

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
 Data File : BG021646.D
 Acq On : 14 Apr 2016 9:32
 Operator : UM/SJ
 Sample : H2418-01
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GMW-11

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:\HPCHEM1\BNA_G\METHODS\8270-BG041316.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	2.914	11	13	21	rVB2	20895	33938	1.14%	0.222%
2	5.299	413	419	427	rVB	34577	56201	1.88%	0.367%
3	5.763	491	498	510	rVB	378941	633456	21.19%	4.137%
4	7.356	762	769	778	rBV	276284	473160	15.83%	3.090%
5	7.743	825	835	846	rBV	645301	1118021	37.40%	7.301%
6	8.219	908	916	922	rBV	114116	203819	6.82%	1.331%
7	8.542	964	971	979	rBV	529272	932639	31.20%	6.090%
8	9.383	1106	1114	1122	rBV	483255	876646	29.32%	5.725%
9	9.465	1122	1128	1137	rVB2	20875	35820	1.20%	0.234%
10	10.446	1288	1295	1300	rBV	40151	75678	2.53%	0.494%
11	11.034	1388	1395	1399	rBV	178334	327840	10.97%	2.141%
12	11.081	1399	1403	1411	rVB	152168	281616	9.42%	1.839%
13	11.786	1515	1523	1528	rBV4	22656	44033	1.47%	0.288%
14	12.667	1666	1673	1681	rBV	19932	35615	1.19%	0.233%
15	12.884	1702	1710	1717	rBV	16398	32558	1.09%	0.213%
16	13.454	1794	1807	1814	rBV	1329763	2102991	70.34%	13.733%
17	14.823	2030	2040	2046	rBV2	277216	462055	15.46%	3.017%
18	14.882	2046	2050	2057	rVB	36757	55251	1.85%	0.361%
19	15.211	2101	2106	2112	rBV2	28472	49919	1.67%	0.326%
20	15.863	2211	2217	2222	rVB	28411	45534	1.52%	0.297%
21	16.298	2281	2291	2299	rBV	962139	1510201	50.52%	9.862%
22	16.380	2300	2305	2312	rVB2	29071	48594	1.63%	0.317%
23	17.297	2457	2461	2465	rBV3	30788	47978	1.60%	0.313%
