

Table S1 the fragmentation of flavones in *Scutellaria baicalensis* extract by HPLC/LTQ-Orbitrap

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
1	4.60	[M+H] ⁺	305.0656	152.9, 195.0, 259.1, 286.9	152.9, 190.9, 219.1, 241.0, 259.0	132.9, 148.8, 164.9, 174.9, 189.1, 213.1, 231.0, 241.2
		[M-H] ⁻	303.0494	124.9, 216.9, 216.9, 259.1, 275.1, 285.1	56.9, 82.9	
2	4.96	[M+H] ⁺	449.1075	273.2, 287.1	107.0, 135.0, 152.9, 161.1, 177.0, 203.0, 219.1, 237.1, 245.1, 269.0, 287.1	96.9, 109.3, 111.0, 125.1
		[M-H] ⁻	447.0924	239.1, 271.2	157.1, 185.2, 197.0, 215.2, 225.2, 243.1, 253.3	
3	5.05	[M+H] ⁺	513.0687			
		[M-H] ⁻	511.0542	269.1, 431.2	165.0, 268.1, 269.1, 281.1, 311.0, 341.2	109.1, 138.1, 163.1, 165.9, 184.0, 196.0, 211.0, 223.1, 239.0, 240.0, 251.0
4	5.55	[M+H] ⁺	597.1811	339.0, 417.2, 441.2, 459.2, 477.2, 525.2, 543.2, 561.2, 579.1 209.1, 239.1, 269.1, 311.3, 329.2, 355.3,		
		[M-H] ⁻	595.1638	385.3, 415.3, 449.2, 457.2, 475.1, 487.2, 505.2, 559.4, 577.3	209.0, 239.0, 329.2, 355.2, 385.2, 439.3, 457.4	144.7, 181.0, 191.0, 209.0, 234.8
5	6.63	[M+H] ⁺	465.1028	168.9, 289.1, 429.1, 447.1	91.0, 107.0, 119.0, 146.9, 168.9, 189.0, 194.9, 201.0, 214.9, 229.2, 243.0, 247.2	84.8, 94.9, 112.9, 122.9, 140.9, 151.0
		[M-H] ⁻	463.0860	174.9, 193.0, 287.1	138.9, 152.9, 166.9, 181.0, 193.0, 201.1, 215.0, 243.1, 259.1, 269.2	108.9, 137.0, 152.9, 162.9
6	4.96	[M+H] ⁺	565.1529	379.3, 391.3, 409.4, 427.3, 445.2, 457.4, 475.4, 481.2, 499.2, 511.3, 529.2, 547.1	307.1, 325.2, 391.3, 409.2, 427.1, 445.1, 481.2, 493.2, 511.2	307.2, 349.2, 373.3, 379.2, 391.3, 409.2, 427.1, 433.3, 445.4, 463.2, 475.2, 493.3
		[M-H] ⁻	563.1370	353.2, 383.3, 425.2, 413.2, 425.3, 443.2, 455.3, 473.2, 485.3, 503.3, 527.4, 545.4	259.1, 297.2, 311.2, 325.3, 353.2, 383.3, 395.1, 413.2, 437.2, 425.2	233.1, 253.1, 297.2, 307.2, 325.2, 335.3
7	7.12	[M+H] ⁺	509.1282	347.1	161.0, 213.0, 314.1, 332.0	134.0, 161.0, 200.0, 242.0, 286.1
8	7.59	[M+H] ⁺	411.0376	331.2	263.1, 270.1, 287.2, 289.1, 298.0, 303.2, 316.2	181.0, 270.1, 287.1, 298.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
9	7.77	[M-H]-	409.0223	314.4, 329.2, 345.2	165.0, 180.0, 195.1, 261.1, 270.1, 299.2, 314.1	165.0, 180.0, 205.1, 245.3, 285.2, 299.0
		[M+H]+	565.1512	307.2, 325.3, 355.4, 379.3, 397.4, 409.4, 427.3, 445.2, 457.3, 469.4, 481.4, 499.4, 511.3, 529.2, 547.4	379.2, 397.3, 409.3, 427.3, 451.2, 457.3, 469.3, 481.2, 493.2, 499.1, 511.2, 529.2	337.3, 349.2, 391.3, 397.1, 409.3, 427.3, 439.3, 451.3, 481.2, 493.3, 499.3, 511.2
		[M-H]-	563.1397	353.2, 383.2, 413.2, 425.2, 443.3, 473.2, 485.2, 503.2, 515.3, 545.3	311.2, 323.2, 335.2, 353.2, 365.2, 383.1, 395.2, 407.2, 413.2, 425.3	191.1, 233.0, 265.1, 297.2, 307.1, 325.2
10	7.41	[M+H]+	567.1675	283.3, 322.5, 387.1, 411.1, 429.0, 435.7, 441.1, 447.2, 459.2, 483.3, 495.2, 501.4, 513.3, 531.2, 549.3	321.3, 363.4, 393.1, 411.2, 465.1, 495.2, 513.2, 531.2	393.2, 411.3, 441.2, 453.3, 465.4, 495.3, 513.3
		[M-H]-	565.1530	209.2, 239.1, 269.1, 299.1, 329.3, 355.1, 385.2, 415.2, 445.2, 475.1, 487.2, 505.3, 547.3	150.9, 167.1, 239.2, 367.2	81.1, 100.8, 122.9, 137.1, 153.0, 167.0, 179.0, 209.1, 221.2
		[M+H]+	579.1666	339.3, 393.3, 423.3, 441.3, 459.2, 483.3, 495.2, 507.3, 513.3, 525.3, 543.1, 561.1	363.3, 405.2, 423.2, 441.2, 465.3, 483.2, 495.2, 513.2, 525.3, 543.2	291.3, 309.3, 363.2, 393.3, 405.3, 423.3
12	9.06	[M-H]-	577.1524	267.3, 295.1, 337.2, 415.1, 439.2, 457.3, 487.2, 559.4	148.8, 191.1, 267.2, 295.1, 319.2, 337.2, 367.4, 429.2	163.1, 190.9, 281.1, 309.1
		[M+H]+	567.1675	411.2, 429.2, 441.2, 447.0, 453.2, 459.1, 465.2, 495.2, 513.2, 531.2, 549.2	393.2, 411.2, 429.3, 465.2, 495.1, 513.1, 531.2	393.2, 411.3, 441.2, 453.3, 465.4, 483.2, 495.3, 513.3
		[M-H]-	565.1531	209.1, 239.1, 269.2, 299.1, 299.1, 329.1, 355.2, 385.2, 415.3, 419.2, 427.3, 445.3, 475.2, 547.3	167.1, 178.9, 209.0, 221.0, 239.0, 265.1, 313.3, 357.2, 367.1	106.7, 122.6, 153.1, 167.0, 179.2, 195.1, 209.1, 221.0
13	10.72	[M+H]+	549.1584	291.3, 309.3, 363.5, 393.2, 411.1, 429.2, 459.4, 465.2, 483.2, 495.2, 513.2, 531.2	279.2, 291.1, 309.2, 321.3, 333.2, 363.1, 375.2, 393.2	279.2, 291.2, 309.2, 321.2, 357.2, 375.2
		[M-H]-	547.1412	337.1, 367.2, 379.2, 409.3, 427.3, 457.2, 487.2, 499.4, 511.3, 529.4	281.1, 309.2, 337.1, 367.3, 397.5	281.3, 309.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
14	10.11	[M-H]-	511.0543	225.2, 241.1, 269.1, 349.2, 431.2	153.1, 169.0, 171.0, 197.1, 213.0, 225.2, 241.1	153.1, 169.1, 181.1, 197.1, 207.1, 213.1, 215.1, 225.1
15	10.86	[M+H]+	509.1297	332.1, 347.1, 413.2, 443.2, 473.2, 491.1	142.1, 169.1, 183.0, 249.0, 314.1, 332.0	142.0, 168.9, 286.0, 314.1
		[M-H]-	507.1115	269.2, 315.1, 330.2, 345.1	192.1, 207.2, 223.1, 251.1, 281.3, 300.3, 330.1	162.9, 165.0, 166.1, 180.5, 191.1, 206.0, 242.0, 284.2, 287.2, 298.2, 312.2, 315.1
16	11.55	[M+H]+	549.1572	363.3, 375.4, 393.4, 411.3, 429.3, 441.3, 459.3, 465.3, 483.3, 495.3, 513.2, 531.1	279.1, 309.1, 321.2, 333.2, 363.1, 375.2, 393.1	279.2, 309.1, 321.3, 331.3, 347.2, 357.2, 375.1
		[M-H]-	547.1435	319.2, 337.2, 349.3, 367.2, 409.2, 427.3, 457.2, 487.3, 499.3, 517.4, 529.3	281.2, 309.0, 337.1, 367.3, 397.4	281.0, 309.1
17	11.61	[M+H]+	625.1744	286.1, 301.1, 463.3	105.0, 153.1, 181.0, 199.1, 255.1, 283.1, 286.1	105.0, 116.0, 128.0, 138.0, 155.9, 172.0, 183.9, 201.9, 212.0, 240.0
18	11.75	[M+H]+	595.1660	271.1, 433.1	122.9, 140.9, 169.0, 197.0, 225.1, 253.0, 271.2	122.9, 168.9, 197.1, 211.1, 225.1, 229.0
