

No.	SMILES	uh/cm ² ·V-1·s-1	ue/cm ² ·V-1·s-1
1	<chem>O=C(C1CC(CCCCCCCC)CCCCCCCC)C2=C(SC(C)=C2)C3=C(C=C(C)S3)C1=O</chem>	0	0.01
2	<chem>CC1=CC(C(CCCCCCCC)(CCCCCCCC)C2=C3C=CC(C4=CC=C(C)C5=NSN=C45)=C2)=C3C=C1</chem>	0	0.0048
3	<chem>CC1=CC(CCCCCCCC)=C(C2=CC=C(C(C3=C(F)C(F)=C(C(C4=CC=C(C5=C(CCCCCCCC)C=C(C)S5)S4)=O)C(F)=C3F)=O)S2)S1</chem>	0	0
4	<chem>CC1=CC(CCCCCC)=C(C2=CC(CCCCCC)=C(C3=CC(CCCCCC)=C(C4=CC(CCCCCC)=C(C)S4)S3)S2)S1</chem>	0.2	0
5	<chem>CC1=CC=C(C2=C3C=C(C4=CC=C(C5=CC=C(C)S5)S4)C=C2)C(C3(CCCCCCCC)CCCCCCCC)=C1</chem>	0.02	0
6	<chem>CCCCCCCCC(CCCCCCCC)N1C2=CC(C3=CC=C(C(C4=NSN=C54)=CC=C5C6=CC=C(S6)C7=CC=CC=C7)S3)=CC=C2C8=CC=C(C9=CC=CC=C9)C=C81</chem>	0.03	0
7	<chem>CC1=CC(CCCCCCCCCCCC)=C(C2=C3C(N=C(C4=CC=CC=C4)C(C5=CC=CC=C5)=N3)=C(C6=C(CCCCCCCCCCCC)C=C(C7=CC(C(CCCCCCCCCCCC)(CCCCCCCCCCCC)C8=C9C=CC(C)=C8)=C9C=C7)S6)S2)S1</chem>	0.03	0
8	<chem>CC(C=C1)=CC2=C1C(C=C3)=C(C2(CCCCCCCCCCCC)CCCCCCCCC)C=C3C(S4)=CC(CCCCCCCCCCCC)=C4C5=C6C(N=C7C8=C(C(C7=N6)=CC=C9)C9=CC=C8)=C(C%10=C(CCCCCCCCCCCC)C=C(C)S%10)S5</chem>	0.2	0
9	<chem>CC1=CC=C(/C=C/C2=CC=C(C3=CC=C(C(C=CC(C)=C4)=C4C5(CCCCCCCC)CCCCCCCC)C5=C3)S2)S1</chem>	0.02	0
10	<chem>CC1=CC2=C(S1)C=C(C3=CC=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)S3)S2</chem>	0.02	0
11	<chem>O=C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C1=O)C2=C(C1=CC(/C=C/C3=C(CCCCCC)C=C(C4=CC(F)=C(/C=C/C5=C(F)C=C(C6=CC(CCCCCC)=C(/C=C/C)S6)C7=NSN=C75)C8=NSN=C48)S3)=C9C(N(CC(CCCCCCCCCCCC)CCCCCCCCC)C%10=O)=O)C9=C%10C=C2C</chem>	0	3.87
12	<chem>O=C(N(CC(CCCCCCCC)CCCCCCCCCCCC)C1=O)C2=C(C1=CC(/C=C/C3=CC=C(C4=C5C(N=S=N5)=C(C6=CC=C(/C=C/C)S6)C7=NN(CC(CC)CCCC)N=C47)S3)=C8C(N(CC(CCCCCCCCCCCC)CCCCCCCCCCC)C9=O)=O)C8=C9C=C2</chem>	0	7.16
13	<chem>CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC(CCCCCCCCCCCC)=C(C6=CC=C(C7=C(CCCCCCCCCCCC)C=C(C)S7)S6)S5)S4)N(CC(CCCCCC)CCCCCCCC)C3=O)S1</chem>	0.015	0.003
14	<chem>CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC(CCCCCCCCCCCC)=C(C6=CC=C(C7=CC=C(C8=C(CCCCCCCCCCCC)C=C(C)S8)S7)S6)S5)S4)N(C(C(CCCCCC)CCCCCCCC)C3=O)S1</chem>	0.05	0.003
15	<chem>CC1=CC=C(C(N(CC(CC)CCCC)C2=O)=C3C2=C(C4=CC=C(C5=C(CCCCCCCCCCCC)C=C(C6=CC=C(/C=C/C7=CC=C(C8=C(CCCCCCCCCCCC)C=C(C)S8)S7)S6)S5)S4)N(CC(CC)CC)CC)C3=O)S1</chem>	0.05	0
16	<chem>CC1=C(C(N2CC(CCCCCC)CCCCCCCC)=O)C3=C(C(C(N4C(C(CCCCCC)CCCCCCCC)=O)=C(C5=CC=C(C6=CC=C(C)S6)S5)C=C3C2=O)C(C4=O)=C1</chem>	0	1.9
17	<chem>CC1=C(C(N2CCCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C)=O)C3=C(C(C(N4CCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)=O)=C(C5=CC=C(C6=CC=C(C)S6)S5)C=C3C2=O)C(C4=O)=C1</chem>	0	1.04
18	<chem>CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCCCC)=O)=C(C4=CC=C(/C=N/N=C/C)S4)N(CC(CCCCCCCCCC)CCCCCCCC)C3=O)S1</chem>	0.36	0.41

19	<chem>CCCCC(C)=O=C(C4=NC=C(C5=CN=C(C6=NC=C(C)S6)S5)S4)N(CCCCC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)S1</chem>	0	0.07
20	<chem>CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCC)CCCCC)CC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)S5)S4)N(CC(CCCCCC)CCCCCCCCCCCCC)C3=O)S1</chem>	4.5	0
21	<chem>CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCC)CCCCC)CC)=O)=C(C4=CC=C(C5=CC6=C(C=C(C)S6)S5)S4)N(CC(CCCCCC)CCCCCCCCCCCCC)C3=O)S1</chem>	1.36	1.56
22	<chem>CC1=CC=C(C2=C3C(C(N2CCCCCCCCCCCCCCCC)=O)=C(C4=CC=C(C5=CC6=C(C(SC(C)=C7)=C7N6CC(CCCCCC)CCCCCCCCC)S5)S4)N(CCCCCCCCCCCCCCCCC)C3=O)S1</chem>	0.41	0
23	<chem>CC1=CC=C(C2=C3C(C(N2CCCC)=O)=C(C4=CC=C(C5=C(C6=C(C(SC(C)=C7)=C7N6C(C(C)CCCCC)C(CCCCCC)CC)S5)S4)N(CCCC)C3=O)S1</chem>	0.05	0
24	<chem>CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCC)CCCCC)CC)=O)=C(C4=CC=C(C5=CC6=C(C(SC(C)=C7)=C7S6)S5)S4)N(CC(CCCCCC)CCCCCCCCCCCCC)C3=O)S1</chem>	0.75	0
25	<chem>CC(S1)=CC=C1C2=C3C(C(N2CC(CCCCCC)CCCCCCCC)CCCC)=O=C(C4=CC=C(C#CC5=C(C=CC(C#CC6=CC=C(CCCCCC)C=C6)=C7)C7=C(C#CC)C8=C5C=C(C#CC9=CC=C(C=C9)CCCCC)C=C8)S4)N(CC(CCCCCC)CCCCCCCCCCCC)C3=O</chem>	0.12	0
26	<chem>CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C)C6=NSN=C65)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)S1</chem>	0.097	0.089
27	<chem>CC(S1)=NC2=C1C(SC(C)=N3)=C3C(N(CC(CCCCC)CCCC)C2=O)=O</chem>	0	0.015
28	<chem>CC1=C(C#N)C(OCC(CC)CCCC)=C(C2=C(OCC(CC)CCCC)C(C#N)=C(C)S2)S1</chem>	0	0.31
29	<chem>CC1=CC(C(N2CC(CCCCC)CCCCCCCC)=O)=C(S1)C3=C(N=C(C(S4)=NC5=C4C(SC(C)=C6)=C6C(N(CC(CCCCC)CCCCC)C5=O)=O)S3)C2=O</chem>	0	1.61
30	<chem>CC1=CC(C(N2CC(CCCCCCCCCC)CCCCCCCC)=O)=C(S1)C(SC(C)=C3)=C3C2=O</chem>	0	3.71
31	<chem>O=C1OC2=C(C=C(OC(/C3=C4C(C=CC(/C=C/C)=C5F)=C5N(CCCC(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCC)CCCC)C4=O)=O)C3=C2)/C1=C(C6=C(N7CCCC(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC)C(F)=C(C)C=C6)\C7=O</chem>	0	1.7
32	<chem>CC1=CC(C(N2CC(CCCCC)CCCCCCCC)=O)=C(S1)C3=C(N=C(C(S4)=NC5=C4C(SC(C6=C(F)C(F)=C(C)S6)=C7)=C7C(N(CC(CCCCC)CCCCCCCC)C5=O)=O)S3)C2=O</chem>	0	0.91
33	<chem>O=C1C2=CC=C3C4=C2C(C(N1CC(CCCCCCCCC)CCCCCCCCC)=O)=CC(C5=CC=C(C(C=CC(C)=C6)=C6C7=O)C7=C5)=C4C8=CC=C9C%10=C(C(N(CC(CCCCCCCCC)CCCCCCCCCCCCC)C9=O)=O)C=C(C)C3=C8%10</chem>	0	0.01
34	<chem>CC1=CC2=C(N=C(C3=CC=C(/C(N(C)C4=O)=N/C)C5=C4C=CC6=C35)N2C6=O)C=C1C</chem>	0	0.1
35	<chem>CC1=CC(C(N2CC(CCCCC)CCCCCCCC)=O)=C(S1)C3=C(N=C(C(S4)=NC5=C4C(SC(C6=CC=C(C)S6)=C7)=C7C(N(C(CCCCC)CCCCCCCC)C5=O)=O)S3)C2=O</chem>	0	0.2
36	<chem>CC1=CC2=C(N=C(C3=CC=C(C4=NC(C=C(C)C(C)=C5)=C5N4C6=O)C7=C6C=CC8=C37)N2C8=O)C=C1C</chem>	0	0
37	<chem>N(CCCC(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC)CCC(C4=O)=O)C3=C2)/C1=C(C6=C(N7CCCC(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC)C=C(C)C=C6)\C7=O</chem>	0	1.4

38	O=C(N1CC(CCCCCCCCCC)CCCCCCCCCCCC)C2=C(SC(C)=C2)C3=C(C=C(C(SC(C4=CC=C(C)S4)=C5)=C5C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C6=O)=O)C6=C3)C1=O	0	0.11
39	=C5C(N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)=O)SC6=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C(C7=C6SC(C)=C7)=	0	2.73
40	CCCCCCCCCCCC)C(/C2=C3C(C=C(OC(/C4=C5C(C=CC(/C=C/C)=C6)=C6N(CC(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C\5=O)=O)C4=C7)=C7OC\3=O)=O)=C	0	0.9
41	CC1=CC=C2C(N(CCCCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C(/C2=C3C(C=C(OC(/C4=C5C(C=C(C(/C=C/C)=C6)=C6N(CCCCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C\5=O)=O)C4=C7)=C7OC\3=O)=O)=C1	0	0.76
42	CC1=CC=C2C(N(CCCCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C(/C2=C3C(C=C(OC(/C4=C5C(C=CC(/C=C/C)=C6)=C6N(CCCCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C\5=O)=O)C4=C7)=C7OC\3=O)=O)=C1	0	0.6
43	O=C(N1CC(CCCCCCCCCC)CCCCCCCCC)C2=C(SC(C)=C2F)C(SC3=C4SC5=C3C(N(CC(CCCCCCCCCC)CCCCCCCCC)C(C6=C5SC(C7=CC=C(C)S7)=C6F)=O)=O)=C4C1=O	0.0001	0
44	O=C(SC1=CC=C(C#CC2=C(OCCCCC)C=C(C#CC(C=C3)=CC=C3SC(C)=O)C(OCCCCC)=C2)C=C1)C	0.1	0
45	O=C(N(CC(CCCCCCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=CC=C(C4=C(F)C(F)=C(C5=CC=C(C)S5)C6=NSN=C64)S3)C=C7C8=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C7=O)=O)C(C)=CC1=C82	0	2.2
46	O=C1C2=CC=C3C4=C2C(C(N1CC(CCCCCCCCCC)CCCCCCCCCCCC)=O)=CC(C5=CC(SC6=C7SC(C)=C6)=C7S5)=C4C8=CC=C9C%10=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C9=O)=O)C=C(C)C3=C8%10	0	0.013
47	O=C1C2=C3C(C(N1CC(CCCCCCCCCC)CCCCCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C6=CC=CC=C6)[Se]5)[Se]4)C=C7C3=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C7=O)=O)C(C8=CC=C(C9=CC=CC=C9)C=C8)=C2	0	0.24
48	O=C(N(CCCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C1=O)C2=C(C3=CC=C(C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CCCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C5=O)=O)C(C)=CC1=C62	0	6.5
49	CC1=CC=C(C2=C3C=C(C)C=C2)C(C3(CCCCCC)CCCCCCC)=C1	0	0
50	O=C(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=C(C=C(C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CC(CCCCCCCCCC)CCCCCCCCC)C5=O)=O)C(C)=CC1=C62	0	3.2
51	O=C(N(CC(CCCCCCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=CC=C(C4=C(F)C(F)=C(C5=CC=C(C)[Se]5)C6=NSN=C64)[Se]3)C=C7C8=C(C(N(CC(CCCCCCCCCC)CCCCCCCCC)C7=O)=O)C(C)=CC1=C82	0	3.5
52	FC1=C(C)C=CC(/C2=C3C(N(CCCC(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)C4=C\3C=CC(C5=C(F)C(F)=C(C6=C(F)C(F)=C(C)S6)S5)=C4F)=O)=C1N(CCCC(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)C2=O	0	1.35
53	O=C(C1=C2C(C3=CC=C24)=C(C5=C6C3=C(C7=CC=C(C8=CC=C(C)S8)S7)C=C9C6=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C9=O)=O)C=C5)C(C)=C1)N(CC(CCCCCC)CCCCCCCCCCCC)C4=O	0	0.002

[illegible]

	O=C(N1CCCCCCCCOCCOCCOCCOC)C2=C(C3=CC=C(C/C		
69	=C/C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CCCCCCCCCOCCO	0	1.64
	CCOCCOC)C5=O)=O)C(C)=CC(C1=O)=C26		
	O=C(C1=C2C(C3=CC(C4=CC=C/C=C/C5=CC=C(C)S5)S4		
70	)=C26)=C(C(N(CCCCCCCCCOCCOCCOCCOCCOCC)C3=O)=O)	0	1.64
	C(C)=C1)N(CCCCCCCCCOCCOCCOCCOCCOCC)C6=O		
	O=C1C2=CC=C3C4=C2C(C(N1CC(CCCCCCCCCC)CCCCC		
71	CCCCCCC)=O)=CC(C5=CC=C(N(CCCCCC)C(C=CC(C)=C6	0	0.05
	)=C6S7)C7=C5)=C4C8=CC=C9C%10=C(C(N(CCCCCC		
	CCCC)CCCCCCCCCCCC)C9=O)=O)C=C(C)C3=C8%10		
	CC(C)(C)C1=CC2=C(C(C=C(C(C3C(C=CC=C4)=C4C5=C3		
72	C=CC=C5)C6=C7C=CC(C(C)(C)C)=C6)C7=C8)=C8C2C9C(	0	0.0001
	C=CC=C%10)=C%10C%11=C9C=CC=C%11)C=C1		
	CC1=CC(CCCCCCCCCCCC)=C(C2=CC(CCCCCCCCCCCC)		
73	=C(C3=CC=C(C(C=C/C(C4=C5C=CC(C6=C(CCCCCCCCCC	0.0002	0.0002
	CCC)C=C(C7=C(CCCCCCCCCCCC)C=C(C)S7)S6)=C4)=C(		
	C#N)/C#N)C5=C8)=C8/C9=C(C#N)/C#N)C9=C3)S2)S1		
	O=C/C1=C2C(C=CC(C3=CC=C(C4=CC=C(C)S4)S3)=C5F		
74	)=C5N(CCCCC(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCC	1.85	0.43
	C\2=O)N(CCCCC(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCC		
	C)C6=C1C=CC(C)=C6F		
	CC1=CN=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCC)=O)=		
75	C(C4=CC=C(C5=C(F)C(F)=C(C)S5)C=N4)N(CC(CCCCCC)C	0	0.13
	CCCCCCC)C3=O)C=C1		
	O=C1C(C2=C(C3=NC=C(C)C=C3)N1CC(CCCCCCCCCC)C		
76	CCCCCCC)=C(C4=NC=C(C5=CC=C(C6=CC=C(C)S6)S5)C	2.78	6.3
	=C4)N(CC(CCCCCCCCCC)CCCCCCCC)C2=O		
	CC1=CC=C(C2=C3C=C(C4=CC(SC(C)=C5)=C5S4)C=C2)C		
77	(C3(CCCCCCCC)CCCCCCCC)=C1	0.0011	0
	O=C1C2=C(C)SC(C3=CC=C(C4=C(CCCCCCCCCCCC)C5=		
78	C(C(CCCCCCCCCCCC)=C(C6=CC=C(C)S6)S5)S4)S3)=C2C(	1.29	0
	N1CC(CCCCCCCC)CCCCCCCCCCC)=O		
	CC1=C(CC(CCCCCCCCCC)CCCCCCCCCCCC)C=C(C(C(S2)		
79	=O)=C3C2=C(C4=CC(CC(CCCCCCCCCCCC)CCCCCCCCC	0	0.25
	C)=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)C(S3)=O)S1		
	C\1=C\1(C\1)C\2=C\2(C\3=C\3(C\4=C\4(C\5=C\5)S		
80	S4)=C6)N(CCCCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C)C\	2.48	0
	3=O)=O)CCCCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C)C=C2C=		
	^1		
81	CC1=CC(N(CC(CCCCCCCC)CCCCCCCCCCC)C/C2=C3C(C=	1.06	0
	CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6N(CC(CCCCCC		
	CCCC)CCCCCCCC)C\3=O)=O)=C2C=C1		
	CC1=CC(N(CCC(CCCCCCCC)CCCCCCCCCCC)C/C2=C3C(C		
82	=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6N(CCC(CCCC	0.4	0
	CCCCC)CCCCCCCC)C\3=O)=O)=C2C=C1		
	CC1=CC(N(CCCC(CCCCCCCC)CCCCCCCCCCC)C/C2=C3C(		
83	C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6N(CCCC(CC	3.62	0
	CCCCCCCC)CCCCCCCC)C\3=O)=O)=C2C=C1		
	CC1=CC(N(CCCCC(CCCCCCCC)CCCCCCCCCCC)C/C2=C3		
84	C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6N(CCCCC	1.76	0
	(CCCCCCCCCCC)CCCCCCCC)C\3=O)=O)=C2C=C1		
	CC1=CN=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCC)=O)=		
85	C(C4=CC=C(C5=CC=C(C)S5)C=N4)N(CC(CCCCCC)CCCC	0	0.55
	CCCC)C3=O)C=C1		
	CC1=C(CCCCCCCCCC)C=C(C(S2)=CC3=C2SC(C4=CC(CC		
86	CCCCCCCC)=C(C)S4)=C3)S1	0.15	0
	O=C1C2=C3C(C(N1CC(CCCCCCCCCC)CCCCCCCCCCCCC		
87	=O)=CC(C4=CC=C5C(SC6=C(C=CC(C)=C6)N5CCCCC)=	0	0.05
	C4)=C7C3=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCCC		
	=O)=O)C=C2C		

