

Roman Szostak

List of Publications by Year in descending order

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89
papers

3,154
citations

159525

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h-index

168321

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90
all docs

90
docs citations

90
times ranked

2435
citing authors

#	ARTICLE	IF	CITATIONS
1	The Nature of Improper, Blue-Shifting Hydrogen Bonding Verified Experimentally. <i>Journal of the American Chemical Society</i> , 2001, 123, 12290-12293.	6.6	306
2	Reversible Twisting of Primary Amides via Ground State N=C(O) Destabilization: Highly Twisted Rotationally Inverted Acyclic Amides. <i>Journal of the American Chemical Society</i> , 2018, 140, 727-734.	6.6	155
3	Suzuki-Miyaura cross-coupling of amides and esters at room temperature: correlation with barriers to rotation around C-N and C-O bonds. <i>Chemical Science</i> , 2017, 8, 6525-6530.	3.7	148
4	Quantitative determination of acetylsalicylic acid and acetaminophen in tablets by FT-Raman spectroscopy. Electronic Supplementary Information available. See http://www.rsc.org/suppdata/an/b1/b108240j/ . <i>Analyst</i> , 2002, 127, 144-148.	1.7	134
5	Ground-State Distortion in N-Acyl-tert-butyl-carbamates (Boc) and N-Acyl-tosylamides (Ts): Twisted Amides of Relevance to Amide N=C Cross-Coupling. <i>Journal of Organic Chemistry</i> , 2016, 81, 8091-8094.	1.7	121
6	N-Acylsaccharins: Stable Electrophilic Amide-Based Acyl Transfer Reagents in Pd-Catalyzed Suzuki-Miyaura Coupling via N=C Cleavage. <i>Organic Letters</i> , 2016, 18, 4194-4197.	2.4	103
7	Quantitative determination of captopril and prednisolone in tablets by FT-Raman spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2006, 40, 1225-1230.	1.4	96
8	Structures of Highly Twisted Amides Relevant to Amide N=C Cross-Coupling: Evidence for Ground-State Amide Destabilization. <i>Chemistry - A European Journal</i> , 2016, 22, 14494-14498.	1.7	94
9	Suzuki-Miyaura Cross-Coupling of N-Acylpyrroles and Pyrazoles: Planar, Electronically Activated Amides in Catalytic N=C Cleavage. <i>Organic Letters</i> , 2017, 19, 3596-3599.	2.4	91
10	Acyl and Decarbonylative Suzuki Coupling of N-Acetyl Amides: Electronic Tuning of Twisted, Acyclic Amides in Catalytic Carbon-Nitrogen Bond Cleavage. <i>ACS Catalysis</i> , 2018, 8, 9131-9139.	5.5	91
11	Resonance Destabilization in N-Acylanilines (Anilides): Electronically-Activated Planar Amides of Relevance in N=C(O) Cross-Coupling. <i>Journal of Organic Chemistry</i> , 2017, 82, 6373-6378.	1.7	82
12	An efficient computational model to predict protonation at the amide nitrogen and reactivity along the N rotational pathway. <i>Chemical Communications</i> , 2015, 51, 6395-6398.	2.2	79
13	Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of N-Mesylamides by N=C Cleavage: Electronic Effect of the Mesyl Group. <i>Organic Letters</i> , 2017, 19, 1434-1437.	2.4	74
14	Electronic structure and vibrational spectra of cis-diammine(oxalato)platinum(II), a potential cisplatin analogue: DFT and experimental study. <i>Chemical Physics</i> , 2007, 333, 37-48.	0.9	71
15	Quantitative determination of diclofenac sodium and aminophylline in injection solutions by FT-Raman spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2006, 40, 1235-1242.	1.4	67
16	C-H...O Halogen Bonding: Interactions of Trifluoromethyl Halides with Dimethyl Ether. <i>ChemPhysChem</i> , 2009, 10, 2105-2115.	1.0	66
17	N-Acyl-glutarimides: Resonance and Proton Affinities of Rotationally-Inverted Twisted Amides Relevant to N=C(O) Cross-Coupling. <i>Organic Letters</i> , 2018, 20, 1342-1345.	2.4	65
18	Determination of Structures and Energetics of Small- and Medium-Sized One-Carbon-Bridged Twisted Amides using ab Initio Molecular Orbital Methods: Implications for Amidic Resonance along the N Rotational Pathway. <i>Journal of Organic Chemistry</i> , 2015, 80, 7905-7927.	1.7	59

