Federico Gago

List of Publications by Year
in descending order

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231 papers	6,344 citations	61857 43 h-index	106150 65 g-index
243 all docs	243 docs citations	243 times ranked	7186 citing authors

#	Article	IF	Citations
1	Prediction of Drug Binding Affinities by Comparative Binding Energy Analysis. Journal of Medicinal Chemistry, 1995, 38, 2681-2691.	2.9	267
2	Molecular Determinants of Topoisomerase I Poisoning by Lamellarins:Â Comparison with Camptothecin and Structureâ˜'Activity Relationships. Journal of Medicinal Chemistry, 2005, 48, 3796-3807.	2.9	207
3	Cross-Talk between Nucleotide Excision and Homologous Recombination DNA Repair Pathways in the Mechanism of Action of Antitumor Trabectedin. Cancer Research, 2006, 66, 8155-8162.	0.4	168
4	The dual role of thymidine phosphorylase in cancer development and chemotherapy. Medicinal Research Reviews, 2009, 29, 903-953.	5.0	166
5	Comparative Binding Energy Analysis of HIV-1 Protease Inhibitors:Â Incorporation of Solvent Effects and Validation as a Powerful Tool in Receptor-Based Drug Design. Journal of Medicinal Chemistry, 1998, 41, 836-852.	2.9	137
6	PM01183, a new DNA minor groove covalent binder with potent in vitro and in vivo antiâ€tumour activity. British Journal of Pharmacology, 2010, 161, 1099-1110.	2.7	120
7	Guanidinium Receptors as Enantioselective Amino Acid Membrane Carriers. Journal of the American Chemical Society, 2003, 125, 8270-8284.	6.6	113
8	ET-18-OCH3 (Edelfosine): A Selective Antitumour Lipid Targeting Apoptosis Through Intracellular Activation of Fas / CD95 Death Receptor. Current Medicinal Chemistry, 2004, 11, 3163-3184.	1.2	113
9	Stacking Interactions and Intercalative DNA Binding. Methods, 1998, 14, 277-292.	1.9	100
10	Mutational Pathways, Resistance Profile, and Side Effects of Cyanovirin Relative to Human Immunodeficiency Virus Type 1 Strains with N-Glycan Deletions in Their gp120 Envelopes. Journal of Virology, 2006, 80, 8411-8421.	1.5	93
11	Regulation of cyclooxygenase activity by metamizol. European Journal of Pharmacology, 1999, 378, 339-347.	1.7	83
12	Synthesis and DNA Binding Properties of Î³-Carbolinium Derivatives and Benzologues. Journal of Organic Chemistry, 1996, 61, 5587-5599.	1.7	82
13	Ab InitioStudy of Stacking Interactions in A- and B-DNA. Journal of Physical Chemistry B, 1997, 101, 3846-3853.	1.2	82
14	Translation Elongation Factor eEF1A2 is a Novel Anticancer Target for the Marine Natural Product Plitidepsin. Scientific Reports, 2016, 6, 35100.	1.6	71
15	Molecular pharmacology and antitumor activity of ZalypsisÂ® in several human cancer cell lines. Biochemical Pharmacology, 2009, 78, 162-170.	2.0	69
16	Quantitative Analysis of Substrate Specificity of Haloalkane Dehalogenase LinB fromSphingomonas paucimobilisUT26â€. Biochemistry, 2005, 44, 3390-3401.	1.2	68
17	Optimization of Taxane Binding to Microtubules: Binding Affinity Dissection and Incremental Construction of a High-Affinity Analog of Paclitaxel. Chemistry and Biology, 2008, 15, 573-585.	6.2	68
18	Three-Dimensional Structure of Ï‰-Conotoxin GVIA Determined by 1H-NMR. Biochemical and Biophysical Research Communications, 1993, 192, 1238-1244.	1.0	67

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19	Identification of a Putative Binding Site for [2â€˜,5â€˜-Bis-O-(tert-butyldimethylsilyl)-Î²-d-ribofuranosyl]-3â€˜-spiro-5â€˜â€‰â€˜-(4â€˜â€‰â€˜-amino-1â€˜â€‰â€˜,2â€˜â€‰â€˜-o (TSAO) Derivatives at the p51â^'p66 Interface of HIV-1 Reverse Transcriptase. Journal of Medicinal Chemistry, 2001, 44, 1853-1865.	2.9	67
