**Beware of external validation! – A Comparative Study of Several Validation Techniques used in QSAR Modelling**

**Supplementary Material**

**Table S1**. Symbols, definitions and classification of topological indices in 95 amines data

|  |  |
| --- | --- |
|  | Topostructural (TS) |
| *IWD* | Information index for the magnitudes of distances between all possible pairs of vertices of a graph |
| *IWD* | Mean information index for the magnitude of distance |
| *W* | Wiener index = half-sum of the off-diagonal elements of the distance matrix of a graph |
| *ID* | Degree complexity |
| *HV* | Graph vertex complexity |
| *HD* | Graph distance complexity |
| *IC* | Information content of the distance matrix partitioned by frequency of occurrences of distance *h* |
| *M1* | A Zagreb group parameter = sum of square of degree over all vertices |
| *M2* | A Zagreb group parameter = sum of cross-product of degrees over all neighboring (connected) vertices |
| *hχ* | Path connectivity index of order *h* = 0-10 |
| *hχC* | Cluster connectivity index of order *h* = 3-5 |
| *hχPC* | Path-cluster connectivity index of order *h* = 4-6 |
| *hχCh* | Chain connectivity index of order *h* = 5, 6, 9, 10 |
| *Ph* | Number of paths of length *h* = 0-10 |
| *J* | Balaban’s *J* index based on topological distance |
| *nrings* | Number of rings in a graph |
| *ncirc* | Number of circuits in a graph |
| DN2S*y* | Triplet index from distance matrix, square of graph order, and distance sum; operation *y* = 1-4 |
| DN21*y* | Triplet index from distance matrix, square of graph order, and number 1; operation *y* = 1-5 |
| AS1*y* | Triplet index from adjacency matrix, distance sum, and number 1; operation *y* = 1-5 |
| DS1*y* | Triplet index from distance matrix, distance sum, and number 1; operation *y* = 1-5 |
| ASN*y* | Triplet index from adjacency matrix, distance sum, and graph order; operation *y* = 1-5 |
| DSN*y* | Triplet index from distance matrix, distance sum, and graph order; operation *y* = 1-5 |
| DN2N*y* | Triplet index from distance matrix, square of graph order, and graph order; operation *y* = 1-5 |
| ANS*y* | Triplet index from adjacency matrix, graph order, and distance sum; operation *y* = 1-2 |
| Triplet index from adjacency matrix, graph order, and distance sum; operation *y* = 3-5 |
| AN1*y* | Triplet index from adjacency matrix, graph order, and number 1; operation *y* = 1-5 |
| ANN*y* | Triplet index from adjacency matrix, graph order, and graph order again; operation *y* = 1-4 |
| ASV*y* | Triplet index from adjacency matrix, distance sum, and vertex degree; operation *y* = 1-5 |
| DSV*y* | Triplet index from distance matrix, distance sum, and vertex degree; operation *y* = 1-2 |
| ANV*y* | Triplet index from adjacency matrix, graph order, and vertex degree; operation *y* = 1-5 |
| *kp0* | Kappa zero |
| *kp1-kp3* | Kappa simple indices |
|  | **Topochemical (TC)** |
| O | Order of neighborhood when *ICr* reaches its maximum value for the hydrogen-filled graph |
| O*orb* | Order of neighborhood when *ICr* reaches its maximum value for the hydrogen-suppressed graph |
