

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
 Data File : BF088142.D
 Acq On : 18 Jun 2016 19:06
 Operator : UM/SJ
 Sample : H3580-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P8-B3(0-5)C

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_F\METHODS\8270-BF060716.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	1.667	6	7	15	rVB	80348	125272	6.35%	0.637%
2	1.781	15	17	23	rVV	664340	938421	47.55%	4.772%
3	1.873	23	25	38	rVB	59830	158222	8.02%	0.805%
4	4.844	283	285	295	rBV	79413	112509	5.70%	0.572%
5	5.290	321	324	326	rBV	1671863	1892730	95.90%	9.625%
6	6.342	413	416	419	rBV2	1405147	1904866	96.52%	9.687%
7	6.456	424	426	429	rBV	1731183	1714187	86.86%	8.717%
8	6.684	444	446	449	rBV	625286	515006	26.09%	2.619%
9	6.845	457	460	462	rBV	1736201	1647231	83.46%	8.377%
10	7.256	493	496	498	rBV	1082154	1027980	52.09%	5.228%
11	7.382	501	507	513	rVV2	32657	62434	3.16%	0.318%
12	7.896	550	552	554	rBV	21654	29452	1.49%	0.150%
13	7.976	556	559	561	rBV	546643	620888	31.46%	3.157%
14	9.050	650	653	655	rBV	2174873	1973599	100.00%	10.037%
15	9.450	686	688	690	rBV	750986	630432	31.94%	3.206%
16	9.553	695	697	700	rBV2	13199	25249	1.28%	0.128%
17	9.668	705	707	709	rBV	54309	47997	2.43%	0.244%
18	9.725	709	712	714	rBV	583520	600980	30.45%	3.056%
19	9.896	723	727	728	rBV	13963	22369	1.13%	0.114%
20	10.136	745	748	749	rBV	17670	21220	1.08%	0.108%
21	10.159	749	750	752	rVB	92010	78159	3.96%	0.397%
22	10.376	766	769	772	rBV	33976	58236	2.95%	0.296%
23	10.513	778	781	783	rBV	774534	900454	45.62%	4.579%
24	10.548	783	784	788	rVV2	17140	28341	1.44%	0.144%
25	10.628	790	791	796	rVV	80446	136436	6.91%	0.694%
