Table S5: compilation of QSPRs for reaction with \*OH

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Endpoint** | **Equation and/or model specifications** | **r2** | **Specifications of training/test set** | **Reference** |
| log(KOH)  reaction rate constant | ANN | 0.9 | 146/31 polar (84%) and non-polar (16%) compounds | Dutot (2003) |
| log(KOH)  reaction rate constant | log kOH = 16.451 - 6.932 Me + 0.159 nDB - 0.679 CH2RX + 0.401 nHAcc - 0.460 Vindex - 0.363 MATS2m - 0.362 Mor27p;  log kOH = 17.215 - 7.564 Me + 0.160 nDB - 0.625 CH2RX + 0.310 nHAcc - 0.563 Vindex - 0.362 MATS2m - 0.427 Mor27p, forward multiple linear regressions | - | N = 88/28. Various chemical classes (phenols, polycyclic aromatic hydrocarbons, alkanes, halogenated aromatic compounds, organophosphorus compounds, etc.) | Jin (2015) |
| log(KOH)  second order degradation rate constant | log kOH\* = -0.628(+-0.408)MW - 2.150(+-0.633)piPC09 + 2.249(0.596)Mor02e - 0.694(0.213)Mor26p + 3.444(0.999)EHOMOa + 11.905(+-0.978), genetic algorithm and multiple regression analysis using several DRAGON descriptors, and parameters from quantum-chemical calculations at semiempirical and at density functional theory level (B3LYP/6-31G(d,p)) | 0.803 | 60 benzene structures with different substitute groups and other heterocycles, containing nitrogen or sulphur | Kusic (2009), Mamy (2014) |
| log(KOH)  degradation rate constant | k\*1000=15.315+291.290Ehomo+ 0.310Cvθ+113.117qH+, stepwise multiple linear regression using fourteen physicochemical and quantum chemical parameters calculated with Gaussian 09 | 0.878 | 17 antimicrobial agents  Fenton-like system Cu2+/H2O2 | Peng (2016) |
| log(KOH)  second order rate constant | kOH = 2.153 + 0.895(DBE) - 0.134(WPSA), several molecular descriptors computed, correlation analysis, principal component analysis and multiple linear regression. | 0.918 | 55/28/28 pharmaceuticals, personal care products or organic solvents | Sudhakaran and Amy (2013), Mamy (2014) |
| log(KOH)  aqueous phase OH-oxidation rate constant | Improved group contribution method (GCM) | 0.89 | 72 alkanes, alcohols, organic acids and bases | Monod (2008), Wang (2009) |
| log(KOH)  aqueous reaction rate for contaminant removal by UV/H2O2 processes | log(KOH) = 0,99 – 0,56qCmean - 0,34BELv1 - 0,42ATS2m + 0,66piPC03, several descriptors computed and MLR | 0.774 | N = 122/25. Various organic micropollutants including solvents, pharmaceuticals and pesticides | Wols and Vries (2012) |
| log(KOH)  hydroxyl radical reaction rate constant | log kOH = - 8.613 - 0.02100 X% + 14.38EHOMO - 0.6430 Mor29u + 0.5870 NdsCH + 0.5870 GATS1e + 0.5770 X3A - 0.2450 SdsCH - 167.0ð1=TÞ + 1.103 BIC1 + 0.1170 RDF015m - 1.044 SpMin8BhðpÞ + 0.2390 nR = Cp - 0.1980 NssssC - 0.5080 F02[F-Br], quantum chemical descriptors and DRAGON descriptors, stepwise MLR analysis | - | N = 1234/309 Various organic chemicals At different temperatures (from 206 K to 1364 K) | Li (2014) |
| log(KOH)  hydroxyl radical reaction rate constant | log kOH = -6.511 + 15.85 EHOMO - 0.03800 AMW + 0.1300 NdsCH + 0.1630 Mor14i + 0.3170 nR = Cp + 0.7790 nP + 0.3930 nRCHO - 0.01900 X% - 0.4550 SpMaxAAEA(dm) + 0.5890(C-020) - 0.05600 nCbH + 0.1410 CATS2D03DL, quantum chemical descriptors and DRAGON descriptors, stepwise MLR analysis | - | 696/176 Various organic chemicals T = 298K | Li (2014) |
| log(KOH)  hydroxyl radical reaction rate constant | log kOH = -6.412 - 0.01900 X% + 13.72EHOMO - 0.07200 nCbH - 0.4510 SpMaxAAEA(dm) - 231.4(1/T) + 0.1710 NdsCH + 0.2100 Mor14i + 0.2390 nR = Cp + 0.5870 nP - 0.02500 AMW + 0.5360 (C - 020) + 0.2580 nRCHO + 0.08700 CATS2D 03 DL, quantum chemical descriptors and DRAGON descriptors, stepwise MLR analysis | - | 1234/309 Various organic chemicals At different temperatures (from 206 K to 1364 K) | Li (2014) |
