

**Supplementary Table S1. Demographics, clinical and molecular outcomes utilized in this study**

| Subject ID | Diagnosis | Sex    | Age | BMI   | mtDNA CN | mtDNA deletions | L/P   | BCAA/AAA | Ceruloplasmin | Total bilirubin | CysCys/Total Cys | Pyruvic acid | L-Glutamic acid | Oxoglutaric acid |
|------------|-----------|--------|-----|-------|----------|-----------------|-------|----------|---------------|-----------------|------------------|--------------|-----------------|------------------|
| M5No_WD    | Control   | Male   | 32  | -0.6  | 0.3      | 0.67            | 0.37  | 1.29     | 0.98          | -0.45           | -1.76            | -0.33        | -1.73           | -1.55            |
| M1No_WD    | Control   | Male   | 27  | -0.4  | 0.95     | -0.31           | -0.41 | 1.7      | 0.83          | 0.14            | -1.5             | 0.01         | -1.5            | -1.33            |
| M4No_WD    | Control   | Male   | 33  | 0.6   | 1.6      | 0.6             | -1.52 | 1        | 1.7           | 0.38            | 1.08             | 1.64         | -2.09           | -0.33            |
| M3No_WD    | Control   | Male   | 28  | 1.1   | 1.37     | 0.47            | -1.44 | 1.4      | 1.33          | 0.54            | 0.97             | 1.03         | -1.75           | -0.8             |
| M2No_WD    | Control   | Male   | 45  | 1.53  | 0.79     | 0.06            | 0.12  | 1.27     | 1.17          | -1.42           | -1.27            | 0.46         | -0.08           | -0.33            |
| K2No_WD    | Control   | Female | 26  | -1.57 | -0.12    | -0.13           | 0.76  | 0.72     | 1.17          | 0.4             | -1               | -0.36        | -0.68           | -1.21            |
| K3No_WD    | Control   | Female | 49  | 0.55  | 1.54     | -0.25           | 0.54  | 0.93     | 0.53          | 0.33            | -0.7             | -0.23        | -1.19           | -0.93            |
| K9No_WD    | Control   | Female | 52  | -0.03 | 0.49     | -0.94           | -2.04 | -0.31    | 0.22          | -0.15           | -1.18            | 1.55         | -1.14           | -0.37            |
| K7No_WD    | Control   | Female | 34  | -1.31 | 0.38     | -1.51           | 0.96  | 0.78     | 1.56          | -0.83           | 0.38             | -0.8         | -1.95           | -1.25            |
| K5No_WD    | Control   | Female | 30  | -1.56 | 1.29     | -0.53           | -0.28 | 1.19     | 1.14          | -2.68           | -1.24            | -0.45        | -1.9            | -2.1             |
| K8No_WD    | Control   | Female | 27  | -0.96 | -0.63    | -1.18           | 1.11  | 1.54     | 1.24          | 0.29            | -0.5             | -1.59        | -1.94           | -0.55            |
| K10No_WD   | Control   | Female | 52  | -0.51 | 0.71     | 1.09            | -0.19 | 1.42     | 1.45          | -0.2            | -1.39            | 0.92         | -0.33           | -0.77            |
| K6No_WD    | Control   | Female | 38  | -1.62 | 0.98     | -0.58           | -1.48 | 1.41     | 1.06          | -1.08           | -1.09            | 1            | -1.84           | -0.43            |
| K1No_WD    | Control   | Female | 38  | -1.16 | 0.72     | -0.34           | -0.38 | 0.96     | 0.69          | -0.62           | 0.79             | 0.59         | -2.02           | -0.72            |
| K4No_WD    | Control   | Female | 31  | -0.39 | 0.26     | -1.02           | -0.84 | 1.13     | 0.89          | -0.32           | 0.45             | 0.69         | -1.86           | -0.74            |
| 1506WD     | WD        | Male   | 41  | 0.52  | -2.92    | -0.19           | -0.77 | -0.79    | -0.96         | -0.64           | -1.47            | 0.88         | 1.05            | 1.35             |
| 1593WD     | WD        | Male   | 25  | -0.49 | -1.49    | -0.77           | -0.06 | 0.92     | 0.24          | -0.49           | -1.46            | -0.34        | 0.21            | 0.63             |
| 1784WD     | WD        | Male   | 39  | 1.42  | 0.08     | 0.17            | -0.07 | 1.04     | 0             | 0.55            | -2.15            | 1.82         | -0.18           | 0.53             |
| 1986WD     | WD        | Male   | 52  | 0.94  | -0.13    | 1.02            | 0.51  | -0.23    | 0.1           | -0.08           | -0.02            | -0.54        | 0.45            | 0.47             |
| 2486WD     | WD        | Male   | 25  | -0.49 | -0.52    | -0.03           | -0.7  | 0.33     | 1.25          | -0.44           | 0.78             | 0.46         | 1.18            | 2.2              |
| 2251WD     | WD        | Male   | 21  | 1.09  | 0.47     | 1.18            | 0.51  | 0.35     | -0.86         | -0.88           | 0.48             | -0.38        | 0.81            | -1.02            |
| 2055WD     | WD        | Female | 20  | 0.36  | -0.27    | 0.06            | -0.13 | -0.45    | 0.4           | -0.19           | -0.21            | 0.48         | 0.1             | 0.94             |
| 2124WD     | WD        | Female | 52  | -0.4  | -0.24    | 0.43            | -0.81 | 0.19     | 0.42          | -1.07           | 0.69             | 0.33         | 0.27            | 0.04             |
| 2275WD     | WD        | Female | 17  | -0.57 | 0.87     | -0.81           | -1.25 | 0.39     | -0.61         | -0.78           | 0.83             | 0.33         | -0.61           | 0.13             |
| 1715WD     | WD        | Female | 30  | -0.8  | 0.38     | -1.7            | -0.4  | -0.01    | 0.3           | 0.02            | -0.89            | -0.8         | 0.21            | 0.58             |
| 1776WD     | WD        | Female | 39  | 0.29  | -2.43    | -0.66           | 0.29  | 0.29     | 0.08          | 0.34            | 0.44             | -0.51        | 0.26            | -0.12            |
| 2452WD-H   | WDHEP     | Male   | 43  | 1.52  | 0.23     | 1.2             | 0.25  | -1.67    | 0.66          | 1.28            | 1.56             | -0.32        | 1.52            | 2                |
| 1864WD-H   | WDHEP     | Male   | 30  | 0.76  | -0.32    | 1.4             | -0.32 | -1.77    | 0.08          | 0.89            | 0.24             | -0.25        | -0.03           | 0.14             |
| 970WD-H    | WDHEP     | Male   | 36  | -0.6  | -0.55    | -0.1            | 0.58  | 0.79     | -2.59         | -0.78           | 0.63             | 0.11         | 0.68            | 0.54             |
| 2210WD-H   | WDHEP     | Male   | 44  | -1.09 | -0.6     | 0.8             | 2.33  | 0.58     | -1.59         | 1.64            | 0.22             | -2.75        | 0.75            | -1.49            |
| 2481WD-H   | WDHEP     | Male   | 43  | -1.1  | -1.44    | -1.49           | -0.52 | -0.85    | 0.1           | -0.36           | -0.12            | 0.54         | 1.3             | 1.93             |
| 1779WD-H   | WDHEP     | Male   | 29  | 1.31  | -1.38    | -0.8            | 0.11  | -2.51    | -0.33         | 1.98            | 0.98             | 0.14         | 0.54            | 0.66             |
| 2415WD-H   | WDHEP     | Male   | 46  | 0.53  | -1.16    | -0.21           | -1.37 | -1.58    | 0.46          | 2.66            | 1.69             | 1.24         | 0.77            | 1.42             |
| 1780WD-H   | WDHEP     | Female | 23  | 0.38  | -0.31    | -1.73           | -0.27 | -1.56    | 0.27          | -0.19           | 0.4              | -0.04        | 0.93            | 0.95             |
| 1866WD-H   | WDHEP     | Female | 24  | 0.39  | -0.63    | 0.89            | -0.38 | -1.81    | 0.43          | 1.9             | 1.91             | 0.86         | 1.54            | 1.79             |
| 1658WD-H   | WDHEP     | Female | 43  | -0.62 | -2.17    | -0.93           | 0.94  | -1.55    | 0.22          | 1.98            | 1.39             | -1.09        | 0.43            | -0.42            |
| 1868WD-H   | WDHEP     | Female | 45  | 1.51  | 0.34     | 1               | 1.16  | 0.43     | 0.39          | 0.02            | -0.42            | -0.87        | -0.45           | -0.37            |

|          |       |        |    |       |       |       |       |       |       |       |       |       |       |       |
|----------|-------|--------|----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1639WD-H | WDHEP | Female | 19 | 0.68  | 0.91  | 1.18  | 2.31  | -1.89 | -0.58 | 1.27  | 0.78  | -2.96 | 1.36  | -1.96 |
| 2065WD-H | WDHEP | Female | 20 | -0.6  | 0.6   | 0.54  | 0.75  | -0.39 | 0.04  | 0.68  | 1.13  | -0.1  | 0.76  | 1.68  |
| 2438WD-H | WDHEP | Female | 19 | -0.24 | 0.44  | -3.36 | -0.53 | 0.29  | -0.03 | -2.09 | -1.05 | 1.94  | 0.45  | 2     |
| 2086WD-H | WDHEP | Female | 32 | -0.39 | -0.2  | 1.27  | 0.3   | 0.41  | -0.7  | 0.02  | -0.08 | -0.48 | 0.86  | 0.64  |
| 972WD-H  | WDHEP | Female | 18 | 0.86  | -1.09 | -0.2  | 0.72  | -0.01 | -2.05 | -0.68 | -0.8  | 0.5   | 1.3   | -0.86 |
| 1843WD-H | WDHEP | Female | 31 | 0.44  | -0.88 | -0.31 | 0.23  | -0.6  | 0.18  | -0.11 | -0.53 | 0.23  | 0.33  | -0.17 |
| 2051WD-H | WDHEP | Female | 56 | -0.83 | 1.3   | 0.67  | 1.12  | 0.38  | 0.61  | -0.05 | -1.01 | -1.04 | 0.82  | 0.05  |
| 1982WD-N | WDNEU | Male   | 34 | 0.73  | -0.16 | 0.69  | 1.97  | -0.19 | -0.51 | 0.11  | -0.26 | -2.08 | 0.63  | -0.76 |
| 2123WD-N | WDNEU | Male   | 24 | -1.37 | 0.41  | -1.03 | -1.05 | -0.04 | -1.13 | -0.41 | -0.02 | 0.85  | -0.34 | 0.32  |
| 2245WD-N | WDNEU | Male   | 23 | 2.4   | -0.59 | 0.51  | 1.86  | 0.52  | -0.49 | 0.85  | 0.21  | -1.28 | 0.9   | 0.91  |
| 2309WD-N | WDNEU | Male   | 44 | -0.18 | -1.29 | 0.33  | -0.28 | -0.84 | 0.23  | -0.3  | 0.99  | -0.48 | 0.7   | -1.26 |
| 2506WD-N | WDNEU | Male   | 52 | -0.36 | -0.19 | 0.24  | -1.67 | -0.75 | -0.18 | 0.35  | 1.04  | 0.85  | 0.11  | 0.7   |
| 2534WD-N | WDNEU | Male   | 21 | 0.94  | -0.02 | 0.4   | -0.92 | -0.5  | -0.42 | -0.49 | 0.85  | 1.05  | 0.3   | 1     |
| 2291WD-N | WDNEU | Male   | 36 | -0.2  | 0.28  | 0.21  | 0.71  | -0.1  | 0.03  | -0.48 | -0.08 | -0.37 | 0.48  | 0.06  |
| 205WD-N  | WDNEU | Male   | 44 | -1.43 | 0.14  | 0.73  | -1.03 | 0.48  | -1.71 | -0.71 | 0.74  | 0.98  | 0.02  | 0.26  |
| 1167WD-N | WDNEU | Male   | 28 | -1.22 | -0.63 | 0.87  | 1.79  | 0.12  | -1.43 | 1.01  | -0.77 | -1.62 | 0.58  | -0.79 |
| 1998WD-N | WDNEU | Male   | 27 | -1.17 | 1.04  | 0.35  | 0.52  | 0.49  | -2.79 | 1.49  | 0.67  | 0.13  | 0.06  | -0.82 |
| 2024WD-N | WDNEU | Male   | 52 | 2.84  | 1.78  | 1.26  | 1.45  | -0.2  | -0.14 | 0.06  | -0.22 | -1.2  | 0.88  | -0.01 |
| 1116WD-N | WDNEU | Female | 25 | 1.25  | -0.18 | 1.75  | -0.58 | -0.4  | -2.61 | 0.42  | 1.03  | 0.46  | 0.13  | -0.52 |
| 2001WD-N | WDNEU | Female | 44 | 0.2   | -1.01 | 0.12  | 0.04  | -1.17 | -0.2  | 0.66  | -0.06 | -0.23 | -0.24 | 0.05  |
| 2354WD-N | WDNEU | Female | 32 | 0.71  | -0.4  | -1.46 | 0.3   | 0.06  | -0.06 | -1.67 | 0.1   | -0.03 | -0.27 | 0.07  |
| 2243WD-N | WDNEU | Female | 46 | -0.32 | 0.56  | -0.56 | -1.24 | -0.12 | -0.34 | 0.17  | -2.38 | 0.9   | 0.02  | -0.32 |
| 2301WD-N | WDNEU | Female | 33 | -0.53 | 1.4   | -1.7  | -1.37 | -0.48 | -0.22 | -1.98 | 0.22  | 0.73  | 0.23  | 0.49  |
| 2508WD-N | WDNEU | Female | 23 | -0.35 | -0.32 | 1.61  | -0.23 | -0.2  | 0.15  | -0.41 | 0.62  | 0.17  | -0.09 | 0.01  |
| 1783WD-N | WDNEU | Female | 46 | -0.38 | 1.67  | 1.05  | -0.08 | -1.79 | -0.08 | 0.57  | 1.35  | -0.36 | 0.28  | -0.23 |

| Glycine | L-Alanine | Succinic acid | L-Lysine | L-Aspartic acid | L-Glutamine | L-Serine | L-Methionine | Ornithine | L-Tryptophan | L-Phenylalanine | L-Tyrosine | Urea  | L-Cysteine | b-Alanine | Glycerol |
|---------|-----------|---------------|----------|-----------------|-------------|----------|--------------|-----------|--------------|-----------------|------------|-------|------------|-----------|----------|
| -0.66   | -0.62     | -0.72         | -2.63    | -1.77           | 0.53        | -0.19    | -0.19        | 0.37      | -0.18        | -1.18           | -0.97      | -0.19 | 1.35       | -0.24     | 0.19     |
| -1.26   | 0.42      | -0.05         | -0.21    | -2.19           | 1.15        | -1.35    | 0.43         | -0.13     | 0.57         | -0.97           | -0.68      | -0.42 | 2.06       | 0.84      | -1.24    |
| -1.77   | 0.54      | -1.72         | -0.29    | -1.97           | 1.05        | -0.85    | -0.09        | -0.09     | 1.15         | -1.33           | 0.15       | -1.41 | 1.83       | -0.9      | 0.42     |
| -1.19   | -1.16     | -0.36         | 0.46     | -2.14           | 0.37        | -1.28    | -1.7         | -0.67     | -0.21        | -1.09           | -0.79      | 1.28  | -0.95      | 0.24      | -0.53    |
| -0.66   | 0.53      | -0.19         | 1.02     | 0.03            | 0.35        | 0.83     | -0.23        | 0.45      | 1.03         | -0.16           | 0.08       | 1.44  | 1.09       | -1.11     | -0.98    |
| 0.26    | -0.65     | 0.62          | -0.42    | -0.38           | 0.75        | 0.47     | -0.37        | 0.44      | 0.22         | -0.84           | -0.69      | -0.1  | 1.26       | -0.43     | -0.02    |
| 0.18    | 2.06      | 0.27          | -0.03    | -0.85           | 0.65        | 1.04     | -0.02        | 0.92      | -0.62        | -0.62           | -0.46      | -0.75 | 1.03       | -0.29     | -1.7     |
| 0.93    | -0.09     | -1.99         | 0.83     | -2.22           | 0.16        | 0.46     | -0.49        | -0.12     | -0.68        | -1.23           | 0.09       | 0.78  | 0.81       | -1.26     | -0.61    |
| -2      | -2.82     | 0.62          | -0.22    | -2.39           | -0.2        | -2.39    | -1.56        | -2.21     | -0.71        | -1.41           | -1.22      | 1.41  | -1.3       | -1.6      | 0.04     |
| -1.04   | -0.61     | 0.55          | 0.38     | -1.47           | 0.73        | -1.5     | -0.18        | -1.1      | -0.01        | -1.83           | -1.63      | 0.33  | 1.51       | 1.34      | -0.25    |
| 0.98    | -0.83     | -0.05         | 1.21     | -1.87           | 1.16        | 0.02     | -0.55        | -0.47     | -0.05        | -2.67           | -1.45      | 1.09  | 1.09       | -0.2      | -0.54    |
| -1.01   | -0.48     | -0.21         | -1.32    | 0.15            | 0.56        | 0.67     | -0.25        | 1.29      | -1.15        | -0.87           | -1.64      | -0.72 | 1.73       | -0.46     | -0.13    |
| -0.56   | -0.24     | -1.55         | 0.66     | -1.7            | 0.88        | -1.75    | -0.37        | -1.53     | 0.24         | -1.83           | -1.24      | 0.76  | 1.45       | 0.44      | -0.24    |
| 0.36    | -0.09     | 0.36          | 0.28     | -1.92           | 0.47        | -1.03    | -0.44        | -0.32     | 0.87         | -1.4            | -0.84      | -0.48 | 1.49       | -1.1      | -0.06    |
| -1.52   | -1.06     | -2.42         | 0.46     | -1.67           | 0.67        | -0.53    | -0.44        | -0.24     | 0.51         | -1.84           | -0.92      | -0.71 | 1.18       | -0.37     | 0.09     |
| -0.02   | 1.11      | 0.56          | 0.23     | 0.74            | -2.81       | 1.05     | 0.51         | -0.22     | 0.01         | 1.01            | 1.09       | -0.14 | -0.7       | 0.57      | 0.16     |
| 0.69    | 0.66      | 0.27          | 1.87     | -0.07           | 0.27        | 0.46     | 0.17         | 0.2       | 0.02         | 0.79            | 0.26       | 1.75  | -0.67      | 0.68      | -0.35    |
| -0.89   | -0.34     | -0.33         | -0.47    | 0.21            | 0.65        | -0.43    | -1.23        | 0.03      | -0.23        | -0.47           | -1.53      | -1.38 | 1.53       | -0.7      | 0.32     |
| -0.78   | -0.58     | 0.79          | 0.4      | 0.81            | -0.78       | -0.42    | -0.46        | -1.18     | 0.14         | 0.5             | -0.08      | 1.46  | -1.54      | 0.87      | 1.36     |
| -0.42   | 0.55      | 1.32          | 1.01     | 0               | -1.87       | -0.48    | -0.14        | 0.16      | 0.63         | 0.24            | -0.5       | -0.89 | 0.29       | -1.15     | -0.21    |
| 0.33    | 1.13      | 0.83          | 0.72     | 0.05            | -0.2        | 0.85     | -0.28        | 0.31      | 0.84         | 0.73            | -0.1       | -1.47 | -0.81      | -1.71     | -0.02    |
| -0.15   | 0.47      | -0.66         | 0.01     | -0.23           | -0.03       | 0.68     | -0.62        | 0.41      | 0.33         | 0.24            | -0.19      | -0.35 | -0.21      | 0.59      | 0.1      |
| -0.47   | 1.08      | 0.36          | -1.92    | 0.17            | 0.27        | -0.14    | -0.28        | -0.3      | 0.85         | 0.24            | -0.2       | -0.08 | 0.45       | -0.41     | 0.42     |
| -0.72   | -0.65     | -0.29         | -2.45    | -0.19           | 0.52        | -1       | -1.45        | -0.64     | 0.21         | 0.05            | -1.51      | 1.35  | -0.32      | 0.48      | 0.1      |
| -0.43   | -0.41     | 1.05          | 0.29     | 0.55            | -0.58       | 0.32     | -0.24        | -0.69     | -0.18        | 0.32            | -0.27      | 0.02  | -0.87      | 1.06      | 0.98     |
| -0.66   | -0.77     | 0.04          | -0.28    | 0.93            | -0.13       | -2.15    | -0.51        | -0.48     | -0.42        | 0.08            | -1.47      | -0.13 | 0.06       | 0.05      | -2.78    |
| 1.74    | -0.83     | 1.55          | -0.16    | 0.77            | -0.07       | -0.78    | 0.98         | 0.9       | -1.58        | 1.3             | 0.99       | 0.14  | 0.22       | -0.71     | 1.16     |
| 1.27    | -0.92     | -0.09         | 0.45     | 0.34            | 1.11        | -0.96    | 2.68         | 0.94      | -0.72        | 0.62            | 1.8        | 1.37  | 0.85       | 2.13      | -0.02    |
| -1.27   | 0.03      | 0.75          | 0.61     | 0.32            | -0.6        | 0.26     | -0.34        | 0.47      | 1.13         | -0.71           | -0.47      | -1.54 | 0.59       | -0.56     | -1.16    |
| -0.8    | -0.51     | -1.93         | 1.22     | 1.11            | 0.38        | -0.29    | 0.3          | 0.41      | 1.38         | 0.19            | 0.33       | 0.92  | -0.06      | 0.91      | 0.27     |
| 2.41    | 1.45      | 1.54          | -2.08    | 1.24            | -0.22       | 0.49     | -0.41        | -0.13     | 0.18         | 1.56            | 0.06       | -0.33 | 0.3        | 0.17      | 0.78     |
| 0.94    | 0.5       | 1.01          | -0.61    | 0.86            | 0.66        | 1.61     | 3.17         | 1.17      | 2.18         | 1.63            | 2.55       | -0.2  | -0.26      | 1.33      | -0.43    |
| 0.7     | 1.53      | 0.58          | 1.03     | 0.78            | 1.16        | -0.37    | 2.82         | 0.91      | -0.23        | 1.48            | 1.49       | -2.1  | 0.32       | -1.05     | 0.37     |
| 2.58    | -0.92     | 1.09          | -0.92    | 0.39            | 0.97        | 0.59     | 0.25         | 0.36      | 1.05         | 0.88            | 1.16       | 0.64  | 0.26       | -0.34     | 1.43     |
| 0.6     | 1.68      | -1.24         | 0.66     | 1.13            | 0.64        | 3.17     | 3.62         | 0.81      | 1.19         | 2.8             | 2.78       | -0.23 | -1.13      | 0.11      | 0.44     |
| 0.68    | 0.02      | 0.34          | -3.39    | 0.18            | -4.31       | -1.57    | 1.65         | -5.46     | -3.15        | -0.14           | 1.65       | -0.11 | -2.46      | -2.05     | 0.46     |
| 0.95    | -0.01     | -0.22         | -1.35    | 0.39            | -0.17       | -0.5     | -0.32        | 0.05      | -1.52        | -0.16           | -0.76      | 1.75  | -1.33      | 2.19      | 0.25     |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| -0.12 | 1.23  | -0.05 | -0.38 | 1.07  | 0.82  | 1.21  | 0.9   | 1.03  | 1.26  | 1.5   | 1.9   | -1.24 | -0.6  | -0.35 | 0.5   |
| -0.23 | -1.26 | 1.84  | -0.34 | 0.43  | 0.09  | -0.1  | 0.02  | 0.87  | -3.57 | 0.22  | -0.73 | -1.92 | -0.29 | -0.32 | 2.07  |
| 1.9   | 2.18  | 2     | 0.14  | -0.2  | -0.31 | 1.61  | -0.47 | -0.79 | 0.31  | -0.22 | 0.03  | -0.52 | 0.84  | -0.67 | 0.53  |
| 0.53  | 0.99  | 0.94  | 0.11  | 0.51  | -0.84 | 0.03  | -0.02 | 0.05  | -0.04 | 0.57  | -0.27 | -0.31 | -0.98 | 0.97  | 0.52  |
| 0.12  | 1.41  | 1.31  | 0.04  | 0.39  | -1.87 | 0.98  | -0.55 | -0.51 | -0.33 | -0.08 | -0.45 | -0.89 | -0.44 | -0.46 | 0.63  |
| 0.88  | -0.61 | 0.4   | 0.51  | 0.77  | 0.22  | 1.37  | -0.01 | 1.18  | -0.04 | -0.03 | 0.29  | -1.6  | -0.04 | -0.78 | 0.42  |
| -0.12 | 0.5   | 0.11  | 1.04  | -0.02 | -0.69 | -0.18 | -0.41 | 0.54  | -0.14 | 0.12  | -0.02 | 0.95  | 0.11  | 1.43  | 0.54  |
| 0.03  | -0.99 | -1.17 | 0.93  | 0.48  | -0.06 | -0.03 | -0.18 | 0.85  | -0.22 | 0.44  | 0.46  | 1.26  | -0.87 | 1.43  | -0.36 |
| -0.42 | 0.43  | -0.8  | 0.4   | 0.5   | -0.18 | -0.99 | 0.28  | 0.27  | -0.01 | 0.37  | 0.26  | -0.28 | -1.01 | 1.15  | 0.55  |
| 0.41  | -1.19 | 0.62  | 1.45  | 1.51  | -1.75 | 0.93  | 0.23  | 0.61  | 0.4   | 1.74  | 0.38  | 1.14  | -0.62 | -0.95 | -0.58 |
| -1.09 | -1.29 | 1.55  | -0.1  | 0.23  | -0.28 | -0.25 | -0.72 | -0.61 | 0.87  | 0.05  | 0.56  | -0.05 | -0.96 | -1.57 | -0.02 |
| -0.99 | 0.47  | -0.84 | 1.35  | 0.44  | 0.84  | 0.17  | 0.74  | -0.45 | 1.77  | 0.32  | 1.36  | 0.2   | 1.12  | -1.08 | -0.22 |
| -0.34 | -0.6  | -0.09 | 0.04  | 0.34  | 0.19  | 1.19  | -0.37 | 0.99  | -0.15 | 0.16  | 0.79  | -0.94 | -0.43 | -0.55 | 1.18  |
| -0.72 | -0.08 | -0.23 | 0.81  | 0.28  | 0.01  | 0.16  | -0.33 | 0.4   | -0.19 | 0.22  | -0.14 | -0.38 | -0.74 | -0.04 | -0.19 |
| 0.12  | 0.36  | -1.07 | 0.58  | 0.29  | 0.22  | 0.79  | -0.26 | 0.64  | -0.02 | 0     | -0.39 | -0.15 | 0.15  | 0.21  | -0.66 |
| 1.24  | -0.11 | 0.05  | -0.53 | 0.73  | -1.27 | 0.97  | -0.74 | -0.72 | -0.58 | -0.03 | 0.01  | 1.05  | -1.66 | 0.62  | 0.82  |
| 1.63  | 1.08  | -0.07 | 0.68  | 0.6   | -1.45 | 0.73  | -0.08 | -0.75 | -1.07 | 0.92  | -0.39 | 1.62  | -1.42 | 1.91  | 0.38  |
| -0.29 | 0.24  | 0.63  | -0.41 | 0.58  | -0.86 | -0.52 | -0.22 | 0.41  | -0.01 | 0.43  | 0.25  | 0.89  | -0.52 | 1.05  | 0.87  |
| -0.8  | 1.4   | -0.42 | -1    | 0.66  | 0.55  | 0.28  | 0.05  | -0.15 | 0.84  | 0.08  | 0.69  | 0.22  | -0.13 | 0.01  | -0.78 |
| -0.49 | -2.5  | -1.73 | -0.3  | -0.17 | 0.6   | -0.67 | -0.94 | -0.11 | -0.21 | -0.33 | 0.18  | 1.06  | -0.99 | 1.8   | 0.02  |
| -0.1  | -0.69 | -2.06 | -0.22 | 0.15  | -0.08 | 0.14  | -0.73 | -0.07 | -0.95 | -0.84 | -0.66 | -0.21 | -0.9  | -0.15 | 0.61  |
| 0.14  | 0.65  | -0.28 | -0.3  | 0.51  | 0.04  | -0.71 | 0.08  | 0.08  | -0.96 | -0.14 | 0.09  | -0.42 | 0.02  | 1.08  | 0.15  |
| -0.83 | -0.29 | -0.32 | 0.12  | 0.63  | 0.24  | -0.65 | -0.27 | 1.02  | -1.4  | 0.16  | -0.37 | -1.85 | 0.04  | -0.75 | 0.78  |
| 0.41  | -0.1  | -0.57 | -0.03 | 0.24  | 0.32  | -0.39 | -0.48 | -0.22 | 0.08  | -0.64 | -0.39 | 0.16  | 0.18  | -0.75 | -0.88 |
| 1.79  | -0.41 | -0.21 | 0.37  | 0.93  | 1.37  | 0.91  | 1.09  | 0.82  | 1.26  | 1.1   | 1.67  | -0.56 | 0.03  | -0.61 | -4.95 |

