Table S1: List of 19 pesticides additionaly included in Split 2

|  |  |  |  |
| --- | --- | --- | --- |
| **ID** | **CAS number** | **SMILES** | **Experimental value LD50 [μg/bee]** |
| **257** | 96489-71-3 | O=C1C(=C(C=NN1C(C)(C)C)SCc2ccc(cc2)C(C)(C)C)Cl | 0.024 |
| **258** | 26002-80-2 | O=C(OCc2cccc(Oc1ccccc1)c2)C3C(C=C(C)C)C3(C)(C) | 0.067 |
| **259** | 54593-83-8 | O(CC)P(OCC)(OC(C(Cl)(Cl)Cl)Cl)=S | 0.09 |
| **260** | 41198-08-7 | O=P(Oc1ccc(cc1Cl)Br)(OCC)SCCC | 0.095 |
| **261** | 122453-73-0 | N#Cc2c(c1ccc(cc1)Cl)n(c(c2Br)C(F)(F)F)COCC | 0.12 |
| **262** | 7696-12-0 | O=C(OCN1C(=O)C2=C(C1(=O))CCCC2)C3C(C=C(C)C)C3(C)(C) | 0.155 |
| **263** | 66230-04-4 | N#CC(OC(=O)C(c1ccc(cc1)Cl)C(C)C)c3cccc(Oc2ccccc2)c3 | 0.41 |
| **264** | 1689-99-2 | N#Cc1cc(c(OC(=O)CCCCCCC)c(c1)Br)Br | 2 |
| **265** | 149877-41-8 | O=C(OC(C)C)NNc1cc(ccc1(OC))c2ccccc2 | 7.8 |
| **266** | 83055-99-6 | O=C(OC)c1ccccc1CS(=O)(=O)NC(=O)Nc2nc(OC)cc(n2)OC | 12.5 |
| **267** | 133-90-4 | O=C(O)c1cc(cc(N)c1Cl)Cl | 14.5 |
| **268** | 76578-14-8 | O=C(OCC)C(Oc3ccc(Oc1nc2ccc(cc2(nc1))Cl)cc3)C | 50 |
| **269** | 55283-68-6 | O=[N+]([O-])c1cc(cc(c1N(CC(=C)C)CC)[N+](=O)[O-])C(F)(F)F | 51 |
| **270** | 131983-72-7 | OC2(C(=Cc1ccc(cc1)Cl)CCC2(C)(C))(Cn3ncnc3) | >  100 |
| **271** | 16672-87-0 | O=P(O)(O)CCCl | >  100 |
| **272** | 150114-71-9 | O=C(O)c1nc(cc(N)c1Cl)Cl | >  100 |
| **273** | 129630-19-9 | O=C(OCC)COc1cc(c(F)cc1Cl)c2nn(c(OC(F)F)c2Cl)C | >  100 |
| **274** | 183675-82-3 | O=C(Nc1ccsc1C(C)CC(C)C)c2cn(nc2C(F)(F)F)C | >  500 |
| **275** | 121552-61-2 | n1c(nc(cc1C)C2CC2)Nc3ccccc3 | >  784 |

Table S2: List of 254 pesticides used for model development with experimental values and model predictions.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **ID** | **Cas NUMBER** | **SMILES** | **Experimental value LD 50 [μg/bee]** | **Dataset** | **C1-1** | | **C100-2** | | **Toxicity level** |
| **1** | 52918-63-5 | CC1(C)C(C=C(Br)Br)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1 | 0,0015 | tr | 1 |  | - | | **H** |
| **2** | 131929-60-7 | CCC1CCCC(OC2CCC(C(C)O2)N(C)C)C(C)C(=O)C2=CC3C4CC(CC4C=CC3C2CC(=O)O1)OC1OC(C)C(OC)C(OC)C1OC | 0,0029 | tr | 1 |  | - | | **H** |
| **3** | 80844-07-1 | CCOc1ccc(cc1)C(C)(C)COCc1cccc(Oc2ccccc2)c1 | 0,0145 | tr | 1 |  | - | | **H** |
| **4** | 66841-24-5 | CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1 | 0,023 | tr | 1 |  | - | | **H** |
| **5** | 52645-53-1 | CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc1cccc(Oc2ccccc2)c1 | 0,024 | v | 1 |  | - | | **H** |
| **6** | 23031-36-9 | CC(C)=CC1C(C(=O)OC2CC(=O)C(CC#C)=C2C)C1(C)C | 0,028 | tr | 1 |  | - | | **H** |
| **7** | 68359-37-5 | CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c1ccc(F)c(Oc2ccccc2)c1 | 0,037 | tr | 1 |  | - | | **H** |
| **8** | 91465-08-6 | CC1(C)C(C=C(Cl)C(F)(F)F)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1 | 0,038 | tr | 1 |  | - | | **H** |
| **9** | 25311-71-1 | CCOP(=S)(NC(C)C)Oc1ccccc1C(=O)OC(C)C | 0,049 | tr | 1 |  | - | | **H** |
| **10** | 10453-86-8 | CC(C)=CC1C(C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C | 0,063 | v | 1 |  | - | | **H** |
| **11** | 7786-34-7 | COC(=O)C=C(C)OP(=O)(OC)OC | 0,07 | tr | 1 |  | - | | **H** |
| **12** | 105827-78-9 | [O-][N+](=O)N=C1NCCN1Cc1ccc(Cl)nc1 | 0,078 | tr | 1 |  | - | | **H** |
| **13** | 66441-23-4 | CCOC(=O)C(C)Oc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1 | 0,1 | tr | 1 |  | - | | **H** |
| **14** | 82-68-8 | [O-][N+](=O)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl | 0,1 | tr | 1 |  | - | | **H** |
| **15** | 298-00-0 | COP(=S)(OC)Oc1ccc(cc1)[N+]([O-])=O | 0,111 | v | 1 |  | - | | **H** |
| **16** | 2921-88-2 | CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl | 0,114 | tr | 1 |  | - | | **H** |
| **17** | 120116-88-3 | CN(C)S(=O)(=O)n1c(nc(Cl)c1-c1ccc(C)cc1)C#N | 0,118 | tr | 1 |  | - | | **H** |
| **18** | 141112-29-0 | CS(=O)(=O)c1cc(ccc1C(=O)c1cnoc1C1CC1)C(F)(F)F | 0,12 | tr | 1 |  | - | | **H** |
| **19** | 66841-25-6 | CC1(C)C(C(Br)C(Br)(Br)Br)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1 | 0,129 | tr | 1 |  | - | | **H** |
| **20** | 60-57-1 | ClC1=C(Cl)C2(Cl)C3C4CC(C5OC45)C3C1(Cl)C2(Cl)Cl | 0,139 | v | 0 |  | 1 |  | **M** |
| **21** | 1563-66-2 | CNC(=O)Oc1cccc2CC(C)(C)Oc12 | 0,16 | tr | 0 |  | 1 |  | **M** |
| **22** | 60-51-5 | CNC(=O)CSP(=S)(OC)OC | 0,16 | tr | 1 |  | - | | **H** |
| **23** | 16752-77-5 | CNC(=O)ON=C(C)SC | 0,16 | tr | 1 |  | - | | **H** |
| **24** | 56-38-2 | CCOP(=S)(OCC)Oc1ccc(cc1)[N+]([O-])=O | 0,175 | tr | 1 |  | - | | **H** |
| **25** | 121-75-5 | CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC | 0,18 | tr | 1 |  | - | | **H** |
| **26** | 113136-77-9 | OC(=O)C1(CC1)C(=O)Nc1ccc(Cl)cc1Cl | 0,18 | tr | 1 |  | - | | **H** |
| **27** | 173584-44-6 | COC(=O)N(C(=O)N1COC2(Cc3cc(Cl)ccc3C2=N1)C(=O)OC)c1ccc(OC(F)(F)F)cc1 | 0,18 | v | 1 |  | - | | **H** |
| **28** | 333-41-5 | CCOP(=S)(OCC)Oc1cc(C)nc(n1)C(C)C | 0,2 | tr | 1 |  | - | | **H** |
| **29** | 950-37-8 | COC1=NN(CSP(=S)(OC)OC)C(=O)S1 | 0,236 | tr | 1 |  | - | | **H** |
| **30** | 2104-64-5 | CCOP(=S)(Oc1ccc(cc1)[N+]([O-])=O)c1ccccc1 | 0,245 | v | 1 |  | - | | **H** |
| **31** | 116-06-3 | CNC(=O)ON=CC(C)(C)SC | 0,285 | tr | 1 |  | - | | **H** |
| **32** | 2032-65-7 | CNC(=O)Oc1cc(C)c(SC)c(C)c1 | 0,3025 | tr | 1 |  | - | | **H** |
| **33** | 254642 | CCOC(=O)C(SP(=S)(OC)OC)c1ccccc1 | 0,306 | tr | 1 |  | - | | **H** |
| **34** | 55-38-9 | COP(=S)(OC)Oc1ccc(SC)c(C)c1 | 0,308 | tr | 1 |  | - | | **H** |
| **35** | 122-14-5 | COP(=S)(OC)Oc1ccc(c(C)c1)[N+]([O-])=O | 0,383 | tr | 1 |  | - | | **H** |
| **36** | 29232-93-7 | CCN(CC)c1nc(C)cc(OP(=S)(OC)OC)n1 | 0,39 | tr | 1 |  | - | | **H** |
| **37** | 86-50-0 | COP(=S)(OC)SCN1N=Nc2ccccc2C1=O | 0,42 | tr | 1 |  | - | | **H** |
| **38** | 22781-23-3 | CNC(=O)Oc1cccc2OC(C)(C)Oc12 | 0,428 | tr | 1 |  | - | | **H** |
| **39** | 300-76-5 | COP(=O)(OC)OC(Br)C(Cl)(Cl)Br | 0,48 | v | 0 |  | 1 |  | **M** |
| **40** | 62-73-7 | COP(=O)(OC)OC=C(Cl)Cl | 0,5 | tr | 0 |  | 1 |  | **M** |
| **41** | 58-89-9 | ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl | 0,56 | tr | 1 |  | - | | **H** |
| **42** | 732-11-6 | COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O | 0,64 | tr | 1 |  | - | | **H** |
| **43** | 298-04-4 | CCOP(=S)(OCC)SCCSCC | 0,96 | tr | 1 |  | - | | **H** |
| **44** | 69409-94-5 | CC(C)C(Nc1ccc(cc1Cl)C(F)(F)F)C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1 | 1,1 | tr | 0 |  | 1 |  | **M** |
| **45** | 139968-49-3 | FC(F)(F)Oc1ccc(NC(=O)NN=C(Cc2ccc(cc2)C#N)c2cccc(c2)C(F)(F)F)cc1 | 1,105 | v | 0 |  | 1 |  | **M** |
| **46** | 63-25-2 | CNC(=O)Oc1cccc2ccccc12 | 1,3 | tr | 0 |  | 1 |  | **M** |
| **47** | 114-26-1 | CNC(=O)Oc1ccccc1OC(C)C | 1,35 | tr | 0 |  | 1 |  | **M** |
| **48** | 22248-79-9 | COP(=O)(OC)OC(=CCl)c1cc(Cl)c(Cl)cc1Cl | 1,37 | tr | 0 |  | 0 |  | **L** |
| **49** | 10265-92-6 | COP(N)(=O)SC | 1,37 | tr | 0 |  | 1 |  | **M** |
| **50** | 13171-21-6 | CCN(CC)C(=O)C(Cl)=C(C)OP(=O)(OC)OC | 1,46 | v | 1 |  | - | | **H** |
| **51** | 22224-92-6 | CCOP(=O)(NC(C)C)Oc1ccc(SC)c(C)c1 | 1,87 | tr | 0 |  | 1 |  | **M** |
| **52** | 72-20-8 | ClC1=C(Cl)C2(Cl)C3C4CC(C5OC45)C3C1(Cl)C2(Cl)Cl | 2,02 | tr | 0 |  | 1 |  | **M** |
| **53** | 8065-48-3 | CCOP(=O)(OCC)SCCSCC | 2,6 | tr | 0 |  | 1 |  | **M** |
| **54** | 128639-02-1 | CCOC(=O)C(Cl)Cc1cc(N2N=C(C)N(C(F)F)C2=O)c(F)cc1Cl | 2,66 | tr | 0 |  | 1 |  | **M** |
| **55** | 301-12-2 | CCS(=O)CCSP(=O)(OC)OC | 3 | v | 0 |  | 1 |  | **M** |
| **56** | 28434-00-6 | CC(C)=CC1C(C(=O)OC2CC(=O)C(CC=C)=C2C)C1(C)C | 3,4 | tr | 1 |  | - | | **H** |
| **57** | 125401-92-5 | COc1cc(OC)nc(Oc2cccc(Oc3nc(OC)cc(OC)n3)c2C(O)=O)n1 | 3,94 | tr | 0 |  | 0 |  | **L** |
| **58** | 13194-48-4 | CCCSP(=O)(OCC)SCCC | 4,09 | tr | 0 |  | 1 |  | **M** |
| **59** | 115-29-7 | ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)C2(Cl)Cl | 4,5 | tr | 0 |  | 1 |  | **M** |
| **60** | 50-29-3 | Clc1ccc(cc1)C(c1ccc(Cl)cc1)C(Cl)(Cl)Cl | 5,15 | v | 0 |  | 1 |  | **M** |
| **61** | 134-20-3 | COC(=O)c1ccccc1N | 7,8 | tr | 0 |  | 1 |  | **M** |
| **62** | 944-22-9 | CCOP(=S)(CC)Sc1ccccc1 | 8,68 | tr | 0 |  | 1 |  | **M** |
| **63** | 74051-80-2 | CCCC(=NOCC)C1=C(O)CC(CC(C)SCC)CC1=O | 10 | tr | 0 |  | 1 |  | **M** |
| **64** | 298-02-2 | CCOP(=S)(OCC)SCSCC | 10,07 | tr | 0 |  | 1 |  | **M** |
