Roman Szostak

List of Publications by Year
in descending order

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89 papers	3,154 citations	159585 30 h-index	168389 53 g-index
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. Journal of the American Chemical Society, 2001, 123, 12290-12293.	13.7	306
2	Reversible Twisting of Primary Amides via Ground State Nâ€“C(O) Destabilization: Highly Twisted Rotationally Inverted Acyclic Amides. Journal of the American Chemical Society, 2018, 140, 727-734.	13.7	155
3	Suzukiâ€“Miyaura cross-coupling of amides and esters at room temperature: correlation with barriers to rotation around Câ€“N and Câ€“O bonds. Chemical Science, 2017, 8, 6525-6530.	7.4	148
4	Quantitative determination of acetylsalicylic acid and acetaminophen in tablets by FT-Raman spectroscopyElectronic Supplementary Information available. See http://www.rsc.org/suppdata/an/b1/b108240j/. Analyst, The, 2002, 127, 144-148.	3.5	134
5	Ground-State Distortion in N-Acyl-tert-butyl-carbamates (Boc) and N-Acyl-tosylamides (Ts): Twisted Amides of Relevance to Amide Nâ€“C Cross-Coupling. Journal of Organic Chemistry, 2016, 81, 8091-8094.	3.2	121
6	N-Acylsaccharins: Stable Electrophilic Amide-Based Acyl Transfer Reagents in Pd-Catalyzed Suzukiâ€“Miyaura Coupling via Nâ€“C Cleavage. Organic Letters, 2016, 18, 4194-4197.	4.6	103
7	Quantitative determination of captopril and prednisolone in tablets by FT-Raman spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2006, 40, 1225-1230.	2.8	96
8	Structures of Highly Twisted Amides Relevant to Amide Nâˆ’C Crossâ€Coupling: Evidence for Groundâ€State Amide Destabilization. Chemistry - A European Journal, 2016, 22, 14494-14498.	3.3	94
9	Suzukiâ€“Miyaura Cross-Coupling of N-Acylpyrroles and Pyrazoles: Planar, Electronically Activated Amides in Catalytic Nâ€“C Cleavage. Organic Letters, 2017, 19, 3596-3599.	4.6	91
10	Acyl and Decarbonylative Suzuki Coupling of N-Acetyl Amides: Electronic Tuning of Twisted, Acyclic Amides in Catalytic Carbonâ€“Nitrogen Bond Cleavage. ACS Catalysis, 2018, 8, 9131-9139.	11.2	91
11	Resonance Destabilization in N-Acylanilines (Anilides): Electronically-Activated Planar Amides of Relevance in Nâ€“C(O) Cross-Coupling. Journal of Organic Chemistry, 2017, 82, 6373-6378.	3.2	82
12	An efficient computational model to predict protonation at the amide nitrogen and reactivity along the Câ€“N rotational pathway. Chemical Communications, 2015, 51, 6395-6398.	4.1	79
13	Palladium-Catalyzed Suzukiâ€“Miyaura Cross-Coupling of N-Mesylamides by Nâ€“C Cleavage: Electronic Effect of the Mesyl Group. Organic Letters, 2017, 19, 1434-1437.	4.6	74
14	Electronic structure and vibrational spectra of cis-diammine(orotato)platinum(II), a potential cisplatin analogue: DFT and experimental study. Chemical Physics, 2007, 333, 37-48.	1.9	71
15	Quantitative determination of diclofenac sodium and aminophylline in injection solutions by FT-Raman spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2006, 40, 1235-1242.	2.8	67
16	Cï£¿Xâ‹…â‹…â‹…O Halogen Bonding: Interactions of Trifluoromethyl Halides with Dimethyl Ether. ChemPhysChem, 2009, 10, 2105-2115.	2.1	66
17	N-Acyl-glutarimides: Resonance and Proton Affinities of Rotationally-Inverted Twisted Amides Relevant to Nâ€“C(O) Cross-Coupling. Organic Letters, 2018, 20, 1342-1345.	4.6	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 Câ€“N Rotational Pathway. Journal of Organic Chemistry, 2015, 80, 7905-7927.	3.2	59

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19	N-Methylamino Pyrimidyl Amides (MAPA): Highly Reactive, Electronically-Activated Amides in Catalytic Nâ€“C(O) Cleavage. Organic Letters, 2017, 19, 4656-4659.	4.6	59