| L-Leucine | L-Histidine | L-Proline | L-Asparagine | Citric acid | L-Valine | Cholesterol | L-Threonine | Arachidonic acid | D-Glucose | Ketoleucine | Taurine | Palmitic acid | Citrulline | Uric acid |
|-----------|-------------|-----------|--------------|-------------|----------|-------------|-------------|------------------|-----------|-------------|---------|---------------|------------|-----------|
| 0.6       | -1.02       | 0.02      | 1.51         | 0.06        | 0.85     | -1.07       | 0.06        | 0.59             | 1.08      | 0.57        | -2.08   | -0.19         | -0.77      | 0.21      |
| 1.7       | 0.6         | 1.15      | 1.65         | -0.88       | 1.81     | -0.82       | 0.66        | 0.33             | 1.39      | 1.5         | 0.27    | -0.63         | -0.07      | 0.76      |
| 1.12      | 0.16        | -0.15     | 1.51         | -1.33       | 1.39     | 1.32        | 0.48        | 0.69             | 1.96      | -0.95       | -2.69   | 1             | -0.78      | 2.2       |
| -0.55     | -0.29       | -0.25     | 0.47         | 0.19        | 2.02     | -0.34       | 0.12        | 0.03             | 0.83      | 1.06        | 1.03    | 0.78          | 2.45       | 0.89      |
| 2.07      | 0.93        | 1.69      | 1.66         | -1.8        | 2.27     | -0.44       | 0.34        | -1.36            | 0.67      | 0.18        | 1.11    | -1.56         | -0.71      | 0.31      |
| 0.02      | 0.23        | -0.09     | -0.08        | -0.21       | 0.36     | -1.5        | -0.44       | -0.35            | 1.35      | 0.42        | -0.2    | -0.43         | -1.12      | 0.85      |
| 0.35      | -0.39       | 2.08      | 2.09         | 0.88        | 0.73     | -0.27       | 1.55        | -1.31            | 0.46      | -1.75       | -0.32   | -3.03         | -1.08      | -0.29     |
| 0.44      | -0.41       | -0.52     | -0.16        | -0.31       | -1.01    | -0.68       | -0.29       | -1.82            | 0.82      | 0.31        | 0.45    | -0.74         | -0.09      | -1.18     |
| -0.63     | -1.65       | -0.77     | -0.75        | -0.41       | -0.89    | -0.56       | -4.01       | 1.63             | 1.46      | 1.39        | 0.59    | 0.8           | -0.55      | 0.62      |
| -0.73     | -0.96       | -0.14     | 1.25         | 0.29        | -0.71    | 1.24        | 0.42        | -0.64            | 0.86      | 0.12        | -0.74   | 0.56          | -0.35      | 0.17      |
| -0.67     | -0.06       | -0.33     | 0.77         | 0.17        | 0        | -0.44       | -0.85       | -0.09            | 1.27      | 0.89        | 0.42    | -0.31         | -0.01      | 0.64      |
| 0.51      | -0.24       | -1        | 1.29         | -1.03       | 0.3      | -0.36       | 0.79        | 0.26             | -1.09     | 0.6         | 0.66    | 0.21          | 0.47       | 0.37      |
| 0.08      | 0.56        | -1.16     | 0.66         | -0.33       | 0.98     | -0.87       | -0.4        | 0.62             | 0         | 1.59        | 0.4     | 0.19          | -0.79      | 0.12      |
| -0.29     | 0.63        | -0.67     | 0.19         | -0.73       | 0.44     | -1.33       | 1.27        | -0.33            | 1.85      | 1.39        | 0.44    | -0.31         | -0.47      | 1.09      |
| -0.13     | -0.55       | -0.8      | 0.05         | 0.41        | 0.68     | -0.03       | 0.47        | 0.15             | 0.67      | 1.05        | -0.26   | 0.43          | -0.76      | 0.92      |
| 0.86      | -0.8        | -0.39     | -1.43        | 0.98        | -0.25    | -1.86       | 0.22        | 0.31             | 0.06      | 1.22        | 0.72    | 0.15          | 2.73       | -0.82     |
| 2.5       | 0.01        | 0.86      | -0.27        | -0.72       | 1.91     | -2.67       | 0.35        | -1.14            | -0.76     | 0.84        | 0.78    | -0.43         | 0.77       | -0.28     |
| -0.82     | -0.71       | -0.9      | -1.41        | -0.25       | -0.11    | 0.84        | -1.32       | -1.88            | 0.38      | 1.01        | 0.82    | 0.42          | -0.86      | 1.54      |
| -0.45     | -0.27       | -0.13     | -0.5         | -1.64       | -0.42    | -0.19       | -0.32       | 1.03             | -0.42     | -1.13       | 1.1     | 0.73          | 2.65       | -0.06     |
| 0.03      | 0.68        | 0.24      | 0.27         | -0.86       | 0.76     | 0.85        | 0.77        | -0.15            | 0.61      | 0.72        | 1.11    | -0.23         | -1.07      | 2.15      |
| 1         | 0.18        | 0.65      | -0.34        | -0.03       | 1.32     | -0.77       | -0.11       | 0.89             | -0.37     | 0.61        | 0.54    | -1.11         | 0.52       | 1.6       |
| -0.41     | -0.4        | -0.32     | -0.13        | -1.26       | -0.97    | 0.3         | -2.13       | -1.73            | -1.03     | 0.4         | 0.54    | -0.19         | 0.23       | 1.13      |
| 0.3       | 1.2         | 0.5       | 0.77         | -1.13       | 0.6      | 0.11        | -0.16       | 1.2              | -0.51     | 0.28        | -0.35   | -0.26         | -0.02      | 1.61      |
| -0.86     | 0.52        | -1        | -0.61        | -0.15       | -0.63    | 0.31        | -2.89       | 0.11             | 0.73      | 0.48        | 0.18    | 0.47          | 0.23       | 0.6       |
| -0.2      | 0.23        | -0.43     | -0.72        | -0.23       | 0.45     | -0.02       | -0.39       | -0.04            | -0.01     | -0.07       | 0.4     | 0.88          | 0.08       | 0.26      |
| -0.58     | 0.2         | -1.66     | -0.37        | 1.02        | -1.11    | 1.56        | -0.23       | 1.38             | 1.23      | 0.6         | 0.36    | 0.94          | -0.87      | 0.07      |
| -0.88     | 1.39        | 0.33      | 0.43         | 1.72        | -1.93    | 2.11        | 0.04        | 2.26             | -0.28     | -0.8        | 0.86    | 0.87          | -0.35      | -1.31     |
| -1.58     | -0.04       | 0.14      | 0.35         | 0.83        | -1.03    | -1.36       | 0.42        | 0.46             | -1.89     | -1.49       | -0.42   | 0.48          | 1.93       | -2.01     |
| 0.62      | 0.84        | -1.37     | -0.52        | -1.32       | 0.34     | 1.36        | 0.33        | 0.99             | 0.83      | 0.77        | 0.58    | -0.56         | -0.33      | 1.53      |
| 1.88      | 0           | -0.04     | 0.14         | -0.64       | 1.49     | -0.33       | 0.16        | 0.04             | -0.78     | -0.37       | 0.29    | 0.32          | 1.69       | 0.36      |
| -1.31     | 1.09        | 0.17      | -0.53        | 0.33        | 0.19     | 1.15        | 0.29        | 0.29             | -0.86     | -1.47       | 0.57    | -0.43         | -1.13      | -0.09     |
| -0.88     | 1.68        | 1.83      | 0.74         | 1.92        | -1.21    | 0.45        | 0.86        | -0.41            | 0.05      | -0.34       | -2      | -2.75         | 0.01       | 0.64      |
| 0.07      | 1.9         | 2.65      | 2.19         | 1.16        | -1.11    | 0.3         | 1.46        | 0.74             | -0.47     | -1.26       | -0.05   | 0.11          | 0.53       | -1.25     |
| -1.73     | 1.37        | 1.15      | 0.69         | 0.63        | -0.8     | 0.94        | 0.47        | -0.39            | 0.49      | -0.52       | 0.61    | 0.33          | -1.15      | -0.03     |
| 0.71      | 1.84        | 2.96      | 1.86         | 1.47        | 0.64     | -0.43       | 1.77        | -0.56            | 0.99      | -0.37       | 0.09    | -1.9          | 0.19       | -1.11     |
| -0.82     | -3.19       | -0.32     | -2.69        | 1.73        | -1.16    | -0.47       | 0.6         | 0.83             | -0.13     | -1.37       | -2.97   | 1.36          | 0.98       | -2.19     |
| -0.37     | 0.52        | 0.29      | -1.81        | 0.01        | -0.65    | -1.31       | -1.12       | -0.06            | -1.54     | -0.87       | 1.05    | 0.19          | -0.51      | -0.33     |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| -0.48 | 0.14  | 1.87  | 0.6   | 0.85  | -0.46 | 0.38  | 1.29  | -0.06 | -0.08 | -2.97 | -0.53 | -0.02 | 1.09  | -0.86 |
| -1.42 | -0.58 | -0.84 | 0.36  | 0.82  | -1.85 | 1.67  | -0.19 | 1.87  | -2.38 | -0.63 | -1.28 | 2.66  | -0.94 | -1.17 |
| -0.11 | 0.66  | -1.34 | -0.5  | -0.35 | -0.17 | 1.91  | -0.28 | -1.87 | -0.13 | 1.95  | 0.95  | -0.38 | -1.32 | 1.39  |
| 0.77  | -1.55 | -0.07 | -1.62 | -1.54 | 0.84  | -0.51 | 0.44  | 0.5   | -0.74 | -0.75 | 0.95  | -0.44 | 0.78  | 0.85  |
| -1.38 | 0.38  | 0.19  | -1.51 | -1.15 | -0.73 | -0.08 | -0.52 | -0.62 | 0.16  | -0.85 | 0.58  | 0.3   | -0.02 | -0.17 |
| -0.05 | 0.97  | -0.99 | -0.27 | 0.38  | -0.43 | 1.09  | 0.86  | 0.4   | -1.74 | -0.34 | 0.21  | -0.95 | -1.71 | -0.96 |
| 0.89  | 0.34  | -0.63 | 0.09  | -0.76 | 0.36  | -0.22 | 0.05  | -0.26 | -0.84 | 0.36  | 0.49  | 0.17  | 1.8   | 0.17  |
| 0.66  | 0.29  | 0.02  | -0.22 | 0.14  | 0.06  | -0.7  | -0.69 | -0.83 | -1.32 | 0.08  | 0.36  | 0.97  | 0.92  | 0.13  |
| 0.38  | -0.69 | -0.78 | 0.1   | 0.37  | 0.21  | -0.74 | 0     | -0.09 | 1.03  | 0.14  | 0.23  | 0.2   | 1.26  | -0.9  |
| 2.43  | 0.49  | -0.61 | 0.35  | -2.83 | 2.3   | -0.21 | 0.05  | -0.98 | -1.12 | 0.19  | 1.09  | -0.26 | -0.55 | -0.5  |
| -0.51 | 0.97  | -1.75 | -0.82 | 0.63  | -0.27 | 1.08  | -0.61 | -2.87 | 0.35  | 0.62  | -0.05 | 0.45  | -0.69 | 0.68  |
| 0.72  | 1.54  | 1.74  | -1.5  | -0.52 | 0.59  | 0.87  | 1.85  | -0.58 | 0.36  | -1.71 | -0.26 | -1.76 | -0.26 | -0.46 |
| 0.47  | -0.52 | 0.48  | 0.12  | -0.05 | -0.26 | 0.77  | 0.08  | 0.21  | 1.42  | 1.2   | -0.62 | 1.89  | -0.86 | 0.31  |
| 0.49  | -0.81 | -0.79 | 0.4   | -0.55 | -0.62 | -0.22 | -0.72 | 0.07  | -0.37 | 1.16  | -0.7  | 0.57  | 0.33  | -0.09 |
| 0.52  | -0.55 | -0.14 | -0.96 | -1.5  | 0.4   | -0.33 | -0.67 | -1.35 | 0.86  | 0.15  | -3.3  | -0.09 | -0.45 | -1.09 |
| 0.23  | -2.12 | 0.07  | -1.17 | -0.91 | -0.25 | -1.94 | 0.39  | -0.82 | -0.52 | -0.1  | 0.92  | 1.04  | 0.69  | -1.45 |
| 0.96  | -1.33 | 0.24  | -0.39 | 1.14  | 0.1   | -0.58 | -0.56 | -0.15 | -1.22 | 0.05  | 0.75  | -0.24 | -0.28 | -0.39 |
| 0.65  | 0.1   | 0.24  | 0.14  | 0.41  | -0.11 | -0.3  | -0.56 | 1.11  | -2.11 | -0.98 | -0.24 | -0.84 | -0.94 | 0.12  |
| -0.01 | -1.44 | -0.02 | -0.91 | 1.3   | 0.14  | -0.83 | -0.51 | 1.05  | 1.08  | 0.49  | -0.09 | -0.97 | 0.29  | -0.26 |
| -2.53 | -0.66 | 0.06  | -0.02 | 0.96  | -2.24 | -0.14 | -1.03 | 0.66  | -0.55 | 0.06  | -0.56 | 1.58  | 0.54  | -1.79 |
| -0.84 | -0.14 | -0.73 | -0.48 | 1.13  | -1.02 | 1.04  | -0.34 | 1.19  | -0.81 | -0.24 | 0.33  | 1.51  | -0.3  | 0.39  |
| 0.09  | -1.67 | -0.66 | -0.37 | 0.63  | -0.12 | 0.66  | 1.33  | -0.3  | -0.52 | -0.42 | -1.68 | 0.11  | -0.26 | -1.49 |
| -0.78 | -1.02 | -0.89 | -0.07 | 0.96  | -0.71 | 0.15  | 0.35  | 1.51  | -0.61 | -0.76 | -0.76 | 0.26  | 0.88  | -0.84 |
| -1.63 | 0.29  | -0.17 | -0.76 | 1.06  | -0.73 | 1.52  | -0.44 | 0.42  | 0.27  | 0.25  | 0.16  | -1.11 | -1.44 | -0.39 |
| -0.5  | 1.17  | 1.22  | 1.18  | 0.84  | -0.57 | 0.91  | 1.19  | -0.76 | -0.38 | -2.19 | -0.82 | -0.84 | -0.19 | -0.95 |

| L-Isoleucine | N-Acetylornithine | Isocitric acid | N-Acetylglutamic acid | Malate | Oleic acid | Creatinine | Indoleacetic acid | g-Hydroxybutyric Acid | 3-Hydroxybutyric acid | 4-Hydroxyproline | Cystine |
|--------------|-------------------|----------------|-----------------------|--------|------------|------------|-------------------|-----------------------|-----------------------|------------------|---------|
| 0.52         | -0.63             | -0.23          | 1.57                  | 0.03   | 0.5        | -0.28      | 0.02              | 0.63                  | 0.92                  | -1.4             | -0.35   |
| 2.19         | -1.27             | -1.2           | 0.14                  | -0.16  | -0.8       | 0.21       | 0.2               | -1.06                 | -1.11                 | 0.77             | 0.16    |
| 1.19         | 0                 | -1.95          | 1.59                  | -1.08  | 1.34       | 0.57       | 0.04              | -0.74                 | 0.18                  | -1.05            | 1.83    |
| 0.36         | -0.23             | 0.13           | -1.04                 | -0.32  | -1.74      | -0.64      | 0.53              | 1.13                  | -0.14                 | 0.75             | 0.18    |
| 1.35         | -1.9              | -1.16          | -2.63                 | -0.38  | -0.41      | 0.23       | 0.1               | -1.47                 | -0.83                 | -0.45            | -0.46   |
| 0.23         | -0.47             | -0.44          | 0.36                  | 0.41   | 0.36       | 0.27       | 0.66              | -1.72                 | -1.74                 | -0.76            | 0       |
| 0.69         | -0.74             | 0.35           | 0.32                  | -0.71  | -2.52      | -0.04      | 0.33              | -0.82                 | -0.08                 | 1.12             | -0.13   |
| -2.83        | -1.76             | 0.76           | 1.12                  | 0.08   | -1.16      | 0.42       | 1.46              | -0.34                 | -0.34                 | 0.03             | -0.37   |
| -0.72        | -2.52             | -3.29          | 1.38                  | 0.49   | 1.3        | 0.35       | 1.74              | -0.05                 | 2.65                  | 0.49             | -0.65   |
| -0.49        | 0.69              | -0.38          | 0.62                  | -0.64  | -0.07      | -0.19      | 0.31              | 1.19                  | -0.28                 | -0.07            | 0.02    |
| 0.09         | 0.03              | 0.01           | 0.64                  | -0.36  | -0.34      | 0.33       | 0.23              | 0.52                  | 0.31                  | -1.05            | 0.17    |
| 0.59         | 1.2               | -1.51          | 0.59                  | 0.47   | 0.16       | 0.47       | 0.5               | 0.33                  | -1.14                 | -0.02            | 0.1     |
| 0.17         | -1.82             | -0.59          | 0.16                  | -0.16  | 0.88       | 0.84       | 0.42              | -1.77                 | 1.23                  | -0.94            | 0.15    |
| -0.42        | -0.08             | -1.43          | 1.57                  | -0.03  | 0.54       | -0.05      | 0.93              | 0.43                  | -1.18                 | 0.08             | 1.54    |
| -0.1         | 0.61              | -0.67          | 0.16                  | -0.56  | 0.85       | -0.08      | 1.32              | 0.49                  | 1.63                  | -0.46            | 1.07    |
| 0.74         | -1.08             | 1.19           | -0.68                 | 0.4    | 0.23       | -1         | -1.22             | 0.85                  | -0.37                 | 2.3              | -1.59   |
| 2.34         | 0.54              | -0.58          | 0.54                  | -0.1   | -2.1       | -1.28      | 1.03              | 0.49                  | -0.72                 | -0.19            | -1.63   |
| -1.36        | -0.3              | 0.58           | 0.13                  | 0.76   | 1.17       | -0.27      | -1.8              | -0.5                  | 2.55                  | -1.07            | -0.54   |
| 0.31         | -0.38             | -1.11          | 0.08                  | -2.46  | 0.04       | -0.33      | 1.44              | 1.18                  | -1.29                 | -0.9             | -1.22   |
| -1.21        | 0.14              | -0.39          | -1.12                 | -0.27  | 0.63       | 0.26       | 2                 | -0.06                 | -0.77                 | 1.72             | 0.8     |
| 0.31         | 0.07              | 0.1            | 0.11                  | -0.5   | -0.13      | 0.86       | 0.61              | -0.49                 | -0.29                 | 0.2              | -0.28   |
| -1.29        | 0.59              | -0.67          | -0.19                 | 2.8    | -0.4       | -0.26      | -0.53             | 0.63                  | -0.11                 | -0.64            | -0.45   |
| -0.15        | -0.84             | -0.43          | -0.63                 | -3.08  | 0.33       | 1.65       | -0.05             | -0.49                 | -0.28                 | 0.57             | 0.8     |
| -0.74        | -1.84             | 0.16           | -0.51                 | -0.98  | -0.44      | 0.85       | -0.26             | 0.31                  | 0.06                  | -0.51            | 0.73    |
| -0.32        | 0.33              | 0.01           | -1.19                 | -0.49  | 1.31       | 0.41       | -0.43             | 0.85                  | 0.86                  | -2.15            | -1.25   |
| -0.84        | 0.3               | 1.09           | -0.47                 | -0.38  | 1.11       | 0.44       | -0.98             | 0.51                  | 0.52                  | -0.05            | 0.37    |
| -0.87        | -0.2              | 1.93           | 1.91                  | 0.78   | 1.78       | -0.7       | -0.1              | -1.72                 | -1.11                 | 1.79             | 2.72    |
| 0.74         | 0.8               | 0.34           | 0.44                  | -0.29  | -0.27      | -1.44      | -0.14             | 1.15                  | 0.08                  | 0.64             | 0.36    |
| 0.72         | 1.01              | -0.72          | -0.43                 | 0.48   | -0.68      | 0.67       | 3.25              | -0.01                 | -1.15                 | -0.63            | 0.71    |
| 1.54         | 0.35              | -0.43          | -1.1                  | -1.13  | -0.91      | 0.85       | 1.45              | 0.46                  | 0.09                  | -0.72            | -0.13   |
| -2.32        | 0.2               | 0.16           | -4.66                 | -0.18  | 0.65       | 0.52       | -0.79             | -1.8                  | -1.59                 | -0.41            | -0.12   |
| -0.35        | -0.63             | 2.17           | -0.02                 | 1.12   | -2.35      | 0.86       | 1.14              | -0.55                 | -0.54                 | 1.83             | 0.24    |
| -0.46        | -0.32             | 0.97           | -0.22                 | 0.73   | 0.75       | 0.5        | -1.54             | -1.58                 | 0.11                  | 1.68             | 3.03    |
| -1.16        | -0.96             | 0.51           | -0.05                 | 0.53   | 0.55       | 0.06       | -0.45             | -2.24                 | 0.65                  | 0.85             | 0.19    |
| 0.75         | -0.78             | 1.46           | -0.98                 | 0.69   | -1.9       | -0.45      | 0.8               | -1.46                 | -0.19                 | 1.19             | 0.81    |
| 0.64         | -0.06             | 1.39           | 0.98                  | 1.2    | 1.17       | -4.88      | -2.03             | 0.66                  | -0.82                 | 0.7              | 0.2     |
| 0.49         | 0.93              | 0.61           | 0.18                  | -0.08  | -0.76      | 0.32       | -0.56             | 0.14                  | -0.25                 | -1.38            | -1.38   |

