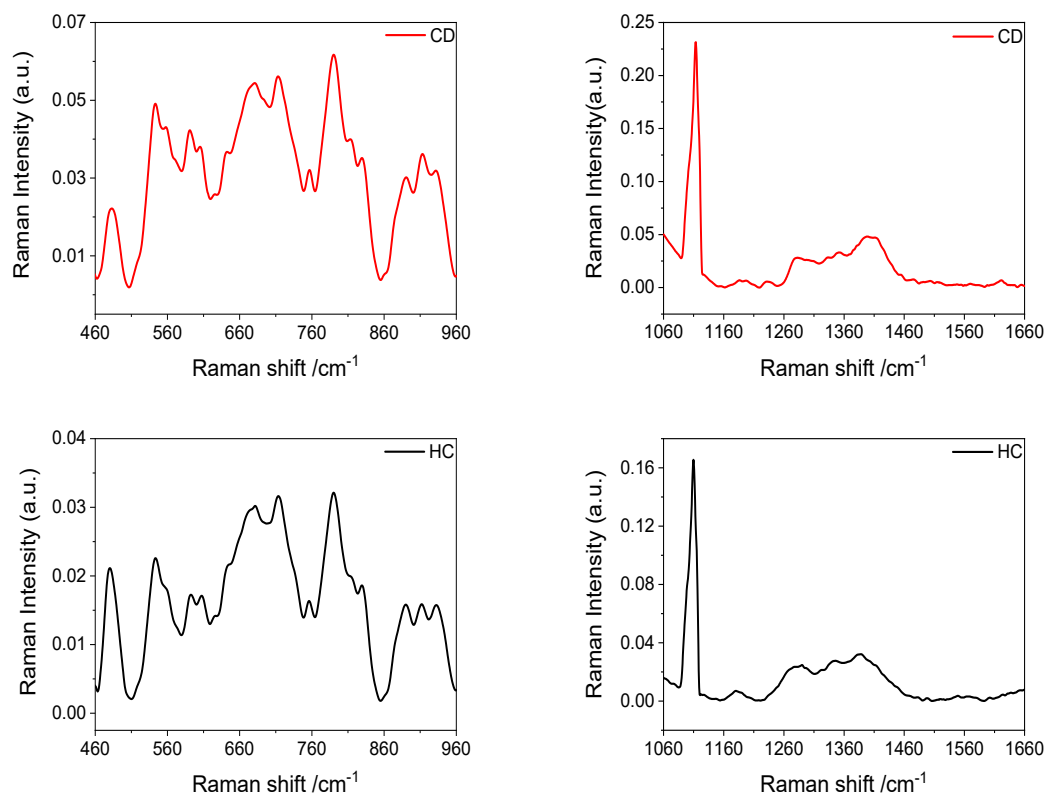# Supplemental Material

Figure S1: Two examples (1 CD + 1 HC) of the average spectra acquired from each sample

Table S1: Tests for normality within disease status (CD/HC). Wilcoxon test between means of Raman intensities at 11 main peaks of CD/HC

Peak (cm^{-1})	Kolmogorov-Smirnov test		Shapiro-Wilk test		Wilcoxon test
	CD	HC	CD	HC	
543	<0.0001	0.012	<0.0001	0.034	<0.0001
559	<0.0001	0.029	<0.0001	0.027	<0.0001
591	0.002	0.192	0.002	0.057	<0.0001
606	0.005	0.056	0.132	0.023	<0.0001
813	0.057	0.2	0.005	0.094	<0.0001
1110	<0.0001	0.2	<0.0001	0.004	<0.0001
1298	0.001	0.166	<0.0001	0.454	<0.0001
1352	0.029	0.093	0.046	0.096	<0.0001
1472	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
1622	<0.0001	0.2	<0.0001	0.026	<0.0001
1643	<0.0001	0.2	<0.0001	0.009	0.014

Table S2: Assignment of the main Raman peaks observed in human urine

Peak Position (cm^{-1})	Assignment
543	Cholesterol
559	Nucleic acid
591	Serine
606	Cholesterol
757	Tryptophan
813	L-serine and glutathione
1110	C-C vibration mode of the gauche-bonded chain
1280	Protein amide III
1298	CH$_2$ bending of lipids and protein
1323	Lipids
1352	Nucleic acid
1472	CH$_2$ bending of lipids and protein
1622	C=C stretching mode of tyrosine and tryptophan
1643	C=C stretching mode of lipids and the protein amide I band

Table S3: The combined effects of age, sex (female/male) and disease status (CD/HC) on the intensities at 11 main Raman peaks analysed by the generalized linear model

