**Modelling of ready biodegradability based on combined public and industrial data sources**

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# Supplementary Material

**Section 1. Data curation**

At the end of the data curation process, the ECHA set consisted of 1671 compounds. With the merging of the remaining datasets (NITE and VEGA, EPI Suite and OPERA training sets), there were roughly 1200 compounds new to the ECHA data (Table 2). Their absence can be explained by the following reasons: (i) exemption from REACH registration (e.g. used in food or feeding stuffs) [5]; (ii) absence of a registration dossier at the time of data collection (e.g. CAS 137-90-2 and 21564-17-0); (iii) exclusion during the data curation process, due to divergence of RB experimental values or chemical structure (e.g. CAS 7173-62-8 and 3886-69-9).

For several chemicals, despite several tens of RB studies were available the concordance between them was rather low. For example, for *tetradec-1-ene* (CAS 1120-36-1) and *octene* (CAS 25377-83-7) more than 50 and 20 independent assays were respectively available, but the classification between B and nB was close to random. Some examples of molecules with highly discordant RB outcomes are reported in Table S1.

*Table* *S1. Compounds with multiple non-concordant RB results.*

|  |  |  |  |
| --- | --- | --- | --- |
| **Name** | **CAS** | **Available study resultsa** | **B / nB** **study results** |
| dodec-1-ene | 112-41-4 | 22 | 13 / 9 |
| 1-decene | 872-05-9 | 21 | 12 / 9 |
| Hexadecene | 26952-14-7 | 63 | 25 / 38 |
| 1-phenylethanamine | 3886-69-9 | 7 | 4 / 3 |
| N-[(9E)-octadec-9-en-1-yl]propane-1,3-diamine | 7173-62-8 | 5 | 3 / 2 |

aNumber of available experimental studies in the substance’s REACH dossier.

As we collected data from multiple sources, there was a significant degree of overlap, and experimentally reported B/nB labels could be in disagreement. In such cases, the most frequent experimental label was assigned to the given compound but, when the repartition of B/nB labels was between 40 and 60 %, the compound was excluded. Table S2 lists all the 125 “close-to-threshold” compounds that were excluded with this filter. The Global model prediction is reported as well.

*Table S2. Excluded compounds with discordant RB labels.*

|  |  |  |  |
| --- | --- | --- | --- |
| **ID** | **Molecule** | **Global model pred.** | **AD** |
| 1 | OCC(Br)(CO)[N+]([O-])=O | 0 | IN |
| 2 | Oc1ccc(cc1)[N+]([O-])=O | 0 | IN |
| 3 | [O-][N+](=O)c1ccccc1 | 0 | IN |
| 4 | BrCCBr | 0 | IN |
| 5 | C[N+]([O-])=O | 1 | OUT |
| 6 | C=CC#N | 1 | IN |
| 7 | C=Cc1ccccc1 | 1 | IN |
| 8 | NCC=C | 1 | OUT |
| 9 | c1nc2ccccc2s1 | 0 | IN |
| 10 | C1CCCCC1 | 1 | IN |
| 11 | C1CCC(CC1)N(Sc1nc2ccccc2s1)C1CCCCC1 | 0 | IN |
| 12 | N(c1ccccc1)c1ccccc1 | 0 | IN |
| 13 | C1CCOC1 | 1 | IN |
| 14 | C1CNCCN1 | 0 | IN |
| 15 | C1CO1 | 1 | IN |
| 16 | C1COCCN1 | 0 | IN |
| 17 | C1CN(CCO1)SSN1CCOCC1 | 0 | IN |
| 18 | C1N2CN3CN1CN(C2)C3 | 1 | IN |
| 19 | CC(=C)C(=O)OC(C)(C)C | 0 | IN |
| 20 | CC(=C)C=C | 1 | OUT |
| 21 | COc1cc(NC(=O)CC(C)=O)c(OC)cc1Cl | 0 | IN |
| 22 | CC(=O)CC(=O)Nc1ccc(C)cc1C | 0 | IN |
| 23 | CC(=O)CC(=O)Nc1ccccc1C | 1 | OUT |
| 24 | COc1ccccc1NC(=O)CC(C)=O | 0 | IN |
| 25 | CCCCOC(=O)CC(CC(=O)OCCCC)(OC(C)=O)C(=O)OCCCC | 0 | IN |
| 26 | CC(Cc1ccc(cc1)C(C)(C)C)C=O | 1 | IN |
| 27 | CC(C)(C)c1ccc(O)cc1 | 0 | IN |
| 28 | CC(C)(C)c1ccccc1O | 0 | IN |
| 29 | CC(C)(C)CC(C)(C)c1ccc(O)cc1 | 0 | IN |
| 30 | CC(C)(C)OOC(=O)c1ccccc1 | 0 | IN |
| 31 | CC(C)(c1ccc(O)cc1)c1ccc(O)cc1 | 0 | IN |
| 32 | CC(C)(CO)COC(=O)C(C)(C)CO | 0 | IN |
| 33 | CC(C)(CO)CO | 0 | IN |
| 34 | CC(C)(N)CO | 0 | IN |
| 35 | CC(C)(OOC(C)(C)c1ccccc1)c1ccccc1 | 0 | IN |
| 36 | CC(C)C(O)C(C)(C)CO | 0 | IN |
| 37 | CC(C)c1ccccc1 | 0 | OUT |
| 38 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | 0 | IN |
| 39 | CC(C)OC(C)C | 0 | IN |
| 40 | CC(CC(C)(C)C)CC(C)(C)CC(C)(C)C | 0 | IN |
| 41 | CC(O)CC(C)(C)O | 1 | OUT |
| 42 | CC(O)CN(CC(C)O)CC(C)O | 0 | IN |
| 43 | CCn1cc[n+](C)c1 | 0 | IN |
| 44 | CC1CC(C)(C)CC(C1)(OOC(C)(C)C)OOC(C)(C)C | 0 | IN |
| 45 | Cc1ncc[nH]1 | 0 | IN |
| 46 | Cc1cccnc1 | 0 | OUT |
| 47 | CC1=CC(=O)CC(C)(C)C1 | 0 | IN |
| 48 | Cc1ccc(N)c(C)c1 | 0 | IN |
| 49 | Cc1cccc(C)c1 | 1 | OUT |
| 50 | CC(C)c1ccc(C)cc1O | 0 | IN |
| 51 | Cc1ccc(C)c(O)c1C | 0 | IN |
| 52 | Cc1ccc(C)cc1 | 1 | IN |
| 53 | Cc1ccc(cc1)S(N)(=O)=O | 0 | IN |
| 54 | Cc1cccc(C)c1N | 0 | IN |
| 55 | Cc1ccccc1 | 1 | IN |
| 56 | CCC(C)c1ccccc1O | 0 | IN |
| 57 | CCC(COC(=O)C(C)=C)(COC(=O)C(C)=C)COC(=O)C(C)=C | 1 | IN |
| 58 | CCC(COC(=O)C=C)(COC(=O)C=C)COC(=O)C=C | 0 | IN |
| 59 | CCC(CO)(CO)COCC(CC)(CO)CO | 0 | IN |
| 60 | CCCCC(CC)COP(=O)(Oc1ccccc1)Oc1ccccc1 | 0 | IN |
| 61 | CCc1ccc2C(=O)c3ccccc3C(=O)c2c1 | 0 | IN |
| 62 | CCc1ccccc1 | 1 | IN |
| 63 | CCC1CO1 | 1 | IN |
| 64 | CCCBr | 0 | OUT |
| 65 | CCCC=O | 1 | IN |
| 66 | CCCCC(CC)C(=O)OOC(C)(C)C | 1 | OUT |
| 67 | CCCCC(CC)COP(O)(=O)OCC(CC)CCCC | 0 | IN |
| 68 | CCCCCCC | 1 | IN |
| 69 | CCCCCCCCCCC | 1 | IN |
| 70 | CCCCCCCCCCCCCCCCCC(=O)NCCNC(=O)CCCCCCCCCCCCCCCCC | 1 | IN |
| 71 | CCCCCCCCCCCCCCCCCCOC(=O)CCc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C | 0 | IN |
| 72 | CCCCCCCCCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCCCCCCCC | 1 | IN |
| 73 | CCCCN(CCCC)CCCC | 0 | IN |
| 74 | CCCCN(CCO)CCCC | 0 | IN |
| 75 | CCCCOCCOCCOC(C)=O | 1 | IN |
| 76 | CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC | 0 | IN |
| 77 | CCCCOP(=O)(OCCCC)OCCCC | 0 | OUT |
| 78 | CCN | 1 | IN |
| 79 | CCN(CC)c1ccccc1 | 0 | IN |
| 80 | CCN(CC)CC | 1 | IN |
| 81 | CCN(CC)CCO | 0 | OUT |
| 82 | CCO[Si](CCCN)(OCC)OCC | 0 | IN |
| 83 | CCOC(=O)C=C | 1 | IN |
| 84 | CCOCCOCCOCCO | 1 | IN |
| 85 | ClC(Cl)(Cl)Cl | 0 | IN |
| 86 | Clc1ccc(Cl)cc1 | 0 | IN |
| 87 | ClCC1CO1 | 0 | IN |
| 88 | ClCCl | 0 | IN |
| 89 | CN(C)C=O | 0 | IN |
| 90 | CN(C)c1ccccc1 | 0 | IN |
| 91 | CN(C)CCCCCCN(C)C | 1 | IN |
| 92 | CN(C)CCOCCN(C)C | 0 | IN |
| 93 | CN(CCO)CCO | 1 | OUT |
| 94 | CNC(=O)NC | 0 | IN |
| 95 | CNc1ccccc1 | 0 | IN |
| 96 | COC(=O)C=C | 1 | IN |
| 97 | COC(=O)CCl | 1 | IN |
| 98 | COC(C)(C)CCO | 0 | IN |
| 99 | COc1ccc(C(=O)c2ccccc2)c(O)c1 | 0 | IN |
| 100 | COc1ccccc1 | 1 | IN |
| 101 | COc1ccccc1N | 0 | IN |
| 102 | CSSC | 0 | IN |
| 103 | N#Cc1ccccc1C#N | 0 | IN |
| 104 | N#CCCCCC#N | 1 | IN |
| 105 | SC#N | 0 | OUT |
| 106 | NC(=O)\N=N\C(N)=O | 0 | IN |
| 107 | NC#N | 0 | IN |
| 108 | Nc1cccc(O)c1 | 1 | IN |
| 109 | Nc1ccc(Nc2ccccc2)cc1 | 0 | IN |
| 110 | NCCCCCCN | 1 | IN |
| 111 | NCCNCCN | 0 | IN |
| 112 | NCCNCCO | 0 | IN |
| 113 | NNC(=O)CCCCC(=O)NN | 0 | IN |
| 114 | O=C(c1ccccc1)c1ccccc1 | 0 | IN |
| 115 | O=C1OC(=O)C=C1 | 1 | IN |
| 116 | O=C1CC(=O)NC(=O)N1 | 1 | IN |
| 117 | O=C1NCCN1 | 0 | IN |
| 118 | Clc1ccccc1C=O | 0 | IN |
| 119 | O=CCCCC=O | 1 | IN |
| 120 | Oc1cc(Cl)ccc1Oc1ccc(Cl)cc1Cl | 0 | IN |
| 121 | Oc1ccc(cc1)-c1ccc(O)cc1 | 0 | IN |
| 122 | Oc1ccc(Cl)cc1 | 0 | IN |
| 123 | OCC(CO)(CO)CO | 0 | IN |
| 124 | OCCNCCO | 1 | IN |
| 125 | OCCSCCO | 0 | IN |

