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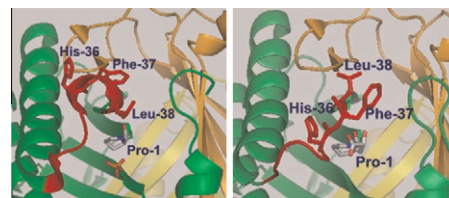
## Regular Articles

### Crystal structures of native and inactivated *cis*-3-chloroacrylic acid dehalogenase: Implications for the catalytic and inactivation mechanisms

pp 1–9

Youzhong Guo, Hector Serrano, William H. Johnson Jr., Stephen Ernst, Marvin L. Hackert\* and Christian P. Whitman\*

The proposed open (left panel) and closed (right panel) states of *cis*-CaaD.

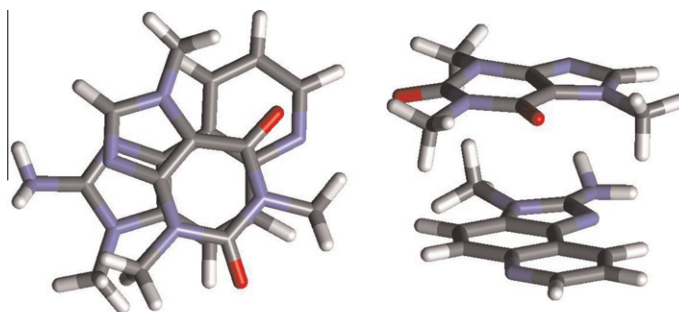


### Caffeine, pentoxifylline and theophylline form stacking complexes with IQ-type heterocyclic aromatic amines

pp 10–17

Anna Woziwodzka, Anna Gwizdek-Wiśniewska and Jacek Piosik\*

Visualization of the most probable lowest energy stacking complex between Caffeine and 2-amino-3-methylimidazo[4,5-f]quinoline (IQ) from the top view (left panel) and from the side view (right panel), obtained by molecular modeling.



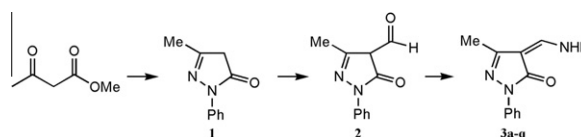
Visualization of spatial structure of Caffeine – IQ hetero-complex

### Synthesis, antitumor activity and QSAR studies of some 4-aminomethylidene derivatives of edaravone

pp 18–27

Violeta Marković, Slavica Erić, Zorica D. Juranić, Tatjana Stanojković, Ljubinka Joksović, Branislav Ranković, Marijana Kosanić and Milan D. Joksović\*

Aminomethylidene derivatives obtained from 4-formylederavone and primary amines were synthesized and tested for their antitumor activity. The compound containing 5-phenylpyrazole moiety was found to be the most active against human breast cancer MDA-MB-361 and MDA-MB-453 cell lines.

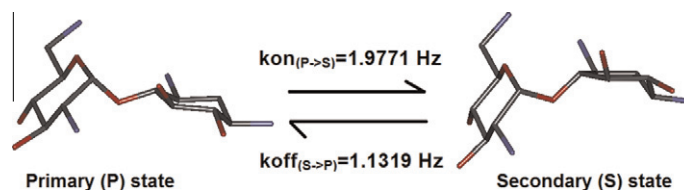


## NMR and amber analysis of the neamine pharmacophore for the design of novel aminoglycoside antibiotics

pp 28–41

Cenk A. Andac,\* Thomas C. Stringfellow, Ulfert Hornemann and Ningur Noyanalpan

Slow conformational exchange between the primary (P) and secondary (S) states of the neamine pharmacophore. Hydrogens are not shown for simplicity.