Peak (cm^{-1})	Parameter	p-value
543	[status CD] - [status HC]	0.007
	[sex female] - [sex male]	0.298
	age	0.936
559	[status CD] - [status HC]	0.016
	[sex female] - [sex male]	0.189
	age	0.965
591	[status CD] - [status HC]	0.017
	[sex female] - [sex male]	0.346
	age	0.968
606	[status CD] - [status HC]	0.040
	[sex female] - [sex male]	0.603
	age	0.934
813	[status CD] - [status HC]	0.022
	[sex female] - [sex male]	0.232
	age	0.964
1110	[status CD] - [status HC]	0.011
	[sex female] - [sex male]	0.800
	age	0.521
1298	[status CD] - [status HC]	<0.0001
	[sex female] - [sex male]	0.951
	age	0.531
1352	[status CD] - [status HC]	0.006
	[sex female] - [sex male]	0.643
	age	0.821
1472	[status CD] - [status HC]	0.015
	[sex female] - [sex male]	0.553
	age	0.503
1622	[status CD] - [status HC]	<0.0001
	[sex female] - [sex male]	0.906
	age	0.579
1643	[status CD] - [status HC]	0.015
	[sex female] - [sex male]	0.822
	age	0.383

Table S4: Eigenvalue, percentage of variance and the cumulative percentage of variance of the first 20 principal components identified by the PCA analysis for CD/HC

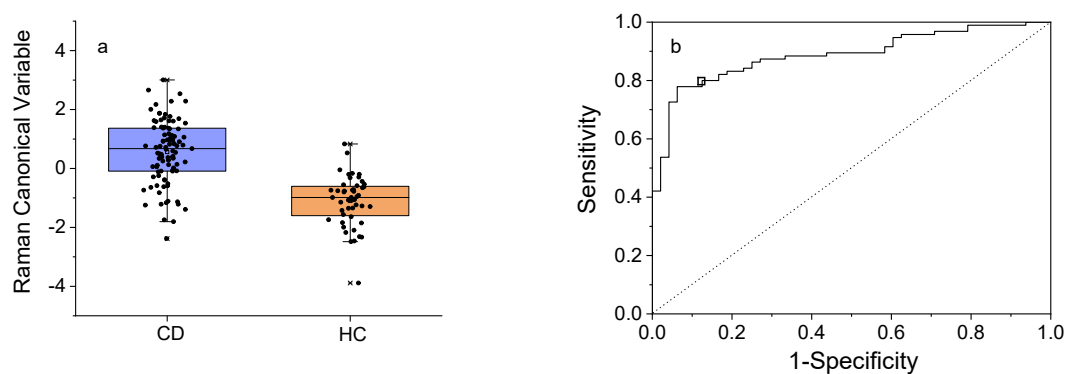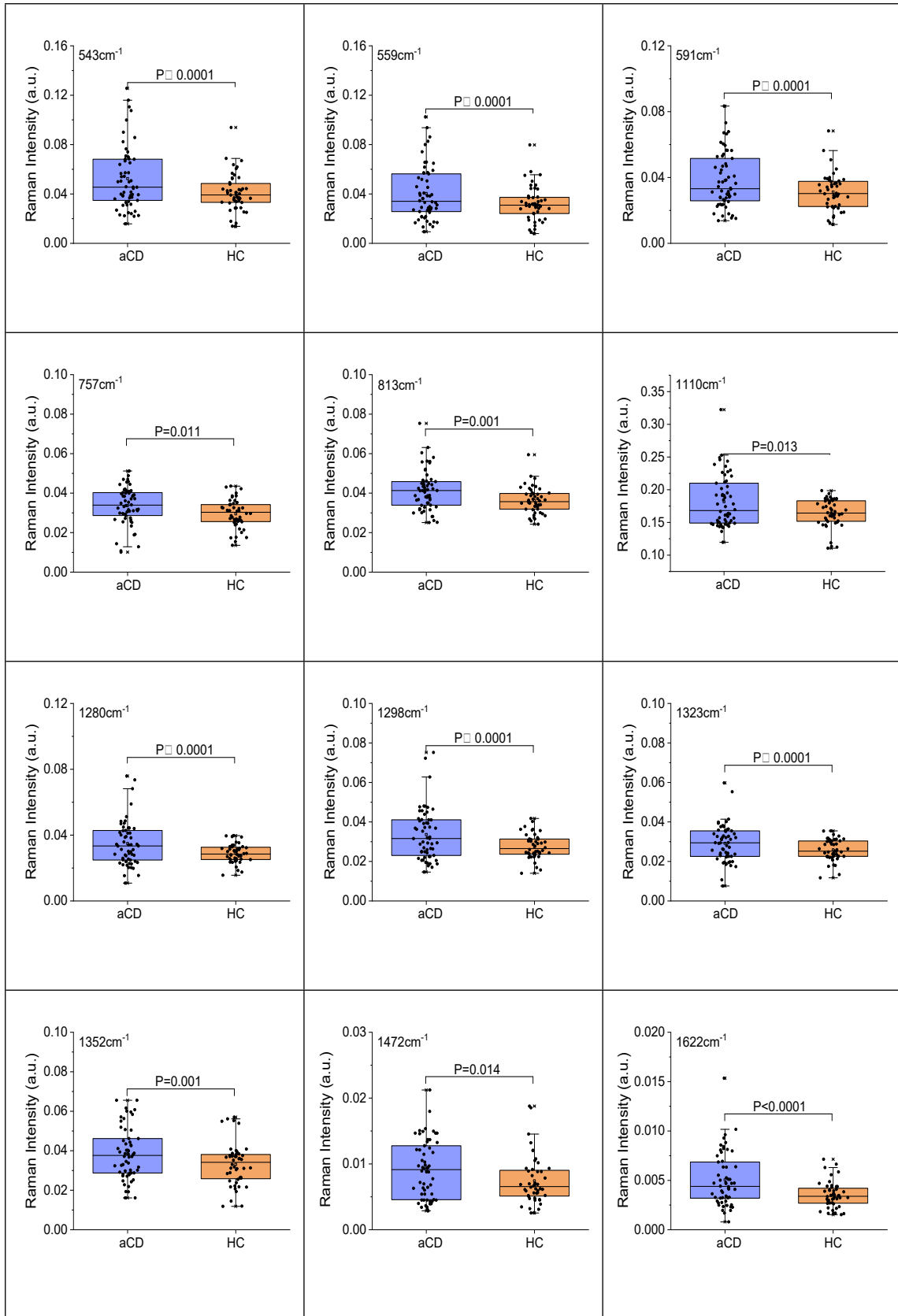| PC number	Eigenvalue	Percentage of Variance (%)	Cumulative (%)
1	0.10455	34.89442	34.89442
2	0.06122	20.4313	55.32573
3	0.03362	11.22009	66.54582
4	0.02577	8.60148	75.14729
5	0.01678	5.59969	80.74698
6	0.01498	5.00067	85.74765
7	0.01246	4.15861	89.90626
8	0.00823	2.74821	92.65447
9	0.0046	1.53513	94.18959
10	0.00325	1.08528	95.27487
11	0.00286	0.9546	96.22947
12	0.00157	0.52322	96.75269
13	0.0011	0.36657	97.11926
14	0.000933732	0.31164	97.4309
15	0.000768392	0.25646	97.68736
16	0.000698389	0.23309	97.92046
17	0.000570682	0.19047	98.11093
18	0.000525439	0.17537	98.2863
19	0.000443079	0.14788	98.43418
20	0.000388619	0.12971	98.56389