|       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| -0.51 | 0.55  | -0.05 | -0.7  | -0.14 | -0.48 | -0.42 | 0.11  | -0.11 | -1.11 | 0.67  | 0     |
| -1.22 | -0.53 | 0.94  | 0.15  | 1.9   | 2.12  | -0.66 | -1.81 | 0.42  | 2.4   | 1.75  | 0.96  |
| -0.7  | -1.81 | 0.43  | 0.12  | 1.46  | 0.24  | 1.06  | 0.13  | -0.83 | -1.1  | -0.55 | -0.58 |
| 0.48  | 1.91  | -0.87 | 0.21  | -0.55 | -0.51 | -0.23 | 0.31  | 1.19  | -0.29 | -1    | -0.92 |
| -0.64 | 0.61  | -0.65 | -0.79 | 0.11  | 0.55  | -3.3  | 0.05  | -0.9  | 1.23  | -0.85 | -1.11 |
| -0.9  | 0.79  | 0.24  | 0.12  | 1.52  | 0.16  | 0.46  | -0.95 | -0.81 | -0.4  | 0.16  | -0.46 |
| 0.78  | 1.82  | -0.66 | -0.13 | -0.24 | -0.74 | 0.44  | -2.11 | 1.36  | -0.46 | -1.26 | -0.85 |
| 0.94  | 0.63  | 0.4   | -0.18 | -0.39 | -0.9  | -0.22 | -0.41 | 0.79  | 0.05  | -0.57 | -0.99 |
| 1.27  | 0.52  | 1.07  | 0.35  | -1.69 | -0.43 | 0.63  | -0.89 | 1.26  | 0.24  | 0.81  | -0.88 |
| 1.67  | 1.22  | -1.45 | -0.57 | 0.37  | 0.56  | 1.44  | -0.39 | 0.96  | 1.36  | -2.6  | -0.6  |
| -1.07 | 0.11  | 0.8   | -1.35 | 2.41  | 0.26  | 0.7   | -0.01 | 0.11  | -0.89 | -0.64 | 0.66  |
| 0.35  | -1.24 | -0.15 | 0.24  | -0.11 | -1.4  | -0.1  | 0.52  | 0.07  | -0.66 | 1.04  | 1.53  |
| -0.08 | 0.63  | -0.62 | 0.6   | 0.38  | 1.94  | -1.19 | -0.14 | 0.75  | 1.09  | 0.13  | 0.19  |
| 0.09  | 1.08  | -0.01 | 0.31  | -0.47 | 0.29  | 0.4   | -0.39 | 0.64  | 0.91  | 0.02  | -0.69 |
| 0.41  | 0.75  | -1.4  | 0.76  | -0.88 | 0.2   | -0.16 | 0.66  | 0.65  | -0.94 | 0.15  | 0.59  |
| 0.72  | -0.04 | 0.11  | 1.02  | -0.66 | 0.3   | -1.53 | -0.79 | 0.47  | 1.13  | 0.89  | -1.82 |
| 1.25  | -0.62 | 0.94  | 1.02  | -0.03 | -1.09 | 0.57  | -0.58 | -1.21 | -0.56 | 0.19  | -0.74 |
| 0.55  | 1.32  | 0.69  | -0.7  | 0.16  | -0.61 | -0.02 | -1.37 | 1.3   | -0.37 | 0.51  | -0.68 |
| 0.21  | 0.61  | 1.47  | 0.15  | 0.7   | -0.55 | -0.06 | 0.13  | 0.16  | -0.36 | 0.89  | 0.71  |
| -1.11 | 0.36  | 0.24  | 0.19  | -0.14 | 0.2   | -0.05 | -1.15 | 1.77  | 1.63  | 0.15  | -0.85 |
| -1.13 | 0.94  | 0.93  | 0.05  | 1.29  | 0.93  | 1.02  | 0.38  | -0.15 | 1.41  | -0.81 | -0.59 |
| 0.33  | 0.39  | 0.65  | 0.5   | 0.61  | -0.26 | 0.18  | -0.06 | 1.43  | -0.02 | -0.73 | -1.45 |
| -0.42 | 2.4   | 0.37  | -0.22 | -1.99 | 0.96  | 0.65  | -0.86 | 0.33  | 0.82  | -0.99 | 0.36  |
| -0.99 | -0.25 | 1.12  | 0.22  | -0.01 | -0.27 | 0.34  | 0.03  | -0.67 | -0.02 | 0.11  | 0.61  |
| -0.59 | -1.12 | -1.32 | -0.03 | -0.27 | -0.13 | 0.04  | -0.04 | -2.1  | -0.61 | 0.68  | 1.95  |



| Lactic acid | Stearic acid | Capric acid | Linoleic acid | Pelargonic acid | Threonic acid | Pyroglutamic acid | 1-Acylglycerol | Indolelactic acid | g-Tocopherol | Dodecanoic acid | N-Methylalanine |
|-------------|--------------|-------------|---------------|-----------------|---------------|-------------------|----------------|-------------------|--------------|-----------------|-----------------|
| 0.15        | 0.39         | -0.08       | 0.11          | -0.1            | 1.42          | 1.91              | -0.35          | 0.51              | 0.2          | 1.11            | 0.08            |
| -0.76       | 0.68         | -0.39       | -0.15         | -0.26           | 1.02          | 1                 | -0.64          | 1.58              | 0.11         | -0.12           | 0.7             |
| 0.19        | 0.03         | -3.51       | 1.21          | -0.42           | 0.61          | 0.96              | -0.97          | 1.34              | 0.37         | -0.85           | -1.86           |
| -0.7        | 1.49         | 0.12        | -0.9          | -0.27           | 0.69          | 1.43              | -0.13          | 0.38              | 0.33         | 0.56            | -0.43           |
| 0.89        | -0.94        | -0.15       | 0.31          | -1.45           | 0.86          | 1.2               | -0.04          | 0.5               | 0.56         | 0.69            | 0.1             |
| 0.87        | -0.52        | -0.28       | 0.71          | -0.65           | 1.19          | 0.85              | -0.61          | 1.46              | 0.71         | -0.13           | 0.26            |
| 0.43        | -2.04        | 0.01        | -1.9          | 0.28            | 1.1           | 1.31              | -0.71          | -0.35             | 1.83         | -1.13           | 0.63            |
| -0.61       | -0.23        | 2.71        | -0.7          | -3.64           | 1.09          | 1.13              | 0.6            | 0.01              | 0.66         | 0.85            | -1.34           |
| 0.32        | 1.09         | 0.6         | 1.11          | 0.24            | 1.59          | 0.78              | 2.28           | 1.63              | 2.06         | 0.43            | 0.46            |
| -1.29       | 1.57         | 0.37        | -1.34         | 0.86            | 1.2           | 0.48              | 0.37           | 0.19              | -2.27        | 0.09            | 0.34            |
| -0.95       | 0.54         | 0.21        | -3.09         | 0.49            | 1.24          | 0.36              | -1.86          | 0.06              | 1.01         | 0.32            | -0.33           |
| 1.65        | 0.78         | -0.3        | 0.3           | -0.21           | 1.07          | 0.91              | -0.23          | -0.54             | 0.11         | 0.17            | 1.4             |
| -0.55       | -0.06        | 0.21        | 1.02          | -1.3            | 1.32          | -0.4              | -1.65          | 0.56              | 0.3          | 0.04            | 0.73            |
| 0.52        | -0.44        | 0.09        | 0.62          | -2.36           | 2.11          | 1.48              | -1.45          | 0.81              | -0.8         | 0.2             | 0.64            |
| -0.05       | 0.51         | -1.95       | 0.49          | -0.39           | 1.68          | -0.24             | -2.1           | 0.55              | 1.76         | -0.19           | 2.19            |
| 0.19        | 0.67         | 0.86        | 0.23          | 1.25            | -1.07         | 0.49              | 1.75           | -0.74             | 0.12         | 0.23            | -3.23           |
| -1.01       | 0.32         | -0.3        | -1.43         | 0.07            | -0.48         | -0.29             | 1.79           | 0.1               | -1.13        | -0.29           | 0.26            |
| 3.31        | -0.33        | 0.89        | 1.01          | 1.67            | -0.61         | -0.06             | 0              | 0.72              | 0.67         | 0.38            | -0.75           |
| -0.1        | 1.12         | 0.09        | -0.28         | 0.75            | 0.47          | -0.73             | 0.18           | 0.29              | 0.53         | 0.17            | -0.26           |
| -0.35       | -1.11        | -1.33       | 0.34          | -0.56           | -1.85         | -2.17             | 0.23           | 1.85              | -0.26        | -0.26           | 1.83            |
| 0.27        | -1.2         | -0.56       | 0.47          | -0.68           | -0.4          | 0                 | -0.9           | 0.11              | 1.08         | -0.6            | -0.08           |
| 0.82        | 0.48         | -0.61       | -0.35         | 0.3             | 0.14          | -0.89             | 2.26           | -0.29             | -1.24        | -1.03           | -1.15           |
| -0.81       | -0.61        | -0.29       | 0.72          | 0.31            | -0.21         | -0.63             | 0.59           | -0.42             | 0.3          | -1.5            | 1.36            |
| -1.49       | 0.52         | -0.09       | 0.39          | -0.72           | 0.36          | -1.25             | 0.06           | 0.26              | 1.82         | -3              | -0.99           |
| -2.17       | 0.08         | 0.36        | 1.03          | 0.48            | 0.19          | -2.27             | -0.33          | -0.94             | -0.45        | 0.16            | 0.44            |
| -0.29       | -0.03        | 0.87        | 0.23          | 0.64            | -2.23         | -0.87             | -0.98          | 0.35              | 0.9          | 1.4             | -0.84           |
| -0.23       | -1.03        | 0.81        | 1.22          | 1.94            | -1.94         | -1.26             | -0.04          | -2.02             | 1.77         | 1.42            | -0.38           |
| -1.25       | 0.5          | 0.18        | -0.51         | -0.64           | -1.2          | 0.75              | 0.62           | -0.44             | 0.76         | 0.16            | 1.44            |
| 1.34        | -0.33        | 0.85        | -0.22         | 0.67            | -0.13         | -0.21             | 0.45           | 0.25              | -0.37        | -0.57           | -0.06           |
| -1.08       | 0.84         | -0.12       | -0.9          | -0.43           | -0.12         | -1.1              | -0.48          | -0.13             | 0.35         | -0.73           | -0.09           |
| 0.12        | -1.42        | -0.43       | 0.71          | -0.44           | 0.47          | -1.83             | -0.04          | 0.19              | -0.56        | 0.47            | 0.5             |
| 0.2         | -2.49        | -0.74       | 0.25          | -0.37           | 0.37          | 0.12              | -0.5           | 3.17              | -1.41        | -3.42           | -1.12           |
| -0.32       | -1.36        | 0.62        | 0.96          | 0.77            | -0.32         | 0.17              | -1.6           | -1.05             | 0.19         | 0.81            | 0.21            |
| -0.67       | -0.7         | 2.34        | 0.56          | -1.13           | 0.16          | 0.03              | -0.13          | 0.67              | -0.53        | 1.79            | 0.31            |
| 0.36        | -1.41        | -1.25       | -2.09         | 0.37            | -2.5          | -0.29             | 0.1            | 0.58              | -1.27        | -0.42           | 0.22            |
| -0.42       | 1.04         | -1.99       | 0.98          | 1.2             | -1.66         | 1.4               | 0.54           | -2.77             | -2.2         | 1.17            | 0.28            |
| 0.45        | 0.85         | 0.08        | -0.45         | 0.71            | -0.86         | -0.81             | 0.24           | -0.61             | -1.06        | -0.16           | -0.09           |

|       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| -1.63 | -0.09 | 0.03  | -0.49 | -0.1  | -0.99 | 0.62  | 0.03  | 0.32  | 0.16  | 0.44  | 0.43  |
| 1.26  | 0.74  | 1.65  | 1.79  | 1.5   | -0.65 | 0.9   | -0.16 | -2.81 | -0.37 | 2.64  | -0.01 |
| 2.45  | -1.43 | 0.24  | 0.64  | 1.42  | 0.63  | -0.36 | 0.23  | -0.55 | 0.1   | 0.15  | 0.81  |
| -0.38 | -0.27 | -0.42 | -0.25 | -0.6  | 0.67  | -0.15 | 1.89  | -0.1  | 0.83  | -1.04 | 0.54  |
| 2.24  | 0.36  | -0.84 | 0.85  | -1.11 | 0.23  | -2.25 | -0.72 | -0.3  | -1.33 | 0.84  | 0.61  |
| 1.15  | -1.7  | 0.23  | -0.87 | -0.42 | -0.98 | 0.19  | 0.36  | 0.59  | 0.5   | 0.33  | -0.02 |
| -0.02 | 0.93  | -0.31 | -0.2  | 0.5   | 0.74  | -0.46 | -0.25 | 0.14  | 0.5   | -1.27 | 1     |
| -0.41 | 1.49  | 0.42  | -0.55 | 0.91  | 0.34  | -0.57 | 1.43  | -0.56 | -2.05 | -0.09 | 0.06  |
| -0.29 | 0.97  | -0.81 | -1.2  | 0.66  | -0.36 | -0.51 | -0.03 | -0.44 | -0.32 | -0.29 | -3.34 |
| 0.82  | -0.5  | -0.65 | 0.62  | -1.61 | -0.52 | -1.62 | -0.72 | 0.49  | -1.33 | -0.52 | -0.46 |
| -1.29 | 0.44  | 0.08  | 0.79  | -0.13 | 0.43  | -0.85 | -1.95 | 0.73  | -0.62 | 0.8   | -1.09 |
| -1.53 | -1.68 | 1.8   | -0.74 | -0.27 | -1.72 | -0.45 | 0.38  | 0.42  | 0.93  | 0.36  | -0.05 |
| 0.22  | -0.05 | 1.58  | 1.63  | 1.2   | -0.08 | 0.4   | -0.22 | 0.03  | -0.36 | 1.4   | -0.37 |
| 0.7   | 0.48  | 0.21  | 0.76  | 0.63  | -0.06 | -0.29 | 0.12  | -0.51 | -1.68 | -0.77 | 0.01  |
| 0.03  | 0.73  | -1.73 | -0.24 | -0.5  | -0.41 | 0.7   | -0.45 | -0.04 | 0.02  | -0.03 | 0.52  |
| 0.11  | 1.36  | 0.47  | 0.12  | 0.96  | -0.72 | 0.51  | 2.24  | -0.9  | -0.71 | 0.75  | 0.94  |
| 1.04  | -0.04 | 0.33  | -1.62 | 1.28  | 0.16  | 2.42  | 1.26  | -0.95 | -1.08 | -0.21 | -0.24 |
| 0.44  | -0.57 | -0.29 | 0.11  | -0.48 | 0.12  | -1.31 | 1.38  | -0.12 | 0.41  | -0.71 | -0.21 |
| -0.25 | -0.28 | -0.53 | -0.18 | -0.77 | -1.2  | 0.34  | 0.26  | 1.06  | -0.1  | -1.88 | 0.86  |
| -0.32 | 2.34  | 0.59  | 0.33  | -0.4  | -0.31 | 0.18  | 0.89  | -1.2  | -1.08 | -0.63 | 0.56  |
| 0.67  | 1.36  | 0.82  | 1.12  | 1.12  | 0.32  | -0.11 | -0.15 | -1.17 | 0.37  | 0.75  | 0.06  |
| -0.44 | 0.51  | -0.25 | -2.32 | 0.03  | 0.2   | 0.27  | 0.08  | -1.24 | 0.55  | 0.31  | -2.21 |
| -0.75 | -0.37 | -1.24 | 1.04  | -1.6  | -0.87 | -0.14 | -0.85 | -0.95 | -0.07 | -0.12 | -0.11 |
| 0.05  | -1.09 | -0.15 | -1.12 | 0.17  | 0.14  | 0.22  | -0.34 | -0.43 | 0.87  | -0.14 | -0.29 |
| -0.84 | -0.93 | 0.89  | -0.69 | 0.63  | 0.13  | 0.81  | -1.03 | 0.69  | 0.91  | 0.72  | 0.64  |

| Glycerolphosphate | 3-Aminoisobutanoic acid | 5-Methoxytryptamine | 2-Hydroxybutyric acid | Myristic acid | Arachidic acid | Palmitoleic acid | Pentadecanoic acid |
|-------------------|-------------------------|---------------------|-----------------------|---------------|----------------|------------------|--------------------|
| 0.44              | -0.1                    | -0.92               | -1.05                 | 0.41          | 1.06           | 0.46             | 1.01               |
| -0.18             | 0.15                    | -1.31               | -1.26                 | -0.45         | 1.28           | -1.12            | 0.76               |
| -1.18             | 0.42                    | 1                   | -1.86                 | 0.29          | -0.14          | 0.7              | 1.36               |
| 0.43              | 0                       | -1.44               | -0.47                 | 0.34          | 0.09           | 0.02             | 0.67               |
| 1.87              | -0.53                   | -1.47               | -1.7                  | -0.14         | -0.97          | -0.66            | 0.44               |
| 0.95              | -0.8                    | -1.04               | -1.08                 | 0.57          | -0.85          | 0.24             | 1.02               |
| 1.19              | 0.03                    | 0.75                | -1.19                 | -1.71         | -1.43          | -2.16            | 0.25               |
| 0.25              | -0.4                    | -1.15               | -0.99                 | 0.48          | -0.16          | -1.64            | 0.45               |
| 0.28              | -1.41                   | -1.13               | 1.23                  | 0.62          | 0.07           | 0.11             | 1.01               |
| 0.82              | 1.52                    | 0.85                | -1.81                 | 0.28          | 0.82           | -0.04            | -0.74              |
| 0.56              | -0.9                    | 0.36                | -0.83                 | -0.28         | 0.28           | -0.95            | 0.92               |
| 1.62              | -1.17                   | -0.14               | -0.11                 | -0.81         | 0.62           | -0.55            | -3.71              |
| 0.93              | 0.26                    | 0.75                | 1.28                  | 0.68          | -0.02          | 0.36             | 0.41               |
| 1.15              | -1.49                   | 1.5                 | -0.81                 | 0.16          | -1.39          | 0.78             | 1.29               |
| 1.25              | -0.03                   | 1.21                | 0.2                   | 0.87          | 0.16           | 0.69             | 0.87               |
| -1.79             | -0.67                   | -1.4                | 0.56                  | 0.08          | 0.59           | 0.41             | 0.14               |
| -0.88             | -0.47                   | -0.86               | -1.63                 | -1.19         | 0.52           | -1.39            | -0.3               |
| 0.27              | 0.21                    | 0.76                | -0.3                  | 0.05          | -0.34          | 0.27             | 0.45               |
| -0.68             | -0.82                   | -1.77               | -0.48                 | 0.22          | 0.38           | 0.4              | 0.23               |
| 0.56              | 0.53                    | 0.27                | 0.9                   | -0.43         | -2.39          | 0.13             | 0.21               |
| -3.67             | -3.19                   | 1.1                 | -0.47                 | -0.61         | -1.32          | -0.41            | -0.45              |
| 1.2               | -1.17                   | 1.49                | 0.03                  | -0.42         | 0.62           | -0.02            | -0.09              |
| 0.63              | 1.72                    | 0.97                | 1.38                  | -0.08         | -0.26          | 0.61             | -0.05              |
| 0.75              | -0.37                   | 1.92                | 0.25                  | -0.56         | 0.3            | -1.81            | 0.44               |
| -0.75             | 1.02                    | -0.05               | 1.54                  | 0.61          | -0.58          | 1.05             | 0.16               |
| 0.51              | 0.61                    | 0.94                | 0.16                  | 0.81          | -0.82          | 1.17             | 1.04               |
| -1.19             | 0.21                    | 0.35                | 1.26                  | 1.72          | 0              | 1.76             | 0.74               |
| -0.09             | 0.32                    | 0.13                | 0.34                  | 0.08          | 0.95           | 0.25             | -0.77              |
| 0.95              | -2.39                   | 0.72                | -0.24                 | -0.46         | -0.53          | -1.01            | 0.35               |
| 0.84              | 0.33                    | 0.38                | -0.24                 | -0.7          | 0.68           | -0.99            | -0.41              |
| -1.04             | -0.07                   | 0.61                | 0.23                  | 0.09          | -1.12          | 0.73             | 0.21               |
| -0.76             | -0.04                   | -0.18               | -1.18                 | -1.83         | -2.51          | -1.53            | -0.12              |
| -1.42             | 1.43                    | -0.15               | 0.2                   | 0.73          | -1.24          | 1.44             | 0                  |
| -0.02             | -0.09                   | 0.22                | 0.51                  | 1.73          | -1.34          | 0.63             | 1.14               |
| -0.42             | 1.22                    | 0.9                 | 0.04                  | -1.08         | -0.93          | -1.13            | 0.43               |
| -1.67             | 2.73                    | -1.88               | 1.51                  | 1.24          | 0.85           | 1.29             | 0.46               |
| -0.85             | 0.1                     | -1.01               | 0.29                  | -0.48         | 0.94           | -0.37            | -0.81              |

|       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.04  | 0.19  | -0.25 | -1.86 | 0.17  | 0.71  | 0.39  | 0.06  |
| 0.56  | 0.52  | 0.17  | 1.17  | 2.73  | 0.44  | 2.28  | 0.01  |
| 1.2   | -0.37 | 1.28  | 1.62  | 0.22  | -0.87 | 0.86  | -0.06 |
| -0.93 | 1.49  | -1.12 | -0.27 | -0.48 | -0.82 | 0.3   | -0.37 |
| 0.7   | 0.5   | 0.22  | 0.57  | 0.43  | 0.55  | 0.45  | 0.53  |
| -0.09 | -0.64 | 0.26  | -0.11 | 0.1   | -1.03 | 0.69  | -0.79 |
| -0.96 | 0.45  | -1.38 | 0.4   | -0.93 | 0.74  | -0.15 | -0.3  |
| -0.6  | 0.42  | -1.95 | 0.54  | 0.1   | 1.9   | -0.39 | -0.34 |
| -0.54 | 0.04  | -0.54 | 0.02  | -0.81 | 0.79  | -2.09 | 0.41  |
| -1.43 | 1.29  | -0.87 | 1.45  | -0.31 | -0.47 | -0.22 | -0.57 |
| 0.98  | -0.82 | 0.82  | 0.37  | 0.21  | 0.67  | 0.36  | 0.15  |
| 0.01  | 1.25  | 0.63  | -1.2  | 0.15  | -0.98 | -1.54 | -2.31 |
| 0.07  | -1.83 | 0.8   | 0.2   | 1.86  | -0.56 | 1.88  | -2.78 |
| -0.74 | -0.69 | -0.05 | 1.98  | -4.65 | 0.41  | 0.67  | 0.1   |
| 1.49  | -0.53 | 1.15  | -0.68 | 0.08  | 1.15  | -0.16 | -3.69 |
| -0.31 | 0.98  | -0.75 | -0.29 | 0.58  | 1.91  | 0.39  | 0.49  |
| -1.04 | 0.81  | -1.33 | -2.19 | -0.39 | 1.52  | -2.54 | -0.44 |
| -0.08 | -0.41 | 0.26  | -0.17 | -0.65 | -0.07 | -0.11 | -1.15 |
| 0.04  | -0.37 | 1.79  | 1.17  | -0.66 | -0.37 | -0.66 | 0.67  |
| -0.44 | -1.11 | -0.59 | 1.46  | 0.31  | 2.66  | 0.05  | 0.48  |
| 1.08  | 0.54  | 0.33  | 0.36  | 1.11  | 0.37  | 0.77  | 0.27  |
| -0.25 | 0.7   | -1.07 | 0.07  | 0.14  | 0.87  | -0.01 | 0.23  |
| -0.09 | 0.34  | -0.15 | -0.05 | -0.11 | -0.27 | 0.74  | 0.15  |
| 0.84  | -0.06 | 1.25  | 0.35  | -0.22 | -0.76 | -0.17 | 0.18  |
| -0.34 | 0.62  | -0.21 | 0.85  | 0.2   | -0.33 | 0.52  | 0.06  |

