Table S11: compilation of QSPRs for bioconcentration

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| --- | --- | --- | --- | --- |
| **Endpoint** | **Equation** | **R2** | **Compound class(es)** | **References** |
| BCF | ? | 0.731 | N= 608/152/76. large variety, includes 138 ionizable chemicals  in fish | Gissi et al. 2013 |
| BCF | VEGA CAESAR | 0.69 | N = 163. Diverse, in fish | Gissi et al. 2013 |
| BCF | VEGA MEYLAN | 0.68 | N = 299. Diverse, in fish | Gissi et al. 2013 |
| BCF | CORAL | 0.60 | N = 335. Diverse, in fish | Gissi et al. 2013 |
| BCF | T.E.S.T. CONSENSUS | 0.50 | N = 291. Diverse, in fish | Gissi et al. 2013 |
| BCF | CORAL | - | N = 851. Diverse, in fish | Gissi et al. (2015) |
| BCF | T.E.S.T.CONSENSUS | - | N = 824. Diverse, in fish | Gissi et al. (2015) |
| BCF | EPISUITEARNOT–GOBAS | - | N = 850. Diverse, in fish | Gissi et al. (2015) |
| BCF | EPISUITEMEYLAN | - | N = 850. Diverse, in fish | Gissi et al. (2015) |
| BCF | VEGAMEYLAN | - | N = 851. Diverse, in fish | Gissi et al. (2015) |
| BCF | VEGACAESAR | - | N = 851. Diverse, in fish | Gissi et al. (2015) |
| BCF | ADMET | - | N = 851. Diverse, in fish | Gissi et al. (2015) |
| BCF | LOGP-BASEDEQUATIONS | - | N = 759. Diverse, in fish | Gissi et al. (2015) |
| BCF | ACD | - | 850, diverse, in fish | Gissi et al. (2015) |
| BCF | CAESAR | - | 483, diverse, in fish | Gissi et al. (2013) |
| BCF | Meylan | - | 676, diverse, in fish | Gissi et al. (2013) |
| BCF | Integrated model relying on the predictions of two among the most used BCF models (CAESAR and Meylan), together with the Applicability Domain Index (ADI) provided by the software VEGA | - | 585, diverse, in fish | Gissi et al. (2013) |
| BCF | Log BCF= 0.542\* Log Kow + 0.124, Linear regression | 0.95 | 7 neutral chemicals: Persistent organic pollutants or polychlorinated biphenyls and polyphenol ether, in rainbow trout | Neely *et al.,* 1974 |
| BCF | Log BCF= 0.85 \* log Kow -0.70, Linear regression | 0.90 | 70 neutral, hydrophobic chemicals, in fathead minnow | Veith *et al.,* 1979 |
| BCF | Log BCF= Log Kow -1.32, Linear regression | 0.95 | 23 neutral, hydrophobic chemicals, in fathead minnow | Mackay (1982) |
| BCF | Log BCF= 0.79\*Log Kow – 0.40, Linear regression | 0.31; 0.19 | 610 non-ionic compounds; 84 ionic compounds, in fish | USA EPA Office of Pollution and Prevention and Toxics (OPPT) model. Veith and Kosian, (1983) |
| BCF | Log BCF= -1.37 \* Log Kow + 14.4 + Σ Fi, Linear regression | 0.62; 0.73 | 84; 610 neutral and ionizable chemicals, in fish | Meylan *et al.,* 1999 model |
| BCF | LogBCF= 3.41-0.508 \* LogS, Linear regression | 0.930 | Pesticides, in mosquito fish | Chiou *et al.,* 1977 |
| BCF | Dimitrov baseline model . log Kow-based relationship | - | 443 highly, moderately and weakly hydrophilic chemicals, in fish | Dimitrov et al. (2002, 2005b). Nendza et al. (2013) |
| BCF | BCFBAF v3.01. log Kow-based relationship | - | 466 non-ionic and 61 ionic non-ionic and ionic compounds (carboxylic acids, sulfonic acids, quats) , in fish | Arnot and Gobas (2003), US EPA (2011a), Nendza et al. (2013) |
| BCF | Nonlinear log Kow-based relationship | - | 154organic compounds, five different families of freshwater fish | Bintein et al. (1993), Nendza et al. (2013) |
| BCF | ChemProp readacross for BCF. ACF-based interpolation from similar reference compounds | - | 1000 organic compounds, in fathead minnow | ChemProp (2012), Nendza et al. (2013) |
