

**LEMONT B. KIER, PH.D.**

Professor of Medicinal Chemistry and Nurse Anesthesia  
Virginia Commonwealth University, Richmond, VA  
Consultant in Medicinal Chemistry *Worldwide*  
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**Education**

Ohio State University, BS in Pharmacy, 1954  
University of Minnesota, Ph.D. 1958 (Medicinal Chemistry)

**Professional Positions**

Assistant Professor of Medicinal Chemistry	1959-1963	University of Florida
Associate Professor of Medicinal Chemistry	1963-1966	Ohio State University
Associate Fellow in Medicinal Chemistry	1966-1972	Battelle Institute, Columbus, Ohio
Professor of Chemistry	1972-1977	Massachusetts College of Pharmacy, Boston, MA
Department Chairman	1972-1974	Department of Medicinal Chemistry, Massachusetts College of Pharmacy, Boston, MA
Division Director	1974-1976	Massachusetts College of Pharmacy, Boston, MA
Department Chairman	1977-1987	School of Pharmacy, Virginia Commonwealth University, Richmond, VA
Professor of Medicinal Chemistry	1987-present	School of Pharmacy, Virginia Commonwealth University, Richmond, VA
Senior Fellow	2002 – present	Center for the Study of Biological Complexity
Visiting Professor	1989-2002	University of Lausanne, Switzerland

**Public Service**

**Military**

Commissioned	1954	2nd Lt., Medical Service Corps, U.S. Army Reserve
Active Duty	1958	Ft. Sam Houston, Texas
Active Reserve participation	1958-1966	

Retired Reserve	1969	Rank: Major
Certificate of Recognition	2001	US Dept. of Defense, Cold War Service

**Government**

Councilman Worthington (Ohio) City Council 1966 – 1972

**Civic**

Hanover Master Gardeners Assoc., founder, first President 1988

**Honors**

Rho Chi Pharmacy honorary fraternity	1953
Fellow of the Academy of Pharmaceutical Sciences	1981
Fellow of the American Association of Pharmaceutical Sciences	1986
Chair of Honor, University of Lausanne	1992
Virginia Life Achievement Award in Science	2004
Educator of Excellence Award, Nurse Anesthesia Program	2004
Distinguished Alumni Award, OSU College of Pharmacy	2006
Chairman's Award for Outstanding Service (Nurse Anesthesia)	2006
Research Achievement Award, Amer. Assoc. Pharm. Sci.	2008

**Professional Activities**

Adjunct Professor of Medicinal Chemistry	1969-1972	University of Michigan, Ann Arbor, MI
Scientific Advisor	1970-1971	Korean Institute of Science and Technology, Department of State, Seoul, South Korea
Chairman, Medicinal Chemistry Section	1972-1973	Academy of Pharmaceutical Science, APHA
Board of Directors	1972-1974	International Society of Quantum Biology
Editor	1972-1974	APHA Book Reviews in Medicinal Chemistry
Editorial Advisory Board	1980-1996	Molecular Pharmacology
Editorial Advisory Board	1992-1997	Quantitative Structure-Activity Relationships
Editorial Advisory Board	1992 –1994	Medicinal Chemistry Research
Editorial Advisory Board	1992-present	QSAR in Toxicology
Board Member	2000-present	QSAR Society
Associate Editor	2003-present	Chemistry & Biodiversity

**Professional Societies**

American Chemical Society  
 American Association of Pharmaceutical Scientist  
 American Association of Colleges of Pharmacy  
 QSAR Society

