

Univ.-Prof. Mag. Dr. Christian Huck

List of publications (all papers)

2023

385. Bec, K.B.; Huck, C.W.

Analytische Vorteile der Nahinfrarot-Spektroskopie. Eine ökonomische Alternative zur konventionellen Analytik.

GIT Labor-Fachzeitschrift 5/6, S. 40-41

384. Woess, C.; Huck, C.W.; Badzoka, J.; Kappacher, C.; Arora, R.; Lindtner, R.A.; Zelger, P.; Schirmer, M.; Rabl, W.; Pallua, J.

Raman spectroscopy for post-mortem interval estimation of human skeletal remains: A scoping review

J. Biophotonics 2023

DOI: 10.1002/jbio.202300189

383. Beć, K.B.; Huck, C.W.

Good vibrations, smooth contours at NIR 2023 Innsbruck: A preview of the conference, NIR News **2023**, 34, 15-28.

DOI: 10.1177/09603360231179427

382. Czarnecki, M.A.; Beć, K.B.; Grabska, J.; Huck, C.W.; Mazurek, S.; Orzechowski, K.

State of water in various environments: aliphatic ketones. MIR/NIR spectroscopic, dielectric and theoretical studies,

Spectrochim. Acta A **2023**, X, 123057.

DOI: 10.1016/j.saa.2023.123057

381. Schlappack, T; Kappacher, C; Demetz, M; Jakschitz, T; Bonn, GK; Huck, CW; Rainer, M

Ambient mass spectrometry and near-infrared spectroscopy – a direct comparison of methods for the quantification of sucralose in e-liquids

Anal. Methods, 2023

DOI: 10.1039/d3ay00380a

380. Grabska, J.; Bec, K.B.; Huck, C.W.

Analyzing the quality parameters of apples by spectroscopy from Vis/NIR to NIR region: A comprehensive review

Foods, 12(10), 1946

DOI: 10.3390/foods12101946

379. Bec, K.B.; Grabska, J.; Huck, C.W.

Xiaoli Chu, Yue Huang, Yong-Huan Yun, Xihui Bian: Chemometric methods in analytical spectroscopy technology

Anal. Bioanal. Chem., 2023

<https://doi.org/10.1007/s00216-023-04642-6>

378. Brunner, A.; Willenbacher, E.; Willenbacher, W.; Zelger, B.; Zelger, P.; Huck, C.W.; Pallua, J.D.

Visible- and near-infrared hyperspectral imaging for the quantitative analysis of PD-L1+ cells in human lymphomas: Comparison with fluorescent multiplex immunohistochemistry.

Spectrochim. Acta A, 2023, 285, 121940

DOI: 10.1016/j.saa.2022.121940

377. Beć, K.B.; Grabska, J.; Huck, C.W.

Near-Infrared (NIR) Sensors for Environmental Analysis.

In: Jafari, R; Mizaikoff, B; Fresco, Cala, B: Encyclopedia of Sensors and Biosensors.

Volume 4, 484-503

Elsevier ISBN 9178-0-12-822549-3

2022

376. Grabska, J.; Beć, K.B.; Huck, C.W. Miniaturized Near-Infrared Spectroscopy – the Ultimate Analytical Tool in Food and Agriculture, Encyclopedia of analytical chemistry: applications, theory and instrumentation, Meyers, R.A.; Ed.; John Wiley & Sons, 2022. DOI: 10.1002/9780470027318.a9790

375. Beć, K.B.; Grabska, J.; Huck, C.W.

Infrared and near-infrared spectroscopic techniques for the quality control of herbal medicines. In: Evidence-based validation of herbal medicine, 2nd edition, Mukherjee, P.K. Ed., Elsevier, 2022, pp. 603-627.

DOI: 10.1016/B978-0-323-85542-6.00018-4

374. Beć, K.B.; Grabska, J.; Huck, C.W.

Miniaturized near-infrared spectroscopy in current analytical chemistry: from natural products to forensics. In: Molecular and laser spectroscopy - Advances and applications. Vol. 3, Gupta, V.P. Ed.; Elsevier, 2022, pp. 141-188.

