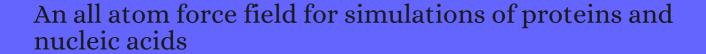
CITATION REPORT List of articles citing



DOI: 10.1002/jcc.540070216 Journal of Computational Chemistry, 1986, 7, 230-252.

Source: https://exaly.com/paper-pdf/18425893/citation-report.pdf

Version: 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
2316	Modeling complex molecular interactions involving proteins and DNA. 1986 , 482, 234-44		12
2315	Computer modeling of actinomycin D interactions with double-helical DNA. 1986 , 191, 495-507		41
2314	Molecular Dynamics Simulations of DNA Double Helices: Studies of Sequence Dependence and the Role of Mismatch Pairs in the DNA Helix. 1986 , 27, 189-197		16
2313	Free energy calculations by computer simulation. 1987 , 236, 564-8		386
2312	Conformational and model-building studies of the hairpin form of the mismatched DNA octamer d(m5C-G-m5C-G-T-G-m5C-G). 1987 , 4, 965-87		36
2311	Molecular mechanics and dynamics in protein design. 1987 , 154, 430-49		9
2310	Conformational properties of 3'-azido-3'deoxy-thymidine (AZT), an inhibitor of HIV reverse transcriptase. 1987 , 145, 1356-61		14
2309	Molecular dynamics simulations of "loop closing" in the enzyme triose phosphate isomerase. 1987 , 198, 533-46		39
2308	Energy minimization and molecular dynamics studies of Asn-102 elastase. 1987 , 1, 211-7		7
2307	Calibration of effective van der Waals atomic contact radii for proteins and peptides. 1987 , 2, 330-9		57
2306	An efficient newton-like method for molecular mechanics energy minimization of large molecules. Journal of Computational Chemistry, 1987 , 8, 1016-1024	3.5	785
2305	Nonbonded interactions. 1. Anisotropic hydrogen-hydrogen interactions. <i>Journal of Computational Chemistry</i> , 1987 , 8, 1124-1130	3.5	20
2304	Benzene-benzene (phenyl-phenyl) interactions in MM2/MMP2 molecular mechanics calculations. Journal of Computational Chemistry, 1987 , 8, 1139-1145	3.5	60
2303	An analysis of the structural and energetic properties of deoxyribose by potential energy methods. Journal of Computational Chemistry, 1987, 8, 1199-1224	3.5	29
2302	PEPCRE: an interactive program to create, manipulate and display oligopeptides. 1987 , 5, 119-125		6
2301	Electrostatic potential and binding of drugs to the minor groove of DNA. 1987, 5, 165-166		16
2300	An NMR study of polymorphous behaviour of the mismatched DNA octamer d(m5C-G-m5C-G-A-G-m5C-G) in solution. The B-duplex and hairpin forms. 1987 , 170, 225-39		35

2299	Conformational analysis of the dinucleotides 5'-methylphospho-N6-dimethyladenylyl-uridine (mpm62A-U) and 5'methylphospho-uridylyl-N6-dimethyladenosine (mpU-m62A) and of the trinucleotide U-m62A-U. A nuclear magnetic resonance and circular dichroic study. 1988 , 171, 143-53		10
2298	Molecular mechanics calculation of geometries of NAD+ derivatives, modified in the nicotinamide group, in a ternary complex with horse liver alcohol dehydrogenase. 1988 , 175, 581-5		9
2297	Secondary structure of the Arg-Gly-Asp recognition site in proteins involved in cell-surface adhesion. Evidence for the occurrence of nested beta-bends in the model hexapeptide GRGDSP. 1988 , 178, 141-54		72
2296	The role of hydroxyproline in collagen folding: conformational energy calculations on oligopeptides containing proline and hydroxyproline. 1988 , 27, 299-312		15
2295	Conformational behavior of ⊞dialkylated peptides: Ab initio and empirical results for cyclopropylglycine. 1988 , 27, 1673-1685		38
2294	Atomic physicochemical parameters for three dimensional structure directed quantitative structure-activity relationships III: Modeling hydrophobic interactions. <i>Journal of Computational Chemistry</i> , 1988 , 9, 80-90	3.5	404
2293	A method for calculating atomic charges in large molecules. <i>Journal of Computational Chemistry</i> , 1988 , 9, 399-405	3.5	17
2292	Determination of the major solution conformation of tyrocidine A, using molecular mechanics energy minimization and NMR-derived distance and torsion angle constraints. <i>Journal of Computational Chemistry</i> , 1988 , 9, 522-538	3.5	9
2291	Representation of the molecular electrostatic potential by atomic multipole and bond dipole models. <i>Journal of Computational Chemistry</i> , 1988 , 9, 745-763	3.5	154
2290	A simple method for calculating reliable atomic charges in large molecules. <i>Journal of Computational Chemistry</i> , 1988 , 9, 764-770	3.5	9
2289	Molecular modelling in design of crop protection chemicals. 1988 , 2, 191-216		7
2288	Unusual Cis ring junction stereochemistry in a lactol derived from photo-oxygenation of abietic acid: An NMR and molecular modeling study. 1988 , 1, 133-139		1
2287	Polar hydrogen positions in proteins: empirical energy placement and neutron diffraction comparison. 1988 , 4, 148-56		467
2286	Electrostatics and molecular recognition. 1988 , 34, 85-93		1
2285	The application of simulated annealing to problems of molecular mechanics. 1988, 34, 611-617		19
2284	Computed redox potentials and the design of bioreductive agents. 1988 , 334, 80-2		74
2283	Location of divalent ion sites in acyl carrier protein using relaxation perturbed 2D NMR. 1988 , 238, 43-8		31
2282	Structural modeling of the distamycin A-d(CGCGAATTCGCG)2 complex using 2D NMR and molecular mechanics. 1988 , 27, 8088-96		90

2281	COMMUNICATIONS. 1988 , 95, 475P-589P	5
2280	Weakly polar interactions in proteins. 1988 , 39, 125-89	604
2279	Using Molecular Mechanics to Model the Movement and Relaxation of Radical Pairs Created By Photolysis of Single Crystals of Acetyl Benzoyl Peroxide (ABP). 1988 , 156, 109-122	1
2278	Increased Rigidity in Complexes Formed from Negatively Charged Lariat Ethers and Alkali Metal Cations. 1988 , 18, 85-91	
2277	Three-dimensional solution structure of plastocyanin from the green alga Scenedesmus obliquus. 1988 , 240, 314-7	91
2276	Experimental DNA-binding and computer modelling studies on an analogue of the anti-tumor drug amsacrine. 1988 , 6, 471-88	11
2275	Stability and motion of a hairpin and the corresponding mismatched duplex: a theoretical exploration using molecular mechanics and normal mode analysis of 2D NMR results on d(GCCGCAGC). 1988 , 6, 525-42	9
2274	Theoretical studies on alpha-helixDNA interactions. 1988 , 5, 859-71	2
2273	Determination of Protein Structures in Solution Using Nmr Data and Impact. 1988 , 2, 41-61	23
2272	Reassessment of structural characteristics of the d(CGCG)2:actinomycin D complex from complete 1H and 31P NMR. 1989 , 7, 557-89	14
2271	A comparison of the CHARMM, AMBER and ECEPP potentials for peptides. I. Conformational predictions for the tandemly repeated peptide (Asn-Ala-Asn-Pro)9. 1989 , 7, 391-419	76
2270	Molecular modeling and energy refinement of supercoiled DNA. 1989 , 7, 661-92	11
2269	A new method for carrying out free energy perturbation calculations: Dynamically modified windows. 1989 , 90, 2460-2470	106
2268	Preliminary Analysis of Water Molecule Distributions in Proteins. 1989 , 3, 167-182	4
2267	The lag between the Hamiltonian and the system configuration in free energy perturbation calculations. 1989 , 91, 7831-7839	110
2266		
2265	Three-dimensional solution structure of a single zinc finger DNA-binding domain. 1989 , 245, 635-7	580
2264	Molecular Design with Transparallel Supercomputers. 1989 , 3, 71-100	6

2263	The influence of the calculation method on conformational analysis of pyrrolidin-2-one derivatives. 1989 , 201, 199-212		7
2262	Molecular dynamics simulation of double helix Z-DNA in solution. 1989 , 129, 175-183		37
2261	Conformational analysis of brominated pA2'-5'A2'-5'A analogs. An NMR and model-building study. 1989 , 182, 629-37		14
2260	Molecular dynamics by the Backward-Euler method. 1989 , 42, 1001-1031		58
2259	On the Macrolactonization of Hydroxy Acids. Crystal structures of the pentolide and the hexolide from (R)-3-hydroxybutanoic acid. Molecular modeling studies of the tetrolide. 1989 , 72, 1704-1717		18
2258	Atomic charge models for polypeptides derived from ab initio calculations. <i>Journal of Computational Chemistry</i> , 1989 , 10, 479-487	3.5	32
2257	An ab initio distributed multipole study of the electrostatic potential around an undecapeptide cyclosporin derivative and a comparison with point charge electrostatic models. <i>Journal of Computational Chemistry</i> , 1989 , 10, 552-567	3.5	39
2256	Locally dense basis sets for chemical shift calculations. <i>Journal of Computational Chemistry</i> , 1989 , 10, 648-659	3.5	213
2255	Force field parameterization for the 4-fluorophenyl group. <i>Journal of Computational Chemistry</i> , 1989 , 10, 711-717	3.5	7
2254	Calculations of a list of neighbors in Molecular Dynamics simulations. <i>Journal of Computational Chemistry</i> , 1989 , 10, 921-927	3.5	29
2253	Simple models for solvation effects on electronic transition energies: Formaldehyde and water. 1989 , 154, 531-535		33
2252	Bioactive conformation of linear peptides in solution: an elusive goal?. 1989 , 28, 91-107		40
2251	Molecular mechanics studies on poly(purine).poly(pyrimidine) sequences in DNA: polymorphism and local variability. 1989 , 28, 531-48		4
2250	Adduct-induced base-shifts: a mechanism by which the adducts of bulky carcinogens might induce mutations. 1989 , 28, 909-27		32
2249	How accurate does a force field need to be?. 1989 , 13, 149-156		30
2248	The oxidation potential of 1,4-diaminobenzene: Calculation versus experiment. 1989 , 258, 79-88		37
2247	Identifying targets for bioreductive agents: using GRID to predict selective binding regions of proteins. 1989 , 7, 103-8, 100		30
2246	Computational and site-specific mutagenesis analyses of the asymmetric charge distribution on calmodulin. 1989 , 6, 70-85		53

2245	Salt or ion bridges in biological systems: a study employing quantum and molecular mechanics. 1989 , 6, 168-92	33
2244	Three-dimensional structure of the neurotoxin ATX Ia from Anemonia sulcata in aqueous solution determined by nuclear magnetic resonance spectroscopy. 1989 , 6, 357-71	71
2243	Use of restrained molecular dynamics in water to determine three-dimensional protein structure: prediction of the three-dimensional structure of Ecballium elaterium trypsin inhibitor II. 1989 , 6, 405-17	64
2242	An empirical potential for interactions of large molecules: Application to binding of dipeptides to DNA. 1989 , 36, 287-298	5
2241	Theoretical calculation of tautomer equilibria in solution: 4-(5-)methylimidazole. 1989 , 993, 134-6	29
2240	Structural versatility of peptides containing C alpha, alpha-dialkylated glycines: conformational energy computations, i.r. absorption and 1H n.m.r. analysis of 1-aminocyclopropane-1-carboxylic acid homopeptides. 1989 , 11, 345-52	30
2239	Solvent bridging sites in A- and B-DNA helices. 1989 , 11, 39-42	12
2238	Three-dimensional structure of a light chain dimer crystallized in water. Conformational flexibility of a molecule in two crystal forms. 1989 , 210, 601-15	57
2237	The different influences of ether and ester phospholipids on the conformation of gramicidin A. A molecular modelling study. 1989 , 979, 321-30	28
2236	A comparison of the CHARMM, AMBER and ECEPP potentials for peptides. II. Phi-psi maps for N-acetyl alanine N'-methyl amide: comparisons, contrasts and simple experimental tests. 1989 , 7, 421-53	152
2235	Computer Simulation by Molecular Dynamics as a Tool for Modelling of Molecular Systems. 1989 , 3, 187-200	7
2234	Molecular Dynamics Calculation for the Complexes of a Macrotricyclic Receptor with Organic Substrates. 1990 , 63, 3566-3570	O
2233	High specificity of a phosphate transport protein determined by hydrogen bonds. 1990 , 347, 402-6	480
2232	A d(GpG)-platinated decanucleotide duplex is kinked. An extended NMR and molecular mechanics study. 1990 , 194, 119-33	90
2231	Pharmacophore Identification in Amnesia-Reversal Compounds Using Conformational Analysis and Chemometric Methods. 1990 , 9, 195-201	14
2230	The theoretical calculation of basicities: an homologous amine series. 1990 , 208, 205-221	8
2229	NAD+ and NAD+ analogues in horse liver alcohol dehydrogenase. Relationship between reactivity and conformation simulated with molecular mechanics. 1990 , 1039, 227-33	12
2228	Molecular modeling studies of O2-alkylthymines and O4-alkylthymines in DNA: structures that may be pertinent to the incorporation of the corresponding dAlkTTP into DNA by DNA polymerases in vitro. 1990 , 233, 39-44	7

2227	Molecular mechanics calculations of the noncovalent interaction of aflatoxin B1 and its ultimate carcinogen with various dna sequences. 1990 , 38, 133-143	1
2226	Cavity search: an algorithm for the isolation and display of cavity-like binding regions. 1990 , 4, 337-54	88
2225	A practical procedure for the determination of electrostatic charges of large molecules. 1990 , 4, 411-26	41
2224	Simulations of the B-DNA molecular dynamics of d(CGCGAATTCGCG)2 and d(GCGCGCGCGC)2: an analysis of the role of initial geometry and a comparison of united and all-atom models. 1990 , 29, 517-32	26
2223	Computational analysis of the effects of site-specific phosphate alkylation in the DNA oligomer (d-[GGAATTCC])2. 1990 , 29, 597-607	3
2222	Restrained energy refinement with two different algorithms and force fields of the structure of the lamylase inhibitor tendamistat determined by nmr in solution. 1990 , 29, 695-706	47
2221	Free energy calculation on base specificity of drugDNA interactions: application to daunomycin and acridine intercalation into DNA. 1990 , 29, 717-27	49
2220	An ellipticine derivative (oxazolopyridocarbazolium) 3' linked to tetrathymidylate stacks intramolecularly with the nearest thymine at low concentration and head-to-tail intermolecularly at high concentration. 1990 , 29, 1077-87	2
2219	The calculated free energy effects of 5-methyl cytosine on the B to Z transition in DNA. 1990 , 29, 1193-209	33
2218	Alanyl dipeptide potential-derived net atomic charges and bond dipoles, and their variation with molecular conformation. 1990 , 29, 1367-1386	71
2217	Analysis of side-chain conformational distributions in neutrophil peptide-5 NMR structures. 1990 , 29, 1807-22	8
2216	Structural versatility of peptides from C⊞disubstituted glycines: Preferred conformation of the C⊞diphenylglycine residue. 1990 , 30, 1-11	37
2215	Molecular dynamics simulation provides a possible structure for substance P-like peptides in aqueous solution. 1990 , 30, 13-23	17
2214	Application of the distance geometry algorithm to cyclic oligopeptide conformation searches. 1990 , 30, 45-56	20
2213	Conformational studies on peptides with proline in the right-handed alpha-helical region. 1990 , 30, 287-98	61
2212	Conformational analysis and helical preferences of normal and Haialkyl amino acids. 1990 , 30, 533-546	57
2211	Thermodynamic cycle-perturbation study of the binding of trifluoroacetyl dipeptide anilide inhibitors with porcine pancreatic elastase. 1990 , 30, 773-80	9
2210	Conformational search in enkephalin analogues containing a disulfide bond. 1990 , 30, 1011-25	24

2209	Restrained and unrestrained molecular dynamics simulations in the NVT ensemble of alamethicin. 1990 , 30, 1083-99		47
2208	Molekldynamik-Computersimulationen; Methodik, Anwendungen und Perspektiven in der Chemie. 1990 , 102, 1020-1055		83
2207	Hydration free energy calculations by the acceptance ratio method. <i>Journal of Computational Chemistry</i> , 1990 , 11, 76-81	3.5	23
2206	Partial electrostatic charges for the active center of Cu, Zn superoxide dismutase. <i>Journal of Computational Chemistry</i> , 1990 , 11, 346-350	3.5	26
2205	Atomic charges derived from semiempirical methods. <i>Journal of Computational Chemistry</i> , 1990 , 11, 43	1-439	2668
2204	MacromodelâĦn integrated software system for modeling organic and bioorganic molecules using molecular mechanics. <i>Journal of Computational Chemistry</i> , 1990 , 11, 440-467	3.5	3405
2203	Variable step molecular dynamics: An exploratory technique for peptides with fixed geometry. Journal of Computational Chemistry, 1990 , 11, 468-486	3.5	50
2202	A vibrational molecular force field of model compounds with biological interest. I. Harmonic dynamics of crystalline urea at 123 K. <i>Journal of Computational Chemistry</i> , 1990 , 11, 560-568	3.5	39
2201	On the use of AM1 and MNDO wave functions to compute accurate electrostatic charges. <i>Journal of Computational Chemistry</i> , 1990 , 11, 909-923	3.5	111
2200	Free energy perturbation calculations on models of active sites: Applications to adenosine deaminase inhibitors. <i>Journal of Computational Chemistry</i> , 1990 , 11, 994-1002	3.5	8
2199	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. Journal of Computational Chemistry, 1990 , 11, 1169-1180	3.5	82
2198	Construction and molecular modeling of phospholipid surfaces. <i>Journal of Computational Chemistry</i> , 1990 , 11, 1181-1186	3.5	52
2197	A novel decomposition of torsional potentials into pairwise interactions: A study of energy second derivatives. <i>Journal of Computational Chemistry</i> , 1990 , 11, 1234-1246	3.5	23
2196	Molecular mechanics parameters for electronically excited states: The (n, 🖹) singlet state of formaldehyde. 1990 , 166, 429-436		12
2195	How does cisplatin alter DNA structure? A molecular mechanics study on double-stranded oligonucleotides. 1990 , 35, 165-78		32
2194	MolStruc: a force field calculation program allowing interactive modifications of the force field parameters. 1990 , 8, 221-7		1
2193	Modelling OH?O hydrogen bonds in carbohydrates. 1990 , 237, 75-79		11
2192	Oligosaccharide conformations: Application of NMR and energy calculations. 1990 , 22, 55-81		90

2191	A microscopic approach to the structure and thermodynamic properties of peptides and proteins. 1990 , 162, 141-154	4
2190	5.3.4 References for 5.3. 453-454	
2189	Dependence of defect-mediated hydrogen-bond melting in the DNA double helix on the size of an induced defect. 1990 , 41, 5677-5682	3
2188	Inelastic neutron scattering analysis of low-frequency motions in proteins: Harmonic and damped harmonic models of bovine pancreatic tryspin inhibitor. 1990 , 93, 2974-2991	78
2187	The effect of polarization energy on the free energy perturbation calculations. 1990 , 92, 7057-7067	16
2186	Multiple intermolecular bend vibrational excitation of a hydrogen bond: An extended infrared study of OCOHF. 1990 , 93, 7716-7730	37
2185	Conformational analysis of the 3'-5'-cyclic dinucleotide d less than pApA greater than by means of molecular mechanics. 1990 , 8, 233-51	3
2184	Molecular-mechanics modelling of drug-DNA structures; the effects of differing dielectric treatment on helix parameters and comparison with a fully solvated structural model. 1990 , 8, 359-73	49
2183	Molecular mechanics and dynamics of an abasic frameshift in DNA and comparison to NMR data. 1990 , 7, 1095-115	14
2182	In search of a Hoogsteen base paired DNA duplex in aqueous solution. 1990 , 8, 461-82	3
	In search of a Hoogsteen base paired DNA duplex in aqueous solution. 1990 , 8, 461-82 Free Energy Calculations of Pharmaceutically Important Properties. 1990 , 5, 265-275	8
2181		
2181	Free Energy Calculations of Pharmaceutically Important Properties. 1990 , 5, 265-275	8
2181 2180	Free Energy Calculations of Pharmaceutically Important Properties. 1990, 5, 265-275 DNA dynamics in aqueous solution: opening the double helix. 1990, 4, 81-96 Structural versatility of peptides from C#disubstituted glycines. Preferred conformation of the	8
2181 2180 2179	Free Energy Calculations of Pharmaceutically Important Properties. 1990, 5, 265-275 DNA dynamics in aqueous solution: opening the double helix. 1990, 4, 81-96 Structural versatility of peptides from Calculations of the Calculation of the Calculation of the Calculation of the 1990, 1481-1487	8 11 16
2181 2180 2179 2178	Free Energy Calculations of Pharmaceutically Important Properties. 1990, 5, 265-275 DNA dynamics in aqueous solution: opening the double helix. 1990, 4, 81-96 Structural versatility of peptides from Cadisubstituted glycines. Preferred conformation of the Cadibenzylglycine residue. 1990, 1481-1487 Interaction of a macrocyclic bisacridine with DNA. 1990, 29, 10918-27 NMR and computational characterization of mitomycin cross-linked to adjacent deoxyguanosines in	8 11 16 34
2181 2180 2179 2178 2177	Free Energy Calculations of Pharmaceutically Important Properties. 1990, 5, 265-275 DNA dynamics in aqueous solution: opening the double helix. 1990, 4, 81-96 Structural versatility of peptides from CHdisubstituted glycines. Preferred conformation of the CHdibenzylglycine residue. 1990, 1481-1487 Interaction of a macrocyclic bisacridine with DNA. 1990, 29, 10918-27 NMR and computational characterization of mitomycin cross-linked to adjacent deoxyguanosines in the minor groove of the d(T-A-C-G-T-A).d(T-A-C-G-T-A) duplex. 1990, 29, 2861-75 A molecular mechanical force field for the conformational analysis of oligosaccharides: comparison	8 11 16 34 82

2173	Atomic charges for DNA constituents derived from single-crystal X-ray diffraction data. 1990 , 211, 171-87	50
2172	SIRIUS. An automated method for the analysis of the preferred packing arrangements between protein groups. 1990 , 211, 595-615	173
2171	Determining local conformational variations in DNA. Nuclear magnetic resonance structures of the DNA duplexes d(CGCCTAATCG) and d(CGTCACGCGC) generated using back-calculation of the nuclear Overhauser effect spectra, a distance geometry algorithm and constrained molecular	66
2170	dynamics. 1990, 214, 711-36 Calculation of the relative binding free energy of 2'GMP and 2'AMP to ribonuclease T1 using molecular dynamics/free energy perturbation approaches. 1990, 212, 197-209	36
2169	Insights into the function of the zinc hydroxide-Thr199-Glu106 hydrogen bonding network in carbonic anhydrases. 1990 , 214, 799-802	88
2168	Computational methods for determining protein structures from NMR data. 1990 , 40, 15-22	62
2167	Probing the role of proline as a recognition element in peptide antigens. 1990 , 40, 119-23	26
2166	Mapping the copper ligands of Cu,Zn superoxide dismutase by nuclear Overhauser enhancement of the isotropically shifted 1H-NMR lines of the Cu,Co derivative. 1990 , 261, 231-6	11
2165	Modeling of the electrostatic potential field of plastocyanin. 1990 , 277, 241-54	38
2164	Electrostatic control of charge separation in bacterial photosynthesis. 1990 , 1017, 251-72	203
2164	Electrostatic control of charge separation in bacterial photosynthesis. 1990 , 1017, 251-72 New features of the delta opioid receptor: conformational properties of deltorphin I analogues. 1990 , 169, 617-22	203
	New features of the delta opioid receptor: conformational properties of deltorphin I analogues.	
2163	New features of the delta opioid receptor: conformational properties of deltorphin I analogues. 1990, 169, 617-22 A molecular model for the enzyme cytochrome P450(17 alpha), a major target for the chemotherapy of prostatic cancer. 1990, 171, 1160-7	40
2163 2162 2161	New features of the delta opioid receptor: conformational properties of deltorphin I analogues. 1990, 169, 617-22 A molecular model for the enzyme cytochrome P450(17 alpha), a major target for the chemotherapy of prostatic cancer. 1990, 171, 1160-7	40
2163 2162 2161	New features of the delta opioid receptor: conformational properties of deltorphin I analogues. 1990, 169, 617-22 A molecular model for the enzyme cytochrome P450(17 alpha), a major target for the chemotherapy of prostatic cancer. 1990, 171, 1160-7 Does anthramycin bind to Z-DNA as well as to B-DNA? A molecular mechanics study. 1990, 167, 477-83	40 86
2163 2162 2161 2160	New features of the delta opioid receptor: conformational properties of deltorphin I analogues. 1990, 169, 617-22 A molecular model for the enzyme cytochrome P450(17 alpha), a major target for the chemotherapy of prostatic cancer. 1990, 171, 1160-7 Does anthramycin bind to Z-DNA as well as to B-DNA? A molecular mechanics study. 1990, 167, 477-83 Histamine tautomerism and its mode of action. 1990, 1036, 158-61	40 86 1 9
2163 2162 2161 2160 2159	New features of the delta opioid receptor: conformational properties of deltorphin I analogues. 1990, 169, 617-22 A molecular model for the enzyme cytochrome P450(17 alpha), a major target for the chemotherapy of prostatic cancer. 1990, 171, 1160-7 Does anthramycin bind to Z-DNA as well as to B-DNA? A molecular mechanics study. 1990, 167, 477-83 Histamine tautomerism and its mode of action. 1990, 1036, 158-61 Theoretical studies of oligosaccharide structure and conformational dynamics. 1991, 1, 711-715 Theoretical and experimental measures of DNA helix stability and their relation to sequence	40 86 1 9 21

Molecular structure and dynamics of dopamine, serotonin and the D2, 5-HT2 and 5-HT1A receptors. **1991**, 1, 310-311

2154	Molecular modeling in food research: technology and techniques. 1991 , 2, 110-115	7
2153	Molecular dynamics of phenol at the liquid-vapor interface of water. 1991 , 94, 5599-605	81
2152	Distance-scaled Force Biased Monte Carlo Simulation for Solutions containing a Strongly Interacting Solute. 1991 , 5, 405-408	15
2151	Combined quantum mechanicalâtholecular mechanical study of catalysis by the enzyme phospholipase A2: an investigation of the potential energy surface for amide hydrolysis. 1991 , 2025-2032	29
2150	Conformation-activity relationship of tachykinin neurokinin A (4-10) and of some [Xaa8] analogues. 1991 , 30, 10175-81	28
2149	Design of a small peptide-based proteinase inhibitor by modeling the active-site region of barley chymotrypsin inhibitor 2. 1991 , 30, 10717-21	20
2148	High-resolution solution structure of reduced French bean plastocyanin and comparison with the crystal structure of poplar plastocyanin. 1991 , 221, 533-55	104
2147	An axial binding site in the Tetrahymena precursor RNA. 1991 , 222, 995-1012	55
2146	RNA recognition by Tat-derived peptides: interaction in the major groove?. 1991 , 66, 577-88	332
2145	Molecular structure and dynamics of serotonin. 1991 , 9, 31-7	6
2144	Potentials for the Classical Simulation of Molecular Systems: Current and Future Model Intermolecular Potentials. 1991 , 183-208	4
2143	Are time-averaged restraints necessary for nuclear magnetic resonance refinement? A model study for DNA. 1991 , 220, 457-79	133
2142	A new method for building protein conformations from sequence alignments with homologues of known structure. 1991 , 217, 1-7	125
2141	Combined procedures of distance geometry and molecular dynamics for determining protein structure from nuclear magnetic resonance data. 1991 , 202, 268-300	13
2140	Aspects of the design of conformationally constrained peptides. 1991 , 202, 411-36	5
2139	Molecular modeling and dynamics of biologically active peptides: application to neuropeptide Y. 1991 , 202, 449-70	3
2138	Molecular modeling in mutagenesis and carcinogenesis. 1991 , 203, 458-76	10

2137	Application of Free-Energy Decomposition to Determine the Relative Stability of R and S Oligodeoxyribonucleotide Methylphosphonates. 1991 , 1, 243-254		10
2136	Molecular modeling to study DNA intercalation by anti-tumor drugs. 1991 , 203, 433-58		11
2135	Vector optimization of amber 3.0 on the NEC SX-2/400 supercomputer. 1991 , 15, 79-85		1
2134	The effects of solvent on the conformation and the collective motions of protein: Normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum. 1991 , 158, 447-472		335
2133	Characterization of proline-containing right-handed alpha-helix by molecular dynamics studies. 1991 , 40, 97-108		9
2132	Efficient method for the generation and display of electrostatic potential surfaces from ab-initio wavefunctions. 1991 , 9, 74-7, 94		22
2131	Efficient techniques for the decomposition of intermolecular interaction energy at SCF level and beyond. 1991 , 234, 387-400		73
2130	Structure of recombinant human rheumatoid arthritic synovial fluid phospholipase A2 at 2.2 A resolution. 1991 , 352, 79-82		213
2129	Molecular modeling of intramolecular hydrogen bonding in simple oligoamides 1. In vacuo 1991 , 32, 3613-3616		6
2128	Structure determination of [d(ATATATAUAT)]2 via two-dimensional NOE spectroscopy and molecular dynamics calculations. 1991 , 197, 583-95		20
2127	Conformational study of a sugar nitroxyl free radical. 1991 , 214, 235-244		8
2126	Minimization and molecular dynamics studies of guanosine and Z-DNA modified by N-2-acetylaminofluorene. <i>Journal of Computational Chemistry</i> , 1991 , 12, 147-166	3.5	17
2125	Free energy difference calculations by thermodynamic integration: Difficulties in obtaining a precise value. <i>Journal of Computational Chemistry</i> , 1991 , 12, 271-275	3.5	149
2124	Conformational dynamics of polypeptides and proteins in the dihedral angle space and in the cartesian coordinate space: Normal mode analysis of deca-alanine. <i>Journal of Computational Chemistry</i> , 1991 , 12, 359-368	3.5	46
2123	Incorporating solvent and ion screening into molecular dynamics using the finite-difference Poissonâ B oltzmann method. <i>Journal of Computational Chemistry</i> , 1991 , 12, 454-468	3.5	120
2122	Can the Lennardâllones 6-12 function replace the 10-12 form in molecular mechanics calculations?. <i>Journal of Computational Chemistry</i> , 1991 , 12, 620-626	3.5	88
2121	A new strategy for the evaluation of force parameters from quantum mechanical computations. Journal of Computational Chemistry, 1991 , 12, 664-674	3.5	36
2120	The use of ultraviolet resonance Raman intensities to test proposed molecular force fields for nucleic acid bases. <i>Journal of Computational Chemistry</i> , 1991 , 12, 731-741	3.5	28

2119	Free energy calculations on calcium and magnesium complexes: Protein and phospholipid model systems. <i>Journal of Computational Chemistry</i> , 1991 , 12, 899-908	3.5	7
2118	Force field parameters for molecular mechanical simulation of dehydroamino acid residues. <i>Journal of Computational Chemistry</i> , 1991 , 12, 934-942	3.5	24
2117	Simulations of lipid crystals: Characterization of potential energy functions and parameters for lecithin molecules. <i>Journal of Computational Chemistry</i> , 1991 , 12, 1033-1046	3.5	45
2116	Long range nonbonded attractive constants for some charged atoms. <i>Journal of Computational Chemistry</i> , 1991 , 12, 1125-1128	3.5	22
2115	Toward accurate transferable electrostatic models for polypeptides: A distributed multipole study of blocked amino acid residue charge distributions. <i>Journal of Computational Chemistry</i> , 1991 , 12, 1187-	131597	42
2114	On the use of electrostatic potential derived charges in molecular mechanics force fields. The relative solvation free energy of cis- and trans-N-methyl-acetamide. <i>Journal of Computational Chemistry</i> , 1991 , 12, 1232-1236	3.5	96
2113	Reactivity in molecular crystals: Radical formation in chiral phosphorus compounds. 1991 , 2, 39-43		5
2112	High directional Monte Carlo procedure coupled with the temperature heating and annealing as a method to obtain the global energy minimum structure of polypeptides and proteins. 1991 , 31, 177-85		31
2111	Conformational energy minimization by simulated annealing using molecular dynamics: Some improvements to the monitoring procedure. 1991 , 31, 663-670		10
2110	New insights on mu/delta selectivity of opioid peptides: conformational analysis of deltorphin analogues. 1991 , 31, 751-60		43
2109	The solution structure of the lantibiotic gallidermin. 1991 , 31, 803-11		69
2108	Prediction of fluorine chemical shifts in proteins. 1991 , 31, 845-58		43
2107	Three-dimensional structure and molecular dynamics of cis(Z)- and trans(E)-chlorprothixene. 1991 , 80, 735-40		7
2106	Stabilization of ⊞elical secondary structure during high-temperature molecular-dynamics simulations of ⊞actalbumin. 1991 , 158, 295-301		14
2105	Free energy evaluation from molecular dynamics simulations using force fields including electronics polarization. 1991 , 177, 433-440		35
2104	Molecular structure and dynamics of acetylcholine. 1991 , 83, 157-70		10
2103	Molecular modeling of intramolecular hydrogen bonding in simple oligoamides 2. GB/SA CH2Cl2 1991 , 32, 3617-3620		9
2102	Automatic creation of drug candidate structures based on receptor structure. Starting point for artificial lead generation 1991 , 47, 8985-8990		138

2101	Free energy calculations on binding and catalysis by alpha-lytic protease: the role of substrate size in the P1 pocket. 1991 , 10, 140-8	18
2100	A model for human cardiac troponin C and for modulation of its Ca2+ affinity by drugs. 1991 , 11, 79-94	30
2099	Effect of Urey-Bradley-Shimanouchi force field on the harmonic dynamics of proteins. 1991 , 11, 120-32	4
2098	DNA bending studied by MD and 2D NMR NOESY simulations: Role of the junction sequence between the A/T tracts. 1991 , 40, 213-229	1
2097	Empirical methods for computing molecular partition coefficients. I. Upon the need to model the specific hydration of polar groups in fragment-based approaches. 1991 , 40, 299-316	8
2096	Molecular dynamics simulations on the protonated 222. H+ and 222.2H+ cryptands in water:Endo versusexo conformations. 1991 , 11, 71-88	12
2095	A potential function for protein folding. 1991 , 6, 91-110	32
2094	COSMIC(90): an improved molecular mechanics treatment of hydrocarbons and conjugated systems. 1991 , 5, 475-504	61
2093	Molecular dynamics simulations of dinucleoside and dinucleoside-drug crystal hydrates. 1991 , 9, 363-86	8
2092	Studies on the cross stand hydrogen bonds in DNA double helices. 1991 , 9, 113-26	13
2091	Modeling of nucleic acid complexes with cationic ligands: a specialized molecular mechanics force field and its application. 1991 , 8, 1119-45	30
2090	Decisions in force field development: an alternative to those described by Roterman et al. (J. Biomol. Struct. Dyn. 7, 421 (1989)). 1991 , 8, 1103-7; discussion 1109-11	26
2089	DNA polymorphism and local variation in base-pair orientation: a theoretical rationale. 1991 , 9, 127-42	12
2088	Molecular modeling of proteins: a strategy for energy minimization by molecular mechanics in the AMBER force field. 1991 , 9, 475-88	31
2087	The overlooked bond-stretching contribution in free energy perturbation calculations. 1991 , 94, 4532-4545	132
2086	Molecular dynamics simulation of a dense model bilayer of chain molecules with fixed head groups. 1991 , 95, 5377-5386	17
2085	Molecular mechanics studies of dinucleoside methylphosphonates: influence of methylphosphonate and its chirality on the phosphodiester conformation. 1991 , 9, 613-31	5
2084	Computer modelling studies on the mechanism of action of ribonuclease T1. 1991 , 9, 215-31	6

2083	MODELING OF MONOLAYERS. 1991 , 305-338	3
2082	Molecular modelling of 9-aminoellipticine interactions with abasic oligonucleotides. 1991 , 9, 579-97	6
2081	Computer Simulations of Mesogenic Molecules Using Realistic Atom-Atom Potentials. 1991 , 198, 465-477	91
2080	Molecular dynamics studies of the behaviour of water molecules and small ions in concentrated solutions of polymeric B-DNA. 1991 , 72, 643-660	39
2079	X-Ray Structural Studies of Adenosine 5?-Triphosphate Metal Compounds. 1992 , 13, 1-34	15
2078	Base sequence criteria and Cartesian coordinates for stable B/Z and B/Z/B junctions in relaxed DNA. 1992 , 9, 1155-83	13
2077	Probing protein stability with unnatural amino acids. 1992 , 256, 1798-802	135
2076	The structures of bacteriorhodopsin with different retinal-Schiff base orientationscomputer modeling and energy minimization studies. 1992 , 9, 1073-95	2
2075	Comparison of protein models minimized by the all-atom and united-atom models in the AMBER force field: correlation of RMS deviation with the crystallographic R factor and size. 1992 , 10, 265-79	4
2074	Conformations of Cyclobut-A and Cyclobut-G: structural resemblance to nucleosides and incorporation into double helical DNA. 1992 , 9, 719-32	3
2073	Flexibility of DNA in 2:1 drug-DNA complexessimultaneous binding of two DAPI molecules to DNA. 1992 , 9, 695-704	10
2072	Free Energy Perturbation Simulations of Cation Binding to Valinomycin. 1992 , 23-53	
2071	Conformation and dynamics of drug-DNA intercalation. 1992 , 10, 97-139	23
2070	van der Waals functional forms for molecular simulations. 1992 , 97, 1109-1115	25
2069	Rigid bender analysis of van der Waals complexes: The intermolecular bending potential of a hydrogen bond. 1992 , 96, 5712-5725	20
2068	Determination of solvation free energy using molecular dynamics with solute Cartesian mapping: An application to the solvation of 18-crown-6. 1992 , 97, 5108-5112	30
2067	Rapid Calculation of Any Dielectric Function for Molecular Dynamics Simulations of Biological Macromolecules. 1992 , 9, 193-200	13
2066	Computer-simulation studies of 町uinol clathrate with various gases. Molecular interactions and crystal structure. 1992 , 97, 8617-8627	22

A molecular mechanics investigation of RNA contract RNA sequence with an unpaired adenosine. 19	omplexes. I. Ethidium intercalation in an HIV-1 TAR 992 , 10, 367-87	12
2064 Molecular dynamics studies on nucleoside 2',3	'-cyclic phosphates. 1992 , 9, 1253-68	
2063 .		3
2062 Sequence effects on the propeller twist of bas	se pairs in DNA helices. 1992 , 9, 1195-211	2
2061 Tetraplex formation of d(GGGGGTTTTT): 1H N	MR study in solution. 1992 , 9, 1131-53	22
Molecular Dynamics Simulations of Proteins in Coulomb Interactions. 1992 , 8, 321-333	n Water Without the Truncation of Long-range	91
2059 Centrally acting dopamine D2 receptor ligands	s: agonists. 1992 , 29, 185-216	11
Applications of molecular physics 'biotechnolo analogue. 1992 , 1, 223-46	ogy' to the rational design of an improved phenytoin	5
2057 Molecular dynamics simulations of dimer oper	ning on a diamond {001}(2x1) surface. 1992 , 255, 835-8	182
A reduced set of coordinates for modeling DN by pseudorotational angle. 1992 , 9, 1185-94	IA structures: (I). A B-to-A transition pathway driven	10
Molecular mechanics calculations of the confo 2055 tripeptide BocâtlyâlleuâtlyâllMe. Searching t 1992, 2263-2270	ormers of the dipetide BocâtlyâlleuâtlMe and the conformational space by the build-up method.	2
First observation of a helical peptide containir preferred screw sense. 1992 , 971-977	ng chiral ⊞nonosubstituted residues without a	6
2053 Electrostatic fields in antibodies and antibody	/antigen complexes. 1992 , 58, 203-24	83
2052 Molecular dynamics of serotonin and ritanseri	n interacting with the 5-HT2 receptor. 1992 , 14, 166-78	39
2051 Hydration of Benzoic Acid in Benzene Solution	n. 1992 , 177, 63-74	2
2050 Model calculations on the amide-I infrared bar	nds of globular proteins. 1992 , 96, 3379-3387	407
The octamer motif in immunoglobulin genes: 6 two-dimensional NMR studies. 1992 , 31, 7477		40
Mambin, a potent glycoprotein IIb-IIIa antagor related to the short neurotoxins. 1992 , 31, 470	nist and platelet aggregation inhibitor structurally 66-72	111

2047	Three-dimensional solution structure of Ca(2+)-loaded porcine calbindin D9k determined by nuclear magnetic resonance spectroscopy. 1992 , 31, 1011-20	43
2046	Molecular-dynamics simulations of interfaces between water and crystalline urea. 1992 , 96, 7010-7018	43
2045	Simulation of the solution structure of the H-ras p21-GTP complex. 1992 , 31, 4951-9	49
2044	The solution structure of a cyclic endothelin antagonist, BQ-123, based on 1H-1H and 13C-1H three bond coupling constants. 1992 , 300, 136-40	38
2043	Do antigenic peptides have a unique sense of direction inside the MHC binding groove? A molecular modelling study. 1992 , 303, 224-8	4
2042	NMR study of self-paired parallel duplex of d(AAAAACCCCC) in solution. 1992 , 306, 223-8	17
2041	Structural determination of the active site of a sweet protein. A 1H NMR investigation of pMNEI. 1992 , 310, 27-30	62
2040	Determination of a high-quality nuclear magnetic resonance solution structure of the bovine pancreatic trypsin inhibitor and comparison with three crystal structures. 1992 , 227, 757-75	168
2039	Structural details of ribonuclease H from Escherichia coli as refined to an atomic resolution. 1992 , 223, 1029-52	211
2038	Three-dimensional structure for the beta 2 adrenergic receptor protein based on computer modeling studies. 1992 , 225, 859-71	87
2037	Design and structural analysis of alternative hydrophobic core packing arrangements in bacteriophage T4 lysozyme. 1992 , 224, 1143-59	120
2036	Investigations on the dynamic structures of adenine- and thymine-containing DNA. 1992 , 223, 455-76	37
2035	Molecular dynamics simulation of the DNA triplex d(TC)5.d(GA)5.d(C+T)5. 1992, 223, 519-29	37
2034	Solution structure of a DNA octamer containing the Pribnow box via restrained molecular dynamics simulation with distance and torsion angle constraints derived from two-dimensional nuclear magnetic resonance spectral fitting. 1992 , 227, 510-31	69
2033	Determination of the nuclear magnetic resonance solution structure of the DNA-binding domain (residues 1 to 69) of the 434 repressor and comparison with the X-ray crystal structure. 1992 , 223, 743-67	62
2032	Structural changes by sulfoxidation of phenothiazine drugs. 1992 , 6, 207-22	10
2031	Computer-aided molecular modeling and design of DNA-inserting molecules. 1992 , 6, 33-46	4
2030	On the suitability of semiempirical calculations as sources of force field parameters. 1992 , 6, 331-48	19

