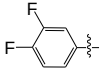
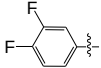
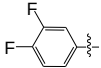
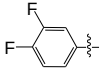
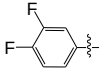
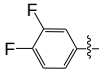
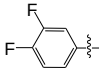
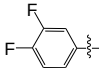
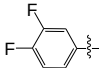
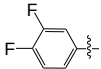
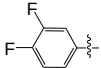
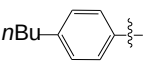
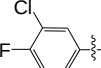
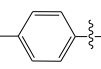
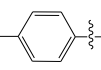
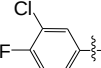
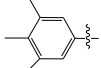
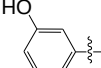
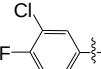
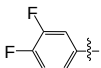


Table S1 Structure of compounds with different skeletons in the data set

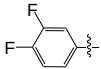
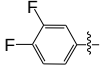
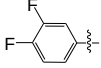
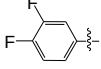
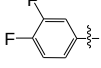
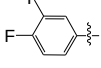
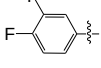
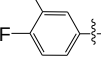
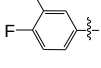
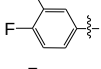
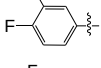
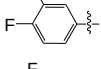
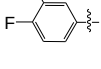
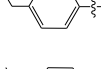
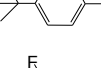
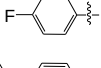
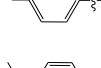
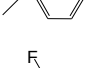
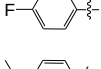
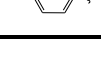
Skeleton A	Skeleton B	Skeleton C	Skeleton D	Skeleton E

NO	Skeleton	R ₁	R ₂	R ₃	IC ₅₀ (μM)
1 ^s	A		H	R ₃ =3-F	20.0
2 ^s	A		H	R ₃ =3-F	29
3	A		H	R ₃ =3-F	32.8
4	A		H	R ₃ =3-F	35.5
5 ^s	A		H	R ₃ =3-F	22.8
6 ^s	A		H	R ₃ =3-F	29.4
7	A		H	R ₃ =4-Me	27.4
8	A		H	R ₃ =3,4-diF	22.5
9 ^s	A		H	R ₃ =3-F	28
10	A		H	R ₃ =3-F	24.8
11	A		H	R ₃ =3-CF ₃	32.2
12	A		H	R ₃ =2-F	33
13	A		H	R ₃ =4-NO ₂	22.4
14	A		Cl	R ₃ =4-NO ₂	21.1
15	A		H	R ₃ =3-F	13.3
16	A		CO ₂ Me	4-F	18.1

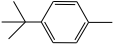
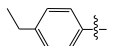
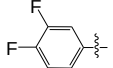
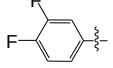
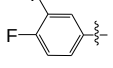
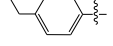
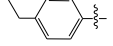
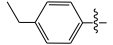
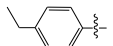
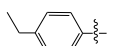
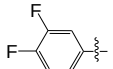
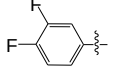
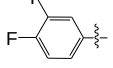
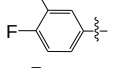
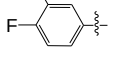
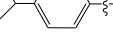
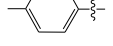
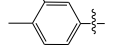
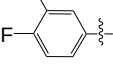
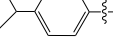
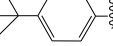
To be continued

NO	Skeleton	R ₁	R ₂	R ₃	IC ₅₀ (μM)
17 [§]	A		CO ₂ Me	4-Cl	14.7
18	A		SO ₂ NH ₂	4-F	16.4
19	A		OMe	4-F	22.1
20	A		OMe	4-Cl	24.2
21 [§]	A		H	4-F	32.3
22	A		F	4-F	27.7
23	A		Cl	4-F	28.5
24	A		H	4-Cl	29.7
25	A		NO ₂	4-Cl	1.8
26	A		F	4-Cl	24.2
27	A		Cl	4-Cl	28
28	A		H	4-F	27.7
29 [§]	A		H	4-F	29.3
30	A		H	4-F	28.2
31	A		NO ₂	4-F	18.4
32	A		NO ₂	4-F	6.5
33	A		NO ₂	4-F	30.5
34	A		NO ₂	4-F	13.7
35	A		NO ₂	4-F	1.8
36	A		OCF ₃	4-F	22.3

