

Yukihio Ozaki

List of Publications by Year in descending order

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437
papers

19,417
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15880

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503
all docs

503
docs citations

503
times ranked

16515
citing authors

#	ARTICLE	IF	CITATIONS
1	Surface-enhanced Raman scattering (SERS) Sensing of Biomedicine and Biomolecules. , 2023, , 441-455.		1
2	A new approach to removing interference of moisture from FTIR spectrum. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 265, 120373.	2.0	11
3	Solvent Effect on Assembling and Interactions in Solutions of Phenol: Infrared Spectroscopic and Density Functional Theory Study. Applied Spectroscopy, 2022, 76, 28-37.	1.2	7
4	Novel Method for Extracting the Spectrum of a Supramolecular Complex via a Comprehensive Approach Involving Two-Dimensional Correlation Spectroscopy, Genetic Algorithm, and Grid Searching. Analytical Chemistry, 2022, 94, 2348-2355.	3.2	3
5	Random swapping, an effective and efficient way to boost the intensities of cross peaks in a 2D asynchronous spectrum. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 272, 120968.	2.0	0
6	An investigation of the effect of high-pressure on charge transfer in dye-sensitized solar cells based on surface-enhanced Raman spectroscopy. Nanoscale, 2022, 14, 373-381.	2.8	2
7	Experimental verification of increased electronic excitation energy of water in hydrate-melt water by attenuated total reflection-far-ultraviolet spectroscopy. Journal of Chemical Physics, 2022, 156, 074705.	1.2	3
8	Attenuated Total Reflection Far-Ultraviolet (ATR-FUV) Spectroscopy is a Sensitive Tool for Investigation of Protein Adsorption. Applied Spectroscopy, 2022, 76, 793-800.	1.2	1
9	<i>In situ</i> SERS monitoring of intracellular H ₂ O ₂ in single living cells based on label-free bifunctional Fe ₃ O ₄ @Ag nanoparticles. Analyst, The, 2022, 147, 1815-1823.	1.7	9
10	Progress of tip-enhanced Raman scattering for the last two decades and its challenges in very recent years. Nanoscale, 2022, 14, 5265-5288.	2.8	18
11	NIR spectroscopy – What a wonderful world!. NIR News, 2022, 33, 10-17.	1.6	1
12	A Study of C=O⋯HO and OH⋯OH (Dimer, Trimer, and Oligomer) Hydrogen Bonding in a Poly(4-vinylphenol) 30%/Poly(methyl methacrylate) 70% Blend and its Thermal Behavior Using Near-Infrared Spectroscopy and Infrared Spectroscopy. Applied Spectroscopy, 2022, 76, 831-840.	1.2	2
13	3D SERS Imaging of Nanoporous Gold-Silver Microstructures: Exploring the Formation Mechanism Based on Galvanic Replacement Reaction. Journal of Physical Chemistry C, 2022, 126, 5617-5627.	1.5	2
14	Two types of C=O⋯HO hydrogen bonds and OH⋯OH (dimer, trimer, oligomer) hydrogen bonds in PVA with 88% saponification/PMMA and PVA with 99% saponification/PMMA blends and their thermal behavior studied by infrared spectroscopy. Polymer, 2022, 246, 124725.	1.8	14
15	Association and solubility of chlorophenols in CCl ₄ : MIR/NIR spectroscopic and DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 274, 121077.	2.0	0
16	Determination of the Influence of Various Factors on the Character of Surface Functionalization of Copper(I) and Copper(II) Oxide Nanosensors with Phenylboronic Acid Derivatives. Langmuir, 2022, 38, 557-568.	1.6	2
17	New Insights of Charge Transfer at Metal/Semiconductor Interfaces for Hot-Electron Generation Studied by Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 3571-3578.	2.1	4
18	Deprotonation from an OH on <i>myo</i> -Inositol Promoted by $\frac{1}{4}$ -Bridges with Possible Regioselectivity/Chiral Selectivity. Inorganic Chemistry, 2022, 61, 6138-6148.	1.9	1

