

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
 Data File : BG043487.D
 Acq On : 4 Nov 2019 19:07
 Operator : JU
 Sample : K5657-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.177	10	15	34	rVB	118641	211555	9.60%	1.434%
2	5.116	340	345	356	rBV	114631	183398	8.32%	1.243%
3	5.597	420	427	441	rBV	529617	932491	42.32%	6.319%
4	7.196	690	699	717	rBV	563636	1087855	49.37%	7.372%
5	7.554	752	760	778	rBV	587387	1068801	48.50%	7.243%
6	8.012	831	838	847	rBV	155563	268611	12.19%	1.820%
7	8.335	882	893	903	rBV	451854	800320	36.32%	5.424%
8	9.176	1027	1036	1056	rBV	293730	628272	28.51%	4.258%
9	10.815	1307	1315	1327	rBV	173890	354321	16.08%	2.401%
10	13.265	1723	1732	1747	rBV	846833	1457390	66.14%	9.877%
11	14.088	1864	1872	1888	rBV	89939	162691	7.38%	1.103%
12	14.640	1959	1966	1982	rBV	325199	543014	24.64%	3.680%
13	16.132	2213	2220	2234	rBV	785235	1345759	61.07%	9.120%
14	17.390	2427	2434	2439	rBV	383182	628521	28.52%	4.259%
