Ingebrigt Sylte

List of Publications by Year in Descending Order

79 papers	1,491 citations	22 h-index	35 g-index
80 ext. papers	1,654 ext. citations	3.9 avg, IF	4.55 L-index

#	Paper	IF	Citations
79	Proposal of selective inhibitor for bacterial zinc metalloprotease: Molecular mechanics and ab initio molecular orbital calculations. *Journal of Molecular Graphics and Modelling*, **2022**, 110, 108047	2.8	1
78	Inhibition of bacterial and human zinc-metalloproteases by bisphosphonate- and catechol-containing compounds. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 819-830	5.6	2
77	Specific interactions between the alkaline protease of P. aeruginosa and its natural peptide inhibitor: ab initio molecular simulations.. *Journal of Molecular Modeling*, **2021**, 28, 10	2	
76	Molecular Interactions Stabilizing the Promatrix Metalloprotease-9□Serglycin Heteromer. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2
75	Exploring Conformational Dynamics of the Extracellular Domain of the GABA Receptor: A Path-Metadynamics Study. *Journal of Chemical Information and Modeling*, **2020**, 60, 2294-2303	6.1	3
74	Homology modeling to screen for potential binding of contaminants to thyroid hormone receptor and transthyretin in glaucous gull (Larus hyperboreus) and herring gull (Larus argentatus). *Computational Toxicology*, **2020**, 13, 100120	3.1	6
73	Protonation states of central amino acids in a zinc metalloprotease complexed with inhibitor: Molecular mechanics optimizations and ab initio molecular orbital calculations. *Biophysical Chemistry*, **2020**, 261, 106368	3.5	3
72	The GABA Receptor-Structure, Ligand Binding and Drug Development. *Molecules*, **2020**, 25,	4.8	22
71	Design of galardine analogs as putative psudolysin inhibitors based on fragment molecular orbital calculations. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3307-3317	3.6	1
70	In Silico Methods for the Discovery of Orthosteric GABA Receptor Compounds. *Molecules*, **2019**, 24,	4.8	6
69	Molecular modelling, synthesis, and biological evaluations of a 3,5-disubstituted isoxazole fatty acid analogue as a PPAR□selective agonist. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 4059-4068	3.4	4
68	In Vitro and in Silico Competitive Binding of Brominated Polyphenyl Ether Contaminants with Human and Gull Thyroid Hormone Transport Proteins. *Environmental Science & Technology*, **2018**, 52, 1533-1541	10.3	10
67	In Silico Site-Directed Mutagenesis Informs Species-Specific Predictions of Chemical Susceptibility Derived From the Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS) Tool. *Toxicological Sciences*, **2018**, 166, 131-145	4.4	12
66	The selectivity of galardin and an azasugar-based hydroxamate compound for human matrix metalloproteases and bacterial metalloproteases. *PLoS ONE*, **2018**, 13, e0200237	3.7	6
65	Synthesis, molecular modeling and biological evaluation of potent analogs of 2-methoxyestradiol. *Steroids*, **2018**, 136, 47-55	2.8	4
64	Regulation of liver X receptor target genes by 22-functionalized oxysterols. Synthesis, in silico and in vitro evaluations. *Steroids*, **2017**, 118, 119-127	2.8	7
63	From Homology Models to a Set of Predictive Binding Pockets-a 5-HT Receptor Case Study. *Journal of Chemical Information and Modeling*, **2017**, 57, 311-321	6.1	22

