Supplementary Materials

Benchmarking Data Sets from PubChem BioAssay Data: Current Scenario and Room for Improvement

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Table S1. Number of PubChem bioactivity assays according to the number of tested substances, the number of active substances, the screening stage, and the target type. Statistics were updated as of April 30, 2020.

| Criteria                                                                 | Assay type          |
|-------------------------------------------------------------------------|---------------------|
|                                                                         | Small-molecule assay| RNA interference assay |
| 1. Number of tested substances ($N_t$):                                  |                     |                       |
|   • $N_t < 100$                                                          | 1,060,707           | 22                    |
|   • $100 \leq N_t < 1,000$                                              | 4,530               | 92                    |
|   • $1,000 \leq N_t < 10,000$                                          | 1,359               | 14                    |
|   • $10,000 \leq N_t < 100,000$                                        | 422                 | 48                    |
|   • $N_t \geq 100,000$                                                  | 701                 | 1                     |
| 2. Number of active substances ($N_a$):                                  |                     |                       |
|   • $N_a < 10$                                                          | 1,000,714           | 28                    |
|   • $10 \leq N_a < 50$                                                  | 60,328              | 57                    |
|   • $50 \leq N_a < 100$                                                 | 3,562               | 18                    |
|   • $100 \leq N_a < 1,000$                                              | 2,399               | 60                    |
|   • $N_a \geq 1,000$                                                   | 716                 | 14                    |
| 3. Screening stage:                                                     |                     |                       |
|   • Primary screening                                                   | 1,416               | 113                   |
|   • Confirmatory, dose-response curves not provided                     | 276,216             | 0                     |
|   • Confirmatory, dose-response curves provided                         | 3,904               | 0                     |
|   • Summary                                                             | 701                 | 10                    |
|   • Screening stage not annotated                                       | 785,482             | 54                    |
| 4. Target type:                                                         |                     |                       |
|   • Single protein                                                      | 238,096             | 0                     |
|   • Single gene                                                         | 17                  | 0                     |
|   • Single nucleotide                                                   | 95,325              | 0                     |
|   • Multiple proteins                                                   | 25,649              | 0                     |
|   • Multiple genes                                                      | 3                   | 0                     |
|   • Multiple nucleotides                                                | 8,646               | 0                     |
|   • Protein-protein interaction                                          | 210                 | 0                     |
|   • None                                                                | 795,301             | 177                   |
| All                                                                    | 1,067,719           | 177                   |
Table S2. Number of compounds featured in PubChem bioactivity assays that satisfy each criterion of the Lipinski’s rule of five, the Ghose filter, and the Veber’s rule. Statistics were updated as of April 30, 2020.

| Criteria | Number of PubChem compounds |
|----------|----------------------------|
| **1. Lipinski’s rule of five:** | |
| ● Molecular mass ≤ 500 Da | 88,667,112 |
| ● ClogP ≤ 5 | 78,183,471 |
| ● Number of hydrogen bond donors ≤ 5 | 101,211,514 |
| ● Number of hydrogen bond acceptors ≤ 10 | 99,344,677 |
| ● Compounds satisfying all criteria | 73,062,126 |
| **2. Ghose filter:** | |
| ● Molecular mass from 180 Da to 480 Da | 82,926,795 |
| ● AlogP from -0.4 to +5.6 | 79,473,661 |
| ● Number of atoms from 20 to 70 | 71,554,127 |
| **3. Veber’s rule:** | |
| ● Number of rotatable bonds not exceeding 10 | 93,857,861 |
| ● Polar surface area not exceeding 140 Å² | 96,031,201 |
| **All** | **102,694,672** |

* The criterion regarding molar refractivity of the Ghose filter is not addressed in this table, as no relevant search option is available on PubChem Compound.
Table S3. Scaffold clusters of PubChem BioAssay active ligands (AID 493208) and the number of their representatives before and after LIT-PCBA filters.

| Scaffold cluster | Scaffold structure             | Number of substances falling into each scaffold cluster | Full data from AID 493208 | Data from the LIT-PCBA MTORC1 ligand set |
|------------------|--------------------------------|--------------------------------------------------------|---------------------------|------------------------------------------|
| 1                | (O=C1CNCCO1)                   | 3                                                      | 1                         |
| 2                | (c1ccnc1c1)                    | 38                                                     | 9                         |
| 3                | (o1cnc1c1)                     | 9                                                      | 5                         |
| 4                | (O=C1CC=CN1)                   | 15                                                     | 9                         |
| 5                | (N=C1NC=CN1)                   | 8                                                      | 5                         |
| 6                | (c1nnc[nH]1)                   | 4                                                      | 1                         |
| 7                | (c1nncnc1c1)                   | 40                                                     | 4                         |
| 8                | (c1ccc1c1)                     | 3                                                      | 0                         |
| 9                | (C1CO=CO1)                     | 1                                                      | 1                         |
| 10               | (O=C1NC=CC1=O)                 | 5                                                      | 5                         |
| 11               | (c1nc[nH]n1)                   | 4                                                      | 1                         |
| 12               | (O=C1NC=CSC=C1)                | 1                                                      | 1                         |
| 13               | (C1CN=CN1)                     | 1                                                      | 0                         |
| 14               | (c1cccccc1c1)                  | 9                                                      | 2                         |
| 15               | (C1CC=CCN1)                    | 5                                                      | 2                         |
| 16               | (c1cn[nH]c1)                   | 20                                                     | 1                         |
| 17               | (c1cc[nH]c1)                   | 13                                                     | 4                         |
| 18               | (C1CCNCC1)                     | 6                                                      | 1                         |
| 19               | (c1nnc[nH]1)                   | 5                                                      | 2                         |
| 20               | (c1csn1c1)                     | 16                                                     | 5                         |
| 21               | (C1OC=CO1)                     | 5                                                      | 3                         |
| 22               | (C1NC=CC1)                     | 2                                                      | 0                         |
| 23               | (C1CCC\(C=C/CC1)              | 2                                                      | 1                         |
| 24               | (c1c[nH]cn1)                   | 13                                                     | 3                         |
| 25               | (C1CNCCN1)                     | 13                                                     | 3                         |
| 26               | (o1cccn1c1)                    | 3                                                      | 2                         |
| 27               | (C1OC=CC1)                     | 1                                                      | 1                         |
| 28               | (c1c[nH]nn1)                   | 2                                                      | 1                         |
| 29               | (C1C=CNC=N1)                   | 1                                                      | 0                         |
| 30               | (O=C1NC=CC=C1)                 | 7                                                      | 4                         |
| 31               | (C1CO=CO1)                     | 3                                                      | 1                         |
| 32               | (C1CC=CN1)                     | 3                                                      | 2                         |
| 33               | (C1CCC=NCC1)                   | 1                                                      | 1                         |
| 34               | (O=C1NN=CC=C1)                 | 8                                                      | 3                         |
|   | Formula                  | Count | Drawings |
|---|-------------------------|-------|---------|
| 35 | (c1ccnc1)               | 4     | 1       |
| 36 | (O=C1NC=CN=C1)          | 2     | 1       |
| 37 | (C1NC=CN=C1)            | 2     | 0       |
| 38 | (C1OC=CN1)              | 1     | 0       |
| 39 | (O=C1NN=CN=C1)          | 3     | 0       |
| 40 | (O=S1(=O)NC=CC=C1)      | 1     | 1       |
| 41 | (o1ccnc1)               | 21    | 1       |
| 42 | (c1nncs1)               | 4     | 2       |
| 43 | (O=C1NC=CC(=O)N1)       | 5     | 1       |
| 44 | (C1CC=CO1)              | 5     | 2       |
| 45 | (C1OC=CC=C1)            | 1     | 0       |
| 46 | (O=C1C=CNC=C1)          | 1     | 0       |
| 47 | (O=C1NC=CS(=O)(=O)C=C1) | 1     | 0       |
| 48 | (C1CN=CO1)              | 3     | 0       |
| 49 | (O=C1C=COC=C1)          | 1     | 1       |
| 50 | (O=C1NC=NC=C1)          | 2     | 1       |
| 51 | (c1ncncn1)              | 5     | 0       |
| 52 | (c1cnncn1)              | 1     | 1       |
| 53 | (C1CCC=CCC1)            | 2     | 0       |
| 54 | (c1cn[nH]n1)            | 1     | 0       |
| 55 | (C1CCCCC1)              | 1     | 0       |
| 56 | (O=C1NCC=C1)            | 1     | 0       |
| 57 | (C1CN=CC=C1)            | 2     | 0       |
| 58 | (S1C=CC=NC=C1)          | 1     | 0       |
| 59 | (o1nccn1)               | 1     | 1       |
| **All** |                   | **342** | **97** |
## Table S4. Scaffold clusters of PubChem BioAssay inactive ligands (AID 493208) and the number of their representatives before and after LIT-PCBA filters.

| Scaffold cluster | Scaffold structure | Number of substances falling into each scaffold cluster | Full data from AID 493208 | Data from the LIT-PCBA MTORC1 ligand set |
|------------------|--------------------|--------------------------------------------------------|---------------------------|----------------------------------------|
| 1                | (c1ccc2ncccc2c1)   | 638                                                    | 288                       |                                        |
| 2                | (O=S(=O)(NC1=NCNC1)c2cccccc2) | 5                                                      | 5                          |                                        |
| 3                | (O=C1NC=Cc2cccccc12) | 196                                                    | 195                       |                                        |
| 4                | (C1OC=Cn2ccnc12)  | 12                                                     | 12                        |                                        |
| 5                | (O=C1NC=Nc2cccccc12) | 256                                                    | 150                       |                                        |
