Electronic Supplementary Material (ESI) for Toxicology Research.

Distribution of toxicity values across different species and modes of action of pesticides from PESTIMEP and PPDB databases

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SUPPORTING INFORMATION

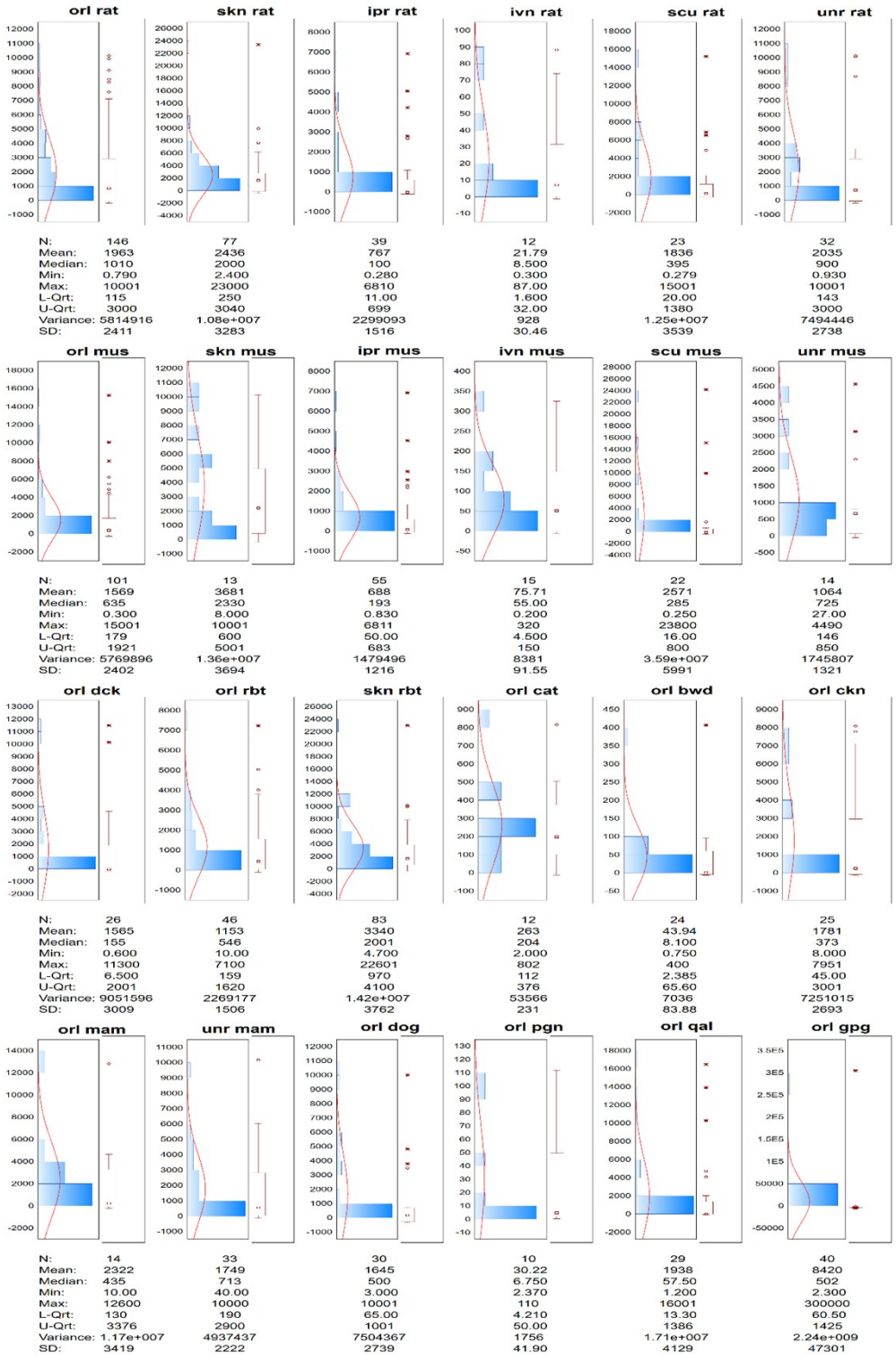

Figure S1. Distributions and descriptive statistics of toxicity endpoints and routes of exposure.