| **65** | 23135-22-0 | CNC(=O)ON=C(SC)C(=O)N(C)C | 10,32 | v | 1 |  | - | | **H** |
| **66** | 142-59-6 | SC(=S)NCCNC(S)=S | 12,09 | tr | 0 |  | 1 |  | **M** |
| **67** | 2439-10-3 | CCCCCCCCCCCCNC(N)=N | 12,1 | tr | 0 |  | 1 |  | **M** |
| **68** | 133-07-3 | ClC(Cl)(Cl)SN1C(=O)c2ccccc2C1=O | 12,1 | tr | 0 |  | 1 |  | **M** |
| **69** | 115-32-2 | OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl | 12,2 | v | 0 |  | 1 |  | **M** |
| **70** | 90982-32-4 | CCOC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(Cl)cc(OC)n1 | 12,5 | tr | 0 |  | 0 |  | **L** |
| **71** | 79277-27-3 | COC(=O)c1sccc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1 | 12,5 | tr | 0 |  | 1 |  | **M** |
| **72** | 150114-71-9 | Nc1cc(Cl)nc(C(O)=O)c1Cl | 12,5 | tr | 0 |  | 1 |  | **M** |
| **73** | 22259-30-9 | CNC(=O)Oc1cccc(c1)N=CN(C)C | 14,27 | v | 1 |  | - | | **H** |
| **74** | 1689-84-5 | Oc1c(Br)cc(cc1Br)C#N | 14,5 | tr | 0 |  | 0 |  | **L** |
| **75** | 1861-40-1 | CCCCN(CC)c1c(cc(cc1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O | 14,5 | tr | 0 |  | 1 |  | **M** |
| **76** | 94-82-6 | OC(=O)CCCOc1ccc(Cl)cc1Cl | 14,5 | tr | 0 |  | 0 |  | **L** |
| **77** | 1918-02-1 | Nc1c(Cl)c(Cl)nc(C(O)=O)c1Cl | 14,5 | tr | 0 |  | 1 |  | **M** |
| **78** | 116714-46-6 | FC(OC(F)(F)F)C(F)(F)Oc1ccc(NC(=O)NC(=O)c2c(F)cccc2F)cc1Cl | 14,5 | v | 0 | x | 0 |  | **L** |
| **79** | 23103-98-2 | CN(C)C(=O)Oc1nc(nc(C)c1C)N(C)C | 18,72 | tr | 0 |  | 1 |  | **M** |
| **80** | 563-12-2 | CCOP(=S)(OCC)SCSP(=S)(OCC)OCC | 20,55 | tr | 0 |  | 1 |  | **M** |
| **81** | 72-43-5 | COc1ccc(cc1)C(c1ccc(OC)cc1)C(Cl)(Cl)Cl | 23,57 | tr | 0 |  | 1 |  | **M** |
| **82** | 741-58-2 | CC(C)OP(=S)(OC(C)C)SCCNS(=O)(=O)c1ccccc1 | 24 | tr | 0 |  | 1 |  | **M** |
| **83** | 1582-09-8 | CCCN(CCC)c1c(cc(cc1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O | 24,2 | tr | 0 |  | 1 |  | **M** |
| **84** | 127-20-8 | CC(Cl)(Cl)C(O)=O | 24,2 | v | 0 |  | 0 |  | **L** |
| **85** | 103361-09-7 | Fc1cc2OCC(=O)N(CC#C)c2cc1N1C(=O)C2=C(CCCC2)C1=O | 28 | tr | 0 |  | 1 |  | **M** |
| **86** | 2008-41-5 | CCSC(=O)N(CC(C)C)CC(C)C | 29 | tr | 0 |  | 1 |  | **M** |
| **87** | 2312-35-8 | CC(C)(C)c1ccc(OC2CCCCC2OS(=O)OCC#C)cc1 | 31,46 | tr | 0 |  | 1 |  | **M** |
| **88** | 88-85-7 | CCC(C)c1cc(cc(c1O)[N+]([O-])=O)[N+]([O-])=O | 32,3 | v | 0 |  | 1 |  | **M** |
| **89** | 13121-70-5 | O[Sn](C1CCCCC1)(C1CCCCC1)C1CCCCC1 | 35,9 | tr | 0 |  | 1 |  | **M** |
| **90** | 156052-68-5 | CCC(C)(NC(=O)c1cc(Cl)c(C)c(Cl)c1)C(=O)CCl | 35,9 | tr | 0 |  | 1 |  | **M** |
| **91** | 1610-18-0 | COc1nc(NC(C)C)nc(NC(C)C)n1 | 36 | tr | 0 |  | 1 |  | **M** |
| **92** | 161050-58-4 | COc1cccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)c1C | 37,8 | tr | 0 |  | 0 |  | **L** |
| **93** | 95266-40-3 | CCOC(=O)C1CC(=O)C(=C(O)C2CC2)C(=O)C1 | 47 | v | 0 |  | 0 |  | **L** |
| **94** | 40487-42-1 | CCC(CC)Nc1c(cc(C)c(C)c1[N+]([O-])=O)[N+]([O-])=O | 49,8 | tr | 0 |  | 1 |  | **M** |
| **95** | 122008-85-9 | CCCCOC(=O)C(C)Oc1ccc(Oc2ccc(cc2F)C#N)cc1 | 51 | tr | 1 |  | - | | **H** |
| **96** | 3547-33-9 | CCCCCCCCSCCO | 56,9 | tr | 0 |  | 1 |  | **M** |
| **97** | 52-68-6 | COP(=O)(OC)C(O)C(Cl)(Cl)Cl | 59,8 | tr | 0 |  | 1 |  | **M** |
| **98** | 21087-64-9 | CSC1=NN=C(C(=O)N1N)C(C)(C)C | 60,4 | tr | 0 | x | 1 |  | **M** |
| **99** | 2439-01-2 | Cc1ccc2nc3SC(=O)Sc3nc2c1 | 66,47 | tr | 0 |  | 0 |  | **L** |
| **100** | 137-42-8 | CNC(S)=S | 66,5 | tr | 0 |  | 1 |  | **M** |
| **101** | 67485-29-4 | CC1(C)CNC(NC1)=NN=C(C=Cc1ccc(cc1)C(F)(F)F)C=Cc1ccc(cc1)C(F)(F)F | 67 | tr | 0 |  | 1 |  | **M** |
| **102** | 759-94-4 | CCCN(CCC)C(=O)SCC | 72,5 | v | 0 |  | 1 |  | **M** |
| **103** | 137-26-8 | CN(C)C(=S)SSC(=S)N(C)C | 74 | tr | 0 |  | 1 |  | **M** |
| **104** | 97886-45-8 | CSC(=O)c1c(nc(c(C(=O)SC)c1CC(C)C)C(F)(F)F)C(F)F | 81 | tr | 0 |  | 1 |  | **M** |
| **105** | 87674-68-8 | COCC(C)N(C(=O)CCl)c1c(C)csc1C | 94 | tr | 0 |  | 1 |  | **M** |
| **106** | 100784-20-1 | COC(=O)c1c(Cl)nn(C)c1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1 | 94 | tr | 0 |  | 1 |  | **M** |
| **107** | 7287-19-6 | CSc1nc(NC(C)C)nc(NC(C)C)n1 | 96,69 | v | 0 |  | 1 |  | **M** |
| **108** | 834-12-8 | CCNc1nc(NC(C)C)nc(SC)n1 | 100 | tr | 0 |  | 1 |  | **M** |
| **109** | 2764-72-9 | C1C[n+]2ccccc2-c2cccc[n+]12 | 100 | tr | 0 |  | 1 |  | **M** |
| **110** | 101200-48-0 | COC(=O)c1ccccc1S(=O)(=O)NC(=O)N(C)c1nc(C)nc(OC)n1 | 100 | tr | 0 |  | 1 |  | **M** |
| **111** | 85-00-7 | C1CN2ccccc2c2ccccN12 | 100 | tr | 0 |  | 1 |  | **M** |
| **112** | 140-56-7 | CN(C)c1ccc(cc1)N=NS(O)(=O)=O | 102 | v | 0 |  | 1 |  | **M** |
| **113** | 150-68-5 | CN(C)C(=O)Nc1ccc(Cl)cc1 | 110 | tr | 1 |  | - | | **H** |
| **114** | 132-66-1 | OC(=O)c1ccccc1C(=O)Nc1cccc2ccccc12 | 113,2 | tr | 0 | x | 0 |  | **L** |
| **115** | 76-87-9 | O[Sn](c1ccccc1)(c1ccccc1)c1ccccc1 | 114,8 | tr | 0 |  | 1 |  | **M** |
| **116** | 330-54-1 | CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1 | 145,03 | tr | 1 |  | - | | **H** |
| **117** | 5234-68-4 | CC1=C(SCCO1)C(=O)Nc1ccccc1 | 181 | v | 0 |  | 1 |  | **M** |
| **118** | 1897-45-6 | Clc1c(Cl)c(C#N)c(Cl)c(C#N)c1Cl | 181,29 | tr | 0 |  | 0 |  | **L** |
| **119** | 314-40-9 | CCC(C)N1C(=O)NC(C)=C(Br)C1=O | 193,38 | tr | 1 |  | - | | **H** |
| **120** | 21725-46-2 | CCNc1nc(Cl)nc(NC(C)(C)C#N)n1 | 193,38 | tr | 0 |  | 0 |  | **L** |
| **121** | 70630-17-0 | COCC(=O)N(C(C)C(=O)OC)c1c(C)cccc1C | 198 | tr | 1 |  | - | | **H** |
| **122** | 1596-84-5 | CN(C)NC(=O)CCC(O)=O | 205,46 | v | 0 | x | 0 |  | **L** |
| **123** | 13684-63-4 | COC(=O)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1 | 241,72 | tr | 0 |  | 0 |  | **L** |
| **124** | 51276-47-2 | CP(O)(=O)CCC(N)C(O)=O | 345,5 | tr | 0 | x | 0 |  | **L** |
| **125** | 135410-20-7 | CN(Cc1ccc(Cl)nc1)C(C)=NC#N | 346 | tr | 0 |  | 0 |  | **L** |
| **126** | 34256-82-1 | CCOCN(C(=O)CCl)c1c(C)cccc1CC | 1720 | tr | 0 |  | 0 |  | **L** |
| **127** | 957-51-7 | CN(C)C(=O)C(c1ccccc1)c1ccccc1 | 2431,7 | v | 0 |  | 0 |  | **L** |
| **128** | 208465-21-8 | COC(=O)c1ccc(CNS(C)(=O)=O)cc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1 | 3980 | tr | 0 |  | 0 |  | **L** |
| **129** | 13356-08-6 | CC(C)(C[Sn](CC(C)(C)c1ccccc1)(CC(C)(C)c1ccccc1)O[Sn](CC(C)(C)c1ccccc1)(CC(C)(C)c1ccccc1)CC(C)(C)c1ccccc1)c1ccccc1 | 3980 | tr | 1 |  | - | | **H** |
| **130** | 114311-32-9 | COCc1cnc(C2=NC(C)(C(C)C)C(=O)N2)c(c1)C(O)=O | >1.83E3 | v | 0 |  | 0 |  | **L** |
| **131** | 57018-04-9 | COP(=S)(OC)Oc1c(Cl)cc(C)cc1Cl | >100 | tr | 0 | x | 0 |  | **L** |
| **132** | 120923-37-7 | COc1cc(OC)nc(NC(=O)NS(=O)(=O)N(C)S(C)(=O)=O)n1 | >100 | tr | 0 |  | 1 |  | **M** |
| **133** | 74070-46-5 | Nc1c(Cl)c(Oc2ccccc2)ccc1[N+]([O-])=O | >100 | tr | 0 |  | 0 |  | **L** |
| **134** | 64902-72-3 | COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2Cl)n1 | >100 | tr | 1 | x | 0 |  | **L** |
| **135** | 19666-30-9 | CC(C)Oc1cc(N2N=C(OC2=O)C(C)(C)C)c(Cl)cc1Cl | >100 | tr | 0 |  | 0 |  | **L** |
| **136** | 90717-03-6 | Cc1cnc2c(C(O)=O)c(Cl)ccc2c1 | >100 | tr | 0 | x | 0 |  | **L** |
| **137** | 101205-02-1 | CCCC(=NOCC)C1=C(O)CC(CC1=O)C1CCCSC1 | >100 | tr | 0 |  | 1 |  | **M** |
| **138** | 51338-27-3 | COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1 | >100 | tr | 1 |  | - | | **H** |
| **139** | 143390-89-0 | CON=C(C(=O)OC)c1ccccc1COc1ccccc1C | >100 | tr | 1 |  | - | | **H** |
| **140** | 119446-68-3 | CC1COC(Cn2cncn2)(O1)c1ccc(Oc2ccc(Cl)cc2)cc1Cl | >100 | tr | 1 |  | - | | **H** |
| **141** | 658066-35-4 | FC(F)(F)c1cnc(CCNC(=O)c2ccccc2C(F)(F)F)c(Cl)c1 | >100 | tr | 0 |  | 0 |  | **L** |
| **142** | 98243-83-5 | COC(=O)C(C)N(C(=O)Cc1ccccc1)c1c(C)cccc1C | >100 | tr | 1 |  | - | | **H** |
| **143** | 422556-08-9 | COc1cc(OC)n2nc(NS(=O)(=O)c3c(OC)nccc3C(F)(F)F)nc2n1 | >100 | tr | 0 |  | 0 |  | **L** |
| **144** | 203313-25-1 | CCOC(=O)OC1=C(C(=O)NC11CCC(CC1)OC)c1cc(C)ccc1C | >100 | tr | 0 |  | 0 |  | **L** |
| **145** | 243973-20-8 | CCc1cc(C)cc(CC)c1C1=C(OC(=O)C(C)(C)C)N2CCOCCN2C1=O | >100 | tr | 0 |  | 0 |  | **L** |
| **146** | 143807-66-3 | Cc1cc(C)cc(c1)C(=O)N(NC(=O)c1ccc2OCCCc2c1C)C(C)(C)C | >100 | tr | 0 | x | 0 |  | **L** |
| **147** | 135158-54-2 | CSC(=O)c1cccc2nnsc12 | >100 | tr | 0 |  | 0 |  | **L** |