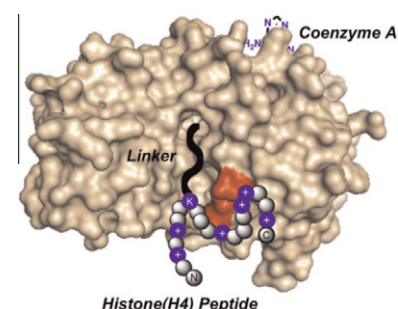


## Probing the reaction coordinate of the p300/CBP histone acetyltransferase with bisubstrate analogs

pp 42–47

Kannan R. Karukurichi and Philip A. Cole\*

We describe here the synthesis and evaluation of bisubstrate analogs as mechanistic probes for p300/CBP histone acetyltransferase. These analogs vary in the linker that conjoins the peptide backbone and coenzyme A.

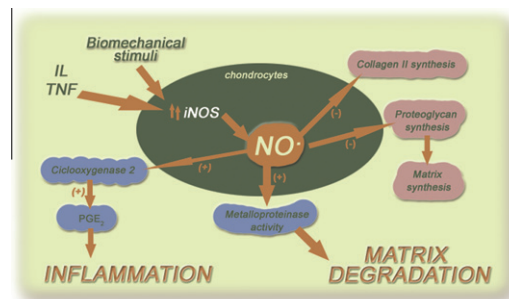


## Heteroarylimino-4-thiazolidinones as inhibitors of cartilage degradation

pp 48–52

Anna Maria Panico,\* Paola Vicini,\* Athina Geronikaki, Matteo Incerti, Venera Cardile, Lucia Crascì, Rossella Messina and Simone Ronsisvalle

Interleukin-1  $\beta$  (IL-1 $\beta$ ), a cytokine produced by chondrocytes induces high levels of prostaglandins E<sub>2</sub> (PGE<sub>2</sub>) and nitric oxide (NO), that has been shown to inhibit collagen and proteoglycans synthesis, increase susceptibility to injury by other oxidant (e.g. H<sub>2</sub>O<sub>2</sub>).

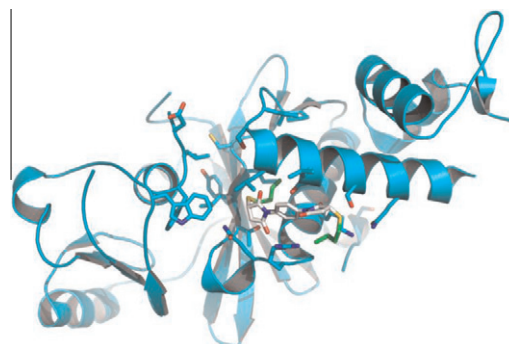


## Small molecule inhibitors of histone acetyltransferase Tip60

pp 53–58

Jiang Wu, Juxian Wang, Minyong Li, Yutao Yang, Binghe Wang and Y. George Zheng\*

Several small molecules were identified as micromolar inhibitors of histone acetyltransferase Tip60. Docking and kinetic analyses suggest that they bind to the active site of the enzyme.



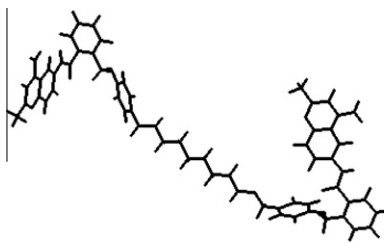
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**High resolution NMR conformational studies of new bivalent NOP receptor antagonists in model membrane systems**

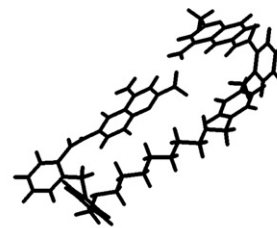
pp 59–66

Anna Borioni,\* Giuditta Bastanzio, Maurizio Delfini,  
Carlo Mustazza, Fabio Sciubba,  
Massimo Tatti and Maria Rosaria Del Giudice

A proton NMR investigation on the behaviour of a bivalent quinolinic ligand of the NOP receptor in the presence of cell membrane models showed a conformational change of the molecule caused by the interaction.



Free ligand



Ligand interacting with liposomes

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\* Corresponding author