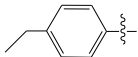
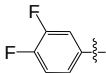
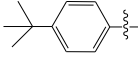
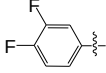
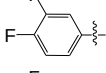
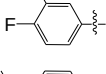
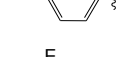
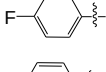
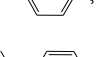
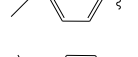
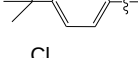
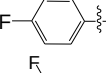
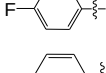
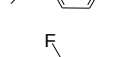
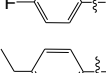
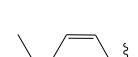
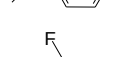
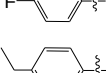
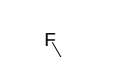
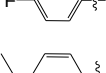
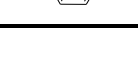
To be continued

NO	Skeleton	R ₁	R ₂	R ₃	IC ₅₀ (μM)
37 ^s	A		OCF ₃	4-Cl	20.5
38	A		NO ₂	4-OMe	22.1
39	A		NO ₂	4-OH	8.2
40	A		NO ₂	3,4,5-Tri-F	6.4
41 ^s	A		NO ₂	3,4-Di-F	4.8
42	A		NO ₂	2- Cl,6-F	7.5
43	A		NO ₂	4-Ph	19.8
44	A		NO ₂	3,4,5-Tri-F	4.7
45	E		NO ₂	-	4
46	A		OCH ₂ -CO ₂ tBu	4-Cl	31.4
47 ^s	A		OCH ₂ -CO ₂ H	4-Cl	20.9
48	A		OCH ₂ -CO ₂ H	4-F	22.5
49 ^s	B		CO ₂ Me	4-F	6
50	B		CO ₂ Me	4-F	5.6
51	B		CO ₂ Me	4-F	4.5
52	B		CO ₂ Me	4-Cl	5.1
53 ^s	B		CO ₂ Me	4-Cl	5.5
54	B		CO ₂ Me	4-Cl	6.2
55	B		SO ₂ NH ₂	4-F	6.9
56	B		SO ₂ NH ₂	4-F	8.3

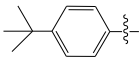
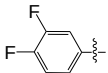
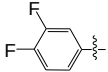
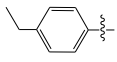
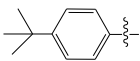
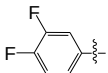
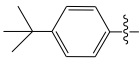
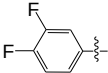
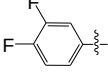
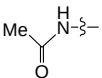
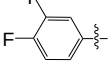
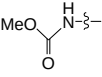
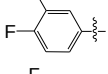
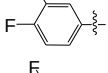
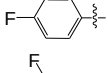
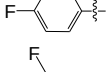
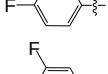
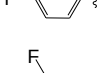
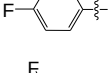
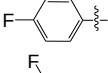
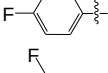
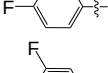
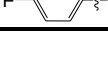
To be continued

57 ^s	B		SO ₂ NH ₂	4-F	3.1
58	B		OMe	4-Cl	14.1
59	B		OMe	4-F	21
60	B		OMe	4-Cl	18.3
61 ^s	B		OMe	3-F	24
62	B		H	4-F	10.5
63 ^s	B		NO ₂	4-F	2.7
64	B		F	4-F	10.9
65 ^s	B		H	4-Cl	22.1
66	B		NO ₂	4-Cl	3.1
67	B		H	4-F	26.1
68	B		NO ₂	4-F	5.1
69 ^s	B		F	4-F	12.3
70	B		NO ₂	3-F	4.3
71 ^s	B		NO ₂	4-Cl	4.5
72	B		H	4-Cl	22.7
73	B		NO ₂	4-F	8.7
74	B		NO ₂	4-F	12.6
75	B		NO ₂	4-F	4.3
76	B		NO ₂	4-F	1.5
77	B		NO ₂	4-F	1.2

