

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
 Data File : BF088569.D
 Acq On : 1 Jul 2016 12:25
 Operator : UM/SJ
 Sample : H3808-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-COMP

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-BF063016.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	1.678	4	8	10	rVB	5201837	8277090	100.00%	16.217%
2	1.735	12	13	23	rVV	616652	974917	11.78%	1.910%
3	1.861	23	24	40	rVB	2568511	5758043	69.57%	11.282%
4	2.067	40	42	77	rVB2	142598	726860	8.78%	1.424%
5	3.130	126	135	138	rBV	248348	944658	11.41%	1.851%
6	4.993	295	298	302	rBV	147693	240188	2.90%	0.471%
7	5.404	331	334	337	rBV	2692686	2927501	35.37%	5.736%
8	6.445	421	425	427	rBV	3006560	3665807	44.29%	7.182%
9	6.570	433	436	439	rBV	2458411	3260678	39.39%	6.389%
10	6.810	454	457	459	rBV	832985	886205	10.71%	1.736%
11	6.959	468	470	473	rVB	1922408	2543289	30.73%	4.983%
12	7.370	503	506	508	rBV	2112031	2189039	26.45%	4.289%
13	8.090	566	569	571	rBV	1342770	1182305	14.28%	2.316%
14	9.176	660	664	666	rBV	2505010	3696786	44.66%	7.243%
15	9.565	695	698	700	rBV	399792	393190	4.75%	0.770%
16	9.839	720	722	724	rVB	1248389	1217007	14.70%	2.384%
17	10.628	788	791	793	rBV	1997790	1997993	24.14%	3.915%
18	11.199	839	841	843	rBV	96201	110216	1.33%	0.216%
19	11.325	849	852	855	rVB	844365	1301820	15.73%	2.551%
20	11.634	877	879	885	rVV	76309	122611	1.48%	0.240%
