Table 1: Biological activity data of the molecules.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sl. No. | Drug name | Structures | IC50(µM) | pIC50(µM) | Reference |
| 1 | Ebselen |  | 0.67 | 0.173 | [10] |
| 2 | Disulfiram |  | 9.35 | -0.970 |
| 3 | Tideglusib |  | 1.55 | -0.190 |
| 4 | Carmofur |  | 1.82 | -0.260 |
| 5 | Shikonin |  | 15.75 | -1.197 |
| 6 | 11a |  | 0.053 | 1.275 | [18] |
| 7 | 11b |  | 0.04 | 1.397 |
| 8 | 11r |  | 0.18 | 0.744 | [19] |
| 9 | 13a |  | 2.39 | -0.378 |
| 10 | 13b(alpha-ketoamide) |  | 0.67 | 0.173 |
| 11 | Simeprevir |  | 13.74 | -1.137 | [20] |
| 12 | Boceprevir |  | 4.13 | -0.615 |
| 13 | Narlaprevir |  | 5.73 | -0.758 |
| 14 | MG-132 |  | 3.9 | -0.591 |
| 15 | Calpeptin |  | 10.69 | -1.028 |
| 16 | Calpain inhibitor I (ALLN) |  | 8.6 | -0.934 |
| 17 | MG-115 |  | 3.14 | -0.496 |
| 18 | Calpain inhibitor II (ALLM) |  | 0.97 | 0.013 |
| 19 | Calpain inhibitor XII |  | 0.45 | 0.346 |
| 20 | PSI |  | 10.38 | -1.016 |
| 21 | Baicalin |  | 6.41 | -0.806 | [21] |
| 22 | Baicalein |  | 0.94 | 0.026 |
| 23 | Chloroquine (Rac) |  | 1.801 | -0.255 | [22] |
| 24 | S-Chloroquine |  | 1.761 | -0.245 |
| \*25 | R-Chloroquine |  | 1.975 | -0.295 |
| 26 | Hydroxychloroquine (Rac) |  | 1.752 | -0.243 |
| 27 | S-Hydroxychloroquine |  | 1.444 | -0.159 |
| 28 | R-Hydroxychloroquine |  | 2.445 | -0.388 |
| 29 | Azithromycin |  | 15.75 | -1.197 |
| 30 | Ivermectin |  | 2.8 | -0.447 | [23] |
| 31 | N1 |  | 1.11 | -0.045 | [18] |
| 32 | N3 |  | 125 | -2.096 | [10] |
| 33 | N9 |  | 0.9 | 0.045 | [18] |
| 34 | UAWJ243 |  | 0.41 | 0.387 | [24] |
| 35 | UAWJ246 |  | 0.045 | 1.346 |
| 36 | UAWJ247 |  | 0.045 | 1.346 |
| 37 | UAWJ248 |  | 0.042 | 1.376 |
| 38 | Manidipine |  | 4.8 | -0.681 | [25] |
| 39 | lercanidipine |  | 16.2 | -1.209 |
| 40 | Bedaquiline |  | 18.7 | -1.271 |

Table 5: External data set along with modeled structural descriptors, observed and predicted activities

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sl. No. | Comp.name | Structures | Modeled parameters | Observed pIC50 | Pred pIC50 |
| ATSC7v | maxHBint10 | VR1\_Dzi | MinsCH3 |
| 41 | GC373 |  | 203.915 | 5.084 | 400.922 | 1.927 | 0.397 | 0.329 |
| 42 | GC376 |  | -229.929 | 5.150 | 351.878 | 1.831 | 0.721 | 0.210 |
| 43 | GC376 derivative 6a |  | -30.378 | 5.050 | 289.682 | 1.952 | 0.086 | 0.258 |
| 44 | GC376 derivative 6c |  | 136.772 | 5.085 | 529.136 | 1.962 | 0.552 | 0.242 |
| 45 | GC376 derivative 6e |  | 160.877 | 5.089 | 404.174 | 1.965 | 0.769 | 0.298 |