		[M-H]-	593.1523	No fragmentation		
19	11.77	[M+H]+	287.0553	97.0, 107.0, 135.0, 137.0, 152.9, 201.0, 219.0, 251.0, 245.0, 259.0, 269.1	66.8, 96.9, 110.9, 125.0, 135.0	
		[M-H]-	285.0390	132.9, 150.9, 199.0, 217.1, 241.1, 267.1	132.9, 145.1, 169.1, 172.9, 199.1, 213.0, 223.0	115.0, 142.9, 157.0, 171.0
20	11.95	[M+H]+	435.1288	279.2, 297.1, 315.1, 321.2, 339.3, 351.2, 363.2, 369.0, 381.1, 391.0, 399.2, 417.2	219.1, 255.2, 267.1, 279.1, 297.1, 321.3, 339.2, 351.2, 363.1, 381.2, 399.2	177.0, 194.9, 211.1, 219.1, 226.9, 240.1, 251.1, 268.1, 279.1
		[M-H]-	433.1138	167.0, 197.1, 269.1, 287.1, 313.1, 343.2, 397.2, 415.2	123.1, 139.1, 167.0	80.9, 949., 122.9, 125.0
21	12.11	[M+H]+	493.1339	331.2	137.1, 182.0, 197.0, 270.2, 287.1, 298.2, 316.0	135.0, 153.0, 181.0, 270.1, 287.2, 298.1
		[M-H]-	491.1169	329.2	118.9, 133.0, 143.3, 152.1, 164.9, 180.0, 195.0, 261.1, 270.3, 282.1, 285.3, 296.1, 299.0, 314.0	152.1, 165.0, 180.1, 205.1, 245.1, 268.2, 285.2, 299.1
22	12.19	[M+H]+	549.1586	363.4, 381.3, 399.3, 411.3, 429.2, 441.3, 453.1, 465.3, 483.2, 495.3, 513.2, 531.1	363.2, 381.3, 393.2, 399.1, 423.2, 435.1, 441.1, 453.2, 465.2, 477.3, 483.2, 495.1, 513.1	381.1, 423.3, 435.4, 447.3, 465.2, 477.2, 495.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
23	12.48	[M-H]-	547.1414	367.3, 379.3, 397.3, 427.3, 439.2, 457.3, 469.3, 487.4, 499.3, 511.3, 529.2	281.2, 309.3, 337.1, 367.2	281.16348, 309.2
		[M+H] ⁺	411.0374	No fragmentation		
		[M-H]-	409.0229	289.1, 327.1, 329.1, 345.1	180.0, 200.0, 253.2, 270.2, 299.2, 314.2	153.0, 179.9, 255.1, 285.1, 296.2, 299.2
24	10.51	[M+H] ⁺	579.1696	399.36877, 423.3, 441.2, 459.3, 465.3, 495.2, 513.2, 525.3, 543.4, 561.1	339.2, 405.3, 423.2, 441.2, 459.2, 495.2, 507.3, 525.2	321.3, 393.1, 405.1, 441.1, 459.2, 471.3, 477.2, 489.2, 507.2
		[M-H]-	577.1589	267.0, 295.1, 337.2, 367.3, 397.2, 439.2, 457.3, 487.3, 517.3, 529.4, 541.2, 559.2	339.2, 367.2, 397.3, 427.2, 469.3	190.9, 235.1, 296.2, 311.2, 324.2, 339.2
25	12.77	[M+H] ⁺	549.1574	363.4, 381.4, 393.4, 411.4, 429.3, 441.3, 453.3, 465.3, 483.3, 495.3, 513.2, 531.2, 309.1, 319.3, 337.2, 349.1, 367.2, 379.2,	363.3, 381.3, 393.2, 405.3, 417.3, 423.3, 435.3, 441.3, 453.3, 465.2, 477.3, 483.1, 495.2	351.3, 381.1, 393.2, 399.2, 465.1
		[M-H]-	547.1435	397.3, 427.2, 439.2, 457.2, 469.2, 487.4, 499.3, 511.3, 529.3	191.1, 221.0, 245.1, 309.3, 337.2, 349.3, 367.1, 391.2, 409.3	163.2, 191.0, 281.2, 309.2
26	12.85	[M+H] ⁺	421.1497	259.2, 293.2, 301.2, 325.2, 337.3, 355.1, 367.1, 385.1, 403.1	235.1, 259.1, 283.3, 325.1, 337.1, 355.2, 367.2, 385.2	104.9, 132.9, 165.0, 193.0, 279.2, 297.3, 307.1
		[M-H]-	419.1336			
26	12.85	[M+H] ⁺	583.1989	301.3, 325.3, 337.3, 367.2, 403.2, 421.1, 445.1, 469.4, 511.2, 529.0, 547.3, 565.4	258.9, 301.2, 325.2, 367.1, 385.3, 403.1	
		[M-H]-	581.1841	299.3, 329.1, 461.2, 491.2, 563.4, 563.4	167.1, 191.0, 299.1, 323.1, 341.1, 353.4	124.9, 167.0, 215.2, 229.2, 255.1, 271.2
27	12.88	[M+H] ⁺	317.0654	137.1, 167.9, 183.0, 302.1	111.9, 140.0, 161.0, 167.9, 185.8, 228.0, 242.0, 256.1, 274.1, 283.9	111.9, 139.9
		[M-H]-	315.0494	151.1, 175.1, 228.0, 243.1, 283.1, 287.2, 300.1	109.9, 137.9, 139.0, 165.9, 167.0, 186.0, 191.0, 216.1, 228.2, 238.2, 244.1, 255.1, 272.0	109.9, 137.9
28	13.00	[M+H] ⁺	579.1697	208.5, 255.3, 267.2, 297.2, 321.2, 351.0, 363.2, 381.2, 399.3, 417.2, 459.2, 513.1,	267.1, 297.1, 321.1, 351.2, 363.2, 381.1, 399.2	267.2, 321.2, 351.1, 363.1, 381.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
				525.2, 543.1, 561.2		
29	13.04	[M+H] ⁺	563.1757	339.4, 363.4, 389.4, 407.3, 425.2, 441.3, 459.2, 465.3, 483.3, 509.2, 527.1, 545.2	321.2, 363.4, 389.3, 407.1, 511.3, 431.3, 443.3, 465.4, 483.3, 491.2, 509.2	291.2, 333.2, 359.3, 371.3, 377.3, 389.3, 411.2, 431.2, 443.3, 455.4, 461.3, 465.3, 476.3, 491.2
		[M-H] ⁻	561.1626	337.2, 349.2, 367.3, 379.3, 397.3, 441.3, 457.3, 471.2, 487.3, 499.3, 517.3, 525.4, 543.3	281.3, 295.1, 309.2, 337.2, 349.3, 367.3	281.1, 309.1
30	13.04	[M+H] ⁺	289.0710	121.0, 147.0, 169.0, 188.9, 194.9, 271.0	84.8, 94.8, 112.9, 122.7, 140.9, 150.9	94.9
		[M-H] ⁻	287.0546	119.0, 139.0, 152.9, 166.9, 181.0, 193.0, 201.0, 215.0, 243.0, 259.1, 269.1	108.9, 124.9, 136.9, 152.9, 163.0	80.9, 82.9, 108.9, 110.9, 136.9
31	13.14	[M+H] ⁺	623.1590	285.0, 461.2	285.1	270.1
		[M-H] ⁻	621.1425	268.1, 283.1, 430.3, 445.2	268.0, 283.0, 430.2	165.9, 184.2, 195.1, 210.9, 223.00, 239.0
32	13.28	[M+H] ⁺	417.1181	267.2, 279.1, 297.2, 321.3, 351.2, 363.2, 381.2, 399.2	267.3, 279.1, 297.0, 321.1, 339.1, 351.1, 363.1, 381.2	219.1, 293.2
		[M-H] ⁻	415.1013	267.3, 295.1, 307.4, 325.2, 337.3	149.0, 187.1, 227.1, 251.2, 267.1	120.9, 144.9, 165.0, 180.0, 194.9, 199.1, 223.1
33	13.57	[M+H] ⁺	289.0707	152.9, 243.1, 271.1	149.1, 153.0, 159.0, 215.1, 243.0	133.0, 148.9, 215.1, 225.2
		[M-H] ⁻	287.0559	124.9, 161.1, 227.1, 269.2	569.9, 82.9, 125.0	
34	13.61	[M+H] ⁺	351.0176	No fragmentation		
		[M-H] ⁻	349.0014	269.1	169.1, 171.0, 181.1, 183.1, 197.1, 213.0, 225.0, 241.0, 251.2	152.8, 169.1, 181.0, 197.1, 207.1, 215.1, 225.1
35	13.71	[M+H] ⁺	347.0739	161.1, 213.1, 242.2, 286.4, 314.2, 317.2, 332.2	134.1, 161.0, 198.0, 200.0, 214.1, 242.0, 258.2, 286.1	168.1, 172.1, 185.1, 186.1, 196.1, 199.2, 200.0, 213.0, 214.0, 224.1, 225.1, 227.2
		[M-H] ⁻	345.0622	149.0, 161.1, 187.0, 226.1, 254.1, 271.2, 286.1, 301.1, 315.2, 330.1	153.0, 168.0, 181.0, 196.0, 243.1, 259.2, 271.2, 287.1, 321.1, 315.0	181.0, 199.1, 215.1, 231.2, 243.2, 271.2, 287.2, 297.0