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19	Development of an amino acid sequence-dependent analytical method for peptides using near-infrared spectroscopy. <i>Analyst</i> , The, 2022, 147, 3634-3642.	1.7	6
20	In-situ fingerprinting phosphorylated proteins via surface-enhanced Raman spectroscopy: Single-site discrimination of Tau biomarkers in Alzheimer's disease. <i>Biosensors and Bioelectronics</i> , 2021, 171, 112748.	5.3	22
21	Method of Monitoring the Number of Amide Bonds in Peptides Using Near-Infrared Spectroscopy. <i>Analytical Chemistry</i> , 2021, 93, 2758-2766.	3.2	9
22	Intensity Enhancement of a Two-Dimensional Asynchronous Spectrum Without Noise Level Fluctuation Escalation Using a One-Dimensional Spectra Sequence Change. <i>Applied Spectroscopy</i> , 2021, 75, 422-433.	1.2	7
23	Recent advances in surface-enhanced Raman scattering-based sensors for the detection of inorganic ions: Sensing mechanism and beyond. <i>Journal of Raman Spectroscopy</i> , 2021, 52, 468-481.	1.2	22
24	Advances, challenges and perspectives of quantum chemical approaches in molecular spectroscopy of the condensed phase. <i>Chemical Society Reviews</i> , 2021, 50, 10917-10954.	18.7	34
25	Solvent effect on the competition between weak and strong interactions in phenol solutions studied by near-infrared spectroscopy and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19188-19194.	1.3	9
26	Half-raspberry-like bimetallic nanoassembly: Interstitial dependent correlated surface plasmon resonances and surface-enhanced Raman spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23875-23885.	1.3	4
27	Investigation on the luminescence behavior of terbium acetylsalicylate/bilirubin system via 2D-COS approaches. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 251, 119427.	2.0	6
28	ATR-far-ultraviolet spectroscopy in the condensed phase—The present status and future perspectives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119549.	2.0	14
29	Electric field analysis, polarization, excitation wavelength dependence, and novel applications of tip-enhanced Raman scattering. <i>Journal of Raman Spectroscopy</i> , 2021, 52, 1997-2017.	1.2	7
30	Understanding phase transition and vibrational mode coupling in ammonium nitrate using 2D correlation Raman spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119581.	2.0	9
31	Anharmonic DFT Study of Near-Infrared Spectra of Caffeine: Vibrational Analysis of the Second Overtones and Ternary Combinations. <i>Molecules</i> , 2021, 26, 5212.	1.7	12
32	Infrared Spectroscopy—Mid-infrared, Near-infrared, and Far-infrared/Terahertz Spectroscopy. <i>Analytical Sciences</i> , 2021, 37, 1193-1212.	0.8	42
33	Far-Ultraviolet Spectroscopy and Quantum Chemical Calculation Studies of the Conformational Dependence on the Electronic Structure and Transitions of Cyclohexane, Methyl and Dimethyl Cyclohexane, and Decalin; Effects of Axial Substitutions on the Electronic Transitions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8205-8214.	1.1	3
34	Effect of Raman exposure time on the quantitative and discriminant analyses of carotenoid concentrations in intact tomatoes. <i>Food Chemistry</i> , 2021, 360, 129896.	4.2	12
35	MCR-ALS with sample insertion constraint to enhance the sensitivity of surface-enhanced Raman scattering detection. <i>Analyst</i> , The, 2021, 146, 3251-3262.	1.7	8
36	Hollow Multi-Shelled V_2O_5 Microstructures Integrating Multiple Synergistic Resonances for Enhanced Semiconductor SERS. <i>Advanced Optical Materials</i> , 2021, 9, 2101866.	3.6	22

