### Supplementary Table 1: The selected JAK1 hits from molecular docking study.

| S. No | Hypothesis | Molecule ID | Fitness | Docking Score SP | Docking Score XP | Glide Energy |
|-------|------------|------------|---------|------------------|------------------|--------------|
| 1     | ADHRRR     | T5920852   | 1.55    | -6.402           | -11.510          | -54.576      |
| 2     | ADPRR      | T5925648   | 1.90    | -7.902           | -11.162          | -50.357      |
| 3     | DDHRR      | ZINC41165444 | 2.05   | -8.509           | -11.097          | -45.811      |
| 4     | ADPRR      | ZINC95449166 | 2.07   | -6.683           | -10.894          | -50.271      |
| 5     | ADPRR      | ZINC65591421 | 2.04   | -5.764           | -10.883          | -46.471      |
| 6     | ADPRR      | F3289-1086 | 2.09    | -7.945           | -10.867          | -57.806      |
| 7     | DDHRR      | T6763842   | 1.83    | -7.550           | -10.671          | -51.703      |
| 8     | DDHRR      | ST088474   | 1.73    | -9.293           | -10.653          | -50.800      |
| 9     | DDHRR      | T6229048   | 1.87    | -8.456           | -10.610          | -51.663      |
| 10    | ADPRR      | T6112362   | 1.84    | -8.158           | -10.532          | -58.182      |
| 11    | DDHRR      | ZINC97480470 | 2.02 | -10.712          | -10.463          | -57.656      |
| 12    | ADPRR      | T5760493   | 1.85    | -7.388           | -10.385          | -48.594      |
| 13    | DRRRR      | T6649932   | 1.55    | -7.536           | -10.335          | -61.771      |
| 14    | ADPRR      | ZINC72148730 | 2.02  | -7.570          | -10.327          | -47.485      |
| 15    | DRRRR      | ZINC77955167 | 2.38  | -6.693           | -10.322          | -53.710      |
| 16    | DDHRR      | ZINC72405250 | 2.15  | -9.124          | -10.306          | -42.617      |
| 17    | DRRRR      | T5923531   | 1.52    | -7.102           | -10.303          | -57.350      |
| 18    | DHRRR      | ZINC68605539 | 2.00  | -7.213           | -10.274          | -45.465      |
| 19    | DPRRR      | ZINC77955168 | 2.06  | -5.524           | -10.266          | -49.226      |
| 20    | DDHRR      | ZINC97480473 | 2.03  | -10.146         | -10.260          | -60.729      |
| 21    | ADPRR      | ZINC65611240 | 2.04  | -7.597           | -10.238          | -45.553      |
| 22    | DDHRR      | ZINC78525289 | 2.19  | -8.123           | -10.230          | -56.090      |
| 23    | ADPRR      | ZINC19741573 | 2.11  | -6.925           | -10.221          | -42.384      |
| 24    | ADPRR      | T6900679   | 1.82    | -6.196           | -10.206          | -49.888      |
| 25    | DRRRR      | ZINC77955172 | 2.13  | -5.963           | -10.201          | -20.930      |
| 26    | ADPRR      | ZINC97159261 | 2.03  | -7.367           | -10.185          | -50.345      |
| 27    | ADPRR      | ZINC97160064 | 2.01  | -8.715           | -10.182          | -46.672      |
| 28    | DHRRR      | ZINC01545892 | 2.00  | -6.951           | -10.137          | -45.520      |
| 29    | ADPRR      | T5919457   | 1.84    | -6.536           | -10.123          | -51.724      |
| 30    | ADPRR      | T5773547   | 1.84    | -6.877           | -10.114          | -57.905      |
| 31    | DDHRR      | ZINC05903136 | 2.11  | -8.228           | -10.111          | -44.202      |
| 32    | DDHRR      | F2491-0101 | 2.12    | -7.766           | -10.105          | -45.273      |
| 33    | ADPRR      | T5661069   | 1.87    | -6.811           | -10.080          | -53.208      |
| 34    | ADPRR      | ZINC73737252 | 2.08  | -7.180           | -10.072          | -46.391      |
| 35    | ADPRR      | T6640882   | 1.83    | -5.524           | -10.071          | -46.301      |
| 36    | ADPRR      | G275-1407  | 1.91    | -7.003           | -10.066          | -48.996      |
| 37    | DDHRR      | ZINC72171525 | 2.22  | -8.156           | -10.062          | -46.311      |
| S. No | Hypothesis | Molecule ID     | Fitness | Docking Score SP | Docking Score XP | Glide Energy |
|-------|------------|----------------|---------|------------------|------------------|--------------|
| 38    | ADPRR      | T6385529       | 1.92    | -7.210           | -10.060          | -48.558      |
| 39    | ADPRR      | ZINC95449165   | 2.02    | -5.933           | -10.059          | -51.392      |
| 40    | ADPRR      | ZINC95469612   | 2.06    | -9.074           | -10.052          | -51.190      |
| 41    | DDHRR      | T6789630       | 1.72    | -8.085           | -10.037          | -58.596      |
| 42    | DDRRR      | ZINC77971158   | 2.37    | -7.943           | -10.037          | -50.510      |
| 43    | ADPRR      | ZINC71839171   | 2.01    | -7.376           | -10.021          | -49.216      |
| 44    | ADPRR      | T6865686       | 1.92    | -6.340           | -10.020          | -52.972      |
| 45    | DDRRR      | T5923555       | 1.77    | -8.482           | -10.015          | -57.500      |
| 46    | ADPRR      | T6466231       | 1.84    | -6.162           | -10.012          | -56.528      |
| 47    | DDHRR      | ZINC50767136   | 2.11    | -8.849           | -10.012          | -47.800      |
