

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090319\
 Data File : BF116779.D
 Acq On : 3 Sep 2019 18:19
 Operator : HP/JU
 Sample : K4554-40
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-8-(5-7)

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_F\METHODS\8270-BF083019.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	4.428	394	398	404	rBB	26054	32438	1.29%	0.142%
2	5.046	499	503	512	rVB	87379	98609	3.94%	0.433%
3	5.463	569	574	577	rBV	2090267	1936950	77.33%	8.498%
4	6.475	741	746	759	rBV	2446479	2255818	90.06%	9.897%
5	6.616	766	770	773	rBV	2599511	2188494	87.37%	9.602%
6	6.845	806	809	813	rBV	951157	715034	28.55%	3.137%
7	7.004	832	836	839	rBV	2108256	1666548	66.53%	7.312%
8	7.404	900	904	907	rBV	1603096	1352938	54.01%	5.936%
9	8.128	1023	1027	1030	rBV	1234421	950825	37.96%	4.172%
10	9.204	1206	1210	1213	rBV	2839468	2504917	100.00%	10.990%
11	9.592	1273	1276	1281	rBV	241917	194645	7.77%	0.854%
12	9.880	1321	1325	1328	rBV	1417530	1115215	44.52%	4.893%
13	10.663	1454	1458	1467	rBV	1392525	1230126	49.11%	5.397%
14	11.363	1573	1577	1580	rBV	1263352	1102402	44.01%	4.837%
15	11.886	1663	1666	1670	rVB2	86275	78851	3.15%	0.346%
16	12.569	1779	1782	1786	rBV	99770	84781	3.38%	0.372%
17	12.798	1817	1821	1824	rBV	84257	75965	3.03%	0.333%
18	12.939	1841	1845	1849	rBV	2363649	2285178	91.23%	10.026%
19	13.127	1869	1877	1880	rBV4	17372	29478	1.18%	0.129%
20	13.416	1924	1926	1933	rVB3	33737	43657	1.74%	0.192%
21	13.839	1994	1998	2006	rBV2	146271	207900	8.30%	0.912%
22	13.992	2019	2024	2027	rBV	945828	911343	36.38%	3.998%
23	14.157	2049	2052	2056	rBV	58911	62740	2.50%	0.275%
24	14.463	2101	2104	2107	rVB	92350	75246	3.00%	0.330%
25	14.768	2152	2156	2159	rBV	102413	98908	3.95%	0.434%
26	15.098	2209	2212	2216	rBV	113278	124960	4.99%	0.548%
27	15.380	2257	2260	2264	rBV	31125	40868	1.63%	0.179%
28	15.445	2266	2271	2274	rVV	730479	904616	36.11%	3.969%
29	15.474	2274	2276	2283	rVB	141265	181864	7.26%	0.798%
