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From Molecules to Metrics: A Physics-Based Python Pipeline for Generating Realistic Synthetic NIRS Datasets

Foundational Principles: The Beer-Lambert Law and its Physical Limitations

The generation of a physically realistic synthetic Near-Infrared Spectroscopy (NIRS) dataset begins with a clear understanding of the foundational principle that links molecular composition to measured spectral intensity: the Beer-Lambert Law (BLL). The law states that the absorbance of light by a material is directly proportional to the concentration of the absorbing analyte and the path length the light travels through the material [60] [66]. Mathematically, this relationship is expressed as $A=\epsilon \cdot c \cdot l$, where A is the absorbance, ϵ is the molar absorptivity (or molar extinction coefficient) of the analyte at a given wavelength, c is its concentration, and l is the effective optical path length [60] [66]. The BLL is widely cited as a fundamental tool for determining the concentration of absorbers in a wide range of media, including various biological tissues [60]. In its basic form, it provides a direct and intuitive link between the chemical makeup of a sample and the resulting spectrum, making it an essential starting point for any spectroscopic simulation.

However, a critical analysis of the literature reveals that the direct application of the standard Beer-Lambert Law is a significant oversimplification for most practical NIRS applications [77]. The primary reason for this limitation is that the law assumes a collimated beam of light traveling in a straight line through a homogeneous, non-scattering medium. This condition is rarely met in real-world scenarios where NIRS is employed. For instance, in biomedical diagnostics, the technique is used to probe biological tissues; in agriculture, it analyzes heterogeneous materials like grains and fruits; and in pharmaceuticals, it assesses solid dosage forms and blends [10] [76] [82]. These sample types are characterized as "turbid media," meaning they contain microscopic structures that cause photons to scatter in multiple directions upon interaction [48]. This intense scattering fundamentally alters the nature of light propagation. Instead of a single, well-defined path length 'l', photons travel along complex, tortuous trajectories of

varying lengths before exiting the sample and reaching the detector [65]. Consequently, the concept of a simple geometric path length becomes obsolete, and the effective path length becomes a stochastic variable dependent on the sample's optical properties [77].

This deviation from the assumptions of the BLL has profound implications for the simulated spectra. Real NIRS spectra are not simple linear functions of concentration but exhibit broad, overlapping peaks and valleys whose shapes and positions are influenced by the underlying scattering properties of the sample matrix [29]. Simply applying the BLL would fail to capture these critical features, producing spectra that lack the characteristic distortions, baseline shifts, and asymmetries observed in experimental data [29]. For example, changes in the sample's temperature can alter the position and intensity of absorption bands, which the simplistic BLL cannot account for, thereby affecting the predictive ability of any subsequent quantitative model built on such flawed data [28]. Therefore, while the BLL correctly identifies the dependence of absorption on concentration and molar absorptivity, relying on it alone to generate a physically realistic dataset is insufficient. It represents a first-order approximation that must be superseded by more sophisticated models capable of describing photon migration in scattering environments. The objective of a high-fidelity simulation pipeline is to move beyond this simplification and incorporate a physically plausible description of light transport, ensuring the final synthetic data accurately reflects the complexities of real-world NIRS measurements. This necessitates moving from the idealized world of the Beer-Lambert Law to computational frameworks based on radiative transfer theory, such as diffusion approximation or Monte Carlo methods, which will be discussed in the following section.

Modeling Light Propagation in Turbid Media

To overcome the limitations of the Beer-Lambert Law in turbid media, it is necessary to employ models that explicitly account for the random walk of photons caused by scattering. The two principal methodologies identified in the scientific literature for this purpose are diffusion theory approximations and Monte Carlo (MC) simulations. Each approach offers a distinct trade-off between computational efficiency and physical fidelity, making them suitable for different stages of algorithm development and validation.

