

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
 Data File : BF092219.D
 Acq On : 12 Jan 2017 20:39
 Operator : UM/SJ
 Sample : I1030-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0013

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	4.721	245	248	260	rBV	1455495	2154092	41.87%	4.862%
2	5.190	287	289	303	rBV	4296141	4512823	87.73%	10.185%
3	6.264	380	383	385	rBV	4591880	5144148	100.00%	11.610%
4	6.367	390	392	395	rVV	4857068	4536140	88.18%	10.238%
5	6.596	410	412	414	rBV	1240623	1211793	23.56%	2.735%
6	6.744	423	425	428	rBV	2795605	3433366	66.74%	7.749%
7	7.167	459	462	464	rBV	3044277	3190500	62.02%	7.201%
8	7.876	522	524	527	rBV	1409243	1553634	30.20%	3.507%
9	8.962	616	619	621	rBV	4935439	4725109	91.85%	10.665%
10	9.362	651	654	656	rBV	1042654	909801	17.69%	2.053%
11	9.625	675	677	680	rBV	1364560	1378395	26.80%	3.111%
12	10.082	715	717	718	rVB	60809	72871	1.42%	0.164%
13	10.413	744	746	749	rBV2	1954167	2617532	50.88%	5.908%
14	10.551	756	758	762	rBV	115384	147785	2.87%	0.334%
15	10.996	795	797	798	rBV2	73326	76242	1.48%	0.172%
