

Supplementary Data

BitterX: a tool for understanding bitter taste in humans

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1 TABLES

Table S1. The 46 physicochemical descriptors used in the model of bitterant estimation. Definitions of how the descriptors were calculated can be found in the *Handbook of Molecular Descriptors* (Todeschini and Consonni, 2000).

Num.	Physicochemical Property
1	Average connectivity index chi-1
2	Binary 2 order of C and O
3	Binary 4 order of C and O
4	Binary 5 order of C and C
5	Binary 5 order of C and N
6	Binary 7 order of C and O
7	Binary 8 order of C and C
8	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic van der Waals volumes
9	Complementary Information Content 0
10	Complementary Information Content 4
11	Conventional bond-order ID number
12	Difference between multiple path count and path count
13	First Mohar index
14	Frequency 2 order of C and N
15	Frequency 2 order of C and O
16	Frequency 4 order of C and C
17	Frequency 9 order of C and O
18	Geary autocorrelation - lag 1 / weighted by atomic polarizabilities
19	Geary autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities
20	Geary autocorrelation - lag 6 / weighted by atomic masses
21	Geary autocorrelation - lag 6 / weighted by atomic Sanderson electronegativities
22	Geary autocorrelation - lag 7 / weighted by atomic masses
23	Geary autocorrelation - lag 8 / weighted by atomic masses
24	Information content index 0
25	Kier&Hall order 1
26	MACCS No 96
27	MACCS No 112
28	MACCS No 131
29	MACCS No 139
30	MACCS No 149
31	MACCS No 153
32	MACCS No 157
33	MACCS No 158
34	MACCS No 159

35	MACCS No 164
36	Maximal electrotopological negative variation
37	Mean topological charge index of order 4
38	Mean topological charge index of order 7
39	Molecular walk count of order 3
40	Moran autocorrelation - lag 2 / weighted by atomic Sanderson electronegativities
41	Moran autocorrelation - lag 5 / weighted by atomic Sanderson electronegativities
42	O atom num
43	Rel C atom num
44	Ring num of member 5
45	Structural information content 2
46	Total information content index 0

Table S2. The 20 physicochemical descriptors used in the model of hTAS2R recognition. Definitions of how the descriptors were calculated can be found in the *Handbook of Molecular Descriptors* (Todeschini and Consonni, 2000).

Num.	Physicochemical Property
1	Average connectivity index chi-3
2	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic polarizabilities
3	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic polarizabilities
4	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic masses
5	Frequency of C-C at topological distance 6 (frequency 6 order of C and C)
6	Frequency of C-C at topological distance 7 (frequency 7 order of C and C)
7	Geary autocorrelation - lag 1 / weighted by atomic Sanderson electronegativities
8	Geary autocorrelation - lag 2 / weighted by atomic Sanderson electronegativities
9	Geary autocorrelation - lag 3 / weighted by atomic masses
10	Geary autocorrelation - lag 7 / weighted by atomic masses
11	Mean atomic polarizability (Average Pol)
12	Mean topological charge index of order 2
13	Mean topological charge index of order 3
14	Relative O atom number
15	Moran autocorrelation - lag 2 / weighted by atomic polarizabilities
16	Moran autocorrelation - lag 3 / weighted by atomic Sanderson electronegativities

17	Moran autocorrelation - lag 5 / weighted by atomic polarizabilities
18	Self returning walk of order 10
19	Structural information content 3
20	Valence average connectivity index chi-6

Table S3. The 15 receptor descriptors used in the model of hTAS2R recognition. Definitions of how the descriptors were calculated can be found in Chou, 2001 and Tian *et al.*, 2007.

Num.	Physicochemical Property
1	Amino Acid Hydropathy Score
2	Normalized frequency of amino acid A
3	Normalized frequency of amino acid F
4	Normalized frequency of amino acid S
5	Normalized frequency of amino acid V
6	Normalized frequency of amino acid Y
7	Pseudo amino acid θ_3
8	Pseudo amino acid θ_{11}
9	Pseudo amino acid θ_{18}
10	Pseudo amino acid θ_{25}
11	Pseudo amino acid θ_{26}
12	Pseudo amino acid θ_{34}
13	Pseudo amino acid θ_{37}
14	Pseudo amino acid θ_{38}
15	Pseudo amino acid θ_{44}

Table S4. Positive bitterant-TAS2R pairs used in the TAS2R recognition model.

Molecule	Target
<chem>CC1=CC(O)C2C(CC(=C)C(CC1)O)OC(=O)C2=C</chem>	TAS2R46
<chem>CN(CCOC(c1ccccc1C)c1ccccc1)C</chem>	TAS2R46
<chem>Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@@H](Cc2c(c1)O)O</chem>	TAS2R5,TAS2R39
<chem>Oc1cc2O[C@H](c3cc(O)c(c(c3)O)O)[C@@H](Cc2c(c1)O)O</chem>	TAS2R39
<chem>Oc1cc(O)c2c(c1)O[C@@H]([C@@H](C2)OC(=O)c1cc(O)c(c(c1)O)O)c1c</chem> <chem>cc(c(c1)O)O</chem>	TAS2R39
<chem>OC[C@H]1O[C@@H](Oc2cc(O)c3c(c2)occ(c3=O)c2ccc(cc2)O)[C@@H]([C@@H]([C@@H]1O)O)O</chem>	TAS2R39
<chem>NC(=S)Nc1ccccc1</chem>	TAS2R38
<chem>CN1CCN(CC1)c1c(F)cc2c3c1OCC(n3cc(c2=O)C(=O)O)C</chem>	TAS2R9
<chem>CCN(CCNC(=O)c1ccc(cc1)N)CC</chem>	TAS2R9
<chem>CN1CCN(CC1)CC(=O)N1C2CCCCC2C(=O)NC2C1NCCCC2</chem>	TAS2R9
<chem>CCCc1cc(=O)[nH]c(=S)[nH]1</chem>	TAS2R38