26	10.719	798	799	806	rVB4	10165	24903	1.26%	0.127%
27	10.822	806	808	813	rBV3	20849	43223	2.19%	0.220%
28	11.016	822	825	827	rVB	20347	22477	1.14%	0.114%
29	11.085	829	831	832	rBV	36844	57208	2.90%	0.291%
30	11.199	839	841	842	rBV	629738	521881	26.44%	2.654%
31	11.268	845	847	850	rVB2	15351	28297	1.43%	0.144%
32	11.451	859	863	865	rBV2	33749	59620	3.02%	0.303%
33	11.508	865	868	869	rVV	31633	32107	1.63%	0.163%
34	11.542	869	871	872	rVV	22669	23432	1.19%	0.119%

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Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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35	11.576	872	874	875	rVB2	16839	21789	1.10%	0.111%
36	11.668	879	882	883	rBV	13340	21195	1.07%	0.108%
37	11.702	883	885	886	rBV	19099	21503	1.09%	0.109%
38	11.736	886	888	892	rVB3	26560	47988	2.43%	0.244%
39	12.125	921	922	925	rBV3	20946	36786	1.86%	0.187%
40	12.194	925	928	931	rBV4	23225	52952	2.68%	0.269%
41	12.251	931	933	934	rBV	38150	41863	2.12%	0.213%
42	12.331	939	940	942	rBV	15750	26124	1.32%	0.133%
43	12.411	945	947	948	rBV	75537	74958	3.80%	0.381%
44	12.639	964	967	968	rBV2	57011	75925	3.85%	0.386%
45	12.674	968	970	971	rVV2	22926	34904	1.77%	0.178%
46	12.788	977	980	982	rBV	1540431	1667508	84.49%	8.480%
47	13.017	998	1000	1002	rBV	36666	56816	2.88%	0.289%
48	13.702	1057	1060	1062	rVB3	84102	154213	7.81%	0.784%
49	13.828	1069	1071	1074	rBV	437889	524055	26.55%	2.665%
50	15.222	1191	1193	1197	rVB	249755	374759	18.99%	1.906%
51	15.817	1243	1245	1252	rVB2	153201	344885	17.47%	1.754%

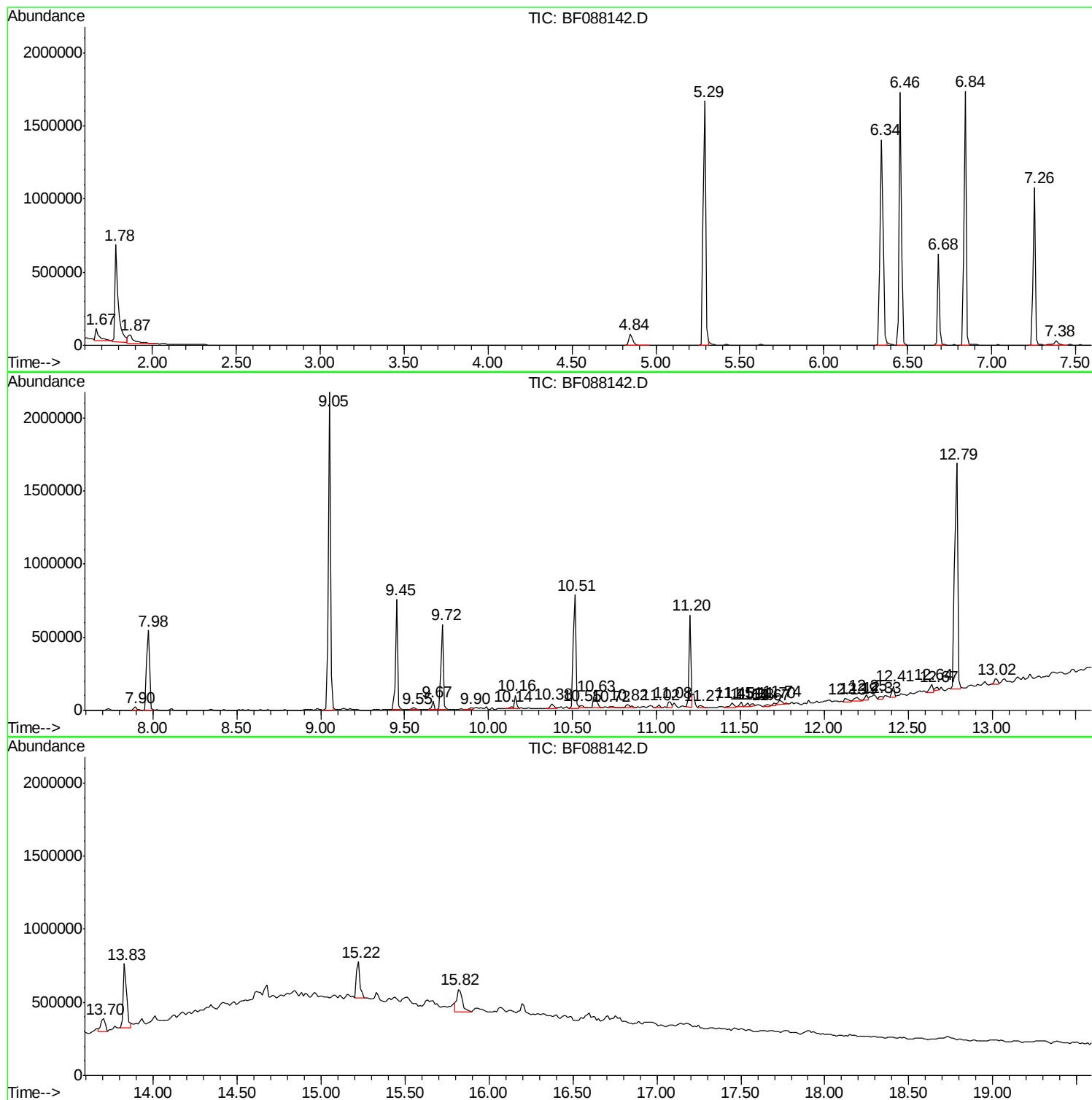