| 6                | (C1OC=Cc2nncccc12) | 28                                                     | 5                         |                                        |
| 7                | (O=C1NC(=O)c2ccccnc2N1) | 160                                                    | 160                       |                                        |
| 8                | (O=C1NNc2nncccc12) | 49                                                     | 48                        |                                        |
| 9                | (O=C1OC=Cc2cccccc12) | 34                                                     | 25                        |                                        |
| 10               | (c1nc2ccnn2c1)    | 439                                                    | 305                       |                                        |
| 11               | (O=C1COc2cccccc2N1) | 402                                                    | 393                       |                                        |
| 12               | (c1ccc2[nH]ccc2c1) | 1139                                                   | 733                       |                                        |
| 13               | (O=C(CN1CCNCN1)c2ccccc2) | 8                                                      | 8                          |                                        |
| 14               | (O=C1C=CNc2ccnn12) | 35                                                     | 31                        |                                        |
| 15               | (C1CCc2cccccc2c1) | 319                                                    | 180                       |                                        |
| 16               | (C1COc2cccccc2O1) | 281                                                    | 250                       |                                        |
| 17               | (c1ccc2ncnc2c1)   | 98                                                     | 16                        |                                        |
| 18               | (O=C(C1CCNCN1)c2ccccc2) | 19                                                     | 19                        |                                        |
| 19               | (C1N=CNc2ccnn12)  | 10                                                     | 10                        |                                        |
| 20               | (c1ncc2cc[nH]c2n1) | 33                                                     | 27                        |                                        |
| 21               | (O=C(NC1C=CNC1)c2ccccc2) | 13                                                     | 13                        |                                        |
| 22               | (O=C1CC2=C(N1)Nc2ccccc2) | 42                                                     | 42                        |                                        |
| 23               | (o1nc2ncccccc12)  | 72                                                     | 65                        |                                        |
| 24               | (O=C(CSC1=NC(=O)C=CN1)c2ccccc2) | 15                                                     | 15                        |                                        |
| 25               | (O=C1CN(=O)Nc2ccccc2) | 7                                                      | 7                         |                                        |
| 26               | (O=C1NC(NS(=O))(=O)c2ccccc2)C(=O)N1) | 15                                                     | 15                        |                                        |
| 27               | (c1nc2ncnn2c1)    | 274                                                    | 205                       |                                        |
| 28               | (c1cn2ncccc2n1)   | 6                                                      | 6                         |                                        |
| 29               | (O=C1NN=C2COC=CN12) | 6                                                      | 6                          |                                        |
| 30               | (O=C1CN=CN1C2CCCCC2) | 5                                                      | 0                          |                                        |
| 31               | (O=C(C1NCCOC1=O)c2ccccc2) | 7                                                      | 7                          |                                        |
| 32               | (N=C1Nc2cccccc2S1) | 8                                                      | 8                         |                                        |
| 33               | (C1C=NNC1c2cn[nH]c2) | 5                                                      | 3                          |                                        |
34 \((O=C(\text{NCS}(=O)(=O)c_1cccccc1)NCc_2cccccc2)\) 14 14
35 \((O=C\text{C}NCc_2cCC=CC=CN1)\) 12 12
36 \((O=C(\text{NCS}(=O)(=O)c_1cccccc1)NCc_2cccccc2)\) 46 39
37 \((c_1ccc(cc1)c_2nn[nH]n2)\) 50 42
38 \((O=C(\text{CNC}1cccccc1)NCc_2cCCCCc2)\) 31 31
39 \((c_1ccc(cc1)nc_2cnnnn)\) 23 23
40 \((O=C(\text{CSc}1nccn1)c_2cccccc2)\) 34 34
41 \((O=C\text{C}2CN3C1C\text{NC}(C2)C_3c4cccccc4)\) 26 23
42 \((O=C\text{C}NCc_2cCCCCc12)\) 5 5
43 \((c_1ccc2cccccc1)\) 604 405
44 \((C(\text{N1CCNC}1)c_2cccccc2)\) 21 21
45 \((O=C\text{C}CCC=CC=CC=CN12)\) 14 14
46 \((c_1ccc(cc1)c_2cc[nH]c2)\) 139 100
47 \((O=S(=O)(c_1cccccc1)c_2ncnc2)\) 14 14
48 \((c_1ccc2nncnc2)\) 175 170
49 \((o_1nc2cCCCCc2n1)\) 68 68
50 \((O=C\text{C}NC(=C\text{C}=C1)SCc_2oncn2)\) 3 3
51 \((O=C(\text{CSC}(=O)(=O)c_1cccccc1)NCc_2cccccc2)\) 12 12
52 \((C(Nc_1ncc[nH]1)c_2cccccc2)\) 9 8
53 \((O=C\text{C}NC(=C(=O)c_1ccccc1)S(=O)(=O)c_2cccccc2)\) 5 5
54 \((N=C\text{C}NC(=C(=O)c_1ccccc1)S(=O)(=O)c_2cccccc2)\) 27 27
55 \((O=C(\text{CNC}1cccccc1)c_2cccccc2)\) 13 13
56 \((C1CN(CCN1)c_2cccccc2)\) 166 151
57 \((O=S(=O)(c_1nccn1)c_2cccccc2)\) 27 27
58 \((O=C\text{C}NCc_2nccn2c=C1)\) 12 12
59 \((O=C\text{C}NC(=O)c_2nccn2N1)\) 190 175
60 \((O=C(\text{CNC}c_1cccccc1)c_2cccccc2)\) 14 14
61 \((O=C(\text{CNC}c_1cccccc1)c_2cccccc2)\) 14 14
62 \((C(c_1nccn1)c_2cccccc2)\) 6 6
63 \((N(c_1cccccc1)c_2ncncs2)\) 17 14
64 \((O=C(\text{CNC}1cccccc1)c_2C2NC(=O)c2)\) 11 11
65 \((O=C(\text{CNC}1cccccc1)c_2cCCc2cCCc2)\) 8 8
66 \((O=C\text{C}NC(=C(=O)c_1ccccc1)CS=CC=CN12)\) 438 424
67 \((O=C(\text{CNC}c_1cccccc1)c_2N2CNCCc2)\) 13 13
68 \((O=C(\text{CSc}1ncn1[nH]1)c_2cCCCCc2)\) 42 15
69 \((O=C\text{C}NC(=O)c_2cccccc2)\) 123 72
70 \((O=C(\text{CSc}(=O)c_1ccn1)NCCc_2cccccc2)\) 13 13
71 \((O=C(\text{CNC}c_1cccccc1)c_2cccccc2)\) 14 14
72 \((O=C(\text{CNC}c_1cccccc1)c_2ccccc2)\) 13 13
73 \((O=C\text{C}oc_2cCCCCc2c=C1)\) 438 336
74 \((C(\text{N1CCNC}1)c_2coccn2)\) 50 44
|   | Chemical Structure                                                                 |   |   |
|---|-----------------------------------------------------------------------------------|---|---|
| 75 | O=C(Nc1ccccc1)c2occcc2                                                             | 30 | 26 |
| 76 | O=C(NCC1CNCC1)Cc2cccccc2                                                            | 12 | 12 |
| 77 | O=C1Sc2cccc2c2N1                                                                  | 138| 134|
| 78 | O1cnc2cccccc12                                                                     | 528| 287|
| 79 | O=C1CCCC2=C1CC=CN2                                                                  | 6  | 6  |
| 80 | c1cnn2cnncc2c1                                                                     | 82 | 75 |
| 81 | c1cccc2[nH]nc2c1                                                                  | 682| 415|
| 82 | O=C(Nc1cccccc1)C2CCCN2                                                             | 5  | 5  |
| 83 | c1cccc2cnnccnc2c1                                                                  | 88 | 40 |
| 84 | O=C1Cc2cccccc2N1                                                                   | 126| 124|
| 85 | O=C1Nc2cccccc2O1                                                                    | 359| 354|
| 86 | O=C1NN=C(C=C1)c2cccccc2                                                             | 70 | 67 |
| 87 | O=C1NC=Cc2ccnn12                                                                   | 13 | 13 |
| 88 | O=S(=O)[NCC1CCCCC1)c2cccccc2                                                      | 18 | 12 |
| 89 | O=C1Nc2cccccc2N1                                                                  | 128| 128|
| 90 | O=C1CN=Cs2cccccc2N1                                                                | 32 | 21 |
| 91 | c1ccc2o2c1                                                                         | 76 | 30 |
| 92 | O=C1NCC2=C1OC=CC2=O                                                                | 110| 97 |
| 93 | c1ccn2[nH]nc2c1                                                                    | 76 | 30 |
| 94 | O=C(NCC1cccc1)Nc2cccccc2                                                            | 17 | 15 |
| 95 | O=C(NCCc1cccc1)c2cccccc2                                                             | 32 | 31 |
| 96 | (c1cccc2n[nH]nc2c1)                                                                 | 76 | 30 |
| 97 | O=C1CCc2cccccc2                                                                   | 123| 123|
| 98 | (c1oc2cccccc2O1)                                                                   | 666| 570|
| 99 | O=C1CNC(=CNc2sccc12)                                                                | 8  | 8  |
| 100| O=C1CC(=NN1)c2cccccc2                                                              | 48 | 48 |
| 101| (C1Cc2scnc2C=C1)                                                                   | 11 | 11 |
| 102| (C1cnc2ncsc12)                                                                     | 13 | 13 |
| 103| (C1Cn2cccccc2N1)                                                                   | 44 | 43 |
| 104| (C1CCn2cccccc2N1)                                                                  | 70 | 63 |
| 105| (C1CC2cccccc2N1)                                                                   | 70 | 63 |
| 106| O=C1CCn2cccccc2                                                                  | 70 | 63 |
| 107| (C1CCn2cccccc2N1)                                                                  | 70 | 63 |
| 108| O=C1CC2=C(COC2=O)N1                                                                | 12 | 12 |
| 109| O=C1CC2=C(O1)C=COC2=O                                                              | 7  | 7  |
| 110| (O=C(COc1cccc1)Nc2cccccc2)                                                         | 8  | 8  |
| 111| (c1ccn2cncnc2c1)                                                                   | 143| 64 |
| 112| (O=C1CN(C2CCCC2)C(=O)CN1)                                                         | 50 | 41 |
| 113| (c1ccc(cc1)c2ccnccn2)                                                              | 11 | 11 |
| 114| (O=C(CSc1cccccc1)NCc2cccccc2)                                                      | 7  | 6  |
| 115| (C1CCc2[nH]nc2c1)                                                                  | 13 | 13 |
| No. | Formula                                                                 | Valency 1 | Valency 2 |
|-----|-------------------------------------------------------------------------|-----------|-----------|
| 116 | (O=C1NC2=CC=CCC2=C1)                                                   | 16        | 16        |
| 117 | (O=C(NCc1cccccc1)c2occcc2)                                             | 37        | 37        |
| 118 | (o1ccnc1c2cccccc2)                                                     | 32        | 32        |
| 119 | (O=S(=O)(NCc1ccccc1)c2cccccc2)                                         | 12        | 5         |
| 120 | (O=C(COc1cccccc1)Nc2cn[nH]c2)                                          | 6         | 6         |
| 121 | (O=C(COc1cccccc1)Nc2cccs2)                                            | 14        | 14        |
| 122 | (o1ccnc1c2cccccc2)                                                     | 36        | 22        |
| 123 | (O=C(Nc1cccccc1)c2c[nH]cn2)                                            | 5         | 5         |
| 124 | (O=S(=O)(N1CCCCC1)c2cccccc2)                                           | 27        | 27        |
| 125 | (O=S(=O)(N1CCOCC1)c2cccccc2)                                           | 27        | 27        |
| 126 | (O=C(Nc1cccccc1)\C=C\c2occcc2)                                       | 26        | 21        |
| 127 | (O=C1NC(=O)c2c[nH]cc2N1)                                              | 59        | 42        |
| 128 | (C1C2cccccc2CN1)                                                      | 142       | 120       |
| 129 | (C(Oc1cccccc1)c2occcc2)                                                | 10        | 10        |
| 130 | (C1CC2(CC1N1)OCCO2)                                                    | 34        | 31        |
| 131 | (O=C(Nc1cccccc1)c2cccccc2)                                             | 133       | 76        |
| 132 | (O=C(COc1cccccc1)NC2CCS(=O)(=O)C2)                                     | 12        | 12        |
| 133 | (O=C1NC=CS(=O)(=O)c2cccccc12)                                         | 170       | 104       |
| 134 | (O=C(NC1CCS(=O)(=O)C1)c2cccccc2)                                      | 32        | 32        |
| 135 | (c1ccc(cc1)n2ccnn2)                                                   | 20        | 20        |
