

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
 Data File : BF093193.D
 Acq On : 25 Feb 2017 15:25
 Operator : SJ/MA
 Sample : I1972-23
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-Y5N-SW2

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-BF013017.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	4.338	195	197	201	rBV	27356	48060	1.15%	0.130%
2	4.453	204	207	210	rBV	417995	616973	14.80%	1.668%
3	4.693	226	228	236	rBV	16144	42120	1.01%	0.114%
4	5.013	253	256	263	rVB	1324903	1735933	41.63%	4.693%
5	5.447	292	294	297	rBV	2819272	3654526	87.64%	9.880%
6	6.499	383	386	389	rBV2	3099989	4169802	100.00%	11.273%
7	6.613	393	396	399	rVV	3722214	3563087	85.45%	9.633%
8	6.842	413	416	418	rBV	712056	864664	20.74%	2.338%
9	6.990	427	429	432	rBV	2378916	3310263	79.39%	8.950%
10	7.413	463	466	468	rBV	2535155	2518627	60.40%	6.809%
11	7.882	502	507	508	rBV	27396	50844	1.22%	0.137%
12	7.905	508	509	515	rVB2	38201	61899	1.48%	0.167%
13	8.122	526	528	531	rBV	987048	1140775	27.36%	3.084%
14	8.499	557	561	563	rBV	31163	62457	1.50%	0.169%
15	8.556	564	566	571	rVB	73723	103715	2.49%	0.280%
16	9.139	614	617	620	rVB	54353	63176	1.52%	0.171%
