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2312	Amphiphilic Cyclodextrin-Based Liquid Crystals for Proton Conduction.		
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2310	Molecular structure and vibrational analysis of 2,4,6-trinitrotoluene and 2,4,6-trinitrotoluene- β -d ₃ . 1989 , 45, 585-588		24
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2307	Hydrogenation Pathway of Quinolines over Raney Nickel and Ru/C. 1990 , 63, 3167-3174		13
2306	Intramolecular hydrogen bonding of malondialdehyde and its monothio and dithio analogues studied by the PM3 method. 1990 , 208, 253-260		12
2305	Theoretical studies of hydrogen-bonded complexes using semiempirical methods. 1990 , 210, 405-426		35
2304	Comparison of semiempirical and bsse corrected mller-plesset ab initio calculations on the direct addition of water to formaldehyde. 1990 , 210, 427-440		19
2303	Molecular modelling of glutathione: a comparison with crystallographic data. 1990 , 210, 467-475		7
2302	Theoretical model of the electrophilic substitution in pentagonal unsaturated heterocycles. 1990 , 209, 361-372		6
2301	Semiempirical calculation of the hyperpolarizabilities of polyenes. 1990 , 38, 791-798		31
2300	Intermediates in the reactions of electron-rich germylenes with an acyl azide: An MNDO-SCF-MO investigation. 1990 , 1, 511-516		0
2299	The use of crystal data together with other experimental and computational results to discuss structure-reactivity and activity relationships. 1990 , 1, 597-616		18
2298	A PM3 SCF-MO study of the structure and bonding in the cage systems S ₄ N ₄ and S ₄ N ₄ X (X = N ⁺ , N ³⁺ , N ₂ S, P ⁺ , C, Si, B and Al). 1990 , 9, 107-111		8
2297	Molecular similarity: the introduction of flexible fitting. 1990 , 4, 231-8		33

2296	MOPAC: a semiempirical molecular orbital program. 1990 , 4, 1-105		2256
2295	Importance of dipolar resonance structures in determining ground state charge distribution. 1990 , 31, 2987-2990		2
2294	Intermolecular potentials of EDA complexes by semi-empirical theory dispersion energy terms in the PM3 method. 1990 , 46, 423-432		5
2293	Semiempirical studies on the structure and bonding of fluorosulfuranes and aminofluorosulfuranes. 1990 , 50, 427-432		
2292	C4O2 (1,2,3-Butatrien-1,4-dion), das erste Dioxid des Kohlenstoffs mit einer geraden Anzahl C-Atome. 1990 , 102, 920-923		21
2291	Calculation of the nonlinear optical properties of molecules. <i>Journal of Computational Chemistry</i> , 1990 , 11, 82-87	3.5	656
2290	Comments on a comparison of AM1 with the recently developed PM3 method. <i>Journal of Computational Chemistry</i> , 1990 , 11, 541-542	3.5	57
2289	Reply to Comments on a comparison of AM1 with the recently developed PM3 method. <i>Journal of Computational Chemistry</i> , 1990 , 11, 543-544	3.5	105
2288	Correlation of the acidity of substituted phenols, anilines, and benzoic acids calculated by MNDO, AM1, and PM3 with Hammett-type substituent constants. <i>Journal of Computational Chemistry</i> , 1990 , 11, 1009-1016	3.5	29
2287	Gas-Phase Thermolysis of 4-Substituted 3,5-Dihydro-3,3,5,5-tetramethyl-4H-pyrazoles Studied by Photoelectron Spectroscopy and Flash Vacuum Pyrolysis. 1990 , 123, 1161-1168		18
2286	N-[(2-Naphthyloxy)methyl] benzazoles: Synthesis and Investigation by X-ray Analysis and by Semiempirical MO Calculations. 1990 , 123, 1185-1191		5
2285	C5S2 (1,2,3,4-Pentatetraen-1,5-dithion), ein neues Sulfid des Kohlenstoffs. 1990 , 123, 1753-1756		31
2284	Molecular dynamics simulations and quantum mechanical studies of the hydrogen bond in water cluster systems. 1990 , 237, 47-61		20
2283	An electron spin resonance study of the 2,5-diphenylchalcophene radical ions. 1990 , 389, 301-313		23
2282	Molecular orbital studies of molecular exciplexes. Part 1: AM1 and PM3 calculations of the ammonia-oxygen complex and its solvation by water. 1990 , 877-883		19
2281	Weak bonds and atomic charge distribution in hydrogenated amorphous silicon. 1991 , 137-138, 295-298		4
2280	Conformation of 1-benzyloxy-4-methoxypyridinium perchlorate: X-ray, AM1 and PM3 studies. 1991 , 69-72		2
2279	Calculations of heats of formation for nitro compounds by semi-empirical mo methods and molecular mechanics. 1991 , 9, 161-171		21

2278	Comparison of hyperpolarizabilities obtained with different experimental methods and theoretical techniques. 1991 , 8, 2269		34
2277	Do Hammett constants model electronic properties in QSARs?. 1991 , 109-110, 221-235		9
2276	Theoretical Studies of Defects, Impurities, and Complexes in Semiconductors. 1991 , 240, 643		6
2275	Negative hyperconjugation does not play an important role in β -fluoro sulfides: An experimental demonstration. 1991 , 32, 1463-1466		11
2274	Semi-empirical studies of torsional potentials in halonitrosomethanes. 1991 , 47, 1661-1671		2
2273	X-ray, NMR and theoretical studies of the structure and conformation of the nootropic agent tenilsetam. 1991 , 26, 443-448		9
2272	DARC/PELCO and OASIS methods I. Methodological comparison. Modeling purine pKa and antitumor activity. 1991 , 26, 575-592		14
2271	Atomic cluster study of chemisorption and epitaxial diamond films on an Si(100) substrate. 1991 , 47, 578-584		4
2270	Conformational analysis of symmetric carbonic acid esters by quantum chemical calculations and dielectric measurements. 1991 , 249, 327-341		13
2269	Molecular and electronic structures of radical-cations derived from diphosphines: a semi-empirical PM3 study. 1991 , 409, 171-178		2
2268	Ames assay mutagenicity and electronic structure calculations of bromomethylfluoranthenes, chloromethylfluoranthenes, and hydroxymethylfluoranthenes. 1991 , 77, 291-302		
2267	About the mutagenicity of chlorine-substituted furanones and halopropenals. A QSAR study using molecular orbital indices. 1991 , 247, 97-102		51
2266	Semiempirical computation of homolytic O-H bond dissociation energies of alcohols: comparison of the AM1 and PM3 methods. 1991 , 236, 211-217		1
2265	Empirical method for the estimation of electron affinities. 1991 , 235, 263-275		1
2264	Structures cristallines et lectroniques de deux dfrivs de l'oxaphthalone: les 2-actyl- et 2-mthoxycarbonyl-6-mthoxynaphto[1,8-bc]pyranes. 1991 , 47, 1667-1670		
2263	Tautomeric equilibria of heterocyclic molecules. A test of the semiempirical AM1 and MNDO-PM3 methods. <i>Journal of Computational Chemistry</i> , 1991 , 12, 17-35	3.5	67
2262	A critical comparison of MINDO/3, MNDO, AM1, and PM3 for a model problem: Carbon clusters C2-C10. An ad hoc reparametrization of MNDO well suited for the accurate prediction of their spectroscopic constants. <i>Journal of Computational Chemistry</i> , 1991 , 12, 52-70	3.5	71
2261	Evaluation of PM3, AM1, and MNDO for calculation of higher energy ionization potentials. <i>Journal of Computational Chemistry</i> , 1991 , 12, 126-134	3.5	10

2260	Comparison of semiempirical MO methods applied to large molecules. <i>Journal of Computational Chemistry</i> , 1991 , 12, 172-174	3.5	34
2259	A comparison of conformational energies calculated by molecular mechanics (MM2(85), Sybyl 5.1, Sybyl 5.21, and ChemX) and semiempirical (AM1 and PM3) methods. <i>Journal of Computational Chemistry</i> , 1991 , 12, 200-208	3.5	51
2258	Optimization of parameters for semiempirical methods. III Extension of PM3 to Be, Mg, Zn, Ga, Ge, As, Se, Cd, In, Sn, Sb, Te, Hg, Tl, Pb, and Bi. <i>Journal of Computational Chemistry</i> , 1991 , 12, 320-341	3.5	553
2257	Hydration of small anions: Calculations by the AM1 semiempirical method. <i>Journal of Computational Chemistry</i> , 1991 , 12, 350-358	3.5	5
2256	Comparison of semiempirical calculations for silicon compounds. <i>Journal of Computational Chemistry</i> , 1991 , 12, 417-420	3.5	13
2255	Correlation of singlet-triplet gaps for aryl carbenes calculated by MINDO/3, MNDO, AM1, and PM3 with Hammett-type substituent constants. <i>Journal of Computational Chemistry</i> , 1991 , 12, 536-545	3.5	15
2254	PM3 study of the proton affinities of 2-, 3-, and 4-monosubstituted pyridines in the gas phase. <i>Journal of Computational Chemistry</i> , 1991 , 12, 675-680	3.5	17
2253	Theoretical kinetic isotope effects for the hydride transfer from formate to carbon dioxide: A comparison of theory with experiment. <i>Journal of Computational Chemistry</i> , 1991 , 12, 1134-1141	3.5	8
2252	Molecular modeling of the Wittig olefination reaction: Part 2: A molecular orbital approach at the MNDO-PM3 level. 1991 , 2, 265-276		19
2251	Crystal structure and theoretical investigation of the configurations of 1,3-dichloro-1,3-diazetidino-2,4-dione and 1,3-bis(trimethylsilyl)-1,3-diazetidino-2,4-dione. 1991 , 2, 487-494		3
2250	Ionization Behavior and Ionization-Dependent Conformation of Raclopride, a Dopamine D2 Receptor Antagonist. 1991 , 74, 956-968		5
2249	Solution and powder X- and Q-band ESR spectra of the 1,3,5- trithia-2,4, 6-triazapentalenyl radical. 1991 , 29, 625-630		18
2248	Substituent effects in the 1,3-dipolar cycloaddition reactions of 2-methylenecephalosporins with diazoalkanes. 1991 , 1991, 699-701		2
2247	3-Methyl-4,6-diphenylfuro[3,4-d]isoxazol [Ein neues heterocyclisches System. 1991 , 124, 2481-2488		13
2246	A PM3 study of the reactions of propene with singlet oxygen and other enophiles. 1991 , 47, 1707-1726		16
2245	Synthese eines oxepino[2,3-d]isoxazol-systems. 1991 , 32, 1161-1164		13
2244	Automatic creation of drug candidate structures based on receptor structure. Starting point for artificial lead generation.. 1991 , 47, 8985-8990		138
2243	MNDO calculations on borazine derivatives. The substitution of one [HNBH] fragment for one [HCCH] fragment in benzene to form the azaborines and the nature of the cyclootrimer of the 1,2-isomer. 1991 , 39, 787-804		24

2242	Theoretical studies of some new Anti-Malarial drugs. 1991 , 40, 231-245	12
2241	Use of AM1 and PM3 methods for the investigation of energies and structures of compounds O=PXYZ, S=PXYZ. 1991 , 31, 684-685	
2240	The discovery of novel auxin transport inhibitors by molecular modeling and three-dimensional pattern analysis. 1991 , 5, 323-34	22
2239	Energetics of the c(2 x 2) reconstruction of the beta -SiC(100) surface. 1991 , 44, 11143-11148	39
2238	Excited state proton transfer in the S1 state of 2-allylphenol, 2-propenylphenol, and 2-propylphenol and their van der Waals clusters with water and ammonia. 1991 , 95, 3290-3301	20
2237	Excited state intermolecular proton transfer in isolated clusters: 1-naphthol/ammonia and water. 1991 , 95, 3119-3128	67
2236	Normal mode analysis of van der Waals vibrations. 1991 , 95, 1577-1587	19
2235	Inhibition of microsomal lipid peroxidation and cytochrome P-450-catalyzed reactions by nitrofurans compounds. 1991 , 14, 419-31	10
2234	Theoretical determination of the geometric and electronic structures of oligorylenes and poly(peri-naphthalene). 1992 , 97, 8470-8480	22
2233	The design, synthesis, and evaluation of chromophores for second-harmonic generation in a polymer waveguide. 1992 , 71, 410-417	53
2232	From uncoupled to coupled Hartree-Fock polarizabilities of infinite polymeric chains. Pariser-Parr-Pople applications to the polyacetylene chains. 1992 , 96, 8330-8337	49
2231	Electronic structure of tetraphenylthiopyranylidene: A valence effective Hamiltonian theoretical investigation. 1992 , 96, 4474-4483	10
2230	Crystal Structure and Spectroscopic Investigation of 1,3-Dichloro-1,3-Diazetidine-2,4-Dione and 1,3-Bis(Trimethylsilyl)-1,3-Diazetidine-2,4-Dione. 1992 , 65, 25-28	1
2229	Calculations of heats of formation for nitroaromatics with PM3 and MM2. 1992 , 10, 173-182	8
2228	PHOTOELECTRON SPECTRA AND QUANTUMCHEMICAL CALCULATIONS OF PERCHLOROCYCLOPOLYSILANES. 1992 , 68, 129-137	7
2227	MO Analysis of Photocycloaddition Reactions of 2-Pyrones. 1992 , 65, 354-359	18
2226	C(9)-C Bonds of 10-Methyl-9-alkyl-9,10-dihydroacridines Acting Like Metal-Carbon Bonds in the Reactions with Electrophiles. 1992 , 21, 1701-1704	
2225	The Effects of Aromaticity and Reduced Bond Length Alternation on Linear and Third-Order Polarizabilities of Conjugated Organic Chromophores. 1992 , 291, 579	

2224	Energy Transfer Dynamics and Impact Sensitivity. 1992 , 296, 35	4
2223	Application of The X β and PM3 Methods to Chloromethanes: Ionization Potentials and Electron Affinities. 1992 , 39, 7-11	0
2222	An SCF Solvation Model for the Hydrophobic Effect and Absolute Free Energies of Aqueous Solvation. 1992 , 256, 213-7	410
2221	Electronic properties and free radical production by nitrofurans compounds. 1992 , 16, 207-15	4
2220	A molecular orbital and crystallographic study of the structure and π -facial regioselectivity of 9-chloro-1,4,5,8-tetrahydro-4a,8a-methanonaphthalene. 1992 , 447-448	5
2219	Novel formation of dienes with greater steric congestion resulting from the Diels-Alder reaction-desulfonylation sequence of 4-acyl-4H,6H-thieno[3,4-c]furan 5,5-dioxides. 1992 , 870-873	12
2218	Aryl group π -facial electrostatic asymmetry as a contributing factor to chiral resolution on β -cyclodextrin HPLC phases. 1992 , 1122-1124	9
2217	Kinetics of the reactions of the nitrate radical with a series of halogenobutenes. A study of the effect of substituents on the rate of addition of NO ₃ to alkenes. 1992 , 88, 1093-1099	36
2216	Electrostatic vs. orbital control in π -facial diastereoselection: a PM3 SCF-MO study of electrophilic reactivity in 7-methylenenorbornanes. 1992 , 998-1000	18
2215	Energetics of the Stone-Wales pyracylene transformation. 1992 , 1665-1666	13
2214	Regioselective Friedel-Crafts acylation of 1,2,3,4-tetrahydroquinoline and related nitrogen heterocycles: effects of NH protective groups and ring size. 1992 , 3401-3406	9
2213	Chemically modified semiconductor surfaces: 1,4-phenylenediamine on Si(100). 1992 , 260, 64-74	52
2212	Formation of the $\sqrt{3}\times\sqrt{3}$ Si c(2 \times 2) reconstructed surface. 1992 , 269-270, 1152-1156	13
2211	Interface structures for epitaxy of diamond on Si(100). 1992 , 1, 195-199	11
2210	Atomic configuration at the $\sqrt{3}\times\sqrt{3}$ Si c(2 \times 2) reconstructed surface. 1992 , 1, 285-289	9
2209	Ab initio study of the thioketo-enethiol tautomerism of dithiomalondialdehyde and dithioacetylacetone. 1992 , 257, 243-257	6
2208	A comparative semiempirical and ab initio study of tautomerization energies. 7-Methyl-2,3,4,7-tetrahydroisothiazolo [5,4b]pyridine-3,4-dione and other models of antibacterial quinolone analogues. 1992 , 257, 475-483	3
2207	Peroxynitrite, a cloaked oxidant formed by nitric oxide and superoxide. 1992 , 5, 834-42	1245

2206	Computer-assisted prediction of gas chromatographic retention times of polychlorinated biphenyls by use of quantum chemical molecular properties. 1992 , 25, 1839-1849	10
2205	Photodegradation mechanism of 2,3,7,8-tetrachlorodibenzo-p-dioxin as studied by the PM3-MNDO method. 1992 , 24, 291-307	8
2204	The hydroxylation of phenylalanine and tyrosine: a comparison with salicylate and tryptophan. 1992 , 296, 521-9	104
2203	Conformational studies on (+)-anatoxin-a and derivatives. 1992 , 6, 287-98	12
2202	AM1-SM2 and PM3-SM3 parameterized SCF solvation models for free energies in aqueous solution. 1992 , 6, 629-66	295
2201	Proton affinities of molecules containing nitrogen and oxygen: comparing ab initio and semiempirical results to experiments. 1992 , 43, 783-800	42
2200	Conformational studies of (S)idazoxan and (S)methoxyidazoxan using AM1 and PM3 semiempirical molecular orbital methods. 1992 , 44, 181-202	3
2199	Quantum mechanical parametrization of a conformationally dependent hydrophobic index. 1992 , 44, 203-218	20
2198	Semiempirical calculations of hyperpolarizabilities for extended π systems: Polyenes, polyynes, and polyphenyls. 1992 , 44, 497-515	45
2197	Consistent parametrization of semiempirical MO methods. 1992 , 44, 517-531	21
2196	A semiempirical study of the reaction of the hemimercaptal of methylglyoxal and glutathione at the active center of glyoxalase I. 1992 , 44, 699-722	2
2195	Semiempirical calculations of molecular polarizabilities and hyperpolarizabilities of polycyclic aromatic compounds. 1992 , 44, 773-784	22
2194	A semiempirical investigation of interelectronic exchange coupling in bisected poly(1,4-phenylene) polycation model systems. 1992 , 44, 785-794	1
2193	Extension of MNDO to d orbitals: Parameters and results for the halogens. 1992 , 44, 807-829	68
2192	A combined quantum chemical/molecular mechanical study of hydrogen-bonded systems. 1992 , 44, 897-930	52
2191	Experimental and theoretical study of the influence of the solvent on asymmetric diels-alders reactions. 1992 , 5, 230-238	62
2190	Stabilization of molecular association: An AM1/PM3 study of tetrahalomethane-arene molecular complexes. 1992 , 5, 253-258	
2189	Comparison of MNDO, AM1 and PM3 rotational barriers in branched alkanes. 1992 , 5, 614-616	6

2188	Significance of the cis-trans isomerization of early intermediates in the carotene biosynthetic pathway. 1992 , 5, 783-786	4
2187	An AM1 and PM3 molecular orbital study of the pericyclic reactivity of aryl carbodiimides.. 1992 , 48, 7425-7434	7
2186	PM3 Calculations on cycloaddition reactions of diimide.. 1992 , 33, 3673-3676	18
2185	¹⁹ F nuclear magnetic resonance studies of halogenated propanes. 1992 , 57, 259-284	10
2184	NMR measurements and semi-empirical calculations in a first approach to elucidate the mechanism of enantioselective cyanohydrin formation catalysed by cyclo-(S)-Phe-(S)-His. 1992 , 3, 401-414	23
2183	Molecular enthalpies: 1. Ground-state thermodynamic and computed enthalpies of the norbornadiene cycle. 1992 , 3, 53-58	1
2182	Extension of the MNDO formalism to d orbitals: Integral approximations and preliminary numerical results. 1992 , 81, 391-404	168
2181	Reaktionen cyclischer Oxalylverbindungen, 34. Mitt.: Synthese von Dibenzoylacet-N-carboxyalkylamiden und semiempirische Rechnungen zur Keto-Enol Tautomerie. 1992 , 123, 265-275	17
2180	Conformational analysis of β -methoxyketones. A photoelectron spectroscopic investigation of 3-methoxybicyclo[2.2.1]heptan-2-ones.. 1992 , 48, 2401-2414	2
2179	Organic paraelectrics resulting from tautomerization coupled with proton-transfer. 1992 , 83, 665-668	18
2178	A quantum chemical study of the degradation and the maximum polyene length in PVC. 1992 , 38, 69-84	35
2177	Second harmonic generation in some donor-acceptor ethylenes[] 1992 , 48, 1647-1656	5
2176	Organotin mediated cycloaddition reactions: a re-investigation of the reaction between organotin azides and isothiocyanates. 1992 , 430, 25-35	32
2175	On the morphology of caprolactam. 1992 , 125, 363-372	20
2174	Quantum-chemical calculations of the hydration energies of organic cations and anions in the framework of a continuum solvent approximation. 1992 , 160, 41-54	86
2173	Quantitative Structure-Activity Relationship of Histamine H2 Antagonists. Electrostatic Similarity of Cimetidine Derivatives. 1992 , 11, 478-485	1
2172	Intramolecular hydrogen bonding of a hydroxy proton to indenide and fluorenone carbanions studied by AM1 and MNDO-PM3 semi-empirical methods. Comparison of calculated OH stretching frequencies with experimental data. 1992 , 276, 141-147	4
2171	AM1 and PM3 MO calculations on D-xylopyranose. 1992 , 276, 341-345	4

2170	Comparative ab initio and semi-empirical study of hydrogen bonded complexes of NH ₃ and H ₂ O. 1992 , 254, 315-328	12
2169	Some comments concerning the use of static charge distributions for predicting chemical reactivity. 1992 , 255, 297-308	9
2168	The hydrolysis of 1,5-gluconolactone: semi-empirical methods and ¹³ C NMR confirmation. 1992 , 258, 235-241	13
2167	Structural and spectroscopic properties of a set of donor-acceptor molecules with and without spacers. 1992 , 262, 273-285	5
2166	Conformations and rotational barriers of aromatic polyesters. 1992 , 259, 331-344	29
2165	Molecular wavefunctions from chemical bonds: the fragment self-consistent field theory. 1992 , 261, 55-62	7
2164	The molecular structure of the urea molecule: is the minimum energy structure planar?. 1992 , 253, 25-33	31
2163	Theoretical modelling of the electrophilic substitution mechanism in furan. 1992 , 253, 243-259	5
2162	Gas- and liquid-phase NMR studies of conformational exchange in N,N-diisopropylacetamide. 1992 , 271, 261-278	6
2161	Theoretical analysis of magnetic vibrational circular dichroism for 1,3,5-trihalobenzene derivatives. 1992 , 198, 511-514	4
2160	Semi-empirical calculations of the isomeric C ₆₀ dihydrides. 1992 , 198, 570-576	38
2159	Theoretical study of buckminsterfullerene derivatives C ₆₀ X _n (X=H, F; n=2, 36, 60). 1992 , 192, 236-242	42
2158	Structures and electron density distributions of [Cl-P(NPCL ₃) ₃] ⁺ .Cl ⁻ and [Cl-P(NPCL ₃) ₃] ⁺ .PCL ₆ ⁻ in C ₂ H ₂ Cl ₄ at 100 K. 1992 , 48, 598-604	2
2157	Inter- and intramolecular hetero diels-alder reactions, 39. Influence of phenylthio and alkylthio substituents on the reactivity of 1-Oxa-1,3-butadienes in hetero diels-alder reactions. 1992 , 125, 1507-1511	13
2156	Photoelectron Spectrum and Electronic Structure of Indigo. 1992 , 125, 1773-1775	7
2155	Some well characterized chemical reactivities of buckminsterfullerene (C ₆₀). 1992 , 30, 1213-1226	24
2154	Quantum-chemical study of C ₇₈ fullerene isomers. 1992 , 197, 324-329	57
2153	Quantum-chemical study of C ₈₄ fulleren isomers. 1992 , 200, 411-417	72

2152	MNDO calculations on boron-nitrogen derivatives of nonbenzenoid aromatics: I. The two fully boron-nitrogen-alternating isomers of inorganic azulene. 1992 , 3, 193-199		2
2151	Comparison of ab initio, semiempirical, and molecular mechanics calculations for the conformational analysis of ring systems. <i>Journal of Computational Chemistry</i> , 1992 , 13, 525-532	3.5	45
2150	Structural studies of aromatic amines and the dna intercalating compounds m-amsa and o-amsa: Comparison of mndo, am1, and pm3 to experimental and ab initio results. <i>Journal of Computational Chemistry</i> , 1992 , 13, 640-650	3.5	33
2149	MO-Studies of enzyme reaction mechanisms. I. Model molecular orbital study of the cleavage of peptides by carboxypeptidase A. <i>Journal of Computational Chemistry</i> , 1992 , 13, 704-717	3.5	36
2148	Analysis of a large data base of electrostatic potential derived atomic charges. <i>Journal of Computational Chemistry</i> , 1992 , 13, 749-767	3.5	110
2147	NDDO fragment self-consistent field approximation for large electronic systems. <i>Journal of Computational Chemistry</i> , 1992 , 13, 830-837	3.5	77
2146	Semiempirical study of compounds with O-H...O intramolecular hydrogen bond. <i>Journal of Computational Chemistry</i> , 1992 , 13, 860-866	3.5	35
2145	Localized electron pair theory for the calculation of ground state energies of large molecules. <i>Journal of Computational Chemistry</i> , 1992 , 13, 901-911	3.5	6
2144	Theoretical studies of organometallic compounds. I. All electron and pseudopotential calculations of Ti(CH ₃) _n Cl _{4-n} (n = 0-4). <i>Journal of Computational Chemistry</i> , 1992 , 13, 919-934	3.5	64
2143	Theoretical studies of [n]paracyclophanes and their valence isomers. I. Geometries, strain energies, and enthalpies of the inter-conversions of [n]paracyclophanes and their Dewar benzene isomers. <i>Journal of Computational Chemistry</i> , 1992 , 13, 1047-1056	3.5	13
2142	PM3-SM3: A general parameterization for including aqueous solvation effects in the PM3 molecular orbital model. <i>Journal of Computational Chemistry</i> , 1992 , 13, 1089-1097	3.5	157
2141	Study of hydrogen bonding interactions relevant to biomolecular structure and function. <i>Journal of Computational Chemistry</i> , 1992 , 13, 1151-1169	3.5	108
2140	Electron-Transfer-Catalyzed cis-trans Isomerization of 1,1'-Azonorborane. Prototype of a reversible two-stage storage system. 1992 , 75, 1607-1612		11
2139	Properties and reactions of protonated molecules in the gas phase. Experiment and theory. 1992 , 11, 389-430		56
2138	A theoretical approach to C ₈₂ and LaC ₈₂ . 1993 , 201, 475-480		141
2137	Theoretical studies of selected C ₆₀ H ₂ and C ₇₀ H ₂ isomers. 1993 , 213, 383-388		66
2136	Theoretical study of thermal dissociation and recombination reactions of XONO ₂ (X = F, Cl, Br, or I). 1993 , 206, 278-284		16
2135	The radical cation of 1,4-dihydropentalene and its photochemical formation from bicyclo [3.3.0] octa-2,6-diene-4,8-diyl cation. 1993 , 212, 144-149		6

2134	Dual fluorescence and excited-state intramolecular proton transfer in jet-cooled 3,4-benzotropolone. 1993 , 215, 641-648	2
2133	MORATE: a program for direct dynamics calculations of chemical reaction rates by semiempirical molecular orbital theory. 1993 , 75, 143-159	105
2132	Synthese, NMR-Spektren und Photoelektronen-Spektren von cyclischen Keten-N,X1-acetalen (2-Alkyliden-N-heterocyclen). 1993 , 126, 503-516	35
2131	AM1 and X-ray Studies of the Structures and Isomerization Reactions of Indigo Dyes. 1993 , 126, 1015-1021	10
2130	FMO Approach in [4 + 2] Cycloadditions. Kinetic Studies with 1,2-Dimethylenecyclopentane. 1993 , 126, 1241-1245	8
2129	Auf dem Weg zu makrocyclischen para-Phenylene. 1993 , 126, 1723-1732	93
2128	Rearrangements of Free Radicals, XIII[1]. Thermal and Photochemical Rearrangements of Cyclic C ₈ H ₉ Radicals in Adamantane Matrix. 1993 , 126, 1917-1927	10
2127	Verkrante-Fullerene. 1993 , 126, 2331-2336	46
2126	Gas-Phase Thermolysis of Pyrazolines, 2[1]. Electronic Structure and Gas-Phase Thermolysis of 4,5-Dihydro-3H-pyrazoles Studied by Photoelectron Spectroscopy, Semiempirical Quantum-Chemical Calculations, and Flash Vacuum Pyrolysis. 1993 , 126, 2675-2681	7
2125	Gasphasenthermolyse von Pyrazolinen, 3[1]. Elektronische Struktur und Gasphasenpyrolyse von 4-substituierten 3,5,5-Trialkyl-3,5-dihydro-4H-1,2,3-triazolen untersucht durch Photoelektronenspektroskopie und semiempirische Rechnungen. 1993 , 126, 2683-2689	5
2124	NMR and computer-aided modeling studies of the interactions between a cyclic hexapeptide and the two enantiomers of some Boc- and Fmoc-amino acids. 1993 , 33, 933-42	4
2123	Absolute asymmetrische Synthese durch Belichtung chiraler Kristalle. 1993 , 105, 727-728	13
2122	Monoklines und triklines Tetraisopropyl-para-phenylendiamin: Wie strukturbestimmend sind nN/E Wechselwirkungen?. 1993 , 105, 1823-1826	10
2121	aci-Nitrodiphenylmethan: Ein über Wasserstoffbrücken verknüpftes Dimer. 1993 , 105, 1826-1828	8
2120	Molecular materials for second-order nonlinear optical applications. 1993 , 5, 804-815	156
2119	Sterically Congested Phosphite Ligands: Synthesis, crystallographic characterization, and observation of unprecedented eight-Bond ³¹ P, ³¹ P coupling in the ³¹ P-NMR spectra. 1993 , 76, 900-914	67
2118	Comparison of computational methods applied to oxazole, thiazole, and other heterocyclic compounds. <i>Journal of Computational Chemistry</i> , 1993 , 14, 75-88	3·5 32
2117	Ability of the PM3 quantum-mechanical method to model intermolecular hydrogen bonding between neutral molecules. <i>Journal of Computational Chemistry</i> , 1993 , 14, 89-104	3·5 145

2116	Reconsideration of solvent effects calculated by semiempirical quantum chemical methods. <i>Journal of Computational Chemistry</i> , 1993 , 14, 371-377	3.5	132
2115	Multicenter point charge model for high-quality molecular electrostatic potentials from AM1 calculations. <i>Journal of Computational Chemistry</i> , 1993 , 14, 503-509	3.5	57
2114	Comparative study between ab initio and semiempirical electrostatic potentials on molecular surfaces. <i>Journal of Computational Chemistry</i> , 1993 , 14, 530-540	3.5	17
2113	Calculation of hydrophobic interactions from molecular dynamics, surface areas, and experimental hydrocarbon solubilities. <i>Journal of Computational Chemistry</i> , 1993 , 14, 741-750	3.5	14
2112	Beyond the MNDO model: Methodical considerations and numerical results. <i>Journal of Computational Chemistry</i> , 1993 , 14, 775-789	3.5	126
2111	Suitability of the PM3-derived molecular electrostatic potentials. <i>Journal of Computational Chemistry</i> , 1993 , 14, 799-808	3.5	56
2110	Analysis of the core-repulsion functions used in AM1 and PM3 semiempirical calculations: Conformational analysis of ring systems. <i>Journal of Computational Chemistry</i> , 1993 , 14, 895-898	3.5	45
2109	MNDO-PM3 study on model cytochrome P450-mediated desulfuration of thiophosphoryl trifluoride, trimethylphosphine sulfide, and trimethyl phosphorothionate. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1250-1257	3.5	3
2108	Optimization and application of lithium parameters for PM3. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1301-1312	3.5	158
2107	Modeling of magic water clusters (H ₂ O) ₂₀ and (H ₂ O) ₂₁ H ⁺ with the PM3 quantum-mechanical method. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1326-1332	3.5	33
2106	Ab initio molecular orbital studies for compounds of magnesium. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1523-1533	3.5	22
2105	Modified neglect of diatomic overlap calculations on boron-nitrogen derivatives of nonbenzenoid aromatics. II. The analysis of the 130 possible nonfully boron-nitrogen-alternating isomers of pentaazapentaborazulene. 1993 , 4, 145-157		1
2104	Pyramidal nitrogen inversion hindered by a strong intramolecular hydrogen bond in 2-diethylaminomethylphenols. 1993 , 31, 1034-1037		11
2103	Application of the configuration interaction method for quantum-chemical calculations of solvation effects. 1993 , 173, 345-355		12
2102	Zeeman effect in T _{1u} symmetry vibrational states of C ₆₀ fullerene. 1993 , 178, 341-348		2
2101	Normal modes of 4-aminobenzonitrile (4-ABN). A comparison of PM3 calculations with experimental jet-cooled spectroscopy. 1993 , 178, 483-491		13
2100	Theoretical aspects of methane dissociation and hydroxylation on metal oxide diatomics in the gas phase. 1993 , 82, 425-442		9
2099	The chemistry of 3-mtro-1,2,4-triazol-5-one (NTO): thermal decomposition. 1993 , 213, 165-175		49

2098	Thermal behaviour and thermochemistry of hexachlorozirconates of mononitrogen aromatic bases. 1993 , 230, 269-292	9
2097	Measurements of standard potentials for nucleophiles by fast cyclic voltammetry: I: 9-substituted fluorenone ions in dimethyl sulphoxide. 1993 , 362, 109-118	8
2096	Photoelectron spectra and electronic structures of some naphtho[1,2-d]thiazoles. 1993 , 296, 115-125	7
2095	The impact of quantum chemical methods on the interpretation of molecular spectra of carbon clusters. 1993 , 294, 21-24	21
2094	AM1 and PM3 semiempirical molecular orbital study of silatranes III. 1-Chlorosilatrane. 1993 , 454, 15-23	20
2093	PM3 study of organometallic radicals formed by elements in periodic Groups 13-16. 1993 , 461, 15-19	10
2092	The overman rearrangement on a diacetone-D-glucose template: kinetic and theoretical studies on the chirality transcription. 1993 , 49, 4527-4540	30
2091	Synthesis and stereochemical behavior of 1-aryloctahydroisobenzofuro[7a,1-d]oxazole ring system: new examples of isolable rotamers.. 1993 , 49, 4549-4558	11
2090	SAM1; The first of a new series of general purpose quantum mechanical molecular models. 1993 , 49, 5003-5038	222
2089	The exo-anomeric effect does not govern the conformation of some 2,2'-O-substituted β,β' -trehalose derivatives. Solid state and solution evidences.. 1993 , 49, 2109-2114	4
2088	Synthesis and conformational study of 1,1'-ethano-9,9'-bifluorenyl. Anti and gauche conformers of a 9,9'-bifluorenyl derivative and chair and twist conformers of a dibenzo-1,5-cyclooctadiene derivative. 1993 , 49, 2437-2446	3
2087	Electrophilic amination of pyrimidine-2-thiones - synthesis of zwitterionic 2-aminothiopyrimidinium-N-ylides, pyrimidine-2-ones and bicyclic pyrimidinium compounds. 1993 , 49, 3767-3780	8
2086	Conformational analysis of the reverse transcriptase inhibitor (+)-(S)-4,5,6,7-tetrahydroimidazo-9-chloro-5-methyl-6-(3-methyl-2-butenyl)imidazo[4,5,1-jk][1,4]-benzodiazepine-2(1H)-thione (TIBO; R82913). 1993 , 34, 2063-2066	5
2085	Synthesis, structure, and physical properties of 1,11-o-benzo[2]orthocyclo[2](1,2)trophyliophane. 1993 , 34, 8493-8496	7
2084	Significant orbital interactions in Efacial stereoselection of electrophilic addition reactions to vinylic sulfoxides. 1993 , 34, 645-648	16
2083	Transition structures for the reformatsky reaction. A theoretical (MNDO-PM3) study.. 1993 , 34, 6111-6114	10
2082	Diarylmethylenecyclopropabenzene in cycloaddition. 1993 , 34, 6151-6154	7
2081	CoMFA validation of the superposition of six classes of compounds which block GABA receptors non-competitively. 1993 , 7, 45-60	28

2080	AMI and PM3 study of a low molecular weight structural mimic of hydrogen exchange within the catalytic center of aspartic proteases. 1993 , 22, 207-212	1
2079	MNDO, AM1 and PM3 calculations in the study of the energy and structure of quinazalone tautomers. 1993 , 29, 1065-1069	
2078	Zur Synthese von Tris(diorganylphosphino)phosphanen mit Substituenten geringen Raumbedarfs. 1993 , 619, 1047-1052	10
2077	A new scaling procedure to correct semiempirical MEP and MEP-derived properties. 1993 , 7, 721-742	25
2076	Helical region of the potential energy surface of β -aminoisobutyric acid: A theoretical study. 1993 , 47, 231-238	10
2075	Semiempirical evaluation for proton affinities of phosphorus compounds. 1993 , 48, 343-354	13
2074	Critical test of PM3-calculated proton affinities. 1993 , 48, 633-641	16
2073	Synthesis and spectroscopy of nitroaceanthrylenes and nitroaceanthrenes. 1993 , 112, 287-302	13
2072	[Computers in pharmacy--an overview]. 1993 , 22, 214-22	1
2071	On the Use of AM1 and PM3 Methods on Energetic Compounds. 1993 , 18, 33-40	30
2070	Photochemical and radiolytic cleavage of 10-methylacridine dimer in solutions and cryogenic glasses. 1993 , 6, 254-256	5
2069	Calculation of non-linear optical properties of pyridinium cyclopentadienylides. 1993 , 6, 531-534	1
2068	Quantum chemical study of molecular ion complexes with hydrogen bonds (Review). 1993 , 33, 899-924	1
2067	Polycyclic aromatic hydrocarbons with five-membered rings: Modeling of experimental X-ray and neutron-diffraction structures. 1993 , 4, 279-285	11
2066	Molecular enthalpies 3: Ground-state thermodynamic and computed enthalpies of the valence isomers of benzene. 1993 , 4, 161-166	4
2065	Structural investigation of [H2cyclam] [O3SCF3]2 (cyclam=1,4,8,11-tetraazacyclotetradecane). 1993 , 23, 755-758	4
2064	Intramolecular charge transfer in 5-phenyl-3H-1,2-dithiole-3-thione and 5-phenyl-3H-1,2-dithiole-3-one derivative molecules for quadratic nonlinear optics. 1993 , 87, 175-194	6
2063	Critical test of PM3 calculated gas-phase acidities. 1993 , 86, 417-427	23

2062	Unexpected behavior of the retinylidene chromophore in the exciton interaction of chiral 1,2-cyclohexanediamine Schiff bases. 1993 , 4, 1-4	11
2061	Dopamine autoreceptor agonists: computational studies, synthesis and biological investigations. 1993 , 3, 1477-1483	16
2060	Aromatic isosteres as conformational probes for an isoprenyl subunit: application to inhibitors of squalene synthase. 1993 , 3, 595-600	19
2059	Characterization of species in ethylaluminum dichloride molten salts by ²⁷ Al NMR. 1993 , 209, 239-240	8
2058	Structure of a powerful mutagenic compound; 6-methoxy-2-nitronaphtho[1,8-bc]pyran. 1993 , 49, 264-267	0
2057	On the mutagenicity of MX compounds. 1993 , 287, 235-41	17
2056	An AM1 and PM3 study of hexafluoroacetylacetone. 1993 , 282, 277-282	6
2055	Conformational studies of imiloxan and imiloxan cation using AM1 and PM3 semiempirical molecular orbital methods. 1993 , 285, 235-250	4
2054	A computational investigation of the molecular geometry and rotational barriers in ethyl methyl ether. 1993 , 288, 215-223	2
2053	Theoretical studies applicable to the design of novel anticonvulsants. 1993 , 281, 173-184	15
2052	Enthalpies of formation of carboxylic acids and proton affinities of carboxylate anions: a comparison of MNDO, AM1 and PM3. 1993 , 281, 259-267	12
2051	A semiempirical AM1, MNDO and PM3 study of the rotational barriers of various ureas, thioureas, amides and thioamides. 1993 , 283, 33-48	18
2050	Energetics of acid-base equilibria in aqueous solution. MNDO, AM1, and PM3 results for compounds with functionalities analogous to the nucleic acids. 1993 , 283, 49-55	19
2049	Theoretical studies on the structure of 1,3-diol systems. 1993 , 283, 191-197	8
2048	Determination of penicillin complexation sites in the presence of Zn(II) ions by AM1 and PM3 methods. 1993 , 283, 213-226	10
2047	AM1 and PM3 semiempirical molecular orbital study of silatranes.. 1993 , 283, 251-259	17
2046	A quantum chemical AM 1 study of some isomeric prostaglandin allylic acetates. 1993 , 279, 127-130	
2045	Ab initio and semiempirical calculations on the interaction of tetramethylammonium with a water molecule. 1993 , 279, 311-319	6

2044 Cotton-Mouton constants for benzoic and phthalic acids. **1993**, 42, 1501-1504

2043 QSAR of Fungicidal β -1,2,4-Thiadiazolines. Reactivity-Activity Correlation of SH-Inhibitors. **1993**, 12, 251-255 28

2042 1,2,3-triazol-1-imines. 2. Electric dipole moments and semiempirical studies of some 2-aryl-N-benzoyl-4,5-dimethyl-1,2,3-triazol-1-imines. **1993**, 30, 1121-1123 2

2041 Cycloaddition behavior of 3,4-diazacyclopentadienone dioxides toward bicyclo[2.2.1]heptadiene derivatives. X-ray analysis of the cycloadduct and reaction pathway. **1993**, 30, 1557-1564 8

2040 Quantum chemical study on the mechanisms of nucleophilic substitution of a nitro group in 2,4,6-trinitrotoluene and 1,3,5-trinitrobenzene. **1993**, 42, 1806-1810

2039 Applicability of PM3 to transphosphorylation reaction path: toward designing a minimal ribozyme. **1993**, 23, 419-27 1

2038 Intramolecular excited state proton transfer in Mannich base \square 3,5,6-trimethyl-2(N,N'-diethylaminomethyl) phenol. **1993**, 72, 123-132 10

2037 Through-space interaction and its influence on the photoreactivity of 2,4-di-(1,2-naphthoquinone-2-diazide-5-sulphonyl-oxy)-benzophenone. **1993**, 69, 313-323 1

2036 The effect of workstation technology on methods in drug design and discovery. **1993**, 1, 359-370 1

2035 The electronic structure of adsorbed aromatic molecules: Perylene and PTCDA on Si(111) and Ag(111). **1993**, 293, 239-244 65

2034 MNDO, AM1 and PM3 semiempirical molecular orbital study of 1-fluorosilatrane. **1993**, 446, 99-106 21

2033 1,4-addition reaction with thiols and conformational analysis with PM3 molecular orbital calculations of 19-oxygenated androst-4-ene-3,6,17-triones. **1993**, 58, 423-8 10