DOI: 10.1016/B978-0-323-91249-5.00009-0

373. Grabska, J.; Beć, K.B.; Huck, C.W.

Current and future applications of IR and NIR spectroscopy in ecology, environmental studies, wildlife and plant investigations. In: Comprehensive analytical chemistry. Infrared Spectroscopy for Environmental Monitoring. Vol. 98, Cozzolino, D. Ed.; 2022, pp. 45-76.

DOI: 10.1016/bs.coac.2020.08.002

372. Grabska, J.; Mizaikoff, B.; Huck, C.W.

Summary of the 12th Advanced Study Course on Optical Chemical Sensors – ASCOS 2022, Obergurgl, Austria

NIR News **2022**, 33, 13-14. DOI: 10.1177/09603360221143435

371. Beć, K.B.; Huck, C.W.

NIR spectroscopy sessions among other disciplines of analytical chemistry – The Great Scientific Exchange 2022 in Cincinnati

NIR News **2022**, 33, 15-17.

DOI: 10.1177/09603360221143436

370. Costa, F.; Zanella, A.; Huck, C.W.; Busatto, N.; Populin, F.; Stürz, S.; Folie, I.; Biasioli, F.; Farneti, B.; Vrhovsek, U.; Ueno, N.; Vittani, L.; Grabska, J.; Beć, K.B.

“Scald-Cold”: comprehensive dissection of the superficial scald in apple.

Acta Hort. 2022, 1344, 7-12.

DOI: 10.17660/ActaHortic.2022.1344.2

369. Beć, K.B.; Grabska, J. Huck, C.W.

The new avenue – theoretical simulation of NIR spectra and its potential in analytical applications In: Chu, X.; Guo, L.; Huang, Y.; Yuan, H. (Eds.): ICNIR 2021, Sense the Real Change: Proceedings of the 20th International Conference on Near Infrared Spectroscopy, Springer, Singapore, 2022, pp. 32–46. DOI: 10.1007/978-981-19-4884-8_3

366. Huck, C.W.; Beć, K.B.; Grabska, J.

Current status and future trends in sensor miniaturization In: X. Chu, X.; Guo, L.; Huang, Y.; Yuan, H. (Eds.): ICNIRS 2021, Sense the Real Change: Proceedings of the 20th International Conference on Near Infrared Spectroscopy, Springer, Singapore, 2022, pp. 59–72.

DOI: 10.1007/978-981-19-4884-8_5

365. Grabska, J.; Beć, K.B.; Huck, C.W.

Theoretical simulation of near-infrared spectrum of piperine. Insight into band origins and the features of regression models from different spectrometers In: Chu, X.; Guo, L.; Huang, Y.; Yuan, H. (Eds.): ICNIR 2021, Sense the Real Change: Proceedings of the 20th International Conference on Near Infrared Spectroscopy, Springer, Singapore, 2022, pp. 253-261. DOI: 10.1007/978-981-19-4884-8_27

364. Huck, C.W.

Present and Future of Miniaturized NIR Spectrometers Combined with Challenging Data Management Strategies

Macedon. Pharm. Bull., 68 (Suppl 2) 9 - 10 (2022) Online ISSN 1857 - 8969 DOI:

10.33320/maced.pharm.bull.2022.68.04.001

363. Beć, K.B.; Grabska, J.; Huck, C.W.

Infrared and near-infrared spectroscopic techniques for the quality control of herbal medicines

In: Evidence-based validation of herbal medicine, 2nd edition, Mukherjee, P.K. (Ed.), Elsevier, 2022, pp. 603-627.

DOI: 10.1016/B978-0-323-85542-6.00018-4

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Near-infrared (NIR) sensors in environmental analysis

In: Encyclopedia of sensor technology, Narayan, R. (Ed.), Elsevier, 2022.

DOI: 10.1016/B978-0-12-822548-6.00093-5

361. Beć, K.B.; Grabska, J.; Huck, C.W.

Miniaturized near-infrared spectroscopy in current analytical chemistry: from natural products to forensics

In: Molecular and laser spectroscopy - Advances and applications. Vol. 3, Gupta, V.P. Ed.; Elsevier, 2022, pp. 141-188.

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360. Grabska, J.; Beć, K.B.; Huck, C.W.

