**Supplementary Material for:**

**Photoprotective Steering of Previtamin D Photochemistry by Phenylalanine in Solution**

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## 1. Excitation Source Spectra

The provitamin D excitation source used to trigger the photochemical reaction was a Xe-arc lamp/monochromator module of a Photon Technology International (PTI) fluorometer. The slit width at the slit just upstream of the sample was kept to 1.0 mm yielding a ~5 nm resolution full-width at half maximum. The spectra for the two excitation wavelengths are shown in Figure S1.
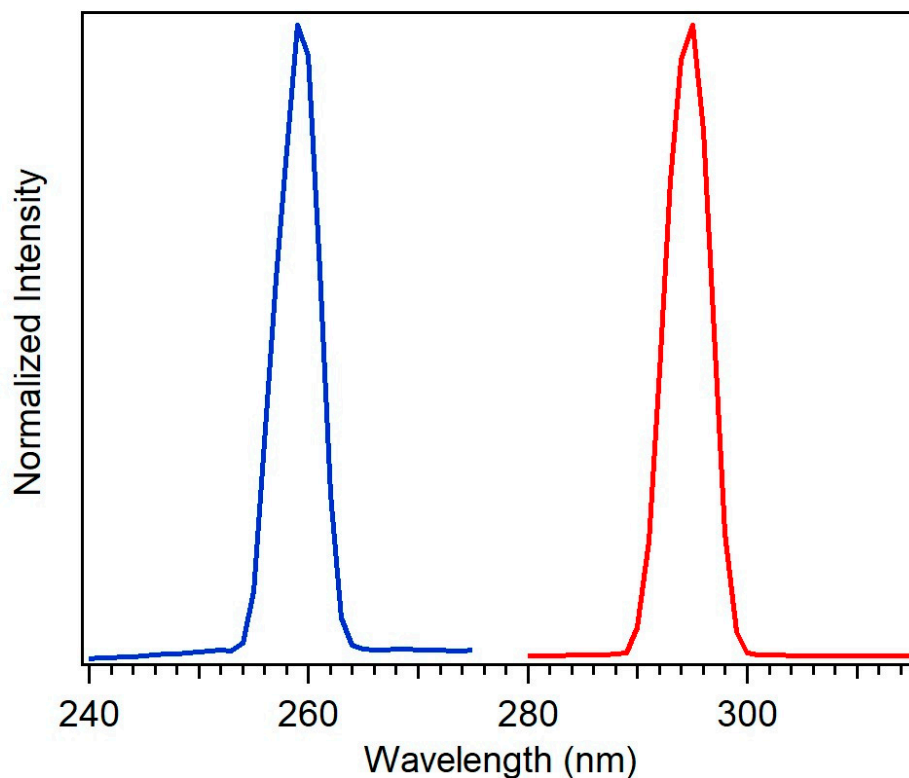


**Figure S1.** Spectra of excitation source used in the photochemistry experiments reported.

## 2. HPLC Data, DAD Spectra, and Gaussian Fitting

HPLC was used to analyze the final relative concentrations of species in the reaction mixture after 90 minutes of illumination. Figure 7 in the manuscript shows chromatograms that reveal the Pre-D, Tachy, and Pro-D elutions measured at an absorption wavelength of 280 nm—a wavelength where all species have some absorption. Figure S2 shows a representative chromatogram and the DAD spectra taken from the peak of each elution. The best separation of the Pre-D, Tachy, and Pro-D elutions was achieved with an isocratic mixture of acetonitrile:methanol:water at 24:69:7

(%v) run at a flow rate of 2.00 ml/min. In Figure S3, the Phe elution is found immediately at ~0.5 minute, and the other species of interest elute significantly later between 7-8.5 minutes. The spectra shown clearly identify each species, with Pre-D eluting first at around 7.3 minutes, Tachy next around 7.8 minutes, and finally the remaining Pro-D population at 8.2 minutes.
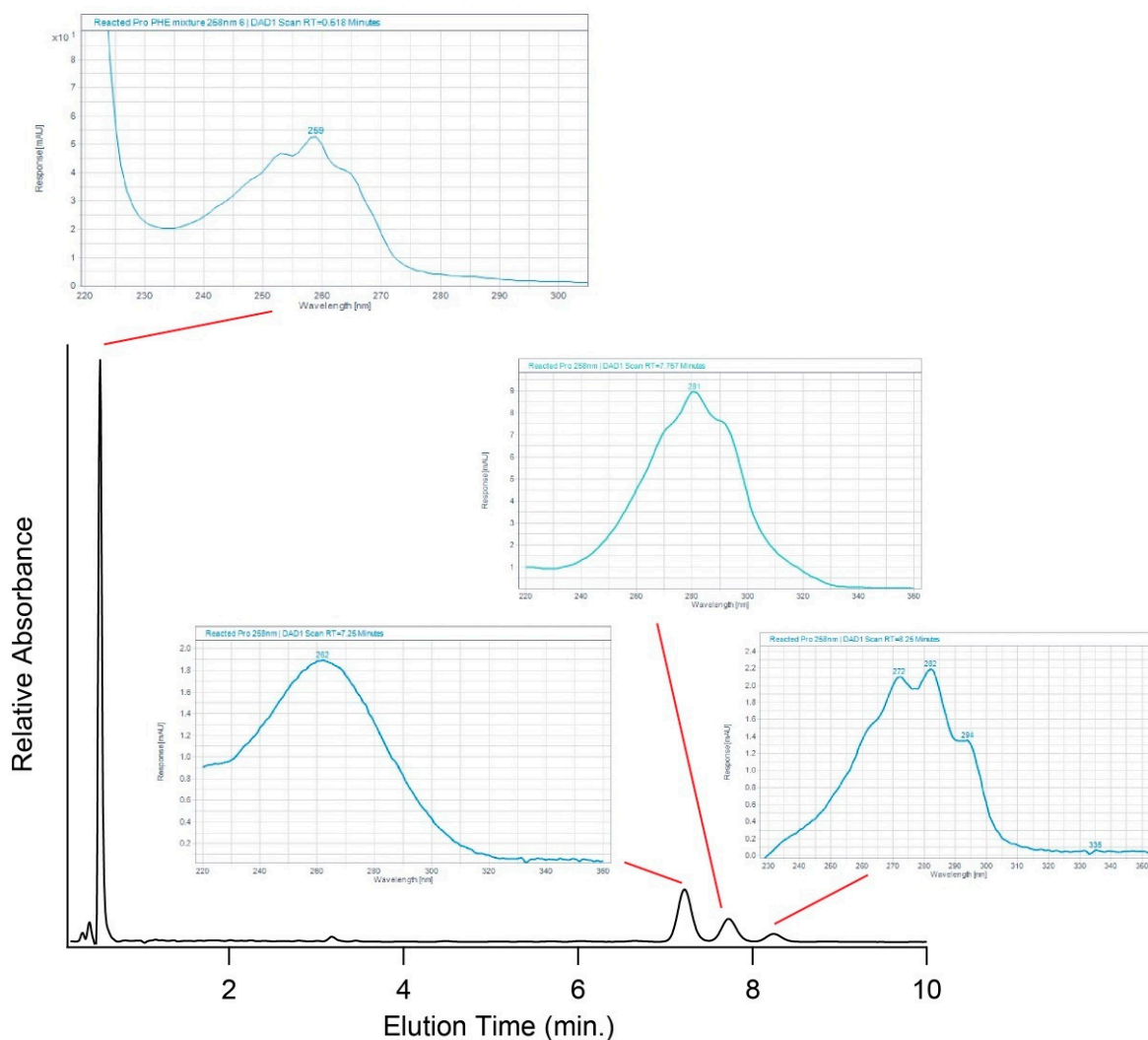