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
36	13.75	[M+H] ⁺	477.1028	301.1	255.2, 269.3, 283.3, 286.1	120.9, 140.0, 168.0, 185.9, 212.1, 240.2, 258.0, 268.1, 285.1
		[M-H] ⁻	475.0875	299.1	284.1	136.8, 166.1, 200.1, 212.0, 227.1, 239.1, 255.0, 256.3, 266.3
37	13.79	[M+H] ⁺	365.0330	No fragmentaion		
		[M-H] ⁻	363.0176	283.0	239.2, 268.1	163.0, 184.1, 196.1, 198.0, 211.1, 212.1, 223.0, 224.2, 239.1, 240.1
38	13.82	[M+H] ⁺	523.1440	361.2	134.1, 161.0, 194.2, 197.1, 212.2, 227.1, 300.2, 313.2, 328.2, 331.2, 346.1	133.9, 161.1, 254.2, 282.2, 300.2, 313.0, 328.1, 331.1
		[M-H] ⁻	521.1274	359.2	133.0, 153.1, 177.0, 194.9, 209.9, 224.9, 234.9, 285.1, 285.1, 329.2, 344.1	195.1, 210.1, 367.1, 329.0
39	13.84	[M+H] ⁺	579.1699	411.3, 417.4, 423.4, 429.2, 441.3, 453.4, 459.3, 471.3, 483.3, 495.4, 513.3, 525.3, 543.3, 561.2	393.4, 411.3, 429.3, 453.3, 465.2, 471.2, 483.2, 495.2, 507.3, 513.1, 525.2, 543.2	309.2, 339.3, 381.3, 393.2, 411.3, 429.2, 495.2
40	13.84	[M+H] ⁺	401.1592	319.1, 323.2, 331.4, 351.2, 369.3, 383.2	229.1, 263.1, 291.2, 319.3, 323.1, 351.2, 368.2	245.1, 263.1, 291.1, 319.1, 323.2, 336.2
41	13.89	[M+H] ⁺	303.0863	167.1, 229.2, 257.1, 285.1	122.9, 167.1, 229.1, 257.1	122.9, 133.0, 229.0
		[M-H] ⁻	301.0706	106.9, 123.9, 132.9, 139.0, 141.0, 160.9, 165.0, 193.0, 225.1, 269.1, 273.1, 283.1	132.9, 161.1	121.2, 133.2
42	13.89	[M+H] ⁺	609.1798	271.1, 285.1	270.0	139.1, 143.9, 155.0, 157.9, 167.9, 178.9, 195.9, 218.1, 224.0, 241.1, 242.1, 252.1
		[M-H] ⁻	607.1977	No fragmentation		
43	14.03	[M+H] ⁺	317.0653	152.9, 177.0, 194.1, 215.1, 219.1, 285.2, 288.2, 302.1	152.9, 176.9, 193.9, 219.1, 245.09357, 260.1, 274.1, 283.9, 285.2	176.0, 193.9
		[M-H] ⁻	315.0492	150.9, 175.9, 217.0, 229.0, 247.1, 256.1, 283.2, 287.2, 300.0	147.9, 150.9, 163.9, 175.9, 190.0, 214.1, 227.1, 244.1, 256.1, 271.2	

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
44	14.05	[M+H] ⁺	477.1031	286.2, 301.1	121.0, 137.0, 165.1, 183.1, 241.30823, 255.2, 269.2, 283.2, 286.0	90.9, 118.9, 139.9, 167.9, 185.8, 240.1, 258.3
		[M-H] ⁻	475.0862	175.0, 284.1, 299.1	108.7, 137.0, 161.1, 187.1, 211.0, 237.2, 255.2, 284.1	110.0, 137.9, 165.8, 200.1, 212.1, 227.2, 240.1, 256.2, 267.0
45	14.25	[M+H] ⁺	289.0710	153.0, 169.1, 243.0, 271.0	66.8, 96.8, 124.9, 152.9	
		[M-H] ⁻	287.0548	124.9, 161.0, 227.0, 243.0, 269.2	56.9, 82.9	
46	14.23	[M-H] ⁻	351.0176	271.0	135.9, 152.0, 157.1, 166.9, 185.0, 199.1, 227.2, 243.2, 253.1	110.8, 123.8, 136.9, 151.9, 173.0, 201.1, 225.1
47	14.34	[M+H] ⁺	463.1240	287.3, 301.1	105.0, 181.2, 199.1, 255.2, 286.1	105.0, 116.0, 138.0, 156.0, 172.1, 184.0, 202.0, 212.0, 240.0, 258.2
		[M-H] ⁻	461.1090	285.1, 299.1	284.1	109.8, 137.9, 165.9, 200.2, 212.1, 214.1, 228.1, 240.3, 256.1, 267.2
48	14.76	[M+H] ⁺	347.0755	142.0, 169.1, 183.1, 249.3, 286.1, 314.1, 332.1	142.0, 168.9, 286.1, 314.1	137.0, 150.0, 165.0, 194.0, 216.1, 242.2, 258.1, 286.2
		[M-H] ⁻	345.0591	165.1, 207.1, 315.2, 330.1	140.0, 165.0, 178.9, 242.1, 270.1, 298.2, 315.2	138.9, 149.1, 164.8, 179.0, 191.0, 215.1, 233.1, 243.1, 271.1, 287.0, 296.9
49	14.53	[M-H] ⁻	349.0007	269.1	141.1, 169.2, 195.0, 197.2, 213.2, 223.0, 225.1, 241.0, 251.0	167.1, 195.0, 213.2, 223.0
50	14.97	[M+H] ⁺	287.0553	90.9, 118.9, 168.9, 213.1, 241.0, 245.1, 269.1, 287.1	118.9, 122.9, 150.9, 213.1, 241.1, 245.1	90.9
		[M-H] ⁻	285.0392	118.9, 136.9, 165.0, 167.1, 185.1, 213.1, 223.0, 239.1, 267.0	167.1, 195.1, 211.1, 223.1, 239.1	167.1, 183.1, 195.1
51	14.96	[M-H] ⁻	349.0023	269.1	169.1, 171.1, 173.1, 181.1, 183.1, 197.2, 213.2, 225.1, 241.2, 251.0, 269.2	169.1, 181.0, 197.0, 215.1, 225.0
52	15.04	[M+H] ⁺	463.1239	301.2	286.1	118.9, 140.1, 168.0, 186.0, 240.1, 258.2

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
		[M-H]-	461.1089	299.1	284.0	109.9, 138.0, 166.0, 186.9, 200.0, 212.0, 214.0, 227.3, 256.1, 267.1
53	15.07	[M+H]+	317.0646	120.9, 139.0, 167.2, 179.1, 215.1, 234.1, 261.1, 271.1, 274.1, 289.1, 299.2, 302.0	120.8, 153.0, 184.0, 202.1, 228.1, 245.1, 256.1, 274.1, 285.1	153.0, 190.1, 218.1, 229.1, 246.1, 256.0
		[M-H]-	315.0504	No fragmentation		
54	15.26	[M+H]+	289.0708	152.9, 169.0, 243.2, 271.0, 288.2	153.0, 215.1, 225.2, 243.2, 253.1	133.0, 148.9, 215.1, 225.2
		[M-H]-	287.0547	124.9, 160.9, 201.2, 243.1, 259.1, 269.1	56.9, 80.8, 82.9	
55	15.39	[M+H]+	563.1741	379.2, 411.4, 425.4, 441.2, 449.3, 467.2, 479.2, 4975.3, 509.3, 527.2, 545.1	363.3, 393.3, 423.2, 441.2, 449.2, 467.2, 479.3, 491.2, 497.2, 509.3, 527.2	309.1, 321.2, 363.2, 393.0, 405.4, 423.2
		[M-H]-	561.1618	337.1, 349.3, 367.2, 379.3, 423.2, 441.3, 457.2, 471.2, 483.3, 501.3, 513.4, 543.3	281.3, 309.3, 337.2, 349.3, 367.2, 379.1, 409.4, 423.4	191.2, 281.1, 309.2
56	15.51	[M+H]+	287.0548	107.0, 137.0, 152.8, 169.0, 183.0, 203.0, 241.1, 269.1, 271.1, 287.1	66.9, 969.9, 124.9, 153.0	
		[M-H]-	285.0400	No fragmentation		
57	15.55	[M-H]-	351.0178	271.0	152.1, 167.0, 185.0, 199.1, 227.1, 243.0, 253.1	124.0, 137.0, 152.0, 173.1, 201.1, 225.1
58	15.86	[M+H]+	447.0916	271.0	102.9, 122.8, 168.9, 224.9, 253.1	103.0, 122.9, 150.9, 169.0, 197.1, 211.1, 225.0
		[M-H]-	445.0749	269.0	169.1, 197.1, 213.1, 223.0, 241.1, 251.1	151.1, 166.7, 195.1, 213.2, 223.1
59	16.04	[M+H]+	507.1121	331.2	180.1, 198.1, 213.2, 301.2, 316.2	180.1, 197.9, 214.1
		[M-H]-	505.0982	329.1	314.1	167.9, 227.0, 240.1, 271.1, 285.0, 299.1
60	15.86	[M-H]-	349.0024	269.1	141.0, 169.1, 197.0, 223.1, 225.1, 241.1, 251.1	167.1, 195.0, 213.2, 223.0
61	16.18	[M+H]+	317.0647	137.0, 168.0, 183.1, 215.1, 243.1, 271.3, 283.2, 302.1	112.0, 140.0, 168.0, 186.0, 228.1, 256.0, 274.2, 284.0	83.9, 111.9, 139.8
		[M-H]-	315.0508	136.9, 177.1, 243.2, 287.1, 300.0	109.9, 123.8, 137.0, 139.0, 166.0, 179.0, 210.1, 228.0, 238.1, 256.2	154.9, 184.0, 212.1, 228.2

