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STUDY ON MOLECULAR MECHANISM OF VASCULAR SMOOTH MUSCLE RELAXATION BY INCORPORATING THE WENXIANG DIAGRAM INTO THE NMR

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Physiologic relaxation of vascular smooth muscle is induced by the cyclic guanosine monophosphate (cGMP)-dependent protein kinase Iα enzyme (cGKIα), which activates myosin phosphatase (MLCP). This activation process is thought to occur through the interaction involving both N- and C-terminal leucine zipper coiled-coil (LZCC) domains of the kinase enzyme (cGKIα) with the myosin binding subunit (MBS) of MLCP. In this study, we summarize how to define the LZCC domains in both N-terminal cGKI$\alpha^{1-59}$and C-terminal MBS proteins using predictive and experimental methods, how to make a rapid and accurate structure determination of a cGKIα^{1-59} molecule using NMR's residual dipolar coupling (RDC) measurements, and how to indentify the existence of a weak protein interaction between N-terminal LZCC domain (cGKI 1-59) and a LZCC domain (MBSCT42) within the C-terminal MBS. In addition, the location and orientation of the residues in LZCC proteins can be readily visualized using a novel diagram, the so-called "wenxiang diagram", which is more advantageous than traditional helical wheel diagrams in analyzing LZCC protein structures and their action mechanisms. Using the composed Wenxiang diagrams, we have characterized the interaction between cGKIα1-59 and another LZCC molecule (MBSCT42), and deduced that the most affected residues of these two LZCC molecules might be at the positions d, a, e and g. It is intriguing to see that the successful incorporation of Wenxiang diagrams and NMR spectroscopy in the LZCC structural and functional studies may provide some insights into molecular mechanism of vascular smooth muscle relaxation and contraction.

Note:

BIOGRAPHY

Guo-Ping Zhou is a current Professor of Gordon Life Science Institute, USA. He is also an Adjunct Professor of several academics in both USA and China. He received his PhD in Biophysics from University of California at Davis, and completed his postdoctoral training at Stanford University and Harvard University, respectively. He has determined the 3D NMR structures of some important biomolecules, and successfully introduced the novel diagram approach to elucidate the mechanisms of the protein-biomolecule interactions, and protein misfolding diseases observed by NMR spectroscopy. His current research is focused on the molecular mechanism of Neural Cell Adhesion Molecule polysialylation using NMR and biophysical approaches. In addition, he has also edited some special issues on the fields of structural biology and medicinal chemistry for several influential scientific journals as an Editorial-Board Member and Guest Editor.

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