# Bibliography of theoretical calculations in molecular pharmacology

# Joanne L Taylor and Julian C Durant

Physical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, UK

## **INTRODUCTION**

A major activity in molecular graphics is to display the results of theoretical calculations on molecules. Nowhere is this more developed than in the area of molecular pharmacology. The extensive literature of calculations published up to the end of 1981 is covered by the bibliographies in the two editions of *Quantum pharmacology* (Richards, W G Butterworths, UK (1977, 1983)). This bibliography extends that coverage to the present time. It provides a background for the next issue of the *Journal of Molecular Graphics* (March 1986), which will be a special issue devoted to drug design.

### **ACETYLCHOLINE**

Hoeltje, H D, Lambrecht, G, Moser, U and Mutschler, E 'Cholinergic properties of isoarecaidine and sulphoarecaidine esters' *Arzneim Forsch* Vol 33 (1983) p 190

Palmer, R A, Tickle, J H and Tickle, I H 'Acetylcholine receptor site by graphics fitting' J. Mol. Graph. Vol I (1983) p 94

Rao, G S, Tyagi, R S and Mishra, R K 'Conformation of acetylcholine using molecular fragments' J. Theor. Biol. Vol 98 (1982) p 543

Zucarello, F, Raudino, A and Buemi, G 'Binding of cholinergic neuro-transmitters to anionic sites of synaptic receptors' J. Mol. Struct. (Theochem) Vol 87 (1982) p 197

# Anticholinergics, cholinesterase inhibitors and related compounds

Goldblum, A 'Affinities of phenyl N-methyl carbamates' Mol. Pharmacol. Vol 24 (1983) p 436

Hariharan, P C, Lewchenko, V, Koski, W S and Kaufman, J J 'Ab initio MODPOT/VRDDO calculations and electrostatic molecular potential contour maps of organophosphorus anticholinesterases' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 259

J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 259
Lewchenko, V, Hariharan, P C, Koski, W S and Kaufman, J J 'The phosphorylation step in the inhibition of AChE by organophosphorus anticholinesterases' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 275

Pauling, P and Datta, N 'Analysis of 24 antagonists of acetylcholine leading to single consistent energetically favourable conformation' *Proc. Natl. Acad. Sci. USA* (1979)

Weinstein, H, Maayani, S, Glick, S D and Meibach, R C 'Multi-disciplinary study of PCP pharmacology including treatment at the molecular level using graphics' in Domino, E F (ed) PCP (phencyclidine): historical and current perspectives NPP Books, USA (1981)

### Muscarine

Aronstam, R S, Triggle, D J and Eldefrawi, M E 'Structural and stereochemical requirements for muscarinic receptor binding' *Mol. Pharmacol.* Vol 15 (1979) p 227

Schulman, J M, Sabio, M L and Disch, R L 'Recognition of cholinergic agonists by the muscarinic receptor. Acetylcholine and other agonists with the NCCOCC backbone' J. Med. Chem. Vol 26 (1983) p 817

Weinstein, H, Maayani, S, Pazhenchevsky, B, Venanzi, C and Osman, R 'Recognition of phencyclidine derivatives at muscarinic cholinergic receptors' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 10 (1983) p 309

### **Nicotine**

Smythies, J R 'Molecular structure of nicotinic acetylcholine receptor' *Med. Hypotheses* Vol 6 (1980) p 943

### ADRENERGIC COMPOUNDS

Lumma, W C (Jr), Randall, W C, Cresson, E L, Huff, J R, Hartman, R D and Lyon, T F 'Piperazinylimidazo(1,2-a)pyrazines with selective affinity for in vitro α-adrenergic receptor subtypes' J. Med. Chem. Vol 26 (1983) p 357

Macchia, B, Balsamo, A, Lapucci, A, Martinelli, A, Macchia, F, Breschi, M C, Fantoni, B amd Martinotti, E 'Design of new structures active at the β-adrenergic receptor: aliphatic oxime ether derivatives' J. Med. Chem. Vol 28 (1985) p 153

### **ANAESTHETICS**

Adams, S M, Murphy, M J and Kaminsky, L S 'Metabolism of fluroxene and analogous anaesthetics' *Mol. Pharmacol.* Vol 20 (1981) n 423

Hobza, P, Mulder, F and Sandorfy, C 'Interaction between chloroform, floroform, and NH...O:C hydrogen bond' J. Am. Chem. Soc. Vol 104 (1982) p 925

Remko, M, Frecer, V and Cizmarik, J 'Conformational analysis of methyl phenyl carbamate and methoxy derivatives' *Archiv. Pharmazie* Vol 316 (1983) p 9

Remko, M, Frecer, V and Cizmarik, J 'Molecular orbital study of carbamate local anaesthetics' *Collect. Czech. Chem. Commun.* Vol 48 (1983) p 533

Remko, M, Sekerka, I and van Duijnen, P Th 'Study of phenyl-carbamates with local anaesthetic activity' *Archiv. Pharmazie* Vol 317 (1984) p 45

Remko, M and van Duijnen, P Th 'Ab initio investigation of procaine, lidocaine and heptacaine' J. Mol. Struct. (Theochem) Vol 105 (1983) p 1

Remko, M and van Duijnen, P Th 'Local anaesthetic-phospholipid interactions' J. Mol. Struct. (Theochem) Vol 104 (1983) p 451 Ruelle, P and Sandorfy, C 'Electrostatic potential around halogenated anaesthetics' Int. J. Quantum Chem. Vol 22 (1982) p 691

### **ANTIBIOTICS**

Cassidei, L, Maestro, M and Sciatovelli, O 'PCILO study on hexahydrorifamycin S' J. Mol. Struct. (Theochem) Vol 86 (1981) p 173 Chatterjee, C L and Saran, A 'Conformation of pyrazofurins by MO theory' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 8 (1981) p 129

Corey, E J and Ponder, J W 'Stereochemistry of the hydrolydins' Tetrahedron Lett. Vol 25 (1984) p 4325

De Beneditti, P G and Frassinetti, C 'Structure-activity relationships in diaryl sulfones, comparison with sulfa drugs' J. Mol. Struct. (Theochem) Vol 92 (1983) p 255

Graves, B J and Boyd, D B 'Correlations between CNDO/2 charge distribution and carbon-13 NMR chemical shift in 7-acylamino side chains of cephalosporins' J. Antibiot. Vol 37 (1984) p 1642

Hirayama, N, Shirahata, K, Ohashi, Y and Sasada, Y 'Conformations of fortimicins and 3D structure-activity relationship in the aminoglycoside antibiotics' *Mol. Pharmacol.* Vol 23 (1983) p 127

Lahiri, J and Basu, R 'Complexes of tetracycline and oxytetracycline drugs with nucleic acid bases and aromatic amino acids' J. Indian Chem. Soc. Vol 59 (1982) p 941

Masut, R A and Kushick, J N 'The molecular mechanics of valinomycin. 1. Energy minimisation calculations on the uncomplexed ionophore' J. Comp. Chem. Vol 5 (1984) p 336 Masut, R A and Kushick, N 'The molecular mechanics of valinomycin.

Masut, R A and Kushick, N 'The molecular mechanics of valinomycin. 2. Comparative studies of alkali ion binding' J. Comput. Chem. Vol. 6 (1985) p 148

Patnaik, L N and Saran, A 'Conformation of 2'-amino-2'-deoxyguano-sine' J. Biol. Phys. Vol 12 (1983) p 12

Sapse, A-M and Snyder, G 'An ab initio study of the reaction pathway between a mitomycin fragment model and ammonia' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 297

Chem. Quantum Biol. Symp. Vol 9 (1982) p 297
Saran, A and Patnaik, L N 'Molecular orbital studies on nucleoside antibiotics. Conformation of 5-vinyl- and 5-ethynyl-2'-deoxyuridines' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 247

Spark, M J, Winkler, D A and Andrews, P R 'Conformational analyses of folates and folate analogues' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 321

Vasudevan, T K and Rao, V S R 'Binding specificities of transpeptidases and penicillinases' Int. J. Biol. Macromol. Vol 4 (1982) p 219

Weinberg, J, Donescu, A and Sahini, V M 'HMO-LCAO calculations of some β-lactam antibiotics' Stud. Biophys. Vol 96 (1983) p 161
Weinberg, J, Donescu, A and Sahini, V M 'MO-LCAO Hückel calculations of some β-lactam antibiotics' Stud. Biophys. Vol 93 (1983) p 161
Zakrzewska, K, Lavery, R and Pullman, B 'Evaluation of the influence of solvent on binding energies to DNA of nonintercalating antibiotics' Nucleic Acids Res. Vol 12 (1984) p 6559