| **148** | 94125-34-5 | COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2CCC(F)(F)F)n1 | >100 | tr | 0 |  | 0 |  | **L** |
| **149** | 53112-28-0 | Cc1cc(C)nc(Nc2ccccc2)n1 | >100 | tr | 1 |  | - | | **H** |
| **150** | 95977-29-0 | CC(Oc1ccc(Oc2ncc(cc2Cl)C(F)(F)F)cc1)C(O)=O | >100 | tr | 0 |  | 0 |  | **L** |
| **151** | 131341-86-1 | FC1(F)Oc2cccc(c2O1)-c1c[nH]cc1C#N | >100 | tr | 0 |  | 0 |  | **L** |
| **152** | 57960-19-7 | CCCCCCCCCCCCC1=C(OC(C)=O)C(=O)c2ccccc2C1=O | >100 | tr | 0 | x | 0 |  | **L** |
| **153** | 56425-91-3 | CC(C)C(O)(c1ccc(OC(F)(F)F)cc1)c1cncnc1 | >100 | tr | 0 |  | 0 |  | **L** |
| **154** | 126535-15-7 | COC(=O)c1cccc(C)c1S(=O)(=O)NC(=O)Nc1nc(OCC(F)(F)F)nc(n1)N(C)C | >100 | tr | 0 | x | 0 |  | **L** |
| **155** | 219714-96-2 | COc1cnc(OC)n2nc(NS(=O)(=O)c3c(OCC(F)F)cccc3C(F)(F)F)nc12 | >100 | tr | 1 |  | - | | **H** |
| **156** | 10004-44-1 | CC1=CC(=O)NO1 | >100 | tr | 0 | x | 0 |  | **L** |
| **157** | 87130-20-9 | CCOc1ccc(NC(=O)OC(C)C)cc1OCC | >100 | tr | 1 |  | - | | **H** |
| **158** | 94361-06-5 | CC(C1CC1)C(O)(Cn1cncn1)c1ccc(Cl)cc1 | >100 | tr | 0 |  | 0 |  | **L** |
| **159** | 42874-03-3 | CCOc1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+]([O-])=O | >100 | tr | 1 |  | - | | **H** |
| **160** | 130561-48-7 | COCCOc1cccc2N(N=C(C(O)=O)C(=O)c12)c1ccc(Cl)cc1 | >100 | tr | 0 | x | 0 |  | **L** |
| **161** | 136426-54-5 | Fc1ccc2N=C(N(C(=O)c2c1)c1ccc(Cl)cc1Cl)n1cncn1 | >100 | tr | 1 |  | - | | **H** |
| **162** | 125225-28-7 | CC(C)C1CCC(Cc2ccc(Cl)cc2)C1(O)Cn1cncn1 | >100 | tr | 0 |  | 0 |  | **L** |
| **163** | 179101-81-6 | FC(F)(F)c1cccc(OCCCOc2c(Cl)cc(OCC=C(Cl)Cl)cc2Cl)n1 | >100 | tr | 1 |  | - | | **H** |
| **164** | 348635-87-0 | CN(C)S(=O)(=O)n1cnc(n1)S(=O)(=O)n1c(C)c(Br)c2ccc(F)cc12 | >100 | tr | 0 |  | 0 |  | **L** |
| **165** | 34014-18-1 | CNC(=O)N(C)c1nnc(s1)C(C)(C)C | >100 | tr | 1 |  | - | | **H** |
| **166** | 51235-04-2 | CN(C)C1=NC(=O)N(C2CCCCC2)C(=O)N1C | >100 | tr | 0 |  | 0 |  | **L** |
| **167** | 122931-48-0 | CCS(=O)(=O)c1cccnc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1 | >100 | tr | 0 |  | 0 |  | **L** |
| **168** | 98-01-1 | O=Cc1ccco1 | >100 | tr | 1 | x | 0 |  | **L** |
| **169** | 23564-05-8 | COC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OC | >100 | tr | 1 | x | 0 |  | **L** |
| **170** | 26644-46-2 | ClC(Cl)(Cl)C(NC=O)N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl | >100 | tr | 0 |  | 0 |  | **L** |
| **171** | 33089-61-1 | CN(C=Nc1ccc(C)cc1C)C=Nc1ccc(C)cc1C | >100 | tr | 1 |  | - | | **H** |
| **172** | 51707-55-2 | O=C(Nc1cnns1)Nc1ccccc1 | >100 | tr | 0 |  | 0 |  | **L** |
| **173** | 67564-91-4 | CC(CN1CC(C)OC(C)C1)Cc1ccc(cc1)C(C)(C)C | >100 | tr | 1 |  | - | | **H** |
| **174** | 81777-89-1 | CC1(C)CON(Cc2ccccc2Cl)C1=O | >100 | tr | 1 |  | - | | **H** |
| **175** | 1928-43-4 | CCCCC(CC)Cc1c(Cl)ccc(OOC(C)=O)c1Cl | >100 | tr | 1 |  | - | | **H** |
| **176** | 624-92-0 | CSSC | >100 | tr | 0 | x | 0 |  | **L** |
| **177** | 81334-34-1 | CC(C)C1(C)N=C(NC1=O)c1ncccc1C(O)=O | >100 | tr | 0 |  | 0 |  | **L** |
| **178** | 75-60-5 | C[As](C)(O)=O | >100 | tr | 1 | x | 0 |  | **L** |
| **179** | 12771-68-5 | COc1ccc(cc1)C(O)(C1CC1)c1cncnc1 | >100 | tr | 0 |  | 0 |  | **L** |
| **180** | 112143-82-5 | CCOC(=O)CSc1nc(nn1C(=O)N(C)C)C(C)(C)C | >100 | tr | 1 |  | - | | **H** |
| **181** | 123343-16-8 | COc1cc(OC)nc(Sc2cccc(Cl)c2C(O)=O)n1 | >100 | tr | 0 | x | 0 |  | **L** |
| **182** | 131807-57-3 | CC1(OC(=O)N(Nc2ccccc2)C1=O)c1ccc(Oc2ccccc2)cc1 | >100 | tr | 1 |  | - | | **H** |
| **183** | 26952-20-5 | CCCCC(CC)COC(=O)c1nc(Cl)c(Cl)c(N)c1Cl | >100 | tr | 0 |  | 0 |  | **L** |
| **184** | 74222-97-2 | COC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(C)cc(C)n1 | >100 | tr | 0 |  | 0 |  | **L** |
| **185** | 112226-61-6 | CC(C)(C)N(NC(=O)c1ccc(Cl)cc1)C(=O)c1ccccc1 | >100 | tr | 0 |  | 0 |  | **L** |
| **186** | 123312-89-0 | CC1=NNC(=O)N(C1)N=Cc1cccnc1 | >100 | tr | 1 |  | - | | **H** |
| **187** | 81335-77-5 | CCc1cnc(C2=NC(C)(C(C)C)C(=O)N2)c(c1)C(O)=O | >100 | tr | 0 |  | 0 |  | **L** |
| **188** | 95737-68-1 | CC(COc1ccc(Oc2ccccc2)cc1)Oc1ccccn1 | >100 | tr | 1 |  | - | | **H** |
| **189** | 25954-13-6 | CCOP(O)(=O)C(N)=O | >100 | tr | 0 | x | 0 |  | **L** |
| **190** | 129909-90-6 | CC(C)C1=NN(C(=O)NC(C)(C)C)C(=O)N1N | >100 | tr | 0 |  | 0 |  | **L** |
| **191** | 178928-70-6 | OC(CN1NC=NC1=S)(Cc1ccccc1Cl)C1(Cl)CC1 | >100 | tr | 1 | x | 0 |  | **L** |
| **192** | 181274-15-7 | CCCOC1=NN(C(O)=NS(=O)(=O)c2ccccc2C(=O)OC)C(=O)N1C | >100 | tr | 0 |  | 0 |  | **L** |
| **193** | 220899-03-6 | COc1ccc(Br)c(C)c1C(=O)c1c(C)cc(OC)c(OC)c1OC | >100 | tr | 1 |  | - | | **H** |
| **194** | 239110-15-7 | FC(F)(F)c1cnc(CNC(=O)c2c(Cl)cccc2Cl)c(Cl)c1 | >100 | tr | 0 |  | 0 |  | **L** |
| **195** | 335104-84-2 | CS(=O)(=O)c1ccc(C(=O)C2C(=O)CCCC2=O)c(Cl)c1COCC(F)(F)F | >100 | tr | 1 | x | - | | **H** |
| **196** | 422556-08-9 | COc1cc(OC)[n+]2[nH]c(NS(=O)(=O)c3c(OC)nccc3C(F)(F)F)nc2n1 | >100 | tr | 0 |  | 0 |  | **L** |
| **197** | 83164-33-4 | Fc1ccc(NC(=O)c2cccnc2Oc2cccc(c2)C(F)(F)F)c(F)c1 | >100 | v | 0 |  | 0 |  | **L** |
| **198** | 139528-85-1 | COc1cc(OC)n2nc(nc2n1)S(=O)(=O)Nc1c(Cl)ccc(C)c1Cl | >100 | v | 1 | x | 0 |  | **L** |
| **199** | 101463-69-8 | Fc1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1NC(=O)NC(=O)c1c(F)cccc1F | >100 | v | 0 | x | 0 |  | **L** |
| **200** | 283159-90-0 | COC(=O)CC(NC(=O)C(NC(=O)OC(C)C)C(C)C)c1ccc(Cl)cc1 | >100 | v | 0 |  | 0 |  | **L** |
| **201** | 145701-23-1 | COc1ncc(F)c2nc(nn12)S(=O)(=O)Nc1c(F)cccc1F | >100 | v | 0 |  | 0 |  | **L** |
| **202** | 116255-48-2 | Clc1ccc(c(Cl)c1)C1(Cn2cncn2)CC(Br)CO1 | >100 | v | 0 |  | 0 |  | **L** |
| **203** | 82558-50-7 | CCC(C)(CC)c1cc(NC(=O)c2c(OC)cccc2OC)on1 | >100 | v | 1 |  | - | | **H** |
| **204** | 1918-00-9 | COc1c(Cl)ccc(Cl)c1C(O)=O | >100 | v | 0 |  | 0 |  | **L** |
| **205** | 1982-49-6 | CC1CCCCC1NC(=O)Nc1ccccc1 | >100 | v | 0 |  | 0 |  | **L** |
| **206** | 55512-33-9 | CCCCCCCCSC(=O)Oc1cc(Cl)nnc1-c1ccccc1 | >100 | v | 0 |  | 0 |  | **L** |
| **207** | 105512-06-9 | CC(Oc1ccc(Oc2ncc(Cl)cc2F)cc1)C(=O)OCC#C | >100 | v | 1 |  | - | | **H** |
| **208** | 118134-30-8 | CCCN(CC)CC1COC2(CCC(CC2)C(C)(C)C)O1 | >100 | v | 1 |  | - | | **H** |
| **209** | 51596-11-3 | CCC1OC2(CCC1C)CC1CC(CC=C(C)CC(C)C=CC=C3COC4C(O)C(C)=CC(C(=O)O1)C34O)O2 | >100 | v | 0 | x | 0 |  | **L** |
| **210** | 64700-56-7 | CCCCOCCOC(=O)COc1nc(Cl)c(Cl)cc1Cl | >100 | v | 0 |  | 0 |  | **L** |
| **211** | 213464-77-8 | COc1cc(OC)nc(NC(=O)NS(=O)(=O)Nc2ccccc2C(=O)N(C)C)n1 | >100 | v | 0 |  | 0 |  | **L** |
| **212** | 8001-35-2 | ClCC1(CCl)C(=C)C2(Cl)C(Cl)C(Cl)C1(Cl)C2(Cl)Cl | >105 | v | 0 |  | 1 |  | **M** |
| **213** | 51218-45-2 | CCc1cccc(C)c1N(C(C)COC)C(=O)CCl | >110 | tr | 1 |  | - | | **H** |
| **214** | 35367-38-5 | Fc1cccc(F)c1C(=O)NC(=O)Nc1ccc(Cl)cc1 | >115 | tr | 1 |  | - | | **H** |
| **215** | 101-05-3 | Clc1ccccc1Nc1nc(Cl)nc(Cl)n1 | >117 | tr | 1 |  | - | | **H** |
| **216** | 1194-65-6 | Clc1cccc(Cl)c1C#N | >120 | tr | 0 |  | 0 |  | **L** |
| **217** | 330-55-2 | CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1 | >121 | v | 1 |  | - | | **H** |
| **218** | 99-30-9 | Nc1c(Cl)cc(cc1Cl)[N+]([O-])=O | >181 | tr | 0 |  | 0 |  | **L** |
| **219** | 5902-51-2 | CC1=C(Cl)C(=O)N(C(=O)N1)C(C)(C)C | >193 | tr | 1 |  | - | | **H** |
| **220** | 731-27-1 | CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccc(C)cc1 | >196 | v | 1 | x | 1 |  | **M** |
| **221** | 53404-31-2 | CCCCOCCOC(=O)C(C)Oc1ccc(Cl)cc1Cl | >1E3 | tr | 1 |  | - | | **H** |
| **222** | 361377-29-9 | CON=C(C1=NOCCO1)c1ccccc1Oc1ncnc(Oc2ccccc2Cl)c1F | >200 | tr | 1 |  | - | | **H** |
| **223** | 283594-90-1 | Cc1cc(C)c(C2=C(OC(=O)CC(C)(C)C)C3(CCCC3)OC2=O)c(C)c1 | >200 | tr | 1 |  | - | | **H** |
| **224** | 42576-02-3 | COC(=O)c1cc(Oc2ccc(Cl)cc2Cl)ccc1[N+]([O-])=O | >200 | tr | 1 |  | - | | **H** |
| **225** | 66332-96-5 | CC(C)Oc1cccc(NC(=O)c2ccccc2C(F)(F)F)c1 | >200 | tr | 0 |  | 0 |  | **L** |
| **226** | 55219-65-3 | CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n1cncn1 | >200 | tr | 0 |  | 0 |  | **L** |
| **227** | 72459-58-6 | [O-][n+]1nc(nc2ccc(Cl)cc12)-n1ccnc1 | >200 | tr | 0 |  | 1 |  | **M** |
| **228** | 64628-44-0 | FC(F)(F)Oc1ccc(NC(=O)NC(=O)c2ccccc2Cl)cc1 | >200 | tr | 0 |  | 0 |  | **L** |
| **229** | 126833-17-8 | CC1(CCCCC1)C(=O)Nc1ccc(O)c(Cl)c1Cl | >200 | tr | 0 |  | 1 |  | **M** |
