

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
 Data File : BM039238.D
 Acq On : 30 Mar 2023 22:12
 Operator : CG/JU
 Sample : 02023-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-12-TEST-PIT-ON-OCEAN

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:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039238.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	288	294	305	rVB	1367079	1917002	26.75%	3.529%
2	5.481	367	373	392	rBV	3315870	4644202	64.81%	8.551%
3	7.087	636	646	662	rBV	2925188	4695792	65.53%	8.646%
4	7.922	780	788	797	rBV	845974	1299823	18.14%	2.393%
5	9.092	979	987	1000	rBV	1825537	3016265	42.09%	5.553%
6	10.733	1255	1266	1273	rBV	1008422	1705065	23.79%	3.139%
7	13.192	1674	1684	1695	rBV	4071326	5827059	81.31%	10.728%
8	13.886	1797	1802	1808	rBV	44166	76632	1.07%	0.141%
9	14.021	1821	1825	1833	rVB2	48479	100088	1.40%	0.184%
10	14.292	1864	1871	1884	rBV	190520	336456	4.70%	0.619%
11	14.398	1884	1889	1897	rBV5	24115	71805	1.00%	0.132%
12	14.568	1906	1918	1924	rBV	1340394	1974664	27.56%	3.636%
13	15.174	2014	2021	2027	rBV3	36634	87871	1.23%	0.162%
14	15.615	2090	2096	2108	rVB2	61321	133264	1.86%	0.245%
15	15.927	2142	2149	2161	rVB	1005309	1390967	19.41%	2.561%
16	16.057	2162	2171	2189	rBV	2904792	4234724	59.09%	7.797%
17	16.292	2208	2211	2222	rVB4	65638	115376	1.61%	0.212%
18	16.486	2239	2244	2250	rVB	102943	142437	1.99%	0.262%
19	16.615	2259	2266	2271	rBV3	36452	74846	1.04%	0.138%
20	17.315	2378	2385	2389	rBV	1531179	2163431	30.19%	3.983%
21	17.356	2389	2392	2399	rVV	275625	370968	5.18%	0.683%
22	17.445	2402	2407	2412	rVV	155460	222278	3.10%	0.409%
23	18.209	2529	2537	2540	rBV2	372932	639531	8.92%	1.177%
24	18.239	2540	2542	2548	rVV	179163	267697	3.74%	0.493%
25	18.321	2552	2556	2561	rVV	89814	156745	2.19%	0.289%
26	18.392	2561	2568	2571	rVV2	254379	488191	6.81%	0.899%
27	18.421	2571	2573	2582	rVB	99950	141336	1.97%	0.260%
28	19.109	2685	2690	2695	rBV	121238	217984	3.04%	0.401%
29	19.168	2696	2700	2703	rVV3	60879	94615	1.32%	0.174%
30	19.368	2730	2734	2741	rVB	489742	633598	8.84%	1.167%
31	19.486	2749	2754	2757	rBV3	124839	200633	2.80%	0.369%