2032 Modulation of interleukin 2 high affinity binding to human T cells by a pyrimidodiazepine insect metabolite. **1993**, 334, 309-12 1

2031 Iminophosphorane-substituted proton sponges. Part 4. Comparison of X-ray molecular structures with solution properties (pKa, ^1H and ^{13}C NMR spectroscopy). **1993**, 709-713 31

2030 Substrate specificity of cytochrome P450cam for L- and D- norcamphor as studied by molecular dynamics simulations. *Journal of Computational Chemistry*, **1993**, 14, 541-548 3.5 10

2029 Oxygen vacancy in α -quartz: A possible bi- and metastable defect. **1993**, 48, 13238-13243 109

2028 SOME WELL CHARACTERIZED CHEMICAL REACTIVITIES OF BUCKMINSTERFULLERENE (C60). **1993**, 75-88 4

2027 Metal/conjugated polymer interfaces: A theoretical investigation of the interaction between aluminum and trans-polyacetylene oligomers. **1993**, 98, 4253-4262 44

2026	Electronic effects in π -facially stereoselective epoxidation of phenyltrifluoromethylpropenol. 1993 , 1337-1340	7
2025	New highly strained adamantanophanes. 1993 , 1168-1170	15
2024	Synthesis and first hyperpolarizabilities of acceptor-substituted β -apo-8'-carotenal derived compounds. 1993 , 432-433	9
2023	3-Ylomethylphenylnitrate a novel quartet species having doubly heterogeneous radical sites (N and C atom; S= 1 and 1/2 center) in a π -conjugated molecule. 1993 , 302-304	4
2022	Photochemistry of uracils in halogenated solvents. 1993 , 1487-1490	1
2021	Formation of a 4H-cyclopenta-1,2,3-thiadiazole by rearrangement of a transient N-(thionitroso)cyclopenta-2,4-diene-1-imine. 1993 , 489-491	2
2020	Structures of base pairs with 5-(hydroxymethyl)-2'-deoxyuridine in DNA determined by NMR spectroscopy. 1993 , 32, 7779-86	38
2019	A Continuum Solvation Model for the AM1 Semi-Empirical Method. 1993 , 33, 427-434	24
2018	NDDO-Based CI Methods for the Prediction of Electronic Spectra and Sum-Over-States Molecular Hyperpolarization. 1993 , 33, 435-448	61
2017	Structure-activity relationships for mitomycins. Application of the distance and charge analysis method. 1993 , 36, 1461-4	14
2016	Abschätzung des umweltchemischen und toxikologischen Verhaltens von Stoffen durch computergestützte Analyse von Struktur und Verhalten sowie von Struktur und Wirkung. 1993 , 5, 11-18	3
2015	Valence electronic structure of C60: Theoretical analysis of photoemission data. 1993 , 56, 3246-3251	2
2014	Theoretical characterization of the electronic properties of unsymmetrical phthalocyanine analogues. 1993 , 57, 4519-4524	6
2013	Comparison of two alternative forms of polysilole: Another quasidegenerate polymer?. 1993 , 57, 4255-4259	15
2012	Geometric and electronic structure of dithiapyranylidine: evolution upon oxidation. 1993 , 57, 4572-4578	
2011	Electronic excitations and alternation of conjugated polymers. 1993 , 54, 35-47	23
2010	Design of one-dimensional ferromagnet based on polyacetylene chain. 1993 , 60, 279-283	10
2009	Prediction of gas chromatographic retention indexes of environmental polychlorinated dibenzo-p-dioxins and dibenzofurans by use of computer-calculated molecular properties. 1993 , 19, 203-210	4

2008	TRANS-CYCLOHEXANE-1,2-DIPHOSPHONATES SYNTHESIS, STRUCTURAL AND NMR SPECTROSCOPIC INVESTIGATIONS. 1993 , 83, 77-98	6
2007	Polymers with conjugated chains in three dimensions. 1993 , 55, 315-320	14
2006	Semiempirical Molecular Orbital Theory: Facts, Myths and Legends. 1993 , 369-380	15
2005	Linear Free Energy Relationships in Kinetic Analyses: Applications of Quantum Chemistry. 1993 , 3, 231-246	14
2004	Estimation of exposure and ecotoxicity related parameters by computer based structure-property and structure-activity relationships. 1993 , 40, 57-69	3
2003	Influence of Structural Isomerism on the Electronic Properties of Extended Phthalocyanines. 1993 , 234, 241-246	3
2002	Sandwich-type molecular recognition of acceptors by a bis-anthracene host. 1993 , 2, 25-31	8
2001	Adiabatic ionization energy of CH ₃ SSCH ₃ . 1993 , 99, 8440-8444	41
2000	Interstitial carbon and the carbon-carbon pair in silicon: Semiempirical electronic-structure calculations. 1993 , 47, 10217-10225	11
1999	A parametric method 3 (PM3) study of trans-stilbene. 1993 , 98, 3016-3021	44
1998	Lifetime of the hypothetical charge transfer state in the phenothiazine crystal. 1993 , 98, 3713-3715	0
1997	Plasma-polymerized C60/C70 mixture films: Electric conductivity and structure. 1993 , 74, 5790-5798	88
1996	Role of gas-phase adducts in the growth of gallium arsenide by metalorganic vapor-phase epitaxy. 1993 , 63, 214-215	10
1995	Excitation and relaxation energies of trans-stilbene: Confined singlet, triplet, and charged bipolarons. 1993 , 47, 1742-1753	100
1994	Modeling study on the cleavage step of the self-splicing reaction in group I introns. 1993 , 10, 945-72	7
1993	Theoretical examination of the mechanism of aldose-ketose isomerization. 1993 , 6, 479-84	28
1992	Fish Toxicity and Dealkylation of Aromatic Phosphorothionates - QSAR* Quantitative structure-activity relationships. Analysis Using NMR Chemical Shifts Calculated by the IGLO Method. 1993 , 28, 899-921	
1991	Photolysis of p-Phenylenebis(chlorodiazirine), Studied by Matrix Isolation Spectroscopy. Generation, Detection and Characterization of p-Phenylenebis(chloromethylene). 1993 , 22, 1291-1294	13

1990	Reaction of C ₆₀ with Chlorophenyl diazirine. Spectral and Electronic Properties of the C ₆₀ -Chlorophenylcarbene 1:1 Adduct. 1993 , 22, 2163-2166	17
1989	Synthesis of Asperuloside Aglucon Silyl Ether and Garjamine from (+)-Genipin via Gardenoside Aglucon Bis(silyl ether) as a Common Intermediate. 1993 , 66, 2646-2652	4
1988	Physicochemical Properties of 2-Methylthio-4-methylphenol, a Model Compound of the Novel Cofactor of Galactose Oxidase. 1993 , 22, 2099-2102	25
1987	An investigation of the interrelationships between linear and nonlinear polarizabilities and bond-length alternation in conjugated organic molecules. 1993 , 90, 11297-301	217
1986	Conformational Analysis of (S)-4,5,6,7-Tetrahydro-5-Methylimidazo [4,5,1-jk][1,4]-Benzodiazepin-2(1H)-one (R78362). 1993 , 26, 1005-1022	1
1985	Calculations of heats of formation for nitroalkanes with PM3 and MM2'. 1993 , 11, 39-46	1
1984	New Classes of Organic High-Spin Molecules Generated with Electron-Doping. 1993 , 233, 9-16	2
1983	Computer-assisted molecular modeling: indispensable tools for molecular pharmacology. 1993 , 33, 1149-64	7
1982	Theoretical and Experimental Investigations of Fullerene Derivatives: C ₆₀ H ₂ , C ₆₀ H ₄ , C ₇₀ H ₂ , AND C ₆₀ (CH ₂) ₂ . 1994 , 349, 145	1
1981	Silicon Cluster Terminated by Hydrogen, Fluorine and Oxygen Atoms: A Correlation with Visible Luminescence of Porous Silicon. 1994 , 33, 909-913	17
1980	Ab initio computation of semiempirical π -electron methods. II. Transferability of H π parameters between ethylene, trans-butadiene, and cyclobutadiene. 1994 , 101, 4011-4027	23
1979	Ab initio computation of semiempirical π -electron methods. III. The benzene molecule, the zero-differential-overlap approximation, and the transferability of parameters. 1994 , 101, 5929-5941	9
1978	Dielectric relaxation derived from collective molecular reorientation of 9-hydroxyphenalenone in the solid state. 1994 , 100, 6646-6648	7
1977	Molecular-dynamics study of oxygenated (100) diamond surfaces. 1994 , 49, 11374-11382	42
1976	Simplified electronic-structure model for hydrogen-bonded systems: Water. 1994 , 50, 10516-10530	32
1975	Optical properties of quasi-one-dimensional thiophene-based oligomers. 1994 , 50, 2301-2305	94
1974	Electronic coupling and conformational barrier crossing of 9,9-bifluorenyl studied in a supersonic jet. 1994 , 100, 3384-3393	11
1973	Low-energy collision-induced dissociation of deprotonated dinucleotides: determination of the energetically favored dissociation pathways and the relative acidities of the nucleic acid bases. 1994 , 137, 121-149	116

1972	The conformational flexibility of aromatic retinoids. 1994 , 51, 59-69	
1971	Structural properties and potential reactivity of substituted 3- aroyldithiocarbazates. 1994 , 5, 147-154	4
1970	Tautomerism of rhodanine. 1994 , 5, 225-231	17
1969	MNDO parameters for As atoms. 1994 , 35, 276-277	
1968	Calculation of vibrational frequencies of sulphur compounds using semiempirical molecular orbital methods (AM1, PM3, MNDO). 1994 , 323, 267-277	8
1967	On the chemical mechanism of aldehyde metabolism by cytochrome P-450. 1994 , 13, 2473-2476	10
1966	Chemical mechanism of olefin oxygenation reaction catalyzed by bis(acetylacetonato)nickel(ii) or cobalt(ii) compounds in the presence of reducing agents. 1994 , 13, 2245-2249	9
1965	Effects of variable selection on CoMFA coefficient contour maps in a set of triazines inhibiting DHFR. 1994 , 8, 97-112	9
1964	Benzotriazole-assisted lithiation of vinyl ethers. 1994 , 50, 6005-6016	12
1963	A study of the interconversion between 3,4-dihydro-4-formyl-2-hydroxy-2H-benzopyran and 2,3,3a,8a-tetrahydro-2-hydroxyfuro[2,3-b]benzofuran moieties, and its application to a formal synthesis of (-)-aflatoxin B1. 1994 , 50, 7597-7610	7
1962	Destabilized vinyl cations. An MO study of the influence of electron-withdrawing substituents. 1994 , 35, 265-268	7
1961	Remarkable kinetic solvent isotope effect on the cycloaromatization of C-1027 chromophore, a 9-membered enediyne, and the thermochemistry. 1994 , 35, 5253-5256	33
1960	Enantioselective dual N π -HO bonding between (R,R)-4,4'-bi [5-((Z)-N-isopropylimino)-1,3-dioxolane] and (S)-1,1'-bi-2-naphthol. 1994 , 35, 9413-9416	6
1959	Modelling the auxin-binding site of auxin-binding protein 1 of maize. 1994 , 35, 1111-1123	40
1958	Stereoselective synthesis of fused lactams by intramolecular nitron cycloaddition. 1994 , 50, 5503-5514	29
1957	Thermal ene reaction of 4-(2-alkenylamino)-3-formyl-2(2H)-chromenones. 1994 , 50, 1063-1072	20
1956	Versatile desilylative cross-coupling of silyl enol ethers and allylic silanes via oxovanadium-induced chemoselective one-electron oxidation. 1994 , 50, 10207-10214	19
1955	New supramolecular host systems. 2. 1,3,5,7-tetraoxadecalin, 1,2-dimethoxyethane and the Gauche effect reappraised. Theory vs. experiment.. 1994 , 50, 9707-9728	36

1954	Effect of zinc halides on the high stereoselectivity of a new mannich type cyclization in the tilivalline synthesis a computational chemical analysis. 1994 , 50, 9775-9780	4
1953	Epimerization of tilivalline. 1994 , 50, 9781-9788	5
1952	Mechanistic and stereochemical studies on Ferrier reaction by means of chirally deuterated glucose. 1994 , 50, 4125-4136	12
1951	Synthesis of new chiral heterocycles of the pyrazole and 2-isoxazoline types from (+)-3-carene.. 1994 , 5, 479-489	21
1950	Bicyclic [b]-heteroannulated pyridazine derivatives--II. Structure-activity relationships in the 6-aryltriazolo-[4,3-b]pyridazine ligands of the benzodiazepine receptor. 1994 , 2, 773-9	6
1949	The oxidative degradation of imide polymers. I: Ozonolysis of a model compound, N-phenylphthalimide. 1994 , 34, 279-284	1
1948	Calibration of a semi-empirical procedure for predicting the ground-state spin multiplicities of open-shell molecules. Applications to new systems. 1994 , 7, 207-217	19
1947	Competition between decarboxylation and isomerization in the C ₃ H ₅ O energy surface. Justification of the experimental results by molecular orbital calculations on the solvated ions. 1994 , 7, 221-226	
1946	AB initio and semi-empirical investigation of gas-phase carbon acidity. 1994 , 7, 268-271	22
1945	Spectrometry and reactivity of phenalenyl anions. 1994 , 7, 296-302	13
1944	AB initio calculations of Diels-Alder transition structures for hetero-dienophile additions to cyclopentadiene. 1994 , 7, 641-645	17
1943	A comparison of semiempirical and ab initio transition states for HF elimination in unimolecular decompositions. 1994 , 51, 161-172	13
1942	Hydrogen bonding of nucleotide base pairs: Application of the PM3 method. 1994 , 52, 95-107	23
1941	The neglect of diatomic differential overlap (NDDO) fragment self-consistent field method for the treatment of very large covalent systems. 1994 , 52, 227-236	4
1940	Quantum-Mechanical investigation of large water clusters. 1994 , 52, 349-360	27
1939	Structure and Tautomerism of ANTA (aminonitrotriazole). 1994 , 19, 32-41	6
1938	Nonlinear optical properties of some substituted biphenyls. 1994 , 3, 329-342	11
1937	Symmetry breaking in charge-transfer compounds. The effects of electric fields and substituents on the properties of bipyrazine cations. 1994 , 4, 339-352	1

1936	Theoretical and experimental studies of intermediate species of photolysis, and phototoxicity of anti-hyperlipoproteinemic drugs (fibrates). 1994 , 4, 451-463	4
1935	Comparison of methods to estimate geometric and electronic properties on sulfur containing compounds. 1994 , 89, 1-12	25
1934	On the selection of the optimal plasticizer for calix[n]arene-based ion-selective electrodes: Possible correlation between the ion selectivity and the softness of the plasticizer. 1994 , 17, 377-392	17
1933	ESR studies on carboxylic esters. Part 13: Electron spin resonance spectroscopy and molecular orbital calculations on the radical anions of 2-oxo-carbothioate and 2-oxo-carbodithioate esters. 1994 , 32, 624-630	6
1932	Study of the kinetics and equilibrium of the benzyl-radical association reaction with molecular oxygen. 1994 , 26, 171-189	41
1931	Syntheses and Reactions of Crown Ether-Bridged Stilbenes. 1994 , 1994, 1199-1209	24
1930	Coronene-Potassium(THF) ₂ (tmeda): X-Ray Structure and MNDO Calculations of a Half-Sandwich Contact Ion Pair as a Model for Potassium(Adsorbate)-Graphite Surface Interactions. 1994 , 127, 1251-1253	27
1929	Thianthren-Radikalkation-Tetrachloroaluminat. 1994 , 127, 2043-2049	41
1928	A Chiral Adamantanophane: Preparation, Enantiomer Separation, Theoretical and Experimental Circular Dichroism and Absolute Configuration. 1994 , 127, 2081-2088	10
1927	Initial stages of electrophilic substitution studied with quantum molecular dynamics. 1994 , 223, 1-6	3
1926	Structure and charge distribution of multiply charged C ₇₀ . 1994 , 223, 149-154	13
1925	The effect of intermolecular interactions on proton tunneling in the tropolone-(CH ₄) ₁ and 5-chlorotropolone-(CH ₄) ₁ van der Waals complexes. 1994 , 224, 563-568	13
1924	The electrostatic potential in the semiempirical molecular orbital approximation. 1994 , 225, 11-17	18
1923	Infrared-active modes of C ₇₀ . 1994 , 227, 365-370	20
1922	Theoretical evaluations of standard heats of formation of fullerenes. 1994 , 231, 331-336	10
1921	Direct measurements of the rates of 1,3- and 1,5-sigmatropic hydrogen shifts in the photo-Fries rearrangements of phenyl acetate. 1994 , 223, 521-526	24
1920	The influence of aluminum trichloride on a configuratively labile lactone-bridged biaryl: quantum chemical calculations and optical spectroscopy. 1994 , 222, 247-253	9
1919	Thermolysis and Chemiluminescence of Monocyclic 1,2,4-Trioxan-5-ones. 1994 , 77, 1851-1860	2

1918	Comparison of NDDO and quasi-ab initio approaches to compute semiempirical molecular electrostatic potentials. <i>Journal of Computational Chemistry</i> , 1994 , 15, 12-22	3.5	39
1917	General parameterization of a reaction field theory combined with the boundary element method. <i>Journal of Computational Chemistry</i> , 1994 , 15, 90-104	3.5	24
1916	Conformation and reactivity of β -oxo-ketenes: Ab initio and semiempirical (AM1, PM3) calculations. <i>Journal of Computational Chemistry</i> , 1994 , 15, 132-143	3.5	13
1915	Semiempirical study of compounds with intramolecular O \cdots H \cdots O hydrogen bonds. II. Further verification of a modified MNDO method. <i>Journal of Computational Chemistry</i> , 1994 , 15, 183-189	3.5	25
1914	Quantum mechanical computations on very large molecular systems: The local self-consistent field method. <i>Journal of Computational Chemistry</i> , 1994 , 15, 269-282	3.5	262
1913	MRD-CI studies of vertical excitation energies of unsaturated hydrocarbon molecules. <i>Journal of Computational Chemistry</i> , 1994 , 15, 424-432	3.5	9
1912	Fast geometry optimization using a modified extended H \ddot{c} kel method: Results for molecules containing H, C, N, O, and F. <i>Journal of Computational Chemistry</i> , 1994 , 15, 733-746	3.5	14
1911	Structure of disiloxane: A semiempirical and Post-HartreeFock study. <i>Journal of Computational Chemistry</i> , 1994 , 15, 925-936	3.5	21
1910	The natural atomic orbital point charge model for PM3: Multipole moments and molecular electrostatic potentials. <i>Journal of Computational Chemistry</i> , 1994 , 15, 1064-1073	3.5	31
1909	3H-Indole. 1994 , 33, 1153-1156		24
1908	N-Heteroarene Dianions as Antiaromatic Ligands Bridging two Lanthanocene Moieties. 1994 , 33, 1171-1174		24
1907	Nonplanar bis(1,3-dithiole) donors affording novel cation radical salts. 1994 , 6, 295-298		24
1906	The First sulfur-containing twin-DCNQI-type acceptor. 1994 , 6, 765-768		9
1905	Ein extrem langlebiges Triplett-Carben; Reaktivit \ddot{a} t, optisches Absorptionsspektrum und Kinetik hochsubstituierter Diarylcarbene. 1994 , 106, 944-946		7
1904	N-Heteroaren-Dianionen als antiaromatische Br \ddot{u} ckenliganden zwischen zwei Lanthanocen-Einheiten. 1994 , 106, 1220-1223		5
1903	3H-Indol. 1994 , 106, 1240-1243		3
1902	Benzobis(thiadiazole) mit hypervalenten Schwefelatomen: neuartige Heterocyclen mit hohen Elektronenaffinit \ddot{a} t \ddot{e} n und kurzen intermolekularen Abst \ddot{a} nden zwischen Heteroatomen. 1994 , 106, 2030-2032		14
1901	Corrphycen: ein neues Porphyrinisomer. 1994 , 106, 2402-2406		33

1900	Spacer-kontrollierte Fernfunktionalisierung von Buckminsterfulleren: regiospezifische Bildung eines Hexaadduktes. 1994 , 106, 2434-2437	70
1899	Comparative semiempirical and ab initio study of the harmonic vibrational frequencies of aniline. The ground state. 1994 , 50, 69-86	55
1898	Hydrogenation of polynuclear aromatic hydrocarbons. 2. quantitative structure/reactivity correlations. 1994 , 49, 4191-4210	44
1897	Molecular dynamics studies in isotropic phase of n-TPEB's by dielectric relaxation method. 1994 , 62, 55-63	5
1896	Structure and optical absorption of oligorylenes upon doping. 1994 , 189, 53-65	19
1895	The role of amphotericin B amino group basicity in its antifungal action. A theoretical approach. 1994 , 49, 241-50	13
1894	Selective cross coupling via oxovanadium(V)-induced oxidative desilylation of benzylic silanes. 1994 , 35, 8005-8008	9
1893	Synthesis of sterically rigid macrocycles by the use of pressure-induced repetitive Diels-Alder reactions. 1994 , 35, 73-76	35
1892	Theoretical consideration on the metalorganic molecular beam epitaxy growth mechanism of III-V semiconductors by molecular orbital calculation. 1994 , 136, 83-88	3
1891	Do gas phase adducts form during metalorganic vapour phase epitaxial growth of gallium arsenide?. 1994 , 145, 104-112	9
1890	Multinuclear NMR spectroscopy and semi-empirical MNDO-PM3 quantum chemical investigations of the compounds C ₆ H ₅ XY (X=S, SO, SO ₂ ; Y=CF ₃ , CH ₃). 1994 , 69, 41-49	12
1889	A new method of calculating interactions between adsorbates and metal oxide surfaces: application to the study of CO ₂ insertion in hydroxyl or methoxy groups on Al ₂ O ₃ and TiO ₂ . 1994 , 320, 49-56	11
1888	Proton sponges. 1994 , 328, 297-323	200
1887	Structures and energetics of radical cations containing tributyltin fragments: A PM3 study. 1994 , 471, 71-76	5
1886	UV laser photolysis and quantum yields of para-substituted phenyldiazosulphonate surfactants. 1994 , 83, 129-140	2
1885	Photochromism of 3-(3-pyridyl): an investigation by electron spectroscopy for chemical analysis (ESCA) and molecular orbital calculations. 1994 , 84, 257-264	11
1884	Role of the 5-aryl moiety in the photophysics of triaryl-2-pyrazolines. 1994 , 77, 133-139	14
1883	Synthesis and antimicrobial activity of novel 3-[(aminopyrimidiniumyl)thio]methyl cephalosporins. 1994 , 37, 3828-33	12

- 1882 Studies on pyrazines. Part 28 . Deoxydative acetoxylation of pyrazine N-oxides. **1994**, 31, 1229-1233 11
- 1881 The utility of the PM3 method for predicting the reactivities of cyanoethenes in diels-alder reactions with pyrrole. **1994**, 31, 1429-1432 22
- 1880 Novel semiempirical method for quantum Monte Carlo simulation: Application to amorphous silicon. **1994**, 100, 3742-3746 17
- 1879 An unequivocal ¹H NMR structural assignment of TOX8 and TOX9, the two most abundant toxaphene congeners in marine mammals. **1994**, 349, 552-558 33
- 1878 Formation of polycyclic hydrocarbons containing a spiropentane or methylenecyclobutane moiety upon thermal decomposition of cyclopropane-containing 1-pyrazolines. **1994**, 43, 612-618 3
- 1877 The effect of substituents (CH₃ and NH₂) in positions 4 and 6 on the acid-base properties of 2(1H)-pyrimidinethiones. **1994**, 43, 2026-2029
- 1876 MNDO method for calculations of magnesium clusters. **1994**, 43, 1310-1314 1
- 1875 Quantum-chemical calculations of the mechanism of some reactions of the insertion of silylenes and dichlorosilylenes into a single bond. **1994**, 43, 751-754 3
- 1874 Acid-base properties and complex-forming ability of 4,6-dimethyl-2-(1H)-pyrimidinone (thione). **1994**, 43, 799-802
- 1873 Combined Use of Factorial Design and Comparative Molecular Field Analysis (CoMFA): a Case Study. **1994**, 13, 249-261 0
- 1872 A Quantitative Structure- Activity Relationship (QSAR) for Prediction of β -2-Microglobulin Nephropathy. **1994**, 13, 275-280 1
- 1871 Modified Hopfinger analysis of the phosphodiesterase inhibiting activity of flavonoids. **1994**, 29, 45-50
- 1870 Semi-empirical molecular orbital calculations on bambuterol, an inhibitor of human butyrylcholinesterase. **1994**, 314, 277-285 3
- 1869 PM3-CI calculation of Diels-Alder transition structures of hetero dienophile addition to butadiene: comparison with PM3 and ab initio generated transition structures. **1994**, 315, 85-90 10
- 1868 Theoretical study of prototropic tautomerism and acidity of tris(fluorosulfonyl)methane. **1994**, 315, 191-196 4
- 1867 On the mechanism of cephalosporin isomerization. **1994**, 315, 1-7 8
- 1866 Computational study of imidazole and methyl imidazoles. **1994**, 304, 45-51 14
- 1865 Investigation of the pyrolysis mechanism of oxazole and maleimide by using the AM1 and PM3 methods. **1994**, 306, 269-287 8

1864	Prediction of geometries and interaction energies of complexes formed by small molecules using semiempirical and ab initio methods. 1994 , 309, 279-294	10
1863	Semiempirical study of the conformation of tetroxane and its halogenated derivatives. 1994 , 309, 315-324	10
1862	The role of electrostatics in the ring opening step of xylose isomerase catalysis. 1994 , 307, 171-178	11
1861	Structural study of β -D-arabinofuranosyluracil derivatives with known antiviral activity. 1994 , 305, 35-53	7
1860	Semiempirical calculation of the ESCA chemical shifts of the group IVA elements in a chemical environment. 1994 , 305, 261-281	6
1859	A comparative molecular mechanics, semiempirical and ab initio study of saturated five-membered rings. 1994 , 303, 205-212	21
1858	AM1, PM3 and MNDO study of SN2 reaction of methylhydroperoxy anion with alkyl chlorides. 1994 , 306, 67-76	3
1857	Strained unsaturated molecules. Theoretical study of acyclic and cyclic cumulenes and acetylenes. 1994 , 313, 335-349	32
1856	Extension of MNDO to d orbitals: parameters and results for silicon. 1994 , 313, 141-154	49
1855	Structure and stability of chlorosiloxanes. 1994 , 313, 155-164	9
1854	Evaporative processes of sputtered alkali halide cluster ions. 1994 , 94, 404-410	1
1853	Hetero-Cope Rearrangement of S-(1,2,3-Triphenylcyclopropenyl)-O-ethyldithiocarbonate. 1994 , 4, 9-11	9
1852	Probing the mechanisms of growth of gallium arsenide by metalorganic vapor phase epitaxy using experimental and theoretical studies of designed precursors. 1994 , 23, 69-74	10
1851	Quantum-chemical calculations of the electronic structure and reactivity of silylenes. 1994 , 43, 941-943	0
1850	Sequential pericyclic reactions of cyclopentadienone with nonconjugated dienes. Intramolecular cycloaddition reactivity of the decarbonylated primary cycloadducts and X-ray structure of DDA adduct. 1994 , 50, 13395-13408	6
1849	An atomistic model for stepped diamond growth. 1994 , 372, 535-537	49
1848	On the reliability of conformational calculations. Comparison of calculated and crystal structures of fenamic acids. 1994 , 312, 115-126	4
1847	Tetrahedral intermediate formation in the acylation step of acetylcholinesterases. A combined quantum chemical and molecular mechanical model. 1994 , 304, 129-141	44

1846	Semiempirical calculations of the ESCA chemical shifts of nitrogen atoms in a chemical environment: failure of the PM3 and AM1 methods. 1994 , 304, 151-161	8
1845	Critical appraisal of the semiempirical wavefunctions by calculating ESCA chemical shifts: inner-shell binding energies in halogen atoms. 1994 , 304, 163-171	4
1844	Functional sites of cytochrome c and other electron carrier proteins: semi-empirical molecular orbital program PM3 applied to the conformational analysis of Cys-X1-X2-Cys peptides. 1994 , 76, 614-21	3
1843	Quantum pharmacologic studies applicable to the design of anticonvulsants: theoretical conformational analysis and structure-activity studies of barbiturates. 1994 , 35, 411-25	10
1842	Light stability of a β -cyclodextrin inclusion complex of a cyanine dye. 1994 , 90, 3517-3520	20
1841	Semiempirical molecular orbital study on the transition states for the anti-selective Michael addition reactions of the lithium Z-enolates of N-alkylideneglycinates to α,β -unsaturated esters. 1994 , 2525-2530	19
1840	Chapter 6 Biochemistry of the penicilloyl serine transferases. 1994 , 27, 103-129	28
1839	One- and two-electron reduction potentials of peroxy radicals and related species. 1994 , 2551-2553	75
1838	Supramolecular complexes based on calixarenes: force field calculations and applications for chemical sensors. 1994 , 1, 11-19	28
1837	Transition between bipolaron and polaron states in doped heterocycle polymers. 1994 , 50, 13364-13370	44
1836	P91 quantitative structure-activity relationships (QSAR) for nitroxanthenes and their antituberculous activity. 1994 , 2, 141	1
1835	Modulation of the kynurenine pathway in search for new neuroprotective agents. Synthesis and preliminary evaluation of (m-nitrobenzoyl)alanine, a potent inhibitor of kynurenine-3-hydroxylase. 1994 , 37, 647-55	126
1834	Synthesis, Isolation, and Equilibration of 1,9- and 7,8-C ₇₀ H ₂ . 1994 , 264, 397-9	88
1833	A PM3 molecular orbital model of silica rings and their vibrational spectra. 1994 , 180, 11-16	36
1832	Chemistry and kinetics of β - and η -naphthyl(phosphonyl)carbenes. Effects of positions on neighbouring phosphonate participation. 1994 , 633-641	5
1831	Asymmetric synthesis of β -aminotetralins by electrophilic amination. 1994 , 50, 10909-10922	10
1830	A semiempirical study of protonated ammonia-triethylamine clusters. 1994 , 312, 85-91	1
1829	Reconstruction of (100) diamond surfaces using molecular dynamics with combined quantum and empirical forces. 1994 , 49, 5662-5671	52

1828	A Quantitative Structure-Activity Relationship (QSAR) for prediction of alpha(2mu)-globulin nephropathy. 1994 , 8, 885-7	8
1827	Molecular orbital calculations of electronic excited states in poly(p-phenylene vinylene). 1994 , 66, 143-148	28
1826	Theoretical study of the electroreduction of halogenated aromatic compounds. Part 3. β -, m- and p-dibromobenzenes studied by AM1 and PM3 methods. 1994 , 90, 3241-3244	3
1825	Remote substituent effects on polar and non-polar covalent bonds. 1994 , 2149-2154	13
1824	Theoretical kinetic isotope effects for the hydride-transfer step in lactate dehydrogenase. 1994 , 90, 1703-1707	31
1823	A theoretical study of protonation and tautomerization of N-substituted aminoazobenzenes. 1994 , 71-75	6
1822	Regioselective Friedel-Crafts acylation of 2,3,4,5-tetrahydro-1H-2-benzazepine and related nitrogen heterocycles. 1994 , 2993-2999	14
1821	Intermolecular interactions responsible for the absence of chiral recognition: aromatic C-H \cdots O hydrogen bonding in the crystal structure of 3-chloro-9,13-dibutylamino-1-hydroxypropyl-6-trifluomethylphenanthrene propan-2-ol solvate hydrochloride. 1994 , 1135-1137	5
1820	Molecular modelling study of a dissymmetric calix[4]arene and its methyl ethers. 1994 , 2259-2267	9
1819	Chlorotropic rearrangements of an β -sulfanyl- β -sulfonylalkanesulfonyl chloride to an β -chloroalkyl disulfide and an S-(β -chloroalkyl) thiosulfonate. 1994 , 1251-1252	5
1818	Utilization of selenium-directed [2 + 2] cycloadditions: concise synthesis of (-)-fraganol. 1994 , 695-700	4
1817	Correlation Between the Chemical Structures of Dialkyl Peroxides and Their Retention in Reversed-Phase High-Performance Liquid Chromatography. 1994 , 17, 3933-3949	13
1816	EINKRISTALL-MOLEKÜLSTRUKTUREN 551,2 DITHIOLO-DITHIOL-DITHION C4S6 UND DITHIOLO-DITHIOL-DION C4O2S4. 1994 , 91, 53-67	5
1815	THE COORDINATION OF AMINOPHOSPHONATES TO CHROMIUM(III). 1994 , 33, 15-32	3
1814	Comparison Between the IR Spectra and the Structure of the Two Conformations of a Diazabicyclanol. 1994 , 27, 1165-1186	3
1813	Possibility of stable spheroid molecules of ZnO. 1994 , 49, R1543-R1546	66
1812	A Molecular Orbital Model of Gel-Silica IR Spectra. 1994 , 346, 727	3
1811	Disilene Addition to C70. 1994 , 359, 363	1

1810	Quantum Chemical Methods for the Design of Molecular Non-Linear Optical Materials. 1994 , 374, 3	
1809	ESR Study of Intramolecular Magnetic Interactions in Bis(nitrenophenyl) Sulfides. 1994 , 23, 1679-1682	4
1808	The Cholesteric Pitch and Its Temperature Dependence of Chiral Nematics Induced by Compounds Having 1-Methyl-Heptyloxy Group. 1994 , 63, 3326-3332	2
1807	Detailed Quantummechanical Calculations of Molecular Vibration Frequencies of Benzene, Naphthalene, Anthracene and Phenanthrene. Comparison of Several Quantumchemical Methods. 1994 , 187, 15-32	5
1806	Vertical Ionization Potentials of Alkoxides in Solution. 1994 , 67, 360-362	4
1805	Structure Correlation and Ligand/Receptor Interactions. 1994 , 543-603	10
1804	Chemically Amplified Resists. V Photochemical Proton Generation Mechanism from Triphenylsulfonium Salts.. 1994 , 7, 483-486	4
1803	Quantum-chemistry calculations of surface complex and orbital control in para/ortho toluene alkylation catalyzed by big pore zeolites. 1994 , 84, 2171-2178	10
1802	SOME EVIDENCE ABOUT THE MECHANISM OF FORMATION OF 5-(1-HYDROXYIMINOALKYL)-1, 2-DITHIOLE-3-THIONES. 1994 , 97, 103-111	1
1801	Quantitative Structure-activity Relationships Of (+)-anatoxin-a Derivatives. 1994 , 4, 121-128	4
1800	Effect of Orbital Overlap in Thermal Reverse Homo-Diels-Alder Reaction and Intramolecular Reverse Ene Reaction. 1994 , 41, 631-634	
1799	Stereoselective synthesis and transformation of siastatin B, A novel glycosidase inhibitor, directed toward new drugs for viral infection and tumor metastasis. 1995 , 75-121	5
1798	Chemically amplified resists VI. photochemical proton generation mechanism from 2-oxocyclohexyl-cyclohexyl-methyl sulfonium salts.. 1995 , 8, 611-614	1
1797	A Theoretical Study of the Energetics and Vibrational Spectra of Oxygenated (100) Diamond Surfaces. 1995 , 416, 281	
1796	Molecular Concepts. 1995 , 15-47	15
1795	Fulgenolides. Thermally Irreversible Photochromic Lactones with Large Quantum Yields of Photoreactions. 1995 , 24, 17-18	2
1794	Important Role of Tetrahydrofuran Ring in Activation of Hydrogen Peroxide in the Presence of Binuclear Iron(III) Complexes with LinearOxo Bridge. 1995 , 24, 885-886	11
1793	Semiconductor Photocatalysis. ZnS-Nanocrystallite-Catalyzed Photooxidation of Organic Compounds. 1995 , 68, 1811-1823	47

- 1792 Photoinduced Hydride Reduction of 10-Methylacridinium Ion by Alkylbenzenes in the Presence of Perchloric Acid. **1995**, 24, 111-112 4
- 1791 Formation and Cycloreversion of Dioxadiazole Intermediates in the Reaction of Diazo Compounds with Singlet Oxygen. **1995**, 24, 545-546 2
- 1790 Preparation and Structural Characterization of the Charge-Transfer Complex (12[ane]S₄.I₂)⁺ (12[ane]S₄ = 1,4,7,10-Tetrathiacyclododecane). **1995**, 51, 697-700 5
- 1789 Two Highly Substituted Methylenecyclopropanes. **1995**, 51, 700-703
- 1788 Structure determination by electron crystallography using both maximum-entropy and simulation approaches. **1995**, 51, 849-868 31
- 1787 Photoacoustic determination of heats of formation and reaction of 5-chloro-1,2-didehydro-1H-azepine, a seven-membered cyclic ketenimine. **1995**, 21, 877-883 4
- 1786 Effects of temperature on the triplet behavior of the styrylphenanthrene isomers. **1995**, 21, 725-734 3
- 1785 Second harmonic generation in ferroelectric liquid crystalline thiadiazole derivatives. **1995**, 7, 170-173 21
- 1784 Novel metallic charge-transfer complexes composed of a [3] radialene type acceptor: A 1,2-Bis(p-benzoquino)-3-12-(dicyanomethylene)-2,5-selenoquinojcyclopropane Derivative**. **1995**, 7, 639-641 9
- 1783 Photoelectron and optical spectroscopic investigations of the electronic structure of oligo(p-phenylenevinylene)s in the solid state**. **1995**, 7, 722-726 37
- 1782 Orthorhombisches und monoklines 2,3,7,8-Tetramethoxythianthren: kleiner Strukturunterschied □ große Gitteränderung. **1995**, 107, 120-122 6
- 1781 Studies on electron transfer as mechanistic concept for [4 + 2] cycloadditions, 2. Cycloadditions of 2,3-bis(dimethylaminomethylene)bicyclo[2.2.1]heptane and 2,3-bis(dimethylaminomethylene)bicyclo[2.2.2]octane with electron-deficient olefins. **1995**, 1995, 1139-1152 11
- 1780 Ab initio and semiempirical calculations of the hetero-Diels-Alder reaction of 1-aza-1,3-butadiene with ethene. **1995**, 1995, 1681-1687 25
- 1779 Influence of conformational factors on acid-catalyzed cyclizations of germacranolides: Molecular structure of the cyclization products of gallicin and 8 β -hydroxygallicin (shonachalin a). **1995**, 1995, 1837-1841 13
- 1778 A molecular orbital description of aromatic cluster ions produced in continuous-flow fast atom bombardment. **1995**, 30, 296-304
- 1777 Mass spectrometric and theoretical determination of polynuclear aromatic hydrocarbon proton affinities. **1995**, 30, 1495-1504 10
- 1776 Oxidation of 4-methylcatechol by dioxygen studied by ESR spectroscopy. The different regioselectivity of OH \cdot and MeO \cdot nucleophilic attack and kinetic deuterium isotope effects. **1995**, 33, 15-19 2
- 1775 Approach to the conformational behaviour of tetraazamacrocycles in the solution state. NMR and molecular modelling studies. **1995**, 33, 128-133 1

1774	Interpretation of substituent-induced chemical shifts in ^{13}C NMR spectra of 2-substituted norbornadienes. Influence of homoconjugation. 1995 , 33, 349-354	5
1773	^{33}S NMR spectroscopy: Substituent effect. Halogen derivatives of tetrahydrothiophene 1,1-dioxide. 1995 , 33, 853-856	3
1772	Efficacy of a 3-substituted versus 17-substituted chemical delivery system for estradiol brain targeting. 1995 , 84, 38-43	8
1771	Surface-enhanced resonance Raman scattering study of the groove binding dye hoechst 33258. 1995 , 26, 435-441	4
1770	Chiral Organometallic Reagents, XIV. Theoretical Investigations into the Mechanism of Inversion of Configuration at the Carbon Center of β -Sulfur-Substituted Carbanions. 1995 , 128, 673-677	28
1769	Aspects of chirality in overcrowded bistricyclic enes. 1995 , 7, 199-205	20
1768	Untersuchungen zur Cyclokondensation von o-aminophenyl-substituierten Ketoximen und Amidoximen mit Carbonylverbindungen zu anellierten Chinazolinderivaten. 1995 , 328, 397-402	9
1767	^{13}C NMR relaxation studies of 1:2 LiCl-ethylaluminum dichloride solutions. 1995 , 230, 185-188	6
1766	^1H NMR relaxation studies of molten salts containing ethylaluminum dichloride. 1995 , 238, 115-120	6
1765	Parameterization of NDDO wavefunctions using genetic algorithms. An evolutionary approach to parameterizing potential energy surfaces and direct dynamics calculations for organic reactions. 1995 , 233, 231-236	164
1764	How reliable is the Lippincott-Schroeder potential for the $\text{OH}\cdots\text{N}$ hydrogen bonded fragment in the gas phase?. 1995 , 244, 89-92	21
1763	First-order hyperpolarizabilities of octupolar aromatic molecules: symmetrically substituted triazines. 1995 , 244, 153-156	41
1762	A theoretical study of C_{80} and $\text{La}_2\text{@C}_{80}$. 1995 , 245, 230-236	124
1761	Synthesis, Structure, and Antimalarial Activity of Some Enantiomerically Pure, cis-fused cyclopenteno-1,2,4-trioxanes. 1995 , 78, 647-662	84
1760	An examination of a density functional/molecular mechanical coupled potential. <i>Journal of Computational Chemistry</i> , 1995 , 16, 113-128	3.5 87
1759	An application of the reaction field theory to hydrated metal cations in the framework of the MNDO, AM1, and PM3 methods. <i>Journal of Computational Chemistry</i> , 1995 , 16, 378-384	3.5 17
1758	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. <i>Journal of Computational Chemistry</i> , 1995 , 16, 563-575	3.5 86
1757	Heterogeneous catalyzed synthesis of 1,1,1,2-tetrafluoroethane from 1,1,1,2-tetrachloroethane: thermodynamics and reaction pathways. 1995 , 75, 103-110	22

