Supporting Information

For

Design, Synthesis, and Structure-Activity Relationship of Novel 2-Substituted Pyranzinoylguanidine Epithelial Sodium Channel Blockers: Drugs for Cystic Fibrosis and Chronic Bronchitis

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Table of Contents

Analytical results of target compounds Table 2 .....S2

Elemental analysis of target compounds Table 3 .....S4

High resolution mass spectrometry of select compounds.....S5-S37

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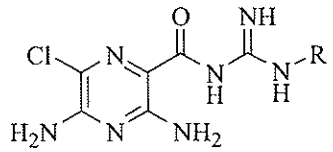
Table 2.

Analytical results of target compounds



Cpd #	R	MW free base	Mp (°C)	HPLC *Rt* (min)	Solvent system	Purity %
2	$(CH_2)_5CH_3$	313.78	230-232	6.6	A	> 99
3	$(CH_2)_7CH_3$	341.83	241-244	7.2	A	> 99
4	$(CH_2)_2OH$	273.67	203-205	7.4	B	95
7	$(CH_2)_2C_6H_5$	333.77	156-160	10.4	B	98.1
8	$(CH_2)_3C_6H_5$	347.80	192-196	6.5	A	98
9	$(CH_2)_4C_6H_5$	361.82	160-162	6.3	A	95
10	$(CH_2)_5C_6H_5$	375.85	240-243	11.3	B	98.3
11	$(CH_2)_6C_6H_5$	389.88	126-129	7.0	A	97
12	$(CH_2)_8C_6H_5$	417.93	171-173	7.1	A	99
				8.4[f]	D	96.5
13	$(CH_2)_2C_6H_4$-4-OH	349.77	Solid[e]	7.5	D	98
14	$(CH_2)_3C_6H_4$-4-OH	363.80	133	9.5	B	95.4
15	$(CH_2)_3C_6H_4$-4-OCH_3	377.82	134	10.1	B	95.8
16	$(CH_2)_4C_6H_4$-4-OH	377.82	160	9.5	B	98.4
17	$(CH_2)_5C_6H_4$-4-OH	391.85	188	9.9	B	95.3
18	$(CH_2)_4C_6H_4$-5-OH	377.82	215	10.3	B	97.2
19	$(CH_2)_4C_6H_4$-2-OH	377.82	240-242	10.8	B	95.6
20	$(CH_2)_4C_6H_4$-4-NH_2	376.85	195-200	9.0	B	98.8
21	$(CH_2)_4C_6H_4$-4-OCH_3	391.85	108-111	6.4	A	> 99
				6.0[f]	D	98
22	$(CH_2)_4C_6H_4$-4 CO_2CH_3	419.86	201	10.7	B	95.2
23	$(CH_2)_5C_6H_4$-4-OCH_3	405.88	132	10.6	B	98.8
24	$(CH_2)_3OC_6H_4$-4OCH_3	393.82	98	10	B	95.9
25	$(CH_2)_4C_6H_4$-4-CO_2H	405.83	123-126	24	C	94.5
26	$(CH_2)_4C_6H_4$-4-SO_3H	441.89	Solid[e]	8.7	B	95
				6.6[f]	D	88
27	$(CH_2)_4C_6H_4$-4CH_2OH	391.85	140	9.5	B	96.1
28	$(CH_2)_3OC_6H_4$-4-OH	379.80	150	9.2	B	94.9
29	$(CH_2)_2OCH_2C_6H_4$-4-OCH_3	393.82	99-102	9.9	B	95.9
30	$(CH_2)_4C_6H_4$-4-O $(CH_2)_2OH$	421.88	218	9.7	B	96.6
31	$(CH_2)_4C_6H_4$-4-O-$(CH_2)_3OH$	435.90	211-213	10.4	B	98.8
32	$(CH_2)_4C_6H_4$-4 – $OCH_2CHOHCH_2OH$	451.90	92-95	9.7	B	95.3
33	$(CH_2)_4C_6H_4$-4 OCH_2CH-(*R*)-$OHCH_2OH$	451.90	167-172	22.8	C	96.8

34	$(CH_2)_4C_6H_4$-4 –OCH_2CH-(*S*)-$OHCH_2OH$	451.90	160-162	23	C	95.9
35	$(CH_2)_4C_6H_4$-3 – $OCH_2CHOHCH_2OH$	451.90	91-93	9.4	B	96.3
36	$(CH_2)_4C_6H_4$-2 – $OCH_2CHOHCH_2OH$	451.90	85-86	9.7	B	95.7
37	$(CH_2)_4C_6H_4$-4-O-CH_2CO_2H	526.80	225	24.4	C	97.8
38	$(CH_2)_4C_6H_4$-4-O-$CH_2CH_2CO_2H$	486.35	198-200	25.8	C	97.1
39	$(CH_2)_4C_6H_4$-3-O-CH_2CH_2OH	490.38	161-163	10.0	B	95
40	$(CH_2)_4C_6H_4$-2-O-CH_2CH_2OH	422.17	115	10.3	B	93.4
41	$(CH_2)_4C_6H_4$-4-O-D-glucuronic acid	575.93	>184	8.6	B	96.1
42	$(CH_2)_4C_6H_3$-3-OH-4-OH	430.28	>154	9.2	B	96.1

Please note for Table 2: Solvent systems include gradient chromatography method: **A**, YMC Pro C8 5 μm column, 1 mL/min. 95:5 (0.4 Acetic acid : 0.4% Acetic acid and MeCN) to 80:20 for 7 min. and 100% (0.4% Acetic acid and MeCN) for 5min, ambient temperature; **B**, Microsorb C8, 5 μm column, 1 mL/min. 95:5 (0.1% TFA: MeCN 0.1%TFA) 1 min then 20:80 at 7 min and 100% (0.1% TFA: MeCN) over 1 min. ambient temperature; **C**, Microsorb C8 5 μm column, 1 mL/min. 95:5 0.05% TFA: MeCN 0.05%TFA 1 min then 20:80 at 7 min and 100% (0.05%TFA MeCN) for 1 min. ambient temperature; **D,** Atlantis C18 5μm column, 1.5 mL/min. 95:5 (0.02% TFA: 0.02% TFA MeCN) to 56:44 at 6.5 min to 90% (0.02% TFA MeCN) for 1 min, at 40°C.

[c] Not analyzed. [f] Data collected using a diverse HPLC system.

Table 3.

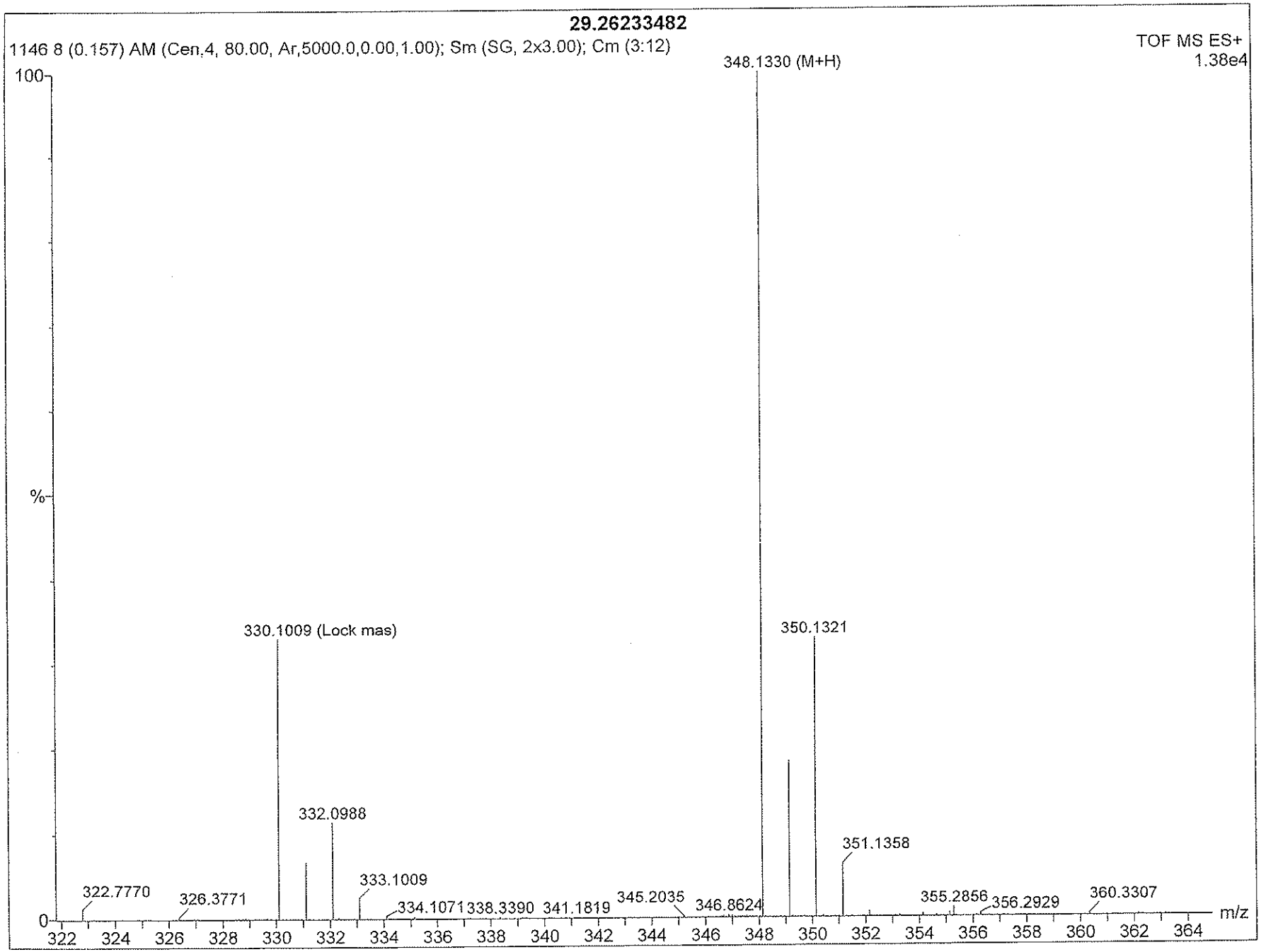
Elemental Analysis

		Calculated			Found		
Cmpd no.	**Formula**[g]	C	H	N	C	H	N
2	$C_{12}H_{20}ClN_7O$•HCl	41.15	6.04	27.99	35.87	5.55	24.26
3	$C_{14}H_{24}ClN_7O$•HCl	44.45	6.66	25.92	45.73	6.82	24.06
4	$C_8H_{12}ClN_7O_2$•HCl	30.98	4.22	31.61	30.50	4.41	27.58
7	$C_{14}H_{16}ClN_7O$•HCl	45.42	4.63	26.48	40.67	4.73	23.28
8	$C_{15}H_{18}ClN_7O$•HCl	46.88	4.98	25.52	43.43	4.43	23.29
9	$C_{16}H_{20}ClN_7O$•HCl	48.25	5.31	24.62	46.59	4.80	23.11
10	$C_{17}H_{20}ClN_7O$•HCl	49.52	5.62	23.78	49.34	5.51	23.48
11	$C_{18}H_{24}ClN_7O$•HCl	50.71	5.91	23.00	49.11	6.49	21.90
13	$C_{14}H_{16}ClN_7O_2$•HCl	43.54	4.44	25.39	40.8	4.86	24.26
14	$C_{15}H_{18}ClN_7O_2$•HCl	45.01	4.79	24.50	42.93	4.81	18.33
15	$C_{16}H_{20}ClN_7O_2$•HCl	46.39	5.11	23.67	49.81	6.14	14.42
16	$C_{16}H_{20}ClN_7O_2$•HCl	46.39	5.11	23.67	45.21	5.92	18.85
17	$C_{17}H_{22}ClN_7O_2$•HCl	47.67	5.41	22.89	45.21	5.92	18.65
18	$C_{16}H_{20}ClN_7O_2$•HCl	46.39	5.11	23.67	45.19	5.34	19.50
19	$C_{16}H_{20}ClN_7O_2$•HCl	46.39	5.11	23.67	46.52	4.42	22.36
20	$C_{16}H_{21}ClN_8O$•2HCl	42.73	5.15	24.91	38.20	5.31	21.08
22	$C_{18}H_{22}ClN_7O_3$•HCl	47.38	5.08	21.49	46.83	5.09	18.33
23	$C_{17}H_{22}ClN_7O_2$•HCl	48.87	5.70	22.17	44.19	5.52	19.53
24	$C_{16}H_{20}ClN_7O_3$•HCl	44.66	4.92	22.79	41.11	5.02	18.99
25	$C_{17}H_{20}ClN_7O_3$•HCl	46.16	4.79	22.17	41.08	4.67	19.42
27	$C_{17}H_{22}ClN_7O_2$•HCl	47.67	5.41	22.89	44.51	5.31	19.28
28	$C_{15}H_{18}ClN_7O_3$•HBr	39.10	4.16	21.28	26.65	2.92	14.11
29	$C_{16}H_{20}ClN_7O_3$•HCl	44.66	4.92	22.79	43.43	4.76	20.22
30	$C_{18}H_{24}ClN_7O_3$•HCl	47.17	5.50	21.39	43.53	5.32	19.90
31	$C_{19}H_{24}ClN_7O_3$•HCl	48.31	5.76	20.76	47.41	5.73	19.89
32	$C_{19}H_{26}ClN_7O_4$•CH_3SO_3H•H_2O	42.44	5.70	17.32	42.75	5.40	17.34
33	$C_{19}H_{26}ClN_7O_4$•CH_3SO_3H•H_2O	42.44	5.70	17.32	42.58	5.13	17.38
34	$C_{19}H_{26}ClN_7O_4$•CH_3SO_3H•H_2O	42.44	5.70	17.32	42.08	5.27	16.95
35	$C_{19}H_{26}ClN_7O_4$•HCl•H_2O	45.07	5.77	19.36	44.85	5.44	19.29
36	$C_{19}H_{26}ClN_7O_4$•HCl	46.73	5.57	20.08	45.34	6.02	19.61
37	$C_{18}H_{22}ClN_7O_4$•HCl	45.77	4.91	20.76	41.04	5.06	18.41
38	$C_{19}H_{24}ClN_7O_4$•HCl	46.92	5.18	20.16	44.90	5.63	19.89
39	$C_{18}H_{24}ClN_7O_3$•HCl	47.17	5.50	21.39	46.18	5.52	20.20
40	$C_{18}H_{24}ClN_7O_3$•HCl	47.17	5.50	21.39	45.70	5.19	20.12
41	$C_{22}H_{27}ClN_7NaO_8$	45.88	4.73	17.02	39.74	4.58	13.79
42	$C_{16}H_{20}ClN_7O_3$•HCl	44.66	4.92	22.79	43.53	5.39	18.52

[g] Residual solvents or acids were not experimentally determined.