Diffusion theory is a mathematical approximation of the radiative transfer equation (RTE), which describes the propagation of light through a medium. It simplifies the RTE by assuming that scattered light is propagated isotropically, effectively treating the light

field as a diffusing quantity. This approach is computationally very efficient and is particularly well-suited for highly scattering media where the mean free path between scattering events is much smaller than the dimensions of the sample [32]. Its utility is demonstrated in the characterization of highly scattering media from time- and/or spatially resolved measurements [49] and in forward modeling for near-infrared optical tomography [67]. Furthermore, analytical solutions derived from diffusion theory have been combined with modified Beer-Lambert formulations to create multi-layer self-calibrated algorithms for probing layered structures like the skin or transabdominal regions [73]. However, the validity of diffusion theory is contingent on certain assumptions. It breaks down in scenarios involving small source-detector separations, highly absorbing media, or near boundaries where the isotropic scattering assumption is invalid [69]. For many NIRS applications, particularly those requiring high accuracy close to the source or detector, these limitations can introduce significant errors.

In contrast, Monte Carlo simulations offer a more physically rigorous and versatile approach. Instead of solving an approximate differential equation, MC methods perform a statistical simulation of the physical process by tracing the paths of thousands or even millions of individual photons as they interact with the modeled medium [31]. At each interaction point, the simulation randomly determines whether a photon will be absorbed or scattered, and if scattered, it calculates a new direction based on a specified phase function (e.g., the Henyey-Greenstein phase function) [48]. By aggregating the results of these individual photon histories, the simulation can produce highly accurate predictions of the total transmitted or reflected light intensity at the detector [33]. The power of MC methods lies in their ability to model complex geometries and optical properties without the restrictive assumptions of diffusion theory. They have been successfully used to investigate optical pathlength in inhomogeneous tissue [65], validate frequency-domain NIRS data [33], estimate blood-glucose concentration via photoplethysmography [46], and determine the optical properties of biological tissues using inverse modeling techniques [70] [72]. Open-source software packages exist to optimize and run these simulations, providing a robust foundation for building a high-fidelity NIRS simulator [68]. While computationally intensive, modern computing resources make these simulations feasible for generating large datasets.

For the purpose of creating a universal and physically realistic synthetic dataset, a dual-pathway strategy is recommended. The core engine of the simulation should be built upon a validated Monte Carlo method to serve as the gold standard, ensuring maximum physical fidelity. This allows for the accurate representation of phenomena in complex, inhomogeneous, or strongly absorbing samples, which is crucial for biomedical and other

advanced applications [50]. Concurrently, an optional module based on diffusion theory should be implemented. This module would provide a much faster alternative for generating spectra, which is advantageous for applications requiring rapid turnaround, such as real-time process analytical technology (PAT) monitoring in pharmaceutical manufacturing [34] or for performing large-scale sensitivity analyses. This hybrid architecture aligns perfectly with the user's goal of covering all NIRS application domains, as it empowers the user to select the appropriate level of complexity and computational cost based on their specific needs, balancing the trade-off between speed and accuracy.

Defining Sample Optical Properties from Analyte Concentrations

The central task of the simulation pipeline is to translate user-defined concentrations of target analytes into a complete optical property spectrum for the sample. This requires a clear methodology for calculating the two fundamental optical coefficients that govern light propagation: the absorption coefficient (μ_a) and the reduced scattering coefficient (μ_s'). The absorption coefficient quantifies how readily the sample removes photons from the light field, while the reduced scattering coefficient describes how frequently photons change direction. Together, these coefficients define the sample's interaction with near-infrared light.

The absorption coefficient, $\mu_a(\lambda)$, at a given wavelength λ, is directly determined by the presence and concentration of light-absorbing molecules, known as chromophores. The calculation follows a straightforward summation principle: the total absorption coefficient is the sum of the individual contributions from each chromophore present in the sample. The contribution of each chromophore 'i' is calculated by multiplying its molar absorptivity (or molar extinction coefficient), $\epsilon_i(\lambda)$, by its molar concentration, c_i. The formula is therefore:

$$\mu_a(\lambda) = \sum_i [\epsilon_i(\lambda) \cdot c_i]$$

This relationship is a cornerstone of quantitative NIR spectroscopy and is consistently referenced across various application areas [12] [47]. The molar absorptivity, $\epsilon_i(\lambda)$, is an intrinsic property of the molecule that depends on its chemical structure and the wavelength of light. High-quality reference data for these values are crucial for a realistic

simulation. The provided literature contains valuable data for several key analytes relevant to different domains.