| 48    | ADPRR      | T5923533       | 2.01    | -6.635           | -10.009          | -59.962      |
| 49    | DDHRR      | T6067538       | 1.71    | -6.545           | -9.987           | -54.848      |
| 50    | DDRRR      | T5923502       | 1.72    | -7.674           | -9.986           | -56.441      |
| 51    | DDRRR      | ZINC77971142   | 2.25    | -8.643           | -9.957           | -53.041      |
| 52    | DDRRR      | ZINC77971114   | 2.24    | -8.639           | -9.953           | -53.005      |
| 53    | DHRRR      | T5923452       | 1.84    | -5.751           | -9.939           | -55.519      |
| 54    | DPRRR      | ZINC13541700   | 2.07    | -8.792           | -9.930           | -52.928      |
| 55    | DDRRR      | T5881519       | 1.51    | -6.373           | -9.882           | -47.103      |
| 56    | DDRRR      | ZINC77971139   | 2.27    | -8.553           | -9.872           | -50.493      |
| 57    | DDRRR      | T5923554       | 1.56    | -7.265           | -9.866           | -57.223      |
| 58    | ADRRR      | T05034595      | 1.72    | -5.378           | -9.852           | -42.346      |
| 59    | DPRRR      | F3234-0530     | 2.05    | -9.017           | -9.841           | -52.467      |
| 60    | DDRRR      | T5927095       | 1.78    | -7.570           | -9.837           | -56.367      |
| 61    | DHRRR      | ZINC77955184   | 2.32    | -6.045           | -9.833           | -50.798      |
| 62    | DDRRR      | T5927094       | 1.56    | -7.686           | -9.827           | -56.589      |
| 63    | DHRRR      | T5707836       | 2.17    | -7.900           | -9.827           | -51.760      |
| 64    | ADRRR      | T5865427       | 1.80    | -8.327           | -9.826           | -51.927      |
| 65    | DDHRR      | T6052252       | 1.68    | -6.692           | -9.819           | -46.423      |
| 66    | DDHRR      | T5506536       | 1.77    | -4.042           | -9.816           | -48.785      |
| 67    | DDHRR      | T6783264       | 1.74    | -7.548           | -9.813           | -52.850      |
| 68    | DDRRR      | F3289-1128     | 1.57    | -5.178           | -9.808           | -55.279      |
| 69    | DHRRR      | F3259-0214     | 1.87    | -8.507           | -9.807           | -49.673      |
| 70    | DDRRR      | T5927106       | 1.83    | -7.125           | -9.803           | -56.420      |
| 71    | DHRRR      | T5769827       | 1.85    | -6.422           | -9.803           | -61.820      |
| 72    | DDRRR      | T5923480       | 1.78    | -6.759           | -9.797           | -57.541      |
| 73    | DDRRR      | T5927092       | 1.50    | -6.235           | -9.794           | -58.554      |
| 74    | DDRRR      | F6000-0016     | 1.75    | -8.034           | -9.793           | -56.378      |
| 75    | DDRRR      | T6649944       | 1.82    | -8.808           | -9.771           | -54.217      |
| S. No | Hypothesis | Molecule ID   | Fitness | Docking Score SP | Docking Score XP | Glide Energy |
|-------|------------|---------------|---------|------------------|------------------|--------------|
| 76    | DDHRR      | T5564236      | 1.79    | -7.526           | -9.762           | -54.207      |
| 77    | DDRRR      | T5923496      | 1.69    | -7.299           | -9.754           | -54.701      |
| 78    | DDRRR      | T5927123      | 1.54    | -5.955           | -9.739           | -56.169      |
| 79    | DHRRR      | T5720930      | 1.81    | -8.840           | -9.729           | -48.047      |
| 80    | DDRRR      | F3289-0901    | 1.81    | -7.839           | -9.727           | -54.174      |
| 81    | DDRRR      | T5927134      | 1.56    | -7.465           | -9.719           | -51.019      |
| 82    | DDRRR      | F3289-1111    | 1.59    | -7.191           | -9.711           | -55.262      |
| 83    | DDHRR      | T5858364      | 1.69    | -8.797           | -9.710           | -49.045      |
| 84    | DHRRR      | T5648531      | 1.72    | -7.520           | -9.707           | -56.272      |
| 85    | DPRRR      | F3234-0076    | 2.06    | -8.958           | -9.703           | -50.851      |
| 86    | DDHRR      | T6215014      | 1.74    | -7.148           | -9.703           | -51.314      |
| 87    | DDRRR      | T6652943      | 1.68    | -7.230           | -9.690           | -46.975      |
| 88    | DDRRR      | T5923437      | 1.84    | -6.298           | -9.684           | -57.616      |
| 89    | DHRRR      | T5941474      | 1.79    | -7.673           | -9.648           | -56.128      |
| 90    | DHRRR      | T5740560      | 1.82    | -7.723           | -9.630           | -56.340      |
Supplementary Figure 1: The contribution maps of highly active compounds in the dataset.

Supplementary Figure 2: The validation of Glide XP docking program using ROC plot.
Supplementary Figure 3 (a)-(f): The representation of docked lead compounds and drug present inside the ATP-binding site of JAK1 after induced fit docking.
**Supplementary Figure 4:** The representation of lead compounds (pink) and drug (green) inside the ATP-binding site after molecular docking and dynamics study.