Solid state NMR structural analysis of designer self-assembling peptides MAX8 and SAF

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Background - MAX8 Application

MAX8 (a designer peptide) has demonstrated utility in both drug delivery and tissue engineering.1

Background - SAF Application

- Two designer peptides which fold and form extended fibers when mixed
- SAF hydrogels were tested as a substrate for cell growth
- Cells seeded on SAF gels could be induced to differentiate into neural cells
- Cell morphology is similar for both SAF (a) and Max8 (b) substrates2

Results and Discussion

- Cyclic crosspeaks in the DARR spectra indicate spatial proximity between V3 and K17 labeled residues

Molecular Modeling

- Obtain predictive distance measurements between atomic sites within a molecule
- Use these distances to select isotopically labeled sites
- Use NMR to obtain experimentally derived constraints
- Use those constraints to further optimize the molecular models3

Summary and Future Work

- Continued studies including CHIC and rotational echo double resonance (REDOR) NMR are being conducted to fully constrain the molecular model of a MAX8 nanofiber
- Although most work to date has been done on MAX8, SAF has been synthesized and preliminary NMR experiments will be conducted in the future to determine SAF’s structural order and characterization

RESEARCH GOAL

Provide a molecular structural basis for the design of peptides that undergo controlled self-assembly into nanofiber networks

Nuclear Magnetic Resonance (NMR) Techniques

A) Magnetic nuclear spins align with a static external magnetic field, B0
B) Radio frequency pulses, B1, are applied to perturb the bulk magnetization, M, from equilibrium
C) M precesses about the external magnetic field inducing a current in the coil

- The free induction decay (FID) is the observed NMR signal generated by the component of magnetization precessing about the external magnetic field on the xy plane
- The FID is Fourier transformed to obtain the frequency domain NMR spectrum
- Cross polarization magic angle spinning (CPMAS) produces a 1D spectrum displaying chemical shifts for distinct carbon labeled sites5

References


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