

COMBINING NMR SPECTRAL INFORMATION WITH ASSOCIATED STRUCTURAL FEATURES TO FORM COMPUTATIONALLY NONINTENSIVE, RUGGED, AND OBJECTIVE MODELS OF BIOLOGICAL ACTIVITY

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1 INTRODUCTION

Nuclear Magnetic Resonance Spectral Information Content
Biological Effect Modeling Based on NMR Spectra and Associated Structural Features
Previous NMR Comparative Spectral Analysis Modeling Approaches
Advantages of Modeling with Simulated Rather Than Experimental NMR Spectra
Adding Structurally Assigned NMR Chemical Shift Information to 2D Templates
Inspiration Based on Extension of Multidimensional NMR Techniques

2 METHODS AND EXAMPLES

Predicted NMR Spectra
Pattern Recognition Methods and Model Development
Linear and Nonlinear Aspects
Model Validation: LOO and LNO
Procedure for Integrating NMR Spectral Information with Molecular Structure