Figure S2: (A) Box plot showing the Raman canonical variable obtained for CD/HC；(B) ROC curve

Table S5: Tests for normality within disease status (aCD/HC). Wilcoxon test between means of Raman intensities at 13 main peaks of aCD/HC

Peak (cm^{-1})	Kolmogorov-Smirnov test		Shapiro-Wilk test		Wilcoxon test
	aCD	HC	aCD	HC	
543	0.012	0.009	0.034	<0.0001	<0.0001
559	0.079	0.003	0.025	0.001	<0.0001
591	0.192	0.015	0.057	0.011	<0.0001
757	0.200	0.200	0.086	0.731	0.011
813	0.200	0.091	0.094	0.033	0.001
1110	0.010	0.200	<0.0001	0.004	0.013
1280	0.200	0.200	0.003	0.578	<0.0001
1298	0.166	0.200	0.454	0.001	<0.0001
1323	0.200	0.200	0.038	0.163	<0.0001
1352	0.033	0.200	0.036	0.063	0.001
1472	<0.0001	0.089	<0.0001	0.007	0.014
1622	0.200	0.004	0.031	<0.0001	<0.0001
1643	0.200	<0.0001	0.009	<0.0001	0.027

Table S6: The combined effects of age, sex (female/male) and disease status (aCD/HC) on the intensities at 13 main Raman peaks analysed by the generalized linear model