21	11.725	885	887	890	rVB	121789	107729	1.30%	0.211%
22	11.862	896	899	900	rBV	125774	156853	1.90%	0.307%
23	12.434	945	949	953	rVB3	268904	512470	6.19%	1.004%
24	12.525	955	957	959	rVB	484578	458503	5.54%	0.898%
25	12.754	973	977	979	rBV	308948	406813	4.91%	0.797%
26	12.902	987	990	993	rVB	2477323	2733621	33.03%	5.356%
27	13.382	1030	1032	1034	rBV	459413	411927	4.98%	0.807%
28	13.691	1057	1059	1061	rBV	57033	89134	1.08%	0.175%
29	13.817	1068	1070	1073	rVB	160761	251514	3.04%	0.493%
30	13.942	1077	1081	1087	rBV2	1141022	1532576	18.52%	3.003%
31	14.525	1130	1132	1135	rBV3	46626	88138	1.06%	0.173%
32	14.800	1154	1156	1158	rVB2	81345	86622	1.05%	0.170%
33	14.948	1167	1169	1174	rVB	181523	352401	4.26%	0.690%
34	15.177	1187	1189	1191	rVB	71606	96096	1.16%	0.188%

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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_F\METHODS\8270-BF063016.M
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35	15.234	1191	1194	1196	rVB	99283	149246	1.80%	0.292%
36	15.280	1196	1198	1201	rBV	105430	136446	1.65%	0.267%
37	15.348	1201	1204	1206	rBV	619805	796843	9.63%	1.561%
38	16.686	1318	1321	1326	rVB2	70301	144933	1.75%	0.284%
39	17.086	1354	1356	1364	rVB	48826	110820	1.34%	0.217%

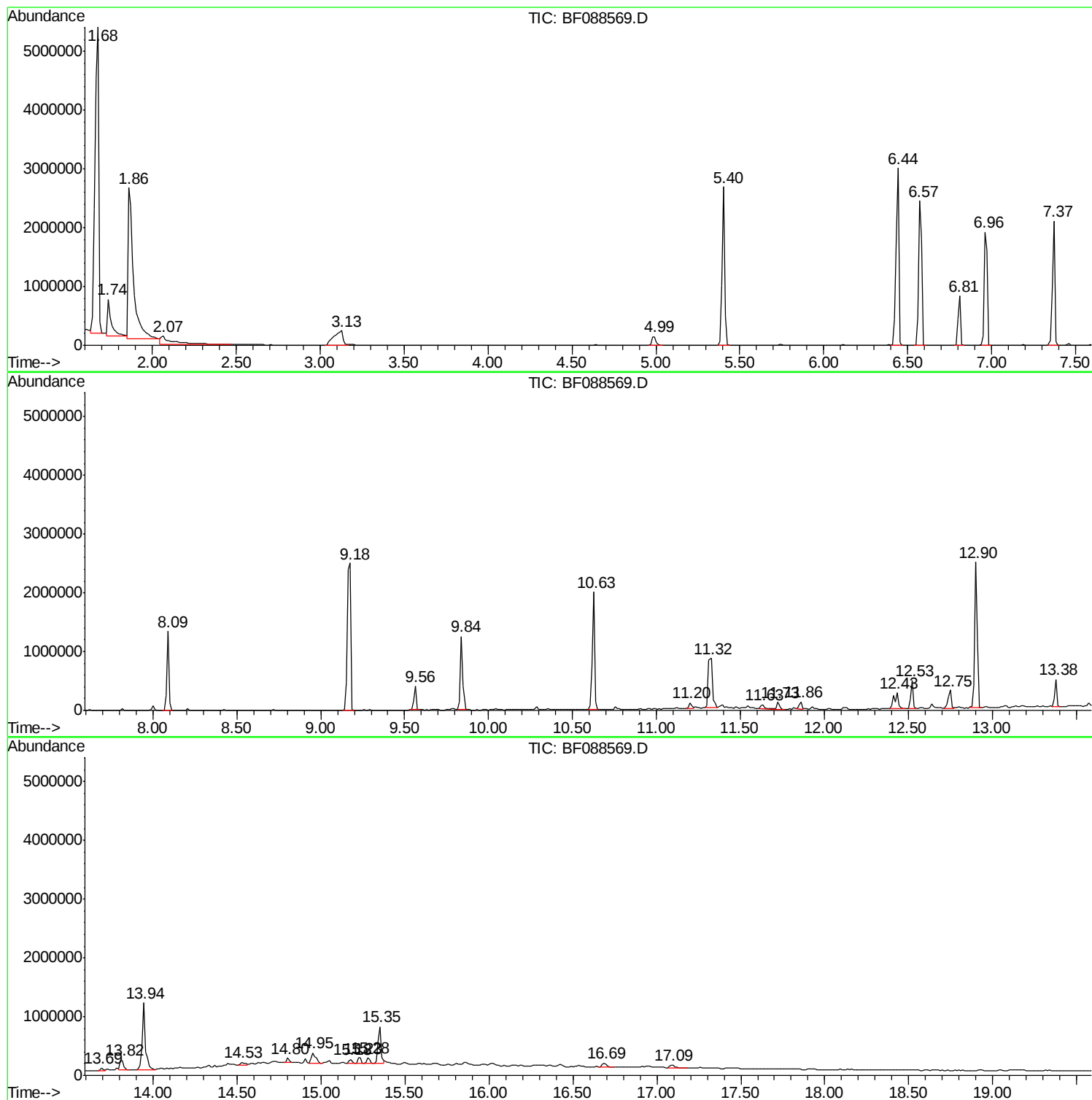
