

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
 Data File : BF102322.D
 Acq On : 23 Jan 2018 1:39
 Operator : SJ/JU
 Sample : J1238-08
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-6.5-7.0

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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	4.922	478	482	490	rVB	156417	213019	6.74%	0.819%
2	5.334	547	552	555	rBV	2933420	3007313	95.21%	11.567%
3	6.369	723	728	740	rBV	2801567	3158521	100.00%	12.149%
4	6.492	744	749	752	rBV	3299104	3079528	97.50%	11.845%
5	6.716	784	787	796	rBV	886660	755222	23.91%	2.905%
6	6.875	810	814	817	rBV	2686770	2307179	73.05%	8.874%
7	7.286	879	884	887	rBV	1942795	1838749	58.22%	7.073%
8	7.998	1002	1005	1009	rBV	1091172	939353	29.74%	3.613%
9	9.080	1184	1189	1192	rBV	2928530	2797949	88.58%	10.762%
10	9.469	1252	1255	1259	rBV	231698	217436	6.88%	0.836%
11	9.680	1288	1291	1296	rBV	87312	76882	2.43%	0.296%
12	9.751	1300	1303	1307	rVV	966088	902149	28.56%	3.470%
13	10.180	1373	1376	1379	rVB	113901	95035	3.01%	0.366%
14	10.398	1407	1413	1416	rBV	27930	40162	1.27%	0.154%
15	10.545	1434	1438	1441	rBV	1618159	1436694	45.49%	5.526%
16	10.657	1453	1457	1461	rBV	87490	85164	2.70%	0.328%
17	11.104	1529	1533	1536	rBV	36719	32690	1.03%	0.126%
18	11.239	1552	1556	1559	rBV	900479	743680	23.55%	2.861%
19	12.827	1821	1826	1829	rBV	1984829	1890913	59.87%	7.273%
20	13.027	1854	1860	1862	rBV2	34136	37690	1.19%	0.145%
21	13.051	1862	1864	1867	rVB	49018	43704	1.38%	0.168%
22	13.715	1974	1977	1984	rBV	517522	525294	16.63%	2.021%
23	13.874	2000	2004	2008	rBV	814008	738736	23.39%	2.842%
24	13.974	2017	2021	2024	rBV	45809	45852	1.45%	0.176%
25	14.351	2080	2085	2090	rBV2	168021	226517	7.17%	0.871%
26	14.962	2186	2189	2191	rBV	31490	33373	1.06%	0.128%
27	14.986	2191	2193	2199	rVB4	36799	47223	1.50%	0.182%
28	15.304	2242	2247	2255	rBV2	452075	592274	18.75%	2.278%
29	15.786	2325	2329	2334	rVB2	53717	89770	2.84%	0.345%