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
62	16.21	[M+H] ⁺	395.0426	No fragmentation		
		[M-H] ⁻	393.0280	298.1, 313.1	152.1, 167.1, 239.3, 254.2, 269.2, 283.3, 298.2	211.1, 255.0, 269.2, 280.1, 283.0
63	16.33	[M-H] ⁻	349.0013	269.1	169.1, 171.1, 197.1, 213.0, 223.1, 241.2, 251.0	194.9, 213.1, 223.0
64	16.57	[M+H] ⁺	507.1115	331.1	180.1, 198.2, 213.2, 298.2, 301.2, 316.2	180.1, 198.0, 298.2, 301.1
		[M-H] ⁻	505.0975	315.1, 329.2	161.1, 196.0, 258.2, 296.2, 314.1	167.9, 196.0, 227.0, 268.0, 299.0
65	16.59	[M+H] ⁺	449.1083	273.1, 431.2	102.9, 131.0, 169.0, 172.9, 255.0	84.9, 94.9, 112.9, 122.9, 141.8, 150.9
		[M-H] ⁻	447.0905	175.0, 271.1	167.0, 185.0, 199.1, 209.0, 227.1, 243.1, 253.0	110.9, 123.9, 137.0, 151.9, 173.0, 201.1, 201.1, 215.1, 225.0
66	16.64	[M+H] ⁺	273.0758	103.1, 131.1, 169.0, 173.1, 187.0, 227.1, 231.1 255.1	84.9, 94.9, 112.9, 122.9, 140.9, 150.9	112.9, 122.9
67	16.76	[M+H] ⁺	493.1334	331.1	118.0, 121.0, 180.0, 195.2, 198.0, 213.2, 298.2, 301.2, 316.1	298.2, 301.1
		[M-H] ⁻	491.1187	269.3, 314.2, 329.1	122.6, 161.2, 196.0, 257.5, 269.2, 296.0, 299.1, 314.1	139.0, 167.9, 196.0, 240.0, 296.1, 299.1
68	16.79	[M+H] ⁺	433.1129	271.1	102.9, 122.9, 169.0, 197.1, 225.0, 253.1	102.8, 122.8, 140.9, 151.1, 169.0, 197.0, 225.0
		[M-H] ⁻	431.0962	269.0	141.0, 169.0, 197.0, 213.2, 223.0, 241.1, 251.0	167.1, 195.2, 207.1, 213.1, 222.9, 239.1
69	16.84	[M+H] ⁺	417.1184	297.2, 321.2, 351.1, 363.1, 381.1, 399.2	267.1, 321.1, 351.1, 363.2, 381.2	265.1, 293.1
		[M-H] ⁻	415.1012	267.3, 295.2, 325.1, 337.2, 397.2	149.1, 185.1, 223.1, 267.2, 277.1	120.9, 145.1, 167.1, 181.1, 195.1, 211.1, 223.1, 239.1
70	16.88	[M+H] ⁺	477.1025	301.1	140.0, 168.0, 186.0, 258.0, 268.2	
		[M-H] ⁻	475.0873	299.1	255.1, 284.2	109.8, 138.0, 166.0, 200.1, 212.0, 214.1, 228.0, 240.0, 256.1, 267.1
71	16.91	[M+H] ⁺	395.0422	No fragmentation		
		[M-H] ⁻	393.0259	298.3, 313.2	152.1, 180.0, 269.3, 283.2, 298.2	152.1, 152.1, 179.9

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
72	17.04	[M+H] ⁺	463.1238	301.1	183.2, 241.3, 255.2, 269.3, 283.3, 286.1	90.9, 112.0, 118.9, 140.0, 168.0, 185.9, 239.9, 244.0, 258.1, 267.9
		[M-H] ⁻	461.1085	299.1	213.2, 255.3, 284.1	110.0, 138.0, 165.9, 200.1, 212.1, 227.0, 240.19794, 256.1, 267.1
73	17.01	[M-H] ⁻	363.0185	283.0	268.1	163.0, 165.9, 184.0, 196.1, 198.1, 211.2, 223.1, 224.1, 239.1, 240.1
74	17.26	[M+H] ⁺	447.0924	271.1	105.0, 123.0, 129.0, 141.0, 151.0, 168.9, 201.1, 225.1, 253.1, 271.0	70.9, 84.8, 95.0, 112.9, 123.0, 140.9, 151.0
		[M-H] ⁻	445.0770	175.0, 269.0	151.0, 153.0, 155.1, 157.0, 169.1, 171.2, 181.1, 197.0, 213.0, 225.0, 241.0, 251.2	155.1, 169.0, 171.0, 181.1, 197.1
75	17.64	[M+H] ⁺	273.0759	103.0, 131.0, 168.9, 173.0, 185.0, 186.9, 195.0, 227.1, 231.0, 255.1, 272.1	70.9, 94.8, 112.8, 122.9, 140.9, 150.9, 168.9	
76	17.91	[M+H] ⁺	447.0927	271.1, 285.0	102.9, 104.9, 122.8, 168.9, 173.0, 201.1, 225.0, 253.0, 253.0	85.0, 112.9, 122.9, 141.0, 150.9, 169.1
		[M-H] ⁻	445.0751	175.1, 197.1, 225.1, 269.1	171.1, 181.1, 197.0, 213.15509, 225.1, 241.0	141.2, 155.1, 169.1, 181.1, 197.0, 215.2
77	17.93	[M+H] ⁺	287.0914	147.2, 166.9, 183.0, 193.0, 245.1, 269.0	97.9, 110.9, 125.0, 137.0, 138.9, 151.9, 167.0	123.9
		[M-H] ⁻	285.0761	124.0, 139.0, 209.0, 241.2, 269.1	110.9, 123.8	95.9
78	18.07	[M+H] ⁺	477.1027	286.2, 301.2	104.9, 127.2, 181.1, 199.1, 255.1, 283.2, 286.1	104.9, 138.0, 156.0, 172.0, 183.9, 201.9, 211.9, 240.0, 259.0
		[M-H] ⁻	475.0845	175.0, 284.2, 299.1	125.0, 153.1, 167.1, 183.1, 211.1, 227.1, 267.2, 284.0	171.0, 181.9, 184.1, 200.0, 212.1, 228.0, 239.2, 256.1, 265.1
79	18.25	[M+H] ⁺	653.2422			
		[M-H] ⁻	651.2243	193.1, 265.2, 337.2, 337.2, 457.3, 475.3	134.8, 161.0, 311.2, 329.3	
80	18.40	[M+H] ⁺	315.0848	104.9, 127.1, 147.1, 167.1, 169.2, 186.2, 195.1, 198.1, 213.2, 254.1, 269.3, 282.2,	197.2, 198.3, 226.3, 254.2, 270.2, 282.1, 285.1	105.0, 129.0, 142.1, 152.1, 169.1, 170.1, 180.1, 198.1, 226.1, 254.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
				285.1, 300.1		
81	18.46	[M+H] ⁺	431.0974	255.1	128.9, 153.0, 171.0, 187.1, 209.1, 231.1, 255.1	66.8, 110.9, 125.1, 142.9
		[M-H] ⁻	429.0797	174.9, 253.1	106.9, 143.1, 150.9, 165.1, 181.2, 209.2, 253.1	139.2, 165.0, 180.0
82	18.46	[M+H] ⁺	301.0703	121.1, 133.1, 139.1, 167.1, 179.1, 199.1, 227.1, 245.2, 255.0, 269.2, 286.0	199.1, 227.1	171.1, 184.0, 199.1, 212.0
		[M-H] ⁻	299.0549	139.0, 165.0, 197.0, 212.1, 227.2, 256.0, 267.1, 271.0, 284.1	157.0, 212.0	167.0, 184.0
83	18.75	[M+H] ⁺	461.1079	270.2, 285.0, 443.2	105.1, 121.5, 137.1, 165.2, 183.2, 197.3, 211.3, 225.0, 239.0, 253.1, 270.1	104.9, 139.9, 167.9, 185.8, 195.9, 213.1, 224.0, 242.0, 252.0
		[M-H] ⁻	459.0904	175.0, 268.1, 283.1	239.2, 268.1	109.9, 137.9, 162.9, 166.1, 184.2, 196.1, 212.0, 223.0, 239.1
84	18.95	[M+H] ⁺	543.1485	No fragmentation		
		[M-H] ⁻	541.1348	295.2, 335.1, 351.3, 377.3, 415.3, 421.3, 441.2, 455.2, 471.2, 497.2, 513.3, 523.3	177.0, 295.2, 323.2, 351.1, 443.2	323.1
85	18.95	[M+H] ⁺	417.1180	255.1	104.8, 129.0, 152.9, 171.0, 187.0, 209.2, 213.1, 227.1, 231.1, 255.1	66.9, 125.0, 152.7
		[M-H] ⁻	415.1028	253.1	143.1, 150.9, 164.9, 181.0, 185.0, 208.9, 255.0	153.0, 165.0, 180.1
86	19.01	[M+H] ⁺	331.0798	182.2, 197.0, 270.2, 287.2, 298.2, 316.2	181.0, 270.1, 287.2, 298.2	270.2, 295.2
		[M-H] ⁻	329.0644	133.1, 165.1, 180.1, 195.1, 299.1, 314.1	133.0, 151.9, 165.1, 179.9, 205.1, 245.14365, 285.1, 299.1	136.9, 164.9, 185.1, 227.1, 255.0, 271.1
87	19.09	[M+H] ⁺	477.1029	286.1, 301.1	105.0, 153.1, 181.1, 199.1, 255.2, 286.1	105.0, 137.9, 155.8, 172.1, 184.0, 201.9, 212.1, 240.0, 258.1
		[M-H] ⁻	475.0857	284.2, 299.2	125.0, 153.0, 201.0, 227.2, 256.1, 284.0	171.0, 184.1, 200.0, 212.0, 228.1, 239.1, 255.1, 265.1
88	19.19	[M+H] ⁺	463.1241	301.1	104.9, 181.1, 199.1, 215.0, 283.2, 286.1	105.0, 116.0, 138.1, 156.0, 171.1, 184.0,

