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## Documents

Aparicio, F., González-Rivas, N., Ireta, J., Rojo, A., Escobar, L.I., Cedillo, A., Galván, M.

**Soft-Soft interactions in the protein-protein recognition process: The K<sup>+</sup> channel-charybdotoxin case**

(2012) *International Journal of Quantum Chemistry*, 112 (22), pp. 3618-3623.

**Document Type:** Article

**Source:** Scopus

Ireta, J.

**Microsolvation effects on the stability of polyalanine in extended and polyproline II conformation**

(2012) *International Journal of Quantum Chemistry*, 112 (22), pp. 3612-3617. Cited 1 time.

**Document Type:** Article

**Source:** Scopus

Ismer, L., Ireta, J., Neugebauer, J.

**A density functional theory based estimation of the anharmonic contributions to the free energy of a polypeptide helix**

(2011) *Journal of Chemical Physics*, 135 (8), art. no. 084122, .

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Ireta, J.

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(2011) *Journal of Chemical Theory and Computation*, 7 (8), pp. 2630-2637. Cited 6 times.

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Tkatchenko, A., Rossi, M., Blum, V., Ireta, J., Scheffler, M.

**Unraveling the stability of polypeptide helices: Critical role of van der Waals interactions**

(2011) *Physical Review Letters*, 106 (11), art. no. 118102, . Cited 12 times.

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(2008) *Journal of Physical Chemistry B*, 112 (13), pp. 4109-4112. Cited 5 times.

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De Gortari, I., Galván, M., Ireta, J., Segall, M., Pickard, C.J., Payne, M.

**Theoretical investigations of oxygen-17 NMR chemical shifts to discriminate among helical forms**

(2007) *Journal of Physical Chemistry A*, 111 (50), pp. 13099-13105. Cited 3 times.

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**Structural transitions in the polyalanine  $\alpha$ -helix under uniaxial strain**

(2005) *Journal of the American Chemical Society*, 127 (49), pp. 17241-17244. Cited 15 times.

**Document Type:** Article

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Ismer, L., Ireta, J., Boeck, S., Neugebauer, J.

**Phonon spectra and thermodynamic properties of the infinite polyalanine  $\alpha$  helix: A density-functional-theory-based harmonic vibrational analysis**

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Ireta, J., Aparicio, F., Viniegra, M., Galván, M.

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**Local reactivity of charybdotoxin, a K<sup>+</sup> channel blocker**

(1998) *Journal of the American Chemical Society*, 120 (38), pp. 9771-9778. Cited 16 times.

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