

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062218\
 Data File : BF106729.D
 Acq On : 23 Jun 2018 00:34
 Operator : JU/SJ
 Sample : J3573-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-49-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.207	484	488	497	rBB	94062	119799	8.04%	1.008%
2	5.607	551	556	559	rBV	1147283	1207712	81.10%	10.166%
3	6.601	720	725	736	rBV	1097663	1266799	85.07%	10.663%
4	6.736	743	748	751	rBV	1252472	1254566	84.24%	10.560%
5	6.960	782	786	789	rBV	343044	277138	18.61%	2.333%
6	7.119	808	813	816	rBV	1115153	1047204	70.32%	8.815%
7	7.525	876	882	885	rBV	836441	848149	56.95%	7.139%
8	8.242	1000	1004	1007	rBV	386297	330943	22.22%	2.786%
9	9.319	1181	1187	1190	rBV	1448727	1489190	100.00%	12.535%
10	9.707	1249	1253	1260	rVB	165777	149479	10.04%	1.258%
11	9.913	1285	1288	1292	rBV	19274	17747	1.19%	0.149%
12	10.001	1299	1303	1309	rVB	382498	351095	23.58%	2.955%
13	10.407	1370	1372	1375	rVB	32321	26244	1.76%	0.221%
14	10.795	1433	1438	1441	rBV	901319	813655	54.64%	6.849%
15	10.883	1450	1453	1460	rBV	32905	31222	2.10%	0.263%
16	11.489	1553	1556	1560	rBV	347764	303368	20.37%	2.554%
17	13.077	1821	1826	1829	rBV	1369135	1273584	85.52%	10.720%
18	13.595	1910	1914	1917	rBV	131563	106589	7.16%	0.897%
19	13.954	1971	1975	1982	rBV	107719	110548	7.42%	0.931%
20	14.142	2003	2007	2011	rVB	355569	328435	22.05%	2.765%
