SI Information

Combining Photo-CIDNP and Long-Lived Spin States Enables High-Contrast Detection of Weak Protein-Ligand Interactions

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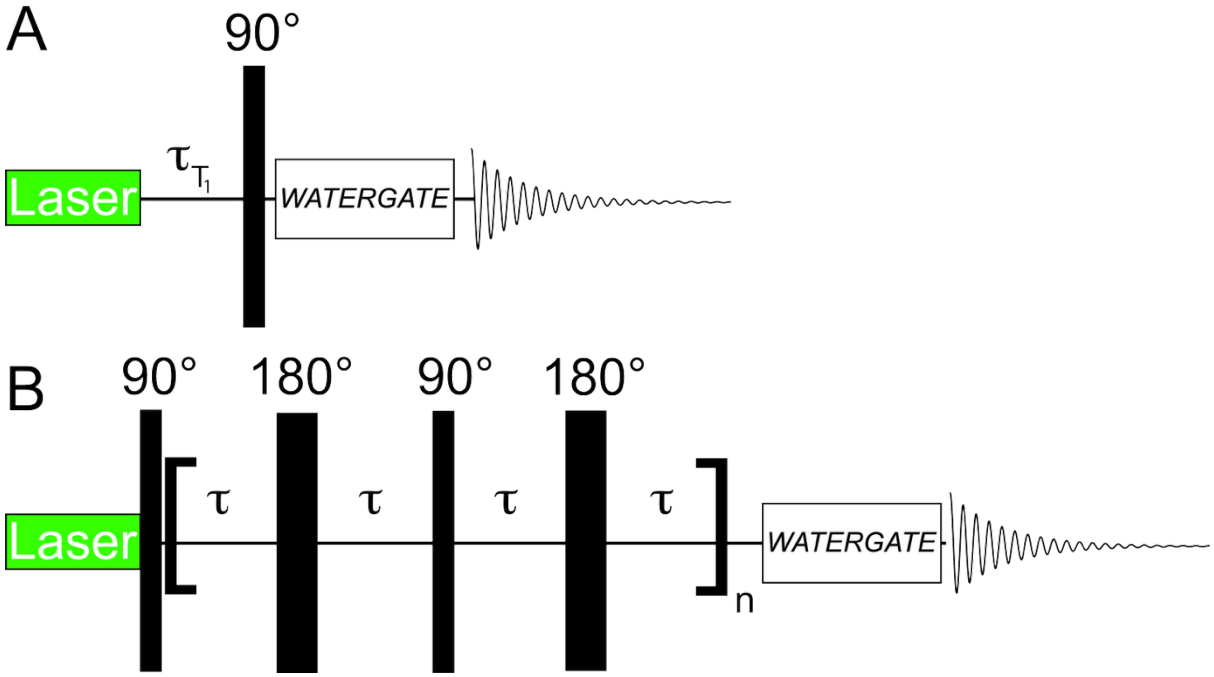

Figure S1. Pulse sequences used for CIDNP-based experiments. (A) ^{1}H CIDNP experiment employing a variable delay after laser irradiation to observe the T_1 relaxation of the photo-CIDNP signal. **(B)** CIDNP-PEARLScreen pulse sequence utilizing so-called perfect echoes enhanced by photo-CIDNP hyperpolarization and WATERGATE for solvent suppression.

