Supplementary Table 1. SERS bands and vibrational mode assignments.

Wavenumber（cm^{-1}）	Vibrational modes	Molecular origin
497	ν(S-S)	collagen and aminoacid cysteine
533	ν(Si-O-Si)	Cholesterol ester
593	ν(C-I)	phosphatidylserine
638	ν(C-S) gauche	aminoacid methionine
726	C-S/ CH_2 rocking	protein, adenine
744	ν(C-Cl)	1,2-dichloroethane
766	ν(C-S)	Pyrimidine ring breathing mode
813	ν(C-O-C)	One of the two most distinct peaks for RNA
887	ν(C-O-C)	disaccharide (cellobiose)
959	$\nu_1PO_4^{3-}$	phosphate of HA
1005	ν(C=S)	Phenylalanine (proteins)
1071	PO_2^-	Glucose
1095	ν(C-N)	Lipid, Phosphodioxy group
1133	ν(C-N)	Proteins
1204	CH_2	Tyrosine, phenylalanine
1270	C-N/ C=C	Typical phospholipids
1330	CH_3CH_2	Nucleic acids and phosphates
1366	vs (CH_3)	phosphplipids

1443	CH_2	lipids and proteins
1500	C=C	benzenoid ring
1580	C-C stretching	cellular pigment
1653	C=O	cytidine

Supplementary Table 2. Area under receiver operating characteristic curves (AUROCs) of AI model for the non-invasive identification of NASH according to different histologic definitions.

The definition of NASH	**AUROC**
NASH with NAS ≥3	0.784
Active NASH with NAS ≥4	0.785
Definite NASH with NAS ≥5	0.828

Supplementary Table 3. Area under receiver operating characteristic curves (AUROCs) of AI model for the non-invasive diagnosis of the stage of liver fibrosis.

The degree of liver fibrosis	**AUROC**
Significant Fibrosis (F ≥2)	0.72
Advanced Fibrosis (F ≥3)	0.96
Cirrhosis (F =4)	NA

Supplementary Table 4. Area under receiver operating characteristic curves (AUROCs) of different machine learning algorithms for the non-invasive identification of NASH.

Machine learning algorithms	AUROC
LightGBM	0.74
XGBoost	0.73
Random forest	0.72
Logistic regression	0.75
Gradient boosting	0.74
Convolutional Neural Network (CNN)	0.75
FCNN	0.83