

CURRICULUM VITAE

DATE: May, 2014

NAME: Laurence A. Nafie

ACADEMIC POSITION: Emeritus Distinguished Professor

ADDRESS: Department of Chemistry
1-014 Center for Science and Technology
Syracuse University
Syracuse, New York 13244-4100

WEB ADDRESS: <http://chemistry.syr.edu/faculty/nafie.html>

EDUCATION:

Ph.D. Chemical Physics, University of Oregon (1973)
M.S. Physics, University of Oregon (1969)
B. Chem. Chemistry, University of Minnesota (1967)

MEMBERSHIP IN PROFESSIONAL AND LEARNED SOCIETIES:

American Association for the Advancement of Science
American Chemical Society
American Physical Society
Biophysical Society
Coblentz Society
Society for Applied Spectroscopy

ACADEMIC POSITIONS:

2010, June Guest Professor, Chinese Academy of Sciences, Dalian, China
2010- present Emeritus Distinguished Professor of Chemistry
2000-2010 Distinguished Professor of Chemistry
1993-1994 Associate Dean for Academic and Fiscal Planning, College of Arts and
 Sciences, Syracuse University
1984-2000 Chair, Department of Chemistry, Syracuse University
1982-1984 Vice Chair, Department of Chemistry, Syracuse University
1982-2000 Professor of Chemistry, Syracuse University
1979-1982 Associate Professor of Chemistry, Syracuse University
1975-1979 Assistant Professor of Chemistry, Syracuse University
1973-1975 Postdoctoral Associate, University of Southern California

OTHER EMPLOYMENT:

1969 - 1971 Science and Engineering Assistant, Nuclear Effects Laboratory,
 Edgewood Arsenal, Maryland (Member, United States Army)
1968 Summer Research Assistant, Lawrence Radiation Laboratory, Livermore, California

AWARDS, HONORS, and PROFESSIONAL OFFICES:

Gold Medal Award of the New York Section of the Society for Applied Spectroscopy, 2014
Pittsburgh Spectroscopy Award of the Spectroscopic Society of Pittsburgh, 2013
Honorary Member of the Coblenz Society, 2012
Editor-in-Chief, *Journal of Raman Spectroscopy*, 2010 to present
Fellow of the Society for Applied Spectroscopy, 2008
Distinguished Service Award of the Society of Applied Spectroscopy, 2007
Editorial Board, *Chirality* 2007 to present
Co-Chair, *Third International Conference on Advanced Vibrational Spectroscopy (ICAVS-3)*, 2005.
Editorial Board, *Applied Spectroscopy*, 2004 to present
President, Society of Applied Spectroscopy, 2003
Meggers Award for the best paper published in *Applied Spectroscopy* in 2000, October 2001
Bomem Michelson Award for Outstanding Achievements in Molecular Spectroscopy, March 2001
Parliamentarian and Executive Committee Member, Society of Applied Spectroscopy, 1999-2001
Editorial Board and Reviewing Editor, *Biopolymers*, 1999 to 2010
Editorial Board Member, *Enantiomer*, 1998 to 2002
Chancellor's Citation for Exceptional Academic Achievement, Syracuse University, February 1998
Co-Founder and Research Consultant, BioTools, Inc., 1996-present
Founding Editor, *Biospectroscopy*, A journal published by John Wiley and Sons, 1994 to 2003
Associate Dean for Academic and Fiscal Planning, College of Arts and Sciences, Syr., N.Y., 1994-1995
President, Coblenz Society, 1993-1995
Dean's Alumni Achievement Award, College of Arts and Sciences, University of Oregon, May 1991.
Advisory Committee, National Center for Biomedical Infrared Spectroscopy, Battelle Columbus Laboratories 1983-1989
Coblenz Society Governing Board Member, 1984 - 1988
Coblenz Award for Outstanding Contributions to Molecular Spectroscopy for a scientist under the age of 35 years, 1981
Alfred P. Sloan Foundation Fellow, 1978 - 1982
National Defense Education Act Fellowship, 1967 - 1969, 1971 - 1972
James Wright Hunt Scholarship, 1966 - 1967

ACADEMIC SPECIALIZATION:

Topics: Physical Chemistry, Chemical Physics, Bio-Analytical Chemistry, Vibrational Spectroscopy, Molecular Optical Activity, Chirality of Biological Molecules, Quantum Chemistry, Electron Transition Current Density, Characterization of Chiral Pharmaceutical Molecules

GRANTS:

- "Vibrational Optical Activity", Research Corporation, 1975 to 1978, \$15,000.
- "Vibrational Optical Activity", Petroleum Research Fund of the American Chemical Society, 1976 to 1979, \$9,000.
- "Vibrational Optical Activity in Proteins and Related Molecules", National Science Foundation, 1976 to 1979, \$88,400.

- "Mid-Infrared Vibrational Circular Dichroism", Senate Research Committee, Syracuse University, 1978, \$3,500.
- "Vibrational Optical Activity", National Institutes of Health, 1978 to 1981, \$177,900.
- Fellowship for Research from the Alfred P. Sloan Foundation, 1978 to 1982, \$19,800.
- "Vibrational Circular Dichroism Spectroscopy", National Science Foundation, 1980 to 1983, \$248,000.
- "Vibrational Optical Activity in Peptide Molecules", National Institutes of Health, 1981 to 1984, \$294,756.
- "Vibrational Circular Dichroism Spectroscopy", National Science Foundation, 1983 to 1986, \$272,500.
- "Vibrational Optical Activity in Peptide Molecules", National Institutes of Health, 1984 to 1989, \$611,355 direct costs.
- "Vibrational Circular Dichroism Spectroscopy", National Science Foundation, 1986 to 1989, \$334,000.
- "Vibrational Optical Activity in Biological Molecules," National Institutes of Health, 1989-1994, \$539,574 direct costs and approximately \$775,000 total costs.
- "Vibrational Optical Activity in Biomolecules" National Institutes of Health, 1994-2000, \$ 637,261 direct costs, and \$851,215 total costs.
- "Near-Infrared VCD of Chiral Pharmaceuticals" National Institutes of Health, 2001-2005, \$1,027,873 total costs.
- "Small Achiral Ligands as Vibrational Circular Dichroism Probes of Active Sites in Metalloproteins", National Science Foundation (NSF), 2001-2004, \$309,500 total costs.
- "Elaboration of VCD method to study of metal-ion induced structural polymorphism of DNA and its polypurine-polypyrimidine sequence", CRDF, 2002-2004, \$6,000 total costs.
- "Miniature Vibrational Circular Dichroism Spectrometer for Detection of Amino Acids and Chirality", Jet Propulsion Lab NASA (JPL), 2002-2005, ~\$100,000 total costs.
- "Detection of Chirality in Amino Acids Using Fourier-Transform Vibrational Circular Dichroism", National Aeronautics and Space Administration (NASA), faculty/graduate student fellowship grant, 2003-2006, \$72,000 total costs.
- BioTools Inc., 2000-2010, \$20,000, Phase one w/R.W. Johnson Pharmaceutical (plus lab equipment and computer donated). Phase two 2001-2002, \$40,000. Phase three 2002-2003, \$40,000. Phase four 2003-2004, \$20,000, 2004-2005, \$30,000. Total \$150,000.
- Small Business Technology Transfer (STTR) Grant "Near-Infrared Surface-Enhanced Raman Optical Activity from Metal Nanoshells" Air Force Office of Scientific Research (AFOSR), Syracuse University and BioTools, Inc., Phase I, \$100,000, 2005-2006.
- Air Force Office of Sponsored Research - Multiple University Research Initiative (AFOSR/MURI Negative Index Materials (NIMS)) "Three-Dimensional Approaches to Assembling Negative Index Metamaterials" \$5,040,000 for five years to the University of Michigan, Syracuse University budget approximately \$500,000 for five years, May 1, 2006 to April 30, 2011. (sub-project PI)
- Small Business Technology Transfer (STTR) Grant "Near-Infrared Surface-Enhanced Raman Optical Activity from Metal Nanoshells" Air Force Office of Scientific Research (AFOSR), BioTools, Inc. and Rice University, Phase II, \$750,000, 2007-2009 (named consultant).
- Small Business Innovation (SBIR) Grant "Vibrational CD Microscopy for Characterizing Supramolecular Bio-Chirality" from the National Science Foundation, Phase I (2010), \$100,000, and Phase II, 2011-2013 (\$500,000)

PUBLICATIONS:

1. "Polarized Laser Raman Studies on Biological Polymers" by B. Fanconi, B. Tomlinson, L.A. Nafie, W. Small and W.L. Peticolas, *J. Chem. Phys.* **51**, 3993-4005 (1969).
2. "Inelastic Light Scattering from Biological and Synthetic Polymers" by W.L. Peticolas, B. Fanconi, B. Tomlinson, L.A. Nafie and W. Small, *Annal. N.Y. Acad. Sci.* **168**, 564-588 (1970).
3. "Quantum Theory of Intensities of Molecular Vibrational Spectra" by W.L. Peticolas, L.A. Nafie, P. Stein and B. Fanconi, *J. Chem. Phys.* **52**, 1576-1584 (1970).
4. "Angular Dependence of Raman Scattering Intensity" by L.A. Nafie, P. Stein, B. Fanconi and W.L. Peticolas, *J. Chem. Phys.* **52**, 1584-1588 (1970).
- 4a. "Reply to Comments by Freund" by L. Nafie, P. Stein, B. Fanconi, and W.L. Peticolas, *The Journal of Chemical Physics*, Vol. **53**, No. 7, 2990-2991 (1970).
5. "Time Ordered Diagrams for the Resonant Raman Effect from Molecular Vibrations" by L.A. Nafie, P. Stein and W.L. Peticolas, *Chem. Phys. Lett.* **12**, 131-136 (1971).
6. "Reorientation and Vibrational Relaxation as Line Broadening Factors in Vibrational Spectroscopy" by L.A. Nafie and W.L. Peticolas, *J. Chem. Phys.* **57**, 3145-3155 (1972).
7. "Origin of the Intensity of the Resonant Raman Bands of Differing Polarization in Heme-Proteins" by L.A. Nafie, M. Pezolet and W.L. Peticolas, *Chem. Phys. Lett.* **20**, 563-568 (1973).
8. "Complete Polarization Measurements for Non-Symmetric Raman Tensors: Symmetry Assignments of Ferrocyclochrom c Vibrations" by M. Pezolet, L.A. Nafie and W.L. Peticolas, *J. Raman Spectrosc.* **1**, 455-464 (1973).
9. "A 10.6 Micron Modulated Light Ellipsometer" by S.D. Allen, A.I. Braunstein, J.C. Cheng and L.A. Nafie, in *Optical Properties of Highly Transparent Solids*, S.S. Mitra and B. Bendow, Eds., Plenum, New York, 1975, pp. 503-514.
10. "Vibrational Circular Dichroism of 2,2,2-Trifluoro-1-phenylethanol" by L.A. Nafie, J.C. Cheng and P.J. Stephens, *J. Am. Chem. Soc.* **97**, 3842 (1975).
11. "Polarization Scrambling Using a Photoelastic Modulator: Application to Circular Dichroism Measurement" by J.C. Cheng, L.A. Nafie and P.J. Stephens, *J. Opt. Soc. Amer.* **65**, 1031-1035 (1975).
12. "Vibrational Circular Dichroism" by L.A. Nafie, T.A. Keiderling and P.J. Stephens, *J. Am. Chem. Soc.* **98**, 2715-2723 (1976).
13. "Photoelastic Modulator for the 0.55-13 μm Range" by J.C. Cheng, L.A. Nafie, S.D. Allen and A.I. Braunstein, *Appl. Optics* **15**, 1960-1965 (1976).
14. "Observation of the Raman Anti-Resonance Effect in Synthetic Metal (II) Porphyrin Analogues" by L.A. Nafie, R.W. Pastor, J.C. Dabrowiak and W.H. Woodruff in *Proceedings of the Fifth International*

Conference on Raman Spectroscopy, E. Schmid et al., Eds., H. Schulz, Freiburg, 1976, pp. 330-331.

