Supplementary Information

A HPLC-MS method for profiling triterpenoid acids and triterpenoid esters in *Osmanthus fragrans* fruits

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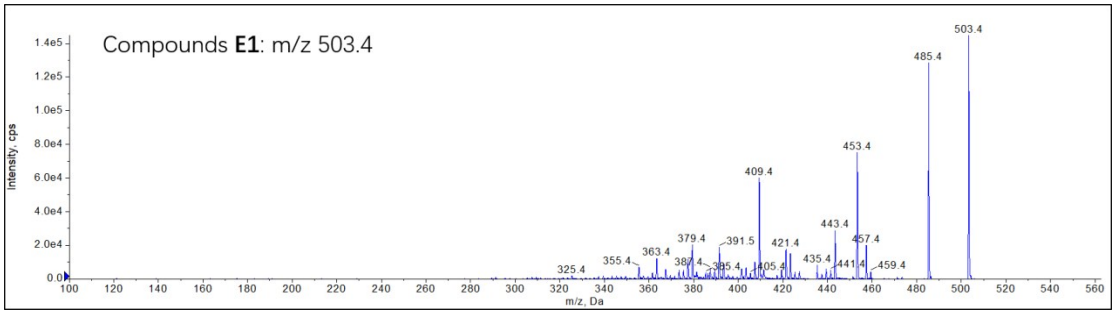
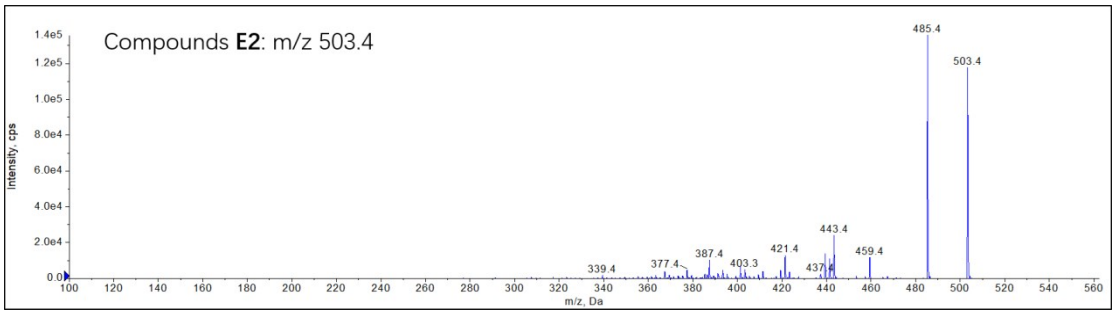
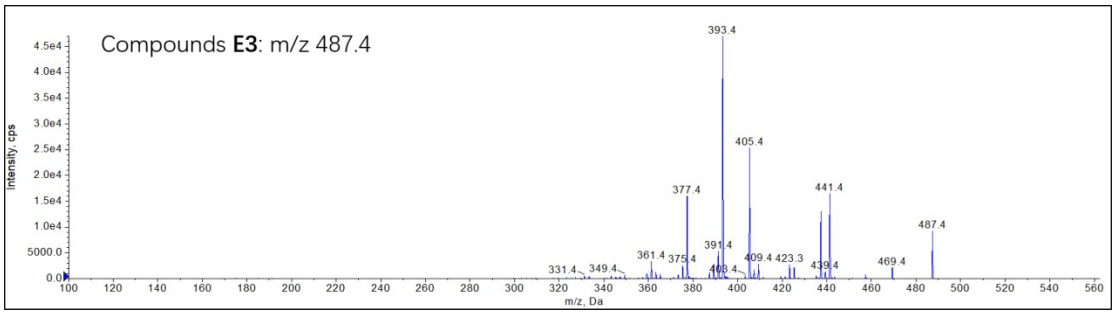
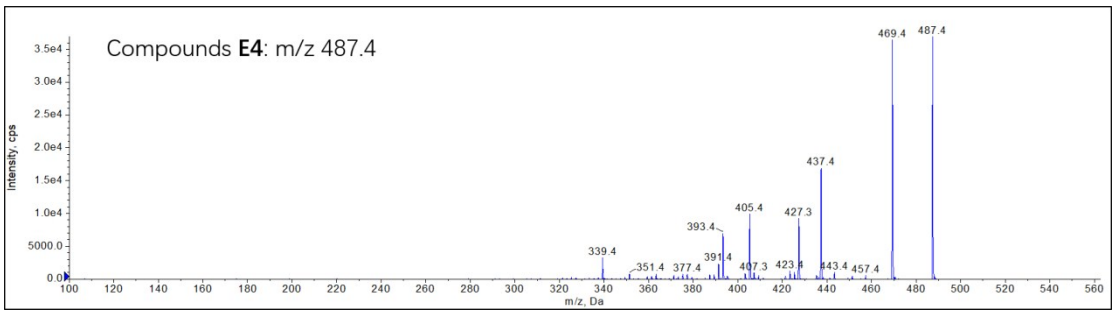
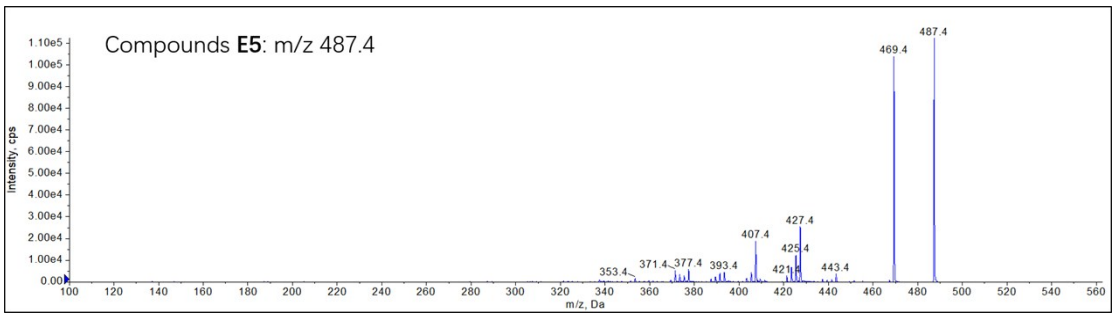
Fig. S1. MS^2 spectra of compounds **E1-E31**