88	O=C1C(C2=C(C3=CC4=C(S3)C=C(C)S4)C1CC(CCCCCCCC CC)CCCCCCCC)=C(C5=CC(SC(C)=C6)=C6S5)C(CC(CCCC CCCC)CCCCCCCCCCC)C2=O	0	0
89	$\text{O}=\text{C}(\text{C}1=\text{C}(\text{C}2=\text{CC}=\text{C}(\text{C}3=\text{C}(\text{C}4=\text{CC}=\text{C}(\text{C}5=\text{CC}=\text{C}(\text{C}6=\text{CC}=\text{C}(\text{C}7=\text{NSN}=\text{C}57)\text{S}4)=\text{C}2)=\text{C}3\text{S}1$ S4)\C#N)S3)S2)N5CC(CCCCCCCCCCCC)CCCCCCCCCCC)N(CC(CCCCCCCCCCCC)CCCCCCCCCCC)C(C6=CC=C(C)S6)=	0.75	7
90	$\text{CC}1=\text{CC}(\text{CCCCCCCCCCCC})=\text{C}(\text{C}2=\text{CC}(\text{SC}(\text{C}3=\text{C}(\text{CCCC}$ CCCCCCCCCCC)C=C(C)S3)=C4)=C4S2)S1	0.72	0
91	CC1=CN=C(C(N(CC(CCCCCCCCCCCC)CCCCCCCCCCC)C2 =O)=C3C2=C(C4=NC=C(C5=CC6=C(C=C(C=C(C)S7)C7= C6)S5)S4)N(CC(CCCCCCCCCCCC)CCCCCCCCCCCC)C3=O)S1	5.47	5.33
92	CC1=CC=C(C2=C3C=C(C4=CC=C(C5=CC=C(C)[Se]5)[Se] 4)C=C2)C(C3(CCCCCCCC)CCCCCCCC)=C1	0.012	0
93	CC1=CC([Ge])(CC(CCCCCCCCCCCC)CCCCCCCC)(CC(CCCCC CCCC)CCCCCCCC)C2=C3SC(C4=CC=C(C5=C(C#N)C(C# N)=C(C6=CC=C(C)S6)C7=NSN=C57)S4)=C2)=C3S1	0	0.0028
94	CC1=CC(CC(CCCCCCCCCCCC)CCCCCCCC)=C(C2=CC3=C(C =C(C4=C(CC(CCCCCCCCCCCC)CCCCCCCC)C=C(C5=C(N=S =N6)C6=C(C)C7=NSN=C75)S4)S3)S2)S1	1	0.7
95	O=C(N1CCCC(CCCCCCCCCCCC)CCCCCCCCCCC)/C(C2=C1C =C(C)C=C2)=C3C(N(CCCCCCCCCCCCC)C4=C/3C=C5C(/C(C(N5CCCCCCCCCCCC)=O)=C6C(N(CCCC(CCCCCCCCCCCC) CCCCCCCCCCC)C7=C\6C=CC(C8=CC=C(/C=C/C9=CC=C(C)S9)S8)=C7)=O)=C4)=O	1.92	0
96	CC1=CC(CCCCCCCCCCCC)=C(C2=CC3=C(C(SC(C4=C(CC CCCCCCCCCCC)C=C(C)S4)=C5)=C5S3)S2)S1	0.5	0
97	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCC)CCCCCCC CCCCCCCC)=O)=C(C4=CC=C(C5=CC6=C(C=C(C=C(C)S7)C7=C6)S5)S4)N(CC(CCCCCCCCCCCCC)CCCCCCCCCCCCC C)C3=O)S1	1.31	0
98	O=C1C(C2=C(C3=CC=C(C4=C(F)C(F)=C(C)C(F)=C4F)S3) N1CC(CCCCCCCC)CCCCCCCCCCC)=C(C5=CC=C(C)S5)N(C C(CCCCCCCCCCCC)CCCCCCCC)C2=O	0	2.36
99	O=C(N1CCCCCCCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)/C(C 2=C1C=C(C)C=C2)=C(C(N3CCCCCCCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)=O)\C4=C3C=C(C5=CC=C(C6=CC=C(C)O 6)O5)C=C4	4.8	0
100	CC1=CC(CCCCCCCCCCCC)=C(C2=NC(CCCCCCCCCCCCC) =C(C3=C(CCCCCCCCCCCCC)N=C(C4=C(CCCCCCCCCCCCC) C=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)S3)S2)S1	0.33	0
101	O=C1C(C2=C(C3=CC=C(C)S3)N1CCCC[Si](C)(O[Si](C)(C) C)O[Si](C)(C)C)=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CCC CC[Si](C)(O[Si](C)(C)C)O[Si](C)(C)C)C2=O	8.84	4.34
102	O=C1C(C2=C(C3=CC=C(C4=CC=C(C)[Se]4)S3)N1CC(CCC CCC)CCCCCCCC)=C(C5=CC=C(C)S5)N(CC(CCCCCC)CCC CCCC)C2=O	1.62	0.14
103	CC(S1)=CC2=C1C3=C(C2(CCCCCCCCCCCCCCCCC)CCCCC CCCCCCCCCCCC)C=C(C4=CC=C(C)C5=NSN=C54)S3	3.3	0
104	O=C(N(C(C1=CC=C(C)S1)=C2C3=O)CC(CCCCCCCCCCCC)CCCCCCCCCCCCCCC)C2=C(C4=CC=C(C5=CC6=C(C(C=C (C=C(C)S7)C7=C8)=C8C=C6)S5)S4)N3CC(CCCCCCCCCCCC C)CCCCCCCCCCCCCCC	0.78	0
105	O=C1C(C2=C(C)N1CC(CCCCCCCCCCCC)CCCCCCCC)=C(C3 =CC=C(C4=CC5=C(C=C(C6=CC=C(C)S6)S5)S4)S3)N(CC(CCCCCCCCCCC)CCCCCCCC)C2=O	10.5	0
106	$\text{CC}1=\text{CC}=\text{C}(\text{C}2=\text{CC}=\text{C}(\text{C}3=\text{C}(\text{C}4=\text{CC}=\text{C}(\text{C}5=\text{CC}6=\text{C}(\text{C}(\text{SC}(\text{C})=\text{C}7)=$ CCCCCCCC)=O)=C(C4=CC=C(C5=CC6=C(C(SC(C)=C7)= C7S6)S5)S4)N(CC(CCCCCCCCCCCCC)CCCCCCCCCCCCCCC) C2=O)C1	2.31	0

107	CCCCCCCCC(CC1=C(C2=CC=C(C(C3=NSN=C3C(C)=C4F)=C4[H])S2)SC(C5=CC(CC(CCCCCCCC)CCCCCCCCC)=C(S5)C(S6)=CC=C6C)=C1)CCCCCCCCC	0	0.39
108	CCCCC1(CCCC)C2=C(C=CC(C3=C(CCCCCC)C=C(C4=CC(SC(C5=CC(CCCCCC)=C(C)S5)=C6)=C6S4)S3)=C2)C7=CC=C(C)C=C71	0.0002	0
109	CCCCC1(CCCC)C2=C(C=CC(C3=CC(CCCCCC)=C(C4=CC(SC(C5=CC(CCCCCC)=C(C)S5)=C6)=C6S4)S3)=C2)C7=CC=C(C)C=C71	0.0005	0
110	CC1=C(CCCCCCCCCC)C=C(C2=CC3=C(C(CCCCCCCCCC)C)=C(C=C(C4=C(C)C=C(C)S4)S5)C5=C3CCCCCCCCCCCCC)S2)S1	0.15	0
111	CC(CCCC(C)C)CCC1(CCC(C)CCCC(C)C)C2=C(SC(C)=C2)C3=C1C=C(C4=CC=C(C)C5=NSN=C54)S3	3.3	0
112	CC1=C(CC(CCCCCCCCCC)CCCCCCCCC)C=C(C2=C(N=S=N3)C3=C(C4=CC(CC(CCCCCCCCCC)CCCCCCCCC)=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)C7=NSN=C72)S1	2.5	0
113	CC1=C(CCCCCCCCCCCCCC)C(SC2=C3SC4=C2SC(C5=CC=C(C6=CC=C(C)S6)S5)=C4CCCCCCCCCCCCC)=C3S1	0.33	0
114	O=C(N1CC(CCCCCCCC)CCCCCCCCC)C(C2=C1C3=CC4=C(S3)C=C(C)S4)=C(C5=CC(SC(C6=CC=C(C)S6)=C7)=C7S5)N(CC(CCCCCCCC)CCCCCCCCC)C2=O	1.95	0
115	CC1=CC(CCCCCCCCCCCCCC)=C(S1)C(S2)=CC3=C2C(SC(C(SC(C)=C4)=C4CCCCCCCCCCCCC)=C5)=C5C=C3	1.95	0
116	CCC(CCCC)CC1=C(C2=CC=C(C3=C(CC(CCCC)CC)C=C(C4=CC(C(CC(CCCC)CC)(CC(CC)CCCC)C5=C6C=CC(C7=CC=CC=C7)=C5)=C6C=C4)S3)S2)SC(C8=CC=CC=C8)=C1	0.07	0.05
117	O=C1C(C2=C(C3=CC=C(C4=CC=C(C)C5=NSN=C45)S3)N1CC(CCCCCCCCCC)CCCCCCCCC)=C(C6=CC=C(C)S6)N(C(C(CCCCCCCC)CCCCCCCCC)C2=O	0.35	0.4
118	CC(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=O)=C(C1=C(C2=CC=C(C3=CC=C(C4=CC=C(C)S4)C5=NSN=C53)S2)N6CC(CCCCCCCC)CCCCCCCCC)C6=O	0.35	0.4
119	O=C1C(C2=C(C3=CC=C(C4=CC=C(C(N5CCOCCOCCOC)=C(C(C5=O)=C(C6=CC=C(C)S6)N7CCOCCOCCOC)C7=O)S4)S3)N1CC(CCCCCCCCCC)CCCCCCCCC)=C(C8=CC=C(C)S8)N(CC(CCCCCCCCCC)CCCCCCCCC)C2=O	0	3
120	O=C1C(C2=C(C3=CC=C(C4=CC=C(C)C5=NSN=C45)[Se]3)N1CC(CCCCCCCCCC)CCCCCCCCC)=C(C6=CC=C(C)[Se]6)N(CC(CCCCCCCC)CCCCCCCCC)C2=O	0.46	0.84
121	CCCCCCCCC(CC1=C(C2=CC=C(C(C3=NSN=C3C(C)=C4F)=C4F)S2)SC(C5=CC(CC(CCCCCCCC)CCCCCCCCC)=C(S5)C(S6)=CC=C6C)=C1)CCCCCCCCC	0	0.29
122	O=C1C(C2=C(C3=CC=C(C4=CC=C(C)C5=NSN=C45)S3)N1CC(CCCCCCCCCC)CCCCCCCCC)=C(C6=CC=C(C)S6)N(CC(CCCCCCCCCCCC)CCCCCCCCC)C2=O	3.4	5.86
123	O=C1C(C2=C(C3=CC=C(C)S3)N1CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)=C(C4=CC=C(C5=CC6=C(C=C/C=C/C7=CC8=C(C=C(C)S8)S7)S6)S5)S4)N(CC(CCCCCCCCCCCC)CCCCCCCCCCCCC)C2=O	7.43	0
124	O=C(C1=C(C2=CC=C(C3=CC=CS3)S2)N4CC(CCCCCCCCCCCC)CCCCCCCCCCCCN(CC(CCCCCCCCCC)CCCCCCCCCCC)C(C5=CC=C(C6=CC=C(C/C=C/C7=CC=C(C8=CC=CS8)[Se]7)[Se]6)S5)=C1C4=O	4.97	0
125	O=C(C1=C(C2=CC=C(C3=CC=C(C/C=C/C4=CC=C(C)[Se]4)[Se]3)S2)N5C(CCCCCCCCCCCCCC)CCCCCCCCC)N(C(CCC(CCCCCCCC)CCCCCCCCC)C(C6=CC=C(C)S6)=C1C5=O	4.4	0

126	$\begin{aligned} & \text{C(C)S5)S4)S3)N1CC(CCCCCCCCCC)CCCCCCCCCCCC)=C(} \\ & \text{C6=CC=C(C)S6)N(CC(CCCCCCCCCCCC)CCCCCCCCCCC)C2} \end{aligned}$	0.749	7
127	$\begin{aligned} & \text{=C4C(N(C5=C4C=CC=C5)C(C(C6=CC=C(C7=C(CCCCCC} \\ & \text{CCCCC)C=C(C8=CC9=C(C(OCC(CCCCCCCCCC)CCCCC} \\ & \text{CC)=C(C=C(C)S\%10)C\%10=C9OCC(CCCCCCCCCC)CCCC} \\ & \text{CCC)S8)S7)S6)=C\%11\%12)=O)=C\%11N1C\%13=C\%12C=CC} \end{aligned}$	1.5	0.41
128	$\begin{aligned} & \text{CC1=C(F)C(F)=C(C2=CC(CC(CCCCCCCCCC)CCCCCCCCC} \\ & \text{CCC)=C(C3=CC=C(C4=CC=C(C5=C(CC(CCCCCCCCCCCC} \\ & \text{)CCCCCCCCC)C=C(C)S5)S4)S3)S2)C6=NSN=C16} \end{aligned}$	1.92	0
129	$\begin{aligned} & \text{O=C1N(CC(CCCCCCCC)CCCCCCCCC)C(C)=C2C(N(CC(C} \\ & \text{CCCCC)CCCCCCCCC)C(C3=CC=C(C4=CC=C(C5=CC} \\ & \text{=C(C6=CC=C(C7=CC=C(C8=CC=C(C)S8)S7)S6)S5)S4)S3)} \\ & \text{=C12)=O} \end{aligned}$	3.94	0
130	$\begin{aligned} & \text{C)C2=C3C=C(C(CCCCCCCCCCCCCC)(CCCCCCCCCCC} \\ & \text{CCCC)C4=C5SC(C6=CC=C(C)C7=NSN=C67)=C4)C5=C} \end{aligned}$	3.6	0
131	$\begin{aligned} & \text{O=C1C(C2=C(C3=CC=C(C)S3)N1CC(CCCCCC)CCCC} \\ & \text{CCCC)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)S} \\ & \text{5)S4)N(CC(CCCCCC)CCCCCCCCC)C2=O} \end{aligned}$	4.5	0
132	$\begin{aligned} & \text{O=C1C(C2=C(C3=CC=C(C)S3)N1CC(CCCCCCCCCC)CCC} \\ & \text{CCCCCCCC)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C} \\ & \text{)S6)S5)S4)N(CCC(CCCCCCCCCC)CCCCCCCCCCCC)C2=O} \end{aligned}$	8.2	0
133	$\begin{aligned} & \text{O=C(C1=C(C2=CC=C(C3=CC=C(/C=C/C4=CC=C(C)S4)S} \\ & \text{3)S2)N5C(CCCCCCCCCCCC)CCCCCCCCC)N(C(CCCCCC} \\ & \text{CCCC)CCCCCCCCC)C(C6=CC=C(C)S6)=C1C5=O} \end{aligned}$	2.8	0
134	$\begin{aligned} & \text{CC1=CC=C(N(C2=CC=C(C)C=C2C)C3=CC=C(C=C3)C)C=} \\ & \text{C1} \end{aligned}$	0.01	0
135	$\begin{aligned} & \text{CC1=CC(SC2=C3C(CCCCCCCCCCCCCC)(CCCCCCCCC} \\ & \text{CCCCC)C4=C2C=C(C(C(CCCCCCCCCCCCCC)(CCCCC} \\ & \text{CCCCCCCCCCC)C5=C6SC7=C5SC(C8=CC=C(C)C9=NSN} \\ & \text{=C98)=C7)C6=C4)=C3S1} \end{aligned}$	8.7	0
136	$\begin{aligned} & \text{O=C1C(C2=C(C3=CC=C(C4=CC5=C(C=C(C(C=C(SC(C)=} \\ & \text{C6)C6=C7)=C7N8CCCCCCCCCCCC)C8=C5)S4)S3)N1CC(} \\ & \text{CCCCCCCC)CCCCCCCCC)=C(C9=CC=C(C)S9)N(CC(CCC} \\ & \text{CCCC)CCCCCCCCC)C2=O} \end{aligned}$	1.36	0
137	$\begin{aligned} & \text{O=C(N(CC(CCCCCC)CCCCCCCCC)C1=C/2SC(C)=C1)} \\ & \text{C2=C3C4=C(C=C(C5=CC=C(C)C6=NSN=C65)S4)N(CC(C} \\ & \text{CCCCCCCC)CCCCCCCC)C/3=O} \end{aligned}$	0.16	0.14
138	$\begin{aligned} & \text{O=C1C(C2=C(C3=CC=C(C4=CC=C(C)[Se]4)[Se]3)N1CC(C} \\ & \text{CCCCCCCC)CCCCCCCC)=C(C5=CC=C(C)S5)N(CC(CCCC} \\ & \text{CCCCC)CCCCCCCC)C2=O} \end{aligned}$	1.57	0.81
139	$\begin{aligned} & \text{O=C1N(CC(CCCCCC)CCCCCCCCC)C(C)=C2C(N(CC(C} \\ & \text{CCCCC)CCCCCCCCC)C(C3=CC=C(C4=CC=C(C5=CC} \\ & \text{=C(C6=CC=C(C7=CC=C(C8=CC=C(C9=CC=C(C)S9)S8)S7} \\ & \text{)S6)S5)S4)S3)=C12)=O} \end{aligned}$	2.82	0
140	$\begin{aligned} & \text{CC1=CC(CCCCCCCCCCCCCC)=C(/C=C/C2=C(CCCCCC} \\ & \text{CCCCC)C=C(C3=CC4=C(C=C(C)S4)S3)S2)S1} \\ & \text{CCCCCCCCCCCCCCCC1(CCCCCCCCCCCCCC)C2=C(S} \\ & \text{C(C3=CN=C(C)S4)=CC5=C4C6=C(C5(CCCCCCCCCCCC} \end{aligned}$	4.6	0
141	$\begin{aligned} & \text{CCC)CCCCCCCCCCCCC)C=C(C7=NC=C(C8=CC=CS8} \\ & \text{)C9=NSN=C79)S6)C\%10=NSN=C\%103)=C2)C\%11=C1C=C} \\ & \text{(S\%11)C\%12=CC=CS\%12} \end{aligned}$	36.3	0
142	$\begin{aligned} & \text{CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC} \\ & \text{CCCCCCCC)=O)=C(C4=CC=C(C5=CC6=C(C(SC7=C8SC(C} \\ & \text{)=C7)=C8S6)S5)S4)N(CC(CCCCCCCCCCCC)CCCCCCCCC} \\ & \text{CCCC)C3=O)S1} \end{aligned}$	3.2	0

143	O=C1N(CC(CCCCCCCCCC)CCCCCCCCC)C(C2=CC=C(C)S2)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCC)C(C4=CC=C(C5=CC=C(C6=CC=C(C=C6)C7=CC=C(C)S7)S5)S4)=C13)=O	3.46	0
144	O=C(/C1=C(C2=C(N3CC(CCCCCCCC)CCCCCCCCC)C=C(C4=CC=C(C=C(C)C=C5)C5=C4)S2)/C3=O)N(CC(CCCCCC)CCCCCCCCC)C6=C1SC(C)=C6	14.4	0
145	CC1=CC(CCCCCCCCCCCCCCCCCC)=C(/C=C/C2=C(CCC(CCCCCCCCCCCCCC)C=C(C3=CC4=C(C(SC(C)=C5)=C5S4)S3)S2)S1	3.91	0
146	CC1=CC=C(C(N(CC(CCCCCCCC)CCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC6=C(/C(C7=C6C=CC=C7)=C8C(C=CC=C9)=C9C%10=C\8SC(C)=C%10)S5)S4)N(CC(CCCCCC)CCCCCCCCC)C3=O)S1	0.68	0.13
147	O=C1N(CC(CCCCCCCC)CCCCCCCCC)C(C2=CC=CC(C)S2)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCC)C(C4=CC=C(C5=CC=C(C6=CC=C(C7=CC=C(C)S7)S6)S5)S4)=C1	3.98	0
148	O=C1N(CC(CCCCCC)CCCCCCCCC)C(C2=CC(SC(C)=C3)=C3S2)=C4C1=C(C5=CC(SC(C6=CC=C(C)S6)=C7)=C7S5)N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O	2	0
149	CC1=CC(CCCCCCCCCCCCCC)=C(C2=CC=C(C3=CC=C(C4=C(CCCCCCCCCCCCCC)C=C(C)S4)S3)S2)S1	0.14	0
150	O=C(C1=C(C2=CC=C(C)S2)N3C(CCCCCCCCCC)CCCCC(CCCCCC)N(C(CCCCCCCCCC)CCCCCCCCCCCC)C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)=C1C3=O	3.37	0
151	O=C(C1=C(C2=CC=C(C)S2)N3CCCC(CCCCCCCCCC)CCC(CCCCCCCC)N(CCCC(CCCCCCCCCC)CCCCCCCCCCCC)C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)=C1C3=O	6.9	0
152	O=C1N(CC(CCCCCCCCCCCC)CCCCCCCCC)C(C2=CC=C(C)S2)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C(C4=CC=C(C5=CC=C(C6=CC=C(C7=CC=C(C)S7)[Se]6)S5)S4)=C13)=O	2.38	0
153	O=C(C1=C(C2=CC=C(C)S2)N3CC(CCCCCCCC)CCCCCCC(CCC)N(CC(CCCCCCCC)CCCCCCCCC)C(C4=CC=C(C5=C(C=C6=CC=C(C)[Se]6)[Se]5)S4)=C1C3=O	1.5	0
154	O=C1N(CC(CCCCCCCCCCCC)CCCCCCCCC)C(C2=CC=C(C)S2)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C(C4=CC=C(C5=CC=C(C6=CC=C(C7=CC=C(C)[Se]7)[Se]6)[Se]5)S4)=C13)=O	5	0
155	CC1=CC=C(C(N(CC(CCCCCCCCCC)CCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C6=CC=C(C7=CC=C(C)S7)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)S1	0.97	0
156	CC1=CC=C(C(N(CC(CCCCCCCCCC)CCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C6=CC=C(C7=CC=C(C)[Se]7)[Se]6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)S1	1.5	0
157	O=C1N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCCC)C(C2=CC=C(C)S2)=C3C1=C(C4=CC=C(C5=CC=C(/C=C/C6=C(C=C(C)[Se]6)[Se]5)S4)N(CCCCCC(CCCCCCCCCC)CCCCC(CCCCCC)C3=O	8.2	0
158	O=C1N(CC(CCCCCCCCCC)CCCCCCCCC)C(C2=CC=C(C)S2)=C3C1=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)[Se]6)[Se]5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C3=O	5	0
159	O=C1N(CC(CCCCCCCCCC)CCCCCCCCC)C(C2=CC=C(C3=CC=C(C4=CC=C(C)S4)S3)O2)=C5C(N(CC(CCCCCCCCCC)CCCCCCCCC)C(C6=CC=C(C)O6)=C15)=O	1.54	0
160	CC1=C(CC(CCCCCCCC)CCCCCCCCC)C=C(C2=C(N=S=N3)C3=C(C4=CC(CC(CCCCCCCCCC)CCCCCCCCC)=C(C5=CC6=C(C=C(C)S6)S5)S4)C7=NSN=C72)S1	1	0.7

