

Supplemental tables

Table S1 a-c. Values of amino acids, of biogenic amines and their derivatives, and of selected sums and ratios for all three groups.

Metabolite concentrations ([$\mu\text{mol/l}$]) for all analytes with selected sums and ratios, grouped by Marfan patients *vs.* controls. Values are given as mean \pm standard deviation. False discovery rate-corrected p ($=q$) < 0.05 was considered statistically significant. Group A, all patients; group AF, patients with preserved systolic ventricular function; group AFV, patients with preserved systolic ventricular function and without major valve regurgitation. FC, fold change (Marfan patients *vs.* controls); HMDB ID, Human Metabolome Database identification; AA, amino acids; AAA, aromatic amino acids; Ac-Orn, acethylornithine; ADMA, asymmetric dimethylarginine; alpha-AAA, alpha aminoadipic acid; Arg, arginine; BCAA, branched-chain amino acids; lysoPC, lysophosphatidylcholine; orn, ornithine; PC, phosphatidylcholine; SM, sphingomyelin; \uparrow , statistically significant higher serum concentration in Marfan patients than in controls; \downarrow , statistically significant lower serum concentration in Marfan patients than in controls. ‘Fischer ratio’ is the ratio of BCAA/AAA.

Table S1 a. Values of amino acids, of biogenic amines and their derivatives, and of selected sums and ratios – all patients (group A).

| Metabolite | HMDB ID | Patients | Controls | p | q | FC |
|------------------|--|----------------------------|----------------------------|-------------|-------------|------------|
| ADMA | HMDB01539 | 0.54 \pm 0.12 | 0.48 \pm 0.13 | 0.14 | 0.56 | 1.11 |
| Alanine | HMDB00161 HMDB01310 | 390 \pm 90 | 400 \pm 110 | 0.72 | 0.90 | 0.98 |
| Arginine | HMDB00517 HMDB03416 | 118 \pm 14 | 120 \pm 20 | 0.64 | 0.85 | 0.98 |
| Asparagine | HMDB00168 HMDB003378 | 48 \pm 10 | 48 \pm 8 | 0.90 | 0.96 | 0.99 |
| Aspartic acid | HMDB00191 HMDB06483 | 19 \pm 3 | 20 \pm 4 | 0.40 | 0.70 | 0.96 |
| C0 | HMDB00062 | 36 \pm 8 | 33 \pm 5 | 0.16 | 0.57 | 1.08 |
| C14:1 | HMDB0002014 | 0.14 \pm 0.05 | 0.13 \pm 0.03 | 0.60 | 0.85 | 1.04 |
| C18:1 | HMDB0006351 HMDB0005065 HMDB06464 HMDB0013338 | 0.15 \pm 0.05 | 0.14 \pm 0.03 | 0.44 | 0.70 | 1.07 |
| C18:2 | HMDB0006469 HMDB0006461 | 0.053 \pm 0.019 | 0.049 \pm 0.017 | 0.43 | 0.70 | 1.08 |
| C2 | HMDB00201 | 7 \pm 3 | 6.4 \pm 1.6 | 0.61 | 0.85 | 1.05 |
| Citrulline | HMDB00904 | 30 \pm 9 | 32 \pm 7 | 0.47 | 0.72 | 0.95 |
| Creatinine | HMDB0000562 | 72 \pm 16 | 83 \pm 14 | 0.02 | 0.38 | 0.88 |
| Glutamine | HMDB00641 HMDB03423 | 740 \pm 90 | 730 \pm 100 | 0.91 | 0.96 | 1.00 |
| Glutamic acid | HMDB00148 HMDB03339 | 45 \pm 22 | 32 \pm 20 | 0.03 | 0.39 | 1.43 |
| Glycine | HMDB00123 | 260 \pm 50 | 310 \pm 80 | 0.03 | 0.39 | 0.87 |
| H1 | | 3800 \pm 1300 | 3700 \pm 500 | 0.87 | 0.95 | 1.01 |
| Histidine | HMDB00177 | 78\pm9 | 87\pm7 | 0.00 | 0.01 | 0.9 |
| Isoleucine | HMDB00172 HMDB0000557 | 70 \pm 14 | 74 \pm 13 | 0.38 | 0.70 | 0.95 |

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|-------------------|---|------------|------------|------|------|------|
| Kynurenine | HMDB00684 | 4.4+-0.7 | 4.8+-0.8 | 0.11 | 0.56 | 0.92 |
| Leucine | HMDB00687 HMDB0013773 | 100+-30 | 110+-30 | 0.22 | 0.62 | 0.90 |
| Lysine | HMDB00182 HMDB03405 | 350+-40 | 320+-50 | 0.02 | 0.38 | 1.10 |
| lysoPC a C16:0 | HMDB10382 HMDB0061702 | 83+-13 | 83+-16 | 0.92 | 0.96 | 1.01 |
| lysoPC a C16:1 | HMDB0010383 | 3+-1.1 | 3.2+-0.8 | 0.42 | 0.70 | 0.93 |
| lysoPC a C17:0 | HMDB12108 | 7+-1 | 7.4+-1.6 | 0.27 | 0.67 | 0.94 |
| lysoPC a C18:0 | HMDB10384 HMDB0011128 | 28+-6 | 28+-5 | 0.95 | 0.96 | 1.00 |
| lysoPC a C18:1 | HMDB02815 HMDB0010385 HMDB0061701 | 23+-6 | 26+-8 | 0.14 | 0.56 | 0.89 |
| lysoPC a C18:2 | HMDB10386 HMDB0061700 | 32+-9 | 37+-15 | 0.19 | 0.57 | 0.87 |
| lysoPC a C20:3 | HMDB10394 HMDB0010393 | 3.1+-1 | 3+-0.8 | 0.89 | 0.96 | 1.01 |
| lysoPC a C20:4 | HMDB10395 HMDB0010396 | 8.4+-2 | 8+-3 | 0.64 | 0.85 | 1.04 |
| lysoPC a C28:0 | HMDB29206 | 0.5+-0.3 | 0.6+-0.3 | 0.23 | 0.62 | 0.81 |
| lysoPC a C28:1 | HMDB0029221 | 0.6+-0.4 | 0.8+-0.4 | 0.02 | 0.38 | 0.65 |
| Methionine | HMDB00696 | 29+-4 | 31+-4 | 0.18 | 0.57 | 0.95 |
| Ornithine | HMDB00214 HMDB03374 | 39+-17 | 46+-23 | 0.23 | 0.62 | 0.85 |
| PC aa C28:1 | HMDB0007867 HMDB0007899 | 2.9+-0.7 | 3.3+-0.7 | 0.12 | 0.56 | 0.90 |
| PC aa C30:0 | HMDB0007934 HMDB0007869 HMDB0007965 | 12+-3 | 12.1+-2.2 | 0.85 | 0.95 | 1.01 |
| PC aa C30:2 | HMDB0007999 | 1.21+-0.23 | 1.1+-0.3 | 0.19 | 0.57 | 1.08 |
| PC aa C32:0 | HMDB00564 HMDB0007871 HMDB0008031 | 14+-4 | 13+-3 | 0.39 | 0.70 | 1.06 |
| PC aa C32:1 | HMDB0007872 HMDB0007873 HMDB0008097 HMDB0007969 | 17+-10 | 17+-7 | 0.97 | 0.97 | 0.99 |
| PC aa C32:2 | HMDB0008002 HMDB0007874 | 4.6+-1.8 | 4.9+-1.7 | 0.46 | 0.71 | 0.92 |
| PC aa C32:3 | HMDB0007876 | 0.7+-0.16 | 0.73+-0.13 | 0.40 | 0.70 | 0.95 |
| PC aa C34:1 | HMDB0007971 HMDB08100 HMDB0008035 HMDB0007972 HMDB0008003 | 240+-60 | 250+-50 | 0.70 | 0.90 | 0.97 |
| PC aa C34:2 | HMDB07973 HMDB0008101 HMDB0008133 HMDB0008005 HMDB0008004 | 390+-50 | 390+-70 | 0.92 | 0.96 | 1.00 |

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|-------------|--|------------|------------|------|------|------|
| PC aa C34:3 | HMDB08006 HMDB0007974 HMDB0007975 | 13+-4 | 15+-6 | 0.18 | 0.57 | 0.87 |
| PC aa C34:4 | HMDB0007883 HMDB0007976 | 1.9+-0.9 | 1.9+-0.7 | 0.87 | 0.95 | 0.98 |
| PC aa C36:0 | HMDB0008265 HMDB0008036 HMDB0008525 HMDB0007886 | 5.8+-1.2 | 5.9+-1.1 | 0.73 | 0.90 | 0.98 |
| PC aa C36:1 | HMDB08038 HMDB0008069 HMDB0007978 HMDB0008102 | 61+-14 | 65+-13 | 0.40 | 0.70 | 0.95 |
| PC aa C36:2 | HMDB08039 HMDB0008070 HMDB08135 HMDB0007979 | 230+-40 | 230+-40 | 0.94 | 0.96 | 1.00 |
| PC aa C36:3 | HMDB08105 HMDB0007980 HMDB0007981 HMDB0008040 | 133+-25 | 130+-30 | 0.82 | 0.95 | 0.99 |
| PC aa C36:4 | HMDB07982 HMDB0008107 HMDB0008138 HMDB0008234 HMDB0008429 HMDB0008170 HMDB0008138 HMDB0008042 HMDB0008203 HMDB0008106 | 170+-40 | 160+-30 | 0.12 | 0.56 | 1.10 |
| PC aa C36:5 | HMDB07984 HMDB0008015 | 20+-13 | 20+-12 | 0.85 | 0.95 | 0.97 |
| PC aa C36:6 | HMDB0008206 HMDB0007892 | 0.8+-0.4 | 0.9+-0.4 | 0.51 | 0.77 | 0.92 |
| PC aa C38:0 | HMDB0007893 HMDB0008528 HMDB0008043 HMDB0008755 HMDB0008267 HMDB0007985 | 3.4+-0.6 | 3.2+-0.7 | 0.42 | 0.70 | 1.05 |
| PC aa C38:1 | HMDB0007894 HMDB0008269 HMDB0007986 HMDB0008268 HMDB0008109 HMDB0008044 | 0.13+-0.18 | 0.23+-0.25 | 0.11 | 0.56 | 0.56 |
| PC aa C38:3 | HMDB0008020 HMDB0008046 HMDB0008047 | 50+-12 | 47+-11 | 0.30 | 0.70 | 1.07 |
| PC aa C38:4 | HMDB0008048 HMDB0008112 HMDB0008113 HMDB0007988 | 101+-23 | 85+-17 | 0.01 | 0.35 | 1.18 |