15	17.507	2449	2454	2462	rVB7	21388	33092	1.50%	0.224%
16	18.277	2579	2585	2595	rBV3	90986	159981	7.26%	1.084%
17	19.440	2778	2783	2789	rBV	48437	79320	3.60%	0.538%
18	19.798	2840	2844	2849	rVB	50993	76353	3.46%	0.517%
19	19.998	2871	2878	2890	rBV	1586232	2203659	100.00%	14.934%
20	20.286	2919	2927	2929	rBV8	14045	35479	1.61%	0.240%
21	21.291	3094	3098	3109	rBV3	125516	219241	9.95%	1.486%
22	21.379	3110	3113	3120	rVB2	23943	41310	1.87%	0.280%
23	21.655	3152	3160	3172	rBV	446934	1014802	46.05%	6.877%
24	22.442	3290	3294	3300	rBV6	20306	40108	1.82%	0.272%
25	23.118	3407	3409	3418	rVB7	26896	52067	2.36%	0.353%
26	23.312	3437	3442	3450	rVB3	75043	152203	6.91%	1.031%
27	24.693	3672	3677	3683	rBV2	21091	48366	2.19%	0.328%
28	24.851	3694	3704	3720	rBV	307124	927063	42.07%	6.283%

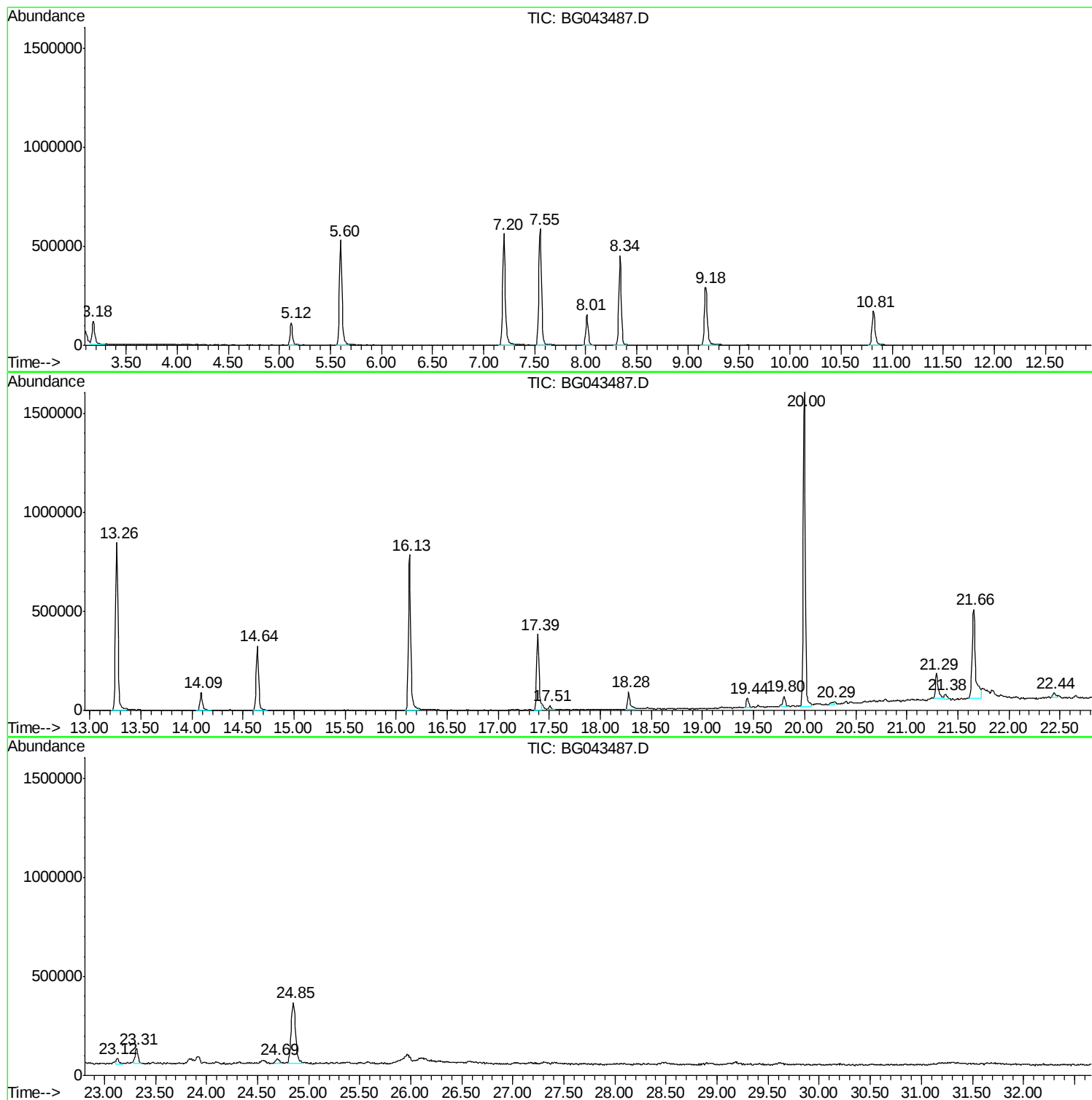
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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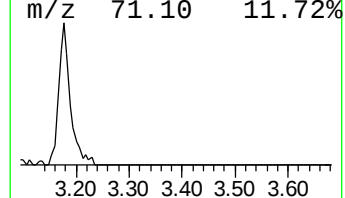