Compound number	molecular Formula	Calculated [M+H]+	Measured [M+H]+	mDa	ppm	EXACT (Measured)
					<5 ppm	H atom
						1.007825
8		348.1339	348.1330	-0.9	-2.6	347.125175
2		314.1496	314.1496	0	0.0	313.141775
11		390.1809	390.1792	-1.7	-4.4	389.171375
12		418.2122	418.2110	-1.2	-2.9	417.203175
21		392.1602	392.1604	0.2	0.5	391.152575
36			452.1816			
16		378.1445	378.1460	1.5	4.0	377.138175

The 330.1009 peak is from the lock mass. Your sample doesn't have this


29.26233482
1146 8 (0.157) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (3:12)
TOF MS ES+
1.38e4
100
%
0
348.1330 (M+H)
330.1009 (Lock mas)
350.1321
332.0988
351.1358
333.1009
322.7770
326.3771
334.1071
338.3390
341.1819
345.2035
346.8624
355.2856
356.2929
360.3307
m/z
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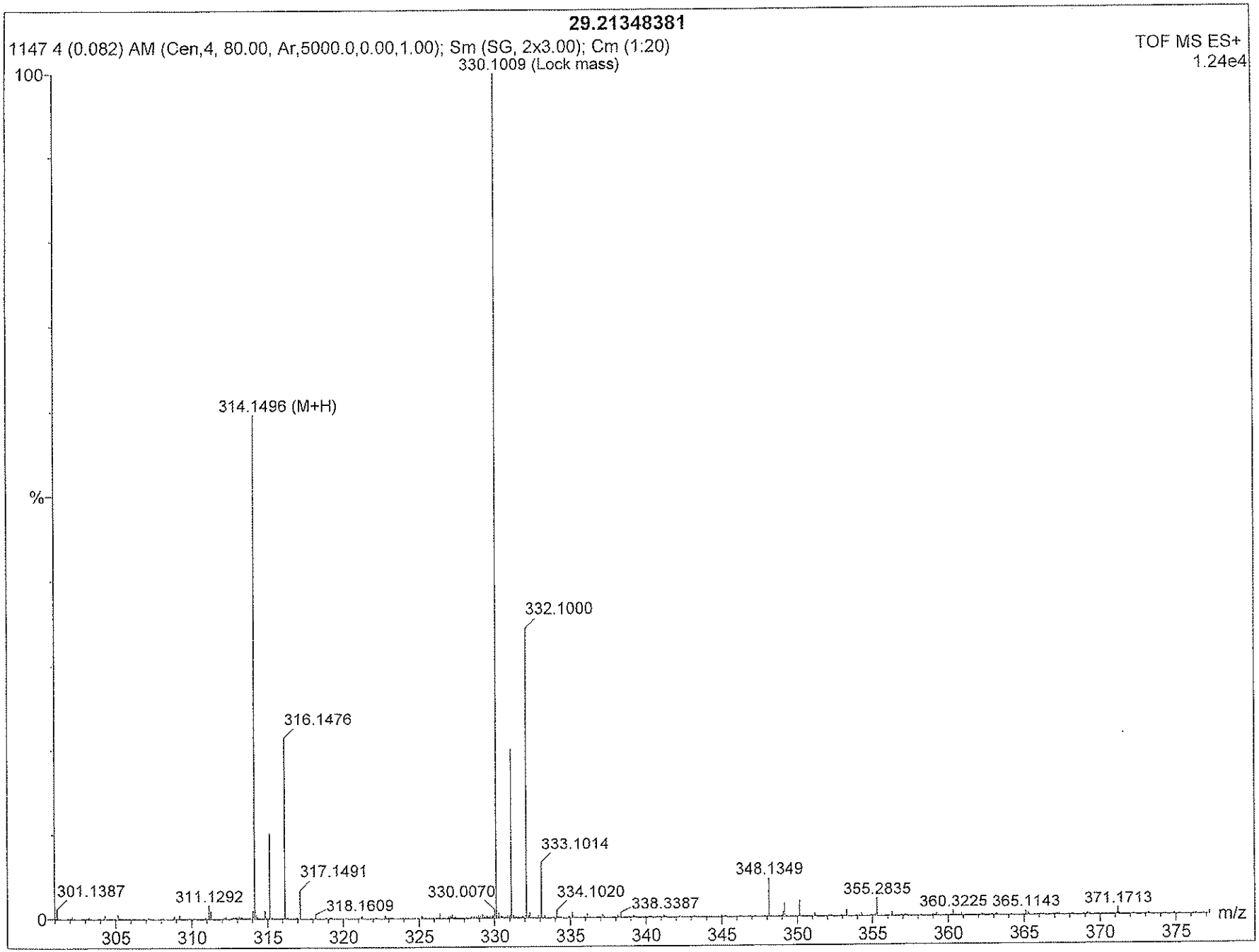
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1147 4 (0.082) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:20)
TOF MS ES+
1.24e4
100
%
0
330.1009 (Lock mass)
314.1496 (M+H)
332.1000
316.1476
333.1014
317.1491
348.1349
301.1387
311.1292
318.1609
330.0070
334.1020
338.3387
355.2835
360.3225
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m/z
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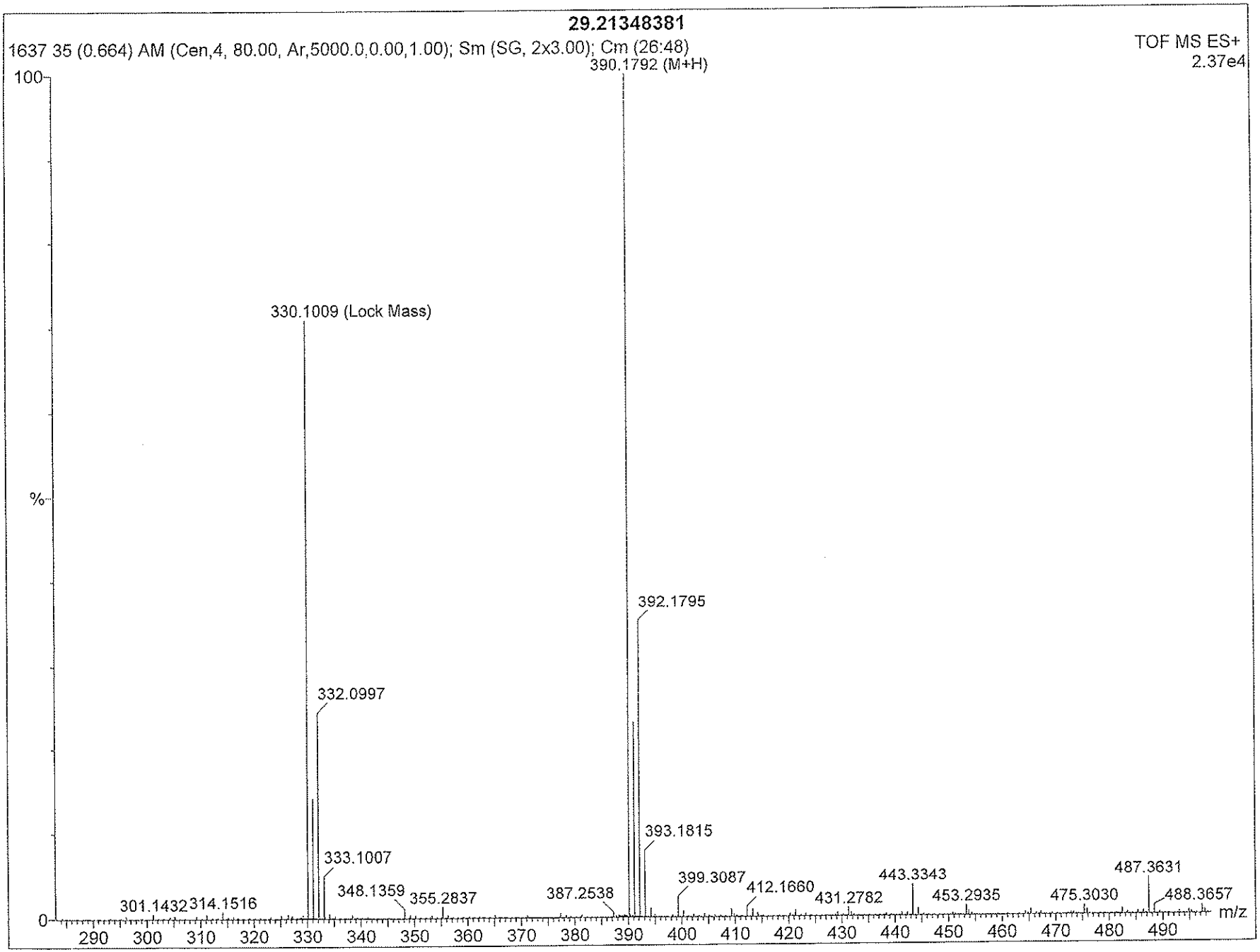
29.21348381
1637 35 (0.664) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (26:48)
TOF MS ES+
2.37e4
390.1792 (M+H)
330.1009 (Lock Mass)
392.1795
332.0997
393.1815
333.1007
348.1359
355.2837
387.2538
399.3087
412.1660
431.2782
443.3343
453.2935
475.3030
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%
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m/z
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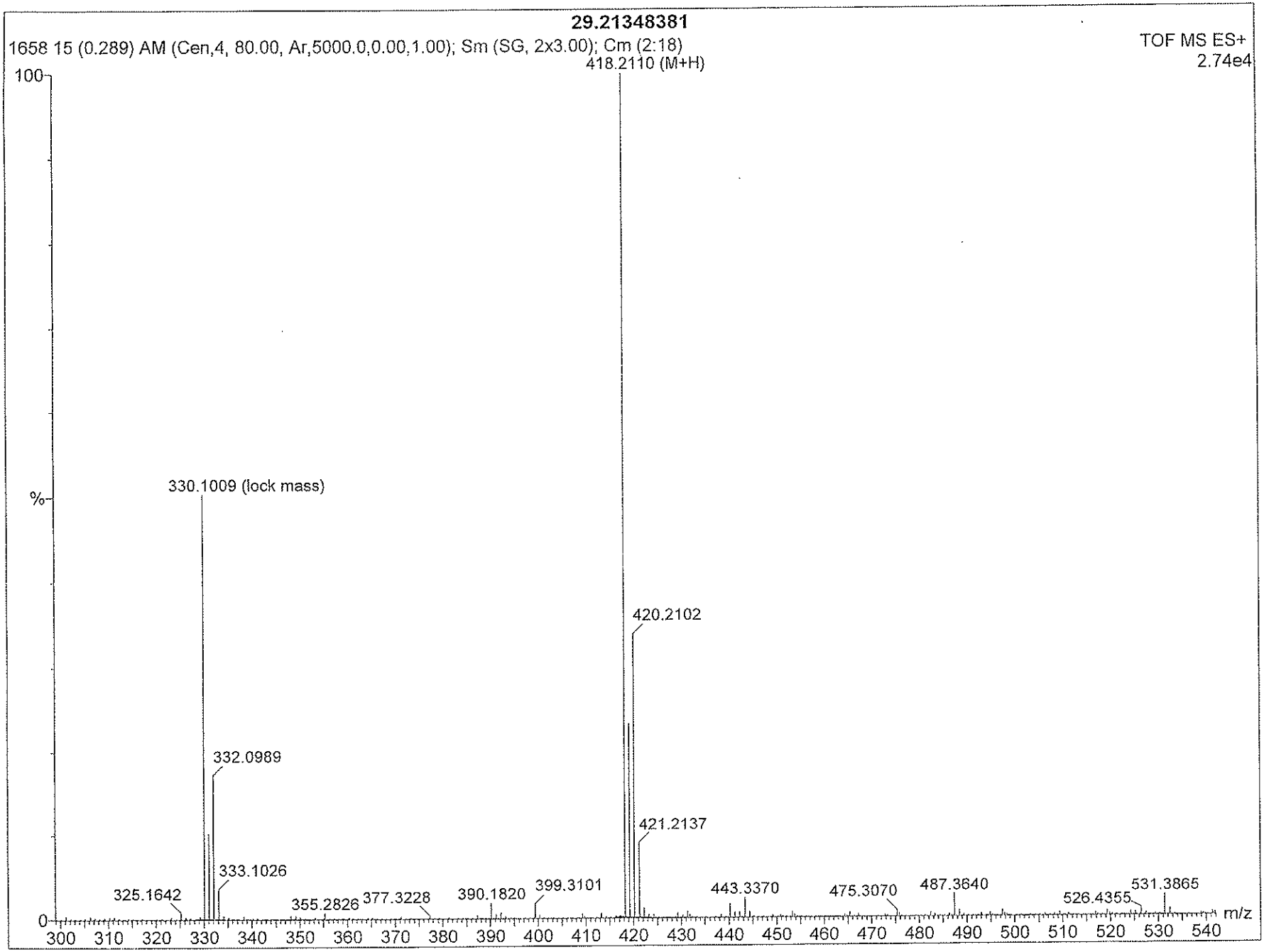
