

	A	B	C	D	E	F	G	H	I	J	K
1	Index	smiles	ring_type	sulfur	selenium	silicon	oxygen	Nitrogen	chlorine	fluorine	polymer_type
2	0	<chem>Cc1scc2c1OCCO2</chem>	double	YES	NO	NO	YES	NO	NO	NO	double-S-O
3	1	<chem>Cc1ccc(C2(C)c3c(sc4cc(C)sc34)-c3sc4c(C)c5c6c(sc5c(C)c4c32)-c2sc3cc(C)sc3c2C6(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
4	2	<chem>CCCCCCCCCCCCCN</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
5	3	<chem>Cc1sc2c3c(sc2c1C)-c1cc2c(cc1C3(C)C)-c1sc3c(C)c(C)sc3c1C2(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
6	4	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3ccc4c5c(ccc4c32)-c2sc(C)cc2C5(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
7	5	<chem>CCCCCCCCCN</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
8	6	<chem>Cc1cc2sc3c(c2s1)C(C)(C)c1cc2c(cc1-3)C(C)(C)c1cc(C)[se]jc1-2</chem>	fused	YES	YES	NO	NO	NO	NO	NO	fused-S-se
9	7	<chem>Cc1cc2sc3c(c2s1)C(C)c1c-3sc2cc(C)sc12</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
10	8	<chem>C=C1Cc2cccc(Cl)c2C1=O</chem>	double	NO	NO	NO	YES	NO	YES	NO	double-O-Cl
11	9	<chem>Cc1cc2sc3c(c2s1)C(C)(C)Oc1cc2c(cc1-3)OC(C)(C)c1c-2sc2cc(C)sc12</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
12	10	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3ccc4c5ccc6c7c(ccc(c8ccc2c3c48)c75)-c2sc(C)cc2C6(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
13	11	<chem>Cc1ccc2c(c1)-c1cccc1C21c2cc(C)ccc2-c2ccc(C)cc21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
14	12	<chem>CCCCCCCCCCCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
15	13	<chem>Cc1ccc2c(c1)[C@H]1c3cccc3[C@@@H]2c2ccc(C)cc21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
16	14	<chem>Cc1cc2c3c(c(C)cc4c3c1C(=O)NC4=O)C(=O)N(C)C2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
17	15	<chem>Cc1cc2c(s1)c1cc3c(cc1n2C)C(C)C1=C3C(C)(C)c2cc3c(cc21)c1sc(C)cc1n3C</chem>	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
18	16	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2)-c1sccc1C3C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
19	17	<chem>Cc1cc2c(s1)-c1cc3c(cc1CO2)-c1sc(C)cc1OC3C</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
20	18	<chem>C=C1Cc2ccc(F)cc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	YES	double-F-O
21	19	<chem>CC1C(=O)NC(=O)N(C)C1=O</chem>	single	NO	NO	NO	YES	YES	NO	NO	single-N-O
22	20	<chem>CCCCCCCCSC</chem>	branch	YES	NO	NO	NO	NO	NO	NO	branch-S

	A	B	C	D	E	F	G	H	I	J	K
23	21	CC=CC#N	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
24	22	C=C1Cc2ccc(Cl)cc2C1=O	double	NO	NO	NO	YES	NO	YES	NO	double-O-Cl
25	23	CC1=c2c3c(c4c(C)cc5c6c(ccc2c64)C(=O)N(C)C5=O)C=CC2C(=O)NC(=O)C(=C1)C32	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
26	24	CN1C(=O)c2ccc3c4c5c(c6ccc(c2c36)C1=O)=CC=C1C(=O)N(C)C(=O)C(C=C4)C15	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
27	25	C=C1Cc2cc(C)c(C)cc2C1=O	double	NO	NO	NO	YES	NO	NO	NO	double-O
28	26	Cc1cc2sc3c(c2s1)N=c1c-3c2c(c3c4sc5cc(C)sc5c4n(C)c13)=NN=N2	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
29	27	Cc1c(C#N)c(C#N)cc2nsnc12	double	YES	NO	NO	NO	YES	NO	NO	double-S-N
30	28	CCCCCCCCOC(C)=O	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
31	29	CCCCCCCCCCCCCCCCC	branch	NO	NO	NO	NO	NO	NO	NO	branch
32	30	CCCC(CC)COC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
33	31	CCCCCCCC(CO)CCCCC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
34	32	Oc1ccccc1	single	NO	NO	NO	YES	NO	NO	NO	single-O
35	33	Cc1sc2c(C)sc2c1F	double	YES	NO	NO	NO	NO	NO	YES	double-S-F
36	34	Cc1c2c(c(-c3ccc3)c3c1-c1ccc(C#N)c4cccc-3c14)C(=O)NC2=O	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
37	35	Cc1cnsc1	single	YES	NO	NO	NO	YES	NO	NO	single-S-N
38	36	Cc1c2nc3c(nc2cc2nc4c(nc12)-c1ccc2c5c(ccc-4c15)C(=O)N(C)C2=O)-c1ccc2c4c(ccc-3c14)C(=O)N(C)C2=O	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
39	37	Cc1ccc(-c2ccc(C)c(C)c2)s1	double	YES	NO	NO	NO	NO	NO	NO	double-S
40	38	CC(C)(C)C	branch	NO	NO	NO	NO	NO	NO	NO	branch
41	39	Cc1cc2csc(C)c2s1	double	YES	NO	NO	NO	NO	NO	NO	double-S
42	40	Cc1cc(F)cc2nsnc12	double	YES	NO	NO	NO	YES	NO	YES	double-S-N-F
43	41	CCOCCOCCOCC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
44	42	CN1C(=O)c2ccc3c4c(C#Cc5ccc(Nc6ccc(C#Cc7cc8c9c(cc%10c%11c%12c(cc%13c%14c(ccc(c7c9%11)c%14%12)C(=O)N(C)C%13=O)OC%10(C)C)C(=O)N(C)C8=O)cc6)cc5)cc5c6c(cc7c(c8c(cc(c2c38)C1=O)OC7(C)C)c64)C(=O)N(C)C5=O	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
45	43	c1ccc2nsnc2c1	double	YES	NO	NO	NO	YES	NO	NO	double-S-N