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
						202.0, 212.0, 240.1, 257.1
		[M-H]-	461.1085	253.2, 283.1, 299.2	125.1, 153.1, 194.8, 211.0, 225.0, 284.1	153.9, 171.0, 184.1, 200.0, 212.2, 228.0, 239.1, 256.0, 256.0
89	19.38	[M+H]+	287.0553	97.0, 107.0, 136.9, 152.8, 201.1, 202.9, 219.1, 241.1, 245.1, 259.1, 269.1	66.9, 96.8, 124.9, 153.0	
		[M-H]-	285.0390	150.9, 185.1, 199.1, 217.0, 241.0, 267.1	132.9, 169.2, 184.9, 196.9, 199.1, 212.9	142.9, 156.9, 185.0
90	19.46	[M+H]+	433.1133	271.1	102.9, 122.8, 169.1, 197.1, 225.1, 253.0, 271.1	94.9, 102.9, 122.9, 151.0, 169.0, 197.0, 211.1, 225.1, 228.9
		[M-H]-	431.0976	269.1	141.0, 141.0, 169.1, 197.0, 223.1, 241.1, 251.1	195.1, 213.2, 223.0
91	19.59	[M+H]+	447.0933	271.1	103.0, 122.8, 150.8, 169.0, 197.1, 225.0, 253.1, 271.0	102.9, 122.9, 141.0, 150.9, 169.0, 197.1, 211.1, 225.1, 228.9
		[M-H]-	445.0769	175.0, 269.1	137.0, 153.0, 165.0, 169.1, 181.1, 195.1, 197.1, 213.1, 223.0, 241.0, 251.1	150.9, 167.1, 179.1, 195.2, 207.3, 213.2, 223.1
92	19.98	[M+H]+	461.1081	270.1, 285.1	105.0, 165.1, 225.1, 239.3, 254.1, 270.2	116.0, 131.0, 144.0, 168.0, 179.1, 213.0, 242.2, 252.1
		[M-H]-	459.0905	175.1, 268.2, 283.2	108.9, 137.1, 268.0	163.1, 183.9, 196.1, 212.1, 224.0, 238.0
93	20.06	[M+H]+	463.1238	287.2	272.1	169.9, 226.1, 243.1, 254.1
		[M-H]-	461.1053	174.9, 270.1, 285.0	137.9, 165.9, 178.9, 270.1	109.8, 137.8, 165.9, 178.9, 214.1, 242.1
94	20.22	[M+H]+	475.1230	285.1	239.2, 267.3, 270.1	105.0, 139.9, 167.9, 185.9, 196.0, 224.0, 242.1, 251.9, 270.1
		[M-H]-	473.1079	269.1, 283.2	239.2, 268.0	162.9, 166.1, 184.0, 191.1, 194.9, 196.1, 198.2, 211.0, 212.2, 223.0, 224.0, 239.1, 240.1
95	20.31	[M+H]+	273.0755	No fragmentation		
		[M-H]-	271.0607	106.9, 124.9, 141.0, 151.0, 164.9, 185.1,	135.0, 148.0, 157.1, 164.9, 181.0, 185.2, 197.1,	150.9, 169.1, 178.9, 197.0