20	MM-ISMSA: An Ultrafast and Accurate Scoring Function for Proteinâ€“Protein Docking. Journal of Chemical Theory and Computation, 2012, 8, 3395-3408.	2.3	65
21	Involvement of Novel Human Immunodeficiency Virus Type 1 Reverse Transcriptase Mutations in the Regulation of Resistance to Nucleoside Inhibitors. Journal of Virology, 2006, 80, 7186-7198.	1.5	64
22	A Designed Non-Peptidic Receptor that Mimics the Phosphocholine Binding Site of the McPC603 Antibody. Angewandte Chemie International Edition in English, 1996, 35, 1712-1715.	4.4	62
23	Reliability of Comparative Molecular Field Analysis Models:â€‰ Effects of Data Scaling and Variable Selection Using a Set of Human Synovial Fluid Phospholipase A2 Inhibitors. Journal of Medicinal Chemistry, 1997, 40, 1136-1148.	2.9	62
24	Azino-Fused Benzimidazolium Salts as DNA Intercalating Agents. 2.. Journal of Organic Chemistry, 1997, 62, 5476-5483.	1.7	61
25	Rational modification of human synovial fluid phospholipase A2 inhibitors. Journal of Medicinal Chemistry, 1994, 37, 337-341.	2.9	60
26	3D-QSAR methods on the basis of ligand-receptor complexes. Application of COMBINE and GRID/GOLPE methodologies to a series of CYP1A2 ligands. Journal of Computer-Aided Molecular Design, 2000, 14, 341-353.	1.3	59
27	Dimerization inhibitors of HIV-1 reverse transcriptase, protease and integrase: A single mode of inhibition for the three HIV enzymes?. Antiviral Research, 2006, 71, 260-267.	1.9	58
28	Antitumor Activity, X-ray Crystal Structure, and DNA Binding Properties of Thiocoraline A, a Natural Bisintercalating Thiodepsipeptide. Journal of Medicinal Chemistry, 2007, 50, 3322-3333.	2.9	58
29	Synthesis, Activity, and Molecular Modeling Studies of Novel Human Aldose Reductase Inhibitors Based on a Marine Natural Product. Journal of Medicinal Chemistry, 2003, 46, 5208-5221.	2.9	56
30	Temperature-induced melting of double-stranded DNA in the absence and presence of covalently bonded antitumour drugs: insight from molecular dynamics simulations. Nucleic Acids Research, 2011, 39, 8248-8257.	6.5	55
31	Development of a New Family of Conformationally Restricted Peptides as Potent Nucleators of Î²-Turns. Design, Synthesis, Structure, and Biological Evaluation of a Î²-Lactam Peptide Analogue of Melanostatin. Journal of the American Chemical Society, 2003, 125, 16243-16260.	6.6	54
32	Identification of the minimal conserved structure of HIV-1 protease in the presence and absence of drug pressure. Aids, 2004, 18, 11-19.	1.0	52
33	HIV Protease Inhibition: Limited Recent Progress and Advances in Understanding Current Pitfalls. Current Topics in Medicinal Chemistry, 2004, 4, 991-1007.	1.0	51
34	The Molecular Basis of Resilience to the Effect of the Lys103Asn Mutation in Non-Nucleoside HIV-1 Reverse Transcriptase Inhibitors Studied by Targeted Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 7570-7578.	6.6	51
35	Recognition and Activation of the Plant AKT1 Potassium Channel by the Kinase CIPK23. Plant Physiology, 2020, 182, 2143-2153.	2.3	51
36	Benzo[f]azino[2,1-a]phthalazinium Cations:Â Novel DNA Intercalating Chromophores with Antiproliferative Activity. Journal of Medicinal Chemistry, 2004, 47, 1136-1148.	2.9	50

