

TIN-a combinatorial compound collection of synthetically feasible multicomponent synthesis products.

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Supplementary Material - Dorschner, KV *et al.*, 2011

Table S1: MOE Descriptors calculated for each TIN molecule.

<u>Descriptor Code</u>	<u>Type of Descriptor</u>	<u>Description</u>
E	Internal energy	Value of the potential energy
weight	Physical properties	Molecular weight including implicit hydrogens
logP(o/w)	Physical properties	Log of the octanol/water partition coefficient including implicit hydrogens
lip_acc	Atom count and Bond count	The number of O and N atoms
lip_don	Atom count and Bond count	The number of OH and NH atoms
lip_violation	Atom count and Bond count	The number of violations of Lipinski's 'Rule of Five'.
lip_druglike	Atom count and Bond count	Displays 1 if violations of lip_violation < 2; otherwise 0
FCharge	Physical properties	Total sum of formal charges of molecule
a_acc	Pharmacophore atom type (descriptor considers only the heavy atoms of a molecule and may take into account implied protonation, deprotonation, keto/enol considerations and tautomerism at a biologically relevant pH)	Number of hydrogen bond acceptor atoms not including acidic atoms
a_don	Pharmacophore atom type	Number of hydrogen bond donor atoms not including basic atoms
a_acid	Pharmacophore atom type	Number of acidic atoms
a_base	Pharmacophore atom type	Number of basic atoms.
a_hyd	Pharmacophore atom type	Number of hydrophobic atoms.
chiral	Atom count and Bond count	Number of chiral centers
chiral_u	Atom count and Bond count	Number of unconstrained chiral centers
rings	Atom count and Bond count	Number of rings
logS	Physical properties	Log of the aqueous solubility
opr_brigid	Atom count and Bond count	The number of rigid bonds.
opr_leadlike	Atom count and Bond count	Displays 1 if violations of opr_violation < 2; otherwise 0
opr_nring	Atom count and Bond count	Number of rings bonds.
opr_violation	Atom count and Bond count	Number of violations of Oprea's lead-like criteria.

<u>Descriptor Code</u>	<u>Type of Descriptor</u>	<u>Description</u>
reactive	Physical properties	Indicator of the presence of reactive groups. Value > 0 indicates molecule contains a reactive group
a_aro	Atom count and Bond count	Number of aromatic atoms
a_count	Atom count and Bond count	Number of atoms including implicit hydrogens
a_heavy	Atom count and Bond count	Number of heavy atoms
a_ICM	Atom information content	Entropy of the element distribution in the molecule including implicit hydrogens (but not lone pair pseudo-atoms)
a_IC	Atom information content	Total atom information content = (a_ICM) x (n)
a_nH	Atom count and Bond count	Number of hydrogen atoms including implicit hydrogens
a_nB	Atom count and Bond count	Number of boron atoms
a_nC	Atom count and Bond count	Number of carbon atoms:
a_nN	Atom count and Bond count	Number of nitrogen atoms
a_nO	Atom count and Bond count	Number of oxygen atoms:
a_nF	Atom count and Bond count	Number of fluorine atoms:
a_nP	Atom count and Bond count	Number of phosphorus atoms
a_nS	Atom count and Bond count	Number of sulfur atoms
a_nCl	Atom count and Bond count	Number of chlorine atoms
a_nBr	Atom count and Bond count	Number of bromine atoms
a_nI	Atom count and Bond count	Number of iodine atoms
b_1rotR	Atom count and Bond count	Number of rotatable single bond not including conjugated single bonds
b_1rotN	Atom count and Bond count	Fraction of rotatable single bonds = b_1rotN divided by b_heavy.
b_ar	Atom count and Bond count	Number of aromatic bonds
b_count	Atom count and Bond count	Number of bonds including implicit hydrogens
b_double	Atom count and Bond count	Number of double bonds (not including aromatic bonds)

Table S2: Structural Fingerprints calculated for TIN and ZINC subsets.

