Bjorn C G Karlsson

List of Publications by Year
in descending order

#	Article	IF	Citations
1	Theoretical and computational strategies for rational molecularly imprinted polymer design. Biosensors and Bioelectronics, 2009, 25, 543-552.	10.1	156
2	Structure and Dynamics of Monomerâ^'Template Complexation: An Explanation for Molecularly Imprinted Polymer Recognition Site Heterogeneity. Journal of the American Chemical Society, 2009, 131, 13297-13304.	13.7	112
3	Rational design of biomimetic molecularly imprinted materials: theoretical and computational strategies for guiding nanoscale structured polymer development. Analytical and Bioanalytical Chemistry, 2011, 400, 1771-1786.	3.7	77
4	Correlated theoretical, spectroscopic and X-ray crystallographic studies of a non-covalent molecularly imprinted polymerisation system. Analyst, The, 2007, 132, 1161.	3.5	63
5	The roles of template complexation and ligand binding conditions on recognition in bupivacaine molecularly imprinted polymers. Analyst, The, 2004, 129, 456.	3.5	55
6	The Spectrophysics of Warfarin: Implications for Protein Binding. Journal of Physical Chemistry B, 2007, 111, 10520-10528.	2.6	51
7	Influence of Composition and Morphology on Template Recognition in Molecularly Imprinted Polymers. Macromolecules, 2013, 46, 1408-1414.	4.8	49
8	Computational Strategies for the Design and Study of Molecularly Imprinted Materials. Industrial & Engineering Chemistry Research, 2013, 52, 13900-13909.	3.7	43
9	On the Influence of Crosslinker on Template Complexation in Molecularly Imprinted Polymers: A Computational Study of Prepolymerization Mixture Events with Correlations to Template-Polymer Recognition Behavior and NMR Spectroscopic Studies. International Journal of Molecular Sciences, 2014, 15, 10622-10634.	4.1	40
10	Mechanisms underlying molecularly imprinted polymer molecular memory and the role of crosslinker: resolving debate on the nature of template recognition in phenylalanine anilide imprinted polymers. Journal of Molecular Recognition, 2012, 25, 69-73.	2.1	38
11	Towards Global QSAR Model Building for Acute Toxicity: Munro Database Case Study. International Journal of Molecular Sciences, 2014, 15, 18162-18174.	4.1	36
12	Dilution of whisky â€" the molecular perspective. Scientific Reports, 2017, 7, 6489.	3.3	34
13	Consequences of Morphology on Molecularly Imprinted Polymer-Ligand Recognition. International Journal of Molecular Sciences, 2013, 14, 1207-1217.	4.1	27
14	Theoretical Studies of 17-Î²-Estradiol-Imprinted Prepolymerization Mixtures: Insights Concerning the Roles of Cross-Linking and Functional Monomers in Template Complexation and Polymerization. Industrial & Engineering Chemistry Research, 2013, 52, 13965-13970.	3.7	26
15	Synthetic Human Serum Albumin Sudlow I Binding Site Mimics. Journal of Medicinal Chemistry, 2010, 53, 7932-7937.	6.4	25
16	A Functional Monomer Is Not Enough: Principal Component Analysis of the Influence of Template Complexation in Pre-Polymerization Mixtures on Imprinted Polymer Recognition and Morphology. International Journal of Molecular Sciences, 2014, 15, 20572-20584.	4.1	24
17	Molecular dynamics approaches to the design and synthesis of PCB targeting molecularly imprinted polymers: interference to monomerâ€"template interactions in imprinting of 1,2,3-trichlorobenzene. Organic and Biomolecular Chemistry, 2014, 12, 844-853.	2.8	24
18	Oxidative hotspots on actin promote skeletal muscle weakness in rheumatoid arthritis. JCI Insight, 2019, 4, .	5.0	23

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19	Warfarin: an environmentâ€dependent switchable molecular probe. Journal of Molecular Recognition, 2010, 23, 604-608.	2.1	22
20	In silico screening of molecular imprinting prepolymerization systems: oseltamivir selective polymers through full-system molecular dynamics-based studies. Organic and Biomolecular Chemistry, 2016, 14, 4210-4219.	2.8	22
21	Hydrogen bond diversity in the pre-polymerization stage contributes to morphology and MIP-template recognition â€" MAA versus MMA. European Polymer Journal, 2015, 66, 558-568.	5.4	19
22	Theoretical and Computational Strategies for the Study of the Molecular Imprinting Process and Polymer Performance. Advances in Biochemical Engineering/Biotechnology, 2015, 150, 25-50.	1.1	18
23	How Warfarinâ€™s Structural Diversity Influences Its Phospholipid Bilayer Membrane Permeation. Journal of Physical Chemistry B, 2013, 117, 2384-2395.	2.6	17
24	Molecular Insights on the Two Fluorescence Lifetimes Displayed by Warfarin from Fluorescence Anisotropy and Molecular Dynamics Studies. Journal of Physical Chemistry B, 2009, 113, 7945-7949.	2.6	16
25	The mechanistic basis for warfarinâ€™s structural diversity and implications for its bioavailability. Computational and Theoretical Chemistry, 2010, 958, 7-9.	1.5	15
26	Monitoring the Distribution of Warfarin in Blood Plasma. ACS Medicinal Chemistry Letters, 2012, 3, 650-652.	2.8	14
27	Key Residues and Phosphate Release Routes in the Saccharomyces cerevisiae Pho84 Transceptor. Journal of Biological Chemistry, 2016, 291, 26388-26398.	3.4	13
28	Spectroscopic evidence for the presence of the cyclic hemiketal form of warfarin in aqueous solution: Consequences for bioavailability. Biochemical and Biophysical Research Communications, 2011, 407, 318-320.	2.1	12
29	Towards a synthetic avidin mimic. Analytical and Bioanalytical Chemistry, 2011, 400, 1397-1404.	3.7	11
30	Simulation of imprinted emulsion prepolymerization mixtures. Polymer Journal, 2015, 47, 827-830.	2.7	11
31	In situ detection of warfarin using time-correlated single-photon counting. Biochemical and Biophysical Research Communications, 2011, 407, 60-62.	2.1	10
32	A Capped Peptide of the Aggregation Prone NAC 71â€"82 Amino Acid Stretch of Î±-Synuclein Folds into Soluble Î²-Sheet Oligomers at Low and Elevated Peptide Concentrations. International Journal of Molecular Sciences, 2020, 21, 1629.	4.1	6
33	Amyloid fibrils prepared using an acetylated and methyl amidated peptide model of the Î±-Synuclein NAC 71â€"82 amino acid stretch contain an additional cross-Î² structure also found in prion proteins. Scientific Reports, 2019, 9, 15949.	3.3	4
34	Synthetic NAC 71-82 Peptides Designed to Produce Fibrils with Different Protofilament Interface Contacts. International Journal of Molecular Sciences, 2021, 22, 9334.	4.1	2
35	CHAPTER 7. Theoretical and Computational Strategies in Molecularly Imprinted Polymer Development. RSC Polymer Chemistry Series, 2018, , 197-226.	0.2	2