

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010317\
 Data File : BF092069.D
 Acq On : 3 Jan 2017 19:14
 Operator : UM/SJ
 Sample : H6322-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP9-COMP9

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-BF122116.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	3.430	130	135	140	rBV	59188	128834	2.53%	0.280%
2	4.184	198	201	205	rVB2	31550	63394	1.25%	0.138%
3	4.813	253	256	270	rVB	1153849	1780433	35.02%	3.874%
4	5.281	294	297	299	rBV	3530003	4461313	87.74%	9.708%
5	6.333	386	389	392	rBV	4587705	5000856	98.35%	10.882%
6	6.447	396	399	401	rBV	4188643	5084578	100.00%	11.064%
7	6.664	416	418	421	rBV	1305644	1200722	23.61%	2.613%
8	6.790	427	429	430	rBV	95407	80985	1.59%	0.176%
9	6.824	430	432	434	rVB	3999003	3549656	69.81%	7.724%
10	7.110	455	457	462	rVB	53742	61778	1.22%	0.134%
11	7.236	465	468	470	rBV	2933244	2867342	56.39%	6.239%
12	7.956	528	531	533	rBV	1409211	1397963	27.49%	3.042%
13	9.030	623	625	628	rVB	3270698	3902608	76.75%	8.492%
14	9.430	658	660	663	rBV	328049	338090	6.65%	0.736%
15	9.648	675	679	681	rBV	62587	94902	1.87%	0.207%
16	9.705	681	684	686	rVB	1800510	1589758	31.27%	3.459%
17	9.933	701	704	706	rBV2	36477	55126	1.08%	0.120%
18	9.979	706	708	710	rBV2	49669	66427	1.31%	0.145%
19	10.128	715	721	722	rBV	35458	76973	1.51%	0.167%
20	10.151	722	723	725	rVB	135864	108925	2.14%	0.237%
21	10.368	739	742	745	rBV	61616	87728	1.73%	0.191%
22	10.493	751	753	756	rBV	2630174	2642543	51.97%	5.750%
23	10.619	761	764	769	rBV2	141069	259522	5.10%	0.565%
24	11.065	802	803	805	rBV	81764	118066	2.32%	0.257%
25	11.191	811	814	816	rBV	1092389	1548674	30.46%	3.370%
26	11.431	833	835	838	rVB2	31637	57004	1.12%	0.124%
27	11.499	838	841	843	rBV	76346	82358	1.62%	0.179%
28	11.659	852	855	856	rBV	31104	51261	1.01%	0.112%
29	11.739	859	862	864	rBV	495368	523020	10.29%	1.138%