Bit Position	Description	SMARTS pattern	ZINC clustered at 60% tanimoto similarity	Diversity subset of TIN	Fingerprint in ZINC	Fingerprint in TIN
0	Primary carbon	[CX4H3][#6]	3769	10911	1	1
1	Secondary carbon	[CX4H2]([#6])[#6]	3547	10845	1	1
2	Tertiary carbon	[CX4H1]([#6])([#6])[#6]	961	10450	1	1
3	Quaternary carbon	[CX4]([#6])([#6])([#6])[#6]	290	3075	1	1
4	Alkene	[CX3;\$([H2]),\$([H1][#6]),\$(C([#6])[#6])]=[CX3;\$([H2]),\$([H1][#6]),\$(C([#6])[#6])]	1680	3393	1	1
5	Alkyne	[CX2]#[CX2]	118	1139	1	1
6	Allene	[CX3]=[CX2]=[CX3]	13	0	1	
7	Alkylchloride	[CIX1][CX4]	126	746	1	1
8	Alkylfluoride	[FX1][CX4]	137	5100	1	1
9	Alkylbromide	[BrX1][CX4]	28	655	1	1
10	Alkyliodide	[IX1][CX4]	2	111	1	1
11	Alcohol	[OX2H][CX4;!\$(C([OX2H])[O,S,#7,#15])]	384	1600	1	1
12	Primary alcohol	[OX2H][CX4H2;!\$(C([OX2H])[O,S,#7,#15])]	206	814	1	1
13	Secondary alcohol	[OX2H][CX4H;!\$(C([OX2H])[O,S,#7,#15])]	219	593	1	1
14	Tertiary alcohol	[OX2H][CX4D4;!\$(C([OX2H])[O,S,#7,#15])]	44	353	1	1
15	Dialkylether	[OX2]([CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])][CX4;!\$(C([OX2])[O,S,#7,#15])]	343	636	1	1
16	Dialkylthioether	[SX2]([CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])][CX4;!\$(C([OX2])[O,S,#7,#15])]	288	114	1	1
17	Alkylarylether	[OX2](c)[CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])]	320	3817	1	1
18	Diarylether	[c][OX2][c]	47	608	1	1
19	Alkylarylthioether	[SX2](c)[CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])]	263	569	1	1
20	Diarylthioether	[c][SX2][c]	85	9	1	1
21	Oxonium	[O+;!\$(O~[!#6]);!\$(S~[#7,#8,#15,#16])]	1	0	1	
22	Amine	[NX3+0,NX4+;!\$(N~[!#6]);!\$(N~[#7,#8,#15,#16])]	184	1395	1	1
23	Primary aliph amine	[NX3H2+0,NX4H3+;!\$(N[!C]);!\$(N~[#7,#8,#15,#16])]	0	0		
24	Secondary aliph amine	[NX3H1+0,NX4H2+;!\$(N[!C]);!\$(N~[#7,#8,#15,#16])]	0	0		
25	Tertiary aliph amine	[NX3H0+0,NX4H1+;!\$(N[!C]);!\$(N~[#7,#8,#15,#16])]	123	169	1	1
26	Quaternary aliph ammonium	[NX4H0+;!\$(N[!C]);!\$(N~[#7,#8,#15,#16])]	14	12	1	1
27	Primary arom amine	[NX3H2+0,NX4H3+]c	496	465	1	1
28	Secondary arom amine	[NX3H1+0,NX4H2+;!\$(N[!c]);!\$(N~[#7,#8,#15,#16])]	0	0		
29	Tertiary arom amine	[NX3H0+0,NX4H1+;!\$(N[!c]);!\$(N~[#7,#8,#15,#16])]	0	0		
30	Quaternary arom ammonium	[NX4H0+;!\$(N[!c]);!\$(N~[#7,#8,#15,#16])]	0	0		

Bit Position	Description	SMARTS pattern	ZINC clustered at 60% tanimoto similarity	Diversity subset of TIN	Fingerprint in ZINC	Fingerprint in TIN
31	Secondary mixed amine	[NX3H1+0,NX4H2+;\$([N]([c])([C]);!\$([N]*~[#7,#8,#15,#16]))]	137	78	1	1
32	Tertiary mixed amine	[NX3H0+0,NX4H1+;\$([N]([c])([C])([6]);!\$([N]*~[#7,#8,#15,#16]))]	46	1215	1	1
33	Quaternary mixed ammonium	[NX4H0+;\$([N]([c])([C])([6])([6]);!\$([N]*~[#7,#8,#15,#16]))]	1	0	1	
34	Ammonium	[N+;!\$([N]~[!#6]);!\$([N]=*);!\$([N]*~[#7,#8,#15,#16]))]	16	12	1	1
35	Alkylthiol	[SX2H][CX4;!\$(C([SX2H])~[O,S,#7,#15])]	9	138	1	1
36	Dialkylthioether	[SX2]([CX4;!\$(C([SX2])(O,S,#7,#15,F,Cl,Br,I))][CX4;!\$(C([SX2])(O,S,#7,#15))])]	180	114	1	1
37	Alkylarylthioether	[SX2](c)[CX4;!\$(C([SX2])(O,S,#7,#15))]	238	569	1	1
38	Disulfide	[SX2D2][SX2D2]	95	57	1	1
39	1,2-Aminoalcohol	[OX2H][CX4;!\$(C([OX2H])(O,S,#7,#15,F,Cl,Br,I))][CX4;!\$(C([N])(O,S,#7,#15))][NX3;!\$(NC=[O,S,N])]	31	0	1	
40	1,2-Diol	[OX2H][CX4;!\$(C([OX2H])(O,S,#7,#15))][CX4;!\$(C([OX2H])(O,S,#7,#15))][OX2H]	71	161	1	1
41	1,1-Diol	[OX2H][CX4;!\$(C([OX2H])([OX2H])(O,S,#7,#15))][OX2H]	1	16	1	1
42	Hydroperoxide	[OX2H][OX2]	0	0		
43	Peroxo	[OX2D2][OX2D2]	24	1565	1	1
44	Organolithium compounds	[LiX1][#6,#14]	0	0		
45	Organomagnesium compounds	[MgX2][#6,#14]	0	0		
46	Organometallic compounds	[!#1;!#5;!#6;!#7;!#8;!#9;!#14;!#15;!#16;!#17;!#33;!#34;!#35;!#52;!#53;!#85]~[#6;-]	0	0		
47	Aldehyde	[\$([CX3H][#6]),\$(CX3H2)]=[OX1]	77	187	1	1
48	Ketone	[#6][CX3](=[OX1])[#6]	1081	2836	1	1
49	Thioaldehyde	[\$([CX3H][#6]),\$(CX3H2)]=[SX1]	2	0	1	
50	Thioketone	[#6][CX3](=[SX1])[#6]	11	0	1	
51	Imine	[NX2;\$([N][#6]),\$([NH]);!\$([N][CX3]=[#7,#8,#15,#16])]=[CX3;\$([CH2]),\$([CH][#6]),\$(C([#6])([#6]))]	550	0	1	
52	Immonium	[NX3+;!\$([N][!#6]);!\$([N][CX3]=[#7,#8,#15,#16]))]	127	0	1	
53	Oxime	[NX2](=[CX3;\$([CH2]),\$([CH][#6]),\$(C([#6])([#6]))][OX2H]	45	0	1	
54	Oximether	[NX2](=[CX3;\$([CH2]),\$([CH][#6]),\$(C([#6])([#6]))][OX2][#6;!\$(C=[#7,#8])]	58	0	1	
55	Acetal	[OX2]([#6;!\$(C=[O,S,N])][CX4;!\$(C(O)(O)[!#6]))][OX2][#6;!\$(C=[O,S,N])]	44	14	1	1
56	Hemiacetal	[OX2H][CX4;!\$(C(O)(O)[!#6]))][OX2][#6;!\$(C=[O,S,N])]	8	0	1	
57	Aminal	[NX3v3;!\$(NC=[#7,#8,#15,#16])][[#6]][CX4;!\$(C(N)(N)[!#6])][NX3v3;!\$(NC=[#7,#8,#15,#16])][[#6]]	3	0	1	