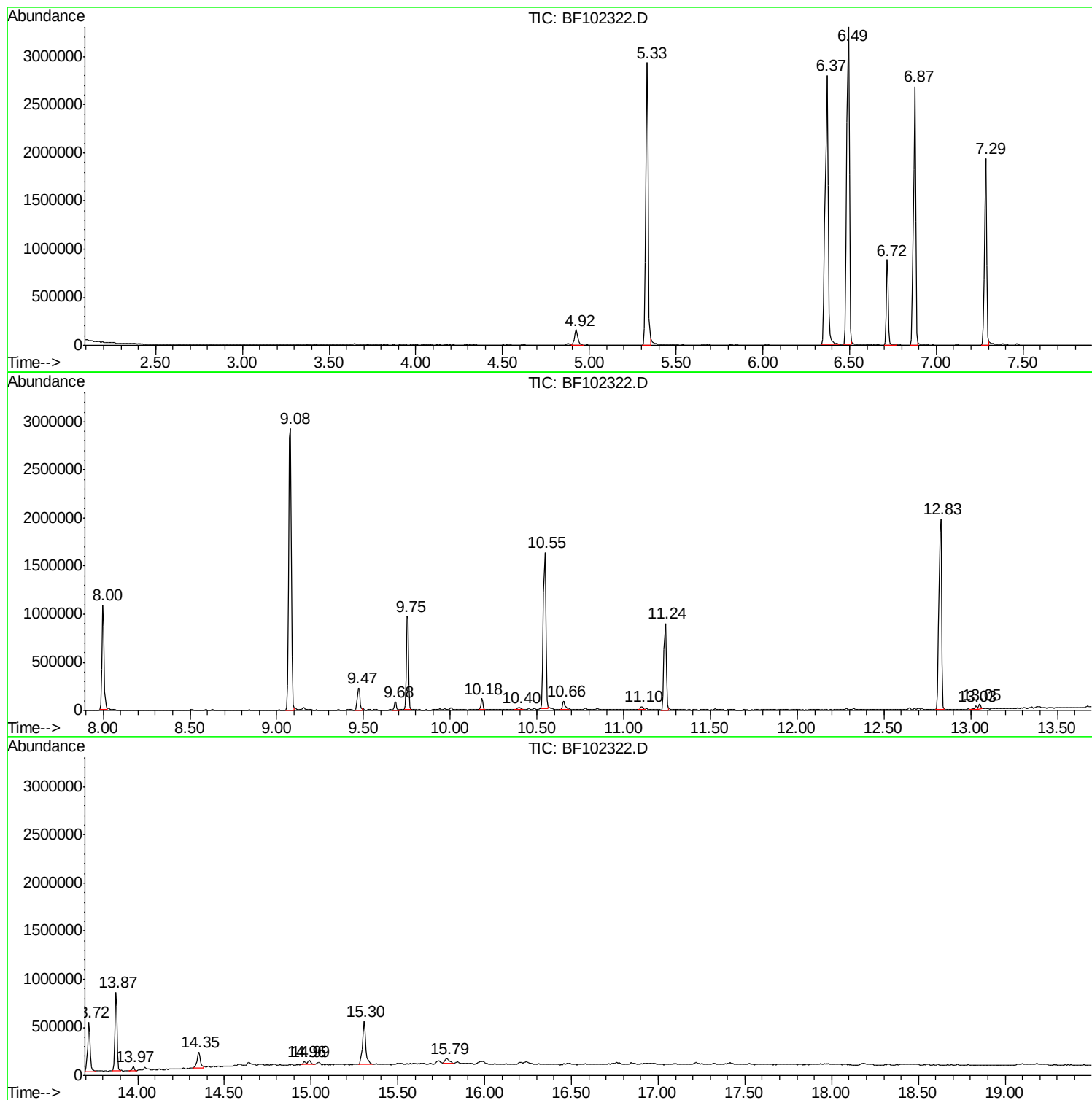
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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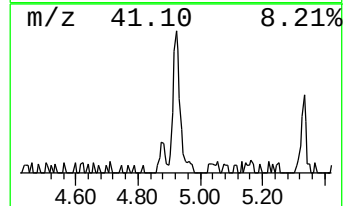
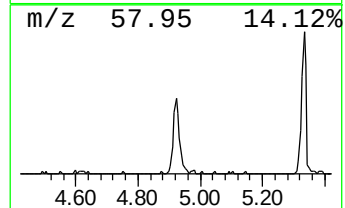
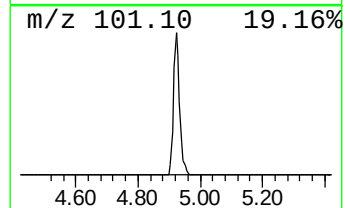
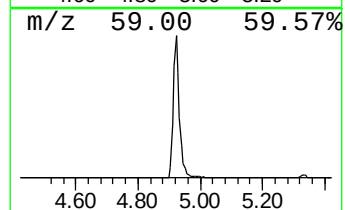
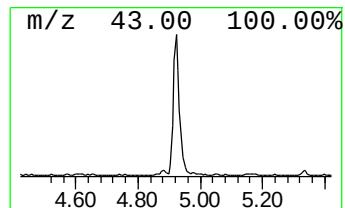
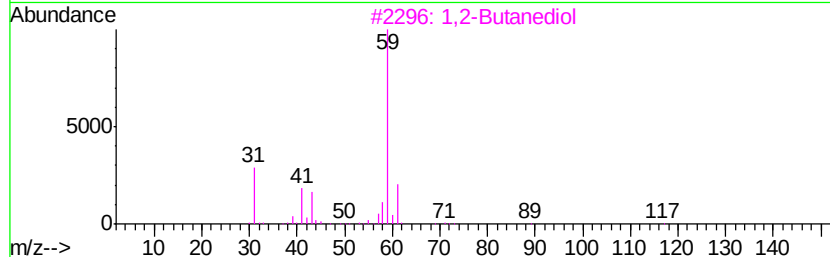
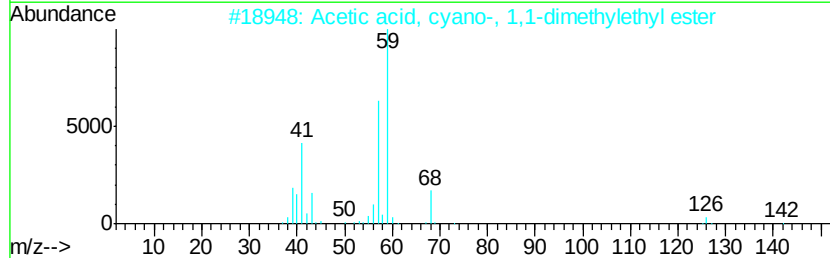
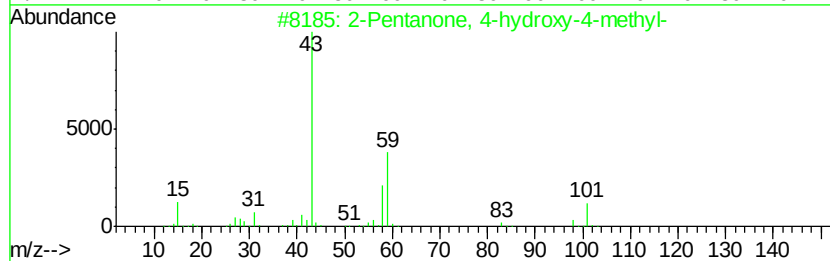
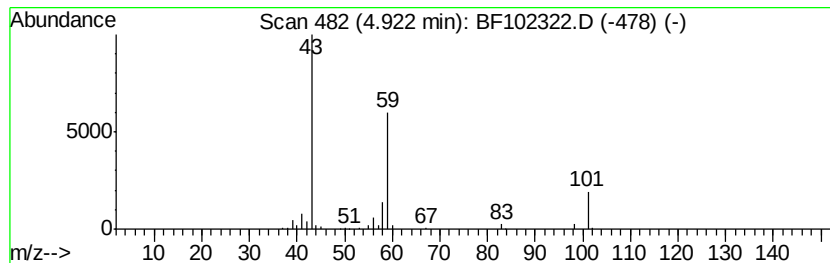
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.64 ng	213019	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			1,2-Butanediol	90	C4H10O2	000584-03-2	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Guanidine	59	CH5N3	000113-00-8	9



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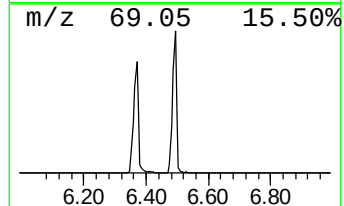
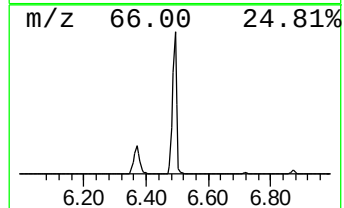
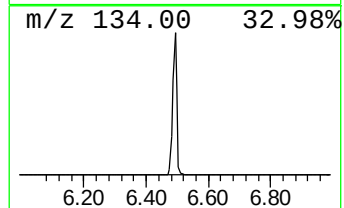
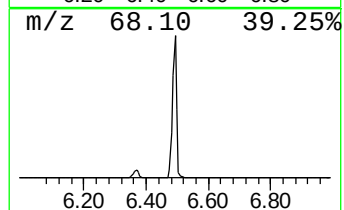