Current and future applications of IR and NIR spectroscopy in ecology, environmental studies, wildlife and plant investigations

In: Comprehensive analytical chemistry. Infrared Spectroscopy for Environmental Monitoring. Vol. 98, Cozzolino, D. Ed.; 2022, pp. 45-72.

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359. Beć, K.B.; Grabska, J.; Huck, C.W.

Portable spectroscopy applications in food, feed and agriculture.

In: Portable spectroscopy and spectrometry 2: Applications. Crocombe, R.A.; Leary, P.E.; Kammrath, B.W. Eds.; John Wiley & Sons, Ltd, 2021, pp. 299-324.

DOI: 10.1002/9781119636489.ch36

358. Huck, C.W.; Beć, K.B.; Grabska, J.

Near infrared spectroscopy in natural product research.

In: Encyclopedia of analytical chemistry: applications, theory and instrumentation, Meyers, R.A.; Ed.; John Wiley & Sons, 2020, pp. 1-29.

DOI: 10.1002/9780470027318.a9909.pub2

357. Beć, K.B.; Grabska, J.; Huck, C.W.

Physical principles of infrared spectroscopy.

In: Comprehensive analytical chemistry. Infrared Spectroscopy for Environmental Monitoring. Vol. 98, Cozzolino, D. Ed.; 2022, pp. 1-39.

DOI: 10.1016/bs.coac.2020.08.001

356. Beć, K.B.; Grabska, J. Huck, C.W.

The new avenue – theoretical simulation of NIR spectra and its potential in analytical applications

In: Chu, X.; Guo, L.; Huang, Y.; Yuan, H. (Eds.): ICNIR 2021, Sense the Real Change: Proceedings of the 20th International Conference on Near Infrared Spectroscopy, Chemical Industry Press, 2022, pp. 32–46. DOI: 10.1007/978-981-19-4884-8_3

355. Huck, C.W.; Beć, K.B.; Grabska, J.

Current status and future trends in sensor miniaturization

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354. Grabska, J.; Beć, K.B.; Huck, C.W.

Theoretical simulation of near-infrared spectrum of piperine. Insight into band origins and the features of regression models from different spectrometers

In: Chu, X.; Guo, L.; Huang, Y.; Yuan, H. (Eds.): ICNIR 2021, Sense the Real Change: Proceedings of the 20th International Conference on Near Infrared Spectroscopy, Chemical Industry Press, 2022, pp. 253-261. DOI: 10.1007/978-981-19-4884-8_27

352. Beć, K.B.; Huck, C.W.

Miniaturization in NIR spectroscopy reshapes chemical analysis

BioPhotonics 2022, 29, 44-51

352. Huck, C.W.; Beć, K.B.; Grabska, J.

Portable near-infrared sensors in medicinal plant quality control.

European Pharmaceutical Review 2022

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'Near-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applications' ranks top 2% among downloaded Springer books in the field of chemistry and materials science.

NIR News 2022, 33, 20-21

DOI: 10.1177/09603360221079454

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SciX 2021 summary including NIR spectroscopy session.

NIR News 2022, 33, 18-19

DOI: 10.1177/09603360221076352

349. Kappacher, C.; Trübenbacher, B.; Losso, K.; Rainer, M.; Bonn, G.K.; Huck, C.W.

Portable vs. benchtop NIR-sensor technology for classification and quality evaluation of black truffle.

Molecules 2022, 27, 589

DOI: 10.3390/molecules27030589

348. Harder, M.; Bakry, R.; Lackner, F.; Mayer, P.; Kappacher, C.; Grießer, C.; Neuner, S.; Huck, C.W.; Bonn, G.K.; Rainer, M.

The crosslinker matters: vinylimidazole-based anion exchange polymer for dispersive solid-phase extraction of phenolic acids.

Separations 2022, 9, 72

DOI: 10.3390/separations9030072

347. Brunner, A.; Schmidt, V.M.; Zelger, B.; Woess, C.; Arora, R.; Zelger, P.; Huck, C.W.; Pallua, J.

Visible and Near-Infrared hyperspectral imaging (HSI) can reliably quantify CD3 and CD45 positive inflammatory cells in myocarditis: Pilot study on formalin-fixed paraffin-embedded specimens from myocard obtained during autopsy.

