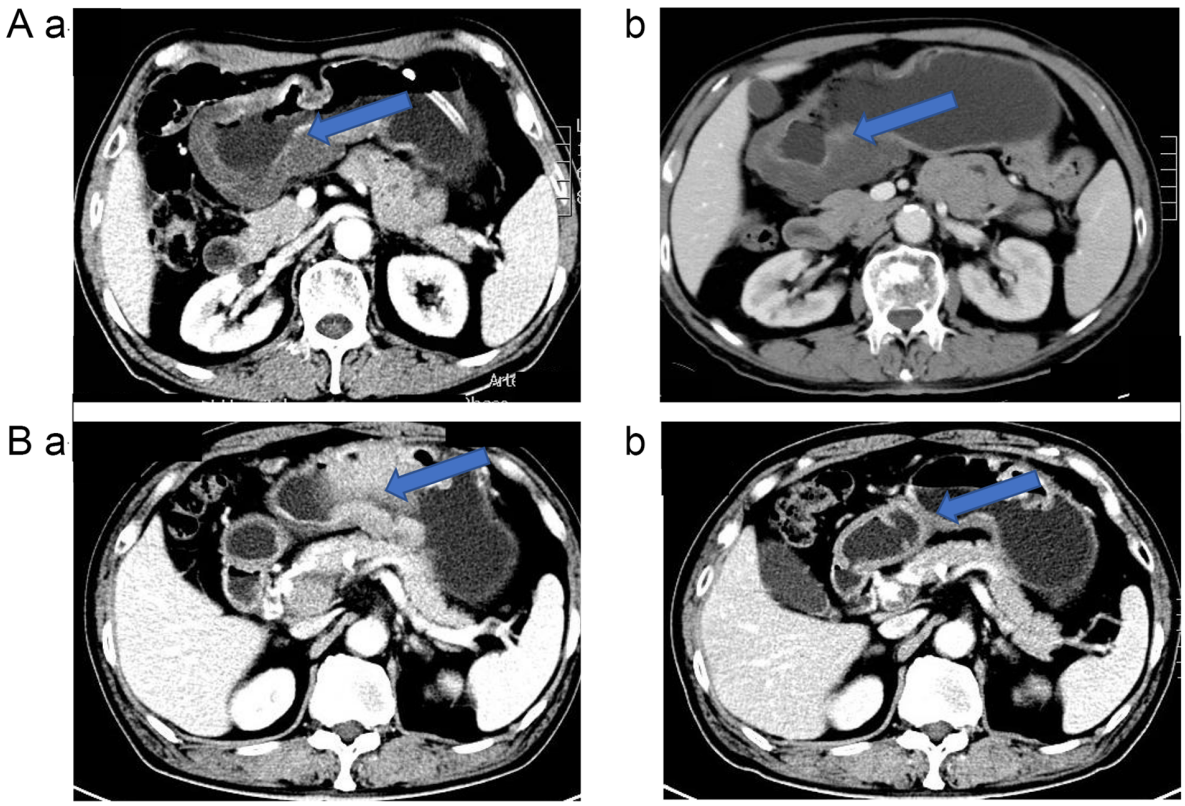
Figure S1. Random images and levels of the four metabolites in the chemo-resistant and chemo-sensitive cases. The blue arrows mark tumor sites. (A-a) Image of chemo-resistant case before chemotherapy. (A-b) Image of chemo-resistant case after chemotherapy. (B-a) Image of chemo-sensitive case before chemotherapy. (B-b) Image of chemo-sensitive case after chemotherapy. (C) Levels of the four metabolites in the chemo-sensitive case and chemo-resistant case. PC, phosphatidylcholine.