| **230** | 1698-60-8 | NC1=C(Cl)C(=O)N(N=C1)c1ccccc1 | >200 | tr | 0 |  | 1 |  | **M** |
| **231** | 272451-65-7 | Cc1cc(ccc1NC(=O)c1cccc(I)c1C(=O)NC(C)(C)CS(C)(=O)=O)C(F)(C(F)(F)F)C(F)(F)F | >200 | tr | 0 | x | 0 |  | **L** |
| **232** | 69327-76-0 | CC(C)N1C(SCN(C1=O)c1ccccc1)=NC(C)(C)C | >200 | tr | 1 |  | - | | **H** |
| **233** | 20354-26-1 | CN1C(=O)ON(C1=O)c1ccc(Cl)c(Cl)c1 | >200 | tr | 0 |  | 1 |  | **M** |
| **234** | 141776-32-1 | CCS(=O)(=O)c1[nH]c2cccc[n+]2c1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1 | >200 | tr | 0 |  | 0 |  | **L** |
| **235** | 104040-78-0 | COc1cc(OC)nc(NC(=O)NS(=O)(=O)c2ncccc2C(F)(F)F)n1 | >200 | tr | 0 |  | 0 |  | **L** |
| **236** | 134605-64-4 | CN1C(=O)N(C(=O)C=C1C(F)(F)F)c1ccc(Cl)c(c1)C(=O)OC(C)(C)C(=O)OCC=C | >200 | tr | 1 |  | - | | **H** |
| **237** | 144550-36-7 | COC(=O)c1ccc(I)cc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1 | >200 | tr | 0 |  | 0 |  | **L** |
| **238** | 147150-35-4 | CCOc1nc(F)cc2[nH]c(n[n+]12)S(=O)(=O)Nc1c(Cl)cccc1C(=O)OC | >200 | tr | 0 |  | 0 |  | **L** |
| **239** | 175013-18-0 | CON(C(=O)OC)c1ccccc1COc1ccn(n1)-c1ccc(Cl)cc1 | >200 | tr | 0 |  | 0 |  | **L** |
| **240** | 179101-81-6 | FC(F)(F)c1ccc(OCCCOc2c(Cl)cc(OCC=C(Cl)Cl)cc2Cl)nc1 | >200 | tr | 1 |  | - | | **H** |
| **241** | 374726-62-2 | COc1cc(CCNC(=O)C(OCC#C)c2ccc(Cl)cc2)ccc1OCC#C | >200 | tr | 1 |  | - | | **H** |
| **242** | 148477-71-8 | CCC(C)(C)C(=O)OC1=C(C(=O)OC11CCCCC1)c1cc(Cl)cc(Cl)c1 | >200 | tr | 1 |  | - | | **H** |
| **243** | 50563-36-5 | COCCN(C(=O)CCl)c1c(C)cccc1C | >200 | v | 0 |  | 0 |  | **L** |
| **244** | 15165-67-0 | CC(Oc1ccc(Cl)cc1Cl)C(O)=O | >200 | v | 0 |  | 0 |  | **L** |
| **245** | 79622-59-6 | [O-][N+](=O)c1cc(c(Cl)c(c1Nc1ncc(cc1Cl)C(F)(F)F)[N+]([O-])=O)C(F)(F)F | >200 | v | 0 |  | 0 |  | **L** |
| **246** | 141517-21-7 | CON=C(C(=O)OC)c1ccccc1CON=C(C)c1cccc(c1)C(F)(F)F | >200 | v | 0 |  | 0 |  | **L** |
| **247** | 188425-85-6 | Clc1ccc(cc1)-c1ccccc1NC(=O)c1cccnc1Cl | >200 | v | 1 |  | - | | **H** |
| **248** | 72490-01-8 | CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1 | >204 | tr | 1 |  | - | | **H** |
| **249** | 133-06-2 | ClC(Cl)(Cl)SN1C(=O)C2CC=CCC2C1=O | >215 | tr | 0 |  | 1 |  | **M** |
| **250** | 84087-01-4 | OC(=O)c1c(Cl)ccc2cc(Cl)cnc12 | >215 | tr | 0 | x | 0 |  | **L** |
| **251** | 112410-23-8 | CCc1ccc(cc1)C(=O)NN(C(=O)c1cc(C)cc(C)c1)C(C)(C)C | >234 | tr | 0 |  | 0 |  | **L** |
| **252** | 114369-43-6 | Clc1ccc(CCC(Cn2cncn2)(C#N)c2ccccc2)cc1 | >292 | v | 1 |  | - | | **H** |
| **253** | 111988-49-9 | Clc1ccc(CN2CCSC2=NC#N)cn1 | >400 | tr | 0 | x | 0 |  | **L** |
| **254** | 145701-23-1 | COc1ncc(F)c2[nH]c(n[n+]12)S(=O)(=O)Nc1c(F)cccc1F | >500 | tr | 1 |  | - | | **H** |

Table S3: Predicted classification for 395 pesticides with CPANN models, K-NN model and experimental data from EPA.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **ID** | **CAS** | **NAME** | **C1-1** | | |  | **C100-2** | | **Toxicity level** | | **out of AD** | **EPA database acute contact LD50 48h exposure [μg/bee]** | **K-NN model** | **out of AD** |
| **1** | 79622-59-6 | Fluazinam | 0 | | x | | 1 | x | 2 | **M** | x | 4.0; 200 | **L** |  |
| **2** | 142459-58-3 | Flufenacet | 0 | x | | | 1 | x | 2 | **M** | x | 25; 100; 109(O2) | **L** | x |
| **3** | 62924-70-3 | Flumetralin | 1 | | x | | 1 | x | 2 | **M** | x | 11 | **M** |  |
| **4** | 87546-18-7 | Flumiclorac pentyl | 0 | |  | | 0 | x | 1 | **L** | x | 106 | **L** |  |
| **5** | 103361-09-7 | Flumioxazin (V-53482) | 1 | | x | | 0 | x | 1 | **L** | x | 105 | **M** |  |
| **6** | 117337-19-6 | Fluthiacet methyl | 0 | |  | | 0 |  | 1 | **L** |  | >100 | **M** |  |
| **7** | 112-05-0 | Nonanoic acid | 0 | |  | | 0 |  | 1 | **L** |  | 25 | **M** |  |
| **8** | 53939-28-9 | Z-11-Hexadecanol | 0 | |  | | 1 |  | 2 | **M** |  | na | **Non Predicted** | na |
| **9** | 118-52-5 | DCDMH(Glychlor Formulation) | 0 | |  | | 1 |  | 2 | **M** |  | na | **L** | x |
| **10** | 542-75-6 | Dichloropropene | 0 | |  | | 0 |  | 1 | **L** |  | 60.3 | **Non Predicted** | na |
| **11** | 86-87-3 | Naphthaleneacetic acid | 0 | | x | | 0 |  | 1 | **L** |  | na | **M** |  |
| **12** | 94-75-7 | 2,4-D Acid | 0 | |  | | 1 | x | 2 | **M** | x | 100 | **L** |  |
| **13** | 1320-18-9 | 2,4-D Propylene Glycol B.E. Ester | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **14** | 7747-35-5 | Oxazolidine E | 0 | |  | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **15** | 301-12-2 | Oxydemeton-methyl | 0 | |  | | 1 | x | 2 | **M** | x | 2.15; 3.0; 24.39; 0.54 | **M** |  |
| **16** | 76738-62-0 | Paclobutrazol | 0 | | x | | 0 |  | 1 | **L** |  | 235; 237(O2) | **L** | x |
| **17** | 106-46-7 | Paradichlorobenzene | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **18** | 1929-73-3 | 2,4-D Butoxyethanol Ester | 0 | |  | | 1 | x | 2 | **M** | x | na | **L** |  |
| **19** | 94-80-4 | 2,4-D Butyl Ester | 0 | |  | | 1 | x | 2 | **M** | x | na | **L** |  |
| **20** | 79270-78-3 | 2,4-DP, 2-EH Ester | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **21** | 120-32-1 | 2-Benzyl-4-chlorophenol | 0 | |  | | 1 |  | 2 | **M** |  | na | **M** |  |
| **22** | 7745-89-3 | 3-Chloro-p-toluidine hydrochloride | 0 | |  | | 0 |  | 1 | **L** |  | 72(O2) | **L** |  |
| **23** | 51200-87-4 | 4,4-Dimethyloxazolidine | 0 | |  | | 1 |  | 2 | **M** |  | na | **Non Predicted** | na |
| **24** | 64359-81-5 | Dichloro-2-n-octyl-3(2H)-isothiazolone | 1 | |  | | - | | 3 | **H** |  | na | **L** | x |
| **25** | 88-04-0 | 4-Chloro-3,5-xylenol | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **26** | 30560-19-1 | Acephate | 1 | |  | | - | | 3 | **H** |  | 1Ibs ai/Acre(O2) | **M** | x |
| **27** | 34256-82-1 | Acetochlor | 0 | |  | | 0 |  | 1 | **L** |  | >100 | **L** |  |
| **28** | 15972-60-8 | Alachlor | 0 | |  | | 0 |  | 1 | **L** |  | 36.2 | **L** |  |
| **29** | 116-06-3 | Aldicarb | 1 | |  | | - | | 3 | **H** |  | 0.29 | **H** |  |
| **30** | 1646-88-4 | Aldoxycarb | 1 | |  | | - | | 3 | **H** |  | na | **H** | x |
| **31** | 834-12-8 | Ametryn | 0 | |  | | 0 |  | 1 | **L** |  | >100; 96.36 | **M** |  |
| **32** | 33089-61-1 | Amitraz | 1 | |  | | - | | 3 | **H** |  | 100; 0.4g/ml(F) | **L** |  |
| **33** | 101-05-3 | Anilazine | 0 | | x | | 0 |  | 1 | **L** |  | 117.23 | **L** |  |
| **34** | 1397-94-0 | Antimycin A | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** | x |
| **35** | 1912-24-9 | Atrazine | 0 | |  | | 0 |  | 1 | **L** |  | 96.69 | **M** |  |
| **36** | 22781-23-3 | Bendiocarb | 0 | |  | | 1 |  | 2 | **M** |  | 0.43; 846 ppm(F) | **H** |  |
| **37** | 17804-35-2 | Benomyl | 0 | |  | | 0 |  | 1 | **L** |  | 120.86 ; 10 | **L** |  |
| **38** | 741-58-2 | Bensulide | 0 | | x | | 0 |  | 1 | **L** |  | 24(C1) | **M** |  |
| **39** | 68359-37-5 | Cyfluthrin | 0 | | x | | 1 | x | 2 | **M** | x | 0.01; 0.04; 0.03 | **H** |  |
| **40** | 3064-70-8 | Bis(trichloromethyl)Sulfone | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **41** | 314-40-9 | Bromacil | 0 | |  | | 0 |  | 1 | **L** |  | 193.38; 11 | **L** |  |
| **42** | 1689-84-5 | Bromoxynil(Phenol) | 0 | |  | | 0 |  | 1 | **L** |  | 14.5 | **M** |  |
| **43** | 1689-99-2 | Bromoxynil octanoate | 0 | |  | | 1 | x | 2 | **M** | x | 14.5 | **L** |  |
| **44** | 3861-41-4 | Bromoxynil(Butyrate) | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **45** | 52-51-7 | Bronopol | 1 | |  | | - | | 3 | **H** |  | na | **L** | x |
| **46** | 33629-47-9 | Butralin | 1 | |  | | - | | 3 | **H** |  | 100; 92.8(O2) | **M** |  |
| **47** | 133-06-2 | Captan | 0 | | x | | 0 | x | 1 | **L** | x | 215; 10 | **L** |  |
| **48** | 63-25-2 | Carbaryl | 0 | | x | | 0 |  | 1 | **L** |  | 1.27; 1.34; 1.1(C1); 0.15(O2); 0.23(O2) | **M** |  |
| **49** | 1563-66-2 | Carbofuran | 0 | |  | | 1 |  | 2 | **M** |  | 0.16 | **H** |  |
| **50** | 5234-68-4 | Carboxin | 0 | |  | | 1 |  | 2 | **M** |  | 100; 181; 104(O2) | **L** |  |
| **51** | 2439-01-2 | Oxythioquinox | 0 | | x | | 0 |  | 1 | **L** |  | 66.47; 80(O2) | **M** |  |
| **52** | 143-50-0 | Kepone (Cancelled in U.S.) | 0 | | x | | 0 | x | 1 | **L** | x | na | **M** | x |
| **53** | 54593-83-8 | Chlorethoxyfos | 1 | |  | | - | | 3 | **H** |  | 0.09 | **H** | x |
| **54** | 55-56-1 | Chlorhexidine diacetate | 0 | | x | | 0 | x | 1 | **L** | x | na | **M** |  |