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
96	20.39	[M+H] ⁺	303.0861	197.0, 215.1, 225.1, 242.9, 253.1	209.0, 225.2	
		[M-H] ⁻	301.0712	119.0, 165.9, 181.0, 195.0, 207.1, 228.1, 286.1	109.9, 138.0, 151.9, 166.0, 179.9, 193.0, 230.2, 258.1, 268.2	123.9, 152.0
97	20.52	[M+H] ⁺	543.1486	393.5, 423.3, 447.3, 477.3, 489.4, 507.3, 525.1	393.4, 447.2, 477.3, 489.3, 507.2	301.1, 327.2, 333.2, 347.1, 361.3, 377.2, 387.2, 401.2, 419.1
		[M-H] ⁻	541.1320	275.1, 305.2, 377.1, 395.2, 451.3, 523.3	275.2, 305.1, 377.3	164.9, 189.0, 203.1, 219.1, 247.1, 257.0
98	20.65	[M+H] ⁺	315.0844	105.0, 167.3, 195.2, 213.2, 254.3, 269.4, 282.3, 285.2, 300.0	282.2, 285.1	180.1, 198.1, 226.1, 254.1
		[M-H] ⁻	313.0699	152.0, 167.1, 283.2, 198.0	201.2, 211.1, 227.0, 239.1, 255.0, 267.1, 269.2, 280.0, 283.1	173.0, 183.0, 201.1, 211.0, 239.0, 255.0
99	20.67	[M+H] ⁺	491.1180	315.2, 472.9	104.9, 167.2, 181.2, 195.2, 198.2, 213.2, 254.2, 269.4, 282.1, 285.1, 300.1	198.3, 226.3, 254.2, 270.2, 282.1, 285.0
		[M-H] ⁻	489.1011	174.9, 298.1, 313.2	152.0, 167.0, 225.2, 239.1, 253.9, 283.2, 298.0	211.1, 227.2, 239.1, 255.2, 283.0
100	20.79	[M+H] ⁺	301.0704	121.0, 139.1, 167.1, 179.1, 199.2, 227.2, 255.3, 268.3, 282.2, 286.1	140.1, 160.0, 168.1, 184.0, 195.0, 234.0, 240.0, 257.1, 268.1	184.0, 195.0, 240.0
		[M-H] ⁻	299.0558	211.0, 227.1, 255.1, 284.1	137.0, 150.1, 200.1, 212.2, 227.1, 239.2, 255.2	118.9, 145.9, 156.1, 174.2, 183.0, 184.1, 202.2
101	20.88	[M+H] ⁺	287.0549	120.9, 133.0, 153.0, 165.0, 183.0, 197.2, 213.1, 231.2, 241.1, 258.1, 269.1, 271.2	129.0, 157.1, 169.2, 197.0, 213.0, 224.9, 241.0, 253.1, 254.1, 269.1	129.1, 139.0, 147.1, 157.1, 170.9, 184.9, 199.0, 213.1
		[M-H] ⁻	285.0397	143.0, 151.0, 163.1, 171.1, 185.0, 199.1, 213.0, 229.1, 241.1, 257.1, 267.1, 269.1	143.0, 169.0, 171.1, 184.9	
102	20.88	[M+H] ⁺	361.0901	227.1, 300.1, 313.2, 328.2, 331.1, 346.2	300.2, 313.2, 328.2, 331.2	169.0, 197.0, 214.9, 285.2, 303.2, 313.1
		[M-H] ⁻	359.0749	329.2, 344.2	194.9, 210.0, 267.2, 285.1, 311.2, 329.1	133.0, 180.1, 195.0, 214.0, 242.1, 270.2, 286.1, 296.1, 314.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
103	20.95	[M+H] ⁺	433.1130	271.1	103.0, 122.9, 168.9, 197.1, 225.1, 253.0	102.8, 122.9, 141.1, 151.0, 197.1, 225.1
		[M-H] ⁻	431.0971	269.1	141.1, 169.1, 197.2, 223.0, 241.0, 251.0	195.1, 213.1, 223.1
104	21.80	[M+H] ⁺	271.0602	102.9, 105.0, 122.9, 151.0, 169.0, 173.0, 201.1, 225.1, 229.1, 242.1, 253.1, 271.1	94.9, 113.1, 122.9, 141.1, 150.9, 168.9	
		[M-H] ⁻	269.0441	171.1, 181.2, 197.0, 213.2, 225.0, 241.0	139.2, 153.0, 169.1, 180.9, 197.1, 215.1, 224.9	153.2, 168.9, 186.9, 197.2
105	21.86	[M+H] ⁺	461.1082	173.1, 271.0	102.9, 122.8, 140.9, 151.0, 169.1, 225.1, 253.1, 271.1	103.0, 122.9, 140.8, 150.9, 169.0, 197.0, 211.1, 225.0, 229.0
		[M-H] ⁻	459.0932	269.1	137.0, 141.0, 169.1, 197.1, 223.0, 241.1, 251.0	150.8, 179.0, 195.1, 213.1, 223.0
106	22.03	[M+H] ⁺	331.0811	197.2, 270.2, 287.2, 298.2, 316.1	181.1, 225.2, 245.2, 270.1, 287.1, 298.1	134.0, 154.0, 163.9, 181.9, 242.2, 270.1
		[M-H] ⁻	329.0665	153.1, 180.2, 195.0, 253.1, 270.2, 285.4, 299.0, 314.0	153.0, 180.0, 227.1, 225.1, 285.1, 296.2, 299.1	164.9, 183.1, 199.0, 227.0, 243.0, 255.0, 271.0
107	22.24	[M+H] ⁺	551.1376	360.4, 375.2	148.1, 195.1, 197.1, 212.1, 227.3, 227.2, 314.2, 324.1, 327.1, 342.1, 345.1, 360.1	148.0, 167.1, 195.1, 211.9, 213.1, 278.1, 296.1, 314.2, 324.2, 327.1, 342.1, 345.1
		[M-H] ⁻	549.1218	175.0, 358.0, 373.1	154.3, 169.1, 181.2, 194.8, 209.1, 225.1, 237.3, 303.3, 343.2, 358.1	169.0, 195.0, 303.1, 343.1
108	22.47	[M+H] ⁺	301.0703	153.0, 286.1	133.9, 152.9, 160.9, 177.9, 201.9, 243.0, 258.1, 268.1, 285.1	160.1, 177.9
		[M-H] ⁻	299.0554	150.9, 223.1, 231.1, 240.0, 255.0, 267.0, 284.1	121.9, 150.9, 171.1, 200.1, 212.1, 228.1, 238.9, 256.2	93.9, 121.8, 160.2, 228.1, 241.11
109	22.56	[M+H] ⁺	537.1588	239.9, 298.7, 360.4, 375.1	151.2, 167.2, 195.2, 197.2, 212.0, 227.1, 327.2, 342.2, 345.2, 360.1	195.1, 314.3, 327.2, 342.2, 345.2
110	22.63	[M+H] ⁺	391.1021	227.2, 312.2, 330.2, 343.2, 361.2, 376.2	191.2, 284.2, 312.2, 330.2, 343.2, 361.1	197.1, 210.9, 318.2, 333.1, 346.2
		[M-H] ⁻	389.0851	No fragmentation		
111	22.65	[M+H] ⁺	361.0902	142.0, 156.2, 169.1, 183.1, 204.1, 300.2, 313.2, 328.2, 331.2, 346.1	142.0, 169.0, 176.1, 204.1, 300.1, 328.1, 331.1	167.0, 189.1, 275.2, 288.1, 303.2, 316.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
		[M-H]-	359.0771	177.2, 221.1, 315.2, 327.3, 329.2, 344.1	109.9, 140.0, 166.0, 179.0, 257.1, 301.2, 311.2, 325.1, 329.1	79.1, 233.1, 301.0, 314.0
112	22.81	[M+H]+	331.0795	141.9, 147.0, 169.0, 183.0, 298.1, 316.1	141.9, 169.0, 174.0, 186.0, 298.1	70.9, 84.8, 94.9, 112.9, 122.9, 140.9, 150.8
		[M-H]-	329.0646	314.1	109.9, 139.9, 165.9, 180.0, 215.1, 227.0, 240.1, 266.9, 283.0, 295.0, 299.0	109.9, 137.8
113	22.81	[M+H]+	521.1280	345.3	227.2, 283.3, 284.3, 297.2, 312.2, 315.2, 330.2	284.2, 297.1, 312.1, 315.1
		[M-H]-	519.1136	343.1	313.2, 328.2	164.0, 171.1, 194.9, 210.1, 241.2, 251.2, 282.2, 295.2, 313.1
114	23.01	[M+H]+	461.1083	271.1	102.8, 122.9, 129.0, 140.9, 151.0, 169.0, 173.1, 197.1, 201.0, 215.1, 225.1, 253.1, 271.0	85.0, 95.0, 112.9, 123.0, 141.0, 151.0, 159.0, 169.1
		[M-H]-	459.0925	269.2	169.1, 171.1, 181.1, 197.0, 213.0, 225.1, 241.1	169.1, 181.1, 197.2, 207.1, 215.1, 225.0
115	23.17	[M+H]+	301.0707	105.0, 181.2, 199.1, 255.4, 272.4, 286.2	102.9, 138.0, 155.9, 172.0, 183.9, 202.0, 211.0, 240.2, 257.0, 286.1	127.8, 137.9, 155.8
		[M-H]-	299.0545	153.1, 227.2, 284.1	110.0, 137.9, 165.9, 171.2, 182.0, 183.9, 200.1, 212.1, 227.9, 239.0, 256.2, 265.1	129.1, 143.1, 156.1, 171.1
116	23.39	[M+H]+	361.0908	213.1, 328.1, 313.1, 331.1, 346.2	148.0, 199.0, 313.1, 331.1	121.1, 149.1, 182.9, 196.9, 214.9, 285.1, 303.2, 313.1
		[M-H]-	359.0746	221.2, 329.2, 344.2	109.9, 154.9, 168.0, 181.1, 196.1, 221.2, 257.1, 301.1, 311.0, 329.0	138.9, 179.1, 257.2, 285.2, 301.2, 314.1
117	23.44	[M+H]+	491.1170	301.2	286.1	105.0, 115.9, 127.9, 155.9, 170.0, 172.1, 183.9, 201.9, 212.1, 240.1, 257.1, 268.2
		[M-H]-	489.1011	No fragmentation		
118	23.48	[M+H]+	461.1066	No fragmentation		
		[M-H]-	459.0910	269.2	169.1, 171.1, 181.1, 197.0, 213.0, 225.1, 241.1	169.1, 181.1, 197.2, 207.1, 215.1, 225.0
119	23.52	[M+H]+	331.0796	169.1, 180.2, 198.1, 213.1, 298.2, 301.2,	118.0, 169.1, 180.1, 197.9, 298.2, 301.1	118.9, 155.0, 182.9, 200.9, 273.0