1756	The ionization energies of polychlorinated dibenzo-p-dioxins: new experimental results and theoretical studies. 1995 , 145, 97-108	40
1755	Analysis of powder EPR and ENDOR spectra of the biphenyl radical cation on H-ZSM-5 zeolite, silica gel and in CFCl ₃ matrix. 1995 , 193, 89-99	30
1754	A theoretical investigation of solvatochromism. Application to merocyanines similar to colored forms obtained by flash-photolysis of spiropyrans. 1995 , 194, 101-116	20
1753	The solvent shift in the excitation of CH ₂ O in H ₂ O: An MRD-CI investigation using effective potentials for the representation of the water molecules. 1995 , 199, 145-153	9
1752	Structure, bonding, and asymmetric induction in (R,R)-2,3-dimethoxy-1,4-bis(dimethylamino)butane complexes with organolithium compounds: A semiempirical computational study. 1995 , 6, 2165-2176	7
1751	A computational study of lithio azaallylic systems. 1995 , 51, 5955-5970	9
1750	Theoretical model of solvated lithium dienediolate of 2-butenic acid. 1995 , 51, 7207-7214	16
1749	A study of the sensitivity and decomposition of 1,3,5-trinitro-2-oxo-1,3,5-triazacyclo-hexane. 1995 , 260, 201-216	9
1748	Correlation between the luminescence and Raman peaks in quantum-confined systems. 1995 , 255, 241-245	7
1747	A quantum-chemical study of para/ortho-toluene alkylation by adsorbed methoxy species on zeolites. 1995 , 100, 75-85	16
1746	Theoretical methods in thermodynamics of condensed phases. 1995 , 45, 829-838	1
1745	Theoretical investigation of isotopic scrambling mechanisms in 2-chloroethyl methyl sulfide. 1995 , 6, 243-254	1
1744	Interaction of divalent metal cations and nucleotides: A computational study. 1995 , 6, 343-348	7
1743	Semiempirical calculation of two-electron integrals using bipolar expansion of the Ohno potential. 1995 , 36, 538-543	2
1742	A molecular mechanics and semiempirical conformational analysis of the herbicide diuron inhibitor of photosystem II. 1995 , 6, 383-389	7
1741	X-ray structure of isomeric 3-chloro-4-(methylthio)- and 4-chloro-3-(methylthio)quinolines. 1995 , 25, 165-169	1
1740	Electronic properties of inorganic benzenes. 1995 , 5, 339-345	1
1739	Self-assembly of frame structures. 10. Stereochemistry of 2,5-dioxabicyclo [2.2.1]heptane-3,6-dione. 1995 , 31, 1280-1288	

1738	Dipyrrolo[1,2-a; 2',1'-c]pyrazines. 1. Quantum-chemical study of dipyrrolo[1,2-a; 2',1'-c]pyrazines in electrophilic substitution reactions. 1995 , 31, 1353-1359	
1737	X-ray crystallographic studies and molecular calculations on 1:1 inclusion complexes of cholic acid with acetophenone and its derivatives. 1995 , 22, 155-168	5
1736	Class IV charge models: a new semiempirical approach in quantum chemistry. 1995 , 9, 87-110	282
1735	Structural model of the photosynthetic reaction center of Rhodobacter capsulatus. 1995 , 22, 226-44	18
1734	The question of pentaphenylethyl: An AM1 study. 1995 , 8, 171-174	1
1733	Quantitative description of acidity of XOH compounds in the gas phase and dimethyl sulphoxide with use of HOMO energies of XO ⁻ anions. 1995 , 8, 364-370	1
1732	Atomic force microscopy and Solid-State rearrangement of benzopinacol. 1995 , 8, 545-551	19
1731	A semiempirical study of heterocycle oligomers and polymers in different dielectric media. 1995 , 54, 369-379	6
1730	Semiempirical study of the bergman reaction: Towards a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. 1995 , 56, 51-59	2
1729	Investigation of the potential energy surface for the first step in the alkaline hydrolysis of methyl acetate. 1995 , 56, 83-93	14
1728	A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. 1995 , 56, 103-112	12
1727	A theoretical investigation of the solution N(7) H ? N(9) H tautomerism of adenine. 1995 , 56, 113-122	37
1726	A theoretical study of lithium ion and aromatic organic cation graphite intercalates. 1995 , 56, 533-539	7
1725	Amino acid composition and wavelength effects in matrix-assisted laser desorption/ionization. 1995 , 9, 744-752	40
1724	Synthesis, spectral characteristics and structure of 1,3- and 1,4-disubstituted tetrazolinones. 1995 , 337, 636-640	5
1723	Molecular Orbital Models of Silica Rings and Their Vibrational Spectra. 1995 , 78, 1093-1096	33
1722	Conformational changes of small molecules binding to proteins. 1995 , 3, 411-28	215
1721	Synthesis, antioxidant properties, biological activity and molecular modelling of a series of chalcogen analogues of the 5-lipoxygenase inhibitor DuP 654. 1995 , 3, 1255-62	110

1720	Inhibition of rat liver mitochondrial monoamine oxidase by hydrazine-thiazole derivatives: structure-activity relationships. 1995 , 3, 1485-91	29
1719	The radiation chemistry of perfluorinated ethers. 1995 , 45, 23-30	14
1718	EPR study of cation-radicals of cyclic alkenes in chlorofluorocarbon matrices. 1995 , 45, 45-49	8
1717	Properties of singlet excited N-(pyrimidin-2-one-4-yl)pyridinium chloride and structurally related organic cations. 1995 , 88, 117-123	3
1716	Photochromic properties of 4?-amino-substituted 2-hydroxychalcones. 1995 , 89, 251-256	36
1715	Molecular design and biological activity of potent and selective protein kinase inhibitors related to balanol. 1995 , 2, 601-8	54
1714	Deuterium isotope effect on ¹³ C NMR spectra of ortho Mannich bases. 1995 , 67, 63-69	15
1713	Site-specific protonation directs low-energy dissociation pathways of dinucleotides in the gas phase. 1995 , 148, 1-23	56
1712	Carbonic anhydrase inhibitors. Part 24. A quantitative structure-activity relationship study of positively charged sulfonamide inhibitors. 1995 , 30, 687-696	59
1711	A study of the carbon-halogen bond breaking in tert-butyl halides by the PM3 quantum chemical method. 1995 , 191, 25-30	12
1710	An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds. 1995 , 195, 107-116	19
1709	Electronic structure of donor-spacer-acceptor molecules of potential interest for molecular electronics. III. Geometry and absorption spectrum of CH ₃ -P3CNQ. 1995 , 196, 407-422	14
1708	Electronic structure of donor-spacer-acceptor molecules of potential interest for molecular electronics. IV. Geometry and device properties of P3CNQ and Q3CNQ. 1995 , 196, 423-436	28
1707	Electron-proton free-energy surfaces for proton transfer reaction in polar solvents: test calculations for carbon-carbon reaction centres. 1995 , 200, 87-106	23
1706	Identification of a predominant keto conformer of malonyl dichloride: An infrared and theoretical study. 1995 , 51, 1891-1901	8
1705	Study of 1-hydroxybenzotriazole/benzotriazole N-oxide tautomerism in the gas phase by photoelectron spectroscopy. 1995 , 51, 1801-1807	14
1704	Cadinane-type sesquiterpenes induced in Gossypium cotyledons by bacterial inoculation. 1995 , 39, 531-536	33
1703	Orientation of molecules of aliphatic alcohols adsorbed on a mercury electrode surface analysis of steric factors of inhibited electrode reactions and quantum-chemical calculations. 1995 , 385, 95-103	18

- 1702 Theoretical studies of electrode potentials in aqueous solution. Investigation of individual contributions from electrostatic, cavity and dispersion interactions to redox potentials. **1995**, 385, 1-8 19
- 1701 Semi-empirical calculations on bis-halomethyl sulfides. A comparison of the structures and other parameters by MNDO, AM1 and PM3 methods. **1995**, 70, 9-17 2
- 1700 Semi-empirical molecular orbital studies of monofluorination reactions: reaction of hydrofluorocarbons over cobalt trifluoride. **1995**, 70, 49-52 2
- 1699 CH₃CF₃BCl_n haloalkanes and CH₂=CF₂BCl_n halo-olefins on γ -alumina catalysts: reactions, kinetics and adsorption. **1995**, 74, 27-35 10
- 1698 Structural chemistry of polycyclic heteroaromatic compounds. Part 6. Photoelectron spectra and electronic structures of polycyclic hetarenes: thienoquinolines and thienoisquinolines. **1995**, 351, 107-117 2
- 1697 Theoretical structure investigations of N-acetyl-L-proline amide. **1995**, 352-353, 59-70 23
- 1696 A semiempirical approach for the calculation of the vibrational spectra of conducting polymers: the case of polyselenophene. **1995**, 348, 91-94 9
- 1695 Electronic properties, polymerization, and cycloaddition of 3,4,7,8-tetragermacycloocta-1,5-diyne and related compounds. **1995**, 499, 123-129 10
- 1694 Interactions in crystals. LXXXIII. The structures of 1,2,4,5-tetrakis(trimethylsilyl)benzene and of its solvent-separated radical anion salt [Na⁺(H₃COCH₂CH_n2OCH₃)₃] [((H₃C)3Si)4H₂C6 $\vec{\sigma}$]. **1995**, 499, 63-71 26
- 1693 Transmission of electronic effects via a SiMe₂ spacer in 4-mono- and 4,4'-disubstituted diphenyldimethylsilanes: ²⁹Si and ¹³C NMR spectroscopy and PM3 semi-empirical calculations. **1995**, 496, 117-125 14
- 1692 Theoretical calculations of heavy-atom isotope effects. **1995**, 19, 11-20 5
- 1691 Theoretical calculations of heavy-atom isotope effects. **1995**, 19, 231-40 20
- 1690 Degradation and stabilization of poly (vinyl chloride). IV. Molecular orbital calculations of activation enthalpies for dehydrochlorination of chloroalkanes and chloroalkenes. **1995**, 47, 9-32 18
- 1689 Competition between cheletropic and homocheletropic additions of sulfur dioxide to 2,3,5,6-tetrakis(methylene)bicyclo[2.2.n]alkanes. Crystal and molecular structures of two 3-thiabicyclo[3.1.0]hexane 3,3-dioxide derivatives.. **1995**, 51, 1685-1696 5
- 1688 Intramolecular addition of aryl radicals to carbon-nitrogen double bonds. **1995**, 51, 2039-2054 18
- 1687 Structure and enantiomerization of helically twisted lactone-bridged biaryls: A theoretical study. **1995**, 51, 3149-3158 24
- 1686 Metallated ketenimines: Deprotonation of N-isopropyl-diphenylketenimine and subsequent trapping reactions with electrophiles A theoretical and experimental study. **1995**, 51, 3767-3786 18
- 1685 Preparation of naphthoquinone imines as NIR dyes. **1995**, 51, 4655-4664 12

1684	Biotransformation of germacrane epoxides by <i>Cichorium intybus</i> . 1995 , 51, 6303-6314	34
1683	Ab initio and PM3 analysis of 1,3-dipolar cycloaddition reaction between pyridine N-oxides and isocyanates. Theoretical evidence of concerted and nonsynchronous mechanism with zwitterionic character. 1995 , 51, 6451-6458	19
1682	NADH mimics on diacetone-d-glucose: Stereoselective biomimetic reduction of benzoylformate and interpretation of chirality transfer deduced by molecular orbital approach. 1995 , 51, 6459-6474	11
1681	1,3-Dipolar cycloaddition of imidate ylides on imino-alcohols: Synthesis of new imidazolones using solvent free conditions. 1995 , 51, 6757-6774	39
1680	High temperature synthesis to bowl-shaped subunits of fullerenes - IV. From 4-[9H-fluorenylidene-(9)]-4H-cyclopenta[def]phenanthrene to fluoreno[1,9,8-abcd]corannulene and difluoreno[1,9,8,7-cdefg;2?,1?,9?,8?-klmno]anthracene. 1995 , 51, 6961-6970	21
1679	On the Equilibrium between Hetareno-annulated 1,2-Dithiines and 12-Membered Cyclic Bis(butadiendiyl) Disulfides. NMR and Molecular Modelling Studies. 1995 , 51, 8853-8862	6
1678	Theoretical Study of the Reaction of Dimethyl Acetylenedicarboxylate with 1-Methyl-2-(1-substituted vinyl)pyrroles. 1995 , 51, 8739-8748	31
1677	Metallated ketenimines: Quinazoline derivatives from base induced dimerization of N-phenyldiethylketenimine. an experimental and theoretical study. 1995 , 51, 9031-9044	10
1676	Studies of proton addition to exo and endo-tricyclo[3.2.1.02,4]octane. 1995 , 51, 11557-11572	0
1675	Easy access to substituted selenazine and selenopyran derivatives by a cycloaddition-cycloreversion process. 1995 , 36, 237-240	34
1674	A theoretical investigation of the N-oxide moiety. 1995 , 36, 699-702	4
1673	Alkylation of 1,4,5-trihydroxyanthraquinone involving nitroalkanes. Syntheses of digitopurpone and (+)-10-deoxy-rhodomyacinone. 1995 , 36, 3729-3730	0
1672	Cycloaddition of imines with allene. formation mechanism of azetidine ring. 1995 , 36, 8031-8034	6
1671	PM3 conformations of C-13 Taxol Ω side chain methyl ester. 1995 , 36, 8849-8852	12
1670	Evidence for reductive elimination of H ₂ in the decomposition of primary arsines. 1995 , 24, 1731-1738	10
1669	Use of comparative molecular field analysis and cluster analysis in series design. 1995 , 70, 149-154	32
1668	A theoretical study of the conformers of trans- and cis-urocanic acid. 1995 , 331, 169-179	17
1667	The relationship of charge transfer complexes to frontier orbital energies in QSAR. 1995 , 331, 63-78	22

1666	Solvent effects on Diels-Alder reactions. A semi-empirical study. 1995 , 331, 37-50	26
1665	Am1 and pm3 transition structure for the hydride transfer. A model of reaction catalyzed by dihydrofolate reductase. 1995 , 330, 411-416	24
1664	MNDO-PM3 investigation of molecule and ion hydration Part 1. Geometry and thermodynamics of H(H ₂ O) _n + water clusters. 1995 , 331, 235-244	3
1663	Diels-Alder transition structures of hetero-dienophile addition to 4H-pyrazole calculated by ab initio methods. 1995 , 331, 229-234	8
1662	PM3 study of the stereochemistry of heterodienophile cycloadditions to pyrrole: endo lone pair effect. 1995 , 332, 39-45	10
1661	Theoretical studies of 5-X-2'-deoxyuracils with known antiviral activity. A comparison of molecular mechanics, AM1, and PM3 semiempirical molecular orbital calculations. 1995 , 332, 75-83	4
1660	The structural and chemical influences on catalytic properties of zeolite clusters. 1995 , 332, 151-159	6
1659	A theoretical study of 2,2';5',2'-terthiophene (T-T) and its analogs. Part 1. Correlation of electronic structure and energies with herbicidal phototoxicity. 1995 , 333, 71-78	10
1658	Theoretical studies of 5-X-2'-deoxyuracils with known antiviral activity. Part 2. A comparison of molecular mechanics, AM1, and PM3 methodologies. 1995 , 333, 111-119	1
1657	MNDO/AM1/PM3 quantum mechanical semiempirical and molecular mechanics barriers to internal rotation: a comparative study. 1995 , 335, 129-139	23
1656	Theoretical study of cluster models and molecular hydrogen interaction with SnO ₂ [110] surface. 1995 , 335, 167-174	15
1655	Conformational analysis of the antiinflammatory fenamates: a molecular mechanics and semiempirical molecular orbital study. 1995 , 335, 215-227	15
1654	Conformational equilibria of 2-substituted 1,3-dithio-5,6-benzocycloheptene and 1,3-dioxa-5,6-benzocycloheptene. 1995 , 334, 59-69	1
1653	Theoretical study of 1,2,4,5-trioxazines. 1995 , 334, 249-255	2
1652	Molecular modelling studies on 1-N-arylamino-1-arylmethanephosphonic acid derivatives. Part 2. Simulated molecular structure of N, N'-ethylenediamino-bis(phenylmethylphosphonic acid diethyl ester). 1995 , 334, 179-185	2
1651	Overlap, pyramidalization and protonation of group 15 heterocycles. The basicities of the higher pyridines 1995 , 338, 51-70	17
1650	Reaction of 2-bromo-2-alkenoic carbonyl compounds with amidines. 1995 , 337, 109-119	1
1649	Charge transfer complexes and frontier orbital energies in QSAR: a congeneric series of electron acceptors. 1995 , 337, 139-150	23

1648	SAR analysis of synthetic neolignans and related compounds which are anti-leishmaniasis active compounds using pattern recognition methods. 1995 , 340, 185-192	16
1647	Theoretical calculations of the structure of a donor-acceptor stilbene, azobenzene and related molecules. 1995 , 340, 45-50	18
1646	Theoretical studies on the structure of chiral 1,2-diol systems. Monomers, dimers and monohydrates. 1995 , 357, 217-223	10
1645	The use of PM3 SCF MO quantum mechanical calculations to refine NMR-determined structures of complexes of antifolate drugs with dihydrofolate reductase in solution. 1995 , 357, 207-216	9
1644	Semiempirical treatment of hydrogen bonding. The acetoin oxime case. 1995 , 342, 33-41	4
1643	Theoretical analysis of the addition of hydroxylamine to uracil and 5-fluorouracil as a model for the thymidylate synthase reaction. 1995 , 343, 1-9	4
1642	A semiempirical conformational analysis of the 3-phenyl-1,2,3-oxathiazolidine 2-oxide. 1995 , 32, 557-562	4
1641	Physicochemical properties of dimethyl sulfoxide-ethanol liquid mixtures. Experimental and semiempirical quantum chemical studies. 1995 , 91, 65-70	59
1640	Flattened fullerenes. 1995 , 44, 1612-1621	
1639	The MNDO-PM3 study of the mechanism of nucleophilic substitution of the phenoxide anion for the nitro group in 1,3,5-trinitrobenzene and 2,4,6-trinitrotoluene in the gas phase and in polar solvents. 1995 , 44, 603-607	
1638	Kinetic studies on the reaction of 9-aryloxy-1,10-anthraquinones with alkyl and arylamines. 1995 , 44, 247-252	
1637	Active centers on the surface of thermoactivated silica. Their reactivity toward organoaluminum compounds. 1995 , 44, 1827-1831	2
1636	Reactions of dimethylzinc on Aerosil. 1995 , 44, 1832-1836	1
1635	Studies of electronic structures of 1,1?-disubstituted silaoxacyclohexa-3,5-dienes. 1995 , 44, 1837-1840	1
1634	Theoretical Investigations on Antimuscarinic Ethylthio and Ethoxy Derivatives of Adiphenine and 4-DAMP. 1995 , 14, 126-133	4
1633	An Experimental and PM3 Semiempirical Quantum-chemical Investigation of Anomalous Aluminium Dissolution in Proton-donor Solvents Containing HCl. 1995 , 5, 207-208	
1632	Rapid and Reversible Migration of the Isothiocyanate Group around the Cyclopropene Ring. 1995 , 5, 213-215	12
1631	Electronic spectra of jet-cooled tropolone-Mn (n=1,2) clusters. Microscopic solvent effects on proton tunneling in the S1 state. 1995 , 103, 3895-3906	19

- 1630 A theoretical analysis of a diamond (100)-(211) dimer bond. **1995**, 102, 5486-5491 37
- 1629 Visible photoluminescence from silicon-backbone polymers. **1995**, 51, 13103-13110 37
- 1628 Dimer-row pattern formation in diamond (100) growth. **1995**, 52, 5426-5432 29
- 1627 Theoretical investigation of the relation of hole-burning properties and the electronic structure of chemisorbed dyes. **1995**, 103, 219-226 2
- 1626 Ultraviolet photoelectron spectroscopy of poly(pyridine-2,5-diyl), poly(2,2'-bipyridine-5,5'-diyl), and their K-doped states. **1995**, 103, 2738-2744 48
- 1625 The Semiempirical Quantum Chemical Studies of Some Properties of Clusters Formed in Formamide-1-Propanol Mixtures. **1995**, 29, 151-158 7
- 1624 THE PHOSPHORYLATION OF 5,12-DIPHENYL-7,14-DIMETHYL-1,4,8,11-TETRAAZACYCLOTETRADECANE. AN NMR AND MOLECULAR MODELLING STUDY OF THE PARENT CYCLE AND THE REACTION PRODUCT. **1995**, 104, 71-80 3
- 1623 X-RAY CRYSTALLOGRAPHIC STRUCTURES OF TWO POLYMORPHIC FORMS OF CIS-6-CARBOXY-2,10-DIOXA-1-PHOSPHABICYCLO-[4.4.0]DECANE 1-OXIDE. **1995**, 102, 115-125 1
- 1622 THE PHOSPHOROTRITHIOUS ACID (HS)₃P IS STABLE IN THE DILUTE GAS PHASE. **1995**, 104, 189-195 5
- 1621 MICRO-STRUCTURES OF PREMIXED HYDROCARBON FLAMES: METHANE. **1995**, 107, 1-19 58
- 1620 Synthesis and Some Physical Properties of Bicyclohexanes Having Fluoro Substituted Alkyl Moiety. **1995**, 260, 277-286 9
- 1619 Constrained search of conformational hyperspace of inactivators of glucosamine-6-phosphate synthase. **1996**, 10, 17-26 4
- 1618 CRYSTAL AND MOLECULAR STRUCTURE OF 4-TERT-BUTYLPHOSPHORINANE 1-SULFIDE DERIVATIVES. **1995**, 103, 137-151 4
- 1617 Second-Order Hyperpolarizabilities of Aromatic Carboxylates without Visible Absorption. **1995**, 34, L1161-L1163 2
- 1616 Assessing Sucrose Hydroxyl Acidities Through Semiempirical Calculations. **1995**, 14, 1117-1132 23
- 1615 Theoretical Estimation of Octanol/Water Partition Coefficient for Organophosphorus Pesticides. **1995**, 48-61 7
- 1614 Covalent interactions in zeolites: The influence of zeolite composition and structure on acid softness and hardness. **1995**, 94, 736-747 8
- 1613 Quantum chemical calculations on cationic positions and adsorption complexes in A-type zeolite. **1995**, 94, 771-778

1612	Isotope Effects on the One- and Two-Electron Reductions of Cyclooctatetraene. A Semiempirical Quantum Chemical Investigation. 1995 , 99, 8033-8037	6
1611	Multidielectric Description of Electrostatic Environment Surrounding a Bound Substrate in Enzymic Systems. 1995 , 99, 12047-12053	6
1610	Synthesis and quantitative structure-activity relationships of dequalinium analogues as K ⁺ channel blockers: investigation into the role of the substituent at position 4 of the quinoline ring. 1995 , 38, 3536-46	24
1609	Three-Dimensional Molecular Descriptors Based on Electron Charge Density Weighted Graphs. 1995 , 35, 708-713	33
1608	The First Long-Lived Olefinic π -Complex of Nitrosonium Cation: Structure and Degenerate Rearrangement of the NO ⁺ -Octamethyl-1,4-cyclohexadiene π -Complex. 1995 , 117, 12863-12864	6
1607	Synthesis and characterization of adducts of alachlor and 2-chloro-N-(2,6-diethylphenyl)acetamide with 2'-deoxyguanosine, thymidine, and their 3'-monophosphates. 1995 , 8, 209-17	14
1606	Contribution to Organophosphorus Compounds. 101. Tropone as Reaction Partner for Kinetically Stabilized Phosphaalkynes. Synthesis and Cycloaddition Behavior of a Tetracyclic Phosphorus-Carbon Cage Compound. 1995 , 60, 5884-5890	17
1605	Thermal features and thermochemistry of hexachlorozirconates of aliphatic and aromatic mono-amines. Stability of hexahalogenozirconates. 1995 , 224, 1-13	4
1604	Molecular and electronic structure of a largely extended tetracyanoquinodimethane. 1995 , 70, 1031-1032	7
1603	Theoretical study of the structures and nonlinear optical properties of hydrogen-bonded nitroaniline systems. 1995 , 71, 1701-1702	2
1602	Novel radical cation salts of organic donors containing iodine atom(s): the first application of strong intermolecular I \cdots X (X = CN, halogen atom) interaction to molecular conductors. 1995 , 73, 117-122	106
1601	Molecular orbital models of strained tetrahedral edge shared active sites on dehydroxylated silica: an AM1 and PM3 study. 1995 , 338, 322-328	11
1600	A semi-empirical study of the chemisorbed state of benzene on Si(100)-(2 \times 1). 1995 , 344, L1226-L1230	47
1599	A dual-level Shepard interpolation method for generating potential energy surfaces for dynamics calculations. 1995 , 103, 5522-5530	130
1598	Geosynthesis of organic compounds: III. Formation of alkyltoluenes and alkylxylenes in sediments. 1995 , 59, 5133-5140	35
1597	Interactions between metal cations and the ionophore lasalocid. Part 13. Structure of 1:1 and 2:1 lasalocid anion-divalent cation complexes in methanol. 1995 , 1939-1947	4
1596	Concepts in Theoretical Heterogeneous Catalytic Reactivity. 1995 , 37, 557-698	250
1595	Using molecular electrostatic potential maps for similarity studies. 1995 , 45-71	22

1594	Molecular Orbital Models of Silica. 1995 , 25, 37-68	31
1593	A MNDO study of carbon clusters with specifically fitted parameters. 1995 , 92, 269-280	16
1592	Transferability of the -COOH...DOC- dyad Geometry from the gas phase to crystals and proteins. 1995 , 90, 41-50	1
1591	¹⁷ O and ¹³ C NMR spectra of stable simple enols. 1995 , 621-637	13
1590	6,11-Bis(dicyanomethylene)-12-methylbenzo[b]phenoxazine and 6,11-dicyanimino-12-methylbenzo[b]phenoxazine as novel donor-acceptor systems. 1995 , 5, 1563-1570	6
1589	Oxidative intramolecular cyclization of 2,2?-bis(1,4-dithiafulven-6-yl)-3,3?-bithienyls affording novel bis(1,3-dithiole) electron donors. 1995 , 1761-1762	21
1588	Organic nitrates, thionitrates, peroxyxynitrites, and nitric oxide: a molecular orbital study of the (X = O, S) rearrangement, a reaction of potential biological significance. 1995 , 73, 1627-1638	45
1587	Solvent effect on the conformational behavior of substituted spiro[4.5]decane and spiro[5.5]undecane. 1995 , 73, 703-709	6
1586	New functionalized tetrathiafulvalenes: X-ray crystal structures and physico-chemical properties of TTF- π (O)NMe ₂ and TTF- π (O)D ₂ 4H ₉ : a joint experimental and theoretical study. 1995 , 5, 1689-1696	50
1585	A theoretical study of the molecular and electronic structure of benzoannulated tetracyanoquinodimethanes. 1995 , 5, 1697-1705	7
1584	Effect of molecular conformation on the electronic properties of donor-acceptor azobenzenes. 1995 , 91, 2067-2069	9
1583	1-N-PHENYLAMINO-1-PHENYL-METHANEPHOSPHONIC ACID DIETHYL ESTER: QUANTUM MECHANICAL AND FORCE FIELD STUDIES. 1995 , 101, 149-160	4
1582	Transition state structures for the molecular mechanism of lactate dehydrogenase enzyme. 1995 , 1551-1558	9
1581	Patterns of muonium addition to imidazoles: a model of radiation-produced hydrogen-atom reactivity with key biological subunits. 1995 , 2107	12
1580	Synthesis and mesomorphic properties of cyanurates and isocyanurates. Branched mesogens as model crosslinks for liquid crystalline thermosets. 1995 , 19, 481-488	9
1579	CRYSTAL AND MOLECULAR STRUCTURE OF 4-tert-BUTYLPHOSPHORINANE 1-SULFIDE DERIVATIVES. PART II. Cis/trans-4-tert-BUTYL-1-CHLOROPHOSPHORINANE 1-SULFIDE. 1995 , 104, 223-233	2
1578	Hydrogen-related defects in crystalline semiconductors: a theorist's perspective. 1995 , 14, 319-412	238
1577	π -Doping of 1,4-polydienes. 1995 , 69, 563-566	19

1576	Modelling of stress-induced diamond nucleation. 1995 , 4, 706-709	11
1575	Calculation of migration barriers on hydrogenated diamond surfaces. 1996 , 5, 613-616	7
1574	Synthesis, biological activity, and SARs of pyrrolobenzoxazepine derivatives, a new class of specific "peripheral-type" benzodiazepine receptor ligands. 1996 , 39, 3435-50	84
1573	Hydrodesulfurization Reactivities of Various Sulfur Compounds in Vacuum Gas Oil. 1996 , 35, 2487-2494	119
1572	A Simplified Perturbed Hard-Sphere Model for the Activity Coefficients of Amino Acids and Peptides in Aqueous Solutions. 1996 , 35, 4319-4327	63
1571	Molecular Orbital Studies of Methoxy-1,3,5-cycloheptatriene Isomers: Results from Semiempirical, ab Initio, and Density Functional Theory Calculations. 1996 , 61, 969-977	12
1570	Control of Diastereo- and Enantioselectivity in Metal-Catalyzed 1,3-Dipolar Cycloaddition Reactions of Nitrones with Alkenes. Experimental and Theoretical Investigations. 1996 , 61, 346-355	134
1569	Selective Oxidation of Monoterpenes with Hydrogen Peroxide Catalyzed by Peroxotungstophosphate (PCWP). 1996 , 61, 5307-5311	74
1568	Thiiranes and Thiirenes: Monocyclic. 1996 , 173-240	9
1567	Ozone-Mediated Nitration of Phenylalkyl Ethers, Phenylacetic Esters, and Related Compounds with Nitrogen Dioxide. The Highest Ortho Substitution Observed in the Electrophilic Nitration of Arenes. 1996 , 61, 5944-5947	19
1566	Interaction between model membranes and a new class of surfactants with antioxidant function. 1996 , 70, 2203-11	10
1565	Free Energy Perturbation Calculations Within Quantum Mechanical Methodologies. 1996 , 142-153	1
1564	Thermal decomposition of methylated β -thiobutyrolactones: a photoelectron spectroscopic study. 1996 , 577-582	6
1563	Superacidity of neutral Brønsted acids in gas phase. <i>Journal of Computational Chemistry</i> , 1996 , 17, 30-41	3.5 40
1562	Properties of Si-H-O clusters and luminescence. 1996 , 35, 13-18	8
1561	Synthesis, Characterization, and Theoretical Study of Sulfur-Containing Donor-Acceptor DCNQI Derivatives with Photoinduced Intramolecular Electron Transfer. 1996 , 61, 3041-3054	16
1560	Bimodal Distribution of Lifetimes for an Intermediate from a Quasiclassical Dynamics Simulation. 1996 , 118, 10329-10330	69
1559	Synthesis of Azinylvinylpyridazines: A General Note on the Isomerization of Hetarylaldienamines. 1996 , 61, 4423-4426	15

1558	Theoretical Bond and Strain Energies of Molecules Derived from Properties of the Charge Density at Bond Critical Points. 1996 , 118, 1529-1534	82
1557	Addition of Aryl and Fluoroalkyl Radicals to Fullerene C70: ESR Detection of Five Regioisomeric Adducts and Density Functional Calculations 1996 , 118, 7608-7617	30
1556	Solvent Effects in Molecular Hyperpolarizability Calculations. 1996 , 8, 428-432	38
1555	Free Radical Ring-Opening Polymerization of 1,1-Bis[(1-adamantyloxy)carbonyl]-2-vinylcyclopropane. 1996 , 29, 1943-1950	25
1554	Quantum Chemical Investigation of the Mechanism of Direct Initiation of Isobutylene Polymerization by Boron Trichloride 1996 , 29, 8696-8701	3
1553	Second-Order Hyperpolarizabilities of Stilbazolium Cations Studied by Semiempirical Calculation. 1996 , 100, 17780-17785	77
1552	Quantum-Chemical Study of the Structure, Aggregation, and NMR Shifts of the Lithium Ester Enolate of Methyl Isobutyrate. 1996 , 118, 8897-8903	31
1551	Ab Initio Study of ¹³ C Shieldings for Linear π -Conjugated Systems. Theoretical Determination of the C12-C13 Conformation in the Chromophore of Rhodopsin. 1996 , 118, 8904-8915	7
1550	On the Crystal Structure of Nylon 55. 1996 , 29, 5406-5415	19
1549	Edge Adjacency Relationships and Molecular Topographic Descriptors. Definition and QSAR Applications. 1996 , 36, 837-843	53
1548	A Time-Resolved Electron Paramagnetic Resonance Study on the Excited States of Tetraphenylporphinatozinc(II) Coordinated by p-Pyridyl Nitronyl Nitroxide. 1996 , 118, 13079-13080	130
1547	Competing Rearrangements of Ammonium Ylides: A Quantum Theoretical Study. 1996 , 61, 7276-7284	19
1546	Atropisomers of Cofacial Heteroaromatic Rings with Two Positive Charges. Derivatives of 1,8-Di(3'-pyridyl)naphthalene. 1996 , 61, 7018-7021	39
1545	Flexible Enantiodivergent Synthesis and Biological Activity of Mannostatin Analogues, New Cyclitol Glycosidase Inhibitors. 1996 , 61, 480-488	21
1544	Water-Soluble Phosphines. 6.(1) Tailor-Made Syntheses of Chiral Secondary and Tertiary Phosphines with Sulfonated Aromatic Substituents: Structural and Quantum Chemical Studies. 1996 , 35, 4103-4113	31
1543	A Theoretical Study of Addition of Organomagnesium Reagents to Chiral β -Alkoxy Carbonyl Compounds. 1996 , 61, 3467-3475	23
1542	Facile 1,3- and 1,5-Chlorine Migration. 1996 , 61, 6809-6813	30
1541	Mass Spectral Analysis of Nitropolycyclic Aromatic Hydrocarbons with Torsion Angle Obtained from Semiempirical Calculations. 1996 , 61, 5271-5273	19

1540	Study of Radical Merostabilization by Electrospray FTICR/MS. 1996 , 118, 11905-11911	7
1539	Control of Three-Dimensional Refractive Indices by Both Drawing and Poling of Functionalized Phenoxy Side-Chain Polymers. 1996 , 29, 7177-7185	3
1538	Synthesis of Alkyl Fructosides Using Solid Acid Catalysts. Part I: Silica-Alumina Cracking Catalysts. 1996 , 15, 331-349	15
1537	Volume 9 References. 1996 , 1039-1146	
1536	Adsorption of some substituted ethylene molecules on Pt(111) at 95 K Part 1: NEXAFS, XPS and UPS studies. 1996 , 350, 60-78	64
1535	First attempts at an elucidation of the interface structure resulting from the interaction between methacrylonitrile and a platinum anode: an experimental and theoretical (ab initio) study. 1996 , 355, 177-202	12
1534	Adsorption of pyrimidine molecules on Pd(110) observed by scanning tunneling microscopy. 1996 , 360, 50-54	12
1533	Two-dimensional self-assembly of DNA base molecules on Cu(111) surfaces. 1996 , 364, L575-L579	66
1532	Quantitative structure-Activity relationships for skin irritation and corrosivity of neutral and electrophilic organic chemicals. 1996 , 10, 247-56	43
1531	Synthesis and quantitative structure-activity relationship of 17 beta-(hydrazonomethyl)-5 beta-androstane-3 beta,14 beta-diol derivatives that bind to Na ⁺ ,K ⁺ -ATPase receptor. 1996 , 39, 3385-93	18
1530	QM/MMpol: A Consistent Model for Solute/Solvent Polarization. Application to the Aqueous Solvation and Spectroscopy of Formaldehyde, Acetaldehyde, and Acetone. 1996 , 100, 14492-14507	227
1529	Comparison of the transmission behavior of a triazeno-polymer with a theoretical model. 1996 , 63, 257-265	31
1528	Importance of steric hindrance in linear coordination of Lewis acids with α -enones. 1996 , 393-394	5
1527	Excited states in bis-substituted polyenes: configuration interaction description of the vertical excitation energies and nonlinear optical properties. 1996 , 80, 211-222	8
1526	First hyperpolarizabilities of some push-pull olefins measured by the hyper-Rayleigh scattering technique. 1996 , 82, 47-51	3
1525	Imidazoles. 1996 , 77-220	69
1524	Mechanism of Atmospheric Photooxidation of Aromatics: A Theoretical Study. 1996 , 100, 10967-10980	141
1523	Quantum Chemical Investigations of the Thermal and Photoinduced Proton-Transfer Reactions of 2-(2,4-Dinitrobenzyl)pyridine. 1996 , 100, 16187-16194	31

1522	Synthesis of a 2,7-Dioxatricyclo[4.2.1.03,8]nonane: A Model Study for Possible Application in a Synthesis of Dictyoxetane. 1996 , 61, 9135-9145	42
1521	Evidence for Reversible Ylide Formation: Equilibrium between Free Alkylidenecarbenes and Etheral Solvent-Alkylidenecarbene Complexes (Oxonium Ylides). 1996 , 118, 10141-10149	41
1520	On Transition Structures for Hydride Transfer Step in Enzyme Catalysis. A Comparative Study on Models of Glutathione Reductase Derived from Semiempirical, HF, and DFT Methods. 1996 , 61, 7777-7783	20
1519	Trajectory Studies of SN2 Nucleophilic Substitution. 5. Semiempirical Direct Dynamics of Cl ⁻ - -CH ₃ Br Unimolecular Decomposition. 1996 , 118, 2257-2266	54
1518	Anionic Polymerization of N-Phenylitaconimide. 1996 , 29, 4473-4477	6
1517	Mechanism of aldehyde oxidation catalyzed by horse liver alcohol dehydrogenase. 1996 , 35, 9782-91	59
1516	Use of (NSCl) ₃ as a Chain-Building Reagent, I: Reaction of ArS ₃ N ₂ Ar with (NSCl) ₃ in the Presence of AgAsF ₆ to Form the Chain-Lengthened Product, [ArS ₄ N ₃ Ar] [AsF ₆]. 1996 , 1, 317-324	6
1515	Influence of Benzoannulation on the Molecular and Electronic Structures of Tetracyanoquinodimethanes. 1996 , 100, 6138-6146	34
1514	Molecular electrostatic potentials and fields: hydrogen bonding, recognition, reactivity and modelling. 1996 , 257-296	26
1513	Theoretical and experimental studies of electronic effects and second-order nonlinear optical properties of some benzenecarbothioates and benzenecarbodithioates. 1996 , 94, 23-37	1
1512	Analytical first derivatives of the energy in the MNDO half-electron open-shell treatment. 1996 , 93, 87-99	4
1511	Mechanism of Mukaiyama-Michael Reaction of Ketene Silyl Acetal: Electron Transfer or Nucleophilic Addition?. 1996 , 61, 2951-2962	30
1510	Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. 1996 , 100, 10400-10407	206
1509	New Diels-Alder reactions of 3-vinylindoles with an aryne: selective access to functionalized [a]annellated carbazoles. 1996 , 1767-1771	20
1508	Temperature dependence of the reactions of the nitrate radical with dichloroalkenes followed by LIF detection. 1996 , 92, 53-58	18
1507	Zinc(II)-catalysed transformation of epoxides to aziridines. 1996 , 1167-1170	10
1506	Theoretical determination of the molecular and solid-state electronic structures of phthalocyanine and largely extended phthalocyanine macrocycles. 1996 , 6, 1751-1761	37
1505	Semiempirical and spectroscopic study of the thermolysis of tetranitromethane. 1996 , 92, 363-368	3

1504	Addition/cyclization reaction of nitroalkane anions with o-quinone derivatives via electron transfer in the charge-transfer complexes. 1996 , 1429-1433	16
1503	Theoretical Simulations of Electron-Induced Degradation of Perfluoropolyether. 1996 , 39, 380-385	9
1502	Ionization Energies of Linear and Cyclic Polysilanes. Application of the Green's Function Method Coupled with Semiempirical Molecular Orbital Calculations. 1996 , 15, 350-360	14
1501	Complexes of Oxygenated trans-Azoalkanes and Tetracyanoethylene. The Interaction of pi Oxygen Dipoles with an Electron Poor Alkene. 1996 , 61, 7895-7903	10
1500	Preparation of delta-Chloro-alpha-allenyl Ketones by Acylation of 3-Buten-1-yne. 1996 , 61, 6678-6684	8
1499	Theoretical Study of the Deprotonation of Nitriles, RCH ₂ CN: Ab Initio and PM3 Calculations of Intermediate Aggregates and Transition States. 1996 , 61, 2523-2529	34
1498	Molecular electronic properties of fused rigid porphyrin-oligomer molecular wires. 1996 , 7, 424-429	32
1497	Sulfonyl esters 7. The second and third sequences in the Trithioorthoformate Reaction. 1996 , 74, 1638-1648	3
1496	Interactions between metal cations and the ionophore lasalocid. Part 14. Structure of lasalocid-alkali metal cation complex salts in methanol from NMR spectroscopy and computational experiments. 1996 , 1971-1979	6
1495	Intercalation of 2-, 4-sulfanylpuridine, 2,2'- and 4,4'-dithiobispyridine into VOPO ₄ and gel-V ₂ O ₅ interlayer spaces. 1996 , 6, 1849-1852	18
1494	Synthesis of 2,2':5,2'-terpyridine and 2,2':5,2':5',2'-quaterpyridine and their photocatalysis of the reduction of water. 1996 , 1963-1969	24
1493	Oxidative rearrangement of 2'-hydroxychalcones having no substituent at the 3'- and 5'-positions with thallium(III) nitrate in methanol. 1996 , 1987-1992	2
1492	Pyryliumolates II: Generation of and cycloaddition reactions with isoxazole annulated pyryliumolates. 1996 , 1035-1040	17
1491	Quantum Chemical Study of the Interaction of Water Molecules with a Partially Oxidized Graphite Surface. 1996 , 14, 383-391	10
1490	Volume 1 References. 1996 , 1215-1369	
1489	Photo Sensitive Phase Behaviour of Mixtures of 4-cyano-4'-n-pentylbiphenyl and a Non-Mesogenic Chromophore methyl 4-(1-naphthyl)propenoate. 1996 , 281, 1-14	
1488	INTERFACIAL ACTIVITY and SEMIEMPIRICAL PM3 CALCULATIONS of 2-ETHYLHEXANOYLBENZOYL METHANE. 1996 , 14, 491-506	8
1487	Structure-activity studies on monoamine oxidase inhibitors by calorimetric and quantum mechanical calculations. 1996 , 10, 215-229	5

1486	Chapter 2. Ionisation Methods in LC-MS and LC-MS-MS (TSP, APCI, ESP and cf-FAB). 1996 , 71-133		5
1485	Analytical second derivatives of the energy in MNDO methods. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1318-27	3.5	17
1484	σ Bonding contribution to restricted internal rotations in saccharides. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1371-84	3.5	2
1483	Dielectric Medium Effects on Absorption Maxima of Protonated Retinylidene Schiff Bases as Models of Rhodopsin. 1996 , 25, 1075-1076		4
1482	Ground State Triplet Cation Diradicals Generated from N,N-Dimethylamino Nitronyl Nitroxide and Its Homologues through One-Electron Oxidation. 1996 , 25, 879-880		18
1481	Theoretical Studies of Carbocations Adsorbed over a Large Zeolite Cluster. Implications on Hydride Transfer Reactions. 1996 , 100, 12418-12423		30
1480	New Method for Derivatization of Squaric Acid to Highly Substituted Cyclobutenones: Lewis Acid-Catalyzed Reaction of Cyclobutene-1,2-dione Monoacetal and Its Vinylog with Unsaturated Organosilanes, and Subsequent Ring Transformation of the Adducts. 1996 , 69, 1353-1362		6
1479	Radical Dissociation of 2,2'-Bis(2-aryl-3-benzothiophenonyl)s by Mechanical Energy. 1996 , 69, 2355-2359		16
1478	Role of the Methoxy Substituents on the Photochromic Indolyfulgides. Absorption Maximum vs. Molar Absorption Coefficient of the Colored Form. 1996 , 25, 587-588		9
1477	Crystal and Molecular Structures of Novel Metal Carbene Complexes IV. Effect of Carbonyl Groups and Formation Mechanism. 1996 , 69, 2771-2780		16
1476	A New Ring Contraction Rearrangement of 2,5- and 3,6-Di-tert-butyl-3H-azepines to Pyridine Derivatives. 1996 , 25, 1129-1130		6
1475	Reactions of Charged Substrates. 6. The Methoxymethyl Carbenium Ion Problem. 1. A Semiempirical Study of the Kinetic and Thermodynamic Stabilities of Linear and Cyclic Oxo- and Thio-carbenium Ions Generated from Pyridinium and Dimethylanilinium Ions. 1996 , 61, 8039-8047		5
1474	Harmonic Vibrational Frequencies: An Evaluation of Hartree-Fock, Møller-Plesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors. 1996 , 100, 16502-16513		6154
1473	Superelectrophiles generated in mBr ₂ nAlBr ₃ systems. 1996 , 6, 175-178		4
1472	Photoisomerization of imidazo[1,2-a]pyridines. 1996 , 6, 225-226		0
1471	Quantum-Chemical Descriptors in QSAR/QSPR Studies. 1996 , 96, 1027-1044		1173
1470	Covalent Fullerene Chemistry. 1996 , 271, 317-324		570
1469	Quantum-chemical calculations of the dissociation energy of the C-H bond in hydrocarbons, alcohols, and ethers. 1996 , 45, 2709-2712		1