21	14.407	2049	2052	2056	rVB	46885	37701	2.53%	0.317%
22	14.601	2079	2085	2090	rBV2	26926	41056	2.76%	0.346%
23	15.065	2160	2164	2168	rBV2	29395	29487	1.98%	0.248%
24	15.677	2262	2268	2273	rBV	223534	286631	19.25%	2.413%
25	16.183	2352	2354	2363	rVB7	7742	15867	1.07%	0.134%
26	18.447	2732	2739	2748	rVB6	23980	56664	3.81%	0.477%
27	18.689	2774	2780	2781	rBV5	11421	18858	1.27%	0.159%
28	18.765	2790	2793	2802	rVB7	16374	40273	2.70%	0.339%

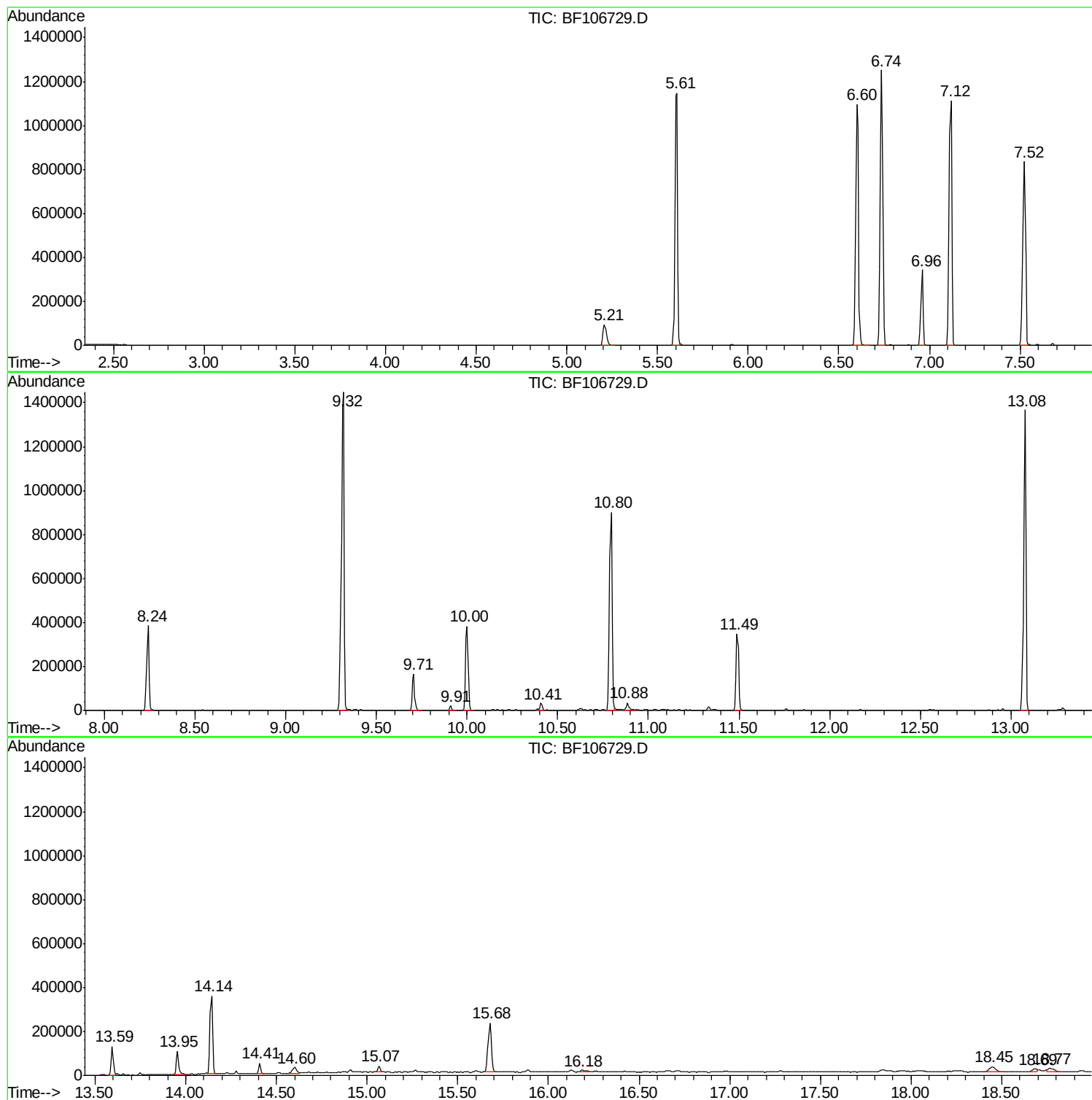
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ClientSampleId :
SB-49-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.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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ClientSampled :
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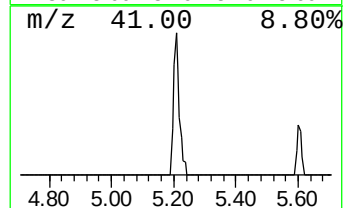
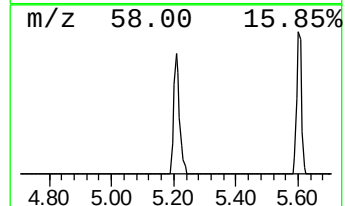
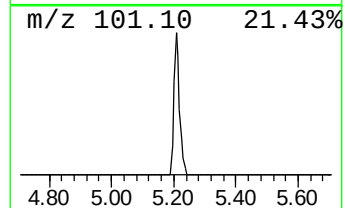
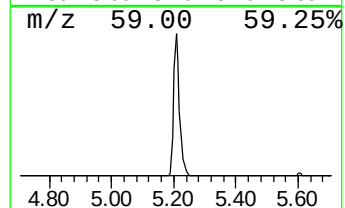
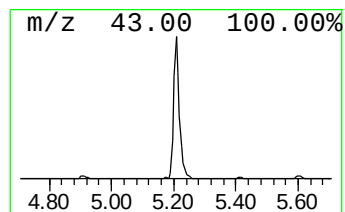
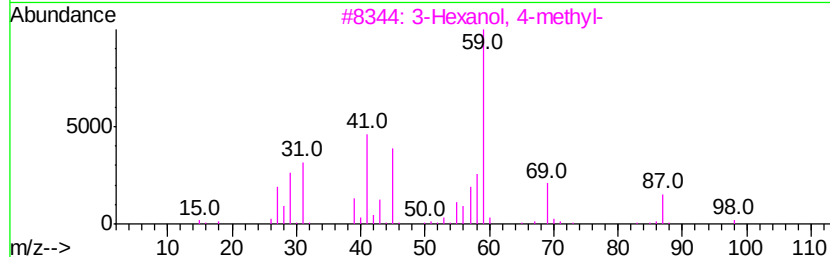
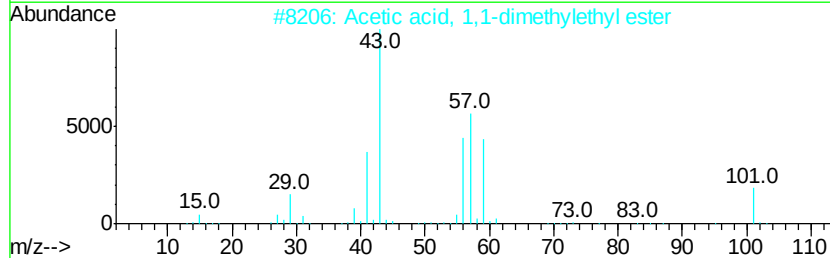
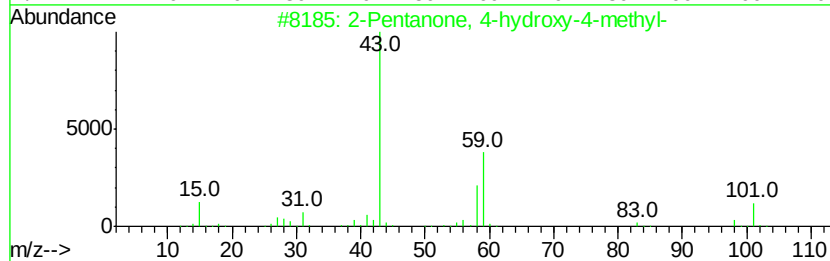
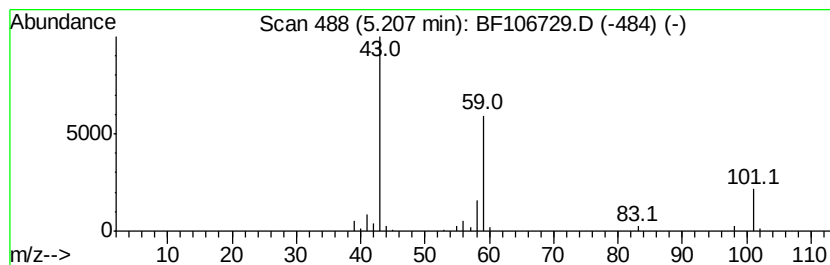
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	8.65 ng	119799	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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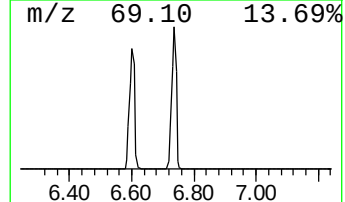