| BCF | CAESAR BCF model. Hybrid model based on 2 radial basis function neural network (RBFNN) using either an heuristic method or a genetic algorithm to descriptors, functional groups, topological select the optimal descriptors (constitutional indices) | 0.83 | 378/95 organic compounds, in fish | Zhao et al. (2008), CAESAR (2011), Vega -2011, Nendza et al. (2013) |
| BCF | CORAL atom indices for BCF. Model based on indices of presence of atoms (e.g. N, O, S, P, halogens) calculated using SMILES codes | - | 1035 (split 50%, 30%, 20%) in fish | CORAL (2011), Toropov et al. (2011), Nendza et al. (2013) |
| BCF | T.E.S.T. v4.0 for BCF. Ensemble of QSARs: hierarchical method, FDA method, single model method, group contribution method, nearest neighbour method and a consensus method that combines the above methods | - | 598 in fish | US EPA (2010), Nendza et al. (2013) |
| BCF | Bayesian consensus for BCF . Aggregated predictions from different in silico BCF models (CAESAR (2011), T.E.S.T. (US EPA,2010), BCFBAF (US EPA, 2011a), ChemProp (2012)) using a continuous Bayes formulation to obtain consensus on bioaccumulation categories (non-B, B, vB) | - | 522 organic compounds, in fish | Fernández et al. -2012, Nendza et al. (2013) |
| BCF | logBCF = 6.598\*Average Bonding Information content (order 1) - 291.721\*Partial Charged (Zefirov) Surface Area of H atoms - 9.189\*Polarity parameter (Zefirov) / distance +12.497.  1D, 2D, and 3D theoretical calculations quantum chemical descriptors derived from MMFFs (vacuum) conformational search and AM1 calculation. Model developed by using multilinear regression. | 0.945 | 58 (split 80%/20%) polychlorinated biphenyls, in rainbow trout | QMRF Database: Q8-10-24-173 |
| BCF | logBCF = 5.78E-002 – 1.16 \* HA dependent HDCA-2 (Zefirov)+ 8.40E-002 \* Lowest exchange energy (AM1) for C - O bonds + 0.40 \* Lowest coulombic interaction (AM1) for C - H bonds + 0.49 \* logP\_calc.  1D, 2D, and 3D theoretical calculations quantum chemical descriptors derived from MMFFs (vacuum) conformational search and AM1 calculation. Model developed by using multilinear regression | 0.83 | 78 (split 2:3) pesticides, in fish | QMRF Database: Q8-10-14-175 |
| BCF | Log(BCF)= -114.12 +29.39 \* Max valency (AM1) -0.94 \* Square root of Charged (Zefirov) Surface Area of C atoms -10.13 \* Square root of Partial Surface Area of H atoms +0.57 \* logP.  1D, 2D, and 3D theoretical calculations quantum chemical descriptors derived from MMFFs (vacuum) conformational search and AM1 calculation. Model developed by using multilinear regression | 0.77 | 156 (split 2:1) non-ionic organic compounds, in fathead minnow | QMRF Database: Q8-10-14-207 |
| BCF | LogBCF= -1.01 (∓0.35) + 2.53 (∓0.13) vIMD,Deg- 1.02 (∓0.12)HIC - 0.46 (∓0.04)nHAcc - 1.13 (∓0.18)GATS1e - 1.70 (∓0.34)MATS1p.  Multiple linear regression (OLS) was applied to generate the QSAR model. Descriptors were generated by DRAGON software. The input files for descriptor calculation contain information on atom and bond types, connectivity, partial charges and atomic spatial coordinates, relative to the minimum energy conformation of the molecule, and were obtained by the Molecular Mechanics method of Allinger (MM+) using the package HYPERCHEM. | 0.807 | 238/179/59 non-ionic organic compounds. rainbow trout, guppies, fathead minnows, bluegill sunfish, golden ide, etc | QMRF Database: Q2-17-16-140 |