2029	Characterization of low-energy conformational domains for Met-enkephalin. 1992 , 6, 175-90	35
2028	Theoretical calculation of electrode potentials: Electron-withdrawing compounds. 1992 , 41, 293-310	42
2027	Investigation on the intermolecular electrostatic interactions of some polar molecules with cumulative potential-derived atomic multipole method. 1992 , 42, 489-499	1
2026	Ab initio force field for simulations of proteins and nucleic acids. 1992 , 42, 1353-1381	25
2025	Empirical methods for computing molecular partition coefficients: II. Inclusion of conformational flexibility within fragmentâBased approaches. 1992 , 44, 219-233	19
2024	The interaction of Na(I), Ca(II), and Mg(II) metal ions with duplex DNA: A theoretical modeling study. 1992 , 44, 145-166	13
2023	Inclusion of solvation free energy with molecular mechanics energy: alanyl dipeptide as a test case. 1992 , 1, 396-400	54
2022	Molecular dynamics studies of a DNA-binding protein: 1. A comparison of the trp repressor and trp aporepressor aqueous simulations. 1992 , 1, 1173-84	20
2021	Molecular dynamics studies of a DNA-binding protein: 2. An evaluation of implicit and explicit solvent models for the molecular dynamics simulation of the Escherichia coli trp repressor. 1992 , 1, 1185-205	93
2020	Evaluation of the conformational, hydrogen bonding and crystal packing preferences of acyclic imides. 1992 , 5, 44-54	22
2019	Re-evaluation of 1,4-Non-bonded interactions in molecular mechanics. 1992 , 5, 567-574	1
2018	A method for determining the positions of polar hydrogens added to a protein structure that maximizes protein hydrogen bonding. 1992 , 12, 266-77	33
2017	Substrate-enzyme interactions and catalytic mechanism in phospholipase C: a molecular modeling study using the GRID program. 1992 , 12, 331-8	25
2016	Continuum electrostatics of the C-peptide: anatomy of the problem. 1992 , 13, 120-31	9
2015	Molecular dynamics characterization of the active cavity of carboxypeptidase A and some of its inhibitor adducts. 1992 , 13, 288-305	35
2014	NMR restraint analysis of transforming growth factor alpha: a key component for NMR structure refinement. 1992 , 13, 306-26	2
2013	Empirical solvation models in the context of conformational energy searches: application to bovine pancreatic trypsin inhibitor. 1992 , 14, 110-9	56
2012	Synthesis of 1?#,2?,3?,4?#,5?,5?-2H6-即-ribonucleosides and 1?#, 2?,2?,3?,4?#,5?,5?-2H7-即-2?-deoxyribonucleosides for selective suppression of proton resonances in partially-deuterated oligo-DNA oligo-RNA and in 2.5A core (1H-NMR window), 1992, 48, 9033-9072	39

2011	NMR and molecular modelling studies of two photoproducts of 2?-deoxy-4- thiouridylyl-(3?,5?)-thymidine 1992 , 48, 1605-1616	5
2010	Free energy perturbation simulations of cation binding to valinomycin. 1992 , 12, 23-53	10
2009	Assessment of competing 2?«5? versus 3?«5? stackings in solution structure of branched-RNA by 1H- & 31 P-NMR spectroscopy. 1992 , 48, 695-718	15
2008	AMBER torsional parameters for the peptide backbone. 1992 , 33, 7743-7746	171
2007	Presto(protein engineering simulator): A vectorized molecular mechanics program for biopolymers. 1992 , 16, 243-248	161
2006	Stereochemical applications of potential energy calculations Part VIII. MM2 conformational analysis of acetyl-l-phenylalanine p-acetyl anilide. 1992 , 269, 223-229	2
2005	NOE R factors and structural refinement using FIRM, an iterative relaxation matrix program. 1992 , 98, 283-298	3
2004	Chemical-shift ranges in proteins. 1992 , 100, 342-357	11
2003	Simulating the effect of the two-spin approximation on the generation of protein structures from NOE data. 1992 , 97, 398-410	1
2002	Object Command Language: a formalism to build molecular models and to analyze structural parameters in macromolecules, with applications to nucleic acids. 1992 , 10, 166-73, 162	15
2001	SAR of Sweet Molecules: Conformational Analysis of Two Hypersweet and Two Conformationally Restricted Aspartame Analogues. 1992 , 11, 486-491	11
2000	Free energy calculations in molecular biophysics. 1992 , 76, 251-275	79
1999	A practical approach to the computation of the electrostatic energy in large molecules. 1992 , 254, 31-42	7
1998	Cumulative multicenter multipole moment databases and their applications. 1992 , 256, 91-112	15
1997	Molecular dynamics study of the effect of ion concentration on the B-DNA, Z-DNA and DNA-daunomycin complex. 1992 , 257, 33-47	2
1996	Molecular to supramolecular design of synthetic polypeptides. 1992 , 17, 699-764	21
1995	Molecular mechanics calculations of systems with strong hydrogen bonds. 1992 , 265, 179-187	3
1994	The conformational behaviour of the cardiac glycoside digoxin as indicated by NMR spectroscopy and molecular dynamics calculations. 1992 , 230, 201-12	15

1993	On the interpretation of biochemical data by molecular dynamics computer simulation. 1992 , 204, 947	-61	105
1992	H8 chemical shifts in oligonucleotide cross-linked at a GpG sequence by cis-Pt(NH3)2(2+): a clue to the adduct structure. 1992 , 205, 895-906		75
1991	The three-dimensional structure of guanine-specific ribonuclease F1 in solution determined by NMR spectroscopy and distance geometry. 1992 , 208, 41-51		5
1990	The structure of the mammalian antibacterial peptide cecropin P1 in solution, determined by proton-NMR. 1992 , 209, 163-9		80
1989	Conformational analysis of a dinucleotide photodimer with the aid of the genetic algorithm. 1992 , 32, 45-52		68
1988	The electrostatic contribution to DNA base-stacking interactions. 1992 , 32, 145-59		84
1987	Molecular dynamics study of the conformational behavior of a representative elastin building block: Boc-Gly-Val-Gly-Leu-OMe. 1992 , 32, 161-72		43
1986	Conformational analysis of an opioid peptide in solvent media that mimic cytoplasm viscosity. 1992 , 32, 367-72		32
1985	A molecular mechanical study of the structure of poly(alpha-aminoisobutyric acid). 1992 , 32, 621-31		40
1984	A molecular dynamics study of conformational changes and hydration of left-handed d(CGCGCGCGCGCG)2 in a nonsalt solution. 1992 , 32, 1035-59		17
1983	The electrostatic potential for the phosphodiester group determined from X-ray diffraction. 1992 , 32, 1141-54		11
1982	Structural investigation of helices II, III, and IV of B. megaterium 5S ribosomal RNA by molecular dynamics calculations. 1992 , 32, 1263-70		2
1981	Flexible-geometry conformational energy maps for the amino acid residue preceding a proline. 1992 , 32, 1443-6		48
1980	Modelization of the protonation of ferrocene using an effective potential parametrized from local-spin density and Hartreeâ E ock calculations. 1992 , 190, 29-35		14
1979	Molecular interactions, structure and stability of Equinol clathrate. 1992 , 195, 135-143		16
1978	Polarization of the nucleic acid bases in aqueous solution. 1992 , 198, 74-80		61
1977	Conformational sampling and ensemble generation by molecular dynamics simulations: 18-Crown-6 as a test case. <i>Journal of Computational Chemistry</i> , 1992 , 13, 33-40	3.5	53
1976	Probing the conformational space available to inhibitors in the thermolysin active site using Monte Carlo/energy minimization techniques. <i>Journal of Computational Chemistry</i> , 1992 , 13, 214-228	3.5	46

1975	Charge distributions of phosphorylcholine and its derivatives. <i>Journal of Computational Chemistry</i> , 1992 , 13, 318-328	3.5	
1974	Standard-geometry chains fitted to X-ray derived structures: Validation of the rigid-geometry approximation. II. Systematic searches for short loops in proteins: Applications to bovine pancreatic ribonuclease A and human lysozyme. <i>Journal of Computational Chemistry</i> , 1992 , 13, 329-350	3.5	25
1973	Free energy perturbation calculations involving potential function changes. <i>Journal of Computational Chemistry</i> , 1992 , 13, 362-370	3.5	29
1972	Automated docking with grid-based energy evaluation. <i>Journal of Computational Chemistry</i> , 1992 , 13, 505-524	3.5	770
1971	Conformational dependence of electrostatic potential derived charges of a lipid headgroup: Glycerylphosphorylcholine. <i>Journal of Computational Chemistry</i> , 1992 , 13, 622-632	3.5	74
1970	Nucleoside free energy perturbation calculations: Mutation of purine-to-pyrimidine and pyrimidine-to-purine nucleosides. <i>Journal of Computational Chemistry</i> , 1992 , 13, 667-673	3.5	5
1969	Conformational analysis of flexible ligands in macromolecular receptor sites. <i>Journal of Computational Chemistry</i> , 1992 , 13, 730-748	3.5	171
1968	Conformational preferences for hydroxyl groups in substituted tetrahydropyrans. <i>Journal of Computational Chemistry</i> , 1992 , 13, 772-791	3.5	33
1967	Localized electron pair theory for the calculation of ground state energies of large molecules. Journal of Computational Chemistry, 1992 , 13, 901-911	3.5	6
1966	Derivation of fluorine and hydrogen atom parameters using liquid simulations. <i>Journal of Computational Chemistry</i> , 1992 , 13, 963-970	3.5	65
1965	How transferable are hydrogen parameters in molecular mechanics calculations?. <i>Journal of Computational Chemistry</i> , 1992 , 13, 971-978	3.5	32
1964	THE weighted histogram analysis method for free-energy calculations on biomolecules. I. The method. <i>Journal of Computational Chemistry</i> , 1992 , 13, 1011-1021	3.5	4722
1963	Study of hydrogen bonding interactions relevant to biomolecular structure and function. <i>Journal of Computational Chemistry</i> , 1992 , 13, 1151-1169	3.5	108
1962	A Monte Carlo method for conformational analysis of saccharides. 1993 , 238, 49-73		115
1961	Vibrational relaxation of Iâ in water and ethanol: molecular dynamics simulation. 1993, 204, 45-52		97
1960	A hybrid approach for the solvent effect on the electronic structure of a solute based on the RISM and Hartree-Fock equations. 1993 , 214, 391-396		203
1959	BenzeneâD2 interaction potential from ab initio calculations. 1993 , 205, 331-336		30
1958	A Monte Carlo method for generating structures of short single-stranded DNA sequences. 1993 , 33, 75-105		20

1957	Molecular dynamics study of iduronate ring conformation. 1993 , 33, 575-588		67
1956	Characterization of the bioactive form and molecular determinants of recognition of cyclic enkephalin peptides at the delta-opioid receptor. 1993 , 33, 647-57		27
1955	Differences in melting behavior between homopolymers and copolymers of DNA: Role of nonbonded forces for GC and the role of the hydration spine and premelting transition for AT. 1993 , 33, 797-812		28
1954	Synthesis, biological activity, and conformational analysis of [pGlu6,N-MePhe8,Aib9] substance P (6-11): a selective agonist for the NK-3 receptor. 1993 , 33, 915-26		21
1953	Conformational transitions using molecular dynamics with minimum biasing. 1993 , 33, 1167-72		40
1952	Molecular dynamics simulations of poly(dA).poly(dT): comparisons between implicit and explicit solvent representations. 1993 , 33, 1537-52		27
1951	A conformational study of the dehydroalanine: dipeptide and homopolypeptide. 1993 , 33, 1811-7		15
1950	Self-consistent reaction field computation of the reactive characteristics of DNA bases in water. 1993 , 33, 1851-1869		32
1949	Cyclische Oligomere von (R)-3-Hydroxybuttersüre: Herstellung und strukturelle Aspekte. 1993 , 76, 200	4-2033	3 55
1948	Warum Pentose- und nicht Hexose-Nucleinsüren??. Teil VI. â⊞omo-DNSâ⊡1H-, 13C-, 31P- und 15N-NMR-spektroskopische Untersuchung von ddGlc(A-A-A-A-A-T-T-T-T) in wßsriger Lಔung. 1993 , 76, 2701-2756		47
1947	A New Helicopodand: Molecular Recognition of Dicarboxylic Acids with High Diastereoselectivity. 1993 , 76, 2757-2774		87
1946	Monte Carlo simulations of the hydration of substituted benzenes with OPLS potential functions. Journal of Computational Chemistry, 1993 , 14, 195-205	3.5	140
1945	MORMIN: A quasi-Newtonian energy minimizer fitting the nuclear overhauser data. <i>Journal of Computational Chemistry</i> , 1993 , 14, 226-236	3.5	5
1944	Conformational and energetic effects of truncating nonbonded interactions in an aqueous protein dynamics simulation. <i>Journal of Computational Chemistry</i> , 1993 , 14, 295-311	3.5	90
1943	AMBERCUBE MD, parallelization of Amber's molecular dynamics module for distributed-memory hypercube computers. <i>Journal of Computational Chemistry</i> , 1993 , 14, 312-329	3.5	26
1942	Conformational dependence of the electrostatic potential-derived charges of dopamine: Ramifications in molecular mechanics force field calculations in the gas phase and in aqueous solution. <i>Journal of Computational Chemistry</i> , 1993 , 14, 353-362	3.5	24
1941	Yammp: Development of a molecular mechanics program using the modular programming method. Journal of Computational Chemistry, 1993 , 14, 455-470	3.5	36
1940	The ethylene group as a peptide bond mimicking unit: A theoretical conformational analysis. Journal of Computational Chemistry, 1993, 14, 471-477	3.5	3

1939	Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. Journal of Computational Chemistry, 1993 , 14, 587-602	3.5	45
1938	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
1937	Suitability of the PM3-derived molecular electrostatic potentials. <i>Journal of Computational Chemistry</i> , 1993 , 14, 799-808	3.5	56
1936	Conformational analysis and molecular dynamics simulation of cellobiose and larger cellooligomers. <i>Journal of Computational Chemistry</i> , 1993 , 14, 831-847	3.5	52
1935	Molecular dynamics simulation of cellobiose in water. <i>Journal of Computational Chemistry</i> , 1993 , 14, 848	3-385,7	56
1934	Efficient calculations of coulombic interactions in biomolecular simulations with periodic boundary conditions. <i>Journal of Computational Chemistry</i> , 1993 , 14, 867-878	3.5	43
1933	Molecular dynamics of 18-crown-6 complexes with alkaliâthetal cations and urea: Prediction of their conformations and comparison with data from the cambridge structural database. <i>Journal of Computational Chemistry</i> , 1993 , 14, 899-906	3.5	18
1932	AMBER force-field parameters for guanosine triphosphate and its imido and methylene analogs. Journal of Computational Chemistry, 1993 , 14, 995-1005	3.5	8
1931	Characterization of force fields for lipid molecules: Applications to crystal structures. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1066-1076	3.5	21
1930	New combining rules for rare gas van der waals parameters. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1077-1084	3.5	269
1929	CONCEPTS: New dynamic algorithm for de novo drug suggestion. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1184-1193	3.5	67
1928	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. Journal of Computational Chemistry, 1993, 14, 1240-1249	3.5	142
1927	Computation of the mean residence time of water in the hydration shells of biomolecules. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1396-1406	3.5	130
1926	Comparison of 6-31G*-based MST/SCRF and FEP evaluations of the free energies of hydration for small neutral molecules. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1498-1503	3.5	59
1925	Conformations of triglycyl-lysylvasopressin: 1H NMR spectroscopic and molecular dynamics study. 1993 , 31, 481-488		4
1924	Enantioselective cathodic reduction of 4-substituted coumarins with alkaloids as catalysts, 2. AM1 and force-field study of the transition-state model. 1993 , 1993, 609-614		8
1923	1,2,4-Oxadiazole derivatives of phenylalanine: potential inhibitors of substance P endopeptidase. 1993 , 28, 801-810		17
1922	A 3D model of the peripheral benzodiazepine receptor and its implication in intra mitochondrial cholesterol transport. 1993 , 11, 236-44, 235		84

1921	Reproduction of correct electrostatic field by charges and dipoles on a closed surface. 1993 , 11, 30-6, 43	5
1920	The dynamics of some metal-organic and organic molecules in water solution studied by molecular mechanical and molecular dynamical methods. 1993 , 174, 127-139	8
1919	Helix propensity of Ala and Val: a free energy perturbation study. 1993 , 47, 113-21	1
1918	Effect of constraints by threonine on proline containing alpha-helixa molecular dynamics approach. 1993 , 46, 77-89	9
1917	Gas-phase fragmentations of anionic complexes of serine- and threonine-containing peptides. 1993 , 127, 17-26	32
1916	Synthesis of thymidine dimer derivatives containing an amide linkage and their incorporation into oligodeoxyribonucleotides. 1993 , 34, 6383-6386	56
1915	Optimization of parameters of nonbonded interactions in a spectroscopically determined force field. 1993 , 17, 67-72	15
1914	PIDOTIMOD, a new immunostimulating dipeptide, studied by molecular mechanics, normal mode analysis and dynamics calculations. 1993 , 298, 177-190	7
1913	Protein 毗urn mimetics II: Design, synthesis, and evaluation in the cyclic peptide gramicidin S. 1993 , 49, 3609-3628	46
1912	Computer-aided drug design: a free energy perturbation study on the binding of methyl-substituted pterins and N5-deazapterins to dihydrofolate reductase. 1993 , 7, 535-55	19
1911	A new scaling procedure to correct semiempirical MEP and MEP-derived properties. 1993 , 7, 721-742	25
1910	Peptide mimetics as enzyme inhibitors: use of free energy perturbation calculations to evaluate isosteric replacement for amide bonds in a potent HIV protease inhibitor. 1993 , 7, 291-304	28
1909	The effects of atomic multipole moments obtained by the potential-derived method on hydrogen bonding. 1993 , 46, 239-255	13
1908	Helical region of the potential energy surface of 🗄 minoisobutyric acid: A theoretical study. 1993 , 47, 231-238	10
1907	Characterization of proline-containing alpha-helix (helix F model of bacteriorhodopsin) by molecular dynamics studies. 1993 , 15, 26-41	34
1906	Novel mechanism-based substrates of dihydrofolate reductase and the thermodynamics of ligand binding: a comparison of theory and experiment for 8-methylpterin and 6,8-dimethylpterin. 1993 , 15, 426-35	7
1905	Fluoride inhibition of yeast enolase: crystal structure of the enolase-Mg(2+)-F(-)-Pi complex at 2.6 A resolution. 1993 , 16, 219-25	36
1904	Absolute and relative binding free energy calculations of the interaction of biotin and its analogs with streptavidin using molecular dynamics/free energy perturbation approaches. 1993 , 16, 226-45	198

1903	Hydrophobic core repacking and aromatic-aromatic interaction in the thermostable mutant of T4 lysozyme Ser 117>Phe. 1993 , 2, 1285-90	72
1902	Application of molecular dynamics and free energy perturbation methods to metalloporphyrin-ligand systems II: CO and dioxygen binding to myoglobin. 1993 , 2, 1975-86	22
1901	The application of the genetic algorithm to the minimization of potential energy functions. 1993 , 3, 49-66	42
1900	Timolol derivatives. I. X-ray, NMR and theoretical studies of the crystallization of (S)-timolol O,O-diacetyl-l-tartaric acid monoester. 1993 , 4, 709-722	12
1899	The NMR solution structure of a Kunitz-type proteinase inhibitor from the sea anemone Stichodactyla helianthus. 1993 , 212, 675-84	50
1898	Structure/activity relationship of adenine-modified NAD derivatives with respect to porcine heart lactate dehydrogenase isozyme H4 simulated with molecular mechanics. 1993 , 213, 947-56	9
1897	Modelling and modification of the binding site of endothelin and other receptors. 1993, 245, 203-14	19
1896	Conformational analysis and structural study by ab initio gradient geometry optimizations of the model tripeptide N-formyl L-alanyl L-alanine amide. 1993 , 286, 149-163	18
1895	A new method for the interpretation of dynamics trajectories in the conformational analysis of HIV receptor mutants. 1993 , 286, 165-182	6
1894	On the use of potential derived (PD) atomic charges for the evaluation of solvation free energy. 1993 , 279, 131-138	9
1893	The relation between ligand structures, coordination stereochemistry, and electronic and thermodynamic properties. 1993 , 123, 1-48	141
1892	NMR spectroscopic properties (1H at 500 MHz) of deuterated* ribonucleotide-dimers ApU*, GpC*, partially deuterated 2'-deoxyribonucleotide-dimers d(TpA*), d(ApT*), d(GpC*) and their comparison with natural counterparts (1H-NMR window). 1993 , 26, 1-26	18
1891	Conformational studies on some Cl'-branched beta-D-nucleosides by 1H-NMR spectroscopy and molecular mechanics calculations. 1993 , 26, 317-34	2
1890	Structural studies of the 5'-phenazinium-tethered matched and G-A-mismatched DNA duplexes by NMR spectroscopy. 1993 , 26, 173-236	19
1889	The three-dimensional structure of the colicin E3 immunity protein by distance geometry calculation. 1993 , 333, 257-60	10
1888	Hydration and heat stability effects on protein unfolding. 1993 , 59, 237-84	163
1887	Aspects of protein energetics and dynamics. 1993 , 60, 73-200	60
1886	Particle mesh Ewald: An N?log(N) method for Ewald sums in large systems. 1993 , 98, 10089-10092	19280

1885	Orientational sampling and rigid-body minimization in molecular docking. 1993, 17, 266-78	132
1884	The effect of long-range electrostatic interactions in simulations of macromolecular crystals: A comparison of the Ewald and truncated list methods. 1993 , 99, 8345-8348	498
1883	Prediction of the global energy minimum conformation of polypeptides by the High Directional Monte Carlo procedure. 1993 , 1, 139-143	3
1882	Conformational analysis by molecular mechanics energy minimizations of the tetrapeptide Boc-Gly-Leu-Gly-GlyâNMe, a recurring sequence of elastin. 1993 , 1951-1961	9
1881	A symmetric inhibitor binds HIV-1 protease asymmetrically. 1993 , 32, 937-47	70
1880	DNA conformational change produced by the site-specific interstrand cross-link of trans-diamminedichloroplatinum(II). 1993 , 32, 11676-81	109
1879	Sampling of the conformations of the d(CGCTGCGGC) hairpin in solution by two-dimensional nuclear magnetic resonance and theoretical methods. 1993 , 32, 948-60	19
1878	Replication of the base pair 6-thioguanine/5-methyl-2-pyrimidine with the large Klenow fragment of Escherichia coli DNA polymerase I. 1993 , 32, 3047-57	39
1877	Theoretical predictions of DNA hairpin loop conformations: correlations with thermodynamic and spectroscopic data. 1993 , 32, 436-54	29
1876	Three-dimensional molecular modeling of bovine caseins: an energy-minimized beta-casein structure. 1993 , 76, 931-45	140
1875	Three-dimensional molecular modeling of bovine caseins: a refined, energy-minimized kappa-casein structure. 1993 , 76, 2507-20	59
1874	Rational protein engineering and industrial application: structure prediction by homology and rational design of protein-variants with improved 'washing performance'the alkaline protease from Bacillus alcalophilus. 1993 , 28, 31-40	16
1873	Protein Structure Prediction with a Combined Solvation Free Energy-Molecular Mechanics Force Field. 1993 , 10, 121-149	69
1872	Computer simulations of biomolecular structure and dynamics using a vibrational empirical potential energy function. 1993 , 3-6	
1871	Stereochemical effects of methylphosphonate in B- and Z-DNA helices: variation in hydrophobicity and effective widths of grooves. 1993 , 10, 1023-45	7
1870	Structure of the retinoid X receptor alpha DNA binding domain: a helix required for homodimeric DNA binding. 1993 , 260, 1117-21	268
1869	Solvent effects on molecular spectra. I. Normal pressure and temperature Monte Carlo simulations of the structure of dilute pyrimidine in water. 1993 , 99, 1482-1495	37
1868	On the use of acceptance ratio methods in free energy calculations. 1993 , 99, 10086-10087	12

1867	Calculations of the relative free energies of aqueous solvation of several fluorocarbons: A test of the bond potential of mean force correction. 1993 , 99, 9103-9110	25
1866	Solvent effects on molecular spectra. III. Absorption to and emission from the lowest singlet (n,图) state of dilute pyrimidine in water. 1993 , 99, 1508-1521	48
1865	Molecular Modelling of Chymotrypsin-Substrate Interactions: Calculation of Enantioselectivity. 1993 , 7, 131-147	46
1864	Theory of pressure-dependent melting of the DNA double helix: Role of strained hydrogen bonds. 1993, 47, 2100-2108	13
1863	Determining the contributions of constraints in free energy calculations: Development, characterization, and recommendations. 1993 , 98, 8946-8957	65
1862	Solvent effects on molecular spectra. II. Simulations of hydrated clusters and dilute solutions of pyrimidine in its lowest (n,🖱) singlet excited state. 1993 , 99, 1496-1507	29
1861	A CHARMm Based Force Field for Carbohydrates Using the CHEAT Approach: Carbohydrate Hydroxyl Groups Represented by Extended Atoms. 1993 , 10, 75-95	56
1860	Computer modelling studies of ribonuclease A-pyrimidine nucleotide complexes. 1993 , 11, 395-415	9
1859	Effects of different continium dielectric models in a molecular dynamics and energy minimization study of the antigenic loop of foot-and-mouth disease virus. 1993 , 11, 429-41	6
1858	Investigation of solution structure of d(GAATTTAAATTC)2 by 1H NMR, molecular dynamics, mechanics, refinement by back-calculation of the NOESY spectrum and analysis of this structure using X-ray data. 1993 , 10, 693-707	3
1857	Theoretical Studies on Hydrogen Bonding Interactions between Peptide Units. 1993 , 66, 3423-3429	13
1856	Theoretical Simulations on d(CGCGAATTCGCG)2withcis-synThymineâIIhymine Cyclobutane Dimer. 1993 , 66, 3132-3134	3
1855	Molecular modeling studies suggest that zinc ions inhibit HIV-1 protease by binding at catalytic aspartates. 1993 , 101, 246-50	9
1854	The Effect of Water on the Low Frequency Motions in BPTI. 1993 , 1207-1210	
1853	Molecular Docking: A Tool for Ligand Discovery and Design. 1994 , 28, 735-749	1
1852	The Genetic Algorithm and the Conformational Search of Polypeptides and Proteins. 1994 , 13, 299-320	17
1851	Molecular dynamics simulations suggest that the Eco RI kink is an example of molecular strain. 1994 , 12, 487-525	16
1850	A study of the interaction of DAPI with DNA containing AT and non-AT sequencesmolecular specificity of minor groove binding drugs. 1994 , 11, 849-67	13

1849	Supercomputing Studies of Biomembranes. 1994 , 8, 6-23	8
1848	Binding of echinomycin to d(GCGC)2 and d(CCGG)2: distinct stacking interactions dictate the sequence-dependent formation of Hoogsteen base pairs. 1994 , 12, 111-29	15
1847	Interactions between amino groups in DNA. An Ab initio study and a comparison with empirical potentials. 1994 , 11, 1357-76	25
1846	Hydration of cytidine, 2'-deoxycytidine and their phosphate salts in the aqueous solutions. A molecular dynamics computer simulation study. 1994 , 11, 1307-25	4
1845	Complexes between osmium tetraoxide bispyridine and DNA: a molecular mechanics study. 1994 , 12, 327-42	1
1844	Molecular dynamics simulations of a r(GA12G).d(CT12C) hybrid duplex. 1994 , 11, 1161-74	13
1843	Characterization of substrate UpA binding to RNase Acomputer modelling and energetics approach. 1994 , 12, 581-603	9
1842	Structure and dynamics of lanthanide ions and lanthanide complexes in solution. 1994 , 6, A137-A140	16
1841	Walking on the free energy hypersurface of the 18-crown-6 ion system using free energy derivatives. 1994 , 101, 627-633	16
1840	Vibrational spectrum of water at the liquid/vapor interface. 1994, 73, 2083-2086	99
1839	NMR solution structure of a peptide nucleic acid complexed with RNA. 1994 , 265, 777-80	198
1838	A deterministic global optimization approach for molecular structure determination. 1994 , 100, 1247-1261	85
1837		
1836	Computer modeling studies of the interaction of water with carbohydrates. 1994 , 22, 43-57	7
1835	A database of 32 DNA triplets to study triple helices by molecular mechanics and dynamics. 1994 , 50, 323-43	23
1834	A view of thermodynamics of hydration emerging from continuum studies. 1994 , 51, 167-90; discussion 190-2	33
1833	An energy-minimized casein submicelle working model. 1994 , 13, 681-700	35
1832	The use of the SPASIBA spectroscopic potential for reproducing the structures and vibrational frequencies of a sries of acids: acetic acid, pivalic acid, succinic acid, adipic acid and l-glutamic acid. 1994 , 317, 171-184	18

1831	Molecular dynamics simulations of the conformational behaviour of the synthetic dipeptide PIDOTIMOD, a new immunostimulating agent. 1994 , 317, 197-214	3
1830	A shape-based machine learning tool for drug design. 1994 , 8, 635-52	75
1829	Finding potential DNA-binding compounds by using molecular shape. 1994 , 8, 731-50	24
1828	GREEN: a program package for docking studies in rational drug design. 1994 , 8, 347-66	32
1827	Comparison of two amides as backbone replacement of the phosphodiester linkage in oligodeoxynucleotides. 1994 , 35, 5225-5228	46
1826	Theoretical studies on specific interactions between biological molecules: interaction of cationic arginine with anionic glutamic acid. 1994 , 311, 45-53	2
1825	Conformational preferences of a few enkephalin unsaturated analogs. 1994 , 311, 255-272	
1824	Solvated structure analysis of a conformationally restricted analogue of phenylalanine in a dipeptide model by the AM1-SM2 method. 1994 , 311, 297-304	
1823	Replacement of the phosphodiester linkage in oligonucleotides: Comparison of two structural amide isomers. 1994 , 4, 873-878	31
1822	Conformational properties of disulphide bridges. 2. Rotational potentials of diethyl disulphide. 1994 , 7, 259-267	11
1821	The relative stability of the tautomers of ⊞ydroxytetronic acid. 1994 , 50, 385-394	1
1820	Response of dynamic structure to removal of a disulfide bond: normal mode refinement of C77A/C95A mutant of human lysozyme. 1994 , 3, 92-102	12
1819	Harmonic and anharmonic aspects in the dynamics of BPTI: a normal mode analysis and principal component analysis. 1994 , 3, 936-43	102
1818	Computer modeling of substrate binding to lipases from Rhizomucor miehei, Humicola lanuginosa, and Candida rugosa. 1994 , 3, 1493-503	58
1817	The NMR solution structure of the pheromone Er-2 from the ciliated protozoan Euplotes raikovi. 1994 , 3, 1515-26	38
1816	The NMR solution structure of the pheromone Er-1 from the ciliated protozoan Euplotes raikovi. 1994 , 3, 1527-36	38
1815	Structure comparison of the pheromones Er-1, Er-10, and Er-2 from Euplotes raikovi. 1994 , 3, 1537-46	46
1814	Determinants of protein side-chain packing. 1994 , 3, 2358-65	64

1813	An evaluation of implicit and explicit solvent model systems for the molecular dynamics simulation of bacteriophage T4 lysozyme. 1994 , 18, 19-33		44
1812	A connected-cluster of hydration around myoglobin: correlation between molecular dynamics simulations and experiment. 1994 , 18, 133-47		101
1811	Molecular dynamics studies on mutants of Cu,Zn superoxide dismutase: the functional role of charged residues in the electrostatic loop VII. 1994 , 18, 216-30		20
1810	Intrinsic pKas of ionizable residues in proteins: an explicit solvent calculation for lysozyme. 1994 , 20, 85-97		84
1809	Polarographic study of Tl+, Li+, Na+, K+, and Cs+ complexes with monensin anion in dipolar aprotic solvents. 1994 , 125, 801-809		7
1808	A computer simulation âl\$tatistical procedure for predicting complexation equilibrium constants. 1994 , 18, 9-26		14
1807	Conformational searches for the global minimum of protein models. 1994 , 4, 209-227		7
1806	Interactive multivariate modeling of ArgGlyAsp (RGD) derivatives. 1994 , 14, 75-126		6
1805	Effect of stereochemistry on hydroxyl proton chemical shifts and coupling constants in carbohydrates. 1994 , 32, 225-230		43
1804	The interaction of intercalators and groove-binding agents with DNA triple-helical structures: the influence of ligand structure, DNA backbone modifications and sequence. 1994 , 7, 89-98		48
1803	Topographical metric to analyze the thermal fluctuations of protein conformation. 1994 , 219, 155-159		5
1802	The electrostatic potential in the semiempirical molecular orbital approximation. 1994 , 225, 11-17		18
1801	On the use of quantum energy surfaces in the derivation of molecular force fields. 1994 , 84, 131-155		69
1800	Simulations of the solution structure of HIV-1 protease in the presence and absence of bound zinc. Journal of Computational Chemistry, 1994 , 15, 61-71	3.5	4
1799	Free energy derivatives: A new method for probing the convergence problem in free energy calculations. <i>Journal of Computational Chemistry</i> , 1994 , 15, 105-123	3.5	51
1798	Derivation of class II force fields. I. Methodology and quantum force field for the alkyl functional group and alkane molecules. <i>Journal of Computational Chemistry</i> , 1994 , 15, 162-182	3.5	659
1797	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
1796	Free energy perturbation calculations on parallel computers: Demonstrations of scalable linear speedup. <i>Journal of Computational Chemistry</i> , 1994 , 15, 351-373	3.5	12

1795	Force field for computation of conformational energies, structures, and vibrational frequencies of aromatic polyesters. <i>Journal of Computational Chemistry</i> , 1994 , 15, 752-768	326
1794	Principal component analysis of dipeptides. <i>Journal of Computational Chemistry</i> , 1994 , 15, 963-980 3.5	7
1793	A force field for monosaccharides and (1 -> 4) linked polysaccharides. <i>Journal of Computational Chemistry</i> , 1994 , 15, 1019-1040	116
1792	Comparison of the molecular mechanics + generalized Born/surface area and the ab initio + Monte Carlo simulation methods in estimating conformational equilibria in aqueous solution. <i>Journal of Computational Chemistry</i> , 1994 , 15, 1228-1240	11
1791	Alpha/3(10)-helix transitions in alpha-methylalanine homopeptides: conformational transition pathway and potential of mean force. 1994 , 34, 75-90	66
1790	Analyzing the normal mode dynamics of macromolecules by the component synthesis method: Residue clustering and multiple-component approach. 1994 , 34, 321-335	13
1789	NMR investigation of cyclo7,10[C7,X9,C10,Nle12] analogues of the alpha-factor from Saccharomyces cerevisiae. 1994 , 34, 709-20	9
1788	Conformation of CD4-derived cyclic hexapeptides by NMR and molecular dynamics. 1994 , 34, 987-1000	6
1787	Solution conformation of a cyclic neurokinin antagonist: a NMR and molecular dynamics study. 1994 , 34, 1165-73	6
1786	Conformational polymorphism in telomeric structures: loop orientation and interloop pairing in d(G4TnG4). 1994 , 34, 1187-211	23
1785	Molecular modeling of the conformational and sodium ion binding properties of the oligosaccharide component of ganglioside GM1. 1994 , 34, 1311-26	12
1784	Amidverbrĉkung, eine neue Art der Modifizierung von Oligonucleotidrĉkgraten. 1994 , 106, 237-240	13
1783	Chiral requirements for tumor promoters: Conformations and activity of benzolactams. 1994 , 4, 491-494	9
1782	A2 agonists: structure-activity relationships of 2-(cycloalkylalkynyl)adenosine derivatives. 1994 , 29, 369-380	8
1781	The hydration and solvent polarization effects of nucleotide bases. 1994 , 51, 253-61	40
1780	Comparison of normal mode analyses on a small globular protein in dihedral angle space and Cartesian coordinate space. 1994 , 52, 107-14	29
1779	Characterization of biomolecular structure and dynamics by NMR cross relaxation. 1994 , 26, 27-58	70
1778	The structures and vibrational frequencies of a series of linear alkenes obtained using the spectroscopic potential SPASIBA. 1994 , 326, 35-58	19

A vibrational molecular force field of model compounds with biological interest. VII. Harmonic dynamics of N-acetyl-Ed-muramic acid and N-acetyl-Ed-neuraminic acid in the crystalline state. **1994**, 327, 1-21

1776	A âllow-coolingâlMonte Carlo conformational space study of 18-crown-6 and its alkali metal cation complexes. 1994 , 308, 125-140	7
1775	Improvements to the molecular dynamics simulated annealing procedures: conformational search of the elastin tetrapeptide Boc-Gly-Leu-Gly-NMe. 1994 , 308, 141-157	9
1774	Conformational effects on vibrational frequencies of cysteine and serine: an ab initio study. 1994 , 305, 205-224	39
1773	Consistent point-charges at the 18-crown-6 atoms from correlated ab initio calculations. 1994 , 305, 249-260	11
1772	Synthesis, molecular modelling, and NMR structure determination of four cyclic peptide antagonists of endothelin. 1994 , 2, 279-96	5
1771	A three-dimensional model of the Rev-binding element of HIV-1 derived from analyses of aptamers. 1994 , 1, 293-300	48
1770	Protein surface oligosaccharides and protein function. 1994 , 1, 499-501	76
1769	Prediction of new serine proteinase inhibitors. 1994 , 1, 735-43	62
1768	High-resolution solution structures of oxidized and reduced Escherichia coli thioredoxin. 1994 , 2, 853-68	267
1767	Geometrical and conformational properties of ganglioside GalNAc-GD1a, IV4GalNAcIV3Neu5AcII3Neu5AcGgOse4Cer. 1994 , 225, 271-88	54
1766	The three-dimensional structure in solution of the paramagnetic high-potential iron-sulfur protein I from Ectothiorhodospira halophila through nuclear magnetic resonance. 1994 , 225, 715-25	87
1765	Crystal structure analysis of a serine proteinase from Streptomyces fradiae at 0.16-nm resolution and molecular modeling of an acidic-amino-acid-specific proteinase. 1994 , 224, 735-42	7
1764	The Solution Structure of a DNA Duplex Containing the cis -Pt(NH3)2[d(-GTG-)-N 7(G), N 7(G)] Adduct, as Determined with High-Field NMR and Molecular Mechanics/Dynamics. 1994 , 225, 1169-1179	40
1763	Conformation analysis of 3'-fluorinated A(2'-5')A(2'-5')A fragments. Relation between conformation and biological activity. 1994 , 221, 759-68	15
1762	Three-dimensional crystal structure of the A-tract DNA dodecamer d(CGCAAATTTGCG) complexed with the minor-groove-binding drug Hoechst 33258. 1994 , 222, 721-6	90
1761	Conversion of enkephalin and dermorphin into delta-selective opioid antagonists by single-residue substitution. 1994 , 224, 241-7	42
1760	Theoretical studies on specific interactions between biological molecules: interaction of cationic arginine with anionic glutamic acid. 1994 , 311, 45-53	2

1759	Conformational preferences of a few enkephalin unsaturated analogs. 1994 , 311, 255-272	4
1758	Solvated structure analysis of a conformationally restricted analogue of phenylalanine in a dipeptide model by the AM1-SM2 method. 1994 , 311, 297-304	7
1757	Solution structure of a specific DNA complex of the Myb DNA-binding domain with cooperative recognition helices. 1994 , 79, 639-48	430
1756	Molecular Dynamics Simulations of Langmuir-Blodgett Monolayers with Explicit Head-group Interactions. 1994 , 13, 77-99	9
1755	Reference interaction site model self-consistent field study for solvation effect on carbonyl compounds in aqueous solution. 1994 , 100, 7443-7453	282
1754	Molecular dynamics simulations of proteins in solution: Artifacts caused by the cutoff approximation. 1994 , 101, 4055-4061	94
1753	Simulation study of poly(Ebenzyl-l-glutamate) in dimethylformamide. 1994 , 81, 369-375	1
1752	The NMR Chemical Shift: Insight into Structure and Environment. 1994 , 29, 1-69	41
1751	Molecular mechanics modeling of shear and the crystal orientation dependence of the elastic precursor shock strength in pentaerythritol tetranitrate. 1994 , 76, 2726-2737	119
1750	NMR solution structure of the recombinant tick anticoagulant protein (rTAP), a factor Xa inhibitor from the tick Ornithodoros moubata. 1994 , 352, 251-7	40
1749	Three-dimensional structure of a type VI turn in a linear peptide in water solution. Evidence for stacking of aromatic rings as a major stabilizing factor. 1994 , 243, 754-66	108
1748	Ligand docking to proteins with discrete side-chain flexibility. 1994 , 235, 345-56	314
1747	Dipole and hydrogen-bonding interactions in polyaniline: a mechanism for conductivity enhancement. 1994 , 65, 123-130	41
1746	A molecular dynamics simulation study of chloroform. 1994 , 83, 381-403	143
1745	The inducible multipole solvation model: A new model for solvation effects on solute electrostatics. 1994 , 100, 5149-5159	33
1744	Molecular modelling study of a dissymmetric calix[4]arene and its methyl ethers. 1994 , 2259-2267	9
1743	Identification of the catalytic base in long chain acyl-CoA dehydrogenase. 1994 , 33, 4258-64	47
1742	Stabilizing and destabilizing effects of placing beta-branched amino acids in protein alpha-helices. 1994 , 33, 12022-31	40

