

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
 Data File : BF095641.D
 Acq On : 2 Jun 2017 19:00
 Operator : SJ/MA
 Sample : I3443-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-RO-6699AA-060117

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-BF050217.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	4.792	524	528	544	rBV	58396	164037	7.15%	0.756%
2	5.451	636	640	682	rBV	1006860	2076555	90.51%	9.565%
3	7.086	914	918	932	rBV	1150131	1925599	83.93%	8.870%
4	7.192	932	936	952	rVB	1453504	2294204	100.00%	10.568%
5	7.533	991	994	1013	rVB	379354	524034	22.84%	2.414%
6	7.775	1030	1035	1055	rBV	1208122	1637907	71.39%	7.544%
7	8.451	1145	1150	1170	rBV	827713	1230436	53.63%	5.668%
8	9.569	1335	1340	1352	rBV	481484	694380	30.27%	3.198%
9	11.345	1636	1642	1654	rBV	1826229	2237377	97.52%	10.306%
10	11.563	1674	1679	1687	rVB3	19250	25085	1.09%	0.116%
11	12.039	1756	1760	1765	rBV	139791	184140	8.03%	0.848%
12	12.392	1815	1820	1835	rBV2	587402	811115	35.35%	3.736%
13	13.239	1960	1964	1969	rBV	59723	68574	2.99%	0.316%
14	13.598	2018	2025	2028	rBV3	17702	32307	1.41%	0.149%
15	13.692	2036	2041	2054	rBV	690313	1075831	46.89%	4.955%
16	14.010	2091	2095	2105	rBV	62885	101108	4.41%	0.466%
17	14.739	2214	2219	2223	rBV	46798	60639	2.64%	0.279%
18	14.792	2224	2228	2233	rBV2	455846	621281	27.08%	2.862%
19	15.415	2330	2334	2341	rVB	33451	39857	1.74%	0.184%
20	15.568	2355	2360	2364	rBV	268461	303489	13.23%	1.398%
21	15.780	2393	2396	2405	rVB2	63496	88374	3.85%	0.407%
22	16.015	2431	2436	2440	rVB2	26585	30428	1.33%	0.140%
23	16.533	2519	2524	2527	rBV	994761	1104433	48.14%	5.087%
24	16.568	2527	2530	2533	rVV	989803	1047132	45.64%	4.823%
25	16.603	2533	2536	2547	rVB2	100383	155802	6.79%	0.718%
26	16.692	2547	2551	2556	rBV	168963	188082	8.20%	0.866%
27	16.880	2579	2583	2585	rBV3	26491	30946	1.35%	0.143%
28	16.909	2585	2588	2593	rVB	73811	93808	4.09%	0.432%
29	17.009	2602	2605	2612	rVB6	22073	31285	1.36%	0.144%
30	17.145	2623	2628	2636	rVB	1376778	1524545	66.45%	7.022%
31	17.421	2672	2675	2678	rBV2	24984	27594	1.20%	0.127%
32	17.533	2691	2694	2700	rVB5	25527	44867	1.96%	0.207%
33	17.662	2713	2716	2719	rVB4	20604	23104	1.01%	0.106%
34	18.386	2835	2839	2848	rBV4	49382	87222	3.80%	0.402%

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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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35	18.492	2853	2857	2873	rBV	441349	681611	29.71%	3.140%
36	18.803	2905	2910	2912	rBV6	18697	33534	1.46%	0.154%
37	20.168	3139	3142	3152	rBV	316668	409237	17.84%	1.885%

