Supplementary Table 1

The differences between the performances obtained from the two approaches (data split by sample and by spectra respectively) are shown in the following table.

Type of specimen (no. of sample)	Cross-validation (data splitting method)	Algorithm	Accuracy (%)	Sensitivity (%)	Specificity (%)	AUC
FFPE (60)	**By sample**	PCA + SVM	82.8	91.9	61.6	0.880
		LSTM	87.4	91.9	77.0	0.930
Frozen (40)		PCA + KNN	87.9	90.8	83.0	0.930
		LSTM	94.4	95.5	92.7	0.980
FFPE (60)	**By spectra**	PCA + SVM	90.7	97.2	75.6	0.950
		LSTM	93.5	96.2	87.2	0.970
Frozen (40)		PCA + KNN	96.5	98.0	94.0	0.960
		LSTM	98.1	98.6	97.3	0.999

Supplementary Table 2

Tissue types	Raman shifts	Assignments
Bone	857	Amino acid side chain vibrations of proline and hydroxyproline, and a (C-C) vibration of the collagen backbone
	961	Phosphate symmetric stretching vibration of calcium hydroxyapatite
	1072	Carbonate symmetric stretching vibration of calcium carbonate apatite
	1248	Amide III (collagen assignment)
	1452	CH_2CH_3 deformation (collagen assignment)
	1663	Proteins, including collagen I
Skeletal muscle	622	(C-C) twisting mode of phenylalanine (proteins)
	755	Symmetric breathing of tryptophan
	856	Amino acid side chain vibrations of proline and hydroxyproline, and a (C-C) vibration of the collagen backbone
	939	Proline, hydroxyproline, ν(C-C) skeletal of collagen backbone
	1004	Phenylalanine (of collagen)
	1103	Phenylalanine (proteins)
	1245	Amide III
	1342	CH deformation (proteins and carbohydrates)
	1451	CH_2CH_3 deformation (collagen assignment)
	1548	Tryptophan
	1666	Collagen
Adipose tissue	725	Adenine (ring breathing mode of DNA/RNA bases)
	870	Single bond stretching vibrations for the amino acid proline, valine and polysaccharides
	972	(C-C) backbone (collagen assignment)
	1083	C-N stretching mode of proteins and lipid mode
	1303	$\delta(CH_2)$ twisting, wagging, phospholipids (lipid assignment)
	1441	CH_2 scissoring & CH_3 bending in lipids
	1657	Fatty acids
Blood cells	622	(C-C) twisting mode of phenylalanine (proteins)
	677	ν_7 , δ (symmetric pyrrole deformation mode)
	755	ν_{15} , ν (pyrrole breathing)
	827	γ_{10} , γ (C-H methine deformation)
	940	C-C stretch backbone
	1003	Phenylalanine, C-C skeletal
	1128	ν_5, ν (C_β–methyl)
	1224	ν_{13} or ν_{42} , δ (C-H methine deformation)
	1342	CH deformation (proteins and carbohydrates)
	1449	δ (CH_2/CH_3)
	1564	ν_{19} , ν ($C_\beta C_\beta$)
	1621	ν (C=C)vinyl

Abbreviations: ν & δ: In-plane modes, Υ: Out -of- plane modes.