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TOF MS ES+
2.74e4
418.2110 (M+H)
330.1009 (lock mass)
420.2102
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333.1026
325.1642
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377.3228
390.1820
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443.3370
475.3070
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%
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m/z
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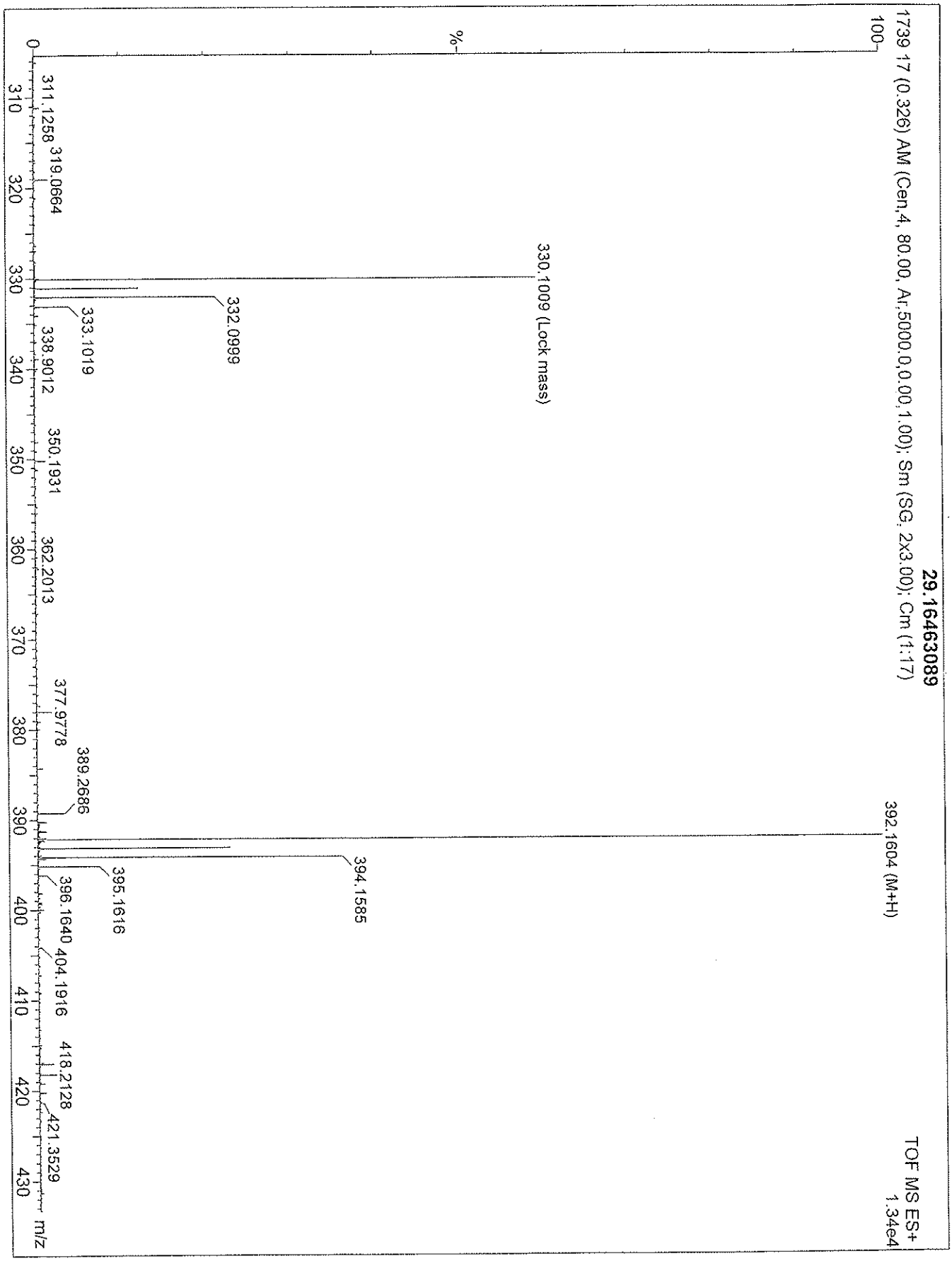
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TOF MS ES+
1.34e4
100
%
0
330.1009 (Lock mass)
392.1604 (M+H)
311.1258
319.0664
332.0999
333.1019
338.9012
350.1931
362.2013
377.9778
389.2686
394.1585
395.1616
396.1640
404.1916
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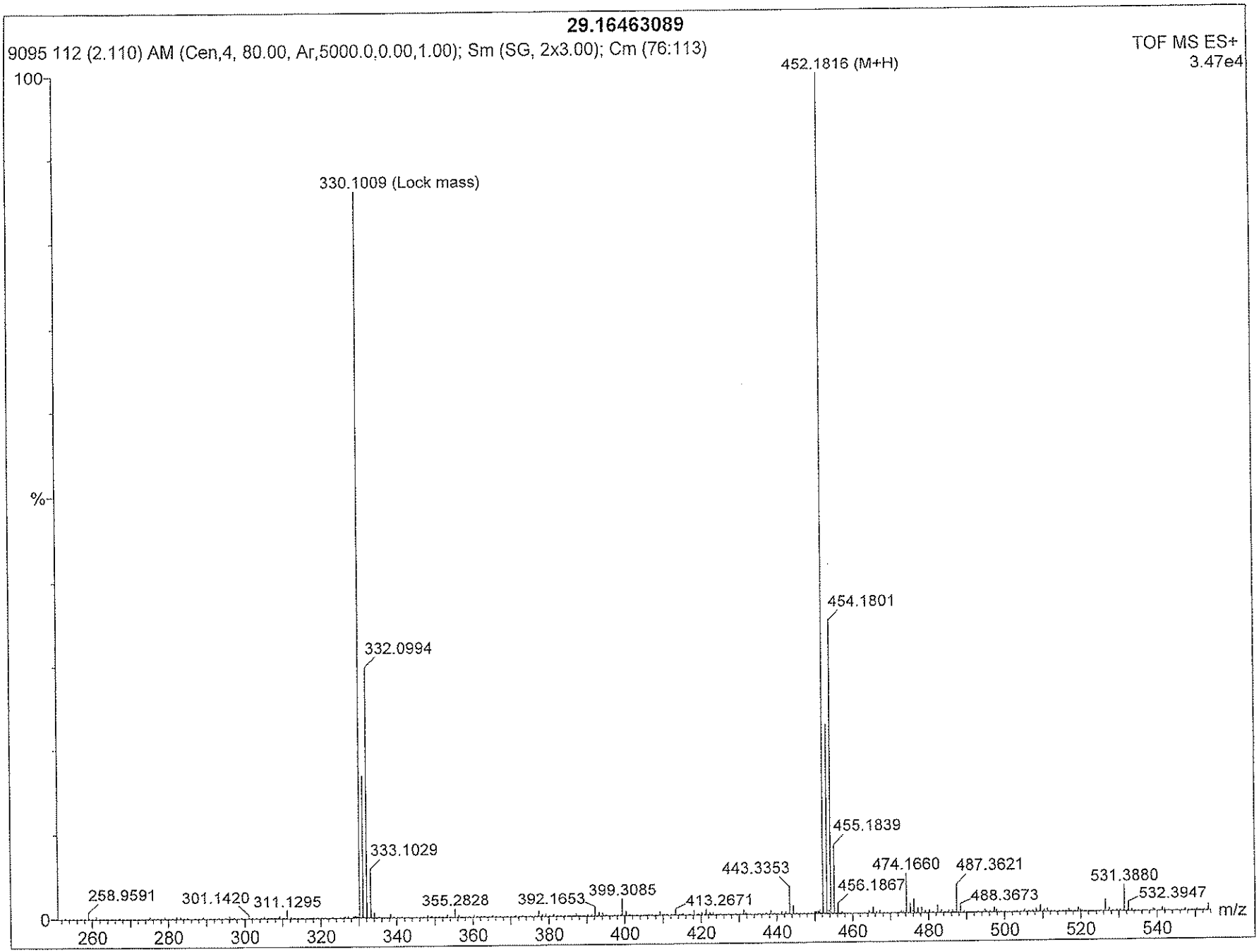
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3.47e4
452.1816 (M+H)
330.1009 (Lock mass)
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332.0994
455.1839
333.1029
443.3353
474.1660
487.3621
531.3880
456.1867
488.3673
532.3947
258.9591
301.1420
311.1295
355.2828
392.1653
399.3085
413.2671
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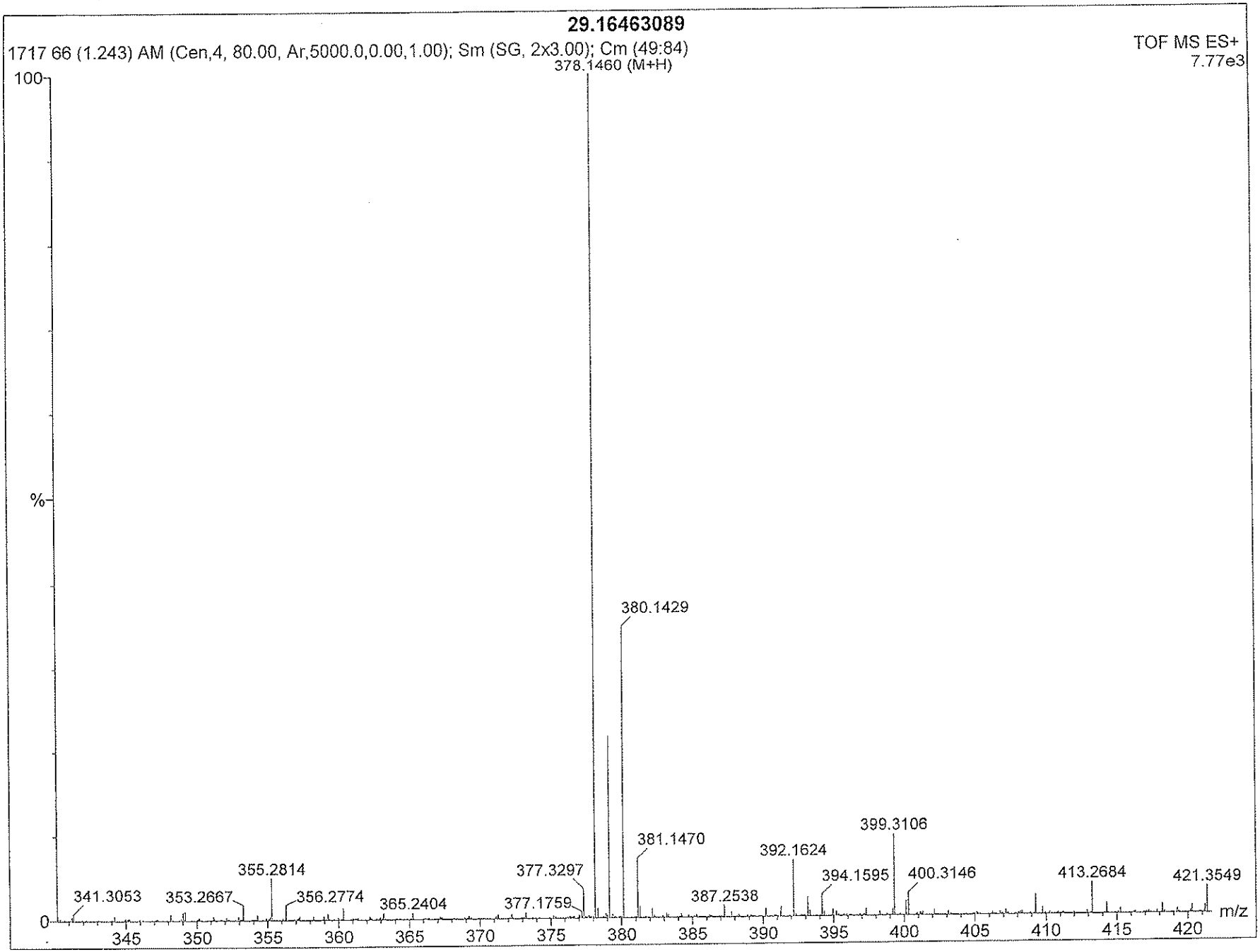
500
520
540
m/z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1717 66 (1.243) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (49:84)
TOF MS ES+
7.77e3
378.1460 (M+H)
100
%
0
380.1429
381.1470
399.3106
392.1624
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400.3146
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377.3297
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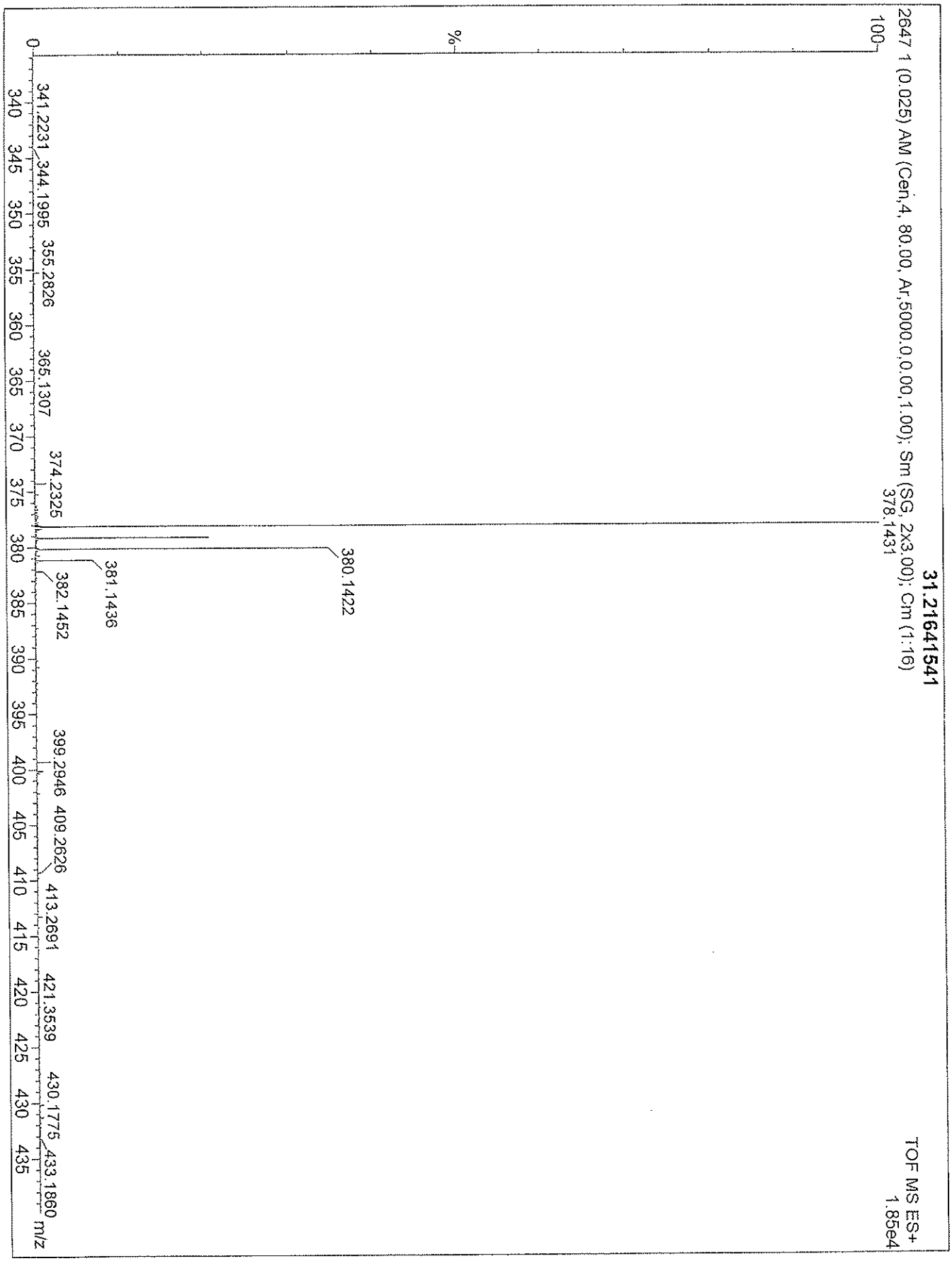
365.2404
377.1759
387.2538
345
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
m/z