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19	<i>N</i> -Methylamino Pyrimidyl Amides (MAPA): Highly Reactive, Electronically-Activated Amides in Catalytic $N=C(O)$ Cleavage. <i>Organic Letters</i> , 2017, 19, 4656-4659.	2.4	59
20	Analysis of milk by FT-Raman spectroscopy. <i>Talanta</i> , 2015, 138, 285-289.	2.9	51
21	IPr# highly hindered, broadly applicable N-heterocyclic carbenes. <i>Chemical Science</i> , 2021, 12, 10583-10589.	3.7	51
22	Quantitative determination of diclofenac sodium in solid dosage forms by FT-Raman spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2008, 48, 814-821.	1.4	45
23	Chemistry of Bridged Lactams: Recent Developments. <i>Molecules</i> , 2019, 24, 274.	1.7	43
24	The Most Twisted Acyclic Amides: Structures and Reactivity. <i>Organic Letters</i> , 2018, 20, 7771-7774.	2.4	41
25	Quantification of atorvastatin calcium in tablets by FT-Raman spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2009, 49, 168-172.	1.4	40
26	FT-Raman quantitative determination of ambroxol in tablets. <i>Journal of Molecular Structure</i> , 2004, 704, 229-233.	1.8	39
27	Quantification of aspartame in commercial sweeteners by FT-Raman spectroscopy. <i>Food Chemistry</i> , 2011, 125, 1051-1057.	4.2	37
28	[(NHC)PdCl ₂ (Aniline)] Complexes: Easily Synthesized, Highly Active Pd(II)-NHC Precatalysts for Cross-Coupling Reactions. <i>Journal of Organic Chemistry</i> , 2021, 86, 15648-15657.	1.7	35
29	Highly Chemoselective Synthesis of Indolizidine Lactams by SmI ₂ -Induced Umpolung of the Amide Bond via Aminoketyl Radicals: Efficient Entry to Alkaloid Scaffolds. <i>Chemistry - A European Journal</i> , 2016, 22, 11949-11953.	1.7	33
30	Triflamides: Highly Reactive, Electronically Activated <i>N</i> -Sulfonyl Amides in Catalytic $N=C(O)$ Amide Cross-Coupling. <i>Organic Letters</i> , 2019, 21, 1253-1257.	2.4	32
31	Quantification of Ash and Moisture in Wheat Flour by Raman Spectroscopy. <i>Foods</i> , 2020, 9, 280.	1.9	31
32	Microheterogeneity in binary mixtures of methanol with aliphatic alcohols: ATR-IR/NIR spectroscopic, chemometrics and DFT studies. <i>RSC Advances</i> , 2016, 6, 37195-37202.	1.7	30
33	Barriers to Rotation in ortho-Substituted Tertiary Aromatic Amides: Effect of Chloro-Substitution on Resonance and Distortion. <i>Journal of Organic Chemistry</i> , 2018, 83, 3159-3163.	1.7	29
34	Quantification of gluten in wheat flour by FT-Raman spectroscopy. <i>Food Chemistry</i> , 2016, 211, 560-563.	4.2	27
35	Sterically Hindered Ketones via Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of Amides by $N=C(O)$ Activation. <i>Organic Letters</i> , 2019, 21, 7976-7981.	2.4	27
36	N-Acylcarbazoles and N-Acylindoles: Electronically Activated Amides for $N=C(O)$ Cross-Coupling by Nlp to Ar Conjugation Switch. <i>Organic Letters</i> , 2020, 22, 4703-4709.	2.4	23