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37	High Sequence Conservation of Human Immunodeficiency Virus Type 1 Reverse Transcriptase under Drug Pressure despite the Continuous Appearance of Mutations. Journal of Virology, 2005, 79, 10718-10729.	1.5	50
38	TSAO Compounds: The Comprehensive Story of a Unique Family of HIV- 1 Specific Inhibitors of Reverse Transcriptase. Current Topics in Medicinal Chemistry, 2004, 4, 945-963.	1.0	49
39	Leishmania infantum expresses a mitochondrial nuclease homologous to EndoG that migrates to the nucleus in response to an apoptotic stimulus. Molecular and Biochemical Parasitology, 2009, 163, 28-38.	0.5	49
40	Identification of Aldo-Keto Reductase AKR1B10 as a Selective Target for Modification and Inhibition by Prostaglandin A1: Implications for Antitumoral Activity. Cancer Research, 2011, 71, 4161-4171.	0.4	49
41	Structure-affinity relationships for the binding of actinomycin D to DNA. Journal of Computer-Aided Molecular Design, 1997, 11, 114-128.	1.3	47
42	Correlation of octanol/water partition coefficients with hydrophobicity measurements obtained by micellar chromatography. Analytical Chemistry, 1987, 59, 921-923.	3.2	46
43	XPF-Dependent DNA Breaks and RNA Polymerase II Arrest Induced by Antitumor DNA Interstrand Crosslinking-Mimetic Alkaloids. Chemistry and Biology, 2011, 18, 988-999.	6.2	46
44	The binding of benzenesulfonamides to carbonic anhydrase enzyme. A molecular mechanics study and quantitative structure-activity relationships. Journal of Medicinal Chemistry, 1989, 32, 951-956.	2.9	45
45	Molecular model of the interaction of bee venom phospholipase A2 with manoalide. Journal of Medicinal Chemistry, 1993, 36, 1866-1879.	2.9	44
46	Relevance of the Fanconi anemia pathway in the response of human cells to trabectedin. Molecular Cancer Therapeutics, 2008, 7, 1309-1318.	1.9	43
47	Comparative Binding Energy Analysis of the Substrate Specificity of Haloalkane Dehalogenase from Xanthobacter autotrophicus GJ10. Biochemistry, 2001, 40, 8905-8917.	1.2	42
48	High-affinity ligands of the colchicine domain in tubulin based on a structure-guided design. Scientific Reports, 2018, 8, 4242.	1.6	42
49	Advances in the Chemistry and Pharmacology of Ecteinascidins, A Promising New Class of Anticancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2001, 1, 257-276.	7.0	40
50	A Series of Enthalpically Optimized Docetaxel Analogues Exhibiting Enhanced Antitumor Activity and Water Solubility. Journal of Natural Products, 2018, 81, 524-533.	1.5	39
51	Assessment of Solvation Effects on Calculated Binding Affinity Differences:Â Trypsin Inhibition by Flavonoids as a Model System for Congeneric Series.. Journal of Medicinal Chemistry, 1997, 40, 4136-4145.	2.9	38
52	Bending of DNA upon Binding of Ecteinascidin 743 and Phthalascidin 650 Studied by Unrestrained Molecular Dynamics Simulations. Journal of the American Chemical Society, 2000, 122, 7172-7182.	6.6	38
53	Increased DNA Binding Specificity for Antitumor Ecteinascidin 743 through Proteinâ^'DNA Interactions?. Journal of Medicinal Chemistry, 2000, 43, 4367-4369.	2.9	38
54	Structural Basis for the Binding of Didemnins to Human Elongation Factor eEF1A and Rationale for the Potent Antitumor Activity of These Marine Natural Products. Journal of Medicinal Chemistry, 2004, 47, 4439-4452.	2.9	38