Where 1 = B and 0 = nB; athe prediction is provided by the Global model.

Table S3. Literature set excluded and corrected entries

|  |  |  |  |
| --- | --- | --- | --- |
| **Molecule** | **CAS** | **Correct Exp** | **Reason** |
| OCc1ccc(Cl)cc1Cl | 1777-82-8 | nB | REACH dossier |
| Oc1ccc(Cl)cc1Cc1ccccc1 | 120-32-1 | nB | REACH dossier |
| Brc1ccc(cc1)-c1ccccc1 | 92-66-0 | Excluded | Inher. biodeg. study |
| CNC(=O)Oc1cccc2ccccc21 | 63-25-2 | Excluded | Inher. biodeg. study |
| [O-][N+](=O)c1cccc(O)c1 | 554-84-7 | Excluded | Inher. biodeg. study |
| Cc1ccc(cc1)OP(=O)(Oc1ccc(C)cc1)Oc1ccc(C)cc1 | 78-32-0 | Excluded | Inher. biodeg. study |

**Section 2. Model generation**

*Employed descriptor spaces*

Table S3 lists all the employed descriptor spaces. The nomenclature of ISIDA descriptors is here briefly described.

T = type of fragmentation. Where 1 = sequences of atom, 3 = sequences of atoms and bonds, 4 = atom centred fragments based on sequences of atoms, 6 = atom centred fragments based on sequences of atoms and bonds, 7 = atom centred fragments based on sequences of atoms (fixed length), 9 = atom centred fragments based on sequences of atoms and bonds (fixed length), 10 = triplets.

L and U = minimum and maximum length

FF = Force Field coloration

AP = Atom pairs (all constitutional details of a sequence are removed and only the number of constitutive atoms is given).

*Table S4. listing all the employed descriptor spaces with the respective number of fragments (Global model).*

|  |  |  |
| --- | --- | --- |
| ISIDA nomenclature | Descriptor space name | No. of fragments |
| IA(1-6)\_AP | t1l2u6\_AP | 295 |
| IA(4-6) | t1l4u6 | 1193 |
| IAB(2-7) | t3l2u7 | 6677 |
| IAB(4-4) | t3l4u4 | 594 |
| IIA(2-3) | t4l2u3 | 2304 |
| IIA(2-3)\_ap | t4l2u3\_ AP | 2055 |
| IIA(2-4) | t4l2u4 | 8258 |
| IIA(2-4)\_ap | t4l2u4\_ AP | 7358 |
| IIA(2-5) | t4l2u5 | 15872 |
| IIA(2-5)\_ap | t4l2u5\_ AP | 14909 |
| IIA(4-4)\_ap | t4l4u4\_ AP | 1120 |
| IIA(4-5)\_ap | t4l4u5\_ AP | 5469 |
| IIAb(2-3) | t6l2u3 | 3694 |
| IIAb(2-3)\_ap | t6l2u3\_ AP | 3561 |
| IIAb(2-4)\_ap | t6l2u4\_ AP | 10837 |
| IIAB(4-4) | t6l4u4 | 5834 |
| IIAB(4-5) | t6l4u5 | 13142 |
| IIAB(4-5)\_AP | t6l4u5\_AP | 9802 |
| Triplets(2-6) | t10l2u6 | 3224 |
|  | AVERAGE | **6115** |

*Figure S1. Modelling workflow.*

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*Evaluation metrics*

*Table S5. Formulas used to assess model performances.*

|  |
| --- |
| Equation |
| Sensitivity | $$Sn=\frac{TP}{TP+FN}$$ |
| Specificity | $$Sp=\frac{TN}{TN+FP}$$ |
| Balanced accuracy | $$BA=\frac{Sn+Sp}{2}$$ |

*TP = True positive; TN = True negative; FN = False negative; FP = False positive*

**Section 3. Datasets comparison**

Figure S2 depicts the Tanimoto pairwise comparison of the datasets: Industrial set/Industrial set; All-Public/All-Public; All-Public/Industrial set. The comparison has been made using the DS IIAB(2-3). The average similarity value between public and industrial data resulted to be 0.405, with the majority of compounds (70 %) having a Tc < 0.6, indicating that the two datasets contain quite dissimilar compounds.

Average similarities:

Industrial set / Industrial set: 0.392

All-Public / All-Public: 0.43

All-Public / Industrial set: 0.405

*Figure S2. Datasets' Tanimoto similarity distributions comparison*

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**Section 4. Criteria for applicability domain definition of benchmarking tools**

1. Compounds found to be inside the training set of the models were excluded.
2. Only predictions for compounds inside AD were retained. The definition of the AD varies, depending on the tool.
* VEGA generates a summary report and assigns a 3-scale reliability score (low, moderate, good). Statistics were calculated both by considering both “moderate” plus “good” and only “good” predictions. Furthermore, for simplicity, the VEGA predictions “possibly B / nB” were considered equivalent to “B / nB”, respectively.
* EPI Suite does not provide a true AD evaluation; it is up to the user to verify if the used descriptors (in this specific case, the Molecular Weight and several functional groups) are within the minimum and maximum value of the training set one’s. The minimum and maximum values of MW for the Industrial set were 28 / 2285; while for EPI Suite 30 / 949. Functional group criteria were not considered, being practically unfeasible when dealing with hundreds of compounds. With these filters, 10 chemicals were out of AD.
* OPERA defines the AD based on structure similarity and the leverage approach. The output is automatically given to the user.
* ToxTree does not provide an AD assessment neither it has a training set. Indeed, it is an ensemble of binary rules based on the chemical structure of the test compound (e.g. presence/absence of a functional group).
1. Performances were compared based on the balanced accuracy and the AD coverage, i.e. the percentage of compounds that felt inside the applicability domain of the model out of the total.

*Table S6. Benchmarking predictions for the 362 compounds of the Literature set.*

*When a molecule was found to be inside the training set of a given tool, its prediction is not reported, but applicability domain results as “in”.*

