Andrei V Afonin

List of Publications by Year
in descending order

48 papers	840 citations	471509 17 h-index	526287 27 g-index
48 all docs	48 docs citations	48 times ranked	729 citing authors

#	Article	IF	Citations
1	Guide to tuning the chalcone molecular properties based on the pushâ€pull effect energy scale created via the molecular tailoring approach. Journal of Computational Chemistry, 2022, 43, 631-643.	3.3	2
2	Molecular tailoring approach as tool for revealing resonanceâ€assisted hydrogen bond: Case study of <scp>Z</scp>â€pyrrolylenones with the Nï£¿Hâ‹¯Oï£¾Đ¡ intramolecular hydrogen bond. Journal of Computational Chemistry, 2022, 43, 1596-1607.	3.3	4
3	Cyanoquinolines and Furo[3,4-b]quinolinones Formation via On-The-Spot 2,3-Functionalization of Quinolines with Cyanopropargylic Alcohols. Journal of Organic Chemistry, 2021, 86, 3800-3809.	3.2	3
4	Localized orbital locator as a descriptor for quantification and digital presentation of lone pairs: benchmark calculations of 4-substituted pyridines. Physical Chemistry Chemical Physics, 2021, 23, 24536-24540.	2.8	5
5	Synthesis of N-(Z)-acylethenyl-6-hydroxydihydrophenanthridines via the stereoselective functionalization of phenanthridine with acylacetylenes and water. Tetrahedron Letters, 2020, 61, 151553.	1.4	5
6	Acylacetylenes in multiple functionalization of hydroxyquinolines and quinolones. Tetrahedron, 2020, 76, 131523.	1.9	1
7	A molecular tailoring approach â€“ a new guide to quantify the energy of pushâ€“pull effects: a case study on (E)-3-(1H-pyrrol-2-yl)prop-2-enones. Physical Chemistry Chemical Physics, 2020, 22, 22190-22194.	2.8	7
8	Cyanoacetylene-driven base catalyzed synthesis of dihydropyrimidophenanthridinones from phenanthridine and water. Mendeleev Communications, 2020, 30, 12-14.	1.6	2
9	KOBu^t/DMSO-Mediated Î±-Câ€“H Vinylation of N-Benzyl Ketimines with Acetylene Gas: Stereoselective Synthesis of (E,Z)-2-Azadienes. Organic Letters, 2020, 22, 2611-2614.	4.6	14
10	Quantitative decomposition of resonanceâ€assisted hydrogen bond energy in Î²â€diketones into resonance and hydrogen bonding (Ï€â€and Ïƒâ€) components using molecular tailoring and functionâ€based approaches. Journal of Computational Chemistry, 2020, 41, 1285-1298.	3.3	17
11	Solvent-induced E/Z isomerization of 2-(furylmethylidene)-1-hydrazinecarbothioamide: The Nâ€“Hâ‹…â‹…â‹…O intramolecular hydrogen bond as promoting factor. Journal of Molecular Structure, 2020, 1207, 127782.	3.6	1
12	Case study of 2-vinyloxypyridine: Quantitative assessment of the intramolecular C Hâ‹¯N hydrogen bond energy and its contribution to the one-bond 13C1H coupling constant. Journal of Molecular Structure, 2019, 1176, 73-85.	3.6	9
13	Cyanoacetylenes as Triggers and Partners in KOH-Assisted Assemblies of Quinoline-Based Dihydropyrimido[1,2-a]quinolin-3-ones on Water. Journal of Organic Chemistry, 2019, 84, 9726-9733.	3.2	10
14	Benchmark calculations of intramolecular hydrogen bond energy based on molecular tailoring and functionâ€based approaches: Developing hybrid approach. International Journal of Quantum Chemistry, 2019, 119, e26001.	2.0	24
15	2H-Indazole Tautomers Stabilized by Intra- and Intermolecular Hydrogen Bonds. Journal of Organic Chemistry, 2019, 84, 9075-9086.	3.2	12
16	Estimating the energy of intramolecular bifurcated (three-centered) hydrogen bond by X-ray, IR and 1 H NMR spectroscopy, and QTAIM calculations. Journal of Molecular Structure, 2018, 1163, 185-196.	3.6	27
17	The intramolecular hydrogen bond as a unit of molecular electronics: Molecular switching controlled by overcrowded intramolecular three-centered hydrogen bond. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850023.	1.8	3
18	Regioselective N(2)-H-functionalization of thiosemicarbazones of aromatic and heteroaromatic aldehydes with acrylonitrile. Synthetic Communications, 2017, 47, 159-168.	2.1	4

