**Supplementary materials**

# 3D-QSAR, molecular docking, and molecular dynamics simulation study of thieno[3,2-b]pyrrole-5- carboxamide derivatives as LSD1 inhibitors

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**Fig. S1**. 3D-QSAR Histogram of activity data distribution



**Fig S2.** Docking-based alignment of training set compounds



**B**

**A**

  

**E**

**D**

**C**

**Fig. S3**. Figures A, B, C, D, and E show the superposition of the crystal pose of the compounds (green) (PDB: 5LGN, 5LGT, 5LGU, 5LHH, 5LHI), and the docked pose of the compounds (cyan), respectively, and the FAD as a reference for orientation is shown in yellow.

**Table S1**. Randomizations of biological activity for the Y-random test.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Random\_1 | Random\_2 | Random\_3 | Random\_4 | Random\_5 | Random\_6 | Random\_7 | Random\_8 | Random\_9 | Random\_10 |
| 4.873 | 6.346 | 4.166 | 5.538 | 6.171 | 8.108 | 4.318 | 8.174 | 8.174 | 4.728 |
| 4.777 | 6.209 | 6.752 | 7.745 | 6.095 | 8.174 | 4.599 | 8.108 | 7.194 | 4.873 |
| 4.599 | 6.171 | 5.538 | 5.886 | 5.886 | 7.194 | 4.281 | 7.745 | 4.166 | 6.171 |
| 4.281 | 8.174 | 7.745 | 7.252 | 8.108 | 4.166 | 4.166 | 7.194 | 4.777 | 7.187 |
| 7.535 | 4.529 | 7.194 | 7.187 | 7.745 | 4.281 | 7.194 | 6.79 | 4.411 | 5.131 |
| 7.067 | 5.658 | 5.027 | 7.18 | 7.194 | 4.599 | 8.174 | 6.752 | 4.048 | 4.599 |
| 8.174 | 5.131 | 6.355 | 7.535 | 4.728 | 4.318 | 8.108 | 6.509 | 5.032 | 4.318 |
| 8.108 | 4.873 | 4.728 | 7.067 | 7.535 | 5.032 | 5.131 | 6.355 | 4.318 | 5.032 |
| 5.602 | 4.777 | 8.108 | 5.131 | 7.067 | 4.048 | 4.873 | 5.824 | 4.599 | 4.048 |
| 5.131 | 4.599 | 6.209 | 4.873 | 5.658 | 4.411 | 4.728 | 5.658 | 4.281 | 4.411 |
| 5.658 | 4.281 | 6.171 | 7.194 | 8.174 | 4.777 | 4.668 | 5.602 | 8.108 | 4.777 |
| 6.509 | 5.027 | 6.095 | 6.917 | 5.602 | 4.654 | 4.654 | 5.538 | 4.654 | 4.654 |
| 4.166 | 5.602 | 5.886 | 6.827 | 5.538 | 4.668 | 4.777 | 5.131 | 4.668 | 6.346 |
| 6.752 | 5.538 | 7.187 | 6.68 | 6.917 | 4.728 | 4.411 | 5.032 | 4.728 | 6.68 |
| 5.824 | 7.745 | 5.658 | 6.346 | 7.252 | 4.873 | 4.048 | 5.027 | 4.873 | 6.827 |
| 5.886 | 7.18 | 5.602 | 6.209 | 7.187 | 5.131 | 5.032 | 4.873 | 5.131 | 6.917 |
| 7.252 | 7.535 | 6.346 | 8.174 | 6.209 | 5.658 | 6.752 | 4.777 | 5.658 | 4.668 |
