# Supplemental Data: Increased Power for the Analysis of Label-Free LC-MS/MS Proteomic Data by Combining Spectral Counts and Peptide Peak Attributes

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**SUPPLEMENTAL FIGURES**

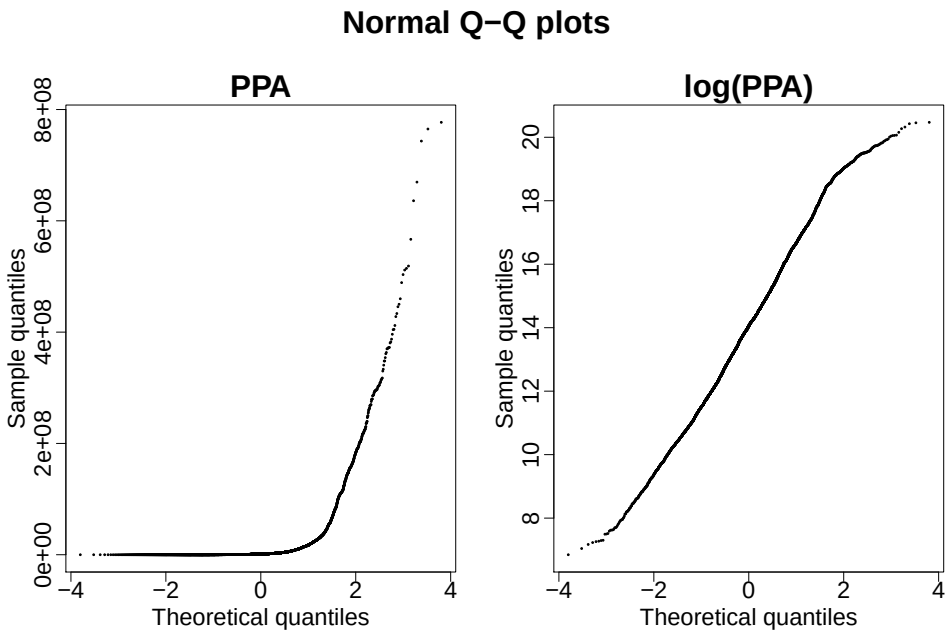



Figure S1: Normal quantile-quantile plots of all msInspect/AMT PPA measurement (left) and log(PPA) measurements (right). Note that log(PPA) measurements appear nearly normally distributed (the points almost form a straight line), when compared with PPA measurements.

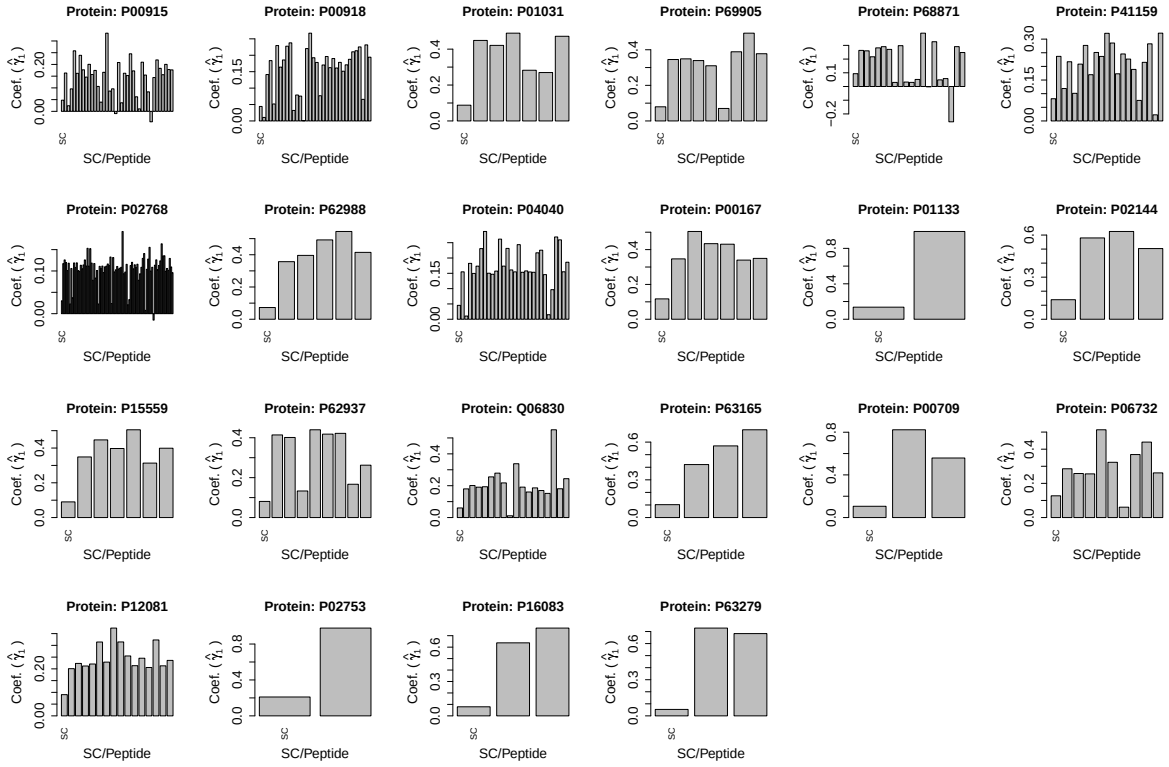



Figure S2: Plots of ProPCA coefficients [$\hat{\gamma}_1 = (\hat{\gamma}_{1jk})$] corresponding to spectral counts and peptides for each protein in the UPS2 standards data. Coefficients for each protein are standardized so that $\sum_{k=1}^{P_j} \hat{\gamma}_{1jk}^2 = 1$. Each plot displays the coefficients for spectral counts and all peptides contributing to the indicated protein's ProPCA estimate. The spectral count coefficient is given on the far-left in each plot (indicated along the horizontal axis); peptides are not labeled, however, more information may be found in Table S4. Table S4 contains a list of ProPCA coefficients for all peptides (along with peptide amino acid sequences) and spectral counts. For each protein, peptides listed from top to bottom in Table S4 correspond to peptides, from left to right, in the above plots.

## SUPPLEMENTAL TABLES

Table S1: UPS2 standard set: Number of LC-MS/MS runs with specified relative protein abundance

| UniProt accession number | UniProt protein name [synonym] | Total amount in UPS2 standard (fmol) | # Distinct peptides * | Sequence Coverage † |
|---|---|---|---|---|
| P00915 | Carbonic anhydrase 1 | 50,000 | 49 | 92% |
| P00918 | Carbonic anhydrase 2 | 50,000 | 38 | 79.2% |
| P01031 | Complement C5 [Complement C5a] | 50,000 | 7 | 28.8% |
| P69905 | Hemoglobin alpha chain | 50,000 | 9 | 90.8% |
| P68871 | Hemoglobin beta chain | 50,000 | 23 | 94.6% |
| P41159 | Leptin | 50,000 | 28 | 77.2% |
| P02768 | Serum albumin | 50,000 | 109 | 84.9% |
| P62988 | Ubiquitin | 50,000 | 9 | 86.8% |
| P04040 | Catalase | 5,000 | 34 | 73.8% |
| P00167 | Cytochrome $b_5$ | 5,000 | 7 | 67.2% |
| P01133 | Epidermal growth factor | 5,000 | 3 | 46.8% |
| P02144 | Myoglobin | 5,000 | 4 | 62.3% |
| P15559 | NAD(P)H dehydrogenase [quinone] 1 [DT Diaphorase] | 5,000 | 6 | 60.6% |
| P62937 | Peptidyl-prolyl cis-trans isomerase A [Cyclophilin A] | 5,000 | 11 | 69.1% |
| Q06830 | Peroxiredoxin 1 | 5,000 | 21 | 84.4% |
| P63165 | Small ubiquitin-related modifier 1 [SUMO-1] | 5,000 | 3 | 18.8% |
| P00709 | Alpha-lactalbumin | 500 | 3 | 45.1% |
| P06732 | Creatine kinase M-type [CK-MM] | 500 | 13 | 69.6% |
| P12081 | Histidyl-tRNA synthetase [Jo-1] | 500 | 19 | 53% |
| P02753 | Retinol-binding protein | 500 | 4 | 32.3% |
| P16083 | Ribosyldihydronicotinamide dehydrogenase (quinone) [Quinone oxidoreductase 2 or NQO2] | 500 | 3 | 38.5% |
| P63279 | Ubiquitin-conjugating enzyme E2 I [UbcH9] | 500 | 4 | 56.3% |

* Number of distinct peptides matched to a protein, across all samples, via tandem MS spectra

† Sequence coverage information obtained from ProteinProphet

Table S2: UPS2 standard set: Number of LC-MS/MS runs with specified relative protein abundance

| Relative protein abundance ($\eta^*$) | Number of LC-MS/MS runs |
|---:|---:|
| 0.0002 | 7 |
| 0.0004 | 3 |
| 0.0006 | 3 |
| 0.001 | 4 |
| 0.0015 | 3 |
| 0.002 | 3 |
| 0.003 | 3 |
| 0.01 | 3 |
| 0.015 | 3 |
| 0.02 | 3 |
| 0.03 | 3 |

* $\eta$ equals the UPS2 protein amount in a given run, as a proportion of the total amount in the UPS2 protein standard set

Table S3: UPS2 standard set: Correlation of log(SC), ProALT, and ProPCA with log-protein abundance for normalized and non-normalized data.

| | | ProALT | | ProPCA | |
|---|---|---|---|---|---|
| UniProt protein name [synonym] | log(SC)* | Normalized data† | Non-normalized data | Normalized data | Non-normalized data |
| Carbonic anhydrase 1 | 0.933 | 0.935 | 0.934 | 0.992 | 0.995 |
| Carbonic anhydrase 2 | 0.944 | 0.969 | 0.975 | 0.994 | 0.994 |
| Complement C5 [Complement C5a] | 0.860 | 0.874 | 0.808 | 0.982 | 0.988 |
| Hemoglobin alpha chain | 0.918 | 0.933 | 0.956 | 0.984 | 0.988 |
| Hemoglobin beta chain | 0.946 | 0.925 | 0.864 | 0.991 | 0.992 |
| Leptin | 0.960 | 0.911 | 0.950 | 0.996 | 0.992 |
| Serum albumin | 0.968 | 0.981 | 0.975 | 0.991 | 0.992 |
| Ubiquitin | 0.824 | 0.976 | 0.896 | 0.985 | 0.988 |
| Catalase | 0.854 | 0.951 | 0.966 | 0.995 | 0.995 |
| Cytochrome $b_5$ | 0.835 | 0.955 | 0.952 | 0.986 | 0.992 |
| Epidermal growth factor | 0.678 | 0.897 | 0.729 | 0.919 | 0.952 |
| Myoglobin | 0.843 | 0.959 | 0.916 | 0.985 | 0.999 |
| NAD(P)H dehydrogenase [quinone] 1 [DT Diaphorase] | 0.739 | 0.859 | 0.731 | 0.954 | 0.982 |
| Peptidyl-prolyl cis-trans isomerase A [Cyclophilin A] | 0.842 | 0.927 | 0.909 | 0.985 | 0.993 |
| Peroxiredoxin 1 | 0.830 | 0.959 | 0.919 | 0.993 | 0.996 |
| Small ubiquitin-related modifier 1 [SUMO-1] | 0.749 | 0.878 | 0.704 | 0.923 | 0.975 |
| Alpha-lactalbumin | 0.662 | 0.738 | 0.797 | 0.858 | 0.985 |
| Creatine kinase M-type [CK-MM] | 0.915 | 0.788 | 0.906 | 0.995 | 0.997 |
| Histidyl-tRNA synthetase [Jo-1] | 0.795 | 0.902 | 0.952 | 0.988 | 0.993 |
| Retinol-binding protein | 0.693 | 0.339 | 0.556 | 0.710 | 0.766 |
| Ribosyldihydronicotinamide dehydrogenase (quinone) [Quinone oxidoreductase 2 or NQO2] | 0.634 | 0.695 | 0.735 | 0.796 | 0.867 |
| Ubiquitin-conjugating enzyme E2 I [UbcH9] | 0.424 | 0.585 | 0.849 | 0.821 | 0.950 |
| **Mean correlation**♯ | **0.811** | **0.861** | **0.863** | **0.947** | **0.971** |

* For log(SC), the normalized and non-normalized data have the same correlation with log-protein abundance because the normalized log(SC) is a linear transformation of the non-normalized log(SC).

† In the normalized data, log(SC) and log(PPA) for each peptide are standardized to have equal means and standard deviations.

♯ Mean correlation across all identified proteins in the UPS2 standards data.

Table S4: Table S4: UPS2 standard set: ProPCA spectral count and peptide coefficient, $\hat{\gamma}_1 = (\hat{\gamma}_{1jk})$ (also see Figure S2).

| UniProt accession number | UniProt protein name [synonym] | SC/Peptide (identified with PPA measurement) * | ProPCA coefficient ($\hat{\gamma}_1$) † |
|---|---|---|---|
| P00915 | Carbonic anhydrase 1 | Spectral count | 0.048 |
| | | ADGLAVIGVLMK | 0.163 |
| | | ADGLAVIGVLMKVGEANPK | 0.024 |
| | | EIINVGHSF | 0.096 |
| | | EIINVGHSFHVNFEDNDNR | 0.258 |
| | | ESISVSSEQLAQ | 0.162 |
| | | ESISVSSEQLAQFR | 0.239 |
| | | FHWGSTNEHGSEHTVDGVK | 0.177 |
| | | GGPFSDSYR | 0.146 |
| | | GLAVIGVLMK | 0.2 |
| | | GSLTHPPLYESVTWIICK | 0.157 |
| | | HDTSLKPISVSYNPATAK | 0.175 |
| | | HVNFEDNDNR | 0.106 |
| | | LFQFHF | 0.039 |
| | | LFQFHFH | 0.166 |
| | | LFQFHFHWGSTN | 0.333 |
| | | LFQFHFHWGSTNEH | 0.087 |
| | | LFQFHFHWGSTNEHGS | 0.096 |
| | | LFQFHFHWGSTNEHGSEHTVDGVK | -0.01 |
| | | LYPIANGNNQSPVDIK | 0.208 |
| | | NGPEQWSK | 0.036 |
| | | PISVSYNPATAK | 0.162 |
| | | RAPFTNFDPSTLLPS | 0.153 |
| | | SAELHVAHWNSAK | 0.245 |
| | | SFHVNFEDNDNR | 0.172 |
| | | SISVSSEQLAQFR | 0.062 |
| | | SLLSNVEGDNAVPMQHN | 0.01 |
| | | SLLSNVEGDNAVPMQHNNRPTQPLK | 0.21 |
| | | SSLAEAASK | 0.155 |
| | | THPPLYESVTWIICK | 0.083 |
| | | VLDALQAIK | -0.045 |
| | | VLDALQAIKTKG | 0.144 |
| | | VNFEDNDNR | 0.219 |
| | | WGSTNEHGSEHTVDGVK | 0.183 |
| | | YSAELHVAHWN | 0.156 |
| | | YSAELHVAHWNS | 0.2 |
| | | YSAELHVAHWNSAK | 0.178 |
| | | YSSLAEAASK | 0.177 |
| P00918 | Carbonic anhydrase 2 | Spectral count | 0.044 |
| | | AFNVEFDDSQDK | 0.011 |
| | | AVQQPDGLAVLGIFLK | 0.141 |
| | | DFPIAK | 0.184 |
| | | EPISVSSEQVLK | 0.052 |
| | | FHWGSLDGQGSEHTVDK | 0.23 |
| | | GGPLDGTYR | 0.164 |
| | | GKSADFTNFDPR | 0.186 |
| | | GLAVLGIFLK | 0.228 |
| | | HWGSLDGQGSEHTVDK | 0.238 |
| | | LECVTWIVLK | 0.032 |
| | | LIQFHFHWGSLDGQ | 0.079 |
| | | LIQFHFHWGSLDGQGSEHTVDK | 0.076 |
| | | LIQFHFHWGSLDGQGSEHTVDKK | 0.001 |
| | | LKPLSVSYDQATSLR | 0.22 |
| | | NVEFDDSQDK | 0.267 |
| | | PLDGTYR | 0.192 |
| | | PLSVSYDQATSLR | 0.178 |
| | | PSLKPLSVSYDQATSLR | 0.077 |