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37	Editorial: Novel SERS-Active Materials and Substrates: Sensing and (Bio)applications. <i>Frontiers in Chemistry</i> , 2021, 9, 784735.	1.8	0
38	Surface-enhanced Raman spectroscopy. <i>Nature Reviews Methods Primers</i> , 2021, 1, .	11.8	183
39	Present and Future of Surface-Enhanced Raman Scattering. <i>ACS Nano</i> , 2020, 14, 28-117.	7.3	2,153
40	Sample- \times Sample Correlation Asynchronous Spectroscopic Method Coupled with Multivariate Curve Resolution-Alternating Least Squares To Analyze Challenging Bilinear Data. <i>Analytical Chemistry</i> , 2020, 92, 1477-1484.	3.2	12
41	Iodine staining as a useful probe for distinguishing insulin amyloid polymorphs. <i>Scientific Reports</i> , 2020, 10, 16741.	1.6	8
42	Nitrosonaphthol reaction-assisted SERS assay for selective determination of 5-hydroxyindole-3-acetic acid in human urine. <i>Analytica Chimica Acta</i> , 2020, 1134, 34-40.	2.6	10
43	Exploration of Insulin Amyloid Polymorphism Using Raman Spectroscopy and Imaging. <i>Biophysical Journal</i> , 2020, 118, 2997-3007.	0.2	12
44	Accurate Monitoring Platform for the Surface Catalysis of Nanozyme Validated by Surface-Enhanced Raman-Kinetics Model. <i>Analytical Chemistry</i> , 2020, 92, 11763-11770.	3.2	36
45	Identification of systematic absence of cross-peaks (SACPs) in a two-dimensional asynchronous Spectrum using an auxiliary 2D quotient Spectrum and a statistical test. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 243, 118789.	2.0	11
46	A Chiral-Label-Free SERS Strategy for the Synchronous Chiral Discrimination and Identification of Small Aromatic Molecules. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19079-19086.	7.2	40
47	A Chiral-Label-Free SERS Strategy for the Synchronous Chiral Discrimination and Identification of Small Aromatic Molecules. <i>Angewandte Chemie</i> , 2020, 132, 19241-19248.	1.6	7
48	SERS Blinking on Anisotropic Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20328-20339.	1.5	5
49	Innentitelbild: A Chiral-Label-Free SERS Strategy for the Synchronous Chiral Discrimination and Identification of Small Aromatic Molecules (<i>Angew. Chem.</i> 43/2020). <i>Angewandte Chemie</i> , 2020, 132, 18982-18982.	1.6	0
50	Attenuated total reflectance far-ultraviolet and deep-ultraviolet spectroscopy analysis of the electronic structure of a dicyanamide-based ionic liquid with Li ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21768-21775.	1.3	7
51	Theoretical Modeling of Electronic Structures of Polyiodide Species Included in β -Cyclodextrin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4089-4096.	1.2	13
52	Assessment of Embryonic Bioactivity through Changes in the Water Structure Using Near-Infrared Spectroscopy and Imaging. <i>Analytical Chemistry</i> , 2020, 92, 8133-8141.	3.2	14
53	Distinguishing Enantiomers by Tip-Enhanced Raman Scattering: Chemically Modified Silver Tip with an Asymmetric Atomic Arrangement. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14564-14569.	7.2	9
54	Enhanced Surface Plasmon Resonance Wavelength Shifts by Molecular Electronic Absorption in Far- and Deep-Ultraviolet Regions. <i>Scientific Reports</i> , 2020, 10, 9938.	1.6	14