| BCF | LogBCF 6.9 10 (logK ) 1.85 10 (logK ) 1.55(logKow)^2 -4.18 logKow + 4.79 |  | 45 mainly chlorinated hydrocarbons. Poecilia reticulata, Carassius auratus, Oncorhynchus mykiss, Pimephales promelas) | Connell and Hawker 1988 |
| BCF | LogBCF a1 + a 2exp(-(log(Kow-logKow0)^2/a3), where a1 = 0.420± 0.214, a2 = 3.321 ± 0.225, a3 = 10.151 ± 2.150 and O LogKOW = 6.348 ± 0.1763 are model parameters.  Non-linear regression | 0.73 | 443 narcotic chemicals, in fish | Pavan, 2006 |
| BCF | Log BCF = 0.85\* logKow - 0.70 | 0.90 | 55, diverse, in fish | Lassiter, R.R. (1975), Pavan, 2006 |
| BCF | Log BCF = 0.79\* logKow - 0.40 | 0.865 | 122, diverse, in fish | Veith, G.D., Kosian, P. (1983)., Pavan, 2006 |
| BCF | Log BCF = 1.00\* logKow - 1.32 | 0.941 | 44, diverse, in fish | Mackay, D. (1982)., Pavan, 2006 |
| BCF | Log BCF = 0.76\* logKow - 0.31 | 0.593 | 38, diverse, in fish | Schüürmann, G., Klein, W. (1988)., Pavan, 2006 |
| BCF | Log BCF = 0.90\* logKow - 0.80 | 0.891 | 80, Diverse nonpolar, in fish | Lu, X.X., Tao, S., Cao, J., Dawson, R.W. (1999)., Pavan, 2006 |
| BCF | Log BCF = 0.74\* logKow + 0.80 | 0.84 | 66, diverse, in fish | Escuder-Gilabert, 2001, Pavan, 2006 |
| BCF | Log BCF = 0.54\* logKow + 0.12 | 0.90 | 8, Halogenated aromatics, in fish | Neely 1974, Pavan, 2006 |
| BCF | Log BCF = 0.67\* logKow - 0.18 | 0.872 | 9, Anilines, in fish | Zok 1991, Pavan, 2006 |
| BCF | Log BCF = 0.910\* logKow - 1.975\*log (6.8E-7\* Kow +1) - 0.786 | 0.90 | 154, Diverse, in fish | Bintein, S., Devillers, J., Karcher, W. (1993)., Pavan, 2006 |
| BCF | LogBCF 0 .42 3.321 e- (logK - logK )2 /10.15 | 0.73 | 443, Diverse narcotics, in fish | Dimitrov, S.D., Mekenyan, O.G., Walker, J.D. (2002)., Pavan, 2006 |
| BCF | Log BCF = 3.41\* logKow - 0.26\*( logKow)2- 5.51 | ? | 6, Chlorobenzenes, in fish | Könemann, H., van Leeuwen, C. (1980)., Pavan, 2006 |
| BCF | Log BCF = -0.44\*logS +3.03 | 0.64 | 29, diverse, in fish | Davies, R.P., Dobbs, A. (1984)., Pavan, 2006 |
| BCF | Log BCF = -0.47\*logS +2.02 | 0.76 | 107, diverse, in fish | Isnard, P., Lambert, S. (1988), Pavan, 2006 |
| BCF | logBCF 0.88 4.39 4.74V /100 0.95, LSER approach | 0.9 | 51, diverse, in fish | Park, J.H., Lee, H.J. (1993)., Pavan, 2006 |
| BCF | LogBCF 0.757 0Xv + 2.6501 1Xv + 3.372 - 1.186 0Xv - 1.807 3Xvc + 0.770, connectivity indices, stepwise regression | 0.907 | 80, non-polar organic ompounds, in fish | Lu, X.X., Tao, S., Cao, J., Dawson, R.W. (1999), Pavan, 2006 |
| BCF | LogBCF = -18.87 + 1.68 IM 0.51 HAcc + 17.09MATS2m -0.40GATS2e | 0.816 | 238, non-ionic organic compounds, in fish | Gramatica, P., Papa, E. (2003)., Pavan, 2006 |
| BCF | LogBCF = 17.58 1.69 IM - 0.45 HAcc + 15.65MATS2m - 0.36GATS2e - 1.64H6p | 0.795 | 179, non-ionic organic compounds, in fish | Gramatica, P., Papa, E. (2003)., Pavan, 2006 |
| BCF | LogBCF = -1.01 + 2.53 IM - 1.02HIC - 0.46nHAcc - 1.13GATS1e - 1.70MATS1p | 0.807 | 179, in fish | Gramatica, P., Papa, E. (2005)., Pavan, 2006 |
| BCF | LogBCF = 0.412logKow + 5.74 | 0.217 | 107, in fish | Dearden, J.C., Shinnawei, N.M. (2004)., Pavan, 2006 |
| BCF | LogBCF = 0.245logSaq + 0.512HDCmax - 0.184DPM - 0.0156PolWMZZ - 0.0380nAtoms + 7.23 | 0.710 | 107, in fish | Dearden, J.C., Shinnawei, N.M. (2004)., Pavan, 2006 |
