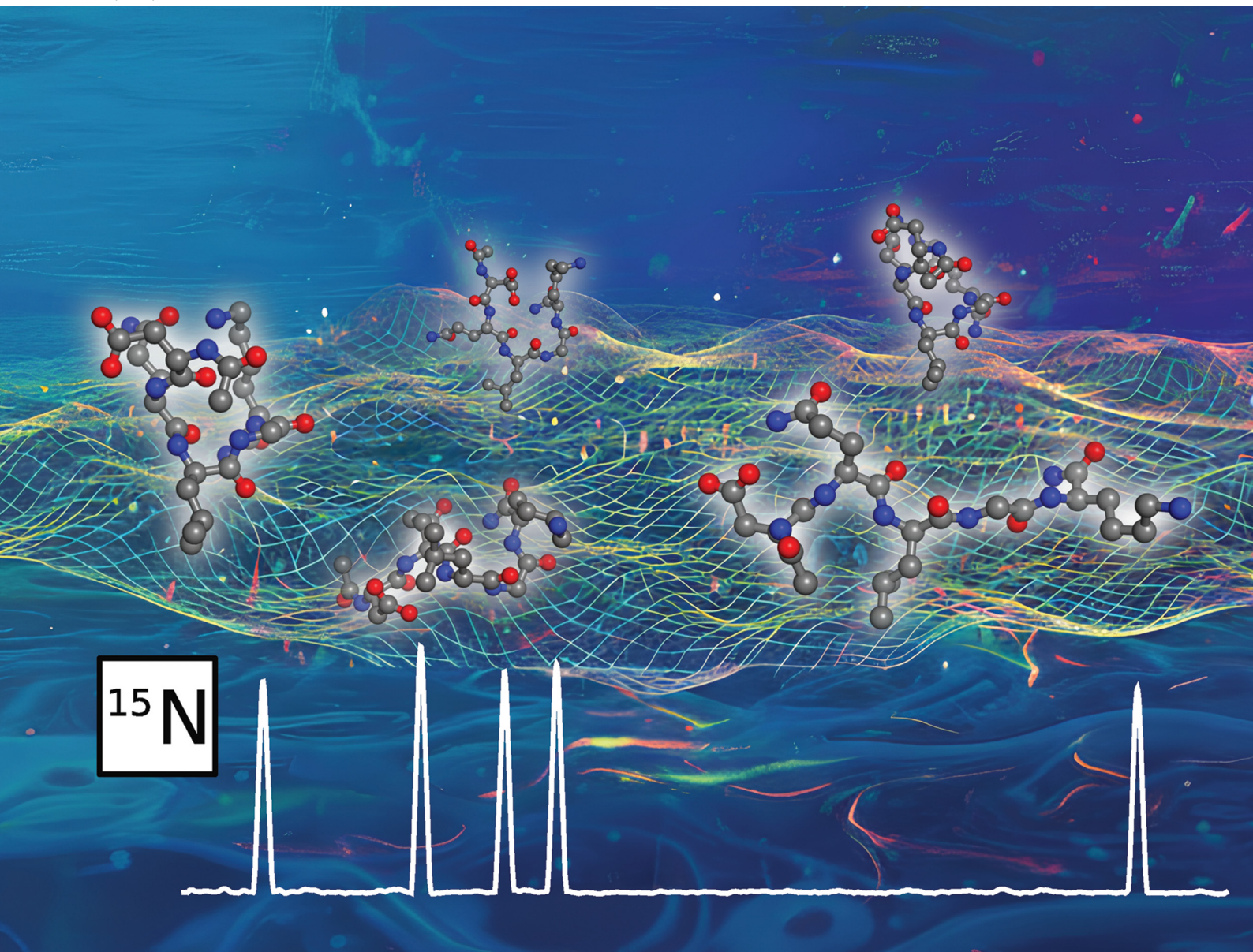


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COMMUNICATION

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A computational protocol for ^{15}N NMR parameter prediction
in aqueous peptide ensembles using optimized DFT methods