24	17.350	2466	2470	2475	rVB6	17643	31020	1.04%	0.203%
25	17.555	2498	2505	2510	rBV2	352138	565221	18.91%	3.691%
26	17.597	2510	2512	2518	rVB	44513	57406	1.92%	0.375%
27	17.949	2568	2572	2578	rVB	64917	95936	3.21%	0.626%
28	18.102	2594	2598	2603	rVB2	18878	30048	1.01%	0.196%
29	18.425	2649	2653	2658	rBV3	45621	68608	2.29%	0.448%
30	18.537	2668	2672	2677	rBV4	18506	33691	1.13%	0.220%
31	19.682	2863	2867	2874	rBV3	66081	117193	3.92%	0.765%
32	19.953	2909	2913	2919	rVB2	49965	80048	2.68%	0.523%
33	20.146	2940	2946	2953	rVB	2199174	2989542	100.00%	19.522%
34	20.934	3078	3080	3084	rVB	43528	37670	1.26%	0.246%

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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:\HPCHEM1\BNA_G\METHODS\8270-BG041316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.433	3162	3165	3166	rBV3	43611	48233	1.61%	0.315%
36	21.827	3226	3232	3241	rVB	412327	712519	23.83%	4.653%
37	22.015	3261	3264	3269	rVB	53691	77309	2.59%	0.505%
38	22.644	3368	3371	3379	rVB2	47609	81808	2.74%	0.534%
39	23.366	3490	3494	3500	rVB2	37607	68519	2.29%	0.447%
40	25.158	3789	3799	3817	rVB3	233837	735132	24.59%	4.801%

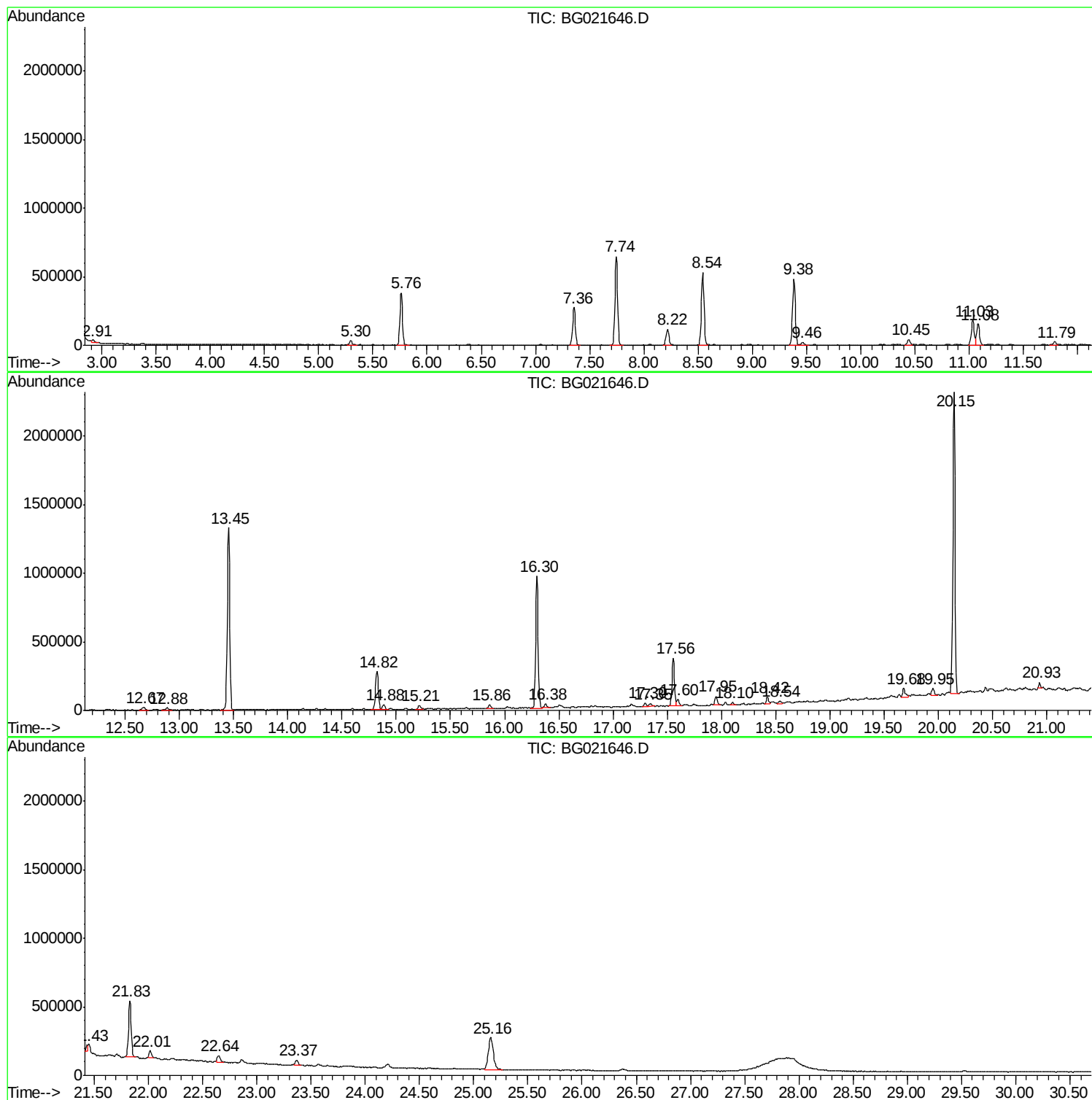
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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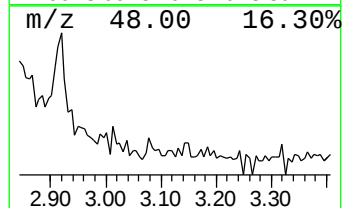
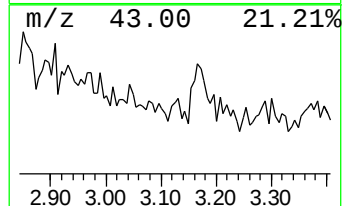
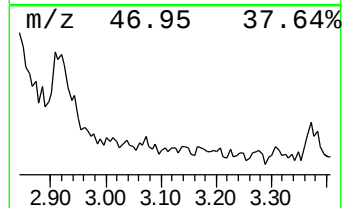
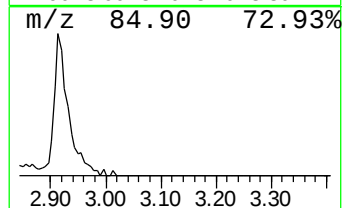
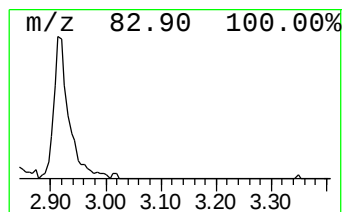
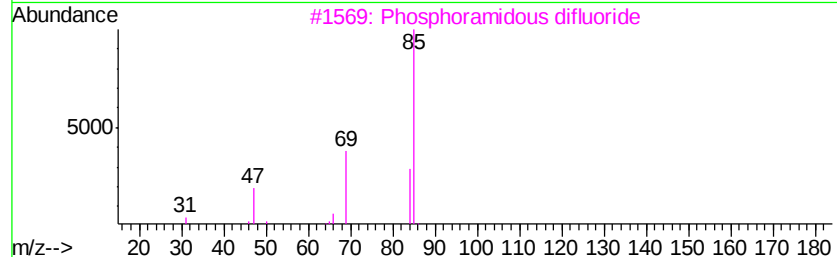
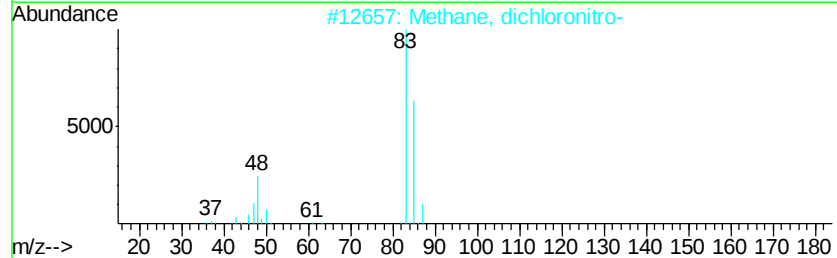
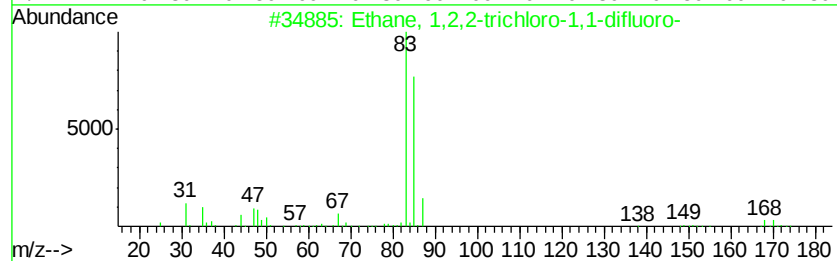
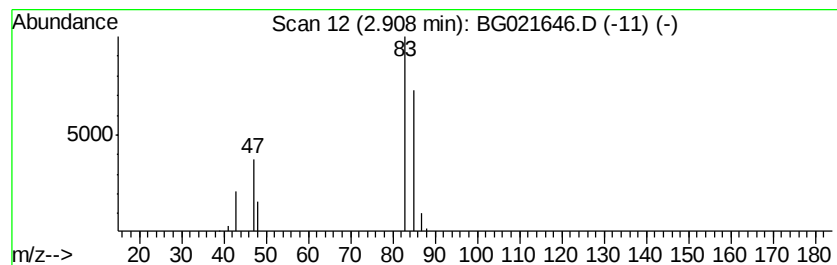
