DCS publications on PubMed: Jun2018-Jan2019

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Methodology. Searches were made in PubMed constraining the search period between June 1, 2018 and February, 28, 2019. These were later processed for readability but no records were otherwise added or removed. In the preparation of this file, the following searches have been executed:

- DCS

Portable system for Time-Domain Diffuse Correlation Spectroscopy.

Tamborini D, Stephens K, Wu M, Farzam P, Siegel A, Shatrovoy O, Blackwell M, Boas D, Carp S, Franceschini MA.

IEEE Trans Biomed Eng. Feb
doi: 10.1109/TBME.2019.[Epub ahead of print]
DOI: 10.1109/TBME.2019.2899762 PMID: 30794161

A Noninvasive Comparison Study between Human Gliomas with IDH1 and IDH2 Mutations by MR Spectroscopy.

Shen X, Voets NL, Larkin SJ, de Pennington N, Plaha P, Stacey R, McCullagh JSO, Schofield CJ, Clare S, Jezzard P, Cadoux-Hudson T, Ansorge O, Emir UE.

Metabolites. Feb 20;9(2). pii: E
doi: 10.3390/metabo9020035.

The oncogenes that are expressed in gliomas reprogram particular pathways of glucose, amino acids, and fatty acid metabolism. Mutations in isocitrate dehydrogenase genes (IDH1/2) in diffuse gliomas are associated with abnormally high levels of 2-hydroxyglutarate (2-HG) levels. The aim of this study was to determine whether metabolic reprogramming associated

with IDH mutant gliomas leads to additional H MRS-detectable differences between IDH1 and IDH2 mutations, and to identify metabolites correlated with 2-HG. A total of 21 glioma patients (age= 37 11, 13 males) were recruited for magnetic resonance spectroscopy (MRS) using semi-localization by adiabatic selective refocusing pulse sequence at an ultra-high-field (7T). For 20 patients, the tumor mutation subtype was confirmed by immunohistochemistry and DNA sequencing. LCModel analysis was applied for metabolite quantification. A two-sample t-test was used for metabolite comparisons between IDH1 (n = 15) and IDH2 (n = 5) mutant gliomas. The Pearson correlation coefficients between 2-HG and associated metabolites were calculated. A Bonferroni correction was applied for multiple comparison. IDH2 mutant gliomas have a higher level of 2-HG/tCho (total choline=phosphocholine+glycerylphosphorylcholine) (2.48 1.01vs.0.72 0.38, Pc $<$ 0.001) and myo-Inositol/tCho (2.70 0.90 vs. 1.46 0.51, Pc = 0.011) compared to IDH1 mutation gliomas. Associated metabolites, myo-Inositol and glucose+taurine were correlated with 2-HG levels. These results show the improved characterization of the metabolic pathways in IDH1 and IDH2 gliomas for precision medicine.

Early microvascular cerebral blood flow response to head-of-bed elevation is related to outcome in acute ischemic stroke.

Gregori-Pla C, Blanco I, Camps-Renom P, Zirak P, Serra I, Cotta G, Maruccia F, Prats-Snchez L, Martnez-Domeo A, Busch DR, Giacalone G, Mart-Fbregas J, Durduran T, Delgado-Mederos R.

J Neurol. Feb

doi: 10.1007/s00415-019-09226-y. [Epub ahead of print]

BACKGROUND AND AIMS: Previously, microvascular cerebral blood flow (CBF) response to a mild head-of-bed (HOB) elevation has been shown to be altered in acute ischemic stroke (AIS) by diffuse correlation spectroscopy (DCS). We have hypothesized that early CBF response is related to the functional outcome. METHODS: Patients with a non-lacunar AIS in the anterior circulation were monitored by DCS to measure relative CBF (?rCBF) on the frontal lobes bilaterally during a 0-30 HOB elevation at early (=?12) or late (>?12) hours from symptom onset. National Institutes of Health Stroke Scale (NIHSS) scores were recorded at baseline at 24 and at 48h. Functional outcome was measured by the modified Rankin Scale (mRS) at 3months. RESULTS: Thirty-eight (n?=?38) AIS patients [baseline NIHSS?=?19 (interquartile range: 16, 21)] were studied. ?rCBF

decreased similarly in both hemispheres (p?=?0.4) when HOB was elevated and was not associated with baseline and follow-up NIHSS scores or patient demographics. At the early phase (n?=?17), a lower or paradoxical ?rCBF response to HOB elevation was associated with an unfavorable functional outcome (mRS?>?2) in the ipsilesional (but not in the contralesional) hemisphere (p?=?0.010). ?rCBF response in the late acute phase was not related to mRS. CONCLUSIONS: Early CBF response to mild HOB elevation in the ipsilesional hemisphere is related to functional outcome. Further studies may enable optical monitoring at the bedside to individualize management strategies in the early phase of AIS.

Synthesis, crystal structure, and two-dimension correlation infrared spectroscopy on two novel Pr carboxylic acid coordination polymers.

Zhao L, Chen Y, Hao Y, Ma P, Wang N, Hu H.

Spectrochim Acta A Mol Biomol Spectrosc. Apr 15;213:430-
doi: 10.1016/j.saa.2019.01.Epub Jan 17.

Two new coordination polymers [Pr(PCPA)3(H2O)]n1 and [Pr2(PCPA)6(H2O)3]nnH2O 2(PCPA?=?p-chlorophenoxyacetic acid) have been synthesized under similar conditions by the hydrothermal method and characterized by single-crystal X-ray diffraction, elemental analyses, powder X-ray diffraction (PXRD) analysis, IR spectroscopy, two-dimensional correlation infrared spectroscopy(2D-IR COS) and ultraviolet-visible diffuse reflection integral spectroscopy (UV-Vis DRIS). 1 displays a 1D infinite chain, which is further linked by O/CH?O hydrogen bonds to form a 3D supra-molecular architecture. 2 shows a 2D layer structure, which is extended by CH?Cl hydrogen bonds generating a 3D network. Noteworthy, we also studied 2D-IR COS under the thermal perturbation to contribute to the development of theory. The 2D-IR correlation spectroscopy analysis is consistent with the analysis of structure and it is superior to 1D IR spectroscopy especially in the coordinated carboxyl group.

Diffuse reflectance spectroscopy to quantify the met-myoglobin proportion and meat oxygenation inside of pork and beef.

Nguyen T, Kim S, Kim JG.

Food Chem. Mar 1;275:369-

doi: 10.1016/j.foodchem.2018.09.Epub 2018 Sep 20.

The potential of diffuse reflectance spectroscopy (DRS) to quantify the met-myoglobin (met-Mb) proportion and meat oxygenation inside of pork and beef was examined. First, reflection spectra were obtained from pork (n?=?52) and beef (n?=?43) samples under fresh and stored conditions. Second, the DRS algorithm was applied to the reflectance spectra to calculate the met-Mb proportion and oxygenation of the meat. Lastly, a regression model was developed showing the change in the met-Mb proportion and oxygenation during met-Mb formation and degradation. A linear relationship existed between the DRS-based computed data and the known met-Mb proportion with a high correlation (R2?=?0.9999) and a low error (0.86%). Measurement of the meat samples revealed a linear increment of the met-Mb proportion (R2?=?0.77) and a quadratic change in the oxygenation (R2?=?0.44) during the met-Mb formation process. This study demonstrated the ability of DRS to quantitatively analyze the relative content of myoglobin derivatives in both pork and beef.

Characterization of the microvascular cerebral blood flow response to obstructive apneic events during night sleep.