17	9.208	620	623	625	rBV	4350283	4067231	97.54%	10.996%
18	9.608	655	658	660	rVB	191469	211279	5.07%	0.571%
19	9.882	680	682	684	rVB	1264011	1082628	25.96%	2.927%
20	10.305	716	719	721	rBV	49907	83993	2.01%	0.227%
21	10.682	749	752	754	rBV	1246581	1602581	38.43%	4.333%
22	10.785	759	761	765	rVB	110581	127597	3.06%	0.345%
23	11.048	782	784	787	rBV	45756	73341	1.76%	0.198%
24	11.231	799	800	802	rBV	83626	80912	1.94%	0.219%
25	11.368	810	812	815	rBV	1000846	940777	22.56%	2.543%
26	11.928	857	861	870	rBV2	681051	1823279	43.73%	4.929%
27	12.362	897	899	902	rBV3	108862	221328	5.31%	0.598%
28	12.774	934	935	938	rVB3	137631	155985	3.74%	0.422%
29	12.957	949	951	954	rBV	2166782	2511677	60.23%	6.791%
30	13.014	954	956	957	rBV	68889	79029	1.90%	0.214%
31	13.185	968	971	974	rBV	230575	300200	7.20%	0.812%
32	13.482	995	997	999	rBV	121370	121800	2.92%	0.329%
33	14.019	1041	1044	1046	rBV	674546	870115	20.87%	2.352%
34	15.448	1167	1169	1173	rVB	447187	627155	15.04%	1.696%

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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

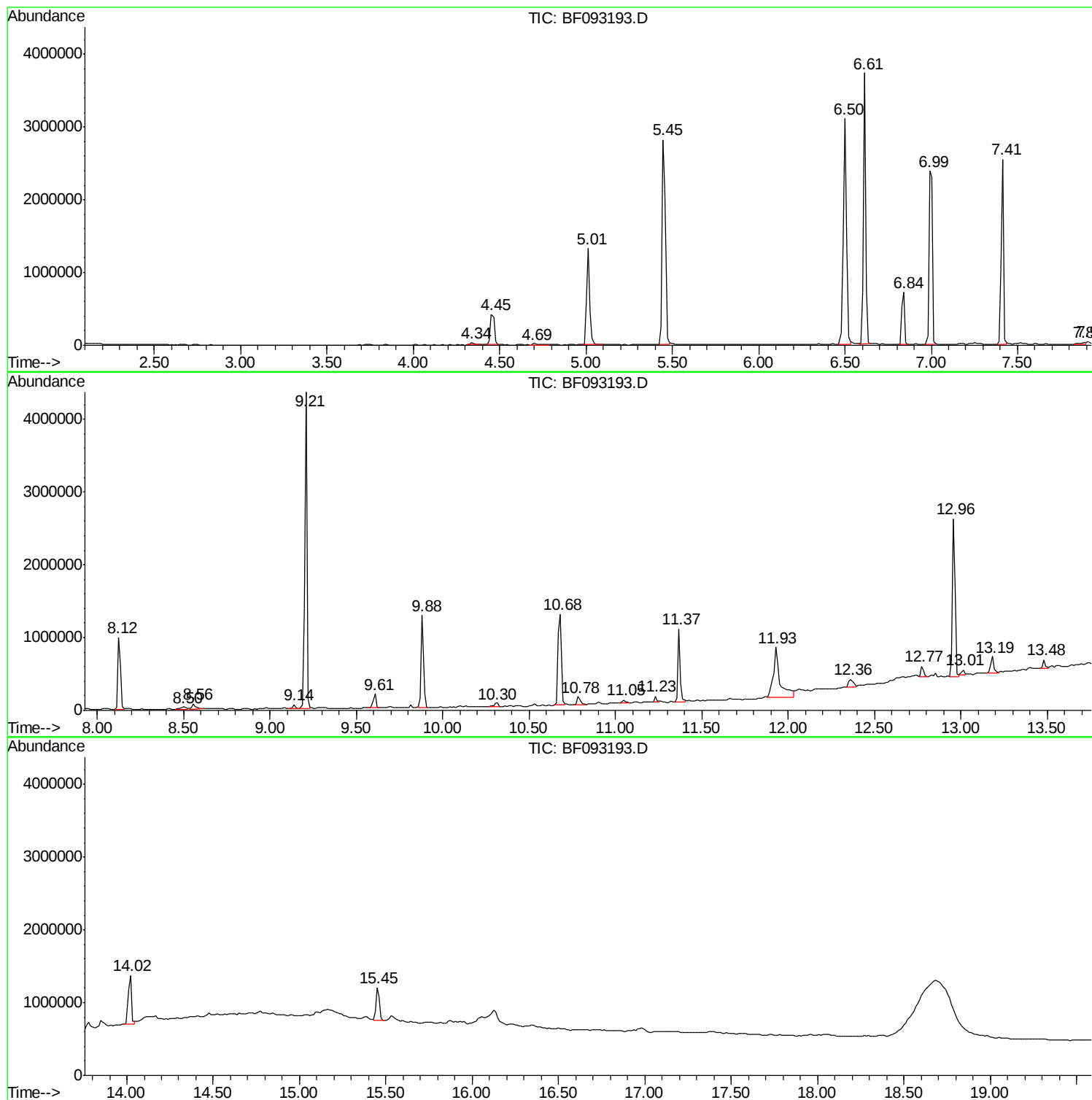