[illegible]

178	<chem>O=C1N(CC(CCCCCCCC)CCCCCCCCC)C(C2=CC=C(C3=CC=C(C4=CC=C(C5=CC=CC=C5)S4)S3)S2)=C6C(N(CC(CCCCCCCC)CCCCCCCC)C(C7=CC=C(S7)C8=CC=CC=C8)=C61)=O</chem>	0.74	0
179	<chem>O=C(/C1=C2C(C=CC(C3=CC=C(C)S3)=C4)=C4N(CC(CCC(CCCCCC)CCCCCCCC)C\2=O)N(CC(CCCCCCCCCC)CCCC(CCC)C5=C1C=CC(C)=C5</chem>	0.4	0.7
180	<chem>O=C(N(CCCCCCCCCC(F)(C(F)(C(F)(C(F)(C(F)(C(F)(F)F)F)F)F)F)C1=O)C2=C(C3=CC=C(C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CCCCCCCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C5=O)=O)C(C)=CC1=C62</chem>	0	6.5
181	<chem>O=C(N(CCCC[Si](C)(O[Si](C)(C)C)O[Si](C)(C)C)C1=O)C2=C(C3=CC=C(C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CCCC[Si](C)(O[Si](C)(C)C)O[Si](C)(C)C)C5=O)=O)C(C)=CC1=C62</chem>	0	1.04
182	<chem>O=C(N(CCCCCCOCOCOCOCOC)C1=O)C2=C(C3=CC=C(/C=C/C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CCCCCCOCOCOCOCOC)C5=O)=O)C(C)=CC1=C62</chem>	0	1.6
183	<chem>C=C(/C(CCO)=C(C4=CC=C(C)[Se]4)\CCO)[Se]3)C=C5C6=C(C(N(CC(CCCCCCCCCC)CCCCCCCC)C5=O)=O)C(C)=CC1=C62</chem>	0	0.65
184	<chem>O=C1C(C2=C(C3=CC=C(C)[Se]3)N1CCCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)=C(C4=CC=C(C)S4)N(CCCCCC[Si](O[Si](C)(C)C)O[Si](C)(C)C)C2=O</chem>	0	1.13
185	<chem>O=C1C(C2=C(C3=CN=C(C4=NC=C(C)S4)S3)N1CC(CCCC(CCCCCC)CCCCCCCCCCCC)=C(C5=CC=C(C)S5)N(CC(CCC(CCCCCCCCCC)CCCCCCCCCCCC)C2=O</chem>	0	1.13
186	<chem>O=C1C(C2=C(C3=C(F)C(F)=C(C)C(F)=C3F)N1CC(CCCCCC(CC)CCCCC)=C(C4=CC=C(C)S4)N(CC(CCCCCC)CCCCC(CC)C2=O</chem>	0	2.36
187	<chem>O=C1C(C2=C(C3=CC=C(C4=CC=C(C)S4)S3)N1CC(CCCC(CCCCCC)CCCCCCCC)=C(C5=CN=C(C)C=C5)N(CC(CCCC(CCCC)CCCCCCCC)C2=O</chem>	0	6.3
188	<chem>O=C1C(C2=C(C3=CC4=C(C=C(C)S4)S3)N1CC(CCCCCC(CCC)CCCCCCCC)=C(C5=CN=C(C)C=C5)N(CC(CCCCCC(C)CCCCCCCC)C2=O</chem>	0	3.36
189	<chem>C2=C3C(C=CC(C4=CC(F)=C(C5=C(F)C=C(C)S5)S4)=C6F)=C6N(CCCC(CCCCCCCCCC)CCCCCCCCC)C\3=O)=O)=^{1F} <chem>O=C(N1C2=C3C=C(OCC(CCCCCCCCCC)CCCCCCCC)C=C2)C(C4=CC=C(C5=CC=C(C)C6=NSN=C65)S4)=C7C8=C1C3=C(C9=CC=C(C)S9)C(N8C%10=C7C=C(OCC(CCCCCC(C)CCCCCCCC)C=C%10)=O</chem></chem>	0	9.7
190	<chem>CC1=NC(CCCCCCCC)=C(C2=CC3=C(C(SC(C4=C(CCCCC(CCC)N=C(C)S4)=C5)=C5N3CC(CCCCCC)CCCCCCCC)S2)S</chem>	0	3.1
191	<chem>CC1=NC(CCCCCCCCCCCC)=C(C2=CC3=C(C(SC(C4=C(C(CCCCCCCCCC)N=C(C)S4)=C5)=C5N3CC(CCCCCC)CCC(CCCCC)S2)S1</chem>	0.14	0
192	<chem>CC1=C(CCCCCCCCCCCCCC)C(SC2=C3SC4=C2SC(C5=CC=C(C)S5)=C4CCCCCCCCCCCCC)=C3S1</chem>	0.1	0
193	<chem>CC1=CC=C(C2=C(C(CCCCCCCCCCCCCC)C(SC3=C4SC5=C3S(C6=CC=C(C)S6)=C5CCCCCCCCCCCCC)=C4S2)S1</chem>	0.042	0
194	<chem>CC1=CC=C(C2=C(C(CCCCCCCCCCCCCC)C(SC3=C4SC5=C3S(C6=CC=C(C7=CC=C(C)S7)S6)=C5CCCCCCCCCCCCC)=C4S2)S1</chem>	0.33	0
195	<chem>CC1=CC=C(C2=C(C(CCCCCCCCCCCCCC)C(SC3=C4SC5=C3S(C6=CC=C(C7=CC=C(C)S7)S6)=C5CCCCCCCCCCCCC)=C4S2)S1</chem>	0.022	0
196	<chem>CC1=CC=C(C2=C(C(CCCCCCCCCC)C(SC3=C4SC5=C3SC6=C5SC(C7=CC=C(C)S7)=C6CCCCCCCCC)=C4S2)S1</chem>	0.01	0
197	<chem>CC1=CC(CCCCCC)=C(C2=CC=C(/C=C/C3=CC=C(C4=C(C(CCCCCC)C=C(C)S4)S3)S2)S1</chem>	0.15	0

198	CC1=CC=C(C2=CC(CCCCCCCCCCCC)=C(C3=NC(CCCCC CCCCCCC)=C(C4=C(CCCCCCCCCCCC)N=C(C5=C(CCCCC CCCCCCC)C=C(C6=CC=C(C)S6)S5)S4)S3)S2)S1	0.33	0
199	CC1=CC(CCCCCCCC)=C(C2=CC(CCCCCCCC)=C(C3=NC(C=C(SC(C4=C(CCCCCCCC)C=C(C5=C(CCCCCCCC)C=C(C)S5)S4)=N6)C6=C7)=C7S3)S2)S1	0.01	0
200	CC1=CC=C(C(C=C(C(CCCCCCCC)(CCCCCCCC)C2=C3C= CC(C4=CC=C(N(C5=CC=C(C)C=C5C)C6=CC=C(C)C=C6) C=C4)=C2)C3=C7)=C7C8(CCCCCCCC)CCCCCCCC)C8=C1	0.02	0
201	CC1=CC=C(C(C=C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C CCCCCCCC)C3=C4SC(C5=CC6=C(C=C(C)S6)S5)=C3)C4 =C7)=C7C2(CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCC C1)C1	0.2	0
202	CC1=CC=C(C2=CC3=C(C(SC(C4=CC=C(C5=CC=C(C6=C C7=C(C(SC(C)=C8)=C8[Si]7(CCCCCCCC)CCCCCCCC)S6)S 5)S4)=C9)=C9[Si]3(CCCCCCCC)CCCCCCCC)S2)C%10=NS N=C%101	0.02	0
203	CC1=CC=C(C2=CC(OCCCCCCCCCCCC)=C(C3=C(OCCCC CCCCCCCC)C=C(C)S3)S2)C(C(N4CCCCCCCCCCCC)=O)= C1C4=O	0.28	0
204	CC1=CC(CCCCCCCC)=C(C)[Se]1	0.09	0.09
205	CC1=CC(CCCCCCCCCC)=C(C2=CC=C(C3=C(CCCCCCCC CC)C=C(C)S3)[Se]2)S1	0.01	0.01
206	CC1=CC(C(N(CC(CC)CCCC)C2=O)=O)=C(C2=C(C3=CC(O CCCCCCCCCCCC)=C(C4=C(OCCCCCCCCCCCC)C=C(C)S4)S3)C=C5C(N6CC(CC)CCCC)=O)C5=C1C6=O	0.04	0.03
207	CC1=C(C)C=C(N=C(C2=CC=C(C3=NC(C)C(C)N3C4=O)C 5=C4C=CC6=C25)N7C6=O)C7=C1	0	0.1
208	O=C1C2=CC=C3C4=C(C5=NC6=CC=CC=C6N5C3=O)C =CC(C7=NC8=CC=CC=C8N71)=C24.CC.CC	0	0.1
209	CC1=CC2=C(C(C=C(C3=CC=C(C)C4=NSN=C34)C=C5)= C5C2(CO)CO)C=C1	0.002	0
210	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5[Si]2(CCC(CO)CCCC)CCC(CO)CCCC)S1	0.003	0
211	CC1=CC2=C(C(SC(C3=CC=C(C4=CC=C(C5=CC=C(C)S5) C6=NSN=C46)S3)=C7)=C7[Si]2(CCC(CO)CCCC)CCC(CO) CCCC)S1	0.001	0
212	CC1=CC(C(OCCCCCCCC)=C(SC(C2=C(SC(C(OCCCCCCCC CCCC)=O)=C3)C3=C(C)S2)=C4)C4=C5OCCCCCCCC)=C5 CC1=CC=C2C(C(CCCCCC)(CCCCC)C3=C2C=CC(C4=CC =C(N(C5=CC=C(C)C=C5)C6=CC=C(/C=C/C7=CC=C(/C= C(C#N)/C#N)C7)C=C6)C=C4)=C3)=C1	0.0001	0
213	CC1=CC=C(C(C=C(C(C=C(C(C=C(C(C=C(C(C=C(C(C=C(C =C(N(C5=CC=C(C)C=C5)C6=CC=C(/C=C/C7=CC=C(/C= C8C(N(CC)C(N(CC)C/8=O)=S)=O)C7)C=C6)C=C4)=C3)=C	0.01	0
214	CC1=CC(C =C(N(C5=CC=C(C)C=C5)C6=CC=C(/C=C/C7=CC=C(/C= C8C(N(CC)C(N(CC)C/8=O)=S)=O)C7)C=C6)C=C4)=C3)=C	0.01	0
215	CC1=CC(CCCCCCCCCCCC)=C(C2=CC(SC(C3=C(CCCCCC CCCCC)C=C(C)S3)=C4)=C4S2)S1	0.3	0
216	CC1=C2C(C(N1CC(CCCCCCCCCC)CCCCCCCC)=O)=C(C3 =CC=C(C4=CC5=C(C(SC(C6=CC=C(C)S6)=C7)=C7C8=CS C=C85)S4)S3)N(CC(CCCCCCCC)CCCCCCCC)C2=O	0.007	0
217	CC1=C2C(C(N1CC(CCCCCCCCCC)CCCCCCCC)=O)=C(C3 =CC=C(C4=CC5=C(C(SC(C6=CC=C(C)S6)=C7)=C7C8=C(CCCCCCCCCCCC)SC(CCCCCCCCCCCC)=C85)S4)S3)N(CC(CCCCCCCC)CCCCCCCC)C2=O	0.2	0
218	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCC) =O)=C(C4=CC=C(C5=CC=C(C)C=C5)S4)N(CC(CCCCCC C)CCCCCCCC)C3=O)S1	0.41	0
219	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCC) =O)=C(C4=CC=C(C5=C(OCCCCCCCC)C=C(C)C(OCCCC CCC)=C5)S4)N(CC(CCCCCCCCCC)CCCCCCCC)C3=O)S1	0.011	0

220	CC1=CC=C2C(/C(C(N2CC(CCCCCCCCCCCC)CCCCCCCCC C)=O)=C3C(OC4=C\3C=CC5=C4C=CC(/C6=C7C(N(CC(C CCCCCCCCC)CCCCCCCCCCCC)C8=C\7C=CC(C(S9)=CC(CCCCCCCCCCCC)=C9C%10=C(C=C(C)S%10)CCCCCCCCC CCC)=C8)=O)=C5OC6=O)=O)=C1	0.37	1.23
221	CC1=CC=C2C(/C(C(N2CC(CCCCCCCCCCCC)CCCCCCCCC C)=O)=C3C(OC4=C\3C=CC5=C4C=CC(/C6=C7C(N(CC(C CCCCCCCCC)CCCCCCCCCCCC)C8=C\7C=CC(C(S9)=C(C CCCCCCCCCCCC)C=C9C%10=CC(CCCCCCCCCCCCC)=C(C)S %10)=C8)=O)=C5OC6=O)=O)=C1	0.0018	0.175
222	F[B-]([N+])1=CC(C2=CC=C(C3=C(CCCCCCCCCCCC)C=C(C4= CC(CCCCCCCCCCCC)=C(C5=CC=C(C)S5)S4)S3)S2)=CC1C 6C7=CC=C(CCCCCCCC)S7)(F)N8C6=CC(C)=C8	0.0005	0
223	F[B-]([N+])1=CC(C2=CC=C(C3=CC(CCCCCCCCCCCC)C=C(C4= C(CCCCCCCCCCCC)C=C(C5=CC=C(C)S5)S4)S3)S2)=CC1C 6C7=CC=C(CCCCCCCC)S7)(F)N8C6=CC(C)=C8	0	0
224	CC1=CC2=C(C=C(C3=C(CCCCCCCCCCCCCC)C=C(/C=C/ C4=CC(CCCCCCCCCCCCCC)=C(C)S4)S3)S2)S1	0.4	0
225	CC1=C(CCCCCCCCCCCCCC)C2=C(C(CCCCCCCCCCCCCC)=C(C3=CC=C(/C=C/C4=CC=C(C)S4)S3)S2)S1	0.1	0
226	O=C1C2=C(C)SC(C3=C(CCCCCCCCCCCCCC)C=C(C4=CC5= C(C=C(C6=CC(CCCCCCCCCCCCCC)=C(C)S6)S5)S4)S3)=C2C(N1CC(CCCCCCCC)CCCCCCCCC)=O	0.15	0
227	O=C1C2=C(C)SC(C3=CC(CCCCCCCCCCCCCC)C=C(C4=CC5= C(C=C(C6=C(CCCCCCCCCCCCCC)C=C(C)S6)S5)S4)S3)=C2C(N1CCCCCCCCCCCCC)=O	0.011	0
228	O=C1N(CCCC(CCCCCC)CCCCCCCCC)C(C2=CC=C(C3= CC(SC(C4=CC=CC=C4)=C5)=C5S3)S2)=C6C(N(CCCCC(C CCCCCCCCC)CCCCC)C(C7=CC=C(C8=CC=CC=C8)S7)= C61)=O	2.1	0
229	O=C1N(CCCC(CCCCCC)CCCCCCCCC)C(C2=CC=C(C3= =CC(SC(C4=CC=CC=C4)=C5)=C5S3)S2)=C6C(N(CCCCC(CCCCCCCCC)CCCCCCC)C(C7=CC=C(C8=CC=CC=C8) S7)=C61)=O	2.5	0
230	O=C1N(CCCC(CCCCCC)CCCCCCCCC)C(C2=CC=C (C3=CC(SC(C4=CC=CC=C4)=C5)=C5S3)S2)=C6C(N(CCC CC(CCCCCCCCCC)CCCCCCCCC)C(C7=CC=C(C8=CC=C C=C8)S7)=C61)=O	2.5	0
231	O=C1N(CCCC(CCCCCC)CCCCCCCCC)C(C2=CC =C(C3=CC(SC(C4=CC=CC=C4)=C5)=C5S3)S2)=C6C(N(C CCCC(CCCCCCCCCC)CCCCCCCCC)C(C7=CC=C(C8= CC=CC=C8)S7)=C61)=O	3.69	0
232	O=C1N(CCCC(CCCCCC)CCCCCCCCC)C(C2= CC=C(C3=CC(SC(C4=CC=CC=C4)=C5)=C5S3)S2)=C6C(N (CCCC(CCCCCCCCCC)CCCCCCCCC)C(C7=CC=C(C8=CC=CC=C8)S7)=C61)=O	1.38	0
233	CC1=CC(N(CC(CCCCCC)CCCCCCCC)C(/C2=C3C(SC(C4=C C(C=C(C)C=C5)=C5C=C4)=C6)=C6N(CC(CCCCCC)CCCC CCCC)C\3=O)=O)=C2S1	1.64	0.0189
234	CC1=CC(N(CC(CCCCCC)CCCCCCCC)C(/C2=C3C(SC (C4=CC(C=C(C)C=C5)=C5C=C4)=C6)=C6N(CC(CCCCCC CCCC)CCCCCCCC)C\3=O)=O)=C2S1	0.606	0.0149
235	CC1=CC(N(CC(CCCCCC)CCCCCCCC)C(/C2=C 3C(SC(C4=CC(C=C(C)C=C5)=C5C=C4)=C6)=C6N(CC(CC CCCCCCCC)CCCCCCCC)C\3=O)=O)=C2S1	0.108	0.0163
236	CC1=CC(C=C(C(CCCCCC)(CCCCCCCC)C2=C3C=C4C(C =C(C5=CC=C(C(N(CC(CCCC)CC)C6=O)=C7C6=C(C8=CC =C(C)S8)N(CC(CCCC)CC)C7=O)S5)S4)=C2)C3=C9)=C9S1	0.012	0

	<chem>CC1=CC(C=C(C(CC(CCCCCC)CCCC)(CC(CCCC)CCCCC)C</chem>		
237	<chem>2=C3C=C4C(C=C(C5=CC=C(C(N(CC(CCCC)CC)C6=O)=C 7C6=C(C8=CC=C(C(S8)N(CC(CCCC)CC)C7=O)S5)S4)=C2) C3=C9)=C9S1</chem>	5.26	0
238	<chem>CC1=CC(C=C(C(CC(CCCCCC)CCCC)(CC(CCCC)CCCCC)C 2=C3C=C4C(C=C(C5=CC=C(C(N(CC(CCCCCCCCCCC)CCC CCCCC)C6=O)=C7C6=C(C8=CC=C(C(S8)N(CC(CCCCCC C)CCCCCCCCCC)C7=O)S5)S4)=C2)C3=C9)=C9S1</chem>	0.001	0
239	<chem>CC1=CC(CCCCCCCCCCCCCC)=C(C2=CC3=C(C(C=C(C CCCCCCCCCCCCC)C4=C5SC(C6=C(CCCCCCCCCCCCCC CCC)C=C(C7=CC(CCCCCCCCCCCCCC)=C(C8=CC9=C(C(C=C(C(CCCCCCCCCCCCCC)C%10=C%11SC(C%12=C(CC CCCCCCCCCCCCC)C=C(C)S%12)=C%10)=C%11C=C9CCC CCCCCCCCCCCCC(S8)S7)S6)=C4)=C5C=C3CCCCCCCCC CCCCC)S2)S1</chem>	0.47	0
240	<chem>CC1=CC(CCCCCCCCCCCCCC)=C(C2=CC(C(C=C(CCCCCC CCCC)C3=C4C=C(C5=C(C(CCCCCCCCCCCCCC)C=C(C6=CC(C CCCCCCCCCCCCC)=C(C7=CC(C(C=C(C(CCCCCCCCCCCCCC)C8= C9C=C(C%10=C(C(CCCCCCCCCCCCCC)C=C(C)S%10)S8)=C9C= C%11CCCCCCCCCCCCC)=C%11S7)S6)S5)S3)=C4C=C%12CC CCCCCCCCC)=C%12S2)S1</chem>	0.042	0
241	<chem>CC1=CC(CCCCCCCCCCCCCC)=C(C2=CC(C(C=C(CCCCC CCCCCCCCCCCCC)C3=C4C=C(C5=C(C(CCCCCCCCCCCCCC CC)C=C(C6=CC(C(CCCCCCCCCCCCCC)=C(C7=CC(C(C= C(CCCCCCCCCCCCCC)C8=C9C=C(C%10=C(C(CCCCCC CCCCCCCCC)C=C(C)S%10)S8)=C9C=C%11CCCCCCCCCCC CCCC)=C%11S7)S6)S5)S3)=C4C=C%12CCCCCCCCCCCCC CCCC)=C%12S2)S1</chem>	0.026	0
242	<chem>CC1=CC(CCCCCCCCCCCCCC)=C(C)S1</chem>	0.0001	0
243	<chem>O=C1/C(C(C=CC(C2=CC=C(C3=CC=C(C(S3)S2)=C4)=C4 N1CCC(CCCCCCCCCC)CCCCCCCCC)=C5C(C=CC(C)=C6)=C6N(CCC(CCCCCCCCCC)CCCCCCCCC)\C\5=O</chem>	0.4	0
244	<chem>O=C1/C(C(C=CC(C2=CC=C(/C=C/C3=CC=C(C(S3)S2)=C 4)=C4N1CCCCC(C(CCCCCCCCCC)CCCCCCCCC)=C5C(C=CC(C)=C6)=C6N(CCCCCC(CCCCCCCCCC)CCCCCCCCC CC)\C\5=O</chem>	1.89	0
245	<chem>C=C1/C(C(C=C(C2=CC=C(/C=C/C3=CC=C(C(S3)S2)=C 4)=C4N1CCCC(C(CCCCCCCCCC)CCCCCCCCC)=C5C(C=C C(C)=C6)=C6N(CCCC(CCCCCCCCCC)CCCCCCCCC)\C\5= ^</chem>	4.07	0
246	<chem>CC1=CC=C(C2=CC(C(CCCCCCCCCC)=C(C3=CC=C(C4= CC=C(C5=CC=C(C6=C(C(CCCCCCCCCC)C=C(C7=CC=C(C8=C9C(C(N8CC(CCCCCCCCCC)CCCCCCCCC)=O)=C (C%10=CC=C(C)S%10)N(CC(CCCCCCCCCC)CCCCCCCCC CC)C9=O)S7)S6)S5)C%11=NSN=C%114)S3)S2)S1</chem>	0.77	0
247	<chem>CC1=CC=C(C2=CC(C(CCCCCCCCCC)=C(C3=CC=C(C4= CC=C(C5=CC=C(C6=C(C(CCCCCCCCCC)C=C(C7=CC=C(C8=C9C(C(N8CCCC(C(CCCCCCCCCC)CCCCCCCCC)= O)=C(C%10=CC=C(C)S%10)N(CCCCC(CCCCCCCCCC)C CCCCCCCCC)C9=O)S7)S6)S5)C%11=NSN=C%114)S3)S2)S 1</chem>	2.95	0
248	<chem>CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCC)CCCCCCC CCC)=O)=C(C4=CC=C(C5=CC=C(C)S5)S4)N(CCCCC(CCC CCCC)CCCCCCCCC)C3=O)S1</chem>	8.32	1.26
249	<chem>CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCC)CCCCCCC CCC)=O)=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CCCCC(C CCCCC)CCCCCCCCC)C3=O)S1</chem>	12.25	2.25
250	<chem>O=C(N1CCCC(CCCCCC)CCCCCCCCC)C(C2=C1C3= CC=CS3)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4) N(CCCCC(CCCCCC)CCCCCCCCC)C2=O</chem>	4.36	0.56