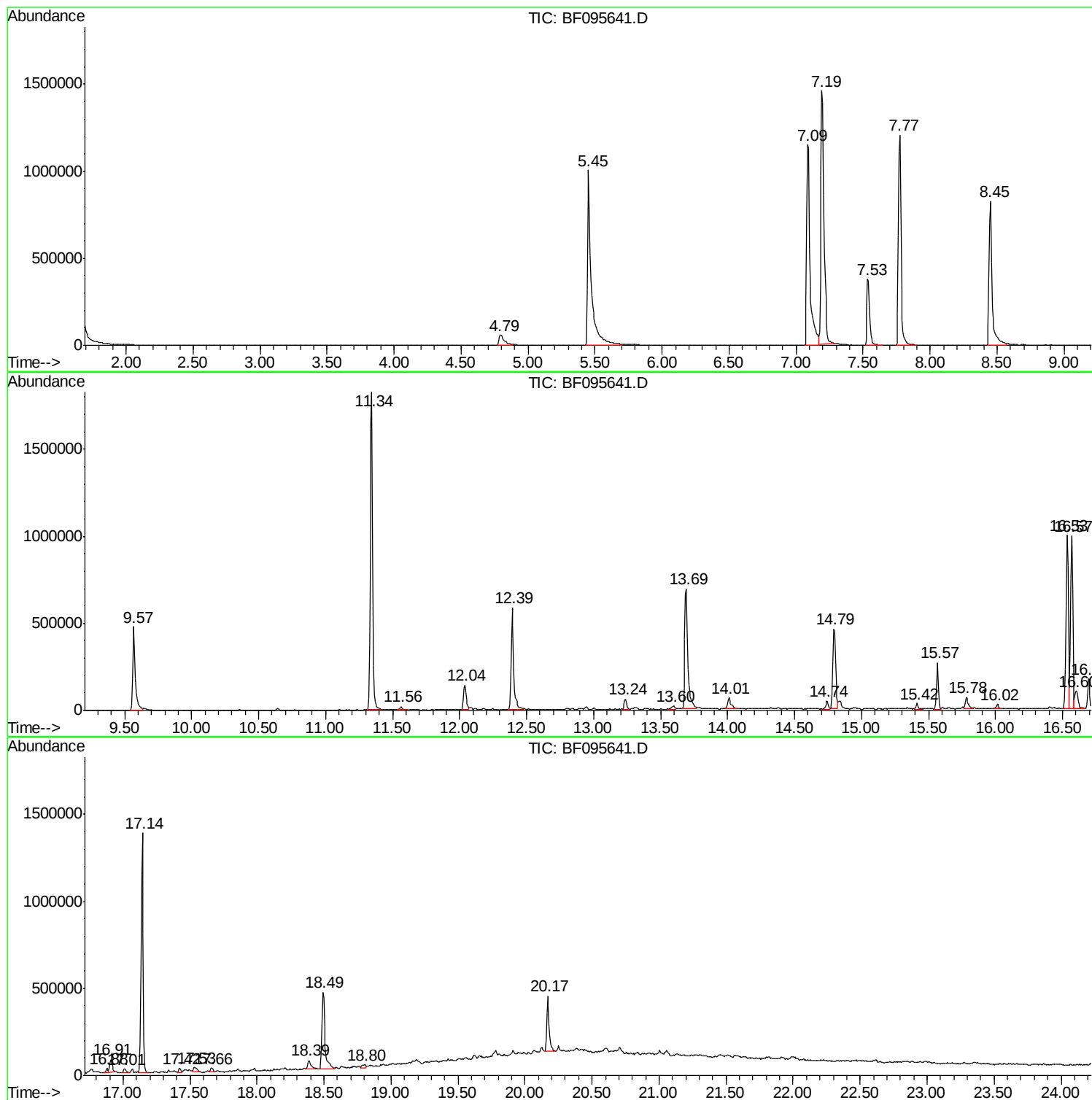
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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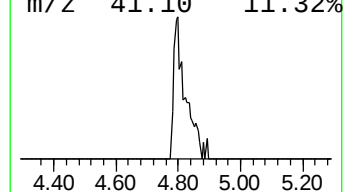
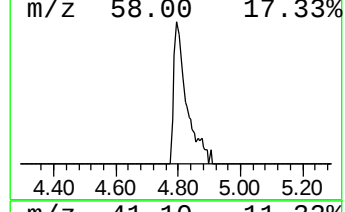
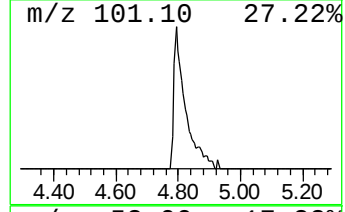
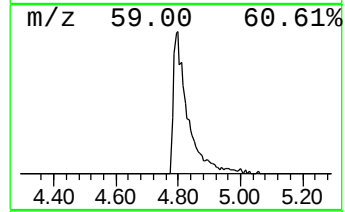
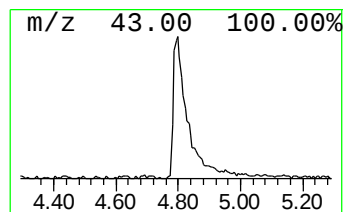
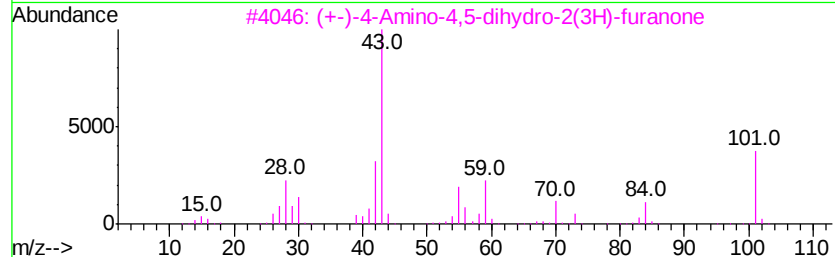
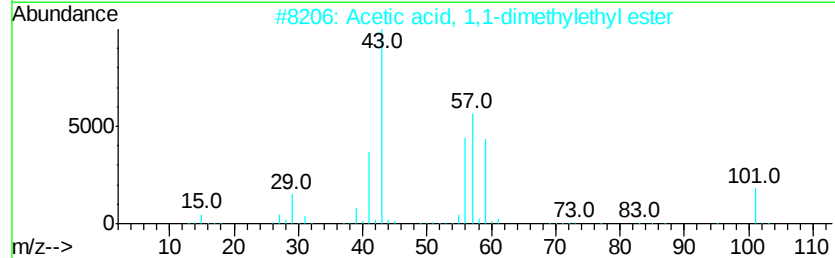
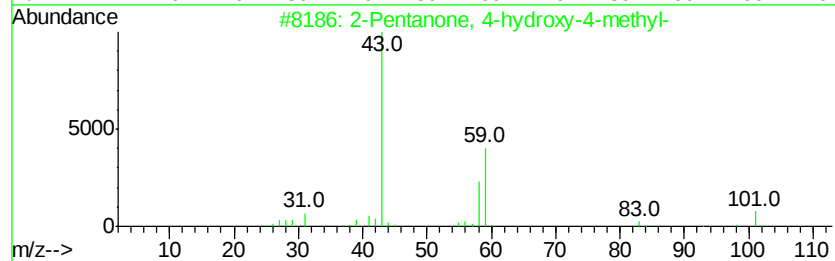
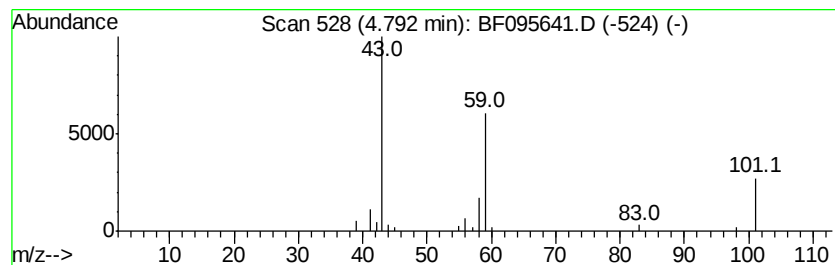
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	6.26 ng	164037	1,4-Dichlorobenzene-d4	7.54