| **55** | 90982-32-4 | Chlorimuron Ethyl | 0 | | x | | 1 | x | 2 | **M** | x | 12.5 | **M** |  |
| **56** | 2675-77-6 | Chloroneb | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **57** | 3691-35-8 | Chlorophacinone | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **58** | 76-06-2 | Chloropicrin | 1 | |  | | - | | 3 | **H** |  | 100 | **Non Predicted** | na |
| **59** | 101-21-3 | Chlorpropham | 0 | |  | | 1 |  | 2 | **M** |  | 36.3 | **L** |  |
| **60** | 2921-88-2 | Chlorpyrifos | 0 | |  | | 1 |  | 2 | **M** |  | 0.06(O1); 0.11(C3) | **H** |  |
| **61** | 5598-13-0 | Chlorpyrifos-methyl | 0 | |  | | 1 | x | 2 | **M** | x | 0.38(C1) | **L** | x |
| **62** | 1861-32-1 | DCPA (Dacthal) | 1 | |  | | - | | 3 | **H** |  | na | **L** |  |
| **63** | 105512-06-9 | Clodinafop-propargyl | 0 | | x | | 1 | x | 2 | **M** | x | 100 | **L** |  |
| **64** | 81777-89-1 | Clomazone | 0 | |  | | 0 |  | 1 | **L** |  | >100; 85.29(O2) | **L** |  |
| **65** | 1134-23-2 | Cycloate | 0 | |  | | 0 |  | 1 | **L** |  | 29 | **M** |  |
| **66** | 13121-70-5 | Cyhexatin (Plictran) | 0 | |  | | 0 | x | 1 | **L** | x | 35.9 | **M** |  |
| **67** | 57966-95-7 | Cymoxanil | 1 | |  | | - | | 3 | **H** |  | 25 | **M** |  |
| **68** | 121552-61-2 | Cyprodinil | 0 | | x | | 1 |  | 2 | **M** |  | 784 | **L** |  |
| **69** | 1596-84-5 | Daminozide | 0 | |  | | 0 |  | 1 | **L** |  | 205.46 | **L** |  |
| **70** | 10222-01-2 | DBNPA | 0 | |  | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **71** | 50-29-3 | DDT (Cancelled in U.S.) | 1 | |  | | - | | 3 | **H** |  | 3.9; 6.4; 7.12 (O2);5.36(O2); 3.7(O2) | **M** |  |
| **72** | 52918-63-5 | Deltamethrin | 0 | | x | | 1 | x | 2 | **M** | x | 0.01; 0.05; 0.11(C3); 0.19(O3) | **H** |  |
| **73** | 35691-65-7 | Dibromodicyanobutane | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **74** | 1194-65-6 | Dichlobenil | 0 | |  | | 0 |  | 1 | **L** |  | 120.86 | **L** |  |
| **75** | 120-36-5 | Dichlorprop(2,4-DP) | 0 | |  | | 1 |  | 2 | **M** |  | 200; 200(O2) | **L** |  |
| **76** | 62-73-7 | Dichlorvos | 1 | |  | | - | | 3 | **H** |  | 0.49 | **H** |  |
| **77** | 99-30-9 | Dicloran (DCNA) | 0 | |  | | 1 | x | 2 | **M** | x | 181 | **L** |  |
| **78** | 141-66-2 | Dicrotophos | 1 | |  | | - | | 3 | **H** |  | 0.08(C1) | **M** | x |
| **79** | 60-57-1 | Dieldrin (Cancelled in U.S.) | 0 | | x | | 1 |  | 2 | **M** |  | 0.14; 0.16; 0.32(O2) | **M** |  |
| **80** | 119446-68-3 | Difenoconazole | 0 | | x | | 0 | x | 1 | **L** | x | >100; 101; 177(O2) | **L** |  |
| **81** | 49866-87-7 | Difenzoquat methyl sulfate | 0 | |  | | 1 |  | 2 | **M** |  | na | **L** |  |
| **82** | 104653-34-1 | Difethialone | 0 | | x | | 0 | x | 1 | **L** | x | na | **Non Predicted** | na |
| **83** | 109293-97-2 | Diflufenzopyr-sodium | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **84** | 87674-68-8 | Dimethenamid | 0 | |  | | 0 |  | 1 | **L** |  | 94; 1000(O2) | **M** |  |
| **85** | 60-51-5 | Dimethoate | 1 | |  | | - | | 3 | **H** |  | 0.01; 0.16; 0.17; 0.29; 0.06(O2); 0.13(O2) | **H** |  |
| **86** | 82-66-6 | Diphacinone | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **87** | 97886-45-8 | Dithiopyr | 0 | |  | | 0 |  | 1 | **L** |  | 81; >100; >100; 119(O2) | **M** |  |
| **88** | 330-54-1 | Diuron | 0 | |  | | 0 |  | 1 | **L** |  | 145.03 | **L** |  |
| **89** | 2439-10-3 | Dodine | 0 | |  | | 0 | x | 1 | **L** | x | 12.1; 200 | **M** |  |
| **90** | 4080-31-3 | Dowicil | 0 | |  | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **91** | 72-20-8 | Endrin (Cancelled in U.S.) | 0 | | x | | 1 |  | 2 | **M** |  | 2.02; 0.65(C1); 0.46(O1) | **M** |  |
| **92** | 2104-64-5 | EPN (Cancelled in U.S.) | 0 | | x | | 1 |  | 2 | **M** |  | 0.25 | **H** |  |
| **93** | 759-94-4 | EPTC | 0 | |  | | 1 |  | 2 | **M** |  | 12.09; 72.5(C3) | **M** |  |
| **94** | 55283-68-6 | Ethalfluralin | 1 | |  | | - | | 3 | **H** |  | 51 | **M** |  |
| **95** | 563-12-2 | Ethion | 0 | |  | | 0 |  | 1 | **L** |  | 20.55; 0.85(C1) | **M** |  |
| **96** | 107-06-2 | Ethylene dichloride | 0 | | x | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **97** | 4602-84-0 | Farnesol | 0 | |  | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **98** | 60168-88-9 | Fenarimol | 0 | | x | | 0 | x | 1 | **L** | x | >100; 10(O2); 100(O2) | **L** | x |
| **99** | 13356-08-6 | Fenbutatin Oxide | 1 | | x | | 0 | x | 1 | **L** | x | 3982 | **L** |  |
| **100** | 66441-23-4 | Fenoxaprop-ethyl | 0 | | x | | 1 |  | 2 | **M** |  | 100 | **H** |  |
| **101** | 79127-80-3 | Fenoxycarb | 0 | | x | | 1 |  | 2 | **M** |  | na | **L** |  |
| **102** | 39515-41-8 | Fenpropathrin | 0 | | x | | 1 | x | 2 | **M** | x | 0.1 Ibs ai/Acre(F) | **H** |  |
| **103** | 68254-10-4 | Fenridazone-sodium | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **104** | 55-38-9 | Fenthion | 0 | |  | | 1 |  | 2 | **M** |  | 0.31 | **H** |  |
| **105** | 76-87-9 | Fentin hydroxide | 0 | |  | | 0 | x | 1 | **L** | x | 114.8 | **L** |  |
| **106** | 59756-60-4 | Fluridone | 0 | | x | | 1 |  | 2 | **M** |  | 100; 362.58 | **L** | x |
| **107** | 56425-91-3 | Flurprimidol | 0 | | x | | 1 | x | 2 | **M** | x | 100 | **L** |  |
| **108** | 66332-96-5 | Flutolanil | 0 | | x | | 1 |  | 2 | **M** |  | 650; 0.32 Ibis ai/Acre(F) | **L** |  |
| **109** | 69409-94-5 | Fluvalinate | 0 | | x | | 0 | x | 1 | **L** | x | 0.20; 0.80; 1.21; 1.9 | **M** |  |
| **110** | 133-07-3 | Folpet | 1 | |  | | - | | 3 | **H** |  | 12.1 | **M** |  |
| **111** | 944-22-9 | Fonofos | 0 | |  | | 0 |  | 1 | **L** |  | 3.3; 8.68; 8.4(O2) | **M** |  |
| **112** | 22259-30-9 | Formetanate Hydrochloride | 0 | |  | | 1 |  | 2 | **M** |  | na | **M** |  |
| **113** | 59682-52-9 | Fosamine ammonium | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **114** | 58-89-9 | Lindane | 1 | |  | | - | | 3 | **H** |  | 0.20; 0.56 | **H** |  |
| **115** | 1071-83-6 | Glyphosate(80WDG) | 1 | |  | | - | | 3 | **H** |  | 103; 182(O2) | **L** | x |
| **116** | 76-44-8 | Heptachlor | 0 | |  | | 1 |  | 2 | **M** |  | na | **M** | x |
| **117** | 53042-79-8 | Hexadecadienol,acetate | 1 | |  | | - | | 3 | **H** |  | na | **M** | x |
| **118** | 67485-29-4 | Hydramethylnon | 0 | |  | | 0 |  | 1 | **L** |  | 67 | **M** |  |
| **119** | 81405-85-8 | Imazethabenz | 0 | |  | | 0 |  | 1 | **L** |  | >100 | **L** |  |
| **120** | 81335-37-7 | Imazaquin | 1 | | x | | 1 | x | 2 | **M** | x | 100 | **L** |  |
| **121** | 81335-77-5 | Imazethapyr(Acid) | 0 | |  | | 0 |  | 1 | **L** |  | 1000 | **L** |  |
| **122** | 36734-19-7 | Iprodione | 1 | | x | | 0 |  | 2 | **L** |  | na | **L** |  |
| **123** | 28159-98-0 | Irgarol | 0 | |  | | 0 |  | 1 | **L** |  | na | **M** |  |
| **124** | 25311-71-1 | Isofenphos | 0 | |  | | 1 |  | 2 | **M** |  | 0.05 | **H** |  |
| **125** | 33820-53-0 | Isopropalin | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **126** | 138-86-3 | Limonene | 0 | | x | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **127** | 330-55-2 | Linuron | 0 | |  | | 1 |  | 2 | **M** |  | 120.86 | **L** |  |
| **128** | 29457-72-5 | Lithium perfluorooctane sulfonate | 0 | | x | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **129** | 121-75-5 | Malathion | 1 | |  | | - | | 3 | **H** |  | 0.16; 0.27; 0.27 | **H** |  |
| **130** | 7085-19-0 | MCPP Acid | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **131** | 104206-82-8 | Mesotrione(AMBA) | 1 | |  | | - | | 3 | **H** |  | 100(C1); 11(O1) | **H** | x |
| **132** | 57837-19-1 | Metalaxyl | 0 | |  | | 0 |  | 1 | **L** |  | >100 | **L** |  |
| **133** | 950-37-8 | Methidathion | 1 | |  | | - | | 3 | **H** |  | 0.24(C3); 5(F) | **H** |  |
| **134** | 16752-77-5 | Methomyl | 0 | |  | | 0 |  | 1 | **L** |  | 0.16 | **H** |  |
| **135** | 134-20-3 | Methyl anthralinate | 0 | |  | | 1 |  | 2 | **M** |  | 25 | **M** |  |
| **136** | 71-55-6 | Methyl chloroform | 0 | | x | | 0 | x | 1 | **L** | x | na | **Non Predicted** | na |
| **137** | 6317-18-6 | Methylenebis(thiocyanate) | 0 | |  | | 0 | x | 1 | **L** | x | na | **Non Predicted** | na |
| **138** | 87392-12-9 | Metolachlor | 0 | |  | | 1 |  | 2 | **M** |  | 200(C3); 85(O3) | **L** |  |
| **139** | 21087-64-9 | Metribuzin | 0 | |  | | 1 |  | 2 | **M** |  | 60.4; 29 | **M** |  |