### **Virginia Commonwealth University Service**

Department <u>Chairman</u>	10 years
MCV Space Committee	4 years
Space Evaluation Team	1 year
Egyptian Building Renovation Committee, <u>Chairman</u>	2 years
VCU Governance Planning Committee	3 years
VCU Governance By Laws Committee, <u>Chairman</u>	1 year
Academic Computer Advisory Committee	3 years
Academic Computer Advisory Committee, <u>Chairman</u>	1 year
VCU Patent Committee, <u>Chairman</u>	3 years
A.D. Williams Grant-in-Aid Committee	4 years
Cancer Center Grant Committee	2 years
Search Committee, Director of MCV Computing	1/2 year
Search Committee, VP for Research	1/2 year
University Graduate Council	13 years
Programs/Courses Committee, <u>Chairman</u>	8 years
VCU Convocation Planning Committee	1 year
A.D. Williams Research Advisory Committee	5 years
VCU Faculty Handbook Committee	2 years
VCU Promotion and Tenure Committee	3 years
VCU Promotion and Tenure Committee, <u>Chairman</u>	2 years
VCU Promotion/Tenure By-Laws Revision Committee	2 years
VCU Graduate School, Development	6 years

### **Industrial and Government Research Grants, Contracts and Consultantships**

NIH CY	1961-1963
Strassenburg Labs	1961-1963
NIH HE	1962-1964
NIH GM	1965-1967
NIH AI	1966-1968
Miles Labs	1967
Mead Johnson	1968
Abbott Labs	1968
NIH GM	1968-1974
Bristol Meyers	1969
A. H. Robins	1969-1970
Norwich Pharmacal	1972
NIMH DA	1975-1979
Dynapol Co.	1979-1980
EPA	1981-1984
Gruppo-Leppitet (Italy)	1983
Mitre Corp	1984-1985
Eastman Kodak	1987
U.S. Army Chem. Res.	1988-1991

Allied Signal	1987
Sterling Research Inc.	1989-1994
DuPont Pharmaceutical	1994
Ares Sorono	1996,1999
SciVision/Academic Press	1998-present
U. S. Dept. of Ed.	2000-2001
Goodwin/Procter	2005-2007
Latham/Watkins	2005
Sapat	2008

### **Graduate Students, Post-Doctoral Fellows, Sabbatical Fellows**

K. K. Kaistha	Ph.D.	1962
D. Dhawan	Ph.D.	1963
T. Stewart	Ph.D.	1964
E. Roche	Ph.D.	1968
H. Aldrich (USA)	Postdoctoral	1973
H.-D. Holtje (Germany)	Postdoctoral	1974
T. DiPaolo (Canada)	Postdoctoral	1975
W. Murray (USA)	Sabbatical Fellow	1976
L. Hall (USA)	Sabbatical Fellow	1976
S. Tovivich	M.S.	1976
M. Tute, (England)	Sabbatical Fellow	1976
M. Lund	M.S.	1981
S. Baldwin, (USA)	Postdoctoral	1981
U. Kim, (Korea)	Sabbatical Fellow	1982
G. Szasz, (Hungary)	Sabbatical Fellow	1983
D. Bonchev, (Bulgaria)	Sabbatical Fellow	1990
A. T. Balaban, (Romania)	Sabbatical Fellow	1991
N. Joshi, (India)	Ph.D.	1993
C. De Gregorio, (Spain)	Graduate Student	1997
G. Gunnarsson, (Iceland)	Graduate Student	1998
P. Seybold (USA)	Sabbatical Fellow	2004

### **Invited Presentations At National And International Symposia \**

1. Buffalo, New York - August, 1968. Buffalo-Milan Symposium On Molecular Pharmacology. "Receptor Mapping Using Molecular Orbital Theory."
2. Seattle, Washington - October, 1969. Battelle Symposium On Quantum Pharmacology. "Molecular Orbital Considerations Of Aminoacid Conformation."
3. Richmond, Virginia - November, 1969. S. E. Regional American Chemical Society Meeting. "Molecular Orbital Calculations Of Preferred Conformation."
4. Toronto, Canada - May 1970. C.I.C.-A.C.S. Meeting. "Molecular Orbital Studies Of Drug Molecule Conformation."
5. Menton, France - July, 1970. International Colloquim On Quantum Chemistry.