32	19.521	2757	2760	2765	rVB	79970	112796	1.57%	0.208%
33	19.733	2788	2796	2805	rBV	908741	1421677	19.84%	2.618%
34	19.809	2806	2809	2814	rVB2	59786	86824	1.21%	0.160%
35	19.939	2825	2831	2842	rVB	5876349	7166117	100.00%	13.194%
36	20.056	2847	2851	2859	rBV3	85420	207076	2.89%	0.381%

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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:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.327	2894	2897	2901	rVB2	110910	134114	1.87%	0.247%
38	20.386	2904	2907	2911	rBV	159483	194413	2.71%	0.358%
39	20.527	2927	2931	2935	rBV2	205124	257006	3.59%	0.473%
40	20.574	2936	2939	2943	rVV3	199283	255299	3.56%	0.470%
41	21.203	3042	3046	3051	rBV2	487875	646680	9.02%	1.191%
42	21.497	3090	3096	3100	rBV2	2090631	3175831	44.32%	5.847%
43	21.533	3100	3102	3109	rVB	381800	459870	6.42%	0.847%
44	23.909	3500	3506	3513	rBV2	1422043	2755171	38.45%	5.073%

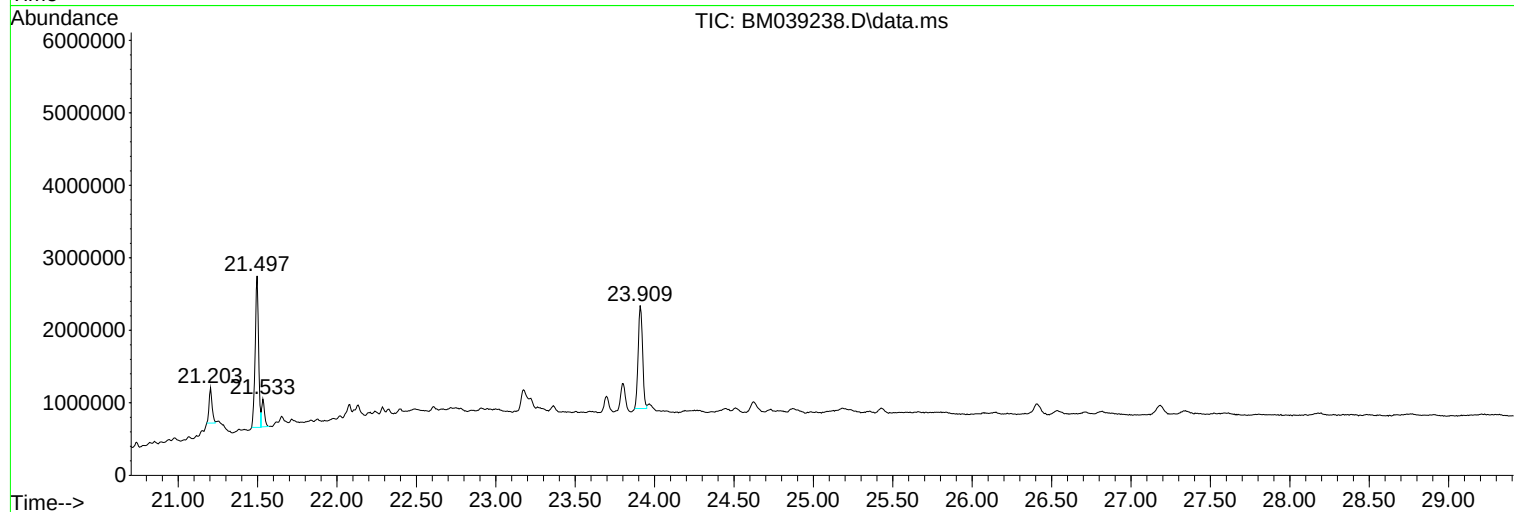
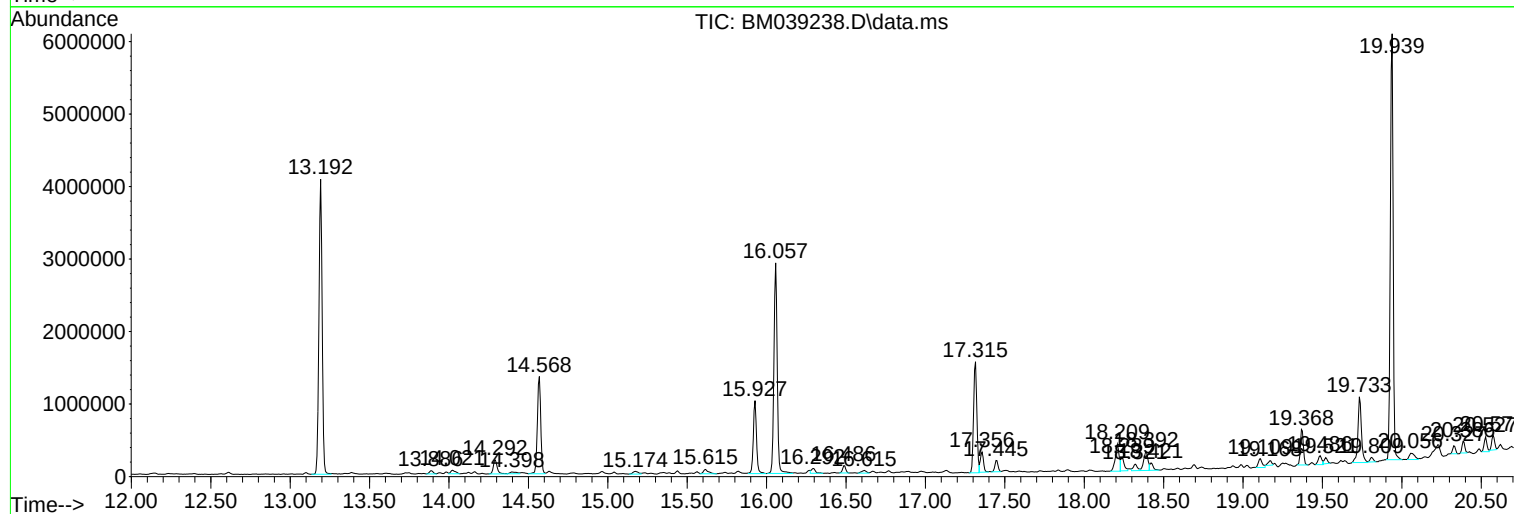
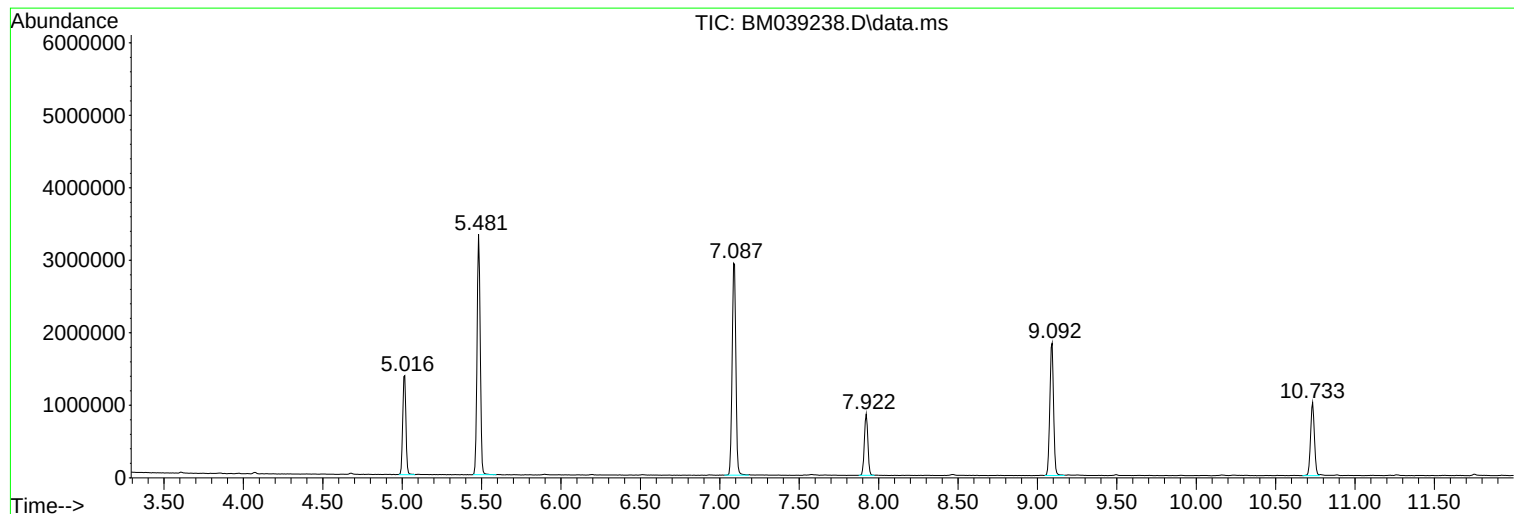