16	11.099	804	806	809	rBV	981544	1384154	26.91%	3.124%
17	11.659	853	855	859	rBV2	468474	441419	8.58%	0.996%
18	12.436	921	923	929	rBV2	130303	177526	3.45%	0.401%
19	12.539	929	932	934	rVB	52621	73887	1.44%	0.167%
20	12.688	943	945	948	rBV	2853424	3490706	67.86%	7.879%
21	13.602	1022	1025	1034	rBV	243761	360927	7.02%	0.815%
22	13.728	1034	1036	1039	rBV	877000	966664	18.79%	2.182%
23	14.231	1076	1080	1088	rBV2	56434	149674	2.91%	0.338%
24	14.585	1109	1111	1113	rVB	52450	58768	1.14%	0.133%
25	14.814	1129	1131	1132	rBV	45875	56378	1.10%	0.127%
26	14.837	1132	1133	1138	rVB2	39760	70624	1.37%	0.159%
27	15.088	1153	1155	1158	rBV	722008	881475	17.14%	1.989%
28	15.500	1188	1191	1193	rBV	52855	72354	1.41%	0.163%
29	15.557	1193	1196	1198	rBV2	31805	72484	1.41%	0.164%
30	16.448	1272	1274	1280	rVV5	35004	74373	1.45%	0.168%
31	16.585	1284	1286	1292	rVB	83304	168232	3.27%	0.380%
32	16.814	1302	1306	1311	rVB8	32000	78644	1.53%	0.178%
33	17.648	1375	1379	1384	rBV5	20335	63882	1.24%	0.144%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

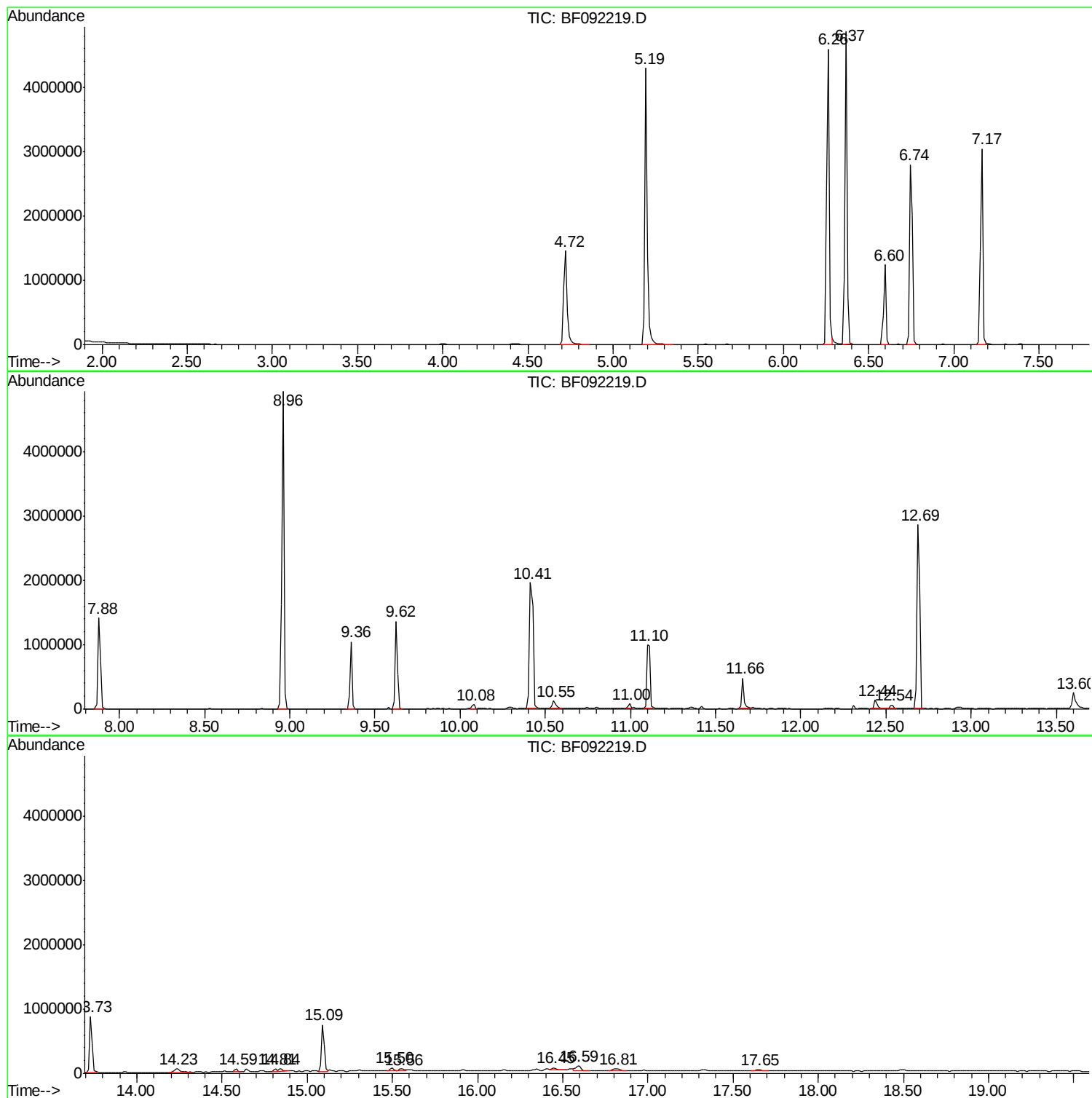