1741	Solution structure of the octamer motif in immunoglobulin genes via restrained molecular dynamics calculations. 1994 , 33, 354-66	79
1740	Molecular dynamics free energy simulations: Influence of the truncation of long-range nonbonded electrostatic interactions on free energy calculations of polar molecules. 1994 , 101, 7953-7962	44
1739	Ab initio SCF and force-field calculations on low-energy conformers of 2-acetylamino-2,N-dimethylpropanamide. 1994 , 563-568	28
1738	The NMR structure of the pulmonary surfactant-associated polypeptide SP-C in an apolar solvent contains a valyl-rich alpha-helix. 1994 , 33, 6015-23	184
1737	Computational chemistry and molecular modeling of electron-transfer proteins. 1994 , 243, 559-607	3
1736	Accounting for molecular mobility in structure determination based on nuclear magnetic resonance spectroscopic and X-ray diffraction data. 1994 , 239, 619-54	28
1735	Derivation of Class II Force Fields. III. Characterization of a Quantum Force Field for Alkanes. 1994 , 34, 195-231	61
1734	Acetylcholine Recognition by an Aromatic Host: the Role of an All-Hydrogen Topology in Simulations of the Cation-Interaction. 1994 , 34, 159-163	6
1733	Molecular volume. 1995 , 259, 377-95	4
1732	How to generate accurate solution structures of double-helical nucleic acid fragments using nuclear magnetic resonance and restrained molecular dynamics. 1995 , 261, 3-44	43
1731	Systems for the NMR study of modified nucleoside-dependent, metal-ion induced conformational changes in nucleic acids. 1995 , 261, 270-99	9
1730	Rational approaches to computer drug design based on drug-receptor interactions. 1995 , 3-48	1
1729	Chapter 12 Simulated annealing applied to crystallographic structure refinement. 1995 , 259-280	1
1728	Structural comparison of the free and DNA-bound forms of the purine repressor DNA-binding domain. 1995 , 3, 1217-24	40
1727	Three-Dimensional Structure of Bovine Heart Fatty-acid-binding Protein with Bound Palmitic Acid, Determined by Multidimensional NMR Spectroscopy. 1995 , 230, 266-280	2
1726	Molecular dynamics study of the binding of elsamicin A to DNA. 1995 , 230, 555-66	8
1725	Solution structure of the oxidized 2[4Fe-4S] ferredoxin from Clostridium pasteurianum. 1995 , 232, 192-205	73
1724	Skalare Kopplungen âlīhre Analyse und ihre Verwendung zur Strukturaufklfung. 1995 , 107, 1813-1838	13

1723	Chelation control by a second nitrogen atom in formal hetero Diels-Alder reactions of N-arylimines. 1995 , 1995, 985-993		13
1722	The Solution Structure of Oxidized HiPIP I from Ectothiorhodospira halophila; Can NMR Spectroscopy Be Used to Probe Rearrangements Associated with Electron Transfer Processes?. 1995 , 1, 598-607		27
1721	A nonhelical, multiple beta-turn conformation in a glycine-rich heptapeptide fragment of trichogin A IV containing a single central alpha-aminoisobutyric acid residue. 1995 , 35, 21-9		26
1720	Molecular dynamics simulations of the effects of ring-saturated thymine lesions on DNA structure. 1995 , 35, 113-24		39
1719	Low-frequency vibrations in alpha-helices: helicoidal analysis of polyalanine and deoxymyoglobin molecular dynamics trajectories. 1995 , 35, 555-71		9
1718	Sequence and temperature dependence of the interbase hydrogen-bond breathing modes in B-DNA polymers: comparison with low-frequency Raman peaks and their role in helix melting. 1995 , 35, 573-82		19
1717	Normal mode calculation of a netropsin-DNA complex: effect of structural deformation on vibrational spectrum. 1995 , 35, 657-66		17
1716	Conformational mimicry: synthesis and solution conformation of a cyclic somatostatin hexapeptide containing a tetrazole cis amide bond surrogate. 1995 , 36, 181-200		54
1715	Controlling enzyme-catalyzed regioselectivity in sugar ester synthesis. 1995 , 45, 426-34		93
1714	Relative melting temperatures of RNase HI mutant proteins from MD simulation/free energy calculations. 1995 , 236, 156-161		18
1713	The solvent effect on the acidities of haloacetic acids in aqueous solution. A RISM-SCF study. 1995 , 240, 199-204		17
1712	Internal motion of benzene. A molecular dynamics simulation study. 1995 , 241, 380-386		10
1711	Can contemporary density functional theory yield accurate thermodynamics for hydrogen bonding?. 1995 , 247, 112-119		47
1710	AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules. 1995 , 91, 1-41		2509
1709	JUMNA (junction minimisation of nucleic acids). 1995 , 91, 135-158		169
1708	Molecular Clefts Derived from 9,9?-spirobi[9H-fluorene] for enantioselective complexation of pyranosides and dicarboxylic acids. 1995 , 78, 367-390		67
1707	An application of the Miertus-Scrocco-Tomasi solvation model in molecular mechanics and dynamics simulations. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1-19	3.5	28
1706	Force field parameters for sulfates and sulfamates based on ab initio calculations: Extensions of AMBER and CHARMm fields. <i>Journal of Computational Chemistry</i> , 1995 , 16, 56-79	3.5	103

1705	An examination of a density functional/molecular mechanical coupled potential. <i>Journal of Computational Chemistry</i> , 1995 , 16, 113-128	3.5	87
1704	A molecular mechanical model that reproduces the relative energies for chair and twist-boat conformations of 1,3-dioxanes. <i>Journal of Computational Chemistry</i> , 1995 , 16, 243-261	3.5	33
1703	Parameterization and evaluation of a flexible water model. <i>Journal of Computational Chemistry</i> , 1995 , 16, 501-511	3.5	112
1702	Efficient conformational space sampling for nucleosides using internal coordinate Monte Carlo simulations and a modified furanose description. <i>Journal of Computational Chemistry</i> , 1995 , 16, 667-680	3.5	12
1701	Accurate modeling of the intramolecular electrostatic energy of proteins. <i>Journal of Computational Chemistry</i> , 1995 , 16, 791-816	3.5	207
1700	An improved molecular modeling method for the prediction of enantioselectivity. <i>Journal of Computational Chemistry</i> , 1995 , 16, 914-922	3.5	15
1699	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1141-1152	3.5	10
1698	Flexible ligand docking without parameter adjustment across four ligandâfeceptor complexes. Journal of Computational Chemistry, 1995 , 16, 1210-1226	3.5	85
1697	Reduced variable molecular dynamics. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1271-1290	3.5	18
1696	Multidimensional free-energy calculations using the weighted histogram analysis method. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1339-1350	3.5	628
1695	Gradient SHAKE: An improved method for constrained energy minimization in macromolecular simulations. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1351-1356	3.5	11
1694	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1357-1377	3 .5	820
1693	A molecular dynamics study of the inhibition of chicken dihydrofolate reductase by a phenyl triazine. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1378-1393	3.5	7
1692	Calculation of molecular geometries, relative conformational energies, dipole moments, and molecular electrostatic potential fitted charges of small organic molecules of biochemical interest by density functional theory. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1483-1506	3.5	90
1691	Toward a more efficient handling of conformational flexibility in computer-assisted modelling of drug molecules. 1995 , 3, 85-105		17
1690	Structural effects of the binding of GTP to the wild-type and oncogenic forms of the ras-gene-encoded p21 proteins. 1995 , 14, 721-9		20
1689	Comparison of the computed three-dimensional structures of oncogenic forms (bound to GDP) of the ras-gene-encoded p21 protein with the structure of the normal (non-transforming) wild-type protein. 1995 , 14, 457-66		21
1688	Calculation of atom-centered partial charges for heme. 1995 , 5, 135-142		2

1687 Construction of a DNA four-way junction: Design and NMR spectroscopy. **1995**, 5, 179-194

PRO-LIGAND: an approach to de novo molecular design. 1. Application to the design of organic molecules. 1995 , 9, 13-32	89
The matching of electrostatic extrema: a useful method in drug design? A study of phosphodiesterase III inhibitors. 1995 , 9, 33-43	31
1684 Class IV charge models: a new semiempirical approach in quantum chemistry. 1995 , 9, 87-110	282
168 ₃ Flexible ligand docking using a genetic algorithm. 1995 , 9, 113-30	204
Modelling and mutation studies on the histamine H1-receptor agonist binding site reveal different binding modes for H1-agonists: Asp116 (TM3) has a constitutive role in receptor stimulation. 1995 , 9, 319-30	46
Structure of Leu5-enkephalin bound to a model membrane as determined by high-resolution NMR. 1995 , 2, 59-70	17
Molecular dynamics simulations of alcohol dehydrogenase with a four- or five-coordinate catalytic zinc ion. 1995 , 21, 40-56	108
1679 Local moves: an efficient algorithm for simulation of protein folding. 1995 , 23, 73-82	58
1678 Parametric sensitivity analysis of avian pancreatic polypeptide (APP). 1995 , 23, 218-32	15
A strategy for theoretical binding constant, Ki, calculations for neuraminidase aromatic inhibitors designed on the basis of the active site structure of influenza virus neuraminidase. 1995 , 23, 264-77	37
1676 Analysis of six protein structures predicted by comparative modeling techniques. 1995 , 23, 463-71	46
1675 Theoretical predictions of the functional interactions of DNA and mutagenic aziridines. 1995 , 56, 29-37	1
De novo prediction of polypeptide conformations using dihedral probability grid Monte Carlo methodology. 1995 , 4, 1203-16	21
1673 Modeled structure of the 75-kDa neurotrophin receptor. 1995 , 4, 1696-707	38
Prediction of polyelectrolyte polypeptide structures using Monte Carlo conformational search methods with implicit solvation modeling. 1995 , 4, 2019-31	13
1671 Structural basis for DNA bending by the architectural transcription factor LEF-1. 1995 , 376, 791-5	524
1670 Flap opening in HIV-1 protease simulated by 'activated' molecular dynamics. 1995 , 2, 334-8	132

1669	The structure of calcyclin reveals a novel homodimeric fold for S100 Ca(2+)-binding proteins. 1995 , 2, 790-6	158
1668	Molecular mechanics and dynamics studies on two structurally related amide-modified DNA backbones for antisense technology. 1995 , 3, 321-35	15
1667	NMR structure of d(CGCA3T3GCG)2:tren-microgonotropen-b:Zn(II) complex and solution studies of metal ion complexes of tren-microgonotropen-b interacting with DNA. 1995 , 3, 631-46	6
1666	Small changes in cationic substituents of diphenylfuran derivatives have major effects on the binding affinity and the binding mode with RNA helical duplexes. 1995 , 3, 785-94	28
1665	Multiple DNA binding modes of anthracene-9-carbonyl-N1-spermine. 1995 , 3, 861-72	65
1664	Molecular approach to protein-polymer interactions in ion-exchange chromatography. 1995 , 664, 33-8	3
1663	Molecular simulation applied to 2-(N?-alkylidenehydrazino)- and 2-(N?-aralkylidenehydrazino)adenosine A2 agonists. 1995 , 30, 15-25	9
1662	Conformation of FK506 in X-ray structures of its complexes with human recombinant FKBP12 mutants. 1995 , 5, 1983-1988	26
1661	An analysis of van der Waals attractive forces in DNA-minor groove binding. 1995 , 5, 2573-2576	7
1660	Applicability of commonly used atom-atom type potential energy functions in structural analysis of nucleic acids. The role of electrostatic interactions. 1995 , 19, 253-258	10
1659	The diastereospecific synthesis of new 2?,3?-Cis-Hused carbocyclic nucleosides. 1995 , 51, 329-342	6
1658	Structure and dynamics of MMI linked nucleotides. 1995 , 51, 6855-6868	15
1657	The interaction of the 2?-OH group with the vicinal phosphate in ribonucleoside 3?-ethylphosphate drives the sugar-phosphate backbone into unique (S,B) conformational state. 1995 , 51, 11775-11792	22
1656	Synthesis and solution conformation of a C2 symmetric macrobicycle. 1995 , 36, 3047-3050	10
1655	Conformational Analysis of a Branched Sugar in Aqueous Solution Based on Molecular Mechanics and 1H-NMR Studies. 1995 , 36, 3185-3188	7
1654	Replacement of the phosphodiester linkage in oligonucleotides by a C=C double bond: Comparison of the cis and trans isomers. 1995 , 36, 6879-6882	11
1653	Synthesis and properties of conformationally rigid cyclouridylic acid having a covalent bonding linker between the uracil 5-position and the 5?-phosphate group. 1995 , 36, 9515-9518	5
1652	Hydration in protein crystallography. 1995 , 64, 105-19	56

1651	Molecular orbital constrained gas electron diffraction study of N-acetyl N?-methyl alanine amide. 1995 , 338, 71-82	8
1650	Comparative study of three systems of potential functions for simulation of nucleic acid hydration. 1995 , 44, 1333-1338	1
1649	Reduced frameshift fidelity and processivity of HIV-1 reverse transcriptase mutants containing alanine substitutions in helix H of the thumb subdomain. 1995 , 270, 19516-23	111
1648	The lattice dynamics of mydroquinone clathrate. 1995 , 103, 2773-2778	4
1647	A new molecular dynamics method combining the reference system propagator algorithm with a fast multipole method for simulating proteins and other complex systems. 1995 , 103, 9444-9459	85
1646	The polarization contribution to the free energy of hydration. 1995 , 102, 6145-6152	40
1645	The dipole moment of 18-crown-6: Molecular dynamics study of the structure and dynamics of the macrocycle in vacuo and in cyclohexane. 1995 , 103, 4637-4652	11
1644	New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulations. 1995 , 103, 10183-10191	46
1643	Solvation dynamics in dielectric solvents with restricted molecular rotations: Polyethers. 1995 , 102, 7180-719	6 65
1642	A new spectroscopic molecular mechanics force field. Parameters for proteins. 1995 , 102, 8586-8605	56
1641	Complexation of alkali cations by calix[4]crown ionophores: Conformation and solvent dependent Na+/Cs+ binding selectivity and extraction: MD simulations in the gas phase, in water and at the chloroform-water interface. 1995 , 6, 187-207	76
1640	Structural polymorphism in d(T)12.d(A)12*d(T)12 triple helices. 1995 , 13, 493-505	13
1639	Computational Techniques in Macromolecular Structural Analysis. 1995 , 433-490	1
1638	Molecular Dynamics Simulations of DNA Triple-Helices. Does The Triplex d(A)10년d(T)10년d(T)10 Have A-Form or B-form Geometry?. 1995 , 14, 275-289	4
1637	Definition and Determination of Molecular Geometry. 1995 , 1-33	
1636	Probing the presumed catalytic triad of selenium-containing peroxidases by mutational analysis of phospholipid hydroperoxide glutathione peroxidase (PHGPx). 1995 , 376, 651-60	191
1635	Interaction with DNA of photoactive viologens based on the 6-(2- pyridinium)phenanthridinium structure. 1995 , 12, 827-46	14
1634	Calculations of the phi-psi conformational contour maps for N-acetyl alanine N'-methyl amide and of the characteristic ratios of poly-L-alanine using various molecular mechanics forcefields. 1995 , 13, 201-18	19

1633	Molecular dynamics simulations of chlorambucil/DNA adducts. A structural basis for the 5'-GNC interstrand DNA crosslink formed by nitrogen mustards. 1995 , 12, 911-36	9
1632	Structural characterization of a (+)-trans-anti-benzo[a]pyrene-DNA adduct using NMR, restrained energy minimization, and molecular dynamics. 1995 , 34, 3152-61	82
1631	Structure and dynamics of a DNA.RNA hybrid duplex with a chiral phosphorothioate moiety: NMR and molecular dynamics with conventional and time-averaged restraints. 1995 , 34, 4969-82	105
1630	Conformational analysis of the disaccharide alpha-L-Rhap-(1>2)-alpha-L-Rhap-OMe: comparison of dynamics simulations with NMR experiments. 1995 , 17, 149-60	38
1629	Modelling of the interaction of verotoxin-1 (VT1) with its glycolipid receptor, globotriaosylceramide (Gb3). 1995 , 17, 199-204	29
1628	About the large fluctuations observed using gas-phase molecular dynamics in the K-ras gene containing a mismatch. 1995 , 77, 835-9	1
1627	Characterization of the internal motions of Escherichia coli ribonuclease HI by a combination of 15N-NMR relaxation analysis and molecular dynamics simulation: examination of dynamic models. 1995 , 34, 6587-601	59
1626	Determination of the solution structure of Apo calbindin D9k by NMR spectroscopy. 1995 , 249, 441-62	133
1625	Solution structure of the DNA binding domain of a nucleoid-associated protein, H-NS, from Escherichia coli. 1995 , 360, 125-31	102
1624	Recognition of 2'-hydroxyl groups by Escherichia coli ribonuclease HI. 1995 , 368, 315-20	14
1623	Conformational analysis of potent and very selective delta opioid dipeptide antagonists. 1995 , 377, 363-7	17
1622	Evaluation of protein 3-D structure prediction: comparison of modelled and X-ray structure of an alkaline serine protease. 1995 , 41, 211-9	4
1621	Electrostatic decoupling of periodic images of plane-wave-expanded densities and derived atomic point charges. 1995 , 103, 7422-7428	190
1620	A nucleic acid triple helix formed by a peptide nucleic acid-DNA complex. 1995 , 270, 1838-41	256
1619	Protein structure prediction: recognition of primary, secondary, and tertiary structural features from amino acid sequence. 1995 , 30, 1-94	113
1618	Calculation of monolayer structures of hydrocarbon chains on transition metal dichalcogenides: Dotriacontane on MoSe2. 1995 , 51, 2090-2098	15
1617	Conformation of 6H,12H,18H-tribenzo[b,f,j][1,5,9]trithiacyclododecin revisited. 1995 , 935-938	
1616	The Influence of Starting Coordinates in Free Energy Simulations of Ligand Binding to Dihydrofolate Reductase. 1995 , 15, 155-175	4

1615	pH Dependence of binding reactions from free energy simulations and macroscopic continuum electrostatic calculations: Application to 2?GMP/3?GMP binding to ribonuclease T1 and implications for catalysis. 1995 , 247, 774-807	31
1614	Conformational study of the Thr-Gly repeat in the Drosophila clock protein, PERIOD. 1995 , 260, 155-63	26
1613	Molecular Dynamics Simulation of Skeletal Muscle Contraction. 1996 , 89-114	
1612	Novel Amphiphilic Phthalocyanines: Formation of Langmuirâ B lodgett and Cast Thin Films. 1996 , 12, 4784-4796	82
1611	Synthesis and DNA Binding Properties of Earbolinium Derivatives and Benzologues. 1996 , 61, 5587-5599	73
1610	Solution structure of the E-domain of staphylococcal protein A. 1996 , 35, 15558-69	49
1609	Molecular Dynamics Potential of Mean Force Calculations: A Study of the TolueneâAmmonium ECation Interactions. 1996 , 118, 2998-3005	85
1608	A Very Fast Molecular Dynamics Method To Simulate Biomolecular Systems with Realistic Electrostatic Interactions. 1996 , 100, 10464-10468	82
1607	Peptide Foldamers: Robust Helix Formation in a New Family of Amino Acid Oligomers. 1996 , 118, 13071-13072	588
1606	New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. 1996 , 100, 11775-11788	852
1605	Glycobiology: Toward Understanding the Function of Sugars. 1996 , 96, 683-720	2497
1604	Gas-Phase Conformation of Biological Molecules: Bradykinin. 1996 , 118, 8355-8364	349
1603	Structural Fluctuations of a Cryptophane Host: A Molecular Dynamics Simulation. 1996, 118, 3237-3246	37
1602	The simulated binding of (+/-)-2,3-dihydro-5,6-dimethoxy-2-[[1-(phenylmethyl)-4-piperidinyl]meth yl] -1H-inden-1-one hydrochloride (E2020) and related inhibitors to free and acylated acetylcholinesterases and corresponding structure-activity analyses. 1996 , 39, 4460-70	57
1601	Analysis of Thermodynamic Determinants in Helix Propensities of Nonpolar Amino Acids through a Novel Free Energy Calculation. 1996 , 118, 995-1001	41
1600	Molecular Mechanics Parameters and Conformational Free Energies of Proline-Containing Peptides. 1996 , 61, 1385-1391	70
1599	An analysis of the conserved residues between halobacterial retinal proteins and G-protein coupled receptors: implications for GPCR modeling. 1996 , 36, 857-61	14
1598	Energetics of Reactions Involving Transition Metal Complexes: Calculation of Relative Electrode Potentials for Cobalt Complexes at Various Ionic Strengths Using Density Functional and PoissonaBoltzmann Methods. 1996, 118, 10545-10550	4

1597	Structural Study on Poly(甲-aspartate)s with Short Alkyl Side Chains:´Helical and Extended Crystal Forms. 1996 , 29, 8449-8459	34
1596	Active site structure of Rieske-type proteins: electron nuclear double resonance studies of isotopically labeled phthalate dioxygenase from Pseudomonas cepacia and Rieske protein from Rhodobacter capsulatus and molecular modeling studies of a Rieske center. 1996 , 35, 7834-45	62
1595	The electrostatic contribution to the B to Z transition of DNA. 1996 , 35, 1115-24	56
1594	Structure of a DNA duplex that contains alpha-anomeric nucleotides and 3'-3' and 5'-5' phosphodiester linkages: coexistence of parallel and antiparallel DNA. 1996 , 35, 9355-65	25
1593	Solvent Effects on Molecular and Ionic Spectra. 7. Modeling the Absorption and Electroabsorption Spectra of Pentaammine- ruthenium(II) Pyrazine and Its Conjugate Acid in Water. 1996 , 118, 2059-2068	82
1592	Structural characterization of the 1:1 adduct formed between the antitumor antibiotic hedamycin and the oligonucleotide duplex d(CACGTG)2 by 2D NMR spectroscopy. 1996 , 35, 9314-24	25
1591	Structural variation among retroviral primer-DNA junctions: solution structure of the HIV-1 (-)-strand Okazaki fragment r(gcca)d(CTGC).d(GCAGTGGC). 1996 , 35, 11070-80	25
1590	Creating RNA bulges: cleavage of RNA in RNA/DNA duplexes by metal ion catalysis. 1996 , 35, 16591-600	73
1589	Delineation of an active fragment and poly(L-proline) II conformation for candidacidal activity of bactenecin 5. 1996 , 35, 4314-25	44
1588	DNA-Mediated Acid Catalysis: Calculations of the Rates of DNA-Catalyzed Hydrolyses of Diol Epoxides1. 1996 , 118, 3325-3331	22
1587	Structural features of a six-nucleotide RNA hairpin loop found in ribosomal RNA. 1996 , 35, 6539-48	62
1586	Electrochemical Cyclization of Dipeptides To Form Novel Bicyclic, Reverse-Turn Peptidomimetics. 2. Synthesis and Conformational Analysis of 6,5-Bicyclic Systems. 1996 , 61, 1198-1204	56
1585	High-affinity partial agonist imidazo[1,5-a]quinoxaline amides, carbamates, and ureas at the gamma-aminobutyric acid A/benzodiazepine receptor complex. 1996 , 39, 158-75	59
1584	Structure-activity relationships for the glutathione conjugation of 2-substituted 1-chloro-4-nitrobenzenes by rat glutathione S-transferase 4-4. 1996 , 9, 527-34	8
1583	High-affinity alpha-aminobutyric acid A/benzodiazepine ligands: synthesis and structure-activity relationship studies of a new series of tetracyclic imidazoquinoxalines. 1996 , 39, 4654-66	36
1582	Investigation of the structural basis for thermodynamic stabilities of tandem GU mismatches: solution structure of (rGAGGUCUC)2 by two-dimensional NMR and simulated annealing. 1996 , 35, 14077-89	303
1581	Benzene Dimer: A Good Model for 🖽 Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. 1996 , 118, 11217-11224	265
1580	Evaluation of the electrostatic effect of the 5'-phosphate of the flavin mononucleotide cofactor on the oxidationreduction potentials of the flavodoxin from desulfovibrio vulgaris (Hildenborough).	30

1579	Three-dimensional models for agonist and antagonist complexes with beta 2 adrenergic receptor. 1996 , 39, 4406-20	34
1578	Theoretical study of inhibition of adenosine deaminase by (8R)-coformycin and (8R)-deoxycoformycin. 1996 , 39, 277-84	35
1577	Secondary Interactions Affecting the Dissociation Patterns of Arginine-Containing Peptide Ions. 1996 , 118, 6252-6256	61
1576	Modeling DNA hydration: comparison of calculated and experimental hydration properties of nuclic acid bases. 1996 , 13, 717-26	23
1575	Experimental (NMR) and Computational (MD) Studies on the Inclusion Complexes of 1-Bromoadamantane with alpha-, beta-, and gamma-Cyclodextrin. 1996 , 61, 7012-7017	44
1574	Carbohydrates: United Atom AMBER* Parameterization of Pyranoses and Simulations Yielding Anomeric Free Energies. 1996 , 118, 2078-2086	90
1573	Contribution to activity of histidine-aromatic, amide-aromatic, and aromatic-aromatic interactions in the extended catalytic site of cysteine proteinases. 1996 , 35, 3970-9	36
1572	Evidence for the existence of a pseudoknot structure at the 3' terminus of the flavivirus genomic RNA. 1996 , 35, 4222-30	113
1571	Computational Simulations of DNA Distortions by a cis,syn-Cyclobutane Thymine Dimer Lesionâl 1996 , 118, 9156-9163	66
1570	Active site of bee venom phospholipase A2: the role of histidine-34, aspartate-64 and tyrosine-87. 1996 , 35, 4591-601	45
1569	Molecular dynamics simulations of the bis-intercalated complexes of ditercalinium and Flexi-Di with the hexanucleotide d(GCGCGC)2: theoretical analysis of the interaction and rationale for the sequence binding specificity. 1996 , 39, 4810-24	19
1568	Structure of chimeric duplex junctions: solution conformation of the retroviral Okazaki-like fragment r(ccca)d(AATGA).d(TCATTTGGG) from Moloney murine leukemia virus. 1996 , 35, 8126-35	22
1567	Understanding the binding of 5-substituted 2'-deoxyuridine substrates to thymidine kinase of herpes simplex virus type-1. 1996 , 39, 4727-37	34
1566	Solution structure of (rGCGGACGC)2 by two-dimensional NMR and the iterative relaxation matrix approach. 1996 , 35, 9677-89	105
1565	CONCERTS: dynamic connection of fragments as an approach to de novo ligand design. 1996 , 39, 1651-63	98
1564	Nonpolar interactions of thrombin and its inhibitors at the fibrinogen recognition exosite: thermodynamic analysis. 1996 , 35, 13021-9	8
1563	Atomic Proximity Due to Molecular Congestion: Rational Design of Bis(phosphite) Ligands by Restriction of Molecular Motion(1). 1996 , 35, 949-958	28
1562	Elucidating the Origin of Conformational Energy Differences in Substituted 1,3-Dioxanes: A Combined Theoretical and Experimental Study. 1996 , 61, 3662-3668	15

1561	A quantum chemical explanation of the antioxidant activity of flavonoids. 1996 , 9, 1305-12	342
1560	Hybrid Models for Combined Quantum Mechanical and Molecular Mechanical Approaches. 1996 , 100, 10580-10594	987
1559	Advances and Continuing Challenges in Achieving Realistic and Predictive Simulations of the Properties of Organic and Biological Molecules. 1996 , 29, 461-469	236
1558	The conformational properties of the highly selective cannabinoid receptor ligand CP-55,940. 1996 , 271, 10640-7	48
1557	Heteroligation of a mouse monoclonal IgE antibody (La2) with small molecules, analysed by computer-aided automated docking. 1996 , 33, 129-44	7
1556	Structural modifications of the omega loop in human acetylcholinesterase. 1996 , 395, 22-8	26
1555	Structural role of a buried salt bridge in the 434 repressor DNA-binding domain. 1996 , 264, 1002-12	42
1554	The coordination of the catalytic zinc in alcohol dehydrogenase studied by combined quantum-chemical and molecular mechanics calculations. 1996 , 10, 153-64	143
1553	Synthesis and DNA interactions of benzimidazole dications which have activity against opportunistic infections. 1996 , 39, 1452-62	108
1552	Hydration and DNA recognition by homeodomains. 1996 , 85, 1057-65	104
1551	Hybrid DFT-MD simulations of geometry and hyperfine structure of the CCH radical in argon matrices at low temperatures. 1996 , 105, 8195-8203	17
1550	Including Side Chain Flexibility in Continuum Electrostatic Calculations of Protein Titration. 1996 , 100, 20156-20163	106
1549	High-resolution solution structure of the EGF-like domain of heregulin-alpha. 1996 , 35, 3402-17	61
1548	Intercalation, DNA kinking, and the control of transcription. 1996, 271, 778-84	270
1547	Catalytic role of 2'-hydroxyl groups within a group II intron active site. 1996 , 271, 1410-3	99
1546	Gating as a control element in constrictive binding and guest release by hemicarcerands. 1996 , 273, 627-9	97
1545	A crystallographic and spectroscopic study of the complex between d(CGCGAATTCGCG)2 and 2,5-bis(4-guanylphenyl)furan, an analogue of berenil. Structural origins of enhanced DNA-binding affinity. 1996 , 35, 5655-61	95
1544	Molecular electrostatic potentials and fields: hydrogen bonding, recognition, reactivity and modelling. 1996 , 257-296	26

1543	that have high affinity at the GABAA/benzodiazepine receptor complex. 1996 , 39, 3820-36	84
1542	A Molecular Dynamics and Quantum Mechanics Analysis of the Effect of DMSO on Enzyme Structure and Dynamics: Subtilisin. 1996 , 118, 4175-4180	91
1541	Model of the Second Most Abundant Cisplatin-DNA Cross-Link: X-ray Crystal Structure and Conformational Analysis of cis-[(NH(3))(2)Pt(9-MeA-N7)(9-EtGH-N7)](NO(3)).2H(2)O (9-MeA = 9-Methyladenine; 9-EtGH = 9-Ethylguanine). 1996 , 35, 1647-1652	40
1540	Intrinsic Torsional Potential Parameters for Conformational Analysis of Peptides and Proteins. 1996 , 100, 15588-15598	29
1539	Hydration of C-H groups in tRNA. 1996 , 151-73	40
1538	A kinetic study of C60/Etyclodextrin inclusion complexation by molecular mechanics. 1996 , 817-818	6
1537	Theoretical Evaluation of Steric Effects in [ReH(5)(PR(3))(2)(SiR(3))(2)] Complexes with the IMOMM Method. 1996 , 35, 6401-6405	24
1536	A configurational bias Monte Carlo method for linear and cyclic peptides. 1996 , 87, 1245-1260	41
1535	Taming the Ewald sum in molecular dynamics simulations of solvated proteins via a multiple time step algorithm. 1996 , 104, 3003-3012	62
1534	A hybrid quantum mechanical force field molecular dynamics simulation of liquid methanol: Vibrational frequency shifts as a probe of the quantum mechanical/molecular mechanical coupling. 1996 , 104, 7261-7269	48
1533	A Comprehensive Analytical Treatment of Continuum Electrostatics. 1996 , 100, 1578-1599	494
1532	NMR studies of the hydration of biological macromolecules. 1996 , 103, 245-253	42
1531	Conformational equilibria of methyl -arabinopyranosides in solution. 1996 , 505-510	2
1530	Computer Methods in Protein Modeling: An Overview. 1996 , 51-73	
1529	A small engineered protein lacks structural uniqueness by increasing the side-chain conformational entropy. 1996 , 93, 13583-8	18
1528	Pbx modulation of Hox homeodomain amino-terminal arms establishes different DNA-binding specificities across the Hox locus. 1996 , 16, 1734-45	253
1527	Three-dimensional structure of G protein-coupled receptors: from speculations to facts. 1996 , 24, 205-214	
1526	Finite element study of protein structure under high pressure. 1996 , 157-162	

1525	Using molecular modeling and molecular dynamics simulation to predict P450 oxidation products. 1996 , 272, 347-57	7
1524	Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. 1996 , 118, 11225-11236	9849
1523	Solvent Effect on Acidity: A Hybrid Approach Based on the RISM and the Hartreeâflock Equations. 1996 , 100, 1111-1117	38
1522	Molecular Dynamics Simulation of Electrolyte Solutions in Ambient and Supercritical Water. 1. Ion Solvation. 1996 , 100, 2706-2715	163
1521	Conformations and vibrations of dicarboxylic acids. An ab initio study. 1996 , 362, 77-99	26
1520	Methodological procedures of Molecular Dynamics Simulated Annealing for the chain folding of the flexible tetrapeptide Boc-Gly-Leu-Gly-Gly-NMe with analysis of the evolution mechanism. 1996 , 363, 43-66	3
1519	A pseudrotation model and ring-puckering of cyclopentane. 1996 , 362, 243-255	35
1518	Solvent and counterion effects on complexation selectivity by conformationally locked calix[4]-bis-crown ligands: Molecular Dynamics and Free Energy Perturbation studies in water and methanol, acetonitrile and chloroform solutions. 1996 , 363, 67-85	37
1517	Vibrational frequencies of proline and hydroxyproline An ab initio study. 1996 , 365, 167-181	17
1516	Kinetic and modelling studies of NAD+ and poly(ethylene glycol)-bound NAD+ in horse liver alcohol dehydrogenase. 1996 , 1295, 125-38	8
1515	On the protein folding problem. 1996 , 47, 188-195	
1514	Interactions of anesthetics with the membrane-water interface. 1996 , 204, 337-45	76
1513	Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics. 1996 , 204, 251-261	15
1512	Molecular dynamics simulations of the bulk phases of 4-cyano-4?-n-pentyloxybiphenyl. 1996 , 208, 57-71	22
1511	Modelling of the inclusion process of 日間 and Ecyclodextrins with 1-bromoadamantane. A comparative molecular mechanics study accounting for the solvent. 1996 , 377, 137-147	12
1510	The structures and vibrational frequencies of a series of aliphatic alcohols as obtained using the spectroscopic potential SPASIBA. 1996 , 378, 249-256	7
1509	Chlorinated ethanes in aqueous solution: parameterization based on thermodynamics of hydration. 1996 , 259, 142-145	1
1508	Particle sizes of purified kappa-casein: metal effect and correspondence with predicted three-dimensional molecular models. 1996 , 15, 435-45	29

1507	Computed three-dimensional structures for the ras-binding domain of the raf-p74 protein complexed with ras-p21 and with its suppressor protein, rap-1A. 1996 , 15, 511-8	7
1506	Design considerations and computer modeling related to the development of molecular scaffolds and peptide mimetics for combinatorial chemistry. 1996 , 2, 46-56	6
1505	Similar conformations of hairpins with TTT and TTTT sequences: NMR and molecular modeling evidence for T.T base pairs in the TTTT hairpin. 1996 , 236, 960-9	19
1504	Conformational and associative behaviours of the third helix of antennapedia homeodomain in membrane-mimetic environments. 1996 , 242, 372-86	138
1503	Synthesis and solution structure of the antimicrobial peptide protegrin-1. 1996 , 237, 575-83	145
1502	The solution structure of paramagnetic metalloproteins. 1996 , 66, 43-80	60
1501	Protein conformational substates from X-ray crystallography. 1996 , 66, 167-96	34
1500	Suggested binding mechanism of the HIV-gp120 to its CD4 receptor. 1996 , 367, 159-186	6
1499	The structure and activity of membrane receptors: computational simulation of histamine H2-receptor activation. 1996 , 371, 279-286	2
1498	Chemical reaction mechanisms in vacuo, in solution and in enzyme fields: isomerization catalyzed by triose phosphate isomerase (TIM). 1996 , 371, 287-298	8
1497	Molecular dynamics of local protein motions in lactate dehydrogenase. 1996 , 368, 205-212	2
1496	Towards a better semiquantitative estimation of binding constants: molecular dynamics exploration of the conformational behavior of isolated sialyllactose and sialyllactose complexed with influenza A hemagglutinin. 1996 , 368, 213-222	10
1495	The structures and vibrational frequencies of a series of aliphatic alcohols as obtained using the spectroscopic potential SPASIBA. 1996 , 378, 249-256	1
1494	Modelling of the inclusion process of 日	3
1493	Two structurally different RNA molecules are bound by the spliceosomal protein U1A using the same recognition strategy. 1996 , 4, 621-31	29
1492	A docking and modelling strategy for peptide-RNA complexes: applications to BIV Tat-TAR and HIV Rev-RBE. 1996 , 1, 463-72	12
1491	Recognition of altered self major histocompatibility complex molecules modulated by specific peptide interactions. 1996 , 26, 949-52	12
1490	Analogs of Cinchona Alkaloids Incorporating a 9,9?-Spirobifluorene Moiety. 1996 , 79, 1338-1360	16

1489	Pyranosyl-RNA (âp-RNAâp NMR and Molecular-Dynamics Study of the Duplex Formed by Self-pairing of Ribopyranosyl-(C-G-A-A-T-T-C-G). 1996 , 79, 2316-2345		36
1488	Stark erhfite Affinitfimodifizierter Oligonucleotide mit in ihrer Konformation eingeschrfikten Furanose-Ringen fr.komplementfie RNA-Strfige. 1996 , 108, 2960-2964		4
1487	A comparison of conformational energies calculated by several molecular mechanics methods. Journal of Computational Chemistry, 1996 , 17, 429-449	3.5	133
1486	Merck molecular force field. I. Basis, form, scope, parameterization, and performance of MMFF94. 1996 , 17, 490-519		3435
1485	Merck molecular force field. II. MMFF94 van der Waals and electrostatic parameters for intermolecular interactions. <i>Journal of Computational Chemistry</i> , 1996 , 17, 520-552	3.5	799
1484	Merck molecular force field. IV. conformational energies and geometries for MMFF94. <i>Journal of Computational Chemistry</i> , 1996 , 17, 587-615	3.5	280
1483	Base stacking in cytosine dimer. A comparison of correlated ab initio calculations with three empirical potential models and density functional theory calculations. <i>Journal of Computational Chemistry</i> , 1996 , 17, 841-850	3.5	134
1482	Alternative approaches to potential of mean force calculations: Free energy perturbation versus thermodynamic integration. Case study of some representative nonpolar interactions. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1112-1131	3.5	52
1481	From secondary structure to three-dimensional structure: Improved dihedral angle probability distribution function for use with energy searches for native structures of polypeptides and proteins. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1453-1480	3.5	2
1480	Structure model of a complex between the factor for inversion stimulation (FIS) and DNA: Modeling protein-DNA complexes with dyad symmetry and known protein structures. 1996 , 25, 486-500		1
1479	Computational design of a substrate specificity mutant of a protein. 1996 , 26, 459-64		3
1478	A technique to study molecular recognition in drug design: preliminary application of free energy derivatives to inhibition of a malarial cysteine protease. 1996 , 9, 103-12		4
1477	Prediction of IgE(Lb4)-ligand complex structures by automated docking. 1996 , 9, 239-46		3
1476	Three-dimensional model of a selective theophylline-binding RNA molecule. 1996, 9, 275-286		
1475	Binding of tacrine and 6-chlorotacrine by acetylcholinesterase. 1996 , 38, 109-17		43
1474	Molecular dynamics of subtilisin Carlsberg in aqueous and nonaqueous solutions. 1996 , 38, 791-9		11
1473	DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations. 1996 , 57, 959-970		179
1472	Diffusion of two different water models and thermal conductivity in a proteinâlvater system. 1996 , 59, 271-279		5