1468	Intermolecular interactions of tetraanions of macrocyclic tetraresorcinol in H ₂ O/DMF solutions. 1996 , 45, 1111-1114	
1467	Crown compounds for anions. MNDO calculations of complexes of halide anions with cyclic pentameric difluoromethylenemercury. 1996 , 45, 37-41	3
1466	Conformational analysis of hydrogen polyoxides. 1996 , 45, 1286-1291	4
1465	On some carbon clusters containing sp ² - and sp ³ -hybridized atoms. 1996 , 45, 511-513	1
1464	Electronic structure, geometry, and stability of organic cations, dications, and donor-acceptor complexes. 1996 , 45, 514-520	5
1463	Semiempirical AM1 and PM3 studies of the enzymatic mechanism of horse liver alcohol dehydrogenase. 1996 , 364, 33-43	7
1462	Theoretical study of the reactions of 1-methyl-2-vinylpyrrole with methyl propiolate and with dimethyl acetylenedicarboxylate. 1996 , 362, 209-213	4
1461	Comparative molecular field analysis (CoMFA) of dye-fibre affinities. Part 2. Symmetrical bisazo dyes. 1996 , 362, 155-162	20
1460	Quantum mechanical investigation of cyclic 3',5'-adenosine monophosphate, the second hormonal messenger. 1996 , 362, 297-304	8
1459	Hydrolysis of adenosine. A semiempirical and ab initio study. 1996 , 363, 191-201	16
1458	CO interaction with ZnO surfaces: an MNDO, AM1 and PM3 theoretical study with large cluster models. 1996 , 363, 249-256	13
1457	A semiempirical quantum mechanical approach towards understanding of cyclopropanone reactivity. 1996 , 364, 45-49	4
1456	Rotational barriers of 2-acetylthiophene and related carbonyl compounds. 1996 , 364, 131-138	12
1455	Semiempirical and ab initio study of closed and open shell derivatives of 10-methylisoalloxazine: a model of flavin redox states. 1996 , 364, 139-149	21
1454	The C-H bond dissociation energies of polycyclic aromatic hydrocarbons. 1996 , 366, 219-226	11
1453	AM1, PM3 and MNDO study of the tautomerism of 2-, 4- or 5-imidazolones and their thio- and azo-analogs. 1996 , 366, 227-231	17
1452	¹³ C NMR studies of the molecular dynamics of chlorpromazine in solution. 1996 , 375, 259-265	
1451	Syntheses of heterocycles by reactions between nucleophilic and electrophilic sites: Course of the reactions and quantum-chemical calculations. 1996 , 71, 109-119	5

1450	Photocontrol of ionic conduction by photochromic crown ethers. 1996 , 148, 41-61	40
1449	A new synthesis of 5-aminolevulinic acid via dye-sensitized oxygenation of N-furfurylphthalimide. 1996 , 94, 167-171	7
1448	A facile and regio- and stereo-selective preparation of bicyclic guanidines by iodocyclization of 3-(alk-2-enyl)-2-(substituted amino)-1-imidazolin-4-ones. 1996 , 52, 2827-2838	33
1447	The role of the hydrogen bonding in cycloadditions of benzonitrile oxide with cyanophenols. 1996 , 52, 7885-7892	9
1446	Mechanistic considerations on the azepine-ring formation through the ene reactions at the periphery of heterocyclic systems. 1996 , 52, 13097-13110	20
1445	1,3-Dipolar cycloaddition reactions of polycyclic aromatic hydrocarbons with 3,5-dichloro-2,4,6-trimethyl- and 2,4,6-trimethylbenzonitrile oxide. 1996 , 52, 13027-13034	9
1444	A theoretical investigation on the reactivity of 6-amino-3-methylpyrimidin-4(3H)-ones towards DMAD. Tandem Diels-Alder retro Diels-Alder (DA/RDA) reaction. 1996 , 52, 13721-13732	6
1443	Sequential pericyclic reaction of unsaturated xanthates. Intramolecular cycloaddition selectivity of the 2,4-alkadienyl 2-alkenyl sulfides. 1996 , 52, 13909-13918	3
1442	Recombination with larger than bandgap energy at centres on the surface of silicon microstructures. 1996 , 276, 290-292	7
1441	Comparative studies in the ¹⁹ F and ¹ H NMR chemical shifts in 2,2-difluorohalogenated propanes. 1996 , 76, 45-48	7
1440	Molecular and crystal structures of dithiosuccinimide and 2,2,3,3-tetramethyldithiosuccinimide. 1996 , 374, 357-362	4
1439	Vibrational properties of C20 isomers, a semi-empirical study. 1996 , 376, 513-523	10
1438	Substituted 1-hetero-3-aza-1,3-butadienes: dipole moments and related structural analysis. 1996 , 382, 39-48	3
1437	Thermodynamic vs. kinetic control in the Diels-Alder cycloaddition of cyclopentadiene to 2,3-dicyano-p-benzoquinone. 1996 , 26, 281-286	8
1436	Electronic and conformational properties of 2,3-benzodiazepine derivatives. 1996 , 18, 389-403	
1435	Comparative studies of the molecular structure of 1-R-1,2,3,4,5,6-hexamethylbenzenonium ions: Molecular and crystal structure of 1-chloromethyl-1,2,3,4,5,6-hexamethylbenzenonium tetrachloroaluminate. 1996 , 37, 464-469	4
1434	Interpretation of low-frequency vibration spectra for crystals of the triglycine sulfate group. 1996 , 63, 49-56	3
1433	Associated species of dimethylsulfoxide: Semiempirical modeling. 1996 , 7, 111-118	13

1432	A new mechanism in serine proteases catalysis exhibited by dipeptidyl peptidase IV (DP IV)--Results of PM3 semiempirical thermodynamic studies supported by experimental results. 1996 , 236, 109-14	11
1431	QSARS of mutagens and carcinogens: two case studies illustrating problems in the construction of models for noncongeneric chemicals. 1996 , 371, 29-46	36
1430	A computational study of mixed aggregate formation in lithio azaallylic systems. 1996 , 367, 33-40	4
1429	Transition structures for hydride transfer reactions in vacuo and their role in enzyme catalysis. 1996 , 371, 299-312	7
1428	PM3 conformational study of some cephalosporins. Comparison with other semiempirical methods. 1996 , 370, 1-10	2
1427	A semiempirical study of 2,2'-dichlorodiethyl sulfide SN2 and neighboring group hydrolysis reaction mechanisms in the gas phase and in aqueous solution. 1996 , 370, 209-220	5
1426	Dependence of isotope effects on conformation in decarboxylation of 3-carboxybenzisoxazoles. 1996 , 370, 237-243	3
1425	Molecular and crystal structures of dithiosuccinimide and 2,2,3,3-tetramethyldithiosuccinimide. 1996 , 374, 357-362	
1424	X-ray crystal structure analyses and atomic charges of color former and developer. I. Color developers. 1996 , 380, 223-233	2
1423	The assignment of lattice vibrations in triglycine sulfate-type crystals. 1996 , 375, 43-51	1
1422	Study of the relationship between decomposition energies of various heterocycles derived by using the PM3 method. 1996 , 375, 143-152	
1421	Theoretical Calculations of β -Lactam Antibiotics. Part VII. Influence of the solvent on the basic hydrolysis of the β -lactam ring. 1996 , 79, 353-362	27
1420	A Reinvestigation of the Oxidative Rearrangement of Yohimbane-Type Alkaloids. Part B. Formation of Oxindol (= 1,3-Dihydro-2H-indol-2-one) Derivatives. 1996 , 79, 1361-1378	24
1419	The Deoxygenation and Isomerization of Artemisinin and Artemether and Their Relevance to Antimalarial Action. 1996 , 79, 1475-1487	85
1418	Synthesis, Separation, and Characterization of Optically Pure C76 Mono-Adducts. 1996 , 79, 1741-1756	27
1417	Ab Initio Molecular Orbital Calculations on Allylic 1,3-Strain of Electron-Donor- and Electron-Acceptor-Substituted Alkenes. 1996 , 1996, 1575-1579	12
1416	Theoretical Study of Pericyclic Reactions of Nitrosoethylene and (Thionitroso)ethylene. 1996 , 1996, 1615-1621	21
1415	A Conformational Study of [3.3](2,6)Pyridinophane by the Dynamic NMR Method and X-ray Structural Analysis. 1996 , 1996, 1645-1649	17

- ¹⁴¹⁴ Asymmetric Alkylation of Chiral 2-Azapentadienyl Metal Compounds: Diastereoselective Synthesis of Alkyl-Substituted N-Allylimines (2-Aza-1,4-pentadienes). **1996**, 1996, 1833-1843 9
- ¹⁴¹³ Solid State and Solution Structures of O-Alkyl- and of O-Acyl Derivatives of 1-Hydroxypyridine-2(1H)-thione. **1996**, 1996, 2091-2097 13
- ¹⁴¹² Eine neue Diradikal-Cyclisierung als Alternative zur Myers-Saito-Cycloaromatisierung bei der thermischen Umsetzung von Eninallenen. **1996**, 108, 1952-1954 31
- ¹⁴¹¹ 5-exo oder 6-endo? Theoretische Untersuchungen von Bergangsstrukturen der Umlagerungen von 4-Penten-1-oxyl-Radikalen. **1996**, 108, 3056-3059 8
- ¹⁴¹⁰ Theoretical investigations on 1,2-ethanediol: The problem of intramolecular hydrogen bonds. *Journal of Computational Chemistry*, **1996**, 17, 133-147 3.5 50
- ¹⁴⁰⁹ Pyrrolizidine alkaloids necine bases: Ab initio, semiempirical, and molecular mechanics approaches to molecular properties. *Journal of Computational Chemistry*, **1996**, 17, 156-166 3.5 9
- ¹⁴⁰⁸ Extension of MST/SCRF method to organic solvents: Ab initio and semiempirical parametrization for neutral solutes in CCl₄. *Journal of Computational Chemistry*, **1996**, 17, 806-820 3.5 104
- ¹⁴⁰⁷ Hybrid supermolecule-polarizable continuum approach to solvation: Application to the mechanism of the Stevens rearrangement. *Journal of Computational Chemistry*, **1996**, 17, 1444-1452 3.5 4
- ¹⁴⁰⁶ Thermal [2 + 2] cycloaddition of (z)-[6]paracycloph-3-ene with tetracyanoethylene. **1996**, 9, 1-6 4
- ¹⁴⁰⁵ Kinetic isotope effects on the Menshutkin reaction: Theory versus experiment. **1996**, 9, 41-49 12
- ¹⁴⁰⁴ Conformational analysis of 2-cyano-1,1-dihydroxyethane in solution. **1996**, 9, 119-127 3
- ¹⁴⁰³ Structure-visible absorption relationship in the photochromic spiro[indoline-naphthoxazine] series. **1996**, 9, 262-264 7
- ¹⁴⁰² Tautomerism in 2,2'-bipyridyl-3,3'-diol. **1996**, 57, 721-728 8
- ¹⁴⁰¹ Molecular orbital studies on the spin states of nitroxide species: Bis- and trisnitroxymetaphenylene, 1,1-bisnitroxylphenylethylene, and 4,6-dimethoxy-1,3-dialkyl nitroxy-benzenes. **1996**, 57, 781-799 73
- ¹⁴⁰⁰ H₂O and H₂ interaction with ZnO surfaces: A MNDO, AM1, and PM3 theoretical study with large cluster models. **1996**, 57, 861-870 41
- ¹³⁹⁹ Theoretical studies on the decarboxylation reaction in thiamin catalysis. **1996**, 57, 943-948 14
- ¹³⁹⁸ Hybrid classical quantum force field for modeling very large molecules. **1996**, 58, 153-159 124
- ¹³⁹⁷ Extension of semiempirical methods to simulation of surfaces. **1996**, 58, 283-295 16

1396	A theoretical analysis of the structure and electronic properties of 2-nitrophenylcyanate and 2-nitrophenylthiocyanate. 1996 , 59, 167-172	
1395	PM3 semiempirical calculations of lithium-cation and proton affinities for XYZPO and XYSO ₂ compounds. 1996 , 59, 409-420	4
1394	Resemblance analysis of molecular systems on the grounds of DFT-evaluated parameters. Platinum complexes and their anticancer activity. 1996 , 60, 1385-1391	3
1393	Modification of the local self-consistent field method for modeling surface reactivity of covalent solids. 1996 , 60, 1525-1536	6
1392	Conformational and solid-state studies of diphenyl 1-hydroxy-1-phenylethylphosphonate. 1996 , 7, 9-16	8
1391	Acid-induced dimerization of imidates derived from glycine: Synthesis of methyl N-(1,2,5-trisubstituted-4-imidazolyl)glycinates. 1996 , 7, 187-194	9
1390	Electronic structures, geometries, and energetics of highly charged cations of the C ₆₀ fullerene. 1996 , 248, 116-120	34
1389	Second-order polarizability of p-substituted cinnamic acids. 1996 , 248, 27-30	9
1388	Radical hydrogen transfer reactions: benchmark calculations on the C ₂ H ₄ H•C ₂ H ₄ transition state. 1996 , 249, 496-500	10
1387	Intramolecular dipolar coupling enhancement of the first-order molecular hyperpolarizability in a polar solvent. 1996 , 253, 141-144	11
1386	Structure and energetics of neutral and negatively charged C ₆₀ dimers. 1996 , 256, 119-125	62
1385	Linear scaling for the charge density fitting procedure of the linear combination of Gaussian-type orbitals density functional method. 1996 , 256, 569-574	45
1384	Ability of empirical potentials (AMBER, CHARMM, CVFF, OPLS, Poltev) and semi-empirical quantum chemical methods (AM1, MNDO/M, PM3) to describe H-bonding in DNA base pairs; comparison with ab initio results. 1996 , 257, 31-35	35
1383	Reaction of O(3P) atoms with CF ₂ ? CXY (X, Y ? H, F, Cl, Br). Discharge flow-chemiluminescence imaging technique. 1996 , 257, 415-420	18
1382	Electrosynthesis of sulfur-containing organic compounds from allene derivatives using a sacrificial mixed sulfur/graphite electrode. 1996 , 41, 1987-1991	10
1381	Thianthrene 5-Oxide as a Mechanistic Probe in Oxygen Transfer Reactions: The Case of Carbonyl Oxides versus Dioxiranes Revisited. 1996 , 2, 255-258	42
1380	The Reduction of Oxalic Amidines with Metallic Lithium: Preparation of Lithiated Bisamides [R?N(RR?N)C=C(NRR?)NR?]Li ₂ and Their Use as Intermediates in a Novel Synthesis of Tetraaminoethenes. 1996 , 129, 39-44	17
1379	Synthesis and Structure of Tris(trialkylstannyl)- and Tris(dialkylhalostannyl)amines; Stabilization of the Sn ₃ N Skeleton by Intramolecular Sn-Sn Bridges. 1996 , 129, 175-189	24

1378	Preparation and Structure of Dithioxo- and Diselenoxophosphoranes Stabilized by Intramolecular Coordination with a Dialkylamino Group. 1996 , 129, 1049-1055	31
1377	P/O Ligand Systems: Synthesis, Reactivity, and Structure of Tertiary o-Phosphanylphenol Derivatives. 1996 , 129, 1547-1560	48
1376	Search for the pharmacophore in kappa-agonistic diazabicyclo[3.3.1]nonan-9-one-1,5-diester and arylacetamides. 1996 , 329, 311-23	22
1375	5-exo or 6-endo? Exploring Transition State Structures in Cyclizations of 4-Penten-1-oxyl Radicals. 1996 , 35, 2820-2823	23
1374	Recognition of the Helical Sense of Polypeptides by a Chiral Metalloporphyrin Receptor. 1996 , 35, 2823-2825	17
1373	Heterocyclic routes to polysubstituted cyclopentanes: Molecular modelling of electrophilic additions to di- and trisubstituted cyclopentenenes. 1996 , 52, 3355-3364	5
1372	Electronic structure and gas-phase thermolysis of 4-substituted 3,3,5,5-Tetramethyl-3,5-dihydro-4H-pyrazoles studied by photoelectron spectroscopy. First evidence for an alkylideneselenirane. 1996 , 52, 1965-1980	10
1371	Theoretical studies of derivatized buckyballs and buckytubes. 1996 , 52, 5247-5256	26
1370	12,13,25,26-Tetraaza-2,15-dithia[3.3]phenanthroline. Synthesis, conformational study and complexation reactions. 1996 , 52, 4673-4678	15
1369	Iodocyclization of 3-alkynyl- and 3-allenyl-2-(substituted amino)-1-imidazolin-4-ones. 1996 , 52, 6581-6590	48
1368	Why are the troponoid rings of the mesylate and tosylate of tropone oxime cleaved easily by nucleophiles?. 1996 , 52, 8439-8450	0
1367	Molecular modelling of the isothiazolo[5,4-b]pyridin-3(2H)-one derivatives. 1996 , 52, 8947-8956	6
1366	Atropisomerism of cofacial pyridine rings. Synthesis, proton NMR spectra and conformations of 1,8-di(3?-pyridyl)naphthalene. 1996 , 52, 8703-8706	28
1365	NMR studies and semiempirical calculations on the structure of glycoamidines. 1996 , 52, 9263-9274	1
1364	On the reason for opposite diastereoselectivities of benzyllithium compounds containing lithium amide and lithium alkoxide functionalities. 1996 , 52, 10025-10042	19
1363	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. 1996 , 52, 10693-10704	30
1362	Theoretical model of solvated lithium dienediolates of methyl substituted 2-butenic acids. 1996 , 52, 11105-11112	14
1361	Vallartanone B: Synthesis and related studies. 1996 , 52, 13901-13908	14

1360	Highly stereocontrolled synthesis of substituted propiolactones and butyrolactones from achiral lithium enolates and homochiral aldehydes. 1996 , 37, 245-248	33
1359	Photoinduced electron transfer reactions of cyclopropanone acetal with conjugated enones in the presence of a redox-type photosensitizer. 1996 , 37, 1833-1836	16
1358	Transformation of 1-alkyl-substituted indene ozonides and the corresponding solvent-derived ozonolysis products to tricyclic peroxides: Isolation and characterization of novel hexoxecane derivative. 1996 , 37, 2093-2096	4
1357	Synthesis of 10-membered masked oxanediene analogue of kedarcidin-chr. and C-1027-chr., and its DNA cleaving activity. 1996 , 37, 2433-2436	9
1356	Retro-ene type fragmentation of allylic dithiolcarbonates. 1996 , 37, 2445-2448	11
1355	Stereoselective conjugate addition of carbon nucleophiles to chiral (E)-nitroalkenes bearing a stereocenter. Origins of the observed anti selectivity. 1996 , 37, 3055-3058	18
1354	Amino acid based diastereoselective synthesis of elsaminose. 1996 , 37, 5743-5746	13
1353	An effective formylation of adamantane with CO initiated by the aprotic organic superacid CBr ₄ /AlBr ₃ under mild conditions. 1996 , 37, 5775-5778	15
1352	Enantioselective syntheses and resolution of the key white intermediate for the synthesis of trisporic acids. 1996 , 7, 1041-1057	9
1351	Conformational analysis of phthalein derivatives acting as thymidylate synthase inhibitors by means of ¹ H NMR and quantum chemical calculations. 1996 , 4, 1783-94	13
1350	MNDO-PM3 MO studies on the thermal isomerization of photochromic 1,3,3,3'-trimethyl-6-nitrospiro[2H-1-benzopyran-2,2'-indoline]. 1996 , 95, 209-214	18
1349	UV-visible absorption and fluorescence studies of 4,4'-diamino-trans-stilbene and its protonated species. 1996 , 99, 23-28	16
1348	Characterization of pyridoxal phosphate as an optical label for measuring electrostatic potentials in proteins. 1996 , 32, 71-9	6
1347	Electronic structure calculations on helicenes. Concerning the chirality of helically twisted aromatic systems. 1996 , 203, 309-316	27
1346	The ground state spin multiplicity of Schlenk-type biradicals and the influence of additional linkage to ladder type structures. 1996 , 206, 339-351	11
1345	Electronic states of multichromophoric phenylethynylbenzene derivatives: exciton theory and CS-INDO-CIPSI calculations. 1996 , 208, 351-373	11
1344	Adsorption and decomposition of hexamethyldisiloxane on platinum: an XPS, UPS and TDS study. 1996 , 99, 245-254	16
1343	A rational approach to the design of flavones as xanthine oxidase inhibitors. 1996 , 31, 693-699	34

- ¹³⁴² Synthesis and pharmacological properties of 4(5)-(2-ethyl-2,3-dihydro-2 silinden-2-yl)imidazole, a silicon analogue of atipamezole. **1996**, 31, 725-729 17
- ¹³⁴¹ Mass-spectrometric study of the pyrolysis reactions in the MOVPE of Ga₂Se₃ by in-situ gas sampling. **1996**, 158, 68-78 5
- ¹³⁴⁰ Examination of the cleavage and formation of the disulfide bond in poly[dithio-2,5-(1,3,4-thiadiazole)] by redox reaction. **1996**, 410, 229-234 21
- ¹³³⁹ Study of the relationship between decomposition energies of various heterocycles derived by using the PM3 method. **1996**, 375, 143-152 1
- ¹³³⁸ The assignment of lattice vibrations in triglycine sulfate-type crystals. **1996**, 375, 43-51 2
- ¹³³⁷ ¹³C NMR studies of the molecular dynamics of chlorpromazine in solution. **1996**, 375, 259-265 1
- ¹³³⁶ X-ray crystal structure analyses and atomic charges of color former and developer. I. Color developers. **1996**, 380, 223-233 16
- ¹³³⁵ X-ray crystal structure analysis and atomic charges of color former and developer: 2. Color formers. **1996**, 380, 235-247 8
- ¹³³⁴ Local and non-local DF calculation of the structure of the helically twisted 1,3-dimethyl-((π -chromium-tricarbonyl)benzo)-[b]naphtho[1,2-d]pyran-6-one: a comparison. **1996**, 520, 261-264 7
- ¹³³³ The ultraviolet and infrared spectroscopy of (benzene)₂-(CH₃OH)₃ isomeric clusters. **1996**, 262, 627-632 16
- ¹³³² Third-order optical nonlinearity in new π -conjugated polymers: polydiethynylsilane and polysilole. **1996**, 263, 119-125 16
- ¹³³¹ Formation and decay of intramolecular exciplexes and bond homolysis of ((N,N-dimethylamino)methyl) arenes. **1996**, 99, 103-114 6
- ¹³³⁰ Origins of selectivity in conjugate additions of alkenylphosphonates to lithiated bislactim ethers: A semiempirical study. **1996**, 7, 3335-3338 2
- ¹³²⁹ Photoemission study on poly(pyridine-2,5-diyl), poly(2,2'-bipyridine-5,5'-diyl), and their K-doped states. **1996**, 78, 399-402 13
- ¹³²⁸ Soft X-ray absorption, UV photoemission, and VUV absorption spectroscopic studies of fluorinated fullerenes. **1996**, 78, 453-456 18
- ¹³²⁷ Kristallstruktur von 1,8-Naphthyridinium-(1)-tetraphenylborat: Einebnung eines verzerrten Molekülskeletts durch Protonierung. **1996**, 127, 391-396 6
- ¹³²⁶ Oxidative cyclocondensation of thio(seleno)-amides and ureas 1. 2-thioxo-4-quinazolone. **1996**, 32, 728-731
- ¹³²⁵ Parallel implementation of semiempirical quantum methods for the Intel platforms. **1996**, 19, 87-109 5

1324	Quantum-chemical analysis of the conformational and diastereomeric composition of 1,3-dimethyl-4-(s-phenylethylimino)piperidine. 1996 , 32, 308-309	
1323	Cation radicals of N-substituted phenothiazines. 1996 , 32, 365-370	2
1322	(2R,3R,5S,6S)-2,3-Diethoxy-5,6-bis(hydroxymethyl)-2,3-dimethyl-1,4-dioxane. 1996 , 52, 669-672	
1321	Two Diastereomers of Benzylidene-D-erythrone. 1996 , 52, 895-899	0
1320	Examination of reactivity of protonated and deprotonated 2,5-dimercapto-1,3,4-thiadiazole and its derivatives by electrochemical experiment and semiempirical MO calculation. 1996 , 417, 17-24	34
1319	Stereopopulation control in 3-(2,4-dimethyl-6-methoxyphenyl)-3-methylbutyric acid and proton stability in hydrogen-bonded carboxylic groups. 1996 , 385, 71-80	3
1318	Potential allelopathic sesquiterpene lactones from sunflower leaves. 1996 , 43, 1205-1215	69
1317	Structure-activity analysis of fluorinated 1-N-arylamino-1-arylmethanephosphonic acid esters as inhibitors of the NADH:ubiquinone oxidoreductase (complex I). 1996 , 10, 100-6	2
1316	Calculation of solvation and binding free energy differences between VX-478 and its analogs by free energy perturbation and AMSOL methods. 1996 , 10, 23-30	16
1315	Mechanism of action of aspartic proteinases: application of transition-state analogue theory. 1996 , 10, 583-8	3
1314	Normal coordinate analysis and vibrational spectra of 9- β -D-arabinofuranosyladenine hydrochloride (ara-A.HCl). 1996 , 24, 149	9
1313	cis/trans-Isomerisierung von 2,2'-Diethyl-5,5'-dimethoxy-4,4'-binaphthyliden-1,1'-dion über eine radikalische Zwischenstufe. 1996 , 338, 69-73	0
1312	Wechselwirkungen in Kristallen. 76. Einkristallstrukturen von 2,5-Bis(trimethylsilyl)hydrochinon ohne Lösungsmittel sowie mit Dimethoxyethan oder Dioxan: Ein Einblick in die Vielfalt von Wasserstoffbrücken-Bindungen desselben Moleküls. 1996 , 338, 363-373	3
1311	Quantenchemische MNDO-, AM1-, und PM3-Untersuchungen von β -D-Glucose-acetaten, -benzoaten und -(trichlor)acetaten als Modelle für die entsprechenden Amyloseverbindungen. 1996 , 48, 29-35	
1310	Modelling pKa of Carboxylic Acids and Chlorinated Phenols. 1996 , 15, 121-132	46
1309	Comparative Molecular Field Analysis (CoMFA) of MX Compounds using different Semi-empirical Methods: LUMO Field and its Correlation with Mutagenic Activity. 1996 , 15, 189-193	13
1308	3D-Quantitative Structure-Activity Relationships for Hydrophobic Interactions: Comparative Molecular Field Analysis (CoMFA) including Molecular Lipophilicity Potentials as Applied to the Glycine Conjugation of Aromatic as well as Aliphatic Carboxylic Acids. 1996 , 15, 194-200	2
1307	Ab Initio Study of β -Chlorinated Ethyl Hydroperoxides CH ₃ CH ₂ OOH, CH ₃ CHClOOH, and CH ₃ CCl ₂ OOH: Conformational Analysis, Internal Rotation Barriers, Vibrational Frequencies, and Thermodynamic Properties. 1996 , 100, 8240-8249	98

1306	X-ray Structure and AM1 Studies of the Proton-Transfer Adduct between 2,5-Dihydroxy-p-quinone and 4-(N,N-Dimethylamino)pyridine. 1996 , 100, 9302-9307	5
1305	Molecular Design of Optical and Structural Properties of Organic Semiconductor Films: Thiophene-Based Oligomers. 1996 , 35, L1097-L1100	2
1304	Ionic Reactions of Sulfonic Acid Esters. 1996 , 19, 1-59	9
1303	PREPARATION OF BICYCLIC GUANIDINES BY THE IODOCYCLIZATION OF 3-ALKENYL-2-(SUBSTITUTED AMINO)- 1-IMIDAZOLIN-4-ONES1. 1996 , 2,	3
1302	A comparative study of first hyperpolarizabilities of the acidic and basic forms of weak organic acids in water. 1996 , 105, 9633-9639	25
1301	Adsorbed state of thiophene on Si(100)-(2 \times 1) surface studied by electron spectroscopic techniques and semiempirical methods. 1996 , 105, 5200-5207	23
1300	Linear-scaling semiempirical quantum calculations for macromolecules. 1996 , 105, 2744-2750	155
1299	Semiempirical MNDO, AM1, and PM3 direct dynamics trajectory studies of formaldehyde unimolecular dissociation. 1996 , 104, 7882-7894	68
1298	Structure-Carcinogenicity Studies for Benz[a]Anthracenes by ¹³ C NMR Spectroscopy and Molecular Orbital Calculation. 1996 , 11, 245-252	2
1297	Atmospheric Photochemical Oxidation of Benzene: Benzene + OH and the BenzeneOH Adduct (Hydroxyl-2,4-cyclohexadienyl) + O ₂ . 1996 , 100, 6543-6554	94
1296	Properties of pure and compound clusters of Si, Ge, and Pb. 1996 , 54, 5970-5977	25
1295	CONFORMATIONAL ISOMERISM IN GLYCINE AND DITHIOGLYCINE: A COMPARATIVE MOLECULAR ORBITAL STUDY. 1996 , 116, 153-173	3
1294	Computational Study on the Endohedral Isomers of C ₆₀ H ₂ . 1996 , 4, 67-86	
1293	Organic Species with Short Cutoff Wavelength and Large Second-Order Hyperpolarizability. 1996 , 280, 1-10	8
1292	Synthesis of 1-Hydroxy-10-methyl-pyrimido [1, 6-C][1, 3]oxazine and the Oxazepine Derivative, Structural Mimicry of Anti-Constrained Acyclic Thymidine. 1996 , 15, 1481-1493	3
1291	Uv Photoemission Study of 8-Hydroxyquinoline Aluminum (ALQ3) / Metal Interfaces. 1996 , 286, 239-244	19
1290	Hydrogen bonding and stacking of DNA bases: a review of quantum-chemical ab initio studies. 1996 , 14, 117-35	202
1289	Transient excited-state absorption of the liquid crystal CB15 [4-(2-methylbutyl)-4-cyanobiphenyl] in its isotropic phase. 1996 , 21, 225-232	3

1288	Synthesis of perfluoroalkylated azo dyes and their application to guest-host liquid crystal display. 1996 , 21, 669-682	19
1287	PAH Formation in the Premixed Flame of Ethane. 1996 , 116-117, 167-181	19
1286	Thiepanes and Thiepines. 1996 , 67-111	6
1285	Unimolecular Decomposition of the Anionic Form of N-Chloro-L-glycine. A Theoretical Study. 1996 , 100, 3561-3568	14
1284	Polarizability/Hyperpolarizability Influences upon Solvatochromism in Polychloroalkane and Polychloroalkene Media. 1996 , 100, 519-522	4
1283	Relative Solution Electron Affinities of Selectively Deuteriated Pyrenes: Correlations between Voltammetric, Electron Paramagnetic Resonance, and Semiempirical PM3 Data. 1996 , 100, 3454-3462	8
1282	Extension of the PM3 Method on s,p,d Basis. Test Calculations on Organochromium Compounds. 1996 , 100, 6354-6358	11
1281	Solvent Effects in Chloroform Solution: Parametrization of the MST/SCRF Continuum Model. 1996 , 100, 4269-4276	110
1280	Ab Initio Molecular Orbital Study of the Structures of Purine Hydrates. 1996 , 100, 4420-4423	24
1279	Electronic Structure of PushPull Molecules Based on Thiophene Oligomers. 1996 , 100, 11029-11032	22
1278	Molecular Orbital Studies of Crystalline Nitroanilines. 1996 , 100, 9638-9648	32
1277	Dynamic Spectral Shift of Benzophenone Radical Anion Caused by the Solvent Molecule Reorientation. Semiempirical PM3-MO and Classical Trajectory Studies. 1996 , 100, 17090-17093	27
1276	Scanning Tunneling Microscopy Observation of Copper-Phthalocyanine and Nucleic Acid Base Molecules on Reduced SrTiO ₃ (100) and Cu(111) Surfaces. 1996 , 35, 3759-3763	16
1275	The Raman activity of and : a computational semiempirical study. 1996 , 29, 5065-5075	13
1274	Preparation of Retardation Film for Supertwisted Nematic Liquid Crystal Display by Drawing and Poling. 1997 , 36, 232-238	3
1273	Crystal structures of (S)- and (R,S)-2,2'-bipyridine-3,3'-dicarboxylic acid 1,1'-dioxides and of their barium salts: absolute configuration and molecular distortion enforced by supramolecular self-assembly. 1997 , 212, 226-233	12
1272	A quantum chemical study of the isomers of bis(methano)fullerene, C ₆₀ (CH ₂) ₂ . 1997 , 91, 561-566	3
1271	Autoxidation Reaction Mechanism for L-Ascorbic Acid in Methanol without Metal Ion Catalysis. 1997 , 61, 2069-75	5

1270	Bond hybridization and structural properties of clusters of group-IV elements. 1997 , 56, 15926-15937	8
1269	What Is the Longest Unbranched Alkane with a Linear Global Minimum Conformation?. 1997 , 37, 876-878	44
1268	Theoretical study of oxygenated (100) diamond surfaces in the presence of hydrogen. 1997 , 55, 1895-1902	40
1267	A semi-empirical scheme for generalized valence bond calculations on water complexes. 1997 , 106, 3248-3257	4
1266	Theoretical evaluation of medium effects on absorption maxima of molecular solutes. I. Formulation of a new method based on the self-consistent reaction field theory. 1997 , 107, 5652-5660	23
1265	On the calculation of G tensors of organic radicals. 1997 , 107, 3905-3913	41
1264	A hybrid semiempirical quantum mechanical and lattice-sum method for electrostatic interactions in fluid simulations. 1997 , 107, 1212-1217	47
1263	A Tersoff potential for clusters. A proposal for a single-binding relation. 1997 , 37, 245-250	2
1262	Electronic and Optical Parameters of the TGM-3 Photopolymer. 1997 , 9, 51-60	13
1261	Excess Li ions in a small graphite cluster. 1997 , 12, 1367-1375	55
1260	Color Prevision of Activated Forms of Photochromic Spirooxazines and Chromenes. 1997 , 298, 21-28	3
1259	Nonlinear Optical Properties of the Thermotropic Liquid-Crystalline Main-Chain Polymers (Aromatic Polyesters). 1997 , 299, 85-90	2
1258	Vibrational Study of a Nucleoside Analogue with Antitumoral and Antiviral Activity, 5-Fluoro-2'-deoxyuridine, FdU. 1997 , 16, 1041-1044	5
1257	Nonenzymatic and enzymatic hydrolysis of alkyl halides: a theoretical study of the SN2 reactions of acetate and hydroxide ions with alkyl chlorides. 1997 , 94, 6591-5	29
1256	Conformation of coenzyme pyrroloquinoline quinone and role of Ca ²⁺ in the catalytic mechanism of quinoprotein methanol dehydrogenase. 1997 , 94, 11881-6	57
1255	Semi-Empirical Calculations and Measurements of Modified Carbocyanines Optical Properties. 1997 , 479, 319	
1254	Structural and Electronic Properties of Self-Assembled Supramolecular Grid Structures: Doping of Supramolecular Thin Films. 1997 , 488, 447	2
1253	Photochemistry of Amino-Linked Bichromophoric Anthracenes. Efficient Cyclomerization of 9-(1-Naphthylmethylaminomethyl)anthracene and Adiabatic Cycloreversion of the Cyclomer. 1997 , 70, 869-875	11

- 1252 Enhanced Nucleophilic Reactivity of a 4-Lithiophenoxide Ion and Its Application to the Synthesis of a Bis(4-hydroxyphenyl)methylenecyclopentadiene and Its Dianion, a Novel Extended Trimethylenemethane Dianion. **1997**, 26, 947-948 3
- 1251 Evidence for Spiro-Conjugation in Perpendicularly-Linked Pentamethinestreptocyanine Dimers. **1997**, 70, 1109-1114 14
- 1250 Biscyanines Linked by a 1,8-Naphthylene Skeleton: Models of Polymethine Dye Aggregates. **1997**, 70, 2287-2296 4
- 1249 Oxidation Mechanism of NAD Dimer Model Compounds. **1997**, 26, 567-568 49
- 1248 On the Basicity of Ozone. **1997**, 26, 835-836 8
- 1247 Transformation of Oximes of Phenethyl Ketone Derivatives to Quinolines and Azaspirotrienones Catalyzed by Tetrabutylammonium Perrhenate and Trifluoromethanesulfonic Acid. **1997**, 70, 965-975 41
- 1246 Hexacyanotriquinarenemethane Dianion. **1997**, 26, 1057-1058 1
- 1245 Rearrangements of Tricyclo[5.3.1.0]undecatrienyl Anion; Chemical Evidence Supporting Cyclopropane Ring Circumambulation of Anionic Species. **1997**, 26, 595-596
- 1244 Crystal and Molecular Structures of Hypervalent Thia/Selena-pentalenes. **1997**, 70, 1267-1275 8
- 1243 5,8,17,20-Tetrakis(3,5-di-*t*-butylphenyl)-6,7,18,19-tetradehydrotetrathia[24]annulene-(4.0.4.0) and Its Dianion: New Thiophene-Derived Paratropic and Diatropic Annulenes. **1997**, 26, 571-572 11
- 1242 Semiquinone production by lipophilic *o*-naphthoquinones. **1997**, 3, 245-52 5
- 1241 Muon spectroscopy applied to biological systems: a study of thiyl radicals, RS. **1997**, 27, 347-52 5
- 1240 Lithio-Aversion of Thiophene Sulfur Atoms in the X-ray Crystal Structures of [LiD₂SiMe₂(2-C₄H₃S)]₆ and [LiD₂CH(i-Pr)(2-C₄H₃S)]₆: Models for Electrostatic Metal-Thiophene Interactions. **1997**, 16, 5032-5041 18
- 1239 Calculation of Quadrupole Moments of Polycyclic Aromatic Hydrocarbons: Applications to Chromatography. **1997**, 101, 5374-5377 18
- 1238 Facile Alkylation of Cobalt(III) Porphyrins by Organosilicon Compounds. **1997**, 16, 3679-3683 13
- 1237 Synthesis and Theoretical Study of Mannich Type Reaction Products of 3-Formylchromones with Triazoles and Amides and Nucleophilic Formation of 2,3-Disubstituted-4-Chromanones. **1997**, 1, 223-235 1
- 1236 Formation Mechanism of Monodehydro-l-ascorbic Acid and Superoxide Anion in the Autoxidation of l-Ascorbic Acid. **1997**, 61, 1693-5 4
- 1235 Conformations and Electronic Structure of Fullerene C₂₄ and C₂₆ Molecules. **1997**, 5, 85-96 9

- 1234 X-Ray Crystallographic Analysis of the Endo-Peroxide of Anthra[1,9-b c:4,10-b?c?]Dichromene. **1997**, 298, 1-6 2
- 1233 Structural stability of hydrogenated (100) surface of cubic boron nitride in comparison with diamond. **1997**, 81, 7798-7805 22
- 1232 Control of Stereochemistry by sigma-Participation of a Silyl Group. A Novel Method for Diastereoselective Polyol Synthesis. **1997**, 62, 4206-4207 28
- 1231 Reaction of C60 with Sultines: Synthesis, Electrochemistry, and Theoretical Calculations of Organofullerene Acceptors. **1997**, 62, 7585-7591 50
- 1230 On The Differences Between Neutral and Negatively Charged C60 Dimers. **1997**, 5, 429-442 1
- 1229 Influence of the Position of an Annular Nitrogen Atom on the Magnitude of the Rotational Barriers in Atropisomers of 1,8-Dihetarylnaphthalenes. **1997**, 62, 3215-3219 24
- 1228 Photo-Induced Cationic Ring-Opening Polymerization of 2-Alkenyl-4-methylene-1,3-dioxolanes by Benzylsulfonium Salt. **1997**, 30, 3414-3416 10
- 1227 CVD Germania on Pyrogenic Silica. **1997**, 13, 250-258 12
- 1226 Stereochemistry of Epoxidation of Some Caryophyllenols. **1997**, 62, 1965-1969 17
- 1225 Radical Cation of Naphthalene on H β SM-5 Zeolite and in CFCl₃ Matrix. A Theoretical and Experimental EPR, ENDOR, and ESEEM Study. **1997**, 101, 2390-2396 21
- 1224 Synthesis, Crystal Structure, and Second-Order Optical Nonlinearity of Bis(2-chlorobenzaldehyde thiosemicarbazone)cadmium Halides (CdL(2)X(2); X = Br, I). **1997**, 36, 1247-1252 167
- 1223 Comparative PM3-M0 Study of the E2O2 and E2N2 (E=P,As) Four Membered Ring Systems. **1997**, 124, 441-444 1
- 1222 Effects of Matrix Structure/Acidity on Ion Formation in Matrix-Assisted Laser Desorption Ionization Mass Spectrometry. **1997**, 119, 2534-2540 37
- 1221 Side-Chain Nitration of Styrene and Para-Substituted Derivatives with a Combination of Nitrogen Dioxide and Ozone. **1997**, 62, 6498-6502 37
- 1220 Quantum Chemical Study of the Different Forms of Nitric Acid Monohydrate. **1997**, 101, 8871-8876 19
- 1219 Synthesis and Conformational Study of Isomers of 9-Methyl-2,11-Dithia[3.3](1,4)triphenylenometacyclophane and 2,23-Dithia[3.3](1,4)triphenylenophane. **1997**, 62, 4500-4503 8
- 1218 Conformations of Azacyclodeca-3,8-diynes and 1,6-Diazacyclodeca-3,8-diynes and the Generalized Anomeric Effect: A Test for Current Conformational Models for Azaheterocycles. **1997**, 119, 10599-10607 17
- 1217 Isolation, Structure Elucidation, and Identification of a Further Major Toxaphene Compound in Environmental Samples. **1997**, 31, 3023-3028 36