30	11.899	872	876	878	rBV2	63569	155947	3.07%	0.339%
31	12.036	887	888	892	rBV2	57031	61609	1.21%	0.134%
32	12.391	918	919	921	rBV	223228	217123	4.27%	0.472%
33	12.436	921	923	926	rVB2	62490	78851	1.55%	0.172%
34	12.516	928	930	934	rVV	274764	340388	6.69%	0.741%

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35	12.619	936	939	941	rVB	198424	215946	4.25%	0.470%
36	12.779	950	953	955	rVB	2304377	3012850	59.25%	6.556%
37	12.905	962	964	965	rBV	60565	52351	1.03%	0.114%
38	12.951	966	968	970	rVB	62789	75965	1.49%	0.165%
39	13.019	972	974	975	rVB	66132	58302	1.15%	0.127%
40	13.054	975	977	982	rBV4	46115	75265	1.48%	0.164%
41	13.259	993	995	998	rBV	98698	146045	2.87%	0.318%
42	13.351	1001	1003	1005	rBV3	52067	89905	1.77%	0.196%
43	13.682	1030	1032	1035	rVB2	183745	244414	4.81%	0.532%
44	13.762	1038	1039	1041	rBV	45484	53954	1.06%	0.117%
45	13.819	1041	1044	1046	rBV	1018644	1208996	23.78%	2.631%
46	14.311	1085	1087	1094	rVB3	85386	179561	3.53%	0.391%
47	14.814	1129	1131	1137	rVV	74222	146235	2.88%	0.318%
48	14.905	1137	1139	1145	rVB2	82912	141921	2.79%	0.309%
49	15.134	1157	1159	1162	rVB	65857	94014	1.85%	0.205%
50	15.191	1162	1164	1167	rBV	677234	958175	18.84%	2.085%
51	15.420	1181	1184	1187	rVB3	52319	90389	1.78%	0.197%
52	15.625	1200	1202	1204	rBV	61224	93503	1.84%	0.203%
53	16.185	1248	1251	1253	rBV3	29322	65372	1.29%	0.142%
54	16.311	1259	1262	1268	rVB3	68750	146106	2.87%	0.318%
55	16.483	1275	1277	1281	rVB2	34108	71190	1.40%	0.155%
56	16.871	1308	1311	1315	rBV	28905	68008	1.34%	0.148%
57	16.997	1319	1322	1327	rVB6	23382	63387	1.25%	0.138%
58	18.769	1472	1477	1489	rVB4	140637	469398	9.23%	1.021%

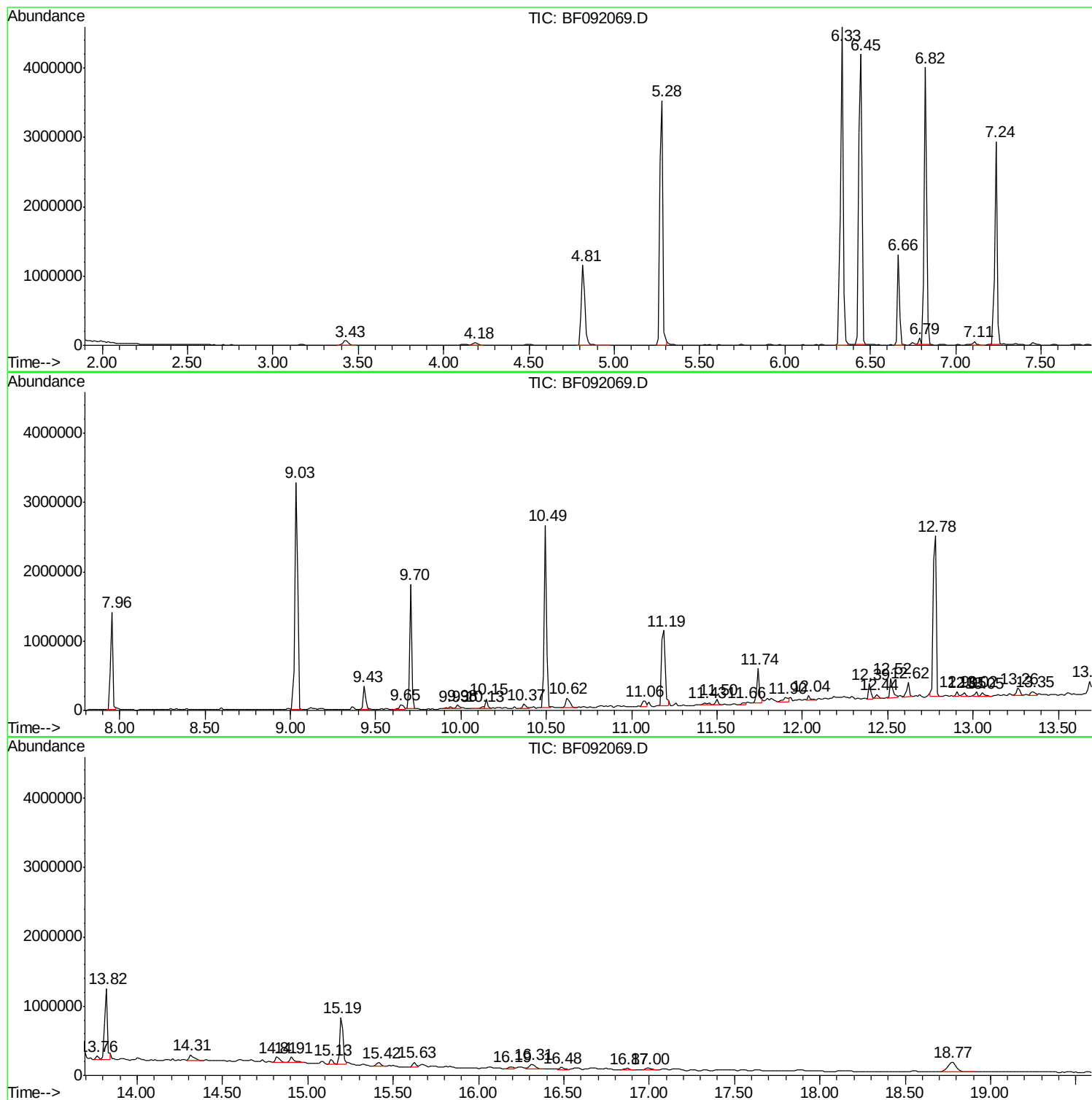
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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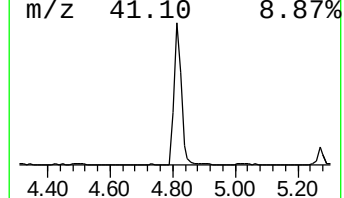