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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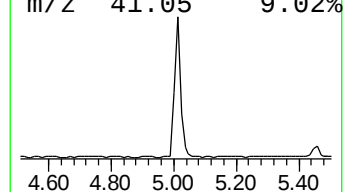
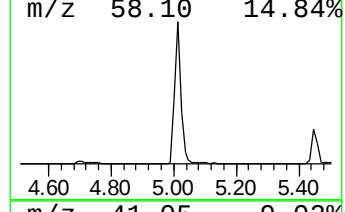
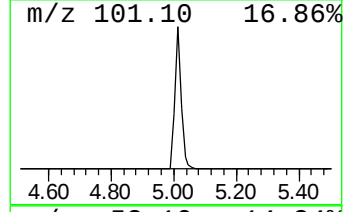
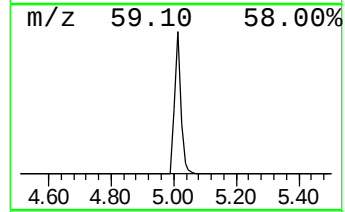
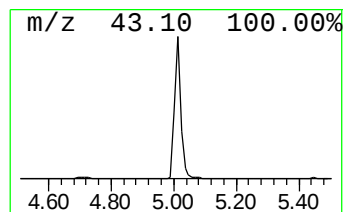
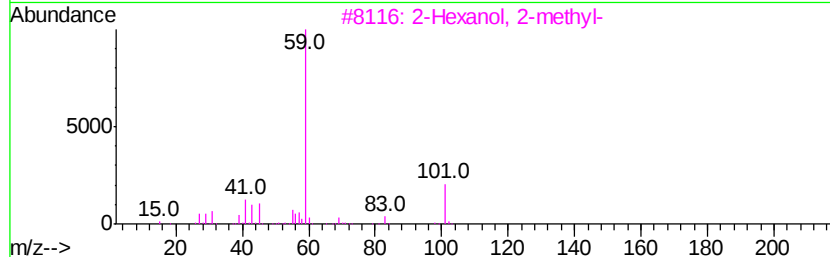
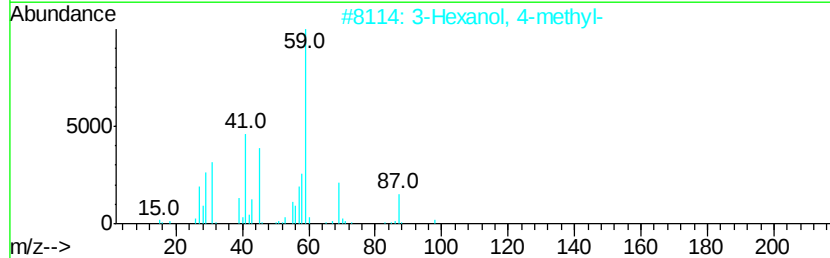
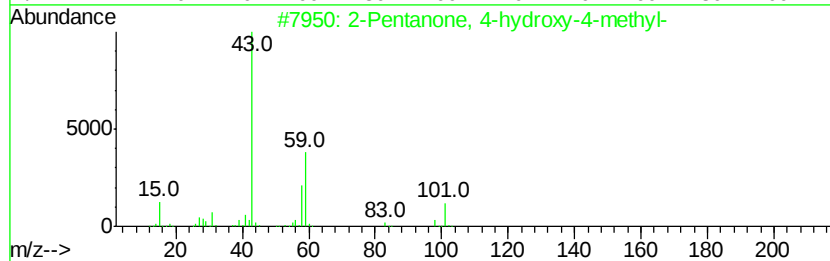
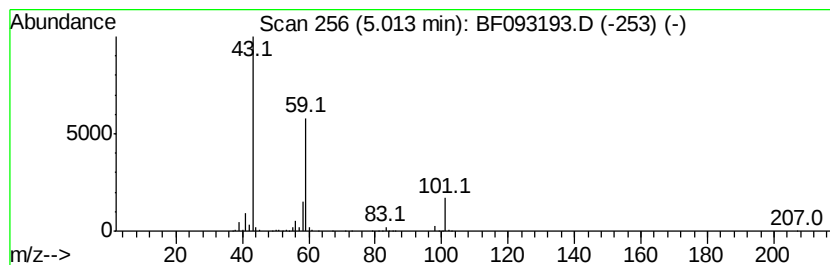
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	40.15 ng	1735930	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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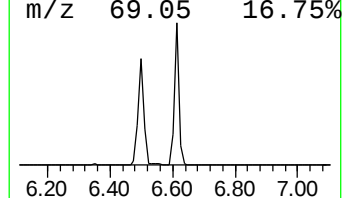
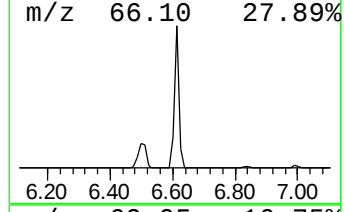
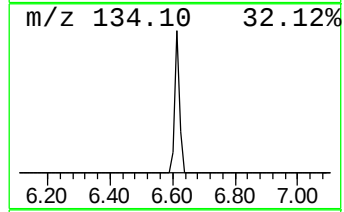
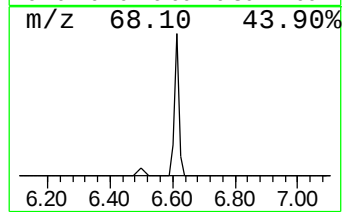
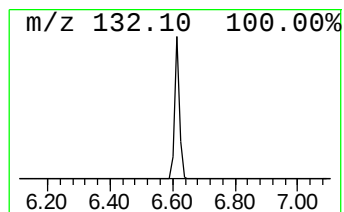
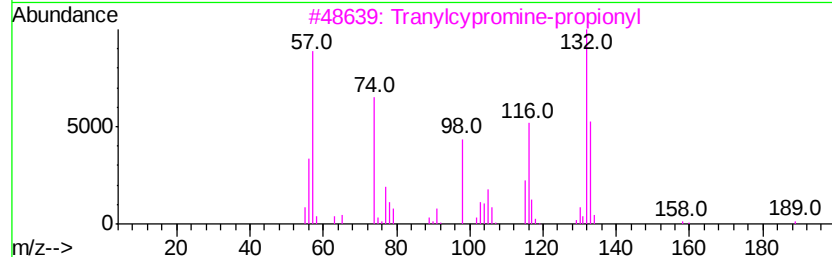
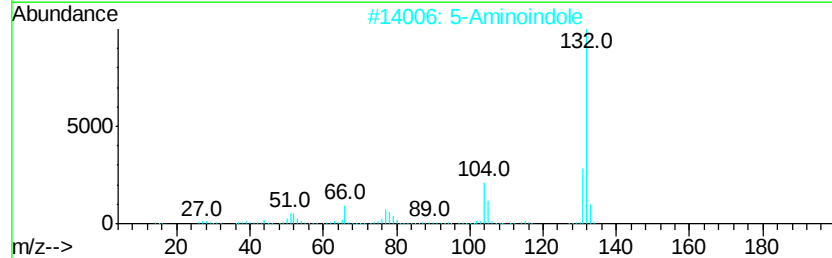
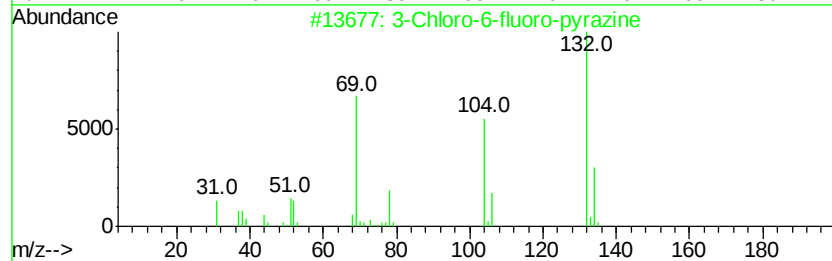
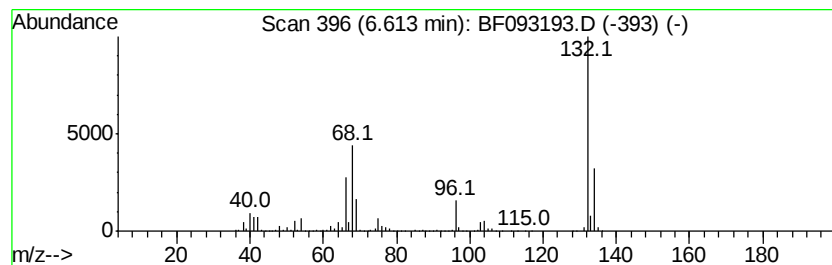
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	82.42 ng	3563090	1,4-Dichlorobenzene-d4	6.84

