Supplemental Materials

ID	Phenotype Detection												Smiles
	Automated Annotation						Manual Annotation						
	P	M	ED	MG	MM	B/E	P	M	ED	MG	MM	B/E	
1	1	0	1	0	0	1	0	0	1	1	0	0	*Not Shown*
2	1	1	1	1	0	0	1	0	0	0	0	0	CN(C)C1=CC=C(C=C1)N=NC2=CC=CC=N2
3	0	0	1	1	0	0	0	0	1	1	0	0	C[N]1N=CC2=C1N=CN=C2SC3=CC=C(Cl)C=C3
4	0	0	1	1	1	1	1	0	0	0	0	0	CCCCN1CCNC1=S
5	0	0	1	1	0	0	0	1	0	1	0	0	*Not Shown*
6	1	1	1	1	0	0	1	0	1	1	0	0	O=C1OCCC1=CC2=CC3=C(OCO3)C=C2
7	0	1	1	0	0	0	0	1	1	0	0	1	CC(C)COC1=NC2=C([N]1C)C(=O)N(C)C(=O)N2C
8	0	0	1	1	1	0	1	0	1	1	0	0	*Not Shown*
9	1	0	1	1	0	0	1	0	0	0	0	0	CC1=NC(=CC=C1)NC(=S)NC2=NC(=CC=C2)C
10	1	0	1	1	0	0	1	0	1	0	0	0	CC1=C(NC(=S)NC2=C(C)C=CC=N2)N=CC=C1
11	1	1	1	1	0	0	1	1	0	0	0	0	CC1=CC=C(C=C1)N=NC2=C(N)N(NC2=N)C3=CC=CC=C3
12	1	0	1	1	1	0	1	0	0	0	0	1	CC(C)C1=CC(=C(C)C=C1O)N=CC2=C(O)C=CC=C2
13	0	1	1	1	0	0	1	1	0	0	0	0	OC(=O)C1=CC2=C([NH]1)C=CC(=C2)OCC3=CC=CC=C3
14	0	1	1	0	0	0	0	0	1	1	0	0	CCOC(=O)NC1=CC=C(C=C1)C(=O)C=CC2=CC=CC=C2
15	0	1	1	1	1	1	0	1	1	0	0	0	CN1C2=C(C=CC=C2)C(C)(C)C1=C=CC3=CC(=C(O)C(=C3)I)I
16	1	0	1	0	0	1	0	1	0	0	1	0	CC(=O)NC1=CC=C(C=C1)[As](O)(=O)C2=CC=C(C=C2)[N+]([O-])=O
17	0	0	1	0	0	0	0	0	0	1	0	0	CN1C(=O)N(C)C2=C(N=C(COC3=CC=C(C=C3)C(C)(C)C)[NH]2)C1=O
18	0	1	1	0	1	1	1	0	0	1	0	0	CC1=CC(=NC(=N1)S)S
19	0	1	1	0	0	1	1	1	0	0	0	0	*Not Shown*
20	1	0	1	1	0	0	1	0	1	0	0	0	*Not Shown*
21	1	0	1	1	0	0	1	0	0	0	0	0	NC(=O)C1=CC=C(C=C1)N=NC2=C(O)N=C3C=CC=CC3=C2O
22	0	1	1	0	0	1	0	1	1	0	1	0	CN(C)S(=O)(=O)C1=C(C=CC(=C1)C)N=NC2=C(O)C3=C(C=CC=C3)N=C2O
23	0	0	1	1	1	0	1	0	1	0	0	0	CC(=O)OC1CCC2(C)C(CCC3C4CC5CC(=CC(=O)C5C4(C)C(=O)CC23)C)C1
24	0	0	1	0	0	0	1	1	0	1	0	0	[NH]1C2=CC=CC=C2N=C1C3=CC=NC=C3
25	1	0	1	1	1	0	1	0	0	0	0	0	S1C2=C(C=CC=C2)N=C1C3=CC=CC=N3
26	0	0	1	0	0	1	0	0	1	1	0	0	ClC1=CC2=C(NC(=O)CN=C2C3=CC=C[NH]3)C=C1
27	1	0	1	0	1	0	0	0	0	0	1	1	OC(=O)C1=C(O)C=CC(=C1)NC(=O)OC2=CC=CC=C2
28	0	1	1	0	0	0	1	1	1	0	0	0	*Not Shown*
29	1	1	1	0	0	1	1	1	1	0	0	1	CCCCNC1=C(C=NC(=N1)N)[N+]([O-])=O
30	1	0	1	1	0	0	1	1	1	0	0	0	COC1=CC(=CC(=C1OC)OC)C(O)C2=NC3=CC=CC=C3S2
31	1	1	1	1	0	1	0	1	0	0	0	0	CC1=NC(=CS1)C2CCC3C4CCC5=CC(=O)CCC5(C)C4CCC23C
32	1	1	1	1	1	0	0	1	0	1	0	0	*Not Shown*
33	1	0	1	1	0	1	1	1	0	0	0	0	CN1((=ONN(CCC2=((N=(([N]]2)CCCNCCCC33)C==S
34	1	0	1	0	0	0	1	0	0	0	0	0	CCN1CCCC(C1)SC2=NC3=C([NH]2)N(C)C(=O)N(C)C3=S
35	1	0	1	1	1	1	1	0	1	1	0	0	CNC(=S)N1NC(=N)N=C1
36	0	0	1	0	1	1	1	1	0	1	0	0	CNC1=NC(=O)N(C=C1)C2CCCO2
37	1	0	1	0	1	0	1	0	0	1	0	0	*Not Shown*
38	1	0	1	1	1	0	1	0	1	0	0	0	[O-][N+](=O)C1=C(OC2=CN=CC=C2)N=CC=C1
39	1	1	1	0	1	0	0	0	1	1	1	1	OC(=O)C1=CC=C2C(=O)C3=CC=CC=C3C(=O)C2=C1SC4=CC=CC=C4
40	1	1	0	0	0	0	1	1	0	1	0	0	NC(=N)NC(=N)NC1=CC=C(O)C=C1
41	1	0	1	0	1	0	0	1	1	1	0	0	COC1=CC=C(C=C1)C(=CC2=CC=CC=N2)C#N

