

Table S4. Comparison of absorbance intensity of major assigned spectral peaks from fecal samples in three types of discrimination models.

Wavenumber (cm ⁻¹)	UC vs. HC			Wavenumber (cm ⁻¹)	RM vs. NRM (W8)			Wavenumber (cm ⁻¹)	RM vs. NRM (W56)		
	VIP value	Fold change (UC/HC)	<i>p</i> -value		VIP value	Fold change (RM/NRM)	<i>p</i> -value		VIP value	Fold change (RM/NRM)	<i>p</i> -value
3271.65	1.99	0.88(↓)	0.000*	3067.23	1.46	0.95(↓)	0.048*	1740.92	1.46	2.50(↑)	0.044*
3271.16	1.99	0.88(↓)	0.000*	3067.71	1.46	0.95(↓)	0.048*	1740.44	1.46	2.46(↑)	0.043*
1629.56	1.74	0.88(↓)	0.000*	2953.45	1.25	0.95(↓)	0.180	1629.56	1.52	0.99(↓)	0.014*
1629.07	1.71	0.88(↓)	0.000*	2953.93	1.24	0.95(↓)	0.188	1629.07	1.60	0.99(↓)	0.019*
1437.67	1.53	1.20(↑)	0.000*	1740.44	1.76	2.09(↑)	0.226	1546.63	1.12	0.93(↓)	0.069
1437.19	1.55	1.20(↑)	0.000*	1740.92	1.74	2.06(↑)	0.226	1546.15	1.15	0.93(↓)	0.076
1408.75	2.09	1.26(↑)	0.000*	1316.18	1.35	1.14(↑)	0.086	1244.82	1.23	1.10(↑)	0.061
1408.26	2.09	1.26(↑)	0.000*	1316.66	1.33	1.14(↑)	0.089	1244.34	1.23	1.10(↑)	0.060
1316.66	1.78	1.37(↑)	0.000*	1244.34	1.68	1.23(↑)	0.038*	1149.37	2.72	1.24(↑)	0.000*
1316.18	1.78	1.38(↑)	0.000*	1244.83	1.68	1.22(↑)	0.038*	1149.85	2.70	1.24(↑)	0.000*
1244.83	1.25	1.29(↑)	0.000*	1149.37	1.60	1.21(↑)	0.032*				
1244.34	1.25	1.29(↑)	0.000*	1149.85	1.60	1.21(↑)	0.033*				
1149.85	1.15	0.82(↓)	0.000*								
1149.37	1.17	0.82(↓)	0.000*								

HC, healthy controls; NRM, patient not in remission; RM, patient in remission; UC, ulcerative colitis; VIP, variable importance of projection; W8, baseline fecal samples from patients after 8 weeks of adalimumab treatment; W56, baseline fecal samples from patients after 56 weeks of adalimumab treatment.

Direction of comparison is UC/HC and RM/NRM with fold change threshold of 1.0. Significant differences between two groups are represented with asterisk mark (*) ($p < 0.05$) in student's *t* test. Bold characters represent selected wavenumbers satisfying both VIP value over 1.0 and *p*-value (student's *t* test) below 0.05.