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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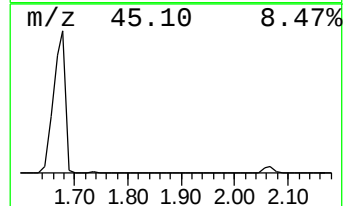
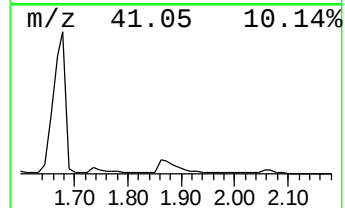
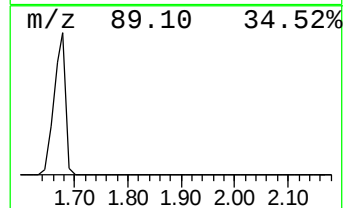
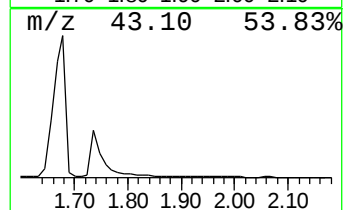
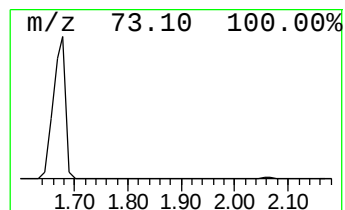
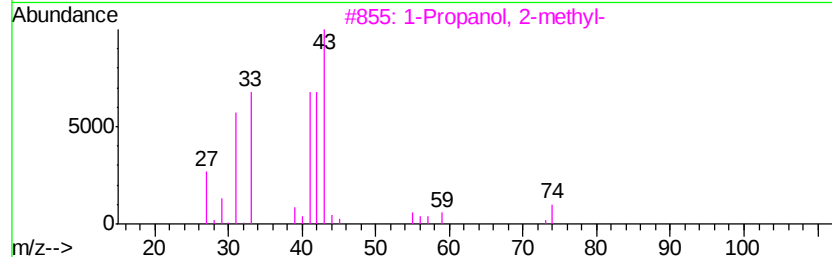
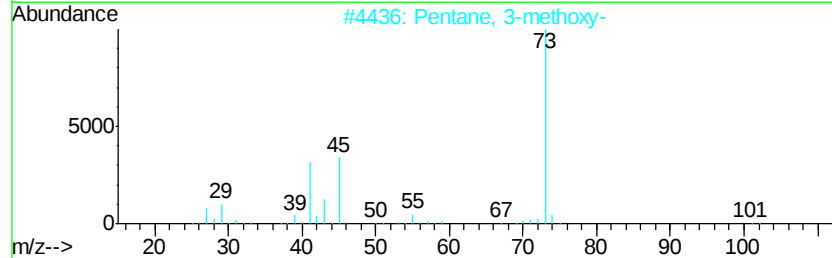
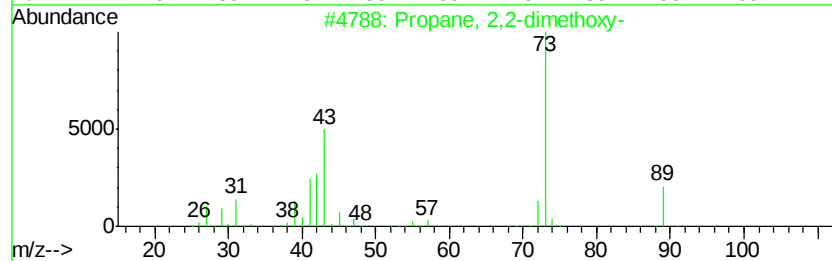
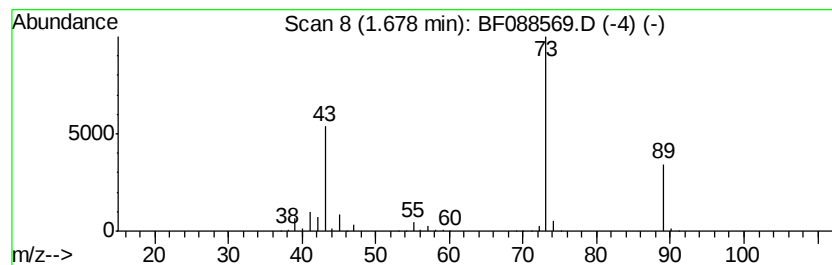
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	186.80 ng	8277090	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9



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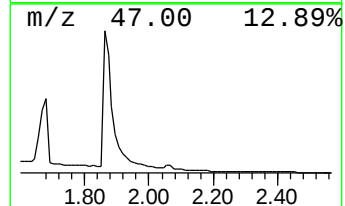
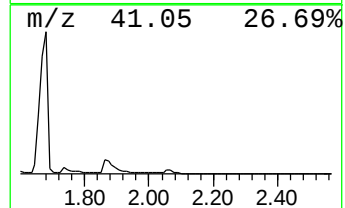
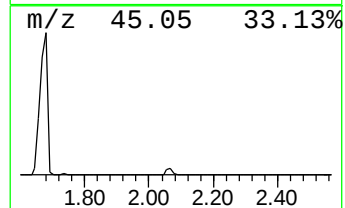
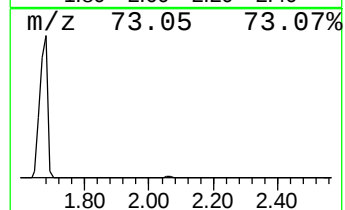
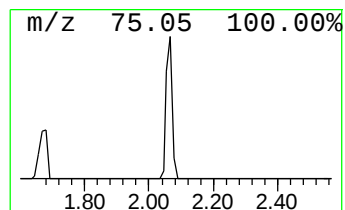
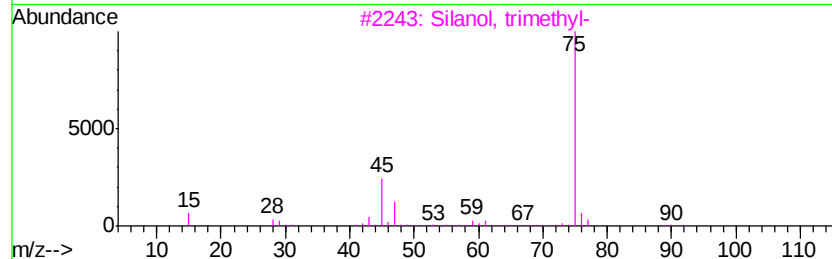
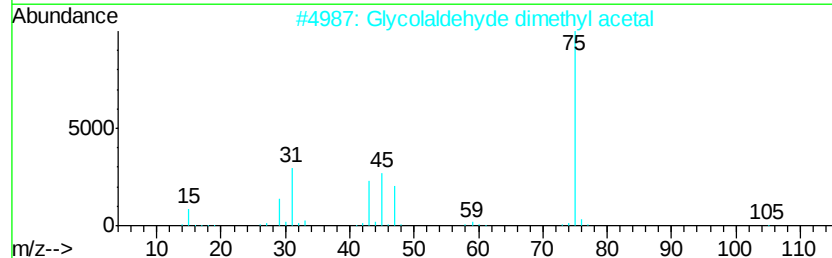
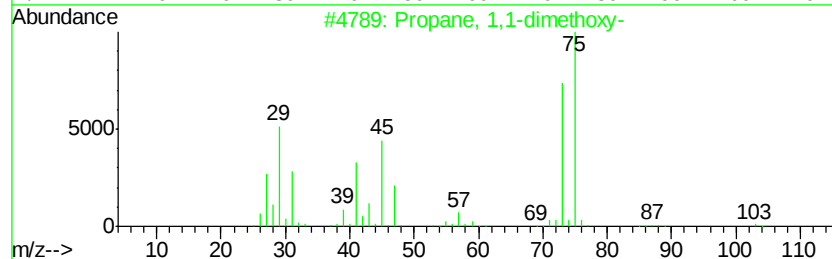
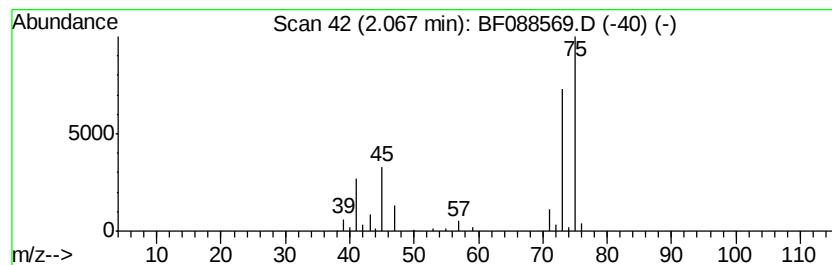
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown2.07 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	16.40 ng	726860	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
3		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
4		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9



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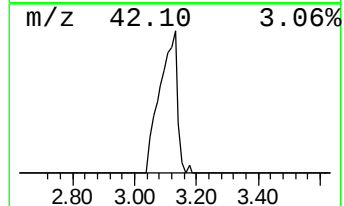
