Supplementary

Table S1 Infrared spectral characteristics and classification of urinary stone components

Stone type	Characteristic peaks (cm^{-1})	Diagnostic criteria	Reference spectrum (CLSI Guidelines)
Infected stones			
Magnesium ammonium phosphate	1,040, 600, 560	Triple phosphate peaks at 1,040 (P-O stretch), 600 (NH_4^+ bend), and 560 (Mg-O stretch)	CLSI C50-A
Carbonate apatite	1,450, 1,030, 600	Broad carbonate peak at 1,450 (CO_3^{2-} stretch), phosphate peak at 1,030 (PO_4^{3-} stretch)	CLSI C50-A
Ammonium urate	1,650, 1,320, 780	Urate peak at 1,650 (C=O stretch), NH_4^+ bend at 1,320, and uric acid ring vibration at 780	CLSI C50-A
Non-infected Stones			
Calcium oxalate monohydrate	1,620, 1,320, 890	Sharp peaks at 1,620 (C=O stretch), 1,320 (O-C-O bend), and 890 (Ca-O lattice)	CLSI C50-A
Calcium oxalate dihydrate	1,640, 1,310, 910	Peaks at 1,640 (C=O stretch), 1,310 (O-C-O bend), and 910 (hydration band)	CLSI C50-A
Uric acid	1,680, 1,250, 800	Uric acid peaks at 1,680 (C=O stretch), 1,250 (N-H bend), and 800 (ring vibration)	CLSI C50-A
Cystine	1,600, 1,200, 500	Disulfide bond peaks at 1,600 (S-S stretch), 1,200 (C-N stretch), and 500 (S-S bend)	CLSI C50-A

CLSI, Clinical and Laboratory Standards Institute. Infrared Spectrophotometric Analysis of Urinary Calculi; Approved Guideline. CLSI document C50-A. 2015.

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