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethane, 1,2,2-trichloro-1,1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.91	3.33 ng	33938	1,4-Dichlorobenzene-d4	8.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2,2-trichloro-1,1-difl...	168	C2HCl3F2	000354-21-2	64
2			Methane, dichloronitro-	129	CHCl2NO2	007119-89-3	43
3			Phosphoramidous difluoride	85	F2H2NP	025757-74-8	7
4			2-Pyrrolidinone	85	C4H7NO	000616-45-5	4
5			Trichloromethane	118	CHCl3	000067-66-3	4



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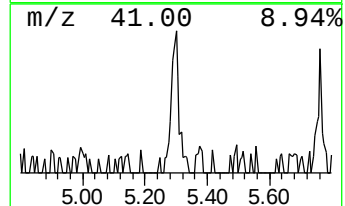
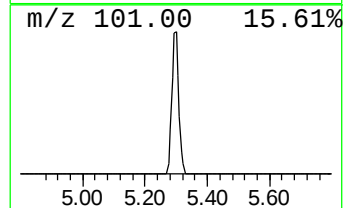
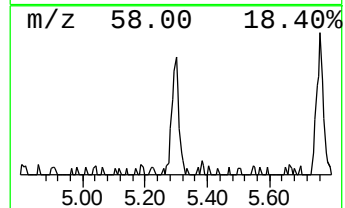
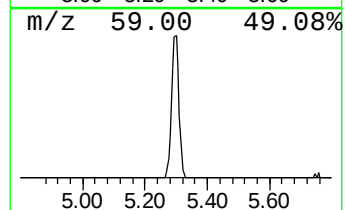
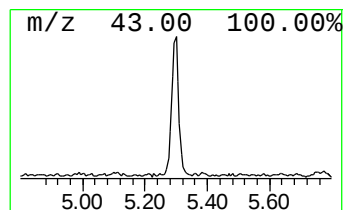
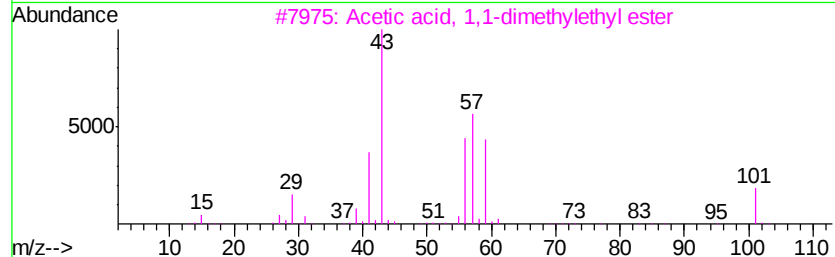
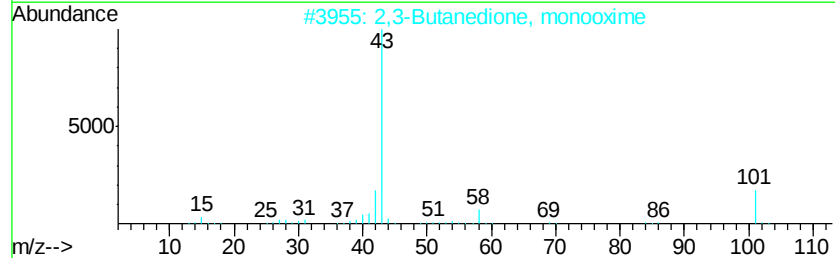
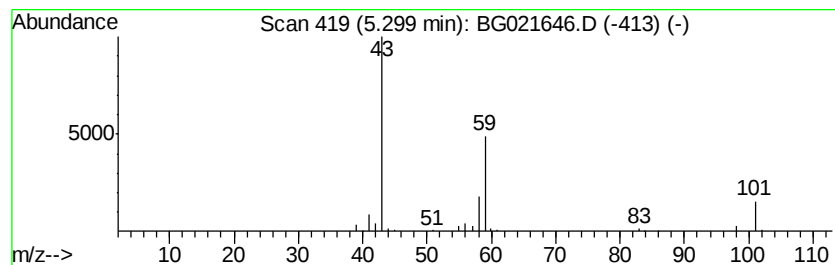
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.30	5.51 ng	56201	1,4-Dichlorobenzene-d4	8.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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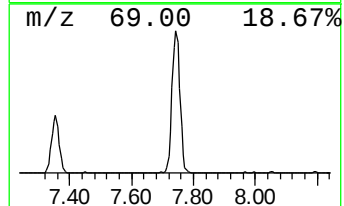
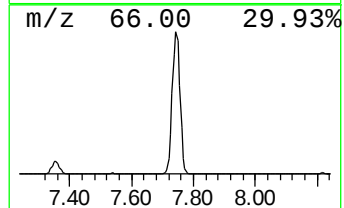
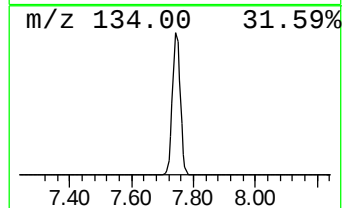
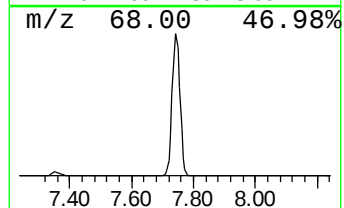
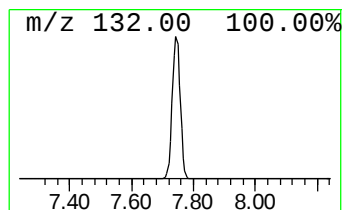
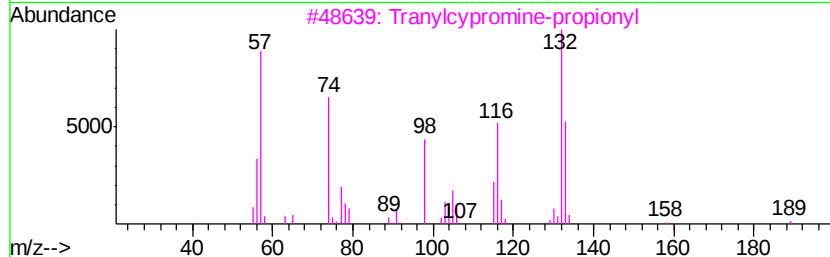
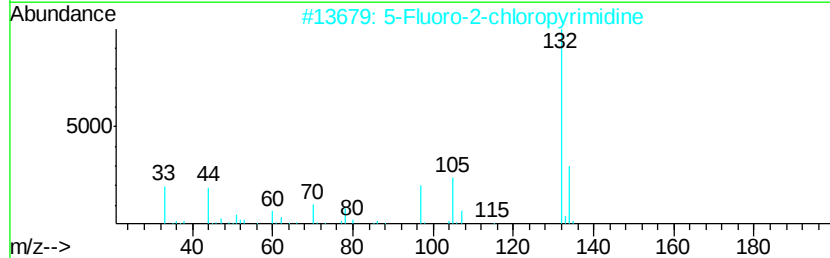
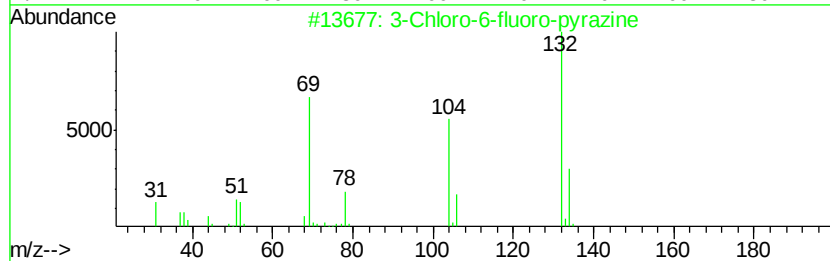
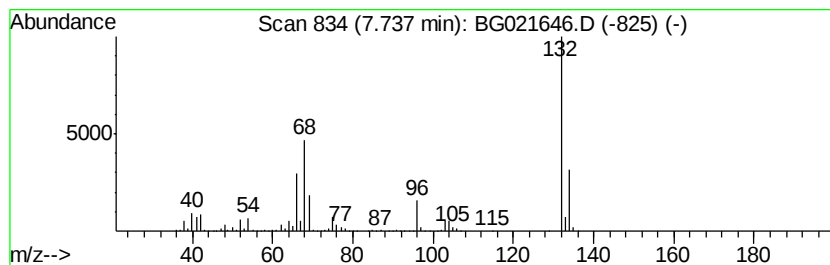
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	109.71 ng	1118020	1,4-Dichlorobenzene-d4	8.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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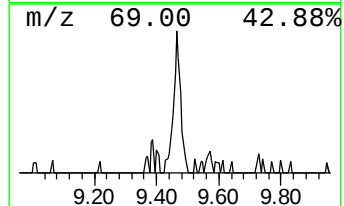