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55	Distinguishing Enantiomers by Tip-Enhanced Raman Scattering: Chemically Modified Silver Tip with an Asymmetric Atomic Arrangement. <i>Angewandte Chemie</i> , 2020, 132, 14672-14677.	1.6	1
56	Lipid Droplet Composition Varies Based on Medaka Fish Eggs Development as Revealed by NIR-, MIR-, and Raman Imaging. <i>Molecules</i> , 2020, 25, 817.	1.7	12
57	Near-infrared spectroscopy and imaging in protein research. , 2020, , 143-176.		10
58	Interactions Between Epitaxial Graphene Grown on the Si- and C-Faces of 4H-SiC Investigated Using Raman Imaging and Tip-Enhanced Raman Scattering. <i>Applied Spectroscopy</i> , 2020, 74, 1384-1390.	1.2	4
59	Glucose Monitoring in Cell Culture with Online Ultrasound-Assisted Near-Infrared Spectroscopy. <i>Analytical Chemistry</i> , 2020, 92, 2946-2952.	3.2	15
60	Solvation effects on wavenumbers and absorption intensities of the OH-stretch vibration in phenolic compounds $\hat{=}$ electrical- and mechanical anharmonicity <i>via</i> a combined DFT/Numerov approach. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13017-13029.	1.3	14
61	Advances in Molecular Spectroscopy in Condensed Phase and Quantum Chemistry. <i>Molecular Science</i> , 2020, 14, A0114.	0.2	0
62	Reusable Silicon-Based SERS Chip for Ratiometric Analysis of Fluoride Ion in Aqueous Solutions. <i>ACS Sensors</i> , 2019, 4, 2336-2342.	4.0	34
63	Plasmon-Enhanced Optical Tweezers for Single Molecules on and near a Colloidal Silver Nanoaggregate. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18001-18006.	1.5	21
64	Enhanced Raman Scattering by ZnO Superstructures: Synergistic Effect of Charge Transfer and Mie Resonances. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 14452-14456.	7.2	133
65	A chiral signal-amplified sensor for enantioselective discrimination of amino acids based on charge transfer-induced SERS. <i>Chemical Communications</i> , 2019, 55, 9697-9700.	2.2	29
66	Enhanced Raman Scattering by ZnO Superstructures: Synergistic Effect of Charge Transfer and Mie Resonances. <i>Angewandte Chemie</i> , 2019, 131, 14594-14598.	1.6	15
67	Innenr¼cktitelbild: Enhanced Raman Scattering by ZnO Superstructures: Synergistic Effect of Charge Transfer and Mie Resonances (<i>Angew. Chem.</i> 41/2019). <i>Angewandte Chemie</i> , 2019, 131, 14915-14915.	1.6	0
68	Crystallization of poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) during melt extrusion promoted by residual crystals. <i>Polymer Crystallization</i> , 2019, 2, e10076.	0.5	6
69	Functional nanomaterials with unique enzyme-like characteristics for sensing applications. <i>Journal of Materials Chemistry B</i> , 2019, 7, 850-875.	2.9	155
70	IR Spectra of Crystalline Nucleobases: Combination of Periodic Harmonic Calculations with Anharmonic Corrections Based on Finite Models. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10001-10013.	1.2	18
71	Phosphoric acid and phosphorylation levels are potential biomarkers indicating developmental competence of matured oocytes. <i>Analyst, The</i> , 2019, 144, 1527-1534.	1.7	7
72	CTAB-triggered Ag aggregates for reproducible SERS analysis of urinary polycyclic aromatic hydrocarbon metabolites. <i>Chemical Communications</i> , 2019, 55, 2146-2149.	2.2	30