**Figure S2.** HPLC-DAD chromatogram showing elution times of various species in a reaction mixture. Each peak is labeled with the full DAD absorption spectrum enabling the identification of each elution.

The relative concentrations were retrieved by referencing each species' molar extinction coefficient at that wavelength to their integrated absorbance found from a fitting of a sum of three gaussian functions to the features in the chromatogram [28].

$$Chromatogram = C_1 e^{-\left(\frac{t-t_{elute1}}{width_1}\right)^2} + C_2 e^{-\left(\frac{t-t_{elute2}}{width_2}\right)^2} + C_3 e^{-\left(\frac{t-t_{elute3}}{width_3}\right)^2} \tag{S1}$$

The quality of those fittings for each chromatogram shown in Figure 7 are given in Figure S3, where the left column shows the full fit function given in equation S1 as the dashed trace against the experimental chromatogram, along with the residual shown below in red. The right column shows the three separate gaussian functions from equation S1 (dashed) against the experimental chromatogram. The three-gaussian fitting yields an excellent fit to the data, and the residuals show that integration of each feature should effectively cancel any the residual portion.
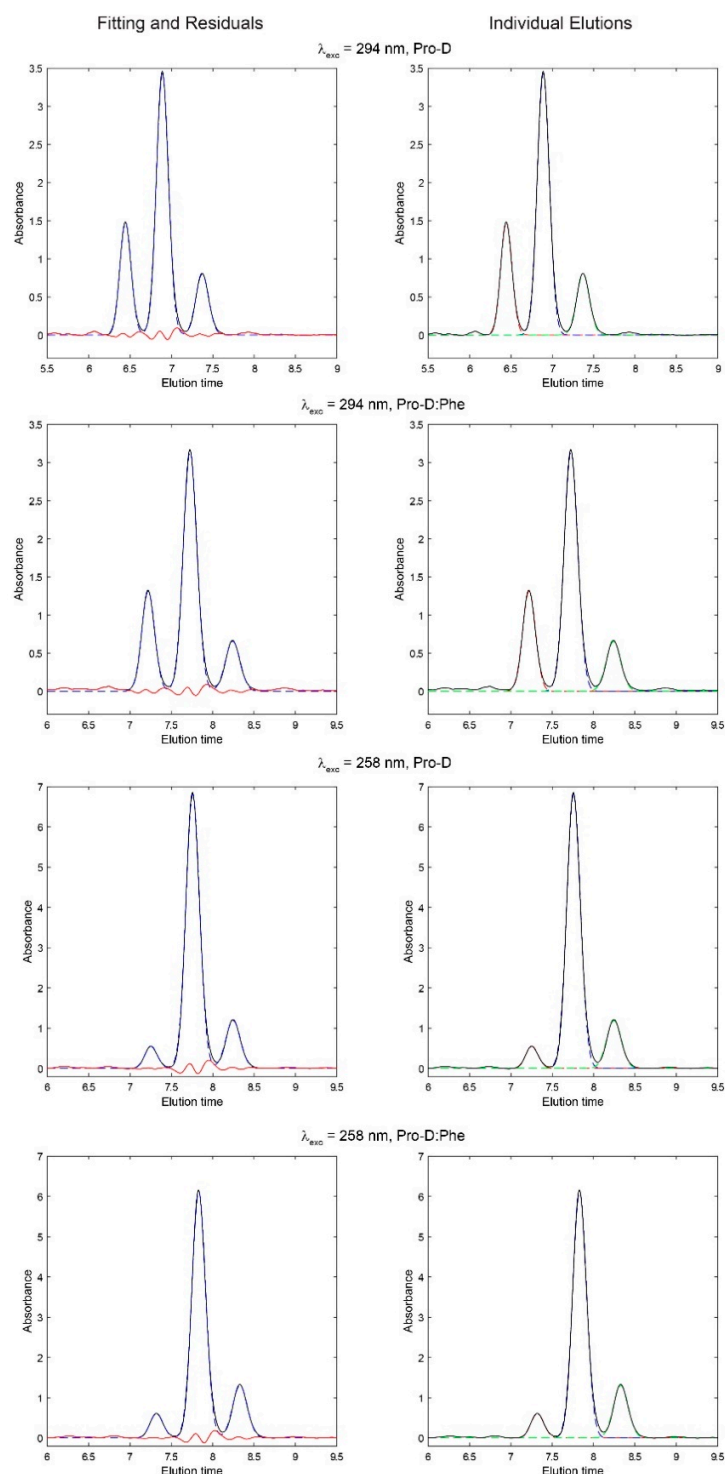
**Figure S3.** HPLC-DAD chromatograms (solid) taken at a detection wavelength of 280 nm for Pro-D and Pro-D:Phe mixtures following 294 and 258 nm illumination. The left column shows a three-gaussian fit function (dashed) along with residuals between the fit and experiment. The right column shows the three individual gaussians fit against their respective elution.