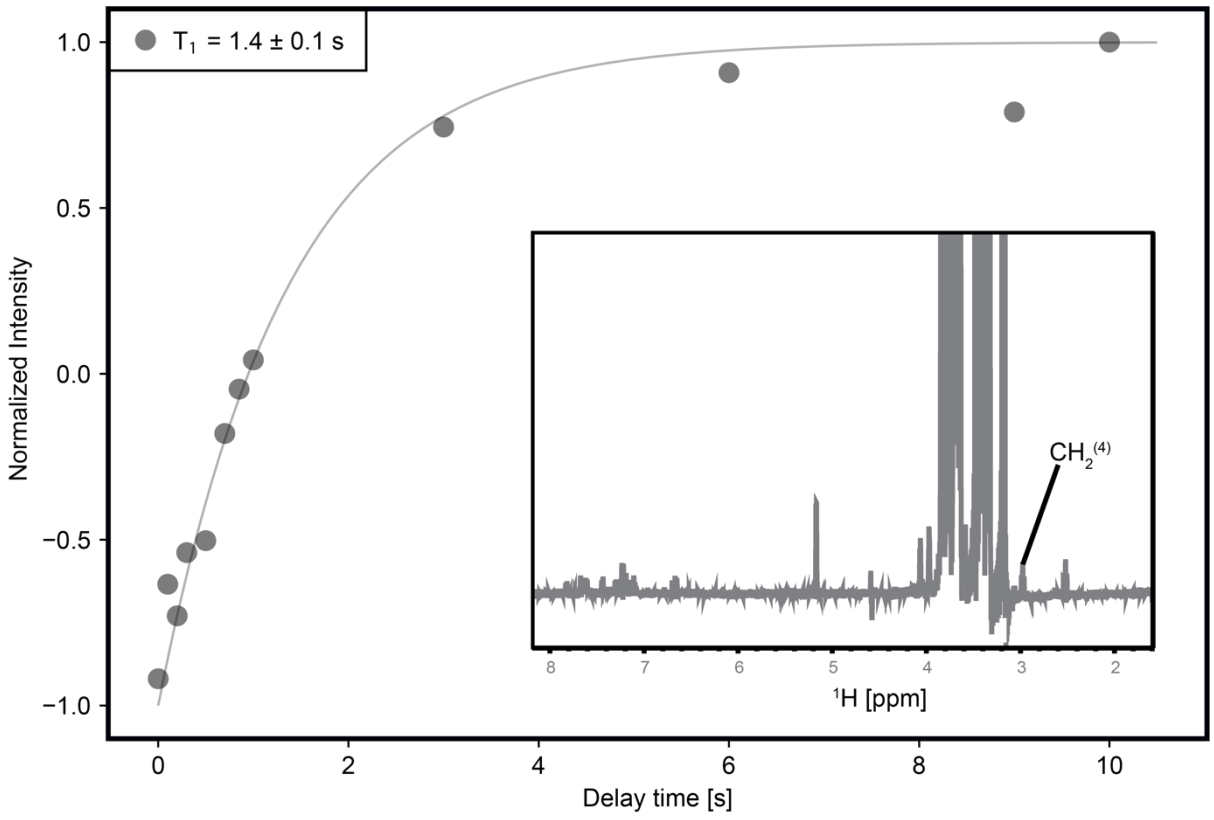

Figure S2. Conventional T_1 Inversion recovery of 50 µM IPA. The T_1 Inversion recovery of 50 µM was measured using thermal polarization. The spectrum shows that IPA is fully relaxed 10 s after inversion. The measurements were conducted with 8 scans.

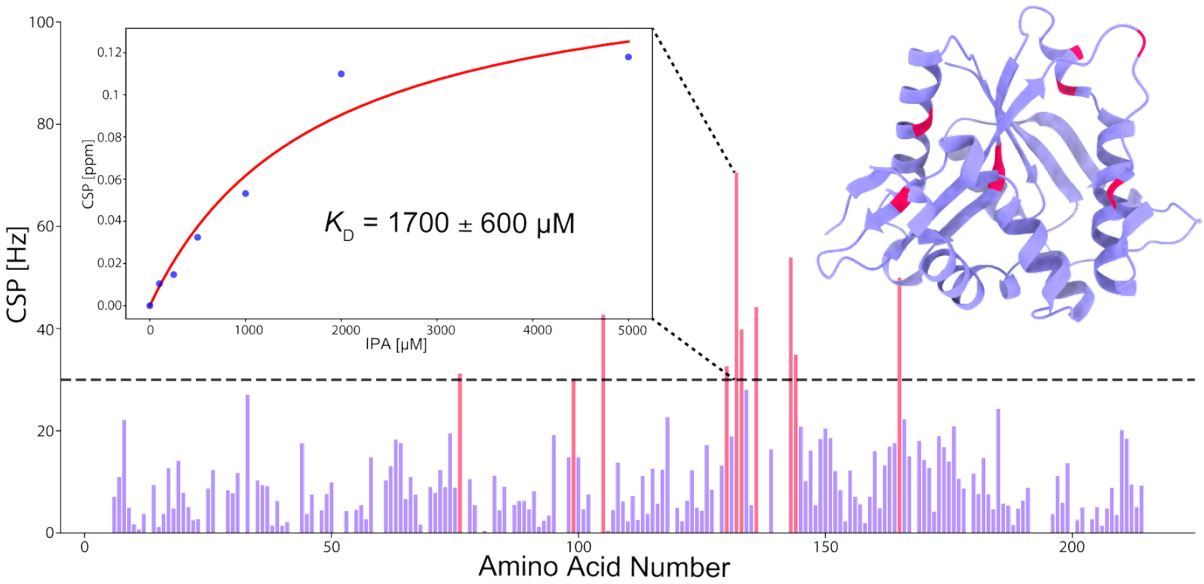

Figure S3. Chemical shift perturbation analysis of the protein AANAT upon IPA binding. ^{15}N, ^{1}H chemical shift perturbation (CSP) map of 100 μM AANAT upon binding to 5 mM IPA. Assignments were taken from BMRB entry 50445. Residues exhibiting CSPs greater than 35 Hz are highlighted in red on the PDB structure 3v8i (apo AANAT). Insert: ^{15}N, ^{1}H HSQC titration curve with corresponding K_D = 1700 μM for residue V132 which has the largest shift.