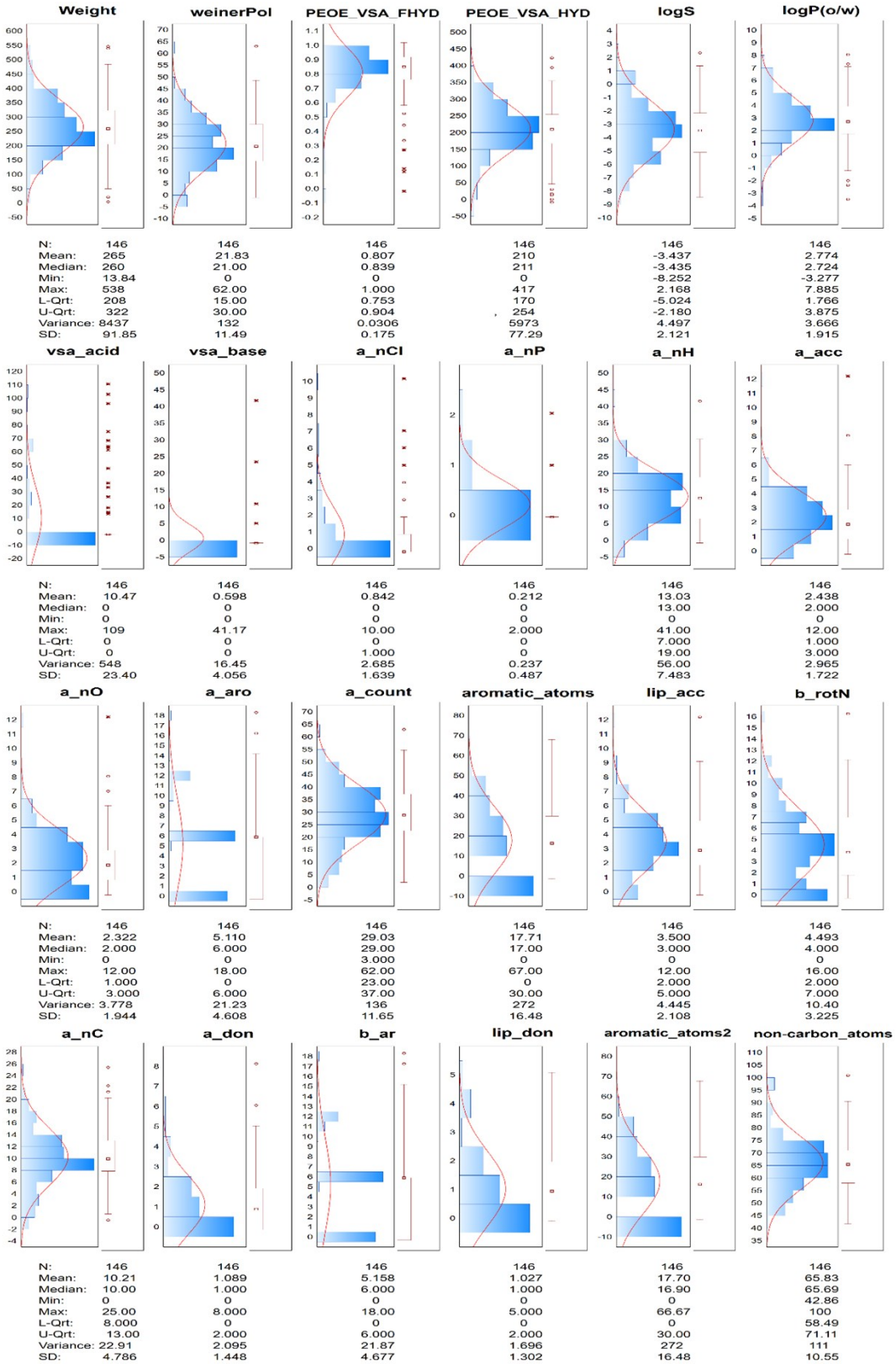

Figure S2. Distributions and descriptive statistics of physicochemical properties.