Bit Position	Description	SMARTS pattern	ZINC clustered at 60% tanimoto similarity	Diversity subset of TIN	Fingerprint in ZINC	Fingerprint in TIN
58	Hemiaminal	[NX3v3;!\$(NC=[#7,#8,#15,#16]))([#6])[CX4;!\$(C(N)(N)![#6])][OX2H]	26	0	1	
59	Thioacetal	[SX2]([#6;!\$(C=[O,S,N]))][CX4;!\$(C(S)(S)![#6])][SX2][#6;!\$(C=[O,S,N])]	4	0	1	
60	Thiohemiacetal	[SX2]([#6;!\$(C=[O,S,N]))][CX4;!\$(C(S)(S)![#6])][OX2H]	5	0	1	
61	Halogen acetal like	[NX3v3,SX2,OX2;!\$(C=[#7,#8,#15,#16]))][CX4;!\$(C([N,S,O])([N,S,O])![#6])][FX1,CIX1,BrX1,IX1]	22	255	1	1
62	Acetal like	[NX3v3,SX2,OX2;!\$(C=[#7,#8,#15,#16]))][CX4;!\$(C([N,S,O])([N,S,O])![#6])][FX1,CIX1,BrX1,IX1,NX3v3,SX2,OX2;!\$(C=[#7,#8,#15,#16])]	146	285	1	1
63	Halogenmethylen ester and similar	[NX3v3,SX2,OX2;\$(*=[#7,#8,#15,#16]))][CX4;!\$(C([N,S,O])([N,S,O])![#6])][FX1,CIX1,BrX1,IX1]	3	0	1	
64	NOS methylen ester and similar	[NX3v3,SX2,OX2;\$(*=[#7,#8,#15,#16]))][CX4;!\$(C([N,S,O])([N,S,O])![#6])][NX3v3,SX2,OX2;!\$(C=[#7,#8,#15,#16])]	91	0	1	
65	Hetero methylen ester and similar	[NX3v3,SX2,OX2;\$(*=[#7,#8,#15,#16]))][CX4;!\$(C([N,S,O])([N,S,O])![#6])][FX1,CIX1,BrX1,IX1,NX3v3,SX2,OX2;!\$(C=[#7,#8,#15,#16])]	94	0	1	
66	Cyanhydrine	[NX1][CX2][CX4;\$([CH2]),\$([CH]([CX2])[#6]),\$(C([CX2])([#6])[#6])][OX2H]	0	0		
67	Chloroalkene	[CIX1][CX3]=[CX3]	96	351	1	1
68	Fluoroalkene	[FX1][CX3]=[CX3]	32	13	1	1
69	Bromoalkene	[BrX1][CX3]=[CX3]	14	278	1	1
70	Iodoalkene	[IX1][CX3]=[CX3]	1	0	1	
71	Enol	[OX2H][CX3;\$([H1]),\$(C[#6])]=[CX3]	110	26	1	1
72	Endiol	[OX2H][CX3;\$([H1]),\$(C[#6])]=[CX3;\$([H1]),\$(C[#6])][OX2H]	8	0	1	
73	Enolether	[OX2]([#6;!\$(C=[N,O,S]))][CX3;\$([H0][#6]),\$([H1])]=[CX3]	290	73	1	1
74	Enolester	[OX2]([CX3]=[OX1])[#6X3;\$([#6][#6]),\$([H1])]=[#6X3;!\$(C[OX2H])]	156	2	1	1
75	Enamine	[NX3;\$([NH2][CX3]),\$([NH1]([CX3])[#6]),\$([N]([CX3])([#6])[#6]);!\$(N*=[#7,#8,#15,#16]))][CX3;\$([CH]),\$(C[#6])]=[CX3]	389	0	1	
76	Thioenol	[SX2H][CX3;\$([H1]),\$(C[#6])]=[CX3]	1	0	1	
77	Thioenolether	[SX2]([#6;!\$(C=[N,O,S]))][CX3;\$([C#H])]=[CX3]	191	26	1	1
78	Acylchloride	[CX3;\$([R0][#6]),\$([H1R0])]=[OX1][CIX1]	1	0	1	
79	Acylfluoride	[CX3;\$([R0][#6]),\$([H1R0])]=[OX1][FX1]	0	0		
80	Acylbromide	[CX3;\$([R0][#6]),\$([H1R0])]=[OX1][BrX1]	0	0		
81	Acyliodide	[CX3;\$([R0][#6]),\$([H1R0])]=[OX1][IX1]	0	0		
82	Acylhalide	[CX3;\$([R0][#6]),\$([H1R0])]=[OX1][FX1,CIX1,BrX1,IX1]	1	0	1	