*aPrediction for the given tool, where 0 = nB and 1 = B*

*bApplicability domain*

*cSource, where C = Cheng et al. and M = Mansouri et al.*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **ID** | **SMILES** | **CASRN** | **EXP** | **Sourcec** | **Global modela** | **Global model ADb** | **EPI Suitea** | **VEGAa** | **VEGA ADb** | **ToxTreea** | **OPERAa** | **OPERA ADb** |
| 1 | [O-][N+](=O)c1cc(ccc1/N=N/c1c(O)c(cc2ccccc21)C(=O)Nc1ccccc1)[N+]([O-])=O | 85005-63-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 2 | [O-][N+](=O)c1cc(ccc1/N=N/c1c(O)ccc2ccccc21)[N+]([O-])=O | 3468-63-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 3 | [O-][N+](=O)c1cc(Cl)c(/N=N/c2ccc(cc2Cl)N(CCO)CCO)c(Br)c1 | 17464-91-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 4 | [O-][N+](=O)c1cc(Cl)c(/N=N/c2ccc(cc2Cl)N(CCO)CCO)c(Cl)c1 | 23355-64-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 5 | [O-][N+](=O)c1cc(Cl)c(cc1)/N=N/c1c(O)ccc2ccccc21 | 2814-77-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 6 | [O-][N+](=O)c1cc(Cl)ccc1/N=N/c1c(O)ccc2ccccc21 | 6410-13-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 7 | [O-][N+](=O)c1ccc(cc1)Nc1ccc(cc1)/N=N/c1c(Cl)cc(cc1Cl)[N+]([O-])=O | 72927-94-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 8 | [O-][N+](=O)c1ccccc1/N=N/c1c(O)ccc2ccccc21 | 6410-09-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 9 | Brc1cc(Br)c(cc1)Oc1cc(Br)c(Br)cc1Br | 32534-81-9 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 10 | Brc1cc(Br)cc(Br)c1 | 626-39-1 | 0 | M | 0 | in | 0 | 0 | in |  | 0 | in |
| 11 | Brc1cc(ccc1)Oc1ccc(Br)c(Br)c1Br | 40088-47-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 12 | Brc1ccc(-c2ccc(Br)c(Br)c2Br)c(Br)c1Br | 36355-01-8 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 13 | BrCCCCBr | 110-52-1 | 0 | C/M | 0 | in | 0 | 0 | in | 1 | 0 | in |
| 14 | C(Oc1ccc(cc1)C(C(c1ccc(cc1)OCC1CO1)c1ccc(cc1)OCC1CO1)c1ccc(cc1)OCC1CO1)C1CO1 | 7328-97-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 15 | C/C=C\C(=O)Oc1c(cc(cc1C(C)CCCCCC)[N+]([O-])=O)[N+]([O-])=O | 131-72-6 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 16 | c1c[n]ccc1C1C2C=CC(N=2)=C(C2C=CC(N=2)=C(C2C=CC(N=2)=C(C2C=CC=1N=2)c1cc[n]cc1)c1cc[n]cc1)c1cc[n]cc1 |c:32,t:13,20,27| | 16834-13-2 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 17 | c1cccc2ccccc21 | 91-20-3 | 0 | C/M | 0 | in | 0 |  | in | 0 | 0 | in |
| 18 | CC(=O)C(/N=N/c1ccc(cc1OC)-c1cc(OC)c(cc1)/N=N/C(C(=O)Nc1ccccc1C)C(C)=O)C(=O)Nc1ccccc1C | 7147-42-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 19 | CC(=O)c1cc(Nc2[n]c(NC(C)C)[n]c([n]2)-c2ccccc2)c2c(c1N)C(=O)c1ccccc1C2=O | 64086-96-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 20 | CC(=O)CCN(CC1(C)CCCC2(C)C1CCc1cc(ccc21)C(C)C)CCC(=O)c1ccccc1 | 70776-86-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 21 | CC(=O)N(CC(O)CO)c1c(I)c(c(I)c(c1I)C(=O)NCC(O)CO)C(=O)NCC(O)CO | 66108-95-0 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 22 | CC(=O)Nc1cc(c(cc1/N=N/c1c(Br)cc(cc1[N+]([O-])=O)[N+]([O-])=O)OC)N(CC=C)CCC#N | 68877-63-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 23 | CC(=O)Nc1cc(c(cc1/N=N/c1c(Br)cc(cc1[N+]([O-])=O)[N+]([O-])=O)OC)N(Cc1ccccc1)CC=C | 42852-92-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 24 | CC(=O)Nc1cc(ccc1/N=N/c1[n][n]c(SCC)[s]1)N(CCC)CCC | 63134-15-6 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 25 | CC(=O)Nc1cc(ccc1/N=N/c1c(Br)cc(cc1[N+]([O-])=O)[N+]([O-])=O)N(CC)CC | 52697-38-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 26 | CC(=O)Nc1cc(ccc1/N=N/c1c(Br)cc(cc1C#N)[N+]([O-])=O)N(CC)CC | 2537-62-4 | 0 | M | 0 | OUT | 0 | 0 | in | 0 | 0 | in |
| 27 | CC(=O)Nc1cc(ccc1/N=N/c1c(Br)cc(cc1C#N)[N+]([O-])=O)N(CCC)CCC | 83249-47-2 | 0 | M | 0 | OUT | 0 | 0 | in | 0 | 0 | in |
| 28 | CC(=O)Nc1cc(ccc1/N=N/c1c(cc(cc1C#N)[N+]([O-])=O)C#N)N(CCC)CCC | 56532-53-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 29 | CC(=O)Nc1cc(ccc1/N=N/c1c(I)cc(cc1C#N)[N+]([O-])=O)N(CC)CC | 55252-53-4 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 30 | CC(=O)Nc1cc(NCC(O)COc2ccccc2)c(Cl)cc1/N=N/c1ccc(cc1Cl)[N+]([O-])=O | 79542-46-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 31 | CC(=O)Nc1ccc(cc1)NC(=O)c1cc2ccccc2c(/N=N/c2cc(ccc2Cl)C(N)=O)c1O | 12236-64-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 32 | CC(=O)OC(C)N(C(C)OC(C)=O)c1cc(NC(=O)c2ccccc2)c(cc1)/N=N/c1ccc(cc1)[N+]([O-])=O | 29765-00-2 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 33 | CC(=O)OCCN(C)S(=O)(=O)c1cc2ccc(O)c(/N=N/c3ccc(cc3)/N=N/c3ccccc3)c2cc1 | 70210-08-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 34 | CC(=O)OCCN(CCC#N)c1cc(C)c(cc1)/N=N/c1ccc(cc1Cl)[N+]([O-])=O | 68516-64-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 35 | CC(=O)OCCN(CCC#N)c1ccc(cc1)/N=N/c1[n]c2cc(Cl)c(Cl)cc2[s]1 | 33979-43-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 36 | CC(=O)OCCN(CCC#N)c1ccc(cc1)/N=N/c1c(Cl)cc(cc1Cl)[N+]([O-])=O | 5261-31-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 37 | CC(=O)OCCN(CCOC(C)=O)c1ccc(cc1)/N=N/c1c(Br)cc(cc1Br)[N+]([O-])=O | 55619-18-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 38 | CC(C)(C)C(=O)C(Oc1ccc(cc1)C(O)=O)C(=O)Nc1ccc(Cl)cc1Cl | 58161-93-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 39 | CC(C)(C)c1cc(cc(C)c1O)Sc1cc(C)c(O)c(c1)C(C)(C)C | 96-66-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 40 | CC(C)(C)c1cc(CCC(=O)OCCNC(=O)C(=O)NCCOC(=O)CCc2cc(c(O)c(c2)C(C)(C)C)C(C)(C)C)cc(c1O)C(C)(C)C | 70331-94-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 41 | CC(C)(C)c1ccc(cc1)-c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C | 6257-39-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 42 | CC(C)(C)c1ccc(cc1)-c1cc(c(O)cc1)C(C)(C)C | 42479-88-9 | 0 | M | 0 | in | 0 |  | out | 0 | 0 | in |
| 43 | CC(C)(C)NC(=O)C1CC2CCCCC2CN1CC(O)C(Cc1ccccc1)NC(=O)C(CC(N)=O)NC(=O)c1ccc2ccccc2[n]1 | 127779-20-8 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 44 | CC(C)(C)OOC(C)(C)C#CC(C)(C)OOC(C)(C)C | 1068-27-5 | 0 | M | 0 | in | 0 |  | out | 0 | 0 | out |
| 45 | CC(C)(c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1ccccc1)c1ccccc1)C(O)=O | 83799-24-0 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 46 | CC(C)(c1ccc(cc1)Oc1ccc(N)cc1)c1ccc(cc1)Oc1ccc(N)cc1 | 13080-86-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 47 | CC(C)(c1ccc(cc1)OP(OCC1(COC1)CC)OCC1(COC1)CC)c1ccc(cc1)OP(OCC1(COC1)CC)OCC1(COC1)CC | 53184-75-1 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 48 | CC(C)C(C)C(CCCCCCCCOCC)C(C)CCN | 68443-10-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 49 | CC(C)c1c2ccccc2ccc1C(C)C | 38640-62-9 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 50 | CC(C)c1cc2ccccc2cc1 | 29253-36-9 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 51 | CC(C)c1ccc(c2cc(ccc21)C(C)C)S(O)(=O)=O | 1322-93-6 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 52 | CC(C)Cc1ccc(cc1)C(C)C(O)=O | 141505-32-0 | 0 | C/M | 0 | in | 0 | 0 | in | 1 | 0 | in |