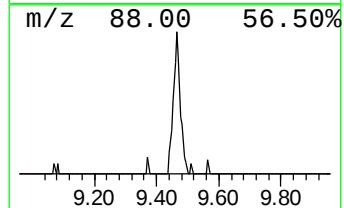
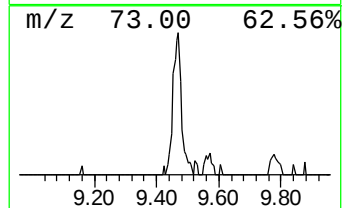
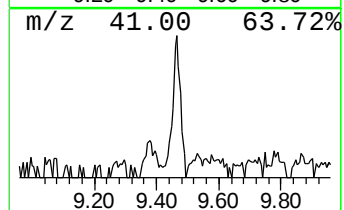
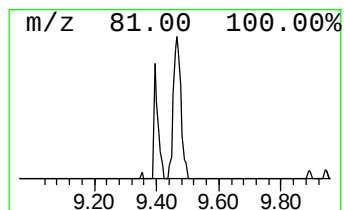
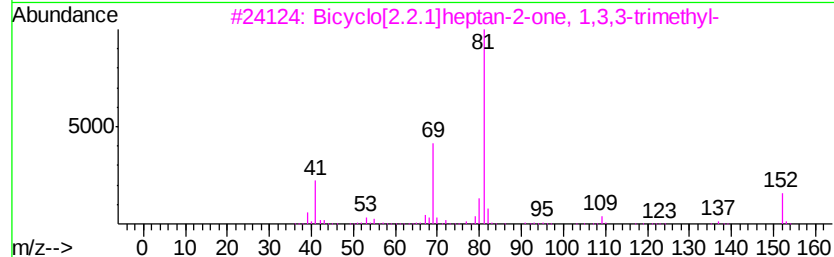
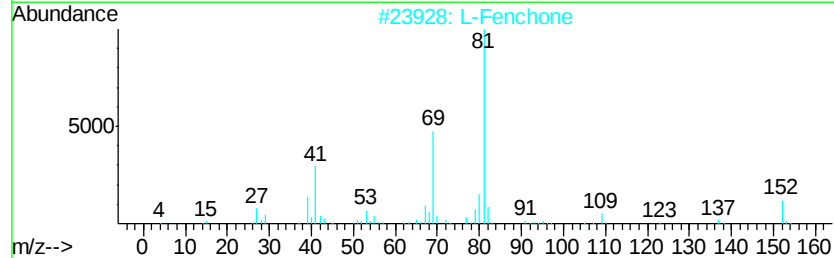
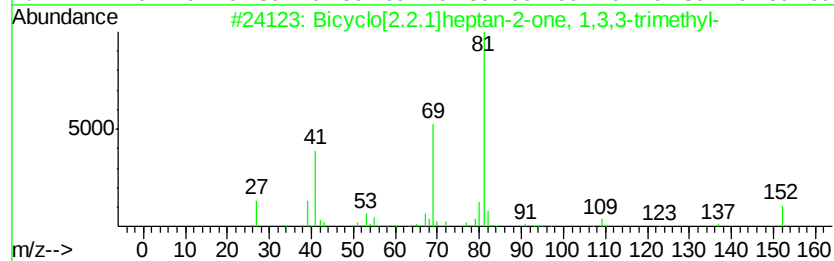
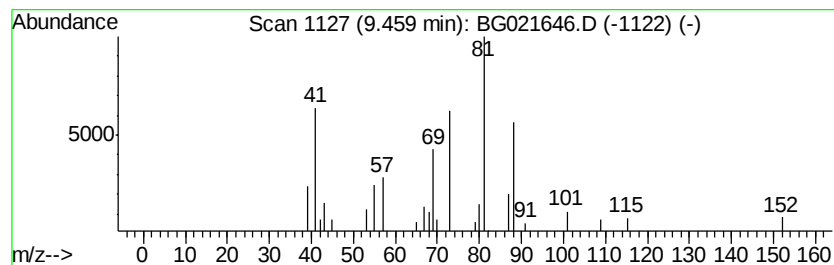
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.46 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.46	3.51 ng	35820	1,4-Dichlorobenzene-d4	8.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	46
2		L-Fenchone	152	C10H16O	000126-21-6	46
3		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	004695-62-9	43
4		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	007787-20-4	38
5		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	27



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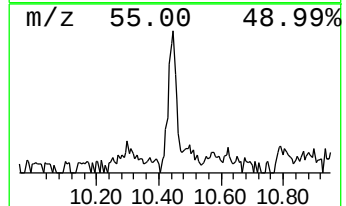
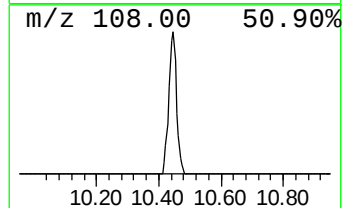
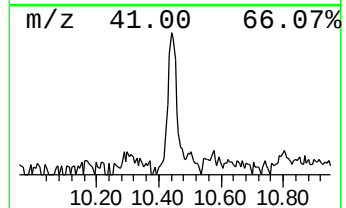
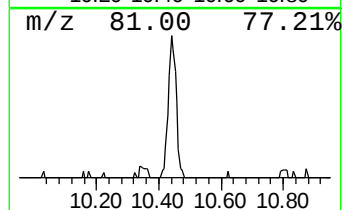
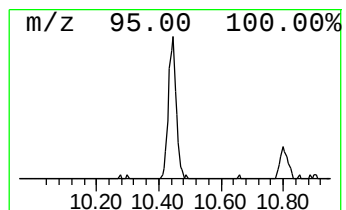
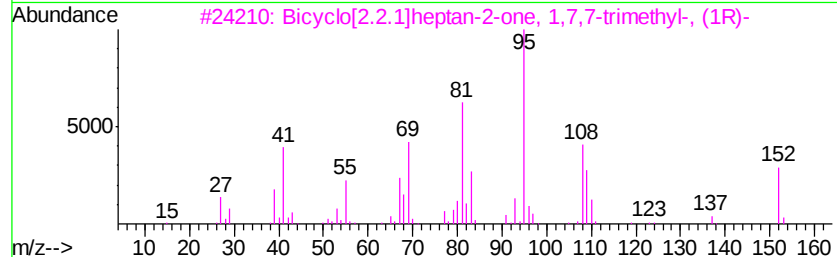
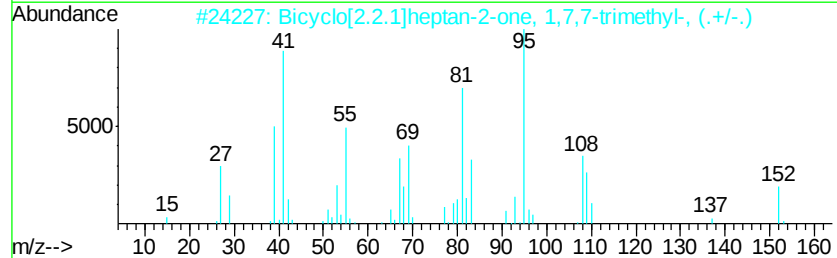
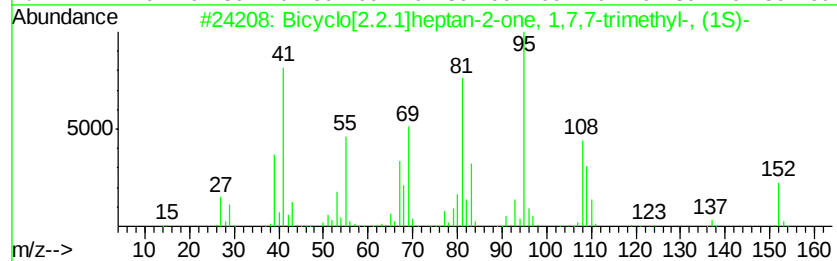
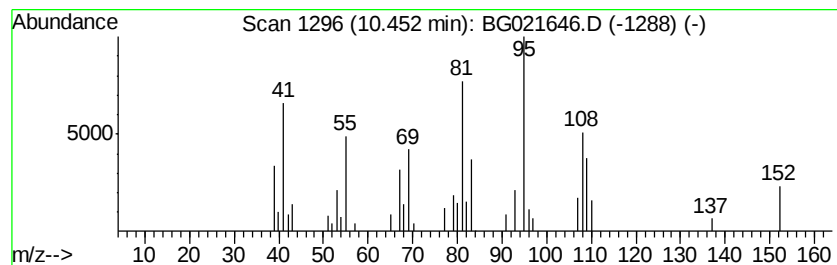
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	4.62 ng	75678	Naphthalene-d8	11.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
2		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	94
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	93
4		Camphor	152	C10H16O	000076-22-2	72
5		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