| I*ORB* | Information content or complexity of the hydrogen-suppressed graph at its maximum neighborhood of vertices |
| IC*r* | Mean information content or complexity of a graph based on the *r*th (*r* = 0-6) order neighborhood of vertices in a hydrogen-filled graph |
| SIC*r* | Structural information content for *r*th (*r* = 0-6) order neighborhood of vertices in a hydrogen-filled graph |
| CIC*r* | Complementary information content for *r*th (*r* = 0-6) order neighborhood of vertices in a hydrogen-filled graph |
| *hχb* | Bond path connectivity index of order *h* = 0-6 |
| *hχbC* | Bond cluster connectivity index of order *h* = 3, 5 |
| *hχbCh* | Bond chain connectivity index of order *h* = 5, 6 |
| *hχbPC* | Bond path-cluster connectivity index of order *h* = 4-6 |
| *hχv* | Valence path connectivity index of order *h* = 0-6 |
| *hχvC* | Valence cluster connectivity index of order *h* = 3, 5 |
| *hχvCh* | Valence chain connectivity index of order *h* = 5, 6, 9, 10 |
| *hχvPC* | Valence path-cluster connectivity index of order *h* = 4-6 |
| *JB* | Balaban’s *J* index based on bond types |
| *JX* | Balaban’s *J* index based on relative electronegativities |
| *JY* | Balaban’s *J* index based on relative covalent radii |
| AZV*y* | Triplet index from adjacency matrix, atomic number, and vertex degree; operation *y* = 1-5 |
| AZS*y* | Triplet index from adjacency matrix, atomic number, and distance sum; operation *y* = 1-5 |
| ASZ*y* | Triplet index from adjacency matrix, distance sum, and atomic number; operation *y* = 1-5 |
| AZN*y* | Triplet index from adjacency matrix, atomic number, and graph order; operation *y* = 1-5 |
| ANZ*y* | Triplet index from adjacency matrix, graph order, and atomic number; operation *y* = 1-5 |
| DSZ*y* | Triplet index from distance matrix, distance sum, and atomic number; operation *y* = 1,2 |
| DN2Z*y* | Triplet index from distance matrix, square of graph order, and atomic number; operation *y* = 1-2 |
| DN2Z*y* | Triplet index from distance matrix, square of graph order, and atomic number; operation 3-5 |
| *nvx* | Number of non-hydrogen atoms in a molecule |
| *nelem* | Number of elements in a molecule |
| *fw* | Molecular weight |
| *si* | Shannon information index |
| *totop* | Total Topological Index *t* |
| *sumI* | Sum of the intrinsic state values *I* |
| *sumdelI* | Sum of delta-*I* values |
| *tets2* | Total topological state index based on electrotopological state indices |
| *phia* | Flexibility index (*kp*1\* *kp*2/*nvx*) |
| *Idcbar* | Bonchev-Trinajstić information index |
| *IdC* | Bonchev-Trinajstić information index |
| *Wp* | Wiener *p* |
| *Pf* | Platt *f* |
| *Wt* | Total Wiener number |
| *knotp* | Difference of chi-cluster-3 and path/cluster-4 |
| *knotpv* | Valence difference of chi-cluster-3 and path/cluster-4 |
| *nclass* | Number of classes of topologically (symmetry) equivalent graph vertices |
| *NumHBd* | Number of hydrogen bond donors |
| *NumHBa* | Number of hydrogen bond acceptors |
| *SHCsats* | E-State of C *sp3* bonded to other saturated C atoms |