| 53 | CC(C)Nc1[n]c([n]c(Nc2cc(Br)c(N)c3c2C(=O)c2ccccc2C3=O)[n]1)-c1ccccc1 | 64086-95-9 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 54 | CC(C)Nc1[n]c(Cl)[n]c(NC(C)C)[n]1 | 139-40-2 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 55 | CC(CC(c1cc(C)c(C)cc1)c1ccccc1)c1ccccc1 | 74921-47-4 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 56 | CC(Cl)CC(Cl)C(Cl)CCC(Cl)CCC(Cl)C(Cl)CC(Cl)CCC(Cl)CCC | 61788-76-9 | 0 | M | 0 | in | 0 | 0 | in | 1 | 0 | in |
| 57 | CC(N)C(O)c1ccccc1 | 3198-15-0 | 0 | C/M | 1 | in | 0 |  | out | 1 | 0 | in |
| 58 | CC(N)c1ccccc1 | 3886-69-9 | 0 | C/M | 0 | in | 0 |  | in |  | 0 | in |
| 59 | CC(O)COC(C)COC(C)CO | 24800-44-0 | 0 | M | 1 | in | 0 | 1 | in | 0 | 0 | in |
| 60 | CC(O)COCC(C)O | 110-98-5 | 0 | C/M | 1 | in | 1 |  | in | 0 | 0 | in |
| 61 | CC(O)COCC(C)OCC(C)O | 24800-44-0 | 0 | C | 1 | in | 0 | 1 | in | 0 | 0 | in |
| 62 | CC1(C)C2CCC3(C)C(CC=C4C5C(C)C(C)CCC5(CCC34C)C(O)=O)C2(C)CCC1O | 77-52-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 63 | CC1(C)CC2(CC(C)(C)N1)OC1(CCCCCCCCCCC1)NC2=O | 64338-16-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 64 | CC1(C)CCCC2(C)C1CCC(C)(O)C2CCC(C)(O)C=C | 515-03-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 65 | CC1(C)SC2C(NC(=O)Cc3ccccc3)C(=O)N2C1C(O)=O | 751-84-8? | 0 | C/M | 0 | OUT | 0 | 1 | out | 0 | 0 | in |
| 66 | CC1(O)C2C(C(=O)c3c1cccc3O)C(=O)C1(O)C(C(C(=O)C(C(N)=O)C1=O)N(C)C)C2O | 15251-48-6 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 67 | CC1(O)C2CC3C(C(=O)C(C(N)=O)C(=O)C3(O)C(=O)C2C(=O)c2c1cccc2O)N(C)C | 60-54-8? | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 68 | Cc1[n]cc([n]1CCO)[N+]([O-])=O | 73334-05-1 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 69 | CC1=CC(C)(C)Nc2ccccc12 | 26780-96-1 | 0 | M | 0 | in | 0 |  | out | 0 | 0 | in |
| 70 | CC1=NN(C(=O)C1/N=N/c1ccccc1Cl)c1ccccc1 | 6407-74-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 71 | CC12CCC3C(CCc4cc(O)ccc43)C1CCC2(O)C#C | 57-63-6 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 72 | Cc1c(C#N)c(NCCCOC)[n]c(NCCCOC)c1/N=N/c1ccc(cc1Cl)/N=N/c1ccccc1 | 85392-21-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 73 | Cc1c(C#N)c(NCCCOCCOc2ccccc2)[n]c(NCCCOCCOc2ccccc2)c1/N=N/c1ccc(cc1Cl)S(C)(=O)=O | 63281-10-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 74 | Cc1c(C#N)c(NCCCOCCOc2ccccc2)[n]c(NCCO)c1/N=N/c1ccc(cc1C#N)[N+]([O-])=O | 63833-78-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 75 | Cc1c(C#N)c(NCCO)[n]c(NCCCOCCOc2ccccc2)c1/N=N/c1ccc(cc1C#N)[N+]([O-])=O | 61799-13-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 76 | Cc1c(C#N)c(NCCOC)[n]c(NCCOC)c1/N=N/c1cc(OC)c(cc1OC)/N=N/c1c(Cl)cc(cc1Cl)[N+]([O-])=O | 73528-78-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 77 | Cc1c(C#N)c(NCCOC)[n]c(NCCOC)c1/N=N/c1cccc2c1C(=O)c1ccccc1C2=O | 73398-96-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 78 | Cc1c(c2ccccc2[n]1CC)C1(OC(=O)c2cc(ccc12)C(=O)OCC)c1ccc(cc1OCC)N(CC)CC | 69898-67-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 79 | Cc1c(c2ccccc2[n]1CC)C1(OC(=O)c2ccc(cc12)C(=O)OCC)c1ccc(cc1OCC)N(CC)CC | 69898-66-4 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 80 | Cc1c(cc(Br)c(O)c1Br)C1(OS(=O)(=O)c2ccccc12)c1cc(Br)c(O)c(Br)c1C | 76-60-8 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 81 | Cc1c(cc(c(OC)c1[N+]([O-])=O)C(C)(C)C)[N+]([O-])=O | 145-39-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 82 | Cc1c(cc2c(c1[N+]([O-])=O)C(C)(C)CC2(C)C)[N+]([O-])=O | 116-66-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 83 | Cc1cc(/N=N/c2ccc(O)cc2)c(cc1/N=N/c1ccccc1OC)OC | 93805-00-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 84 | Cc1cc(Br)c(/N=N/c2ccc(cc2C)N(CC)CC)c(c1)C#N | 83249-49-4 | 0 | M | 0 | OUT | 0 | 0 | in | 0 | 0 | in |
| 85 | Cc1cc(Br)c(Br)c(c1)OCC1CO1 | 30171-80-3 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 86 | Cc1cc(c(N)cc1Cl)S(O)(=O)=O | 6627-59-4 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 87 | CC1CC(C)(C)N(CCOC(=O)Nc2ccccc2)c2ccc(C=C(C#N)C#N)cc21 | 63467-19-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 88 | Cc1cc(C)c(C)cc1C | 12408-10-5 | 0 | M | 0 | in | 0 |  | out |  | 0 | in |
| 89 | Cc1cc(C)c(cc1)/N=N/C1C(=O)N(N=C1C)c1ccccc1 | 6407-78-9 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 90 | Cc1cc(C)c(cc1)/N=N/c1c(O)ccc2ccccc21 | 3118-97-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 91 | Cc1cc(C#N)c(/N=N/c2ccc(cc2NS(C)(=O)=O)N(CC)CC)c(Br)c1 | 83249-53-0 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 92 | Cc1cc(C#N)c(/N=N/c2ccc(cc2NS(C)(=O)=O)N(CCC)CCC)c(Br)c1 | 83249-54-1 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 93 | Cc1cc(C#N)c(/N=N/c2ccc(cc2NS(C)(=O)=O)N(CCC)CCC)c(c1)C#N | 72968-82-2 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 94 | Cc1cc(cc(Br)c1O)C1(OS(=O)(=O)c2ccccc12)c1cc(C)c(O)c(Br)c1 | 115-40-2 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 95 | Cc1cc(cc(c1)[N+]([O-])=O)[N+]([O-])=O | 25321-14-6 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 96 | Cc1cc(ccc1)-c1ccccc1 | 28652-72-4 | 0 | C/M | 0 | in | 0 |  | out | 0 | 0 | in |
| 97 | Cc1cc(ccc1)Nc1ccc(NC)c2c1C(=O)c1ccccc1C2=O | 6408-50-0 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 98 | Cc1cc(ccc1/N=N/c1[n]c2ccc(cc2[s]1)[N+]([O-])=O)N(CCC#N)CC | 16586-42-8 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 99 | Cc1cc(ccc1/N=N/c1c(Cl)cc(cc1Cl)[N+]([O-])=O)N(CCOC(=O)OC)CCOC(=O)OC | 73003-64-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 100 | Cc1cc(ccc1/N=N/c1ccc(cc1)NC(=O)OC)/N=N/c1ccc(O)cc1 | 6465-02-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 101 | Cc1cc(ccc1C=C(C#N)C#N)N(CCCC)CCOC(=O)Nc1cc(Cl)c(Cl)cc1 | 59583-77-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 102 | Cc1cc(ccc1C=C(C#N)C#N)N(CCOC(=O)CCCCC(=O)OCCN(CC)c1cc(C)c(C=C(C#N)C#N)cc1)CC | 25857-05-0 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 103 | Cc1cc(ccc1C=C(C#N)C#N)N(CCOc1ccc(cc1)C1CCCCC1)CC | 54079-53-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 104 | Cc1cc(ccc1C=C(C#N)C#N)N(CCOc1ccccc1C1CCCCC1)CC | 54079-60-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 105 | Cc1cc(ccc1N(C)C)OC(=O)NC | 2032-59-9 | 1 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 106 | Cc1cc(ccc1O)/N=N/c1ccc(cc1)/N=N/c1ccccc1 | 6300-37-4 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 107 | Cc1cc(Cl)c(C)c2c1S/C(=C1/Sc3c(C/1=O)c(C)c(Cl)cc3C)/C2=O | 2379-75-1 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 108 | Cc1cc(Cl)cc2S/C(=C3\Sc4c(C\3=O)c(C)c(Cl)cc4Cl)/C(=O)c12 | 6371-23-9 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 109 | Cc1cc(Cl)cc2S/C(=C3\Sc4cc(Cl)cc(C)c4C\3=O)/C(=O)c12 | 2379-74-0 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 110 | Cc1cc(Cl)ccc1NC(=O)c1cc2ccccc2cc1O | 92-76-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 111 | Cc1cc(N)ccc1C | 95-64-7 | 0 | C/M | 0 | in | 0 |  | in | 0 | 0 | in |
| 112 | Cc1cc(NS(=O)(=O)c2ccc(N)cc2)[n]o1 | 129378-89-8 | 0 | C/M | 0 | OUT | 0 | 1 | out | 0 | 0 | in |