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19	Study of spontaneous E/Z isomerization of bis[(Z)â€cyanomethylidene]â€diazapentacyclodienedicarboxylates by ¹H, ¹³C, and ¹⁵N NMR spectroscopy, Xâ€ray, and quantum chemical calculation data. Magnetic Resonance in Chemistry, 2017, 55, 563-569.	1.9	8
20	Aluminium oxide-mediated cross-coupling of pyrroles with 1-bromo-2-(trifluoroacetyl)acetylene: a quantum-chemical insight. Mendeleev Communications, 2016, 26, 480-482.	1.6	11
21	Estimating the energy of intramolecular hydrogen bonds from¹H NMR and QTAIM calculations. Organic and Biomolecular Chemistry, 2016, 14, 11199-11211.	2.8	119
22	(Imidazolâ€2â€yl)methylâ€1,3â€propanediones: Regioselective Câ€“H Functionalization of the Imidazole Ring by Acylacetylene/Aldehyde Pairs. European Journal of Organic Chemistry, 2016, 2016, 1199-1204.	2.4	8
23	Ringâ€Opening of Pyridines with AcylÂacetylenes and Water: Straightforward Access to 5â€[(Z)â€Acylethenyl]aminoâ€2,4â€pentadienals. European Journal of Organic Chemistry, 2015, 2015, 7876-7879.	2.4	12
24	Vinylation of trialkylamines with acyl- and cyanoacetylenes via Câ€“N bond cleavage in the presence of water. Mendeleev Communications, 2014, 24, 209-210.	1.6	5
25	Experimental and theoretical study of the intramolecular Câ€“HÂ·Â·Â·N and Câ€“HÂ·Â·Â·S hydrogen bonding effects in the ¹H and ¹³C NMR spectra of the 2â€(alkylsulfanyl)â€5â€aminoâ€1â€vinylpyrroles: a particular state of amine nitrogen. Magnetic Resonance in Chemistry, 2013, 51, 414-423.	1.9	17
26	Structural studies of meso-CF3-3(5)-aryl(hetaryl)- and 3,5-diaryl(dihetaryl)-BODIPY dyes by 1H, 13C and 19F NMR spectroscopy and DFT calculations. Journal of Fluorine Chemistry, 2013, 145, 51-57.	1.7	11
27	Structural peculiarities of configurational isomers of 1â€styrylpyrroles according to ¹Ð¸ ¹³Ð¸ and ¹⁵N NMR spectroscopy and density functional theory calculations: electronic and steric hindrance for planar structure. Magnetic Resonance in Chemistry, 2013, 51, 339-349.	1.9	5
28	Stereospecificity of ¹H, ¹³C and ¹⁵N shielding constants in the isomers of methylglyoxal bisdimethylhydrazone: problem with configurational assignment based on ¹H chemical shifts. Magnetic Resonance in Chemistry, 2012, 50, 502-510.	1.9	10
29	Study of stereospecificity of ¹H, ¹³C, ¹⁵N and ⁷⁷Se shielding constants in the configurational isomers of the selenopheneâ€2â€carbaldehyde azine by NMR spectroscopy and MP2â€GIAO calculations. Magnetic Resonance in Chemistry, 2011, 49, 740-748.	1.9	8
30	C2â€Functionalization of 1â€Substituted Imidazoles with Aldehydes and Electronâ€Deficient Acetylenes: A Novel Threeâ€Component Reaction. European Journal of Organic Chemistry, 2010, 2010, 1772-1777.	2.4	32
31	Theoretical study of bifurcated hydrogen bonding effects on the ¹J(N,H), ^{1h}J(N,H), ^{2h}J(N,N) couplings and ¹H, ¹⁵N shieldings in model pyrroles. Magnetic Resonance in Chemistry, 2010, 48, 309-317.	1.9	17
32	Study of conformations and hydrogen bonds in the configurational isomers of pyrroleâ€2â€carbaldehyde oxime by ¹H, ¹³C and ¹⁵N NMR spectroscopy combined with MP2 and DFT calculations and NBO analysis. Magnetic Resonance in Chemistry, 2010, 48, 685-692.	1.9	36
33	DFT prediction of anomalously large blue shift of the Câ€“H stretching frequency in 2-vinyloxypyridine and -quinoline due to the intramolecular Câ€“HÂ·Â·Â·N hydrogen bonding. Computational and Theoretical Chemistry, 2010, 940, 56-60.	1.5	14
34	Cï£¿HÂ·Â·Â·N and Cï£¿HÂ·Â·Â·O intramolecular hydrogen bonding effects in the ¹H, ¹³C and ¹⁵ N NMR spectra of the configurational isomers of 1â€vinylpyrroleâ€2â€carbaldehyde oxime substantiated by DFT calculations. Magnetic Resonance in Chemistry, 2009, 47, 105-112.	1.9	46
35	1-Vinylpyrrole-2-carbaldehyde oximes: synthesis, isomerization, and spectral properties. Monatshefte FÃ¼r Chemie, 2009, 140, 1475-1480.	1.8	7
36	Comparative analysis of hydrogen bonding with participation of the nitrogen, oxygen and sulfur atoms in the 2(2â€²â€heteroaryl)pyrroles and their trifluoroacetyl derivatives based on the ¹H, ¹³C, ¹⁵N spectroscopy and DFT calculations. Magnetic Resonance in Chemistry, 2008, 46, 441-447.	1.9	18

