Table S10: compilation of QSPRs for other tertiary treatment methods

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| --- | --- | --- | --- | --- | --- |
| **Symbol** | **Endpoint** | **Equation** | **R2** | **Compound class(es)** | **References** |
| % | rejection | compound descriptors; membrane characteristics; opetating conditions. ANN, eleven neurons for NN1 | 0.833204 | 956 (split up 80%, 10%, 10%) organic compounds (neutral and ionic) | Ammi (2015) |
| % | rejection | compound descriptors; membrane characteristics; opetating conditions. ANN, eleven neurons for NN1 | 0.887176 | 701 (split up 80%, 10%, 10%) organic compounds (neutral and ionic) | Ammi (2015) |
| % | rejection | compound descriptors; membrane characteristics; opetating conditions. ANN, eleven neurons for NN1 | 0.907637 | 701 (split up 80%, 10%, 10%) organic compounds (neutral and ionic) | Ammi (2015) |
| % | retention | R = a0 + ad several molecular descriptors | ~0.99 | 6; 6 saturated and aromatic hydrocarbons; substituted aromatic hydrocarbons with heteroatoms | Koter (2009) |
| % | retention | R = a0 + ad1d1+ ad2d2 several molecular descriptors | ~0.999 | 6; 6 saturated and aromatic hydrocarbons; substituted aromatic hydrocarbons with heteroatoms | Koter (2009) |
| % | rejection | R = 0.81 x depth - 6.38 - 10^8 x Ds + 0.0796 x Ln(Jv) + 0.553 ; rejection = R (if o<R<1), 1 (if R>1), 0 (if <0) | ? | - | Shahmansouri (2013) |
| % | percent removal by riverbank filtration (RBF) | % Removal=174.8 (#imidazoles)+158.4 (AR)−98.1 (#CONN)−1830.3 (ME)+1851.1 several molecular descriptors. Multi-criteria analysis (MCA) | 0.84 | 25(?) | Sudhakaran (2013) |
| % | percent removal by nanofiltration (NF) | % Rejection=265.15eqwidth−117.36 (depth)+81.66 (length)−5.23 (logD)+1348.09 (SR)−1447.82 several molecular descriptors. Multi-criteria analysis (MCA) | 0.75 | 25(?) | Sudhakaran (2013) |
| % | rejection | Principal component analysis (PCA) and multivariate regressions. Membrane characteristics related to hydrophobicity (contact angle), salt rejection, and surface charge (zeta potential [ZP]); compound properties describing hydrophobicity (log Kow, log D), polarity (dipole moment), and size (molar volume,molecular length, molecular depth, equivalent width, molecular weight); and operating conditions (flux, pressure, cross flow velocity) were identified and evaluated as candidate variables for rejection prediction. | 0.93 | - | Yangali-Quintanilla (2010) |
| % | rejection | rejection = 265.150 eqwidth - 117.356 depth + 81.662 length - 5.229 logD + 1358.090 SR - 1447.817 several compound, membrane, and operating conditions. Principal component analysis, partial least square regression and multiple linear regressions | 0.75 | 14 pharmaceuticals, endocrine disruptors, pesticides and other organic compounds | Yangali-Quintanilla (2010) |
| % | rejection | rejection = 265.150 eqwidth - 117.356 depth + 81.662 length - 5.229 logD - 0.272 MWCO - 62.565 several compound, membrane, and operating conditions. Principal component analysis, partial least square regression and multiple linear regressions | 0.75 | 14 pharmaceuticals, endocrine disruptors, pesticides and other organic compounds | Yangali-Quintanilla (2010) |
| % | rejection | solute properties, membrane characteristics and operating conditions. ANN | 0.9 | 50, 161 rejections of 50 organic neutral compounds (including pharmaceuticals, endocrine disrupting compounds, pesticides, alcohols, phenols and solvents) by six NF | Yangali-Quintanilla (2010) |
| % | rejection | rejection = 183.920 eqwidth + 31.830 length − 0.549 log Kow +883.294 SR − 945.133 F32 solute properties, membrane characteristics and operating conditions. Principal component analysis and multiple linear regressions | ? | 50, 161 rejections of 50 organic neutral compounds (including pharmaceuticals, endocrine disrupting compounds, pesticides, alcohols, phenols and solvents) by six NF | Yangali-Quintanilla (2010) |
| %GAC | percent removal by adsorption by granular activated carbon (GAC) | Relative adsorbability=0.2730 (8Xp)+0.00106 (FOSA) several molecular descriptors. Multi-criteria analysis (MCA) | 0.86 | 25(?) | Sudhakaran (2013) |
| %RO | percent removal by reverse osmosis (RO) | % Rejection=252.714eqwidth+35.104length+485.839SR−590.714 several molecular descriptors. Multi-criteria analysis (MCA) | 0.882 | 25(?) | Sudhakaran (2013) |
| refl | reflection coefficient | /- ; R = r(1 - F) / (1 - rF) ANN | 0.89 | 200 rejection conditions for training. 55 rejection conditions for validation | Shahmansouri (2013) |
| refl | reflection coefficient | r = -9.786x10^8 x Ds - 8.35x10^4 x SASA + 1.824 ; R = r(1 - F) / (1 - rF) MLR | 0.51 | 200 rejection conditions for training. 55 rejection conditions for validation | Shahmansouri (2013) |
| perm | permeability coefficient | Log(P) = - 8.98 x 10^3 x VLaBas - 4.156 | 0.95 | 200 rejection conditions for training. 55 rejection conditions for validation | Shahmansouri (2013) |