| 113 | Cc1cc(O)c(C)cc1C1(OS(=O)(=O)c2ccccc12)c1cc(C)c(O)cc1C | 125-31-5 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 114 | Cc1cc2c(cc1/N=N/c1c(Cl)cc(cc1[N+]([O-])=O)[N+]([O-])=O)C(C)CC(C)(C)N2CCO | 63133-84-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 115 | Cc1cc2c(cc1C)N=C1C(=NC(=O)NC1=O)N2CC(O)C(O)C(O)CO | 83-88-5 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 116 | Cc1cc2c(cc1C=C(C#N)C#N)C(C)CC(C)(C)N2CCC(=O)Nc1ccccc1 | 63467-15-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 117 | Cc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC | 473-41-6? | 0 | C/M | 0 | in | 0 | 1 | in |  | 0 | in |
| 118 | Cc1ccc(cc1)S(=O)(=O)Nc1cc(OC)c(N)c2c1C(=O)c1ccccc1C2=O | 81-68-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 119 | Cc1ccc(cc1[N+]([O-])=O)[N+]([O-])=O | 25321-14-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 120 | Cc1ccc(cc1Cl)NC(=O)N(C)C | 15545-48-9 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 121 | Cc1cccc(Cc2ccccc2)c1Cc1ccccc1 | 26898-17-9 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 122 | Cc1ccccc1/N=N/c1c(O)ccc2ccccc21 | 2646-17-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 123 | CCC(=O)OC(Cc1ccccc1)(C(C)CN(C)C)c1ccccc1 | 469-62-5? | 0 | C/M | 0 | in | 0 | 1 | out | 0 | 0 | in |
| 124 | CCC(C)(C)O | 75-85-4 | 0 | C/M | 0 | OUT | 1 | 1 | in | 1 | 0 | in |
| 125 | CCC(Cl)CCC(Cl)C(Cl)CC(Cl)C(Cl)C(Cl)CCl | 63449-39-8 | 0 | M | 0 | in | 0 | 0 | in | 1 | 0 | in |
| 126 | CCc1cc(ccc1)-c1cc(CC)cc(CC)c1 | 42343-17-9 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 127 | CCc1cc(ccc1)-c1ccc(CC)cc1 | 28575-17-9 | 0 | C/M | 0 | in | 0 |  | out | 0 | 0 | in |
| 128 | CCCC(C)(COC(N)=O)COC(N)=O | 57-53-4 | 0 | C/M | 0 | in | 0 | 1 | in |  | 0 | in |
| 129 | CCCC(C)CC(C)=C | 13987-01-4 | 0 | C | 1 | in | 0 | 0 | in |  | 0 | in |
| 130 | CCCC[Sn](CCCC)(CCCC)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl | 3644-38-0 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 131 | CCCc1cc(ccc1Cl)-c1cc[n]cc1 | 73398-87-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 132 | CCCc1ccccc1 | 103-65-1 | 1 | C/M | 1 | in | 0 |  | out |  | 0 | in |
| 133 | CCCCC/C(/C=O)=C\c1ccccc1 | 122-40-7 | 1 | C | 1 | in |  |  | in | 1 | 0 | in |
| 134 | CCCCc1cc2cc(ccc2cc1)S(O)(=O)=O | 25638-17-9 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 135 | CCCCCC1OC1CC1OC1CCCCCCCC(=O)OC(COC(=O)CCCCCCCC1OC1CC1OC1CCCCC)COC(=O)CCCCCCCC1OC1CC1OC1CCCCC | 8013-07-8 | 1 | M | 1 | OUT | 0 | 1 | in | 0 | 0 | in |
| 136 | CCCCCCC(=O)OCCN1CCN(CCCN2c3cc(ccc3Sc3ccccc23)C(F)(F)F)CC1 | 2746-81-8 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 137 | CCCCCCCC=C | 124-11-8 | 0 | C/M | 1 | in | 1 |  | in |  | 0 | in |
| 138 | CCCCCCCCCc1ccc(cc1)OP(Oc1ccc(CCCCCCCCC)cc1)Oc1ccc(CCCCCCCCC)cc1 | 26523-78-4 | 0 | C/M | 0 | in | 0 | 1 | out | 0 | 0 | in |
| 139 | CCCCCCCCCc1ccc(O)cc1 | 25154-52-3 | 0 | C | 1 | in |  | 1 | out | 1 | 0 | in |
| 140 | CCCCCCCCCc1cccc(O)c1CCCCCCCCC | 1323-65-5 | 0 | C/M | 0 | OUT | 0 | 0 | in | 1 | 0 | in |
| 141 | CCCCCCCCCCCCc1cc(cc(c1)S(O)(=O)=O)Oc1ccc(cc1)S(O)(=O)=O | 28519-02-0 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 142 | CCCCCCCCCCCCCCCc1cccc(O)c1 | 501-24-6 | 1 | M | 1 | in | 0 | 1 | out | 1 | 0 | in |
| 143 | CCCCCCCCCCCCCCCCCCC1CC(=O)OC1=O | 47458-32-2 | 0 | C/M | 1 | in | 0 |  | in | 1 | 0 | in |
| 144 | CCCCN(CCOC(C)=O)c1cc(C)c(cc1)/N=N/c1c(Br)cc(cc1C#N)[N+]([O-])=O | 72828-63-8 | 0 | M | 0 | OUT | 0 | 0 | in | 0 | 0 | in |
| 145 | CCCCN(CCOC(C)=O)c1cc(C)c(cc1)/N=N/c1c(cc(cc1C#N)[N+]([O-])=O)C#N | 72828-64-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 146 | CCCN(CCC)N=O | 621-64-7 | 0 | C/M | 0 | in | 0 | 1 | out | 0 | 0 | in |
| 147 | CCN(CCC#N)c1ccc(cc1)/N=N/c1[n]c2cc(Cl)c(Cl)cc2[s]1 | 25176-89-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 148 | CCN(CCC#N)c1ccc(cc1)/N=N/c1[n]c2cc(Cl)cc(Cl)c2[s]1 | 25150-28-1 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 149 | CCN(CCC#N)c1ccc(cc1)/N=N/c1c(Br)cc(cc1Br)[N+]([O-])=O | 55281-26-0 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 150 | CCN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 1691-99-2 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 151 | CCN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68555-73-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 152 | CCN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 34455-03-3 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 153 | CCN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68555-72-6 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 154 | CCN(CCOc1ccccc1)c1ccc(cc1)/N=N/c1ccc(cc1Cl)[N+]([O-])=O | 31030-27-0 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 155 | CCNc1ccc2ccccc2c1/N=N/c1ccc(cc1)/N=N/c1ccccc1 | 6368-72-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 156 | CCNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68957-62-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 157 | CCOC(=O)c1ccccc1C(c1cc(Br)c(O)c(Br)c1)=C1C=C(Br)C(=O)C(Br)=C1 | 1176-74-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 158 | CCOC(=O)CCc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C | 36294-24-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 159 | CCOc1cc(c(NC(C)=O)c(c1)/N=N/c1c(Br)cc(cc1[N+]([O-])=O)[N+]([O-])=O)N(CCOC(C)=O)CCOC(C)=O | 12239-34-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 160 | CCOc1ccc(cc1)/N=N/c1ccc(O)c2ccccc12 | 6535-42-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 161 | CCOc1ccccc1NC(=O)c1cc2ccccc2c(/N=N/c2ccccc2[N+]([O-])=O)c1O | 94199-57-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 162 | CCOCC | 60-29-7 | 0 | C/M | 1 | in | 1 |  | in | 0 | 0 | in |
| 163 | CCOCCOC(=O)Nc1cc(ccc1/N=N/c1ccc(cc1Cl)[N+]([O-])=O)N(CC)CC | 68214-66-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 164 | ClC(Cl)C(c1ccccc1Cl)c1ccc(Cl)cc1 | 53-19-0 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 165 | Clc1c2ccccc2c(Cl)c(Cl)c1Cl | 70776-03-3 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 166 | Clc1cc(cc(Cl)c1Cl)-c1cc(Cl)c(Cl)c(Cl)c1 | 1336-36-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 167 | Clc1cc(ccc1)-c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl | 26601-64-9 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 168 | Clc1cc2Oc3cc(Cl)c(Cl)cc3Oc2cc1Cl | 1746-01-6 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 169 | Clc1ccc(cc1Cl)-c1ccccc1 | 25512-42-9 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 170 | CN(C)C(=N)NC(N)=N | 657-24-9 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 171 | CN(C)C(=O)C1CC(CN1)SC1C(C)C2C(C(C)O)C(=O)N2C=1C(O)=O | 119478-56-7 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 172 | CN(C)C(=O)Nc1ccc(cc1)Oc1ccc(Cl)cc1 | 1982-47-4 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 173 | CN(C)C(=S)S[Sn](c1ccccc1)(c1ccccc1)c1ccccc1 | 1803-12-9 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 174 | CN(C)c1ccc(cc1)C(c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C | 603-48-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 175 | CN(C)c1ccc(cc1)C(c1ccc(cc1)N(Cc1cc(ccc1)S(O)(=O)=O)CC)=C1C=CC(C=C1)=[N+](Cc1cc(ccc1)S(O)(=O)=O)CC |c:32,t:39| | 1694-09-3 | 0 | C | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 176 | CN(C)c1ccc(cc1)C(O)(c1ccc(Nc2ccccc2)c2ccccc12)c1ccc(cc1)N(C)C | 6786-83-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 177 | CN(C)CC[n]1[n][n][n]c1SCC1CSC2C(NC(=O)Cc3c[s]c(N)[n]3)C(=O)N2C=1C(O)=O | 66309-69-1? | 0 | C/M | 0 | OUT | 0 | 1 | out | 0 | 0 | out |