30	15.910	2346	2350	2354	rBV	92228	127244	5.08%	0.558%
31	16.409	2430	2435	2439	rBV2	74700	113573	4.53%	0.498%

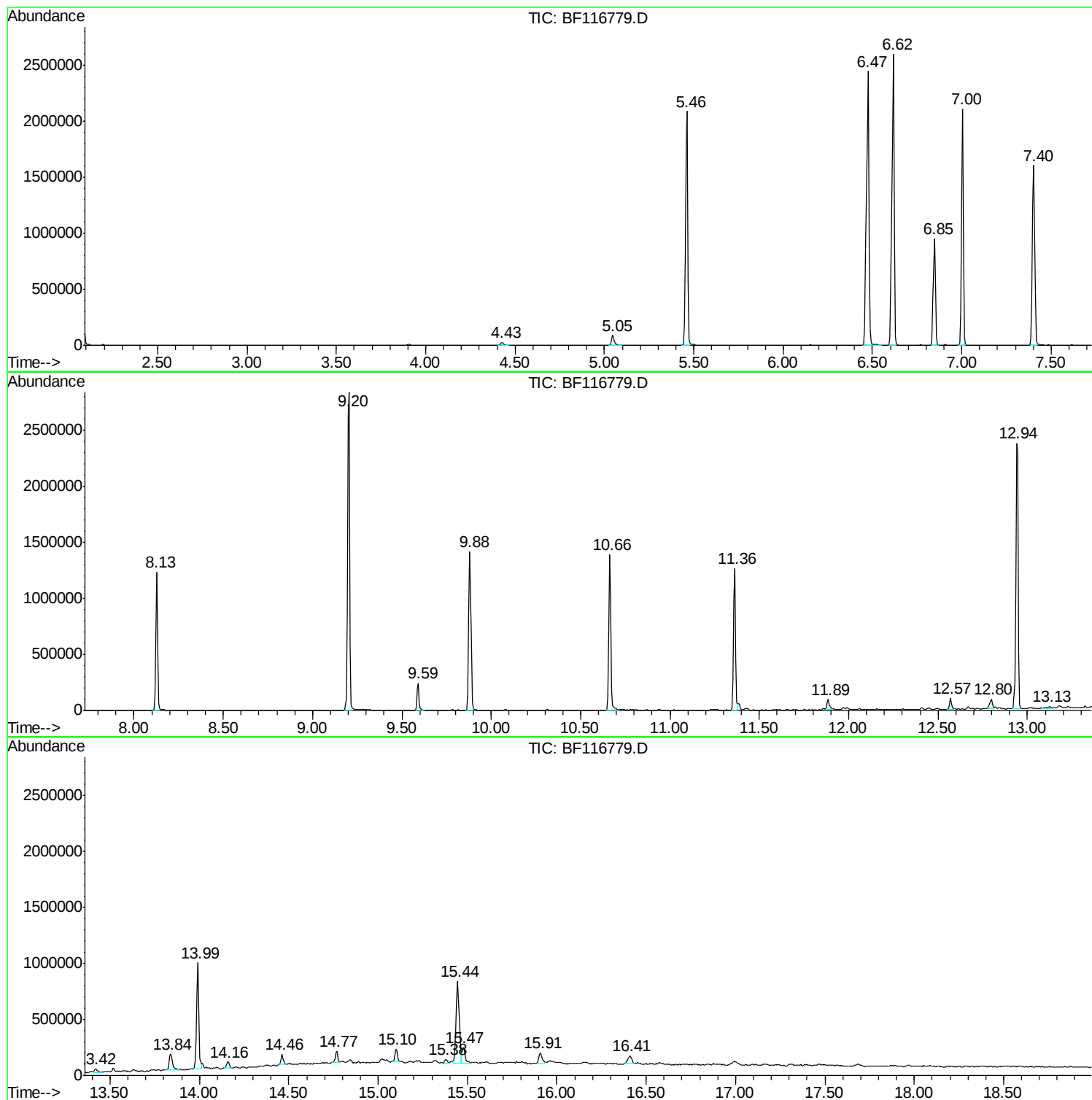
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ClientSampleId :
SB-8-(5-7)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.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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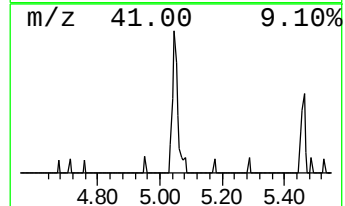
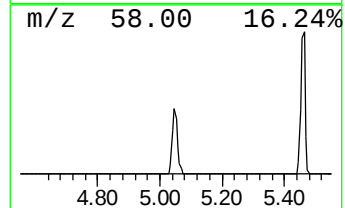
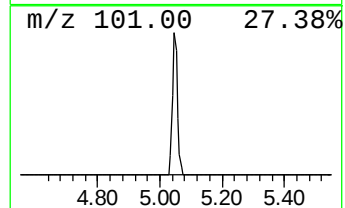
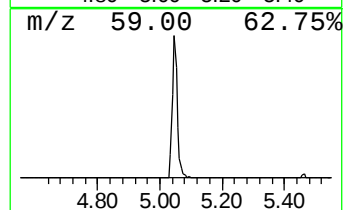
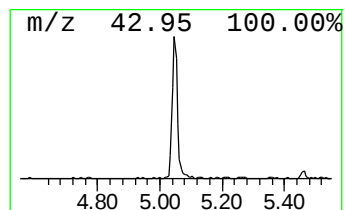
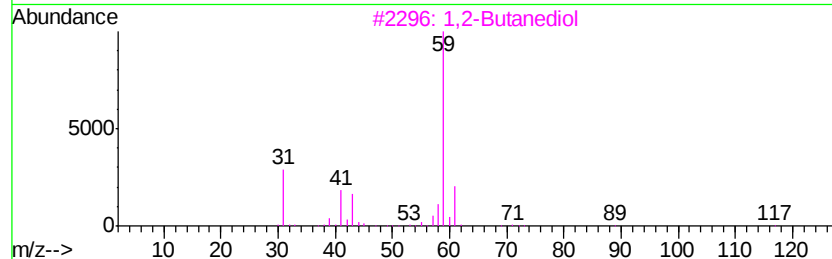
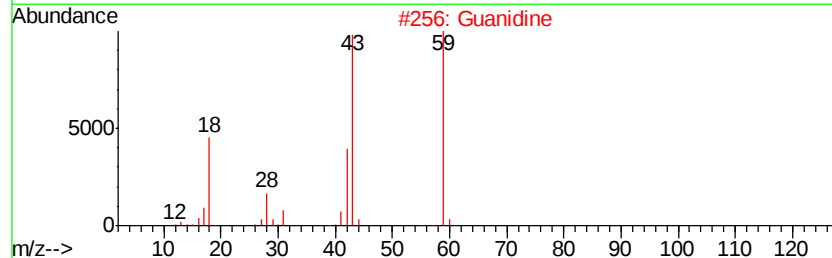
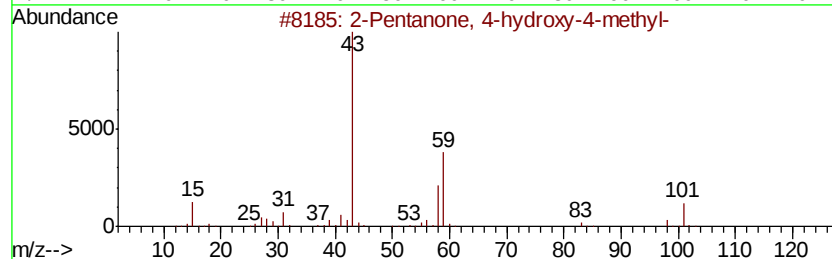
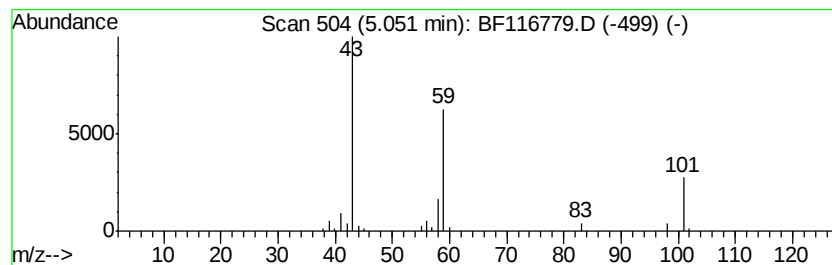
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.05	2.76 ng	98609	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	1,2-Butanediol	90	C4H10O2	000584-03-2	23