S5

## 3. Global Analysis Modeling and Fits

Global spectral analysis was performed on the time-dependent absorption spectra for Pro-D and Pro-D:Phe solutions under 258 nm illumination wavelength to extract the rate/time constants for decay of each separate time-evolving population. The evolution-associated spectra and their rate/time constants are given in Figure 8 and Table 1 of the manuscript respectively. In Figure S4, the fits from the model are shown against the experimental traces taken from the same wavelengths given in Figure 5 of the manuscript (albeit here raw absorbance is modeled). Inspection of the fits shows excellent agreement with the experimental data validating the A→B→C sequential model used.
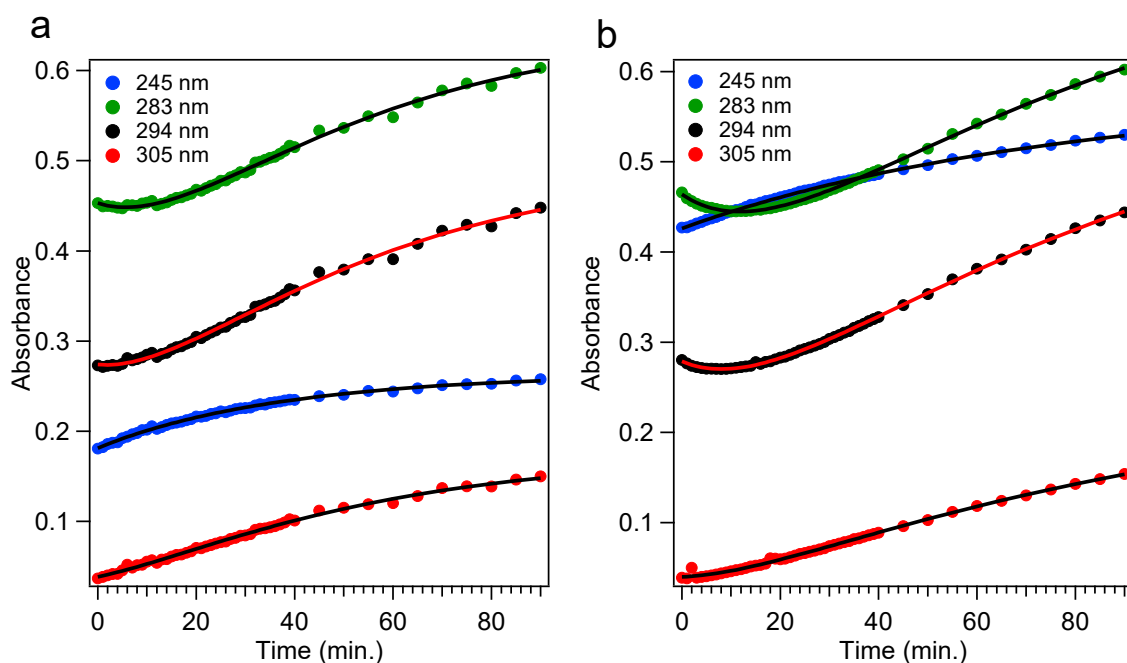


**Figure S4.** Experimental absorbance transients taken from a (a) Pro-D and (b) Pro-D:Phe mixture at 245 nm (blue), 283 nm (green), 294 nm (black), and 305 nm (red) detection wavelengths following 258 nm light exposure. Solid lines are from global spectra fitting of the data.

## 4. Atomic Coordinates of Calculated Pro-D, Phe, and Pro-D•••Phe Structures

Below are the atomic coordinates for calculated structures reported in Figure 9 of the manuscript. The structures have been calculated at the DFT//M06-2X/6-31+G(d) level of theory.

Pro-D

| | x | y | z |
|---|---|---|---|
| C | 6.00968 | 1.099472 | -1.04859 |
| C | 5.763742 | 2.209261 | -0.0334 |
| C | 5.242569 | 1.61689 | 1.275574 |
| C | 4.045632 | 0.71561 | 1.094695 |
| C | 4.069296 | -0.2799 | -0.06052 |
| C | 4.721119 | 0.32218 | -1.32435 |
| C | 3.07584 | 0.636894 | 2.022912 |
| C | 1.997974 | -0.35499 | 1.949818 |
| C | 1.813153 | -1.08601 | 0.838902 |
| C | 2.642135 | -0.78654 | -0.388 |
| C | 0.678928 | -2.03026 | 0.542861 |
| C | -0.19314 | -1.44904 | -0.6596 |
| C | 0.258837 | -0.007 | -0.96651 |
| C | 1.763404 | 0.151356 | -1.26042 |
| C | -0.30311 | -2.30467 | 1.689645 |
| C | -1.48691 | -1.38268 | 1.417053 |
| C | -1.66223 | -1.47242 | -0.10701 |
| C | -2.67122 | -0.45302 | -0.67775 |
| C | -3.99636 | -0.52694 | 0.103696 |
| C | -5.11105 | 0.38617 | -0.41263 |
| C | -6.27907 | 0.470365 | 0.571387 |
| C | -7.52113 | 1.192291 | 0.036218 |
| C | -7.2129 | 2.634664 | -0.37122 |
| C | -8.64196 | 1.162 | 1.076738 |
| C | -0.02093 | -2.34899 | -1.89006 |
| C | -2.92225 | -0.64932 | -2.17628 |
| C | 4.907078 | -1.48713 | 0.418692 |
| O | 4.820163 | 3.109715 | -0.61467 |
| H | 6.798864 | 0.443844 | -0.66081 |
| H | 6.385733 | 1.536804 | -1.98041 |
| H | 6.701988 | 2.746008 | 0.163971 |
| H | 5.009789 | 2.413037 | 1.994402 |
| H | 6.070202 | 1.038039 | 1.714272 |
| H | 4.914733 | -0.489 | -2.0389 |
| H | 4.023867 | 1.011256 | -1.80761 |