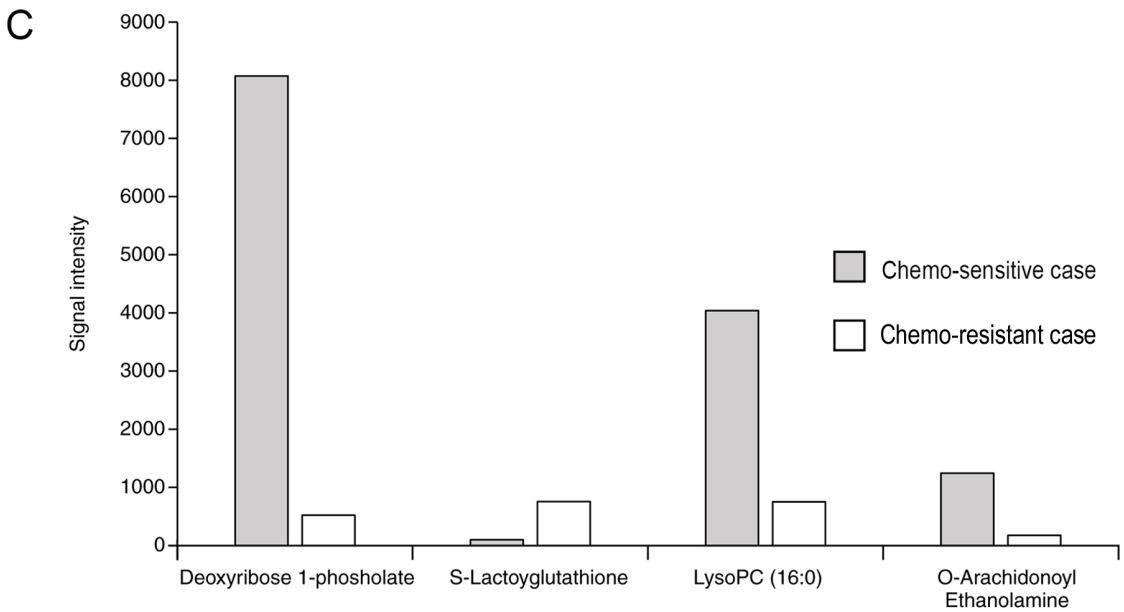


Table SI. Metabolites with significant differences between serum samples from chemo-sensitive and -resistant patients in positive ion mode.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
99.0452	7.3	0.00±0.00	22.93±39.23	0.02631[a]
127.0397	7.3	4.90±13.51	58.21±95.97	0.03586[a]
183.1013	7.28	0.00±0.00	34.26±65.82	0.04602[a]
215.0315	9.52	7598.48±955.87	2482.61±811.16	0.00141[b]
228.2321	6.91	48.81±15.56	61.92±19.96	0.04984[a]
230.2479	7.35	776.44±133.73	929.68±113.94	0.00187[b]
235.1685	9.55	54.04±37.07	25.46±38.48	0.04402[a]
243.1211	8.59	13.67±31.07	71.87±108.22	0.04802[a]
255.1225	8.88	8.64±24.73	79.61±128.93	0.03898[a]
256.261	7.31	59.63±33.10	80.24±18.30	0.04223[a]
262.2374	5.53	117.85±34.48	161.44±23.44	0.00031[c]
266.1717	6.91	7.10±8.05	1.81±4.92	0.03681[a]
273.438	7.28	480.30±92.54	564.61±103.37	0.02327[a]
274.274	7.28	55738.16±9069.52	63255.79±9878.32	0.03522[a]
276.2793	7.28	1245.56±226.72	1429.11±254.23	0.04228[a]
278.2464	8.66	0.00±0.00	33.11±50.25	0.01326[a]
299.1452	6.84	1.45±5.78	63.60±121.25	0.04948[a]
299.1833	8.61	16.19±37.58	147.43±251.04	0.04758[a]
300.289	8.29	170.80±83.97	317.52±187.12	0.00801[b]
301.3817	8.08	199.96±94.48	263.2±73.06	0.04702[a]
306.2635	5.73	41.80±32.88	93.46±24.20	0.00238[b]
311.1833	8.92	7.46±29.85	168.51±299.09	0.04047[a]
315.1778	8.69	3.12±12.46	64.05±117.33	0.04772[a]
328.739	7.07	4.35±17.3900	60.84±105.67	0.04353[a]
337.2829	11.25	317.19±208.99	712.77±687.66	0.03612[a]
344.3503	9.62	306.32±150.54	426.84±147.59	0.03229[a]
345.2252	9.23	0.00±0.00	42.14±65.86	0.01587[a]
351.1753	8.92	5.15±20.62	55.74±85.63	0.02911[a]
354.2279	7.63	99.04±46.10	137.03±48.50	0.03320[a]
357.2698	10.25	592.5±293.41	806.27±197.34	0.02502[a]
357.2762	7.55	40.66±57.17	281.79±450.34	0.04215[a]
357.3092	10.16	13.69±24.44	0.00±0.00	0.03865[a]
358.3661	10.31	86465.19±39985.12	111731.61±24379.47	0.04394[a]
360.2512	11.16	0.00±0.00	25.83±43.27	0.02353[a]
360.3712	10.36	2954.95±1379.86	3805.46±831.50	0.04838[a]
371.2024	9.76	6.38±23.08	91.93±135.71	0.01893[a]
376.2425	10.49	22.17±41.16	0.00±0.00	0.04610[a]
380.1122	11.3	312.26±148.42	855.95±103.00	0.00616[b]
382.7683	6.6	0.00±0.00	24.30±47.33	0.04883[a]
383.2033	9.99	48.74±85.74	376.40±634.11	0.04958[a]
395.3994	9.31	290.26±291.23	622.29±483.62	0.02678[a]
396.7837	7.85	3.95±8.55	57.64±99.57	0.03997[a]
397.2824	7.89	0.00±0.00	18.55±33.91	0.03664[a]
