Supplementary Table S2. Docking results of compounds in NCI Diversity Set II to lanthionine synthetase C-like 2, ranked by the lowest binding energy (N=1,364 compounds).

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| --- | --- | --- | --- |
| **ZINC Number** | **Name** | **Chemical Structure** | **Lowest**  **Binding**  **Energy**  **(**kcal/mol**)** |
| ZINC01690699  (NSC61610) | 1-N,4-N-bis[3-(1H-benzimidazol-2-yl)phenyl]benzene-1,4-dicarboxamide | http://www.chemspider.com/ImagesHandler.ashx?id=216405 | -11.1 |
| ZINC29589888 | 2-[2-[(6-oxo-5H-phenanthridin-3-yl)carbamoyl]phenyl]benzoic acid | http://www.chemspider.com/ImagesHandler.ashx?id=244735 | -10.5 |
| ZINC13130018 | 6-(1,3-dihydrophenanthro[9,10-d]imidazol-2-ylidene)cyclohexa-2, 4-dien-1-one | http://www.chemspider.com/ImagesHandler.ashx?id=4531769 | -10.3 |
| ZINC01726776 | 3-(4-chloro-6-phenoxy-1,3,5-triazin-2-yl)-1-phenylindole | http://www.chemspider.com/ImagesHandler.ashx?id=251607 | -10.2 |
| ZINC01736228 | (2R)-5-phenyl-2-[(2R)-5-phenyl-2,3-dihydro-1,3-benzoxazol-2-yl]-2, 3-dihydro-1,3-benzoxazole | http://www.chemspider.com/ImagesHandler.ashx?id=225214 | -10.2 |
| ZINC04783229 | 1-N,4-N-bis(3-phenylphenyl)piperazine-1,4-dicarboxamide | http://www.chemspider.com/ImagesHandler.ashx?id=205764 | -10.1 |
| ZINC00990239 | 3-(4,5-dimethylbenzo[h][1, 6]naphthyridin-1-ium-2-yl)-2-methylquinolin-4-amine | http://www.chemspider.com/ImagesHandler.ashx?id=5345128 | -10 |
| ZINC18057104 | 4-[(1-methyl-6-nitroquinolin-1-ium-4-yl)amino]-N-[4-[(1-methylpyridin-1- ium-4-yl)amino]phenyl]benzamide | http://www.chemspider.com/ImagesHandler.ashx?id=4380602 | -10 |
| ZINC04214344 | Genostrychnine | http://www.chemspider.com/ImagesHandler.ashx?id=66110 | -9.7 |
| ZINC04720972 | 2-hydroxy-N-(4-methoxyphenyl)-11H-benzo[a]carbazole-3-carboxamide | http://www.chemspider.com/ImagesHandler.ashx?id=59942 | -9.6 |