### Anticancer drugs and carcinogens

Abdul-Ahad, P G and Webb, G A 'Molecular orbital calculations on quinazolines and correlations with inhibitory potencies of DHFR' J. Mol. Struct. (Theochem) Vol 88 (1982) p 15

Adams, S M and Kaminsky, L S 'Molecular orbital studies of epoxide stability of carcinogenic polycyclic aromatic hydrocarbon diol epoxides' Mol. Pharmacol. Vol 22 (1982) p 459

Bakale, G, McCreary, R D and Gregg, E C 'Quasifree electron attachment to carcinogens' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 15

Balasubramanian, K, Kaufman, J J, Koski, W S and Balaban, A T 'Computer generation of carcinogenic benzenoid hydrocarbons' *J. Comput. Chem.* Vol 1 (1980) p 149

**Ball, J R and Thomson, C** 'Electronic theory of cancer — interaction of formamide and glyoxals' *J. Mol. Struct. (Theochem)* Vol 109 (1984) p 73

Blair, T and Webb, G A 'Anti-tumour activity of α-(N)-formyl isoquinoline thiosemicarbazones' J. Mol. Struct. (Theochem) Vol 89 (1982) p 35

Ferrel, J E and Loew, G H 'Mechanistic studies of arene oxide and diol epoxide rearrangement and hydrolysis reactions using MINDO/3' J. Am. Chem. Soc. Vol 101 (1979) p 1385

Guerch, G, Faucher, J-P, Graffeuil, M, Levy, G and Labarre, J-F 'Role of aziridinyl cyclophospazones as anticancer agents' J. Mol. Struct. (Theochem) Vol 88 (1982) p 317

Hariharan, P C, Popkie, H E and Kaufman, J J 'Attack of CH3(+)on guanine' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 13 (1979) p 225

**Imamura, A and Ohsaku, M A** 'Reactivity of polycyclic aromatic hydrocarbon diol epoxides' *J. Theoret. Biol.* Vol 102 (1983) p 511

Islam, S A, Neidle, S, Gandecha, B M and Brown, J R 'Experimental and computer graphics analyses of the DNA interaction of 1,8-bis-(2-diethylaminoethylamino)anthracene-9,10-dione as model for doxorubicin' *Biochem. Pharmacol.* Vol 32 (1983) p 2801

Kaufman, J J, Hariharan, P C, Koski, W S and Balasubramian, K 'Quantum chemical and other theoretical studies of carcinogens, their metabolic activation and attack on DNA constituents' *Prog. Clin. Biol. Res.* Vol 172 (Mol. Basis Cancer, Pt. A) (1985) p 263

Kikuchi, O, Karasawa, Y, Susiki, J and Hopfinger, A J 'Reactivity of methylazoxymethanol and metabolites with nucleophilic centres of DNA bases' Cancer Biochem. Biophys. Vol 6 (1982) p 75

Laurence, P R and Thomson, C 'Ab initio calculations of charge transfer interactions involving ascorbic acid and its metabolites' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 8 (1981) p 81

Liu, C, Shi, Z, Wang, Y and Dai, S 'Superdelocalizability and carcinogenesis of polycyclic aromatic hydrocarbons' *Fenzi Kexui Xuebao* Vol 1 (1981) p 19

Loew, GH, Phillips, J, Wong, J, Hjelmeland, L and Pack, G'Quantum mechanical studies of metabolism of polycyclic aromatic hydrocarbons—bay region reactivity as a criterion for carcinogenic potency' Cancer Biochem. Biophys. Vol 2 (1978) p 113

Loew, G, Poulsen, M, Ferrel, J and Chaet, D 'Studies of methyl benzo(A)anthracenes: metabolism and correlations with carcinogenicity' Chem. Biol. Interactions Vol 31 (1980) p 319

Loew, G H, Poulsen, M T, Spangler, D and Kirkjian, E 'Structure-activity studies of dialkylnitrosamines' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 10 (1983) p 201

Loew, G H, Sudhindra, B S and Ferrel, J E (Jr) 'Quantum mechanical studies of polycyclic aromatic hydrocarbons and metabolites — correlations with carcinogenesis' *Chem. Biol. Interactions* Vol 26 (1979) p. 75

Loew, G H, Sudhindra, B S, Walker, J M, Sigman, C C and Johnson, H L 'Mutagenic properties of aniline derivatives' J. Env. Path. and Tox. Vol 2 (1979) p 1069

Lowe, J P 'Theoretical study of relations between bay-region and K-region indices of carcinogenicity' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 5

Mohammad, S N 'Metabolic activation and carcinogenicity of extended anilines and aminoazo compounds' *Mol. Pharmacol.* Vol 27 (1985) p l

Perrin-Roussel, O, Croisy-Delcey, M, Mispelter, J, Saad, S, Chalvet, O, Ekert, B, Fouquet, J, Jacquignon, P, Lhoste, J-M, Muel, B and Zajdela, F E 'Study of metabolites of dibenzo(a,e) fluoranthene (DBF). Calculations of the relative stabilities of diol epoxides' *Cancer Res.* Vol 40 (1980) p 1742

Pullman, A and Pullman, B 'Mechanism of interaction of DNA with carcinogens' *INSERM* Vol 117 (1983) p 51

Pullman, B 'Polycyclic hydrocarbon carcinogenesis — an overall view with results of Hückel calculations on BP. epoxides' in *Polycyclic hydrocarbons and cancer* Vol 2 (1978) p 419

Reynolds, G and Thompson, C 'Nitrosation of amines' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 11 (1984) p 167

Rhee, J D and Yakhak Hoe Chi 'N'-nitrosonornicotine and its metabolic intermediates' Vol 26 (1982) p 175

Richards, W G and Cuthbertson, A F 'Binding of methotrexate to DHFR by quantum chemical calculation' J. Chem. Soc. Chem. Commun. Vol 167 (1984)

Sapse, A-M and Snyder, G 'An ab initio study of the reaction pathway between a mitomycin fragment model and ammonia' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 297

Sapse, A-M and Snyder, G'Molecular orbital calculations of properties of nitroso-ureas' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 10 (1983) p 175

Spark, M J, Winkler, D A and Andrews, P R 'Conformational analysis of folates and folate analogs' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 321

Szent-Györgyi, A 'Biological oxidation and cancer' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 27

Wang, Y and Zhou, S 'Structure-activity relations of sesquiterpenoid antitumour agents by MO theory' Yaoxue Xuebao Vol 18 (1983) p 25 Yukta, K and Jurs, P C 'Computer-assisted structure activity studies of chemical carcinogens. Aromatic amines' J. Med. Chem. Vol 24 (1981) p 241

Zhu, L, Qu, Y, Tang, W and Dai, A 'CNDO/2 study of mechanism of cisplatin binding to DNA' *Huaxue Xuebao* Vol 41 (1983) p 673

### **ANTIHYPERTENSIVES**

Burkert, U 'Conformational and constitutional equilibria of tetraoxabicyclo-[4.4.0]- and [5.3.0]-decanes, bicyclic diacetals of alditols' J. Comput. Chem. Vol 1 (1980) p 192

### **ANTIMALARIALS**

Wu, J, Chen, K and Ji, R 'EHT calculations of artemisinine and its derivatives Fenzi Kexue Xuebao Vol 1 (1981) p 27

### CARBOHYDRATES

Jeffrey, G A and Yates, J H 'Ab initio calculations of 1-methoxyethanol as a model for anomeric effect in pyranoses' Carbohydr. Res. Vol 96 (1981) p 205

Khodyreva, N V, Stolyarova, T V and Ivanov, M A 'Conformational analysis of \beta-D-glucose by zero differential overlap method' Khim. Drev. Vol 6 (1981) p 56

Leps, B, Barnickel, G, Bradaczek, H and Labischinski, H 'Structural studies of glycan strands of bacterial cell wall peptidoglycan pseudomurein' J. Theoret. Biol. Vol 107 91984) p 85

Tho, N X, Tronchet, J M J and Bill, H 'Study of conformational equilibria of E-1,3-disubstituted propenes as model for carbohydrates' Helv. Chim. Acta Vol 64 (1981) p 1949

Tvaroska, I 'Theoretical study of stereochemistry of methoxy(methylthio)methane as a model of the thioacetal segment in thiosaccharides' Collect. Czech. Chem. Commun. Vol 49 (1984) p 345

