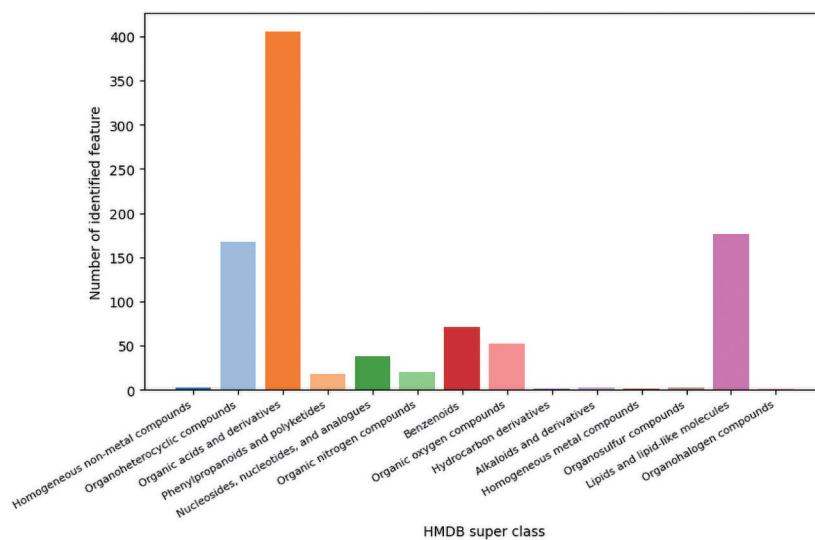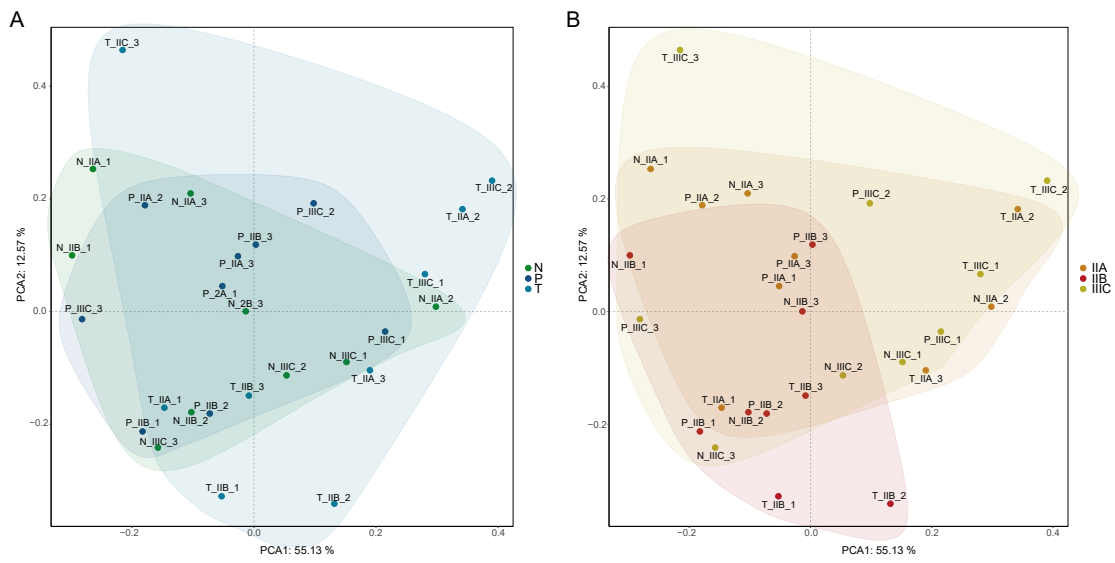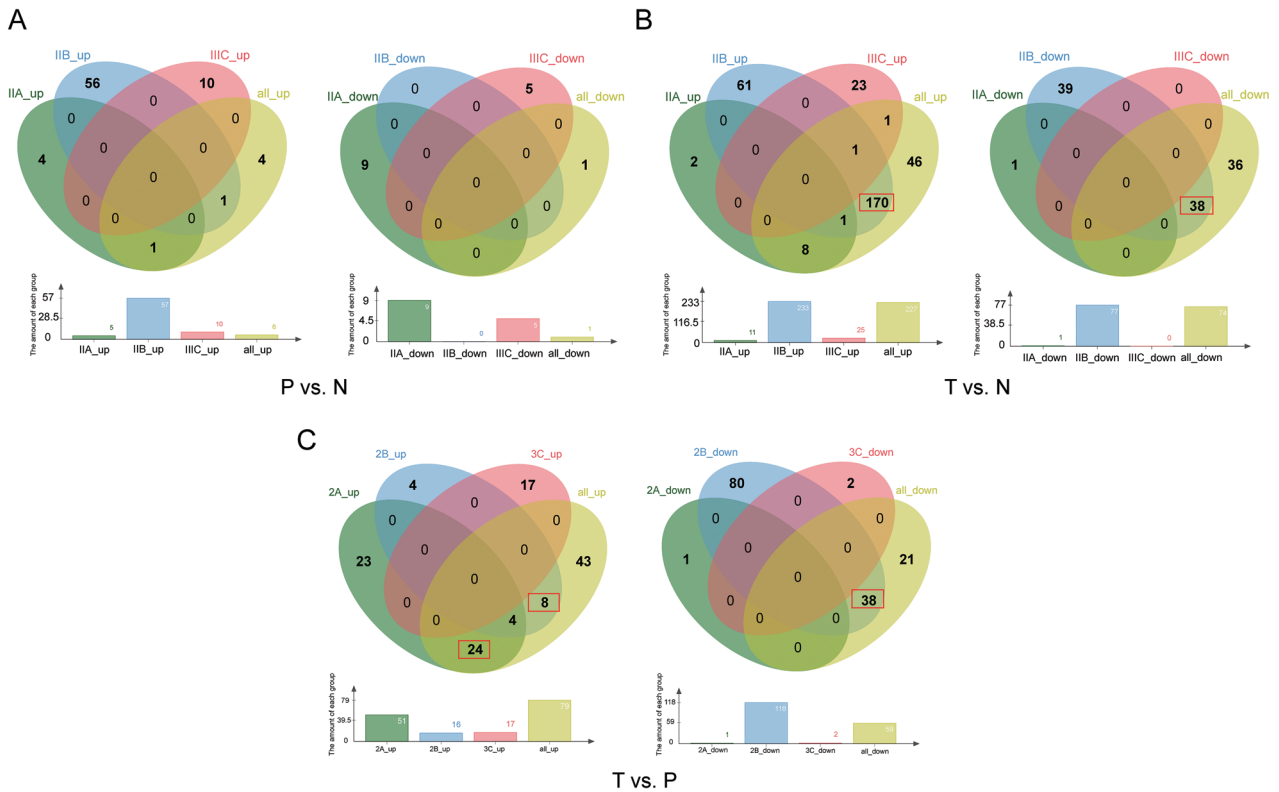**Table S1** Clinicopathologic characteristics of the included samples