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
				316.2		
		[M-H]-	329.0647	161.0, 195.9, 269.2, 299.3, 314.2	167.9, 196.0, 227.2, 240.2, 271.1, 285.0, 299.1	154.9, 182.9, 200.9, 227.1, 255.1, 271.1
120	23.87	[M+H]+	271.0601	102.9, 122.9, 168.9, 197.1, 225.1, 242.1, 253.0, 271.0	102.9, 122.9, 150.9, 169.1, 196.9, 211.9, 225.1, 228.9	94.9
		[M-H]-	269.0441	136.9, 141.1, 150.9, 153.1, 157.1, 169.2, 197.0, 223.1, 241.1, 251.1	151.0, 167.0, 178.9, 195.1, 207.1, 213.0, 223.0	150.9, 179.0, 195.0, 213.1
121	23.97	[M+H]+	301.0699	121.0, 183.1, 241.2, 255.2, 286.1	90.9, 118.9, 139.9, 168.0, 185.9	111.9, 139.9
		[M-H]-	299.0540	166.1, 213.1, 227.2, 240.1, 284.0	109.9, 137.9, 165.9, 200.1, 212.1, 227.1, 240.2, 256.0, 267.1	109.9, 137.9
122	24.06	[M+H]+	491.1183	301.1	286.1	105.0, 116.0, 127.8, 138.0, 156.0, 183.9, 201.9, 212.0, 240.1, 258.1
		[M-H]-	489.1036	No fragmentation		
123	24.55	[M+H]+	331.0801	180.1, 198.1, 213.1, 226.2, 270.3, 298.2, 301.1, 316.1	180.0, 184.0, 198.0, 214.0, 226.0, 242.0, 270.0	198.1, 184.1
		[M-H]-	329.0660	171.2, 183.2, 196.1, 211.1, 238.1, 255.2, 270.1, 296.2, 299.3, 314.1	137.9, 153.0, 166.0, 168.0, 183.1, 193.9, 196.1, 201.1, 227.3, 240.1, 255.1, 268.1, 271.0, 285.2, 296.1, 299.0	139.0, 155.1, 183.1, 199.1, 201.0, 227.1, 255.1, 271.1
124	24.64	[M+H]+	445.1134	No fragmentation		
		[M+HA c-H]-	489.1036	253.0, 443.2	107.0, 143.1, 165.1, 180.1, 185.0, 197.3, 209.1, 225.0, 253.1	78.8, 118.8, 132.1, 153.1, 164.9, 180.1, 181.1, 191.0
125	24.71	[M+H]+	475.1241	285.2	105.0, 137.2, 165.1, 183.2, 225.1, 242.3, 253.4, 267.3, 270.0	115.9, 131.0, 140.1, 144.1, 168.0, 179.1, 224.1, 241.2, 242.0, 270.0
		[M-H]-	473.1105	268.1, 283.2	224.1, 239.1, 253.1, 268.0	166.0, 184.0, 196.1, 211.1, 212.0, 223.1, 224.0, 239.1, 240.1
126	24.86	[M+H]+	257.0808	No fragmentation		

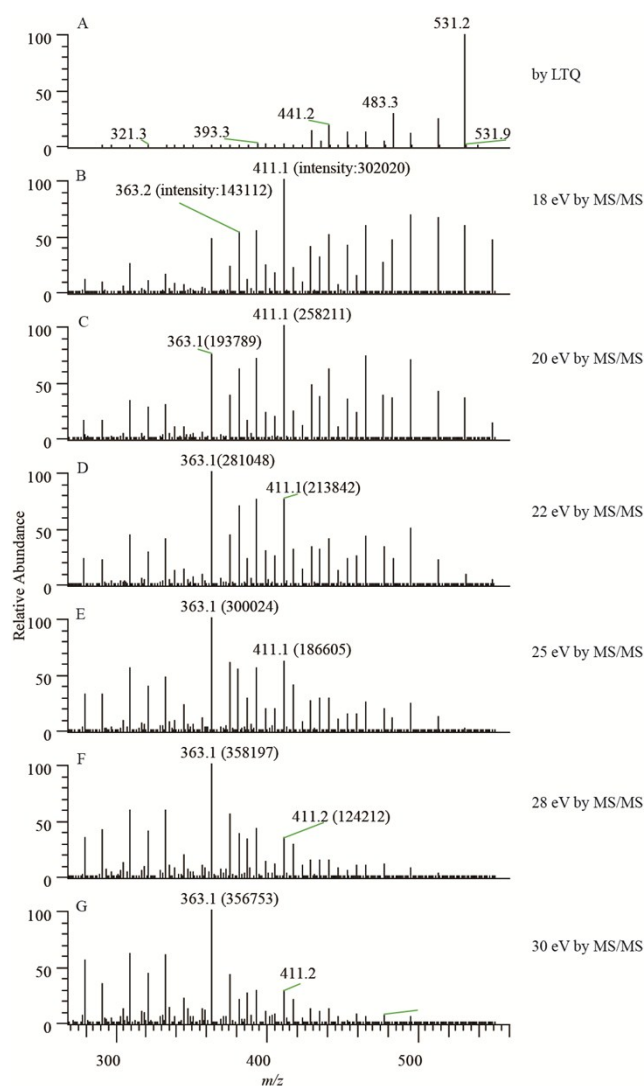
No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
		[M-H]-	255.0647	133.1, 145.1, 151.0 164.0, 167.1, 169.0, 211.1, 213.1, 227.1	140.9, 145.1, 169.0, 185.1, 195.1	141.1, 143.1, 157.0
127	25.51	[M+H]+	315.0855	No fragmentation		
		[M-H]-	313.0712	181.0, 209.1, 237.2, 253.2, 281.1, 298.1	181.1, 209.1, 222.2, 237.2, 253.1	150.0, 181.1, 209.0, 225.0
128	25.52	[M+H]+	475.1237	270.1, 285.0	104.9, 139.2, 183.1, 225.2, 239.2, 254.2, 270.1	168.0, 179.0, 224.1, 241.1, 252.1, 270.1
		[M-H]-	473.1061	268.1, 283.1	122.0, 187.3, 192.2, 195.0, 197.4, 224.0, 239.1, 268.0	110.0, 137.9, 162.8, 165.9, 184.0, 191.0, 196.0, 211.1, 223.1, 239.0, 240.0
129	26.49	[M+H]+	331.0796	197.2, 287.3, 298.1, 316.0	134.1, 270.0	166.1, 186.0, 214.0, 242.1
		[M-H]-	329.0660	152.1, 180.0, 211.0, 229.0, 299.2, 314.2	152.1, 179.9, 205.0, 268.2, 285.1, 296.2, 299.2	165.0, 199.1, 227.1, 243.1, 255.1, 271.1
130	26.52	[M+H]+	391.1014	227.2, 343.2, 358.2, 361.1, 376.1	325.1, 343.2, 361.2	196.9, 214.9, 333.1, 346.2
		[M-H]-	389.0853	207.1, 329.2, 342.2, 359.2, 374.1	183.1, 285.1, 300.1, 331.2, 341.1, 359.1	272.1, 285.1, 300.1, 331.1, 344.0
131	27.14	[M+H]+	313.1067	253.1, 269.2, 283.2, 298.2	252.2, 255.2, 269.2, 283.1	152.9, 227.0, 255.0
132	27.95	[M+H]+	361.0899	227.3, 310.3, 313.2, 328.2, 331.2, 346.1	211.1, 310.2, 313.2, 328.2, 331.1	135.0, 169.0, 197.0, 214.9, 257.0, 285.1, 303.1, 313.0, 316.0
		[M-H]-	359.0767	329.2, 344.2	298.2, 329.2	283.1, 286.1, 299.2, 311.1, 314.1
133	28.37	[M+H]+	345.0952	165.1, 183.0, 197.1, 270.1, 284.1, 301.1, 312.1, 315.1, 330.2	165.1, 183.0, 284.1, 301.1, 312.1, 315.2	255.1, 284.1, 296.2
		[M-H]-	343.0798	152.0, 165.1, 180.1, 195.1, 237.1, 273.1, 313.2, 328.2	139.0, 165.0, 180.1, 219.1, 273.2, 295.1, 313.2	137.0, 165.1, 241.2, 269.2, 285.2, 298.2
134	28.52	[M+H]+	285.0757	105.0, 165.1, 183.2, 270.1	103.0, 139.9, 167.9, 186.0, 179.0, 196.0, 213.1, 223.9, 241.1, 242.0, 252.1	
		[M-H]-	283.0597	163.2, 195.1, 211.2, 239.2, 255.2, 268.1	109.8, 163.0, 183.9, 196.1, 210.9, 224.1, 239.2	136.9, 166.9, 182.9, 195.1, 211.0, 239.2
135	28.95	[M+H]+	255.0648	102.9, 104.9, 128.9, 146.9, 152.9, 171.0, 187.0, 209.1, 212.94884, 230.98114	66.8, 96.9, 112.9, 125.0, 135.0	
		[M-H]-	253.0489	143.1, 151.0, 165.2, 181.1, 209.1, 253.2	115.1, 140.9, 153.1, 165.1, 180.1, 208.5	138.9, 153.1, 171.1