- "Quantum Pharmacology: Molecular Orbital Studies Of Drug Molecule Conformations", plus seminars at Battelle Frankfort and Battelle Geneva.
6. Chonju, Korea - November, 1970. Korean Chemical Society. "Molecular Orbital Theory In Drug Research."
  7. Los Angeles, California - April, 1971. Pesticide Division, American Chemical Society. "Molecular Orbital Studies Of Drug And Hormone Molecule Conformation."
  8. Cincinnati, Ohio - June, 1971. Central Regional Meeting, American Chemical Society. "Molecular Orbital Considerations In Conformational Specificity."
  9. Andover, New Hampshire - July, 1971. Gordon Conference On Molecular Pharmacology. "Extended Huckel Calculations On Acetylcholine."
  10. Burlington, Vermont - August, 1971. American Society For Pharmacol. & Exp. Ther. And Division Of Medicinal Chemistry, A.C.S. "Molecular Orbital Studies Of Conformation And Physiological Activity In The Prostaglandins."
  11. New Orleans, Louisiana - February, 1972. American Chemical Society Mardi Gras Symposium. "Molecular Orbital Studies of Biological Molecule Conformations."
  12. Milan, Italy - September, 1972. International Symposium On Medicinal Chemistry. "The Prediction Of Molecular Conformation As A Biologically Significant Property."
  13. London, England - September, 1972. Society For Drug Research, Conference On Conformation And Drug Action. "Drug Conformation Calculated By Molecular Orbitals"
  14. Cambridge, Massachusetts - December, 1972. N. E. Regional Meeting, Medicinal Chemistry Division, A.C.S. "Molecular Orbital Studies Of Drug Molecules."
  15. Prague, Czechoslovakia - June, 1973. Conference On Structure-Activity Relationships. "Molecular Orbital Predictions Of Properties Influencing Biological Phenomena."
  16. Stockholm, Sweden - September, 1973. Federation Internationale Pharmaceutique. "Molecular Orbital Studies In Chemical Pharmacology."
  17. Noordwijkerhout, Netherlands - September, 1974. International Symposium On Medicinal Chemistry. "SAR Studies On GABA-Like Agents."
  18. Wadenswil, Switzerland - September, 1975. European Chemoreception Research Organization. "Theoretical Studies On The Sweet-Taste Glucophore."
  19. Atlanta, Georgia - November, 1975. Academy Of Pharmaceutical Sciences. "Molecular Connectivity In Drug Research."
  20. Gregynog, Wales, U. K. - May, 1976. European Symposium On Bioorganic Chemistry. "Theoretical Approaches To Drug SAR Studies."
  21. Namur, Belgium - May, 1976. International Symposium On Drug-Receptor And Drug-Enzyme Interactions. "Molecular Connectivity In Chemistry And Drug Research."
  22. Hollywood, Florida - November, 1978. Academy Of Pharmaceutical Sciences Symposium On Methods In SAR. "Molecular Connectivity In Drug Research."
  23. Kyoto, Japan - August, 1982. Fifth International Congress Of Pesticide Chemistry. "Recent Advances In Molecular Connectivity Analysis Of Biological Molecules."
  24. Portoroz, Yugoslavia Sept. 1986. Sixth European Conference on QSAR. "Molecular Shape from Chemical Graphs."
  25. Interlaken, Switzerland 1988. Seventh European Conference on QSAR. "Flexibility Quantitation."
  26. Lausanne, Switzerland March 1995. Lipophilicity Symposium "A Cellular Automata

- Model of Partitioning".
27. Valencia, Spain June 1997 "Molecular Connectivity Difference Indices" Girona, Spain  
1999 "The E-State Indices in Similarity Searching"
  28. Washington, D. C. 2000, Am. Chem. Soc., 25<sup>th</sup> Anniv. Symposium on Molecular  
Connectivity "The Meaning of Molecular Connectivity"
  29. Lugano, Switzerland, 2005, Computational methods in Drug Design, "The Prediction  
of ADMET Properties using Structure Information Representation"
  30. Honolulu, Hawaii 2005. Pacificchem Meeting, "Ligand Passage over Protein Surfaces"