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73	A novel systematic absence of cross peaks-based 2D-COS approach for bilinear data. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 220, 117103.	2.0	19
74	Low-Frequency Vibrational Modes of Nylon 6 Studied by Using Infrared and Raman Spectroscopies and Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5368-5376.	1.2	23
75	Recent Advances in Molecular Spectroscopy of Electronic and Vibrational Transitions in Condensed Phase and Its Application to Chemistry. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 629-654.	2.0	28
76	A Novel Approach Based on Two-Dimensional Correlation Spectroscopy to Determine the Stoichiometric Ratio of Two Substances Involved in Intermolecular Interactions. <i>Applied Spectroscopy</i> , 2019, 73, 1051-1060.	1.2	12
77	Overtone of $\frac{1}{2}C\alpha\%_iN$ Vibration as a Probe of Structure of Liquid CH_3CN , CD_3CN , and CCl_3CN : Combined Infrared, Near-Infrared, and Raman Spectroscopic Studies with Anharmonic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4431-4442.	1.1	27
78	A preliminary study on constructing a high-dimensional asynchronous spectrum to analyze bilinear data. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 216, 76-84.	2.0	14
79	Effect of TiO_2 on Altering Direction of Interfacial Charge Transfer in a TiO_2 -Ag-MPY-FePc System by SERS. <i>Angewandte Chemie</i> , 2019, 131, 8256-8260.	1.6	12
80	Effect of TiO_2 on Altering Direction of Interfacial Charge Transfer in a TiO_2 -Ag-MPY-FePc System by SERS. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8172-8176.	7.2	66
81	Distinct Difference in Sensitivity of NIR vs. IR Bands of Melamine to Inter-Molecular Interactions with Impact on Analytical Spectroscopy Explained by Anharmonic Quantum Mechanical Study. <i>Molecules</i> , 2019, 24, 1402.	1.7	38
82	Simulated NIR spectra as sensitive markers of the structure and interactions in nucleobases. <i>Scientific Reports</i> , 2019, 9, 17398.	1.6	20
83	NIR spectroscopy research in the Ozaki group for the last 30 years. <i>NIR News</i> , 2019, 30, 16-20.	1.6	1
84	Nickel Nanowires Combined with Surface-Enhanced Raman Spectroscopy: Application in Label-Free Detection of Cytochrome c-Mediated Apoptosis. <i>Analytical Chemistry</i> , 2019, 91, 1213-1216.	3.2	24
85	FT-IR Spectroscopic Imaging of Endothelial Cells Response to Tumor Necrosis Factor- α : To Follow Markers of Inflammation Using Standard and High-Magnification Resolution. <i>Analytical Chemistry</i> , 2018, 90, 3727-3736.	3.2	12
86	<i>In situ</i> formation of SERS hot spots by a bis-quaternized perylene dye: a simple strategy for highly sensitive detection of heparin over a wide concentration range. <i>Analyst</i> , 2018, 143, 1899-1905.	1.7	21
87	Noninvasive, high-speed, near-infrared imaging of the biomolecular distribution and molecular mechanism of embryonic development in fertilized fish eggs. <i>Journal of Biophotonics</i> , 2018, 11, e201700115.	1.1	17
88	Three different kinds of weak C-H \cdots O=C inter- and intramolecular interactions in poly(μ -caprolactone) studied by using terahertz spectroscopy, infrared spectroscopy and quantum chemical calculations. <i>Polymer</i> , 2018, 137, 245-254.	1.8	44
89	Tip-Enhanced Raman Scattering in Liquid/Solution. , 2018, , 299-321.		3
90	Exploring the difference in xerogels and organogels through <i>in situ</i> observation. <i>Royal Society Open Science</i> , 2018, 5, 170492.	1.1	6