Analyte	Domain	Relevant Wavelength(s) / Range	Molar Absorptivity Value(s)
Hemoglobin (HbO_2)	Biomedical	673 nm	~290 $cm^{-1}M^{-1}$ [12]
Water (H_2O)	Biomedical, General	NIR region	Measured values exist [54]
Glucose	Biomedical	1000–1700 nm	Informative bands identified [13] [45]
Glycated Hemoglobin (HbA1c)	Biomedical	450–700 nm	Experimentally measured [25]
Protein	Agricultural, Food	Not Specified	Correlation with absorbance shown [19] [20] [39]
Starch	Agricultural, Food	Not Specified	Correlation with absorbance shown [19] [20] [22]
Moisture	Agricultural, Food	Not Specified	Correlation with absorbance shown [19] [20] [36]
Fat / Oil	Agricultural, Food	Not Specified	Correlation with absorbance shown [20] [21]
Active Pharmaceutical Ingredient (API)	Pharmaceutical	Reflectance mode	Demonstrated for quantitative analysis [81] [83]

The second key parameter, the reduced scattering coefficient, $\mu_s'(\lambda)$, primarily characterizes the scattering properties of the sample matrix—the background material in which the analytes are dissolved or dispersed. Unlike μ_a, μ_s' is often considered to be relatively independent of wavelength in the NIR region for many biological tissues [74]. Its value is determined by the size, shape, and refractive index of the scattering particles within the medium. In a practical simulation framework, μ_s' is typically treated as a bulk parameter for the sample. It can be determined experimentally using specialized setups, such as an integrating sphere system in combination with an inverse Monte Carlo model, to deconvolve the scattering and absorption properties of a sample [55] [70] [74]. For the purposes of the synthetic data generator, the user should be able to specify a value or a simple functional form for $\mu_s'(\lambda)$, allowing for the simulation of different sample types with varying degrees of opacity and granularity. By combining the calculated wavelength-dependent $\mu_a(\lambda)$ with the user-defined $\mu_s'(\lambda)$, the simulation creates a complete optical description of the sample, ready for input into the light propagation model.

Implementing a Multi-Sourced Noise Model for Realism

A physically grounded simulation of light-sample interaction is incomplete without a comprehensive model of the imperfections and variabilities inherent in real-world measurement systems. Incorporating a realistic noise model is a critical requirement for generating synthetic data that can be used to develop and validate robust chemometric algorithms. The literature identifies several distinct sources of noise and artifacts that contribute to the final measured spectrum, which can be broadly categorized into electronic noise, photon statistics, and systematic instrumental drift.

Electronic noise originates from the components of the spectrometer's detection system. This includes Johnson-Nyquist (thermal) noise, which arises from the random motion of charge carriers in resistive elements and is a primary noise source in detectors like pyroelectric sensors [52]. Another component is dark current noise, which is the small electrical current that flows through a photodetector even in the absence of light; this current is subject to its own fluctuations [41]. The total noise current in a photodetector is generally modeled as the sum of the shot noise current, thermal noise current, and a 1/f noise current [42] [53]. Shot noise is an intrinsic physical phenomenon arising from the discrete, particle-like nature of both light (photons) and electricity (electrons) [61]. It is characterized by a Poisson distribution and manifests as random fluctuations in the detected signal intensity [61]. Additionally, certain types of detectors, like organic photodiodes, are known to exhibit prominent 1/f noise, a type of low-frequency noise that can significantly impact measurements [41] [53].

Beyond these random noise sources, a major challenge in NIRS is the presence of systematic artifacts, most notably baseline drift. This refers to a slow, non-linear shift in the entire spectral baseline over time or between measurements. The literature suggests several root causes for this phenomenon. Fluctuations in the temperature of the light source or the ambient environment are a primary contributor, as changes in temperature can alter the output characteristics of the source and the optical components, leading to a drifting baseline [28] [29]. Some instruments employ temperature feedback compensation systems to stabilize the light source and control wavelength drift within tight tolerances, highlighting the importance of this factor [57]. However, baseline shift may also arise from other instrumental factors, such as the specific algorithm used by the instrument's control IC or the mechanical structure of the device itself, suggesting that not all drift is purely thermally induced [40].