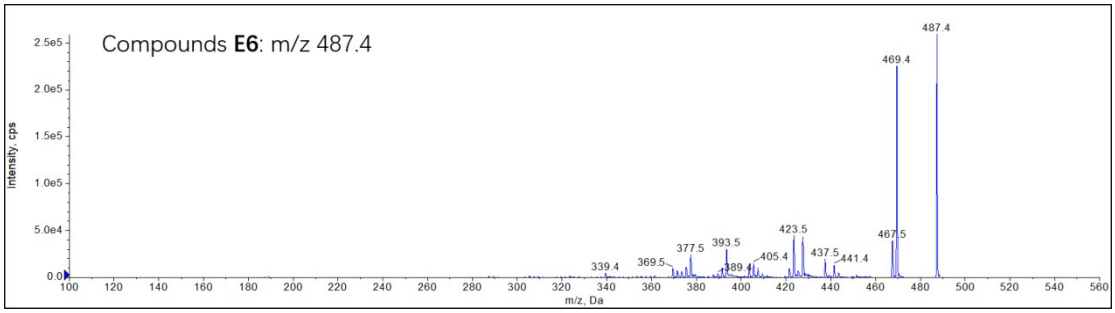











Compounds **E6**: m/z 487.4
Intensity, cps
m/z, Da
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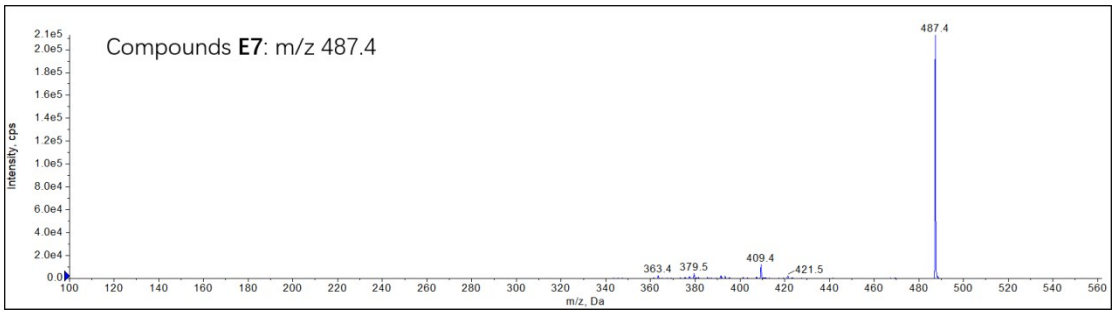
423.5
467.5
393.5
377.5
405.4
437.5
441.4
339.4
369.5
389.4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Intensity, cps
m/z, Da
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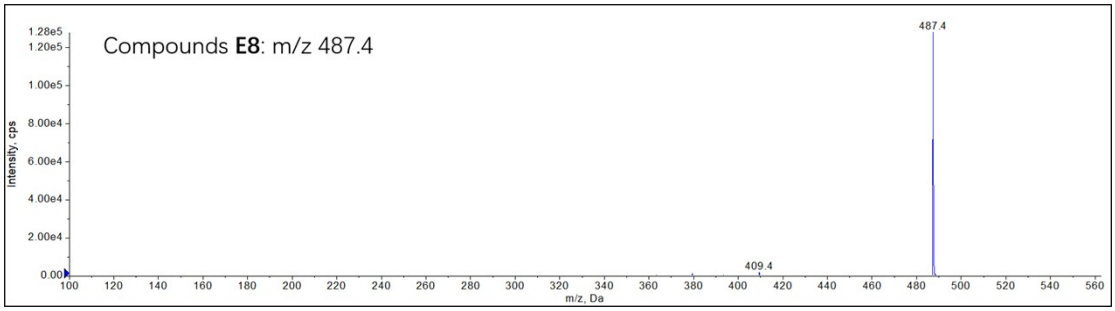
363.4
379.5
421.5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m/z, Da
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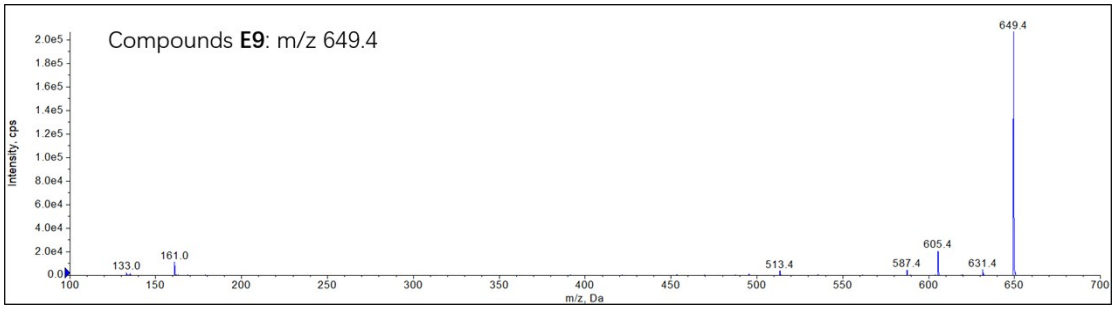
Compounds **E9**: m/z 649.4
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m/z, Da
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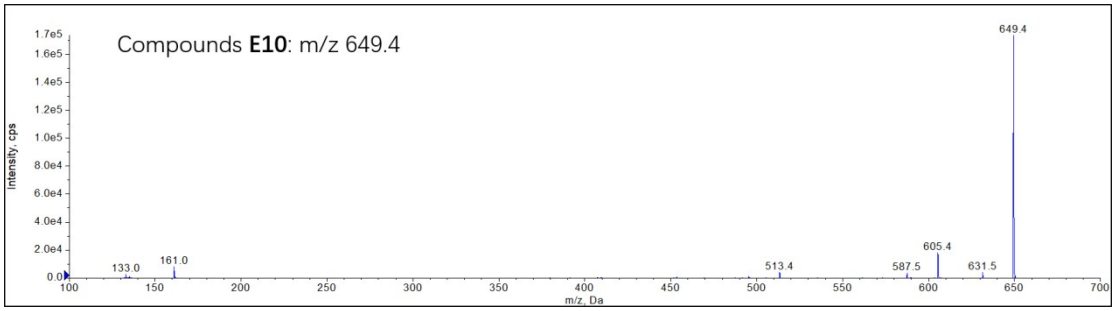
605.4
161.0
133.0
513.4
587.4
631.4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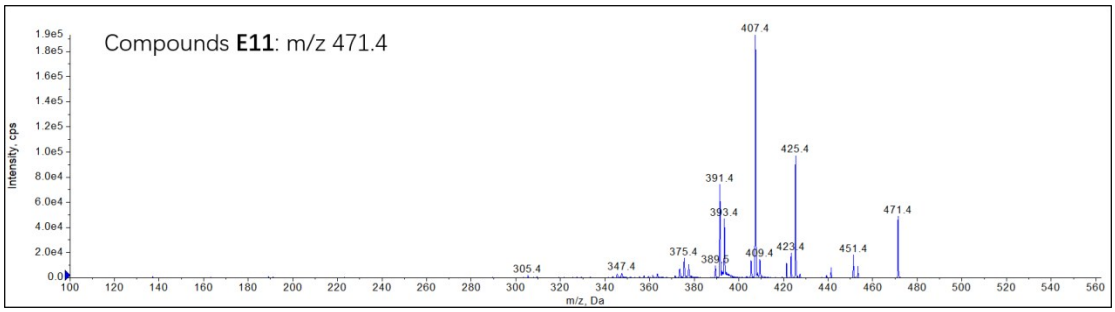
161.0
133.0
513.4
587.5
631.5