| BCF | Log BCF = (0.85\*log Kow) - 0.70 | 0.90 | 55, in fish | Veith, G.D., DeFoe, D.L., Bergstedt, B.V. (1979)., Pavan, 2006 |
| BCF | Log BCF)0.2432 × Log P-1.601 × ABSQon-0.9529 × MaxNeg-55.85 × xch10+1.392 × xvp10+ 168.7 × xvch9+0.09185 × SaasC\_acnt- 2.861 × SssNH\_acnt+0.5661 × SssO\_acnt+ 0.7797 × SdssS\_acnt+1.078 × SssNH- 1.886 × SssssNp+0.2769 × 0.04637 × SHBint6+0.2835 × SHBint2\_Acnt+SdsssP+ 0.09498 × SHBint6\_Acnt+1.45606 | 0.80 | 93 Pesticides, in fish | Jackson 2009 |
| BCF | - | 0.68 (acids); 0.75 (bases) | 211 ionogenic organic chemicals, in fish | Armitage 2013 |
| BCF | log BCF = 3.036 ClogP - 0.197 ClogP^2 - 0.808 MgVol | 0.817 | 28, diverse group of organic chemicals including halogenated, nonhalogenated, and phosphate containing chemicals, (highly hydrophobic chemicals ) in fathead minnow | Garg and Smith 2014 |
| BCF | Log BCF = 0.337(SaasC)+ 25.462(X3Av) + 1.147(MAXDN) - 7.437(MSD) + 0.908(S3K) - 1.243 | 0.923 | 47 polychlorinatedbiphenyls(PCBs), in fish | de Melo (2012) |
| BCF | GANN | 0.8836 | 53 polycyclic aromatic hydrocarbons, heterocyclic compounds and benzene derivatives, in Poecillia reticulata | Fatemi et al. 2003 |
| BCF | stepwise-NN | 0.7921 | 53 polycyclic aromatic hydrocarbons, heterocyclic compounds and benzene derivatives, in Poecillia reticulata | Fatemi et al. 2003 |
| BCF | log BCFmale guppy = 0.91(0.45) log Poct - 1.14(1.72), linear regression | 0.74 | 10 organophosphorus pesticides, in male guppies | Fujikawa et al (2009) |
| BCF | log BCFmale guppy = 2.02(0.38) log PM + 1.60(0.19), linear regression | 0.95 | 10 organophosphorus pesticides, in fish | Fujikawa et al (2009) |
| BCF | logBCF =-17.58 (1.64)+1.69 (0.01) VIMD deg - 0.45 ( 0.03) nHAccþ + 15.65 ( 1.70) MATS2m - 0.36 ( 0.09) GATS2e - 1.64 ( 0.56) H6p, multiple linear regression models (OLS-Ordinary Least Squares) selected by genetic algorithm |  | 179/59 non-ionic organic compounds, in fish | Gramatica and Papa 2005 |
| BCF | logBCF =-1.01(0.35)+2.53 (0.13) VIMD deg - 1.02 ( 0.12)HIC - 0.46 ( 0.04) nHAcc - 1.13 ( 0.18) GATS1e - 1.70 ( 0.34) MATS1p, multiple linear regression models (OLS-Ordinary Least Squares) selected by genetic algorithm |  | 179/59 non-ionic organic compounds, in fish | Gramatica and Papa 2005 |
| BCF | MLR model | 0.931 | 27, In fish | Wei et al., Hong et al. (2009) |
| BCF | MLR model | 0.810 | 239, In fish | Lu et al., Hong et al. (2009) |
| BCF | MLR model | 0.851 | 122, In fish | Sacan et al., Hong et al. (2009) |
| BCF | GA-OLS model | 0.816 | 238, In fish | Gramatica and Papa, Hong et al. (2009) |
| BCF | logBCF = −7.043×10−1 + 9.937×10−3CMA+1.212 ×10−2α + 5.017×10−3 MW + 1.817q−c, PLS regression | 0.868 | 122 nonionic organic compounds, including chlorinated aliphatic hydrocarbons, monocyclic aromatic hydrocarbons, polycyclic aromatic hydrocarbons, halogenated benzenes, halogenated biphenyls, phenols, anilines and nitroaromatics, in fish | Hong et al. (2009) |
| BCF | posetic quantitative super-structure/activity relationship | 0.8154-0.8742 | 20 polychlorinated biphenyls, in fish | Ivanciuc et al. (2006) |
| BCF | Fuzzy filtering | 0.7905 - 0.9144 | 511 alkanes, alkenes, mono- and diaromatic hydrocarbons, polycyclic aromatic hydrocarbons (PAH), polychlorinated dibenzofuranes (PCDF), polychlorinated dibenzodioxines (PCDD), polychlorinated biphenyls (PCB), cycloalkanes and cycloalkenes, chloraromatic chemicals, perfluorinated acids (PFA), chlorinated biphenyl esters, aliphatic esters, chlororganic chemicals, aliphatic and aromatic N-containing compounds, polycyclic aromatic N-containing compounds, organotin compounds, and sulphur-containing heterocyclic compounds, in fish | Kumar et al. (2009) |