CC(=O)Nc1ccc(cc1)O	TAS2R39
CC1=CC(=NS(=O)(=O)O1)[O-]	TAS2R44,TAS2R43
OCc1cc(O)c2c(c1)C(C1OC(CO)C(C(C1O)O)O)c1c(C2=O)c(O)ccc1	TAS2R44,TAS2R43
CC1C(=O)CC2C1C1OC(=O)C(=C)C1C(CC2=C)O	TAS2R46,TAS2R43
O=C1NS(=O)(=O)c2c1cccc2	TAS2R44,TAS2R43
OCC1(C)C(O)CCC2(C1CCC(=C)C2C/C=C/1\C(O)COC1=O)C	TAS2R46,TAS2R47,TAS2R50
OCC1=CC2OC(=O)C(=C)C2C(CC(=CCC1)C)OC(=O)C(=C)C(CO)O	TAS2R46
OOCC1CCC2(CC1=CCC1C(C2O)OC(=O)C1=C)C	TAS2R46
OCC(=O)C1(O)CCC2C1(C)CC(O)C1C2CCC2=CC(=O)CCC12C	TAS2R46
S=C=NCCc1cccc1	TAS2R38
N/C(=N\CCCCC/N=C(/N=C(/Nc1ccc(cc1)Cl)\N)\N)/N=C(/Nc1ccc(cc1)Cl)\N	TAS2R14
CCCC(COC(=O)N)(COC(=O)NC(C)C)C	TAS2R14
COC1=CC(C)C2C(C1=O)(C)C1C(=O)C(=C(C3C1(C(C2)OC(=O)C3)C)C)OC	TAS2R46,TAS2R47,TAS2R4,TA S2R10,TAS2R14
CC1=CCCC2(C)OC2C2C(CC1)C(=C)C(=O)O2	TAS2R46,TAS2R44,TAS2R1,TA S2R4,TAS2R8,TAS2R10,TAS2R 14
NC(=O)c1cccc1	TAS2R14
Cn1cnc(c1Sc1ncnc2c1[nH]cn2)[N+](=O)[O-]	TAS2R46,TAS2R4,TAS2R10,TA S2R14
CCCCCCC/C=C/C(C#CC#CC(C=C)O)O	TAS2R43,TAS2R14
CC(=O)OC/C=C/C(=O)C(C1C(O)CC2(C1(C)CC(=O)C1(C2CC=C2C1CC(O)C(=O)C2(C)C)C)C(O)C(C)C	TAS2R10,TAS2R14
COc1ccc(cc1OC)Cc1nccc2c1cc(OC)c(c2)OC	TAS2R7,TAS2R10,TAS2R14
COc1ccc2c(c1OC)C(=O)OC2C1N(C)CCc2c1c(OC)c1c(c2)OCO1	TAS2R14
Oc1ccc2c(c1)oc(=O)c1c2oc2c1ccc(c2)O	TAS2R39,TAS2R14
S=C1NCCN1C	TAS2R38
O=C1OCC23C(C1)OC(C2CC(=O)C1(C3CCC2(C31OC3C(=O)OC2c1cocc1)C)C(C)C	TAS2R38
CNC(=S)N	TAS2R38
CC(=C)C1C2OC(=O)C1C1(C3(C2OC(=O)C23C(C1)O2)C)O	TAS2R46,TAS2R47,TAS2R1,TA S2R10,TAS2R14
CCc1cncn1	TAS2R38
S=CN(C)C	TAS2R38
S=C1NCCN1	TAS2R38
CCNC(=S)N	TAS2R38
CC(=CCC(=O)C1(O)C(=C(C(=O)C1CC=C(C)C)C(=O)C(C)C)O)C	TAS2R1,TAS2R14
CC(=CCC(=O)C1(O)C(=C(C(=O)C1CC=C(C)C)C(=O)C(C)C)O)C	TAS2R1,TAS2R14
CCC(C(=O)C1=C(O)C(C(=O)C(=C1O)CC=C(C)C)(CC=C(C)C)CC=C(C)C)C	TAS2R1,TAS2R14
[O-]S(=O)(=O)NC1CCCCC1	TAS2R1,TAS2R38
CCN(CCCC(Nc1cnc2c1ccc(c2)Cl)C)CC	TAS2R3,TAS2R10,TAS2R39,TA S2R14

CCC(C(=O)C1=C(O)C(C(C1=O)CC=C(C)C)(O)C(=O)CC=C(C)C)C	TAS2R1,TAS2R14
CCC(C(=O)C1=C(O)C(C(C1=O)CC=C(C)C)(O)C(=O)CC=C(C)C)C	TAS2R1,TAS2R14
CC(=O)NC(=S)N	TAS2R38
O=C1CCCCCN1	TAS2R38
OCC1OC(OCC2OC(OC(c3ccccc3)C#N)C(C(C2O)O)O)C(C(C1O)O)O	TAS2R16
OCC1OC(Oc2ccc(cc2)O)C(C(C1O)O)O	TAS2R16
O=C1CC2OCC=C3C4C2C2N1c1ccccc1C12CCN(C1C4)C3	TAS2R46,TAS2R10
NC(=Nc1scc(n1)CSCC/C(=N/S(=O)(=O)N)/N)N	TAS2R44,TAS2R10
C=CC/C(=N)OS(=O)(=O)[O-]/SC1OC(CO)C(C(C1O)O)O	TAS2R38,TAS2R16
C=CCN=C=S	TAS2R38
OCC1OC(Oc2ccccc2C=O)C(C(C1O)O)O	TAS2R43,TAS2R16
OCC1OC(Oc2ccccc2CO)C(C(C1O)O)O	TAS2R16
C=CC1CN2CCC1CC2C(c1cnc2c1cc(OC)cc2)O	TAS2R46,TAS2R44,TAS2R43,TAS2R40,TAS2R4,TAS2R7,TAS2R10,TAS2R39,TAS2R14
CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)CC(C)C)(CC=C(C)C)CC=C(C)C)C	TAS2R1,TAS2R14
)C	
OC(C(=O)c1ccccc1)c1ccccc1	TAS2R10,TAS2R14
CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)CC(C)C)(O)CC=C(C)C)C	TAS2R40,TAS2R1
OCC1OC(Oc2ccccc2)C(C(C1O)O)O	TAS2R16
CN(CCC(c1cccn1)c1ccc(cc1)Cl)C	TAS2R46,TAS2R40,TAS2R4,TAS2R7,TAS2R10,TAS2R39,TAS2R38,TAS2R14
CN(CCOC(c1ccccc1)c1ccccc1)C	TAS2R14
OC(c1ccccc1)(c1ccccc1)CCCN1CCCCC1	TAS2R49,TAS2R46,TAS2R47,TAS2R44,TAS2R43,TAS2R40,TAS2R1,TAS2R4,TAS2R7,TAS2R13,TAS2R10,TAS2R39,TAS2R38,TAS2R14,TAS2R16
S=C(Nc1ccccc1)Nc1ccccc1	TAS2R1,TAS2R38,TAS2R14
C=CS(=O)C=C	TAS2R14
OC(=O)c1ccccc1Nc1cccc(c1)C(F)(F)F	TAS2R14
Fc1ccc(cc1)C(=O)CCCN1CCC(CC1)(O)c1ccc(cc1)Cl	TAS2R10,TAS2R14
[O-]C(=O)c1ccccc1	TAS2R14,TAS2R16
OCCc1sc[n+](c1C)Cc1cnc(nc1N)C	TAS2R1,TAS2R39
OCC(C(c1ccc(cc1)[N+](=O)[O-])O)NC(=O)C(Cl)Cl	TAS2R46,TAS2R43,TAS2R1,TAS2R8,TAS2R10,TAS2R39,TAS2R41
OCC1OC(Oc2ccccc2CO)C(C(C1O)O)O	TAS2R16
CC1CC(C)C(=O)C(C1)C(CC1CC(=O)NC(=O)C1)O	TAS2R10
COc1cc2c(cc1OC)N1C3C42CCN2C4CC4C3C(CC1=O)OCC=C4C2	TAS2R46,TAS2R4
O=C1CC2(C(C1C)C2)C(C)C	TAS2R10,TAS2R14
Nc1ccc(cc1)S(=O)(=O)c1ccc(cc1)N	TAS2R40,TAS2R4,TAS2R10
COc1c(OC)cc2c(c1OC)c1ccc(c(=O)cc1C(CC2)NC(=O)C)OC	TAS2R46,TAS2R4,TAS2R39