| UniProt accession number | UniProt protein name [synonym] | SC/Peptide (identified with PPA measurement) | ProPCA coefficient ($\hat{\gamma}_1$) |
|---|---|---|---|
| P00918 | Carbonic anhydrase 2 (continued) | QSPVDIDTH | 0.17 |
| | | QSPVDIDTHTAK | 0.196 |
| | | SADFTNFDPR | 0.162 |
| | | SPVDIDTHTAK | 0.19 |
| | | SVSYDQATSLR | 0.161 |
| | | VTWIVLK | 0.178 |
| | | VVDVLDSIK | 0.151 |
| | | VVDVLDSIKTK | 0.171 |
| | | WGSLDGQGSEHTVDK | 0.188 |
| | | YAAELHLVH | 0.211 |
| | | YAAELHLVHWN | 0.214 |
| | | YAAELHLVHWNTK | 0.225 |
| | | YDPSLKPLSVSYDQAT | 0.066 |
| | | YDPSLKPLSVSYDQATSLR | 0.232 |
| | | YGDFGK | 0.194 |
| P01031 | Complement C5 [Complement C5a] | Spectral count | 0.088 |
| | | AFTECCVVASQLR | 0.449 |
| | | CVVASQLR | 0.421 |
| | | DMQLGR | 0.489 |
| | | IEEIAAK | 0.282 |
| | | KIEEIAAK | 0.27 |
| | | TECCVVASQLR | 0.472 |
| P69905 | Hemoglobin alpha chain | Spectral count | 0.079 |
| | | AAHLPAEFTPAVHASLDK | 0.345 |
| | | AGEYGAEALER | 0.349 |
| | | FLASVSTVLTSK | 0.339 |
| | | LRVDPVNFK | 0.31 |
| | | MFLSFPTTK | 0.07 |
| | | TYFPHFDLSHGSAQVK | 0.389 |
| | | VADALTNAVAHVDDMPNALSALSDLHAHK | 0.493 |
| | | VGAHAGEYGAEALER | 0.378 |
| P68871 | Hemoglobin beta chain | Spectral count | 0.094 |
| | | EFTPPVQAAY | 0.263 |
| | | EFTPPVQAAYQK | 0.26 |
| | | FFESFGDLSTPDAVMGNPK | 0.217 |
| | | GAFSDGLAHLDNLK | 0.282 |
| | | GTFATLSELH | 0.291 |
| | | GTFATLSELHCDK | 0.271 |
| | | KVLGAFSDGLAHLDNLK | 0.03 |
| | | LHVDPENFR | 0.298 |
| | | LLGNVLVCVLAH | 0.032 |
| | | LLGNVLVCVLAHH | 0.03 |
| | | LLVVYPWTQ | 0.051 |
| | | LLVVYPWTQR | 0.389 |
| | | SAVTALWGK | -0.002 |
| | | SDGLAHLDNLK | 0.327 |
| | | VHLTPEEK | 0.048 |
| | | VLGAFSDGLAHLDNL | 0.058 |
| | | VLGAFSDGLAHLDNLK | -0.258 |
| | | VLVCVLAHHFGK | 0.291 |
| | | VVAGVANALAHK | 0.248 |
| P41159 | Leptin | Spectral count | 0.081 |
| | | DISHTQSVSSK | 0.237 |
| | | DLLHVLAF | 0.119 |
| | | DLLHVLAFSK | 0.217 |
| | | GLDFIPGLHPILTLSK | 0.101 |
| | | GYSTEVVALSR | 0.208 |
| | | INDISHTQSVS | 0.277 |
| | | INDISHTQSVSSK | 0.17 |
| | | MDQTLAVYQQILTSMPSR | 0.251 |
| | | NDISHTQSVSSK | 0.237 |
| | | NVIQISNDLENL | 0.321 |
| | | NVIQISNDLENLR | 0.286 |
| | | SCHLPWASGL | 0.173 |
| | | SCHLPWASGLETL | 0.246 |
| | | SGYSTEVVALSR | 0.227 |
| | | STEVVALSR | 0.189 |

| UniProt accession number | UniProt protein name [synonym] | SC/Peptide (identified with PPA measurement) | ProPCA coefficient ($\hat{\gamma}_1$) |
|---|---|---|---|
| P41159 | Leptin (continued) | TGLDFIPGLHPILTLSK | 0.075 |
| | | VIQISNDLENLR | 0.215 |
| | | VQDDTKTLIK | 0.283 |
| | | VTGLDFIPGLHPI | 0.022 |
| | | VTGLDFIPGLHPILTLSK | 0.322 |
| P02768 | Serum albumin | Spectral count | 0.03 |
| | | AACLLPK | 0.117 |
| | | AAFTECCQAADK | 0.126 |
| | | ADDKETCFAEEGK | 0.12 |
| | | ADICTLSEK | 0.101 |
| | | AEFAEVSK | 0.118 |
| | | AEFAEVSKLVTDLTK | 0.023 |
| | | AFHDNEETFLK | 0.106 |
| | | ALVLIAFAQY | 0.037 |
| | | APELLFFAK | 0.119 |
| | | AQYLQQCPFEDHVK | 0.108 |
| | | AWAVAR | 0.119 |
| | | CCAAADPHECYAK | 0.101 |
| | | CCTESLVNR | 0.099 |
| | | CELFEQLGEYK | 0.113 |
| | | CTAFHDNEETFLK | 0.105 |
| | | DDFAAFVEK | 0.114 |
| | | DDNPNLPR | 0.126 |
| | | DLGEENFK | 0.112 |
| | | DLPSLAADFVESK | 0.153 |
| | | DNEETFLK | 0.112 |
| | | DYSVVLLLR | 0.152 |
| | | ECCEKPLLEK | 0.119 |
| | | EFAEVSK | 0.078 |
| | | EFNAETFTFH | 0.117 |
| | | EFNAETFTFHADICTLSEK | 0.084 |
| | | ETCFAEEGK | 0.101 |
| | | ETCFAEEGKK | 0.023 |
| | | ETYGEMADCCAK | 0.111 |
| | | FAEVSK | 0.106 |
| | | FLYEYAR | 0.111 |
| | | FQNALLVR | 0.096 |
| | | FSALEVDETYVPK | 0.11 |
| | | FYAPELLFFAK | 0.111 |
| | | HADICTLSEK | 0.116 |
| | | HDNEETFLK | 0.113 |
| | | HPDYSVVLLLR | 0.133 |
| | | HPDYSVVLLLRLAK | 0.024 |
| | | IAFAQYLQQCPFEDHVK | 0.131 |
| | | KLVAASQAALGL | 0.098 |
| | | KQTALVELVK | 0.103 |
| | | KVPQVSTPTLVEVSR | 0.111 |
| | | KYLYEIAR | 0.105 |
| | | LAADFVESK | 0.107 |
| | | LCTVATLR | 0.109 |
| | | LPSLAADFVESK | 0.192 |
| | | LVAASQAALGL | 0.094 |
| | | LVNEVTEFAK | 0.098 |
| | | LVRPEVDVMCTAF | 0.116 |
| | | LVRPEVDVMCTAFHDNEETFLK | 0.021 |
| | | LVRPEVDVMCTAFHDNEETFLKK | 0.033 |
| | | LVTDLTK | 0.113 |
| | | NECFLQHK | 0.12 |
| | | NQLCVLHEK | 0.105 |
| | | PADLPSLAADFVESK | 0.115 |
| | | PLVEEPQNLIK | 0.108 |
| | | QEPERNECFLQHK | 0.116 |
| | | QNCELFEQLGEYK | 0.078 |
| | | QTALVELVK | 0.093 |
| | | RHPDYSVVLLLR | 0.109 |
| | | RHPDYSVVLLLRLAK | 0.13 |
| | | RHPYFYAPELL | 0.141 |

| UniProt accession number | UniProt protein name [synonym] | SC/Peptide (identified with PPA measurement) | ProPCA coefficient ($\hat{\gamma}_1$) |
|---|---|---|---|
| P02768 | Serum albumin (continued) | RHPYFYAPELLF | 0.008 |
| | | RPCFSAL | 0.104 |
| | | RPCFSALEVDE | 0.128 |
| | | RPCFSALEVDETYVPK | 0.155 |
| | | SALEVDETYVPK | 0.1 |
| | | SLHTLFGDK | 0.109 |
| | | TCVADESAENCDK | -0.015 |
| | | TFHADICTLSEK | 0.114 |
| | | TYETTLEK | 0.126 |
| | | VFDEFK | 0.103 |
| | | VFDEFKPLVEEPQ | 0.113 |
| | | VFDEFKPLVEEPQN | 0.124 |
| | | VFDEFKPLVEEPQNLIK | 0.164 |
| | | VHTECCHGDLLECADDR | 0.135 |
| | | VHTECCHGDLLECADDRADLAK | 0.136 |
| | | VPQVSTPTLVEVSR | 0.1 |
| | | VTDLTK | 0.106 |
| | | YAPELLFFAK | 0.101 |
| | | YICENQDSISSK | 0.129 |
| | | YLQQCPFEDHVK | 0.109 |
| | | YLYEIAR | 0.096 |
| P62988 | Ubiquitin | Spectral count | 0.073 |
| | | ESTLHLVLR | 0.357 |
| | | LIFAGK | 0.396 |
| | | QLEDGRTLSDYNIQK | 0.492 |
| | | TITLEVEPSDTIENVK | 0.544 |
| | | TLSDYNIQK | 0.415 |
| P04040 | Catalase | Spectral count | 0.045 |
| | | ADVLTTGAGNPVGDK | 0.155 |
| | | AETFPFNPFDLTK | 0.01 |
| | | AFYVNVLNEEQR | 0.182 |
| | | DAQIFIQK | 0.15 |
| | | DLFNAIATGK | 0.173 |
| | | DPASDQMQHWK | 0.231 |
| | | DPILFPSFIHSQK | 0.287 |
| | | FNTANDDNVTQVR | 0.15 |
| | | FSTVAGESGSADTVR | 0.147 |
| | | FSTVAGESGSADTVRDPR | 0.157 |
| | | GAGAFGYFEVTHDITK | 0.262 |
| | | GYFEVTHDITK | 0.174 |
| | | IRDPILFPSFIHSQK | 0.231 |
| | | LCENIAGHLK | 0.161 |
| | | LFAYPDTHR | 0.155 |
| | | LGPNYLHIPVNCPYR | 0.244 |
| | | LNVITVGPR | 0.153 |
| | | LSQEDPDYGIR | 0.158 |
| | | LVNANGEAVYCK | 0.154 |
| | | NAIHTFVQS | 0.153 |
| | | NAIHTFVQSGSHLAAR | 0.217 |
| | | NFTEVHPDYGSHIQALLDK | 0.225 |
| | | NLSVEDAAR | 0.146 |
| | | QAETFPFNPFDLTK | 0.015 |
| | | RLCENIAGHLK | 0.097 |
| | | SFGAPEQQPSALEHSIQYSGEVR | 0.269 |
| | | SLRPESLHQVSFLFSDR | 0.259 |
| | | VFEHIGK | 0.155 |
| | | YLHIPVNCPYR | 0.186 |
| P00167 | Cytochrome $b_5$ | Spectral count | 0.117 |
| | | FLEEHPG | 0.347 |
| | | ISAVAVALMYR | 0.504 |
| | | STWLILHHK | 0.434 |
| | | TFIIGELHPDDRPK | 0.431 |
| | | VYDLTK | 0.34 |
| | | YYTLEEIQK | 0.35 |
| P01133 | Epidermal growth factor | Spectral count | 0.136 |
| | | YACNCVVGY | 0.991 |
| P02144 | Myoglobin | Spectral count | 0.139 |

| UniProt accession number | UniProt protein name [synonym] | SC/Peptide (identified with PPA measurement) | ProPCA coefficient ($\hat{\gamma}_1$) |
|---|---|---|---|
| P02144 | Myoglobin (continued) | HGATVLTALGGILK | 0.579 |
| | | HPGDFGADAQGAMNK | 0.625 |
| | | VEADIPGHGQEVLIR | 0.504 |
| P15559 | NAD(P)H dehydrogenase [quinone] 1 | Spectral count | 0.09 |
| | [DT Diaphorase] | ALIVLAHSER | 0.349 |
| | | ALIVLAHSERT | 0.447 |
| | | FGLSVGHHLGK | 0.397 |
| | | HLSPDIVAEQK | 0.505 |
| | | IQILEGWK | 0.313 |
| | | KLEAADLVIF | 0.399 |
| P62937 | Peptidyl-prolyl cis-trans isomerase A [Cyclophilin A] | Spectral count | 0.081 |
| | | FDIAVDGEPLGR | 0.414 |
| | | FEDENFILK | 0.401 |
| | | IIPGFMCQGGDFTR | 0.133 |
| | | ITIADCGQLE | 0.44 |
| | | KITIADCGQLE | 0.418 |
| | | TEWLDGK | 0.422 |
| | | VFFDIAVDGEPLGR | 0.167 |
| | | VSFELFADK | 0.262 |
| Q06830 | Peroxiredoxin 1 | Spectral count | 0.06 |
| | | ADEGISFR | 0.18 |
| | | ATAVMPDGQFK | 0.201 |
| | | DISLSDYK | 0.191 |
| | | GLFIIDDK | 0.193 |
| | | HGEVCPAGWK | 0.255 |
| | | HGEVCPAGWKPGSDTIKPDVQK | 0.279 |
| | | IGHPAPNFK | 0.218 |
| | | KLNCQVIGASVDSHFCHLAWVNTPK | 0.011 |
| | | LNCQVIGASVDSHFCHLAWVNTPK | 0.338 |
| | | LVQAFQFTDK | 0.191 |
| | | PGSDTIKPDVQK | 0.16 |
| | | QITVNDLPVGR | 0.186 |
| | | RTIAQDYGVLK | 0.17 |
| | | SVDETLR | 0.152 |
| | | TFVCPTEIIAFSDR | 0.551 |
| | | TIAQDYGVLK | 0.181 |
| | | VCPTEIIAFSDR | 0.244 |
| P63165 | Small ubiquitin-related modifier 1 [SUMO-1] | Spectral count | 0.103 |
| | | FLFEGQR | 0.421 |
| | | SSEIHFK | 0.57 |
| | | VIGQDSSEIHFK | 0.698 |
| P00709 | Alpha-lactalbumin | Spectral count | 0.106 |
| | | FLDDDITDDIMCAK | 0.823 |
| | | NICDISCDK | 0.558 |
| P06732 | Creatine kinase M-type [CK-MM] | Spectral count | 0.127 |
| | | ELFDPIISDR | 0.285 |
| | | FCVGLQK | 0.258 |
| | | IEEIFK | 0.255 |
| | | LGSSEVEQVQLVVDGVK | 0.513 |
| | | LNYKPEEEYPDLSK | 0.323 |
| | | LSVEALNSLTGEFK | 0.061 |
| | | RGTGGVDTAAVGSVFDVSNADR | 0.369 |
| | | SFLVWVNEEDHLR | 0.441 |
| | | VLTLELYK | 0.261 |
| P12081 | Histidyl-tRNA synthetase [Jo-1] | Spectral count | 0.09 |
| | | AALEELVK | 0.201 |
| | | AELLYK | 0.223 |
| | | ASAELIEEEVAK | 0.212 |
| | | DQGGELLSLR | 0.221 |
| | | HGAEVIDTPVFELK | 0.314 |
| | | IFSIVEQR | 0.229 |
| | | IGDYVQQHGGVSLVEQLLQDPK | 0.374 |
| | | ISFDLSLAR | 0.315 |
| | | LVSELWDAGIK | 0.255 |
| | | QALEGLGDLK | 0.214 |
| | | REDLVEEIK | 0.245 |
| | | VFDVIIR | 0.206 |

| UniProt accession number | UniProt protein name [synonym] | SC/Peptide (identified with PPA measurement) | ProPCA coefficient ($\hat{\gamma}_1$) |
|---|---|---|---|
| P12081 | Histidyl-tRNA synthetase [Jo-1] (continued) | VPCVGLSIGVER | 0.323 |
| | | VSWEEVK | 0.213 |
| | | YDLTVPFAR | 0.236 |
| P02753 | Retinol-binding protein | Spectral count | 0.21 |
| | | DPNGLPPEAQK | 0.978 |
| P16083 | Ribosyldihydronicotinamide dehydrogenase (quinone) [Quinone oxidoreductase 2 or NQO2] | Spectral count | 0.079 |
| | | NVAVDELSR | 0.638 |
| | | VLAPQISFAPEIASEEER | 0.766 |
| P63279 | Ubiquitin-conjugating enzyme E2 I [UbcH9] | Spectral count | 0.053 |
| | | DDYPSSPPK | 0.729 |
| | | DWRPAITIK | 0.683 |

* Not all peptides identified by tandem MS spectra have corresponding high-quality PPA measurements which may be used to compute ProPCA estimates. Those peptides with no high-quality PPA measurements are omitted from this table – the corresponding ProPCA coefficient for such a peptide is $\hat{\gamma}_{1jk} = 0$.