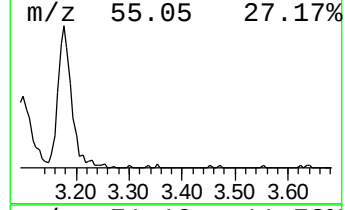
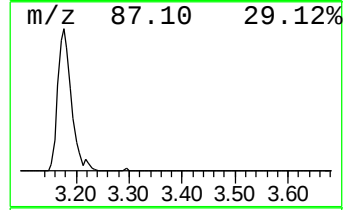
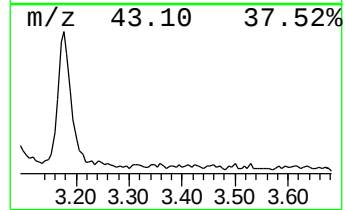
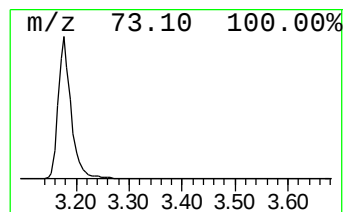
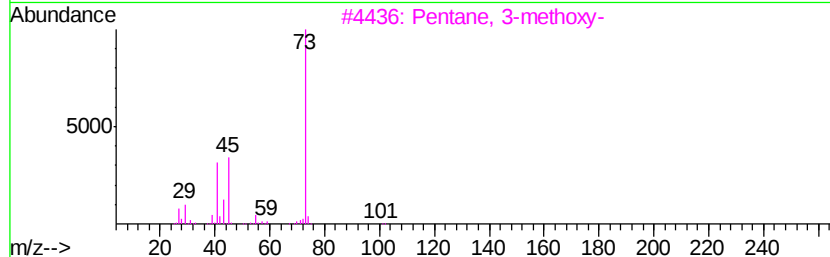
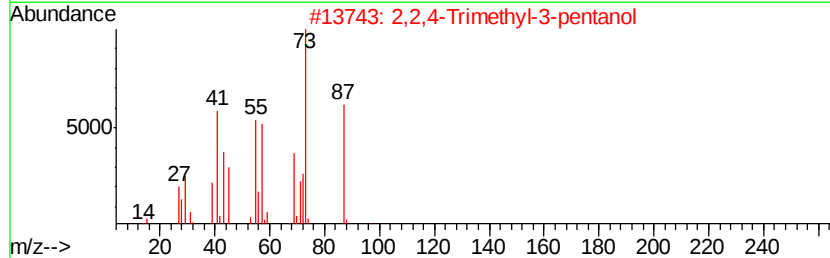
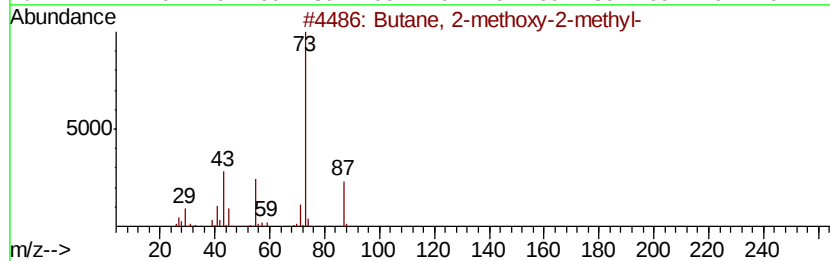
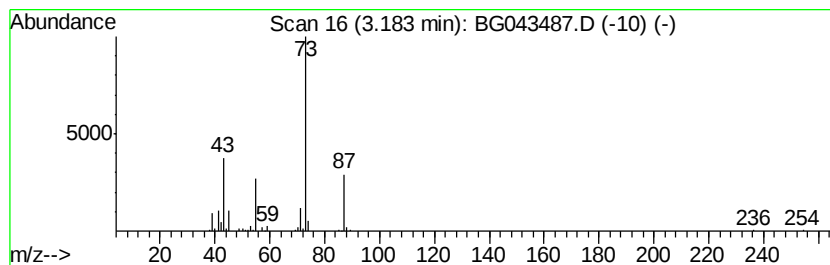
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	15.75 ng	211555	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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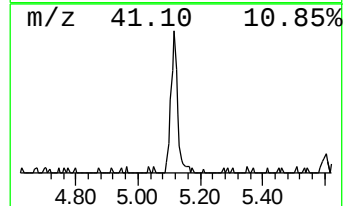
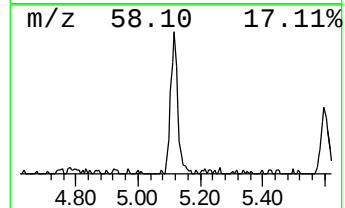
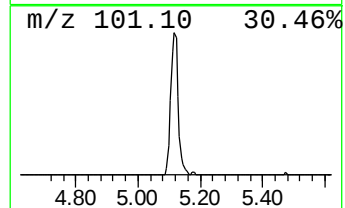
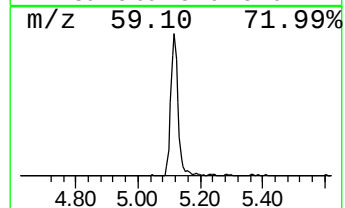
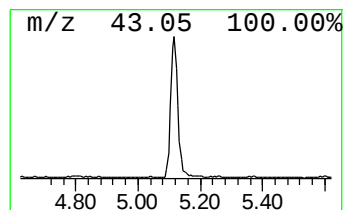
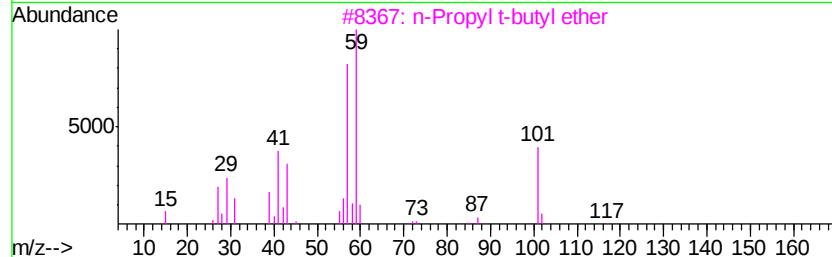
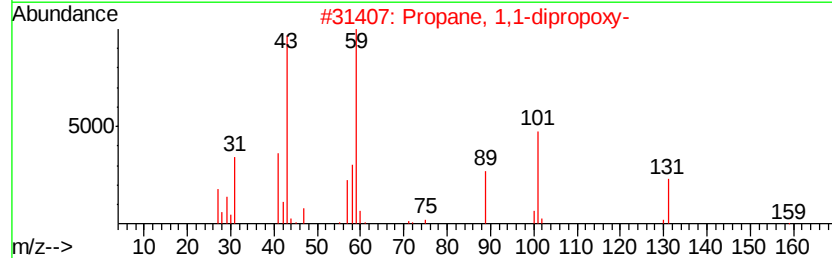
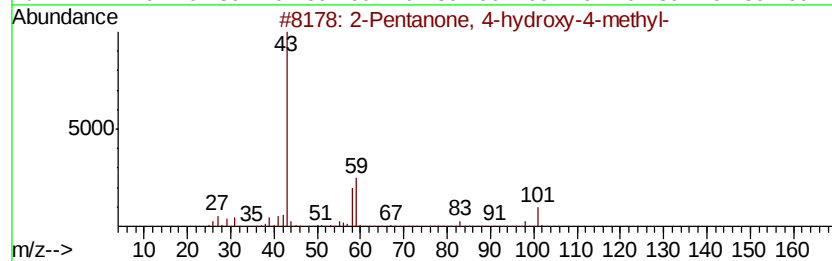
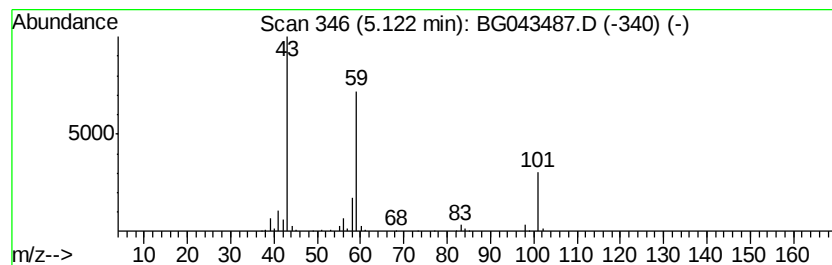