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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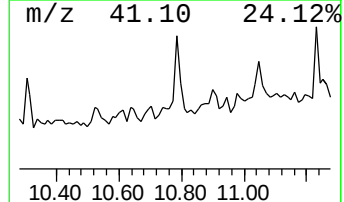
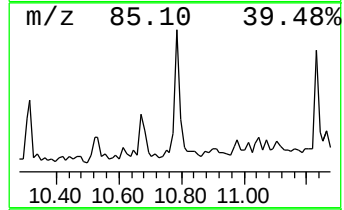
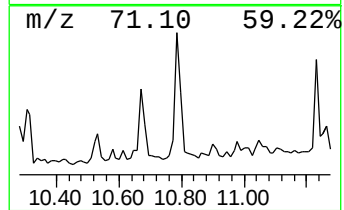
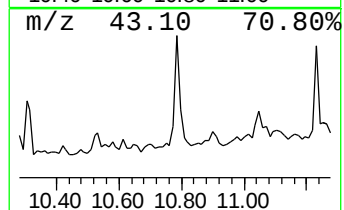
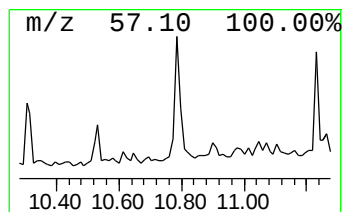
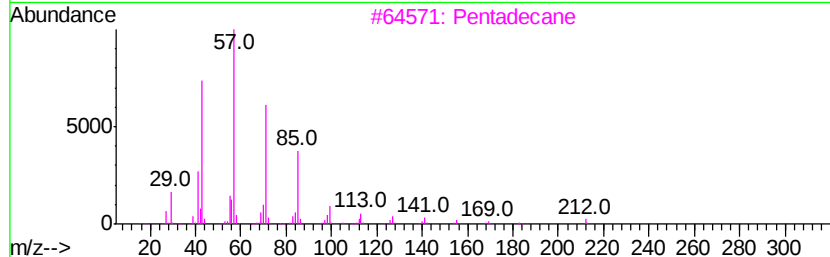
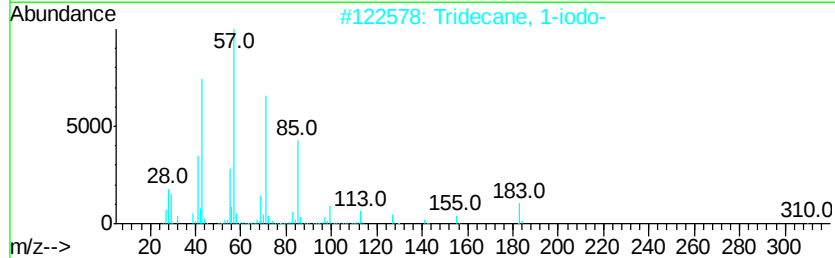
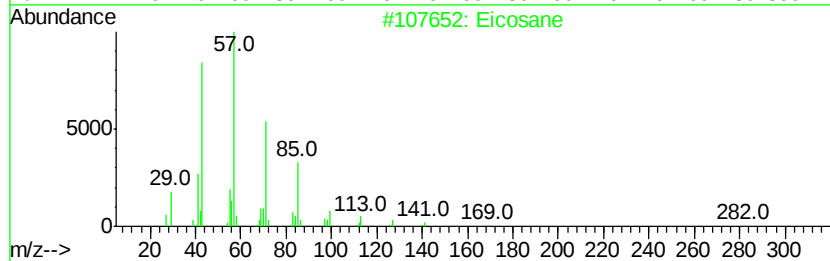
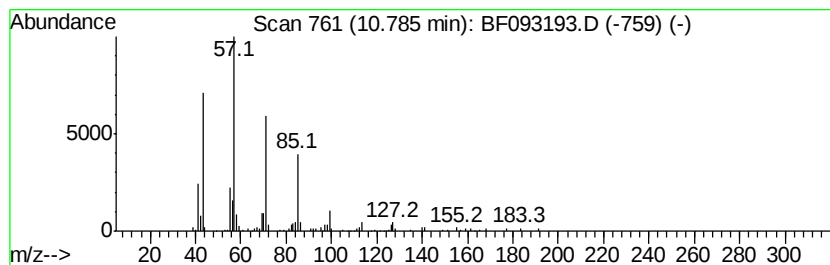
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	2.71 ng	127597	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	90
3	Pentadecane		212	C15H32	000629-62-9	90
4	2-Bromo dodecane		248	C12H25Br	013187-99-0	80
5	Hexadecane		226	C16H34	000544-76-3	64



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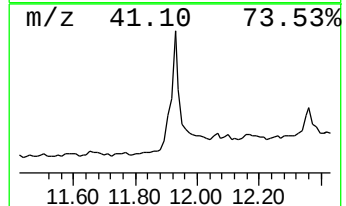
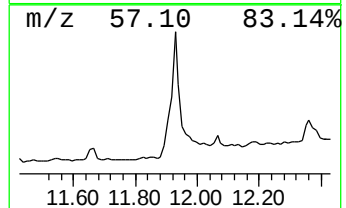
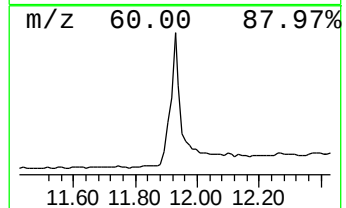
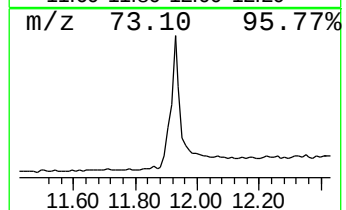
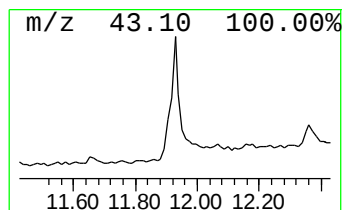
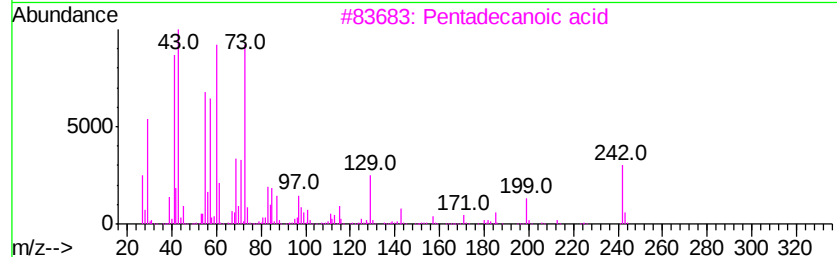
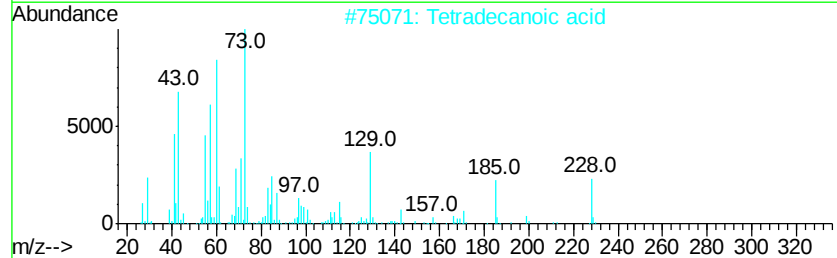
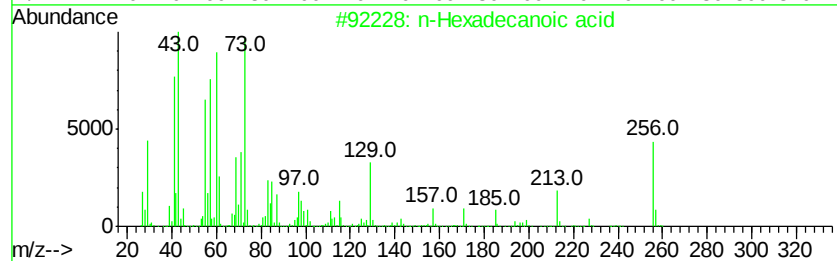
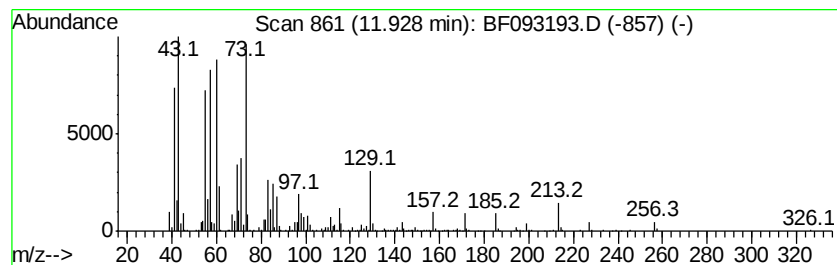