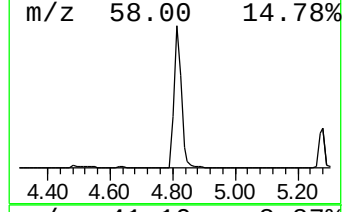
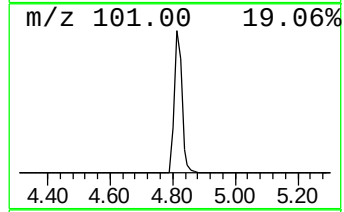
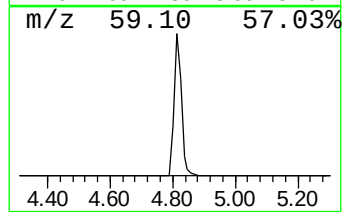
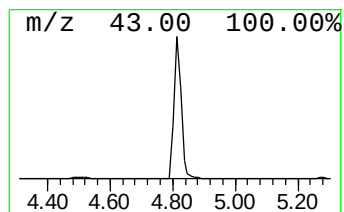
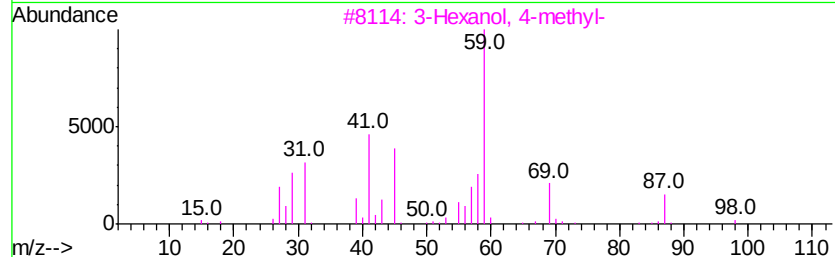
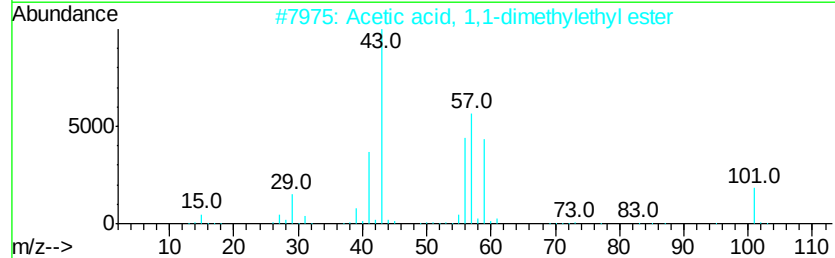
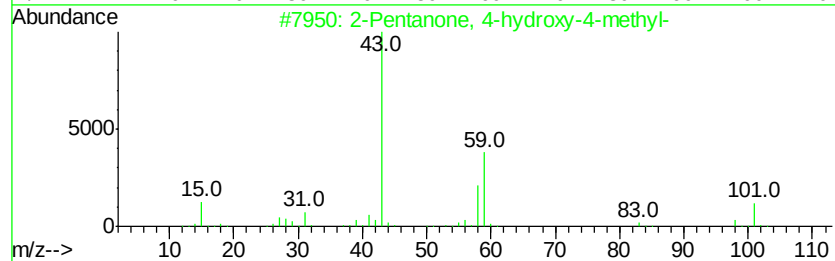
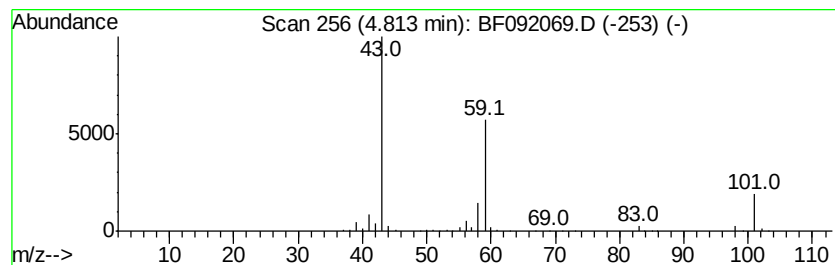
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	29.66 ng	1780430	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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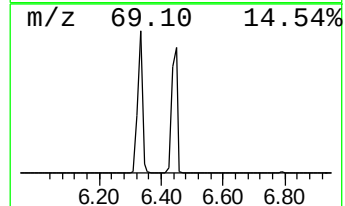
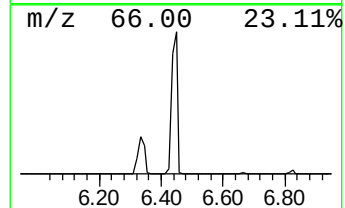
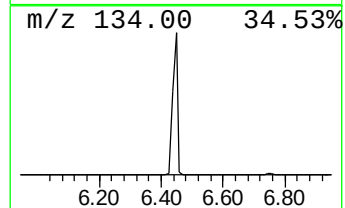
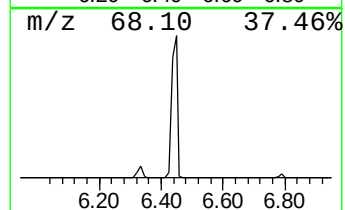
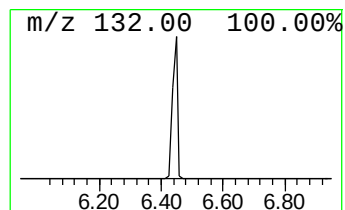
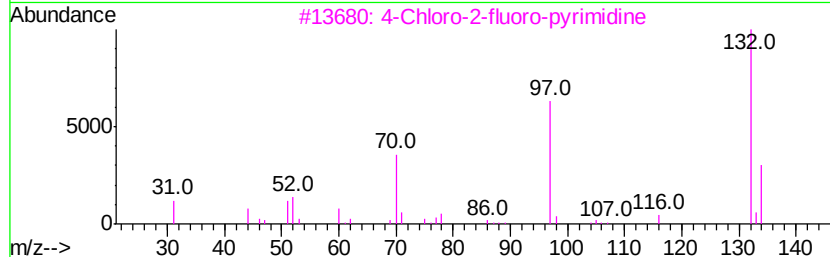
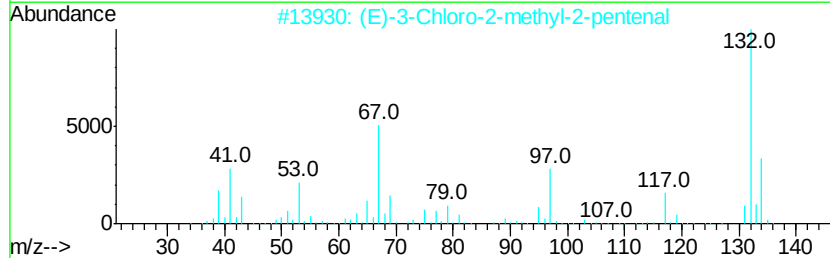
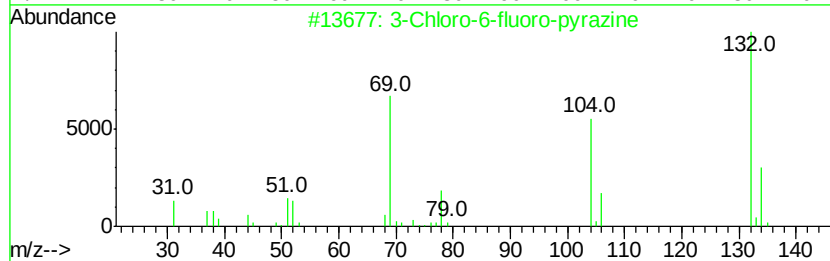
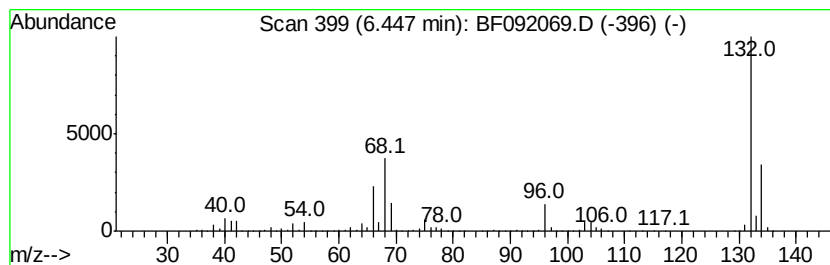
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	84.69 ng	5084580	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3		Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4		Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4		Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4		Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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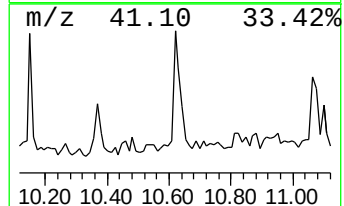
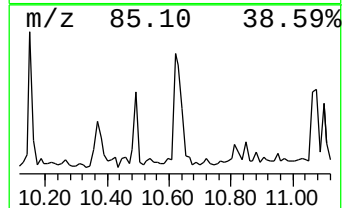
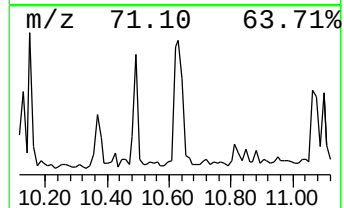
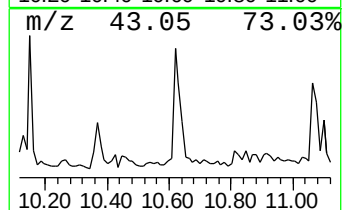
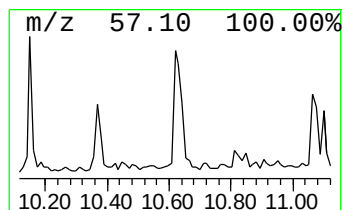
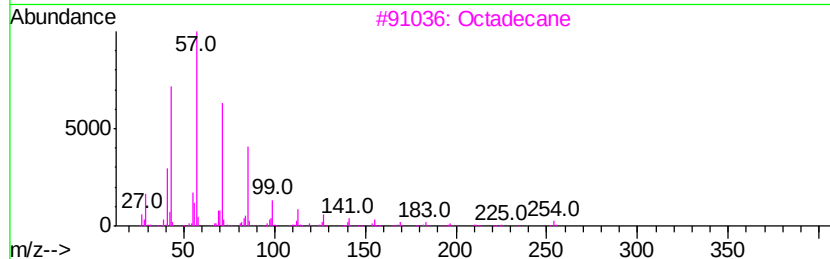
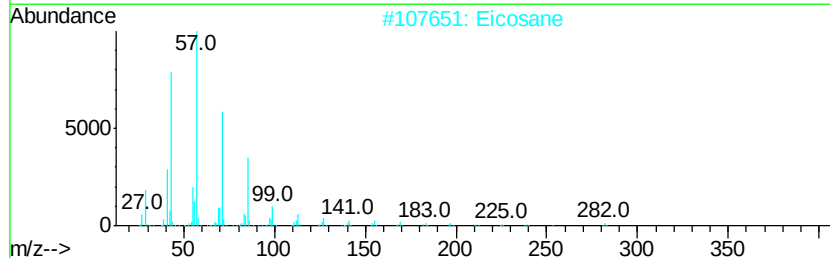
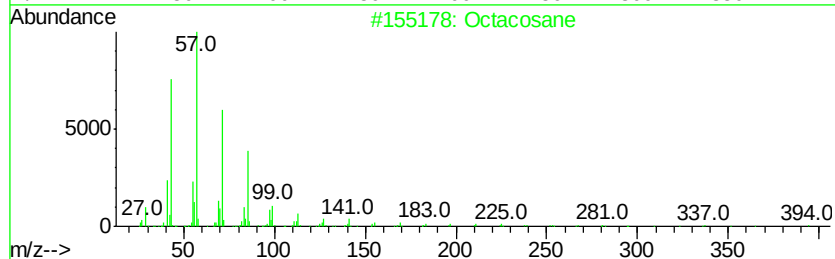
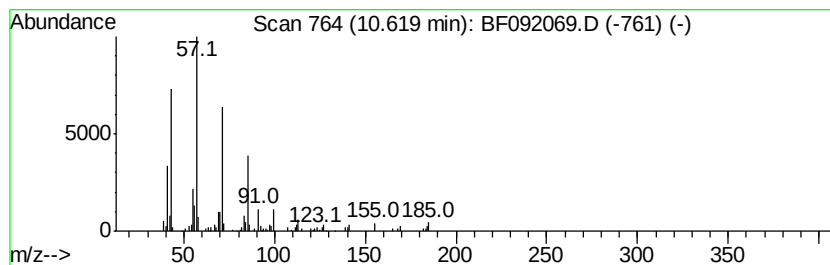
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	3.35 ng	259522	Phenanthrene-d10	11.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	Eicosane		282	C20H42	000112-95-8	83
3	Octadecane		254	C18H38	000593-45-3	80