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : H3580-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
P8-B3(0-5)C

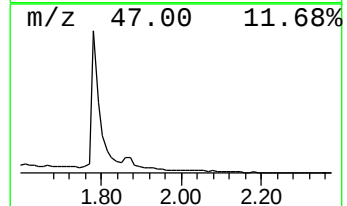
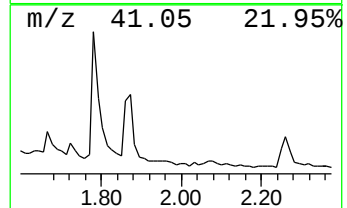
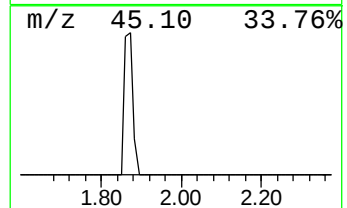
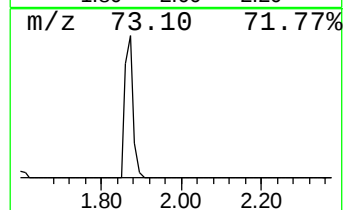
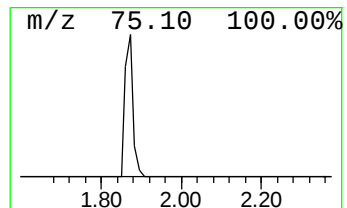
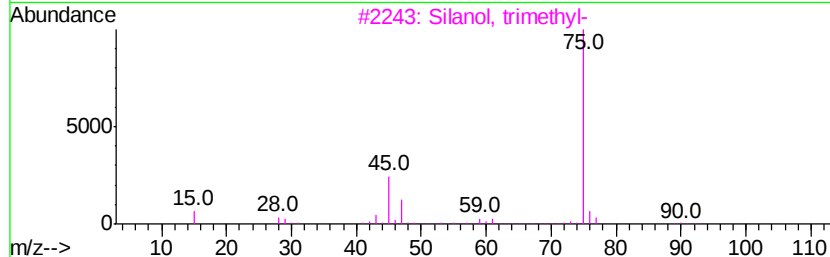
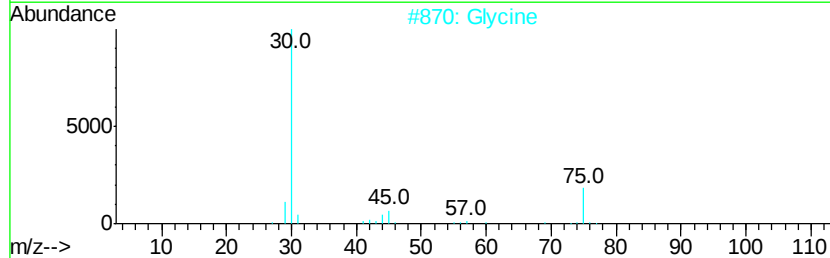
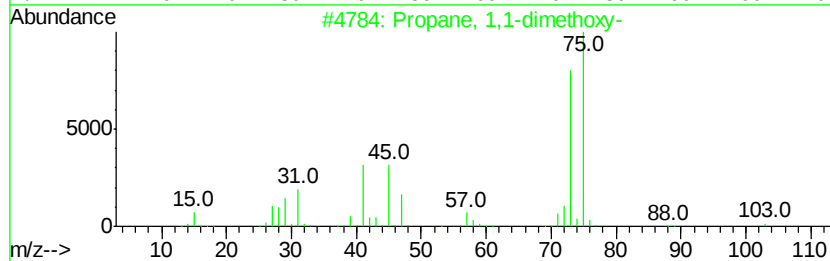
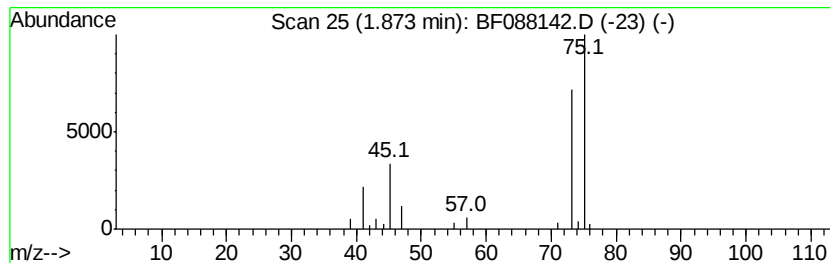
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	6.14 ng	158222	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Glycine	75	C2H5NO2	000056-40-6	9
3		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9



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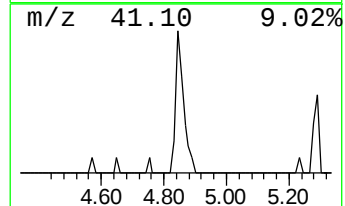
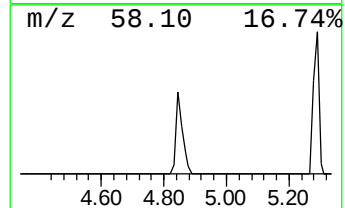
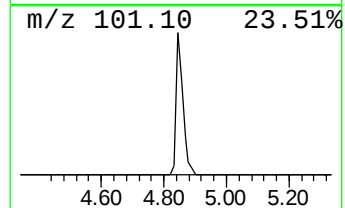
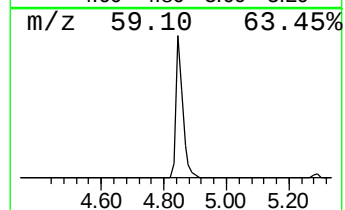
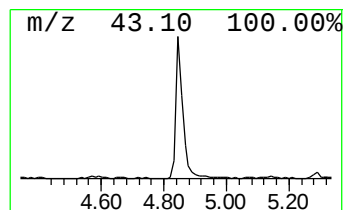
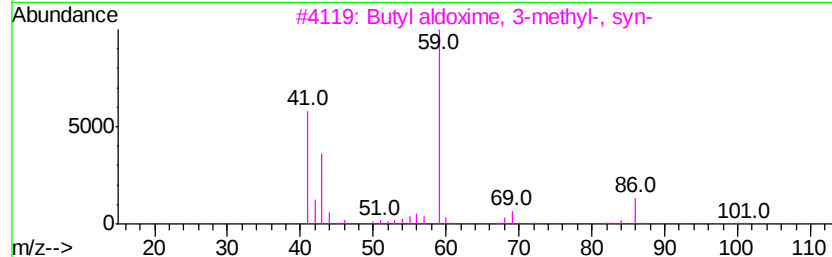
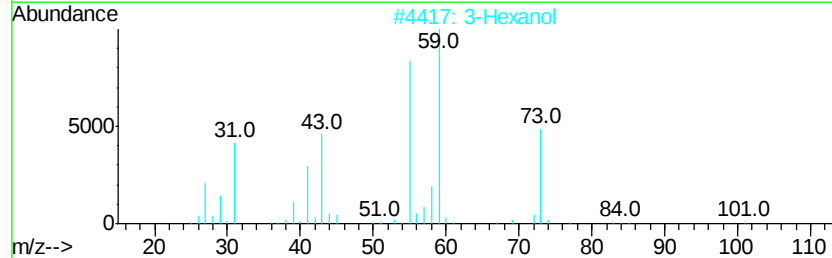
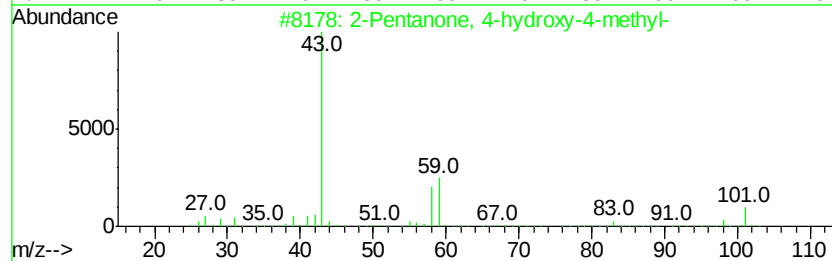
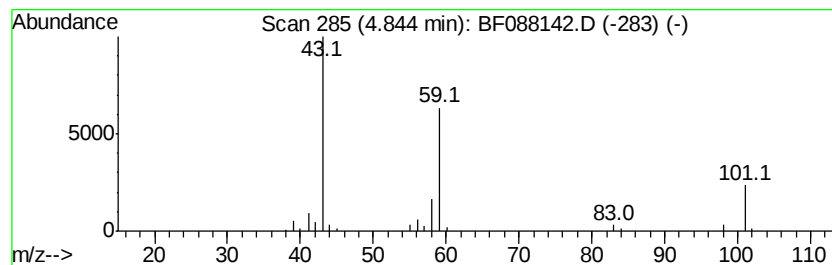
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.37 ng	112509	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol	102	C6H14O	000623-37-0	28
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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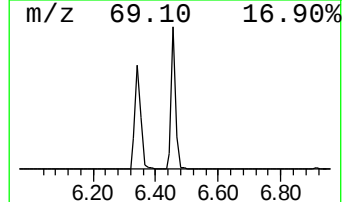
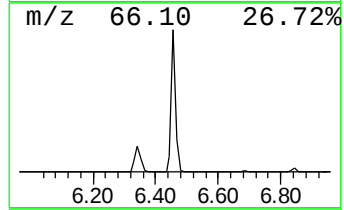
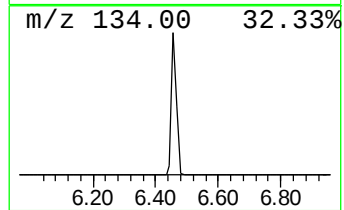
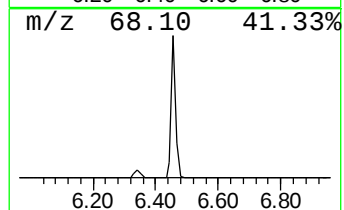
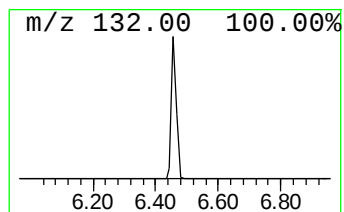
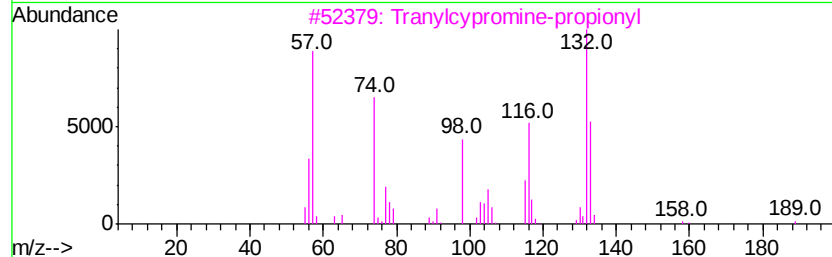