**Supplementary Table S2. Results from SFAM algorithm**

| Subject ID | Diagnosis | Predicted | Sex | Age | BMI   | mtDNA CN | mtDNA deletions | L/P   | BCAA/AAA | CP    | Total BR | CysCys/Total Cys | Pyruvic acid | L-Glutamic acid |
|------------|-----------|-----------|-----|-----|-------|----------|-----------------|-------|----------|-------|----------|------------------|--------------|-----------------|
| K10No_WD   | Control   | Control   | 2   | 52  | -0.51 | 0.71     | 1.09            | -0.19 | 1.42     | 1.45  | -0.2     | -1.39            | 0.92         | -0.33           |
| K6No_WD    | Control   | Control   | 2   | 38  | -1.62 | 0.98     | -0.58           | -1.48 | 1.41     | 1.06  | -1.08    | -1.09            | 1            | -1.84           |
| M2No_WD    | Control   | Control   | 1   | 45  | 1.53  | 0.79     | 0.06            | 0.12  | 1.27     | 1.17  | -1.42    | -1.27            | 0.46         | -0.08           |
| K1No_WD    | Control   | Control   | 2   | 38  | -1.16 | 0.72     | -0.34           | -0.38 | 0.96     | 0.69  | -0.62    | 0.79             | 0.59         | -2.02           |
| K4No_WD    | Control   | Control   | 2   | 31  | -0.39 | 0.26     | -1.02           | -0.84 | 1.13     | 0.89  | -0.32    | 0.45             | 0.69         | -1.86           |
| 2275WD     | WD        | WDNEU     | 2   | 17  | -0.57 | 0.87     | -0.81           | -1.25 | 0.39     | -0.61 | -0.78    | 0.83             | 0.33         | -0.61           |
| 2251WD     | WD        | WDNEU     | 1   | 21  | 1.09  | 0.47     | 1.18            | 0.51  | 0.35     | -0.86 | -0.88    | 0.48             | -0.38        | 0.81            |
| 1715WD     | WD        | WDNEU     | 2   | 30  | -0.8  | 0.38     | -1.7            | -0.4  | -0.01    | 0.3   | 0.02     | -0.89            | -0.8         | 0.21            |
| 1776WD     | WD        | WDNEU     | 2   | 39  | 0.29  | -2.43    | -0.66           | 0.29  | 0.29     | 0.08  | 0.34     | 0.44             | -0.51        | 0.26            |
| 1779WD-H   | WDHEP     | WDHEP     | 1   | 29  | 1.31  | -1.38    | -0.8            | 0.11  | -2.51    | -0.33 | 1.98     | 0.98             | 0.14         | 0.54            |
| 2086WD-H   | WDHEP     | WD        | 2   | 32  | -0.39 | -0.2     | 1.27            | 0.3   | 0.41     | -0.7  | 0.02     | -0.08            | -0.48        | 0.86            |
| 2415WD-H   | WDHEP     | WDHEP     | 1   | 46  | 0.53  | -1.16    | -0.21           | -1.37 | -1.58    | 0.46  | 2.66     | 1.69             | 1.24         | 0.77            |
| 972WD-H    | WDHEP     | WD        | 2   | 18  | 0.86  | -1.09    | -0.2            | 0.72  | -0.01    | -2.05 | -0.68    | -0.8             | 0.5          | 1.3             |
| 1843WD-H   | WDHEP     | WDNEU     | 2   | 31  | 0.44  | -0.88    | -0.31           | 0.23  | -0.6     | 0.18  | -0.11    | -0.53            | 0.23         | 0.33            |
| 2051WD-H   | WDHEP     | WDNEU     | 2   | 56  | -0.83 | 1.3      | 0.67            | 1.12  | 0.38     | 0.61  | -0.05    | -1.01            | -1.04        | 0.82            |
| 205WD-N    | WDNEU     | WDNEU     | 1   | 44  | -1.43 | 0.14     | 0.73            | -1.03 | 0.48     | -1.71 | -0.71    | 0.74             | 0.98         | 0.02            |
| 1167WD-N   | WDNEU     | WDNEU     | 1   | 28  | -1.22 | -0.63    | 0.87            | 1.79  | 0.12     | -1.43 | 1.01     | -0.77            | -1.62        | 0.58            |
| 1998WD-N   | WDNEU     | WDNEU     | 1   | 27  | -1.17 | 1.04     | 0.35            | 0.52  | 0.49     | -2.79 | 1.49     | 0.67             | 0.13         | 0.06            |
| 2024WD-N   | WDNEU     | WDNEU     | 1   | 52  | 2.84  | 1.78     | 1.26            | 1.45  | -0.2     | -0.14 | 0.06     | -0.22            | -1.2         | 0.88            |
| 2508WD-N   | WDNEU     | WDNEU     | 2   | 23  | -0.35 | -0.32    | 1.61            | -0.23 | -0.2     | 0.15  | -0.41    | 0.62             | 0.17         | -0.09           |
| 1783WD-N   | WDNEU     | WDHEP     | 2   | 46  | -0.38 | 1.67     | 1.05            | -0.08 | -1.79    | -0.08 | 0.57     | 1.35             | -0.36        | 0.28            |

| Oxoglutaric acid | Glycine | L-Alanine | Succinic acid | L-Lysine | L-Aspartic acid | L-Glutamine | L-Serine | L-Methionine | Ornithine | L-Tryptophan | L-Phenylalanine | L-Tyrosine | Urea  |
|------------------|---------|-----------|---------------|----------|-----------------|-------------|----------|--------------|-----------|--------------|-----------------|------------|-------|
| -0.77            | -1.01   | -0.48     | -0.21         | -1.32    | 0.15            | 0.56        | 0.67     | -0.25        | 1.29      | -1.15        | -0.87           | -1.64      | -0.72 |
| -0.43            | -0.56   | -0.24     | -1.55         | 0.66     | -1.7            | 0.88        | -1.75    | -0.37        | -1.53     | 0.24         | -1.83           | -1.24      | 0.76  |
| -0.33            | -0.66   | 0.53      | -0.19         | 1.02     | 0.03            | 0.35        | 0.83     | -0.23        | 0.45      | 1.03         | -0.16           | 0.08       | 1.44  |
| -0.72            | 0.36    | -0.09     | 0.36          | 0.28     | -1.92           | 0.47        | -1.03    | -0.44        | -0.32     | 0.87         | -1.4            | -0.84      | -0.48 |
| -0.74            | -1.52   | -1.06     | -2.42         | 0.46     | -1.67           | 0.67        | -0.53    | -0.44        | -0.24     | 0.51         | -1.84           | -0.92      | -0.71 |
| 0.13             | -0.72   | -0.65     | -0.29         | -2.45    | -0.19           | 0.52        | -1       | -1.45        | -0.64     | 0.21         | 0.05            | -1.51      | 1.35  |
| -1.02            | 0.33    | 1.13      | 0.83          | 0.72     | 0.05            | -0.2        | 0.85     | -0.28        | 0.31      | 0.84         | 0.73            | -0.1       | -1.47 |
| 0.58             | -0.43   | -0.41     | 1.05          | 0.29     | 0.55            | -0.58       | 0.32     | -0.24        | -0.69     | -0.18        | 0.32            | -0.27      | 0.02  |
| -0.12            | -0.66   | -0.77     | 0.04          | -0.28    | 0.93            | -0.13       | -2.15    | -0.51        | -0.48     | -0.42        | 0.08            | -1.47      | -0.13 |
| 0.66             | 0.94    | 0.5       | 1.01          | -0.61    | 0.86            | 0.66        | 1.61     | 3.17         | 1.17      | 2.18         | 1.63            | 2.55       | -0.2  |
| 0.64             | 0.53    | 0.99      | 0.94          | 0.11     | 0.51            | -0.84       | 0.03     | -0.02        | 0.05      | -0.04        | 0.57            | -0.27      | -0.31 |
| 1.42             | 0.7     | 1.53      | 0.58          | 1.03     | 0.78            | 1.16        | -0.37    | 2.82         | 0.91      | -0.23        | 1.48            | 1.49       | -2.1  |
| -0.86            | 0.12    | 1.41      | 1.31          | 0.04     | 0.39            | -1.87       | 0.98     | -0.55        | -0.51     | -0.33        | -0.08           | -0.45      | -0.89 |
| -0.17            | 0.88    | -0.61     | 0.4           | 0.51     | 0.77            | 0.22        | 1.37     | -0.01        | 1.18      | -0.04        | -0.03           | 0.29       | -1.6  |
| 0.05             | -0.12   | 0.5       | 0.11          | 1.04     | -0.02           | -0.69       | -0.18    | -0.41        | 0.54      | -0.14        | 0.12            | -0.02      | 0.95  |
| 0.26             | 0.12    | 0.36      | -1.07         | 0.58     | 0.29            | 0.22        | 0.79     | -0.26        | 0.64      | -0.02        | 0               | -0.39      | -0.15 |
| -0.79            | 1.24    | -0.11     | 0.05          | -0.53    | 0.73            | -1.27       | 0.97     | -0.74        | -0.72     | -0.58        | -0.03           | 0.01       | 1.05  |
| -0.82            | 1.63    | 1.08      | -0.07         | 0.68     | 0.6             | -1.45       | 0.73     | -0.08        | -0.75     | -1.07        | 0.92            | -0.39      | 1.62  |
| -0.01            | -0.29   | 0.24      | 0.63          | -0.41    | 0.58            | -0.86       | -0.52    | -0.22        | 0.41      | -0.01        | 0.43            | 0.25       | 0.89  |
| 0.01             | 0.41    | -0.1      | -0.57         | -0.03    | 0.24            | 0.32        | -0.39    | -0.48        | -0.22     | 0.08         | -0.64           | -0.39      | 0.16  |
| -0.23            | 1.79    | -0.41     | -0.21         | 0.37     | 0.93            | 1.37        | 0.91     | 1.09         | 0.82      | 1.26         | 1.1             | 1.67       | -0.56 |

| L-Cysteine | Beta-Alanine | Glycerol | L-Leucine | L-Histidine | L-Proline | L-Asparagine | Citric acid | L-Valine | Cholesterol | L-Threonine | Arachidonic acid | D-Glucose | Ketoleucine |
|------------|--------------|----------|-----------|-------------|-----------|--------------|-------------|----------|-------------|-------------|------------------|-----------|-------------|
| 1.73       | -0.46        | -0.13    | 0.51      | -0.24       | -1        | 1.29         | -1.03       | 0.3      | -0.36       | 0.79        | 0.26             | -1.09     | 0.6         |
| 1.45       | 0.44         | -0.24    | 0.08      | 0.56        | -1.16     | 0.66         | -0.33       | 0.98     | -0.87       | -0.4        | 0.62             | 0         | 1.59        |
| 1.09       | -1.11        | -0.98    | 2.07      | 0.93        | 1.69      | 1.66         | -1.8        | 2.27     | -0.44       | 0.34        | -1.36            | 0.67      | 0.18        |
| 1.49       | -1.1         | -0.06    | -0.29     | 0.63        | -0.67     | 0.19         | -0.73       | 0.44     | -1.33       | 1.27        | -0.33            | 1.85      | 1.39        |
| 1.18       | -0.37        | 0.09     | -0.13     | -0.55       | -0.8      | 0.05         | 0.41        | 0.68     | -0.03       | 0.47        | 0.15             | 0.67      | 1.05        |
| -0.32      | 0.48         | 0.1      | -0.86     | 0.52        | -1        | -0.61        | -0.15       | -0.63    | 0.31        | -2.89       | 0.11             | 0.73      | 0.48        |
| -0.81      | -1.71        | -0.02    | 1         | 0.18        | 0.65      | -0.34        | -0.03       | 1.32     | -0.77       | -0.11       | 0.89             | -0.37     | 0.61        |
| -0.87      | 1.06         | 0.98     | -0.2      | 0.23        | -0.43     | -0.72        | -0.23       | 0.45     | -0.02       | -0.39       | -0.04            | -0.01     | -0.07       |
| 0.06       | 0.05         | -2.78    | -0.58     | 0.2         | -1.66     | -0.37        | 1.02        | -1.11    | 1.56        | -0.23       | 1.38             | 1.23      | 0.6         |
| -0.26      | 1.33         | -0.43    | -0.88     | 1.68        | 1.83      | 0.74         | 1.92        | -1.21    | 0.45        | 0.86        | -0.41            | 0.05      | -0.34       |
| -0.98      | 0.97         | 0.52     | 0.77      | -1.55       | -0.07     | -1.62        | -1.54       | 0.84     | -0.51       | 0.44        | 0.5              | -0.74     | -0.75       |
| 0.32       | -1.05        | 0.37     | 0.07      | 1.9         | 2.65      | 2.19         | 1.16        | -1.11    | 0.3         | 1.46        | 0.74             | -0.47     | -1.26       |
| -0.44      | -0.46        | 0.63     | -1.38     | 0.38        | 0.19      | -1.51        | -1.15       | -0.73    | -0.08       | -0.52       | -0.62            | 0.16      | -0.85       |
| -0.04      | -0.78        | 0.42     | -0.05     | 0.97        | -0.99     | -0.27        | 0.38        | -0.43    | 1.09        | 0.86        | 0.4              | -1.74     | -0.34       |
| 0.11       | 1.43         | 0.54     | 0.89      | 0.34        | -0.63     | 0.09         | -0.76       | 0.36     | -0.22       | 0.05        | -0.26            | -0.84     | 0.36        |
| 0.15       | 0.21         | -0.66    | 0.52      | -0.55       | -0.14     | -0.96        | -1.5        | 0.4      | -0.33       | -0.67       | -1.35            | 0.86      | 0.15        |
| -1.66      | 0.62         | 0.82     | 0.23      | -2.12       | 0.07      | -1.17        | -0.91       | -0.25    | -1.94       | 0.39        | -0.82            | -0.52     | -0.1        |
| -1.42      | 1.91         | 0.38     | 0.96      | -1.33       | 0.24      | -0.39        | 1.14        | 0.1      | -0.58       | -0.56       | -0.15            | -1.22     | 0.05        |
| -0.52      | 1.05         | 0.87     | 0.65      | 0.1         | 0.24      | 0.14         | 0.41        | -0.11    | -0.3        | -0.56       | 1.11             | -2.11     | -0.98       |
| 0.18       | -0.75        | -0.88    | -1.63     | 0.29        | -0.17     | -0.76        | 1.06        | -0.73    | 1.52        | -0.44       | 0.42             | 0.27      | 0.25        |
| 0.03       | -0.61        | -4.95    | -0.5      | 1.17        | 1.22      | 1.18         | 0.84        | -0.57    | 0.91        | 1.19        | -0.76            | -0.38     | -2.19       |

| Taurine | Palmitic acid | Citrulline | Uric acid | L-Isoleucine | N-Acetyloronithine | Isocitric acid | N-Acetylglutamic acid | Malate | Oleic acid | Creatinine | Indoleacetic acid |
|---------|---------------|------------|-----------|--------------|--------------------|----------------|-----------------------|--------|------------|------------|-------------------|
| 0.66    | 0.21          | 0.47       | 0.37      | 0.59         | 1.2                | -1.51          | 0.59                  | 0.47   | 0.16       | 0.47       | 0.5               |
| 0.4     | 0.19          | -0.79      | 0.12      | 0.17         | -1.82              | -0.59          | 0.16                  | -0.16  | 0.88       | 0.84       | 0.42              |
| 1.11    | -1.56         | -0.71      | 0.31      | 1.35         | -1.9               | -1.16          | -2.63                 | -0.38  | -0.41      | 0.23       | 0.1               |
| 0.44    | -0.31         | -0.47      | 1.09      | -0.42        | -0.08              | -1.43          | 1.57                  | -0.03  | 0.54       | -0.05      | 0.93              |
| -0.26   | 0.43          | -0.76      | 0.92      | -0.1         | 0.61               | -0.67          | 0.16                  | -0.56  | 0.85       | -0.08      | 1.32              |
| 0.18    | 0.47          | 0.23       | 0.6       | -0.74        | -1.84              | 0.16           | -0.51                 | -0.98  | -0.44      | 0.85       | -0.26             |
| 0.54    | -1.11         | 0.52       | 1.6       | 0.31         | 0.07               | 0.1            | 0.11                  | -0.5   | -0.13      | 0.86       | 0.61              |
| 0.4     | 0.88          | 0.08       | 0.26      | -0.32        | 0.33               | 0.01           | -1.19                 | -0.49  | 1.31       | 0.41       | -0.43             |
| 0.36    | 0.94          | -0.87      | 0.07      | -0.84        | 0.3                | 1.09           | -0.47                 | -0.38  | 1.11       | 0.44       | -0.98             |
| -2      | -2.75         | 0.01       | 0.64      | -0.35        | -0.63              | 2.17           | -0.02                 | 1.12   | -2.35      | 0.86       | 1.14              |
| 0.95    | -0.44         | 0.78       | 0.85      | 0.48         | 1.91               | -0.87          | 0.21                  | -0.55  | -0.51      | -0.23      | 0.31              |
| -0.05   | 0.11          | 0.53       | -1.25     | -0.46        | -0.32              | 0.97           | -0.22                 | 0.73   | 0.75       | 0.5        | -1.54             |
| 0.58    | 0.3           | -0.02      | -0.17     | -0.64        | 0.61               | -0.65          | -0.79                 | 0.11   | 0.55       | -3.3       | 0.05              |
| 0.21    | -0.95         | -1.71      | -0.96     | -0.9         | 0.79               | 0.24           | 0.12                  | 1.52   | 0.16       | 0.46       | -0.95             |
| 0.49    | 0.17          | 1.8        | 0.17      | 0.78         | 1.82               | -0.66          | -0.13                 | -0.24  | -0.74      | 0.44       | -2.11             |
| -3.3    | -0.09         | -0.45      | -1.09     | 0.41         | 0.75               | -1.4           | 0.76                  | -0.88  | 0.2        | -0.16      | 0.66              |
| 0.92    | 1.04          | 0.69       | -1.45     | 0.72         | -0.04              | 0.11           | 1.02                  | -0.66  | 0.3        | -1.53      | -0.79             |
| 0.75    | -0.24         | -0.28      | -0.39     | 1.25         | -0.62              | 0.94           | 1.02                  | -0.03  | -1.09      | 0.57       | -0.58             |
| -0.24   | -0.84         | -0.94      | 0.12      | 0.55         | 1.32               | 0.69           | -0.7                  | 0.16   | -0.61      | -0.02      | -1.37             |
| 0.16    | -1.11         | -1.44      | -0.39     | -0.99        | -0.25              | 1.12           | 0.22                  | -0.01  | -0.27      | 0.34       | 0.03              |
| -0.82   | -0.84         | -0.19      | -0.95     | -0.59        | -1.12              | -1.32          | -0.03                 | -0.27  | -0.13      | 0.04       | -0.04             |



| g-Hydroxybutyric Acid | 3-Hydroxybutyric acid | 4-Hydroxyproline | Cystine | Lactic acid | Stearic acid | Capric acid | Linoleic acid | Pelargonic acid | Threonic acid | Pyroglutamic acid |
|-----------------------|-----------------------|------------------|---------|-------------|--------------|-------------|---------------|-----------------|---------------|-------------------|
| 0.33                  | -1.14                 | -0.02            | 0.1     | 1.65        | 0.78         | -0.3        | 0.3           | -0.21           | 1.07          | 0.91              |
| -1.77                 | 1.23                  | -0.94            | 0.15    | -0.55       | -0.06        | 0.21        | 1.02          | -1.3            | 1.32          | -0.4              |
| -1.47                 | -0.83                 | -0.45            | -0.46   | 0.89        | -0.94        | -0.15       | 0.31          | -1.45           | 0.86          | 1.2               |
| 0.43                  | -1.18                 | 0.08             | 1.54    | 0.52        | -0.44        | 0.09        | 0.62          | -2.36           | 2.11          | 1.48              |
| 0.49                  | 1.63                  | -0.46            | 1.07    | -0.05       | 0.51         | -1.95       | 0.49          | -0.39           | 1.68          | -0.24             |
| 0.31                  | 0.06                  | -0.51            | 0.73    | -1.49       | 0.52         | -0.09       | 0.39          | -0.72           | 0.36          | -1.25             |
| -0.49                 | -0.29                 | 0.2              | -0.28   | 0.27        | -1.2         | -0.56       | 0.47          | -0.68           | -0.4          | 0                 |
| 0.85                  | 0.86                  | -2.15            | -1.25   | -2.17       | 0.08         | 0.36        | 1.03          | 0.48            | 0.19          | -2.27             |
| 0.51                  | 0.52                  | -0.05            | 0.37    | -0.29       | -0.03        | 0.87        | 0.23          | 0.64            | -2.23         | -0.87             |
| -0.55                 | -0.54                 | 1.83             | 0.24    | 0.2         | -2.49        | -0.74       | 0.25          | -0.37           | 0.37          | 0.12              |
| 1.19                  | -0.29                 | -1               | -0.92   | -0.38       | -0.27        | -0.42       | -0.25         | -0.6            | 0.67          | -0.15             |
| -1.58                 | 0.11                  | 1.68             | 3.03    | -0.32       | -1.36        | 0.62        | 0.96          | 0.77            | -0.32         | 0.17              |
| -0.9                  | 1.23                  | -0.85            | -1.11   | 2.24        | 0.36         | -0.84       | 0.85          | -1.11           | 0.23          | -2.25             |
| -0.81                 | -0.4                  | 0.16             | -0.46   | 1.15        | -1.7         | 0.23        | -0.87         | -0.42           | -0.98         | 0.19              |
| 1.36                  | -0.46                 | -1.26            | -0.85   | -0.02       | 0.93         | -0.31       | -0.2          | 0.5             | 0.74          | -0.46             |
| 0.65                  | -0.94                 | 0.15             | 0.59    | 0.03        | 0.73         | -1.73       | -0.24         | -0.5            | -0.41         | 0.7               |
| 0.47                  | 1.13                  | 0.89             | -1.82   | 0.11        | 1.36         | 0.47        | 0.12          | 0.96            | -0.72         | 0.51              |
| -1.21                 | -0.56                 | 0.19             | -0.74   | 1.04        | -0.04        | 0.33        | -1.62         | 1.28            | 0.16          | 2.42              |
| 1.3                   | -0.37                 | 0.51             | -0.68   | 0.44        | -0.57        | -0.29       | 0.11          | -0.48           | 0.12          | -1.31             |
| -0.67                 | -0.02                 | 0.11             | 0.61    | 0.05        | -1.09        | -0.15       | -1.12         | 0.17            | 0.14          | 0.22              |
| -2.1                  | -0.61                 | 0.68             | 1.95    | -0.84       | -0.93        | 0.89        | -0.69         | 0.63            | 0.13          | 0.81              |

| 1-Acylglycerol | Indolelactic acid | g-Tocopherol | Dodecanoic acid | N-Methylalanine | Glycerolphosphate | 3-Aminoisobutanoic acid | 5-Methoxytryptamine | 2-Hydroxybutyric acid |
|----------------|-------------------|--------------|-----------------|-----------------|-------------------|-------------------------|---------------------|-----------------------|
| -0.23          | -0.54             | 0.11         | 0.17            | 1.4             | 1.62              | -1.17                   | -0.14               | -0.11                 |
| -1.65          | 0.56              | 0.3          | 0.04            | 0.73            | 0.93              | 0.26                    | 0.75                | 1.28                  |
| -0.04          | 0.5               | 0.56         | 0.69            | 0.1             | 1.87              | -0.53                   | -1.47               | -1.7                  |
| -1.45          | 0.81              | -0.8         | 0.2             | 0.64            | 1.15              | -1.49                   | 1.5                 | -0.81                 |
| -2.1           | 0.55              | 1.76         | -0.19           | 2.19            | 1.25              | -0.03                   | 1.21                | 0.2                   |
| 0.06           | 0.26              | 1.82         | -3              | -0.99           | 0.75              | -0.37                   | 1.92                | 0.25                  |
| -0.9           | 0.11              | 1.08         | -0.6            | -0.08           | -3.67             | -3.19                   | 1.1                 | -0.47                 |
| -0.33          | -0.94             | -0.45        | 0.16            | 0.44            | -0.75             | 1.02                    | -0.05               | 1.54                  |
| -0.98          | 0.35              | 0.9          | 1.4             | -0.84           | 0.51              | 0.61                    | 0.94                | 0.16                  |
| -0.5           | 3.17              | -1.41        | -3.42           | -1.12           | -0.76             | -0.04                   | -0.18               | -1.18                 |
| 1.89           | -0.1              | 0.83         | -1.04           | 0.54            | -0.93             | 1.49                    | -1.12               | -0.27                 |
| -1.6           | -1.05             | 0.19         | 0.81            | 0.21            | -1.42             | 1.43                    | -0.15               | 0.2                   |
| -0.72          | -0.3              | -1.33        | 0.84            | 0.61            | 0.7               | 0.5                     | 0.22                | 0.57                  |
| 0.36           | 0.59              | 0.5          | 0.33            | -0.02           | -0.09             | -0.64                   | 0.26                | -0.11                 |
| -0.25          | 0.14              | 0.5          | -1.27           | 1               | -0.96             | 0.45                    | -1.38               | 0.4                   |
| -0.45          | -0.04             | 0.02         | -0.03           | 0.52            | 1.49              | -0.53                   | 1.15                | -0.68                 |
| 2.24           | -0.9              | -0.71        | 0.75            | 0.94            | -0.31             | 0.98                    | -0.75               | -0.29                 |
| 1.26           | -0.95             | -1.08        | -0.21           | -0.24           | -1.04             | 0.81                    | -1.33               | -2.19                 |
| 1.38           | -0.12             | 0.41         | -0.71           | -0.21           | -0.08             | -0.41                   | 0.26                | -0.17                 |
| -0.34          | -0.43             | 0.87         | -0.14           | -0.29           | 0.84              | -0.06                   | 1.25                | 0.35                  |
| -1.03          | 0.69              | 0.91         | 0.72            | 0.64            | -0.34             | 0.62                    | -0.21               | 0.85                  |

| Myristic acid | Arachidic acid | Palmitoleic acid | Pentadecanoic acid |
|---------------|----------------|------------------|--------------------|
| -0.81         | 0.62           | -0.55            | -3.71              |
| 0.68          | -0.02          | 0.36             | 0.41               |
| -0.14         | -0.97          | -0.66            | 0.44               |
| 0.16          | -1.39          | 0.78             | 1.29               |
| 0.87          | 0.16           | 0.69             | 0.87               |
| -0.56         | 0.3            | -1.81            | 0.44               |
| -0.61         | -1.32          | -0.41            | -0.45              |
| 0.61          | -0.58          | 1.05             | 0.16               |
| 0.81          | -0.82          | 1.17             | 1.04               |
| -1.83         | -2.51          | -1.53            | -0.12              |
| -0.48         | -0.82          | 0.3              | -0.37              |
| 0.73          | -1.24          | 1.44             | 0                  |
| 0.43          | 0.55           | 0.45             | 0.53               |
| 0.1           | -1.03          | 0.69             | -0.79              |
| -0.93         | 0.74           | -0.15            | -0.3               |
| 0.08          | 1.15           | -0.16            | -3.69              |
| 0.58          | 1.91           | 0.39             | 0.49               |
| -0.39         | 1.52           | -2.54            | -0.44              |
| -0.65         | -0.07          | -0.11            | -1.15              |
| -0.22         | -0.76          | -0.17            | 0.18               |
| 0.2           | -0.33          | 0.52             | 0.06               |