					<5 ppm		H atom
Compound number	molecular Formula	Calculated [M+H]+	Measured [M+H]+	mDa	ppm	EXACT (Measured)	1.007825
15		378.1445	378.1431	-1.4	-3.7	377.135275	
14		364.1289	364.1276	-1.3	-3.6	363.119775	
17		392.1602	392.1588	-1.4	-3.6	391.150975	
29		394.1394	394.1376	-1.8	-4.6	393.129775	


31.21641541
2647 1 (0.025) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:16)
TOF MS ES+
1.85e4
100
%
0
378.1431
380.1422
381.1436
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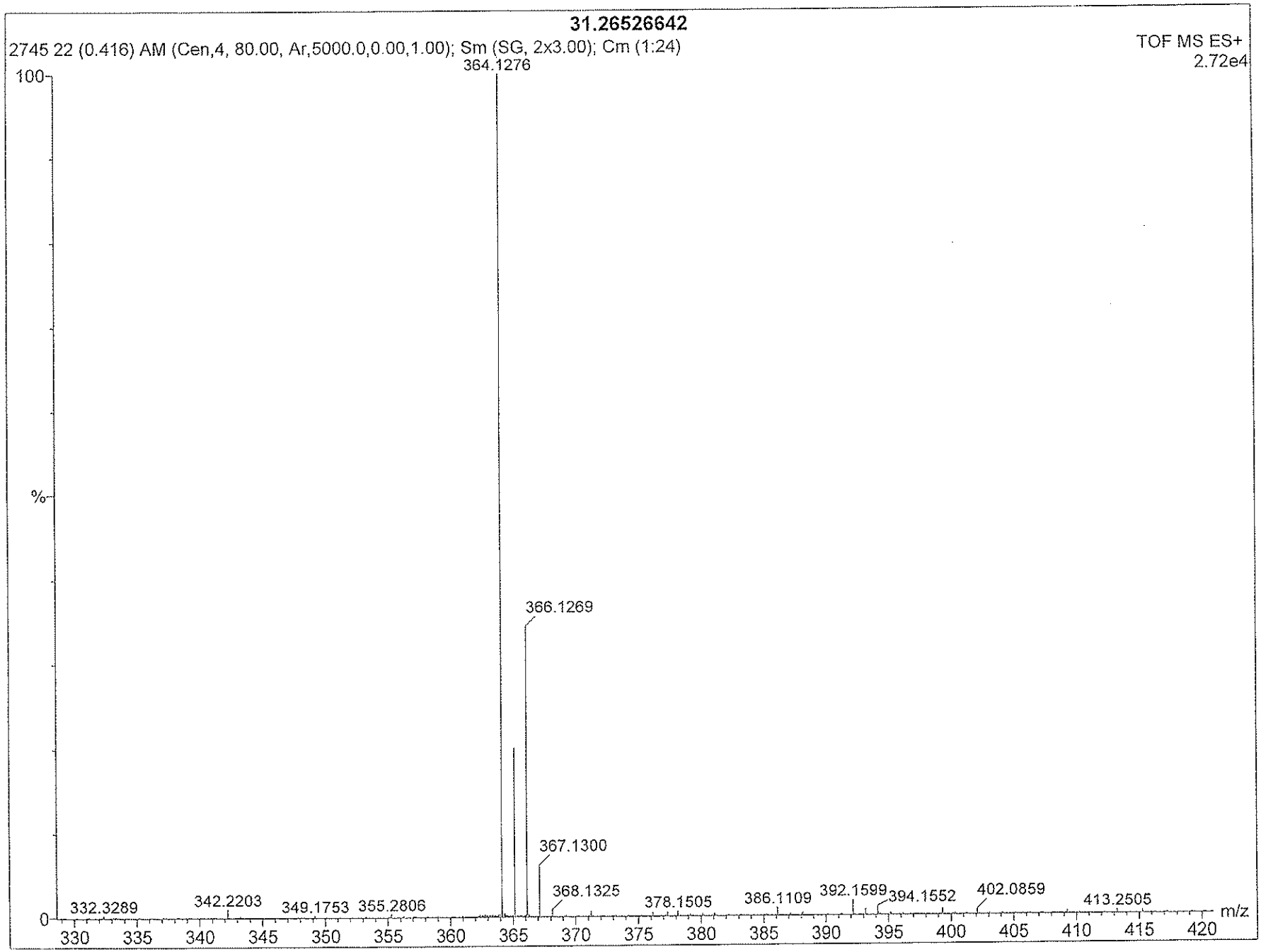
31.26526642
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TOF MS ES+
2.72e4
100
%
0
364.1276
366.1269
367.1300
368.1325
332.3289
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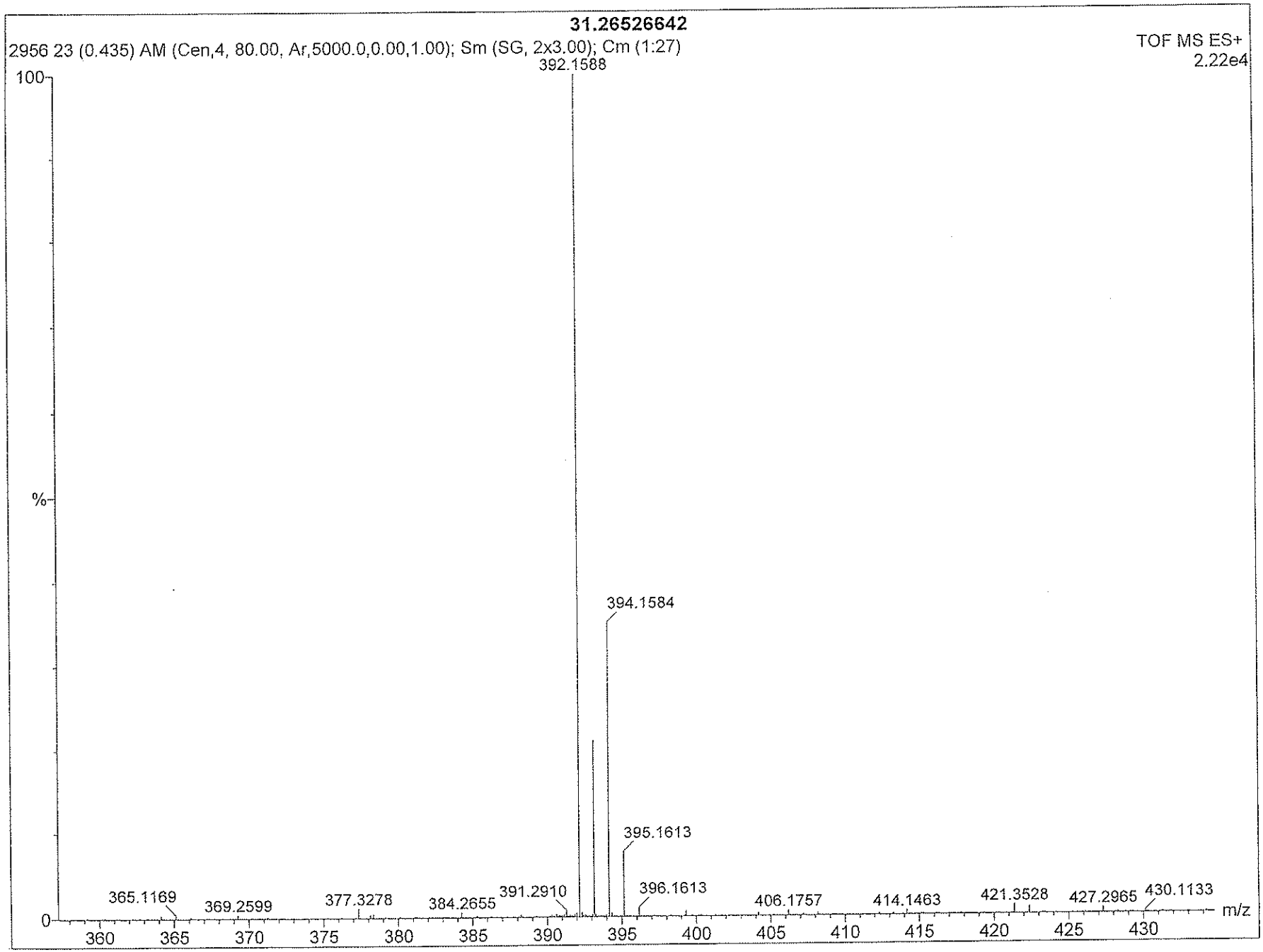
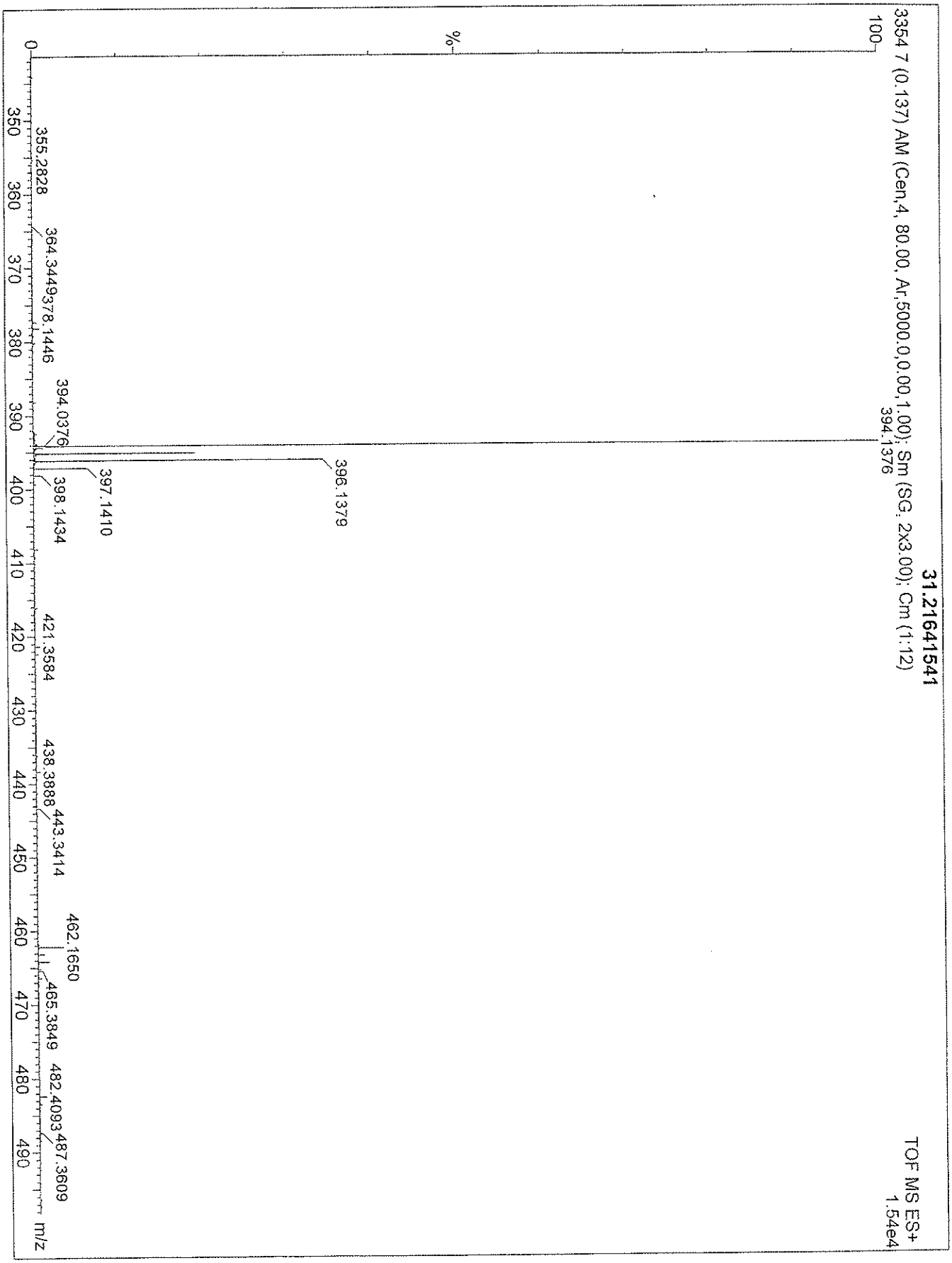
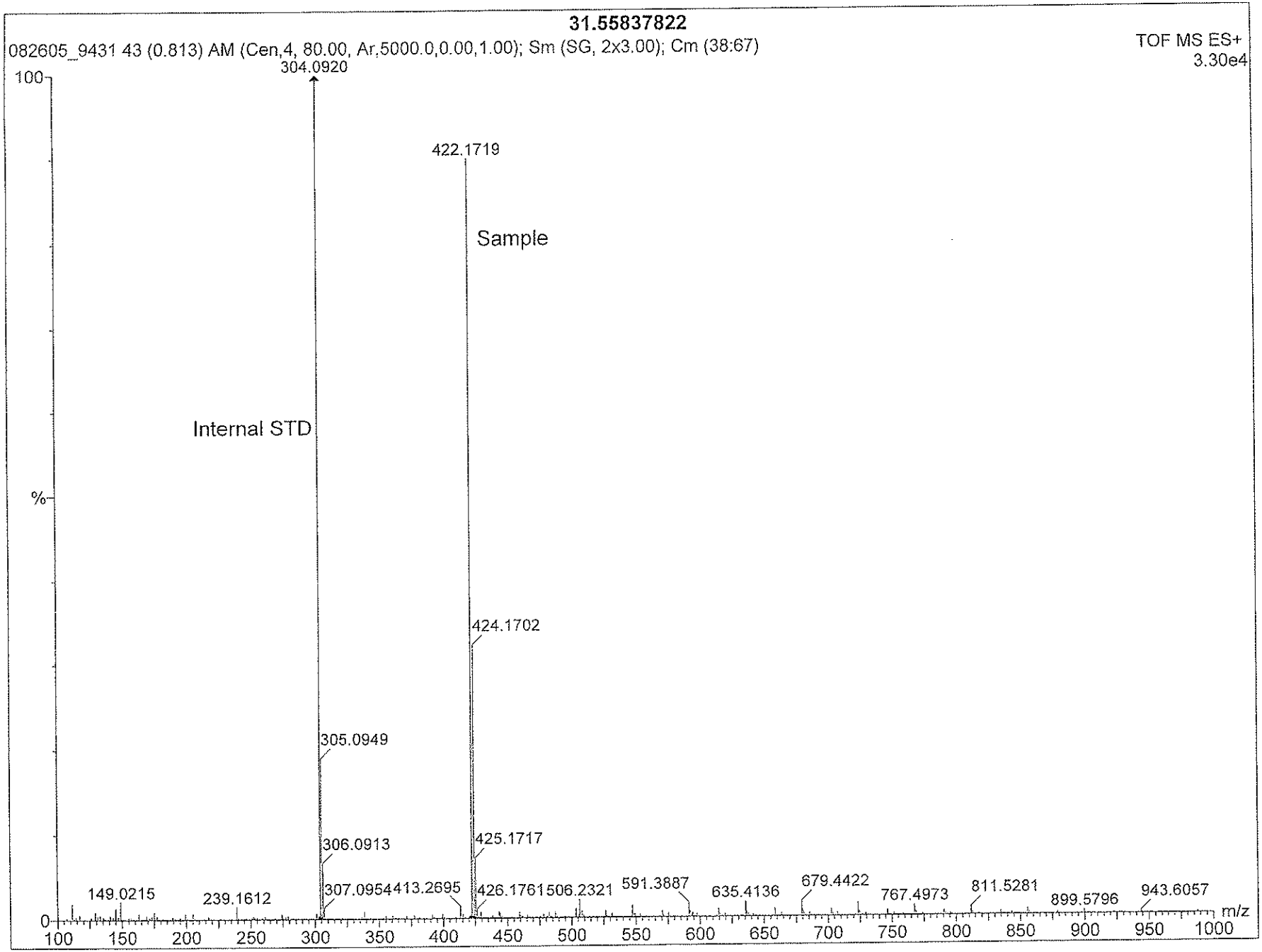
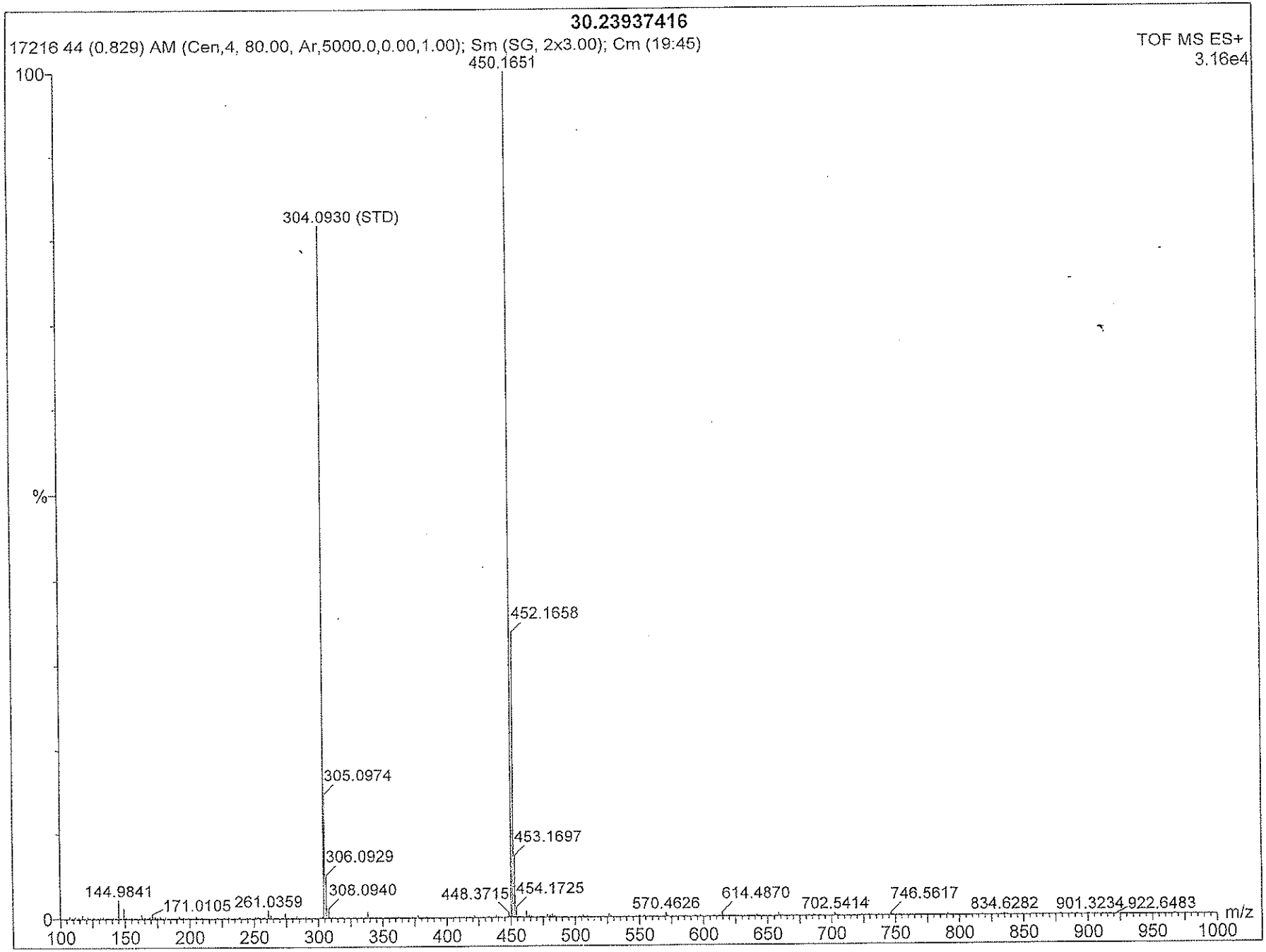

31.26526642
2956 23 (0.435) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:27)
TOF MS ES+
2.22e4
100
%
0
392.1588
394.1584
395.1613
365.1169
369.2599
377.3278
384.2655
391.2910
396.1613
406.1757
414.1463
421.3528
427.2965
430.1133
360
365
370
375
380
385
390
395
400
405
410
415
420
425
430
m/z