Yadav, J S, Barnickel, G, Bradaczek, H and Labischinski, H 'Conformational structure of bacterial peptidoglycan -- calculations on the monosaccharides' J. Theoret. Biol. Vol 95 (1982) p 151

Yadav, J S, Barnickel, G, Bradaczek, H and Labischinski, H 'Conformational structure of bacterial peptidoglycan — calculations on the N-acetyl glucosamine' J. Theoret. Biol. Vol 95 (1982) p 167

### CENTRAL NERVOUS SYSTEM DRUGS

### **Amphetamine**

Anderson, G M, Castagnoli, N (Jr) and Kollman, P A 'Structure-activity relationships in 2,4,5 ring substituted phenylisopropylamines — conformational perturbations by PCILO and ab initio molecular orbital methods' in Barnett, G, Trsic, M and Willette, R (eds) "QuaSAR' Research Monograph 22 Nat. Inst. Drug Abuse (1978)

Anderson, G M, Kollman, P A, Domelsmith, L N and Houk, K N 'Predictive model for conformations and rotational barriers for alkoxy aromatics — hallucinogenic properties of polyalkoxy-amphetamines' J. Am. Chem. Soc. Vol 101 (1979) p 2344

### **Analgesics**

Chen, C and Li, L 'Mechanism of analgesia of 3-methylfentanyl and analogs' Int. J. Quantum Chem. Vol 23 (1983) p 1597

Cheney, V, Zichi, D A and Miller, A B 'N-protonated benzomorphan molecules — binding at agonist and antagonist states of opioid receptor' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 10 (1983) p 43

Froimowitz, M 'Conformation-activity study of 4-phenylpiperidine analgesics' J. Med. Chem. Vol 25 (1982) p 1127

Froimowitz, M 'Conformation-activity study of methadone and related compounds' J. Med. Chem. Vol 25 (1982) p 689

Froimowitz, M 'Preferred conformers of polymorphan opiates' J. Med. Chem. Vol 27 (1984) p 1234

Froimowitz, M and Kollman, P 'A study of the biologically active conformers for proline opiates and their derivatives' J. Comput. Chem. Vol 5 (1984) p 507

Froimowitz, M, Salva, P, Hite, G J, Gianutsos, G, Suzdak, P and Heyman, R 'Conformational properties of α- and β-azabicyclane opiates. The effect of conformation on pharmacological activity' J. Comput. Chem. Vol 5 (1984) p 291

Loew, G H and Berkowitz, D S 'Effect of C7 substitution on agonist/ antagonist activity in oripavines' in Van Ree and Trenius (eds) Characteristics and function of opioids Biomedical Press, Elsevier, Netherlands (1978) p 223

Mazurek, A P, Weinstein, H, Osman, R, Topiol, S and Ebersole, B J 'Determinants for recognition of 5-hydroxytryptamine analogs' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 11 (1984) p 183

Miyashita, Y, Seki, T, Yotsui, Y, Yamazaki, K, Sano, M, Abe, H and Sasaki, S 'Analgesic activity in pyrazolylpyrimidine derivatives' Bull. Chem. Soc. Jpn. Vol 55 (1982) p 1489

### Antianxiety and antipsychotic drugs

Crasnier, F, Mouzin, G and Cousse, H 'Seven-membered structure of glycylanilide anxiolytics' J. Mol. Struct. (Theochem) Vol 85 (1981) p 311

Loew, G H, Nienow, J R and Poulsen, M 'Structure-activity studies for benzodiazepines' Mol. Pharmacol. Vol 26 (1984) p 19

### Psychotropic drugs

Reggio, P H, Weinstein, H, Osman, R and Topiol, S'Binding of methylenedioxytryptamines at 5-HT/LSD receptors' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 8 (1981) p 373

Weinstein, H, Osman, R, Green, J P and Topiol, P 'The basis for successful predictions of biological activity using electrostatic potentials — example LSD' in Politzer, P and Truhlar, D G (eds) Chemical applications of atomic and molecular electrostatic potentials Plenum Press, USA (1980) Chapter 16

### **DOPAMINE**

Burlamacchi, L, Lai, A, Monduzzi, M and Saba, G 'Complexes of dopamine with Cu(2+), Mn(2+) and Fe(3+)' J. Magn. Reson. Vol

Kocjan, D, Solmajer, T and Hadzi, D 'Conformational studies of dopaminergic ligands by molecular mechanics' Stud. Phys. Theor. Chem. Vol 18 (1982) p 79

Richards, W G 'Non-equilibrium conformations' Proc. Symp. on Steric

Effects in Biomolecules Eger, Hungary (1981) p 61 Richards, W G and Wallis, J 'The distribution of charge (within spheres) in biologically active amines (dopamine - neutral and monocation)' Proc. R. Soc. Lond. Ser. B. Vol 199 (1977) p 291

van der Waterbeemd, H and Testa, B 'Theoretical conformational studies of some dopamine antagonistic benzamide drugs: 3-pyrrolidyl and 4-pyrrolidyl derivatives' J. Med. Chem. Vol 26 (1983) p 203

### **ENZYMES**

Abdul-Ahad, P G and Webb, G A 'Inhibitory potency of pteridines and triazines on DHFR' J. Mol. Struct. (Theochem) Vol 89 (1982) p 25

Abdul-Ahad, P G and Webb, G A 'Molecular orbital calculations on quinazolines and correlations with inhibitory potencies of DHFR' J. Mol. Struct. (Theochem) Vol 88 (1982) p 15

Alagona, G, Desmeules, P, Ghio, C and Kollman, P A 'Quantum mechanical and molecular mechanical studies on a model for the dihydroxyacetone phosphate — glyceraldehyde phosphate isomerisation catalysed by TIM' J. Am. Chem. Soc. Vol 106 (1984) p 3623

Andrews, P R, Cain, E N, Rizzardo, E and Smith, G D 'Transition-state structure for chorismate-prephenate rearrangement' Biochem. Vol. 16 (1977) p 4848

Brandt, R B, Brandt, M E and April, M E 'Potential transition-state inhibitors of glyoxalase-I' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 335

Christianson, D W and Lipscomb, W N 'A molecular orbital evaluation of possible factors affecting the homolytic activation of coenzyme B12' J. Am. Chem. Soc. Vol 107 (1985) p 2682

Clementi, E, Corongui, G, Gratarola, M, Habitz, P, Lupo, C, Otto, P and Vercauteren, D 'Solvation of DNA and proteins (enzymes)' Int. J. Quantum Chem. Quantum Chem. Symp. Vol 16 (1982) p 409

Cook, C M, Haydock, K, Lee, R H and Allen, L C 'Electronic structure investigations of catalysis: carbonic anhydrase' J. Phys. Chem. Vol 88 (1984) p 4875

Cook, CM, Lee, RH and Allen, LC 'Inhibition of carbonic anhydrase' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 10 (1983) p 263

Dive, G, Peeters, D, Leroy, G and Ghysen, J M 'C-N bond cleavage by serine peptidases' J. Mol. Struct. (Theochem) Vol 107 (1984) p 117 Etzler, F M, Hristea, M and Comorosan, S 'Effect of electromagnetic field on enzymic substrate, a time dependent perturbation analysis' Rev. Roum. Biochim. Vol 19 (1982) p 267

Ferreira, R and Gomes, M A F 'Electronic aspects of enzymatic catalysis' Int. J. Quantum Chem. Vol 22 (1982) p 537

Gready, J E 'Geometries of substrates and inhibitors of dihydrofolate and dihydropteridine reductases' J. Mol. Struct. (Theochem) Vol 109 (1984) p 231

Gresh, N and Pullman, B 'Interaction of ammonium and guanidinium ions with phosphodiester linkage' *Theor. Chim. Acta* Vol 52 (1979) p 67

Hopfinger, A J 'A quantitative structure-activity relationship study of 2,4-diamino-5-benzylpyrimidines as DHFR inhibitors' J. Med. Chem. Vol 26 (1983) p 990

Hopfinger, A J 'Inhibition of DHFR: structure-activity correlations of 2,4-diamino-5-benzylpyramidines based upon molecular shape analysis' J. Med. Chem. Vol 24 (1981) p 818

Hosoya, T, Fujii, T and Ogawa, S 'Oxidation of hydrogen donor

Hosoya, T, Fujii, T and Ogawa, S 'Oxidation of hydrogen donor molecules by peroxidase compound II' J. Theor. Biol. Vol 100 (1983) p 283

Humphries, R L 'Computer simulation of binding between flexible ligand and polymeric receptor e.g. enzyme and substrate' J. Theor. Biol. Vol 91 (1981) p 477