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55	Molecular dynamics simulations of the conformational changes of the glutamate receptor ligand-binding core in the presence of glutamate and kainate. Proteins: Structure, Function and Bioinformatics, 2001, 44, 460-469.	1.5	37
56	Assessment by Molecular Dynamics Simulations of the Structural Determinants of DNA-binding Specificity for Transcription Factor Sp1. Journal of Molecular Biology, 2003, 328, 9-32.	2.0	37
57	Overcoming the Inadequacies or Limitations of Experimental Structures as Drug Targets by Using Computational Modeling Tools and Molecular Dynamics Simulations. ChemMedChem, 2007, 2, 1388-1401.	1.6	36
58	Investigation of the complexation between cyclodextrins and medetomidine enantiomers by capillary electrophoresis, NMR spectroscopy and molecular modeling. Journal of Chromatography A, 2018, 1567, 198-210.	1.8	36
59	Implications of a consensus recognition site for phosphatidylcholine separate from the active site in cobra venom phospholipases A2. Biochemistry, 1992, 31, 2887-2896.	1.2	35
60	Stepwise dissection and visualization of the catalytic mechanism of haloalkane dehalogenase LinB using molecular dynamics simulations and computer graphics. Journal of Molecular Graphics and Modelling, 2007, 26, 643-651.	1.3	35
61	Hiv-1 Specific Reverse Transcriptase Inhibitors: why are Tsao-Nucleosides so Unique?. Journal of Carbohydrate Chemistry, 2000, 19, 451-469.	0.4	34
62	Role of Histidine-85 in the Catalytic Mechanism of Thymidine Phosphorylase As Assessed by Targeted Molecular Dynamics Simulations and Quantum Mechanical Calculations. Biochemistry, 2004, 43, 405-414.	1.2	34
63	Role of stacking interactions in the binding sequence preferences of DNA bis-intercalators: insight from thermodynamic integration free energy simulations. Nucleic Acids Research, 2005, 33, 6214-6224.	6.5	34
64	Tubulin-based Structure-affinity Relationships for Antimitotic Vinca Alkaloids. Anti-Cancer Agents in Medicinal Chemistry, 2012, 12, 219-225.	0.9	34
65	DNA Sequence-Specific Reading by Echinomycin: Role of Hydrogen Bonding and Stacking Interactions. Journal of Medicinal Chemistry, 1994, 37, 1602-1609.	2.9	33
66	Novel DNA Intercalators Based on the Pyridazino[1â€˜,6â€˜:1,2]pyrido[4,3-b]indol-5-inium System. Journal of Organic Chemistry, 1999, 64, 3907-3915.	1.7	33
67	Exploring Acyclic Nucleoside Analogues as Inhibitors of Mycobacterium tuberculosis Thymidylate Kinase. ChemMedChem, 2008, 3, 1083-1093.	1.6	33
68	3â€²-[4-Aryl-(1,2,3-triazol-1-yl)]-3â€²-deoxythymidine Analogues as Potent and Selective Inhibitors of Human Mitochondrial Thymidine Kinase. Journal of Medicinal Chemistry, 2010, 53, 2902-2912.	2.9	33
69	A molecular dynamics study of the bis-intercalation complexes of echinomycin with d(ACGT)2 and d(TCGA)2: rationale for sequence-specific Hoogsteen base pairing. Journal of Medicinal Chemistry, 1993, 36, 1548-1561.	2.9	32
70	Modular Architecture and Unique Teichoic Acid Recognition Features of Choline-Binding Protein L (CbpL) Contributing to Pneumococcal Pathogenesis. Scientific Reports, 2016, 6, 38094.	1.6	32
71	Molecular model of the interaction between nimesulide and human cyclooxygenase-2. British Journal of Rheumatology, 1999, 38, 14-18.	2.5	30
72	A 3Â·(ET743)-DNA Complex That Both Resembles an RNA-DNA Hybrid and Mimicks Zinc Finger-Induced DNA Structural Distortions. Journal of Medicinal Chemistry, 2002, 45, 871-880.	2.9	30