4	Hexadecane		226	C16H34	000544-76-3	80
5	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	80



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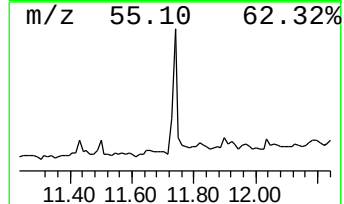
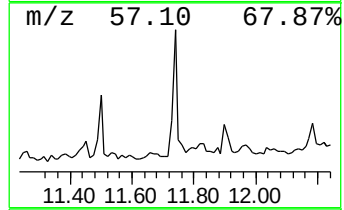
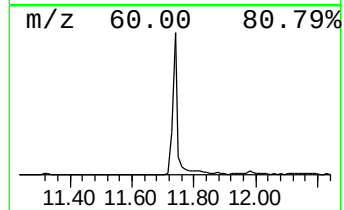
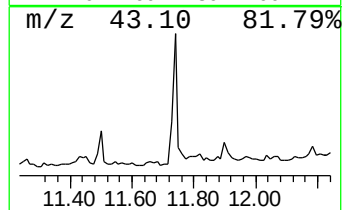
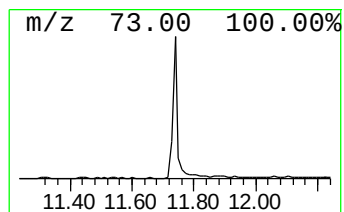
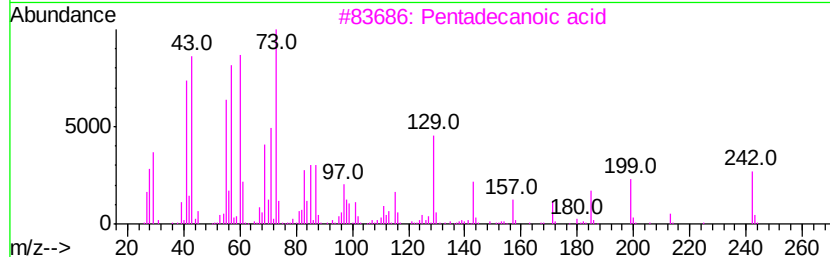
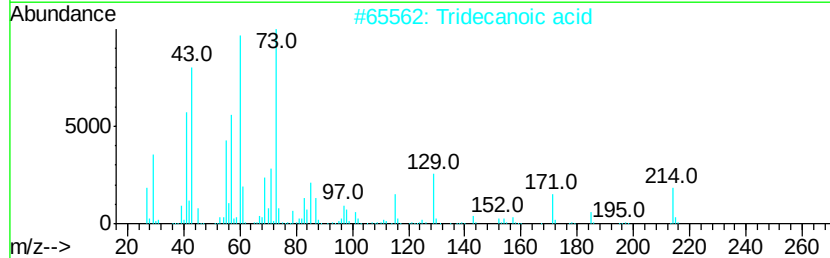
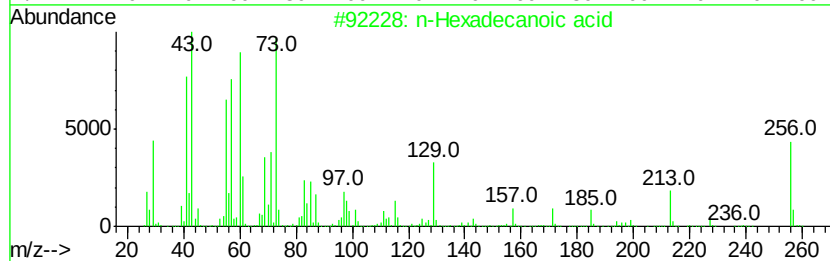
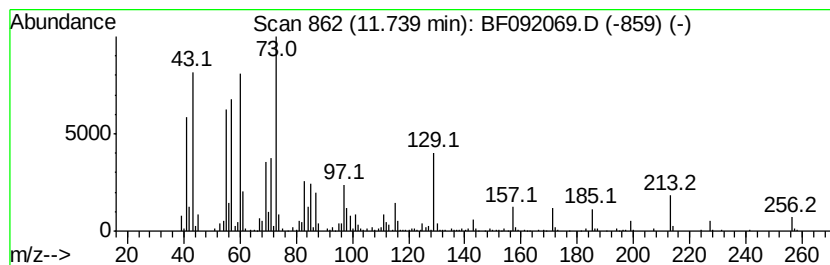
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.74	6.75 ng	523020	Phenanthrene-d10	11.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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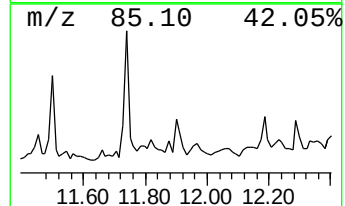
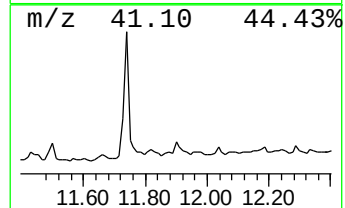
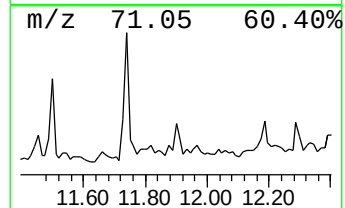
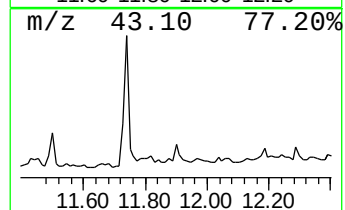
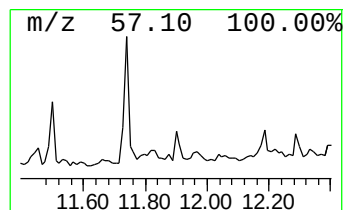
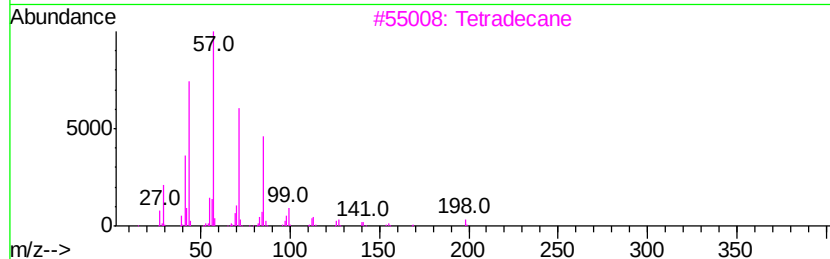
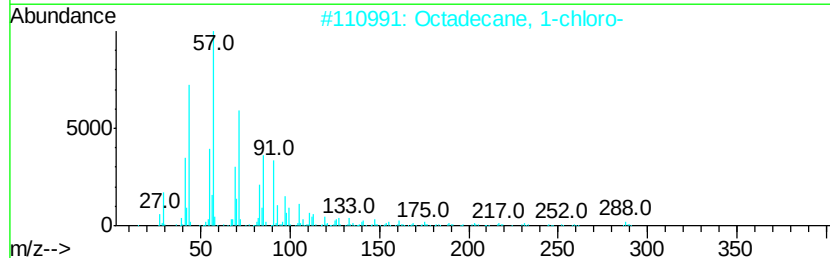
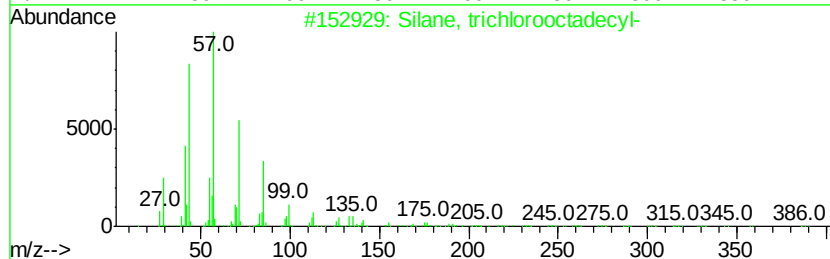
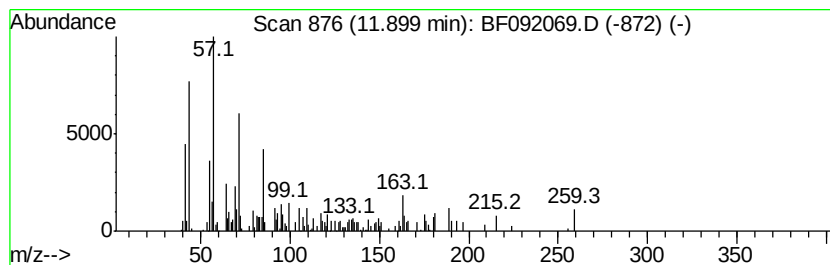
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown11.90 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.01 ng	155947	Phenanthrene-d10	11.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	46
2		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	43
3		Tetradecane	198	C14H30	000629-59-4	43
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	38
5		Tridecane	184	C13H28	000629-50-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010317\
Data File : BF092069.D
Acq On : 3 Jan 2017 19:14
Operator : UM/SJ
Sample : H6322-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

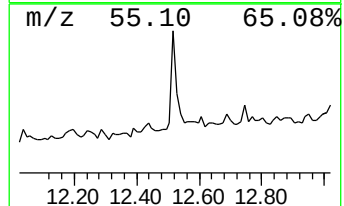
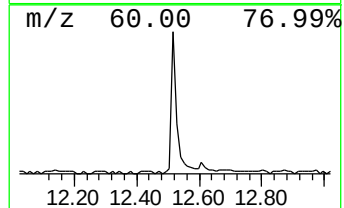
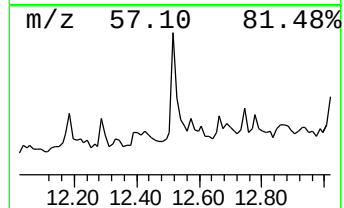