Data File : BG021646.D
Acq On : 14 Apr 2016 9:32
Operator : UM/SJ
Sample : H2418-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GMW-11

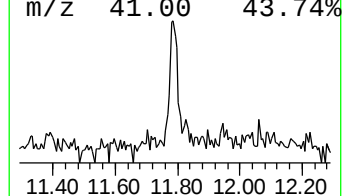
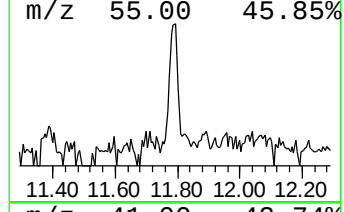
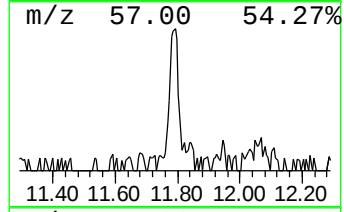
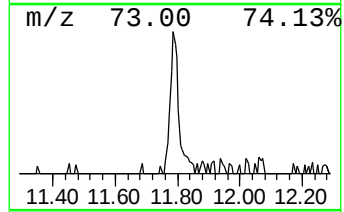
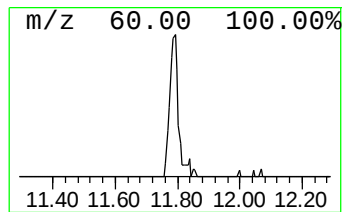
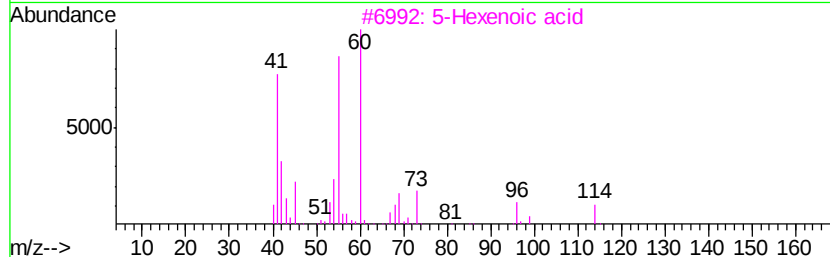
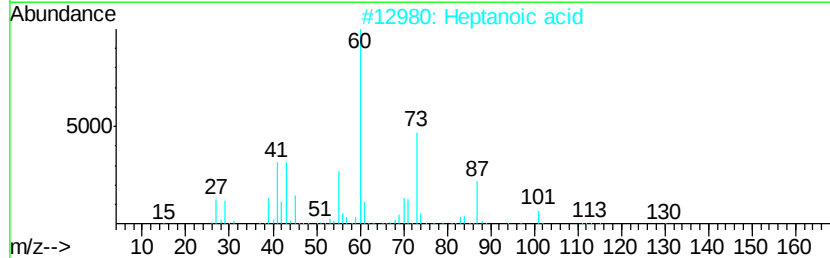
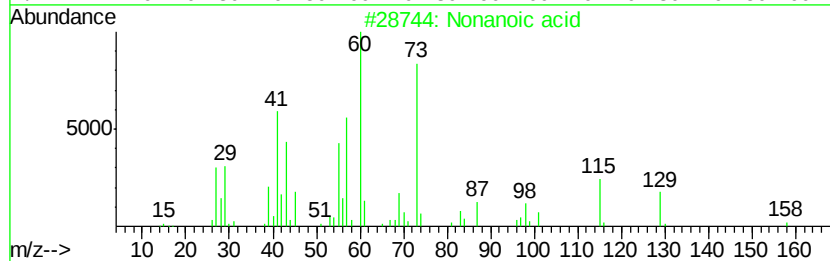
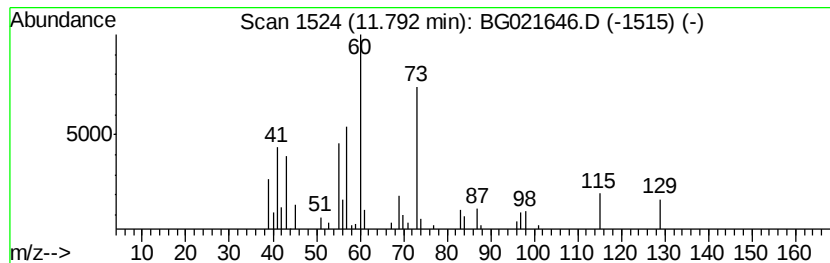
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown11.79 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.69 ng	44033	Napthalene-d8	11.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	45
2		Heptanoic acid	130	C7H14O2	000111-14-8	42
3		5-Hexenoic acid	114	C6H10O2	001577-22-6	37
4		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	33
5		Hexanoic acid	116	C6H12O2	000142-62-1	28



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
Data File : BG021646.D
Acq On : 14 Apr 2016 9:32
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Sample : H2418-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
GMW-11

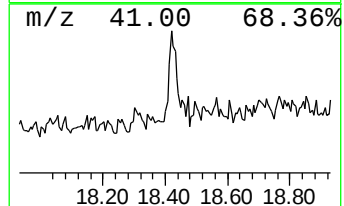
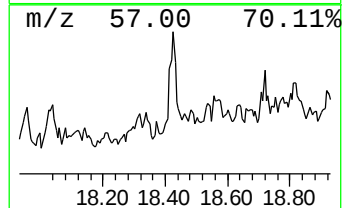
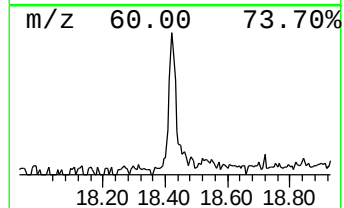
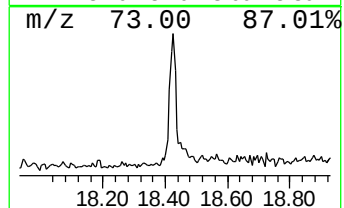
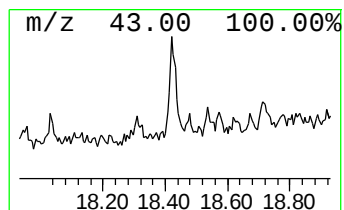
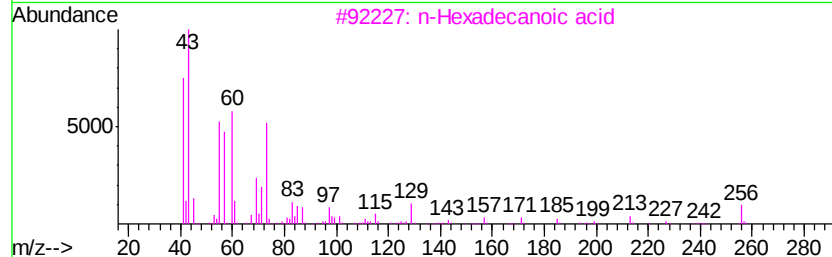
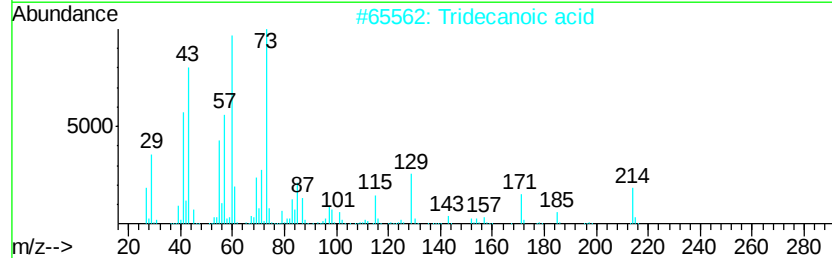
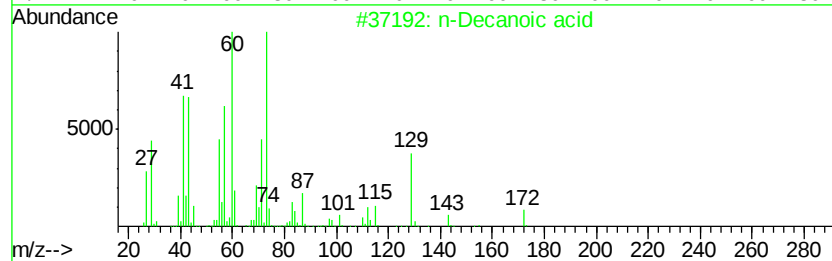
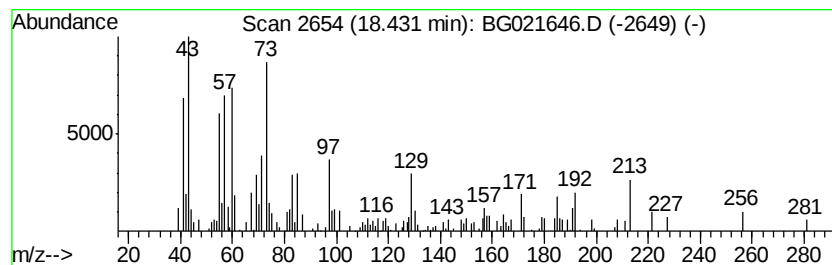