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73	Molecular Recognition of Epothilones by Microtubules and Tubulin Dimers Revealed by Biochemical and NMR Approaches. ACS Chemical Biology, 2014, 9, 1033-1043.	1.6	30
74	Further Insight into the DNA Recognition Mechanism of Trabectedin from the Differential Affinity of Its Demethylated Analogue Ecteinascidin ET729 for the Triplet DNA Binding Site CGA. Journal of Medicinal Chemistry, 2006, 49, 6925-6929.	2.9	29
75	First example of peptides targeting the dimer interface of Leishmania infantum trypanothione reductase with potent inÂvitro antileishmanial activity #. European Journal of Medicinal Chemistry, 2017, 135, 49-59.	2.6	29
76	Azinium-N-(2â€²-azinyl)aminides: synthesis, structure and reactivity. Tetrahedron, 1994, 50, 4995-5012.	1.0	28
77	Binding of 5â€˜-GMP to the GluR2 AMPA Receptor:Â Insight from Targeted Molecular Dynamics Simulationsâ€. Biochemistry, 2005, 44, 14470-14476.	1.2	28
78	Structural rationale for the chiral separation and migration order reversal of clenpenterol enantiomers in capillary electrophoresis using two different Î²-cyclodextrins. Physical Chemistry Chemical Physics, 2017, 19, 27935-27939.	1.3	28
79	Enzymatic Synthesis of Therapeutic Nucleosides using a Highly Versatile Purine Nucleoside 2â€™â€Deoxyribosyltransferase from Trypanosoma brucei. ChemCatChem, 2018, 10, 4406-4416.	1.8	28
80	Understanding the Basis of Resistance in the Irksome Lys103Asn HIV-1 Reverse Transcriptase Mutant through Targeted Molecular Dynamics Simulations. Journal of the American Chemical Society, 2004, 126, 15386-15387.	6.6	27
81	Improving the Antiviral Efficacy and Selectivity of HIV-1 Reverse Transcriptase Inhibitor TSAO-T by the Introduction of Functional Groups at the N-3 Position. Journal of Medicinal Chemistry, 2005, 48, 6653-6660.	2.9	26
82	Viral engagement with host receptors blocked by a novel class of tryptophan dendrimers that targets the 5-fold-axis of the enterovirus-A71 capsid. PLoS Pathogens, 2019, 15, e1007760.	2.1	26
83	Pyrrolopyrimidine vs Imidazole-Phenyl-Thiazole Scaffolds in Nonpeptidic Dimerization Inhibitors of Leishmania infantum Trypanothione Reductase. ACS Infectious Diseases, 2019, 5, 873-891.	1.8	26
84	Automated docking and molecular dynamics simulations of nimesulide in the cyclooxygenase active site of human prostaglandin-endoperoxide synthase-2 (COX-2). Journal of Computer-Aided Molecular Design, 2000, 14, 147-160.	1.3	25
85	Synthesis of 3â€˜Ââ€˜-Substituted TSAO Derivatives with Anti-HIV-1 and Anti-HIV-2 Activity through an Efficient Palladium-Catalyzed Cross-Coupling Approach. Journal of Medicinal Chemistry, 2002, 45, 3934-3945.	2.9	25
86	Abasic Analogues of TSAO-T as the First Sugar Derivatives That Specifically Inhibit HIV-1 Reverse Transcriptase. Journal of Medicinal Chemistry, 1998, 41, 4636-4647.	2.9	24
87	The Amino Acid Asn136 in HIV-1 Reverse Transcriptase (RT) Maintains Efficient Association of Both RT Subunits and Enables the Rational Design of Novel RT Inhibitors. Molecular Pharmacology, 2005, 68, 49-60.	1.0	24
88	Binding of eEF1A2 to the RNA-dependent protein kinase PKR modulates its activity and promotes tumour cell survival. British Journal of Cancer, 2018, 119, 1410-1420.	2.9	24
89	The N137 and P140 amino acids in the p51 and the P95 amino acid in the p66 subunit of human immunodeficiency virus type 1 (HIV-1) reverse transcriptase are instrumental to maintain catalytic activity and to design new classes of anti-HIV-1 drugs. FEBS Letters, 2005, 579, 2294-2300.	1.3	23