| BCF | log BCF = -1.474(0.443)1wp + 1.812 (0.3394)wpc - 1.901(0.779)7wp + 7.558(1.577), Molecular connectivity indices method | 0.815409 | 16 substituted nitrobenzene and aniline compounds, in carp | Lin et al. 2009 |
| BCF | log BCF = (1.2006+-0.0848) + (0.0621 +- 0.0075) \* x15 (0.1374 +- 0.0340) \* x17 + (0.0736 0.0189) \* x25 + (0.0679 +- 0.0062) \* x36 + (0.0651 +- 0.0167) \* x91, Molecular electronegativity distance vector model | 0.9500 | 122 nonionic organic compounds, in fish | Liu et al. (2007) |
| BCF | CoMFA | 0.926 | 58 polychlorinated biphenyls, in fish | Liu et al. 2014 |
| BCF | logBCF = 1.6(0.12) + 1.45(0.08)H2p - 0.008( 0.001)TPSA(tot) - 0.39(0.1)Max(Ea) + 0.26(0.08)Max(Ca) + 0.16(0.03)Cl - 089, genetic algorithm and linear regression | 0.73 | 290/315, in fish | Papa et al. (2007) |
| BCF | log BCF = 2.77(0.4) - 1.32(0.3)BELe7 - 0.75(0.2)H6u + 2.39ð(0.7)R6v - 1.05(0.3)Hy, genetic algorithm and linear regression | 0.77 | 53/31 highly hydrophobic compounds, in fish | Papa et al. (2007) |
| BCF | Log BCF = − 0.420 × log S – 0.005 × WPSA-1 + 0.252 × LUMO + 0.004 × THSA – 0.096 × min(#HA,#HD) – 0.405, linear regression | 0.75 | 310 156; 161, diverse, in fish | Piir (2015) |
| BCF | log BCF = 6.340 + 35.356 \* [0.040 −ΔεD] + 67.375 \* [ε3 − 0.420] + 11.470 \* X SUM Bns(δ) −7.731 - [2.851 − ηlocal] −3.767 \* ΔΨB + 1.567 [hΔεA−0.108], Genetic function approximation followed by multiple linear regression algorithm | 0.641 | 522, diverse, in fish | Pramanik and Roy 2014 |
| BCF | molecular electronegativity distance vector model | 0.92256 | 58 polychlorinated biphenyls, in fish | Qin et al. (2008) |
| BCF | log BCF = (1.3238 ± 0.0778) + (0.0643 ± 0.0048)x15 +(0.0709±0.0102)x25−(0.0636±0.01380)x26 +(0.0858 ± 0.0282)x27 +(0.1098 ± 0.0093)x36, molecular electronegativity distance vector method | 0.9271 | 85/29 nonpolar organic compounds, in fish | Qin et al. (2010) |
| BCF | log BCF = 4.623 + 1.045CRI + 0.546EHOMO, forward multiple linear regression | 0.848241 | 122, diverse, in fish | Sacan et al. (2004) |
| BCF | pBCF = 0.00250227 MW – 0.0723952 ET – 0.21352 eHOMO – 0.892481 eLUMO – 2.58291, multi linear regression | 0.871 | 131 organic compounds of different chemical structures, in fish | Sahu and Singh 2009 |
| BCF | logBCF = (1.34144 ± 0.07119) + (0.05419 ± 0.00426)x15 + (0.07706 ± 0.01698)x22 + (0.07885 ± 0.01061)x25 − (0.08285 ± 0.01386)x33 + (0.04996 ± 0.00536)x36 + (0.28660 ± 0.06546)x43 + (0.07013 ± 0.01703)x91, molecular electronegativity-distance vector method | 0.803 | 200/7 aromatic hydrocarbons, chlorinated aliphatic hydrocarbons, anilines, nitroaromatics, halogenated phenols, esters, ethers, chlo-rinated dibenzo-dioxins, chlorinated dibenzofurans, and some organic pesticides, in fish | Shihai et al. (2007) |
| BCF | Two tiered BCF assessment. Conditional inference trees and random forests. Nendza et al. (2013). Two tiered method with a) B/non-B/notcovered classification rules derived from conditional inference trees and b) BCF estimation using random forests | 0.836 | 713, 560 (78.5%) chemicals with a BCF below 2,000 and 153 (21.5%) with a BCF equal to or above 2,000, in fish? | Strempel et al. (2013) |