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.66 ng	183398	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
3		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5		Ether, hexyl t-butyl	158	C10H22O	069775-79-7	23



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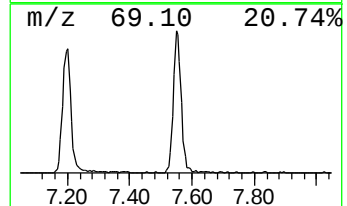
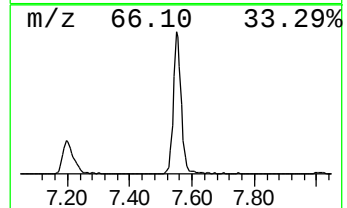
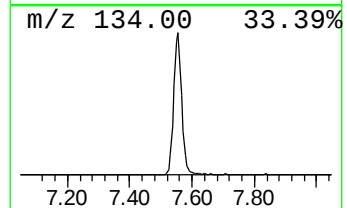
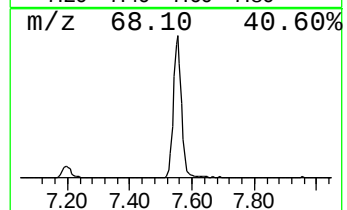
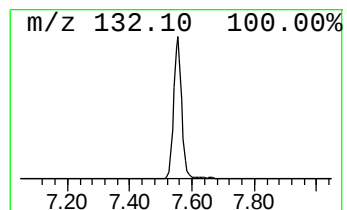
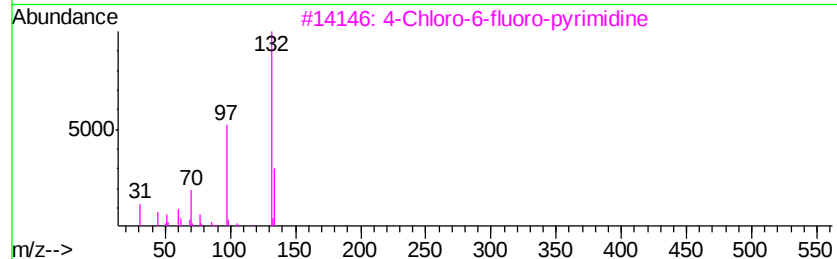
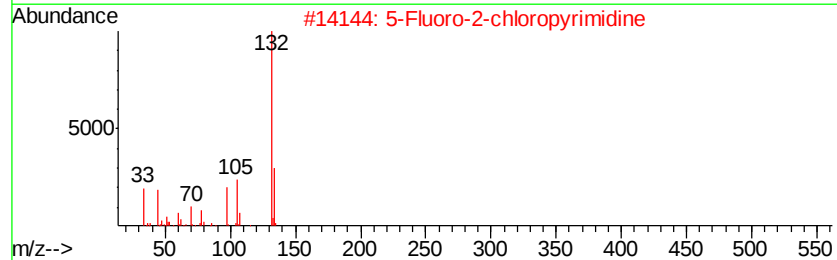
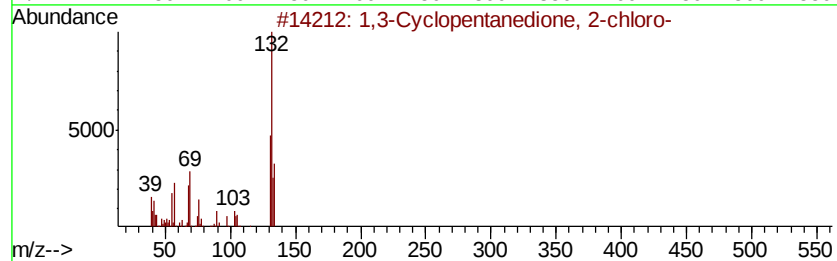
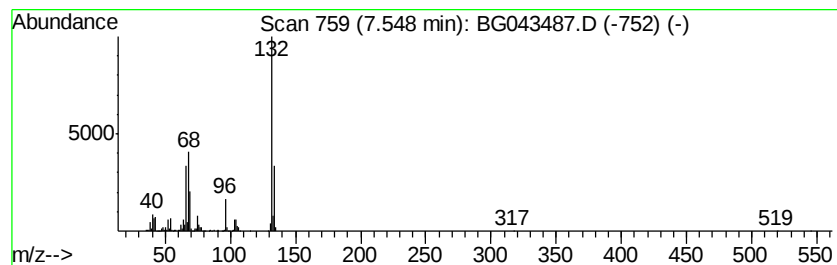
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Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	79.58 ng	1068800	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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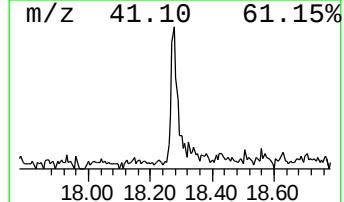