90	Structure, physiological role, and specific inhibitors of human thymidine kinase 2 (TK2): Present and future. Medicinal Research Reviews, 2008, 28, 797-820.	5.0	23

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91	Antiviral Agents: Structural Basis of Action and Rational Design. Sub-Cellular Biochemistry, 2013, 68, 599-630.	1.0	23
92	Probing the Dimerization Interface of Leishmania infantum Trypanothione Reductase with Siteâ€Directed Mutagenesis and Short Peptides. ChemBioChem, 2013, 14, 1212-1217.	1.3	23
93	Esterase LpEst1 from Lactobacillus plantarum: A Novel and Atypical Member of the Î±Î² Hydrolase Superfamily of Enzymes. PLoS ONE, 2014, 9, e92257.	1.1	23
94	Chemometrical Identification of Mutations in HIV-1 Reverse Transcriptase Conferring Resistance or Enhanced Sensitivity to Arylsulfonylbenzonitriles. Journal of the American Chemical Society, 2004, 126, 2718-2719.	6.6	22
95	Phosphorylation modulates the alpha-helical structure and polymerization of a peptide from the third tau microtubule-binding repeat. Biochimica Et Biophysica Acta - General Subjects, 2005, 1721, 16-26.	1.1	22
96	The Protein Kinase Inhibitor Balanol: Structure â€“ Activity Relationships and Structure-Based Computational Studies. Anti-Cancer Agents in Medicinal Chemistry, 2008, 8, 638-645.	0.9	22
97	Understanding the Key Factors that Control the Inhibition of Typeâ€…II Dehydroquinase by (2R)â€2â€Benzylâ€3â€dehydroquinic Acids. ChemMedChem, 2010, 5, 1726-1733.	1.6	22
98	A structure-based design of new C2- and C13-substituted taxanes: tubulin binding affinities and extended quantitative structureâ€“activity relationships using comparative binding energy (COMBINE) analysis. Organic and Biomolecular Chemistry, 2013, 11, 3046.	1.5	22
99	Structural Determinants of the Dictyostatin Chemotype for Tubulin Binding Affinity and Antitumor Activity Against Taxane- and Epothilone-Resistant Cancer Cells. ACS Omega, 2016, 1, 1192-1204.	1.6	22
100	Generation of endoplasmic reticulum stress and inhibition of autophagy by plitidepsin induces proteotoxic apoptosis in cancer cells. Biochemical Pharmacology, 2020, 172, 113744.	2.0	22
101	Structural rationale for the cross-resistance of tumor cells bearing the A399V variant of elongation factor eEF1A1 to the structurally unrelated didemnin B, ternatin, nannocystin A and ansatrienin B. Journal of Computer-Aided Molecular Design, 2017, 31, 915-928.	1.3	22
102	Exploring the role of the 5â€²-position of TSAO-T. Synthesis and anti-HIV evaluation of novel TSAO-T derivatives. Antiviral Research, 2001, 50, 207-222.	1.9	21
103	In silico activation of Src tyrosine kinase reveals the molecular basis for intramolecular autophosphorylation. Journal of Molecular Graphics and Modelling, 2004, 23, 189-198.	1.3	21
104	gCOMBINE: A graphical user interface to perform structureâ€based comparative binding energy (COMBINE) analysis on a set of ligandâ€receptor complexes. Proteins: Structure, Function and Bioinformatics, 2010, 78, 162-172.	1.5	21
105	Characterization of pyrimidine nucleoside phosphorylase of Mycoplasma hyorhinis: implications for the clinical efficacy of nucleoside analogues. Biochemical Journal, 2012, 445, 113-123.	1.7	21
106	Molecular Dynamics Simulations of the Bis-Intercalated Complexes of Ditercalinium and Flexi-Di with the Hexanucleotide d(GCGCGC)2:Â Theoretical Analysis of the Interaction and Rationale for the Sequence Binding Specificity. Journal of Medicinal Chemistry, 1996, 39, 4810-4824.	2.9	20