| *SHCsatu* | E-State of C *sp3* bonded to unsaturated C atoms |
| *SHarom* | E-State of C *sp2* which are part of an aromatic system |
| *SHHBd* | Hydrogen bond donor index, sum of Hydrogen E-State values for *–OH*, *=NH*, -*NH2*, *-NH-,-SH*, and *#CH* |
| *SHHBa* | Hydrogen bond acceptor index, sum of the *E*-State values for *–OH*, *=NH*, *-NH2*, -*NH-*, *>N*, *-O-*, *-S-*, along with –F and –Cl |
| *Qv* | General Polarity descriptor |
| *NHBinty* | Count of potential internal hydrogen bonders (*y* = 3-10) |
| *SHBinty* | E-State descriptors of potential internal hydrogen bond strength (*y =*3, 4) |
| *ka1-ka3* | Kappa alpha indices |
|  | Electrotopological State index values for atom types:  *SHsOH, SHsNH2, SHssNH, SHother, Hmax, Gmax, Hmin, Gmin, SsCH3, SssCH2, SdsCH, SaaCH, SsssCH, SaaaC, SssssC, SsNH2, SssNH, SaaNH, SaaN, SddsN, SsOH, SdO, SssO, SsF, SssS, SsCl, SsBr,* |
|  | **Geometrical (3-D)** |
| *3DW* | 3D Wiener number based on the hydrogen-suppressed geometric distance matrix |
| *3DW H* | 3D Wiener number based on the hydrogen-filled geometric distance matrix |
| *VW* | Van der Waal’s volume |
|  | Quantum Chemical (QC) |
| *EHOMO* | Energy of the highest occupied molecular orbital |
| *EHOMO-1* | Energy of the second highest occupied molecular |
| *ELUMO* | Energy of the lowest unoccupied molecular orbital |
| *ELUMO+1* | Energy of the second lowest unoccupied molecular orbital |
| *ΔHf* | Heat of formation |
| *μ* | Dipole moment |

Table S2: MSPE and external validation *q*2 values from individual splits in the three simulated datasets

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Dataset 1: *p* = 100** | | | **Dataset 2: *p* = 500** | | | **Dataset 3: *p* = 1000** | | |
| **Split no.** | **MSPE** | ***q*2** | **Split no.** | **MSPE** | ***q*2** | **Split no.** | **MSPE** | ***q*2** |
| **1** | 2.042 | 0.810 | **1** | 3.126 | 0.679 | **1** | 3.723 | 0.710 |
| **2** | 1.027 | 0.852 | **2** | 2.549 | 0.779 | **2** | 1.661 | 0.707 |
| **3** | 1.257 | 0.884 | **3** | 4.565 | 0.615 | **3** | 1.903 | 0.767 |
| **4** | 2.354 | 0.651 | **4** | 1.924 | 0.443 | **4** | 3.385 | 0.564 |
| **5** | 0.608 | 0.710 | **5** | 0.870 | 0.605 | **5** | 2.409 | 0.762 |
| **6** | 0.684 | 0.871 | **6** | 2.769 | 0.551 | **6** | 4.993 | 0.461 |
| **7** | 1.932 | 0.796 | **7** | 1.701 | 0.476 | **7** | 4.959 | 0.508 |
| **8** | 1.822 | 0.731 | **8** | 3.738 | 0.678 | **8** | 5.241 | 0.578 |
| **9** | 0.897 | 0.891 | **9** | 1.951 | 0.753 | **9** | 2.306 | 0.498 |
| **10** | 1.263 | 0.825 | **10** | 1.713 | 0.666 | **10** | 4.832 | 0.572 |
| **11** | 3.434 | 0.616 | **11** | 2.180 | 0.255 | **11** | 12.969 | 0.119 |
| **12** | 0.589 | 0.918 | **12** | 4.174 | 0.418 | **12** | 10.945 | 0.079 |
| **13** | 1.121 | 0.813 | **13** | 2.254 | 0.648 | **13** | 1.600 | 0.734 |
| **14** | 0.789 | 0.913 | **14** | 0.862 | 0.830 | **14** | 3.975 | 0.534 |
| **15** | 1.949 | 0.718 | **15** | 1.818 | 0.752 | **15** | 3.329 | 0.668 |
| **16** | 1.251 | 0.805 | **16** | 1.717 | 0.657 | **16** | 3.211 | 0.526 |
| **17** | 1.691 | 0.712 | **17** | 6.616 | 0.524 | **17** | 18.971 | -0.130 |