397.3754	11.68	94.82±82.96	170.21±116.48	0.04586[a]
402.3902	10.29	21683.77±9549.55	27643.98±5856.49	0.04672[a]
403.2285	10.43	20.14±36.53	0.00±0.00	0.04150[a]
403.2885	7.48	2.94±11.77	40.35±70.18	0.04423[a]
405.2572	11.35	38.71±37.19	14.40±27.12	0.04772[a]
405.7983	7.82	0.00±0.00	32.58±60.31	0.03889[a]
410.3143	10.92	98.70±154.52	0.00±0.00	0.01958[a]
412.3027	8.21	0.00±0.00	105.64±182.42	0.02764[a]
413.7948	6.6	2.10±8.41	38.15±69.57	0.04858[a]
414.2964	6.84	14.44±33.48	251.30±446.64	0.04293[a]
418.7969	7.74	4.87±13.35	72.19±129.9	0.04812[a]
425.8038	8.13	1.40±5.60	112.22±193.05	0.02898[a]
426.3365	8.25	0.00±0.00	231.80±435.41	0.04161[a]

Table SI. Continued.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
427.3102	7.77	22.33±48.03	179.53±293.93	0.04345[a]
431.2915	8.29	0.00±0.00	50.94±95.32	0.04090[a]
431.3109	9.48	694.53±94.61	316.66±39.18	0.00180[b]
433.2511	9.93	0.00±0.00	34.72±56.26	0.01957[a]
434.3169	8.11	10.94±30.18	187.38±325	0.03884[a]
434.3327	7.87	0.00±0.00	324.1±632.86	0.04942[a]
434.8173	8.13	3.28±2.28	75.10±34.81	0.04223[a]
436.7931	8.09	0.00±0.00	42.49±74.43	0.02973[a]
438.2935	8.95	302.03±142.41	626.39±520.36	0.02295[a]
440.8087	7.74	0.00±0.00	58.10±104.17	0.03340[a]
441.325	8.58	0.00±0.00	266.94±466.56	0.02941[a]
443.2587	9.83	0.00±0.00	79.99±139.01	0.02856[a]
445.2742	9.76	47.62±112.92	348.48±526.50	0.03336[a]
447.8163	8.06	10.4±18.63	107.8±182.79	0.04249[a]
448.3163	8.03	0.00±0.00	40.57±75.69	0.04032[a]
450.3167	6.88	48.58±65.4	485.30±795.4	0.03665[a]
451.7993	7.67	0.00±0.00	27.59±49.65	0.03401[a]
454.2874	8.6	2729.15±1072.99	3837.61±1680.84	0.03567[a]
454.8237	8.38	0.00±0.00	128.57±224.07	0.02898[a]
456.3284	8.06	26.24±50.51	368.29±637.39	0.04074[a]
456.3454	7.56	0.00±0.00	500.79±979.46	0.04976[a]
457.2732	10.01	141.81±294.42	1471.25±2454.12	0.03978[a]
458.8065	8.08	1.74±6.96	58.11±96.72	0.02714[a]
462.2986	9.76	42.25±99.4	299.41±446.00	0.03221[a]
463.3352	8.41	14.17±33.12	393.76±675.68	0.03243[a]
464.3084	9.23	127.33±120.8	375.71±358.31	0.01382[a]
464.3243	7.34	0.00±0.00	63.60±124.31	0.04962[a]
465.2401	9.8	21.78±87.11	171.67±267.39	0.04204[a]
469.8284	7.96	9.43±20.4	97.68±158.19	0.03483[a]
470.3607	8.13	0.00±0.00	472.32±888.17	0.04182[a]
471.1001	11.82	882.39±1562.64	31.68±80.06	0.04420[a]
473.0967	11.84	538.67±978.53	12.01±46.53	0.04647[a]
474.3009	9.99	123.08±247.55	1154.77±1909.71	0.04053[a]
476.8342	8.31	6.64±14.72	142.14±238.13	0.03054[a]
