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	Rapid discrimination of Curcuma longa and Curcuma xanthorrhiza using Direct Analysis in Real Time Mass Spectrometry and Near Infrared Spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 265, 120347.	3.9	14
2	Quantification of Silymarin in Silybi mariani fructus: Challenging the Analytical Performance of Benchtop vs. Handheld NIR Spectrometers on Whole Seeds. Planta Medica, 2022, 88, 20-32.	1.3	6
3	Physical principles of infrared spectroscopy. Comprehensive Analytical Chemistry, 2022, , 1-43.	1.3	9
4	Miniaturized NIR Spectroscopy in Food Analysis and Quality Control: Promises, Challenges, and Perspectives. Foods, 2022, 11, 1465.	4.3	64
5	In silico NIR spectroscopy â€“ A review. Molecular fingerprint, interpretation of calibration models, understanding of matrix effects and instrumental difference. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 279, 121438.	3.9	13
6	Infrared and near-infrared spectroscopic techniques for the quality control of herbal medicines. , 2022, , 603-627.		1
7	Theae nigrae folium: Comparing the analytical performance of benchtop and handheld near-infrared spectrometers. Talanta, 2021, 221, 121165.	5.5	39
8	Near-infrared spectroscopy in quality control of Piper nigrum: A comparison of performance of benchtop and handheld spectrometers. Talanta, 2021, 223, 121809.	5.5	36
9	Issues in Hyperspectral Traceability of Foods. , 2021, , 258-289.		2
10	Challenging handheld NIR spectrometers with moisture analysis in plant matrices: Performance of PLSR vs. GPR vs. ANN modelling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119342.	3.9	29
11	NIR spectroscopy of natural medicines supported by novel instrumentation and methods for data analysis and interpretation. Journal of Pharmaceutical and Biomedical Analysis, 2021, 193, 113686.	2.8	43
12	Principles and Applications of Miniaturized Nearâ€Infrared (NIR) Spectrometers. Chemistry - A European Journal, 2021, 27, 1514-1532.	3.3	169
13	The comprehensive sourcebook for modern NIR spectroscopy: A commentary on â€œNear-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applicationsâ€• NIR News, 2021, 32, 5-10.	0.3	1
14	Novel near-infrared and Raman spectroscopic technologies for print and photography identification, classification, and authentication. NIR News, 2021, 32, 11-16.	0.3	2
15	Current and future research directions in computer-aided near-infrared spectroscopy: A perspective. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 254, 119625.	3.9	26
16	Theoretical Simulation of Near-Infrared Spectrum of Piperine: Insight into Band Origins and the Features of Regression Models. Applied Spectroscopy, 2021, 75, 1022-1032.	2.2	20
17	Anharmonic DFT Study of Near-Infrared Spectra of Caffeine: Vibrational Analysis of the Second Overtones and Ternary Combinations. Molecules, 2021, 26, 5212.	3.8	12
18	Spectra-structure correlations in NIR region of polymers from quantum chemical calculations. The cases of aromatic ring, C=O, Câ‰¡N and C-Cl functionalities. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 262, 120085.	3.9	26

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19	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. Molecules, 2021, 26, 6390.	3.8	25
20	Current frontiers in quantum chemical simulations of NIR spectra â€“ Polymers, biomolecules, aqueous matrix and interpretation of instrumental difference of handheld spectrometers. NIR News, 2021, 32, 7-14.	0.3	5
21	Anharmonicity and Spectraâ€“Structure Correlations in MIR and NIR Spectra of Crystalline Menadione (Vitamin K3). Molecules, 2021, 26, 6779.	3.8	5
22	Near-Infrared (NIR) Sensors in Environmental Analysis. , 2021, , .		2
23	Scald-Cold: Joint Austrian-Italian consortium in the Euregio project for the comprehensive dissection of the superficial scald in apples. NIR News, 2020, 31, 5-9.	0.3	1
24	Principles and Applications of Vibrational Spectroscopic Imaging in Plant Science: A Review. Frontiers in Plant Science, 2020, 11, 1226.	3.6	35
25	Near-Infrared Spectroscopy as a Rapid Screening Method for the Determination of Total Anthocyanin Content in Sambucus Fructus. Sensors, 2020, 20, 4983.	3.8	29
26	Effect of conformational isomerism on NIR spectra of ethanol isotopologues. Spectroscopic and anharmonic DFT study. Journal of Molecular Liquids, 2020, 310, 113271.	4.9	14
27	Vibrational coupling to hydration shell â€“ Mechanism to performance enhancement of qualitative analysis in NIR spectroscopy of carbohydrates in aqueous environment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 237, 118359.	3.9	17
28	Near-Infrared Spectroscopy in Bio-Applications. Molecules, 2020, 25, 2948.	3.8	185
29	Biomolecular and bioanalytical applications of infrared spectroscopy â€“ A review. Analytica Chimica Acta, 2020, 1133, 150-177.	5.4	107
30	Handheld near-infrared spectrometers: Where are we heading?. NIR News, 2020, 31, 28-35.	0.3	96
31	IR Spectra of Crystalline Nucleobases: Combination of Periodic Harmonic Calculations with Anharmonic Corrections Based on Finite Models. Journal of Physical Chemistry B, 2019, 123, 10001-10013.	2.6	18
32	The essential role of omni-capable research laboratories in advancing analytical spectroscopy. NIR News, 2019, 30, 30-34.	0.3	0
33	Spectraâ€“Structure Correlations in Isotopomers of Ethanol (CX3CX2OX; X = H, D): Combined Near-Infrared and Anharmonic Computational Study. Molecules, 2019, 24, 2189.	3.8	19
34	The fundamental handbook for analytical spectroscopy. Release of the second edition of â€˜Chemometrics in spectroscopyâ€™ by Howard Mark and Jerry Workman, Jr. and its impact on the spectroscopic community. NIR News, 2019, 30, 11-13.	0.3	0
35	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. Molecules, 2019, 24, 1402.	3.8	38
36	Simulated NIR spectra as sensitive markers of the structure and interactions in nucleobases. Scientific Reports, 2019, 9, 17398.	3.3	20