	A	B	C	D	E	F	G	H	I	J	K
46	44	CCCCCCCCC(CC)CCCCC	branch	NO	NO	NO	NO	NO	NO	NO	branch
47	45	Cc1c2c(c(-c3cccs3)c3c1-c1ccc(C)c4ccc-3c14)C(=O)NC2=O	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
48	46	CCCCC1(CCCC)c2cccc2-c2ccc(C)cc21	fused	NO	NO	NO	NO	NO	NO	NO	fused
49	47	Cc1c(F)ccc2nsnc12	double	YES	NO	NO	NO	YES	NO	YES	double-S-N-F
50	48	C#Cc1ccc(C)s1	single	YES	NO	NO	NO	NO	NO	NO	single-S
51	49	CCCCCCC(CC)CCCC	branch	NO	NO	NO	NO	NO	NO	NO	branch
52	50	c1ccc2sc2c1	double	YES	NO	NO	NO	NO	NO	NO	double-S
53	51	Cc1ccc2c(c1)Cc1cc3c(cc1-2)C(C)c1cc(C)ccc1-3	fused	NO	NO	NO	NO	NO	NO	NO	fused
54	52	Cc1cccc(F)c1	single	NO	NO	NO	NO	NO	NO	YES	single-F
55	53	C=C1Cc2cc(C)ccc2C1=O	double	NO	NO	NO	YES	NO	NO	NO	double-O
56	54	C=C1C(=O)c2ccccc2C1=C(C#N)c1cc(F)cc(F)c1	fused	NO	NO	NO	YES	YES	NO	YES	fused-N-F-O
57	55	CCCCCCCCCCCCC	branch	NO	NO	NO	NO	NO	NO	NO	branch
58	56	N#CC=C(C#N)C#N	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
59	57	CCCCCCCCOC=O	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
60	58	Cc1sc(C)c2c1C(=O)NC2=O	double	YES	NO	NO	YES	YES	NO	NO	double-S-N-O
61	59	C=C1Cc2cc(F)ccc2C1=O	double	NO	NO	NO	YES	NO	NO	YES	double-F-O
62	60	C=C1Cc2cc(F)c(OC)cc2C1=O	double	NO	NO	NO	YES	NO	NO	YES	double-F-O
63	61	Cc1ccc(C2(C)c3cc(C)sc3-c3ccc4cc5c6c(ccc7cc2c3c4c76)-c2sc(C)cc2C5(C)C)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
64	62	Cc1cc2sc3c(c2s1)C(C)c1cc2c(cc1-3)C(C)c1cc3c(cc1-2)C(C)(C)c1c-3sc2cc(C)sc12	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
65	63	CCCCC(CC)CN	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
66	64	CCCCCCN	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
67	65	CCCCCCCCS	branch	YES	NO	NO	NO	NO	NO	NO	branch-S
68	66	C=C1Cc2cc(l)ccc2C1=O	double	NO	NO	NO	YES	NO	NO	NO	double-O
69	67	C#Cc1ccc2c(n1)C(=O)N(C)C2=O	double	NO	NO	NO	YES	YES	NO	NO	double-N-O
70	68	C=C1c2cccc2-c2nc(C#N)c(C#N)nc21	fused	NO	NO	NO	NO	YES	NO	NO	fused-N
71	69	Cc1cc2c(s1)-c1sc(C)cc1C2C	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
72	70	N#CCC#N	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
73	71	CC1c2cc3ccccc3cc2-c2cc3ccccc3cc21	fused	NO	NO	NO	NO	NO	NO	NO	fused
74	72	CCCCC(CC)COC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O



	A	B	C	D	E	F	G	H	I	J	K
97	95	<chem>Cc1cc2sc3c(c2s1)C(C)(C)c1cc2c(cc1-3)C(C)(C)c1c-2sc2c1sc1cc(C)sc12</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
98	96	<chem>Cc1cccc2nsc12</chem>	double	YES	NO	NO	NO	YES	NO	NO	double-S-N
99	97	<chem>C=C1Cc2cc(C)c(C)cc2C1=O</chem>	double	NO	NO	NO	YES	NO	YES	NO	double-O-Cl
100	98	<chem>COc1cc(F)c(OC)c(C)c1F</chem>	single	NO	NO	NO	YES	NO	NO	YES	single-F-O
101	99	<chem>Cc1ccccc1</chem>	single	NO	NO	NO	NO	NO	NO	NO	single
102	100	<chem>C#CC#CC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
103	101	<chem>CCCO(C)C</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
104	102	<chem>Cc1c(F)c(F)c(F)c1F</chem>	single	NO	NO	NO	NO	NO	NO	YES	single-F
105	103	<chem>CB1n2c3c4cc5cc6c(cc5cc4c2N=c2c4cc5cc7c(cc5cc4c(n21)=NC1=NC(=N3)c2cc3cc4c(cc3cc21)C(=O)NC4=O)C(=O)N(C)C7=O)C(=O)N(C)C6=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
106	104	<chem>c1cc2ccc3ccc4ccc5ccc1c1c2c3c4c51</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
107	105	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2(C)C)-c1sc(C)cc1C3(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
108	106	<chem>CCCCCCCCCCCCCCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
109	107	<chem>CC1=C2C=CC(=N2)C(C)=c2ccc3n2[Zn]n2c1ccc2C(C)=C1C=CC(=N1)C=3c1cc(C)c(C)c(C)c1</chem>	fused	NO	NO	NO	NO	YES	NO	NO	fused-N
110	108	<chem>Cc1ccc(C2=CC3C(=O)N(C)C(=O)C4=CC5=c6c(c2c2ccc7c8c(cc(c6c28)OC5(C)C)C(=O)NC7=O)C43)cc1</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
111	109	<chem>C=C1Cc2c(OC)cccc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
112	110	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3sc4c(C)c5c(sc6c7c(sc65)-c5sc(C)cc5C7(C)C)c(C)c4c32)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
113	111	<chem>CC1=CC2C(=O)N(C)C(=O)C3=CC=c4c(c1c1ccc5c6c(ccc4c16)C(=O)N(C)C5=O)C32</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
114	112	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3[se]j4cc5c6c([se]j5cc4c32)-c2sc(C)cc2C6(C)C)cc1</chem>	fused	YES	YES	NO	NO	NO	NO	NO	fused-S-se

