

Table 1. Name, CAS number, toxicity to *T. pyriformis*, physicochemical descriptors, and absolute residual from Equation (1) for the 384 aromatic compounds in the training set.

| Chemical name | Probable MOA ^a | CAS | log (IGC ₅₀ ⁻¹) | log <i>K</i> _{ow} | <i>A</i> _{max} | Absolute residual ^b |
|---------------------------------------|---------------------------|-------------|--|----------------------------|-------------------------|--------------------------------|
| 3-Aminobenzyl alcohol | 1 | 1877-77-6 | -1.13 | -0.55 | 0.2928 | 0.33 |
| 2-Aminobenzyl alcohol | 1 | 5344-90-1 | -1.07 | -0.17 | 0.2958 | 0.14 |
| Benzyl alcohol | 1 | 100-51-6 | -0.83 | 1.05 | 0.2852 | 0.12 |
| 4-Hydroxyphenethyl alcohol | 1 | 501-94-0 | -0.83 | 0.52 | 0.3026 | 0.10 |
| 4-Aminobenzyl cyanide | 2 | 3544-25-0 | -0.76 | 0.34 | 0.3022 | 0.07 |
| 2-Nitrobenzamide | 2 | 610-15-1 | -0.72 | -0.12 | 0.3321 | 0.13 |
| 4-Hydroxy-3-methoxybenzyl alcohol | 1 | 498-00-0 | -0.70 | 0.29 | 0.3002 | 0.19 |
| 2-Anisidine | 1 | 90-04-0 | -0.69 | 1.18 | 0.2951 | 0.21 |
| (<i>sec</i>)Phenethyl alcohol | 1 | 98-85-1 | -0.66 | 1.42 | 0.2852 | 0.14 |
| Resorcinol | 1 | 108-46-3 | -0.65 | 0.80 | 0.3074 | 0.16 |
| 1-Phenyl-2-propanol | 1 | 14898-87-4 | -0.62 | 1.97 | 0.2825 | 0.36 |
| Phenethyl alcohol | 1 | 60-12-8 | -0.59 | 1.36 | 0.2861 | 0.06 |
| 2-Phenyl-2-propanol | 1 | 617-94-7 | -0.57 | 1.81 | 0.2877 | 0.31 |
| 3-Amino-2-cresol | 1 | 53222-92-7 | -0.55 | 0.70 | 0.3013 | 0.10 |
| 2,4,6-Tris(dimethylaminomethyl)phenol | 1 | 90-72-2 | -0.52 | 0.92 | 0.3016 | 0.00 |
| 4-Methylbenzyl alcohol | 1 | 589-18-4 | -0.49 | 1.58 | 0.2836 | 0.04 |
| Phenylacetic acid hydrazide | 2 | 937-39-3 | -0.48 | 0.14 | 0.3194 | 0.18 |
| 3-Cyanoaniline | 1 | 2237-30-1 | -0.47 | 1.07 | 0.3056 | 0.09 |
| Acetophenone | 1 | 98-86-2 | -0.46 | 1.63 | 0.3178 | 0.59 |
| 2-Methylbenzyl alcohol | 1 | 89-95-2 | -0.43 | 1.55 | 0.2851 | 0.01 |
| (±)1-Phenyl-1-propanol | 1 | 93-54-9 | -0.43 | 1.94 | 0.2857 | 0.21 |
| 2,3-Dimethylaniline | 1 | 87-59-2 | -0.43 | 1.81 | 0.2935 | 0.26 |
| 2,6-Dimethylaniline | 1 | 87-62-7 | -0.43 | 1.84 | 0.2944 | 0.29 |
| <i>n</i> -Methylphenethylamine | 1 | 589-08-2 | -0.41 | 1.43 | 0.2854 | 0.09 |
| 2-Methyl-1-phenyl-2-propanol | 1 | 100-86-7 | -0.41 | 1.86 | 0.2852 | 0.13 |