## **PUBLICATIONS**

### **Books (authored)**

1. Molecular Orbital Theory In Drug Research. L. B. Kier, Academic Press, New York (1971).
  - a. Translated into Japanese in 1975, b. Translated into Indonesian in 1996
2. Molecular Connectivity In Chemistry and Drug Research. L. B. Kier and L. H. Hall, Academic Press, New York (1976)
3. Molecular Connectivity in Structure-Activity Analysis. L. B. Kier and L. H. Hall, John Wiley Publ, London (1986)
4. Molecular Structure Description: The Electrotopological State L. B. Kier and L. H. Hall, Academic Press, San Diego, (1999)
5. Medicinal Chemistry and Physics for Nurse Anesthetists L. B. Kier and C. Dowd Amer. Assoc. of Nurse Anesthetists, Chicago (2004)
6. Cellular Automata Modeling of Chemical Systems. L. B. Kier, P. G. Seybold and C.-K. Cheng, Springer, Amsterdam (2005)
7. Science and Complexity for Life Science Students. L. B. Kier, Kendall/Hunt, Dubuque, IO, (2007).

### **Books (edited)**

1. Molecular Orbital Studies In Chemical Pharmacology. L. B. Kier (Ed.). Springer-Verlag, New York (1970).

### **Book Chapters**

1. Drug-Receptor Interactions: Molecular Orbital Approaches. L. B. Kier, In Current Concepts In The Pharmaceutical Sciences (J. Swarbrick, Ed.) Lea and Febiger, Phila. (1970)

2. Molecular Orbital Theory In Drug Design. L. B. Kier, In Principles Of Medicinal Chemistry. (W. O. Foye, Ed.) Lea and Febiger, Phila. (1974)
3. Parasite Chemotherapy. L. B. Kier, In Principles Of Medicinal Chemistry. (W. O. Foye, Ed.) Lea and Febiger, Phila. (1974)
4. Theoretical Aspects of Drug Design. L. B. Kier and M. S. Tute, In Principles of Medicinal Chemistry. (W. O. Foye, Ed.) Lea Febiger, Phila. (1981). Revised 1989, 1994
5. Parasite Chemotherapy. E. B. Roche and L. B. Kier, Principles of Medicinal Chemistry. (W.O. Foye, Ed.) Lea Febiger, Phila. (1981). Revised 198
6. Electrotopological State Indices to Assess Molecular and ADMET Properties”, Chapter L. H. Hall, L. B. Kier and L. M. Hall 5 in Comprehensive Medicinal Chemistry, /Second Edition, eds. John Taylor and David Triggle, Elsevier Limited, Oxford, UK (2007).
7. Structure Information Representation (SIR) in Drug Discovery, L. B. Kier. L. H. Hall and L. Mark Hall, Chapter 4, in Comprehensive Medicinal Chemistry, /Second Edition, eds. John Taylor and David Triggle, Elsevier Limited, Oxford, UK (2007).