**Supplementary Table S3. Results from Visual Rule Extraction algorithm**

| Subject ID | Diagnosis | Predicted | Sex | Age | BMI   | mtDNA CN | mtDNA deletions | L/P   | BCAA/AAA | CP    | Total BR | CysCys/Total Cys | Pyruvic acid | L-Glutamic acid |
|------------|-----------|-----------|-----|-----|-------|----------|-----------------|-------|----------|-------|----------|------------------|--------------|-----------------|
| K10No_WD   | Control   | WD        | 2   | 52  | -0.51 | 0.71     | 1.09            | -0.19 | 1.42     | 1.45  | -0.2     | -1.39            | 0.92         | -0.33           |
| K6No_WD    | Control   | Control   | 2   | 38  | -1.62 | 0.98     | -0.58           | -1.48 | 1.41     | 1.06  | -1.08    | -1.09            | 1            | -1.84           |
| M2No_WD    | Control   | WD        | 1   | 45  | 1.53  | 0.79     | 0.06            | 0.12  | 1.27     | 1.17  | -1.42    | -1.27            | 0.46         | -0.08           |
| K1No_WD    | Control   | Control   | 2   | 38  | -1.16 | 0.72     | -0.34           | -0.38 | 0.96     | 0.69  | -0.62    | 0.79             | 0.59         | -2.02           |
| K4No_WD    | Control   | Control   | 2   | 31  | -0.39 | 0.26     | -1.02           | -0.84 | 1.13     | 0.89  | -0.32    | 0.45             | 0.69         | -1.86           |
| 2275WD     | WD        | WDNEU     | 2   | 17  | -0.57 | 0.87     | -0.81           | -1.25 | 0.39     | -0.61 | -0.78    | 0.83             | 0.33         | -0.61           |
| 2251WD     | WD        | WD        | 1   | 21  | 1.09  | 0.47     | 1.18            | 0.51  | 0.35     | -0.86 | -0.88    | 0.48             | -0.38        | 0.81            |
| 1715WD     | WD        | WDNEU     | 2   | 30  | -0.8  | 0.38     | -1.7            | -0.4  | -0.01    | 0.3   | 0.02     | -0.89            | -0.8         | 0.21            |
| 1776WD     | WD        | WDNEU     | 2   | 39  | 0.29  | -2.43    | -0.66           | 0.29  | 0.29     | 0.08  | 0.34     | 0.44             | -0.51        | 0.26            |
| 1779WD-H   | WDHEP     | WDHEP     | 1   | 29  | 1.31  | -1.38    | -0.8            | 0.11  | -2.51    | -0.33 | 1.98     | 0.98             | 0.14         | 0.54            |
| 2086WD-H   | WDHEP     | WD        | 2   | 32  | -0.39 | -0.2     | 1.27            | 0.3   | 0.41     | -0.7  | 0.02     | -0.08            | -0.48        | 0.86            |
| 2415WD-H   | WDHEP     | WDHEP     | 1   | 46  | 0.53  | -1.16    | -0.21           | -1.37 | -1.58    | 0.46  | 2.66     | 1.69             | 1.24         | 0.77            |
| 972WD-H    | WDHEP     | WD        | 2   | 18  | 0.86  | -1.09    | -0.2            | 0.72  | -0.01    | -2.05 | -0.68    | -0.8             | 0.5          | 1.3             |
| 1843WD-H   | WDHEP     | WDNEU     | 2   | 31  | 0.44  | -0.88    | -0.31           | 0.23  | -0.6     | 0.18  | -0.11    | -0.53            | 0.23         | 0.33            |
| 2051WD-H   | WDHEP     | WD        | 2   | 56  | -0.83 | 1.3      | 0.67            | 1.12  | 0.38     | 0.61  | -0.05    | -1.01            | -1.04        | 0.82            |
| 205WD-N    | WDNEU     | WDNEU     | 1   | 44  | -1.43 | 0.14     | 0.73            | -1.03 | 0.48     | -1.71 | -0.71    | 0.74             | 0.98         | 0.02            |
| 1167WD-N   | WDNEU     | WD        | 1   | 28  | -1.22 | -0.63    | 0.87            | 1.79  | 0.12     | -1.43 | 1.01     | -0.77            | -1.62        | 0.58            |
| 1998WD-N   | WDNEU     | WD        | 1   | 27  | -1.17 | 1.04     | 0.35            | 0.52  | 0.49     | -2.79 | 1.49     | 0.67             | 0.13         | 0.06            |
| 2024WD-N   | WDNEU     | WDHEP     | 1   | 52  | 2.84  | 1.78     | 1.26            | 1.45  | -0.2     | -0.14 | 0.06     | -0.22            | -1.2         | 0.88            |
| 2508WD-N   | WDNEU     | WDNEU     | 2   | 23  | -0.35 | -0.32    | 1.61            | -0.23 | -0.2     | 0.15  | -0.41    | 0.62             | 0.17         | -0.09           |
| 1783WD-N   | WDNEU     | WDHEP     | 2   | 46  | -0.38 | 1.67     | 1.05            | -0.08 | -1.79    | -0.08 | 0.57     | 1.35             | -0.36        | 0.28            |

| Oxoglutaric acid | Glycine | L-Alanine | Succinic acid | L-Lysine | L-Aspartic acid | L-Glutamine | L-Serine | L-Methionine | Ornithine | L-Tryptophan | L-Phenylalanine | L-Tyrosine | Urea  |
|------------------|---------|-----------|---------------|----------|-----------------|-------------|----------|--------------|-----------|--------------|-----------------|------------|-------|
| -0.77            | -1.01   | -0.48     | -0.21         | -1.32    | 0.15            | 0.56        | 0.67     | -0.25        | 1.29      | -1.15        | -0.87           | -1.64      | -0.72 |
| -0.43            | -0.56   | -0.24     | -1.55         | 0.66     | -1.7            | 0.88        | -1.75    | -0.37        | -1.53     | 0.24         | -1.83           | -1.24      | 0.76  |
| -0.33            | -0.66   | 0.53      | -0.19         | 1.02     | 0.03            | 0.35        | 0.83     | -0.23        | 0.45      | 1.03         | -0.16           | 0.08       | 1.44  |
| -0.72            | 0.36    | -0.09     | 0.36          | 0.28     | -1.92           | 0.47        | -1.03    | -0.44        | -0.32     | 0.87         | -1.4            | -0.84      | -0.48 |
| -0.74            | -1.52   | -1.06     | -2.42         | 0.46     | -1.67           | 0.67        | -0.53    | -0.44        | -0.24     | 0.51         | -1.84           | -0.92      | -0.71 |
| 0.13             | -0.72   | -0.65     | -0.29         | -2.45    | -0.19           | 0.52        | -1       | -1.45        | -0.64     | 0.21         | 0.05            | -1.51      | 1.35  |
| -1.02            | 0.33    | 1.13      | 0.83          | 0.72     | 0.05            | -0.2        | 0.85     | -0.28        | 0.31      | 0.84         | 0.73            | -0.1       | -1.47 |
| 0.58             | -0.43   | -0.41     | 1.05          | 0.29     | 0.55            | -0.58       | 0.32     | -0.24        | -0.69     | -0.18        | 0.32            | -0.27      | 0.02  |
| -0.12            | -0.66   | -0.77     | 0.04          | -0.28    | 0.93            | -0.13       | -2.15    | -0.51        | -0.48     | -0.42        | 0.08            | -1.47      | -0.13 |
| 0.66             | 0.94    | 0.5       | 1.01          | -0.61    | 0.86            | 0.66        | 1.61     | 3.17         | 1.17      | 2.18         | 1.63            | 2.55       | -0.2  |
| 0.64             | 0.53    | 0.99      | 0.94          | 0.11     | 0.51            | -0.84       | 0.03     | -0.02        | 0.05      | -0.04        | 0.57            | -0.27      | -0.31 |
| 1.42             | 0.7     | 1.53      | 0.58          | 1.03     | 0.78            | 1.16        | -0.37    | 2.82         | 0.91      | -0.23        | 1.48            | 1.49       | -2.1  |
| -0.86            | 0.12    | 1.41      | 1.31          | 0.04     | 0.39            | -1.87       | 0.98     | -0.55        | -0.51     | -0.33        | -0.08           | -0.45      | -0.89 |
| -0.17            | 0.88    | -0.61     | 0.4           | 0.51     | 0.77            | 0.22        | 1.37     | -0.01        | 1.18      | -0.04        | -0.03           | 0.29       | -1.6  |
| 0.05             | -0.12   | 0.5       | 0.11          | 1.04     | -0.02           | -0.69       | -0.18    | -0.41        | 0.54      | -0.14        | 0.12            | -0.02      | 0.95  |
| 0.26             | 0.12    | 0.36      | -1.07         | 0.58     | 0.29            | 0.22        | 0.79     | -0.26        | 0.64      | -0.02        | 0               | -0.39      | -0.15 |
| -0.79            | 1.24    | -0.11     | 0.05          | -0.53    | 0.73            | -1.27       | 0.97     | -0.74        | -0.72     | -0.58        | -0.03           | 0.01       | 1.05  |
| -0.82            | 1.63    | 1.08      | -0.07         | 0.68     | 0.6             | -1.45       | 0.73     | -0.08        | -0.75     | -1.07        | 0.92            | -0.39      | 1.62  |
| -0.01            | -0.29   | 0.24      | 0.63          | -0.41    | 0.58            | -0.86       | -0.52    | -0.22        | 0.41      | -0.01        | 0.43            | 0.25       | 0.89  |
| 0.01             | 0.41    | -0.1      | -0.57         | -0.03    | 0.24            | 0.32        | -0.39    | -0.48        | -0.22     | 0.08         | -0.64           | -0.39      | 0.16  |
| -0.23            | 1.79    | -0.41     | -0.21         | 0.37     | 0.93            | 1.37        | 0.91     | 1.09         | 0.82      | 1.26         | 1.1             | 1.67       | -0.56 |

| L-Cysteine | b-Alanine | Glycerol | L-Leucine | L-Histidine | L-Proline | L-Asparagine | Citric acid | L-Valine | Cholesterol | L-Threonine | Arachidonic acid | D-Glucose | Ketoleucine | Taurine |
|------------|-----------|----------|-----------|-------------|-----------|--------------|-------------|----------|-------------|-------------|------------------|-----------|-------------|---------|
| 1.73       | -0.46     | -0.13    | 0.51      | -0.24       | -1        | 1.29         | -1.03       | 0.3      | -0.36       | 0.79        | 0.26             | -1.09     | 0.6         | 0.66    |
| 1.45       | 0.44      | -0.24    | 0.08      | 0.56        | -1.16     | 0.66         | -0.33       | 0.98     | -0.87       | -0.4        | 0.62             | 0         | 1.59        | 0.4     |
| 1.09       | -1.11     | -0.98    | 2.07      | 0.93        | 1.69      | 1.66         | -1.8        | 2.27     | -0.44       | 0.34        | -1.36            | 0.67      | 0.18        | 1.11    |
| 1.49       | -1.1      | -0.06    | -0.29     | 0.63        | -0.67     | 0.19         | -0.73       | 0.44     | -1.33       | 1.27        | -0.33            | 1.85      | 1.39        | 0.44    |
| 1.18       | -0.37     | 0.09     | -0.13     | -0.55       | -0.8      | 0.05         | 0.41        | 0.68     | -0.03       | 0.47        | 0.15             | 0.67      | 1.05        | -0.26   |
| -0.32      | 0.48      | 0.1      | -0.86     | 0.52        | -1        | -0.61        | -0.15       | -0.63    | 0.31        | -2.89       | 0.11             | 0.73      | 0.48        | 0.18    |
| -0.81      | -1.71     | -0.02    | 1         | 0.18        | 0.65      | -0.34        | -0.03       | 1.32     | -0.77       | -0.11       | 0.89             | -0.37     | 0.61        | 0.54    |
| -0.87      | 1.06      | 0.98     | -0.2      | 0.23        | -0.43     | -0.72        | -0.23       | 0.45     | -0.02       | -0.39       | -0.04            | -0.01     | -0.07       | 0.4     |
| 0.06       | 0.05      | -2.78    | -0.58     | 0.2         | -1.66     | -0.37        | 1.02        | -1.11    | 1.56        | -0.23       | 1.38             | 1.23      | 0.6         | 0.36    |
| -0.26      | 1.33      | -0.43    | -0.88     | 1.68        | 1.83      | 0.74         | 1.92        | -1.21    | 0.45        | 0.86        | -0.41            | 0.05      | -0.34       | -2      |
| -0.98      | 0.97      | 0.52     | 0.77      | -1.55       | -0.07     | -1.62        | -1.54       | 0.84     | -0.51       | 0.44        | 0.5              | -0.74     | -0.75       | 0.95    |
| 0.32       | -1.05     | 0.37     | 0.07      | 1.9         | 2.65      | 2.19         | 1.16        | -1.11    | 0.3         | 1.46        | 0.74             | -0.47     | -1.26       | -0.05   |
| -0.44      | -0.46     | 0.63     | -1.38     | 0.38        | 0.19      | -1.51        | -1.15       | -0.73    | -0.08       | -0.52       | -0.62            | 0.16      | -0.85       | 0.58    |
| -0.04      | -0.78     | 0.42     | -0.05     | 0.97        | -0.99     | -0.27        | 0.38        | -0.43    | 1.09        | 0.86        | 0.4              | -1.74     | -0.34       | 0.21    |
| 0.11       | 1.43      | 0.54     | 0.89      | 0.34        | -0.63     | 0.09         | -0.76       | 0.36     | -0.22       | 0.05        | -0.26            | -0.84     | 0.36        | 0.49    |
| 0.15       | 0.21      | -0.66    | 0.52      | -0.55       | -0.14     | -0.96        | -1.5        | 0.4      | -0.33       | -0.67       | -1.35            | 0.86      | 0.15        | -3.3    |
| -1.66      | 0.62      | 0.82     | 0.23      | -2.12       | 0.07      | -1.17        | -0.91       | -0.25    | -1.94       | 0.39        | -0.82            | -0.52     | -0.1        | 0.92    |
| -1.42      | 1.91      | 0.38     | 0.96      | -1.33       | 0.24      | -0.39        | 1.14        | 0.1      | -0.58       | -0.56       | -0.15            | -1.22     | 0.05        | 0.75    |
| -0.52      | 1.05      | 0.87     | 0.65      | 0.1         | 0.24      | 0.14         | 0.41        | -0.11    | -0.3        | -0.56       | 1.11             | -2.11     | -0.98       | -0.24   |
| 0.18       | -0.75     | -0.88    | -1.63     | 0.29        | -0.17     | -0.76        | 1.06        | -0.73    | 1.52        | -0.44       | 0.42             | 0.27      | 0.25        | 0.16    |
| 0.03       | -0.61     | -4.95    | -0.5      | 1.17        | 1.22      | 1.18         | 0.84        | -0.57    | 0.91        | 1.19        | -0.76            | -0.38     | -2.19       | -0.82   |

| Palmitic acid | Citrulline | Uric acid | L-Isoleucine | N-Acetylornithine | Isocitric acid | N-Acetylglutamic acid | Malate | Oleic acid | Creatinine | Indoleacetic acid | g-Hydroxybutyric Acid |
|---------------|------------|-----------|--------------|-------------------|----------------|-----------------------|--------|------------|------------|-------------------|-----------------------|
| 0.21          | 0.47       | 0.37      | 0.59         | 1.2               | -1.51          | 0.59                  | 0.47   | 0.16       | 0.47       | 0.5               | 0.33                  |
| 0.19          | -0.79      | 0.12      | 0.17         | -1.82             | -0.59          | 0.16                  | -0.16  | 0.88       | 0.84       | 0.42              | -1.77                 |
| -1.56         | -0.71      | 0.31      | 1.35         | -1.9              | -1.16          | -2.63                 | -0.38  | -0.41      | 0.23       | 0.1               | -1.47                 |
| -0.31         | -0.47      | 1.09      | -0.42        | -0.08             | -1.43          | 1.57                  | -0.03  | 0.54       | -0.05      | 0.93              | 0.43                  |
| 0.43          | -0.76      | 0.92      | -0.1         | 0.61              | -0.67          | 0.16                  | -0.56  | 0.85       | -0.08      | 1.32              | 0.49                  |
| 0.47          | 0.23       | 0.6       | -0.74        | -1.84             | 0.16           | -0.51                 | -0.98  | -0.44      | 0.85       | -0.26             | 0.31                  |
| -1.11         | 0.52       | 1.6       | 0.31         | 0.07              | 0.1            | 0.11                  | -0.5   | -0.13      | 0.86       | 0.61              | -0.49                 |
| 0.88          | 0.08       | 0.26      | -0.32        | 0.33              | 0.01           | -1.19                 | -0.49  | 1.31       | 0.41       | -0.43             | 0.85                  |
| 0.94          | -0.87      | 0.07      | -0.84        | 0.3               | 1.09           | -0.47                 | -0.38  | 1.11       | 0.44       | -0.98             | 0.51                  |
| -2.75         | 0.01       | 0.64      | -0.35        | -0.63             | 2.17           | -0.02                 | 1.12   | -2.35      | 0.86       | 1.14              | -0.55                 |
| -0.44         | 0.78       | 0.85      | 0.48         | 1.91              | -0.87          | 0.21                  | -0.55  | -0.51      | -0.23      | 0.31              | 1.19                  |
| 0.11          | 0.53       | -1.25     | -0.46        | -0.32             | 0.97           | -0.22                 | 0.73   | 0.75       | 0.5        | -1.54             | -1.58                 |
| 0.3           | -0.02      | -0.17     | -0.64        | 0.61              | -0.65          | -0.79                 | 0.11   | 0.55       | -3.3       | 0.05              | -0.9                  |
| -0.95         | -1.71      | -0.96     | -0.9         | 0.79              | 0.24           | 0.12                  | 1.52   | 0.16       | 0.46       | -0.95             | -0.81                 |
| 0.17          | 1.8        | 0.17      | 0.78         | 1.82              | -0.66          | -0.13                 | -0.24  | -0.74      | 0.44       | -2.11             | 1.36                  |
| -0.09         | -0.45      | -1.09     | 0.41         | 0.75              | -1.4           | 0.76                  | -0.88  | 0.2        | -0.16      | 0.66              | 0.65                  |
| 1.04          | 0.69       | -1.45     | 0.72         | -0.04             | 0.11           | 1.02                  | -0.66  | 0.3        | -1.53      | -0.79             | 0.47                  |
| -0.24         | -0.28      | -0.39     | 1.25         | -0.62             | 0.94           | 1.02                  | -0.03  | -1.09      | 0.57       | -0.58             | -1.21                 |
| -0.84         | -0.94      | 0.12      | 0.55         | 1.32              | 0.69           | -0.7                  | 0.16   | -0.61      | -0.02      | -1.37             | 1.3                   |
| -1.11         | -1.44      | -0.39     | -0.99        | -0.25             | 1.12           | 0.22                  | -0.01  | -0.27      | 0.34       | 0.03              | -0.67                 |
| -0.84         | -0.19      | -0.95     | -0.59        | -1.12             | -1.32          | -0.03                 | -0.27  | -0.13      | 0.04       | -0.04             | -2.1                  |

| 3-Hydroxybutyric acid | 4-Hydroxyproline | Cystine | Lactic acid | Stearic acid | Capric acid | Linoleic acid | Pelargonic acid | Threonic acid | Pyroglutamic acid | 1-Acylglycerol |
|-----------------------|------------------|---------|-------------|--------------|-------------|---------------|-----------------|---------------|-------------------|----------------|
| -1.14                 | -0.02            | 0.1     | 1.65        | 0.78         | -0.3        | 0.3           | -0.21           | 1.07          | 0.91              | -0.23          |
| 1.23                  | -0.94            | 0.15    | -0.55       | -0.06        | 0.21        | 1.02          | -1.3            | 1.32          | -0.4              | -1.65          |
| -0.83                 | -0.45            | -0.46   | 0.89        | -0.94        | -0.15       | 0.31          | -1.45           | 0.86          | 1.2               | -0.04          |
| -1.18                 | 0.08             | 1.54    | 0.52        | -0.44        | 0.09        | 0.62          | -2.36           | 2.11          | 1.48              | -1.45          |
| 1.63                  | -0.46            | 1.07    | -0.05       | 0.51         | -1.95       | 0.49          | -0.39           | 1.68          | -0.24             | -2.1           |
| 0.06                  | -0.51            | 0.73    | -1.49       | 0.52         | -0.09       | 0.39          | -0.72           | 0.36          | -1.25             | 0.06           |
| -0.29                 | 0.2              | -0.28   | 0.27        | -1.2         | -0.56       | 0.47          | -0.68           | -0.4          | 0                 | -0.9           |
| 0.86                  | -2.15            | -1.25   | -2.17       | 0.08         | 0.36        | 1.03          | 0.48            | 0.19          | -2.27             | -0.33          |
| 0.52                  | -0.05            | 0.37    | -0.29       | -0.03        | 0.87        | 0.23          | 0.64            | -2.23         | -0.87             | -0.98          |
| -0.54                 | 1.83             | 0.24    | 0.2         | -2.49        | -0.74       | 0.25          | -0.37           | 0.37          | 0.12              | -0.5           |
| -0.29                 | -1               | -0.92   | -0.38       | -0.27        | -0.42       | -0.25         | -0.6            | 0.67          | -0.15             | 1.89           |
| 0.11                  | 1.68             | 3.03    | -0.32       | -1.36        | 0.62        | 0.96          | 0.77            | -0.32         | 0.17              | -1.6           |
| 1.23                  | -0.85            | -1.11   | 2.24        | 0.36         | -0.84       | 0.85          | -1.11           | 0.23          | -2.25             | -0.72          |
| -0.4                  | 0.16             | -0.46   | 1.15        | -1.7         | 0.23        | -0.87         | -0.42           | -0.98         | 0.19              | 0.36           |
| -0.46                 | -1.26            | -0.85   | -0.02       | 0.93         | -0.31       | -0.2          | 0.5             | 0.74          | -0.46             | -0.25          |
| -0.94                 | 0.15             | 0.59    | 0.03        | 0.73         | -1.73       | -0.24         | -0.5            | -0.41         | 0.7               | -0.45          |
| 1.13                  | 0.89             | -1.82   | 0.11        | 1.36         | 0.47        | 0.12          | 0.96            | -0.72         | 0.51              | 2.24           |
| -0.56                 | 0.19             | -0.74   | 1.04        | -0.04        | 0.33        | -1.62         | 1.28            | 0.16          | 2.42              | 1.26           |
| -0.37                 | 0.51             | -0.68   | 0.44        | -0.57        | -0.29       | 0.11          | -0.48           | 0.12          | -1.31             | 1.38           |
| -0.02                 | 0.11             | 0.61    | 0.05        | -1.09        | -0.15       | -1.12         | 0.17            | 0.14          | 0.22              | -0.34          |
| -0.61                 | 0.68             | 1.95    | -0.84       | -0.93        | 0.89        | -0.69         | 0.63            | 0.13          | 0.81              | -1.03          |



| Indolelactic acid | Gamma-Tocopherol | Dodecanoic acid | N-Methylalanine | Glycerolphosphate | 3-Aminoisobutanoic acid | 5-Methoxytryptamine | 2-Hydroxybutyric acid |
|-------------------|------------------|-----------------|-----------------|-------------------|-------------------------|---------------------|-----------------------|
| -0.54             | 0.11             | 0.17            | 1.4             | 1.62              | -1.17                   | -0.14               | -0.11                 |
| 0.56              | 0.3              | 0.04            | 0.73            | 0.93              | 0.26                    | 0.75                | 1.28                  |
| 0.5               | 0.56             | 0.69            | 0.1             | 1.87              | -0.53                   | -1.47               | -1.7                  |
| 0.81              | -0.8             | 0.2             | 0.64            | 1.15              | -1.49                   | 1.5                 | -0.81                 |
| 0.55              | 1.76             | -0.19           | 2.19            | 1.25              | -0.03                   | 1.21                | 0.2                   |
| 0.26              | 1.82             | -3              | -0.99           | 0.75              | -0.37                   | 1.92                | 0.25                  |
| 0.11              | 1.08             | -0.6            | -0.08           | -3.67             | -3.19                   | 1.1                 | -0.47                 |
| -0.94             | -0.45            | 0.16            | 0.44            | -0.75             | 1.02                    | -0.05               | 1.54                  |
| 0.35              | 0.9              | 1.4             | -0.84           | 0.51              | 0.61                    | 0.94                | 0.16                  |
| 3.17              | -1.41            | -3.42           | -1.12           | -0.76             | -0.04                   | -0.18               | -1.18                 |
| -0.1              | 0.83             | -1.04           | 0.54            | -0.93             | 1.49                    | -1.12               | -0.27                 |
| -1.05             | 0.19             | 0.81            | 0.21            | -1.42             | 1.43                    | -0.15               | 0.2                   |
| -0.3              | -1.33            | 0.84            | 0.61            | 0.7               | 0.5                     | 0.22                | 0.57                  |
| 0.59              | 0.5              | 0.33            | -0.02           | -0.09             | -0.64                   | 0.26                | -0.11                 |
| 0.14              | 0.5              | -1.27           | 1               | -0.96             | 0.45                    | -1.38               | 0.4                   |
| -0.04             | 0.02             | -0.03           | 0.52            | 1.49              | -0.53                   | 1.15                | -0.68                 |
| -0.9              | -0.71            | 0.75            | 0.94            | -0.31             | 0.98                    | -0.75               | -0.29                 |
| -0.95             | -1.08            | -0.21           | -0.24           | -1.04             | 0.81                    | -1.33               | -2.19                 |
| -0.12             | 0.41             | -0.71           | -0.21           | -0.08             | -0.41                   | 0.26                | -0.17                 |
| -0.43             | 0.87             | -0.14           | -0.29           | 0.84              | -0.06                   | 1.25                | 0.35                  |
| 0.69              | 0.91             | 0.72            | 0.64            | -0.34             | 0.62                    | -0.21               | 0.85                  |

| Myristic acid | Arachidic acid | Palmitoleic acid | Pentadecanoic acid |
|---------------|----------------|------------------|--------------------|
| -0.81         | 0.62           | -0.55            | -3.71              |
| 0.68          | -0.02          | 0.36             | 0.41               |
| -0.14         | -0.97          | -0.66            | 0.44               |
| 0.16          | -1.39          | 0.78             | 1.29               |
| 0.87          | 0.16           | 0.69             | 0.87               |
| -0.56         | 0.3            | -1.81            | 0.44               |
| -0.61         | -1.32          | -0.41            | -0.45              |
| 0.61          | -0.58          | 1.05             | 0.16               |
| 0.81          | -0.82          | 1.17             | 1.04               |
| -1.83         | -2.51          | -1.53            | -0.12              |
| -0.48         | -0.82          | 0.3              | -0.37              |
| 0.73          | -1.24          | 1.44             | 0                  |
| 0.43          | 0.55           | 0.45             | 0.53               |
| 0.1           | -1.03          | 0.69             | -0.79              |
| -0.93         | 0.74           | -0.15            | -0.3               |
| 0.08          | 1.15           | -0.16            | -3.69              |
| 0.58          | 1.91           | 0.39             | 0.49               |
| -0.39         | 1.52           | -2.54            | -0.44              |
| -0.65         | -0.07          | -0.11            | -1.15              |
| -0.22         | -0.76          | -0.17            | 0.18               |
| 0.2           | -0.33          | 0.52             | 0.06               |