| | | | |
|---|---|---|---|
| H | 3.105169 | 1.296893 | 2.889056 |
| H | 1.339402 | -0.45525 | 2.809606 |
| H | 2.773809 | -1.72657 | -0.94518 |
| H | 1.134628 | -2.97232 | 0.204948 |
| H | -0.31097 | 0.393162 | -1.8128 |
| H | 0.008403 | 0.620437 | -0.10216 |
| H | 1.96967 | -0.03356 | -2.32107 |
| H | 2.036017 | 1.195389 | -1.06348 |
| H | -0.64473 | -3.34535 | 1.631587 |
| H | 0.142244 | -2.17132 | 2.68006 |
| H | -1.25085 | -0.34758 | 1.70705 |
| H | -2.38159 | -1.68486 | 1.968407 |
| H | -2.06775 | -2.47629 | -0.32432 |
| H | -2.26692 | 0.559443 | -0.52593 |
| H | -4.35485 | -1.56879 | 0.10769 |
| H | -3.80653 | -0.2625 | 1.151314 |
| H | -4.69872 | 1.388775 | -0.59406 |
| H | -5.48864 | 0.023745 | -1.37802 |
| H | -6.56621 | -0.54978 | 0.866334 |
| H | -5.94434 | 0.974581 | 1.491461 |
| H | -7.86624 | 0.649305 | -0.85666 |
| H | -8.12356 | 3.152567 | -0.69225 |
| H | -6.49332 | 2.683903 | -1.19451 |
| H | -6.79285 | 3.188829 | 0.478755 |
| H | -9.55453 | 1.630485 | 0.692033 |
| H | -8.88471 | 0.134756 | 1.371 |
| H | -8.33939 | 1.708048 | 1.979583 |
| H | -0.31918 | -3.37729 | -1.6517 |
| H | -0.62305 | -2.01378 | -2.73897 |
| H | 1.025038 | -2.37642 | -2.21672 |
| H | -3.31754 | -1.65555 | -2.3714 |
| H | -3.64838 | 0.076461 | -2.55382 |
| H | -2.01271 | -0.52531 | -2.76762 |
| H | 5.918715 | -1.18825 | 0.711945 |
| H | 4.431443 | -1.96343 | 1.282882 |
| H | 4.991729 | -2.23041 | -0.38369 |
| H | 4.61203 | 3.800676 | 0.031872 |

Phe

|   | x | y | z |
|---|---|---|---|
| C | 2.903042 | 0.196743 | -0.03663 |
| N | 1.170417 | -1.1131 | 1.111663 |
| C | 1.409844 | 0.185138 | 0.399166 |
| C | 0.496503 | 0.283634 | -0.82871 |
| C | -0.96952 | 0.186734 | -0.47553 |
| C | -1.70327 | -0.96577 | -0.77378 |
| C | -3.04829 | -1.0693 | -0.40985 |
| C | -3.67256 | -0.01824 | 0.257575 |
| C | -2.94826 | 1.13803 | 0.55909 |
| C | -1.60748 | 1.237575 | 0.196841 |
| O | 3.343447 | 1.302467 | -0.39849 |
| O | 3.474257 | -0.92269 | -0.01169 |
| H | 0.721155 | 1.243441 | -1.30344 |
| H | 0.767984 | -0.50454 | -1.54146 |
| H | -1.22394 | -1.78477 | -1.30656 |
| H | -1.05037 | 2.142717 | 0.430157 |
| H | -3.60438 | -1.96992 | -0.65274 |
| H | -3.43079 | 1.963282 | 1.074475 |
| H | -4.71839 | -0.09488 | 0.539475 |
| H | 1.205155 | 0.99606 | 1.099545 |
| H | 1.365159 | -1.0428 | 2.114294 |
| H | 0.212548 | -1.46563 | 1.001593 |
| H | 1.861139 | -1.77679 | 0.715359 |

Pro-D•••Phe dimer 1 ($\Delta G_{binding}$ -2.77 kJ/mol)

|   | x | y | z |
|---|---|---|---|
| C | -5.59965 | -0.37103 | 0.862632 |
| C | -5.38707 | 0.592778 | -0.29743 |
| C | -4.91821 | -0.17671 | -1.53049 |
| C | -3.67964 | -0.99475 | -1.25591 |
| C | -3.62967 | -1.82195 | 0.027076 |
| C | -4.29867 | -1.09343 | 1.216755 |
| C | -2.72261 | -1.14897 | -2.18926 |
| C | -1.5737 | -2.03811 | -2.00096 |
| C | -1.3224 | -2.59188 | -0.80402 |
| C | -2.17087 | -2.21488 | 0.390858 |
| C | -0.09795 | -3.38108 | -0.42008 |
| C | 0.744359 | -2.55835 | 0.655097 |
| C | 0.136802 | -1.15109 | 0.809584 |