| 136 | (O=C1NN=Nc2ccccc12)                                                   | 80        | 34        |
| 137 | (c1ccc2scnc2c1)                                                       | 819       | 610       |
| 138 | (O=C1NCc2cn[nH]c12)                                                   | 118       | 91        |
| 139 | (o1ccnc(n1)c2cccccc2)                                                 | 75        | 72        |
| 140 | (O=C(NCC12CC3CC(CC(C3)C1)C2)c4cc[nH]n4)                               | 6         | 0         |
| 141 | (o1ccnc(n1)c2ccncnc2)                                                 | 20        | 20        |
| 142 | (c1ncnc2en[nH]c2n1)                                                   | 225       | 175       |
| 143 | (O=C(CSc1ocnn1)Nc2cccccc2)                                            | 36        | 36        |
| 144 | (C1C=CNc2ncnn12)                                                     | 273       | 164       |
| 145 | (C(Oc1cccccc1)c2oncn2)                                                | 13        | 13        |
| 146 | (c1ncnc2cc[nH]c2n1)                                                   | 76        | 3         |
| 147 | (O=C1NN=Cc2cccccc12)                                                 | 75        | 70        |
| 148 | (O=C(CN1CCNCC1)Nc2cccccc2)                                            | 26        | 26        |
| 149 | (c1nc2sccc2c1)                                                       | 168       | 111       |
| 150 | (o1cnc(n1)c2occc2)                                                   | 21        | 21        |
| 151 | (O=C1NC(=O)c2ccsc2N1)                                                | 305       | 200       |
| 152 | (c1ccn2cnnc2c1)                                                       | 33        | 24        |
| 153 | (O=C1NC=Nc2ccsc12)                                                   | 114       | 46        |
| 154 | (O=C(Nc1cccccc1)C2CCNCC2)                                             | 40        | 40        |
| 155 | (c1cc2nccn2cn1)                                                      | 167       | 83        |
| 156 | (O=C1Nc2cccccc2S(=O)(=O)N1)                                           | 58        | 37        |
|   | Chemical Structure |   |   |
|---|--------------------|---|---|
| 157 | (O=C1NC=NC2ccc12) | 203 | 151 |
| 158 | (C1CN2CCC1c3cccc23) |   | 16 |
| 159 | (O=C1NC2=C(CNC2=O)N1) | 13 | 13 |
| 160 | (O=C1NC(=O)c2cccccc2N1) | 571 | 501 |
| 161 | (O=C1CC2=C1CC=CN2) | 11 | 11 |
| 162 | (O=C(CSc1nc[nH]1)Nc2cccccc2) | 89 | 72 |
| 163 | (C1CNC2cccccc2C1) | 299 | 264 |
| 164 | (O=C(CSC1=NC(=O)c1)Nc2cccccc2) | 13 | 13 |
| 165 | (O=S(=O)(Cc1occc1)c2cccs2) | 39 | 39 |
| 166 | (C1C=CNc2nnnn12) | 24 | 24 |
| 167 | (O=C(NCCc1occc1)C(=O)NCCc2cccccc2) | 12 | 12 |
| 168 | (O=C(NCCc1occc1)C(=O)NCc2cccccc2) | 11 | 11 |
| 169 | (C(N1CCNCC1)c2occ2c2) | 18 | 18 |
| 170 | (C1CC(CCO1)c2cccs2) | 24 | 24 |
| 171 | (O=C1Nc2nccn2C=C1) | 12 | 12 |
| 172 | (O=C1Nc=NC1NS(=O)(=O)c2cccccc2) | 6 | 6 |
| 173 | (O=C1NC=COc2cccccc2) | 4 | 4 |
| 174 | (O=C1CC(=O)Nc2cccccc2N1) | 25 | 25 |
| 175 | (O=C(NCCc1occc1)C(=O)NCCc2cccccc2) | 12 | 12 |
| 176 | (O=C(NCCc1occc1)C(=O)NCc2cccccc2) | 13 | 13 |
| 177 | (c1cncc2[nH]cc2n1) | 17 | 17 |
| 178 | (C(N1CCNCC1)c2ccnc2c2) | 63 | 63 |
| 179 | (O=C(CSc1ccccc1)Nc2cccccc2) | 56 | 19 |
| 180 | (O=C(CNS(=O)(=O)c1conc1)Nc2cccccc2) | 13 | 13 |
| 181 | (c1conc1)n2ccnc2) | 13 | 13 |
| 182 | (C1NC=Cc2nncnc2O1) | 33 | 18 |
| 183 | (O=C1NC=NC2cc[nH]c12) | 175 | 74 |
| 184 | (O=C1CCCC2=C1CC=CC(=O)N2) | 62 | 42 |
| 185 | (O=C1NC=CC(N1)c2cn[nH]c2) | 13 | 13 |
| 186 | (c1cncc2nccn2c1) | 89 | 65 |
| 187 | (O=C(CSC1=NC=CC(=O)N1)Nc2cccccc2) | 49 | 45 |
| 188 | (O=C1C2CN3CC1CN(C2)C3c4cc[nH]c4) | 14 | 14 |
| 189 | (O=C(CNc1cccccc1)NCCc2cccccc2) | 14 | 14 |
| 190 | (C1CC2NC=CN2C1) | 26 | 26 |
| 191 | (O=C1CNC2nncnc12N1) | 86 | 86 |
| 192 | (O=C1NN=CC2c[nH]nc12) | 105 | 105 |
| 193 | (O=C1CCc2cccccc2N1) | 107 | 107 |
| 194 | (c1cncc2[nH]cc2c1) | 25 | 6 |
| 195 | (O=S1(=O)NC=CC2nccncc12) | 106 | 75 |
| 196 | (O=C(CNS(=O)(=O)c1cc[nH]c1)N2CCNCC2) | 13 | 13 |
| 197 | (c1ccc(cc1)n2cnnc2) | 9 | 9 |
|   | Molecular Structure                                                                 | Num1 | Num2 |
|---|-----------------------------------------------------------------------------------|------|------|
| 198 | (O=C1NC(=O)C2CCCCCN12)                                                           | 19   | 19   |
| 199 | (C1n2cnnc2S1)                                                                    | 37   | 37   |
| 200 | (C1Cc2ccsc2CN1)                                                                   | 86   | 53   |
| 201 | (C(C1CCNCC1)N2CCCCCC2)                                                           | 13   | 13   |
| 202 | (O=C(NCCc1occc1)c2cccccc2)                                                        | 13   | 13   |
| 203 | (C(C1CCNCC1)N2CCCC2)                                                              | 13   | 13   |
| 204 | (c1cn22cnc2c1)                                                                    | 13   | 13   |
| 205 | (C(C1CCNCC1)N2CCOC2C2)                                                            | 13   | 13   |
| 206 | (O=S(=O)(Cc1cccs1)c2cccs2)                                                        | 26   | 26   |
| 207 | (C(C1CCNCC1)N2CCCC2)                                                              | 18   | 18   |
| 208 | (C1COc2ccccc2N1)                                                                  | 214  | 212  |
| 209 | (O=C(CNS(=O)(=O)c1cc[nH]c1)NCc2cccccc2)                                           | 13   | 13   |
| 210 | (O=C(CNS(=O)(=O)c1cc[nH]c1)NCc2cccccc2)                                           | 31   | 31   |
| 211 | (O=S(=O)N1CCCCCC1)c2cc[nH]c2)                                                     | 99   | 99   |
| 212 | (O=C(NCc1cccccc1)2c2ccn[nH]2)                                                     | 13   | 13   |
| 213 | (O=C1C=CN=C2SC=NN12)                                                              | 649  | 595  |
| 214 | (O=C1CCc2cccccc2N1)                                                               | 93   | 93   |
| 215 | (C1Sc2ccccc2N1)                                                                   | 137  | 99   |
| 216 | (c1cn2ncsc2n1)                                                                    | 69   | 69   |
| 217 | (C1CCc2nnncn2CC1)                                                                 | 24   | 24   |
| 218 | (c1cn2ccscn2n1)                                                                   | 99   | 87   |
| 219 | (O=C1OC2(CCNCC2)C=C1)                                                              | 25   | 25   |
| 220 | (o1cccc1c2oncc2)                                                                  | 12   | 12   |
| 221 | (O=C1NC=CC=C1CN2CCCC2C2)                                                          | 25   | 25   |
| 222 | (O1ncc1c2cccs2)                                                                   | 36   | 36   |
| 223 | (o1ncc1c2ccccc2)                                                                  | 112  | 110  |
| 224 | (O=C1NC2ccccc12)                                                                  | 206  | 205  |
| 225 | (O=S(=O)N1CCNC1)c2cccccc2)                                                        | 80   | 54   |
| 226 | (C(C1CCCC1)N2cccccc2)                                                              | 12   | 12   |
| 227 | (O=S(=O)C1=NCC=N1)NCC2cccccc2)                                                     | 12   | 12   |
| 228 | (O=C1C=CNc2nnccc12)                                                               | 75   | 66   |
| 229 | (O=C1OC=Cc2[nH]ncnc12)                                                             | 22   | 22   |
| 230 | (O=C1NC=CC=C1CN2CCNC2)                                                             | 43   | 43   |
| 231 | (O=C(COCc1cccon1)Nc2cccccc2)                                                       | 12   | 12   |
| 232 | (O=C(NCc1nnn[nH]1)c2cccccc2)                                                        | 13   | 13   |
| 233 | (O=S(=O)N1CCCCC1)c2cn[nH]c2)                                                       | 20   | 20   |
| 234 | (O=S(=O)N1CCCCC1)c2cn[nH]c2)                                                       | 35   | 35   |
| 235 | (O=C(NCCS(=O)(=O)N1CCNC1)C2CNC(=O)C2)                                              | 11   | 11   |
| 236 | (O=C1NC=C(CN2CCNC2)N1)                                                             | 17   | 17   |
| 237 | (O=C(NC1=NCC(=O)N1)c2cccccc2)                                                      | 13   | 13   |
| 238 | (o1ncc2cnnc12)                                                                    | 164  | 127  |
|   | Chemical Structure          | Score1 | Score2 |
|---|-----------------------------|--------|--------|
| 239 | (C(Oc1cccc1)c2cocn2)       | 23     | 18     |
| 240 | (C1NCc2ccnn2C1)            | 13     | 13     |
| 241 | (C1Ne2ccnn2OC=O1)          | 47     | 38     |
| 242 | (c1nc2[nH]nc2c1)           | 164    | 99     |
| 243 | (c1nc2[nH]nc2c1)           | 388    | 296    |
| 244 | (C1NCc2ccnn2O1)            | 43     | 23     |
| 245 | (O=C(N1CCCCC1)c2cn[nH]c2)  | 45     | 42     |
| 246 | (O=C1CCSc2ccccc2N1)        | 67     | 62     |
| 247 | (c1ccn(c1)n2ccn[nH]2)      | 79     | 59     |
| 248 | (C1CCc2cc[nH]c2CC1)        | 23     | 18     |
| 249 | (C(Sc1nc[nH]1)c2ccccc2)    | 13     | 13     |
| 250 | (C1CCN(C1)c2ccnn2)        | 23     | 22     |
| 251 | (C1CN(CCO1)c2ccnn2)       | 13     | 13     |
| 252 | (C1CCN(CC1)c2ccnn2)       | 42     | 20     |
| 253 | (O=C1Nc2nnn2C=C1)          | 241    | 230    |
| 254 | (c1ccc(cc1)c2ccnn2)       | 30     | 30     |
| 255 | (O=C1CN(Cc2occc2)(C=O)N1)  | 13     | 13     |
| 256 | (O=S(=O)(N1CCCC1)c2cc{nH}c2) | 25   | 25     |
| 257 | (O=C1CN(Cc2cccs2)(C=O)N1)  | 13     | 13     |
| 258 | (O=C(C1NC=O)=O)c2ccccc2)   | 69     | 68     |
| 259 | (C1CCN(CC1)c22ncs2)       | 111    | 87     |
| 260 | (C1C=CNc2ccnn12)          | 39     | 33     |
| 261 | (c1ccn(cc1)n2ccn[nH]2)    | 129    | 79     |
| 262 | (C1CC(CCN1)c2ccn[nH]2)    | 65     | 65     |
| 263 | (o1nncc1c2c[nH]nn2)       | 39     | 39     |
| 264 | (O=C1C=CSc2ccccc12)       | 202    | 108    |
| 265 | (O=C1NC=CSc2ccccc12)      | 220    | 198    |
| 266 | (c1cn2nncn2s1)            | 129    | 79     |
| 267 | (O=S(=O)(NCc1csn1)c2cccccc2) | 13   | 13     |
| 268 | (O=C1Nc2ccccc2C=C1)       | 244    | 237    |
| 269 | (O=C(NCCc1csn1)(C=O)Nc2ccccc2) | 31   | 31     |
| 270 | (C1Cc2ccccc2N1)           | 884    | 872    |
| 271 | (O=C1NC=(=O)c2[nH]ccc2N1) | 158    | 73     |
| 272 | (O=C1NC=Nc2ccc12)         | 69     | 69     |
| 273 | (O1cccc2cncc12)           | 151    | 151    |
| 274 | (c1cn2nnnc2cn1)           | 52     | 52     |
| 275 | (O=S(=O)(N1CCOCC1)c2cc[nH]c2) | 13   | 13     |
| 276 | (O=C(Cc1ccccc1)NCCc2csn2) | 12     | 12     |
| 277 | (O=C(NCCc1cscn1)c2ccccc2) | 31     | 27     |
| 278 | (O=S(=O)(NCc1csn1)c2ccccc2) | 17   | 17     |
| 279 | (O=C(NCCc1cscn1)(C=O)Nc2ccccc2) | 29   | 29     |
|   | Chemical Structure                                                                 |   |   |
|---|-----------------------------------------------------------------------------------|---|---|
| 280| \((O=C(NCCc1cnccs1)c2cccccc2)\)                                                 | 31| 28|
| 281| \((O=C(NCCc1cccs1)c2cccccc2)\)                                                 | 13| 10|
| 282| \((O=S1(=O)CCCCN1c2cccccc2)\)                                                 | 42| 42|
| 283| \((O=C1Ne2cccccc2NC1=O)\)                                                      | 130| 130|
| 284| \((O=C1CC(=O)c2cccccc2)\)                                                     | 21| 13|
| 285| \((O=C(NCc1cccccc1)c2cnccn2)\)                                                | 20| 20|
| 286| \((O=C(Nc1cccccc1)c2cnccn2)\)                                                | 18| 17|
| 287| \((O=C1NN=Cc2cc[nH]c12)\)                                                     | 353| 246|
| 288| \((C1CCc2cncc2C1)\)                                                          | 18| 18|
| 289| \((O=C(NCCc1cccccc1)c2c[nH]nn2)\)                                             | 13| 13|
| 290| \((O=C(Ncc1cccccs1)c2c[nH]nn2)\)                                             | 13| 13|
| 291| \((O=C(NCc1cccccc1)c2c[nH]nn2)\)                                             | 19| 19|
| 292| \((C(N1CCOCC1)c2cccccc2)\)                                                   | 39| 39|
| 293| \((C(N1CCCCC1)c2cccccc2)\)                                                   | 16| 16|
| 294| \((O=C(CN1C=CC=CC1=O)Nc2cccccc2)\)                                           | 13| 13|
| 295| \((O=C(Nc1cccccc1)c2cccon2)\)                                               | 29| 25|
| 296| \((o1cncc1c2cccnc2c1)\)                                                        | 45| 45|
| 297| \((O=C(NGc1cccn[nH]1)Nc2cccccc2)\)                                           | 12| 12|
| 298| \((O=C(Nc1cnccn1)c2cccnc2)\)                                               | 17| 17|
| 299| \((O=C(COC1cccccc1)c2c[nH]nn2)\)                                             | 29| 25|
| 300| \((O=C(Nc1cccccc1)c2c[nH]nn2)\)                                             | 69| 69|
| 301| \((c1nncc2nc[nH]c2n1)\)                                                        | 32| 32|
| 302| \((O=S(=O)(N1CCNCC1)c2cc[nH]c2)\)                                           | 87| 87|