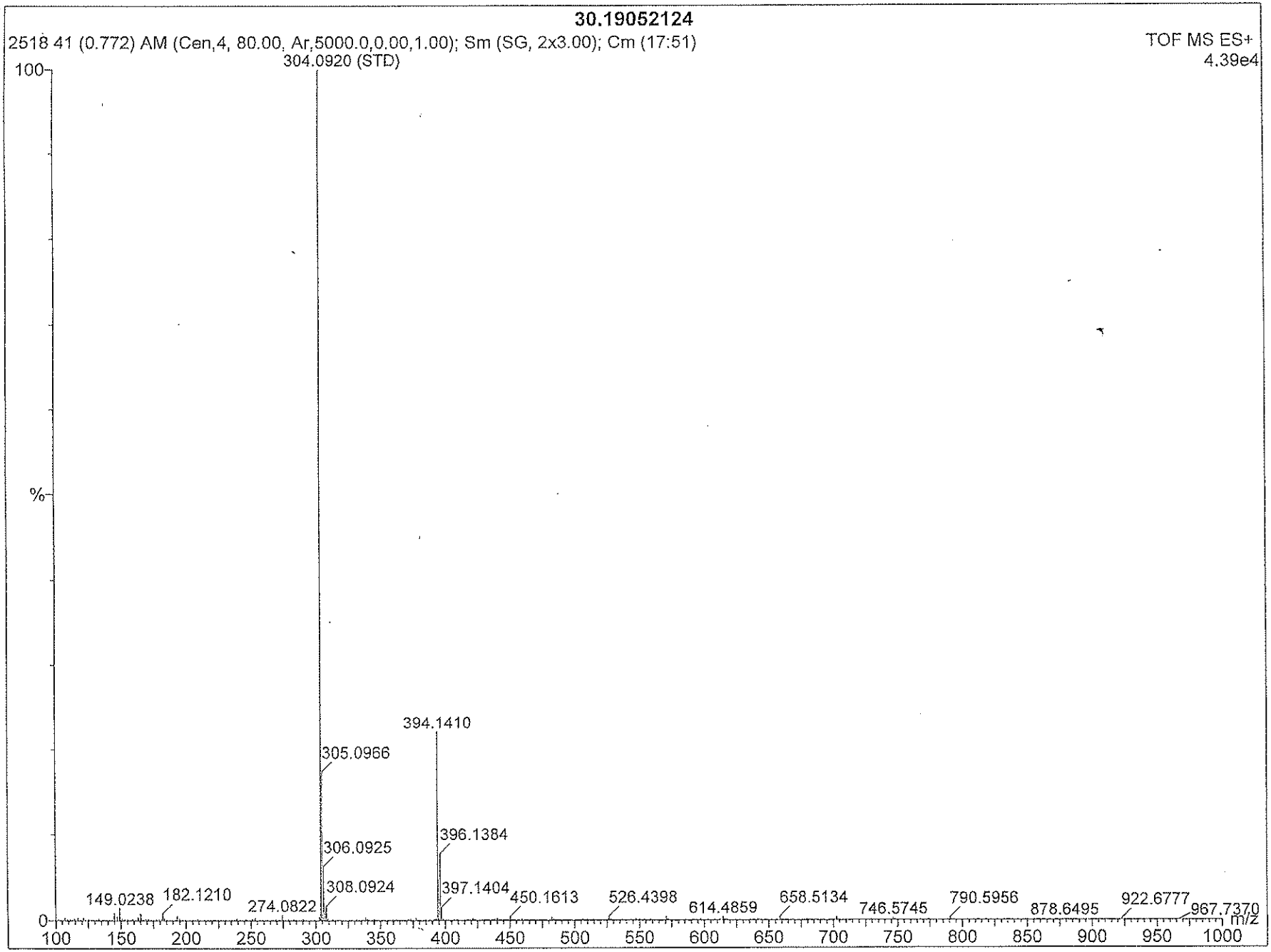

3354 7 (0.137) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:12)
31.21641541
TOF MS ES+
1.54e4
100
%
0
394.1376
396.1379
397.1410
398.1434
394.0376
378.1446
364.3449
355.2828
421.3584
438.3888
443.3414
462.1650
465.3849
482.4093
487.3609
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
m/z

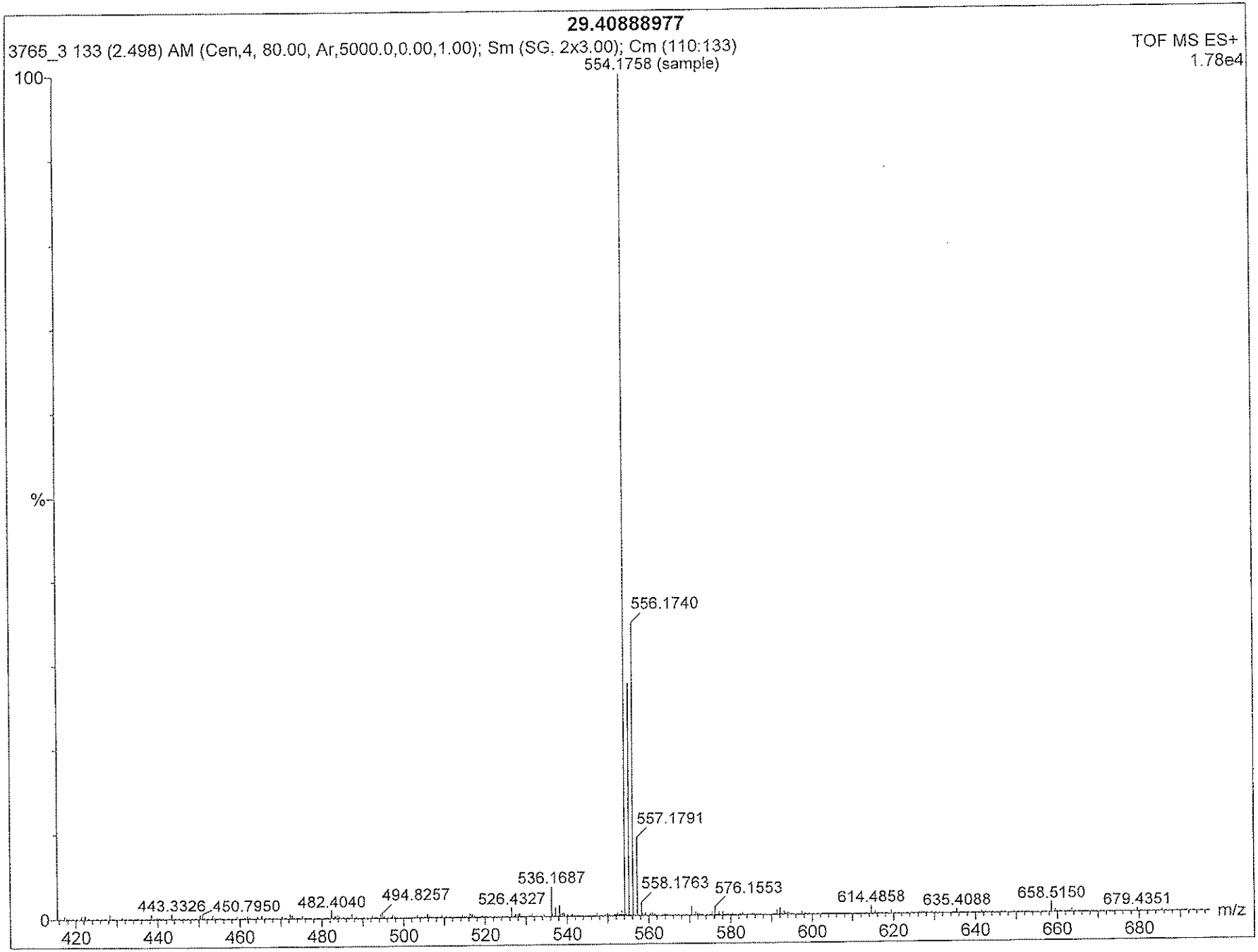
						<5 ppm		H atom
Compound number	molecular Formula	Calculated [M+H]+	Measured [M+H]+	mDa	ppm	EXACT (Measured)		1.007825
38		422.1707	422.1719	1.2	2.8	421.164075		


31.55837822
082605_9431 43 (0.813) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (38:67)
TOF MS ES+
3.30e4
100
%
0
304.0920
422.1719
Sample
Internal STD
424.1702
305.0949
306.0913
425.1717
149.0215
239.1612
307.0954
413.2695
426.1761
506.2321
591.3887
635.4136
679.4422
767.4973
811.5281
899.5796
943.6057
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000

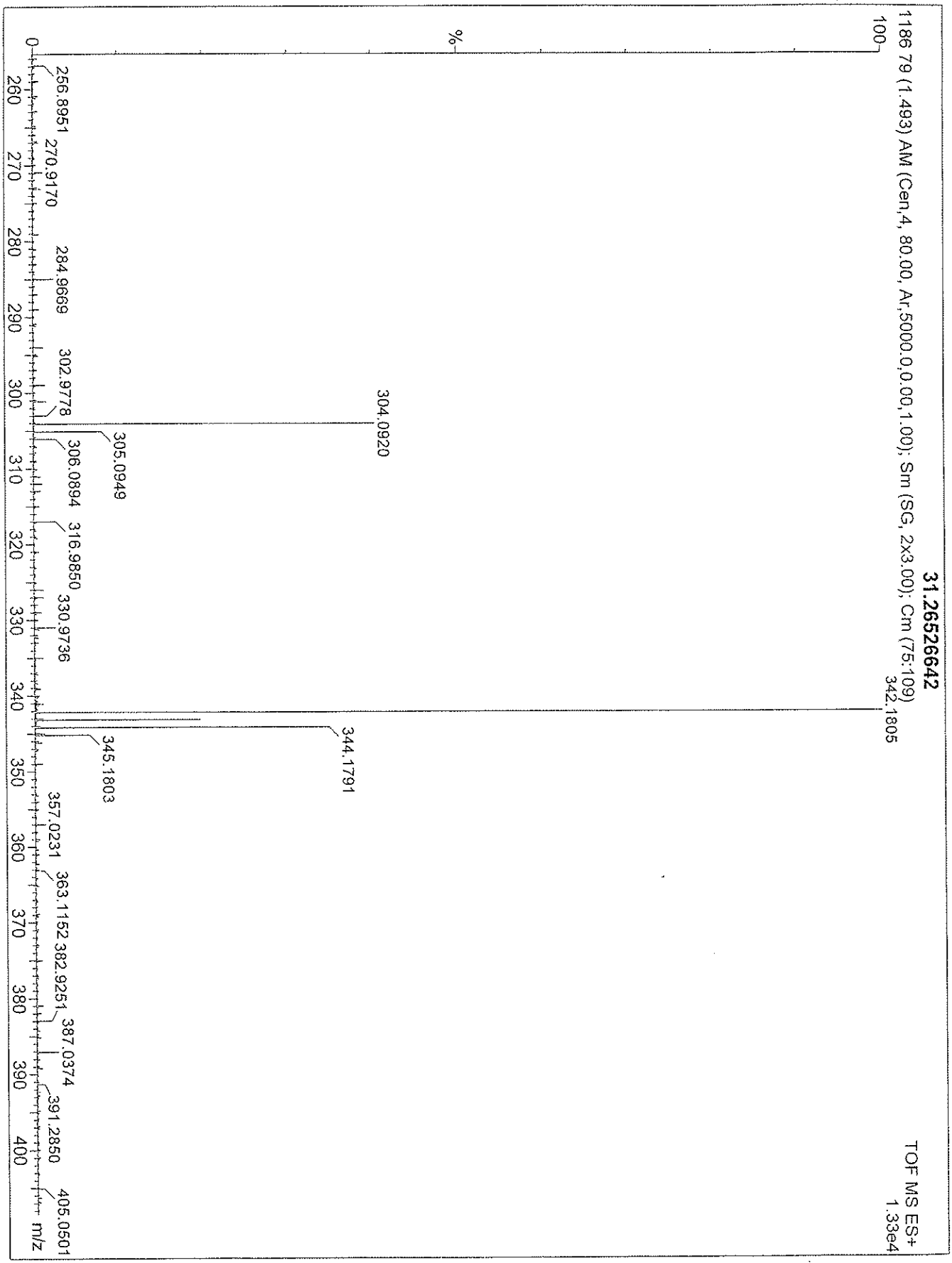
					<5 ppm		H atom
Compound number	molecular Formula	Calculated [M+H]+	Measured [M+H]+	mDa	ppm	EXACT (Measured)	1.007825
40		450.1656	450.1651	-0.5	-1.1	449.157275	
42		394.1394	394.1410	1.6	4.1	393.133175	
41		576.1585					

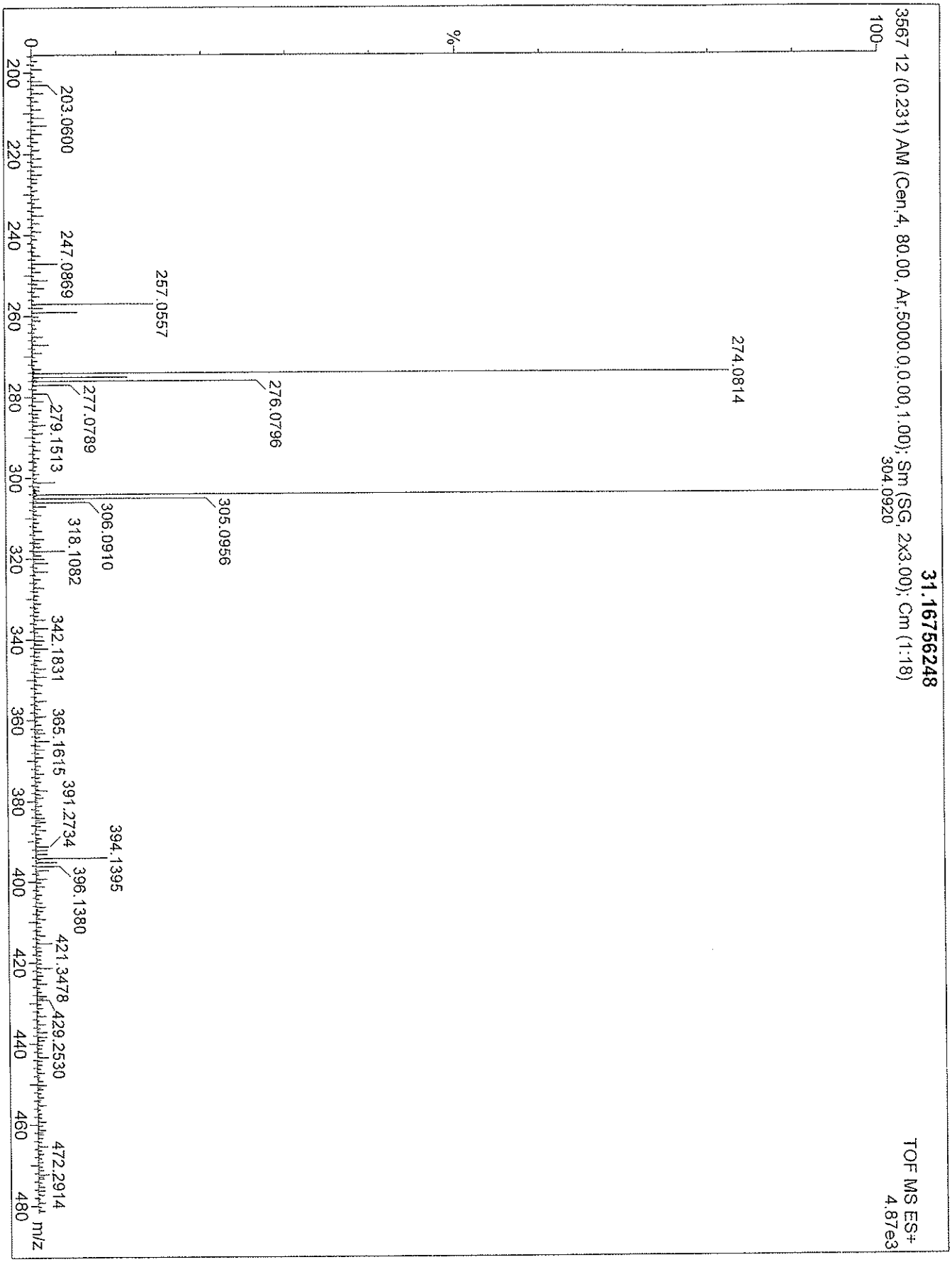

30.23937416
17216 44 (0.829) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (19:45)
TOF MS ES+
3.16e4
100
%
0
450.1651
304.0930 (STD)
452.1658
305.0974
453.1697
306.0929
308.0940
454.1725
144.9841
171.0105
261.0359
448.3715
570.4626
614.4870
702.5414
746.5617
834.6282
901.3234
922.6483
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