20	Analysis of milk by FT-Raman spectroscopy. Talanta, 2015, 138, 285-289.	5.5	51
21	IPr# â€“ highly hindered, broadly applicable N-heterocyclic carbenes. Chemical Science, 2021, 12, 10583-10589.	7.4	51
22	Quantitative determination of diclofenac sodium in solid dosage forms by FT-Raman spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2008, 48, 814-821.	2.8	45
23	Chemistry of Bridged Lactams: Recent Developments. Molecules, 2019, 24, 274.	3.8	43
24	The Most Twisted Acyclic Amides: Structures and Reactivity. Organic Letters, 2018, 20, 7771-7774.	4.6	41
25	Quantification of atorvastatin calcium in tablets by FT-Raman spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2009, 49, 168-172.	2.8	40
26	FT-Raman quantitative determination of ambroxol in tablets. Journal of Molecular Structure, 2004, 704, 229-233.	3.6	39
27	Quantification of aspartame in commercial sweeteners by FT-Raman spectroscopy. Food Chemistry, 2011, 125, 1051-1057.	8.2	37
28	[(NHC)PdCl₂(Aniline)] Complexes: Easily Synthesized, Highly Active Pd(II)â€“NHC Precatalysts for Cross-Coupling Reactions. Journal of Organic Chemistry, 2021, 86, 15648-15657.	3.2	35
29	Highly Chemoselective Synthesis of Indolizidine Lactams by SmI₂â€Induced Umpolung of the Amide Bond via Aminoketyl Radicals: Efficient Entry to Alkaloid Scaffolds. Chemistry - A European Journal, 2016, 22, 11949-11953.	3.3	33
30	Triflamides: Highly Reactive, Electronically Activated N-Sulfonyl Amides in Catalytic Nâ€“C(O) Amide Cross-Coupling. Organic Letters, 2019, 21, 1253-1257.	4.6	32
31	Quantification of Ash and Moisture in Wheat Flour by Raman Spectroscopy. Foods, 2020, 9, 280.	4.3	31
32	Microheterogeneity in binary mixtures of methanol with aliphatic alcohols: ATR-IR/NIR spectroscopic, chemometrics and DFT studies. RSC Advances, 2016, 6, 37195-37202.	3.6	30
33	Barriers to Rotation in ortho-Substituted Tertiary Aromatic Amides: Effect of Chloro-Substitution on Resonance and Distortion. Journal of Organic Chemistry, 2018, 83, 3159-3163.	3.2	29
34	Quantification of gluten in wheat flour by FT-Raman spectroscopy. Food Chemistry, 2016, 211, 560-563.	8.2	27
35	Sterically Hindered Ketones via Palladium-Catalyzed Suzukiâ€“Miyaura Cross-Coupling of Amides by Nâ€“C(O) Activation. Organic Letters, 2019, 21, 7976-7981.	4.6	27
36	N-Acylcarbazoles and N-Acylindoles: Electronically Activated Amides for Nâ€“C(O) Cross-Coupling by Nlp to Ar Conjugation Switch. Organic Letters, 2020, 22, 4703-4709.	4.6	23

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37	Palladium-NHC (NHC = N-heterocyclic Carbene)-Catalyzed Suzukiâ€“Miyaura Cross-Coupling of Alkyl Amides. ACS Catalysis, 2022, 12, 2426-2433.	11.2	23
38	Application of infrared reflection and Raman spectroscopy for quantitative determination of fat in potato chips. Journal of Molecular Structure, 2016, 1126, 213-218.	3.6	22
39	Determination of nutritional parameters of bee pollen by Raman and infrared spectroscopy. Talanta, 2020, 212, 120790.	5.5	22
40	Quantification of active ingredients in Potentilla tormentilla by Raman and infrared spectroscopy. Talanta, 2018, 189, 308-314.	5.5	21
41	N-Acyl-glutarimides: Effect of Glutarimide Ring on the Structures of Fully Perpendicular Twisted Amides and Nâ€“C Bond Cross-Coupling. Journal of Organic Chemistry, 2020, 85, 5475-5485.	3.2	21
42	Microheterogeneity in binary mixtures of water with CH3OH and CD3OH: ATR-IR spectroscopic, chemometric and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 197, 88-94.	3.9	20
43	Pentafluorophenyl Esters: Highly Chemoselective Ketyl Precursors for the Synthesis of Î±,Î±-Dideuterio Alcohols Using SmI₂ and D₂O as a Deuterium Source. Organic Letters, 2020, 22, 1249-1253.	4.6	20