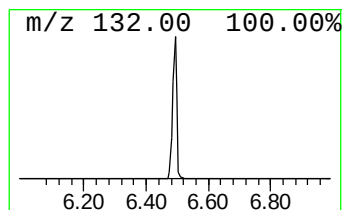
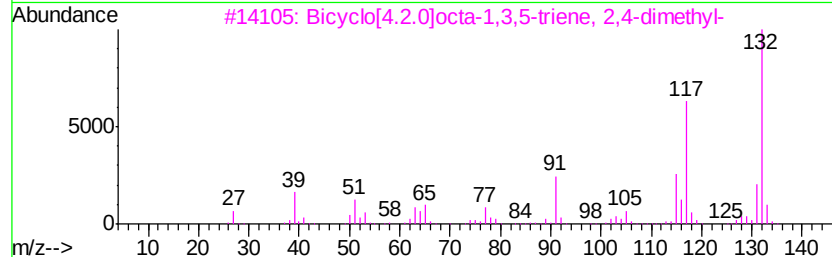
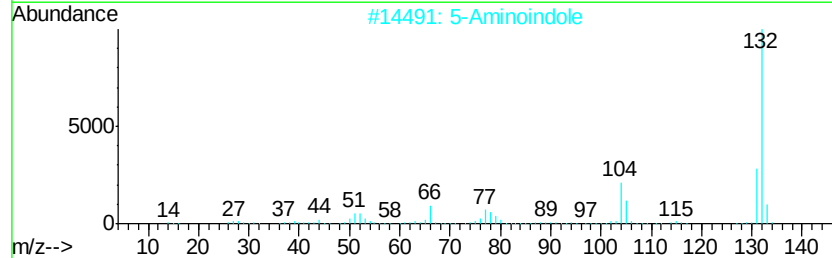
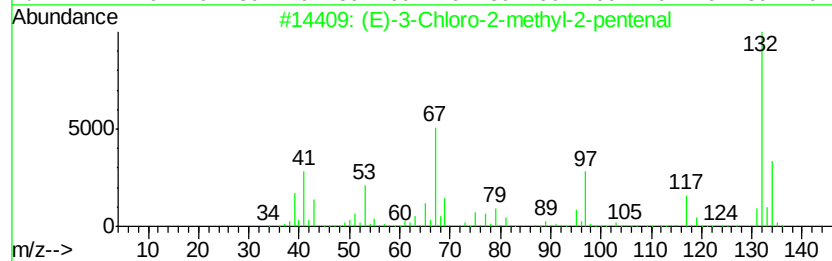
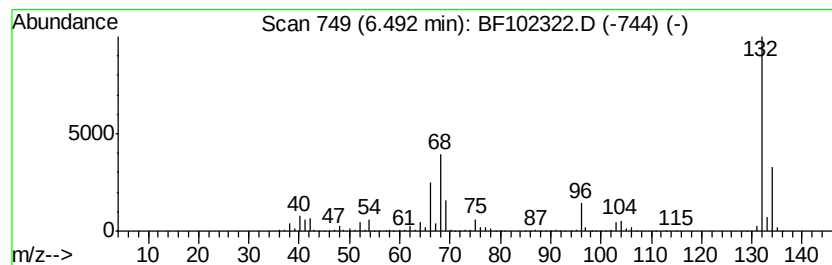
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	81.55 ng	3079530	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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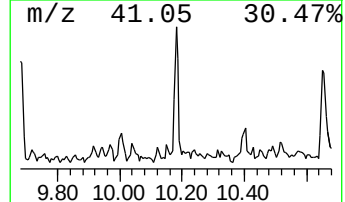
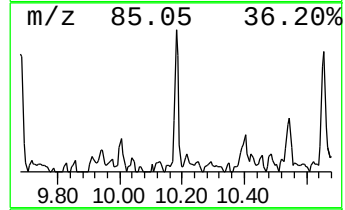
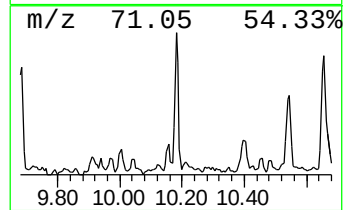
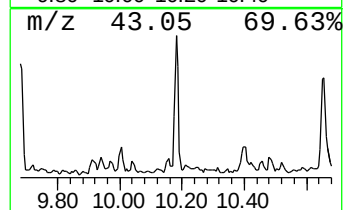
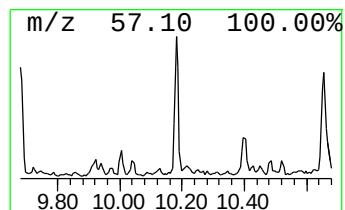
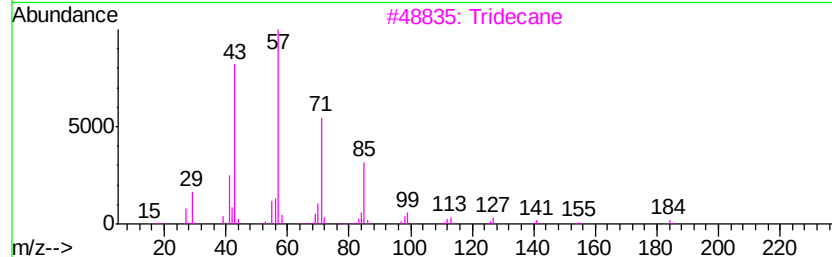
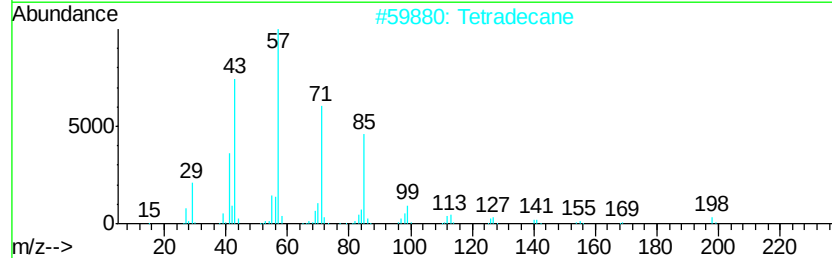
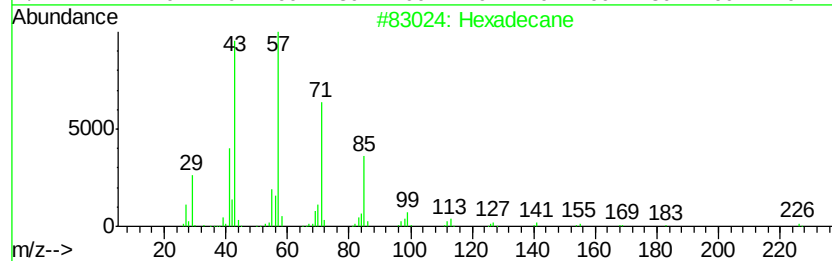
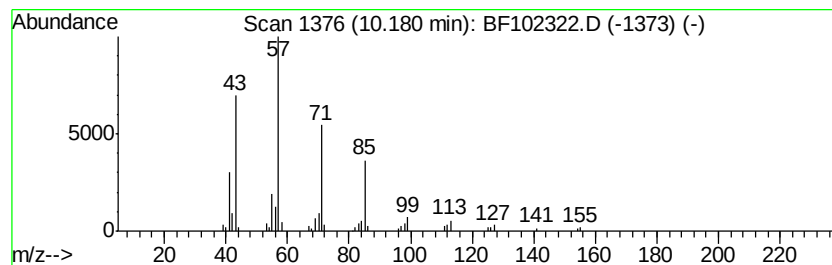
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Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	2.11 ng	95035	Acenaphthene-d10	9.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Tetradecane	198 C14H30	000629-59-4	91