477.3361	8.27	0.00±0.00	55.45±98.33	0.03162[a]
478.3238	8.76	752.77±201.33	1019.17±306.70	0.00745[b]
478.3414	7.96	56.48±101.34	413.76±677.12	0.04568[a]
480.8198	7.98	0.00±0.00	57.10±99.01	0.02824[a]
481.0033	7.9	6.05±16.91	34.90±52.17	0.04460[a]
482.3187	9.73	2399.39±1107.66	3422.60±1013.56	0.01208[a]
484.3243	9.71	0.00±0.00	53.58±79.83	0.01178[a]
484.3756	8.72	0.00±0.00	240.19±447.95	0.04026[a]
485.3472	8.31	38.71±69.54	515.41±869.90	0.03695[a]
487.827	8.35	0.00±0.00	75.26±126.04	0.02350[a]
490.3306	10.32	0.00±0.00	66.33±104.42	0.01656[a]
491.0031	7.14	0.00±0.00	26.43±47.04	0.03221[a]
491.3094	7.09	0.00±0.00	39.22±76.31	0.04865[a]
491.8424	7.91	9.89±21.40	88.18±143.82	0.03964[a]
492.3395	7.87	0.00±0.00	46.62±80.37	0.02742[a]
492.3555	8.72	7.46±20.41	334.45±627.44	0.04590[a]
494.8101	8.68	1624.18±458.68	2231.47±774.97	0.01213[a]
496.3331	8.78	6637.71±2345.54	1033.40±342.01	0.02887[a]
498.8489	8.26	10.50±22.64	146.97±245.69	0.03482[a]
499.3416	8.78	1611.18±465.13	2175.7±683.84	0.01136[a]
499.349	8.21	0.00±0.00	69.19±116.78	0.02451[a]
502.8316	7.87	7.81±16.89	51.14±82.00	0.04752[a]
503.3324	7.87	0.00±0.00	25.60±42.28	0.02178[a]

Table SI. Continued.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
505.8571	8.58	0.00±0.00	164.35±283.57	0.02752[a]
506.3582	8.62	0.00±0.00	68.11±125.93	0.03867[a]
507.36	8.2	64.44±116.29	607.95±1009.81	0.04088[a]
509.8387	8.21	8.32±18.16	87.23±144.62	0.03859[a]
514.3668	8.62	0.00±0.00	639.70±1073.96	0.02382[a]
514.3853	7.96	6.32±25.29	629.41±1170.62	0.04169[a]
515.8611	7.53	3.98±15.91	71.01±129.27	0.04849[a]
518.737	8.41	543.45±323.18	864.39±332.16	0.01075[a]
520.3325	8.37	94077.98±37345.01	136482.56±54014.90	0.01607[a]
520.8599	8.16	15.01±27.14	138.42±227.67	0.03965[a]
521.3777	9.1	0.00±0.00	446.56±774.48	0.02826[a]
522.426	8.09	0.00±0.00	23.20±41.58	0.03335[a]
523.3396	8.37	666.57±299.46	940.63±338.46	0.02350[a]
524.8432	7.8	5.07±14.38	51.28±82.40	0.03512[a]
525.0271	7.74	6.65±18.32	50.50±80.22	0.04176[a]
527.8695	8.53	3.51±14.03	174.76±303.41	0.03166[a]
528.3993	8.49	0.00±0.00	589.86±1073.13	0.03583[a]
529.3719	8.15	80.04±143.36	637.20±1053.33	0.04478[a]
531.8504	8.16	5.45±14.93	82.18±135.51	0.03199[a]
535.8657	7.75	0.00±0.00	62.05±98.01	0.01688[a]
536.3793	8.48	59.21±109.91	733.22±1224.57	0.03634[a]
537.3721	7.51	6.69±26.77	95.01±169.34	0.04836[a]
539.7014	7.22	0.00±0.00	36.74±66.96	0.03615[a]
539.8487	6.94	0.00±0.00	24.76±48.29	0.04916[a]