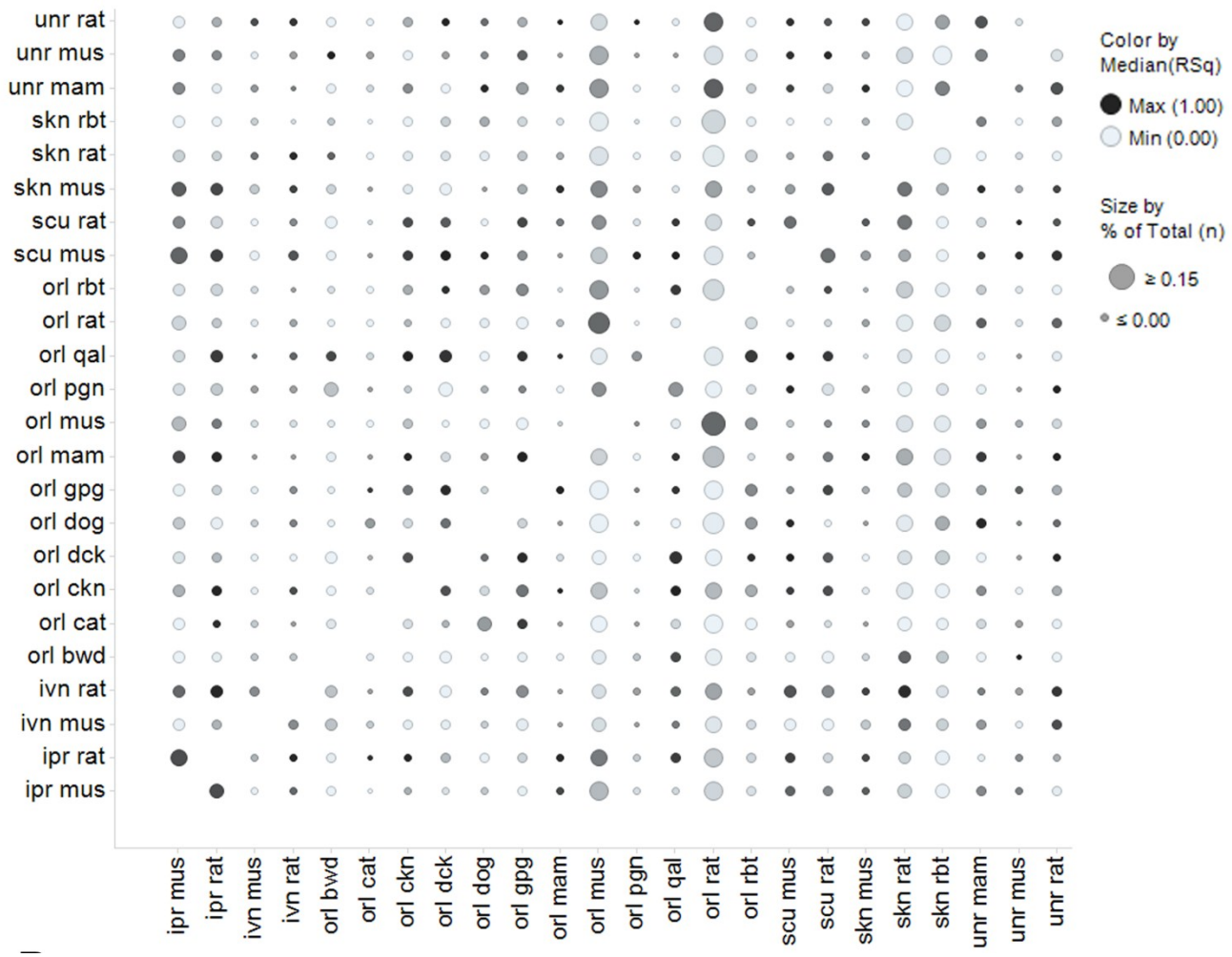

Figure S3. Graphical representation of the pair-wise linear regressions.

Table S1. Number of molecules evaluated at a given experimental assay in PESTIMEP.

		#molecules evaluated
rat	orl	147
mus	orl	102
rbt	skn	85
rat	skn	77
mus	ipr	55
rbt	orl	47
gpg	orl	40
rat	ipr	39
rat	unr	33
mam	unr	33
dog	orl	31
qal	orl	29
dck	orl	26
ckn	orl	25
bwd	orl	24
rat	scu	23
mus	scu	22
mus	ivn	17
mus	unr	14
mam	orl	14
mus	skn	13
rat	ivn	12
cat	orl	12
pgn	orl	10
gpg	skn	8
dom	orl	6
gpg	ipr	6
rat	par	5
brd	orl	5
dcl	orl	5
qal	unr	5
ham	orl	5
rbt	ivn	4
rat	ims	3
dck	skn	3
ctl	orl	3
mam	skn	3
ham	ipr	3
dck	unr	2

		#molecules evaluated
rbt	scu	2
rbt	unr	2
ckn	scu	2
ckn	unr	2
mky	orl	2
dog	ipr	2
dog	ivn	2
grb	ipr	2
rat	ro	1
rat	ihl	1
rat	ice	1
rat	itr	1
mus	ice	1
mus	ims	1
brd	rec	1
prn	orl	1
dcl	skn	1
rbt	ipr	1
rbt	ocu	1
cat	skn	1
cat	ipr	1
cat	unr	1
ctl	unr	1
bwd	skn	1
mam	ipr	1
mam	ivn	1
man	orl	1
man	unr	1
dog	scu	1
dog	unr	1
frg	par	1
pgn	ivn	1
qal	skn	1
gpg	ivn	1
gpg	scu	1
gpg	unr	1
hmn	orl	1
hmn	ims	1
trk	orl	1
	TOTAL	**1043**

Table S2. Coefficients of the first five principal components (PC) for the descriptors used in the PCA of FDA and pesticides databases based on druglike properties.