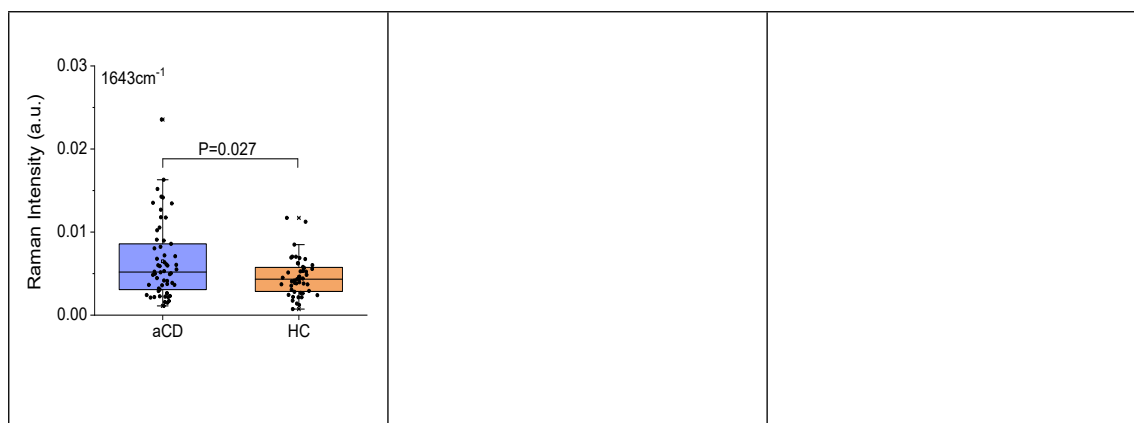| Peak (cm^{-1})	Parameter	p-value
543	[status aCD] - [status HC]	0.008
	[sex female] - [sex male]	0.152
	age	0.599
559	[status aCD] - [status HC]	0.024
	[sex female] - [sex male]	0.123
	age	0.699
591	[status aCD] - [status HC]	0.015
	[sex female] - [sex male]	0.259
	age	0.654
757	[status aCD] - [status HC]	0.015
	[sex female] - [sex male]	0.669
	age	0.615
813	[status aCD] - [status HC]	0.002
	[sex female] - [sex male]	0.349
	age	0.573
1110	[status aCD] - [status HC]	0.008
	[sex female] - [sex male]	0.817
	age	0.232
1280	[status aCD] - [status HC]	0.004
	[sex female] - [sex male]	0.443
	age	0.472
1298	[status aCD] - [status HC]	0.004
	[sex female] - [sex male]	0.383
	age	0.372
1323	[status aCD] - [status HC]	0.032
	[sex female] - [sex male]	0.324
	age	0.75
1352	[status aCD] - [status HC]	0.024
	[sex female] - [sex male]	0.453
	age	0.669
1472	[status aCD] - [status HC]	0.037
	[sex female] - [sex male]	0.985
	age	0.135
1622	[status aCD] - [status HC]	0.001
	[sex female] - [sex male]	0.694
	age	0.299
1643	[status aCD] - [status HC]	0.010
	[sex female] - [sex male]	0.620
	age	0.469

Figure S3: Box plots of the Raman intensities at 13 main Raman peaks in aCD/HC

Table S7: Eigenvalue, percentage of variance and the cumulative percentage of variance of the first 20 principal components identified by the PCA analysis for aCD/HC

PC number	Eigenvalue	Percentage of Variance (%)	Cumulative (%)
1	0.10119	37.7101	37.7101
2	0.04595	17.12467	54.83477
3	0.03589	13.37359	68.20836
4	0.02502	9.32306	77.53142
5	0.01575	5.86843	83.39985
6	0.01437	5.35506	88.7549
7	0.00846	3.15153	91.90643
8	0.00653	2.43394	94.34037
9	0.00412	1.53503	95.8754
10	0.00193	0.71886	96.59425
11	1.47E-03	0.54941	97.14366
12	1.01E-03	0.37547	97.51913
13	8.29E-04	0.30887	97.82801
14	6.64E-04	0.24733	98.07533
15	6.08E-04	0.22673	98.30206
16	4.85E-04	0.18071	98.48277
17	4.39E-04	0.16357	98.64635
18	3.49E-04	0.13019	98.77654
19	2.60E-04	0.09683	98.87336
20	2.35E-04	0.08771	98.96108

Table S8: Tests for normality within disease status (iCD/HC). Wilcoxon test between means of Raman intensities at four main peaks of iCD/HC