Lambros, S A, Richards, W G and Marchington, A F 'Binding of n-alkylboronic acids to α-chromotrypsin A' J. Mol. Struct. (Theochem) Vol 109 (1984) p 61

Lavery, R, Pullman, A and Wen, Y K 'Electrostatic potentials and fields created by papain (thiol protease)' *Int. J. Quantum Chem.* Vol 24 (1983) p 353

Maggiora, G M and Christoffersen, R E 'Quantum mechanical approaches to enzyme transition states' in Showen, R L and Gardour, R D (eds) Transition states of biochemical processes Plenum Press (1977) Martin, M, Sanz, F, Campillo, M, Pardo, L, Perez, J and Turmo, J 'Molecular patterns of MAO inhibitors and substrates' Int. J. Quantum Chem. Vol 23 (1983) p 1627

Nakagawa, S and Umeyama, H 'Proton transfer energetics between glu 270 and Zn-coordinated H20 in carboxypeptidase A' J. Theor. Biol. Vol 96 (1982) p 473

Naray-Szabo, G 'Quantum chemical calculation of the enzyme-ligand interaction energy for trypsin inhibition by benzamidines' J. Am. Chem. Soc. Vol 106 (1984) p 4584

Naray-Szabo, G and Bleha, T 'Quantum chemical studies on the mechanism of enzyme action' *Prog. Theor. Org. Chem.* Vol 3 (1982) p 267

Naray-Szabo, G, Polgar, L, Kapur, A and Mezey, P G 'Serine proteases — protonation of the histidine-aspartate diad of subtilisin' J. Mol. Struct. (Theochem) Vol 90 (1982) p 137

Pudzianowski, A T, Loew, G H, Mico, B A, Blanchflower, R V and Pohl, L R 'A molecular orbital study of model cytochrome P450 oxidation of CC14 and CHC13' J. Am. Chem. Soc. Vol 105 (1983) p 3434

Richards, W G and Cuthbertson, A F 'Binding of methotrexate to DHFR by quantum chemical calculation' J. Chem. Soc., Chem. Commun. Vol 167 (1984)

Sapse, A M, Russell, C S and Snyder, G 'SCF calculations on 2-aminomethyl-3-carboxymethyl pyrrole, a substrate analog of PBG deaminase. Evidence of intramolecular hydrogen bonding' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 8 (1981) p 73

Shea, J P, Nelson, S D and Ford, G P 'MNDO calculation of kinetic isotope effects in model cytochrome P450 oxidations' J. Am. Chem. Soc. Vol 105 (1983) p 5451

Strich, A and Veillard, V 'The structure of the active oxygen complex of catalase: model calculations' *Theor. Chim. Acta* Vol 60 (1981) p 379 **Thomson, C and Brandt, R** 'Structure of glyoxalase-I inhibitors' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 10 (1983) p 357

Umeyama, H 'Quantum chemical studies on enzymic reaction mechanisms' Yakugaku Zasshi Vol 102 (1982) p 503

Venanzi, C A, Weinstein, H, Corongiu, G and Clementi, E 'The solvent effect in enzyme-substrate interactions: models of carboxypeptidase' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 355

Vol-Kenshtein, M V, Golovanov, I B and Sobolev, V M in Molecular orbitals in enzymology, Nauka, Moscow, USSR (1982) p 239

### GABA (gamma. amino butyric acid)

Andrews, P R, Iskander, M N, Jones, G P and Winkler, D A 'Design of transition-state analogues for GABA-transaminase' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 345

**Armstrong, D R, Breckenbridge, R J and Suckling, C J** 'Muscimol and aza analogs as GABA mimetics by molecular orbital theory' *J. Theor. Biol.* Vol 97 (1982) p 267

Blake, I O, Les, A and Rybak, S'Interaction of GABA with hydrated Ca(2+) and Mg(2+)' J. Theor. Biol. Vol 104 (1983) p 571

Richards, W G 'Non-equilibrium conformations' Proc. Symp. on Steric Effects in Biomolecules Eger, Hungary (1981) p 61

Richards, W G and Wallis, J 'The distribution of charge (within spheres) in biologically active amines (GABA — neutral and zwitterion)' Proc. R. Soc. Lond. Ser. B. Vol 199 (1977) p 291

Steward, E G, Borthwick, P W, Clarke, G R and Warner, D 'Agonism and antagonism of GABA. Analysis of the role of agonist flexibility' *Nature* Vol 256 (1975) p 600

Steward, E G and Lowe, R H 'Structure-activity relationships in inhibitory processes in the GABA-nergic system' in Ryall and Kelly (eds) Iontophoresis and transmitter mechanisms in the mammalian CNS (1978) p 394

### **GENERAL DRUG DESIGN**

Davies, R H, Smith, D A, McNellie, D J and Morris, T R 'The identification of biologically active conformations in flexible drug molecules' Sanibel-Palm Coast Symp., Quant. Biol. (1979)

Goodford, P J 'Drug design by the method of receptor fit' J. Med. Chem. Vol 27 (1984) p 557

Kaufman, J J 'General account of theoretical approaches to pharmacology' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 4 (1977) p 375

**Kaufman**, J J 'Quantum chemical and physicochemical influences on the structure-activity relations and drug design' *Int. J. Quantum Chem.* Vol 16 (1979) p 221

Kollman, P Theory of complex molecular reactions: computer graphics, distance geometry, molecular mechanics and quantum mechanics' Acc. Chem. Res. Vol 18 (1985) p 105

Lukovits, I 'Quantitative structure-activity relationships employing independent quantum chemical indices' J. Med. Chem. Vol 26 (1983) p 1104

Richards, W G and Black, M E 'Quantum chemistry in drug research' *Prog. Med. Chem.* Vol 11 (1975) p 67

### **HISTAMINE**

Carpy, A, Leger, J M, Leclerc, G, Decker, N, Rouot, B and Wermuth, C G 'Crystallographic and quantum mechanical analysis for imidazolidines compared with pharmacology' *Mol. Pharmacol.* Vol 21 (1982) p 400

Chen, K, Ji, R, Liu, H, Chen, N, Wu, G and Liao, M 'Ab initio calculations of molecular electrostatic potential of histamine and its derivatives' Fenzi Kexue Yu Huaxue Yanjiu Vol 3 (1983) p 25

Durant, G J, Emmett, J C, Ganellin, C R, Miles, P D, Parsons, M E, Prain, H D and White, G R 'Cyanoguanidine-thiourea equivalence in the development of cimetidine' J. Med. Chem. Vol 20 (1977) p 901 Mazurek, A P, Topiol, S, Weinstein, H and Osman, R 'Histamine H2 receptor. Role of guanidine substitution in partial agonism of N(α) guanylhistamine' Int. J. Quantum Chem. Quantum Biol. Symp.

Vol 10 (1983) p 293

Rao, G S, Mahajan, S and Mishra, R K 'Conformations and receptor maps of histamine' Int. J. Quantum Chem. Quantum Biol. Symp. Vol. 10 (1983) p 5

Richards, W G 'Non-equilibrium conformations' Proc. Symp. on Steric Effects in Biomolecules Eger, Hungary (1981) p 61

Richards, W G and Ganellin, C R 'Calculations of unstable conformations of histamine and methyl histamines' in Bergmann, E D and Pullmann, B (eds) Molecular and quantum pharmacology Proc. 7th Jerusalem Symp. on Quantum Chemistry and Biochemistry Academic Press, USA (1974) p 391

Richards, W G and Wallis, J 'Distribution of charge (within spheres) in biologically active amines (histamine — neutral and monocation) *Proc. Soc. Lond. Ser. B.* Vol 199 (1977) p 291

### **HORMONES**

Humphries, R L 'Computer simulation of binding between flexible ligand and polymeric receptor; e.g. peptide hormoes (enzyme substrates, neurotransmitters, drugs)' J. Theor. Biol. Vol. 91 (1981) p 477 Viana, L M and Takahata, Y 'PCILO study of conformation of 20-oxopregnane hormones' Int. J. Quantum Chem. Vol 22 (1982) p 265

### ION CHANNELS

Etchebest, C, Ranganathan, S and Pullman, A 'Energy profiles of Cs(+), K(+) and Na(+) in gramicidin A channel' *Fed. Eur. Biochem. Soc. Lett.* Vol 173 (1984) p 301