† The ProPCA coefficients $\hat{\gamma}_1 = (\hat{\gamma}_{1jk})$ are standardized for each protein so that $\sum_{k=1}^{P_j} \hat{\gamma}_{1jk}^2 = 1$.

## PEPTIDE AND PROTEIN PLOTS

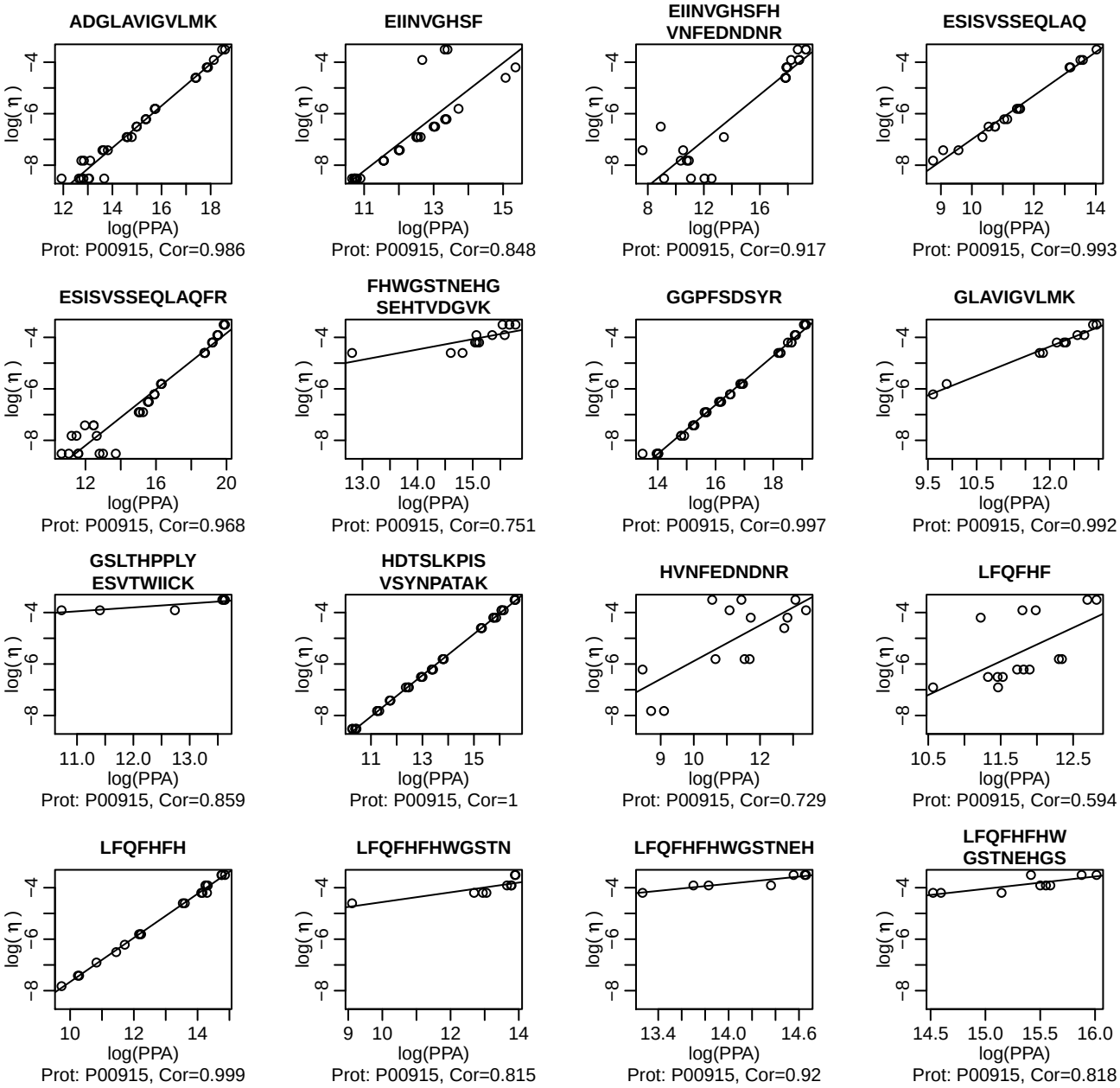
The following pages contain plots of

(i) log-protein abundance versus log(PPA) for all peptides identified in the UPS2 standards (corresponding protein and correlation are listed for each peptide) and

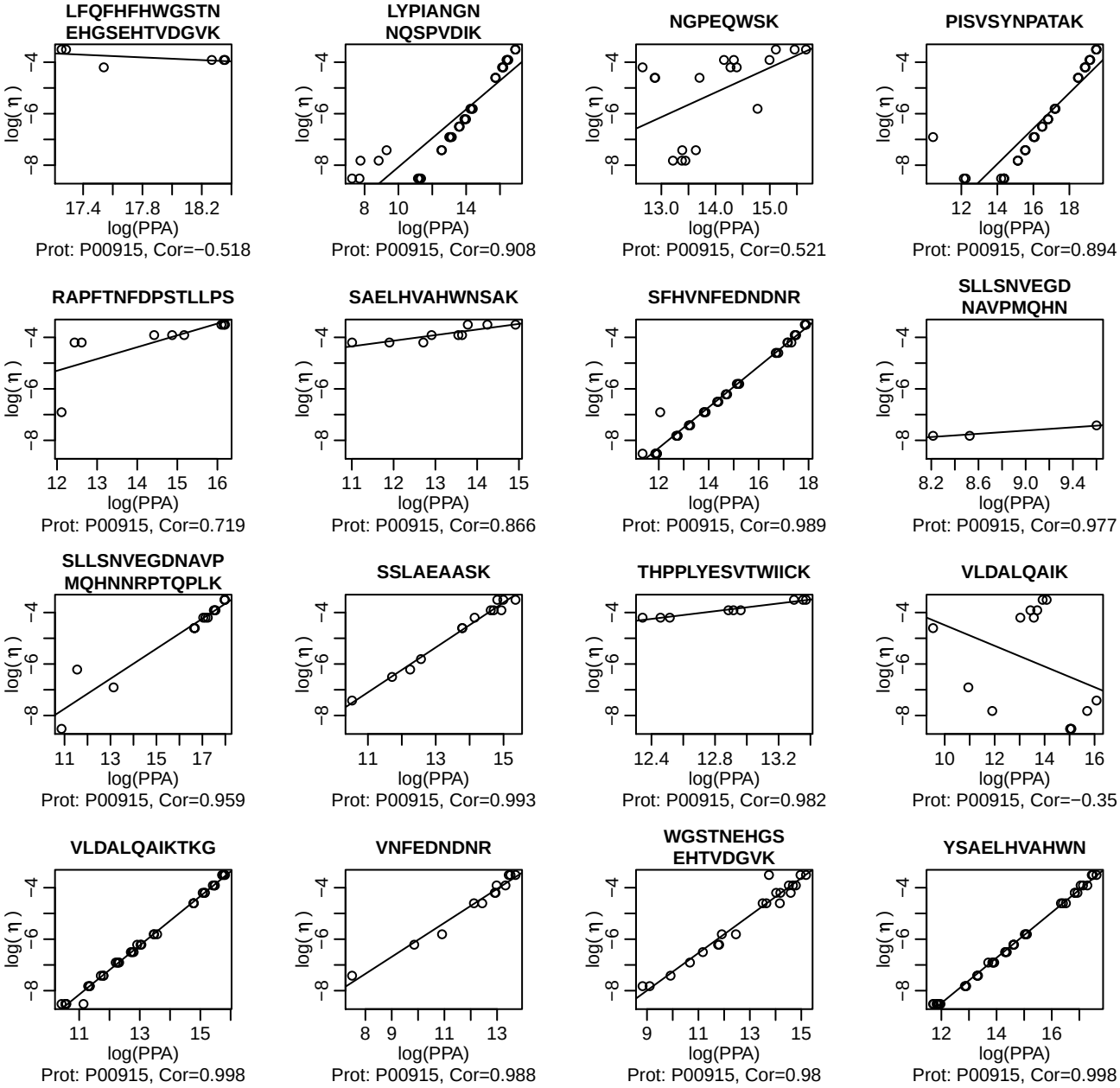
(ii) log-protein abundance versus ProPCA, log(SC), and ProALT for all proteins identified in the UPS2 standards (correlation is listed for each protein).

These plots are based on PPA measurements obtained using msInspect/AMT.

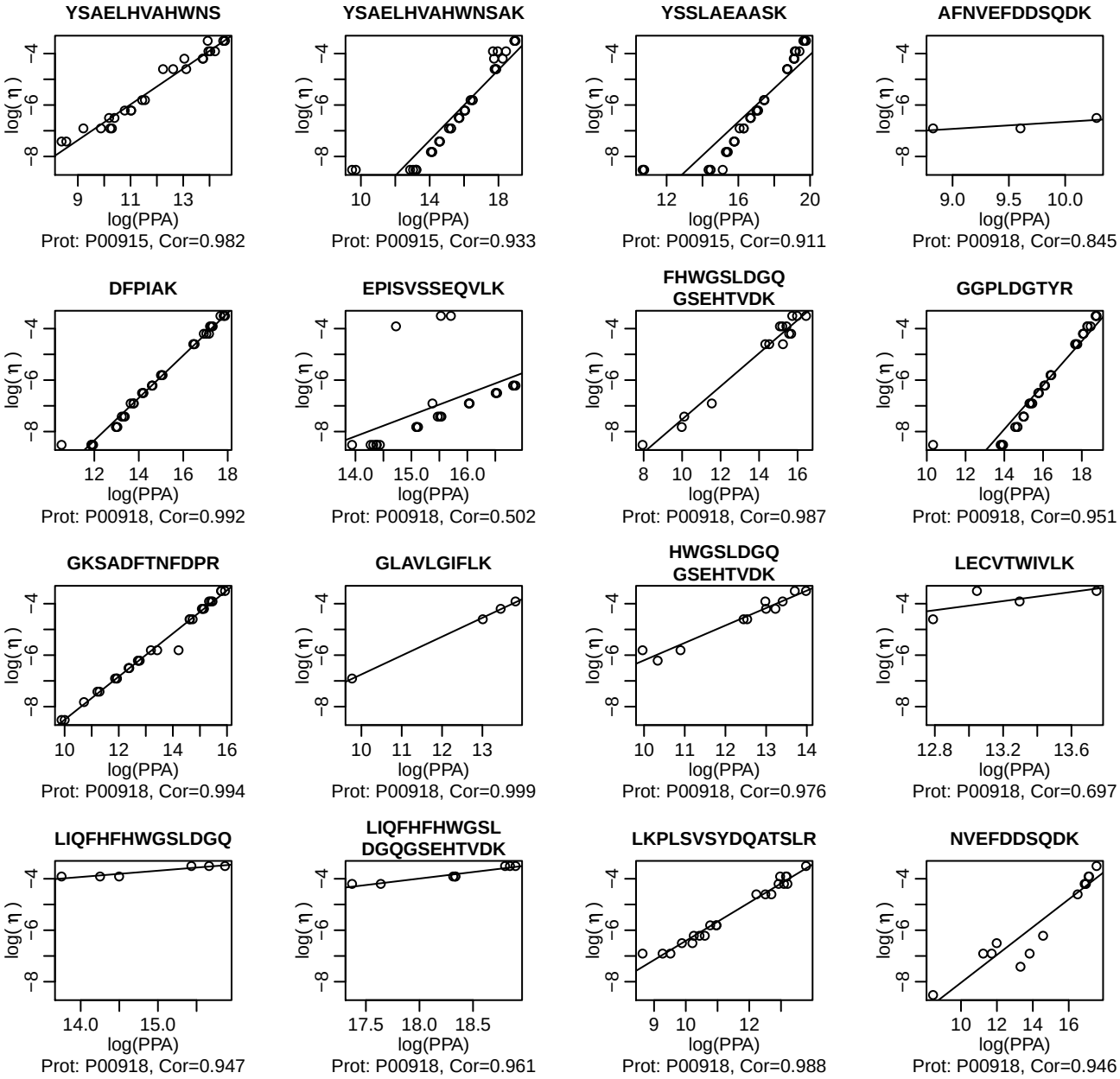
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



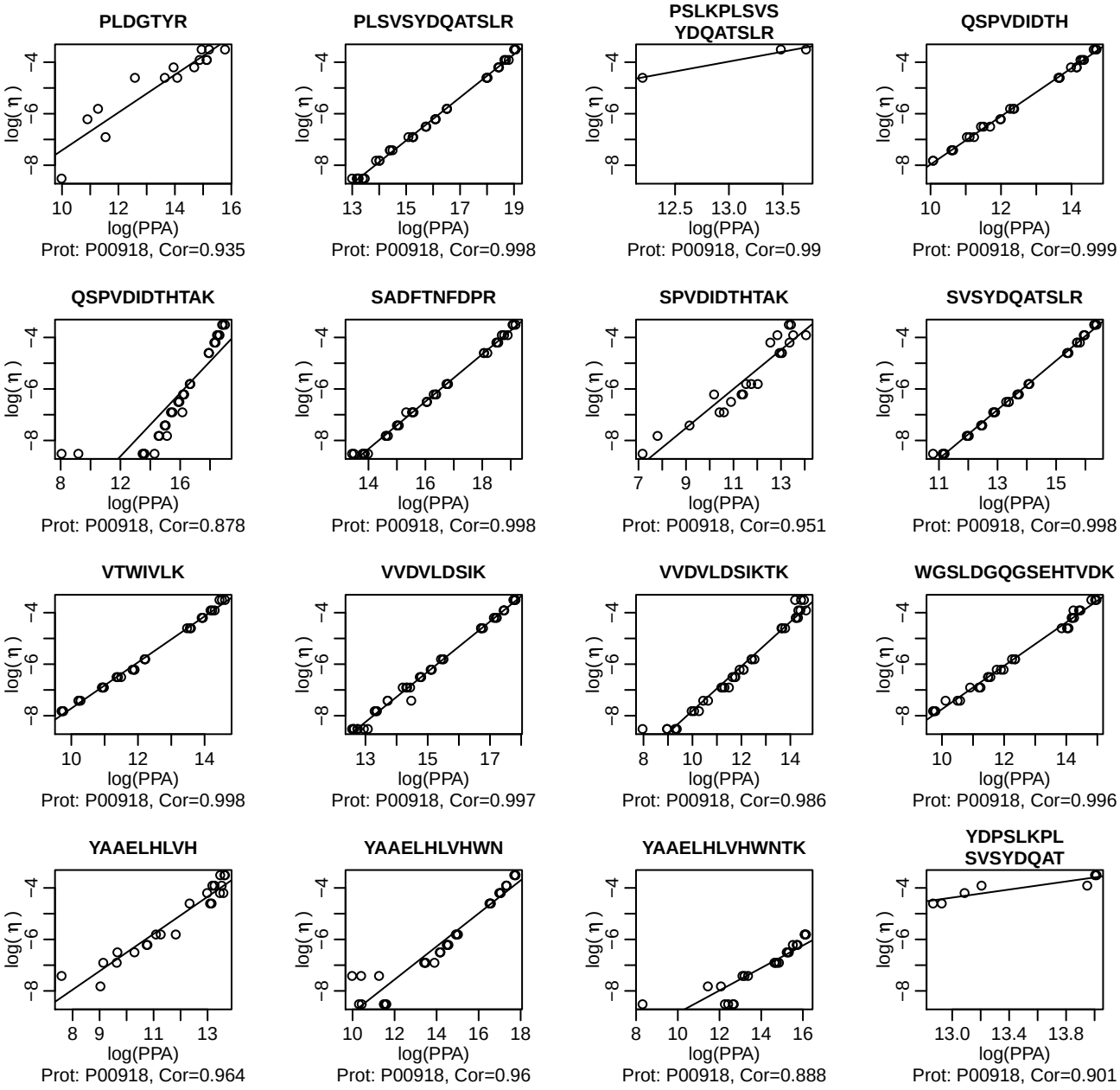
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