Zirak P, Gregori-Pla C, Blanco I, Fortuna A, Cotta G, Bramon P, Serra I, Mola A, Sol-Soler J, Giraldo-Giraldo BF, Durduran T, Mayos M.

Neurophotonics. Oct;5(4):
doi: 10.1117/1.NPh.5.4.Epub 2018 Nov 3.

Obstructive apnea causes periodic changes in cerebral and systemic hemodynamics, which may contribute to the increased risk of cerebrovascular disease of patients with obstructive sleep apnea (OSA) syndrome. The improved understanding of the consequences of an apneic event on the brain perfusion may improve our knowledge of these consequences and then allow for the development of preventive strategies. Our aim was to characterize the typical microvascular, cortical cerebral blood flow (CBF) changes in an OSA population during an apneic event. Sixteen patients (age 58 8 ?? years , 75% male) with a high risk of severe OSA were measured with a polysomnography device and with diffuse correlation spectroscopy (DCS) during one night of sleep with 1365 obstructive apneic events detected. All patients were later confirmed to suffer from severe OSA syndrome with a mean of 83 15 apneas and hypopneas per hour. DCS has been shown to be able to characterize the microvascular CBF response to each event with a sufficient contrast-to-noise ratio to reveal its dynamics. It has also revealed

that an apnea causes a peak increase of microvascular CBF (30 17 %) at the end of the event followed by a drop (- 20 12 %) similar to what was observed in macrovascular CBF velocity of the middle cerebral artery. This study paves the way for the utilization of DCS for further studies on these populations.

Investigation of the buried planar interfaces in multi-layered inverted organic solar cells using x-ray reflectivity and impedance spectroscopy.

Srivastava SB, Modi MH, Ghosh SK, Singh SP.

J Phys Condens Matter. Mar 27;31(12):
doi: 10.1088/1361-648X/aafe Epub Jan 14.

The hole and electron extracting interlayers in the organic solar cells (OSCs) play an important role in high performing devices. The present work focuses on an investigation of Zinc oxide/bulk heterojunction (ZnO/BHJ) and BHJ/MoO x (Molybdenum oxide) buried planar interfaces in inverted OSC devices using the optical contrast in various layers along with the electrical measurements. The x-ray reflectivity (XRR) analysis demonstrates the formation of additional intermixing layers at the interfaces of ZnO/BHJ and BHJ/MoO x . Our results indicate infusion of PC71BM into ZnO layer up to 4?nm which smoothen the ZnO/BHJ interface. In contrast, thermally evaporated MoO x molecules diffuse into PTB7-Th dominant upper layers of BHJ active layer resulting in an intermixed layer at the interface of MoO x /BHJ. The high recombination resistance (5 kO cm2) and electron lifetime (70 s), obtained from the impedance spectroscopy (IS), support such vertical segregation of PTB7-Th and PC71BM in the active layer. The OSC devices, processed in ambient condition, exhibit high power conversion efficiency of 6.4%. We consider our results have great significance to understand the structure of buried planar interfaces at interlayers and their correlation with the electrical parameters representing various interfacial mechanisms of OSCs.

Muscular blood flow responses as an early predictor of the severity of diabetic neuropathy at a later stage in streptozotocin-induced type I diabetic rats: a diffuse correlation spectroscopy study.

Ono Y, Esaki K, Takahashi Y, Nakabayashi M, Ichinose M, Lee K.
Biomed Opt Express. Aug 29;9(9):4539-
doi: 10.1364/BOE.9.004539. eCollection Sep 1.

We propose a novel application of diffuse correlation spectroscopy to evaluate microvascular malfunctions of muscle tissue affected by hyperglycemia and determine their correlation with the severity of diabetic neuropathy at a later stage. Microvascular responses of the thigh muscle and the mechanical pain threshold of the hind paw of streptozotocin-induced type I diabetic rats were continuously monitored once per week for 70 days. Significantly decreased baseline blood flow and reactive hyperemia responses were observed as early as 1 week after hyperglycemia induction. The reactive hyperemia response at 2 weeks of hyperglycemia was highly correlated with the mechanical pain threshold at 8 weeks, at which time a decreased pain threshold was statistically confirmed in hyperglycemic rats relative to controls.

Estimation of free hemoglobin concentrations in blood bags by diffuse reflectance spectroscopy.

Can OM, lgen Y.
J Biomed Opt. Dec;23(12):1-
doi: 10.1117/1.JBO.23.12.127001.

Free hemoglobin (FHB) concentration is considered a prospect quality indicator for erythrocyte suspensions (ES) under storage. Storage lesions alter the optical properties of ES and can be monitored by diffuse reflectance spectroscopy. Due to storage lesions, erythrocytes lyse and release hemoglobin into the extracellular medium. The purpose of the study is to model and assess the quality of ES units in a blood bank with diffuse reflectance measurements together with hematological variables reflecting absorption and scattering characteristics of ES. FHB concentrations were modeled based on the increased scattering in the extracellular medium. A semiempirical model was used for relating optical properties of ES to the diffuse reflectance measurements. The attenuation in the blood bag was computed and its influence was discarded via normalization, in accordance with Monte Carlo simulations. In the experiments, 40 ES units were measured multiple times during prolonged storage of 70 days. A generalized linear model was used for modeling the training set, and, in the validation, the highest correlation coefficient between predicted and actual FHB concentrations was 0.89. Predicting the actual value was accurate at a maximum level of R2??=??0.80. The error rate of the model in diagnosing the true quality was about 10%.

Towards the use of diffuse reflectance spectroscopy for real-time in vivo detection of breast cancer during surgery.

de Boer LL, Bydlon TM, van Duijnhoven F, Vranken Peeters MTFD, Loo CE, Winter-Warnars GAO, Sanders J, Sterenborg HJCM, Hendriks BHW, Ruers TJM.

J Transl Med. Dec 19;16(1):
doi: 10.1186/s12967-018-1747-5.

BACKGROUND: Breast cancer surgeons struggle with differentiating healthy tissue from cancer at the resection margin during surgery. We report on the feasibility of using diffuse reflectance spectroscopy (DRS) for real-time in vivo tissue characterization. METHODS: Evaluating feasibility of the technology requires a setting in which measurements, imaging and pathology have the best possible correlation. For this purpose an optical biopsy needle was used that had integrated optical fibers at the tip of the needle. This approach enabled the best possible correlation between optical measurement volume and tissue histology. With this optical biopsy needle we acquired real-time DRS data of normal tissue and tumor tissue in 27 patients that underwent an ultrasound guided breast biopsy procedure. Five additional patients were measured in continuous mode in which we obtained DRS measurements along the entire biopsy needle trajectory. We developed and compared three different support vector machine based classification models to classify the DRS measurements. RESULTS: With DRS malignant tissue could be discriminated from healthy tissue. The classification model that was based on eight selected wavelengths had the highest accuracy and Matthews Correlation Coefficient (MCC) of 0.93 and 0.87, respectively. In three patients that were measured in continuous mode and had malignant tissue in their biopsy specimen, a clear transition was seen in the classified DRS measurements going from healthy tissue to tumor tissue. This transition was not seen in the other two continuously measured patients that had benign tissue in their biopsy specimen. CONCLUSIONS: It was concluded that DRS is feasible for integration in a surgical tool that could assist the breast surgeon in detecting positive resection margins during breast surgery. Trail registration NIH US National Library of Medicine-clinicaltrails.gov, NCT01730365. Registered: 10/04/2012 https://clinicaltrials.gov/ct2/show/study/NCT01730365.