251	CC1=CC=C(C2=C3C(C(N2CCCCC(CCCCCCCC)CCCCCCC CCC)=O)=C(C4=CC=C(C5=CC=C(C/C=C/C6=CC=C(C(S6)S 5)S4)N(CCCCC(CCCCCCCC)CCCCCCCCCCC)C3=O)S1	5.2	0.19
252	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C 2(CCCCC(CCCC)CC)CCCCC(CCCC)CC)S1	0	0.004
253	CC1=CC(C(CC(CCCCCC)CCCC)(CC(CCCCCC)CCCC)C2=C3 SC(C4=CC(F)=C(C5=CC(C(CC(CCCCCC)CCCC)(CC(CCCCC C)CCCC)C6=C7SC(C8=C(F)C=C(C)C9=NSN=C98)C6)=C7 S5)C%10=NSN=C%104)=C2)=C3S1	0.0004	0
254	CC1=CC(C(CCCC(CCCCCC)CCCC)(CCCC(CCCCCC)CCCC) C2=C3SC(C4=CC(F)=C(C5=CC(C(CCCC(CCCCCC)CCCC)(C CCC(CCCCCC)CCCC)C6=C7SC(C8=C(F)C=C(C)C9=NSN= C98)C6)=C7S5)C%10=NSN=C%104)=C2)=C3S1	0.0035	0
255	CC1=CC(C(CCCCC(CCCCCC)CCCC)(CCCC(CCCCCC)CCC C)C2=C3SC(C4=CC(F)=C(C5=CC(C(CCCCC(CCCCCC)CCC C)(CCCCC(CCCCCC)CCCC)C6=C7SC(C8=C(F)C=C(C)C9= NSN=C98)C6)=C7S5)C%10=NSN=C%104)=C2)=C3S1	0.0154	0
256	CC1=CC(C(CCCCCC(CCCCCC)CCCC)(CCCCC(CCCCCC)C CCC)C2=C3SC(C4=CC(F)=C(C5=CC(C(CCCCC(CCCCCC) CCCC)(CCCCC(CCCCCC)CCCC)C6=C7SC(C8=C(F)C=C(C)C9=NSN=C98)C6)=C7S5)C%10=NSN=C%104)=C2)=C3S1	0.0201	0
257	CC1=CC(C(CCCCCCCCCCCCCC(CCCCCC)CCCC)(CCCCCCCC CCCC(CCCCCC)CCCC)C2=C3SC(C4=CC(F)=C(C5=CC(C(C CCCCCCCCCCCC(CCCCCC)CCCC)(CCCCCCCCCCCC(CCCC CC)CCCC)C6=C7SC(C8=C(F)C=C(C)C9=NSN=C98)C6)=C 7S5)C%10=NSN=C%104)=C2)=C3S1	0.408	0
258	O=C(N(CC(CCCCCC)CCCCC)C1=O)C2=CC(C3=CC=C(C) S3)=C4C5=C(C(N(CC(CCCCCC)CCCCC)C4=O)=O)C=C(C)C1=C52	0	0.034
259	O=C(N(CCC(CCCCCC)CCCCC)C1=O)C2=CC(C3=CC=C(C)S3)=C4C5=C(C(N(CCC(CCCCCC)CCCCC)C4=O)=O)C= C(C)C1=C52	0	0.093
260	O=C(N(CCCC(CCCCCC)CCCCC)C1=O)C2=CC(C3=CC=C (C)S3)=C4C5=C(C(N(CCCC(CCCCCC)CCCCC)C4=O)=O) C=C(C)C1=C52	0	0.142
261	O=C(N(CCCCC(CCCCCC)CCCCC)C1=O)C2=CC(C3=CC= C(C)S3)=C4C5=C(C(N(CCCCC(CCCCCC)CCCCC)C4=O)= O)C=C(C)C1=C52	0	0.217
262	O=C1C(C2=CC=C(C3=CC=C(C)S3)S2)=C4C5=C6N1C(C= CC(OCC(CCCCCCCCCC)CCCCCCCC)=C7)=C7C6=C(C)C(N 5C8=C4C=C(OCC(CCCCCCCC)CCCCCCCCC)C=C8)=O	0.29	0.31
263	O=C1C(C2=CC=C(C3=CC=C(C)S3)S2)=C4C5=C6N1C(C= CC(OCCCC(CCCCCCCCCC)CCCCCCCC)=C7)=C7C6=C(C) C(N5C8=C4C=C(OCCCC(CCCCCCCC)CCCCCCCCC)C=C 8)=O	0.11	1.01
264	O=C1C(C2=CC=C(C3=CC=C(C)S3)S2)=C4C5=C6N1C(C= C=CC(OCC(CCCCCCCCCC)CCCCCCCC)=C7)=C7C6=C(C) C(N5C8=C4C=C(OCC(CCCCCCCC)CCCCCCCCC)C=C8)= O	0.2	0.99
265	O=C1C(C2=CC=C(C3=CC=C(C)S3)S2)=C4C5=C6N1C(C= C=CC(OCCCC(CCCCCCCCCC)CCCCCCCC)=C7)=C7C6=C(C)C(N5C8=C4C=C(OCCCC(CCCCCCCC)CCCCCCCCC)C= 8)=O	0.13	1.04
266	O=C1C(C2=CC=C(C3=CC=C(C)C4=NSN=C43)S2)=C5C6 =C7N1C(C=CC(OCC(CCCCCCCCCC)CCCCCCCC)=C8)=C8 C7=C(C)C(N6C9=C5C=C(OCC(CCCCCCCC)CCCCCCCCC)C=C9)=O	0.52	3.11
267	O=C1C(C2=CC=C(C3=CC=C(C)C4=NSN=C43)S2)=C5C6 =C7N1C(C=CC(OCCCC(CCCCCCCCCC)CCCCCCCC)=C8) =C8C7=C(C)C(N6C9=C5C=C(OCCCC(CCCCCCCC)CCCCC CCCC)C=C9)=O	0.38	0.63

[illegible]

[illegible]

	CC1=CC=C(C2=CC=C(C3C(C(N2CCCC[Si](O[Si](C)(C)(C)O[Si](C)(C)(C)=O)=C(C4=CC=C(C5=CC=C(C(C=C(C(C)S6)S5)S4)N(CCCC[Si](O[Si](C)(C)(C)(C)O[Si](C)(C)(C)C3=O)S1	4.55	0
302	CC1=CC=C(C(N(CCCCC[Si](O[Si](C)(C)(C)(C)O[Si](C)(C)(C)C/2=O)=CC2=C3C=C(C4=CC=C(C5=CC=C(C(C)S5)S4)N(CCC	0.74	0.87
303	CC[Si](O[Si](C)(C)(C)(O[Si](C)(C)(C)C\3=O)S1		
304	CC1=CC=C(C(N(CCCCC[Si](O[Si](C)(C)(C)(C)O[Si](C)(C)(C)C/2=O)=CC2=C3C=C(C4=CC=C(C5=CC=C(C(C)[Se]5)S4)N(C	0.52	0.35
	CCCC[Si](O[Si](C)(C)(C)(O[Si](C)(C)(C)C\3=O)S1		
305	C=C(C(N(CCCCC[Si](O[Si](C)(C)(C)(C)O[Si](C)(C)(C)C\3=O)S1		
	=C(C3=CC=C(C4=CC=C(C(C)S4)S3)C=C5C6=C(C(N(CCCCC	0	1.04
	C[Si](O[Si](C)(C)(C)(C)O[SiH](C)(C)C5=O)=O)C(C)=CC1=C6		
306	=C(C3=CC=C(C/C=C/C4=CC=C(C(C)S4)S3)C=C5C6=C(C(N(C	0	0.93
	CCCCC[Si](O[Si](C)(C)(C)(C)O[SiH](C)(C)C5=O)=O)C(C)=CC		
	1=C6		
307	CC1=CC2=C/C(C(N2CCCCCCC[Si](C)(C#CC#CC#C)CCCCC	3.22	0
	C)=O)=C3C(N(CCCCCC[Si](CCCCC)(CCCCC)C4=C\3		
	C=CC(C5=CC=C(C6=CC=C(C(C)S6)S5)=C4)=O)C=C1		
308	=C1C=C(C(C)C=C2)=C3C(N(CCCCCCCC[Si](O[Si](C)(C)(C)(C)	0.78	0
	O[Si](C)(C)(C)C4=C/3C=CC(C5=CC=C(C6=CC=C(C(C)S6)S5)		
309	CC1=CC(COCCOCCOCCOC)=C(C)S1	0.0002	0
	O=C(C1=C2C(C3=CC(C4=CC=C(C/C=C/C5=CC=C(C(C)S5)S4		
310	)=C26)=C(C(N(CCCCCCOCCCOCCOCCOC)C3=O)=O)C(	0	1.64
	C)=C1)N(CCCCCCCCOCOCOCOCOC)C6=O		
	O=C(C1=C2C(C(C3=O)=CC(C4=CC=C(C/C=C/C5=CC=C(C		
311	)S5)S4)=C26)=C(C(N3OCCOCCOCCOCCCCCCCCC)=O)C(	0	0.11
	C)=C1)N(OCCCOCCOCCOCCCCCCCC)C6=O		
312	CC1=CC=C(C2=C3C(C(N2CCOCCOCCOC)=O)=C(C4=CC		
	=C(C5=CC=C(C6=CC=C(C(N(CC(CCCCCCCC)CCCCCCCC	0.65	0
	CC)C7=O)=C8C7=C(C9=CC=C(C%10=CC=C(C(S%10)S9)N		
	(CC(CCCCCCCCCC)CCCCCCCC)C8=O)S6)S5)S4)N(CCOCC		
	OCCOC)C3=O)S1		
313	CC1=CC=C(C2=C3C(C(N2CCOCCOCCOC)=O)=C(C4=CC	2.6	0
	=C(C5=CC=C(C(C)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCC)C		
	3=O)S1		
314	CC1=CC=C(C2=C3C(C(N2CCOCCOCCOCCOC)=O)=C(C4	0.04	0
	=CC=C(C5=CC=C(C(C)S5)S4)N(CC(CCCCCCCCCC)CCCCC		
	CCCC)C3=O)S1		
315	CC1=CC=C(C2=C3C(C(N2CCOCCOCCOCCOC)=O)=C(C4=CC	0.84	0
	=C(C5=CC=C(C6=CC=C(C(C)S6)S5)S4)N(CCCC(OCC(CCCCCCCCCC)CCCCCCCC		
	=O)C3=O		
316	CC1=CC=C(C2=C3C(C(N2CCCCC(OCC(CCCCCCCC)CCC	1.56	0
	CCCCCCC)=O)=O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C		
	S6)S5)S4)N(CCCCC(OCC(CCCCCCCCCC)CCCCCCCC)=O)		
	C3=O)S1		
317	CC1=CC=C(C2=C3C(C(N2CCCC(OCC(CCCCCCCCCCCC)C	2.3	0
	CCCCCCCCC)=O)=O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C		
	C)S6)S5)S4)N(CCCC(OCC(CCCCCCCCCC)CCCCCCCCCCC		
	C)=O)C3=O)S1		
318	CC1=CC=C(C2=C3C(C(N2CCCCC(OCC(CCCCCCCCCCCC	2.3	0
	C)CCCCCCCCC)=O)=O)=C(C4=CC=C(C5=CC=C(C6=CC		
	=C(C)S6)S5)S4)N(CCCCC(OCC(CCCCCCCCCC)CCCCCCC		
	CCCCC)=O)C3=O)S1		
319	CC1=CC2=C(C(SC(C3=CC=C(C(C)C4=NSN=C34)=C5)=C5C	0.61	0
	2(CCCCCC/C=C/C(CCCCCC)CCCCC/C=C/C(CCCCCC)S		
320	CC1=CC(C(C(C#C)CO)(CC(C#C)CO)C2=C3C=C4C(C(SC	0.003	0
	C5=CC=C(C(C)C6=NSN=C65)=C7)=C7C4(CC(C#C)CO)CC(C		
	#C)CO)=C2)=C3S1		

321	CC1=CC(N(CC(CCCCCCCCCCCC)CCCCCCCCCCCCCCC)C2=C3C=C4C(C(SC(C5=CC=C(C)C6=NSN=C65)=C7)=C7N4CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)=C2)=C3S1	0.03	0
322	CC1=CC=C(C2=C(CCCCCCCCCC)N=C(C)S2)S1	0.0025	0
323	CC1=NN=C(C2=CC=C(C)S2)S1	0.0054	0
324	CC1=CC(CCCCCC)=C(C2=NN=C(C3=C(CCCCCC)C=C(C)S3)C=C2)S1	0.003	0
325	CC1=CC=C(C2=CC=C(C)C3=C2N=C(CCCCCC)C(CCCCCC)=N3)S1	0.0036	0
326	CC(S1)=CC(CCCCCCCCCCCC)=C1C2=C(N=CC=N3)C3=C(C4=C(CCCCCCCCCCCC)C=C(C)S4)S2	0.0007	0
327	CC(S1)=CC(CCCCCCCCCCCC)=C1C2=C(N=CC=N3)C3=C(C4=C(CCCCCCCCCCCC)C=C(C5=CC(C(CCCCCCCC)(CCCCCCCC)C6=C7C=C(C)C=C6)=C7C=C5)S4)S2	0.0016	0
328	CC1=CC(CCCCCCCCCCCC)=C(C2=C(N=CC=N3)C3=C(C4=C(CCCCCCCCCCCC)C=C(C5=C(OCCCCCCCCCCC)C=C(C)C(OCCCCCCCCCCC)=C5)S4)S2)S1	0.0011	0
329	CC1=CC(CCCCCCCCCCCC)=C(C2=C(N=CC=N3)C3=C(C4=C(CCCCCCCCCCCC)C=C(C5=CC=C(C)S5)S4)S2)S1	0.0004	0
330	CC1=CC=C(C2=C(N=C(CCCCCC)C(CCCCCC)=N3)C3=C(C)S2)S1	0	0
331	CC(S1)=C2C(N=C(CCCCCC)C(CCCCCC)=N2)=C1C3=C(C=C(C4=CC=C(C)S4)S3	0.0001	0
332	CC1=CC=C(C2=C(N=C(CCCCCCCCCCCC)C(CCCCCCCCCC)=N3)C3=C(C)S2)S1	0.011	0
333	CC(S1)=CC=C1C(C2=NSN=C23)C4C(N=C(C5=CC=CC=C5)C(C6=CC=CC=C6)=N4)C3C7=CC=C(S7)C8=CC9=C(C=C8)C%10=CC=C(C)C=C%10C9(CCCCCCCC)CCCCCCCC	0.03	0
334	CC1=C(CCCCCC)C=C(C2=C(N=C(CCCCCC)C(CCCCCC)=N3)C3=C(C4=CC(CCCCCC)=C(C)S4)C5=NSN=C52)S1	0.0002	0
335	CC(S1)=C(CCCCCC)C=C1C(C2=NSN=C23)=C4C(N=C(CCCCCC)C(CCCCCC)=N4)=C3C5=CC(CCCCCC)=C(C6=C(C=C(C)S6)S5	0.0038	0
336	CC(S1)=C(CCCCCC)C=C1C(C2=NSN=C23)=C4C(N=C(CCCCCC)C(CCCCCC)=N4)=C3C5=CC(CCCCCC)=C(C6=C(C(C(CCCCCC))(CCCCCCCC)C7=C8C=CC(C)=C7)=C8C=C6)C5	0.0002	0
337	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C2(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCC)S1	22.2	0
338	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C2(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCC)S1	11.4	0
339	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C2(CC(CC)CCCC)CC(CC)CCCC)S1	0.015	0
340	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C2(CCCC(CC)CCCC)CCCC(CC)CCCC)S1	0.09	0
341	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C2(CC(C)CCCC(C)C)CC(C)CCCC(C)C)S1	0.4	0
342	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5C2(CC(CCCCCCCCCC)CCCCCCCCCCCC)CC(CCCCCCCCCC)CCCCCCCCCCC)S1	0.0001	0
343	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5[Sij]2(CC(CC)CCCC)CC(CC)CCCC)S1	0.1	0
344	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5[Sij]2(CCCCCCCCCC)CCCCCCCCCCC)S1	0.01	0
345	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C34)=C5)=C5[Ge]2(CC(CCCC)CC)CC(CCCC)CC)S1	0.11	0
346	CC1=CC2=C(C(SC(C3=NC=C(C)C4=NSN=C34)=C5)=C5[Ge]2(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCC)S1	0.005	0

347	CC1=CC2=C(C(SC(C3=CN=C(C4=CC5=C(C(CC(C6=NC=C(C)C7=NSN=C67)=C8)=C8C5(CCCCCCCCCCCCCC)C CCCCCCCCCCCCCCCC)C4)C9=NSN=C39)=C%10)=C%10C2 (CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)S1	71	0
348	CC1=CC2=C(C([Se]C(C3=CC=C(C)C4=NSN=C34)=C5)=C 5C2(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)[Se]1	0.15	0
349	CC1=CC(C(N2CC(CC)CCCC)=O)=C3C(C4=CC=C3C2=O) =C1C5=C(C4=C(C(S6)=CC7=C6C(S8)=C(N7C(CC(CCCC)C C)CC(CCCC)CC)C=C8C)C=C9C(N(CC(CCCC)CC)C%10=O) =O)C9=C%10C=C5	0	0.0002
350	CC1=CC(C(N2CC(CC)CCCC)=O)=C3C(C4=CC=C3C2=O) =C1C5=C(C4=C(C(S6)=CC7=C6C(S8)=C(N7C(CCCCCCCC)CCCCCCCC)C=C8C)C=C9C(N(CC(CCCC)CC)C%10=O)=O) C9=C%10C=C5	0	0.0002
351	CC1=CC=C(N2C(C3=CC=C(C4=C(OC5=CC=C(C(C)(C)C)C =C5)C=C(C(N(C6=CC=C(/C=C/C7=C(OCCCCC)C=C(/C =C/C)C(OCCCCC)=C7)C=C6)C8=O)=O)C9=C8C=CC%10 =C49)C%11=C%10C(OC%12=CC=C(C(C)(C)C)C=C%12)=CC (C2=O)=C3%11)=O)C=C1	0	0.0085
352	CC1=CC2=C3C(C4=CC(C5=C(C(CCCCCCCCC)C6=C(C(SC7 =C8SC(C)=C7CCCCCCCC)=C8S6)S5)=C3C(N(CC(CCCC CCCC)CCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCC)CC CCCCC)C4=O)=O	0	0.012
353	CC1=CC(C(CC(CCCC)CC)(CC(CC)CCCC)C2=C3C=C4C(C(S C(C5=CN=C(C6=CC=C(C7=NC=C(C)S7)C8=NSN=C86)S5)=C9)=C9C4(CC(CC)CCCC)CC(CCCC)CC)=C2)=C3S1	0	0.011
354	O=C1C(C2=C(C3=CC=C(C4=CC=C(C)C5=NSN=C54)C=C 3)N1CC(CCCCCC)CCCCCCCC)=C(C6=CC=C(C)C=C6)N(C C(CCCCCCCC)CCCCC)C2=O	0	0
355	O=C1C(C2=C(C3=CC=C(C4=CC=C(C)S4)C=C3)N1CC(CC CCCC)CCCCCCCC)=C(C5=CC=C(C)C=C5)N(CC(CCCCCC C)CCCCC)C2=O	0	0
356	O=C1C(C2=C(C3=CC=C(C4=CC=C(C(C=CC(C)=C5)=C5C 6(CCCCCCCC)CCCCCCCC)C6=C4)S3)N1CC(CCCCCC)CCC C)=C(C7=CC=C(C)S7)N(CC(CCCC)CCCCC)C2=O	0	0
357	CC1=CC2=C(C(C3=CC=C(C)S3)=C(C=C(C4=C5C(SC(C(O CC(CCCC)CC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(CC(CC)CCCC)S7)S1	0.0011	0
358	CC1=CC2=C(C(C3=CC=C(C)S3)=C(C=C(C4=C5C(SC(C(O CC(CCCC)CC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(CC(CC)CCCC)S7)S1	0.0001	0
359	CC1=CC2=C(C(C3=CC=C(C)S3)=C(C=C(C4=C5C(SC(C(O CC(CCCC)CC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(CC(CC)CCCC)S7)S1	0.0001	0
360	CC1=CC2=C(C(C3=CC=C(C)S3)=C(C=C(C4=C5C(SC(C(O CC(CCCC)CC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(CC(CC)CCCC)S7)S1	0.0001	0
361	CC1=CC2=C(C(C3=CC=C(C)S3)=C(C=C(C4=C5C(SC(C(O CC(CCCC)CC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(CC(CC)CCCC)S7)S1	0.0001	0
362	CC1=CC2=C(C(C3=CC=C(C)S3)=C(C=C(C4=C5C(SC(C(O CC(CCCC)CC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(CC(CC)CCCC)S7)S1	0.0003	0
363	CC1=CC2=C(C(OC(CCCC)CC)=C(C=C(C3=C4C(SC(C(OC(CCCC)CC)=O)=C4F)=C(C)S3)S5)C5=C2OC(CC)CCCC)S1	0.0006	0