Kim, K S. Nguyen, H L, Swaminathan, P K and Clementi, E 'Transport of Na(+) and K(+) through Gramicidin A transmembrane channel. Study by molecular mechanics using parallel processors' *J. Phys. Chem.* Vol 89 (1985) p 2870

Nagata, C and Aida, M J 'Ab initio study of interaction of Li(+), Na(+) and K(+) with the pore components of the channels' J. Theor. Biol. Vol 110 (1984) p 505

Pullman, A 'Cation-ionophore interactions' in Pach, G (ed) Physical chemistry of transmembrane ion motions (1983) p 153

Pullman, A 'Specificity in ionophore-cation interactions' Pont. Acad. Sci. Scripta Varia. Vol 55 (1984) p 303

Venkatachalam, C M, Alonzo-Romanowski, S, Prasad, K U and Urry, D W 'Leu gramicidin A analog' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 11 (1984) p 315

Venkatachalam, C M and Urry, D W 'Theoretical analysis of gramicidin A trans-membrane channel: energetics of helical vibrational states of channel' J. Comput. Chem. Vol 5 (1984) p 64

### MOLECULAR GRAPHICS

Barrett, A N 'Determination of biomolecular charge distributions using interactive computer graphics' J. Mol. Graph. Vol 1 (1983) p 71

Morffew, A J Bibliography for molecular graphics' J. Mol. Graph. Vol 1 (1983) p 17

Morffew, A J 'Bibliography for molecular graphics' J. Mol. Graph. Vol 2 (1984) p 124

Richards, W G and Sackwild, V 'Computer graphics in drug research' Chem. Br. Vol 635 (1982)

### **NUCLEIC ACIDS**

Aida, M, Nagata, C, Ohmine, I and Morokuma, K 'Thermostability of extreme thermophile tRNA' J. Theor. Biol. Vol 99 (1982) p 599 Aktekin, N and Pamuk, H O 'Ab initio computation of ground state electronic properties of RNA and DNA II' Chim. Acta Turc. Vol 10 (1982) p 1

Angeli, R.P., Hornung, S.D. and Christoffersen, R. E. 'Developments in ab initio techniques applied to large molecules. Studies in DNA components' in Ludeva, E. V., Sabelli, N. H. and Wahl, A. C. (eds). Computers in chemical education and research Plenum Press (1977) p. 357

Balasubramian, R and Seetharamulu, P 'Conformational energy calculations on primitive tRNA nestling an amino acid' *J. Theor. Biol.* Vol 113 (1985) p 15

Beaconsfield, P and Balanovski, E 'Energy transfer in B-DNA: mechanism and effects' *Phys. Lett. A.* Vol 95A (1983) p 454

Broch, H, Cabrol, D and Vasilescu, D 'Electrostatic properties of sulphur containing radioprotectors: interactions with DNA by PCILO method' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p. 111

Buda, A and Sygula, A 'MNDO study of tautomers of nucleic bases; uracil, thymine and cytosine' J. Mol. Struct. (Theochem) Vol 92 (1983) p 255

Cizek, J, Förner, W and Ladik, J 'Localisation of the filled and virtual orbitals in the nucleotide bases' *Theor. Chim. Acta* Vol 64 (1983) p 107

Clementi, E and Corongui, G 'Charge transfer in nucleic acids' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 213

Clementi, E and Corongui, G 'Theoretical and computational chemistry for large molecular systems' Stud. Phys. Theor. Chem. Vol 27 (1983) p 397

Clementi, E, Corongui, G, Gratarola, M, Habitz, P, Lupo, C, Otto, P and Vercauteren, D'Solvation of DNA and proteins' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 16 (1982) p 409

Corbin, S, Lavery, R and Pullman, B 'The molecular electrostatic potential of DNA: the effect of countercation screening on various allomorphic forms' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 103

De Giambiagi, M S, Giambiagi, M and Esquivel, D M S 'Hydrogen bond indexes and tertiary structure of yeast tRNAphe' Z. Naturforsch, C. Vol 38C (1983) p 621

Dean, P M and Wakelin, L P G 'A quantum mechanical study of the intercalative attack on ethidium and carboxylated derivatives on a DNA fragment' *Phil. Trans. R. Soc. London, Ser. B.* Vol 287 (1979) p 571

Dean, P M and Wakelin, L P G 'Electrostatic potential of nucleotides' Proc. R. Soc. Ser. B. Vol 209 (1980) p 453

Del Bene, J 'Molecular orbital study of the Li(+) complexes of the DNA bases' J. Phys. Chem. Vol 88 (1984) p 5927

Del Bene, J E 'Molecular orbital study of the protonation of DNA bases' J. Phys. Chem. Vol 87 (1983) p 367

Eisenmenger, F, Sklenar, H and Behlka, J 'Stabilisation of secondary structure of RNA by divalent cations' *Stud. Biophys.* Vol 96 (1983) p 187

Furois-Corbin, S, Pullman, B and Lavery, R 'Guanine reactivity in B-DNA toward aflatoxin B, by accessible surface integrated field' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 11 (1984) p 273

Giessner-Prettre, C and Pullman, B 'Ab initio quantum mechanical calculation of the magnetic shielding constants of the different nuclei of cytosine' J. Am. Chem. Soc. Vol 104 (1982) p 70

Gresh, N and Pullman, B 'Affinities of aliphatic and aromatic bisguanylhydrazone for minor groove of double stranded(dA-dT) oligomers' *Theor. Chim. Acta* Vol 64 (1984) p 383

Gresh, N and Pullman, B 'Binding of berenil and stibamidine to double stranded (dA-dT)n oligomers' *Molec. Pharmac*. Vol 25 (1984) p 452

Gresh, N and Pullman, B 'Interaction specificities of tetramethyl ammonium for double stranded oligonucleotides held in B conformation' *Int. J. Quantum Chem.* Vol 24 (1983) p 491

Gresh, N and Pullman, B 'Theoretical study of the interaction of ammonium and guanidium ions with the phosphodiester linkage' *Theor. Chim. Acta* Vol 52 (1979) p 67

Hass, E C, Mezey, P G and Ladik, J J 'Non-empirical SCF molecular orbital studies on the protonation of biopolymer constituents. Protonation of cytosine, thymine and their tautomeric forms' *Theor. Chim. Acta* Vol 60 (1981) p 283

Hingerty, B E and Broyde, S 'Base displacement in AAF and AF modified dCpdG: syn and anti guanine' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 125

Ishida, T, Katsuta, M, Inoue, M, Yamagata, Y and Tomita, K 'Stacking interactions on 7-methylguanine-tryptophan systems, model for interaction of CAP structure of mRNA and its binding protein' *Biochem. Biophys. Res. Commun.* Vol 115 (1983) p 849

Kaiser, P M 'Geometry of stacked nucleobases derived from quantum chemical calculations' *Nucleic Acids Symp*. Vol 9 (1981) p 1

Kollman, P, Keepers, J W and Weiner, P 'Molecular-mechanics studies on d(CGCGAATTCGCG)2 and dA12.cntdot.dT12 illustrating coupling between sugar repuckering and DNA twisting' *Biopolymers* Vol 21 (1982) p 2345

Kollman, P A, Weiner, P K and Dearing, A 'Relative stabilities of double helical B-DNA sequence isomers' *Biopolymers* Vol 20 (1981) p. 2583

Ladik, J 'Electronic structures of polymers, specifically polycytosine' in Nicolaides, C A and Beck, D R (eds) Excited states in quantum chemistry (1978) p 495

Ladik, J J 'Band structures of periodic DNA molecules and treatment of aperiodicity' in Struct. Dyn.: Nucleic acids, proteins, Proc. Int. Symp. Adenine Press, USA (1982) p 261

Ladik, J, Otto, P and Förner, W 'Quantum mechanistic investigation of DNA — new results' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 10 (1983) p 73

Ladik, J, Suhai, S, Otto, P and Collins, T C 'DNA band structure from ab initio calculations on polycytosine' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 4 (1977) p 55

Lal, K B, Agrawal, V K, Srivastawa, A K and Krishna, B 'HOMO and LUMO energy values for bases of nucleic acids' *Indian J. Pure Appl. Phys.* Vol 21 (1983) p 670

Lavery, R, Corbin, S and Pullman, B 'The molecular electrostatic potential and steric accessibility of C-DNA' *Theor. Chim. Acta* Vol 60 (1982) p 513

Lavery, R and Pullman, A 'New theoretical index of biochemical reactivity combining steric and electrostatic factors — an application to tRNA' *Biophys. Chem.* Vol 19 (1984) p 171