	A	B	C	D	E	F	G	H	I	J	K
115	113	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2C)-c1cc2c(cc1C3C)-c1cc3c(cc1C2(C)C)-c1sc(C)cc1C3(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
116	114	<chem>Cc1ccc(C2(C)Oc3cc(C)sc3-c3cc4c(cc32)-c2sc(C)cc2OC4(C)C)cc1</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
117	115	<chem>CC1(C)c2ccccc2C2C=CC=CC21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
118	116	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2(C)C)-c1sc2c(c1C3(C)C)C(C)(C)c1c-2sc2cc(C)sc12</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
119	117	<chem>CCCCCCO</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
120	118	<chem>Cc1ccc2c3c(cccc13)C(=O)NC2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
121	119	<chem>Cc1cc2c(s1)-c1cc3cc4c(cc3cc1C2(C)C)-c1sc(C)cc1C4(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
122	120	<chem>C=C1SC(=S)N(C)C1=O</chem>	single	YES	NO	NO	YES	YES	NO	NO	single-S-N-O
123	121	<chem>Cc1ccc(-c2cnc3c(C)c4nsnc4c(C)c3n2)cc1</chem>	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
124	122	<chem>Cc1ccc(C)c2nsnc12</chem>	double	YES	NO	NO	NO	YES	NO	NO	double-S-N
125	123	<chem>CCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
126	124	<chem>C=C1Cc2cc(OC)c(OC)cc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
127	125	<chem>CCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
128	126	<chem>CC1=Cc2c3c(c4cccc5cccc2c54)=CC(C)=C2C(=O)N(C)C(=O)C1C23</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
129	127	<chem>Cc1sc(F)c1C</chem>	single	YES	NO	NO	NO	NO	NO	YES	single-S-F
130	128	<chem>CC1=CC2C(C=C1)c1ccc(C)cc1C21c2ccccc2C2C=CC=CC21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
131	129	<chem>CC1=CC2C(C=C1)c1ccc(C)cc1C21c2ccccc2-c2ccccc21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
132	130	<chem>C=C1SC(=S)N(CCC)C1=O</chem>	single	YES	NO	NO	YES	YES	NO	NO	single-S-N-O
133	131	<chem>Cc1c2nc3c(nc2c(C)c2nc4c(nc12)-c1ccc2c5c(ccc-4c15)C(=O)N(C)C2=O)-c1ccc2c4c(ccc-3c14)C(=O)NC2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O

	A	B	C	D	E	F	G	H	I	J	K
134	132	<chem>CN1C(=O)C2=CC(c3cc4c(=O)n(C)c(=O)c5cc6[se]c7cc8c(=O)n(C)c(=O)c9ccc%10c3c(c45)c6c7c%10c98)c3c4c5c6c(cc7[se]c8cc(c2c3c8c75)C1=O)C(=O)NC(=O)C6=CC4</chem>	fused	NO	YES	NO	YES	YES	NO	NO	fused-N-O-se
135	133	<chem>Cc1cc2c(s1)-c1sc3c(c1C2(C)C)c1sc2c(c1c1sc4c(c31)C(C)C)c1cc(C)sc1-4)C(C)(C)c1cc(C)sc1-2</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
136	134	<chem>Cc1cc2c3c(cc4c5c6c(cc7c8c(ccc(c1c35)c86)C(=O)NC7=O)C(C)(C)O4)C(=O)N(C)C2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
137	135	<chem>Cc1c2c(nc3cc4c(-c5ccccc5)c5c(nc4cc13)-c1ccc3c4c(ccc-5c14)C(=O)NC3=O)-c1ccc3c4c(ccc-2c14)C(=O)N(C)C3=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
138	136	<chem>CC1=C2C=CC(=N2)C(c2cccc2C)=c2ccc3c2[Zn]n2c1ccc2C(c1c1cccc1C)=C1C=CC(=N1)C=3C</chem>	fused	NO	NO	NO	NO	YES	NO	NO	fused-N
139	137	<chem>CCOCCOCCOC</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
140	138	<chem>Cc1cccc1F</chem>	single	NO	NO	NO	NO	NO	NO	YES	single-F
141	139	<chem>Cc1cc2c3c(ccc4c3c1C(=O)N(C)C4=O)C(=O)N(C)C2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
142	140	<chem>C=C1Cc2cc(Cl)sc2C1=O</chem>	double	YES	NO	NO	YES	NO	YES	NO	double-S-O-Cl
143	141	<chem>C=C1Cc2c(sc3cccc23)C1=O</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
144	142	<chem>Cc1cc2c(s1)-c1cc3c(c(C)c1C2(C)C)-c1sc(C)cc1C3(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
145	143	<chem>CC1=CC2C(S1)c1cccc3c4c5c(cccc5c(c13)C2(C)c1ccc(C)cc1)-c1sc(C)cc1C4(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
146	144	<chem>C#Cc1cc2c(s1)C(=O)N(C)C2=O</chem>	double	YES	NO	NO	YES	YES	NO	NO	double-S-N-O
147	145	<chem>CC1=CC2C(=O)N(C)C(=O)C3=CC4=c5c(c1c1ccc6c7c(cc(c5c17)OC4(C)C)C(=O)N(C)C6=O)C32</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
148	146	<chem>Cc1cc2c(s1)-c1cc3c(cc1OC2C)-c1sc(C)cc1C(C)(C)O3</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O

	A	B	C	D	E	F	G	H	I	J	K
149	147	<chem>Cc1cccc(C2(C)c3cc4c(cc3-c3sc(C)cc32)C(C)(c2cccc(C)c2)c2c-4sc3c4c(sc23)-c2cc3c(cc2C4(C)C)-c2sc(C)cc2C3(C)C)c1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
150	148	<chem>Cc1ccc(C#Cc2ccc3c4c(cccc24)C(=O)N(C)C3=O)s1</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
151	149	<chem>CN1C(=O)c2ccc3c4c5c(c6ccc(c2c36)C1=O)=CC=C1C(=O)N(C)C(=O)C(C=C4)C15</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
152	150	<chem>CCCCCCCCO</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
153	151	<chem>CCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
154	152	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3sc4c(c(C)cc5c4cc(C)c4c6c(sc45)-c4sc(C)cc4C6(C)C)c32)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
155	153	<chem>C=C1Cc2c(C)sc(C)c2C1=O</chem>	double	YES	NO	NO	YES	NO	NO	NO	double-S-O
156	154	<chem>CCCCCCCCCCCCO</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
157	155	<chem>C#Cc1ccc2c(c1)C(=O)N(C)C2=O</chem>	double	NO	NO	NO	YES	YES	NO	NO	double-N-O
158	156	<chem>CCCCCCCCC(C)CCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
159	157	<chem>Cc1cc2sc3c(c2s1)C(C)(C)c1c-3sc2c(C)c3c4c(sc3cc12)-c1sc2cc(C)sc2c1C4(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
160	158	<chem>CC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
161	159	<chem>CN1C(=O)c2ccc3c4c5c6c([se]c7cc(c2c3c76)C1=O)=CC1C(=O)N(C)C(=O)C(=CC=4)C51</chem>	fused	NO	YES	NO	YES	YES	NO	NO	fused-N-O-se
162	160	<chem>CCCCCCCC[Si]</chem>	branch	NO	NO	YES	NO	NO	NO	NO	branch-Si
163	161	<chem>C=C1Cc2scoc2C1=O</chem>	double	YES	NO	NO	YES	NO	NO	NO	double-S-O
164	162	<chem>CCCC(C)CSC</chem>	branch	YES	NO	NO	NO	NO	NO	NO	branch-S
165	163	<chem>CC1=c2c3c(c4ccc5c6c(ccc2c46)C(=O)NC5=O)C=CC2C(=O)N(C)C(=O)C(=C1)C32</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
166	164	<chem>CCCCCCC(CCN)CCCC</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
167	165	<chem>CC1=c2c3c(c4ccc5c6c(ccc2c46)C(=O)N(C)C5=O)C=CC2C(=O)N(C)C(=O)C(=C1)C32</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
168	166	<chem>COc1ccc(OC)c(C)c1</chem>	single	NO	NO	NO	YES	NO	NO	NO	single-O
169	167	<chem>CCCCCCCCCCCCC(C)CCCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
170	168	<chem>Cc1cc2cc3c(cc2s1)-c1cc2sc(C)cc2cc1C3C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
171	169	<chem>C=C1SC(=S)N(CC)C1=O</chem>	single	YES	NO	NO	YES	YES	NO	NO	single-S-N-O