Microfluidics-based self-assembly of peptide-loaded microgels: Effect of three dimensional (3D) printed micromixer design.

Borro BC, Bohr A, Bucciarelli S, Boetker JP, Foged C, Rantanen J, Malmsten M.

J Colloid Interface Sci. Mar 7;538:559-
doi: 10.1016/j.jcis.2018.12.010. Epub Dec 4.

In an effort to contribute to research in scalable production systems for polymeric delivery systems loaded with antimicrobial peptides (AMPs), we here investigate effects of hydrodynamic flow conditions on microfluidic particle generation. For this purpose, rapid prototyping using 3D printing was applied to prepare micromixers with three different geometric designs, which were used to prepare Ca2+-cross-linked alginate microgels loaded with the AMP polymyxin B in a continuous process. Based on fluid dynamic simulations, the hydrodynamic flow patterns in the micromixers were designed to be either (i) turbulent with chaotic disruption, (ii) laminar with convective mixing, or (iii) convective with microvortex formation. The physicochemical properties of the microgels prepared with these micromixers were characterized by photon correlation spectroscopy, laser-Doppler micro-electrophoresis, small-angle x-ray scattering, and ellipsometry. The particle size and compactness were found to depend on the micromixer geometry: From such studies, particle size and compactness were found to depend on micromixer geometry, the smallest and most compact particles were obtained by preparation involving microvortex flows, while larger and more diffuse microgels were formed upon laminar mixing. Polymyxin B was found to be localized in the particle interior and to cause particle growth with increasing peptide loading. Ca2+-induced cross-linking of alginate, in turn, results in particle contraction. The peptide encapsulation efficiency was found to be higher than 80% for all investigated micromixer designs; the highest encapsulation efficiency observed for the smallest particles generated by microvortex-mediated self-assembly. Ellipsometry results for surface-immobilized microgels, as well as results on peptide encapsulation, demonstrated electrolyte-induced peptide release. Taken together, these findings demonstrate that rapid prototyping of microfluidics using 3D-printed micromixers offers promises for continuous manufacturing of AMP-loaded microgels. Although the micromixer combining turbulent flow and microvortexes was demonstrated to be the most efficient, all three micromixer designs were found to mediate self-assembly of small microgels displaying efficient peptide encapsulation. This demonstrates the robustness of employing 3D-printed micromixers for microfluidic assembly of AMP-loaded microgels during continuous production.

Noninvasive continuous optical monitoring of absolute cerebral blood flow in critically ill adults.

He L, Baker WB, Milej D, Kavuri VC, Mesquita RC, Busch DR, Abramson K, Jiang JY, Diop M, St Lawrence K, Amendolia O, Quattrone F, Balu R, Kofke WA, Yodh AG.

Neurophotonics. Oct;5(4):
doi: 10.1117/1.NPh.5.4.Epub 2018 Nov 23.

We investigate a scheme for noninvasive continuous monitoring of absolute cerebral blood flow (CBF) in adult human patients based on a combination of time-resolved dynamic contrast-enhanced near-infrared spectroscopy (DCE-NIRS) and diffuse correlation spectroscopy (DCS) with semi-infinite head model of photon propogation. Continuous CBF is obtained via calibration of the DCS blood flow index (BFI) with absolute CBF obtained by intermittent intravenous injections of the optical contrast agent indocyanine green. A calibration coefficient (?) for the CBF is thus determined, permitting conversion of DCS BFI to absolute blood flow units at all other times. A study of patients with acute brain injury (N = 7) is carried out to ascertain the stability of ? . The patient-averaged DCS calibration coefficient across multiple monitoring days and multiple patients was determined, and good agreement between the two calibration coefficients measured at different times during single monitoring days was found. The patient-averaged calibration coefficient of 1.24 10 9 ?? (mL / 100 ?? g / min) / (cm 2 / s) was applied to previously measured DCS BFI from similar brain-injured patients; in this case, absolute CBF was underestimated compared with XeCT, an effect we show is primarily due to use of semi-infinite homogeneous models of the head.

White powder identification using broadband coherent light in the molecular fingerprint region.

Maidment L, Schunemann PG, Reid DT.

Opt Express. Sep 17;26(19):25364-
doi: 10.1364/OE.26.025364.
DOI: 10.1364/OE.26.025364 PMID: 30469638

Small separation diffuse correlation spectroscopy for measure-

ment of cerebral blood flow in rodents.

Sathialingam E, Lee SY, Sanders B, Park J, McCracken CE, Bryan L, Buckley EM.

Biomed Opt Express. Oct 25;9(11):5719-
doi: 10.1364/BOE.9.005719. eCollection Nov 1.

Diffuse correlation spectroscopy (DCS) has shown promise as a means to non-invasively measure cerebral blood flow in small animal models. Here, we characterize the validity of DCS at small source-detector reflectance separations needed for small animal measurements. Through Monte Carlo simulations and liquid phantom experiments, we show that DCS error increases as separation decreases, although error remains below 12% for separations > 0.2 cm. In mice, DCS measures of cerebral blood flow have excellent intra-user repeatability and strongly correlate with MRI measures of blood flow (R = 0.74, p<0.01). These results are generalizable to other DCS applications wherein short-separation reflectance geometries are desired.

Prolonged monitoring of cerebral blood flow and autoregulation with diffuse correlation spectroscopy in neurocritical care patients.

Selb J, Wu KC, Sutin J, Lin PI, Farzam P, Bechek S, Shenoy A, Patel AB, Boas DA, Franceschini MA, Rosenthal ES.

Neurophotonics. Oct;5(4):
doi: 10.1117/1.NPh.5.4.Epub 2018 Nov 13.

Monitoring of cerebral blood flow (CBF) and autoregulation are essential components of neurocritical care, but continuous noninvasive methods for CBF monitoring are lacking. Diffuse correlation spectroscopy (DCS) is a noninvasive diffuse optical modality that measures a CBF index (CBF i) in the cortex microvasculature by monitoring the rapid fluctuations of near-infrared light diffusing through moving red blood cells. We tested the feasibility of monitoring CBF i with DCS in at-risk patients in the Neurosciences Intensive Care Unit. DCS data were acquired continuously for up to 20h in six patients with aneurysmal subarachnoid hemorrhage, as permitted by clinical care. Mean arterial blood pressure was recorded synchronously, allowing us to derive autoregulation curves and to compute an autoregulation index. The autoregulation curves suggest disrupted cerebral autoregulation in most patients, with the severity of disruption and the limits of preserved autoregulation varying between subjects. Our findings suggest the potential of the DCS modality for noninvasive, long-term monitoring of cerebral

perfusion, and autoregulation.

Diffuse Speckle Contrast Analysis Assisted Intraoperative Blood Flow Monitoring in the Rat Model of Femoral Arterial Occlusion.

Yeo CB, Jo WR, Kim HJ, Song C.

Conf Proc IEEE Eng Med Biol Soc. Jul;2018:858-
doi: 10.1109/EMBC.2018.8512382.

DOI: 10.1109/EMBC.2018.8512382 PMID: 30440526

Neurologic phenotypes associated with COL4A1/2 mutations: Expanding the spectrum of disease.