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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TP-12-TEST-PIT-ON-OCEAN

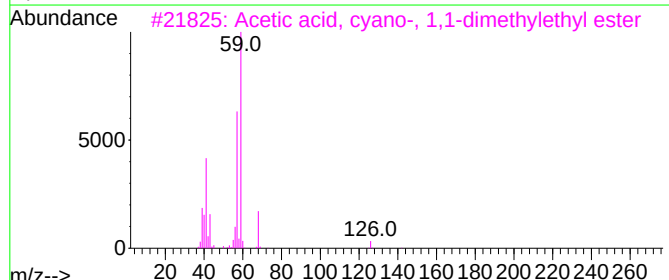
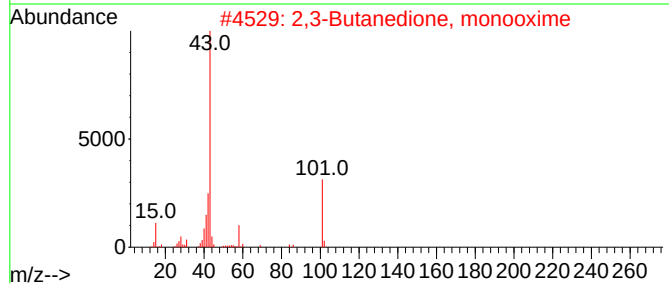
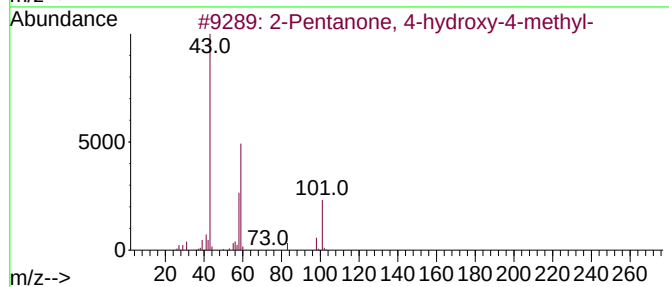
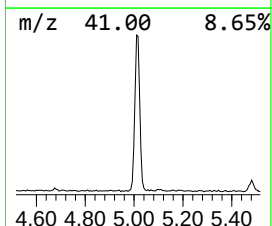
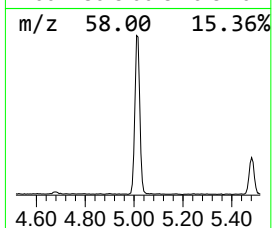
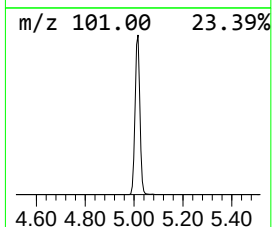
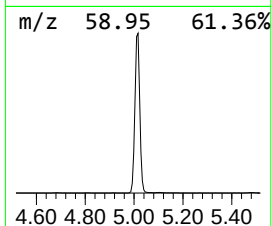
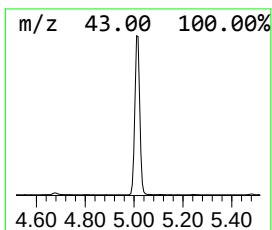
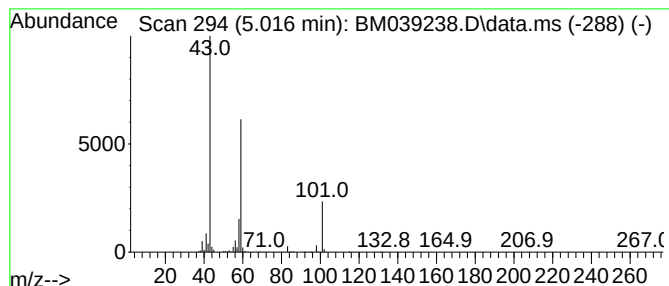
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	29.50 ng	1917000	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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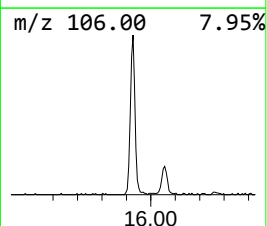
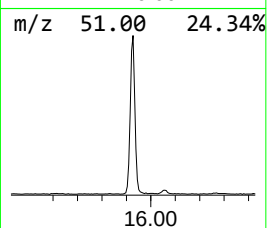
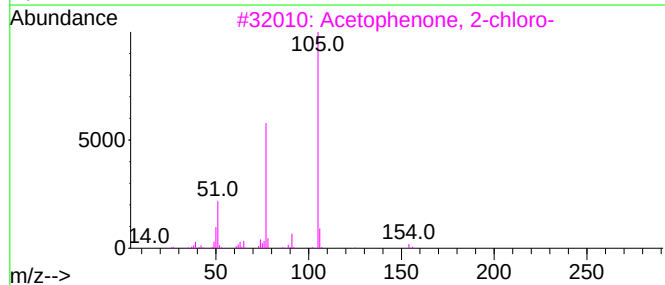
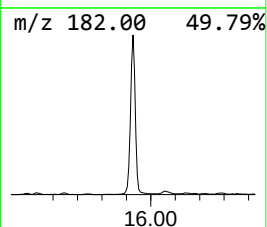
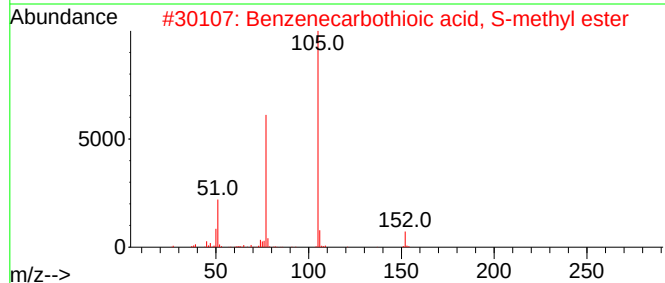
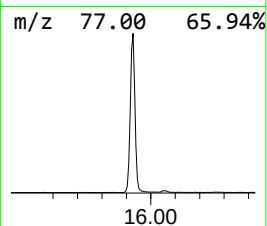
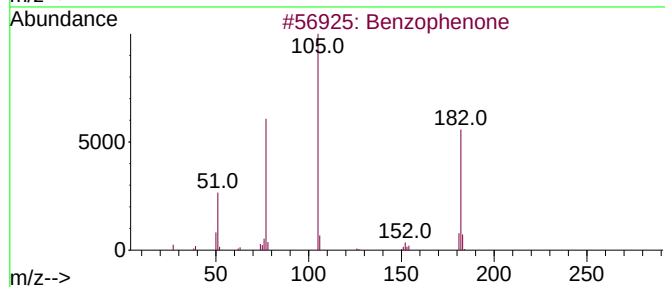
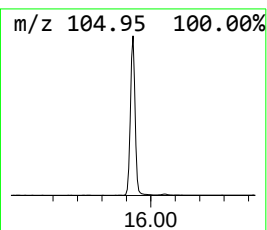
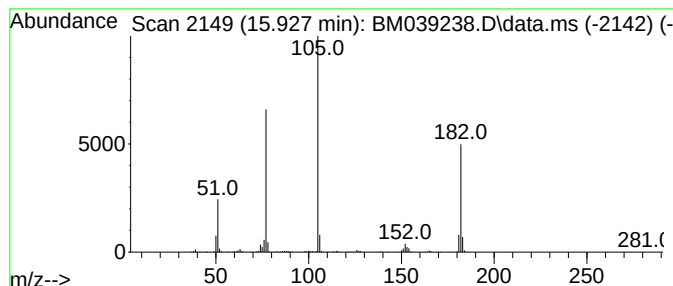
