Table S11: Scaled residuals from MCR-ALS model

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Al | Ba | Ca | Mg | Sr | Co | Cr | Cu | Fe | Ga | Zn | K | Li | Mn | Na | Ni | Pb | Rb |
| 1 | -0.18832 | 0.511374 | -1.43609 | 0.360577 | -3.67788 | -0.15338 | -0.00152 | -0.19113 | -0.32141 | 0.071646 | -1.7575 | 0.325164 | 0.028729 | -0.5353 | 0.624882 | -0.05969 | -0.76266 | 0.209193 |
| 2 | -0.09942 | 0.552478 | -0.82831 | 0.371556 | -3.94262 | -0.01754 | -0.00032 | -0.15088 | -0.25105 | 0.065619 | -1.51058 | 0.306527 | 0.000858 | -0.18967 | 0.639988 | -0.03622 | -0.37064 | -0.17652 |
| 3 | -0.12971 | 0.6578 | -0.3668 | 0.300335 | -3.80379 | -0.02187 | -0.00444 | -0.17346 | -0.29957 | 0.002524 | 1.616089 | -0.00581 | 0.013384 | -0.20994 | 0.459566 | -0.04635 | -0.37773 | 0.112501 |
| 4 | -0.08452 | -0.11102 | -0.72613 | 0.117459 | -0.37813 | -0.06636 | 0.016921 | -0.10986 | -0.37821 | 0.092778 | -4.30462 | 0.43005 | -0.0052 | -0.38482 | 0.281389 | -0.02897 | -0.32538 | 0.076022 |
| 5 | -0.08676 | 0.429765 | -1.11878 | 0.345213 | -3.38835 | -0.01075 | 0.000492 | -0.11245 | -0.27 | 0.081787 | -2.51407 | 0.382512 | -0.00756 | -0.35578 | 0.617303 | -0.02999 | -0.41115 | 0.039019 |
| 6 | -0.22763 | -0.31286 | -1.36981 | -0.00922 | 1.089272 | 0.260896 | 0.001069 | -0.32034 | -0.52433 | 0.074542 | -3.92961 | 0.355209 | 0.027519 | -0.55185 | 0.070534 | -0.09351 | -0.002 | 0.143607 |
| 7 | -0.10611 | 0.620232 | -1.65675 | 0.351803 | -3.92592 | -0.18809 | -0.00268 | -0.18599 | -0.45663 | 0.03813 | -0.07393 | 0.191468 | -0.01119 | -0.49395 | 0.583384 | 0.010844 | 0.090953 | -0.21969 |
| 8 | -0.12994 | 0.369054 | -0.02435 | 0.322974 | -3.16567 | 0.017574 | -0.00055 | -0.19179 | -0.12233 | 0.084964 | -2.8957 | 0.385798 | 0.015913 | -0.06241 | 0.592535 | -0.0584 | 0.20729 | -0.25406 |
| 9 | -0.19588 | -0.33525 | -1.36256 | -0.26916 | 2.905676 | -0.27395 | 0.002874 | -0.39081 | -0.94733 | -0.05268 | 2.132202 | -0.26293 | -0.00718 | -0.89464 | -0.48468 | -0.15853 | -0.53018 | -0.76916 |
| 10 | -0.08489 | 0.369365 | -0.36607 | 0.321979 | -3.13568 | -0.01444 | 0.007061 | 0.098382 | 0.468532 | 0.083005 | -2.85183 | 0.386939 | -0.00141 | -0.02165 | 0.583076 | -0.03907 | -0.13808 | -0.36497 |
| 11 | -0.07368 | 0.360497 | -0.40181 | 0.32004 | -3.12193 | 0.012137 | 0.010327 | 0.114026 | 0.207078 | 0.080702 | -2.87046 | 0.394567 | -0.00905 | 0.273514 | 0.579607 | 0.048443 | -0.39297 | -0.20112 |
| 12 | -0.04678 | 0.089862 | -0.38857 | 0.207393 | -1.66297 | 0.126623 | 0.018842 | 0.132421 | 0.218329 | 0.079057 | -3.75086 | 0.427435 | -0.00567 | 1.010481 | 0.413732 | 0.060742 | -0.20054 | 0.105409 |