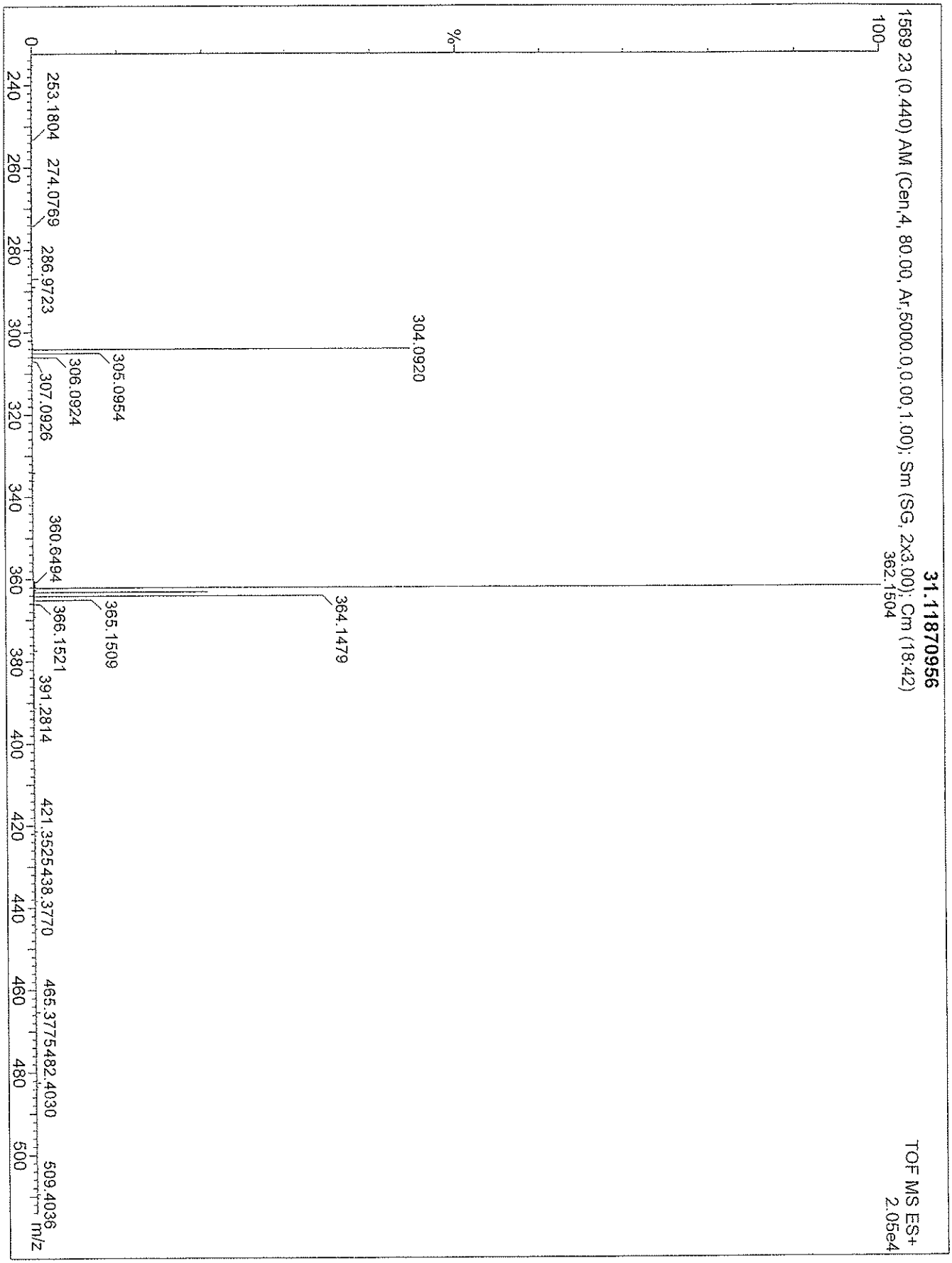

30.19052124
2518 41 (0.772) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (17:51)
TOF MS ES+
4.39e4
100
%
0
304.0920 (STD)
394.1410
305.0966
396.1384
306.0925
308.0924
397.1404
149.0238
182.1210
274.0822
450.1613
526.4398
614.4859
658.5134
746.5745
790.5956
878.6495
922.6777
967.7370
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

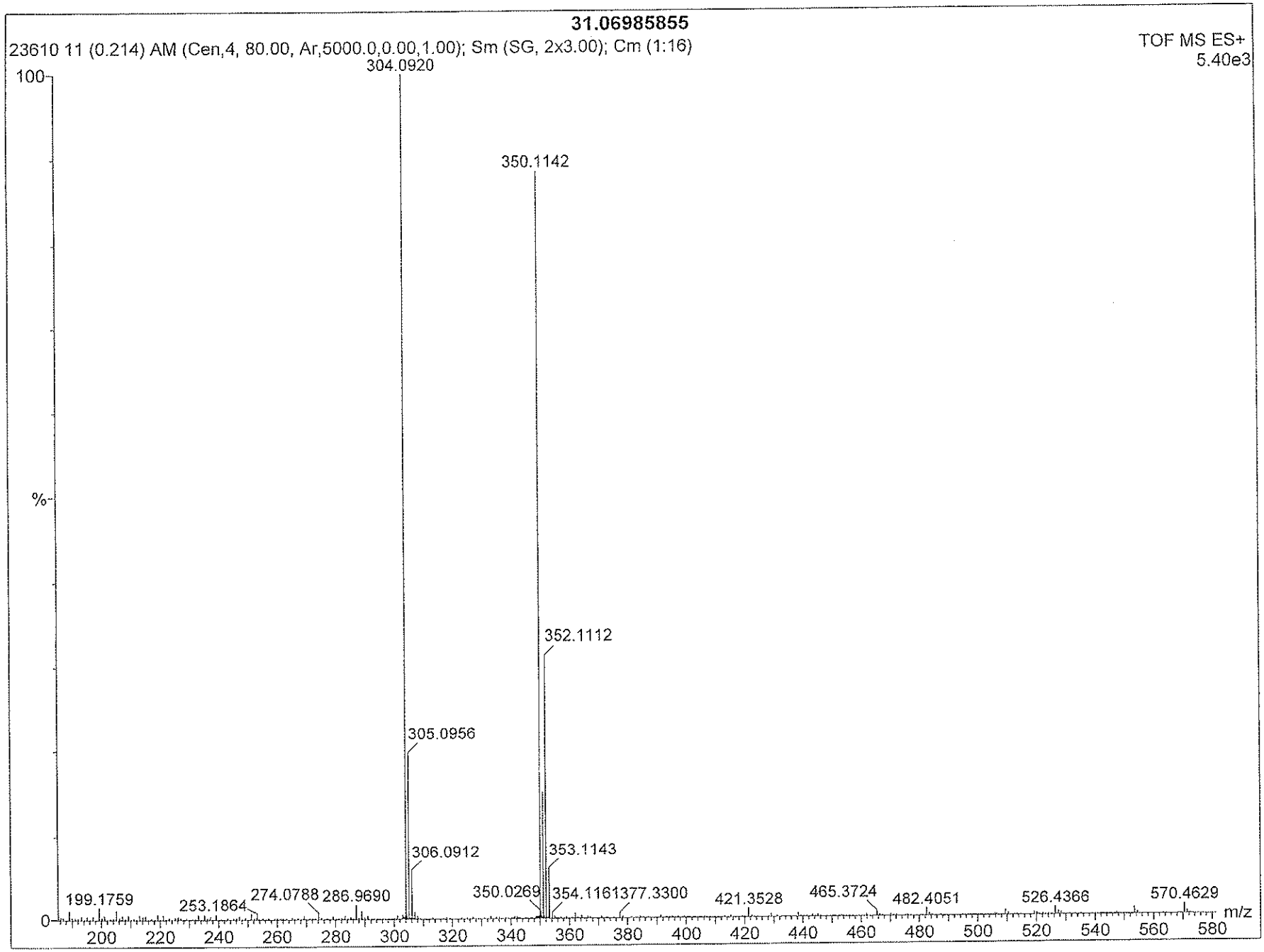

29.40888977
3765_3 133 (2.498) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (110:133)
554.1758 (sample)
TOF MS ES+
1.78e4
100
%
0
556.1740
557.1791
558.1763
536.1687
526.4327
576.1553
614.4858
635.4088
658.5150
679.4351
443.3326
450.7950
482.4040
494.8257
420
440
460
480
500
520
540
560
580
600
620
640
660
680
m/z

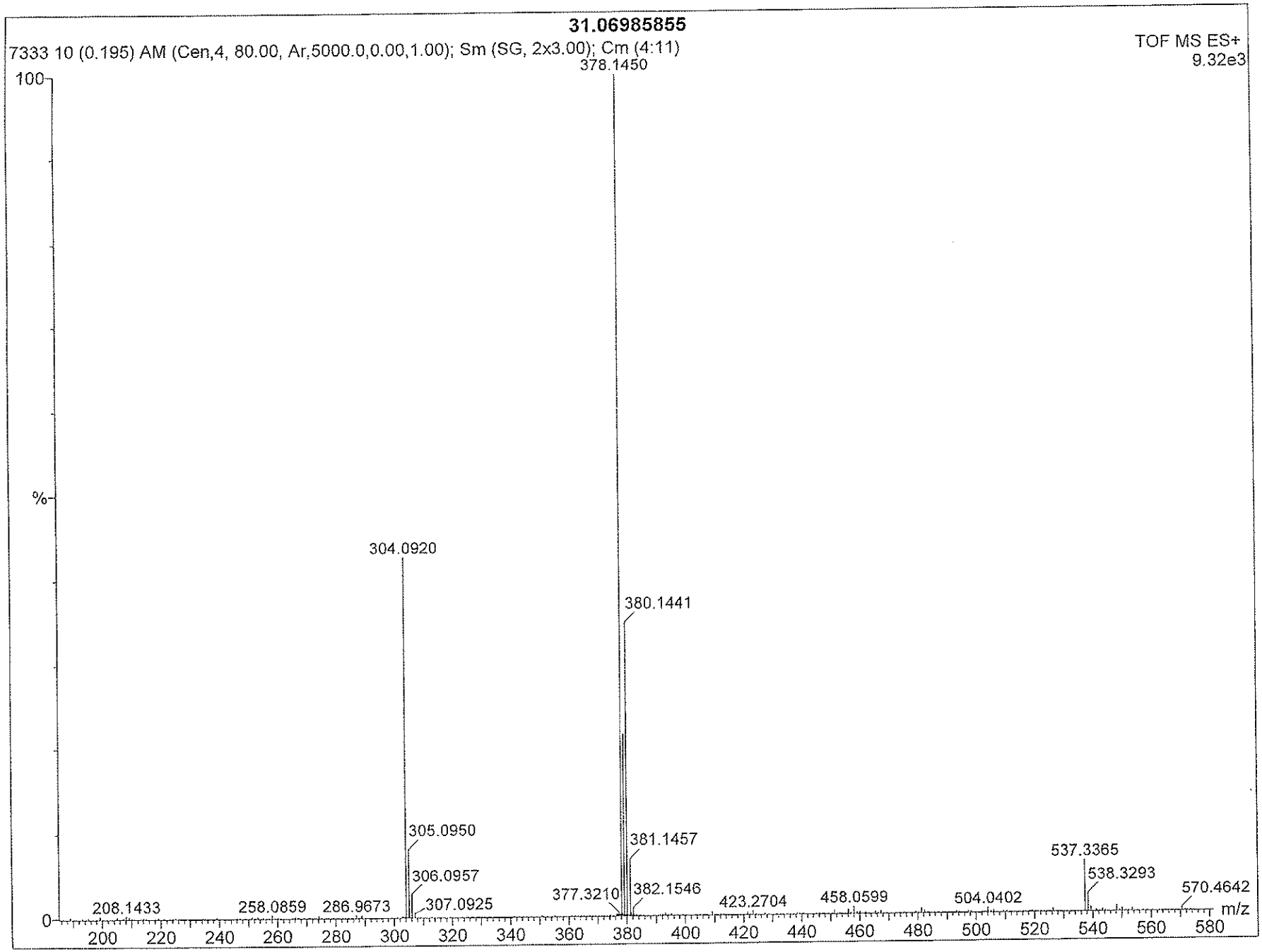
	Sep-19-05				<5 ppm		H atom
Compound number	molecular Formula	Calculated [M+H]+	Measured [M+H]+	mDa	ppm	EXACT (Measured)	1.007825035
3		342.1809	342.1805	-0.4	-1.2	341.172675	
4		274.0819	274.0814	-0.5	-1.8	273.073575	
9		378.1445	362.1504	0.8	2.1	377.137475	Lost Oxygen
13		350.1132	350.1142	1	2.9	349.106375	
18		378.1445	378.145	0.5	1.3	377.137175	
19		378.1445	378.144	-0.5	-1.3	377.136175	
20		377.1605	377.1607	0.2	0.5	376.152875	
22		420.1551	420.1544	-0.7	-1.7	419.146575	
23		406.1758	406.1743	-1.5	-3.7	405.166475	
25		406.1394	406.1395	0.1	0.2	405.131675	
27		392.1602	392.1588	-1.4	-3.6	391.150975	
28		380.1238	380.1239	0.1	0.3	379.116075	
31		436.1864	436.1852	-1.2	-2.8	435.177375	

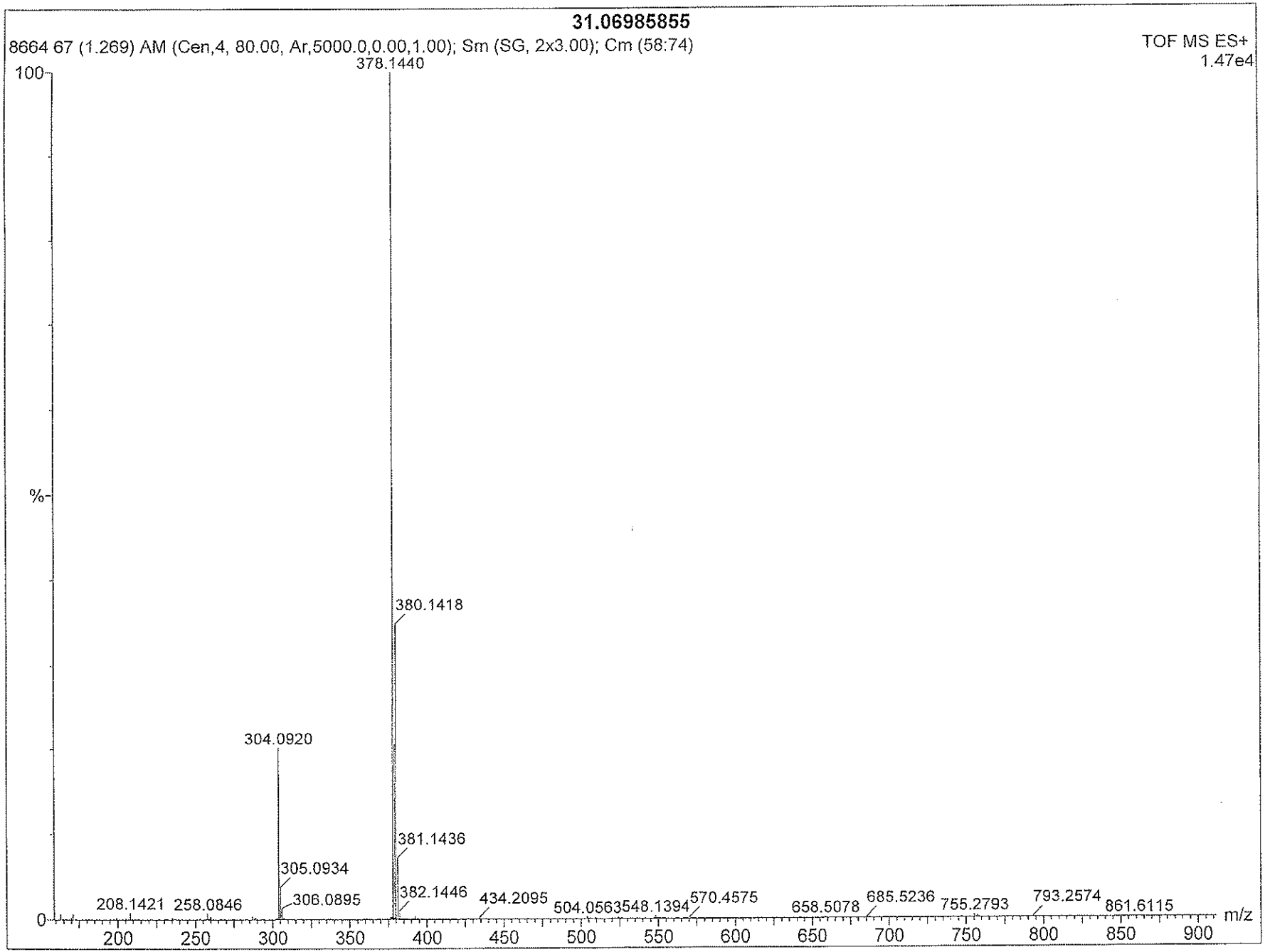

31.26526642
1186 79 (1.493) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (75:109)
TOF MS ES+
1.33e4
100
%
0
342.1805
344.1791
345.1803
304.0920
305.0949
306.0894
316.9850
330.9736
302.9778
284.9669
270.9170
256.8951
357.0231
363.1152
382.9251
387.0374
391.2850
405.0501
260
270
280
290
300
310
320
330
340
350
360
370
380
390
400
m/z