364	CC(S1)=CC2=C1C(C3=CC=C(SCCCCCCCC)S3)=C(C=C(C4=C5C(SC(C(OC(CC)CCCC)=O)=C5F)=C(C)S4)S6)C6=C2C7=CC=C(SCCCCCCCC)S7	0.0109	0
365	CC1=CC2=C(C(C3=CC=C(SCCCCCCCC)S3)=C(C=C(C4=C(C(OC(CC)CCCC)=O)=C(C5=C(C(OC(CCCC)CC)=O)C=C(C)S5)S4)S6)C6=C2C7=CC=C(SCCCCCCCC)S7)S1	0	0
366	CC1=CC2=C(C(C3=CC=C(SCCCCCCCC)S3)=C(C=C(C4=C(C(OC(CC)CCCC)=O)=C(C5=CC=C(C(SC(C)=C6)=C6C(OC(CC)CCCC)=O)S5)S4)S7)C7=C2C8=CC=C(SCCCCCCCC)S	0.0001	0
367	CC1=CC(C(C2=CC=C(CC(CC)CCCC)S2)=C(SC(C3=CC=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CCCC)CC)=C6C5=O)=O)=C(C7=CC=C(C)S7)S4)S3)=C8)C8=C9C%10=CC=C(CC(CCCC)CC)S%10)=C9S1	0.0001	0
368	CC1=CC(C(C2=CC(F)=C(CC(CCCC)CC)S2)=C(SC(C3=CC=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CC)CCCC)=C6C5=O)=O)=C(C7=CC=C(C)S7)S4)S3)=C8)C8=C9C%10=CC(F)=C(CC(CC)CCCC)S%10)=C9S1	0.0003	0
369	CC1=CC(C(C2=CC(Cl)=C(CC(CCCC)CC)S2)=C(SC(C3=CC=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CC)CCCC)=C6C5=O)=O)=C(C7=CC=C(C)S7)S4)S3)=C8)C8=C9C%10=CC(Cl)=C(CC(CC)CCCC)S%10)=C9S1	0.0007	0
370	CC1=CC(C(C2=CC=CC(OC(CCCC)CC)=C2)=C(SC(C3=CC=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CCCC)CC)=C6C5=O)=O)=C(C7=CC=C(C)S7)S4)S3)=C8)C8=C9C%10=CC=CC(OC(CC)CCCC)=C%10)=C9S1	0.0008	0
371	CC1=CC(C(C2=CC=C(CC(CCCCCC)CCCC)C=C2)=C(SC(C3=C(Cl)C=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CCCC)C=C6C5=O)=O)=C(C7=CC(Cl)=C(C)S7)S4)S3)=C8)C8=C9C%10=CC=C(CC(CCCC)CCCCC)C=C%10)=C9S1	0.0013	0
372	CC1=CC(C(C2=CC=C(OC(CCCCCC)CCCC)C=C2)=C(SC(C3=CC=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CCCC)CC)=C6C5=O)=O)=C(C7=CC=C(C)S7)S4)S3)=C8)C8=C9C%10=CC=C(OC(CCCC)CCCCC)C=C%10)=C9S1	0.0004	0
373	CC1=CC(C(C2=CC(F)=C(OC(CCCCCC)CCCC)C(F)=C2)=C(SC(C3=CC=C(C4=C5C(C(C6=C(CC(CC)CCCC)SC(CC(CCC)CC)=C6C5=O)=O)=C(C7=CC=C(C)S7)S4)S3)=C8)C8=C9C%10=CC(F)=C(OC(CCCC)CCCCC)C(F)=C%10)=C9S1	0.0015	0
374	CC(S1)=CC2=C1C(C3=CC(Cl)=C([Si](CCC)(CCC)CCC)S3)=C(C=C(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NN(CC(CCCCCC)CCCCC)N=C75)S4)S8)C8=C2C9=CC(Cl)=C([Si](CCC)(CCC)CCC)S9	0.001	0
375	CC1=CC2=C(C(C3=CC=CC(OC(CCCC)CC)=C3)=C(C=C(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NN(CC(CCCC)CCCCC)N=C75)S4)S8)C8=C2C9=CC=CC(OC(CC)CCCC)=C9)S1	0.0007	0
376	CC(S1)=CC2=C1C(C3=CC=C(OC(CCCCCC)CCCC)C=C3)=C(C=C(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NN(CC(CCCCCC)CCCCC)N=C75)S4)S8)C8=C2C9=CC=C(OC(CCCC)CCCCC)C=C9	0.0007	0
377	CC(S1)=CC2=C1C(C3=CC(C(F)(F)F)=C(OC(CCCCCC)CCC)C=C3)=C(C=C(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NN(CC(CCCCCC)CCCCC)N=C75)S4)S8)C8=C2C9=CC(C(F)(F)F)=C(OC(CCCC)CCCCC)C=C9	0.0008	0
378	CC1=CC2=C(C(C3=CC(F)=C(SC(CCCCCC)CCCCC)C=C3)=C(C=C(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NN(CC(CCCCCC)CCCCC)N=C75)S4)S8)C8=C2C9=C(C(F)=C(SC(CCCCCC)CCCCC)C=C9)S1	0.0006	0

379	CC1=CC2=C(C(C3=CC=C(SC(CCCCCCCC)CCCCC)C=C3)=C(C=C(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NN(C(C(CCCCCCCC)CCCCC)N=C75)S4)S8)C8=C2C9=CC=C(SC(CCCCCC)CCCCCCC)C=C9)S1	0.0006	0
380	CC1=CC2=C(C3=CC(CI)=C(CC(CC)CCCC)S3)C(SC(C4=C(C(C(CCCCC)CCCC)C=C(C5=CC6=C(C(SC(C7=CC(CC(CCCC)CCCCC)=C(C)S7)=C8)=C8C9=C6N=C%10C(C=CC=C%10)=N9)S5)S4)=C%11)=C%11C(C%12=CC(CI)=C(CC(CCCC)C)S%12)=C2S1	0.0002	0
381	CC1=CC2=C(C3=CC(CI)=C(CC(CC)CCCC)S3)C(SC(C4=C(C(C(CCCCC)CCCC)C=C(C5=CC6=C(C(SC(C7=CC(CC(CCCC)CCCCC)=C(C)S7)=C8)=C8C9=C6N=C%10C(C=C(F)C(F)=C%10)=N9)S5)S4)=C%11)=C%11C(C%12=CC(CI)=C(CC(CCCC)C)CC)S%12)=C2S1	0.0008	0
382	CC1=CC=C(S1)C2=NC3=C(C4=CC=C(CC(CCCCCCCC)CCCC)S4)C(S5)=C(C(C6=CC=C(CC(CCCCC)CCCCCCCC)S6)=C3S2)N=C5C7=CC=C(S7)C8=CC9=C(C%10=CC=C(CC(CCCCC)CCCCCCCC)S%10)C(SC(C)=C%11)=C%11C(C%12=CC=C(CC(CCCCC)CCCCCCCC)S%12)=C9S8	0.0001	0
383	CC1=CC=C(S1)C2=NC3=C(C4=CC=C(CC(CCCCCCCC)CCCC)S4)C(S5)=C(C(C6=CC=C(CC(CCCCC)CCCCCCCC)S6)=C3S2)N=C5C7=CC=C(S7)C8=CC9=C(C%10=CC(F)=C(CC(CCCCC)CCCCCCCC)S%10)C(SC(C)=C%11)=C%11C(C%12=CC(F)=C(CC(CCCCC)CCCCCCCC)S%12)=C9S8	0	0
384	CC1=CC=C(S1)C2=NC3=C(C4=CC=C(CC(CCCCCCCC)CCCC)S4)C(S5)=C(C(C6=CC=C(CC(CCCCC)CCCCCCCC)S6)=C3S2)N=C5C7=CC=C(S7)C8=CC9=C(C%10=CC(CI)=C(CC(CCCCC)CCCCCCCC)S%10)C(SC(C)=C%11)=C%11C(C%12=CC(CI)=C(CC(CCCCC)CCCCCCCC)S%12)=C9S8	0	0
385	CC1=CC2=C(C(C3=CC=C(CC(CCCC)CC)S3)=C(C=C(C4=C(CC(CCCC)CC)C=C(C5=CC6=C(C(SC(C7=CC(CC(CC)CCCC)=C(C)S7)=C8)=C8OC6=O)S5)S4)S9)C9=C2C%10=CC=C(CC(CC)CCCC)S%10)S1	0.0007	0
386	CC1=CC2=C(C(C3=CC=C(CC(CCCC)CC)S3)=C(C=C(C4=C(CC(CCCC)CCCCC)C=C(C5=CC6=C(C(SC(C7=CC(CC(CC)CCCC)=C(C)S7)=C8)=C8SC6=O)S5)S4)S9)C9=C2C%10=CC=C(CC(CC)CCCC)S%10)S1	0.0012	0
387	CC1=CC2=C(C(C3=CC(F)=C(CC(CCCC)CC)S3)=C(C=C(C4=C(CC(CCCC)CCCCC)C=C(C5=CC6=C(C(SC(C7=CC(CC(CCCC)CCCCC)=C(C)S7)=C8)=C8C9=NSN=C96)S5)S4)S%10)C%10=C2C%11=CC(F)=C(CC(CC)CCCC)S%11)S1	0.0016	0
388	CC1=CC=C(C(N(CC(CCCCCCCC)CCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C(N(CCOCCOCCOC)C6=O)=C7C6=C(C8=CC=C(C)S8)N(CCOCCOCCOC)C7=O)S5)S4)N(CC(CCCCCCCCC)CCCCCCCC)C3=O)S1	0.0002	0
389	CC1=C(N=C(C2=CC(OCCCCCCC)=CC=C2)C(C3=CC=C(C(OCCCCCCC)=C3)=N4)C4=C(C5=CC=C(C)S5)C=C1F	0.002	0
390	CC1=C(OC)C=C(/C=C/C)C(OCC(CCCC)CC)=C1	0	0
391	CC1=CC(C(C2=CC=C(CC(CC)CCCC)S2)=C(SC(C3=CC=C(C(N(CC(CCCCC)CCCC)C4=O)=C5C4=C(C6=CC=C(C)S6)N(CC(CCCC)CCCCC)C5=O)S3)=C7)C7=C8C9=CC=C(C(C(CCC)CC)S9)=C8S1	0.0001	0
392	CC1=CC(C(C2=CC=C(CC(CC)CCCC)S2)=C(SC(C3=CC=C(C(N(CC(CCCCC)CCCC)C4=O)=C5C4=C(C6=CC=C(C7=C(C(C8=CC=C(CC(CCCC)CC)S8)=C(SC(C9=CC=C(C(N(CC(OCCOCCOC)C%10=O)=C%11C%10=C(C%12=CC=C(C)S%12)N(CCOCOCOC)C%11=O)S9)=C%13)C%13=C%14C%15=C(C=C(C(CCCC)CC)S%15)=C%14S7)S6)N(CC(CCCC)CCCCC)C5=O)S3)=C%16)C%16=C%17C%18=CC=C(C(CCCC)CC)S%18)=C%17S1	0.0001	0

393	CC1=CC=C(C(N(CC(COCCOC)COCCOC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C(C)S5)S4)N(CC(COCCOC)COCCOC)C3=O)S1	0.0041	0
394	CC1=CC=C(C2=C(N3CCCCCCCCC)C(N(CCCCCCCCCC)C2=O)=C(C4=CC=C(C5=CC6=C(C(SC(C)=C7)=C7[Si]6(CCCC(CCCCCC)CCCCCCCC)S5)S4)C3=O)S1	0.03	0
395	O=C(N(C=C1)C(C2=C1C=C(C)S2)=C34)C3=C(C5=CC=C(C6=C(F)C(F)=C(C)S6)S5)N(CCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC)C4=O	2.33	0
396	CC1=CC(CCCC)=C(C)S1	0.017	0
397	CC1=CC(CCCCCC)=C(C)S1	0.2	0
398	CC1=CC(CCCCCCCC)=C(C)S1	0.02	0
399	CC1=CC([Si](CC(CCCC)CC)(CC(CCCC)CC)C2=C3SC(C4=C(F)C(F)=C(C5=CSC6=C5[Si](CC(CC)CCCC)(CC(CC)CCCC)C7=C6C=C(C8=CC=C(C)S8)S7)C9=NSN=C94)=C2)=C3S1	0.48	0
400	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC(CCCC)=O)=C(C4=CC=C(C5=CC=C(C)S5)S4)N(CCOCCOC(COCCOC)C3=O)S1	0.0065	0
401	CC1=CC=C(C2=C3C(C(N(CC(CCCCCCCCCC)CCCCCCCCC(CCC)C3=O)=O)=C(C4=C(C(N(CC(CCCCCCCCCCCCCC)CCCC(CCCCCC)C5=O)=O)C5=C(C6=C(C(CCCCCCCCCCCCCC)C=C(C7=CC(F)=C(C8=C(F)C=C(C)S8)S7)S6)S4)S2)S1	0	0
402	CC1=CC(CCCCC)=C(C2=CC(CCCCC)=C(C)S2)S1	0.1	0
403	CC1=CC=C(C2=C(C(CCCCCCCCC)C(CCCCCCCCC)=C(C3=C(C=C(C)S3)S2)S1	0.01	0
404	CC1=CC=C(C2=C(C(CCCCCC)C(CCCCCC)=C(C3=CC=C(C)S3)S2)S1	0.17	0
405	CC1=CC(CCCCCCCCC)=C(C2=CC=C(C3=C(C(CCCCCC)C=C(C)S3)S2)S1	0.03	0
406	CC1=CC(CCCCCCCCCCCCC)=C(C2=CC(C=C(C3=C(C(CCCCC(CCCCCC)C=C(C)S3)S4)=C4S2)S1	0.15	0
407	CC1=CC(CCCCCCCCCCCCC)=C(C2=CC(C(CCCCCCCCCCCCC)=C(/C=C/C3=C(C(CCCCCCCCCCCCC)C=C(C4=C(C(CCCCCC(CCCC)C=C(C)S4)S3)S2)S1	1.05	0
408	CC1=CC=C(C2=C(C(CCCCCCCCCC)C(SC3=C4SC(C5=CC=C(C)S5)=C3CCCCCCCCC)=C4S2)S1	0.002	0
409	CC1=CC=C(C2=C(C(CCCCCCCCCC)C(SC3=C4SC5=C3SC(C6=CC=C(C)S6)=C5CCCCCCCCC)=C4S2)S1	0.09	0
410	CC1=CC(CCCCC)=C(C2=CC3=C(C(CCCCC)=C(C=C(C4=C(C(CCCCC)C=C(C)S4)S5)C5=C3CCCCC)S2)S1	0.25	0
411	CC(S1)=CC=C1C2=CC3=C(S2)C4=C(C=C(C)S4)C5=C3C=C(C(C(CCCCCC)CCCCCCCC)S5	0.24	0
412	CC(S1)=CC2=C1C(SC(C3=CC(SC(C)=C4)=C4S3)=C5)=C5C6=C2SC(C(CCCCCC)CCCCCCCC)=C6	0.025	0
413	CC1=CC(CCCCC)=C(S1)C(S2)=CC3=C2C(SC(C4=C(CCC(CCC)C=C(C)S4)=C5)=C5C6=C3SC(C(CCCCCCCCCCCCCC)S1	0.27	0
414	CC1=CC2=C(C(SC(C3=CC=C(C)S3)=C4)=C4[Si]2(CCCCCC)CCCCC)S1	0.05	0
415	CC1=CC2=C(C(SC(C3=CC=C(C4=CC=C(C)S4)S3)=C5)=C5[Si]2(CCCCC)CCCCC)S1	0.08	0
416	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C43)=C5)=C5[Si]2(C(CCCC)CC)C(CCCC)CC)S1	0.01	0
417	CC(S1)=CC(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)=C1C2=CC=C(S2)C(S3)=CC=C3C4=C(CC(C(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)C=C(S4)C5=C(N=S=N6)C6=C(C)C7=NSN=C75	2.5	0

418	CC1=CC(CC(CCCCCCCCCCCCCC)CCCCCCCCC)=C(C2=CC=C(C3=CC=C(C4=C(CC(CCCCCCCCCCCCCC)CCCCCCCCC)C=C(C5=CC(C6=NSN=C6C(C)=C7)=C7C8=NSN=C85)S4)S3)S2)S1	3.5	0
419	CC1=CC=C(C2=C(CCCCCCCCCCCCCC)C=C(C3=C(CCCCCCCCCCCCCC)C=C(C4=CC(CCCCCCCCCCCCCC)=C(C5=CC(CCCCCCCCCC)=C(C6=CC=C(C7=CC=C(C)C8=NSN=C87)S6)S5)S4)S3)S2)S1	3.7	0
420	CC1=CC(CCCCCCCCCCCCCC)=C(C2=CC=C(C3=C(CCCCCCCCCCCCCC)C=C(C4=C5C(N=S=N5)=C(C)S4)S3)S2)S1	3.5	0
421	CC1=CN=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)S1	3.05	0
422	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCCC)=O)=C(C4=NC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)S1	3.05	0
423	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CN=C(C6=NC=C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)S1	1.87	0
424	CC1=CC=C(C2=C3C(CN2CC(CCCCCCCCCC)CCCCCCCCC=O)=C(C4=CC=C(C5=C(F)C(F)=C(/C=C/C6=C(F)C(F)=C(C)S6)S5)S4)N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)C3)S1	3.4	5.86
425	CCCCCCCCC=C(C4=CC=C(C5=CC=C(C6=C7C(CN6CC(CCCCCCCCCC)CCCCCCCCCCCCC)=C(C8=CC=C(C9=CC=C(C%10=CC=C(C)S%10)S9)S8)N(CC(CCCCCCCCCCCCCC)CCCCCCCCC)C7)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC	2.99	2.6
426	CCCCCCCCC=C(C4=CC=C(C5=CC=C(C6=C7C(CN6CC(CCCCCCCCCC)CCCCCCCCCCCCC)=C(C8=CC=C(C9=CC(SC(C)=C%10)=C%10S9)S8)N(CC(CCCCCCCCCCCCCC)CCCCCCCCC)C7)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C2=	4.16	3.01
427	CC1=CC=C(C2=C3C4=C(C5=C(C6=CC=C(C7=CC=C(C)C8=NSN=C87)S6)C(N4C9=C3C=C(OC(CCCCCCCCCC)CCCCCCCCC)C=C9)=O)N(C%10=CC=C(OC(CCCCCCCCCC)CCCCCCCCC)C=C5%10)C2=O)S1	0.52	3.11
428	O=C(N1CC(CCCCCCCCCC)CCCCCCCCC)C2C(SC(C3=NC4C(C5SC(C)=CC5C(N(C4=O)CC(CCCCCCCC)CCCCCCCCC)=O)S3)=N2)C6C(C=C(C)S6)C1=O	0	1.61
429	CC1=CC2=C(C(CC(C3=C(F)C(F)=C(C4=CC([Si](C(CCCC)C(C)(C(CCCC)CC)C5=C6SC(C7=CC=C(C)[Se]7)=C5)=C6S4)C8=NSN=C83)=C9)=C9[Si]2(C(CC)CCCC)C(CC)CCCC)C1	20.3	0
430	CC1=CC2=C(C(CC(C3=C(F)C(F)=C(C4=CC([Si](C(CCCC)C(C)(C(CCCC)CC)C5=C6SC(C7=CC=C(C)S7)=C5)=C6S4)C8=NSN=C83)=C9)=C9[Si]2(C(CC)CCCC)C(CC)CCCC)C1	9.05	0
431	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=C(CCCCCCCC)C=C(C6=CC([H])=C(C7=CC(CCCCCCCC)=C(C)S7)C=C6[H])S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)S1	0.24	0
432	CC1=C(CC(CCCCCCCCCC)CCCCCCCCC)C=C(C2=C(N=S=N3)C3=C(C4=CC(CC(CCCCCCCC)CCCCCCCCCCC)=C(C5=CC(SC(C)=C6)=C6S5)S4)C7C2N=S=N7)S1	1	0.7
433	O=C1C(C2=C(C3=CC=C(C)O3)N1CC(CCCCCCCC)CCCCCCCCCCCCC=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)S5)O4)N(CC(CCCCCCCCCCCCCC)CCCCCCCCC)C2=O	0.13	0
434	CC1=CC=C(C(N(CCCCCCCCCCCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC(N(CC(CCCCCCCC)CCCCCCCCC)C6=C7SC(C)=C6)=C7S5)S4)N(CCCCCCCCCCCCCCCCCC)C3=O)S1	0.41	0

