Supplementary Data

Topological Features in Profiling the Antimalarial Activity Landscape of Anilinoquinolines: A Multi-Pronged QSAR Study

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CP-MLR and GA identified descriptors' values (delimited by comma) of compounds used in regression equations.

Compd,MATS4m,MATS8m,MATS5e,MATS7e,nNR2,H-047,H-052,RDF085p,Mor15m,Mor17p,Mor30p,E1m,E2m,R6m,R7m,R7m+,R6e+,RTe+
AQ01(V),1.004,1.008,0.007,-0.05,0,9,0,3.827,1.502,0.409,0.474,0.803,0.216,0.262,0.237,0.025,0.036,0.267
AQ02(V),1.012,0.993,-0.059,0.013,1,13,4,10.811,1.701,-0.032,0.434,0.664,0.191,0.309,0.277,0.026,0.02,0.181
AQ03(T),1.008,0.991,0.053,-0.087,1,15,4,12.472,1.475,0.031,0.545,0.666,0.227,0.297,0.247,0.023,0.019,0.177
AQ04(T),1.007,0.994,0.008,0.058,1,15,6,10.437,1.815,-0.124,0.68,0.683,0.274,0.3,0.264,0.024,0.018,0.174
AQ05(Tr),1.007,1.002,0.015,0.087,1,15,6,10.856,1.484,-0.202,0.699,0.681,0.305,0.307,0.27,0.025,0.018,0.167
AQ06(V),1.006,0.999,0.026,0.018,1,15,6,10.233,1.564,-0.396,0.597,0.703,0.327,0.302,0.262,0.023,0.017,0.164
AQ07(Tr),1.005,1,0.042,0.039,1,15,6,10.952,1.342,-0.608,0.748,0.742,0.402,0.297,0.255,0.021,0.015,0.158
AQ08(Tr),1.008,1,-0.078,-0.039,1,13,4,9.986,1.75,0.026,0.478,0.68,0.184,0.305,0.264,0.027,0.021,0.185
AQ09(T),1.012,0.995,-0.076,0.027,2,20,0,10.964,2.011,0.002,0.419,0.662,0.192,0.311,0.277,0.026,0.02,0.183
AQ10(Tr),1.01,1,-0.066,0.123,1,14,0,9.722,1.829,0.042,0.536,0.712,0.187,0.314,0.285,0.026,0.02,0.182
AQ11(T),1.008,1.002,-0.119,0.018,1,13,4,9.513,2.035,0.11,0.655,0.692,0.189,0.298,0.271,0.03,0.022,0.191
AQ12(Tr),1.011,1.007,-0.113,0.006,1,13,0,10.273,1.85,0.146,0.601,0.769,0.187,0.303,0.291,0.03,0.022,0.196
AQ13(T),1.02,0.987,0.036,0.044,0,9,9,9.901,1.564,0.129,0.557,0.692,0.207,0.286,0.25,0.026,0.021,0.174