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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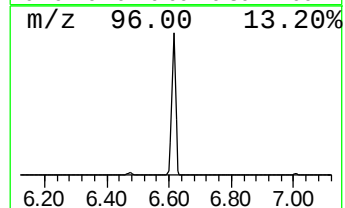
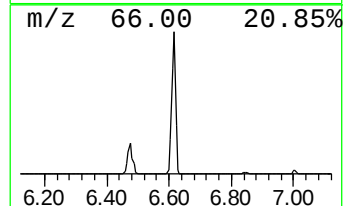
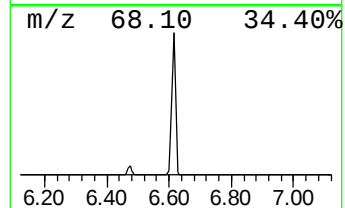
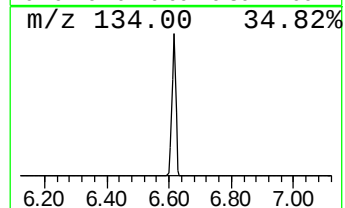
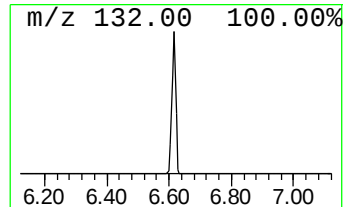
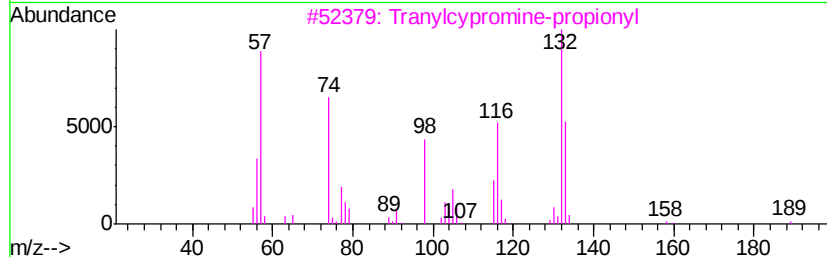
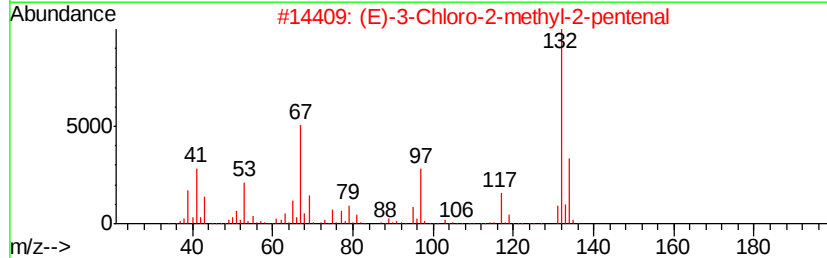
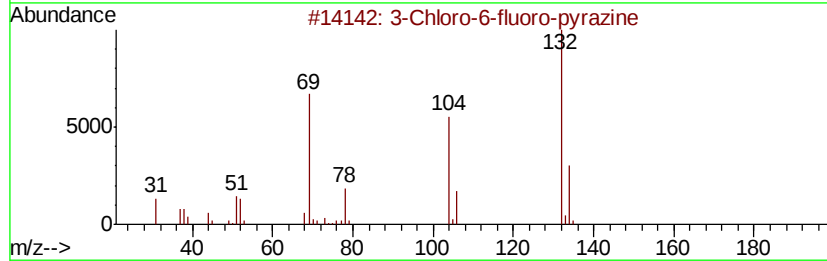
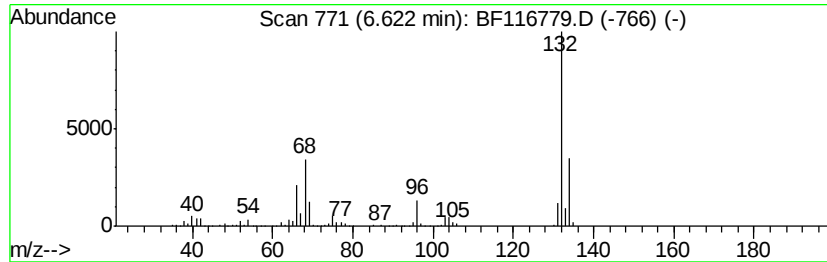
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	61.21 ng	2188490	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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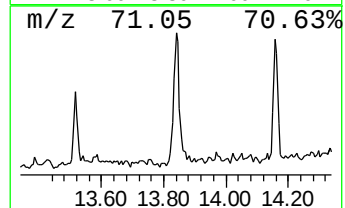
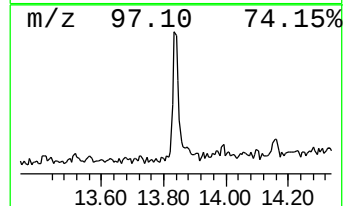
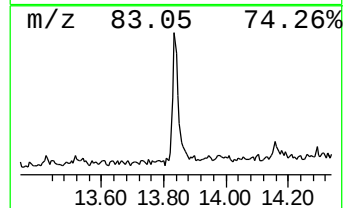
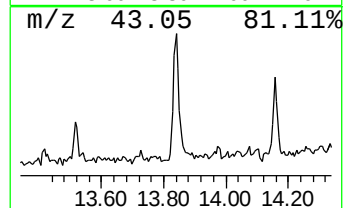
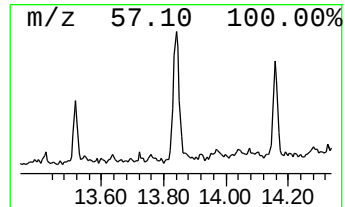
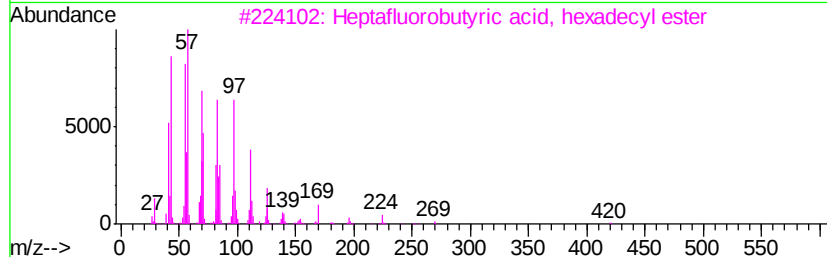
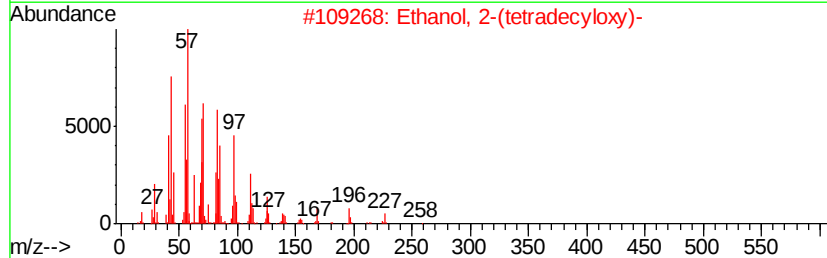
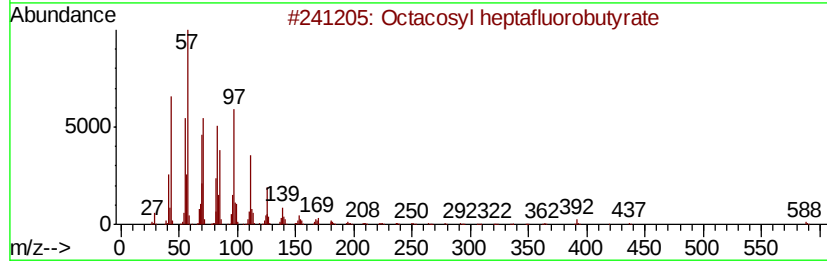
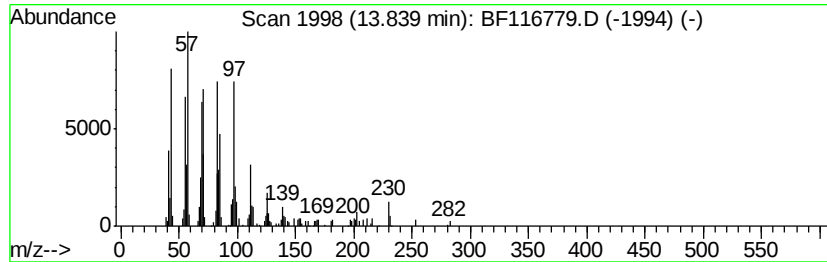