Zagaglia S, Selch C, Nisevic JR, Mei D, Michalak Z, Hernandez-Hernandez L, Krithika S, Vezyroglou K, Varadkar SM, Pepler A, Biskup S, Leo M, Grtner J, Merkenschlager A, Jaksch M, Mller RS, Gardella E, Kristiansen BS, Hansen LK, Vari MS, Helbig KL, Desai S, Smith-Hicks CL, Hino-Fukuyo N, Talvik T, Laugesaar R, Ilves P, unap K, Krber I, Hartlieb T, Kudernatsch M, Winkler P, Schimmel M, Hasse A, Knuf M, Heinemeyer J, Makowski C, Ghedia S, Subramanian GM, Striano P, Thomas RH, Micallef C, Thom M, Werring DJ, Kluger GJ, Cross JH, Guerrini R, Balestrini S, Sisodiya SM.

Neurology. Nov 27;91(22):e2078-e
doi: 10.1212/WNL.0000000000006567. Epub Nov 9.

OBJECTIVE: To characterize the neurologic phenotypes associated with COL4A1/2 mutations and to seek genotype-phenotype correlation. METHODS: We analyzed clinical, EEG, and neuroimaging data of 44 new and 55 previously reported patients with COL4A1/COL4A2 mutations. RESULTS: Childhood-onset focal seizures, frequently complicated by status epilepticus and resistance to antiepileptic drugs, was the most common phenotype. EEG typically showed focal epileptiform discharges in the context of other abnormalities, including generalized sharp waves or slowing. In 46.4% of new patients with focal seizures, porencephalic cysts on brain MRI colocalized with the area of the focal epileptiform discharges. In patients with porencephalic cysts, brain MRI frequently also showed extensive white matter abnormalities, consistent with the finding of diffuse cerebral disturbance on EEG. Notably, we also identified a subgroup of patients with epilepsy as their main clinical feature, in which brain MRI showed

nonspecific findings, in particular periventricular leukoencephalopathy and ventricular asymmetry. Analysis of 15 pedigrees suggested a worsening of the severity of clinical phenotype in succeeding generations, particularly when maternally inherited. Mutations associated with epilepsy were spread across COL4A1 and a clear genotype-phenotype correlation did not emerge. CONCLUSION: COL4A1/COL4A2 mutations typically cause a severe neurologic condition and a broader spectrum of milder phenotypes, in which epilepsy is the predominant feature. Early identification of patients carrying COL4A1/COL4A2 mutations may have important clinical consequences, while for research efforts, omission from large-scale epilepsy sequencing studies of individuals with abnormalities on brain MRI may generate misleading estimates of the genetic contribution to the epilepsies overall.

Non-invasive optical neuromonitoring of the temperature-dependence of cerebral oxygen metabolism during deep hypothermic cardiopulmonary bypass in neonatal swine.

Ko TS, Mavroudis CD, Baker WB, Morano VC, Mensah-Brown K, Boorady TW, Schmidt AL, Lynch JM, Busch DR, Gentile J, Bratinov G, Lin Y, Jeong S, Melchior RW, Rosenthal TM, Shade BC, Schiavo KL, Xiao R, Gaynor JW, Yodh AG, Kilbaugh TJ, Licht DJ.

J Cereb Blood Flow Metab. Oct 30:271678X
doi: 10.1177/0271678X[Epub ahead of print]

Management of deep hypothermic (DH) cardiopulmonary bypass (CPB), a critical neuroprotective strategy, currently relies on non-invasive temperature to guide cerebral metabolic suppression during complex cardiac surgery in neonates. Considerable inter-subject variability in temperature response and residual metabolism may contribute to the persisting risk for postoperative neurological injury. To characterize and mitigate this variability, we assess the sufficiency of conventional nasopharyngeal temperature (NPT) guidance, and in the process, validate combined non-invasive frequency-domain diffuse optical spectroscopy (FD-DOS) and diffuse correlation spectroscopy (DCS) for direct measurement of cerebral metabolic rate of oxygen (CMRO2). During CPB, n?=?8 neonatal swine underwent cooling from normothermia to 18?, sustained DH perfusion for 40?min, and then rewarming to simulate cardiac surgery. Continuous non-invasive and invasive measurements of intracranial temperature (ICT) and CMRO2 were acquired. Significant hysteresis (p?<?0.001) between cooling and rewarming periods in the NPT versus ICT and NPT versus CMRO2 relationships were found.

Resolution of this hysteresis in the ICT versus CMRO2 relationship identified a crucial insufficiency of conventional NPT guidance. Non-invasive CMRO2 temperature coefficients with respect to NPT (Q10?=?2.0) and ICT (Q10?=?2.5) are consistent with previous reports and provide further validation of FD-DOS/DCS CMRO2 monitoring during DH CPB to optimize management.

Comparing Geometry and Chemistry When Confined Molecules Diffuse in Monodisperse Metal-Organic Framework Pores.

Jee AY, Yanai N, Granick S.

J Phys Chem Lett. Nov 15;9(22):6399-
doi: 10.1021/acs.jpclett.8b Epub Oct 26.

The monodisperse pore structure of MOFs (metal-organic frameworks) is advantageous for investigating how porosity influences diffusion. Here we report translational and rotational diffusion using fluorescence correlation spectroscopy and time-correlated single-photon counting, using the three-dimensional pores of the zeolitic-like metal-organic framework family. We compare the influence of size and electric charge as well as dependence on pore size that we controlled through postsynthetic cation-exchange modifications. Charge-charge interactions with the MOF appeared to produce transient adsorption, manifested as a relatively fast and a slower diffusion process, but diffusants without net electric charge displayed a single diffusion process. Obtained from this family of guest molecules selected to be fluorescent, these findings suggest potentially useful general design rules to predict how pore size, guest size, and host-guest interaction control guest mobility within nanopores. With striking fidelity, diffusion coefficient scales with the ratio of cross-sectional areas of diffusant and host pores when charge is taken into account.

In vivo characterization of light scattering properties of human skin in the 475- to 850-nm wavelength range in a Swedish cohort.

Jonasson H, Fredriksson I, Bergstrand S, stgren CJ, Larsson M, Strmberg T.

J Biomed Opt. Sep;23(12):1-
doi: 10.1117/1.JBO.23.12.121608.

We have determined in vivo optical scattering properties of normal human skin in 1734 subjects, mostly with fair skin type, within the Swedish CArdioPulmonary bioImage Study. The measurements were performed with a noninvasive system, integrating spatially resolved diffuse reflectance spectroscopy and laser Doppler flowmetry. Data were analyzed with an inverse Monte Carlo algorithm, accounting for both scattering, geometrical, and absorbing properties of the tissue. The reduced scattering coefficient was found to decrease from 3.16 0.72 to 1.13 0.27mm-1 (mean SD) in the 475- to 850-nm wavelength range. There was a negative correlation between the reduced scattering coefficient and age, and a significant difference between men and women in the reduced scattering coefficient as well as in the fraction of small scattering particles. This large study on tissue scattering with mean values and normal variation can serve as a reference when designing diagnostic techniques or when evaluating the effect of therapeutic optical systems.

Simultaneous monitoring of cerebral perfusion and cytochrome c oxidase by combining broadband near-infrared spectroscopy and diffuse correlation spectroscopy.

Rajaram A, Bale G, Kewin M, Morrison LB, Tachtsidis I, St Lawrence K, Diop M.

Biomed Opt Express. May 10;9(6):2588-
doi: 10.1364/BOE.9.002588. eCollection Jun 1.