Peak (cm^{-1})	Kolmogorov-Smirnov test		Shapiro-Wilk test		Wilcoxon test
	iCD	HC	iCD	HC	
1110	0.2	0.2	0.476	0.004	0.018
1298	0.003	0.166	<0.0001	0.454	<0.0001
1351	0.068	0.15	0.071	0.118	<0.0001
1623	0.136	0.2	0.03	0.031	0.01

Table S9: The combined effects of age, sex (female/male) and disease status (iCD/HC) on the intensities at four main Raman peaks analysed by the generalized linear model

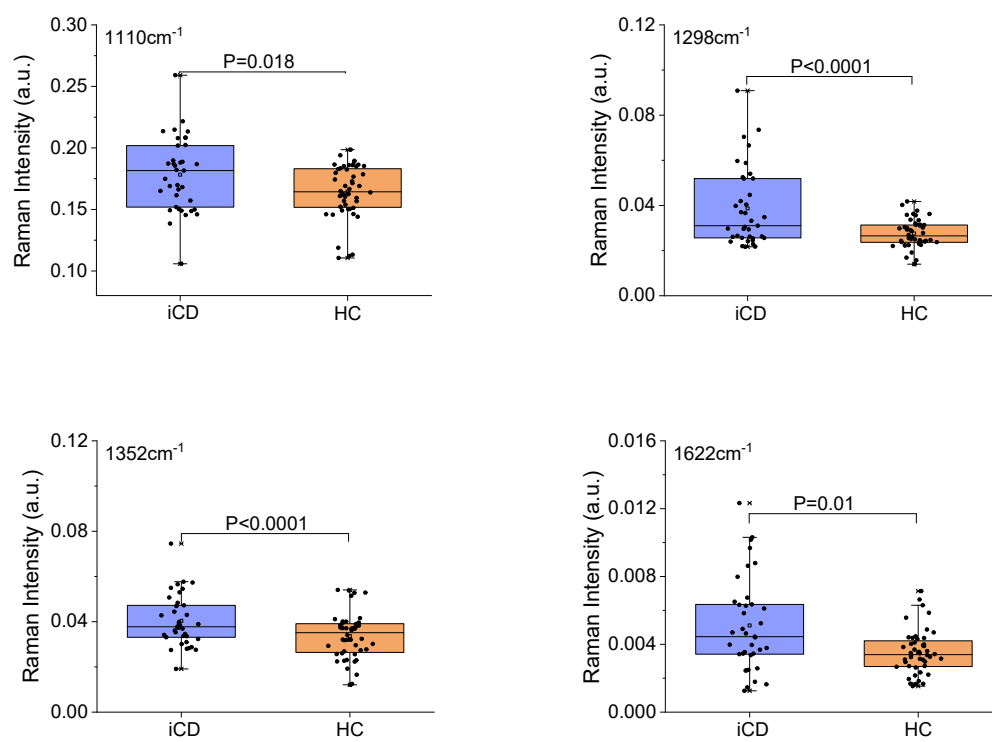| Peak (cm^{-1})	Parameter	p-value
1110	[status iCD] - [status HC]	0.015
	[sex female] - [sex male]	0.505
	age	0.968
1298	[status iCD] - [status HC]	<0.0001
	[sex female] - [sex male]	0.518
	age	0.998
1352	[status iCD] - [status HC]	0.005
	[sex female] - [sex male]	0.939
	age	0.723
1622	[status iCD] - [status HC]	0.001
	[sex female] - [sex male]	0.367
	age	0.583

Figure S4: Box plots of the Raman intensities at four main Raman peaks in iCD/HC

Table S10: Eigenvalue, percentage of variance and the cumulative percentage of variance of the first 20 principal components identified by the PCA analysis for iCD/HC

PC number	Eigenvalue	Percentage of Variance (%)	Cumulative (%)
1	0.08781	32.52619	32.52619
2	0.05663	20.97624	53.50243
3	0.03602	13.34367	66.8461
4	0.02231	8.26283	75.10893
5	0.01605	5.94714	81.05607
6	0.01285	4.75867	85.81474
7	0.00972	3.60024	89.41499
8	0.00673	2.49329	91.90828
9	0.00486	1.80143	93.70971
10	0.00332	1.22804	94.93775
11	2.79E-03	1.03202	95.96976
12	1.64E-03	0.60873	96.5785
13	1.12E-03	0.41323	96.99172
14	9.07E-04	0.33595	97.32767
15	8.34E-04	0.30883	97.6365
16	7.22E-04	0.26747	97.90397
17	5.51E-04	0.20415	98.10813
18	4.98E-04	0.18456	98.29268
19	4.33E-04	0.16054	98.45322
20	4.28E-04	0.15863	98.61185