c1ccc2c(n1)c1ncccc1cc2	TAS2R5
CC[N+](Cc1ccccc1)(CC(=O)Nc1c(C)cccc1C)CC	TAS2R46,TAS2R47,TAS2R43,TA AS2R4,TAS2R8,TAS2R13,TAS2 R10,TAS2R39
CC(=O)OC(/C=C/C(=O)C(C1C(O)CC2(C1(C)CC(=O)C1(C2CC=C2C1C=C C(O)C(=O)C2(C)C)C)C(O)C)C)C	TAS2R10
OC(COc1ccccc2c1c(=O)cc(o2)C(=O)O)COc1ccc2c(c1)c(=O)cc(o2)C(=O)O	TAS2R49,TAS2R43,TAS2R7
CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccc(cc1)O)O)C	TAS2R14
Cc1cc(O)nc(n1)S	TAS2R38
Oc1cc(O)c2c(c1)O[C@@H]([C@H]([C@@H]2c1c(O)cc(c2c1O[C@H](c1c cc(c(c1)O)O)[C@H]([C@@H]2c1c(O)cc(c2c1O[C@H]([C@H](C2)O)c1 ccc(c(c1)O)O)O)O)c1ccc(c(c1)O)O	TAS2R5
C[C@@H]1C(=O)O[C@H]2[C@H]1CC[C@@]1(C2=C(C)C(=O)C=C1)C	TAS2R10
OC[C@H]1O[C@@H](Oc2cc3c(O)cc(cc3[o+]c2c2cc(OC)c(c(c2)OC)O)O)[C@@H]([C@H]([C@@H]1O)O)O	TAS2R5,TAS2R7
O=C(c1cc(O)c(c(c1)O)O)O[C@@H]1[C@@H](OC(=O)c2cc(O)c(c(c2)O) O)[C@@H](OC([C@@H]1OC(=O)c1cc(O)c(c(c1)O)O)OC(=O)c1cc(O)c(c (c1)O)O)OC(=O)c1cc(O)c(c(c1)O)O	TAS2R39
O=CC1(CC(c2cocc2)O)C(C)C(OC(=O)C)CC2(C1CCC(C2(C)O)O)C	TAS2R46,TAS2R47,TAS2R1,TA S2R10,TAS2R14
O=c1ccc2c(o1)ccccc2	TAS2R10,TAS2R14
Cn1cnc2c1c(=O)n(C)c(=O)n2C	TAS2R46,TAS2R43,TAS2R7,TA S2R10,TAS2R14
O=C1OC(=O)C2(C(C1CC2)(C)C)C	TAS2R47,TAS2R4,TAS2R10,TA S2R14
COc1ccccc2c1cc([N+](=O)[O-])c1c2c2OCOc2cc1C(=O)O	TAS2R44,TAS2R43,TAS2R14
CC1=CC2OC(=O)C(=C)C2CCC(=C)C(CC1)O	TAS2R46,TAS2R47,TAS2R4,TA S2R10,TAS2R14
CC1=CCC23C1C1OC(=O)C(C1CCC3(O2)C)C	TAS2R46,TAS2R43,TAS2R1,TA S2R4,TAS2R10,TAS2R14
CC1=CCC23C1C1OC(=O)C(=C)C1CCC3(O2)C	TAS2R46,TAS2R43,TAS2R10,T AS2R14
CC1C(=O)OC2C1CCC(C1C2=C(C)C2C1C1C3C2(C(=C1)C)C1OC(=O)C(C1CCC3(C)O)C)C)O	TAS2R46,TAS2R47,TAS2R10,T AS2R14
COc1ccc2c(c1)C13CCCCC3C(C2)N(CC1)C	TAS2R1,TAS2R10
COc1cc(O)c(c(c1C(=O)/C=C/c1ccc(cc1)O)O)CC=C(C)C	TAS2R40,TAS2R1,TAS2R14
COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1)O)CC=C(C)C	TAS2R40,TAS2R1,TAS2R14
CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)C(C)C)(CC=C(C)C)CC=C(C)C) C	TAS2R40,TAS2R1
CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)C(C)C)(O)CC=C(C)C)C	TAS2R40,TAS2R1
CCC(C(=O)C1=C(O)C(C(=O)C(C1=O)CC=C(C)C)(O)CC=C(C)C)C	TAS2R46,TAS2R47,TAS2R43,T AS2R1,TAS2R4,TAS2R39,TAS2 R50
OCC1OC(OC2OC=C3C(C2C=C)CCOC3=O)C(C(C1O)O)OC(=O)c1c(O)cc (cc1c1ccccc(c1)O)O	

<chem>COC(=O)C1C(O)CCC2C1CC1N(C2)CCc2c1[nH]c1c2cccc1</chem>	TAS2R46,TAS2R1,TAS2R4,TAS2R10,TAS2R38
<chem>CC(CC(=O)C1=C(O)C(C(C1=O)CC=C(C)C)(O)C(=O)CC=C(C)C)C</chem>	TAS2R1,TAS2R14
<chem>Oc1cc(O)c2c(c1)O[C@@H]([C@@H](C2)OC(=O)c1cc(O)c(c(c1)O)O)c1c</chem>	TAS2R39
<chem>c(O)c(c(c1)O)O</chem>	
<chem>Oc1ccc(cc1)[C@H]1COc2c(C1)ccc(c2)O</chem>	TAS2R39,TAS2R14
<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O</chem>	TAS2R39,TAS2R14

Table S5. Negative bitterant-TAS2R pairs used in the TAS2R recognition model.