### **Research Articles**

1. A Note on Tigogenin From Digitalis Lanata. L. B. Kier and O. Gisvold, *J. Am. Pharm. Assoc., Sci. Ed.*, 45, 8 (1956)
2. The Alkaloids of Argemone Munita Subsp. Rotundata. L. B. Kier and T. O. Soine, *J. Am. Pharm. Assoc., Sci. Ed.*, 49, 187 (1960)
3. Reaction of Aniline with 3-Phenoxy-1,2-Epoxy Propane. L. B. Kier and R. B. Penland, *J. Org. Chem.*, 25, 1965 (1960)
4. Structural Studies on Related Argemone Alkaloids. L. B. Kier and T. O. Soine, *J. Pharm. Sci.*, 50, 321 (1961)
5. Triterpenes of Poria Obliqua. L. B. Kier, *J. Pharm. Sci.*, 50, 471 (1961)
6. Structural Studies on Terebinthone from Schinus Terebinthefolius. K. K. Kaistha and L. B. Kier, *J. Pharm. Sci.*, 51, 245 (1962)
7. A New Class of Central Nervous System Stimulants. L. B. Kier, L. E. Fox, D. Dhawan and I. W. Waters, *Nature* 195, 817 (1962)
8. Structural Studies on the Triterpenes of Schinus Terebinthefolius. K. K. Kaistha and L. B. Kier, *J. Pharm. Sci.*, 51, 1136 (1962)
9. The Synthesis of Sydnones as Potential Therapeutic Agents. L. B. Kier and D. Dhawan, *J. Pharm. Sci.*, 51, 1058 (1962)
10. On the Structure of Argemonine. T. O. Soine and L. B. Kier, *J. Pharm. Sci.*, 51, 1196 (1962)
11. Structural Studies on the Triterpene Obliquol. L. B. Kier and W. S. Brey, Jr., *J. Pharm. Sci.*, 52, 465 (1963)
12. Isolation of Podophyllotoxin from Callitrus Drummondii. L. B. Kier, D. B. Fitzgerald and S. Burgett, *J. Pharm. Sci.*, 52, 502 (1963)
13. The Structure of Argemonine, Identification as N-Methylpavine. M. Martell, T. O. Soine and L. B. Kier, *J. Am. Chem. Soc.* 85, 1022 (1963)
14. Nuclear Magnetic Resonance of Natural Products IV. Structure and Stereochemistry of Terebinthone and Schinol. L. B. Kier, "J. M. Lehn and G. Ourisson, *Bull. Soc. Chim. France*, 911 (1963)

15. The Structure of Bisnorargemonine. T. O. Soine and L. B. Kier, *J. Pharm. Sci.*, 52, 1013 (1963)
16. Derivatives of 1-Phenyl-4-(2-Hydroxy-3-Methoxypropyl) Piperazine. H. Howell, C.B. Pollard, L. B. Kier and H. H. Sisler, *J. Med. Chem.*, 6, 604 (1963)
17. Identification of Methyl Esters of Krebs Cycle Acids by Gas-Liquid Chromatography. H. H. Luke, T. E. Freeman and L. B. Kier, *Anal. Chem.*, 35, 1916 (1963)
18. Synthesis of Several Disubstituted Sydnone. D. Dhawan and L. B. Kier *J. Pharm. Sci.*, 53, 677 (1964)
19. Chloruretic, Naturetic and Depressor Activities of Some Substituted Sydnone. M. J. Fregley, L. B. Kier and D. Dhawan, *Tox. & Appl. Pharmacol.*, 6, 529 (1964)
20. Synthesis of 3-Alkylsydnone-4-Carboxylic Acids. L. B. Kier, D. Dhawan and M. J. Fregley, *J. Pharm. Sci.*, 53, 677 (1964)
21. Hydrogen Chemical Shifts of 3-Alkyl and 3-Phenylsydnone. K. D. Lawson, W. S. Brey and L. B. Kier, *J. Am. Chem. Soc.*, 86, 436 (1964)
22. A New Class of Antimicrobial Agents. L. B. Kier, M. C. Dodd, P. Sapko and T. G. Stewart, *Nature*, 204, 697 (1964)
23. Synthesis of Several Mesoionic 1,3,4-Thiadiazoles. T. G. Stewart and L. B. Kier, *J. Pharm. Sci.*, 54, 731 (1965)
24. Synthesis of Two 4,5-Dialkylsydnone. E. B. Roche and L. B. Kier, *J. Pharm. Sci.*, 54, 1700 (1965)
25. Calculation of Dipole Moments of Heteroatom Molecules. L. B. Kier, *Tetrahedron Letters*, 3273 (1965)
26. Molecular Orbital Localization Energies and Carbonyl Nucleophilic Reactivity. L. B. Kier, *J. Pharm. Sci.*, 55, 98 (1966)
27. Effect of Substituted Sulfamic Acid Compounds on Development of Renal Hypertension in Rats. M. J. Fregley and L. B. Kier, *Tox. & Appl. Pharmacol.*, 9, 124 (1966)
28. A New Class of Hypotensive Agents. L. B. Kier, A. Al-Shamma, R. Hahn and A. Tye, *Nature*, 210, 742 (1966)
29. Molecular Orbital Calculations of the Electronic Structure of the Sydnone. L. B. Kier and E. B. Roche, *J. Pharm. Sci.*, 55, 807 (1966)
30. Mesoionic Pseudo-Oxatriazoles as Hypotensive Agents. L. B. Kier, A. Al-Shamma, R. Hahn, and A. Tye, *J. Pharm. Sci.*, 55, 1467 (1966)
31. Medicinal Chemistry of the Mesoionic Compounds. L. B. Kier and E. B. Roche, *J. Pharm. Sci.*, 56, 149 (1966)
32. Acylation of 3-Phenylsydnone with Carboxylic Acids and Phosphorus Pentoxide. C. V. Greco, J. Tobias and L. B. Kier, *J. Hetero. Chem.*, 4, 160 (1967)
33. The Preferred Conformation of 3-Phenylsydnone an EHT-MO Calculation. L. B. Kier, *Tetrahedron Letters*, 1233 (1967)
34. Structure of Argemonine. Identification as (-)-N-Methylpavine. M. J. Martell, T. O. Soine and L. B. Kier, *J. Pharm. Sci.*, 56, 973 (1967)
35. Molecular Orbital Calculation of the Preferred Conformation of Acetylcholine, Muscarine and Muscarone. L. B. Kier, *Molec. Pharmacol.*, 3, 487 (1967)
36. A Molecular Orbital Study of the Reactions of Sydnone. E. B. Roche and L. B. Kier, *Tetrahedron*, 24, 1673 (1968)
37. A Molecular Orbital Calculation of the Preferred Conformation of Nicotine. L. B. Kier,