Preterm infants born with very low birth weights are at a high risk of brain injury, in part because the premature brain is believed to be prone to periods of low cerebral blood flow (CBF). Tissue damage is likely to occur if reduction in CBF is sufficient to impair cerebral energy metabolism for extended periods. Therefore, a neuromonitoring method that can detect reductions in CBF, large enough to affect metabolism, could alert the neonatal intensive care team before injury occurs. In this report, we present the development of an optical system that combines diffuse correlation spectroscopy (DCS) for monitoring CBF and broadband near-infrared spectroscopy (B-NIRS) for monitoring the oxidation state of cytochrome c oxidase (oxCCO) - a key biomarker of oxidative metabolism. The hybrid instrument includes a multiplexing system to enable concomitant DCS and B-NIRS measurements while avoiding crosstalk between the two subsystems. The ability of the instrument to monitor dynamic changes in CBF and oxCCO was demonstrated in a piglet model of neonatal hypoxia-ischemia (HI). Experiments

conducted in eight animals, including two controls, showed that oxCCO exhibited a delayed response to ischemia while CBF and tissue oxygenation (StO2) responses were instantaneous. These findings suggest that simultaneous neuromonitoring of perfusion and metabolism could provide critical information regarding clinically significant hemodynamic events prior to the onset of brain injury.

Current Progress in CNS Imaging of Myotonic Dystrophy.
Minnerop M, Gliem C, Kornblum C.
Front Neurol. Aug 21;9:
doi: 10.3389/fneur.2018.eCollection 2018.

Neuroimaging in myotonic dystrophies provided a major contribution to the insight into brain involvement which is highly prevalent in these multisystemic disorders. Particular in Myotonic Dystrophy Type 1, conventional MRI first revealed hyperintense white matter lesions, predominantly localized in the anterior temporal lobe. Brain atrophy and ventricle enlargement were additional early findings already described almost 30 years ago. Since then, more advanced and sophisticated imaging methods have been applied in Myotonic Dystrophy Types 1 and 2. Involvement of actually normal appearing white matter and widespread cortical affection in PET studies were key results toward the recognition of diffuse and not only focally localized brain pathology in vivo. Later, structural abnormalities of both, gray and white matter, have been found in both forms of the disorder, albeit more prominent in myotonic dystrophy type 1. In Type 1, a consistent widespread cortical and subcortical involvement of gray and white matter affecting all lobes, brainstem and cerebellum was observed. Spectroscopy studies gave additional evidence of neuronal and glial damage in both types. Central questions regarding the origin and spatiotemporal evolution of the CNS involvement and its relevance for clinical symptoms had already been raised 30 years ago, however are still not answered. Results of correlation analyses between neuroimaging and clinical parameters are diverse and with few exceptions not well reproducible across studies. It may be related to the fact that most of the reported studies included only small numbers of subjects, sometimes even not separating Myotonic Dystrophy Type 1 from Type 2. But this heterogeneity may also support the current point of view that the clinical impairments are not simply linked to specific and regionally circumscribed structural or functional brain alterations. It seems more convincing that disturbed networks build the functional and structural substrate of

clinical symptoms in these disorders as it is proposed in other neuropsychiatric diseases. Consecutively, structural and functional network analyses may provide additional information regarding the link between brain pathology and clinical symptoms. Up to now, only cross-sectional neuroimaging studies have been published. To analyze the temporal evolution of brain affection, longitudinal studies are urgently needed, and systematic natural history data would be useful to identify potential biomarkers for therapeutic studies.

Accurate and rapid detection of soil and fertilizer properties based on visible/near-infrared spectroscopy.

Lin Z, Wang R, Wang Y, Wang L, Lu C, Liu Y, Zhang Z, Zhu L.

Appl Opt. Jun 20;57(18):D69-D

doi: 10.1364/AO.57.000D69.

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Estimating soil heavy metals concentration at large scale using visible and near-infrared reflectance spectroscopy.

Yousefi G, Homaee M, Norouzi AA.

Environ Monit Assess. Aug 13;190(9):

doi: 10.1007/s10661-018-6898-6.

This study was aimed (i) to examine using diffuse reflectance spectra within VNIR region to estimate soil heavy metals concentrations at large scale, (ii) to compare the influence of different pre-processing models on predictive model accuracy, and (iii) to explore the best predictive models. A number of 325 topsoil samples were collected and their spectral data, pH, clay content, organic matter, Ni, and Cu concentrations were determined. To improve spectral data, various pre-processing methods including Savitzky-Golay smoothing filter, Savitzky-Golay smoothing filter with first and second derivatives, and standard normal variant (SNV) were used. Partial least squares regression (PLSR), principal component regression (PCR), and support vector machine regression (SVMR) models were employed to build calibration models for estimating soil heavy metals concentration followed by evaluation of provided predictive models. Results indicated that Cu had stronger correlation coefficients with spectral bands compared to Ni. Cu and Ni demonstrated strongest correlations at wavelengths 1925 and

1393nm, respectively. Based on RMSE, R2, and RPD statistics, the PLSR model with Savitzky-Golay filter pretreatment provided the most accurate predictions for both Cu and Ni (R2?=?0.905, RMSE = 0.00123, RPD = 2.80 for Ni; R2 = 0.825, RMSE = 0.00467, RPD = 2.04 for Cu) where such prediction was much better for Ni than for Cu. Reasonable results with lower accuracy and stability were obtained for PCR (R2 = 0.742, RMSE = 0.00181, RPD = 1.91 for Ni; R2 = 0.731, RMSE = 0.00578, RPD = 1.65 for Cu) and SVMR (R2 = 0.643, RMSE = 0.00091, RPD = 3.80 for Ni; R2 = 0.505, RMSE = 0.00296, RPD = 3.22 for Cu). We concluded that reflectance spectroscopy technique could be applied as a reliable tool for detection and prediction of soil heavy metals.

Band Gap Implications on Nano-TiO2 Surface Modification with Ascorbic Acid for Visible Light-Active Polypropylene Coated Photocatalyst.

D'Amato CA, Giovannetti R, Zannotti M, Rommozzi E, Minicucci M, Gunnella R, Di Cicco A.

Nanomaterials (Basel). Aug 7;8(8). pii: E
doi: 10.3390/nano8080599.

The effect of surface modification using ascorbic acid as a surface modifier of nano-TiO2 heterogeneous photocatalyst was studied. The preparation of supported photocatalyst was made by a specific paste containing ascorbic acid modified TiO2 nanoparticles used to cover Polypropylene as a support material. The obtained heterogeneous photocatalyst was thoroughly characterized (scanning electron microscope (SEM), RAMAN, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), photoluminescence (PL), and Diffuse Reflectance Spectra (DRS) and successfully applied in the visible light photodegradation of Alizarin Red S in water solutions. In particular, this new supported TiO2 photocatalyst showed a change in the adsorption mechanism of dye with respect to that of only TiO2 due to the surface properties. In addition, an improvement of photocatalytic performances in the visible light photodegration was obtained, showing a strict correlation between efficiency and energy band gap values, evidencing the favorable surface modification of TiO2 nanoparticles.

Microstructural and Neurochemical Changes in the Rat Brain

After Diffuse Axonal Injury.

Chen X, Chen Y, Xu Y, Gao Q, Shen Z, Zheng W.