	A	B	C	D	E	F	G	H	I	J	K
172	170	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2C)-c1sc(C)cc1C3C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
173	171	<chem>C=C1SC(C)=C(C)S1</chem>	single	YES	NO	NO	NO	NO	NO	NO	single-S
174	172	<chem>C=C(C)C#N</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
175	173	<chem>C=C1C(=O)N(C)C(=O)N(C)C1=O</chem>	single	NO	NO	NO	YES	YES	NO	NO	single-N-O
176	174	<chem>Cc1ccc(C2(C)c3cc4c(cc3-c3sccc32)C(C)(c2ccc(C)cc2)c2cc(C)sc2-4)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
177	175	<chem>C=C1Cc2ccsc2C1=O</chem>	double	YES	NO	NO	YES	NO	NO	NO	double-S-O
178	176	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3sc4c(sc5c(C)c6c(sc7c8c(sc76)-c6sc(C)cc6C8(C)C)c(C)c54)c32)c1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
179	177	<chem>CCCCCCCC(CC)CCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
180	178	<chem>CC1=c2c3c4c(n(C)c5cc6c7c(ccc2c7c45)C(=O)N(C)C6=O)=CC2C(=O)N(C)C(=O)C(=C1)C32</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
181	179	<chem>CCCCCC[Si]</chem>	branch	NO	NO	YES	NO	NO	NO	NO	branch-Si
182	180	<chem>C=C1Cc2csc(Cl)c2C1=O</chem>	double	YES	NO	NO	YES	NO	YES	NO	double-S-O-Cl
183	181	<chem>CCCc1ccccc1</chem>	single	NO	NO	NO	NO	NO	NO	NO	single
184	182	<chem>Cc1sc(C)c2sccc12</chem>	double	YES	NO	NO	NO	NO	NO	NO	double-S
185	183	<chem>Cc1cccc2nonc12</chem>	double	NO	NO	NO	YES	YES	NO	NO	double-N-O
186	184	<chem>Cc1scc(F)c1F</chem>	single	YES	NO	NO	NO	NO	NO	YES	single-S-F
187	185	<chem>CCCCC1(CCCC)c2cccc2-c2cccc21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
188	186	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2(C)C)-c1sc2c(c1C3C)C(C)(C)c1cc3c(cc1-2)C(C)(C)c1cc(C)sc1-3</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
189	187	<chem>CCCCCSC</chem>	branch	YES	NO	NO	NO	NO	NO	NO	branch-S
190	188	<chem>Cc1cc2c(s1)-c1sc3c4c(sc3c1OC2(C)C)-c1sc(C)cc1C(C)(C)O4</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
191	189	<chem>Cc1ccc(C2C3C(=O)NC(c4cccs4)=C3C(=O)N2C)s1</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
192	190	<chem>Cc1ccc2c(c1)C(C)c1cccc1-2</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
193	191	<chem>C=C1Cc2cc(Cl)ccc2C1=O</chem>	double	NO	NO	NO	YES	NO	YES	NO	double-O-Cl
194	192	<chem>CCC(C)CC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
195	193	<chem>CC1=C2C(=O)NC(c3ccc(C)s3)=C2C(=O)N1C</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O



	A	B	C	D	E	F	G	H	I	J	K
218	216	<chem>Cc1ccc(-c2cc3c(s2)-c2sc(C)cc2C3)s1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
219	217	<chem>Cc1ccc(C2(C)c3cc4c(cc3-c3sc5cc(C)sc5c32)C(C)(c2ccc(C)cc2)c2c-4sc3c4c(sc23)-c2cc3c(cc2C4(C)C)-c2sc4cc(C)sc4c2C3(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
220	218	<chem>CCCC(CC)COC=O</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
221	219	<chem>COc1csc(C)c1OC</chem>	single	YES	NO	NO	YES	NO	NO	NO	single-S-O
222	220	<chem>C=C1Cc2sc(Cl)cc2C1=O</chem>	double	YES	NO	NO	YES	NO	YES	NO	double-S-O-Cl
223	221	<chem>Cc1sc2c(sc3c4c5nsnc5c5c6sc7c(c8cccc8)c(C)sc7c6n(C)c5c4n(C)c23)c1C</chem>	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
224	222	<chem>CN1C(=O)c2ccc3c4c5c6c7c(cc(c2c73)C1=O)C(C)(C)OC6=CC1C(=O)N(C)C(=O)C(=CC=4)C51</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
225	223	<chem>c1ccccc1</chem>	single	NO	NO	NO	NO	NO	NO	NO	single
226	224	<chem>CCCCc1ccccc1</chem>	single	NO	NO	NO	NO	NO	NO	NO	single
227	225	<chem>Cc1ccc2c(c1)C(C)c1cc(C)ccc1-2</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
228	226	<chem>Cc1ccsc1</chem>	single	YES	NO	NO	NO	NO	NO	NO	single-S
229	227	<chem>CC#Cc1ccc2c(c1)C(C)C(C)C2=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
230	228	<chem>Cc1cc(F)ccc1F</chem>	single	NO	NO	NO	NO	NO	NO	YES	single-F
231	229	<chem>CCCCCCCCCCN</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
232	230	<chem>CCCCC(CC)CO</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
233	231	<chem>Cc1ccc2c(c1)C(=O)NC2=O</chem>	double	NO	NO	NO	YES	YES	NO	NO	double-N-O
234	232	<chem>C[Si]</chem>	branch	NO	NO	YES	NO	NO	NO	NO	branch-Si
235	233	<chem>CCCCC(C)CC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
236	234	<chem>COc1c2c(c(OC)c3c1-c1sc(C)cc1C3C)-c1sc(C)cc1C2</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
237	235	<chem>Cc1c(F)c(F)cc2nsnc12</chem>	double	YES	NO	NO	NO	YES	NO	YES	double-S-N-F
238	236	<chem>Cc1ccco1</chem>	single	NO	NO	NO	YES	NO	NO	NO	single-O
239	237	<chem>Cc1cc2c(C)c3sc(C4=CC5C(=O)N(C)C(=O)C6=CC=c7c(c4c4ccc8c9c(cc(C)c7c49)C(=O)NC8=O)C65)cc3c(C)c2s1</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
240	238	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2C)-c1cc2c(cc1C3C)-c1sc(C)cc1C2(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
241	239	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2(C)C)-c1sc2cc(C)sc2c1C3(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S