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	14.09 ng	1390970	Acenaphthene-d10	14.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47



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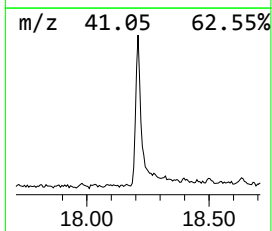
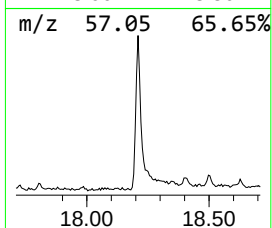
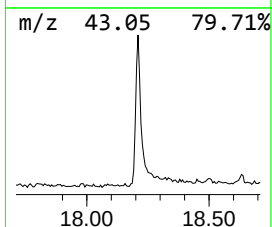
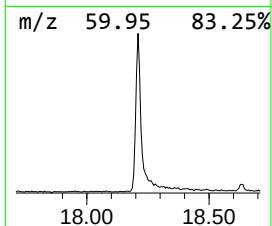
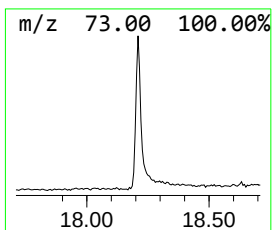
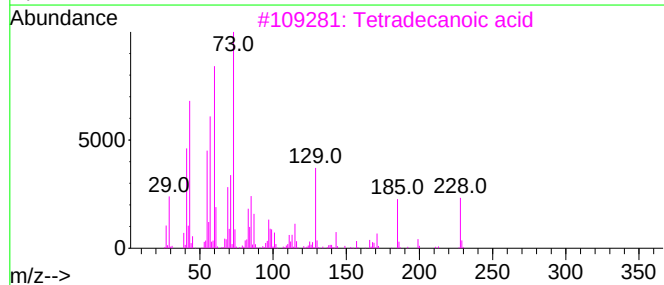
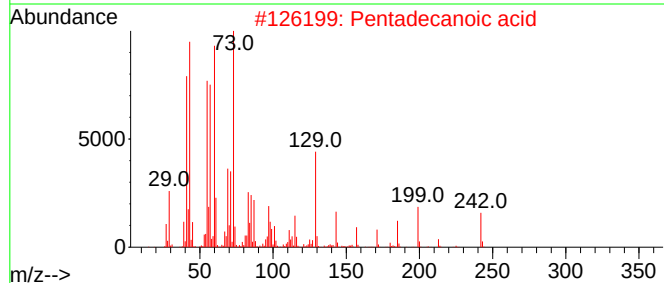
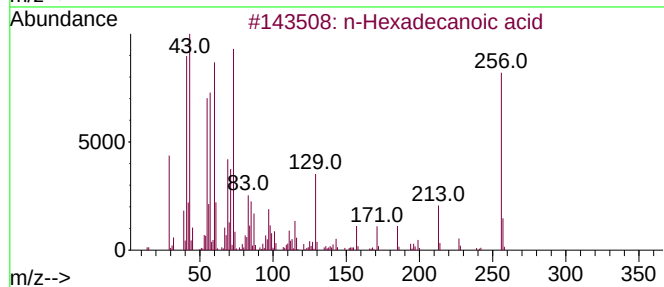
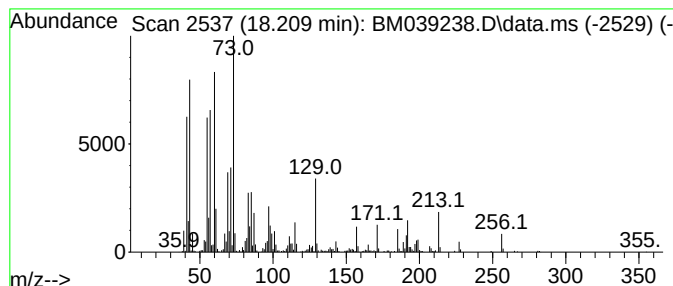
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.209	5.91 ng	639531	Phenanthrene-d10		17.315	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	89
4	Tridecanoic acid		214	C13H26O2	000638-53-9	89
5	Nonanoic acid		158	C9H18O2	000112-05-0	45



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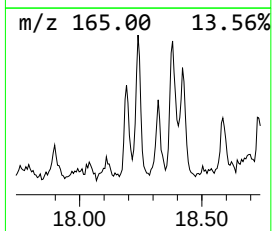
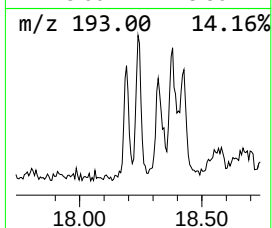
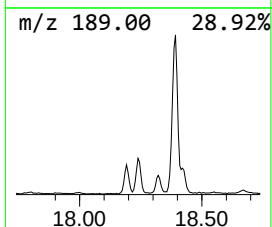
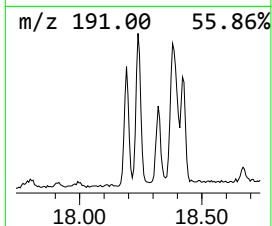
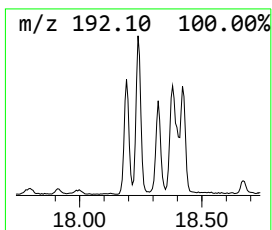
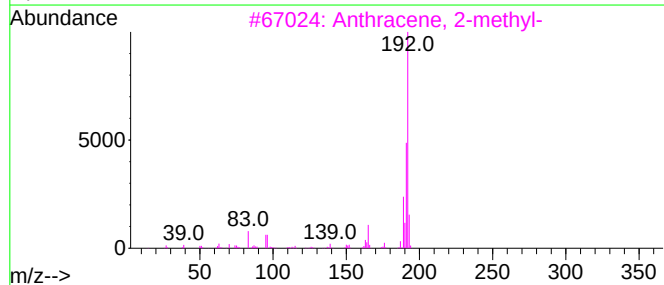