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|-------------|---|------------|------------|------|------|------|
| PC aa C38:5 | HMDB0007990 HMDB0007989 HMDB0008050 HMDB0008114 | 51+-11 | 48+-11 | 0.43 | 0.70 | 1.05 |
| PC aa C38:6 | HMDB0008725 HMDB0008116 HMDB0008434 HMDB0007991 HMDB0008147 HMDB0008083 HMDB0008499 | 61+-15 | 59+-16 | 0.75 | 0.90 | 1.03 |
| PC aa C40:2 | HMDB0008308 HMDB0008276 | 0.45+-0.08 | 0.42+-0.11 | 0.34 | 0.70 | 1.06 |
| PC aa C40:3 | HMDB0008278 HMDB0008277 HMDB0008086 HMDB0008119 | 0.77+-0.13 | 0.76+-0.12 | 0.71 | 0.90 | 1.02 |
| PC aa C40:4 | HMDB0008279 HMDB0008628 HMDB0008054 | 4+-1 | 3.6+-0.8 | 0.08 | 0.56 | 1.13 |
| PC aa C40:5 | HMDB0008056 HMDB0008055 HMDB0008120 | 9.8+-2.1 | 8.6+-2 | 0.05 | 0.51 | 1.13 |
| PC aa C40:6 | HMDB08057 HMDB0008089 | 20+-5 | 18+-4 | 0.17 | 0.57 | 1.11 |
| PC aa C42:0 | HMDB0008537 HMDB0008760 HMDB0008282 HMDB0008058 | 0.46+-0.1 | 0.48+-0.09 | 0.34 | 0.70 | 0.95 |
| PC aa C42:1 | HMDB0008762 HMDB0008124 HMDB0008283 HMDB0008538 HMDB0008059 | 0.26+-0.09 | 0.28+-0.08 | 0.45 | 0.71 | 0.93 |
| PC aa C42:2 | HMDB0008157 HMDB0008795 HMDB0008125 HMDB0008763 HMDB0008092 HMDB0008316 HMDB0008794 HMDB0008602 HMDB0008284 HMDB0008348 HMDB0008539 HMDB0011330 HMDB0008570 | 0.25+-0.06 | 0.24+-0.07 | 0.70 | 0.90 | 1.03 |
| PC aa C42:4 | HMDB0008191 | 0.26+-0.09 | 0.23+-0.08 | 0.25 | 0.64 | 1.13 |
| PC aa C42:5 | HMDB08287 | 0.33+-0.09 | 0.35+-0.11 | 0.54 | 0.79 | 0.95 |
| PC aa C42:6 | HMDB0008288 | 0.42+-0.09 | 0.41+-0.14 | 0.61 | 0.85 | 1.04 |
| PC ae C30:0 | HMDB0013341 | 0.55+-0.21 | 0.61+-0.11 | 0.09 | 0.56 | 0.90 |
| PC ae C30:1 | HMDB0013402 | 0.72+-0.16 | 0.78+-0.11 | 0.16 | 0.57 | 0.93 |

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|--------------------|---|-----------------|-------------------|-------------|-------------|-------------|
| PC ae C32:1 | HMDB0013404 HMDB0007896 HMDB0007994 | 2.6+-0.6 | 2.7+-0.5 | 0.33 | 0.70 | 0.94 |
| PC ae C32:2 | HMDB0013411 | 1.2+-0.3 | 1.28+-0.23 | 0.58 | 0.82 | 0.96 |
| PC ae C34:0 | HMDB0013405 | 1.9+-0.6 | 2+-0.5 | 0.38 | 0.70 | 0.93 |
| PC ae C34:1 | HMDB0013426 | 9.2+-2.3 | 10.2+-1.9 | 0.13 | 0.56 | 0.91 |
| PC ae C34:2 | HMDB0011151 | 10.6+-2.4 | 11.2+-2.2 | 0.37 | 0.70 | 0.95 |
| PC ae C34:3 | HMDB0013413 | 8.1+-1.8 | 8.4+-1.9 | 0.57 | 0.82 | 0.96 |
| PC ae C36:0 | HMDB13406 HMDB0013417 | 1.2+-0.3 | 1.34+-0.25 | 0.21 | 0.62 | 0.93 |
| PC ae C36:1 | HMDB0013427 HMDB0013414 | 7.6+-1.8 | 8.6+-1.6 | 0.06 | 0.51 | 0.89 |
| PC ae C36:2 | HMDB0013418 HMDB0013428 HMDB0011243 | 13+-3 | 14+-3 | 0.35 | 0.70 | 0.94 |
| PC ae C36:3 | HMDB0013429 HMDB0013425 | 8.1+-1.9 | 8.1+-1.5 | 0.96 | 0.97 | 1.00 |
| PC ae C36:4 | HMDB0013435 HMDB0013407 | 15+-4 | 13+-4 | 0.14 | 0.56 | 1.14 |
| PC ae C36:5 | HMDB0013415 HMDB0011220 | 31+-7 | 30+-5 | 0.74 | 0.90 | 1.02 |
| PC ae C38:0 | HMDB0013408 HMDB0013419 | 1.9+-0.5 | 2.1+-0.5 | 0.18 | 0.57 | 0.90 |
| PC ae C38:1 | HMDB0013419 HMDB0013408 | 1.4+-0.3 | 1.5+-0.3 | 0.03 | 0.39 | 0.88 |
| PC ae C38:2 | HMDB0013416 HMDB0013430 | 2.3+-0.5 | 2.6+-0.5 | 0.07 | 0.56 | 0.90 |
| PC ae C38:3 | HMDB0013436 HMDB0013431 | 4+-0.9 | 4.3+-0.7 | 0.31 | 0.70 | 0.94 |
| PC ae C38:4 | HMDB0013420 | 13+-3 | 12.2+-2.1 | 0.53 | 0.79 | 1.04 |
| PC ae C38:5 | HMDB11253 HMDB0013432 | 16+-3 | 15+-3 | 0.06 | 0.51 | 1.12 |
| PC ae C38:6 | HMDB0013409 | 6.4+-1.3 | 5.9+-1.7 | 0.37 | 0.70 | 1.07 |
| PC ae C40:1 | HMDB0013433 | 1.09+-0.21 | 1.2+-0.3 | 0.13 | 0.56 | 0.91 |
| PC ae C40:2 | HMDB0013437 | 1.4+-0.3 | 1.6+-0.3 | 0.14 | 0.56 | 0.91 |
| PC ae C40:3 | HMDB0013445 HMDB0013446 | 1.03+-0.17 | 1.11+-0.16 | 0.07 | 0.56 | 0.92 |
| PC ae C40:4 | HMDB0013442 | 2.1+-0.4 | 2.2+-0.4 | 0.71 | 0.90 | 0.98 |
| PC ae C40:5 | HMDB0013444 | 3+-0.4 | 3+-0.5 | 0.81 | 0.95 | 0.99 |
| PC ae C40:6 | HMDB0013422 | 3.7+-0.8 | 3.7+-0.8 | 0.93 | 0.96 | 0.99 |
| PC ae C42:1 | HMDB0013434 HMDB0013447 | 0.34+-0.07 | 0.32+-0.06 | 0.27 | 0.67 | 1.07 |
| PC ae C42:2 | HMDB0013438 | 0.53+-0.13 | 0.57+-0.09 | 0.12 | 0.56 | 0.91 |
| PC ae C42:3 | HMDB0013458 HMDB0013459 | 0.7+-0.1 | 0.82+-0.12 | 0.00 | 0.03 | 0.86 |
| PC ae C44:3 | HMDB0013449 HMDB0013452 | 0.15+-0.06 | 0.15+-0.06 | 0.86 | 0.95 | 0.98 |
| PC ae C44:4 | HMDB0013455 HMDB0013453 HMDB0013460 | 0.46+-0.1 | 0.49+-0.11 | 0.32 | 0.70 | 0.94 |
| PC ae C44:5 | HMDB0013456 | 1.6+-0.4 | 1.7+-0.4 | 0.17 | 0.57 | 0.91 |
| PC ae C44:6 | HMDB0013450 HMDB0013457 | 0.99+-0.17 | 1+-0.24 | 0.80 | 0.95 | 0.98 |