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91	An Application for the Quantitative Analysis of Pharmaceutical Tablets Using a Rapid Switching System Between a Near-Infrared Spectrometer and a Portable Near-Infrared Imaging System Equipped with Fiber Optics. <i>Applied Spectroscopy</i> , 2018, 72, 551-561.	1.2	14
92	Novel Method of Constructing Two-Dimensional Correlation Spectroscopy without Subtracting a Reference Spectrum. <i>Journal of Physical Chemistry A</i> , 2018, 122, 788-797.	1.1	19
93	Nonstaining Blood Flow Imaging Using Optical Interference Due to Doppler Shift and Near-Infrared Imaging of Molecular Distribution in Developing Fish Egg Embryos. <i>Analytical Chemistry</i> , 2018, 90, 5217-5223.	3.2	19
94	Excitation wavelength selection for quantitative analysis of carotenoids in tomatoes using Raman spectroscopy. <i>Food Chemistry</i> , 2018, 258, 308-313.	4.2	37
95	Rydberg transitions as a probe for structural changes and phase transition at polymer surfaces: an ATR-FUV-DUV and quantum chemical study of poly(3-hydroxybutyrate) and its nanocomposite with graphene. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8859-8873.	1.3	20
96	Advances in Far-Ultraviolet Spectroscopy in the Solid and Liquid States. , 2018, , 251-285.		12
97	Study on phase separation in an ultra-thin poly(methyl methacrylate)/poly(4-vinyl phenol) film by infrared reflection absorption spectroscopy. <i>Polymer</i> , 2018, 135, 69-75.	1.8	4
98	Electronic Spectra of Graphene in Far- and Deep-Ultraviolet Region: Attenuated Total Reflection Spectroscopy and Quantum Chemical Calculation Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28998-29008.	1.5	9
99	Blinking Surface-Enhanced Raman Scattering and Fluorescence From a Single Silver Nanoaggregate Simultaneously Analyzed by Bi-Color Intensity Ratios and a Truncated Power Law. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22106-22113.	1.5	7
100	Design of a Novel Apparatus to Enrich Analytes via a Diffuse-Evaporation Process for HPLC-FTIR Analysis. <i>Analytical Sciences</i> , 2018, 34, 1351-1356.	0.8	3
101	Investigation of charge-transfer between a 4-mercaptobenzoic acid monolayer and TiO ₂ nanoparticles under high pressure using surface-enhanced Raman scattering. <i>Chemical Communications</i> , 2018, 54, 6280-6283.	2.2	27
102	A dual colorimetric and SERS detection of Hg ²⁺ based on the stimulus of intrinsic oxidase-like catalytic activity of Ag-CoFe ₂ O ₄ /reduced graphene oxide nanocomposites. <i>Chemical Engineering Journal</i> , 2018, 350, 120-130.	6.6	87
103	Local structural changes in graphene oxide layers induced by silver nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21498-21505.	1.3	4
104	Reduced Charge-Transfer Threshold in Dye-Sensitized Solar Cells with an Au@Ag/N ₃ -TiO ₂ Structure As Revealed by Surface-Enhanced Raman Scattering. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12748-12760.	1.5	13
105	NIR Spectra Simulations by Anharmonic DFT-Saturated and Unsaturated Long-Chain Fatty Acids. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6931-6944.	1.2	39
106	Recent Developments in Plasmon-Supported Raman Spectroscopy. , 2018, , .		22
107	Unsaturated lipid bodies as a hallmark of inflammation studied by Raman 2D and 3D microscopy. <i>Scientific Reports</i> , 2017, 7, 40889.	1.6	75
108	Low-Frequency Vibrational Modes of Poly(glycolic acid) and Thermal Expansion of Crystal Lattice Assigned On the Basis of DFT-Spectral Simulation Aided with a Fragment Method. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1128-1138.	1.2	33