15. "Resonance Raman Studies of Macrocyclic Complexes II. Anti-Resonance and Selective Intensity Enhancement in Synthetic Metal (II) Porphyrin Analogues" by L.A. Nafie, R.W. Pastor, J.C. Dabrowiak and W.H. Woodruff, *J. Am. Chem. Soc.* **98**, 8007-8014 (1976).
16. "Calculation of Excitation Profiles from the Vibronic Theory for Raman Scattering" by B.B. Johnson, L.A. Nafie and W.L. Peticolas, *Chem. Phys.* **19**, 303-311 (1977).
17. "Near-Infrared Magnetic Circular Dichroism of Cytochrome c" by J. Rawlings, P.J. Stephens, L.A. Nafie and M. Kamen, *Biochemistry* **16**, 1725-1729 (1977).
18. "Accessibility of Manganese Oxidation States. Control by Pentaazo Macrocyclic Ligands" by J.C. Dabrowiak, L.A. Nafie, P.S. Bryan and A.T. Torkelson, *Inorg. Chem.* **16**, 540-544 (1977).
19. "Vibrational Circular Dichroism Theory: A Localized Molecular Orbital Model" by L.A. Nafie and T.H. Walnut, *Chem. Phys. Lett.* **49**, 441-446 (1977).
20. "Infrared Absorption and the Born-Oppenheimer Approximation I. Vibrational Intensity Expressions" by T.H. Walnut and L.A. Nafie, *J. Chem. Phys.* **67**, 1491-1500 (1977).
21. "Infrared Absorption and the Born-Oppenheimer Approximation II. Vibrational Circular Dichroism" by T.H. Walnut and L.A. Nafie, *J. Chem. Phys.* **67**, 1501-1510 (1977).
22. "Vibrational Circular Dichroism in Amino Acids and Peptides. 1. Alanine" by M. Diem, P.J. Gotkin, J.M. Kupfer, A.G. Tindall and L.A. Nafie, *J. Am. Chem. Soc.* **99**, 8103-8104 (1977).
23. "Analysis of the Gas Phase Infrared Spectrum of Bromochlorofluoromethane: Calculated and Observed Band Contours and Intensities" by M. Diem, L.A. Nafie and D.F. Burow, *J. Molec. Spectrosc.* **71**, 446-457 (1978).
24. "Vibrational Circular Dichroism in Amino Acids and Peptides. 2. Simple Alanyl Peptides" by M. Diem, P.J. Gotkin, J.M. Kupfer and L.A. Nafie, *J. Am. Chem. Soc.* **100**, 5644-5650 (1978).
25. "Theory of High Frequency Differential Interferometry: Application to Infrared Circular and Linear Dichroism via Fourier Transform Spectroscopy" by L.A. Nafie and M. Diem, *Appl. Spectrosc.* **33**, 130-135 (1979).
26. "Fourier Transform Infrared Vibrational Circular Dichroism" by L.A. Nafie, M. Diem and D.W. Vidrine, *J. Am. Chem. Soc.* **101**, 496-498 (1979).
27. "Optical Activity in Vibrational Transitions: Vibrational Circular Dichroism and Raman Optical Activity" by L.A. Nafie and M. Diem, *Acc. Chem. Res.* **12**, 296-302 (1979).
28. "The Atom Dipole Interaction Model of Raman Optical Activity: Reformulation and Comparison to the Two-Group Model" by P.L. Prasad and L.A. Nafie, *J. Chem. Phys.* **70**, 5582-5588 (1979).
29. "Raman Optical Activity. Spectral Simulation of the Conformer Dependent C-Cl Stretching Vibrations

- in 1-Chloro-2-Methylbutane" by P.L. Prasad, L.A. Nafie and D.F. Burow, *J. Raman Spectrosc.* **8**, 255-258 (1979).
30. "Vibrational Circular Dichroism in Amino Acids and Peptides. 3. Solution and Solid Phase Spectra of Serine and Alanine" by M. Diem, E. Photos, H. Khouri and L.A. Nafie, *J. Am. Chem. Soc.* **101**, 6829-6837 (1979).
 31. "Vibrational Circular Dichroism in Peptides" by L.A. Nafie, P.L. Prasad, H. Khouri and E. Doorly, *Polymer Preprints* **20**(2), 85-89 (1979).
 32. "Differential Absorption at High Modulation Frequencies Using a Fourier Transform Infrared Spectrometer" by L.A. Nafie and D.W. Vidrine, *Proc. Soc. Photo. Inst. Eng.* **191**, 56-63 (1979).
 33. "Vibrational Optical Activity: Comparison of Theoretical and Experimental Results for (+)-(3R)-Methylcyclohexanone" by P.L. Polavarapu and L.A. Nafie, *J. Chem. Phys.* **73**, 1567-1575 (1980).
 34. "Vibrational Optical Activity in Para-Substituted 1-Methylcyclo-hex-1-enes" by P.L. Polavarapu, M. Diem and L.A. Nafie, *J. Am. Chem. Soc.* **102**, 5549-5453 (1980).
 35. "Experimental Observations and Theoretical Predictions of Raman Optical Activity" by P.L. Prasad and L.A. Nafie, in *Proceedings of the VIIIth International Conference on Raman Spectroscopy*, W.F. Murphy, Ed., North-Holland, New York, 1980, pp. 252-253.
 36. "Vibrational Optical Activity in Perturbed Degenerate Modes: Concepts and Model Calculations in 1-Substituted Haloethanes" by L.A. Nafie, P.L. Polavarapu and M. Diem, *J. Chem. Phys.* **73**, 3530-3540 (1980).
 37. "Infrared and Raman Vibrational Optical Activity" by L.A. Nafie in *Vibrational Spectra and Structure*, Vol. 10, J.R. Durig, Ed., Elsevier, Amsterdam, 1981, pp. 153-225.
 38. "Optical Activity Due to Isotopic Substitution. Vibrational Circular Dichroism and the Absolute Configuration of α -Deuterated Cyclohexanones" by P.L. Polavarapu, L.A. Nafie, S.A. Benner and T.H. Morton, *J. Am. Chem. Soc.* **103**, 5349-5354 (1981).
 39. "Localized Molecular Orbital Calculations of Vibrational Circular Dichroism. I. General Theoretical Formalism and CNDO Results for the Carbon Deuterium Stretching Vibration in Neopentyl-1-d-Chloride" by L.A. Nafie and P.L. Polavarapu, *J. Chem. Phys.* **75**, 2935-2944 (1981).
 40. "Localized Molecular Orbital Calculations of Vibrational Circular Dichroism. II. CNDO Formulation and Results for the Hydrogen Stretching Vibrations of (+)-(3R)-Methylcyclohexanone" by P.L. Polavarapu and L.A. Nafie, *J. Chem. Phys.* **75**, 2945-2951 (1981).
 41. "Fourier Transform Infrared Circular Dichroism: A Double Modulation Approach" by L.A. Nafie, E.D. Lipp and C.G. Zimba in *Proceedings of the 1981 International Conference on Fourier Transform Infrared Spectroscopy*, J. Sakal, Ed., SPIE Vol. 289, 1981, pp. 457-468.
 42. "A Unified Approach to the Determination of Infrared and Raman Vibrational Optical Activity

- Intensities Using Localized Molecular Orbitals" by L.A. Nafie and T.B. Freedman, *J. Chem. Phys.* **75**, 4847-4851 (1981).
- 42a. Book Review of *Vibrational Spectra and Structure*, Vol. 9, J.R. Durig, Ed. Elsevier Publishing Co., *J. Am. Chem. Soc.* **103**, 7699-7700 (1981).
43. "Double Modulation Fourier Transform Spectroscopy" by L.A. Nafie and D.W. Vidrine in *Fourier Transform Infrared Spectroscopy*, J.R. Ferraro and L.J. Basile, Eds., Academic Press, New York, Vol. 3, 1982, pp. 83-123.
- 43a. Book Review of *Fourier Transform Infrared Spectroscopy*, Vol. 1, J.R. Ferraro and L.J. Basile, Eds., Academic Press Inc., *J. Chem. Soc.* **104**, 3329-3336 (1982).
44. "Vibrational Circular Dichroism in Amino Acids and Peptides. 4. Vibrational Analysis, Assignments and Solution Phase Raman Spectra of Deuterated Isotopomers of Alanine" by M. Diem, P.L. Polavarapu, M. Oboodi and L.A. Nafie, *J. Am. Chem. Soc.* **104**, 3329-3336 (1982).
45. "Vibrational Circular Dichroism in Amino Acids and Peptides. 5. Carbon-Hydrogen Stretching VCD and Fixed Partial Charge Calculations for Deuterated Isotopomers of Alanine" by B.B. Lal, M. Diem, P.L. Polavarapu, M. Oboodi, T.B. Freedman and L.A. Nafie, *J. Am. Chem. Soc.* **104**, 3336-3342 (1982).
46. "Vibrational Circular Dichroism in Amino Acids and Peptides. 6. Localized Molecular Orbital Calculations of the Carbon-Hydrogen Stretching VCD in Deuterated Isotopomers of Alanine" by T.B. Freedman, M. Diem, P.L. Polavarapu and L.A. Nafie, *J. Am. Chem. Soc.* **104**, 3343-3349 (1982).
47. "The Emergence and Exploration of Vibrational Optical Activity" by L.A. Nafie, *Appl. Spectrosc.* **36**, 489-495 (1982).
48. "Polarization Demodulation: A New Approach to the Reduction of Polarization Artifacts from Vibrational Circular Dichroism Spectra" by E.D. Lipp, C.G. Zimba, L.A. Nafie and D.W. Vidrine, *Appl. Spectrosc.* **36**, 496-498 (1982).
49. "Molecular Orbital Formulations of Raman Optical Activity" by T.B. Freedman and L.A. Nafie in *Raman Spectroscopy: Linear and Nonlinear*, J. Lascombe and P.V. Huong, Eds., Wiley Heyden, New York, 1982, pp. 13-14.
50. "Spectroscopic Studies of Copper(II) Bound at the Native Copper Site or Substituted at the Native Zinc Site of Bovine Erythrocyte (Superoxide Dismutase) by M.W. Pantoliano, J.S. Valentine and L.A. Nafie, *J. Am. Chem. Soc.* **104**, 6310-6317 (1982).
51. "Vibrational Circular Dichroism in the Mid-Infrared Using Fourier Transform Spectroscopy" by E.D. Lipp, C.G. Zimba and L.A. Nafie, *Chem. Phys. Lett.* **90**, 1-5 (1982).
52. "Vibrational Circular Dichroism in Amino Acids and Peptides. 7. Amide Stretching Vibrations in Polypeptides" by B.B. Lal and L.A. Nafie, *Biopolymers* **21**, 2161-2183 (1982).
53. "Vibrational Optical Activity Calculations Using Infrared and Raman Atomic Polar Tensors" by T.B. Freedman and L.A. Nafie, *J. Chem. Phys.* **78**, 27-31 (1983).

- 53a. "Erratum: Vibrational optical activity calculations using infrared and Raman atomic polar tensors" by Teresa B. Freedman and Laurence A. Nafie, *J. Chem. Phys.* **97**(2), 1104 (1983).
54. "Experimental and Theoretical Advances in Vibrational Optical Activity" by L.A. Nafie in *Advances in Infrared and Raman Spectroscopy*, Vol. 11, R.J.H. Clark and R.E. Hester, Eds., Heyden, London, 1984, pp. 49-93.
55. "Vibronic Coupling Theory of Infrared Vibrational Intensities" by L.A. Nafie and T.B. Freedman, *J. Chem. Phys.* **78**, 7108-7116 (1983).
56. "Raman Spectral Studies of Bleomycin A₂ and Related Structural Fragments. A Probe of Bleomycin-DNA Interactions" by T.B. Freedman, F.S. Santillo, C.G. Zimba, L.A. Nafie and J.C. Dabrowiak, *J. Raman Spectrosc.* **14**, 266-270 (1983).
57. "Adiabatic Behavior Beyond the Born-Oppenheimer Approximation. Complete Adiabatic Wavefunctions and Vibrationally Induced Electronic Current Density" by L.A. Nafie, *J. Chem. Phys.* **79**, 4950-4957 (1983).
58. "Vibrational Circular Dichroism in Amino Acids and Peptides. 8. A Chirality Rule for the Methine C*H Stretching Mode" by L.A. Nafie, M.R. Oboodi and T.B. Freedman, *J. Am. Chem. Soc.* **105**, 7449-7450 (1983).
59. "An Alternative View on the Sign Convention of Raman Optical Activity" *Chem. Phys. Lett.* **102**, 287-288 (1983).
60. "Fourier Transform Vibrational Circular Dichroism: Improvements in Methodology and Mid-Infrared Spectral Results" by E.D. Lipp and L.A. Nafie, *Appl. Spectrosc.* **38**, 20-25 (1984).
61. "Molecular Orbital Approaches to the Calculation of Vibrational Circular Dichroism" by T.B. Freedman and L.A. Nafie, *J. Phys. Chem.* **88**, 496-500 (1984).
62. "Raman Optical Activity in the Skeletal Motions of (+)-(3R)-Methylcyclohexanone. Chiral Mixing of Inherently Achiral Vibrations" by T.B. Freedman, J. Kallmerten, C.G. Zimba, W.M. Zuk and L.A. Nafie, *J. Am. Chem. Soc.* **106**, 1244-1252 (1984).
63. "Application of Fourier Self-Deconvolution to Vibrational Circular Dichroism Spectra" by E.D. Lipp and L.A. Nafie, *Appl. Spectrosc.* **38**, 774-778 (1984).
64. "Fourier Transform Vibrational Circular Dichroism in the Carbonyl Region of Peptides and Polypeptides" by L.A. Nafie, E.D. Lipp, A. Farrel and G. Paterlini, *Polymer Preprints* **25**(2), 145-146 (1984).
65. "Vibrational Circular Dichroism in Amino Acids and Peptides. 9. Carbon-Hydrogen Stretching Spectra of the Amino Acids and Selected Transition Metal Complexes" by M.R. Oboodi, B.B. Lal, D.A. Young, T.B. Freedman and L.A. Nafie, *J. Am. Chem. Soc.* **107**, 1547-1556 (1985).
66. "Vibrational Circular Dichroism in Amino Acids and Peptides. 10. Fourier Transform VCD and Fourier