| log(KOH)  reaction rate constant | Group contribution method (GCM) | 0.3364 | 310/124 Various organic compounds with a variety of functional groups. Includes 66 group rate constants and 80 group contribution factors | Minekata (2009) |
| log(KOH)  degradation rate constant in water | y=0.499x+13.503, HOMO-SOMO (ev) descriptor as x Dewar et al., 1985 with the HyperChem software, linear regression | 0.512 | 477 Various organic compounds with a variety of functional groups | Minekata (2009) |
| log(KOH) (log(kox)) [1/M·sec]  the second-order hydroxyl radical rate constant | logkox(water) = 0.805 log kox(air) + 1.682, linear regression | - | ? Extrapolation from air to water | Güsten et al. (1981), Lim (2011) |
| log(KOH) (log(kox)) [1/M·sec]  the second-order hydroxyl radical rate constant | logkox(water) = 0.88 log kox(air) + 0.98, linear regression | - | ? Extrapolation from air to water | Yao (1992), Lim (2011) |
| log(KOH) (log(kox)) [1/M·sec]  the second-order hydroxyl radical rate constant | logkox(water) = 1.22 log kox(air) - 1.45, linear regression | - | ? Extrapolation from air to water | Klöpffer et al. (1985), Lim (2011) |
| log(KOH) (log(kox)) [1/day]  the first-order oxidation reaction rate constant | logkox(water) = log kox(air) - 3.29, linear regression | - | ? Extrapolation from air to water | Lim (2011) |
| log(KOH) (log(kgas)) (M-1/s-1) | log kgas = (2.54+-2.19) + (1.31 +- 0.24) log(kaq) , linear regression | 0.81 | Various organic compounds including alcohols, ketones, aldehydes and acids 31  H-abstraction reactions of OH with a series of organic compounds versus corresponding aqueous phase rate constants | Gligorovski, 2015 |
| log(KOH (log(k)) M-1S-1 Reaction rate constant in water | log k (water) = 1.68 + 0.81 log k (air) , linear regression | 0.76 | 45Alkanes | Haag and Yao (1992), Canonica and Tratnyek(2003) |
| log(KOH (logk k) | log k = 8.58(+-0.05) - 0.21(+-0.06)s+, linear regression | 0.88 | 12Benzene derivatives, (X–C6H5), where only one Substituent, X, was varied at a fixed position | Hansch and Gao (1997), Canonica and Tratnyek(2003) |
| log(KOHrel | log krel = -0.40(+-0.03) - 0.24(+-0.07)s, linear regression | 0.9 | 9Benzene derivatives, (X–C6H5), where only one substituent, X, was varied at a fixed position | Hansch and Gao (1997), Canonica and Tratnyek(2003) |
| log(KOH (log(k)) | log k = 8.70(+-0.02) - 0.27(+-0.04)s+, linear regression | 0.98 | 9 X–C6H4–COO2 compounds | Hansch and Gao (1997), Canonica and Tratnyek(2003) |
| log(KOH)  second order degradation rate constant | logkOH\* = -0.908(+-0.433)piPC08 + 0.512(+-0.291)GATS2p + 0.515(0.176)HATS7p + 4.404(0.992)EHOMO + 13.255(+-0.930), genetic algorithm and multiple regression analysis using several DRAGON descriptors, and parameters from quantum-chemical calculations at semiempirical and at density functional theory level (B3LYP/6-31G(d,p)) | 0.735 | 60 Benzene structures with different substitute groups and other heterocycles, containing nitrogen or sulphur | Kusic (2009), Mamy (2014) |
| log(KOH)  reaction rate constant | log kOH = (−0.28+-0.07)sT + (9.50+-0.06), linear regression | 0.6241 | 10 Phenolic acids | Peres (2010) |
| log(KOH)  Aqueous-Phase Reaction Rate Constants | log kOH = 1.507\*10 + 5.036\*10^-1 EHOMO - 4.881QH + 4.623\*10^-3 MSA - 5.118\*10^-2mu, several quantum chemical descriptors and multiple linear regressions (MLR) | 0.905 | 44/11 Phenols, alkanes and alcohols | Wang (2009) |
| log(KOH)  Aqueous-Phase Reaction Rate Constants | log kOH = 1.097\*10 - 4.883QH - 6.612\*10^-2mu, several quantum chemical descriptors and multiple linear regressions (MLR) | 0.686 | 17 Phenols | Wang (2009) |
| log(KOH)  Aqueous-Phase Reaction Rate Constants | log kOH = 1.903\*10 + 7.577\*10^-1 EHOMO - 2.222\*10 QH + 3.503\*10^-3 MSA, several quantum chemical descriptors and multiple linear regressions (MLR) | 0.974 | 16 Alkanes | Wang (2009) |