Lavery, R, Pullman, A and Pullman, B 'The electrostatic field of B-DNA' Theor. Chim. Acta Vol 62 (1982) p 93

Lavery, R and Pullman B 'The electrostatic field of DNA: the role of the nucleic acid conformation' *Nucleic Acids Res.* Vol 10 (1982) p 4383

Lavery, R, Pullman, B and Zakrzewska, K 'Electrostatic properties and base sequence effects in oligonucleotide structure' *Biophys. Chem.* Vol 15 (1982) p 343

Lavery, R, Zakrzewska, K and Pullman, A 'Optimised monopole expansions for the representation of electrostatic properties of nucleic acids' J. Comput. Chem. Vol 5 (1984) p 363

Lybrand, T, Dearing, A, Weiner, K and Kollman, P 'Complexes of 4-nitroquinoline-N-oxide with dinucleoside phosphates' *Nucleic Acids Res.* Vol 9 (1981) p 6995

Maranon, J and Grinberg, H 'Molecular orbital correlation and orbital energy shifts in the double H-bonding of the adenine-thymine base pair' J. Mol. Struct. (Theochem) Vol 88 (1982) p 283

Maranon, J, Grinberg, H and Nudelman, N S 'Charge-transfer character of intermolecular hydrogen bond in singlet and triplet excited states of the adenine-thymine base pair' *Int. J. Quantum Chem.* Vol 22 (1982) p 69

Miertus, S and Trebaticka, M 'Semiempirical calculation of alkylation

and protonation energies of bases of nucleic acids' Collect. Czech. Chem. Commun. Vol 48 (1983) p 3517

Miertus, S and Trebaticka, M 'Theoretical study of alkylation and protonation of nucleic acid bases' J. Theor. Biol. Vol 108 (1984) p 509 Miller, K J and Kowalczyk, P J 'Interactions of molecules with nucleic acids' J. Comput. Chem. Vol. 5 (1984) p 89

Nishimura, Y, Tsuboi, M, Kato, S and Morokuma, K 'Vibrational modes of nucleic acid bases by ab initio SCF MO calculation' *Raman Spectrosc.*, Proc. Int. Conf., 8th Wiley, UK (1982) p 703

Olson, W K 'Computational studies of polynucleotide flexibility' Nucleic Acids Res. Vol 10 (1982) p 777

Otto, P 'Large scale ab initio band structure calculations: polynucleotides' *NATO Adv. Study Inst. Ser., Ser. C.* Vol 123 (Quantum Chem. Polym.: Solid State Aspects) (1984) p 361

Otto, P, Clementi, E and Ladik, J 'Electronic structure of DNA related periodic polymers' J. Chem. Phys. Vol 78 (1983) p 4547

Pack, G R 'Theory of ion effects on DNA conformation: a high salt model' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p. 81

Pack, G R and Loew, G H 'Theoretical analysis of origins of specificity in intercalation of ethidium into nucleic acids' *Biochim. Biophys. Acta* Vol 519 (1978) p 163

Pechenaya, V I and Volkov, S N 'Hydrogen exchange mechanism in DNA' Mol. Biol. (Moscow) Vol 18 (1984) p 1134

Platt, E and Robson, D 'Refinement of orbital-centred force field e.g. DNA' J. Theor. Biol. Vol 96 (1982) p 381

Pohorille, M J, Burt, S K and MacEiroy, R D 'Monte-Carlo simulations of the influence of solvent on nucleic acid base associations' J. Am. Chem. Soc. Vol 106 (1984) p 402

Ponnuswamy, P K and Anukanth, A 'Conformational characteristics of modified nucleotides' J. Theor. Biol. Vol 96 (1982) p 233

Pullman, A 'Nucleophilic affinity of conjugated heterocycles' in Pullman, A, Salem, L and Veillard, A (eds) Quantum theory of chemical reactions Vol 1 (1979) p 229

Pullman, A and Perahia, D 'Hydration of uracil and cytosine — electrostatic and complete supermolecule computations compared' *Theor. Chim. Acta* Vol 48 (1978) p 29

Pullman, B 'Electrostatics and specificity in nucleic acid reactions' Pont. Acad. Sci. Scripta Varia. Vol 55 (1984) p 1

Pullman, B 'Macromolecular electrostatic effect in biochemical reactivity of nucleic acids' in Pullman, B (ed) Catalysis in chemical and biochemical theory and experiment (1979) p 1

Pullman, B 'Recognitory interaction of non-intercalating drugs with DNA' in Ovchinnikov, Yu A (ed) Progress in bioorganic chemistry and molecular biology (1984) p 395

Ray, N K, Bolis, G B, Shibata, M and Rein, R 'Electrostatic interaction energies in complexes of water with uracil, thymine and cytosine' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 11 (1984) p 257

Sarai, A and Saito, M 'Ab initio calculation for the effect of hydrogenbonding interaction of proteins on stability of adenine-uracil pair' Int. J. Quantum Chem. Vol 25 (1984) p 527

Sarma, R H 'Structures of the DNA double helix' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 65

Scanlan, M J and Hillier, I H 'An ab initio study of tautomerism of uracil, thymine, 5-fluorouracil and cytosine' J. Am. Chem. Soc. Vol 106 (1984) p 3737

Sevilla, M D and McGlashen, M 'ESR and INDO study of the cations of (hydroxymethyl)uracil and (hydroxymethyl)cytosine' J. Phys. Chem. Vol 87 (1983) p 634

Sygula, A and Buda, A 'Amino-type tautomers of nucleic bases' J. Mol. Struct. (Theochem) Vol 121 (1985) p 133

Tilton, R F (Jr), Weiner, P K and Kollman, P A 'Molecular mechanics analysis of sequence dependence of structure and energy of A- and B-DNA molecules' *Biopolymers* Vol 22 (1983) p 969

Tosi, C and Lipari, G 'Molecular orbital computations of the conformational energy of ethyl methyl phosphate' *Theoret. Chim. Acta* Vol 60 (1981) p 41

Van Lier, J J C, Koole, L H and Buck, H M 'Dynamics of DNA. A quantum chemical study' Recl: J. R. Neth. Chem. Soc. Vol 102 (1983) p 148

Van Lier, J J C, Smits, M T and Buck, H M 'B-Z transition in methylated DNA. A quantum-chemical study' Eur. J. Biochem. Vol 132 (1983) p 55

Wang, J, Wu, J and Xu, S 'Radiation sensitivity of bases in the nucleic acid' *Tongi Daxue Xuebao* Vol 1 (1983) p 113

Weiner, S. J., Kollman, P A, Case, D A, Singh, U C, Ghio, C, Alagona, G, Profeta, S (Jr) and Weiner, P 'A new force field for molecular mechanical simulation of nucleic acids and proteins' J. Am. Chem. Soc. Vol 106 (1984) p 765

Zakrzewska, K, Lavery, R and Pullman, B 'The solvation contribution

to the binding energy of DNA with non-intercalating antibiotics' Nucleic Acids Res. Vol 12 (1984) p 6559

Zakrzewska, K, Lavery, R and Pullman, B 'Theoretical studies of the selective binding to DNA of two non-intercalating ligands: nitropsin and SN18071' Nucleic Acids Res. Vol 11 (1983) p 8825

### PEPTIDES AND PROTEINS

Bonaccorsi, R, Palla, P and Tomasi, J 'Conformational energy of glycine in aqueous solutions and relative stability of the zwitterionic and neutral forms. An ab initio study' J. Am. Chem. Soc. Vol 104 (1984) p 1945

Broch, H, Cabrol, D and Vasilescu, D 'Implications of aminoacyladenylate conformations in prebiotic polypeptide synthesis' Int. Quantum Chem. Quantum Biol. Symp. Vol 8 (1981) p 139

Cabrol, D, Broch, H and Vasilescu, D 'Conformational study of tripeptide sequences of collagen' *Biochimie* Vol 63 (1981) p 851

Ciarkowski, J 'CNDO/2 calculations of conformational flexibility of diketopiperazine skeleton' *Biopolymers* Vol 23 (1984) p 397

Day, R. S., Suhai, S. and Ladik, J. 'Electronic structure in large finite aperiodic polypeptide chains' J. Chem. Phys. Vol 62 (1981) p 165

Duben, A J and Miertus, S 'Effect of solvent on the internal rotation of formamide: a CNDO/2 solvation method study (formamide representative of polypeptides)' *Theor. Chim. Acta* Vol 60 (1981) p 327 Edwards, R A and Woody, R W 'Molecular orbital calculations of