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	38.76 ng	1823280	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94	
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93	
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74	
5	Undecanoic acid	186	C11H22O2	000112-37-8	53	



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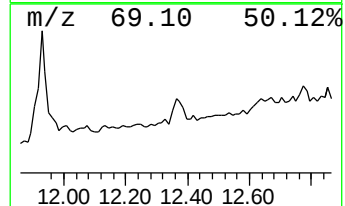
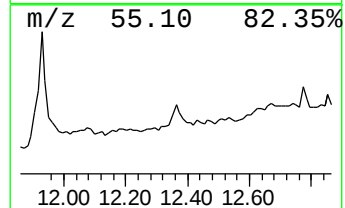
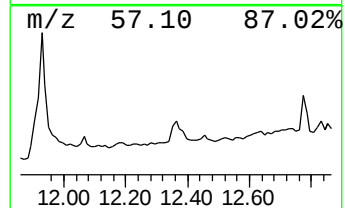
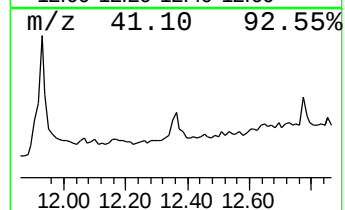
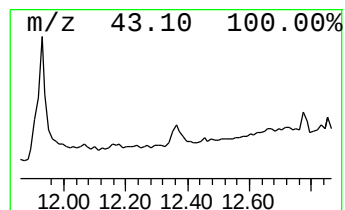
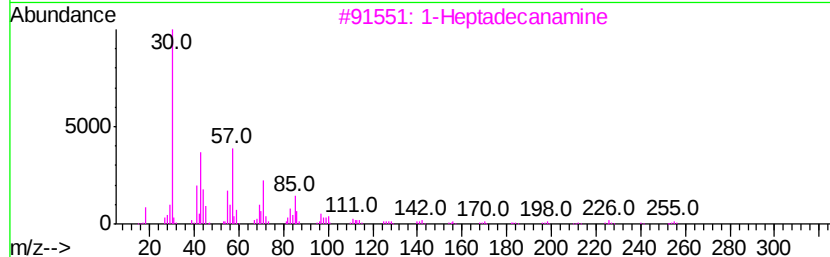
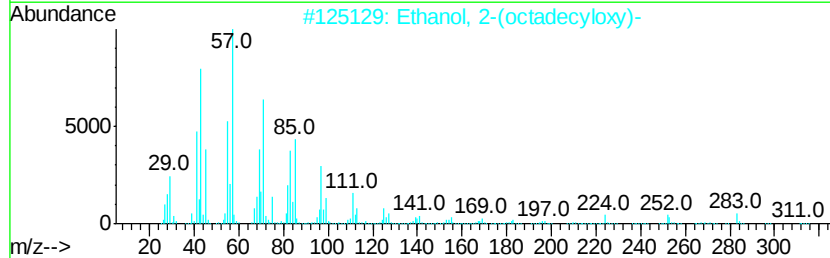
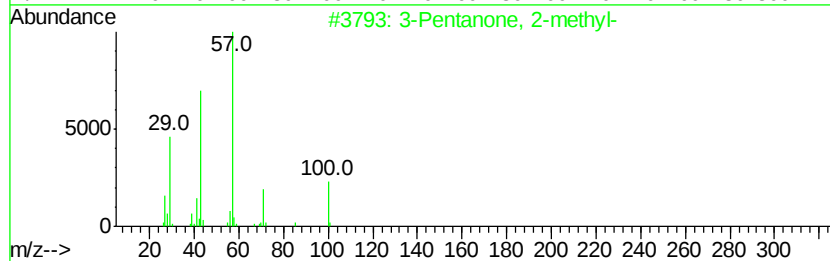
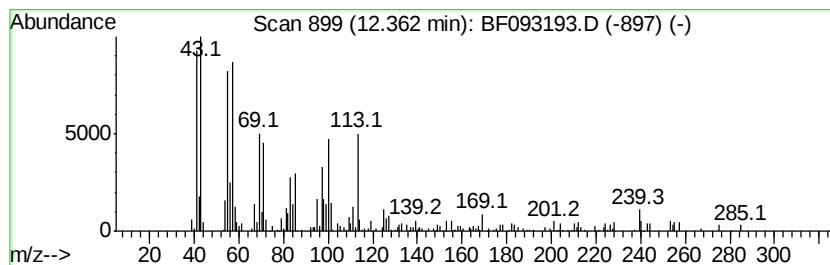
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Peak Number 7 unknown12.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	4.71 ng	221328	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	35
2		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	35
3		1-Heptadecanamine	255	C17H37N	004200-95-7	30
4		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	30
5		Octadecane	254	C18H38	000593-45-3	30