| **18** | 0.263 | 0.946 | **18** | 1.528 | 0.640 | **18** | 2.040 | 0.562 |
| **19** | 1.967 | 0.784 | **19** | 2.680 | 0.627 | **19** | 2.201 | 0.602 |
| **20** | 2.035 | 0.717 | **20** | 1.740 | 0.767 | **20** | 5.781 | 0.326 |
| **21** | 1.749 | 0.706 | **21** | 1.395 | 0.627 | **21** | 3.082 | 0.628 |
| **22** | 1.695 | 0.880 | **22** | 2.765 | 0.724 | **22** | 3.311 | 0.534 |
| **23** | 2.387 | 0.731 | **23** | 1.065 | 0.768 | **23** | 1.839 | 0.763 |
| **24** | 0.770 | 0.483 | **24** | 1.757 | 0.826 | **24** | 1.334 | 0.854 |
| **25** | 1.575 | 0.846 | **25** | 4.205 | 0.692 | **25** | 3.112 | 0.723 |
| **26** | 2.440 | 0.797 | **26** | 2.384 | 0.741 | **26** | 1.539 | 0.695 |
| **27** | 2.457 | 0.720 | **27** | 2.496 | 0.596 | **27** | 5.242 | 0.498 |
| **28** | 1.579 | 0.839 | **28** | 2.658 | 0.640 | **28** | 3.398 | 0.615 |
| **29** | 2.642 | 0.684 | **29** | 1.074 | 0.766 | **29** | 6.677 | 0.526 |
| **30** | 1.404 | 0.778 | **30** | 4.286 | 0.651 | **30** | 3.709 | 0.521 |
| **31** | 1.162 | 0.803 | **31** | 1.928 | 0.757 | **31** | 4.551 | 0.301 |
| **32** | 0.923 | 0.896 | **32** | 2.988 | 0.687 | **32** | 1.013 | 0.874 |
| **33** | 1.248 | 0.822 | **33** | 3.303 | 0.721 | **33** | 1.284 | 0.607 |
| **34** | 1.245 | 0.732 | **34** | 2.849 | 0.636 | **34** | 3.222 | 0.478 |
| **35** | 0.966 | 0.872 | **35** | 1.326 | 0.794 | **35** | 2.976 | 0.744 |
| **36** | 1.378 | 0.829 | **36** | 3.954 | 0.455 | **36** | 3.451 | 0.722 |
| **37** | 2.211 | 0.777 | **37** | 2.154 | 0.626 | **37** | 2.697 | 0.621 |
| **38** | 1.437 | 0.868 | **38** | 1.848 | 0.815 | **38** | 3.926 | 0.337 |
| **39** | 2.166 | 0.712 | **39** | 2.691 | 0.689 | **39** | 3.549 | 0.550 |
| **40** | 1.858 | 0.811 | **40** | 1.285 | 0.893 | **40** | 3.319 | 0.712 |
| **41** | 2.096 | 0.811 | **41** | 2.366 | 0.507 | **41** | 4.437 | 0.457 |
| **42** | 1.087 | 0.873 | **42** | 2.819 | 0.799 | **42** | 2.037 | 0.776 |
| **43** | 0.261 | 0.905 | **43** | 3.452 | 0.750 | **43** | 1.927 | 0.512 |
| **44** | 2.068 | 0.774 | **44** | 1.189 | 0.811 | **44** | 3.298 | 0.671 |
| **45** | 1.867 | 0.793 | **45** | 5.388 | 0.516 | **45** | 9.745 | 0.297 |
| **46** | 0.992 | 0.778 | **46** | 4.972 | 0.627 | **46** | 3.164 | 0.537 |
| **47** | 1.731 | 0.760 | **47** | 2.647 | 0.693 | **47** | 3.998 | 0.656 |
| **48** | 1.422 | 0.705 | **48** | 2.657 | 0.744 | **48** | 2.658 | 0.745 |
| **49** | 1.637 | 0.764 | **49** | 2.293 | 0.568 | **49** | 1.320 | 0.733 |
| **50** | 1.865 | 0.743 | **50** | 1.010 | 0.805 | **50** | 2.599 | 0.667 |
| **51** | 1.781 | 0.629 | **51** | 2.575 | 0.706 | **51** | 2.795 | 0.514 |
| **52** | 1.363 | 0.849 | **52** | 2.354 | 0.507 | **52** | 2.848 | 0.628 |
| **53** | 1.615 | 0.641 | **53** | 3.298 | 0.524 | **53** | 4.263 | 0.700 |
| **54** | 1.190 | 0.696 | **54** | 3.110 | 0.694 | **54** | 2.243 | 0.851 |
| **55** | 2.097 | 0.773 | **55** | 2.684 | 0.638 | **55** | 2.801 | 0.634 |
| **56** | 1.662 | 0.805 | **56** | 1.061 | 0.783 | **56** | 4.350 | 0.685 |
| **57** | 1.723 | 0.691 | **57** | 1.493 | 0.709 | **57** | 3.547 | 0.622 |