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 n-Decanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	2.43 ng	68608	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	68
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		Tridecane	184	C13H28	000629-50-5	53



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
Data File : BG021646.D
Acq On : 14 Apr 2016 9:32
Operator : UM/SJ
Sample : H2418-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleID :
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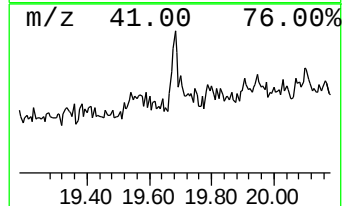
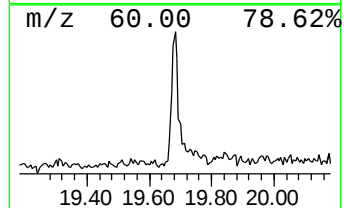
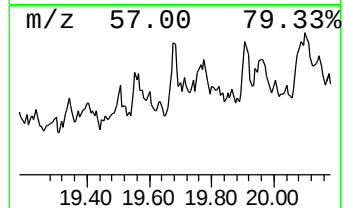
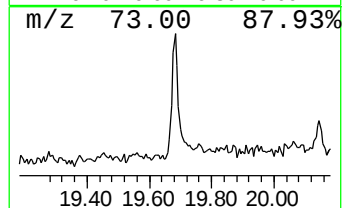
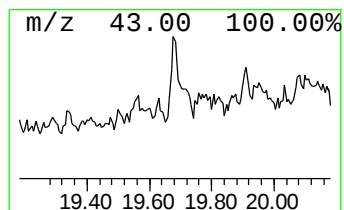
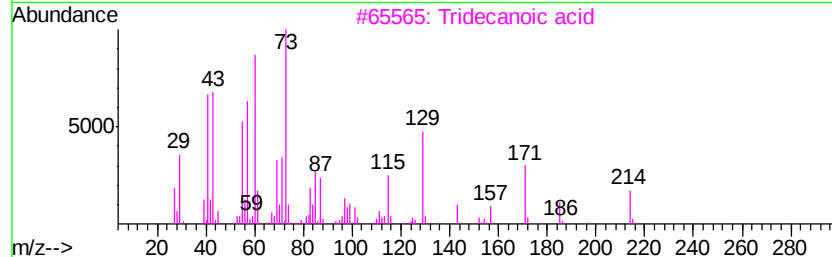
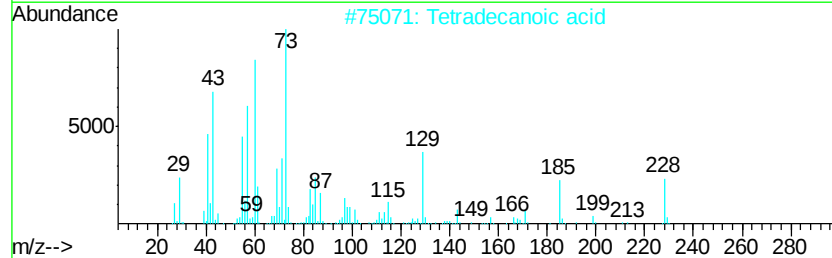
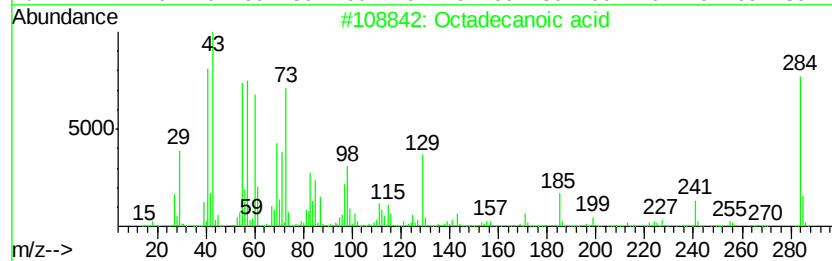
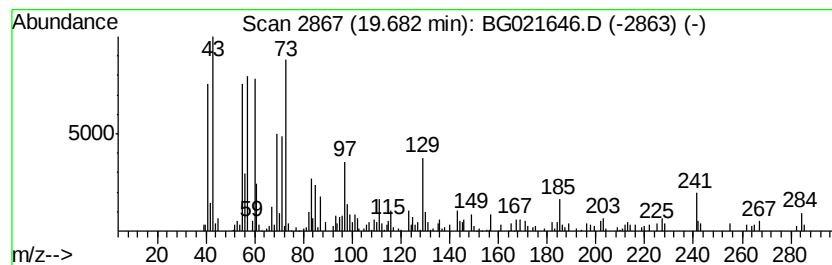
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	4.15 ng	117193	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3		Tridecanoic acid	214	C13H26O2	000638-53-9	62
4		n-Decanoic acid	172	C10H20O2	000334-48-5	53
5		Tridecane	184	C13H28	000629-50-5	25



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
Data File : BG021646.D
Acq On : 14 Apr 2016 9:32
Operator : UM/SJ
Sample : H2418-01
Misc :
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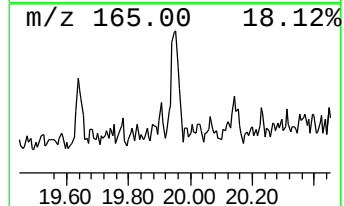
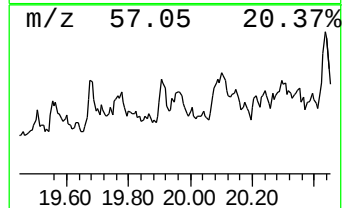
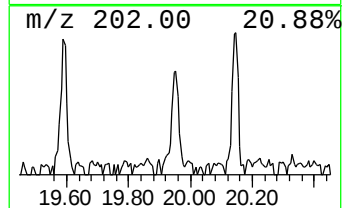
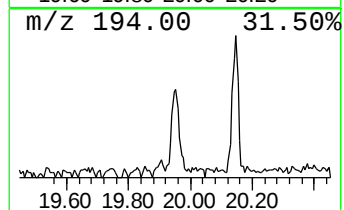
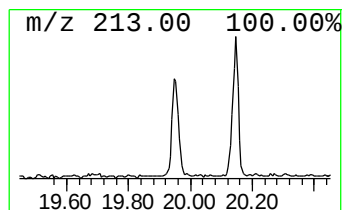
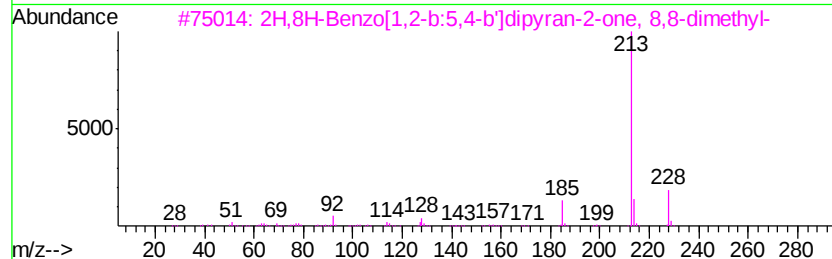
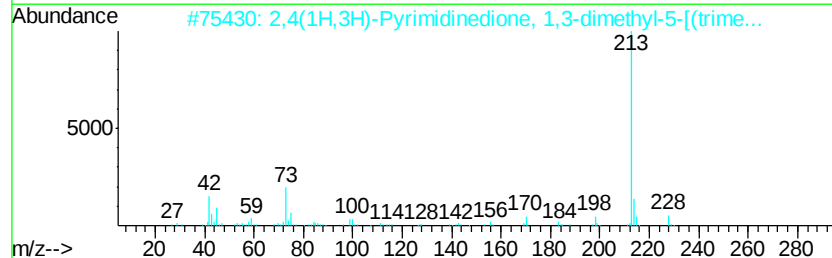
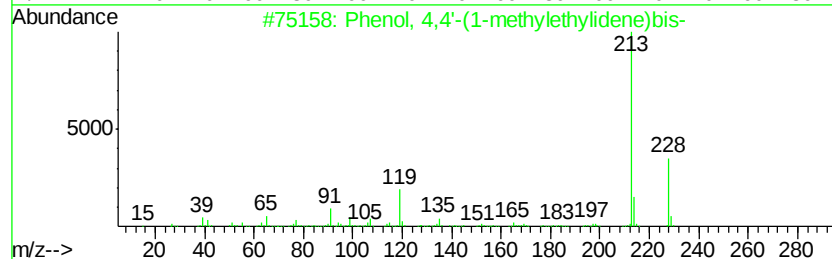