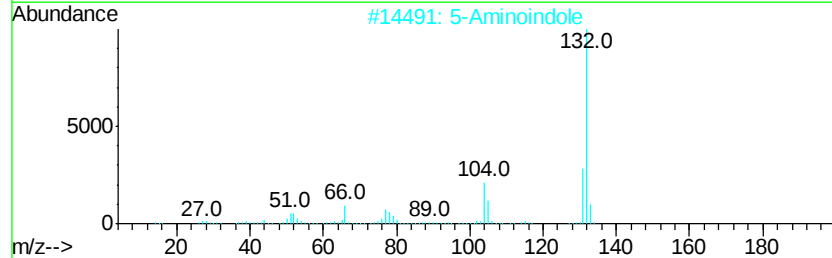
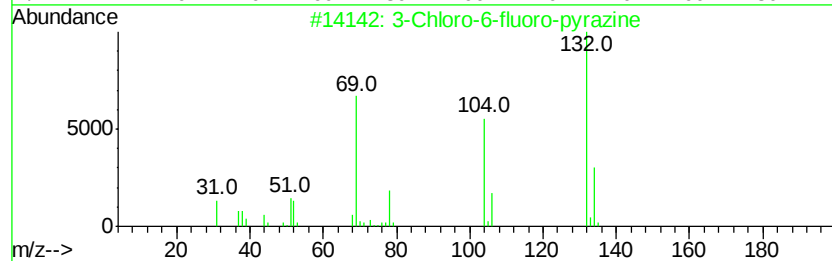
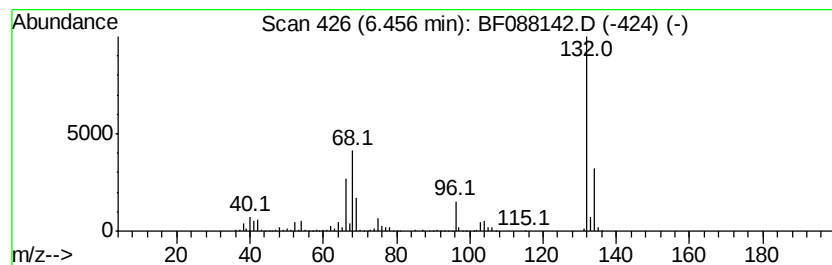
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	66.57 ng	1714190	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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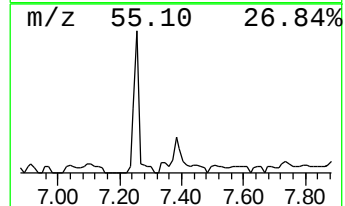
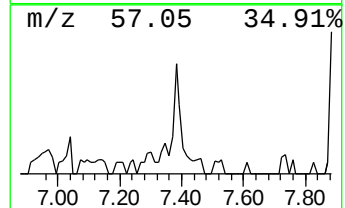
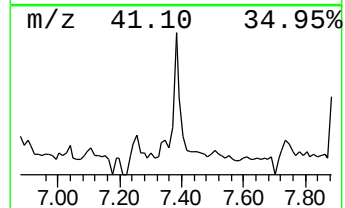
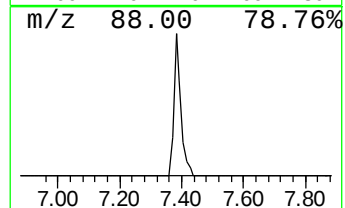
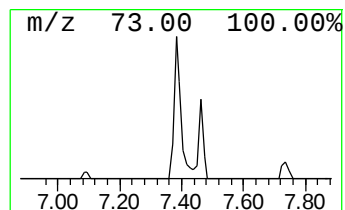
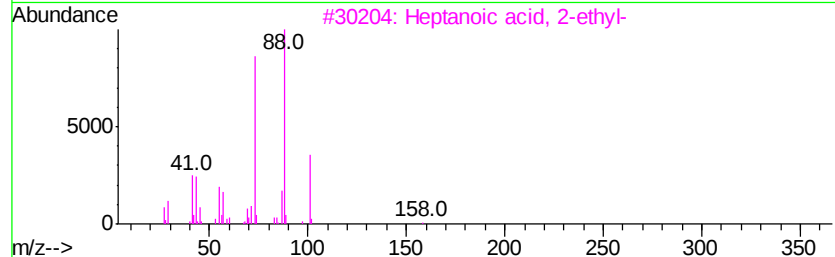
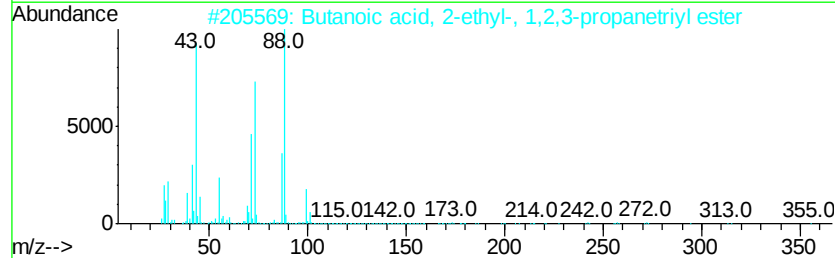
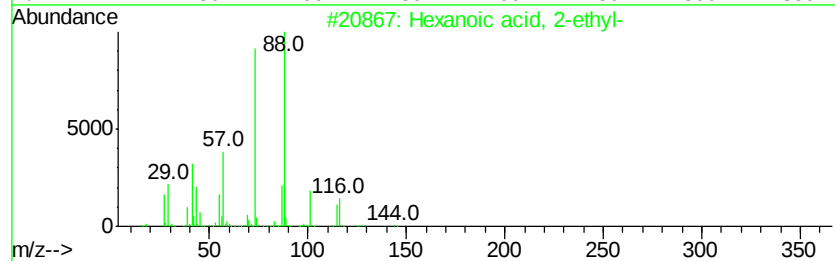
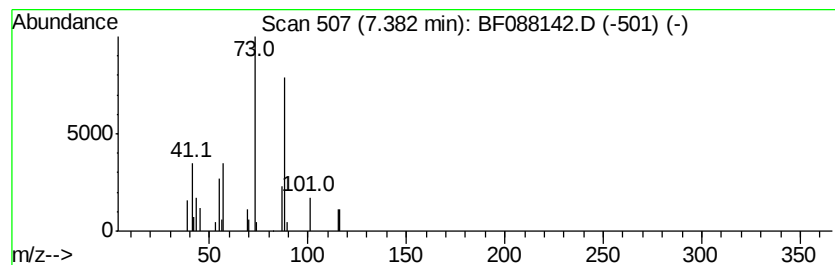
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	2.01 ng	62434	Naphthalene-d8	7.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
4		Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	40
5		Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	40



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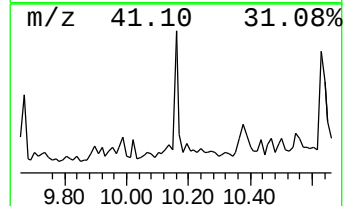
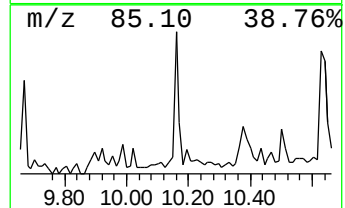
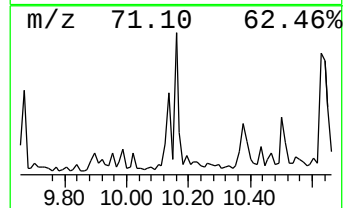
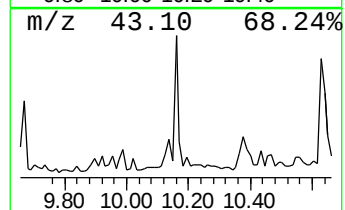
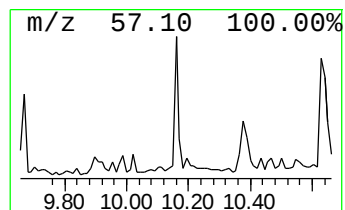
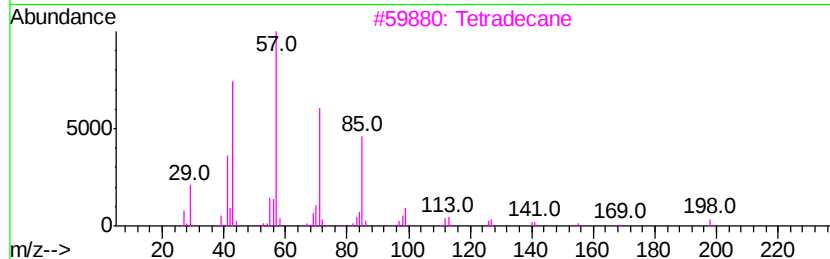
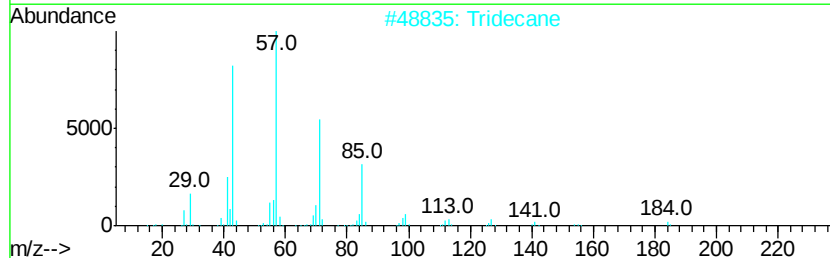
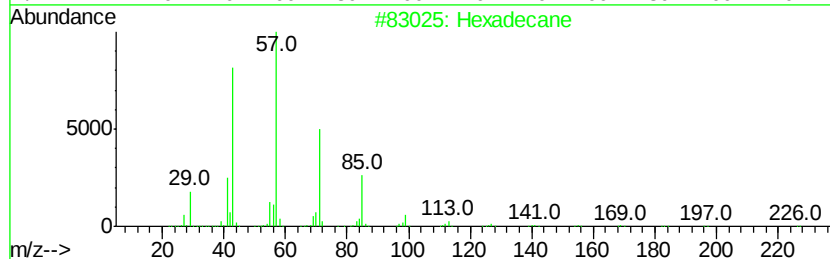
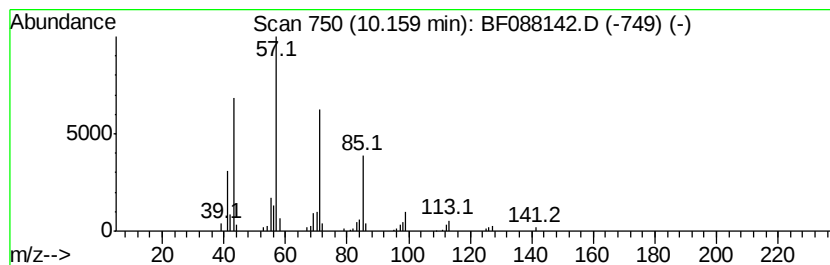
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.60 ng	78159	Acenaphthene-d10	9.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Tridecane		184	C13H28	000629-50-5	86
3	Tetradecane		198	C14H30	000629-59-4	86