- Self-Deconvolution of the Amide I Region of Poly(γ -Benzyl-L-Glutamate)" by E.D. Lipp and L.A. Nafie, *Biopolymers* **24**, 799-812 (1985).
67. "Vibrational Circular Dichroism in Bis(acetylacetonato) (L-alaninato)cobalt(III). Isolated Occurrences of the Coupled Oscillator and Ring Current Intensity Mechanisms" by D.A. Young, E.D. Lipp and L.A. Nafie, *J. Am. Chem. Soc.* **107**, 6205-6213 (1985).
68. "Enhanced Vibrational Circular Dichroism via Vibrationally Generated Electronic Ring Currents" by T.B. Freedman, G.A. Balukjian and L.A. Nafie, *J. Am. Chem. Soc.* **107**, 6213-6222 (1985).
69. "Vibrational Circular Dichroism Spectroscopy and the Ring Current Intensity Mechanism" by L.A. Nafie and T.B. Freedman in *Proceedings of the International Conference on Circular Dichroism*, Bulgarian Academy of Sciences, Sofia, 1985, pp. 218-232.
70. "Fourier Transform Vibrational Circular Dichroism of Carbonyl Stretching Modes in N-Urethanyl- α -Amino Acids" by A.C. Chernovitz, T.B. Freedman and L.A. Nafie in *1985 Conference on Fourier and Computerized Infrared Spectroscopy*, J. Grasselli et al. eds. Proc. SPIE Vol., pp. 222-223 (1985).
71. "Fourier Transform Vibrational Circular Dichroism in the Amide I Band of Polypeptides" by M.G. Paterlini, T.B. Freedman and L.A. Nafie, in *1985 Conference on Fourier and Computerized Infrared Spectroscopy*, J. Grasselli et al. eds. Proc. SPIE Vol., pp. 274-275 (1985).
72. "The VCD Spectrum of 2-Methyl Oxetan" by R.A. Shaw, N. Ibrahim, L.A. Nafie, A. Rank and H. Wieser in *1985 Conference on Fourier and Computerized Infrared Spectroscopy*, J. Grasselli et al. eds. Proc. SPIE Vol., pp. 433-434 (1985).
73. "Ring Current Mechanism of Vibrational Circular Dichroism" by L.A. Nafie and T.B. Freedman, *J. Phys. Chem.* **90**, 763-767 (1986).
74. "Ring Current Enhanced Vibrational Circular Dichroism in the CH-Stretching Motion of the Sugars" by M.G. Paterlini, T.B. Freedman and L.A. Nafie, *J. Am. Chem. Soc.* **108**, 1389-1397 (1986).
75. "Molecular Orbital Calculations of Infrared Intensities Beyond the Born-Oppenheimer Approximation Using the Dipole Momentum Operator" by T.B. Freedman and L.A. Nafie, *Chem. Phys. Lett.* **126**, 441-446 (1986).
76. "Biologically Relevant Applications of Vibrational Circular Dichroism" by L.A. Nafie in *Spectroscopy in the Biomedical Sciences*, R.N. Gendreau, Ed., CRC Press, Boca Raton, Florida, 1986, pp. 141-150.
77. "Raman Optical Activity Spectra of (+)-(3R)-Methylcyclohexanone Obtained with a Soleil-Babinet Compensator" by C.G. Zimba, T.B. Freedman, K.M. Spencer, X.M. Hu and L.A. Nafie in *Proceedings of the Tenth International Conference on Raman Spectroscopy*, Eugene, Oregon, 1986, p. 20-26.
78. "Vibrational Circular Dichroism Spectra of Three Conformationally Distinct States and an Unordered State of Poly(L-lysine) in Deuterated Aqueous Solution" by M.G. Paterlini, T.B. Freedman and L.A. Nafie, *Biopolymers* **25**, 1751-1765 (1986).

79. "Vibrational Circular Dichroism in Transition Metal Complexes. 2. Ion Association, Ring Conformation and Ring Currents of Ethylenediamine Ligands" by D.A. Young, T.B. Freedman, E.D. Lipp and L.A. Nafie, *J. Am. Chem. Soc.* **108**, 7255-7263 (1986).
80. "Vibrational Spectra of Methylthiirane" by P.L. Polavarapu, B.A. Hess, Jr., L.J. Schaad, D.O. Henderson, L.P. Fontana, H.E. Smith, L.A. Nafie, T.B. Freedman and W.M. Zuk, *Phys. Chem.* **86**, 1140-1146 (1987).
81. "Raman Optical Activity and Related Techniques" by L.A. Nafie and C.G. Zimba in *Biological Applications of Raman Spectroscopy* Vol. 1, T.G. Spiro, ed., Wiley, New York, 1987, pp. 307-343.
82. "A Bond Origin Independent Formulation of the Bond Dipole Model of Vibrational Circular Dichroism" by J.R. Escribano, T.B. Freedman and L.A. Nafie, *J. Phys. Chem.* **91**, 46-49 (1987).
83. "Vibrational Circular Dichroism Theory: Formulation Defining Magnetic Dipole Atomic Polar Tensors and Vibrational Nuclear Magnetic Shielding Tensors" by L.A. Nafie and T.B. Freedman, *Chem. Phys. Lett.* **134**, 225-232 (1987).
84. "A Soleil-Babinet Compensator Based Raman Optical Activity Spectrometer: Interpretation of ROA Couplets in (+)-(3R) Methylcyclohexanone" by C.G. Zimba, T.B. Freedman, K.M. Spencer, X.-M. Hu and L.A. Nafie, *Chem. Phys. Lett.* **134**, 233-238 (1987).
85. "Vibrational Circular Dichroism in Transition Metal Complexes. 3. Ring Currents and Ring Conformation of Amino Acid Ligands" by T.B. Freedman, D.A. Young, M.R. Oboodi and L.A. Nafie, *J. Am. Chem. Soc.* **109**, 1551-1559 (1987).
86. "Stereochemical Aspects of Vibrational Optical Activity" by T.B. Freedman and L.A. Nafie in *Topics in Stereochemistry*, Vol. 17, E.L. Eliel and S.H. Wilen, Eds., Wiley, New York 1987 pp. 113-206.
87. "Fourier Transform Infrared Vibrational Circular Dichroism in the Carbonyl Stretching Region of Polypeptides and Urethane Amino Acid Derivatives" by L.A. Nafie, E.D. Lipp, A. Chernovitz and G. Paterlini in *FT-IR Characterization of Polymers*, H. Ishida, Ed., Plenum, New York 1987, pp. 81-95.
88. "Vibrational Circular Dichroism in the Carbon-Hydrogen and Carbon-Deuterium Stretching Modes of (S,S)-[2,3-²H₂]Oxirane" by T.B. Freedman, M.G. Paterlini, N.-S. Lee, L.A. Nafie, J.M. Schwab and T. Ray, *J. Am. Chem. Soc.* **109**, 4727-4728 (1987).
89. "Bond Polarizability and Vibronic Coupling Theory of Raman Optical Activity: The Electric-Dipole Magnetic Dipole Optical Activity Tensor" by J.R. Escribano, T.B. Freedman and L.A. Nafie, *J. Chem. Phys.* **87**, 3366 (1987).
90. "Vibrational CD Studies of the Solution Conformation of N-Urethanyl L-Amino Acid Derivatives" by A.C. Chernovitz, T.B. Freedman and L.A. Nafie, *Biopolymers* **26**, 1879-1900 (1987).
91. "Vibrational Circular Dichroism Spectroscopy" by L.A. Nafie and T.B. Freedman, *Spectroscopy* **2** (12), 24-29 (1987).
92. "Vibrational Circular Dichroism in Transition Metal Complexes. 4. Solution Conformation of α -mer and

- `-fac-Tris(-alaninato) Cobalt (III)" by D.A. Young, T.B. Freedman and L.A. Nafie, *J. Am. Chem. Soc.* **109**, 7674-7677 (1987).
93. "Polarization Modulation FTIR Spectroscopy" by L.A. Nafie in *Advances in Applied FTIR Spectroscopy*, M.W. Mackenzie, ed., John Wiley and Sons, New York, 1988.
 94. "Vibrational Circular Dichroism in the CH-Stretching Region of (+)-(3R)-Methylcyclohexanone and Chiral Deuterated Isotopomers" by T.B. Freedman, J. Kallmerten, E.D. Lipp, D.A. Young and L.A. Nafie, *J. Am. Chem. Soc.* **110**, 689-698 (1988).
 95. "Vibronic Coupling Calculations of Vibrational Circular Dichroism Intensities Using Floating Basis Sets" by T.B. Freedman and L.A. Nafie, *J. Chem. Phys.* **89**, 374-384 (1988).
 96. "Polarization Modulation Fourier Transform Infrared Spectroscopy" by L.A. Nafie, N.S. Lee, G. Paterlini and T.B. Freedman, *Microchim. Acta* **1987 III**, 93-104 (1988).
 97. "Scattered Circular Polarization Raman Optical Activity" by K.M. Spencer, T.B. Freedman and L.A. Nafie, *Chem. Phys. Lett.* **149**, 367-374 (1988).
 98. "Vibrational Circular Dichroism in the Methine Bending Modes of Amino Acids and Dipetides" by T.B. Freedman, A.C. Chernovtitz, W.M. Zuk, M.G. Paterlini and L.A. Nafie, *J. Am. Chem. Soc.* **110**, 6970-6974 (1988).
 99. "Vibrational Circular Dichroism in the CH-Stretching Modes of L- α -Amino Acids as a Function of pH", by W.M. Zuk, T.B. Freedman and L.A. Nafie, *J. Phys. Chem.*, **93**, 1771-1779 (1989).
 100. "Dual Circular Polarization Raman Optical Activity" by L.A. Nafie and T.B. Freedman, *Chem. Phys. Lett.*, **154**, 260-266 (1989).
 101. "Synthesis and Gas-Phase Vibrational Circular Dichroism of (+)-(S,S)-Cyclopropane-1,2-²H₂", by S.J. Cianciosi, K.M. Spencer, T.B. Freedman, L.A. Nafie and J.E. Baldwin, *J. Am. Chem. Soc.* **111**, 1913-1915 (1989).
 102. "Vibrational CD Studies of the Solution Conformation of Simple Alanyl Peptides as a Function of pH", by W.M. Zuk, T.B. Freedman and L.A. Nafie, *Biopolymers* **28**, 2025-2044 (1989).
 103. "Vibrational Optical Activity in Amino Acids, Peptides and Proteins" by Teresa B. Freedman and Laurence A. Nafie, in *Biomolecular Spectroscopy*, R.R. Birge and H.H. Mantsch, eds., Proc. SPIE Vol. 1057, 1989, pp 15-25.
 104. "Vibrational Circular Dichroism of Simple Chiral Molecules in the Gas Phase," by T. B. Freedman, K. M. Spencer, C. McCarthy, S. J. Cianciosi, J. E. Baldwin and L. A. Nafie, in *7th International Conference on Fourier Transform Spectroscopy*, D. G. Cameron, Ed., Proc. SPIE Vol. 1145, 1989, pp 273-274.
 105. "Circular Dichroism Measurement using Fourier Transform Interferometry," by N. Ragunathan, L. A. Nafie and T. B. Freedman, in *7th International Conference on Fourier Transform Spectroscopy*, D. G.

Cameron, Ed., Proc. SPIE Vol. 1145, 1989, pp 148-149.

106. "Vibrational Circular Dichroism Studies of Interchain Hydrogen Bonding in Tripodal Peptide Molecules," by M. G. Paterlini, T. B. Freedman and L. A. Nafie, in *7th International Conference on Fourier Transform Spectroscopy*, D. G. Cameron, Ed., Proc. SPIE Vol. 1145, 1989, pp 150-151.
107. "Measurement of Vibrational Circular Dichroism Using a Polarizing Michelson Interferometer" by N. Rangunathan, N.-S. Lee, T.B. Freedman, L.A. Nafie, C. Tripp and H. Buijs, *Appl. Spectrosc.* **44**, 5-7 (1990).
108. "Determination of Enantiomeric Excess in Deuterated Chiral Hydrocarbons by Vibrational Circular Dichroism Spectroscopy" by K.M. Spencer, S.J. Cianciosi, J.E. Baldwin, T.B. Freedman and L.A. Nafie, *Appl. Spectrosc.*, **44**, 235-238 (1990).
109. "Comparison of Incident and Scattered Circular Polarization Raman Optical Activity" by D. Che, L. Hecht and L.A. Nafie in *Twelfth International Conference on Raman Spectroscopy*, J.R. Durig and J.F. Sullivan, Eds., Wiley, New York, 1990, p.846.
110. "Electronic Current Models of Vibrational Circular Dichroism" by L.A. Nafie and T.B. Freedman, *J. Molec. Structure*, **224**, 121-132 (1990).
111. "Linear Polarization Raman Optical Activity: A New Form of Natural Optical Activity" by L. Hecht and L.A. Nafie, *Chem. Phys. Lett.* **174**, 575 (1990).
- 111a. "Reply to a Comment concerning "Linear polarization Raman optical activity as a new form of natural optical activity" by Lutz Hecht and Laurence A. Nafie, *Chem. Phys. Lett.* **195**, 637-640 (1992).
112. "Racemization and Geometrical Isomerization of (-)-(R,R)-Cyclopropane 1,2-²H₂" by S.J. Cianciosi, N. Rangunathan, T.B. Freedman, L.A. Nafie, and J.E. Baldwin, *J. Am. Chem. Soc.* **112**, 8204-8206 (1990).
113. "Vibrational Circular Dichroism is a Sensitive Probe Study of Heme-Protein-Ligand Interactions" S.A. Asher, R.W. Bormett. P.J. Larkin, W.G. Gustafson, N. Rangunathan, T.B. Freedman, L.A. Nafie, N.-T. Yu, K. Gersonde, R.W. Noble, B.A. Springer, S. Balasubramanian, and S.G. Boxer in *Spectroscopy of Biological Molecules*, R.E. Hester R.B. Girling Eds., Royal Society of Chemistry, Cambridge, England, 1991, pp. 139-140.
114. "Theory of Natural Raman Optical Activity I. Complete Circular Polarization Formalism" by L. Hecht and L.A. Nafie, *Mol. Phys.* **72**, 441-469 (1991).
115. "A New Scattered Circular Polarization Raman Optical Activity Instrument Equipped with a Charged-Coupled-Device Detector" by L. Hecht, D. Che and L.A. Nafie, *Appl. Spectrosc.* **45**, 18-25 (1991).
116. "Racemization and Geometrical Isomerization of (2S,3S)-Cyclopropane-1-¹³C,2-²H-2,3-²H₂ at 407 C: Kinetically Competitive One-Center and Two-Center Thermal Epimerizations in an Isotopically Substituted Cyclopropane" by S.J. Cianciosi, N. Rangunathan, T.B. Freedman, L. A. Nafie, D.K. Lewis, D.A. Glenar and J.E. Baldwin, *J. Am. Chem. Soc.*, **113**, 1864-1866 (1991).

