

Justyna Grabska

List of Publications by Year in descending order

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55
papers

1,576
citations

279798

23
h-index

315739

38
g-index

63
all docs

63
docs citations

63
times ranked

779
citing authors

#	ARTICLE	IF	CITATIONS
1	Near-Infrared Spectroscopy in Bio-Applications. <i>Molecules</i> , 2020, 25, 2948.	3.8	185
2	Principles and Applications of Miniaturized Near-Infrared (NIR) Spectrometers. <i>Chemistry - A European Journal</i> , 2021, 27, 1514-1532.	3.3	169
3	Biomolecular and bioanalytical applications of infrared spectroscopy – A review. <i>Analytica Chimica Acta</i> , 2020, 1133, 150-177.	5.4	107
4	Handheld near-infrared spectrometers: Where are we heading?. <i>NIR News</i> , 2020, 31, 28-35.	0.3	96
5	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.	2.5	64
6	Miniaturized NIR Spectroscopy in Food Analysis and Quality Control: Promises, Challenges, and Perspectives. <i>Foods</i> , 2022, 11, 1465.	4.3	64
7	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.	2.5	48
8	NIR spectroscopy of natural medicines supported by novel instrumentation and methods for data analysis and interpretation. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2021, 193, 113686.	2.8	43
9	NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features. <i>Journal of Molecular Liquids</i> , 2018, 268, 895-902.	4.9	42
10	NIR Spectra Simulations by Anharmonic DFT-Saturated and Unsaturated Long-Chain Fatty Acids. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6931-6944.	2.6	39
11	<i>Theae nigrae folium</i> : Comparing the analytical performance of benchtop and handheld near-infrared spectrometers. <i>Talanta</i> , 2021, 221, 121165.	5.5	39
12	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.	3.9	38
13	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.	3.8	38
14	Near-infrared spectroscopy in quality control of <i>Piper nigrum</i> : A comparison of performance of benchtop and handheld spectrometers. <i>Talanta</i> , 2021, 223, 121809.	5.5	36
15	Principles and Applications of Vibrational Spectroscopic Imaging in Plant Science: A Review. <i>Frontiers in Plant Science</i> , 2020, 11, 1226.	3.6	35
16	Spectra-structure correlations in NIR region: Spectroscopic and anharmonic DFT study of n-hexanol, cyclohexanol and phenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 197, 176-184.	3.9	33
17	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.	2.5	29
18	Near-Infrared Spectroscopy as a Rapid Screening Method for the Determination of Total Anthocyanin Content in <i>Sambucus Fructus</i> . <i>Sensors</i> , 2020, 20, 4983.	3.8	29

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19	Challenging handheld NIR spectrometers with moisture analysis in plant matrices: Performance of PLSR vs. GPR vs. ANN modelling. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119342.	3.9	29
20	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.	2.5	27
21	Current and future research directions in computer-aided near-infrared spectroscopy: A perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119625.	3.9	26
22	Spectra-structure correlations in NIR region of polymers from quantum chemical calculations. The cases of aromatic ring, C=O, C-N and C-Cl functionalities. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 262, 120085.	3.9	26
23	Insect Protein Content Analysis in Handcrafted Fitness Bars by NIR Spectroscopy. Gaussian Process Regression and Data Fusion for Performance Enhancement of Miniaturized Cost-Effective Consumer-Grade Sensors. <i>Molecules</i> , 2021, 26, 6390.	3.8	25
24	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.	2.8	20
25	Simulated NIR spectra as sensitive markers of the structure and interactions in nucleobases. <i>Scientific Reports</i> , 2019, 9, 17398.	3.3	20
26	Theoretical Simulation of Near-Infrared Spectrum of Piperine: Insight into Band Origins and the Features of Regression Models. <i>Applied Spectroscopy</i> , 2021, 75, 1022-1032.	2.2	20
27	Spectra-Structure Correlations in Isotopomers of Ethanol (CX ₃ CX ₂ OX; X = H, D): Combined Near-Infrared and Anharmonic Computational Study. <i>Molecules</i> , 2019, 24, 2189.	3.8	19
28	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.	2.6	18
29	Vibrational coupling to hydration shell - Mechanism to performance enhancement of qualitative analysis in NIR spectroscopy of carbohydrates in aqueous environment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 237, 118359.	3.9	17
30	Effect of conformational isomerism on NIR spectra of ethanol isotopologues. Spectroscopic and anharmonic DFT study. <i>Journal of Molecular Liquids</i> , 2020, 310, 113271.	4.9	14
31	Rapid discrimination of <i>Curcuma longa</i> and <i>Curcuma xanthorrhiza</i> using Direct Analysis in Real Time Mass Spectrometry and Near Infrared Spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120347.	3.9	14
32	In silico NIR spectroscopy - A review. Molecular fingerprint, interpretation of calibration models, understanding of matrix effects and instrumental difference. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 279, 121438.	3.9	13
33	Quantum chemical calculation of NIR spectra of practical materials. <i>NIR News</i> , 2017, 28, 13-20.	0.3	12
34	Anharmonic DFT Study of Near-Infrared Spectra of Caffeine: Vibrational Analysis of the Second Overtones and Ternary Combinations. <i>Molecules</i> , 2021, 26, 5212.	3.8	12
35	Computational and quantum chemical study on high-frequency dielectric function of tert-butylmethyl ether in mid-infrared and near-infrared regions. <i>Journal of Molecular Liquids</i> , 2016, 224, 1189-1198.	4.9	9
36	Advances in Anharmonic Methods and Their Applications to Vibrational Spectroscopies. , 2018, , 483-512.		9