3	Tridecane	184 C13H28	000629-50-5	86
4	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	86
5	Octadecane	254 C18H38	000593-45-3	72



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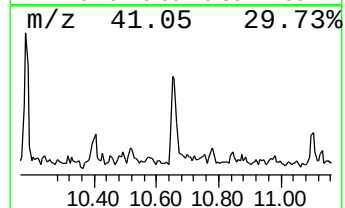
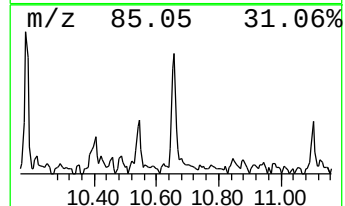
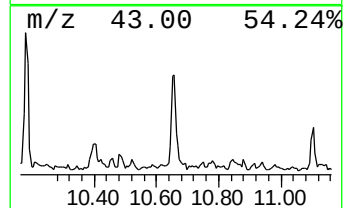
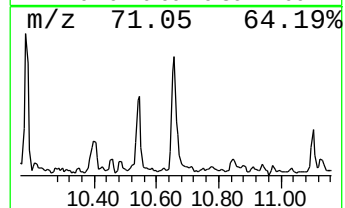
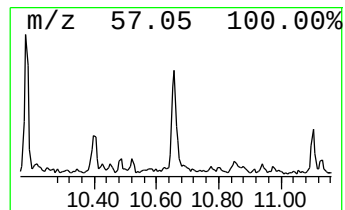
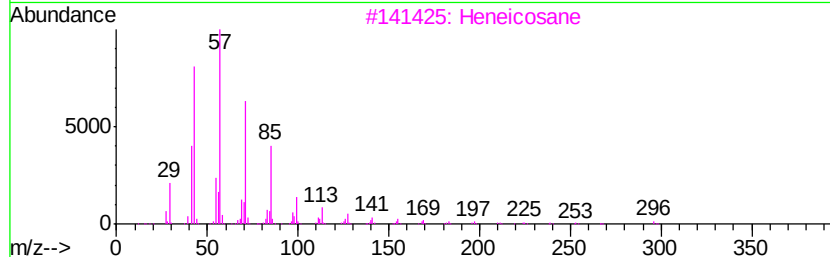
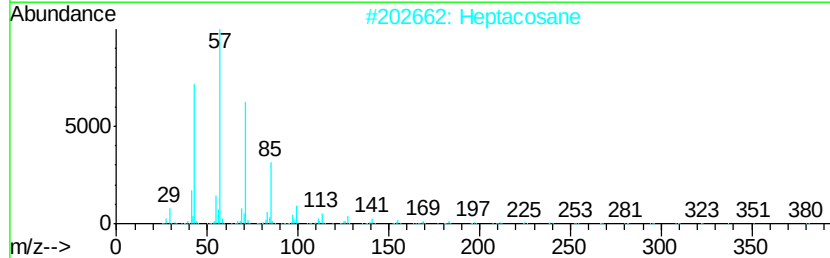
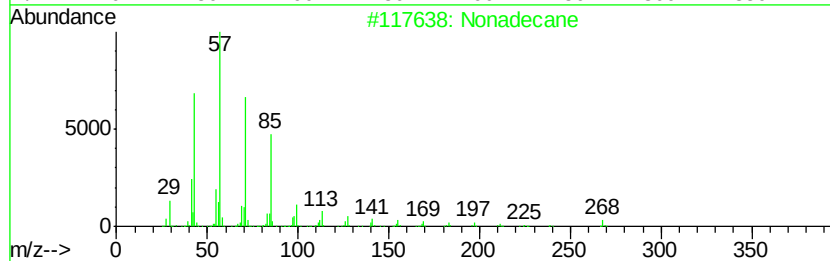
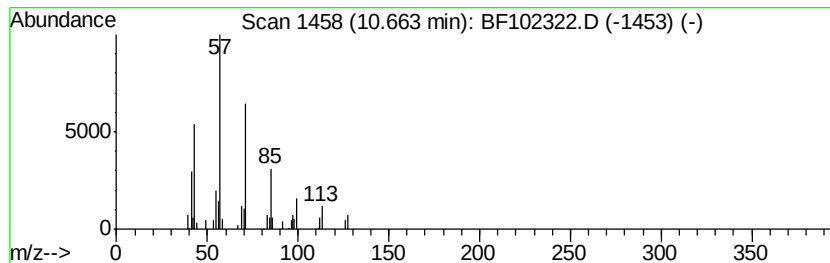
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Peak Number 5 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.29 ng	85164	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	90
2	Heptacosane		380	C27H56	000593-49-7	90
3	Heneicosane		296	C21H44	000629-94-7	90
4	Tetracosane		338	C24H50	000646-31-1	86
5	Heptadecane		240	C17H36	000629-78-7	86