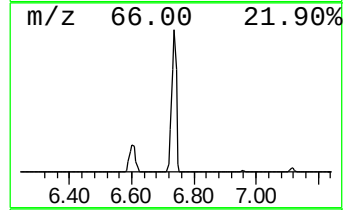
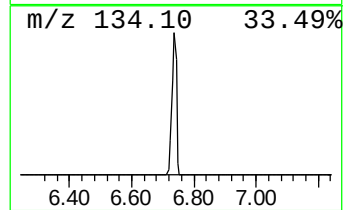
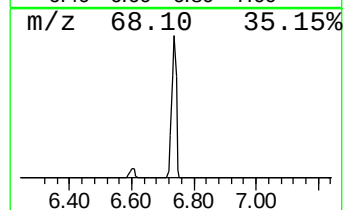
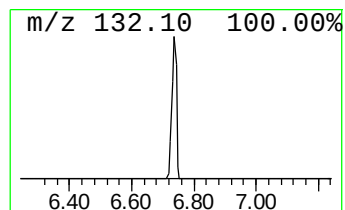
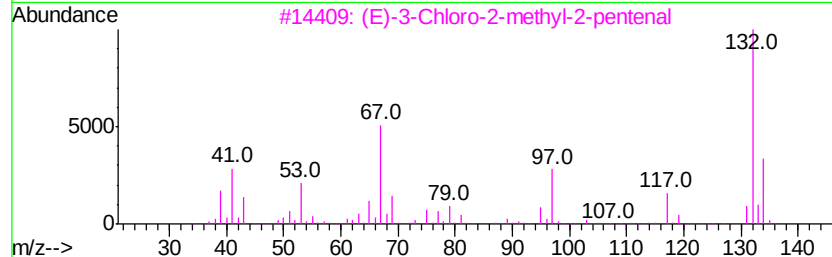
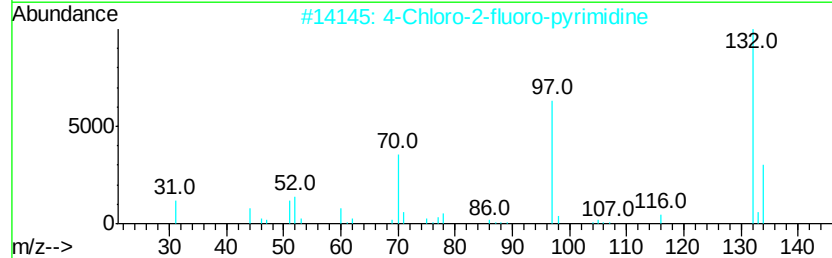
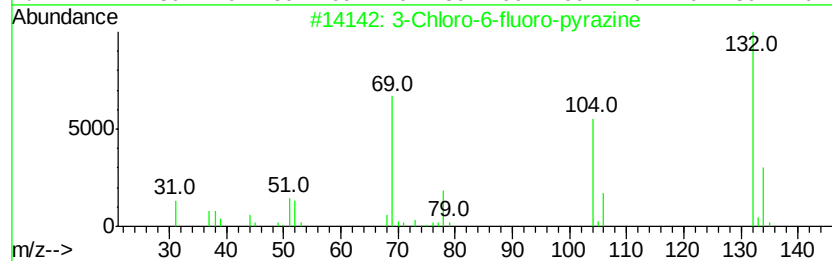
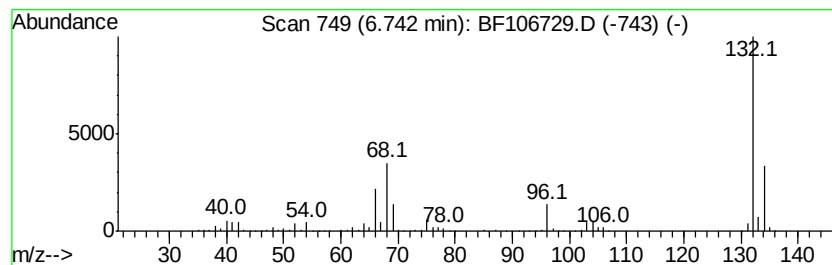
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	90.54 ng	1254570	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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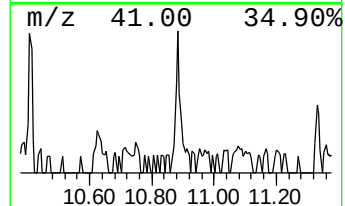
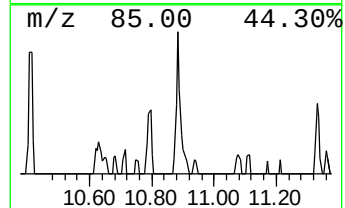
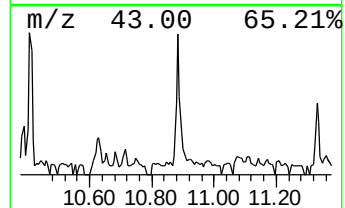
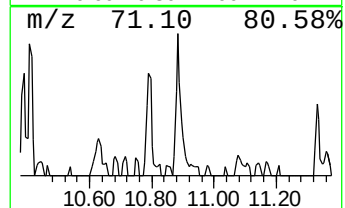
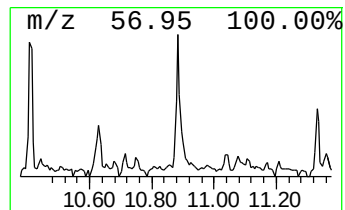
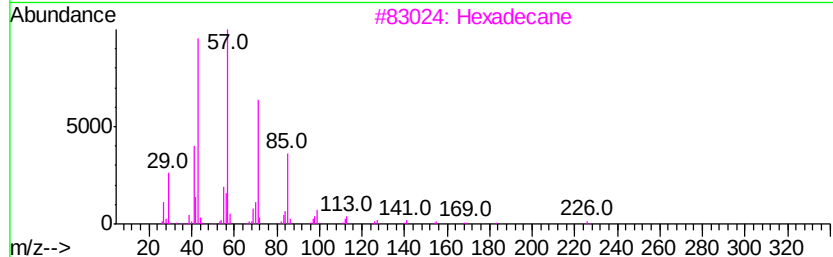
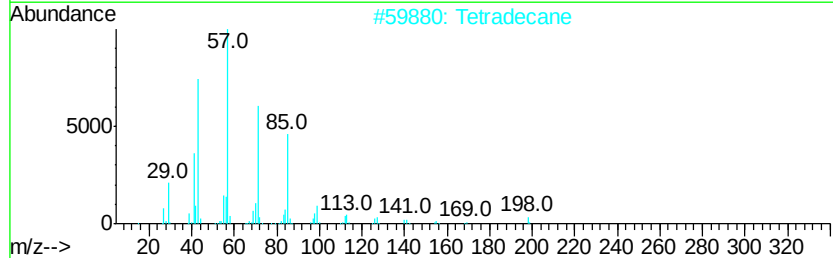
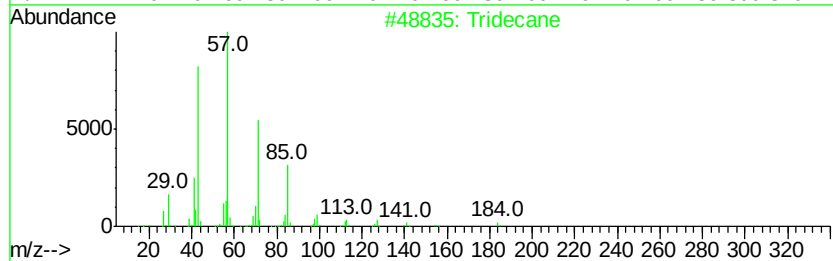
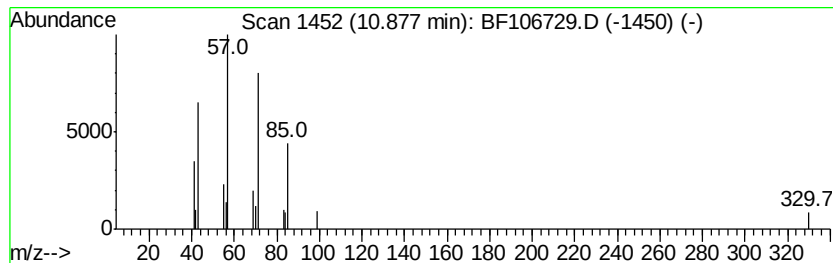
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.06 ng	31222	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	78
2		Tetradecane	198	C14H30	000629-59-4	78
3		Hexadecane	226	C16H34	000544-76-3	78
4		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	78
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72



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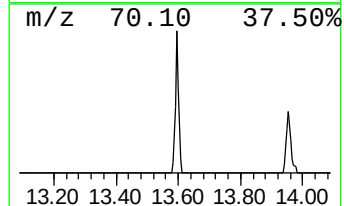
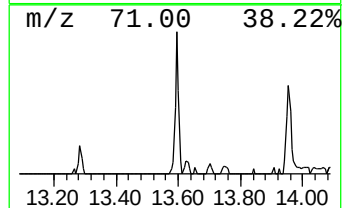