| 13 | 0.030742 | 0.328956 | -1.11147 | 0.311877 | -2.87298 | -0.15564 | -0.00297 | -0.09535 | -0.04366 | 0.089553 | -3.05357 | 0.41242 | -0.01782 | -0.43202 | 0.567171 | -0.01411 | -0.95405 | 0.092078 |
| 14 | -0.00046 | 0.070982 | 0.118879 | -0.13655 | 0.679375 | 0.021221 | 0.00071 | 0.011063 | 0.064734 | -0.09213 | 4.279832 | -0.42435 | 0.001183 | 0.084424 | -0.31048 | 4.17E-05 | 0.18673 | -0.00917 |
| 15 | -0.01451 | 0.475232 | -0.62912 | 0.120103 | -2.0946 | -0.05523 | 0.006839 | -0.00684 | -0.21865 | -0.05285 | 3.57118 | -0.24021 | 0.00342 | -0.04964 | 0.123005 | -0.02591 | -0.31958 | 0.146839 |
| 16 | 0.028411 | -0.63771 | -0.22628 | -0.35238 | 4.153996 | 0.125966 | -0.00148 | -0.01114 | -0.07295 | -0.03316 | -0.01141 | -0.1429 | -0.00017 | -0.07443 | -0.579 | -0.00996 | -0.12566 | 0.052985 |
| 17 | -0.04354 | -0.244 | 3.853336 | -0.18732 | 1.677484 | -0.04621 | -0.00705 | -0.18268 | -0.16225 | -0.02643 | 0.973528 | -0.25638 | 0.00448 | -0.25845 | -0.32958 | -0.05573 | -0.32208 | 0.131337 |
| 18 | -0.00681 | -0.51045 | 2.562421 | -0.31945 | 3.379137 | 0.017694 | 0.000107 | -0.08393 | -0.06151 | -0.03859 | 0.69366 | -0.25524 | 0.003336 | -0.05153 | -0.53999 | -0.02533 | -0.15193 | 0.102693 |
| 19 | -0.0287 | 0.443279 | -3.15366 | 0.289567 | -2.92054 | 0.066014 | -0.00415 | 0.013235 | 0.085626 | 0.041777 | -0.83681 | 0.263576 | 0.011002 | -0.30886 | 0.490318 | -0.00542 | -0.31986 | -0.1121 |
| 20 | 0.042962 | -0.6555 | -0.33703 | -0.33732 | 4.097656 | 0.027512 | 0.009474 | 0.01013 | 0.03797 | -0.02336 | -0.6019 | -0.07966 | -0.0047 | 0.203003 | -0.54291 | 0.00634 | -0.06246 | -0.06486 |
| 21 | 0.020764 | -0.60798 | 0.580381 | -0.36286 | 4.021139 | 0.084322 | 0.015446 | 0.202323 | 0.041528 | -0.05343 | 0.571771 | -0.20663 | 0.003039 | 0.649257 | -0.59811 | 0.025069 | 1.226852 | -0.0514 |
| 22 | 0.145326 | -0.253 | -2.20512 | 0.008659 | 0.764845 | -0.03991 | 0.050638 | 0.37781 | 0.302888 | 0.052332 | -3.44961 | 0.361056 | -0.01525 | 0.553821 | 0.087158 | 0.088476 | 0.527278 | -0.23568 |
| 23 | 0.22079 | -0.53044 | -2.31747 | -0.24768 | 3.257874 | 0.182083 | 0.020716 | 0.321462 | 0.247866 | -0.01599 | -0.93967 | 0.038706 | -0.03307 | 0.591135 | -0.3887 | 0.048337 | 0.212249 | -0.09976 |
| 24 | 0.096639 | -0.31901 | -0.07253 | -0.05081 | 1.210873 | -0.17813 | -0.01654 | 0.407477 | -0.00319 | 0.043039 | -3.15999 | 0.250862 | 0.013549 | 0.34232 | 0.001196 | 0.09106 | 2.469967 | -0.05878 |
| 25 | -0.02583 | 0.625752 | -0.56581 | 0.369618 | -4.15663 | -0.09735 | -0.00764 | -0.07161 | -0.10029 | 0.046449 | -0.50505 | 0.209898 | -0.00391 | -0.22669 | 0.616505 | -0.00279 | -0.22333 | 0.017858 |
| 26 | 0.045008 | 0.251101 | 2.718102 | 0.153968 | -1.97693 | -0.09944 | -0.00792 | 0.273153 | 0.155271 | 0.018945 | -0.64815 | 0.063151 | 0.001905 | 0.531572 | 0.286385 | 0.073476 | 2.588492 | -0.15738 |