107	Simulation of alternative binding modes in a structure-based QSAR study of HIV-1 protease inhibitors. Journal of Molecular Graphics and Modelling, 1997, 15, 364-371.	1.3	20
108	Scaffold Simplification Strategy Leads to a Novel Generation of Dual Human Immunodeficiency Virus and Enterovirus-A71 Entry Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 349-368.	2.9	20

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109	Comparative binding energy analysis of haloalkane dehalogenase substrates: modelling of enzyme-substrate complexes by molecular docking and quantum mechanical calculations. Journal of Computer-Aided Molecular Design, 2003, 17, 299-311.	1.3	19
110	Modulation of Binding Strength in Several Classes of Active Site Inhibitors of Acetylcholinesterase Studied by Comparative Binding Energy Analysis. Journal of Medicinal Chemistry, 2004, 47, 4471-4482.	2.9	19
111	N1-Substituted Thymine Derivatives as Mitochondrial Thymidine Kinase (TK-2) Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 7766-7773.	2.9	18
112	VSDMIP 1.5: an automated structure- and ligand-based virtual screening platform with a PyMOL graphical user interface. Journal of Computer-Aided Molecular Design, 2011, 25, 813-824.	1.3	18
113	Binding of Echinomycin to d(GCGC)2and d(CCGG)2: Distinct Stacking Interactions Dictate the Sequence-Dependent Formation of Hoogsteen Base Pairs. Journal of Biomolecular Structure and Dynamics, 1994, 12, 111-129.	2.0	17
114	Mitochondrial Thymidine Kinase Inhibitors. Current Topics in Medicinal Chemistry, 2005, 5, 1205-1219.	1.0	17
115	Proteinâ€“protein interactions at an enzymeâ€“substrate interface: Characterization of transient reaction intermediates throughout a full catalytic cycle of Escherichia coli thioredoxin reductase. Proteins: Structure, Function and Bioinformatics, 2010, 78, 36-51.	1.5	17
116	Characterization of an atypical, thermostable, organic solvent- and acid-tolerant 2â€²-deoxyribosyltransferase from Chroococcidiopsis thermalis. Applied Microbiology and Biotechnology, 2018, 102, 6947-6957.	1.7	17
117	Comparative binding energy analysis. Journal of Computer - Aided Molecular Design, 1998, 9/11, 19-34.	1.0	16
118	Solution Structure and Stability of Tryptophan-Containing Nucleopeptide Duplexes. ChemBioChem, 2003, 4, 40-49.	1.3	16
119	Synthesis, modeling and evaluation of 3â€²-(1-aryl-1H-tetrazol-5-ylamino)-substituted 3â€²-deoxythymidine derivatives as potent and selective human mitochondrial thymidine kinase inhibitors. Organic and Biomolecular Chemistry, 2011, 9, 892-901.	1.5	16
120	Molecular Interactions and Implications of Aldose Reductase Inhibition by PGA₁ and Clinically Used Prostaglandins. Molecular Pharmacology, 2016, 89, 42-52.	1.0	16
121	Trypanothione reductase inhibition and anti-leishmanial activity of all-hydrocarbon stapled Î±-helical peptides with improved proteolytic stability. European Journal of Medicinal Chemistry, 2018, 149, 238-247.	2.6	16
122	Synthesis and Structural Characterization of Pyrimidine Bi- and Tricyclic Nucleosides with Sugar Puckers Conformationally Locked into the Eastern Region of the Pseudorotational Cycleâ€. Journal of Organic Chemistry, 2003, 68, 6695-6704.	1.7	15
123	The Role of Thr139 in the Human Immunodeficiency Virus Type 1 Reverse Transcriptase Sensitivity to (+)-Calanolide A. Molecular Pharmacology, 2005, 68, 652-659.	1.0	15