Molecule	Target
<chem>CC1=CC(O)C2C(CC(=C)C(CC1)O)OC(=O)C2=C</chem>	TAS2R43, TAS2R47, TAS2R9
<chem>CN(CCOC(c1ccccc1C)c1ccccc1)C</chem>	TAS2R48, TAS2R8, TAS2R60
<chem>OCC1OC(OCC2OC(O)C(C(C2O)O)O)C(C(C1O)O)O</chem>	TAS2R1
<chem>Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@@H](Cc2c(c1)O)O</chem>	TAS2R4
<chem>Oc1cc2O[C@H](c3cc(O)c(c(c3)O)O)[C@@H](Cc2c(c1)O)O</chem>	TAS2R47
<chem>Oc1cc(O)c2c(c1)O[C@@H]([C@@H](C2)OC(=O)c1cc(O)c(c(c1)O)O)c1</chem>	TAS2R1, TAS2R16, TAS2R4
<chem>ccc(c(c1)O)O</chem>	
<chem>OC[C@H]1O[C@@H](Oc2cc(O)c3c(c2)occ(c3=O)c2ccc(cc2)O)[C@@H]</chem>	TAS2R43
<chem>][C@H]([C@@H]1O)O)O</chem>	
<chem>CCN(CCCC(Nc1ccnc2c1ccc(c2)Cl)C)CC</chem>	TAS2R60, TAS2R5, TAS2R49
<chem>CN1CCN(CC1)c1c(F)cc2c3c1OCC(n3cc(c2=O)C(=O)O)C</chem>	TAS2R42, TAS2R46
<chem>CCN(CCN(C=O)c1ccc(cc1)N)CC</chem>	TAS2R13, TAS2R43, TAS2R46
<chem>CN1CCN(CC1)CC(=O)N1C2CCCCC2C(=O)NC2C1NCCCC2</chem>	TAS2R8, TAS2R43, TAS2R10
<chem>CCCc1cc(=O)[nH]c(=S)[nH]1</chem>	TAS2R60, TAS2R50, TAS2R16
<chem>CC(=O)Nc1ccc(cc1)O</chem>	TAS2R9, TAS2R7, TAS2R16
<chem>CC1=CC(=NS(=O)(=O)O1)[O-]</chem>	TAS2R39, TAS2R40
<chem>OCc1cc(O)c2c(c1)C(C1OC(CO)C(C(C1O)O)O)c1c(C2=O)c(O)ccc1</chem>	TAS2R1, TAS2R3
<chem>CC1C(=O)CC2C1C1OC(=O)C(=C)C1C(CC2=C)O</chem>	TAS2R44, TAS2R47, TAS2R9
<chem>O=C1NS(=O)(=O)c2c1ccccc2</chem>	TAS2R10, TAS2R5, TAS2R45
<chem>OCC1(C)C(O)CCC2(C1CCC(=C)C2C/C=C/1\C(O)COC1=O)C</chem>	TAS2R9, TAS2R14
<chem>OCC1=CC2OC(=O)C(=C)C2C(CC(=CCC1)C)OC(=O)C(=C)C(CO)O</chem>	TAS2R40, TAS2R50, TAS2R14
<chem>OOCC1CCC2(CC1=CCC1C(C2O)OC(=O)C1=C)C</chem>	TAS2R45, TAS2R10, TAS2R43
<chem>OCC(=O)C1(O)CCC2C1(C)CC(O)C1C2CCC2=CC(=O)CCC12C</chem>	TAS2R42, TAS2R38
<chem>N/C(=N\CCCCC/N=C/N=C/Nc1ccc(cc1)Cl)\N)\N)/N=C/Nc1ccc(cc1)</chem>	TAS2R42, TAS2R5, TAS2R44
<chem>Cl)\N</chem>	
<chem>CCCC(COC(=O)N)(COC(=O)NC(C)C)C</chem>	TAS2R3, TAS2R38
<chem>COC1=CC(C)C2C(C1=O)(C)C1C(=O)C=C(C3C1(C(C2)OC(=O)C3)C)C</chem>	TAS2R5, TAS2R50
<chem>)OC</chem>	
<chem>CC1=CCCC2(C)OC2C2C(CC1)C(=C)C(=O)O2</chem>	TAS2R7, TAS2R50
<chem>NC(=O)c1ccccc1</chem>	TAS2R38, TAS2R44
<chem>Cn1nc(c1Sc1ncnc2c1[nH]cn2)[N+](=O)[O-]</chem>	TAS2R7, TAS2R38
<chem>CCCCCCC/C=C/C(C#CC#CC(C=C)O)O</chem>	TAS2R9, TAS2R42
<chem>CC(=O)OC/C=C/C(=O)C(C1C(O)CC2(C1(C)CC(=O)C1(C2CC=C2)C1C</chem>	TAS2R45, TAS2R43, TAS2R42

<chem>C(O)C(=O)C2(C)C)C(O)C(C)C</chem>	
<chem>COc1ccc(cc1OC)Cc1nccc2c1cc(OC)c(c2)OC</chem>	TAS2R46
<chem>COc1ccc2c(c1OC)C(=O)OC2C1N(C)CCc2c1c(OC)c1c(c2)OCO1</chem>	TAS2R50, TAS2R42
<chem>Oc1ccc2c(c1)oc(=O)c1c2oc2c1ccc(c2)O</chem>	TAS2R7, TAS2R40
<chem>S=C1NCCN1C</chem>	TAS2R5, TAS2R60, TAS2R39
<chem>O=C1OCC23C(C1)OC(C2CC(=O)C1(C3CCC2(C31OC3C(=O)OC2c1coc</chem>	TAS2R1, TAS2R14
<chem>c1)C)C(C)C</chem>	
<chem>CNC(=S)N</chem>	TAS2R60, TAS2R44, TAS2R14
<chem>Cc1cc(O)nc(n1)S</chem>	TAS2R5, TAS2R13
<chem>CCc1cnccn1</chem>	TAS2R3, TAS2R10
<chem>S=CN(C)C</chem>	TAS2R40, TAS2R1
<chem>S=C1NCCN1</chem>	TAS2R48, TAS2R1
<chem>CCNC(=S)N</chem>	TAS2R16, TAS2R8
<chem>CC(=CCC(=O)C1(O)C(=C(C(=O)C1CC=C(C)C)C(=O)C(C)C)O)C</chem>	TAS2R16, TAS2R47, TAS2R10
<chem>CC(=CCC(=O)C1(O)C(=C(C(=O)C1CC=C(C)C)C(=O)C(C)C)O)C</chem>	TAS2R4, TAS2R40
<chem>CCC(C(=O)C1=C(O)C(C(=O)C(=C1O)CC=C(C)C)(CC=C(C)C)CC=C(C</chem>	TAS2R16, TAS2R60
<chem>)C)C</chem>	
<chem>NC(=S)Nc1cccc1</chem>	TAS2R16, TAS2R14, TAS2R13
<chem>S=C=NCCc1cccc1</chem>	TAS2R13, TAS2R60, TAS2R39
<chem>CCC(C(=O)C1=C(O)C(C(C1=O)CC=C(C)C)(O)C(=O)CC=C(C)C)C</chem>	TAS2R45, TAS2R44, TAS2R39
<chem>CCC(C(=O)C1=C(O)C(C(C1=O)CC=C(C)C)(O)C(=O)CC=C(C)C)C</chem>	TAS2R9, TAS2R47
<chem>CC(=O)NC(=S)N</chem>	TAS2R1, TAS2R50
<chem>O=C1CCCCCN1</chem>	TAS2R5, TAS2R48, TAS2R60
<chem>OCC1OC(OCC2OC(OC(c3ccccc3)C#N)C(C(C2O)O)O)C(C(C1O)O)O</chem>	TAS2R40
<chem>OCC1OC(Oc2ccc(cc2)O)C(C(C1O)O)O</chem>	TAS2R38, TAS2R7
<chem>O=C1CC2OCC=C3C4C2C2N1c1cccc1C12CCN(C1C4)C3</chem>	TAS2R9
<chem>NC(=Nc1sc(n1)CSCC/C(=N/S(=O))(=O)N)/N)N</chem>	TAS2R7, TAS2R16
<chem>C=CC/C(=N)OS(=O)(=O)[O-]/SC1OC(CO)C(C(C1O)O)O</chem>	TAS2R44, TAS2R3, TAS2R10
<chem>C=CCN=C=S</chem>	TAS2R48, TAS2R44
<chem>OCC1OC(Oc2ccccc2C=O)C(C(C1O)O)O</chem>	TAS2R40
<chem>OCC1OC(Oc2ccccc2CO)C(C(C1O)O)O</chem>	TAS2R38, TAS2R39
<chem>C=CC1CN2CCC1CC2C(c1cnc2c1cc(OC)cc2)O</chem>	TAS2R50
<chem>CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)CC(C)C)(CC=C(C)C)CC=C(C</chem>	TAS2R46
<chem>)C)C</chem>	
<chem>OC(C(=O)c1cccc1)c1cccc1</chem>	TAS2R48, TAS2R8, TAS2R38
<chem>CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)CC(C)C)(O)CC=C(C)C)C</chem>	TAS2R4, TAS2R48
<chem>OCC1OC(Oc2ccccc2)C(C(C1O)O)O</chem>	TAS2R50, TAS2R47, TAS2R13
<chem>CN(CCC(c1ccccc1)c1ccc(cc1)Cl)C</chem>	TAS2R48, TAS2R3, TAS2R49
<chem>CN(CCOC(c1ccccc1)c1cccc1)C</chem>	TAS2R1, TAS2R42, TAS2R9
<chem>OC(c1ccccc1)(c1cccc1)CCCN1CCCC1</chem>	TAS2R3
<chem>S=C(Nc1cccc1)Nc1cccc1</chem>	TAS2R44, TAS2R49, TAS2R45
<chem>C=CS(=O)C=C</chem>	TAS2R42
<chem>OC(=O)c1cccc1Nc1cccc(c1)C(F)(F)F</chem>	TAS2R42, TAS2R7, TAS2R39
<chem>Fc1ccc(cc1)C(=O)CCCN1CCC(CC1)(O)c1ccc(cc1)Cl</chem>	TAS2R60, TAS2R39