62	Serotonin transporter and receptor ligands with antidepressant activity as neuroprotective and proapoptotic agents. *Pharmacological Reports*, **2017**, 69, 469-478	3.9	16
61	Specific interactions between zinc metalloproteinase and its inhibitors: Ab initio fragment molecular orbital calculations. *Journal of Molecular Graphics and Modelling*, **2017**, 75, 277-286	2.8	5
60	Ligand-guided homology modelling of the GABAB2 subunit of the GABAB receptor. *PLoS ONE*, **2017**, 12, e0173889	3.7	16
59	Synthesis, in vitro and in vivo biological evaluation of new oxysterols as modulators of the liver X receptors. *Journal of Steroid Biochemistry and Molecular Biology*, **2017**, 165, 323-330	5.1	5
58	Synthesis, experimental evaluation and molecular modelling of hydroxamate derivatives as zinc metalloproteinase inhibitors. *European Journal of Medicinal Chemistry*, **2016**, 108, 141-153	6.8	12
57	Environmental Chemicals Modulate Polar Bear (Ursus maritimus) Peroxisome Proliferator-Activated Receptor Gamma (PPARG) and Adipogenesis in Vitro. *Environmental Science & Technology*, **2016**, 50, 10708-10720	10.3	33
56	The catalytic reaction mechanism of drosophilid alcohol dehydrogenases. *Perspectives in Science*, **2015**, 4, 46-54	0.8	5
55	Synthesis, biological evaluation and molecular modeling of new analogs of the anti-cancer agent 2-methoxyestradiol: potent inhibitors of angiogenesis. *RSC Advances*, **2015**, 5, 32497-32504	3.7	7
54	Inhibition of pseudolysin and thermolysin by hydroxamate-based MMP inhibitors. *European Journal of Medicinal Chemistry*, **2015**, 89, 340-8	6.8	14
53	Functional Selectivity and Antidepressant Activity of Serotonin 1A Receptor Ligands. *International Journal of Molecular Sciences*, **2015**, 16, 18474-506	6.3	60
52	High-level expression of pseudolysin, the extracellular elastase of Pseudomonas aeruginosa, in Escherichia coli and its purification. *Protein Expression and Purification*, **2015**, 113, 79-84	2	6
51	Synthesis, biological evaluation and molecular modeling studies of the PPAR□ antagonist CC618. *European Journal of Medicinal Chemistry*, **2015**, 94, 229-36	6.8	8
50	Ligand-directed trafficking of receptor stimulus. *Pharmacological Reports*, **2014**, 66, 1011-21	3.9	5
49	PAC-1 and isatin derivatives are weak matrix metalloproteinase inhibitors. *Biochimica Et Biophysica Acta - General Subjects*, **2014**, 1840, 3162-9	4	12
48	Identification of novel serotonin transporter compounds by virtual screening. *Journal of Chemical Information and Modeling*, **2014**, 54, 933-43	6.1	27
47	Development of new LXR modulators that regulate LXR target genes and reduce lipogenesis in human cell models. *European Journal of Medicinal Chemistry*, **2014**, 74, 258-63	6.8	4
46	Comparative molecular dynamic simulations of wild type and Thr114Val mutated Scaptodrosophila lebanonensis alcohol dehydrogenase. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 465-76	3.6	1
45	Studies of synthetic chalcone derivatives as potential inhibitors of secretory phospholipase A2, cyclooxygenases, lipoxygenase and pro-inflammatory cytokines. *Drug Design, Development and Therapy*, **2014**, 8, 1405-18	4.4	32

44	Comparative molecular dynamics simulations of mitogen-activated protein kinase-activated protein kinase 5. *International Journal of Molecular Sciences*, **2014**, 15, 4878-902	6.3	5
43	Synthesis and initial biological evaluation of new mimics of the LXR-modulator 22(S)-hydroxycholesterol. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 643-50	3.4	5
42	Homology modeling and ligand docking of Mitogen-activated protein kinase-activated protein kinase 5 (MK5). *Theoretical Biology and Medical Modelling*, **2013**, 10, 56	2.3	12
41	Synthesis, antidepressant evaluation and docking studies of long-chain alkylnitroquipazines as serotonin transporter inhibitors. *Chemical Biology and Drug Design*, **2013**, 81, 695-706	2.9	7
40	A linear combination of pharmacophore hypotheses as a new tool in search of new active compounds--an application for 5-HT1A receptor ligands. *PLoS ONE*, **2013**, 8, e84510	3.7	29
39	Large-scale expression and purification of active pseudolysin in Escherichia coli. *FASEB Journal*, **2013**, 27, 984.4	0.9	1
38	Molecular mechanism of serotonin transporter inhibition elucidated by a new flexible docking protocol. *European Journal of Medicinal Chemistry*, **2012**, 47, 24-37	6.8	20
37	Synthesis, in vitro binding studies and docking of long-chain arylpiperazine nitroquipazine analogues, as potential serotonin transporter inhibitors. *European Journal of Medicinal Chemistry*, **2012**, 49, 200-10	6.8	4
36	An intact eight-membered water chain in drosophilid alcohol dehydrogenases is essential for optimal enzyme activity. *FEBS Journal*, **2012**, 279, 2940-56	5.7	8
35	Specific interactions and binding energies between thermolysin and potent inhibitors: molecular simulations based on ab initio molecular orbital method. *Journal of Molecular Graphics and Modelling*, **2012**, 33, 1-11	2.8	8
34	Substrate binding and translocation of the serotonin transporter studied by docking and molecular dynamics simulations. *Journal of Molecular Modeling*, **2012**, 18, 1073-85	2	25
33	The liver X receptor modulator 22(S)-hydroxycholesterol exerts cell-type specific effects on lipid and glucose metabolism. *Journal of Steroid Biochemistry and Molecular Biology*, **2012**, 128, 154-64	5.1	25
32	Dipeptide Inhibitors of Thermolysin and Angiotensin I-Converting Enzyme. *Current Topics in Medicinal Chemistry*, **2012**, 12, 1748-1762	3	6
31	Regulation of matrix metalloproteinase activity in health and disease. *FEBS Journal*, **2011**, 278, 28-45	5.7	262
30	Protein binding site analysis by means of structural interaction fingerprint patterns. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 6816-9	2.9	31
29	Specific interactions and binding free energies between thermolysin and dipeptides: molecular simulations combined with ab initio molecular orbital and classical vibrational analysis. *Journal of Computational Chemistry*, **2011**, 32, 3047-57	3.5	11
28	Identification of novel quinazolin-4(3H)-ones as inhibitors of thermolysin, the prototype of the M4 family of proteinases. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 4317-27	3.4	21
27	The development and validation of a novel virtual screening cascade protocol to identify potential serotonin 5-HT(7)R antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 2465-8	2.9	26