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octacosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.56 ng	207900	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	93
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	76



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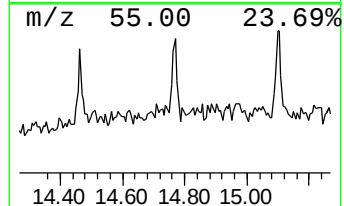
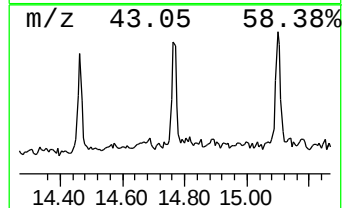
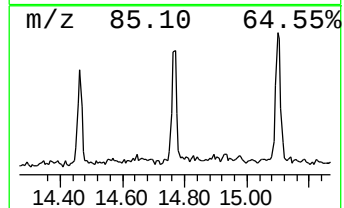
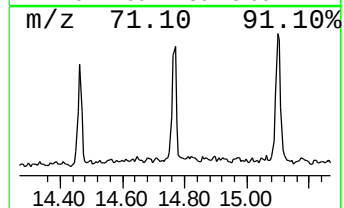
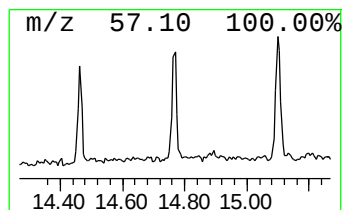
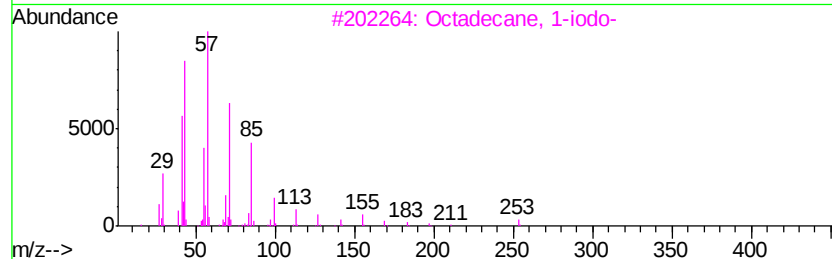
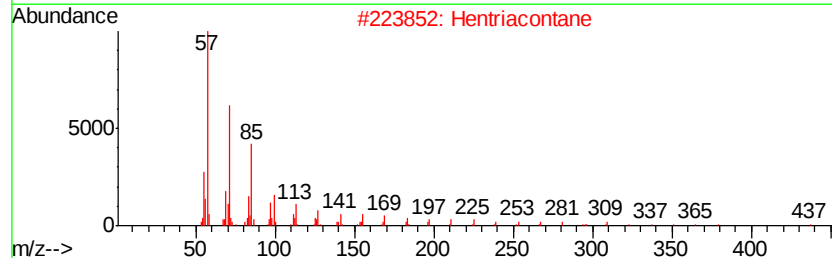
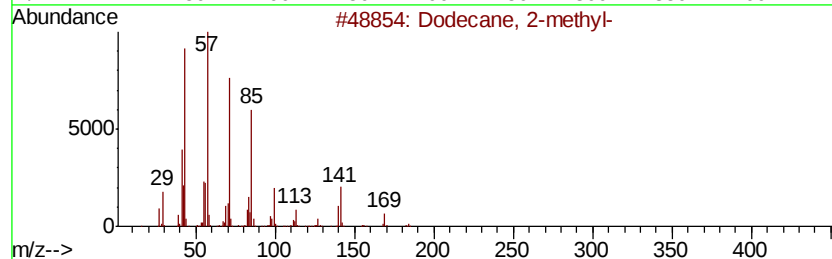
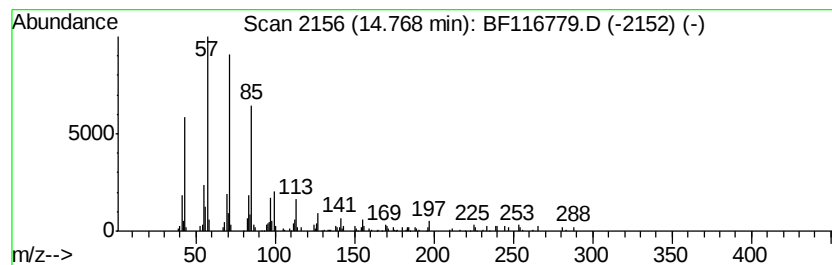
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Peak Number 5 Dodecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	2.19 ng	98908	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4		Hexadecane	226	C16H34	000544-76-3	80
5		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	74



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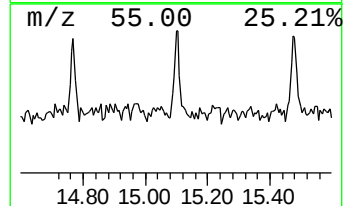