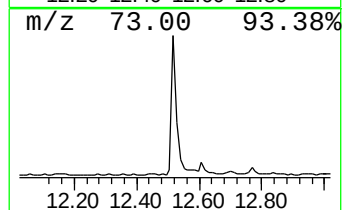
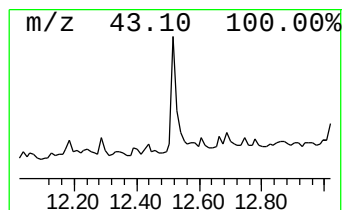
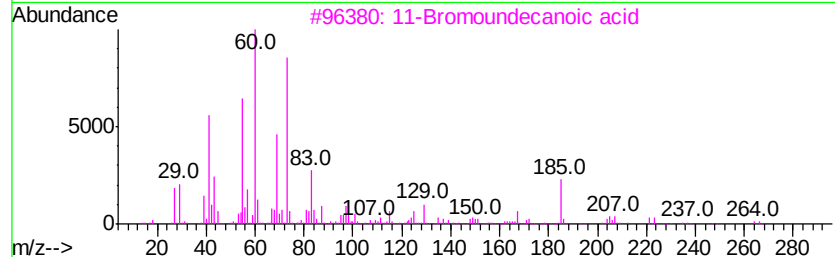
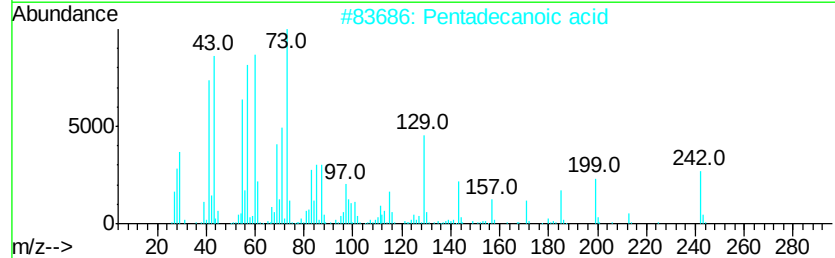
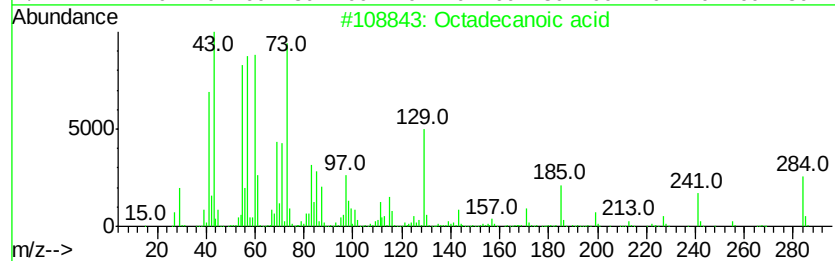
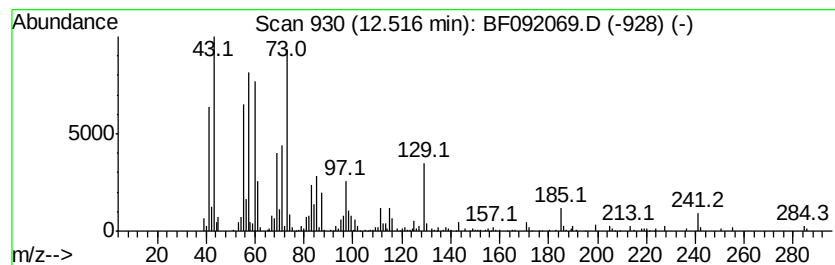
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.52	5.63 ng	340388	Chrysene-d12		13.82	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
4		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25
5		Tetradecane	198	C14H30	000629-59-4	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010317\
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Misc :
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Instrument :
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ClientSampleId :
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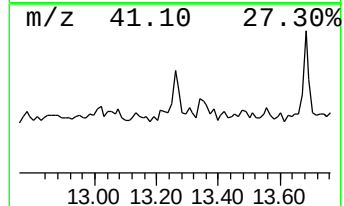
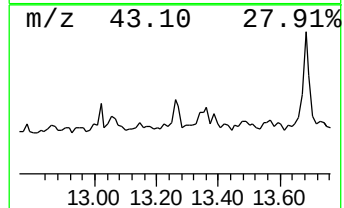
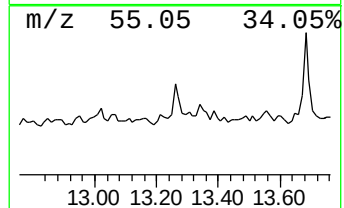
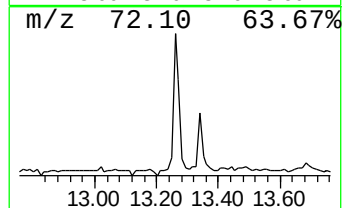
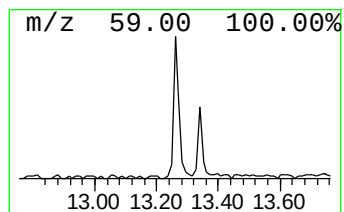
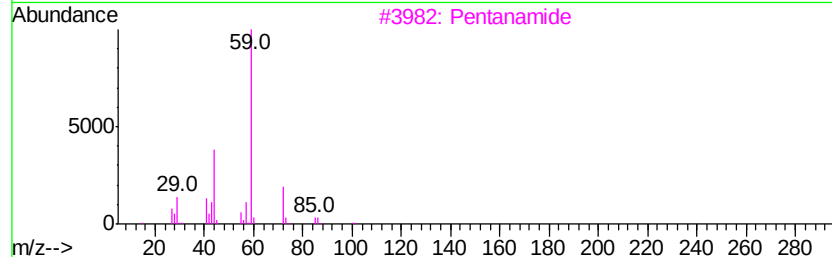
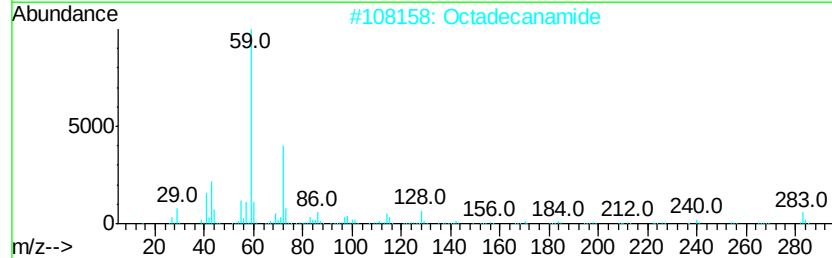
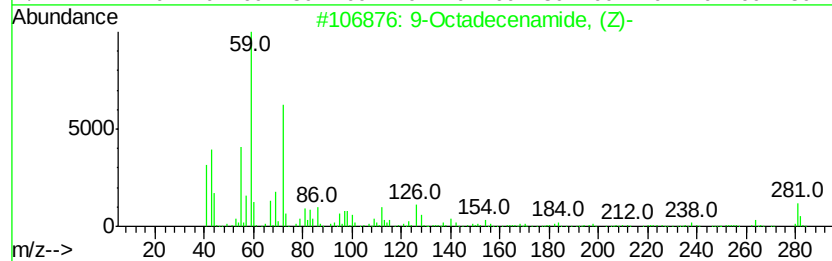
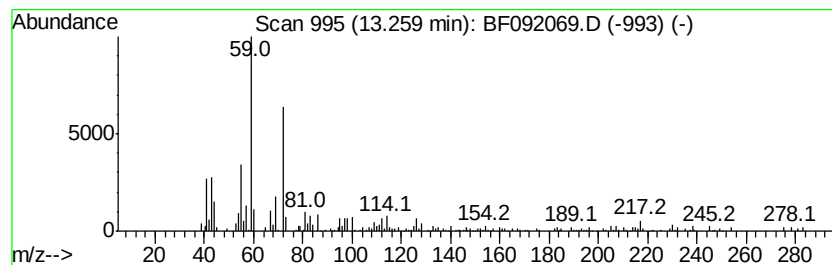
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	2.42 ng	146045	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Octadecanamide	283	C18H37NO	000124-26-5	78
3		Pentanamide	101	C5H11NO	000626-97-1	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Octanamide	143	C8H17NO	000629-01-6	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010317\
Data File : BF092069.D
Acq On : 3 Jan 2017 19:14
Operator : UM/SJ
Sample : H6322-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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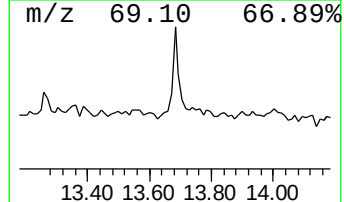
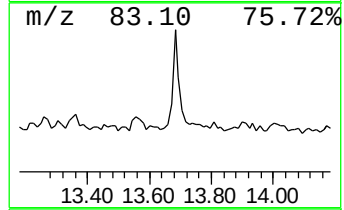
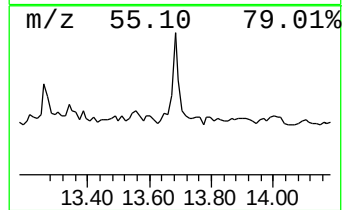
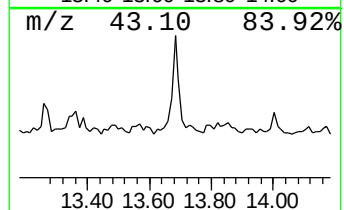