Compounds **E11**: m/z 471.4
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m/z, Da
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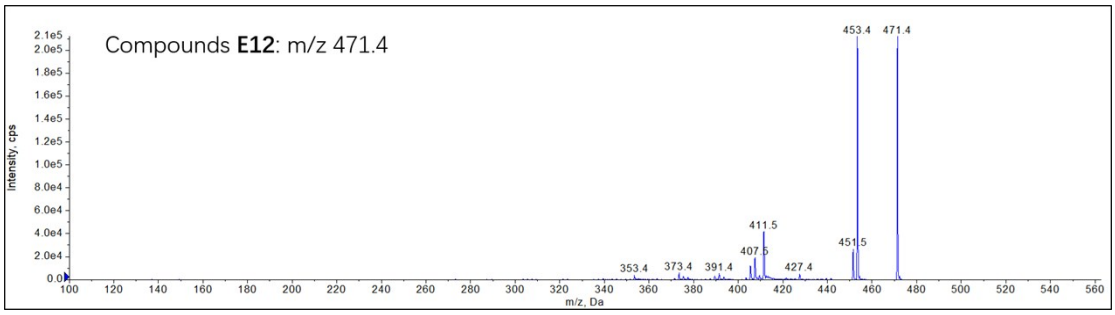
391.4
393.4
471.4
423.4
451.4
375.4
389.5
409.4
305.4
347.4


Compounds **E12**: m/z 471.4
Intensity, cps
m/z, Da
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407.5
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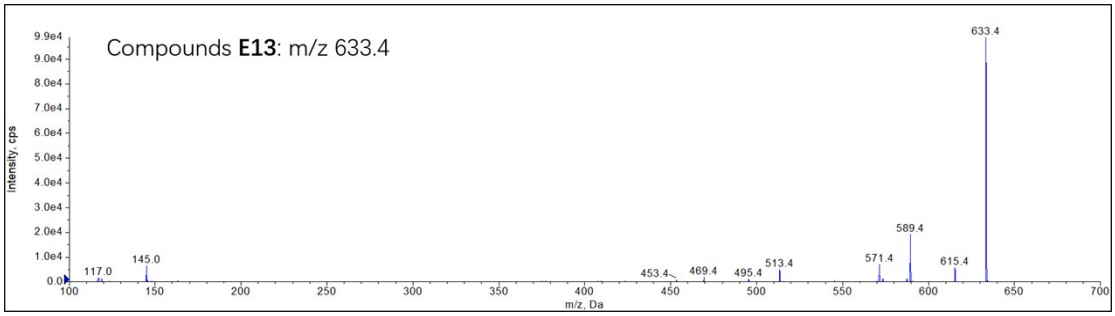
373.4
391.4
427.4


Compounds **E13**: m/z 633.4
Intensity, cps
m/z, Da
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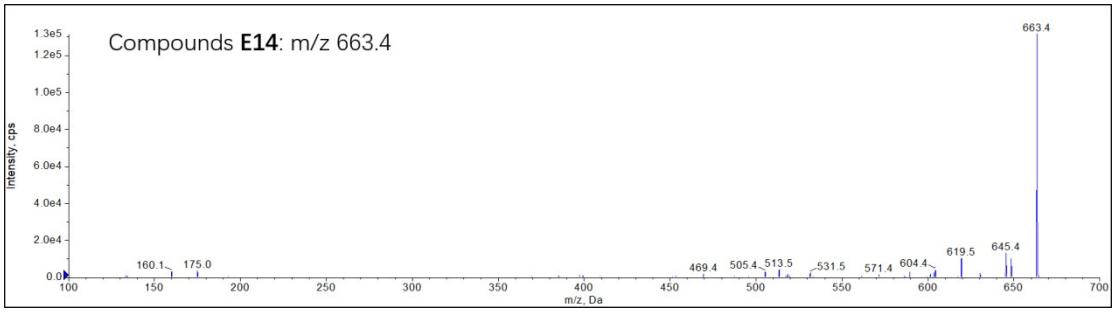
589.4
145.0
117.0
571.4
615.4
453.4
469.4
495.4
513.4