| 27 | 0.144096 | 0.552753 | -1.41039 | 0.232454 | -3.04939 | -0.17235 | -0.00437 | 0.589483 | 0.914405 | -0.02414 | 1.869907 | -0.0262 | -0.01413 | 0.313107 | 0.34881 | 0.165672 | 1.22109 | -0.11481 |
| 28 | 0.309195 | 0.347984 | -1.12879 | 0.065578 | -1.42821 | -0.16436 | -0.012 | 0.841636 | 1.21641 | -0.06949 | 3.130741 | -0.20901 | 0.013116 | 0.859775 | 0.051626 | 0.179713 | 1.894518 | 0.050788 |
| 29 | 0.096781 | 0.45701 | -0.77684 | 0.33298 | -3.48378 | -0.04287 | -0.00047 | 0.469578 | 0.679232 | 0.056378 | -1.87397 | 0.316067 | -0.00153 | 0.528187 | 0.582451 | 0.108057 | 0.157975 | 0.436339 |
| 30 | 0.378165 | 0.102747 | -1.50695 | 0.193839 | -1.54905 | -0.15721 | -0.03258 | 0.614101 | 0.963011 | 0.061363 | -3.16374 | 0.397192 | -0.00975 | 1.239619 | 0.371505 | 0.228088 | -0.32774 | 0.174574 |
| 31 | 0.38137 | 0.315907 | -2.05861 | 0.250445 | -2.45138 | -0.05703 | -0.00893 | 0.63727 | 1.805433 | 0.042402 | -1.67798 | 0.300534 | -0.02777 | 0.695294 | 0.427988 | 0.186966 | -0.59586 | -0.20333 |
| 32 | 0.244759 | -0.35369 | 0.079329 | -0.21844 | 2.342333 | -0.03928 | -0.01974 | 0.447918 | 1.123569 | -0.04992 | 0.396838 | -0.12751 | 0.019542 | 1.128019 | -0.34363 | 0.103128 | 3.646423 | 0.228893 |
| 33 | 0.477021 | -0.62732 | -0.31695 | -0.32911 | 4.025678 | -0.14612 | -0.03548 | 0.005183 | 0.298612 | -0.01754 | -0.52486 | -0.09489 | -0.0014 | -0.38473 | -0.53124 | 0.134355 | 0.563136 | -0.27509 |
| 34 | -0.04769 | 0.542358 | -1.4098 | 0.356407 | -3.812 | -0.15059 | 0.00131 | -0.02226 | -0.36863 | 0.052599 | -1.20432 | 0.293004 | 0.01495 | 0.513112 | 0.609907 | -0.0096 | -0.10705 | -0.07661 |
| 35 | 0.154124 | 0.397504 | -0.65452 | 0.333738 | -3.2764 | -0.0116 | -0.01533 | 0.086038 | -0.0398 | 0.08155 | -2.70369 | 0.387258 | -0.00423 | -0.11398 | 0.600914 | 0.031164 | -0.23754 | 0.028708 |
| 36 | 0.067528 | -0.43558 | 3.114718 | -0.28226 | 2.89523 | 0.274191 | -0.02293 | -0.05266 | 0.226369 | -0.03321 | 0.734149 | -0.25992 | 0.003907 | -0.26468 | -0.48315 | -0.02735 | -0.33968 | 0.141343 |
| 37 | -0.15233 | 0.276566 | -2.24643 | 0.248468 | -2.05137 | -0.28144 | -0.04389 | -0.2689 | -0.43354 | 0.089634 | -2.26106 | 0.313952 | 0.00627 | -2.73199 | 0.448636 | 0.008592 | -1.19149 | -0.21433 |
| 38 | -0.02696 | -0.11961 | -0.77299 | -0.20617 | 1.847037 | 0.075211 | -0.02717 | -0.20232 | -0.30287 | -0.07075 | 3.413501 | -0.38133 | 0.021489 | -1.27535 | -0.4089 | -0.0523 | -0.44661 | 0.319091 |
| 39 | -0.06484 | 0.206974 | -1.35415 | 0.262737 | -2.22069 | -0.02205 | 0.016599 | 0.019712 | 0.021787 | 0.087147 | -3.45579 | 0.436512 | -0.02101 | -0.23862 | 0.496166 | 0.010115 | -1.00945 | 0.246657 |
