

HOT PAPERS IN VCD

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Empowering Characterization

Metamaterial using nanorod plasmonic resonators for enhanced vibrational circular dichroism sensor and applications of the same

National University of Singapore

July 2024

application no: <https://patents.justia.com/patent/20250020589>

Vibrational circular dichroism of adenosine crystals

Krupova, Monika; Leszczenko, Patrycja; Sierka, Ewa; Hamplova, Sara Emma; Klepetarova, Blanka; Pelc, Radek; Andrushchenko, Valery

Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2024), 319, 124381

doi: <https://doi.org/10.1016/j.saa.2024.124381>

Solid-state vibrational circular dichroism for pharmaceutical applications: Polymorphs and cocrystal of sofosbuvir

Sklenar, Adam; Ruzickova, Lucie; Schrenkova, Vera; Bednarova, Lucie; Pazderkova, Marketa; Chatziadi, Argyro; Zmeskalova Skorepova, Eliska; Soos, Miroslav; Kaminsky, Jakub

Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2024), 318, 124478

doi: <https://doi.org/10.1016/j.saa.2024.124478>

Increased accuracy of vibrational circular dichroism calculations for isotopically labeled helical peptides

Cheeseman, James R.; Frisch, Michael J.; Keiderling, Timothy A.

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doi: <https://doi.org/10.1016/j.saa.2024.124097>

Probing solution conformations of L-DOPA: Integration of experiment and simulation via vibrational optical activity

Spasovova, Monika; Kapitan, Josef; Jilek, Stepan; Siddhique Para Kkadan, Mohammed; Klener, Jakub; Scott Lynn, Nicolas Jr.; Kopecky, Vladimir Jr.; Baumruk, Vladimir; Profant, Vaclav

Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2024), 313, 124119

doi: <https://doi.org/10.1016/j.saa.2024.124119>

Chiroptical Properties of a Cryptophane Soluble at Neutral pH

Brotin, Thierry; Daugey, Nicolas; Jean, Marion; Vanthuyne, Nicolas; Buffeteau, Thierry

European Journal of Organic Chemistry (2024), 27(18), e202400136

doi: <https://doi.org/10.1002/ejoc.202400136>

Vibrational circular dichroism spectroscopy with a classical polarizable force field: alanine in the gas and condensed phases

Bowles, Jessica; Jahnigen, Sascha; Agostini, Federica; Vuilleumier, Rodolphe; Zehnacker, Anne; Calvo, Florent; Clavaguera, Carine

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Rode, Joanna E; Lyczko, Krzysztof; Kaczorek, Dorota; Kawecki, Robert; Dobrowolski, Jan Cz.

Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2024), 310, 123939

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Rode, Joanna E; Wasilczenko, Justyna; Gorecki, Marcin

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Multidimensional vibrational circular dichroism for insect wings: Comparison of species

Sato, Hisako ; Koshoubu, Jun; Inoue, Sayako; Kawamura, Izuru; Yamagishi, Akihiko
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Mid-IR and CH stretching vibrational circular dichroism spectroscopy to distinguish various sources of chirality: The case of quinophaneoxazoline based ruthenium(II) complexes

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Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2024), 307, 123634
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O'Neill, Nichole ; Lima, Thamires A. ; Furlan Ferreira, Fabio; Alvarez, Nicolas J.; Schweitzer-Stenner, Reinhard
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Exploring the Influence of the Phosphorus-Heteroatom Substitution in Nicotine on Its Electronic and Vibrational Spectroscopic Properties

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Pushing measurements and interpretation of VCD spectra in the IR, NIR and visible ranges to the detectability and computational complexity limits

Fuse, Marco; Mazzeo, Giuseppe; Bloino, Julien; Longhi, Giovanna; Abbate, Sergio
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Pitfalls in the Optimization of Conformer Populations to Maximize the Similarity between Predicted and Experimental Chiroptical Spectra

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"Nature or nurture" - How environmental factors influence the conformational memory of amyloid fibrils

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Stereo-Differentiating Asymmetric Rh(I)-Catalyzed Pauson-Khand Reaction: A DFT-Informed Approach to Thapsigargin Stereoisomers

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McGown, Andrew; Renault, Nicolas; Barczyk, Amelie; Nafie, Jordan; Barluzzi, Luciano; Guest, Daniel; Tizzard, Graham J.; Coles, Simon J.; Leach, David; von Emlöh, Daniel; et al
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Ziadi, Kamal

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VCD Analysis of Axial Chirality in Synthetic Stereoisomeric Biaryl-Type bis-Isochroman Heterodimers with Isolated Blocks of Central and Axial Chirality

Czenke, Zoltan; Mandi, Attila; Kiraly, Sandor Balazs; Kiss-Szikszai, Attila ; Konya-Abraham, Anita; Kurucz-Szabados, Anna; Cserepes, Krisztian; Benyei, Attila; Zhang, Changsheng ; Kicsak, Mate; et al

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Unveiling chiral optical constants of α -pinene and propylene oxide through ATR and VCD spectroscopy in the mid-infrared range

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