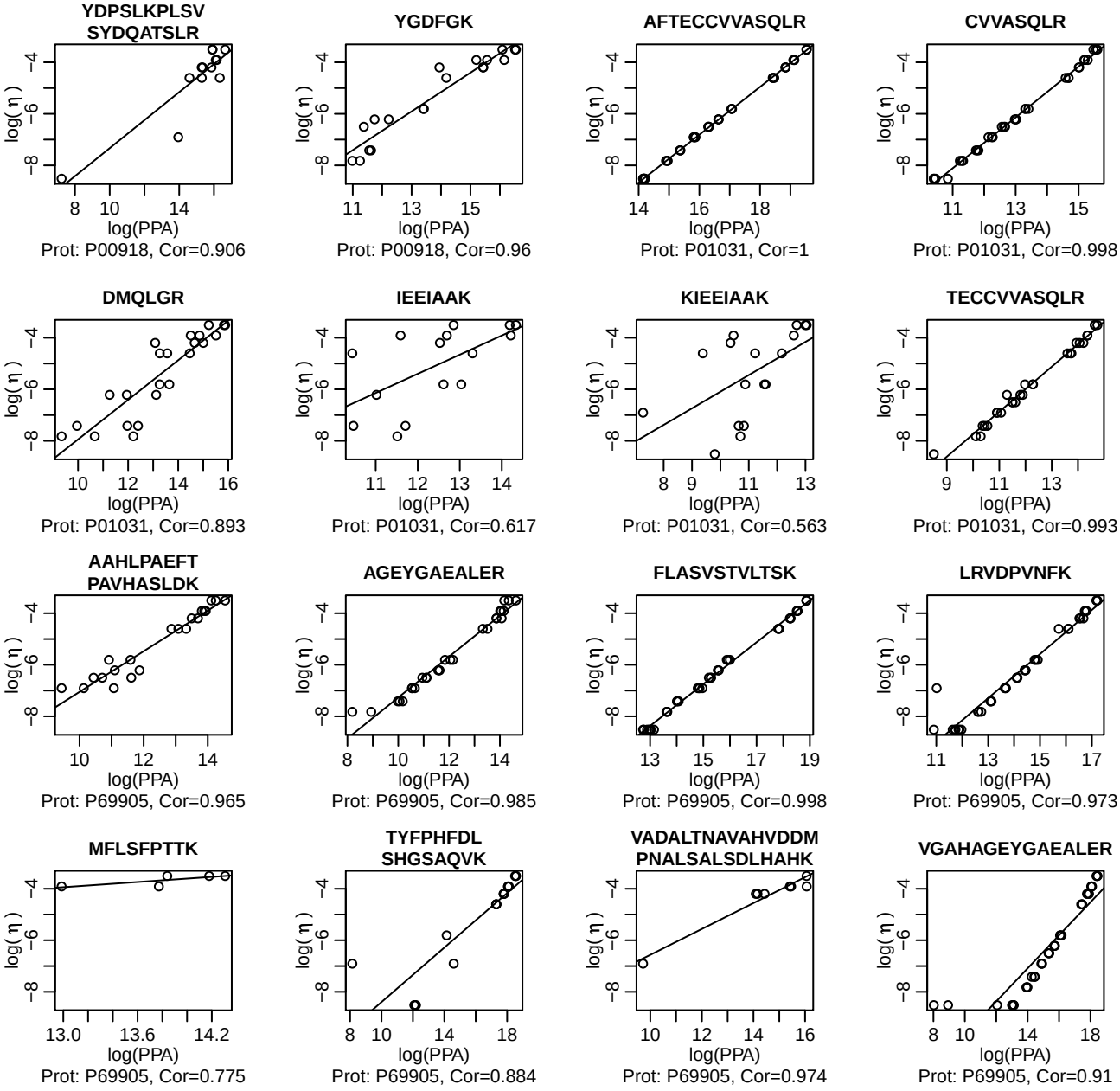
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



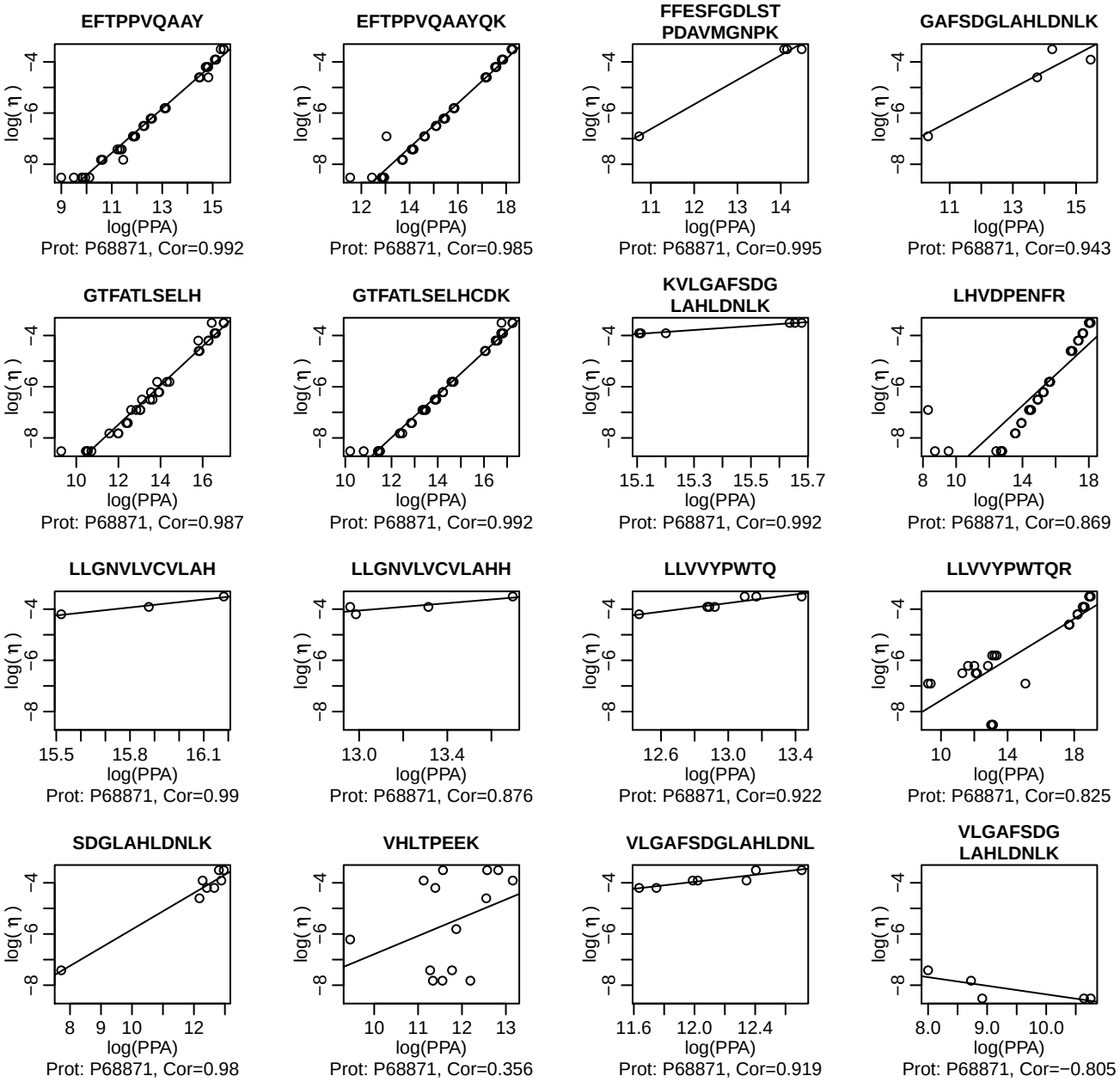
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



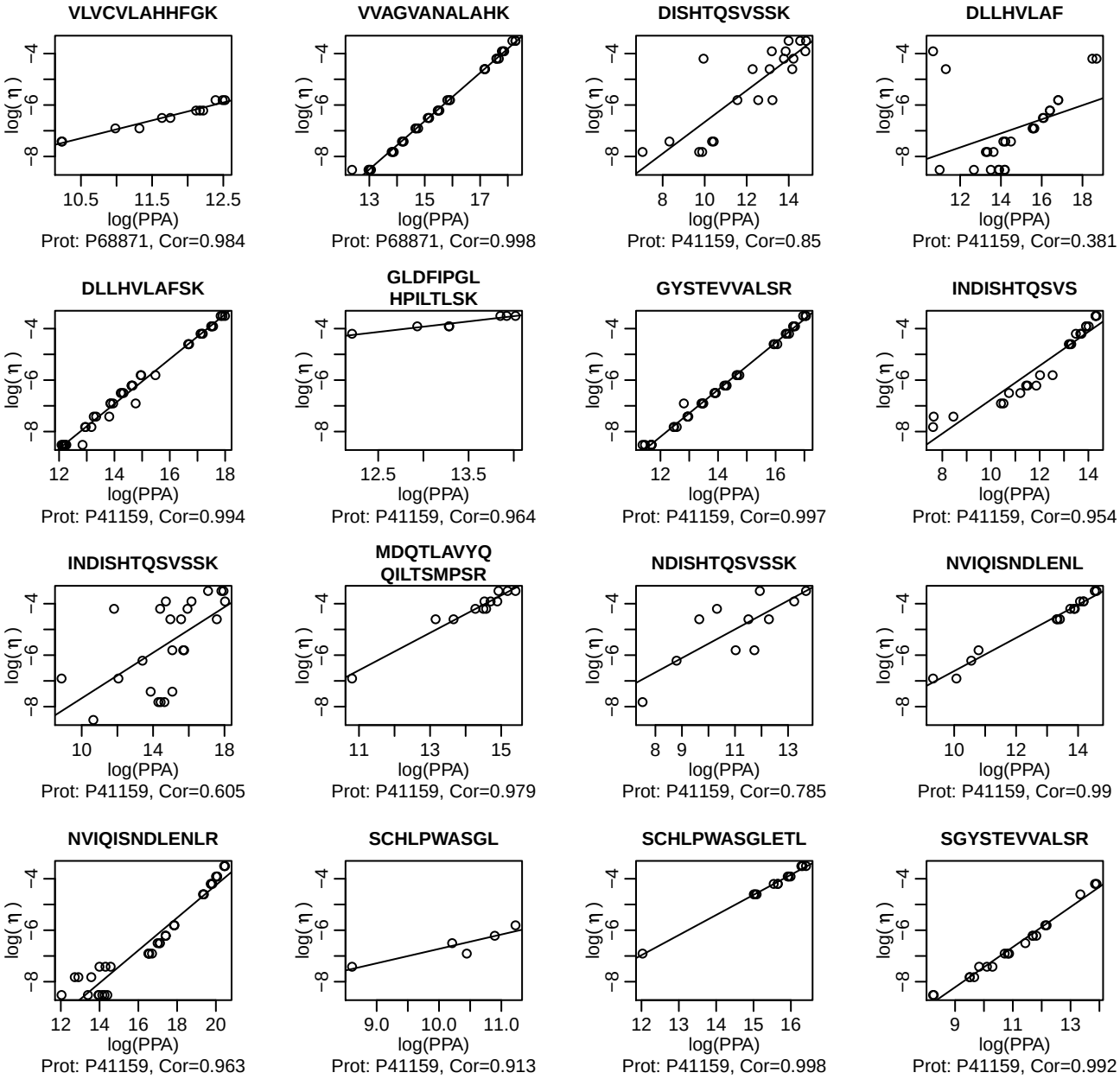
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



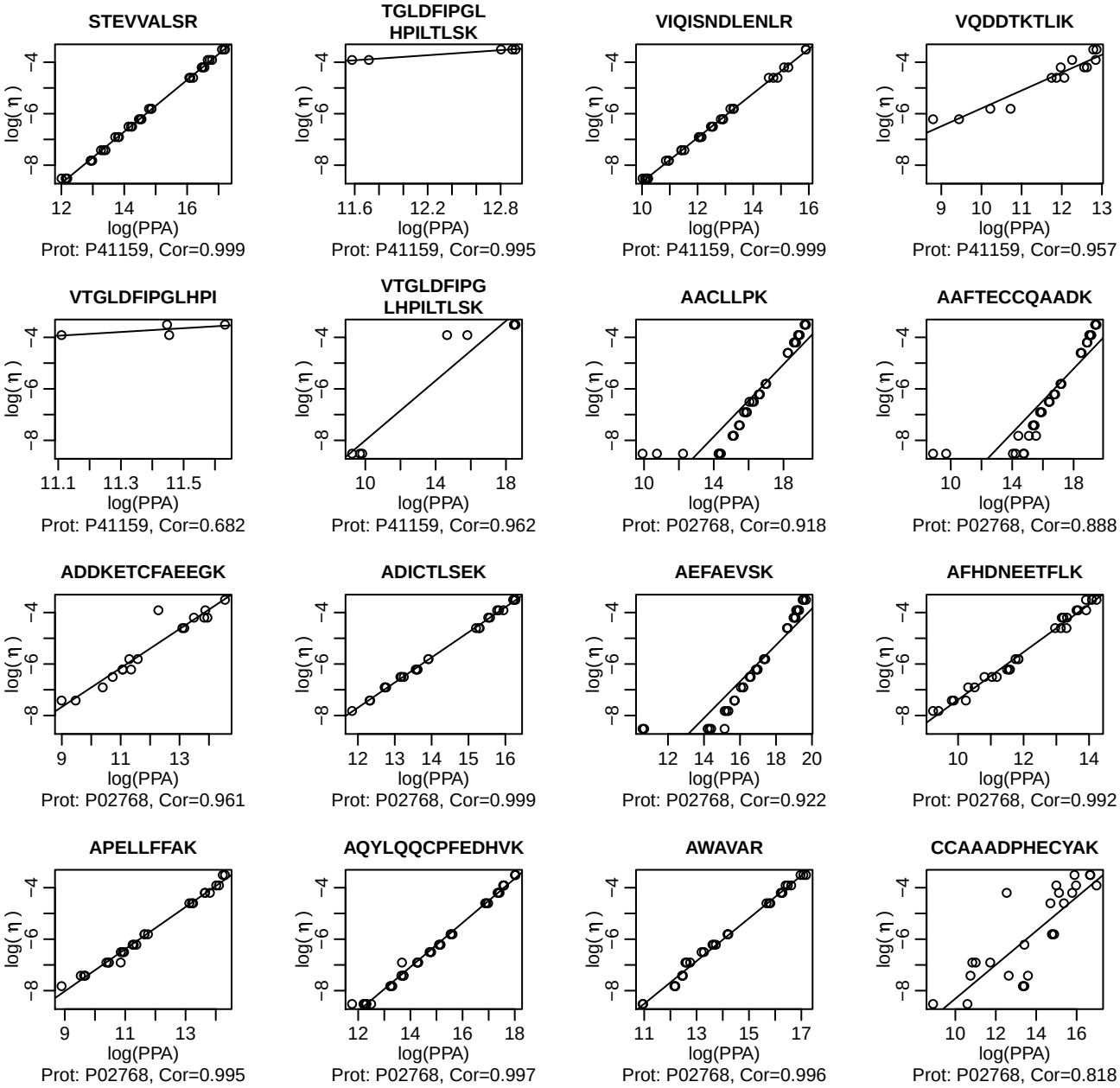
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