| BCF | log BCF = -71.0448 (0.1775) + 67.1911 (0.1631)DCW(14), Balance of correlations approach | 0.771 | 193, diverse, in fish | Toporov et al. (2009) |
| BCF | log BCF = 0.0037(0.0037) + 0.0922(0.0001)\*DCW(1), Based on indices of the presence of atoms (IPA) encode the presence or absence of atoms, such as nitrogen, oxygen, sulphur, phosphorus, fluorine, chlorine, and bromine in a molecule | 0.6803 | 502/322/165, diverse, in fish | Toropov et al. (2011), CORAL |
| BCF | shuffling multivariate adaptive regression splines and adaptive neuro-fuzzy inference system | 0.9663 | 58, polychlorinated biphenyls, in fish | Zarei and Salehabadi (2012) |
| BCF | ANN | 0.765 | 624, In fish | Dearden and Hewitt (2010) |
| BCF | Density functional theory (DFT) | 0.981 | 12, chloroanilines, in fish | Feng and Wei-Hua(2014) |
| BCF | model based on fragment constants and structural correction factors |  | 337, very hydrophobic to the very hydrophilic with logKow values between 0.39 and 8.60, in fish | Tao (2001) |
| BCF | Log BCF= 0.85\* log Kow -0.70, Linear regression | 0.91 | 73, monovalent acids, in fish | Fu *et al.,* ( 2009) |
| BCF | Log BCF= -0.2\*logKow^2 +2.74 \* log Kow -4.72, Linear regression | 0.80 | 65, monovalent bases, in fish | Fu *et al.,* ( 2009) |
| BCF | Log BCF= 0.858\* Log Kow – 0.808, Linear regression | ? | neutral chemicals, in Daphnia magna | Geyer *et al.,* 1991 |
| BCF | LogBCF = 0.71logDlipw-0.23, Linear regression | 0.89 | 6 (moclobemide, 5-fluoruracil, carbamazepine, diazepam, carvedilol, fluoxetine), in G. pulex | Meredith and Williams model, 2012 |
| BCF | LOGBCF= 1.3 LogVd +1.2, Linear regression | 0.50 | 6 (moclobemide, 5-fluoruracil, carbamazepine, diazepam, carvedilol, fluoxetine), in G. pulex | Meredith and Williams model, 2012 |
| BCF | Log BCF = 0.90\* logKow - 1.32 | 0.922 | 12, Diverse, in Daphnia magna | Hawker, D.W., Connell, D.W. (1986). |
| BCF | Log BCF = 0.85\* logKow - 1.10 | 0.913 | 52, Diverse, in Daphnia magna | Geyer, 1991 |
| BCF | Log BCF = 0.898 log Kow − 1.315, Linear regression | 0.93 | 22, Organochlorines and PAH, in G pulex | Hawker and Connell 1986 |
| BCF | Log BCF = 4.82 3χc v + 1.276, Linear regression | 0.89 | 6 PAHs, in G pulex | Govers et al. (1984) |
| BCF | Log BCF = 0.752 log Kow − 0.4362, Linear regression | 0.85 | 7 PAHs, in G pulex | Southworth et al. (1978) |
| BCF | Log BCF = 0.850 log Kow − 1.10, Linear regression | 0.91 | 52 Pesticides, PAHs, PCBs, in Daphnia magna | Geyer et al. (1991) |
| BCF | Log BCF = 0.7207 log Kow − 0.334, Linear regression | 0.89 | 11 PAHs, in Daphnia pulex and magna | Axelman et al. (1995) |
| BCF | Log BCF = 1.1 log Kow − 1.8, Linear regression | 0.88 | PAHs, in Asellus aquaticus | van Hattum and Cid Montanes (1999) |
| BCF | Log BCF = 0.38 log Kow + 3.78, Linear regression | 0.93 | 10 PAHs, in Asellus aquaticus | Curto et al. (1993) |
| BCF | Log BCF = 0.65 log Kow + 1.8, Linear regression | 0.99 | 4 PAHs, in curstacea (Pontoporeia hoyi) | Landrum (1988) |
| BCF | Log BCF = 0.681 log Kow + 0.164, Linear regression | 0.81 | 41 Pesticides and organics, in green algae (Chlorella fusca) | Geyer et al. (1984) |
| BCF | Log BCF = 0.53 log kw + 0.99, Linear regression | 0.56 | 15 Urea herbicides, in green algae (Chlorella fusca) | Manthey et al. (1993) |