1471	A test of the new âIhtegrated MO + MMâ[(IMOMM) method for the conformational energy of ethane and n-butane. 1996 , 60, 1101-1109	163
1470	Direct reaction field force field: A consistent way to connect and combine quantum-chemical and classical descriptions of molecules. 1996 , 60, 1111-1132	56
1469	Analysis of interfacial water structure and dynamics in #maltose solution by molecular dynamics simulation. 1996 , 251, 268-274	20
1468	Correlated solvent-induced forces on a protein at single residue resolution: relation to conformation, stability, dynamics and function. 1996 , 254, 292-301	12
1467	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
1466	Thermodynamic characteristics for the formation of H-bonded DNA base pairs. 1996 , 261, 379-384	38
1465	Molecular dynamics simulations of glycosides in aqueous solution. 1996 , 282, 13-23	22
1464	Complexation of the p-t-butyl-calix[4]arene anion with alkali metal cations in polar, non-aqueous solvents: experimental and theoretical studies. 1996 , 246, 275-286	29
1463	Oxygen and Nitrogen in Competitive Situations: Which is the Hydrogen-Bond Acceptor?. 1996 , 2, 1509-1513	87
1462	Design and synthesis of a heterocyclic amine receptor. 1996 , 52, 10441-10454	9
1462 1461	Design and synthesis of a heterocyclic amine receptor. 1996 , 52, 10441-10454 Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison between carbon-, sulfur-, and oxygen-containing analogs. 1996 , 37, 5511-5514	9
	Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison	
1461	Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison between carbon-, sulfur-, and oxygen-containing analogs. 1996 , 37, 5511-5514 Charge is the major discriminating factor for glutathione reductase versus trypanothione reductase	12
1461 1460	Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison between carbon-, sulfur-, and oxygen-containing analogs. 1996 , 37, 5511-5514 Charge is the major discriminating factor for glutathione reductase versus trypanothione reductase inhibitors. 1996 , 4, 1247-53	12 63
1461 1460 1459	Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison between carbon-, sulfur-, and oxygen-containing analogs. 1996, 37, 5511-5514 Charge is the major discriminating factor for glutathione reductase versus trypanothione reductase inhibitors. 1996, 4, 1247-53 The rationale for E2020 as a potent acetylcholinesterase inhibitor. 1996, 4, 1429-46 Synthesis and biochemical activity of novel amidine derivatives as m1 muscarinic receptor agonists.	1263106
1461 1460 1459 1458	Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison between carbon-, sulfur-, and oxygen-containing analogs. 1996, 37, 5511-5514 Charge is the major discriminating factor for glutathione reductase versus trypanothione reductase inhibitors. 1996, 4, 1247-53 The rationale for E2020 as a potent acetylcholinesterase inhibitor. 1996, 4, 1429-46 Synthesis and biochemical activity of novel amidine derivatives as m1 muscarinic receptor agonists. 1996, 4, 1605-15 The importance of charge-separation reactions in tandem mass spectrometry of doubly protonated angiotensin II formed by electrospray ionization: Experimental considerations and structural implications. 1996, 7, 30-41	12 63 106 20
1461 1460 1459 1458	Replacement of the phosphodiester linkage in oligonucleotides by an acetylenic bond: Comparison between carbon-, sulfur-, and oxygen-containing analogs. 1996, 37, 5511-5514 Charge is the major discriminating factor for glutathione reductase versus trypanothione reductase inhibitors. 1996, 4, 1247-53 The rationale for E2020 as a potent acetylcholinesterase inhibitor. 1996, 4, 1429-46 Synthesis and biochemical activity of novel amidine derivatives as m1 muscarinic receptor agonists. 1996, 4, 1605-15 The importance of charge-separation reactions in tandem mass spectrometry of doubly protonated angiotensin II formed by electrospray ionization: Experimental considerations and structural implications. 1996, 7, 30-41	12 63 106 20 32

1453	Molecular simulation of 5,6-substituted 1-[(2-hydroxyethoxy)methyl]uracils with anti-HIV-1 activity. 1996 , 31, 701-712	9
1452	The structures and vibrational frequencies of a series of aliphatic ethers obtained using the spectroscopic potential SPASIBA. 1996 , 377, 47-56	9
1451	Correlations between the sugar-backbone conformation and the third strand orientation in triple helices. 1996 , 377, 57-74	2
1450	Solvent effects on the conformational behavior of model peptides. A comparison between different continuum models. 1996 , 263, 113-118	26
1449	Electronic energy transfer in supersonic jet expanded naphthalene-(CH2)n-anthracene bichromophoric molecules. 1996 , 263, 441-448	14
1448	Synthesis and conformational studies of the tyvelose capped, Lewis-x like tetrasaccharide epitope of Trichinella spiralis. 1996 , 4, 1989-2001	18
1447	Hydrogen bonding effects on amine rotation rates in crystalline amino acids. 1996 , 7, 161-72	51
1446	DL_POLY_2.0: a general-purpose parallel molecular dynamics simulation package. 1996 , 14, 136-41	1827
1445	Modeling polysaccharides: present status and challenges. 1996 , 14, 307-21, 361-2	56
1444	The spasiba force field of model compounds related to lipids of biomembranes. 1996 , 384, 55-71	11
1443	Ab initio calculations of the NMR chemical shift. 1996 , 29, 229-278	209
1442	Molecular dynamics simulations of peptides from BPTI: a closer look at amide-aromatic interactions. 1996 , 8, 229-38	79
1441	Comparative docking studies on ligand binding to the multispecific antibodies IgE-La2 and IgE-Lb4. 1996 , 10, 305-20	18
1440	Evolutionary algorithms in computer-aided molecular design. 1996 , 10, 337-58	102
1439	Simulations of CRP:(cAMP)2 in noncrystalline environments show a subunit transition from the open to the closed conformation. 1996 , 5, 62-71	46
1438	A structural basis for enantioselective inhibition of Candida rugosa lipase by long-chain aliphatic alcohols. 1996 , 5, 83-8	59
1437	Improving the quality of NMR and crystallographic protein structures by means of a conformational database potential derived from structure databases. 1996 , 5, 1067-80	180
1436	Experimentally observed conformation-dependent geometry and hidden strain in proteins. 1996 , 5, 1406-20	214

1435	1996 , 5, 1512-22	21
1434	A distant evolutionary relationship between bacterial sphingomyelinase and mammalian DNase I. 1996 , 5, 2459-67	58
1433	Delta-selective opioid peptides containing a single aromatic residue in the message domain: an NMR conformational analysis. 1996 , 2, 290-308	14
1432	Processes Underlying Interactions of Human Lactoferrin with the Jurkat Human Lymphoblastic T-cell Line Receptor. II - Comparative Molecular Field Analysis. 1996 , 15, 102-107	2
1431	A molecular mechanics and dynamics study of alternate triple-helices involving the integrase-binding site of the HIV-1 virus and oligonucleotides having a 3'-3' internucleotide junction. 1996 , 13, 835-53	16
1430	Binding of Net-Fla, a netropsin-flavin hybrid molecule, to DNA: molecular mechanics and dynamics studies in vacuo and in water solution. 1996 , 13, 963-77	16
1429	Solution structures of the individual single strands of the fragile X DNA triplets (GCC)n.(GGC)n. 1996 , 24, 784-92	71
1428	Comparative studies on the substrate specificity of avian myeloblastosis virus proteinase and lentiviral proteinases. 1996 , 271, 6781-8	29
1427	Structure and dynamics of the DNA hairpins formed by tandemly repeated CTG triplets associated with myotonic dystrophy. 1996 , 24, 775-83	59
1426	Stabilization of helical peptides by mixed spaced salt bridges. 1996 , 14, 285-91	4
1425	Human immunodeficiency virus, type 1 protease substrate specificity is limited by interactions between substrate amino acids bound in adjacent enzyme subsites. 1996 , 271, 4709-17	43
1424	Molecular Dynamics Simulation of Electrolyte Solutions in Ambient and Supercritical Water. 2. Relative Acidity of HCl. 1996 , 100, 2716-2722	41
1423	Molecular modelling of liquid crystal systems: An internal coordinate Monte Carlo approach. 1996 , 21, 437-447	30
1422	Molecular modeling of drug-DNA interactions. 1996 , 2, 29-58	2
1421	Quantum-mechanical derivation of angular and torsional forces in well-bonded systems. 1996 , 54, 13656-1360	54
1420	Calculation of nuclear magnetic resonance order parameters in proteins by normal mode analysis. II. Contribution from localized high frequency motions. 1996 , 105, 6560-6564	4
1419	The Jacobian factor in free energy simulations. 1996 , 105, 5145-5154	56
1418	Solvation energies and electronic spectra in polar, polarizable media: Simulation tests of dielectric continuum theory. 1996 , 104, 1293-1308	90

1417	Analytical energy gradient for the reference interaction site model multiconfigurational self-consistent-field method: Application to 1,2-difluoroethylene in aqueous solution. 1996 , 105, 1546-1551	227
1416	Epitaxial interactions between molecular overlayers and ordered substrates. 1996 , 54, 14037-14051	130
1415	1H NMR studies of the 5-(hydroxymethyl)-2'-deoxyuridine containing TF1 binding site. 1996 , 24, 2740-5	14
1414	Oncogenic amino acid substitutions in the inhibitory rap-1A protein cause it to adopt a ras-p21-like conformation as computed using molecular dynamics. 1996 , 13, 925-33	1
1413	Gibbs-Ensemble Molecular Dynamics: Liquid-Gas Equilibria for Lennard-Jones Spheres and n-Hexane. 1996 , 17, 95-112	16
1412	DNA binding by TATA-box binding protein (TBP): a molecular dynamics computational study. 1996 , 13, 593-600	28
1411	FORCE FIELD CALCULATIONS OF ANTITUMOR PLATINUM(II) COMPLEX SYSTEMS. 1996 , 37, 305-314	5
1410	Structure of the Trinucleotide D-acp3U-A with Coordinated Mg2+ Demonstrates that Modified Nucleosides Contribute to Regional Conformations of RNA. 1996 , 15, 1009-1028	16
1409	Computer-Assisted New Lead Design. 1996 , 93-137	2
1408	Are There Water-Bridge-Induced Hydrophilic Interactions?. 1996 , 100, 6760-6763	7
1407	Structural Analysis of the Solution Conformation of Methyl 4-O-时-Glucopyranosyl-时-Glucopyranoside by Molecular Mechanics and ab Initio Calculation, Stochastic Dynamics Simulation, and NMR Spectroscopy. 1996 , 100, 9187-9192	22
1406	Prediction of pKa Shifts without Truncation of Electrostatic Interactions: An Explicit Solvent Calculation for Succinic Acid. 1996 , 100, 6389-6392	34
1405	New Technique for Conformational Sampling of Cyclic Molecules Using the AMBER Force Field: Application to 18-Crown-6. 1996 , 100, 14339-14342	21
1404	Orientation of the OH Dipole of Tyrosine (M)210 and Its Effect on Electrostatic Energies in Photosynthetic Bacterial Reaction Centers. 1996 , 100, 16761-16770	84
1403	Solvent Effects on Molecular and Ionic Spectra IX: The Change in Dipole Moment Accompanying Metal to Ligand Charge Transfer Absorption in Pentaaminopyridylruthenium(II). 1996 , 100, 19292-19294	27
1402	Binding of Azide to Human Carbonic Anhydrase II: The Role Electrostatic Complementarity Plays in Selecting the Preferred Resonance Structure of Azide. 1996 , 100, 17414-17420	26
1401	Solvent Effects on Molecular and Ionic Spectra. VIII. The 1(n,图) Excited States of Pyridazine in Water. 1996 , 100, 9561-9567	30
1400	The J-coupling restrained molecular mechanics (JrMM) protocolan efficient alternative for deriving DNA endocyclic torsion angle constraints. Part I: Correlation of endocyclic torsion angles and vicinal torsion angle phi 1'2' 1996, 13, 803-14	2

1399	A molecular dynamics study of the conformation of the alanine dipeptide in aqueous solution using a quantum mechanical potential. 1997 , 90, 787-792	14
1398	Thermodynamic investigation of enzyme and inhibitor interactions with high affinity. 1997 , 8, 513-521	
1397	Empirical potential for methyl-radical association with diamond surfaces. 1997 , 56, 13543-13555	1
1396	The Molecular Structure of Sodium Octanoate Micelles Studied by Molecular Dynamics Computer Experiments. 1997 , 101, 1485-1492	23
1395	Calculation of the binding affinity of the anticancer drug daunomycin to DNA by a statistical mechanics approach. 1997 , 55, 7390-7395	2
1394	Synthesis and Properties of Conformationally Rigid Cyclouridylic Acids Having Covalent Bonding Linkers Between the Uracil 5-Position and the 5?-Phosphate Group. 1997 , 16, 1023-1032	4
1393	What Is the Longest Unbranched Alkane with a Linear Global Minimum Conformation?. 1997 , 37, 876-878	44
1392	Diffusive motions in liquid 18-crown-6: A molecular dynamics study. 1997 , 106, 8140-8148	2
1391	Direct identification of a distinct site of interaction between the carboxyl-terminal residue of cholecystokinin and the type A cholecystokinin receptor using photoaffinity labeling. 1997 , 272, 24393-401	83
1390	Alanine exchanges of polar amino acids in the transmembrane domains of a platelet-activating factor receptor generate both constitutively active and inactive mutants. 1997 , 272, 7846-54	58
1389	Potassium and Sodium Complexes of 1,3-calix[4]-bis-crown-6: Crystal and Molecular Structures, 1H-NMR Investigation and Molecular Dynamics Simulation. 1997 , 8, 319-332	19
1388	Temperature-Dependent Changes in the Folding Patterns of the Łoop (Tyr181 to Tyr188) of HIV-1 Reverse Transcriptase. 1997 , 19, 117-129	
1387	Crystallographic refinement by simulated annealing: methods and applications. 1997 , 277, 243-69	86
1386	Chapter 17. Sorption rate processes in carbon molecular sieves. 1997 , 837-880	5
1385	Revised intermolecular potential with parameters depending on partial atomic charges for aromatic molecular systems. 1997 , 90, 705-712	
1384	Azino-Fused Benzimidazolium Salts as DNA Intercalating Agents. 2 1997 , 62, 5476-5483	52
1383	The Consistent Force Field. 5. PEF95SAC: Optimized Potential Energy Function for Alcohols and Carbohydrates. 1997 , 16, 751-772	21
1382	Conformation Control of Peptides by Metal Ions. Coordination Conformation Correlation Observed in a Model for Cys-X-Y-Cys/M(2+) in Proteins. 1997 , 36, 4849-4859	14

1381	Variation of the Energy Landscape of a Small Peptide under a Change from the ECEPP/2 Force Field to ECEPP/3. 1997 , 101, 3304-3310	43
1380	Selective Extraction of Cesium at Tracer Level Concentration from a Sodium Nitrate Solution with Calix-Crowns. Molecular Modeling Study of the Cs+/Na+ Selectivity. 1997 , 32, 175-191	29
1379	Conformational properties of the TATA-box binding sequence of DNA. 1997 , 14, 757-65	40
1378	Thermodynamic Decomposition of Hydration Free Energies by Computer Simulation: Application to Amines, Oxides, and Sulfides. 1997 , 101, 10527-10534	53
1377	Multivariate Investigations of Random-Coil and Ordered-Structure Conformations of the TYR181-to-TYR188 Segment of HIV-1 Reverse Transcriptase. 1997 , 19, 17-41	1
1376	Theoretical Prediction of Vibrational Spectrum of N-Glycylglycine Hydrochloride: An ab Initio Study. 1997 , 101, 6964-6969	19
1375	Binding affinities for sulfonamide inhibitors with human thrombin using Monte Carlo simulations with a linear response method. 1997 , 40, 1539-49	162
1374	The role of phenylalanine at position 6 in glucagon's mechanism of biological action: multiple replacement analogues of glucagon. 1997 , 40, 2555-62	21
1373	Classical and Quantum Simulations of Tryptophan in Solution. 1997 , 101, 1935-1945	29
1372	Molecular mechanics calculations of proteins. Comparison of different energy minimization strategies. 1997 , 15, 473-88	19
1371	Structural model of a cyclic dynorphin A analog bound to dodecylphosphocholine micelles by NMR and restrained molecular dynamics. 1997 , 40, 2148-55	19
1370	Evidence by site-directed mutagenesis that arginine 203 of thermolysin and arginine 717 of neprilysin (neutral endopeptidase) play equivalent critical roles in substrate hydrolysis and inhibitor binding. 1997 , 36, 13938-45	40
1369	Solution structure of (rGGCAGGCC)2 by two-dimensional NMR and the iterative relaxation matrix approach. 1997 , 36, 4449-60	55
1368	Trimethyl-p-benzoquinone Provides Excellent Structural, Spectroscopic, and Thermochemical Models for Plastoquinone-1 and Its Radical Anion. 1997 , 101, 1160-1165	33
1367	A Quantum Mechanically Derived All-Atom Force Field for Pyranose Oligosaccharides. AMBER* Parameters and Free Energy Simulations. 1997 , 62, 1427-1438	65
1366	A new type of DNA minor-groove complex: carbazole dication-DNA interactions. 1997 , 36, 15315-25	52
1365	Solution conformation of an abasic DNA undecamer duplex $d(CGCACXCACGC) \times d(GCGTGTGTGCG)$: the unpaired thymine stacks inside the helix. 1997 , 36, 4817-30	79
1364	Molecular Modeling of Vanadium Peroxides. 1997 , 36, 4029-4034	12

1363	A molecular mechanics and dynamics study of the minor adduct between DNA and the carcinogen 2-(acetylamino)fluorene (dG-N2-AAF). 1997 , 10, 1123-32	15
1362	Synthesis and opioid activity of conformationally constrained dynorphin A analogues. 2. Conformational constraint in the "address" sequence. 1997 , 40, 1211-8	55
1361	The Molecular Sieving Mechanism in Carbon Molecular Sieves: A Molecular Dynamics and Critical Path Analysis. 1997 , 13, 1199-1204	58
1360	Assessment of solvation effects on calculated binding affinity differences: trypsin inhibition by flavonoids as a model system for congeneric series. 1997 , 40, 4136-45	35
1359	Protein structure-based design, synthesis, and biological evaluation of 5-thia-2,6-diamino-4(3H)-oxopyrimidines: potent inhibitors of glycinamide ribonucleotide transformylase with potent cell growth inhibition. 1997 , 40, 2502-24	39
1358	Modeling of End-On (&mgr-Peroxo)dicopper(II) Complexes. 1997 , 36, 2309-2313	25
1357	Structural Fluctuations of a Cryptophaneâlletramethylammonium Hostâlluest System: A Molecular Dynamics Simulation. 1997 , 119, 8015-8022	15
1356	Structure and Dynamics of Water in the Presence of Charged Surfactant Monolayers at the WaterâtCl4 Interface. A Molecular Dynamics Study. 1997 , 101, 10775-10780	55
1355	Proteins as Solvents: The Role of Amino Acid Composition in the Excited-State Charge Transfer Dynamics of Plastocyanins. 1997 , 119, 896-905	46
1354	Conformation and Crystal Structure of Poly(⊞ycloalkyl-間-aspartate)s. 1997 , 101, 4215-4223	14
1353	NMR solution structures of stereoisometric covalent polycyclic aromatic carcinogen-DNA adduct: principles, patterns, and diversity. 1997 , 10, 111-46	314
1352	Assignment and analysis of fluorine nuclear magnetic resonance spectra of 4-fluorotryptophan myoglobins and hemoglobins. 1997 , 36, 3590-9	24
1351	Self-Assembling Ternary Complex Stabilities and Template Ratios in Carceplex Formation. 1997 , 119, 4321-4322	29
1350	Interactions of anesthetics with the water-hexane interface. A molecular dynamics study. 1997 , 101, 782-91	79
1349	Intermolecular Potential for the Hexahydro-1,3,5-trinitro-1,3,5-s-triazine Crystal (RDX): A Crystal Packing, Monte Carlo, and Molecular Dynamics Study. 1997 , 101, 798-808	107
1348	Investigation of Hydrophobic Interactions in Colloidal and Biological Systems by Molecular Dynamics Simulations and NMR Spectroscopy. 1997 , 13, 2007-2018	28
1347	Nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: methyl scan of the inhibitor linker. 1997 , 36, 13494-502	14
1346	Mapping the suramin-binding sites of human neutrophil elastase: investigation by fluorescence resonance energy transfer and molecular modeling. 1997 , 36, 15624-31	12

1345	Conformational analysis of three NK1 tripeptide antagonists: a proton nuclear magnetic resonance study. 1997 , 40, 594-601	5
1344	Combining Quantum Mechanical Reaction Pathways with Force Field Lattice Interactions To Model a Solid-State Phototransformation. 1997 , 119, 1474-1475	17
1343	Electrostatic effects on substrate activation in para-hydroxybenzoate hydroxylase: studies of the mutant lysine 297 methionine. 1997 , 36, 7548-56	33
1342	Synthesis and Separation of Atropisomers of 9,10-Dipivaloylanthracene and 9,10-Bis(1-imino-2,2-dimethylpropyl)anthracene. Structural Study by NMR, Molecular Mechanics, and X-ray Diffraction. 1997 , 62, 899-902	4
1341	Constructing protein models for ligand-receptor binding thermodynamic simulations: an application to a set of peptidometic renin inhibitors. 1997 , 37, 779-91	34
1340	Hydrogen Bonding between Amino Acid Backbone and Side Chain Analogues: A High-Level ab Initio Study. 1997 , 119, 12952-12961	61
1339	Solution Conformations of Potent Bicyclic Antagonists of Oxytocin by Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics Simulations. 1997 , 119, 5833-5846	21
1338	Dielectric Constant and Structure of Liquid 18-Crown-6 Calculated from Molecular Dynamics Simulations. 1997 , 101, 1024-1034	10
1337	NMR and structural model of dynorphin A (1-17) bound to dodecylphosphocholine micelles. 1997 , 36, 1971-81	51
1336	Quantitative Analysis of Hydrophobically Induced Folding in a Minimal Model System. 1997 , 119, 5041-5042	38
1335	Development of Weiner et al. force field parameters suitable for conformational studies of [1,4]-benzodiazepines and related compounds. 1997 , 37, 951-6	12
1334	Potent alpha 4 beta 1 peptide antagonists as potential anti-inflammatory agents. 1997 , 40, 3359-68	78
1333	Quantum Mechanics and Molecular Mechanics Studies of the Low-Energy Conformations of 9-Crown-3. 1997 , 101, 1920-1926	11
1332	Synthesis of C-Alkylcalix[4]arenes. 5. Design, Synthesis, Computational Studies, and Homodimerization of Polymethylene-Bridged Resorc[4]arenes. 1997 , 62, 1788-1794	19
1331	Hybrid Quantum and Molecular Mechanical (QM/MM) Studies on the Pyruvate to l-Lactate Interconversion in l-Lactate Dehydrogenase. 1997 , 101, 5614-5618	53
1330	What Controls Partitioning of the Nucleic Acid Bases between Chloroform and Water?. 1997 , 101, 5084-5088	31
1329	Crystal Packing and Molecular Dynamics Studies of the 5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one Crystal. 1997 , 101, 3605-3613	31
1328	Ab Initio Calculations of Conformational Effects on 13C NMR Spectra of Amorphous Polymers. 1997 , 1-121	9

1327	Carrier-Based Ion-Selective Electrodes and Bulk Optodes. 1. General Characteristics. 1997, 97, 3083-3132	1884
1326	Receptor site and stereospecifity of dihydrolipoamide dehydrogenase for R- and S-lipoamide: a molecular modeling study. 1997 , 58, 89-100	23
1325	Structure-based drug design: computational advances. 1997 , 37, 71-90	117
1324	Molecular Modeling of Proteins and Mathematical Prediction of Protein Structure. 1997 , 39, 407-460	120
1323	Accurate ab Initio Quantum Chemical Determination of the Relative Energetics of Peptide Conformations and Assessment of Empirical Force Fields. 1997 , 119, 5908-5920	323
1322	Multicanonical Ensemble Generated by Molecular Dynamics Simulation for Enhanced Conformational Sampling of Peptides. 1997 , 101, 817-824	352
1321	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
1320	4-Substituted 1-chloro-2-nitrobenzenes: structure-activity relationships and extension of the substrate model of rat glutathione S-transferase 4-4. 1997 , 10, 439-49	7
1319	Adsorption and solvation of ethanol at the water liquid-vapor interface: a molecular dynamics study. 1997 , 101, 3130-5	95
1318	Binding of Bicarbonate to Human Carbonic Anhydrase II: A Continuum of Binding States. 1997 , 119, 863-871	70
1318	Binding of Bicarbonate to Human Carbonic Anhydrase II: A Continuum of Binding States. 1997 , 119, 863-871 A refined substrate model for human cytochrome P450 2D6. 1997 , 10, 41-8	7° 66
		,
1317	A refined substrate model for human cytochrome P450 2D6. 1997 , 10, 41-8 Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum	66
1317 1316	A refined substrate model for human cytochrome P450 2D6. 1997 , 10, 41-8 Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). 1997 , 101, 4851-4859	66
1317 1316 1315	A refined substrate model for human cytochrome P450 2D6. 1997 , 10, 41-8 Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). 1997 , 101, 4851-4859 [18] Kinetics, molecular modeling, and synthetic applications with microbial lipases. 1997 , 386-405 The role in cell binding of a beta-bend within the triple helical region in collagen alpha 1 (I) chain:	66 92 11
1317 1316 1315	A refined substrate model for human cytochrome P450 2D6. 1997, 10, 41-8 Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). 1997, 101, 4851-4859 [18] Kinetics, molecular modeling, and synthetic applications with microbial lipases. 1997, 386-405 The role in cell binding of a beta-bend within the triple helical region in collagen alpha 1 (I) chain: structural and biological evidence for conformational tautomerism on fiber surface. 1997, 14, 547-60 Biologically important conformations of aminoglycoside antibiotics bound to an aminoglycoside 3'-phosphotransferase as determined by transferred nuclear Overhauser effect spectroscopy. 1997	66 92 11
1317 1316 1315 1314	A refined substrate model for human cytochrome P450 2D6. 1997, 10, 41-8 Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). 1997, 101, 4851-4859 [18] Kinetics, molecular modeling, and synthetic applications with microbial lipases. 1997, 386-405 The role in cell binding of a beta-bend within the triple helical region in collagen alpha 1 (I) chain: structural and biological evidence for conformational tautomerism on fiber surface. 1997, 14, 547-60 Biologically important conformations of aminoglycoside antibiotics bound to an aminoglycoside 3'-phosphotransferase as determined by transferred nuclear Overhauser effect spectroscopy. 1997, 36, 2353-9 Prediction of ligand-receptor binding thermodynamics by free energy force field (FEFF) 3D-QSAR	66 92 11 109 46

1309	Solution conformation of nociceptin. 1997 , 233, 640-3	24
1308	NMR solution structure of the pathogenesis-related protein P14a. 1997 , 266, 576-93	123
1307	Molecular docking to ensembles of protein structures. 1997 , 266, 424-40	362
1306	Structural rules and conformational compensations in the tRNA L-form. 1997 , 266, 269-82	59
1305	Electrostatic effects in homeodomain-DNA interactions. 1997 , 267, 368-81	50
1304	Solution structure of the HIV-2 TAR-argininamide complex. 1997 , 267, 624-39	129
1303	The NMR solution structure of the non-classical homeodomain from the rat liver LFB1/HNF1 transcription factor. 1997 , 267, 673-83	18
1302	Solution structure of r(gaggacug):d(CAGTCCTC) hybrid: implications for the initiation of HIV-1 (+)-strand synthesis. 1997 , 269, 225-39	61
1301	Thermodynamics of a reverse turn motif. Solvent effects and side-chain packing. 1997 , 270, 305-17	38
1300	The NMR solution conformation of unligated human cyclophilin A. 1997 , 272, 64-81	66
1299	Kinetics of peptide folding: computer simulations of SYPFDV and peptide variants in water. 1997 , 272, 423-42	67
1298	Molecular dynamics simulation study of DNA dodecamer d(CGCGAATTCGCG) in solution: conformation and hydration. 1997 , 272, 553-72	98
1297	Cystosine-rich strands of the insulin minisatellite adopt hairpins with intercalated cytosine+.cytosine pairs. 1997 , 272, 369-82	66
1296	Helix-loop-helix motif in GnRH associated peptide is critical for negative regulation of prolactin secretion. 1997 , 272, 731-40	19
1295	Solution structure of the first three zinc fingers of TFIIIA bound to the cognate DNA sequence: determinants of affinity and sequence specificity. 1997 , 273, 183-206	171
1294	Centromeric pyrimidine strands fold into an intercalated motif by forming a double hairpin with a novel T:G:G:T tetrad: solution structure of the d(TCCCGTTTCCA) dimer. 1997 , 273, 840-56	59
1293	Design of mu selective opioid dipeptide antagonists. 1997 , 417, 141-4	25
1292	Calculated One-Electron Reduction Potentials and Solvation Structures for Selected p-Benzoquinones in Water. 1997 , 101, 623-631	62

1291	Natural steric analysis: Ab initio van der Waals radii of atoms and ions. 1997 , 107, 5422-5432	146
1290	Natural bond orbital analysis of steric interactions. 1997 , 107, 5406-5421	228
1289	Modeling of anti-nucleosome immunoglobulin Fv domains: analysis of electrostatic interactions. 1997 , 34, 793-807	8
1288	Molecular adaptation to cold of an Antarctic bacterial lipase. 1997 , 3, 29-35	40
1287	Selectivity of lipases: Conformational analysis of suggested intermediates in ester hydrolysis of chiral primary and secondary alcohols. 1997 , 3, 83-98	46
1286	Predicting RNA structures: the model of the RNA element binding Rev meets the NMR structure. 1997 , 2, 141-7	5
1285	Homology modelling of an antimicrobial protein, Ace-AMP1, from lipid transfer protein structures. 1997 , 2, 183-92	15
1284	Configurations of diastereomeric hydroxyethylene isosteres strongly affect biological activities of a series of specific inhibitors of human-immunodeficiency-virus proteinase. 1997 , 250, 559-66	21
1283	Design and solution structure of a partially rigid opioid antagonist lacking the basic centermodels of antagonism. 1997 , 247, 66-73	21
1282	How to develop force fields: An account of the emergence of potential energy functions for saccharides. 1997 , 395-396, 91-106	4
1281	Reconsidering the conformational flexibility of Eyclodextrin. 1997, 395-396, 451-468	15
1280	Ab initio investigation of conformation-transmission effects in 4,4-dimethylandrostan-3-one. 1997 , 389, 241-250	
1279	Ab initio explorative survey of the mechanism catalyzed by mandelate racemase. 1997 , 390, 217-223	7
1278	Molecular structure and conformational analysis of chiral alcohols. Application to the enantioselectivity study of lipases. 1997 , 390, 225-237	7
1277	The glycosidic linkage flexibility and time-scale similarity hypotheses. 1997 , 395-396, 187-200	27
1276	Nature of H-bonding in clusters, liquids, and enzymes: an ab initio, natural bond orbital perspective. 1997 , 398-399, 181-197	199
1275	A carbohydrate force field for amber and its application to the study of saccharide to surface adsorption. 1997 , 395-396, 157-171	20
1274	Molecular force field development for saccharides using the SPASIBA spectroscopic potential. Force field parameters for Ħ-glucose. 1997 , 395-396, 81-90	14

1273	Molecular dynamics simulation of EGF and TGF-Econformation and receptor binding properties. 1997 , 398-399, 543-550	5
1272	The effects of basis set and blocking groups on the conformational energies of glycyl and alanyl dipeptides A Hartree-Fock and MP2 study. 1997 , 392, 101-109	18
1271	Computational methods for the prediction of protein folds. 1997 , 1343, 1-15	6
1270	Computer simulation of molecular diffusion in amorphous polymers. 1997 , 48, 57-66	43
1269	Simulation of Sodium Dodecyl Sulfate at the Waterâldapor and Waterâldarbon Tetrachloride Interfaces at Low Surface Coverage. 1997 , 101, 3793-3799	191
1268	Development of a Hybrid Quantum Chemical and Molecular Mechanics Method with Application to Solvent Effects on the Electronic Spectra of Uracil and Uracil Derivatives. 1997 , 101, 2478-2488	51
1267	Micro-environment effect on the structure of synthetic substrates of thermolysin. 1997 , 4, 391-395	1
1266	Effect of loop on the stability of intramolecular triplex DNA. 1997 , 40, 650-656	1
1265	Angular and torsional forces via quantum mechanics. 1997, 18, 608-613	
1264	Prediction of titration properties of structures of a protein derived from molecular dynamics trajectories. 1997 , 6, 373-82	37
1263	IL-8 single-chain homodimers and heterodimers: interactions with chemokine receptors CXCR1, CXCR2, and DARC. 1997 , 6, 609-17	44
1262	Predicted structure of the extracellular region of ligand-gated ion-channel receptors shows SH2-like and SH3-like domains forming the ligand-binding site. 1997 , 6, 983-98	32
1261	Template-based docking of a prolactin receptor proline-rich motif octapeptide to FKBP12: implications for cytokine receptor signaling. 1997 , 6, 999-1008	5
1260	Conformational analysis using distance geometry methods. 1997 , 15, 18-36	56
1259	Aspartame dipeptide analogues: effect of number of side-chain methylene group spacers and Clmethylation in the second position. 1997 , 8, 1305-1314	35
1258	Studies on the active conformation of the NK1 antagonist CGP 49823. Part 21. Fluoro-olefin analogs of tertiary amide rotamers 1997 , 7, 351-354	10
1257	Molecular modeling of the interaction of trypanocide guanyl hydrazones with B-DNA. 1997 , 7, 1797-1802	17
1256	Amide backbone modifications for antisense oligonucleotides carrying potential intercalating substituents: Influence on the thermodynamic stability of the corresponding duplexes with RNA-and DNA-complements. 1997 , 7, 1869-1874	5

1255	Mercaptoacyl matrix metalloproteinase inhibitors: The effect of substitution at the mercaptoacyl moiety. 1997 , 7, 2765-2770	19
1254	Synthesis of N-glyoxylyl peptides and their in vitro evaluation as HIV-1 protease inhibitors. 1997 , 5, 707-14	14
1253	Alkylation of a catalytic aspartate group of the SIV protease by an epoxide inhibitor. 1997 , 5, 2019-27	9
1252	Conformational preference for segetalins G and H, cyclic peptides with estrogen-like activity from seeds of Vaccaria segetalis. 1997 , 5, 2063-7	11
1251	Bioactive conformation of a potent stromelysin inhibitor determined by X-nucleus filtered and multidimensional NMR spectroscopy. 1997 , 5, 2193-201	40
1250	Vibrational analysis and spectra of cytidine 3?-monophosphate (3?-CMP). 1997 , 15, 1-16	20
1249	Synthesis and characterization of [RhIIICl2(II-C6H5)(PYR)2(SbPh3)], [RhIIICl2)(II-C6H5)(PY)2(THZ)], [RHIIICl2(II-C6H5(PY)2(PYR)], and [RhIIICl2(II-C6H5)(CEP)(SbPh3)2] [PYR = pyrazine; PY = pyridine; THZ = thiazole; CEP =	7
1248	N-(2-cyanoethylpyrrole)]. Crystal and molecular structure of [RhIIICl2(回-C6H5)(PYR)2(SbPh3)] and The conformational study of 聞-GlcA-(1,4)-l-Rha in solution by NMR and molecular dynamics simulations. 1997 , 224, 81-94	3
1247	A comparative study of the DG-OMEGA (DGI) DGII, and GAT method for the structure elucidation of a methylene-acetal linked thymine dinucleotide. 1997 , 21, 281-297	2
1246	Combined quantum chemical and MM-approach to the endo/exo selectivity of diels-alder reactions in polar media. 1997 , 53, 119-132	7
1245	Solution state conformation of an immunosuppressive cyclic dodecapeptide, cycloleonurinin. 1997 , 53, 7469-7478	13
1244	Vicinal tetrahydrofuran polysubstitution of simulated fatty acids. 1997 , 53, 7403-7416	7
1243	Synthesis of a branched oligosaccharide by remote glycosidation. 1997 , 38, 391-394	23
1242	Molecular packing and conformational behaviour of poly (則 -aspartate)s containing medium size linear alkyl side-chain. 1997 , 38, 3477-3484	16
1241	A combined density functional theory/molecular mechanics formalism and its application to small water clusters. 1997 , 412, 121-133	20
1240	The SPASIBA force field of esters. 1997 , 405, 113-122	8
1239	Conformational study of glyoxal bis(amidinohydrazone) by ab initio methods. 1997 , 415, 135-151	
1238	Use of T cell receptor/HLA-DRB1*04 molecular modeling to predict site-specific interactions for the DR shared epitope associated with rheumatoid arthritis. 1997 , 40, 1316-1326	3

1237	Molecular Recognition and Enantiomer Separations on a novel chiral stationary phase based on a 9,9?-spirobi[9H-fluorene]-derived molecular cleft. 1997 , 80, 897-911		32
1236	New Cyclophanes as Initiator Cores for the Construction of Dendritic Receptors: Host-guest complexation in aqueous solutions and structures of solid-state inclusion compounds. 1997 , 80, 2368-2	2390	34
1235	Nucleic Acid Analogs with Constraint Conformational Flexibility in the Sugar-Phosphate Backbone âllricyclo-DNAâllPart 1. Preparation of [(5?R,6?R)-2?-deoxy-3?,5?-ethano-5?,6?-methano-D-ribofuranosyl]thymine and -adenine, and the		35
1234	corresponding phosphoramidites for oligonucleotide synthesis. 1997, 80, 2426-2439 Adsorption of Ionophores and of Their Cation Complexes at the Water/Chloroform Interface: A Molecular Dynamics Study of a [2.2.2]Cryptand and of Phosphoryl-Containing Podands. 1997, 3, 552-56	50	21
1233	Molecular docking of superantigens with class II major histocompatibility complex proteins. 1997 , 10, 277-89		10
1232	MOLECULAR DYNAMICS STUDY OF THE COMPLEXATION OF LUMINESCENT CATIONS BY ENCAPSULATING LIGANDS WITH BIPYRIDINE UNITS. 1997 , 10, 292-304		11
1231	A computational analysis of interaction energies in methane and neopentane dimer systems. Journal of Computational Chemistry, 1997 , 18, 70-79	3.5	19
1230	Finite difference Poisson-Boltzmann electrostatic calculations: Increased accuracy achieved by harmonic dielectric smoothing and charge antialiasing. <i>Journal of Computational Chemistry</i> , 1997 , 18, 268-276	3.5	60
1229	Free energy calculation methods: A theoretical and empirical comparison of numerical errors and a new method qualitative estimates of free energy changes. <i>Journal of Computational Chemistry</i> , 1997 , 18, 902-919	3.5	94
1228	Internal coordinate modeling of DNA: Force field comparisons. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1043-1055	3.5	36
1227	An assessment of the accuracy of the RRIGS hydration potential: Comparison to solutions of the Poissonâ B oltzmann equation. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1072-1078	3.5	7
1226	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio HartreeâHock method for interaction of DNA bases: Comparison with nonempirical beyond HartreeâHock results.		239
1225	Molecular mechanics study of transannular amineâlletone (N->C(DOUBLE BOND)O) interaction in medium-sized heterocycles. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1211-1221	3.5	5
1224	SONHICA (Simple optimized non-Hierarchical Cluster Analysis): A new tool for analysis of molecular conformations. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1295-1311	3.5	12
1223	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
1222	Fast and accurate molecular dynamics simulation of a protein using a special-purpose computer. 1997 , 18, 1546-1563		64
1221	Advancing beyond the atom-centered model in additive and nonadditive molecular mechanics. Journal of Computational Chemistry, 1997 , 18, 1632-1646	3.5	116
1220	Development and validation of force-field parameters for molecular simulations of peptides and proteins containing open-shell residues. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1720-1728	3.5	10

1219	Automated flexible ligand docking method and its application for database search. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1812-1825	121	
1218	ORAC: A Molecular dynamics program to simulate complex molecular systems with realistic electrostatic interactions. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1848-1862	152	
1217	Ricin A-chain structural determinant for binding substrate analogues: a molecular dynamics simulation analysis. 1997 , 27, 80-95	30	
1216	Model-free methods of analyzing domain motions in proteins from simulation: a comparison of normal mode analysis and molecular dynamics simulation of lysozyme. 1997 , 27, 425-37	227	
1215	High resolution fast quantitative docking using fourier domain correlation techniques. 1997 , 27, 493-506	28	
1214	Automated multiple analysis of protein structures: application to homology modeling of cytochromes P450. 1997 , 28, 388-404	14	
1213	Accuracy and precision of NMR relaxation experiments and MD simulations for characterizing protein dynamics. 1997 , 28, 481-493	49	
1212	On the reaction mechanism of class Pi glutathione S-transferase. 1997 , 28, 530-542	8	
1211	Pseudocontact shifts as constraints for energy minimization and molecular dynamics calculations on solution structures of paramagnetic metalloproteins. 1997 , 29, 68-76	94	
1210	A predictive method for the evaluation of peptide binding in pocket 1 of HLA-DRB1 via global minimization of energy interactions. 1997 , 29, 87-102	19	
1209	Variations on a theme by Debye and Waller: From simple crystals to proteins. 1997 , 29, 153-160	51	
1208	Ab initio MO study of the chlorophyll dimer in the photosynthetic reaction center. I. A theoretical treatment of the electrostatic field created by the surrounding proteins. 1997 , 61, 137-151	33	
1207	A check on rational drug design: molecular simulation of the allosteric inhibition of HIV-1 reverse transcriptase. 1997 , 17, 235-76	16	
1206	Design of peptides, proteins, and peptidomimetics in chi space. 1997 , 43, 219-66	287	
1205	Conformational analysis and molecular dynamics simulation of alpha-(1>2) and alpha-(1>3) linked rhamnose oligosaccharides: reconciliation with optical rotation and NMR experiments. 1997 , 41, 83-96	17	
1204	Effect of the side group on the helix-forming tendency of	19	
1203	Comparison of van der Waals and semiempirical calculations of the molecular volumes of small molecules and proteins. 1997 , 42, 191-202	24	
1202	Substrate binding and catalytic mechanism in phospholipase C from Bacillus cereus: a molecular mechanics and molecular dynamics study. 1997 , 42, 319-36	14	