117. "Dual and Incident Circular Polarization Raman Optical Activity Backscattering of (-)-Trans-Pinane" by D. Che, L. Hecht and L.A. Nafie, *Chem. Phys. Lett.*, **180**, 182-190 (1991).
118. "New Experimental Methods and Theory of Raman Optical Activity" by L.A. Nafie, D. Che, G.-S. Yu and T.B. Freedman, in *Biomolecular Spectroscopy II*, R.R. Birge and L.A. Nafie, eds., SPIE, Vol. 1432, 1991, pp. 37-49.
- 118a. *Biomolecular Spectroscopy II*, R.R. Birge and L.A. Nafie, eds, SPIE, Vol 1432, 1991.
119. "Optical Activity Arising from ^{13}C Substitution: Vibrational Circular Dichroism Study of (2S,3S)-Cyclopropane-1- ^{13}C ,2H-2,3- $^2\text{H}_2$ " by T.B. Freedman, S.J. Cianciosi, N. Rangunathan, J.E. Baldwin and L.A. Nafie, *J. Am. Chem. Soc.*, **113**, 8298-8305 (1991).
120. "Methods and Applications of Infrared and Raman Vibrational Optical Activity" by L.A. Nafie in *Lectures and Posters of the Fourth International Conference on Circular Dichroism*, Bochum, Germany, H. Klein and G. Snatzke, eds., Ruhrgebiet, Essen, 1991, pp. 101-114.
121. "Vibrational Circular Dichroism of (S,S)-[2,3- $^2\text{H}_2$]Oxirane in the Gas Phase and in Solution" by T.B. Freedman, K. M. Spencer, N. Rangunathan, L.A. Nafie, J.A. Moore and J.M. Schwab, *Can. J. Chem.*, **69**, 1619-1629 (1991).
122. "Isolation of Raman Optical Activity Invariants" by D. Che and L. A. Nafie, *Chem. Phys. Lett.*, **189**, 35-42 (1992).
123. "Velocity-Gauge Formalism in the Theory of Vibrational Circular Dichroism and Infrared Absorption" by L. A. Nafie, *J. Chem. Phys.*, **96**, 5687-5702 (1992).
124. "Experimental Comparison of Scattered and Incident Circular Polarization Raman Optical Activity in Pinanes and Pinenes" by L. Hecht, D. Che and L. A. Nafie, *J. Phys. Chem.* **96**, 4266-4270 (1992).
125. "Vibrational Circular Dichroism Studies of Interchain Hydrogen Bonded Model Tripeptides" by M.G. Paterlini, T.B. Freedman, L.A. Nafie, Y. Tor, and A. Shanzer, *Biopolymers*, **32**, 765-782 (1992).
126. "Selective Examination of Heme Protein Azide Ligand-Distal Globin Interactions by Vibrational Circular Dichroism" by R.W. Bormett, S.A. Asher, P.J. Larkin, W.G. Gustafson, N. Rangunathan, T.B. Freedman, L.A. Nafie, S. Balasubramanian, S.G. Boxer, N.-T. Yu, K. Gersonde, R.W Noble, B.A. Springer and S.G. Sligar, *J. Am. Chem. Soc.* **114**, 6864-6867 (1992).
127. "Instrumental Techniques for Infrared and Raman Vibrational Optical Activity" by L.A. Nafie, in *Optically Based Methods for Process Analysis*, J.M. Lerner, ed., SPIE Vol. 1681, 1992, pp. 29-40.
128. "Fourier Transform Vibrational Circular Dichroism Studies of Model Peptide Molecules" by M.J. Citra, M.G. Paterlini, T.B. Freedman, L.A. Nafie, A. Shanzer, Y. Tor, C. Pratesi and O. Pieroni, in *8th International Conference on Fourier Transform Spectroscopy*, H.M. Heise, E.H. Korte, H.W. Siesler, Proc. SPIE, Vol. 1575, (1992) p.406-407.

129. "Spectral and Kinetic Investigations of Chirally-Deuterated Three-Membered Ring Molecules using Fourier Transform Vibrational Circular Dichroism Spectroscopy" by T.B. Freedman, N. Rangunathan, S.J. Cianciosi, J.E. Baldwin, L.A. Nafie, J.A. Moore and J.M. Schwab, in *8th International Conference on Fourier Transform Spectroscopy*, H.M. Heise, E.H. Korte, H.W. Siesler, Proc. SPIE 1575, 1992, pp.408-409.
130. "Backscattering Dual Circular Polarization Raman Optical Activity in Ephedrine Molecules" by G.-S. Yu, D. Che, T.B. Freedman and L.A. Nafie, *Tetrahedron Asym.* **4**, 511-516 (1993).
131. "Theory and Reduction of Artifacts in Incident, Scattered and Dual Circular Polarization Raman Optical Activity" by D. Che and L.A. Nafie, *Appl. Spectrosc.* **47**, 544-555 (1993).
132. "Raman Optical Activity" by L.A. Nafie and T.B. Freedman, in *Metallochemistry, Methods in Enzymology, Part C*, J.F. Riordan and B.L. Vallee, eds., Academic Press, New York, 1993, pp. 470-482.
133. "Vibrational Circular Dichroism" by T.B. Freedman and L.A. Nafie, in *Metallochemistry, Methods in Enzymology, Part C*, J.F. Riordan and B.L. Vallee, eds., Academic Press, Orlando, 1993, pp. 306-319.
134. *Biomolecular Spectroscopy III*, L.A. Nafie and H.H. Mantsch, Eds., Proc.SPIE 1890, 1993.
135. "Vibrational Circular Dichroism of 1-Amino-2-propanol and 2-Amino-1-propanol: Experiment and Calculation" X. Qu, M. Citra, N. Rangunathan, T.B. Freedman and L.A. Nafie, in *9th International Conference on Fourier Transform Spectroscopy*, J.E. Bertie and H. Wieser, Eds. Proc. SPIE 2089, 1993, pp. 142-143.
136. "Vibrational circular dichroism studies of 3_{10} -helical solution conformers in dehydro-peptides" by Mario J. Citra, M. Germana Paterlini, Teresa B. Freedman, Laurence A. Nafie, Adriano Fissi and Osvaldo Pieroni, in *9th International Conference on Fourier Transform Spectroscopy*, J.E. Bertie and H. Wieser, eds., Proc. SPIE 2089, 1993, pp. 478-479.
137. "Theory and Measurement of Raman Optical Activity" by L.A. Nafie and D. Che, in *Modern Nonlinear Optics, Part 3*, M. Evans and S. Kielich eds., *Adv. Chem. Phys. Series* **85**, 105-149 (1994).
138. "Theoretical Formalism and Models for Vibrational Circular Dichroism Intensity" by T.B. Freedman and L.A. Nafie, in *Modern Nonlinear Optics, Part 3*, M. Evans and S. Kielich eds., *Adv. Chem. Phys. Series* **85**, 207-263 (1994).
139. "Instrumental Methods of Infrared and Raman Vibrational Optical Activity" by L.A. Nafie, M. Citra, N. Rangunathan and D. Che in *Analytical Applications of Circular Dichroism*, N. Purdie and H.G. Brittain, eds., Elsevier, Amsterdam, 1994, pp.53-89.
140. "Isolation of Preresonance and Out-of-Phase Dual Circular Polarization Raman Optical Activity" by G.-S. Yu and L.A. Nafie, *Chem. Phys. Lett.* **222**, 403-410 (1994).
141. "Raman Optical Activity of Biomolecules" by L.A. Nafie in *Proceedings of the PharmAnalysis Conference and Exhibition*, Advanstar Communications Inc., Eugene, 1994, pp. 306-317.

- 141a. "Book Review of *Biomolecular Spectroscopy, Part A, Advances in Spectroscopy*, Vol. 20, R.J.H. Clark and R.E. Hester, eds., John Wiley & Sons, New York, 1993" by L.A. Nafie, *Spectroscopy* **9**, 41 (1994).
142. "Molecular Electronic Transition Current Density: Simple Orbital Transitions" by L.A. Nafie, in *Molecular and Biomolecular Electronics*, R.R. Birge, ed., ACS Advances in Chemistry, Vol. 240, Washington D.C., 1994, pp. 63-80.
143. "Raman Optical Activity of Biological Molecules" by L.A. Nafie, G.-S. Yu and T.B. Freedman, *Vibrational Spectrosc.* **8**, 231-239 (1995).
144. "Ab Initio Locally Distributed Origin Gauge Calculations of Vibrational Circular Dichroism Intensity: Formulation and Application to (S,S)-Oxirane-2,3-²H₂" by T.B. Freedman, L.A. Nafie and D. Yang, *Chem. Phys. Lett.* **227**, 419-428 (1994).
145. "Ab Initio Calculations of DCP_I ROA in Alanine and Alanyl Peptides" by L.A. Nafie, G.-S. Yu, P.L. Polavarpu, Z. Deng and T.B. Freedman, in *XIVth International Conference on Raman Spectroscopy*, N.-T. Yu and X.-Y. Li, eds., Wiley, New York, 1994, pp. 1088-1089.
146. "Backscattering Dual Circular Polarization Raman Optical Activity" by L.A. Nafie, G.-S. Yu and T.B. Freedman, in *XIVth International Conference on Raman Spectroscopy*, N.-T. Yu and X.-Y. Li, eds., Wiley, New York, 1994, pp. 244-245.
147. "Comparison of IR and Raman Forms of Vibrational Optical Activity" by L.A. Nafie, *Faraday Discuss.* **99**, 13-34 (1994).
148. "Circular Polarization Spectroscopy of Chiral Molecules" by L.A. Nafie, *J. Molec. Struct.* **347**, 83-100 (1995).
149. "Experimental Measurement and Ab Initio Calculation of Raman Optical Activity of L-Alanine and its Deuterated Isotopomers" by G.S. Yu, T.B. Freedman, L.A. Nafie, Z.Y. Deng and P.L. Polavarapu, *J. Phys. Chem.* **99**, 835-843 (1995).
150. "Vibrational Optical Activity of Oligopeptides" by T.B. Freedman, L.A. Nafie and T.A. Keiderling, *Biopolymers (Peptide Science)* **37**, 265-279 (1995).
- 150a. "An Editorial Letter of Introduction" L.A. Nafie, *Biospectroscopy*, **1**, 1 (1995).
151. "Raman Optical Activity of Simple Alanyl Peptides: Backscattering In-Phase Dual Circular Polarization Measurements in Aqueous Solution" by G.S. Yu, D. Che, T.B. Freedman and L.A. Nafie, *Biospectroscopy*, **1**, 113-123 (1995).
152. "Infrared and Raman Vibrational Optical Activity of Biomolecules" by L.A. Nafie in *Spectroscopy of Biological Molecules*, J.C. Merlin, S. Turrell and J.P. Huvenne, Eds., Kluwer Academic Publishers, Dordrecht, 1995 pp. 7-10.
153. "Raman Optical Activity of Small Peptides and Terpene Molecules", G.-S. Yu, M. Vargek, T.B. Freedman and L.A. Nafie in *Spectroscopy of Biological Molecules*, J.C. Merlin, S. Turrell and J.P.

Huvenne, Eds., Kluwer Academic Publishers, Dordrecht, 1995 pp. 77-78.

