

Supplementary material

Title: Identification of fluoroquinolone-resistant *Mycobacterium tuberculosis* through high-level data fusion of Raman and laser-induced breakdown spectroscopy

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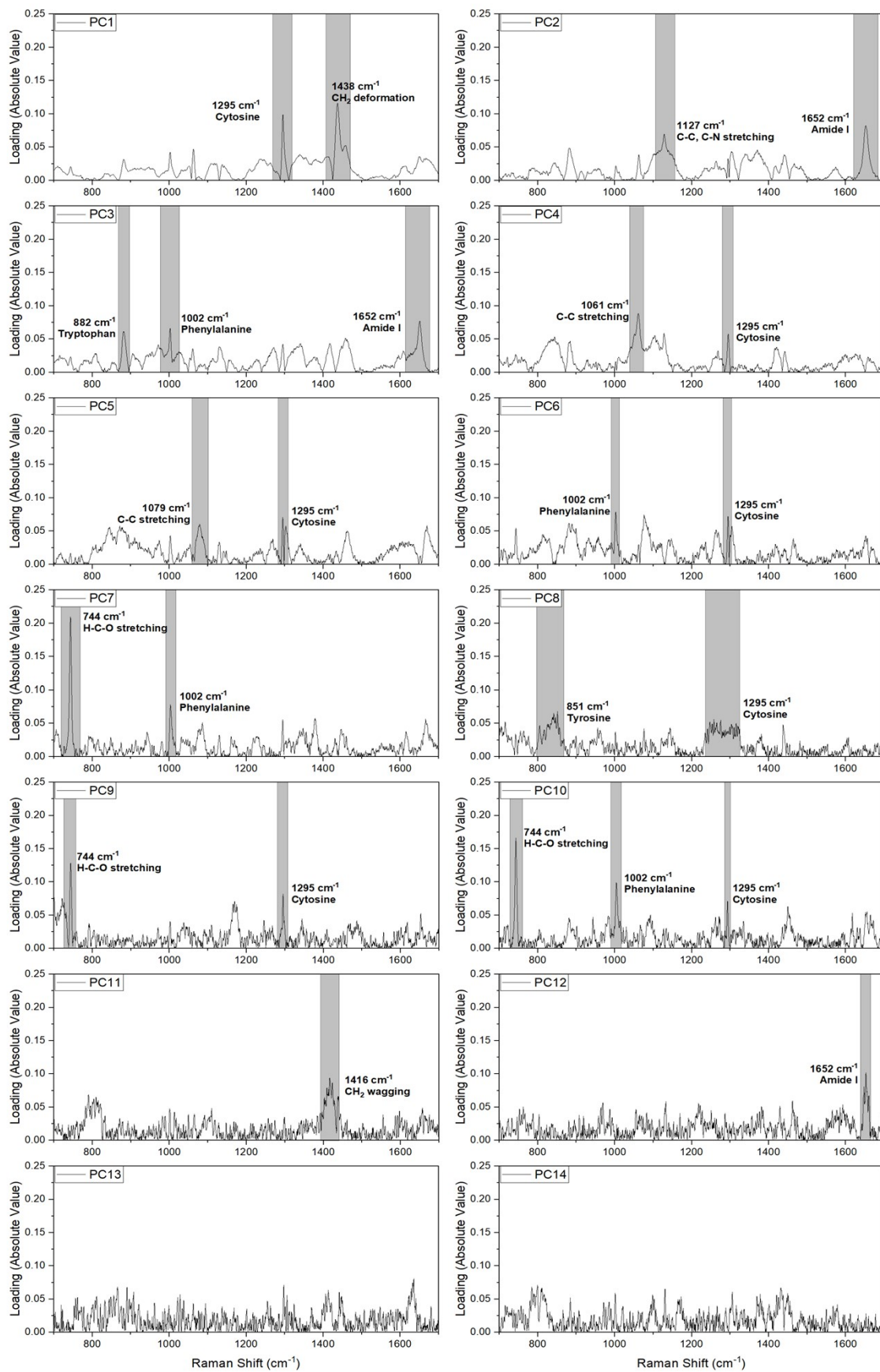
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FIG

URE S1. The loading plots of the principal components for the Raman spectra of the samples.