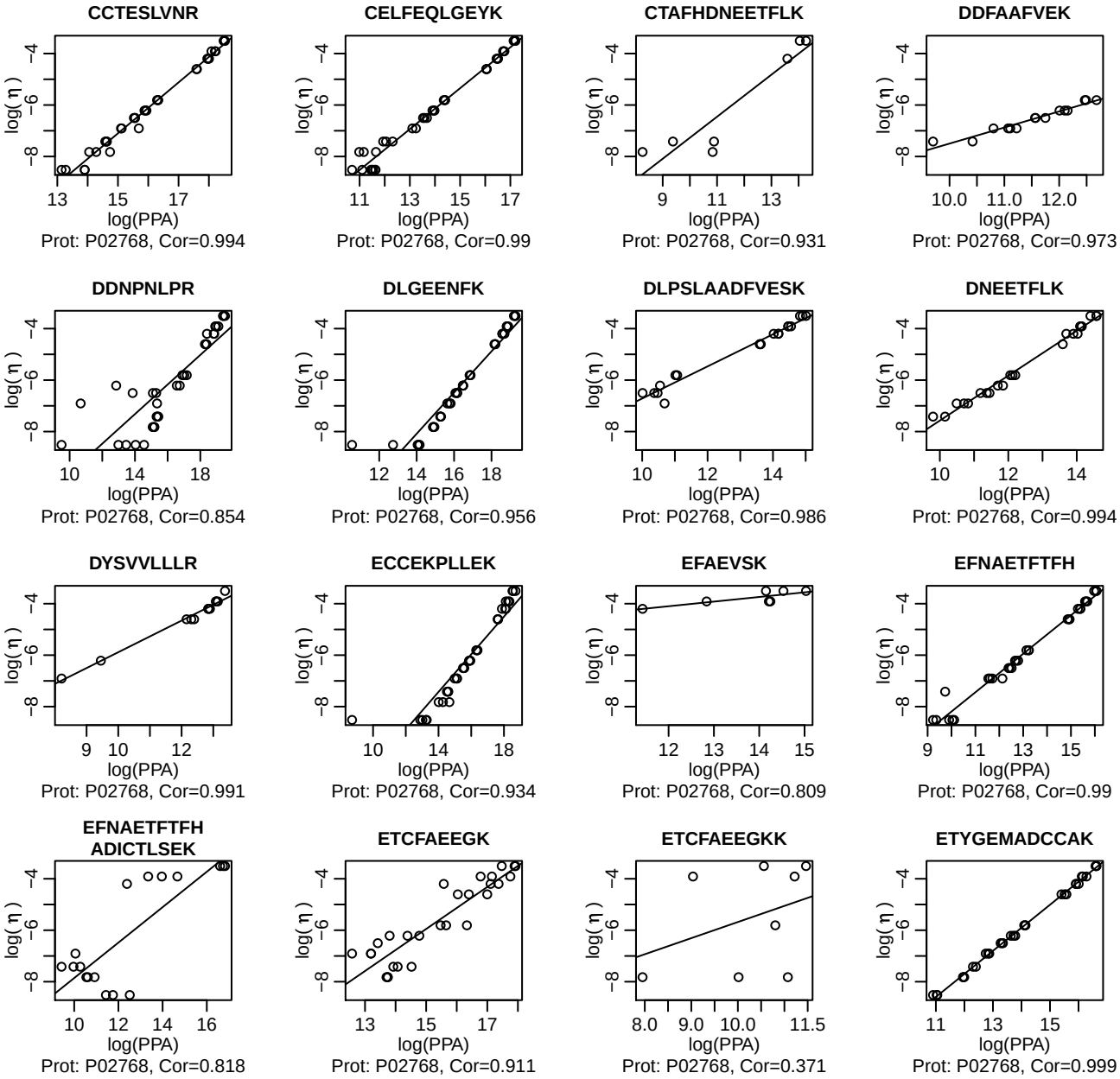
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



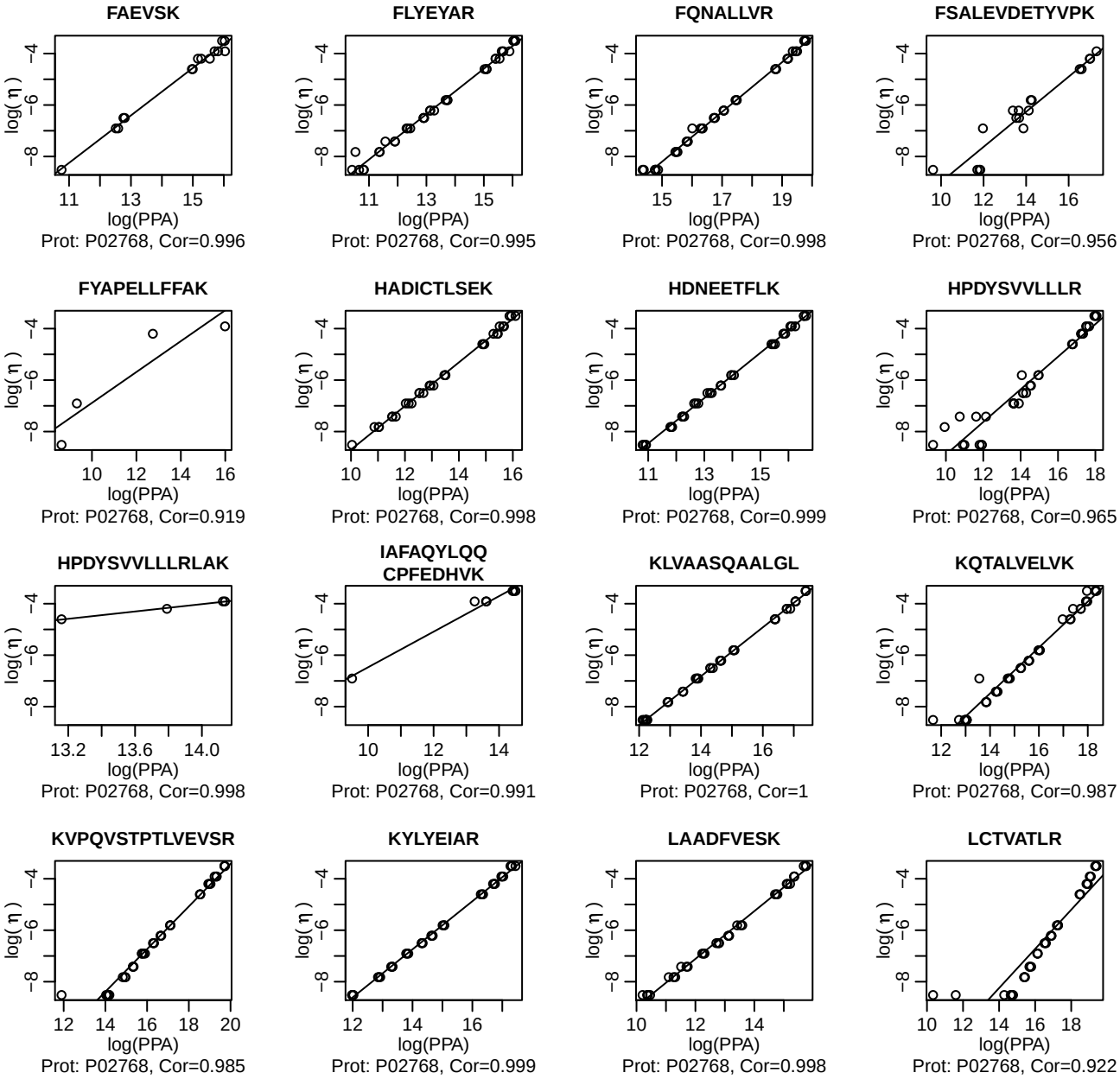
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



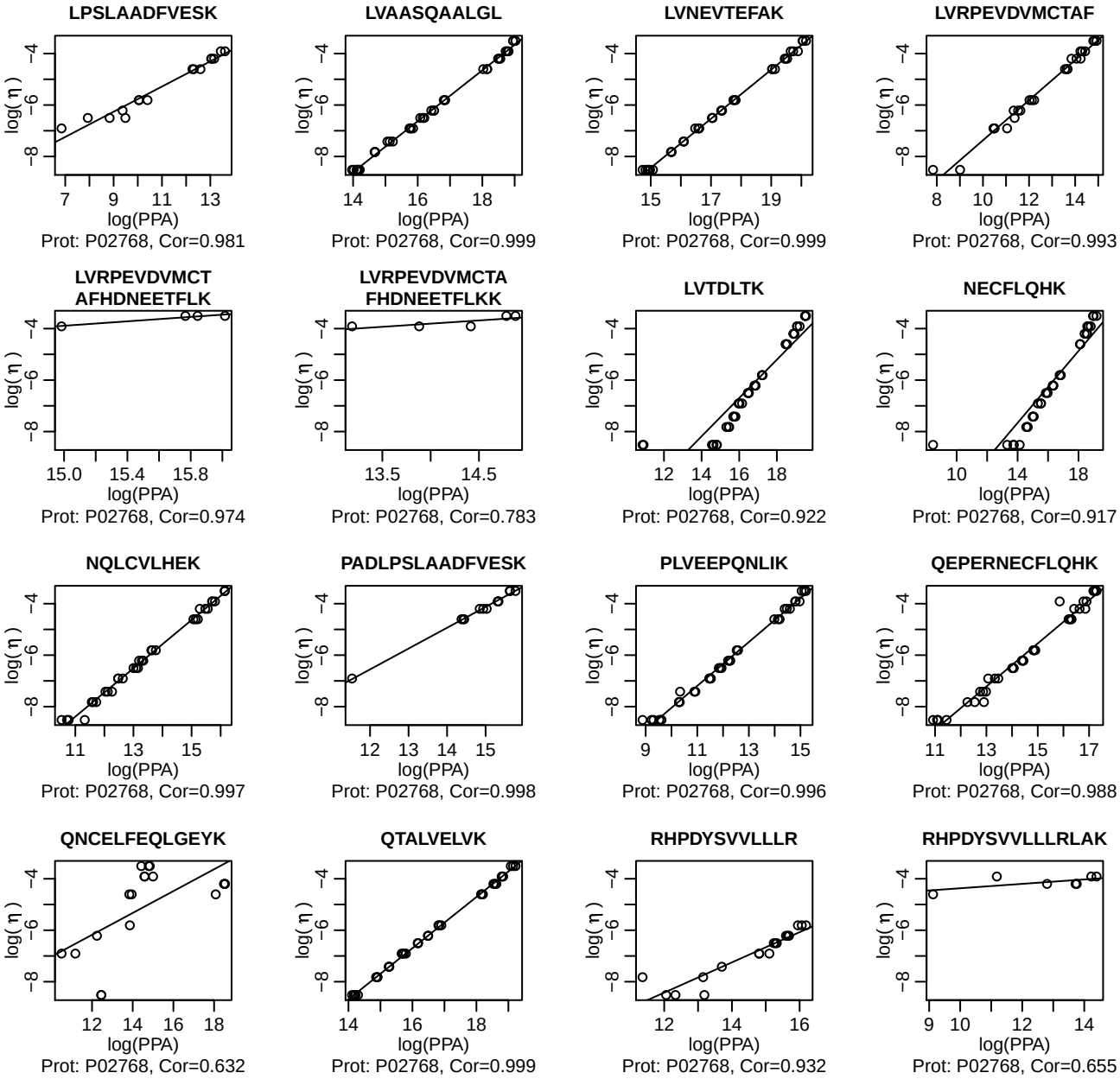
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



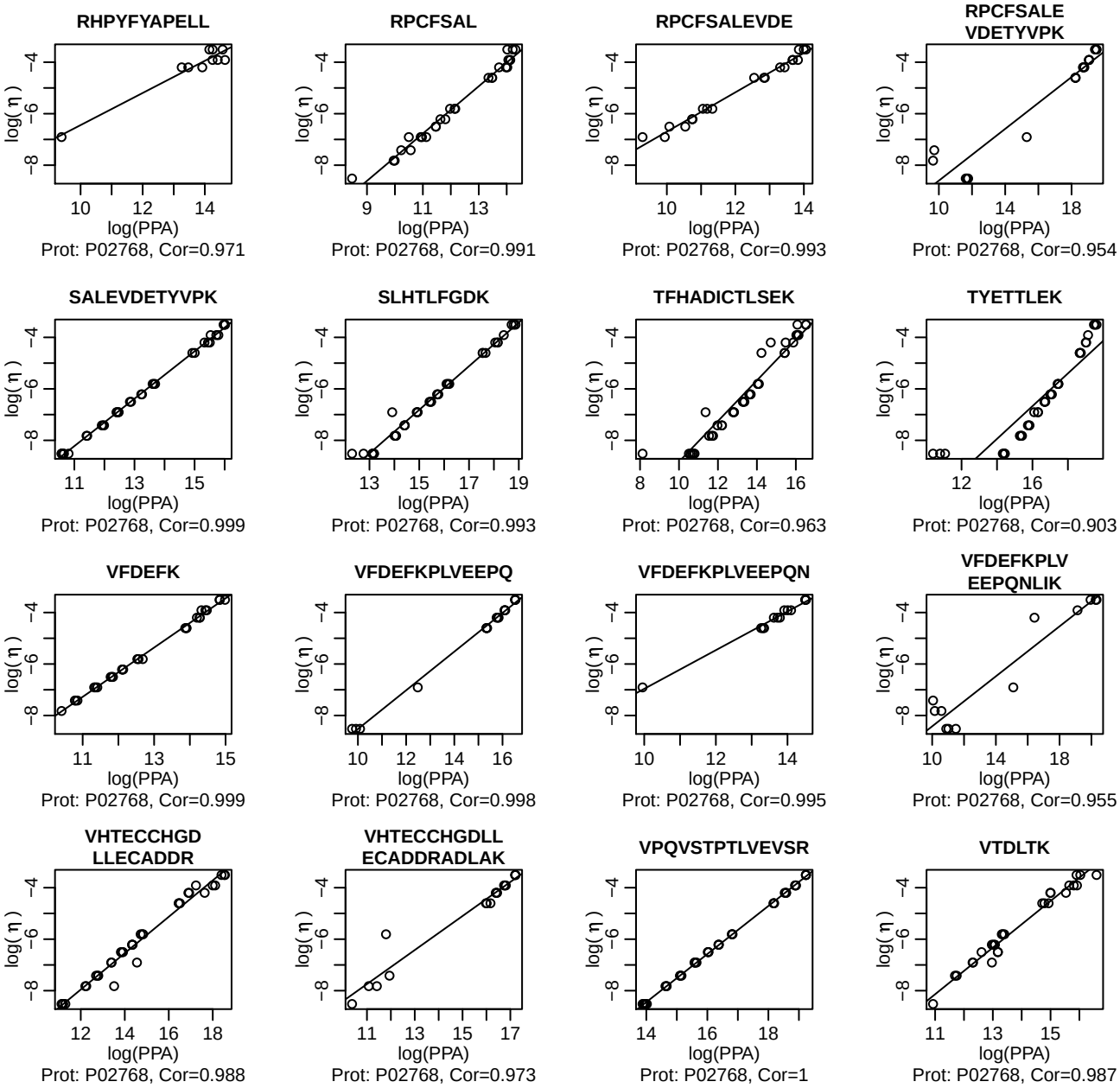
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