| 46 | GC376 derivative 6h |  | 34.737 | 5.135 | 8217.574 | 1.871 | 0.366 | -2.605 |
| 47 | GC376 derivative 6j |  | 133.887 | 5.100 | 402.192 | 1.884 | 0.318 | 0.317 |
| 48 | GC376 derivative 7a |  | -429.898 | 5.115 | 331.929 | 1.856 | 0.187 | 0.119 |
| 49 | GC376 derivative 7c |  | -13.570 | 5.135 | 1383.37 | 1.864 | 0.638 | -0.094 |
| 50 | GC376 derivative 7e |  | -115.938 | 5.137 | 499.692 | 1.866 | 0.698 | 0.188 |
| 51 | GC376 derivative 7h |  | -383.017 | 5.201 | 468.35 | 1.775 | 0.387 | 0.130 |
| 52 | GC376 derivative 7j |  | -275.647 | 5.166 | 911.423 | 1.787 | 0.346 | 0.001 |
| 53 | Walrycin B |  | -413.339 | 0 | 196.972 | 1.260 | 0.585 | -0.406 |
| 54 | AMG-837 |  | -144.346 | 0 | 312.661 | 1.671 | -1.382 | -0.481 |
| 55 | Z-DEVD-FMK (Caspase-3 Inhibitor) |  | -628.969 | 5.508 | 2468.365 | 1.041 | -0.833 | -0.406 |
| 56 | Z-FA-FMK |  | 311.686 | 0 | 278.213 | 1.395 | -1.055 | -0.179 |
| 57 | LLL-12 |  | -269.232 | 0 | 189.301 | 0 | -0.993 | 0.101 |
| 58 | DA-3003-1 |  | -221.67 | 0 | 228.057 | 0 | -0.419 | 0.107 |
| 59 | CAY-10581 |  | -418.67 | 0 | 376.209 | 1.719 | -0.963 | -0.636 |
| 60 | Fascaplysin |  | 108.049 | 0 | 198.823 | 0 | -0.998 | 0.256 |
| 61 | β-Lapachone |  | -948.459 | 0 | 179.88 | 2.000 | -1.124 | -0.886 |
| 62 | Sepantronium bromide |  | -1466.7 | 0 | 1948.568 | 1.612 | -1.133 | -1.621 |
| 63 | NSC95397 |  | -1377.94 | 0 | 214.219 | 0 | -1.253 | -0.372 |
| 64 | 4E1RCat |  | 157.9256 | 0 | 405.7154 | 0 | -1.261 | 0.201214 |
| 65 | TBB |  | 0 | 0 | 268.491 | 0 | -1.311 | 0.185 |
| 66 | GW-0742 |  | 91.393 | 0 | 379.674 | 1.881 | -1.347 | -0.481 |
| 67 | Agaric acid |  | 3.916 | 0 | 270.743 | 2.222 | -1.371 | -0.597 |
| 68 | MK0893 |  | -315.615 | 0 | 456.294 | 1.674 | -1.386 | -0.607 |
| 69 | SU 16f |  | -925.42 | 8.139 | 335.422 | 1.931 | -1.397 | 0.351 |
| 70 | Penta-O-galloyl-Beta-D-glucose hydrate |  | -456.249 | 6.948 | 1050.838 | 0 | -1.443 | 0.781 |
| 71 | SP100030 |  | 46.220 | 0 | 235.287 | 0 | -1.460 | 0.217 |
| 72 | Anacardic acid |  | 48.263 | 0 | 241.401 | 2.258 | -1.042 | -0.581 |
| 73 | Adomeglivant |  | 476.373 | 6.011 | 515.548 | 1.953 | -1.282 | 0.536 |
| 74 | Eltrombopag olamine |  | -513.675 | 0 | 441.005 | 1.723 | -1.332 | -0.702 |
| 75 | GSK-3965 |  | -390.592 | 1.420 | 399.888 | 0 | -1.332 | 0.193 |
| 76 | GW5074 |  | 531.705 | 0 | 261.699 | 0 | -1.332 | 0.411 |
| 77 | Hexachlorophene |  | -115.812 | 0 | 499.692 | 0 | -1.332 | 0.051 |
| 78 | MK-886 |  | -1415.59 | 0 | 519.189 | 1.866 | -1.332 | -1.160 |
| 79 | MG149 |  | 262.264 | 0 | 343.371 | 2.231 | -1.432 | -0.519 |