Ground truth	LIBS				Raman				Fusion model
	Control	<i>Gyr A</i>	<i>Gyr B</i>	Prediction result	Control	<i>Gyr A</i>	<i>Gyr B</i>	Prediction result	Prediction result
Control	0.888367	0.068291	0.043342	Control	0.436609	0.227114	0.336277	Control	Control
Control	0.704504	0.236775	0.05872	Control	0.853505	0.058979	0.087516	Control	Control
Control	0.66474	0.26935	0.065909	Control	0.987077	0.008325	0.004599	Control	Control
Control	0.821866	0.134258	0.043876	Control	0.985765	0.012965	0.00127	Control	Control
Control	0.919178	0.058729	0.022093	Control	0.73819	0.173335	0.088476	Control	Control
Control	0.549346	0.415994	0.034661	Control	0.928299	0.035284	0.036417	Control	Control
Control	0.790227	0.17056	0.039213	Control	0.963231	0.013251	0.023518	Control	Control
Control	0.359267	0.612857	0.027876	<i>Gyr A</i>	0.796706	0.119775	0.083519	Control	Control
Control	0.741499	0.225746	0.032755	Control	0.905821	0.049857	0.044322	Control	Control
Control	0.543043	0.42653	0.030428	Control	0.681307	0.108273	0.21042	Control	Control
Control	0.831542	0.145237	0.023221	Control	0.594109	0.350347	0.055545	Control	Control
Control	0.701223	0.290233	0.008544	Control	0.986579	0.008593	0.004828	Control	Control
Control	0.36996	0.588502	0.041538	<i>Gyr A</i>	0.743564	0.183197	0.07324	Control	Control
Control	0.230911	0.712822	0.056267	<i>Gyr A</i>	0.984929	0.010734	0.004336	Control	Control
Control	0.808284	0.161933	0.029782	Control	0.99218	0.004397	0.003423	Control	Control
Control	0.313056	0.315103	0.371842	Control	0.921533	0.043115	0.035353	Control	Control
Control	0.177093	0.744585	0.078322	<i>Gyr A</i>	0.87034	0.042313	0.087347	Control	Control
Control	0.618393	0.35703	0.024578	Control	0.882018	0.040937	0.077046	Control	Control
Control	0.69676	0.281015	0.022224	Control	0.980736	0.010347	0.008917	Control	Control
Control	0.387454	0.560084	0.052462	<i>Gyr A</i>	0.447403	0.236982	0.315614	Control	Control
<i>gyrA</i>	0.167414	0.791645	0.04094	<i>Gyr A</i>	0.001853	0.694202	0.303945	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.264245	0.676642	0.059113	<i>Gyr A</i>	0.023365	0.221305	0.755331	<i>Gyr B</i>	<i>Gyr A</i>
<i>gyrA</i>	0.721112	0.224272	0.054616	Control	0.001358	0.660233	0.338409	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.309918	0.63197	0.058112	<i>Gyr A</i>	0.364354	0.21313	0.422515	<i>Gyr B</i>	<i>Gyr A</i>
<i>gyrA</i>	0.021406	0.930457	0.048137	<i>Gyr A</i>	0.000593	0.575374	0.424033	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.016131	0.910695	0.073174	<i>Gyr A</i>	0.000699	0.551876	0.447425	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.267757	0.708559	0.023684	<i>Gyr A</i>	0.082306	0.493738	0.423956	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.200563	0.696552	0.102886	<i>Gyr A</i>	0.043869	0.946313	0.009817	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.231198	0.510485	0.258317	<i>Gyr A</i>	0.000631	0.692285	0.307084	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.402096	0.471142	0.126763	<i>Gyr A</i>	0.083358	0.441327	0.475315	<i>Gyr B</i>	<i>Gyr A</i>
<i>gyrA</i>	0.083621	0.898931	0.017448	<i>Gyr A</i>	0.078593	0.761591	0.159816	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.012724	0.184093	0.803182	<i>Gyr B</i>	0.003071	0.988563	0.008366	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.630496	0.338182	0.031322	Control	0.080396	0.844091	0.075513	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.856189	0.129617	0.014193	Control	0.209291	0.51102	0.279689	<i>Gyr A</i>	Control
<i>gyrA</i>	0.24531	0.695818	0.058872	<i>Gyr A</i>	0.039522	0.916326	0.044152	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.393436	0.534797	0.071768	<i>Gyr A</i>	0.107034	0.644966	0.247999	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.291194	0.639548	0.069258	<i>Gyr A</i>	0.005804	0.778165	0.216032	<i>Gyr A</i>	<i>Gyr A</i>