Bit Position	Description	SMARTS pattern	ZINC clustered at 60% tanimoto similarity	Diversity subset of TIN	Fingerprint in ZINC	Fingerprint in TIN
83	Carboxylic acid	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])\$([OX2H]),\$([OX1-])]	401	396	1	1
84	Carboxylic ester	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])[OX2][#6;!\$(C=[O,N,S])]	460	613	1	1
85	Lactone	[#6][#6X3R](=[OX1])[#8X2][#6;!\$(C=[O,N,S])]	303	0	1	
86	Carboxylic anhydride	[CX3;\$([H0][#6]),\$([H1]))(=[OX1])[#8X2][CX3;\$([H0][#6]),\$([H1]))(=[OX1])]	2	0	1	
87	Carboxylic acid derivative	[\$([#6X3H0][#6]),\$([#6X3H])](=[#6])[!#6]	6344	8906	1	1
88	Carbothioic acid	[CX3;!R;\$([C][#6]),\$([CH]);\$([C](=[OX1])\$([SX2H]),\$([SX1-]))),\$([C](=[SX1])\$([OX2H]),\$([OX1-]))]	0	0		
89	Carbothioic S ester	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])[SX2][#6;!\$(C=[O,N,S])]	14	0	1	
90	Carbothioic S lactone	[#6][#6X3R](=[OX1])[#16X2][#6;!\$(C=[O,N,S])]	33	0	1	
91	Carbothioic O ester	[CX3;\$([H0][#6]),\$([H1]))(=[SX1])[OX2][#6;!\$(C=[O,N,S])]	0	0		
92	Carbothioic O lactone	[#6][#6X3R](=[SX1])[#8X2][#6;!\$(C=[O,N,S])]	0	0		
93	Carbothioic halide	[CX3;\$([H0][#6]),\$([H1]))(=[SX1])[FX1,CIX1,BrX1,IX1]	0	0		
94	Carbodithioic acid	[CX3;!R;\$([C][#6]),\$([CH]);\$([C](=[SX1])\$([SX2H]))]	1	0	1	
95	Carbodithioic ester	[CX3;!R;\$([C][#6]),\$([CH]);\$([C](=[SX1])\$([SX2][#6;!\$(C=[O,N,S])]))]	1731	963	1	1
96	Carbodithiolactone	[#6][#6X3R](=[SX1])[#16X2][#6;!\$(C=[O,N,S])]	8	0	1	
97	Amide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]]]	0	0		
98	Primary amide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])[NX3H2]	118	0	1	
99	Secondary amide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])[#7X3H1][#6;!\$(C=[O,N,S])]	167	487	1	1
100	Tertiary amide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1])[#7X3H0][#6;!\$(C=[O,N,S])][#6;!\$(C=[O,N,S])]	63	171	1	1
101	Lactam	[#6R][#6X3R](=[OX1])[#7X3;\$([H1][#6;!\$(C=[O,N,S])]),\$([H0])([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]]]	0	0		
102	Alkyl imide	[#6X3;\$([H0][#6]),\$([H1]))(=[OX1])[#7X3H0][#6][#6X3;\$([H0][#6]),\$([H1]))(=[OX1])]	24	0	1	
103	N hetero imide	[#6X3;\$([H0][#6]),\$([H1]))(=[OX1])[#7X3H0][!#6][#6X3;\$([H0][#6]),\$([H1]))(=[OX1])]	10	0	1	
104	Imide acidic	[#6X3;\$([H0][#6]),\$([H1]))(=[OX1])[#7X3H1][#6X3;\$([H0][#6]),\$([H1]))(=[OX1])]	22	0	1	
105	Thioamide	[\$([CX3;!R][#6]),\$([CX3H;!R]))(=[SX1])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]]]	0	0		