Compounds **E14**: m/z 663.4
Intensity, cps
m/z, Da
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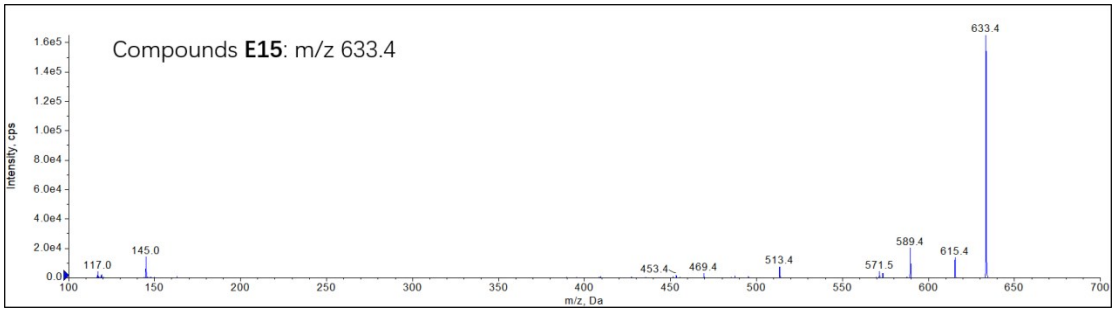
619.5
645.4
160.1
175.0
469.4
505.4
513.5
531.5
571.4
604.4


Compounds **E15**: m/z 633.4
Intensity, cps
m/z, Da
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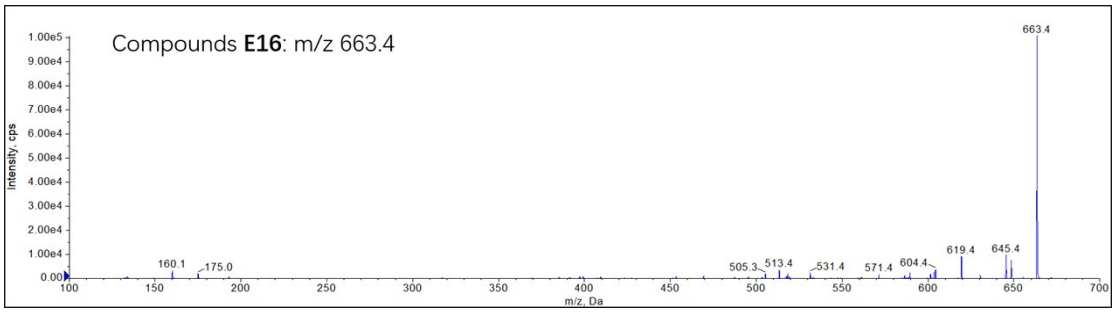
589.4
145.0
117.0
615.4
453.4
469.4
513.4
571.5


Compounds **E16**: m/z 663.4
Intensity, cps
m/z, Da
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160.1
175.0
505.3
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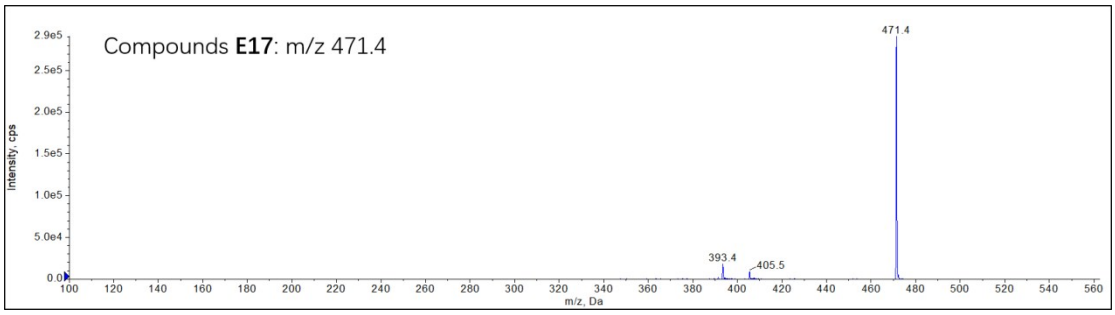
571.4
604.4
619.4
645.4


Compounds **E17**: m/z 471.4
Intensity, cps
m/z, Da
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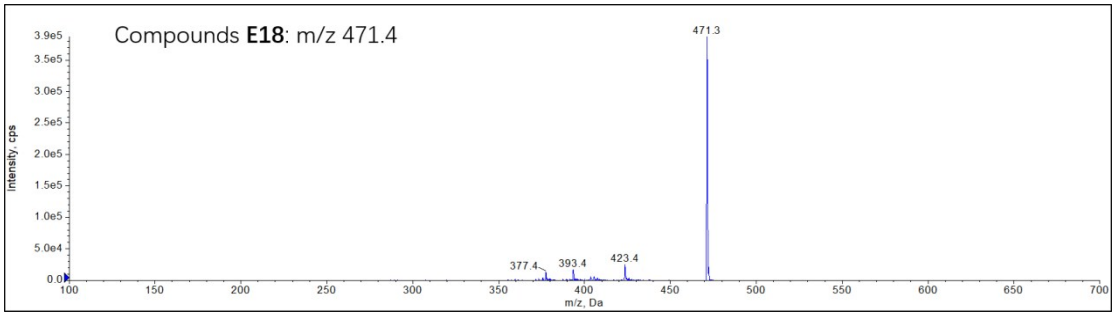
393.4
405.5


Compounds **E18**: m/z 471.4
Intensity, cps
m/z, Da
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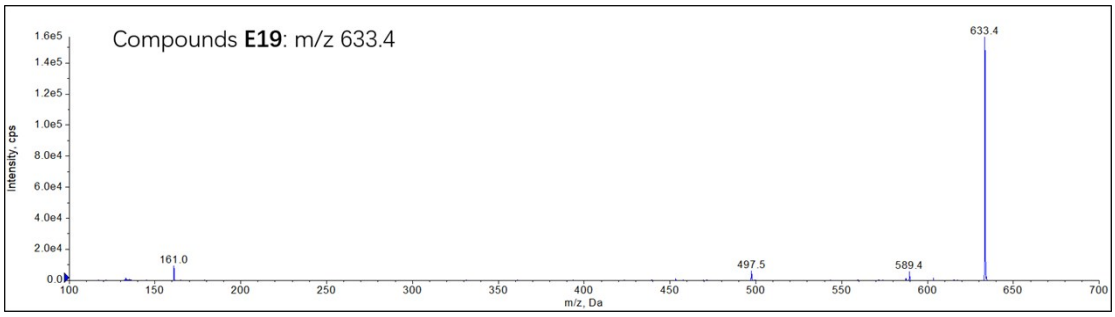
377.4
393.4
423.4