	A	B	C	D	E	F	G	H	I	J	K
242	240	<chem>CC1=C2C=CC(=N2)C(C)=c2ccc3n2[Zn]n2c1ccc2C(C)=C1C=CC(=N1)C=3c1cc(C)cc(C)c1</chem>	fused	NO	NO	NO	NO	YES	NO	NO	fused-N
243	241	<chem>C=C1Cc2cc(Br)ccc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
244	242	<chem>Cc1ccc2c(c1)Sc1cccc1N2CCCCCn1c2cccc2c2cc(C)ccc21</chem>	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
245	243	<chem>CN1c2cccc2C(=O)C2C=C3NC4C=CC=CC4C(=O)C3=CC21</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
246	244	<chem>Cc1ccc(C2(C)c3c(cc4ccc5c6c(cc7ccc3c4c75)-c3sc4cc(C)sc4c3C6(C)C)-c3sc4cc(C)sc4c32)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
247	245	<chem>C#CC1=CC2C(C=C1)c1ccc(C)cc1C21c2cc(C)ccc2C2C=CC(C)=CC21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
248	246	<chem>Cc1cc2c(s1)-c1sc3c(C)c4c5c(sc4cc3c1C2(C)C)-c1sc(C)cc1C5(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
249	247	<chem>CCCCC(CC)CO</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
250	248	<chem>Cc1cc2c3c(ccc4c5ccc6c7c(ccc(c1c34)c75)C(=O)NC6=O)C(=O)N(C)C2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
251	249	<chem>C=C1C(=O)N(C)C(C)=S)N(CC)C1=O</chem>	single	YES	NO	NO	YES	YES	NO	NO	single-S-N-O
252	250	<chem>CN1C(=O)c2cccc3cccc(c23)C1=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
253	251	<chem>Fc1cccc(F)c1F</chem>	single	NO	NO	NO	NO	NO	NO	YES	single-F
254	252	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3sc4c5c(sc4c32)-c2sc(C)cc2C5(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
255	253	<chem>Cc1sc1F</chem>	single	YES	NO	NO	NO	NO	NO	YES	single-S-F
256	254	<chem>Cc1ccc(C(C#N)=Cc2ccc(C)c(C)c2)s1</chem>	double	YES	NO	NO	NO	YES	NO	NO	double-S-N
257	255	<chem>Cc1ccc2c(c1)C1(c3cc(C)ccc3-2)c2cc(C)ccc2-c2ccc(C3C=C4C(=O)N(C)C(=O)c5ccc6c(c54)c3c3c4c5c(ccc46)C(=O)NC(=O)C5=CC3)cc21</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
258	256	<chem>Cc1ccsc1C</chem>	single	YES	NO	NO	NO	NO	NO	NO	single-S
259	257	<chem>CCCCCCCCCN</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N

	A	B	C	D	E	F	G	H	I	J	K
260	258	<chem>Cc1ccc(C2(C)c3c(sc4cc(C)sc34)-c3sc4c5c(sc4c32)-c2sc3cc(C)sc3c2C5(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
261	259	<chem>CN1C(=O)c2ccc3c4ccc5c6c(ccc(c7ccc(c2c37)C1=O)c64)C(=O)N(C)C5=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
262	260	<chem>Cc1ccc2c(c1)=c1cc3c(cc1N=2)=c1cc(C)ccc1=N3</chem>	fused	NO	NO	NO	NO	YES	NO	NO	fused-N
263	261	<chem>Cc1cc2c(s1)-c1cc3cc4c(cc3cc1C2C)-c1sc(C)cc1C4(C)C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
264	262	<chem>CN1C(=O)C2=CC(c3cc4c(=O)n(C)c(=O)c5cc6sc7cc8c(=O)n(C)c(=O)c9ccc%10c3c(c45)c6c7c10c98)c3c4c5c6c(cc7sc8cc(c2c3c8c75)C1=O)C(=O)NC(=O)C6=CC4</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
265	263	<chem>COC=O</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
266	264	<chem>CCCCC(CC)CCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
267	265	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3sc4c(cc(C)c5c4ccc4c6c(sc45)-c4sc(C)cc4C6(C)c4ccc(C)cc4)c32)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
268	266	<chem>Cc1ccc(C2(C)c3cc(C)sc3-c3sc4cc5c(cc4c32)C(C)c2cc3c4c(sc3cc2-5)-c2sc(C)cc2C4(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
269	267	<chem>CC1=CC2C(C=C1)c1cccc1C21c2cc(C)ccc2C2C=CC(C)=CC21</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
270	268	<chem>C=C(C#N)C#N</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
271	269	<chem>CCCCCCCC[Si]</chem>	branch	NO	NO	YES	NO	NO	NO	NO	branch-Si
272	270	<chem>C=C1Cc2cc(Br)c(Br)cc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
273	271	<chem>Fc1ccnc1F</chem>	single	NO	NO	NO	NO	YES	NO	YES	single-N-F
274	272	<chem>CCOCCOC</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
275	273	<chem>CC1=c2c3c(c4c(C)cc5c6c(ccc2c64)C(=O)N(C)C5=O)C=CC2C(=O)N(C)C(=O)C(=C1)C32</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
276	274	<chem>Cc1cc2c(s1)-c1cc3c(cc1C2(C)CCCCc1cccc1)-c1sc(C)cc1C3(C)CCCCc1cccc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
277	275	<chem>Cc1cccc2nn(C)nc12</chem>	double	NO	NO	NO	NO	YES	NO	NO	double-N