- Molec. Pharmacol.*, 4, 70 (1968)
38. Molecular Orbital Calculations of the Preferred Conformations of Histamine and a Theory on its Dual Activity. L. B. Kier, *J. Med. Chem.* 11, 4411 (1968)
  39. The Synthesis of Dialkyl Mesoionic 1,3,4-Thiadiazoles. L. B. Kier and M. K. Scott, *J. Hetero. Chem.*, 5, 277 (1968)
  40. Preferred Conformation of Serotonin and a Postulate on the Nature of its Receptor from MO Calculations. L. B. Kier, *J. Pharm. Sci.*, 57, 1188 (1968)
  41. The Conformation of 20-Oxopregnane Hormones from M.O. Calculations and A Consideration of the Cortisol Receptor. L. B. Kier, *J. Med. Chem.*, 11, 915 (1968)
  42. Similarities in the Interatomic Distances of Some Anti-inflammatory Agents and Inflammagenic Amines: A Possible Insight into their Common Receptors. L. B. Kier and M. W. Whitehouse, *J. Pharm. and Pharmacol.*, 20, 793 (1968)
  43. The Preferred Conformations of Ephedrine Isomers and the Nature of the Adrenergic Receptor. L. B. Kier, *J. Pharmacol. Exptl. Therap.*, 164, 75 (1968)
  44. The Preferred Conformation of Norepinephrine and A Consideration of the Alpha-Adrenergic Receptor. L. B. Kier, *J. Pharm. Pharmacol.*, 21, 93 (1969)
  45. The Conformation of Aminoacid Residues from M. O. Theory. L. B. Kier and J. M. George, *Theor. Chim. Acta*, 14, 258 (1969)
  46. Semi-empirical Quantum Mechanical Studies on Some Hydrogen Bonded Systems. J. R. Hoyland and L. B. Kier, *Theor. Chim. Acta*, 15, 1, (1969)
  47. Nieuwe Geneesmiddelen. L. B. Kier, *Natuur en Techniek*, 37, 229 (1969)
  48. Molecular Orbital Conformation of Oxotremorine and A Comparison with the Muscarinic Pattern. L. B. Kier, *J. Pharm. Sci.*, 59, 112 (1970)
  49. The Preferred Conformation of Dopamine From M. O. Theory. L. B. Kier and E. B. Truitt, *J. Pharmacol. Expt. Ther.*, 174, 94 (1970)
  50. M.O. Approaches to the Interpretation of Organic Mass Spectra. The Mass Spectra of Mesoionic Compounds. R. C. Dougherty, R. L. Foltz and L. B. Kier, *Tetrahedron*, 26, 1989 (1970)
  51. Conformations of Amino acids Calculated From M. O. Theory. J. M. George and L. B. Kier, *Experientia*, 26, 952 (1970)
  52. M. O. Studies on the Conformation of Gamma-Amino- butyric Acid and Muscimol. L. B. Kier and E. B. Truitt, *Experientia*, 26, 988 (1970)
  53. A Molecular Orbital Study of 3,5,3'-Trihalothyronine Analogues. L. B. Kier and J. R. Hoyland, *J. Med. Chem.*, 13, 1182 (1970)
  54. Molecular Orbital Consideration of Amino Acid Conformation. L. B. Kier and J.M. George, In Molecular Orbital Studies In Chemical Pharmacology. (L. B. Kier, Ed.). Springer-Verlag, New York (1970)
  55. Receptor Mapping Using Molecular Orbital Theory. L.B. Kier, In Fundamental Concepts In Drug-Receptor Interaction. (J.F. Moran and D.J. Trigg, Eds.). Academic Press, New York (1970)
  56. Quantum Pharmacology: Molecular Orbital Studies of Drug Molecule Conformations. L. B. Kier, In Current Concepts In the Pharmaceutical Sciences (J. Swarbrick, Ed.) Lea and Febiger, Phila. (1970)
  57. Molecular Orbital Conformation of Phenylcholine Ether. L. B. Kier and J. M. George, *J. Med. Chem.*, 14, 80 (1971)