J Magn Reson Imaging. Aug
doi: 10.1002/jmri.[Epub ahead of print]

BACKGROUND: Diffuse axonal injury (DAI) is one of the devastating types of traumatic brain injury, but is difficult to detect on conventional imaging in its early stages. PURPOSE: To test the technical feasibility and diagnostic value of diffusion kurtosis imaging (DKI) and glutamate chemical exchange saturation transfer (GluCEST) imaging in the brain after DAI. STUDY TYPE: Prospective. ANIMAL MODEL: Sixty Sprague-Dawley rats. The DAI model was induced by using the impact acceleration model of Marmarou et al with modified settings. FIELD STRENGTH/SEQUENCE: A 7.0T animal MR scanner with a fast spin-echo sequence (T2 -weighted imaging), fast spin-echo multislice sequence (DKI), echo planar imaging in the signal of the chemical exchange saturation transfer sequence (CEST), and point-resolved spectroscopy sequence (hydrogenproton magnetic resonance spectroscopy, 1 H-MRS). ASSESSMENT: Brain MRI scanned before and 2 hours after injury. DKI images were processed with MatLab and MRIcro software, GluCEST images were processed using software routines written in MatLab, and spectroscopic data were postprocessed with LCModel. STATISTICAL TESTS: The parameters of these techniques were assessed using the independent sample t-test and Pearson correlation. RESULTS: Mean kurtosis and mean diffusivity values were significantly higher than controls in the parietal lobe, hippocampus, and thalamus (P?<? 0.01). However, fractional anisotropy was lower only in the parietal lobe, with no detectable changes in the hippocampus and thalamus. GluCEST values of the parietal lobe, hippocampus, and thalamus were significantly higher than controls in DAI rats (P?<? 0.01). This change was further validated through 1 H-MRS. A positive correlation was observed between glutamate (Glu) and glutamate compound (Glx) concentrations and GluCEST values (Glu: R2 ?=?0.589, Glx: R2 ?=?0.878). DATA CONCLUSION: DKI and GluCEST might be acceptably sensitive for tracking microstructural and neurochemical changes in the brain following DAI. LEVEL OF EVIDENCE: 1 Technical Efficacy: Stage 2 J. Magn. Reson. Imaging 2018.

Detection of Brain Hypoxia Based on Noninvasive Optical Monitoring of Cerebral Blood Flow with Diffuse Correlation Spectroscopy.

Busch DR, Balu R, Baker WB, Guo W, He L, Diop M, Milej D, Kavuri V, Amendolia O, St Lawrence K, Yodh AG, Kofke WA.
Neurocrit Care. Feb;30(1):72-
doi: 10.1007/s12028-018-0573-1.

BACKGROUND: Diffuse correlation spectroscopy (DCS) noninvasively permits continuous, quantitative, bedside measurements of cerebral blood flow (CBF). To test whether optical monitoring (OM) can detect decrements in CBF producing cerebral hypoxia, we applied the OM technique continuously to probe brain-injured patients who also had invasive brain tissue oxygen (PbO2) monitors. METHODS: Comatose patients with a Glasgow Coma Score (GCS) <?8) were enrolled in an IRB-approved protocol after obtaining informed consent from the legally authorized representative. Patients underwent 6-8h of daily monitoring. Brain PbO2 was measured with a Clark electrode. Absolute CBF was monitored with DCS, calibrated by perfusion measurements based on intravenous indocyanine green bolus administration. Variation of optical CBF and mean arterial pressure (MAP) from baseline was measured during periods of brain hypoxia (defined as a drop in PbO2 below 19mmHg for more than 6min from baseline (PbO2?>?21mmHg). In a secondary analysis, we compared optical CBF and MAP during randomly selected 12-min periods of "normal" (>?21mmHg) and "low" (<?19mmHg) PbO2. Receiver operator characteristic (ROC) and logistic regression analysis were employed to assess the utility of optical CBF, MAP, and the two-variable combination, for discrimination of brain hypoxia from normal brain oxygen tension. RESULTS: Seven patients were enrolled and monitored for a total of 17days. Baseline-normalized MAP and CBF significantly decreased during brain hypoxia events (p?<?0.05). Through use of randomly selected, temporally sparse windows of low and high PbO2, we observed that both MAP and optical CBF discriminated between periods of brain hypoxia and normal brain oxygen tension (ROC AUC 0.761, 0.762, respectively). Further, combining these variables using logistic regression analysis markedly improved the ability to distinguish low- and high-PbO2 epochs (AUC 0.876). CONCLUSIONS: The data suggest optical techniques may be able to provide continuous individualized CBF measurement to indicate occurrence of brain hypoxia and guide brain-directed therapy.

Silver-modified octahedral anatase particles as plasmonic photocatalyst.

Wei Z, Janczarek M, Endo M, Colbeau-Justin C, Ohtani B, Kowalska E.

Catal Today. Jul 15;310:19-
doi: 10.1016/j.cattod.2017.05.039.

Octahedral anatase particles (OAPs) were modified with silver nanoparticles (NPs) by photodeposition method. The properties of OAPs influenced the properties of silver deposits, and thus the photocatalytic activity of the obtained silver-modified OAPs. Photocatalytic activities were tested under UV and vis irradiation for oxidative decomposition of acetic acid and oxidation of 2-propanol, respectively. The properties of silver-modified OAPs were investigated by XRD, STEM, DRS, XPS and time-resolved microwave conductivity (TRMC) method. It was found that electron traps (ETs) worked as nucleation sites for silver, resulting in formation of smaller silver NPs on smaller OAPs with larger content of ETs. The modification with silver resulted in enhanced photocatalytic activity under both UV and vis irradiation. It was found that larger crystallite size of silver NPs, and thus larger polydispersity of silver deposits resulted in broad and intense plasmon resonance peak causing enhanced visible activity. The correlation between photocatalytic activity and TRMC data, e.g., slower decay of TRMC signal for more active samples, allowed discussion on property-governed photocatalytic activities of silver-modified titania.

A Protein-Based Encapsulation System with Calcium-Controlled Cargo Loading and Detachment.

Lizatovic R, Assent M, Barendregt A, Dahlin J, Bille A, Satzinger K, Tupina D, Heck AJR, Wennmalm S, Andr I.

Angew Chem Int Ed Engl. Aug 27;57(35):11334-
doi: 10.1002/anie.Epub Jul 30.

Protein-based encapsulation systems have a wide spectrum of applications in targeted delivery of cargo molecules and for chemical transformations in confined spaces. By engineering affinity between cargo and container proteins it has been possible to enable the efficient and specific encapsulation of target molecules. Missing in current approaches is the ability to turn off the interaction after encapsulation to enable the cargo to freely diffuse in the lumen of the container. Separation between cargo and container is desirable in drug delivery applications and in the use of capsids as catalytic nanoparticles. We describe an encapsulation system based on the hepatitis B virus capsid in which an engineered high-affinity interaction between cargo and capsid proteins can be modulated by Ca2+ . Cargo proteins are loaded into capsids in the presence of Ca2+ , while ligand removal triggers unbinding

inside the container. We observe that confinement leads to hindered rotation of cargo inside the capsid. Application of the designed container for catalysis was also demonstrated by encapsulation of an enzyme with -glucosidase activity.

Particle Diffusion in Polymeric Hydrogels with Mixed Attractive and Repulsive Interactions.

Hansing J, Duke JR 3rd, Fryman EB, DeRouchey JE, Netz RR.

Nano Lett. Aug 8;18(8):5248-
doi: 10.1021/acs.nanolett.8bEpub Jul 5.