Edwards, R A and Woody, R W 'Molecular orbital calculations of the optical properties of congo red and cibacron blue and their complexes with proteins' J. Phys. Chem. Vol 87 (1983) p 1329

Förner, W, Otto, P, Bernhardt, J and Ladir, J J 'Model study of intermolecular interactions of amino acids in aqueous solution. The glycine-water system' *Theor. Chim. Acta* Vol 60 (1981) p 269

Gresh, N, Claverie, P and Pullman, A 'Computation of macromolecular conformations, intramolecular interactions-SIBFA' *Theor. Chim. Acta* Vol 66 (1984) p 1

Gresh, N, Pullman, A and Claverie, P 'SIBFA method extended to conformation of peptides' *Theor. Chim. Acta* Vol 67 (1985) p 11

Gresh, N and Pullman, B 'Binding of sodium to serine phosphate' in Srinivasan, R (ed) Biomolecular structure, conformation, function and evolution Vol 2 (Physicochemical and Theoretical Studies) (1980) Hall, D and Pavitt, N 'An appraisal of molecular force fields for

representation of polypeptides' *J. Comput. Chem.* Vol 5 (1984) p 441 **Hamed, M M, Robinson, R M and Mattis, W L** 'Behaviour of amphipathic helices on analysis by matrix methods, application to glucagon, secretin and vasoactive intestinal peptide' *Biopolymers* Vol 22 (1983)

p 1003

Klimenko, V E, Kuprievich, V A and Shramko, O V 'Dynamics of electron transfer through a polypeptide chain' Fiz. Mnogochastichnykh

Sist Vol 2 (1982) p 26

Mehler, E L and Paul, C H 'Small Gaussian sets for ab initio calculations on large biomolecules' Chem. Phys. Lett. Vol 63 (1979) p 145

Mehrota, P K, Mezei, M and Beveridge, D L 'Hydration of aladipeptide by Monte-Carlo methods' Int. J. Quantum Chem. Quantum Biol. Symp. Vol. 11 (1984) p 301

Mezei, M, Mehrotra, P K and Beveridge, D L 'Monte-Carlo determination of the free energy and internal energy of hydration for the ala dipeptide at 25°C' J. Am. Chem. Soc. Vol 107 (1985) p 2239

Mezey, P G, Del Re, G, Otto, P, Suhai, S and Ladik, J 'Charge transfer and induced polarisation in peptide-ion complexes' *Int. Quantum Chem.* Vol. 21 (1982) p 677

Naray-Szabo, G 'Electrostatic isopotential maps for large bio-molecules' Int. J. Quantum Chem. Vol 16 (1979) p 265

Ohsaku, M, Taketoshi, M and Imamura, A 'Interchain interactions in poly (amino acids)' J. Mol. Struct. (Theochem) Vol 119 (1985) p 307

Oie, T, Loew, G H, Burt, S K, Binkley, J S and MacElroy, R D 'Ab initio study of catalysed and uncatalysed amide bond formation as a model for peptide bond formation: ammonia-formic acid and ammonia-glycine reactions' J. Int. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 223

Oie, T, Loew, G H, Burt, S K, Binkley, J S and MacElroy, R D 'Quantum chemical studies of a model for peptide bond formation: Formation of formamide and water from ammonia and formic acid' J. Am. Chem. Soc. Vol. 104 (1982) p 6169

Oie, T, Loew, G H, Burt, S K and MacElroy, R D 'Ab initio study of amide bond formation as a model for peptide bond formation: ammonia-glycine reactions' J. Comput. Chem. Vol 4 (1983) p 449

Oie, T, Loew, G H, Burt, S K and MacElroy, R D 'Quantum chemical studies of a model for peptide bond formation: Role of amine catalyst in formation of formamide and water from ammonia and formic acid' J. Am. Chem. Soc. Vol 105 (1983) p 2221

Oie, T, Loew, G H, Burt, S K and MacElroy, R D 'Quantum chemical studies of a model for peptide bond formation: The role of the magnesium cation in formation of amide and water from ammonia and glycine.

Otto, P 'Large scale ab initio band structure calculations: polypeptides' NATO Adv. Study Inst. Ser., Ser. C. Vol 123 (Quantum Chem. Polym.: Solid State Aspects) (1984) p 361

Parra-Mouchet, J, Fink, W H and Nash, C P 'Ab initio STO-NG Hartree-Fock-Roothaan calculations of the ammonia-formic acid complex as a model for hydrogen bonding in crystalline amino acids' J. Phys. Chem. Vol 89 (1985) p 524

Peters, D and Peters, J 'Asparagine dipeptide' J. Mol. Struct. (Theochem) Vol 109 (1984) p 127

Peters, D and Peters, J 'Aspartic acid dipeptide' J. Mol. Struct. (Theochem) Vol 109 (1984) p 137

Peters, D and Peters, J 'β-branched side chains in valine and isoleucine'

J. Mol. Struct. (Theochem) Vol 88 (1982) p 137

Peters, D and Peters, J 'C10 H-bonds and β-bends in peptides and proteins' J. Mol. Struct. (Theochem) Vol 85 (1981) p 267

Peters, D and Peters, J 'Conformational analysis of side chains and the ethyl group as model side chain' J. Mol. Struct. (Theochem) Vol 88 (1982) p 157

Peters, D and Peters, J 'Proline dipeptide' J. Mol. Struct. (Theochem) Vol 85 (1981) p 257

Peters, D and Peters, J 'Serine dipeptide' J. Mol. Struct. (Theochem) Vol 90 (1982) p 321

Peters, D and Peters, J 'Simplified method applied to α-amino-isobutyric acid residue' J. Mol. Struct. (Theochem) Vol 86 (1982) p 341

Peters, D and Peters, J 'Structure and bonding in ala-dipeptide' J. Mol. Struct. (Theochem) Vol 85 (1981) p 107

Peters, D and Peters, J 'Threonine dipeptide' J. Mol. Struct. (Theochem) Vol 90 (1982) p 305

Platt, E and Robson, B 'Refinement of orbital-centered force field e.g. peptides' J. Theor. Biol. Vol 96 (1982) p 381

Ramani, R and Boyd, R J 'Cis-trans conformations of the peptide bond by ab initio method' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 8 (1981) p 117

Rao, G S, Tyagi, R S and Mishra, R K 'Conformations of glycine, di-, tri- and tetra-peptides' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 10 (1983) p 1

Remko, M, Sekerka, I and Frecer, V 'N-methylacetamide and N,N'-dimethylacetamide as models for peptidic bond in hydrogen bond interaction with water, methanol and phenol' Collect. Czech. Chem. Commun. Vol 48 (1983) p 3214

Sawaryn, A and Yadav, J S 'Ab initio studies of non-planarity of peptide unit' Int. J. Quantum Chem. Vol. 22 (1982) p 547

Scarsdale, J N, Van Alsenoy, C, Klimkowski, V J, Schafer, L and Homany, F A 'Ab initio studies of molecular geometries: Optimised molecular structures and conformational analysis of N-acetyl-N-methylalaninamide and comparison with peptide crystal data and empirical calculations' J. Am. Chem. Soc. Vol 105 (1983) p 3438

Schaefer, L, Van Alsenoy, C and Scarsdale, J N 'Molecular structures and conformational analysis of dipeptide N-acetyl-N'-methyl glycyl amide and significance of local geometries for peptide structures' J. Chem. Phys. Vol 76 (1982) p 1439

Siam, K, Klimkowski, V J, Ewbank, J D, Shäfer, L and Van Alsenoy, C 'Conformational analysis of alanine and glycine' J. Mol. Struct. (Theochem) Vol 110 (1984) p 171

Snyder, J P 'Unimportance of intramolecular hydrogen bonds in determination of secondary structure of cyclic hexapeptides. Roseotoxin B' J. Am. Chem. Soc. Vol 106 (1984) p 2393

Vasilescu, D, Cabrol, D and Broch, H 'Conformons in tripeptide units in collagen' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 10 (1983) p 109

Voogd, J, Derissen, J L and Van Duijneveldt, F B 'Proton transfer energies and electrostatic lattice energies of some amino acids and peptides by CNDO/2 and ab initio SCF methods' J. Am. Chem. Soc. Vol 103 (1981) p 7701

Weiner, S J, Kollman, P A, Case, D A, Singh, U C, Ghio, C, Alagona, G, Profeta, S (Jr) and Weiner, P 'A new force field for molecular mechanical simulation; proteins' J. Am. Chem. Soc. Vol 106 (1984) p. 765