| **58** | 2.281 | 0.751 | **58** | 5.617 | 0.558 | **58** | 5.448 | 0.545 |
| **59** | 1.535 | 0.886 | **59** | 3.122 | 0.804 | **59** | 1.857 | 0.770 |
| **60** | 2.100 | 0.743 | **60** | 3.455 | 0.788 | **60** | 3.429 | 0.684 |
| **61** | 1.353 | 0.838 | **61** | 2.393 | 0.693 | **61** | 6.167 | 0.502 |
| **62** | 0.901 | 0.794 | **62** | 2.744 | 0.357 | **62** | 2.640 | 0.759 |
| **63** | 1.752 | 0.716 | **63** | 2.314 | 0.710 | **63** | 4.374 | 0.436 |
| **64** | 3.137 | 0.690 | **64** | 5.257 | 0.269 | **64** | 3.189 | 0.711 |
| **65** | 1.980 | 0.725 | **65** | 2.002 | 0.836 | **65** | 3.395 | 0.653 |
| **66** | 3.613 | 0.829 | **66** | 1.309 | 0.805 | **66** | 2.844 | 0.641 |
| **67** | 1.888 | 0.856 | **67** | 1.144 | 0.696 | **67** | 5.661 | 0.583 |
| **68** | 1.543 | 0.781 | **68** | 2.987 | 0.779 | **68** | 4.205 | 0.396 |
| **69** | 1.023 | 0.901 | **69** | 2.332 | 0.621 | **69** | 2.996 | 0.475 |
| **70** | 3.735 | 0.730 | **70** | 1.810 | 0.778 | **70** | 3.240 | 0.470 |
| **71** | 1.628 | 0.343 | **71** | 3.761 | 0.619 | **71** | 6.346 | 0.647 |
| **72** | 1.179 | 0.677 | **72** | 3.531 | 0.669 | **72** | 4.198 | 0.447 |
| **73** | 1.941 | 0.849 | **73** | 1.655 | 0.656 | **73** | 17.880 | -0.091 |
| **74** | 1.236 | 0.793 | **74** | 1.695 | 0.732 | **74** | 5.903 | 0.404 |
| **75** | 2.328 | 0.773 | **75** | 3.132 | 0.692 | **75** | 7.409 | 0.178 |
| **76** | 3.118 | 0.793 | **76** | 2.955 | 0.639 | **76** | 5.447 | 0.585 |
| **77** | 0.846 | 0.726 | **77** | 3.697 | 0.680 | **77** | 8.661 | 0.008 |
| **78** | 1.443 | 0.665 | **78** | 2.156 | 0.727 | **78** | 6.148 | 0.313 |
| **79** | 2.082 | 0.802 | **79** | 2.312 | 0.799 | **79** | 2.506 | 0.700 |
| **80** | 3.055 | 0.831 | **80** | 3.844 | 0.648 | **80** | 2.852 | 0.552 |
| **81** | 1.579 | 0.818 | **81** | 2.701 | 0.708 | **81** | 9.658 | 0.276 |
| **82** | 1.874 | 0.832 | **82** | 2.469 | 0.422 | **82** | 3.357 | 0.419 |
| **83** | 1.536 | 0.559 | **83** | 2.022 | 0.585 | **83** | 3.127 | 0.552 |
| **84** | 1.226 | 0.677 | **84** | 2.507 | 0.655 | **84** | 1.932 | 0.626 |
| **85** | 1.010 | 0.813 | **85** | 2.622 | 0.760 | **85** | 3.344 | 0.527 |
| **86** | 1.475 | 0.902 | **86** | 1.980 | 0.465 | **86** | 2.159 | 0.427 |
| **87** | 1.551 | 0.871 | **87** | 1.959 | 0.856 | **87** | 2.867 | 0.401 |
| **88** | 2.339 | 0.700 | **88** | 3.176 | 0.062 | **88** | 4.550 | 0.551 |
| **89** | 2.222 | 0.762 | **89** | 3.520 | 0.654 | **89** | 2.953 | 0.677 |
| **90** | 1.944 | 0.812 | **90** | 0.954 | 0.890 | **90** | 1.887 | 0.677 |
| **91** | 2.014 | 0.859 | **91** | 2.783 | 0.701 | **91** | 3.522 | 0.721 |
| **92** | 0.996 | 0.649 | **92** | 2.068 | 0.688 | **92** | 10.644 | 0.192 |
| **93** | 1.701 | 0.749 | **93** | 2.979 | 0.652 | **93** | 2.327 | 0.818 |
| **94** | 3.417 | 0.640 | **94** | 1.140 | 0.814 | **94** | 7.593 | 0.509 |
| **95** | 3.086 | 0.583 | **95** | 1.336 | 0.734 | **95** | 4.000 | 0.571 |
| **96** | 2.089 | 0.725 | **96** | 2.492 | 0.695 | **96** | 3.187 | 0.663 |
| **97** | 1.138 | 0.894 | **97** | 2.183 | 0.810 | **97** | 5.404 | 0.477 |