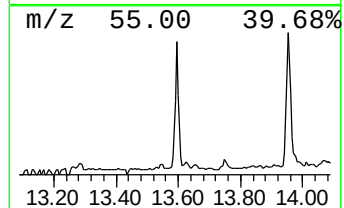
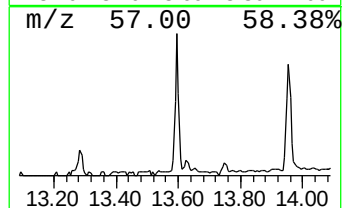
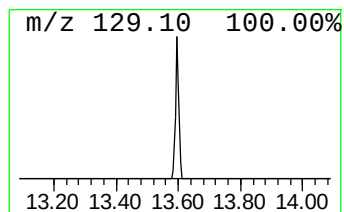
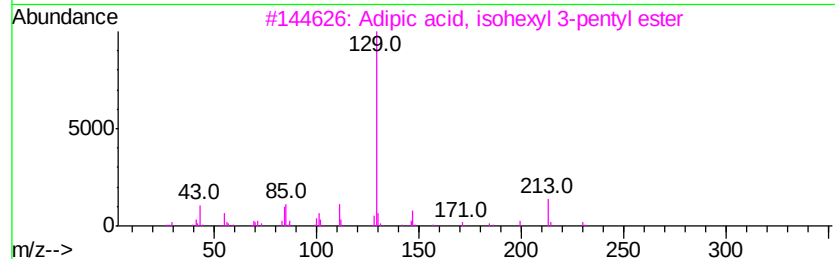
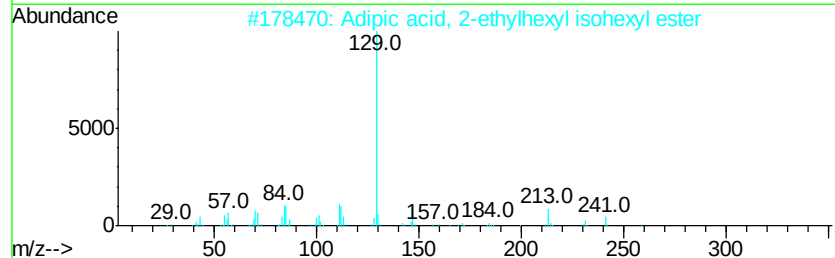
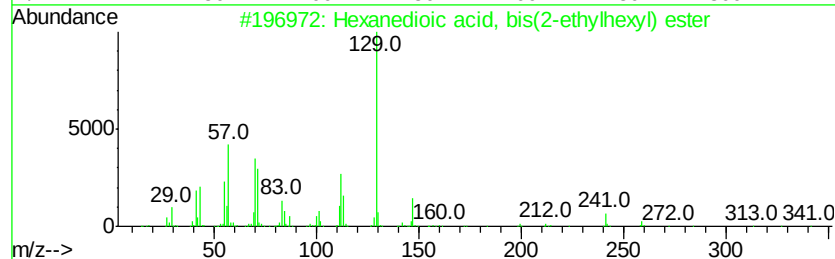
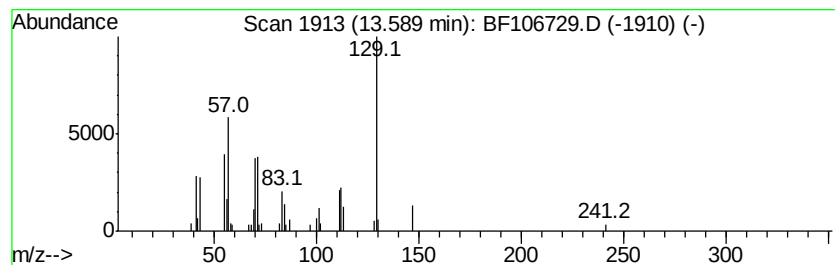
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Peak Number 5 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	6.49 ng	106589	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2		Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	50
3		Adipic acid, isohexyl 3-pentyl e...	300	C17H32O4	1000324-60-7	47
4		Adipic acid, isobutyl 2-methylbu...	272	C15H28O4	1000324-67-1	47
5		Adipic acid, isohexyl 2-octyl ester	342	C20H38O4	1000324-44-8	43



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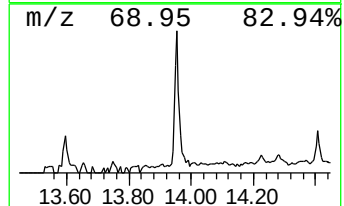
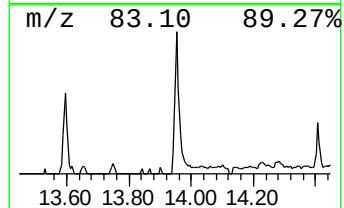
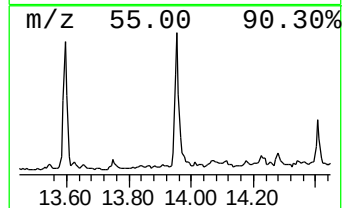
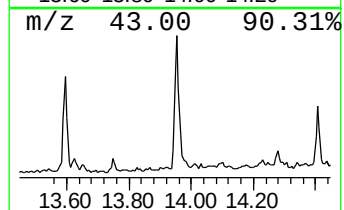
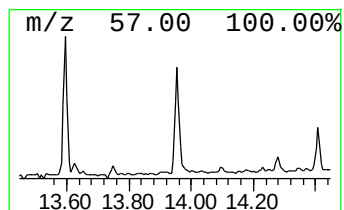
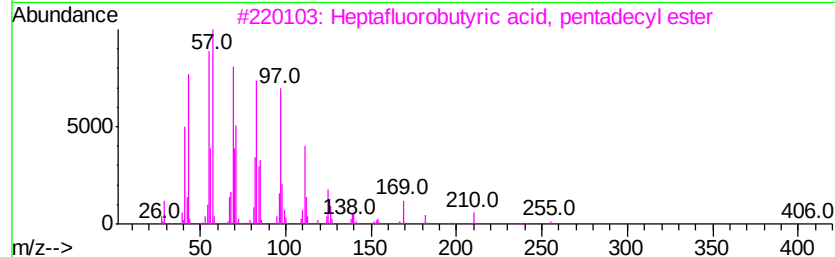
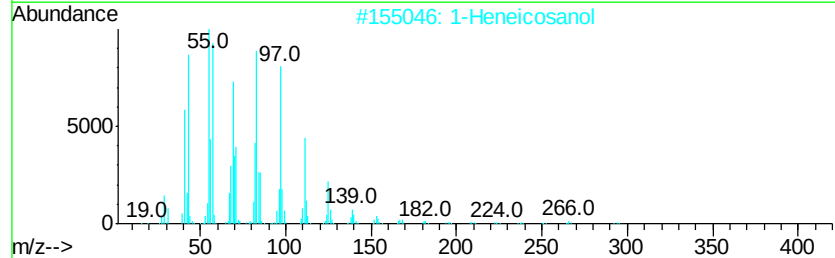
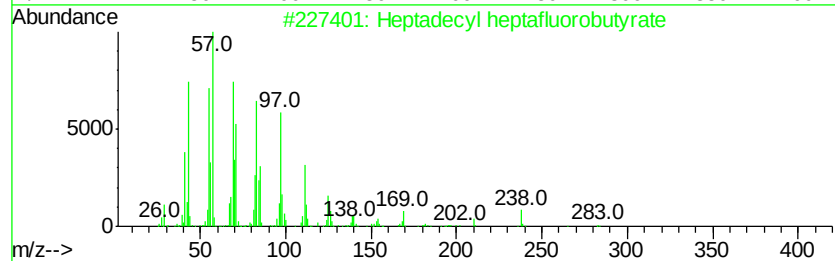
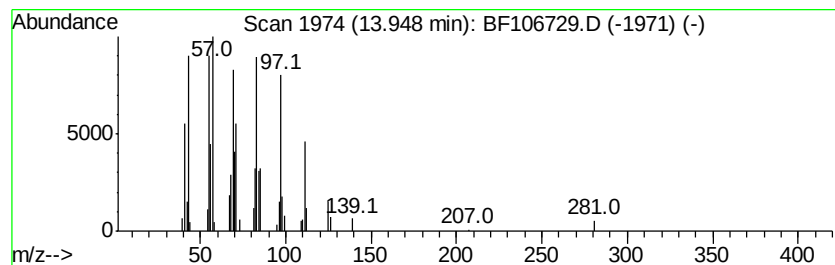
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	6.73 ng	110548	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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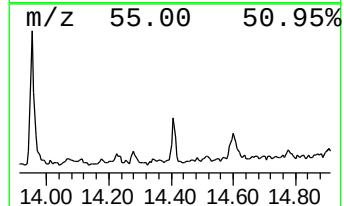