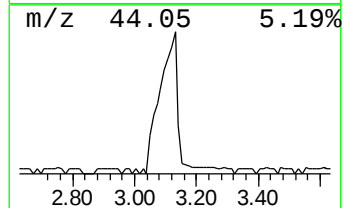
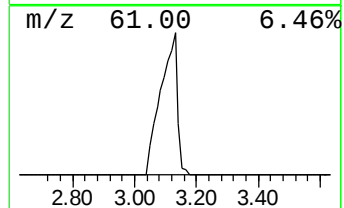
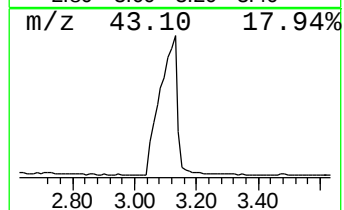
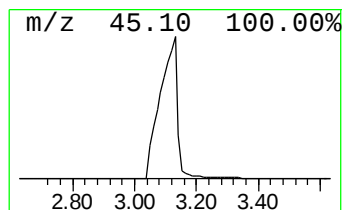
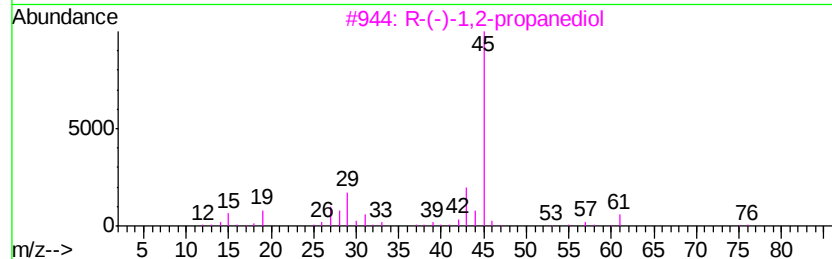
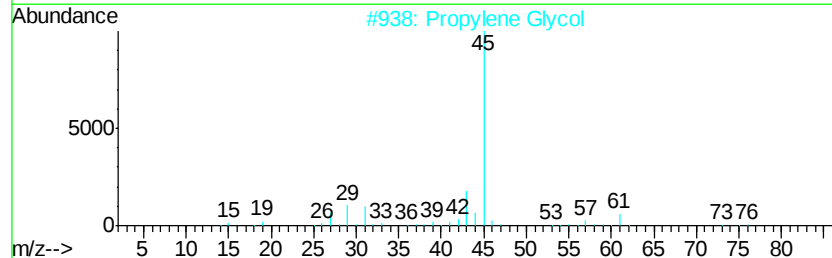
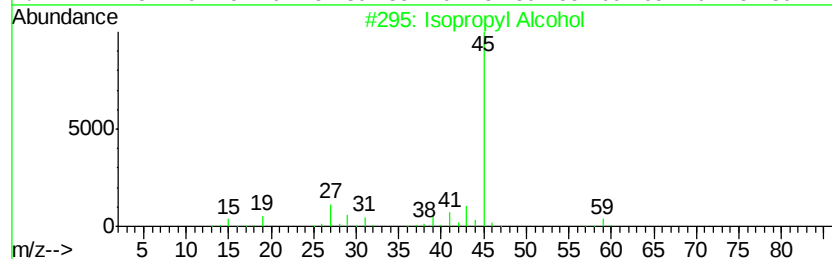
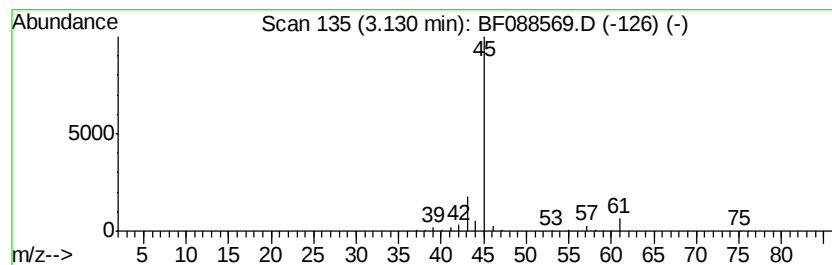
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	21.32 ng	944658	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2		Propylene Glycol	76	C3H8O2	000057-55-6	43
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



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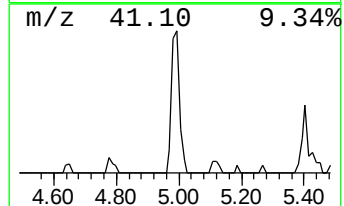
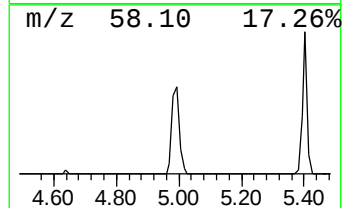
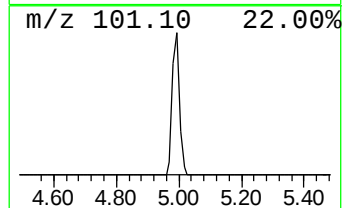
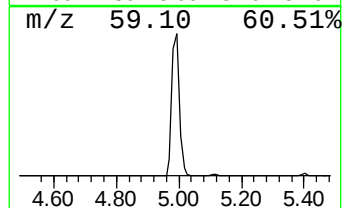
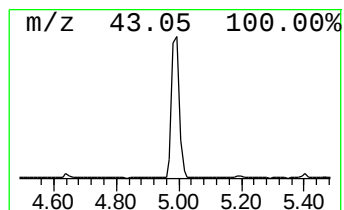
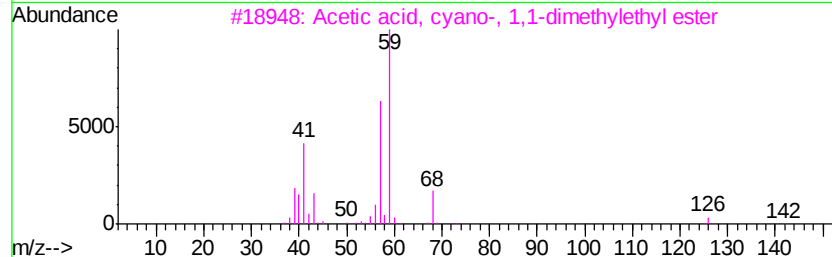
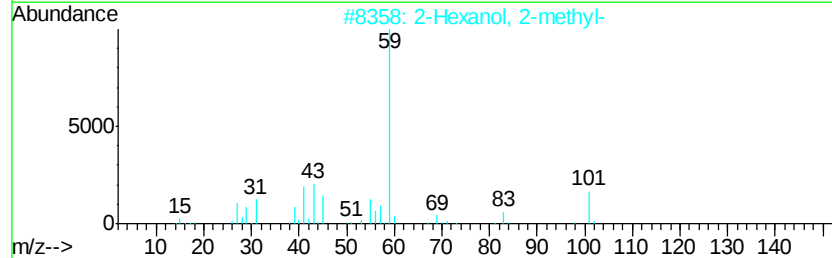
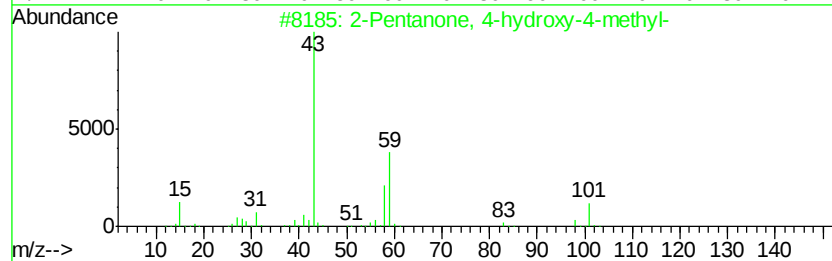
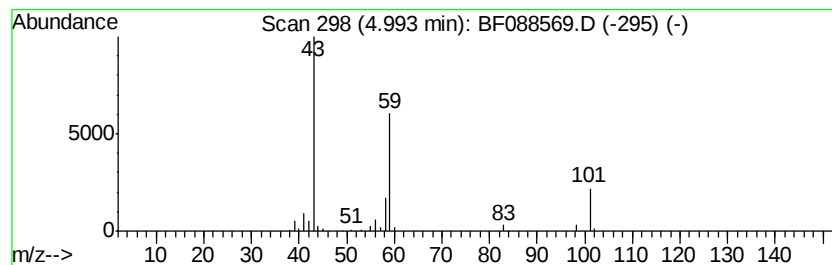
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	5.42 ng	240188	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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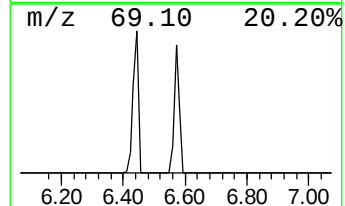
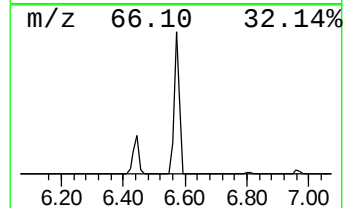
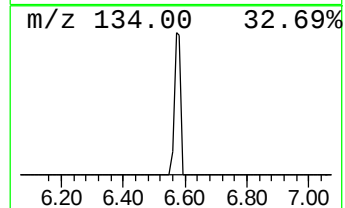
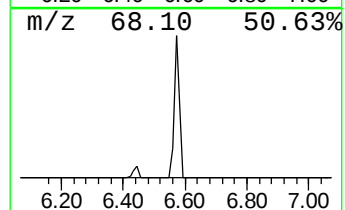
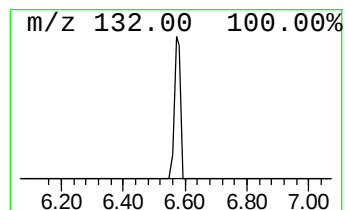
