

Appendix 2: Descriptor values (atomic signatures) for the 20 new pesticides

N°	Compound	Atomic signatures							logkow
		X3	X6	X14	X17	X20	X29	X32	
1	C6H14OS2	17	2	0	0	0	0	0	1.8849246
2	C9H19N2O4PS4	17	2	2	0	1	0	0	2.1957886
3	C13H23N4O5PS2	17	2	2	0	0	0	0	2.6154626
4	C6H16NO2PS2	17	2	2	0	0	0	0	2.6154626
5	C9H22N3O3PS3	17	2	2	0	0	0	0	2.6154626
6	C6H14NO3PS4	17	2	2	0	1	0	0	2.1957886
7	C10H15N2O4PS2	17	2	2	0	1	0	0	2.1957886
8	C6H16NO5PS2	17	2	2	0	0	0	0	2.6154626
9	C16H26N3O7PS3	17	2	0	0	1	0	0	1.4652506
10	C8H18N3O2PS3	17	2	2	0	0	0	0	2.6154626
11	C8H20NO3PS2	17	2	2	0	0	0	0	2.6154626
12	C5H15N2O4PS	17	2	2	0	1	0	0	2.1957886
13	C7H17O2PS4	17	2	2	0	0	0	0	2.6154626
14	C6H15O2PS3	17	2	2	0	0	0	0	2.6154626
15	C7H15N2O4PS3	17	2	2	0	1	0	0	2.1957886
16	C8H17N2O4PS3	17	2	2	0	1	0	0	2.1957886
17	C9H17Cl2N2O3PS2	17	2	2	0	1	0	0	2.1957886
18	C7H18NO2PS2	17	2	2	0	0	0	0	1.3610566
19	C5H12NO5PS	17	0	2	0	1	0	0	2.6154626
20	C7H16NO4PS	17	2	2	0	1	0	0	2.1957886