**Table S1.** Experimental and estimated HHVs obtained for each ML(N)R and ANN model using mixture samples.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **Type of equation** | **Equation** | **Ref** | **Estimation HHV** | **Experimental HHV** | **Relative error %** |
| S1 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 21.092 | 20.713 | 1.83 |
| S1 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.153 | 20.713 | 2.12 |
| S1 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 20.164 | 20.713 | 2.65 |
| S1 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 20.928 | 20.713 | 1.04 |
| S1 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 20.399 | 20.713 | 1.52 |
| S1 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 20.471 | 20.713 | 1.17 |
| S1 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 20.499 | 20.713 | 1.03 |
| S2 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 21.407 | 21.963 | 2.53 |
| S2 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.218 | 21.963 | 3.39 |
| S2 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 20.656 | 21.963 | 5.95 |
| S2 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 21.620 | 21.963 | 1.56 |
| S2 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 20.905 | 21.963 | 4.82 |
| S2 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 21.262 | 21.963 | 3.19 |
| S2 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 22.199 | 21.963 | 1.07 |
| S3 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 21.522 | 22.663 | 5.03 |
| S3 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.285 | 22.663 | 6.08 |
| S3 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 21.149 | 22.663 | 6.68 |
| S3 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 22.330 | 22.663 | 1.47 |
| S3 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 20.484 | 22.663 | 9.61 |
| S3 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 21.180 | 22.663 | 6.34 |
| S3 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 25.269 | 22.663 | 11.49 |
| S4 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 21.437 | 22.816 | 6.04 |
| S4 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.349 | 22.816 | 6.43 |
| S4 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 21.639 | 22.816 | 5.16 |
| S4 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 23.003 | 22.816 | 0.82 |
| S4 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 19.239 | 22.816 | 15.68 |
| S4 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 20.110 | 22.816 | 11.86 |
| S4 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 31.074 | 22.816 | 36.19 |
| S5 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 21.153 | 23.162 | 8.67 |
| S5 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.418 | 23.162 | 7.53 |
| S5 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 22.133 | 23.162 | 4.44 |
| S5 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 23.681 | 23.162 | 2.24 |
| S5 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 17.291 | 23.162 | 25.35 |
| S5 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 17.958 | 23.162 | 22.47 |
| S5 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 40.952 | 23.162 | 76.80 |
| S6 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 20.667 | 24.520 | 15.71 |
| S6 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.467 | 24.520 | 12.45 |
| S6 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 22.615 | 24.520 | 7.76 |
| S6 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 24.320 | 24.520 | 0.82 |
| S6 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 14.701 | 24.520 | 40.04 |
| S6 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 14.538 | 24.520 | 40.71 |
|  | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 56.411 | 24.520 | 130.06 |
| S7 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 19.989 | 25.326 | 21.07 |
| S7 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.635 | 25.326 | 14.57 |
| S7 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 23.169 | 25.326 | 8.51 |
| S7 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 25.405 | 25.326 | 0.31 |
| S7 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 11.890 | 25.326 | 53.05 |
| S7 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 10.372 | 25.326 | 59.04 |
| S7 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 77.526 | 25.326 | 206.1 |
| S8 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 20.208 | 26.120 | 22.63 |
| S8 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.640 | 26.120 | 17.15 |
| S8 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 23.624 | 26.120 | 9.55 |
| S8 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 25.880 | 26.120 | 0.92 |
| S8 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 8.323 | 26.120 | 68.13 |
| S8 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | 4.023 | 26.120 | 84.59 |
| S8 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 108.395 | 26.120 | 314.99 |
| S9 | MNLR | HHV=20.137+0.008L+0.131E-0.004E2 | Rhen2004 | 18.014 | 26.378 | 31.70 |
| S9 | MLR1 | HHV=14.3377+0.1228L+0.1353E | MLR23,2011 | 21.681 | 26.378 | 17.81 |
| S9 | MLR2 | HHV=15.605+0.074L+0.172E | MLR3 | 24.101 | 26.378 | 8.63 |
| S9 | MLR3 | HHV=-28.179+0.880L+1.019E | This study | 26.486 | 26.378 | 0.41 |
| S9 | ANN1 | HHV=17.0000+0.0337689[L]-0.370197[E]+0.0217811[EL]-0.0001237[EL2]-0.00026906[LE2] | MLR3 | 4,554 | 26.378 | 82.73 |
| S9 | ANN2 | HHV=18.9886-0.0821496[L]-0.788837[E]+0.047379[LE]-0.00044862[EL2]-0.000301034[LE2]+0.00146961[L2] | MLR3 | -3,744 | 26.378 | 114.19 |
| S9 | ANN3 | HHV=20.7165-0.141898[L]-1.78999[E]+0.0763139[LE]-0.0006305[EL2]-0.00244972[LE2]+0.00194996[L2]+0.112698[E2] | MLR3 | 148,569 | 26.378 | 463.23 |