Molecular Imaging and Biology (2025) 27 (Suppl 2):S761–S1256
https://doi.org/10.1007/s11307-024-01977-z

ABSTRACTS

2024 World Molecular Imaging Congress Program

Published online: 7 February 2025

Selected abstracts from the World Molecular Imaging Congress 2024 meeting of the World Molecular Imaging Society

WMIC 2024, Montreal, Canada
Sponsorship: Publication of this supplement was funded by the World Molecular Imaging Society. All content was reviewed and approved by the 2024 WMIC Program Committee, which held full responsibility for the abstract selections. Presenting authors have asterisks in the contributor lists.

GA16- Development and Evaluation of D-Fluoroalanine and D-Fluoroalanine-d3 as PET Imaging Agents for Bacterial Infection

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Category: Infection

Abstract Body: Novel positron emission tomography (PET) imaging agents are needed to detect and diagnose deep-seated bacterial infections.[1] D-amino acids, which are selectively taken up by bacteria, are attractive targets for radiotracer development.[2] This has resulted in the synthesis and evaluation of several ^{11}C-labeled D-amino acids including D-Met,[3] D-Ala,[4] and D-Gln.[5] Given that D-alanine is an essential component of bacterial peptidoglycan, and in order to expand the studies to ^{18}F tracers which have a longer half-life than ^{11}C, D-FAla and D-FAla-d_3 were synthesized and evaluated in a soft-tissue infection model, laying the groundwork for the wider application of ^{18}F-labeled D-amino acids for bacterial imaging.

D-FAla and D-FAla-d_3 were synthesized using cyclic D-sulfamidate precursors involving a 2-step radiofluorination followed by acidic deprotection. Uptake experiments were performed with both Gram-negative (*Escherichia coli*) and Gram-positive (*Staphylococcus aureus*) bacteria, and a *S. aureus* Xen29 rat soft-tissue infection model was utilized for *in vivo* PET imaging. *In vivo* bioluminescent imaging was used to monitor the bacterial infection starting from the 2nd day post inoculation. Once a robust infection had developed, 90-min dynamic PET imaging was used to analyze the biodistribution of D-FAla (n=4) and D-FAla-d_3 (n=4), while the *ex vivo* biodistribution was evaluated at the conclusion of the PET imaging. Heat killed bacteria were used to generate an inflammatory response in the contralateral triceps to compare and contrast with radiotracer accumulation in the infected triceps.

D-FAla and D-FAla-d_3 were prepared with radiochemical yields (decay corrected) of 19–21% and radiochemical purities of >98%. For D-FAla and D-FAla-d_3, the uptake in heat-killed *E. coli* was reduced to 2%−4% of the uptake in live *E. coli*, while the uptake in heat-killed *S. aureus* was decreased to 31–41% of that observed in live bacteria. The uptake of both tracers in bacteria was dose-dependently blocked by D-alanine. *In vivo* PET imaging was initiated when a strong bioluminescent signal was detected in the infected (right) triceps which *ex vivo* analysis of the tissue showed was due to ~10^7 colony-forming units (CFU)/ml of *S. aureus* Xen29. Based on the PET data, the uptake in the infected triceps at 15 min post injection of D-FAla and D-FAla-d_3 was 0.78 ± 0.07 %ID/cc and 0.64 ± 0.03 %ID/cc, respectively, which was ~2-fold higher than the uptake at the site of sterile inflammation.

The PET imaging data demonstrated that both D-FAla and D-FAla-d_3 can detect and localize bacterial infection. Subsequent studies will involve the evaluation of the radiotracers in models of prosthetic joint infection and endocarditis, and extending the studies to fungal infections. The future studies will support the clinical translation of D-FAla and D-FAla-d_3 for the management of infection.

Disclosures: The authors have no conflicts of interest to disclose.

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was then extracted as numpy arrays. Equation (1) is the generalized partial differential equation for describing the dynamics of fluid spins under the influence of B_0 and B_1 field. After making a reasonable assumption, equation (3) can be derived from equation (1). A solution to equation (3) is given as equation (4), which was then used to filter the extracted image data (achieved by using this solution as an image filter). With this, the image data has been assigned to appropriate MR diffusion physics parameters. Traditional ML algorithms implemented in Python programming were then used to train the extracted image fitted data so as to learn the three tissue clusters.

The performances of the ML models have been presented in table 1 showing how the diffusion images predicted with the models compare with the ground truth. Figures 1–3 show the predicted images using 12 models. The parameters of some of the models were tuned to check their influence on image prediction.

Obviously, figure 1 and 2 show that most of the models performed poorly. However, figure 3b, 3c and 3d had perfect performance on the training set but performance on the testing set was not good enough. Overall, random forest classifier with max_depth of 2000, was the best performing model.

This study has addressed an imaging challenge often encountered in low-resource settings and methods consistent with this inadequacy has been presented. The results were not very impressive because the resolutions of the MRI scan used was low but we were able to demonstrate how ML and AI could help improve MRI analyses. Using larger dataset could prove to be very important to optimizing these models. Future studies making use of hyperparameter tuning and/or U-Net could lead to improvements in the performance of the models.

Disclosures: The authors have no conflicts of interest to disclose.