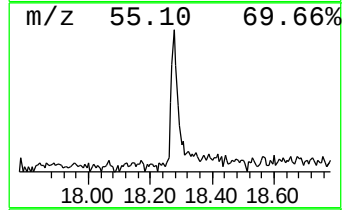
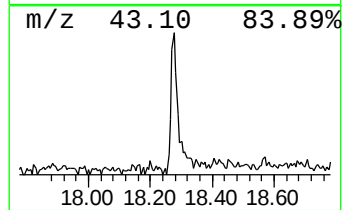
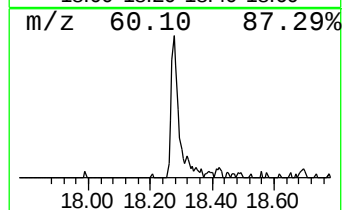
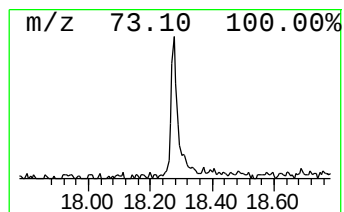
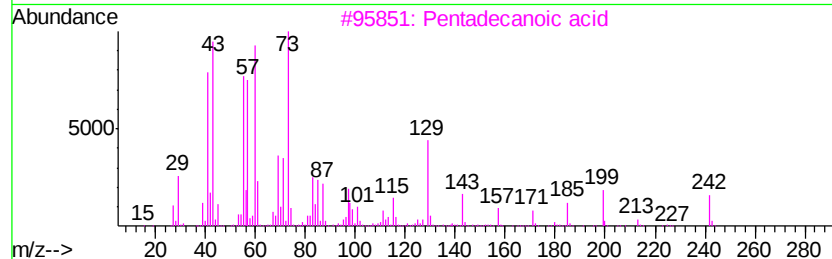
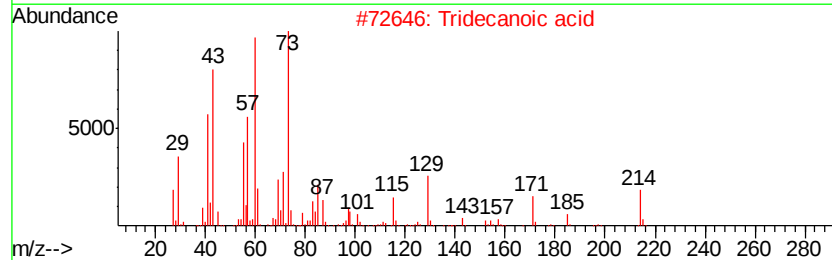
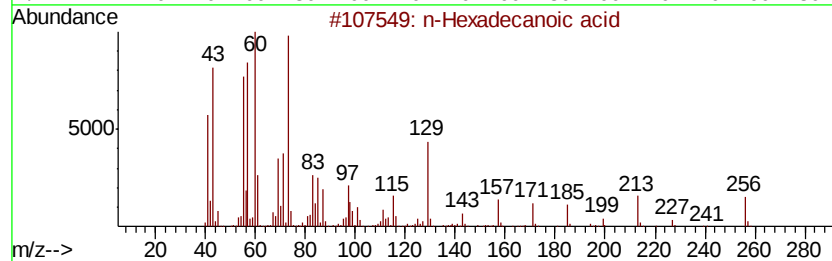
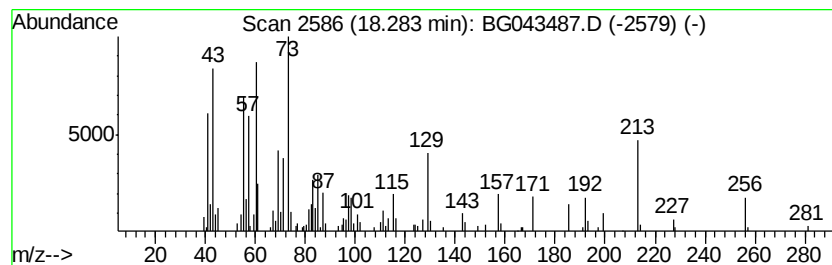
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.28	5.09 ng	159981	Phenanthrene-d10	17.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	68
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64



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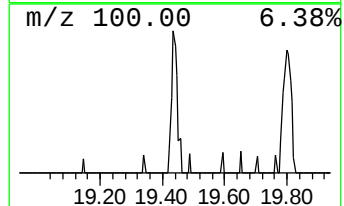
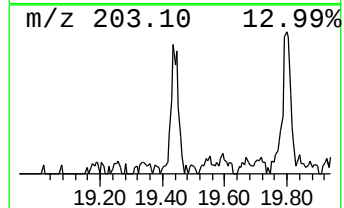
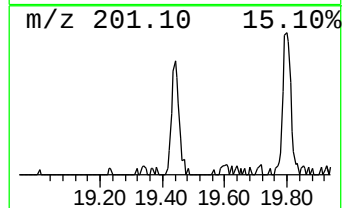
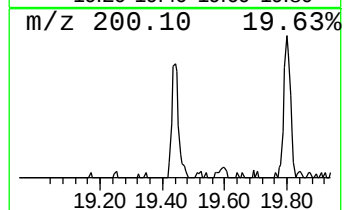
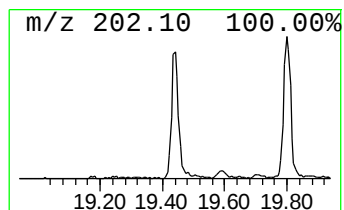
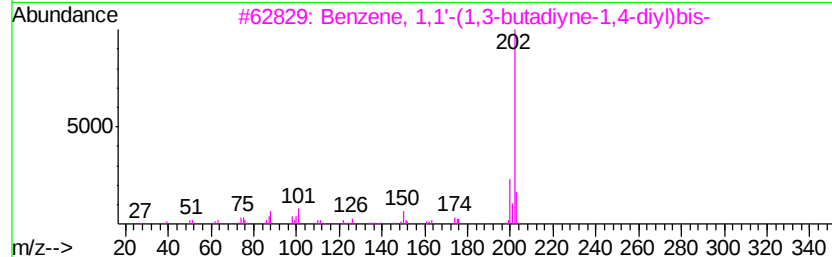
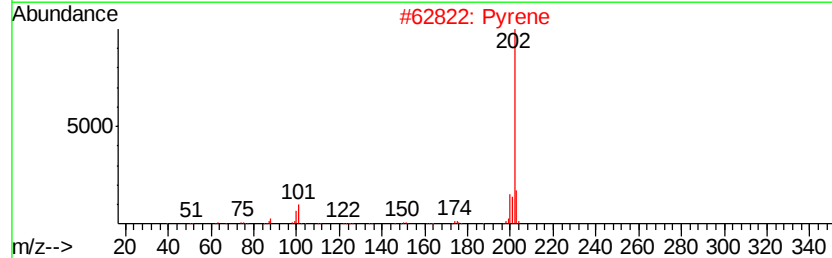
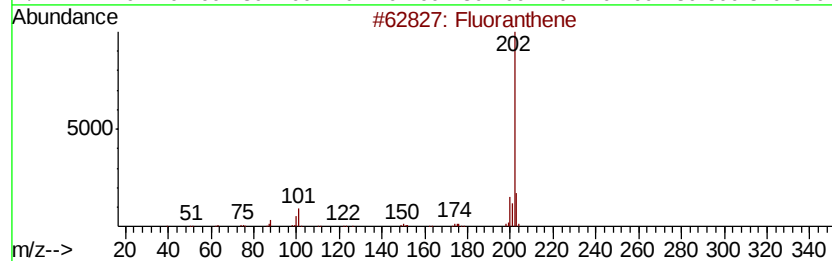