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	83
5	Heptadecane		240	C17H36	000629-78-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088142.D
Acq On : 18 Jun 2016 19:06
Operator : UM/SJ
Sample : H3580-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

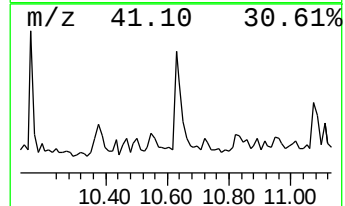
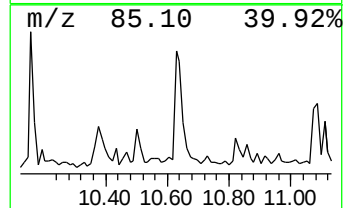
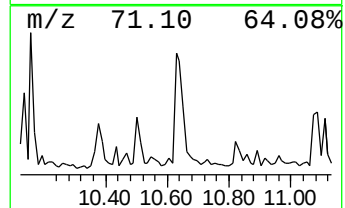
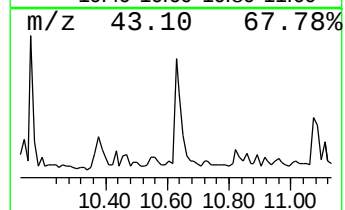
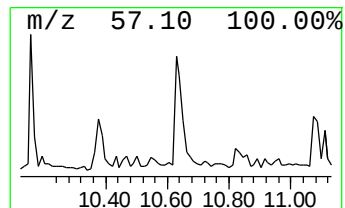
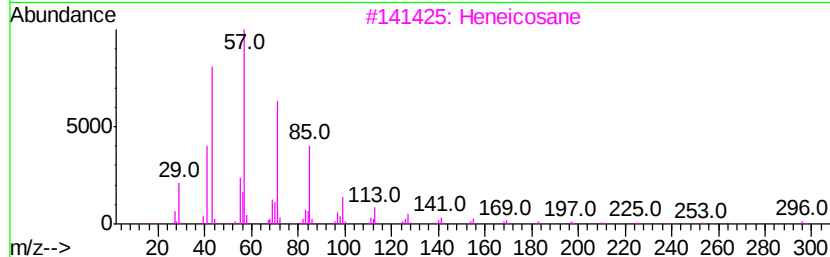
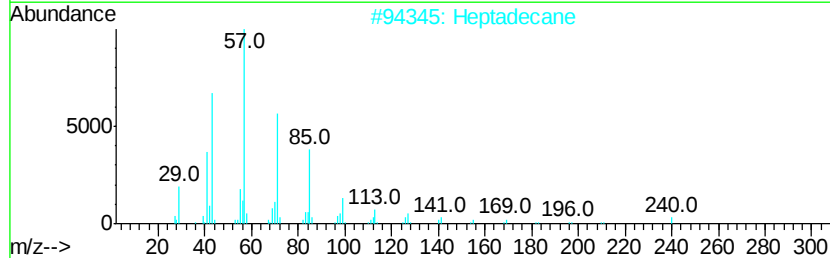
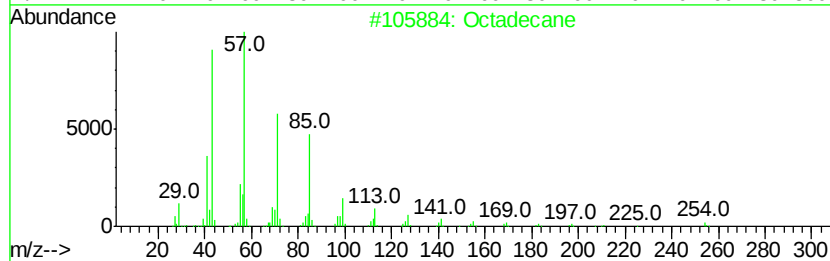
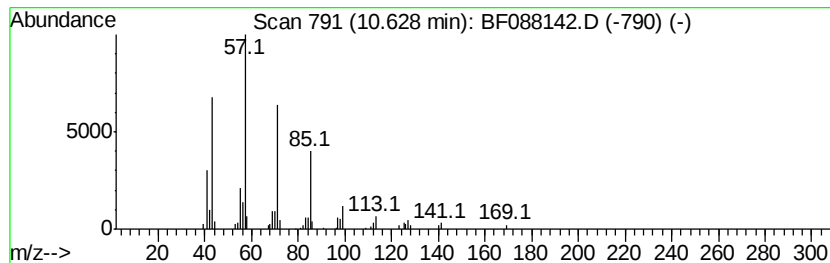
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P8-B3(0-5)C

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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 9 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.63	5.23 ng	136436	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Hexadecane	226	C16H34	000544-76-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
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Operator : UM/SJ
Sample : H3580-01
Misc :
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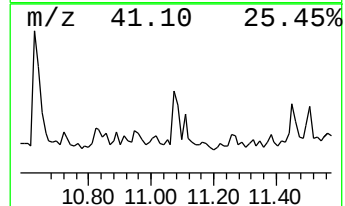
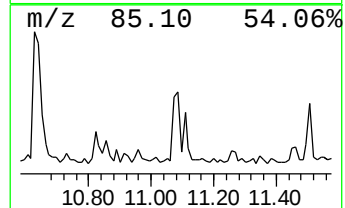
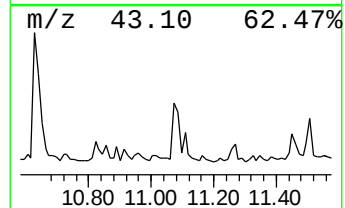
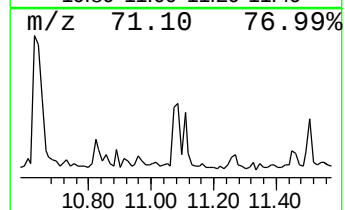
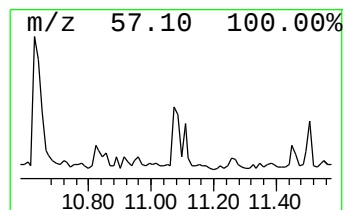
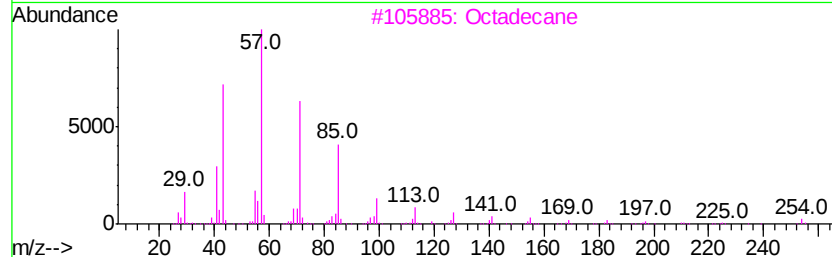
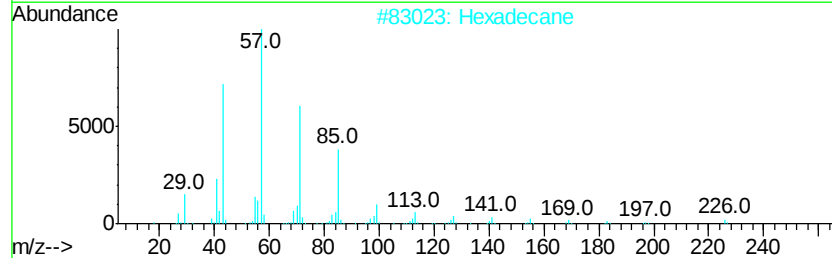
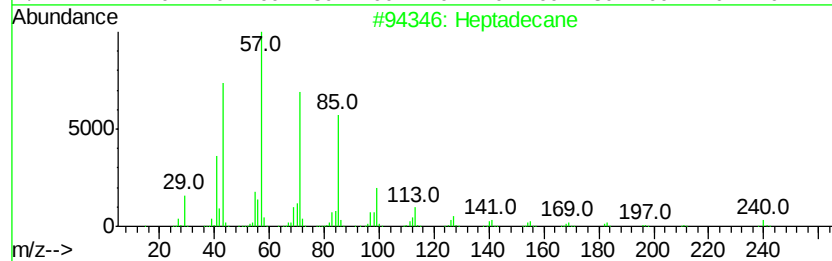
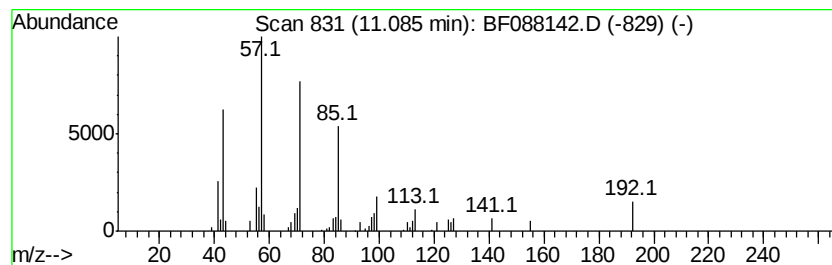
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	2.19 ng	57208	Phenanthrene-d10	11.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	90