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|------------------|----------------------------|-------------------|------------------|-------------|-------------|-------------|
| Phenylalanine | HMDB00159 | 66+-8 | 70+-22 | 0.34 | 0.70 | 0.93 |
| Proline | HMDB00162 HMDB03411 | 230+-60 | 200+-40 | 0.11 | 0.56 | 1.12 |
| Putrescine | HMDB01414 | 0.16+-0.07 | 0.19+-0.06 | 0.14 | 0.56 | 0.85 |
| Serine | HMDB00187 HMDB03406 | 117+-22 | 121+-20 | 0.45 | 0.71 | 0.96 |
| Serotonin | HMDB00259 | 0.8+-0.4 | 0.9+-0.4 | 0.39 | 0.70 | 0.89 |
| SM (OH) C14:1 | HMDB0013462 | 5.8+-2 | 6.5+-1.6 | 0.23 | 0.62 | 0.90 |
| SM (OH) C16:1 | HMDB0013463 | 4.2+-1.2 | 4.2+-0.9 | 0.81 | 0.95 | 0.98 |
| SM (OH) C22:1 | HMDB0013466 | 17+-4 | 19+-4 | 0.30 | 0.70 | 0.94 |
| SM (OH) C22:2 | HMDB0013467 | 14+-3 | 15+-3 | 0.19 | 0.57 | 0.92 |
| SM (OH) C24:1 | HMDB0013469 | 1.8+-0.4 | 1.9+-0.5 | 0.62 | 0.85 | 0.96 |
| SM C16:0 | HMDB0061712 HMDB0010169 | 146+-22 | 140+-20 | 0.35 | 0.70 | 1.04 |
| SM C16:1 | HMDB0029216 | 21+-4 | 20+-3 | 0.35 | 0.70 | 1.05 |
| SM C18:0 | HMDB01348 | 29+-7 | 28+-6 | 0.67 | 0.88 | 1.03 |
| SM C18:1 | HMDB0012100 HMDB0012101 | 14+-4 | 13+-3 | 0.44 | 0.70 | 1.06 |
| SM C20:2 | | 0.5+-0.18 | 0.5+-0.16 | 0.94 | 0.96 | 0.99 |
| SM C22:3 | | 2.7+-1.1 | 2.6+-1.1 | 0.85 | 0.95 | 1.02 |
| SM C24:0 | HMDB11697 | 37+-6 | 36+-6 | 0.43 | 0.70 | 1.04 |
| SM C24:1 | HMDB12107 | 70+-11 | 65+-11 | 0.14 | 0.56 | 1.08 |
| SM C26:0 | HMDB0011698 | 0.38+-0.15 | 0.41+-0.15 | 0.54 | 0.79 | 0.94 |
| SM C26:1 | HMDB0013461 | 0.44+-0.21 | 0.41+-0.15 | 0.63 | 0.85 | 1.06 |
| Taurine | HMDB00251 | 61+-12 | 83+-20 | 0.00 | 0.01 | 0.74 |
| Threonine | HMDB04041 HMDB00167 | 121+-24 | 130+-30 | 0.41 | 0.70 | 0.95 |
| Tryptophane | HMDB00929 HMDB0013609 | 64+-13 | 70+-10 | 0.13 | 0.56 | 0.93 |
| Tyrosine | HMDB00158 | 69+-16 | 68+-12 | 0.78 | 0.93 | 1.02 |
| Valine | HMDB00883 | 240+-50 | 270+-50 | 0.03 | 0.39 | 0.89 |
| BCAA | | 416+-87 | 460+-85 | | | |
| AAA | | 277+-30 | 295+-33 | | | |
| Fischer ratio | | 1.5+-0.25 | 1.57+-0.27 | | | |
| ADMA/Arg | | 0.0046+- 0.001 | 0.004+- 0.001 | | | |
| Cit/Arg | | 0.26+-0.07 | 0.27+-0.05 | | | |
| Cit/Orn | | 0.94+-0.49 | 1.3+-2.3 | | | |
| Orn/Arg | | 0.33+-0.14 | 0.39+-0.21 | | | |

Table S1 b. Values of amino acids, of biogenic amines and their derivatives, and of selected sums and ratios – patients with preserved systolic ventricular function (group AF).

| Metabolite | HMBD ID | Patients | Controls | p | q | FC |
|-------------------|--|-----------------|------------------|-------------|-------------|-------------|
| ADMA | HMDB01539 | 0.54+-0.12 | 0.48+-0.13 | 0.12 | 0.73 | 1.13 |
| Alanine | HMDB00161 HMDB01310 | 400+-90 | 390+-80 | 0.59 | 0.84 | 1.03 |
| Arginine | HMDB00517 HMDB03416 | 119+-14 | 119+-20 | 0.87 | 0.96 | 0.99 |
| Asparagine | HMDB00168 HMDB003378 | 48+-10 | 48+-9 | 0.94 | 0.98 | 1.00 |
| Aspartic acid | HMDB00191 HMDB06483 | 18.8+-2.4 | 20+-4 | 0.36 | 0.83 | 0.94 |
| C0 | HMDB00062 | 36+-7 | 33+-5 | 0.10 | 0.73 | 1.10 |
| C14:1 | HMDB0002014 | 0.14+-0.05 | 0.13+-0.03 | 0.71 | 0.90 | 1.03 |
| C18:1 | HMDB0006351 HMDB0005065 HMDB06464 HMDB0013338 | 0.15+-0.05 | 0.14+-0.03 | 0.57 | 0.84 | 1.05 |
| C18:2 | HMDB0006469 HMDB0006461 | 0.053+- 0.02 | 0.049+- 0.018 | 0.50 | 0.84 | 1.08 |
| C2 | HMDB00201 | 7+-3 | 6.5+-1.7 | 0.71 | 0.90 | 1.04 |
| Citrulline | HMDB00904 | 30+-9 | 32+-7 | 0.57 | 0.84 | 0.95 |
| Creatinine | HMDB0000562 | 72+-16 | 82+-14 | 0.04 | 0.50 | 0.88 |
| Glutamine | HMDB00641 HMDB03423 | 740+-80 | 740+-110 | 0.88 | 0.96 | 1.01 |
| Glutamic acid | HMDB00148 HMDB03339 | 47+-23 | 33+-20 | 0.04 | 0.50 | 1.42 |
| Glycine | HMDB00123 | 270+-60 | 310+-80 | 0.06 | 0.59 | 0.87 |
| H1 | | 3800+- 1300 | 3700+-600 | 0.79 | 0.95 | 1.02 |
| Histidine | HMDB00177 | 78+-10 | 87+-7 | 0.00 | 0.03 | 0.89 |
| Isoleucine | HMDB00172 HMDB0000557 | 71+-14 | 73+-13 | 0.59 | 0.84 | 0.97 |
| Kynurenine | HMDB00684 | 4.5+-0.7 | 4.8+-0.9 | 0.16 | 0.73 | 0.93 |
| Leucine | HMDB00687 HMDB0013773 | 100+-30 | 110+-30 | 0.31 | 0.81 | 0.92 |
| Lysine | HMDB00182 HMDB03405 | 360+-30 | 320+-50 | 0.01 | 0.16 | 1.13 |
| lysoPC a C16:0 | HMDB10382 HMDB0061702 | 83+-13 | 83+-17 | 0.95 | 0.98 | 1.00 |
| lysoPC a C16:1 | HMDB0010383 | 3+-1.1 | 3.2+-0.8 | 0.53 | 0.84 | 0.94 |
| lysoPC a C17:0 | HMDB12108 | 7+-1 | 7.4+-1.6 | 0.27 | 0.77 | 0.94 |
| lysoPC a C18:0 | HMDB10384 HMDB0011128 | 28+-6 | 28+-5 | 0.88 | 0.96 | 1.01 |
| lysoPC a C18:1 | HMDB02815 HMDB0010385 HMDB0061701 | 23+-6 | 26+-8 | 0.21 | 0.75 | 0.90 |
| lysoPC a C18:2 | HMDB10386 HMDB0061700 | 33+-9 | 37+-15 | 0.29 | 0.81 | 0.89 |
| lysoPC a C20:3 | HMDB10394 HMDB0010393 | 3+-0.9 | 3+-0.8 | 0.98 | 0.98 | 1.00 |

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|-------------------|---|------------|------------|------|------|------|
| lysoPC a C20:4 | HMDB10395 HMDB0010396 | 8.3+-2 | 8+-3 | 0.50 | 0.84 | 1.06 |
| lysoPC a C28:0 | HMDB29206 | 0.5+-0.3 | 0.6+-0.3 | 0.13 | 0.73 | 0.77 |
| lysoPC a C28:1 | HMDB0029221 | 0.6+-0.4 | 0.8+-0.4 | 0.04 | 0.50 | 0.68 |
| Methionine | HMDB00696 | 29+-4 | 30+-4 | 0.49 | 0.84 | 0.97 |
| Ornithine | HMDB00214 HMDB03374 | 41+-16 | 46+-23 | 0.37 | 0.83 | 0.88 |
| PC aa C28:1 | HMDB0007867 HMDB0007899 | 3+-0.8 | 3.3+-0.7 | 0.15 | 0.73 | 0.90 |
| PC aa C30:0 | HMDB0007934 HMDB0007869 HMDB0007965 | 12+-3 | 12.1+-2.2 | 0.82 | 0.96 | 1.02 |
| PC aa C30:2 | HMDB0007999 | 1.2+-0.23 | 1.1+-0.3 | 0.20 | 0.75 | 1.09 |
| PC aa C32:0 | HMDB00564 HMDB0007871 HMDB0008031 | 14+-4 | 14+-3 | 0.44 | 0.83 | 1.06 |
| PC aa C32:1 | HMDB0007872 HMDB0007873 HMDB0008097 HMDB0007969 | 17+-11 | 17+-7 | 0.98 | 0.98 | 1.00 |
| PC aa C32:2 | HMDB0008002 HMDB0007874 | 4.6+-1.9 | 5+-1.7 | 0.50 | 0.84 | 0.93 |
| PC aa C32:3 | HMDB0007876 | 0.69+-0.16 | 0.74+-0.13 | 0.27 | 0.77 | 0.93 |
| PC aa C34:1 | HMDB0007971 HMDB08100 HMDB0008035 HMDB0007972 HMDB0008003 | 240+-60 | 250+-50 | 0.67 | 0.89 | 0.97 |
| PC aa C34:2 | HMDB07973 HMDB0008101 HMDB0008133 HMDB0008005 HMDB0008004 | 390+-50 | 390+-70 | 0.97 | 0.98 | 1.00 |
| PC aa C34:3 | HMDB08006 HMDB0007974 HMDB0007975 | 14+-4 | 16+-6 | 0.20 | 0.75 | 0.87 |
| PC aa C34:4 | HMDB0007883 HMDB0007976 | 1.9+-0.9 | 2+-0.7 | 0.83 | 0.96 | 0.97 |
| PC aa C36:0 | HMDB0008265 HMDB0008036 HMDB0008525 HMDB0007886 | 5.9+-1.3 | 6+-1.1 | 0.67 | 0.89 | 0.97 |
| PC aa C36:1 | HMDB08038 HMDB0008069 HMDB0007978 HMDB0008102 | 62+-14 | 65+-13 | 0.42 | 0.83 | 0.95 |
| PC aa C36:2 | HMDB08039 HMDB0008070 HMDB08135 HMDB0007979 | 230+-40 | 230+-40 | 0.87 | 0.96 | 1.01 |