435	CC1=CC=C(C(N(CCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC(N(CC(CC(CCCC)CC(CCCC)CC)C6=C7SC(C)=C6)=C7S5)S4)N(CCCCC)C3=O)S1	0.05	0
436	CC1=CC=C(C2=C3C(C(N2CC(CCCCC)CC)=O)=C(C4=CC=C(C5=CC(CCCCCCCCCC)=C(C6=CC=C(/C=C/C7=CC=C(C8=C(CCCCCCCCCC)C=C(C)S8)S7)S6)S5)S4)N(CC(C)CCCCC)C3=O)S1	0.05	0
437	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=C(CCCCCCCCCC)C=C(C6=C(N=S=N7)C7=C(C8=CC(CCCCCCCCCC)=C(C)S8)C9=NSN=C96)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCC)C3=O)S1	1.17	1.32
438	O=C1C(C2=C(C3=CC=C(C)O3)N1CC(CCCCCC)CCCCCCCCC)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)O4)N(CC(CCCCCCCCCC)CCCCCCCC)C2=O	1.54	0
439	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCCCCC)=O)=C(C4=CC=C(C5=C([H])C(F)=C(/C=C/C6=CC=C(C)C([H])=C6F)C=C5)S4)N(CCCCC(CCCCCCCCC)CCCCCCCC)C3=O)S1	1.4	0
440	O=C1N(CC(CCCCCCCCC)CCCCCCCCCCCC)C2=CC(C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C(F)=C5F)S4)=C7)=C7N(CC(CCCCCCCCCCCCC)CCCCCCCC)C/3=O	0.028	0
441	$\bigcup_{i=1}^n \bigcup_{j=1}^m \bigcup_{k=1}^p \bigcup_{l=1}^q \bigcup_{m=1}^n \bigcup_{j=1}^m \bigcup_{k=1}^p \bigcup_{l=1}^q$ =CC(CCCCCCCCCC)=C(C)S5)S4)S3)N1CC(CCCCC)CCCCCCCC)=C(C6=CC=C(C)S6)N(CC(CCCCCC)CCCCC)	0.1	0.09
442	$\bigwedge_{i=1}^n \bigwedge_{j=1}^m$ CC1=CC=C(C(N(CCCCCOCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)N(CCCCCOCCCCCCCC)C3=O)S1	0.085	0
443	CC1=CC=C(C2=C3C(C(N2CCCCCCCCCCCC)=O)=C(C4=CC=C(C5=CC6=C(C(C=C([Si](CCCCCCCC)(CCCCCCCC)C7=C8SC(C)=C7)C8=C9)=C9[Si]6(CCCCCC)CCCCCCCC)S5)S4)N(CCCCCCCCCCCCC)C3=O)S1	0.65	0.1
444	$\bigcup_{i=1}^n \bigcup_{j=1}^m \bigcup_{k=1}^p \bigcup_{l=1}^q \bigcup_{m=1}^n \bigcup_{j=1}^m \bigcup_{k=1}^p \bigcup_{l=1}^q$ CCCCC)=C(C4=CC=C(C5=CC=C6C(C=C(C=CC(C)=C7)C7=C6)=C5)O4)N(CC(CCCCCCCCCCCCC)CCCCCCCC)C2=	0.07	0
445	$\bigwedge_{i=1}^n \bigwedge_{j=1}^m$ CC1=CC=C(C2=C3C(C(N2CC(CCCCCC)CCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C)C5(C)C)S4)N(CC(CCCCCC)CCCCCCCC)C3=O)S1	3.1	0
446	O=C1C(C2=C(C3CCC(C)O3)N1CC(CCCCC)CCCCCCCCC)C)=C(C4CCC(C5=CC=C(C)C=C5)O4)N(CC(CCCCCCCCC)CCCCC)C2=O	0.003	0.007
447	O=C1C(C2=C(C3CCC(C)O3)N1CC(CCCCCC)CCCCCCCCCCCCC)=C(C4CCC(C5=CC=C(C)C=C5)O4)N(CC(CCCCCCCCCCCCC)CCCCCCCC)C2=O	0.04	0
448	$\bigcup_{i=1}^n \bigcup_{j=1}^m \bigcup_{k=1}^p \bigcup_{l=1}^q \bigcup_{m=1}^n \bigcup_{j=1}^m \bigcup_{k=1}^p \bigcup_{l=1}^q$ CC)=O)=C(C4=CC=C(C5=C(CCCCCCCCCC)C=C(C6=C(N=S=N7)C7=C(C8=CC(CCCCCCCCCC)=C(C)S8)C9=NSN=C96)S5)S4)N(CC(CCCCCC)CCCCCCCCCCCC)C3=O	1.17	1.32
449	$\bigwedge_{i=1}^n \bigwedge_{j=1}^m$ O=C1C(C2=C(C3=CC=C(C)S3)N1CC(CCCCCCCCC)CCCCCCCCC)=C(C4=CC=C(C5=CC(SC(C)=C6)=C6S5)S4)N(CC(CCCCCC)CCCCCCCC)C2=O	1.6	2
450	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCC)CCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)[Se]5)S4)N(CC(CCCCCCCCCCCCC)CCCCCCCC)C3=O)S1	3	0
451	CC1=CC=C(C2=C3C(C(N2CCCCC(CCCCCCCCC)CCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)[Se]5)S4)N(CCCCCC(CCCCCCCCCCCCC)CCCCCCCC)C3=O)S1	8.2	0

452	O=C1C(C2=C(C3=CC=C(C(C)O3)N1CC(CCCCCCCC)CCCCC CCCCCCC)=C(C4=CC=C(C5=CC=C6C(C=CC(C)=C6)=C5) O4)N(CC(CCCCCCCCCCCC)CCCCCCCC)C2=O	0.11	0
453	CC(C1=NSN=C12)=C(F)C(F)=C2C3=CC(C4(CCCCCCCCCC CCCCCC)CCCCCCCCCCCCCCCC)=C(S3)C5=C4C=CS5 CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=C(CCCCCCCC)C=C(C6=CC(F)=C(C7=CC(CCCCCCCC)=C(C)S7)C=C6F)S5)S4)N(CC(CCC CCCCCCC)CCCCCCCCCCCC)C3=O)S1	0.3	0
454	CCCCCCCCCCC=C(C4=CC=C(C5=C(CCCCCCCC)C=C(C6=CC(F)=C(C7=CC(CCCCCCCC)=C(C)S7)C=C6F)S5)S4)N(CC(CCC CCCCCCC)CCCCCCCCCCCC)C3=O)S1	1.32	0
455	CCCCCCCCCCC=C(C4=CC(C)=C(C5=CC([H])=C(C6=C([H]) C=C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C C1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCCCC CC)=O)=C(C4=CC=C(C5=C(CCCCCCCCCCCC)C=C(C6=C C=C(C7=CC(CCCCCCCCCCCC)=C(C)S7)C=C6)S5)S4)N(CC (CCCCCCCCCCCC)CCCCCCCC)C3=O)S1	11.16	0
456	CCCCCCCCCCC=C(C4=CC=C(C5=C(CCCCCCCCCCCC)C=C(C6=C C=C(C7=CC(CCCCCCCCCCCC)=C(C)S7)C=C6)S5)S4)N(CC (CCCCCCCCCCCC)CCCCCCCC)C3=O)S1	0.27	0
457	CCCCCCCCCCC=C(C4=CC=C(C5=CC=C(/C=C/C6=CC =C(C)S6)S5)S4)N(CCCCCC(CCCCCCCCCCCC)CCCCCCC CCC)C3=O)S1	8.74	0
458	CCCCCCCCCCC=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)[S e]6)S5)S4)N(CC(CCCCCCCCCCCC)CCCCCCCCCCCC)C3=O)S 1	3	0
459	CCCCCCCCCCC=C(C4=CC=C(C5=CC=C(/C=C/C6=CC =C(C)[Se]6)S5)S4)N(CCCCCC(CCCCCCCCCCCC)CCCCCCC CCCC)C3=O)S1	8.2	0
460	CC(S1)=CC=C1C(N(CCCCCCCC(CCCCCCCCCC)CCCCCCC CCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6= CC=C(C)[Se]6)[Se]5)S4)N(CCCCCCCC(CCCCCCCCCC)CCC CCCCCCCC)C3=O	10.3	0
461	CC(S1)=CC=C1C(N(CCCCCCCCCC(CCCCCCCCCC)CCCCCCC CCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6= =CC=C(C)[Se]6)[Se]5)S4)N(CCCCCCCCCC(CCCCCCCCCC)C CCCCCCCCCCCC)C3=O	7.27	0
462	CC(S1)=CC=C1C(N(CCCCCCCCCC(CCCCCCCCCC)CCCCCCC CCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)[Se]6)[Se]5)S4)N(CCC(CCCCCCCCCC)CCCCCCCCCCCCC) C1=CC=C(C(N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCCC CC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6=CC= C(C)[Se]6)[Se]5)S4)N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCC CCC)C3=O	4.59	0
463	CC(S1)=CC=C1C(N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCCC CC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6=CC= C(C)[Se]6)[Se]5)S4)N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCC CCC)C3=O	4.23	0
464	CC(S1)=CC=C1C(N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCCC CCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6=CC =C(C)[Se]6)[Se]5)S4)N(CCCCCC(CCCCCCCCCC)CCCCCCCC CCCCC)C3=O	0.54	0
465	CC(S1)=CC=C1C(N(CCCCCC(CCCCCCCCCC)CCCCCCCCCCCC C)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C (C)[Se]6)[Se]5)S4)N(CCCC(CCCCCCCCCC)CCCCCCCCCCCC C)C3=O	0.5	0
466	CCCCC3=C1C=C(N(CC(CCCCCCCCCC)CCCCCCCCCCCCC) C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6C7=O)C7 C1=CC=C(C(N(CC(CCCCCCCC)CCCCCCCCCCCC)C2=O)=C 3C2=C(C4=CC=C(C5=C(CCCCCCCCCCCC)C=C(C6=CC= C(C7=C(CCCCCCCCCCCC)C=C(C)S7)C=C6)S5)S4)N(CC(C CCCCCCCCC)CCCCCCCC)C3=O)S1	0.16	0
467	CCCCCCCCCCC=C(C4=CC=C(C5=C(CCCCCCCCCCCC)C=C(C6=CC= C(C7=C(CCCCCCCCCCCC)C=C(C)S7)C=C6)S5)S4)N(CC(C CCCCCCCCC)CCCCCCCC)C3=O)S1	0	0.027

468	CC1=CC2=C(C(SC(C3=CN=C(C4=CC(C(CCCCCCCCCCCC CCCC)(CCCCCCCCCCCCCCCC)C5=C6SC(C7=NC=C(C)C8 =NSN=C87)=C5)=C6S4)C9=NSN=C93)=C%10)=C%10C2(CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)S1	47	0
469	CC1=CC=C(C(N(CC(CC)CCCCC)C2=O)=C3C2=C(C4=CC =C(C5=C(CCCC(CCCC)CC)C(SC(C)=C6CCCC(CC)CCCC)=C 6S5)S4)N(CC(CC)CCCCC)C3=O)S1	0.01	0.002
470	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCCCCCC)C2=O) =C3C2=C(C4=CC=C(C5=C(CCCCCC)C=C(C6=C(N=S=N7)C7=C(C8=CC(CCCCCC)=C(C)S8)C9=NSN=C96)S5)S4)N(CC(CCCCCCCCCCCC)CCCCCCCCC)C3=O)S1	0.83	1.36
471	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC CC)=O)=C(C4=CC=C(C5=C(CCCCCCCCCCCC)C=C(C6=C C=C(C7=CC(CCCCCCCCCCCC)=C(C)S7)C8=NSN=C86)S5)S4)N(CC(CCCCCCCC)CCCCCCCCCCCC)C3=O)S1	0.23	0
472	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCCCC) =O)=C(C4=CC=C(C5=CC(SC6=C7SC(C)=C6)=C7S5)O4)N (CC(CCCCCCCC)CCCCCCCCCCC)C3=O)O1	4.1	0
473	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=C(F)C([H])=C(/C=C/C6=CC= C(C)C(F)=C6[H])C=C5)S4)N(CCCCC(CCCCCCCCCC)CCCC CCCC)C3=O)S1	0.3	0
474	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	8.2	0
475	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	0.28	0
476	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C2= C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	0.91	0
477	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	0.2	0
478	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	12.5	0
479	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	5.23	0
480	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	5.87	0
481	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	6.2	0
482	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	0.246	0
483	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	1.95	0.063
484	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	0.22	0
485	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S 6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCCCCC)C3=O)	1.5	0

486	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCC)CCCCCCCCC CC)=O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)N(CC(CCCCCCCCCCCCC)CCCCCCCCC)C3=O)S1	1.57	0.18
487	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCCC)C2=O)=C3C2= C(C4=CC=C(C5=CC(CCCCCCCCCCCCC)=C(C6=CC=C(C7= C(CCCCCCCCCCCCC)C=C(C)S7)C=C6)S5)S4)N(CC(CCCCCC)CCCCCCCCC)C3=O)S1	0.035	0.005
488	CC(C=C1)=CC2=C1/C(C(N2CC(CCCCCCCCC)CCCCCCC C)=O)=C3C(N(C4=C\3C=CC(C5=CC=C(C6=CC=C(C)O6) O5)=C4)CC(CCCCCCCCC)CCCCCCCCC)=O	1.1	0
489	CC1=CC(C(CCCCCCCCCCCCCCCCC)(CCCCCCCCCCCCCCCC C)C2=C3C=C4C(C([Se]C(C5=CC=C(C)C6=NSN=C56)=C7) =C7C4(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC)= C2)=C3[Se]1	6.4	0
490	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCC)CCCCCCCCC =O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C7=C8C(C(N7CC(CCCCCCCCC)CCCCCCCCC)=O)=C(C9=CC=C(C%10=CC= C(C)[Se]%10)S9)N(CC(CCCCCCCCC)CCCCCCCCC)C8=O)S 6)C%11=NSN=C5%11)S4)N(CC(CCCCCCCCC)CCCCCCCCC C2=O)S1	8.9	7.71
491	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCC)CCCCCCCCC =O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)N(CC(CCCCCCCCC)CCCCCCCCC)C3=O)S1	5.5	0
492	CC1=CC=C(C2=C3C(C(N2CCC(CCCCCCCCC)CCCCCCCC CCC)=O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4) N(CCC(CCCCCCCCC)CCCCCCCCC)C3=O)S1	2	0
493	O=C(N1CCCC(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCC CCCCCCC)/C(C2=C1C=C(C)C=C2)=C3C(OC4=C/3C=CC5 =C4C=CC(/C6=C7C(N(CCCC(CCCCCCCCCCCCCCCCC)C CCCCCCCCCCCCCCCCC)C8=C\7C=CC(C9=CC(SC(C)=C% 10)=C%10S9)=C8)=O)=C5OC6=O)=O	0.12	0.14
494	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCC)CCCCCCC)=O)=C(C4=CC=C(C5=CC(CCCCCCCCCCCCC)=C(C6=C(CCCC CCCCCCCCC)C=C(C)S6)S5)S4)N(CC(CCCCCC)CCCCCCCCC C)C3=O)S1	0.11	0.09
495	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCC)CCCCCCCCC =O)=C(C4=CC=C(C(S5)=CC=C5C6=C(C(N7CCCCOCCOC COC)=O)C(C(N6CCCCOCCOCCOC)=O)=C7C8=CC=C(C) S8)S4)N(CC(CCCCCCCCC)CCCCCCCCC)C3=O)S1	0	3
496	CC1=CC=C(C(N(CCCCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C) C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CCC CCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C)C3=O)S1	3.97	2.2
497	CC1=CC=C(C2=C([H])C([H])=C(C)C3=NN(CC(CCCCCC)CCCCC)N=C32)S1	0.007	0
498	O=C1C(C2=C(C3=CC=C(C)S3)N1CC(CCCCCCCCCCCCC)C CCCCCCCCC)=C(C4=CC(C)=C(C5=CC(F)=C(C6=C(F)C=C(C)S6)S5)S4)N(CC(CCCCCCCCC)CCCCCCCCCCCCC)C2=O	1.66	0
499	CC1=CC=C(C2=C3C(C(N2C(CCCCCCCCC)CCCCCCCCC CCC)=O)=C(C4=CC=C(C5=CC=C(C6=C([H])C([H])=C(C7 =CC=C(C)S7)C([H])=C6[H])S5)S4)N(C(CCCCCCCCC)CCC CCCCCCCCC)C3=O)S1	0.058	0.0002
500	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCCCCCCC)CC CCCCCCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C#CC6=C C=C(C)S6)S5)S4)N(CC(CCCCCCCCCCCCC)CCCCCCCCC CCCCCCC)C3=O)S1	2.19	0.38
501	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCC)CCCCCCC)=O)= C(C4=CC=C(C5=C([H])C([H])=C(C)S5)S4)N(CC(CCCCCC)C CCCCCCC)C3=O)S1	0.53	0

502	CC1=CC=C(C(N(CCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC(N(C(CCCCCCCC)CCCCCCCC)C6=C7C=CC(C)=C6)=C7C=C5)S4)N(CCCCCCCC)C3=O)S1	0.02	0
503	CC1=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C2=O)=O)C2=C(C3=C4C(C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O)=C(C5=CC=C(C6=C(F)C(F)=C(C7=CC=C(C)S7)C8=NSN=C68)S5)S3)S1	0.16	0.36
504	O=C1C(C2=C(C3=CC=C(C)[Se]3)N1CC(CCCCCCCC)CCCCCCCCC)=C(C4=CC=C(C5=CC6=C(C=C(C)S6)S5)[Se]4)N(CC(CCCCCCCCCC)CCCCCCCC)C2=O	1.1	0.15
505	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCC)C2=O)=C3C2=C(C4=CC=C(/C=C/C)C=C4)N(CC(CCCCCCCC)CCCCC)C3=O)C=C1	0.2	0.03
506	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CC(CCCCCCCC)CCCCCCCC)C3=O)S1	12.25	0
507	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCC)CCCC)=O)=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CCCCCCCC)C3=O)S1	8.1	0
508	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCC)CCCC)=O)=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CCCCCCCC)C3=O)S1	9.4	0
509	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CC(CCCCCCCC)CCCCCCCC)C3=O)S1	1.62	0.14
510	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCC)=O)=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CC(CCCCCC)CCCCCCCC)C3=O)S1	1.62	0.14
511	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C)S5)S4)N(CC(CCCCCCCC)CCCCCCCC)C3=O)S1	8.32	0
512	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCC)CC)=O)=C(C4=CC=C(C5=CC=C(C)S5)S4)N(CC(CCCCCCCC)CCCCC)CCCCCCCC)C3=O)S1	0.6	0.012
513	CC1=CC=C(C2=C3C(C(N2CC(CCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C)S5)S4)N(CC(CCCCCCCCCC)CCCCC)C3=O)S1	0.3	0.12
514	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC6=C(C=C(C)S6)S5)S4)N(CCCC(CCCCCCCCCC)CCCCCCCCCCCC)C3=O)S1	3.7	0
515	CC1=CC=C(C(N(CC(CCCCCCCCCC)CCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC(SC(C)=C6)=C6S5)S4)N(CC(CCCCCCCC)CCCCC)C3=O)S1	0.9	0.05
516	CC1=CC=C(C2=C3C(C(N2CCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C(C=CC(C)=C6)=C6[Ge]7(CCCC)CCCC)C7=C5)S4)N(CCCCCCCC)C3=O)S1	0.04	0
517	O=C1C(C2=C(C3=CC=C(C)[Se]3)N1CC(CCCCCCCC)CCCCCCCCC)=C(C4=CC=C(C5=CC=C(C)[Se]5)[Se]4)N(CC(CCCCCCCCCC)CCCCCCCC)C2=O	0.1	0.1
518	CC1=CC2=C(C(SC(C3=C(F)C=C(C4=CC(C(CCCCCCCCCC)CCCCC)(CCCCCCCCCCCCCCCC)C5=C6SC(C7=CC(F)=C(C)C(F)=C7)=C5)=C6S4)C=C3F)=C8)=C8C2(CCCCCCCCCC)CCCCCCCCCCCCCCCC)S1	5.7	0
519	CC1=CC=C(C2=C3C(C(N2CC(CCCCCC)CCCCCCCCC)=O)=C(C4=CC=C(/C=C/C)S4)N(CC(CCCCCCCCCC)CCCCC)C3=O)S1	0.013	0.025
520	CC1=CC=C(C2=C3C(C(N2C(CCCCCCCC)CCCCCCCCCCCC)=O)=C(C4=NC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)N(C(CCCCCCCCCC)CCCCCCCC)C3=O)S1	3.05	0

