| **ID** | **Complex** | **pV5βII conc. (mM)** | **Pin1 conc. (mM)** | **Bound pV5βII,%** | **Bound Pin1, %** | **Experiments** |
| --- | --- | --- | --- | --- | --- | --- |
| 1 | [U-13C, 15N] Pin1 + pV5βII | 1.05 | 0.9 | 98 | 84 | --2D experiments: [15N, 1H] HSQC, ct [13C, 1H] HSQC, (HB)CB(CGCDCE)HE, (HB)CB(CGCD)HD  --3D experiments for backbone assignment: HNCACB, CBCA(CO)NH, HNCO, HN(CA)CO  --3D experiments for side-chain assignments: C(CO)NH, H(CCO)NH, HNHA, HNHB  --NOESY experiments: 3D 15N-edited NOESY-HSQC, 3D [F1] 13C,15N-filtered NOESY-15N-HSQC |
| 2\* | [U-13C, 15N] Pin1 + pV5βII | 1.05 | 0.9 | 98 | 84 | --1H/2D exchange  --2D ct [13C, 1H] HSQC, 2D ct 1H-13C aromatic HSQC  --3D experiments for sidechain assignments: HCCH-COSY, HCCH-TOCSY  --NOESY experiments: 3D 13C-edited NOESY-HSQC, 3D Caro-edited NOESY-HSQC, 3D [F1] 13C,15N-filtered NOESY-13C-HSQC |
| 3 | [U-13C, 15N] Pin1 + pV5βII | 1.0 | 1.3 | 76 | 99 | --2D [F1] 13C,15N-filtered NOESY  --2D [F2] 13C,15N-filtered NOESY  --2D [F1, F2] 13C,15N-filtered NOESY  --2D [F1, F2] 13C,15N-filtered TOCSY |
| 4 | [U-13C, 15N] PPIase + pHMβII | 0.8 | 5.5 | 97 | 14 | --3D [F1] 13C, 15N-filtered NOESY-15N-HSQC  --3D [F1] 13C, 15N-filtered NOESY-13C-HSQC |
| 5 | [U-13C, 15N] PPIase + pHMβII | 0.5 | 1.8 | 25 | 91 | --2D [F1] 13C,15N-filtered NOESY  --2D [F2] 13C,15N-filtered NOESY  --2D [F1, F2] 13C,15N-filtered NOESY  --2D [F1, F2] 13C,15N-filtered TOCSY |
| 6 | PPIase + [U-13C,15N Phe] pHMβII  *peptide ID #15 (Supplementary File 1)* | 0.5 | 2.5 | 19 | 93 | --3D [F1] 13C,15N-filtered NOESY-15N-HSQC  --3D [F1] 13C,15N-filtered NOESY-13Caro-HSQC  --3D [F1] 13C,15N-filtered NOESY-13Cali-HSQC |
| 7 | Pin1 + [U-13C,15N Pro, Ile, Val] pTMβII  *peptide ID #14 (Supplementary File 1)* | 1.0 | 1.5 | 66 | 98 | --3D [F1] 13C,15N-filtered NOESY-15N-HSQC  --3D [F1] 13C,15N-filtered NOESY-13C-HSQC |
| 8 | [U-13C, 15N] Pin1 + Ext-pV5βII  *peptide ID #13 (Supplementary File 1)* | 1.3 | 1.0 | >95% |  | --3D [F1] 13C,15N-filtered NOESY-15N-HSQC  --3D [F1] 13C,15N-filtered NOESY-13C-HSQC |
| 9 | [U-13C, 15N] Pin1 + Ext-pV5βII  *peptide ID #13 (Supplementary File 1)* | 0.8 | 1.3 |  | >95% | --2D [F1] 13C,15N-filtered NOESY  --2D [F2] 13C,15N-filtered NOESY  --2D [F1, F2] 13C,15N-filtered NOESY  --2D [F1, F2] 13C,15N-filtered TOCSY |