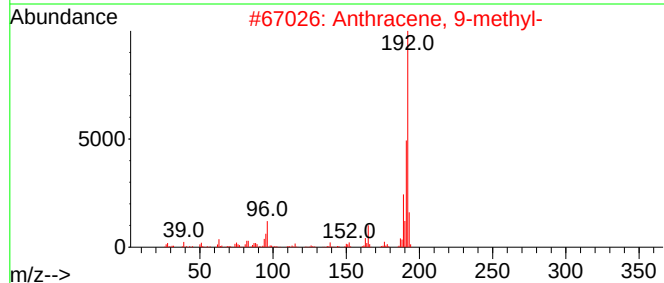
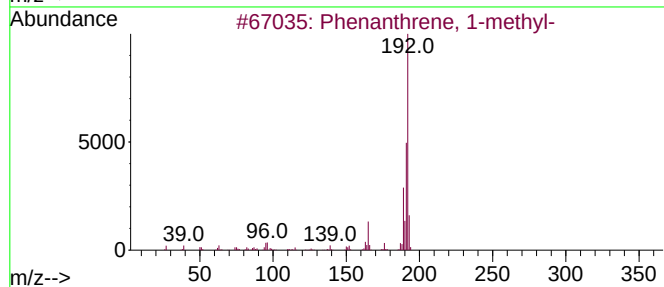
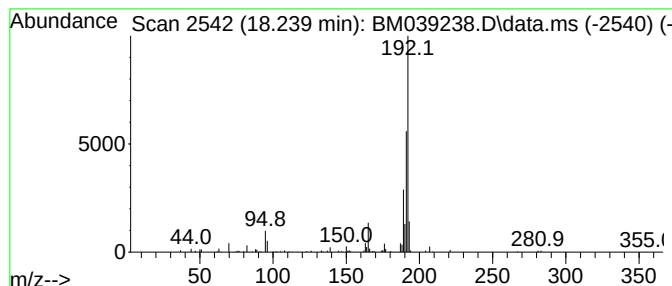
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	2.47 ng	267697	Phenanthrene-d10	17.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87



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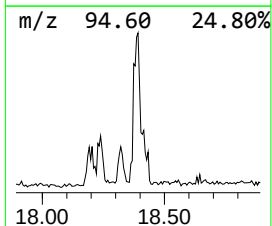
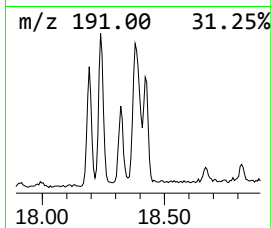
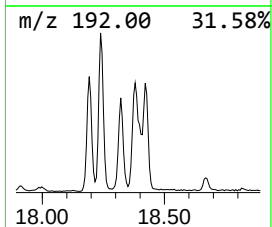
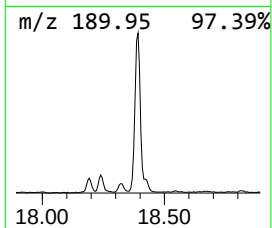
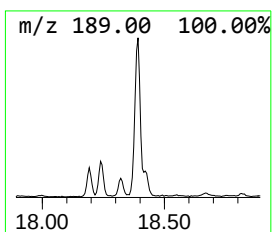
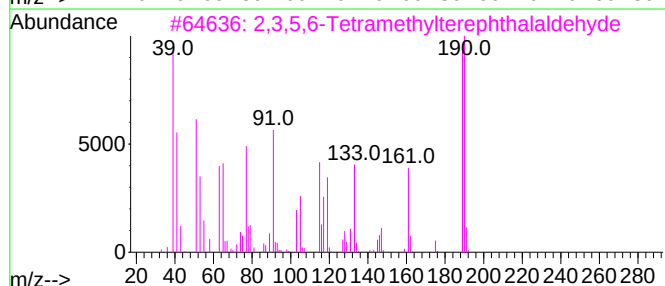
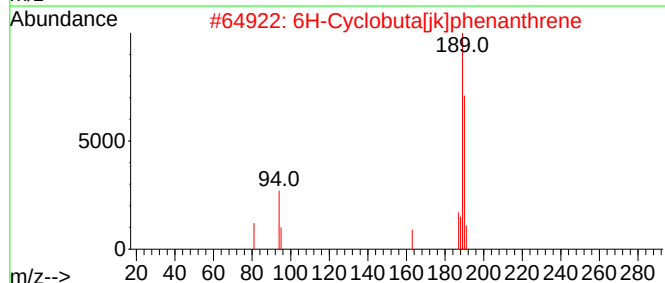
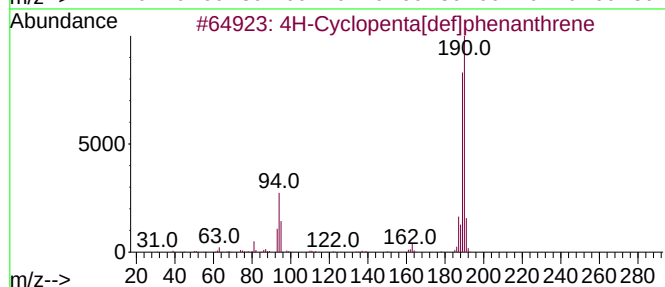
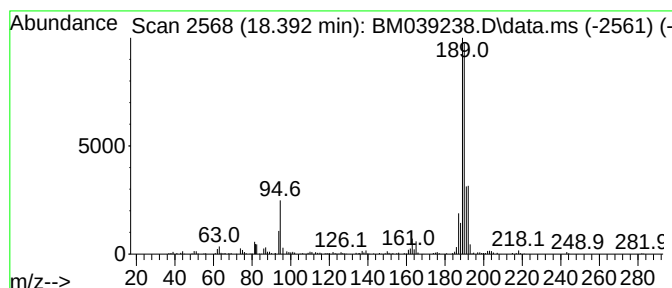
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.392	4.51 ng	488191	Phenanthrene-d10	17.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4			1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	35
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039238.D
Acq On : 30 Mar 2023 22:12
Operator : CG/JU
Sample : 02023-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-12-TEST-PIT-ON-OCEAN