[O-]C(=O)c1ccccc1	TAS2R43, TAS2R8, TAS2R42
OCCc1sc[n+](c1C)Cc1cnc(nc1N)C	TAS2R8, TAS2R49
OCC(C(c1ccc(cc1)[N+](=O)[O-])O)NC(=O)C(Cl)Cl	TAS2R40, TAS2R14, TAS2R5
O=C(c1cc(O)c(c(c1)O)O)O[C@@H]1[C@@H](OC(=O)c2cc(O)c(c(c2)O)O)[C@@H](OC([C@@H]1OC(=O)c1cc(O)c(c(c1)O)O)OC(=O)c1cc(O)c(c(c1)O)O)OC(=O)c1cc(O)c(c(c1)O)O	TAS2R4, TAS2R49, TAS2R46
CCC1CN2CCc3c(C2CC1CC1NCCc2c1cc(OC)c(c2)OC)cc(c(c3)OC)OC	TAS2R13
OCC1OC(Oc2ccccc2CO)C(C(C1O)O)O	TAS2R45, TAS2R7, TAS2R47
CC1CC(C)C(=O)C(C1)C(CC1CC(=O)NC(=O)C1)O	TAS2R9, TAS2R43, TAS2R46
COc1cc2c(cc1OC)N1C3C42CCN2C4CC4C3C(CC1=O)OCC=C4C2	TAS2R43, TAS2R8, TAS2R47
O=C1CC2(C(C1C)C2)C(C)C	TAS2R4, TAS2R48, TAS2R38
Nc1ccc(cc1)S(=O)(=O)c1ccc(cc1)N	TAS2R46, TAS2R47, TAS2R14
O=C1OC2C(C1C)(O)C13C4(C2)C(OC3=O)CC(C24C(O1)OC(=O)C2O)C(C)(C)C	TAS2R8, TAS2R16, TAS2R9
c1ccc2c(n1)c1cccc1cc2	TAS2R14, TAS2R38, TAS2R45
CC[N+](Cc1ccccc1)(CC(=O)Nc1c(C)cccc1C)CC	TAS2R49, TAS2R48, TAS2R1
CC(=O)OC(/C=C/C(=O)C(C1C(O)CC2(C1(C)CC(=O)C1(C2CC=C2C1C=C(O)C(=O)C2(C)C)C)(O)C)(C)C	TAS2R50, TAS2R45, TAS2R46
OC(COc1cccc2c1c(=O)cc(o2)C(=O)O)COc1ccc2c(c1)c(=O)cc(o2)C(=O)O	TAS2R3, TAS2R40
CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccc(cc1)O)O)C	TAS2R43, TAS2R10
CC(=C)C1C2OC(=O)C1C1(C3(C2OC(=O)C23C(C1)O2)C)O	TAS2R13, TAS2R49, TAS2R48
Oc1cc(O)c2c(c1)O[C@@H]([C@H]([C@@H]2c1c(O)cc(c2c1O[C@H](c1ccc(c(c1)O)O)[C@H]([C@@H]2c1c(O)cc(c2c1O[C@H]([C@H](C2)O)c1ccc(c(c1)O)O)O)O)c1ccc(c(c1)O)O	TAS2R45, TAS2R14
C[C@@H]1C(=O)O[C@H]2[C@H]1CC[C@@]1(C2=C(C)C(=O)C=C1)C	TAS2R16, TAS2R5, TAS2R47
C/C1=C\C[C@H]2OC(=O)C(=C)[C@@H]2CC/C(=C/CC1)/C	TAS2R60, TAS2R8, TAS2R1
Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@H](Cc2c(c1)O)O	TAS2R39
OC[C@H]1O[C@@H](Oc2cc3c(O)cc(cc3[o+]c2c2cc(OC)c(c(c2)OC)O)O)[C@@H]([C@H]([C@@H]1O)O)O	TAS2R13, TAS2R4, TAS2R49
NCCS(=O)(=O)O	TAS2R43, TAS2R4, TAS2R39
O=CC1(CC(c2cocc2)O)C(C)C(OC(=O)C)CC2(C1CCC(C2(C)O)O)C	TAS2R50, TAS2R4
O=c1ccc2c(o1)cccc2	TAS2R38, TAS2R39
Cn1cnc2c1c(=O)n(C)c(=O)n2C	TAS2R3, TAS2R13, TAS2R44
[O-]S(=O)(=O)NC1CCCCC1	TAS2R45, TAS2R14, TAS2R7
COc1cccc2c1cc([N+](=O)[O-])c1c2c2OCOc2cc1C(=O)O	TAS2R49, TAS2R13
CC1=CC2OC(=O)C(=C)C2CCC(=C)C(CC1)O	TAS2R40, TAS2R45, TAS2R44
CC1=CCC23C1C1OC(=O)C(C1CCC3(O2)C)C	TAS2R50, TAS2R8
CC1=CCC23C1C1OC(=O)C(=C)C1CCC3(O2)C	TAS2R48, TAS2R3, TAS2R8
CC1C(=O)OC2C1CCC(C1C2=C(C)C2C1C1C3C2(C(=C1)C)C1OC(=O)C(C1CCC3(C)O)C)(C)O	TAS2R5, TAS2R1, TAS2R39
COc1ccc2c(c1)C13CCCCC3C(C2)N(CC1)C	TAS2R14
COc1cc(O)c(c(c1C(=O)/C=C/c1ccc(cc1)O)O)CC=C(C)C	TAS2R9, TAS2R49, TAS2R42

<chem>COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1)O)CC=C(C)C</chem>	TAS2R3
<chem>CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)C(C)C)(CC=C(C)C)CC=C(C)C</chem>	TAS2R5
<chem>C)C</chem>	
<chem>CC(=CCC1=C(O)C(C(=O)C(=C1O)C(=O)C(C)C)(O)CC=C(C)C)C</chem>	TAS2R38
<chem>CCC(C(=O)C1=C(O)C(C(=O)C(C1=O)CC=C(C)C)(O)CC=C(C)C)C</chem>	TAS2R13, TAS2R10
<chem>OCC1OC(OC2OC=C3C(C2C=C)CCOC3=O)C(C(C1O)O)OC(=O)c1c(O)</chem>	TAS2R16, TAS2R10
<chem>cc(cc1c1cccc(c1)O)O</chem>	
<chem>COC(=O)C1C(O)CCC2C1CC1N(C2)CCc2c1[nH]c1c2cccc1</chem>	TAS2R3
<chem>CC(CC(=O)C1=C(O)C(C(C1=O)CC=C(C)C)(O)C(=O)CC=C(C)C)C</chem>	TAS2R4, TAS2R7
<chem>CC(=O)c1cncn1</chem>	TAS2R47
<chem>O=C1OC(=O)C2(C(C1CC2)(C)C)C</chem>	TAS2R46
<chem>Oc1ccc(cc1)[C@H]1COc2c(C1)ccc(c2)O</chem>	TAS2R7, TAS2R40, TAS2R44
<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O</chem>	TAS2R60, TAS2R4, TAS2R49

Table S6. The in-house library composed of 220 chemical probes in the SMILES format.