542.6585	8.44	9.55±26.28	77.23±126.29	0.04473[a]
542.8749	8.09	16.37±29.55	118.02±194.43	0.04765[a]
543.3715	8.05	3.85±15.39	55.64±96.31	0.04227[a]
543.3904	8.97	24.1±45.24	508.90±856.04	0.03119[a]
544.881	7.75	8.60±34.40	162.99±281.37	0.03752[a]
548.2656	8.23	188.65±90.9	121.67±84.34	0.04242[a]
548.3629	9.44	1094.15±842.46	2001.38±1467.84	0.04197[a]
548.3858	9.07	43.99±81.62	0.00±0.00	0.04595[a]
549.8819	8.4	0.00±0.00	167.16±273.40	0.02063[a]
550.4376	10.24	1772.24±706.03	2431.53±879.76	0.02830[a]
551.3859	8.08	87.57±157.31	597.72±979.80	0.04879[a]
553.8644	8.09	9.57±20.99	72.12±114.62	0.04027[a]
556.8864	8.82	0.00±0.00	130.35±227.50	0.02919[a]
558.4112	7.88	15.63±38.04	720.43±1360.53	0.04710[a]
560.8712	8.38	0.00±0.00	81.84±141.93	0.02827[a]
565.3886	8	1.94±7.74	61.72±101.59	0.02583[a]
569.383	7.2	0.00±0.00	66.78±118.38	0.03157[a]
571.8926	8.37	12.22±26.41	143.95±231.55	0.03133[a]
572.4091	9.31	0.00±0.00	474.84±818.18	0.02733[a]
572.4273	8.37	0.00±0.00	813.81±1486.27	0.03650[a]
578.9014	8.7	0.00±0.00	148.41±259.28	0.02934[a]
582.884	8.31	5.39±15.39	87.68±142.74	0.02919[a]
585.2595	8.58	1269.05±813.73	661.47±744.06	0.03876[a]
586.898	7.92	3.67±14.68	78.43±135.64	0.03645[a]
587.4148	8.69	76.82±140.35	625.32±1053.08	0.04784[a]
587.9167	8.72	42.39±95.91	393.76±679.34	0.04955[a]
593.9052	8.26	17.7±38.63	128.31±206.42	0.04390[a]
594.4078	8.24	0.00±0.00	73.28±121.58	0.02233[a]
594.4219	9.15	34.59±64.94	563.23±949.99	0.03418[a]
595.4113	7.93	19.78±79.14	374.47±645.68	0.03733[a]
600.4562	9.62	7.91±31.65	167.62±302.16	0.04413[a]
600.911	8.57	0.00±0.00	139.52±241.95	0.02825[a]
601.4299	9.6	8.84±35.37	353.71±585.78	0.02562[a]

Table SI. Continued.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
602.4159	8.2	42.40±124.03	527.58±915.89	0.04446[a]
602.4365	7.78	39.87±71.4	773.13±1430.61	0.04952[a]
604.8958	8.29	10.99±30.29	87.48±138.78	0.03978[a]
605.3994	8.26	0.00±0.00	43.70±76.12	0.02889[a]
607.3328	10.9	269.51±356.60	725.91±569.03	0.01160[a]
607.9218	9	0.00±0.00	132.28±227.74	0.02721[a]
608.9102	7.91	0.00±0.00	61.64±96.06	0.01558[a]
609.4267	8.63	102.25±185.89	752.20±1227.12	0.04497[a]
610.9192	7.59	0.00±0.00	147.17±268.75	0.03647[a]
611.9058	8.63	0.00±0.00	86.48±149.98	0.02826[a]
612.8934	7.09	0.00±0.00	21.59±41.59	0.04659[a]
616.4495	8.2	5.07±20.28	1016.94±1830.76	0.03491[a]
619.9034	7.9	0.00±0.00	31.54±54.68	0.02823[a]
622.924	8.52	0.00±0.00	130.81±207.05	0.01709[a]