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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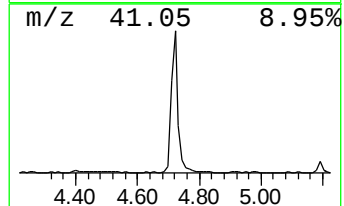
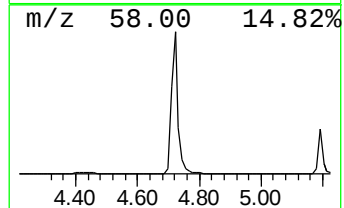
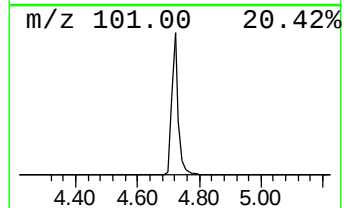
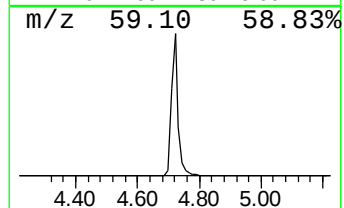
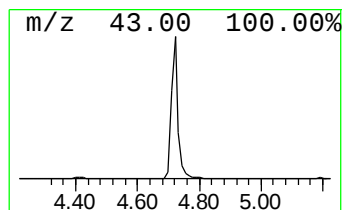
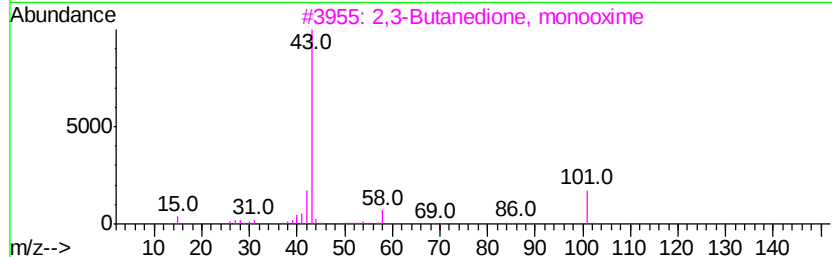
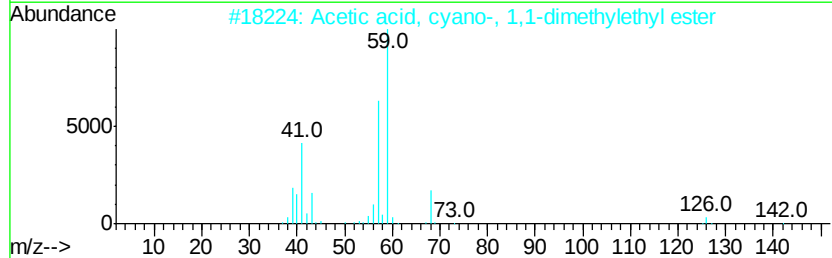
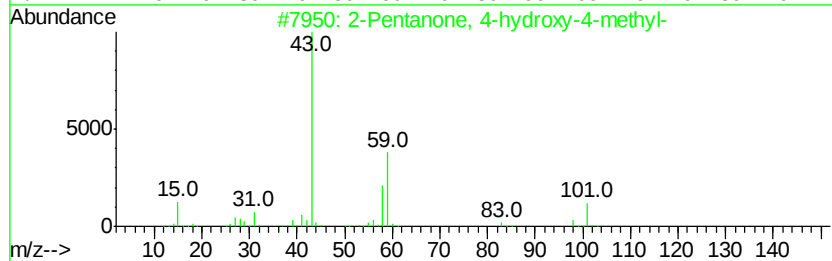
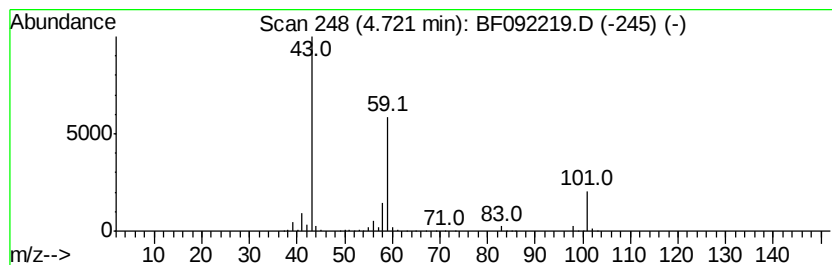
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	35.55 ng	2154090	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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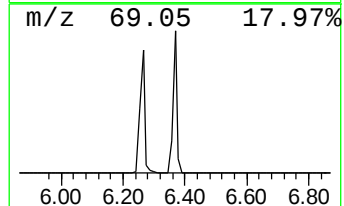
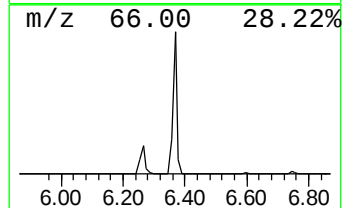
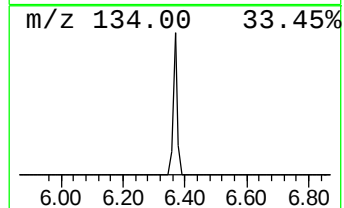
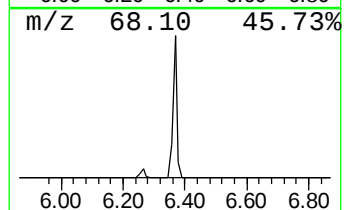
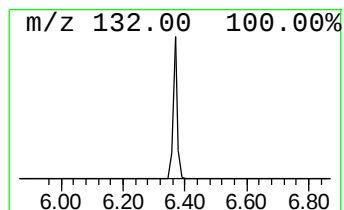
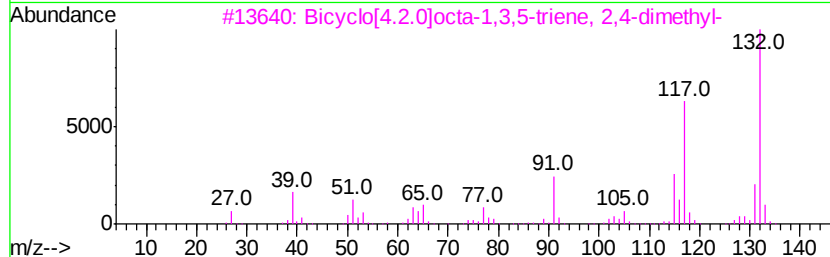
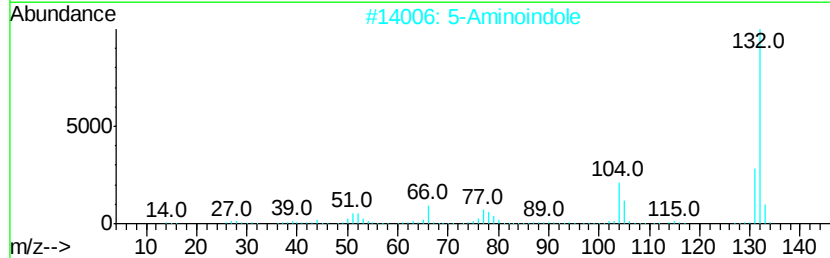
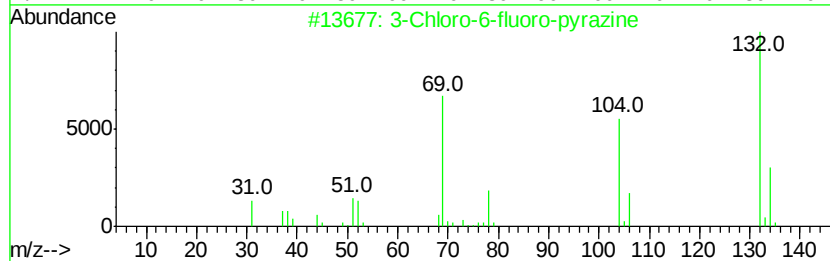
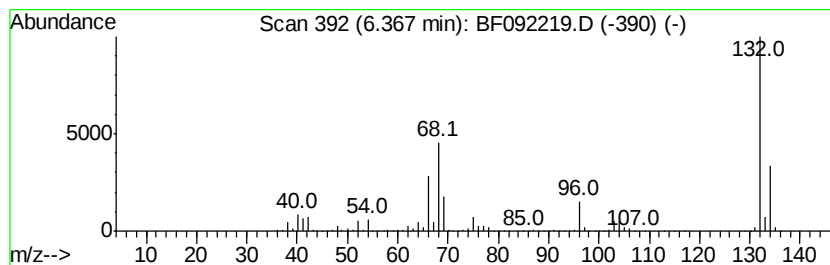