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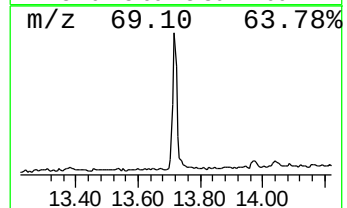
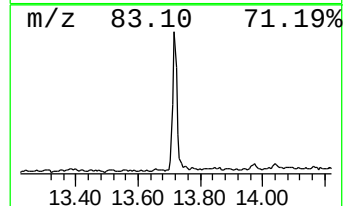
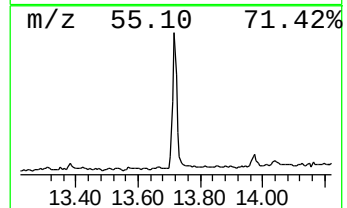
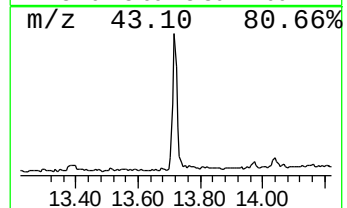
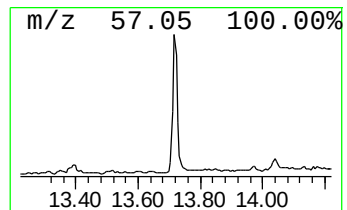
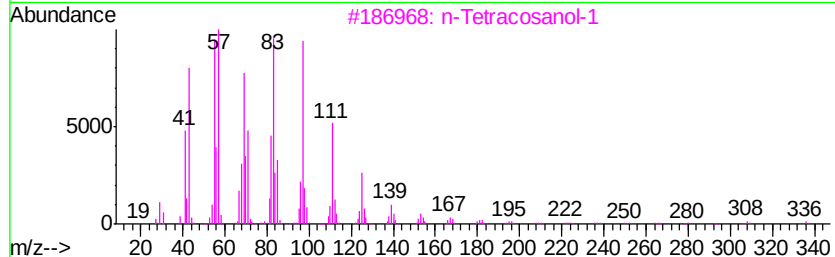
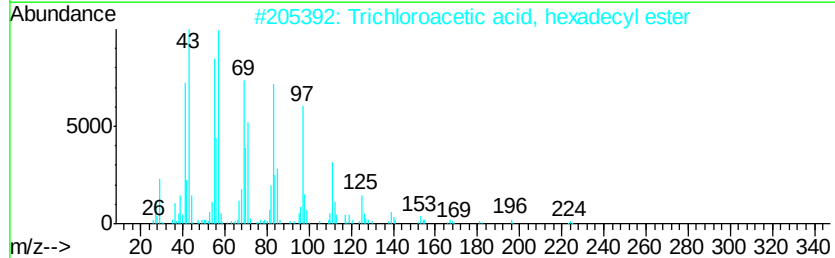
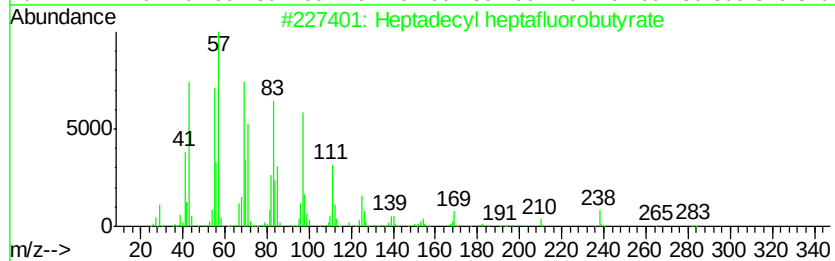
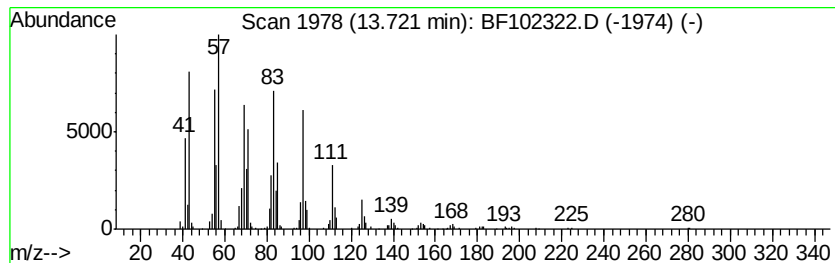
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	14.22 ng	525294	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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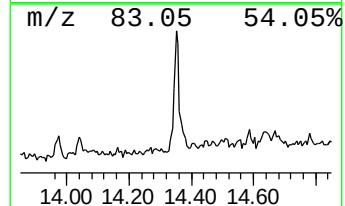
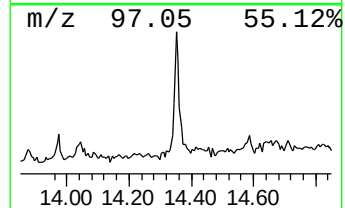
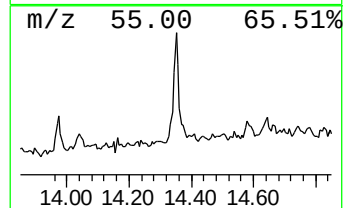
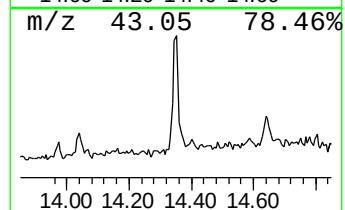
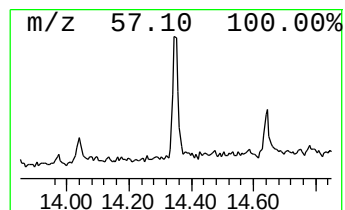
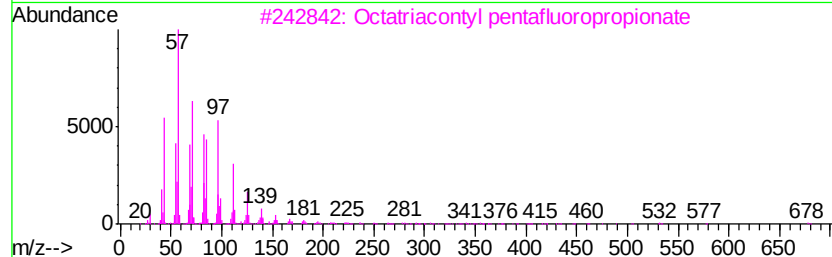
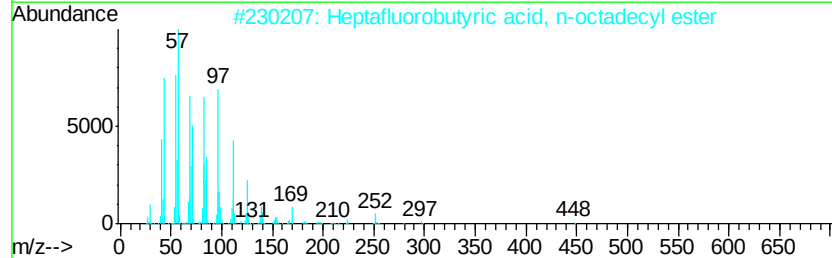
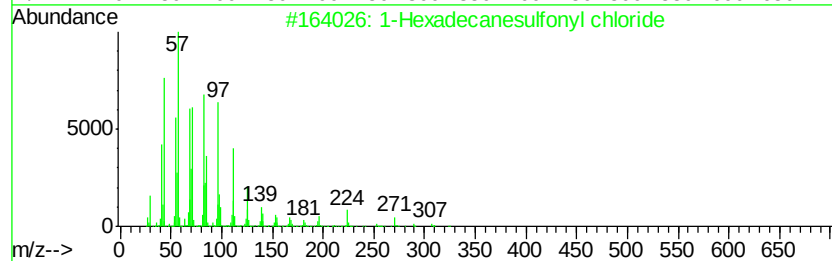
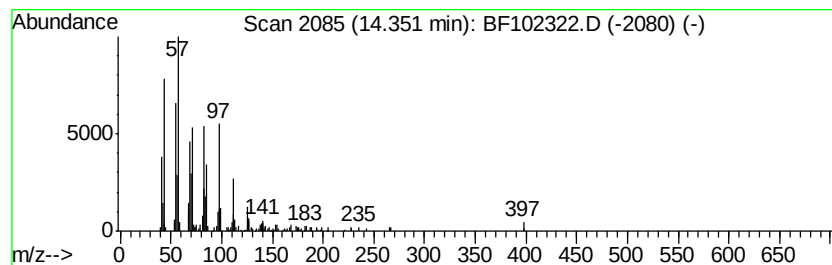