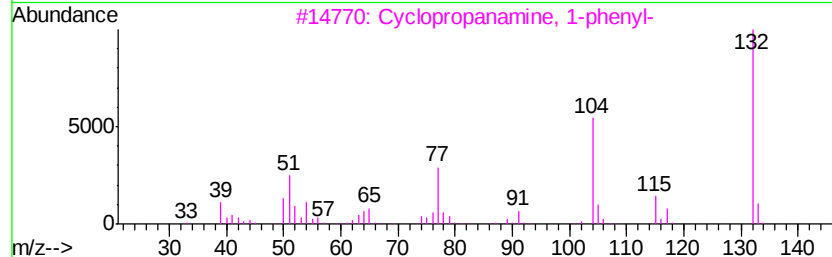
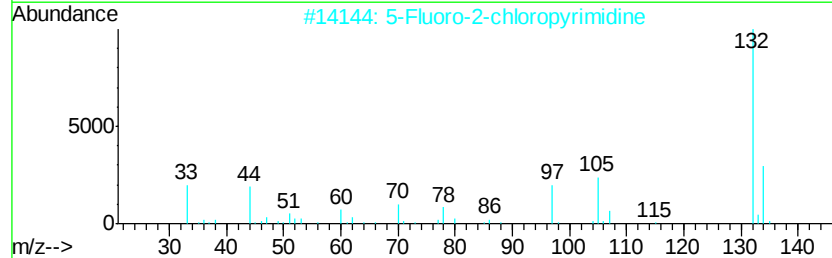
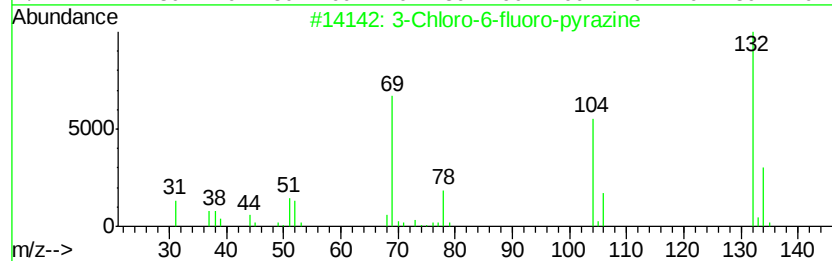
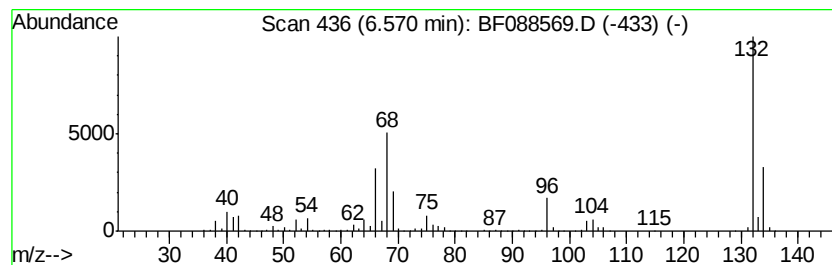
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Peak Number 7 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	73.59 ng	3260680	1,4-Dichlorobenzene-d4	6.81

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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088569.D
Acq On : 1 Jul 2016 12:25
Operator : UM/SJ
Sample : H3808-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-COMP

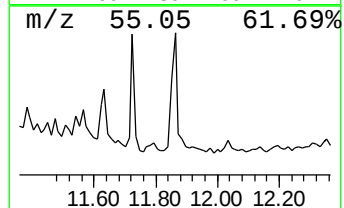
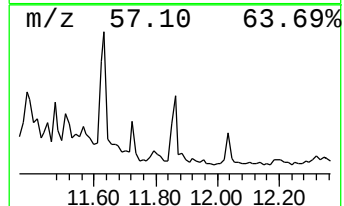
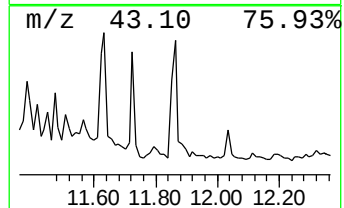
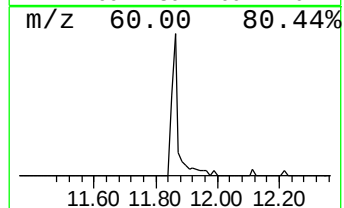
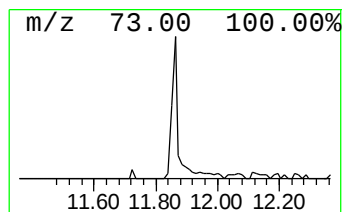
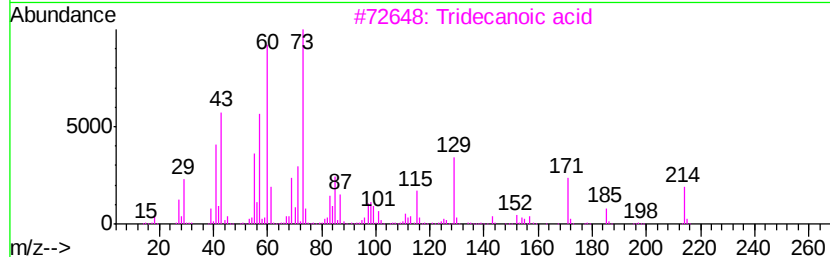
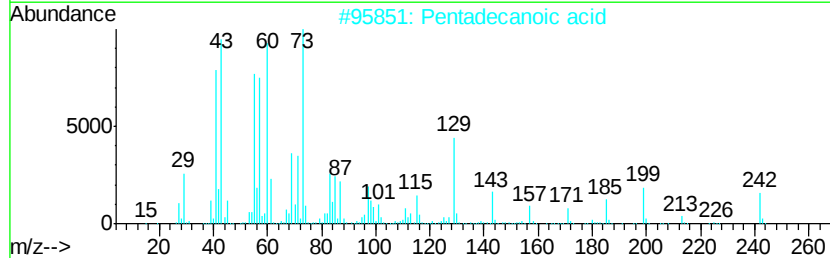
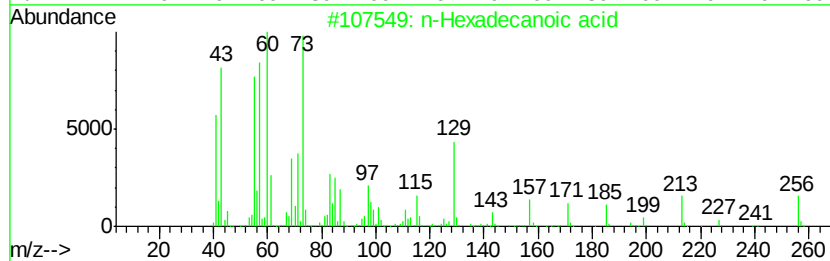
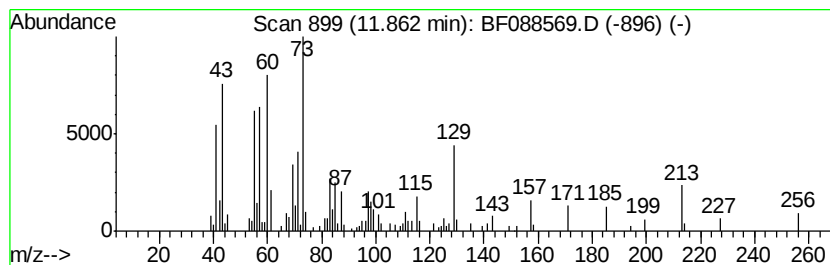
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.41 ng	156853	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Nonanoic acid	158	C9H18O2	000112-05-0	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
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Operator : UM/SJ
Sample : H3808-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-COMP

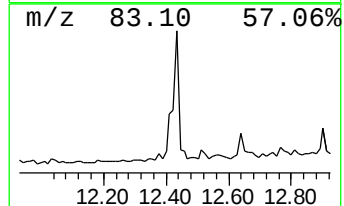