42	1	0	1	1	1	0	1	1	0	0	0	0	*Not Shown*
43	1	0	1	0	0	1	1	1	0	0	0	0	*Not Shown*
44	1	0	0	1	1	1	0	0	0	1	1	0	*Not Shown*
45	1	0	1	1	1	0	1	0	0	0	0	0	S=C1NC2=CC3=CC=CC=C3C=C2N1
46	0	0	1	0	0	0	0	1	0	0	1	0	*Not Shown*
47	0	0	0	0	1	0	0	0	0	1	0	0	OC1=C(N=NC2=NC=CS2)C3=C(C=CC=C3)C=C1
48	1	0	1	1	0	1	0	1	0	1	0	0	[O-][N+](=O)C=CC1=CC2=CC=CC=C2[NH]1
49	1	1	1	1	1	0	0	1	0	0	0	0	BrC1=CC=C(C=C1)C(=CC2=CC=CN=C2)C#N
50	0	0	1	0	0	0	1	0	0	0	0	0	*Not Shown*
51	0	0	1	1	1	0	1	0	1	1	0	0	CC1=N[N]2C=NC3=C(C=CC=C3)C2=C1
52	1	0	1	1	1	0	1	0	0	0	0	0	NC(=S)NC1=CC(=CC=C1)Cl
53	1	0	1	0	1	1	0	0	1	1	1	0	ClC1=C(Cl)C=C(NC(=O)OC2=CC=C(NC(=S)NCC=C)C=C2)C=C1
54	1	1	1	1	1	1	1	1	1	0	0	1	*Not Shown*
55	0	1	1	1	1	0	1	1	0	0	0	0	*Not Shown*
56	1	0	1	0	0	0	0	0	1	1	0	0	COC1=CC=C(C=C1OC)C2C=C(OC3=C2C(=O)OC4=CC=CC=C34)C5=CC(=C(OC)C=C5)OC
57	1	1	1	1	0	1	1	1	1	1	1	1	*Not Shown*
58	1	0	1	1	0	0	0	0	1	0	1	1	*Not Shown*
59	0	0	0	0	1	0	0	0	0	0	1	1	CN(C)CCN1C(=O)C2=CC=CC3=CC(=CC(=C23)C1=O)N
60	1	0	1	0	0	0	1	1	0	0	0	0	CC(C)(C)CC(C)(C)N1CNC(=S)NC1
61	1	0	1	1	0	0	1	0	0	0	0	0	*Not Shown*
62	0	0	1	0	1	1	1	1	1	0	0	0	CCN1CN(C2=CC(=CC=C2)Cl)C3=C4C=C(OC)C=CC4=NC(=C3C1)C=CC5=CC=CC=C5
63	1	1	1	0	0	1	1	1	1	0	0	1	NC1=C(C=CC=C1)C(=O)NC2=C(Cl)C=C(Cl)C=C2
64	1	1	1	0	1	0	1	1	1	1	0	0	O=C(NC1=CC=C(C=C1)C#N)NC2=CC(=CC=C2)C#N
65	1	0	1	1	0	0	0	0	1	0	1	0	COC1=CC=C(NC=C2C(=O)CCC3=C2OC4=CC(=C(O)C(=C34)Cl)Cl)C=C1
66	1	1	1	1	0	0	1	1	1	0	0	0	OC1=CC(=C(C=C1)N=NC2=CC=C(Br)C=C2)O
67	1	0	1	1	0	0	1	0	0	0	0	0	S=C1NC2(CCCCC2)NC13CCCCC3
68	0	1	1	1	0	0	1	1	1	0	0	0	OC1=CC(=C(O)C=C1[N]2C=CC=N2)[N]3C=CC=N3
69	1	1	1	0	1	0	1	1	1	0	1	0	CN(C)C1=CC(=CC=C1)C=C(C#N)C2=CC=CC=C2

Table 1. Comparison of manual and automated phenotype detection outcomes per compound along with the corresponding compound smiles. Some entries cannot be shown due to follow-up experiments and are annotated accordingly.