154. "Vibrational Circular Dichroism of Ephedrine and Related Molecules", G.-S. Yu, A. Potts, S. Alexander, F. Long, T.B. Freedman and L.A. Nafie in *Spectroscopy of Biological Molecules*, J.C. Merlin, S. Turrell and J.P. Huvenne, Eds., Kluwer Academic Publishers, Dordrecht, 1995 pp. 575-576.
155. "Dual Circular Polarization Raman Optical Activity of Related Terpene Molecules: Comparison of Backscattering DCP₁ and Right-Angle ICP Spectra" by Gu-Sheng Yu, Teresa B. Freedman and Laurence A. Nafie, *J. Raman Spectrosc.* **26**, 733-743 (1995).
156. "Theory of Resonance Raman Optical Activity: The Single Electronic State Limit" by L.A. Nafie, *Chem. Phys.* **205**, 309-322 (1996).
157. "Quantitative Comparison of Experimental Infrared and Raman Optical Activity Spectra" by X. Qu, E. Lee, G.-S. Yu, T.B. Freedman and L.A. Nafie, *Appl. Spectrosc.* **50**, 649-657 (1996).
158. "Vibrational Optical Activity" by L.A. Nafie, *Appl. Spectrosc.* (Invited Focal Point article) **50**(5), 14A-26A (1996).
159. "Theory of Resonance Raman Optical Activity in the Strong Resonance Limit" by L.A. Nafie, in *Fifteenth International Conference on Raman Spectroscopy*, Vol. 2, P. Stein and S.A. Asher, Eds., McGraw-Hill, New York, 1996, pp. 7-8.
160. "Advances in Backscattering Dual Circular Polarization Raman Optical Activity" by L.A. Nafie, M. Vargheese and T.B. Freedman, in *Fifteenth International Conference on Raman Spectroscopy*, Vol. 2, P. Stein and S.A. Asher, Eds., McGraw-Hill, New York, 1996, pp. 123-124.
161. "Optical Design and Sampling Methods for the Measurement of Vibrational Circular Dichroism using an FTIR Spectrometer" by L.A. Nafie, X. Qu, F. Long and T.B. Freedman, *Mikrochim. Acta, Supplement* **14**, 803-805 (1997).
162. "Comparison of Fourier Transform Vibrational Circular Dichroism and Multichannel Detected Raman Optical Activity" by L.A. Nafie, X. Qu, E. Lee, G.-S. Yu and T.B. Freedman, *Mikrochim. Acta, Supplement* **14**, 807-808 (1997).
163. "Step-Scan Fourier Transform Vibrational Circular Dichroism Measurements in the Vibrational Region above 2000 cm⁻¹", by F. Long, T.B. Freedman, T.J. Tague, Jr. and L.A. Nafie, *Appl. Spectrosc.* **51**, 508-511 (1997).
164. "Comparison of Step-Scan and Rapid-Scan Approaches to the Measurement of Mid-Infrared Fourier Transform Vibrational Circular Dichroism" by F. Long, T.B. Freedman, R. Hapanowicz and L.A. Nafie, *Appl. Spectrosc.* **51**, 504-507 (1997).
165. "New Improved Backscattering Dual Circular Polarization Raman Optical Activity Spectrometer with Enhanced Performance for Biomolecular Applications" *J. Raman Spectrosc.* **28**, 627-633 (1997).

166. "Resonance and Non-Resonance Raman Optical Activity in Pharmaceutical Analgesic Molecules" by Maria Vargek, Teresa B. Freedman and Laurence A. Nafie, *Spectroscopy of Biological Molecules: Modern Trends*, P. Carmona et al. (eds.), Kluwer Academic Publishers, 1997, pp. 459-460.
167. "Step-Scan Fourier Transform Vibrational Circular Dichroism Spectra of Pharmaceutical Molecules" by Fujin Long, Teresa B. Freedman and Laurence A. Nafie, in *Spectroscopy of Biological Molecules: Modern Trends*, P. Carmona et al. (eds.), Kluwer Academic Publishers, 1997, pp. 461-462.
168. "Infrared and Raman Vibrational Optical Activity: Theoretical and Experimental Aspects" by L.A. Nafie, *Ann. Rev. Phys. Chem.* **48**, 357-386 (1997).
169. "Electron Transition Current Density in Molecules. 1. Non-Born-Oppenheimer Theory of Vibronic and Vibrational Transitions" by L.A. Nafie, *J. Phys. Chem.* **101**, 7826-7833 (1997).
170. "Electron Transition Current Density in Molecules. 3. Ab Initio Calculations for Vibrations Transitions in Ethylene and Formaldehyde" by T.B. Freedman, M.-L. Shih, E. Lee and L.A. Nafie, *J. Am. Chem. Soc.*, **119**, 10620-10626 (1997).
171. "Progress in Vibrational Circular Dichroism and Raman Optical Activity" by Laurence A. Nafie and Teresa B. Freedman, in the 6th *International Conference on Circular Dichroism*, Pisa Italy, 1997, pp. 18.
172. "CH-Stretching Vibrational Circular Dichroism of α -Hydroxy Acids and Related Molecules" by Teresa B. Freedman, Denise Gigante, Eunah Lee, and Laurence A. Nafie, in the 6th *International Conference on Circular Dichroism*, Pisa Italy, 1997, pp. 77.
173. "Electron Transition Current Density in Molecules. 2. Ab Initio Calculations for Electronic Transitions in Ethylene and Formaldehyde" by T.B. Freedman, M.-L. Shih and L.A. Nafie, *J. Phys. Chem.*, **102**, 3352-3357 (1998).
174. "Experimental Observation of Resonance Raman Optical Activity" by M. Vargek, T.B. Freedman, E. Lee and L.A. Nafie, *Chem. Phys. Lett.* **287**, 359-364 (1998).
175. "CH-Stretching Vibrational Circular Dichroism of α -Hydroxy Acids and Related Molecules" by T.B. Freedman, D. Gigante, E. Lee, and L.A. Nafie, in *11th International Conference on Fourier Transform Spectroscopy*, J.A. de Haseth, ed., American Institute of Physics, Woodbury, NY, 1998, pp.723-725.
176. "Step-Scan Versus Rapid-Scan FTIR-VCD Spectroscopy Using HgCdTe and InSb Detectors" by F. Long, T.B. Freedman and L.A. Nafie, in *11th International Conference on Fourier Transform Spectroscopy*, J.A. de Haseth, ed., American Institute of Physics, Woodbury, NY, 1998, pp.375-376.
177. "Fourier Transform Vibrational Circular Dichroism of Small Pharmaceutical Molecules" by F. Long, T.B. Freedman and L.A. Nafie, in *11th International Conference on Fourier Transform Spectroscopy*, J.A. de Haseth, ed., American Institute of Physics, Woodbury, NY, 1998, pp.706-707.
178. "The Determination of Enantiomeric Purity and Absolute Configuration by Vibrational Circular Dichroism Spectroscopy" by L.A. Nafie, F. Long, T.B. Freedman, H. Buijs, A. Rilling, J.-R. Roy and R.K. Dukor, in *11th International Conference on Fourier Transform Spectroscopy*, J.A. de Haseth, ed., American Institute of Physics, Woodbury, NY, 1998, pp.432-434.

179. "Vibrational Circular Dichroism: An Incisive Tool for Stereochemical Applications" by L.A. Nafie and T. B. Freedman, *Enantiomer* **3**, 283-297 (1998).
180. "Hydrogen Stretching Vibrational Circular Dichroism in Methyl Lactate and Related Molecules" by D.M.P. Gigante, F. Long, L.A. Bodack, Jeffrey M. Evans, J. Kallmerten, L. A. Nafie and T.B. Freedman, *J. Phys. Chem. A* **103**, 1523-1537 (1999).
181. "Hydrogen-Stretching Vibrational Circular Dichroism Spectroscopy: Absolute Configuration and Solution Conformation of Selected Pharmaceutical Molecules" by T.B. Freedman, F. Long, M. Citra and L.A. Nafie, *Enantiomer* **4**, 103-119 (1999).
182. "Vibrational Circular Dichroism Studies of the Solution Conformation of Selected Tripeptides" by L.A. Bodack, T.B. Freedman, M. Plass and L.A. Nafie, in *Proceeding of the 12th International Conference on Fourier Transform Spectroscopy*, M. Tasumi and K. Itoh, eds., Waseda Univ. Press, 1999. pp. 265-266.
183. "The Determination of Enantiomeric Purity by Vibrational Circular Dichroism Spectroscopy" by R.K. Dukor, J.-R. Roy and L.A. Nafie, in *Proceeding of the 12th International Conference on Fourier Transform Spectroscopy*, M. Tasumi and K. Itoh, eds., Waseda Univ. Press, 1999, pp. 263-264.
184. "Theory of Raman Optical Activity" by Laurence A. Nafie, in *Encyclopedia of Spectroscopy and Spectrometry*, J. Lindon, G. Tranter and J. Holmes, Eds., Academic Press, Ltd., London, 2000, pp. 1976-1985. Also *Encyclopedia of Spectroscopy and Spectrometry II*, 2010, pp. 2397-2405.
185. "Vibrational Transition Current Density in (*S*)-Methyl Lactate: Visualizing the origin of the methine-stretching vibrational circular dichroism intensity" T.B. Freedman, E. Lee and L.A. Nafie, *J. Phys. Chem.* **104**, 3944-3951 (2000).
186. "Vibrational CD Spectrometer" by L.A. Nafie, in *Encyclopedia of Spectroscopy and Spectrometry*, J.C. Lindon, G.E. Tranter and J.L. Holmes, eds., Academic Press, Ltd., London, 2000, pp. 2391-2402. Also *Encyclopedia of Spectroscopy and Spectrometry II*, 2010, pp. 2899-2909
187. "Vibrational Optical Activity Theory" by Laurence A. Nafie and Teresa B. Freedman, in *Circular Dichroism: Principles and Applications for Biologists*, Second Edition, K. Nakanishi, N. Berova, R. Woody, eds., John Wiley and Sons, New York, 2000, pp. 97-131.
188. "Vibrational Transition Current Density in (2*S*,3*S*)-Oxirane-*d*₂: Visualizing Electronic and Nuclear Contributions to IR Absorption and Vibrational Circular Dichroism Intensities" by T.B. Freedman, E. Lee and L.A. Nafie, *J. Molec. Struct.* **550-551**, 123-134 (2000).
189. "Vibrational Optical Activity of Pharmaceuticals and Biomolecules" by R.K. Dukor and L.A. Nafie in *Encyclopedia of Analytical Chemistry: Instrumentation and Applications*, R.A. Meyers, Ed., John Wiley and Sons Ltd., Chichester, 2000, pp. 662-676.
190. "Dual Polarization Modulation: Real-Time, Spectral Multiplex Separation of Circular Dichroism from Linear Birefringence Spectral Intensities", L.A. Nafie, *Appl. Spectrosc.* **54**, 1634-1645 (2000).
191. "Theory of Raman Spectroscopy" by L. A. Nafie, in *Encyclopedia of Raman Spectroscopy*, Ian R. Lewis

- and Howell G.M. Edwards, Eds., Marcel Dekker Inc., New York, 2001. pp. 1-10.
192. “Biological and Pharmaceutical Applications of Vibrational Optical Activity” by L.A. Nafie and T.B. Freedman in *Infrared and Raman Spectroscopy of Biological Materials*, H.-U. Gremlich and B. Yan, eds., Marcel Dekker, Inc. New York, 2001. pp. 15-54.
193. “A Chiral 1,4-Oxazin-2-one: asymmetric synthesis versus resolution, Structure, Conformation and VCD Absolute Configuration” by A. Solladie-Cavallo, O. Sedy, M. Salisova, M. Biba, C.J. Welch, L. Nafie and T. Freedman, *Tetrahedron: Asymmetry* **12**, 2703-2707, (2001).
194. “Ab initio VCD calculation of a transition-metal containing molecule and new intensity enhancement mechanism for VCD” by Y. He, X. Cao, L.A. Nafie, T.B. Freedman, *J. Am. Chem. Soc.* **123**, 11320-11321 (2001).
195. “A New Chiral Oxathiane: Synthesis, Resolution and Absolute Configuration Determination by Vibrational Circular Dichroism” by A. Solladie-Cavallo, M. Balaz, M. Salisova, C. Suteu, L.A. Nafie, X. Cao and T. B. Freedman, *Tetrahedron: Asymmetry* **12**, 2605-2611, (2001).
196. “Spectroscopic methods for determining enantiomeric purity and absolute configuration in chiral pharmaceutical molecules” by Rekha D. Shah and Laurence A. Nafie, *Current Opinion in Drug Discovery & Development* **4**, 764-775 (2001).
197. “Role of Solvent and Secondary Doping in Polyaniline Films Doped with Chiral Camphorsulfonic Acid: Preparation of a Chiral Metal” by Dean M. Tigelaar, Wonpil Lee, Kenn A. Bates, Alexei Sapringin, Vladimir N. Prigodin, Xiaolin Cao, Laurence A. Nafie, Matthew S. Platz, and Arthur J. Epstein, *Chem. Materials* **14**, 1430-1438, (2002).
198. “The Use of Dual Polarization Modulation in Vibrational Circular Dichroism Spectroscopy” by L.A. Nafie and R. K. Dukor, in *Chirality: Physical Chemistry*, ACS Symposium Series 810, J.M. Hicks, Ed., American Chemical Society, Washington, D.C., 2002, pp. 79-88.
199. “Vibrational Circular Dichroism” by Laurence A. Nafie, Rina K. Dukor and Teresa B. Freedman, *Handbook of Vibrational Spectroscopy*, John M Chalmers and Peter R. Griffiths eds., John Wiley & Sons Ltd. Chichester, 2002, pp. 731-744.
200. “Determination of the Absolute Configuration of a Key Tricyclic Component of a Novel Vasopressin Receptor Antagonist by Use of Vibrational Circular Dichroism” by Alexey B. Dyatkin, Teresa B. Freedman, Xiaolin Cao, Rina K. Dukor, Bruce E. Maryanoff, Cynthia A. Maryanoff, Jay M. Matthews, Rekha D. Shah and Laurence A. Nafie, *Chirality* **14**, 215-219 (2002).
201. “Density Functional Theory Calculations of Vibrational Circular Dichroism in Transition Metal Complexes: Identification of Solution Conformations and Mode of Chloride Ion Association for (+)-Tris(ethylenediaminato)cobalt(III)” by Teresa B. Freedman, Xiaolin Cao, Daryl A. Young and Laurence A. Nafie, *J. Phys. Chem.* **106**, 3560-3565, (2002).
202. “(R)-(+)- and (S)-(-)-1-(9-Phenanthryl)ethylamine: Assignment of Absolute Configuration by CD Tweezer and VCD Methods, and Difficulties Encountered with the CD Exciton Chirality Method” by Arlette Solladie-Cavallo, Claire Marsol, Gennaro Pescitelli, Lorenzo Di Bari, Piero Salvadori, Xuefei