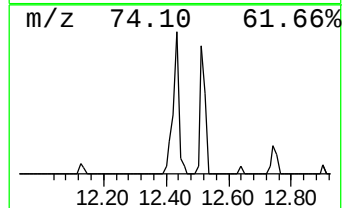
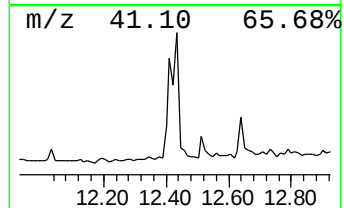
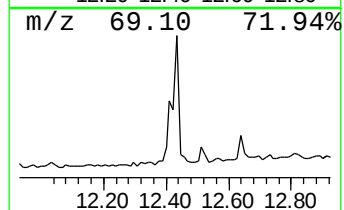
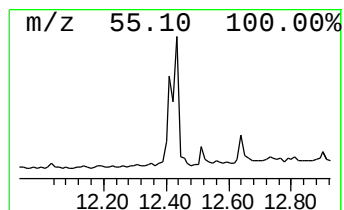
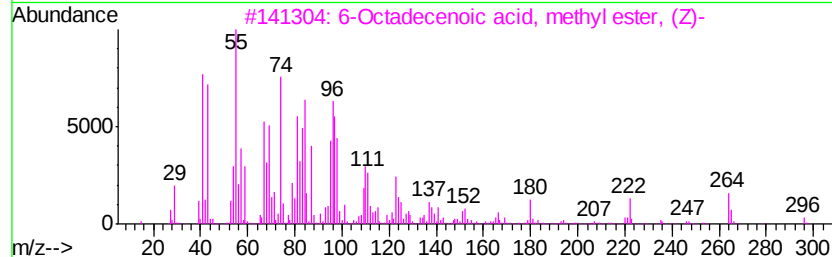
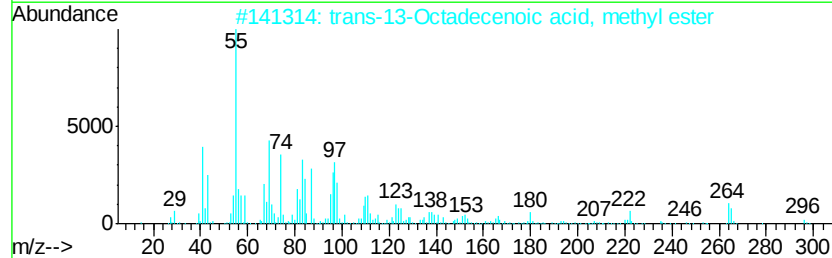
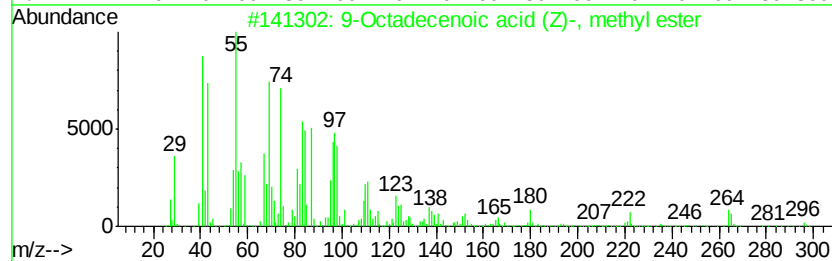
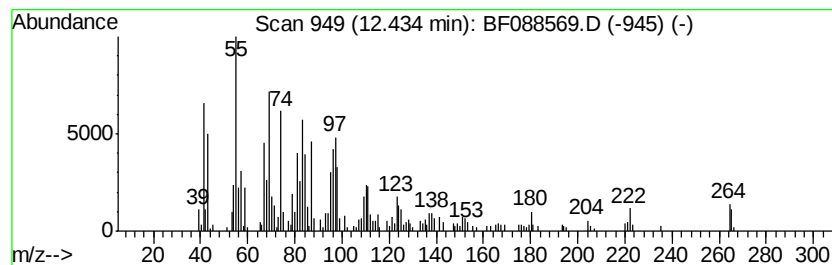
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenoic acid (Z)-, m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	7.87 ng	512470	Phenanthrene-d10	11.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
3			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	93
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088569.D
Acq On : 1 Jul 2016 12:25
Operator : UM/SJ
Sample : H3808-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

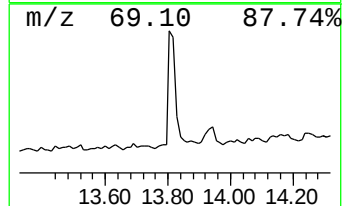
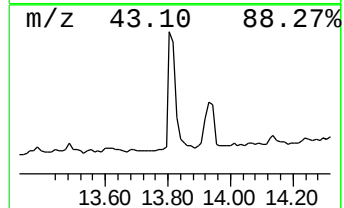
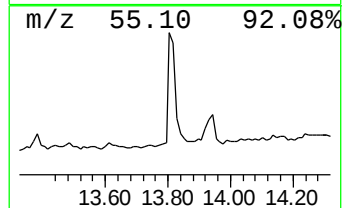
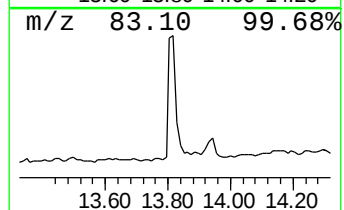
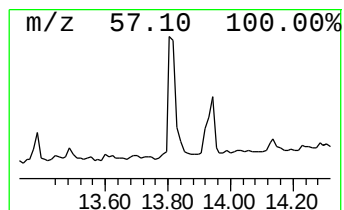
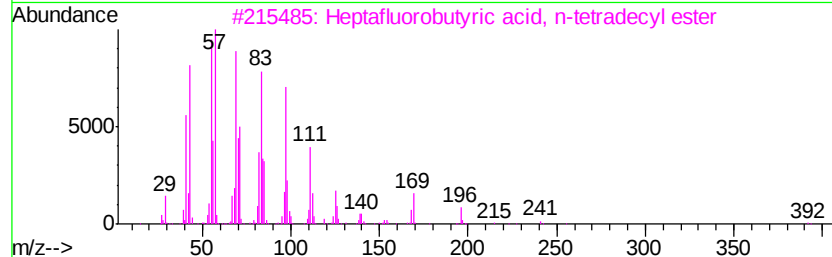
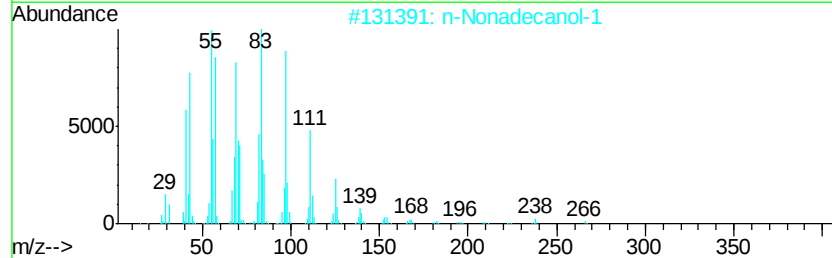
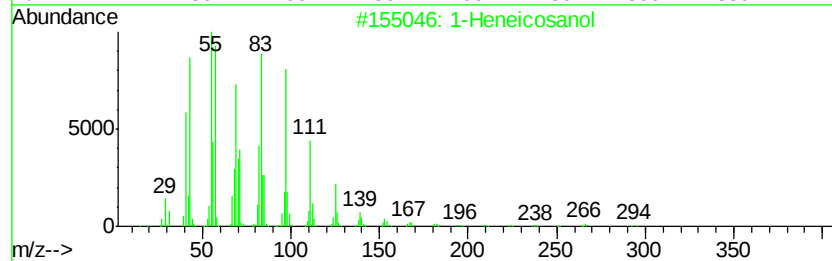
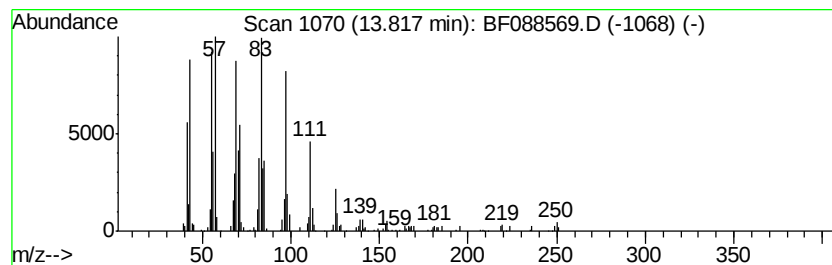
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ClientSampleId :