| | | | |
|---|---:|---:|---:|
| C | -1.3533 | -1.15002 | 1.176976 |
| C | 0.881465 | -3.71539 | -1.55288 |
| C | 1.949133 | -2.6288 | -1.47372 |
| C | 2.185052 | -2.47748 | 0.037254 |
| C | 3.062887 | -1.26634 | 0.41919 |
| C | 4.343925 | -1.24119 | -0.43361 |
| C | 5.319522 | -0.11068 | -0.09804 |
| C | 6.415265 | 0.031019 | -1.15541 |
| C | 7.543208 | 1.001868 | -0.78736 |
| C | 7.019007 | 2.416668 | -0.53185 |
| C | 8.607202 | 1.019687 | -1.88617 |
| C | 0.716085 | -3.30993 | 1.992111 |
| C | 3.411413 | -1.25344 | 1.910306 |
| C | -4.41339 | -3.11957 | -0.27476 |
| O | -4.40391 | 1.561054 | 0.09018 |
| C | -2.54358 | 3.932678 | -1.56769 |
| N | -1.72777 | 1.667806 | -0.94041 |
| C | -1.44615 | 3.133549 | -0.8201 |
| C | -1.41957 | 3.521765 | 0.65961 |
| C | -0.43088 | 2.742386 | 1.501719 |
| C | 0.936822 | 2.739397 | 1.193777 |
| C | 1.849711 | 2.084274 | 2.018845 |
| C | 1.408881 | 1.427779 | 3.169754 |
| C | 0.048656 | 1.403457 | 3.47203 |
| C | -0.8641 | 2.050961 | 2.637616 |
| O | -2.27536 | 5.124964 | -1.78377 |
| O | -3.59822 | 3.297376 | -1.84828 |
| H | -6.38712 | -1.07974 | 0.578158 |
| H | -5.96306 | 0.180387 | 1.736813 |
| H | -6.32518 | 1.114883 | -0.52354 |
| H | -4.73791 | 0.511295 | -2.36587 |
| H | -5.73874 | -0.84193 | -1.83923 |
| H | -4.47832 | -1.82369 | 2.016478 |
| H | -3.62112 | -0.34215 | 1.630261 |
| H | -2.816 | -0.63001 | -3.14388 |
| H | -0.91338 | -2.20118 | -2.84915 |
| H | -2.24797 | -3.10249 | 1.036812 |
| H | -0.45262 | -4.30478 | 0.058694 |
| H | 0.687649 | -0.57529 | 1.560091 |
| H | 0.274599 | -0.62374 | -0.14641 |
| H | -1.47911 | -1.30312 | 2.255685 |
| H | -1.75551 | -0.14939 | 0.9861 |
| H | 1.349403 | -4.68599 | -1.34806 |

| | | | |
|---|---|---|---|
| H | 0.399889 | -3.79543 | -2.53192 |
| H | 1.575343 | -1.6824 | -1.89333 |
| H | 2.856625 | -2.89756 | -2.02158 |
| H | 2.727023 | -3.38054 | 0.367844 |
| H | 2.508859 | -0.34264 | 0.188839 |
| H | 4.862034 | -2.20884 | -0.33844 |
| H | 4.066863 | -1.14221 | -1.49063 |
| H | 4.758483 | 0.830664 | -0.00952 |
| H | 5.790544 | -0.28677 | 0.87822 |
| H | 6.853005 | -0.96016 | -1.34508 |
| H | 5.963691 | 0.355684 | -2.10593 |
| H | 8.011688 | 0.636488 | 0.139026 |
| H | 7.844833 | 3.108828 | -0.33329 |
| H | 6.339034 | 2.454353 | 0.325218 |
| H | 6.475102 | 2.785778 | -1.41161 |
| H | 9.446096 | 1.670827 | -1.61692 |
| H | 9.002623 | 0.01517 | -2.07413 |
| H | 8.179631 | 1.394118 | -2.8252 |
| H | 1.1537 | -4.30834 | 1.872167 |
| H | 1.272865 | -2.79027 | 2.77685 |
| H | -0.31233 | -3.44281 | 2.347964 |
| H | 3.981932 | -2.15313 | 2.178638 |
| H | 4.017244 | -0.3796 | 2.170376 |
| H | 2.519938 | -1.21903 | 2.539714 |
| H | -5.44518 | -2.90772 | -0.57352 |
| H | -3.93271 | -3.67766 | -1.08551 |
| H | -4.44175 | -3.75771 | 0.616571 |
| H | -4.37741 | 2.268982 | -0.59452 |
| H | -1.1851 | 4.590938 | 0.694192 |
| H | -2.42873 | 3.400982 | 1.073539 |
| H | 1.296251 | 3.274108 | 0.316732 |
| H | -1.92481 | 2.033365 | 2.88027 |
| H | 2.907593 | 2.096643 | 1.769933 |
| H | -0.30548 | 0.881824 | 4.356617 |
| H | 2.122259 | 0.931251 | 3.820975 |
| H | -0.47832 | 3.309764 | -1.29429 |
| H | -0.9755 | 1.107755 | -0.52272 |
| H | -2.6307 | 1.418772 | -0.47957 |
| H | -1.82424 | 1.382499 | -1.91997 |