No.	t _R (min)	Ions	m/z	MS ²	MS ³	MS ⁴
136	29.19	[M+H] ⁺	315.0852	169.1, 195.1, 213.2, 282.2, 285.1, 300.1	153.0, 178.9, 197.1, 226.1, 254.2, 282.2, 285.1	198.1, 226.2, 254.0
		[M-H] ⁻	313.0696	151.9, 167.0, 180.2, 254.2, 283.2, 298.2	152.1, 180.1, 211.2, 239.1, 255.0, 269.2, 283.0	154.9, 172.9, 183.0, 201.0, 211.0, 239.0, 255.1
137	29.31	[M+H] ⁺	375.1057	168.9, 183.0, 192.1, 208.1, 229.2, 314.2, 327.2, 342.2, 345.2, 360.1	168.9, 183.1, 192.1, 218.0, 314.1, 316.1, 327.2, 342.2, 345.2	167.1, 314.2, 327.2
		[M-H] ⁻	373.0923	180.1, 195.1, 210.2, 258.2, 313.2, 343.2, 358.1	151.8, 166.0, 205.0, 284.2, 299.1, 315.1, 328.1, 343.1	165.0, 241.0, 256.0, 283.2, 300.2, 315.1, 328.2
138	29.62	[M+H] ⁺	257.0802	102.9, 130.9, 152.9, 173.0, 179.9, 190.9, 215.1	66.7, 127.1	
		[M-H] ⁻	255.0660	106.9, 125.0, 145.1, 151.0, 169.0, 186.9, 213.1, 227.1, 237.1, 255.1	121.9, 145.0, 169.1, 185.0, 195.1	108.1, 143.1, 157.1, 184.9
139	29.95	[M+H] ⁺	285.0761	165.2, 197.1, 225.0, 239.2, 270.1	105.0, 139.9, 167.9, 186.0, 196.1, 242.1	83.9, 98.9, 111.9, 139.9
		[M-H] ⁻	283.0599	211.2, 239.2, 241.2, 268.0	110.1, 118.9, 138.0, 156.1, 163.0, 166.0, 183.9, 196.1, 211.0, 223.0, 224.1, 239.2, 240.1	139.1, 167.0, 171.2, 183.0, 195.1, 211.0, 229.1, 239.0
140	30.02	[M+H] ⁺	375.1068	147.8, 195.0, 197.0, 212.0, 227.1, 314.2, 324.2, 327.2, 342.1, 345.1, 360.0	148.1, 195.1, 314.2, 327.0, 345.1	149.1, 168.9, 196.9, 215.0, 302.1, 317.1, 327.1
		[M-H] ⁻	373.0897	169.0, 195.2, 235.3, 267.1, 303.2, 325.0, 343.1, 358.1	169.0, 194.9, 210.1, 303.1, 343.2	153.9, 169.0, 271.0, 300.1, 328.1
141	30.21	[M+H] ⁺	287.0913	131.1, 145.1, 167.9, 182.9, 245.1, 271.1	137.0, 167.9, 185.9	119.9, 139.9
		[M-H] ⁻	285.0749	137.2, 166.0, 199.1, 241.2, 270.1	109.9, 138.0, 165.9, 178.9, 214.02438, 242.0	109.9, 137.9
142	30.29	[M+H] ⁺	315.0852	197.1, 254.2, 271.2, 282.2, 300.1	153.1, 181.1, 254.1, 271.1, 282.1	154.0, 229.1
		[M-H] ⁻	313.0700	180.0, 195.1, 269.1, 283.2, 298.12	151.9, 180.0, 269.1, 283.02	109.0, 136.8, 165.0, 183.0, 211.0, 227.1, 239.1, 255.1
143	31.82	[M+H] ⁺	345.0954	227.2, 284.3, 297.1, 312.1, 315.1, 330.2	284.2, 297.1, 315.1	168.9, 197.0, 215.0, 269.02, 287.2, 297.0
		[M-H] ⁻	343.0801	195.1, 209.1, 210.1, 243.2, 313.1, 328.0	195.1, 209.2, 241.0, 251.1, 269.2, 295.1, 313.2	153.0, 242.1, 270.2, 285.2, 295.2, 298.1

Supplementary information Fig. S1 (A) the peak 22 in LTQ-Orbitrap-MS give the different MS² spectrum with (B) that of the peak m/z 549.2 eluted at 1.99 min in HPLC/MS-MS; (C-G) the MS² spectra with different CE values in HPLC/MS-MS.

Supplementary information Fig. S2 (A-D) the elution order was reversed when the elution gradient was shortened, which is consistent with that of HPLC-MS-MS separation system; (E) the four different elution gradient

Supplementary information Fig. S3 A total of 12 components were detected by HPLC/LTQ-Orbitrap-MS of dosed plasma at 4 h after administration



Supplementary Fig. S1

Fig. S1

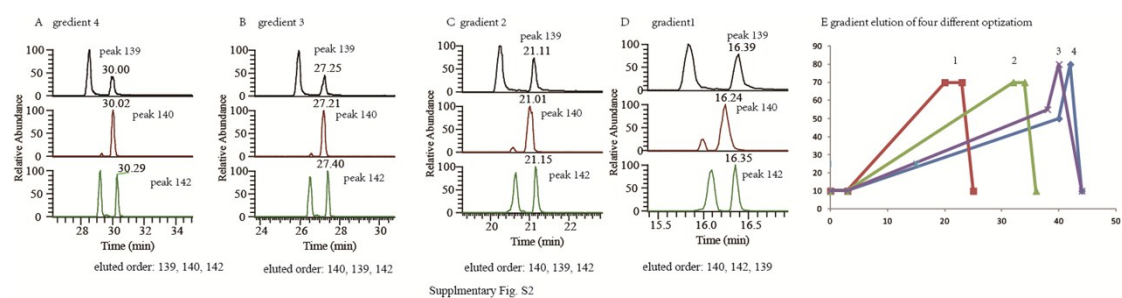
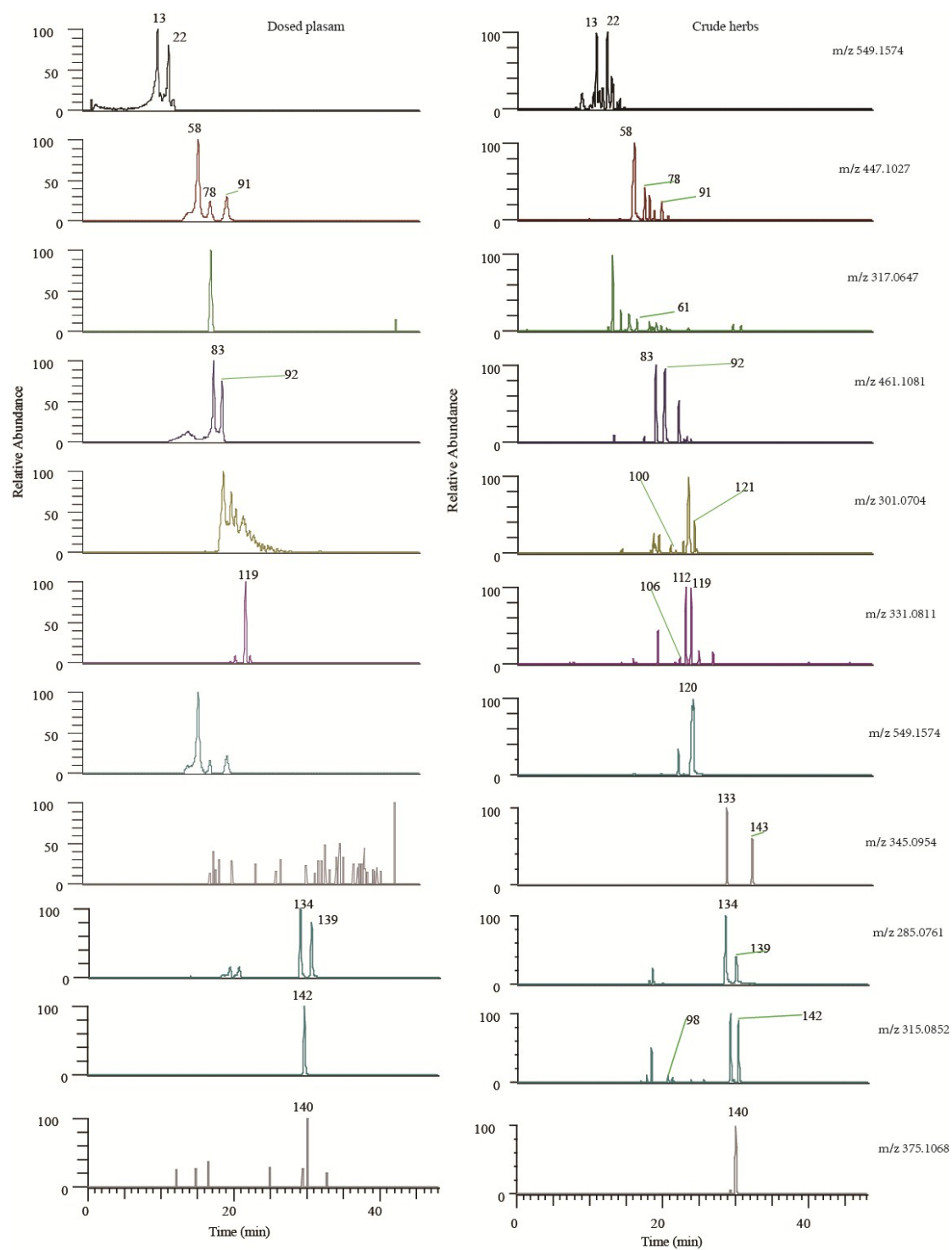


Fig. S2



Supplementary Fig. S3

Fig. S3