- Huang, Naoko Fujioka, Nina Berova, Xiaolin Cao, Teresa B. Freedman and Laurence A. Nafie, *Eur. J. Org. Chem.*, 1788-1796, (2002).
203. "Determination of the Absolute Configuration of (-)-Mirtazapine by Vibrational Circular Dichroism" by Teresa B. Freedman, Rina K. Dukor, Peter J.C.M. van Hoof, Edwin R. Kellenbach, and Laurence A. Nafie, *Helvetica Chimica Acta*. **85**, 1160-1165, (2002).
204. "Tripeptides Adopt Stable Structures in Water. A Combined Polarized Visible Raman, FTIR and VCD Spectroscopy Study" by Fatma Eker, Xiaolin Cao, Laurence A. Nafie, and Reinhard Schweitzer-Stenner, *J. Am. Chem. Soc.*, 14330-14341, (2002).
205. "Vibrational Optical Activity: Circular Polarization Forms, and Excited State Electronic Intensity Enhancement for ROA and VCD" by Laurence A. Nafie, in *Proceedings of XVIIIth International Conference on Raman Spectroscopy*, Janos Mink, Gyorgy Jalsovszky, and Gabor Keresztury eds., John Wiley & Sons Ltd. Chichester, 2002, pp. 59-61.
206. "Comparison of Raman Optical Activity and Vibrational Circular Dichroism of Proteins: What You Get and What You Don't" by Rina K. Dukor and Laurence A. Nafie, in *Proceedings of XVIIIth International Conference on Raman Spectroscopy*, Janos Mink, Gyorgy Jalsovszky, and Gabor Keresztury eds., John Wiley & Sons Ltd. Chichester, 2002, pp. 417-418.
207. "Performance Characteristics of a Dual Circular Polarization Raman Optical Activity Spectrometer" by David A. Dunmire and Laurence A. Nafie, in *Proceedings of XVIIIth International Conference on Raman Spectroscopy*, Janos Mink, Gyorgy Jalsovszky, and Gabor Keresztury eds., John Wiley & Sons Ltd. Chichester, 2002, pp. 423-424.
208. "Vibrational circular dichroism of chiral pesticides: cis-permethrin, malathion, and heptachlor" by Hiroshi Izumi, Shigeru Futamura, Laurence A. Nafie, Rina K. Dukor, ACS National Meeting, Am. Chem. Soc., Division of Environmental Chemistry, 42, 177-182, (2002).
209. "Structure Analysis of DI- and Tripeptides by FTIR, Polarized Raman and VCD Spectroscopy" by R. Schweitzer-Stenner, F. Eker, P. Mroz, P.M. Kozlowski, X. Cao and L. Nafie, in *Proceedings of XVIIIth International Conference on Raman Spectroscopy*, Janos Mink, Gyorgy Jalsovszky, and Gabor Keresztury eds., John Wiley & Sons Ltd. Chichester, 2002, pp. 733-734.
210. "The Structure of Alanine Based Tripeptides in Water and Dimethylsulfoxide Probed by Vibrational Spectroscopy" by Fatma Eker, Xiaolin Cao, Laurence A. Nafie, Qing Huang and Reinhard Schweitzer-Stenner, *J. Phys.Chem. A*, **107**, 358-365, (2003).
211. "Determination of the Absolute Configuration and Solution Conformation of Gossypol by Vibrational Circular Dichroism" by Teresa B. Freedman, Xiaolin Cao, Regina V. Oliveira, Quezia B. Cass, and Laurence A. Nafie, *Chirality*, **15**, 196-200, (2003)
212. "Vibrational absorption spectra, DFT and SCC-DFTB conformational study and analysis of [Leu]enkephalin" by Salim Abdali, T.A. Nichaus, Karl J. Jalkanen, Xiaolin Cao, Laurence A. Nafie, Th. Frauenheim, S. Suhai, and Henryk Bohr, *Phys. Chem. Chem. Phys.* **5**, 1295-1300, (2003).

213. "Structural Studies on McN-5652-X, a High-Affinity Ligand for the Serotonin Transporter in Mammalian Brain" by Bruce E. Maryanoff, David F. McComsey, Rina K. Dukor, Laurence A. Nafie, Teresa B. Freedman, Xiaolin Cao, and Victor W. Day, *Biorg. Med. Chem.* **11**, 2463-2470, (2003).
214. "Determination of Molecular Stereochemistry Using Vibrational Circular Dichroism Spectroscopy: Absolute Configuration and Solution Conformation of 5-Formyl-cis,cis-1,3,5-trimethyl-3-hydroxymethylcyclohexane-1-carboxylic Acid Lactone" by Hiroshi Izumi, Shigeru Futamura, Laurence A. Nafie, and Rina K. Dukor, *The Chemical Record* **3**, 112-119, (2003).
215. "Observation of Fourier Transform Near-Infrared Vibrational Circular Dichroism to 6150 cm^{-1} " by Laurence A. Nafie, Rina K. Dukor, Jean-René Roy, Allan Rilling, Xiaolin Cao and Henry Buijs, *Appl. Spectrosc.* **57** (10), 1245-1249, (2003).
216. Preparation of cruciferous phytoalexin related metabolites, (-)-dioxibrassinin and (-)-3-cyanomethyl-3-hydroxyoxindole, and determination of their absolute configurations by vibrational circular dichroism (VCD)" by Kenji Monde, Tohru Taniguchi, Nobuaki Miura, Sin-Ichiro Nishimura, Nobuyuki Harada, Rina K. Dukor and Laurence A. Nafie, *Tetrahedron Lett.* **44**, 6017-6020, (2003).
217. "An Unexpected Atropisomerically Stable 1,1-Biphenyl at Ambient Temperature in Solution, Elucidated by Vibrational Circular Dichroism (VCD)" by Teresa B. Freedman, Xiaolin Cao, Laurence A. Nafie, Monica Kalbermatter, Anthony Linden and Andreas Johannes Rippert, *Helvetica Chimica Acta.* **86**, 3141-3155, (2003).
218. "Erythro-1-Naphtyl-1-[2-piperidyl]-methanol: ^1H NMR and Absolute Configuration Determined by VCD" by L. Nafie, T.B. Freedman, X. Cao, A. Solladie-Cavallo, K Azyat and M. Roje, *J. Org. Chem.* **68**, 7308-7315, (2003).
219. "Absolute Configuration Determination of Chiral Molecules in the Solution State Using Vibrational Circular Dichroism" by T.B. Freedman, X. Cao, R. K. Dukor and L.A. Nafie, *Chirality* **15**, 743-758 (2003).
220. "The Structure of Tri-Proline in Water Probed by Polarized Raman, Fourier Transform Infrared, Vibrational Circular Dichroism, and Electric Ultraviolet Circular Dichroism Spectroscopy" by Reinhard Schweitzer-Stenner, Fatma Eker, Alejandro Perez, Kai Griebenow, Xiaolin Cao and Laurence A. Nafie, *Biopolymers (Peptide Science)*, **71**, 558-568, (2003).
221. "Presidential Reflections" by Laurence A. Nafie, *Appl. Spectrosc.*, **57**, 349A-351A, (2003).
222. "Determination of Absolute Configuration in Molecules with Chiral Axes by Vibrational Circular Dichroism: A C_2 -Symmetric Annelated Heptathiophene and a D_2 -Symmetric Dimer of 1,1'-Binaphtyl" by Teresa B. Freedman, Xiaolin Cao, Andrzej Rajca, Hua Wang, and Laurence A. Nafie, *J. Phys. Chem. A*, **107**, 7692-7696, (2003).
223. "Direct Observation of Odd-Even Effect for Chiral Alkyl Alcohols in Solution Using Vibrational Circular Dichroism Spectroscopy" by Hiroshi Izumi, Souko Yamagami, Shigeru Futamura, Laurence A. Nafie, Rina K. Dukor, *J. Am. Chem. Soc.*, **126**, 194-198, (2004).

224. "Tripeptides with Ionizable Side Chains Adopt a Perturbed Polyproline II Structure in Water" by Fatma Eker, Kai Griebenow, Xiaolin Cao, Laurence A. Nafie, Reinhard Schweitzer-Stenner, *Biochemistry*, **43**, 613-621, (2004).
225. "Solution conformation of Cyclosporins and Magnesium-Cyclosporin Complexes Determined by Vibrational Circular Dichroism" by Louise A. Bodack, Teresa B. Freedman, Babur Z. Chowdhry, and Laurence A. Nafie, *Biopolymers*, **73**, 163-177, (2004).
226. "New Approaches to the Determination of Absolute Configuration for Chiral Pharmaceuticals" by Laurence A. Nafie, *Business Briefing – PharmaTech*, (2004).
227. "The Conformation of Tetra-Alanine in Water Determination by Polarized Raman, FT-IR and VCD Spectroscopy" by Reinhard Schweitzer-Stenner, Fatma Eker, Kai Griebenow, Xiaolin Cao and Laurence A. Nafie, *J. Am. Chem. Soc.*, **126**, 2768-2776, (2004).
228. "Dual Source Fourier Transform Polarization Modulation Spectroscopy: An Improved Method for the Measurement of Circular and Linear Dichroism" by Laurence A. Nafie, Henry Buijs, Allan Rilling, Xiaolin Cao and Rina K. Dukor, *Appl. Spectrosc.*, **58**, 647-654, (2004).
229. "Theory of Vibrational Circular Dichroism and Infrared Absorption: Extension to Molecules with Low-Lying Excited Electronic States" by Laurence A. Nafie, *J. Phys. Chem. A*, **108**, 7222-7231, (2004).
230. "Extension of Fourier Transform Vibrational Circular Dichroism into the Near-Infrared Region: Continuous Spectral Coverage from 800 to 10,000 cm^{-1} " by Xiaolin Cao, Rekha D. Shah, Rina K. Dukor, Changning Guo, Teresa B. Freedman and Laurence A. Nafie, *Appl. Spectrosc.*, **58**, 1057-1064, (2004).
231. "Preferred peptide backbone conformations in the unfolded state revealed by the structure analysis of alanine-based (AXA) tripeptides in aqueous solution" by Fatma Eker, Kai Griebenow, Xiaolin Cao, Laurence A. Nafie, Reinhard Schweitzer-Stenner, *Proc. Nat. Acad. Sci.- PNAS*, **101**, 10054-10059, (2004).
- 231a. Correction: "Preferred peptide backbone conformations in the unfolded state revealed by the structure analysis of alanine-based (AXA) tripeptides in aqueous solution" by Fatma Eker, Kai Griebenow, Xiaolin Cao, Laurence A. Nafie, Reinhard Schweitzer-Stenner, *Proceedings of the National Academy of Sciences of the United States of America - PNAS*, **101**, 12777, (2004).
232. "VCD configuration of enantiopure/-enriched tetrasubstituted α -fluoro cyclohexanones and their use of epoxidation of trans-olefins" by T.B. Freedman, X. Cao, L.A. Nafie, A. Solladie-Cavallo, L. Jierry, L. Bouverat, *Chirality*, **16**, 467-474, (2004).
233. "Conformation determination of [Leu]enkephalin based on theoretical and experimental VA and VCD spectral analyses" by S. Abdali, K.J. Jalkanen, X. Cao, L.A. Nafie, H. Bohr, *Physical Chemistry Chemical Physics*, **6**, 2434-2439, (2004).
234. "Determination of enantiomeric excess in samples of chiral molecules using Fourier transform vibrational circular dichroism spectroscopy: Simulation of real-time reaction monitoring" by Changning