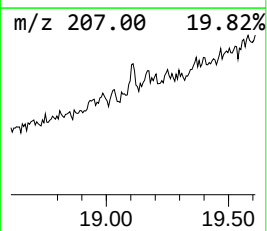
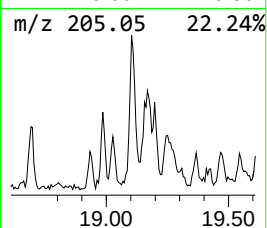
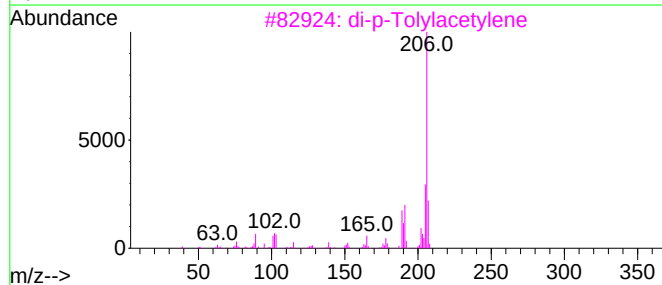
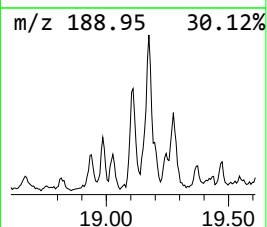
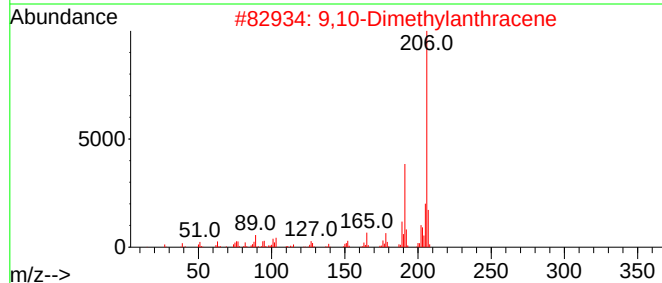
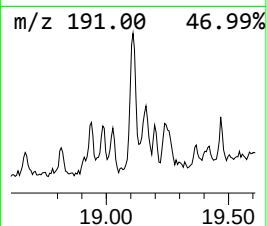
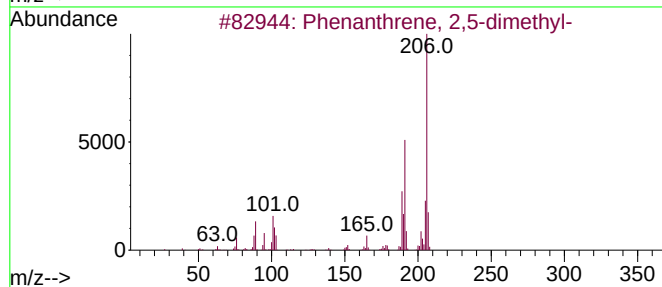
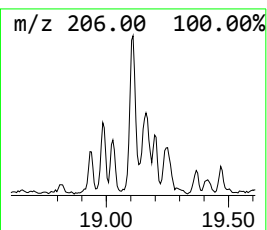
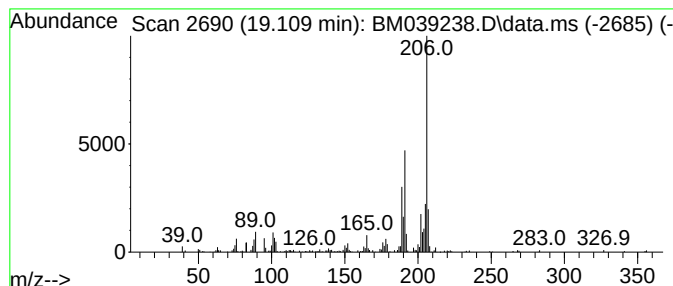
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.109	2.02 ng	217984	Phenanthrene-d10	17.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2			9,10-Dimethylantracene	206	C16H14	000781-43-1	95
3			di-p-Tolylacetylene	206	C16H14	002789-88-0	94
4			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
5			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039238.D
Acq On : 30 Mar 2023 22:12
Operator : CG/JU
Sample : 02023-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-12-TEST-PIT-ON-OCEAN

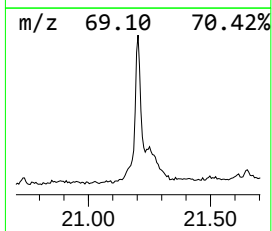
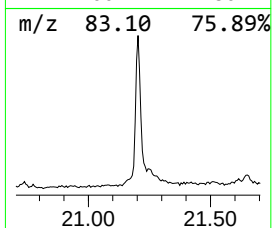
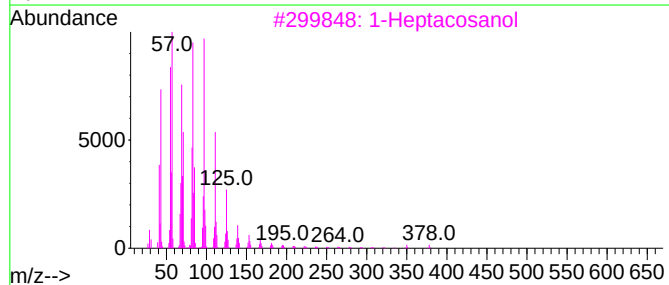
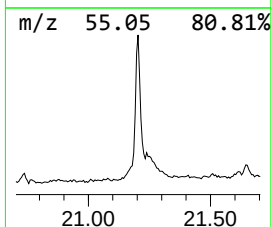