2	Hexadecane	226 C16H34	000544-76-3	86
3	Octadecane	254 C18H38	000593-45-3	86
4	Heneicosane	296 C21H44	000629-94-7	83
5	Hexacosane	366 C26H54	000630-01-3	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
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Sample : H3580-01
Misc :
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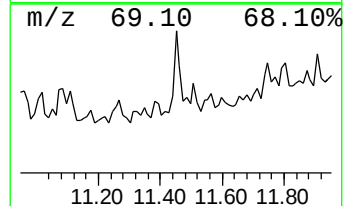
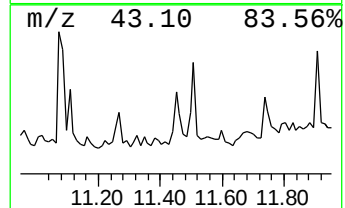
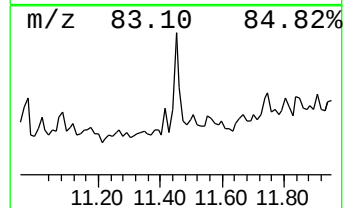
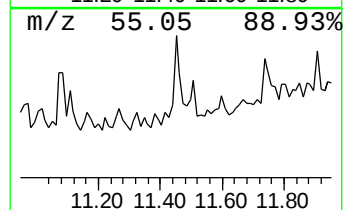
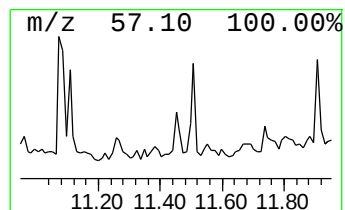
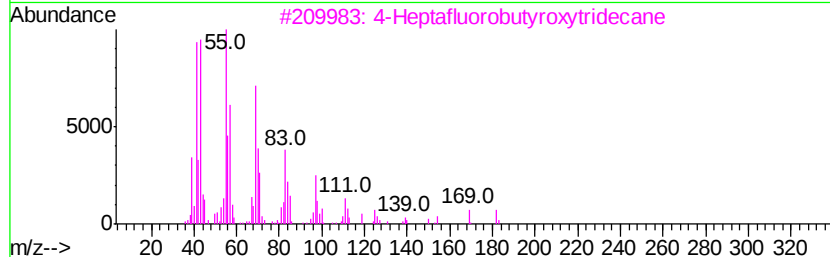
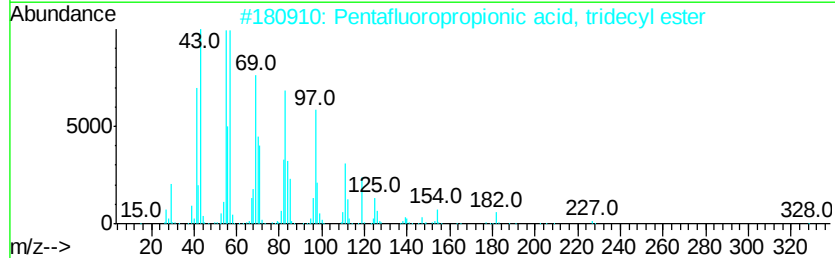
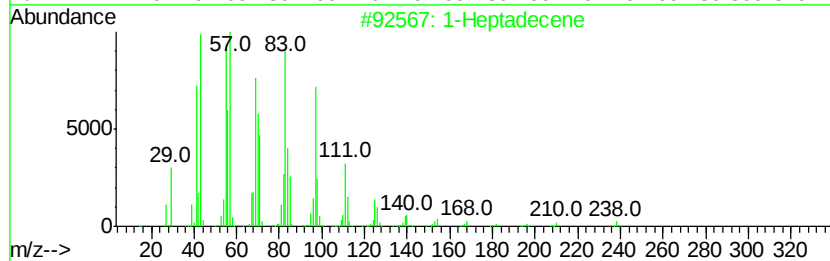
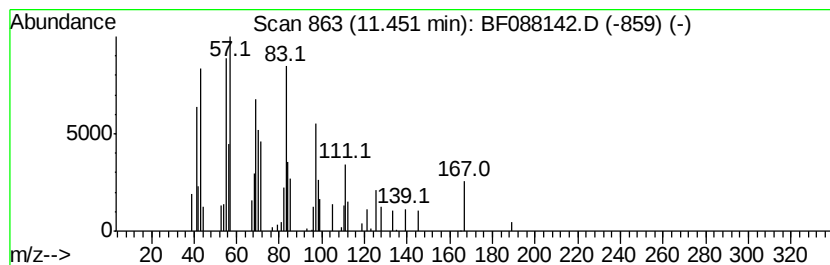
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heptadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	2.28 ng	59620	Phenanthrene-d10	11.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptadecene	238 C17H34	006765-39-5	90
2	Pentafluoropropionic acid, tridecyl ester	346 C16H27F5O2	959261-22-4	90
3	4-Heptafluorobutyltridecane	396 C17H27F7O2	1000245-49-6	90
4	Trichloroacetic acid, tetradecyl ester	358 C16H29Cl3O2	074339-52-9	87
5	1-Octadecene	252 C18H36	000112-88-9	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088142.D
Acq On : 18 Jun 2016 19:06
Operator : UM/SJ
Sample : H3580-01
Misc :
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Instrument :
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ClientSampleId :
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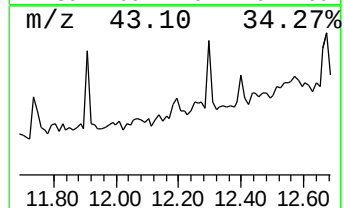