| **140** | 82633-79-2 | MTI | 0 | |  | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **141** | 134-62-3 | N,N-Diethyl-meta-toluamide(DEET) | 0 | |  | | 1 |  | 2 | **M** |  | na | **L** |  |
| **142** | 300-76-5 | Naled | 0 | |  | | 0 | x | 1 | **L** | x | 0.48 | **H** |  |
| **143** | 15299-99-7 | Napropamide | 0 | | x | | 1 |  | 2 | **M** |  | 113.5(O2) | **L** |  |
| **144** | 132-66-1 | Naptalam, Sodium | 0 | | x | | 0 |  | 1 | **L** |  | 113.2 | **L** |  |
| **145** | 7212-44-4 | Neurolidol | 0 | |  | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **146** | 1929-82-4 | Nitrapyrin | 0 | |  | | 1 |  | 2 | **M** |  | 100; 100(O2) | **M** | x |
| **147** | 105726-67-8 | N-methylneodecanamide | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **148** | 27314-13-2 | Norflurazon | 0 | |  | | 0 |  | 1 | **L** |  | 236; 90.6 | **L** |  |
| **149** | 105827-78-9 | Imidacloprid | 0 | |  | | 1 |  | 2 | **M** |  | na | **H** |  |
| **150** | 58-36-6 | OBPA | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** | x |
| **151** | 26530-20-1 | Octhilinone | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** | x |
| **152** | 19044-88-3 | Oryzalin | 1 | |  | | - | | 3 | **H** |  | 11 | **M** | x |
| **153** | 19666-30-9 | Oxadiazon | 1 | |  | | - | | 3 | **H** |  | 21.7; 25 | **L** |  |
| **154** | 23135-22-0 | Oxamyl | 0 | |  | | 1 |  | 2 | **M** |  | 10.32; 0.47; 0.31 | **M** |  |
| **155** | 100-02-7 | Paranitrophenol | 0 | | x | | 0 |  | 1 | **L** |  | na | **M** |  |
| **156** | 56-38-2 | Parathion (Ethyl) | 0 | |  | | 1 |  | 2 | **M** |  | 0.17 | **H** |  |
| **157** | 298-00-0 | Methyl Parathion | 0 | |  | | 1 |  | 2 | **M** |  | 0.29; 0.11; 0.21 | **H** |  |
| **158** | 40487-42-1 | Pendimethalin | 1 | |  | | - | | 3 | **H** |  | 49.8; 100; 101.2(O2) | **M** |  |
| **159** | 13684-63-4 | Phenmedipham | 0 | | x | | 1 |  | 2 | **M** |  | 100; 241.72 | **L** |  |
| **160** | 298-02-2 | Phorate | 0 | |  | | 0 |  | 1 | **L** |  | 0.24; 10.07; 0.32(C1) | **M** |  |
| **161** | 732-11-6 | Phosmet | 1 | |  | | - | | 3 | **H** | x | 1.06; 1Ibis ai/acre(F) | **H** |  |
| **162** | 83-26-1 | Pival | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **163** | 51-03-6 | Piperonyl butoxide | 1 | |  | | - | | 3 | **H** |  | 11 | **M** | x |
| **164** | 86209-51-0 | Primisulfuron-methyl | 0 | | x | | 0 |  | 1 | **L** |  | >100 | **L** | x |
| **165** | 41198-08-7 | Profenofos | 0 | |  | | 0 |  | 1 | **L** |  | 0.09; 3.46; 1 Ibs ai/Acre(F) | **H** | x |
| **166** | 1610-18-0 | Prometon | 1 | |  | | - | | 3 | **H** |  | 36 | **M** |  |
| **167** | 7287-19-6 | Prometryn | 1 | |  | | - | | 3 | **H** |  | 96.69 | **M** |  |
| **168** | 1918-16-7 | Propachlor | 0 | |  | | 0 |  | 1 | **L** |  | 25 | **L** |  |
| **169** | 709-98-8 | Propanil | 0 | |  | | 0 |  | 1 | **L** |  | 24.17 | **L** |  |
| **170** | 2312-35-8 | Propargite | 0 | | x | | 1 | x | 2 | **M** | x | 51.3; 18.13; 15 | **M** |  |
| **171** | 31218-83-4 | Propetamphos | 0 | |  | | 1 | x | 2 | **M** | x | na | **H** | x |
| **172** | 10453-86-8 | Resmethrin | 0 | | x | | 1 |  | 2 | **M** |  | 0.02; 0.06 | **H** |  |
| **173** | 83-79-4 | Rotenone | 0 | | x | | 1 |  | 2 | **M** |  | 2.42; 60; 30(O2) | **L** |  |
| **174** | 74051-80-2 | Sethoxydim | 1 | |  | | - | | 3 | **H** |  | 10 | **M** |  |
| **175** | 1982-49-6 | Siduron | 0 | |  | | 1 |  | 2 | **M** |  | 100; 120.86 | **L** |  |
| **176** | 122-34-9 | Simazine | 0 | |  | | 0 |  | 1 | **L** |  | 96.7 | **M** |  |
| **177** | 149-30-4 | Sodium 2-mercaptobenzothiolate | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** | x |
| **178** | 144-49-0 | Sodium fluroacetate | 0 | |  | | 0 |  | 1 | **L** |  | na | **M** | x |
| **179** | 131929-60-7 | Spinosad | 0 | | x | | 0 | x | 1 | **L** | x | 0.0029 | **H** |  |
| **180** | 3689-24-5 | Sulfotepp | 1 | |  | | - | | 3 | **H** |  | na | **M** | x |
| **181** | 1983-10-4 | Tributyltin fluoride(TBTF) | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **182** | 72-54-8 | TDE (Cancelled in U.S.) | 0 | | x | | 0 | x | 1 | **L** | x | na | **M** | x |
| **183** | 96182-53-5 | Phostebupirim | 1 | |  | | - | | 3 | **H** |  | na | **H** |  |
| **184** | 34014-18-1 | Tebuthiuron | 0 | |  | | 0 |  | 1 | **L** |  | >100 | **L** |  |
| **185** | 3383-96-8 | Temephos | 0 | |  | | 1 | x | 2 | **M** | x | na | **H** |  |
| **186** | 5902-51-2 | Terbacil | 0 | |  | | 0 |  | 1 | **L** |  | 193 | **L** |  |
| **187** | 13071-79-9 | Terbufos | 1 | |  | | - | | 3 | **H** |  | 4.09(O2) | **M** |  |
| **188** | 5915-41-3 | Terbuthylazine | 0 | |  | | 0 |  | 1 | **L** |  | na | **M** |  |
| **189** | 117718-60-2 | Thiazopyr | 0 | |  | | 0 | x | 1 | **L** | x | >100 | **L** | x |
| **190** | 28249-77-6 | Thiobencarb | 0 | |  | | 0 |  | 1 | **L** |  | >100; 100(O2) | **L** | x |
| **191** | 137-26-8 | Thiram | 0 | |  | | 1 |  | 2 | **M** |  | 73.72 | **M** |  |
| **192** | 66841-25-6 | Tralomethrin | 0 | | x | | 1 | x | 2 | **M** | x | 0.13 | **H** |  |
| **193** | 43121-43-3 | Triadimefon | 0 | | x | | 0 |  | 1 | **L** |  | 25; 25(O2) | **L** |  |
| **194** | 55219-65-3 | Triadimenol | 0 | | x | | 0 |  | 1 | **L** |  | 200; 224.8(O2) | **L** |  |
| **195** | 2303-17-5 | Triallate | 1 | |  | | - | | 3 | **H** |  | 25; 36.26 | **M** |  |
| **196** | 78-48-8 | Tribuphos | 1 | |  | | - | | 3 | **H** |  | 44.2 | **M** | x |
| **197** | 7673-09-8 | Trichloromelamine | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** | x |
| **198** | 55335-06-3 | Triclopyr, acid | 0 | |  | | 0 | x | 1 | **L** | x | >100; 99(O2) | **L** |  |
| **199** | 3380-34-5 | Triclosan | 0 | |  | | 1 | x | 2 | **M** | x | na | **L** |  |
| **200** | 58138-08-2 | Tridiphane | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **201** | 68694-11-1 | Triflumizole | 0 | | x | | 0 |  | 1 | **L** |  | 160 | **L** | x |
| **202** | 1582-09-8 | Trifluralin | 1 | |  | | - | | 3 | **H** |  | 24.17; 100(C1); 50(O1) | **M** |  |
| **203** | 126535-15-7 | Trisulfuron methyl | 0 | | x | | 0 | x | 1 | **L** | x | 25 | **L** |  |
| **204** | 2686-99-9 | Trimethacarb | 0 | |  | | 1 |  | 2 | **M** |  | 0.1(C1) | **H** |  |
| **205** | 126-11-4 | Tris(hydroxymethyl)nitromethane | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** | x |
| **206** | 83657-17-4 | Uniconazole | 0 | | x | | 0 |  | 1 | **L** |  | 20(C1) | **L** | x |
| **207** | 1929-77-7 | Vernolate | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **208** | 56-35-9 | Tributyltin oxide | 0 | | x | | 0 |  | 1 | **L** |  | na | **M** | x |
| **209** | 67-63-0 | Isopropanol | 0 | | x | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **210** | 79-09-4 | Proprionic acid | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **211** | 3244-90-4 | Aspon (Cancelled in U.S.) | 0 | |  | | 0 |  | 1 | **L** |  | na | **M** | x |
| **212** | 7779-27-3 | 1,3,5-Triethylhexahydro-s-triazine | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **213** | 26532-25-2 | Acetaldehyde | 0 | |  | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **214** | 85264-33-1 | 3,5 Dimethyl-1-(hydroxymethyl)pyrazole | 0 | |  | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **215** | 643-79-8 | 1,2-Benzenedicarboxaldehyde | 0 | |  | | 1 |  | 2 | **M** |  | na | **M** | x |
| **216** | 94-11-1 | 2,4-D Isopropyl Ester | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **217** | 3547-33-9 | 2-Hydroxyethyl octyl sulfide | 0 | |  | | 0 |  | 1 | **L** |  | 56.9 | **M** |  |
| **218** | 55406-53-6 | 3-Iodo-2-propynyl butylcarbamate | 1 | |  | | - | | 3 | **H** |  | na | **H** | x |
| **219** | 1192-52-5 | 4,5-Dichloro-1,2-dithio-3-one | 0 | |  | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **220** | 135158-54-2 | Acibenzolar-s-methyl | 0 | | x | | 0 |  | 1 | **L** |  | >100; 128.3(O2) | **L** |  |
| **221** | 131860-33-8 | Azoxystrobin | 0 | | x | | 0 | x | 1 | **L** | x | 200 | **L** | x |
| **222** | 1861-40-1 | Benfluralin | 1 | |  | | - | | 3 | **H** |  | 14.5; 101 | **M** |  |
| **223** | 25057-89-0 | Bentazon Sodium Salt | 0 | | x | | 1 | x | 2 | **M** | x | na | **H** |  |
| **224** | 2634-33-5 | Benzisothiazolin-3-one | 0 | |  | | 0 |  | 1 | **L** |  | na | **M** | x |
| **225** | 66841-24-5 | Beta Cypermethrin | 0 | | x | | 1 | x | 2 | **M** | x | na | **H** |  |