| | | | | | | |
|-------------|--|------------|------------|------|------|------|
| PC aa C36:3 | HMDB08105 HMDB0007980 HMDB0007981 HMDB0008040 | 130+-30 | 140+-30 | 0.78 | 0.95 | 0.98 |
| PC aa C36:4 | HMDB07982 HMDB0008107 HMDB0008138 HMDB0008234 HMDB0008429 HMDB0008170 HMDB0008138 HMDB0008042 HMDB0008203 HMDB0008106 | 170+-40 | 160+-30 | 0.13 | 0.73 | 1.11 |
| PC aa C36:5 | HMDB07984 HMDB0008015 | 20+-14 | 21+-12 | 0.79 | 0.95 | 0.95 |
| PC aa C36:6 | HMDB0008206 HMDB0007892 | 0.9+-0.4 | 0.9+-0.4 | 0.52 | 0.84 | 0.92 |
| PC aa C38:0 | HMDB0007893 HMDB0008528 HMDB0008043 HMDB0008755 HMDB0008267 HMDB0007985 | 3.4+-0.6 | 3.2+-0.7 | 0.53 | 0.84 | 1.04 |
| PC aa C38:1 | HMDB0007894 HMDB0008269 HMDB0007986 HMDB0008268 HMDB0008109 HMDB0008044 | 0.14+-0.18 | 0.22+-0.24 | 0.22 | 0.75 | 0.64 |
| PC aa C38:3 | HMDB0008020 HMDB0008046 HMDB0008047 | 50+-12 | 47+-11 | 0.42 | 0.83 | 1.06 |
| PC aa C38:4 | HMDB0008048 HMDB0008112 HMDB0008113 HMDB0007988 | 101+-24 | 85+-17 | 0.02 | 0.46 | 1.18 |
| PC aa C38:5 | HMDB0007990 HMDB0007989 HMDB0008050 HMDB0008114 | 51+-11 | 49+-11 | 0.58 | 0.84 | 1.04 |
| PC aa C38:6 | HMDB0008725 HMDB0008116 HMDB0008434 HMDB0007991 HMDB0008147 HMDB0008083 HMDB0008499 | 60+-16 | 59+-17 | 0.81 | 0.96 | 1.02 |
| PC aa C40:2 | HMDB0008308 HMDB0008276 | 0.45+-0.08 | 0.42+-0.11 | 0.44 | 0.83 | 1.06 |
| PC aa C40:3 | HMDB0008278 HMDB0008277 HMDB0008086 HMDB0008119 | 0.77+-0.14 | 0.77+-0.13 | 0.92 | 0.98 | 1.01 |

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|-------------|---|------------|------------|------|------|------|
| PC aa C40:4 | HMDB0008279 HMDB0008628 HMDB0008054 | 4+-1 | 3.6+-0.8 | 0.15 | 0.73 | 1.11 |
| PC aa C40:5 | HMDB0008056 HMDB0008055 HMDB0008120 | 9.8+-2.2 | 8.8+-2 | 0.13 | 0.73 | 1.11 |
| PC aa C40:6 | HMDB08057 HMDB0008089 | 20+-5 | 18+-4 | 0.23 | 0.75 | 1.10 |
| PC aa C42:0 | HMDB0008537 HMDB0008760 HMDB0008282 HMDB0008058 | 0.46+-0.1 | 0.48+-0.09 | 0.48 | 0.84 | 0.96 |
| PC aa C42:1 | HMDB0008762 HMDB0008124 HMDB0008283 HMDB0008538 HMDB0008059 | 0.26+-0.09 | 0.28+-0.08 | 0.44 | 0.83 | 0.93 |
| PC aa C42:2 | HMDB0008157 HMDB0008795 HMDB0008125 HMDB0008763 HMDB0008092 HMDB0008316 HMDB0008794 HMDB0008602 HMDB0008284 HMDB0008348 HMDB0008539 HMDB0011330 HMDB0008570 | 0.25+-0.06 | 0.24+-0.07 | 0.58 | 0.84 | 1.05 |
| PC aa C42:4 | HMDB0008191 | 0.26+-0.09 | 0.23+-0.08 | 0.21 | 0.75 | 1.15 |
| PC aa C42:5 | HMDB08287 | 0.33+-0.09 | 0.36+-0.11 | 0.43 | 0.83 | 0.93 |
| PC aa C42:6 | HMDB0008288 | 0.42+-0.09 | 0.41+-0.14 | 0.67 | 0.89 | 1.04 |
| PC ae C30:0 | HMDB0013341 | 0.55+-0.21 | 0.61+-0.12 | 0.16 | 0.73 | 0.90 |
| PC ae C30:1 | HMDB0013402 | 0.72+-0.16 | 0.79+-0.11 | 0.11 | 0.73 | 0.91 |
| PC ae C32:1 | HMDB0013404 HMDB0007896 HMDB0007994 | 2.6+-0.6 | 2.7+-0.5 | 0.33 | 0.81 | 0.94 |
| PC ae C32:2 | HMDB0013411 | 1.2+-0.3 | 1.29+-0.24 | 0.49 | 0.84 | 0.95 |
| PC ae C34:0 | HMDB0013405 | 1.9+-0.6 | 2.1+-0.5 | 0.40 | 0.83 | 0.93 |
| PC ae C34:1 | HMDB0013426 | 9.3+-2.4 | 10.2+-1.9 | 0.17 | 0.73 | 0.91 |
| PC ae C34:2 | HMDB0011151 | 11+-3 | 11.2+-2.3 | 0.33 | 0.81 | 0.94 |
| PC ae C34:3 | HMDB0013413 | 8+-1.9 | 8.5+-2 | 0.45 | 0.84 | 0.95 |
| PC ae C36:0 | HMDB13406 HMDB0013417 | 1.2+-0.3 | 1.4+-0.3 | 0.23 | 0.75 | 0.93 |
| PC ae C36:1 | HMDB0013427 HMDB0013414 | 7.7+-1.8 | 8.7+-1.7 | 0.06 | 0.63 | 0.88 |
| PC ae C36:2 | HMDB0013418 HMDB0013428 HMDB0011243 | 13+-3 | 14+-3 | 0.39 | 0.83 | 0.95 |
| PC ae C36:3 | HMDB0013429 HMDB0013425 | 7.9+-1.9 | 8.1+-1.6 | 0.78 | 0.95 | 0.98 |
| PC ae C36:4 | HMDB0013435 HMDB0013407 | 15+-4 | 13+-4 | 0.27 | 0.77 | 1.11 |