1216	Parametrized Model for Aqueous Free Energies of Solvation Using Geometry-Dependent Atomic Surface Tensions with Implicit Electrostatics. 1997 , 101, 7147-7157	73
1215	Electronic Effects of para- and meta-Substituents on the EPR D Parameter in 1,3-Arylcyclopentane-1,3-diyl Triplet Diradicals. A New Spectroscopic Measure of π Spin Densities and Radical Stabilization Energies in Benzyl-Type Monoradicals. 1997 , 62, 1419-1426	25
1214	Relative Basicities of Some Endo and Exo Norbornylamines. 1997 , 62, 7205-7209	4
1213	Theoretical Insights Regarding the Cycloaddition Behavior of Push-Pull Stabilized Carbonyl Ylides. 1997 , 62, 2001-2010	46
1212	Additivity of the Electronic Meta-Substituent Effect in 3,5-Disubstituted Cumyl Radicals Assessed by the EPR D Parameter of 1,3-Arylcyclopentane-1,3-diyl Triplet Diradicals. 1997 , 62, 7263-7266	1
1211	Theoretical Investigation of the Reaction between Aluminum and Propene. Comparison between Calculated and Experimental ESR Results. 1997 , 101, 4814-4820	5
1210	A Theoretical Examination of the Factors Controlling the Catalytic Efficiency of a Transmethylation Enzyme: Catechol O-Methyltransferase. 1997 , 119, 8137-8145	72
1209	7,14-Dichloro[1.1]metacyclophane: A Highly Strained Aromatic Intermediate. 1997 , 62, 7090-7091	4
1208	Insertion of Amines and Alcohols into Proton-Bound Dimers. A Density Functional Study. 1997 , 101, 2597-2606	15
1207	Hydrogen Bonding in Copoly(ether-urea)s and Its Relationship with the Physical Properties. 1997 , 30, 3584-3592	96
1206	Formation of Trace Byproducts in the Premixed Flames of CH ₃ Cl/C ₂ H ₄ . 1997 , 31, 1372-1381	11
1205	Electrochemical and Spectroscopic Investigation of the Influence of Acid-Base Chemistry on the Redox Properties of 2,5-Dimercapto-1,3,4-thiadiazole. 1997 , 101, 2861-2866	41
1204	Molecular Modeling Studies on Aromatic Sulfonation. 1. Intermediates Formed in the Sulfonation of Toluene. 1997 , 62, 7358-7363	17
1203	Synthesis and antimetastatic activity of L-iduronic acid-type 1-N-iminosugars. 1997 , 40, 2626-33	63
1202	Resistance of the Bianthrone Radical Anion toward Oxidation by Dioxygen. 1997 , 101, 8227-8232	4
1201	A Semiempirical PM3 Treatment of Benzotetrazepinone Decomposition in Acid Media. 1997 , 62, 7006-7014	12
1200	Ab Initio and Semiempirical Studies on the Transition Structure of the Baeyer and Villiger Rearrangement. The Reaction of Acetone with Performic Acid \square 1997 , 101, 192-200	31
1199	Notable Substituent Electronic Effects on the Regioselectivity of an Oxygen-Atom Abstraction in the Reaction of Unsymmetrically Substituted Monocyclic 1,2-Dioxolanes with Triphenylphosphine. 1997 , 62, 752-754	7

1198	Synthesis and Diatropicity of trans-10b,10c-Dimethylenacenaphthylene[1,2:e]-10b,10c-dihdropyrene: A Model Aromatic Molecule To Verify the Effect of Conjugation on the Diatropicity of an Annulene. 1997 , 62, 916-924	10
1197	Trends in Inversion Barriers of Group 15 Compounds. 3. Are Fluorinated Pyridone Derivatives Planar or Nonplanar?. 1997 , 62, 8063-8070	10
1196	Deuterium Nuclear Quadrupole Coupling and cis↔trans Isomerization in Poly(phenylacetylene-d1). 1997 , 30, 1074-1078	30
1195	Ab Initio and Semiempirical Calculations of Geometry and Electronic Spectra of Ruthenium Organic Complexes and Modeling of Spectroscopic Changes upon DNA Binding. 1997 , 36, 2544-2553	63
1194	Ab Initio and Semiempirical Study of the Effect of Ethereal Solvent on Aggregation of a Lithium Enolate. 1997 , 119, 11255-11268	90
1193	Thermodynamic Parameters and Group Additivity Ring Corrections for Three- to Six-Membered Oxygen Heterocyclic Hydrocarbons. 1997 , 101, 2471-2477	39
1192	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. 1997 , 101, 1859-1865	44
1191	Catenation of Heterocyclic Non-Kekulé Biradicals to Tetraradical Prototypes of Conductive or Magnetic Polymers. 1997 , 119, 1428-1438	22
1190	Quantum semiempirical study of the reactivity of monomers in the synthesis of aromatic polyamides and polyimides. 1997 , 122, 197-202	1
1189	Synthesis and Proton Conductivity of Highly Sulfonated Poly(thiophenylene). 1997 , 30, 2941-2946	65
1188	(E)- and (Z)-7-arylidenealtrexones: synthesis and opioid receptor radioligand displacement assays. 1997 , 40, 749-53	13
1187	Why Is the Rearrangement of [6,5] Open Fulleroids to [6,6] Closed Fullerenes Zero Order?. 1997 , 119, 1149-1150	21
1186	Development of Weiner et al. force field parameters suitable for conformational studies of [1,4]-benzodiazepines and related compounds. 1997 , 37, 951-6	12
1185	Tuning the Singlet↔Triplet Energy Gap in a Non-Kekulé Series by Designed Structural Variation. The Singlet States of N-Substituted-3,4-dimethylenepyrrole Biradicals. 1997 , 119, 1406-1415	31
1184	Surface Migration in Diamond Growth. 1997 , 101, 3025-3036	68
1183	New Insights into the Dynamics of Concerted Proton Tunneling in Cyclic Water and Hydrogen Fluoride Clusters. 1997 , 101, 4707-4716	35
1182	Structures of C _n H _x ⁺ Molecules for n ≥ 2 and x ≤ 5: Emergence of PAHs and Effects of Dangling Bonds on Conformation. 1997 , 101, 2096-2102	28
1181	Quantum Mechanics and Molecular Mechanics Studies of the Low-Energy Conformations of 9-Crown-3. 1997 , 101, 1920-1926	11

1180	Diastereoselective Synthesis of Cycloalkylamines by Samarium Diiodide-Promoted Cyclizations of β -Amino Radicals Derived from β -Benzotriazolylalkenylamines. 1997 , 62, 1125-1135	20
1179	Effect of substitution site upon the oxidation potentials of alkylanilines, the mutagenicities of N-hydroxyalkylanilines, and the conformations of alkylaniline-DNA adducts. 1997 , 10, 1266-74	47
1178	Formation of 2-[1-(Trimethylsilyl)alkylidene]-4-cyclopentene-1,3-dione from Lewis Acid-Catalyzed Reaction of Cyclobutenedione Monoacetal with Alkynylsilane: Novel Cationic 1,2-Silyl Migrative Ring Opening and Subsequent 5-Exo-Trig Ring Closure. 1997 , 62, 1292-1298	21
1177	Alkaline Degradation of Resorcinol-Formaldehyde Resins: Solid-State NMR, Thermal Adsorption and Desorption Analysis, and Molecular Modeling. 1997 , 34, 281-289	5
1176	Synthesis and Diatropicity of trans-10b-Methyl-10c-undecyl- and trans-10b-Methyl-10c-pentadecyl-10b,10c-dihydropyrene. An Empirical Approach to a Semiquantitative Assessment of the Diamagnetic Ring Current in a [14]Annulene. 1997 , 62, 925-931	12
1175	New Photochromic 10?-Substituted Spiro[Indoline-Naphthoxazines]. 1997 , 298, 7-11	
1174	Modeling interface structures of cubic boron nitride films deposited heteroepitaxially and via a hexagonal boron nitride interlayer on silicon (001) surfaces. 1997 , 6, 589-593	3
1173	Stokes Shift as a Tool for Probing the Solvent Reorganization Energy. 1997 , 101, 3433-3442	46
1172	Comparison of photoinduced electron transfer reactions of C60 and aromatic carbonyl compounds. 1997 , 23, 519-539	5
1171	Synthesis and cytotoxic evaluation of substituted sulfonyl-N-hydroxyguanidine derivatives as potential antitumor agents. 1997 , 40, 2276-86	42
1170	Porphyrin Isomers: Geometry, Tautomerism, Geometrical Isomerism, and Stability. 1997 , 62, 9240-9250	74
1169	Synthesis of 2-Aryl-10b,10c-dimethyl-10b,10c-dihydropyrenes and a Study of Their Conjugation Behavior: Linear Relationship between the Degree of Conjugation and the Electronic Nature of Substituents. 1997 , 62, 4412-4417	16
1168	Chemical Ionization of TNT and RDX with Trimethylsilyl Cation. 1997 , 69, 1092-1101	25
1167	Calculation of the Molecular Ordering Parameters of (-)-3-Butyn-2-ol Dissolved in an Organic Solution of Poly(β benzyl-L-glutamate). 1997 , 101, 5719-5724	63
1166	1,3,2-Dioxathiolane Oxides: Epoxide Equivalents and Versatile Synthons. 1997 , 89-180	32
1165	Steric Consequences on the Conformation of Medium-Sized Rings: Solution NMR, Solid-State Crystallographic, ab Initio Molecular Orbital Calculations, and Molecular Mechanics Studies on Substituted Eight-Membered Organosilicon Ring Systems1. 1997 , 119, 8313-8323	18
1164	Simulation of the enzyme reaction mechanism of malate dehydrogenase. 1997 , 36, 4800-16	68
1163	Use of Electron Diffraction and High-Resolution Imaging To Explain Why the Non-dipolar 1,3,5-Triamino-2,4,6-trinitrobenzene Displays Strong Powder Second Harmonic Generation Efficiency. 1997 , 101, 7265-7276	31

1162	Oxidation of Diols and Ethers by NaBrO ₃ /NaHSO ₃ Reagent. 1997 , 70, 2561-2566	40
1161	True Polyazulene: Soluble Precursor of So-Called Polyazulene 1997 , 30, 6385-6387	6
1160	Synthesis, Crystal Structure, and Explosive Decomposition of 1,2:5,6:11,12:15,16-Tetrabenzotriaza-3,7,9,13,17,19-hexadehydro[20]annulene: Formation of Onion- and Tube-like Closed-Shell Carbon Particles. 1997 , 119, 2052-2053	129
1159	[21] Stereoselectivity of lipase from <i>Rhizopus oryzae</i> toward triacylglycerols and analogs: Computer-aided modeling and experimental validation. 1997 , 353-376	11
1158	Fundamental Studies on Brooker's Merocyanine. 1997 , 119, 10192-10202	90
1157	Towards mechanosynthesis of diamondoid structures: I. Quantum-chemical molecular dynamics simulations of sila-adamantane synthesis on hydrogenated Si(111) surface with the STM. 1997 , 8, 132-144	5
1156	Absolute Binding Energies of Lithium Ions to Short Chain Alcohols, C _n H _{2n+2} O, n = 1-14, Determined by Threshold Collision-Induced Dissociation. 1997 , 101, 2614-2625	102
1155	Charged and Betainic Nucleobases. On Syntheses and Properties of First Mesomeric Uracilybetaines, Uracilates, and Novel Uracilium Salts. 1997 , 62, 3910-3918	18
1154	Semiempirical methods with conjugate gradient density matrix search to replace diagonalization for molecular systems containing thousands of atoms. 1997 , 107, 425-431	128
1153	Low dimensional self-organization of DNA-base molecules on Cu(111) surfaces. 1997 , 386, 124-136	75
1152	Monte Carlo study on formation of periodic structures on Si(111) surfaces. 1997 , 389, 375-381	4
1151	Scanning tunneling microscopy observation of two-dimensional self-assembly formation of adenine molecules on Cu(111) surfaces. 1997 , 392, L33-L39	44
1150	The octanol-water partition coefficient of benzene derivatives based on three dimensional structure directed molecular properties. 1997 , 35, 993-1002	6
1149	Short-chain (C ₂₁ and C ₂₂) diasteranes in petroleum and source rocks as indicators of maturity and depositional environment. 1997 , 61, 2653-2667	49
1148	Substituents Effect on the Electronic Properties of Aniline and Oligoanilines. 1997 , 101, 6945-6950	39
1147	Conformational equilibria of 5-substituted-1,3-dithianes. Study of solvent effects. 1997 , 418, 113-118	2
1146	Future ESR and optical dating of outer planet ICY materials. 1997 , 16, 431-435	2
1145	Heavy metal tolerance of <i>Minuartia verna</i> . 1997 , 151, 101-108	90

1144	Inhibitory effects on Epstein-Barr virus activation of anthraquinones: correlation with redox potentials. 1997 , 115, 179-83	15
1143	Unravelling Mango's mysteries: a kinetic scheme describing the diagenetic fate of C7-alkanes in petroleum systems. 1997 , 27, 597-599	16
1142	Electronic structure and optical properties of conducting and semiconducting conjugated oligomers and polymers: An overview of the quantum-mechanical approaches. 1997 , 84, 3-10	20
1141	Non-enzymatic and enzymatic hydrolysis of alkyl halides: a haloalkane dehalogenation enzyme evolved to stabilize the gas-phase transition state of an SN2 displacement reaction. 1997 , 94, 8417-20	51
1140	Interaction of Water and other Polar Substances with Hydrophilic Centres on the Surface of Hydrophobic Adsorbents. 1997 , 15, 497-505	7
1139	An elongation method to calculate the electronic structure of non-periodical and periodical polymers. 1997 , 71-72, 147-164	2
1138	Bisacetals of aromatic ring-annelated . [3.3][3.3]Orthocyclophanes with triple-layered benzo/benzo/benzo- and naphtho/benzo/naphtho-system. 1997 , 53, 3015-3026	7
1137	Substituent effects on the regiochemistry of enone-alkene 2+2-photocycloadditions. Experimental results and FMO analysis. 1997 , 53, 3545-3556	23
1136	Synthesis and Properties of Benzobis(thiadiazole)s with Nonclassical π -Electron Ring Systems. 1997 , 53, 10169-10178	67
1135	Regiochemistry of Wacker-type oxidation of vinyl group in the presence of neighboring oxygen functions. Part 1. 1997 , 53, 7577-7586	31
1134	Determining factors in the assignment of the absolute configuration of alcohols by NMR. The use of anisotropic effects on remote positions. 1997 , 53, 8541-8564	46
1133	The determination of the absolute configuration of a chiral molecular tweezer using CD spectroscopy. 1997 , 38, 8655-8658	28
1132	Calculation of the solvent reorganization free energy in the dielectric cavity model. 1997 , 215, 355-370	9
1131	Electronic structure of docosahexaenoic acid studied by photoelectron spectroscopy. 1997 , 85, 47-52	3
1130	Conformational analysis of the antimalarial agent quinidine. 1997 , 5, 353-61	9
1129	Molecular modeling of (E)-1-alkyl-4(3)-[2-(1H-azolyl)vinyl]-pyridinium salts and evaluation of their behavior towards choline acetyltransferase. 1997 , 5, 949-54	2
1128	Synthesis, structure and quantitative structure-activity relationships of sigma receptor ligands, 1-[2-(3,4-dimethoxyphenyl)ethyl]-4-(3-phenylpropyl) piperazines. 1997 , 5, 1675-83	35
1127	Introduction of solvent-accessible surface area in the calculation of the hydrophobicity parameter log P from an atomistic approach. 1997 , 86, 57-63	18

1126	Computer-aided modelling of stereoselective triglyceride hydrolysis catalyzed by <i>Rhizopus oryzae</i> lipase. 1997 , 3, 73-82	24
1125	Structure and isomerization of β -phenylcinnamic acid stereoisomers [Reaction pathway and transition-state structure by semiempirical methods. 1997 , 391, 189-192	1
1124	Semiempirical and ab initio calculations on the alkaline hydrolysis of the β -lactam ring Influence of the solvent. 1997 , 390, 247-254	20
1123	Semiempirical calculations of the hydrolysis of penicillin G. 1997 , 390, 255-263	8
1122	Semiempirical determination of torsional potentials and electronic properties of bithiophene, terthiophene and 3,4'-dihexyl-2,2':5,2'-terthiophene in their ground and first excited singlet and triplet electronic states. 1997 , 391, 85-99	24
1121	Ab initio studies on four alkyl nitric esters. 1997 , 393, 207-212	17
1120	Computational study of the addition of molecular oxygen to benzene. 1997 , 397, 13-20	8
1119	Scaled semiempirical method for the calculation of vibrational spectra Molecular vibrational frequencies of monosaccharides and disaccharides by PM3 method. 1997 , 395-396, 71-80	13
1118	Ab initio and PM3 studies of hydrogen bonding of acetoin (E)- and (Z)-oxime dimers. Cooperativity and competition. 1997 , 393, 177-187	1
1117	Bond and atomization energies of C60 and C70 fullerenes. 1997 , 398-399, 301-305	5
1116	Ab initio and semiempirical MO studies using large cluster models of CO and H2 adsorption and dissociation on ZnO surfaces with the formation of ZnH and OH species. 1997 , 397, 147-157	11
1115	Monte Carlo simulation of amorphous systems with the fragment self-consistent field method. 1997 , 398-399, 129-133	3
1114	Ab initio study, semiempirical calculation and NMR spectroscopy of keto-enol tautomerism of triazolopyrimidines. 1997 , 401, 1-14	14
1113	Analysis of permanent electric dipole moments of aliphatic hydrocarbon molecules. 1997 , 401, 21-27	12
1112	A theoretical study of the structure, electronic properties, and reactivity of phenylcyanates. 1997 , 401, 69-76	
1111	NDDO semiempirical approximations coupled with Green's function technique [reliable approach for calculating ionization potentials. 1997 , 401, 235-252	7
1110	Semiempirical molecular orbital theory in carcinogenesis research. 1997 , 401, 253-266	9
1109	Hydrogen bonds: a comparison of semiempirical and ab initio treatments. 1997 , 401, 279-286	45

1108	Applicability of semi-empirical methods to the study of small water clusters: cubic structures for (H ₂ O) _n (n = 8, 12, 16). 1997 , 417, 35-47	22
1107	Computational methods for large molecules. 1997 , 398-399, 1-6	17
1106	Computational modeling of the mechanisms of circumambulatory rearrangements of main-group migrants in the cyclopropene ring. 1997 , 398-399, 237-253	4
1105	Conformational analysis of 2-substituted-1,3-diheteroanes. A theoretical study of solvent effects. 1997 , 418, 41-47	3
1104	PM3 study of cyclization of β - and β -glucosyl azides into 1,2-cyclic carbamates. 1997 , 395-396, 61-69	15
1103	Parallelization strategies and experiences with the dynamically defined reaction path (DDRP) method. 1997 , 398-399, 111-119	4
1102	Semiempirical characterization of substituted bis-pyrazolopyridines as new bulky electron donor-acceptor systems in their electronic ground state. 1997 , 419, 63-75	16
1101	Quantum chemical modelling of thyroid hormone analogues. 1997 , 419, 121-131	1
1100	Theoretical study of the dissociative process of the 4-chlorotoluene radical anion. 1997 , 392, 87-94	8
1099	A theoretical study of the cationic dimerization and polymerization of isobutene. 1997 , 392, 111-124	1
1098	Semiempirical quantum chemical methods: testing of physicochemical properties of acyclic and aromatic compounds. 1997 , 392, 137-140	7
1097	Quantum chemical modelling of electronic charge density distribution in several tetrathiafulvalene derivatives. 1997 , 51, 135-141	4
1096	Isomerisation of deuterated cyclopropanes – The possibility for stereochemical control. 1997 , 101, 414-422	11
1095	Quantum chemical study of the intramolecular transfer of hydrogen in o- methylacetophenone and 1- alkylanthraquinones. 1997 , 38, 536-543	1
1094	Exchange and magnetic dipole-dipole interactions in bi- and triradical complexes of Al(III), Ga(III), In(III), and Sn(IV) witho-semiquinones. PM3 calculation. 1997 , 38, 884-889	2
1093	Ab initio investigation of the electronic structure of malonic dialdehyde derivatives. 1997 , 38, 890-894	
1092	On the nature of the isomer shift in tin(IV) tetrachloride complexes with organic ligands from quantum chemical data. 1997 , 38, 970-973	2
1091	Exchange interactions in biradical complexes of metals (II) witho-semiquinones. PM3 calculation. 1997 , 38, 41-46	3

1090	Stereo- and regioselective cycloaddition of norbornene to 2,4,9-triazidopyridine. 1997 , 33, 1315-1324	5
1089	Structure dependence of intramolecular photoinduced electron transfer in 9-aminoacridine benzoyl esters dyads linked by a polyether chain. 1997 , 42, 1619-1624	1
1088	Study of the mechanism of recyclization of furans into thiophenes and selenophenes in conditions of acid catalysis. 5. Direction of protonation of furans. 1997 , 33, 898-902	4
1087	Conformational analysis of the antimalarial agent quinine. 1997 , 8, 95-107	14
1086	Quantum chemical study of the nature of regioselectivity in reactions of 2,4,6-triazidopyridines with tert-butylphosphaacetylene. 1997 , 33, 587-595	4
1085	Effect of substituents in the ring on the structure and electron density distribution in benzyl halides. 1997 , 46, 1996-2005	1
1084	Electrochemical activation of the alkylation of GeI ₂ by n-butyl bromide and methylcobalt(III) bisdimethylglyoximate. 1997 , 46, 2044-2047	1
1083	Functionalization of saturated hydrocarbons by aprotic superacids. 1997 , 46, 491-495	6
1082	Quantum-chemical study of possible structural transformations in 3-methylthio-3-phenyl-2-propenethial. 1997 , 46, 1216-1220	
1081	Synthesis and structure of 2,4-di-tert-butyl-1-chloro-6-methyltricyclo[4.1.0.0 ^{2,7}]hept-4-en-3-one. 1997 , 46, 1565-1568	
1080	Cyclopentadienyl type π - π -complexes of C ₆₀ fullerene derivatives with indium and thallium: simulation of molecular and electronic structure by the MNDO/PM3 method of C ₆₀ fullerene derivatives with indium and thallium: simulation of molecular and electronic structure by the MNDO/PM3 method. 1997 , 46, 1832-1837	7
1079	The ESR study of reactivity of perfluoroacetyl diisopropylmethyl radical. 1997 , 46, 1851-1854	
1078	Structural dependence of non-linear optical properties of 4-Dimethylamino-3-cyanobiphenyl. 1997 , 275, 18-37	10
1077	Electrostatic modulation of electron transfer in the active site of heme peroxidases. 1997 , 2, 135-138	23
1076	Wechselwirkungen in Kristallen. 96. Darstellung und Strukturen von Salzen [RnN ⁺ H ₂ N ⁺ Rn][B ⁻ (C ₆ H ₅) ₄] mit Prototyp-Wasserstoffbrücken N ⁺ H ⁺ N ⁺ . 1997 , 339, 26-37	10
1075	Wechselwirkungen in Kristallen. 98. Mitt. Protonierte Hexamethylmelamin-Salze mit verschiedenen Anionen: Monomeres Tetraphenylborat, dimeres Trifluoracetat und polymeres Chlorid-Dihydrat. 1997 , 339, 525-533	4
1074	Simple Quantum Chemical Parameters as an Alternative to the Hammett Sigma Constants in QSAR Studies. 1997 , 16, 377-382	38
1073	Effect of solvents on the electronic absorption spectra of some substituted diarylformazans. 1997 , 128, 981-990	11

1072	Interaction of flutriafol with the surface of silica and layer silicates. 1997 , 127, 187-199	7
1071	Photophysics of a simple cyanide dye. 1997 , 104, 179-187	17
1070	Photoinitiated electron transfer interaction of all-trans retinal with electron donors and acceptors. 1997 , 107, 55-62	8
1069	Chemical studies on the nonlinear optics of coordination compounds. 1997 , 106, 85-90	9
1068	Comparison of the photochromic properties of fulgides and fulgimides. 1997 , 108, 239-245	41
1067	Role of structural flexibility in the fluorescence and photochromism of salicylideneaniline: the general scheme of the phototransformations. 1997 , 110, 267-270	47
1066	Local electrostatic potentials in pyridoxal phosphate labelled horse heart cytochrome c. 1997 , 37, 74-83	9
1065	Synthesis of (2S,1? S,2? S)-2-methyl-2-(carboxycyclopropyl)glycine and (S)-2-amino-2-methyl-4-phosphonobutyric acid from l-alanine. 1997 , 8, 889-893	12
1064	Modulation of nucleic acid structure by ligand binding: induction of a DNA.RNA.DNA hybrid triplex by DAPI intercalation. 1997 , 5, 1137-47	34
1063	Vibrational analysis and spectra of cytidine 3'-monophosphate (3'-CMP). 1997 , 15, 1-16	20
1062	Stationary and time-resolved fluorescence investigations combined with studies of tautomeric phenomena in neutral and protonated 9-acridinamine. 1997 , 53, 1723-1733	14
1061	Electronic transitions and intramolecular hydrogen bonding in anthralin. UV-VIS linear dichroism spectroscopy and quantum chemical calculations. 1997 , 53, 2615-2625	16
1060	New pyrrolobenzothiazepine derivatives as molecular probes of the peripheral-type benzodiazepine receptor (PBR) binding site. 1997 , 32, 241-251	24
1059	Carbonic anhydrase inhibitors. Part 41. Quantitative structure-activity correlations involving kinetic rate constants of 20 sulfonamide inhibitors from a non-congeneric series. 1997 , 32, 311-319	35
1058	Intramolecular orbital interactions in 9,10-disilatriptycene studied by photoelectron spectroscopy. 1997 , 83, 165-172	3
1057	Site-specific lithium ion attachment directs low-energy dissociation pathways of dinucleotides in the gas phase. Application to nucleic acid sequencing by mass spectrometry. 1997 , 161, 193-216	14
1056	Generation and characterization of ionic and neutral (methylthio)oxophosphane (CH ₃ S ⁺ P ⁺ O) ⁺ and (methoxy)oxophosphane (CH ₃ O ⁺ P ⁺ O) ⁺ by neutralization-reionization mass spectrometry. 1997 , 171, 79-82	14
1055	Chemical ionization of the nitrate ester explosives EGDN and PETN by trimethylsilyl cation and comparison of the reactivity of nitrate ester and nitro explosives toward trimethylsilyl cation. 1997 , 165-166, 641-653	10

1054	Mechanism of H ₂ desorption from H-terminated Si(001) surfaces. 1997 , 117-118, 67-71	6
1053	Synthesis and crystal structure of the cadmium complex of 2-bromobenzaldehyde thiosemicarbazone. 1997 , 16, 2857-2861	11
1052	Using triazine as coupling unit for intra and intermolecular ferromagnetic coupling I. 1997 , 214, 291-299	22
1051	C ₉₀ temperature effects on relative stabilities of the IPR isomers. 1997 , 219, 193-200	47
1050	Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones. 1997 , 224, 143-155	80
1049	The use of maximum entropy statistics combined with simulation methods to determine the structure of 4-dimethylamino-3-cyanobiphenyl. 1997 , 68, 43-59	26
1048	Zur Komplexbildung neuer Podanden vom Bis(phenoxyalkyl)sulfan-Typ mit AgI und HgII. 1997 , 623, 340-346	3
1047	The Use of Structure Analysis Methods in Combination with Semi-empirical Quantum-Chemical Calculations for the Estimation of Quadratic Nonlinear Optical Coefficients of Organic Crystals. 1997 , 53, 603-614	19
1046	Charge-transfer complex formation and photo-induced electron-transfer reaction of dibenzo-7-silabicyclo[2.2.1]hepta-2,5-dienes. 1997 , 53, 1265-1274	10
1045	Unexpected stability of β -lactones with axial substituents rather than equatorial ones. Conformational evaluation by molecular mechanics and molecular orbital calculations. 1997 , 53, 2013-2024	9
1044	Cycloadditions to [60]fullerene using microwave irradiation: A convenient and expeditious procedure. 1997 , 53, 2599-2608	68
1043	Conformational analysis of 4-aryl-dihydropyrimidine calcium channel modulators. A comparison of ab initio, semiempirical and X-ray crystallographic studies. 1997 , 53, 2803-2816	352
1042	Studies on novel and chiral 1,4-dihydropyridines. IV. Mechanistic aspects of the asymmetric reduction with chiral NADH model compounds, (SS)-3-(p-tolylsulfinyl)-1,4-dihydropyridines. 1997 , 53, 3073-3082	15
1041	Asymmetric allylation of aromatic aldehydes catalyzed by chiral phosphoramides prepared from (S)-proline. 1997 , 53, 3513-3526	83
1040	Unexpected double benzylation of acetophenone under phase transfer catalysis conditions. Acidity or π -Interaction effect?. 1997 , 53, 3659-3668	11
1039	Cyclization of 1,5-dinitrile systems with hydrogen halides: A search for the undetected key tautomer. 1997 , 53, 4487-4496	3
1038	Total synthesis of balanol, part 2. Completion of the synthesis and investigation of the structure and reactivity of two key heterocyclic intermediates. 1997 , 53, 4857-4868	41
1037	Diastereomers of a cofacial ternaphthalene and two azaternaphthalenes. Syntheses and barriers to isomerization. 1997 , 53, 5379-5388	27

1036	Mediation of substituent effects via monoatomic SiMe ₂ , CMe ₂ and CH ₂ spacers. An NMR investigation. 1997 , 53, 5825-5830	3
1035	Factors Affecting Conformation of (R,R)-Tartaric Acid Ester, Amide and Nitrile Derivatives. X-Ray Diffraction, Circular Dichroism, Nuclear Magnetic Resonance and Ab Initio Studies. 1997 , 53, 6113-6144	49
1034	A new route to 2-oxazolines, bis-oxazolines, and 2-imidazoline-5-ones from imidates using solvent-free cycloadditions: Synthesis, chemical properties, and PM3 MO calculations. 1997 , 53, 6351-6364	33
1033	SOLUTION AND SOLID STATE STUDIES OF SOME NEW SILICON AND GERMANIUM COMPOUNDS STABILIZED BY TRIDENTATE LIGANDS. 1997 , 53, 10133-10154	19
1032	Novel heterocyclic dyes as DNA markers. Part II. Structure and biological activity. 1997 , 53, 12605-12614	6
1031	Selective derivatisation of resorcarenes: 1. The regioselective formation of tetra-benzoxazine derivatives. 1997 , 53, 10709-10724	64
1030	Ab initio study of formation and structure of double Diels-Alder cycloadduct derived from sequential pericyclic reactions of 2-pyrone with cycloocta-1,5-diene. 1997 , 53, 12415-12424	2
1029	Tautomeric and conformational preferences in nitraminopyridines: Comparison of theoretical and experimental data. 1997 , 53, 17211-17220	18
1028	NMR and semiempirical conformational analysis of the 2-aryl-1,3-dihydroxy-4,4,5,5-tetramethylimidazolidines. 1997 , 53, 16911-16922	7
1027	Crown compounds for anions. A new approach to the description of chemical bonds in the complexes of halide anions with polymcury-containing macrocycles. 1997 , 53, 413-424	38
1026	Phospholes with reduced pyramidal character from steric crowding III NMR and X-ray diffraction studies on 1-(2,4,6-tri-isopropylphenyl)-3-methylphosphole. 1997 , 53, 109-116	39
1025	Electronic structures of linear germanesilane copolymer radical anions [Me(SiMe ₂) _n (GeMe ₂) _n Me] (n = 3-7) in ground and low-lying excited states. A theoretical study. 1997 , 54, 337-341	3
1024	Complexation between a mixed methylalkenylcuprate and an alkyne. Further insight into the mechanism of organocopper additions to ynones. 1997 , 54, 591-595	14
1023	Restriction of the Inversion Process of the 1,3-Bridged Ring in the Rigid Conformer of 24-Methyl-2,17-Dithia[3.3](2,2')Biphenylene(1,3)Cyclophane. 1997 , 38, 2553-2556	5
1022	Electron-transfer reaction of 1,2-disila-3,5-cyclohexadienes. 1997 , 38, 3525-3528	6
1021	The first tandem inter-intramolecular catalytic asymmetric nitroaldol reaction utilizing a LnLi ₃ tris((R)-binaphthoxide) complex ((R)-LnLB) (Ln: Lanthanoid). 1997 , 38, 6031-6034	40
1020	[2.2.2]Metacyclophane-1,9,17-triyne. 1997 , 38, 6681-6684	35
1019	Theoretical simulation of resonance Raman bands of amorphous carbon. 1997 , 306, 17-22	16

1018	Staggered and eclipsed conformations of C ₂ F ₆ : A systematic ab initio study. 1997 , 83, 51-60	6
1017	¹³ C NMR studies of hydrochlorofluoropropanes and chlorofluoropropanes. 1997 , 84, 13-17	3
1016	Proton affinities of some polyfluoroalkanes in comparison to the unsubstituted alkanes. The estimation of the proton affinities of polytetrafluoroethylene and polyethylene by applying theoretical methods. 1997 , 82, 55-71	7
1015	Anomalous strengthening of the intramolecular hydrogen bond by steric repulsion. 1997 , 404, 67-74	15
1014	Structure and phenomenon relationships: a theoretical study. 1997 , 404, 87-90	0
1013	NMR spectroscopic and theoretical structural analysis of 5,5-disubstituted hydantoins in solution. 1997 , 403, 111-122	22
1012	Direct synthesis of organometallics V. Direct synthesis of isopropylcyclopentadienyl M(I) compounds of Ga, Tl, Mn and Cu via metal vapour cocondensation, and their spectroscopic characterization. 1997 , 408-409, 507-512	5
1011	Acyclic purine nucleoside analogues: computational and NMR studies of conformational behaviour. 1997 , 410-411, 31-33	1
1010	Conformational study and ground state dipole moments of two ketene dithioacetal compounds. 1997 , 405, 133-138	2
1009	A practical method for diffraction analysis of equilibrium geometries of molecules without refined force fields. 1997 , 413-414, 463-470	4
1008	Structure of dicyano-pyridinium methyldide and amidocyano-pyridinium methyldide using ab initio and semi-empirical methods. 1997 , 435, 35-47	13
1007	Intramolecular C ⁺ H ⁺ N hydrogen bond interactions in 1-(2-hydroxy-iminopyranosyl)pyrazoles. Results of crystallographic and semiempirical studies. 1997 , 436-437, 173-179	5
1006	Resonance Raman investigation and semi-empirical calculation of the natural carotenoid bixin. 1997 , 435, 101-107	23
1005	Conformational properties and electronic structure of tetrahydrotetrazines studied by photoelectron spectroscopy and quantum chemical calculations. 1997 , 435, 157-167	15
1004	Multiple Linear Regression (MLR) and Neural Network (NN) calculations of some disazo dye adsorption on cellulose. 1997 , 34, 181-193	23
1003	2-Amino-2-Oxazolines, Part VIII. Calculated Molecular Properties of Tautomeric Species. 1997 , 330, 367-371	9
1002	Spektroskopischer Nachweis und theoretische Untersuchungen eines 2:1-Brom-Olefin-Komplexes. 1997 , 109, 1339-1343	7
1001	[2+2]-Cycloaddukte von Tetrahydrodianthracen: experimenteller und theoretischer Nachweis außergewöhnlich langer C-C-Einfachbindungen. 1997 , 109, 1825-1828	16

1000	Enantioselective Synthese mit Lithium/(β -Sparte in-Carbanion-Paaren. 1997 , 109, 2376-2410	208
999	Stabilisierung von atomarem Stickstoff im Innenraum von C ₆₀ . 1997 , 109, 2858-2861	26
998	Strukturelle Reorganisation von Stilbenanalogen Verbindungen mit ausgedehnten π -Elektronensystemen durch Oxidation und Reduktion. 1997 , 109, 2926-2929	4
997	Study of bimolecular interactions by molecular modeling and surface acoustic wave device. 1997 , 9, 1054-1061	2
996	Multiple Adducts of C ₆₀ by Tether-Directed Remote Functionalization and synthesis of soluble derivatives of new carbon allotropes C _n (60+5). 1997 , 80, 317-342	77
995	TADDOLs under closer scrutiny – why bulky substituents make it all different. 1997 , 80, 2073-2083	9
994	Chemistry of Opium Alkaloids, XLIII – A PM3 Computational Approach to the Selectivity in the Diels-Alder Reactions of Thebaine and Analogues with Methyl Propenoate. 1997 , 1997, 13-19	3
993	Addition and Cycloaddition Reactions of Arenediazonium Ions with 1,3-Dienes: A Shift From a Concerted to a Stepwise Mechanism. 1997 , 1997, 71-80	15
992	The Effect of Pressure on the Cycloadditions of Cyanoacetylene to Furan Derivatives – [2.2](2,5)Furanoparacyclophane, [8](2,5)Furanophane, and Furan. 1997 , 1997, 127-137	5
991	Synthesis of Sterically Rigid Macrocycles by The Use of Pressure-Induced Repetitive Diels-Alder Reactions. 1997 , 1997, 501-516	24
990	Highly Selective Alkylation of 5-Amino-1-methyl-1H-1,2,4-triazole with 1-(1-Chloroalkyl)pyridinium Chlorides under Formation of Novel Geminal Bis(heteroarylium) Salts: A Combined Experimental/MO-Theoretical Study. 1997 , 1997, 745-752	14
989	Diels-Alder Reactions of Tetradehydroanthracene with Electron-Deficient Dienes. 1997 , 1997, 1473-1479	9
988	Direct Iodination of Sydnones and Their Cycloadditions to Form 5-Iodopyrazoles. 1997 , 1997, 2613-2616	19
987	Gas phase thermolysis of pyrazolines. 5. Electronic structure and gas phase thermolysis of tetrazole derivatives studied by photoelectron spectroscopy. 1997 , 34, 113-122	23
986	1,3-Dipolar cycloaddition reactions of cyclooctyne with pyridinium dicynomethylides. 1997 , 34, 203-208	7
985	Bicyclic [b]-heteroannulated pyridazine derivatives. 4. Cyclization reactions of 4-aryl-tetrahydropyridazine-3,6-dione 3-hydrazones with some keto esters. 1997 , 34, 389-396	8
984	Molecular structure and electronic spectrum of ellagic acid: Semiempirical molecular orbital calculations. 1997 , 34, 665-667	6
983	Synthesis of pteridine derivatives related to folic acid and methanopterin from pyrazine-2,3-dicarbonitrile. 1997 , 34, 973-981	7

982	Singlet and triplet photocycloaddition reactions of 2-pyridones with propenoate and 2,4-pentadienones, and the frontier molecular orbital analysis. 1997 , 34, 1005-1011		5
981	Reactions of O-methyl o-quinone monoximes with methyl-, methylene- and methine- substituted aromatic compounds. Synthesis of benzo[d]oxazole and 1,4-benzoxazine derivatives. 1997 , 34, 1651-1656		7
980	Acid-Base Properties of Adenosine 5'-O-Thiomonophosphate in Aqueous Solution. 1997 , 3, 29-33		36
979	Investigations into the biosynthesis of porphyrins and corrins calculations on 1,3-allylic strain and [1,5]-sigmatropic rearrangements in pyrroles, furans, and thiophenes. 1997 , 3, 523-529		12
978	Acid-Catalyzed degradation mechanism of poly(phthalaldehyde): Unzipping reaction of chemical amplification resist. 1997 , 35, 77-89		34
977	A computational study of a host-guest complex. 1997 , 10, 159-68		3
976	MECHANISTICALLY OPTIMIZED INTRAMOLECULAR CATALYSIS IN THE HYDROLYSIS OF ESTERS. GLOBAL CHANGES INVOLVED IN MOLECULAR REACTIVITY. 1997 , 10, 461-465		8
975	Photoinduced intramolecular electron transfer in dichromophore-appended α -helical peptides: spectroscopic properties and preferred conformations. 1997 , 10, 484-498		18
974	Cobalt(III) Porphyrin-catalysed Hydride Reduction of 10-Methylacridinium ion and Hydrometallation of Alkenes and Alkynes by Tributyltin Hydride. 1997 , 01, 251-258		7
973	Sites of Action of Noncompetitive GABA Antagonists in Houseflies and Rats: Three-Dimensional QSAR Analysis. 1997 , 49, 319-332		27
972	Stereochemistry and active conformation of a novel insecticide, acetamiprid. 1997 , 51, 157-164		18
971	A computational analysis of interaction energies in methane and neopentane dimer systems. <i>Journal of Computational Chemistry</i> , 1997 , 18, 70-79	3.5	19
970	Quantum-mechanical and molecular mechanics conformational analysis of 1,5-cyclooctadiene. <i>Journal of Computational Chemistry</i> , 1997 , 18, 254-259	3.5	17
969	Ab initio and density functional study of the conformational space of 1C4 β -L-fucose. <i>Journal of Computational Chemistry</i> , 1997 , 18, 330-342	3.5	37
968	Proton affinities of polybenzenoid aromatic hydrocarbons and those with five-membered rings. <i>Journal of Computational Chemistry</i> , 1997 , 18, 629-637	3.5	13
967	Transfer of molecular property tensors in cartesian coordinates: A new algorithm for simulation of vibrational spectra. <i>Journal of Computational Chemistry</i> , 1997 , 18, 646-659	3.5	199
966	VESPA: A new, fast approach to electrostatic potential-derived atomic charges from semiempirical methods. <i>Journal of Computational Chemistry</i> , 1997 , 18, 744-756	3.5	34
965	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio Hartree-Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree-Fock results. 1997 , 18, 1136-1150		239

964	Coupled semiempirical molecular orbital and molecular mechanics model (QM/MM) for organic molecules in aqueous solution. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1496-1512	3.5	62
963	Calculation of molecular vibrations: Selective scaling factors for semiempirical force constants. <i>Journal of Computational Chemistry</i> , 1997 , 18, 2050-2059	3.5	14
962	A theoretical study of bond energies in model SiH ₄ Cl molecules using density functional approaches for representing Si surface chemistry. <i>Journal of Computational Chemistry</i> , 1997 , 18, 2075-2085	3.5	4
961	Acetyl-CoA enolization in citrate synthase: A quantum mechanical/molecular mechanical (QM/MM) study. 1997 , 27, 9-25		89
960	The reaction pathway of the isomerization of D-xylose catalyzed by the enzyme D-xylose isomerase: a theoretical study. 1997 , 27, 545-55		29
959	Role of electrostatics at the catalytic metal binding site in xylose isomerase action: Ca(2+)-inhibition and metal competence in the double mutant D254E/D256E. 1997 , 28, 183-93		18
958	A temperature dependence study of the gas-phase reaction of the nitrate radical with 3-fluoropropene followed by laser induced fluorescence detection. 1997 , 29, 927-932		9
957	Calculations of the structure and electronic properties of extended polar hydrocarbons. 1997 , 61, 991-996		11
956	Electronic structure of testosterone: A semiempirical and ab initio assessment. 1997 , 62, 279-289		7
955	Complexes between divalent metals and carboxylic acids: Semiempirical study. 1997 , 62, 653-658		5
954	Long-range electronic interactions in androstanediones. 1997 , 63, 797-803		1
953	A semiempirical study on the ring-opening process for the cyclopropanone, 2,2-dimethylcyclopropanone, trans-2,3-di-tert-butylcyclopropanone, and spiro(bicyclo[2.2.1]heptane-2.1'-cyclopropan)-2'-one systems in solution. 1997 , 65, 729-738		4
952	Dimerization of dexanabinol by hydrogen bonding accounts for its hydrophobic character. 1997 , 65, 1057-1064		9
951	The x-ray structure determinations and semiempirical PM3 calculations of two chloro(piperidyl)cyclotri(phosphazenes). 1997 , 8, 267-271		3
950	The x-ray structure determination and semiempirical PM3 calculations of 2,4,4,6,6-pentachloro-2-(piperidyl)cyclotri(phosphazene). 1997 , 8, 283-286		1
949	Structures of dibenzocycloheptenylidene- and fluorenylidene-(2,4,6-tri-t-butylphenyl)phosphines and their reactions with sulfur. 1997 , 8, 375-382		11
948	Normal coordinate analysis and vibrational spectra of adenosine. 1997 , 3, 47-59		24
947	Identifying the Intermediate in the Dioxygen Transfer from 4a-Hydroperoxyflavin Anion to Phenolate and Indole Anions. 1997 , 25, 331-336		4