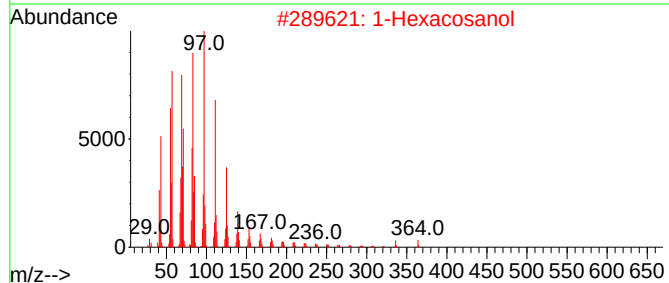
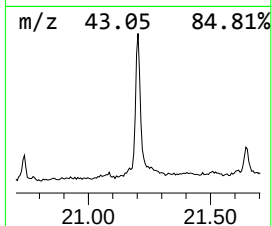
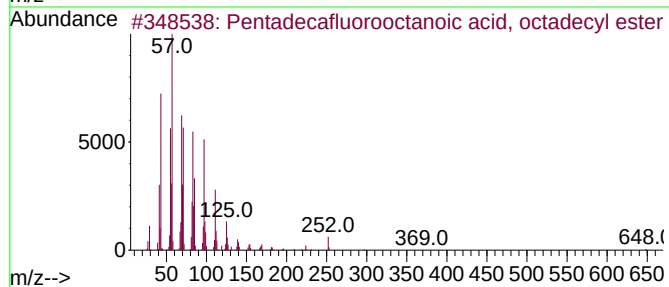
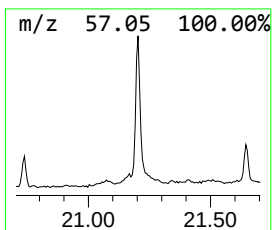
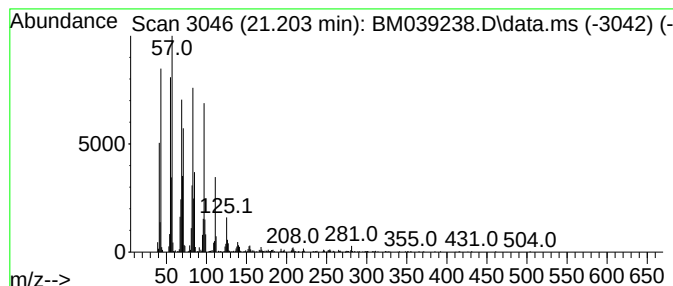
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.203	4.07 ng	646680	Chrysene-d12	21.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Hexacosanol	382	C26H54O	000506-52-5	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
Data File : BM039238.D
Acq On : 30 Mar 2023 22:12
Operator : CG/JU
Sample : 02023-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-12-TEST-PIT-ON-OCEAN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	29.5	ng	1917000	1	7.922	1299820	20.0
Benzophenone	15.927	14.1	ng	1390970	3	14.568	1974660	20.0
n-Hexadecanoic ...	18.209	5.9	ng	639531	4	17.315	2163430	20.0
Phenanthrene, 1...	18.239	2.5	ng	267697	4	17.315	2163430	20.0
4H-Cyclopenta[d...	18.392	4.5	ng	488191	4	17.315	2163430	20.0
Phenanthrene, 2...	19.109	2.0	ng	217984	4	17.315	2163430	20.0
Pentadecafluoro...	21.203	4.1	ng	646680	5	21.497	3175830	20.0