Table S5. The predicted ADME properties of the selected hits and the Metabolite.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MOL ID | Molecular Weight | AlogP | H-bond Acceptor | H-bond Donor | Molar Refractivity | BBB Permeation |
| MOL003130 | 640.54 | -2.41 | 17 | 10 | 147.01 | No |
| MOL002037 | 538.46 | 5.13 | 10 | 6 | 146.97 | No |
| MOL000010 | 578.52 | -1.10 | 14 | 8 | 137.33 | No |
| MOL003008 | 788.66 | -1.04 | 20 | 12 | 185.94 | No |
| MOL003337 | 756.71 | -2.55 | 19 | 11 | 178.84 | No |
| MOL003332 | 640.58 | -1.52 | 16 | 10 | 149.58 | No |
| MOL003316 | 640.59 | -1.52 | 16 | 10 | 149.58 | No |
| MOL003313 | 622.57 | -0.48 | 15 | 8 | 146.23 | No |
| MOL003013 | 546.65 | 1.76 | 11 | 4 | 138.08 | No |
| MOL000415 | 610.52 | -1.69 | 16 | 10 | 141.38 | No |
| MOL001875 | 516.45 | 1.03 | 11 | 7 | 126.90 | No |
| MOL003051 | 594.52 | -1.39 | 15 | 9 | 139.36 | No |
| MOL003336 | 462.45 | -2.69 | 12 | 8 | 105.03 | No |
| MOL003284 | 478.45 | 0.13 | 11 | 7 | 117.20 | No |
| MOL003334 | 478.45 | -3.20 | 13 | 9 | 106.19 | No |
| Metabolite | 316.26 | 2.29 | 7 | 4 | 82.50 | No |