	A	B	C	D	E	F	G	H	I	J	K
278	276	Cc1ccc(C2(C)c3cc(C)sc3-c3sc4c(C)c5c6c(sc5c(C)c4c32)-c2sc(C)cc2C6(C)C)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
279	277	Cc1cc2c(s1)-c1cc3c(cc1C2(C)C)-c1sc2c(sc4cc(C)sc42)c1C3(C)C	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
280	278	CC(C)C	branch	NO	NO	NO	NO	NO	NO	NO	branch
281	279	CCCCCCCCCOC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
282	280	C#Cc1ccccc1	single	NO	NO	NO	NO	NO	NO	NO	single
283	281	Cc1cc2c(s1)-c1cc3ccc4cc5c(c6ccc(c1C2(C)C)c3c46)C(C)(C)c1cc(C)sc1-5	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
284	282	Cc1ccc(C=C2SC(=S)N(C)C2=O)s1	double	YES	NO	NO	YES	YES	NO	NO	double-S-N-O
285	283	Cc1cc2sc3c4c5nsnc5c5c6sc7c(C)c(C)sc7c6n(C)c5c4n(C)c3c2s1	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
286	284	Cc1ccc(C2(C)c3c(sc4cc(C)sc34)-c3sc4c5c(sc4c32)-c2sc3c4c(sc3c2C5(C)c2ccc(C)cc2)-c2sc3cc(C)sc3c2C4(C)C)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
287	285	Cn1c(=O)c2ccc3c4ccc5c(=O)n(C)c(=O)c6cc7c8c9cc%10c(=O)n(C)c(=O)c%11cc(-c%12cccc(-c%13cc%14c(=O)n(C)c(=O)c%15c%16c%17c%18cc%19c(=O)n(C)c(=O)c%20ccc%21c%22ccc%23c(=O)n(C)c(=O)c%24cc(c%17c%17cc%25c(=O)n(C)c(=O)c%26ccc%27c%13c(c%14%15)c%16c%17c%27c%26%25)c(c%22c%23%24)c%18c%21c%20%19)c%12)c%12c%13ccc%14c(=O)n(C)c(=O)c%15cc(c8c8cc(c1=O)c2c3c8c7c4c56)c(c%13c%14%15)c9c%12c%11%10	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
288	286	CCC(N)CC	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
289	287	Cc1ccc(-c2cc(C)c(C)c(C)c2C)cc1	double	NO	NO	NO	NO	NO	NO	NO	double
290	288	C#[N+]	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
291	289	c1ccc2occc2c1	double	NO	NO	NO	YES	NO	NO	NO	double-O
292	290	Cc1cc2sc3c(c2s1)C(C)(C)Oc1c-3sc2c3c(sc12)-c1sc2cc(C)sc2c1C(C)(C)O3	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O



	A	B	C	D	E	F	G	H	I	J	K
318	316	<chem>Cc1scc2c1C(=O)N(C)C2=O</chem>	double	YES	NO	NO	YES	YES	NO	NO	double-S-N-O
319	317	<chem>C=C1Cc2ccc(Br)cc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
320	318	<chem>CCCCC(C)CC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
321	319	<chem>CC1Cc2ccccc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
322	320	<chem>C=C1Cc2cc(OC)ccc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
323	321	<chem>C=C1Cc2cc3ccccc3cc2C1=O</chem>	fused	NO	NO	NO	YES	NO	NO	NO	fused-O
324	322	<chem>CCCCCOC</chem>	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
325	323	<chem>C=C(C#N)C(=O)OCC</chem>	branch	NO	NO	NO	YES	YES	NO	NO	branch-N-O
326	324	<chem>Cn1c(=O)c2ccc3c4ccc5c(=O)n(C)c(=O)c6cc7c8c9cc%10c(=O)n(C)c(=O)c%11cc%12c%13c%14cc%15c(=O)n(C)c(=O)c%16cc(-c%17cccc(-c%18cc%19c(=O)n(C)c(=O)c%20cc%21c%22c%23cc%24c(=O)n(C)c(=O)c%25cc%26c%27c%28cc%29c(=O)n(C)c(=O)c%30ccc%31c%32cc%33c(=O)n(C)c(=O)c%34cc(c%27c%27cc%35c(=O)n(C)c(=O)c%36cc(c%22c%22cc%37c(=O)n(C)c(=O)c%38ccc%39c%18c(c%19%20)c%21c%22c%39c%38%37)c%18c%23c(c%25%24)c%26c%27c%18c%35%36)c(c%32c%33%34)c%28c%31c%30%29)c%17)c%17c%18ccc%19c(=O)n(C)c(=O)c%20cc(c%13c%13cc%21c(=O)n(C)c(=O)c%22cc(c8c8cc(c1=O)c2c3c8c7c4c56)c1c9c(c%10%11)c%12c%13c1c%22%21)c(c%18c%19%20)c%14c%17c%16%15</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
327	325	<chem>CCCCC(CC)CN</chem>	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
328	326	<chem>c1ccsc1</chem>	single	YES	NO	NO	NO	NO	NO	NO	single-S
329	327	<chem>CCCCC1(CCCC)c2ccc(C)cc2-c2c1c1c(c3c2C(CCCC)(CCCC)c2ccc(C)cc2-3)C(CCCC)(CCCC)c2ccc(C)cc2-1</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
330	328	<chem>Cc1cc2sc3cc4c(cc3c2s1)C1=C(c2cc3c(cc2C1(C)C)sc1cc(C)sc13)C4C</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
331	329	<chem>CC1C=C2C(=O)N(C)C(=O)c3cc4c(c32)c1c1c2c3c(ccc24)C(=O)N(C)C(=O)C3=CC1</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O