Num.	Fragments
1	<chem>ON1C(C)(C)CC(CC1(C)C)N=C=S</chem>
2	<chem>FC1(F)C(F)(F)OS1(=O)=O</chem>
3	<chem>c1(noc(c1)c1ccc(cc1)Br)C(=O)O</chem>
4	<chem>N#CCc1c(C)c(C)c(c(c1C)C)C</chem>
5	<chem>O/N=C(\Cc1cccc1)/C</chem>
6	<chem>C[Si]1(C)N[Si](C)(C)N[Si](N1)(C)C</chem>
7	<chem>C[Si](P([Si](C)(C)C)[Si](C)(C)C)(C)C</chem>
8	<chem>N#CCCS1sc(=O)sc1SCCC#N</chem>
9	<chem>c1(csc(n1)C)C(=O)OCC</chem>
10	<chem>FS(=O)(=O)C(F)(F)F</chem>
11	<chem>Sc1nc(=O)n2c(n1)ccc(c2)Cl</chem>
12	<chem>C12(CC(=O)N(C(=O)C1)CCC)CCCC2</chem>
13	<chem>N#CC1=CC[C@@]23[C@@]1(CCC2)C(=CC3)C#N</chem>
14	<chem>FCCN1CCN(CC1)C(=O)Cl</chem>
15	<chem>O[C@H]1C[C@@H](C)[C@H]2[C@H](C=C1)C)CC(=C(C)C)C2</chem>
16	<chem>Nc1nc(N)nc(n1)N</chem>
17	<chem>CN([Si](N(C)C)(N(C)C)C)C</chem>
18	<chem>[C@]12([C@@H](O1)C[C@@H](CC2)C(=C)C)C</chem>
19	<chem>N(CCCCCC)(CCCCC)N=O</chem>
20	<chem>C(=O)(N1CCN(CC1)CC=C)CC(=O)NN</chem>
21	<chem>Fc1ccc2c3c1ccc1c3c(cc2)ccc1</chem>
22	<chem>CCCN1CCC(=O)CC1</chem>
23	<chem>c12c([nH]nc1O)cc(cc2Cl)I</chem>
24	<chem>FC(C1=[NH]S(=O)(=O)NC(=C1)C)(F)F</chem>
25	<chem>Fc1ccc(c2c1cn[nH]2)I</chem>
26	<chem>c1nc(=O)c(c[nH]1)Br</chem>

27 COc1ccc(cc1)c1ncc[nH]1
28 C[SiH](C(C)(C)C)C(C)(C)C
29 COCCN1CCN(CC1)CC[N]#C
30 c1(c(c(cc(c1)/C=C\C(=O)O)OC)OC)S(=O)(=O)Nc1ccc(cc1)C(=O)O
31 c12c([nH]c(c1)C(=O)OC)cccc2
32 c1(cc(cc(c1)C(C)C)C(C)C)C(C)C
33 O[C@H]1CCC(=C1)I
34 C1(=O)[C@H]2[C@@H](C1)C=CC2
35 CCN1CCOCC1
36 CCOP(OP(OCC)OCC)OCC
37 c1(n2cccc2)ccc(en1)I
38 FC(=C(C(F)(F)F)Br)F
39 CC([NH2]NC(C)(C)C)(C)C
40 COP(=O)(SCc1nc(N)nc(n1)N)OC
41 COCCOCOCCOC
42 C12([C@@H](O1)C(=O)OC)CCCCC2
43 CN(/C=N/c1cc[nH]c(=O)n1)C
44 COC1CSC1
45 Cl[C@H]1CC[C@@H]2[C@@H](C1)NON2O
46 Fc1ccc(c2c1cn[nH]2)Br
47 BrC[C@@H]1CC[C@H](O1)c1ccncc1
48 O=CCC(C(C(F)(F)F)(F)F)(F)F
49 n12c(=NCC1)ssc2=S
50 Brc1n[nH]cn1
51 CC(SSC(C)(C)C)(C)C
52 CC1CCN(CC1)CCCS(=O)(=O)O
53 o1nc2c(n1)nc1c(n2)[nH]c2c([nH]1)c1nsnc1cc2
54 C12=CNCCC[C@@H]1C=C(C=C2)OC
55 C\1=C/C=N\[C@H]2C[C@@H]2N/C=C/C=N\[C@@H]2[C@@H](N1)C2
56 COP(=O)OC
57 N#Cc1ncn2c1nmn(c2=O)C
58 O=S1(=O)CC=CC1
59 c1(/C=C\2/C(=C(C=N2)C)C)c(c(c[nH]1)C)C
60 CSc1scc(c1)/C=N/NC(=O)N
61 O=CN1CCN(CC1)C=O
62 Cc1cc(C)nc(n1)Nc1ccc(cc1)OC(F)(F)F
63 ICC(C(F)F)(F)F
64 C[C@H]1CCCC[C@H]1N[C@H]1CCS(=O)(=O)C1
65 C1CCCC(CC1)NC1CCOCC1
66 c1(mnc1)SCC(=O)N
67 OCCCCCCCCCCCCO
68 C1=CC=CC=c2c(=C1)nc1cccc1n2
69 NCCOCCN
70 c1(c(ccn(c1=O)C)OC)C#N