521	CC1=CC=C(C2=C3C(C(N2C(CCCCCCCCCC)CCCCCCCCC CCC)=O)=C(C4=CC=C(C5=CC=C(C6=C([H])C(F)=C(C7=C C=C(C)S7)C([H])=C6F)S5)S4)N(C(CCCCCCCCCC)CCCCC CCCCC)C3=O)S1	0.025	0.008
522	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=CC(F)=C(C6=C(F)C=C(C)S6) S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C3=O)S1	1.8	0
523	O=C1C(C2=C(C3=CC=C(C)[Se]3)N1CC(CCCCCC)CCCC CCCCCCCC)=C(C4=CC=C(C5=CC=C(C)C6=NSN=C65)[Se]4)N(CC(CCCCCCCCCC)CCCCCCCC)C2=O	0.46	0.84
524	CC1=CC2=C(C(SC(C3=CC(F)=C(C4=CC5=C(C(SC(C6=C(F) C=C(C)C7=NSN=C76)=C8)=C8C5(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)S4)C9=NSN=C93)=C%10)=C%10 C2(CCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC)S1	1.2	0
525	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCC CCCC)=O)=C(C4=CC=C(C5=C(F)C([H])=C(/C=C/C6=CC= C(C)C(F)=C6[H])C=C5)S4)N(CC(CCCCCCCCCC)CCCCC CCCC)C3=O)S1	0.3	0
526	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=C(F)C([H])=C(/C=C/C6=CC= C(C)C(F)=C6[H])C=C5)S4)N(CCCC(CCCCCCCCCC)CCCC CCCC)C3=O)S1	0.3	0
527	CC1=CC=C(C2=C3C(C(N2CCCCCCCCCCCCCCCCC)=O) =C(C4=CC=C(C5=CC=C(C)C6=NN(C(CCCCCCCCCCCCCC CCCC)CCCCCCCCCCCCCCCC)N=C56)S4)N(CCCCCC CCCCCCCCCCCC)C3=O)S1	2.4	1.5
528	CC1=CC=C(C(N(CCCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C)C2 =O)=C3C2=C(C4=CC=C(C5=CC=C(C)[Se]5)S4)N(CCCC[Si](O[Si](C)(C)C)(O[Si](C)(C)C)C3=O)S1	6.16	3.07
529	CC1=CC([Si](CCCCCCCC)(CCCCCCCC)C2=C3C=C4C(C(SC (C5=CC=C(C6=C(F)C(F)=C(C7=CC=C(C)S7)C8=NSN=C86)S5)=C9)=C9[Si]4(CCCCCC)CCCCCCCC)=C2)=C3S1	0.19	0
530	CC1=CC=C(C2=C3C(C(N2CC(CCCCCC)CCCCCCCCC CC)=O)=C(C4=CC=C(C5=CC(C=CC(C)=C6)=C6C=C5)S4) N(CC(CCCCCCCCCC)CCCCCCCC)C3=O)S1	0.98	0
531	CC1=CC=C(C(N(CC(CCCCC)CCCCCCCC)C2=O)=C3C2= C(C4=CC=C(C5=CC=C(C)C=C5)S4)N(CC(CCCCCC)CCC CCC)C3=O)S1	0.05	0.03
532	CC1=CC=C(C2=C3C(C(N2CC(CCCCC)CCCCCCCCC)=O)=C(C4=CC=C(C5=CC=C(C)C=C5)S4)N(CC(CCCCCCCC C)CCCCC)C3=O)S1	0.04	0.02
533	C=C1C(C2=C(C3=CC=C(C)C)S5)N1CC(CCCCCCCCCC)C CCCCCCCC)=C(C4=CC=C(C5=CC(F)=C(/C=C/C6=C(F)C (F)=C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCC)	3.4	5.86
534	CC1=CC=C(C(N(CC(CCCCCCCCCC)CCCCCCCC)C2=O)=C 3C2=C(C4=CC=C(C)S4)N(CC(CCCCCC)CCCCCCCCC) C3=O)S1	0.006	0.025
535	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCC CC)=O)=C(C4=CC=C(C5=CC=C(C6=CC=C(C)C7=NSN=C 67)C8=NSN=C85)S4)N(CC(CCCCCC)CCCCCCCCCCCC) C3=O)S1	0.53	0.58
536	O=C1C(C2=C(C3=CC=C(C)O3)N1CC(CCCCCC)CCCCC CCCCC)=C(C4=CC=C(C5=CC=C(C)C6=NSN=C65)O4) N(CC(CCCCCCCCCC)CCCCCCCC)C2=O	0.2	0.56
537	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC(C)=C(C5=CC(SC6=C7SC(C)=C6)=C 7S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)S1	5.27	0

538	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCC)=O)=C(C4=CC=C(C5=C(F)C(F)=C(C)S5)S4)N(CC(CCCCCC)CCCCC)C3=O)S1	0.22	0.19
539	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC(CCCC)=O)=C(C4=CC=C(C5=CC6=C(C=C(C=C(C)S7)C7=C6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)S1	7.42	0
540	CC1=CC=C(C2=C3C(C(N2C(CCCCCCCCCC)CCCCCCCCC(CCC)=O)=C(C4=CC=C(C5=CC=C(C6=C(F)C(F)=C(C7=CC=C(C)S7)C(F)=C6F)S5)S4)N(C(CCCCCCCCCC)CCCCCCCCC(CCC)C3=O)S1	0.015	0.013
541	O=C(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=C(C(Cl)=C(C4=C(Cl)C=C(C)S4)S3)C=C5C6=C(C(N(CC(CCCC(CCCC)CCCCCCCCC)C5=O)=O)C(C)=CC1=C62	0	0.06
542	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCCC(CCCC)=O)=C(C4=CC=C(C5=C([H])C(F)=C(/C=C/C6=CC=C(C)C([H])=C6F)C=C5)S4)N(CC(CCCCCCCCCC)CCCCCCC(CCCCC)C3=O)S1	1.4	0
543	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCC)CCCCC(CCCC)=O)=C(C4=CC=C(C5=C([H])C(F)=C(/C=C/C6=CC=C(C)C([H])=C6F)C=C5)S4)N(CCCC(CCCCCCCCCC)CCCCC(CCCCC)C3=O)S1	1.4	0
544	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCC)=O)=C(C4=CC=C(C5=C(F)C([H])=C(C)C(F)=C5[H])S4)N(CC(CC(CCCC)CCCCCCCC)C3=O)S1	0.003	0.009
545	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCC)=O)=C(C4=CC=C(C)S4)N(CC(CCCCCC)CCCCCCCC)C3=O)S1	0	0.3
546	CC1=CC=C(C(NC2=O)=C3C2=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)NC3=O)S1	0.078	0
547	CCCCCCCCCCCC(CCCCCCCCCC)CC1=C(SC(C2=C(F)C=C(C)C3=NSN=C23)=C1)C(S4)=CC=C4C(S5)=CC=C5C6=C(CC(CCCCCCCCCC)CCCCCCCCC)C=C(C)S6	1.06	0
548	CC1=CC2=C(C(SC(C3=CC=C(C)C4=NSN=C43)=C5)=C5C2(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC(C)S1	11.4	0
549	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC(CCCC)=O)=C(C4=CC=C(C5=C(CCCCCC)C=C(C6=CC(OC)=C(C7=CC(CCCCCC)=C(C)S7)C=C6OC)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)S1	0.12	0
550	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(C(N(OCCOCOCOC)C6=O)=C7C6=C(C8=CC=C(C)S8)N(OCCOCOCOC)C7=O)S5)S4)N(CC(CCCCCC)CCCCCCCCC)C3=O)S1	0.01	0.01
551	CC1=CC=C(C(N(CC(CCCCCC)CCCCCCCCC)C/2=O)=CC2=C3C=C(C4=CC=C(C5=CC(SC(C)=C6)=C6S5)S4)N(C(CCCCCCCCCC)CCCCCCCC)C\3=O)S1	1.37	0
552	CC1=C(CCCCC)C(SC(C2=C(F)C(F)=C(C3=CC4=C(C(CCC(CCC)=C(C5=CC6=C(C(OC(CCCCCC)CCCCCCCCC)=C(C=C(C)S7)C7=C6OC(CCCCCCCCCC)CCCCCCCC)S5)S4)S3)C8=NSN=C82)=C9)=C9S1	0.0175	0
553	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC(CCCC)=O)=C(C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)S5)S4)N(CC(CCCCCCCCCC)CCCCCCCCC)C3=O)S1	8.2	0
554	CC1=CC(C(CCCCCC)(CCCCCCCC)C2=C3C=CC(C4=CC=C(C5=C(OC(CCCC)C(OC(CCCC)=C(C6=CC=C(C)S6)C7=NSN=C75)S4)=C2)=C3C=C1	0	0
555	CC1=CC=C(/C(C(N2CC(CCCCCCCCCCCC)CCCCCCCCC)=O)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C4=C\3C=CC(C5=C(F)C(F)=C(/C=C/C6=C(F)C(F)=C(C)S6)S5)=C4F)=O)C2=C1F	3.94	3.5

556	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCC)=O)=C(C4=CC=C(C5=C(F)C(F)=C(C)C(F)=C5F)S4)N(CC(CCCCC)CCCCCCCC)C3=O)S1	0.23	2
557	C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(O5)C)O4)=C6)=C6N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C/3=	3.2	0
558	O=C1N(CCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C2=CC(C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(O5)C)O4)=C6)=C6N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C/	3.2	0
559	C(C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(O5)C)O4)=C6)=C6N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C	3	0
560	O=C1N(CCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C2=CC(C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(O5)C)O4)=C6)=C6N(CCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C/3=O	2	0
561	O=C1N(CCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C2=CC(C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(O5)C)O4)=C6)=C6N(CCCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C/3=O	2	0
562	O=C1N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C2=CC(C)=CC=C2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(O5)C)O4)=C6)=C6N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C/3=O	1.9	0
563	CC1=C(C)SC(C2=C([H])C(N(CCCCCC)C)/C3=C4C(C=C(C5=CC(C)=C(C6=CC([H])=C(C7=C([H])C=C(C)S7)S6)S5)=C8[H])=C8N(CCCCCC)C\4=O)=O)=C3C=C2)=C1	0.0064	0
564	O=C(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=CC=C(C4=C(N=S=N5)C5=C(C6=CC=C(C)S6)C7=NN(CC(CCCC)CC)N=C74)S3)C=C8C9=C(C(N(CC(CCCCCC)CCCCCCCCC)C8=O)=O)C(C)=CC1=C92	0	5.35
565	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCC)CCCCC)CCCC)=O)=C(C4=CC=C(C5=C(F)C(F)=C(C)C(F)=C5F)S4)N(CC(CCCCCCCC)CCCCCCCCCCC)C3=O)S1	2.36	0
566	CC1=CC=C(/C(C(N2CC(CCCCCCCCCC)CCCCCCCCC)=O)=C3C(OC4=C\3C=C5C(/C(C(O5)=O)=C6C(N(CC(CCC)CCCCC)CCCCCCCCCCC)C7=C\6C=CC(C8=CC(CCCC)CCCCC)=C(C9=C(CCCCCCCCCC)C=C(C)S9)S8)=C7)=O)=C4)=O)C2=C1	0.37	1.23
567	CC1=CC2=C(C(SC(C3=CC(F)=C(C)C=C3F)=C4)=C4C2(CC(CCCCCCCCCCCC)CCCCCCCCCCCCCCC)S1	4.2	0
568	CC1=NC=C(C2=CN=C(C3=CC(CC(CCCCCCCCCC)CCCCCCCCC)=C(/C=C/C4=C(CC(CCCCCCCCCC)CCCCCCCCC)C=C(C)S4)S3)C5=NSN=C25)C6=NSN=C61	6.87	8.49
569	CC1=CC2=C(C(SC(C3=CC=C(C)C(F)=C3F)=C4)=C4C2(CC(CCCCCCCCCCCC)CCCCCCCCCCCCCCC)S1	2.8	0
570	CC1=CC(C(CC(CC)CCCC)(CC(CC)CCCC)C2=C3C=C4C(C(S(C5=CC=C(C6=C(F)C(F)=C(C7=CC=C(C)S7)C8=NSN=C86)S5)=C9)C9C4(CC(CCCC)CC)CC(CCCC)CC)=C2)=C3S1	0.065	0
571	O=C1/C(C2=CC=C(C)C=C2N1CCCCC(CCCCCCCCCC)CCCCCCCCC)=C3C4=CC=C(C5=CC=C(/C=C/C6=CC=C(C)S6)S5)C=C4N(CCCCCC(CCCCCCCCCC)CCCCCCCCC)C\3=O	2.13	0
572	CC1=CN=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCC)=O)=C(C4=CC=C(C5=CC(SC(C)=C6)=C6S5)C=N4)N(CC(CCCCCCCC)CCCCCCC)C3=O)C=C1	2.04	3.36
573	CC1=CC=C(S1)C(C2=NSN=C23)=C(OCCCCC)C(OCCCCC)=C3C(S4)=CC=C4C(C=C5)=CC6=C5C7=CC=C(C)C=C7C6(CCOCOC)CCOCOC	0	0

574	CC1=CC=C(S1)C(C2=NSN=C23)=C(OCCCCC)C(OCCCC CC)=C3C(S4)=CC=C4C(C=C5)=CC6=C5C7=CC=C(C)C=C 7C6(CCOCCOCCOC)CCOCCOCCOC	0	0
575	CC1=CC=C(S1)C(C2=NSN=C23)=C(OCCCCC)C(OCCCC CC)=C3C(S4)=CC=C4C(C=C5)=CC6=C5C7=CC=C(C)C=C 7C6(CCOCCOCCOCCOC)CCOCCOCCOCCOC	0	0
576	CC1=CC=C(S1)C(C2=NSN=C23)=C(OCCCCC)C(OCCCC CC)=C3C(S4)=CC=C4C(C=C5)=CC6=C5C7=CC=C(C)C=C 7C6(CCOCCOCCOCCOC)CCOCCOCCOCCOC =C(S2)C=C(C)S3)=C4C(N(CC(CCCCCCCCCC)CCCCCCCC CCC)C5=C/4SC6=C5SC(C7=CC=C(C)C8=NSN=C87)=C6)	0.4	0.7
577	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC CC)=O)=C(C4=CC=C(/C=N/N=C/C)S4)N(CC(CCCCCCCC CCCCCCCCCCCC)C3=O)S1	0.36	0.41
578	CC(S1)=CC=C1C(N(CCCCCCCCCC(CCCCCCCCCC)CCCC CCCCCCC)C2=O)=C3C2=C(C4=CC=C(C5=CC=C(/C=C/C 6=CC=C(C)[Se]6)[Se]5)S4)N(CCCCCCCCCC(CCCCCCCC C)CCCCCCCCCCCC)C3=O	4.75	0
579	O=C(C1=CC(C2=CC=C(S2)C(C3C4N=S=N3)C(C(C4C5=C C=CS5)=N6)=NN6CC(CC)CCCC)=C(C(N7CC(CCCCCCCCC C)CCCCCCCCCCCC)=O)C8=C1C9=C(C)C=C8C7=O)N(CC (CCCCCCCCCCC)CCCCCCCCCCCC)C9=O	5.35	0
580	O=C(N1CC(CCCCCCCCCC)CCCCCCCCCCCC)C(C2=C1C3 =NC=C(C=C(C)C=C4)C4=C3)=C(C5=NC=C(C=C(C6=C(F) C(F)=C(C)S6)C=C7)C7=C5)N(CC(CCCCCCCCCC)CCCCC CCCCC)C2=O	6.04	0
581	O=C1C2=CC(C)=CC=C2N(CCCC(CCCCCCCCCC)CCCCC CCCCC)C3=C1C=C(N(CCCC(CCCCCCCCCC)CCCCCCCC CCCC)C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6C7 =O)C7=C3	0.33	0
582	O=C1C2=CC(C)=CC=C2N(CCCC(CCCCCCCCCC)CCCCC CCCCC)C3=C1C=C(N(CCCC(CCCCCCCCCC)CCCCCCCC CCCC)C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6 C7=O)C7=C3	0.22	0
583	CC1=CC=C(S1)C(C2=NSN=C23)=C(OCCCCC)C(OCCCC CC)=C3C(S4)=CC=C4C(C=C5)=CC6=C5C7=CC=C(C)C=C 7C6(CCOCCOCCOCCOC)CCOCCOCCOCCOC	0.15	0
584	CC1=CC=C(S1)C(C2=NSN=C23)=C(OCCCCC)C(OCCCC CC)=C3C(S4)=CC=C4C(C=C5)=CC6=C5C7=CC=C(C)C=C 7C6(CCOCCOCCOCCOC)CCOCCOCCOCCOC =C(S2)C=C(C)S3)=C4C(N(CC(CCCCCCCCCC)CCCCCCCC CCC)C5=C/4SC6=C5SC(C7=CC=C(C)C8=NSN=C87)=C6)	0.32	0
585	CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCCCCCC)CCCCC CCCC)=O)=C(C4=CC=C(C5=C(F)C(F)=C(/C=C/C6=C(F)C F)=C(C)S6)S5)C=N4)N(CC(CCCCCCCCCC)CCCCCCCCCCCC C)C3=O)N=C1	0	1.19
586	CC1=CC=C(C2=C3C(C(N2CCCC(CCCCCCCCCCCCCC)CC CCCCCCCCCCCC)=O)=C(C4=CC=C(C5=C(F)C(F)=C(/C=C /C6=C(F)C(F)=C(C)S6)S5)C=N4)N(CCCC(CCCCCCCCCCCC CC)CCCCCCCCCCCC)C3=O)N=C1	0	1.35
587	CC1=C(Cl)C=C2C(N(CCCC(CCCCCCCCCCCCCC)CCCCC CCCCCCCC)C(/C2=C3C(C=C(Cl)C(C4=CC=C(C5=CC=C(C S5)S4)=C6)=C6N(CCCC(CCCCCCCCCCCCCC)CCCCCCCC CCCCC)C\3=O)=O)=C1	0.62	0.54
588	CC(S1)=CC=C1C2=C3C(C(N2CCCC(CCCCCCCCCCCCCC CCCCCCCCCCCCCCCC)=O)=C(C4=CC=C(C5=CC(C#N)=C/ C=C/C6=C(C#N)C=C(C)S6)S5)S4)N(CCCCCC(CCCCCC CCCCC)CCCCCCCCCCCC)C3=O	0	1.2
589	CC1=CC=C(C2=C(C(CCCCCCCCCCCC)C=C(C3=C([H])C=C4 C(N(CC(CCCCCCCCCC)CCCCCCCCCCCC)C(/C4=C5C(C=C ([H])C(C6=CC(CCCCCCCCCCCC)=C(C7=CC=C(C)S7)S6)= C8F)=C8N(CC(CCCCCCCCCCCC)CCCCCCCCCCC)C\5=O)= O)=C3F)S2)S1	0.75	0

590	O=C1C(C2=C(C3=CC=C(C)C=N3)N1CCCC(CCCCCCCCCC CCCCC)CCCCCCCCCCCCC)=C(C4=CC=C(C5=C(F)C(F)= C(C6=C(F)C(F)=C(C)S6)S5)C=N4)N(CCCC(CCCCCCCCCC CCC)CCCCCCCCCCCCC)C2=O	0	2.45
591	CC1=CC=C(C(N(C(C(CCCCCCCCCC)CCCCCCCCC)=O)C 2=O)=C3C2=C(C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)S 4)N(C(C(CCCCCCCCCC)CCCCCCCCC)=O)C3=O)S1	0.096	0
592	CC1=CC2=C(CI)C3=C(/C(C(N3CC(CCCCCCCCCC)CCCC CCC)=O)=C4C(N(CC(CCCCCC)CCCCCCCCC)C5=C\4 C=C6C(C=C(C7=CC=C(C)S7)S6)=C5CI)=O)C=C2S1	0.018	0.029
593	CC1=C(CCCC(CCCCCCCCCC)CCCCCCCCCCCCC)C=C(C(C(S2)=O)=C3C2=C(C4=CC(CCCC(CCCCCCCCCC)CCCC CCCC)=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)C(S3)=O)S1	0.34	0.16
594	CC1=CC2=C(C4=CC(CCCC(CCCCCCCCCC)CCC CCCCC)=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)C(S3)=O)	0.2	0.093
595	CC1=C(CCC(CCCCCCCCCC)CCCCCCCCCCCCC)C=C(C(C(S2)=O)=C3C2=C(C4=CC(CCC(CCCCCCCCCC)CCCCCCCC CC)=C(C5=CC=C(C6=CC=C(C)S6)S5)S4)C(S3)=O)S1	0.11	0.054
596	CC1=CC2=C(CI)C3=C(/C(C(N3CC(CCCCCCCCCC)CCCC CCC)=O)=C4C(N(CC(CCCCCC)CCCCCCCCC)C5=C\4 C=C6C(C=C(C7=CC=C(/C=C/C8=CC=C(C)S8)S7)S6)=C5 CI)=O)C=C2S1	0.037	0.004
597	C5=CC(C(N(CC(CCCCCCCCCC)CCCCCCCCC)C6=O)= O)=C(C6=CC(C)=C7C(N8CC(CCCCCCCCCC)CCCCCCCC CCC)=O)C7=C5C8=O)S4)C9=NN(CC(CCCC)CC)N=C29)S	7.37	0
598	CC1=CN=C(C2=C3C(C(N2CC(CCCCCCCCCC)CCCCCCCC CCCC)=O)=C(C4=NC=C(C5=CC=C(C6=CC=C(C)S6)S5)C =C4)N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C3=O)C=C1	0.86	1.05
599	O=C1N(CC(CCCCCCCCCC)CCCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC=C(C5=CC=C(C)[Se]5)[Se]4)=C6) =C6N(CC(CCCCCC)CCCCCCCCC)C/3=O	0.66	0
600	CC1=CC(N(CC(CCCCCCCCCC)CCCCCCCCCCCCC) C(/C2=C3C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6 N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C\3=O)= O)=C2C=C1	1.27	0.01
601	CC1=CC=C(C2=C3C(C(N2CC(CCCCCC)CCCCC)=O)= C(C4=CC=C(/C=C/C)S4)N(CC(CCCCCC)CCCCCCCC)C3= CC1=CC=C2C(N(CCCCC(CCCCCCCCCC)CCCCCCCCC)C(/C2=C3C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6)=C6N (CCCC(CCCCCCCCCC)CCCCCCCCC)C\3=O)=O)=C1	0	0
602	O=C1/C(C2=CC=C(C)C=C2N1CCCC(CCCCCCCCCC)CCC CCCCC)=C3C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)C =C4N(CCCC(CCCCCCCCCC)CCCCCCCCC)C\3=O	1.76	0
603	O=C1/C(C2=CC=C(C)C=C2N1CCCC(CCCCCCCCCC)CCC CCCCC)=C3C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)C =C4N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C\3=O	3.62	0
604	O=C1/C(C2=CC=C(C)C=C2N1CCCC(CCCCCCCCCC)CCC CCCCC)=C3C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)C =C4N(CCCCC[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C\3=O	5.1	0
605	O=C1/C(C2=CC=C(C)C=C2N1CCCC(CCCCC[Si](CCCCC)(CCC CCC)C)=C3C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)C=C4 N(CCCCC[Si](C)(CCCCC)CCCCC)C\3=O	3.22	0
606	O=C1/C(C2=CC=C(C)C=C2N1CCCC(CCCCC[Si](CCCCC)(C CCCC)C)=C3C4=CC=C(C5=CC=C(C6=CC=C(C)S6)S5)C =C4N(CCCCC[Si](C)(CCCCC)CCCCC)C\3=O	8.06	0
607	C[Si](C(C1)CCS1=O)(C(CC2)CS2=O)CCCCCN(C/3=O)C4 =CC(C5=CC=C(C6=CC=C(C)S6)S5)=CC=C4C3=C7C(C=C C(C)=C8)=C8N(C[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C\7=O	2.48	0