To implement a realistic noise model in the synthetic data pipeline, these effects should be incorporated through a combination of additive and multiplicative processes. Additive

noise, representing dark current and thermal noise, can be modeled as a zero-mean Gaussian-distributed random variable added to the simulated signal at each wavelength point. The standard deviation of this Gaussian distribution should be calibrated based on the expected detector sensitivity and integration time. Multiplicative noise, representing shot noise, should be modeled as a Poisson-distributed random variable multiplied by the signal intensity. This accounts for the statistical fluctuation in the number of photons detected. Finally, to simulate baseline drift, a slowly varying polynomial function (e.g., of 2nd or 3rd order) can be added to the entire spectrum. The coefficients of this polynomial should be randomized within a plausible range for each generated spectrum to mimic the variability seen in real experiments. By combining these elements—a Gaussian additive term, a Poisson multiplicative term, and a randomized polynomial drift term—the synthetic dataset will accurately reflect the statistical and systematic imperfections of real-world instruments, making it an invaluable resource for testing the robustness of spectral analysis algorithms.

Architectural Design for a Universal and Reproducible Framework

To fulfill the user's goal of a universal, multi-domain synthetic NIRS dataset generator, the Python implementation must be designed with modularity, extensibility, and scientific reproducibility at its core. A monolithic script would be difficult to maintain, extend to new application domains, or use reliably in a research context. Instead, a modular architecture, inspired by best practices in scientific computing, is essential. This approach breaks the complex simulation process into a series of distinct, interchangeable components, each responsible for a specific part of the workflow.

The pipeline can be logically divided into four primary modules: 1. **`AnalyteDefinition`**: This module would be responsible for defining the chemical constituents of the sample. It should allow the user to input a dictionary specifying the name of each analyte, its concentration, and its corresponding molar absorptivity spectrum. The module should also include functionality to load pre-existing molar absorptivity data from curated databases or text files, supporting the addition of new analytes for different domains. 2. **`OpticalPropertyCalculator`**: This module takes the analyte definitions as input and computes the sample's wavelength-dependent absorption coefficient, $\mu_a(\lambda)$. It would apply the summation formula, leveraging the data from the `AnalyteDefinition` module. It would also accept a definition for the reduced scattering coefficient, $\mu_s'(\lambda)$, either as a constant value, a function of

wavelength, or a lookup table, allowing the user to configure the optical properties of the sample matrix. 3. **`LightTransportSimulator`**: This is the computational heart of the framework. It would take the full set of optical properties (μ_a, μ_s') and the geometry of the measurement setup (e.g., source-detector separation, sample thickness) as inputs. Crucially, this module should be designed with a choice of backends. It could feature an option to use a fast diffusion theory approximation for quick simulations or switch to a more accurate Monte Carlo simulation engine for high-fidelity results. This flexibility directly addresses the need to cover all application domains, from rapid PAT to detailed biomedical research. 4. **`NoiseInjector`**: This final module takes the clean spectrum generated by the `LightTransportSimulator` and adds the various sources of noise described previously. It would apply the additive Gaussian noise (for dark current/ thermal noise), the multiplicative Poisson noise (for shot noise), and a randomized polynomial function (for baseline drift). Parameters for each noise source (e.g., noise level, drift magnitude) would be configurable inputs.

Beyond modularity, ensuring full reproducibility is paramount for scientific rigor. The framework should adopt a logging philosophy similar to that of ASpecD, a modular Python framework for analyzing spectroscopic data [80]. Every single parameter, choice, and calculation performed during the simulation process must be recorded. This includes the analyte names and concentrations, the specific molar absorptivity data used, the values of μ_a and μ_s', the chosen light transport model and its parameters, the noise model settings, and any random seeds used for generating stochastic variables. This complete history should be stored as metadata alongside the final generated spectra, creating a self-contained, traceable scientific artifact. This ensures that any synthetic dataset produced by the framework can be exactly reproduced at a later date, fulfilling a key tenet of good scientific practice. This reproducible framework would enable researchers to share not just their data, but also the exact provenance of how that data was created, greatly enhancing the validity and comparability of their work.