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106	Thiolactam	[#6R][#6X3R](=[SX1])[#7X3;\$([H1][#6!\$(C=[O,N,S])])\$([H0][#6!\$(C=[O,N,S])])][#6!\$(C=[O,N,S])])]	0	0		
107	Oximester	[#6X3;\$([H0][#6]),\$([H1]))(=[OX1])[#8X2][#7X2]=,.[#6X3;\$([H0][#6])[#6]),\$([H1][#6]),\$([H2])]	15	0	1	
108	Amidine	[NX3!\$(NC=[O,S])[CX3;\$([CH]),\$([C][#6])]=[NX2!\$(NC=[O,S])]	377	5	1	1
109	Hydroxamic acid	[CX3;\$([H0][#6]),\$([H1]))(=[OX1])[#7X3;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])][([OX2H]),\$([OX1-])]	0	0		
110	Hydroxamic acid ester	[CX3;\$([H0][#6]),\$([H1]))(=[OX1])[#7X3;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])][OX2][#6!\$(C=[O,N,S])]	0	0		
111	Imidoacid	[CX3R0;\$([H0][#6]),\$([H1]))(=[NX2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])\$([OX2H]),\$([OX1-])]	0	0		
112	Imidoacid cyclic	[#6R][#6X3R](=,.[#7X2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])\$([OX2H]),\$([OX1-])]	0	0		
113	Imidoester	[CX3R0;\$([H0][#6]),\$([H1]))(=[NX2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])][OX2][#6!\$(C=[O,N,S])]	0	0		
114	Imidolactone	[#6R][#6X3R](=,.[#7X2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])][OX2][#6!\$(C=[O,N,S])]	0	0		
115	Imidothioacid	[CX3R0;\$([H0][#6]),\$([H1]))(=[NX2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])\$([SX2H]),\$([SX1-])]	0	0		
116	Imidothioacid cyclic	[#6R][#6X3R](=,.[#7X2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])\$([SX2H]),\$([SX1-])]	0	0		
117	Imidothioester	[CX3R0;\$([H0][#6]),\$([H1]))(=[NX2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])][SX2][#6!\$(C=[O,N,S])]	0	0		
118	Imidothiolactone	[#6R][#6X3R](=,.[#7X2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])][SX2][#6!\$(C=[O,N,S])]	0	0		
119	Amidine	[#7X3v3!\$(N([#6X3]=[#7X2])C=[O,S])[CX3R0;\$([H1]),\$([H0][#6])]=[NX2v3!\$(N([#6X3]=[#7X3])C=[O,S])]	24	0	1	
120	Imidolactam	[#6][#6X3R;\$([H0])(=[NX2!\$(N([#6X3][#7X3])C=[O,S])])][#7X3!\$(N([#6X3]=[#7X2])C=[O,S])])\$([H0])(-[NX3!\$(N([#6X3]=[#7X2])C=[O,S])])=,.[#7X2!\$(N([#6X3][#7X3])C=[O,S])])]	0	0		
121	Imidoylhalide	[CX3R0;\$([H0][#6]),\$([H1]))(=[NX2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])][FX1,CIX1,BrX1,IX1]	0	0		
122	Imidoylhalide cyclic	[#6R][#6X3R](=,.[#7X2;\$([H1]),\$([H0][#6!\$(C=[O,N,S])])])][FX1,CIX1,BrX1,IX1]	0	0		
123	Amidrazone	[\$([#6X3][#6]),\$([#6X3H]))(=[#7X2v3])[#7X3v3][#7X3v3],[\$([#6X3][#6]),\$([#6X3H]))([#7X3v3])=[#7X2v3][#7X3v3]	0	0		
124	Alpha aminoacid	[NX3,NX4+!\$([N]-[#6])!\$([N]*-[#7,#8,#15,#16])][C][CX3](=[OX1])[OX2H,OX1-]	2	0	1	

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125	Alpha hydroxyacid	[OX2H][C][CX3](=[OX1])[OX2H,OX1-]	2	2	1	1
126	Peptide middle	[NX3;\$([N][CX3](=[OX1])[C][NX3,NX4+))][C][CX3](=[OX1])[NX3;\$([N][C][CX3](=[OX1])[NX3,OX2,OX1-])]	23	0	1	
127	Peptide C term	[NX3;\$([N][CX3](=[OX1])[C][NX3,NX4+))][C][CX3](=[OX1])[OX2H,OX1-]	3	0	1	
128	Peptide N term	[NX3,NX4+;!\$([N]~[!#6]);!\$([N]*~[!#7,#8,#15,#16])][C][CX3](=[OX1])[NX3;\$([N][C][CX3](=[OX1])[NX3,OX2,OX1-])]	0	0		
129	Carboxylic orthoester	[#6][OX2][CX4;\$([C#6]),\$([CH])][OX2][#6][OX2][#6]	4	0	1	
130	Ketene	[CX3]=[CX2]=[OX1]	1	0	1	
131	Ketenacetal	[#7X2,#8X3,#16X2;\$(*[!#6,#14])][#6X3]([#7X2,#8X3,#16X2;\$(*[!#6,#14]))=[#6X3]	186	0	1	
132	Nitrile	[NX1][CX2]	678	0	1	
133	Isonitrile	[CX1-][NX2+]	1	0	1	
134	Vinylogous carbonyl or carboxyl derivative	[#6X3](=[OX1])[#6X3]=.:[#6X3][#7,#8,#16,F,Cl,Br,I]	1472	1580	1	1
135	Vinylogous acid	[#6X3](=[OX1])[#6X3]=.:[#6X3]([OX2H]),\$([OX1-])]	187	150	1	1
136	Vinylogous ester	[#6X3](=[OX1])[#6X3]=.:[#6X3][#6;!\$(C=[O,N,S])]	2005	3602	1	1
137	Vinylogous amide	[#6X3](=[OX1])[#6X3]=.:[#6X3][#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([!#6;!\$(C=[O,N,S])]))][#6;!\$(C=[O,N,S])]	0	0		
138	Vinylogous halide	[#6X3](=[OX1])[#6X3]=.:[#6X3][FX1,CIX1,BrX1,IX1]	37	297	1	1
139	Carbonic acid diester	[#6;!\$(C=[O,N,S])][#8X2][#6X3](=[OX1])[#8X2][#6;!\$(C=[O,N,S])]	14	0	1	
140	Carbonic acid esterhalide	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[OX1])[OX2][FX1,CIX1,BrX1,IX1]	0	0		
141	Carbonic acid monoester	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[OX1])\$([OX2H]),\$([OX1-])]	0	0		
142	Carbonic acid derivatives	[!#6][#6X3](=[!#6])[!#6]	3590	2174	1	1
143	Thiocarbonic acid diester	[#6;!\$(C=[O,N,S])][#8X2][#6X3](=[SX1])[#8X2][#6;!\$(C=[O,N,S])]	0	0		
144	Thiocarbonic acid esterhalide	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[SX1])[OX2][FX1,CIX1,BrX1,IX1]	0	0		
145	Thiocarbonic acid monoester	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[SX1])\$([OX2H]),\$([OX1-])]	0	0		
146	Urea	[#7X3;!\$([#7][!#6])][#6X3](=[OX1])[#7X3;!\$([#7][!#6])]	41	0	1	
147	Thiourea	[#7X3;!\$([#7][!#6])][#6X3](=[SX1])[#7X3;!\$([#7][!#6])]	6	0	1	