58. Theoretical Considerations of Alpha and Beta Adrenergic Activity. J. M. George, L. B. Kier and J. R. Hoyland, *Molec. Pharmacol.*, 7, 328 (1971)
59. Molecular Orbital Theory in Drug Research. L. B. Kier, Prog. In Chem. and Chem. Ind. (Korea) 11, 18 (1971)
60. The Preferred Conformation of Prostaglandin E-1. J. R. Hoyland and L. B. Kier, *J. Med. Chem.*, 15, 84 (1972)
61. Mechanism of Action of Amodiaquin. Synthesis of its Indol- oquinoline Analog. V.E. Marquez, J.W. Cranston, R.W. Ruddon, L.B. Kier, and J.H. Burckhalter, *J. Med. Chem.*, 15, 36 (1972)
62. Molecular Orbital Studies of Ethylenediamine Conformation. M. S. Jhon, U. L. Cho, L. B. Kier and H. Eyring, *Proc. Nat. Acad. Sci.*, 69, 121 (1972)
63. Conformation of Gastrin Tetrapeptide. L. B. Kier and J. M. George, *J. Med. Chem.*, 15, 384 (1972)
64. A Molecular Theory of Sweet Taste. L. B. Kier, *J. Pharm. Sci.*, 61, 394 (1972)
65. The Preferred Conformation of the Muscarinic Agent L(+)-Acetylmethylcholine. M. S. Jhon, U. I. Cho, Y. B. Chae and L. B. Kier, *J. Korean Chem. Soc.*, 16, 70 (1972)
66. Molecular Orbital Studies Of Biological Molecule Conformations. L. B. Kier In, Biological Correlations: The Hansch Approach. (W. Van Valkenburg, ed.) American Chemical Society, Wash. D.C. (1972)
67. M. O. Studies on the Conformations of Bicuculline and Beta-Hydroxy GABA. L. B. Kier and J. M. George, *Experientia*, 29, 501 (1973)
68. Chlorpromazine and Serotonin: Conformational Similarities Correlating with Activities. L. B. Kier, *J. Theor. Biol.*, 40, 211 (1973)
69. Conformation of Thyrotropin-Releasing Hormone: Prediction From M. O. Theory. J. M. George and L. B. Kier, *J. Theor. Biol.*, 40, 393 (1973)
70. The Prediction of Molecular Conformation As A Biologically Significant Property. L. B. Kier, *Pure and Appl. Chem.*, 35, 509 (1973)
71. M. O. Studies of the Conformation Around the 5 Position in Angiotensin II. J. M. George and L. B. Kier, *J. Theor. Biol.*, 46, 111 (1974)
72. A Theoretical Approach to Structure-Activity Relationships of Chloamphenicol and Congeners. H. D. Holtje and L. B. Kier, *J. Med. Chem.*, 71, 814 (1974)
73. Structure-Activity Studies on GABA-Like Agents. L. B. Kier, J. M. George and H. D. Holtje, *J. Pharm. Sci.*, 63, 1435 (1974)
74. Studies on Sweet Taste Receptor Using Model Interaction Energy Calculations. H. D. Holtje and L. B. Kier, *J. Pharm. Sci.*, 63, 1722 (1974)
75. M. O. Calculations on Antiepileptic Compounds. H. S. Aldrich and L. B. Kier, *Molecular and Quantum Pharmacology* (E. Bergmann and B. Pullman, Eds.), Reidel Publ., Dordrecht, Holland (1974) p. 229
76. A Theoretical Study of Receptor Site Models for Trimethylammonium Group Interaction. L. B. Kier and H. S. Aldrich, *J. Theor. Biol.*, 46, 521 (1974)
77. Structure-Activity Studies of Enzyme Substrates Using Model Interaction Calculations. H. D. Holtje and L. B. Kier, *J. Theor. Biol.*, 48, 197 (1974)
78. Theoretical Studies on the Nature of the Alpha Site of Cholinesterase. H. D. Holtje and L. B. Kier, *J. Pharm. Sci.*, 64, 418 (1975)
79. A Stochastic Model of the Remote Recognition of Preferred Conformation in A