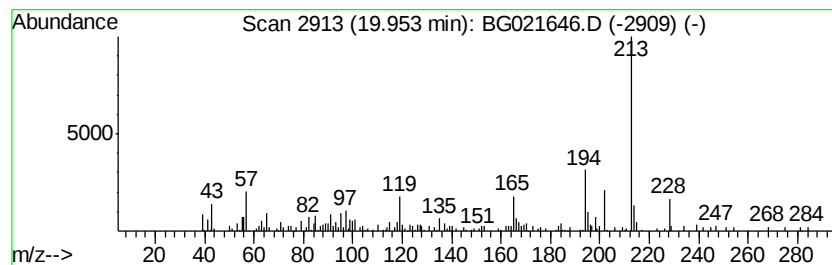
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Phenol, 4,4'-(1-methylethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.95	2.25 ng	80048	Chrysene-d12	21.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	60	
2	2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	47	
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	46	
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	43	
5	Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	43	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
Data File : BG021646.D
Acq On : 14 Apr 2016 9:32
Operator : UM/SJ
Sample : H2418-01
Misc :
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Instrument :
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ClientSampleId :
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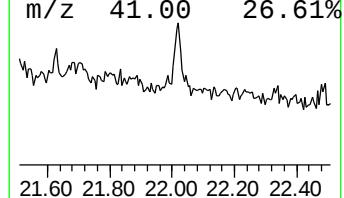
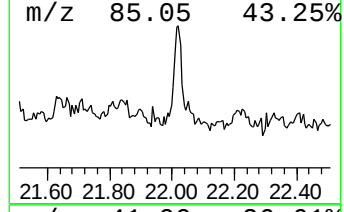
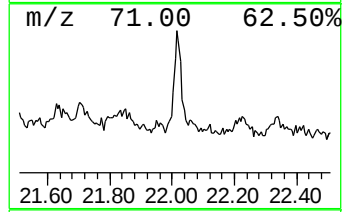
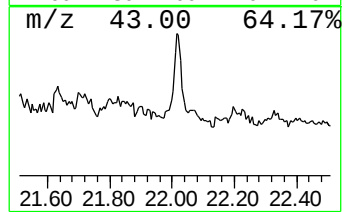
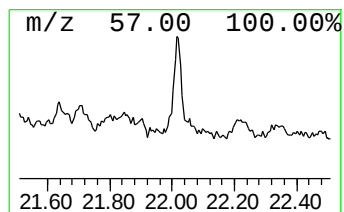
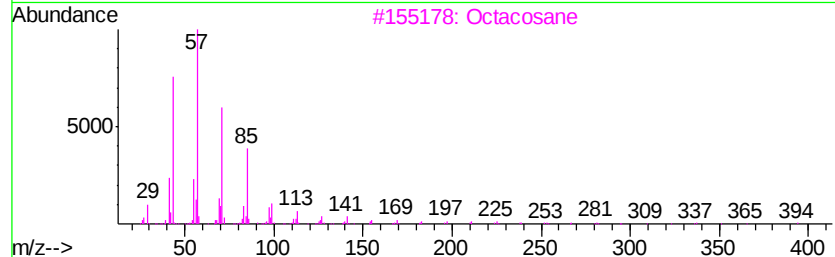
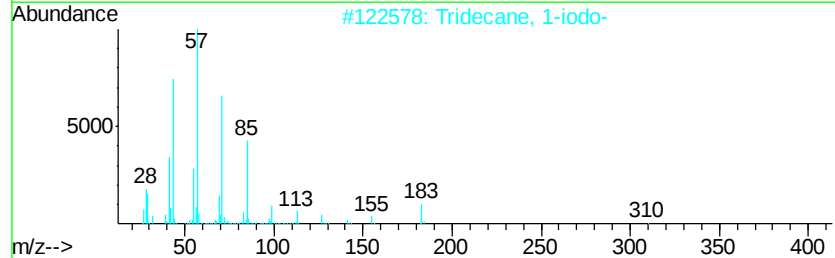
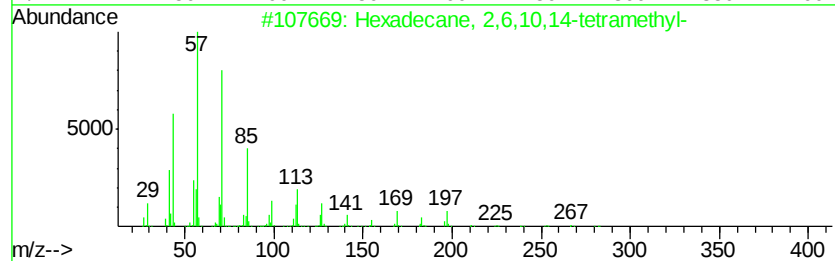
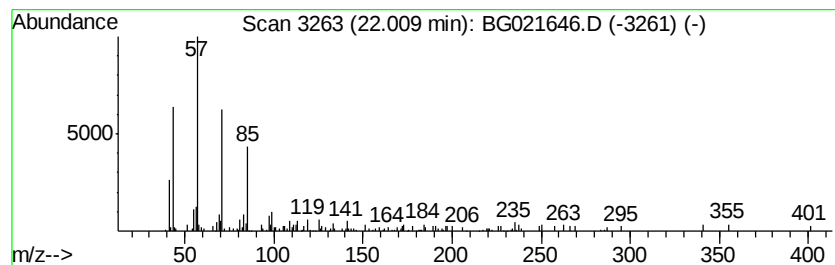
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Hexadecane, 2,6,10,14-tetra... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.01	2.17 ng	77309	Chrysene-d12	21.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
3			Octacosane	394	C28H58	000630-02-4	80
4			Nonadecane	268	C19H40	000629-92-5	80
5			Pentadecane	212	C15H32	000629-62-9	80



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
Data File : BG021646.D