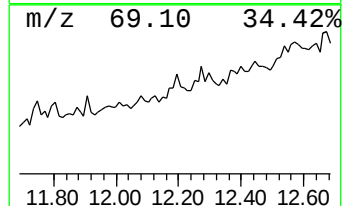
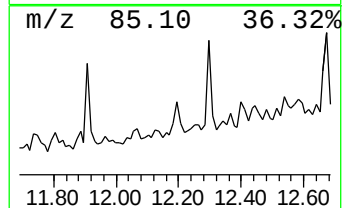
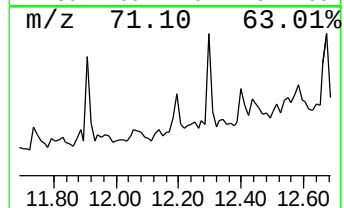
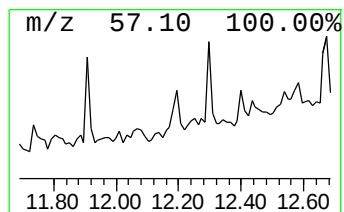
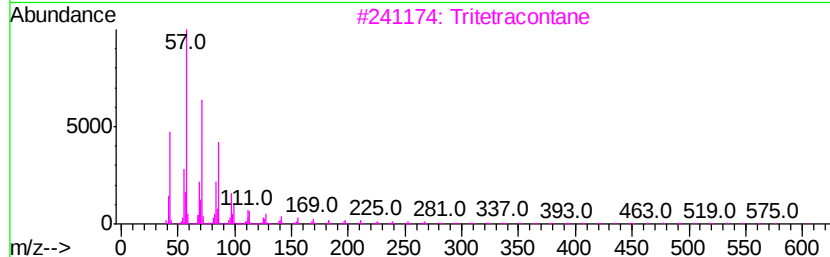
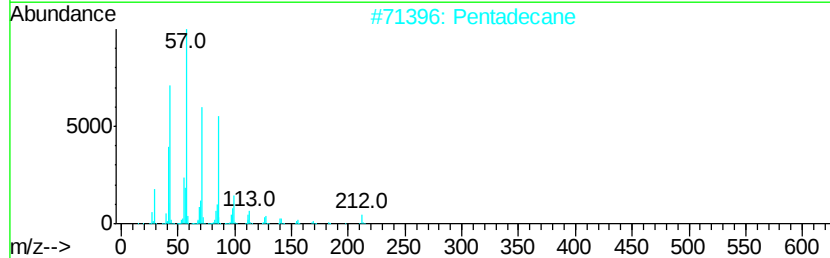
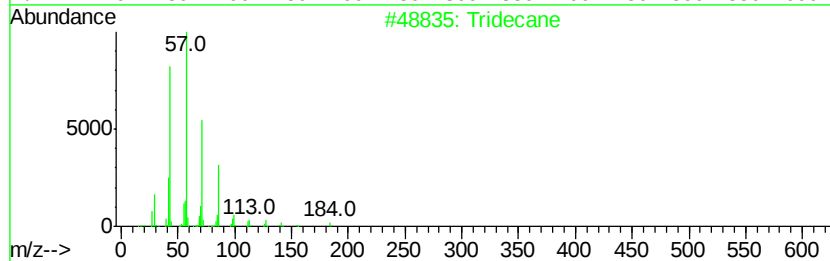
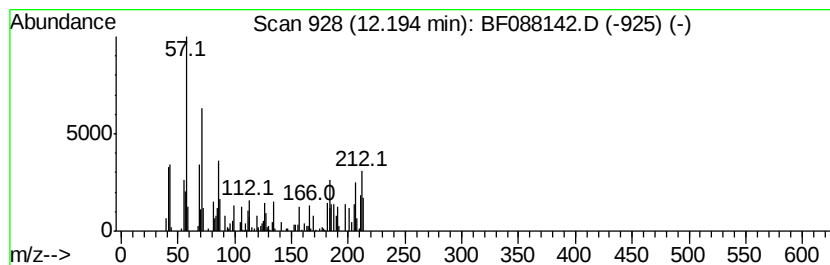
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown12.19 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	2.03 ng	52952	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	42
2		Pentadecane	212	C15H32	000629-62-9	38
3		Tritetracontane	605	C43H88	007098-21-7	25
4		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	25
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088142.D
Acq On : 18 Jun 2016 19:06
Operator : UM/SJ
Sample : H3580-01
Misc :
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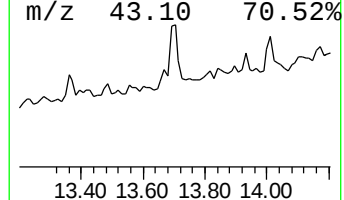
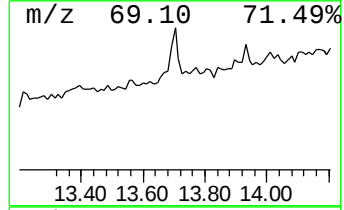
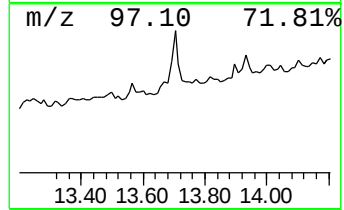
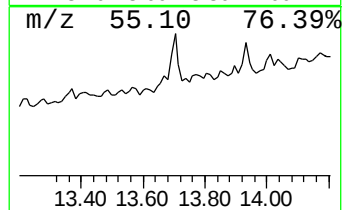
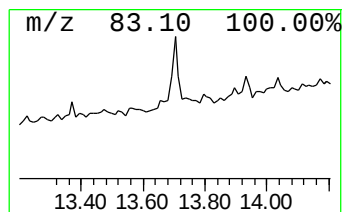
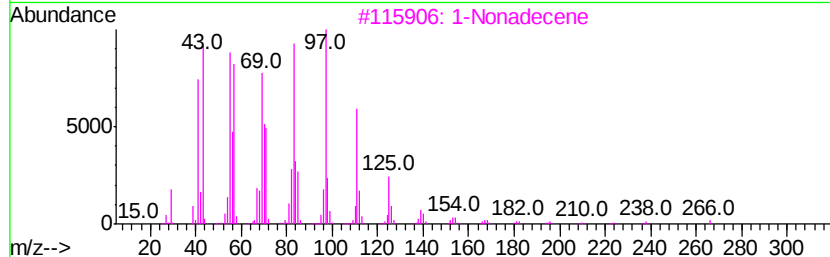
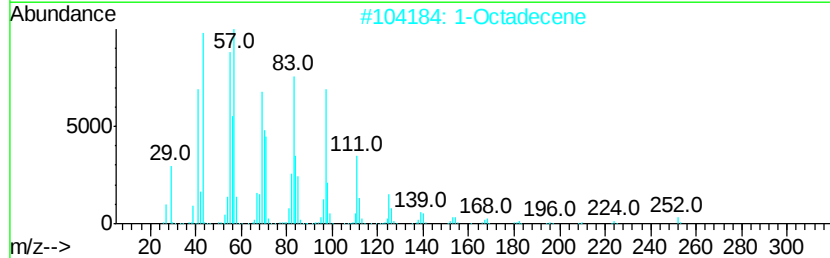
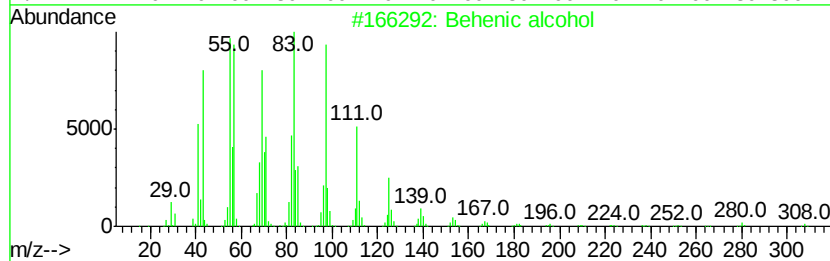
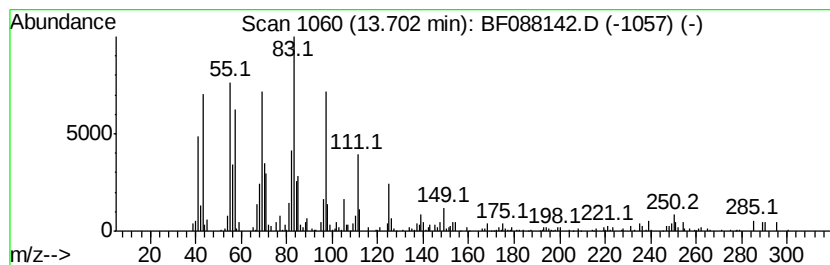
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.70	5.89 ng	154213	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Octadecene	252	C18H36	000112-88-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088142.D
Acq On : 18 Jun 2016 19:06
Operator : UM/SJ
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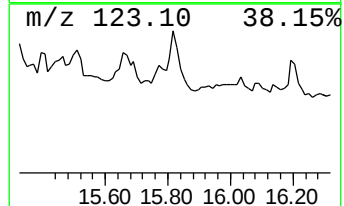
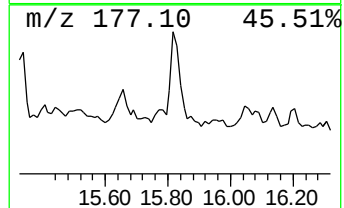