623.443	9.44	29.67±66.78	409.61±671.81	0.03200[a]
629.9303	8.88	3.86±15.44	119.59±194.45	0.02436[a]
630.4099	10.87	12.57±34.72	131.07±220.78	0.04255[a]
630.4632	8.75	0.00±0.00	564.79±1032.32	0.03664[a]
630.9242	7.85	3.04±12.15	39.68±69.09	0.04555[a]
633.9163	8.52	0.00±0.00	88.85±135.88	0.01389[a]
634.4174	8.52	0.00±0.00	38.02±73.53	0.04739[a]
637.4332	7.59	25.52±47.36	0.00±0.00	0.04600[a]
637.9288	8.08	12.67±27.28	89.46±143.27	0.04398[a]
638.4322	8.11	2.41±9.63	52.81±92.78	0.03892[a]
644.4827	9.39	0.00±0.00	409.51±728.18	0.03206[a]
644.9385	8.4	0.00±0.00	111.18±172.72	0.01529[a]
645.4513	9.29	33.28±94.08	633.45±1050.77	0.03031[a]
646.4056	6.49	60.47±73.15	4.45±11.82	0.00659[b]
651.3986	11.23	6.15±24.61	42.34±66.04	0.04977[a]
651.9441	8.75	0.00±0.00	99.39±155.89	0.01620[a]
652.4622	9.86	0.00±0.00	222.03±386.99	0.02899[a]
654.4363	7.05	427.61±115.87	49.90±20.11	0.00475[b]
659.9398	8.01	7.44±20.39	61.43±96.19	0.03627[a]
659.9726	10.38	0.00±0.00	47.54±85.01	0.03294[a]
660.4729	8.11	20.70±44.66	1004.16±1803.81	0.03730[a]
661.9507	7.74	17.33±44.84	192.64±311.17	0.03355[a]
667.4519	8.35	0.00±0.00	52.14±79.55	0.01369[a]
674.4717	9.57	0.00±0.00	265.41±428.37	0.01914[a]
674.4912	8.6	0.00±0.00	1053.69±1862.41	0.03111[a]
674.974	9.67	6.40±25.60	158.91±275.16	0.03520[a]
680.9665	9.03	5.09±20.38	69.31±121.53	0.04599[a]
681.4815	10.17	0.00±0.00	95.01±164.66	0.02816[a]
681.9533	7.95	2.87±11.48	40.26±69.95	0.04358[a]
683.4617	7.71	6.35±25.41	92.93±165.56	0.04764[a]
683.9625	7.69	6.71±14.63	131.34±227.04	0.03644[a]
688.5071	9.15	0.00±0.00	639.01±1119.63	0.02978[a]
695.9702	8.58	6.30±25.22	76.82±120.06	0.02894[a]
701.52	7.09	0.00±0.00	32.64±62.93	0.04679[a]
701.5476	8.89	16.98±67.91	170.2±264.19	0.03260[a]
703.4867	10.41	0.00±0.00	94.03±146.9	0.01582[a]
703.9956	9.98	5.89±23.57	85.80±152.46	0.04723[a]
704.4994	8.03	43.92±78.70	966.77±1719.31	0.04028[a]
718.5128	8.46	419.98±152.03	817.05±101.27	0.04175[a]
732.5286	8.96	0.00±0.00	759.57±1328.89	0.02955[a]
734.998	7.87	3.58±14.31	77.28±139.06	0.04357[a]
746.5434	9.52	0.00±0.00	456.01±801.59	0.03027[a]
748.5258	7.91	63.82±115.05	782.80±1372.77	0.04554[a]

Table SI. Continued.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
756.5079	7.8	0.00±0.00	84.99±138.68	0.02035[a]
762.5351	8.33	32.75±59.38	1028.43±1786.84	0.03364[a]
765.9736	8.93	182.70±117.91	99.65±92.87	0.03845[a]
776.5512	8.8	0.00±0.00	664.59±1170.24	0.03053[a]