Weiner, S J, Singh, U C, O'Donnell, T J and Kollman, P A 'Quantum and molecular mechanical studies on alanyl dipeptide' J. Am. Chem. Soc. Vol 106 (1984) p 6243

Wright, L R 'Ab initio SCF studies of amino acids and peptides' (Dissertation) Univ. Microfilms Int. Order No. DA8208804 (1981) p 117

Wright, L R and Borkman, R F 'Ab initio self-consistent field studies

of the peptides Gly-Gly, Gly-Ala, Ala-Gly and Gly-Gly-Gly' J. Phys. Chem. Vol 86 (1982) p 3956

Wright, L R, Borkman, R F and Gabrielli, A M 'Protonation of glycine: an ab initio self-consistent field study' J. Phys. Chem. Vol 86 (1982) p. 3951

Yamanobe, T., Ando, I, Saito, H, Tabeta, R, Shoji, A and Ozaki, T 'Carbon-13 NMR chemical shift and electronic structure of solid poly-peptides from tight binding MO theory. Polyglycine and poly(L-alanine)' Bull. Chem. Soc. Jpn. Vol 58 (1985) p 23

### **PROSTAGLANDINS**

Kothekar, V 'Conformational and quantum chemical studies on prostaglandins' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 281

Kothekar, V 'Conformational energy of PGE2, PGF2α and 15-(S) methyl PGF2α' J. Theor. Biol. Vol 101 (1983) p 233

Kothekar, V 'Prostaglandins — conformation energy calculations on PGA1, PGB1 and PGE1' J. Theor. Biol. Vol 94 (1982) p 943

**Kothekar, V and Kailash, S** 'Relative affinities of cations Na(1+), Mg(2+) and Ca(2+) to carboxylic group' *J. Theor. Biol.* Vol 101 (1983) p 225

### **SULPHONAMIDES**

Platt, E and Robson, B 'Refinement of orbital-centred forcefields e.g. sulphonamides' J. Theor. Biol. Vol 96 (1982) p 381

### **MISCELLANEOUS**

Bandoli, G, Clemente, D A, Grassi, A and Pappalardo, G C 'Structure and conformation of nootropic agent 2-pyrrolidone-N-acetamide by X-ray and molecular orbital calculation' *Mol. Pharmacol.* Vol 30 (1981) p 558

Bartzch, C, Hofmann, H J and Weiss, C 'Theoretical description of some tautomeric equilibria of chemical and biological importance' Stud. Biophys. Vol 93 (1983) p 197

Brandi, H S, Koiller, B and Ferreira, R 'Localised states of polymeric molecules' *Theor. Chin. Acta* Vol 60 (1981) p 89

Brugman, C J M, van den Hoof, H and Blange, T 'Role of quantum mechanics in theory of muscle contraction' J. Theor. Biol. Vol 107 (1984) p 173

Chandler, D 'Quantum theory of solvation' J. Phys. Chem. Vol 88 (1984) p 3400

Cheney, B V and Christoffersen, R E 'Structure-activity correlations for a series of antiallergy agents. Development of a quantitative model' J. Med. Chem. Vol 26 (1983) p 726

Cheney, B V, Duchamp, D J and Christoffersen, R E, 'Geometric and electronic characterisation of some oxamic and dioxamic acids as antiallergy agents' J. Med. Chem. Vol 26 (1983) p 719

**Del Bene, J** E 'Ab initio molecular orbital calculations on 2- and 4-monosubstituted pyridines' *J. Am. Chem. Soc.* Vol 101 (1979) p 21 **Demoulin, D and Pullman, A** 'Ab initio theoretical studies of binding of ZnII with CO<sub>2</sub>, H<sub>2</sub>O, OH(-), imidazole and imidazolate' *Theor. Chim. Acta* Vol 49 (1978) p 161

**Denner, V and Kaiser, F** Phase transition behaviour of a greater membrane model' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 9 (1982) p 41

Edwards, R A and Woody, R W 'Molecular orbital calculations of the optical properties of congo red and cibacron blue and their complexes with proteins' J. Phys. Chem. Vol. 87 (1983) p 1329

Graf, P and Mehler, E L 'Evaluation of small Gaussian basis sets for ab initio calculations on biologically active molecules' *Int. J. Quantum Chem. Quantum Biol. Symp.* Vol 8 (1981) p 49

Gray, B F and Gonda, I 'Quantum mechanics in muscle contraction' J. Theor. Biol. Vol 110 (1984) p 131

Gruendler, W. Friedemann, R, Brandt, W and Walther, P 'Detailed potential models for biomolecules' *Stud. Biophys.* Vol 96 (1983) p 249 Kao Lee, L, Sabelli, N H and Le Breton, P R 'Theoretical characterisation of phthalocyanin, tetraazaporphyrin, tetrabenzoporphyrin and porphyrin electronic structure' *J. Phys. Chem.* Vol 86 (1982) p 3926

Kaufman, J J, Popkie, H E and Preston, H J T 'Ab initio and approximate rigorous calculations on small, medium and large systems' *Int. J. Quantum Chem.* Vol 11 (1977) p 1005

Kolb, V M and Scheiner, S 'Angular dependence of the interaction energy between the N lone pair of amines and a proton: relevance to drug receptor systems' J. Pharm. Sci. Vol 73 (1984) p 389

Larsson, S'Electron transfer in biological systems' Int. J. Quantum

Chem. Quantum Biol. Symp. Vol 9 (1982) p 385

Loewdin, P O 'On the theoretical background of molecular biology' Struct. Dyn.: Nucleic acids, Proteins, Proc. Int. Symp. Adenine Press, USA (1982) p 13

Long, G A, Hiskey, R G, Pedersen, L G and Koehler, K A 'Role of gamma-carboxyglutamic acid in blood clotting proteins. Mg-malonate complexes' J. Mol. Struct. (Theochem) Vol 108 (1984) p 173 Lozes, R L and Sabin, J R Localised electronic excitation in a hydrogen bond' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 289 Lumbroso, H, Liegeois, C, Pappalardo, G C and Grassi, A 'Ab initio study of nootropic agent piracetam' J. Mol. Struct. (Theochem) Vol 87 (1982) p 229

Nagata, C and Imamura, A 'Application of frontier molecular orbital theory to biology' Kagaku Sosetsu Vol 38 (1983) p 164

Nichols, D E and Weintraub, J R 'Effects of steric interactions on models of charger-transfer complexes' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 205

Orita, Y, Ando, A and Abe, H 'Quantum mechanical studies of environmental effects in biomolecules; structure and hydration of thiourea' Theor. Chim. Acta Vol 54 (1979) p 73

Pullman, B and Courriere, P H 'Quantum-mechanical studies on conformation of sphingomyelins' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 3 (1976) p 29

Raudino, A, Zuccarello, F, Buemi, G and Rigano, C 'Medium and long range interactions between characteristic fragments of lipid-

protein systems' Bull. Chem. Soc. Jpn. Vol 55 (1982) p 1628

Rawlings, D C, Davidson, E R and Gouterman, M 'Porphyrins. Ground and excited state calculations on the isomers of free base porphine and sirohydrochlorin' *Theor. Chim. Acta* Vol 61 (1982) p 227

Sackwild, V and Richards, W G 'Conformational analysis — new method' J. Mol. Struct. (Theochem) Vol 89 (1982) p 269

Saran, A and Dhingra, M M 'Structure of the intermediate species of the photoreaction cycle of rhodopsin' Int. J. Quantum Chem. Quantum Biol. Symp. Vol 9 (1982) p 145

Steiner, E 'Density difference maps in quantum chemistry' Theor. Chim. Acta Vol 60 (1982) p 561

Teitell, M F, Suck, S-H and Fox, J L 'A MINDO/3 molecular orbital study of oxidised flavins' *Theor. Chim. Acta* Vol 60 (1981) p 127

Veerkamp, W, Serne, P and Hutzinger, O 'Prediction of hydroxylated metabolites in polychlorodibenzo-p-dioxins and polychlorodibenzo-furans by Hückel molecular orbital calculations' J. Chem. Soc. Perkin. Trans. II (1983)

Waleh, A and Loew, G H 'Quantum mechanical studies of the photodissociation of carbonylheme complexes' J. Am. Chem. Soc. Vol 104 (1982) p 2346

Waleh, A and Loew, G H 'Quantum mechanical studies of the photodissociation of oxyheme complexes' J. Am. Chem. Soc. Vol 104 (1982) p 2352

Williams, J M 'Computer calculations on stable compounds related to thromboxane A2' J. Chem. Soc. Perkin Trans. II (1984) p 1567