44	Proton-coupled electron transfer in the reduction of carbonyls using SmI₂â€“H₂O: implications for the reductive coupling of acyl-type ketyl radicals with SmI₂â€“H₂O. Organic and Biomolecular Chemistry, 2016, 14, 9151-9157.	2.8	19
45	Thiazol-2-ylidenes as N-Heterocyclic carbene ligands with enhanced electrophilicity for transition metal catalysis. Communications Chemistry, 2022, 5, .	4.5	17
46	Quantitative analysis of topical gels and ointments by FT-Raman spectroscopy. Vibrational Spectroscopy, 2016, 83, 1-7.	2.2	16
47	TrÃ¶gerâ€™s Base Twisted Amides: High Amide Bond Twist and N-/O-Protonation Aptitude. Journal of Organic Chemistry, 2019, 84, 1510-1516.	3.2	16
48	Buchwaldâ€“Hartwig Amination of Coordinating Heterocycles Enabled by Largeâ€butâ€Flexible Pdâ€BIANâ€NHC Catalysts**. Chemistry - A European Journal, 2022, 28, .	3.3	16
49	Determining moisture content in pasta by vibrational spectroscopy. Talanta, 2018, 178, 294-298.	5.5	15
50	Twisted N-Acyl-hydantoins: Rotationally Inverted Urea-Imides of Relevance in Nâ€“C(O) Cross-coupling. Journal of Organic Chemistry, 2018, 83, 14676-14682.	3.2	13
51	Polypyrroleâ€“Methyl Orange Raman pH Sensor. Polymers, 2019, 11, 715.	4.5	13
52	Electrophilicity Scale of Activated Amides: 17 Oâ€¦NMR and 15 Nâ€¦NMR Chemical Shifts of Acyclic Twisted Amides in Nâ^'C(O) Crossâ€Coupling. Chemistry - A European Journal, 2020, 26, 16246-16250.	3.3	13
53	Conversion of esters to thioesters under mild conditions. Organic and Biomolecular Chemistry, 2021, 19, 2991-2996.	2.8	13
54	Methylenecyclopropaneâ^'Boron Trifluoride van der Waals Complexes; an Infrared and DFT Study. Journal of Physical Chemistry A, 2000, 104, 8480-8488.	2.5	12

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55	Quantification of active ingredients in suppositories by FTâ€Raman spectroscopy. Drug Testing and Analysis, 2013, 5, 126-129.	2.6	12
56	¹⁷O NMR and¹⁵N NMR chemical shifts of sterically-hindered amides: ground-state destabilization in amide electrophilicity. Chemical Communications, 2019, 55, 4423-4426.	4.1	12
57	Preference of cis-Thioamide Structure in N-Thioacyl-N-methylanilines. Organic Letters, 2020, 22, 9500-9505.	4.6	12
58	Evaluation of Cyclic Amides as Activating Groups in Nâ€“C Bond Cross-Coupling: Discovery of N-Acyl-Î´-valerolactams as Effective Twisted Amide Precursors for Cross-Coupling Reactions. Journal of Organic Chemistry, 2021, 86, 10455-10466.	3.2	12
59	N-Heterocyclic Carbene Complexes of Nickel(II) from Caffeine and Theophylline: Sustainable Alternative to Imidazol-2-ylidenes. Organometallics, 2022, 41, 1806-1815.	2.3	12
60	A quantitative analysis of liquid hydrocarbon mixtures on the basis of FT-Raman spectra registered under unstable conditions. Journal of Molecular Structure, 2004, 704, 235-245.	3.6	11
61	The influence of sample area on diclofenac sodium quantification by diffuse reflectance IR spectroscopy. Talanta, 2011, 84, 583-586.	5.5	11
62	Microheterogeneity in CH3OH/CD3OH mixture. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 349-354.	3.9	11
63	Acyl fluorides as direct precursors to fluoride ketyl radicals: reductive deuteration using SmI₂ and D₂O. Chemical Communications, 2021, 57, 5195-5198.	4.1	11
64	Application of Indazolin-3-ylidenes in Catalysis: Steric Tuning of Nonclassical Formally Normal N-Heterocyclic Carbenes with Dual Electronic Character for Catalysis. Organometallics, 2022, 41, 1115-1124.	2.3	11
65	Redox switching hysteresis in polyanilineâ€“acetate systems: a search of molecular factors important for the dynamics of the polymer reaction. Journal of Electroanalytical Chemistry, 2004, 571, 51-57.	3.8	10
66	Comparison of infrared attenuated total reflection and Raman spectroscopy in the quantitative analysis of diclofenac sodium in tablets. Vibrational Spectroscopy, 2011, 57, 157-157.	2.2	10