Spectrochim. Acta A 2022, 274, 121092

DOI: 10.1016/j.saa.2022.121092

346. Losso, K.; Beć, K.B.; Mayr, S.; Grabska, J.; Stuppner, S.; Jones, M.; Jakschitz, T.; Rainer, M.; Bonn, G.K.; Huck, C.W.

Rapid discrimination of Curcuma longa and Curcuma xanthorrhiza using direct analysis in real time mass spectrometry and near infrared spectroscopy.

Spectrochim. Acta A 2022, 265, 120347

DOI: 10.1016/j.saa.2021.120347

345. Gigopulu, O.; Geskovski, N.; Stefkov, G.; Gjorgievska, V.S.; Spirevska, I.S.; Huck, C.W.; Makreski, P.

A unique approach for in-situ monitoring of the THCA decarboxylation reaction in solid state

Spectrochim. Acta A 2022, 267, 120471

DOI: 10.1016/j.saa.2021.120471

344. Mayr, S.; Strasser, S.; Kirchler, C.G.; Meischl, F.; Stuppner, S.; Beć, K.B.; Grabska, J.; Sturm, S.; Popp, M.; Stuppner, H.; Bonn, G.K.; Huck, C.W.

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.

DOI: 10.1055/a-1326-2497

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343. Beć, K.B.; Grabska, J.; Huck, C.W.

X-Ray, LIBS, NMR, and MS applications in food, feed, and agriculture. In: Portable spectroscopy and spectrometry 2: Applications. Crocombe, R.A.; Leary, P.E.; Kammrath, B.W. Eds.; John Wiley & Sons, Ltd, 2021, p. 299-324.

DOI: 10.1002/9781119636489.ch36

342. Huck, C.W.

SAS – Society for Applied Spectroscopy Fellow Award for Christian Huck.

NIR News 2021, 32, 5-6

DOI: 10.1177/09603360211067097

341. Beć, K.B.; Grabska, J.; Huck, C.W.; Mazurek S.; Czarnecki, M.A.

Anharmonicity and structure–structure correlations in MIR and NIR Spectra of crystalline menadione (Vitamin K₃).

Molecules 2021, 26, 6779

DOI: 10.3390/molecules26226779

341. Beć, K.B.; Grabska, J.; Plewka, N.; Huck, C.W.

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

DOI: 10.3390/molecules26216390

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Theoretical simulation of near-infrared spectrum of piperine. Insight into band origins and the features of regression models.

App. Spectr. 2021 75, 1022-1032

DOI: 10.1177/00037028211027951

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Anharmonic DFT study of near-infrared spectra of caffeine. Vibrational analysis of the second overtones and ternary combinations.

Molecules 2021, 26, 5212

DOI: 10.3390/molecules26175212

338. Beć, K.B.; Grabska, J.; Huck, C.W.

The comprehensive sourcebook for modern NIR spectroscopy: A commentary on “Near-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applications”.

NIR News 2021, 32, 5-10

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Novel near-infrared (NIR) and Raman spectroscopic technologies for print and photography identification, classification and authentication.

NIR News 2021, 32, 11-16

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336. Ozaki, Y.; Bec, KB; Morisawa, Y.; Yamamoto, S.; Tanabe, I.; Huck, C.W.; Hofer, T.S.

Advances, challenges and perspectives of quantum chemical approaches in molecular spectroscopy of the condensed phase

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Innovative combination of dispersive solid phase extraction followed by NIR-detection and multivariate data analysis for prediction of total polyphenolic content.

Molecules 2021, 26, 4807

DOI: 10.3390/molecules26164807

334. Pallua, J.D.; Brunner, A.; Zelger, B.; Huck, C.W.; Schirmer, M.; Laimer, J.; Putzer, D.; Thaler, M.; Zelger, B.

New perspectives of hyperspectral imaging for clinical research.

NIR News 2021, 32, 3-4

DOI: 10.1177/09603360211024971

333. Willenbacher, E.; Brunner, A.; Zelger, B.; Unterberger, S.H.; Stalder, R.; Huck, C.W.; Willenbacher, W.; Pallua, J.D.