Compounds **E19**: m/z 633.4
Intensity, cps
m/z, Da
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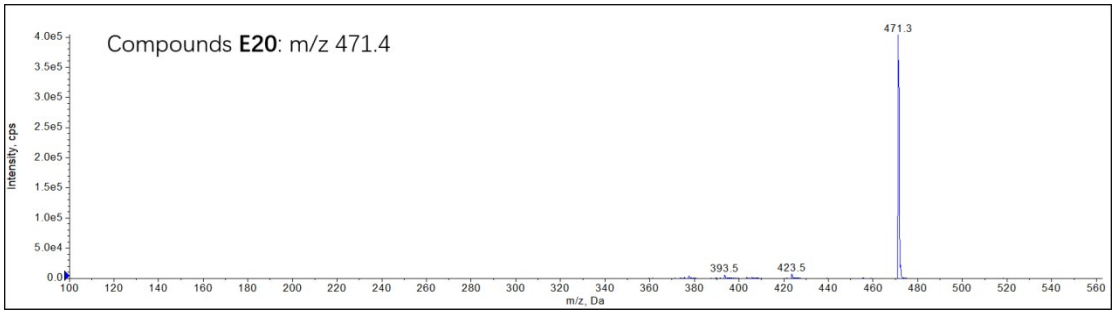
161.0
497.5
589.4


Compounds **E20**: m/z 471.4
Intensity, cps
m/z, Da
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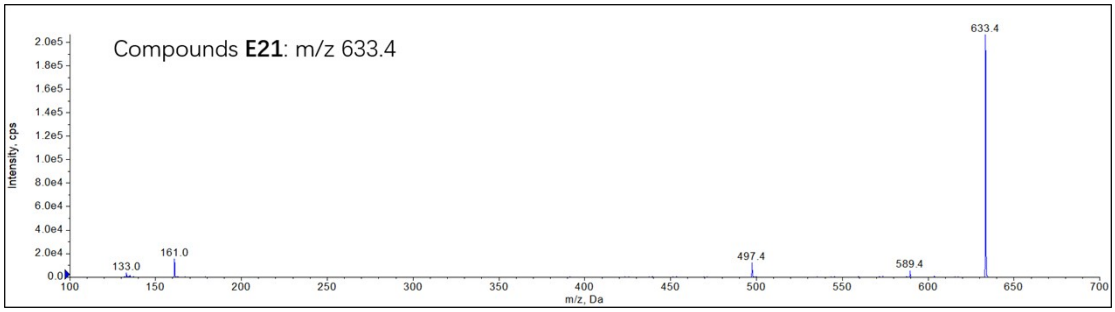
393.5
423.5


Compounds **E21**: m/z 633.4
Intensity, cps
m/z, Da
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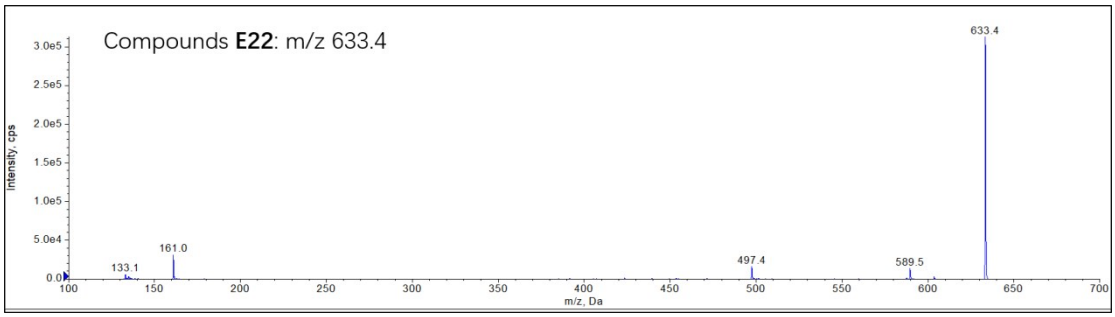
161.0
133.0
497.4
589.4


Compounds **E22**: m/z 633.4
Intensity, cps
m/z, Da
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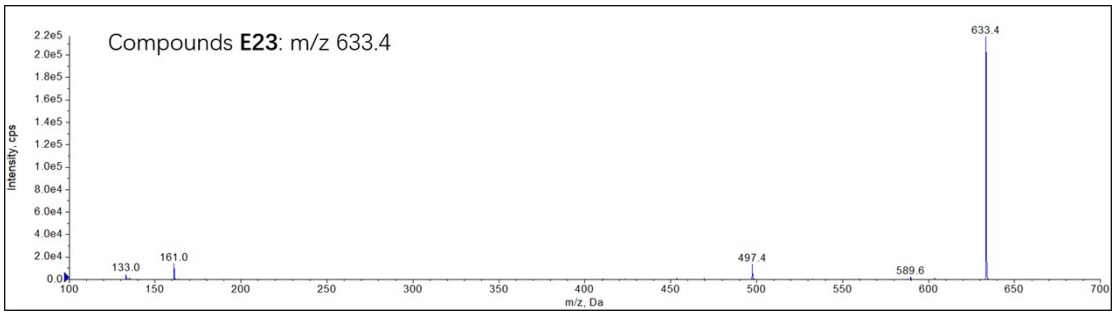
161.0
133.1
497.4
589.5