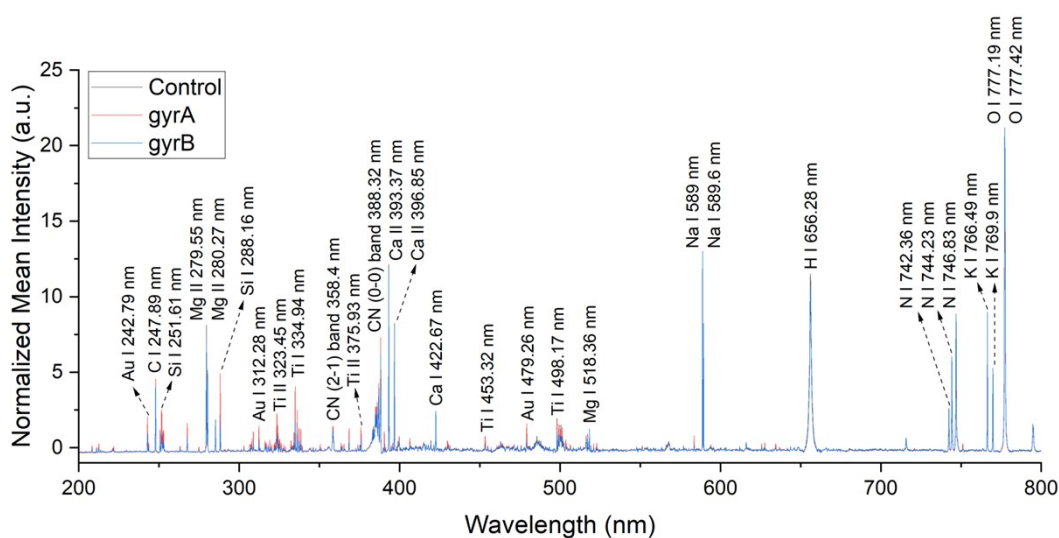


FIGURE S2. The normalized mean LIBS spectra for each sample.

<i>gyrA</i>	0.400698	0.506356	0.092946	<i>Gyr A</i>	0.053138	0.825617	0.121245	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.433741	0.490466	0.075793	<i>Gyr A</i>	0.077366	0.483662	0.438973	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrA</i>	0.091027	0.871019	0.037954	<i>Gyr A</i>	0.03476	0.957947	0.007294	<i>Gyr A</i>	<i>Gyr A</i>
<i>gyrB</i>	0.112683	0.334871	0.552445	<i>Gyr B</i>	0.023653	0.169152	0.807195	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.012216	0.031103	0.956681	<i>Gyr B</i>	0.140884	0.403713	0.455404	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.156169	0.259372	0.584458	<i>Gyr B</i>	0.00115	0.431963	0.566887	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.231881	0.139707	0.628412	<i>Gyr B</i>	0.019556	0.241658	0.738786	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.030228	0.272312	0.69746	<i>Gyr B</i>	0.006364	0.631784	0.361852	<i>Gyr A</i>	<i>Gyr B</i>
<i>gyrB</i>	0.36963	0.460177	0.170193	<i>Gyr A</i>	0.08861	0.192044	0.719346	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.007308	0.037667	0.955025	<i>Gyr B</i>	0.001108	0.449456	0.549436	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.062411	0.155053	0.782536	<i>Gyr B</i>	0.0429	0.356622	0.600478	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.006576	0.005707	0.987717	<i>Gyr B</i>	0.005208	0.291882	0.70291	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.005687	0.003697	0.990616	<i>Gyr B</i>	0.240596	0.107358	0.652045	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.060149	0.079849	0.860002	<i>Gyr B</i>	0.002435	0.62382	0.373745	<i>Gyr A</i>	<i>Gyr B</i>
<i>gyrB</i>	0.038515	0.2332	0.728285	<i>Gyr B</i>	0.066259	0.152731	0.78101	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.016277	0.009005	0.974717	<i>Gyr B</i>	0.01282	0.178054	0.809126	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.034796	0.355524	0.60968	<i>Gyr B</i>	0.137232	0.193903	0.668865	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.009405	0.012877	0.977718	<i>Gyr B</i>	0.130614	0.243741	0.625645	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.016411	0.655215	0.328374	<i>Gyr A</i>	0.036245	0.280374	0.683382	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.022857	0.074297	0.902845	<i>Gyr B</i>	0.060166	0.282981	0.656853	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.004241	0.005554	0.990205	<i>Gyr B</i>	0.015584	0.280586	0.70383	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.078993	0.337363	0.583644	<i>Gyr B</i>	0.248302	0.314028	0.43767	<i>Gyr B</i>	<i>Gyr B</i>
<i>gyrB</i>	0.127667	0.368539	0.503794	<i>Gyr B</i>	0.098254	0.311991	0.589755	<i>Gyr B</i>	<i>Gyr B</i>

Table S1. The probabilities derived from each model and the resulting prediction