| 303| \((C1CCc2nnccn2CC1)\)                                                         | 65| 65|
| 304| \((O=C1NC=Nc2onncc12)\)                                                      | 24| 24|
| 305| \((O=C1NC=Cc2nccnc12)\)                                                      | 99| 99|
| 306| \((O=S1(=O)N=Cc2cccccc12)\)                                                 | 9| 9|
| 307| \((O=C(CCn1cccn1)Nc2cccccc2)\)                                              | 10| 10|
| 308| \((O=S(=O)(NCc1oncn1)c2cccccc2)\)                                           | 11| 11|
| 309| \((O=C(CCN1cccn1)Nc2cccccc2)\)                                              | 13| 13|
| 310| \((O=C(CCc1nccn1)c2ncncn2)\)                                                | 63| 27|
| 311| \((O=C(CSc1nnc[nH]1)c2oncn2)\)                                              | 29| 29|
| 312| \((O=C(CSc1nnc[nH]1)c2oncn2)\)                                              | 13| 13|
| 313| \((O=C(CCSc1nncn1)c2ncncn2)\)                                               | 22| 19|
| 314| \((O=C(CNc1cccn1)Nc2cccccc12)\)                                             | 50| 46|
| 315| \((O=C1CSC2(N1)C=CNc2=O)\)                                                  | 102| 84|
| 316| \((O=C1OC2(CCCCC2)C=C1)\)                                                   | 18| 18|
| 317| \((O=C1OC2(CCCCC2)C=C1)\)                                                   | 35| 35|
| 318| \((O=C1OC2(CCCCC2)C=C1)\)                                                   | 13| 13|
| 319| \((O=C(CN1cccn1)Nc2cccccc2)\)                                               | 10| 10|
|  | | |
|---|---|---|
| 321 | (c1cc2nncn2cn1) | 37 | 33 |
| 322 | (O=C(CNS(=O)(=O)c1ccsc1)Nc2ccccc2) | 12 | 12 |
| 323 | (O=5(=O)(Nc1ccccccc1)c2ccsc2) | 28 | 20 |
| 324 | (O=S(=O)(N1CCNCC1)c2ccsc2) | 24 | 22 |
| 325 | (O=C(CNS(=O)(=O)c1cccs1)Nc2ccccc2) | 39 | 37 |
| 326 | (O=C1Nc2[nH]ncc2C=c1) | 176 | 166 |
| 327 | (O=C(Nc1nncc1)c2ccccc2) | 54 | 54 |
| 328 | (O=S1(=O)NCCCCN1Cc2ccccc2) | 9 | 9 |
| 329 | (O=C(N1CCNCC1)=O)Nc2ccccc2) | 10 | 10 |
| 330 | (c1cn2cnncc2cn1) | 64 | 55 |
| 331 | (C1Cn2cnncc2C=N1) | 23 | 7 |
| 332 | (C1CSc2ncccc2N1) | 63 | 60 |
| 333 | (C1CCc2[nH]ccc2C1) | 43 | 16 |
| 334 | (C1CCc2cccccc2NC1) | 51 | 35 |
| 335 | (O=C1NC=Nc2[nH]ncc12) | 68 | 44 |
| 336 | (O=C(NC1CCCCC1)C2CNCC(=O)N2) | 12 | 12 |
| 337 | (O=C1NC= Coc2ncccc212) | 58 | 58 |
| 338 | (C1nncc2n[nH]cc12) | 122 | 86 |
| 339 | (C(N1CCNCC1)c2ccccc2) | 6 | 6 |
| 340 | (C1CCN2CCNCC2C1) | 13 | 13 |
| 341 | (C(NC1CCNCC1)c2occcc2) | 13 | 13 |
| 342 | (O=S1(=O)C=CC(=N1)N2CCCCC2) | 49 | 49 |
| 343 | (O=C1NN2C=NC=NCc2ccccc2) | 72 | 50 |
| 344 | (c1nncc2cccccc12) | 61 | 60 |
| 345 | (O=C1C=CN=C2CCCCCN12) | 77 | 76 |
| 346 | (O=C1NC=CN=C1NCCc2cccccc2) | 13 | 13 |
| 347 | (O=C1NC=CN=C1Ncc2ccccc2) | 13 | 13 |
| 348 | (c1nc(ns1)c2c[nH]nn2) | 34 | 23 |
| 349 | (O=C(NCc1oncn1)c2ccccc2) | 30 | 27 |
| 350 | (C1Nc2sccc2C=N1) | 13 | 11 |
| 351 | (c1ccsc(c1)c2cccn2) | 13 | 4 |
| 352 | (O=C1NC=Cc2sccc12) | 90 | 83 |
| 353 | (O=C(NCc1cccccc1)C2CCCCC2) | 7 | 7 |
| 354 | (O=C(NCCc1ccccccc1)C2CCCCC2) | 11 | 9 |
| 355 | (O=C1OC=Cc2sccc12) | 65 | 39 |
| 356 | (O=S1(=O)NC=Cc2cccccc12) | 56 | 53 |
| 357 | (N1C=CS/C=1=Nc2ccccc2) | 5 | 5 |
| 358 | (O=C1CCc2ncnc212) | 6 | 6 |
| 359 | (c1cccc(c1)c2cc[nH]n2) | 14 | 10 |
| 360 | (O=S1(=O)CCC(C1)Ncc2cccs2) | 23 | 23 |
| 361 | (o1cccc1c2ccccc2) | 11 | 4 |
|   | Formula | Count | Count |
|---|---------|-------|-------|
| 362 | (O=C1C=CNc2ncnn12) | 19 | 18 |
| 363 | (C(CSc1nnnn[nH]1)NC2cccccc2) | 36 | 36 |
| 364 | (O=C1CC2C=(N1)NC(=O)NC2=O) | 6 | 6 |
| 365 | (C1CCNCC1) | 13 | 13 |
| 366 | (c1c[nH]c(c1)c2cccs2) | 13 | 7 |
| 367 | (O=C(CSc1nnc[nH]1)Nc2ccccc2) | 42 | 42 |
| 368 | (C1Cc2nccccc2CN1) | 26 | 26 |
| 369 | (O=S(=O)(Nc1ccccc1)c2cccs2) | 13 | 13 |
| 370 | (O=C1NN=Nc2ccsc12) | 13 | 5 |
| 371 | (O=C(NCc1cccccc1)C2CCNCC2) | 16 | 16 |
| 372 | (c1ncn2ncnc2c1) | 48 | 47 |
| 373 | (O=S(=O)(N1CCCCC1)c2concc2) | 120 | 108 |
| 374 | (O=C(Nc1cccs1)\(\text{C}c2cccccc2) | 11 | 8 |
| 375 | (O=C1C=COc2cccccc12) | 204 | 170 |
| 376 | (C(=C\(\text{C}1nccs1)2cccccc2) | 10 | 1 |
| 377 | (O=C(COc1cccccc1)Nc2nnc[nH]2) | 6 | 6 |
| 378 | (N=C1Ncc2cccccc2N1) | 5 | 5 |
| 379 | (O=C1NC(=O)2c=CC=CNC2=N1) | 23 | 23 |
| 380 | (O=C1OCc2cccccc12) | 27 | 19 |
| 381 | (c1nncc2c[nH]cc12) | 1 | 1 |
| 382 | (O=S(=O)(N1CCCCC1)c2cccccc2) | 12 | 12 |
| 383 | (C(Sc1ocnn1)c2cccccc2) | 18 | 18 |
| 384 | (O=C(NCC1CCO1)\(\text{C}c2cccccc2) | 6 | 6 |
| 385 | (O=C(CSc1nnc[nH]1)N2CCCCC2) | 12 | 12 |
| 386 | (O=C1NCC(=C(N2CCCCC2))N1) | 6 | 6 |
| 387 | (O=C1Ccccccc1)c2concc2) | 17 | 17 |
| 388 | (O=C1Ccccccc1)c2concc2) | 11 | 11 |
| 389 | (N(c1ccccc1)c2nncnn2) | 2 | 2 |
| 390 | (O=C(CSc1nccnn1)Nc2ccccc2) | 22 | 12 |
| 391 | (c1ncc2ccsc2n1) | 63 | 22 |
| 392 | (O=C(Nc1ccccc1)c2concc2) | 11 | 11 |
| 393 | (O=C(CCn1cccccc1)NC2CCCCC2) | 8 | 8 |
| 394 | (O=C(NO(=O)(=O)c1ccccc1)c2cccccc2) | 13 | 5 |
| 395 | (O=C(COc1cccccc1)NCc2oncn2) | 13 | 13 |
| 396 | (O=C(Nc1ncns1)c2cccccc2) | 13 | 13 |
| 397 | (c1ccc(cc1)n2ccc2c2) | 9 | 0 |
| 398 | (c1ccc(cc1)n2ncnc[nH]2) | 7 | 7 |
| 399 | (O=C(CCC(=O)c1ccccc1)Nc2ccccc2) | 11 | 11 |
| 400 | (O=S(=O)(N1CCNCC1)c2cccs2) | 17 | 15 |
| 401 | (O=C1NC=C(=O)\(\text{N}O)S(=O)(=O)N2CCNCC2) | 5 | 5 |
| 402 | (O=C(Cn1cccccc1)NC2CCCCC2) | 5 | 5 |
|   | Molecular Formula               | Score1 | Score2 |
|---|--------------------------------|--------|--------|
| 403 | (O=C(Cn1cccc1)NC2CCCCCC2)      | 5      | 3      |
| 404 | (O=S(=O)(NCC1CCCCC1)c2cccs2)  | 12     | 12     |
| 405 | (O=C(C1CCCCC1)N2CCNCC2)        | 8      | 8      |
| 406 | (O=S(=O)(N1CCCCC1)c2cccs2)    | 20     | 20     |
| 407 | (C1C=CNc2nccn12)              | 31     | 13     |
| 408 | (C1Ccc2ccsc2CC1)              | 92     | 35     |
| 409 | (O=C(CS(=O)Cc1cocn1)N2CCNCC2) | 9      | 9      |
| 410 | (O=C1CN(C2CCCCCC2)C(=O)CN1)  | 37     | 27     |
| 411 | (C1Cc2ccsc2C1)                | 62     | 56     |
| 412 | (O=C1NC2cccs2SC=C1)           | 5      | 0      |
| 413 | (O=C(NCc1ccccc1)c2ccccc2)     | 22     | 21     |
| 414 | (O=C(NCC1cccccc1)c2ccccc2)    | 5      | 5      |
| 415 | (C1CC(N1)c2ccccc2)            | 8      | 8      |
| 416 | (O=C(S1=O)Cc1coen1)NCc2cccccc2) | 12     | 12     |
| 417 | (O=C(CCSSCCc1ccccc1)c2ccccc2) | 7      | 7      |
| 418 | (O=C1CN(C2CCCCC2)(=O)CN1)     | 37     | 27     |
| 419 | (O=C(CSc1ccccc1)C2CCCCC2)     | 11     | 1      |
| 420 | (O=C(CS1hccccc1)c2ccccc2)     | 20     | 3      |
| 421 | (O=C(CN1hcccc1)c2cccccc2)    | 14     | 1      |
| 422 | (O=C(CN1cccccc1)C2CNCC(=O)C2) | 6      | 6      |
| 423 | (O=C(NCC1cccccc1)c2ccccc2)   | 5      | 5      |
| 424 | (O=C1CN(C2CCCCC2)(=O)CN1)     | 37     | 27     |
| 425 | (O=C(CSc1ccccc1)C2CCS CCC2)  | 11     | 1      |
| 426 | (O=C(NCCc1cccccc1)NCC2cccccc2) | 8      | 0      |
| 427 | (O=C1CN(C2CCCCC2)(=O)CN1)     | 37     | 27     |
| 428 | (O=C(CSc1ccccc1)c2ccccc2)     | 7      | 0      |
| 429 | (O=C(CSc1cccccc1)c2ccccc2)   | 7      | 0      |
| 430 | (O=C(CSc1cccccc1)c2ccccc2)   | 7      | 0      |
| 431 | (O=C1CC(C2CCCCC2)(=O)CN1)     | 37     | 27     |
| 432 | (O=C(NCC1cccccc1)C2CNCC(=O)C2) | 6      | 6      |
| 433 | (O=C1CN(C2CCCCC2)(=O)CN1)     | 37     | 27     |
| 434 | (O=C(CSc1cccccc1)c2ccccc2)   | 7      | 0      |
| 435 | (O=C1CN(C2CCCCC2)(=O)CN1)     | 37     | 27     |
| 436 | (O=C(CNC(=O)CNS1cccccc1)Nc2cccccc2) | 6      | 0      |
| 437 | (O=C(CSc1cccccc1)c2ccccc2)   | 7      | 0      |
| Number | Structure                                                                 | Adj | Dist |
|--------|---------------------------------------------------------------------------|-----|------|
| 444    | (c1cc2scc2[nH]1)                                                          | 111 | 70   |
| 445    | (O=S(=O)(NC1CCCCC1)c2cccccc2)                                            | 14  | 14   |
| 446    | (c1cccc2cccccc2c1)                                                       | 42  | 25   |
| 447    | (C1Cc2cc[nH]c2CN1)                                                        | 49  | 3    |
| 448    | (O=S1(=O)Cc2c[nH]nc2C1)                                                  | 14  | 14   |
| 449    | (O=C1C=CN=C2SCC=NN12)                                                    | 9   | 0    |
| 450    | (O=C1CN=C2C=CN=CN12)                                                     | 191 | 129  |
| 451    | (O=S1(=O)N=Cnc2cccccc12)                                                 | 17  | 17   |
| 452    | (O=S1(=O)NC=Nc2cccccc12)                                                 | 11  | 11   |
| 453    | (O=C(1cccccc1)c2cccs2)                                                   | 29  | 0    |
| 454    | (N(1cccccc1)c2cccs2)                                                     | 33  | 12   |
| 455    | (O=C1Nc2ccnnn2C=C1)                                                      | 12  | 12   |
| 456    | (O=C(Nc1cccccn1)C2CCNC2)                                                 | 8   | 8    |
| 457    | (O=C(1CCCCNC1)N2CCNCC2)                                                  | 22  | 18   |
| 458    | (c1cn2nc[nH]2n1)                                                         | 11  | 11   |
| 459    | (O1ccc2ncncc12)                                                          | 11  | 11   |
| 460    | (O=C1CNCC(=O)c2cccccc2N1)                                                | 7   | 7    |
| 461    | (O=C(Cc1cc[nH]1)Nc2cccccc2)                                              | 12  | 12   |
| 462    | (O=C(Nc1ccccn1)C2CCNCC2)                                                 | 6   | 6    |
| 463    | (O=C(Cc1cc[nH]1)NCc2cccccc2)                                             | 9   | 9    |
| 464    | (O=C(Cc1cc[nH]1)N2CCNCC2)                                                | 11  | 11   |
| 465    | (O=C1Nc2cccccc2N=C1)                                                     | 66  | 64   |
| 466    | (C1CC(CCN1)c2ccncc2)                                                     | 17  | 17   |
| 467    | (O=C1NCCN(C2CCNCC2)C1=O)                                                 | 47  | 47   |
| 468    | (O=C1NN=C(N=C1)c2cccccc2)                                                | 5   | 5    |
| 469    | (C1CN(CCN1)c2ccccc2)                                                     | 3   | 3    |
| 470    | (C1CN(CC=C=C1)c2cccccc2)                                                 | 1   | 0    |
| 471    | (C1CCN(CC1)c2CCNCC2)                                                     | 14  | 14   |
| 472    | (O=C(CN1CCNC1)c2cccccc2)                                                 | 3   | 3    |
| 473    | (C1CC(=CCN1)c2cccccc2)                                                   | 1   | 0    |
| 474    | (C(CN1CCOC1)c2CCNCC2)                                                    | 1   | 1    |
| 475    | (O=C1C=CNC(=C1)CN2CCCCC2)                                                | 9   | 9    |
| 476    | (C1CN(CCO1)c2cccccc2)                                                    | 2   | 2    |
| 477    | (O=C(Nc1cccccc1)c2=NNC(=O)C=C2)                                          | 7   | 7    |
| 478    | (C(Nc1cccccc1)c2cccccc2)                                                 | 20  | 17   |
| 479    | (C1CCN(CC1)c2cccccc2)                                                    | 1   | 1    |
| 480    | (O=C(CNC1cccc1)NCCc2cccccc2)                                             | 8   | 8    |
| 481    | (O=C(CSc1nncc[nH]1)c2cccccc2)                                            | 20  | 11   |
| 482    | (O=C1NC=C2ncn12)                                                         | 44  | 36   |
| 483    | (O=C(Nc1cccccc1)C2=CC=CNC2=O)                                            | 28  | 28   |
| 484    | (O=C(Nc1nnccs1)C2=CC=CNC2=O)                                             | 10  | 10   |
|   | Formula                                                                 |   |   |
|---|------------------------------------------------------------------------|---|---|
| 485 | (O=C(Nc1cccon1)C2=CC=CNC2=O)                                          | 8 | 8 |
| 486 | (O=S(=O)(Cc1cccs1)c2cccc2)                                            | 7 | 7 |
| 487 | (C1cn2cccc2CN1)                                                       | 18| 12|
| 488 | (O=S(=O)(Cc1occ1)c2cccc2)                                            | 9 | 9 |
| 489 | (O=C1NC2=C(CCC2)C=N1)                                                | 82| 82|
| 490 | (N1C=CSc2nncc1n12)                                                   | 30| 30|
| 491 | (C1Sc2n[nH]cc12)                                                     | 23| 23|
| 492 | (O=C(Nc1ccccc1)C2=CNC(=O)C=C2)                                        | 9 | 9 |
| 493 | (C1CCc2cccc2C1)                                                      | 11| 5 |
| 494 | (O=C1NC(=NC=C1)n2cccn2)                                              | 9 | 9 |
| 495 | (O=C1NC2=C(CCCC2)C=N1)                                               | 19| 19|
| 496 | (C1CSC1=NC(=O)NC=C1)NC2cccc2)                                        | 8 | 8 |
| 497 | (C1CN(CC1)C2cccn2)                                                   | 7 | 7 |
| 498 | (O=C1NC(=O)c2cn[nH]c2N1)                                             | 6 | 6 |
| 499 | (O=C(NC1CNC(=O)C1)c2cccs2)                                           | 10| 10|
| 500 | (O=C(NC1CNC(=O)C1)c2occc2)                                           | 12| 12|