26	Structure and localisation of drug binding sites on neurotransmitter transporters. *Journal of Molecular Modeling*, **2009**, 15, 1155-64	2	27
25	Molecular recognition of long chain fatty acids by peroxisome proliferator-activated receptor *Medicinal Chemistry Research*, **2009**, 18, 8-19	2.2	4
24	The thermolysin family (M4) of enzymes: therapeutic and biotechnological potential. *Chemical Biology and Drug Design*, **2009**, 73, 7-16	2.9	103
23	A combined simulation with ab initio MO and classical vibrational analysis on the specific interactions between thermolysin and dipeptide ligands. *Chemical Physics Letters*, **2009**, 479, 290-295	2.5	10
22	Discovery of potent thermolysin inhibitors using structure based virtual screening and binding assays. *Journal of Medicinal Chemistry*, **2009**, 52, 48-61	8.3	26
21	Determinants for Psychrophilic and Thermophilic Features of Metallopeptidases of the M4 Family. *In Silico Biology*, **2009**, 9, 105-124	2	10
20	Multivariate Linear Regression Models Based on ADME Descriptors and Predictions of ADMET Profile for Structurally Diverse Thermolysin Inhibitors. *Letters in Drug Design and Discovery*, **2009**, 6, 428-436	0.8	3
19	Theoretical calculations of the catalytic triad in short-chain alcohol dehydrogenases/reductases. *Biophysical Journal*, **2008**, 94, 1412-27	2.9	19
18	Membrane Transporters: Structure, Function and Targets for Drug Design. *Topics in Medicinal Chemistry*, **2008**, 15-51	0.4	5
17	Molecular model of the outward facing state of the human P-glycoprotein (ABCB1), and comparison to a model of the human MRP5 (ABCC5). *Theoretical Biology and Medical Modelling*, **2007**, 4, 33	2.3	39
16	Molecular insight into pseudolysin inhibition using the MM-PBSA and LIE methods. *Journal of Structural Biology*, **2006**, 153, 129-44	3.4	18
15	A homology model of SERT based on the LeuT(Aa) template. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 5594-7	2.9	25
14	Putative drug binding conformations of monoamine transporters. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 666-75	3.4	34
13	Conformational restrictions in ligand binding to the human intestinal di-/tripeptide transporter: implications for design of hPEPT1 targeted prodrugs. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 1977-88	3.4	7
12	The protein-protein interactions between SMPI and thermolysin studied by molecular dynamics and MM/PBSA calculations. *Journal of Biomolecular Structure and Dynamics*, **2005**, 22, 521-31	3.6	11
11	Structures and models of transporter proteins. *Journal of Pharmacology and Experimental Therapeutics*, **2004**, 309, 853-60	4.7	62
10	Molecular mechanism of citalopram and cocaine interactions with neurotransmitter transporters. *Journal of Pharmacology and Experimental Therapeutics*, **2003**, 307, 34-41	4.7	52
9	Molecular model of the neural dopamine transporter. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 367-82	4.2	30

8	Molecular dynamics of 5-HT1A and 5-HT2A serotonin receptors with methylated buspirone analogues. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 1005-23	4.2	10
7	Comparative molecular dynamics of mesophilic and psychrophilic protein homologues studied by 1.2 ns simulations. *Journal of Biomolecular Structure and Dynamics*, **1999**, 17, 493-506	3.6	31
6	The catalytic triad in Drosophila alcohol dehydrogenase: pH, temperature and molecular modelling studies. *Journal of Molecular Biology*, **1999**, 294, 601-16	6.5	30
5	A Three Dimensional Model of Human Thiopurine Methyltransferase; Ligand Interactions and Structural Consequences of Naturally Occurring Mutations. *Journal of Molecular Modeling*, **1998**, 4, 211-220	2	5
4	Molecular Modeling of the NPY Binding Site on the Y1 Receptor. *Journal of Molecular Modeling*, **1998**, 4, 221-233	2	5
3	Mapping the suramin-binding sites of human neutrophil elastase: investigation by fluorescence resonance energy transfer and molecular modeling. *Biochemistry*, **1997**, 36, 15624-31	3.2	12
2	Molecular structure and dynamics of cis(Z)-and trans(E)-flupenthixol and clopenthixol. *Pharmaceutical Research*, **1991**, 8, 462-70	4.5	8
1	Stereochemical activity of lone pairs. The crystal and molecular structure of a complex of 18-crown-6 (1,4,7,10,13,16-hexaoxacyclooctadecane) with bismuth(III) chloride. *Inorganica Chimica Acta*, **1990**, 171, 11-15	2.7	20