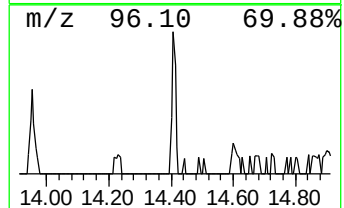
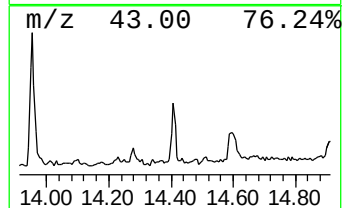
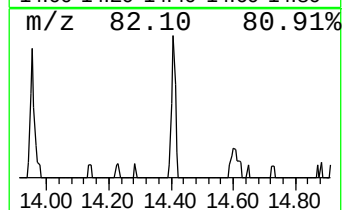
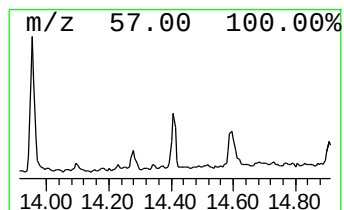
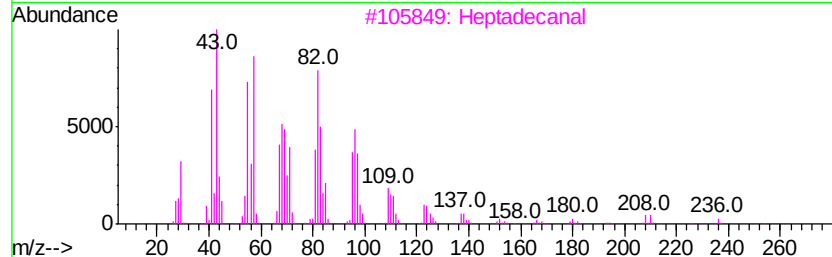
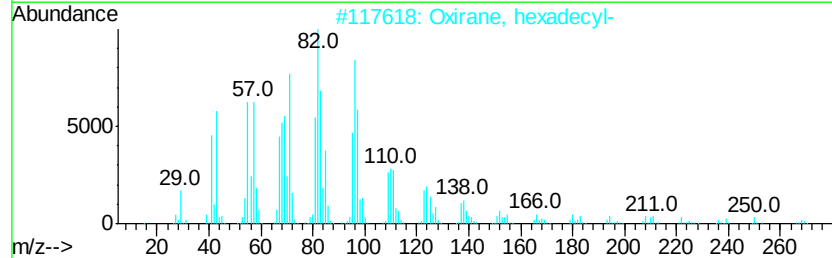
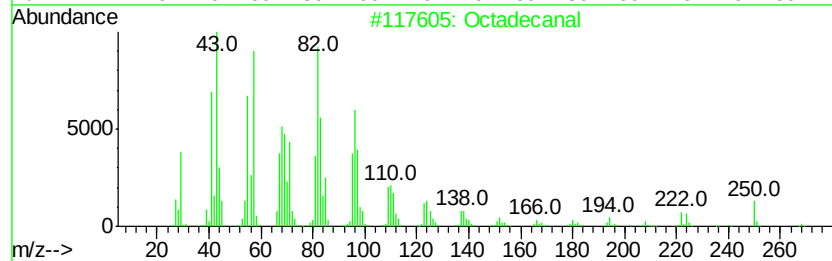
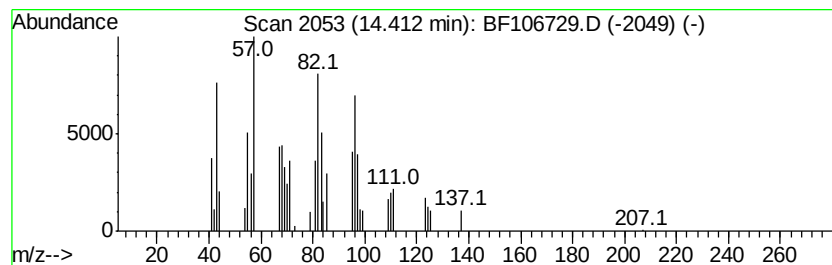
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.30 ng	37701	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	91
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Heptadecanal	254	C17H34O	1000376-70-0	91
4		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5		Pentadecanal	226	C15H30O	002765-11-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062218\
Data File : BF106729.D
Acq On : 23 Jun 2018 00:34
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49-COMP

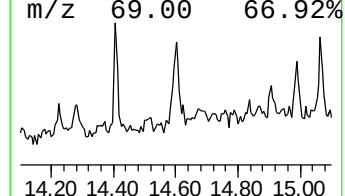
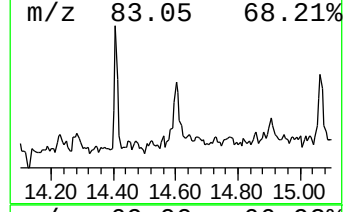
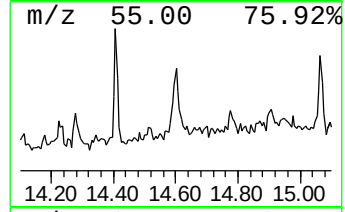
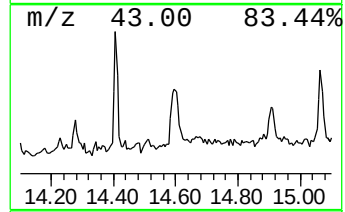
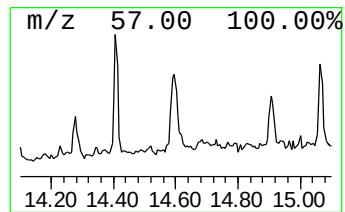
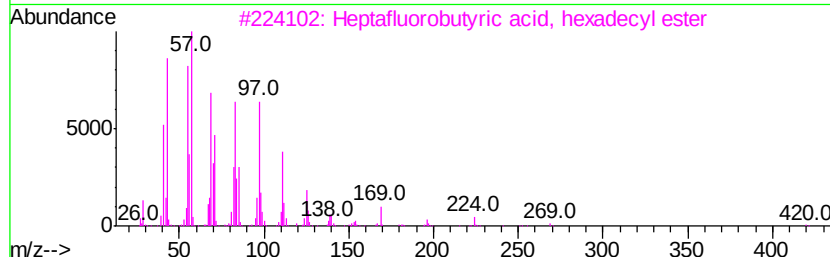
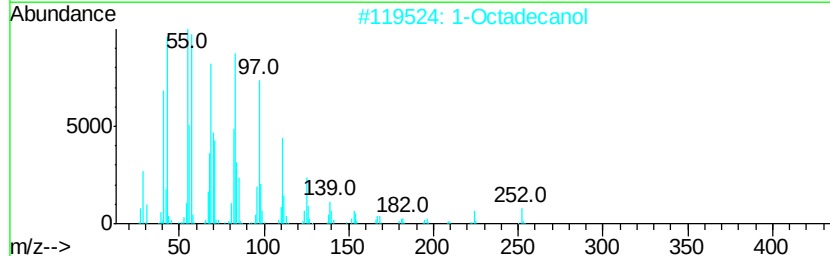
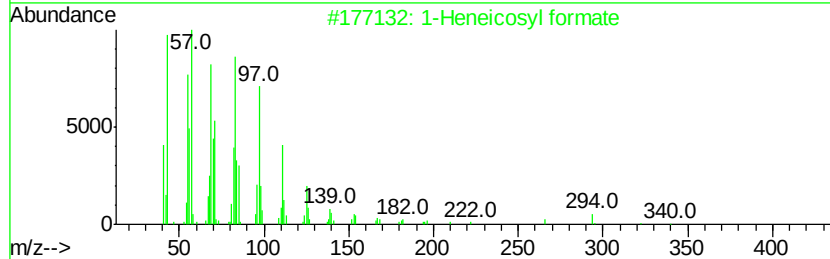
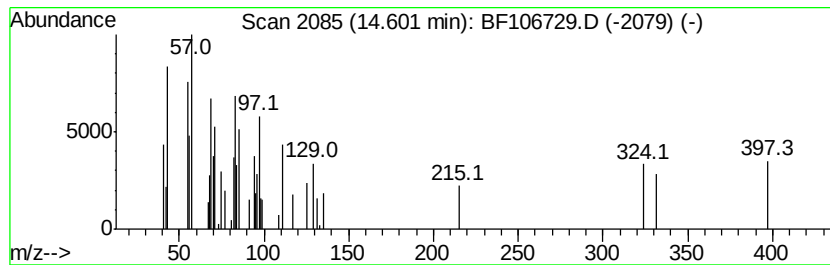
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.60 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.50 ng	41056	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	46