| | | | | | | |
|------------------|---|------------------|-------------------|-------------|-------------|-------------|
| PC ae C36:5 | HMDB0013415 HMDB0011220 | 30+-7 | 30+-5 | 0.84 | 0.96 | 1.01 |
| PC ae C38:0 | HMDB0013408 HMDB0013419 | 1.9+-0.6 | 2.1+-0.6 | 0.21 | 0.75 | 0.90 |
| PC ae C38:1 | HMDB0013419 HMDB0013408 | 1.4+-0.3 | 1.6+-0.3 | 0.03 | 0.50 | 0.88 |
| PC ae C38:2 | HMDB0013416 HMDB0013430 | 2.3+-0.5 | 2.6+-0.5 | 0.12 | 0.73 | 0.91 |
| PC ae C38:3 | HMDB0013436 HMDB0013431 | 4+-0.9 | 4.3+-0.7 | 0.33 | 0.81 | 0.94 |
| PC ae C38:4 | HMDB0013420 | 13+-3 | 12.1+-2.1 | 0.56 | 0.84 | 1.04 |
| PC ae C38:5 | HMDB11253 HMDB0013432 | 16+-3 | 14+-3 | 0.10 | 0.73 | 1.11 |
| PC ae C38:6 | HMDB0013409 | 6.3+-1.4 | 6+-1.8 | 0.57 | 0.84 | 1.05 |
| PC ae C40:1 | HMDB0013433 | 1.09+-0.22 | 1.2+-0.3 | 0.17 | 0.73 | 0.91 |
| PC ae C40:2 | HMDB0013437 | 1.4+-0.3 | 1.6+-0.3 | 0.12 | 0.73 | 0.90 |
| PC ae C40:3 | HMDB0013445 HMDB0013446 | 1.03+-0.17 | 1.12+-0.17 | 0.09 | 0.73 | 0.92 |
| PC ae C40:4 | HMDB0013442 | 2.1+-0.4 | 2.1+-0.4 | 0.79 | 0.95 | 0.99 |
| PC ae C40:5 | HMDB0013444 | 3+-0.4 | 3+-0.5 | 0.89 | 0.96 | 0.99 |
| PC ae C40:6 | HMDB0013422 | 3.7+-0.8 | 3.7+-0.8 | 0.85 | 0.96 | 0.99 |
| PC ae C42:1 | HMDB0013434 HMDB0013447 | 0.33+-0.07 | 0.32+-0.06 | 0.50 | 0.84 | 1.04 |
| PC ae C42:2 | HMDB0013438 | 0.52+-0.13 | 0.57+-0.09 | 0.19 | 0.75 | 0.92 |
| PC ae C42:3 | HMDB0013458 HMDB0013459 | 0.69+-0.1 | 0.82+-0.12 | 0.00 | 0.02 | 0.84 |
| PC ae C44:3 | HMDB0013449 HMDB0013452 | 0.15+-0.06 | 0.15+-0.06 | 0.97 | 0.98 | 1.00 |
| PC ae C44:4 | HMDB0013455 HMDB0013453 HMDB0013460 | 0.46+-0.1 | 0.47+-0.09 | 0.66 | 0.89 | 0.97 |
| PC ae C44:5 | HMDB0013456 | 1.6+-0.4 | 1.7+-0.4 | 0.35 | 0.82 | 0.93 |
| PC ae C44:6 | HMDB0013450 HMDB0013457 | 0.99+-0.18 | 0.99+-0.24 | 0.95 | 0.98 | 1.00 |
| Phenylalanine | HMDB00159 | 66+-8 | 70+-23 | 0.43 | 0.83 | 0.94 |
| Proline | HMDB00162 HMDB03411 | 230+-50 | 200+-40 | 0.03 | 0.50 | 1.17 |
| Putrescine | HMDB01414 | 0.17+-0.07 | 0.19+-0.06 | 0.32 | 0.81 | 0.89 |
| Serine | HMDB00187 HMDB03406 | 118+-22 | 119+-18 | 0.87 | 0.96 | 0.99 |
| Serotonin | HMDB00259 | 0.8+-0.4 | 0.8+-0.3 | 0.68 | 0.89 | 0.94 |
| SM (OH) C14:1 | HMDB0013462 | 5.9+-2.1 | 6.6+-1.6 | 0.25 | 0.76 | 0.90 |
| SM (OH) C16:1 | HMDB0013463 | 4.2+-1.2 | 4.3+-0.9 | 0.68 | 0.89 | 0.97 |
| SM (OH) C22:1 | HMDB0013466 | 17+-4 | 19+-4 | 0.31 | 0.81 | 0.93 |
| SM (OH) C22:2 | HMDB0013467 | 14+-3 | 16+-3 | 0.17 | 0.73 | 0.92 |
| SM (OH) C24:1 | HMDB0013469 | 1.8+-0.4 | 1.9+-0.5 | 0.70 | 0.90 | 0.97 |
| SM C16:0 | HMDB0061712 HMDB0010169 | 146+-23 | 140+-20 | 0.41 | 0.83 | 1.04 |
| SM C16:1 | HMDB0029216 | 21+-4 | 20+-3 | 0.34 | 0.82 | 1.05 |
| SM C18:0 | HMDB01348 | 28+-7 | 28+-6 | 0.92 | 0.98 | 1.01 |

| | | | | | | |
|----------------|----------------------------|-------------------|------------------|-------------|-------------|-------------|
| SM C18:1 | HMDB0012100 HMDB0012101 | 14+-3 | 13+-3 | 0.64 | 0.89 | 1.04 |
| SM C20:2 | | 0.49+-0.19 | 0.51+-0.16 | 0.73 | 0.92 | 0.96 |
| SM C22:3 | | 2.7+-1.2 | 2.6+-1.2 | 0.95 | 0.98 | 1.01 |
| SM C24:0 | HMDB11697 | 37+-6 | 36+-7 | 0.52 | 0.84 | 1.03 |
| SM C24:1 | HMDB12107 | 69+-12 | 65+-12 | 0.27 | 0.77 | 1.06 |
| SM C26:0 | HMDB0011698 | 0.39+-0.16 | 0.42+-0.15 | 0.49 | 0.84 | 0.92 |
| SM C26:1 | HMDB0013461 | 0.44+-0.22 | 0.41+-0.16 | 0.58 | 0.84 | 1.08 |
| Taurine | HMDB00251 | 61+-11 | 84+-21 | 0.00 | 0.01 | 0.72 |
| Threonine | HMDB04041 HMDB00167 | 121+-25 | 120+-30 | 0.60 | 0.84 | 0.97 |
| Tryptophane | HMDB00929 HMDB0013609 | 65+-13 | 69+-10 | 0.24 | 0.75 | 0.94 |
| Tyrosine | HMDB00158 | 71+-16 | 67+-12 | 0.40 | 0.83 | 1.05 |
| Valine | HMDB00883 | 240+-48 | 270+-40 | 0.05 | 0.59 | 0.90 |
| BCAA | | 416+-90 | 455+-81 | | | |
| AAA | | 279+-30 | 294+-34 | | | |
| Fischer ratio | | 1.49+-0.25 | 1.56+-0.26 | | | |
| ADMA/Arg | | 0.0046+- 0.001 | 0.004+- 0.001 | | | |
| Cit/Arg | | 0.26+-0.08 | 0.27+-0.05 | | | |
| Cit/Orn | | 0.85+-0.38 | 1.34+-2.3 | | | |
| Orn/Arg | | 0.35+-0.13 | 0.39+-0.21 | | | |

Table S1 c. Values of amino acids, of biogenic amines and their derivatives, and of selected sums and ratios – patients with preserved systolic function and without major valve regurgitation (group AFV).

| Metabolite | HMDB ID | Patients | Controls | p | q | FC |
|-------------------|--|------------------|--------------|-------------|-------------|-------------|
| ADMA | HMDB01539 | 0.53+-0.12 | 0.48+-0.1 | 0.28 | 0.84 | 1.10 |
| Alanine | HMDB00161 HMDB01310 | 430+-70 | 380+-80 | 0.14 | 0.84 | 1.11 |
| Arginine | HMDB00517 HMDB03416 | 123+-13 | 121+-20 | 0.71 | 0.92 | 1.02 |
| Asparagine | HMDB00168 HMDB003378 | 50+-12 | 51+-7 | 0.69 | 0.92 | 0.97 |
| Aspartic acid | HMDB00191 HMDB06483 | 18.9+-2.4 | 20+-4 | 0.43 | 0.85 | 0.95 |
| C0 | HMDB00062 | 36+-9 | 33+-4 | 0.31 | 0.84 | 1.08 |
| C14:1 | HMDB0002014 | 0.13+-0.04 | 0.14+-0.03 | 0.47 | 0.85 | 0.93 |
| C18:1 | HMDB0006351 HMDB0005065 HMDB06464 HMDB0013338 | 0.14+-0.05 | 0.15+-0.04 | 0.65 | 0.92 | 0.95 |
| C18:2 | HMDB0006469 HMDB0006461 | 0.049+- 0.022 | 0.052+-0.02 | 0.79 | 0.92 | 0.96 |
| C2 | HMDB00201 | 6+-3 | 6.6+-1.6 | 0.57 | 0.91 | 0.93 |
| Citrulline | HMDB00904 | 31+-9 | 33+-7 | 0.57 | 0.91 | 0.94 |
| Creatinine | HMDB0000562 | 76+-19 | 83+-17 | 0.27 | 0.84 | 0.91 |
| Glutamine | HMDB00641 HMDB03423 | 750+-80 | 730+-110 | 0.58 | 0.91 | 1.03 |
| Glutamic acid | HMDB00148 HMDB03339 | 45+-23 | 35+-24 | 0.24 | 0.84 | 1.30 |
| Glycine | HMDB00123 | 270+-50 | 290+-50 | 0.19 | 0.84 | 0.91 |
| H1 | | 3900+-1600 | 3700+-400 | 0.61 | 0.92 | 1.06 |
| Histidine | HMDB00177 | 81+-10 | 87+-9 | 0.07 | 0.84 | 0.92 |
| Isoleucine | HMDB00172 HMDB0000557 | 76+-15 | 74+-12 | 0.66 | 0.92 | 1.03 |
| Kynurenine | HMDB00684 | 4.4+-0.8 | 4.6+-0.8 | 0.45 | 0.85 | 0.95 |
| Leucine | HMDB00687 HMDB0013773 | 120+-30 | 110+-30 | 0.95 | 0.98 | 1.01 |
| Lysine | HMDB00182 HMDB03405 | 370+-40 | 320+-60 | 0.01 | 0.29 | 1.16 |
| lysoPC a C16:0 | HMDB10382 HMDB0061702 | 85+-14 | 80+-11 | 0.35 | 0.84 | 1.06 |
| lysoPC a C16:1 | HMDB0010383 | 3.2+-1 | 3+-0.5 | 0.61 | 0.92 | 1.05 |
| lysoPC a C17:0 | HMDB12108 | 7.1+-1 | 7.3+-1.1 | 0.66 | 0.92 | 0.98 |
| lysoPC a C18:0 | HMDB10384 HMDB0011128 | 28+-6 | 28+-4 | 0.83 | 0.92 | 1.02 |
| lysoPC a C18:1 | HMDB02815 HMDB0010385 HMDB0061701 | 24+-6 | 26+-6 | 0.41 | 0.84 | 0.93 |
| lysoPC a C18:2 | HMDB10386 HMDB0061700 | 35+-10 | 38+-15 | 0.56 | 0.91 | 0.92 |
| lysoPC a C20:3 | HMDB10394 HMDB0010393 | 3.1+-1 | 3+-0.9 | 0.81 | 0.92 | 1.03 |