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ClientSampleId :
E2-Y5N-SW2

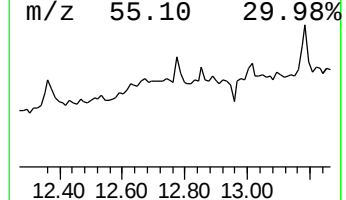
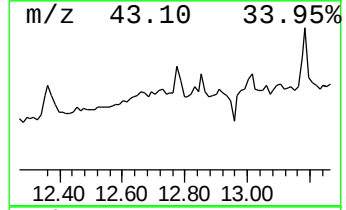
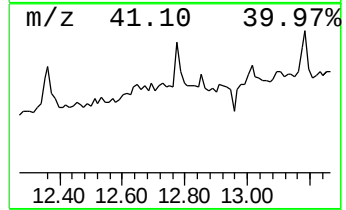
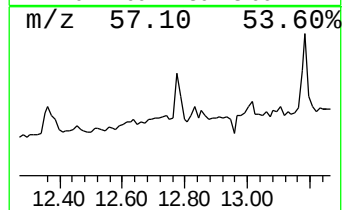
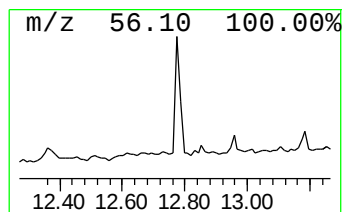
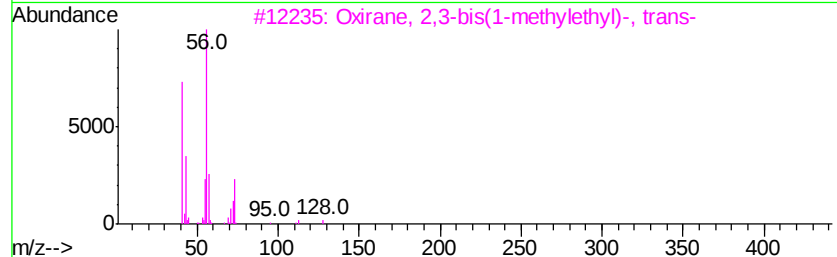
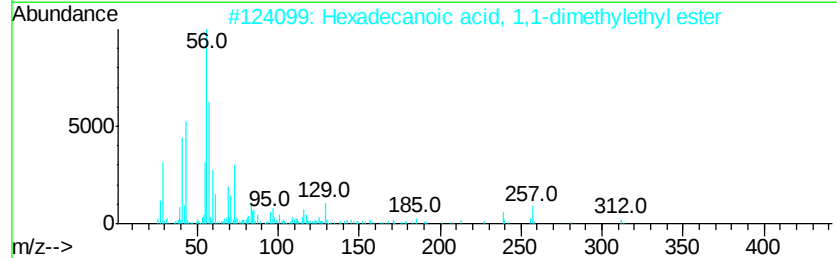
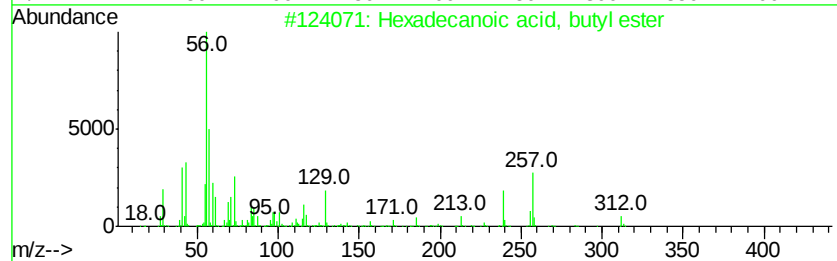
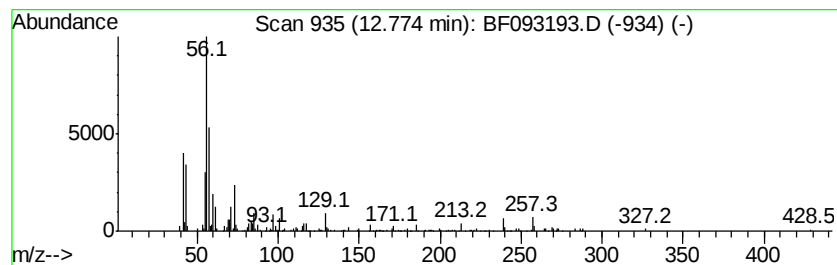
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.59 ng	155985	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	47
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	43
5		Pentanal, 3-methyl-	100	C6H12O	015877-57-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022417\
Data File : BF093193.D
Acq On : 25 Feb 2017 15:25
Operator : SJ/MA
Sample : I1972-23
Misc :
ALS Vial : 46 Sample Multiplier: 1

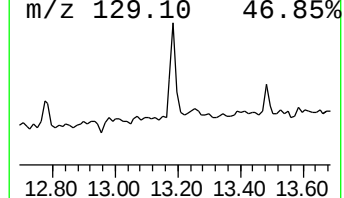
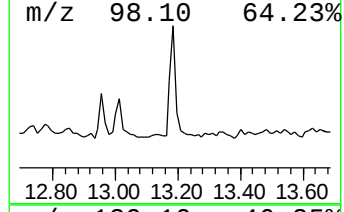
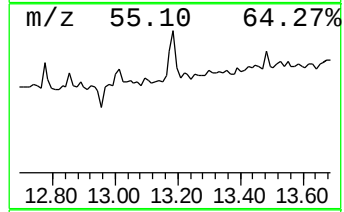
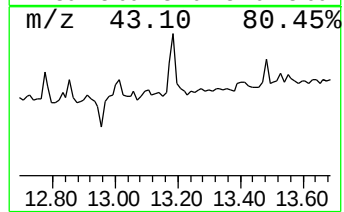
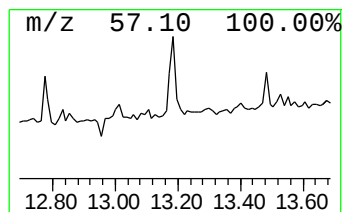
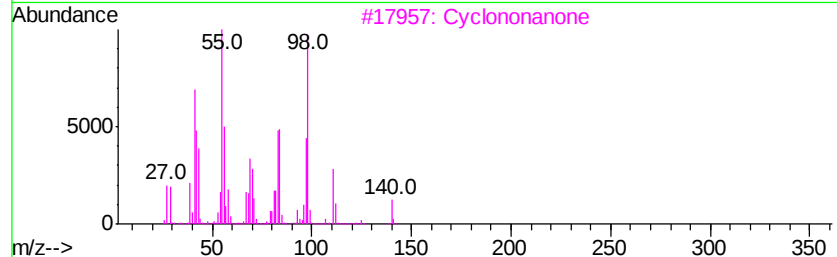