| 501 | (O=C(NC1CNC(=O)C1)c2cccc2)                                           | 21| 21|
| 502 | (O=C(Cc1ccccc1)NC2CNC(=O)C2)                                         | 12| 12|
| 503 | (O=C(Cc1cccs1)NC2CNC(=O)C2)                                          | 10| 10|
| 504 | (O=C(Cc1ccccc1)NC2CNC(=O)C2)                                         | 18| 18|
| 505 | (O=C(COc1ccccc1)NC2CNC(=O)C2)                                        | 8 | 8 |
| 506 | (O=C(Nc1ccccc1)Nc2nnccs2)                                            | 10| 8 |
| 507 | (O=C(NC1CNC(=O)C1)\C=C/c2cccccc2)                                    | 8 | 8 |
| 508 | (O=C(NC1CNC(=O)C1)C2CCCCC2)                                          | 10| 10|
| 509 | (O=C(CSc1nncc1)N2CCCCC2)                                             | 4 | 4 |
| 510 | (O=C1CCCN1cc2cccccc2)                                                | 17| 17|
| 511 | (O=C(NC1CCCC1)Nc2nnccs2)                                             | 6 | 6 |
| 512 | (O=C(CCCc1ccccc1)NC2CNC(=O)C2)                                       | 6 | 6 |
| 513 | (c1ncn2nn[nH]c2n1)                                                   | 73| 66|
| 514 | (C(N1CCOC21)c2cccs2)                                                 | 9 | 9 |
| 515 | (O=C(COc1ccccc1)NCCc2occc2)                                          | 5 | 5 |
| 516 | (O=C(CSC1=NC=CC(=O)N1)NC2cccon2)                                     | 5 | 5 |
| 517 | (O=C(CSC1=NC=CC(=O)N1)N2CCOCC2)                                      | 6 | 6 |
| 518 | (O=C(Cc1ccccc1)NCCc2cccs2)                                           | 9 | 8 |
| 519 | (O=C(COc1ccccc1)NCCc2cccs2)                                          | 5 | 5 |
| 520 | (O=C(CCCc1ccccc1)NCCc2ccsn2)                                         | 6 | 6 |
| 521 | (c1ncnc(c1)c2ncss2)                                                 | 10| 10|
| 522 | (c1ccnc(c1)c2cncs2)                                                 | 31| 19|
| 523 | (C(c1ccccc1)n2ccnc2)                                                | 5 | 5 |
| 524 | (O=C(CSc1ncn[nH]1)Nc2nnccs2)                                         | 13| 13|
| 525 | (O=C1NC(=O)C=C(N1)N2CCNCC2)                                         | 5 | 5 |
|   | Molecular Structure                                                                 | Count | Count |
|---|----------------------------------------------------------------------------------|------|------|
| 526 | (O=C(CSc1ncc[nH]1)NCc2occc2)                                                     | 5    | 5    |
| 527 | (O=C(CSc1ncc[nH]1)NCc2cccccc2)                                                   | 11   | 11   |
| 528 | (O=C(COC1cccccc1)NCCc2csn2)                                                      | 7    | 7    |
| 529 | (O=C(NCCc1cncs1)c2occc2)                                                         | 5    | 5    |
| 530 | (O=C(Cc1cccccc1)NCCc2cncs2)                                                      | 7    | 7    |
| 531 | (O=C(NCCc1cncs1)c2cccs2)                                                         | 5    | 5    |
| 532 | (O=C(NCCc1cncs1)c2occc2)                                                         | 8    | 8    |
| 533 | (C1CCC(NC1)c2ccccc2)                                                             | 5    | 5    |
| 534 | (c1cn2cnc2s1)                                                                    | 16   | 14   |
| 535 | (O=S(=O)(c1cccccc1)c2cocn2)                                                       | 2    | 2    |
| 536 | (C1CN(CCO1)c2ocnc2)                                                              | 5    | 5    |
| 537 | (C1CCN(C1)c2ocnc2)                                                               | 39   | 30   |
| 538 | (O=C(Nc1ccccc1)N2CCCCC2)                                                          | 7    | 7    |
| 539 | (O=S(=O)(NCc1ccccc1)c2cccs2)                                                      | 7    | 7    |
| 540 | (O=C(CNS(=O)(=O)c1cccs1)N2CCNCC2)                                                | 8    | 8    |
| 541 | (O=C(CNS(=O)(=O)c1cccs1)Ncc2cccccc2)                                             | 7    | 7    |
| 542 | (o1cnc(c1)c2cccccc2)                                                              | 21   | 21   |
| 543 | (O=C1NN=C(C=C1)e2ccncc2)                                                         | 5    | 5    |
| 544 | (C1CCCCc2[nH]c2ccc2C1)                                                            | 8    | 4    |
| 545 | (O=C1NN=C2CCCCC2=C1)                                                              | 16   | 16   |
| 546 | (c1cccc2cncc2c1)                                                                 | 75   | 59   |
| 547 | (O=S(=O)(NCc1ccccc1)c2cncc2)                                                      | 12   | 12   |
| 548 | (O=S(=O)(Nc1cccccc1)c2cncc2)                                                      | 8    | 8    |
| 549 | (O=S(=O)(N1CCNCC1)c2cncc2)                                                        | 2    | 2    |
| 550 | (o1ccc2cccccnc12)                                                                | 27   | 24   |
| 551 | (C(Sc1ncccn1)c2oncn2)                                                             | 20   | 11   |
| 552 | (c1cccc2sncc2c1)                                                                 | 92   | 88   |
| 553 | (O=C(CCC1cc[nH]c1)NCc2cccccc2)                                                    | 12   | 12   |
| 554 | (O=C(CCc1cc[nH]c1)Nc2ccccc2)                                                      | 11   | 11   |
| 555 | (O=C(CCc1cc[nH]c1)N2CCNCC2)                                                       | 7    | 7    |
| 556 | (C1CN(CCN1)c2oncc2)                                                               | 8    | 6    |
| 557 | (O=C(NCc1occc1)c2concc2)                                                          | 5    | 5    |
| 558 | (O=C1C=CN=C2SC=CN12)                                                              | 311  | 311  |
| 559 | (C1CC(=CCN1)c2ncon2)                                                              | 5    | 5    |
| 560 | (O=C(COc1cccccc1)Nc2cccn[nH]2)                                                    | 12   | 1    |
| 561 | (O=C(Nc1ccn[nH]1)c2ccccc2)                                                        | 11   | 2    |
| 562 | (O=C1NC(=O)c2cnccc2N1)                                                             | 45   | 45   |
| 563 | (c1cnc(nc1)n2cccn2)                                                               | 16   | 9    |
| 564 | (C1CCN(C1)c2ccn[nH]2)                                                             | 14   | 14   |
| 565 | (C1CCN(C1)c2oncc2)                                                                | 13   | 11   |
| 566 | (C1COc2cccccc2C1)                                                                 | 60   | 60   |
|   | Formula                                    |    |    |
|---|--------------------------------------------|----|----|
| 567| (C1CC2(CCN1)NC=CN=C2)                      | 7  | 6  |
| 568| (O=C(CSc1nnc[nH]1)N2CCNCC2)                | 9  | 9  |
| 569| (O=C(CSc1nnc[nH]1)NCc2ccccc2)              | 9  | 9  |
| 570| (O=C1N=CNc2ncccc12)                       | 13 | 9  |
| 571| (C1CCCN2CCN=C2CC1)                        | 26 | 26 |
| 572| (C1CC2=NCCN2C1)                           | 17 | 17 |
| 573| (O=C(CSc1nnc[nH]1)NCCc2ccccc2)             | 7  | 7  |
| 574| (O=C(NCc1nnn[nH]1)C2NCN(=O)C2)             | 5  | 5  |
| 575| (O=C(CSc1nnc[nH]1)NCCc2ccccc2)             | 7  | 7  |
| 576| (O=C1NN=Cc2n[nH]cc12)                     | 24 | 23 |
| 577| (O=C(CCc1ccc[nH]1)NCCc2ccccc2)             | 10 | 10 |
| 578| (O=C(CCc1ccc[nH]1)NCc2ccccc2)              | 3  | 3  |
| 579| (O=C(CCc1ccc[nH]1)Ne2ccccc2)               | 9  | 9  |
| 580| (C1CN2CCN=c2co1)                          | 21 | 21 |
| 581| (O=S(=O)(N1CCNCC1)c2cc[nH]n2)              | 12 | 12 |
| 582| (O=S(=O)(Nc1cccnc1)c2cc[nH]n2)             | 11 | 11 |
| 583| (O=C(CCc1cccnc1)NCc5(=O)(=O)N22CCNCC2)     | 5  | 5  |
| 584| (O1cccnc1c2c[nH]nn2)                       | 5  | 5  |
| 585| (C1C=Nc2ccccc2N=c1)                       | 24 | 9  |
| 586| (O=S(=O)(N1CCOC1)c2cn[nH]c2)              | 12 | 12 |
| 587| (O=S(=O)(NCc1cccnc1)c2cc[nH]n2)            | 4  | 4  |
| 588| (O=C(Nc1cccnc1)c2=NcN(=O)NC2=cO)           | 12 | 12 |
| 589| (O=C(N1CCNCC1)c2=NcN(=O)NC2=cO)            | 7  | 7  |
| 590| (O=C(N1CCCNCC1)c2=NcN(=O)NC2=cO)           | 5  | 5  |
| 591| (O=C1NC(=O)(N=N(c1)c2cncccc2)              | 8  | 8  |
| 592| (O=C1Nc2ccccc2S1)                         | 27 | 24 |
| 593| (O=C1NC=CN2CCCC12)                        | 28 | 28 |
| 594| (C10c2ccccc2c=C1)                         | 10 | 10 |
| 595| (O=C1NC=Nc2ncccc12)                       | 28 | 28 |
| 596| (O=C1Nc2ncnc2N1)                          | 44 | 44 |
| 597| (O=C(N1CCNCC1)c2cc[nH]2)                  | 18 | 18 |
| 598| (O=S(=O)(Nc1cccnc1)c2c[nH]cn2)             | 6  | 6  |
| 599| (O=S(=O)(N1CCNCC1)c2c[nH]cn2)              | 7  | 7  |
| 600| (C1CCCN(CCC1)c2ccncn2)                    | 21 | 13 |
| 601| (O=S(=O)(N1CCCNCC1)c2cc[nH]c2)             | 27 | 27 |
| 602| (C1CCCan2ccnc2C1)                         | 5  | 4  |
| 603| (C1CN=C2Sc=C2c=C1)                        | 5  | 4  |
| 604| (O=C(NCCc1csnc1)c2cccs2)                  | 3  | 3  |
| 605| (O=C(CSC1=Nc=CC(=O)N1)NCc2ccccc2)         | 9  | 9  |
| 606| (O=C1NNCCN2ccnc12)                        | 29 | 29 |
| 607| (C1SC=C2c[nH]nc12)                        | 42 | 39 |
|   | Chemical Structure | Value1 | Value2 |
|---|--------------------|--------|--------|
| 608| (O1ccc1c2ocnc2)    | 12     | 12     |
| 609| (O=C1Nc2ccccc2C=N1) | 61     | 42     |
| 610| (C1CCN(C1)c2ccccc2) | 33     | 25     |
| 611| (O=C(NCCc1cn[nH]c1)Nc2ccccc2) | 29     | 29     |
| 612| (O=S(=O)(NCc1ccc[nH]1)c2ccccc2) | 12     | 12     |
| 613| (O=C1Nc2[nH]1nc2N=C1) | 4      | 4      |
| 614| (C1Cc2ncncc2CN1)   | 78     | 75     |
| 615| (O=C1NC=Cn2ncccc12) | 22     | 22     |
| 616| (C1CCN(C1)c2ncncc2) | 19     | 19     |
| 617| (O=C(N1CCNCC1)c2cncnc2) | 14     | 14     |
| 618| (O=C1Oc2cnccc2C=C1) | 11     | 11     |
| 619| (O=S(=O)(N1CCCC1)c2c[nH]cn2) | 43     | 43     |
| 620| (O=C(CN1c1ccn1)NC2CCNCC2) | 5      | 5      |
| 621| (O=C1NCCN(C2CCNCC2)C1=O) | 7      | 7      |
| 622| (O=C(N1CCOCC1)c2cccs2) | 6      | 6      |
| 623| (O=C1NCCN(Cc2cccccc2)C1=O) | 4      | 4      |
| 624| (c1cccc[nH]1nc2c1) | 46     | 44     |
| 625| (O=C(NCc1ccc1)NC2CCNCC2) | 7      | 7      |
| 626| (O=C(NCc1ccc1)NC2ccccc2) | 7      | 7      |
| 627| (O=C(N1CCCCC1)c2cc[nH]c2) | 21     | 21     |
| 628| (O=S(=O)(NC1c1ccnc1)c2ccccc2) | 4      | 4      |
| 629| (O=C(CN1Cc1ccn1)Nc2ccccc2) | 27     | 27     |
| 630| (O=C(CN1CCCC1=O)=O)NC2ccccc2) | 4      | 4      |
| 631| (c1cc2[nH]1nc2cn1) | 79     | 19     |
| 632| (O=C1CC=NCe2ccccc2N1) | 17     | 15     |
| 633| (O=C1NC=O)c25ccccc2N1) | 255    | 192    |
| 634| (C1CN2C=NC=CC2=N1) | 12     | 12     |
| 635| (C(N1CCOC1)c2oncc2) | 12     | 12     |
| 636| (O=C1CSc2[nH]1nc2N1) | 27     | 27     |
| 637| (C(N1CCOCC1)c2oncc2) | 12     | 12     |
| 638| (O=S(=O)(N1CCCOCC1)c2c[nH]cn2) | 8      | 8      |
| 639| (c1ccnnc(c1)ncc2cn2) | 70     | 68     |
| 640| (O=C(CCC1cn[nH]c1)N2CCNCC2) | 6      | 5      |
| 641| (O=C1CC(CN1)c2oncn2) | 10     | 10     |
| 642| (O=C(N1CCCCOC1)c2cc[nH]c2) | 17     | 17     |
| 643| (O=C(CNS(=O)=O)c1ccs1)c2ccccc2) | 10     | 10     |
| 644| (C(Nc1ccc1cc1)c2oconn2) | 29     | 3      |
| 645| (C(N1CCNCC1)c2oconn2) | 29     | 17     |
| 646| (O=C1C=SC(=O)=O)NC1c2ccccc2) | 23     | 21     |
| 647| (O=C1NCc2ccccc12) | 45     | 40     |
| 648| (o1ncnc1c2ccn[nH]2) | 22     | 22     |
(O=S(=O)(c1ccccc1)c2cn[nH]c2) 23 23
(c1ccn2ccccc2c1) 33 25
(O=C1NC-CN=C1NCc2cccs2) 5 5
(O=C1NC-CN2CCCC12) 8 8
(O=S(=O)[NCC1CNCNCC1]c2cc[nH]c2) 8 8
(O=S1(=O)CCCN1ccccc2) 19 19
(o1ccc(n1)c2cccs2) 9 9
(O=C1NC=Nc2c[nH]nc12) 30 8
(c1ccn(c1)c2nncc2) 15 9
(C1CN(CC1N)c2nncc2) 4 4
(C1CCN(C1)c2nncc2) 18 18
(O=S(=O)[NCC1CCCC1]c2ccsc2) 6 6
(O=S(=O)[NCC1cccacc1]c2ccsc2) 11 11
(C1CCC2=C(CC1)NCC2) 22 15
(C1(N1CCCNCC1)c2cn[nH]c2) 86 53
(O=C(NC1CCCNCC1)c2cn[nH]c2) 6 6
(O=C(=O)[N1CCCCC1]c2ccsc2) 6 6
(O=C(=O)[N1CCCCC1]c2ccsc2) 12 12
(c1ccn2nncc2c1) 10 6
(c1ccn2nncc2c1) 29 29
(O=C1NN=C(C=C1)N2CCNCC2) 42 42
(O=C(CS1oncn1)N2CCNCC2) 8 8
(O=C(CS1oncn1)Nc2ccccc2) 9 8
(O=C(CS1oncn1)N2CCCCC2) 6 6
(O=C(NC1=NC(=O)NC1=O)Nc2ccccc2) 12 12
(O=C(CN=CCN(CC1)N=CC=N2) 11 2
(C1Nc2ccccc2C=N1) 5 5
(O=C(NCCN1CCNCC1)c2cn[nH]c2) 23 19
(O=C1CS(=O)[N2c(N1)C=NC2=O) 40 40
(C1CCN(CC1)c2nncc2) 8 8
(O=C(NCCN1CCNCC1)c2cn[nH]c2) 8 8
(C1CCN(C1)c2ccncc2) 5 5
(O=C(N1CCOC1)c2cn[nH]c2) 8 8
(O=C(NCC1CCOC1)c2cn[nH]c2) 8 8
(O=C1CCCS2(N1)C=NC2=O) 9 8
(C1CCCN(C1)c2nncc2) 14 12
(C1CN(CCO1)c2nncc2) 5 5
(C1CCc2oncc2CC1) 9 9
(O=C(NCC1cccacc1)c2c[nH]nn2) 7 7
(O=C(Cn1cccacc1)N2CCNCC2) 8 8
|   | Chemical Structure                                      | Count1 | Count2 |
|---|--------------------------------------------------------|--------|--------|
| 690| (O=S(=O)(NC1cccccc1)c2nncc2)                           | 8      | 8      |
| 691| (O=C1NCc2cc[nH]c12)                                    | 16     | 10     |
| 692| (C(N1CCNC1C)c2no[nH])                                  | 7      | 7      |
| 693| (O=C(NCCc1cccccc1)c2ccn[nH]2)                          | 8      | 8      |
| 694| (O=C(Nc1cccccc1)c2ccn[nH]2)                            | 10     | 10     |
| 695| (O=C1NN=C2=CNC=C12)                                   | 11     | 11     |