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148	Isourea	[#7X2;!\$([#7]!#6))=,:[#6X3]([#8X2&!\$([#8]!#6)),OX1-)[#7X3;!\$([#7]!#6)]	27	0	1	
149	Isothiourea	[#7X2;!\$([#7]!#6))=,:[#6X3]([#16X2&!\$([#16]!#6)),SX1-)[#7X3;!\$([#7]!#6)]	73	0	1	
150	Guanidine	[N;v3X3,v4X4+][CX3](=[N;v3X2,v4X3+])[N;v3X3,v4X4+]	262	4	1	1
151	Carbaminic acid	[NX3]C(=[OX1])[O;X2H,X1-]	1	0	1	
152	Urethan	[#7X3][#6](=[OX1])[#8X2][#6]	187	9	1	1
153	Biuret	[#7X3][#6](=[OX1])[#7X3][#6](=[OX1])[#7X3]	12	0	1	
154	Semicarbazide	[#7X3][#7X3][#6X3]([#7X3;!\$([#7]!#6))=([OX1])	60	0	1	
155	Carbazide	[#7X3][#7X3][#6X3]([#7X3][#7X3])=([OX1])	3	0	1	
156	Semicarbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3;!\$([#7]!#6))=([OX1])	46	0	1	
157	Carbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3][#7X3])=([OX1])	4	0	1	
158	Thiosemicarbazide	[#7X3][#7X3][#6X3]([#7X3;!\$([#7]!#6))=([SX1])	21	0	1	
159	Thiocarbazide	[#7X3][#7X3][#6X3]([#7X3][#7X3])=([SX1])	4	0	1	
160	Thiosemicarbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3;!\$([#7]!#6))=([SX1])	36	0	1	
161	Thiocarbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3][#7X3])=([SX1])	5	0	1	
162	Isocyanate	[NX2]=[CX2]=[OX1]	4	0	1	
163	Cyanate	[OX2][CX2]#[NX1]	0	0		
164	Isothiocyanate	[NX2]=[CX2]=[SX1]	13	0	1	
165	Thiocyanate	[SX2][CX2]#[NX1]	8	0	1	
166	Carbodiimide	[NX2]=[CX2]=[NX2]	3	0	1	
167	Orthocarbonic derivatives	[CX4H0]([O,S,#7])([O,S,#7])([O,S,#7])([O,S,#7,F,Cl,Br,I])	3	0	1	
168	Phenol	[OX2H][c]	156	3233	1	1
169	1,2-Diphenol	[OX2H][c][c][OX2H]	7	387	1	1
170	Arylchloride	[Cl][c]	203	1469	1	1
171	Arylfluoride	[F][c]	93	672	1	1
172	Arylbromide	[Br][c]	13	1021	1	1
173	Aryliodide	[I][c]	3	458	1	1
174	Arylthiol	[SX2H][c]	5	49	1	1
175	Iminoarene	[c]=[NX2;\$([H1]),\$([H0][#6;!\$([C]=[N,S,O])))]	0	0		
176	Oxoarene	[c]=[OX1]	0	0		
177	Thioarene	[c]=[SX1]	0	0		
178	Hetero N basic H	[nX3H1+0]	732	2449	1	1
179	Hetero N basic no H	[nX3H0+0]	1510	5830	1	1
180	Hetero N nonbasic	[nX2,nX3+]	3644	10984	1	1
181	Hetero O	[o]	1145	5696	1	1
182	Hetero S	[sX2]	1058	0	1	
183	Heteroaromatic	[a;!c]	4507	10984	1	1