Synthesis and Final Recommendations for Implementation

The creation of a physically realistic, multi-domain synthetic NIRS dataset in Python is an ambitious undertaking that requires a departure from simplistic models toward a more sophisticated, physics-based simulation framework. The analysis of the provided materials indicates that a successful implementation must pivot away from the direct application of the Beer-Lambert Law, which fails to account for the dominant effects of

light scattering in most NIRS applications. Instead, the core of the simulation must be a model of light propagation through a turbid medium. The evidence strongly supports the use of Monte Carlo methods as the preferred engine for achieving maximum physical realism, as they can accurately simulate photon transport in complex geometries and media [31] [33]. However, to ensure broad applicability and usability across different domains, this high-fidelity engine should be complemented by a computationally cheaper diffusion theory approximation, allowing users to choose the appropriate level of complexity for their specific needs [32] [67].

The proposed pipeline begins with user-defined concentrations of target analytes. From these inputs, the framework must calculate the sample's absorption coefficient spectrum (μ_a) by summing the contributions of each analyte, weighted by its molar absorptivity [12] [47]. The reduced scattering coefficient (μ_s') serves as a configurable bulk parameter representing the sample matrix [74]. These two spectra then feed into the light transport simulator to generate a base spectrum representing the interaction of light with the sample. Critically, this base spectrum must then be corrupted with a comprehensive, multi-sourced noise model to bridge the gap between the idealized simulation and real-world measurement conditions. This involves adding components for electronic noise (modeled as Gaussian), photon statistics (modeled as Poisson), and systematic artifacts like baseline drift (modeled as a slowly varying polynomial) [29] [42] [61].

Finally, the entire process must be encapsulated within a modular and transparent Python framework designed for reproducibility. Following the principles of frameworks like ASpecD, every parameter and decision made during the simulation—from analyte definitions to noise levels—must be meticulously logged as metadata [80]. This creates a complete, auditable record of how each synthetic dataset was generated, ensuring that the results are not only scientifically valuable but also rigorously verifiable. By adopting this hierarchical, modular, and transparent architecture, the resulting Python pipeline will serve as a powerful and versatile tool for the scientific community. It will enable the development and validation of robust chemometric algorithms, facilitate the training of machine learning models on controlled data, and provide an educational resource for teaching the fundamental principles of NIRS, all grounded in established physical and optical principles.

Reference

1. (PDF) Physics-Informed Neural Networks vs. ... https://www.researchgate.net/publication/395541911_Physics-Informed_Neural_Networks_vs_Physics_Models_for_Non-Invasive_Glucose_Monitoring_A_Comparative_Study_Under_Realistic_Synthetic_Conditions
2. Review of shortwave infrared imaging and spectroscopy in ... https://pmc.ncbi.nlm.nih.gov/articles/PMC12698095/
3. Artifact Management for Cerebral Near-Infrared ... https://www.mdpi.com/2306-5354/11/9/933
4. A Motion Artifact Correction Procedure for fNIRS Signals ... https://www.mdpi.com/1424-8220/21/15/5117
5. The Effect of Motion Artifacts on Near-Infrared ... https://pubmed.ncbi.nlm.nih.gov/29430243/
6. Improved Motion Artifact Correction in fNIRS Data by ... https://www.mdpi.com/1424-8220/23/8/3979
7. Hammerstein–Wiener Motion Artifact Correction for ... https://www.mdpi.com/1424-8220/24/10/3173
8. Estimation of Respiratory Rate from Functional Near ... https://www.mdpi.com/2079-6374/12/12/1170
9. Non-invasive blood glucose estimation method based on ... https://pmc.ncbi.nlm.nih.gov/articles/PMC10913690/
10. Near-infrared spectroscopy for medical, food and forage ... https://www.sciencedirect.com/science/article/abs/pii/B9780323912495000168
11. A Feasibility Study on Noninvasive Blood Glucose ... https://www.mdpi.com/2079-6374/15/11/711
12. Wavelength-Dependent Optical Sensing of Glucose in ... https://link.springer.com/article/10.1007/s11220-025-00714-2
13. Miniaturized Optical Glucose Sensor Using 1600–1700 nm ... https://advanced.onlinelibrary.wiley.com/doi/10.1002/adsr.202300160
14. (PDF) Non-invasive Blood Glucose Measurement Using ... https://www.researchgate.net/publication/398191919_Non-