1201	Effects of substrate binding on the dynamics of RNase A: Molecular dynamics simulations of UpA bound and native RNase A. 1997 , 42, 505-520	16
1200	SulfurâAromatic Interactions: A Computational Study of the Dimethyl Sulfideâ B enzene Complex. 1997 , 25, 213-219	26
1199	Solving the multiple instance problem with axis-parallel rectangles. 1997 , 89, 31-71	1457
1198	Generalized linear response approximation in discrete methods. 1997 , 265, 473-480	20
1197	Flexible docking of a ligand peptide to a receptor protein by multicanonical molecular dynamics simulation. 1997 , 278, 297-301	81
1196	Isolation, stereochemical assignments and molecular mechanics calculation of ethyl 眼-arabinopyranoside. 1998 , 311, 85-88	2
1195	Symplectic integrator for molecular dynamics of a protein in water. 1998 , 282, 115-120	10
1194	Simulation studies for liquid phenol: properties evaluated and tested over a range of temperatures. 1998 , 294, 135-142	68
1193	Pd(gly-l-his-l-lys)Cl: Solution structure and ternary complex formation with mono- and tetranucleotides. 1998 , 273, 31-40	9
1192	All-atom empirical potential for molecular modeling and dynamics studies of proteins. 1998 , 102, 3586-616	11429
1192 1191	All-atom empirical potential for molecular modeling and dynamics studies of proteins. 1998 , 102, 3586-616 New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998 , 102, 1820-1831	11429 241
	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998 ,	
1191	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998 , 102, 1820-1831 Specific interactions between the syntrophin PDZ domain and voltage-gated sodium channels.	241
1191 1190 1189	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998, 102, 1820-1831 Specific interactions between the syntrophin PDZ domain and voltage-gated sodium channels. 1998, 5, 19-24 Solution structure of the fourth metal-binding domain from the Menkes copper-transporting	197
1191 1190 1189	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998, 102, 1820-1831 Specific interactions between the syntrophin PDZ domain and voltage-gated sodium channels. 1998, 5, 19-24 Solution structure of the fourth metal-binding domain from the Menkes copper-transporting ATPase. 1998, 5, 47-54	241197196
1191 1190 1189 1188	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998, 102, 1820-1831 Specific interactions between the syntrophin PDZ domain and voltage-gated sodium channels. 1998, 5, 19-24 Solution structure of the fourth metal-binding domain from the Menkes copper-transporting ATPase. 1998, 5, 47-54 Structure of a stereoregular phosphorothioate DNA/RNA duplex. 1998, 5, 271-6 CH/pi interactions as demonstrated in the crystal structure of guanine-nucleotide binding proteins, Src homology-2 domains and human growth hormone in complex with their specific ligands. 1998,	24119719639
1191 1190 1189 1188 1187	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. 1998, 102, 1820-1831 Specific interactions between the syntrophin PDZ domain and voltage-gated sodium channels. 1998, 5, 19-24 Solution structure of the fourth metal-binding domain from the Menkes copper-transporting ATPase. 1998, 5, 47-54 Structure of a stereoregular phosphorothioate DNA/RNA duplex. 1998, 5, 271-6 CH/pi interactions as demonstrated in the crystal structure of guanine-nucleotide binding proteins, Src homology-2 domains and human growth hormone in complex with their specific ligands. 1998, 6, 493-504 Evaluation of docking strategies for virtual screening of compound databases: cAMP-dependent	24119719639104

1183	Experimental and molecular modeling studies on interactions between drugs and Eudragit RL/RS resins in aqueous environment. 1998 , 73, 57-62	4
1182	Models of HIV-1 protease with peptides representing its natural substrates. 1998 , 423, 1-12	6
1181	A molecular modeling study of antibioticsâ R NA interactions: application to HIV-1 Rev response element. 1998 , 423, 125-136	1
1180	Stability of a constrained peptide-based antagonist of neurokinin A, as described by ab initio, semiempirical and empirical calculations. 1998 , 426, 339-347	2
1179	Simulated annealing and molecular dynamics of an elastin-related tetrapeptide in aqueous solution. 1998 , 431, 205-218	10
1178	Theoretical study of methylene blue: a new method to determine partial atomic charges; investigation of the interaction with guanine. 1998 , 432, 235-245	28
1177	An ab initio study of pyruvic acid. 1998 , 430, 51-56	21
1176	Protein hydration and unfoldinginsights from experimental partial specific volumes and unfolded protein models. 1998 , 3, 105-18	81
1175	Computational analysis of thermal stability: effect of Ile>Val mutations in human lysozyme. 1998 , 3, 173-81	13
1174	Solution structure of the heparin-binding domain of vascular endothelial growth factor. 1998 , 6, 637-48	166
1174 1173	Solution structure of the heparin-binding domain of vascular endothelial growth factor. 1998 , 6, 637-48 Cation binding to the integrin CD11b I domain and activation model assessment. 1998 , 6, 923-35	166 64
1173		
1173	Cation binding to the integrin CD11b I domain and activation model assessment. 1998 , 6, 923-35 The crystal structure of pyrimidine nucleoside phosphorylase in a closed conformation. 1998 , 6, 1467-79 Searching for the Lowest Energy Conformation of Substrates in the Carboxypeptidase A Active Site Using Monte Carlo/Energy Minimization Techniques. 1998 , 26, 295-308	64
1173	Cation binding to the integrin CD11b I domain and activation model assessment. 1998, 6, 923-35 The crystal structure of pyrimidine nucleoside phosphorylase in a closed conformation. 1998, 6, 1467-79 Searching for the Lowest Energy Conformation of Substrates in the Carboxypeptidase A Active Site Using Monte Carlo/Energy Minimization Techniques. 1998, 26, 295-308 Macrotricyclic Steroid Receptors by Pd°-Catalyzed Cross-Coupling Reactions: Dissolution of	64
1173 1172 1171	Cation binding to the integrin CD11b I domain and activation model assessment. 1998, 6, 923-35 The crystal structure of pyrimidine nucleoside phosphorylase in a closed conformation. 1998, 6, 1467-79 Searching for the Lowest Energy Conformation of Substrates in the Carboxypeptidase A Active Site Using Monte Carlo/Energy Minimization Techniques. 1998, 26, 295-308 Macrotricyclic Steroid Receptors by Pd°-Catalyzed Cross-Coupling Reactions: Dissolution of cholesterol in aqueous solution and investigations of the principles governing selective molecular recognition of steroidal substrates. 1998, 81, 109-144 \$\mathbb{P}\$- and \$\mathbb{P}\$-Peptides with Proteinaceous Side Chains: Synthesis and solution structures of	64 61 2
1173 1172 1171 1170 1169	Cation binding to the integrin CD11b I domain and activation model assessment. 1998, 6, 923-35 The crystal structure of pyrimidine nucleoside phosphorylase in a closed conformation. 1998, 6, 1467-79 Searching for the Lowest Energy Conformation of Substrates in the Carboxypeptidase A Active Site Using Monte Carlo/Energy Minimization Techniques. 1998, 26, 295-308 Macrotricyclic Steroid Receptors by Pd°-Catalyzed Cross-Coupling Reactions: Dissolution of cholesterol in aqueous solution and investigations of the principles governing selective molecular recognition of steroidal substrates. 1998, 81, 109-144 \$\mathbb{P}\$- and \$\mathbb{P}\$-Peptides with Proteinaceous Side Chains: Synthesis and solution structures of constitutional isomers, a novel helical secondary structure and the influence of solvation and	64 61 2 21
1173 1172 1171 1170 1169	Cation binding to the integrin CD11b I domain and activation model assessment. 1998, 6, 923-35 The crystal structure of pyrimidine nucleoside phosphorylase in a closed conformation. 1998, 6, 1467-79 Searching for the Lowest Energy Conformation of Substrates in the Carboxypeptidase A Active Site Using Monte Carlo/Energy Minimization Techniques. 1998, 26, 295-308 Macrotricyclic Steroid Receptors by Pd°-Catalyzed Cross-Coupling Reactions: Dissolution of cholesterol in aqueous solution and investigations of the principles governing selective molecular recognition of steroidal substrates. 1998, 81, 109-144 \$\mathbb{P}\$- and \$\mathbb{P}\$-Peptides with Proteinaceous Side Chains: Synthesis and solution structures of constitutional isomers, a novel helical secondary structure and the influence of solvation and hydrophobic interactions on folding. 1998, 81, 932-982	64 61 2 21 287

1165	Conformational properties of a model alanyl dipeptide and of alanine-derived oligopeptides: Effects of solvation in water and in organic solventsâl combined SIBFA/continuum reaction field, ab initio self-consistent field, and density functional theory investigation. 1998 , 45, 405-425		20	
1164	Derivation of class II force fields. VI. Carbohydrate compounds and anomeric effects. 1998 , 45, 435-68		75	
1163	Structural similarities and differences between H1- and H2-family DNA minihairpin loops: NMR studies of octameric minihairpins. 1998 , 46, 375-393		19	
1162	Molecular-modeling calculations of enzymatic enantioselectivity taking hydration into account. 1998 , 57, 741-5		17	
1161	. 1998 , 1998, 1559-1568		54	
1160	Conformational sampling of bioactive conformers: a low-temperature NMR study of 15N-Leuâlnkephalin. 1998 , 4, 253-265		24	
1159	1H NMR conformational study on N-terminal nonapeptide sequences of HIV-1 Tat protein: a contribution to structure-activity relationships. 1998 , 4, 400-10		4	
1158	Molecular dynamics simulations of biomembrane models. 1998 , 4, S41-6		1	
1157	SHAKE, rattle, and roll: Efficient constraint algorithms for linked rigid bodies. <i>Journal of Computational Chemistry</i> , 1998 , 19, 102-111	3.5	77	
1156	Derivation of class II force fields: V. Quantum force field for amides, peptides, and related compounds. <i>Journal of Computational Chemistry</i> , 1998 , 19, 430-458	3.5	119	
1155	Parametrization of aliphatic CHn united atoms of GROMOS96 force field. 1998 , 19, 535-547		335	
1154	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	
1153	Fast summation boundary element method for calculating solvation free energies of macromolecules. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1494-1504	3.5	86	
1152	ELECT++: Faster conformational search method for docking flexible molecules using molecular similarity. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1834-1852	3.5	10	
1151	Mapping the active site of factor Xa by selective inhibitors: an NMR and MD study. 1998 , 30, 264-74		10	
1150	Characterization of receptors with a new negative image: Use in molecular docking and lead optimization. 1998 , 30, 321-336		18	
1149	Improved protein free energy calculation by more accurate treatment of nonbonded energy: Application to chymotrypsin inhibitor 2, V57A. 1998 , 30, 388-400		37	
1148	The role played by environmental residues on sidechain torsional angles within homologous families of proteins: A new method of sidechain modeling. 1998 , 31, 355-369		15	

1147	Species dependence of enzyme-substrate encounter rates for triose phosphate isomerases. 1998 , 31, 406-416	20
1146	A set of van der Waals and coulombic radii of protein atoms for molecular and solvent-accessible surface calculation, packing evaluation, and docking. 1998 , 32, 111-127	131
1145	Interaction of explicit solvent with hydrophobic/philic/charged residues of a protein: Residue character vs. conformational context. 1998 , 32, 129-135	12
1144	Solution structure of human calcitonin in membrane-mimetic environment: The role of the amphipathic helix. 1998 , 32, 314-323	59
1143	A new method for predicting binding free energy between receptor and ligand. 1998 , 33, 62-73	20
1142	Exploring the conformational space of protein side chains using dead-end elimination and the A* algorithm. 1998 , 33, 227-39	167
1141	Kinetic steps for alpha-helix formation. 1998 , 33, 343-57	42
1140	Energy landscape of a native protein: jumping-among-minima model. 1998 , 33, 496-517	224
1139	Characterization of N93S, I312T, and A333P missense mutations in two Japanese families with mitochondrial acetoacetyl-CoA thiolase deficiency. 1998 , 12, 245-54	33
1138	Molecular dynamics simulations of the oligonucleotide with the modified phosphate/phosphonate internucleotide linkage. 1998 , 48, 409-415	4
1138		4
	internucleotide linkage. 1998 , 48, 409-415 Atom-atom potential functions for simulation of DNAâdounterion interaction in aqueous solution.	19
1137	internucleotide linkage. 1998, 48, 409-415 Atom-atom potential functions for simulation of DNAâdounterion interaction in aqueous solution. 1998, 47, 2098-2105 Predicting solvated peptide conformations via global minimization of energetic atom-to-atom	
1137	internucleotide linkage. 1998, 48, 409-415 Atom-atom potential functions for simulation of DNAâdounterion interaction in aqueous solution. 1998, 47, 2098-2105 Predicting solvated peptide conformations via global minimization of energetic atom-to-atom interactions. 1998, 22, 765-788 A global optimization method, BB, for general twice-differentiable constrained NLPsâll.	19
1137 1136 1135	Atom-atom potential functions for simulation of DNAâdounterion interaction in aqueous solution. 1998, 47, 2098-2105 Predicting solvated peptide conformations via global minimization of energetic atom-to-atom interactions. 1998, 22, 765-788 A global optimization method, BB, for general twice-differentiable constrained NLPsâll. Implementation and computational results. 1998, 22, 1159-1179	19 238
1137 1136 1135	Atom-atom potential functions for simulation of DNAâdounterion interaction in aqueous solution. 1998, 47, 2098-2105 Predicting solvated peptide conformations via global minimization of energetic atom-to-atom interactions. 1998, 22, 765-788 A global optimization method, BB, for general twice-differentiable constrained NLPsâll. Implementation and computational results. 1998, 22, 1159-1179 Molecular dynamics simulation of the water nitrobenzene interface. 1998, 450, 335-345	19 238 63
1137 1136 1135 1134	Atom-atom potential functions for simulation of DNAâBounterion interaction in aqueous solution. 1998, 47, 2098-2105 Predicting solvated peptide conformations via global minimization of energetic atom-to-atom interactions. 1998, 22, 765-788 A global optimization method, BB, for general twice-differentiable constrained NLPsâII. Implementation and computational results. 1998, 22, 1159-1179 Molecular dynamics simulation of the water nitrobenzene interface. 1998, 450, 335-345 Loop and water effect on stability of intertriplex DNA. 1998, 442, 275-280 W.a.x.s. and force field constrained RIETVELD modelling of meta-linked fully aromatic copolyesters:	19 238 63

1129	Calculated electrostatic gradients in recombinant human H-chain ferritin. 1998, 7, 1083-91	139
1128	Dynamic properties of individual water molecules in a hydrophobic pore lined with acyl chains: a molecular dynamics study. 1998 , 71, 35-50	6
1127	Glycated human hemoglobin (HbA1c): functional characteristics and molecular modeling studies. 1998 , 72, 323-35	46
1126	Enhancing the relaxivity of paramagnetic coordination complexes through the optimization of the molecular electrostatic potential. 1998 , 16, 811-28	5
1125	The structural basis for DNA binding by an anti-DNA autoantibody. 1998, 35, 1207-17	34
1124	On the helical conformation of un-ionized poly(gamma-D-glutamic acid). 1998 , 23, 175-84	52
1123	Nucleic Acid Interactions of Unfused Aromatic Cations: Evaluation of Proposed Minor-Groove, Major-Groove, and Intercalation Binding Modes. 1998 , 120, 10310-10321	74
1122	Ribozyme catalysis from the major groove of group II intron domain 5. 1998 , 1, 433-41	78
1121	Application of molecular dynamics to the evaluation of dielectric properties of model compounds with flexible side groups of acrylic polymer chains. 1998 , 235-237, 353-361	1
1120	Molecular modeling studies of human A3 adenosine antagonists: structural homology and receptor docking. 1998 , 38, 1239-48	43
1119	Computational analysis of the thermal stability in thioredoxins: a molecular dynamics approach. 1998 , 16, 437-46	14
1118	Chapter 3. Quantum mechanical treatment of enzyme reactions. 1998 , 94, 49	
1117	Critical Evaluation of Metal Complex Molecular Mechanics. Part 1. Cobalt(III) Hexaamines. 1998, 37, 4795-480	6 18
1116	Hydrophobic solvation in aqueous trifluoroethanol solution. 1998 , 39, 43-50	40
1115	Tertiary contacts in alpha-lactalbumin at pH 7 and pH 2: a molecular dynamics study. 1998 , 16, 355-65	3
1114	Mapping the charged residues in the second immunoglobulin-like domain of the vascular endothelial growth factor/placenta growth factor receptor Flt-1 required for binding and structural stability. 1998 , 273, 3216-22	39
1113	Chromophore-in-Protein Modeling of the Structures and Resonance Raman Spectra for Type 1 Copper Proteins. 1998 , 120, 12791-12797	36
1112	Diffusion Equation and Distance Scaling Methods of Global Optimization: Applications to Crystal Structure Prediction. 1998 , 102, 2904-2918	40

1111	Protein Electron Transfer Reorganization Energy Spectrum from Normal Mode Analysis. 2. Application to Ru-Modified Cytochromec. 1998 , 102, 2085-2094	34
1110	Comparison of ring current methods for use in molecular modeling refinement of NMR derived three-dimensional structures. 1998 , 38, 702-9	23
1109	Solution structure of N-(2-deoxy-D-erythro-pentofuranosyl)urea frameshifts, one intrahelical and the other extrahelical, by nuclear magnetic resonance and molecular dynamics. 1998 , 37, 1083-93	15
1108	Polarity and Conformational Characteristics of Semialiphatic Poly(imideâlster)s. 1998 , 31, 1972-1978	1
1107	Solution studies of isepamicin and conformational comparisons between isepamicin and butirosin A when bound to an aminoglycoside 6'-N-acetyltransferase determined by NMR spectroscopy. 1998 , 37, 3638-44	29
1106	Helical Nylons 3. Synthesis and Crystal Structure of Poly(粗-aspartate)s with Branched Alkyl Side Chains. 1998 , 31, 124-134	24
1105	Structure, Dynamics, and Electronic Spectrum of N, NâEDiethyl-p-nitroaniline at Water Interfaces. A Molecular Dynamics Study. 1998 , 102, 5145-5151	55
1104	Thermodynamic and Conformational Implications of Glycosidic Rotamers Preorganized for Binding. 1998 , 120, 5317-5318	50
1103	Molecular Modeling and Solid-State NMR of Short-Chain Molecules in Dianin's Compound and Zeolite 5A. 1998 , 120, 8113-8123	12
1102	Use of X-ray Co-crystal Structures and Molecular Modeling To Design Potent and Selective Non-peptide Inhibitors of Cathepsin K. 1998 , 120, 9114-9115	36
1101	A molecular dynamics computer simulation study of nucleotide analogues. Comparison of the hydration pattern of dithymidine phosphate with those of the dithymidine methylphosphonate diastereomers. 1998 , 15, 987-98	3
1100	Proteins as Solvents: Blue Copper Proteins as a Molecular Ruler for Solvent Effects on Resonance Raman Intensities. 1998 , 102, 7659-7665	28
1099	Structural basis for different inhibitory specificities of human cystatins C and D. 1998 , 37, 4071-9	56
1098	Proton transfer in benzyl alcohol dehydrogenase during catalysis: alternate proton-relay routes. 1998 , 37, 3305-11	22
1097	Migration of Ionophores and Salts through a Waterâthloroform Liquidâtiquid Interface: Molecular Dynamicsâthotential of Mean Force Investigations. 1998 , 102, 245-256	80
1096	Dual recognition of double-stranded DNA by 2'-aminoethoxy-modified oligonucleotides: the solution structure of an intramolecular triplex obtained by NMR spectroscopy. 1998 , 37, 17714-25	61
1095	Modeling the mechanics of a DNA oligomer. 1998 , 16, 593-604	23
1094	Dynamic Flexibility of Proteinâlhhibitor Complexes: A Study of the HIV-1 Protease/KNI-272 Complex. 1998 , 120, 12410-12418	8

1093	Behavior of the 9-Anthryl-tert-butylcarbinol as a Chiral Solvating Agent. Study of Diastereochemical Association by Intermolecular NOE and Molecular Dynamics Calculations. 1998 , 63, 8689-8695	18
1092	Metal Ion Induced Self-Assembly of a Designed Peptide into a Triple-Stranded ⊞elical Bundle: A Novel Metal Binding Site in the Hydrophobic Core. 1998 , 120, 13008-13015	80
1091	Derivatives of the triazoloquinazoline adenosine antagonist (CGS 15943) having high potency at the human A2B and A3 receptor subtypes. 1998 , 41, 2835-45	98
1090	Atomic Charges of the Water Molecule and the Water Dimer. 1998 , 102, 7686-7691	47
1089	Conformational studies on a diastereoisomeric pair of tricyclic nonclassical cannabinoids by NMR spectroscopy and computer molecular modeling. 1998 , 41, 167-74	17
1088	Solution Structure of a Metallointercalator Bound Site Specifically to DNA. 1998 , 120, 6877-6888	97
1087	Pyranose Ring Flexibility. Mapping of Physical Data for Iduronate in Continuous Conformational Space. 1998 , 120, 2099-2107	53
1086	Actinomycin D binds to metastable hairpins in single-stranded DNA. 1998 , 37, 11915-23	65
1085	A new method for predicting the alignment of flexible molecules and orienting them in a receptor cleft of known structure. 1998 , 41, 691-8	6
1084	Substitutions of conserved aromatic amino acid residues in subunit I perturb the metal centers of the Escherichia coli bo-type ubiquinol oxidase. 1998 , 37, 1632-9	18
1083	Conformational Analysis of Reverse-Turn Constraints by N-Methylation and N-Hydroxylation of Amide Bonds in Peptides and Non-Peptide Mimetics. 1998 , 120, 5363-5372	110
1082	Theoretical and Experimental Study on the TimeâDipole Correlation Function of 2-(Acetyloxy)ethyl-2-(2-naphthyl) Acetate (ANA)â 1998, 102, 5763-5768	4
1081	5-Substituted pyrimidines with a 1,5-anhydro-2, 3-dideoxy-D-arabino-hexitol moiety at N-1: synthesis, antiviral activity, conformational analysis, and interaction with viral thymidine kinase. 1998, 41, 4343-53	48
1080	A Quantum Mechanical and Molecular Mechanical Method Based on CM1A Charges: Applications to Solvent Effects on Organic Equilibria and Reactions. 1998 , 102, 1787-1796	109
1079	Bactericidal activity and poly-L-proline II conformation of the tandem repeat sequence of human salivary mucin glycoprotein (MG2). 1998 , 356, 197-206	31
1078	Protein phosphatase 1 catalytic subunit isoforms from alfalfa: biochemical characterization and cDNA cloning. 1998 , 360, 206-14	7
1077	Ion pairs involved in maintaining a thermostable structure of glutamate dehydrogenase from a hyperthermophilic archaeon. 1998 , 248, 920-6	44
1076	Self-Guided Molecular Dynamics Simulation for Efficient Conformational Search. 1998 , 102, 7238-7250	96

1075	An all-atom distance-dependent conditional probability discriminatory function for protein structure prediction. 1998 , 275, 895-916	383
1074	Conformational sampling of CDR-H3 in antibodies by multicanonical molecular dynamics simulation. 1998 , 278, 481-96	52
1073	Solution-state structure of a DNA dodecamer duplex containing a Cis-syn thymine cyclobutane dimer, the major UV photoproduct of DNA. 1998 , 282, 1013-32	111
1072	Stepping through an RNA structure: A novel approach to conformational analysis. 1998 , 284, 1465-78	110
1071	Structure determination and analysis of helix parameters in the DNA decamer d(CATGGCCATG)2 comparison of results from NMR and crystallography. 1998 , 284, 1453-63	35
1070	Chemical Synthesis and Properties of Conformationally Fixed Diuridine Monophosphates as Building Blocks of the RNA Turn Motif. 1998 , 63, 1429-1443	28
1069	A Transferable Intermolecular Potential for Nitramine Crystals. 1998 , 102, 8386-8392	50
1068	Molecular Dynamics Simulation of Li+BF4-in Ethylene Carbonate, Propylene Carbonate, and Dimethyl Carbonate Solvents. 1998 , 102, 1055-1061	148
1067	Human P2Y1 receptor: molecular modeling and site-directed mutagenesis as tools to identify agonist and antagonist recognition sites. 1998 , 41, 1456-66	138
1066	Sequence-dependent dynamics of TATA-Box binding sites. 1998 , 75, 372-81	54
1065	Electrostatic contributions to heat capacity changes of DNA-ligand binding. 1998, 75, 769-76	94
1064	Structural changes of creatine kinase upon substrate binding. 1998 , 75, 1016-23	66
1063	Dependence of protein stability on the structure of the denatured state: free energy calculations of I56V mutation in human lysozyme. 1998 , 75, 2178-87	27
1062	Electrostatic contributions to the binding free energy of the lambdacl repressor to DNA. 1998 , 75, 2262-73	96
1061	Importance of explicit salt ions for protein stability in molecular dynamics simulation. 1998 , 74, 2906-11	87
1060	Computer simulation study of synthetic 4-helix bundle that binds halothane. 1998 , 100-101, 377-85	1
1059	Parallel molecular dynamics simulations of biomolecular systems. 1998 , 296-303	6
1058	Strong Trans Influence Methoxymethyl Ligand in B(12) Cobaloxime and Imine/Oxime Model Complexes: Structural, Spectroscopic, and Molecular Mechanics Investigations. 1998 , 37, 6890-6897	62

1057	Modeling of Peptide Hydrolysis by Thermolysin. A Semiempirical and QM/MM Study. 1998 , 120, 8825-8833	68
1056	Solubility of nonpolar solutes in water: Computer simulations using the CF1 central force model. 1998 , 109, 7991-8002	22
1055	NMR solution structure of the N3'> P5' phosphoramidate duplex d(CGCGAATTCGCG)2 by the iterative relaxation matrix approach. 1998 , 37, 12082-93	25
1054	Conformationally constrained 1,3-diamino ketones: a series of potent inhibitors of the cysteine protease cathepsin K. 1998 , 41, 3563-7	53
1053	Identification of CD44 residues important for hyaluronan binding and delineation of the binding site. 1998 , 273, 338-43	140
1052	Solvation and conformational dynamics of dicarboxylic suberic acid. 1998 , 109, 2403-2412	6
1051	Sequence-dependent binding of metal ion to DNA oligomeres. A comparison of molecular electrostatic potentials with NMR data. 1998 , 16, 631-7	17
1050	Hydration of a BâDNA fragment in the method of atomâBtom correlation functions with the reference interaction site model approximation. 1998 , 109, 1528-1539	3
1049	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. 1998 , 80, 5011-5014	63
1048	High resolution mapping of the binding site of TrkA for nerve growth factor and TrkC for neurotrophin-3 on the second immunoglobulin-like domain of the Trk receptors. 1998 , 273, 5829-40	54
1047	Solvation free energies of methane and alkali halide ion pairs: An expanded ensemble molecular dynamics simulation study. 1998 , 108, 227-233	54
1046	Constant temperature molecular dynamics of a protein in water by high-order decomposition of the Liouville operator. 1998 , 109, 3276-3284	13
1045	Electrostatic calculations and multiple time scales in molecular dynamics simulation of flexible molecular systems. 1998 , 108, 8799-8803	46
1044	Helix-Coil Transition and 1/f Fluctuation in a Polypeptide. 1998 , 80, 5691-5694	30
1043	The role of bound water in the stability of the triple-helical conformation of (Pro-Pro-Gly)10. 1998 , 15, 1029-37	10
1042	THEORETICAL STUDIES ON TRI-n-BUTYL PHOSPHATE: MD SIMULATIONS IN VACUO, IN WATER, IN CHLOROFORM, AND AT A WATER / CHLOROFORM INTERFACE 1998 , 16, 597-618	49
1041	The glycosylation and structure of human serum IgA1, Fab, and Fc regions and the role of N-glycosylation on Fc#eceptor interactions. 1998 , 273, 2260-72	316
1040	Prion protein NMR structure and familial human spongiform encephalopathies. 1998 , 95, 11667-72	235

1039	Molecular Simulation of the Amyloid Peptide A順1-40) of Alzheimer's Disease. 1998 , 20, 201-222	13
1038	Interfacial Behavior of Ionophoric Systems: Molecular Dynamics Studies on 18-Crown-6 and Its Complexes at the Water-Chloroform Interface 1998 , 14, 43-56	42
1037	Structure comparison of human glioma pathogenesis-related protein GliPR and the plant pathogenesis-related protein P14a indicates a functional link between the human immune system and a plant defense system. 1998 , 95, 2262-6	93
1036	A conserved tyrosine residue (Y601) in transmembrane domain 5 of the human thyrotropin receptor serves as a molecular switch to determine G-protein coupling. 1998 , 12, 1461-71	74
1035	DNA-binding preferences of bisantrene analogues: relevance to the sequence specificity of drug-mediated topoisomerase II poisoning. 1998 , 54, 1036-45	12
1034	Redox regulation of c-Jun DNA binding by reversible S-glutathiolation. 1999 , 13, 1481-90	251
1033	A Sos-derived peptidimer blocks the Ras signaling pathway by binding both Grb2 SH3 domains and displays antiproliferative activity. 1999 , 13, 31-8	85
1032	Simulating synthetic polymer chains in parallel. 1999 , 13-22	
1031	Amino acid neighbours and detailed conformational analysis of cysteines in proteins. 1999 , 12, 535-48	136
1030	Molecular modeling of the amyloid-beta-peptide using the homology to a fragment of triosephosphate isomerase that forms amyloid in vitro. 1999 , 12, 959-66	11
1029	Automated docking of peptides and proteins by using a genetic algorithm combined with a tabu search. 1999 , 12, 639-48	40
1028	SOLVENT EXTRACTION OF METAL PICRATES BY PHOSPHORYL-CONTAINING PODANDS. 1999 , 17, 495-523	17
1027	Structural requirements of the higher order RNA kissing element in the enteroviral 3'UTR. 1999 , 27, 485-90	46
1026	Structure-function analysis of tritrypticin, an antibacterial peptide of innate immune origin. 1999 , 274, 23296-304	34
1025	Differential stability of the triple helix of (Pro-Pro-Gly)10 in H2O and D2O: thermodynamic and structural explanations. 1999 , 17, 481-91	8
1024	Assessment of the bioactive conformation of the farnesyltransferase protein binding recognition motif by computational methods. 1999 , 16, 1043-52	3
1023	Calculations of the phonon dispersion curves of C2H2, OC(ND2)2, and Na2CO3 from generic force field. 1999 , 110, 6406-6411	9
1022	New methods for incorporating nonholonomic constraints into molecular dynamics simulations. 1999 , 111, 1394-1406	16

1021	Accurate dipole moments from HartreeâHock calculations by means of class IV charges. 1999 , 111, 885-892	22
1020	Dynamic properties of double-stranded DNA by normal mode analysis. 1999 , 110, 11070-11075	41
1019	"RKKH" peptides from the snake venom metalloproteinase of Bothrops jararaca bind near the metal ion-dependent adhesion site of the human integrin alpha(2) I-domain. 1999 , 274, 31493-505	30
1018	Three-dimensional models of alpha(2A)-adrenergic receptor complexes provide a structural explanation for ligand binding. 1999 , 274, 23405-13	25
1017	Mutational analysis of the antagonist-binding site of the histamine H(1) receptor. 1999 , 274, 29994-30000	97
1016	Conformational analysis of the 13/4 to 4/1 helical transition in poly(日sobutyl 乱-aspartate). 1999 , 40, 5647-5654	
1015	PCSP: a computer program to predict and analyze the packing in crystalline polymers. 1999 , 40, 7351-7358	23
1014	Thionucleoside disulfide cross-linked duplex DNA. 1999 , 40, 13-16	6
1013	Thionucleoside disulfides as covalent constraints of DNA conformation. 1999 , 55, 12009-12022	14
1012	The SPASIBA force field of aldehydes. Part I: Structure and vibrational wavenumbers of methanal, ethanal and propanal. 1999 , 476, 261-270	7
1011	Conformation and packing of poly(alkylene phosphate) chains in the crystal lattice. Part I: molecular modelling and wide-angle X-ray scattering. 1999 , 474, 55-64	1
1010	Molecular scaffold-based design and comparison of combinatorial libraries focused on the ATP-binding site of protein kinases. 1999 , 17, 1-9, 51-2	23
1009	Improved AMBER torsional parameters for the N-N rotational barrier in diacylhydrazines. 1999 , 17, 315-24	9
1008	Structural basis of the dynamic mechanism of ligand binding to cyclooxygenase. 1999 , 9, 2779-84	49
1007	Docking experiments in the flexible non-nucleoside inhibitor binding pocket of HIV-1 reverse transcriptase. 1999 , 7, 1163-70	19
1006	Towards an understanding of drug resistance in malaria: three-dimensional structure of Plasmodium falciparum dihydrofolate reductase by homology building. 1999 , 7, 1003-11	48
1005	Detection of nascent polyproline II helices in solution by NMR in synthetic insect kinin neuropeptide mimics containing the X-Pro-Pro-X motif. 1999 , 53, 294-301	6
1004	Strategies toward predicting peptide cellular permeability from computed molecular descriptors. 1999 , 53, 355-69	32

1003	A novel approach to thermophysical properties prediction for chloro-fluoro-hydrocarbons. 1999 , 166, 21-37	22
1002	Molecular modelling study for chiral separation of equol enantiomers by ∉yclodextrin. 1999 , 240, 101-108	11
1001	A comparative study of MP2, B3LYP, RHF and SCC-DFTB force fields in predicting the vibrational spectra of N-acetyl-L-alanine-N'-methyl amide: VA and VCD spectra. 1999 , 246, 13-36	72
1000	Collisional deactivation of CF3I âla molecular dynamics simulation. 1999 , 248, 195-211	6
999	Heat capacity and compactness of denatured proteins. 1999 , 78, 207-17	22
998	Solvent effects on the 1(n,图) transition of formaldehyde in liquid water. A QM/MM study using the mean field approximation. 1999 , 310, 195-200	28
997	Roles of threonine 192 and asparagine 382 in agonist and antagonist interactions with M1 muscarinic receptors. 1999 , 126, 735-45	40
996	The structure of cobalt corrinoids based on molecular mechanics and NOE-restrained molecular mechanics and dynamics simulations. 1999 , 190-192, 127-153	18
995	Structural modeling of DNA mini-hairpin molecules with various loop sequences. 1999 , 308, 267-273	4
994	Ab initio and lattice dynamics studies of the vibrational and geometrical properties of the molecular complex of hydroquinone and C60. 1999 , 312, 299-305	5
993	Replica-exchange molecular dynamics method for protein folding. 1999 , 314, 141-151	3402
992	Synthesis, CoMFA analysis, and receptor docking of 3,5-diacyl-2, 4-dialkylpyridine derivatives as selective A3 adenosine receptor antagonists. 1999 , 42, 706-21	171
991	Pressure Dependence of Protein Electron Transfer Reactions: Theory and Simulation. 1999 , 103, 562-571	23
990	A theoretical evaluation of the ionization potentials for one-electron oxidized states of cytochrome c3. 1999 , 461-462, 325-334	1
989	Structure determination and prediction: A study on human Tom20. 1999 , 468, 127-134	2
988	On the pair potential in dense fluid methane. 1999 , 464, 107-119	25
 987	Studies on aliphatic polyesters I: Ab initio, density functional and force field studies of esters with one carboxyl group. 1999 , 488, 247-262	25
986	Isomers of adenine. 1999 , 493, 275-285	3

985	Molecular docking studies on interaction of diverse retinol structures with human alcohol dehydrogenases predict a broad role in retinoid ligand synthesis. 1999 , 1432, 239-50	12
984	Biodegradable cross-linked prodrug of the bronchial dilator Vephylline. 2. Kinetics and quantum chemical studies on the release mechanism. 1999 , 58, 189-94	3
983	Inhibition of tumor necrosis factor-alpha (TNF-alpha)/TNF-alpha receptor binding by structural analogues of suramin. 1999 , 58, 851-9	37
982	Structure of a CXC chemokine-receptor fragment in complex with interleukin-8. 1999 , 7, 157-68	142
981	The atomic-resolution structure of human caspase-8, a key activator of apoptosis. 1999 , 7, 1135-43	146
980	Solution structure of the alpha-subunit of human chorionic gonadotropin. 1999 , 260, 490-8	42
979	A molecular mechanism for the cleavage of a disulfide bond as the primary function of agonist binding to G-protein-coupled receptors based on theoretical calculations supported by experiments. 1999 , 261, 89-97	38
978	A Model for Nonstoichiometric, Cotranslational Protein Scission in Eukaryotic Ribosomes. 1999 , 27, 55-79	52
977	Structural identification of a novel degradant of the antibiotic pirlimycin formed under thermal stress conditions. 1999 , 36, 1049-1055	2
976	Inhibitors of cytochrome P450 catalyzed insecticide metabolism: A rational approach. 1999 , 73, 123-135	13
975	Peptides and proteins in neurodegenerative disease: helix propensity of a polypeptide containing helix 1 of the mouse prion protein studied by NMR and CD spectroscopy. 1999 , 51, 145-52	30
974	Conformation in solution and dynamics of a structurally constrained linear insect kinin pentapeptide analogue. 1999 , 49, 403-13	40
973	Cyclic pentapeptides of chiral sequence DLDDL as scaffold for antagonism of G-protein coupled receptors: synthesis, activity and conformational analysis by NMR and molecular dynamics of ITF 1565 a substance P inhibitor. 1999 , 50, 211-9	20
972	600 ps molecular dynamics reveals stable substructures and flexible hinge points in cAMP dependent protein kinase. 1999 , 50, 513-24	45
971	MMFF VII. Characterization of MMFF94, MMFF94s, and other widely available force fields for conformational energies and for intermolecular-interaction energies and geometries. <i>Journal of Computational Chemistry</i> , 1999 , 20, 730-748	597
970	Molecular dynamics of cryptophane and its complexes with tetramethylammonium and neopentane using a continuum solvent model. <i>Journal of Computational Chemistry</i> , 1999 , 20, 956-970 ^{3.5}	9
969	Coupled semiempirical quantum mechanics and molecular mechanics (QM/MM) calculations on the aqueous solvation free energies of ionized molecules. <i>Journal of Computational Chemistry</i> , 1999 , 20, 1028-1038	22
968	Statistical analysis of computational docking of large compound data bases to distinct protein binding sites. <i>Journal of Computational Chemistry</i> , 1999 , 20, 1634-1643	6

967	Protein tertiary structure prediction using a branch and bound algorithm. 1999 , 35, 41-57	44
966	Effective energy function for proteins in solution. 1999 , 35, 133-52	1044
965	Major subdomain rearrangement in HIV-1 reverse transcriptase simulated by molecular dynamics. 1999 , 35, 332-337	20
964	Flexible ligand docking: A multistep strategy approach. 1999 , 36, 1-19	119
963	A fast and simple method to calculate protonation states in proteins. 1999 , 36, 474-83	47
962	Efficacy and selectivity in flexible database docking. 1999 , 37, 334-45	40
961	Study of the electrostatics treatment in molecular dynamics simulations. 1999 , 37, 417-28	23
960	Enhanced conformational diversity search of CDR-H3 in antibodies: Role of the first CDR-H3 residue. 1999 , 37, 683-696	32
959	Multinuclear NMR Study of the Conformational Changes in MepdG and dGpMe upon Interaction with Mg2+, Zn2+ and Hg2+ Ions Reveals the Strengthening of the Anomeric Effect by Soft M2+ Ions. 1999 , 1999, 547-555	8
958	Conformational Preferences of Peptides Containing Reverse-Turn Mimetic Bicyclic Lactams: Inverse ETurns versus Type-II? 町urns âInsights into 冊airpin Stability. 1999 , 1999, 389-400	88
957	Crown EtherâAmmonium Complexes: Binding Mechanisms and Solvent Effects. 1999 , 1999, 1847-1856	65
956	Solution structure of human beta-endorphin in helicogenic solvents: an NMR study. 1999 , 5, 410-22	19
955	4-[3,5-Bis(2-hydroxyphenyl)-1,2,4-triazol-1-yl]benzoesüre: ein neuartiger, effizienter und selektiver Eisen(III)-Komplexbildner. 1999 , 111, 2733-2736	8
954	De novo design and structural characterization of proteins and metalloproteins. 1999 , 68, 779-819	529
953	Derivation of Class II Force Fields. 7. Nonbonded Force Field Parameters for Organic Compounds. 1999 , 103, 6998-7014	45
952	DNA Binding of Ruthenium Tris(1,10-phenanthroline): Evidence for the Dependence of Binding Mode on Metal Complex Concentration. 1999 , 38, 4486-4497	93
951	Binding preferences of hydroxamate inhibitors of the matrix metalloproteinase human fibroblast collagenase. 1999 , 42, 1225-34	42
950	Chiral resolution and stereospecificity of 6-phenyl-4-phenylethynyl- 1,4-dihydropyridines as selective A(3) adenosine receptor antagonists. 1999 , 42, 3055-65	54

949	Piperazine imidazo[1,5-a]quinoxaline ureas as high-affinity GABAA ligands of dual functionality. 1999 , 42, 1123-44	63
948	Analytical rebridging Monte Carlo: Application to cis/trans isomerization in proline-containing, cyclic peptides. 1999 , 111, 6625-6632	60
947	DNA bending induced by high mobility group proteins studied by fluorescence resonance energy transfer. 1999 , 38, 12150-8	65
946	Conformational Change of an Azamacrocycle Containing Nitrophenol Side Arms by Proton Coordination. Crystal Structures, Heat of reaction and Molecular Mechanics Calculations. 1999 , 10, 243-252	4
945	Evaluation of PMF scoring in docking weak ligands to the FK506 binding protein. 1999 , 42, 2498-503	124
944	Modeling the Bacterial Photosynthetic Reaction Center. 2. A Combined Quantum Mechanical/Molecular Mechanical Study of the Structure of the Cofactors in the Reaction Centers of Purple Bacteria. 1999 , 103, 4906-4915	47
943	Docking of Glycosaminoglycans to Heparin-Binding Proteins: Validation for aFGF, bFGF, and Antithrombin and Application to IL-8. 1999 , 121, 3004-3013	80
942	Molecular modelling of conformational changes in solvated ₹1-casein peptides. 1999, 9, 207-213	5
941	Ovalbumin(323-339) peptide binds to the major histocompatibility complex class II I-A(d) protein using two functionally distinct registers. 1999 , 38, 16663-70	61
940	Free energy calculations for peptides via deterministic global optimization. 1999 , 110, 7491-7512	53
939	Novel DNA Intercalators Based on the Pyridazino[1â[͡ʁât͡l],2]pyrido[4,3-b]indol-5-inium System. 1999 , 64, 3907-3915	31
938	Molecular dynamics simulation of a synthetic four-alpha-helix bundle that binds the anesthetic halothane. 1999 , 455, 332-8	8
937	Prediction of q-values and conformations of gadolinium chelates for magnetic resonance imaging. 1999 , 10, 958-64	3
936	Ab initio study of the role of lysine 16 for the molecular switching mechanism of Ras protein p21. 1999 , 77, 3287-92	32
935	Brownian dynamics simulations of interactions between aldolase and G- or F-actin. 1999, 76, 17-27	47
934	Free energy determinants of binding the rRNA substrate and small ligands to ricin A-chain. 1999 , 76, 28-39	31
933	Computational Prediction of the Enantioselectivity of a Solid-State Photoreaction. 1999 , 1, 1279-1281	8
932	CationâlInteractions in Proteins: Can Simple Models Provide an Accurate Description?. 1999 , 121, 10366-1037	72 169