All biogels are heterogeneous, consisting of functional groups with different biophysical properties arrayed on spatially disordered polymer networks. Nanoparticles diffusing in such biogels experience a mixture of attractive and repulsive interactions. Here, we present experimental and theoretical studies of charged particle diffusion in gels with a random distribution of attractive and repulsive electrostatic interaction sites inside the gel. In addition to interaction disorder, we theoretically investigate the effect of spatial disorder of the polymer network. Our coarse-grained simulations reveal that attractive interactions primarily determine the diffusive behavior of the particles in systems with mixed attractive and repulsive interactions. As a consequence, charged particles of either sign are immobilized in mixed cationic/anionic gels because they are trapped near oppositely charged interaction sites, whereas neutral particles diffuse rapidly. Even small fractions of oppositely charged interaction sites lead to strong trapping of a charged particle. Translational diffusion coefficients of charged probe molecules in gels consisting of mixed cationic and anionic dextran polymers are determined by fluorescence correlation spectroscopy and quantitatively confirm our theoretical predictions.

Promotional effect of antimony on the selective catalytic reduction NO with NH3 over V-Sb/Ti catalyst.

Kwon DW, Kim DH, Hong SC.

Environ Technol. Jul 4:1-
doi: 10.1080/09593330.2018.[Epub ahead of print]

The effect of antimony on the selective catalytic reduction (SCR) performance and SO2 durability of V-Sb/Ti was investigated. The physicochem-

ical characteristics of catalyst were characterized by various techniques, including Brunauer-Emmett-Teller (BET) surface area analysis, X-ray diffraction (XRD), NH3/SO2-temperature programmed desorption (TPD), diffuse reflectance infrared Fourier transform spectroscopy (DRIFTs), X-ray photoelectron spectroscopy (XPS), and H2-temperature programmed reduction (H2-TPR). The V-Sb/Ti catalyst showed excellent activity in the range 200-300C (compared with V/Ti), with an optimum achieved for 2 wt.% antimony. The total amount of acidic sites and NH3 adsorption characteristics did not affect the catalytic efficiency. The Sb5+ fraction was highest for V-2.0Sb/Ti and exhibited a positive correlation with the V4+ fraction. This phenomenon is related to the effect of synergistic between vanadium and antimony, promoting the conversion of V5+ to V4+ by Sb5+. Increasing the V4+ fraction in V-Sb/Ti increased the catalytic activity, which was mainly attributed to enhanced catalyst re-oxidation capability due to the addition of antimony. Furthermore, the addition of antimony delayed the adsorption of SO2 onto the V-Sb/Ti catalyst surface, improving the resistance to this gas. Therefore, the addition of antimony to V/Ti improved NOx conversion and SO2 durability.

Time domain diffuse correlation spectroscopy: modeling the effects of laser coherence length and instrument response function.

Cheng X, Tamborini D, Carp SA, Shatrovoy O, Zimmerman B, Tyulmankov D, Siegel A, Blackwell M, Franceschini MA, Boas DA.

Opt Lett. Jun 15;43(12):2756-

doi: 10.1364/OL.43.002756.

DOI: 10.1364/OL.43.002756 PMCID: PMC6197052 [Available on 2019-06-15] PMID: 29905681

Optical spectroscopic sensing of tumor hypoxia.

Dadgar S, Troncoso JR, Rajaram N.

J Biomed Opt. Jun;23(6):1-

doi: 10.1117/1.JBO.23.6.067001.

Tumor hypoxia is a critical indicator of poor clinical outcome in patients with cancers of the breast, cervix, and oral cavity. The ability to noninvasively and reliably monitor tumor oxygenation both prior to and

during therapy can aid in identifying poor treatment response earlier than is currently possible and lead to effective changes in treatment regimen. Diffuse reflectance spectroscopy (DRS) has been used in several studies to measure tissue scattering, total hemoglobin content (THb), and vascular oxygenation (sO2) in tissue. In this study, we validate in vivo DRS-based measurements of vascular oxygenation using immunohistochemical staining of tumor hypoxia using pimonidazole, an established hypoxia marker. Using tumor xenografts grown from two different head and neck cell lines-UM-SCC-22B and UM-SCC-47-we demonstrate statistically significant negative correlations between tumor hypoxic fraction (HF) and THb (r??=????-??0.45; p??=??0.04) and sO2 (r??=????-??0.50; p??=??0.02). In addition, we also found a statistically significant positive correlation between HF and mean reduced scattering coefficient (r??=??0.60; p??=??0.005). Our results demonstrate that DRS-based measures of sO2 can provide reliable indirect measurements of tumor hypoxia that can be of significant utility in preclinical and clinical studies.

Preoperative cerebral hemodynamics from birth to surgery in neonates with critical congenital heart disease.

Lynch JM, Ko T, Busch DR, Newland JJ, Winters ME, Mensah-Brown K, Boorady TW, Xiao R, Nicolson SC, Montenegro LM, Gaynor JW, Spray TL, Yodh AG, Naim MY, Licht DJ.

J Thorac Cardiovasc Surg. Oct;156(4):1657-

doi: 10.1016/j.jtcvs.2018.04.Epub May 3.

Comment in J Thorac Dis. 2018 Nov;10(Suppl 33):S3973-S3975.

In vivo time-gated diffuse correlation spectroscopy at quasi-null source-detector separation.

Pagliazzi M, Sekar SKV, Di Sieno L, Colombo L, Durduran T, Contini D, Torricelli A, Pifferi A, Mora AD.

Opt Lett. Jun 1;43(11):2450-

doi: 10.1364/OL.43.002450.

DOI: 10.1364/OL.43.002450 PMID: 29856401 [Indexed for MEDLINE]

Identification of tumor margins using diffuse reflectance spec-

troscopy with an extended-wavelength spectrum in a porcine model.

Dahlstrand U, Sheikh R, Nguyen CD, Hult J, Reistad N, Malmsj M.

Skin Res Technol. Nov;24(4):667-
doi: 10.1111/srt.Epub May 17.

OBJECTIVE: A novel extended-wavelength diffuse reflectance spectroscopy (EWDRS) technique is being developed for future clinical non-invasive tumor margin delineation. In this study, the ability of EWDRS to identify the margins of pigmented skin lesions in an in vivo pig model was evaluated. MATERIALS AND METHODS: Extended-wavelength diffuse reflectance spectroscopy recordings (350-1550nm) were made on 13 pigmented skin lesions and non-pigmented skin, as a reference. The hand-held probe was swept toward the pigmented area until the signal changed, thus indicating that the margin had been identified. A needle was inserted as a marker, and tissue samples were sent for histological analysis. The distance between the EWDRS-defined border and the histological border was measured by 3 independent examiners. RESULTS: The median difference between the EWDRS-defined border and the histological border was 70m toward the pigmented tissue (range: -579 to 538m). A Pearson correlation coefficient of .95 was obtained for the examiners. CONCLUSIONS: Extended-wavelength diffuse reflectance spectroscopy can be used in vivo to delineate the border of pigmented skin lesions in a porcine model with high accuracy, indicating that it may be a useful tool for non-invasive tumor margin delineation in the future.

Near-Infrared Diffuse Reflectance Measurement Method Based on Temperature-Insensitive Radial Distance.

Wu M, Liu R, Xu K.

Appl Spectrosc. Jul;72(7):1021-
doi: 10.1177/Epub Jun 18.