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AQ14(V),0.994,0.997,-
0.047,0.027,1,13,6,9.491,1.651,0.031,0.581,0.703,0.183,0.298,0.265,0.029,0.023,0.18
AQ15(V),1.003,1.003,-0.07,-
0.036,0,16,0,10.874,2.065,0.18,0.57,0.664,0.297,0.333,0.298,0.027,0.021,0.198
AQ16(Tr),1.007,1.006,-0.068,-
0.061,0,15,0,12.559,2.047,0.28,0.504,0.734,0.482,0.372,0.333,0.038,0.021,0.196
AQ17(Tr),1.006,1.002,-
0.077,0.003,1,17,2,11.977,1.859,0.126,0.551,0.701,0.18,0.333,0.294,0.024,0.019,0.153
AQ18(Tr),1,1.006,-0.062,-
0.125,0,10,3,10.42,1.705,0.354,0.553,0.71,0.214,0.32,0.285,0.03,0.022,0.202
AQ19(Tr),1.003,1.006,-0.033,-
0.023,0,9,0,5.244,1.522,0.421,0.457,0.845,0.185,0.321,0.284,0.046,0.031,0.238
AQ20(Tr),1.01,0.986,-0.124,0.007,2,17,8,18.619,1.796,-
0.428,0.503,0.613,0.3,0.239,0.179,0.008,0.015,0.074
AQ21(T),1.007,0.985,0.003,-0.037,2,19,8,15.991,1.882,-
0.633,0.514,0.571,0.302,0.239,0.178,0.01,0.017,0.07
AQ22(V),1.006,0.985,-0.043,0.105,2,19,10,17.871,1.691,-
0.651,0.609,0.602,0.304,0.243,0.189,0.009,0.014,0.07
AQ23(Tr),1.006,0.991,-0.035,0.129,2,19,10,19.524,1.91,-
0.744,0.678,0.538,0.337,0.241,0.181,0.009,0.014,0.074
AQ24(V),1.005,0.988,-0.021,0.061,2,19,10,19.228,1.853,-
0.921,0.832,0.551,0.337,0.242,0.186,0.009,0.013,0.067
AQ25(Tr),1.007,0.984,-0.061,0.098,2,19,10,17.295,2.146,-
0.593,0.717,0.553,0.324,0.238,0.185,0.009,0.014,0.071
AQ26(Tr),1.006,0.986,-0.06,0.058,2,23,6,17.387,1.806,-
0.683,0.644,0.588,0.336,0.251,0.196,0.009,0.014,0.071
AQ27(T),1.008,0.986,-0.046,0.091,3,26,6,16.705,1.748,-
0.549,0.613,0.595,0.327,0.251,0.2,0.009,0.013,0.076
AQ28(Tr),0.997,0.983,-0.028,0.106,2,19,12,18.166,1.692,-
0.497,0.75,0.554,0.322,0.247,0.203,0.009,0.022,0.068
AQ29(Tr),1.004,0.994,-0.116,0.061,1,15,6,14.762,1.948,-
0.241,0.752,0.839,0.446,0.348,0.193,0.022,0.018,0.089
AQ30(T),1.007,0.997,-0.127,0.053,1,18,4,15.93,1.995,-
0.024,0.465,0.633,0.362,0.232,0.191,0.01,0.016,0.077
AQ31(Tr),1.004,0.997,-0.053,0.011,1,18,4,17.221,2.734,-
0.119,0.547,0.628,0.325,0.266,0.202,0.012,0.019,0.085
AQ32(T),1.012,1.001,-0.074,-
0.037,1,11,4,9.78,1.676,0.058,0.442,0.661,0.24,0.341,0.299,0.037,0.025,0.132
AQ33(T),1.012,0.983,-0.134,-0.081,2,23,4,15.686,1.937,-
0.293,0.397,0.703,0.225,0.2,0.155,0.008,0.017,0.084
AQ34(Tr),1.011,0.993,-0.072,-0.081,2,23,4,13.853,1.629,-
0.336,0.471,0.701,0.262,0.207,0.156,0.008,0.016,0.076
AQ35(V),1.014,0.986,-0.138,-0.082,3,26,4,15.741,2.043,-
0.464,0.449,0.688,0.243,0.202,0.153,0.006,0.016,0.075
AQ36(T),1.009,0.987,-0.104,-0.08,2,21,8,14.057,2.107,-
0.493,0.515,0.686,0.273,0.221,0.168,0.008,0.017,0.087