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	74.87 ng	4536140	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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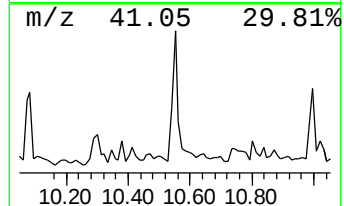
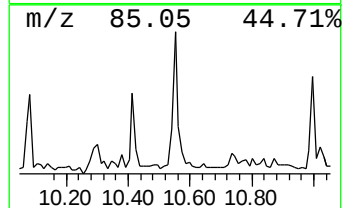
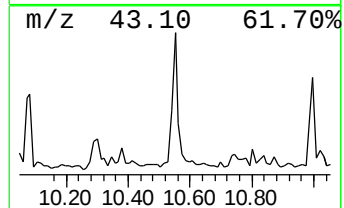
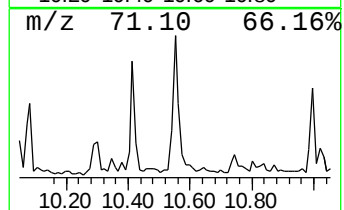
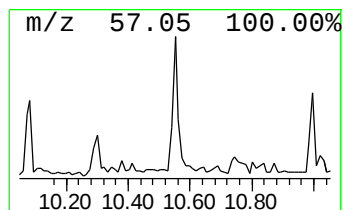
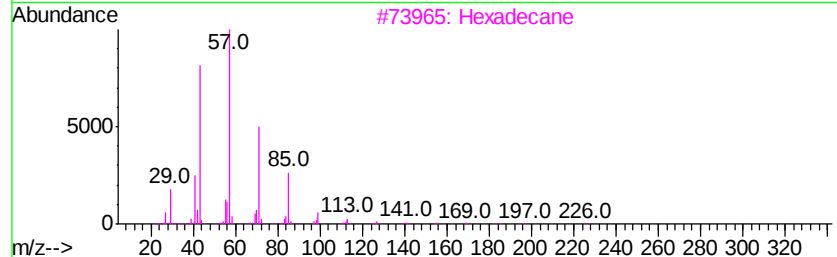
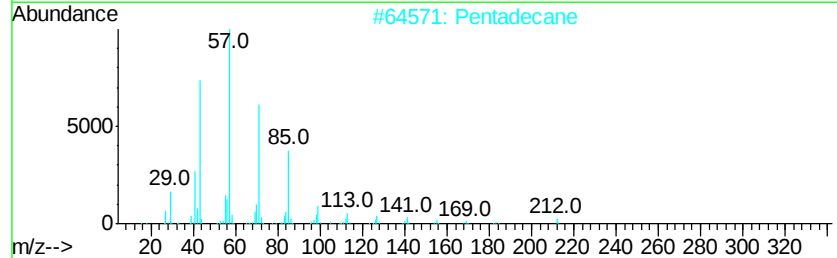
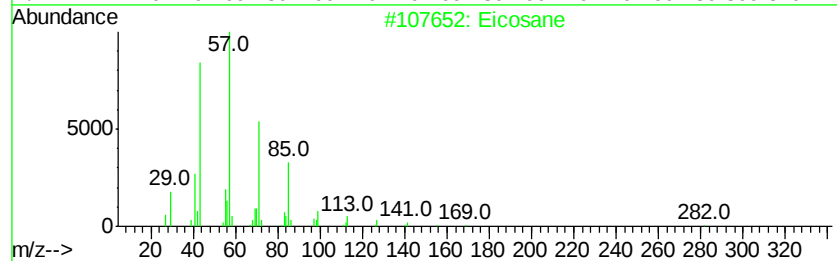
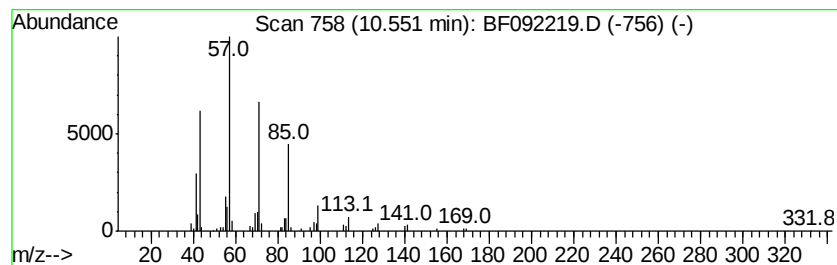
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.14 ng	147785	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Pentadecane		212	C15H32	000629-62-9	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Heneicosane		296	C21H44	000629-94-7	90
5	Tritetracontane		605	C43H88	007098-21-7	90



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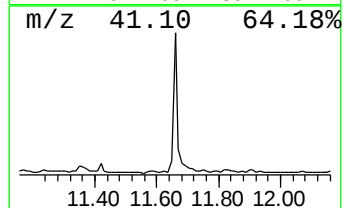
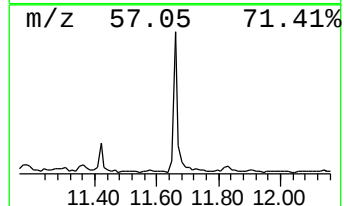
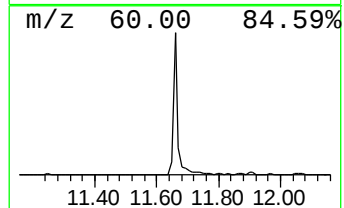
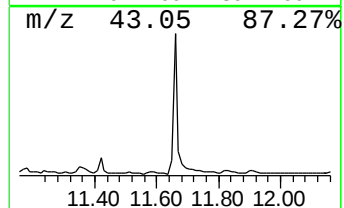
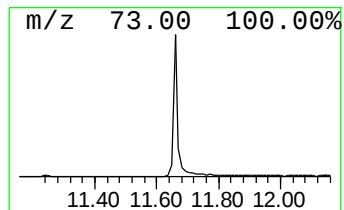
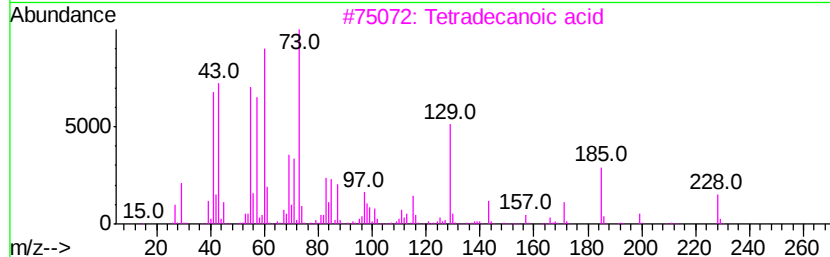