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37	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.	3.1	9
38	Physical principles of infrared spectroscopy. <i>Comprehensive Analytical Chemistry</i> , 2022, , 1-43.	1.3	9
39	Infrared dispersion of liquid di-n-propylether. <i>Journal of Molecular Liquids</i> , 2013, 181, 127-132.	4.9	6
40	Quantification of Silymarin in <i>Silybi mariani fructus</i> : Challenging the Analytical Performance of Benchtop vs. Handheld NIR Spectrometers on Whole Seeds. <i>Planta Medica</i> , 2022, 88, 20-32.	1.3	6
41	Current frontiers in quantum chemical simulations of NIR spectra – Polymers, biomolecules, aqueous matrix and interpretation of instrumental difference of handheld spectrometers. <i>NIR News</i> , 2021, 32, 7-14.	0.3	5
42	Anharmonicity and Spectra – Structure Correlations in MIR and NIR Spectra of Crystalline Menadione (Vitamin K3). <i>Molecules</i> , 2021, 26, 6779.	3.8	5
43	Dielectric functions of iso -propanol and di- iso -propylether in the infrared. <i>Journal of Molecular Liquids</i> , 2015, 203, 143-152.	4.9	3
44	Quantum mechanically calculated NIR spectra of fatty acids. <i>NIR News</i> , 2017, 28, 11-16.	0.3	3
45	Computer simulations of NIR spectra of thymol – Towards linking basic and analytical NIRS. <i>NIR News</i> , 2018, 29, 13-16.	0.3	3
46	Quantum mechanical simulations of near-infrared spectra of biomolecules – Long-chain fatty acids. <i>NIR News</i> , 2018, 29, 13-19.	0.3	3
47	Issues in Hyperspectral Traceability of Foods. , 2021, , 258-289.		2
48	Novel near-infrared and Raman spectroscopic technologies for print and photography identification, classification, and authentication. <i>NIR News</i> , 2021, 32, 11-16.	0.3	2
49	Near-Infrared (NIR) Sensors in Environmental Analysis. , 2021, , .		2
50	On optimization of absorption – dispersion spectra. <i>Journal of Molecular Structure</i> , 2016, 1126, 11-18.	3.6	1
51	Scald-Cold: Joint Austrian-Italian consortium in the Euregio project for the comprehensive dissection of the superficial scald in apples. <i>NIR News</i> , 2020, 31, 5-9.	0.3	1
52	The comprehensive sourcebook for modern NIR spectroscopy: A commentary on – Near-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applications – <i>NIR News</i> , 2021, 32, 5-10.	0.3	1
53	Infrared and near-infrared spectroscopic techniques for the quality control of herbal medicines. , 2022, , 603-627.		1
54	The essential role of omni-capable research laboratories in advancing analytical spectroscopy. <i>NIR News</i> , 2019, 30, 30-34.	0.3	0

#	ARTICLE	IF	CITATIONS
55	The fundamental handbook for analytical spectroscopy. Release of the second edition of "Chemometrics in spectroscopy"™ by Howard Mark and Jerry Workman, Jr. and its impact on the spectroscopic community. NIR News, 2019, 30, 11-13.	0.3	0