124	Recent Advances in Thymidine Kinase 2 (TK2) Inhibitors and New Perspectives for Potential Applications. Current Pharmaceutical Design, 2012, 18, 2981-2994.	0.9	15
125	CRDOCK: An Ultrafast Multipurpose Proteinâ€“Ligand Docking Tool. Journal of Chemical Information and Modeling, 2012, 52, 2300-2309.	2.5	15
126	Comparison of ultraâ€fast 2<scp>D</scp> and 3<scp>D</scp> ligand and target descriptors for side effect prediction and network analysis in polypharmacology. British Journal of Pharmacology, 2013, 170, 557-567.	2.7	15

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127	A Supramolecular Stabilizer of the 14â€3â€3Î¶/ERÎ± Proteinâ€Protein Interaction with a Synergistic Mode of Action. Angewandte Chemie - International Edition, 2020, 59, 5284-5287.	7.2	15
128	Hakin-1, a New Specific Small-Molecule Inhibitor for the E3 Ubiquitin-Ligase Hakai, Inhibits Carcinoma Growth and Progression. Cancers, 2020, 12, 1340.	1.7	15
129	Tuning melatonin receptor subtype selectivity in oxadiazolone-based analogues: Discovery of QR2 ligands and NRF2 activators with neurogenic properties. European Journal of Medicinal Chemistry, 2020, 190, 112090.	2.6	15
130	On the Need to Tell Apart Fraternal Twins eEF1A1 and eEF1A2, and Their Respective Outfits. International Journal of Molecular Sciences, 2021, 22, 6973.	1.8	15
131	Improving the selectivity of acyclic nucleoside analogues as inhibitors of human mitochondrial thymidine kinase: replacement of a triphenylmethoxy moiety with substituted amines and carboxamides. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 3027-3030.	1.0	14
132	DNA Structural Similarity in the 2:1 Complexes of the Antitumor Drugs Trabectedin (Yondelis) and Chromomycin A3 with an Oligonucleotide Sequence Containing Two Adjacent TGG Binding Sites on Opposing Strands. Molecular Pharmacology, 2005, 68, 1559-1567.	1.0	14
133	Identification of aspartic acid-203 in human thymidine phosphorylase as an important residue for both catalysis and non-competitive inhibition by the small molecule â€œcrystallization chaperoneâ€• 5â€²-O-tritylinosine (KIN59). Biochemical Pharmacology, 2009, 78, 231-240.	2.0	14
134	Efficient Dimerization Disruption of Leishmania infantum Trypanothione Reductase by Triazole-phenyl-thiazoles. Journal of Medicinal Chemistry, 2021, 64, 6137-6160.	2.9	14
135	Molecular modeling of the interaction of polyproline-based peptides with the Abl-SH3 domain: rational modification of the interaction. Protein Engineering, Design and Selection, 1994, 7, 1455-1462.	1.0	13
136	Rationale for the opposite stereochemistry of the major monoadducts and interstrand crosslinks formed by mitomycin C and its decarbamoylated analogue at CpG steps in DNA and the effect of cytosine modification on reactivity. Organic and Biomolecular Chemistry, 2012, 10, 1543.	1.5	13
137	Comparative Binding Energy (COMBINE) Analysis Supports a Proposal for the Binding Mode of Epothilones to Î²â€Tubulin. ChemMedChem, 2012, 7, 836-843.	1.6	13
138	ALFA: Automatic Ligand Flexibility Assignment. Journal of Chemical Information and Modeling, 2014, 54, 314-323.	2.5	13
139	Comparison of hydrocarbon-and lactam-bridged cyclic peptides as dimerization inhibitors of Leishmania infantum trypanothione reductase. RSC Advances, 2015, 5, 55784-55794.	1.7	13
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