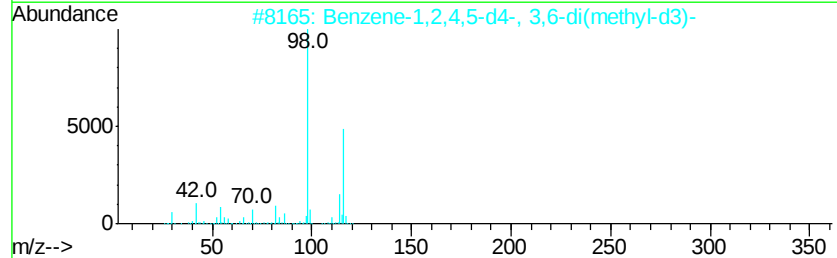
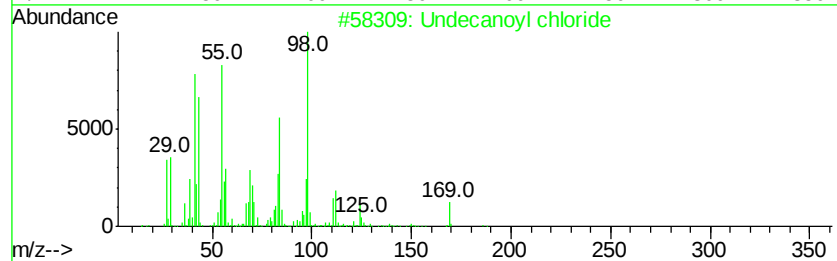
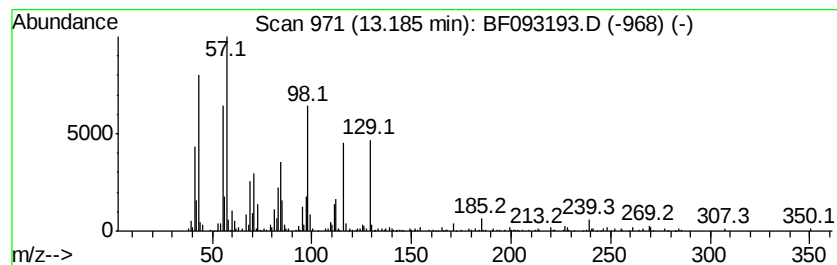
Instrument :
BNA_F
ClientSampleId :
E2-Y5N-SW2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.19 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.19	6.90 ng	300200	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoyl chloride	204	C11H21ClO	017746-05-3	43
2	Benzene-1,2,4,5-d4-, 3,6-di(meth...	116	C8D10	041051-88-1	30
3	Cyclohexanone	140	C9H16O	003350-30-9	22
4	Cyclohexanone, 4-(1,1-dimethylet...	154	C10H18O	000098-53-3	22
5	Z-8-Methyl-9-tetradecenoic acid	240	C15H28O2	1000130-84-5	20



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
Data File : BF093193.D
Acq On : 25 Feb 2017 15:25
Operator : SJ/MA
Sample : I1972-23
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-Y5N-SW2

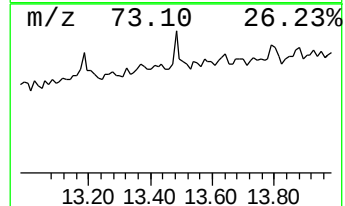
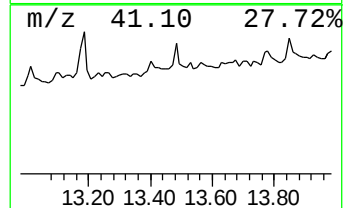
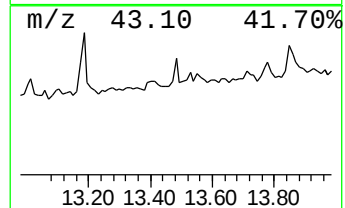
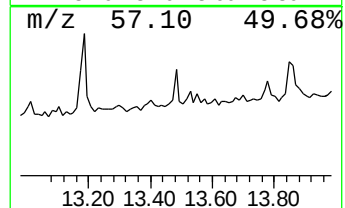
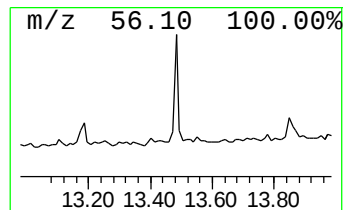
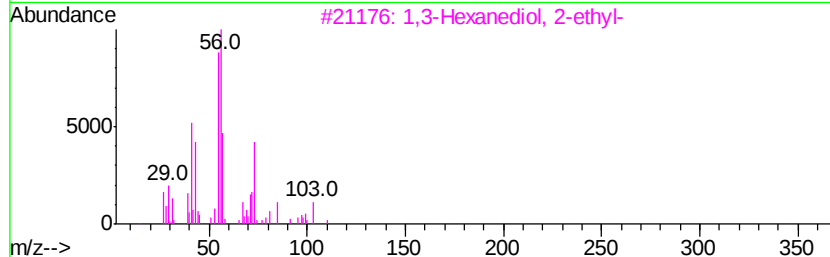
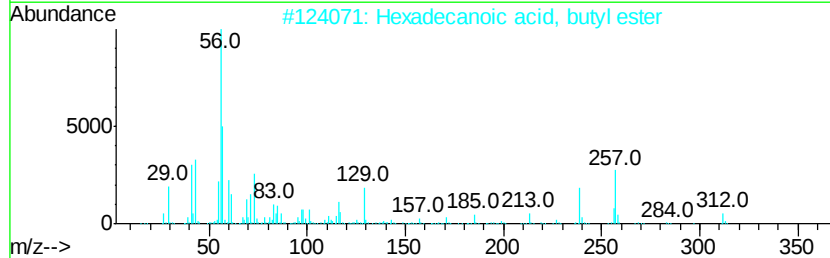
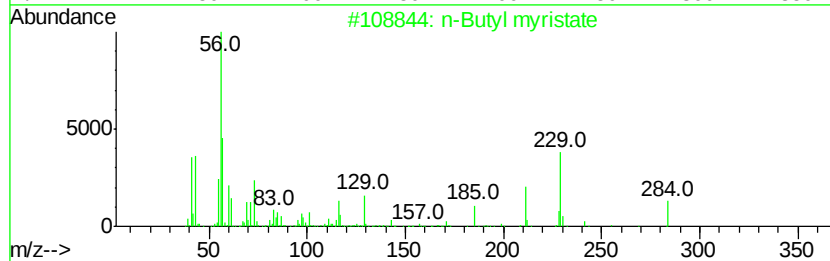