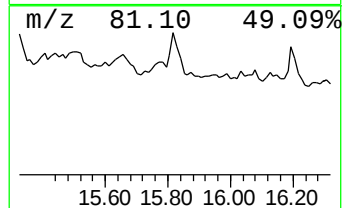
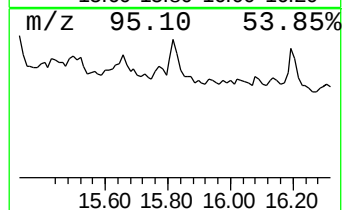
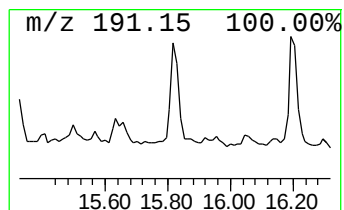
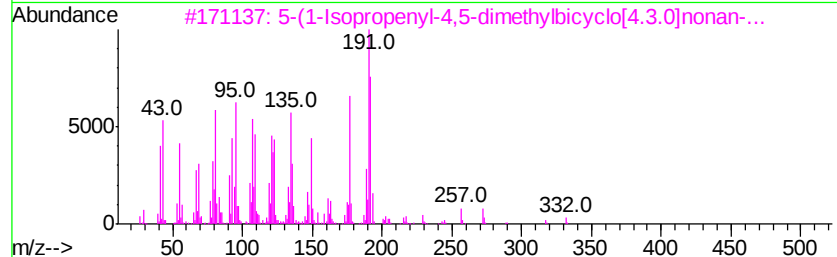
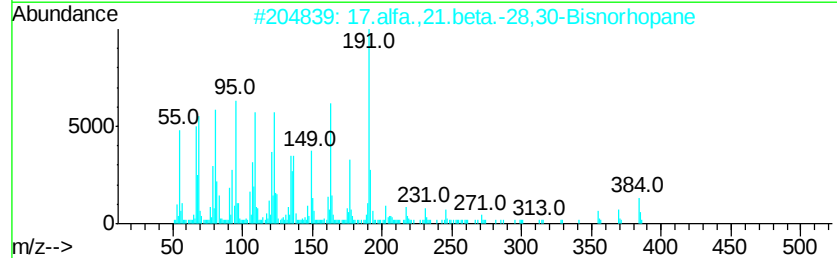
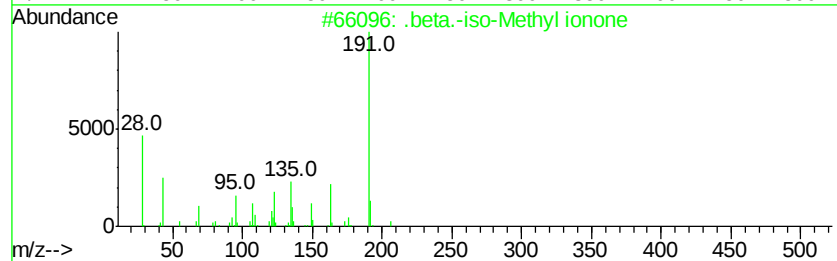
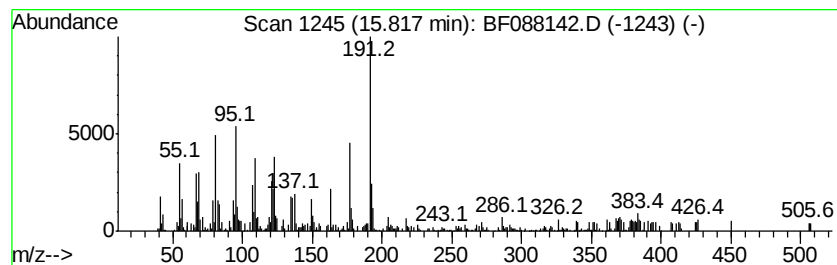
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 .beta.-iso-Methyl ionone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	18.41 ng	344885	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	60
2		17.alfa.,21.beta.-28,30-Bisnorho...	384	C28H48	1000360-26-1	46
3		5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8	41
4		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	35
5		3-Fluoro-4-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-94-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
 Data File : BF088142.D
 Acq On : 18 Jun 2016 19:06
 Operator : UM/SJ
 Sample : H3580-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 P8-B3(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
Propane, 1,1-dime...	1.87	6.1 ng		158222	1	6.68	515006	20.0
2-Pentanone, 4-hy...	4.84	4.4 ng		112509	1	6.68	515006	20.0
unknown6.46	6.46	66.6 ng		1714190	1	6.68	515006	20.0
Hexanoic acid, 2-...	7.38	2.0 ng		62434	2	7.98	620888	20.0
Hexadecane	10.16	2.6 ng		78159	3	9.72	600980	20.0
Octadecane	10.63	5.2 ng		136436	4	11.20	521881	20.0
Heptadecane	11.08	2.2 ng		57208	4	11.20	521881	20.0
1-Heptadecene	11.45	2.3 ng		59620	4	11.20	521881	20.0
unknown12.19	12.19	2.0 ng		52952	4	11.20	521881	20.0
Behenic alcohol	13.70	5.9 ng		154213	5	13.83	524055	20.0
.beta.-iso-Methyl...	15.82	18.4 ng		344885	6	15.22	374759	20.0