71 S(Cc1nnn[nH]1)Cc1nnn[nH]1
72 CN1CCN(CC1)C(=O)NC(C)(C)C
73 CN1CCN(CC1)C(=O)N
74 FC(C(Cl)(Cl)Cl)(C(Cl)(F)F)F
75 OC(=O)Cn1nc2c(n1)cccc2
76 ClC(=O)CCC[Si](Cl)(Cl)C
77 c1(c2ccc(cc2)OC)ccc(cc1)OC
78 Br1ccc(cc1)c1cccc(c1)Cl
79 CO[Si](OC)(OC)OC
80 BrCc1onc(c1)Br
81 c1(c2cncn2)ccn1
82 NN1C(=S)S[C@H]2[C@@H]1CS(=O)(=O)C2
83 Nc1ccc2=c3c(=c2c1)cccc3
84 N#Cc1c(N)onc1c1ccc(cc1)Br
85 O=Nc1c(N)nc(nc1N)N
86 Cn1c(COc2cccc2)mmc1S
87 N#CCSSCCC#N
88 CCCCCCC[C@H]1CO1
89 c1(c2cccc2)nc2c(s1)cccc2
90 CCSc1nccc(c1C#N)c1ccc(cc1)Cl
91 C=CS(=O)(=O)O
92 O=C1CNc2c(N1)cnc(n2)N
93 NC[C@@H]1N[C@H](CCl)CN([C@H]1N)O
94 N[C@]12C[C@H]3C[C@@H](C2)C[C@@H](C1)C3
95 c1(C(=O)NC2CC2)cn(nc1)CCC(=O)O
96 OC(C#CC(C)(C)C)C#CC(C)(C)C
97 C(C(=C/C=N/C(C)(C)C)C[Si](C)(C)C)[Si](C)(C)C
98 Fe1ccc2c(c1)c(=O)n1c(n2)CCCC1
99 C1CC(C1)CNC[C@H]1CCCO1
100 ClCCNC(=O)N(CCCl)CCCl
101 O=Cc1cccc1OC
102 Clc1ncc(nc1)OC
103 n1(c2ccc(cc2)C)c(ccc1)C=O
104 ClC[C@@H]1CN(O)[C@H]([C@@H](N1)C#N)N
105 CCCn1ccc(n1)C=O
106 c12c3c([nH]c1C(=O)CCC2)cccc3
107 Nc1ccc(c(c1)Cl)Oc1cc(C)cc(c1)C
108 c1(c(n[nH]c(=O)n1)C)N/N=C/c1cccc1
109 c12n(c(nc1cccc2)CC)CC(=O)O
110 NCCc1c(C)nn(c1N1CCOCC1)C
111 COCCN(CCCl)CCCl
112 COS(=O)(=O)OC
113 n1ccc2[nH]cc(c2c1)Br
114 BrN1C(=O)CCC1=O

115 c1(/C(=C/C=O)/Cl)cccc(cc1)F
116 OCc1[nH]c2c(n1)cc1c(c2)[nH]cn1
117 N[C@H]1CCN(CC1)C(=O)c1cccc1
118 C[Si]1(C)CCC1
119 c1(n(nnn1)CCCC)NCc1cccc1
120 O=C=NC[C@@H]1CCC[C@H](C1)CN=C=O
121 c1(C(=O)CSc2[nH]c(nn2)N)cccc1
122 c1ccc(cc1)c1nc2c([nH]1)cccc2
123 NN1C(=O)CCC1=O
124 C(#CC=O)[Si](C)(C)C
125 c1ccc2c(c1)c1cccc1c1c2cccc1
126 N#CC1=CC[C@]2([C@]1(CC)CC=C2C#N)C
127 CC(=O)Nc1nc2c(s1)ccc(c2)Br
128 N#CC(=C(C#N)C#N)C#N
129 Sc1[nH]c(=O)c2c(n1)n(nc2)c1cccc1
130 C1CCCC(CC1)NC1CCOCC1
131 c1(c2ccc(cc2)OC)nc(ncc1)N
132 Br1ccc(s1)CCc1c[nH]cn1
133 CCSc1nc(N)cc(=O)[nH]1
134 n1(c(cc(cc1=O)C)C)N
135 N[C@@H]1CONC1=O
136 c12c([nH]c(=S)nc1)CC[C@H](C2)N
137 N/N=c/1\sc2c([nH]1)c(Cl)cc(c2)Br
138 c12c(nc([nH]1)CCN)cccc2
139 OS(=O)(=O)c1ccccn1
140 [Si](CC)(F)(F)F
141 Sc1nnc(n1N)S
142 c1([C@@H](CN2CCN(CC2)C)N)cccc1
143 CCCCn1ccnc1CNCCOC
144 [C@@]12(c3c([C@H](C1(C)C)CC2)nnc(n3)S)C
145 Cc1cc(Nc2cccc2)c2c(n1)c1cccc1cc2
146 OS(=O)(=O)CCS(=O)(=O)O
147 NC(=N)N/N=C/1\C=CC(=O)C=C1
148 C1(=C(N[C@H](N1)C=C)C)C(=O)C
149 BrC1=CCCS1(=O)=O
150 C[C@]1(CSC(=O)S1)/C=N/O
151 FC(c1cc(Cl)c(cc1Cl)C(F)(F)F)(F)F
152 ClC(=O)CCc1c(F)c(F)c(c(c1F)F)F
153 ClC(=O)N1CCCCC1
154 CCCCOP(=O)(OCCCC)OCCCC
155 Fe1ccc(c(c1)F)Oc1ccc(c(c1)C(F)(F)F)N
156 Br1csc(c1)Cl
157 CC(C#C[Si](C)(C)C)(C)C
158 N1[C@@H](O)CCCC1

159 Clc1cc(nc(n1)C(F)(F)F)N1CCOCC1
160 C1(C([C@@H]2[C@@H]3[C@H]1[C@@H]1[C@H]2[C@@H]1C3)(C#N)C#N)(C#N)C#N
161 c1(ccc(cc1)C(=O)O)c1nc(no1)C
162 c12c(ccc(c1)C(F)(F)F)[nH]c(n2)C
163 ClCc1ccn1
164 ON1C[C@@H](C)[C@H]([C@@H](C1)C)[N](=O)O
165 N=C(Nc1ccccc1)NC(=N)N
166 C1CN=C(N1)CC2=CC=CC=C2
167 C=C/C=C/C(C(F)(F)F)(C(F)(F)F)C(F)(F)F
168 ClCCn1nnc2n(c1=O)cnc2C(=O)N
169 OC[C@H]1CN1[C@@H](c1ccccc1)C
170 O=Cc1c2=Nc3c(c2cc2=c4c(=Nc12)cccc4)cccc3
171 NCCCCC(=O)O
172 CCCCC/C=C/CCCCCCCC(=O)Cl
173 c1ccc(cc1)[C@@H]1NN=C(C1)c1ccccc1
174 CN(S(=O)(=O)N(C)C)C
175 COc1nc(nc(n1)N)NC(C)(C)C
176 C12(C(=O)OC[C@H](N1)CC)CCCC2
177 CSC[C@@H]1CO1
178 Cc1cc(Br)c(=O)[nH]n1
179 P(=O)(OCCCC)(OCCCC)CCCC
180 NCc1nnc(o1)C1CCCC1
181 CN(S(=O)(=O)N1CCNCC1)C
182 [C@@H]1([C@H]([C@H](C=C[C@@H]1O)O)O)O
183 c12c3c(ccc1oc(n2)C)n3
184 CC(CC([NH3])(C)C)([NH3])C
185 c12c(sc(c1C)C=O)sc2C
186 OC(=O)Cn1nnc(n1)N1CCOCC1
187 O=CN(CCC#N)CCC#N
188 CO[Si](Cl)(C)C
189 CCOc1ccc(cc1Cl)F
190 c12c3c([nH]c1nc(c2)C(=O)OC)cccc3
191 c1(c(cc(cc1)Br)Br)OCC#N
192 c1(c(n[nH]c1N)C)Cl
193 FC(C(C(C([C@]1(F)OC1(F)F)(F)F)(F)F)(F)F)F
194 n1(c2nc(cc(n2)C)C)nc(cc1C)C
195 C=CCSc1nc2cc(C)ccn2c(=O)n1
196 OC(=O)c1c(C)cc(cc1C)C(C)(C)C
197 c12c(C(=O)c3c(C1=O)cccc3)ccc(c2)C
198 CN(C(=O)N(C)C)C
199 Sc1nn2c(s1)nnc(c2=O)C(C)(C)C
200 c1(c2cc(c(cc2)Cl)Cl)cc(c(cc1)Cl)Cl
201 [C@H]12[C@H](C(=O)OC1=O)CC=CC2