608	<chem>O=C1/C(C2=CC=C(C)C=C2)N(CCCCCCCCCC[Si](CCCCCCC C)(CCCCCCCC)C)=C3C(N(CCCCCCCC[Si](CCCCCCCC)(CC CCCCC)C)C4=C/C3C=CC(C5=CC=C(C6=CC=C(C)S6)S5)=</chem>	8.06	0
609	<chem>CC1=CC(CCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) =C(C2=CC=C(C3=CC=C(C4=C(CCCCC(F)(F)C(F)(F)C(F)(F))C(F)(F)C(F)(F)C(F)(F)C=C(C)S4)S3)S2)S1</chem>	3.22	0
610	<chem>CC1=C([H])C=C2C(N(CCCC(CCCCCCCCCCCCC)CCCCCCC CCCCCCCC)C(/C2=C3C(C=C([H])C(C4=CC=C(C5=CC=C(C C)S5)S4)=C6)=C6N(CCCC(CCCCCCCCCCCCC)CCCCCCC CCCCCCC)C\3=O)=O)=C1</chem>	0.79	0
611	<chem>O=C1C(C2=C(C3=CC=C(C)S3)N1CC(CCCCCCCCC)CCC CCCC)=C(C4=CC(C)=C(C5=CC(SC6=C7SC(C)=C6)=C7S 5)S4)N(CC(CCCCCCCC)CCCCCCCC)C2=O</chem>	5.32	0
612	<chem>CC1=CC=C(C2=C(CCCCCCCCCCCC)C=C(C3=C(Cl)C=C4 C(N(CC(CCCCCCCCC)CCCCCCCCCCCC)C(/C4=C5C(C=C (Cl)C(C6=CC(CCCCCCCCCCCC)=C(C7=CC=C(C)S7)S6)=C 8[H])=C8N(CC(CCCCCCCCCCCC)CCCCCCCC)C\5=O)= O)=C3[H])S2)S1</chem>	0.1	0
613	<chem>CC1=CC=C(C2=C3C(C(N2CC(CCCCCCCC)CCCCCCCCCCC) =O)=C(C4=CC=C(C5=C(C#N)C=C(C)C(C#N)=C5)S4)N(C C(CCCCCCCCC)CCCCCCCC)C3=O)S1</chem>	0.0086	0.18
614	<chem>O=C1/C(N(CCCC(CCCCCCCCC),CCCCCCCC),C1=C/C2=C C(C3=CC(F)=C(C4=C(F)C=C(C)S4)S3)=C1[H])C2=C(C(N5C CCC(CCCCCCCCC)CCCCCCCC)=O)/C6=C5C([H])=C(CC1=C(F)C(N(CC(CCCCCCCCCCCCC)CCCCCCCCCCCCC C)C(/C2=C3C(C=CC(C4=CC=C(C5=CC=C(C)S5)S4)=C6F) =C6N(CC(CCCCCCCCCCCCC)CCCCCCCCCCCC)C\3= O)=O)=C2C=C1</chem>	6.41	6.76
615	<chem>CC1=C(C)SC(C2=C([H])C(N(CCCCCCCC)C(/C3=C4C(C=C C(C5=CC(C)=C(C6=CC(F)=C(C7=C(F)C=C(C)S7)S6)S5)=C 8[H])=C8N(CCCCCCCC)C\4=O)=O)=C3C=C2)=C1</chem>	1.87	0.43
616	<chem>CC1=CC=C(C2=C(C3=CC(C4=CC(C5=CC(C(C)S6)S5)S4)C3=O)S1 O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	0.0034	0
617	<chem>O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 3/C1=C3C(C=CC(C4=CC(C5=CC(C6=CC(C)S6)S5)S4)C3=O)S1 O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	0.14	0.14
618	<chem>O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	0.34	0
619	<chem>C3=CC=C(C/C=C/C4=CC=C(C)[Se]4)[Se]3C=C5C6=C(C(N CC(CCCCCCCCC)CCCCCCCC)C5=O)=O)C(C)=CC1 CC1=C(C)SC(C2=C(F)C(N(CCCCCCCC)C(/C3=C4C(C=CC C5=CC(C)=C(C6=CC([H])=C(C7=C([H])C=C(C)S7)S6)S5)= C8F)=C8N(CCCCCCCC)C\4=O)=O)=C3C=C2)=C1</chem>	0	2.4
620	<chem>CC1=CC=C(C2=C(C3=CC(C4=CC(C5=CC(C(C)S6)S5)S4)C3=O)S1 O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	0.002	0
621	<chem>CC1=CC=C(C2=C(C3=CC(C4=CC(C5=CC(C6=CC(C)S6)S5)S4)C3=O)S1 O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	3.49	2.77
622	<chem>CC1=CC=C(C2=C(C3=CC(C4=CC(C5=CC(C6=CC(C)S6)S5)S4)C3=O)S1 O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	1.9	0
623	<chem>CC1=CC=C(C2=C(C3=CC(C4=CC(C5=CC(C6=CC(C)S6)S5)S4)C3=O)S1 O=C1N(CC(CCCCCCCCC)CCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC(SC(C)=C5)=C5S4)=C6)=C6N(CC (CCCCCCCC)CCCCCCCC)C/3=O</chem>	7.28	0
624	<chem>O=C1N(CC(CCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) (F)C(F)(F)C1=O)C2=C(C3=CC=C(C/C=C/C4=CC=C(C)S4) S3)C=C5C6=C(C(N(CCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) (F)C(F)(F)C(F)(F)C5=O)=O)C(C)=CC1=C62</chem>	0	6.5
625	<chem>CC1=C(C)SC(C2=C(F)C(N(CCCCCCCC)C(/C3=C4C(C=CC C5=CC(C)=C(C6=CC([H])=C(C7=C([H])C=C(C)S7)S6)S5)= C8F)=C8N(CCCCCCCC)C\4=O)=O)=C3C=C2)=C1</chem>	0	0.93

626	CC(C=C1)=CC2=C1/C(C(N2CCCCCCC(CCCCCCCCCCCC) CCCCCCCCCCC)=O)=C(C3=C4C=C(C=C3)C5=CC=C(/C=C /C6=CC=C(C)[Se]6)[Se]5)\C(N4CCCCCCC(CCCCCCCCCC) CCCCCCCCCCC)=O	5.83	0
627	O=C(N(CCCCCCCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F) (F)C(F)(F)C1=O)C2=C(C3=CC=C(/C=C/C4=CC=C(C)S4) S3)C=C5C6=C(C(N(CCCCCCCCCC(F)(F)C(F)(F)C(F)(F) (F)C(F)(F)C(F)(F)C5=O)=O)C(C)=CC1=C62	5.64	0
628	O=C(N1CC(CCCCCCCCCC)CCCCCCCCCCC)C2=CC(C3= CC=C(N(CCCCCC)C(C=C(C)C=C4)=C4S5)C5=C3)=C6C7= C(C8=C9C6=CC=C%10C9=C(C(N(CC(CCCCCCCCCCCC)C CCCCCCCCC)C%10=O)=O)C=C8C)C=CC(C1=O)=C27	0	0.05
629	O=C(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=C/2C=CC(C3= C(F)C=C(C4=CC(F)=C(C)S4)S3)=C1)C2=C(C(N5CC(CCCCC CCC)CCCCCCCCC)=O)/C6=C5C=C(C)C=C6	0.09	0.09
630	O=C1N(CC(CCCCCCCCCC)CCCCCCCCC)C2=CC(C)=CC=C 2/C1=C3C(C=CC(C4=CC5=C(C=C(C=C(C)S6)C6=C5)S4)= C7)=C7N(CC(CCCCCCCC)CCCCCCCCC)C/3=O	0.48	0
631	2/C1=C3C(C=CC(C4=CC5=C(C(C=CC6=C7SC(C)=C6)=C7 C=C5)S4)=C8)=C8N(CC(CCCCCCCC)CCCCCCCCC)C/3= CC1=NC2=C(/C(C(N2CC(CCCCCCCCCCCC)CCCCCCCCC)=O)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C4=C\ 3C=CC(C5=CC=C(C6=CC=C(C)S6)S5)=N4)=O)C=C1	0.32	0
632	C3=CC(F)=C(/C=C/C4=C(F)C=C(C)S4)S3)C=C5C6=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C5=O)=O)C(C)=CC1	0.45	0.47
633	CC1=CC=C2C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C(/ C2=C3C(C=CC(C4=CC=C(C5=C(F)C(F)=C(C6=CC=C(C)S6)C7=NSN=C75)S4)=C8)=C8N(CC(CCCCCCCCCCCC)CCCC CCCCC)C\3=O)=O)=C1	3.2	0
634	CC1=CC(CCCCCCCCCCCCCCCC)=C(C2=CC(SC(C3=C(CC CCCCCCCCCCCCC)C=C(C)S3)=C4)=C4S2)S1	0.073	0
635	CC1=CC(N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC) C(/C2=C3C(C=C(Cl)C(C4=CC=C(C5=CC=C(C)[Se]5)[Se]4) =C6)=C6N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC) C\3=O)=O)=C2C=C1Cl	0.32	0
636	CC1=CC=C(/C(C(N2CCCC(CCCCCCCCCCCCCCCCCC)CCC CCCCCCCCCCCCCCC)=O)=C3S(/C(CC\3)=C4CC/C(S\4(= O)=O)=C5C(N(CCCC(CCCCCCCCCCCCCCCCCC)CCCCC CCCCCCCCCCCCC)C6=C\5C=CC(C7=CC=C(C8=CC=C(C)S 8)S7)=C6)=O)(=O)=O)C2=C1	0.81	0.66
637	CC1=CC2=C(/C(C(N2CCCC(OC(CCCCCCCCCCCCCCCC)C CCCCCCCCCCCCCCC)=O)=O)=C3C(OC4=C\3C=C5C(/C(C(O5)=O)=C6C(N(CCCC(OC(CCCCCCCCCCCCCCCC)CCC CCCCCCCCCCCCC)=O)C7=C\6C=CC(C8=CC=C(C9=CC= C(C)S9)S8)=C7)=O)=C4)=O)C=C1	0	0.18
638	CC1=CC=C(/C(C(N2CC(CCCCCCCCCCCCCC)CCCCCCCCC) =O)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C4=C\3 C=CC(C5=C(F)C(F)=C(/C=C/C6=C(F)C(F)=C(C)S6)S5)=C4[H])=O)C2=C1[H]	0.2	0.35
639	CC1=CC=C(/C(C(N2CCCC(CCCCCCCCCCCCCC)CCCCCCCCC) =O)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C4=C\3 C=CC(C5=C(F)C(F)=C(/C=C/C6=C(F)C(F)=C(C)S6)S5)=C4[H])=O)C2=C1[H]	0.89	1.63
640	CC1=CC(N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC) C(/C2=C3C(C=C(Cl)C(C4=CC=C(C5=CC=C(C)S5)S4)=C6) =C6N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)C\3= O)=O)=C2C=C1Cl	0	4.97
641	CC1=CC(N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC) C(/C2=C3C(C=C(Cl)C(C4=CC=C(C5=CC=C(C)S5)S4)=C6) =C6N(CC(CCCCCCCCCCCCCC)CCCCCCCCCCCCC)C\3= O)=O)=C2C=C1Cl	0.54	0.48

642	CC1=CC=C(/C(C(N2CCCC(CCCCCCCCCCCCCC)CCCCCCC CCCCCCC)=O)=C3C(N(CCCC(CCCCCCCCCCCCCC)CCCC CCCCCCCCC)C4=C\3C=CC(C5=CC=C(C6=CC=C(C)[Se] 6)[Se]5)=C4Cl)=O)C2=C1Cl	1.05	0.72
643	CC1=C(Cl)C=C2C(N(CCCC(CCCCCCCCCCCCCC)CCCCC CCCCCCCCC)C(/C2=C3C(C=C(Cl)C(C4=CC=C(C5=CC=C(C)[Se]5)[Se]4)=C6)=C6N(CCCC(CCCCCCCCCCCCCC)CCCC CCCCCCCCC)C\3=O)=O)=C1	1.05	0.72
644	CCCCC)=O)=C3C(N(C4=C\3C=CC(C5=CC=C(/C=C/C6=C C=C(C)S6)S5)=C4)CC(CCCCCCCCCC)CCCCCCCCCCCC)= O=C(O1)/C(C2=C1C=C(/C(C(O3)=O)=C(C4=C(C(F)=C(C) C=C4)N5CCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCC CCCCCCCCC)\C5=O)C3=C2)=C6C(N(CCCC(CCCCCCCCCC CCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C7=C/6C=CC(C8= CC=C(C9=CC=C(C)[Se]9)[Se]8)=C7F)=O	2.2	0
645	O=C(O1)/C(C2=C1C=C(/C(C(O3)=O)=C(C4=C(C(F)=C(C) C=C4)N5CCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCC CCCCCCCCC)\C5=O)C3=C2)=C6C(N(CCCC(CCCCCCCCCC CCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C7=C/6C=CC(C8= CC=C(C9=CC=C(C)[Se]9)[Se]8)=C7F)=O	6.14	0
646	O=C(O1)/C(C2=C1C=C(/C(C(O3)=O)=C(C4=C(C(F)=C(C) C=C4)N5CCCC(CCCCCCCCCCCCCCCCCC)CCCCCCCCC CCCCCCCCC)\C5=O)C3=C2)=C6C(N(CCCC(CCCCCCCCCC CCCCCCCCC)CCCCCCCCCCCCCCCCCCCC)C7=C/6C=CC(C8= CC=C(C9=CC=C(C)S9)S8)=C7F)=O	14.9	0
647	CC1=C(F)C2=C(/C(C(N2CCCC(CCCCCCCCCCCCCCCCCC) CCCCCCCCCCCCCCCCC)=O)=C3C(OC4=C\3C=C5C(/C(C(O5)=O)=C6C(N(CCCC(CCCCCCCCCCCCCCCCCC)CCCC CCCCCCCCCCCCCCCC)C7=C\6C=C(F)C(C8=CC=C(C9=CC= C(C)S9)S8)=C7F)=O)=C4)=O)C=C1F	0	14.9
648	CC1=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C2=O)= O)C2=C(C3=C4C(C(N(CC(CCCCCCCCCCCCCC)CCCCCCCCC C)C4=O)=O)=C(C5=CC=C(C6=C([H])C([H])=C(C7=CC=C(C)S7)C8=NSN=C68)S5)S3)S1	0.33	1.02
649	CC1=CC=C(C2=CC(CCCCCCCCCC)=C(C3=CC=C(C4= CC=C(C5=CC=C(C6=C(CCCCCCCCCC)C=C(C7=CC=C(C(N(CC(CCCCCCCCCC)CCCCCCCCCCCCC)C8=O)=C9C8=C (C)N(CC(CCCCCCCCCC)CCCCCCCCC)C9=O)S7)S6)S5)C%10=NSN=C%104)S3)S2)S1	0.81	0
650	O=C(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=CC=C(C4=C([H])C([H])=C(C5=CC=C(C)[Se]5)C6=NSN =C64)[Se]3)C=C7C8=C(C(N(CC(CCCCCCCCCC)CCCCC CCCCC)C7=O)=O)C(C)=CC1=C82	1.7	8.5
651	CC1=CC=C(/C(C(N2CCCC(CCCCCCCCCCCCCCCCCC)CCC CCCCCCCCCCCCCCCC)=O)=C3S(/C(CC\3)=C4CC/C(S\4= O)=O)=C5C(N(CCCC(CCCCCCCCCCCCCCCCCC)CCCCC CCCCCCCCCCCCC)C6=C\5C=CC(C7=CC8=C(C=C(C)S8)S7)=C6)=O)(=O)=O)C2=C1	0	0.14
652	FC1=C2C(/C(C(N2CC(CCCCC)CCCCCCCC)=O)=C3C(N(C C(CCCCCC)CCCCC)C4=C\3C=CC(C(C=C5)=NC6=C5/ C(C(N6CC(CCCCCC)CCCCC)=O)=C7C8=CC=C(C9=C(F)C(F)=C(C%10=C(F)C(F)=C(C)S%10)S9)C(F)=C8N(CC(CCC CCC)CCCCCCCC)C/7=O)=N4)=O)=CC=C1C	0	1.24
653	CC1=CC=C(/C(C(N2CC(CCCCC)CCCCCCCC)=O)= C3C(N(CC(CCCCCCCCCC)CCCCCCCC)C4=C\3C=CC(C5= CC=C(C)[Se]5)=N4)=O)C2=N1	0.2	0.5
654	O=C(N(CC(CCCCCCCCCC)CCCCCCCCC)C1=O)C2=C(C3=CC=C(C4=C([H])C([H])=C(C5=CC=C(C)S5)C6=NSN= C64)S3)C=C7C8=C(C(N(CC(CCCCCCCCCC)CCCCCCCCC CC)C7=O)=O)C(C)=CC1=C82	0.7	3.1
655	C=C(C3=CC=C(C4=CC=C(C)S4)S3)C=C5C6=C(C(N(CCCCC C[Si](O[Si](C)(C)C)(C)O[Si](C)(C)C)C5=O)=O)C(C)=CC1=C	0	1.04

671	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C([H])C([H])=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O O=C(N1CC(CCCCCCCCCC)CCCCCCCC)C2C(SC3=C2SC4=C3C(N(CC(CCCCCCCCCC)CCCCCCCC)C(C5=C4SC(C)=C5)=O)=O)C6C(C=C(C)S6)C1=O	0.7	3.1
672	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C([H])C([H])=C(C)C7=NON=C76)[Se]5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O	0	1.34
673	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)[Se]5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O	0	2.43
674	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O O=C(N(CC(CCCCCCCCCC)CCCCCCCC)C1=O)C2=C(C3=CC(Cl)=C(C4=C(Cl)C=C(C)S4)S3)C=C5C6=C(C(N(CC(CCCCCC)CCCCCCCC)C5=O)=O)C(C)=CC1=C62	0	1.1
675	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)[Se]5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O O=C(N1CC(CCCCCCCCCC)CCCCCCCC)C2C(SC(C)=C2)C3C(C=C(C)S3)C1=O	0	3.5
676	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O O=C(N(CC(CCCCCCCCCC)CCCCCCCC)C1=O)C2=C(C3=CC(Cl)=C(C4=C(Cl)C=C(C)S4)S3)C=C5C6=C(C(N(CC(CCCCCC)CCCCCCCC)C5=O)=O)C(C)=CC1=C62	0	2.2
677	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O O=C(N1CC(CCCCCCCCCC)CCCCCCCC)C2C(SC(C)=C2)C3C(C=C(C)S3)C1=O	0	0.03
678	CC1=CC2=C3C(C4=CC(C5=CC=C(C6=C(F)C(F)=C(C)C7=NSN=C76)S5)=C3C(N(CC(CCCCCCCCCC)CCCCCCCCCCC)C2=O)=O)=C1C(N(CC(CCCCCCCCCC)CCCCCCCCC)C4=O)=O O=C(N(CC(CCCCCCCCCC)CCCCCCCC)C1=O)C2=C(C3=CC(Cl)=C(C4=C(Cl)C=C(C)S4)S3)C=C5C6=C(C(N(CC(CCCCCC)CCCCCCCC)C5=O)=O)C(C)=CC1=C62	0	3.71