| 178 | CN(C)CCC=C1c2ccccc2CCc2ccccc21 | 50-48-6 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 179 | CN(c1c(I)c(c(I)c(c1I)C(=O)NC(CO)C(O)CO)C(=O)NC(CO)C(O)CO)C(=O)CC(=O)N(C)c1c(I)c(c(I)c(c1I)C(=O)NC(CO)C(O)CO)C(=O)NC(CO)C(O)CO | 79770-24-4 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 180 | CN(c1ccc(c2ccccc21)C(O)(c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C)c1ccccc1 | 1325-85-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 181 | CN(Cc1c[n]c2[n]c(N)[n]c(N)c2[n]1)c1ccc(cc1)C(=O)NC(CCC(O)=O)C(O)=O | 133073-73-1? | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 182 | CN(CCC#N)c1ccc(cc1)/N=N/c1[n]c2cc(Cl)c(Cl)cc2[s]1 | 41362-82-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 183 | CN(CCO)c1ccc(cc1)/N=N/c1c(Cl)cc(cc1Cl)[N+]([O-])=O | 6232-56-0 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 184 | CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 24448-09-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 185 | CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68555-76-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 186 | CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68555-75-9 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 187 | CN1C(=O)c2[nH]c[n]c2N(C)C1=O | 58-55-9 | 1 | C/M | 0 | in | 0 |  | out | 0 | 0 | in |
| 188 | CN1c2[n]c[n](C)c2C(=O)NC1=O | 83-67-0 | 0 | C/M | 0 | in | 0 |  | out | 0 | 0 | in |
| 189 | CN1C2C3(CCN4CC=CC(CC)(C34)C(O)C2(O)C(N)=O)c2cc(c(cc12)OC)C1(CC2CC(O)(CN(C2)CCc2c1[nH]c1ccccc21)CC)C(=O)OC | 53643-48-4 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 190 | CN1C2C3(CCN4CC=CC(CC)(C34)C(OC(C)=O)C2(O)C(=O)OC)c2cc(c(cc12)OC)C1(CC2CC(O)(CN(C2)CCc2c1[nH]c1ccccc21)CC)C(=O)OC | 865-21-4 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 191 | CN1CCN(CCCN2c3ccccc3Sc3ccc(cc23)C(F)(F)F)CC1 | 440-17-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 192 | CN1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc23)CC1 | 58-38-8 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 193 | CNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68259-14-3 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 194 | CNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68259-15-4 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 195 | CNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68298-13-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 196 | CO[Si](CCCSC(=O)NCCCCCCNC(=O)N(CCCCCCN=C=O)C(=O)NCCCCCCN=C=O)(OC)OC | 85702-90-5 | 0 | M | 1 | OUT | 0 | 0 | out | 0 | 0 | out |
| 197 | COC(=O)CCN(CCC(=O)OC)c1ccc(cc1)/N=N/c1c(Cl)cc(cc1Br)[N+]([O-])=O | 59709-38-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 198 | COC1(C)CC(OC2C(C)C(=O)OC(CC)C(C)(O)C(O)C(C)C(=O)C(C)CC(C)(O)C(OC3OC(C)CC(C3O)N(C)C)C2C)OC(C)C1O | 114-07-8 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 199 | COc1[n]c([n]c([n]1)OC)-c1ccc2ccc3cccc4ccc1c2c34 | 3271-22-5 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 200 | COc1c(OC)c(Cl)c(Cl)c(Cl)c1Cl | 944-61-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 201 | COc1c[n]c(NS(=O)(=O)c2ccc(N)cc2)[n]c1 | 127-73-1 | 0 | C/M | 0 | in | 0 | 1 | out | 0 | 0 | in |
| 202 | COc1cc(/N=N/c2c(Cl)cc(cc2[N+]([O-])=O)[N+]([O-])=O)c(cc1N(Cc1ccccc1)CCOC(C)=O)NC(C)=O | 16421-40-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 203 | COc1cc(/N=N/c2ccc(cc2[N+]([O-])=O)[N+]([O-])=O)c(cc1N(Cc1ccccc1)CCOC(C)=O)NC(C)=O | 16421-41-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 204 | COc1cc(ccc1/N=N/c1ccc(O)cc1)/N=N/c1ccc(cc1)[N+]([O-])=O | 19800-42-1 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 205 | COc1cc(ccc1Nc1ccc(cc1[N+]([O-])=O)[N+]([O-])=O)-c1cc(OC)c(cc1)Nc1ccc(cc1[N+]([O-])=O)[N+]([O-])=O | 29398-96-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 206 | COc1cc(OC)c(Cl)cc1NC(=O)c1cc2ccccc2c(/N=N/c2cc(ccc2OC)S(=O)(=O)N(CC)CC)c1O | 6410-41-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 207 | COc1cc2ccc(cc2cc1)C(C)C(O)=O | 26159-31-9 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 208 | COc1ccc(cc1)C(Cl)(c1ccccc1)c1ccc(cc1)OC | 40615-36-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 209 | COc1ccc(cc1)C(OCC1OC(CC1O)[n]1c[n]c2c1[n]c[n]c2NC(=O)c1ccccc1)(c1ccccc1)c1ccc(cc1)OC | 64325-78-6 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 210 | COc1ccc(cc1)Oc1cc(O)c2c(C(=O)c3ccccc3C2=O)c1N | 54243-60-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 211 | COc1ccc(cc1/N=N/c1c(O)c(cc2ccccc21)C(=O)Nc1cc(Cl)c(cc1OC)OC)C(=O)Nc1ccc(cc1)C(N)=O | 59487-23-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 212 | COc1ccc(N)cc1 | 104-94-9 | 1 | C/M | 0 | in |  |  | in | 0 | 0 | in |
| 213 | COc1ccc2CC3C4C=CC(O)C5Oc1c2C45CCN3C | 76-57-3 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 214 | COc1ccccc1/N=N/c1c(O)ccc2ccccc21 | 1229-55-6 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 215 | COc1ccccc1Nc1ccc(N)c2c1C(=O)c1ccccc1C2=O | 27341-33-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 216 | COCC(=O)Nc1c(I)c(c(I)c(c1I)C(=O)N(C)CC(O)CO)C(=O)NCC(O)CO | 73334-07-3 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 217 | COCCCNc1ccc(/N=N/c2c(Br)cc(cc2[N+]([O-])=O)[N+]([O-])=O)c2ccccc21 | 70660-55-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 218 | CS(=O)(=O)Oc1ccc(cc1)Nc1ccc(O)c2c1C(=O)c1ccccc1C2=O | 1594-08-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 219 | N#Cc1cc(ccc1/N=N/c1ccc(cc1)N(CCc1ccccc1)CCC#N)[N+]([O-])=O | 24610-00-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 220 | N#CC1SC2=C(SC=1C#N)C(=O)c1ccccc1C2=O | 3347-22-6 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 221 | N#CCCN(CCc1ccccc1)c1ccc(cc1)/N=N/c1[n]cc([s]1)[N+]([O-])=O | 19745-44-9 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 222 | N#CCCN(CCOC(=O)Nc1ccccc1)c1ccc(cc1)/N=N/c1ccc(cc1)[N+]([O-])=O | 15958-27-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 223 | N#CCCNCCc1ccc(cc1)/N=N/c1[n]c2c(cc(Br)cc2Br)[s]1 | 28824-41-1 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 224 | Nc1c2c(ccc1-c1[n][n]c(o1)-c1ccc(cc1)-c1[n][n]c(o1)-c1ccc3c(C(=O)c4ccccc4C3=O)c1N)C(=O)c1ccccc1C2=O | 52671-38-2 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 225 | Nc1c2c(ccc1-c1[n][n]c(o1)-c1ccc3c(C(=O)c4ccccc4C3=O)c1N)C(=O)c1ccccc1C2=O | 52591-25-0 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 226 | Nc1c2c(ccc1/C=N/N=C/c1ccc3c(C(=O)c4ccccc4C3=O)c1N)C(=O)c1ccccc1C2=O | 6409-68-3 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 227 | Nc1cc(Cl)cc(C(O)=O)c1Cl | 133-90-4 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 228 | Nc1ccc(cc1)S(=O)(=O)NC(=O)c1ccccc1 | 127-71-9 | 0 | C/M | 0 | in | 0 | 1 | out | 0 | 0 | in |