Compounds **E23**: m/z 633.4
Intensity, cps
m/z, Da
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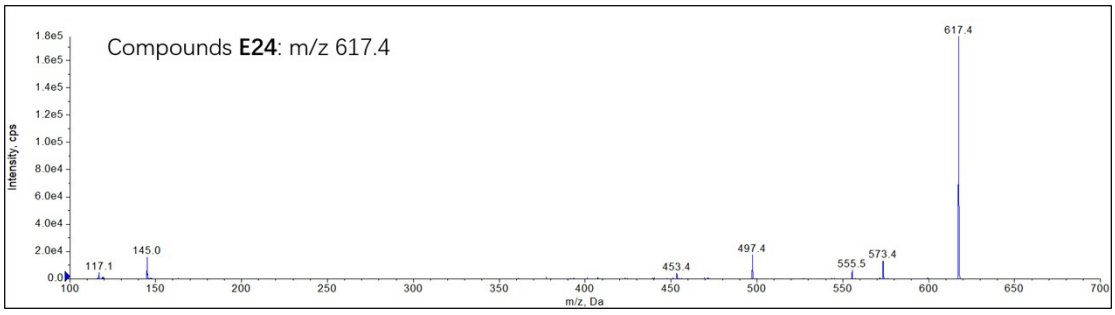
133.0
497.4
589.6


Compounds **E24**: m/z 617.4
Intensity, cps
m/z, Da
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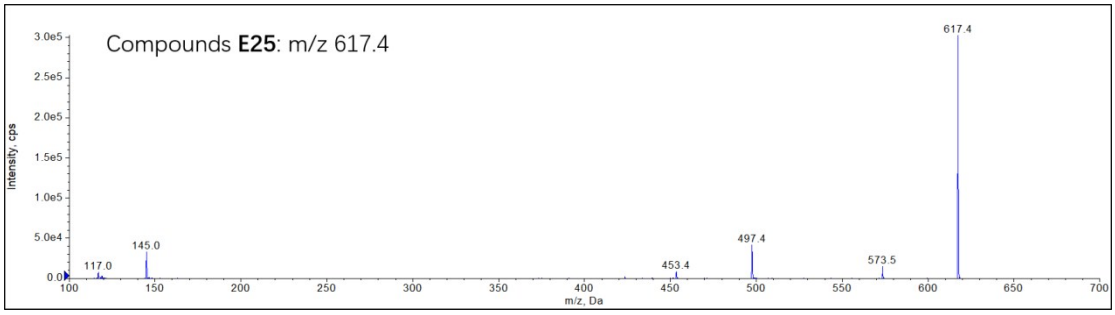
145.0
117.1
497.4
453.4
555.5
573.4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Intensity, cps
m/z, Da
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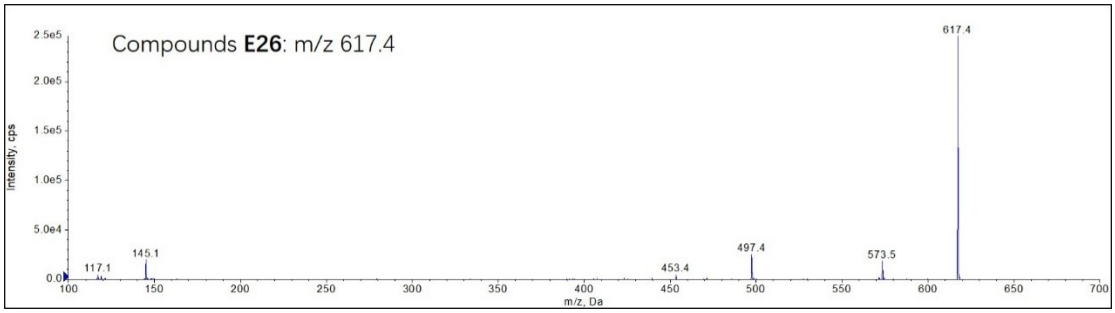
145.0
117.0
497.4
453.4
573.5


Compounds **E26**: m/z 617.4
Intensity, cps
m/z, Da
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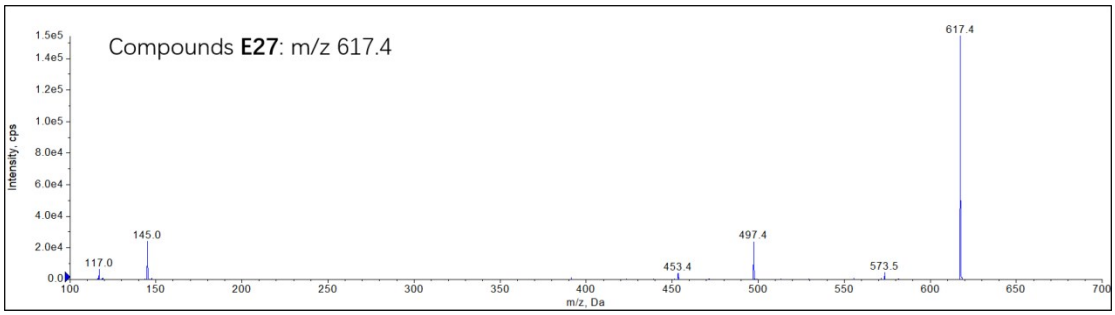
497.4
573.5
145.1
117.1
453.4