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37	Palladium-NHC (NHC = N-heterocyclic Carbene)-Catalyzed Suzuki–Miyaura Cross-Coupling of Alkyl Amides. <i>ACS Catalysis</i> , 2022, 12, 2426-2433.	5.5	23
38	Application of infrared reflection and Raman spectroscopy for quantitative determination of fat in potato chips. <i>Journal of Molecular Structure</i> , 2016, 1126, 213-218.	1.8	22
39	Determination of nutritional parameters of bee pollen by Raman and infrared spectroscopy. <i>Talanta</i> , 2020, 212, 120790.	2.9	22
40	Quantification of active ingredients in <i>Potentilla tormentilla</i> by Raman and infrared spectroscopy. <i>Talanta</i> , 2018, 189, 308-314.	2.9	21
41	<i>N</i> -Acyl-glutarimides: Effect of Glutarimide Ring on the Structures of Fully Perpendicular Twisted Amides and $\text{N}=\text{C}$ Bond Cross-Coupling. <i>Journal of Organic Chemistry</i> , 2020, 85, 5475-5485.	1.7	21
42	Microheterogeneity in binary mixtures of water with CH ₃ OH and CD ₃ OH: ATR-IR spectroscopic, chemometric and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 197, 88-94.	2.0	20
43	Pentafluorophenyl Esters: Highly Chemoselective Ketyl Precursors for the Synthesis of H, D -Dideuterio Alcohols Using Sml_2 and D_2O as a Deuterium Source. <i>Organic Letters</i> , 2020, 22, 1249-1253.	2.4	20
44	Proton-coupled electron transfer in the reduction of carbonyls using $\text{Sml}_2 \cdot \text{H}_2\text{O}$: implications for the reductive coupling of acyl-type ketyl radicals with $\text{Sml}_2 \cdot \text{H}_2\text{O}$. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 9151-9157.	1.5	19
45	Thiazol-2-ylidenes as N-Heterocyclic carbene ligands with enhanced electrophilicity for transition metal catalysis. <i>Communications Chemistry</i> , 2022, 5, .	2.0	17
46	Quantitative analysis of topical gels and ointments by FT-Raman spectroscopy. <i>Vibrational Spectroscopy</i> , 2016, 83, 1-7.	1.2	16
47	Tröger's Base Twisted Amides: High Amide Bond Twist and N-/O-Protonation Aptitude. <i>Journal of Organic Chemistry</i> , 2019, 84, 1510-1516.	1.7	16
48	Buchwald–Hartwig Amination of Coordinating Heterocycles Enabled by Large–but–Flexible Pd–BINAP–NHC Catalysts**. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	16
49	Determining moisture content in pasta by vibrational spectroscopy. <i>Talanta</i> , 2018, 178, 294-298.	2.9	15
50	Twisted <i>N</i> -Acyl-hydantoin: Rotationally Inverted Urea-Imides of Relevance in $\text{N}=\text{C}(\text{O})$ Cross-coupling. <i>Journal of Organic Chemistry</i> , 2018, 83, 14676-14682.	1.7	13
51	Polypyrrole–Methyl Orange Raman pH Sensor. <i>Polymers</i> , 2019, 11, 715.	2.0	13
52	Electrophilicity Scale of Activated Amides: 17 $\text{O}=\text{C}$...NMR and 15 $\text{N}=\text{C}$...NMR Chemical Shifts of Acyclic Twisted Amides in $\text{N}=\text{C}(\text{O})$ Cross–Coupling. <i>Chemistry - A European Journal</i> , 2020, 26, 16246-16250.	1.7	13
53	Conversion of esters to thioesters under mild conditions. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 2991-2996.	1.5	13
54	Methylenecyclopropane–Boron Trifluoride van der Waals Complexes; an Infrared and DFT Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8480-8488.	1.1	12

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55	Quantification of active ingredients in suppositories by FT-Raman spectroscopy. <i>Drug Testing and Analysis</i> , 2013, 5, 126-129.	1.6	12
56	¹⁷ O NMR and ¹⁵ N NMR chemical shifts of sterically-hindered amides: ground-state destabilization in amide electrophilicity. <i>Chemical Communications</i> , 2019, 55, 4423-4426.	2.2	12
57	Preference of <i>cis</i> -Thioamide Structure in <i>N</i> -Thioacyl- <i>N</i> -methylanilines. <i>Organic Letters</i> , 2020, 22, 9500-9505.	2.4	12
58	Evaluation of Cyclic Amides as Activating Groups in N=C Bond Cross-Coupling: Discovery of <i>N</i> -Acyl- <i>l</i> -valerolactams as Effective Twisted Amide Precursors for Cross-Coupling Reactions. <i>Journal of Organic Chemistry</i> , 2021, 86, 10455-10466.	1.7	12
59	<i>N</i> -Heterocyclic Carbene Complexes of Nickel(II) from Caffeine and Theophylline: Sustainable Alternative to Imidazol-2-ylidenes. <i>Organometallics</i> , 2022, 41, 1806-1815.	1.1	12
60	A quantitative analysis of liquid hydrocarbon mixtures on the basis of FT-Raman spectra registered under unstable conditions. <i>Journal of Molecular Structure</i> , 2004, 704, 235-245.	1.8	11
61	The influence of sample area on diclofenac sodium quantification by diffuse reflectance IR spectroscopy. <i>Talanta</i> , 2011, 84, 583-586.	2.9	11
62	Microheterogeneity in CH ₃ OH/CD ₃ OH mixture. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 349-354.	2.0	11
63	Acyl fluorides as direct precursors to fluoride ketyl radicals: reductive deuteration using Sml ₂ and D ₂ O. <i>Chemical Communications</i> , 2021, 57, 5195-5198.	2.2	11
64	Application of Indazolin-3-ylidenes in Catalysis: Steric Tuning of Nonclassical Formally Normal <i>N</i> -Heterocyclic Carbenes with Dual Electronic Character for Catalysis. <i>Organometallics</i> , 2022, 41, 1115-1124.	1.1	11
65	Redox switching hysteresis in polyaniline acetate systems: a search of molecular factors important for the dynamics of the polymer reaction. <i>Journal of Electroanalytical Chemistry</i> , 2004, 571, 51-57.	1.9	10
66	Comparison of infrared attenuated total reflection and Raman spectroscopy in the quantitative analysis of diclofenac sodium in tablets. <i>Vibrational Spectroscopy</i> , 2011, 57, 157-157.	1.2	10
67	Quantitative Determination of Prednisone in Tablets by Infrared Attenuated Total Reflection and Raman Spectroscopy. <i>Journal of AOAC INTERNATIONAL</i> , 2012, 95, 744-750.	0.7	10
68	Quantitative analysis of thiamine hydrochloride in tablets—Comparison of infrared attenuated total reflection, diffuse reflectance infrared and Raman spectroscopy. <i>Vibrational Spectroscopy</i> , 2012, 62, 10-16.	1.2	10
69	Modeling red coral (<i>Corallium rubrum</i>) and African snail (<i>Helix aspersa</i>) shell pigments: Raman spectroscopy versus DFT studies. <i>Journal of Raman Spectroscopy</i> , 2016, 47, 908-916.	1.2	10
70	Determination of nutritional parameters of yoghurts by FT Raman spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 196, 413-417.	2.0	9
71	Ring-Opening Olefin Metathesis of Twisted Amides: Activation of Amide Bonds by C=C Cleavage. <i>ACS Catalysis</i> , 2020, 10, 737-742.	5.5	9
72	On the HCl and DCl complexes of methylenecyclopropane in liquid argon. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 3983-3991.	1.3	8

