

Supporting Table S1. The optimised temperature program of GC/MS.

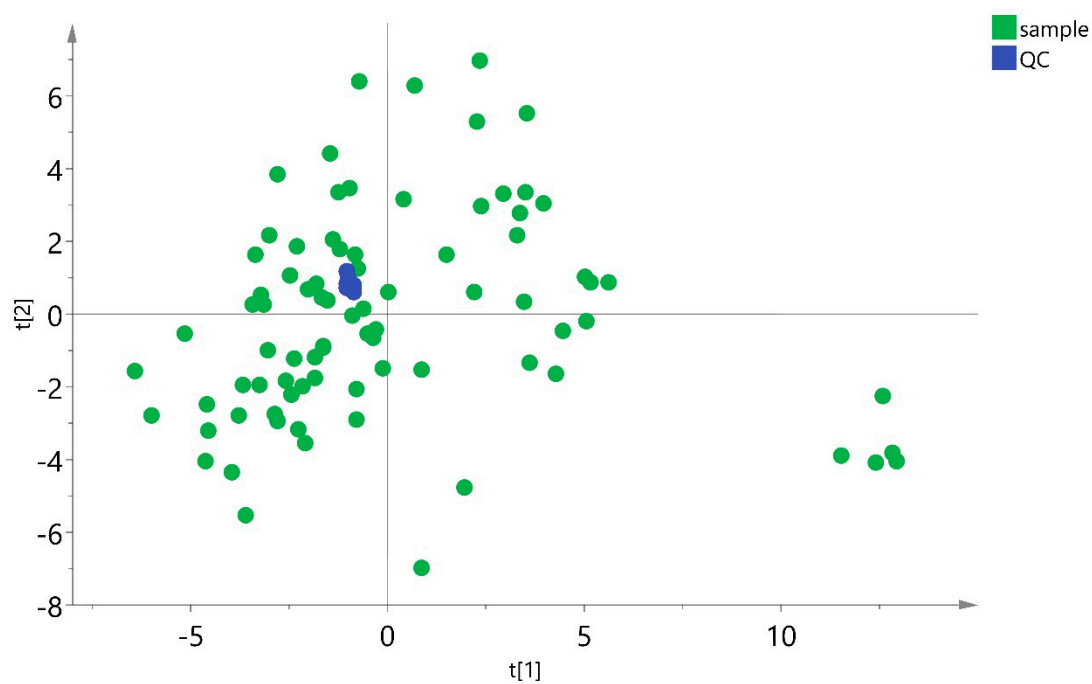
	Rate (°C/min)	Value (°C)	Hold Time (min)	Run Time (min)
(Initial)		50	0.00	0.00
Ramp 1	30	120	5.50	7.83
Ramp 2	30	140	3.00	11.50
Ramp 3	30	150	3.00	14.83
Ramp 4	30	280	2.00	21.17

Supporting Table S2. Selected ions used in SIM mode.