2		1-Octadecanol	270	C18H38O	000112-92-5	46
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	45
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	41
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062218\
Data File : BF106729.D
Acq On : 23 Jun 2018 00:34
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Sample : J3573-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

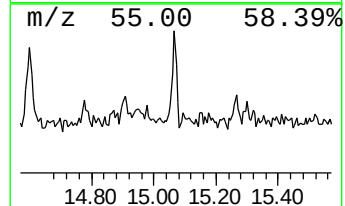
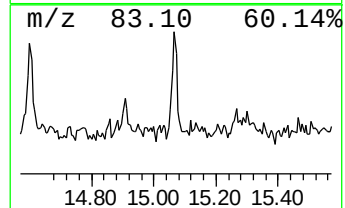
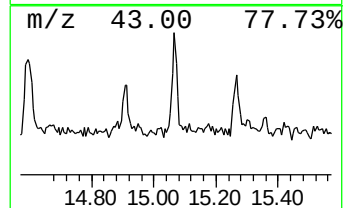
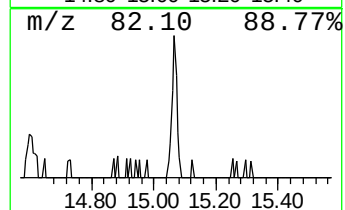
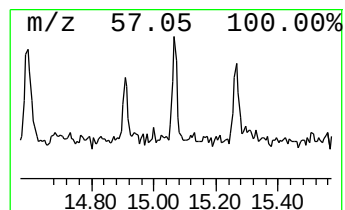
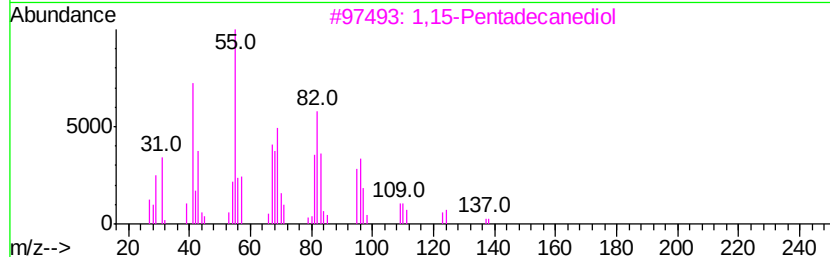
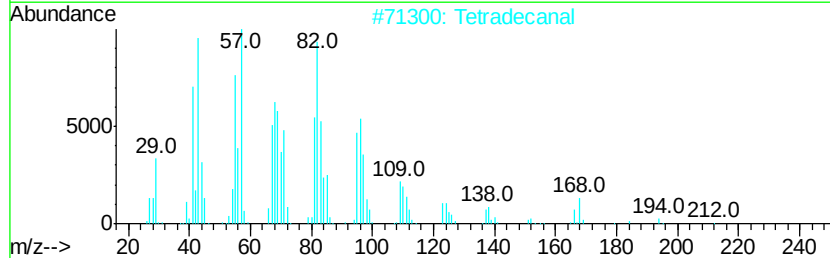
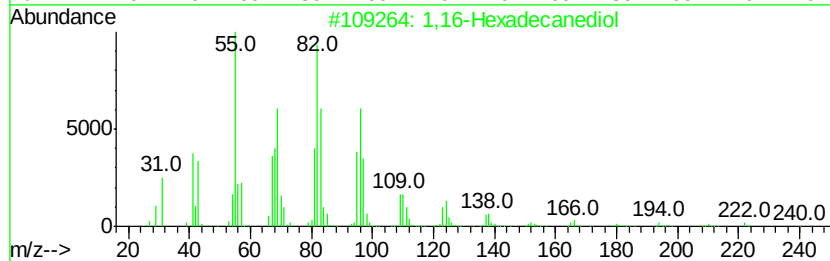
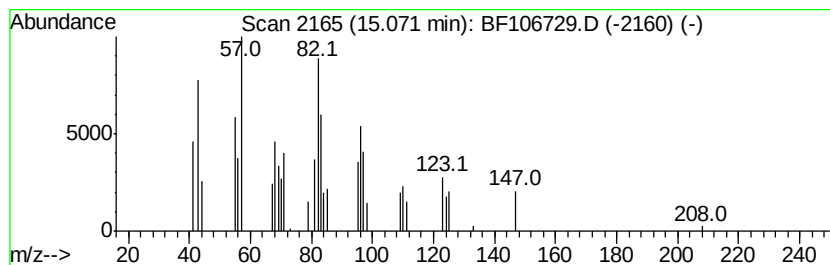
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,16-Hexadecanediol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.07	2.06 ng	29487	Perylene-d12	15.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	72
2	Tetradecanal	212	C14H28O	000124-25-4	72
3	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	58
4	Pentadecanal-	226	C15H30O	002765-11-9	50
5	trans-11-Tetradecenyl acetate	254	C16H30O2	033189-72-9	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062218\
Data File : BF106729.D
Acq On : 23 Jun 2018 00:34
Operator : JU/SJ