invasive_Blood_Glucose_Measurement_Using_Near-infrared_Spectroscopy_and_Microcontroller_Equipment

15. Noninvasive Blood Glucose Monitoring Systems Using ... https://pdfs.semanticscholar.org/659a/3b802993ab126b48f70e456ddc87728f58d7.pdf
16. Systematic Analysis for fNIRS Measurement Combining ... https://ieeexplore.ieee.org/iel7/4563994/9116844/09126139.pdf
17. Experimental setup used to validate the predictions of our ... https://www.researchgate.net/figure/Experimental-setup-used-to-validate-the-predictions-of-our-noise-model-Light-is_fig1_336902162
18. Physics-Informed Neural Networks vs. Physics Models for ... https://arxiv.org/html/2509.12253v1
19. Rapid determination of protein, starch and moisture content ... https://www.sciencedirect.com/science/article/abs/pii/S088915752300008X
20. (PDF) Determination of Moisture, Starch, Protein, and Fat in ... https://www.researchgate.net/publication/6871759_Determination_of_Moisture_Starch_Protein_and_Fat_in_Common_Beans_Phaseolus_vulgaris_L_by_Near_Infrared_Spectroscopy
21. Detection of protein, starch, oil, and moisture content ... https://pmc.ncbi.nlm.nih.gov/articles/PMC10280583/
22. Near Infrared Spectroscopic Evaluation of Starch ... https://www.mdpi.com/2227-9717/9/11/1942
23. Research progress in near-infrared spectroscopy for detecting ... https://link.springer.com/article/10.1186/s40538-025-00747-5
24. A near-infrared spectroscopy method for detecting corn ... https://www.sciencedirect.com/science/article/abs/pii/S0889157525012372
25. Optical Measurement of Molar Absorption Coefficient ... https://www.mdpi.com/1424-8220/22/21/8179
26. Coefficient of determination between NIR absorbance and ... https://www.researchgate.net/figure/Coefficient-of-determination-between-NIR-absorbance-and-API-content-as-a-function-of_fig1_7416074
27. Near-infrared spectroscopy-based methods for quantitative ... https://www.tandfonline.com/doi/full/10.1080/00387010.2019.1681459
28. Influence of Temperature on the Predictive Ability of near ... https://www.researchgate.net/publication/244738624_Influence_of_Temperature_on_the_Predictive_Ability_of_near_Infrared_Spectroscopy_Models
29. Origins of Baseline Drift and Distortion in Fourier Transform ... https://pmc.ncbi.nlm.nih.gov/articles/PMC9268569/

