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USING PAPER SPRAY ION MOBILITY SPECTROMETRY-MASS SPECTROMETRY (PSI-MS) TO AID THE DIAGNOSIS OF THYROID CANCER

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Introduction

Thyroid ultrasound and ultrasound-guided fine-needle aspiration cytology (FNAC) is a standard of care technique for preoperative diagnosis of imaging suspicious thyroid lesions. However, discrimination between malignant and benign thyroid nodules from FNAC can be challenging. Those indeterminate cytology results mainly include atypia of undetermined significance (AUS) and follicular neoplasm (FN). The final malignancy rate is about 6-18% for AUS and 10-40% for FN. In those nodules with FNAC indeterminate results, a correct diagnosis can only be achieved by final surgical pathology. So, a quick, low cost and correct preoperative diagnostic method are compelling needed.

Mass spectrometry (MS) provides an ability to obtain the chemical fingerprint of a biological tissue based on the mass-to-charge (m/z) ratio of its constituent molecules. Paper spray ionization Mass spectrometry (PSI-MS), as only a small amount of sample and minimal pretreatment is required, diagnoses using Field asymmetry waveform ion mobility spectrometry (FAIMS) could greatly reduce the invasiveness and waiting time for patients.

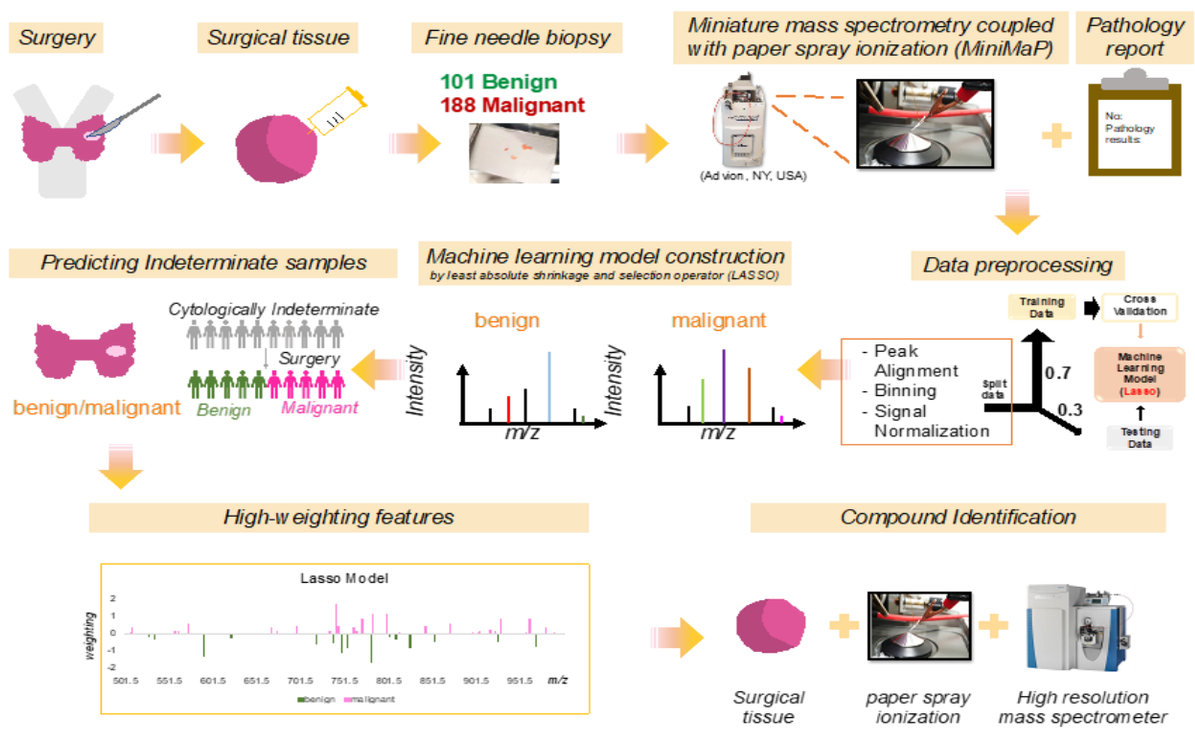
In this study, we aim to test the feasibility of PSI-MSl in the diagnosis of thyroid tumors.

Materials and Methods

Totally 289 thyroid tumors operated were included. Fresh tissue samples and ex vivo FNAC samples were collected from the same tumor in the operation. 101 benign and 188 malignant tumors included. The age, gender, preoperative thyroid function, size of tumors, results of FNAC and postoperative pathologic reports were collected from each participant. There were 66 benign tumors and 91 malignant tumors in Bethesda category III-V of the preoperative FNAC results. All experiments were carried out using Orbitrap Elite mass spectrometer (Thermo Scientific, USA). Data were acquired then were converted to mzXML format using open-source software ProteoWizard (version 3.0.100521) and were imported into MATLAB software for further processing. After MS data were pretreated, they were transferred into the RapidMiner (version 9.2.001). In this software, the machine learning model was trained using training data sets and external validation on the testing set was applied.

Results

The sensitivity of training set and testing set in Bethesda III-V were 92.86% and 90.48% respectively. The specificity of training set and testing set in Bethesda III-V were 78.72% and 84.21 respectively. The accuracy of training set and testing set in Bethesda III-V were 86.67% and 86.36 respectively. Using paper spray ion mobility spectrometry-mass spectrometry (PSI-MS) can aid the diagnosis of thyroid cancer, especially for those nodules with indeterminate FNAC result.



The machine learning model for BSRTC II-VI and performance of BSRTC III-V in training and testing set

Sample Type	Dataset	Pathologist Diagnosis		Sensitivity	Specificity	Accuracy
BSRTC II,III,IV,V,VI	Training Set	Malignant	132	125/132	57/71	182/203
		Benign	71	94.70%	80.28%	89.66%
	Testing Set	Malignant	56	53/56	26/30	79/86
		Benign	30	94.64%	86.67%	91.86%
	BSRTC III,IV,V in training set	Malignant	70	65/70	37/47	102/117
		Benign	47	92.86%	78.72%	87.18%
	BSRTC III,IV,V in testing set	Malignant	21	19/21	16/19	35/40
		Benign	19	90.48%	84.21%	87.50%

Performance of each BSRTC III, IV and V with PPV in testing set

Sample Type	Dataset	Pathologist Diagnosis		Sensitivity	Specificity	PPV
BSRTC II,III,IV,V,VI	BSRTC III,IV,V in testing set	Malignant	21	19/21	16/19	86.36%
		Benign	19	90.48%	84.21%	
	BSRTC III in testing set	Malignant	4	4/4	9/9	100.00%
		Benign	9	100.00%	100.00%	
	BSRTC IV in testing set	Malignant	2	1/2	3/6	25.00%
		Benign	6	50.00%	50.00%	
	BSRTC V in testing set	Malignant	15	14/15	4/4	100.00%
		Benign	4	93.33%	100.00%	

Conclusion

Using paper spray ion mobility spectrometry-mass spectrometry (PSI-MS) can aid the diagnosis of thyroid cancer, even for those nodules with indeterminate FNAC result.

Reference

Huang, Y.C., et al., Predicting Breast Cancer by Paper Spray Ion Mobility Spectrometry Mass Spectrometry and Machine Learning. Anal Chem, 2020. 92(2): p. 1653-1657.