**Supplementary Table S4. PCA  
variance when using all outcomes**

|      | Individual | Cumulative  |
|------|------------|-------------|
| PC1  | 0.15       | <b>0.15</b> |
| PC2  | 0.12       | <b>0.27</b> |
| PC3  | 0.10       | <b>0.37</b> |
| PC4  | 0.07       | <b>0.44</b> |
| PC5  | 0.05       | <b>0.48</b> |
| PC6  | 0.04       | <b>0.52</b> |
| PC7  | 0.04       | <b>0.56</b> |
| PC8  | 0.04       | <b>0.60</b> |
| PC9  | 0.03       | <b>0.63</b> |
| PC10 | 0.03       | <b>0.66</b> |
| PC11 | 0.03       | <b>0.69</b> |
| PC12 | 0.02       | <b>0.71</b> |
| PC13 | 0.02       | <b>0.73</b> |
| PC14 | 0.02       | <b>0.75</b> |
| PC15 | 0.02       | <b>0.77</b> |
| PC16 | 0.02       | <b>0.79</b> |
| PC17 | 0.02       | <b>0.80</b> |
| PC18 | 0.02       | <b>0.82</b> |
| PC19 | 0.01       | <b>0.83</b> |
| PC20 | 0.01       | <b>0.85</b> |
| PC21 | 0.01       | 0.86        |
| PC22 | 0.01       | 0.87        |
| PC23 | 0.01       | 0.88        |
| PC24 | 0.01       | 0.89        |
| PC25 | 0.01       | 0.90        |
| PC26 | 0.01       | 0.91        |
| PC27 | 0.01       | 0.91        |
| PC28 | 0.01       | 0.92        |
| PC29 | 0.01       | 0.93        |
| PC30 | 0.01       | 0.94        |
| PC31 | 0.01       | 0.94        |
| PC32 | 0.01       | 0.95        |
| PC33 | 0.00       | 0.95        |
| PC34 | 0.00       | 0.96        |
| PC35 | 0.00       | 0.96        |
| PC36 | 0.00       | 0.97        |
| PC37 | 0.00       | 0.97        |
| PC38 | 0.00       | 0.97        |
| PC39 | 0.00       | 0.98        |
| PC40 | 0.00       | 0.98        |

|      |      |      |
|------|------|------|
| PC41 | 0.00 | 0.98 |
| PC42 | 0.00 | 0.98 |
| PC43 | 0.00 | 0.99 |
| PC44 | 0.00 | 0.99 |
| PC45 | 0.00 | 0.99 |
| PC46 | 0.00 | 0.99 |
| PC47 | 0.00 | 0.99 |
| PC48 | 0.00 | 0.99 |
| PC49 | 0.00 | 0.99 |
| PC50 | 0.00 | 1.00 |
| PC51 | 0.00 | 1.00 |
| PC52 | 0.00 | 1.00 |
| PC53 | 0.00 | 1.00 |
| PC54 | 0.00 | 1.00 |
| PC55 | 0.00 | 1.00 |
| PC56 | 0.00 | 1.00 |
| PC57 | 0.00 | 1.00 |
| PC58 | 0.00 | 1.00 |
| PC59 | 0.00 | 1.00 |
| PC60 | 0.00 | 1.00 |
| PC61 | 0.00 | 1.00 |
| PC62 | 0.00 | 1.00 |

Supplementary Table S5. PCA loadings when using all outcomes

|                           | PC1   | PC2   | PC3   | PC4   | PC5   | PC6   | PC7   | PC8   | PC9   | PC10  | PC11  | PC12  | PC13  | PC14  | PC15  | PC16  | PC17  | PC18  | PC19  | PC20  | PC21  | PC22  | PC23  | PC24  | PC25  | PC26  | PC27  | PC28  | PC29  | PC30  |
|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| BCAA/AAA                  | 0.26  | 0.03  | -0.06 | 0.07  | -0.03 | -0.11 | 0.09  | -0.01 | -0.03 | 0.03  | 0.10  | 0.08  | -0.17 | 0.08  | -0.05 | 0.00  | -0.04 | 0.06  | -0.03 | 0.08  | -0.02 | 0.06  | -0.01 | -0.04 | 0.04  | -0.10 | 0.05  | -0.04 | 0.01  | 0.02  |
| Threonic acid             | 0.22  | -0.01 | 0.00  | -0.02 | 0.07  | 0.03  | 0.09  | -0.08 | -0.09 | -0.09 | 0.07  | -0.07 | 0.18  | -0.06 | 0.14  | 0.01  | 0.15  | -0.09 | -0.03 | 0.03  | 0.18  | 0.01  | 0.06  | 0.04  | -0.16 | 0.19  | 0.15  | -0.14 | 0.08  | -0.01 |
| Ketoleucine               | 0.18  | 0.05  | 0.02  | 0.14  | 0.13  | -0.05 | -0.07 | 0.06  | 0.17  | 0.18  | 0.00  | -0.10 | -0.05 | 0.29  | 0.10  | -0.13 | 0.07  | 0.03  | -0.19 | 0.01  | -0.03 | 0.12  | -0.15 | -0.06 | 0.00  | 0.00  | 0.02  | 0.08  | 0.13  | 0.02  |
| Uric acid                 | 0.18  | -0.09 | 0.06  | 0.20  | -0.07 | -0.06 | -0.11 | -0.01 | 0.08  | -0.06 | 0.15  | -0.01 | -0.02 | 0.09  | 0.16  | 0.19  | -0.06 | 0.02  | 0.08  | 0.12  | 0.02  | -0.02 | -0.07 | -0.06 | -0.10 | 0.09  | 0.14  | 0.16  | -0.04 | 0.11  |
| L-Cysteine                | 0.17  | -0.14 | 0.13  | -0.06 | -0.04 | -0.01 | 0.18  | 0.05  | -0.11 | 0.04  | 0.00  | 0.00  | -0.01 | 0.05  | 0.04  | -0.02 | -0.10 | 0.06  | -0.13 | -0.01 | -0.28 | -0.11 | 0.03  | -0.04 | -0.17 | 0.08  | -0.21 | -0.06 | -0.04 | -0.02 |
| Glycerolphosphate         | 0.15  | -0.02 | 0.09  | 0.01  | 0.05  | 0.11  | 0.11  | 0.06  | -0.06 | -0.18 | -0.24 | 0.06  | 0.00  | 0.19  | -0.08 | 0.10  | -0.19 | 0.20  | 0.02  | -0.05 | 0.02  | 0.19  | 0.24  | 0.07  | -0.02 | 0.06  | -0.14 | -0.13 | 0.33  | -0.02 |
| D-Glucose                 | 0.15  | -0.08 | 0.09  | -0.11 | 0.08  | -0.14 | -0.23 | 0.01  | 0.11  | 0.01  | -0.10 | -0.08 | -0.10 | -0.04 | 0.06  | 0.14  | 0.07  | 0.14  | 0.03  | 0.00  | -0.07 | -0.15 | -0.13 | 0.01  | 0.16  | -0.12 | -0.05 | -0.09 | 0.22  | 0.13  |
| L-Valine                  | 0.14  | -0.14 | -0.15 | 0.08  | -0.12 | -0.22 | 0.01  | -0.11 | -0.04 | 0.11  | 0.00  | -0.03 | -0.11 | -0.01 | -0.10 | 0.03  | -0.02 | 0.04  | -0.07 | 0.07  | 0.03  | 0.18  | -0.09 | 0.03  | 0.02  | -0.01 | 0.15  | 0.13  | 0.14  | -0.13 |
| mtDNA CN                  | 0.13  | -0.05 | -0.01 | -0.09 | -0.12 | 0.09  | 0.19  | 0.04  | -0.05 | 0.00  | 0.18  | 0.16  | 0.14  | -0.09 | -0.11 | 0.11  | 0.04  | -0.15 | 0.14  | 0.04  | 0.37  | -0.03 | -0.17 | -0.13 | -0.02 | 0.13  | -0.05 | -0.03 | 0.12  | -0.21 |
| Indoleacetic acid         | 0.13  | -0.13 | -0.02 | 0.03  | 0.00  | 0.02  | -0.14 | -0.07 | 0.16  | -0.06 | -0.22 | 0.17  | 0.02  | 0.06  | 0.13  | -0.09 | 0.07  | 0.04  | 0.22  | 0.12  | -0.02 | 0.06  | 0.29  | 0.05  | 0.18  | 0.25  | -0.08 | -0.01 | -0.01 | 0.08  |
| Indolelactic acid         | 0.12  | -0.19 | 0.00  | 0.05  | 0.00  | 0.03  | -0.18 | -0.09 | 0.12  | -0.09 | 0.00  | -0.18 | 0.12  | -0.02 | 0.08  | 0.04  | -0.06 | -0.01 | 0.05  | -0.07 | -0.25 | -0.10 | 0.03  | -0.17 | 0.01  | -0.05 | 0.22  | 0.02  | 0.02  | -0.12 |
| CP                        | 0.12  | -0.02 | 0.12  | -0.11 | -0.04 | -0.02 | 0.04  | -0.21 | -0.14 | 0.11  | 0.13  | -0.14 | 0.12  | 0.11  | 0.13  | -0.07 | -0.34 | -0.17 | 0.10  | -0.08 | 0.02  | 0.01  | -0.02 | 0.28  | 0.07  | -0.19 | -0.01 | 0.19  | -0.07 | 0.21  |
| Creatinine                | 0.10  | -0.13 | 0.04  | 0.13  | -0.08 | 0.26  | -0.01 | 0.05  | -0.05 | 0.12  | 0.16  | 0.00  | -0.09 | -0.01 | -0.01 | 0.03  | 0.24  | -0.23 | -0.04 | -0.08 | 0.00  | 0.20  | 0.11  | -0.09 | -0.07 | 0.03  | 0.06  | 0.20  | 0.04  | 0.15  |
| L-Glutamine               | 0.10  | -0.15 | 0.08  | -0.15 | -0.08 | 0.30  | 0.12  | 0.03  | -0.01 | 0.05  | 0.00  | -0.07 | 0.08  | 0.04  | 0.01  | 0.07  | 0.08  | 0.08  | -0.04 | 0.01  | -0.10 | -0.06 | -0.08 | 0.08  | -0.02 | -0.06 | 0.06  | 0.06  | -0.07 | -0.04 |
| Gamma-Tocopherol          | 0.09  | -0.06 | 0.10  | -0.05 | -0.04 | 0.12  | -0.02 | -0.06 | 0.10  | 0.10  | 0.16  | 0.31  | -0.12 | -0.25 | -0.17 | -0.07 | -0.05 | 0.04  | 0.00  | -0.07 | -0.15 | -0.05 | 0.06  | 0.50  | -0.20 | 0.09  | 0.13  | -0.01 | 0.12  | -0.15 |
| Stearic acid              | 0.08  | 0.25  | -0.13 | -0.08 | -0.06 | 0.07  | -0.02 | 0.01  | 0.01  | 0.05  | -0.13 | -0.08 | 0.03  | 0.09  | 0.08  | 0.14  | -0.01 | 0.10  | -0.09 | 0.02  | 0.12  | -0.05 | 0.07  | 0.01  | 0.03  | 0.00  | -0.02 | 0.03  | -0.02 | 0.00  |
| Pyroglutamic acid         | 0.07  | -0.01 | -0.03 | -0.30 | 0.14  | -0.12 | 0.18  | 0.03  | 0.20  | -0.03 | 0.04  | 0.05  | 0.06  | -0.04 | 0.05  | 0.01  | 0.09  | -0.05 | -0.09 | -0.08 | 0.09  | 0.07  | 0.06  | -0.13 | 0.01  | 0.03  | 0.22  | 0.15  | 0.16  | 0.05  |
| L-Leucine                 | 0.06  | -0.12 | -0.19 | 0.08  | -0.09 | -0.22 | 0.08  | -0.05 | 0.10  | 0.19  | 0.00  | -0.02 | -0.14 | 0.03  | -0.11 | 0.04  | 0.09  | -0.15 | -0.03 | -0.05 | -0.06 | 0.22  | -0.06 | 0.01  | -0.06 | 0.04  | -0.16 | 0.13  | -0.02 | -0.02 |
| N-Acetylglutamic acid     | 0.06  | 0.08  | 0.00  | -0.21 | 0.04  | -0.06 | 0.09  | 0.10  | 0.26  | 0.01  | 0.05  | 0.07  | 0.03  | 0.08  | -0.01 | -0.17 | 0.16  | -0.25 | 0.17  | 0.20  | -0.20 | -0.24 | -0.16 | -0.04 | -0.06 | 0.14  | -0.23 | -0.03 | 0.02  | 0.20  |
| L-Asparagine              | 0.06  | -0.17 | 0.04  | -0.16 | -0.13 | 0.08  | 0.17  | -0.09 | -0.04 | 0.12  | 0.15  | -0.14 | 0.04  | 0.17  | 0.12  | 0.04  | 0.05  | 0.04  | 0.02  | -0.14 | 0.18  | 0.08  | 0.06  | -0.01 | 0.12  | -0.10 | -0.20 | -0.03 | 0.18  | 0.02  |
| Pyruvic acid              | 0.05  | -0.08 | 0.16  | 0.03  | 0.15  | -0.14 | 0.02  | 0.28  | -0.01 | 0.30  | -0.03 | 0.02  | 0.16  | 0.01  | -0.13 | 0.00  | -0.10 | 0.04  | -0.08 | 0.06  | 0.07  | -0.13 | 0.13  | -0.09 | 0.06  | 0.04  | 0.16  | -0.03 | -0.03 | -0.01 |
| L-Tryptophan              | 0.05  | -0.24 | -0.04 | 0.08  | -0.05 | 0.07  | -0.19 | -0.04 | 0.06  | -0.04 | -0.13 | -0.14 | 0.04  | -0.02 | 0.05  | 0.18  | 0.09  | 0.08  | 0.00  | -0.04 | -0.11 | -0.11 | -0.13 | -0.02 | -0.08 | 0.18  | 0.02  | 0.12  | 0.02  | -0.02 |
| Urea                      | 0.04  | 0.06  | -0.20 | -0.02 | 0.13  | 0.19  | -0.12 | -0.23 | -0.06 | 0.05  | -0.02 | 0.03  | 0.09  | 0.11  | -0.18 | 0.02  | -0.11 | -0.15 | -0.12 | 0.20  | -0.06 | 0.05  | -0.07 | 0.01  | 0.20  | 0.04  | -0.01 | -0.06 | 0.17  | 0.04  |
| Pentadecanoic acid        | 0.04  | 0.02  | 0.08  | -0.07 | 0.12  | -0.01 | -0.22 | -0.18 | -0.06 | -0.02 | 0.26  | -0.20 | -0.16 | -0.09 | 0.06  | -0.04 | 0.13  | 0.26  | 0.08  | 0.07  | 0.13  | -0.22 | 0.16  | -0.08 | -0.04 | 0.04  | -0.30 | 0.22  | 0.22  | -0.18 |
| (R)-3-Hydroxybutyric acid | 0.04  | 0.16  | 0.07  | 0.00  | -0.05 | 0.10  | 0.04  | 0.01  | 0.11  | 0.10  | 0.09  | -0.25 | 0.01  | 0.05  | -0.32 | -0.10 | 0.15  | 0.25  | 0.36  | -0.12 | -0.05 | 0.04  | -0.11 | -0.06 | -0.05 | -0.09 | 0.15  | -0.15 | 0.01  | -0.07 |
| L-Isoleucine              | 0.03  | -0.04 | -0.26 | -0.06 | -0.14 | -0.19 | 0.04  | -0.03 | 0.07  | 0.11  | 0.09  | -0.02 | -0.13 | 0.16  | -0.02 | 0.03  | 0.07  | -0.04 | -0.11 | 0.04  | -0.11 | 0.09  | -0.04 | 0.06  | 0.14  | 0.15  | -0.02 | -0.20 | 0.06  | -0.19 |
| 5-Methoxytryptamine       | 0.03  | -0.10 | 0.19  | 0.08  | -0.08 | 0.10  | -0.08 | 0.26  | 0.02  | -0.15 | -0.07 | 0.07  | -0.04 | 0.13  | -0.09 | 0.01  | 0.04  | 0.13  | -0.01 | 0.18  | -0.04 | 0.01  | -0.32 | 0.13  | -0.04 | -0.09 | -0.15 | 0.01  | 0.02  | -0.12 |
| N-Methylalanine           | 0.03  | -0.02 | 0.04  | 0.00  | -0.15 | -0.02 | 0.09  | -0.20 | -0.11 | -0.24 | -0.08 | 0.21  | 0.20  | 0.34  | -0.07 | -0.27 | -0.01 | 0.23  | 0.01  | 0.02  | 0.01  | 0.03  | -0.10 | -0.05 | -0.04 | 0.12  | 0.20  | 0.10  | -0.07 | -0.01 |
| Gamma Hydroxybutyric Acid | 0.03  | 0.17  | -0.16 | 0.01  | -0.13 | 0.06  | -0.06 | 0.19  | 0.03  | 0.07  | -0.11 | -0.04 | 0.01  | -0.04 | 0.18  | -0.09 | -0.22 | -0.07 | 0.18  | -0.06 | -0.05 | 0.07  | -0.14 | 0.05  | -0.10 | 0.02  | 0.05  | -0.08 | 0.31  | 0.05  |
| L-Lysine                  | 0.03  | -0.10 | -0.09 | 0.07  | -0.05 | 0.08  | 0.10  | -0.07 | 0.11  | 0.27  | -0.24 | -0.04 | -0.22 | 0.06  | 0.03  | -0.20 | 0.08  | -0.04 | 0.28  | 0.09  | 0.19  | -0.16 | -0.04 | -0.04 | -0.06 | -0.03 | 0.02  | -0.09 | -0.20 | -0.25 |
| Taurine                   | 0.03  | -0.01 | -0.05 | 0.24  | 0.12  | 0.14  | 0.01  | -0.26 | 0.02  | 0.17  | 0.06  | 0.15  | -0.13 | 0.03  | 0.01  | -0.10 | -0.11 | 0.22  | -0.03 | 0.19  | 0.13  | -0.09 | 0.01  | -0.09 | -0.11 | -0.03 | 0.02  | 0.10  | -0.08 | 0.05  |
| Arachidic acid            | 0.02  | 0.21  | -0.17 | -0.12 | -0.02 | 0.09  | 0.09  | 0.06  | 0.00  | 0.00  | -0.09 | -0.05 | 0.02  | 0.09  | -0.06 | 0.19  | 0.08  | 0.04  | -0.21 | 0.02  | 0.08  | -0.08 | 0.04  | 0.08  | 0.00  | 0.03  | -0.20 | 0.06  | -0.13 | -0.09 |
| Lactic acid               | 0.01  | 0.02  | 0.06  | 0.19  | 0.12  | -0.15 | 0.26  | 0.11  | 0.22  | -0.10 | 0.19  | -0.07 | 0.02  | 0.09  | -0.11 | -0.03 | -0.03 | 0.11  | -0.02 | 0.05  | 0.06  | -0.17 | 0.31  | -0.07 | 0.09  | 0.06  | 0.06  | -0.14 | -0.02 | 0.10  |
| Oleic acid                | 0.00  | 0.18  | 0.24  | 0.05  | -0.16 | -0.11 | 0.04  | -0.06 | 0.02  | 0.05  | -0.01 | -0.04 | 0.01  | -0.04 | -0.03 | 0.03  | 0.16  | -0.01 | -0.07 | -0.04 | -0.13 | -0.08 | -0.04 | 0.02  | 0.03  | -0.06 | -0.05 | 0.03  | 0.03  | -0.02 |
| Palmitic acid             | 0.00  | 0.28  | 0.08  | -0.02 | -0.15 | 0.02  | 0.02  | -0.04 | 0.02  | 0.13  | -0.09 | -0.07 | 0.01  | 0.06  | 0.07  | 0.16  | 0.08  | 0.03  | -0.05 | 0.10  | 0.05  | -0.04 | 0.02  | -0.05 | 0.00  | -0.03 | 0.03  | 0.06  | 0.02  | 0.02  |
| Linoleic acid             | -0.01 | 0.10  | 0.20  | 0.12  | -0.15 | -0.13 | -0.04 | -0.08 | 0.10  | 0.04  | 0.07  | -0.09 | 0.26  | -0.03 | -0.04 | 0.05  | 0.08  | 0.02  | -0.17 | -0.08 | -0.02 | 0.12  | -0.02 | -0.17 | -0.13 | 0.13  | -0.01 | -0.11 | -0.11 | 0.04  |
| Cystine                   | -0.02 | -0.13 | 0.22  | -0.17 | -0.18 | 0.00  | -0.07 | 0.01  | 0.07  | 0.01  | -0.06 | 0.10  | -0.07 | 0.12  | -0.04 | 0.01  | -0.04 | -0.11 | -0.13 | 0.14  | 0.10  | -0.04 | 0.04  | -0.07 | -0.12 | -0.06 | -0.08 | -0.03 | -0.01 | 0.01  |