Patient ID	Age (years)	Gender	Tissue	Type	TNM	Size (cm)	Date of birth	Date of diagnosis	Metastatic type	Country	City
IIA_1	67	Male	Rectum	Adenocarcinoma	T3N0M0	5.5×4.0×1.5	1952	2020	No	China	Ningbo
IIA_2	68	Male	Rectum	Adenocarcinoma	T3N0M0	3.0×2.0×0.8	1950	2020	No	China	Ningbo
IIA_3	66	Male	Rectum	Adenocarcinoma	T3N0M0	5.0×3.5×2.0	1953	2020	No	China	Ningbo
IIB_1	62	Male	Rectum	Adenocarcinoma	T4aN0M0	3.7×3.2×0.8	1957	2020	No	China	Ningbo
IIB_2	57	Male	Rectum	Adenocarcinoma	T4aN0M0	5.5×4.0×1.0	1962	2020	No	China	Ningbo
IIB_3	57	Male	Rectum	Adenocarcinoma	T4aN0M0	4.0×3.0×1.0	1963	2020	No	China	Ningbo
IIIC_1	66	Male	Rectum	Adenocarcinoma	T4aN2bM0	4.0×3.0×0.8	1954	2021	No	China	Ningbo
IIIC_2	68	Male	Rectum	Adenocarcinoma	T3N2bM0	6.5×6.0×5.0	1951	2019	No	China	Ningbo
IIIC_3	66	Male	Rectum	Adenocarcinoma	T4aN2bM0	3.8×3.0×0.5	1954	2021	No	China	Ningbo

Figure S1 HMDB (The Human Metabolome Database) Super class classification map of the included samples.

Figure S2 PCA (principal component analysis) models for the classification of colorectal cancer. PCA of cancer tissue, its adjacent tissues, and normal tissues (A) and the different stages of cancers, including stages IIA, IIB, and IIIC (B). N, normal tissues; P, paracancerous tissues; T, tumor tissues.

Figure S3 Venn diagram for intersection analysis of the differential metabolites of the various groups. The bar graph shows the number of differential metabolites for each corresponding set. N, normal tissues; P, paracancerous tissues; T, tumor tissues.