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|-------------------|---|------------|------------|------|------|------|
| lysoPC a C20:4 | HMDB10395 HMDB0010396 | 9+-2 | 8+-3 | 0.38 | 0.84 | 1.10 |
| lysoPC a C28:0 | HMDB29206 | 0.5+-0.3 | 0.6+-0.3 | 0.33 | 0.84 | 0.80 |
| lysoPC a C28:1 | HMDB0029221 | 0.6+-0.4 | 0.7+-0.5 | 0.40 | 0.84 | 0.82 |
| Methionine | HMDB00696 | 30+-4 | 31+-4 | 0.58 | 0.91 | 0.97 |
| Ornithine | HMDB00214 HMDB03374 | 42+-16 | 51+-25 | 0.23 | 0.84 | 0.81 |
| PC aa C28:1 | HMDB0007867 HMDB0007899 | 3+-0.8 | 3.1+-0.6 | 0.67 | 0.92 | 0.96 |
| PC aa C30:0 | HMDB0007934 HMDB0007869 HMDB0007965 | 12+-3 | 11.3+-1.6 | 0.36 | 0.84 | 1.08 |
| PC aa C30:2 | HMDB0007999 | 1.21+-0.24 | 1+-0.3 | 0.08 | 0.84 | 1.17 |
| PC aa C32:0 | HMDB00564 HMDB0007871 HMDB0008031 | 14+-4 | 12.8+-2.4 | 0.20 | 0.84 | 1.14 |
| PC aa C32:1 | HMDB0007872 HMDB0007873 HMDB0008097 HMDB0007969 | 17+-12 | 14+-6 | 0.41 | 0.84 | 1.21 |
| PC aa C32:2 | HMDB0008002 HMDB0007874 | 4.8+-2.1 | 4.3+-1.6 | 0.51 | 0.89 | 1.11 |
| PC aa C32:3 | HMDB0007876 | 0.69+-0.18 | 0.71+-0.13 | 0.74 | 0.92 | 0.97 |
| PC aa C34:1 | HMDB0007971 HMDB08100 HMDB0008035 HMDB0007972 HMDB0008003 | 240+-60 | 230+-40 | 0.48 | 0.85 | 1.06 |
| PC aa C34:2 | HMDB07973 HMDB0008101 HMDB0008133 HMDB0008005 HMDB0008004 | 400+-50 | 370+-60 | 0.10 | 0.84 | 1.10 |
| PC aa C34:3 | HMDB08006 HMDB0007974 HMDB0007975 | 14+-5 | 15+-7 | 0.74 | 0.92 | 0.95 |
| PC aa C34:4 | HMDB0007883 HMDB0007976 | 2+-1 | 1.7+-0.6 | 0.34 | 0.84 | 1.18 |
| PC aa C36:0 | HMDB0008265 HMDB0008036 HMDB0008525 HMDB0007886 | 5.9+-1.3 | 5.8+-1 | 0.74 | 0.92 | 1.02 |
| PC aa C36:1 | HMDB08038 HMDB0008069 HMDB0007978 HMDB0008102 | 63+-14 | 62+-13 | 0.93 | 0.97 | 1.01 |
| PC aa C36:2 | HMDB08039 HMDB0008070 HMDB08135 HMDB0007979 | 240+-40 | 220+-40 | 0.25 | 0.84 | 1.08 |
| PC aa C36:3 | HMDB08105 HMDB0007980 HMDB0007981 HMDB0008040 | 140+-30 | 124+-23 | 0.20 | 0.84 | 1.10 |

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|-------------|--|------------|-----------|------|------|------|
| PC aa C36:4 | HMDB07982 HMDB0008107 HMDB0008138 HMDB0008234 HMDB0008429 HMDB0008170 HMDB0008138 HMDB0008042 HMDB0008203 HMDB0008106 | 190+-40 | 150+-30 | 0.01 | 0.29 | 1.24 |
| PC aa C36:5 | HMDB07984 HMDB0008015 | 19+-11 | 18+-8 | 0.71 | 0.92 | 1.08 |
| PC aa C36:6 | HMDB0008206 HMDB0007892 | 0.9+-0.4 | 0.8+-0.3 | 0.57 | 0.91 | 1.09 |
| PC aa C38:0 | HMDB0007893 HMDB0008528 HMDB0008043 HMDB0008755 HMDB0008267 HMDB0007985 | 3.4+-0.7 | 3.2+-0.7 | 0.39 | 0.84 | 1.07 |
| PC aa C38:1 | HMDB0007894 HMDB0008269 HMDB0007986 HMDB0008268 HMDB0008109 HMDB0008044 | 0.15+-0.2 | 0.2+-0.3 | 0.42 | 0.85 | 0.67 |
| PC aa C38:3 | HMDB0008020 HMDB0008046 HMDB0008047 | 50+-12 | 44+-10 | 0.16 | 0.84 | 1.14 |
| PC aa C38:4 | HMDB0008048 HMDB0008112 HMDB0008113 HMDB0007988 | 106+-24 | 84+-17 | 0.01 | 0.29 | 1.26 |
| PC aa C38:5 | HMDB0007990 HMDB0007989 HMDB0008050 HMDB0008114 | 51+-10 | 47+-10 | 0.25 | 0.84 | 1.09 |
| PC aa C38:6 | HMDB0008725 HMDB0008116 HMDB0008434 HMDB0007991 HMDB0008147 HMDB0008083 HMDB0008499 | 60+-15 | 55+-16 | 0.45 | 0.85 | 1.08 |
| PC aa C40:2 | HMDB0008308 HMDB0008276 | 0.45+-0.07 | 0.4+-0.12 | 0.21 | 0.84 | 1.12 |
| PC aa C40:3 | HMDB0008278 HMDB0008277 HMDB0008086 HMDB0008119 | 0.76+-0.11 | 0.73+-0.1 | 0.41 | 0.84 | 1.05 |
| PC aa C40:4 | HMDB0008279 HMDB0008628 HMDB0008054 | 4+-0.9 | 3.5+-0.8 | 0.12 | 0.84 | 1.15 |
| PC aa C40:5 | HMDB0008056 HMDB0008055 HMDB0008120 | 9.5+-1.7 | 8.6+-2 | 0.18 | 0.84 | 1.11 |
| PC aa C40:6 | HMDB08057 HMDB0008089 | 19+-5 | 17+-4 | 0.21 | 0.84 | 1.13 |

| | | | | | | |
|-------------|---|------------|------------|------|------|------|
| PC aa C42:0 | HMDB0008537 HMDB0008760 HMDB0008282 HMDB0008058 | 0.45+-0.09 | 0.49+-0.09 | 0.28 | 0.84 | 0.92 |
| PC aa C42:1 | HMDB0008762 HMDB0008124 HMDB0008283 HMDB0008538 HMDB0008059 | 0.27+-0.08 | 0.28+-0.09 | 0.73 | 0.92 | 0.96 |
| PC aa C42:2 | HMDB0008157 HMDB0008795 HMDB0008125 HMDB0008763 HMDB0008092 HMDB0008316 HMDB0008794 HMDB0008602 HMDB0008284 HMDB0008348 HMDB0008539 HMDB0011330 HMDB0008570 | 0.24+-0.05 | 0.24+-0.05 | 0.79 | 0.92 | 0.98 |
| PC aa C42:4 | HMDB0008191 | 0.26+-0.09 | 0.22+-0.07 | 0.28 | 0.84 | 1.16 |
| PC aa C42:5 | HMDB08287 | 0.33+-0.11 | 0.34+-0.11 | 0.85 | 0.93 | 0.98 |
| PC aa C42:6 | HMDB0008288 | 0.41+-0.09 | 0.37+-0.14 | 0.35 | 0.84 | 1.12 |
| PC ae C30:0 | HMDB0013341 | 0.52+-0.24 | 0.59+-0.11 | 0.32 | 0.84 | 0.88 |
| PC ae C30:1 | HMDB0013402 | 0.71+-0.18 | 0.77+-0.12 | 0.36 | 0.84 | 0.92 |
| PC ae C32:1 | HMDB0013404 HMDB0007896 HMDB0007994 | 2.7+-0.7 | 2.7+-0.5 | 0.83 | 0.92 | 0.98 |
| PC ae C32:2 | HMDB0013411 | 1.2+-0.4 | 1.23+-0.22 | 0.97 | 0.98 | 1.00 |
| PC ae C34:0 | HMDB0013405 | 1.9+-0.7 | 2+-0.4 | 0.76 | 0.92 | 0.97 |
| PC ae C34:1 | HMDB0013426 | 9+-3 | 9.9+-1.9 | 0.46 | 0.85 | 0.93 |
| PC ae C34:2 | HMDB0011151 | 11+-3 | 11.4+-2.4 | 0.53 | 0.89 | 0.94 |
| PC ae C34:3 | HMDB0013413 | 8.4+-2 | 8.5+-1.9 | 0.88 | 0.95 | 0.99 |
| PC ae C36:0 | HMDB13406 HMDB0013417 | 1.2+-0.3 | 1.3+-0.3 | 0.36 | 0.84 | 0.93 |
| PC ae C36:1 | HMDB0013427 HMDB0013414 | 7.5+-2 | 8.2+-1.4 | 0.30 | 0.84 | 0.92 |
| PC ae C36:2 | HMDB0013418 HMDB0013428 HMDB0011243 | 13+-3 | 13+-3 | 0.77 | 0.92 | 0.97 |
| PC ae C36:3 | HMDB0013429 HMDB0013425 | 8.3+-2.1 | 8.1+-1.7 | 0.79 | 0.92 | 1.02 |
| PC ae C36:4 | HMDB0013435 HMDB0013407 | 16+-5 | 14+-5 | 0.27 | 0.84 | 1.15 |
| PC ae C36:5 | HMDB0013415 HMDB0011220 | 31+-7 | 28+-4 | 0.18 | 0.84 | 1.11 |
| PC ae C38:0 | HMDB0013408 HMDB0013419 | 1.9+-0.6 | 2+-0.4 | 0.75 | 0.92 | 0.97 |
| PC ae C38:1 | HMDB0013419 HMDB0013408 | 1.4+-0.3 | 1.5+-0.3 | 0.38 | 0.84 | 0.93 |
| PC ae C38:2 | HMDB0013416 HMDB0013430 | 2.3+-0.6 | 2.4+-0.5 | 0.66 | 0.92 | 0.96 |
| PC ae C38:3 | HMDB0013436 HMDB0013431 | 4+-1 | 4+-0.6 | 0.93 | 0.97 | 0.99 |
| PC ae C38:4 | HMDB0013420 | 13+-3 | 12.2+-2.3 | 0.39 | 0.84 | 1.08 |