|                         |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Myristic acid           | -0.03 | 0.13  | 0.19  | -0.09 | 0.01  | -0.04 | 0.08  | -0.18 | 0.00  | 0.08  | -0.17 | 0.05  | -0.02 | -0.13 | -0.05 | 0.20  | 0.00  | 0.05  | -0.01 | 0.26  | -0.17 | 0.10  | 0.02  | 0.00  | 0.04  | 0.15  | 0.13  | 0.04  | 0.11  | -0.23 |
| Beta-Alanine            | -0.03 | 0.05  | -0.21 | -0.02 | 0.00  | 0.25  | 0.04  | 0.11  | -0.18 | 0.08  | 0.11  | -0.03 | 0.10  | 0.18  | 0.11  | 0.11  | 0.02  | 0.06  | -0.06 | 0.13  | -0.21 | -0.13 | 0.05  | -0.14 | 0.06  | 0.11  | 0.16  | -0.07 | 0.07  | -0.22 |
| Capric acid             | -0.03 | 0.04  | 0.07  | 0.01  | 0.22  | 0.27  | 0.15  | -0.18 | 0.11  | 0.16  | -0.13 | 0.12  | -0.08 | -0.07 | 0.03  | 0.04  | 0.04  | 0.02  | 0.02  | -0.13 | -0.09 | 0.08  | -0.19 | -0.26 | -0.19 | 0.15  | 0.00  | -0.08 | 0.00  | 0.25  |
| Dodecanoic acid         | -0.04 | 0.12  | 0.14  | -0.08 | 0.06  | -0.09 | 0.25  | -0.23 | 0.02  | 0.11  | -0.23 | 0.01  | -0.18 | -0.11 | 0.03  | 0.05  | -0.02 | 0.08  | -0.01 | 0.00  | 0.03  | 0.02  | -0.03 | -0.01 | 0.17  | -0.09 | 0.00  | 0.03  | -0.03 | -0.03 |
| Ornithine               | -0.04 | -0.16 | -0.01 | 0.07  | -0.15 | 0.23  | 0.29  | 0.10  | 0.11  | 0.11  | 0.02  | -0.06 | 0.06  | -0.06 | 0.11  | -0.04 | 0.06  | 0.09  | -0.03 | -0.05 | -0.08 | -0.02 | 0.09  | -0.01 | 0.03  | -0.16 | -0.06 | 0.05  | 0.17  | -0.06 |
| Arachidonic acid        | -0.04 | 0.10  | 0.08  | -0.09 | -0.22 | 0.02  | -0.11 | -0.03 | 0.09  | 0.09  | 0.28  | 0.26  | -0.01 | -0.04 | 0.12  | -0.14 | 0.10  | 0.10  | 0.00  | -0.01 | -0.18 | 0.16  | 0.20  | -0.07 | 0.23  | 0.12  | -0.03 | 0.04  | -0.11 | -0.06 |
| L-Histidine             | -0.04 | -0.22 | 0.11  | 0.09  | -0.06 | 0.16  | -0.01 | -0.16 | -0.07 | 0.09  | -0.03 | -0.07 | -0.01 | 0.10  | 0.04  | 0.08  | -0.05 | -0.05 | -0.16 | 0.13  | 0.00  | -0.01 | 0.04  | 0.01  | 0.06  | 0.05  | -0.10 | -0.14 | -0.21 | 0.09  |
| Cholesterol             | -0.05 | -0.02 | 0.25  | 0.07  | -0.07 | 0.11  | 0.03  | 0.10  | -0.05 | -0.07 | -0.02 | 0.03  | -0.21 | 0.00  | 0.02  | 0.26  | -0.10 | -0.19 | 0.21  | -0.04 | 0.09  | -0.05 | 0.11  | -0.06 | 0.06  | 0.18  | 0.00  | 0.03  | 0.02  | 0.01  |
| N-Acetylmethionine      | -0.06 | 0.07  | -0.10 | 0.10  | -0.29 | 0.02  | 0.12  | 0.21  | -0.07 | -0.11 | -0.06 | -0.07 | -0.06 | -0.09 | 0.22  | -0.24 | -0.08 | 0.02  | 0.08  | 0.14  | -0.01 | -0.06 | -0.01 | -0.11 | 0.08  | -0.08 | 0.09  | 0.15  | -0.02 | -0.02 |
| L/P                     | -0.06 | 0.08  | -0.14 | 0.08  | -0.08 | 0.05  | 0.12  | -0.25 | 0.14  | -0.36 | 0.13  | -0.07 | -0.16 | 0.06  | 0.07  | 0.00  | 0.09  | 0.03  | 0.09  | -0.02 | -0.03 | 0.03  | 0.03  | 0.06  | -0.01 | 0.00  | -0.13 | -0.06 | 0.03  | 0.06  |
| Citrulline              | -0.06 | 0.07  | -0.21 | -0.08 | -0.08 | 0.01  | -0.15 | -0.01 | 0.03  | 0.22  | -0.05 | 0.05  | 0.07  | -0.07 | 0.21  | -0.01 | -0.04 | 0.17  | -0.10 | -0.04 | 0.23  | -0.16 | 0.09  | 0.14  | -0.26 | 0.14  | 0.08  | -0.08 | 0.00  | 0.13  |
| mtDNA deletions         | -0.06 | -0.03 | -0.12 | -0.07 | -0.24 | 0.05  | 0.09  | 0.00  | 0.28  | -0.09 | 0.03  | 0.12  | 0.02  | -0.04 | -0.11 | 0.05  | -0.24 | 0.05  | -0.23 | 0.09  | -0.02 | -0.15 | -0.08 | -0.11 | -0.10 | -0.10 | -0.05 | 0.17  | 0.12  | 0.09  |
| 1-Acylglycerol          | -0.07 | 0.10  | -0.16 | 0.07  | 0.17  | 0.01  | -0.01 | -0.01 | 0.13  | 0.05  | 0.04  | 0.21  | 0.25  | 0.10  | -0.03 | 0.15  | -0.11 | -0.03 | 0.25  | -0.13 | -0.15 | -0.02 | 0.07  | -0.11 | -0.01 | -0.03 | -0.17 | 0.39  | -0.01 | -0.13 |
| Palmitoleic acid        | -0.07 | 0.14  | 0.22  | 0.03  | -0.18 | -0.10 | 0.08  | -0.11 | -0.02 | 0.02  | -0.04 | -0.08 | 0.07  | -0.01 | 0.14  | -0.03 | -0.02 | 0.05  | -0.05 | -0.07 | -0.03 | -0.13 | -0.14 | 0.06  | 0.02  | 0.12  | 0.05  | 0.20  | 0.12  | -0.03 |
| Glycerol                | -0.07 | 0.12  | 0.03  | 0.09  | -0.04 | -0.07 | 0.05  | 0.02  | -0.05 | 0.12  | 0.11  | -0.01 | 0.27  | -0.05 | 0.16  | 0.14  | 0.11  | 0.11  | 0.22  | 0.44  | -0.06 | 0.33  | 0.00  | 0.15  | -0.20 | -0.09 | -0.13 | -0.08 | 0.00  | 0.11  |
| Malate                  | -0.08 | 0.02  | 0.11  | 0.05  | 0.21  | -0.02 | 0.14  | 0.02  | 0.21  | -0.13 | -0.06 | -0.26 | -0.04 | 0.15  | 0.06  | -0.04 | -0.20 | -0.18 | -0.03 | 0.09  | 0.04  | 0.18  | 0.06  | 0.08  | -0.23 | 0.07  | 0.00  | 0.16  | -0.11 | -0.37 |
| L-Alanine               | -0.08 | -0.17 | -0.06 | 0.07  | 0.08  | -0.24 | 0.04  | 0.17  | -0.16 | -0.01 | 0.12  | 0.15  | -0.01 | -0.01 | 0.00  | 0.09  | 0.05  | 0.18  | -0.02 | 0.04  | 0.11  | -0.10 | -0.13 | 0.05  | -0.12 | 0.07  | -0.12 | 0.05  | -0.08 | -0.05 |
| 2-Hydroxybutyric acid   | -0.09 | 0.14  | 0.12  | 0.14  | -0.06 | 0.05  | -0.13 | -0.03 | -0.03 | 0.06  | 0.02  | -0.03 | 0.05  | 0.24  | -0.17 | -0.28 | 0.04  | -0.03 | -0.12 | -0.22 | 0.15  | -0.04 | -0.09 | 0.11  | -0.03 | 0.23  | -0.09 | 0.01  | 0.17  | 0.02  |
| L-Threonine             | -0.10 | -0.17 | -0.01 | -0.14 | -0.09 | -0.18 | 0.16  | 0.00  | -0.15 | 0.07  | -0.14 | 0.00  | -0.14 | -0.05 | 0.18  | -0.11 | -0.05 | 0.11  | 0.06  | -0.02 | -0.04 | 0.04  | 0.00  | -0.13 | -0.03 | 0.21  | 0.06  | 0.09  | 0.10  | 0.11  |
| Succinic acid           | -0.10 | 0.00  | 0.08  | 0.17  | 0.07  | -0.11 | 0.02  | -0.17 | -0.03 | -0.09 | 0.13  | 0.17  | 0.00  | 0.02  | 0.35  | 0.03  | -0.06 | -0.17 | -0.01 | -0.07 | -0.01 | -0.07 | -0.16 | -0.12 | -0.09 | -0.13 | 0.01  | -0.37 | 0.21  | -0.21 |
| Pelargonic acid         | -0.10 | 0.11  | 0.01  | -0.01 | 0.01  | -0.01 | 0.08  | 0.05  | 0.09  | 0.03  | 0.18  | 0.09  | -0.27 | 0.36  | 0.12  | 0.34  | 0.02  | -0.02 | 0.08  | -0.09 | -0.02 | -0.18 | -0.11 | 0.25  | 0.07  | 0.13  | 0.23  | 0.01  | -0.09 | 0.11  |
| 3-Aminoisobutanoic acid | -0.11 | 0.03  | -0.02 | -0.13 | -0.07 | -0.12 | -0.02 | -0.05 | -0.37 | 0.02  | 0.03  | -0.05 | -0.12 | 0.16  | -0.29 | 0.09  | -0.10 | -0.02 | 0.22  | -0.01 | -0.08 | -0.02 | 0.04  | -0.25 | -0.20 | 0.09  | 0.01  | 0.06  | 0.11  | 0.11  |
| BMI                     | -0.11 | -0.05 | -0.01 | 0.08  | -0.07 | 0.06  | 0.06  | -0.04 | 0.22  | 0.05  | 0.20  | -0.20 | 0.06  | -0.22 | -0.13 | -0.01 | -0.42 | 0.07  | 0.02  | 0.11  | 0.07  | -0.01 | -0.16 | -0.04 | 0.26  | 0.30  | -0.06 | -0.11 | 0.03  | 0.04  |
| L-Proline               | -0.12 | -0.20 | -0.06 | -0.15 | 0.00  | -0.04 | 0.05  | -0.16 | 0.01  | 0.02  | 0.06  | 0.01  | 0.16  | 0.05  | -0.06 | 0.14  | -0.02 | 0.19  | 0.16  | -0.02 | 0.01  | 0.01  | -0.15 | 0.04  | 0.11  | -0.11 | 0.04  | -0.09 | -0.15 | 0.06  |
| L-Serine                | -0.12 | -0.16 | -0.05 | 0.13  | 0.11  | -0.05 | 0.20  | 0.05  | 0.09  | -0.08 | -0.11 | -0.08 | 0.12  | 0.01  | -0.03 | 0.05  | 0.20  | 0.11  | 0.06  | 0.01  | 0.10  | 0.05  | -0.04 | 0.23  | 0.07  | 0.03  | 0.08  | 0.11  | 0.16  | 0.19  |
| CysCys/Total Cys        | -0.13 | -0.06 | 0.11  | -0.10 | -0.18 | 0.03  | -0.24 | -0.01 | 0.18  | -0.07 | -0.08 | 0.10  | -0.01 | 0.10  | -0.07 | 0.04  | 0.07  | -0.12 | 0.04  | 0.22  | 0.29  | 0.09  | 0.03  | -0.10 | 0.08  | -0.12 | 0.14  | 0.01  | 0.09  | 0.02  |
| 4-Hydroxyproline        | -0.13 | -0.07 | 0.06  | -0.18 | 0.11  | -0.02 | -0.07 | 0.02  | 0.20  | 0.11  | 0.03  | 0.23  | 0.06  | 0.18  | 0.14  | 0.02  | -0.10 | 0.16  | 0.00  | -0.19 | 0.05  | 0.11  | -0.04 | -0.13 | -0.06 | -0.16 | -0.07 | -0.05 | 0.02  | -0.12 |
| Citric acid             | -0.15 | 0.02  | 0.10  | -0.22 | 0.14  | 0.14  | -0.06 | 0.11  | -0.01 | -0.06 | 0.15  | -0.05 | -0.13 | 0.01  | 0.12  | -0.09 | 0.02  | 0.10  | -0.04 | -0.01 | 0.04  | 0.20  | -0.11 | 0.04  | 0.11  | 0.08  | 0.17  | 0.08  | -0.09 | -0.13 |
| Oxoglutaric acid        | -0.15 | -0.04 | 0.12  | 0.17  | 0.03  | -0.03 | -0.02 | 0.06  | -0.04 | 0.31  | 0.00  | 0.06  | 0.08  | 0.17  | -0.03 | -0.05 | -0.05 | -0.09 | 0.11  | 0.08  | -0.05 | -0.11 | 0.15  | 0.10  | 0.10  | -0.09 | 0.03  | 0.02  | 0.21  | -0.01 |
| Total BR                | -0.17 | -0.04 | -0.06 | -0.18 | -0.04 | -0.01 | -0.02 | -0.10 | 0.14  | -0.05 | 0.09  | -0.16 | -0.10 | 0.07  | -0.12 | -0.02 | -0.03 | -0.03 | -0.04 | 0.19  | -0.07 | -0.05 | 0.23  | 0.03  | -0.37 | -0.18 | 0.19  | -0.06 | 0.10  | 0.09  |
| Glycine                 | -0.17 | -0.05 | 0.02  | 0.01  | 0.22  | 0.03  | 0.14  | -0.12 | -0.16 | -0.07 | 0.01  | 0.07  | 0.06  | 0.00  | 0.00  | -0.17 | 0.21  | -0.15 | -0.13 | 0.24  | -0.04 | -0.22 | -0.08 | 0.03  | 0.13  | -0.05 | 0.06  | 0.13  | 0.17  | 0.02  |
| D-threo-Isocitric acid  | -0.19 | 0.01  | 0.04  | -0.06 | 0.19  | 0.11  | -0.05 | 0.18  | -0.07 | 0.03  | 0.15  | -0.08 | -0.21 | -0.01 | 0.06  | -0.07 | -0.08 | 0.13  | -0.09 | 0.17  | -0.01 | 0.24  | -0.12 | -0.08 | -0.01 | 0.08  | -0.06 | 0.03  | 0.08  | 0.15  |
| L-Methionine            | -0.19 | -0.15 | -0.02 | -0.17 | -0.04 | -0.08 | -0.01 | -0.01 | -0.02 | 0.05  | 0.00  | -0.13 | 0.05  | 0.17  | 0.06  | -0.11 | 0.03  | -0.04 | 0.03  | 0.00  | -0.14 | 0.01  | 0.11  | 0.05  | -0.04 | 0.13  | -0.06 | -0.14 | -0.07 | -0.04 |
| L-Tyrosine              | -0.23 | -0.12 | -0.04 | -0.10 | 0.00  | -0.04 | -0.08 | -0.05 | 0.08  | 0.05  | -0.12 | -0.15 | 0.14  | -0.03 | 0.01  | 0.03  | 0.05  | -0.07 | 0.03  | -0.03 | 0.03  | 0.00  | -0.05 | 0.11  | -0.02 | 0.24  | -0.06 | 0.07  | 0.04  | -0.09 |
| L-Aspartic acid         | -0.24 | -0.02 | -0.05 | 0.16  | -0.10 | 0.06  | 0.04  | 0.05  | -0.03 | -0.04 | -0.05 | 0.04  | -0.10 | -0.05 | -0.07 | 0.07  | 0.08  | 0.01  | -0.09 | -0.11 | -0.12 | 0.02  | 0.09  | -0.01 | 0.04  | 0.00  | 0.08  | -0.06 | 0.09  | 0.05  |
| L-Glutamic acid         | -0.25 | -0.02 | -0.02 | 0.20  | -0.06 | -0.01 | 0.02  | -0.03 | 0.02  | -0.02 | -0.07 | 0.06  | -0.03 | -0.02 | 0.03  | 0.06  | 0.03  | 0.06  | -0.04 | -0.08 | 0.02  | 0.02  | 0.04  | 0.01  | -0.06 | -0.01 | -0.11 | 0.02  | 0.03  | -0.01 |
| L-Phenylalanine         | -0.25 | -0.09 | -0.06 | 0.10  | -0.05 | 0.01  | -0.03 | -0.04 | 0.02  | 0.08  | 0.02  | -0.02 | 0.08  | -0.01 | -0.05 | 0.10  | 0.09  | -0.05 | -0.04 | -0.07 | 0.02  | 0.00  | 0.02  | -0.04 | 0.01  | -0.12 | 0.03  | 0.02  | 0.08  | -0.08 |