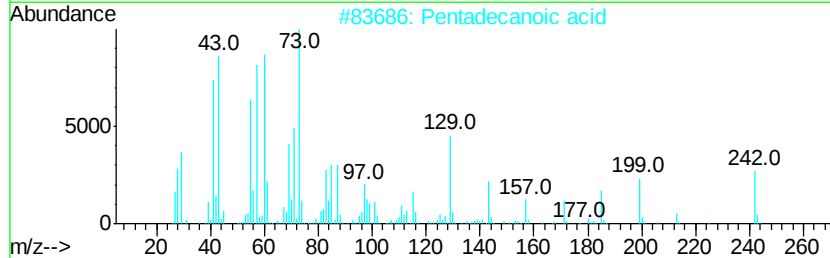
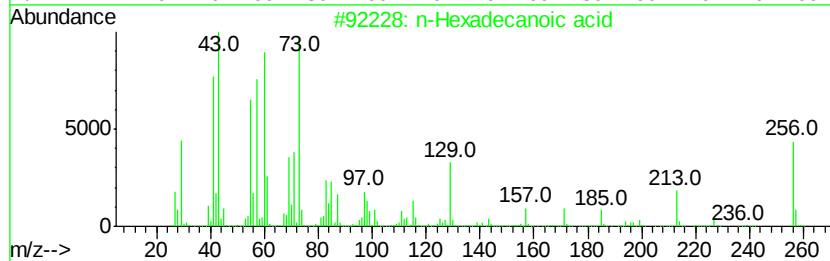
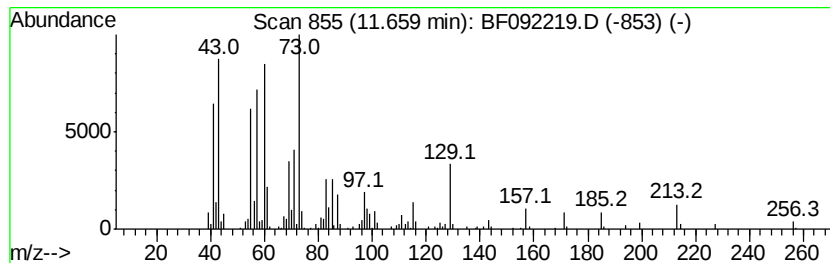
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	6.38 ng	441419	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	25



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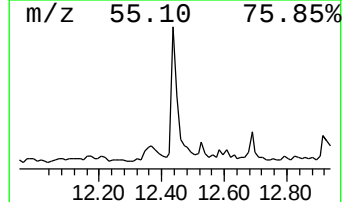
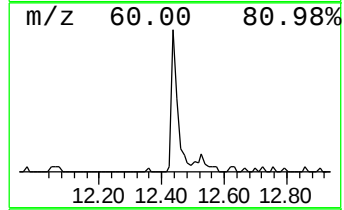
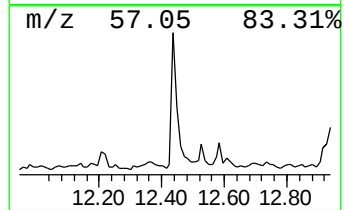
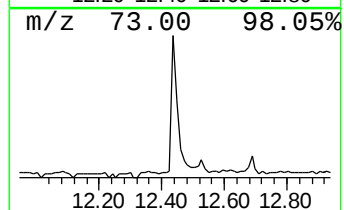
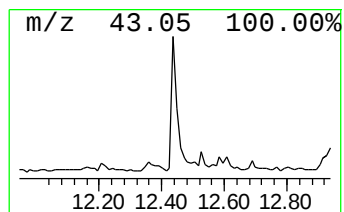
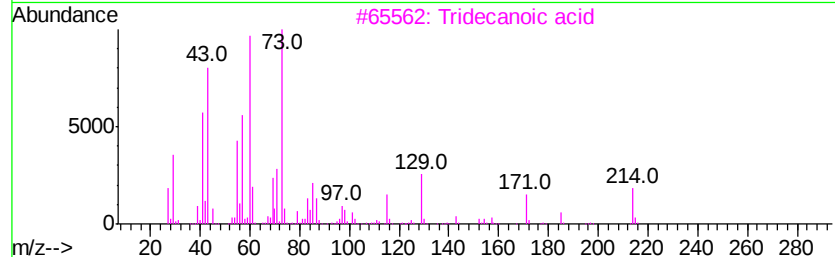
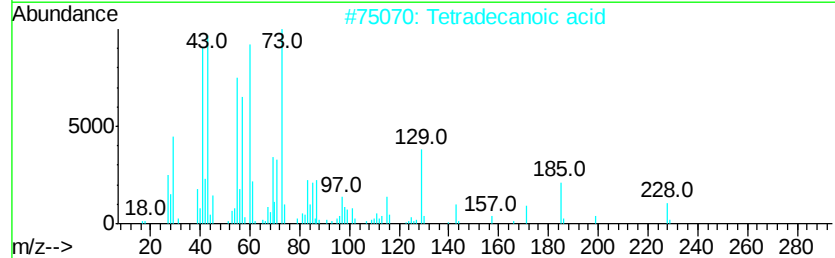
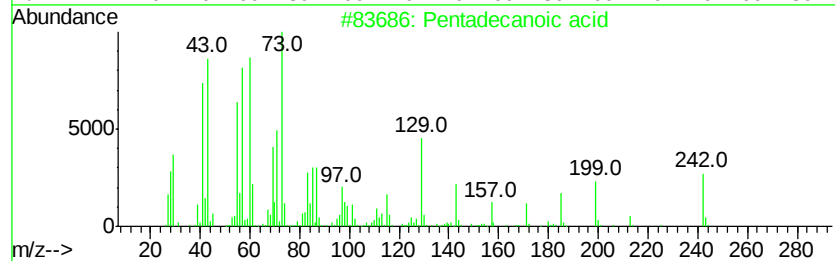
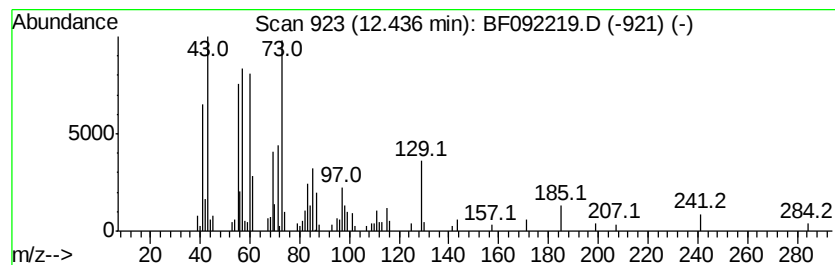
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	3.67 ng	177526	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3		Tridecanoic acid	214	C13H26O2	000638-53-9	46
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	15
5		Undecane	156	C11H24	001120-21-4	11



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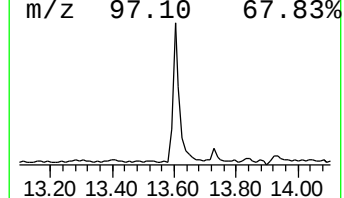
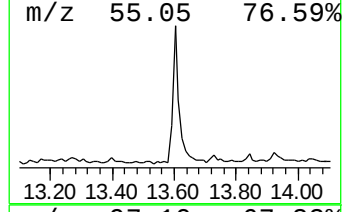