| BCF | Log BCF = 0.70 log Kow − 0.26, Linear regression | 0.93 | 8 Pesticides, in green algae (Scenedesmus acutus) | Ellgehausen et al. (1980) |
| BCF | Log BCF = 0.28 log Kow + 2.6, Linear regression | 0.64 | 5 Organochlorines and pesticides, in green algae (Selenastrum capricornutum) | Mailhot (1987) |
| BCF | Log BCF = 0.46 log Kow + 2.36, Linear regression | 0.83 | 8 Aromatics, in green algae (Selenastrum capricornutum) | Casserly et al. (1983) |
| BCF | Log BCF = 0.681\* logKow+0.164 | 0.814 | 41, Diverse, in algae | Geyer, H.J., Politzki, G., Freitag, D. (1984). |
| BCF | Log BCF = 0.70\* logKow - 0.26 | 0.93 | 8 Pesticides, in algae | Ellgenhausen, H., Guth, J.A., Esser, H.O. (1980). |
| BCF | log BCF = 0.51 + 0.64 log Pow, Linear regression | 0.86 | 9, mostly low-polarity compounds, in green algae (Selenastrum capricornutum) | Mallhot 1987 |
| lipid-normalized algae–water distribution coefficient | log Kaw/lipid = 0.983(±0.014) log Ktw + 0.134(±0.061) , Linear regression | 0.999 | 53 low-polarity compounds, in Chlorella sorokiniana | Hung et al. 2014 |
| BCF | Log BCF = 0.98 log Kow – 2.24, Linear regression | 0.97 | 9 Chlorobenzenes and PCBs, in aquatic plant (Myriophyllum spicatum) | Gobas et al. (1991) |
| BCF | Log BCF = 0.491 log Kow + 0.0562, Linear regression | 0.96 | 10 Pesticides, PCBs, in common duckweed (Lemna minor) | Lockhart et al. (1983) |
| BCF | Log BCF = 0.86\* logKow - 0.81 | 0.912 | 16 Diverse, in mussels | Geyer 1982 |
| BCR | log BCR plant-soil = - 0.204 1c - 0.385 Σ(NpPf) + 0.589, Linear regression | 0.830 | 30 Miscellaneous organic compounds, in plants (from soil) | Dowdy and McKone (1997) |
| BCR | log BCR root-soil = 0.718 1c + a Σ(NpPf) - 2.372, Linear regression | 0.840 | 16 Miscellaneous organic compounds, in plant roots (from soil) | Dowdy and McKone (1997) |
| BCR | log BCR plant-air = 0.480 1c + 0.907 Σ(NpPf) + 3.285, Linear regression | 0.780 | 14 Miscellaneous organic compounds, in plants (from air) | Dowdy and McKone (1997) |
| RCF | Log (RCF -0.82) = 0.77 \* Log Kow -1.52 , Linear regression. estimation the uptake of non-ionised chemicals in plant roots. | ? | neutral chemicals, in plant roots | Briggs *et al.,* (1983) |
| BCF | LogBCF = 0.27logDlipw-0.93, Linear regression | 0.83 | 6 (moclobemide, 5-fluoruracil, carbamazepine, diazepam, carvedilol , fluoxetine), in tree tobacco plant (N. glauca) | Meredith and Williams model, 2012 |
| BCF | LogBCF=-0.5 LogVd+0.4, Linear regression | 0.70 | 6 (moclobemide, 5-fluoruracil, carbamazepine, diazepam, carvedilol , fluoxetine), in tree tobacco plant (N. glauca) | Meredith and Williams model, 2012 |
| BCF | Log BCF = 0.844 log Kow − 1.235, Linear regression | 0.69 | 34 Organochlorines and pesticides, in snail (Molluscs, four species) | Hawker and Connell 1986 |
| BCF | Log BCF = −0.58 log WS (ppb) + 4.5, Linear regression | 0.92 | 4 Herbicides, in blue mussel (Mytilus edulis) | Watanabe et al. (1985) |
| BCF | Log BCF = 0.66 log Kow − 0.05, Linear regression | 0.96 | 6 Insecticides, in blue mussel (Mytilus edulis) | Zaroogian et al. (1985) |
| BCF | Log BCF = 0.858 log Kow − 0.808, Linear regression | 0.91 | 16 Pesticides, in blue mussel (Mytilus edulis) | Geyer et al. (1982) |
| BCF | Log BCF = −0.843 log WS (ppb) + 5.15, Linear regression | 0.87 | 17 Chlorinated aromatics, in blue mussel (Mytilus edulis) | Ernst (1977) |