| PC31  | PC32  | PC33  | PC34  | PC35  | PC36  | PC37  | PC38  | PC39  | PC40  | PC41  | PC42  | PC43  | PC44  | PC45  | PC46  | PC47  | PC48  | PC49  | PC50  | PC51  | PC52  | PC53  | PC54  | PC55  | PC56  | PC57  | PC58  | PC59  | PC60  | PC61  | PC62  |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.08  | -0.05 | 0.03  | -0.05 | -0.01 | 0.01  | -0.04 | 0.02  | 0.00  | -0.01 | 0.03  | -0.03 | -0.04 | 0.00  | 0.06  | 0.07  | 0.13  | -0.02 | -0.02 | 0.04  | -0.01 | -0.08 | 0.01  | 0.01  | 0.05  | -0.01 | 0.11  | -0.20 | 0.12  | 0.08  | -0.05 | -0.22 |
| 0.20  | -0.05 | -0.09 | -0.19 | -0.18 | -0.16 | 0.12  | -0.20 | 0.05  | 0.05  | -0.43 | 0.05  | 0.03  | 0.07  | -0.15 | -0.05 | 0.14  | -0.06 | 0.05  | -0.08 | -0.07 | 0.09  | -0.19 | -0.13 | 0.06  | 0.19  | -0.15 | -0.16 | -0.09 | -0.09 | 0.04  | -0.01 |
| -0.11 | 0.01  | -0.05 | -0.08 | 0.04  | -0.03 | 0.07  | 0.14  | 0.12  | 0.06  | 0.01  | -0.11 | -0.04 | -0.07 | -0.31 | 0.02  | 0.10  | 0.12  | -0.24 | -0.20 | -0.05 | 0.04  | 0.02  | 0.10  | -0.22 | 0.04  | -0.15 | 0.11  | -0.12 | -0.11 | -0.01 | 0.09  |
| 0.07  | 0.05  | 0.10  | -0.14 | 0.00  | 0.10  | -0.19 | -0.01 | -0.13 | 0.15  | 0.01  | -0.13 | 0.13  | -0.08 | -0.12 | 0.07  | -0.40 | 0.00  | -0.03 | 0.15  | -0.21 | 0.01  | -0.19 | -0.11 | -0.03 | -0.08 | 0.01  | 0.15  | 0.10  | -0.04 | 0.27  | -0.14 |
| 0.09  | 0.08  | -0.03 | 0.02  | 0.21  | -0.07 | -0.01 | 0.17  | -0.05 | 0.29  | -0.05 | 0.02  | 0.16  | -0.05 | 0.18  | -0.07 | 0.03  | 0.05  | 0.02  | 0.18  | -0.10 | 0.18  | -0.01 | -0.10 | -0.04 | -0.05 | -0.07 | 0.04  | -0.27 | -0.03 | -0.17 | 0.04  |
| -0.10 | 0.26  | 0.06  | 0.07  | -0.23 | -0.09 | -0.03 | -0.15 | -0.01 | -0.11 | 0.03  | -0.10 | -0.03 | -0.11 | -0.06 | 0.00  | -0.19 | -0.10 | -0.16 | -0.01 | 0.08  | 0.09  | 0.05  | 0.04  | -0.03 | 0.10  | -0.04 | 0.13  | 0.15  | 0.01  | -0.03 | 0.08  |
| -0.15 | -0.05 | 0.22  | 0.05  | 0.04  | -0.29 | 0.31  | -0.04 | 0.13  | 0.05  | 0.04  | -0.06 | 0.05  | 0.04  | 0.09  | 0.06  | 0.13  | 0.29  | 0.07  | 0.12  | 0.05  | -0.09 | -0.04 | -0.04 | 0.02  | 0.10  | 0.02  | -0.10 | 0.01  | 0.06  | 0.23  | 0.03  |
| 0.03  | -0.13 | -0.02 | 0.09  | 0.11  | 0.07  | -0.17 | -0.02 | -0.08 | 0.07  | -0.08 | -0.11 | 0.03  | -0.03 | 0.04  | 0.00  | 0.15  | 0.04  | -0.07 | 0.14  | 0.16  | 0.01  | 0.11  | -0.04 | 0.25  | 0.20  | -0.07 | 0.17  | 0.10  | 0.10  | -0.04 | 0.04  |
| -0.34 | -0.09 | 0.09  | 0.11  | 0.12  | -0.13 | 0.02  | -0.10 | -0.23 | 0.18  | 0.27  | 0.01  | 0.05  | -0.03 | -0.04 | -0.04 | 0.08  | -0.09 | -0.16 | -0.04 | -0.07 | -0.15 | -0.04 | 0.16  | -0.12 | 0.04  | -0.08 | -0.03 | -0.09 | -0.02 | -0.03 | -0.02 |
| -0.11 | -0.34 | 0.11  | -0.13 | -0.17 | 0.08  | -0.18 | 0.19  | -0.24 | -0.07 | -0.13 | 0.06  | 0.09  | 0.02  | 0.10  | -0.02 | 0.14  | 0.08  | -0.06 | 0.07  | 0.00  | 0.01  | 0.08  | 0.11  | -0.11 | 0.04  | 0.04  | 0.04  | -0.10 | 0.06  | -0.09 | 0.05  |
| -0.28 | 0.03  | -0.06 | -0.02 | 0.05  | 0.06  | 0.13  | 0.03  | -0.07 | 0.02  | 0.08  | -0.21 | -0.06 | 0.17  | 0.11  | -0.10 | 0.00  | -0.33 | 0.16  | -0.19 | 0.07  | 0.13  | 0.11  | 0.00  | 0.04  | 0.03  | 0.07  | -0.04 | -0.09 | -0.24 | 0.06  | 0.11  |
| -0.13 | 0.05  | -0.06 | 0.05  | -0.07 | 0.04  | -0.02 | -0.09 | -0.08 | 0.03  | 0.08  | 0.08  | -0.05 | 0.03  | -0.04 | 0.11  | 0.01  | 0.11  | 0.09  | 0.05  | -0.03 | 0.05  | -0.12 | -0.04 | -0.17 | 0.01  | 0.01  | 0.10  | -0.15 | 0.14  | -0.12 | 0.18  |
| -0.03 | 0.05  | -0.10 | -0.03 | -0.07 | 0.10  | 0.14  | 0.11  | 0.09  | -0.31 | 0.13  | 0.06  | 0.33  | 0.00  | 0.23  | 0.09  | 0.01  | 0.00  | -0.01 | 0.16  | 0.11  | -0.08 | -0.02 | -0.02 | -0.17 | 0.04  | -0.03 | -0.10 | -0.02 | -0.18 | 0.01  | 0.04  |
| 0.02  | -0.06 | 0.13  | 0.33  | -0.05 | -0.02 | -0.22 | 0.09  | 0.03  | -0.21 | -0.05 | -0.20 | 0.03  | -0.18 | -0.03 | 0.08  | 0.29  | -0.05 | 0.17  | -0.20 | -0.04 | 0.06  | -0.35 | 0.02  | 0.02  | 0.03  | 0.01  | 0.10  | 0.14  | 0.17  | 0.16  | 0.02  |
| -0.12 | 0.11  | 0.05  | -0.12 | 0.06  | 0.01  | 0.04  | 0.02  | 0.06  | -0.08 | -0.10 | -0.06 | -0.07 | 0.24  | -0.01 | 0.04  | -0.10 | 0.14  | 0.00  | -0.04 | -0.05 | -0.23 | 0.00  | -0.03 | 0.01  | 0.04  | 0.13  | 0.08  | -0.04 | -0.02 | 0.01  | -0.03 |
| 0.00  | -0.04 | 0.06  | -0.07 | 0.05  | 0.10  | 0.09  | 0.00  | -0.01 | -0.05 | 0.02  | -0.08 | 0.05  | 0.11  | 0.15  | 0.24  | 0.06  | -0.06 | 0.11  | -0.01 | -0.19 | -0.25 | -0.06 | -0.10 | -0.04 | 0.10  | -0.08 | -0.08 | 0.08  | -0.08 | -0.15 | -0.13 |
| 0.11  | 0.21  | -0.08 | 0.21  | -0.03 | 0.02  | -0.07 | 0.19  | 0.12  | 0.00  | 0.06  | 0.01  | 0.04  | 0.02  | 0.10  | 0.10  | -0.15 | 0.20  | -0.04 | -0.02 | -0.05 | 0.06  | 0.18  | -0.05 | -0.02 | 0.14  | -0.09 | -0.10 | 0.08  | 0.15  | -0.11 | 0.06  |
| 0.04  | 0.05  | 0.15  | -0.13 | -0.06 | -0.12 | 0.05  | 0.03  | -0.07 | -0.06 | -0.04 | -0.03 | -0.10 | 0.12  | -0.09 | -0.18 | 0.08  | -0.13 | 0.20  | -0.17 | -0.12 | -0.05 | 0.03  | -0.06 | -0.13 | -0.26 | -0.04 | -0.02 | 0.33  | 0.08  | -0.08 | 0.13  |
| -0.18 | 0.05  | 0.11  | -0.02 | -0.03 | 0.21  | 0.04  | -0.12 | 0.06  | -0.15 | 0.00  | 0.01  | -0.11 | 0.00  | -0.16 | 0.18  | -0.06 | -0.16 | -0.06 | 0.13  | 0.09  | 0.15  | -0.05 | -0.13 | 0.13  | 0.01  | -0.04 | -0.05 | 0.10  | 0.04  | -0.09 | -0.05 |
| 0.12  | -0.04 | -0.01 | -0.08 | -0.01 | 0.10  | 0.28  | 0.21  | -0.11 | 0.02  | -0.09 | 0.08  | -0.16 | -0.04 | -0.16 | -0.02 | -0.21 | -0.13 | 0.15  | 0.05  | 0.27  | -0.16 | 0.07  | 0.02  | 0.17  | 0.03  | 0.22  | 0.05  | -0.04 | 0.01  | 0.07  | -0.05 |
| -0.06 | -0.09 | -0.03 | 0.09  | -0.03 | 0.05  | 0.01  | 0.03  | 0.06  | -0.10 | -0.11 | 0.03  | -0.04 | 0.02  | -0.08 | -0.06 | -0.05 | -0.02 | 0.09  | 0.11  | -0.06 | -0.14 | -0.02 | 0.06  | 0.00  | -0.09 | 0.01  | 0.08  | 0.03  | -0.04 | -0.05 | -0.21 |
| 0.05  | 0.07  | -0.25 | 0.09  | 0.11  | -0.01 | 0.09  | -0.10 | 0.02  | -0.04 | -0.08 | 0.03  | 0.03  | -0.01 | -0.06 | 0.02  | -0.03 | -0.15 | -0.26 | 0.12  | 0.01  | -0.15 | -0.12 | 0.10  | 0.10  | 0.00  | 0.22  | -0.08 | 0.00  | 0.31  | -0.36 | 0.00  |
| -0.03 | 0.16  | -0.12 | 0.04  | -0.04 | -0.16 | 0.02  | 0.15  | -0.03 | 0.04  | -0.15 | 0.02  | -0.10 | 0.15  | 0.09  | 0.09  | 0.02  | -0.10 | 0.15  | 0.30  | -0.03 | 0.02  | -0.08 | 0.20  | -0.12 | -0.23 | -0.20 | 0.00  | -0.04 | 0.09  | 0.11  | -0.17 |
| 0.03  | -0.01 | 0.04  | 0.11  | 0.00  | -0.01 | -0.25 | 0.00  | 0.16  | -0.08 | 0.01  | 0.21  | 0.00  | 0.12  | -0.01 | 0.01  | -0.03 | -0.10 | 0.07  | -0.04 | -0.11 | -0.08 | 0.05  | -0.07 | 0.00  | -0.10 | -0.21 | 0.06  | -0.01 | -0.06 | -0.07 | 0.11  |
| 0.11  | -0.10 | -0.07 | 0.01  | -0.04 | 0.19  | -0.07 | -0.01 | -0.02 | 0.14  | -0.14 | -0.06 | 0.02  | 0.16  | 0.00  | 0.07  | -0.11 | 0.05  | -0.04 | 0.02  | 0.09  | 0.07  | 0.00  | 0.24  | -0.23 | -0.06 | -0.04 | -0.15 | -0.04 | 0.20  | 0.03  | 0.05  |
| 0.00  | 0.07  | 0.04  | 0.24  | 0.04  | 0.06  | -0.09 | -0.18 | 0.04  | -0.03 | -0.10 | 0.01  | -0.03 | -0.09 | 0.05  | 0.12  | -0.16 | 0.10  | 0.02  | -0.02 | -0.03 | 0.04  | -0.10 | -0.05 | -0.06 | -0.02 | 0.17  | -0.15 | -0.28 | -0.26 | -0.03 | -0.01 |
| 0.24  | 0.04  | -0.10 | 0.14  | -0.08 | 0.14  | 0.06  | 0.05  | -0.29 | -0.02 | 0.02  | 0.12  | -0.14 | 0.11  | 0.00  | -0.01 | 0.10  | 0.05  | 0.08  | 0.09  | 0.05  | -0.10 | 0.02  | -0.15 | -0.14 | 0.11  | -0.12 | 0.00  | 0.05  | -0.30 | 0.00  | 0.03  |
| -0.10 | 0.02  | 0.11  | 0.01  | 0.24  | -0.05 | 0.01  | 0.28  | 0.20  | -0.11 | 0.04  | 0.12  | 0.02  | 0.11  | -0.08 | -0.04 | -0.07 | -0.06 | 0.09  | -0.03 | 0.00  | -0.06 | 0.01  | -0.05 | 0.16  | -0.04 | -0.10 | -0.14 | 0.00  | -0.02 | 0.02  | -0.05 |
| 0.21  | 0.00  | -0.03 | -0.02 | 0.09  | -0.01 | 0.05  | 0.04  | 0.06  | -0.11 | 0.19  | 0.15  | 0.22  | 0.21  | -0.15 | -0.10 | 0.09  | 0.02  | 0.00  | 0.02  | -0.15 | 0.04  | -0.15 | 0.24  | 0.24  | -0.07 | 0.01  | 0.12  | 0.01  | -0.09 | -0.07 | 0.14  |
| -0.09 | 0.24  | -0.25 | -0.14 | -0.13 | -0.21 | -0.09 | 0.15  | 0.13  | 0.00  | 0.06  | 0.07  | -0.07 | -0.17 | 0.06  | 0.02  | 0.02  | 0.05  | 0.07  | 0.13  | -0.01 | -0.02 | -0.04 | -0.07 | 0.11  | 0.15  | 0.03  | 0.11  | -0.03 | -0.03 | 0.10  | 0.08  |
| -0.08 | 0.06  | 0.10  | 0.21  | -0.05 | 0.15  | 0.39  | -0.14 | -0.09 | -0.02 | -0.10 | 0.19  | 0.02  | -0.04 | 0.05  | -0.06 | -0.02 | 0.16  | -0.07 | -0.22 | 0.00  | 0.23  | -0.09 | 0.08  | 0.02  | -0.05 | 0.09  | -0.01 | 0.08  | 0.00  | -0.13 | -0.08 |
| -0.06 | -0.08 | -0.02 | -0.08 | 0.22  | 0.13  | 0.03  | 0.08  | 0.20  | -0.13 | -0.10 | 0.04  | 0.06  | 0.16  | 0.06  | -0.19 | -0.02 | -0.03 | -0.20 | 0.00  | 0.07  | 0.15  | -0.11 | 0.03  | -0.20 | 0.12  | 0.19  | 0.22  | -0.01 | 0.01  | 0.22  | 0.02  |
| -0.02 | 0.12  | -0.19 | 0.11  | 0.07  | -0.01 | 0.04  | -0.05 | -0.05 | -0.02 | 0.08  | -0.06 | 0.14  | 0.11  | -0.15 | -0.04 | 0.24  | 0.01  | 0.18  | 0.13  | -0.05 | -0.17 | -0.03 | 0.01  | -0.02 | -0.08 | 0.17  | 0.18  | 0.03  | -0.03 | 0.00  | 0.07  |
| -0.08 | 0.06  | -0.09 | -0.04 | -0.09 | -0.07 | 0.20  | 0.09  | -0.13 | 0.03  | -0.04 | 0.15  | 0.09  | -0.10 | 0.16  | -0.08 | -0.13 | -0.03 | -0.18 | -0.01 | -0.19 | -0.03 | 0.02  | 0.09  | 0.18  | 0.03  | -0.17 | 0.09  | 0.14  | 0.14  | 0.25  | -0.12 |
| -0.01 | 0.02  | 0.11  | -0.06 | 0.07  | 0.01  | -0.05 | 0.08  | -0.21 | -0.09 | -0.01 | -0.08 | -0.17 | -0.01 | 0.05  | 0.07  | -0.08 | 0.08  | 0.25  | -0.03 | -0.31 | 0.06  | 0.07  | 0.22  | 0.14  | 0.21  | 0.15  | -0.03 | -0.09 | -0.05 | -0.23 | 0.06  |
| -0.08 | 0.22  | 0.22  | -0.10 | -0.02 | -0.12 | -0.17 | -0.04 | -0.09 | -0.02 | -0.04 | 0.25  | -0.10 | 0.15  | 0.13  | 0.11  | 0.08  | 0.18  | 0.00  | 0.06  | 0.34  | -0.01 | -0.20 | 0.07  | 0.05  | 0.02  | 0.03  | 0.10  | 0.09  | -0.06 | -0.08 | 0.19  |
| 0.11  | 0.08  | 0.12  | 0.01  | 0.01  | -0.03 | 0.00  | 0.00  | 0.10  | 0.13  | -0.13 | 0.03  | 0.11  | 0.02  | 0.02  | -0.14 | 0.13  | -0.15 | -0.09 | 0.03  | -0.16 | -0.05 | 0.09  | 0.07  | -0.07 | -0.18 | 0.19  | -0.14 | -0.01 | 0.16  | 0.04  | 0.18  |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.08  | 0.02  | 0.04  | -0.21 | -0.01 | 0.26  | 0.15  | -0.06 | 0.15  | 0.13  | 0.23  | 0.13  | 0.19  | -0.26 | -0.19 | 0.07  | 0.12  | -0.07 | 0.28  | -0.02 | 0.17  | 0.00  | 0.01  | -0.02 | -0.13 | -0.03 | -0.05 | 0.04  | -0.07 | 0.09  | -0.03 | 0.01  |
| 0.00  | -0.09 | -0.04 | -0.14 | -0.09 | -0.15 | 0.01  | -0.07 | -0.12 | -0.06 | 0.19  | 0.08  | -0.11 | 0.07  | 0.03  | -0.01 | -0.09 | 0.24  | -0.08 | -0.02 | 0.03  | -0.03 | 0.03  | -0.30 | -0.02 | -0.21 | 0.08  | 0.00  | 0.12  | 0.19  | 0.00  | 0.16  |
| 0.19  | -0.13 | 0.12  | 0.15  | -0.01 | -0.18 | -0.03 | -0.05 | -0.02 | 0.07  | 0.05  | -0.07 | -0.08 | 0.12  | 0.02  | -0.06 | -0.10 | -0.08 | 0.10  | 0.01  | -0.06 | -0.11 | 0.18  | -0.13 | -0.08 | 0.08  | 0.09  | 0.21  | -0.11 | 0.00  | 0.00  | -0.04 |
| -0.07 | -0.10 | -0.08 | 0.08  | -0.04 | -0.05 | -0.04 | 0.01  | -0.15 | -0.09 | 0.00  | -0.22 | 0.21  | 0.24  | -0.06 | -0.16 | -0.15 | -0.07 | -0.15 | 0.13  | 0.14  | -0.01 | -0.34 | -0.17 | 0.08  | -0.14 | -0.12 | -0.18 | 0.02  | -0.17 | -0.09 | 0.13  |
| -0.09 | 0.02  | 0.22  | -0.18 | 0.00  | 0.08  | -0.12 | -0.14 | 0.10  | 0.06  | -0.07 | -0.09 | 0.05  | 0.03  | 0.06  | -0.06 | 0.04  | 0.15  | 0.00  | 0.09  | -0.06 | 0.18  | 0.11  | 0.13  | 0.17  | -0.24 | -0.09 | -0.09 | -0.03 | -0.10 | 0.03  | -0.13 |
| 0.19  | -0.11 | -0.11 | 0.10  | -0.05 | -0.12 | 0.17  | -0.05 | 0.13  | 0.11  | 0.13  | -0.18 | -0.24 | 0.01  | 0.01  | 0.01  | 0.03  | -0.14 | -0.11 | 0.08  | -0.04 | 0.06  | -0.20 | 0.11  | 0.06  | 0.08  | -0.10 | 0.21  | -0.01 | -0.03 | -0.02 | 0.04  |
| 0.02  | 0.01  | -0.05 | -0.03 | 0.04  | 0.13  | -0.12 | -0.27 | 0.23  | -0.02 | 0.21  | -0.09 | -0.10 | 0.18  | -0.15 | -0.11 | -0.02 | 0.14  | -0.01 | 0.11  | -0.04 | -0.13 | 0.15  | 0.20  | 0.08  | 0.24  | -0.24 | -0.20 | 0.10  | 0.01  | 0.03  | 0.00  |
| 0.02  | -0.07 | -0.14 | 0.01  | 0.27  | -0.05 | 0.10  | 0.22  | 0.07  | 0.05  | -0.16 | -0.10 | -0.21 | 0.01  | -0.07 | 0.19  | 0.05  | 0.25  | -0.01 | -0.14 | 0.11  | 0.17  | -0.02 | -0.03 | 0.05  | -0.20 | -0.11 | -0.07 | 0.16  | -0.08 | -0.12 | -0.02 |
| -0.01 | 0.10  | 0.23  | 0.06  | 0.02  | -0.09 | 0.15  | -0.14 | 0.11  | 0.03  | -0.26 | -0.13 | 0.05  | 0.01  | 0.06  | -0.03 | -0.09 | -0.03 | 0.06  | 0.07  | 0.18  | -0.24 | 0.04  | -0.03 | -0.26 | 0.08  | -0.16 | 0.14  | -0.03 | 0.13  | -0.17 | -0.02 |
| 0.06  | 0.17  | -0.07 | -0.02 | 0.08  | -0.07 | 0.01  | -0.02 | -0.09 | 0.09  | 0.16  | -0.07 | 0.13  | 0.06  | 0.01  | 0.05  | 0.20  | 0.07  | 0.04  | -0.02 | 0.03  | 0.07  | 0.00  | -0.02 | -0.04 | 0.07  | 0.10  | 0.00  | 0.06  | 0.06  | 0.01  | -0.26 |
| 0.05  | 0.16  | 0.07  | 0.12  | -0.06 | 0.18  | 0.02  | 0.16  | -0.08 | 0.24  | 0.10  | -0.18 | -0.06 | -0.04 | 0.01  | 0.10  | 0.15  | -0.12 | -0.10 | 0.14  | 0.23  | 0.01  | 0.07  | -0.01 | -0.01 | -0.16 | -0.09 | -0.11 | 0.11  | -0.09 | 0.13  | 0.07  |
| -0.13 | -0.31 | -0.33 | -0.07 | -0.30 | -0.06 | -0.08 | -0.01 | 0.11  | 0.20  | -0.07 | 0.11  | 0.05  | 0.08  | 0.02  | 0.11  | -0.06 | 0.04  | 0.12  | -0.09 | 0.07  | 0.04  | 0.00  | 0.04  | 0.01  | 0.10  | 0.02  | 0.01  | 0.11  | -0.07 | -0.02 | 0.06  |
| 0.14  | 0.08  | 0.07  | 0.10  | 0.01  | -0.02 | -0.01 | -0.04 | 0.01  | 0.05  | -0.11 | 0.01  | 0.01  | -0.15 | -0.09 | -0.21 | 0.07  | 0.18  | 0.05  | 0.13  | 0.07  | -0.15 | -0.08 | 0.08  | 0.08  | 0.11  | 0.04  | -0.26 | -0.05 | -0.09 | 0.16  | 0.07  |
| 0.03  | 0.07  | -0.11 | -0.03 | -0.27 | -0.14 | -0.11 | 0.02  | 0.01  | -0.20 | 0.07  | -0.11 | -0.16 | -0.06 | -0.06 | -0.10 | 0.20  | 0.01  | -0.18 | 0.01  | 0.01  | -0.02 | 0.15  | 0.01  | -0.20 | -0.13 | 0.20  | -0.16 | -0.12 | -0.09 | -0.01 | -0.29 |
| -0.20 | -0.02 | -0.25 | 0.19  | 0.08  | -0.08 | 0.02  | 0.03  | 0.08  | -0.05 | -0.12 | -0.11 | 0.06  | 0.01  | 0.07  | -0.04 | 0.00  | -0.01 | 0.01  | -0.02 | -0.03 | 0.00  | 0.24  | -0.12 | 0.06  | -0.05 | 0.04  | -0.04 | 0.00  | 0.03  | 0.05  | 0.09  |
| 0.06  | -0.18 | 0.16  | 0.10  | -0.10 | -0.03 | 0.16  | -0.03 | 0.04  | 0.01  | 0.05  | -0.03 | -0.08 | 0.15  | 0.18  | 0.30  | 0.03  | -0.08 | -0.12 | 0.10  | -0.02 | -0.06 | 0.03  | 0.08  | 0.16  | -0.08 | 0.01  | 0.02  | -0.08 | 0.03  | 0.13  | -0.02 |
| 0.11  | -0.02 | 0.03  | -0.13 | -0.20 | -0.16 | 0.14  | 0.08  | -0.02 | -0.23 | 0.18  | -0.22 | 0.08  | 0.13  | 0.03  | 0.08  | -0.12 | -0.01 | 0.19  | 0.06  | 0.07  | 0.30  | -0.04 | 0.23  | -0.02 | 0.05  | -0.06 | -0.07 | -0.17 | 0.19  | -0.05 | 0.03  |
| -0.04 | -0.28 | -0.06 | 0.02  | 0.06  | -0.02 | 0.06  | -0.21 | 0.01  | -0.01 | 0.01  | -0.21 | 0.18  | -0.22 | 0.09  | 0.01  | -0.01 | 0.07  | 0.18  | 0.12  | 0.00  | 0.04  | 0.07  | -0.18 | 0.11  | -0.09 | 0.05  | -0.01 | 0.04  | 0.06  | 0.00  | 0.11  |
| 0.00  | -0.08 | -0.14 | 0.07  | 0.20  | 0.08  | 0.00  | -0.23 | -0.13 | -0.14 | -0.03 | 0.24  | -0.11 | 0.14  | 0.02  | 0.14  | 0.06  | 0.03  | 0.03  | 0.01  | -0.06 | 0.05  | 0.02  | 0.09  | -0.14 | 0.01  | 0.05  | 0.00  | 0.02  | 0.02  | 0.42  | 0.00  |
| -0.03 | -0.14 | 0.03  | 0.11  | -0.08 | 0.23  | -0.07 | 0.17  | 0.20  | -0.10 | -0.07 | 0.00  | -0.04 | -0.06 | 0.14  | -0.10 | -0.02 | 0.02  | 0.05  | 0.12  | -0.02 | -0.05 | -0.12 | 0.09  | -0.15 | 0.02  | 0.07  | 0.05  | 0.17  | 0.04  | -0.07 | 0.01  |
| -0.05 | 0.00  | 0.05  | 0.03  | -0.06 | -0.04 | -0.07 | -0.07 | 0.01  | 0.01  | -0.11 | 0.14  | 0.08  | 0.04  | 0.09  | -0.17 | 0.03  | -0.16 | 0.03  | -0.06 | 0.16  | -0.05 | 0.18  | 0.09  | 0.08  | 0.00  | -0.21 | 0.07  | -0.12 | 0.04  | 0.01  | 0.10  |
| -0.11 | 0.08  | 0.04  | -0.08 | -0.20 | 0.17  | 0.07  | 0.00  | 0.13  | 0.05  | -0.09 | -0.22 | -0.07 | 0.07  | 0.12  | -0.05 | 0.18  | 0.04  | -0.08 | 0.05  | -0.11 | -0.04 | -0.07 | -0.04 | 0.04  | 0.14  | 0.05  | 0.13  | 0.01  | -0.12 | -0.01 | 0.01  |
| 0.13  | 0.09  | 0.10  | -0.10 | 0.05  | 0.08  | 0.06  | 0.19  | -0.02 | -0.22 | -0.06 | -0.06 | 0.02  | -0.11 | 0.13  | -0.10 | 0.01  | -0.04 | -0.11 | -0.07 | -0.10 | 0.02  | 0.06  | -0.16 | -0.01 | 0.18  | -0.07 | -0.10 | -0.02 | 0.07  | 0.10  | 0.15  |
| 0.12  | -0.08 | 0.11  | -0.10 | -0.05 | -0.16 | 0.07  | -0.03 | 0.17  | -0.07 | -0.05 | 0.06  | 0.19  | -0.11 | -0.03 | 0.30  | 0.04  | -0.02 | -0.21 | 0.05  | -0.11 | -0.05 | 0.12  | 0.05  | -0.03 | -0.16 | 0.06  | 0.19  | 0.11  | -0.33 | -0.13 | 0.04  |
| -0.02 | -0.06 | 0.02  | -0.09 | 0.00  | 0.15  | 0.06  | -0.01 | 0.18  | 0.21  | 0.17  | 0.09  | -0.35 | -0.04 | 0.30  | -0.18 | 0.02  | -0.03 | -0.02 | 0.05  | -0.16 | -0.03 | -0.29 | -0.10 | -0.05 | -0.05 | -0.03 | 0.01  | -0.03 | 0.01  | -0.10 | 0.06  |
| 0.13  | 0.14  | 0.02  | 0.05  | -0.05 | 0.02  | -0.02 | -0.12 | 0.06  | -0.04 | 0.04  | -0.08 | 0.02  | 0.14  | 0.05  | -0.11 | -0.07 | 0.10  | 0.04  | -0.08 | 0.00  | 0.09  | -0.09 | -0.12 | 0.04  | -0.14 | 0.12  | 0.08  | -0.21 | 0.05  | 0.07  | 0.02  |
| -0.05 | 0.15  | -0.22 | -0.30 | 0.19  | 0.11  | 0.00  | -0.21 | -0.17 | -0.15 | -0.11 | -0.10 | 0.01  | -0.04 | 0.17  | 0.09  | 0.14  | -0.05 | -0.01 | -0.07 | -0.06 | -0.07 | -0.07 | -0.09 | -0.05 | -0.03 | -0.22 | 0.02  | -0.03 | 0.14  | -0.05 | -0.07 |
| -0.20 | 0.07  | 0.05  | -0.04 | -0.03 | -0.04 | 0.05  | 0.00  | -0.06 | 0.14  | -0.10 | 0.07  | 0.04  | 0.04  | -0.11 | -0.13 | 0.05  | -0.02 | 0.08  | 0.35  | -0.17 | 0.23  | 0.05  | 0.00  | -0.07 | 0.15  | 0.21  | -0.13 | 0.32  | -0.08 | -0.08 | 0.08  |
| 0.16  | 0.00  | 0.10  | -0.01 | 0.14  | -0.21 | -0.13 | -0.02 | 0.02  | 0.15  | 0.08  | 0.12  | 0.12  | 0.14  | 0.14  | 0.13  | -0.01 | -0.29 | -0.08 | -0.16 | 0.09  | 0.18  | -0.06 | -0.09 | -0.12 | 0.29  | 0.12  | -0.15 | 0.17  | -0.03 | -0.03 | -0.14 |
| 0.06  | -0.21 | 0.06  | -0.06 | 0.20  | -0.21 | 0.04  | 0.03  | -0.17 | -0.23 | 0.07  | 0.01  | -0.14 | -0.27 | -0.08 | -0.18 | -0.07 | 0.02  | -0.07 | 0.17  | 0.07  | -0.01 | -0.10 | 0.07  | -0.13 | 0.08  | -0.14 | -0.06 | 0.00  | -0.07 | -0.06 | -0.01 |
| 0.14  | 0.10  | -0.02 | -0.13 | 0.09  | 0.08  | -0.01 | 0.00  | -0.20 | 0.03  | -0.12 | -0.23 | 0.04  | 0.03  | 0.03  | 0.11  | 0.03  | 0.05  | -0.12 | -0.08 | 0.04  | -0.12 | 0.06  | 0.20  | 0.08  | 0.02  | 0.07  | 0.13  | 0.04  | -0.08 | 0.03  | 0.27  |
| -0.17 | 0.03  | 0.02  | -0.13 | -0.02 | -0.06 | -0.20 | 0.11  | 0.03  | 0.08  | -0.03 | 0.02  | 0.04  | -0.06 | 0.01  | 0.00  | 0.04  | -0.04 | 0.00  | -0.13 | 0.18  | -0.18 | -0.22 | 0.07  | 0.20  | -0.03 | 0.11  | -0.04 | -0.18 | 0.02  | -0.02 | -0.18 |
| -0.01 | -0.01 | 0.01  | 0.09  | -0.23 | 0.08  | 0.11  | 0.16  | -0.12 | 0.16  | 0.08  | -0.03 | 0.22  | 0.11  | -0.03 | -0.07 | -0.08 | 0.20  | -0.03 | -0.27 | -0.10 | -0.23 | -0.11 | 0.00  | 0.00  | 0.05  | -0.07 | -0.09 | 0.06  | 0.06  | -0.01 | -0.08 |
| -0.05 | 0.07  | -0.07 | 0.11  | 0.09  | -0.08 | -0.02 | -0.05 | 0.00  | 0.01  | -0.08 | -0.06 | 0.11  | -0.03 | 0.04  | -0.13 | -0.13 | 0.10  | 0.20  | -0.05 | 0.08  | 0.06  | -0.01 | 0.15  | -0.10 | 0.00  | -0.09 | 0.22  | 0.18  | -0.14 | -0.10 | -0.28 |
| -0.11 | 0.09  | 0.00  | 0.18  | -0.11 | 0.00  | 0.04  | 0.00  | -0.09 | -0.04 | -0.09 | 0.16  | 0.00  | -0.17 | -0.07 | 0.19  | 0.03  | -0.17 | 0.03  | 0.02  | -0.21 | -0.02 | -0.04 | 0.05  | 0.08  | -0.04 | -0.12 | -0.10 | -0.11 | -0.02 | 0.04  | 0.14  |
| -0.15 | -0.02 | 0.02  | -0.06 | 0.09  | -0.07 | -0.02 | 0.12  | 0.07  | 0.08  | -0.08 | -0.10 | -0.02 | 0.04  | -0.25 | 0.25  | -0.12 | -0.03 | 0.05  | 0.04  | -0.08 | -0.09 | -0.11 | -0.03 | -0.20 | 0.11  | 0.07  | -0.12 | -0.05 | 0.09  | 0.09  | 0.19  |
| -0.08 | -0.02 | 0.13  | 0.08  | -0.06 | 0.09  | 0.05  | 0.13  | -0.08 | -0.04 | -0.02 | 0.07  | 0.02  | 0.23  | -0.30 | 0.02  | 0.19  | 0.05  | -0.11 | 0.16  | -0.06 | 0.17  | 0.08  | -0.31 | 0.08  | 0.12  | -0.11 | 0.18  | -0.20 | 0.15  | -0.05 | -0.21 |



**Supplementary Table S6. PCA  
variance when using the  
outcomes selected by the visual  
extraction rule**

|     | Individual  | Cumulative |
|-----|-------------|------------|
| PC1 | <b>0.43</b> | 0.43       |
| PC2 | <b>0.29</b> | 0.72       |
| PC3 | 0.21        | 0.93       |
| PC4 | 0.07        | 1.00       |

**Supplementary Table S7. PCA  
loadings when using outcomes  
selected by Visual Extraction**

| Algorithm       |       |       |       |       |
|-----------------|-------|-------|-------|-------|
|                 | PC1   | PC2   | PC3   | PC4   |
| L-Glutamic acid | 0.69  | 0.13  | -0.26 | -0.67 |
| Taurine         | -0.01 | 0.81  | -0.48 | 0.33  |
| L-Asparagine    | -0.32 | -0.45 | -0.83 | -0.10 |
| BCAA/AAA        | -0.65 | 0.35  | 0.14  | -0.66 |