- Guo, Rekha D. Shah, Rina K. Dukor, Xiaolin Cao, Teresa Freedman, Laurence A. Nafie, *Anal. Chem.*, **76**, 6956-6966 (2004).
235. "Determination of the Absolute Configuration of the Anti-Fungal Pharmaceutical Agents: Ketoconazole, Itraconazole and Miconazole using Vibrational Circular Dichroism Measurements and Calculations" by D.A. Dunmire, T.B. Freedman, L.A. Nafie, C. Aeschlimann, J.G. Gerber and J. Gal, *Chirality*, **17**, S101-S108 (2005).
236. "Enantiomeric excess determination by Fourier transform near-infrared vibrational circular dichroism spectroscopy: Simulation of real-time process monitoring" by Changning Guo, Rekha D. Shah, Rina K. Dukor, Xiaolin Cao, Teresa B. Freedman and Laurence A. Nafie, *Appl. Spec.* **59**, 1114-1124, (2005).
237. "Determination of the atropisomeric stability and solution conformation of asymmetrically substituted biphenyls by means of vibrational circular dichroism (VCD)" by Teresa B. Freedman, Xiaolin Cao, Laurence A. Nafie, Monica Kalbermatter, Anthony Linden and Andreas Johannes Rippert, *Helvetica Chimica Acta*, **88**, 2304-2314, (2005).
238. "Stereochemical determination and bioactivity assessment of (S)-(+)-curcuphenol dimmers isolated from the marine sponge *didiscus aceratus* and synthesized through laccase biocatalysis" by Robert H. Cichewicz, Laura J. Clifford, Peter R. Lassen, Xiaolin Cao, Teresa B. Freedman, Laurence A. Nafie, Joshua D. Deschamps, Victor A. Kenyon, Jocelyn R. Flanary, Theodore R. Holman and Phillip Crews, *Bioorganic & Medicinal Chemistry*, **13**, 5600-5612, (2005).
239. "Phase equilibrium in poly(rA): poly(rU) complexes with Cd²⁺ and Mg²⁺ ions, studied by ultraviolet, infrared, and vibrational circular dichroism spectroscopy" by Yurii Blagoi, Galina Gladchenko, Laurence A. Nafie, Teresa B. Freedman, Victor Sorokin, Vladimir Valeev, and Yanan He, *Biopolymers*, **78**, 275-286, (2005).
240. "Chlorofluoroiodomethane as a potential candidate for parity violation measurements. Spectroscopic features: supersonic beam spectroscopy and VCD in the gas phase. Preparation of its partially resolved enantiomers and enantioselective recognition by a chiral cryptophane" by Pascale Soulard, Pierre Asselin, Arnaud Cuisset, Juan Ramon Aviles Moreno, Thérèse R. Huet, Denis Petitprez, Jean Demaison, Teresa B. Freedman, Xiaolin Cao, Laurence A. Nafie and Jeanne Crassous, *Phys. Chem. Chem. Phys.* **8**, 79-92 (2006).
241. "Structure and Absolute Configuration of Nyasol and Hirekiresinol Determined by Synthesis and Vibrational Circular Dichroism Spectroscopy" by Peter R. Lassen, Dorthe Mondrup Skytte, Lars Hemmingsen, Simon Feldbaek Nielson, Teresa B. Freedman, Laurence A. Nafie and S. Brogger Christensen, *J. Nat. Prod.*, **68**, 1603-1609 (2005).
242. "Determination of the Absolute Configuration and Solution Conformation of a Novel Disubstituted Pyrrolidine Acid A by Vibrational Circular Dichroism" by Teresa B. Freedman, Xiaolin Cao, Linda M. Phillips, Peter T. W. Cheng, Richard Dalterio, Yue-Zhong Shu, Hao Zhang, Ning Zhao, Rajesh, B. Shukla, Adirenne Tymiak, Stephen K. Gozo, Laurence A. Nafie, and Jack Z. Gougoutas, *Chirality*, **18**, 746-753 (2006).

243. “Fourier Transform Near-Infrared Vibrational Circular Dichroism Used for On-Line Monitoring of the Epimerization of 2,2-Dimethyl-1,3-Dioxolane-4-Methanol – A Pseudo Racemization Reaction” by Changning Guo, Rekha D. Shah, John Mills, Rina K. Dukor, Xiaolin Cao, Teresa B. Freedman and Laurence A. Nafie, *Chirality*, **18**, 775-782, (2006).
244. “Fourier transform near-infrared vibrational circular dichroism from 800 to 10,000 cm⁻¹: Near-IR spectral standards for terpenes and related molecules” by Changning Guo, Xiaolin Cao, Teresa B. Freedman and Laurence A. Nafie, *Vibrational Spectroscopy*, **42**, 254-272 (2006).
245. “Two Dimensional Vibrational Circular Dichroism Correlation Spectroscopy: pH Induced Spectral Changes in L-Alanine”, by Shengli Ma, T.B. Freedman, X. Cao and L.A. Nafie, *J. Mol. Struct.*, **799**, 226-238, (2006).
246. “Raman spectroscopic study of the L-type straight flagellar filament of *Salmonella*” by T. Uchihayama, M. Sonoyama, Y. Hamada, M. Komatsu, R.K. Dukor, L.A. Nafie, and K. Oosawa, *Vibrational Spectroscopy*, **42**, 192-194 (2006).
247. “Synthesis and vibrational circular dichroism of enantiopure chiral oxorhenium(V) complexes containing the hydrotris(1-pyrazolyl)borate ligand” by Peter R. Lassen, Laure Guy, Iyad Karame, Thierry Roisnel, Nicolas Vanthuyne, Christian Roussel, Xiaolin Cao, Rosina Lombardi, Jeanne Crassous, Teresa B. Freedman, and Laurence A. Nafie, *Inorg. Chem.* **45**, 10230-10239 (2006)
248. “Vibrational Optical Activity in Chiral Analysis” by Laurence A. Nafie and Rina K. Dukor, in *Chiral Analysis*, K.W. Busch and M.A. Busch, Eds, Elsevier, Amsterdam, 505-544, (2006).
249. “Applications of Vibrational Optical Activity in the Pharmaceutical Industry” by Laurence A. Nafie and Rina K. Dukor, in *Applications of Vibrational Spectroscopy in Pharmaceutical Research and Development*, Edited by Don Pivonka, John M. Chalmers and Peter R. Griffiths, John Wiley & Sons, Ltd., Chichester, pp. 129-154 (2007).
250. “Near-Infrared Excited Raman Optical Activity” by Laurence A. Nafie, Bruce E. Brinson, Xiaolin Cao, David A. Rice, Omar M. Rahim, Rina K. Dukor and Naomi J. Halas, *Appl. Spectrosc.* **61**, 1103-1106 (2007).
251. “Vibrational Circular Dichroism Shows Unusual Sensitivity to Protein Fibril Formation and Development in Solution” by Shengli Ma^a Xiaolin Cao, Mimi Mak, Adeola Sadik, Christoph Walkner, Teresa B. Freedman, Igor Lednev, Rina K. Dukor and Laurence A. Nafie, *J. Am. Chem. Soc.* **129**, 12364-12365 (2007).
252. “The Structural and Optical Isomers of Nonamethoxy Cyclotrimeratrylene – Separation and Physical Characterization” by Zeev Luz, Raphy Poupko, Ellen J. Wachtel, Hailin Zheng, Noga Friedman¹ Xiaolin Cao, Teresa B. Freedman Laurence A. Nafie and Herbert Zimmermann, *J. Phys. Chem. A* **111**, 10507-10516 (2007).
253. “Absolute configuration determination of chiral molecules without crystallisation by vibrational circular dichroism (VCD)” by Edwin R. Kellenbach, Rina K. Dukor and Laurence A. Nafie, *Spectroscopy Europe*, **19 (4)**, 15-19 (2007).

254. "HPLC separation and VCD spectroscopy of chiral pyrazoles from (5*R*)-dihydrocarvone" by Eva Tur, Guillaume Vives, Gwénaél Rapenne, Jeanne Crassous, Nicolas Vanthuylne, Christian Roussel, Rosina Lombardi, Teresa B. Freedman, and Laurence A. Nafie, *Tetrahedron Asymmetry* **18**, 1911-1917 (2007).
255. "Theory of Raman Scattering and Raman Optical Activity: Near-Resonance Theory and Levels of Approximation" by Laurence A. Nafie, *Theo. Chem. Acc.*, **119**, 39-55 (2008).
256. "Reduction of Linear Birefringence in Vibrational Circular Dichroism Measurements: Use of a Rotating Half-Wave Plate" by Xiaolin Cao, Rina K. Dukor and Laurence A. Nafie, *Theo. Chem. Acc.*, **119**, 69-79 (2008).
257. "A Combined Theoretical and Experimental Study of the Structure and Vibrational Absorption, Vibrational Circular Dichroism, Raman and Raman Optical Activity Spectra of the L-Histidine Zwitterion" by E. Deplazes, W. van Brownsjik, F. Zhu, L.D. Barron, S. Ma, L.A. Nafie and K.L. Jalkanen, *Theo. Chem. Acc.*, **119**, 155-176 (2008).
258. "Role of Hydration in Determining the Structure and Vibrational Spectra of L-Alanine and N-Acetyl L-Alanine N'-Methylamide in Aqueous Solution: A Combined Theoretical and Experimental Approach" by K.J. Jalkanen, I. M. Degryarenko, R.M. Nieminen, X. Cao, L.A. Nafie, F. Zhu and L.D. Barron, *Theo. Chem. Acc.*, **119**, 191-210 (2008).
259. "Vibrational Circular Dichroism (VCD) Analysis Reveals and Conformational Change of the Baccatin III Ring of Paclitaxel: Visualization of Conformations using a New Code for Structure-Activity Relationships" by Hiroshi Izumi, Atsushi Ogata, Laurence A. Nafie and Rina K. Dukor, *J. Org. Chem.* **73**, 2367-2372 (2008).
260. "Vibrational Circular Dichroism: A New Tool for the Solution-State Determination of the Structure and Absolute Configuration of Chiral Natural Product Molecules" by Laurence A. Nafie, *Nat. Prod. Comm.* **3**, 451-466 (2008).
261. "Isotopic Spectral Shifts as an Aide in Determining Absolute Configuration using Vibrational Optical Activity: VCD of ¹³C-Labelled Cyclotrimeratrylene" by T.B. Freedman, Xiaolin Cao, Zeev Luz, Herbert Zimmermann, Raphy Poupko and Laurence A. Nafie, *Chirality* **20**, 673-680 (2008).
262. "Raman optical activity of flagellar filaments of *Salmonella*: Increase in ROA intensity upon formation of certain self-assembled protein filaments and their possible higher level structures" by Tomonori Uchiyama, Masashi Sonoyama, Yoshiaki Hamada, Rina K. Dukor, Laurence A. Nafie, Fumio Hayashi and Kenji Oosawa *Vibrational Spectroscopy* **48**, 65-68(2008).
263. "Solvent Induced Conformational Changes of Secondary Structure of Amylose Carbamate using Vibrational Circular Dichroism" by Shengli Ma, Sherry Shen, Heewon Lee, Nathan Yee, Chris Senanayake, Laurence A. Nafie, Nelu Grinberg, *Tetrahedron: Asymmetry* **19**, 2111-2114 (2008).
264. "A Revised Conformational Code for the Exhaustive Analysis of Conformers with One-to-One Correspondence between Conformation and Code: Application to the VCD Analysis of(S)-

- Ibuprofen” by Hiroshi Izumi, Atsushi Ogata, Laurence A. Nafie and Rina K. Dukor, *J. Org. Chem.* **74**, 1231-1236 (2009).
265. “Subtle Chirality in Oxo- and Sulfhydro-Rhenium Complexes” by Frederi De Montigny, Laure Guy, Guillaume Pilet, Nicolas Vanthuyne, Christian Roussel, Rosina Lombardi, Teresa B. Freedman, Laurence A. Nafie and Jeanne Crassous, *Chem. Comm.* (32) 4841-4843 (2009).
266. “Structural determination of molecular stereochemistry using VCD spectroscopy and a conformational code: Absolute configuration and solution conformation of a chiral liquid pesticide, (*R*)-(+)-malathion” by Hiroshi Izumi, Atsushi Ogata, Laurence A. Nafie, Rina K. Dukor, *Chirality* **21**, E172-E180 (2009).
267. “Observation and calculation of vibrational circular birefringence: A new form of vibrational optical activity” by Rosina A. Lombardi, Laurence A. Nafie, *Chirality*, **21**, E277-E286 (2009).
268. “Structure and absolute configuration of ginkgolide B characterized by IR- and VCD spectroscopy” by N.H. Andersen, N.J. Christiansen, P.R. Lassen, T.B. Freedman, L.A. Nafie, K. Stromgaard, and L. Hemmingsen. *Chirality*, **22**, 217-223 (2010).
269. “Near-Infrared and Mid-Infrared Fourier Transform Vibrational Circular Dichroism of Proteins in Aqueous Solution” by Shengli Ma, Teresa B. Freedman, Rina K. Dukor, and Laurence A. Nafie, *Appl. Spectrosc.* **64**, 615-626 (2010).
270. “Observation of resonance electronic and non-resonance enhanced vibrational natural Raman optical activity” by Christian Merten, Honggang Li, Xuefang Lu, Andreas Hartwig and Laurence A. Nafie, DOI 10.1002/jrs.2750, *J. Raman Spectrosc.* **41**, 1272-1275 (2010).
271. “Direct Observation of pH Control of Reversed Supramolecular Chirality in Insulin Fibrils by Vibrational Circular Dichroism” by Dmitry Kurovski, Rosina A. Lombardi, Rina K. Dukor, Igor K. Lednev and Laurence A. Nafie, DOI: 10.1039/C0CC02423F, *Chem Comm.* **46**, 7154-7156 (2010).
272. “Absolute configuration reassignment of two chromanes from *Peperomia obtusifolia* (Piperaceae) using VCD and DFT calculations” by João Marcos Batista Jr., Andrea N. L. Batista, Daniel Rinaldo, Wagner Vilegas, Quezia B. Cass, Vanderlan S. Bolzani, Massuo J. Kato^c, Silvia N. López, Maysa Furlan and Laurence A. Nafie, DOI: 10.1016/j.tetasy.2010.09.004, *Tetra. Asym.* **21**, 2702-2706 (2010).
273. “Recent Advances in Linear and Non-Linear Raman Spectroscopy. Part IV” by Laurence A. Nafie, DOI 10.1002/jrs.2859, *J. Raman Spectrosc.* **41**, 1566-1586 (2010).
274. “Structure Elucidation and Absolute Stereochemistry of Isomeric Monoterpene Chromane Esters” by João M. Batista Jr, Andrea N. L. Batista, Jonas S. Mota, Quezia B. Cass, Massuo J. Kato, Vanderlan S. Bolzani, Teresa B. Freedman, Silvia N. López, Maysa Furlan and Laurence A. Nafie, Dxdoi.org/10/1021/jo1025089, *J. Org. Chem.* **76**, 2603-2612 (2011).