| 696| (O=S(=O)(Cc1co[cn]1)c2ccccc2)                          | 10     | 10     |
| 697| (C(S1cccccc1)c2co[cn]2)                                | 29     | 10     |
| 698| (O=C(N1CCNC1C)c2ccccc2)                               | 7      | 1      |
| 699| (O=C1CN(CCc2ccncc2)C(=O)N1)                           | 7      | 7      |
| 700| (O=C1CN(Cc2ccncc2)C(=O)N1)                            | 9      | 9      |
| 701| (O=C(N1CCNC1C)c2ccccc2)                               | 5      | 5      |
| 702| (C1CN(CC1)c2on[nn]2)                                  | 10     | 10     |
| 703| (C1CCc2ccnnc2CC1)                                     | 30     | 11     |
| 704| (c1ccn2ccnn2c1)                                        | 225    | 128    |
| 705| (O=C(NC1CCCCC1C)C2CNCC(=O)N2)                         | 11     | 11     |
| 706| (O=C1CNCC1Nc2ccccc2)                                  | 4      | 4      |
| 707| (O=C(NCc1cccccc1)c2ccccc2)                            | 1      | 1      |
| 708| (O=C(N1CCNC1C)c2ccccc2)                               | 1      | 1      |
| 709| (O=C(N1CCNC1C)c2ccn[nH]2)                             | 13     | 13     |
| 710| (c1cc2ccsc2[nH]c2s1)                                  | 11     | 1      |
| 711| (O=C(COCc1ccon1)N2CCNCC2)                             | 3      | 3      |
| 712| (O=C1NC=CC1C)c2ccccc2)                                | 19     | 19     |
| 713| (c1cc2cn[nH]c2s1)                                     | 62     | 38     |
| 714| (C1SC=CN=C2=Cc=C12)                                   | 8      | 2      |
| 715| (O=C1CCC=C2SCN1C12)                                   | 8      | 7      |
| 716| (C1CCc2ncccc2C1)                                      | 39     | 6      |
| 717| (O=C1NC=Cc2[nH]ccc12)                                 | 24     | 24     |
| 718| (O=S(=O)(Nc1cccccc1)c2cooncc2)                        | 5      | 5      |
| 719| (O=C1OC=Cc2[nH]nc12)                                  | 39     | 39     |
| 720| (O=C(CNS(=O)(=O)c1cn[nH]c1)Nc2ccccc2)                 | 12     | 12     |
| 721| (O=C(CNS(=O)(=O)c1concc1)N2CCNCC2)                    | 12     | 12     |
| 722| (O=C(CNS(=O)(=O)c1concc1)Ncc2ccccc2)                  | 12     | 12     |
| 723| (O=C(CNS(=O)(=O)c1concc1)NCCc2ccccc2)                 | 7      | 7      |
| 724| (O=C(Cc1concc1)Nc2ccccc2)                             | 10     | 10     |
| 725| (c1ccc(nc1)c2ccnn2)                                   | 3      | 3      |
| 726| (c1ccnnc1)c2cccs2                                     | 17     | 13     |
| 727| (O=C1NC(=O)c2occcc2N1)                                | 83     | 65     |
| 728| (C1C=COC2ncccc2)                                      | 98     | 25     |
| 729| (O=C(NCCCN1CCNC1)c2occcc2)                            | 1      | 1      |
| 730| (O=C(N1CCNC1C)c2occcc2)                               | 13     | 10     |
|    | Chemical Structure                                                                 | 8    | 8    |
|----|-----------------------------------------------------------------------------------|------|------|
| 772| (O=C(Nc1nncs1)c2cccs2)                                                          |      |      |
| 773| (O=S(=O)(N1CCCC1)c2nncs2)                                                        | 12   | 12   |
| 774| (O=S(=O)(N1CCCC1)c2nncs2)                                                        | 10   | 10   |
| 775| (c1cnc2scnc2c1)                                                                  | 31   | 29   |
| 776| (O=C(Nc1cccccc1)c2cc[nH]c2)                                                       | 12   | 12   |
| 777| (O=C(Nc1cccccc1)c2cc[nH]c2)                                                       | 11   | 11   |
| 778| (O=C(Nc1cccccc1)c2cn[nH]c2)                                                       | 12   | 4    |
| 779| (O=C1NN=CN2cccc12)                                                                | 270  | 261  |
| 780| (O=S1(=O)NC=CC(=N1)c2cccs2)                                                       | 10   | 10   |
| 781| (O=S1(=O)NC=CC(=N1)c2cccs2)                                                       | 7    | 7    |
| 782| (O=C1NN=CN2cccc12)                                                                | 696  | 66   |
| 783| (O=C1NC=NC2=C1CNCC2)                                                              | 25   | 25   |
| 784| (O=C(Nc1cccccc1)C2=CC=NS(=O)(=O)N2)                                              | 12   | 12   |
| 785| (O=C(Nc1cccccc1)C2=CC=NS(=O)(=O)N2)                                              | 5    | 5    |
| 786| (C1OC=CCnncocc12)                                                                | 9    | 0    |
| 787| (C1OC=CC[nc]nncc12)                                                               | 34   | 34   |
| 788| (C1SC=CC2oncc12)                                                                  |      |      |
| 789| (c1cccs2[nc]nncc2c1)                                                              |      |      |
| 790| (O=S1(=O)C=CC(=N1)N2CCNCC2)                                                      | 12   | 12   |
| 791| (O=S1(=O)C=CC(=N1)N2CCNCC2)                                                      | 7    | 7    |
| 792| (N(c1ccccc1)c2cccs2)                                                              | 9    | 9    |
| 793| (O=C1NCNc2cccc2N1)                                                                | 5    | 3    |
| 794| (C1Ccc2cn[nH]c2C=C1)                                                              | 12   | 12   |
| 795| (C1CCCC(CC1)Ne2nncs2)                                                             | 12   | 12   |
| 796| (O=C1NC2(CCNCC2)OC=C1)                                                            | 12   | 5    |
| 797| (O=C1NN=CN2nnc12)                                                                 | 10   | 10   |
| 798| (c1cc2[nc]nncc2n1)                                                                | 20   | 20   |
| 799| (O=C(NCc1cn[nH]c1)Ne2ccccc2)                                                      | 6    | 0    |
| 800| (O=C(Nc1nncs1)c2ccccc2)                                                           | 11   | 11   |
| 801| (o1nnc1c1c2ccccc2)                                                                | 142  | 138  |
| 802| (O=C1Ccc2cn[nH]c2N1)                                                               | 28   | 24   |
| 803| (O=C1NC=CN2cccc12)                                                                | 16   | 10   |
| 804| (O=C(Nc1cccccc1)Ne2ccccc2)                                                        | 8    | 8    |
| 805| (O=C(CSc1oconn1)Oc2ccccc2)                                                        | 15   | 15   |
| 806| (O=C1C=CNCC2=C1CCCC2)                                                             | 7    | 7    |
| 807| (O=C(Nc1connon1)c2ccccc2)                                                         | 12   | 12   |
| 808| (O=C1NC=NC2=C1CCCC2)                                                               | 17   | 17   |
| 809| (O=C(NCCSCc1cccccc1)C2CCNCC2)                                                     | 6    | 6    |
| 810| (o1ncnc1c1c2ccccc2)                                                                | 24   | 24   |
| 811| (O=C1NC=NC2=C1CCCC2)                                                               | 17   | 16   |
| 812| (O=C(NCc1occc1)c2cccon2)                                                           | 6    | 1    |
|   | Chemical Structure                                                                 | T   | A  |
|---|-----------------------------------------------------------------------------------|-----|----|
| 813| (C1CNC2nccn2C1)                                                                   | 7   | 5  |
| 814| (C1CC=NC2ccccccc2S1)                                                              | 5   | 0  |
| 815| (O=C(Nc1cccs1)c2cccon2)                                                           | 26  | 18 |
| 816| (O=C1CCNC(C1)c2cccs2)                                                             | 5   | 5  |
| 817| (O=C(N1CCNCC1)c2cccon2)                                                            | 12  | 12 |
| 818| (O=C1CSCc2cn[nH]c2N1)                                                              | 11  | 11 |
| 819| (O=C(CSc1ocnn1)NCc2cccccc2)                                                        | 6   | 6  |
| 820| (C(CSc1ocnn1)Oc2cccccc2)                                                           | 10  | 10 |
| 821| (O=C(CSc1ocnn1)NC2CCCC2)                                                           | 8   | 8  |
| 822| (O=C(Nc1ccccccc1)c2nc[nH]n2)                                                        | 24  | 24 |
| 823| (o1cncc(n1)c2cccncc2)                                                              | 18  | 8  |
| 824| (O=C(CCc1oncn1)Ne2cccccc2)                                                          | 29  | 29 |
| 825| (o1ncnc1c2ccencc2)                                                                 | 17  | 11 |
| 826| (o1cncc(n1)c2ccencc2)                                                              | 14  | 14 |
| 827| (C1CCc2scnc2C1)                                                                    | 35  | 35 |
| 828| (O=C1NC(=O)c2cc[nH]c2N1)                                                           | 29  | 29 |
| 829| (C(Cc1ccccn1)N2CCNCC2)                                                              | 23  | 23 |
| 830| (O=C(Oc1ccccccc1)Ne2cccccc2)                                                        | 15  | 2  |
| 831| (C(Nc1cccccn1)c2ccccc2)                                                             | 31  | 30 |
| 832| (O=C(NCc1ccccc1)c2ccccc2)                                                            | 11  | 4  |
| 833| (O=C(NCc1ccccc1)c2ccccc2)                                                            | 5   | 5  |
| 834| (O=C(COc1ccccccc1)NCc2cccs2)                                                        | 12  | 6  |
| 835| (C(Nc1cccccn1)c2occc2)                                                              | 23  | 23 |
| 836| (C(Cc1ccccn1)N2CCNCC2)                                                              | 20  | 20 |
| 837| (O=C(Oc1ccccccc1)c2cccon2)                                                           | 12  | 5  |
| 838| (C1CCC(CC1)N2CCOCC2)                                                                | 21  | 21 |
| 839| (O=C(NCc1ccccccc1)c2cccon2)                                                          | 17  | 17 |
| 840| (O=C(Oc1ccccccc1)NCC2CCCC2)                                                          | 10  | 10 |
| 841| (C1CCCCC1)                                                                         | 9   | 7  |
| 842| (O=C(NCC1CCCC1)c2cccccc2)                                                            | 10  | 10 |
| 843| (C1CC(CC1NC1)c2ocnn2)                                                               | 24  | 24 |
| 844| (Oc1ccccccc1)c2nccs2                                                                | 12  | 12 |
| 845| (o1ccccc1c2nc[nH]n2)                                                                  | 43  | 38 |
| 846| (C1CCC(CC1)N2CCNCC2)                                                                | 3   | 3  |
| 847| (C1CCC2(CC1)CCNC=N2)                                                                | 37  | 25 |
| 848| (c1cnnc(c1)c2nccs2)                                                                  | 30  | 5  |
| 849| (O=C1C=CC=CCc2occc12)                                                               | 24  | 21 |
| 850| (O=S1(=O)CCC(C1)NCc2occcc2)                                                          | 22  | 22 |
| 851| (o1nce(n1)c2cccs2)                                                                   | 5   | 5  |
| 852| (O=C(Oc1ccccccc1)c2cnnns2)                                                           | 9   | 9  |
| 853| (c1csc(c1)c2ccsc2)                                                                   | 15  | 13 |
| ID  | Structure                                                                 | Adsorption   | Desorption  |
|-----|---------------------------------------------------------------------------|--------------|-------------|
| 854 | (C(NCc1ccccc1)C2CCCO2)                                                   | 22           | 22          |
| 855 | (O=C(Nc1ccccc1)c2csnn2)                                                   | 11           | 11          |
| 856 | (O=S(=O)(c1ccccc1)c2|nH|cn2)                                                                                 | 7            | 6           |
| 857 | (c1sc(c1)c2ncsn2)                                                       | 6            | 6           |
| 858 | (O=C(COc1ccccc1)Nc2ncns2)                                               | 11           | 11          |
| 859 | (C(N1CCCCC1)c2ccccc2)                                                   | 17           | 16          |
| 860 | (O=C(CSc1ccncn1)Nc2cccccc2)                                             | 12           | 12          |
| 861 | (o1ccccc1c2occcn2)                                                      | 56           | 33          |
| 862 | (C(Nc1ocnc1)c2ccccc2)                                                   | 5            | 5           |
| 863 | (C1CN(CCN1)c2ocnc2)                                                     | 42           | 25          |
| 864 | (C1Cc2cnnc2C1)                                                          | 1            | 1           |