946	Studies on alpha-sialylation using sialyl donors with an auxiliary 3-thiophenyl group. 1997 , 302, 123-9	23
945	Comparative study on the vibrational IR spectra of cytosine and thiocytosine by various semi-empirical quantum mechanical methods. 1997 , 264, 92-100	6
944	Electronic structures of linear polysilane radical cations in ground and low-lying excited states: a theoretical study. 1997 , 265, 455-459	10
943	Enthalpies of formation of cyclic alkyl peroxides: dioxirane, 1,2-dioxetane, 1,2-dioxolane, and 1,2-dioxane. 1997 , 268, 175-179	13
942	Models of the stable dumbbell-like C120 cluster and crimped nanotubes constructed from C60 fullerenes. 1997 , 269, 85-87	9
941	Electronic transition moment directions and tautomerization of 9,10,19,20-tetra-n-propylporphycene. 1997 , 271, 341-348	12
940	Electronic structures of linear polysilane radical anions for ground and low-lying excited states: a theoretical study. 1997 , 281, 221-225	8
939	Protonation effects on the chromophore of green fluorescent protein. Quantum chemical study of the absorption spectrum. 1997 , 272, 162-167	82
938	Anodic oxidation of carbamates using organothio groups as electroauxiliaries. 1997 , 42, 1995-2003	31
937	Role of heteropolar bonds in OCM-2 oligocarbonatemetacrylate. 1997 , 33, 1441-1447	26
936	Mixed aggregation between lithium diisopropylamide and lithium chloride: NMR, solid-state structure and ab initio calculations. 1997 , 258, 1-9	12
935	Molecular orbital simulations on electron-induced degradation of perfluoropolyethers with several types of segments. 1997 , 30, 121-128	8
934	Charge transfer complexes and electron transfer reaction of organosilicon and related compounds. 1998 , 176, 87-112	16
933	Electronic charge density distributions in tetrathiafulvalene derivatives. 1998 , 34, 455-462	2
932	Benzene/Si(100): metastable chemisorption and binding state conversion. 1998 , 282, 305-312	99
931	Is a 1.90 Å bond length in polymeric fullerenes possible?. 1998 , 282, 318-324	17
930	Electron-energy-loss spectroscopy of solid phenylacetylene. 1998 , 285, 246-251	9
929	Elementary processes in pressure-induced polymerization of C60. 1998 , 285, 289-293	24

928	Theoretical study of the radiationless decay channels of triplet state norbornene. 1998 , 287, 601-607	9
927	Molecular structure of the fullerene C70 at 825°C:: quantum-chemical molecular dynamics simulations. 1998 , 288, 183-187	3
926	X-ray spectroscopic and quantum-chemical study of carbon tubes produced in arc-discharge. 1998 , 289, 341-349	16
925	Electron beam induced fragmentation of fullerene derivatives. 1998 , 289, 586-590	33
924	Excited-state intramolecular proton transfer in anthralin.. 1998 , 291, 51-56	21
923	Role of the intramolecular hydrogen bond and ligand rigidity in the complexation of trifluoroacetylcycloalkanones with lanthanides: novel strategy for the design of organic ligands of high selectivity. 1998 , 267, 201-207	9
922	A linear open-chain piperazine-pyridine ligand and its meso-helical Co complex. 1998 , 277, 55-60	20
921	A Theoretical Approach to the Description of the Thermal Dissociation of N,N,N-Trimethylmethanaminium Halides. 1998 , 54, 189-195	7
920	Carbon particle phase stability as a function of size. 1998 , 5, 279-294	63
919	A quantum-chemical study of the formation mechanism and nature of tert-butyl carbenium ions in 100% sulfuric acid. 1998 , 55, 7-14	11
918	ORGANOPHOSPHOROUS CHEMISTRY: SELECTIVE TRANSFORMATION OF BENZOIN TO BENZIL, DESYL BROMIDE, OR BENZYL PHENYL KETONE. 1998 , 143, 85-99	
917	Diversity of excited state deactivation paths in heteroazaaromatics with multiple intermolecular hydrogen bonds. 1998 , 102, 469-475	19
916	Flavonols and Crown-Flavonols as Metal Cation Chelators. The Different Nature of Ba ²⁺ and Mg ²⁺ Complexes. 1998 , 102, 5907-5914	140
915	Mechanism of Micelle to Vesicle Transition in Cationic-Anionic Surfactant Mixtures. 1998 , 14, 3778-3782	76
914	Rational de novo design of NADH mimic for stereoselective reduction based on molecular orbital calculation. 1998 , 54, 705-714	8
913	Dialkylation of acetophenones and acetophenone ethylene ketals with 1,8-bis(trimethylsilyl)-2,6-octadiene (BISTRO). Semi-empirical SCF studies of β -methoxy- β -methylbenzyl cations. 1998 , 54, 2075-2086	6
912	Synthesis of (-)-B(9a)-Homo-C-nor-3-methoxy-12-oxa-17-vinylestra-1,3,5(10)-trienes. 1998 , 54, 13805-13812	15
911	Synthesis of angular triquinanes from (+)- β -cedrol. 1998 , 54, 14803-14810	7

- 910 Enhanced endo selectivity in 1,3-dipolar cycloaddition of pyrazolone N,N -dioxides with dipolarophiles having ether and carbonyl groups. Role of the remarkably long N-N bond. **1998**, 39, 2761-2764 9
- 909 New phototautomerizing systems: non-symmetric derivatives of [2,2'-bipyridyl]-3,3'-diol. **1998**, 291, 351-359 23
- 908 Intramolecular proton-transfer cycle of 2,4-dimethoxy-6-(1-hydroxy-2-naphthyl)-s-triazine studied by laser photolysis. **1998**, 231, 205-214 7
- 907 Fragmentation of semiconductor and metallic clusters. Calculations of a quantum mechanical type. **1998**, 142, 17-29 2
- 906 Electronic structure and optical spectra of MDF-2 oligoetheracrylate. **1998**, 56, 7-13 15
- 905 Quantum chemical approach to isomerization of 1,2-dihydro-1,2-epoxybenzene and its derivatives involving hydration. **1998**, 422, 1-12
- 904 Molecular structure of divalent metal ion fulvic acid complexes. **1998**, 423, 203-212 8
- 903 Electronic structure of chromone and its hydroxylated derivatives on positions 2 and 3. **1998**, 423, 235-243 17
- 902 Computational design of clay minerals: hydration of Mg-exchange cation located in ditrigonal cavity. **1998**, 425, 129-135 13
- 901 Investigation of the structure and the properties of the potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in the gas and aqueous phases using semiempirical methods. **1998**, 427, 65-77 8
- 900 Solvation dynamics of the fluorenone radical anion by methanol: a direct MO dynamics study. **1998**, 427, 191-198 1
- 899 On the origin of long-lived spin isomerism in π -conjugated non-Kekulé molecules. **1998**, 424, 21-27 6
- 898 Semi-empirical atomic charges and dipole moments in hypervalent sulfonamide molecules: descriptors in QSAR studies. **1998**, 428, 109-121 12
- 897 A PM3 theoretical study of the adsorption and dissociation of water on MgO surfaces. **1998**, 426, 199-205 10
- 896 A theoretical study of the addition of CH_3MgCl to chiral β -alkoxy carbonyl compounds. **1998**, 426, 263-275 3
- 895 A PM3 semiempirical study of the molecular mechanism for the Favorskii rearrangement of the β -chlorocyclobutanone. **1998**, 426, 299-306 3
- 894 Alkaline hydrolysis of N-methylazetidin-2-one. Hydration effects. **1998**, 426, 313-321 11
- 893 Theoretical studies on the biocidal activity of 5-chloro-3-isothiazolone. **1998**, 429, 103-110 29

892	Modulation of the proton-transfer equilibrium of the adducts between 2-hydroxy-p-quinones and 4-(N,N-dimethyl)aminopyridine: a semiempirical MO study. 1998 , 429, 197-206	4
891	Toward a platelet-activating factor pseudoreceptor: Semiempirical modeling of cation- π and hydrogen bond interactions in agonist binding. 1998 , 429, 217-227	4
890	Ab initio calculations in tricyclo[3,3,1,13,7]decane, tricyclo[3,3,1,13,7]decsilane and their silicon-carbon mixed derivatives, C10 H _n Si _n H ₁₆ (n = 0, 4, 6, 10). 1998 , 432, 105-113	1
889	A computational study of imidazole, 4-nitroimidazole, 5-nitroimidazole and 4,5-dinitroimidazole. 1998 , 432, 41-53	37
888	Theoretical study of hydrogen bonding in the 1-hydroperoxy-1-(p-nitrophenyl) ethanol. 1998 , 433, 227-230	
887	On the geometry of 3-amino-sydnones. 1998 , 433, 291-299	3
886	Theoretical study of cis- and trans-3,6-dimethoxy-1,2,4,5-tetroxane molecule. 1998 , 433, 311-317	4
885	Nonlinear optical properties of push pull molecules grafted onto chloromethylstyrene. Hyperpolarizabilities of first- and second-order obtained by PM3, AM1 and MNDO methods. Correlation of EFISH measures on side-chain polymer with quantum chemistry results. 1998 , 451, 277-293	5
884	Effects of hydration on the molecular structure of divalent metal ion-fulvic acid complexes: a MOPAC (PM3) study. 1998 , 431, 267-275	4
883	Hartree-Fock and density functional studies on the molecular structure of (E)-2-methoxy-4-[2-(4-nitrophenyl)ethenyl]-phenol. 1998 , 432, 161-167	1
882	NMR-K reduced coupling constant calculations within the CLOPPA-PM3 approach: I. General results. 1998 , 452, 1-11	15
881	NMR-K reduced coupling constants within the CLOPPA-PM3 approach. II: shortcomings and how to overcome them. 1998 , 452, 13-23	17
880	PM3 semi-empirical study of stereoelectronic effects in the Baeyer-Villiger reaction. 1998 , 434, 183-191	16
879	Semiempirical quantum chemical methods: testing of thermodynamic and molecular properties of cyclic non-aromatic hydrocarbons and unsaturated heterocycles. 1998 , 453, 7-15	18
878	Molecular orbital modeling of solvent effects on excited states of organic molecules. 1998 , 453, 49-57	5
877	Ab initio study of solvent effects on the structure and vibrational frequencies of methyl nitrate. 1998 , 453, 141-147	4
876	Are mutated enzymes good models for interpretation of intrinsic isotope effects?. 1998 , 454, 69-75	6
875	Investigation of the structure and properties of the potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and aqueous phases using the AM1 and PM3/COSMO solvation method. 1998 , 430, 85-95	9

874	Distamycin-NA: A DNA Analog with an Aromatic Heterocyclic Polyamide Backbone. Part 1. Synthesis and structural analysis of monomers and dimers containing the nucleobase uracil. 1998 , 81, 14-34	5
873	Hydrolysis of genotoxic methyl-substituted oxiranes: Experimental kinetic and semiempirical studies. 1998 , 17, 2141-2147	14
872	Photoelectron-Spectrum and Electronic Structure of Perfluoro(2,4-dimethyl-3-oxa-2,4-diazapentane) (CF ₃) ₂ N ₂ O(CF ₃) ₂ . 1998 , 1998, 1377-1380	1
871	. 1998 , 1998, 585-592	11
870	. 1998 , 1998, 1231-1236	8
869	First Synthesis and Investigation of Two Hydroxyalkyl-Substituted 2-Tetrazenes. 1998 , 1998, 1431-1440	6
868	Structure/Chiroptics Relationships of Planar Chiral and Helical Molecules. 1998 , 1998, 1491-1509	182
867	. 1998 , 1998, 1629-1637	29
866	. 1998 , 1998, 1759-1762	14
865	Generation and Diels-Alder Trapping of 4,5-Bis(bromomethylene)-4,5-dihydrothiazole. 1998 , 1998, 2047-2050	4
864	Synthesis of Enantiomerically Pure trans-1,2-Disubstituted Cyclopentanes and Cyclohexanes by Intramolecular Allylsilane Addition to Chiral Alkylidene-1,3-dicarbonyl Compounds. 1998 , 1998, 2089-2099	17
863	Stereoselective Intramolecular Hetero Diels-Alder Reactions of Cyclic Benzylidenesulfoxides and DFT Calculations on the Transition Structures. 1998 , 1998, 2733-2741	27
862	Syntheses of a Novel Class of 5/6/5-Heterocycles: Convenient Routes from Aldehydes to Bis(1,3,4-thiadiazolo)-1,3,5-triazinium Halides. 1998 , 1998, 2923-2930	9
861	Changes of structure and energy on the route from dioxetane to carbonyl products. A quantum chemical study. 1998 , 13, 69-74	10
860	Theoretical studies on the gas-phase nucleophilic substitution reactions of benzyl chlorides with phenoxides and thiophenoxides. 1998 , 11, 115-124	9
859	Base-catalysed hydrolysis of lactones: reactivity-structure correlations for 3-(substituted phenoxy- and thiophenoxymethylene)-(Z)-1(3H)-isobenzofuranones. 1998 , 11, 467-474	3
858	Conformational analysis of substituted 5,6,7,8-tetrahydrodibenzo[a,c]cyclo-octene: comparison of ¹ H NMR, molecular mechanics and semiempirical methods. 1998 , 11, 781-786	5
857	Synthese des Trinaphthophenaleniumions. 1998 , 110, 95-96	1

856	Triphenylphosphonioacetylid: eine mit Isocyaniden isovalenzelektronische Spezies. 1998 , 110, 347-351		6
855	Gemischte Liganden aus Elementen der 5. und 6. Hauptgruppe: Schnittstelle zwischen Festkörper- und Molekülchemie. 1998 , 110, 782-800		29
854	Eine spontane Fragmentierung vom Criegee-Zwitterion zur 'eingeschnittenen' Möbius-Aromatizität. 1998 , 110, 1951-1954		4
853	Das thermische Verhalten der Spiroozonide aus Formaldehyd-O-oxid und Troponderivaten: eine eingeschnittene Reaktion. 1998 , 110, 1954-1957		5
852	Dynamisches Verhalten von organischen reaktiven Intermediaten. 1998 , 110, 3532-3543		22
851	Convenient Catalytic Synthesis and Assignment of the Absolute Configuration of Enantiomerically Pure Dihydronaphthalenes and Their Corresponding Epoxides. 1998 , 4, 1944-1951		16
850	Synthesis of the Trinaphthophenalenium Cation. 1998 , 37, 90-91		4
849	Parallel Differentiated Recognition of Ketones and Acetals. 1998 , 37, 91-93		23
848	A Spontaneous Fragmentation: From the Criegee Zwitterion to Coarctate Möbius Aromaticity. 1998 , 37, 1850-1853		16
847	Dynamic Behavior of Organic Reactive Intermediates. 1998 , 37, 3340-3350		147
846	Electronic Properties of Nanosize Silicon-Dioxygen Clusters. 1998 , 165, 57-61		1
845	Quantitative correlation between molecular similarity and receptor-binding activity of neonicotinoid insecticides. 1998 , 52, 104-110		22
844	Quantitative structure-Activity studies of insect growth regulators xiv. Three-dimensional quantitative structure-Activity relationship of ecdysone agonists including dibenzoylhydrazine analogs. 1998 , 53, 267-277		42
843	Prediction of the binding mode of imidacloprid and related compounds to house-fly head acetylcholine receptors using three-dimensional QSAR analysis. 1998 , 54, 134-144		47
842	Quantum mechanical/molecular mechanical self-consistent Madelung potential method for treatment of polar molecular crystals. <i>Journal of Computational Chemistry</i> , 1998 , 19, 38-50	3.5	23
841	Evaluation of reactivity for nitroxide radical trapping by correlation analysis using steric substituent parameter (S). <i>Journal of Computational Chemistry</i> , 1998 , 19, 215-221	3.5	14
840	Comparison of ab initio and density functional methods for vibrational analysis of TeCl ₄ . <i>Journal of Computational Chemistry</i> , 1998 , 19, 308-318	3.5	9
839	Quantum chemical studies on structures and spectra of 2,5-distyrylpyrazine (DSP) laser dye. <i>Journal of Computational Chemistry</i> , 1998 , 19, 585-592	3.5	2

838	Solvation free energies calculated using the GB/SA model: Sensitivity of results on charge sets, protocols, and force fields. <i>Journal of Computational Chemistry</i> , 1998 , 19, 769-780	3.5	36
837	Parallel implementation of divide-and-conquer semiempirical quantum chemistry calculations. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1101-1109	3.5	17
836	Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/vinylamine systems. 1998 , 66, 9-24		28
835	Theoretical studies on the structure and electronic properties of aryl sulfides and sulfones. 1998 , 66, 141-147		7
834	Theoretical study of fullerene derivatives: C ₂₈ H ₄ and C ₂₈ X ₄ cluster molecules. 1998 , 67, 187-197		21
833	Theoretical study of aminoalkylation in the Mannich reaction of furan with methyleneiminium salt. 1998 , 67, 359-366		2
832	Theoretical study of fullerene derivatives: C ₄₀ H ₄ and C ₄₀ X ₄ cluster molecules. 1998 , 68, 273-284		8
831	CO ₂ and NH ₃ interaction with ZnO surface: An AM1 study. 1998 , 70, 367-374		15
830	GROMOS-MD simulations on the coenzyme thiamin diphosphate in apoenzyme environment. 1998 , 70, 407-413		5
829	Cyclic anhydride ring opening reactions: theory and application. 1998 , 41, 8-17		8
828	Conformational behavior on 2,2,3-trisubstituted 1,2,3,4-tetrahydroquinoline alkaloids, virantmycin, benzastatins, and their congeners, evaluated by semi-empirical molecular orbital calculations. 1998 , 35, 279-284		7
827	Substitution reactions of phenanthro[9,10-d]triazole with benzyl chlorides. 1998 , 35, 365-369		5
826	Asymmetric imine-ene reactions: diastereofacial selective reactions with chiral glyoxylate-derived alpha-imino esters and asymmetric catalysis of enantiofacial selective reactions with prochiral alpha-imino esters. 1998 , 14, 311-8		10
825	Quantum chemical study of 2-substituted 4-oxo-and 4-thioxospiro(benzo[h]quinazoline-5,1'-cycloalkanes) in alkylation reactions. 1998 , 34, 964-970		
824	Simulation of molecular and electronic structure of π - π -complexes of fullerene I _h -C ₆₀ with half-sandwich XCp species (X=Si, Ge, Sn). 1998 , 47, 2087-2097		8
823	Molecular and electronic structures of some trimers of polyhedral carbon clusters. 1998 , 47, 1-7		3
822	The ESR study of the structure and reactivity of β -ketoradicals, derivatives of (CF ₃) ₃ CC(O)C(O)CF ₃ . 1998 , 47, 60-65		1
821	MNDO/PM3 study of the mechanism of a model reaction between methane and Br ⁺ cation. 1998 , 47, 1666-1669		1

820	Indium-containing heterofullerenes and their π - π complexes. 1998 , 47, 851-854	1
819	Fast and reversible migrations of N,S-centered groups around the perimeter of cyclopropene and cycloheptatriene rings. 1998 , 47, 884-894	11
818	Role of water traces in the liquid-phase catalytic hydrochlorination of olefins in organic solvents. 1998 , 47, 243-246	1
817	Quantum chemical analysis of the effect of the outer-spheric cation on the electronic state of the tin atom and isomer shift in hexafluorostannates. 1998 , 39, 125-127	
816	Resolution of racemic R,S- α -arylethylamine by a new resolving agent (R)thiazolidine-2-thione-4-carboxylic acid. 1998 , 41, 361-370	1
815	PM3 computation for the DNA complementary base pair cross-linked by the metabolite of Benzo[a]pyrene. 1998 , 43, 175-175	
814	Reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines. 1998 , 34, 1050-1065	
813	Determination of consistent semiempirical one-centre integrals based on coupled-cluster theory. 2017 , 115, 538-544	5
812	Effect of mutation on the stabilization energy of HIV-1 zinc fingers: a hybrid local self-consistent field/molecular mechanics investigation. 2017 , 22, 109-119	5
811	Modulating hydrogen-bond basicity within the context of protein-ligand binding: A case study with thrombin inhibitors that reveals a dominating role for desolvation. 2017 , 125, 975-991	6
810	Exploring potential energy surfaces of biological molecules using a Multi-Niche Crowding genetic algorithm. 2017 , 17, 595-609	1
809	Excited state molecular polarizability estimated by solvatochromic means. 2017 ,	1
808	A peony-leaves-derived liquid corrosion inhibitor: protecting carbon steel from NaCl. 2017 , 10, 359-379	11
807	Investigation of naproxen drug using mass spectrometry, thermal analyses and semi-empirical molecular orbital calculation. 2017 , 10, 351-359	5
806	Cation, Anion and Ion-Pair Complexes with a G-3 Poly(ethylene imine) Dendrimer in Aqueous Solution. 2017 , 22,	2
805	Synthesis, Structure, Surface and Antimicrobial Properties of New Oligomeric Quaternary Ammonium Salts with Aromatic Spacers. 2017 , 22,	19
804	Semiempirical Theoretical Studies of 1,3-Benzodioxole Derivatives as Corrosion Inhibitors. 2017 , 2017, 1-10	5
803	Computational Studies of Supramolecular Systems: Resorcinarenes and Pyrogallolarenes. 2017 , 303-342	2

802	Analysis of the retention behavior of selected antipsychotics and their impurities by thin-layer chromatography. 2017 , 30, 340-349		2
801	Alkylaromatics in Detergents Manufacture: Modeling and Optimizing Linear Alkylbenzene Sulfonation. 2018 , 21, 175-184		8
800	Investigation of indole chalcones encapsulation in β -cyclodextrin: determination of stoichiometry, binding constants and thermodynamic parameters. 2018 , 90, 305-320		2
799	Unimolecular Fragmentation of Deprotonated Diproline [Pro-H] Studied by Chemical Dynamics Simulations and IRMPD Spectroscopy. 2018 , 122, 2612-2625		17
798	Automated error control in divide-and-conquer self-consistent field calculations. <i>Journal of Computational Chemistry</i> , 2018 , 39, 909-916	3.5	10
797	Molecular modeling and cyclization reactions of 2-(4-oxothiazolidine-2-ylidene) acetonitrile. 2018 , 15, 1243-1254		3
796	Random versus Systematic Errors in Reaction Enthalpies Computed Using Semiempirical and Minimal Basis Set Methods. 2018 , 3, 4372-4377		9
795	An efficient implementation of semiempirical quantum-chemical orthogonalization-corrected methods for excited-state dynamics. 2018 , 148, 154103		16
794	Exciton Dynamics from Strong to Weak Coupling Limit Illustrated on a Series of Squaraine Dimers. 2018 , 122, 8082-8093		33
793	Adsorption of basic dyes onto activated carbon: Experimental and theoretical investigation of chemical reactivity of basic dyes using DFT-based descriptors. 2018 , 448, 662-670		72
792	Theoretical Studies on the Catalytic Mechanism and Substrate Diversity for Macrocyclization of Pikromycin Thioesterase. 2018 , 8, 4323-4332		33
791	The evaluation of Cr-curcumin-DNA complexation by experimental and theoretical approaches. 2018 , 37, 35-52		6
790	Sugar moiety has a synergistic effect on hydroxylated xanthone for better antioxidant activity of mangiferin. 2018 , 27, 1276-1282		11
789	Photoferroelectricity in di-phenylalanine peptide nanotubes. 2018 , 14, 94-100		3
788	Synthesis, X-Ray diffraction, theoretical and anti-bacterial studies of bis-thiourea secondary amine. 2018 , 1159, 96-102		7
787	Interpretation of ANN-based QSAR models for prediction of antioxidant activity of flavonoids. <i>Journal of Computational Chemistry</i> , 2018 , 39, 953-963	3.5	28
786	Structural determinants in the bulk heterojunction. 2018 , 20, 5708-5720		3
785	Nucleic Bases Alkylation with Acrylonitrile and Cyanoethylene Oxide: A Computational Study. 2018 , 31, 97-104		7

784	TGA, Hirshfeld, Raman spectroscopy and computational studies of diethylammonium hexachloroplumbate [(C ₂ H ₅) ₂ NH ₂] ₂ PbCl ₆ . 2018 , 1157, 621-630	4
783	Designing of calixarene based drug carrier for dasatinib, lapatinib and nilotinib using multilevel molecular docking and dynamics simulations. 2018 , 90, 157-169	8
782	One pot synthesis, X-ray crystal structure of 2-(2'-hydroxyphenyl)oxazolo[4,5-b]pyridine derivatives and studies of their optical properties. 2018 , 1157, 119-126	3
781	Atom-Centered Potentials with Dispersion-Corrected Minimal-Basis-Set Hartree-Fock: An Efficient and Accurate Computational Approach for Large Molecular Systems. 2018 , 14, 726-738	14
780	Modeling molecular boiling points using computed interaction energies. 2017 , 24, 21	1
779	The structures of liquid pyridine and naphthalene: the effects of heteroatoms and core size on aromatic interactions. 2018 , 20, 2704-2715	14
778	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. 2018 , 122, 869-877	15
777	Synthesis and comparison of mesomorphic behaviour of a cholesterol-based liquid crystal dimer and analogous monomers. 2018 , 45, 1164-1176	12
776	Overview of Computational Methods for Organic Chemists. 2018 , 31-67	3
775	Photo-Driven Chirality Switching in a Dark Conglomerate Phase of an Achiral Liquid Crystal Trimer. 2018 , 3, 3278-3283	5
774	A Direct, Quantitative Connection between Molecular Dynamics Simulations and Vibrational Probe Line Shapes. 2018 , 9, 2560-2567	20
773	NAMD goes quantum: an integrative suite for hybrid simulations. 2018 , 15, 351-354	88
772	A chemical rationalization of the processing and application of the mortar coatings: Structural, thermodynamic, and fluorescence properties. 2018 , 1164, 546-555	5
771	Generating Converged Accurate Free Energy Surfaces for Chemical Reactions with a Force-Matched Semiempirical Model. 2018 , 14, 2207-2218	25
770	A novel tetra-stilbene-based fluorescent compound: Synthesis, characterization and photophysical properties evaluation. 2018 , 199, 165-173	10
769	Experimental and theoretical investigations of a newly synthesized azomethine compound as inhibitor for mild steel corrosion in aggressive media: A comprehensive study. 2018 , 259, 199-208	17
768	Modeling Protein S-Aromatic Motifs Reveals Their Structural and Redox Flexibility. 2018 , 122, 3760-3770	18
767	Furoxan Derivatives of Pyrene: A DFT Study. 2018 , 38, 257-271	3

766	QSAR, DFT and molecular modeling studies of peptides from HIV-1 to describe their recognition properties by MHC-I. 2018 , 36, 2312-2330	7
765	Contemplation on some cyclic N 8 isomers-A DFT treatment. 2018 , 14, 19-27	9
764	Computational study of the phosphoryl donor activity of dihydroxyacetone kinase from ATP to inorganic polyphosphate. 2018 , 118, e25520	2
763	A DFT study on TNGU isomers and aluminized cis-TNGU composites. 2018 , 14, 109-118	1
762	Schiff-base derivatives as corrosion inhibitors for carbon steel materials in acid media: quantum chemical calculations. 2018 , 53, 36-43	10
761	A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor. 2018 , 116, 323-337	0
760	Synthesis, chematin inhibition studies and antimalarial evaluation of new dehydroxy isoquine derivatives against Plasmodium berghei: A promising antimalarial agent. 2018 , 148, 498-506	9
759	Theoretical approaches for dynamical ordering of biomolecular systems. 2018 , 1862, 212-228	5
758	Reaction profiling of a set of acrylamide-based human tissue transglutaminase inhibitors. 2018 , 79, 157-165	3
757	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. 2018 , 8, 815-827	4
756	Effect of magnesium on FOX-7 and its tautomers-A DFT treatment. 2018 , 14, 179-187	2
755	Synthesis and preliminary structure-activity relationship study of 2-aryl-2H-pyrazolo[4,3-c]quinolin-3-ones as potential checkpoint kinase 1 (Chk1) inhibitors. 2017 , 33, 171-183	5
754	Synthesis, structural configuration and DFT molecular orbital studies of [Mn-2[benzo[b]oxazole] acetonitrile] complexes encapsulated in ZSM-5: Direct synthesis of phenol by benzene hydroxylation. 2018 , 262, 35-48	5
753	Rigorous and Empirical Approaches to Correlated Single-Particle Theories. 2018 , 1-20	1
752	Theoretical study: Electronic structure and receptor interaction of four type bis-1,4-dihydropyridine molecules. 2018 , 1123, 102-110	0
751	Charge calculation studies done on a single walled carbon nanotube using MOPAC. 2018 , 92, 479-485	4
750	Fast and accurate prediction of the regioselectivity of electrophilic aromatic substitution reactions. 2018 , 9, 660-665	39
749	Mechanistic Insights on Human Phosphoglucomutase Revealed by Transition Path Sampling and Molecular Dynamics Calculations. 2018 , 24, 1978-1987	7

748	Quantum chemical investigation of new model bent-shaped bis-azomethines for nonlinear optics applications. 2018 , 671, 113-127	2
747	Correlation between photochemical reaction and structural feature of benzyliden derivatives. 2018 , 673, 16-22	
746	Bibliography. 2018 , 209-228	
745	Dual QM and MM Approach for Computing Equilibrium Isotope Fractionation Factor of Organic Species in Solution. 2018 , 23,	2
744	New Strategy of the Synthesis of 3,4-Dihydropyrimido[1,2-a]benzimidazol-2(1H)-ones. 2018 , 54, 1363-1368	
743	Exploring the Reactivity of Hydrofluoropolyethers toward OH through a Cost-Effective Protocol for Calculating Multiconformer Transition State Theory Rate Constants. 2018 , 122, 9721-9732	8
742	High-throughput quantum-mechanics/molecular-mechanics (ONIOM) macromolecular crystallographic refinement with PHENIX/DivCon: the impact of mixed Hamiltonian methods on ligand and protein structure. 2018 , 74, 1063-1077	12
741	QSAR and Molecular Docking Studies of the Inhibitory Activity of Novel Heterocyclic GABA Analogues over GABA-AT. 2018 , 23,	4
740	A Feynman dispersion correction: a proof of principle for MNDO. 2018 , 24, 338	7
739	. 2018 , 62, 5:1-5:9	
738	Big data analysis of ab Initio molecular integrals in the neglect of diatomic differential overlap approximation. <i>Journal of Computational Chemistry</i> , 2019 , 40, 638-649	3.5 6
737	Studies on the Dual Activity of EGFR and HER-2 Inhibitors Using Structure-Based Drug Design Techniques. 2018 , 19,	8
736	Surface manipulation of a curved polycyclic aromatic hydrocarbon-based nano-vehicle molecule equipped with triptycene wheels. 2018 , 29, 495401	11
735	Water Distribution within Wild-Type NRas Protein and Q61 Mutants during Unrestrained QM/MM Dynamics. 2018 , 115, 1417-1430	7
734	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. 2018 , 23,	23
733	Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. 2018 , 118, e25799	29
732	Could the presence of sodium ion influence the accuracy and precision of the ligand-posing in the human A adenosine receptor orthosteric binding site using a molecular docking approach? Insights from Dockbench. 2018 , 32, 1337-1346	6
731	Binding, and thermodynamics of β -cyclodextrin inclusion complexes with some coumarin laser dyes and coumarin-based enzyme substrates: a simulation study. 2018 , 92, 319-327	7

730	Charge transfer dynamics at the boron subphthalocyanine chloride/C interface: non-adiabatic dynamics study with Libra-X. 2018 , 20, 25275-25294	15
729	Accelerated Computation of Free Energy Profile at ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semi-Empirical Reference Potential. I. Weighted Thermodynamics Perturbation. 2018 , 14, 5583-5596	30
728	Comprehensive Analysis of the Neglect of Diatomic Differential Overlap Approximation. 2018 , 14, 5169-5179	12
727	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. 2018 , 149, 104102	19
726	On the Possibility of Endohedrally Helium-doped TEX Δ DFT Treatment. 2018 , 644, 1096-1102	2
725	Accurate or Fast Prediction of Solid-State Formation Enthalpies Using Standard Sublimation Enthalpies Derived From Geometrical Fragments. 2018 , 57, 13856-13865	8
724	Modeling zinc-oxygen coordination in histone deacetylase: A comparison of semiempirical methods performance. 2018 , 118, e25720	3
723	Application of Semiempirical Methods to Transition Metal Complexes: Fast Results but Hard-to-Predict Accuracy. 2018 , 14, 3428-3439	29
722	Interaction energy profile for diphenyl diselenide in complex with β -aminolevulinic acid dehydratase enzyme using quantum calculations and a molecular fragmentation method. 2018 , 7, 9-19	5
721	A DFT study of inclusion complexes of substituted calix[n]arenes with dasatinib and lapatinib. 2018 , 84, 160-165	3
720	Virtual Screening of Hole Transport, Electron Transport, and Host Layers for Effective OLED Design. 2018 , 58, 2440-2449	13
719	Ab Initio Molecular Local Nuclear Magnetic Shielding Tensors. 2018 , 167-183	
718	A random forest learning assisted "divide and conquer" approach for peptide conformation search. 2018 , 8, 8796	2
717	Transition State Search Using rPM6: Iron- and Manganese-Catalyzed Oxidation Reactions as a Test Case. 2018 , 91, 1377-1389	3
716	Can Path Integral Molecular Dynamics Make a Good Approximation for Vapor Pressure Isotope Effects Prediction for Organic Solvents? A Comparison to ONIOM QM/MM and QM Cluster Calculation. 2018 , 122, 7353-7364	4
715	Effect of β -dextrin nanoparticles on the structure of iodine complexes with polypeptides and alkali metal halogenides, and on the mechanisms of their anti-human immunodeficiency virus and anticancer activity. 2018 , 637-685	1
714	Behavior of the E-E' Bonds (E, E' = S and Se) in Glutathione Disulfide and Derivatives Elucidated by Quantum Chemical Calculations with the Quantum Theory of Atoms-in-Molecules Approach. 2018 , 23,	4
713	An Antioxidant Potential, Quantum-Chemical and Molecular Docking Study of the Major Chemical Constituents Present in the Leaves of Linn. 2018 , 11,	21

712	EUV photofragmentation and oxidation of a polyarylene sulfonium resist: XPS and NEXAFS study. 2018 , 364, 373-381	7
711	Comprehensive adsorption characteristics of a newly synthesized and sustainable anti-corrosion catalyst on mild steel surface exposed to a highly corrosive electrolytic solution. 2018 , 268, 37-48	6
710	Computational Simulation Studies on the Binding Selectivity of 1-(1H-Benzimidazol-5-yl)-5-aminopyrazoles in Complexes with FGFR1 and FGFR4. 2018 , 23,	3
709	The Design, Synthesis, and Characterizations of Spore Germination Inhibitors Effective against an Epidemic Strain of <i>Clostridium difficile</i> . 2018 , 61, 6759-6778	10
708	Testing new chromophores for singlet fission: A computational protocol applied to 2,3-diamino-1,4-benzoquinone. 2018 , 515, 635-642	4
707	Benchmarking Semiempirical Methods To Compute Electrochemical Formal Potentials. 2018 , 122, 6809-6818	9
706	Chloride Ion Transport by the CLC Cl/H Antiporter: A Combined Quantum-Mechanical and Molecular-Mechanical Study. 2018 , 6, 62	4
705	Influence of piperidine ring on stability and reactivity of piperine. 2018 , 17-18, 138-142	5
704	Analytic gradient and derivative couplings for the spin-flip extended configuration interaction singles method: Theory, implementation, and application to proton transfer. 2018 , 148, 244108	8
703	Highly efficient and reusable mesoporous zeolite synthesized from a biopolymer for cationic dyes adsorption. 2018 , 556, 43-50	61
702	A Study of the Terahertz Spectra of Crystalline Materials (Polyethylene, Poly(Vinylidene Fluoride) form II, and β -D-Glucose) Using NDDO Semiempirical Methods. 2018 , 85, 552-559	4
701	Vibrational spectroscopic investigation of the gold complexation within the cascade structure of phosphorus-containing dendrimer. 2018 , 203, 118-126	2
700	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. 2018 , 9, 2316	48
699	Investigation of intermolecular interactions and stability of verubecestat in the active site of BACE1: Development of first model from QM/MM-based charge density and MD analysis. 2019 , 37, 2339-2354 ¹¹	
698	A density functional study on some cyclic N10 isomers. 2019 , 15, 154-161	7
697	Regulation of Cell Membrane Transport by Plasma. 2019 , 173-247	
696	Use of Surfactants in Manufacture of Catalysts for Conversion of Methane. 2019 , 92, 639-646	
695	Study of the Properties of Oxide Melts in a Model Experiment. 2019 , 2019, 176-181	1

- 694 Effects of Processed Agro-Residues on the Performance of Sodium Chloride Brine Anti-Icer. **2019**, 7, 13655-13667 8
- 693 Application of Quantum Chemical Calculation for Prediction of Ultraviolet-vis Spectrum of Plant Self-protective Metabolites Produced by UV-B Irradiation. **2019**, 18, 108-114
- 692 Competition between dispersion interactions and conventional hydrogen bonding: insights from a theoretical study on Z-Arg-OH. **2019**, 21, 17893-17900 1
- 691 Functionalised novel gemini surfactants as corrosion inhibitors for mild steel in 50 mM NaCl: Experimental and theoretical insights. **2019**, 580, 123699 24
- 690 Reactivity of the Intermediate Products of the Pulsed Photolysis of Iodophenol. **2019**, 93, 1417-1419
- 689 A procedure combining molecular docking and semiempirical method PM7 for identification of selective Shp2 inhibitors. **2019**, 110, e23320 3
- 688 Contemplation on Some Prismatic Polynitrogen Structures [A DFT Treatment]. **2019**, 645, 1118-1126 2
- 687 Examination of the performance of semiempirical methods in QM/MM studies of the SN2-like reaction of an adenylyl group transfer catalysed by ANT4?. **2019**, 138, 1 1
- 686 Small atomic clusters: quantum chemical research of isomeric composition and physical properties. **2019**, 30, 2057-2084 15
- 685 Modeling molecularly imprinted polymer mechanics. **2019**, 51-75 2
- 684 Reductive Cleavage of Unactivated Carbon-Cyano Bonds under Ammonia-Free Birch Conditions. **2019**, 84, 15827-15833 14
- 683 . **2019**, 7
- 682 Graphynes: Advanced Carbon Materials with Layered Structure. **2019**, 113-150 7
- 681 Fragmentation Spectra Prediction and DNA Adducts Structural Determination. **2019**, 30, 2771-2784 8
- 680 Remote-controlled nucleophilicity III: A valuable model to explain and predict the observed regioselectivity of the electrophilic attack on substituted 4-methylpyridine anions. **2019**, 900, 120919 1
- 679 Anisotropic Hydrolysis Susceptibility in Deformed Polydimethylsiloxanes. **2019**, 123, 7926-7935 4
- 678 Synthesis, structural studies and biological properties of some phosphono-perfluorophenylalanine derivatives formed by SAR reactions.. **2019**, 9, 24117-24133 1
- 677 The role of regioselective hydroxylation on toxicity of diclofenac and related derivatives. **2019**, 45, 1454-1458 1

676	Accelerated computation of free energy profile at ab initio quantum mechanical/molecular mechanical accuracy via a semi-empirical reference potential. II. Recalibrating semi-empirical parameters with force matching. 2019 , 21, 20595-20605	20
675	Anti-parallel dimer and tetramer formation of cyclic and open structure tertiary amides, N-methyl-2-pyrrolidone and N,N-dimethylacetamide, in solution of a non-polar solvent, benzene. 2019 , 21, 22081-22091	3
674	A new luminescent organic-inorganic hybrid material based on cadmium iodide. 2019 , 109, 107572	2
673	Improved Eco-Friendliness of a Common Flame Retardant through Inclusion Complexation with Cyclodextrins. 2019 , 1, 2768-2777	4
672	Supramolecular forces and their interplay in stabilizing complexes of organic anions: tuning binding selectivity in water. 2019 , 6, 75-86	15
671	A C-substituted cyclotrimeratriylene derivative with 8-quinolinyl groups as a fluorescence-enhanced probe for the sensing of Cu ions. 2019 , 144, 1140-1146	6
670	Morphing of Ibogaine: A Successful Attempt into the Search for Sigma-2 Receptor Ligands. 2019 , 20,	6
669	Heteroatoms and π -electrons as favorable factors for efficient corrosion protection. 2019 , 70, 1099-1110	13
668	Exploring the first-shell and second-shell structures arising in the microsolvation of Li ⁺ by rare gases. 2019 , 119, e25860	7
667	Molecular modeling and computational study of the chiral-dependent structures and properties of self-assembling diphenylalanine peptide nanotubes. 2019 , 25, 199	20
666	Multi niche crowding genetic algorithm parameter tuning for molecular potential energy surface computation. 2019 , 19, 1127-1136	
665	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. 2019 , 58, 11078-11087	38
664	Mechanism of Graphene Formation via Detonation Synthesis: A DFTB Nanoreactor Approach. 2019 , 15, 3654-3665	13
663	Temperature effects on anharmonic infrared spectra of large compact polycyclic aromatic hydrocarbons. 2019 , 622, A152	4
662	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. 2019 , 131, 11195-11204	13
661	Synthesis, structural investigation, antibacterial and DFT studies of complexes derived from a cholesteryl dithiophosphonate ligand with some thio-metallolane and thio-metallocane heterocycles of As(III) and Sb(III). 2019 , 495, 118943	2
660	In silico identification of genetic mutations conferring resistance to acetohydroxyacid synthase inhibitors: A case study of <i>Kochia scoparia</i> . 2019 , 14, e0216116	5
659	Effect of the alkyl chain length on micelle formation for bis(N-alkyl-N,N-dimethylethylammonium)ether dibromides. 2019 , 22, 386-392	11