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73	Blue or red $\hat{\nu}_{1/2}XH$ complexation shift in $X\hat{A}^{\ominus}H\hat{A}^{\ominus}CO_2$ hydrogen-bonded complexes?. <i>Chemical Physics Letters</i> , 2011, 516, 166-170.	1.2	8
74	Determination of Antioxidant Activity and Polyphenols Content in Chips by Raman and IR Spectroscopy. <i>Food Analytical Methods</i> , 2017, 10, 3964-3971.	1.3	8
75	Quantification of active ingredients in pharmaceutical suspensions by FT Raman spectroscopy. <i>Vibrational Spectroscopy</i> , 2017, 93, 57-64.	1.2	8
76	Simple transformation of spectra to effectively reduce quantification errors in FT-Raman multivariate analysis of complex systems. <i>Vibrational Spectroscopy</i> , 2009, 49, 298-302.	1.2	7
77	Quantitative Determination of Vitamins A and E in Ointments Using Raman Spectroscopy. <i>Processes</i> , 2021, 9, 8.	1.3	6
78	Chemometric Detection of Acetaminophen in Pharmaceuticals by Infrared Spectroscopy Combined with Pattern Recognition Techniques: Comparison of Attenuated Total Reflectance-FTIR and Raman Spectroscopy. <i>Journal of AOAC INTERNATIONAL</i> , 2011, 94, 743-749.	0.7	5
79	Why the $\hat{\nu}_{1/2}CH$ blue shift is larger in chloral than in dichloroacetyl chloride dimers?. <i>Journal of Raman Spectroscopy</i> , 2011, 42, 1185-1192.	1.2	5
80	Modeling of Antioxidant Activity, Polyphenols and Macronutrients Content of Bee Pollen Applying Solid-State ^{13}C NMR Spectra. <i>Antioxidants</i> , 2021, 10, 1123.	2.2	4
81	Quantification of Salicylates and Flavonoids in Poplar Bark and Leaves Based on IR, NIR, and Raman Spectra. <i>Molecules</i> , 2022, 27, 3954.	1.7	4
82	Quantitative analysis of solid samples using modified specular reflectance accessory. <i>Talanta</i> , 2016, 161, 655-659.	2.9	3
83	Silver(I) chloride-polypyrrole composite: electrochemical preparation, characterization, and application as a SERS platform. <i>Journal of Solid State Electrochemistry</i> , 2017, 21, 823-832.	1.2	3
84	Structures of the Most Twisted Thioamide and Selenoamide: Effect of Higher Chalcogens of Twisted Amides on $N\hat{a}^{\ominus}C(X)$ Resonance. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	3
85	On the blue-shifting hydrogen bond in tribromoacetaldehyde dimers. <i>Chemical Physics Letters</i> , 2011, 514, 49-53.	1.2	2
86	Electrocrystallization of silver nanoparticles from silver halides in polypyrrole evidenced by their SERS activity—thermodynamic and kinetic conditions. <i>Journal of Solid State Electrochemistry</i> , 2018, 22, 3933-3945.	1.2	2
87	pH determination of small sample volumes using Raman spectra of azo dyes. <i>Journal of Molecular Structure</i> , 2022, 1253, 132226.	1.8	2
88	ATR-IR Spectroscopy Application to Diagnostic Screening of Advanced Endometriosis. <i>Oxidative Medicine and Cellular Longevity</i> , 2022, 2022, 1-13.	1.9	2
89	Structures and energetic properties of 4-halobenzamides. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 1395-1402.	0.2	1