275. “Determination of Absolute Configuration of Chiral Molecules Using Vibrational Optical Activity: A Review” (Focal Point Review) by Yanan He, Bo Wang, Rina K. Dukor and Laurence A. Nafie, *Appl. Spectrosc.* **65**, 699-723 (2011).
276. “Vibrational Circular-Dichroism Spectroscopy of Homologous Cyclic Peptides Designed to Fold into β Helices of Opposite Chirality” by John L. Kulp III and Jeffrey C. Owirutsky, Dmitri Y. Petrovykh, Kenan P. Fears, Rosina Lombardi and Laurence A. Nafie, doi:10.1116/1.3548075, *Biointerphases* **6**, 1-7 (2011).
277. “A Confidence Level Algorithm for the Determination of Absolute Configuration using Vibrational Circular Dichroism or Raman Optical Activity” Elke Debie, Ewoud De Gussem, Rina K. Dukor, Wouter Herrebout, Laurence A. Nafie, Patrick Bultinck, DOI: 10.1002/cphc.201100050, *ChemPhysChem*, **12**, 1542-1549 (2011).
278. “Recent Advances in Linear and Non-Linear Raman Spectroscopy. Part V” by Laurence A. Nafie, DOI 10.1002/jrs.3115 *J. Raman Spectrosc.* **42**, 2049-2068 (2011).
279. “Absolute Configuration and Selective Trypanocidal Activity of Gaudichaudianic Acid Enantiomers” by João M. Batista Jr., Andrea N. L. Batista, Daniel Rinaldo, Wagner Vilegas, Daniela L. Ambrósio, Regina M. B. Cicarelli, Vanderlan S. Bolzani, Massuo J. Kato, Laurence A. Nafie, Silvia N. López, and Maysa Furlan, DOI: dxdoi.org/10.1021/np200085h, *J. Nat. Prod.* **74**, 1154-1160 (2011).
280. “Chirality and diastereoselection of Δ/Λ -configured tetrahedral zinc complexes through enantiopure Schiff base complexes: Combined VCD (vibrational circular dichroism), DFT, ^1H NMR and X-ray structural studies” Anne-Christine Chamayou, Steffen Lüdeke, Volker Brecht, Teresa B. Freedman, Laurence A. Nafie and Christoph Janiak, *Inorg. Chem.*, 11363-11374 (2011).
281. “Simultaneous Acquisition of All Four Forms of Circular Polarization Raman Optical Activity: Results for α -Pinene and Lysozyme” by Honggang Li and Laurence A. Nafie, DOI: 10.1002/jrs.3000, *J. Raman Spectrosc.* **43**, 89-94 (2012).
282. “Spontaneous Inter-Conversion of Insulin Fibril Chirality” by Dmitry Kurouski, Rina K. Dukor, Xuefang Lu, Laurence A. Nafie and Igor K. Lednev, DOI: 10.1039/c2cc16895b, *Chem Comm.* **48**, 2837-2839 (2012).
283. “Experimental and theoretical polarized Raman linear difference spectroscopy of small molecules with a new alignment method using stretched polyethylene film” Patrycja Kowalski, James R. Cheeseman, Kasra Razmkah, Ben Green, Laurence A. Nafie and Alison Rodger, dx.doi.org/10.1021/ac202432e, *Anal. Chem.*, **84**, 1394-1401 (2012).
284. “Analysis of the Molten Globule State of Bovine α -Lactalbumin by Using Vibrational Circular Dichroism” Soo Ryeon Ryu, Bogusława Czarnik-Matusiewicz, Rina K. Dukor, Laurence A. Nafie, and Young Mee Jung, doi:10.1016/j.vibspec.2012.02.006, *Vibr. Spectrosc.*, **60**, 68-72 (2012).

285. "Albendazole sulfoxide enantiomers: preparative chiral separation and absolute stereochemistry" by Tiago C. Lourenço, João M. Batista Jr., Maysa Furlan, Yanan He, Laurence A. Nafie, Cesar C. Santana and Quezia B. Cass, <http://dx.doi.org/10.1016/j.chroma.2012.01.070>, *J. Chrom. A*, **1230**, 61-65 (2012).
286. "Normal and Reversed Supramolecular Chirality of Insulin Fibrils Probed by VCD at the Proto-Filament Level of Fibril Structure" by Dmitry Kurouski, Xuefang Lu, Rina K. Dukor, Laurence A. Nafie and Igor K. Lednev, *Biophys. J.*, **103** 522-531 (2012).
287. "Infrared Vibrational Optical Activity: Measurement and Instrumentation" by Laurence A. Nafie, in *Comprehensive Chiroptical Spectroscopy, Volume 1: Instrumentation, Methodologies, and Theoretical Simulations*, Edited by N. Berova, P. L. Polavarapu, K. Nakanishi, and R. W. Woody, 2012 John Wiley & Sons, Inc. (2012) pp. 115-146.
288. VCD to determine absolute configuration of natural product molecules: secolignans from *Peperomia blanda* by Lidian G. Felipe, João M. Batista Jr., Debora C. Baldoqui, Isabele R. Nascimento, Massuo J. Kato, Yanan He, Laurence A. Nafie, and Maysa Furlan, DOI: 10.1039/C2OB25109D *Org. Biomolec. Chem.* **10**, 4208-4214 (2012).
289. "Vibrational Circular Dichroism" by Laurence A. Nafie, in *Comprehensive Chirality, Volume 8: Spectroscopic Analysis*, Edited by George Tranter, Elsevier, Amsterdam, (2012) pp. 478-497.
290. "Simultaneous Resonance Raman Optical Activity Involving Two Electronic States" by Christian Merten, Honggang Li and Laurence A. Nafie, dx.doi.org/10.1021/jp3036082 *J. Phys. Chem. A*, **116**(27), 7329-7336, (2012).
291. "Further monoterpene chromane esters from *Peperomia obtusifolia*: VCD determination of the absolute configuration of a new diastereomeric mixture" by João M. Batista Jr., Andrea N. L. Batista, Massuo J. Kato, Vanderlan S. Bolzani, Silvia N. López, Laurence A. Nafie, Maysa Furlan, <http://dx.doi.org/10.1016/j.tetlet.2012.08.113> *Tet. Lett.* **53**, 6051-6054 (2012).
292. "Recent Advances in Linear and Non-Linear Raman Spectroscopy. Part VI" by Laurence A. Nafie, DOI 10.1002/jrs.4221 *J. Raman Spectrosc.* **43**, 1845-1863 (2012).
293. "Vibrational Circular Dichroism Spectra of Lysozyme Solutions: Solvent Effects on Thermal Denaturation Processes" by Alessandra Giugliarelli, Paola Sassi, Marco Paolantoni, Assunta Morresi, Rina K. Dukor, and Laurence A Nafie, DOI: 10.1021/jp311268x *J. Phys. Chem. B* **117**, 2645-2652 (2013).
294. "Data Mining of Supersecondary Structure Homology between Light Chains of Immunoglobulins and MHC Molecules: Absence of the Common Conformational Fragment in the Human IgM Rheumatoid Factor" by Hiroshi Izumi, Akihiro Wakisaka; Laurence Nafie; Rina Dukor, *J. Chem. Infor. & Model.* **53**, 584-591 (2013).
295. "Handedness Detected by Microwaves" by Laurence A. Nafie, *Nature*, **297**, 446-448 (2013).
296. "Levels of Supramolecular Chirality in Polyglutamine Aggregates Revealed by Vibrational Circular Dichroism" by Dmitry Kurouski, Karunakar Kar, Ronald Wetzel, Rina K. Dukor, Igor

- K. Lednev and Laurence A. Nafie, DOI 10.1016/j.febslet.2013.03.038, *FEBS Lett.* **587**, 1638-1643 (2013).
297. “A combined experimental and theoretical analysis of the structure and vibrational spectra of Nacetyl L-histidine N'-methylamide in aqueous solution” by Karl James Jalkanen, Karin Bagger Stibius Jensen, Laurence A Nafie, Fujiang Zhu, Laurence D Barron, Yuriko Aoki, Berit Mannfors, Risto M. Nieminen, Vladimir Pomogaev, Carolina Silva Carvalho, Airton A. Martin, *Theo. Chem. Accts.* in press (2013).
298. “Vibrational circular dichroism as a new technology for determining the absolute configuration, conformation, and enantiomeric purity of chiral pharmaceutical ingredients” Laurence A. Nafie, Oliver McConnell, Doug Minick, Edwin Kellenbach, Yanan He, Bo Wang and Rina K. Dukor, www.usp.org/usp-nf/pharmacopeial-forum, *Pharmacopeial Forum* 39(4), (2013).
299. “Challenges in the assignment of relative and absolute configurations of complex molecules: computation can resolve conflicts between theory and experiment” Jie Ren, Guo-You Li, Lan Shen, Guo-Lin Zhang, Laurence A. Nafie, Hua-Jie Zhu, <http://dx.doi.org/10.1016/j.tet.2013.10.004>. *Tetrahedron* **69**, 10351-10356 (2013)
300. “Recent Advances in Linear and Non-Linear Raman Spectroscopy. Part VII” by Laurence A. Nafie, DOI 10.1002/jrs.4119 *J. Raman Spectrosc.* **44**, 1629-1648 (2013).
301. “The transition from the native to the acid-state characterized by multi-spectroscopy approach: Study for the holo-form of bovine α -lactalbumin” by Adriana Litwińczuk, Soo Ryeon Ryu, Laurence A Nafie, Jong Wha Lee, Hugh I Kim, Young Mee Jung, Bogusława Czarnik-Matusiewicz, DOI:10.1016/j.bbapap.2013.12.018 *Biochimica et Biophysica Acta*, **1844**, 593-606 (2014).
302. “Is Supramolecular Chirality the Underlying Cause of Major Morphology Differences in Amyloid Fibrils” by Dmitry Kurovski, Xuefang Lu, Ludmila Popova, William Wan, Maruda Shanmugasundaram, Gerald Stubbs, Rina K. Dukor, Igor K. Lednev and Laurence A. Nafie, DOI: <http://dx.doi.org/10.1021/ja407583r>, *J. Am. Chem. Soc.* **136**, 2302-2312 (2014).
303. “Amplified Vibrational Circular Dichroism as a Probe of Local Biomolecular Structure” by Sérgio R. Domingos, Adriana Huerta-Viga, Lambert Baij, Saeed Amirjalayer, Dorien A. E. Dunnebier, Annemarie J. C. Walters, Markus Finger, Laurence A. Nafie, Bas de Bruin, Wybren Jan Buma, and Sander Woutersen, DOI: <http://dx.doi.org/10.1021/ja411405s>, *J. Am. Chem. Soc.* **136**, 3530-3535 (2014).

BOOK

1. *Vibrational Optical Activity: Principles and Applications* by Laurence A. Nafie, John Wiley & Sons, Ltd., Chichester, (2011).

PATENTS

1. “Dual Circular Polarization Circular Dichroism Spectrometer” Laurence A. Nafie, U.S. Patent Number 6,480,277, filed October 18, 2001, issued November 12, 2002.
2. “Reaction Monitoring of Chiral Molecules using Fourier Transform Vibrational Circular Dichroism Spectroscopy” Laurence A. Nafie, Changning Guo and Rina K. Dukor, U.S. Patent Number 7,378,283, filed October 14, 2003, issued May 27, 2008, expires December 26, 2025.
3. “Methods and Apparatus for the Improvement of the Measurement of Circular and Linear Dichroism and Uses Thereof” Laurence A. Nafie and Henry Buijs, U.S. Patent Application Number 11/358,531, filed February 21, 2006, issued December 20, 2008. U.S. (2009), U.S. Patent Number 7,522,283 B2 20090421