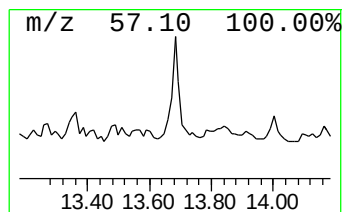
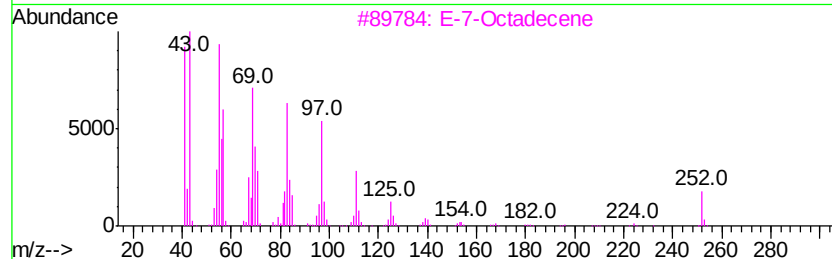
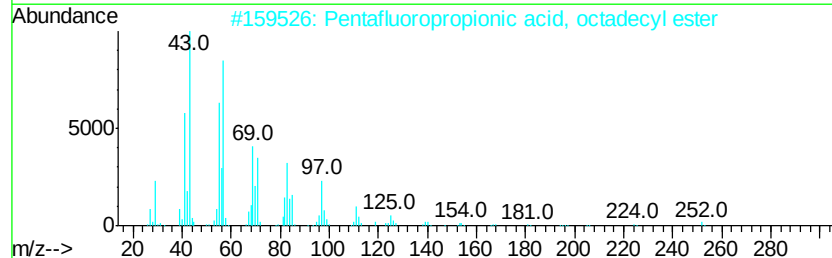
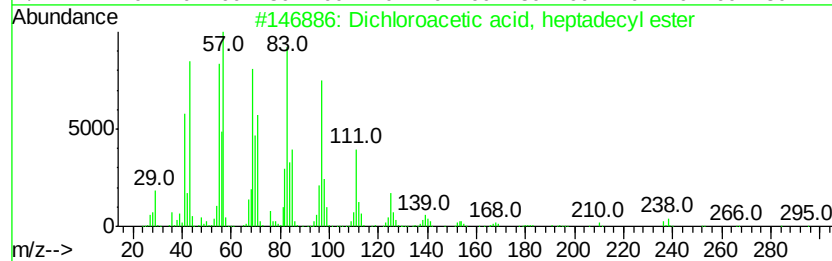
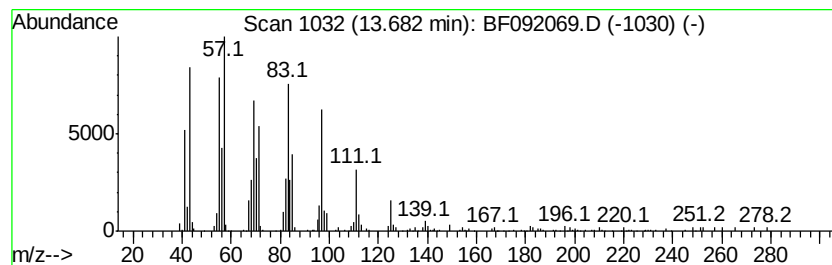
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.04 ng	244414	Chrysene-d12	13.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
3			E-7-Octadecene	252	C18H36	1000130-92-0	89
4			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010317\
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Misc :
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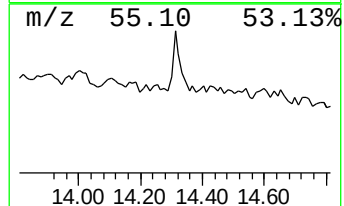
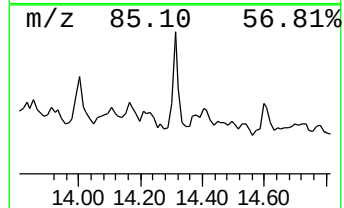
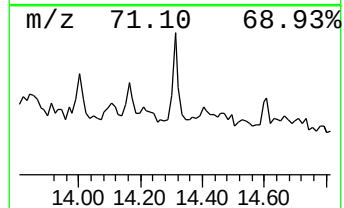
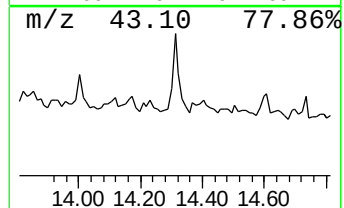
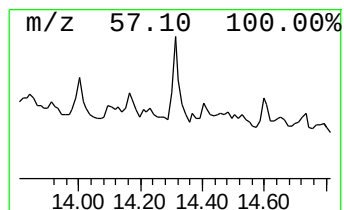
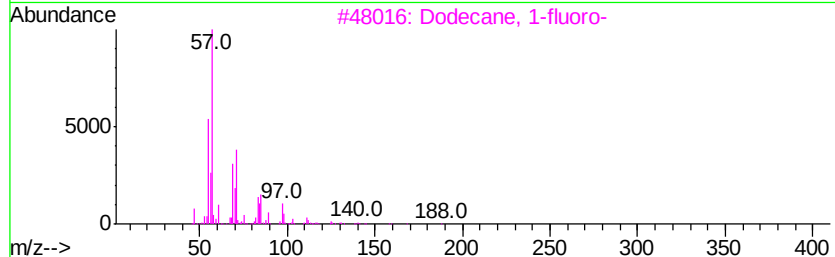
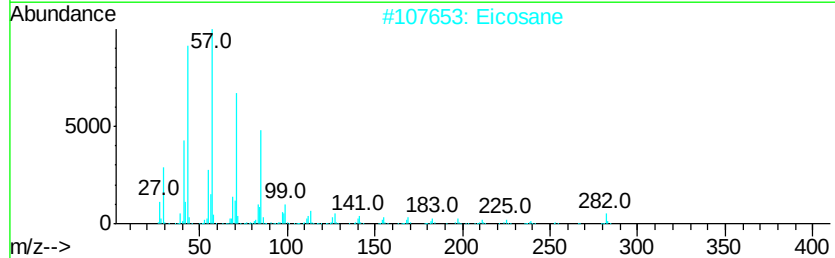
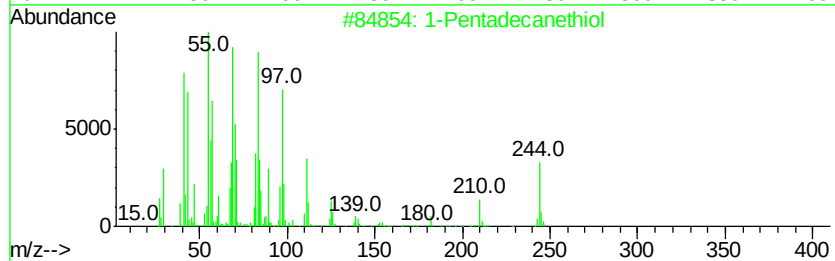
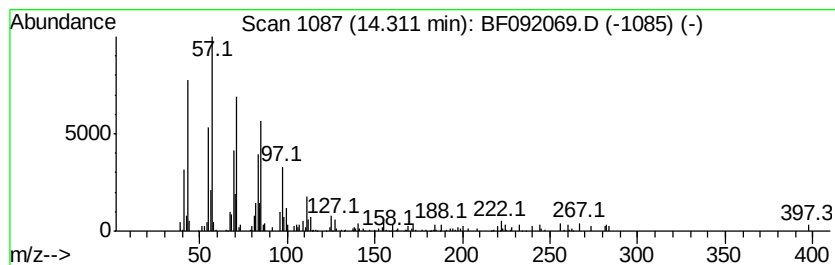
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Pentadecanethiol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.31	2.97 ng	179561	Chrysene-d12		13.82		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecanethiol	244	C15H32S	025276-70-4	90
2			Eicosane	282	C20H42	000112-95-8	78
3			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	74
4			Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	72
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010317\
Data File : BF092069.D
Acq On : 3 Jan 2017 19:14
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Misc :
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Instrument :
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ClientSampleId :
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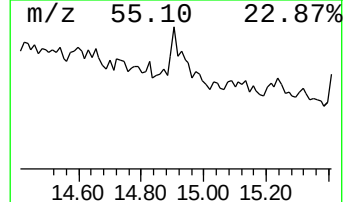
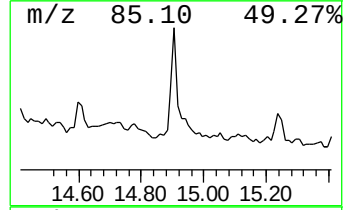
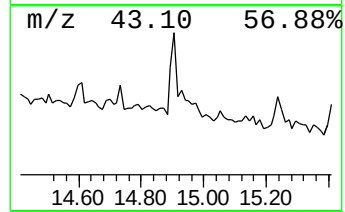