Instrument :
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ClientSampleId :
SB-01-6.5-7.0

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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-Hexadecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.35	6.13 ng	226517	Chrysene-d12	13.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	90
3		Octatriacontyl pentafluoropropionic acid, heptafluorobutyrate	697	C41H77F5O2	1000351-89-1	90
4		Pentafluoropropionic acid, heptafluorobutyrate	402	C20H35F5O2	959218-78-1	90
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102322.D
Acq On : 23 Jan 2018 1:39
Operator : SJ/JU
Sample : J1238-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-6.5-7.0

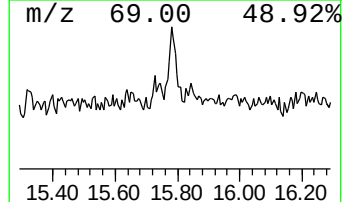
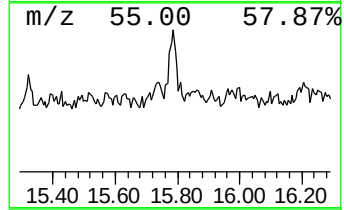
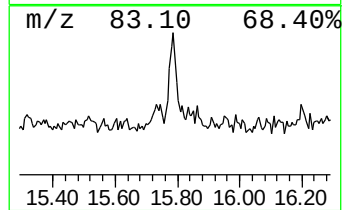
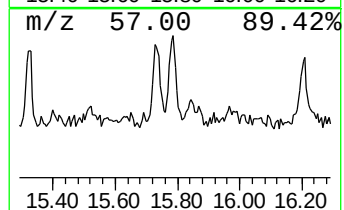
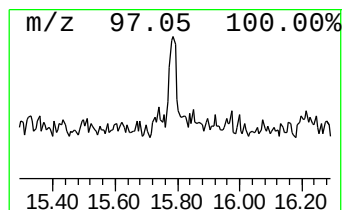
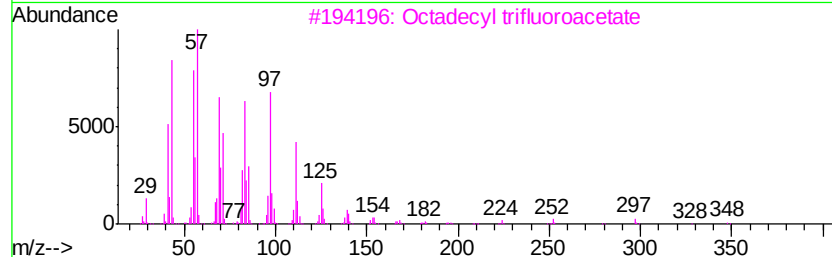