| **226** | 149877-41-8 | Bifenazate | 0 | | x | | 1 |  | 2 | **M** |  | 7.93 | **L** |  |
| **227** | 82657-04-3 | Bifenthrin | 0 | | x | | 1 |  | 2 | **M** |  | 0.02; 0.2 Ibis ai/Acre(F) | **H** |  |
| **228** | 2224-44-4 | Bioban P-1487 | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** | x |
| **229** | 2665-13-6 | Biobor | 1 | |  | | - | | 3 | **H** |  | na | **H** | x |
| **230** | 56073-10-0 | Brodifacoum | 0 | | x | | 0 | x | 1 | **L** | x | na | **H** | x |
| **231** | 7166-19-0 | Bromonitrostyrene | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** | x |
| **232** | 116255-48-2 | Bromuconazole | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **233** | 128639-02-1 | Carfentrazone-ethyl (F8246) | 0 | |  | | 0 | x | 1 | **L** | x | 27.2; 200(C1) | **M** |  |
| **234** | 122453-73-0 | Chlorfenapyr (Pirate) | 0 | | x | | 1 | x | 2 | **M** | x | 0.12 | **L** | x |
| **235** | 2536-31-4 | Chlorflurenol methyl | 0 | |  | | 1 |  | 2 | **M** |  | na | **-** | na |
| **236** | 95266-40-3 | Cimecticarb | 0 | |  | | 0 | x | 1 | **L** | x | 193.6; 47; 193.6(O2) | **M** |  |
| **237** | 39515-40-7 | Cyphenothrin | 0 | | x | | 1 | x | 2 | **M** | x | na | **H** |  |
| **238** | 7173-51-5 | DDAC | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **239** | 115-32-2 | Dicofol | 0 | | x | | 0 | x | 1 | **L** | x | 12.2(C3) | **M** |  |
| **240** | 38727-55-8 | Diethyl ethyl | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **241** | 35367-38-5 | Diflubenzuron | 0 | | x | | 0 |  | 1 | **L** |  | 114.8; 30; 30(O2); 2(F) | **L** |  |
| **242** | 20018-09-1 | Diiodomethyl p-tolyl sulfone | 0 | | x | | 0 |  | 1 | **L** |  | na | **H** | x |
| **243** | 55290-64-7 | Dimethepin | 0 | |  | | 0 |  | 1 | **L** |  | >100; 100(O2) | **M** | x |
| **244** | 122-39-4 | Diphenylamine | 1 | |  | | - | | 3 | **H** |  | na | **L** |  |
| **245** | 136-45-8 | Dipropyl isocinchomeronate | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **246** | 29873-30-1 | DTEA | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **247** | 91-53-2 | Ethoxyquin | 0 | | x | | 1 |  | 2 | **M** |  | na | **L** |  |
| **248** | 2593-15-9 | Etridiazole | 0 | |  | | 1 | x | 2 | **M** | x | 100; 77(O2) | **Non Predicted** | na |
| **249** | 114369-43-6 | Fenbuconazole | 0 | | x | | 0 | x | 1 | **L** | x | 292 | **L** |  |
| **250** | 35554-44-0 | Imazalil | 0 | | x | | 0 | x | 1 | **L** | x | 5.9; 27(O2) | **L** |  |
| **251** | 143390-89-0 | Kresoxim methyl | 0 | | x | | 1 |  | 2 | **M** |  | 25 | **L** |  |
| **252** | 91465-08-6 | Lambda-Cyhalothrin | 0 | | x | | 0 | x | 1 | **L** | x | 0.04; 0.096; 0.48(O2); 0.91(O2) | **H** |  |
| **253** | 556-61-6 | Methyl isothiocyanate | 0 | | x | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **254** | 112-12-9 | Methyl nonyl ketone | 1 | |  | | - | | 3 | **H** |  | na | **M** | x |
| **255** | 113-48-4 | MGK-264 | 1 | |  | | - | | 3 | **H** |  | 25 | **L** | x |
| **256** | 91-20-3 | Naphthalene | 0 | | x | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **257** | 50-65-7 | Niclosamide (ethanolamine salt) | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **258** | 90-43-7 | O-Phenylphenol | 0 | | x | | 1 |  | 2 | **M** |  | na | **L** |  |
| **259** | 42874-03-3 | Oxyfluorfen | 0 | | x | | 1 | x | 2 | **M** | x | 100(C3) | **L** |  |
| **260** | 59-50-7 | Parachlorometacresol | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **261** | 82-68-8 | PCNB | 1 | |  | | - | | 3 | **H** |  | 100; 100 | **H** |  |
| **262** | 23103-98-2 | Pirimicarb | 0 | |  | | 1 |  | 2 | **M** |  | 12.56; 18.72 | **M** |  |
| **263** | 29232-93-7 | Pirimiphos-methyl | 0 | |  | | 1 |  | 2 | **M** |  | 0.39; 0.36(O2) | **H** |  |
| **264** | 112-80-1 | Potassium salt of Oleic Acid | 1 | |  | | - | | 3 | **H** |  | na | **M** | x |
| **265** | 23031-36-9 | Prallethrin | 1 | |  | | - | | 3 | **H** |  | 0.23 | **H** |  |
| **266** | 96489-71-3 | Pyridaben | 0 | | x | | 0 | x | 1 | **L** | x | 0.02; 1.81; 2.63(O2) | **L** | x |
| **267** | 57-24-9 | Strychnine | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **268** | 107534-96-3 | Tebuconazole | 0 | | x | | 1 | x | 2 | **M** | x | 200 | **L** |  |
| **269** | 79538-32-2 | Tefluthrin | 0 | |  | | 0 |  | 1 | **L** |  | 0.17; 1.74(O2) | **H** |  |
| **270** | 59669-26-0 | Thiodicarb | 0 | |  | | 0 | x | 1 | **L** | x | 2.11; 25; 0.13(O2) | **H** | x |
| **271** | 64700-56-7 | Triclopyr BEE | 0 | | x | | 0 |  | 1 | **L** |  | >100; 25 | **L** |  |
| **272** | 141517-21-7 | Trifloxystrobin | 0 | | x | | 1 |  | 2 | **M** |  | 200; 200(O2) | **L** |  |
| **273** | 156052-68-5 | Zoxamide | 1 | |  | | - | | 3 | **H** |  | 100 | **M** |  |
| **274** | 1702-17-6 | Clopyralid,monoethanolamine salt | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **275** | 2782-57-2 | Sodium dichloro-s-triazinetrione | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **276** | 34375-28-5 | 2-(Hydroxymethylamino)ethanol | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** | x |
| **277** | 25168-26-7 | 2,4-D Isooctyl Ester | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **278** | 94-82-6 | 2,4-DB | 0 | |  | | 0 | x | 1 | **L** | x | 14.5 | **M** |  |
| **279** | 3337-71-1 | Asulam | 0 | |  | | 0 |  | 1 | **L** |  | 36.2 | **L** |  |
| **280** | 86-50-0 | Azinphos-methyl | 0 | | x | | 1 |  | 2 | **M** |  | 0.06; 0.42; 0.15(O2) | **H** |  |
| **281** | 28772-56-7 | Bromadiolone | 0 | | x | | 0 | x | 1 | **L** | x | na | **H** | x |
| **282** | 63333-35-7 | Bromethalin | 0 | | x | | 1 | x | 2 | **M** | x | na | **M** | x |
| **283** | 16079-88-2 | Bromo-3-chloro-5,5-dimethylhydantoin(BCDMH) | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** | x |
| **284** | 56634-95-8 | Bromoxynil heptanoate | 0 | |  | | 1 | x | 2 | **M** | x | na | **L** |  |
| **285** | 2425-06-1 | Captafol | 1 | |  | | - | | 3 | **H** |  | na | **L** | x |
| **286** | 10605-21-7 | Carbendazim | 1 | |  | | - | | 3 | **H** |  | 50 | **M** |  |
| **287** | 7003-89-6 | Chloroethyl trimethyl ammonium chloride | 0 | |  | | 1 | x | 2 | **M** | x | na | **Non Predicted** | na |
| **288** | 1897-45-6 | Chlorothalonil | 0 | |  | | 1 | x | 2 | **M** | x | 181.29 | **L** |  |
| **289** | 64902-72-3 | Chlorsulfuron | 0 | | x | | 1 | x | 2 | **M** | x | 25 | **L** |  |
| **290** | 56-72-4 | Coumaphos | 0 | | x | | 0 |  | 1 | **L** |  | na | **H** |  |
| **291** | 21725-46-2 | Cyanazine | 0 | |  | | 0 | x | 1 | **L** | x | 193.38 | **L** |  |
| **292** | 113136-77-9 | Cyclanilide | 0 | |  | | 0 |  | 1 | **L** |  | >100; 89.5(O2) | **H** |  |
| **293** | 34375-28-6 | Cyproconazole | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **294** | 25168-26-8 | Decanol | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** | x |
| **295** | 94-82-7 | Diazinon | 0 | |  | | 0 |  | 1 | **L** |  | na | **H** |  |
| **296** | 3337-71-2 | Dicamba (Acid) | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **297** | 86-50-1 | Diclofop-methyl | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **298** | 28772-56-8 | Diphenamid | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **299** | 63333-35-8 | Endosulfan | 1 | | x | | 1 | x | 2 | **M** | x | na | **M** |  |
| **300** | 134098-61-6 | Fenpyroximate | 0 | | x | | 0 | x | 1 | **L** | x | 479.8(C3); 118.5(O3) | **L** |  |
| **301** | 16079-88-3 | Endothall | 0 | |  | | 1 |  | 2 | **M** |  | na | **L** |  |
| **302** | 56634-95-9 | Ethephon | 0 | |  | | 0 | x | 1 | **L** | x | na | **M** | x |
| **303** | 2425-06-2 | Ethofenprox | 0 | | x | | 1 | x | 2 | **M** | x | na | **H** |  |
| **304** | 10605-21-8 | Ethoprop | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **305** | 34375-28-6 | Fenamiphos | 0 | |  | | 1 |  | 2 | **M** |  | na | **M** |  |
| **306** | 25168-26-8 | Fenitrothion | 0 | |  | | 1 |  | 2 | **M** |  | na | **H** |  |
| **307** | 2008-41-5 | Butylate | 0 | |  | | 1 |  | 2 | **M** |  | 26; 72.5 | **M** |  |
| **308** | 533-74-4 | Dazomet | 0 | |  | | 1 |  | 2 | **M** |  | 24; 50; 10(O2) | **M** | x |
| **309** | 94-82-7 | Fluchloralin | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **310** | 3337-71-2 | Flumetsulam | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **311** | 86-50-1 | Fluometuron | 0 | |  | | 1 |  | 2 | **M** |  | na | **L** |  |