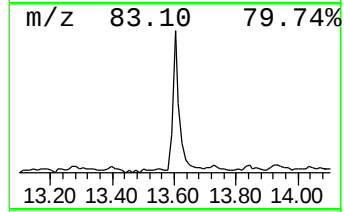
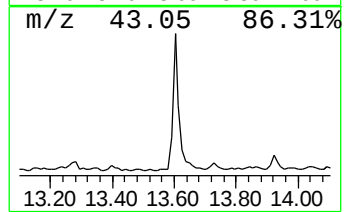
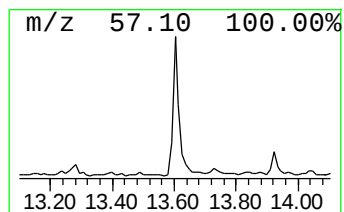
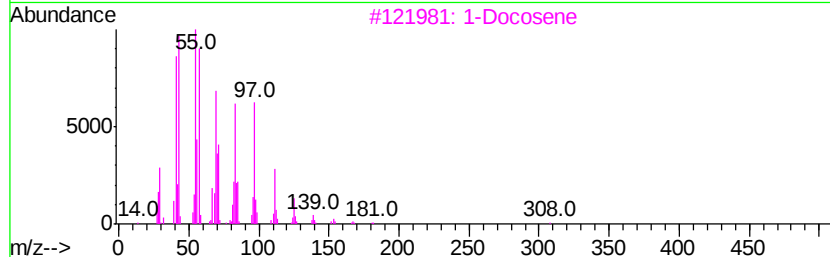
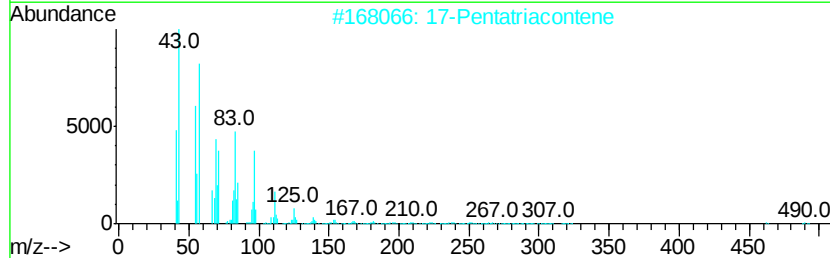
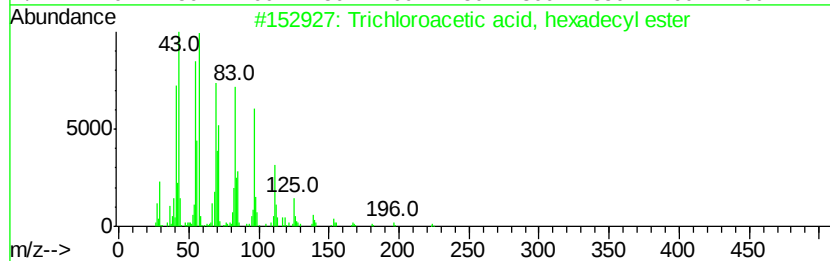
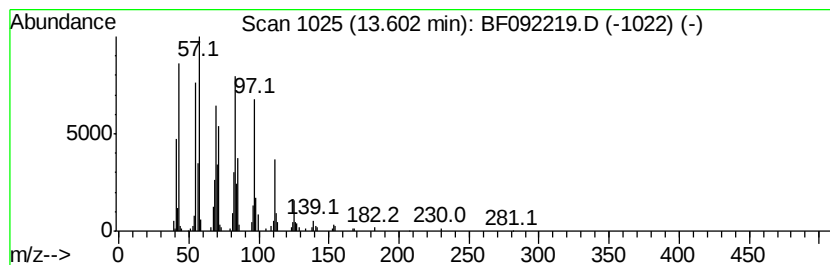
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	7.47 ng	360927	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		1-Docosene	308	C22H44	001599-67-3	90
4		1-Tetracosanol	354	C24H50O	000506-51-4	90
5		1-Pentadecanol	228	C15H32O	000629-76-5	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092219.D
Acq On : 12 Jan 2017 20:39
Operator : UM/SJ
Sample : I1030-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0013

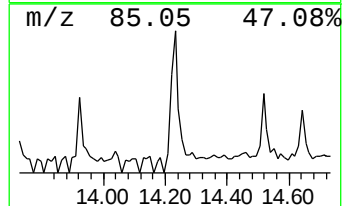
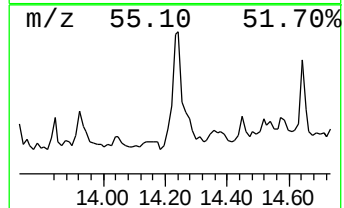
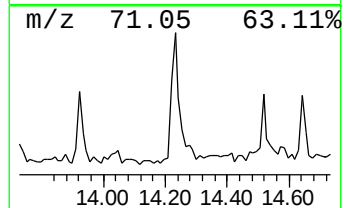
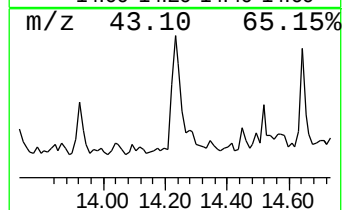
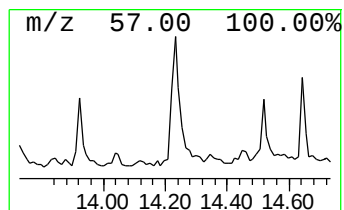
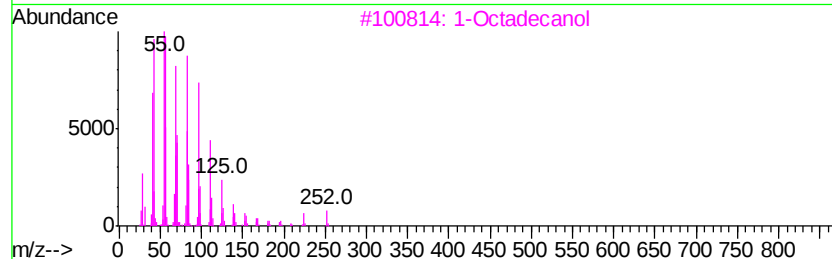
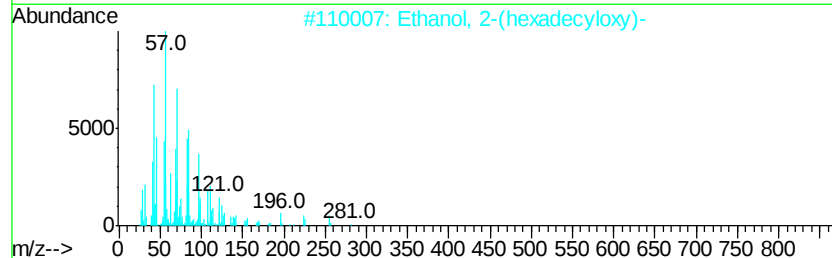
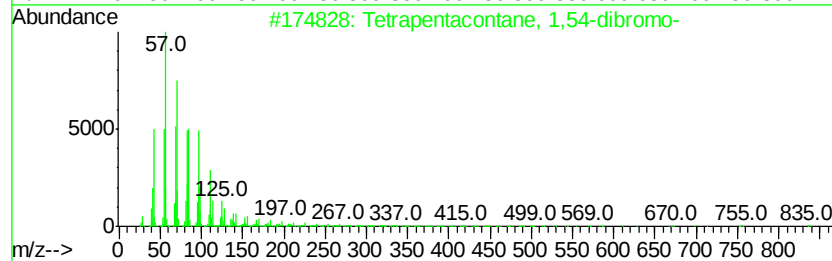