| 7.187 | 7.067 | 4.048 | 6.171 | 6.827 | 4.529 | 5.824 | 4.728 | 4.529 | 6.752 |
| 6.917 | 4.318 | 5.032 | 6.095 | 6.68 | 4.577 | 5.658 | 4.668 | 4.577 | 6.209 |
| 6.827 | 4.728 | 4.318 | 8.108 | 6.346 | 6.509 | 5.602 | 4.654 | 6.509 | 8.108 |
| 6.68 | 4.668 | 7.18 | 4.281 | 5.658 | 6.355 | 5.538 | 4.599 | 6.68 | 8.174 |
| 6.346 | 8.108 | 7.535 | 4.411 | 5.131 | 6.79 | 7.745 | 4.577 | 6.346 | 7.194 |
| 6.209 | 6.095 | 7.067 | 4.048 | 4.281 | 4.046 | 5.027 | 4.529 | 6.209 | 4.166 |
| 7.18 | 5.886 | 8.174 | 5.032 | 5.032 | 5.027 | 4.046 | 4.411 | 6.752 | 4.281 |
| 7.194 | 7.252 | 6.917 | 5.027 | 4.318 | 7.745 | 6.79 | 4.318 | 5.824 | 7.067 |
| 4.529 | 7.187 | 4.529 | 4.166 | 7.18 | 5.538 | 6.355 | 7.535 | 5.658 | 5.886 |
| 6.171 | 4.046 | 5.658 | 4.577 | 5.027 | 5.602 | 6.509 | 7.252 | 5.602 | 6.095 |
| 6.095 | 6.79 | 5.131 | 6.509 | 4.411 | 5.658 | 4.577 | 7.187 | 5.538 | 7.252 |
| 4.411 | 6.355 | 6.509 | 4.046 | 4.048 | 5.824 | 4.529 | 7.18 | 7.745 | 7.535 |
| 4.048 | 6.509 | 4.046 | 4.318 | 6.79 | 6.752 | 5.658 | 7.067 | 5.027 | 7.18 |
| 5.032 | 7.194 | 4.411 | 5.658 | 4.668 | 6.209 | 7.18 | 6.917 | 4.046 | 5.658 |
| 4.318 | 5.824 | 4.281 | 5.602 | 4.654 | 6.346 | 7.535 | 6.827 | 6.79 | 4.529 |
| 4.728 | 5.658 | 5.824 | 6.79 | 4.577 | 6.68 | 7.252 | 6.68 | 6.355 | 4.577 |
| 4.046 | 6.752 | 6.79 | 6.355 | 4.529 | 6.827 | 7.187 | 6.346 | 6.827 | 6.509 |
| 6.79 | 6.917 | 4.577 | 6.752 | 4.046 | 6.917 | 6.171 | 6.209 | 6.917 | 6.355 |
| 6.355 | 6.827 | 4.873 | 5.824 | 4.166 | 7.067 | 6.095 | 6.171 | 7.067 | 6.79 |
| 5.538 | 6.68 | 4.777 | 4.728 | 6.752 | 5.886 | 5.886 | 6.095 | 5.886 | 4.046 |
| 7.745 | 5.032 | 4.599 | 4.668 | 4.873 | 6.095 | 7.067 | 5.886 | 6.095 | 5.027 |
| 5.658 | 4.654 | 7.252 | 4.654 | 6.355 | 6.171 | 6.917 | 5.658 | 6.171 | 7.745 |
| 5.027 | 4.577 | 6.827 | 4.777 | 6.509 | 7.187 | 6.827 | 4.281 | 7.187 | 5.538 |
| 4.668 | 4.411 | 6.68 | 4.529 | 4.777 | 7.252 | 6.68 | 4.166 | 7.252 | 5.602 |
| 4.654 | 4.048 | 4.668 | 5.658 | 4.599 | 7.535 | 6.346 | 4.048 | 7.535 | 5.658 |
| 4.577 | 4.166 | 4.654 | 4.599 | 5.824 | 7.18 | 6.209 | 4.046 | 7.18 | 5.824 |



**Fig. S4**. Temperature fluctuation plot in MD



**Fig. S5**. Total energy fluctuation plot in MD



**Fig. S6**. BOILED-Egg model plot