| log(KOH)  Aqueous-Phase Reaction Rate Constants | log kOH = 2.062\*10 + 9.985\*10^-1 EHOMO - 5.547QH + 3.821\*10^-3 MSA, several quantum chemical descriptors and multiple linear regressions (MLR) | 0.871 | 22 Alcohols | Wang (2009) |
| log(KOH)  aqueous phase OH-oxidation rate constant normalised for the number of equivalnet hydrogen atoms | ln k(OHaq/nH) = (27+-4) - (0.05+-0.01)BDE(C-H), Evans – Polanyi-type correlations | 0.81 | 22 Alkanes, alcohols, organic acids and bases | Monod (2005), Wang (2009) |
| log(KOH)  aqueous phase OH-oxidation rate constant | Log(kOHaq298K) = 0.71(+-0.03) Log(kOHgas298 K), gas and aqueous-phase correlations | 0.74 | 143 Alkanes, alcohols, organic acids and bases | Monod (2005), Wang (2009) |
| log(KOH)  aqueous phase OH-oxidation rate constant | LogkOHaq298 = 0.57(+-0.02) Log(kOHgas298 K) | 0.9604 | 23 Alkanes | Monod (2005) |
| log(KOH)  kobs, first-order degradation rate constant by UV/H2O2 | A quadratic polynomial function: Y = AX1 + BX1^2 + CX2 + DX2^2 + EX1X2 + F. The coefficients pertaining to each term were used as responses in QSPR modeling to establish their dependence on the structural features of studied aromatics. Variable selection Genetic Algorithm (GA) and Multiple Linear Regression Analysis (MLRA) methods | 0.9556 to 0.9988 | 30 Single-benzene-ring compounds | Smidt (2015) |
| log(KOH)  hydroxyl radical reaction rate constant | y = −0.4 ± 1.3) × 10^8 + 1.01 ± 0.06 · x, gem-diols descriptors, linear regression | 0.79 | 72 Carbonyl compounds | Doussin and Monod (2013), Doussin and Monod (2013) |
| log(KOH)  hydroxyl radical reaction rate constant | y = (−0.8 ± 1.4) × 10^8 + 0.80 ± 0.06 · x, gem-diols descriptors, linear regression | 0.73 | 53 Carbonyl compounds | Minakata et al. (2009), Doussin and Monod (2013) |
| log(KOH)  hydroxyl radical reaction rate constant | y = (2.0 ± 3.9) × 10^9 + 7.5 ± 1.7 · x, gem-diols descriptors, linear regression | 0.26 | 56 Carbonyl compounds | Monod et al. (2005), Doussin and Monod (2013) |
| log(KOH)  hydroxyl radical reaction rate constant | y = (4.3 ± 1.9) × 10^7 + 0.15 ± 0.01 · x, gem-diols descriptors, linear regression | 0.83 | 25 Carbonyl compounds | Ervens et al. (2003), Doussin and Monod (2013) |
| KHabs  H-atom abstraction | Relationship with the Taft constant, σ\* y=-0.32x+1.04, linear regression | 0.8281 | 12 Alkyl, oxygenated, and halogenated functional groups | Minekata (2009) |
| KHabs  H-atom abstraction | Relationship with the Taft constant, σ\* y=-0.68x+2.43, linear regression | 0.9801 | 4 compounds with S-, N-, or P-atom-containing functional groups | Minekata (2009) |
| KOHadd  HO• addition to aromatic compounds | Relationship with electrophilic substituent parameter, σ+ y=-0.51x+0.82, linear regression | 0.7921 | 13 Benzene compounds | Minekata (2009) |
| KOHadd  HO• addition to aromatic compounds | Relationship with electrophilic substituent parameter, σ+ y=-1.21x+0.73, linear regression | 0.8649 | 6 Pyridine compounds | Minekata (2009) |
| KOHadd  HO• addition to aromatic compounds | Relationship with electrophilic substituent parameter, σ+ y=-0.34x+0.81, linear regression | 0.4225 | 7 Furan compounds | Minekata (2009) |