781.5706	10.56	5.56±22.24	305.61±558.54	0.04008[a]
790.5659	9.36	0.00±0.00	696.12±1217.38	0.02949[a]
806.5619	8.21	27.05±59.67	814.50±1422.86	0.03484[a]
820.5813	8.66	0.00±0.00	878.87±1543.27	0.03011[a]
825.6519	9.02	2087.54±1451.45	3400.35±977.26	0.00649[b]
834.5959	9.18	0.00±0.00	732.10±1281.34	0.02961[a]
846.4894	8.88	0.00±0.00	108.91±166.83	0.01404[a]
850.5888	8.13	41.19±74.13	572.74±991.30	0.04082[a]
864.6057	8.66	4.12±16.48	720.45±1258.95	0.03025[a]
869.6742	9.07	53.59±100.55	169.79±148.80	0.01584[a]
894.6149	8.03	34.80±62.52	368.73±626.89	0.04251[a]
908.5086	8.33	320.41±292.09	542.87±300.67	0.04557[a]
908.624	8.4	0.00±0.00	523.22±914.08	0.02934[a]
924.6253	7.62	11.75±32.29	111.79±185.84	0.04253[a]
933.6086	8.94	13.74±54.96	304.52±390.01	0.00616[b]
938.6393	8	25.17±45.25	231.68±378.33	0.03839[a]
939.5717	11.62	419.64±354.89	176.88±161.37	0.02186[a]
952.6556	8.34	13.86±30.97	339.69±575.89	0.03135[a]
982.6635	7.88	3.55±14.19	138.40±228.21	0.02513[a]
988.5866	8.78	154.23±180.32	421.95±454.59	0.03738[a]
989.6534	6.6	7.60±30.41	125.81±226.30	0.04727[a]
991.6469	8.78	72502.61±34209.43	135323.94±100784.87	0.02550[a]
994.6572	8.78	2739.97±1326.63	4715.69±2785.68	0.01641[a]
996.6774	8.24	0.00±0.00	228.81±385.48	0.02427[a]

[a]P<0.05, [b]P<0.01, [c]P<0.001.

Table SII. Metabolites with significant differences between serum samples from chemo-sensitive and -resistant patients in negative ion mode.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
80.9163	10.35	6.94±20.3	33.12±40.4	0.02871a
80.9165	9.11	4.01±11.66	19.39±19.64	0.01227[a]
131.0862	7.37	0.66±2.65	20.32±37.39	0.04454[a]
141.0551	7.72	1.03±4.12	14.63±24.52	0.03684[a]
144.0117	2.17	0.00±0.00	14.31±25.39	0.03169[a]
155.1087	7.31	68.32±174.02	918.78±1580.14	0.04077[a]
171.1395	9.25	1628.89±2757.23	159.94±116.17	0.04853[a]
177.092	7.55	1.72±6.90	35.37±58.59	0.02997[a]
183.1392	8.05	2.06±5.65	56.90±103.56	0.04296[a]
197.0803	7.65	0.00±0.00	5.97±11.16	0.04063[a]
205.1603	9.95	75.43±62.9	128.76±47.72	0.01303[a]
211.1688	10.17	6.25±10.17	0.00±0.00	0.02427[a]
213.114	7.65	0.00±0.00	6.01±9.91	0.02160[a]
215.1294	7.73	3.19±8.75	73.22±136.51	0.04952[a]
279.1994	8.71	13.30±36.66	124.82±193.81	0.03141[a]
297.6274	2.47	14.52±25.21	0.67±2.60	0.04317[a]
301.2201	9.7	8.10±32.38	124.66±168.29	0.01091[a]
307.228	11.46	24.87±38.14	3.17±8.39	0.03971[a]
317.219	9.71	16.50±40.84	79.62±102.91	0.03068[a]