Sample : J3573-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49-COMP

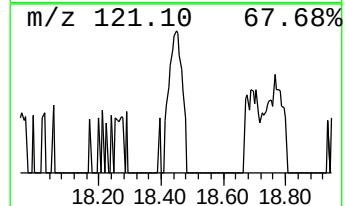
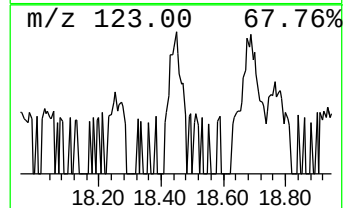
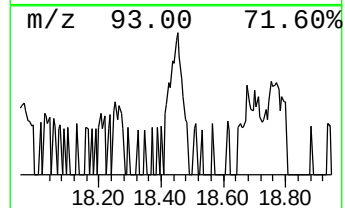
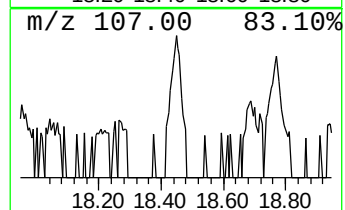
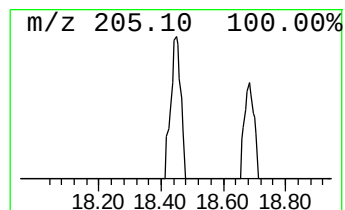
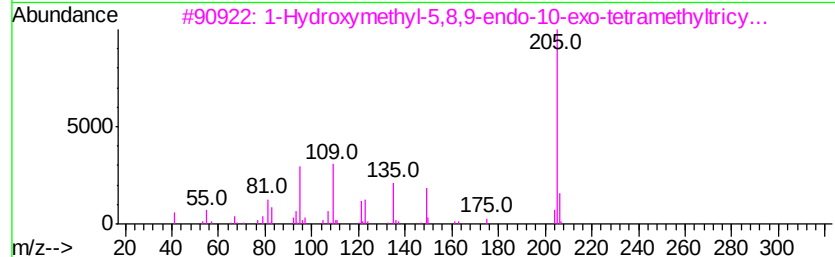
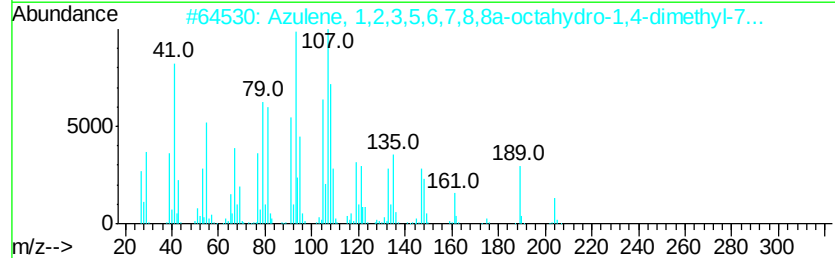
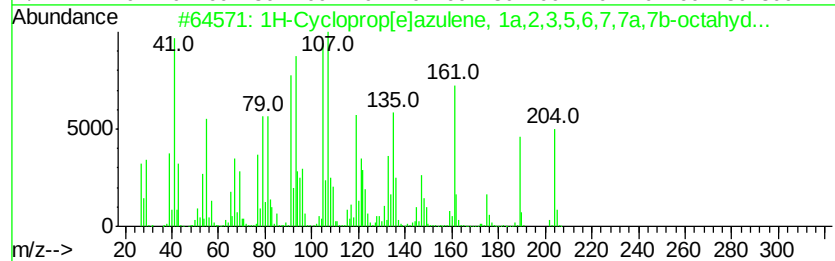
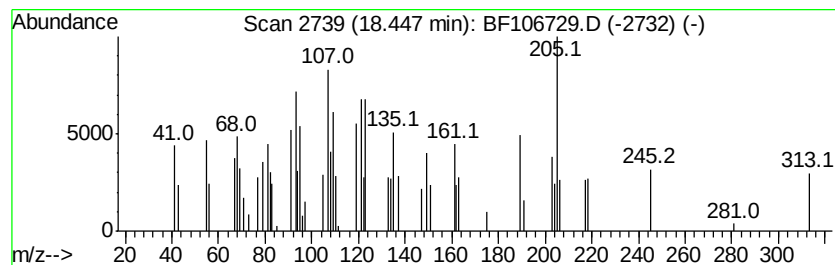
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.45	3.95 ng	56664	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Cycloprop[elazulene, 1a,2,3,5...	204	C15H24	021747-46-6	55
2		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	38
3		1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	35
4		But-3-enal, 2-methyl-4-(2,6,6-tr...	206	C14H22O	104900-59-6	22
5		Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062218\
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Acq On : 23 Jun 2018 00:34
Operator : JU/SJ
Sample : J3573-04
Misc :
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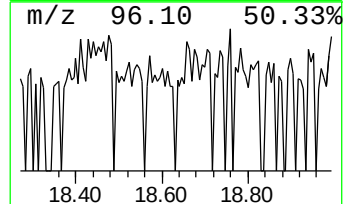
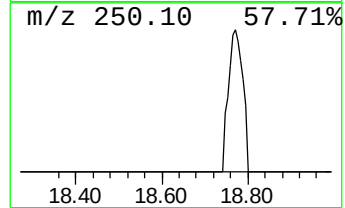
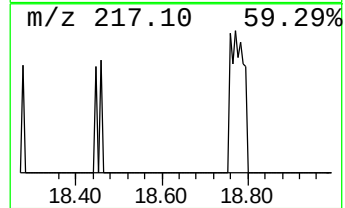
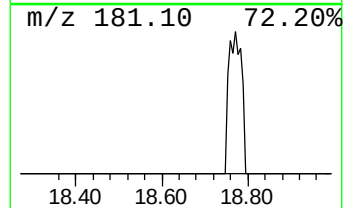
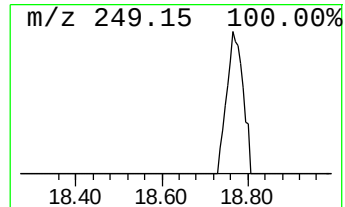
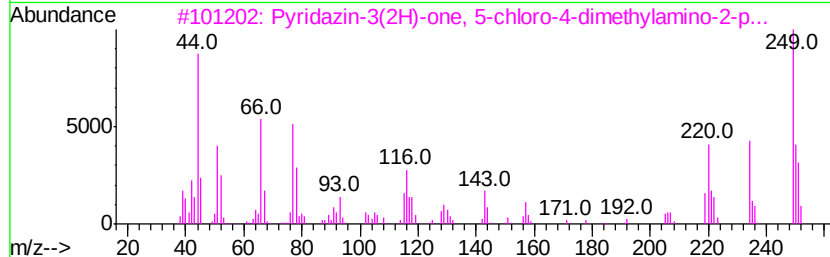
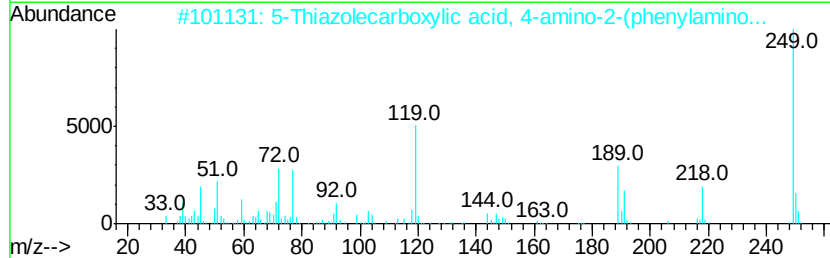
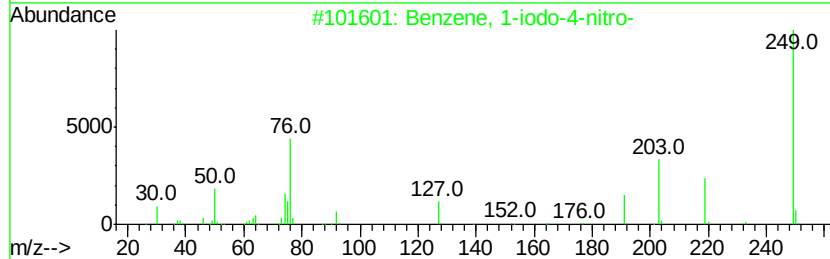