| KHabs  H-abstraction from C-H | y = -0.295x + 23.086, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.755 | 53 Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| KOHadd  HO addition to C=C of alkenes | y = -0.425x + 21.213, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.699 | 12 Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| KO2add  O2 addition to aliphatic C-centered radicals | y = -0.088x + 19.931, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.827 | Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| KO2add  O2 addition to aromatic C-centered radicals | y = -0.407x + 13.621, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.871 | Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| Kbidecay  Bidecay of peroxyl radical | y = -0.720x + 19.465, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.768 | Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| Ktetr  Tetroxide formation | y = -0.350x + 11.778, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.881 | Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| KO2add  HO addition to aromatic | y = -0.847x + 20.914, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.882 | 15 Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| Kuni  Unidecay of peroxyl radical | y = -0.1871x + 19.84, Linear regression, LFER: calculations on the aqueous phase reaction rate constant using Transition State Theory (TST) lnkexp = -ρΔGact aq, calc + σ | 0.7079 | 9 Various organic compounds | Minakata and Crittenden (2011); Minakata, Song, and Crittenden (2011); Minakata (2014) |
| ln(KOHag/nH)  aqueous reaction rate normalised for the number of equivalnet hydrogen atoms | ln kOHaq/nH = (28+-4) - (0.05+-0.01)BDE(C-H) | 0.8649 | 16 what compounds? | Herman (2003), Monod (2005) |
| ln kOHag/nH  aqueous reaction rate normalised for the number of equivalnet hydrogen atoms | ln kOHaq nH = (28+-4) - (0.05+-0.01)BDE(C-H) | 0.9801 | 10 what compounds? | Gligorovski and Herman (2004) |
| log(KOH) (log(Ks))  hydroxyl-radical quenching reactivity of phenolic compounds (log Ks) | logKs = -0.300(+-0.019)DHf + 16.568(+-0.470), Several descriptors and MLR | 0.8416 | 13 Phenolic compounds | Cheng (2002) |
| log(KOH) (log(Ks))  hydroxyl-radical quenching reactivity of phenolic compounds (log Ks) | Log Ks = -0.227(+-0.028)DHf + 0.171(+-0.047) Ea + 0.169(+-0.043)EHOMO - 9.807(+-3.600)Dsr +20.4949(+-1.091), Several descriptors and MLR | 0.989 | 13 Phenolic compounds | Cheng (2002) |
| Abs, z  the absorption competitiveness between parent pollutant and H2O2 for irradiation energy (z) | log(z) = 3.680(+-1.107)BIC1 - 0.961(+-0.812)Mor21e + 0.543(+-0358)Mor29p + 9.652(+-2.587)EHOMO + 4.036(+-1.661), Variable selection Genetic Algorithm (GA) and Multiple Linear Regression Analysis (MLRA) methods. The combination of GA-MLRA was used to build models using the BuildQSAR 2.1.0.0 program | 0.837 | 29/10/1 Single-benzene ring compounds | Juretic (2014) |
| Rate, u  the rate of BP1 degradation (u) | u = 1.537(+-0.452)SPI - 0.590(+-0.517)MAXDP + (0.637(+-0.439)G2e - 2.044(+-0.348)dðHfÞ + (0.250+-0.402), Variable selection Genetic Algorit hm (GA) and Multiple Linear Regression Analysis (MLRA) methods. The combination of GA-MLRA was used to build models using the BuildQSAR 2.1.0.0 program | 0.912 | 29/10/1 Single-benzene ring compounds | Juretic (2014) |
| Ratio, w  the ratio of ‘‘fast’’ and ‘‘slow’’ mineralizing by-products (w) | w = 0.466(+-0.109)Mor18v + 0.039(+-0.015)Mor14p - 0.148(0.053)R1u + 0.170(+-0.043)R4u + 1.034(+-0.101), variable selection Genetic Algorit hm (GA) and Multiple Linear Regression Analysis (MLRA) methods. The combination of GA-MLRA was used to build models using the BuildQSAR 2.1.0.0 program | 0.889 | 29/10/1 Single-benzene ring compounds | Juretic (2014) |
| profile  concentration time profiles | log(z), u, and w were used to parametrize a mechanistic model (MM) based on simplified degradation scheme for UV/H2O2 process, variable selection Genetic Algorit hm (GA) and Multiple Linear Regression Analysis (MLRA) methods. The combination of GA-MLRA was used to build models using the BuildQSAR 2.1.0.0 program | - | 29/10/1 Single-benzene ring compounds | Juretic (2014) |
| %COD  antibiotic removal in aqueous solution by the Fenton process | ANN | 0.997 | 60/30/30 Antibiotics | Elmolla (2010) |