Figure 1	Upper panel, right	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_1_DrBphP_CD_Pr_Pfr.csv**; this dataset was extracted from Rockwell et al., 2009 using "Starry Digitizer" followed by smoothing as mentioned in the manuscript.
Figure 1	Lower panel, right	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_1_SynCph1-N514_CD_dark_light.csv**; this dataset was extracted from the data repository accompanying the publication Rockwell et al., 2025 followed by smoothing as mentioned in the manuscript.
Figure 2	C	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_2C_IsPadC_FL_BV_dark_vs_light_Absorption_spectrum.csv**
Figure 2	D	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_2D_IsPadC_FL_PCB_dark_vs_light_Absorption_spectrum.csv**
Figure 2	E	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_2E_thermal_reversion_IsPadC_BV_IsPadC_PCB.csv**
Figure 2	F	Sample names are provided in the file header; the column separator is a comma "," The unit on the y axis is µmol product/min µmol (*Is*PadC)$_2$. Note that IsPadC forms a dimer where each protomer contributes a half of the active center which is why concentration of the dimer (IsPadC)$_2$ is used. File name: **Figure_2F_enzyme_kinetics_IsPadC_BV_IsPadC_PCB.csv**
Figure 3	A	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_3A_IsPadC_FL_BV_dark_vs_light_CD_spectrum.csv**
Figure 3	B	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_3B_IsPadC_FL_PCB_dark_vs_light_CD_spectrum.csv**
Figure 3	C	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". Note that there are values for a continuous spectrum and single transition values in the file. File name: **Figure_3C_IsPadC_BV_computational_Pr_vs_Pfr_CD_spectrum.csv**
Figure 3	D	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". Note that there are values for a continuous spectrum and single transition values in the file. File name: **Figure_3D_IsPadC_PCB_computational_Pr_vs_Pfr_CD_spectrum.csv**
Figure 4	B	The presented traces were extracted for a direct Pr and Pfr comparison from Figures 3C and 3D.
Figure 5	C	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_5C_IsPadC_BV_Pfr_computational_A_ring_rotation csv**
Figure 5	D	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_5D_IsPadC_PCB_Pfr_computational_A_ring_rotation.csv**
Figure 6	A, left	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_6A_left_IsPadC_BV_Pr_computational_bond_saturation.csv**

Figure 6	A, right	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Figure_6A_right_IsPadC_BV_Pfr_computational_bond_saturation.csv**
Figure 6	B	Chemical structures of BV as shown in the Figure. File name: **Figure_6B_BV_A_D_ring_saturation.cdxml**
Supplementary Figure 2	A	Intact MS raw data was deconvoluted using the Bruker DataAnalysis Tools followed by exporting the data in csv format; the column separator is a comma ",".File name: **IsPadC_BV.csv**
Supplementary Figure 2	B	Intact MS raw data was deconvoluted using the Bruker DataAnalysis Tools followed by exporting the data in csv format; the column separator is a comma ",".File name: **IsPadC_PCB.csv**
Supplementary Figure 3	A	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_3A_IsPadC_BV_denaturation_dark_versus_light.csv**
Supplementary Figure 3	B	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_3B_IsPadC_PCB_denaturation_dark_versus_light.csv**
Supplementary Figure 4		The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_4_icOS_data_IsPadC_Reg2_PCB.csv**
Supplementary Figure 5	A	Mapping of changes in deuterium incorporation after 10 s of *Is*PadC PSM light versus dark. The differences in deuterium incorporation are plotted on pdb 5llw and can be visualized by Pymol and the corresponding session file **IsPadC_Reg2_BV_dark_versus_PCB_dark_curated_bfactors.pse**. Within the file, the HDX data for all time points can be accessed (t1=10 s, t2=30 s, t3=3 min, t4=15 min, t5=60 min). The filtered raw data can be found in **0_240205_IsPadC_FL_Reg2_PCB_dark_filtered.yaml** and **1_240206_IsPadC_FL_Reg2_BV_dark_filtered.yaml**. The files can be opened using HXViewer, freely available from https://hx2.mr.mpg.de/. To visualize the HDX-MS data, tables containing the delta deuterium values are generated by providing a .yaml dataset containing single peptides spanning each region and setting the dark dataset as reference. The corresponding tables can be found under HDX_tables\WT_dark_vs_light. Using a script, these values are inserted into the B-factor column of a .pdb file and visualized with a custom color gradient.
Supplementary Figure 5	B	Hydrogen-deuterium exchange MS results plotted against time points for three example peptides. Find the filtered raw data in the following .yaml files which can be opened using HXViewer within the Hexicon2 package, freely available from https://hx2.mr.mpg.de/. File names: **0_240205_IsPadC_FL_Reg2_PCB_dark_filtered.yaml** and **1_240206_IsPadC_FL_Reg2_BV_dark_filtered.yaml**
Supplementary Figure 6	A	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_6A_IsPadC_Reg2_FL_BV_dark_vs_light_Absorption_spectrum.csv**
Supplementary Figure 6	B	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_6B_IsPadC_Reg2_FL_PCB_dark_vs_light_Absorption_spectrum.csv**

Supplementary Figure 6	C	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_6C_IsPadC_Reg2_FL_BV_dark_vs_light_CD_spectrum.csv**
Supplementary Figure 6	D	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_6D_IsPadC_Reg2_FL_PCB_dark_vs_light_CD_spectrum.csv**
Supplementary Figure 7	A	Please refer to the raw data uploaded for Figure 3D.
Supplementary Figure 7	B	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". Note that there are values for a continuous spectrum and single transition values in the file. File name: **Supp_Figure_7B_oat_phyA_beta_slump_geometry_computational_CD_calculations.csv**
Supplementary Figure 8	A	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_8A_CD_IsPadC_BV_Pr_computational_CD_spectra_gas_phase_vs_in_protein.csv**
Supplementary Figure 8	B	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_8B_CD_IsPadC_BV_Pfr_computational_CD_spectra_gas_phase_vs_in_protein.csv**
Supplementary Figure 8	C	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_8C_CD_IsPadC_PCB_Pr_computational_CD_spectra_gas_phase_vs_in_protein.csv**
Supplementary Figure 8	D	The axis title, units and sample name are provided in the file header; the column separator is a comma ",". File name: **Supp_Figure_8D_CD_IsPadC_PCB_Pfr_computational_CD_spectra_gas_phase_vs_in_protein.csv**