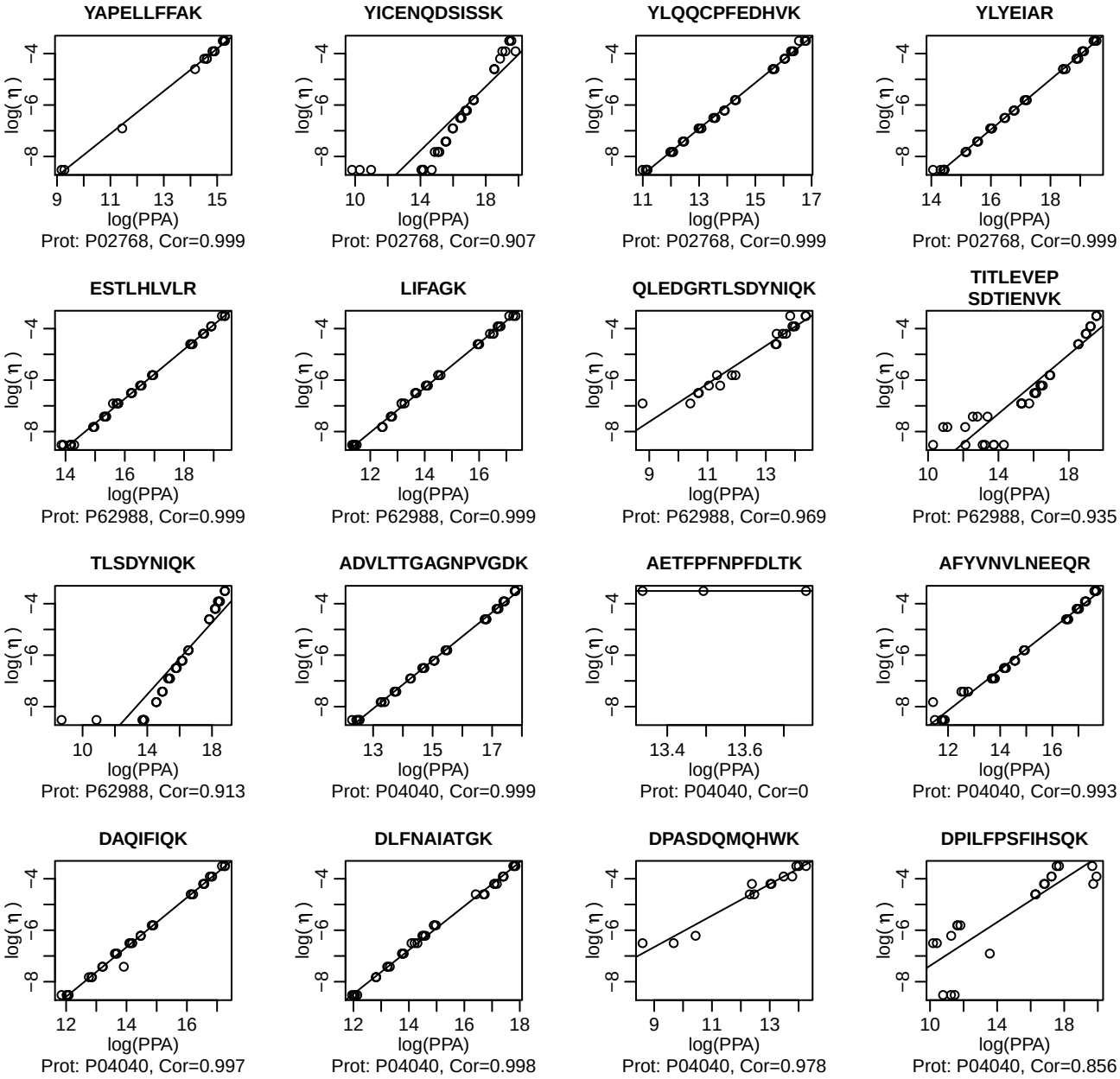
# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



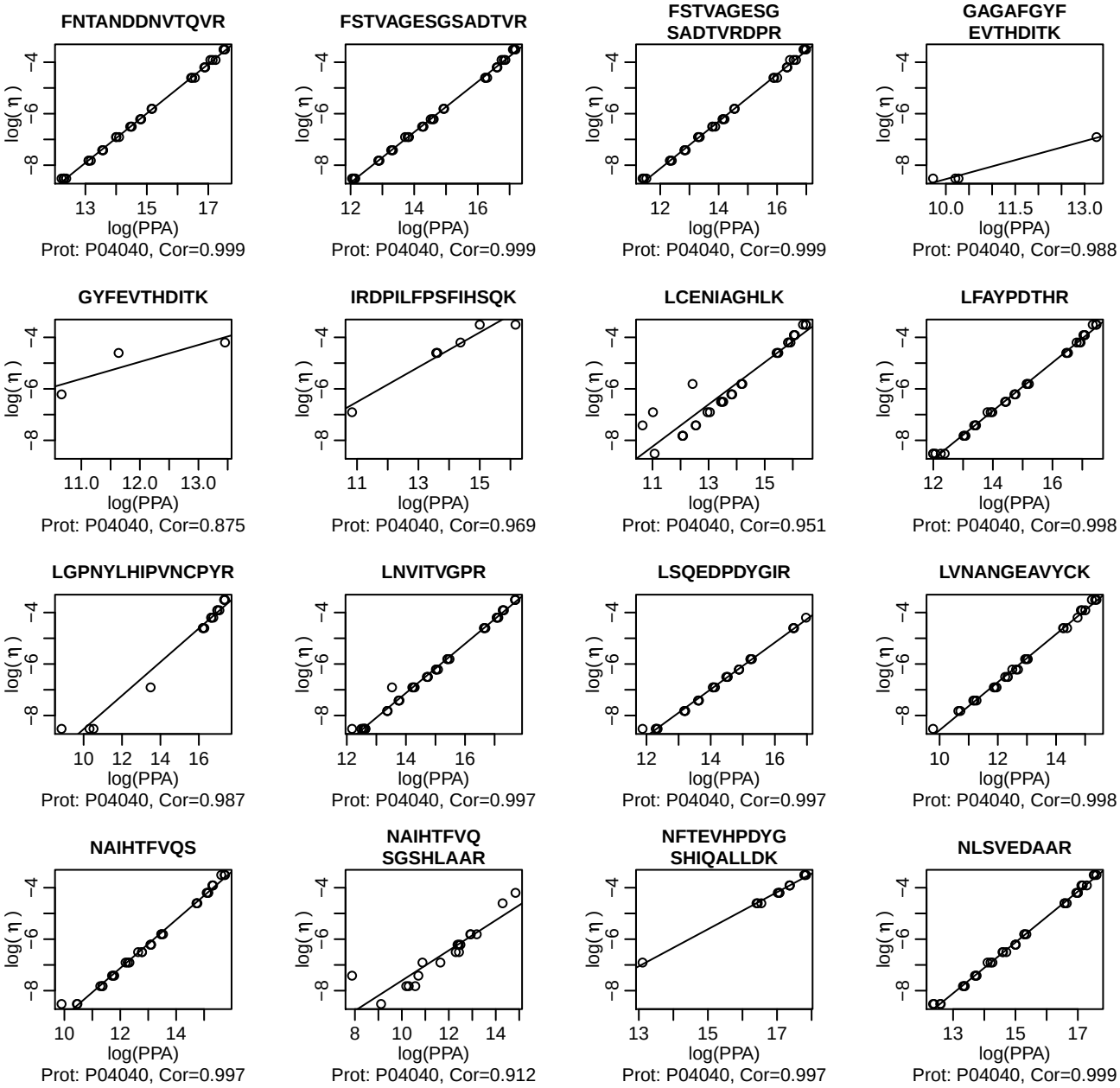
log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



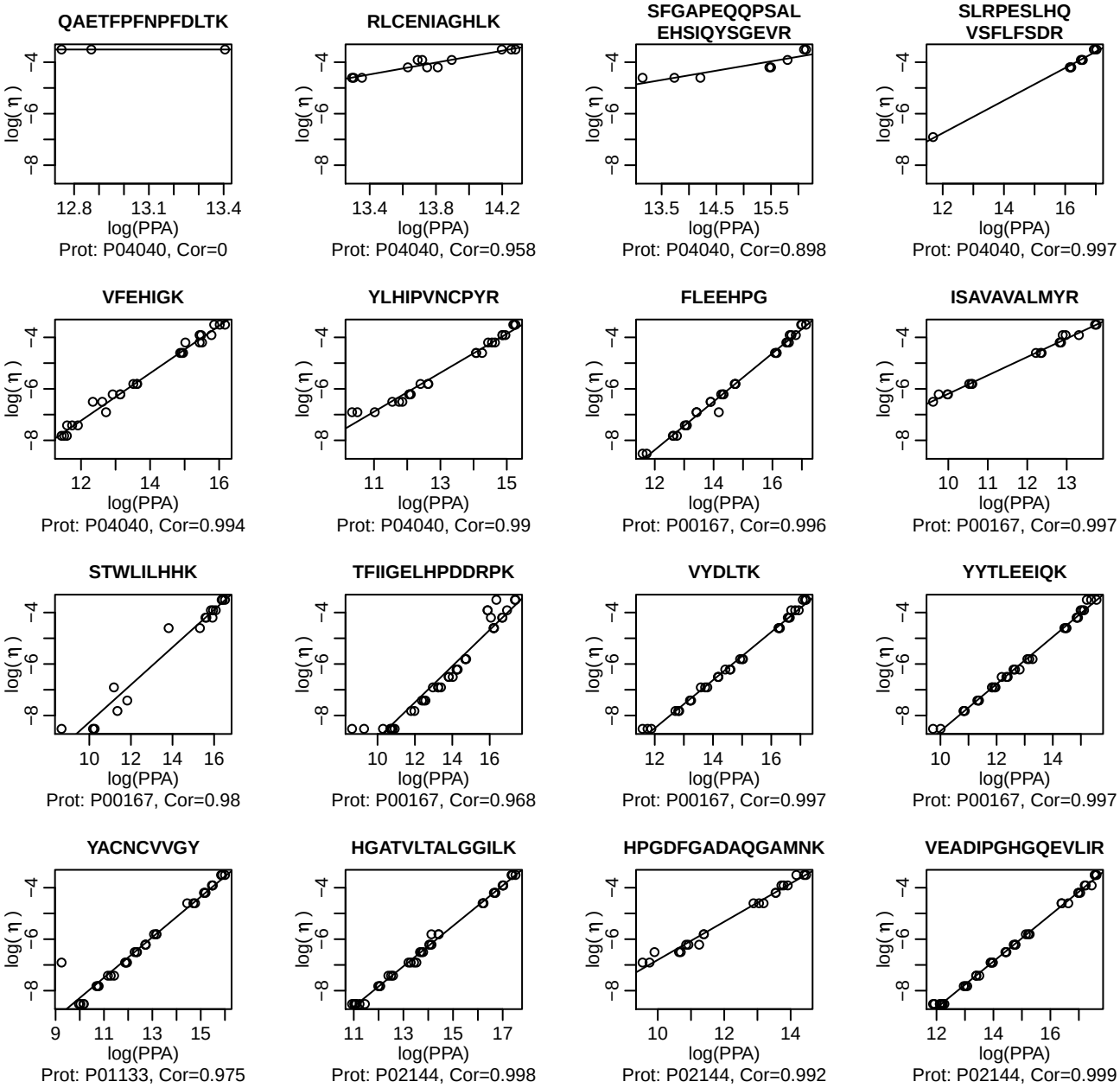
log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