| 865 | (O=C(COc1ccccc1)Nc2oncc2)                                               | 12           | 12          |
| 866 | (O=C1CC(CN1)c2ncns2)                                                    | 7            | 7           |
| 867 | (N(c1ccccc1)c2ccncn2)                                                   | 37           | 28          |
| 868 | (O=C1NC=NC(=C1)c2cccccc2)                                               | 1            | 1           |
| 869 | (C(CNCc1occcc1)CSc2nnn[nH]2)                                            | 5            | 5           |
| 870 | (C(CNCc1ccccc1)CSc2nnn[nH]2)                                            | 23           | 23          |
| 871 | (C(Nc1ncnc1)c2occc2)                                                    | 41           | 24          |
| 872 | (o1ncn(n1)c2nncc[nH]2)                                                  | 36           | 36          |
| 873 | (O=C(CSc1ccccc1)c2cccccc2)                                              | 5            | 1           |
| 874 | (C(CSc1nnn[nH]1)Nc2occcc2)                                              | 6            | 5           |
| 875 | (O=C1CCCC2=C(NC=NC2=O)N1)                                               | 11           | 11          |
| 876 | (C1CCN(CC1)c2ncncn2)                                                    | 21           | 21          |
| 877 | (O=C1CCC2=C(N1)N=CNC2=O)                                                | 7            | 7           |
| 878 | (O=C(Nc1oncc1)c2cccccc2)                                                | 11           | 11          |
| 879 | (O=C1NN=Nc2cccccc1)                                                     | 12           | 12          |
| 880 | (O=C(NCC1CCNC1)Nc2cccccc2)                                              | 2            | 2           |
| 881 | (O=C(NCCN1CCNC1)Nc2cccccc2)                                             | 6            | 6           |
| 882 | (O=C(NCc1oncn1)c2occc2)                                                 | 9            | 9           |
| 883 | (o1nc2nccnc2n1)                                                         | 2            | 1           |
| 884 | (O=C(NCC1CCNC1)Nc2cccccc2)                                              | 6            | 5           |
| 885 | (C1CCN(CC1)c2ncccn2)                                                    | 8            | 8           |
| 886 | (O=C(Nc1ccccc1)C2=CC=NNC2=O)                                            | 12           | 12          |
| 887 | (O=C(Nc1ncns1)C2=CC=NNC2=O)                                             | 5            | 5           |
| 888 | (O=C1NN=CC2=C1CCCC2)                                                    | 12           | 5           |
| 889 | (O=C(Cc1csn1)Nc2cccccc2)                                                | 12           | 12          |
| 890 | (O=C(Nc1ccccc1)c2ncncn2)                                                | 33           | 33          |
| 891 | (O=C(Nc1nnns1)c2ccncn2)                                                 | 14           | 14          |
| 892 | (C(Sc1ncncn1)c2cccccc2)                                                 | 38           | 15          |
| 893 | (C(NCc1ccccc1)c2occc2)                                                  | 41           | 22          |
| 894 | (C(NCc1occcc1)c2occc2)                                                  | 24           | 24          |
| ID  | Molecular Formulas                                                                 | H   | W  |
|-----|------------------------------------------------------------------------------------|-----|----|
| 895 | O=C(NC1CCS(=O)(=O)C1)c2cccn2                                                      | 12  | 12 |
| 896 | O=C(Nc1cccs1)c2cccn2                                                             | 10  | 7  |
| 897 | C(NCc1cccs1)c2occc2                                                              | 4   | 4  |
| 898 | O=C(NCc1cccccc1)c2cn[nH]n2                                                        | 12  | 12 |
| 899 | O=C(NCc1cccs1)c2cn[nH]n2                                                           | 7   | 7  |
| 900 | (c1ccc(cc1)n2nccn2)                                                               | 12  | 12 |
| 901 | O=C(NCCCCc1cccccc1)c2cn[nH]n2                                                      | 8   | 8  |
| 902 | O=C(NCCCCc1cccccc1)c2cn[nH]n2                                                      | 6   | 6  |
| 903 | O=C(NCc1ccccc1)c2cn[nH]n2                                                           | 6   | 6  |
| 904 | O=C(NCc1ccccc1)c2cn[nH]n2                                                           | 7   | 7  |
| 905 | O=C(NCCCCc1cccccc1)c2cn[nH]n2                                                      | 13  | 13 |
| 906 | O=C(NCc1ccccc1)c2cccn2                                                             | 9   | 6  |
| 907 | (C1CCC(C1)c2cccccc2)                                                              | 12  | 12 |
| 908 | (C1CC(CC1N)c2nncn2)                                                               | 5   | 5  |
| 909 | (C1CC(CC1N)c2oncn2)                                                                | 9   | 9  |
| 910 | (C=NC(C2N3CC4CN2CC(C3)C4=O)(=O)N1)                                               | 5   | 5  |
| 911 | (CN1CCOCC1)C2CCCCN2                                                               | 9   | 9  |
| 912 | (c1nncc2[nH]nnc12)                                                                | 13  | 8  |
| 913 | (c1ccc(cc1)c2nnn[nH]2)                                                             | 8   | 8  |
| 914 | (CN1CCCCC1)C2CCCCN2                                                               | 11  | 11 |
| 915 | (O=S(=O)(c1ccccc1)c2ccsn2)                                                         | 15  | 13 |
| 916 | (O=c1cccn1)c2nccn2                                                                | 18  | 12 |
| 917 | (O=C12CN3CC1CN(C2)C3c4ccccn4)                                                     | 5   | 5  |
| 918 | (c1csc(c1)c2c[nH]cn2)                                                              | 3   | 0  |
| 919 | (c1ccc(cc1)c2c[nH]cn2)                                                             | 6   | 0  |
| 920 | (O=C1NN=C(Oc2nncn2)C=C1)                                                          | 11  | 11 |
| 921 | (C1CC(CC1N)c2nnn[nH]2)                                                             | 10  | 10 |
| 922 | (N1C=NC=Ne2ccccc12)                                                               | 43  | 23 |
| 923 | (C1CC(CC1N)Oc2ccccc2)                                                              | 4   | 4  |
| 924 | (C1CC(CC1N)Ne2oacen2)                                                              | 4   | 4  |
| 925 | (C(Nc1oacen1)c2ccccc2)                                                             | 24  | 13 |
| 926 | (C1CCCN(CC1)c2oacen2)                                                              | 14  | 4  |
| 927 | (N(c1oacen1)c2ccccc2)                                                              | 10  | 10 |
| 928 | (O=C1NCNc2ccsc12)                                                                  | 7   | 5  |
| 929 | (O1ccnc1\C=C\c2ccccc2)                                                            | 9   | 9  |
| 930 | (C(Cc1ccccc1)Ne2oacen2)                                                             | 13  | 13 |
| 931 | (N(c1ccccc1)c2cn[nH]n2)                                                             | 10  | 0  |
| 932 | (O(c1ccccc1)c2cccn2)                                                                | 6   | 0  |
| 933 | (O=C1Cc2ccccc2CN1)                                                                  | 10  | 8  |
| 934 | (c1ncncc(c1)c2nc[nH]n2)                                                             | 17  | 17 |
| 935 | (O=C(CCCc1oncn1)NCc2occc2)                                                         | 3   | 3  |
| Number | Chemical Structure                                                                 | X Value | Y Value |
|--------|------------------------------------------------------------------------------------|---------|---------|
| 936    | (C1CC2nocc2C1)                                                                      | 11      | 11      |
| 937    | (O=C(Cc1cccc1)NCc2oncn2)                                                            | 5       | 5       |
| 938    | (C(NC1CCCCC1)c2oncn2)                                                                | 9       | 7       |
| 939    | (o1ccnc1c2cccc2)                                                                     | 29      | 5       |
| 940    | (O=C(CSC1=NC=CC(=O)N1)N2CCNCC2)                                                     | 6       | 6       |
| 941    | (O=C1NC(=NC=C1)SCCOc2cccc2)                                                          | 6       | 3       |
| 942    | (O=C1NC(=NC=C1)Nc2cccccc2)                                                           | 11      | 11      |
| 943    | (O=C(NCc1occ1c2cccn2)                                                                | 4       | 3       |
| 944    | (O=C1NC2(C=CNC2=O)C=C1)                                                              | 11      | 11      |
| 945    | (O=C(N1CCNCC1)c2ccncn2)                                                              | 4       | 4       |
| 946    | (O=C(COC1cccccc1)Ncc2occcc2)                                                         | 3       | 1       |
| 947    | (O=C(NCc1occc1)c2cccccc2)                                                             | 2       | 0       |
| 948    | (O=C1Nc2cccccc2C1=O)                                                                  | 4       | 4       |
| 949    | (C1CC2OCOC2CO1)                                                                      | 11      | 11      |
| 950    | (c1ccc2snnc2c1)                                                                      | 22      | 22      |
| 951    | (O=C(Nc1ccsc1)c2cccccc2)                                                              | 6       | 5       |
| 952    | (O=C1NN=Cc2c[nH][cc12]                                                                | 85      | 85      |
| 953    | (O=C(Nc1ccsc1)c2ccsc2)                                                                | 7       | 4       |
| 954    | (O=S(=O)(NCc1cscn1)c2cccccc2)                                                        | 9       | 9       |
| 955    | (C1SC=Cc2sccl2)                                                                      | 20      | 3       |
| 956    | (O=C1NC2(CCCCC2)N=C1)                                                                 | 12      | 12      |
| 957    | (O=C1NCN=C1c2cccccc2)                                                                | 12      | 12      |
| 958    | (O=C1NC2(CCCCC2)N=C1)                                                                 | 12      | 12      |
| 959    | (O=C(Nc1ccsc1)c2ccsc2)                                                                | 17      | 13      |
| 960    | (C1CC2c[nH]nc2CC1)                                                                   | 3       | 3       |
| 961    | (C[NCc1cc[nH]c1)cccccc2)                                                               | 30      | 30      |
| 962    | (C(CNc1cc[nH]c1)Cc2cccccc2)                                                            | 7       | 7       |
| 963    | (C(Cc1cccc1)NCc2cc[nH]c2)                                                             | 12      | 12      |
| 964    | (C[NC1CCCCC1)c2cc[nH]c2)                                                               | 10      | 10      |
| 965    | (C[NC1CCCCC1)c2cc[nH]c2)                                                               | 5       | 5       |
| 966    | (C1CC2n[nH]cc2C1)                                                                     | 12      | 12      |
| 967    | (c1cc2nc[nH]c2cn1)                                                                    | 111     | 38      |
| 968    | (C(Nc1ccns1)c2cccccc2)                                                                | 11      | 4       |
| 969    | (O=C(CNS(=O)(=O)c1c[nH]cn1)Nc2cccccc2)                                               | 6       | 6       |
| 970    | (O=C(1ccccccc1)c2cc[nH]2)                                                              | 9       | 9       |
| 971    | (C(NCc1cccs1)c2cccccc2)                                                                | 13      | 13      |
| 972    | (O=C1CSc2ncccc2N1)                                                                    | 5       | 5       |
| 973    | (O=C(CS(=O)(=O)c1cocn1)NCc2cccccc2)                                                   | 12      | 12      |
| 974    | (O=C1NCCc2cccccc12)                                                                   | 12      | 10      |
| 975    | (O=C(N1CCCCC1)c2cccs2)                                                                  | 8       | 8       |
| 976    | (c1ccn(c1)c2cccs2)                                                                    | 12      | 10      |
| Line | Chemical Structure                                                                 | Rows | Columns |
|------|-----------------------------------------------------------------------------------|------|---------|
| 977  | (O=C(NCc1cCCCCC1)c2cn[nH]c2)                                                       | 6    | 6       |
| 978  | (O=C1CCCC1NCc2ncns2)                                                              | 7    | 3       |