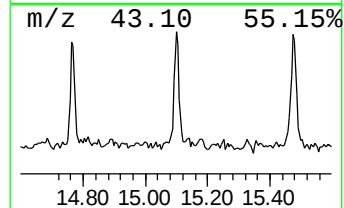
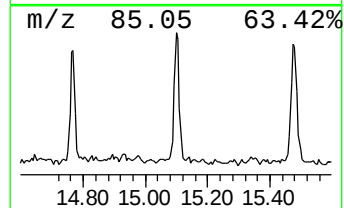
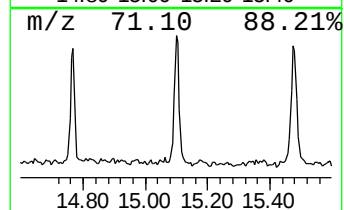
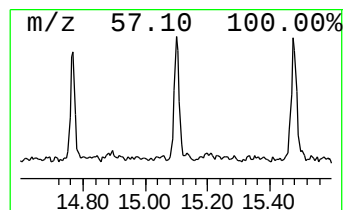
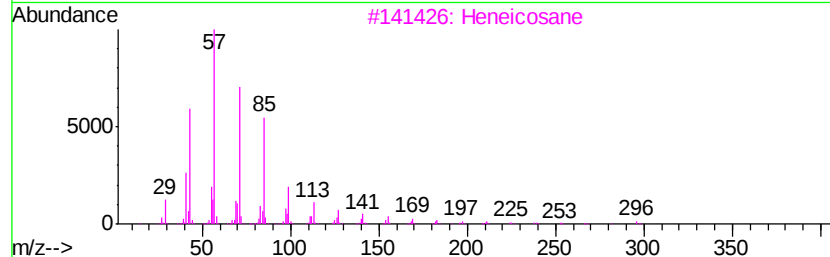
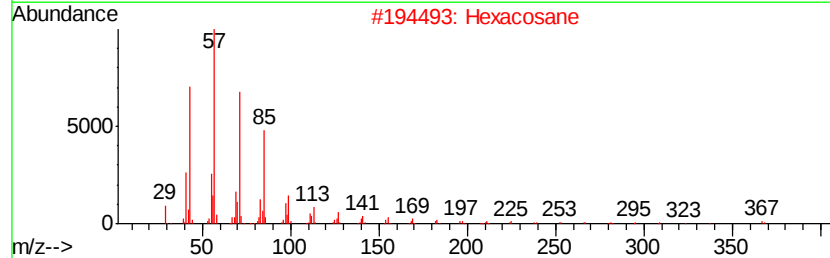
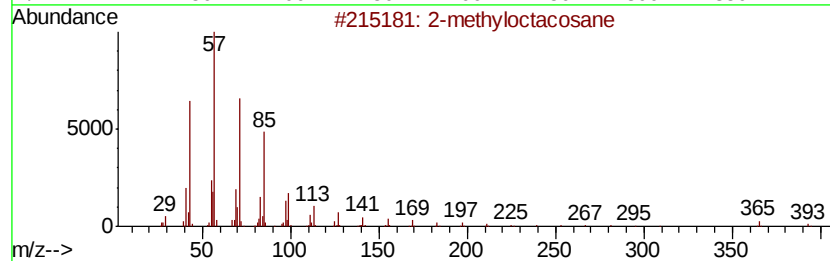
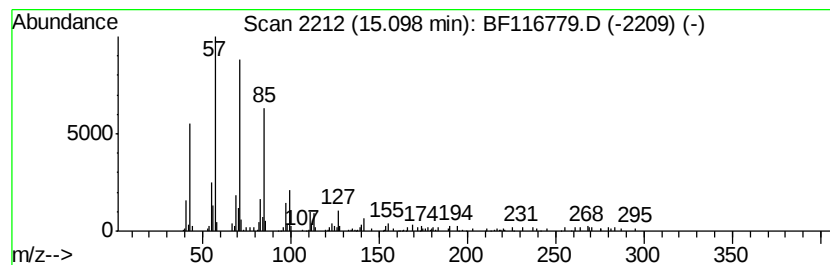
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	2.76 ng	124960	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91	
2	Hexacosane	366	C26H54	000630-01-3	90	
3	Heneicosane	296	C21H44	000629-94-7	87	
4	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	86	
5	Methoxyacetic acid, 4-hexadecyl ...	314	C19H38O3	1000282-99-0	86	



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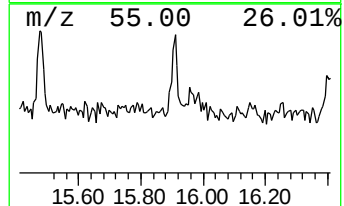
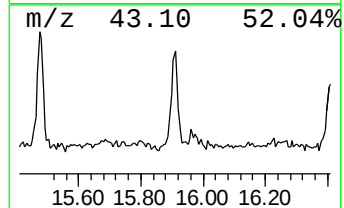
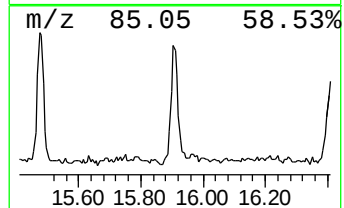
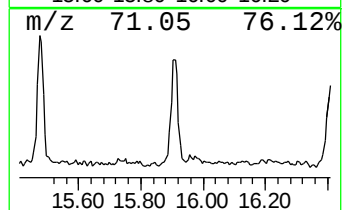
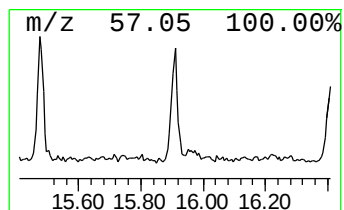