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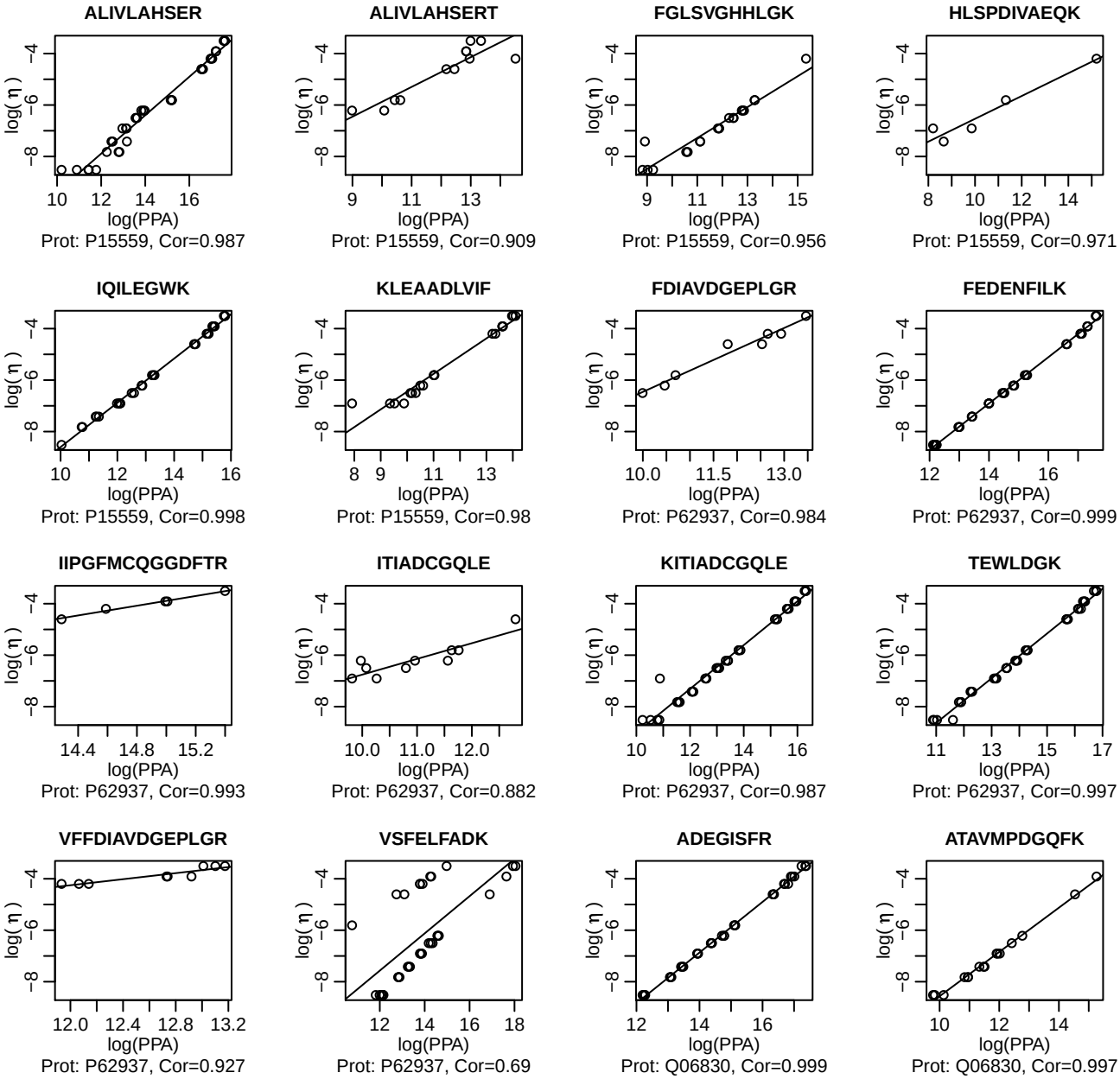
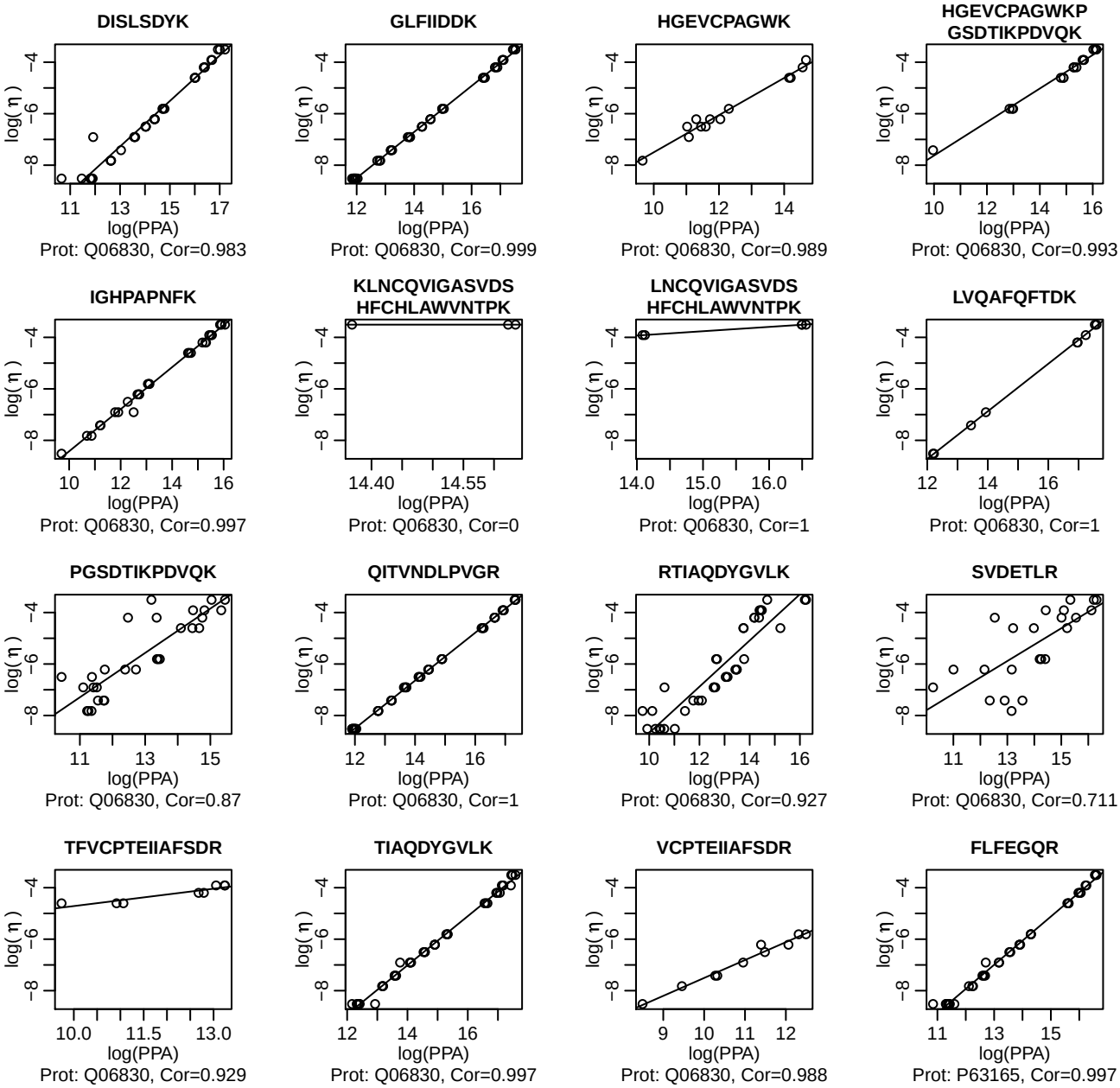


# log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample



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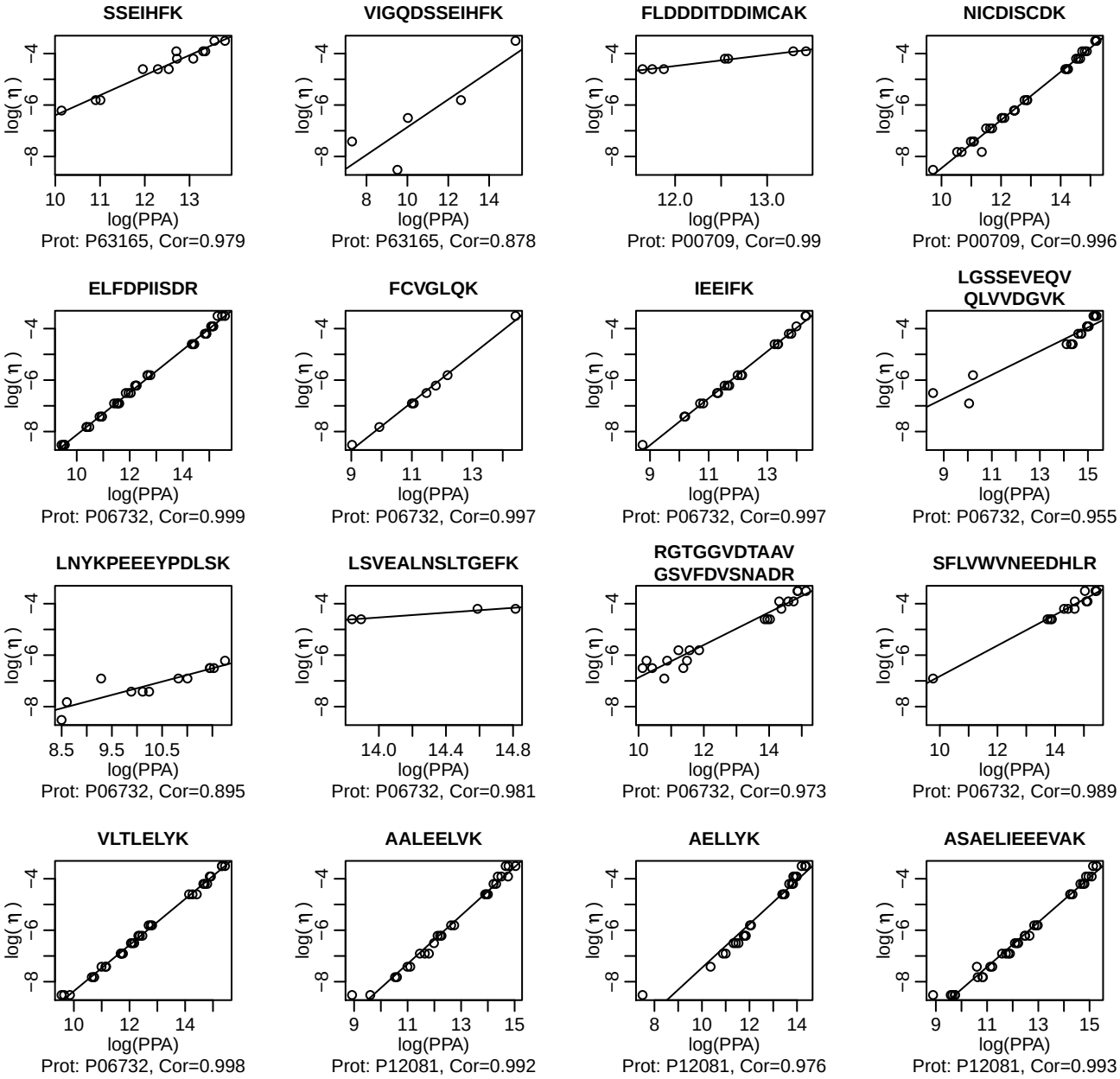

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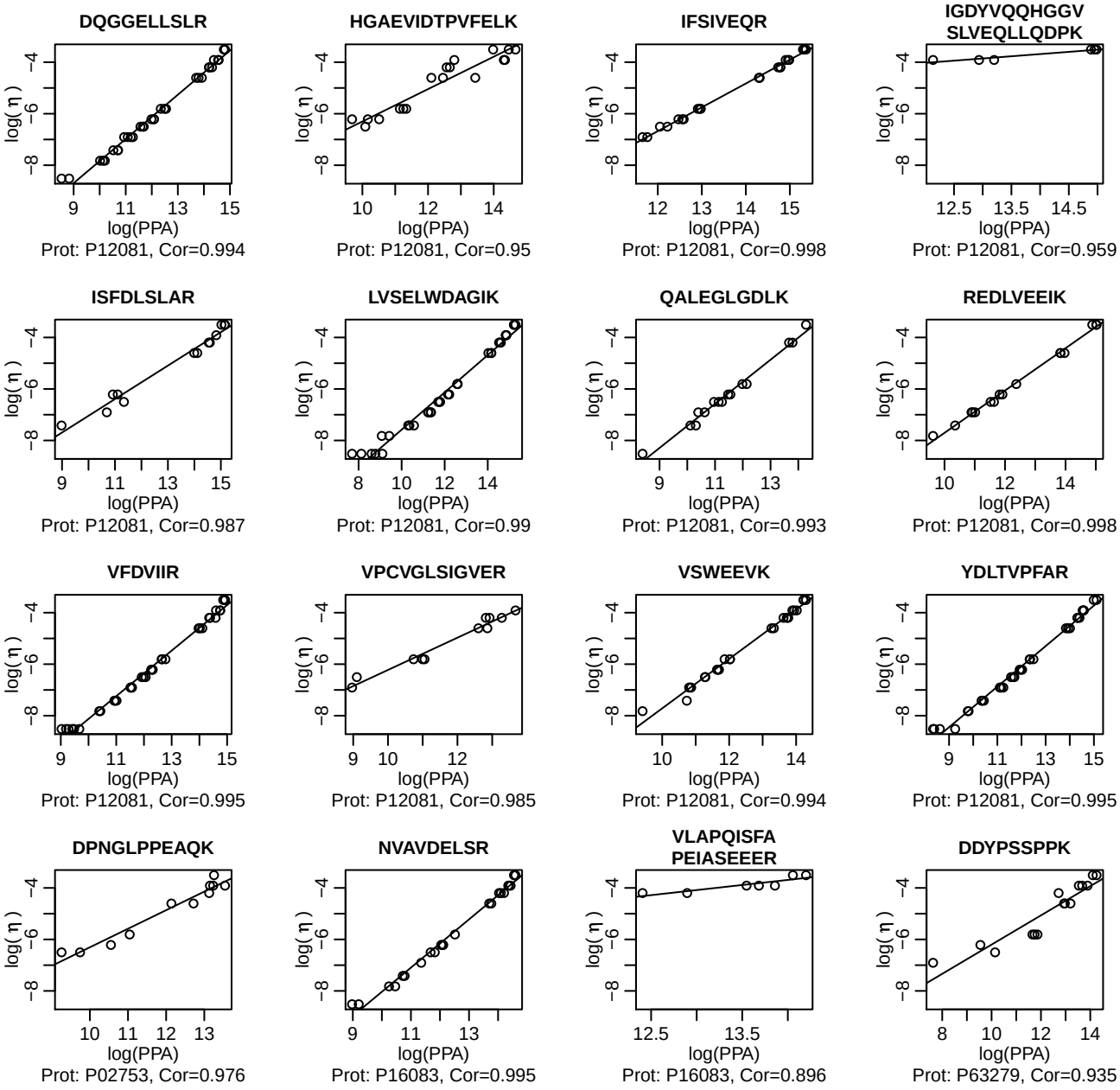
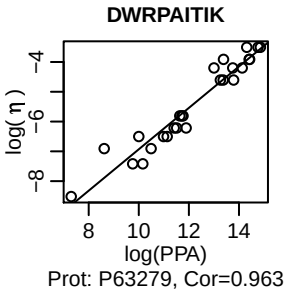
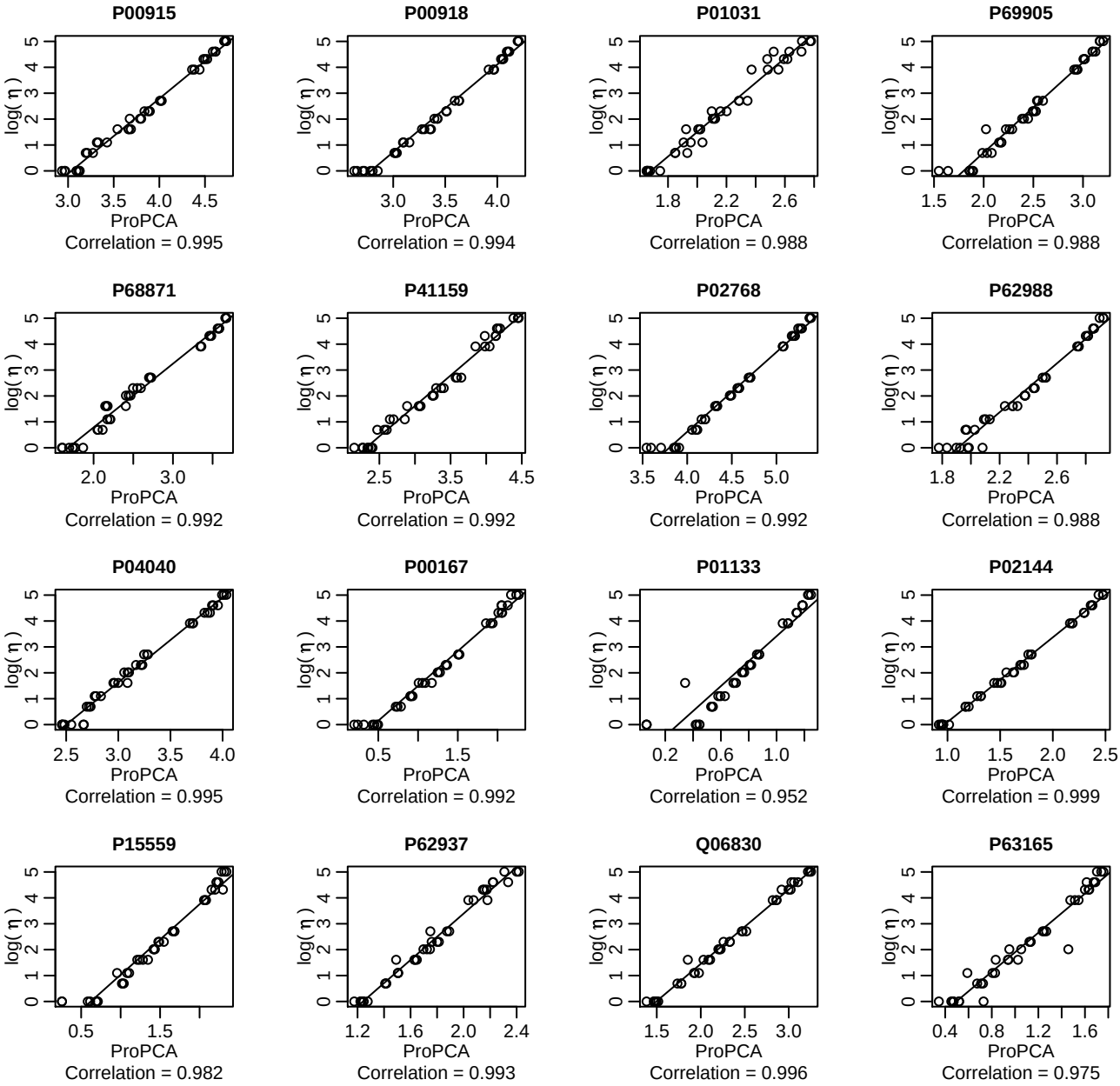