| | | | | | | |
|--------------------|---|-------------------|-------------------|-------------|-------------|-------------|
| PC ae C38:5 | HMDB11253 HMDB0013432 | 17+-4 | 15+-3 | 0.11 | 0.84 | 1.15 |
| PC ae C38:6 | HMDB0013409 | 6.5+-1.3 | 6+-2 | 0.40 | 0.84 | 1.09 |
| PC ae C40:1 | HMDB0013433 | 1.14+-0.24 | 1.12+-0.23 | 0.89 | 0.95 | 1.01 |
| PC ae C40:2 | HMDB0013437 | 1.4+-0.4 | 1.5+-0.3 | 0.36 | 0.84 | 0.92 |
| PC ae C40:3 | HMDB0013445 HMDB0013446 | 1.02+-0.19 | 1.1+-0.17 | 0.31 | 0.84 | 0.93 |
| PC ae C40:4 | HMDB0013442 | 2.2+-0.4 | 2.1+-0.4 | 0.68 | 0.92 | 1.03 |
| PC ae C40:5 | HMDB0013444 | 3+-0.5 | 3+-0.5 | 0.82 | 0.92 | 1.01 |
| PC ae C40:6 | HMDB0013422 | 3.7+-0.9 | 3.6+-0.8 | 0.93 | 0.97 | 1.01 |
| PC ae C42:1 | HMDB0013434 HMDB0013447 | 0.34+-0.07 | 0.31+-0.06 | 0.20 | 0.84 | 1.10 |
| PC ae C42:2 | HMDB0013438 | 0.55+-0.15 | 0.58+-0.08 | 0.52 | 0.89 | 0.95 |
| PC ae C42:3 | HMDB0013458 HMDB0013459 | 0.71+-0.11 | 0.81+-0.11 | 0.01 | 0.29 | 0.87 |
| PC ae C44:3 | HMDB0013449 HMDB0013452 | 0.16+-0.07 | 0.15+-0.08 | 0.77 | 0.92 | 1.06 |
| PC ae C44:4 | HMDB0013455 HMDB0013453 HMDB0013460 | 0.47+-0.11 | 0.47+-0.08 | 0.99 | 0.99 | 1.00 |
| PC ae C44:5 | HMDB0013456 | 1.7+-0.4 | 1.7+-0.4 | 0.62 | 0.92 | 0.96 |
| PC ae C44:6 | HMDB0013450 HMDB0013457 | 1.02+-0.19 | 1.01+-0.24 | 0.89 | 0.95 | 1.01 |
| Phenylalanine | HMDB00159 | 69+-7 | 68+-7 | 0.72 | 0.92 | 1.01 |
| Proline | HMDB00162 HMDB03411 | 250+-50 | 200+-40 | 0.01 | 0.29 | 1.25 |
| Putrescine | HMDB01414 | 0.16+-0.06 | 0.19+-0.07 | 0.21 | 0.84 | 0.84 |
| Serine | HMDB00187 HMDB03406 | 116+-22 | 123+-21 | 0.39 | 0.84 | 0.94 |
| Serotonin | HMDB00259 | 0.8+-0.3 | 0.9+-0.3 | 0.27 | 0.84 | 0.86 |
| SM (OH) C14:1 | HMDB0013462 | 5.5+-2 | 6.3+-1.5 | 0.24 | 0.84 | 0.87 |
| SM (OH) C16:1 | HMDB0013463 | 4+-1.1 | 4.2+-0.9 | 0.46 | 0.85 | 0.93 |
| SM (OH) C22:1 | HMDB0013466 | 18+-4 | 18+-4 | 0.94 | 0.97 | 0.99 |
| SM (OH) C22:2 | HMDB0013467 | 14+-3 | 15+-2.1 | 0.48 | 0.85 | 0.94 |
| SM (OH) C24:1 | HMDB0013469 | 1.8+-0.5 | 1.8+-0.5 | 0.96 | 0.98 | 1.00 |
| SM C16:0 | HMDB0061712 HMDB0010169 | 147+-22 | 140+-18 | 0.34 | 0.84 | 1.05 |
| SM C16:1 | HMDB0029216 | 21+-4 | 19+-3 | 0.09 | 0.84 | 1.12 |
| SM C18:0 | HMDB01348 | 29+-5 | 27+-6 | 0.59 | 0.92 | 1.04 |
| SM C18:1 | HMDB0012100 HMDB0012101 | 13.6+-2.3 | 13+-3 | 0.41 | 0.84 | 1.07 |
| SM C20:2 | | 0.5+-0.19 | 0.48+-0.15 | 0.70 | 0.92 | 1.05 |
| SM C22:3 | | 2.6+-0.7 | 2.4+-0.8 | 0.48 | 0.85 | 1.09 |
| SM C24:0 | HMDB11697 | 38+-7 | 35+-6 | 0.18 | 0.84 | 1.10 |
| SM C24:1 | HMDB12107 | 70+-9 | 65+-11 | 0.14 | 0.84 | 1.09 |
| SM C26:0 | HMDB0011698 | 0.42+-0.19 | 0.43+-0.16 | 0.80 | 0.92 | 0.96 |
| SM C26:1 | HMDB0013461 | 0.45+-0.19 | 0.44+-0.15 | 0.87 | 0.95 | 1.03 |
| Taurine | HMDB00251 | 61+-12 | 88+-20 | 0.00 | 0.03 | 0.69 |
| Threonine | HMDB04041 HMDB00167 | 125+-24 | 130+-30 | 0.69 | 0.92 | 0.97 |

| | | | | | | |
|---------------|--------------------------|-------------------|-------------------|------|------|------|
| Tryptophane | HMDB00929 HMDB0013609 | 66+-10 | 73+-10 | 0.08 | 0.84 | 0.91 |
| Tyrosine | HMDB00158 | 76+-16 | 70+-11 | 0.30 | 0.84 | 1.08 |
| Valine | HMDB00883 | 260+-50 | 270+-50 | 0.70 | 0.92 | 0.97 |
| BCAA | | 450+-92 | 454+-72 | | | |
| AAA | | 291+-23 | 298+-25 | | | |
| Fischer ratio | | 1.55+-0.28 | 1.52+-0.22 | | | |
| ADMA/Arg | | 0.0043+- 0.001 | 0.0041+- 0.001 | | | |
| Cit/Arg | | 0.25+-0.07 | 0.27+-0.05 | | | |
| Cit/Orn | | 0.82+-0.37 | 0.88+-0.7 | | | |
| Orn/Arg | | 0.33+-0.11 | 0.44+-0.23 | | | |

Table S2. Multivariate regression analysis.

Table S2 a. Multivariate regression analysis, clinical and imaging parameters as outcome variables. Correlation of variables which were different between patients and controls and the outcome variables ‘group assignment to patients vs. controls’, ‘evidence of diastolic dysfunction’, ‘history of aortic root surgery’ and aortic root dimensions. False discovery rate-adjusted $p (=q) \leq 0.05$ was considered statistically significant. Group A, all patients; group AF, patients with preserved systolic ventricular function; group AFV, patients with preserved systolic ventricular function and without major valve regurgitation. β , beta coefficient in multivariate regression; NT-proBNP, N-terminal prohormone of brain natriuretic peptide R^2 , R squared referring to the regression analysis of the group of the variables listed straight above (corresponding line and column), respectively.