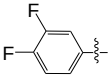
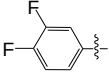
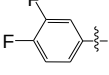
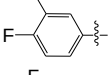
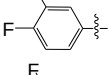
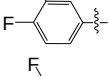
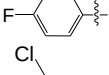
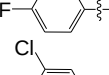
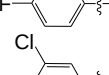
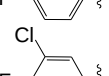
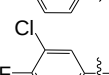
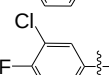
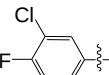
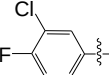
To be continued

78 ^s	B		Cl	4-Cl	7.6
79	B		Cl	4-Cl	8.9
80	B		H	4-F	12.7
81 ^s	B		H	4-Me	25.9
82	B		F	3-F	25
83	B		H	2-F	30.2
84	B		H	3-F	27.5
85 ^s	B		H	4-NO ₂	18.2
86	B		NO ₂	4-Cl	5.4
87	B		NO ₂	4-Cl	2.9
88	B		NO ₂	4-Cl	1.5
89 ^s	B		NO ₂	4-Cl	2.2
90	B		NO ₂	4-Br	2.6
91	B		NO ₂	4-Br	3.8
92	B		OCF ₃	4-F	6.1
93 ^s	B		OCF ₃	4-F	13.1
94	B		NO ₂	4-F	1.4
95	B		NO ₂	4-OMe	9.3
96	B		NO ₂	4-OMe	14.3
97	B		OCH ₂ -CO ₂ <i>t</i> Bu	4-F	8.7
98	B		OCH ₂ -CO ₂ <i>t</i> Bu	4-F	28.7

To be continued

99	B		OCH ₂ -CO ₂ tBu	4-F	9.2
100	B		OCH ₂ -CO ₂ tBu	4-Cl	8.3
101 ^s	B		OCH ₂ -CO ₂ H	4-F	9.6
102	B		OCH ₂ -CO ₂ H	4-F	8.7
103	B		OCH ₂ -CO ₂ H	4-F	3.9
104	B		OCH ₂ -CO ₂ H	4-Cl	8.2
105 ^s	B		OCH ₂ -CO ₂ H	4-Cl	3
106	A		NH ₂	3-F	31.4
107	A			3-F	33.1
108	A			3-F	34.7
109 ^s	C		NO ₂	3-F	9.6
110	D		NO ₂	4-F	4.8
111 ^s	D		NO ₂	4-Cl	2.9
112	D		NO ₂	4-Br	2.6
113 ^s	D		NO ₂	3-Cl	2.3
114	D		NO ₂	3-CF ₃	2.4
115	A		NO ₂	3-F	3.9
116	A		NO ₂	3-F	0.32
117 ^s	A		NO ₂	4-F	5.8
118	A		NO ₂	4-F	0.52
119	A		NO ₂	4-Br	2.9

To be continued

120	A		NO ₂	4-Br	0.28
121 [§]	A		NO ₂	4-CN	8.8
122	A		NO ₂	4-CN	1.3
123	A		NO ₂	3-Cl	9.6
124	A		NO ₂	3-Cl	0.94
125 [§]	A		NO ₂	3-CF ₃	7.9
126	A		NO ₂	3-CF ₃	0.38
127	A		NO ₂	3-Cl	8.9
128	A		NO ₂	3-Cl	0.51
129 [§]	A		NO ₂	3,4-Di F	11
130	A		NO ₂	3,4-Di F	1.3
131	A		NO ₂	3-CF ₃	9.1
132	A		NO ₂	3-CF ₃	1.4
133 [§]	A		NO ₂	4-Cl	9.5
134	A		NO ₂	4-Cl	1.24

[§] Molecules Belonged to the Test Set.