Pro-D•••Phe dimer 2 (ΔG_binding -2.65 kJ/mol)

|   | x | y | z |
|---|---|---|---|
| C | -4.50329 | -1.106 | 1.671104 |
| C | -5.3109 | -0.83568 | 0.405397 |
| C | -5.07304 | -1.92827 | -0.65644 |
| C | -3.59241 | -2.05157 | -0.89176 |
| C | -2.75975 | -2.43568 | 0.327256 |
| C | -3.01304 | -1.33427 | 1.384511 |
| C | -3.02834 | -1.59314 | -2.02423 |
| C | -1.59424 | -1.31228 | -2.11932 |
| C | -0.75858 | -1.64154 | -1.12045 |
| C | -1.24811 | -2.57171 | -0.02796 |
| C | 0.657987 | -1.14384 | -1.05389 |
| C | 1.692632 | -2.15719 | -0.48443 |
| C | 1.117918 | -2.9356 | 0.737463 |
| C | -0.29257 | -2.51944 | 1.170476 |
| C | 0.804036 | 0.151661 | -0.20411 |
| C | 2.119851 | -0.01477 | 0.575529 |
| C | 2.852858 | -1.19444 | -0.08707 |
| C | 4.014037 | -1.71538 | 0.777033 |
| C | 5.034361 | -0.59889 | 1.080837 |
| C | 5.671702 | 0.067902 | -0.14003 |
| C | 6.79781 | 1.024275 | 0.255799 |
| C | 7.348231 | 1.881115 | -0.89017 |
| C | 7.909953 | 1.024216 | -2.02668 |
| C | 8.420002 | 2.839692 | -0.3682 |
| C | 2.048573 | -3.13965 | -1.60794 |
| C | 4.712195 | -2.94335 | 0.18117 |
| C | -3.21979 | -3.80294 | 0.870568 |
| O | -4.88379 | 0.442973 | -0.0666 |
| C | -4.34162 | 3.160777 | -1.65114 |
| N | -2.57954 | 1.489459 | -1.17379 |
| C | -2.97802 | 2.913074 | -0.95049 |
| C | -3.04768 | 3.199365 | 0.551979 |
| C | -1.77977 | 2.834457 | 1.293859 |
| C | -1.80915 | 1.887641 | 2.32241 |
| C | -0.64569 | 1.541577 | 3.013475 |
| C | 0.565963 | 2.144038 | 2.681496 |
| C | 0.60957 | 3.087203 | 1.652834 |
| C | -0.55342 | 3.428751 | 0.965416 |
| O | -4.76965 | 4.326494 | -1.57138 |
| O | -4.86375 | 2.164237 | -2.21822 |

| H | -4.92909 | -1.97859 | 2.178589 |
| H | -4.62845 | -0.25657 | 2.352903 |
| H | -6.37995 | -0.78491 | 0.646042 |
| H | -5.59057 | -1.65612 | -1.58393 |
| H | -5.52155 | -2.86094 | -0.29275 |
| H | -2.50261 | -1.58855 | 2.321843 |
| H | -2.55157 | -0.4001 | 1.031781 |
| H | -3.66871 | -1.28033 | -2.84862 |
| H | -1.23203 | -0.73986 | -2.97333 |
| H | -1.14248 | -3.58477 | -0.45972 |
| H | 0.976774 | -0.90102 | -2.07658 |
| H | 1.084247 | -4.00462 | 0.487763 |
| H | 1.790882 | -2.84992 | 1.596987 |
| H | -0.63185 | -3.19527 | 1.963627 |
| H | -0.278 | -1.51248 | 1.606873 |
| H | 0.83414 | 1.027169 | -0.86364 |
| H | -0.04333 | 0.296168 | 0.479537 |
| H | 1.912114 | -0.26796 | 1.625736 |
| H | 2.714999 | 0.904027 | 0.583757 |
| H | 3.281198 | -0.84314 | -1.04047 |
| H | 3.605028 | -2.01121 | 1.75365 |
| H | 4.561701 | 0.174361 | 1.700945 |
| H | 5.832774 | -1.03446 | 1.698812 |
| H | 6.058954 | -0.70194 | -0.82007 |
| H | 4.911383 | 0.628749 | -0.70265 |
| H | 6.431435 | 1.692777 | 1.048847 |
| H | 7.625813 | 0.447291 | 0.696734 |
| H | 6.516549 | 2.480644 | -1.2904 |
| H | 8.355597 | 1.652824 | -2.80562 |
| H | 7.137369 | 0.4079 | -2.49705 |
| H | 8.692575 | 0.354007 | -1.64678 |
| H | 8.789073 | 3.495225 | -1.16464 |
| H | 8.031467 | 3.470476 | 0.439208 |
| H | 9.275631 | 2.276807 | 0.026598 |
| H | 2.574867 | -2.62886 | -2.42353 |
| H | 2.672518 | -3.96729 | -1.26385 |
| H | 1.128739 | -3.57451 | -2.02158 |
| H | 4.93371 | -2.80881 | -0.88417 |
| H | 5.658281 | -3.13573 | 0.700356 |
| H | 4.094739 | -3.84075 | 0.281767 |
| H | -4.25032 | -3.79203 | 1.232297 |
| H | -3.14901 | -4.56537 | 0.08737 |
| H | -2.58384 | -4.1126 | 1.706776 |

| | | | |
|---|---|---|---|
| H | -5.34556 | 0.723002 | -0.88139 |
| H | -3.26551 | 4.266646 | 0.656169 |
| H | -3.89484 | 2.648287 | 0.976419 |
| H | -2.75544 | 1.42321 | 2.592179 |
| H | -0.50849 | 4.173314 | 0.172994 |
| H | -0.69066 | 0.802626 | 3.808846 |
| H | 1.551549 | 3.55815 | 1.385987 |
| H | 1.474064 | 1.87674 | 3.214154 |
| H | -2.21547 | 3.53396 | -1.42871 |
| H | -2.59901 | 1.269541 | -2.17373 |
| H | -1.64327 | 1.278602 | -0.80901 |
| H | -3.28207 | 0.859456 | -0.72315 |