| 2-Phenyl-1-propanol | 1 | 1123-85-9 | -0.40 | 1.58 | 0.2862 | 0.01 |
| 3-Fluorobenzyl alcohol | 1 | 456-47-3 | -0.39 | 1.25 | 0.3051 | 0.11 |
| 4-Hydroxybenzyl cyanide | 1 | 14191-95-8 | -0.38 | 0.90 | 0.3089 | 0.03 |
| 4-Cyanobenzamide | 1 | 3034-34-2 | -0.38 | 0.48 | 0.3218 | 0.06 |
| 2-Fluoroaniline | 1 | 348-54-9 | -0.37 | 1.26 | 0.3021 | 0.05 |
| Benzyl cyanide | 1 | 140-29-4 | -0.36 | 1.56 | 0.2936 | 0.06 |
| 3,5-Dimethylaniline | 1 | 108-69-0 | -0.36 | 1.91 | 0.2928 | 0.24 |
| Phenol | 1 | 108-95-2 | -0.35 | 1.50 | 0.3013 | 0.14 |
| 2,5-Dimethylaniline | 1 | 95-78-3 | -0.33 | 1.83 | 0.2936 | 0.18 |
| 3-Methoxyphenol | 1 | 150-19-6 | -0.33 | 1.58 | 0.3051 | 0.22 |
| 2-Cresol | 1 | 95-48-7 | -0.29 | 1.98 | 0.3007 | 0.34 |
| 2,4-Dimethylaniline | 1 | 95-68-1 | -0.29 | 1.68 | 0.2933 | 0.05 |
| β-Methylphenethylamine | 1 | 582-22-9 | -0.28 | 1.68 | 0.2854 | 0.09 |
| 3-Methylaniline | 1 | 108-44-1 | -0.28 | 1.40 | 0.2936 | 0.11 |
| 4-Methylphenethyl alcohol | 1 | 699-02-5 | -0.26 | 1.68 | 0.2850 | 0.11 |
| Benzylamine | 1 | 100-46-9 | -0.24 | 1.09 | 0.2843 | 0.46 |
| 3-Methylbenzyl alcohol | 1 | 587-03-1 | -0.24 | 1.60 | 0.2845 | 0.19 |
| 2-Tolunitrile | 1 | 529-19-1 | -0.24 | 2.21 | 0.3021 | 0.43 |
| Aniline | 1 | 62-53-3 | -0.23 | 0.90 | 0.2945 | 0.42 |
| 3-Nitrobenzyl alcohol | 1 | 619-25-0 | -0.22 | 1.21 | 0.3151 | 0.08 |
| 2-Ethylaniline | 1 | 578-54-1 | -0.22 | 1.74 | 0.2946 | 0.03 |
| 3-Phenyl-1-propanol | 1 | 122-97-4 | -0.21 | 1.88 | 0.2851 | 0.06 |
| Benzaldehyde | 1 | 100-52-7 | -0.20 | 1.48 | 0.3170 | 0.23 |
| (±)-α-Methylbenzylamine | 1 | 618-36-0 | -0.18 | 1.40 | 0.2850 | 0.35 |
| 2-Phenyl-3-butyn-2-ol | 2 | 127-66-2 | -0.18 | 1.88 | 0.3001 | 0.16 |
| 2-Chloroaniline | 1 | 95-51-2 | -0.17 | 1.88 | 0.3043 | 0.22 |
| Hydrocinnamitrile | 2 | 645-59-0 | -0.16 | 1.72 | 0.2935 | 0.05 |
| (±)-α-Ethylphenethyl alcohol | 1 | 120055-09-6 | -0.16 | 2.02 | 0.2836 | 0.05 |
| 4-Cresol | 1 | 106-44-5 | -0.16 | 1.97 | 0.3001 | 0.19 |
| 2-Methylaniline | 1 | 95-53-4 | -0.16 | 1.43 | 0.2944 | 0.20 |
| 3,4-Dimethylaniline | 1 | 95-64-7 | -0.16 | 1.86 | 0.2926 | 0.00 |
| 3-Acetamidophenol | 1 | 621-42-1 | -0.16 | 0.73 | 0.3215 | 0.15 |
| 4-Methoxyphenol | 1 | 150-76-5 | -0.14 | 1.34 | 0.2980 | 0.21 |
| Isovanillin | 1 | 621-59-0 | -0.14 | 0.97 | 0.3169 | 0.10 |