化学医学

支持信息

合成和生物评价:Dantrolene-like

Synthesis and Biological Evaluation of Dantrolene-Like

Hydrazide and Hydrazone Analogues as Multitarget Agents

for Neurodegenerative Diseases

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SUPPORTING INFORMATION

Table S1. Calculated log P values of compounds 1-21

Figure S1. Plots of pIC$_{50}$ values of enzymatic activities vs.

a) calculated Clog P values; b) log $k'$ values experimentally determined
| Entry | Clog P$^a$ | Entry | Clog P$^a$ |
|-------|-----------|-------|-----------|
|       |           |       |           |
| 1.63  | 3.15      | 1.65  | 4.28      |
| DAN   | 1.43±0.59 | 11    | 3.12±0.66 |
|       |           | 2.63  | 3.19      |
| 4.18  | 2.58      | 3.84  | 3.92      |
| 1     | 2.94±0.61 | 12    | 2.95±0.64 |
|       |           |       |           |
| 2.63  | 3.19      | 3.01  | 4.57      |
| 1     | 1.75±0.58 | 13    | 3.27±0.58 |
|       |           |       |           |
| 2.58  | -0.21     | 2.17  | -0.24     |
| 3     | 1.27±0.55 | 14    | 0.02±0.49 |
|       |           |       |           |
| 3.12  | 1.59      | 3.72  | 2.34      |
| 4     | 2.64±0.63 | 15    | 1.54±0.57 |
|       |           |       |           |
| 2.32  | 1.27      | 3.03  | 0.54      |
| 5     | 1.45±0.60 | 16    | -0.13±0.39|
|       |           |       |           |
| 1.88  | 1.89      | 2.73  | 2.42      |
| 6     | 1.88±0.64 | 17    | 2.55±0.58 |
|       |           |       |           |
| 1.32  | 1.03      | 2.02  | 2.07      |
| 7     | 1.13±0.61 | 18    | 1.84±0.58 |
|       |           |       |           |
| 3.43  | 1.69      | 3.98  | 1.97      |
| 8     | 3.65±0.64 | 19    | 1.36±0.36 |
|       |           |       |           |
| 3.95  | 2.09      | 4.87  | 2.63      |
| 9     | 3.08±0.60 | 20    | 3.13±0.58 |
|       |           |       |           |
| 4.14  | -0.081    | 4.67  | 1.08      |
| 10    | 4.09±0.64 | 21    | 1.22±0.51 |

$^a$) First value: ChemDraw 15.0; second value: ALOGPS 2.1; third value: ChemSketch 2017.
Figure S1. Plots of pIC$_{50}$ values of enzymatic activities vs. a) calculated Clog P values (ChemDraw); b) log $k'$ values experimentally determined (eluent mixture: MeOH/PBS buffer 60:40 v/v); only compounds with finite IC$_{50}$ values are shown.