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37	Annelation of Benzimidazoles with Î±,Î²-Acetylenic Î³-Hydroxyacid Nitriles and Hydrolytic Rearrangement of the Cycloadducts on Alumina. European Journal of Organic Chemistry, 2007, 2007, 1018-1025.	2.4	18
38	Bifurcated hydrogen-bonding effect on the shielding and coupling constants in trifluoroacetyl pyrroles as studied by1H,13C and15N NMR spectroscopy and DFT calculations. Magnetic Resonance in Chemistry, 2007, 45, 220-230.	1.9	25
39	Reaction of Pyridine with Phenylcyanoacetylene: A New Route to Functionalized Polyconjugated 1,4-Dihydropyridine Systems. European Journal of Organic Chemistry, 2006, 2006, 1581-1585.	2.4	4
40	2-Arylazo-1-vinylpyrroles: A Novel Promising Family of Reactive Dyes. European Journal of Organic Chemistry, 2006, 2006, 4021-4033.	2.4	43
41	Different types of hydrogen bonds in 2-substituted pyrroles and 1-vinyl pyrroles as monitored by1H,13C and15N NMR spectroscopy andab initio calculations. Magnetic Resonance in Chemistry, 2006, 44, 59-65.	1.9	36
42	Synthesis, Structure, and Spectral Properties of Bis(pyrrol-2-yl)pyridines. European Journal of Organic Chemistry, 2005, 2005, 4338-4345.	2.4	27
43	Influence of the C?Hï¿½ ï¿½ ï¿½N intramolecular interaction on the spatial structures and1H and13C NMR parameters of heteroaryl vinyl ethers and sulfides. Magnetic Resonance in Chemistry, 2003, 41, 557-566.	1.9	15
44	Cascade cyclization of quinoline and quinoxaline with nitriles of Î±,Î²-acetylenic Î³-hydroxy acids. Mendeleev Communications, 2003, 13, 186-188.	1.6	26
45	C?Hï¿½ï¿½ï¿½X (X = N, O, S) intramolecular interaction in 1-vinyl-2-(2?-heteroaryl)pyrroles as monitored by1H and13C NMR spectroscopy. Magnetic Resonance in Chemistry, 2002, 40, 114-122.	1.9	31
46	Configurational and conformational analysis ofO-vinyl ketoximes by1H and13C NMR spectroscopy. Magnetic Resonance in Chemistry, 2000, 38, 994-1000.	1.9	25
47	Specific intramolecular interactions C-HÂ·Â·Â·N in heteroaryl vinyl ethers and heteroaryl vinyl sulfides studied by 1H, 13C, and 15N NMR spectroscopies and by ab initio calculations on molecular structures as well as on nuclear shieldings. Canadian Journal of Chemistry, 1999, 77, 416-424.	1.1	31
48	Structural Effects in NMR Spectroscopy of Vinylic Compound 1. Investigation of Intramolecular Specific Interactions Câ€“HÂ·Â·Â·N in Hetaryl Vinyl Ethers by1H,13C,15N, and17O NMR Spectroscopies and Quantum-Chemical Calculations. Bulletin of the Chemical Society of Japan, 1996, 69, 933-945.	3.2	25