Pro-D•••Phe dimer 3 ($\Delta G_{\text{binding}}$ -2.61 kJ/mol)

| | x | y | z |
|---|---|---|---|
| C | 5.727365 | -0.83889 | -1.64546 |
| C | 5.727944 | 0.440064 | -0.81768 |
| C | 5.30971 | 0.139868 | 0.620956 |
| C | 3.993691 | -0.59435 | 0.702419 |
| C | 3.794097 | -1.7878 | -0.22634 |
| C | 4.34598 | -1.49626 | -1.63968 |
| C | 3.111768 | -0.35014 | 1.688283 |
| C | 1.922891 | -1.1819 | 1.903382 |
| C | 1.566365 | -2.11789 | 1.008998 |
| C | 2.302784 | -2.21046 | -0.30708 |
| C | 0.343993 | -2.9973 | 1.03997 |
| C | -0.56668 | -2.70515 | -0.23429 |
| C | -0.06943 | -1.42131 | -0.92882 |
| C | 1.418799 | -1.4472 | -1.32844 |
| C | -0.57336 | -2.86024 | 2.263669 |
| C | -1.72761 | -1.98254 | 1.790303 |
| C | -1.9992 | -2.49613 | 0.367692 |
| C | -2.99872 | -1.63243 | -0.42847 |
| C | -4.2661 | -1.37877 | 0.408234 |
| C | -5.35318 | -0.56899 | -0.30329 |
| C | -6.39374 | -0.00816 | 0.665995 |
| C | -7.42466 | 0.930466 | 0.027725 |
| C | -8.36019 | 1.494664 | 1.098546 |
| C | -8.23403 | 0.237439 | -1.07072 |
| C | -0.5072 | -3.90399 | -1.19045 |
| C | -3.35931 | -2.24223 | -1.7867 |

| C | 4.577705 | -2.96362 | 0.399882 |
|---|---|---|---|
| O | 4.818697 | 1.365254 | -1.42042 |
| C | 3.305451 | 3.102087 | 1.080885 |
| N | 2.182201 | 2.302244 | -0.97425 |
| C | 1.968421 | 2.604069 | 0.477257 |
| C | 0.879836 | 3.670543 | 0.636403 |
| C | -0.44724 | 3.261848 | 0.041376 |
| C | -1.27969 | 2.360992 | 0.718441 |
| C | -2.50499 | 1.982252 | 0.174247 |
| C | -2.90784 | 2.48686 | -1.06446 |
| C | -2.08167 | 3.373261 | -1.75187 |
| C | -0.86002 | 3.761219 | -1.19826 |
| O | 4.194558 | 3.437571 | 0.248 |
| O | 3.343089 | 3.158853 | 2.319946 |
| H | 6.490989 | -1.51273 | -1.23824 |
| H | 6.021561 | -0.60613 | -2.67513 |
| H | 6.733365 | 0.881414 | -0.82079 |
| H | 5.263165 | 1.065128 | 1.208836 |
| H | 6.10137 | -0.47871 | 1.070621 |
| H | 4.370903 | -2.43464 | -2.20952 |
| H | 3.666264 | -0.8255 | -2.17296 |
| H | 3.305235 | 0.461055 | 2.390048 |
| H | 1.342439 | -1.01046 | 2.806768 |
| H | 2.307229 | -3.26647 | -0.61433 |
| H | 0.708943 | -4.03194 | 0.960684 |
| H | -0.67279 | -1.21839 | -1.82135 |
| H | -0.2335 | -0.57458 | -0.24796 |
| H | 1.545142 | -1.88616 | -2.32474 |
| H | 1.764449 | -0.40962 | -1.40388 |
| H | -0.96844 | -3.84787 | 2.530387 |
| H | -0.06093 | -2.4753 | 3.149715 |
| H | -1.42817 | -0.92322 | 1.756838 |
| H | -2.59861 | -2.05877 | 2.446869 |
| H | -2.4514 | -3.49835 | 0.469783 |
| H | -2.5386 | -0.64977 | -0.60959 |
| H | -4.68447 | -2.34241 | 0.739676 |
| H | -3.98429 | -0.84001 | 1.321686 |
| H | -4.88634 | 0.264445 | -0.85117 |
| H | -5.84913 | -1.19065 | -1.05692 |
| H | -6.92395 | -0.84098 | 1.154535 |
| H | -5.87391 | 0.538434 | 1.466528 |
| H | -6.8755 | 1.769871 | -0.42622 |
| H | -9.07145 | 2.208431 | 0.668672 |

| | | | |
|---|---|---|---|
| H | -7.79932 | 2.006596 | 1.888462 |
| H | -8.93705 | 0.685789 | 1.56519 |
| H | -9.00962 | 0.904783 | -1.46259 |
| H | -7.60656 | -0.07339 | -1.9118 |
| H | -8.73073 | -0.65643 | -0.67044 |
| H | -0.85051 | -4.81155 | -0.67922 |
| H | -1.13149 | -3.76202 | -2.07619 |
| H | 0.516112 | -4.0886 | -1.53585 |
| H | -3.77881 | -3.24947 | -1.66036 |
| H | -4.10087 | -1.63111 | -2.30967 |
| H | -2.49168 | -2.31893 | -2.4456 |
| H | 5.635435 | -2.72236 | 0.542787 |
| H | 4.15509 | -3.22291 | 1.377015 |
| H | 4.515071 | -3.84567 | -0.24898 |
| H | 4.83608 | 2.190923 | -0.88588 |
| H | 0.781576 | 3.848522 | 1.711322 |
| H | 1.227338 | 4.607152 | 0.182588 |
| H | -0.97099 | 1.968519 | 1.685777 |
| H | -0.23012 | 4.472854 | -1.72852 |
| H | -3.15026 | 1.29854 | 0.720954 |
| H | -2.3902 | 3.773404 | -2.71312 |
| H | -3.86495 | 2.197819 | -1.48885 |
| H | 1.666364 | 1.66559 | 0.949437 |
| H | 1.313028 | 2.013407 | -1.43734 |
| H | 2.545014 | 3.138268 | -1.4482 |
| H | 2.914666 | 1.575665 | -1.10622 |