30. Application of the near-infrared spectroscopy in ... https://www.researchgate.net/publication/223982056_Application_of_the_near-infrared_spectroscopy_in_the_pharmaceutical_technology
31. Mesh Optimization for Monte Carlo-Based Optical Tomography https://pmc.ncbi.nlm.nih.gov/articles/PMC4640680/
32. Tutorial on methods for estimation of optical absorption and ... https://pmc.ncbi.nlm.nih.gov/articles/PMC11166171/
33. Single-distance, phase-only frequency-domain NIRS for ... https://pmc.ncbi.nlm.nih.gov/articles/PMC12530142/
34. The application of Near-Infrared Spatially Resolved ... https://www.sciencedirect.com/science/article/abs/pii/S0378517323004842
35. Guideline on the use of Near Infrared Spectroscopy (NIRS) by ... https://www.ema.europa.eu/en/documents/scientific-guideline/draft-guideline-use-near-infrared-spectroscopy-pharmaceutical-industry-and-data-requirements-new-submissions-and-variations-revision-2_en.pdf
36. Rapid determination of protein, starch and moisture content ... https://www.researchgate.net/publication/366906888_Rapid_determination_of_protein_starch_and_moisture_contents_in_wheat_flour_by_near-infrared_hyperspectral_imaging?_share=1
37. High-throughput near-infrared spectroscopy for detection of ... https://pmc.ncbi.nlm.nih.gov/articles/PMC11663664/
38. A Nondestructive Detection Method for the Muti-Quality ... https://www.mdpi.com/2304-8158/13/22/3560
39. Comparison of NIR and Raman spectra combined with ... https://www.sciencedirect.com/science/article/abs/pii/S0956713522006910
40. Online Removal of Baseline Shift with a Polynomial ... https://www.mdpi.com/1424-8220/18/1/312
41. Noise Suppression in Organic Photodiodes - PubMed Central https://pmc.ncbi.nlm.nih.gov/articles/PMC12802548/
42. Noise current and specific detectivity of photodetector. a) ... https://www.researchgate.net/figure/Noise-current-and-specific-detectivity-of-photodetector-a-The-total-noise-current-in-a_fig2_334889850
43. Integrating Biometric and Environmental Monitoring in Next ... https://www.mdpi.com/2079-6374/16/1/43
44. Determination of glycated hemoglobin using near-infrared ... https://www.sciencedirect.com/science/article/abs/pii/S0169743915000982
45. Evaluation and Validation on Sensitivity of Near-Infrared ... https://www.researchgate.net/publication/

383939837_Evaluation_and_Validation_on_Sensitivity_of_Near-Infrared_Diffuse_Reflectance_in_Non-Invasive_Human_Blood_Glucose_Measurement

46. Noninvasive In Vivo Estimation of Blood-Glucose ... https://pmc.ncbi.nlm.nih.gov/articles/PMC8309922/
47. Derivation and validation of gray-box models to estimate ... https://www.nature.com/articles/s41598-021-91527-2
48. Optical Characterization of Two-Layered Turbid Media for Non ... https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0064095
49. Characterization of the reduced scattering coefficient for ... https://www.researchgate.net/publication/230968564_Characterization_of_the_reduced_scattering_coefficient_for_optically_thin_samples_Theory_and_experiments
50. Hemodynamics of the sternocleidomastoid measured with ... https://pmc.ncbi.nlm.nih.gov/articles/PMC8367268/
51. Deep learning-enabled high-speed, multi-parameter diffuse ... https://core.ac.uk/download/614692835.pdf
52. Emerging Thermal Detectors Based on Low-Dimensional ... https://pmc.ncbi.nlm.nih.gov/articles/PMC11945977/
53. Emerging optoelectronic architectures in carbon nanotube ... https://www.sciencedirect.com/science/article/pii/S2667325823002923
54. Molar Absorptivities of Glucose and Other Biological ... https://www.researchgate.net/publication/8192209_Molar_Absorptivities_of_Glucose_and_Other_Biological_Molecules_in_Aqueous_Solutions_over_the_First_Overtone_and_Combination_Regions_of_the_Near-Infrared_Spectrum
55. Detecting hemoglobin content blood glucose using surface ... https://www.researchgate.net/publication/334140956_Detecting_hemoglobin_content_blood_glucose_using_surface_plasmon_resonance_in_D-shaped_photonic_crystal_fiber
56. Diffuse reflectance spectra measurement in vivo skin tissue ... https://www.researchgate.net/publication/362217652_Diffuse_reflectance_spectra_measurement_in_vivo_skin_tissue_based_on_the_integrated_single_integrating_sphere_system
57. Issue 4 - Volume 36 - Measurement Science and Technology https://iopscience.iop.org/issue/0957-0233/36/4
58. (PDF) On feasibility of near-infrared spectroscopy for ... https://www.researchgate.net/publication/331236808_On_feasibility_of_near-infrared_spectroscopy_for_noninvasive_blood_glucose_measurements