658	QM/MM Benchmarking of Cyanobacteriochrome Slr1393g3 Absorption Spectra. 2019 , 24,	15
657	Synthesis, molecular structure, spectroscopic properties and biological evaluation of 4-substituted-N-(1H-tetrazol-5-yl)benzenesulfonamides: Combined experimental, DFT and docking study. 2019 , 1195, 119-130	11
656	Learning by Computing: A First Year Honors Chemistry Curriculum. 2019 , 127-138	2
655	Stretching of -formic acid: warm-up and cool-down as molecular work-out. 2019 , 10, 6285-6294	13
654	Vase-Kite Equilibrium of Resorcin[4]arene Cavitands Investigated Using Molecular Dynamics Simulations with Ball-and-Stick Local Elevation Umbrella Sampling. 2019 , 102, e1900060	3
653	Formation of polyynes and ring-polyynes molecules following fragmentation of polycyclic aromatic hydrocarbons. 2019 , 486, 1875-1881	5
652	End functionalization of a double walled carbon nanotube for biomedical application. 2019 ,	
651	Synthesis, crystal structure, vibrational and optical properties of chlorometalate hybrids incorporating (DABCOH ₂) ₂ ⁺ cations. 2019 , 105, 230-239	3
650	Simulation of the Electronic Structure of Graphene/Polyvinylidene Fluoride Composite Material. 2019 , 61, 56-61	2
649	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. 2019 , 15, 3008-3020	27
648	Liquid crystalline lithium-ion electrolytes derived from biodegradable cyclodextrin. 2019 , 7, 12201-12213	12
647	The comparison of retention behaviour of imidazoline and serotonin receptor ligands in non-aqueous hydrophilic interaction chromatography and supercritical fluid chromatography. 2019 , 1603, 371-379	1
646	New aspects in the study of carbon-hydrogen interaction in hydrogenated carbon nanotubes for energy storage applications. 2019 , 792, 713-720	16
645	Nickel Complexes of Guanidine Functionalized Trisiloxane. 2019 , 29, 2024-2034	0
644	Dynamic exciton localisation in a pyrene-BODIPY-pyrene dye conjugate. 2019 , 21, 9013-9025	7
643	Thermal behavior of poly[3,3-bis(azidomethyl)oxetane] compositions with an energetic plasticizer: Calorimetric and optical studies. 2019 , 283, 366-373	5
642	Structure and vibrational spectra of p-coumaric acid dimers by DFT methods. 2019 , 101, 100-108	4
641	Characterization and spectroscopic study of enzymatic oligomerization of phenazopyridine hydrochloride. 2019 , 1188, 76-85	8

640	A Comparison in the Use of the Crystallographic Structure of the Human A1 or the A2A Adenosine Receptors as a Template for the Construction of a Homology Model of the A3 Subtype. 2019 , 9, 821	4
639	Nitric oxide-releasing molecules at the interface of inorganic chemistry and biology: a concise overview. 2019 , 39, 91-112	8
638	Selective synthesis of N-protected exo-spiro[oxirane-3,2'-tropanes]. 2019 , 6, 1692-1697	2
637	Analysis of the retention behavior of selected antiarrhythmics by means of thin-layer chromatography. 2019 , 42, 317-323	1
636	Electrical Functionalization and Fabrication of Nanostructured Hydroxyapatite Coatings. 2019 , 149-190	1
635	Efficient determination of excitation energies and absorption spectra for quantum dots and large systems from ab initio data. 2019 , 721, 12-17	0
634	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. 2019 , 15, 1743-1760	25
633	Improving the accuracy of predicting protein-ligand binding-free energy with semiempirical quantum chemistry charge. 2019 , 11, 303-321	9
632	Multiconformer transition state theory rate constants for the reaction between OH and -dimethoxyfluoropolyethers. 2019 , 51, 358-366	3
631	Argo: a data analysis program for quantum chemical calculations. 2019 , 25, 82	2
630	Circularly polarized luminescence of Sm (III) and Eu (III) complexes with chiral ligand (R/S)-BINAPO. 2019 , 31, 301-311	12
629	Investigation of the structural and physicochemical requirements of quinoline-arylamidine hybrids for the growth inhibition of K562 and Rajileukemia cells. 2019 , 43, 251-265	1
628	Mitigating Alzheimer's Disease with Natural Polyphenols: A Review. 2019 , 16, 529-543	27
627	A theoretical, dynamical evaluation method of the steric hindrance in nitroxide radicals using transition states of model reactions. 2019 , 9, 20339	2
626	Why does tautomycin thioesterase prefer hydrolysis to macrocyclization? Theoretical study on its catalytic mechanism. 2019 , 9, 6391-6403	5
625	Molecular motions, structure and hydration behaviour of glucose oligomers in aqueous solution. 2019 , 21, 25379-25388	8
624	Can Alkaline Hydrolysis of H ₂ CH Serve as a Model Reaction to Study Its Aerobic Enzymatic Dehydrochlorination by LinA?. 2019 , 20,	2
623	Solutions 201 D250. 2019 , 601-719	

- 622 Dependence of the Enthalpy of Formation of Phenols on Molecular Structure [Semiempirical Study]. **2019**, 1-12
- 621 Carbocatalysed hydrolytic cleaving of the glycosidic bond in fucoidan under microwave irradiation.. **2019**, 9, 30325-30334 4
- 620 Loss of mass, structural, and thermodynamic properties of concretes under rainy conditions. **2019**, 1176, 622-632 4
- 619 Structure, stability, and nature of bonding between high energy water clusters confined inside cucurbituril: A computational study. **2019**, 1148, 44-54 7
- 618 An examination of the nature of localized molecular orbitals and their value in understanding various phenomena that occur in organic chemistry. **2018**, 25, 7 8
- 617 Magnetic iron oxide nanoparticles modified with vanadate and phosphate salts for purification of alkaline phosphatase from the bovine skim milk. **2019**, 175, 644-653 5
- 616 Lone pairs vs. covalent bonds: conformational effects in bicyclo[3.3.1]nonane derivatives. **2019**, 30, 509-522 5
- 615 Theoretical study on polyglycerine polynitrates for potential high-energy plasticizers of propellants. **2019**, 97, 287-295
- 614 Design, synthesis and QSAR study of 2'-hydroxy-4'-alkoxy chalcone derivatives that exert cytotoxic activity by the mitochondrial apoptotic pathway. **2019**, 27, 43-54 13
- 613 An Apparent Binary Choice in Biochemistry: Mutual Reactivity Implies Life Chooses Thiols or Nitrogen-Sulfur Bonds, but Not Both. **2019**, 19, 579-613 6
- 612 Inclusion complexes of β -cyclodextrin and polymorphs of mebendazole: Physicochemical characterization. **2019**, 127, 330-338 9
- 611 Investigation and prediction of retention characteristics of imidazoline and serotonin receptor ligands and their related compounds on mixed-mode stationary phase. **2019**, 1585, 92-104 7
- 610 Semi-Empirical Born-Oppenheimer Molecular Dynamics (SEBOMD) within the Amber Biomolecular Package. **2019**, 59, 206-214 2
- 609 Prediction of ion selectivity by quantum chemical calculations X: A recent (personal) review. **2019**, 73, 445-505 6
- 608 Protonation of Curcumin Triggers Sequential Double Cyclization in the Gas-Phase: An Electrospray Mass Spectrometry and DFT Study. **2019**, 438, 107-114
- 607 Density functional theories study of the interactions between host β -Cyclodextrin and guest 8-Anilinonaphthalene-1-sulfonate: Molecular structure, HOMO, LUMO, NBO, QTAIM and NMR analyses. **2019**, 280, 218-229 20
- 606 Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spin-polarized DFTB3 model. *Journal of Computational Chemistry*, **2019**, 40, 400-413 3.5 11
- 605 Aromaticity, Coulomb repulsion, π -delocalization or strain: who is who in endohedral metallofullerene stability?. **2018**, 21, 124-131 4

604	Multistep Explicit Solvation Protocol for Calculation of Redox Potentials. 2019 , 15, 52-67	24
603	Chiral Inductions in Excited State Reactions: Photodimerization of Alkyl 2-Naphthoates as a Model. 2019 , 95, 24-32	2
602	Computational chemistry in drug lead discovery and design. 2019 , 119, e25678	29
601	Urinary tract anti-infectious potential of DFT-experimental composite analyzed ruthenium nitrosyl complex of N-dehydroacetic acid-thiosemicarbazide. 2019 , 31, 89-100	16
600	Binding and stability of indirubin-3-monoxime in the GSK3 β enzyme: a molecular dynamics simulation and binding free energy study. 2020 , 38, 957-974	9
599	Charge calculation studies done on an end-functionalized double-walled carbon nanotube using MOPAC. 2020 , 94, 189-194	
598	Alignment independent 3D-QSAR studies and molecular dynamics simulations for the identification of potent and selective S1P receptor agonists. 2020 , 94, 107459	3
597	Theoretical study on the heat of formation of some polycyclic aromatic hydrocarbons. 2020 , 74, 829-836	
596	Effect of hydrophobic and hydrogen bonding interactions on the potency of Alanine analogs of G-protein coupled glucagon receptor inhibitors. 2020 , 88, 327-344	9
595	Bioinspired surface activators for wet/dry environments through greener epoxy-catechol amine chemistry. 2020 , 505, 144414	8
594	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. <i>Journal of Computational Chemistry</i> , 2020 , 41, 427-438	3.5 18
593	MOA-based linear and nonlinear QSAR models for predicting the toxicity of organic chemicals to <i>Vibrio fischeri</i> . 2020 , 27, 9114-9125	7
592	Investigation of the aromaticity of mono, di, tri and tetraazaphenanthrene derivatives. 2020 , 5,	
591	Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. 2020 , 1205, 127517	2
590	Hydrophobic boron organic polymers: Ultra-high capacity of enrichment and storage for chloroform. 2020 , 385, 123827	5
589	Are the Absorption Spectra of Doxorubicin Properly Described by Considering Different Tautomers?. 2020 , 60, 513-521	2
588	Quantitative assessment of reparameterized PM6 (rPM6) for hydrogen abstraction reactions. 2020 , 118, e1700313	3
587	Minimum Mode Saddle Point Searches Using Gaussian Process Regression with Inverse-Distance Covariance Function. 2020 , 16, 499-509	11

586	Alkaloid from Colchicum species in complexes with lithium, sodium, potassium and magnesium cations: Spectroscopic characterization, semiempirical and theoretical calculation, fungicidal and cytotoxic activity. 2020 , 1204, 127520	4
585	Preclinical toxicity of innovative molecules: In vitro, in vivo and metabolism prediction. 2020 , 315, 108896	10
584	Identification of novel inhibitors for the tyrosyl-DNA-phosphodiesterase 1 (Tdp1) mutant SCAN1 using virtual screening. 2020 , 28, 115234	7
583	Novel trivalent europium β -diketonate complexes with N-(pyridine-2-yl)amides and N-(pyrimidine-2-yl)amides as ancillary ligands: Photophysical properties and theoretical structural modeling. 2020 , 219, 116884	14
582	Energy-Screened Many-Body Expansion: A Practical Yet Accurate Fragmentation Method for Quantum Chemistry. 2020 , 16, 475-487	27
581	Accelerated Computation of Free Energy Profile at Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 3. Gaussian Smoothing on Density-of-States. 2020 , 16, 6814-6822	5
580	Comparative Studies of Infrared Spectral Simulation of Some Benzoyl Derivatives of N-Heterocyclic Compounds Using Semi-Empirical Methods. 2020 , 32, 2463-2468	
579	Encompassment of phthalyl sulfacetamide in β - and γ -cyclodextrin using ultrasonication: Physicochemical and computational modeling investigations. 2020 , 319, 114184	0
578	Investigating the pernicious effects of heparan sulfate in serum amyloid A1 protein aggregation: a structural bioinformatics approach. 2020 , 1-15	3
577	Pillar[5]arenes as potential personage for DNA compactization and gene therapy. 2020 , 319, 114178	3
576	Synthesis, spectral studies, molecular structure determination by single crystal X-ray diffraction of (E)-1-(((3-fluoro-4-morpholinophenyl)imino)methyl)naphthalen-2-ol and computational studies by Austin model-1(AM1), MM2 and DFT/B3LYP. 2020 , 2, 1	
575	Controlling the outcome of S ₂ reactions in ionic liquids: from rational data set design to predictive linear regression models. 2020 , 22, 23009-23018	5
574	Benchmark and parameter tuning of hybrid functionals for fast calculation of excitation energies of AIEgens. 2020 , 22, 18035-18039	5
573	Polynitro-acetone, dimethyl ether, and dimethylamine: a series of potential green and powerful oxidants for propellants. 2020 , 26, 347	1
572	-(Pyrimidin-2-yl)-1,2,3,4-tetrahydroisoquinolin-6-amine Derivatives as Selective Janus Kinase 2 Inhibitors for the Treatment of Myeloproliferative Neoplasms. 2020 , 63, 14921-14936	4
571	New Aspects of the Airglow Problem and Reactivity of the Dioxygen Quintet O(Π) State in the MLT Region as Predicted by DFT Calculations. 2020 , 124, 9638-9655	3
570	Quantum Chemical Calculations of Carbon Nanoscroll Energy Rolled from Zigzag Graphene Nanoribbon. 2020 , 54, 1678-1681	2
569	Lipoxygenase Inhibition Activity of Coumarin Derivatives-QSAR and Molecular Docking Study. 2020 , 13,	11

568	Lanthanide Contraction in Lanthanide Organic Frameworks: A Theoretical and Experimental Study. 2020 , 124, 7678-7684	3
567	Antileishmanial activity of 4-phenyl-1-[2-(phthalimido-2-yl)ethyl]-1H-1,2,3-triazole (PT4) derivative on <i>Leishmania amazonensis</i> and <i>Leishmania braziliensis</i> : In silico ADMET, in vitro activity, docking and molecular dynamic simulations. 2020 , 105, 104437	6
566	Structures and Properties of the Self-Assembling Diphenylalanine Peptide Nanotubes Containing Water Molecules: Modeling and Data Analysis. 2020 , 10,	11
565	Electrochemical preparation and physicochemical study of polymers obtained from carbazole and N-((methoxycarbonyl)methyl)carbazole. 2020 , 270, 116584	4
564	Catalytic activity of water molecules in gas-phase glycine dimerization. 2020 , 120, e26469	2
563	The Antineoplastic Properties and Mechanism of Interaction of an Antioxidant, Sodium 2-Carboxy-2-(N-ABtylamino)-3-(3,5-di-tert-Butyl-4-Hydroxyphenyl)Propionate, with Peptides in an Aqueous Environment According to the Data of the Calculation by Quantum Chemistry Methods. 2020 , 11, 113-119	1
562	Understanding Enzyme Catalysis Mechanism Using QM/MM Simulation Methods. 2020 , 121-137	1
561	Real-Time Time-Dependent Electronic Structure Theory. 2020 , 120, 9951-9993	60
560	Putative SARS-CoV-2 M Inhibitors from an In-House Library of Natural and Nature-Inspired Products: A Virtual Screening and Molecular Docking Study. 2020 , 25,	21
559	Bi-Stability of a Pyramidal Structure of NH ₂ Groups in Nitrous Bases and its Role in the Structural and Functional Organization of the Genomic DNA. 2020 , 63, 1322-1338	
558	Computer simulation of collision induced dissociation and isolobal analogy: The case of biotin and its analogs. 2020 , 457, 116417	
557	10-Methylthiocolchicine complexes with lithium, sodium, potassium, rubidium and cesium metal cations salts [Cytotoxic, semi-empirical and molecular modelling studies. 2020 , 190, 114791	0
556	Glucuronidation of Methylated Quercetin Derivatives: Chemical and Biochemical Approaches. 2020 , 68, 14790-14807	4
555	Alkaline Phosphatases: Study on the Catalytic Effect of Conserved Active Site Residues Using Human Placental Alkaline Phosphatase (PLAP) As a Model Protein. 2020 , 60, 6228-6241	
554	Study of Synergistic Effect of Some Pyrazole Derivatives as Corrosion Inhibitors for Mild Steel in 1 M H ₂ SO ₄ . 2020 , 56, 601-609	3
553	Molecular modeling and computational study of the chiral-dependent structures and properties of the self-assembling diphenylalanine peptide nanotubes, containing water molecules. 2020 , 26, 326	3
552	Quantum mechanics/molecular mechanics multiscale modeling of biomolecules. 2020 , 143-183	0
551	Monolayer self-organization of cyclodextrins on carbon surface. 2020 , 67, 1778-1782	0

550	Quantitative structure-activity relationships of xanthen-3-one and xanthen-1,8-dione derivatives and design of new compounds with enhanced antiproliferative activity on HeLa cervical cancer cells. 2021 , 39, 4026-4036	1
549	A search for the physical basis of the genetic code. 2020 , 195, 104148	3
548	Simulations of dielectric constants and viscosities of organic electrolytes by quantum mechanics and molecular dynamics. 2020 , 312, 113288	9
547	The inclusion behavior of 8-Anilino-1-naphthalene sulfonate into Cucurbit[7]uril: A DFT approach. 2020 , 1217, 128390	3
546	Theoretical investigation of the molecular structure, vibrational spectra, thermodynamic and nonlinear optical properties of 4, 5-dibromo-2, 7-dinitro- fluorescein. 2020 , 52, 1	5
545	Origin of optical bandgap fluctuations in graphene oxide. 2020 , 93, 1	2
544	Supramolecular polyelectrolyte complexes based on cyclodextrin-grafted chitosan and carrageenan for controlled drug release. 2020 , 245, 116592	12
543	On the Potential of Silicon as a Building Block for Life. 2020 , 10,	25
542	Chemical Bonding: The Journey from Miniature Hooks to Density Functional Theory. 2020 , 25,	5
541	The strategy for improving the stability of nitroform derivatives-high-energetic oxidant based on hexanitroethane. 2020 , 26, 181	2
540	Novel Quinazolin-2,4-Dione Hybrid Molecules as Possible Inhibitors Against Malaria: Synthesis and Molecular Docking Studies. 2020 , 7, 105	14
539	Predicting oxidative stress induced by organic chemicals by using quantitative Structure-Activity relationship methods. 2020 , 201, 110817	7
538	EMPIRE: a highly parallel semiempirical molecular orbital program: 3: Born-Oppenheimer molecular dynamics. 2020 , 26, 43	5
537	Bicyclic β -Iminophosphonates as High Affinity Imidazoline I Receptor Ligands for Alzheimer's Disease. 2020 , 63, 3610-3633	8
536	Experimental and theoretical study of isorecticular lanthanoid organic framework (LOF): Structure and luminescence. 2020 , 223, 117179	1
535	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. 2020 , 16, 5771-5783	27
534	Mixing and Solvent Effects on Kinetics of Supercritical Hydrothermal Synthesis: Reaction of Nickel Nitrate to Nickel Oxide. 2020 , 124, 4772-4780	6
533	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. 2020 , 120, 2215-2287	113

532	Evolved <i>Fusarium oxysporum</i> laccase expressed in <i>Saccharomyces cerevisiae</i> . 2020 , 10, 3244	9
531	Density-functional tight-binding: basic concepts and applications to molecules and clusters. 2020 , 5, 1710252	19
530	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. 2020 , 16, 2002-2012	32
529	Exploring the charge configuration of an armchair single walled carbon nanotube for drug delivery. 2020 , 28, 185-187	2
528	Theoretical Spectroscopic Studies on Chemical and Electronic Structures of Selenocysteine and Pyrrolysine. 2020 , 124, 2215-2224	1
527	Novel computational approaches to retention modeling in dual hydrophilic interactions/reversed phase chromatography. 2020 , 1619, 460951	6
526	Fast Evaluation of Two-Center Integrals over Gaussian Charge Distributions and Gaussian Orbitals with General Interaction Kernels. 2020 , 16, 2570-2583	7
525	Encapsulation of essential oil components with methyl- β -cyclodextrin using ultrasonication: Solubility, characterization, DPPH and antibacterial assay. 2020 , 64, 104997	28
524	Investigation of the polymer-salt interactions in polymeric light emitting electrochemical cells: Electronic structure calculations and experimental studies. 2020 , 79, 105629	5
523	Cucurbit[7]uril as a catalytic nanoreactor for one-pot synthesis of isoxazolidines in water. 2020 , 18, 1194-1203	7
522	Elucidation of the atroposelectivity in the synthesis of axially chiral thiohydantoin derivatives. 2020 , 18, 2233-2241	2
521	Quantum Mechanics in Drug Discovery. 2020 ,	10
520	Impact of conformational and solubility properties on psycho-activity of cannabidiol (CBD) and tetrahydrocannabinol (THC). 2020 , 26, 100345	2
519	Potential of Mean Force Calculations for an S2 Fluorination Reaction in Five Different Imidazolium Ionic Liquid Solvents Using Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulations. 2020 , 124, 4338-4357	7
518	Computational strategies towards developing novel antimelanogenic agents. 2020 , 250, 117602	
517	Exploring enthalpies of formation of imidazolium-, pyridinium-, and pyrrolidinium-based ionic liquids with dicyanamide anion using quantum chemical methods. 2020 , 308, 113137	4
516	identification of novel 5-HT antagonists supported with ligand- and target-based drug design methodologies. 2021 , 39, 1819-1837	6
515	Supercritical CO ₂ /subcritical H ₂ O system: A green reactive separation medium for selective conversion of glucose to 5-hydroxymethylfurfural. 2021 , 168, 105079	3

- 514 Assessing conformer energies using electronic structure and machine learning methods. **2021**, 121, e26381 23
- 513 Bond dissociation energy and thermal stability of energetic materials. **2021**, 143, 3439-3445 1
- 512 Improving the solubility of an antifungal thiazolyl hydrazone derivative by cyclodextrin complexation. **2021**, 156, 105575 3
- 511 Synthesis and antimicrobial activity evaluation of some new 7-substituted quinolin-8-ol derivatives: POM analyses, docking, and identification of antibacterial pharmacophore sites. **2021**, 31, 100593 5
- 510 Functional roles of the hexamer structure of C-phycocyanin revealed by calculation of absorption wavelength. **2021**, 11, 164-172 1
- 509 Reactivities of electrophilic N-F fluorinating reagents. **2021**, 57, 683-712 11
- 508 Observation of quantum signature in rivastigmine chemical bond break-up and quantum energetics, spectral studies of anti-Alzheimer inhibitors. **2021**, 39, 118-128 1
- 507 Comparison of theoretical and experimental investigation of protonation process of some thiones in acid media. **2021**, 62, 9-21
- 506 Computational study of IR, Raman, and NMR spectra of 4-methylmethcathinone drug. **2021**, 27, 3 2
- 505 Computational Study for the Aromatic Nucleophilic Substitution of 4-Dimethylamino-3-trifluoroacetyl- quinoline with Various Nucleophiles. **2021**, 103, 918
- 504 Exploring the stability of inhibitor binding to SIK2 using molecular dynamics simulation and binding free energy calculation. **2021**, 23, 13216-13227 4
- 503 Mechanism of zinc ejection by disulfiram in nonstructural protein 5A. **2021**, 23, 12204-12215 7
- 502 A comparative theoretical mechanism on simplified flavonoid derivatives and isoxazolone analogous as Michael system inhibitor. **2021**, 27, 26 2
- 501 Destructive Reduction of TEX by Lithium-DFT Treatment. 249-260
- 500 Theoretical and Computational Investigations of Carbon Nanostructures. **2021**, 139-164
- 499 Quantitative Structure-Activity Relationship Study of DPP-4 Enzyme Inhibitors as Drugs in Therapy of Type 2 Diabetes Mellitus. **2021**, 481-488
- 498 Reactivity of 1,3-dichloro-1,3-bis(dimethylamino)-propenium salts with primary amines. **2021**, 45, 13558-13570 0
- 497 CID Fragmentation of Deprotonated -Acyl Aromatic Sulfonamides. Smiles-Type and Nitrogen-Oxygen Rearrangements. **2021**, 32, 806-814 2

496	Design, synthesis and biological evaluation of new benzoxazolone/benzothiazolone derivatives as multi-target agents against Alzheimer's disease. 2021 , 212, 113124	8
495	Bond order predictions using deep neural networks. 2021 , 129, 064701	1
494	Comparative Approach to Interaction of Zinc Dication with Theobromine and Theophylline-A DFT Treatment. 295-306	
493	RegioSQM20: improved prediction of the regioselectivity of electrophilic aromatic substitutions. 2021 , 13, 10	3
492	Synthesis, in silico, and in vitro studies of novel dopamine D and D receptor ligands. 2021 , 354, e2000486	2
491	Theoretical investigations on the density, detonation performance and stability of fluorinated hexanitroadamantanes. 2021 , 32, 1651-1657	
490	High throughput virtual screening of 230 billion molecular solar heat battery candidates. 3, e16	7
489	Synthesis of arylfuran derivatives as potential antibacterial agents. 2021 , 30, 1074-1086	1
488	Theoretical insights into molecular mechanism and energy criteria of PARP-2 enzyme inhibition by benzimidazole analogues. 2021 , 89, 988	3
487	Condensed-phase relative Gibbs free energy and E/Z descriptors for 2-acetylthiophene and 2-acetylthiophene-N1-phenyl thiosemicarbazones. 2021 , 27, 101	1
486	Effect of Electric Field on ANTA. 329-345	1
485	Isomers of (L)-Diiodotyrosine - A DFT Treatise. 347-361	
484	A Quire Polycyclic Structure of N8 - A DFT Treatise. 1-14	
483	Dasatinib-SIK2 Binding Elucidated by Homology Modeling, Molecular Docking, and Dynamics Simulations. 2021 , 6, 11025-11038	5
482	DFT Treatment of ANTA and Some of its Tautomers. 23-36	
481	Simplified Protocol for the Calculation of Multiconformer Transition State Theory Rate Constants Applied to Tropospheric OH-Initiated Oxidation Reactions. 2021 , 125, 4499-4512	2
480	Detonation Parameters of the Pentaerythritol Tetranitrate and Some Structures Descriptors in Different Solvents - Computational Study.	
479	Spectroscopic Determination of Dissociation Constants of Some 4-nitrobenzaldehyde-4-substituted phenyl-1-carbonylhydrazones in Sodium Hydroxide Media. 2021 , 17, 812-821	0

478	Diagonally Compressed TNAZ - A DFT Treatment. 65-84	
477	Polyphenol-Peptide Interactions in Mitigation of Alzheimer's Disease: Role of Biosurface-Induced Aggregation. 2021 , 81, 33-55	0
476	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. 2021 , 47, 762-770	0
475	How to face COVID-19: proposed treatments based on remdesivir and hydroxychloroquine in the presence of zinc sulfate. Docking/DFT/POM structural analysis. 2021 , 1-14	3
474	Optical and structural properties of cyanine dyes via electronic structure calculations. 2021 , 1199, 113197	0
473	Automated Construction of Quantum-Classical Hybrid Models. 2021 , 17, 3797-3813	8
472	Some Trinitroazetidine Isomers - A DFT Treatment. 85-98	
471	Prediction of organic compounds adsorbed by polyethylene and chlorinated polyethylene microplastics in freshwater using QSAR. 2021 , 197, 111001	4
470	SAMPL7 blind challenge: quantum-mechanical prediction of partition coefficients and acid dissociation constants for small drug-like molecules. 2021 , 35, 841-851	3
469	Coumarin Derivatives Act as Novel Inhibitors of Human Dipeptidyl Peptidase III: Combined In Vitro and In Silico Study. 2021 , 14,	2
468	Prediction of essential binding domains for the endocannabinoid N-arachidonylethanolamine (AEA) in the brain cannabinoid CB1 receptor. 2021 , 16, e0229879	0
467	Using Atomic Charges to Describe the p of Carboxylic Acids. 2021 , 61, 2733-2743	3
466	STUDY OF THE INTERACTION BETWEEN OXICAM DERIVATIVES AND COX1 USING FINGERPRINT DESCRIPTORS AND MOLECULAR DOCKING. 2021 , 21, 529-538	1
465	Revealing generation, migration, and dissociation of electron-hole pairs and current emergence in an organic photovoltaic cell. 2021 , 7,	1
464	Isolable Pyridinium Trifluoromethoxide Salt for Nucleophilic Trifluoromethoxylation. 2021 , 23, 5138-5142	8
463	Effect of Selenium on TNAZ Molecule - A DFT Treatment. 119-135	1
462	Effect of ether functionalization and alkyl chain length on the structure and electronic properties of ammonium ionic liquids. 2021 , 775, 138650	2
461	Synthesis, FT-IR and NMR Characterization, Antibacterial and Antioxidant Activities, and DNA Docking Analysis of a New Vanillin-Derived imine Compound. 2021 , 1236, 130288	4

460	Machine learning approach to discovery of small molecules with potential inhibitory action against vasoactive metalloproteases. 2021 , 1	1
459	Nifuroxazide as JAK2 inhibitor: A binding mode proposal and Hel cell proliferation assay. 2021 , 162, 105822	0
458	Synthesis, antioxidant and cytoprotective activity evaluation of C-3 substituted indole derivatives. 2021 , 11, 15425	5
457	Design of Dual COX-2 and 5-LOX Inhibitors with Iron-Chelating Properties Using Structure-Based and Ligand-Based Methods. 2021 , 18,	
456	Rhodamine 6G-Ligand Influencing G-Quadruplex Stability and Topology. 2021 , 22,	1
455	Biological Activities Related to Plant Protection and Environmental Effects of Coumarin Derivatives: QSAR and Molecular Docking Studies. 2021 , 22,	3
454	Some Diazodinitrophenol Isomers - A DFT Treatment. 137-154	
453	Quantum-Chemical Calculations for the Electronic Absorption Spectra of Certain Anthocyanidins. 2021 , 95, 1378-1385	
452	On the Mechanism of Soot Nucleation. III. The Fate and Facility of the E-Bridge. 2021 , 125, 6789-6795	2
451	New Approach for Correcting Noncovalent Interactions in Semiempirical Quantum Mechanical Methods: The Importance of Multiple-Orientation Sampling. 2021 , 17, 5556-5567	3
450	Investigation of electrochemical oxidative coupling of 3 and 6 substituted carbazoles. 2021 , 894, 115356	3
449	Energy and reactivity profile and proton affinity analysis of rimegepant with special reference to its potential activity against SARS-CoV-2 virus proteins using molecular dynamics. 2021 , 27, 276	4
448	Molecular Docking, Modeling, Semiempirical Calculations Studies and In Vitro Evaluation of New Synthesized Pyrimidin-imide Derivatives. 2021 , 131548	4
447	Some Ions of TNAZ - A DFT Study. 215-228	
446	Molecular modelling of two coordination states of Zn(II) ion at the active site of human carbonic anhydrase II. 2021 , 549, 111281	0
445	Connecting Gas-Phase Computational Chemistry to Condensed Phase Kinetic Modeling: The State-of-the-Art. 2021 , 13,	4
444	Benzofuranyl-2-imidazoles as imidazoline I receptor ligands for Alzheimer's disease. 2021 , 222, 113540	2
443	Molecular structure, spectral and thermal properties and in silico biological activity of new bis-phthalimidopropylalkylammonium conjugates of bile acids. 2021 , 1243, 130814	0

442	Study on Clitoria ternatea extracts doped sol-gel coatings for the corrosion mitigation of mild steel. 2021 , 6, 100177	2
441	A study of products of tetrakis(hydroxymethyl)glycoluril dehydroxymethylation in aqueous solutions. 2021 , 70, 140-147	1
440	Development and Applications of the ReaxFF Reactive Force Field for Biological Systems. 2021 , 157-182	4
439	Microwave Assisted Synthesis of Quinoline Fused Benzodiazepines as Anxiolytic and Antimicrobial Agents. 2021 , 33, 1107-1114	1
438	Multiscale modelling of charge transport in P3HT:DIPBI bulk heterojunction organic solar cells. 2021 , 23, 12233-12250	2
437	Prediction of Antagonistic Activity of β -Carboline and Its Derivatives Using Topological Descriptors. 2021 , 11, 577-584	
436	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. 2021 , 23, 8181-8199	7
435	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. 2021 , 9, 13557-13583	4
434	MSINDO.	4
433	Tellurophenes, Dihydrotellurophenes, and Tetrahydrotellurophenes and their Benzo and Dibenzo Analogs. 31-145	1
432	Quantitative Structure-Property Relationships. 1314-1335	2
431	Tris(chlordimethylstannyl)amin, ein durch intramolekulare Sn-Cl-Sn-Brücken stabilisiertes Molekül mit planarem Sn ₃ N-Gerüst. 1993 , 105, 1693-1695	2
430	Polymerization of Chrysoidine with chemical and enzymatic oxidative preference: Synthesis, characterization, and spectroscopic study. 2018 , 29, 2515-2528	9
429	Molecular Orbital Calculations and Optical Transitions of PAHs and Asphaltenes. 2007 , 95-137	18
428	Dynamics Studies of the O(3P) + CH ₄ , C ₂ H ₆ and C ₃ H ₈ Reactions. 2004 , 329-348	3
427	Encyclopedia of Complexity and Systems Science. 2009 , 7931-7953	1
426	Structure-Based Drug Design. 2007 , 135-176	2
425	User-Friendly Quantum Mechanics: Applications for Drug Discovery. 2020 , 2114, 231-255	5

424	Binding Free Energy Calculation Using Quantum Mechanics Aimed for Drug Lead Optimization. 2020 , 2114, 257-268	16
423	QM Calculations in ADMET Prediction. 2020 , 2114, 285-305	4
422	INFLUENCE OF IMPURITIES AND DEFECTS ON ELECTRONIC STRUCTURE OF CARBON NANOTUBES. 2007 , 795-799	3
421	CUBIC POLYMERIZED STRUCTURES OF SMALL FULLERENES C20, C24, C28, C32. 2007 , 713-719	1
420	Quantifying Solvation Effects on Peptide Conformations: A QM/MM Replica Exchange Study. 2008 , 507-518	2
419	Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. 2009 , 377-408	1
418	Towards an Accurate Semi-Empirical Molecular Orbital Treatment of Covalent and Non-Covalent Biological Interactions. 2009 , 105-136	1
417	Correlation of Crystal Data and Charge Density with the Reactivity and Activity of Molecules: Towards a Description of Elementary Steps in Enzyme Reactions. 1991 , 287-318	4
416	Rotamers of tolrestat and their binding mode to aldose reductase. 1999 , 463, 465-72	1
415	Partitioning of Free Energies of Solvation into Fragment Contributions: Applications in Drug Design. 2001 , 143-168	8
414	Hybrid quantum and classical methods for computing kinetic isotope effects of chemical reactions in solutions and in enzymes. 2008 , 443, 37-62	4
413	Semiempirical Calculations. 2016 , 421-482	1
412	Nano-Modeling Structure and Micromechanical Properties of Mesoscopic Composite Systems. 2006 , 129-138	1
411	Cerium (III) Complexes Modeling with Sparkle/PM3. 2007 , 312-318	13
410	The Linear Scaling Semiempirical LocalSCF Method and the Variational Finite LMO Approximation. 2011 , 409-437	2
409	Quantum Parabolic Effects of Electronegativity and Chemical Hardness on Carbon ESystems. 2011 , 1-32	5
408	Theoretical Studies of the Energetics of Radicals. 1996 , 110-149	1
407	The Role of Trivalent Oxygen in Electrically Active Complexes. 1996 , 163-177	2

406	Building A Bridge Between AB Initio and Semiempirical Theories of Molecular Electronic Structure. 1995 , 25-67	3
405	An Application of Theoretical Models to Understand Chemical Reactions: The Electrophilic Substitution in Furan. 1992 , 71-98	0
404	Molecular Modelling. Semi-Empirical and Empirical Methods of Theoretical Chemistry. 1991 , 229-259	1
403	Computational Modeling of Surface Layers of Refractory Compounds. 1999 , 155-186	1
402	Semi-Empirical Mo Calculations on Enzyme Reaction Mechanisms. 1997 , 307-317	5
401	Structure Determination by Electron Crystallography Using a Simulation Approach Combined with Maximum Entropy with the Aim of Improving Material Properties. 1997 , 273-284	1
400	On the Electronic Structure of Oxo-Metalloporphyrins and Mechanistic Aspects of Oxygen-Transfer Reactions. 1994 , 207-238	0
399	Electronic and Nonlinear Optical Properties of Conjugated Molecules and Polymers: A Quantum Chemistry Approach. 1993 , 127-153	2
398	SOFT AND HARD ACIDITY IN ZEOLITES AND ZEOTYPES: EVALUATION AND CATALYTIC IMPLICATIONS. 1993 , 379-387	1
397	Electrochemical, morphological and theoretical insights of a new environmentally benign organic inhibitor for mild steel corrosion in acidic media. 2017 , 241, 9-19	29
396	Effectiveness of O-bridged cationic gemini surfactants as corrosion inhibitors for stainless steel in 3 M HCl: Experimental and theoretical studies. 2018 , 249, 1113-1124	58
395	Synthesis, crystal structure, antibacterial, antiproliferative and QSAR studies of new bismuth(III) complexes of pyrrolidinedithiocarbamate of dithia-bismolane and bismane, oxodithia- and trithia-bismocane. 2020 , 1217, 128456	3
394	Electrostatic potential surfaces of the transition state for AMP deaminase and for (R)-coformycin, a transition state inhibitor.. 1994 , 269, 22385-22390	14
393	Overcrowded polycyclic aromatic enes. 1998 , 245-322	17
392	Computational and spectroscopic studies on hydrated molecules. 1995 , 227-260	0
391	Symmetry-broken inversion structures for group 15 EX3 halides. 1999 , 223-262	14
390	Methods of incorporating quantum mechanical calculations into molecular dynamics simulations. 1999 , 7, 1-29	2
389	Relative stabilities of isomeric fullerenes. 1999 , 185-235	22

388	A Cyclic Periodic Wave Function Approach for the Study of Infinitely Periodic Solid-State Systems: II. Application to Helical Polysaccharides. 2020 , 5, 27556-27565	3
387	CHAPTER 3: Metal-free Azide-Alkyne Click Polymerization. 2018 , 86-121	1
386	Chapter 3: Quantum Catalysis in Enzymes. 2009 , 36-78	7
385	Chapter 5: Kinetic Isotope Effects from Hybrid Classical and Quantum Path Integral Computations. 2009 , 105-131	5
384	Characterization and application studies of ProxyPhos, a chemosensor for the detection of proximally phosphorylated peptides and proteins in aqueous solutions. 2017 , 142, 2451-2459	7
383	Heteronuclear cobalt(iii)/sodium complexes with salen type compartmental Schiff base ligands: methylene spacer regulated variation in nuclearity. 2018 , 47, 331-347	45
382	Fragmentation and isomerization of polycyclic aromatic hydrocarbons in the interstellar medium: Coronene as a case study. 2020 , 633, A103	2
381	Natural Commiphora Caudata extract as corrosion inhibitor for mild steel in acid media. 2020 ,	1
380	Domain and homogeneous switching in ferroelectrics. 2020 , 569, 164-181	1
379	Concurrent Coupling of Atomistic and Continuum Models. 2009 , 93-133	3
378	Prediction of photofading of N-(4-hydroxyethylamino)-o-nitrophenyl derivatives: a theoretical study. 2021 , 137, 134-144	1
377	Synthesis and Resolution of a New C ₂ -Symmetric Chiral Bis-Aniline, trans-1,2-Bis(2-aminophenyl)cyclopentane. 2000 , 65, 549-554	2
376	Steric Hindrance in the Solute-Solvent Interactions of 2-Substituted 4,5-Dimethoxypyridazin-3(2H)-ones: An Infrared Spectral and Theoretical Study. 2002 , 67, 1790-1804	2
375	Mechanism of corrosion protection in chloride solution by an apple-based green inhibitor: experimental and theoretical studies. 2020 , 1,	14
374	Quantum Chemical Descriptors in Structure-Activity Relationships II: Calculation, Interpretation, and Comparison of Methods. 2004 ,	1
373	Chlorine Kinetic Isotope Effects on Biological Systems. 2005 , 875-892	1
372	SMx Continuum Models for Condensed Phases. 2006 , 112-139	14
371	A New Free Volume Theory Based on Microscopic Concept of Molecular Collisions for Penetrant Self-Diffusivity in Polymers. 2009 , 42, 86-94	9

370	Quantum chemical studies of the myosin ATPase mechanism. 2007 , 74, 4-10	2
369	The energy computation paradox and ab initio protein folding. 2011 , 6, e18868	41
368	Membrane-lipid therapy in operation: the HSP co-inducer BGP-15 activates stress signal transduction pathways by remodeling plasma membrane rafts. 2011 , 6, e28818	59
367	The Effectiveness of Natural Diarylheptanoids against Trypanosoma cruzi: Cytotoxicity, Ultrastructural Alterations and Molecular Modeling Studies. 2016 , 11, e0162926	14
366	QM/MM simulations provide insight into the mechanism of bioluminescence triggering in ctenophore photoproteins. 2017 , 12, e0182317	6
365	Computational methods for calculation of protein-ligand binding affinities in structure-based drug design. 2020 ,	1
364	Quantitative structure-retention relationships (QSRR) of biogenic amine neurotransmitters and their metabolites on RP-18 plates in thin-layer chromatography. 2003 , 16, 102-106	5
363	Inhibitors of human collagenase, MMP1. 2009 , 34, 87-102	3
362	Aplicaciones de los métodos computacionales al estudio de la estructura y propiedades de polímeros. 2003 , 13, 250-264	2
361	Chiral Peculiar Properties of Self-Organization of Diphenylalanine Peptide Nanotubes: Modeling Of Structure and Properties. 2019 , 14, 94-125	5
360	Modeling of helix formation in peptides containing aspartic and glutamic residues. 2010 , 2, 83-90	0
359	Integrated Protocol to Design Potential Inhibitors of Dipeptidyl Peptidase- 4 (DPP-4). 2020 , 20, 209-226	1
358	Synthesis, Characterization, Antibacterial and Antioxidant Potency of NSubstituted-2-Sulfanylidene-1,3-Thiazolidin-4-one Derivatives and QSAR Study. 2019 , 15, 840-849	4
357	Thermodynamic properties of cadmium compounds from quantum chemical evaluations. 2002 , 67, 339-346	10
356	Structure and stereochemistry of electrochemically synthesized poly-(l-naphthylamine) from neutral aceto- nitrile solution. 2002 , 67, 867-877	33
355	An approach to quantum chemical consideration of "hydride" transfer reaction. 2004 , 69, 431-439	3
354	Activation energies of H2O and H2 diffusions in silica glass: Semi-empirical molecular orbital study.. 1997 , 19, 13-19	2
353	Prediction of High-Spin Ground States of Biguanide Trication and Biuret Trication as a Design for Novel Polymer Ferrromagnets. 2005 , 4, 101-106	7