SB-02-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heneicosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	3.28 ng	251514	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Trifluoroacetoxyl hexadecane	338	C18H33F3O2	006222-03-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
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Operator : UM/SJ
Sample : H3808-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-COMP

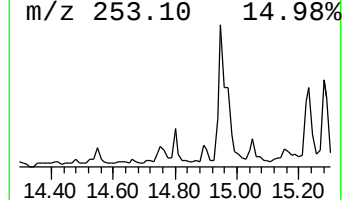
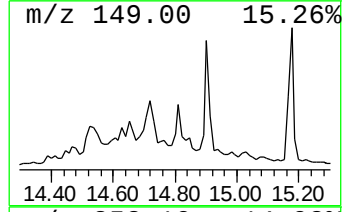
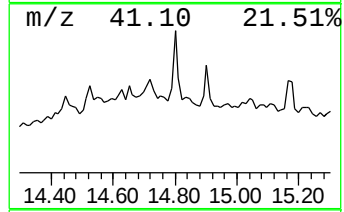
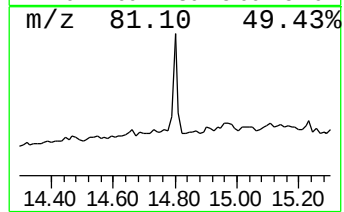
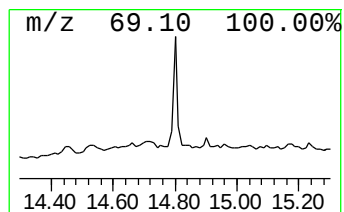
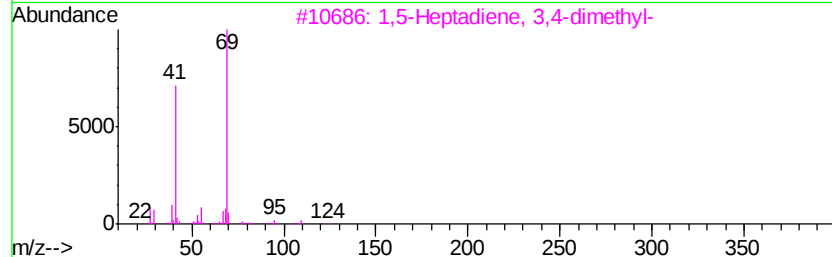
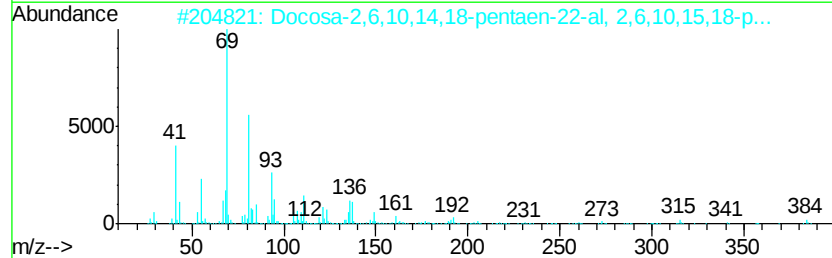
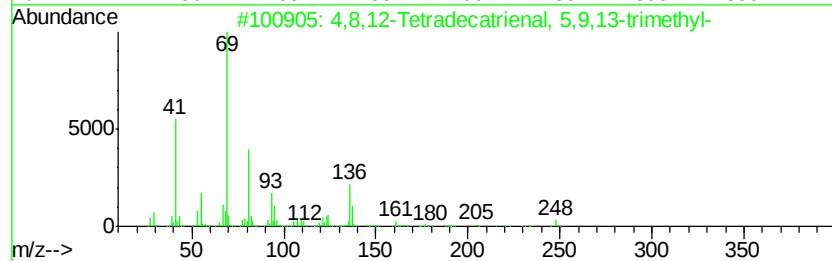
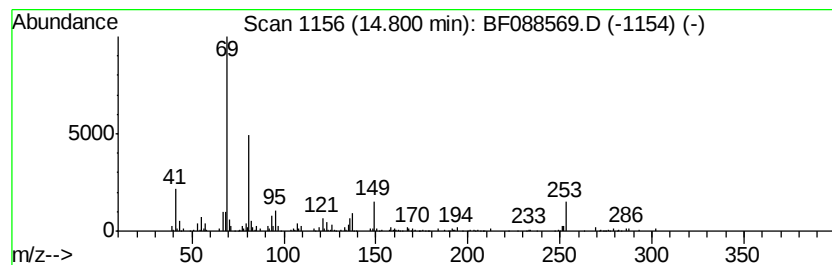
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 4,8,12-Tetradecatrienal, 5,... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.17 ng	86622	Perylene-d12	15.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	53
3			1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50
4			1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47
5			2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	47



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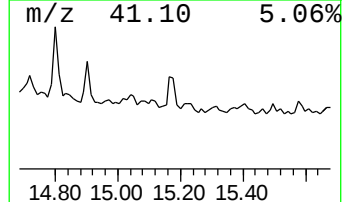
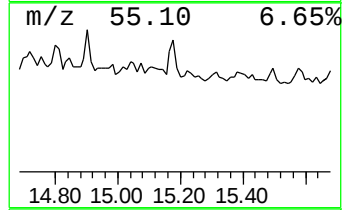
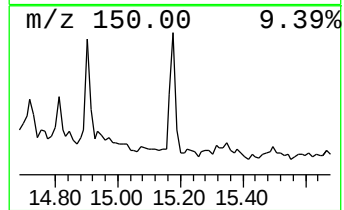
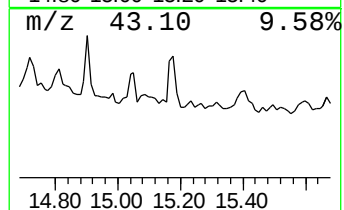
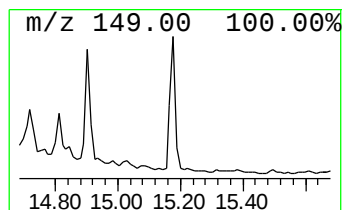