Acq On : 14 Apr 2016 9:32
Operator : UM/SJ
Sample : H2418-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
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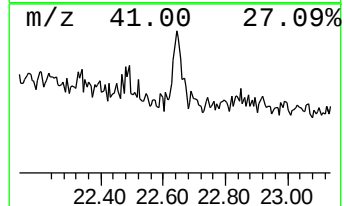
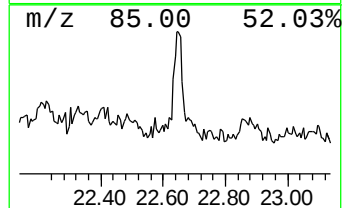
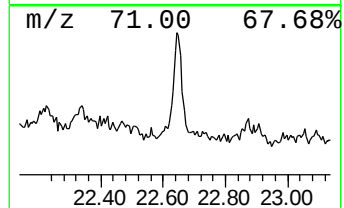
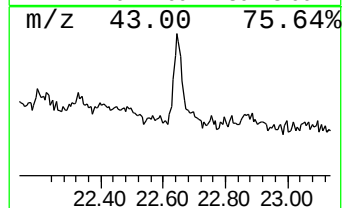
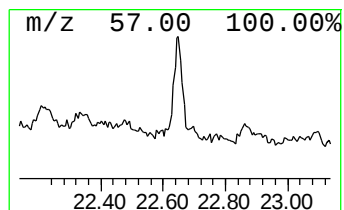
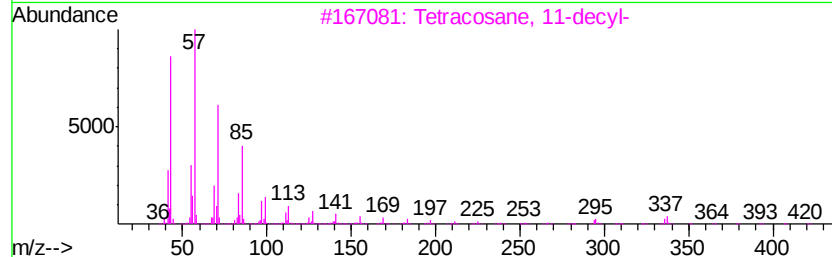
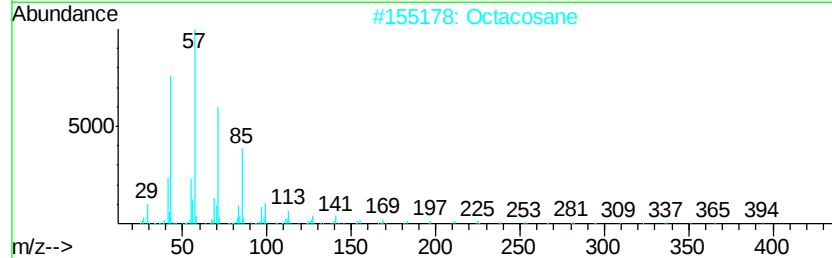
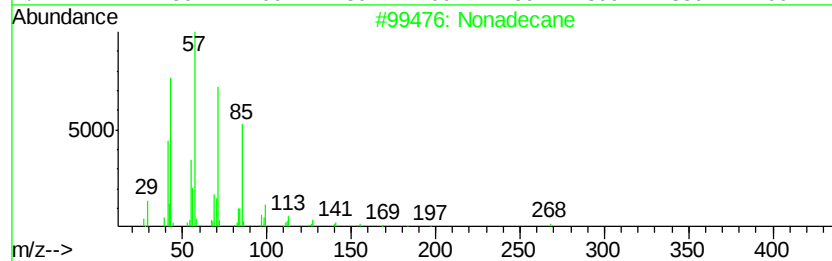
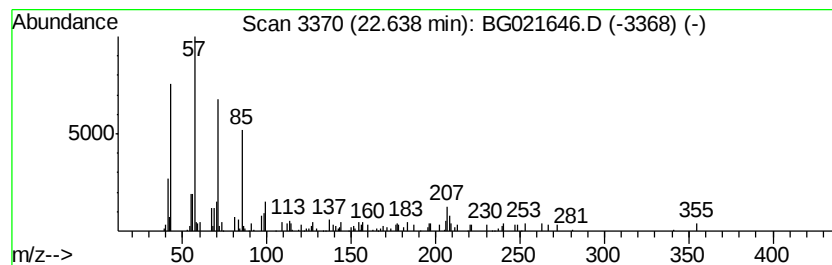
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.64	2.30 ng	81808	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	87
2		Octacosane	394	C28H58	000630-02-4	86
3		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	78
4		2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	72
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
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Acq On : 14 Apr 2016 9:32
Operator : UM/SJ
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Misc :
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.30	5.5	ng	56201	1	8.22	203819	20.0
unknown7.74	7.74	109.7	ng	1118020	1	8.22	203819	20.0
unknown9.46	9.46	3.5	ng	35820	1	8.22	203819	20.0
Bicyclo[2.2.1]hep...	10.45	4.6	ng	75678	2	11.03	327840	20.0
unknown11.79	11.79	2.7	ng	44033	2	11.03	327840	20.0
n-Decanoic acid	18.43	2.4	ng	68608	4	17.56	565221	20.0
Octadecanoic acid	19.68	4.2	ng	117193	4	17.56	565221	20.0
Phenol, 4,4'-(1-m...	19.95	2.3	ng	80048	5	21.83	712519	20.0
Hexadecane, 2,6,1...	22.01	2.2	ng	77309	5	21.83	712519	20.0
Nonadecane	22.64	2.3	ng	81808	5	21.83	712519	20.0