| **98** | 1.355 | 0.888 | **98** | 2.304 | 0.686 | **98** | 3.838 | 0.656 |
| **99** | 1.231 | 0.704 | **99** | 4.563 | 0.681 | **99** | 6.992 | 0.447 |
| **100** | 1.551 | 0.868 | **100** | 3.385 | 0.348 | **100** | 1.691 | 0.651 |

Table S3: MSPE and external validation *q*2 values from individual splits in the 95 amines data

|  |  |  |
| --- | --- | --- |
| **Split no.** | **MSPE** | ***q*2** |
| **1** | 0.932 | 0.754 |
| **2** | 1.037 | 0.611 |
| **3** | 1.198 | 0.705 |
| **4** | 1.877 | 0.648 |
| **5** | 0.844 | 0.857 |
| **6** | 0.524 | 0.868 |
| **7** | 0.858 | 0.794 |
| **8** | 0.820 | 0.478 |
| **9** | 0.412 | 0.793 |
| **10** | 0.893 | 0.754 |
| **11** | 0.549 | 0.826 |
| **12** | 0.807 | 0.712 |
| **13** | 1.169 | 0.772 |
| **14** | 0.341 | 0.944 |
| **15** | 1.289 | 0.718 |
| **16** | 1.146 | 0.753 |
| **17** | 1.152 | 0.712 |
| **18** | 1.542 | 0.562 |
| **19** | 1.293 | 0.465 |
| **20** | 0.983 | 0.691 |
| **21** | 1.104 | 0.387 |
| **22** | 0.860 | 0.833 |
| **23** | 0.918 | 0.152 |
| **24** | 1.592 | 0.706 |
| **25** | 0.656 | 0.871 |
| **26** | 0.943 | 0.604 |
| **27** | 0.583 | 0.841 |
| **28** | 1.789 | 0.558 |
| **29** | 0.526 | 0.869 |
| **30** | 1.636 | 0.678 |
| **31** | 0.400 | 0.795 |
| **32** | 1.239 | 0.712 |
| **33** | 0.653 | 0.799 |
| **34** | 1.171 | 0.664 |
| **35** | 0.467 | 0.903 |
| **36** | 0.640 | 0.887 |
| **37** | 1.286 | 0.666 |
| **38** | 0.882 | 0.788 |
| **39** | 1.361 | 0.395 |
| **40** | 0.777 | 0.740 |
| **41** | 1.362 | 0.630 |
| **42** | 0.656 | 0.652 |
| **43** | 1.002 | 0.726 |
| **44** | 0.988 | 0.735 |
| **45** | 0.846 | 0.717 |
| **46** | 0.854 | 0.748 |
| **47** | 1.406 | 0.716 |
| **48** | 0.553 | 0.733 |
| **49** | 1.271 | 0.649 |
| **50** | 1.864 | 0.605 |
| **51** | 2.010 | 0.593 |
| **52** | 0.346 | 0.906 |
| **53** | 0.960 | 0.703 |
| **54** | 1.327 | 0.647 |
| **55** | 0.764 | 0.835 |
| **56** | 0.274 | 0.900 |
| **57** | 0.876 | 0.763 |
| **58** | 1.700 | 0.658 |
| **59** | 1.280 | 0.331 |
| **60** | 0.875 | 0.732 |
| **61** | 0.324 | 0.832 |
| **62** | 0.392 | 0.700 |
| **63** | 0.581 | 0.856 |
| **64** | 0.572 | 0.808 |
| **65** | 0.457 | 0.882 |
| **66** | 0.623 | 0.867 |
| **67** | 0.344 | 0.884 |
| **68** | 0.465 | 0.848 |
| **69** | 0.568 | 0.840 |
| **70** | 0.595 | 0.824 |
| **71** | 1.496 | 0.437 |
| **72** | 0.777 | 0.699 |
| **73** | 0.587 | 0.675 |
| **74** | 0.904 | 0.648 |
| **75** | 1.172 | 0.695 |
| **76** | 0.999 | 0.625 |
| **77** | 0.752 | 0.607 |
| **78** | 0.518 | 0.869 |
| **79** | 1.499 | 0.793 |
| **80** | 1.140 | 0.608 |
| **81** | 0.603 | 0.878 |
| **82** | 0.831 | 0.745 |
| **83** | 1.271 | 0.627 |
| **84** | 0.615 | 0.769 |
| **85** | 1.368 | 0.492 |
| **86** | 1.434 | -0.003 |
| **87** | 0.502 | 0.753 |
| **88** | 1.547 | 0.749 |
| **89** | 0.633 | 0.871 |
| **90** | 1.577 | 0.682 |
| **91** | 1.507 | 0.647 |
| **92** | 1.455 | 0.742 |
| **93** | 1.243 | 0.723 |
| **94** | 0.844 | 0.774 |
| **95** | 1.513 | 0.535 |
| **96** | 0.718 | 0.872 |
| **97** | 1.129 | 0.781 |
| **98** | 1.693 | 0.609 |
| **99** | 0.778 | 0.744 |
| **100** | 0.269 | 0.924 |