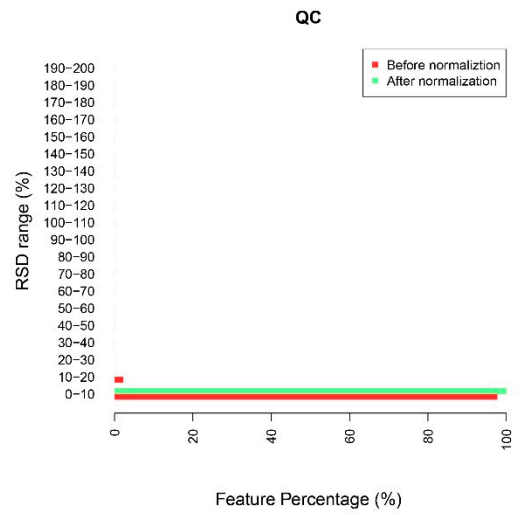
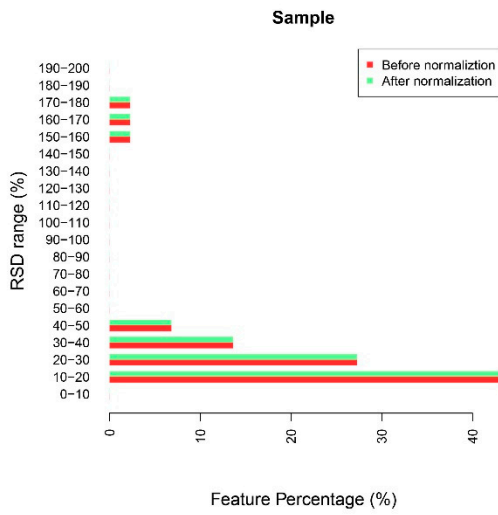
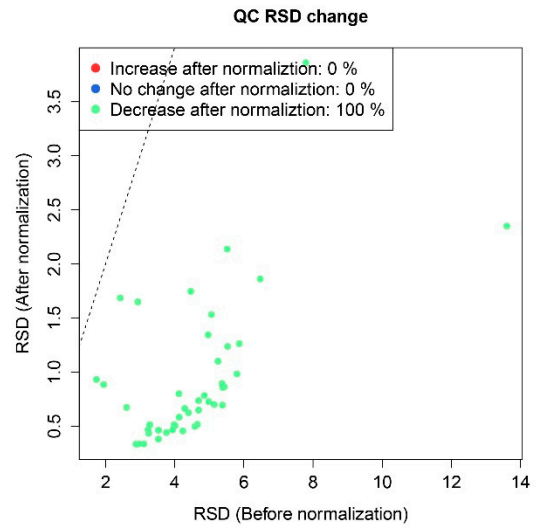
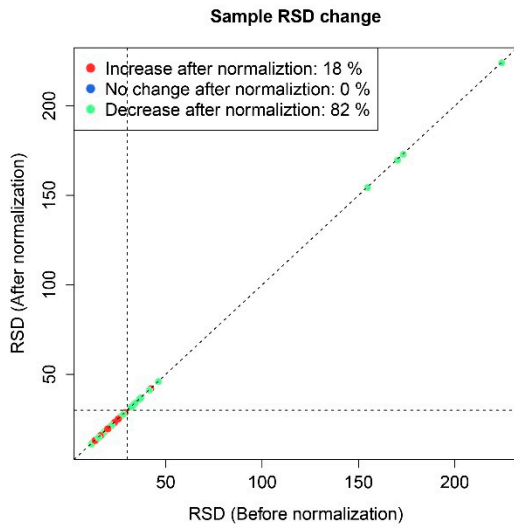
No.	Retention Time (min)	Selected Ions (m/z)					Time Segment
1	5.14	41	55	<u>69</u>			
2	5.86	91	92	<u>93</u>			
3	5.99	79	91	92	<u>93</u>	1	
4	6.42	43	79	91	<u>93</u>		
5	6.50	41	<u>69</u>	91	93		
6	6.65	<u>43</u>	56	84			
7	6.84	77	91	<u>93</u>	136		
8	7.01	93	<u>121</u>	136		2	
9	7.12	91	117	<u>119</u>	134		
10	7.32	<u>43</u>	81	108	154	3	
11	7.54	40	55	57	<u>70</u>	83	
12	7.68	91	<u>93</u>	121	136	4	
13	7.88	71	91	<u>93</u>	121		
14	8.27	91	93	121	<u>136</u>		
15	8.30	69	<u>71</u>	93		5	
16	8.80	91	93	<u>121</u>	136		
17	9.42	67	81	<u>91</u>	94	109	
18	9.67	<u>59</u>	81	93			
19	9.77	81	94	<u>109</u>		7	
20	9.91	<u>71</u>	93	111			
21	10.05	55	69	<u>83</u>			
22	10.15	<u>59</u>	93	136		8	
23	10.25	<u>43</u>	55	57			
24	10.76	83	<u>84</u>	91	119	134	
25	11.18	41	<u>69</u>	93	94		
26	11.39	41	<u>69</u>	93			
27	11.46	<u>91</u>	117	119		10	
28	11.63	41	43	<u>70</u>			
29	11.87	41	<u>69</u>	83			
30	12.63	<u>91</u>	117	119	148		
31	13.06	<u>91</u>	119	148		11	
32	13.55	79	91	<u>94</u>			
33	13.75		91	<u>117</u>	119	148	
34	14.02		115	117	<u>146</u>		

35	14.39	<u>91</u>	119	148		
36	14.59	91	117	119	<u>148</u>	
37	14.69	41	68	<u>69</u>	93	12
38	14.92	91	115	117	<u>145</u>	
39	15.09	<u>91</u>	115	117		13
40	15.37	<u>43</u>	54	55	67	96
41	16.36	91	105	133	134	<u>162</u>
42	16.54	43	55	57	<u>70</u>	83
43	17.74	41	<u>69</u>	81	93	
44	18.09	<u>43</u>	81	82		17
45	18.65	41	55	<u>70</u>	83	18

The underlined ions are quantifiers.



Supporting Figure S1. PCA score plot of samples and QC.



Supporting Figure S2. Change of RSD after SVR normalization.