| 229 | Nc1ccc(cc1)S(=O)(=O)Nc1[n]ccc[n]1 | 116-44-9? | 0 | C/M | 0 | in | 0 | 1 | out | 0 | 0 | in |
| 230 | Nc1ccc(cc1)S(O)(=O)=O | 121-57-3 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 231 | Nc1ccc(Nc2ccccc2)c2c1C(=O)c1ccccc1C2=O | 4395-65-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 232 | Nc1ccc(Sc2[n]c3ccccc3[s]2)c2c1C(=O)c1ccccc1C2=O | 3767-68-8 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 233 | Nc1ccc[n]c1N | 452-58-4 | 0 | C/M | 0 | in | 0 |  | out | 0 | 0 | in |
| 234 | Nc1ccc2c(-c3ccc4c5c3c(ccc5c3ccc5c6c3c4ccc6-c3ccccc3C5=O)C2=O)c1N | 58019-27-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 235 | O=C1C(Nc2c1cc(Br)cc2Br)C1=Nc2c(Cl)cc(Br)cc2C1=O | 85702-64-3 | 0 | M | 0 | OUT | 0 | 0 | in | 0 | 0 | in |
| 236 | O=C1C(Sc2c3c(Cl)cccc3ccc12)C1=Nc2ccc(Br)cc2C1=O | 3687-67-0 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 237 | O=C1c2c(S/C/1=C1\Sc3c(c(Cl)ccc3Cl)C\1=O)c(Cl)ccc2Cl | 14295-43-3 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 238 | O=C1c2c3[nH]c4c(cc(Cl)cc4Cl)c(=O)c3cc(Cl)c2C(=O)c2ccccc12 | 6373-31-5 | 0 | M | 0 | in | 0 |  | out | 0 | 0 | in |
| 239 | O=C1c2ccc3c([nH]c4ccc(cc4c3=O)C(=O)Nc3cccc4c3C(=O)c3cccc(NC(=O)c5ccccc5)c3C4=O)c2C(=O)c2ccccc12 | 6417-38-5 | 0 | M | 0 | in | 0 |  | out | 0 | 0 | out |
| 240 | O=C1c2cccc(Nc3ccc(cc3)S(=O)(=O)c3ccccc3)c2C(=O)c2ccccc12 | 15958-61-9 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 241 | O=C1CN2C3CC1CC2CC(C3)OC(=O)c1c[nH]c2ccccc12 | 115956-12-2 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 242 | O=S(=O)(CCl)Nc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)ccc1 | 100468-92-6 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 243 | OC(=O)c1cc(ccc1O)/N=N/c1ccc(cc1)S(=O)(=O)Nc1cccc[n]1 | 599-79-1 | 0 | C/M | 0 | in | 0 | 0 | out | 0 | 0 | in |
| 244 | OC(=O)c1cccc(Cl)c1 | 535-80-8 | 0 | C/M | 0 | in | 0 |  | in | 0 | 0 | in |
| 245 | Oc1c(Br)c2Oc3c(cc(Br)c(O)c3Br)C3(OC(=O)c4c3c(Cl)c(Cl)c(Cl)c4Cl)c2cc1Br | 2134-15-8 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 246 | Oc1c(Br)cc(cc1Br)C1(OS(=O)(=O)c2ccccc12)c1cc(Br)c(O)c(Br)c1 | 115-39-9 | 0 | M | 0 | OUT | 0 | 0 | out | 0 | 0 | out |
| 247 | Oc1c(cc(Br)cc1Br)C(=O)Nc1ccc(Br)cc1 | 87-10-5 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 248 | Oc1c(cc(Cl)cc1Cl)C(=O)Nc1cc(Cl)c(Cl)cc1 | 1154-59-2 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 249 | Oc1c(Cl)cc(Cl)cc1Cl | 88-06-2 | 1 | C/M | 0 | in |  |  | in | 0 | 0 | in |
| 250 | Oc1cc(Cc2ccccc2O)ccc1 | 1333-16-0 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 251 | Oc1cc2[nH]c3ccccc3c2cc1C(=O)Nc1ccc(Cl)cc1 | 132-61-6 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 252 | Oc1ccc(cc1)/N=N/c1ccc(/N=N/c2ccccc2)c2ccccc12 | 6253-10-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 253 | Oc1ccc(cc1)/N=N/c1ccc(cc1)/N=N/c1ccc(O)cc1 | 21811-64-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 254 | Oc1ccc(cc1)/N=N/c1ccc(cc1)/N=N/c1ccccc1 | 6250-23-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 255 | Oc1ccc(I)cc1 | 540-38-5 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 0 | in |
| 256 | Oc1ccc(O)c2c1C(=O)c1c(c(ccc1NCCNCCO)NCCNCCO)C2=O | 65271-80-9? | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 257 | Oc1ccc2c([nH]c3ccccc23)c1C(=O)Nc1ccc(Cl)cc1 | 23077-61-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 258 | Oc1ccc2ccccc2c1/N=N/c1ccc(cc1)/N=N\c1ccccc1 | 85-86-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 259 | Oc1ccc2ccccc2c1/N=N/c1cccc2ccccc21 | 2653-64-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 260 | Oc1ccc2ccccc2c1/N=N/c1ccccc1 | 842-07-9 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 261 | Oc1ccccc1I | 533-58-4 | 0 | C/M | 1 | OUT | 0 | 0 | out | 0 | 0 | in |
| 262 | OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 68391-08-2 | 0 | M | 0 | in | 0 | 0 | out | 0 | 0 | out |
| 263 | OS(=O)(=O)c1cc2ccc(Cc3cc4ccc(cc4cc3)S(O)(=O)=O)cc2cc1 | 26545-58-4 | 0 | C | 0 | in | 0 | 0 | in | 0 | 0 | out |
| 264 | OS(=O)(=O)c1cccc2c(cccc21)S(O)(=O)=O | 81-04-9 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 265 | Sc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl | 133-49-3 | 0 | M | 0 | in | 0 | 0 | in | 0 | 0 | in |
| 266 | C[N+](C)(C)CCOP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1O)N1C=CC(N)=NC1=O | 987-78-0 | 1 | C | 1 | in | 0 | 0 | out | 0 | 1 | out |
| 267 | C[N+](C)(C)OP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1O)N1C=CC(N)=NC1=O | 987-78-0 | 1 | M | 0 | OUT | 0 | 0 | out | 0 | 1 | in |
| 268 | C[Si](C)(C)O[Si](O[Si](C)(C)C)(O[Si](C)(C)C)O[Si](C)(C)C | 3555-47-3 | 0 | M | 0 | in | 0 |  | out |  | 1 | out |
| 269 | C[Si](C)(O[Si](C)(C)O[SiH](C)C)O[SiH](C)C | 1000-05-1 | 0 | M | 0 | in | 0 |  | out |  | 1 | out |
| 270 | C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1 | 541-02-6 | 0 | M | 0 | in | 0 |  | out |  | 1 | out |
| 271 | C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1 | 556-67-2 | 0 | M | 0 | in | 0 |  | out |  | 1 | out |
| 272 | C[Si]1(O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1)c1ccccc1 | 10448-09-6 | 0 | M | 0 | OUT | 0 |  | out | 0 | 1 | out |
| 273 | C=CC(=O)NCO | 924-42-5 | 0 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 274 | CC(=O)C=C | 78-94-4 | 0 | C/M | 1 | in | 1 | 1 | in | 0 | 1 | in |
| 275 | CC(=O)O[Sn](CCCC)(CCCC)CCCC | 56-36-0 | 0 | M | 0 | in | 0 | 0 | in |  | 1 | in |
| 276 | CC(C)(C)CCCCCC(=O)OCC1CO1 | 26761-45-5 | 0 | C | 1 | OUT | 0 | 1 | in | 0 | 1 | in |
| 277 | CC(C)(Oc1ccc(Cl)cc1)C(=O)OCC | 637-07-0 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 1 | in |
| 278 | CC(C)(Oc1ccc(Cl)cc1)C(O)=O | 882-09-7 | 0 | C/M | 0 | in | 0 | 0 | in | 0 | 1 | in |
| 279 | CC(C)CC(NC=O)C(=O)OC(CC1OC(=O)C1CCCCCC)CCCCCCCCCCC | 96829-58-2 | 0 | C/M | 1 | in | 1 | 0 | out | 1 | 1 | in |
| 280 | CC(N)(Cc1cc(O)c(O)cc1)C(O)=O | 133161-54-3 | 0 | C/M | 1 | OUT | 0 | 1 | out | 1 | 1 | in |
| 281 | CC(O)COC(=O)C=C | 25584-83-2 | 1 | C | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 282 | CC/C=C\CCO | 928-96-1 | 1 | C/M | 1 | in | 1 |  | out | 1 | 1 | in |
| 283 | CC1(C)CC(CC(C)(C)N1C)OC(=O)CCCCCCCCC(=O)OC1CC(C)(C)N(C)C(C)(C)C1 | 41556-26-7 | 0 | M | 0 | in | 0 | 0 | out | 0 | 1 | out |
| 284 | Cc1ccc(cc1)OP(=O)(Oc1ccccc1)Oc1ccccc1 | 26444-49-5 | 0 | C/M | 1 | OUT | 0 |  | out | 0 | 1 | in |
| 285 | CCCC[Sn](CCCC)(CCCC)OC(=O)/C=C/C(O)=O | 4027-18-3 | 0 | M | 0 | in | 0 | 0 | in | 1 | 1 | in |
| 286 | CCCC[Sn](CCCC)(CCCC)OC(=O)c1ccccc1O | 4342-30-7 | 0 | M | 0 | in | 0 | 0 | out | 1 | 1 | in |
| 287 | CCCC[Sn](CCCC)(CCCC)OC(=O)CC(CCCCCCCC)C(=O)O[Sn](CCCC)(CCCC)CCCC | 67701-37-5 | 0 | M | 0 | in | 0 | 0 | in |  | 1 | out |
| 288 | CCCC[Sn](CCCC)CCCC | 688-73-3 | 0 | M | 0 | in | 0 | 0 | out |  | 1 | in |
| 289 | CCCC[Sn](Cl)(CCCC)CCCC | 1461-22-9 | 0 | M | 0 | OUT | 0 | 0 | out |  | 1 | in |