- Drug-Receptor Interaction. L. B. Kier and H. D. Holtje, *J. Theor. Biol.*, 49, 401 (1975)
80. Molecular Connectivity I. Relationship To Non-Specific Local Anesthetic Activity. L. B. Kier, L. H. Hall, W. J. Murray and M. Randic, *J. Pharm. Sci.*, 64, 1971 (1975)
  81. Molecular Connectivity II. Relationship to Water Solubility and Boiling Point. L. H. Hall, L. B. Kier and W. J. Murray, *J. Pharm. Sci.*, 64, 1974 (1975)
  82. Molecular Connectivity III. Relationship to Partition Coefficient. W. J. Murray, L. H. Hall and L. B. Kier, *J. Pharm. Sci.*, 64, 1978 (1975)
  83. Molecular Connectivity IV. Relationship to Biological Activity. L. B. Kier, W. J. Murray and L. H. Hall, *J. Med. Chem.*, 18, 1272 (1975)
  84. A Model for Drug Receptor Remote Recognition Applied to Certain Hydrogen Bonding Systems. L. H. Hall and L. B. Kier, *J. Theor. Biol.*, 58, 77 (1976)
  85. Molecular Connectivity V. Relationship to Density. L. B. Kier, L. H. Hall, M. Randic and W. J. Murray, *J. Pharm. Sci.*, 65, 1226 (1976)
  86. Molecular Connectivity VI. Examination of the Parabolic Relationship Between Molecular Connectivity and Biological Activity. L. B. Kier and L. H. Hall, *J. Med. Chem.*, 19, 578 (1976)
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### **Patents**

Certain Pseudo Oxatriazole Derivatives  
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