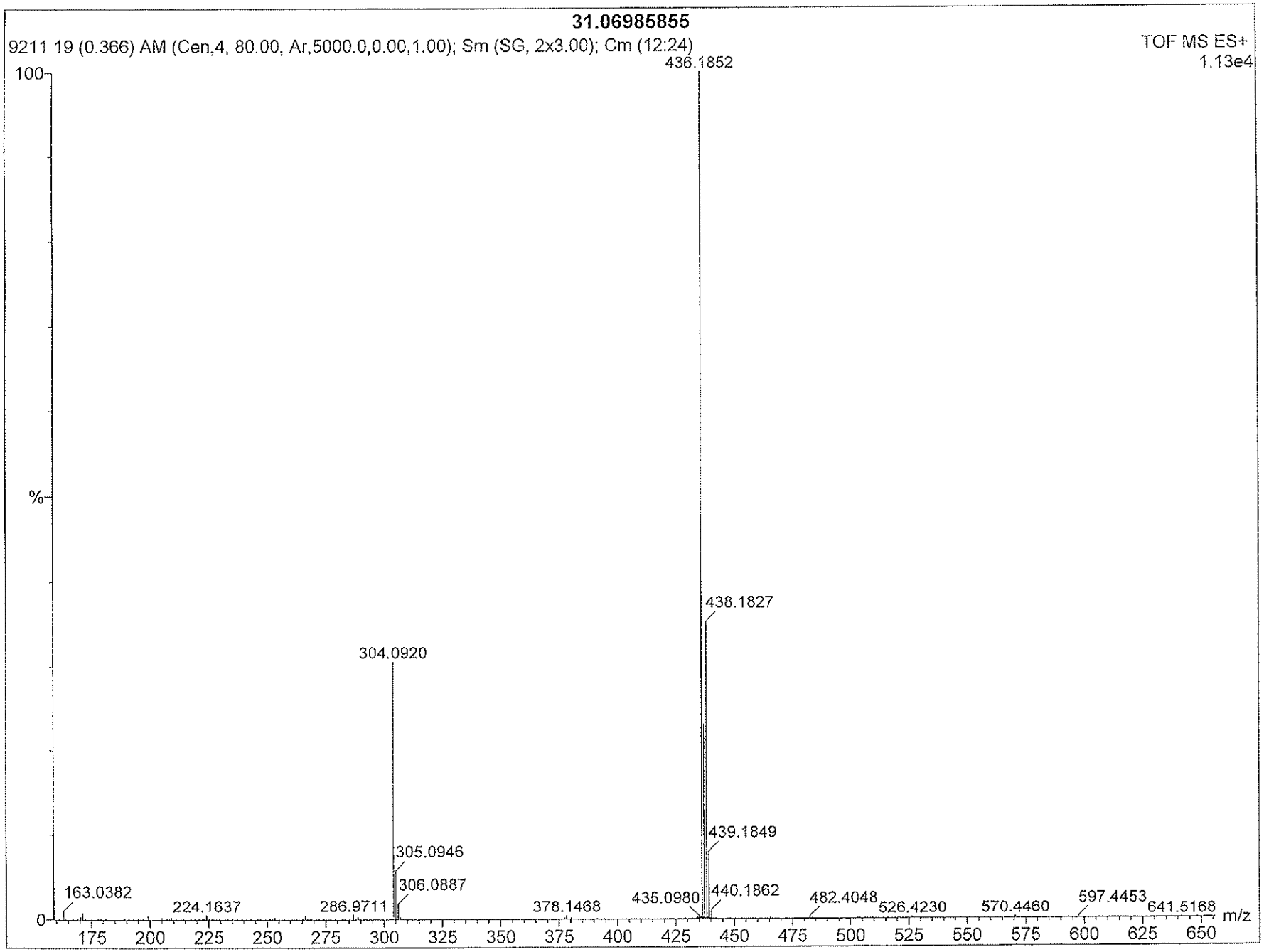

31.16756248
3567 12 (0.231) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:18)
TOF MS ES+
4.87e3
100
%
0
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
m/z
203.0600
247.0869
257.0557
274.0814
276.0796
277.0789
279.1513
304.0920
305.0956
306.0910
318.1082
342.1831
365.1615
391.2734
394.1395
396.1380
421.3478
429.2530
472.2914

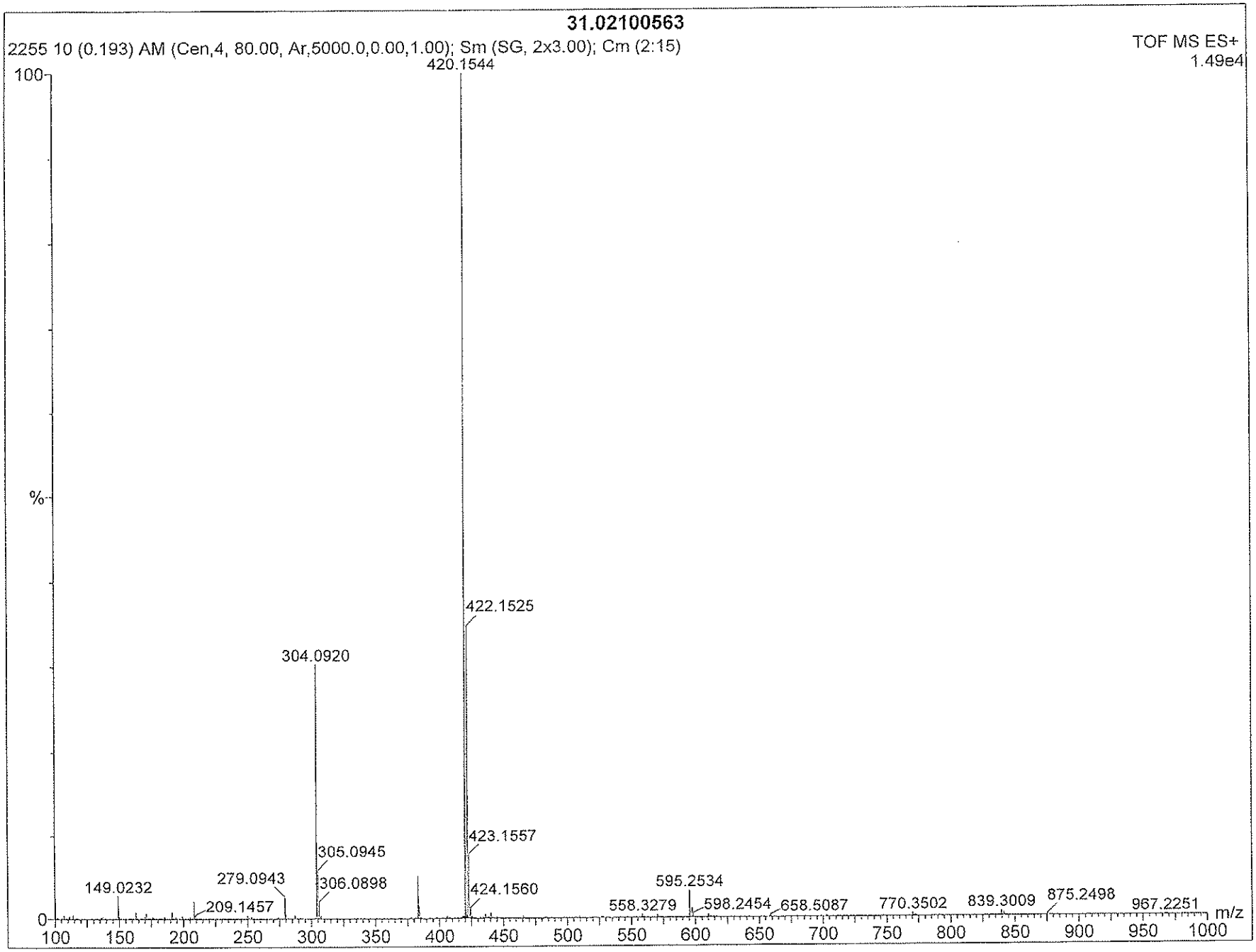

31.11870956
1569 23 (0.440) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (18:42)
TOF MS ES+
2.05e4
100
%
0
362.1504
304.0920
364.1479
305.0954
306.0924
307.0926
253.1804
274.0769
286.9723
360.6494
365.1509
366.1521
391.2814
421.3525
438.3770
465.3775
482.4030
509.4036
240
260
280
300
320
340
360
380
400
420
440
460
480
500
m/z

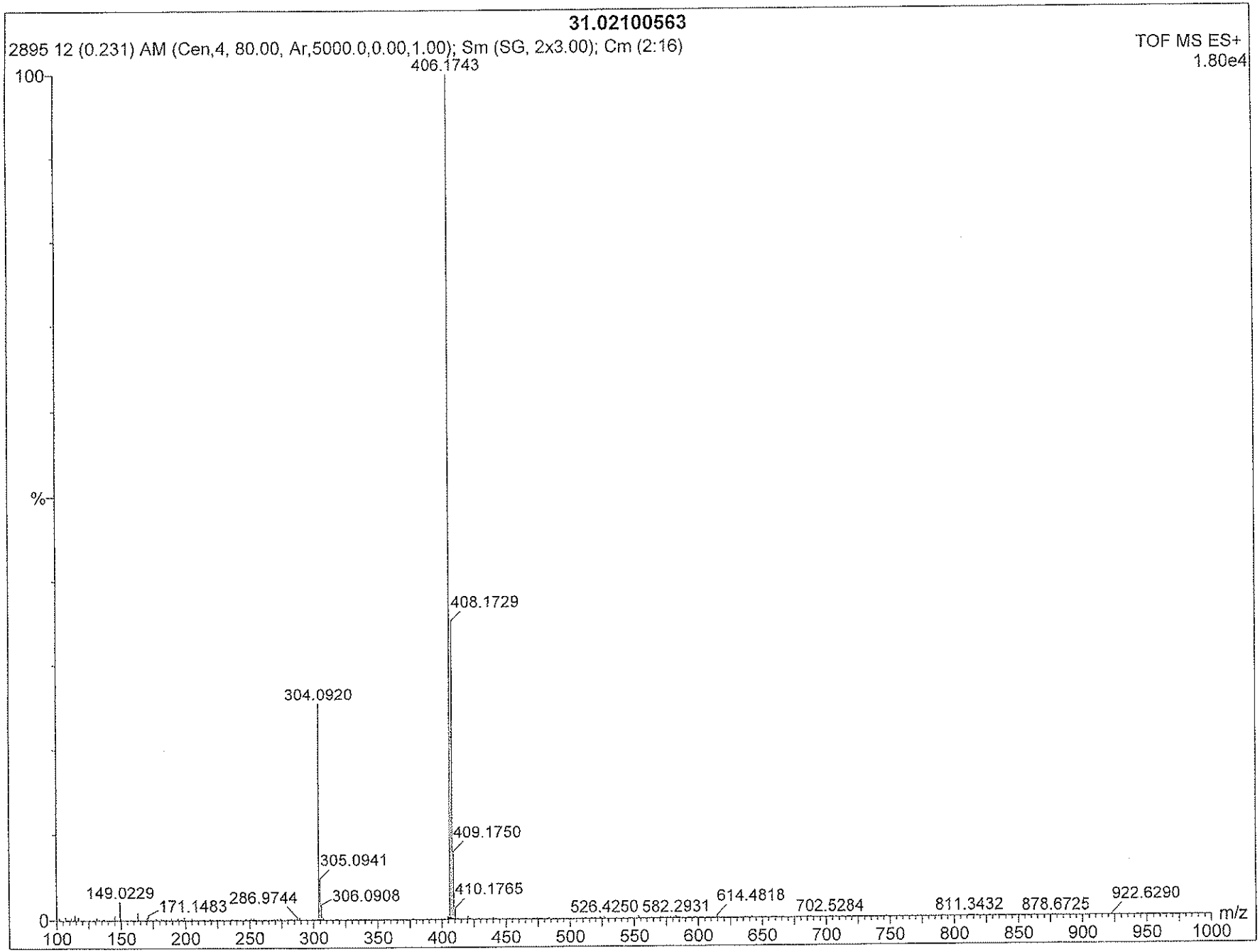

31.06985855
23610 11 (0.214) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:16)
TOF MS ES+
5.40e3
100
%
0
304.0920
350.1142
352.1112
305.0956
306.0912
353.1143
199.1759
253.1864
274.0788
286.9690
350.0269
354.1161
377.3300
421.3528
465.3724
482.4051
526.4366
570.4629
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580
m/z

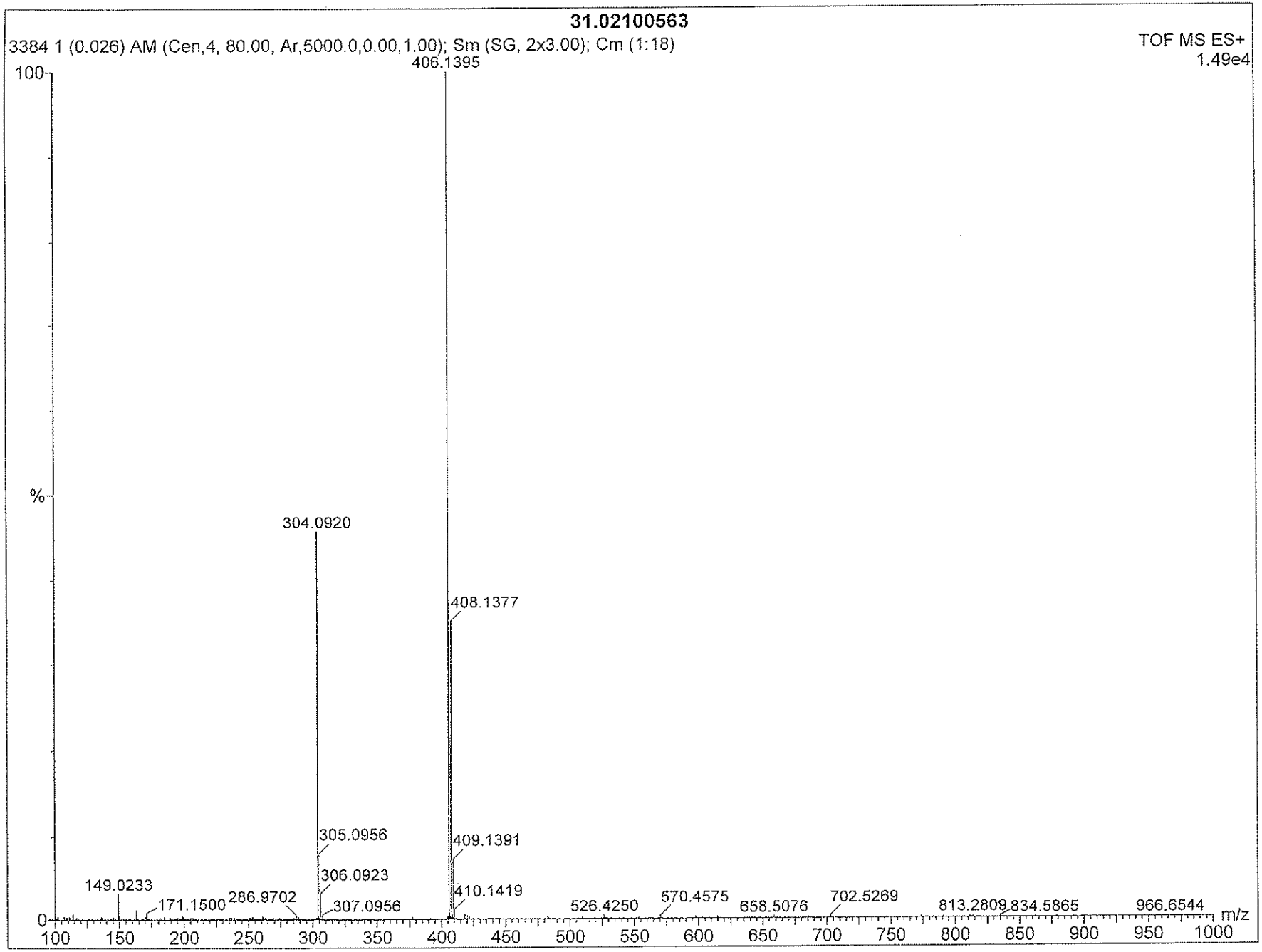

31.06985855
7333 10 (0.195) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (4:11)
TOF MS ES+
9.32e3
100
%
0
378.1450
304.0920
380.1441
305.0950
381.1457
306.0957
307.0925
377.3210
382.1546
208.1433
258.0859
286.9673
423.2704
458.0599
504.0402
537.3365
538.3293
570.4642
m/z
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580