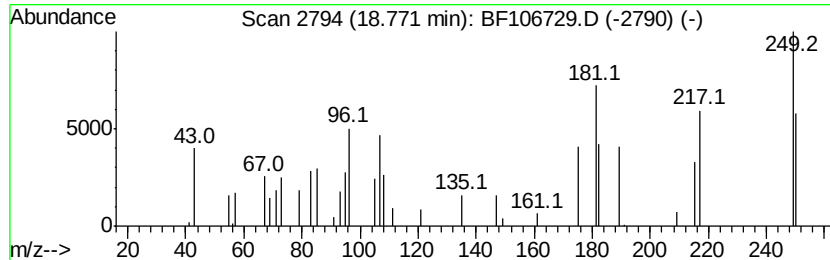
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, 1-iodo-4-nitro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.77	2.81 ng	40273	Perylene-d12	15.68		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-iodo-4-nitro-	249	C6H4IN02	000636-98-6	9
2		5-Thiazolecarboxylic acid, 4-ami...	249	C11H11N3O2S	1000362-79-7	9
3		Pyridazin-3(2H)-one, 5-chloro-4-...	249	C12H12ClN3O	091396-18-8	9
4		12H-Benzo[alphenothiazine	249	C16H11NS	000225-83-2	9
5		Benzene, 1-nitro-2-hydroxy-4-(p-...	249	C12H8FN04	189214-56-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062218\
 Data File : BF106729.D
 Acq On : 23 Jun 2018 00:34
 Operator : JU/SJ
 Sample : J3573-04
 Misc :
 ALS Vial : 21 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\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	8.7	ng	119799	1	6.96	277138	20.0
unknown6.74	6.74	90.5	ng	1254570	1	6.96	277138	20.0
Tridecane	10.88	2.1	ng	31222	4	11.49	303368	20.0
Hexanedioic acid,...	13.59	6.5	ng	106589	5	14.14	328435	20.0
Heptadecyl heptaf...	13.95	6.7	ng	110548	5	14.14	328435	20.0
Octadecanal	14.41	2.3	ng	37701	5	14.14	328435	20.0
unknown14.60	14.60	2.5	ng	41056	5	14.14	328435	20.0
1,16-Hexadecanediol	15.07	2.1	ng	29487	6	15.68	286631	20.0
1H-Cycloprop[e]az...	18.45	4.0	ng	56664	6	15.68	286631	20.0
Benzene, 1-iodo-4...	18.77	2.8	ng	40273	6	15.68	286631	20.0