Compounds **E27**: m/z 617.4
Intensity, cps
m/z, Da
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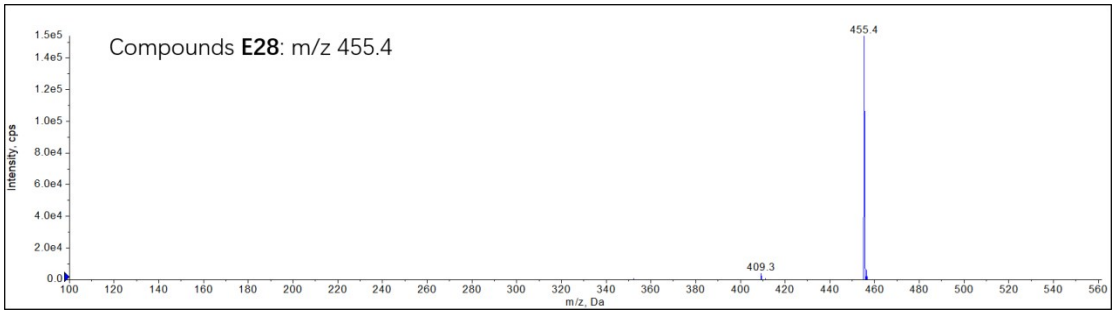
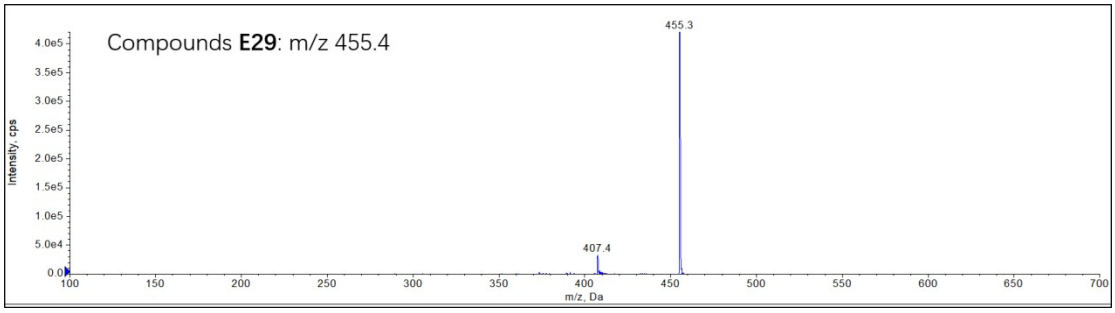
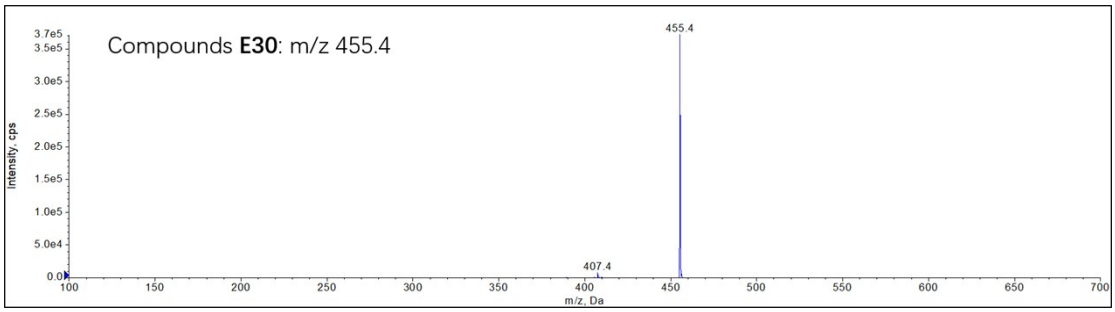
145.0
117.0
453.4
573.5


Compounds **E28**: m/z 455.4
Intensity, cps
m/z, Da
455.4
409.3


Compounds **E29**: m/z 455.4
Intensity, cps
m/z, Da
455.3
407.4


Compounds **E30**: m/z 455.4
Intensity, cps
m/z, Da
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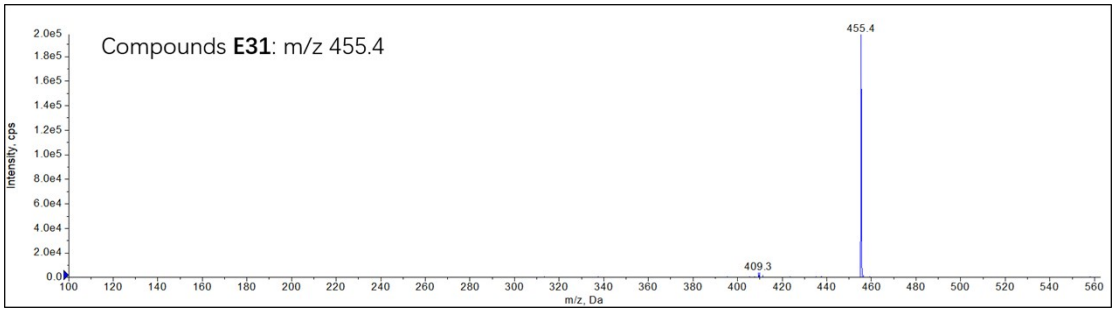
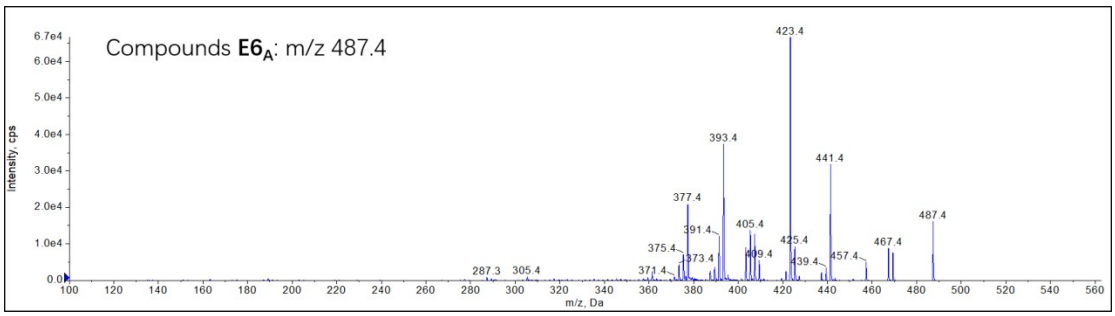
407.4


Compounds **E31**: m/z 455.4
Intensity, cps
m/z, Da
455.4
409.3


Compounds **E6$_A$**: m/z 487.4
Intensity, cps
m/z, Da
423.4
393.4
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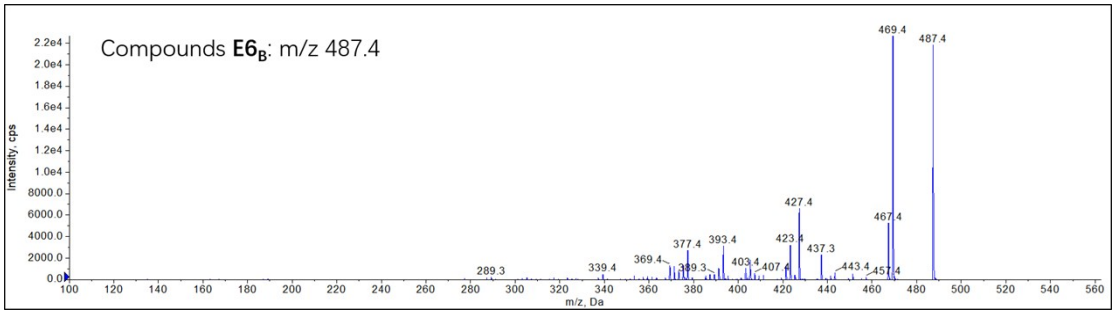
405.4
391.4
425.4
467.4
375.4
457.4
287.3
305.4
371.4