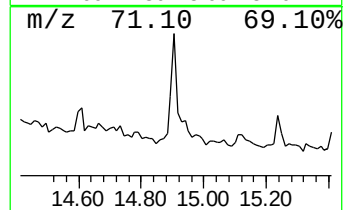
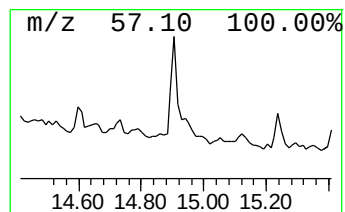
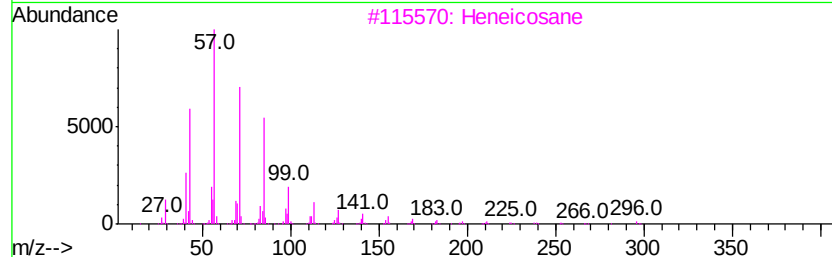
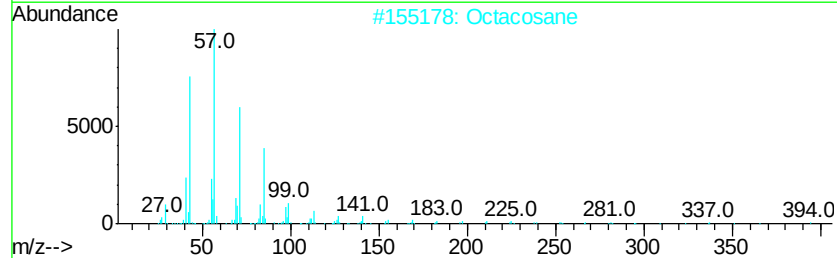
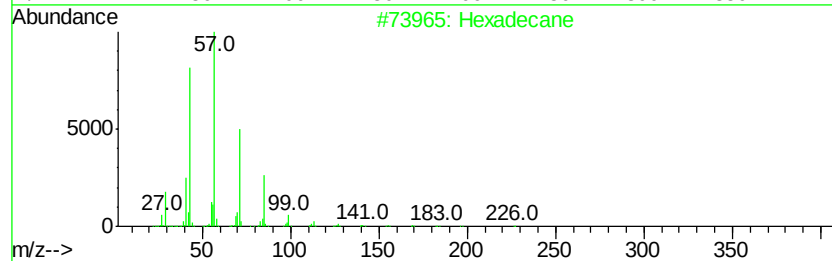
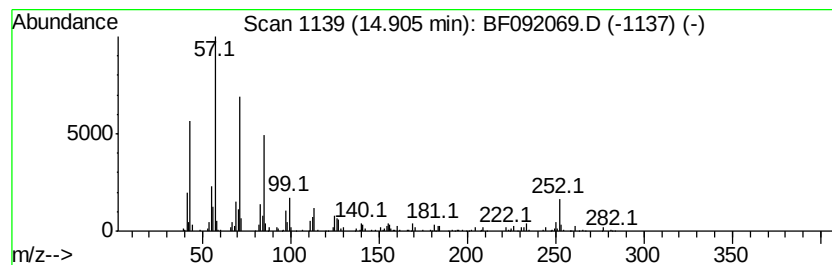
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	2.96 ng	141921	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Octacosane	394	C28H58	000630-02-4	87
3		Heneicosane	296	C21H44	000629-94-7	83
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010317\
Data File : BF092069.D
Acq On : 3 Jan 2017 19:14
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Misc :
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Instrument :
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ClientSampled :
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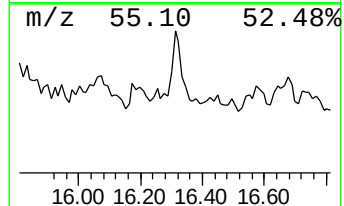
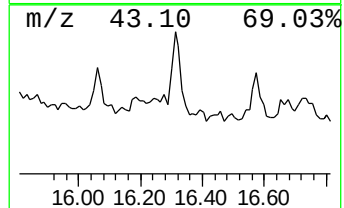
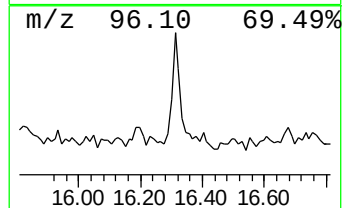
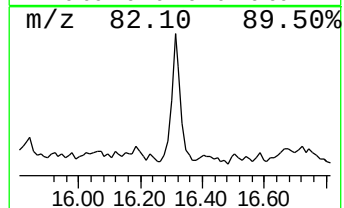
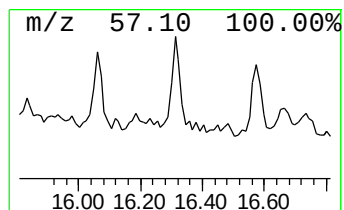
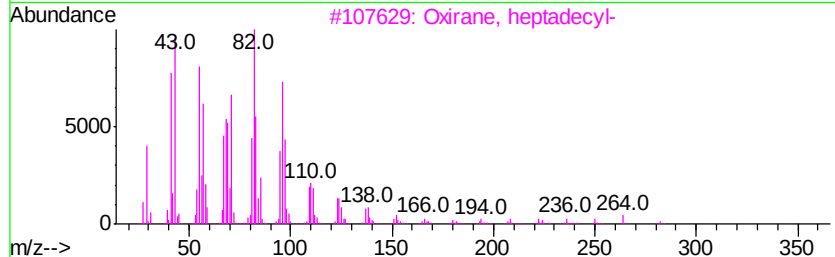
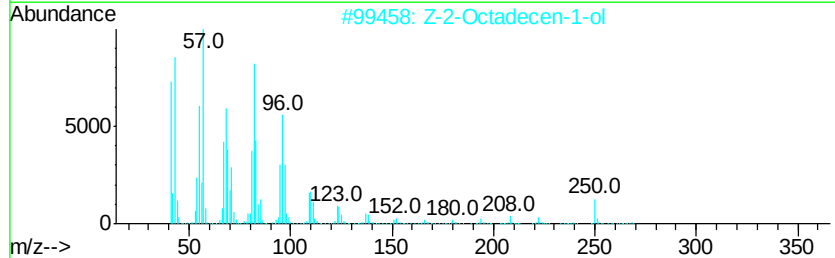
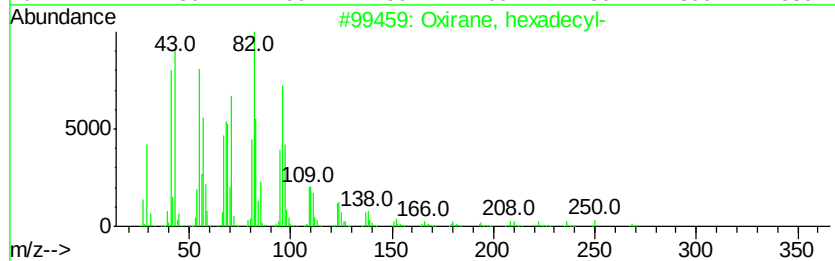
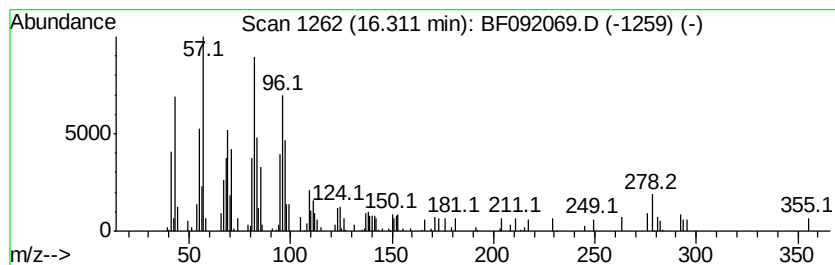
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	3.05 ng	146106	Perylene-d12	15.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
2			Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	86
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	86
4			17-Octadecenal	266	C18H34O	056554-86-0	80
5			E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010317\
Data File : BF092069.D
Acq On : 3 Jan 2017 19:14
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP9-COMP9

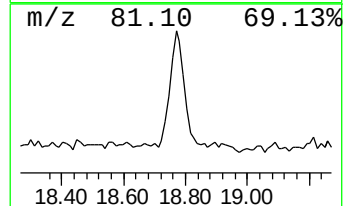
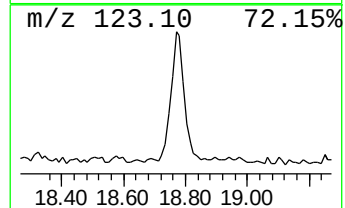
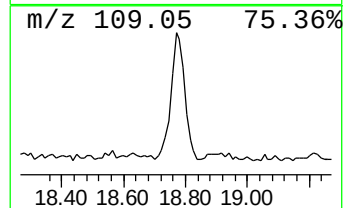
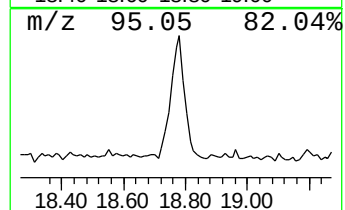
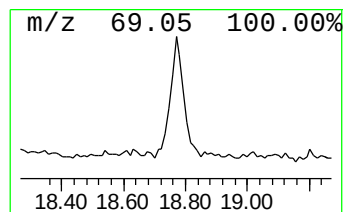