| BCF | Log BCF = 0.72 log Kow + 0.41, Linear regression | 0.29 | 17 Organochlorines and pesticides, in easern oyster (Crassostrea virginica) | Zaroogian et al. (1985) |
| BCF | Log BCF = 1.76 log Kow − 6.33, Linear regression | 0.97 | 4 Chlorobenzenes, in snail (Lymnaea stagnalis) | Legierse et al. (1998) |
| BCF | ? | ? | 23 pesticides, PBBs, in earthworm | Pflugmacher, 1992 |
| BCF | Log BCF = −0.75 (log Kow – 6.84)^2 + 6.25, quadratic regression | 0.96 | 15 Chlorobenzenes and PCBs, in Oligochaetes (two aquatic and terrestrial earthworm species) | Connell et al. (1988) |
| BCF | BCF waiving scheme, Decision tree | - | 999 | Nendza and Herbst (2011). ChemProp -2012. Nendza et al. (2013). |
| BCF | EUSES equations, Two linear log Kow-based relationships | - | 55; 43 | European Commission -1996. Nendza et al. (2013). |
| BCF | BiLin worst-case model, Bilinear log Kow-based relationship | - | 132 | Nendza (1991). Nendza et al. (2013). |
| BCF | LogBCF -0.041 (0Xv)^2 -5.809 (1Xv)^0.5 + 0.615 2X - 0.785 3Xc + 1.564 0Xv +sum(Ffnf) +3.179 | 0.810 | - | Pavan, 2006 |
| BCF | LogBCF =13.82 +1.51 3Xc −1.50 4Xv −154.25 6Xvch, BCF model based on fragment constants | 0.780; 0.880; 0.911 | 40 PCBs | Jorgensen, S. L., Sorensen, B. H., Mahier, H. (1998). Pavan, 2006 |
| BCF | LogBCF = 0.64nCl − 0.062nCln2,6 − 0.044nCln3,5 + 2.697, BCF model based on fragment constants | 0.889 | ? | Pavan, 2006 |
| BCF | LogBCF = 10.4678(0.8129)+ 0.0033( 0.0014)a+ 0.7415( 0.0751) Ehomo + 0.5696( 0.0751)Elumo 0.0266( 0.0102)CCR, BCF model based on quantum chemical descriptors | 0.8613 | 31 | Pavan, 2006 |
| BCF | LogBCF = 10.8570( 0.4286) + 0.7479( 0.0439)Ehomo 0.0465 ( 0.0498)Elumo + 0.0200( 0.0068)CCR | | 27 | Pavan, 2006 |
| BCF | LogBCF = 0.475logKow + 0.237 | 0.550 | 540 | Pavan, 2006 |
| BCF | LogBCF = 0.39logKow + 0.00925Polmw + 0.398nNH2 -0.435HAEmax - 0.147d4Xpv +0.740 | 0.664 | 540 | Pavan, 2006 |
| BCF | LogBCF = 1.52( 0.09) + 1.14( 0.16)H2p - 0.44( 0.08)MaxEa + 0.34( 0.08)BEHm7 - 0.17( 0.02)nHbondAcc + 0.03( 0.005)Sum(Ead) 0.22( 0.07)MaxCa(o) | 0.72 | 318/292, diverse | Papa, E., Gramatica, P., Dearden J.C. (2005). Pavan, 2006 |
| BCF | LogBCF = 5.70( 0.50) - 1.69( 0.19)BELv8 + 0.33( 0.05)logWS + 3.09( 0.65)R6v - 0.64( 0.15)GroupCountHydroxy | 0.79 | 88 highly hydrophobic chemicals | Papa, E., Gramatica, P., Dearden J.C. (2005). Pavan, 2006 |
| BCF | ANN | 0.747 | 239 organic pollutants | Feng et al. (2008 |
| BCF | ANN | 0.829 | 239 organic pollutants | Feng et al. (2008 |
| BCF | ? | 0.821 | 239 organic pollutants | Feng et al. (2008) |
| BCF | Log BCF= 0.85\* log Kow -0.70 (Where 1≤ log Kow ≤6); Log BCF= -0.2\*logKow^2 +2.74 \*log Kow- 4.72 (Where 6< log Kow <10 . Very liphofilic compounds.), Linear regression. TDG model | 0.90 | 50 lipophillic and very lipophillic compounds, generic QSPR? | Veith *et al.,* (1979) |
| BCF | Log BCF = –1.67 (0.26) + 1.02\*(0.06) log Kow, Linear regression | r²= 0.70 all autotroph; r²= 0.88 acceptable autotroph; r²= 0.23 all invertebrates BCF; r²= 0.61 acceptable invertebrates BCF; r²= 0.38 all invertebrates BAF; r²=0.55 acceptable invertebrate BAF; r²= 0.38 all fish BCF; r²= acceptable fish BCF; r²= 0.52 acceptable fish BCF; r²= 0.55 all fish BAF; r²= 0.55 acceptable fish BAF. | 22 neutral chemicals, generic QSPR (218 invertebrates) | Arnot and Gobas2006 model |
| BCF | Log BCF = -0.564\*logS +2.79 | 0.49 | 36 Diverse, in daphnia and fish? | Kenaga, E.E., Goring, C.A.I. (1980). Pavan, 2006 |