

with spectral phasor analysis on UV-excited autofluorescence in *Saccharomyces cerevisiae* suspensions. The approach provides real time, dynamical information on cellular pyridine nucleotide conformation to chemically-induced metabolic change. We demonstrate the ability to sense a broad range of responses, including concentration-dependent-differences in the acute toxicity response to cyanide, discrimination between NADH- and NADPH-linked responses, and the ability to sense metabolic response under pressurized (several hundred atm) conditions. Emphasis is placed on interpreting the non-two-component behavior in the spectral response in terms of the affected biochemical pathways.

### 2817-Pos

#### Infrared Spectroscopy Offers Tremendous Potential in Cancer Diagnosis

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All over the world, scientists are actively engaged in the characterization, screening and diagnosis of different pathological conditions. Ideally, the aim is to monitor the system of interest, without disturbing it, in a sensitive, rapid and operated manner at minimum cost. Infrared spectroscopy is one of the few analytical techniques that fulfill all of these requirements. Recently, the power of infrared spectroscopy in diagnosis of bladder cancer from the bladder wash was reported by our group [Gok et al., 2016]. Here, we will show the potential of infrared spectroscopy coupled with chemometrics in the determination of disease specific diagnostic biomarkers and differentiation of malignant pleural mesothelioma (MPM), lung cancer (LC), metastatic lung cancers and benign pleural effusions from pleural fluids and serum. Spectral analysis indicated significant differences in lipid, protein, nucleic acid, glycogen content, lipid order and fluidity and protein structure especially for MPM group. Disease induced specific biomarkers have also been determined for different groups. Unsupervised (hierarchical cluster analysis, HCA and principal component analysis, PCA) and supervised (Soft Independent Modeling by Class Analogy, SIMCA) chemometric analyses methods were applied to the infrared spectra. Based on the spectral differences successful differentiations with 85-100% sensitivity and 84-100% specificity for pleural fluid, with 71-95% sensitivity and 80-94% specificity for serum were obtained when MPM, LC and control samples (benign transudative effusion for pleural fluid and healthy control for serum) were taken into consideration. The differentiation with 80-85% sensitivity and 84-88% specificity for pleural fluid was achieved with the inclusion of all the groups. This study demonstrated that ATR-FTIR spectroscopy coupled with chemometrics is a novel, rapid, non-invasive diagnostic method with higher sensitivity, specificity and accuracy in differentiation of different malignant and benign lung diseases. (This study was supported by TUBITAK- SBAG-113S294 project).

### 2818-Pos

#### Early Warning Detection of Carcinogens and Other Contaminants for Surface Water Treatment Plants using Simultaneous Absorbance-Transmittance and Fluorescence Excitation-Emission Spectroscopy

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Most surface water treatment plants remain prone to contaminations by petroleum-derived carcinogens because they lack detectors upstream or even at their intakes. Early spill warnings require that water-soluble fluorescent or chromophoric components, including Benzene, Toluene, Ethylbenzene and Xylenes (BTEX), be discriminated from the high fluorescent backgrounds of the natural Dissolved Organic Matter (DOM) components. Benzene is believed to be the most toxic BTEX component and has a low (around 1%) fluorescence quantum yield in water; benzene's EPA regulated maximum contamination limit in the distribution system is 5 µg/L. In contrast, typical surface water DOM concentrations range from 1 to 20 mg/L and most DOM components have higher fluorescent quantum yields than BTEX compounds. Here we present a sensitive method for rapid (3-5 min) reagent- and extraction-free detection of all BTEX compounds in typical raw surface water with respective Limits of Detection (LOD) and Quantification (LOQ) of 1 and 3 µg/L. The method uses a patented simultaneous Absorbance-Transmittance and fluorescence Excitation-Emission (A-TEEM) instrument. Importantly the method employs an exclusive automated, sequential and targeted variable selection Partial Least Squares (PLS) library analysis. The instrument can be equipped for automated surface water sampling and html based communication at the plant intake or upstream for early warning of carcinogens and other contamination events.