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184	Nitrite	[NX2](=[OX1])[O;\$([X2]),\$(X1-)]	0	0		
185	Thionitrite	[SX2][NX2]=[OX1]	0	0		
186	Nitrate	[\$([NX3](=[OX1])(=[OX1])[O;\$([X2]),\$(X1-)])),\$(NX3+)([OX1-])(=[OX1])[O;\$([X2]),\$(X1-)]))]	0	0		
187	Nitro	[\$([NX3](=O)=O),\$(NX3+)(=O)[O-])[!#8]	353	4706	1	1
188	Nitroso	[NX2](=[OX1])[!#7;!#8]	69	0	1	
189	Azide	[NX1]~[NX2]~[NX2,NX1]	16	0	1	
190	Acylazide	[CX3](=[OX1])[NX2]~[NX2]~[NX1]	0	0		
191	Diazo	[\$([#6]=[NX2+]=[NX1-]),\$(#6-)[NX2+]#(NX1)]	22	0	1	
192	Diazonium	[#6][NX2+]#(NX1)	3	0	1	
193	Nitrosamine	[#7;!\$(N*=O)][NX2]=[OX1]	0	0		
194	Nitrosamide	[NX2](=[OX1])N*=O	1	0	1	
195	N-Oxide	[\$([#7+][OX1-]),\$(#7v5=[OX1]);!\$(#7)(-[O])~[O]);!\$(#7)=[#7]]	71	0	1	
196	Hydrazine	[NX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6];!\$(NC=[O,N,S])[NX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6];!\$(NC=[O,N,S])]	100	77	1	1
197	Hydrazone	[NX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6];!\$(NC=[O,N,S])[NX2]=[#6]	255	0	1	
198	Hydroxylamine	[NX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6];!\$(NC=[O,N,S])[OX2;\$([H1]),\$(O[#6];!(C=[N,O,S])))]	0	0		
199	Sulfon	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$(SX4+2)([OX1-])([OX1-])([#6])[#6])]	169	0	1	
200	Sulfoxide	[\$([SX3](=[OX1])([#6])[#6]),\$(SX3+)([OX1-])([#6])[#6])]	27	0	1	
201	Sulfonium	[S+;!\$(S)~[!#6]);!\$(S)*~[#7,#8,#15,#16]]	8	0	1	
202	Sulfuric acid	[SX4](=[OX1])(=[OX1])([O2H]),\$(OX1-))][\$(OX2H),\$(OX1-)]	0	5		1
203	Sulfuric monoester	[SX4](=[OX1])(=[OX1])([O2H]),\$(OX1-))][OX2][#6;!\$(C=[O,N,S])]	3	0	1	
204	Sulfuric diester	[SX4](=[OX1])(=[OX1])(OX2)[#6;!\$(C=[O,N,S])][OX2][#6;!\$(C=[O,N,S])]	0	0		
205	Sulfuric monoamide	[SX4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$(H1)[#6;!\$(C=[O,N,S])]),\$(#7)([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])[\$(OX2H),\$(OX1-)]	0	0		
206	Sulfuric diamide	[SX4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$(H1)[#6;!\$(C=[O,N,S])]),\$(#7)([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),\$(H1)[#6;!\$(C=[O,N,S])]),\$(#7)([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]	0	0		
207	Sulfuric esteramide	[SX4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])][OX2][#6;!\$(C=[O,N,S])]	2	0	1	
208	Sulfuric derivative	[SX4D4](=[!#6])(=[!#6])([!#6])[!#6]	77	5	1	1

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244	Phosphoric monoesterdiamide	[PX4D4](=[OX1])([OX2][#6!\$(C=[O,N,S])])([#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])])[#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])])]	0	0		
245	Phosphoric acid derivative	[PX4D4](=[#6])([!#6])([!#6])[!#6]	89	2	1	1
246	Phosphinic acid	[PX4;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])(=[OX1])[\$([OX2H]),\$(OX1-)]	28	0	1	
247	Phosphinic ester	[PX4;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])(=[OX1])[OX2][#6!\$(C=[O,N,S])]	15	0	1	
248	Phosphinic amide	[PX4;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])(=[OX1])[#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])]	0	0		
249	Phosphinic acid derivative	[PX4;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])(=[!#6])[!#6]	67	0	1	
250	Phosphonous acid	[PX3;\$([H1]),\$(H0)[#6])([OX2H]),\$(OX1-)]\$([OX2H]),\$(OX1-)]	0	0		
251	Phosphonous monoester	[PX3;\$([H1]),\$(H0)[#6])([OX2H]),\$(OX1-)]\$([OX2][#6!\$(C=[O,N,S])])	0	0		
252	Phosphonous diester	[PX3;\$([H1]),\$(H0)[#6])([OX2][#6!\$(C=[O,N,S])])\$([OX2][#6!\$(C=[O,N,S])])	1	0	1	
253	Phosphonous monoamide	[PX3;\$([H1]),\$(H0)[#6])([OX2H]),\$(OX1-)]\$([#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])]	0	0		
254	Phosphonous diamide	[PX3;\$([H1]),\$(H0)[#6])([#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])])\$([#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])]	0	0		
255	Phosphonous esteramide	[PX3;\$([H1]),\$(H0)[#6])([OX2][#6!\$(C=[O,N,S])])\$([#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])]	0	0		
256	Phosphonous derivatives	[PX3;\$([D2]),\$(D3)[#6])([!#6])[!#6]	6	0	1	
257	Phosphinous acid	[PX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])\$([OX2H]),\$(OX1-)]	0	0		
258	Phosphinous ester	[PX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])[OX2][#6!\$(C=[O,N,S])]	0	0		
259	Phosphinous amide	[PX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])[#7X3;\$([H2]),\$(H1)[#6!\$(C=[O,N,S])]),\$([#7]([#6!\$(C=[O,N,S])])[#6!\$(C=[O,N,S])])]	0	0		
260	Phosphinous derivatives	[PX3;\$([H2]),\$(H1)[#6]),\$(H0)([#6])[#6])[!#6]	5	0	1	
261	Quart silane	[SiX4]([#6])([#6])([#6])[#6]	0	0		
262	Non-quart silane	[SiX4;\$([H1])([#6])([#6])[#6]),\$(H2)([#6])[#6]),\$(H3)[#6]),\$(H4)]	0	0		