The variation of temperature is one of the main interference factors that affect the detection accuracy of near-infrared (NIR) diffuse reflectance. In this paper, a measurement method based on temperature-insensitive radial distance was proposed, and its feasibility and effectiveness were verified in Intralipid solutions. First, the possibility of temperature-insensitive radial distance was deduced based on the analytic solution of the steady-state diffusion equation in an infinite media, and the temperature-insensitive radial distances of 3% Intralipid solution in the wavelength range of 1000-1600?nm

was calculated. Second, a detection system was designed to measure the diffuse reflectance of 3% Intralipid solutions at multiple radial distances with different glucose concentration (0-100?mM) and different temperatures (35-40??). Both theoretical calculations and experimental results demonstrated the existence of temperature-insensitive radial distances in the range of 1000-1340?nm and 1440-1600?nm, and the distances were hardly affected by glucose variations. Finally, the glucose information extracted from the diffuse reflectance of Intralipid solutions at different radial distances under random temperature variations and constant temperature were compared. The result showed that the correlation between the glucose concentration and the diffuse reflectance obtained at the temperature-insensitive radial distance was significantly better than that of other radial distances, which was almost close to the situation of constant temperature. Therefore, the measurement method based on temperature-insensitive radial distance can effectively reduce the influence of temperature variations on NIR diffuse reflectance, and it is expected to improve the accuracy of diffuse reflectance in human body components detection and industrial field analysis.

The size effect to O2- -Ce4+ charge transfer emission and band gap structure of Sr2 CeO4.

Wang W, Pan Y, Zhang W, Liu X, Li L.

Luminescence. Aug;33(5):907-
doi: 10.1002/bio.Epub Apr 24.

Sr2 CeO4 phosphors with different crystalline sizes were synthesized by the sol-gel method or the solid-state reaction. Their crystalline size, luminescence intensity of O2- -Ce4+ charge transfer and energy gaps were obtained through the characterization by X-ray diffraction, photoluminescence spectra, as well as UV-visible diffuse reflectance measurements. An inverse relationship between photoluminescence (PL) spectra and crystalline size was observed when the heating temperature was from 1000C to 1300C. In addition, band energy calculated for all samples showed that a reaction temperature of 1200C for the solid-state method and 1100C for sol-gel method gave the largest values, which corresponded with the smallest crystalline size. Correlation between PL intensity and crystalline size showed an inverse relationship. Band structure, density of states and partial density of states of the crystal were calculated to analyze the mechanism using the cambrige sequential total energy package (CASTEP) module integrated with Materials Studio software.

Sympathoexcitation constrains vasodilation in the human skeletal muscle microvasculature during postocclusive reactive hyperemia.

Ichinose M, Nakabayashi M, Ono Y.

Am J Physiol Heart Circ Physiol. Aug 1;315(2):H242-H
doi: 10.1152/ajpheart.00010.Epub Apr 13.

We used diffuse correlation spectroscopy to investigate sympathetic vasoconstriction, local vasodilation, and integration of these two responses in the skeletal muscle microvasculature of 20 healthy volunteers. Diffuse correlation spectroscopy probes were placed on the flexor carpi radialis muscle or vastus lateralis muscle, and a blood flow index was derived continuously. We measured hemodynamic responses during sympathoexcitation induced by forehead cooling, after which the effects of the increased sympathetic tone on vasodilatory responses during postocclusive reactive hyperemia (PORH) were examined. PORH was induced by releasing arterial occlusion (3 min) in an arm or leg. To increase sympathetic tone during PORH, forehead cooling was begun 60 s before the occlusion release and ended 60 s after the release. During forehead cooling, mean arterial pressure rose significantly and was sustained at an elevated level. Significant vasoconstriction and decreases in blood flow index followed by gradual blunting of the vasoconstriction also occurred. The time course of these responses is in good agreement with previous observations in animals. The acute sympathoexcitation diminished the peak vasodilation during PORH only in the vastus lateralis muscle, but it hastened the decline in vasodilation after the peak in both the flexor carpi radialis muscle and vastus lateralis muscle. Consequently, the total vasodilatory response assessed as the area of the vascular conductance during the first minute of PORH was significantly diminished in both regions. We conclude that, in humans, the integrated effects of sympathetic vasoconstriction and local vasodilation have an important role in vascular regulation and control of perfusion in the skeletal muscle microcirculation. NEW & NOTEWORTHY We used diffuse correlation spectroscopy to demonstrate that acute sympathoexcitation constrains local vasodilation in the human skeletal muscle microvasculature during postocclusive reactive hyperemia. This finding indicates that integration of sympathetic vasoconstriction and local vasodilation is importantly involved in vascular regulation and the control of perfusion of the skeletal muscle microcirculation in humans.

Study on the prediction of soil heavy metal elements content based on visible near-infrared spectroscopy.

Liu J, Zhang Y, Wang H, Du Y.

Spectrochim Acta A Mol Biomol Spectrosc. Jun 15;199:43-
doi: 10.1016/j.saa.2018.03.Epub Mar 14.

The estimation of soils heavy metal content can reflect the impending surroundings of surface, which lays theoretical foundation for using covered vegetation to monitor environment and investigate resource. In this study, the contents of Cr, Mn, Ni, Cu, Zn, As, Cd, Hg and Pb in 44 soil samples were collected from Fufeng County, Yangling County and Wugong County, Shaanxi Province and were used as data sources. ASD FieldSpec HR (350-2500nm), and then the NOR, MSC and SNV of the reflectance were pretreated, the first deviation, second deviation and reflectance reciprocal logarithmic transformation were carried out. The optimal spectroscopy estimation model of nine heavy metal elements of Cr, Mn, Ni, Cu, Zn, As, Cd, Hg and Pb was established by regression method. Comparing the diffuse reflectance characteristics of different heavy metal contents and the effect of different pretreatment methods on the establishment of soil heavy metal spectral inversion model. The results of chemical analysis show that there was a serious Hg pollution in the study area, and the Cd content was close to the critical value. The results show that: (1) NOR, MSC and SNV were adopted for the acquisition of visible near-infrared. Combining differential transformation can improve the information of heavy metal elements in the soil, and use the correlation band energy Significantly improve the stability and predictability of the model. (2) The modeling accuracy of the optimal model of nine heavy metal spectra of Cr, Mn, Ni, Cu, Zn, As, Cd, Hg and Pb by PLSR method were 0.70, 0.79, 0.69, 0.81, 0.86, 0.58, 0.55, 0.99, 0.62. (3) The optimal estimation model of different elements using different treatment methods has better stability and higher precision, and can realize the rapid prediction of nine kinds of heavy metal elements in this region.

Optical monitoring of cerebral microcirculation in neurointensive care.

Rejmstad P, Haj-Hosseini N, neman O, Wrdell K.

Med Biol Eng Comput. Jul;56(7):1201-
doi: 10.1007/s11517-017-1725-8. Epub Dec 8.

Continuous optical monitoring of local cerebral microcirculation could benefit neurointensive care patients treated for subarachnoid hemorrhage

(SAH). The aim of the study was to evaluate laser Doppler flowmetry (LDF) and diffuse reflectance spectroscopy (DRS) for long-term monitoring of brain microcirculation and oxygen saturation (SO2) in the neurointensive care unit (NICU). A fiber optic probe was designed for intraparenchymal use and connected to LDF and DRS for assessment of the local blood flow (perfusion and tissue reflectance (TLI)) and SO2 in the brain. The optically monitored parameters were compared with conventional NICU monitors and Xe-CT. The LDF signals were low with median and 25 to 75% interquartiles of perfusion=70 (59 to 83) a.u. and TLI=2.0 (1.0 to 2.4) a.u. and showed correlation with the NICU monitors in terms of heart rate. Median and interquartiles of SO2 were 17.4 (15.7 to 19.8) %. The lack of correlation between local perfusion and cerebral perfusion pressure indicated intact cerebral autoregulation. The systems were capable of monitoring both local perfusion and SO2 with stable signals in the NICU over 4days. Further clinical studies are required to evaluate the optical systems' potential for assessing the onset of secondary brain injury.