59. Noninvasive blood glucose assay using a newly ... https://www.researchgate.net/publication/3409605_Noninvasive_blood_glucose_assay_using_a_newly_developed_near-infrared_system
60. Beer–Lambert law for optical tissue diagnostics https://pmc.ncbi.nlm.nih.gov/articles/PMC8553265/
61. Shot Noise - an overview https://www.sciencedirect.com/topics/mathematics/shot-noise
62. NIR Calibrations for Soybean Seeds and Soy Food ... https://www.nature.com/articles/npre.2011.6611.1.pdf
63. A Review of Optical Nondestructive Visual and Near − ... https://onlinelibrary.wiley.com/doi/10.1155/2013/341402
64. Near-infrared spectroscopy for analysing livestock diet quality https://pmc.ncbi.nlm.nih.gov/articles/PMC11609248/
65. A Monte Carlo investigation of optical pathlength in ... https://pubmed.ncbi.nlm.nih.gov/8108489/
66. A Review of Machine Learning for Near-Infrared ... https://www.mdpi.com/1424-8220/22/24/9764?type=check_update&version=1
67. Validation and Comparison of Monte Carlo and Finite ... https://pubmed.ncbi.nlm.nih.gov/31893425/
68. Optimizing the Monte-Carlo simulation program for NIRS ... https://hal.science/hal-04709286v1/file/2024274708.pdf
69. Small separation frequency-domain near-infrared spectroscopy ... https://pdfs.semanticscholar.org/e947/9b40c73399e66103dda5b5ac1a13c0e0b020.pdf
70. Measurement of Ex Vivo and In Vivo Tissue Optical ... https://www.researchgate.net/publication/226532817_Measurement_of_Ex_Vivo_and_In_Vivo_Tissue_Optical_Properties_Methods_and_Theories
71. Multimodal analysis of neurovascular coupling in the ... https://theses.hal.science/tel-03648471v1/file/TheseNourhashemi.pdf
72. Diffuse Reflectance Spectroscopy to Quantify in vivo Tissue ... https://search.proquest.com/openview/04c6057a05a64c8d9bc80e2ee822dc37/1?pq-origsite=gscholar&cbl=18750&diss=y
73. Multi-layer self-calibrated algorithm for transabdominal ... https://iopscience.iop.org/article/10.1088/2515-7647/ae1a27
74. Temperature Dependence of the Visible-Near-Infrared ... https://www.researchgate.net/publication/

231629610_Temperature_Dependence_of_the_Visible-Near-Infrared_Absorption_Spectrum_of_Liquid_Water

75. Visible-NIR 'point' spectroscopy in postharvest fruit and ... https://www.sciencedirect.com/science/article/pii/S0925521419303230
76. Applications of Photonics in Agriculture Sector: A Review https://pmc.ncbi.nlm.nih.gov/articles/PMC6571790/
77. Relating Near-Infrared Light Path-Length Modifications to ... https://www.researchgate.net/publication/351071702_Relating_Near-Infrared_Light_Path-Length_Modifications_to_the_Water_Content_of_Scattering_Media_in_Near-Infrared_Spectroscopy_Toward_a_New_Bouguer-Beer-Lambert_Law
78. Exploratory multivariate spectroscopic study on human skin https://www.researchgate.net/publication/10792726_Exploratory_multivariate_spectroscopic_study_on_human_skin
79. Visible-NIR 'point' spectroscopy in postharvest fruit and https://www.sciencedirect.com/science/article/am/pii/S0925521419303230
80. ASpecD: A Modular Framework for the Analysis of ... https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/cmtd.202100097
81. API Determination by NIR Spectroscopy Across ... https://pmc.ncbi.nlm.nih.gov/articles/PMC2628264/
82. Analysis of pharmaceuticals using near-infrared ... https://www.metrohm.com/content/dam/metrohm/shared/documents/application-bulletins/AB-410_1.pdf
83. Monitoring low dose API blend uniformity with Parteck® M ... https://www.sigmaaldrich.com/deepweb/assets/sigmaaldrich/product/documents/116/623/monitoring-whitepaper-wp11825en-ms.pdf?srsltid=AfmBOoowDDy0vzHjHBYrUTpA2SO5mK0szLv-pzpJ_DhNipPrvBVdENVn