352	Evaluation of Several Computational Methods for the Purpose of Predicting the Structure of a Dinuclear Zinc(II) Complex. 2008 , 7, 27-32	5
351	Binding energy between lactose repressor protein and DNA: semiempirical molecular orbital calculations. 2003 , 4, 35-41	3
350	Semiempirical MO calculations for double-strand DNA and its base-mismatched ones. 2003 , 4, 42-51	1
349	Electronic Properties for Medicine Inhibiting Cancer Metastasis (1) : Molecular Orbital Calculations for Physiological Substance Bikunin. 2004 , 5, 62-69	4
348	Electronic Properties for Medicine Inhibiting Cancer Metastasis (2) : Molecular Mechanics and Molecular Orbital Calculations for Urokinase. 2004 , 5, 70-78	4
347	Molecular Mechanics and Molecular Orbital Simulations on The Specific Interactions between Lactose Repressor Protein and Its Inducer and Anti-Inducer Molecules. 2008 , 9, 17-29	2
346	METHYLCYTISINE ALCALOID POTENTIALLY ACTIVE AGAINST DENGUE VIRUS: A MOLECULAR DOCKING STUDY AND ELECTRONIC STRUCTURAL CHARACTERIZATION. 2020 , 8, 221-236	7
345	Computational Surface Modelling of Ices and Minerals of Interstellar Interest Insights and Perspectives. 2021 , 11, 26	2
344	A DFT Treatment of Some Aluminized 1,3,3-Trinitroazetidine (TNAZ) Systems - A Deeper Look. 121-140	4
343	Bischler-Napieralski Reaction of N-[2-(2-Bromo-4,5-dialkyloxyphenyl)-ethyl]-N-(1-phenylethyl)-2-(2-bromo-4,5-dimethoxyphenyl)acetamides. 2002 , 57, 2149	2
342	Synthesis, Tautomerism and Calculations of Mesomeric Betaines of Guanine. 2002 , 57, 2231	9
341	1,3-Dipolar Cycloaddition of Ethyl 2,3-Pentadienoate with Pyridinium Dicyanomethylides: Regiospecific Formation of Ethyl 3-Cyano-2-ethylindolizine-1-carboxylates and a Novel Formation of Tricyclic Compounds. 2005 , 66, 175	2
340	A Convenient Synthesis of Functionalized 1H-Pyrimidine-2-ones/thiones, Pyridazine and Imidazole; Experimental Data and PM3 Calculations. 2006 , 68, 2045	2
339	Tandem Catalysis Strategy for Direct Glycosylation of 1-Hydroxy Sugars. Methoxyacetic Acid as an Effective Catalytic Mediator. 2009 , 79, 967	6
338	Relative Stability of Cryptolepinone and Hydroxycryptolepine. 2009 , 78, 1823	1
337	Formation Pathway of Novel Cycloadduct Obtained by Reaction of 3,5-Disubstituted 4-Oxo-4H-pyrazole 1,2-Dioxide with Dimethyl Acetylenedicarboxylate. 2009 , 78, 2777	4
336	Computational Study for 1,5-Sigmatropic Hydrogen Shift on Trifluoromethylazadiene Derivatives - The Key Step in the Synthesis of Fluorine-Containing Oxazines -. 2016 , 93, 243	1
335	Selective Aromatic Nucleophilic Substitution of 4-Dimethylamino-2-methoxy-3-(trifluoroacetyl)quinoline with Alcohols [DFT Calculation Study. 2020 , 101, 692	2

- 334 Synthesis of Polycyclic Systems via Diels-Alder Reactions of Sugar Derived Dienes. **2000**, 53, 81 3
- 333 Cycloadditions of 5,6-Unsaturated N,N-Dimethylhydrazones. A Diels-Alder Strategy for the Building of Aza-Hetero Rings. **2001**, 54, 1095 30
- 332 Structure and Reactivity of Cycloimmonium Ylides. **1999**, 51, 863 23
- 331 Computational Study for the Aromatic Nucleophilic Substitution Reaction on 1-Dimethylamino-2,4-bis(trifluoroacetyl)-naphthalene with Amines. **2018**, 08, 273-281 3
- 330 A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. **2014**, 05, 1185-1191 6
- 329 Hydration of Formaldehyde in Water: Insight from ONIOM Study. **2008**, 29, 2528-2530 5
- 328 Enantiomeric Recognition in Host-Guest Complexation Using Chiral Bis-pyridino-18-crown-6 Ethers, by Electrospray Ionization Mass Spectrometry (ESI-MS) Enantiomer-Labelled (EL) Guest Method. **2008**, 29, 1069-1072 3
- 327 A Comparative QSPR Study of Alkanes with the Help of Computational Chemistry. **2009**, 30, 67-76 6
- 326 Structural and Molecular Orbital Properties of Some Boroxine Derivatives-A Theoretical Study. **2009**, 30, 2233-2239 14
- 325 Synthesis of Some Novel Pyrimidine Derivatives and Investigation of their Electrochemical Behavior. **2010**, 31, 3632-3638 7
- 324 Studies on the Different Reaction Pathways between 3-Acetyl-5-benzoyl-6-methyl-2-phenyl-4H-pyran-4-one and Alkylamines. **2010**, 31, 2633-2636 3
- 323 Theoretical Studies on Nitramine Explosives with -NH₂ and -F Groups. **2012**, 33, 1913-1918 3
- 322 Molecular Orbital Interpretation on the Inhibitory Effect of the Ni(II) Complexes with Polyamines and Imidazole Derivatives. **2004**, 48, 123-128 1
- 321 Exploration of Novel Medicinal Leads by Use of Natural Products Inhibiting Nuclear Export of Proteins as Scaffolds. **2011**, 69, 393-402 0
- 320 From quantum chemical formation free energies to evaporation rates. 3
- 319 Photocatalytic Degradation of Surfactants. XX. Photooxidation of Sodium Butylnaphthalenesulfonates. **2003**, 52, 245-253 2
- 318 Unimolecular Metastable Decomposition of Bis(2,2,2-trifluoroethyl) Ether, CF₃CH₂OCH₂CF₃, and Ethyl 2,2,2-Trifluoroethyl Ether, CH₃CH₂OCH₂CF₃, upon Electron Ionization.. **2002**, 50, 193-198 3
- 317 Unimolecular Reactions of Diethyl Malonate Cation in Gas-phase. **2004**, 52, 263-270 1

- 316 Collision-Induced Dissociation (CID) Spectra versus Collision Energy Using a Quadrupole Ion Trap Mass Spectrometer IV -Dissociation of Ionized Maleamide and Fumaramide-. **2004**, 52, 57-62 1
- 315 Lignin-Derived Materials for Supercapacitors. **2021**, 1-51
- 314 Interaction of TATP with Some Group II Metals - A DFT Treatment. 1-16 1
- 313 Charged Forms of 2,6-Dinitro-1-oxidopyridin-1-ium-3,5-diamine - A DFT Treatment. 17-34
- 312 Local perturbations of periodic systems. Chemisorption and point defects by GoGreenGo. *Journal of Computational Chemistry*, **2021**, 42, 2352-2368 3.5
- 311 Implications of the Conformationally Flexible, Macrocyclic Structure of the First-Generation, Direct-Acting Anti-Viral Paritaprevir on Its Solid Form Complexity and Chameleonic Behavior. **2021**, 143, 17479-17491 4
- 310 Design, synthesis, spectral and theoretical study of new bile acid-sterol conjugates linked via 1,2,3-triazole ring. **2021**, 176, 108934 0
- 309 Photoinduced Electron-Transfer Reactions between C60 and Cyclic Disiliranes (c-R2Si-X-SiR2; X=SiR2, CH2, O, NPh, S). **2001**, 54, 777
- 308 Applications: Pharmaceuticals and Life Sciences. **2002**, 71-81
- 307 Free Energy Perturbation Calculations within Quantum Mechanical Methodologies. **2002**, 103-123
- 306 Science: Electronic Structure, Thermochemistry and Kinetics. **2002**, 9-22
- 305 Semiempirical Vibrational Frequencies (Including Scaling).
- 304 Semiempirical Methods: Integrals and Scaling.
- 303 MNDO/d.
- 302 Hydrogen Bonds: Semiempirical Methods.
- 301 Green's Function Ionization Potentials in Semiempirical MO Theory.
- 300 Quantitative Structure-Property Relationships (QSPR).
- 299 Divide and Conquer for Semiempirical MO Methods.

298 PM3.

297 MNDO.

296 Population Analyses for Semiempirical Methods.

295 Configuration Interaction: Semiempirical Calculations.

294 Quantum Mechanical/Molecular Mechanical (QM/MM) Coupled Potentials.

293 Parameterization of Semiempirical MO Methods.

292 Rotational Barriers and Molecular Mechanics Corrections.

291 AM1.

290 DNA Bases and Base Pairs: Ab Initio Calculations.

289 On Construction of Molecular Memory Based on Fullerene Adducts. **2003**, 293-303

288 Theoretical Study on Mechanism of Initiation Reaction of Asymmetric Anionic Polymerization of N-Substituted Maleimide with a Zn catalyst. **2003**, 4, 52-59

287 Electronic States of Chemically Modified CdS Nanoparticles. **2003**, 253-264

286 Surface Reactions at Metal Oxides: Relaxation Spectroscopy and Charge Transfer. **2003**, 41-53

285 Molecular-Level Machines: The Clockwork Model. **2003**, 343-354

284 Molecular Modeling of Fulvic and Humic Acids. **2003**,

283 In Silico Application of Quantum Chemical Methods for Relating Toxicity to Chemical Reactivity. **2003**,

282 Photochemically Induced Tautomerism of Salicylic Acid and Its Related Derivatives. **2003**,

281 Semiempirical Methods. **2003**,

280 Quantum-Chemical Descriptors in QSAR. **2003**,

279 Hybrid Quantum Mechanical/Molecular Mechanical Methods. **2003**,

278 Accuracy and Applicability of Quantum Chemical Methods in Computational Medicinal Chemistry. **2003**,

277 Molecular Mechanics and Comparison of Force Fields. **2003**,

276 Molecular Clockworks as Potential Models for Biological Chirality. **2004**, 29-37

275 T-Nanoconstructions on the (0001)-Surface of Graphite Based on Carbon (6,6)-Nanotubes. **2004**, 325-328

274 Charge Transfer through Single and Double-strand DNAs : Theoretical Analysis Based on Molecular Orbital Calculations. **2004**, 5, 52-61

273 Specific Interaction between Catabolite Activator Protein and Cyclic AMP: Molecular Mechanics and Molecular Orbital Calculations. **2005**, 6, 67-82

272 Cis-trans-regulation mechanism and multiplicity in ionic-coordinate polymerization of dienes. **2005**, 251-368

271 Polaronic charge transport mechanism in DNA. **2006**, 429-450

270 Structures and Electronic Properties of Calcium Binding Proteins with EF-hand Motif :Semiempirical Molecular Orbital Calculations. **2006**, 7, 78-86

269 Density Functional Studies on ATP, ADP, AMP, GTP and Their Mg²⁺ Complexes in Solvated States. **2006**, 7, 178-189

1

268 Structures of B-Podands Complexes with Cations Calculated by PMS Semiempirical Method. **2006**, 1102-1106

267 Two-Way Intramolecular Transfer of Chirality in Organocobalt Complexes. **2007**, 421-439

266 Vibrons in DNA: Their Influence on Transport. **2007**, 249-262

265 Nanomolecular Switches Operated by Clockwork Mechanism. **2007**, 441-452

264 Molecular Mechanics and Molecular Orbital Simulations on Specific Interactions between Peroxisome Proliferator-Activated Receptor PPAR and Plasticizers. **2007**, 8, 1-11

263 Calculation of Solubility of Organic Compounds in Supercritical CO₂ based on Quantitative Structure-Activity Relationships. **2007**, 21, 137-142

1

262 Models of Molecular Structure: Hybrid Perspective. **2008**, 95-204

261 EQUILIBRIUM CONFIGURATION AND ELECTRONIC STRUCTURE OF THE C₃₂H₈ MOLECULE ISOMERS. **2008**, 375-378

260 INFLUENCE OF IMPURITIES AND DEFECTS ON ELECTRONIC STRUCTURE OF CARBON NANOTUBES. **2008**, 365-368

259 Quantum Mechanics. 947-976

258 Toxicophores and Quantitative Structure -Toxicity Relationships for Some Environmental Pollutants. **2008**, 3, 94-104

2

257 Interpreting The Observed Substrate Selectivity And The Product Regioselectivity In Orf2-Catalyzed Prenylation From X-Ray Structures. **2009**, 351-375

256 Several Molecular Orbital Computations for a Dinuclear Nickel(II) Complex. **2009**, 8, 87-92

3

255 Electronic Properties and Reactivities of Perfect, Defected, and Doped Single-Walled Carbon Nanotubes. **2010**, 421-471

254 Structure and Function: Insights into Bioinorganic Systems from Molecular Mechanics Calculations. **2010**, 87-109

253 QM/MM Energy Functions, Configuration Optimizations, and Free Energy Simulations of Enzyme Catalysis. **2010**, 331-353

252 Transport Mechanism in the Escherichia coli Ammonia Channel AmtB: A Computational Study. **2010**, 397-429

251 Evaluation of the Correlation between the Onset Temperature and the Elongation of Bond Length by Temperature Rise. **2010**, 9, 47-54

250 Quantum-chemical study of degradation of molecular analogs of butadiene-styrene copolymer fragments during stretching by end atoms. **2010**, 50, 335

249 Design of Gas Barrier Membrane / Vapor Permeation Membrane - Approach from Diffusivity Prediction Model in Polymer Matrices -. **2011**, 36, 71-78

248 Theoretical Methods for Nonadiabatic Dynamics On the fly In Complex Systems and its Control by Laser Fields. **2012**, 299-325

247 A Review of Bonding in Dendrimers and Nano-Tubes. **2012**, 611-623

246 Recent Advances of Carbon Nanotube/Biopolymers Nanocomposites: A Technical Review. **2011**, 120-135

245 The first solvation shell of Reichardt's dye in ionic liquids: a semiempirical study. **2013**, 299-305

244 Topological Mechanochemistry of Graphene. **2013**, 285-301

243 Size effect of silk fibroin peptide chains in the growth process. **2013**, 62, 236101

2

242 Thermodynamics of Synthesis of New Phenoxazine Derivatives.

241 Nitrogen Acids. **2013**, 77-92

240 A Step Back: Hydrogen Abstraction from Methane Using a Semiempirical Molecular Orbital Method. **1991**, 525-531

239 A Theoretical Treatment of the Structural Aspects of the Topochemical Polymerization of Diacetylenes. **1992**, 161-170

238 A Strategy for Modelling of Chemical Reactivity using MC-SCF and MM-VB Methods. **1992**, 237-250

237 A Perspective of Peptide Modelling. **1994**, 377-416

236 A Theoretical Study on the Protonation of Nucleic Acid Pyrimidine and Purine Bases. **1994**, 331-351

235 Effect of Surface Termination of Si-Cluster on the Visible Luminescence of Porous-Si: A Correlation with Hydrogen, Fluorine, and Oxygen Atoms. **1994**, 417-422

234 Molecular Mechanics: Problems and Potential. **1994**, 53-88

233 Molecular Modelling Methods. **1994**, 1-52

232 FT-IR and FT-Raman Spectra of 5'-AMP. Application of Different Force Fields to Their Assignment. **1995**, 291-292

231 Theoretical Studies of Semiconductor Surfaces with Particular Reference to Fluorine and Chlorine Chemisorption on Si(001). **1995**, 175-189

230 Ten-membered Rings or Larger with One or More Oxygen and Sulfur Atoms. **1996**, 893-923

229 Soft X-ray absorption, UV photoemission, and VUV absorption spectroscopic studies of fluorinated fullerenes. **1996**, 453-456

228 Volume 2 References. **1996**, 969-1102

227 Second Order Static Hyperpolarizabilities of Unsaturated Polymers. **1996**, 297-311

- 226 Computer Modelling of Metal-Based Radiopharmaceuticals. **1996**, 201-217
- 225 Volume 3 References. **1996**, 817-932
- 224 Synthesis and Characterization of Carbon Electrode Materials for Rechargeable Batteries. **1996**, 349-362 1
- 223 Photoemission Study on Poly(pyridine-2,5-diyl), Poly(2,2'-bipyridine-5,5'-diyl), and their K-doped States. **1996**, 399-402
- 222 Key features of quantum chemistry methods used in CAMD. **1996**, 266-300
- 221 2,5-Dimethoxy-1,4-bis[2-(2,4-dimethoxyphenyl) ethenyl]benzene studied by quantum chemical calculations and single crystal X-ray diffraction. *Journal of Computational Chemistry*, **1996**, 17, 1820-1835^{3,5}
- 220 Infrared Scaled Frequencies by Semiempirical Methods in Several Local Anesthetics of Procaine Type. **1997**, 541-542
- 219 The Role of Electrostatics at the Catalytic Metal Binding Site in Xylose Isomerase Action. **1997**, 419-439
- 218 Frequencies and Structure of the 1,3-Deimethyluracil Devier. **1997**, 215-216
- 217 Structure and solvation effects of PO₄³⁻, HPO₄²⁻, H₂PO₄⁻ and H₃PO₄ from AM1 and PM3. **1997**, 245-248
- 216 Geometries and Stabilities of G₃GC, T₃AT, A₃AT and C₃GC Nucleic Acid Base Triplets. **1997**, 285-297
- 215 Sensor Response and Computational Molecular Modelling. **1998**, 27-40
- 214 MOLECULAR ORBITAL MODELS OF SPECIES INVOLVED IN THE BONE BONDING OF BIOACTIVE GLASSES AND GLASS-CERAMICS. **1998**,
- 213 Structure-Activity Relationship and Molecular Design of Peroxidizing Herbicides with Cyclic Imide Structures and Their Relatives. **1999**, 91-139 2
- 212 Modified Uracils Convertible between Cations, Conjugated, and Cross-conjugated Mesomeric Betaines. Syntheses, Semiempirical Study, and X-Ray Analysis. **1999**, 51, 237 1
- 211 Quantum Chemistry: Integrated Methods. 3961-3974
- 210 A Theoretical Approach to Ion-Molecule Complexation. **2015**, 41-81 0
- 209 Guide to Programs for Nonrelativistic Quantum Chemistry Calculations. **2015**, 1-23

208 Molecular Structure and Vibrational Spectra. **2015**, 1-74

207 Evaluation of Homolytic Dissociation Energies by Quantum Mechanical Methods. **2015**, 127, 891-894

206 Study of Carbon Nanostructures for Soil Fertility Improvement. **2016**, 85-104

205 An Approach to Developing Electronic Laboratory TextbookExperimental Program of Esterification of Acetic Acid and Ethanol. **2016**, 289-296

204 Fundamental Structural, Electronic, and Chemical Properties of Carbon Nanostructures: Graphene, Fullerenes, Carbon Nanotubes, and Their Derivatives. **2016**, 1-84

203 Quantum Mechanics for Quantum Chemistry. **2016**, 357-549

202 Modeling Molecular Aromaticity. **2016**, 441-522

201 3D-QSAR study and development of pharmacophore for serotonin 5-HT_{2A} receptors agonists. **2017**, 67, 165-179

200 3D-QSAR modeling and pharmacophore study of serotonin 5HT-_{2A} receptors antagonists. **2017**, 67, 233-247

199 Quantum Chemical Computational Studies on a vic-Dioxime Ligand and Its Nickel Complex. 1-1

198 ~~600-4-001,2-a]E(1H)-E-~~
~~"EPL-2018~~, 1350-1354

197 Computational Study for the Selective Aromatic Nucleophilic Substitution on 4-Dimethylamino-2-methoxy-3-trifluoroacetylquinoline. **2018**, 97, 451

3

196 Crystal structure and theoretical study of (2)-1-[4-hy-droxy-3-(morpholin-4-ylmeth-yl)phen-yl]-3-(thio-phen-2-yl)prop-2-en-1-one. **2018**, 74, 960-963

2

195 Quantum Mechanics. 320-344

194 A participatory action research on the improvement of outdoor play in kindergarten. **2018**, 38, 83-107

193 Selective Aromatic Nucleophilic Substitution of 4-(Dimethylamino)-2-methoxy-3-(trifluoroacetyl)quinoline with Thiols DFT Calculation Study. **2019**, 99, 694

2

192 Some DADNE Embedded Push-Pull Type Structures - A DFT Study. 1-23

191 Copper (I) Nicotinate complex Abrogates Acrylamide Induced Hepatotoxicity in Male Rats: Biochemical and Histological Studies. **2019**, 6, 21-31

- 190 Epoxides of DADNE Isomers - A DFT Study. 121-139 1
- 189 Interaction of TNT with Dopamine - A DFT Treatment. 175-188
- 188 Interaction of CL-20 and Zinc Δ A DFT Treatment. 205-215
- 187 Interaction of 1,1-Diamino-2,2-Dinitroethylene and Gallium - DFT Treatment. 271-291 3
- 186 Destructive Effect of Zinc on TEX - A DFT Treatment. 1-15
- 185 Tautomerism in Pindone Δ A DFT Study. 35-50 1
- 184 cis- and trans-2,5,7,9-Tetranitro-2,5,7,9-tetraazabicyclo[4,3,0]nonan-8-one and Some of its Isomers-A DFT Treatise. 77-88
- 183 Tautomerism in Flindersine - A DFT Treatment. 89-104
- 182 Deciphering the structure of itaconate-based unsaturated polyester resins by high resolution mass spectrometry. **2020**, 69, 1140-1151 0
- 181 Some Curcumin Isomers and Their Enol Tautomers - A DFT Treatment. 183-197
- 180 Compatibility of Diborane and Borane with FOX-7 - A DFT Treatment. 209-225
- 179 Inhomogeneities of charge distribution in porous graphitic carbon nitride g-CxNy nanosheets. **2020**, 74, 1
- 178 Computational studies of biologically active alkaloids of plant origin: an overview. **2020**,
- 177 1,3,5-Triamino-2,4,6-trinitrobenzene and Magnesium Interaction-A DFT Treatment. 175-190
- 176 Dinitro Derivatives of 3,6,7,8-tetraazatricyclo $[1^{\{1,5\}}. 1^{\{1,5\}}.1^{\{2,4\}}. 1^{\{2,4\}}]$ octa-1,4-diene Δ A DFT Treatment. 151-165
- 175 Molecular Modelling. **2020**, 3-48
- 174 Interaction of Pindone and its Tautomers with Calcium Dication Δ A DFT Study. 77-91
- 173 Dinitro Derivatives of 3,6,7,8-tetraazatricyclo[11,5. 11,5.12,4. 12,4]octa-1,4-diene Δ A DFT Treatment. 151-165

- 172 Computational Study of the Stability of Natural Amino Acid isomers. **2021**, 1 0
- 171 Application of in vitro PAMPA technique and in silico computational methods for blood-brain barrier permeability prediction of novel CNS drug candidates. **2021**, 168, 106056 5
- 170 Multidimensional Free Energy and Accelerated Quantum Library Methods Provide a Gateway to Glycoenzyme Conformational, Electronic, and Reaction Mechanisms. **2021**, 54, 4120-4130 0
- 169 Some DADNE Originated Cyclic Isomers - A DFT Study. 137-153 0
- 168 Homolytic C-NO₂ Bond Cleavage in Diaminodinitroethylene Isomers - A DFT Treatment. 115-136
- 167 On the Mechanisms of Proteinases. **2002**, 295-340 1
- 166 Theoretical Study of Circular Dichroism Spectra in the Vacuum-Ultraviolet. **1999**, 93-119
- 165 Semiempirical Thermochemistry: A Brief Survey. **2001**, 235-245
- 164 Theoretical Studies of Growth Reactions on Diamond Surfaces. **2004**, 266-307 1
- 163 Towards Fast and Reliable Quantum Chemical Modelling of Macromolecules. **2006**, 315-341 0
- 162 ELECTRONIC STRUCTURE OF Y-JUNCTIONS OF CARBON NANOTUBES. **2007**, 801-804
- 161 ELECTRONIC STRUCTURE OF CARBON NANOTUBES OF VARIABLE DIAMETER. **2007**, 707-712
- 160 ELECTRONIC STRUCTURE OF T-JUNCTIONS OF CARBON NANOTUBES. **2007**, 721-728
- 159 An Introduction to Molecular Modeling. 1-25
- 158 Tin-DNA complexes investigated by nuclear inelastic scattering of synchrotron radiation. **2006**, 299-302
- 157 Tautomerism in Fusicin - A DFT Treatment. 243-259
- 156 Effect of Copper on 1,1-Diamino-2,2-dinitroethene - A DFT Treatment. 1-17
- 155 Effect of Titanium on FOX-7 - A DFT Treatment. 19-34

154 Some Novel Tricyclic Caged-Nitramines - A DFT Study. 35-48

153 About the Creation of Sensor of New Firefighting, Devices Based on Nanostructures for Determination of Carbon Monoxide and Carbon Dioxide Components. **2021**, 277-287

152 Two-dimensional ferroelectrics and uniform switching. To the 75th anniversary of the Landau-Ginzburg theory of ferroelectricity. **2020**, 190,

o

151 Theoretical and experimental studies for different compounds to calculate: electronic transfer, energy gap and NLO properties. **2020**, 928, 072010

150 Integrated Ligand and Structure based approaches towards developing novel Janus Kinase 2 inhibitors for the treatment of myeloproliferative neoplasms.

149 Interaction of Carmustine Tautomers with Adenine - DFT Study. 63-76

o

148 Interaction of 1,1-Diamino-2,2-Dinitroethylene with Aluminum and Gallium Admixture - DFT Treatment. 87-103

147 Computer modeling and numerical studies of peptide nanotubes based on diphenylalanine. **2021**, 1-54

o

146 A review of quantum chemical methods for treating energetic molecules. **2021**, 2, 292-292

3

145 Charged Forms of Diacetone Diperoxide - DFT Treatment. 53-65

144 Direct evidence of edge-to-face CH/π interaction for PAR-1 thrombin receptor activation. **2021**, 51, 116498

o

143 Parametric method three (PM3) study of the tautomerization of 2- pyridone systems. **1994**, 106, 163-168

142 Experimental and computational (AM1, MNDO, PM3) studies on the hydrolysis rates of ethylene ketals in 1,3-cyclohexanediones. **1996**, 108, 51-56

141 Iron(III) complexes of phenolate ligands as models for catechol dioxygenases. **1996**, 108, 235-249

3

140 A semiempirical MO study of tautomerism and the electronic structure of barbituric acid. **1998**, 110, 535

8

139 Solvatochromism of 4-(diethylamino)-4-nitroazobenzene: explanation based on CNDO/S calculation results. **2021**, 22, 8-16

138 Dinitrohydrazines and Interaction of Them with Some Group-II Metals - DFT Treatment. 115-126

137 Spectroanalytical, computational, DNA/BSA binding and in vitro cytotoxic activity studies of new transition metal complexes of novel aryl hydrazone. **2022**, 1252, 132126

- 136 A Cyclic Periodic Wave Function Approach for the Study of Infinitely Periodic Solid-State Systems. I. Application to the CH₃C≡C Hydrogen Bonding Systems. **2020**, 5, 27546-27555 4
- 135 Two-dimensional ferroelectrics and homogeneous switching. On the 75th anniversary of the Landau-Ginzburg theory of ferroelectricity. **2021**, 63, 1140-1147
- 134 Nanostructured Bismuth Electrodes for Non-Enzymatic Paracetamol Sensing: Development, Testing, and Computational Approach. **2021**, 5, 33
- 133 The Study of Steroid Keys for Androgen Receptors. **2021**, 66, 738-745
- 132 Dicyanofuroxan and Its Charged Forms - A DFT Study. 127-142
- 131 Testing and Optimizing the Drude Polarizable Force Field for Blocked Amino Acids Based on High-Level Quantum-Mechanical Energy Surfaces. 1-9 1
- 130 Superior performance of the machine-learning GAP force field for fullerene structures. **2022**, 33, 505 1
- 129 Capturing non-local through-bond effects in molecular mechanics force fields: II. Using fractional bond orders to fit torsion parameters. 1
- 128 The binding mechanism of NHWD-870 to bromodomain-containing protein 4 based on molecular dynamics simulations and free energy calculation.. **2022**, 1
- 127 Inhibition of mitochondrial LonP1 protease by allosteric blockade of ATP -binding and -hydrolysis via CDDO and its derivatives.. **2022**, 101719 0
- 126 The reaction path of cyclooctatetraene dimerization revisited. 1
- 125 PM3 Method based QSAR Study of the Derivatives of Thiadiazole and Quinoxaline for Antiepileptic Activity using Topological Descriptors. **2022**, 7, 99-110
- 124 Theoretical studies of gas-phase decomposition of single-source precursors. **2022**, 123-161
- 123 Molecular Interactions of Tannic Acid with Proteins Associated with SARS-CoV-2 Infectivity.. **2022**, 23, 1
- 122 Structure-Activity Relationship of -Phenylthieno[2,3-]pyridine-2-carboxamide Derivatives Designed as Forkhead Box M1 Inhibitors: The Effect of Electron-Withdrawing and Donating Substituents on the Phenyl Ring.. **2022**, 15, 0
- 121 Eco-friendly dyeing of cationised cotton with reactive dyes: mechanism of bonding reactive dyes with CHPTAC cationised cellulose. 1 2
- 120 Effect of Nitro-Iodol Group Replacement on TNT - A DFT Treatment. 53-67
- 119 Molecular Dynamics Simulation Study of the Self-Assembly of Phenylalanine Peptide Nanotubes.. **2022**, 12, 0

118	Molecular modelling and computational studies of peptide diphenylalanine nanotubes, containing waters: structural and interactions analysis.. 2022 , 28, 81	1
117	Effects of Coumarinyl Schiff Bases against Phytopathogenic Fungi, the Soil-Beneficial Bacteria and Entomopathogenic Nematodes: Deeper Insight into the Mechanism of Action.. 2022 , 27,	1
116	Benchmarking Semiempirical QM Methods for Calculating the Dipole Moment of Organic Molecules.. 2022 ,	4
115	Some Ions of Hexamethylene Triperoxide Diamine - A DFT Treatment. 1-12	
114	A Data Resource for Prediction of Gas-Phase Thermodynamic Properties of Small Molecules. 2022 , 7, 33	0
113	Catechin mediated green synthesis of Au nanoparticles: Experimental and theoretical approaches to the determination HOMO-LUMO energy gap and reactivity indexes for the (+)-epicatechin (2S, 3S). 2022 , 15, 103758	0
112	Substitution-inert polynuclear platinum complexes and Glycosaminoglycans: A molecular dynamics study of its non-covalent interactions.. 2022 , 232, 111811	
111	Isotope Effects on the Vaporization of Organic Compounds from an Aqueous Solution-Insight from Experiment and Computations.. 2021 , 125, 13868-13885	1
110	Comparison of Oxidative Powers of DADP and TATP - A DFT Treatise. 67-80	
109	Enantioselective Voltammetric Sensors Based on Amino Acid Complexes of Cu(II), Co(III), and Zn(II). 2021 , 76, 1438-1448	1
108	Quantum Mechanical Investigation on Decomposition Pathways of BuNENA. 2022 , 47,	
107	Molecular Docking Analysis of Used Drugs for the Treatment of Cancer. 539-547	
106	OUP accepted manuscript.	0
105	Mechanism of E-bridge formation by various PAH molecules: A theoretical study. 2022 , 139637	2
104	Review on the QM/MM Methodologies and Their Application to Metalloproteins.. 2022 , 27,	1
103	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations.. 2022 , 23,	0
102	Presentation1.PDF. 2018 ,	
101	Data_Sheet_1.PDF. 2020 ,	

- 100 Alkaline-earth metal(II) complexes of salinomycin: Spectral properties and antibacterial activity. **2022**, 0
- 99 Computational vibrational spectroscopy of molecule-surface interactions: what is still difficult and what can be done about it.. **2022**, 3
- 98 Computational Modeling of Supramolecular Metallo-organic Cages: Challenges and Opportunities. 5806-5826 3
- 97 Synthesis, characterization and investigation of fluorescent Sn²⁺ probe potential of pyrene-derived monomer and its oligo(azomethine) compound. **2022**, 172, 111229 0
- 96 Mononitro-monoperchlorylbenzenes - A DFT Treatment. 77-95
- 95 3D QSAR Analysis of Flavones as Antidiabetic agents. **2022**, 1689-1695
- 94 Combining classical molecular docking with self-consistent charge density-functional tight-binding computations for the efficient and quality prediction of ligand binding structure. **2022**, 46, 174751982211019
- 93 Regression Modeling for the Prediction of Hydrogen Atom Transfer Barriers in Cytochrome P450 from Semi-empirically Derived Descriptors.
- 92 Accelerating Ab Initio Quantum Mechanical and Molecular Mechanical (QM/MM) Molecular Dynamics Simulations with Multiple Time Step Integration and a Recalibrated Semiempirical QM/MM Hamiltonian.
- 91 DFT Treatment of Hydrazine - Nitroform Interaction. 131-145
- 90 Role of an intramolecular H-bond in lidocaine conformer distribution and polymorph stability. **2022**, 360, 119461 1
- 89 In silico drug repurposing for coronavirus (COVID-19): screening known HCV drugs against the SARS-CoV-2 spike protein bound to angiotensin-converting enzyme 2 (ACE2) (6M0J).
- 88 Electrodeposition and Characterization of Conducting Polymer Films Obtained from Carbazole and 2-(9H-carbazol-9-yl)acetic Acid. **2022**, 3, 322-336
- 87 In silico study to identify novel potential thiadiazole-based molecules as anti-Covid-19 candidates by hierarchical virtual screening and molecular dynamics simulations. 3
- 86 Efficient and Accurate Description of Diels-Alder Reactions using Density Functional Theory. 0
- 85 A Simple Molecular Model to Study the Substrate Diffusion into the Active Site of a Lipase-Catalyzed Esterification of Ibuprofen and Ketoprofen with Glycerol. 0
- 84 Effect of Aluminum on Nitroform - A DFT Study. 147-162
- 83 The Conformational Landscape Of β -Aminoglycine. **2022**, 111667

81 Discovery of new chemotypes of dual 5-HT_{2A}/D₂ receptor antagonists with a strategy of drug design methodologies. **2022**, 14, 963-989

64	ULYSSES: An Efficient and Easy to Use Semiempirical Library for C++. 2022 , 62, 3685-3694	2
63	A Study on Repositioning Nalidixic Acid via Lanthanide Complexation: Synthesis, Characterization, Cytotoxicity and DNA/Protein Binding Studies. 2022 , 15, 1010	1
62	Understanding the anti-corrosion characteristics of a newly synthesized Schiff's base: an experimental and computational approach. 2022 ,	1
61	MagicMolecules and a New Look at Chemical Diversity of Hydrocarbons. 2022 , 13, 7600-7606	0
60	Carbon Nanodots from an In Silico Perspective. 2022 , 122, 13709-13799	2
59	Effect of Isotopic Nitrogen Exchange on NTO Molecule-A DFT Approach. 193-204	
58	Design, synthesis, and in vitro anticancer activity of thiophene substituted pyridine derivatives. 2023 , 127-143	0
57	Computer Simulations of MOF Systems: Key Applications. 2022 , 231-253	0
56	Density Functional Theory on the CO ₂ Absorption Process with Ionic Liquids. 2022 , 967-972	0
55	Partition of the electronic energy of the PM7 method via the interacting quantum atoms approach. 2022 , 24, 19521-19530	1
54	Molecular Docking, Molecular Dynamics Simulations, and Free Energy Calculation Insights into the Binding Mechanism between VS-4718 and Focal Adhesion Kinase. 2022 , 7, 32442-32456	1
53	Association of 5,5'-Dibromo-o-Cresolsulfonphthalein Anions with Dye Cations in Aqueous Solution. 2022 , 16, 387-397	0
52	Experimental and computational evaluation of dipeptidyl peptidase III inhibitors based on quinazolinone-Schiff bases. 1-15	0
51	Effect of Aluminum on 1,3,5,5-tetranitrohexahydropyrimidine (DNNC) - A DFT Treatment. 1-16	0
50	Some Tautomers of Dacarbazine - A DFT Study. 47-62	0
49	Allyl Aryl Ether Cleavage by Blautia sp. MRG-PMF1 Cocorrinoid O -Demethylase.	0
48	Conformational preferences of tolfenamic acid in DMSO-CO ₂ solvent system by 2D NOESY. 2022 , 367, 120481	2
47	A computational study of the inclusion of β -cyclodextrin and nicotinic acid: DFT, DFT-D, NPA, NBO, QTAIM, and NCI-RDG studies. 2022 , 28,	2

46	Prediction of the photofading of 1-H or 1-ethyl derivatives of 3-cyano-6-hydroxy-4-methyl-5-(p-X-phenylazo)-2-pyridone dyes and their azo-hydrazone tautomerism: a theoretical study.	0
45	Tautomers of Ethosuximide and their Interaction with Calcium Cation - A DFT Treatment. 103-119	0
44	Pillar[5]arene-induced DNA condensation: liquid-liquid phase separation in pillar[5]arene-oligonucleotide system. 2022 , 120683	1
43	Multiple Logistic Regression Modeling of Compound Class as Active or Inactive Against COX-2 and Prediction on Designed Coxib Derivatives and Similar Compounds. 2022 , 22, 63-87	0
42	Identification of defactinib derivatives targeting focal adhesion kinase using ensemble docking, molecular dynamics simulations and binding free energy calculations. 1-17	0
41	Unexpected Gas-Phase Nitrogen-Oxygen Smiles Rearrangement: Collision-Induced Dissociation of Deprotonated 2-(N-Methylanilino)ethanol and Morpholinylbenzoic Acid Derivatives. 2022 , 33, 2120-2128	0
40	Reliable gas-phase tautomer equilibria of drug-like molecule scaffolds and the issue of continuum solvation.	2
39	Quantitative structure-property relationships in the series of diazonium cations, intermediate products in the synthesis of analytical forms and dyes. 2005 , 60, 130-136	1
38	Redshifting and Blueshifting of π 2 Chromophores in the Phycocyanin Hexamer of Porphyridium purpureum Phycobilisomes Due to Linker Proteins. 2022 , 12, 1833	0
37	Structural and vibrational investigations and molecular docking studies of a vinca alkaloid, vinorelbine. 1-20	0
36	Interaction of DMAZ and TEMED - A DFT Treatise. 163-176	0
35	Characterization of a bioscaffold containing polysaccharide acemannan and native collagen for pulp tissue regeneration. 2022 ,	0
34	Study of methylene blue dye elimination from water using polyaniline (PANI) and PANI/SiO ₂ composite. 2022 , 30, 096739112211417	0
33	Photochemistry of Biological Systems: Excited-State Electronic Structure Calculations and Nonadiabatic Dynamics Simulations with QM/MM Methods. 2022 ,	0
32	Some Tautomers of Amrinone and their Interaction with Calcium Cation - DFT Treatment. 209-226	0
31	Synthesis, Antiproliferative Evaluation and QSAR Analysis of Novel Halogen- and Amidino-Substituted Benzothiazoles and Benzimidazoles. 2022 , 23, 15843	0
30	An Improved Parameterization Procedure for NDDO-Descendant Semiempirical Methods.	0
29	On the Origin of the Blue Color in The Iodine/Iodide/Starch Supramolecular Complex. 2022 , 27, 8974	0

- 28 The Effects of BTTN, TMETN and DEGDN Molecules on the Explosion Properties of PETN Molecule. 366-371 ○
- 27 Effects of Encapsulating Tube and Encapsulated Molecular Chain Length on the Second-Order Nonlinear Optical Responses of Carbon Nanotubes Filled with Head-To-Tail Polar Molecules. **2022**, 126, 21328-21337 ○
- 26 Ultra-Fast Semi-Empirical Quantum Chemistry for High-Throughput Computational Campaigns with Sparrow. ○
- 25 Diazoxide and its Tautomers - A DFT Treatment. 249-265 ○
- 24 QM/MM Studies on Enzyme Catalysis and Insight into Designing of New Inhibitors by ONIOM Approach: Recent Update. **2023**, 8, ○
- 23 Long-range Corrected Fragment Molecular Orbital Density-Functional Tight-binding Method for Excited States in Large Molecular Systems. 1
- 22 Origin of Catalysis by Nitroalkane Oxidase. **2023**, 127, 151-162 ○
- 21 Discovery of a Novel Covalent EZH2 Inhibitor Based on Tazemetostat Scaffold for the Treatment of Ovarian Cancer. **2023**, 66, 1725-1741 ○
- 20 The inhibitory activity of Ruxolitinib against COVID-19 major protease enzyme and SARS CoV-2 spike glycoprotein: A molecular docking study. **2023**, 8, 1-9 ○
- 19 Using Stationary Points on Potential Energy Surfaces to Model Intermolecular Interactions and Retention in Gas Chromatography. **2004**, 59, 329-334 ○
- 18 Flow Synthesis of Gigantic Porphyrinic Cages: Facile Synthesis of P12L24 and Discovery of Kinetic Product P9L18. ○
- 17 Predicted Structure of the BciC Enzyme Catalyzing the Removal of the C132-Methoxycarbonyl Group for Biosynthesis of Chlorosomal Chlorophylls: A Mechanism for Dual Catalytic Functions of Hydrolysis and Decarboxylation inside Its Active Site. ○
- 16 A modified bonded model approach for molecular dynamics simulations of New Delhi Metallo- β -lactamase. **2023**, 121, 108431 ○
- 15 Synthesis and molecular structure of V-shaped liquid crystalline compounds: Spectroscopic, mesomorphic, DFT investigations, electrochemical and fluorescence studies. **2023**, 1283, 135304 ○
- 14 Design, synthesis and biological evaluation of purine-based derivatives as novel JAK2/BRD4(BD2) dual target inhibitors. **2023**, 132, 106386 ○
- 13 Study of Some Azo Derivatives as Corrosion Inhibitors for Mild Steel in 1 M H₂SO₄. **2022**, 58, 708-719 ○
- 12 Molecular Mechanism of Conformational Crossover of Mefenamic Acid Molecules in scCO₂. **2023**, 16, 1403 ○
- 11 Comparison of theoretical methods via different ways for assessing the heat of formation of cubane. ○

- 10 Doping of Graphene Nanostructure with Iron, Nickel and Zinc as Selective Detector for the Toxic Gas Removal: A Density Functional Theory Study. **2023**, 9, 20 ○
- 9 Mechanistic Modeling of Lys745 Sulfonylation in EGFR C797S Reveals Chemical Determinants for Inhibitor Activity and Discriminates Reversible from Irreversible Agents. **2023**, 63, 1301-1312 ○
- 8 A Computational Study on the Role of Lubricants under Boundary Lubrication. **2023**, 11, 80 ○
- 7 DFT Treatment of Some Cantharidine Isomers and Some Radicals from Them. 77-91 ○
- 6 An improved parameterization procedure for NDDO-descendant semi-empirical methods. **2023**, 29, ○
- 5 Synthesis, Computational Studies, Molecular Docking, Anti-inflammatory and Antioxidant Activities of β -Aminophosphonates Incorporating an Azo Chromophore for Polyester Printing Application. **2023**, 8, ○
- 4 Benzo[g]quinazolines as antifungal against candidiasis: screening, molecular docking, and QSAR investigations. **2023**, ○
- 3 Some Isomers of Nevirapine - A DFT Study. 93-109 ○
- 2 Discovery of pyrimidine-5-carboxamide derivatives as novel salt-inducible kinases (SIKs) inhibitors for inflammatory bowel disease (IBD) treatment. **2023**, 256, 115469 ○
- 1 Insights into the carbonization mechanism of PAN-derived carbon precursor fibers and establishment of a kinetics-driven accelerated reaction template for atomistic simulation. ○