| **312** | 28772-56-8 | Fomesafen | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **313** | 63333-35-8 | Glufosinate-ammonium | 1 | |  | | - | | 3 | **H** |  | na | **L** |  |
| **314** | 16079-88-3 | Halofenoxide | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **315** | 56634-95-9 | Hexaflumuron | 1 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **316** | 2425-06-2 | Hexazinone | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **317** | 10605-21-8 | Hymexazol | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **318** | 126833-17-8 | Fenhexamid | 1 | |  | | - | | 3 | **H** |  | 0.22; >100(O2) | **L** |  |
| **319** | 7003-89-7 | Indole-3-butyric acid | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **320** | 1897-45-7 | Kinoprene | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **321** | 64902-72-4 | Maleic Hydrazide | 0 | |  | | 1 |  | 2 | **M** |  | na | **L** |  |
| **322** | 56-72-5 | Methiocarb | 0 | |  | | 1 |  | 2 | **M** |  | na | **H** |  |
| **323** | 21725-46-3 | Methoprene | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **324** | 113136-77-10 | Methoxyfenozide | 0 | | x | | 0 | x | 1 | **L** | x | na | **M** |  |
| **325** | 34375-28-7 | Methyl Bromide | 0 | | x | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **326** | 25168-26-9 | N6-Benzuladenine | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **327** | 94-82-8 | Oxadixyl | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **328** | 3337-71-3 | Phosphamidon | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **329** | 86-50-2 | Picloram (Acid) | 0 | |  | | 0 | x | 1 | **L** | x | na | **M** |  |
| **330** | 28772-56-9 | Piperalin | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **331** | 63333-35-9 | Propiconazole | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **332** | 16079-88-4 | Propoxur | 0 | |  | | 1 |  | 2 | **M** |  | na | **M** |  |
| **333** | 56634-95-10 | Pymetrozine | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **334** | 2425-06-3 | Pyraclostrobin | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **335** | 83055-99-6 | Bensulfuron Methyl | 0 | | x | | 0 | x | 1 | **L** | x | 12.5 | **L** |  |
| **336** | 72-43-5 | Methoxychlor | 1 | |  | | - | | 3 | **H** |  | 23.57 | **M** |  |
| **337** | 10605-21-9 | Pyridate | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **338** | 34375-28-7 | Pyriproxyfen | 0 | | x | | 1 |  | 2 | **M** |  | na | **L** |  |
| **339** | 25168-26-9 | Quinclorac | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **340** | 94-82-8 | Rimsulfuron | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **341** | 3337-71-3 | Sodium 2-phenylphenate | 0 | | x | | 1 |  | 2 | **M** |  | na | **L** |  |
| **342** | 86-50-2 | Streptomycin | 0 | | x | | 0 | x | 1 | **L** | x | na | **H** | x |
| **343** | 28772-56-9 | Sulfentrazone | 0 | |  | | 1 | x | 2 | **M** | x | na | **L** |  |
| **344** | 2764-72-9 | Diquat | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **345** | 26002-80-2 | D-Phenothrin | 0 | | x | | 1 | x | 2 | **M** | x | 0.07 | **H** |  |
| **346** | 140-56-7 | Fenaminosulf | 0 | |  | | 1 |  | 2 | **M** |  | 102 | **L** |  |
| **347** | 63333-35-9 | Sulfluramid | 0 | | x | | 0 | x | 1 | **L** | x | na | **Non Predicted** | na |
| **348** | 16079-88-4 | TCMTB | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** | x |
| **349** | 56634-95-10 | Tetrachlorvinphos | 0 | |  | | 1 | x | 2 | **M** | x | na | **M** |  |
| **350** | 2425-06-3 | Tetramethrin | 1 | |  | | - | | 3 | **H** |  | na | **M** | x |
| **351** | 10605-21-9 | Thiabendazole | 1 | |  | | - | | 3 | **H** |  | na | **L** | x |
| **352** | 7003-89-8 | Thidiazuron | 0 | | x | | 1 | x | 2 | **M** | x | na | **L** |  |
| **353** | 1897-45-8 | Thiophanate-methyl | 1 | |  | | - | | 3 | **H** |  | na | **L** |  |
| **354** | 64902-72-5 | Tricosene | 1 | |  | | - | | 3 | **H** |  | na | **Non Predicted** | na |
| **355** | 56-72-6 | Triforine | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **356** | 298-04-4 | Disulfoton | 1 | |  | | - | | 3 | **H** |  | 0.96; 1.11; 4.3 | **H** |  |
| **357** | 21725-46-4 | Triticonazole | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **358** | 113136-77-11 | Vinclozolin | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **359** | 34375-28-8 | Warfarin | 0 | | x | | 0 | x | 1 | **L** | x | na | **L** |  |
| **360** | 504-24-5 | 4-Aminopyridine | 0 | |  | | 1 |  | 2 | **M** |  | na | **Non Predicted** | na |
| **361** | 510-15-6 | Chlorobenzilate | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **362** | 101-10-0 | Chloroprop, Sodium salt | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** |  |
| **363** | 66215-27-8 | Cyromazine | 0 | |  | | 1 |  | 2 | **M** |  | 25 | **M** |  |
| **364** | 138698-36-9 | Decyl isonomyl dimethyl ammonium chloride | 1 | |  | | - | | 3 | **H** | x | na | **M** | x |
| **365** | 828-00-2 | Dimethoxane | 0 | |  | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **366** | 66230-04-4 | Esfenvalerate | 0 | | x | | 1 | x | 2 | **M** | x | 0.02 | **H** |  |
| **367** | 4719-04-4 | Grotan | 1 | |  | | - | | 3 | **H** |  | na | **L** | x |
| **368** | 94-74-6 | MCPA Acid | 0 | |  | | 0 |  | 1 | **L** |  | >100; 24.17; 10(O2) | **L** |  |
| **369** | 16484-77-8 | Mecoprop-P | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **370** | 70630-17-0 | Mefenoxam | 0 | |  | | 0 |  | 1 | **L** |  | 25 | **L** |  |
| **371** | 10265-92-6 | Methamidophos | 0 | | x | | 0 |  | 1 | **L** |  | 1.37 | **M** |  |
| **372** | 123342-93-8 | Pyrithiobac-sodium | 0 | | x | | 0 |  | 1 | **L** |  | na | **L** |  |
| **373** | 27176-87-0 | Sodium dodecylbenzenesulfonate | 0 | |  | | 0 |  | 1 | **L** |  | na | **L** | x |
| **374** | 35400-43-2 | Sulprofos | 0 | |  | | 0 | x | 1 | **L** | x | na | **H** |  |
| **375** | 87-90-1 | Trichloro-s-triazinetrione | 0 | |  | | 0 | x | 1 | **L** | x | na | **Non Predicted** | na |
| **376** | 65195-55-3 | Avermectin | 1 | | x | | 0 | x | 1 | **L** | x | na | **H** | x |
| **377** | 70124-77-5 | Flucythrinate | 0 | | x | | 0 | x | 1 | **L** | x | 0.05 Ibis ai/Acre(F) | **H** | x |
| **378** | 108-80-5 | Isocyanuric acid | 0 | |  | | 0 |  | 1 | **L** |  | na | **Non Predicted** | na |
| **379** | 7786-34-7 | Mevinphos (cancelled in U.S.) | 0 | |  | | 1 | x | 2 | **M** | x | 0.07; 0.03(O2) | **H** |  |
| **380** | 2385-85-5 | Mirex (Cancelled in U.S.) | 0 | | x | | 0 | x | 1 | **L** | x | na | **H** | x |
| **381** | 28434-00-6 | s-Bioallethrin | 1 | |  | | - | | 3 | **H** |  | na | **M** |  |
| **382** | 133-90-4 | Chloramben | 0 | |  | | 0 | x | 1 | **L** | x | na | **L** |  |
| **383** | 52-68-6 | Trichlorfon | 1 | |  | | - | | 3 | **H** |  | 59.8 | **M** |  |
| **384** | 173584-44-6 | Indoxacarb(DPX-MP062) | 0 | | x | | 1 | x | 2 | **M** | x | 0.07; 0.2(O2) | **H** |  |
| **385** | 150-68-5 | Monuron | 0 | |  | | 1 |  | 2 | **M** |  | 110 | **L** |  |
| **386** | 142-59-6 | Nabam | 0 | |  | | 0 |  | 1 | **L** |  | 12.09 | **M** |  |
| **387** | 52645-53-1 | Permethrin | 0 | | x | | 1 |  | 2 | **M** |  | 0.02; 0.05(C3); 0.11(C3); 0.13(O2) | **H** |  |
| **388** | 76578-14-8 | Quizalofop,Ethyl | 0 | | x | | 0 | x | 1 | **L** | x | 50 | **L** |  |
| **389** | 88-85-7 | Dinoseb acid (Cancelled in U.S.) | 0 | |  | | 1 | x | 2 | **M** | x | 36.26 | **M** |  |
| **390** | 144-21-8 | Disodium methanearsonate | 0 | | x | | 0 | x | 1 | **L** | x | 217; 20.7 | **L** | x |
| **391** | 127-20-8 | Dalapon | 0 | |  | | 0 |  | 1 | **L** |  | 24.2 | **M** |  |
| **392** | 79277-27-3 | Thiameturon-methyl | 0 | | x | | 0 | x | 1 | **L** | x | 12.5 | **M** |  |
| **393** | 87-86-5 | Pentachlorophenol | 0 | |  | | 1 |  | 2 | **M** |  | 48.34 | **L** |  |
| **394** | 1114-71-2 | Pebulate | 0 | |  | | 1 | x | 2 | **M** | x | 29 | **M** |  |
| **395** | 101200-48-0 | Tribenuron methyl | 0 | | x | | 0 | x | 1 | **L** | x | >100 | **M** | x |

x - prediction is out of AD; if the predictions in both model were out of AD, then compound was sorted as out of AD.

Toxicity levels: L – low toxic, M – moderate toxic, H – high toxic.

na - not available

C1 - acute contact LD50 - 24h exposure

C3 - acute contact LD50 - 72h exposure

O1 - oral LD50 - 24h exposure

O2 - oral LD50 - 48h exposure

O3 - oral LD50 ->72h exposure

F - foliage exposure