| 979  | (C(Cn1cccc1)c2ccccccc2)                                                           | 12   | 12      |
| 980  | (C(OC=Cc2cccccc2))                                                                | 68   | 36      |
| 981  | (O=C1NN=Cc2cccc12)                                                                | 6    | 6       |
| 982  | (C1NC2ncccc2N1)                                                                   | 6    | 6       |
| 983  | (O=C(CS1=O)(=O)Cc1ccn1)N2CCNC2)                                                    | 9    | 9       |
| 984  | (O=C(CS1=O)(=O)Cc1ccn1)NCCc2cccccc2)                                              | 12   | 12      |
| 985  | (O=C(CS1=O)(=O)Cc1ccn1)NCCc2cccccc2)                                              | 4    | 4       |
| 986  | (O=C(Nc1ccoc1)C23CC4CC(CC(C4)C2)C3)                                               | 7    | 3       |
| 987  | (C(N1CCCNCC1)c2oncn2)                                                             | 5    | 5       |
| 988  | (N(c1concn1)c2oncn2)                                                              | 4    | 1       |
| 989  | (C1SC=Cc2n[nH]cc12)                                                                | 1    | 1       |
| 990  | (O=C(CNS1=O)(=O)c1cncn[nH]c1)NCCCCc2cccccc2)                                       | 8    | 8       |
| 991  | (O=C(CNS1=O)(=O)c1cncn[nH]c1)N2CCNC2)                                             | 8    | 8       |
| 992  | (O=C1CN(CCC2=CCCCC2)(=O)N1)                                                       | 12   | 12      |
| 993  | (O=C1CN(C2CCCCC2)(=O)N1)                                                           | 12   | 12      |
| 994  | (o1cc2cccccc2n1)                                                                  | 11   | 4       |
| 995  | (O=C1CN(Cc2cccccc2)C(=O)N1)                                                       | 5    | 5       |
| 996  | (O=C1CN(Cc2cccccc2)C(=O)N1)                                                       | 12   | 12      |
| 997  | (c1cc2sccc2ncn1)                                                                  | 38   | 10      |
| 998  | (O=C(CCCc1ccon1)NCCc2cccccc2)                                                     | 5    | 2       |
| 999  | (O=C1NC(=O)N2CCSC12)                                                              | 7    | 7       |
| 1000 | (O=C(Cnc1nncn[nH]1)C23CC4CC(CC(C4)C2)C3)                                           | 8    | 8       |
| 1001 | (O=C1CCCC2c[nH]cc12)                                                              | 60   | 7       |
| 1002 | (O=C(CNS1=O)(=O)c1cncn1)cnc1cncn1cnc2cccccc2)                                     | 12   | 12      |
| 1003 | (O=C(CNS1=O)(=O)c1cncn1)cnc1cncn1cnc2cccccc2)                                     | 9    | 9       |
| 1004 | (O=C(CS1=O)(=O)Cc1ccn1)NCCCN2CCNC2)                                               | 4    | 4       |
| 1005 | (O=C(CS1=O)(=O)Cc1ccn1)Ncc2cccccc2)                                               | 12   | 12      |
| 1006 | (O=C(NCCCN1CCNCC1)C2CCNC2)                                                        | 3    | 3       |
| 1007 | (O=C(Ncn1ccn1)cnc1cnc2cccccc2)                                                    | 12   | 12      |
| 1008 | (C(c1cc2ncnc1)c2cccccc2)                                                           | 7    | 2       |
| 1009 | (O=C(CSc1nnncn[nH]1)NCCc2cccccc2)                                                  | 6    | 6       |
| 1010 | (O=C(OCC1cccccc1)c2cn[nH]n2)                                                       | 7    | 7       |
| 1011 | (O=C1NC(C=C1)c2cccccc2)                                                            | 9    | 3       |
| 1012 | (O=C(Nc1ccccc1)c2=CC(=O)NC(=O)N2)                                                 | 1    | 1       |
| 1013 | (C1NC=Nc2ncnc12)                                                                  | 3    | 3       |
| 1014 | (O=C(Nc1ncnc1)cnc1cnc2cccccc2)                                                    | 5    | 5       |
| 1015 | (O=C(NC1NC(=O)NC1=O)c2cccccc2)                                                    | 7    | 7       |
| 1016 | (O=C(Nc1ccccc1)C=C\c1cc2ncn[nH]c2)                                                | 5    | 2       |
| 1017 | (N=C1NC(=CS1)c2cccccc2)                                                            | 3    | 3       |
| No.  | Structure                                                                 | Frequency | Weight |
|------|---------------------------------------------------------------------------|-----------|--------|
| 1018 | (O=S(=O)(Nc1cccccc1)c2cccccc2)                                             | 12        | 7      |
| 1019 | (O=C(Nc1cccccc1)(=O)c1cccccc2)                                             | 10        | 8      |
| 1020 | (O=S(=O)(NCCSc1nnc[nH]1)c2cccccc2)                                         | 5         | 5      |
| 1021 | (O=C1C-CN=C2NC=NN12)                                                       | 1         | 1      |
| 1022 | (O=C(Nc1cccccc1)(=O)c1cccccc2)                                             | 10        | 7      |
| 1023 | (c1cccc(nc1)c2ccccs2)                                                     | 13        | 0      |
| 1024 | (c1ccc(cc1)c2cccccn2)                                                     | 23        | 5      |
| 1025 | (O=C(Nc1cccccc1)\(C=c/2cccccc2)                                           | 1         | 0      |
| 1026 | (O=C(NCc1cccccc1)C(=O)Nc2cccccc2)                                          | 10        | 10     |
| 1027 | (O=C(CC1CCNC1)Nc2cccccc2)                                                 | 8         | 8      |
| 1028 | (C(=C/c1nccs1)/c2cccccc2)                                                 | 7         | 0      |
| 1029 | (o1ncn(\C=c\c2cccccc2)n1)                                                | 5         | 5      |
| 1030 | (C1CCc2ccoc2C1)                                                           | 12        | 6      |
| 1031 | (O=C(NCc1cccccc1)NCCsc2cccccc2)                                            | 8         | 8      |
| 1032 | (O=C(NCCNC1cccccc1)c2cnnon2)                                              | 6         | 6      |
| 1033 | (O=C1C=CC=C2OC=CN12)                                                      | 6         | 6      |
| 1034 | (O=C(CSc1ncncn1)NCCc2cccccc2)                                             | 5         | 0      |
| 1035 | (O=C(CSc1ncncn1)N2CCCCCC2)                                                | 8         | 4      |
| 1036 | (o1cccc1c2ccncn2)                                                         | 22        | 17     |
| 1037 | (O=C1CN=C2C=CC=C2N1)                                                      | 4         | 4      |
| 1038 | (O=C1CN=C2=CC=CCC2-CN1)                                                   | 2         | 2      |
| 1039 | (O=C(CSc1ncncn1)Nc2cccs2)                                                 | 5         | 0      |
| 1040 | (O=C1NC(=CC(=O)N1)Nc2ccccc2)                                              | 2         | 2      |
| 1041 | (C1Cc2ccncoc2CO1)                                                         | 5         | 5      |
| 1042 | (C(Nc1ncn[nH]1)c2ccccc2)                                                  | 4         | 4      |
| 1043 | (C(Nc1ncn[nH]1)c2cccccc2)                                                 | 12        | 2      |
| 1044 | (O=C(c1occc1)n2ccncn2)                                                    | 5         | 4      |
| 1045 | (O=S(=O)(Nc1ccncn1)c2cccccc2)                                             | 6         | 6      |
| 1046 | (O=C1OC=NC2cccccc12)                                                      | 6         | 5      |
| 1047 | (O=C(CSc1ncncn1)Nc2cccccc2)                                               | 12        | 0      |
| 1048 | (O=C(CSc1nc[nH]n1)Nc2cccccc2)                                             | 3         | 3      |
| 1049 | (C1Cc2ccn[nH]c2C1)                                                        | 8         | 8      |
| 1050 | (O=S(=O)(Nc1ccncn1)c2cccccc2)                                             | 15        | 15     |
| 1051 | (O=C(CCSc1ncncn1)Nc2cccccc2)                                              | 10        | 1      |
| 1052 | (O=C1CCSc2ncnn12)                                                         | 10        | 10     |
| 1053 | (C1CCc2ccncce2C1)                                                         | 8         | 0      |
| 1054 | (C1=C=OC2cccccc12)                                                        | 8         | 5      |
| 1055 | (O=C1OC=NC2cccccc12)                                                      | 6         | 5      |
| 1056 | (O=C(Nc1cccc1)c2cccccc2)                                                  | 9         | 3      |
| 1057 | (C1Cc2cccccc2CO1)                                                         | 4         | 4      |
| 1058 | (O=C1CCSC2=NC=CCN12)                                                      | 6         | 4      |
|   | Formula | 1059 | 1060 | 1061 | 1062 | 1063 | 1064 | 1065 | 1066 | 1067 | 1068 | 1069 | 1070 | 1071 | 1072 | 1073 | 1074 | 1075 | 1076 | 1077 | 1078 | 1079 | 1080 | 1081 | 1082 | 1083 | 1084 | 1085 | 1086 | 1087 | 1088 | 1089 | 1090 | 1091 | 1092 | 1093 | 1094 | 1095 | 1096 | 1097 | 1098 | 1099 |
|---|--------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| ID   | Reaction                                      | Frequency | Precision |
|------|-----------------------------------------------|-----------|-----------|
| 1100 | (O=C(COc1cccccc1)Nc2nc[nH]n2)                 | 1         | 1         |
| 1101 | (C1CN=C(O1)c2ccc[nH]2)                        | 2         | 1         |
| 1102 | (C1Cc2[nH]nc2C=N1)                            | 1         | 0         |
| 1103 | (c1ccc(cc1)c2nc[nH]2)                         | 22        | 16        |
| 1104 | (O=C(CSc1c[nH]cn1)NCC2CCCO2)                  | 11        | 9         |
| 1105 | (O=C(CCc1oncn1)NCC2cccccc2)                   | 5         | 5         |
| 1106 | (O=C1NC=Cc2cc[nH]c12)                         | 34        | 24        |
| 1107 | (O=C1OC=Cc2ncccc12)                           | 6         | 6         |
| 1108 | (O=C(CSc1c[nH]cn1)Nc2cccccc2)                 | 12        | 0         |
| 1109 | (O=C(CN1CCNC1=O)NCCc2cccccc2)                 | 6         | 6         |
| 1110 | (O=C1C=Cc2ncccc12)                            | 15        | 0         |
| 1111 | (C(Cc1cccccc1)Nc2ocnn2)                       | 10        | 0         |
| 1112 | (O=C1CC(CN1)c2ocnn2)                          | 10        | 10        |
| 1113 | (O=C(CSc1ocnn1)N2CCCC2)                       | 12        | 12        |
| 1114 | (O=C(C0CC1CCCC1)c2=NCN(=O)CC2)                | 9         | 9         |
| 1115 | (O=C1CC(C=CN1)c2cccccc2)                      | 7         | 7         |
| 1116 | (O=C(C0CC1CCCCC1)c2=CCN(=O)CC2)               | 6         | 6         |
| 1117 | (O=C1NC=(C(=O)N1)S(=O)(=O)N2CCCC2)            | 8         | 8         |
| 1118 | (O=C(NC1=CCNC1=O)Nc2cccccc2)                  | 12        | 12        |
| 1119 | (O=C(Nc1cccccc1)C2CC2)                        | 9         | 9         |
| 1120 | (O=C1NC(=O)C2=NCN=C2N1)                      | 6         | 6         |
| 1121 | (O=C1NC(=O)c2ncnc2N1)                         | 3         | 3         |
| 1122 | (C1Cc2cnoc2=C1)                               | 22        | 13        |
| 1123 | (O=C(Nc1cccccc1)c2con2)                       | 7         | 7         |
| 1124 | (O=C(NC1=CCNC1=O)c2con2)                      | 10        | 10        |
| 1125 | (O=C(N1CCCCC1)c2con2)                         | 8         | 8         |
| 1126 | (O=C(NCCc1cccccc1)c2con2)                     | 7         | 7         |
| 1127 | (O=C(Nc1cc[nH]n1)c2con2)                      | 6         | 1         |
| 1128 | (O=C(Nc1ccn[nH]1)c2con2)                      | 5         | 4         |
| 1129 | (O=C(Nc1cn[nH]1)c2con2)                       | 19        | 19        |
| 1130 | (O=C(CS(=O)[=O]c1cccs1)Nc2cccccc2)            | 19        | 19        |
| 1131 | (O=C(CCNS(=O)[=O]c1cccs1)Nc2cccccc2)          | 4         | 4         |
| 1132 | (C(c1ccn1)n2ccnn2)                            | 8         | 8         |
| 1133 | (c1cc2cnccn2n1)                               | 4         | 0         |
| 1134 | (c1ccs(n1)c2nccs2)                            | 7         | 0         |
| 1135 | (O=C1NC=Nc2cnnc12)                            | 5         | 5         |
| 1136 | (O=S(=O)(Nc1cccccc1)c2ccn[nH]2)               | 1         | 1         |
| 1137 | (C(c1ccccc1)c2cncc2)                          | 1         | 1         |
| 1138 | (O=C1NC(=O)c2[nH]nc2N1)                       | 15        | 15        |
| 1139 | (O=C(Cn1ccnn1)NC(=O)Ncc2cccccc2)              | 7         | 7         |
| 1140 | (O=C(CS(=O)[=O]c1ncc[nH]1)Nc2cccccc2)         | 10        | 3         |
|   | Molecular Structure |   |   |
|---|-------------------|---|---|
| 1141 | (O=C(CN(=O)C1CCCCC1)Nc2cccccc2) | 12 | 12 |
| 1142 | (c1cn2ccnc2cn1) | 10 | 8 |
| 1143 | (O=C(CSc1ocnc1)Nc2cccccc2) | 9 | 1 |
| 1144 | (O=C(CSc1ocnc1)NC2CCCCC2) | 7 | 0 |
| 1145 | (O=C(CSc1ocnc1)c2cccccc2) | 7 | 0 |
| 1146 | (C(Cc1cccccc1)Nc2ncccn2) | 8 | 0 |
| 1147 | (C(Nc1ncccn1)c2cccccc2) | 11 | 0 |
| 1148 | (O=C(Cc1cccs1)NCC(=O)Nc2cccccc2) | 4 | 3 |
| 1149 | (O=C(CCCS(=O)(=O)c1ncccn1)Nc2cccccc2) | 4 | 2 |
| 1150 | (O=C(CNCc1ccccc1)NC2CCCCC2) | 4 | 1 |
| 1151 | (O=C(NC1N=CNC1=O)c2cccccc2) | 8 | 1 |
| **All** | **41294** | **32972** |