AQ37(Tr),1.008,0.986,-0.081,-0.083,2,21,8,16.371,1.852,-
0.462,0.523,0.664,0.295,0.207,0.155,0.008,0.015,0.078
AQ38(V),1.008,0.989,-0.093,-0.083,2,25,4,16.484,2.137,-
0.346,0.488,0.688,0.316,0.228,0.174,0.008,0.016,0.085
AQ39(Tr),1,0.988,-0.057,-0.116,2,17,10,16.596,1.629,-
0.413,0.606,0.666,0.219,0.219,0.186,0.009,0.021,0.07
AQ40(Tr),1.019,0.978,-0.068,-0.025,1,13,13,17.619,1.776,-
0.317,0.581,0.675,0.231,0.2,0.166,0.009,0.017,0.077
AQ41(V),1.011,0.992,-0.08,-0.129,2,17,8,20.692,1.745,-
0.357,0.54,0.63,0.258,0.255,0.212,0.009,0.017,0.079
AQ42(V),1.012,0.994,-0.106,-0.135,2,17,8,16.237,2.081,-
0.302,0.603,0.652,0.226,0.221,0.187,0.009,0.016,0.069
AQ43(T),1.013,0.988,-0.082,-0.123,3,24,4,17.024,1.802,-
0.539,0.499,0.614,0.265,0.266,0.22,0.009,0.016,0.076
AQ44(Tr),1.01,0.994,-0.096,-0.146,2,21,4,16.415,2.06,-
0.245,0.6,0.607,0.303,0.22,0.184,0.009,0.016,0.073
AQ45(Tr),1.012,0.995,-0.126,-0.146,2,18,8,16.993,1.711,-
0.51,0.547,0.604,0.305,0.27,0.223,0.009,0.016,0.078
AQ46(V),1.008,0.989,-0.097,-0.107,3,25,4,19.387,2.026,-
0.408,0.507,0.548,0.435,0.276,0.223,0.009,0.016,0.102
AQ47(T),1.005,0.995,-0.07,-0.119,3,26,4,25.688,2.44,-
0.584,0.575,0.395,0.636,0.282,0.22,0.009,0.016,0.075
AQ48(Tr),1.011,0.996,-0.081,-0.093,3,28,4,30.307,2.08,-
0.453,0.44,0.387,0.67,0.294,0.233,0.008,0.016,0.076
AQ49(Tr),1.003,1.006,-0.085,-0.059,3,32,4,37.878,2.171,-
0.495,0.426,0.364,0.576,0.352,0.258,0.009,0.014,0.068
AQ50(T),1.014,0.993,-0.072,-0.084,3,27,4,31.397,2.199,-
0.355,0.488,0.492,0.598,0.313,0.259,0.015,0.016,0.076
AQ51(T),1.007,0.994,-0.055,-0.077,3,30,4,30.217,2.375,-
0.499,0.422,0.325,0.632,0.298,0.242,0.008,0.016,0.076
AQ52(Tr),1.013,0.997,-0.092,-0.048,3,27,4,33.249,1.62,-
0.454,0.54,0.449,0.591,0.311,0.255,0.008,0.016,0.077
AQ53(Tr),0.998,0.985,-0.043,-0.059,3,31,10,38.571,2.311,-
0.717,0.644,0.299,0.61,0.286,0.233,0.007,0.014,0.07
AQ54(V),1.013,0.996,-0.092,-0.083,3,27,4,31.406,2.002,-
0.65,0.408,0.417,0.631,0.312,0.253,0.008,0.016,0.077
AQ55(T),1.011,0.992,-0.049,-0.12,3,26,4,26.792,2.661,-
0.849,0.363,0.381,0.606,0.314,0.259,0.008,0.016,0.068
AQ56(V),1.007,0.992,-0.114,-0.067,1,18,4,16.457,2.07,-
0.528,0.328,0.568,0.383,0.241,0.205,0.011,0.015,0.08
AQ57(Tr),1.008,0.996,-0.118,-0.106,1,20,4,17.024,1.842,-
0.762,0.197,0.605,0.323,0.232,0.191,0.01,0.015,0.085
AQ58(T),1.002,0.998,-0.11,-0.046,1,24,4,23.605,2.012,-
0.823,0.355,0.482,0.494,0.28,0.215,0.008,0.013,0.08
AQ59(Tr),1.012,0.999,-0.109,-0.115,1,19,4,18.201,1.895,-
0.728,0.156,0.58,0.465,0.281,0.222,0.029,0.019,0.077