	A	B	C	D	E	F	G	H	I	J	K
332	330	Cc1cc2sc3c(c2s1)C(C)(C)c1cc2c(cc1-3)C(C)(C)c1c-2sc2cc(C)sc12	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
333	331	Cc1ccc2c(c1)C(C)c1cc(C)sc1-2	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
334	332	Cc1cc2c3c(sc2s1)-c1cc2c(cc1C3(C)C)-c1sc3cc(C)sc3c1C2(C)C	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
335	333	Cn1c(=O)c2ccc3sc4cccc4c4ccc(c1=O)c2c34	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
336	334	Cc1cc2c(s1)-c1cc3sc4cc5c(cc4c3cc1C2(C)C)C(C)(C)c1cc(C)sc1-5	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
337	335	Cc1ccc(C2(C)c3c(ccc4c5c(ccc34)-c3sc4cc(C)sc4c3C5(C)C)-c3sc4cc(C)sc4c32)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
338	336	Cc1cc2c(s1)-c1sc3c(c1C2(C)C)c1ccc2nc(C)c4c5sc6c(c5c5ccc7nc(C)c3c3c7c5c4c2c13)C(C)(C)c1cc(C)sc1-6	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
339	337	CN1C(=O)C2=CCc3c4c5c6c(ccc5c5ccc(c2c35)C1=O)C(=O)N(C)C(=O)C6=CC4	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
340	338	Cc1cc2c(s1)-c1scoc1[Si]2	fused	YES	NO	YES	NO	NO	NO	NO	fused-S-Si
341	339	CCCC(CC)CS	branch	YES	NO	NO	NO	NO	NO	NO	branch-S
342	340	C[Ge]	branch	NO	NO	NO	NO	NO	NO	NO	branch
343	341	Cc1ccc2c(c1)C(C)C1C=CC=CC21	fused	NO	NO	NO	NO	NO	NO	NO	fused
344	342	Cc1cc2c(s1)-c1cc3c(cc1C2)C(C)C1=C3C(C)(C)c2cc3c(cc21)-c1sc(C)cc1C3	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
345	343	C=C1Cc2cc(C#CC)ccc2C1=O	double	NO	NO	NO	YES	NO	NO	NO	double-O
346	344	Cc1cc2sc3c(c2s1)C(C)c1cc2c(cc1-3)C(C)(C)c1c-2sc2cc(C)sc12	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
347	345	C#Cc1ccc(C)cc1	single	NO	NO	NO	NO	NO	NO	NO	single
348	346	COCCOC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
349	347	CCCCCS	branch	YES	NO	NO	NO	NO	NO	NO	branch-S
350	348	Cc1ccc(-c2cc(C)c(C)s2)cc1C	double	YES	NO	NO	NO	NO	NO	NO	double-S
351	349	Cc1cc2sc3c4c(sc3c2s1)-c1c(C)c2c(c(C)c1C4(C)C)-c1sc3c(sc4cc(C)sc43)c1C2(C)C	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
352	350	C=C1Cc2ccc(C)cc2C1=O	double	NO	NO	NO	YES	NO	NO	NO	double-O
353	351	Cc1cnc2c(c1)C(=O)NC2=O	double	NO	NO	NO	YES	YES	NO	NO	double-N-O

	A	B	C	D	E	F	G	H	I	J	K
354	352	CCCCCCC(N)CCCC	branch	NO	NO	NO	NO	YES	NO	NO	branch-N
355	353	Cc1ccc(- c2c3c(c(C)c4nsnc24)C(=O)NC3 =O)s1	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
356	354	CN1C(=O)c2cc3cc4c5n6c(c4cc3 cc2C1=O)N=c1c2cc3cc4c(cc3cc 2c(n1B6F)=NC1=NC(=N5)c2cc 3cc5c(cc3cc21)C(=O)NC5=O)C( =O)N(C)C4=O	fused	NO	NO	NO	YES	YES	NO	YES	fused-N-F-O
357	355	C1(C=CS2)=C2C=CS1	double	YES	NO	NO	NO	NO	NO	NO	double-S
358	356	Cc1cc2[se]c3c(c2s1)C(C)(C)c1cc 2c(cc1-3)C(C)(C)c1c- 2[se]c2cc(C)sc12	fused	YES	YES	NO	NO	NO	NO	NO	fused-S-se
359	357	C#Cc1ccc2c3c(cccc13)C(=O)N( C)C2=O	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
360	358	Cc1cc2c(ccc3nsnc32)c2nsnc12	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
361	359	Cc1cc2sccc2s1	double	YES	NO	NO	NO	NO	NO	NO	double-S
362	360	Cc1ccc(C2(C)c3cc4c(cc3- c3sc(C)cc32)C(C)(c2ccc(C)cc2)c 2c-4sc3c4c(sc23)- c2cc3c(cc2C4(C)C)- c2sc(C)cc2C3(C)C)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
363	361	CCC	branch	NO	NO	NO	NO	NO	NO	NO	branch
364	362	Cc1ccc(-c2nc3sc(C)nc3s2)s1	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
365	363	Cc1cc2sc3c(c2s1)C(C)(C)c1c(C)c 2c(c(C)c1-3)C(C)(C)c1c- 2sc2cc(C)sc12	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
366	364	C#[N+]C1=C(C)C(C)C(=O)N(CC CC)C1=O	single	NO	NO	NO	YES	YES	NO	NO	single-N-O
367	365	Cc1cc2c(s1)-c1scccc1C2	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
368	366	Cc1ccc(C)s1	single	YES	NO	NO	NO	NO	NO	NO	single-S
369	367	C=C1SC(=O)N(CC)C1=O	single	YES	NO	NO	YES	YES	NO	NO	single-S-N-O
370	368	CN1C(=O)c2ccc3c4cccc5cccc(c 6ccc(c2c36)C1=O)c54	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
371	369	Cc1ccc(-c2cc3c(s2)- c2sc(C)cc2[Si]3)s1	fused	YES	NO	YES	NO	NO	NO	NO	fused-S-Si
372	370	Cc1csc(C)c1C	single	YES	NO	NO	NO	NO	NO	NO	single-S
373	371	CCCCCCC(C)CCCC	branch	NO	NO	NO	NO	NO	NO	NO	branch
374	372	Cc1ccc(C2(C)c3cc(C)sc3- c3ccc4cc5c6c(ccc5cc4c32)- c2sc(C)cc2C6(C)C)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S