	PC1	PC2	PC3	PC4	PC5
Weight	0.5005	0.37877	0.38767	0.27076	0.61841
logP(o/w)	0.09008	0.73269	0.3243	0.45241	0.38107
a_acc	0.57605	0.16351	0.23975	0.36007	0.67401
a_don	0.48082	0.3904	0.09341	0.76894	0.12809
b_rotN	0.42233	0.3749	0.82361	0.03308	0.04064

Table S3. Coefficients of the first five principal components (PC) for the descriptors used in the PCA of FDA and pesticides databases based on pesticides properties.

	PC1	PC2	PC3	PC4	PC5
weinerPol	0.49167	0.03691	0.03278	0.01893	0.03669
PEOE_VSA_HYD	0.49457	0.03522	0.06162	0.05536	0.027
logS	0.38326	0.29492	0.1884	0.04434	0.09114
vsa_acid	0.0678	0.08849	0.535	0.37777	0.03307
vsa_base	0.01779	0.02091	0.08505	0.48102	0.81922
reactive	0.10514	0.18917	0.02127	0.62962	0.43812
a_nCl	0.01923	0.27107	0.52827	0.41984	0.1817
a_nP	0.0493	0.22789	0.59026	0.07161	0.20948
a_nH	0.47037	0.16033	0.10665	0.10553	0.00578
a_nO	0.30682	0.35848	0.0983	0.08317	0.15304
aromatic_carbons	0.02932	0.54181	0.0909	0.1568	0.15832
non-carbon_atoms	0.17818	0.54147	0.09459	0.00835	0.00518

Table S4. Coefficients of the first five principal components (PC) for the descriptors used in the PCA of FDA database based on pesticide-like properties.

	PC1	PC2	PC3	PC4	PC5
weinerPol	0.49169	0.02309	0.00239	0.00985	0.03329
PEOE_VSA_HYD	0.49237	0.0582	0.02621	0.01769	0.10274
logS	0.38701	0.31408	0.03046	0.08315	0.04462
vsa_acid	0.00757	0.07779	0.69457	0.01738	0.05595
vsa_base	0.01843	0.0399	0.68386	0.05414	0.22635
reactive	0.1179	0.17753	0.17883	0.32065	0.75538
a_nCl	0.00853	0.28609	0.02044	0.65445	0.17498
a_nP	0.02878	0.22202	0.08704	0.65405	0.49698
a_nH	0.47362	0.1387	0.02617	0.12285	0.06537
a_nO	0.31814	0.3453	0.00273	0.05292	0.15136
aromatic_carbons	0.05073	0.53907	0.08727	0.0687	0.2268
non-carbon_atoms	0.15081	0.54595	0.0005131	0.08907	0.07184

Table S5. Coefficients of the first five principal components (PC) for the descriptors used in the PCA of pesticides database based on pesticide-like properties

	PC1	PC2	PC3	PC4	PC5
weinerPol	0.44496	0.21068	0.23106	0.07116	0.03227
PEOE_VSA_HYD	0.46606	0.26846	0.1564	0.00613	0.06307
logS	0.47727	0.03927	0.0082	0.12848	0.13119
vsa_acid	0.14188	0.162	0.52858	0.12444	0.06178
vsa_base	0.02329	0.0023	0.29726	0.40607	0.68288
reactive	0.04135	0.07183	0.35611	0.42343	0.40731
a_nCl	0.24258	0.21203	0.16629	0.55092	0.46392
a_nP	0.04261	0.42465	0.061	0.15113	0.14369
a_nH	0.21659	0.43166	0.3463	0.33674	0.10064
a_nO	0.06281	0.46308	0.45549	0.05925	0.08189
aromatic_carbons	0.22933	0.37211	0.24671	0.37437	0.23596
non-carbon_atoms	0.41293	0.29336	0.08872	0.18788	0.1826