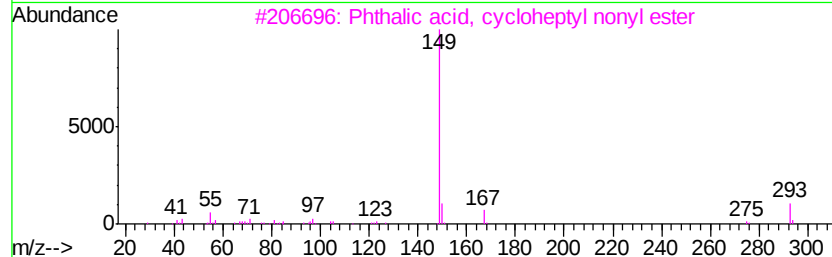
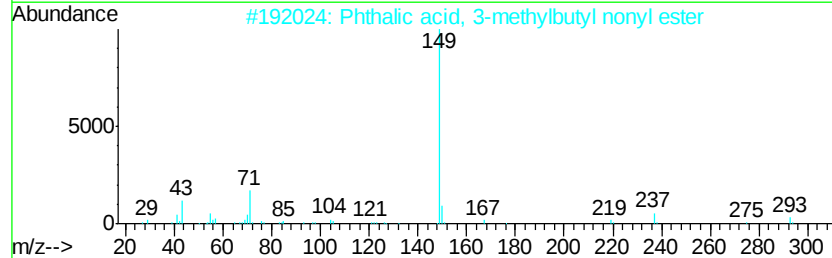
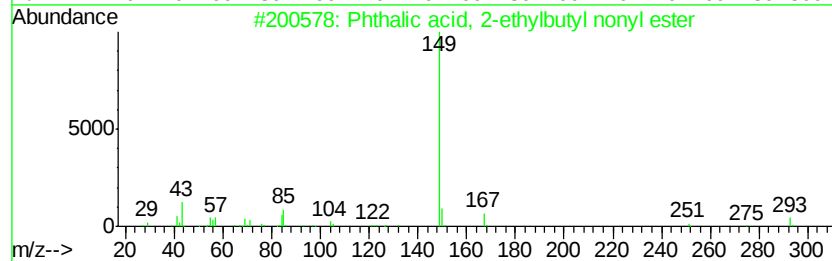
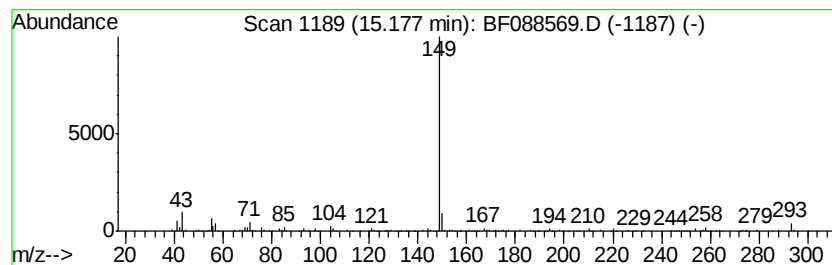
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Phthalic acid, 2-ethylbutyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	2.41 ng	96096	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 2-ethylbutyl nonyl...	376	C23H36O4	1000356-89-4	80
2		Phthalic acid, 3-methylbutyl non...	362	C22H34O4	1000356-81-0	80
3		Phthalic acid, cycloheptyl nonyl...	388	C24H36O4	1000322-83-4	72
4		Phthalic acid, 2-methylbutyl non...	362	C22H34O4	1000322-81-7	72
5		Phthalic acid, dodecyl pentyl ester	404	C25H40O4	1000308-93-0	72



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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, 2,2-dime...	1.68	186.8	ng	8277090	1	6.81	886205	20.0
unknown2.07	2.07	16.4	ng	726860	1	6.81	886205	20.0
Isopropyl Alcohol	3.13	21.3	ng	944658	1	6.81	886205	20.0
2-Pentanone, 4-hy...	4.99	5.4	ng	240188	1	6.81	886205	20.0
unknown6.57	6.57	73.6	ng	3260680	1	6.81	886205	20.0
n-Hexadecanoic acid	11.86	2.4	ng	156853	4	11.32	1301820	20.0
9-Octadecenoic ac...	12.43	7.9	ng	512470	4	11.32	1301820	20.0
1-Heneicosanol	13.82	3.3	ng	251514	5	13.94	1532580	20.0
4,8,12-Tetradecat...	14.80	2.2	ng	86622	6	15.35	796843	20.0
Phthalic acid, 2-...	15.18	2.4	ng	96096	6	15.35	796843	20.0