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37	Spectra-structure correlations in NIR region: Spectroscopic and anharmonic DFT study of n-hexanol, cyclohexanol and phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 197, 176-184.	3.9	33
38	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. Physical Chemistry Chemical Physics, 2018, 20, 8859-8873.	2.8	20
39	Advances in Anharmonic Methods and Their Applications to Vibrational Spectroscopies. , 2018, , 483-512.		9
40	Electronic Spectra of Graphene in Far- and Deep-Ultraviolet Region: Attenuated Total Reflection Spectroscopy and Quantum Chemical Calculation Study. Journal of Physical Chemistry C, 2018, 122, 28998-29008.	3.1	9
41	Computer simulations of NIR spectra of thymol â€“ Towards linking basic and analytical NIRS. NIR News, 2018, 29, 13-16.	0.3	3
42	Quantum mechanical simulations of near-infrared spectra of biomolecules â€“ Long-chain fatty acids. NIR News, 2018, 29, 13-19.	0.3	3
43	NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features. Journal of Molecular Liquids, 2018, 268, 895-902.	4.9	42
44	NIR Spectra Simulations by Anharmonic DFT-Saturated and Unsaturated Long-Chain Fatty Acids. Journal of Physical Chemistry B, 2018, 122, 6931-6944.	2.6	39
45	Influence of Non-fundamental Modes on Mid-infrared Spectra: Anharmonic DFT Study of Aliphatic Ethers. Journal of Physical Chemistry A, 2017, 121, 1412-1424.	2.5	27
46	Correlations between Structure and Near-Infrared Spectra of Saturated and Unsaturated Carboxylic Acids. Insight from Anharmonic Density Functional Theory Calculations. Journal of Physical Chemistry A, 2017, 121, 3437-3451.	2.5	64
47	Spectra-structure correlations of saturated and unsaturated medium-chain fatty acids. Near-infrared and anharmonic DFT study of hexanoic acid and sorbic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 35-44.	3.9	38
48	Temperature Drift of Conformational Equilibria of Butyl Alcohols Studied by Near-Infrared Spectroscopy and Fully Anharmonic DFT. Journal of Physical Chemistry A, 2017, 121, 1950-1961.	2.5	48
49	Quantum mechanically calculated NIR spectra of fatty acids. NIR News, 2017, 28, 11-16.	0.3	3
50	Spectroscopic and Quantum Mechanical Calculation Study of the Effect of Isotopic Substitution on NIR Spectra of Methanol. Journal of Physical Chemistry A, 2017, 121, 7925-7936.	2.5	29
51	Quantum chemical calculation of NIR spectra of practical materials. NIR News, 2017, 28, 13-20.	0.3	12
52	Computational and quantum chemical study on high-frequency dielectric function of tert-butylmethyl ether in mid-infrared and near-infrared regions. Journal of Molecular Liquids, 2016, 224, 1189-1198.	4.9	9
53	On optimization of absorptionâ€“dispersion spectra. Journal of Molecular Structure, 2016, 1126, 11-18.	3.6	1
54	Dielectric functions of iso -propanol and di- iso -propylether in the infrared. Journal of Molecular Liquids, 2015, 203, 143-152.	4.9	3

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55	Infrared dispersion of liquid di-n-propylether. Journal of Molecular Liquids, 2013, 181, 127-132.	4.9	6