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Poster Presentation

GA262- Physics-informed Machine Learning Approach for Denoising Low Resolution Diffusion Magnetic Resonance Images

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Category: Computational & Data Science

Abstract Body: Image denoising is to remove noise from a noisy image for the purpose of restoration to the true image. Meanwhile, since noise, edge and texture are high frequency components, it is difficult to distinguish them in during denoising and the denoised images could inevitably lose some details. However, recovering meaningful information from noisy images in the process of noise removal to obtain high quality images is an important research problem in recent time. Although, image denoising is a classic problem which has been subject to studies for a long time, it remains a challenging and open task. This is because from a mathematical perspective, image denoising is an inverse problem with a non-unique solution. In recent time, various deep learning methods have been adopted to address denoising problem. Therefore, there have been efforts to develop machine learning methods with Physics contraints. This study attempts developing a Physics-informed machine learning model in which a modified Bloch-Torrey formulation of diffusion signal is used as a constraint.

The MRI dataset was obtained from W-ResearchWorks Archive which is a digital library of Washington education platform (https://digital.lib.washington.edu/researchworks/handle/1773/33311?show=full). In this dataset, diffusion MRI at multiple b-values (200, 400, 1000, 2000, and 3000) was collected on a 3T Siemens Prisma MRI instrument in a single healthy individual. For this study, the scan at b = $200 s/mm^2$ was used and image processing was then carried out with FSL software (created by the Analysis Group, FMRIB, Oxford, UK). BET was used to extract brain tissues and then the slices of the resulting image volume was then extracted as 72 2D images. The central slice was then selected as the reference image. Using python programming, gaussian and impulse noises were then added to this image so that we check how our model performs in removing them. Equation (1) is the generalized partial differential equation for describing the dynamics of fluid spins under the influence of B0 and B1 fields. After making a reasonable assumption, equation (3) can be derived from equation (1). A solution to equation (3) is given as equation (4),

which was then used to filter the noisy images. The filter developed from equation (3) is called ADF (Analytical diffusion filter). Other common filters such as GF (Gaussian filter), BF (Bilateral filter), TVF (Total variation (TV) filter), WF (Wavelet filter), SIWF (Shift invariant wavelet filter), NLM (Non-local means filter), FNLM (Fast non-local means filter) and BM3D (Block-matching and 3D filter) were also implemented to compare with ADF. PSNR, SSIM, SNR and NRMSE were used as the performance metrics.
Table 1 shows the performance of ADF and other filters on the image polluted with gaussian noise while table 2 shows the performance of the filters on the image polluted with impulse noise. Figures 1 and 2 illusrates the predicted images after denoising performed on image polluted with gaussian and impulse noises respectively.
When denoising Gaussian noise, the "ADF" comes out as a superior method. In comparison, the PSNR values of the cleaned image outputs from approaches such as "GF," "TVF," "WF," "SIWF," "BM3D," "NLM," 'FNLM," and "BF" vary from 11 to 13, exhibiting various degrees of quality. Similarly, impulse noise provides the same PSNR value for the noisy image across all filters. However, for denoised image (impulse noise), "BM3D" and "TVF" perform the best with values of 25.87136 and 20.98943, respectively. The "ADF" approach ranks fourth in terms of denoising impulse noise performance.
Noises in MR images are primarily Rician noise, Gaussian Noise and Rayleigh noise. We observed that ADF had the best performance for gaussian noise. It will be interest to implement this model on images polluted with Rician and Rayleigh noises.
Disclosures: The authors have no conflicts of interest to disclose.

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Poster Presentation

GA266- Structural Properties of Squaraine Dyes and their Influence on Optoacoustic Signal

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Category: New Chemistry, Materials & Probes

Abstract Body: While optoacoustic imaging is frequently used to identify endogenous chromophores such as hemoglobin, it has the capability to identify multiple reporter dyes or nanoparticles that generate unique spectral shapes. This study assesses the influence of halogens within squaraine dyes to assess potential changes in optoacoustic signal. We synthesized squaraine dye to contain hydrogen, fluorine, chlorine, or bromine at the same position. Computational modeling suggests the origin of increased optoacoustic signal is due to increases in transition dipole moment and vibrational entropy, which manifested experimentally as increased absorbance in the NIR wavelength range and decreased fluorescence quantum yield, respectively. Optoacoustic signal was identified from each dye in tissue mimicking phantoms which demonstrated that Br containing dyes resulted in the greatest optoacoustis signals. Specifically, *in vivo* MSOT signals related to halogenation were as follows: bromine-2.12 a.u., chlorine-0.81 a.u., fluorine- 0.58 a.u., no halogen-0.44 a.u. ($p<0.001$). This study provides an insight into the structure-function relationships that lead to guiding principles for designing optoacoustic-specific contrast agents. Further developments of squaraines and other types of optoacoustic agents will further expand the potential of generating novel exogenous reporters that can facilitate multiplexed optoacoustic imaging.
Disclosures: The authors have no conflicts of interest to disclose.

Poster Presentation

GA272- Rapid Detection of Viral Antibodies in Camel Sera – the COMPASS POC Device

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Category: New Chemistry, Materials & Probes

Abstract Body: Camels are known reservoirs and carriers of various coronavirus strains . The growing trade of camels