67	Quantitative Determination of Prednisone in Tablets by Infrared Attenuated Total Reflection and Raman Spectroscopy. Journal of AOAC INTERNATIONAL, 2012, 95, 744-750.	1.5	10
68	Quantitative analysis of thiamine hydrochloride in tabletsâ€”Comparison of infrared attenuated total reflection, diffuse reflectance infrared and Raman spectroscopy. Vibrational Spectroscopy, 2012, 62, 10-16.	2.2	10
69	Modeling red coral (Corallium rubrum) and African snail (Helixia aspersa) shell pigments: Raman spectroscopy versus DFT studies. Journal of Raman Spectroscopy, 2016, 47, 908-916.	2.5	10
70	Determination of nutritional parameters of yoghurts by FT Raman spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 196, 413-417.	3.9	9
71	Ring-Opening Olefin Metathesis of Twisted Amides: Activation of Amide Bonds by Câ•C Cleavage. ACS Catalysis, 2020, 10, 737-742.	11.2	9
72	On the HCl and DCl complexes of methylenecyclopropane in liquid argon. Physical Chemistry Chemical Physics, 2000, 2, 3983-3991.	2.8	8

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73	Blue or red Î”Î½XH complexation shift in Xâ€“Hâ‹¯CO2 hydrogen-bonded complexes?. Chemical Physics Letters, 2011, 516, 166-170.	2.6	8
74	Determination of Antioxidant Activity and Polyphenols Content in Chips by Raman and IR Spectroscopy. Food Analytical Methods, 2017, 10, 3964-3971.	2.6	8
75	Quantification of active ingredients in pharmaceutical suspensions by FT Raman spectroscopy. Vibrational Spectroscopy, 2017, 93, 57-64.	2.2	8
76	Simple transformation of spectra to effectively reduce quantification errors in FT-Raman multivariate analysis of complex systems. Vibrational Spectroscopy, 2009, 49, 298-302.	2.2	7
77	Quantitative Determination of Vitamins A and E in Ointments Using Raman Spectroscopy. Processes, 2021, 9, 8.	2.8	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. Journal of AOAC INTERNATIONAL, 2011, 94, 743-749.	1.5	5
79	Why the Î”Î½_{CH} blue shift is larger in chloral than in dichloroacetyl chloride dimers?. Journal of Raman Spectroscopy, 2011, 42, 1185-1192.	2.5	5
80	Modeling of Antioxidant Activity, Polyphenols and Macronutrients Content of Bee Pollen Applying Solid-State 13C NMR Spectra. Antioxidants, 2021, 10, 1123.	5.1	4
81	Quantification of Salicylates and Flavonoids in Poplar Bark and Leaves Based on IR, NIR, and Raman Spectra. Molecules, 2022, 27, 3954.	3.8	4
82	Quantitative analysis of solid samples using modified specular reflectance accessory. Talanta, 2016, 161, 655-659.	5.5	3
83	Silver(I) chloride-polypyrrole composite: electrochemical preparation, characterization, and application as a SERS platform. Journal of Solid State Electrochemistry, 2017, 21, 823-832.	2.5	3
84	Structures of the Most Twisted Thioamide and Selenoamide: Effect of Higher Chalcogens of Twisted Amides on Nâˆ’C(X) Resonance. Angewandte Chemie - International Edition, 2022, 61, .	13.8	3
85	On the blue-shifting hydrogen bond in tribromoacetaldehyde dimers. Chemical Physics Letters, 2011, 514, 49-53.	2.6	2
86	Electrocrystallization of silver nanoparticles from silver halides in polypyrrole evidenced by their SERS activityâ€”thermodynamic and kinetic conditions. Journal of Solid State Electrochemistry, 2018, 22, 3933-3945.	2.5	2
87	pH determination of small sample volumes using Raman spectra of azo dyes. Journal of Molecular Structure, 2022, 1253, 132226.	3.6	2
88	ATR-IR Spectroscopy Application to Diagnostic Screening of Advanced Endometriosis. Oxidative Medicine and Cellular Longevity, 2022, 2022, 1-13.	4.0	2
89	Structures and energetic properties of 4-halobenzamides. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1395-1402.	0.5	1