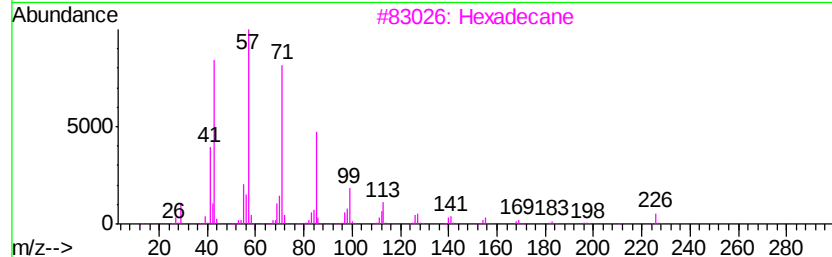
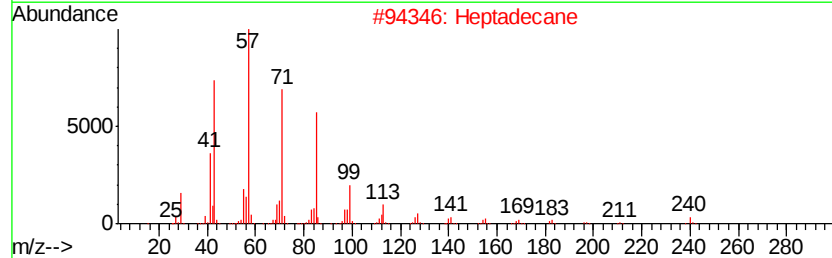
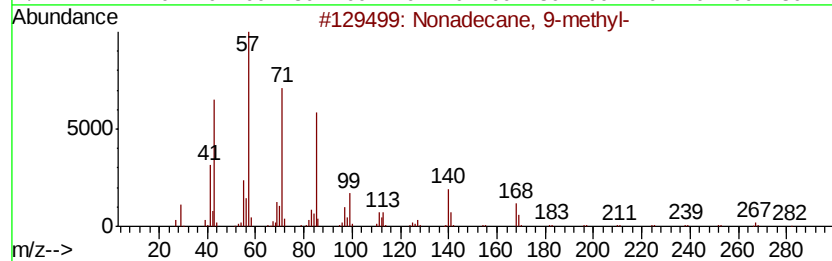
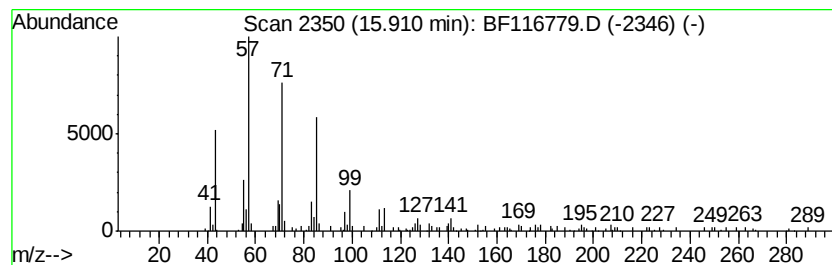
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.81 ng	127244	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
2		Heptadecane	240	C17H36	000629-78-7	86
3		Hexadecane	226	C16H34	000544-76-3	86
4		Hexacosane	366	C26H54	000630-01-3	86
5		Tridecane, 3-methyl-	198	C14H30	006418-41-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116779.D
Acq On : 3 Sep 2019 18:19
Operator : HP/JU
Sample : K4554-40
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8-(5-7)

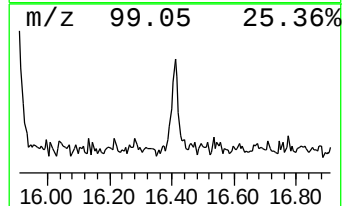
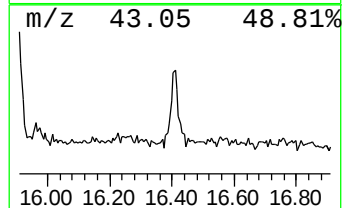
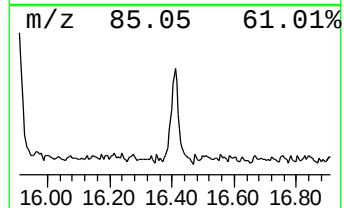
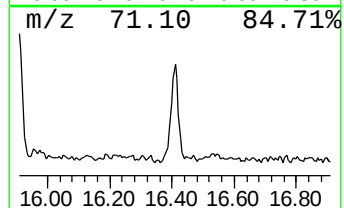
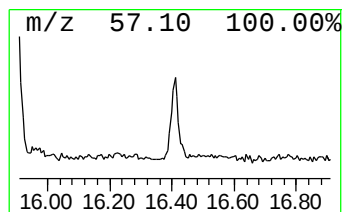
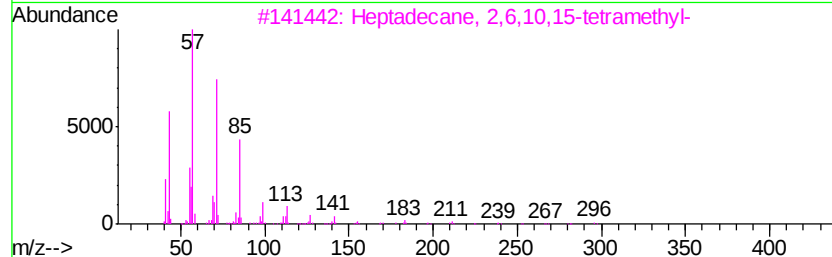
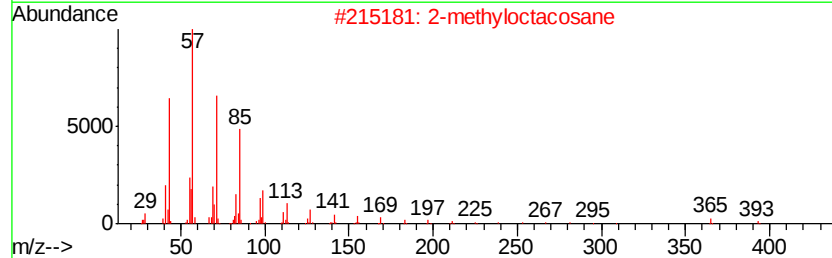
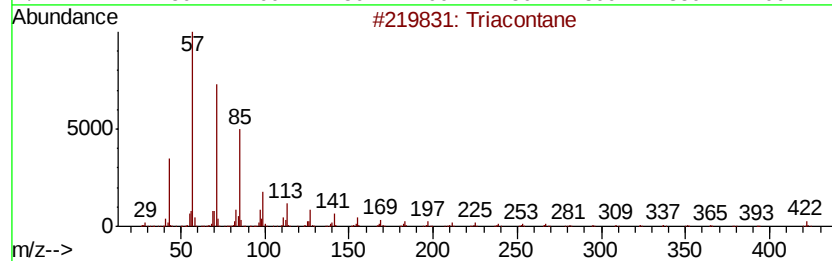
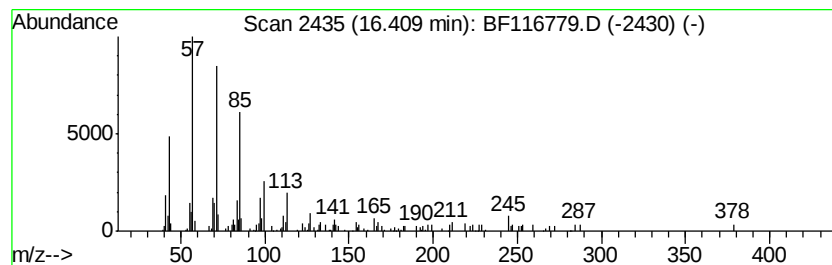
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	2.51 ng	113573	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	86
2		2-methyloctacosane	408	C29H60	1000376-72-8	80
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
4		Hexacosane	366	C26H54	000630-01-3	72
5		Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090319\
Data File : BF116779.D
Acq On : 3 Sep 2019 18:19
Operator : HP/JU
Sample : K4554-40
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8-(5-7)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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...	5.05	2.8	ng	98609	1	6.85	715034	20.0
unknown6.62	6.62	61.2	ng	2188490	1	6.85	715034	20.0
Octacosyl heptafl...	13.84	4.6	ng	207900	5	13.99	911343	20.0
Dodecane, 2-methyl-	14.77	2.2	ng	98908	6	15.44	904616	20.0
2-methyloctacosane	15.10	2.8	ng	124960	6	15.44	904616	20.0
Nonadecane, 9-met...	15.91	2.8	ng	127244	6	15.44	904616	20.0
Triacontane	16.41	2.5	ng	113573	6	15.44	904616	20.0