| Groups | Independent variables | Outcome variable: patients vs. controls $\beta/R^2 (q)$ |
|------------------|-----------------------|--|
| A Pat. + Ctrl. | NT-proBNP | 0.002 (0.0055) |
| | PCaC42:3 | -0.07 (0.3) |
| | Taurine | -0.009 (0.004) |
| | Histidine | -0.02 (0.004) |
| | Adjusted $R^2 (q)$ | 0.53 (<0.0001) |
| AF Pat. + Ctrl. | NT-proBNP | 0.002 (0.016) |
| | PCaC42:3 | -0.06 (0.35) |
| | Taurine | -0.009 (0.003) |
| | Histidine | -0.02 (0.01) |
| | Adjusted $R^2 (q)$ | 0.51 (<0.0001) |
| AFV Pat. + Ctrl. | NT-proBNP | 0.002 (0.05) |
| | PCaC42:3 | 0.05 (0.59) |
| | Taurine | -0.012 (0.003) |
| | Histidine | -0.007 (0.3) |
| | Adjusted $R^2 (q)$ | 0.52 (0.0004) |
| Groups | Independent variables | Outcome variable: evidence of diastolic dysfunction $\beta/r^2 (q)$ |
| A Pat. | NT-proBNP | 0.0007 (0.59) |
| | PCaC42:3 | -0.08 (0.65) |
| | Taurine | 0.004 (0.77) |
| | Histidine | 0.002 (0.89) |
| | Adjusted $R^2 (q)$ | -0.2 (0.97) |
| AF Pat. | NT-proBNP | 0.0004 (0.76) |
| | PCaC42:3 | -0.03 (0.88) |
| | Taurine | -0.002 (0.89) |
| | Histidine | 0.0004 (0.98) |
| | Adjusted $R^2 (q)$ | -0.24 (0.99) |
| AFV Pat. | NT-proBNP | -0.0018 (0.27) |
| | PCaC42:3 | 0.21 (0.39) |
| | Taurine | 0.018 (0.36) |
| | Histidine | 0.02 (0.33) |
| | Adjusted $R^2 (q)$ | -1.5 (0.67) |
| Groups | Independent variables | Outcome variable: history of aortic root surgery $\beta/r^2 (q)$ |
| A Pat. | NT-proBNP | 0.0002 (0.15) |
| | PCaC42:3 | 0.03 (0.85) |
| | Taurine | -0.005 (0.77) |
| | Histidine | 0.008 (0.89) |
| | Adjusted $R^2 (q)$ | -0.03 (0.52) |
| AF Pat. | NT-proBNP | 0.001 (0.19) |
| | PCaC42:3 | 0.09 (0.57) |
| | Taurine | -0.01 (0.34) |
| | Histidine | 0.01 (0.40) |
| | Adjusted $R^2 (q)$ | -0.005 (0.49) |
| AFV Pat. | NT-proBNP | 0.002 (0.18) |
| | PCaC42:3 | 0.12 (0.52) |
| | Taurine | -0.006 (0.69) |
| | Histidine | 0.008 (0.61) |
| | Adjusted $R^2 (q)$ | -0.02 (0.47) |
| Groups | Independent variables | Outcome variable: aortic root dimension $\beta/r^2 (q)$ |
| A Pat. | NT-proBNP | 0.008 (0.23) |
| | PCaC42:3 | -0.69 (0.34) |
| | Taurine | 0.02 (0.7) |
| | Histidine | -0.07 (0.37) |
| | Adjusted $R^2 (q)$ | -0.08 (0.56) |
| AF Pat. | NT-proBNP | 0.01 (0.16) |
| | PCaC42:3 | -0.2 (0.8) |

| | | |
|---------------|------------------------------|--|
| | Taurine | -0.005 (0.9) |
| | Histidine | - 0.02 (0.87) |
| | Adjusted R ² (q) | -0.08 (0.57) |
| AFV Pat. | NT-proBNP | -0.003 (0.93) |
| | PCaC42:3 | -0.58 (0.7) |
| | Taurine | -0.02 (0.85) |
| | Histidine | -0.0007 (0.99) |
| | Adjusted R ² (q) | -1.15 (0.85) |
| Groups | Independent variables | Outcome variable: ascending aorta dimension β/r² (q) |
| A Pat. | NT-proBNP | 0.01 (0.008) |
| | PCaC42:3 | 0.1 (0.85) |
| | Taurine | -0.004 (0.93) |
| | Histidine | -0.05 (0.36) |
| | Adjusted R ² (q) | -0.42 (0.048) |
| AF Pat. | NT-proBNP | 0.01 (0.003) |
| | PCaC42:3 | -0.72 (0.17) |
| | Taurine | -0.04 (0.29) |
| | Histidine | 0.002 (0.97) |
| | Adjusted R ² (q) | 0.6 (0.01) |
| AFV Pat. | NT-proBNP | 0.008 (0.11) |
| | PCaC42:3 | 0.73 (0.37) |
| | Taurine | -0.04 (0.51) |
| | Histidine | 0.02 (0.78) |
| | Adjusted R ² (q) | 0.45 (0.19) |

Table S2 b. Multivariate regression analysis, biochemical parameters as outcome variables. Correlation of the variables ‘diastolic dysfunction’, ‘history of surgery’, and aortic root dimensions and the outcome variables ‘serum concentration of Histidine’, ‘serum concentration of Taurine’, ‘serum concentration of PCaC42:3’ and ‘serum concentration of NT-proBNP’. False discovery rate-adjusted $p (=q) \leq 0.05$ was considered statistically significant. Group A, all patients; group AF, patients with preserved systolic ventricular function; group AFV, patients with preserved systolic ventricular function and without major valve regurgitation. Asc., ascending; β , beta coefficient in multivariate regression; dim., dimension; hx, history; NT-proBNP, N-terminal prohormone of brain natriuretic peptide R^2 , R squared referring to the regression analysis of the group of the variables listed straight above (corresponding line and column), respectively; z-sc., z-score.

| Group | Independent variables | Outcome variable: Histidine β/R^2 (q) |
|----------|-------------------------|--|
| A Pat. | Diastolic dysfunction | -1.7 (0.76) |
| | Hx of surgery | -2.8 (0.72) |
| | Aortic root dim. z-sc. | -1.4 (0.61) |
| | Asc. aorta dim. z-sc. | -0.3 (0.89) |
| | Adjusted R^2 (q) | 0.13 (0.88) |
| AF Pat. | Diastolic dysfunction | -1.3 (0.83) |
| | Hx of surgery | -4.7 (0.59) |
| | Aortic root dim. z-sc. | -1.4 (0.61) |
| | Asc. aorta dim. z-sc. | 0.1 (0.96) |
| | Adjusted R^2 (q) | -0.48 (0.93) |
| AFV Pat. | Diastolic dysfunction | -0.96 (0.95) |
| | Hx of surgery | -23.7 (0.5) |
| | Aortic root dim. z-sc. | -0.01 (0.99) |
| | Asc. aorta dim. z-sc. | 6.3 (0.62) |
| | Adjusted R^2 (q) | -1.5 (0.88) |
| Groups | Independent variables | Outcome variable: Taurine β/r^2 (q) |
| A Pat. | Diastolic dysfunction | -14.6 (0.004) |
| | Hx of surgery | -34.4 (0.0002) |
| | Aortic root diam. z-sc. | -8.6 (0.0017) |
| | Asc. aorta dim. z-sc. | 5.33 (0.0064) |
| | Adjusted R^2 (q) | 0.83 (0.002) |
| AF Pat. | Diastolic dysfunction | -14.1 (0.005) |
| | Hx of surgery | -36.3 (0.0003) |
| | Aortic root dim. z-sc. | -8.1 (0.002) |
| | Asc. aorta dim. z-sc. | 5.7 (0.005) |
| | Adjusted R^2 (q) | 0.96 (0.002) |
| AFV Pat. | Diastolic dysfunction | -14.7 (0.15) |
| | Hx of surgery | -32.4 (0.13) |
| | Aortic root dim. z-sc. | -7.6 (0.12) |
| | Asc. aorta dim. z-sc. | 5.7 (0.27) |
| | Adjusted R^2 (q) | 0.9 (0.18) |
| Groups | Independent variables | Outcome variable: PCaC42:3 β/r^2 (q) |
| A Pat. | Diastolic dysfunction | -0.8 (0.28) |
| | Hx of surgery | -1.5 (0.17) |
| | Aortic root dim. z-sc. | -0.53 (0.15) |
| | Asc. aorta dim. z-sc. | 0.45 (0.16) |
| | Adjusted R^2 (q) | 0.03 (0.43) |
| AF Pat. | Diastolic dysfunction | -0.7 (0.29) |
| | Hx of surgery | -1.9 (0.08) |
| | Aortic root dim. z-sc. | -0.55 (0.11) |
| | Asc. aorta dim. z-sc. | 0.54 (0.08) |
| | Adjusted R^2 (q) | 0.18 (0.3) |
| AFV Pat. | Diastolic dysfunction | -14.2 (0.24) |
| | Hx of surgery | -1.7 (0.9) |
| | Aortic root dim. z-sc. | -3.4 (0.37) |
| | Asc. aorta dim. z-sc. | 4.7 (0.45) |
| | Adjusted R^2 (q) | 0.77 (0.32) |
| Groups | Independent variables | Outcome variable: NT-proBNP β/r^2 (q) |
| A Pat. | Diastolic dysfunction | 14.6 (0.78) |
| | Hx of surgery | -4.2 (0.95) |
| | Aortic root dim. z-sc. | -3.7 (0.87) |
| | Asc. aorta dim. z-sc. | 35.3 (0.11) |
| | Adjusted R^2 (q) | 0.2 (0.26) |

| | | |
|-----------------|-----------------------------|--------------|
| AF Pat. | Diastolic dysfunction | 26 (0.4) |
| | Hx of surgery | -48 (0.3) |
| | Aortic root dim. z-sc. | -5.6 (0.7) |
| | Asc. aorta dim. z-sc. | 45.1 (0.01) |
| | Adjusted R ² (q) | 0.7 (0.02) |
| AFV Pat. | Diastolic dysfunction | -18.2 (0.38) |
| | Hx of surgery | 6.7 (0.81) |
| | Aortic root dim. z-sc. | -1.2 (0.85) |
| | Asc. aorta dim. z-sc. | 13.7 (0.36) |
| | Adjusted R ² (q) | 0.78 (0.31) |