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290	Mixed anhydrides	[\$(*=O),\$(#16,#14,#5)],\$(#7)([6]=[OX1]))[#8X2][\$(*=O),\$(#16,#14,#5)],\$(#7)([6]=[OX1]))]	24	0	1	
291	Halogen on hetero	[FX1,ClX1,BrX1,IX1][!#6]	11	430	1	1
292	Halogen multi subst	[F,Cl,Br,I;!\$(X1);!\$(X0-)]	1	12	1	1
293	Trifluoromethyl	[FX1][CX4;!\$(H0)[Cl,Br,I];!\$(F)[C]([F])(F)[F])([FX1])([FX1])]	86	4897	1	1
294	C ONS bond	[#6]~[#7,#8,#16]	10000	11000	1	1
295	Charged	[!+0]	3340	9950	1	1
296	Anion	[-1,-2,-3,-4,-5,-6,-7]	1890	4729	1	1
297	Kation	[+1,+2,+3,+4,+5,+6,+7]	2299	9942	1	1
298	Salt	([-1,-2,-3,-4,-5,-6,-7]).([+1,+2,+3,+4,+5,+6,+7])	1890	4729	1	1
299	1,3-Tautomerizable	[\$([#7X2,OX1,SX1]=*!H0;!\$(a;!n))],[\$([#7X3,OX2,SX2;!H0]*=*)],[\$([#7X3,OX2,SX2;!H0]*:n))]	9627	10999	1	1
300	1,5-Tautomerizable	[\$([#7X2,OX1,SX1]=:*~,*!H0;!\$(a;!n))],[\$([#7X3,OX2,SX2;!H0]*==*)],[\$([#7X3,OX2,SX2;!H0]*=:*~:n))]	9627	10999	1	1
301	Rotatable bond	[!\$(*)&!D1]-!@[!\$(*)&!D1]	7396	11000	1	1
302	Michael acceptor	[CX3]=[CX3][\$(CX3=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-])]	2489	642	1	1
303	Dicarbodiazene	[CX3](=[OX1])[NX2]=[NX2][CX3](=[OX1])	7	0	1	
304	CH-acidic	[\$([CX4;!\$(H0)];!\$(C[!#6;!\$(P,S)=O];!\$(N(~O)~O)))]([\$(CX3=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(S,O,N;H1,H2);!\$(+0)[S,O:X1-]))],[\$([CX4;!\$(H0)])1[CX3]=[CX3][CX3]=[CX3]1)]	0	0		
305	CH-acidic strong	[CX4;!\$(H0)];!\$(C[!#6;!\$(P,S)=O];!\$(N(~O)~O)))]([\$(CX3=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(S,O,N;H1,H2);!\$(+0)[S,O:X1-])))]([\$(CX3=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(S,O,N;H1,H2);!\$(+0)[S,O:X1-]))]	0	0		
306	Chiral center specified	[\$([*@](-*)(~*)(*)*),\$([*@H](-*)(~*)(*)*),\$([*@](-*)(*)*),\$([*@H](-*)(~*)(*)*)]	10081	11000	1	1

Table S3: Bioactive molecules using TIN scaffold substructures.

Scaffold substructure	Name	Pubchem			ChEMBL		
		All compounds	Active compounds*	No. Targets	All compounds	Positive Assay results*	No. Targets
<chem>o1nc(C)c(CCC(O)=O)c1C</chem>	MA01_00001	1337	11	1	35	114	17
<chem>o1nc(C)c(Cc2onc(C)c2[N+](=O)[O-])c1C</chem>	MA02_00001	0	0	0	0	0	0
<chem>o1nc(C)c(Cc2onc(C)c2[NH2+]C=O)c1C</chem>	MA03_00001	0	0	0	0	0	0
<chem>o1nc(C)c([N+](=O)[O-])c1CCC(C(=O)C)C(=O)C</chem>	MA04_00001	4	0	0	0	0	0
<chem>O1N=C(C)C([N+](=O)[O-])C12CC(=O)C(CC2)C</chem>	MA05_00001	10	0	0	0	0	0
<chem>o1nc(C)c([N+](=O)[O-])c1CCC(C(O)=O)C(O)=O</chem>	MA06_00001	5	0	0	0	0	0
<chem>o1nc(C)c([N+](=O)[O-])c1CCC=O</chem>	MA07_00001	6	0	0	0	0	0
<chem>o1nc(c2NC(=O)CCCc12)C</chem>	MA08_00001	6	0	0	0	0	0
<chem>[oH+]1nc(c2nc(O)ccc12)C</chem>	MA11_00001	0	0	0	0	0	0
<chem>O=Cc1c(cc(nc1C)C#CCCC)C=O</chem>	MA16_00001	0	0	0	0	0	0
<chem>FC(F)(F)CON1N=C(C=C(N=C1C)C=O)C#Cc1cccc1</chem>	MA20_00001	0	0	0	0	0	0
<chem>FC(F)(F)CON1[NH+]C(N=C(C=C1C#Cc1cccc1)C=O)C</chem>	MA21_00001	0	0	0	0	0	0

* ChEMBL Positive Assay result: Activation/Inhibition either IC50, EC50, Ki < 10000 nM; Max Inhibition, Activity, Recovery > 50%. PubChem compounds returned as “Active in any Assay” from search.