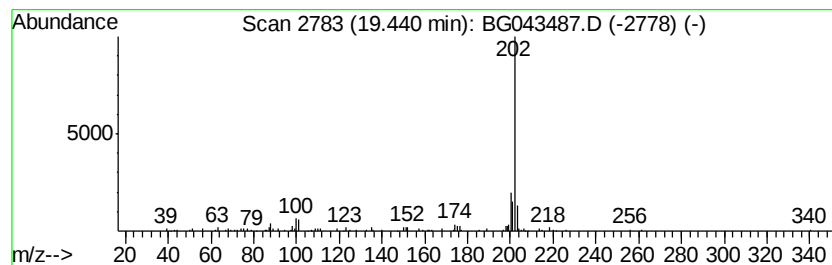
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Peak Number 6 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.44	2.52 ng	79320	Phenanthrene-d10	17.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	81
2	Pyrene	202	C16H10	000129-00-0	74
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	74
4	1-Methyl-7,11-dithiaspiro[5.5] u...	202	C10H18S2	107678-22-8	46
5	l-Leucine, N-methyl-N-(2-methoxy...	373	C20H39NO5	1000328-54-4	40



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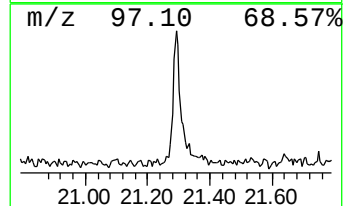
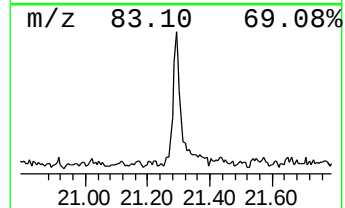
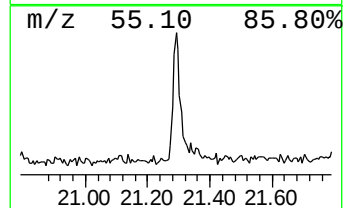
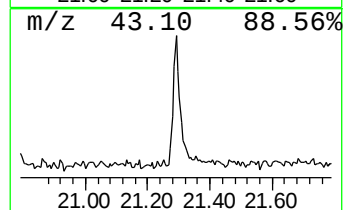
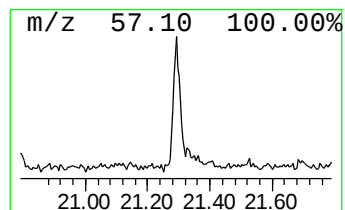
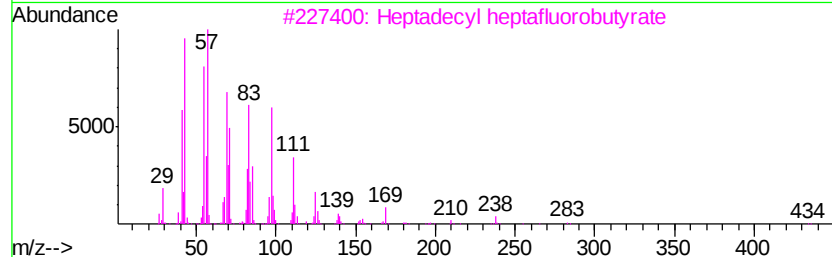
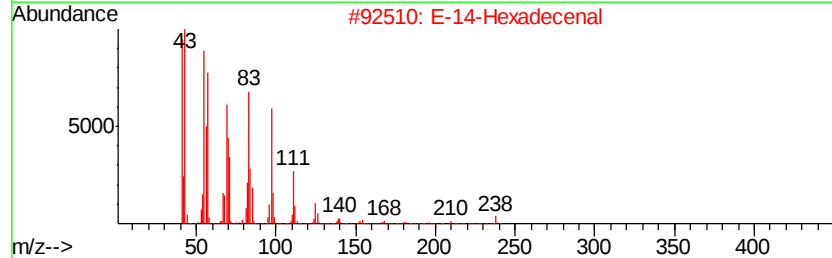
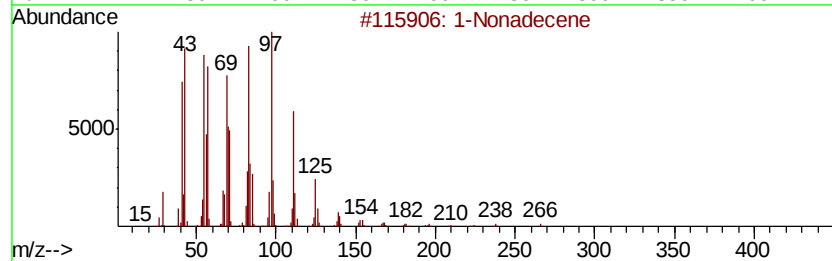
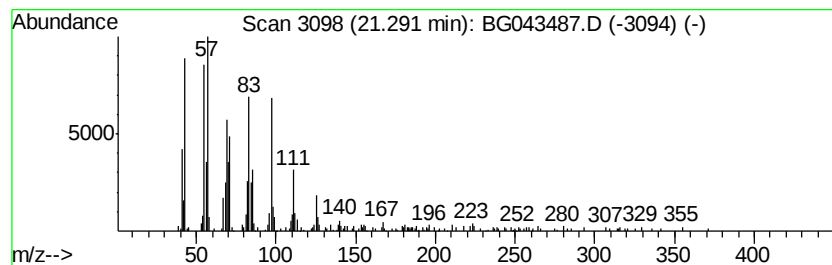
