PAPERS IN VCD

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1. **Metamaterial using nanorod plasmonic resonators for enhanced vibrational circular dichroism sensor and applications of the same**
   National University of Singapore. (2025). (U.S. Patent Application No. US20250020589A1). United States Patent and Trademark Office

2. **Exploring naproxen cocrystals through solid-state vibrational circular dichroism**
   Sklenář, A., Zehnacker-Rentien, A., Kaminsky, J., Rohlicek, J., & Bour, P. (2025). *Chirality, 37*(3), e70027. https://doi.org/10.1002/chir.70027

3. **Analytic computation of vibrational circular dichroism spectra using second-order Møller–Plesset perturbation theory**
   Shumberger, B. M., Pearce, K. C., & Crawford, T. D. (2025). *Journal of Chemical Theory and Computation, 21*(4), 1234–1245. https://doi.org/10.1021/acs.jctc.5c00047

4. **Solvent effects in furofuran lignans revealed by vibrational CD spectroscopy**
   Lee, E. Y., Sousa, V. M. S., Mestriner, E. R., Bernardino, K., Nascimento, I. R., & Batista, J. M. Jr. (2025). *Physical Chemistry Chemical Physics, 27*(7), 3908–3915. https://doi.org/10.1039/D4CP04673K

5. **Cycloartane-type triterpenoids from *Combretum quadrangulare* Kurz with PCSK9 secretion inhibitory activities**
   An, C.-Y., Pel, P., Bae, M., Park, C.-W., Kwon, H., Lee, H. S., Dung, L. V., Kim, C., Lee, D., Choi, Y. H., et al. (2025). *Phytochemistry, 230*, 114330. https://doi.org/10.1016/j.phytochem.2024.114330

6. **Spectroscopic response of chiral proteophenes binding to two chiral insulin amyloids**
   Watanabe, T., Swaminathan, P., Bjork, L., Nakanishi, A., Sato, H., Zako, T., Nilsson, K. P. R., & Lindgren, M. (2025). *ChemPhotoChem, 9*(1), e202400225. https://doi.org/10.1002/cptc.202400225

7. **Induced axial chirality in near-infrared-absorbing ball-shaped ruthenium complexes**
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8. **Vibrational circular dichroism of adenosine crystals**
   Krupova, M., Leszczenko, P., Sierka, E., Hamplova, S. E., Klepetarova, B., Pelc, R., & Andrushchenko, V. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 319*, 124381. https://doi.org/10.1016/j.saa.2024.124381

9. **Solid-state vibrational circular dichroism for pharmaceutical applications: Polymorphs and cocrystal of sofosbuvir**
   Sklenar, A., Ruzickova, L., Schrenkova, V., Bednarova, L., Pazderkova, M., Chatziadi, A., Zmeskalova Skorepova, E., Soos, M., & Kaminsky, J. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 318*, 124478. https://doi.org/10.1016/j.saa.2024.124478

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    Cheeseman, J. R., Frisch, M. J., & Keiderling, T. A. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 313*, 124097. https://doi.org/10.1016/j.saa.2024.124097

11. **Probing solution conformations of L-DOPA: Integration of experiment and simulation via vibrational optical activity**
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13. **Vibrational circular dichroism spectroscopy with a classical polarizable force field: Alanine in the gas and condensed phases**
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14. **VCD spectra of chiral naphthalene-1-carboxamides in the solid-state**
    Rode, J. E., Łyczko, K., Kaczorek, D., Kawęcki, R., & Dobrowolski, J. Cz. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 310*, 123939. https://doi.org/10.1016/j.saa.2024.123939

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17. **Mid-IR and CH stretching vibrational circular dichroism spectroscopy to distinguish various sources of chirality: The case of quinophaneoxazoline based ruthenium(II) complexes**
Fusè, M., Mazzeo, G., Abbate, S., Ruzziconi, R., Bloino, J., & Longhi, G. (2024). *Chirality, 36*(3), e23649. https://doi.org/10.1002/chir.23649

18. **Near-field coupling induced less chiral responses in chiral metamaterials for surface-enhanced vibrational circular dichroism.**
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19. **Conformational distributions of tetrahydro-2-furoic acid in water at different pH values by their IR and vibrational circular dichroism spectra.**
Yang, Y., Alshalalfeh, M., & Xu, Y. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 307*, 123634. https://doi.org/10.1016/j.saa.2023.123634

20. **Determining the nanostructure and main axis of gly-his-gly fibrils using the amide I′ bands in FTIR, VCD, and Raman spectra.**
O'Neill, N., Lima, T. A., Ferreira, F. F., Alvarez, N. J., & Schweitzer-Stenner, R. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 306*, 123584. https://doi.org/10.1016/j.saa.2023.123584

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23. **Pushing measurements and interpretation of VCD spectra in the IR, NIR and visible ranges to the detectability and computational complexity limits.**
Fusè, M., Mazzeo, G., Bloino, J., Longhi, G., & Abbate, S. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 305*, 123496. https://doi.org/10.1016/j.saa.2023.123496

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Dobsikova, K., Tausova, T., Fagan, P., Paskanova, N., Kuchar, M., Cejka, J., & Setnicka, V. (2024). *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 305*, 123486. https://doi.org/10.1016/j.saa.2023.123486

25. **Pitfalls in the optimization of conformer populations to maximize the similarity between predicted and experimental chiroptical spectra.**
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26. **"Nature or nurture" – How environmental factors influence the conformational memory of amyloid fibrils.**
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33. **Structurally diverse duclauxins from a coral-derived *Talaromyces* sp. and insight into determining the configuration at C-1 of heptacyclic duclauxins by ^1H NMR.**
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34. **Use of deperturbed and generalized second-order vibrational perturbation theories to study vibrational spectra intensity and the role of cubic force constant and total anharmonic matrix contributions to anharmonicity: α-thujone and S-camphor.**
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35. **VCD analysis of axial chirality in synthetic stereoisomeric biaryl-type bis-isochroman heterodimers with isolated blocks of central and axial chirality.**
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