Application of mid-infrared microscopic imaging for the diagnosis and classification of human lymphomas

J. Biophotonics 2021, 14, e202100079

DOI: 10.1002/jbio.202100079

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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

Spectrochim. Acta A 2021, 262, 120085

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Simultaneous quantification of 14 compounds in *Achillea millefolium* by GC-MS analysis and near-infrared spectroscopy combined with multivariate techniques.

J. Anal. Methods Chem. 2021, 2021, 5566612.

DOI: 10.1155/2021/5566612

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Principles and applications of miniaturized near-infrared (NIR) spectrometers.

Chemistry - A European Journal 2021, 27, 1514-1532

DOI: 10.1002/chem.202002838

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Current and future research directions in computer-aided near-infrared spectroscopy: a perspective.

Spectrochim. Acta A 2021, 254, 119625

DOI: 10.1016/j.saa.2021.119625

328. Mayr, S.; Beć, K.B.; Grabska, J.; Wiedemair, V.; Pürgy, V.; Popp, M.A.; Bonn, G.K.; Huck, C.W.

Challenging handheld NIR spectrometers with moisture analysis in plant matrices: Performance of PLSR vs. GPR vs. ANN modelling

Spectrochim. Acta A 2021, 249, 119342

DOI: 10.1016/j.saa.2020.119342

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Mid-infrared spectroscopy as process analytical technology tool for estimation of THC and CBD content in Cannabis flowers and extracts.

Spectrochim. Acta A 2021, 251, 119422

DOI: 10.1016/j.saa.2020.119422

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Near-Infrared Spectra of High-Density Crystalline H₂O Ices II, IV, V, VI, IX, and XII

J. Phys. Chem. A 2021, 125, 1062–1068

DOI: 10.1021/acs.jpca.0c09764

325. Laimer, J.; Bruckmoser, E.; Helten, T.; Kofler, B.; Zelger, B.; Brunner, A.; Zelger, B.; Huck, C.W.; Tappert, M.; Rogge, D.; Schirmer, M.; Pallua, J.D.

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DOI: 10.1002/jbio.202000424

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Fatty acid profiling of bovine milk and cheese from six European areas by GC-FID and GC-MS

Int. J. Dairy Technol 2021, 74, 215-224

DOI: 10.1111/1471-0307.12749

323. Mayr, S.; Beć, K.B.; Grabska, J.; Schneckenreiter, E.; Huck, C.W.

Near-infrared spectroscopy in quality control of Piper nigrum: A Comparison of performance of benchtop and handheld spectrometers.

Talanta 2021, 223, 121809

DOI: 10.1016/j.talanta.2020.121809

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Theae nigrae folium: Comparing the analytical performance of benchtop and handheld near-infrared spectrometers.

Talanta 2021, 221, 121165

DOI: 10.1016/j.talanta.2020.121165

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Suitability of biodegradable materials in comparison with conventional packaging materials for the storage of fresh pork products over extended shelf-life periods.

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DOI: 10.1016/j.aca.2020.04.015

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Molecules 2020, 25, 2948

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Near infrared spectroscopy as a rapid screening method for the determination of total anthocyanin content in sambucus fructus.

Sensors 2020, 20, 4983

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Solvation effects on wavenumbers and absorption intensities of the OH-stretch vibration in phenolic compounds - electrical - and mechanical anharmonicity via a combined DFT/Numerov approach.

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Near-infrared spectroscopy with linear discriminant analysis for green 'Robusta' coffee bean sorting.

International Food Research Journal 2020, 27, 287 – 294

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Vibrational coupling to hydration shell – Mechanism to performance enhancement of qualitative analysis in NIR spectroscopy of carbohydrates in aqueous environment.

Spectrochim. Acta A 2020, 237, 118359

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Effect of conformational isomerism on NIR spectra of ethanol isotopologues. Spectroscopic and anharmonic DFT study.

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DOI: 10.1016/j.molliq.2020.113271

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Preliminary study on using near-infrared spectroscopy at 1.6–2.4 μm for document examination.

Infrared Physics and Technology 2020, 105, 103212

DOI: 10.1016/j.infrared.2020.103212

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NIR News 2020, 31, 28–35

DOI: 10.1177/0960336020916815

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