| 40 | -0.41803 | -0.18809 | -1.70934 | -0.20959 | 1.985725 | 0.366206 | 0.01689 | -0.06871 | -0.30594 | -0.076 | 2.830225 | -0.27293 | -0.02725 | 0.674448 | -0.40997 | -0.05451 | -1.36771 | -0.27216 |
| 41 | -0.02565 | -0.59728 | 0.557658 | -0.36438 | 3.999267 | 0.088149 | 0.015943 | 0.205642 | 0.067469 | -0.05742 | 0.756484 | -0.22297 | 0.003697 | 0.691094 | -0.6041 | 0.024723 | 1.227727 | -0.03154 |
| 42 | -0.09919 | 0.337403 | -0.5937 | 0.025254 | -1.0904 | -0.17872 | 0.003521 | -0.06277 | -0.21405 | -0.07345 | 3.974897 | -0.31907 | -0.01821 | -0.06957 | -0.02987 | 0.023311 | 0.801439 | 0.348452 |
| 43 | 0.067275 | -0.5934 | 0.226472 | -0.37209 | 4.072593 | 0.060988 | 0.030557 | 0.17743 | 0.151149 | -0.06099 | 1.063323 | -0.24496 | 0.01006 | 0.690607 | -0.63415 | 0.041748 | 0.070167 | 0.029048 |
| 44 | 0.128009 | 0.0214 | -0.76416 | -0.14707 | 0.858323 | 0.172754 | 0.029571 | 0.406595 | 0.725256 | -0.10155 | 3.958949 | -0.35874 | -0.01323 | 0.974271 | -0.31866 | 0.066145 | 0.913963 | -0.50036 |
| 45 | 0.436519 | -0.15778 | -0.48876 | -0.23507 | 2.11152 | -0.16099 | -0.03896 | -0.18047 | 0.778841 | -0.07943 | 3.521698 | -0.40591 | 0.007921 | -0.64782 | -0.46563 | 0.033825 | 0.077285 | -0.14387 |
| 46 | 0.135899 | 0.566865 | -0.69781 | 0.318583 | -3.7543 | 0.002847 | 0.001238 | 0.333435 | 0.603006 | 0.016956 | 0.004579 | 0.162138 | 0.018442 | 1.476324 | 0.517481 | 0.053345 | 0.061514 | 0.146048 |
| 47 | 0.077867 | 0.044969 | -1.92466 | 0.185318 | -1.2009 | -0.00284 | 0.01136 | -0.00473 | 0.249458 | 0.085677 | -3.72956 | 0.447556 | -0.02225 | -0.34484 | 0.37182 | 0.015621 | -1.03499 | -0.34697 |
| 48 | 0.075009 | -0.58854 | 0.3631 | -0.36677 | 4.012641 | 0.05479 | 0.003038 | 0.094494 | 0.578697 | -0.06076 | 0.924407 | -0.23697 | 0.001152 | 0.727038 | -0.61672 | 0.005657 | 1.028329 | -0.07061 |
| 49 | 0.243829 | -0.58374 | -0.44842 | -0.34393 | 3.869113 | 0.329763 | 0.033876 | 0.277896 | 0.149666 | -0.05301 | 0.606319 | -0.16479 | -0.01971 | 1.473501 | -0.58527 | 0.065455 | -0.29493 | -0.31292 |
| 50 | 0.047385 | -0.64692 | -0.28683 | -0.29015 | 3.786465 | -0.03128 | 0.005839 | -0.05199 | -0.18696 | 0.004487 | -1.64097 | 0.025936 | -0.00578 | -0.16613 | -0.44503 | -0.011 | -0.31418 | -0.16244 |
| 51 | 0.162457 | -0.13973 | -0.8773 | 0.099986 | -0.16341 | 0.032587 | 0.005723 | -0.07773 | -0.38246 | 0.092197 | -4.24312 | 0.425218 | -0.00048 | -0.61136 | 0.247183 | -0.03068 | -0.73598 | -0.06915 |
| 52 | -0.2231 | -0.40765 | 2.853718 | -0.25765 | 2.729887 | 0.260046 | -0.01478 | -0.40365 | -0.39526 | -0.01877 | 0.520692 | -0.23268 | -0.002 | -1.04558 | -0.43481 | -0.12383 | -0.62495 | 0.109651 |