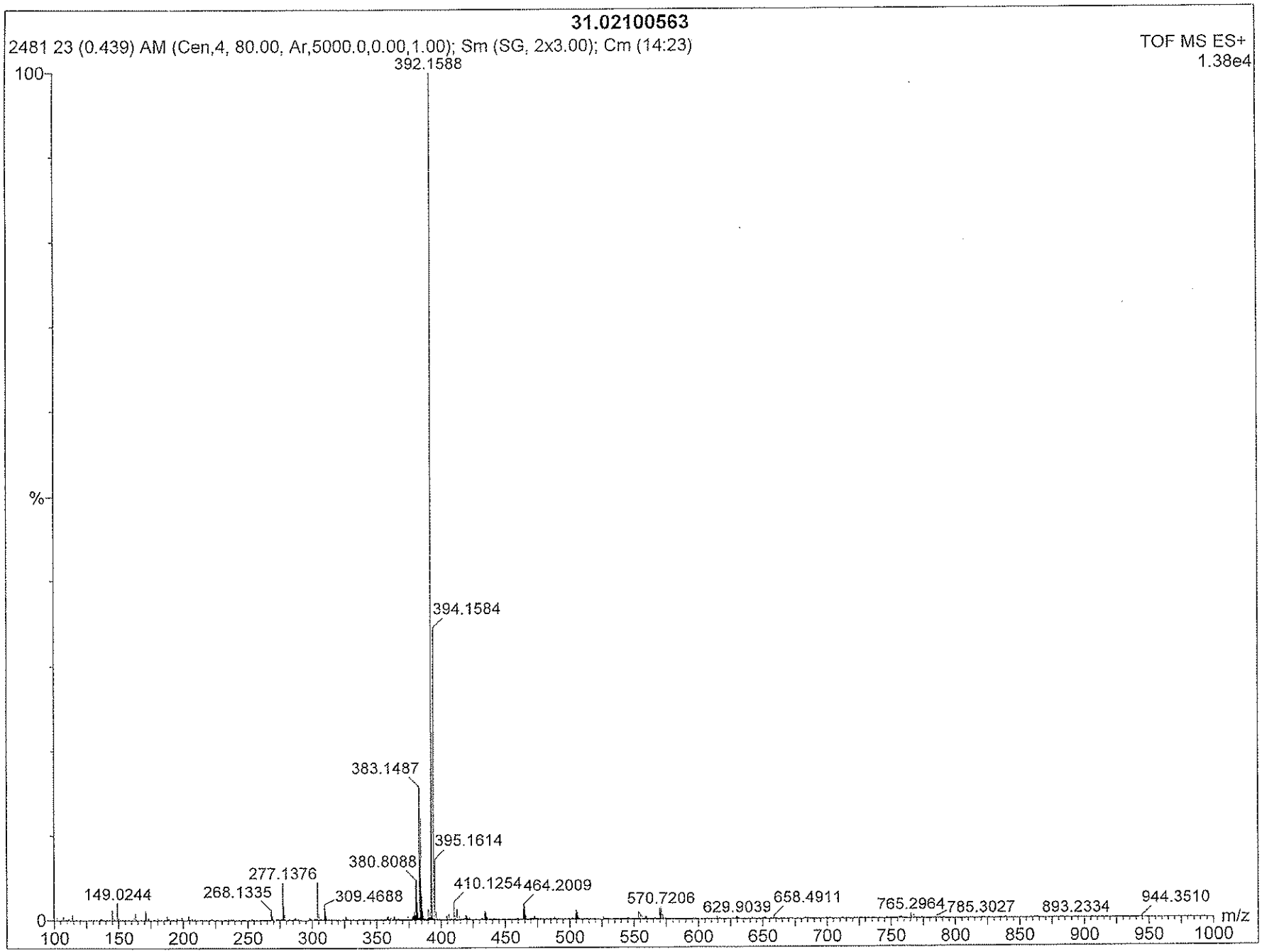

31.06985855
8664 67 (1.269) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (58:74)
TOF MS ES+
1.47e4
100
%
0
378.1440
380.1418
304.0920
381.1436
305.0934
382.1446
306.0895
208.1421
258.0846
434.2095
504.0563
548.1394
570.4575
658.5078
685.5236
755.2793
793.2574
861.6115
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z

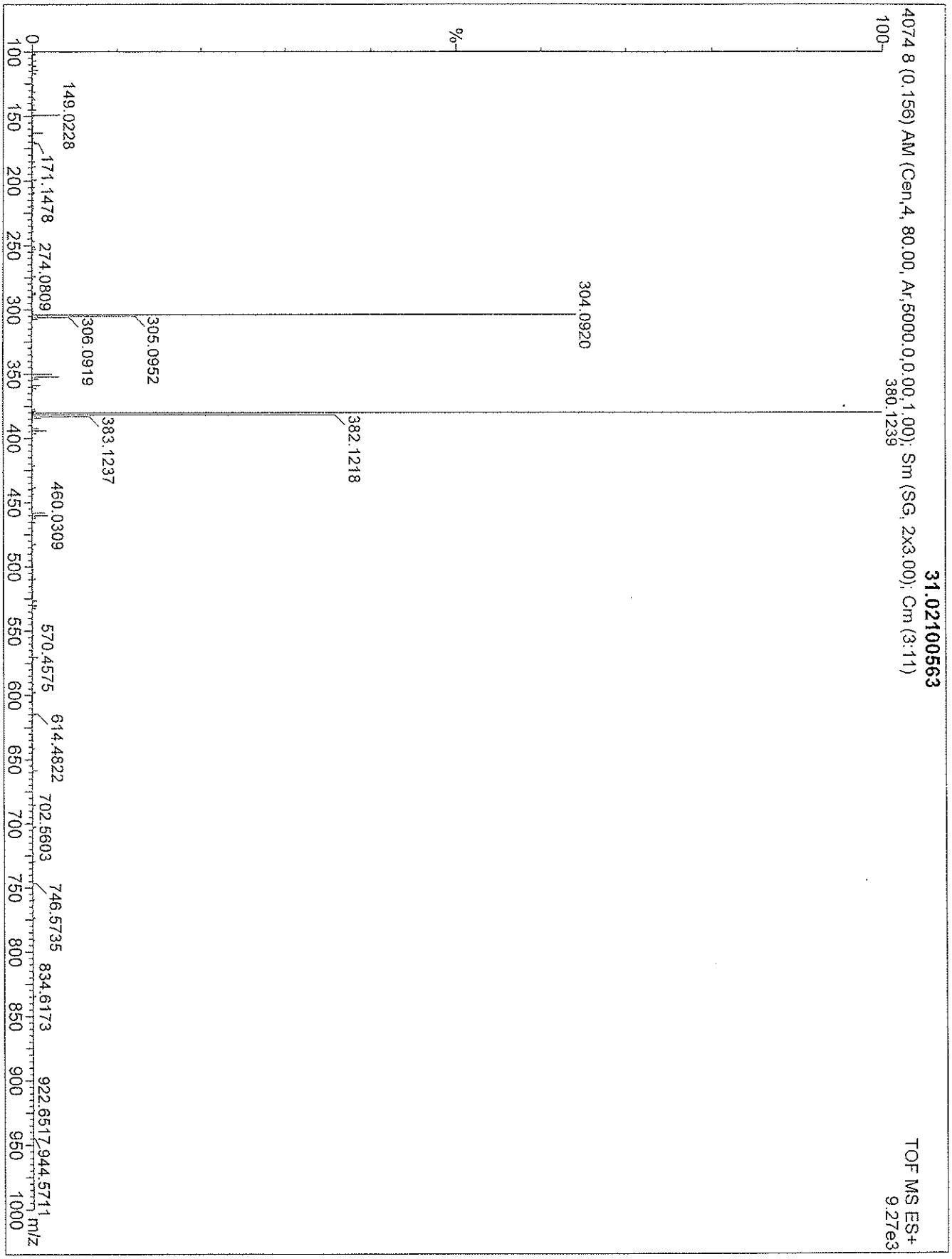

31.06985855
9211 19 (0.366) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (12:24)
TOF MS ES+
1.13e4
100
%
0
436.1852
438.1827
304.0920
439.1849
305.0946
306.0887
163.0382
224.1637
286.9711
378.1468
435.0980
440.1862
482.4048
526.4230
570.4460
597.4453
641.5168
m/z
175
200
225
250
275
300
325
350
375
400
425
450
475
500
525
550
575
600
625
650

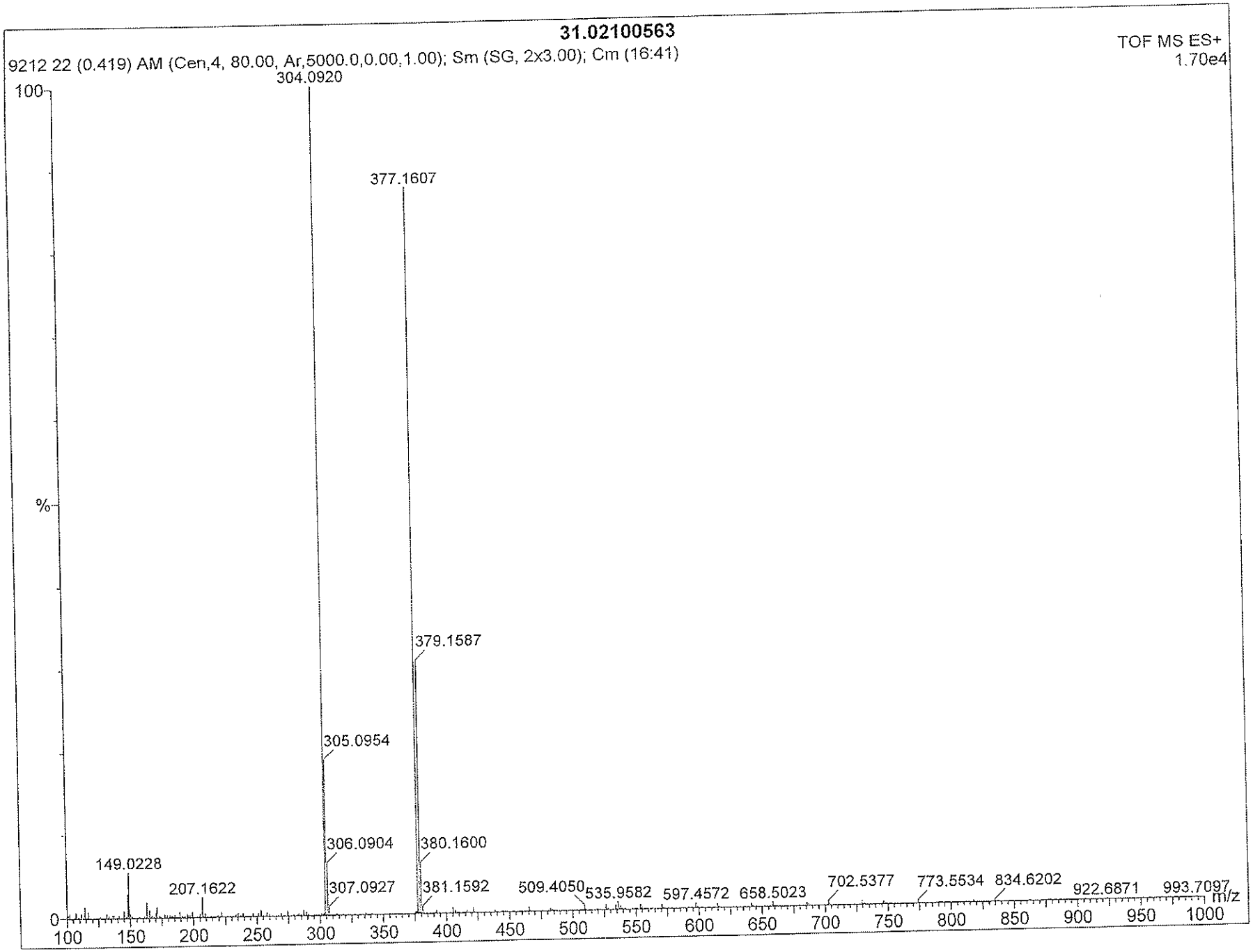

31.02100563
2255 10 (0.193) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (2:15)
TOF MS ES+
1.49e4
100
%
0
420.1544
422.1525
304.0920
423.1557
305.0945
306.0898
149.0232
279.0943
209.1457
424.1560
595.2534
558.3279
598.2454
658.5087
770.3502
839.3009
875.2498
967.2251
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000


31.02100563
2895 12 (0.231) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (2:16)
TOF MS ES+
1.80e4
100
%
0
406.1743
408.1729
304.0920
409.1750
305.0941
149.0229
171.1483
286.9744
306.0908
410.1765
526.4250
582.2931
614.4818
702.5284
811.3432
878.6725
922.6290
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000


31.02100563
3384 1 (0.026) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:18)
TOF MS ES+
1.49e4
406.1395
304.0920
408.1377
305.0956
409.1391
306.0923
410.1419
149.0233
171.1500
286.9702
307.0956
526.4250
570.4575
658.5076
702.5269
813.2809
834.5865
966.6544
100
%
0
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z


31.02100563
2481 23 (0.439) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (14:23)
TOF MS ES+
1.38e4
100
%
0
392.1588
394.1584
383.1487
395.1614
380.8088
277.1376
149.0244
268.1335
309.4688
410.1254
464.2009
570.7206
629.9039
658.4911
765.2964
785.3027
893.2334
944.3510
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000


31.02100563
4074 8 (0.156) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (3:11)
TOF MS ES+
9.27e3
%
100
0
380.1239
304.0920
305.0952
306.0919
382.1218
383.1237
149.0228
171.1478
274.0809
460.0309
570.4575
614.4822
702.5603
746.5735
834.6173
922.6517
944.5711
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z


31.02100563
9212 22 (0.419) AM (Cen,4, 80.00, Ar,5000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (16:41)
TOF MS ES+
1.70e4
100
%
0
304.0920
377.1607
379.1587
305.0954
306.0904
380.1600
149.0228
207.1622
307.0927
381.1592
509.4050
535.9582
597.4572
658.5023
702.5377
773.5534
834.6202
922.6871
993.7097
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000