

3RD EUROCC VILNIUS WORKSHOP

ON USING HPC

Abstract book

https://doi.org/10.5281/zenodo.14748386

January 20-21, 2025

Vilnius, Lithuania



Workshop organizers

Local organizing committee

Mindaugas Mačernis Laura Baliulytė Jonas Franukevičius

Scientific committee

Mindaugas Mačernis Jevgenij Chmeliov Andrius Gelžinis



Funding



Co-funded by the European Union



Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.



Bendrai finansuoja Europos Sąjunga

Projektas bendrai finansuojamas 2021–2027 metų ES fondų investicijų programos (sutartis Nr. 10-051-P-0001).

EuroCC2-EuroCC4SEE Project Organiser



Project Implementers









Matematikos ir informatikos fakultetas







Towards an automated diagnosis of well-differentiated thyroid carcinomas based on wide field second harmonic generation microscopy imaging

<u>Yaraslau Padrez</u>¹, Lena Golubewa^{1,2}, Adrian Enache³, Lucian G. Eftimie^{3,4}, Radu Hristu⁵, Danielis Rutkauskas¹

¹Department for Molecular Compound Physics, Centre for Physical Sciences and Technology, Vilnius, Lithuania

²Institute for Chemical Physics, Vilnius University, Vilnius, Lithuania ³Pathology Department, Central University Emergency Military Hospital, Bucharest, Romania

⁴Department of Special Motricity and Medical Recovery, the National University of Physical Education and Sports, Bucharest, Romania
⁵Centre for Microscopy-Microanalysis and Information Processing, National University of Science and Technology Politehnica Bucharest, Bucharest, Romania

E-mail: yaraslau.padrez@ftmc.lt

Papillary thyroid carcinoma (PTC) and follicular thyroid carcinoma (FTC) are both welldifferentiated tumors and together account for up to 88% of all cases of thyroid cancer [1]. The collagen capsule surrounding PTC or FTC nodules is an important histopathologic feature that provides valuable information about the malignancy, invasiveness of the tumor, and prognosis for cure. Wide field second harmonic generation microscopy enables label-free, rapid visualization of collagen networks in cancer tissue sections on centimeter-sized areas with submicrometer resolution. Applying machine learning algorithms to the large datasets of SHG images can help identify specific features associated with either PTC or FTC, enabling accurate diagnosis of well-differentiated thyroid carcinomas. In the present study, we applied three monolithic (logistic regression, RG; C-support vector classifier, C-SVC; and a multilayer perceptron MLP) and three ensemble (random forest, RF; eXtreme gradient boosting, XGBoost and light gradient-boosting machine, LightGBM) classifiers to (i) diagnose PTC and FTC based on the texture features of SHG images of collagen networks in the whole scans of thyroid tissue sections, (ii) analyze how the heterogeneity of collagen structure within the capsules and the similarities between PTC and FTC affect the prediction performance of the models, and (iii) to evaluate the feasibility of SHG-based discrimination between PTC and FTC. Three different approaches were applied to pre-process the data, aiming at accurate selection of collagenous structures for training and testing the models. The best performance was achieved by the C-SVC, MLP and XGBoost models with accuracies of 84.73%, 81.76% and 81.42%, respectively, when forming the training and validation sets considering the heterogeneity of the capsules as a whole, with the C-SVC model showing the best classification performance on the completely unknown dataset. Similarities in the textural features of PTC and FTC nodules and the heterogeneity of collagen structures throughout the capsule complicate the diagnosis of PTC and FTC. The developed predictive models can serve as a reliable complement to histopathologic examinations to enable accurate diagnosis.

REFERENCES

[1] L. Boucai, M. Zafereo, M.E. Cabanillas, Thyroid Cancer: A Review, JAMA 331, 425-435 (2024).