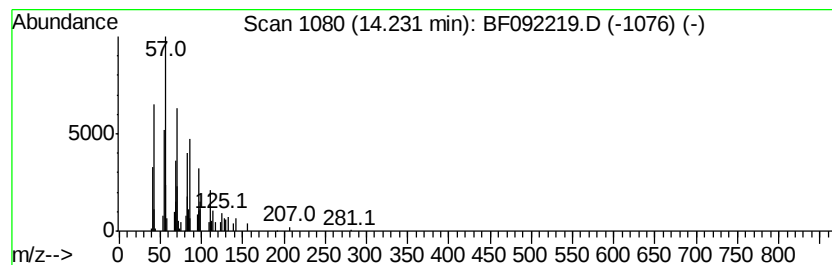
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetrapentacontane, 1,54-dib... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	3.10 ng	149674	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	86
2		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	80
3		1-Octadecanol	270	C18H38O	000112-92-5	60
4		1-Docosene	308	C22H44	001599-67-3	58
5		17-Pentatriacontene	491	C35H70	006971-40-0	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092219.D
Acq On : 12 Jan 2017 20:39
Operator : UM/SJ
Sample : I1030-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0013

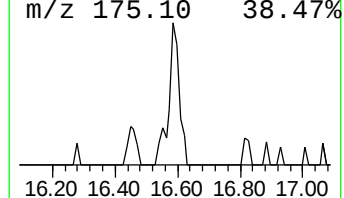
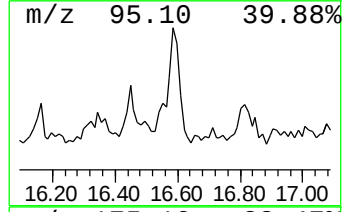
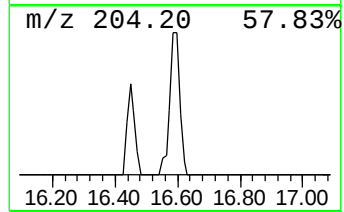
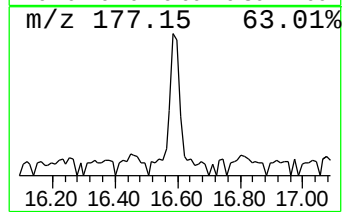
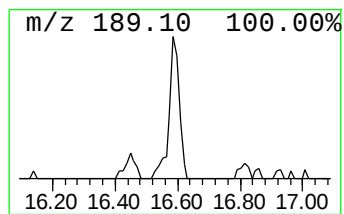
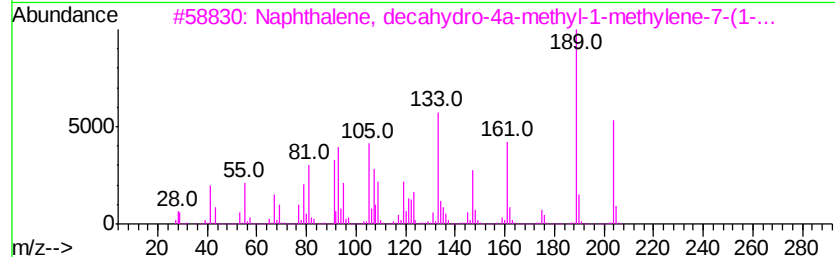
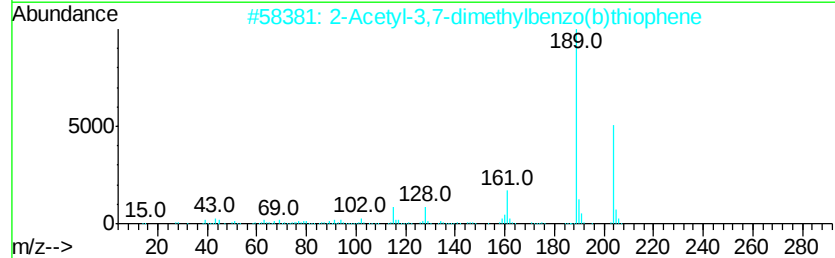
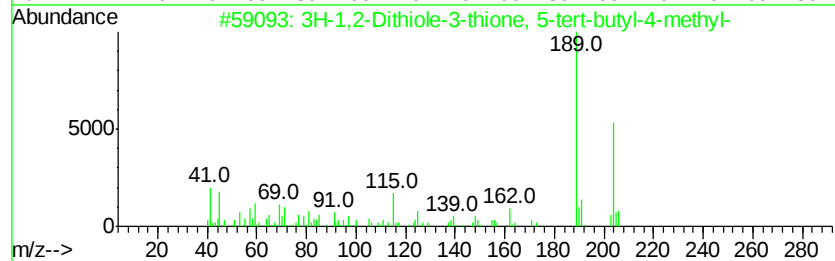
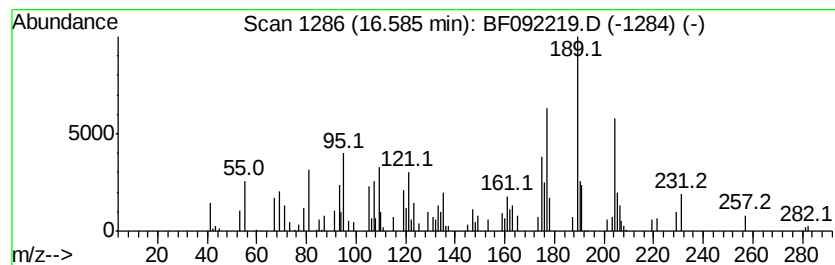
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.59 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	3.82 ng	168232	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiole-3-thione, 5-tert...	204	C8H12S3	013120-76-8	38
2		2-Acetyl-3,7-dimethylbenzo(b)thi...	204	C12H12OS	006179-06-2	30
3		Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	30
4		Benzenepropanal, 3-(1,1-dimethyl...	204	C14H20O	062518-65-4	30
5		2-Acetyl-3,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-05-1	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092219.D
Acq On : 12 Jan 2017 20:39
Operator : UM/SJ
Sample : I1030-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0013

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...	4.72	35.5	ng	2154090	1	6.60	1211790	20.0
unknown6.37	6.37	74.9	ng	4536140	1	6.60	1211790	20.0
Eicosane	10.55	2.1	ng	147785	4	11.11	1384150	20.0
n-Hexadecanoic acid	11.66	6.4	ng	441419	4	11.11	1384150	20.0
Pentadecanoic acid	12.44	3.7	ng	177526	5	13.73	966664	20.0
Trichloroacetic a...	13.60	7.5	ng	360927	5	13.73	966664	20.0
Tetrapentacontane...	14.23	3.1	ng	149674	5	13.73	966664	20.0
unknown16.59	16.59	3.8	ng	168232	6	15.09	881475	20.0