AQ60(V),1.004,0.997,-0.081,-0.107,1,22,4,19.679,2.028,-
0.743,0.232,0.617,0.32,0.248,0.208,0.011,0.015,0.09
AQ61(T),1.012,1.004,-0.128,-0.036,1,19,4,17.811,2.024,-
0.786,0.266,0.621,0.458,0.283,0.258,0.02,0.016,0.107
AQ62(Tr),0.985,1.02,0.039,-0.142,1,13,6,6.328,1.54,-
0.388,0.379,0.765,0.205,0.328,0.231,0.014,0.024,0.102
AQ63(Tr),0.991,0.999,0.066,0.006,1,13,6,6.187,1.754,-
0.461,0.32,0.758,0.211,0.332,0.27,0.027,0.031,0.151
AQ64(Tr),0.993,1.01,0.049,-0.072,1,14,6,7.712,1.337,-
0.604,0.212,0.808,0.191,0.276,0.196,0.014,0.024,0.106
AQ65(T),0.996,1.001,0.024,-0.168,1,13,6,7.46,1.485,-
0.585,0.21,0.759,0.23,0.317,0.285,0.027,0.022,0.225
AQ66(Tr),0.995,1.007,0.017,-0.143,1,13,6,6.806,1.564,-
0.58,0.26,0.784,0.211,0.285,0.251,0.022,0.02,0.156
AQ67(Tr),0.995,0.986,0.033,-0.08,2,25,6,12.441,1.837,-
0.975,0.178,0.764,0.263,0.268,0.239,0.01,0.015,0.07
AQ68(V),1.002,1.001,-0.074,0.161,1,18,4,17.244,2.24,-
0.476,0.485,0.606,0.319,0.275,0.221,0.015,0.017,0.077
AQ69(Tr),1.002,0.999,-0.093,0.017,1,18,4,16.273,1.909,-
0.339,0.509,0.57,0.308,0.253,0.205,0.009,0.013,0.073
AQ70(Tr),1.002,0.999,-0.081,-0.021,1,18,4,23.267,1.856,-
0.396,0.583,0.709,0.26,0.3,0.235,0.008,0.014,0.077
AQ71(V),1.002,1,-0.055,-0.005,1,17,4,16.498,1.959,-
0.291,0.574,0.599,0.305,0.255,0.206,0.009,0.014,0.09
AQ72(Tr),1.002,1,-0.043,-0.038,1,17,4,24.33,2.275,-
0.563,0.552,0.701,0.251,0.311,0.244,0.009,0.014,0.074
AQ73(Tr),1.005,0.992,-0.054,0.042,1,18,4,17.487,2.006,-
0.391,0.685,0.642,0.276,0.261,0.206,0.009,0.014,0.072
AQ74(T),1.002,0.999,-0.054,-0.018,1,19,6,28.615,1.931,-
0.312,0.577,0.656,0.268,0.324,0.267,0.01,0.014,0.087
AQ75(Tr),1.01,0.984,-0.05,-0.088,2,23,4,16.809,1.861,-
0.317,0.458,0.588,0.29,0.25,0.183,0.008,0.015,0.074
AQ76(Tr),1.007,0.978,-0.004,-0.017,2,21,8,16.42,1.78,-
0.484,0.567,0.522,0.326,0.242,0.191,0.009,0.014,0.071
AQ77(Tr),1.007,0.981,-0.031,-0.044,2,25,4,15.509,2.176,-
0.296,0.593,0.541,0.348,0.254,0.204,0.01,0.016,0.076
AQ78(Tr),0.997,0.98,-0.03,0.091,2,21,10,17.039,1.771,-
0.578,0.516,0.506,0.313,0.24,0.195,0.009,0.022,0.074
AQ79(V),1.009,0.984,-0.048,0.104,3,28,4,16.546,2.395,-
0.525,0.705,0.513,0.333,0.234,0.192,0.009,0.012,0.069
AQ80(Tr),1.006,0.995,-0.058,0.028,1,20,4,15.516,2.214,-
0.277,0.56,0.608,0.319,0.259,0.197,0.014,0.019,0.073
AQ81(Tr),1.009,0.98,0.007,-0.08,2,21,4,18.145,1.676,-
0.27,0.439,0.605,0.218,0.294,0.255,0.018,0.016,0.08
AQ82(Tr),1.009,0.978,0.009,0.046,2,21,4,16.184,1.645,-
0.505,0.569,0.65,0.215,0.248,0.212,0.012,0.016,0.082

AQ83(V),1.007,0.984,0,-0.071,2,24,4,18.001,1.578,-0.46,0.472,0.606,0.239,0.264,0.216,0.01,0.016,0.076
AQ84(Tr),1.006,0.976,0.034,-0.033,2,19,8,17.42,2.055,-0.487,0.546,0.598,0.266,0.278,0.247,0.012,0.016,0.076
AQ85(Tr),1.005,0.977,0.015,-0.054,2,23,4,16.603,2.04,-0.307,0.654,0.62,0.281,0.292,0.252,0.012,0.016,0.077
AQ86(Tr),1.003,0.99,-0.033,0.004,1,15,8,19.053,1.706,-0.429,0.621,0.634,0.227,0.229,0.206,0.015,0.017,0.082
AQ87(Tr),1.003,0.991,0.032,-0.039,1,19,4,16.09,1.989,-0.14,0.632,0.591,0.28,0.234,0.216,0.015,0.016,0.071
AQ88(Tr),1.006,0.985,0.014,-0.059,2,22,4,17.356,1.91,-0.231,0.547,0.624,0.227,0.24,0.211,0.017,0.016,0.07
AQ89(Tr),0.999,0.987,0.024,0.004,2,24,4,20.266,2.258,-0.328,0.648,0.556,0.347,0.259,0.227,0.015,0.014,0.07
AQ90(V),1.005,0.992,0.016,-0.011,2,26,4,20.323,2.421,-0.42,0.558,0.287,0.587,0.277,0.237,0.015,0.014,0.066