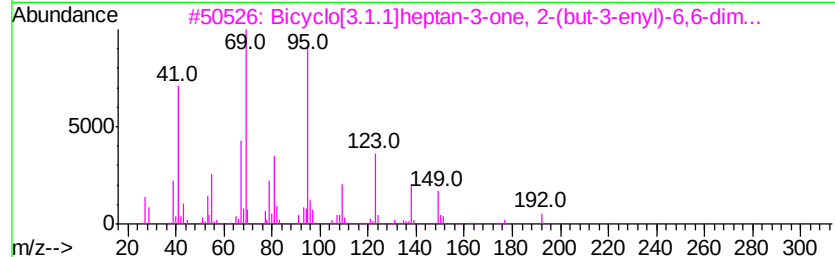
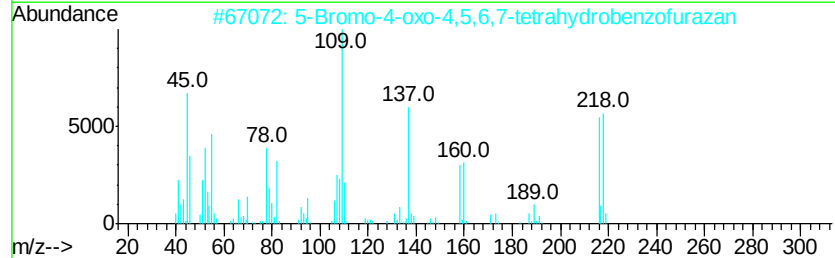
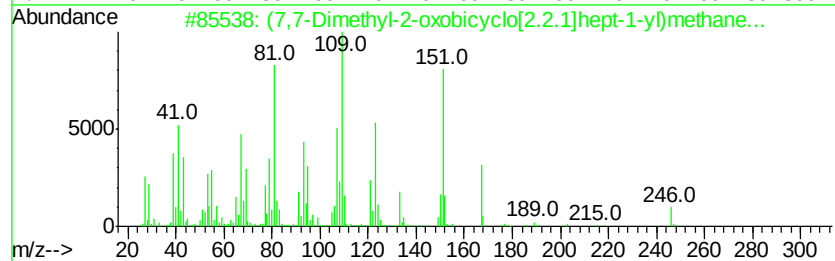
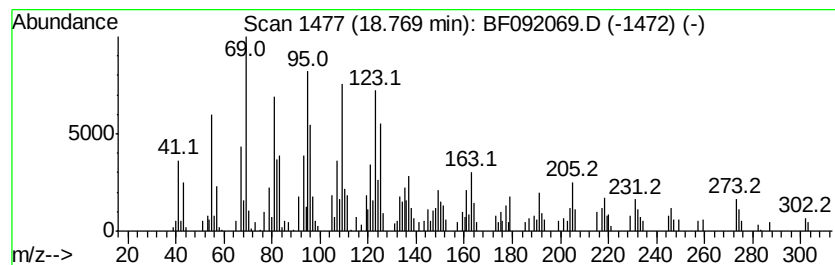
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 (7,7-Dimethyl-2-oxobicyclo[...] Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	9.80 ng	469398	Perylene-d12	15.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(7,7-Dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methane...	246	C11H18O4S	1000197-55-6	60
2			5-Bromo-4-oxo-4,5,6,7-tetrahydrobenzofuran	216	C6H5BrN2O2	300574-36-1	59
3			Bicyclo[3.1.1]heptan-3-one, 2-(but-3-enyl)-6,6-dimethyl-	192	C13H20O	1000163-96-1	43
4			2,4a,8,8-Tetramethyldecahydrocyclopenta[b]pyridine	206	C15H26	074022-04-1	38
5			2,2,6-Trimethyl-1-(2-methyl-cyclopentyl)pyridine	218	C15H22O	1000188-72-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010317\
 Data File : BF092069.D
 Acq On : 3 Jan 2017 19:14
 Operator : UM/SJ
 Sample : H6322-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP9-COMP9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
 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
2-Pentanone, 4-hy...	4.81	29.7	ng	1780430	1	6.66	1200720	20.0
unknown6.45	6.45	84.7	ng	5084580	1	6.66	1200720	20.0
Octacosane	10.62	3.4	ng	259522	4	11.19	1548670	20.0
n-Hexadecanoic acid	11.74	6.8	ng	523020	4	11.19	1548670	20.0
unknown11.90	11.90	2.0	ng	155947	4	11.19	1548670	20.0
Octadecanoic acid	12.52	5.6	ng	340388	5	13.82	1209000	20.0
9-Octadecenamide,...	13.26	2.4	ng	146045	5	13.82	1209000	20.0
Dichloroacetic ac...	13.68	4.0	ng	244414	5	13.82	1209000	20.0
1-Pentadecanethiol	14.31	3.0	ng	179561	5	13.82	1209000	20.0
Hexadecane	14.91	3.0	ng	141921	6	15.19	958175	20.0
Oxirane, hexadecyl-	16.31	3.0	ng	146106	6	15.19	958175	20.0
(7,7-Dimethyl-2-o...	18.77	9.8	ng	469398	6	15.19	958175	20.0