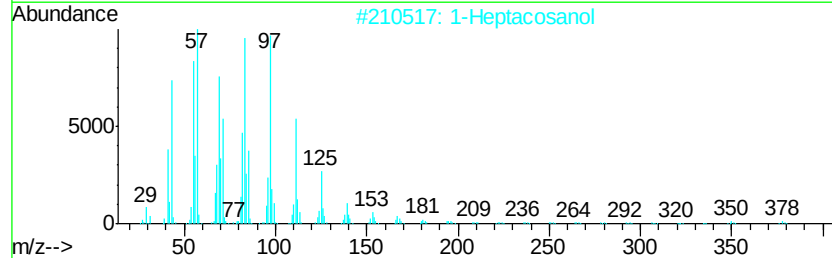
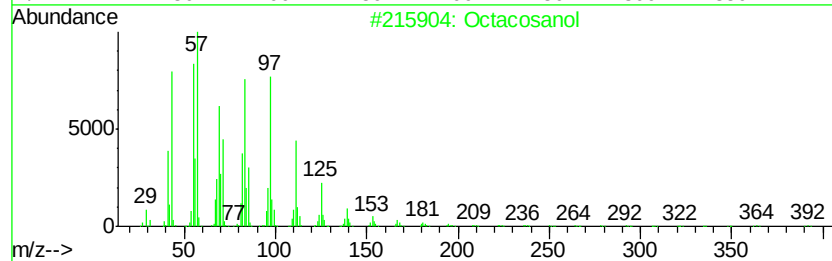
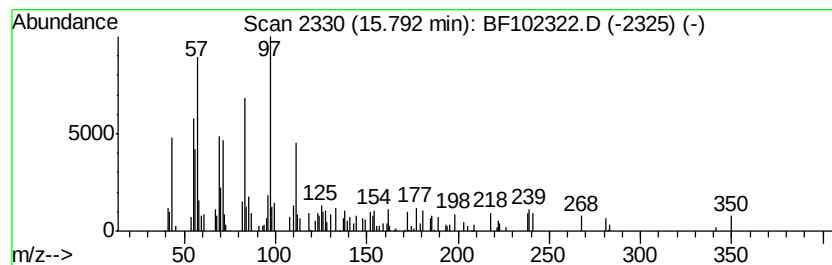
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.03 ng	89770	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	87
2		1-Heptacosanol	396	C27H56O	002004-39-9	83
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	62
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102322.D
Acq On : 23 Jan 2018 1:39
Operator : SJ/JU
Sample : J1238-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-6.5-7.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
2-Pentanone, 4-hy...	4.92	5.6	ng	213019	1	6.72	755222	20.0
unknown6.49	6.49	81.5	ng	3079530	1	6.72	755222	20.0
Hexadecane	10.18	2.1	ng	95035	3	9.75	902149	20.0
Nonadecane	10.66	2.3	ng	85164	4	11.24	743680	20.0
Heptadecyl hepta...	13.72	14.2	ng	525294	5	13.87	738736	20.0
1-Hexadecanesulfo...	14.35	6.1	ng	226517	5	13.87	738736	20.0
Octacosanol	15.79	3.0	ng	89770	6	15.30	592274	20.0