

SUPPLEMENTARY MATERIAL APPENDIX

Table 3 : Freundlich coefficients K and $1/n$, and Chi indices of the 55 organic compounds

Organic compound	n°	log K	1/n	r
toluene	1	2.179	0.519	0.99
benzaldehyde	2	2.027	0.276	0.98
benzoic acid	3	1.914	0.384	0.97
chlorobenzene	4	2.478	0.430	0.97
anisole	5	2.158	0.338	0.99
nitrobenzene	6	2.308	0.279	0.98
fluorobenzene	7	2.142	0.466	0.99
acetophenone	8	2.271	0.258	0.99
dimethyl acetalbenzaldehyde	9	2.248	0.267	0.99
bromobenzene	10	2.680	0.372	0.99
4-chlorophenol	11	2.119	0.206	0.99
4-nitrophenol	12	2.264	0.125	0.98
diethylphtalate	13	2.347	0.226	0.95
4-methoxyphenol	14	2.192	0.162	0.99
4-cresol	15	2.101	0.177	0.98
salycilic acid	16	1.955	0.318	0.95
4-aminophenol	17	2.355	0.105	0.97
2-carboxybenzaldehyde	18	2.009	0.201	0.99
4-iodoaniline	19	2.608	0.210	0.99
3-nitrobenzoic acid	20	2.105	0.360	0.97
3-aminobenzoic acid	21	1.925	0.273	0.96
catechol	22	1.953	0.265	0.99
4-tertbutyl phenol	23	2.475	0.136	0.99
4-ethyl phenol	24	2.277	0.200	0.99
vaniline	25	2.211	0.175	0.99
2-tertbutyl-4-methyl phenol	26	2.479	0.117	0.99
atrazine	27	2.270	0.351	0.99

3-chloro-4-fluoroaniline	28	2.292	0.280	0.98
chlorohydroquinone	29	2.326	0.190	0.99
2,3-dichloroaniline	30	2.605	0.191	0.99
2-chloro-5-nitrobenzoic acid	31	1.974	0.405	0.93
2,4-dichlorobenzoic acid	32	2.067	0.487	0.97
2,5-dimethyl phenol	33	2.273	0.173	0.99
4-amino-2,6-dichloro phenol	34	2.353	0.243	0.97
2,4,6-trimethyl aniline	35	2.392	0.176	0.99
4,6-dinitro-o-cresol	36	1.906	0.184	0.99
2,3,5-trimethyl phenol	37	2.396	0.207	0.98
dl-tryptophane	38	2.304	0.109	0.98
amino-4-benzenesulfonamide	39	1.968	0.455	0.98
1-ethoxy-2-tertbutoxy ethane	40	1.040	0.175	0.96
ethylbenzene	41	2.580	0.336	0.98
phenol	42	1.808	0.287	0.99
aniline	43	1.785	0.315	0.99
4-tertbutyl benzoic acid	44	1.603	0.209	0.99
hydroquinone	45	1.684	0.177	0.99
phtalic acid	46	1.754	0.390	0.96
4-chlorobenzoic acid	47	1.260	0.275	0.99
3,5-dimethoxybenzoic acid	48	1.622	0.231	0.99
3-methylsalycilic acid	49	1.286	0.326	0.99
dl-tyrosine	50	1.897	0.272	0.99
dl-phenylalanine	51	1.876	0.205	0.96
phenyl salycilate	52	1.137	0.343	0.99
bromophenol	53	1.684	0.199	0.98
p-anisidine	54	1.435	0.559	0.96
methylethyldioxalane	55	1.316	0.544	0.98

Table 4 : Correlation coefficients between the Chi indices and the first four PCs

	PC1	PC2	PC3	PC4
${}^0\chi$	-0.932	0.259	-0.220	-0.008
${}^1\chi$	-0.892	0.406	-0.158	-0.056
${}^2\chi$	-0.964	0.104	-0.221	0.013
${}^3\chi$	-0.912	0.336	0.011	0.204
${}^4\chi$	-0.863	0.431	-0.050	0.092
${}^5\chi$	-0.820	0.485	-0.070	-0.032
${}^6\chi$	-0.896	0.318	-0.123	-0.053
${}^0\chi^v$	-0.937	-0.022	0.003	-0.228
${}^1\chi^v$	-0.943	-0.030	0.094	-0.262
${}^2\chi^v$	-0.886	-0.417	0.041	-0.170
${}^3\chi^v$	-0.911	-0.158	0.345	0.114
${}^4\chi^v$	-0.929	-0.044	0.299	0.049
${}^5\chi^v$	-0.872	-0.004	0.318	-0.126
${}^6\chi^v$	-0.927	-0.092	0.160	-0.095
${}^3\chi_c$	-0.743	-0.533	-0.351	0.037
${}^3\chi_c^v$	-0.496	-0.774	-0.258	-0.159
${}^4\chi_{pc}$	-0.875	-0.175	-0.083	0.430
${}^4\chi_{pc}^v$	-0.735	-0.599	0.105	0.256

Table 5 : Eigenvalues and associated proportions of the first four PCs

	PC1	PC2	PC3	PC4
Eigenvalue	13.612	2.361	0.698	0.524
Proportion	0.756	0.131	0.039	0.029
Cumulative	0.756	0.887	0.926	0.955

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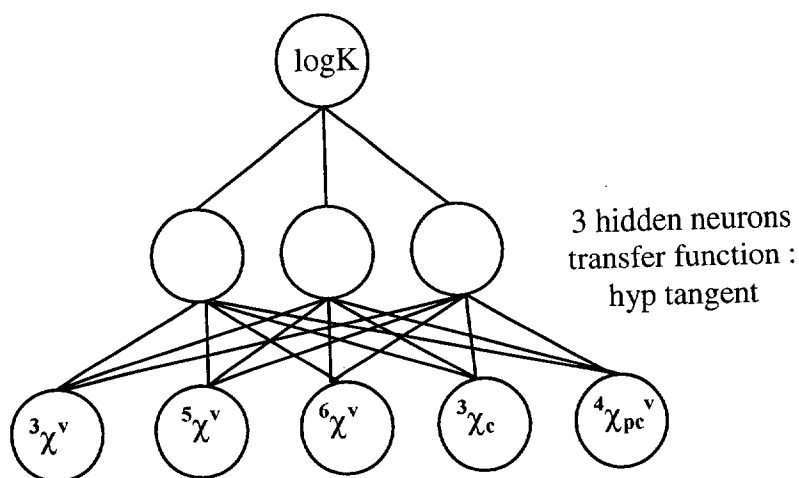


Figure 4 : Final architecture of the neural network