931	Solution structure and energy calculation of bis-intercalation of homodimeric thiazole orange dye derivatives in DNA: effects of modifying the linker. 1999 , 10, 735-44	8
930	Binding of Pyrimidine Model Dimers to the Photolyase Enzyme: A Molecular Dynamics Study. 1999 , 103, 2001-2007	23
929	Searching the Conformational Space of Cyclic Molecules: A Molecular Mechanics and Density Functional Theory Study of 9-Crown-3. 1999 , 103, 10993-10997	18
928	SATIS: Atom Typing from Chemical Connectivity. 1999 , 39, 751-757	10
927	2'-deoxyribonolactone lesion in DNA: refined solution structure determined by nuclear magnetic resonance and molecular modeling. 1999 , 38, 3985-95	38
926	Hydrolysis Mechanism of the Phenylalanineâ B roline Peptide Bond Specific to HIV-1 Protease: Investigation by the ab Initio Molecular Orbital Method. 1999 , 121, 7349-7354	41
925	Solution structure of a five-adenine bulge loop within a DNA duplex. 1999 , 38, 12860-8	38
924	Differences in conformational behavior of ATA and TAT sequences in single strand DNA trimer. 1999 , 16, 1087-95	1
923	Human cathepsin X: A cysteine protease with unique carboxypeptidase activity. 1999 , 38, 12648-54	114
922	Modeling the 3D Structure of Rhodopsin Using a De Novo Approach to Build G-proteinâ © oupled Receptors. 1999 , 103, 2520-2527	9
921	Ab Initio Quantum Mechanical Study of the Structures and Energies for the Pseudorotation of 5âDehydroxy Analogues of 2âDeoxyribose and Ribose Sugars. 1999 , 121, 985-993	71
920	Role of the extracellular loops of G protein-coupled receptors in ligand recognition: a molecular modeling study of the human P2Y1 receptor. 1999 , 38, 3498-507	113
919	Molecular Dynamics of a 15-Residue Poly(l-alanine) in Water: Helix Formation and Energetics. 1999 , 121, 605-612	80
918	Solution structure and dynamics of a complex between DNA and the antitumor bisnaphthalimide LU-79553: intercalated ring flipping on the millisecond time scale. 1999 , 38, 15104-15	55
917	Modeling Internal Energy Distributions in Ion Clusters: Comparison between Experiment and Simulations. 1999 , 103, 8777-8791	43
916	Threading bis-intercalation of a macrocyclic bisacridine at abasic sites in DNA: nuclear magnetic resonance and molecular modeling study. 1999 , 38, 14205-13	51
915	Structural study of homeodomain protein-DNA complexes using a homology modeling approach. 1999 , 17, 347-54	10
914	Selective Adsorption of Sterically Hindered Phenols through a Single-Point Binding Mechanism. 1999 , 38, 3076-3082	7

913	Computer Simulation of the Cryoprotectant Disaccharide #Trehalose in Aqueous Solution. 1999 , 103, 4049-4055	121
912	Inclusion of Solvation in Ligand Binding Free Energy Calculations Using the Generalized-Born Model. 1999 , 121, 8033-8043	211
911	Design, synthesis, and evaluation of Phe-Gly mimetics: heterocyclic building blocks for pseudopeptides. 1999 , 42, 4331-42	140
910	Polycarbonate Simulations with a Density Functional Based Force Field. 1999 , 103, 5387-5398	15
909	Anhydrous protein ions. 1999 , 99, 3037-80	301
908	Prediction of ligand-receptor binding thermodynamics by free energy force field three-dimensional quantitative structure-activity relationship analysis: applications to a set of glucose analogue inhibitors of glycogen phosphorylase. 1999 , 42, 2169-79	41
907	Efficient Monte Carlo methods for cyclic peptides. 1999 , 97, 559-580	55
906	Transport Diffusion of Oxygenâ⊠itrogen Mixtures in Graphite Pores: A Nonequilibrium Molecular Dynamics (NEMD) Studyâ□ 1999 , 15, 6050-6059	44
905	Stable-Isotope-Assisted NMR Studies on 13C-Enriched Sialyl Lewisx in Solution and Bound to E-Selectin. 1999 , 121, 2546-2551	55
904	Free energy grids: a practical qualitative application of free energy perturbation to ligand design using the OWFEG method. 1999 , 42, 4313-24	32
903	Molecular Dynamics Computer Simulations of Surfactant Monolayers: Monododecyl Pentaethylene Glycol at the Surface between Air and Water. 1999 , 103, 8493-8501	55
902	Three-dimensional quantitative structure-activity relationship study on cyclic urea derivatives as HIV-1 protease inhibitors: application of comparative molecular field analysis. 1999 , 42, 249-59	78
901	The folding of centromeric DNA strands into intercalated structures: a physicochemical and computational study. 1999 , 285, 1039-52	35
900	A branch and bound algorithm for protein structure refinement from sparse NMR data sets. 1999 , 285, 1691-710	28
899	The high-resolution structure of the triplex formed by the GAA/TTC triplet repeat associated with Friedreich's ataxia. 1999 , 285, 2035-52	73
898	Molecular modeling of the three-dimensional architecture of the RNA component of yeast RNase MRP. 1999 , 292, 827-36	14
897	Solution structure of the VEGF-binding domain of Flt-1: comparison of its free and bound states. 1999 , 293, 531-44	50
896	Crystal structure of the catalytic subunit of Cdc25B required for G2/M phase transition of the cell cycle. 1999 , 293, 559-68	172

(2000-1999)

895	studies. 1999 , 294, 601-16	30
894	The recognition of distorted DNA structures by HMG-D: a footprinting and molecular modelling study. 1999 , 294, 79-91	43
893	Transfer of a Tetramethylammonium Ion across the WaterâNitrobenzene Interface: Potential of Mean Force and Nonequilibrium Dynamics. 1999 , 103, 10274-10279	63
892	A 12-Porphyrin System: Syntheses of Peptide Porphyrins with Multiple Histidines and the Aggregation Behavior in the Presence of Hemin. 1999 , 72, 1351-1364	4
891	Conformational study of Ac-Xaa-Pro-NHMe dipeptides: proline puckering and trans/cis imide bond. 1999 , 53, 30-40	25
890	Molecular dynamics of pectic substances. 1999 , 7, 899-932	O
889	The Calculation of Relative Binding Thermodynamics of Molecular Associations in Aqueous Solvents. 1999 , 8, 325-368	1
888	Molecular dynamics and NMR studies of proteins in ionic solutions. 1999 , 140, 217-223	
887	Selective Anion Complexation by a Calix[4]pyrrole Investigated by Monte Carlo Simulations. 1999 , 64, 7439-7444	32
886	DNA structure control by polycationic species: polyamine, cobalt ammines, and di-metallo transition metal chelates. 2000 , 12, 221-36	44
885	Solution structure of nocistatin, a new peptide analgesic. 2000 , 53, 257-64	7
884	An NMR study of conformations of substituted dipeptides in dodecylphosphocholine micelles: implications for drug transport. 2000 , 53, 396-410	14
883	A three-dimensional model of the delta-opioid pharmacophore: comparative molecular modeling of peptide and nonpeptide ligands. 2000 , 53, 565-80	39
882	Improved treatment of cyclic mmino acids and successful prediction of meptide secondary structure using a modified force field: AMBER*C. <i>Journal of Computational Chemistry</i> , 2000 , 21, 763-773 ^{3.5}	29
881	Transcriptional repressor CopR: Structure model-based localization of the deoxyribonucleic acid binding motif. 2000 , 38, 393-406	15
880	An atoms-in-molecules study of the genetically-encoded amino acids: I. Effects of conformation and of tautomerization on geometric, atomic, and bond properties. 2000 , 40, 310-29	60
879	Flexible ligand docking using a robust evolutionary algorithm. <i>Journal of Computational Chemistry</i> , 2000 , 21, 988-998	37
878	Computational analysis of two similar neuropeptides yields distinct conformational ensembles. 2000 , 40, 367-77	4

877	Similarity-driven flexible ligand docking. 2000 , 40, 623-36	74
876	Structure and morphology of nylon 46 lamellar crystals: Electron microscopy and energy calculations. 2000 , 38, 41-52	26
875	Rationally Designed Bicyclic Lactams Control Different Turn Motifs and Folding Patterns in Hexapeptide Mimics. 2000 , 2000, 695-699	14
874	NMR analysis of the configuration and conformation of N-acetylneuraminosyl-(2 -> 3)-lactose. 2000 , 38, 751-756	4
873	Nature of the special-pair radical cation in bacterial photosynthesis. 2000 , 80, 1224-1243	22
872	A new all-atom force field for crystalline cellulose I. 2000 , 78, 1939-1946	36
871	A qualitative model for the histamine H3 receptor explaining agonistic and antagonistic activity simultaneously. 2000 , 333, 254-60	28
870	Conformational Analysis of Azabicycloalkane Amino Acid Scaffolds as Reverse-Turn Inducer Dipeptide Mimics. 2000 , 2000, 2563-2569	41
869	Ionization state and molecular docking studies for the macrophage migration inhibitory factor: the role of lysine 32 in the catalytic mechanism. 2000 , 13, 146-56	26
868	Entropic and energetic selectivity in air separation with microporous materials. 2000 , 46, 99-109	14
867	Bivalency and epitope specificity of a high-affinity IgG3 monoclonal antibody to the Streptococcus group A carbohydrate antigen. Molecular modeling of a Fv fragment. 2000 , 324, 17-29	21
866	Crystal structure and conformational stability of N -acetyl- l -prolyl- l -leucinamide. Comparison between structural and thermophysical data. 2000 , 553, 117-130	3
865	Conformational stability of avarol-type molecules. Crystal structure of 3?-methylaminoavarone, a metabolite from Dysidea avara. 2000 , 516, 31-41	3
864	Comparison of lamellar crystal structure and morphology of nylon 46 and nylon 5. 2000 , 41, 8961-8973	34
863	A conformational model for poly(dichlorophosphazene) derived from molecular dynamics simulations. 2000 , 41, 3337-3347	18
862	Wide angle X-ray diffraction and force field constrained Rietveld modelling of m-linked fully aromatic copolyesters. 2. Poly(p-phenylene terephthalate-co-p-phenylene isophthalate). 2000 , 41, 3791-3795	1
861	Enantiodifferentiation by Complexation with Ecyclodextrin: Experimental (NMR) and Theoretical (MD, FEP) Studies. 2000 , 56, 3035-3041	25
860	Dynamics of p-Menthan-3,9-diols. A Computational Study in Aqueous and Chloroform Solutions of Two Epimers. 2000 , 56, 6089-6097	2

(2000-2000)

859	Chemical fragmentation in quantum mechanical methods. 2000 , 24, 287-94	19
858	The conformational characteristics of Congo red, Evans blue and Trypan blue. 2000 , 24, 429-50	39
857	Fundamental factors controlling the exchange of multidentate ligands: displacement of 12-crown-4 and triglyme from complexes with divalent alkaline earth cations. 2000 , 195-196, 639-652	28
856	Conformational properties of a cyclic peptide bradykinin B2 receptor antagonist using experimental and theoretical methods. 2000 , 55, 63-71	7
855	Primary and secondary locations of charge sites in angiotensin II (M + 2H)2+ ions formed by electrospray ionization. 2000 , 11, 40-53	19
854	Monte Carlo structural investigation of helical poly(⊞l -aspartate)s containing linear alkyl side chains. 2000 , 10, 177-187	10
853	QM/MM and SCRF studies of the ionization state of 8-methylpterin substrate bound to dihydrofolate reductase: existence of a low-barrier hydrogen bond. 2000 , 18, 42-9	10
852	An automatic homology modeling method consisting of database searches and simulated annealing. 2000 , 18, 258-72, 305-6	79
851	Docking of sulfonamides to carbonic anhydrase II and IV. 2000 , 18, 283-9, 307-8	39
850	Adsorption of melittin to a lipid bilayer : A molecular dynamics study. 2000 , 84, 89-98	7
849	Simulating synthetic polymer chains in parallel. 2000 , 16, 513-522	
848	Thermodynamic, structural, and dynamic study of the NâH?O?C hydrogen bond association in aqueous solution. 2000 , 255, 73-84	11
847	DFT studies on helix formation in N-acetyl-(L-alanyl)n-N?-methylamide for n=1â00. 2000 , 256, 15-27	94
846	1H-NMR and molecular modelling techniques for the investigation of the inclusion complex of econazole with alpha-cyclodextrin in the presence of malic acid. 2000 , 23, 25-31	38
845	Potential of mean force between two ions in a sucrose rich aqueous solution. 2000, 329, 221-227	14
844	Syntheses, antitumor activity, and molecular mechanics studies of cis-PtCl2(pzH)2 (pzH=pyrazole) and related complexes. Crystal structure of a novel Magnus-type double-salt [Pt(pzH)4][PtCl4][cis-PtCl2(pzH)2]2 involving two perpendicularly aligned 1D chains. 2000 , 297, 64-71	73
843	Nucleic acids: theory and computer simulation, Y2K. 2000 , 10, 182-96	197
842	A family competition evolutionary algorithm for automated docking of flexible ligands to proteins. 2000 , 4, 225-37	11

841	Molecular mechanics and molecular dynamics calculations of the Ecyclodextrin inclusion complexes with m-, and p-nitrophenyl alkanoates. 2000 , 530, 155-163	15
840	Molecular mechanics calculations of molecular and chiral recognition by cyclodextrins. Is it reliable? The selective complexation of decalins by tyclodextrin. 2000 , 503, 221-230	28
839	Theoretical study on the nitric oxide binding to nitrophorin 1, an NO-carrier protein from a blood-sucking insect. 2000 , 503, 51-58	2
838	Interactions between DNA and benzo- and tetrahydrobenzofurocoumarins: thermodynamic and molecular modeling studies. 2000 , 55, 276-86	9
837	A knowledge-based scoring function for protein-ligand interactions: Probing the reference state. 2000 , 20, 99-114	105
836	Dual epitope recognition by the VASP EVH1 domain modulates polyproline ligand specificity and binding affinity. 2000 , 19, 4903-14	103
835	Aminoglycoside antibiotics bound to aminoglycoside-detoxifying enzymes and RNA adopt similar conformations. 2000 , 33, 297-308	7
834	Synthesis, biological activity, and molecular modeling of ribose-modified deoxyadenosine bisphosphate analogues as P2Y(1) receptor ligands. 2000 , 43, 829-42	113
833	Exploiting the Peptide âlMHC Water Interface in the Computer-Aided Design of Non-Natural Peptides that Bind to the Class I MHC Molecule HLA-A2. 2000 , 24, 215-228	1
832	A conformational analysis of biologically active RGD-containing cyclopentapeptides. 2000 , 26, 262-270	
831	Is the Folded-chain Structure Possible in Cellulose Molecule?. 2000 , 56, 402-409	5
830	COMPUTER SIMULATION OF STRUCTURAL CHANGES IN PHOSPHOLIPID BILAYERS. 2000 , 11, 153-158	4
829	DNA binding site selection of dimeric and tetrameric Stat5 proteins reveals a large repertoire of divergent tetrameric Stat5a binding sites. 2000 , 20, 389-401	158
828	Direct identification of a peptide binding region in the opioid receptor-like 1 receptor by photoaffinity labeling with [Bpa(10),Tyr(14)]nociceptin. 2000 , 275, 29268-74	23
827	Reprogrammable recognition codes in bicoid homeodomain-DNA interaction. 2000 , 20, 7673-84	40
826	Charge engineering of a protein domain to allow efficient ion-exchange recovery. 2000 , 13, 703-9	33
825	Surface of active polarons: A semiexplicit solvation method for biomolecular dynamics. 2000, 112, 7723-7734	18
824	On the spatial disposition of the fifth transmembrane helix and the structural integrity of the transmembrane binding site in the opioid and ORL1 G protein-coupled receptor family. 2000 , 13, 477-90	3

(2008-2000)

823	Molecular dynamics simulation of human prion protein including both N-linked oligosaccharides and the GPI anchor. 2000 , 10, 959-74		81
822	Improving the oral bioavailability of the iron chelator HBED by breaking the symmetry of the intramolecular H-bond network. 2000 , 43, 1467-75		27
821	THE INFLUENCE OFSTRUCTURAL EFFECTS ON THE CMPLEXINGABILITY & CROWEIHERS. II. CESIUM COMPLEXES FORMED BY THE LIGANDS OF THE 18C6 TYPE. 2000 , 23,		
820	Requirement of specific intrahelical interactions for stabilizing the inactive conformation of glycoprotein hormone receptors. 2000 , 275, 37860-9		28
819	Homology models of mu-opioid receptor with organic and inorganic cations at conserved aspartates in the second and third transmembrane domains. 2000 , 375, 31-49		15
818	The role of the loop in binding of an actinomycin D analog to hairpins formed by single-stranded DNA. 2000 , 384, 199-203		21
817	Succinyl-CoA:3-ketoacid CoA transferase (SCOT): cloning of the human SCOT gene, tertiary structural modeling of the human SCOT monomer, and characterization of three pathogenic mutations. 2000 , 68, 144-51		40
816	Specific interactions for ab initio folding of protein terminal regions with secondary structures. 2008 , 72, 793-803		194
815	FURSMASA: a new approach to rapid scoring functions that uses a MD-averaged potential energy grid and a solvent-accessible surface area term with parameters GA fit to experimental data. 2008 , 71, 1519-38		6
814	Molecular dynamics study on the conformational flexibility and energetics in aqueous solution of methylated beta-cyclodextrins. 2008 , 20, 1127-33		5
813	A potent integrin antagonist from a small library of cyclic RGD pentapeptide mimics including benzyl-substituted azabicycloalkane amino acids. 2008 , 3, 1589-603		23
812	Lipid thermodynamics: melting is molecular. 2008 , 9, 2321-4		17
811	Stability of Hoogsteen-Type Triplexes âl Electrostatic Attraction between Duplex Backbone and Triplex-Forming Oligonucleotide (TFO) Using an Intercalating Conjugate. 2008 , 91, 805-818		6
810	GLYCAM06: a generalizable biomolecular force field. Carbohydrates. <i>Journal of Computational Chemistry</i> , 2008 , 29, 622-55	.5	1387
809	Macrocyclic 14-Membered Ring Diketal Diamines: Synthesis, Conformational Analysis and 99mTc Radiolabeling Evaluation. 2008 , 2008, 2039-2048		1
808	Structural Features of the (+)-Yatakemycin/d(GACTAATTGAC)-(GTCAATTAGTC) Complex â de Quantum Mechanical Calculation of NMR Parameters as a Tool for the Characterization of Ligand/DNA Interactions. 2008 , 2008, 2454-2462		4
807	Conformational studies of the alpha-helical 28-43 fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. 2008 , 89, 1032-44		10
806	Influence of charge and size of terminal amino-acid residues on local conformational states and shape of alanine-based peptides. 2008 , 90, 772-82		17

805	Molecular simulation of sodium butyl benzene sulfonate at airâlvater interface and in aqueous solution. 2008 , 142, 143-149	3
804	3D-QSAR and molecular docking studies of 1,3,5-triazene-2,4-diamine derivatives against r-RNA: novel bacterial translation inhibitors. 2008 , 26, 1338-52	8
803	Non-covalent inclusion of ferulic acid with alpha-cyclodextrin improves photo-stability and delivery: NMR and modeling studies. 2008 , 46, 645-52	59
802	Experimental and theoretical studies of NLO properties of organicalhorganic materials base on p-nitroaniline. 2008 , 455, 270-274	31
801	Pyrene-perylene as a FRET pair coupled to the N2'-functionality of 2'-amino-LNA. 2008 , 16, 94-9	48
800	Discovery of novel inhibitors of 11beta-hydroxysteroid dehydrogenase type 1 by docking and pharmacophore modeling. 2008 , 18, 1340-5	44
799	Molecular recognition of a DNA:RNA hybrid: sub-nanomolar binding by a neomycin-methidium conjugate. 2008 , 18, 4142-5	58
798	Study on the molecular mechanism of inhibiting HIV-1 integrase by EBR28 peptide via molecular modeling approach. 2008 , 132, 69-80	20
797	Scoring functions for de novo protein structure prediction revisited. 2008 , 413, 243-81	8
796	Conformational studies of highly potent 1-aminocyclohexane-1-carboxylic acid substituted V2 vasopressin agonists. 2008 , 66, 30-40	3
795	Identification of novel HCV RNA-dependent RNA polymerase inhibitors using pharmacophore-guided virtual screening. 2008 , 72, 585-91	12
794	Molecular dynamics of oligopeptides. A comparative study of residue interactions in dipeptides. 2008 , 53, 260-263	
793	AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening. 2008, 9, 438	39
79 ²	Equilibrium Molecular Dynamics Simulations. 2009 , 255-290	9
791	Extension of the GLYCAM06 Biomolecular Force Field to Lipids, Lipid Bilayers and Glycolipids. 2008 , 34, 349-363	8o
790	Ab initio folding of terminal segments with secondary structures reveals the fine difference between two closely related all-atom statistical energy functions. 2008 , 17, 1212-9	117
789	Transferred-NOE NMR experiments on intact human platelets: receptor-bound conformation of RGD-peptide mimics. 2008 , 6, 258-62	21
788	Synthesis and conformational studies of peptidomimetics containing a new bifunctional diketopiperazine scaffold acting as a beta-hairpin inducer. 2008 , 73, 652-60	45

787	Temperature Effects in Multiscale Modeling of Polymer Materials. 2008,	O
786	Docking, synthesis, and NMR studies of mannosyl trisaccharide ligands for DC-SIGN lectin. 2008 , 6, 2743-54	34
7 ⁸ 5	Features of the alkynyl ruthenium chromophore with modified anionic subsystem UV absorption. 2008 , 69, 178-82	14
7 ⁸ 4	Experimental and theoretical studies of the structures and interactions of vancomycin antibiotics with cell wall analogues. 2008 , 130, 13013-22	24
783	Structural similarities between thiamin-binding protein and thiaminase-I suggest a common ancestor. 2008 , 47, 1346-57	35
782	Hydrogen-bond structure and dynamics at the interface between water and carboxylic acid-functionalized self-assembled monolayers. 2008 , 112, 227-31	56
781	Energy landscape of an electron hole in hydrated DNA. 2008 , 112, 13945-50	9
780	New bis-cresol-bridged bis(1,4,7-triazacyclononane) ligand as receptor for metal cations and phosphate anions. 2008 , 47, 6551-63	27
779	Conformational simulations of aqueous solvated alpha-conotoxin GI and its single disulfide analogues using a polarizable force field model. 2008 , 112, 9854-67	20
778	Molecular Modeling of Geometries, Charge Distributions, and Binding Energies of Small, Drug-Like Molecules Containing Nitrogen Heterocycles and Exocyclic Amino Groups in the Gas Phase and Aqueous Solution. 2008 , 4, 1718-1732	12
777	Characterizing the properties of the N7,N9-dimethylguaninium chloride ion pairs: prospecting for the design of a novel ionic liquid. 2008 , 112, 106-16	9
776	An efficient method for calculating atomic charges of peptides and proteins from electronic populations. 2008 , 112, 5470-8	12
775	Density functional theory-based conformational analysis of a phospholipid molecule (dimyristoyl phosphatidylcholine). 2008 , 112, 13433-42	36
774	NMR solvent shifts of acetonitrile from frozen density embedding calculations. 2008, 112, 2640-7	37
773	Substituent effects on the rearrangements of cyclohexyl to cyclopentyl radicals involving avermectin-related radicals. 2008 , 73, 8175-81	19
772	Binding properties of Cu(+/2+)-(glycyl)n glycine complexes (n = 1-3). 2008 , 112, 3444-53	18
771	Coordination properties of lysine interacting with Co(I) and Co(II). A theoretical and mass spectrometry study. 2008 , 112, 12385-92	8
770	The importance of micelle-bound states for the bioactivities of bifunctional peptide derivatives for delta/mu opioid receptor agonists and neurokinin 1 receptor antagonists. 2008 , 51, 6334-47	31

769	Crystal structure of a sulfur carrier protein complex found in the cysteine biosynthetic pathway of Mycobacterium tuberculosis. 2008 , 47, 10354-64	29
768	Access and binding of local anesthetics in the closed sodium channel. 2008 , 74, 1033-45	54
767	Introduction to Protein Modeling. 2008 , 77-132	
766	Molecular modeling of benzothiazepine binding in the L-type calcium channel. 2008 , 283, 17594-604	45
765	Novel macromolecular inhibitors of human immunodeficiency virus-1 protease. 2008 , 21, 453-61	7
764	On the dynamics of some small structural motifs in rRNA upon ligand binding. 2008, 73, 41-53	
763	Scripting approach in hybrid organicâlhorganic condensation simulation: the GPTMS proof-of-concept. 2008 , 34, 1215-1236	12
762	Determination of ligand-binding sites on proteins using long-range hydrophobic potential. 2008 , 31, 1552-8	15
761	Dynamic interaction among the platform domain and two membrane-proximal immunoglobulin-like domains of class I major histocompatibility complex: normal mode analysis. 2008 , 56, 635-41	5
760	Theoretical Calculation of Partition Coefficients. 2008 , 173-180	3
760 759	Theoretical Calculation of Partition Coefficients. 2008, 173-180 Thermodynamics of van der Waals and Hydrophobic Interactions. 2008, 27-48	3
		3
759	Thermodynamics of van der Waals and Hydrophobic Interactions. 2008 , 27-48 C-terminal residues of mature human T-lymphotropic virus type 1 protease are critical for	
759 75 ⁸	Thermodynamics of van der Waals and Hydrophobic Interactions. 2008, 27-48 C-terminal residues of mature human T-lymphotropic virus type 1 protease are critical for dimerization and catalytic activity. 2008, 416, 357-64	11
759 758 757	Thermodynamics of van der Waals and Hydrophobic Interactions. 2008, 27-48 C-terminal residues of mature human T-lymphotropic virus type 1 protease are critical for dimerization and catalytic activity. 2008, 416, 357-64 Subdiffusive dynamics of a liquid crystal in the isotropic phase. 2008, 128, 194501 Towards a comprehensive model for the electronic and vibrational structure of the Creutz-Taube	11 12
759 758 757	Thermodynamics of van der Waals and Hydrophobic Interactions. 2008, 27-48 C-terminal residues of mature human T-lymphotropic virus type 1 protease are critical for dimerization and catalytic activity. 2008, 416, 357-64 Subdiffusive dynamics of a liquid crystal in the isotropic phase. 2008, 128, 194501 Towards a comprehensive model for the electronic and vibrational structure of the Creutz-Taube ion. 2008, 366, 15-31	11 12 27
759 758 757 756 755	Thermodynamics of van der Waals and Hydrophobic Interactions. 2008, 27-48 C-terminal residues of mature human T-lymphotropic virus type 1 protease are critical for dimerization and catalytic activity. 2008, 416, 357-64 Subdiffusive dynamics of a liquid crystal in the isotropic phase. 2008, 128, 194501 Towards a comprehensive model for the electronic and vibrational structure of the Creutz-Taube ion. 2008, 366, 15-31 Dinfinica molecular: teoria e aplica sem planejamento de filmacos. 2008, 33, 13-24	11 12 27 20

751	Structural model for dihydropyridine binding to L-type calcium channels. 2009 , 284, 19006-17	66
75°	Water in the Neck-Zipper Region of Kinesin. 2009 , 26, 078701	2
749	Structural model for phenylalkylamine binding to L-type calcium channels. 2009 , 284, 28332-28342	39
748	An electrostatic switch displaces phosphatidylinositol phosphate kinases from the membrane during phagocytosis. 2009 , 187, 701-14	71
747	Protein Dynamics: From Structure to Function. 2009 , 217-249	
746	N,N?-dimethylperylene-3,4,9,10-bis(dicarboximide) on alkali halide (001) surfaces. 2009 , 105, 094311	13
745	A systematic understanding of orbital energy shift in polar solvent. 2009 , 130, 044107	11
744	Correlated movements of ions and water in a nanochannel. 2009 , 35, 13-23	8
743	An effective docking strategy for virtual screening based on multi-objective optimization algorithm. 2009 , 10, 58	29
742	Effect of calcium (II) and magnesium (II) ions on the 18-23 gamma-carboxyglutamic acid containing cyclic peptide loop of bovine prothrombin. An AMBER molecular mechanics study. 1988 , 31, 137-49	8
741	Divalent metal ion mediated interaction of proteins with negatively charged membranes. A model study employing molecular mechanics. 1990 , 35, 111-6	1
740	Dimensional oscillation. 2009, 38, 161-168	2
739	Peptides from chiral C alpha,alpha-disubstituted glycines. Synthesis and characterization, conformational energy computations and solution conformational analysis of C alpha-methyl, C alpha-isopropylglycine [(alpha Me)Val] derivatives and model peptides. 1991, 38, 242-52	30
738	Conformations of cyclic pentapeptide endothelin receptor antagonists. 1994 , 44, 223-32	13
737	A crystal-state, solution and theoretical study of the preferred conformation of linear C alpha, alpha-diphenylglycine derivatives and dipeptides with potential anticonvulsant activity. 1994 , 44, 85-95	16
736	Solution conformation of c-[Gln-Trp-Phe-Gly-Leu-Met], a NK-2 tachykinin antagonist. 1994 , 44, 556-61	3
735	Effect of the environment and role of the Estacking interactions in the stabilization of the 310-helix conformation in dehydroalanine oligopeptides. 2009 , 46, 408-418	15
734	Combined use of NMR, distance geometry and MD calculations for the conformational analysis of opioid peptides of the type [D(L)-Cys2, D(L)-Cys5]enkephalin. 1996 , 48, 443-51	1

733	Evidence for a C-terminal turn in PBAN. An NMR and distance geometry study. 1996 , 47, 361-8		13
732	In silico platform for xenobiotics ADME-T pharmacological properties modeling and prediction. Part I: Beyond the reduction of animal model use. 2009 , 14, 401-5		14
731	Cyclic RGD-containing functionalized azabicycloalkane peptides as potent integrin antagonists for tumor targeting. 2009 , 4, 615-32		40
730	Design, Synthesis, and Hybridisation of Water-Soluble, Peptoid Nucleic Acid Oligomers Tagged with Thymine. 2009 , 2009, 6113-6120		10
729	A novel method for enzyme design. <i>Journal of Computational Chemistry</i> , 2009 , 30, 256-67	3.5	13
728	Rotamer optimization for protein design through MAP estimation and problem-size reduction. Journal of Computational Chemistry, 2009 , 30, 1923-45	3.5	20
727	The SAAP force field: development of the single amino acid potentials for 20 proteinogenic amino acids and Monte Carlo molecular simulation for short peptides. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2039-55	3.5	6
726	Conformational studies of the C-terminal 16-amino-acid-residue fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. 2009 , 91, 37-51		12
725	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. 2009 , 15, 1175-84		11
724	DFT study of electronic properties, structure and spectra of aryl diazonium cations. 2009 , 904, 14-20		17
723	Synthesis and structural characterization of dicopper(II) and dipalladium(II) complexes of 1,1,2,2-tetrakis(carboxamido-2-methylpyridyl)ethane. 2009 , 936, 250-256		1
722	?-SHAKE: An extension to SHAKE for the explicit treatment of angular constraints. 2009 , 180, 360-364		8
721	Docking and scoring with alternative side-chain conformations. 2009 , 74, 712-26		29
720	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. I. Importance of hydrophobic interactions in stabilization of beta-hairpin structure. 2009 , 75, 931-53		22
719	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. II. Interplay of local backbone conformational dynamics and long-range hydrophobic interactions in hairpin formation. 2009 , 76, 637-54		17
718	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. III. Dynamics of long-range hydrophobic interactions. 2010 , 78, 723-37		8
717	Complex mathematical models of biology at the nanoscale. 2009 , 1, 650-9		13
716	Molecular mechanics studies of sequence-specific repair of DNA alkylated by EMS in the laci gene of Escherichia coli. 2009 , 36, 35-44		_

(2009-2009)

715	The representation of molecular electrostatics using interactive graphics. 2009 , 36, 73-85	1
714	Molecular Modeling and Receptor-Dependent (RD) 3D-QSAR Approach to a Set of Antituberculosis Derivatives. 2009 , 28, 1455-1464	3
713	Comparative modeling of DNA and RNA polymerases from Moniliophthora perniciosa mitochondrial plasmid. 2009 , 6, 22	7
712	Solution conformational analysis of sodium complexed [Gly6]- and [Gly9]-antamanide analogs. 1998 , 51, 180-7	12
711	Conformational behaviour of the TraM headpiece. 1998 , 51, 244-50	3
710	Computer simulations of amorphous polymers: From quantum mechanical calculations to mesoscopic models. 2009 , 898, 62-72	10
709	On some strategies to design new high energy density molecules. 2009 , 897, 42-47	27
708	QM/MM study of the insertion of metal ion into protoporphyrin IX by ferrochelatase. 2009 , 103, 1680-6	16
707	Morpholine-based RGD-cyclopentapeptides as alphavbeta3/alphavbeta5 integrin ligands: role of configuration towards receptor binding affinity. 2009 , 17, 1542-9	23
706	Discovery of novel Trypanosoma cruzi glyceraldehyde-3-phosphate dehydrogenase inhibitors. 2009 , 17, 2476-82	53
705	Rational design, synthesis and characterization of potent, non-peptidic Smac mimics/XIAP inhibitors as proapoptotic agents for cancer therapy. 2009 , 17, 5834-56	33
704	Distance-scaled, finite ideal-gas reference state improves structure-derived potentials of mean force for structure selection and stability prediction. 2002 , 11, 2714-26	717
703	Discovering potent inhibitors against the beta-hydroxyacyl-acyl carrier protein dehydratase (FabZ) of Helicobacter pylori: structure-based design, synthesis, bioassay, and crystal structure determination. 2009 , 52, 2465-81	40
702	Anion binding by protonated forms of the tripodal ligand tren. 2009 , 48, 2391-8	47
701	Role of triplet states of aryldiazonium cations in the Meerwein reaction. 2009, 82, 840-845	11
700	Molecular dynamics simulations of a hyperbranched poly(ester amide): statics, dynamics, and hydrogen bonding. 2009 , 113, 5356-68	31
699	TraPPE-UA force field for acrylates and Monte Carlo simulations for their mixtures with alkanes and alcohols. 2009 , 113, 6415-25	69
698	Configuration effects of H-bonded sites and rigid core lengths on h-bonded banana-shaped liquid crystalline supramolecules consisting of symmetric trimers and asymmetric heterodimers. 2009 , 113, 14648-60	22

697	Functionalized 2'-amino-alpha-L-LNA: directed positioning of intercalators for DNA targeting. 2009 , 74, 1070-81	43
696	Docking ligands into flexible and solvated macromolecules. 5. Force-field-based prediction of binding affinities of ligands to proteins. 2009 , 49, 2564-71	29
695	Generation and integration of NaOH into NaCl clusters in supercritical water: a molecular dynamics study on hydrolysis product partitioning. 2009 , 113, 14681-8	7
694	Improving metabolic stability by glycosylation: bifunctional peptide derivatives that are opioid receptor agonists and neurokinin 1 receptor antagonists. 2009 , 52, 5164-75	40
693	Predictions of hydration free energies from all-atom molecular dynamics simulations. 2009, 113, 4533-7	76
692	Coordination of (glycyl)(n)glycine (n = 1-3) to Co+ and Co2+. 2009 , 113, 8883-92	8
691	Reoptimization of the AMBER force field parameters for peptide bond (Omega) torsions using accelerated molecular dynamics. 2009 , 113, 16590-5	64
690	Carbon dioxide capture at the molecular level. 2009 , 11, 8556-9	31
689	Local Dynamics and Hydrogen Bonding in Hyperbranched Aliphatic Polyesters. 2009 , 42, 9581-9591	25
688	Conformational study of the PCU cage monopeptide: a key role of some force-field parameters. 2009 , 113, 5234-8	
687	New insights into the design of inhibitors of human S-adenosylmethionine decarboxylase: studies of adenine C8 substitution in structural analogues of S-adenosylmethionine. 2009 , 52, 1388-407	23
686	Fluorescent J-aggregates of core-substituted perylene bisimides: studies on structure-property relationship, nucleation-elongation mechanism, and sergeants-and-soldiers principle. 2009 , 131, 6719-32	292
685	Association of a weakly acidic anti-inflammatory drug (ibuprofen) with a poly(amidoamine) dendrimer as studied by molecular dynamics simulations. 2009 , 113, 10984-93	71
684	Molecular dynamics simulations of polyamidoamine dendrimers and their complexes with linear poly(ethylene oxide) at different pH conditions: static properties and hydrogen bonding. 2009 , 11, 10017-28	44
683	Structure and stability of (alpha-CD)3 aggregate and OEG@(alpha-CD)3 pseudorotaxane in aqueous solution: a molecular dynamics study. 2009 , 113, 9762-9	16
682	Conserved water mediated H-bonding dynamics of inhibitor, cofactor, Asp 364 and Asn 303 in human IMPDH II. 2009 , 26, 497-507	25
681	Gas phase supramolecular cluster ions of deoxyguanosine induced by binding to (2,2':6'2"-terpyridine)-platinum(II) and (diethylenetriamine)-platinum(II). 2009 , 1542-8	2
68o	Structure of the alanine hydration shell as probed by NMR chemical shifts and indirect spin-spin coupling. 2009 , 113, 14698-707	45

(2010-2009)

679	Hydrogen bonding and pi-stacking: how reliable are force fields? A critical evaluation of force field descriptions of nonbonded interactions. 2009 , 49, 944-55	146
678	Recognition and discrimination of DNA quadruplexes by acridine-peptide conjugates. 2009, 7, 76-84	50
677	Functionalization of 2'-amino-LNA with additional nucleobases. 2009 , 7, 1793-7	35
676	Extending the Time Scale in Atomically Detailed Simulations. 2009 , 367-420	1
675	Dynamic influence of the two membrane-proximal immunoglobulin-like domains upon the peptide-binding platform domain in class I and class II major histocompatibility complexes: normal mode analysis. 2009 , 57, 1193-9	5
674	Molecular Mechanics Calculations. 2009,	1
673	Reactivity of Lignin-Correlation with Molecular Orbital Calculations. 2010, 321-347	6
672	Predicting Solid Compounds Using Simulated Annealing. 2010 , 67-105	5
671	Structure and spectral properties of phenyldiazonium tetrachlorocuprate (II). 2010, 83, 36-43	7
670	Conformational analysis of tripeptide Ac-Lys-Pro-Val-NH2, COOH-terminal sequence of alpha-MSH. 2001 , 53, 949-53	3
669	Third-Generation Hydrogen-Bonding Corrections for Semiempirical QM Methods and Force Fields. 2010 , 6, 3808-3816	187
668	Mercaptophosphonate compounds as broad-spectrum inhibitors of the metallo-beta-lactamases. 2010 , 53, 4862-76	105
667	Docking of calcium ions in proteins with flexible side chains and deformable backbones. 2010 , 39, 825-38	7
666	Structural modeling of calcium binding in the selectivity filter of the L-type calcium channel. 2010 , 39, 839-53	14
665	Efficient RNA-targeting by the introduction of aromatic stacking in the duplex major groove via 5-(1-phenyl-1,2,3-triazol-4-yl)-2'-deoxyuridines. 2010 , 18, 4702-10	33
664	Analogues of both Leu- and Met-enkephalin containing a constrained dipeptide isostere prepared from a Baylis-Hillman adduct. 2010 , 38, 1057-65	12
663	MOLS sampling and its applications in structural biophysics. 2010 , 2, 169-179	О
662	Docking flexible ligands in proteins with a solvent exposure- and distance-dependent dielectric function. 2010 , 24, 91-105	62

661	Investigation of structure-activity relationships in organophosphates-cholinesterase interaction using docking analysis. 2010 , 187, 153-6	3
660	Molecular Dynamics Simulation of HIV-1 Integrase Dimer Complexed with Viral DNA. 2010 , 28, 33-40	7
659	Effect of Electronic Structures of Enantiomers of Ruthenium(II) Polypyridyl Complexes on DNA Binding Behaviors. 2010 , 28, 1317-1321	4
658	Macrocyclic 14-Membered-Ring Diketal Dilactams: Spectroscopic Studies and Conformational Analysis of Their Complexes with Divalent Cations. 2010 , 2010, 3278-3289	2
657	Significantly enhanced DNA thermal stability resulting from porphyrin H-aggregate formation in the minor groove of the duplex. 2010 , 11, 1833-9	23
656	SYNTHETIC MODIFICATIONS OF ANTISENSE OLIGONUCLEOTIDES: NOVEL BACKBONE REPLACEMENTS WITH IMPROVED PROPERTIES. 2010 , 103, 705-717	7
655	Oligonucleotides with sugars other than ribo- and 2'-deoxyribofuranose in the backbone: the solution structures determined by NMR in the context of the 'Etiology of nucleic acids' project of Albert Eschenmoser. 2010 , 7, 2103-28	9
654	PhthalaPhos: Chiral Supramolecular Ligands for Enantioselective Rhodium-Catalyzed Hydrogenation Reactions. 2010 , 122, 6783-6787	12
653	PhthalaPhos: chiral supramolecular ligands for enantioselective rhodium-catalyzed hydrogenation reactions. 2010 , 49, 6633-7	46
652	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin-binding protein G from Streptococcus. IV. Implication for the mechanism of folding of the parent protein. 2010 , 93, 469-80	16
651	Relaxation of amorphous multichain polymer systems using inverse kinematics. 2010 , 51, 4008-4014	5
650	Atomistic theoretical models for nanoporous hybrid materials. 2010 , 129, 304-318	46
649	Semisynthesis and pharmacological activities of thyroxine analogs: Development of new angiogenesis modulators. 2010 , 20, 3394-8	5
648	Evaluation of Density Functionals, SCC-DFTB, Neglect of Diatomic Differential Overlap (NDDO) Models and Molecular Mechanics Methods for Prolyl-Leucyl-Glycinamide (PLG) and Structural Derivatives. 2010 , 944, 76-82	1
647	Molecular mechanics modeling of the adsorption of methionine on graphite. 2010 , 604, 2084-2090	6
646	Pharmacophore identification, synthesis, and biological evaluation of carboxylated chalcone derivatives as CysLT1 antagonists. 2010 , 18, 5519-27	5
645	Synthesis and bio-evaluation of alkylaminoaryl phenyl cyclopropyl methanones as antitubercular and antimalarial agents. 2010 , 18, 8289-301	24
644	Improved side-chain torsion potentials for the Amber ff99SB protein force field. 2010 , 78, 1950-8	3395

