

Supporting Information Table S1

Parameters for simulation and preparation of ^{13}C - and ^{15}N -resolved NOESY spectra obtained from the experimental data

| NMR Spectra | ^{13}C -resolved NOESY | ^{15}N -resolved NOESY |
|--|---|---|
| Number of transients | 8 | 8 |
| Inter-scan delay (D1), sec | 1.0 | 1.0 |
| Time domain sizes, complex points | | |
| ^{13}C , indirect | 64 | - |
| ^{15}N , indirect | - | 64 |
| ^1H , indirect (points studied) | 28, 37, 52, 74, 101, 135, 175, 221, 273, 331, 395, 466, 542, 625, 714, 809, 910, 1017, 1130, 1250 | 28, 37, 52, 74, 101, 135, 175, 221, 273, 331, 395, 466, 542, 625, 714, 809, 910, 1017, 1130, 1250 |
| ^1H , direct detection | 1024 | 1024 |
| Spectral Width, Hz | | |
| ^{13}C , indirect | 10752.6881 | - |
| ^{15}N , indirect | - | 2000.0000 |
| ^1H , indirect | 6596.3058 | 7194.2446 |
| ^1H , direct detection | 6602.1126 | 7211.5384 |
| Spectrometer Carrier Position, MHz | | |
| ^{13}C , indirect | 150.8458 | - |
| ^{15}N , indirect | - | 60.7924 |
| ^1H , indirect | 599.8828 | 599.8828 |
| ^1H , direct detection | 599.8828 | 599.8828 |
| Number of FIDs | 4320 | 4320 |
| NUS sampling bias, T_2 , sec | | |
| ^{13}C indirect | 0.1 | - |
| ^{15}N indirect | - | 0.1 |
| ^1H , direct detection | 1.0 | 1.0 |
| Calculated T_2 (^1H direct), sec | | |
| PDB ID (Mw), (Da) | | |
| 2BBX (5440) | 0.061275 | 0.061275 |
| 1D5G (10008) | 0.033307 | 0.033307 |
| 1XKE (15117) | 0.022050 | 0.022050 |
| 1JBj (20602) | 0.016180 | 0.016180 |
| 1TTE (24154) | 0.013800 | 0.013800 |
| 2JT2 (31267) | 0.010661 | 0.010661 |