### 2819-Pos

#### SERS as an Effective Probe to Adsorption and Conformation of Biomolecules on the Metal Surfaces

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Adsorption/conformation of biomolecules on metal surfaces is a long-standing issue which requires development of new tools and methods to settle the existing controversies. In this regard, surface enhanced Raman spectroscopy (SERS) emerges as an alternative approach which may provide a solution for it is highly sensitive with even single molecular detection ability and it can provide structural information which also depends on the adsorption and conformation of the examined molecules on the metal surface. Therefore, our group combined SERS experiments with other methods such as density functional theory computation to analyze conformations and adsorptions of small biomolecules such as tyrosine [1], adenine [2] and cysteine [3], as well as the larger biomolecules such as some sequences of DNA molecules as they are attached to the metal surfaces and interact with other molecules (e.g. coralyne and PCB-77) [4-6] and ions (e.g. Hg<sup>2+</sup>) [7]. With this idea, we are also developing this approach in combination with more advanced tools to investigate more complex biomolecules.

References:

- [1] G. Yao et al. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 2015, 151: 111-123.
- [2] G. Yao, et al. J. Phys. Chem. C 2017, 121, 9869-9878.
- [3] G. Yao and Q. Huang. J. Phys. Chem. C 2018, 122, 15241-15251.
- [4] Y. Lu, Qing Huang. Analytical Methods 2013, 5:3927-3932.
- [5] Y. Lu, et al. Analyst 2014, 139, 3083-3087.
- [6] K. Sun, et al. ACS Appl. Mater. Interfaces 2016, 8:5723-5728.
- [7] Y. Lu, et al. Sensors and Actuators B: Chemical 2018, 258:365-372.

### 2820-Pos

#### Structural and Spectroscopic Study of the Tyrosine Kinase Inhibitor PD-153035

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Our study revolves around investigating the spectroscopic properties of the tyrosine kinase inhibitor, PD-153035, both experimentally and theoretically. The UV-Vis absorption spectrum of PD-153035 exhibited four absorption peaks at ca. 220, 250, 330, and 340 nm. The position and relative optical density of the two lowest energy bands at 330 and 340 nm were significantly altered depending on solvent used in UV-Vis measurements. We therefore prompted to computationally examine PD-153035 structures. The potential energy surface scan revealed four energetically stable conformers of PD-153035 calculated through rotation of the dihedral angle between the anilino and quinazolinyl moieties. Two structures have planar conformations while the other two have twisted conformations. The energy difference between the global minimum structure and the highest energy conformer was estimated at 2.12 kcal/mol. The HOMO-LUMO energy gap was calculated at  $(4.3140 \pm 0.0196)$  eV for the four conformers. The time-dependant Density Functional Theory (td-DFT) calculations employing B3LYP/6-311++G\*\* level of theory revealed that the 330 nm peak can be attributed to the planar conformers while the 340 nm peak can be due to the twisted conformers. The computed oscillator strength of the planar isomers in various solvents had values double that of the twisted isomers. Taken together, these results showed how the absorption spectrum is sensitive to PD-153035 conformation. Hence, our findings assume relevance in understanding the structure and environment of PD-153035 in the ATP binding pocket of its target proteins. Our future work is to identify the fluorescence spectra of PD-153035 in different solvents and when it bounds to its target proteins.

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### 2821-Pos

#### Fluorophore-Induced Plasmonic Current

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Fluorophore-induced plasmonic current is generated when a near-field excited fluorophore in proximity to a metal nanoparticle film induces plasmon resonance in the metal, subsequently generating electrical current, only if certain conditions are met. This highly novel technology allows for the detection of fluorescent molecules without the need for traditional detectors such as photomultiplier tubes, avalanche photodiodes, and linear arrays. In this paper, we describe our recent photophysical experiments which describe how plasmonic current can be generated. For example, we discuss the excitation polarization, fluorophore oscillator strength, nanoparticle spacing, and solution dielectric. In