(2010-2010)

643	An abasic site induces a bulged conformation in the single-stranded DNA trimer d(Ap(ab)pA). An NMR and model-building study. 2010 , 114, 79-86	
642	Emodin, a natural product, selectively inhibits 11beta-hydroxysteroid dehydrogenase type 1 and ameliorates metabolic disorder in diet-induced obese mice. 2010 , 161, 113-26	92
641	Potassium channel block by a tripartite complex of two cationophilic ligands and a potassium ion. 2010 , 78, 588-99	23
640	A homology model of the pore domain of a voltage-gated calcium channel is consistent with available SCAM data. 2010 , 135, 261-74	13
639	Similarity and Diversity in Chemical Design. 2010 , 519-553	
638	Implementing Quantum Mechanics into Molecular Mechanicsâ©ombined QM/MM Modeling Methods. 2010 , 1-15	9
637	Theoretical modeling of magnesium ion imprints in the Raman scattering of water. 2010 , 114, 3574-82	28
636	HMP binding protein ThiY and HMP-P synthase THI5 are structural homologues. 2010 , 49, 8929-36	11
635	Biological and conformational evaluation of bifunctional compounds for opioid receptor agonists and neurokinin 1 receptor antagonists possessing two penicillamines. 2010 , 53, 5491-501	20
634	Merging Implicit with Explicit Solvent Simulations: Polyethylene Glycol. 2010 , 6, 1871-83	8
633	Nuclear magnetic resonance structure of the prohead RNA E-loop hairpin. 2010 , 49, 5989-97	13
632	RISM-SCF-SEDD study on the symmetry breaking of carbonate and nitrate anions in aqueous solution. 2010 , 114, 10513-9	26
631	Docking and Scoring in Drug Discovery. 2010 , 601-684	2
630	Synthesis and biophysical studies of coronene functionalized 2'-amino-LNA: a novel class of fluorescent nucleic acids. 2010 , 21, 513-20	20
629	Transport Properties of Aqueous Solutions of (1R,2S)-(â∄ and (1S,2R)-(+)-Ephedrine Hydrochloride at Different Temperatures. 2010 , 55, 1145-1152	10
628	Structure-based design of novel small-molecule inhibitors of Plasmodium falciparum. 2010 , 50, 840-9	41
627	The R.E.D. tools: advances in RESP and ESP charge derivation and force field library building. 2010 , 12, 7821-39	631
626	Calorimetric and spectroscopic studies of aminoglycoside binding to AT-rich DNA triple helices. 2010 , 92, 514-29	31

625	Computational analysis of the structural basis of ligand binding to the crustacean retinoid X receptor. 2010 , 5, 317-24	5
624	Scoring functions and their evaluation methods for protein-ligand docking: recent advances and future directions. 2010 , 12, 12899-908	308
623	Molecular Dynamics Simulations: Difficulties, Solutions and Strategies for Treating Metalloenzymes. 2010 , 299-330	10
622	Estimation on the intramolecular hydrogen-bonding energies in proteins and peptides by the analytic potential energy function. 2010 , 956, 38-43	51
621	Structure-based discovery of A2A adenosine receptor ligands. 2010 , 53, 3748-55	195
620	Mean-Force Scoring Functions for Proteinâ∐igand Binding. 2010 , 280-296	11
619	On potential energy models for EA-based ab initio protein structure prediction. 2010 , 18, 255-75	4
618	Inclusion of solvation and entropy in the knowledge-based scoring function for protein-ligand interactions. 2010 , 50, 262-73	100
617	Intramolecular cation-pi interactions as the driving force to restrict the conformation of certain nucleosides. 2010 , 75, 1974-81	5
616	Atomic charges derived from electrostatic potentials for molecular and periodic systems. 2010 , 114, 10225-33	62
615	Unveiling the unfolding pathway of FALS associated G37R SOD1 mutant: a computational study. 2010 , 6, 1032-9	11
614	N,N-dimethylformamide-induced phase separation of hexafluoroisopropanol-water mixtures. 2011 , 13, 11222-32	16
613	An atomistic simulation of the liquid-crystalline phases of sexithiophene. 2011 , 21, 125-133	55
612	Computer simulation to investigate the FRET application in DNA hybridization systems. 2011 , 13, 10364-71	4
611	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. 2011 , 7, 2886-2902	569
610	Understanding the molecular conformations of Na-dimyristoylphosphatidylglycerol (DMPG) using DFT-based method. 2011 , 37, 953-963	2
609	Intraligand hydrophobic interactions rationalize drug affinities for peptidyl-prolyl cis-trans isomerase protein. 2011 , 115, 6193-201	11
608	Ligand Identification Scoring Algorithm (LISA). 2011 , 51, 1296-306	23

607	Theoretical study of magnesium fluoride in aqueous solution. 2011 , 115, 10553-9	10
606	Ion-Pair Association Constant for LiOH in Supercritical Water. 2011 , 56, 3637-3642	28
605	Discovery of a potent and efficacious peptide derivative for Appioid agonist/neurokinin 1 antagonist activity with a 2',6'-dimethyl-L-tyrosine: in vitro, in vivo, and NMR-based structural studies. 2011 , 54, 2029-38	26
604	Pyrene intercalating nucleic acids with a carbon linker. 2011 , 30, 210-26	4
603	GOAP: a generalized orientation-dependent, all-atom statistical potential for protein structure prediction. 2011 , 101, 2043-52	192
602	Exploring the binding ability of polyammonium hosts for anionic substrates: selective size-dependent recognition of different phosphate anions by bis-macrocyclic receptors. 2011 , 50, 7202-16	34
601	First-principles-based multiscale, multiparadigm molecular mechanics and dynamics methods for describing complex chemical processes. 2012 , 307, 1-42	8
600	Dynamics on the electronically excited state surface of the bioluminescent firefly luciferase-oxyluciferin system. 2011 , 133, 12040-9	48
599	Combination of spectroscopic and computational methods to get an understanding of supramolecular chemistry of drugs: from simple host systems to biomolecules. 2011 , 13, 20893-905	25
598	The Challenge of Affinity Prediction: Scoring Functions for Structure-Based Virtual Screening. 2011 , 177-221	14
597	Argiotoxin in the closed AMPA receptor channel: experimental and modeling study. 2011 , 50, 8213-20	14
596	Modeling of hyperbranched polyesters as hosts for the multifunctional bioactive agent Shikonin. 2011 , 13, 10808-17	15
595	The 5-HT(1A) agonism potential of substituted piperazine-ethyl-amide derivatives is conserved in the hexyl homologues: molecular modeling and pharmacological evaluation. 2011 , 51, 2961-6	8
594	Structural basis for the potential antitumour activity of DNA-interacting benzo[kl]xanthene lignans. 2011 , 9, 701-10	28
593	HL005a new selective PPAR[antagonist specifically inhibits the proliferation of MCF-7. 2011 , 124, 112-20	19
592	Characterization of the structure and function of Klebsiella pneumoniae allantoin racemase. 2011 , 410, 447-60	11
591	The ligand-binding site of buspirone analogues at the 5-HT1A receptor. 1997 , 49, 698-705	22
590	Solution-structure of a peptide designed to mimic the C-terminal hexapeptide of endothelin. 1998 , 50, 837-44	_

589	Application of Molecular Dynamics Simulations in Molecular Property Prediction I: Density and Heat of Vaporization. 2011 , 7, 2151-2165	85
588	Tracing protein evolution through ancestral structures of fish galectin. 2011 , 19, 711-21	13
587	Simulations of docking C60 in €Cyclodextrin. 2011 , 162, 69-77	11
586	Theoretical Study of Hydration Effects on the Selectivity of 18-Crown-6 Between K+ and Na+. 2011 , 19, 212-216	21
585	Duplex and triplex formation of mixed pyrimidine oligonucleotides with stacking of phenyl-triazole moieties in the major groove. 2011 , 76, 6177-87	30
584	Interaction of clozapine and its nitrenium ion with rat D2 dopamine receptors: in vitro binding and computational study. 2011 , 25, 163-9	6
583	A homology model for Clostridium difficile methionyl tRNA synthetase: active site analysis and docking interactions. 2011 , 17, 1679-93	9
582	Charge sensitivity analysis in force-field-atom resolution. 2011 , 17, 2217-26	12
581	Molecular dynamics simulations of the growth of poly(chloro-para-xylylene) films. 2011, 17, 2725-33	4
580	Trends in template/fragment-free protein structure prediction. 2011 , 128, 3-16	41
579	Structural solution using molecular dynamics: Fundamentals and a case study of epoxy-silica	
	interface. 2011 , 48, 2131-2140	96
578		96 152
57 ⁸	interface. 2011 , 48, 2131-2140	
	interface. 2011 , 48, 2131-2140 Confab - Systematic generation of diverse low-energy conformers. 2011 , 3, 8	152
577	interface. 2011, 48, 2131-2140 Confab - Systematic generation of diverse low-energy conformers. 2011, 3, 8 Structure-guided forcefield optimization. 2011, 79, 1898-909 Protein loop selection using orientation-dependent force fields derived by parameter optimization.	152
577 576	Confab - Systematic generation of diverse low-energy conformers. 2011, 3, 8 Structure-guided forcefield optimization. 2011, 79, 1898-909 Protein loop selection using orientation-dependent force fields derived by parameter optimization. 2011, 79, 2260-7 Synthesis, biological activity and solution structure of new analogues of the antimicrobial	152 42 6
577 576 575	Confab - Systematic generation of diverse low-energy conformers. 2011, 3, 8 Structure-guided forcefield optimization. 2011, 79, 1898-909 Protein loop selection using orientation-dependent force fields derived by parameter optimization. 2011, 79, 2260-7 Synthesis, biological activity and solution structure of new analogues of the antimicrobial Gramicidin S. 2011, 17, 211-7 Development of force field parameters for oxyluciferin on its electronic ground and excited states.	152 42 6

571	development of the molecular mechanics-based program ACE and application to asymmetric 3.5 epoxidation reactions. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2878-89	25
570	Effects of water miscible organic solvents on the activity and conformation of the Baeyer-Villiger monooxygenases from Thermobifida fusca and Acinetobacter calcoaceticus: a comparative study. 2011 , 108, 491-9	39
569	Synthesis of tyrrolic-modified porphyrins and their incorporation into DNA. 2011 , 17, 6227-38	30
568	STD and trNOESY NMR study of receptor-ligand interactions in living cancer cells. 2011 , 12, 695-9	29
567	Synthesis and structural characterization of 2'-fluoro-—RNA-modified oligonucleotides. 2011 , 12, 1904-11	7
566	Towards more specific O6-methylguanine-DNA methyltransferase (MGMT) inactivators. 2011 , 19, 1658-65	5
565	Assessment of dynamic properties of water around a monovalent ion: A classical molecular dynamics simulation study. 2011 , 966, 26-30	11
564	Prediction of the PPAR gonism of fibrates by combined MM-docking approaches. 2011 , 29, 865-75	4
563	PTCDA on Cu(111) partially covered with NaCl. 2011 , 22, 295305	15
562	Calculating solvation energies by means of a fluctuating charge model combined with continuum solvent model. 2011 , 134, 194115	12
561	Prediction and interpretation of the hydration entropies of monovalent cations and anions. 2011 , 109, 37-48	23
560	Why does the inner-helix mutation A413C double the stoichiometry of Kv1.3 channel block by emopamil but not by verapamil?. 2011 , 79, 681-91	10
559	Molecular engineering of RANTES peptide mimetics with potent anti-HIV-1 activity. 2011 , 25, 1230-43	16
558	Batrachotoxin, pyrethroids, and BTG 502 share overlapping binding sites on insect sodium channels. 2011 , 80, 426-33	8
557	Possible roles of exceptionally conserved residues around the selectivity filters of sodium and calcium channels. 2011 , 286, 2998-3006	30
556	Identification of new batrachotoxin-sensing residues in segment IIIS6 of the sodium channel. 2011 , 286, 13151-60	44
555	Task-parallel global optimization with application to protein folding. 2011,	2
554	Computational design of a PDZ domain peptide inhibitor that rescues CFTR activity. 2012 , 8, e1002477	89

553	Naphthyridine tetramer with a pre-organized structure for 1:1 binding to a CGG/CGG sequence. 2012 , 40, 2771-81	27
552	Architecture and pore block of eukaryotic voltage-gated sodium channels in view of NavAb bacterial sodium channel structure. 2012 , 82, 97-104	88
551	Multiscale, Multiparadigm Modeling for Nanosystems Characterization and Design. 2012, 935-982	
550	Close intramolecular sulfur-oxygen contacts: modified force field parameters for improved conformation generation. 2012 , 26, 1195-205	18
549	Transferable potentials for phase equilibria-united atom description of five- and six-membered cyclic alkanes and ethers. 2012 , 116, 11234-46	79
548	Poissonâ B oltzmann Implicit Solvation Models. 2012 , 149-162	11
547	Phase transition study of confined water molecules inside carbon nanotubes: hierarchical multiscale method from molecular dynamics simulation to ab initio calculation. 2012 , 38, 40-9	11
546	Structure-based virtual screening of small-molecule antagonists of platelet integrin 日本 that do not prime the receptor to bind ligand. 2012 , 26, 1005-15	18
545	Optimizing solute-water van der Waals interactions to reproduce solvation free energies. 2012 , 116, 4524-34	116
544	Long-range hydrogen-bond structure in aqueous solutions and the vapor-water interface. 2012 , 137, 034508	31
543	Comparative modeling of 25-hydroxycholesterol-7 hydroxylase (CYP7B1): ligand binding and analysis of hereditary spastic paraplegia type 5 CYP7B1 mutations. 2012 , 18, 441-53	10
542	Superstructure based on €CD self-assembly induced by a small guest molecule. 2012 , 14, 1934-44	39
541	Hydrogen bonding and reactivity of water to azines in their S1 (n,图) electronic excited states in the gas phase and in solution. 2012 , 14, 8791-802	31
540	Proton transfer step in the carbon dioxide capture by monoethanol amine: a theoretical study at the molecular level. 2012 , 116, 2244-8	28
539	Methodologies for computing UVâl/IS spectra and nonlinear properties of azo-azulene derivatives. 2012 , 34, 1639-1643	16
538	Computational enzymatic catalysisclarifying enzymatic mechanisms with the help of computers. 2012 , 14, 12431-41	44
537	Quantum Chemical Calculation of Chemical Shifts in the Stereochemical Determination of Organic Compounds: A Practical Approach. 2012 , 571-599	3
536	Amide-induced phase separation of hexafluoroisopropanol-water mixtures depending on the hydrophobicity of amides. 2012 , 14, 8335-47	16

535	comprehensive assessments of protein structures. 2012 , 20, 3756-67	9
534	Structural and molecular basis of interaction of HCV non-structural protein 5A with human casein kinase 1\text{\text{B}} nd PKR. 2012 , 12, 28	11
533	Scoring Functions for Proteinâlligand Interactions. 2012 , 237-263	9
532	Substituent effect on the structural behavior of modified cyclodextrin: a molecular dynamics study on methylated ICDs. 2012 , 116, 3477-89	11
531	A force field for naproxen. 2012 , 38, 152-160	0
530	Stabilizing effect of solvent and guest residue amino acids on a model alpha-helix peptide. 2012 , 998, 80-86	1
529	Synthesis and conformational studies of a hybrid 陶lanineâ印orpholine tetramer. 2012 , 68, 9701-9705	8
528	Bespoke Force Field for Simulating the Molecular Dynamics of Porous Organic Cages. 2012 , 116, 16639-16651	36
527	Distance-dependent atomic knowledge-based force in protein fold recognition. 2012 , 80, 683-90	7
526	Boron containing compounds as protease inhibitors. 2012 , 112, 4156-220	251
525	Recent advances in wave function-based methods of molecular-property calculations. 2012 , 112, 543-631	453
524	An improved structural characterisation of reduced French bean plastocyanin based on NMR data and local-elevation molecular dynamics simulation. 2012 , 41, 579-95	2
523	Atomistic and Coarse-Grained Molecular Dynamics Simulation of a Cross-Linked Sulfonated Poly(1,3-cyclohexadiene)-Based Proton Exchange Membrane. 2012 , 45, 6669-6685	20
522	Molecule-specific determination of atomic polarizabilities with the polarizable atomic multipole model. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1662-72	5
521	Novel (phenylethynyl)pyrene-LNA constructs for fluorescence SNP sensing in polymorphic nucleic acid targets. 2012 , 13, 1509-19	24
520	A library approach to the development of BenzaPhos: highly efficient chiral supramolecular ligands for asymmetric hydrogenation. 2012 , 18, 10368-81	29
519	Synthesis of Gd and (68)Ga complexes in conjugation with a conformationally optimized RGD sequence as potential MRI and PET tumor-imaging probes. 2012 , 7, 1084-93	40

517	Molecular modeling of the Toxoplasma gondii adenosine kinase inhibitors. 2012 , 21, 590-600	20
516	Prediction of SAMPL3 host-guest binding affinities: evaluating the accuracy of generalized force-fields. 2012 , 26, 517-25	27
515	Monte Carlo simulation of several biologically relevant molecules and zwitterions in water. 2012 , 524, 90-95	
5 ¹ 4	Revealing interaction mode between HIV-1 protease and mannitol analog inhibitor. 2012 , 79, 916-25	
513	Multi-scale models for cross-linked sulfonated poly (1, 3-cyclohexadiene) polymer. 2012 , 53, 1517-1528	14
512	Rhodium-catalyzed asymmetric hydrogenation of olefins with PhthalaPhos, a new class of chiral supramolecular ligands. 2012 , 18, 1383-400	54
511	Like-charged residues at the ends of oligoalanine sequences might induce a chain reversal. 2012 , 97, 240-9	6
510	The internal rotational barriers about NC⊞and C∉ backbone bonds of polypeptides. 2012, 41, 53-61	4
509	Ab initio parameterization of YFF1, a universal force field for drug-design applications. 2012 , 18, 663-73	14
508	Temperature dependence of the molecular conformations of dilauroyl phosphatidylcholine: A density functional study. 2013 , 113, 631-636	7
507	Experimental and Computation Studies on Candida antarctica Lipase B-Catalyzed Enantioselective Alcoholysis of 4-Bromomethyl-⊞actone Leading to Enantiopure 4-Bromo-3-hydroxybutanoate. 2013 , 355, 1808-1816	8
506	Recent advances in computational predictions of NMR parameters for the structure elucidation of carbohydrates: methods and limitations. 2013 , 42, 8376-415	93
505	Recent Progress in Density Functional Methodology for Biomolecular Modeling. 2013, 1-64	7
504	Self-association and complexation of the anti-cancer drug doxorubicin with PEGylated hyperbranched polyesters in an aqueous environment. 2013 , 117, 2564-75	21
503	Investigation by MD simulation of the key residues related to substrate-binding and heme-release in human ferrochelatase. 2013 , 19, 2509-18	6
502	An efficient fluctuating charge model for transition metal complexes. <i>Journal of Computational Ghemistry</i> , 2013 , 34, 1598-608	13
501	On the inner workings of Monte Carlo codes. 2013 , 39, 1253-1292	238
500	Functional validation of virtual screening for novel agents with general anesthetic action at ligand-gated ion channels. 2013 , 84, 670-8	16

499	Forcefield_PTM: Charge and AMBER Forcefield Parameters for Frequently Occurring Post-Translational Modifications. 2013 , 9, 5653-5674		68	
498	Modeling active GPCR conformations. 2013 , 522, 21-35		11	
497	Toward Reproducing Sequence Trends in Phosphorus Chemical Shifts for Nucleic Acids by MD/DFT Calculations. 2013 , 9, 1641-56		21	
496	The enzyme 3-hydroxykynurenine transaminase as potential target for 1,2,4-oxadiazoles with larvicide activity against the dengue vector Aedes aegypti. 2013 , 21, 6996-7003		14	
495	Complementarity between in silico and biophysical screening approaches in fragment-based lead discovery against the A(2A) adenosine receptor. 2013 , 53, 2701-14		55	
494	Differential Recognition of Mannose-Based Polysaccharides by Tripodal Receptors Based on a Triethylbenzene Scaffold Substituted with Trihydroxybenzoyl Moieties. 2013 , 2013, 65-76		11	
493	Is it possible for Fe2+ to approach protoporphyrin IX from the side of Tyr-13 in Bacillus subtilis ferrochelatase? An answer from QM/MM study. 2013 , 19, 963-71		5	
492	Avian lipocalin expression in chickens following Escherichia coli infection and inhibition of avian pathogenic Escherichia coli growth by Ex-FABP. 2013 , 152, 156-67		15	
491	Protein-specific force field derived from the fragment molecular orbital method can improve protein-ligand binding interactions. <i>Journal of Computational Chemistry</i> , 2013 , 34, 1251-7	3.5	14	
490	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. 2013 , 15, 3736-51		69	
489	Understanding the orientation of water molecules around the phosphate and attached functional groups in a phospholipid molecule: a DFT-based study. 2013 , 39, 937-955		3	
488	Structure and proton transport in proton exchange membranes based on cross-linked sulfonated poly (1, 3-cyclohexadiene) with varying local acid environment. 2013 , 54, 2299-2307		7	
487	Structure and Diffusion in Cross-Linked and Sulfonated Poly(1,3-cyclohexadiene)/Polyethylene Glycol-Based Proton Exchange Membranes. 2013 , 117, 4901-4912		9	
486	The interactions of apamin and tetraethylammonium are differentially affected by single mutations in the pore mouth of small conductance calcium-activated potassium (SK) channels. 2013 , 85, 560-9		7	
485	Methanol clusters (CH3OH)n: putative global minimum-energy structures from model potentials and dispersion-corrected density functional theory. 2013 , 138, 224303		38	
484	Peptide-LNA oligonucleotide conjugates. 2013 , 11, 4240-9		20	
483	Recombinant 即,3-1,4-glucanase from Theobroma cacao impairs Moniliophthora perniciosa mycelial growth. 2013 , 40, 5417-27		8	
482	Metal ion binding by a G-2 poly(ethylene imine) dendrimer. Ion-directed self-assembling of hierarchical mono- and two-dimensional nanostructured materials. 2013 , 52, 2125-37		26	

481	Influence of Grid Spacing in Poisson-Boltzmann Equation Binding Energy Estimation. 2013, 9, 3677-3685	23
480	Preparation and characterization of a monoclonal antibody against the refolded and functional extracellular domain of rat P2X4 receptor. 2013 , 153, 275-82	9
479	Molecular evidence for dual pyrethroid-receptor sites on a mosquito sodium channel. 2013 , 110, 11785-90	175
478	A methodology for constitutive relationships estimation for SWNT reinforced composites. 2013 , 30, 409-447	
477	A possible molecular mechanism of immunomodulatory activity of bilirubin. 2013, 2013, 467383	5
476	Toward Structure Prediction for Short Peptides Using the Improved SAAP Force Field Parameters. 2013 , 2013, 1-13	3
475	Study on the interactions between diketo-acid inhibitors and prototype foamy virus integrase-DNA complex via molecular docking and comparative molecular dynamics simulation methods. 2013 , 31, 734-47	12
474	Interaction of local anesthetics with the K (+) channel pore domain: KcsA as a model for drug-dependent tetramer stability. 2013 , 7, 182-93	6
473	Structure-based discovery of antagonists of nuclear receptor LRH-1. 2013 , 288, 19830-44	68
472	Rapid genotyping using pyrene-perylene locked nucleic acid complexes. 2013 , 4, 58-68	17
471	Topology of the Interconversion Pathway Networks of Cycloheptane Conformations and Those of Relatedn-Membered Rings. 2013 , 86, 230-242	5
470	Towards an understanding of Mesocestoides vogae fatty acid binding proteins' roles. 2014 , 9, e111204	2
469	A multi-scale-multi-stable model for the rhodopsin photocycle. 2014 , 19, 14961-78	8
468	Application of 4D-QSAR studies to a series of benzothiophene analogs. 2014 , 20, 2420	6
467	Hydration free energies calculated using the AMBER ff03 charge model for natural and unnatural amino acids and multiple water models. 2014 , 71, 745-752	7
466	Biological applications of classical electrostatics methods. 2014 , 13, 1440008	15
465	Fluoxetine blocks Nav1.5 channels via a mechanism similar to that of class 1 antiarrhythmics. 2014 , 86, 378-89	19
464	Graphene/Hyperbranched Polymer Nanocomposites: Insight from Molecular Dynamics Simulations. 2014 , 47, 8833-8845	26

463	Validation and application of modeling algorithms for the design of molecularly imprinted polymers. 2014 , 37, 3579-86	8
462	The effects of conformational constraints in the polyamine moiety of philanthotoxins on AMPAR inhibition. 2014 , 9, 1725-31	5
461	A study of the influence of charged residues on thairpin formation by nuclear magnetic resonance and molecular dynamics. 2014 , 33, 525-35	8
460	Interaction of the BKCa channel gating ring with dendrotoxins. 2014 , 8, 421-32	2
459	A computational analysis for amino acid adsorption. 2014 , 624, 118-129	7
458	Bio-inspired benzo[k,l]xanthene lignans: synthesis, DNA-interaction and antiproliferative properties. 2014 , 12, 2686-701	27
457	A Bayesian statistical approach of improving knowledge-based scoring functions for protein-ligand interactions. <i>Journal of Computational Chemistry</i> , 2014 , 35, 932-43	8
456	Anchor Points Reactive Potential for Bond-Breaking Reactions. 2014 , 10, 924-33	15
455	Properties of LiOH and LiCl at sub and supercritical water conditions. 2014 , 190, 30-33	4
454	Delaunay-based nonlocal interactions are sufficient and accurate in protein fold recognition. 2014 , 82, 415-23	7
453	Homology modeling of Kv1.5 channel block by cationic and electroneutral ligands. 2014 , 1838, 978-87	9
452	On the reaction mechanism of the complete intermolecular O2 transfer between mononuclear nickel and manganese complexes with macrocyclic ligands. 2014 , 20, 13296-304	4
45 ¹	Protein Ligand Docking in Drug Discovery. 2014 , 249-286	5
450	A consistent force field parameter set for zwitterionic amino acid residues. 2014 , 20, 2478	25
449	Bicontinuity and multiple length scale ordering in triphilic hydrogen-bonding ionic liquids. 2014 , 118, 12706-16	61
448	Molecular Modeling and Evaluation of Novel Dibenzopyrrole Derivatives as Telomerase Inhibitors and Potential Drug for Cancer Therapy. 2014 , 11, 1196-207	8
447	In vitro and in silico analysis of the Aspergillus nidulans DNA-CreA repressor interactions. 2014 , 32, 2033-41	6
446	Cyclopropane pipecolic acids as templates for linear and cyclic peptidomimetics: application in the synthesis of an Arg-Gly-Asp (RGD)-containing peptide as an ₩ integrin ligand. 2014 , 20, 11187-203	15

Functionalization of 2?-C-(Piperazinomethyl)-2?,3?-BcNA (Bicyclic Nucleic Acids) with Pyren-1-ylcarbonyl Units. **2014**, 97, 1204-1218

444	High Temperature Diffusion Coefficients for O2, H2, and OH in Water, and for Pure Water. 2014 , 59, 1964-1969	27
443	Strategies for improved modeling of GPCR-drug complexes: blind predictions of serotonin receptors bound to ergotamine. 2014 , 54, 2004-21	19
442	Molecular mechanics investigation of some acrylic polymers using SPASIBA force field. 2014 , 74, 20-32	15
441	Folding similarity of the outer pore region in prokaryotic and eukaryotic sodium channels revealed by docking of conotoxins GIIIA, PIIIA, and KIIIA in a NavAb-based model of Nav1.4. 2014 , 144, 231-44	28
440	Toward a molecular dynamics force field for simulations of 40% trifluoroethanol-water. 2014 , 118, 1471-80	16
439	Structural insights into Estrogen Related Receptor-modulation: 4-methylenesterols from Theonella swinhoei sponge as the first example of marine natural antagonists. 2014 , 80, 51-63	14
438	Molecular dynamics simulations of sodium dodecyl sulfate micelles in water-the effect of the force field. 2014 , 118, 3864-80	111
437	Conformational sensitivity of conjugated poly(ethylene oxide)-poly(amidoamine) molecules to cations adducted upon electrospray ionization - a mass spectrometry, ion mobility and molecular modeling study. 2014 , 808, 163-74	16
436	Drug-induced conformational population shifts in topoisomerase-DNA ternary complexes. 2014 , 19, 7415-28	7
435	Encyclopedia of Applied and Computational Mathematics. 2015, 940-951	O
434	Computational Approaches to Understanding the Self-assembly of Peptide-based Nanostructures. 2015 , 55, 724-734	21
433	A Study of the Solvation Structure of L-Leucine in Alcohol-Water Binary Solvents through Molecular Dynamics Simulations and FTIR and NMR Spectroscopy. 2015 , 16, 3190-9	9
432	The Orientational Order of the Helical Backbone of Poly(Benzyl L-Glutamate) âlà Molecular Dynamics Simulation. 2015 , 23, 51-58	2
431	Double-headed nucleotides introducing thymine nucleobases in the major groove of nucleic acid duplexes. 2015 , 13, 7040-9	11
430	QuickFF: A program for a quick and easy derivation of force fields for metal-organic frameworks from ab initio input. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1015-27	105
429	Biomolecular recognition of antagonists by # nicotinic acetylcholine receptor: Antagonistic mechanism and structure-activity relationships studies. 2015 , 76, 119-32	4
428	Oligonucleotides containing a piperazino-modified 2'-amino-LNA monomer exhibit very high duplex stability and remarkable nuclease resistance. 2015 , 51, 4024-7	15

427	Selectivity Mechanism of ATP-Competitive Inhibitors for PKB and PKA. 2015 , 86, 9-18	4
426	Use of 1-4 interaction scaling factors to control the conformational equilibrium between 由elix and 縣trand. 2015 , 457, 183-6	11
425	Understanding the structural differences between spherical and rod-shaped human insulin nanoparticles produced by supercritical fluids precipitation. 2015 , 16, 476-82	7
424	Molecular docking screening using agonist-bound GPCR structures: probing the A2A adenosine receptor. 2015 , 55, 550-63	55
423	Thermodynamic Driving Forces for Dye Molecule Position and Orientation in Nanoconfined Solvents. 2015 , 119, 9150-9	7
422	Classification of current scoring functions. 2015 , 55, 475-82	150
421	Non-classical mechanism of ⊞mino-3-hydroxy-5-methyl-4-isoxazolepropionic acid receptor channel block by fluoxetine. 2015 , 41, 869-77	4
420	Effect of partial atomic charges on the calculated free energy of solvation of poly(vinyl alcohol) in selected solvents. 2015 , 21, 58	4
419	Polarized Water Wires under Confinement in Chiral Channels. 2015 , 119, 8707-17	9
418	Receptor-based virtual screening protocol for drug discovery. 2015 , 582, 56-67	74
417	Liposome-based gene delivery systems containing a steroid derivative: computational and small angle X-ray diffraction study. 2015 , 5, 54070-54078	16
416	MoDock: A multi-objective strategy improves the accuracy for molecular docking. 2015 , 10, 8	11
415	A hybrid-type approach with MD and DFT calculations for evaluation of redox potential of molecules. 2015 , 41, 936-941	1
414	Domain Based Pair Natural Orbital Coupled Cluster Studies on Linear and Folded Alkane Chains. 2015 , 11, 2137-43	45
413	Multiscale Modeling of the Active Site of [Fe] Hydrogenase: The H2 Binding Site in Open and Closed Protein Conformations. 2015 , 127, 6344-6348	2
412	Towards metal-mediated g-quartet analogues: 1,2,4-triazole nucleotides. 2015 , 34, 277-88	2
411	Multiscale modeling of the active site of [Fe] hydrogenase: the Hâlbinding site in open and closed protein conformations. 2015 , 54, 6246-50	18
410	Developing accurate molecular mechanics force fields for conjugated molecular systems. 2015 , 17, 25123-32	17

409	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. 2015, 11, 5897-905	43
408	Quantum Derivative Fitting and Biomolecular Force Fields: Functional Form, Coupling Terms, Charge Flux, Nonbond Anharmonicity, and Individual Dihedral Potentials. 2015 , 11, 5555-72	23
407	Domain Motion Enhanced (DoME) Model for Efficient Conformational Sampling of Multidomain Proteins. 2015 , 119, 14584-93	8
406	Studying the structure of single-component ceramide bilayers with molecular dynamics simulations using different force fields. 2015 , 41, 1122-1136	8
405	Effect of confinement on the hydration and diffusion of chloride at high temperatures. 2015 , 97, 22-30	4
404	Adaptive molecular docking method based on information entropy genetic algorithm. 2015 , 26, 299-302	25
403	Binding isotope effects as a tool for distinguishing hydrophobic and hydrophilic binding sites of HIV-1 RT. 2015 , 119, 917-27	30
402	Molecular Dynamics Simulation of Heavy Metal Ions in Aqueous Solution Using Lennard-Jones 12-6 Potential. 2015 , 202, 1685-1692	10
401	Electron Transport in a Dioxygenase-Ferredoxin Complex: Long Range Charge Coupling between the Rieske and Non-Heme Iron Center. 2016 , 11, e0162031	5
400	Unexpected Hydration of a Triple Bond During DNA Synthesis: Conjugating 3-(Pyren-1-ylethynyl)indole to DNA for Triplex Studies. 2016 , 2016, 3528-3535	3
399	Probing the binding of Cu(2+) ions to a fragment of the At 1-42) polypeptide using fluorescence spectroscopy, isothermal titration calorimetry and molecular dynamics simulations. 2016 , 216, 44-50	9
398	Synthesis of New DNA G-Quadruplex Constructs with Anthraquinone Insertions and Their Anticoagulant Activity. 2016 , 99, 116-124	6
397	Atomistic Molecular Dynamics Simulations of Carbon Dioxide Diffusivity in n-Hexane, n-Decane, n-Hexadecane, Cyclohexane, and Squalane. 2016 , 120, 12890-12900	39
396	Insights into the Interaction Energy for Cs+âtrown Ether Complex by Molecular Dynamics Simulations. 2016 , 90, 395-400	4
395	Modeling interactions between blocking and permeant cations in the NavMs channel. 2016 , 780, 188-93	2
394	Coarse-grained modeling of RNA 3D structure. 2016 , 103, 138-56	35
393	Elucidating Hyperconjugation from Electronegativity to Predict Drug Conformational Energy in a High Throughput Manner. 2016 , 56, 788-801	8
392	A unified description of the double perovskite family SrMWO within a rigid ion model. 2016 , 18, 26033-26039	1

391	Force Field Application and Development. 2016 , 33-75	2
390	Prediction of cyclohexane-water distribution coefficient for SAMPL5 drug-like compounds with the QMPFF3 and ARROW polarizable force fields. 2016 , 30, 977-988	10
389	The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations. 2016 , 6, 27190	20
388	Geometric and energetic considerations of surface fluctuations during ion transfer across the water-immiscible organic liquid interface. 2016 , 145, 014701	25
387	Chondroitin Sulfate Tetrasaccharides: Synthesis, Three-Dimensional Structure and Interaction with Midkine. 2016 , 22, 2356-69	39
386	Assessing the Current State of Amber Force Field Modifications for DNA. 2016 , 12, 4114-27	203
385	Analysis of inter-residue contacts reveals folding stabilizers in P-loops of potassium, sodium, and TRPV channels. 2016 , 45, 321-9	6
384	Investigation by molecular dynamics simulation of the glass transition temperature and elastic properties of amorphous polymers PMMA, PMAAM and PMMA co PMAAM copolymers. 2016 , 73, 3007-3017	12
383	The dielectric properties of LiOH aqueous solution under external electromagnetic fields by molecular dynamics simulation. 2016 , 216, 747-753	0
382	New potent ∰ integrin ligands based on azabicycloalkane (∰dipeptide mimics. 2016 , 14, 3221-33	4
381	Graphene/poly(ethylene glycol) nanocomposites as studied by molecular dynamics simulations. 2016 , 97, 163-174	33
380	Cyclic RGD peptidomimetics containing 4- and 5-amino-cyclopropane pipecolic acid (CPA) templates as dual 紀 and 5 and 5 integrin ligands. 2016 , 24, 703-11	12
379	Analysis of cyclosporin A and a set of analogs as inhibitors of a T. cruzi cyclophilin by docking and molecular dynamics. 2016 , 34, 399-413	4
378	Conformation-dependent affinity of Cu(II) ions peptide complexes derived from the human Pin1 protein. 2017 , 127, 1431-1443	8
377	Structure and stability of clusters of halanine in the gas phase: importance of the nature of intermolecular interactions. 2017 , 19, 5465-5476	4
376	Molecular dynamics study of thermal transport in a dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) organic semiconductor. 2017 , 9, 2262-2271	27
375	Exploring the binding sites of Staphylococcus aureus phenylalanine tRNA synthetase: A homology model approach. 2017 , 73, 36-47	5
374	Mechanism of sodium channel block by local anesthetics, antiarrhythmics, and anticonvulsants. 2017 , 149, 465-481	55

373	Molecular inclusion process of urease inhibitors into cyclodextrins: A theoretical study. 2017, 675, 69-74	3
372	Transforming the Energy Landscape of a Coiled-Coil Peptide via Point Mutations. 2017 , 13, 1468-1477	12
371	Feature functional theoryâBinding predictor (FFTâBP) for the blind prediction of binding free energies. 2017 , 136, 1	20
370	Protein Dynamics: From Structure to Function. 2017 , 393-425	O
369	Exploring biomolecular energy landscapes. 2017 , 53, 6974-6988	48
368	Accuracy Test of the OPLS-AA Force Field for Calculating Free Energies of Mixing and Comparison with PAC-MAC. 2017 , 13, 1911-1923	14
367	Biological effects of ⊞drenergic phentolamine on erythrocyte hemeprotein: Molecular insights from biorecognition behavior, protein dynamics and flexibility. 2017 , 171, 75-84	1
366	Mitochondria-dependent benzothiadiazole-based molecule probe for quantitatively intracellular pH imaging. 2017 , 145, 576-583	26
365	Extractive insights in the cesium ion partitioning with bis(2-propyloxy)-calix [4]crown-6 and dicyclohexano-18-crown-6 in ionic liquid-water biphasic systems. 2017 , 241, 279-291	6
364	Development of efficient docking strategies and structure-activity relationship study of the c-Met type II inhibitors. 2017 , 75, 241-249	8
363	Integrated In Silico Fragment-Based Drug Design: Case Study with Allosteric Modulators on Metabotropic Glutamate Receptor 5. 2017 , 19, 1235-1248	20
362	Searching for bioactive conformations of drug-like ligands with current force fields: how good are we?. 2017 , 9, 29	16
361	Synthesis and Molecular Modeling of Thermally Stable DNA G-Quadruplexes with Anthraquinone Insertions. 2017 , 2017, 3092-3100	4
360	Metal Ion Modeling Using Classical Mechanics. 2017 , 117, 1564-1686	189
359	Molecular modeling, simulation and docking study of ebola virus glycoprotein. 2017, 72, 266-271	13
358	Elastic properties of the hydrogen-bonded liquid and glassy glycerol under high pressure: comparison with propylene carbonate. 2017 , 7, 33278-33284	9
357	Analysis of the binding sites of vitamin D 1\(\text{Hydroxylase}\) (CYP27B1) and vitamin D 24-hydroxylase (CYP24A1) for the design of selective CYP24A1 inhibitors: Homology modelling, molecular dynamics simulations and identification of key binding requirements. 2017 , 25, 5629-5636	8
356	OPUS-DOSP: A Distance- and Orientation-Dependent All-Atom Potential Derived from Side-Chain Packing. 2017 , 429, 3113-3120	18

355	Improved i-motif thermal stability by insertion of anthraquinone monomers. 2017 , 15, 6613-6621	2
354	Evaluating amber force fields using computed NMR chemical shifts. 2017 , 85, 1944-1956	4
353	Oxygen binding isotope effects of triazole-based HIV-1 reverse transcriptase inhibitors indicate the actual binding site. 2017 , 635, 87-95	2
352	Perfluoropolyethers: Development of an All-Atom Force Field for Molecular Simulations and Validation with New Experimental Vapor Pressures and Liquid Densities. 2017 , 121, 6588-6600	8
351	AMMOS2: a web server for protein-ligand-water complexes refinement via molecular mechanics. 2017 , 45, W350-W355	21
350	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. 2017 , 7, e1281	104
349	Interfacial insights on the dibenzo-based crown ether assisted cesium extraction in [BMIM][Tf2N]âWater binary system. 2017 , 311, 427-438	18
348	Diffusion and hydration of oxygen confined in Fe(OH)2 nano-cracks at high temperatures. 2017 , 120, 345-354	2
347	Fixed-Charge Atomistic Force Fields for Molecular Dynamics Simulations in the Condensed Phase: An Overview. 2018 , 58, 565-578	94
346	Energy Landscapes for the Aggregation of A# 2018 , 140, 4018-4027	22
345	Molecular dynamics analysis of stabilities of the telomeric Watson-Crick duplex and the associated i-motif as a function of pH and temperature. 2018 , 237, 22-30	12
344	Interfacial Behavior of Cs, K, Na, and Rb Extraction in the Presence of Dibenzo-18-Crown-6 from the Nitrobenzene-Water Biphasic System: Experimental, Quantum Chemical, and Molecular Dynamic Studies. 2018 , 3, 1663-1674	5
343	Dynamical heterogeneities of rotational motion in room temperature ionic liquids evidenced by molecular dynamics simulations. 2018 , 148, 193811	13
342	Partitioning of Cs+ and Na+ ions by dibenzo-18-crown-6 ionophore in biphasic aqueous systems of octanol and ionic liquid. 2018 , 106, 477-495	5
341	Alkali Metal Ion Partitioning with Calix[4]arene-benzo-crown-6 Ionophore in Acidic Medium: Insights from Experiments, Statistical Mechanical Framework, and Molecular Dynamics Simulations. 2018 , 122, 2102-2112	5
340	Modeling of Diffusion in MOFs. 2018 , 63-97	
339	OPUS-CSF: A C-atom-based scoring function for ranking protein structural models. 2018, 27, 286-292	12
338	Atom Types Independent Molecular Mechanics Method for Predicting the Conformational Energy of Small Molecules. 2018 , 58, 194-205	11