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.32 ng	219241	Chrysene-d12	21.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	99
2	E-14-Hexadecenal		238	C16H30O	330207-53-9	95
3	Heptadecyl heptafluorobutvrate		452	C21H35F7O2	959085-66-6	94
4	9-Eicosene, (E)-		280	C20H40	074685-29-3	93
5	Cycloeicosane		280	C20H40	000296-56-0	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043487.D
Acq On : 4 Nov 2019 19:07
Operator : JU
Sample : K5657-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP

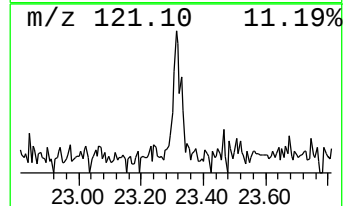
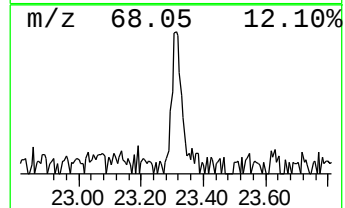
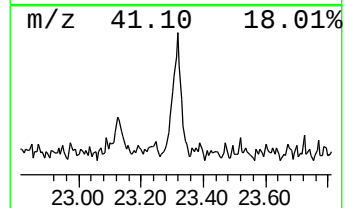
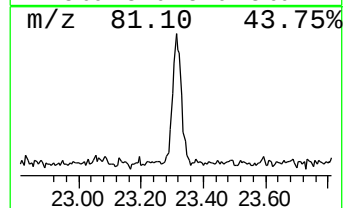
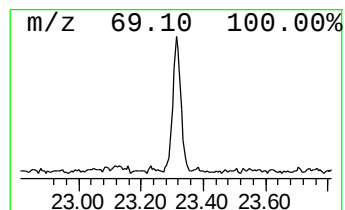
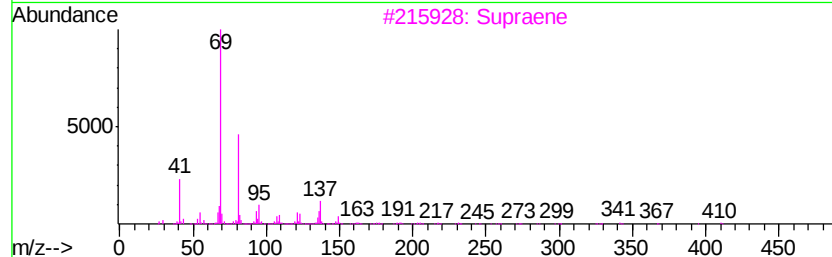
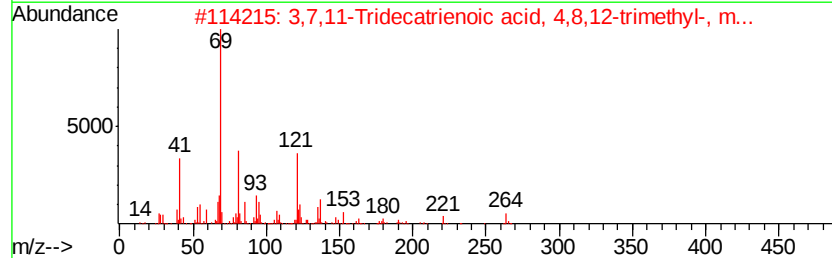
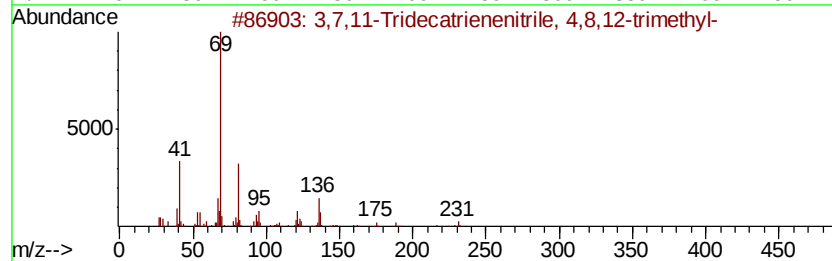
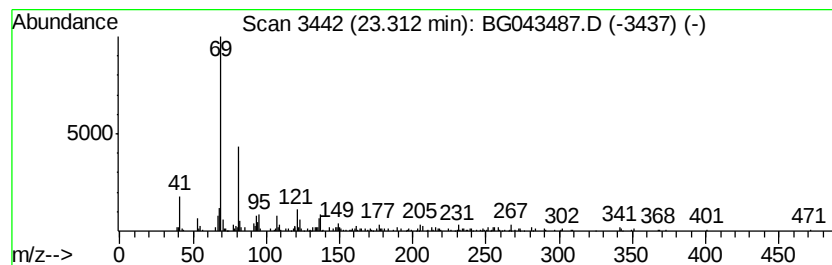
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 3,7,11-Tridecatrienitrile... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	3.28 ng	152203	Perylene-d12	24.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
2		3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	64
3		Supraene	410	C30H50	007683-64-9	64
4		trans-Farnesol	222	C15H26O	000106-28-5	64
5		Squalene	410	C30H50	000111-02-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110419\
Data File : BG043487.D
Acq On : 4 Nov 2019 19:07
Operator : JU
Sample : K5657-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.18	15.8	ng	211555	1	8.01	268611	20.0
2-Pentanone, 4-hy...	5.12	13.7	ng	183398	1	8.01	268611	20.0
unknown7.55	7.55	79.6	ng	1068800	1	8.01	268611	20.0
n-Hexadecanoic acid	18.28	5.1	ng	159981	4	17.39	628521	20.0
Benzene, 1,1'-(1,...	19.44	2.5	ng	79320	4	17.39	628521	20.0
1-Nonadecene	21.29	4.3	ng	219241	5	21.66	1014800	20.0
3,7,11-Tridecatri...	23.31	3.3	ng	152203	6	24.85	927063	20.0