	A	B	C	D	E	F	G	H	I	J	K
375	373	Cc1cc2c(s1)- c1sc3c(c1C2(C)C)C(C)(C)c1cc2c( cc1-3)C(C)(C)c1c- 2sc2c1C(C)(C)c1cc(C)sc1-2	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
376	374	Cc1cc2c(s1)-c1cc3c(cc1C2C)- c1cc2c(cc1C3(C)C)- c1sc(C)cc1C2(C)C	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
377	375	Cc1ccc(-c2cnc(C)c(C)n2)cc1	double	NO	NO	NO	NO	YES	NO	NO	double-N
378	376	CC1=Cc2c3c(c4cc(C)c5c6c(c(C) cc2c64)C(=O)NC5=O)=CC(C)= C2C(=O)N(C)C(=O)C1C23	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
379	377	Cc1ccc(C2(C)c3cc4c5cc6c(cc5n( C)c4cc3-c3sc(C)cc32)- c2sc(C)cc2C6(C)C)cc1	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
380	378	Cc1cc2c(s1)- c1c(ccc3c4c(ccc13)C(C)(C)c1cc( C)sc1-4)C2C	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
381	379	CCC(C)(C)C	branch	NO	NO	NO	NO	NO	NO	NO	branch
382	380	CC1=C2C(=O)N(C)C(C)=C2C(= O)N1	double	NO	NO	NO	YES	YES	NO	NO	double-N-O
383	381	CCCC(C)CC	branch	NO	NO	NO	NO	NO	NO	NO	branch
384	382	CC1=CC2=CSC=C2C1=O	double	NO	NO	YES	YES	NO	NO	NO	double-S-O
385	383	CCCCCCCCOC	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
386	384	CCC[Si](CCC)CCC	branch	NO	NO	YES	NO	NO	NO	NO	branch-Si
387	385	Cc1ccc(C2(C)c3cc4c5cc6c(cc5n( C)c4cc3-c3sc4cc(C)sc4c32)- c2sc3cc(C)sc3c2C6(C)C)cc1	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
388	386	CCOCCOCCO	branch	NO	NO	NO	YES	NO	NO	NO	branch-O
389	387	Cc1nc2cccc(C)c2nc1C	double	NO	NO	NO	NO	YES	NO	NO	double-N
390	388	Cc1ccc(C2(C)c3cc(C)sc3- c3sc4cc5c6c(sc5cc4c32)- c2sc(C)cc2C6(C)C)cc1	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
391	389	Cc1cc2sc3c4c(sc3c2s1)- c1cc2c(cc1C4(C)C)- c1[se]c(C)cc1C2(C)C	fused	YES	YES	NO	NO	NO	NO	NO	fused-S-se
392	390	Cc1cc2c(s1)c1sc3c(c1n2C)C(C)( C)c1cc2c(cc1-3)C(C)(C)c1c- 2sc2c3sc(C)cc3n(C)c12	fused	YES	NO	NO	NO	YES	NO	NO	fused-S-N
393	391	C=C1Cc2cc(OC)c(F)cc2C1=O	double	NO	NO	NO	YES	NO	NO	YES	double-F-O
394	392	Cc1ccc(C2(C)Oc3cc(C)sc3- c3cc4c(cc32)-c2sc(- c3ccc(C)s3)cc2OC4(C)C)cc1	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O

	A	B	C	D	E	F	G	H	I	J	K
395	393	<chem>Cc1cc2c3c(ccc4c5c6c(c1c43)=C C=C1C(=O)N(C)C(=O)C(C=C5c 3cccs3)C16)C(=O)NC2=O</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
396	394	<chem>CCCCCCCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
397	395	<chem>CC1c2cc(- c3cc4c5cc6c(=O)n(C)c(=O)c7cc c8c9ccc%10c(=O)n(C)c(=O)c%11 cc(c4o3)c(c9c%10%11)c5c8c76)c cc2-c2ccc(- c3cc4c5cc6c(=O)n(C)c(=O)c7cc c8c9ccc%10c(=O)n(C)c(=O)c%11 cc(c4o3)c(c9c%10%11)c5c8c76)c c21</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
398	396	<chem>Cc1cc2c(s1)- c1cc3c(cc1OC2(C)C)- c1sc(C)cc1C(C)(C)O3</chem>	fused	YES	NO	NO	YES	NO	NO	NO	fused-S-O
399	397	<chem>CCCCN1C2=CC3C(=O)c4ccccc 4N(CCCC)C3C=C2C(=O)C2C=C C=CC21</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
400	398	<chem>CCCCCCCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
401	399	<chem>Cc1cc2sc3c(c2s1)C(C)(C)c1cc2c( cc1-3)C(C)(C)c1c-2sc2ccsc12</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
402	400	<chem>CCCCC1(CCCC)c2cc(C)ccc2- c2c1c1c(c3c2C(CCCC)(CCC)c2 cc(C)ccc2- 3)C(CCCC)(CCC)c2cc(C)ccc2-1</chem>	fused	NO	NO	NO	NO	NO	NO	NO	fused
403	401	<chem>Cc1ccc(C2=CC3C(=O)N(C)C(= O)C4=CC=c5c(c2c2ccc6c7c(cc( C)c5c27)C(=O)NC6=O)C43)s1</chem>	fused	YES	NO	NO	YES	YES	NO	NO	fused-S-N-O
404	402	<chem>C=C1Cc2ccc(OC)cc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
405	403	<chem>Cc1ccc(C2(C)c3c(sc4c(C)csc34)- c3sc4c5c(sc4c32)- c2sc3c4c(sc3c2C5(C)c2ccc(C)cc 2)-c2sc3cc(C)sc3c2C4(C)C)cc1</chem>	fused	YES	NO	NO	NO	NO	NO	NO	fused-S
406	404	<chem>Cc1cc2c3c(ccc4c3c1C(=O)N(C) C4=O)C(=O)NC2=O</chem>	fused	NO	NO	NO	YES	YES	NO	NO	fused-N-O
407	405	<chem>CCCCCCCCCCC</chem>	branch	NO	NO	NO	NO	NO	NO	NO	branch
408	406	<chem>Cc1cc(F)c(C)s1</chem>	single	YES	NO	NO	NO	NO	NO	YES	single-S-F
409	407	<chem>Cc1cc(C)c(C)s1</chem>	single	YES	NO	NO	NO	NO	NO	NO	single-S
410	408	<chem>C=C1C(=O)c2ccccc2C1=O</chem>	double	NO	NO	NO	YES	NO	NO	NO	double-O
411	409	<chem>C#Cc1ccccc1</chem>	single	NO	NO	NO	NO	NO	NO	NO	single
412	410	<chem>C#[N+ ]C1=C(C)C(C)C(=O)N(CC</chem>	single	NO	NO	NO	YES	YES	NO	NO	single-N-O

		CC)C1=O									
413	411	Cc1ccc[se]1	single	NO	YES	NO	NO	NO	NO	NO	single-se
414	412	c1ccc2nsnc2c1	double	YES	NO	NO	NO	YES	NO	NO	double-S-N