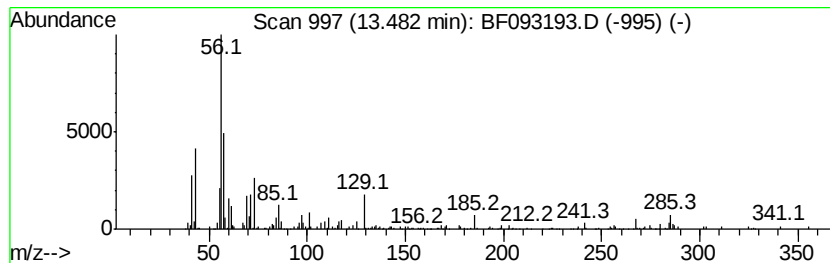
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Butyl myristate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.80 ng	121800	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Butyl myristate	284	C18H36O2	000110-36-1	64
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
3		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	47
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022417\
Data File : BF093193.D
Acq On : 25 Feb 2017 15:25
Operator : SJ/MA
Sample : I1972-23
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-Y5N-SW2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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...	5.01	40.1	ng	1735930	1	6.84	864664	20.0
unknown6.61	6.61	82.4	ng	3563090	1	6.84	864664	20.0
Eicosane	10.78	2.7	ng	127597	4	11.37	940777	20.0
n-Hexadecanoic acid	11.93	38.8	ng	1823280	4	11.37	940777	20.0
unknown12.36	12.36	4.7	ng	221328	4	11.37	940777	20.0
Hexadecanoic acid...	12.77	3.6	ng	155985	5	14.02	870115	20.0
unknown13.19	13.19	6.9	ng	300200	5	14.02	870115	20.0
n-Butyl myristate	13.48	2.8	ng	121800	5	14.02	870115	20.0