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109	Analysis of blinking from multicoloured SERS-active Ag colloidal nanoaggregates with poly-L-lysine via truncated power law. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 570-577.	1.2	9
110	Semiconductor-enhanced Raman scattering: active nanomaterials and applications. <i>Nanoscale</i> , 2017, 9, 4847-4861.	2.8	289
111	Terahertz Imaging of the Distribution of Crystallinity and Crystalline Orientation in a Poly(ϵ -caprolactone) Film. <i>Applied Spectroscopy</i> , 2017, 71, 1537-1542.	1.2	17
112	Charge Transfer at the TiO ₂ /N ₃ /Ag Interface Monitored by Surface-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5145-5153.	1.5	11
113	Influence of Non-fundamental Modes on Mid-infrared Spectra: Anharmonic DFT Study of Aliphatic Ethers. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1412-1424.	1.1	27
114	Facile synthesis of silver nanoparticles/carbon dots for a charge transfer study and peroxidase-like catalytic monitoring by surface-enhanced Raman scattering. <i>Applied Surface Science</i> , 2017, 410, 42-50.	3.1	34
115	Non-destructive monitoring of mouse embryo development and its qualitative evaluation at the molecular level using Raman spectroscopy. <i>Scientific Reports</i> , 2017, 7, 43942.	1.6	25
116	Changes in the Electronic States of Low-Temperature Solid <i>n</i> -Tetradecane: Decrease in the HOMO-LUMO Gap. <i>ACS Omega</i> , 2017, 2, 618-625.	1.6	25
117	Distribution of Polymorphic Crystals in the Ring-Banded Spherulites of Poly(butylene adipate) Studied Using High-Resolution Raman Imaging. <i>Macromolecules</i> , 2017, 50, 3377-3387.	2.2	18
118	The Born-Oppenheimer molecular simulations of infrared spectra of crystalline poly-(R)-3-hydroxybutyrate with analysis of weak C-H \cdots O C hydrogen bonds. <i>Chemical Physics Letters</i> , 2017, 678, 112-118.	1.2	11
119	Correlations between Structure and Near-Infrared Spectra of Saturated and Unsaturated Carboxylic Acids. Insight from Anharmonic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3437-3451.	1.1	64
120	Reinvestigation of the β -to- α Crystal Phase Transition of Poly(butylene adipate) by the Time-Resolved X-ray Scattering and FTIR Spectral Measurements in the Temperature-Jump Process. <i>Macromolecules</i> , 2017, 50, 3883-3889.	2.2	35
121	Polarization dependence of tip-enhanced Raman and plasmon-resonance Rayleigh scattering spectra. <i>Applied Physics Letters</i> , 2017, 110, 233104.	1.5	7
122	Spectra-structure correlations of saturated and unsaturated medium-chain fatty acids. Near-infrared and anharmonic DFT study of hexanoic acid and sorbic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 35-44.	2.0	38
123	Investigation on intermolecular interaction between berberine and β -cyclodextrin by 2D UV-Vis asynchronous spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 343-348.	2.0	18
124	Critical Evaluation of NIR and ATR-IR Spectroscopic Quantifications of Rosmarinic Acid in Rosmarini folium Supported by Quantum Chemical Calculations. <i>Planta Medica</i> , 2017, 83, 1076-1084.	0.7	25
125	Temperature Drift of Conformational Equilibria of Butyl Alcohols Studied by Near-Infrared Spectroscopy and Fully Anharmonic DFT. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1950-1961.	1.1	48
126	Infrared Spectroscopy and Born-Oppenheimer Molecular Dynamics Simulation Study on Deuterium Substitution in the Crystalline Benzoic Acid. <i>Journal of Physical Chemistry B</i> , 2017, 121, 479-489.	1.2	9

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127	Critical evaluation of spectral information of benchtop vs. portable near-infrared spectrometers: quantum chemistry and two-dimensional correlation spectroscopy for a better understanding of PLS regression models of the rosmarinic acid content in Rosmarini folium. <i>Analyst, The</i> , 2017, 142, 455-464.	1.7	94
128	Rapid analysis of chemical composition in intact and milled rice cookies using near infrared spectroscopy. <i>Journal of Near Infrared Spectroscopy</i> , 2017, 25, 330-337.	0.8	17
129	Spectroscopic and Quantum Mechanical Calculation Study of the Effect of Isotopic Substitution on NIR Spectra of Methanol. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7925-7936.	1.1	29
130	Investigation on the Behavior of Noise in Asynchronous Spectra in Generalized Two-Dimensional (2D) Correlation Spectroscopy and Application of Butterworth Filter in the Improvement of Signal-to-Noise Ratio of 2D Asynchronous Spectra. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7524-7533.	1.1	21
131	Unveiling the Aggregation of Lycopene in Vitro and in Vivo: UV-Vis, Resonance Raman, and Raman Imaging Studies. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8046-8057.	1.2	35
132	Interpretation of the $\tilde{\nu}_{\text{OH}}$ transition of hydrated protons in aqueous solutions observed in the far-UV region with quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21490-21499.	1.3	6
133	Temperature compensation for determination of moisture and reducing sugar of longan honey by near infrared spectroscopy. <i>Journal of Near Infrared Spectroscopy</i> , 2017, 25, 36-44.	0.8	18
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