337	PEG-coumarin nanoaggregates as Estacking derived small molecule lipophile containing self-assemblies for anti-tumour drug delivery. 2018 , 29, 360-375	13
336	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. 2018 , 118, 4177-4338	235
335	Combined QSAR, molecular docking and molecular dynamics study on new Acetylcholinesterase and Butyrylcholinesterase inhibitors. 2018 , 74, 304-326	40
334	Perspective: Ab initio force field methods derived from quantum mechanics. 2018 , 148, 090901	36
333	Incorporation of Hydrogen Bond Angle Dependency into the Generalized Solvation Free Energy Density Model. 2018 , 58, 761-772	2
332	Does an electronic continuum correction improve effective short-range ion-ion interactions in aqueous solution?. 2018 , 148, 222816	25
331	Potentiation and Block of ASIC1a by Memantine. 2018, 38, 869-881	6
330	5-Acetyl-6-methyl-4-aryl-3,4-dihydropyrimidin-2(1H)-ones: As potent urease inhibitors; synthesis, in vitro screening, and molecular modeling study. 2018 , 76, 37-52	23
329	Theoretical investigation on the molecular inclusion process of urease inhibitors into p-sulfonic acid calix[4,6]arenes. 2018 , 692, 117-123	2
328	Polymer Electrolytes Containing Solvate Ionic Liquids: A New Approach To Achieve High Ionic Conductivity, Thermal Stability, and a Wide Potential Window. 2018 , 30, 252-261	42
327	Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures. 2018 , 470, 109-119	12
326	Phase-Transferable Force Field for Alkali Halides. 2018 , 14, 5933-5948	24
325	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. 2018 , 122, 8982-8988	14
324	Dislocations in molecular crystals. 2018 , 81, 096501	27
323	Identification by Molecular Docking ofHomoisoflavones from Leopoldia comosa as Ligands of Estrogen Receptors. 2018 , 23,	38
322	Theoretical Study of the tCyclodextrin Inclusion Complex Formation of Eugenol in Water. 2018 , 23,	5
321	Molecular Docking: From Lock and Key to Combination Lock. 2017 , 2,	23
320	Protein-RNA Docking Using ICM. 2018 , 14, 4971-4984	7

319	A Force Balanced Fragmentation Method for Molecular Dynamic Simulation of Protein. 2018 , 6, 189	5
318	Study on mechanical properties of polyethylene with chain branching in atomic scale by molecular dynamics simulation. 2018 , 44, 1016-1024	10
317	Molecular dynamics simulation of methane hydrate formation in presence and absence of amino acid inhibitors. 2018 , 269, 721-732	24
316	Computational Molecular Modeling Techniques of Biomacromolecular Systems. 2018 , 295-322	
315	Toward a unified scoring function for native state discrimination and drug-binding pocket recognition. 2018 , 20, 17148-17155	2
314	Development of New Transferable Coarse-Grained Models of Hydrocarbons. 2018 , 122, 7143-7153	17
313	An in silico study of the citrus dioxygenases CCD4 family substrates. 2019 , 37, 2086-2097	2
312	Atomic Mechanisms of Timothy Syndrome-Associated Mutations in Calcium Channel Cav1.2. 2019 , 10, 335	5
311	Correlating structure and transport behavior in Li and O containing pyrrolidinium ionic liquids. 2019 , 21, 17176-17189	5
310	OPUS-SSF: A side-chain-inclusive scoring function for ranking protein structural models. 2019 , 28, 1157-1162	4
309	OPUS-SSF: A side-chain-inclusive scoring function for ranking protein structural models. 2019 , 28, 1157-1162 Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. 2019 , 21, 9-35	67
	Recent progress in theoretical and computational studies on the utilization of lignocellulosic	
309	Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. 2019 , 21, 9-35 Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in	67
309	Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. 2019 , 21, 9-35 Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. 2019 , 2, 1900135	67
309 308 307	Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. 2019, 21, 9-35 Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. 2019, 2, 1900135 A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. 2019, 20,	67 27 10
309 308 307 306	Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. 2019, 21, 9-35 Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. 2019, 2, 1900135 A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. 2019, 20, A novel protein descriptor for the prediction of drug binding sites. 2019, 20, 478	67 27 10
309 308 307 306	Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. 2019, 21, 9-35 Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. 2019, 2, 1900135 A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. 2019, 20, A novel protein descriptor for the prediction of drug binding sites. 2019, 20, 478 Mechanism of oligosaccharide synthesis via a mutant GH29 fucosidase. 2019, 4, 402-409 Molecular simulation of peptides coming of age: Accurate prediction of folding, dynamics and	67 27 10 9

301	Molecular Simulation of the Separation of Isoleucine Enantiomers by € Cyclodextrin. 2019 , 24,	10
300	Flexible and Transferable ab Initio Force Field for Zeolitic Imidazolate Frameworks: ZIF-FF. 2019 , 123, 3000-3012	12
299	Molecular Dynamics Insights for Screening the Ability of Polymers to Remove Pesticides from Water. 2019 , 8, 438-446	6
298	Assessment of Multi-Scale Approaches for Computing UV-Vis Spectra in Condensed Phases: Toward an Effective yet Reliable Integration of Variational and Perturbative QM/MM Approaches. 2019 , 15, 3170-318	34 ¹²
297	Equation of State of Fluid Methane from First Principles with Machine Learning Potentials. 2019 , 15, 2574-2586	26
296	Random Forest Refinement of the KECSA2 Knowledge-Based Scoring Function for Protein Decoy Detection. 2019 , 59, 1919-1929	9
295	Interaction of Human Telomeric i-Motif DNA with Single-Walled Carbon Nanotubes: Insights from Molecular Dynamics Simulations. 2019 , 123, 10343-10353	12
294	CherryPicker: An Algorithm for the Automated Parametrization of Large Biomolecules for Molecular Simulation. 2019 , 7, 400	4
293	Computational systems pharmacology analysis of cannabidiol: a combination of chemogenomics-knowledgebase network analysis and integrated in silico modeling and simulation. 2019 , 40, 374-386	22
292	G-Quadruplex and I-Motif Structures within the Telomeric DNA Duplex. A Molecular Dynamics Analysis of Protonation States as Factors Affecting Their Stability. 2019 , 123, 468-479	16
291	Biomolecular force fields: where have we been, where are we now, where do we need to go and how do we get there?. 2019 , 33, 133-203	35
290	Force field development phase II: Relaxation of physics-based criteriaâlbr inclusion of more rigorous physics into the representation of molecular energetics. 2019 , 33, 205-264	26
289	Duffy binding-like 1\textbf{\textit{B}}dhesin from Plasmodium falciparum recognizes ABH histo-blood group saccharide in a type specific manner. 2019 , 207, 266-275	
288	Intersegment contacts determine geometry of the open and closed states in P-loop channels. 2020 , 38, 1012-1027	3
287	Novel assemblies based on oligonucleotides containing intercalating nucleic acid monomers. 2020 , 39, 82-96	
286	Mechanisms of NMDA receptor inhibition by diarylamidine compounds. 2020 , 51, 1573-1582	3
285	Application of computational chemistry for adsorption studies on metalâBrganic frameworks used for carbon capture. 2020 , 5,	
284	ff19SB: Amino-Acid-Specific Protein Backbone Parameters Trained against Quantum Mechanics Energy Surfaces in Solution. 2020 , 16, 528-552	197

(2020-2020)

283	A coarse-grained potential for liquid water by spherically projected hydrogen-bonding interactions. 2020 , 300, 112246	1
282	Periodic Coulomb Tree Method: An Alternative to Parallel Particle Mesh Ewald. 2020, 16, 7-17	7
281	Molecular Simulation of the Separation of Some Amino Acid Enantiomers by ¶Cyclodextrin in Gas-Phase. 2020 , 8, 823	1
280	Energy Landscape for the Membrane Fusion Pathway in Influenza A Hemagglutinin From Discrete Path Sampling. 2020 , 8, 575195	3
279	Demystifying the Molecular Basis of Pyrazoloquinolinones Recognition at the Extracellular 日+/即-Interface of the GABA Receptor by Molecular Modeling. 2020 , 11, 561834	1
278	Effect of Vitamin K Inhibiting the Function of NorA Efflux Pump and Its Gene Expression on. 2020 , 10,	14
277	Application of a Distance-Dependent Sigmoidal Dielectric Constant to the REMC/SAAP3D Simulations of Chignolin, Trp-Cage, and the G10q Mutant. 2020 , 39, 402-410	О
276	Fast Rescoring Protocols to Improve the Performance of Structure-Based Virtual Screening Performed on Protein-Protein Interfaces. 2020 , 60, 3910-3934	6
275	Solution structure of macromolecules using small angle neutron scattering and molecular simulations. 2020 , 236, 03003	
274	Probing the conformational landscape and thermochemistry of DNA dinucleotide anions via helium nanodroplet infrared action spectroscopy. 2020 , 22, 18400-18413	10
273	Carbazole modified oligonucleotides: synthesis, hybridization studies and fluorescence properties. 2020 , 18, 6935-6948	1
272	Atypical structures of GAA/TTC trinucleotide repeats underlying Friedreich's ataxia: DNA triplexes and RNA/DNA hybrids. 2020 , 48, 9899-9917	8
271	Evolution of Alchemical Free Energy Methods in Drug Discovery. 2020 , 60, 5308-5318	24
270	Comparison of Methods for Bulk Automated Simulation of Glycosidic Bond Conformations. 2020 , 21,	1
269	Numeric analysis of reversibility of classic movement equations and constructive criteria of estimating quality of molecular dynamic simulations. 2021 , 39, 4066-4076	5
268	Molecular Dynamics Study of the Interaction of Carbon Nanotubes With Telomeric DNA Fragment Containing Noncanonical G-quadruplex and i-Motif Forms. 2020 , 21,	7
267	Phenylalkylamines in calcium channels: computational analysis of experimental structures. 2020 , 34, 1157-1169	2
	Pair Potentials as Machine Learning Features. 2020 , 16, 5385-5400	

265	Pairwise-additive and polarizable atomistic force fields for molecular dynamics simulations of proteins. 2020 , 170, 1-71	5
264	Hydrogen-bond network in liquid methanol as studied by neutron Scattering, DFT calculations and molecular dynamics simulations. 2021 , 1227, 129683	4
263	A second generation of 1,2,4-oxadiazole derivatives with enhanced solubility for inhibition of 3-hydroxykynurenine transaminase (HKT) from. 2021 , 12, 222-236	2
262	COMPASS III: automated fitting workflows and extension to ionic liquids. 2021 , 47, 540-551	15
261	Effect of water nanoconfinement on the dynamic properties of paramagnetic colloidal complexes. 2021 , 23, 16948-16957	О
260	The development of an Amber-compatible organosilane force field for drug-like small molecules. 2021 , 23, 12582-12591	3
259	Construction of DNA/RNA Triplex Helices Based on GAA/TTC Trinucleotide Repeats. 2021 , 11, e4155	O
258	Possible Mechanism of Ion Selectivity in Eukaryotic Voltage-Gated Sodium Channels. 2021 , 125, 2074-2088	1
257	Molecular mechanics approaches for rational drug design: forcefields and solvation models. 2021,	О
256	Docking, Scoring, and Virtual Screening in Drug Discovery. 1-102	1
255	Protonation of Cytosine-Rich Telomeric DNA Fragments by Carboxylated Carbon Nanotubes: Insights from Computational Studies. 2021 , 125, 5526-5536	1
254	VirtualFlow Ants-Ultra-Large Virtual Screenings with Artificial Intelligence Driven Docking Algorithm Based on Ant Colony Optimization. 2021 , 22,	4
253	Molecular Dynamics Study of the Photodissociation of ICN in Ethanol: Effect of Solvent Polarity. 2021 , 50, 894-919	
252	Specificity of the HIV-1 Protease on Substrates Representing the Cleavage Site in the Proximal Zinc-Finger of HIV-1 Nucleocapsid Protein. 2021 , 13,	O
251	Mapping the interaction surface of scorpion ∉oxins with an insect sodium channel. 2021 , 478, 2843-2869	1
251 250	Mapping the interaction surface of scorpion toxins with an insect sodium channel. 2021 , 478, 2843-2869 Computational Analysis of the Crystal and Cryo-EM Structures of P-Loop Channels with Drugs. 2021 , 22,	0
	Computational Analysis of the Crystal and Cryo-EM Structures of P-Loop Channels with Drugs. 2021	

247	Performance-Based Screening of Porous Materials for Carbon Capture. 2021 , 121, 10666-10741	28
246	Transferable Gaussian Attractive Potentials for Organic/Oxide Interfaces. 2021 , 125, 10843-10853	2
245	In Silico Approach in Drug Design and Drug Discovery: An Update. 2021 , 245-271	1
244	AMBER: A Program for Simulation of Biological and Organic Molecules.	2
243	Nucleic Acids: Molecular Dynamic Simulations.	2
242	OPLS Force Fields.	7
241	Molecular Modeling in Drug Design. 2003 , 77-168	2
240	Virtual Screening. 2003 , 243-279	3
239	Docking and Scoring Functions/Virtual Screening. 2003, 281-331	11
238	Use of T cell receptor/HLA-DRB1*04 molecular modeling to predict site-specific interactions for the DR shared epitope associated with rheumatoid arthritis. 1997 , 40, 1316-26	25
237	Computer Simulation of Biomolecular Systems Using Molecular Dynamics and Free Energy Perturbation Methods. 295-320	16
236	Computer Simulation of Lipid Systems. 269-298	13
235	Computer Graphics and Molecular Modeling in the Analysis of Synthetic Targets. 1-85	4
234	Supramolecular Inorganic Chemistry. 137-233	9
233	The Docking Problem. 1732-1768	2
232	Structure model of a complex between the factor for inversion stimulation (FIS) and DNA: modeling protein-DNA complexes with dyad symmetry and known protein structures. 1996 , 25, 486-500	19
231	Molecular Mechanics Calculations on Protein-Ligand Complexes. 2002 , 115-127	2
230	Protein-Ligand Interactions. 2002 , 363-374	1

229	New Molecular Mechanism of Dextran Extension in Single Molecule AFM. 2006 , 711-720	2
228	Atomistic Simulations of Liquid Crystals. 1999 , 41-64	8
227	Hybrid Quantum Mechanics/Molecular Mechanics Methods in Transition Metal Chemistry. 1999 , 165-191	31
226	Interaction of alcohols and anesthetics with the water-hexane interface: A molecular dynamics study. 1997 , 29-40	30
225	Simulations of Protein Aggregation. 2006 , 47-77	2
224	Refinement of Three-dimensional Structures of Proteins and Nucleic Acids. 1991 , 137-178	2
223	The Calculation, Representation and Analysis of Molecular Fields. 1994 , 266-304	1
222	Modeling of G-Protein-Coupled Receptors. 1994 , 237-255	3
221	Pursuing Laplaceâ⊞ Vision on Modern Computers. 1996 , 219-247	11
220	NMR Structural Studies of Flexible Molecules. 1996 , 245-249	1
219	Computational Complexity, Protein Structure Prediction, and the Levinthal Paradox. 1994 , 433-506	18
218	The Genetic Algorithm and Protein Tertiary Structure Prediction. 1994, 109-124	6
217	An Empirical Potential Energy Function for Phospholipids: Criteria for Parameter Optimization and Applications. 1996 , 31-81	154
216	Refinement of Three-Dimensional Protein and DNA Structures in Solution from NMR Data. 1991 , 331-347	2
215	Computational evaluation of protein stability change upon mutations. 2010 , 634, 189-201	7
214	Nanotribology: Nonlinear Mechanisms of Friction. 2015, 175-208	4
213	The Adaptive Cartesian Grid-Based Poissonâ B oltzmann Solver: Energy and Surface Electrostatic Properties. 2015 , 73-110	1
212	Data Mining in Organic Crystallography. 2009 , 89-134	5

211	Design of Protein-Protein Interactions with a Novel Ensemble-Based Scoring Algorithm. 2011 , 361-376	2
210	Empirical Classical Force Fields for Molecular Systems. 1999 , 177-214	6
209	Free-Energy Calculations in Protein Folding by Generalized-Ensemble Algorithms. 2002, 304-332	21
208	A Test Set for Molecular Dynamics Algorithms. 2002 , 73-103	3
207	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems. 1991 , 1-49	6
206	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems. 1991 , 1-49	2
205	Molecular Dynamics in Systems with Multiple Time Scales: Reference System Propagator Algorithms. 1999 , 297-317	1
204	Molecular Dynamics Simulations of Proteins and Protein-Protein Complexes. 1990, 68-84	3
203	Computer modelling and drug design. 1992 , 133-162	1
202	Solvent and Dynamic Effects on the Structure of Alkali Cation Complexes of the t-Butyl-calix[4]arene Anion: MD and FEP Computer Investigations on the Na+/Cs+ Binding Affinity. 1996 , 67-99	5
201	Monte Carlo and Molecular Dynamics Simulations. 1990 , 805-888	4
200	Molecular Simulations of Protein Structure, Dynamics and Thermodynamics. 1990 , 289-334	2
199	Minihairpin Loops in DNA: Experimental and Theoretical Studies. 1988, 93-124	3
198	Monte Carlo and Molecular Dynamics Simulations. 1989 , 363-423	3
197	Trends in Molecular Dynamics Simulation Technique. 1995 , 217-253	2
196	Calculation of Atom-Centered Partial Charges for Heme. 1995 , 181-188	3
195	Construction of a DNA Four-Way Junction: Design and NMR Spectroscopy. 1995 , 289-304	1
194	Isomerization Reactions at Aqueous Interfaces. 1994 , 207-226	5

193	Molecular Recognition of Dinucleotides and Amino Acids by Artificial Receptors Containing a Bicyclic Guanidinium Subunit. 1994 , 79-99	7
192	The treatment of conformationally flexible molecules in similarity and complementarity searching. 1995 , 57-88	2
191	Time scales and fluctuations of protein dynamics: metmyoglobin in aqueous solution. 1993, 168-193	1
190	AB Initio Studies and Quantum-Classical Molecular Dynamics Simulations for Proton Transfer Processes in Model Systems and in Enzymes. 1992 , 299-326	8
189	Design of Bifunctional Nucleic Acid Ligands. 1990 , 275-290	5
188	The Effects of Ligand Structure on Binding Mode and Specificity in the Interaction of Unfused Aromatic Cations with DNA. 1990 , 331-353	12
187	Contrasting Mechanisms for the Sequence Recognition of DNA by (+)- and (-)-CC-1065. 1990 , 531-550	5
186	Structure and Dynamics of Adenosine Loops in RNA Bulge Duplexes. RNA Hydration at the Bulge Site. 1999 , 73-87	1
185	Computer Modelling of the Structures of Host-Guest Complexes. 1992 , 207-237	5
184	Empirical classical interaction functions for molecular simulation. 1997 , 3-82	
	Empirical classical interaction functions for molecular simulation. 1991, 5-62	25
183	The development/application of a âthinimalistât brganic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. 1997 , 83-96	25 156
183	The development/application of a âfhinimalistâlorganic/biochemical molecular mechanic force field	
	The development/application of a âthinimalistâtbrganic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. 1997 , 83-96	156
182	The development/application of a âfhinimalistâlbrganic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. 1997 , 83-96 Reduced variable molecular dynamics. 1997 , 122-149	156 1
182	The development/application of a âfininimalistâlbrganic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. 1997, 83-96 Reduced variable molecular dynamics. 1997, 122-149 SOLUTION STRUCTURE OF TGFBY 2D 1H NMR AND MOLECULAR MODELLING. 1989, 223-232 Molecular dynamics simulations of proteins in aqueous solution without the truncation of	156 1
182 181 180	The development/application of a âfhinimalistâlbrganic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. 1997, 83-96 Reduced variable molecular dynamics. 1997, 122-149 SOLUTION STRUCTURE OF TGFBY 2D 1H NMR AND MOLECULAR MODELLING. 1989, 223-232 Molecular dynamics simulations of proteins in aqueous solution without the truncation of long-range Coulomb interactions. 1993, 1185-1188 Improving small molecule virtual screening strategies for the next generation of therapeutics. 2018	156 1 1
182 181 180	The development/application of a âfhinimalistâlbrganic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. 1997, 83-96 Reduced variable molecular dynamics. 1997, 122-149 SOLUTION STRUCTURE OF TGF®Y 2D 1H NMR AND MOLECULAR MODELLING. 1989, 223-232 Molecular dynamics simulations of proteins in aqueous solution without the truncation of long-range Coulomb interactions. 1993, 1185-1188 Improving small molecule virtual screening strategies for the next generation of therapeutics. 2018, 44, 87-92	156 1 1 1 24

175	Kinetic analysis of a mutant (His107â⊠Tyr) responsible for human carbonic anhydrase II deficiency syndrome 1993 , 268, 4775-4779	12
174	Charged collagen structure mediates the recognition of negatively charged macromolecules by macrophage scavenger receptors 1993 , 268, 2126-2133	188
173	Identification of an extracytoplasmic region of H+,K(+)-ATPase labeled by a K(+)-competitive photoaffinity inhibitor 1991 , 266, 18976-18988	85
172	Free energy perturbation calculations on binding and catalysis after mutating threonine 220 in subtilisin. 1991 , 266, 11801-11809	17
171	The binding of human factor IX to endothelial cells is mediated by residues 3-11 1992 , 267, 20529-20531	49
170	The Salmonella typhimurium his operon leader region contains an RNA hairpin-dependent transcription pause site. 1989 , 264, 20796-20804	51
169	Molecular mechanism for familial protein C deficiency and thrombosis in protein CVermont (Glu20âBAla and Val34âBMet) 1994 , 269, 29032-29038	15
168	Design of bioactive peptides based on antibody hypervariable region structures. Development of conformationally constrained and dimeric peptides with enhanced affinity 1991 , 266, 5182-5190	92
167	Methods of incorporating quantum mechanical calculations into molecular dynamics simulations. 1999 , 7, 1-29	2
166	Solute location in a nanoconfined liquid depends on charge distribution. 2015 , 143, 044701	3
165	Open Force Field Consortium: Escaping atom types using direct chemical perception with SMIRNOFF v0.1.	11
164	Three-dimensional structure of bovine heart fatty-acid-binding protein with bound palmitic acid, determined by multidimensional NMR spectroscopy. 1995 , 230, 266-80	49
163	Kissing of the two predominant hairpin loops in the coxsackie B virus 3' untranslated region is the essential structural feature of the origin of replication required for negative-strand RNA synthesis. 1997 , 71, 686-96	119
162	Conformational Analysis, Solvent-Accessible Surface and Geometric Extent of Inhibitors and Substrates. 2006 , 71, 842-858	1
161	Background. 2004 ,	1
160	Nucleic Acid Simulations. 2001,	1
159	Docking and Scoring. 2003 ,	1
158	Photoinduced SHG in Push-Pull Chromophores 1,3-dithiol-2-yliedene Moieties Embedded in Photopolymer Matrices. 2003 , 103, 293-300	1

157	PROPERTIES OF AQUEOUS SYSTEMS RELEVANT TO THE SCWR VIA MOLECULAR DYNAMICS SIMULATIONS. 2015 , 4, 9-22	7
156	An estimate of the numbers and density of low-energy structures (or decoys) in the conformational landscape of proteins. 2009 , 4, e5148	3
155	Conformational determinants of phosphotyrosine peptides complexed with the Src SH2 domain. 2010 , 5, e11215	10
154	TRPV1 activation power can switch an action mode for its polypeptide ligands. 2017 , 12, e0177077	22
153	Anti-angiogenic peptides for cancer therapeutics. 2011 , 12, 1101-16	119
152	Recent Trends in Drug Design and Discovery. 2020 , 20, 1761-1770	4
151	Computational Chemical Analysis of Firefly Luciferase Catalyzed Enantioselective Thioester Formation toward Ketoprofen. 2008 , 7, 143-150	1
150	Carbon Nanotubes and Short Cytosine-Rich Telomeric DNA Oligomeres as Platforms for Controlled Release of Doxorubicin-A Molecular Dynamics Study. 2020 , 21,	11
149	Peptoids with aliphatic sidechains as helical structures without hydrogen bonds and collagen/inverse-collagen type structures. 2011 , 02, 37-48	7
148	Functional group based Ligand binding affinity scoring function at atomic environmental level. 2009 , 3, 268-74	2
147	A Possible Mechanism of Modulation of Slow Sodium Channels in the Sensory Neuron Membrane by Short Peptides. 2021 , 66, 579-588	1
146	Possible Interactions of Extracellular Loop IVP2-S6 With Voltage-Sensing Domain III in Cardiac Sodium Channel. 2021 , 12, 742508	O
145	Molecular insights into complex formation between scandenin and various types of tyclodextrin. 2021 , 344, 117774	
144	Structure Prediction of Binding Sites of MHC Class II Molecules based on the Crystal of HLA-DRB1 and Global Optimization. 2000 , 157-189	
143	Flexible Ligand Docking Using a Robust Evolutionary Algorithm. 2000 , 95-106	
142	Molecular Dynamics Simulation of Biological Molecules. (1). Methods 2000 , 6, 1-36	2
141	3D QSAR on Mutagenic Heterocyclic Amines That are Substrates of Cytochrome P450 1A2. 2000 , 321-322	
140	Methodology for Elucidating the Folding Dynamics of Peptides : Met-enkephalin Case Study. 2000 , 19-46	1

139	Proline. 2000 , 63-73
138	Multiple Time Steps Algorithms for the Atomistic Simulations of Complex Molecular Systems. 2000 , 333-387
137	Molecular Modelling of DNA Adducts of BBR3464: A New Phase I Clinical Agent. 2000 , 375-376
136	The Alpha Factor. 2000 , 97-112
135	Modeling of Suramin-TNF#Interactions. 2000 , 359-360
134	Makrokonformationen. 2000 , 66-137
133	Electrostatic and Hydrophobic Nature of the Binding of Gelsolin 135â¶42 and Gelsolin 150â¶69 Fragments to the PIP2-Containing Lipid Bilayer. 2001 , 420-421
132	Molecular Docking and Structure-based Design.
131	Free Energy Simulations.
130	Force Fields: A General Discussion.
129	Nucleic Acid Force Fields.
128	Free Energy Calculations: Methods and Applications.
127	Charge Distribution Calculations: Alternative Approaches.
126	Protein Force Fields. 1
125	ProteinâNucleic Acid Interactions.
124	Quantum Mechanical/Molecular Mechanical (QM/MM) Coupled Potentials.
123	Hydrogen Bonding: 2.
122	DNA Bases and Base Pairs: Ab Initio Calculations.

121	Macromolecular Structure Calculation and Refinement by Simulated Annealing: Methods and Applications.
120	Cyclodextrins.
119	Development of an Assisting System to Add New Residues to the Standard AMBER Residue Database 2003 , 2, 135-142
118	Studies of the Monodipole-macrodipole Interactions within Helices Using the Point-charge Systems for Alanine. 2003 , 24, 824-828
117	Molecular Mechanics and Comparison of Force Fields. 2003,
116	New Algorithms and the Physics of Protein Folding. 2004 , 173-192
115	Computational Experiments with an Adaptive Genetic Algorithm for Global Minimization of Potential Energy Functions. 2004 , 71-82
114	Reducing the Cost of Evaluation of the Gradient and Hessian of Molecular Potential Energy Functions. 2004 , 275-287
113	Development of Modrast-P with GTK+. 2005 , 4, 119-126
112	Computer simulation of isothermal mass transport in graphite slit pores. 2005 ,
112	Computer simulation of isothermal mass transport in graphite slit pores. 2005 , Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006 , 71, 691-697
	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity.
111	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006 , 71, 691-697
111	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006, 71, 691-697 Theoretical and empirical approaches to protein-structure prediction and analysis. 1991, 35, 1-86 Molecular Dynamics Study for the Base Sequence Recognition Probe of Nucleic Acids Modified with
111 110 109	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006, 71, 691-697 Theoretical and empirical approaches to protein-structure prediction and analysis. 1991, 35, 1-86 Molecular Dynamics Study for the Base Sequence Recognition Probe of Nucleic Acids Modified with the Pyrenyl Group. 2007, 6, 227-234
111 110 109 108	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006, 71, 691-697 Theoretical and empirical approaches to protein-structure prediction and analysis. 1991, 35, 1-86 Molecular Dynamics Study for the Base Sequence Recognition Probe of Nucleic Acids Modified with the Pyrenyl Group. 2007, 6, 227-234 Molecular Mechanics. 920-946
111 110 109 108	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006, 71, 691-697 Theoretical and empirical approaches to protein-structure prediction and analysis. 1991, 35, 1-86 Molecular Dynamics Study for the Base Sequence Recognition Probe of Nucleic Acids Modified with the Pyrenyl Group. 2007, 6, 227-234 Molecular Mechanics. 920-946 Computational Analysis of Switchable Rotaxanes. 2008, 939-953

Theoretical Calculations of the Electrostatic Potential of Some Tumor Promoters. 1988, 301-311 103 Molecular graphics of antidepressant drugs and metabolites. 1989, 7, 60-7 102 Protein-Struktur und Funktion: Die M\(Glichkeiten und Probleme der Computersimulation aus der 101 Sicht des Experimentators. 1990, 258-274 Computer Simulation of Zinc-Containing Enzymes. 1990, 199-209 100 Theories and simulation of protein folding. 1990, 14, 1-19 99 Normal modes of crambin and molecular dynamics for structure prediction. 1991, 220-228 98 Conformational Analysis of Multifidene and Its Synthetic Analogues. 1991, 23-33 97 Semiclassical Methods for Large Molecules of Biological Importance. 1991, 51-64 96 The development of molecular mechanics parameters for carbohydrates. 1991, 372-378 95 Semiclassical Methods for Large Molecules of Biological Importance. 1991, 51-64 94 Modeling DNA Backbone Structures. 1993, 87-97 93 Vibration analysis of transfer RNAs using normal mode calculation. 1993, 1203-1206 92 Molecular modeling of neurotransmitter receptors and ligands. 1993, 10, 1-8 91 Hydrophobic energy estimation for bio-molecules using liquid statistical mechanics theory. 1993, 1311-1314 90 Modeling three-dimensional structure and electrostatics of alkali-stable cyclomaltodextrin 89 1 glucanotransferase. 1993, 47, 291-298 88 On the interpretation of biochemical data by molecular dynamics computer simulation. 1993, 63-77 Conformational properties of the transmembrane domains of the human D2-receptor: Comparison 87 with bacteriorhodopsin. 1993, 420-421 The effects of solvent on the conformation and the collective motions of protein. 1993, 1211-1214 86

85	Molecular Dynamics Studies of H-ras p21-GTP. 1993 , 235-245
84	The effect of codon 31 on the relative affinities for the binding of designed 8-alkyl-pterins to dihydrofolate reductase: a statistical perturbation theory and molecular dynamics simulation study. 1993 , 338, 511-4
83	Receptor-Ligand Interactions in Pharmacology and Drug Design. 1994 , 151-159
82	Conformational Analysis of Dolavaline, Dolaisoleuine, Dolaproine and Dolaphenine Unusual Amino Acids. 1994 , 405-413
81	Computer Modeling Studies of the Interaction of Water With Carbohydrates. 1994 , 43-57
80	Computer-Assisted Structure Determination of Biomacromolecules by NMR. 1994 , 67-85
79	Molecular Modelling Methods. 1994 , 1-52
78	Hydration and Association Abilities of Cytidine, 2âDeoxycytidine and Their Phosphate Salts in the Aqueous Solutions by Molecular Dynamics Simulations and FTIR Spectroscopy. 1994 , 509-512
77	3D QSAR The Integration of QSAR with Molecular Modeling. 1994 , 9-88
76	Conformational properties of new cyclic bradykinin antagonists. 1995 , 527-528
75	The Effect of Hydrostatic Pressure on Protein Crystals Investigated by Molecular Simulation. 1995 , 203-215
74	
	The Structures and Vibrational Frequencies of a Series of Linear Ethers, Alcohols and Acetals using the Spectroscopic Potential Spasiba. 1995 , 117-118
73	
73 72	the Spectroscopic Potential Spasiba. 1995 , 117-118 Molecular Dynamics Simulations of a Hydrated Phospholipid Bilayer with the Force Field Spasiba.
	the Spectroscopic Potential Spasiba. 1995, 117-118 Molecular Dynamics Simulations of a Hydrated Phospholipid Bilayer with the Force Field Spasiba. 1995, 385-386 Molecular Force Field Development for Saccharides Using the Spasiba Spectroscopic Potential.
72	the Spectroscopic Potential Spasiba. 1995, 117-118 Molecular Dynamics Simulations of a Hydrated Phospholipid Bilayer with the Force Field Spasiba. 1995, 385-386 Molecular Force Field Development for Saccharides Using the Spasiba Spectroscopic Potential. Force Field Parameters for Glucose. 1995, 435-435 Use of Molecular Dynamics for the Reconstruction of Complete Structures: A Study on Thioredoxin.
72 71	Molecular Dynamics Simulations of a Hydrated Phospholipid Bilayer with the Force Field Spasiba. 1995, 385-386 Molecular Force Field Development for Saccharides Using the Spasiba Spectroscopic Potential. Force Field Parameters for Glucose. 1995, 435-435 Use of Molecular Dynamics for the Reconstruction of Complete Structures: A Study on Thioredoxin. 1995, 103-110

67	Substrate Binding and Catalytic Mechanism in Phospholipase C from Bacillus cereus. 1997, 93-96	
66	Typische Modelle und Programme. 1997 , 85-206	
65	The Role of Electrostatics at the Catalytic Metal Binding Site in Xylose Isomerase Action. 1997, 419-439	
64	Characterization of the effect of functional groups substitution at the 2-position of adenine on the stability of a duplex dodecamer d(CGCGAATTCGCG)2 by molecular mechanics and free energy perturbation method. 1997 , 563-600	
63	Molecular Dynamics Simulations of Biomembrane Models. 1997 , 293-296	
62	Incorporation of solvation energy contributions for energy refinement and folding of proteins. 1997 , 270-283	
61	The Role of Ca2+ in the Binding of Carbohydrates to C-Type Lectins as Revealed by Molecular Mechanics and Molecular Dynamics Calculations. 1997 , 167-190	
60	Semiempirical and Ab Initio Modeling of Chemical Processes. 1997 , 47-77	
59	Chapter 4 Computational methods relating protein sequence and structure. 1997 , 165-268	
58	Modelling DNA Stretching for Physics and Biology. 1999 , 115-131	
57	Development of Support Program for AMBER 1999 , 5, 39-48	3
56	Introduction to Packing Patterns and Packing Energetics of Crystalline Self-Assembled Structures. 1999 , 23-42	
55	A New Automated Method for Modeling Non-Covalent Macro-Molecular Interactions. 1999 , 205-223	
54	Dynamic Docking Study of the Binding of 1-Chloro-2,4- Dinitrobenzene in the Putative Electrophile Binding Site of Naturally Occurring Human Glutathione. 1999 ,	
53	TcCYPR04, a Cacao Papain-Like Cysteine-Protease Detected in Senescent and Necrotic Tissues Interacts with a Cystatin TcCYS4. 2015 , 10, e0144440	2
52	Molecular Docking at a Glance. 2016 , 1-38	1
51	Modelling and simulation of DNA hydrogel with a coarse-grained model. 2017, 66, 150201	2
50	Molecular Docking at a Glance. 2017 , 764-803	

49 OPUS-CSF: A C-atom-based Scoring Function for Ranking Protein Structural Models.

48	Molecular Mechanics. 279-300	
47	Basic concepts and physical-chemical phenomena, that have conceptual meaning for the formation of systemic clinical thinking and formalization of the knowledge of systemic structural-functional organization of the humanâl organism. 2020 , 5, 15-62	
46	Thermal transport in organic semiconductors. 2021 , 130, 170902	5
45	Intersegment Contacts of Potentially Damaging Variants of Cardiac Sodium Channel. 2021, 12, 756415	O
44	On the Mechanisms of Proteinases. 2002 , 295-340	1
43	Structure of Met30-Ser40 Segment in N-Terminus of Human Tyrosine Hydroxylase Type1. 2004 , 57-67	
42	5.2.3 Nonbonded interactions. 416-419	
41	5.2.7 References for 5.2. 434-435	
40	5.3.2 Molecular mechanics and dynamics theory. 437-442	
39	Effect of the valine-threonine constraint on the dynamics of the proline helix â[A molecular dynamics study. 1994 , 106, 579-589	
38	Synthetic and conformational studies of branched and lariat RNAs. Modelling the lariat formed in the splicing reaction â[A critical review. 1994 , 106, 1023-1050	
37	Structural and morphological changes of breast cancer cells induced by iron(II) complexes 2022,	1
36	Structural Characterization of a New Collagen Biomimetic Octapeptide with Nanoscale Self-Assembly Potential: Experimental and Theoretical Approaches 2022 , 87, e202100462	2
35	Prediction of the structure and mechanical properties of polycaprolactone-silica nanocomposites and the interphase region by molecular dynamics simulations: the effect of PEGylation 2022 ,	
34	Molecular Forcefield Methods for Describing Energetic Molecular Crystals: A Review 2022 , 27,	Ο
33	Integration of Experimental Data and Use of Automated Fitting Methods in Developing Protein Force Fields 2022 , 5,	1
32	A refined photo-switchable cyclic peptide scaffold for use in 毗urn activation.	

31	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022 , 156, 175101	2
30	Energy Landscapes for Base-Flipping in a Model DNA Duplex 2022,	O
29	Simulations of Protein Aggregation. 2006 , 47-77	
28	Data_Sheet_1.PDF. 2019 ,	
27	Data_Sheet_1.PDF. 2019 ,	
26	Data_Sheet_2.PDF. 2019 ,	
25	DataSheet_1.pdf. 2020 ,	
24	A new insight into the transfer and delivery of anti-SARS-CoV-2 drug Carmofur with the assistance of graphene oxide quantum dot as a highly efficient nanovector toward COVID-19 by molecular dynamics simulation 2022 , 12, 14167-14174	O
23	Self-Consistent Parameterization of DNA Residues for the Non-Polarizable AMBER Force Fields. 2022 , 12, 666	
22	DFT studies on the physicochemical properties of a new potential drug carrier containing cellobiose units and its complex with paracetamol.	O
21	Regulation of water access, storage, separation and release of drugs from the carbon nanotube functionalized by cytosine rich DNA fragments. 2022 , 212835	
20	Progress in Simulation Studies of Insulin Structure and Function. 13,	2
19	Energy landscapes in inorganic chemistry. 2022 ,	0
18	Modeling Metal Ions in Enzyme Catalysis. 2022 ,	O
17	Evaluating the performance of ReaxFF potentials for sp2 carbon systems (graphene, carbon nanotubes, fullerenes) and a new ReaxFF potential. 10,	0
16	Computational Studies on Selected Macrolides Active against Escherichia coli Combined with the NMR Study of Tylosin A in Deuterated Chloroform. 2022 , 27, 7280	O
15	Exploiting Sequence-Dependent Rotamer Information in Global Optimization of Proteins. 2022 , 126, 8381-8390	O
14	RNA as a Major-Groove Ligand: RNAâRNA and RNAâDNA Triplexes Formed by GAA and UUC or TTC Sequences. 2022 , 7, 38728-38743	O

13	Mechanisms of acid-sensing ion channels inhibition by nafamostat, sepimostat and diminazene. 2022 , 175394	1
12	Molecular Modeling of Cardiac Sodium Channel with Mexiletine. 2022 , 12, 1252	О
11	Shape Theory Applied to Molecular Docking and Automatic Localization of Ligand Binding Pockets in Large Proteins. 2022 , 7, 45991-46002	1
10	The development of nucleic acids force fields: From an unchallenged past to a competitive future. 2022 ,	O
9	The MHC Class I-Restricted Immune Response to HIV-gag in BALB/c Mice Selects a Single Epitope That Does Not Have a Predictable MHC-Binding Motif and Binds to Kd Through Interactions Between a Glutamine at P3 and Pocket D. 1998 , 161, 2985-2993	21
8	A Guide to In Silico Drug Design. 2023 , 15, 49	О
7	3D MODELS OF HORMONE RECEPTORS : EXPERIMENTAL VALIDATION. 1995 , 30, 189s-199s	1
6	Analysis of residueâlesidue interactions in the structures of ASIC1a suggests possible gating mechanisms.	О
5	The inorganic chemistry of the cobalt corrinoids âlan update. 2023 , 242, 112154	О
4	The Ku complex promotes DNA end-bridging and this function is antagonized by Tel1/ATM kinase. 2023 , 51, 1783-1802	0
3	Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. 1-39	О
2	Are computational approaches critically important for solving real-world problems?. 2023, 567-583	0
1	Extremely Tough, Stretchable Gel Electrolytes with Strong Interpolymer Hydrogen Bonding Prepared Using Concentrated Electrolytes to Stabilize Lithium-Metal Anodes.	0