**S6 Table**. Comparison Results of Secondary Matching

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Vorinostat** | **Trichostatin** | **Anisomycin** |
| **Rank** | **DNN** | **GEO2R** | **DNN** | **GEO2R** | **DNN** | **GEO2R** |
| 1 | lycorine | lycorine | lycorine | anisomycin\* | vorinostat\* | trichostatin A\* |
| 2 | anisomycin\* | anisomycin\* | anisomycin\* | lycorine | trichostatin A\* | vorinostat\* |
| 3 | emetine\* | tanespimycin | emetine\* | tanespimycin | midecamycin | tanespimycin |
| 4 | lobeline | trichostatin A\* | lanatoside C | lanatoside C | lobeline | lanatoside C |
| 5 | lanatoside C | emetine\* | digoxigenin | emetine\* | lycorine | lycorine |
| 6 | cephaeline | lanatoside C | midecamycin | digoxigenin | tanespimycin | emetine\* |
| 7 | midecamycin | digoxigenin | proscillaridin | helveticoside | clindamycin | 15-delta prostaglandin J2 |
| 8 | helveticoside | helveticoside | helveticoside | digitoxigenin | emetine\* | clindamycin |
| 9 | digoxigenin | digitoxigenin | lobeline | proscillaridin | danazol | digoxigenin |
| 10 | digitoxigenin | clindamycin | cephaeline | 8-azaguanine | digoxigenin | helveticoside |
| 11 | tanespimycin | 15-delta prostaglandin J2 | digitoxigenin | vorinostat\* | glibenclamide | digitoxigenin |
| 12 | proscillaridin | proscillaridin | vorinostat\* | sanguinarine | helveticoside | alprostadil |
| 13 | clindamycin | 8-azaguanine | tanespimycin | ouabain | lanatoside C | proscillaridin |
| 14 | 8-azaguanine | alprostadil | 8-azaguanine | clindamycin | luteolin | sanguinarine |
| 15 | trichostatin A\* | sanguinarine | apigenin | midecamycin | proscillaridin | lobeline |
| 16 | cicloheximide | ouabain | luteolin | 15-delta prostaglandin J2 | chlortetracycline | danazol |
| 17 | danazol\* | pergolide | clindamycin | apigenin | thiostrepton | ouabain |
| 18 | glibenclamide\* | cephaeline | cicloheximide | alprostadil | apigenin | midecamycin |
| 19 | apigenin | lobeline | digoxin | lobeline | cephaeline | pergolide |
| 20 | digoxin | midecamycin | thiostrepton | cephaeline | digitoxigenin | 8-azaguanine |
| 21 |  |  | ouabain | strophanthidin |  |  |
| 22 |  |  | danazol\* | luteolin |  |  |
| 23 |  |  | glibenclamide\* | digoxin |  |  |
| 24 |  |  | chlortetracycline | cicloheximide |  |  |
| 25 |  |  | strophanthidin | verteporfin |  |  |
| 26 |  |  | chlorzoxazone | danazol\* |  |  |
| 27 |  |  | ampyrone\* | pergolide |  |  |
| 28 |  |  | 15-delta prostaglandin J2 | chlortetracycline |  |  |
| 29 |  |  | baclofen | thiostrepton |  |  |
| 30 |  |  | azacyclonol | geldanamycin |  |  |