log( η ) v. log(PPA);  η = Proportion of UPS2 standard in sample

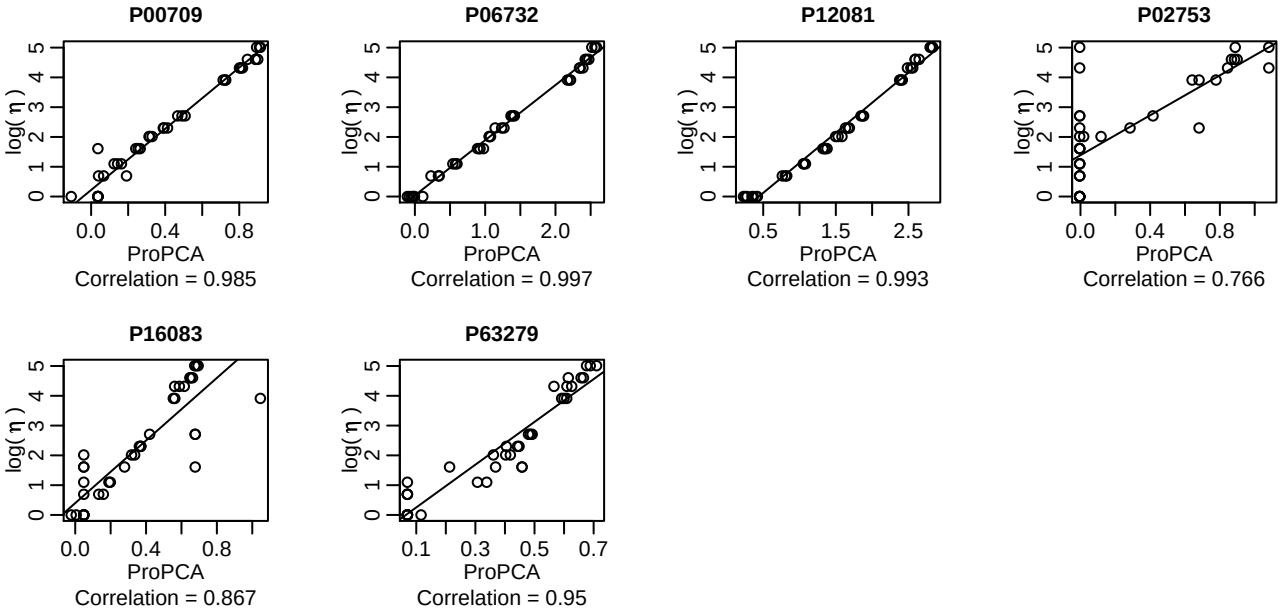



Prot: P63279, Cor=0.963

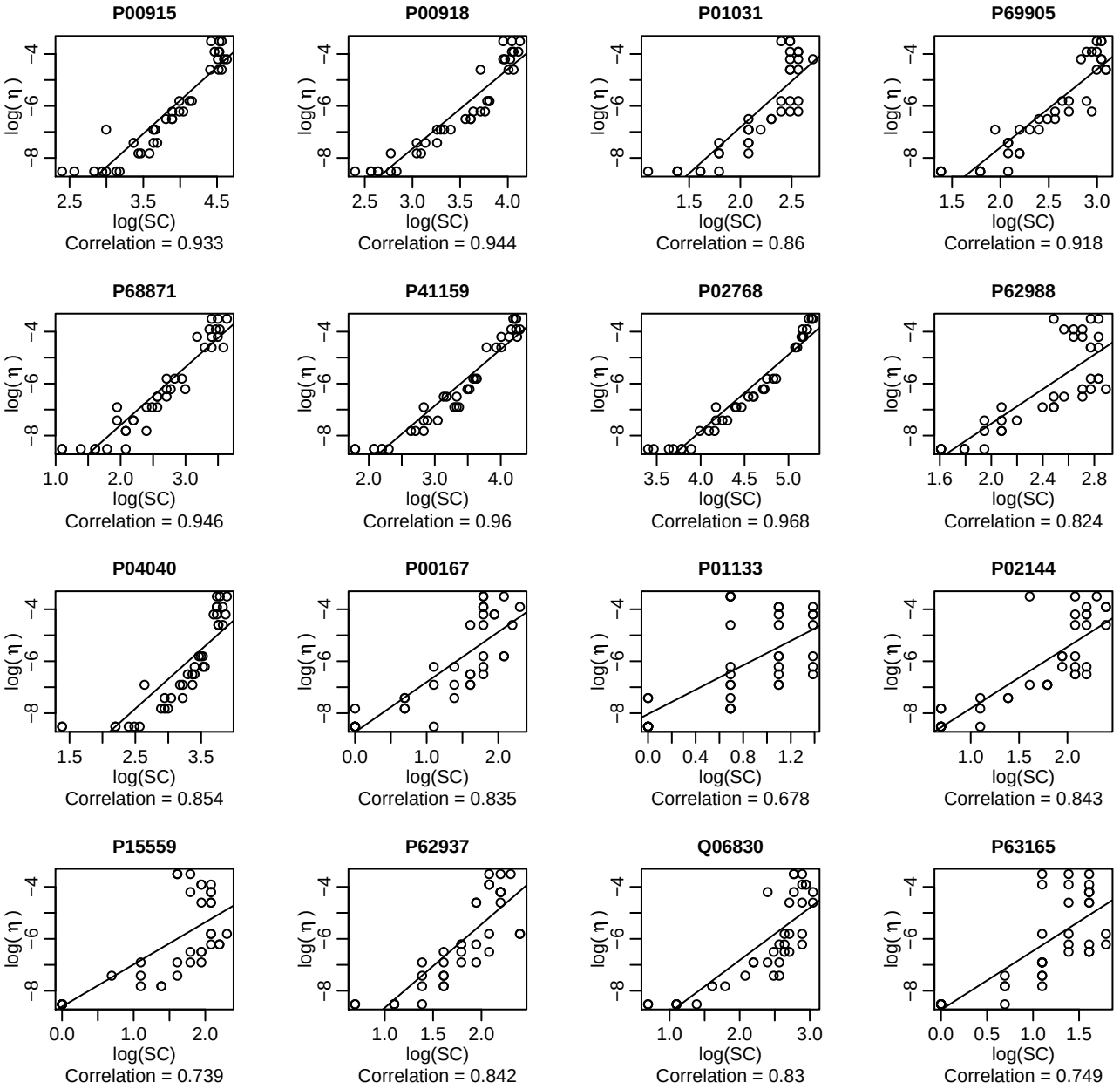
# log( η ) v. ProPCA;  η = Proportion of UPS2 standard in sample



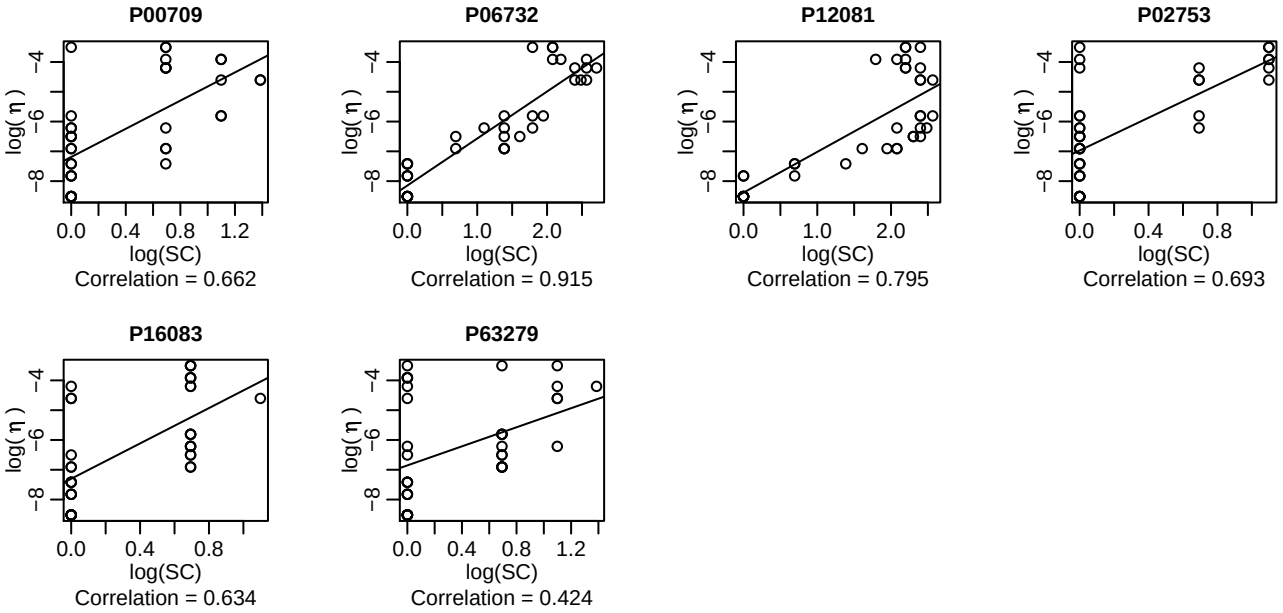
log( η ) v. ProPCA;  η = Proportion of UPS2 standard in sample



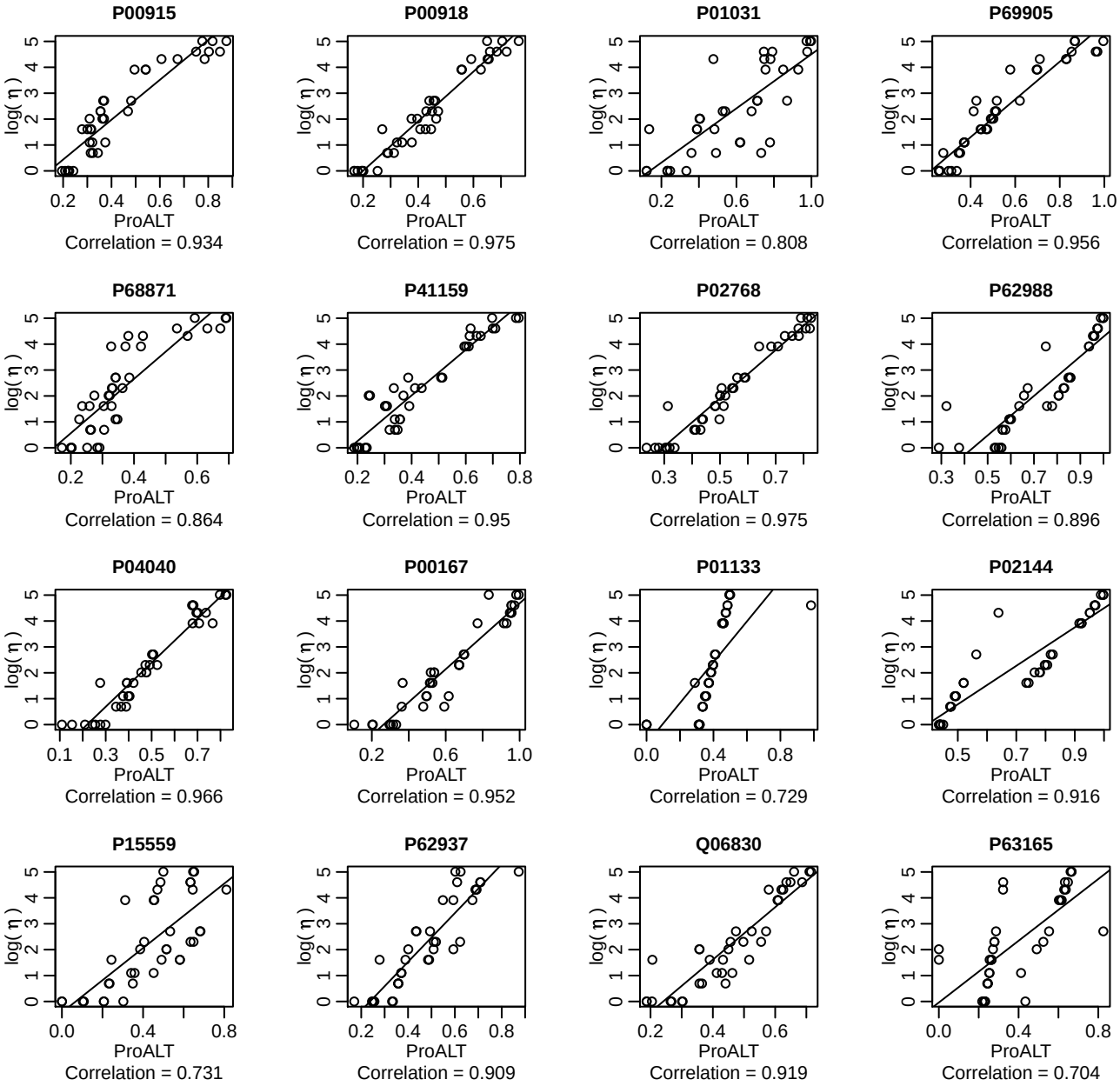
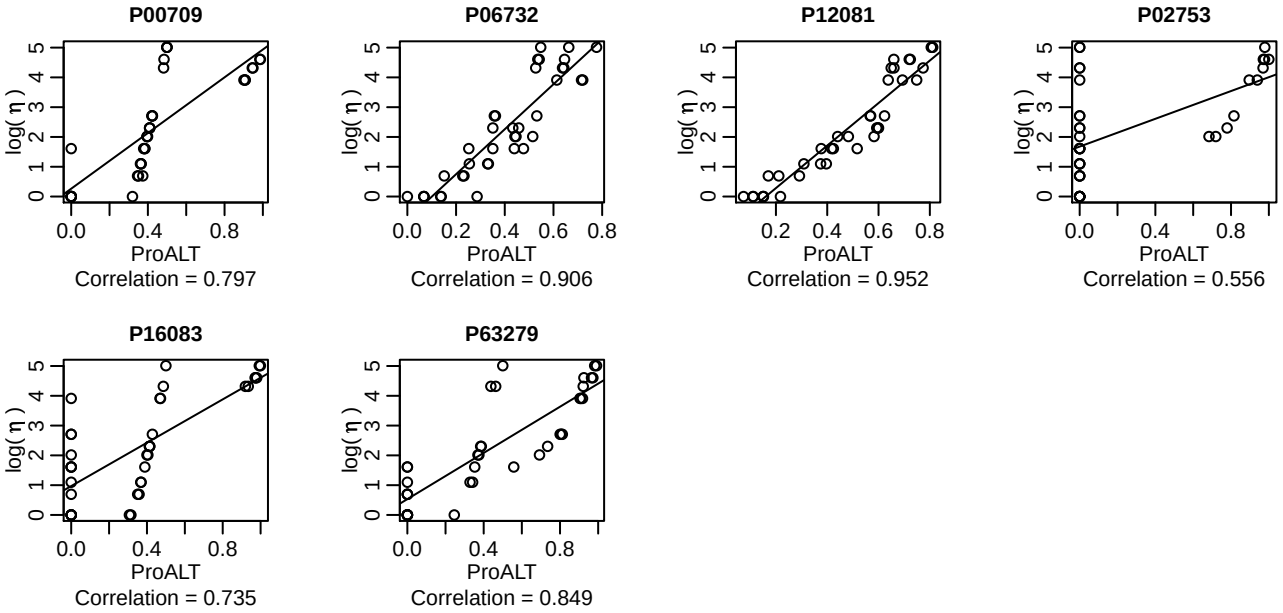
# log( η ) v. log(SC);  η = Proportion of UPS2 standard in sample



log( η ) v. log(SC);  η = Proportion of UPS2 standard in sample



# log( η ) v. ProALT ; η = Proportion of UPS2 standard in sample



log( η ) v.  ProALT ;  η = Proportion of UPS2 standard in sample