202 ClC(P(Cl)(Cl)(Cl)Cl)(Cl)Cl
203 c1ccc2c(c1)c1c3c2cccc3cc2c1cccc2
204 c1esc(c1)c1cccs1
205 O=C(CN1CCNCC1)NC1CC1
206 c1(c2n(c(=O)cc1O)cccc2)C(=O)OC
207 Clc1ncc(nc1)Cl
208 CCC(NC(CC)(C)C)(C)C
209 CCCN1CCC(CC1)NC[C@H]1CCCO1
210 S(=O)(=O)(c1ccc(N2CCNCC2)cc1)N
211 CCCCCCCCCCCCCCP(=O)(O)O
212 S=C=Nc1ccc(cc1C)C(C)(C)C
213 ClP1OCCO1
214 CSCC[C@H]1NCCNC1=O
215 n1(c(=S)[nH]nc1)N1CCCCC1
216 Sc1nn2c(s1)nnc(c2=O)C
217 C1CCc2c(C1)c1CCCc3c1c1e2CCCc1cc3
218 C1=CC=C(C(=C1)C(=O)N)O
219 N(=C=NC(C)(C)C)C(C)(C)C
220 Cc1ccc(cc1)OCc1nnc(s1)N

2 FIGURES

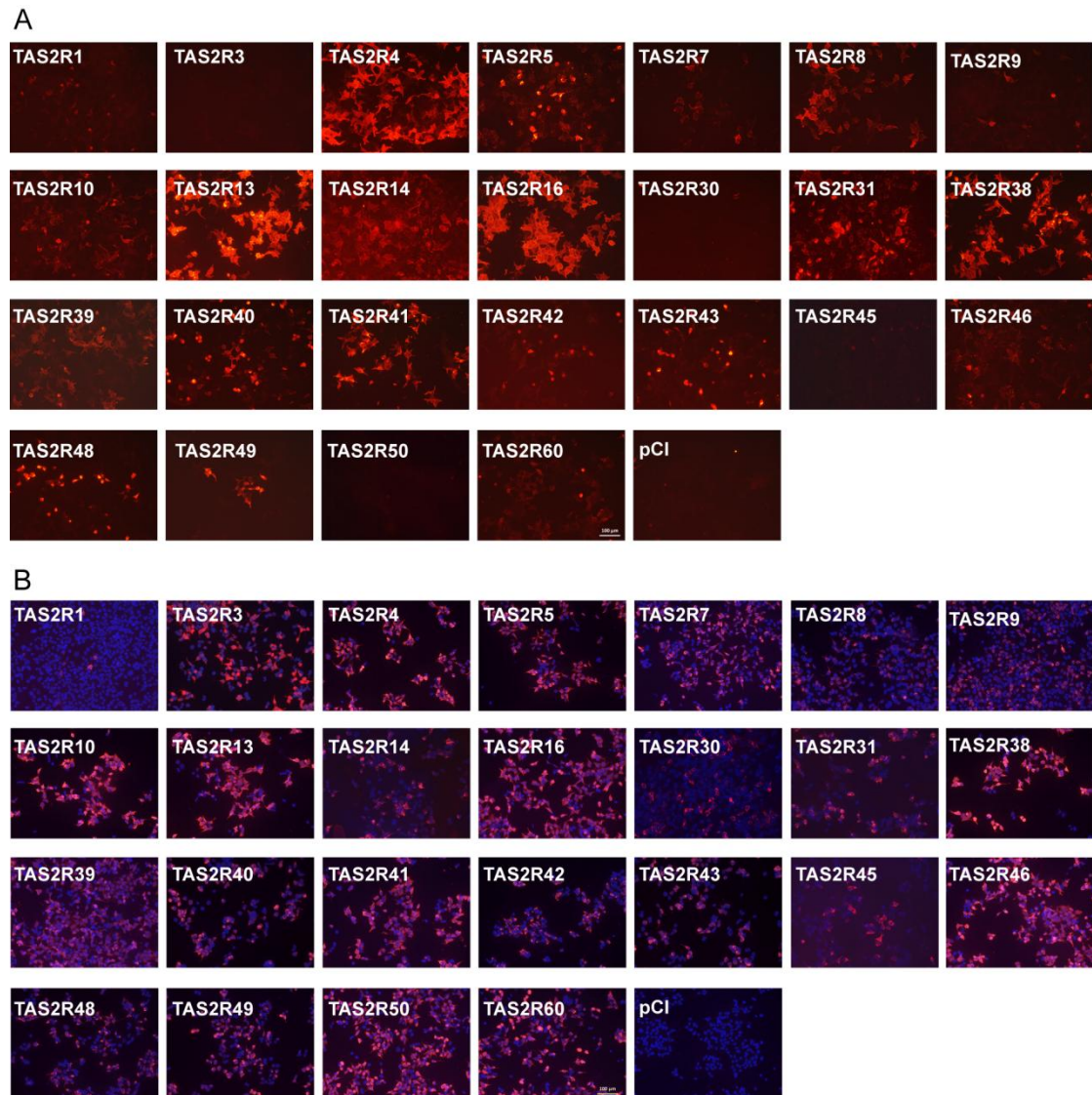


Figure S1. The (A) cell-surface expression and (B) total expression of all TAS2R constructs when transfected into HEK293T cells. For optimal expression, RTP3 were co-transfected with TAS2R7, TAS2R8, TAS2R9, TAS2R40, TAS2R43, and TAS2R49, and RTP4 were co-transfected with TAS2R3, TAS2R42, TAS2R48, and TAS2R60. (Scale bar = 100 μ m).

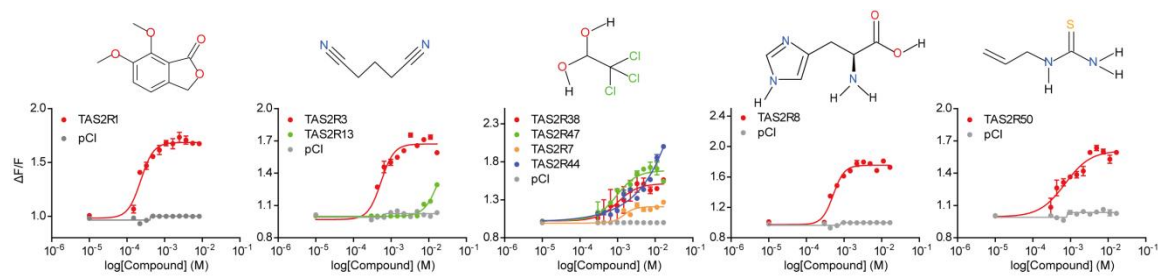


Figure S2. The positive-control dose-response curves of 9 TAS2Rs that tested negative in our system (Ji et al. 2015). y-axis represents $\Delta F/F \pm \text{SEM}$ ($N = 2$). “pCI” denotes the response of mock-transfected cells to each compound. The structures of the compounds tested are shown above each graph.