Compounds **E6$_B$**: m/z 487.4
Intensity, cps
m/z, Da
469.4
487.4
427.4
467.4
377.4
393.4
423.4
437.3
369.4
289.3
339.4
403.4
443.4

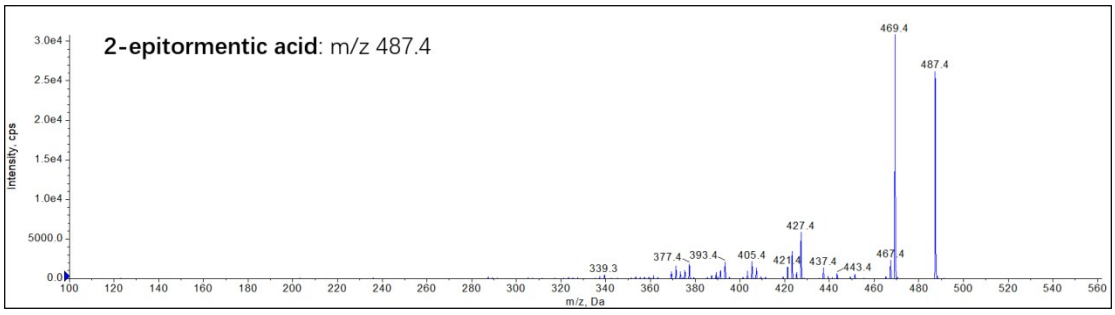

2-epitormentic acid: m/z 487.4
Intensity, cps
m/z, Da
469.4
487.4
427.4
377.4
393.4
405.4
467.4
339.3
437.4
443.4

Table S1 HPLC-MS/MS parameters for semi-quantitative determination of triterpenoid acids and triterpenoid esters

Q1 (m/z)	Q3 (m/z)	CE (V)
455.4	455.4*	-10
	409.4	-55
	407.4	-55
471.4	471.4*	-10
	453.4	-40
	423.4	-55
	405.4	-60
	393.4	-60
	377.4	-68
487.4	487.4*	-10
	469.4	-40
	427.4	-55
	425.4	-35
	423.4	-55
	409.4	-50
503.4	503.4*	-10
	485.4	-40
617.4	617.4	-10
	497.4	-60
	145.0*	-60
633.4	633.4	-10
	497.4	-60
	161.0*	-60
	145.0*	-60

649.4	649.4	-10
	605.4	-60
	161.0*	-60
663.4	663.4*	-10
	645.4	-60
	160.0	-60

* Semi-quantitative ions

Table S2 Method validation for semiquantitative determination of triterpenoid acids and triterpenoid esters by HPLC-MS

Compound	Calibration curve	Linear range [a]	*r*	Stability (%)
E1	Y=2130492.7x-1566.6	0.05-1	0.9999	1.5
E2	Y=712231.1x-1783.8	0.05-1	0.9999	3.4
E3	Y=602469.1x+4578.6	0.05-1	0.9998	3.7
E4	Y=453981.9x+2698.3	0.05-1	0.9995	2.8
E5	Y=1533955.8x+4128.0	0.05-1	0.9999	2.1
E6	Y=38354251.4x-42850.3	0.005-0.2	0.9998	1.1
$E6_B$	Y=280036.6x+1771.1	0.01-0.5	0.9994	4.8
E7	-	-	-	-
E8	Y=388114.6x+1580.6	0.05-1	0.9997	3.0
E9	Y=640750.8x+1456.0	0.01-1	0.9998	3.5
E10	Y=2607369.1x+12217.8	0.01-1	0.9996	4.0
E11	Y=14795606.0x-51202.0	0.005-0.3	0.9998	1.1
E12	Y=75990617.5x+432609.9	0.005-0.3	0.9988	0.6
E13	Y=4785408.6x+7685.4	0.001-0.5	0.9995	3.7
E14	Y=18026.0x+344.1	0.1-1	0.9995	1.1
E15	Y=10483746.44x+65745.3	0.001-0.3	0.9979	3.1
E16	Y=29406.6x+670.8	0.1-1	0.9990	4.2

E17	-	-	-	-
E18	Y=37310466.2x+262841.7	0.005-0.3	0.9978	1.1
E19 [a]	Y=1365534.6x+1523.0	0.005-0.3	0.9996	4.2
E20	Y=18939136.2x+76312.4	0.005-0.3	0.9992	0.7
E21	Y=244012.5x+795.1	0.05-0.5	0.9989	4.3
E22	Y=4310168.1x+23628.9	0.005-0.5	0.9990	4.8
E23 [a]	Y=845150.2x+7491.6	0.01-0.5	0.9987	4.0
E24	Y=5805087.2x+28232.9	0.005-0.5	0.9989	4.6
E25	Y=1337238.3x-2687.9	0.005-0.3	0.9998	4.0
E26	Y=9798596.1x+16690.1	0.005-0.3	0.9998	4.2
E27	Y=2716866.9x-4301.2	0.05-1	0.9996	4.9
E28	Y=1947993.0x+4019.2	0.05-1	0.9997	2.2
E29	Y=116209063.4x+328435.1	0.001-0.1	0.9974	0.6
E30	Y=30427012.2x+60729.0	0.001-0.1	0.9982	1.0
E31	Y=3180698.7x+8243.7	0.05-1	0.9998	3.5

[a] Dilution rate