.2295 | 3 |
| 27 | Hellicoside               | 10  | -1.16 | 11 | 17 | 656.59  | 12 | 2.1005 | 3 |
| 28 | 2'-Methoxykurarinone      | 9.9 | 5.9   | 2  | 6  | 452.547 | 8  | 3.1774 | 3 |
| 29 | Mangiferin                | 9.9 | -0.16 | 8  | 11 | 422.342 | 2  | 2.3664 | 4 |
| 30 | Luteolin 7-galactoside    | 9.9 | 0.19  | 7  | 11 | 448.38  | 4  | 2.3869 | 3 |
| 31 | Isosalvianolic acid C     | 9.9 | 3.38  | 6  | 10 | 492.436 | 7  | 3.4184 | 2 |
| 32 | Melittoside               | 9.9 | -4.64 | 10 | 15 | 524.472 | 7  | 2.6373 | 4 |
| 33 | 3,5-Dicaffeoylquinic acid | 9.9 | 1.42  | 6  | 12 | 515.447 | 9  | 2.4214 | 3 |
| 34 | Baicalein                 | 9.9 | 2.68  | 3  | 5  | 270.24  | 1  | 3.02   | 2 |
| 35 | Isoacteoside              | 9.8 | -0.23 | 9  | 15 | 624.592 | 11 | 2.0947 | 3 |
| 36 | Arctigenin                | 9.8 | 2.22  | 1  | 6  | 372.417 | 7  | 2.5844 | 3 |
| 37 | Nystose                   | 9.8 | -5.08 | 14 | 21 | 666.579 | 13 | 1.3683 | 3 |
| 38 | Narirutin 4'-glucoside    | 9.8 | -2.9  | 11 | 19 | 742.68  | 9  | 2.0375 | 3 |
| 39 | Lucidumoside A            | 9.8 | 0.54  | 5  | 12 | 526.535 | 12 | 2.585  | 3 |
| 40 | Quercetin                 | 9.8 | 1.68  | 5  | 7  | 302.238 | 1  | 3.02   | 2 |
| 41 | Lobetyolinin              | 9.7 | -1.64 | 9  | 13 | 558.577 | 12 | 1.6964 | 2 |
| 42 | Curcumin                  | 9.6 | 2.3   | 2  | 6  | 368.385 | 8  | 2.5468 | 3 |
| 43 | Isoangustone A            | 9.4 | 6.04  | 4  | 6  | 422.477 | 5  | 3.0645 | 3 |
| 44 | Lycoponic acid B          | 9.2 | 2.63  | 8  | 16 | 718.62  | 14 | 3.3595 | 2 |
| 45 | Andrographolide           | 9   | 1.05  | 3  | 5  | 350.455 | 3  | 3.0943 | 3 |
| 46 | Cynaroside                | 8.9 | 0.19  | 7  | 11 | 448.38  | 4  | 2.3869 | 3 |
| 47 | Astringin                 | 8.8 | 0.71  | 7  | 9  | 406.387 | 5  | 2.1382 | 3 |
| 48 | Oleracein A               | 8.8 | -2.01 | 7  | 11 | 503.46  | 6  | 2.3343 | 3 |
| 49 | Ursolic acid              | 8.7 | 6.79  | 1  | 3  | 455.703 | 1  | 2.1645 | 3 |
| 50 | Sanggenol A               | 8.7 | 5.92  | 4  | 6  | 424.493 | 6  | 3.3264 | 3 |

## S2. The JAK3 Kinase Activity Inhibitory Effects of 12 Phytochemicals

| No. | Phytochemical      | Docking Results | JAK3 Kinase Activity Inhibitory Effect (%) |                   |                  |                  |                  |                  |
|-----|--------------------|-----------------|--|-------------------|------------------|------------------|------------------|------------------|
|     |                    |                 | 3.125 $\mu$ M                              | 6.25 $\mu$ M      | 12.5 $\mu$ M     | 25 $\mu$ M       | 50 $\mu$ M       | 100 $\mu$ M      |
| 1   | Andrographolide    | 9               | 75.82 $\pm$ 2.86                           | 68.84 $\pm$ 2.16  | 68.35 $\pm$ 1.06 | 59.44 $\pm$ 1.78 | 60.33 $\pm$ 2.08 | 60.72 $\pm$ 3.86 |
| 2   | Arctigenin         | 9.8             | 90.35 $\pm$ 1.76                           | 77.28 $\pm$ 1.94  | 79.24 $\pm$ 2.75 | 78.12 $\pm$ 3.05 | 76.54 $\pm$ 1.64 | 72.89 $\pm$ 1.67 |
| 3   | Baicalein          | 9.9             | 85.32 $\pm$ 2.22                           | 86.35 $\pm$ 3.16  | 84.47 $\pm$ 2.86 | 83.88 $\pm$ 1.88 | 78.25 $\pm$ 2.32 | 71.45 $\pm$ 3.18 |
| 4   | Berbamine          | 10.5            | 79.36 $\pm$ 3.42                           | 78.33 $\pm$ 3.81  | 75.42 $\pm$ 2.85 | 71.65 $\pm$ 3.26 | 70.73 $\pm$ 2.89 | 66.82 $\pm$ 2.18 |
| 5   | Cryptotanshinone   | 10.5            | 67.48 $\pm$ 1.79                           | 53.18 $\pm$ 2.19  | 47.71 $\pm$ 1.96 | 43.60 $\pm$ 2.19 | 39.63 $\pm$ 2.46 | 32.18 $\pm$ 3.16 |
| 6   | Curcumin           | 9.6             | 88.04 $\pm$ 3.56                           | 78.51 $\pm$ 3.62  | 80.36 $\pm$ 2.91 | 72.64 $\pm$ 2.43 | 62.66 $\pm$ 1.07 | 61.83 $\pm$ 3.92 |
| 7   | Ginkgolide B       | 10              | 100.31 $\pm$ 2.61                          | 98.62 $\pm$ 4.06  | 96.34 $\pm$ 2.89 | 91.85 $\pm$ 3.71 | 91.67 $\pm$ 2.99 | 88.19 $\pm$ 2.84 |
| 8   | Icaritin           | 11.1            | 56.84 $\pm$ 2.10                           | 52.73 $\pm$ 2.07  | 45.17 $\pm$ 2.04 | 41.09 $\pm$ 2.23 | 37.43 $\pm$ 0.55 | 34.81 $\pm$ 2.62 |
| 9   | Indirubin          | 10.2            | 64.39 $\pm$ 3.24                           | 54.45 $\pm$ 2.18  | 50.14 $\pm$ 2.74 | 44.85 $\pm$ 1.40 | 42.28 $\pm$ 2.25 | 38.47 $\pm$ 3.05 |
| 10  | Quercetin          | 9.8             | 86.45 $\pm$ 2.37                           | 81.76 $\pm$ 2.98  | 82.67 $\pm$ 3.28 | 75.06 $\pm$ 3.33 | 72.82 $\pm$ 2.75 | 71.67 $\pm$ 2.66 |
| 11  | Salvianolic acid B | 10.4            | 82.85 $\pm$ 3.83                           | 83.20 $\pm$ 1.85  | 81.64 $\pm$ 2.48 | 82.60 $\pm$ 3.76 | 78.54 $\pm$ 4.51 | 80.28 $\pm$ 3.45 |
| 12  | Ursolic acid       | 8.7             | 101.36 $\pm$ 3.78                          | 102.81 $\pm$ 4.24 | 98.37 $\pm$ 1.96 | 85.25 $\pm$ 1.26 | 87.36 $\pm$ 4.26 | 75.06 $\pm$ 2.98 |