319.2316	9.7	1286.64±3197.64	6461.94±8960.08	0.03836[a]
327.2643	10.27	32.79±61.52	0.00±0.00	0.04825[a]
334.2397	11.46	15.51±27.95	0.00±0.00	0.04034[a]
342.56	6.53	2.81±8.35	57.25±88.28	0.02021[a]
369.1794	6.42	1959.43±2993.87	5229.94±4008.68	0.01504[a]
376.2258	6.68	214.11±162.42	328.33±119.74	0.03470[a]
383.1773	8.58	0.00±0.00	24.79±43.13	0.02874[a]
389.2728	7.56	25.44±41.96	2.65±10.26	0.04998[a]
391.2714	11.67	8.93±16.48	54.52±82.45	0.03851[a]
393.1172	7.1	0.00±0.00	117.22±208.32	0.03197[a]
398.9475	6.76	28.96±42.03	130.65±190.11	0.04567[a]
407.2875	6.84	0.00±0.00	30.97±52.94	0.02621[a]
411.2457	7.56	0.00±0.00	8.31±13.18	0.01726[a]
428.1936	8.16	15.79±19.29	34.50±25.13	0.02669[a]
437.1678	6.42	1.85±7.41	25.72±34.19	0.01071[a]
447.2166	7.16	11.89±20.63	0.00±0.00	0.03374[a]
449.1916	8.35	792.5±1262.94	76.88±297.77	0.04112[a]
473.2349	8.34	37.19±51.74	6.45±24.98	0.04613[a]
493.1314	8.33	4.29±17.17	22.87±29.87	0.04084[a]
500.2912	8.33	4724.75±4994.74	8372.98±3946.14	0.03247[a]
508.355	9.97	142.92±169.88	333.90±307.29	0.03917[a]
516.3336	9.12	12.40±34.87	100.46±159.51	0.03948[a]
526.3666	9.09	173.90±252.83	623.42±802.14	0.04147[a]
536.3074	7.68	34.86±31.83	6.40±16.99	0.00455[b]
536.3176	7.74	2.02±8.07	25.87±37.05	0.01772[a]
537.2686	8.59	0.00±0.00	12.40±22.37	0.03441[a]
537.3455	8.67	704.87±715.98	1229.92±552.89	0.03055[a]
540.3447	8.68	13281.30±20364.88	28726.85±21107.94	0.04712[a]
544.3341	9.27	27.07±56.19	128.54±162.66	0.02565[a]
544.9786	8.11	129.02±352.55	479.69±537.40	0.03903[a]
552.3467	8.51	75.32±104.96	211.21±216.06	0.03220[a]
552.3848	9.39	215.70±255.92	586.01±498.88	0.01367[a]
554.3639	9.3	330.12±332.65	795.02±812.75	0.04368[a]
561.3563	8.4	561.35±284.94	764.83±267.15	0.04975[a]
562.5871	8.4	26.69±53.20	74.20±69.37	0.04019[a]
565.3792	9.94	251.98±208.42	470.18±276.74	0.01874[a]
574.4153	11.2	0.00±0.00	430.40±774.18	0.03392[a]

Table SII. Continued.

m/z	Retention time, min	Signal intensity, mean ± standard deviation		P-value
		Sensitive	Resistant	
593.149	8.02	13.41±21.26	67.77±71.48	0.00686[b]
600.2688	8.36	8.92±35.67	84.98±129.73	0.03163[a]
600.285	8.98	76.04±108.28	171.28±140.29	0.04232[a]
610.391	9.01	80.76±126.42	193.23±175.27	0.04854[a]
826.5665	8.74	327.43±598.88	0.00±0.00	0.04312[a]
828.5959	8.88	0.00±0.00	61.29±106.1	0.02800[a]
947.6478	8.59	0.00±0.00	349.31±551.19	0.01678[a]
973.6725	8.84	0.00±0.00	139.48±210.15	0.01266[a]

[a]P<0.05, [b]P<0.01, [c]P<0.001.