| 290 | CCCc1cc(Cl)cc(c1)-c1cc[n]cc1 | 73398-86-4 | 0 | M | 0 | in | 0 | 0 | in | 0 | 1 | in |
| 291 | CCCCCC/C=C/CCCCCCCc1cccc(O)c1 | 50985-45-0 | 1 | C | 1 | in | 0 | 1 | out | 1 | 1 | in |
| 292 | CCCCCCC(C)=O | 111-13-7 | 1 | C/M | 1 | in | 1 | 1 | in | 0 | 1 | in |
| 293 | CCCCCCCC/C=C/CCCCCCCC(=O)N(C)CCS(O)(=O)=O | 137-20-2 | 1 | C | 1 | in | 0 | 1 | in | 0 | 1 | in |
| 294 | CCCCCCCC/C=C\CCCCCCCC(O)=O | 112-80-1 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 295 | CCCCCCCC/C=C\CCCCCCCCN | 112-90-3 | 0 | C/M | 1 | in | 1 | 1 | in |  | 1 | in |
| 296 | CCCCCCCCCCCCc1ccc(O)cc1 | 27193-86-8 | 0 | C | 1 | in | 0 | 1 | out | 1 | 1 | in |
| 297 | CCCCCCCCCCCCc1ccccc1O | 27193-86-8 | 0 | M | 1 | in | 0 | 1 | out | 1 | 1 | in |
| 298 | CCCCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCCCCCCC | 504-53-0 | 0 | C | 1 | in | 0 | 1 | in | 0 | 1 | in |
| 299 | CCCCCCCCCCCCCCCCCCCCCC(O)=O | 112-85-6 | 0 | C | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 300 | CCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCO | 26787-65-5 | 0 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 301 | CCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 630-03-5 | 0 | C | 1 | in |  | 1 | in |  | 1 | in |
| 302 | CCCCCCCCCCCCCCCCCCN(C)C | 124-28-7 | 0 | C/M | 1 | in | 0 |  | in | 0 | 1 | in |
| 303 | CCCCCCCCCCCCCCCCCCN=C=O | 112-96-9 | 0 | C/M | 1 | in |  |  | in |  | 1 | in |
| 304 | CCCCCCCCCCCCS(O)(=O)=O | 1510-16-3 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 305 | CCCCCCCCOC1OC(CO)C(O)C(O)C1O | 29836-26-8 | 1 | C | 1 | in | 1 | 1 | in | 0 | 1 | in |
| 306 | CCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCC | 3648-21-3 | 0 | C | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 307 | CCOC(=O)/C(/Cl)=C/C(=O)OCC | 10302-94-0 | 0 | C | 1 | in | 1 | 0 | out | 1 | 1 | in |
| 308 | CCOc1cc(O)c(cc1)C(O)=O | 10435-55-9 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 309 | Clc1cc(CCCc2cccc[n]2)ccc1 | 101200-53-7 | 0 | M | 0 | in | 0 | 0 | in | 0 | 1 | in |
| 310 | Clc1ccc(cc1)-c1ccccc1 | 2051-62-9 | 1 | C/M | 0 | in | 0 | 0 | in | 0 | 1 | in |
| 311 | COc1cc(/C=C/C(O)=O)ccc1O | 1135-24-6 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 312 | CS(=O)(=O)OCC(O)C(O)COS(C)(=O)=O | 299-75-2 | 0 | C/M | 1 | in | 0 | 1 | out | 1 | 1 | in |
| 313 | FC(F)C(F)F | 1652-63-7 | 0 | M | 0 | in | 0 | 0 | out | 1 | 1 | out |
| 314 | O=P(Oc1ccccc1-c1ccccc1)(Oc1ccccc1)Oc1ccccc1 | 132-29-6 | 0 | C/M | 0 | in | 0 |  | out | 0 | 1 | out |
| 315 | O=P1(NCCCl)OCCCN1CCCl | 36341-88-5 | 0 | C/M | 0 | in | 0 | 1 | out | 1 | 1 | in |
| 316 | OC(=O)/C=C\C(O)=O | 110-16-7 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 317 | OC(=O)C1CC(C(C1C(O)=O)C(O)=O)C(O)=O | 3786-91-2 | 0 | C/M | 0 | in | 1 | 1 | in | 1 | 1 | in |
| 318 | OC(=O)c1cc(cc[n]1)C(O)=O | 499-80-9 | 1 | C/M | 1 | in | 1 |  | out | 0 | 1 | in |
| 319 | OC(=O)c1ccc(c[n]1)C(O)=O | 100-26-5 | 0 | M | 1 | in | 1 |  | in | 0 | 1 | in |
| 320 | OC(=O)c1cccc[n]1 | 98-98-6 | 1 | C/M | 1 | in | 1 |  | out | 0 | 1 | in |
| 321 | OC(=O)CC(O)=O | 141-82-2 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 322 | OC/C=C/CO | 110-64-5 | 0 | C | 1 | in | 1 |  | out | 1 | 1 | in |
| 323 | Oc1cc(ccc1O)C(O)=O | 99-50-3 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 324 | Oc1ccc(/C=C/C(O)=O)cc1 | 7400-08-0 | 1 | C/M | 1 | in | 1 | 1 | in | 1 | 1 | in |
| 325 | OCCCOCCCO | 2396-61-4 | 0 | C/M | 1 | in | 1 |  | in | 0 | 1 | in |
| 326 | OP(O)(=O)C(Sc1ccc(Cl)cc1)P(O)(O)=O | 89987-06-4 | 0 | C/M | 0 | OUT | 0 | 0 | out | 0 | 1 | out |
| 327 | OS(=O)(=O)c1ccc(Cl)cc1 | 98-66-8 | 1 | C/M | 0 | in | 0 |  | in | 0 | 1 | in |
| 328 | [O-][N+](=O)c1ccc(cc1)C(O)=O | 62-23-7 | 1 | C/M | 0 | in |  |  | in | 0 |  | in |
| 329 | [O-][N+](=O)c1ccccc1C(O)=O | 552-16-9 | 1 | C/M | 0 | in |  |  | in | 0 |  | in |
| 330 | C/C=C/C/C=C/C/C=C/CC=C | 6842-15-5 | 0 | M | 1 | in | 0 |  | out |  |  | in |
| 331 | C1CC=CCCC=CCCC=C1 |c:2,6,10| | 4904-61-4 | 0 | C/M | 1 | OUT |  | 1 | in | 0 |  | in |
| 332 | c1ccc[nH]1 | 109-97-7 | 1 | C | 1 | in |  |  | in | 0 |  | in |
| 333 | c1ccccc1-c1ccccc1 | 92-52-4 | 1 | C/M | 0 | in |  |  | in | 0 |  | in |
| 334 | c1ccccc1[Bi](c1ccccc1)c1ccccc1 | 603-33-8 | 0 | M | 0 | OUT | 0 |  | out | 0 |  | in |
| 335 | C1CCCCCCCCCCC1 | 294-62-2 | 0 | C/M | 1 | in |  | 1 | in | 0 |  | in |
| 336 | CC(C)C#N | 78-82-0 | 1 | C/M | 1 | in |  | 1 | in | 1 |  | in |
| 337 | CC(C)CC(C)CC(C)/C=C/C | 6842-15-5 | 0 | C | 0 | in | 0 | 1 | in |  |  | in |
| 338 | CC(C)OC(=O)Cl | 108-23-6 | 0 | C/M | 1 | in | 0 |  | out | 1 |  | in |
| 339 | Cc1c(C#N)c(=O)[n](CCCC)c(O)c1/N=N/c1ccc(cc1[N+]([O-])=O)C(=O)c1ccc(Cl)cc1 | 90729-40-1 | 0 | M | 0 | in | 0 |  | out | 0 |  | in |
| 340 | CCC1CCCCC1 | 1678-91-7 | 0 | C/M | 1 | in | 1 | 1 | out |  |  | in |
| 341 | CCCC[Sn](=O)CCCC | 818-08-6 | 0 | M | 1 | in | 0 | 0 | out |  |  | in |
| 342 | CCCC[Sn](F)(CCCC)CCCC | 1983-10-4 | 0 | M | 0 | in | 0 | 0 | out |  |  | in |
| 343 | CCCCCC=O | 66-25-1 | 0 | C | 1 | in | 1 | 1 | in | 1 |  | in |
| 344 | CCCCCCCC(=O)OC | 544-01-4 | 0 | M | 1 | in |  | 1 | in | 1 |  | in |
| 345 | CCCCCCCC/C=C/CCCCCCCCC1CC(=O)OC1=O | 28777-98-2 | 0 | C | 1 | in | 0 | 0 | in | 1 |  | in |
| 346 | CCCCCCCCCCCCCCCC/C=C/C1CC(=O)OC1=O | 28777-98-2 | 0 | M | 1 | in | 0 | 1 | in | 1 |  | in |
| 347 | CCCCCCCCCCCCCCCCCCCCCC(N)=O | 3061-75-4 | 0 | C/M | 1 | in | 0 | 1 | in | 1 |  | in |
| 348 | CCCCCCCCCCCCCCCCCCNC(=O)C(O)C(O)C(O)C(O)CO | 18375-66-1 | 0 | C/M | 1 | in | 1 | 1 | in | 1 |  | in |
| 349 | CCCCCCCCCCCCCCCCCCS | 2885-00-9 | 0 | C/M | 1 | in |  |  | in |  |  | in |
| 350 | CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCC | 119-06-2 | 0 | C/M | 1 | in | 1 | 1 | in | 1 |  | in |
| 351 | Clc1cccc2c1c1:[n]:c3:[n]:c(:[n]:c4c5ccccc5c5:[n]:c6:[n]:c(:[n]:c2[n]1[Cu][n]54)-c1ccccc1-6)-c1ccccc1-3 | 12239-87-1 | 0 | M | 0 | OUT | 0 | 0 | out |  |  | in |
| 352 | CN1CCN(CC1)c1c(F)cc2c3c1OCC(C)[n]3cc(C(O)=O)c2=O | 82419-36-1 | 0 | C/M | 0 | OUT | 0 |  | out | 0 |  | in |
| 353 | COc1ccc(cc1)C(OCC1OC(CC1O)[n]1ccc(NC(=O)c2ccccc2)[n]c1=O)(c1ccccc1)c1ccc(cc1)OC | 67219-55-0 | 0 | M | 0 | in | 0 |  | out | 0 |  | in |
| 354 | COCCl | 107-30-2 | 1 | C | 1 | in |  |  | out | 0 |  | in |
| 355 | Nc1cc[n](C2OC(CO)C(O)C2(F)F)c(=O)[n]1 | 122111-03-9 | 0 | C/M | 0 | OUT | 0 |  | out | 0 |  | in |
| 356 | Nc1cc[n](C2OC(CO)C(O)C2O)c(=O)[n]1 | 147-94-4 | 0 | C/M | 0 | in | 1 |  | out | 0 |  | in |
| 357 | O=c1[nH]c2ccccc2[n]1C1CCN(CCCC(c2ccc(F)cc2)c2ccc(F)cc2)CC1 | 2062-78-4 | 0 | M | 0 | in | 0 |  | out | 0 |  | in |
| 358 | O=c1[nH]cc(F)c(=O)[nH]1 | 1004-03-1? | 0 | C/M | 0 | OUT | 0 |  | out |  |  | in |
| 359 | O=C1c2ccccc2C(=O)c2ccccc12 | 84-65-1 | 0 | C/M | 0 | in |  | 0 | in | 0 |  | in |
| 360 | OC(=O)c1c[n](C2CC2)c2cc(c(F)cc2c1=O)N1CCNCC1 | 85721-33-1 | 0 | C/M | 0 | in | 0 |  | out | 0 |  | in |
| 361 | Oc1cc2ccccc2cc1 | 135-19-3 | 1 | C/M | 0 | in |  |  | in | 0 |  | in |
| 362 | OS(=O)(=O)c1ccccc1 | 98-11-3 | 1 | C/M | 0 | in |  |  | in | 0 |  | in |