Pro-D•••Phe dimer 4 ($\Delta G_{binding}$ -2.52 kJ/mol)

| | x | y | z |
|---|---|---|---|
| C | -5.24933 | -1.84143 | 1.040965 |
| C | -5.37059 | -1.13859 | -0.30496 |
| C | -4.58064 | -1.90707 | -1.36194 |
| C | -3.13616 | -2.09397 | -0.96681 |
| C | -2.83008 | -2.54674 | 0.459529 |
| C | -3.78915 | -1.90815 | 1.492326 |
| C | -2.15035 | -2.04978 | -1.88164 |
| C | -0.75595 | -2.35532 | -1.55285 |
| C | -0.36762 | -2.50365 | -0.27616 |
| C | -1.35415 | -2.24732 | 0.841825 |
| C | 1.048317 | -2.64208 | 0.219575 |
| C | 1.441482 | -1.34187 | 1.055317 |

| | | | |
|---|---|---|---|
| C | 0.321885 | -0.29199 | 0.923791 |
| C | -1.06309 | -0.80404 | 1.343355 |
| C | 2.132867 | -2.79327 | -0.857 |
| C | 2.677368 | -1.38144 | -1.05456 |
| C | 2.765521 | -0.84282 | 0.380108 |
| C | 3.086725 | 0.662724 | 0.468391 |
| C | 4.265353 | 1.055934 | -0.44356 |
| C | 5.596634 | 0.364469 | -0.14186 |
| C | 6.691116 | 0.784126 | -1.12403 |
| C | 8.093959 | 0.263493 | -0.78968 |
| C | 9.111123 | 0.796788 | -1.80019 |
| C | 8.142433 | -1.26538 | -0.74476 |
| C | 1.645148 | -1.72173 | 2.526852 |
| C | 3.351986 | 1.122846 | 1.906515 |
| C | -3.02686 | -4.07963 | 0.469706 |
| O | -4.85747 | 0.19303 | -0.17088 |
| C | -4.00701 | 2.735857 | -2.31453 |
| N | -2.39015 | 1.15156 | -1.28093 |
| C | -2.73817 | 2.600412 | -1.43507 |
| C | -2.98506 | 3.208439 | -0.05259 |
| C | -1.83514 | 3.058661 | 0.921648 |
| C | -2.04421 | 2.463918 | 2.169862 |
| C | -1.01578 | 2.396416 | 3.111302 |
| C | 0.242259 | 2.913565 | 2.807944 |
| C | 0.473017 | 3.479202 | 1.552171 |
| C | -0.55917 | 3.553508 | 0.618028 |
| O | -4.21545 | 3.870659 | -2.77198 |
| O | -4.70554 | 1.691913 | -2.44356 |
| H | -5.68473 | -2.84355 | 0.943422 |
| H | -5.84092 | -1.30495 | 1.791032 |
| H | -6.42555 | -1.08152 | -0.60084 |
| H | -4.64289 | -1.39922 | -2.33235 |
| H | -5.0601 | -2.88976 | -1.4871 |
| H | -3.71053 | -2.46765 | 2.433555 |
| H | -3.47928 | -0.88394 | 1.714379 |
| H | -2.39259 | -1.82061 | -2.91985 |
| H | -0.04307 | -2.4167 | -2.37136 |
| H | -1.1083 | -2.93231 | 1.667287 |
| H | 1.066127 | -3.50459 | 0.90086 |
| H | 0.562107 | 0.599805 | 1.511815 |
| H | 0.287513 | 0.029552 | -0.1281 |
| H | -1.1707 | -0.75724 | 2.433729 |
| H | -1.82002 | -0.11353 | 0.957534 |

| | | | |
|---|---|---|---|
| H | 2.937449 | -3.43066 | -0.47044 |
| H | 1.768171 | -3.26381 | -1.77476 |
| H | 1.977712 | -0.77132 | -1.64547 |
| H | 3.641507 | -1.37201 | -1.57337 |
| H | 3.588365 | -1.38485 | 0.874754 |
| H | 2.217078 | 1.221831 | 0.09256 |
| H | 3.996291 | 0.865577 | -1.4911 |
| H | 4.408222 | 2.14304 | -0.3614 |
| H | 5.920116 | 0.602017 | 0.881735 |
| H | 5.465504 | -0.7242 | -0.18266 |
| H | 6.418556 | 0.441929 | -2.13517 |
| H | 6.725757 | 1.882488 | -1.16922 |
| H | 8.365665 | 0.645626 | 0.205973 |
| H | 10.12792 | 0.476396 | -1.54781 |
| H | 9.098806 | 1.891814 | -1.83814 |
| H | 8.881409 | 0.422585 | -2.8062 |
| H | 9.165508 | -1.61831 | -0.57356 |
| H | 7.51178 | -1.67381 | 0.051078 |
| H | 7.797247 | -1.68523 | -1.69907 |
| H | 2.443742 | -2.46771 | 2.618264 |
| H | 1.916936 | -0.85826 | 3.141366 |
| H | 0.735019 | -2.16018 | 2.952555 |
| H | 4.102947 | 0.490278 | 2.395089 |
| H | 3.721174 | 2.155699 | 1.918913 |
| H | 2.446451 | 1.09301 | 2.517809 |
| H | -4.04408 | -4.35728 | 0.174773 |
| H | -2.32856 | -4.56047 | -0.22382 |
| H | -2.84471 | -4.4756 | 1.475979 |
| H | -5.07865 | 0.697698 | -0.98761 |
| H | -3.20564 | 4.268695 | -0.21575 |
| H | -3.88785 | 2.754363 | 0.375041 |
| H | -3.02616 | 2.062232 | 2.412205 |
| H | -0.37533 | 4.023959 | -0.34582 |
| H | -1.20048 | 1.940514 | 4.079837 |
| H | 1.455395 | 3.871825 | 1.30374 |
| H | 1.042244 | 2.869915 | 3.541324 |
| H | -1.89279 | 3.077783 | -1.93481 |
| H | -1.50447 | 1.033554 | -0.77527 |
| H | -3.14169 | 0.638545 | -0.76972 |
| H | -2.29701 | 0.688242 | -2.19021 |