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			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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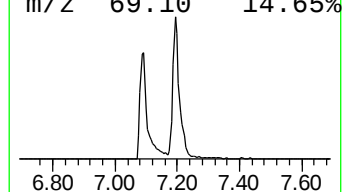
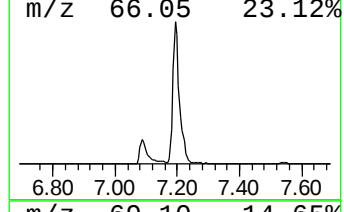
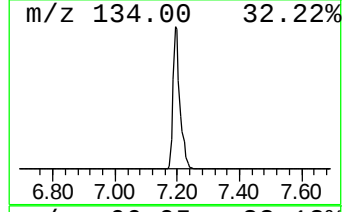
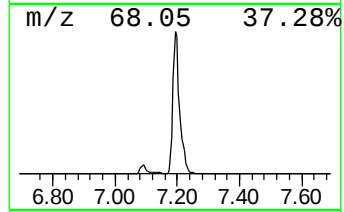
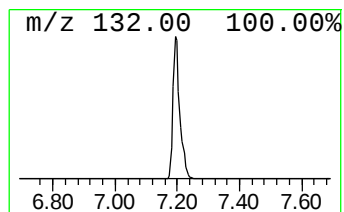
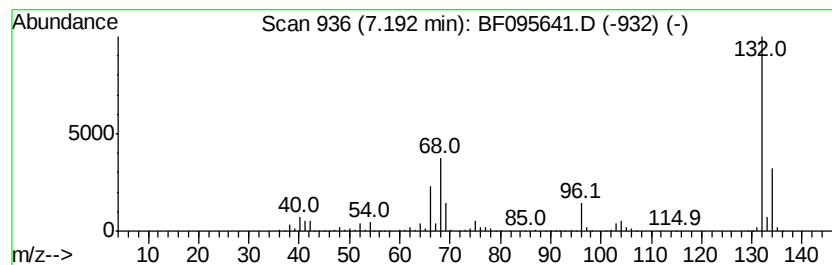
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	87.56 ng	2294200	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1-Aminoindan	133	C9H11N	034698-41-4	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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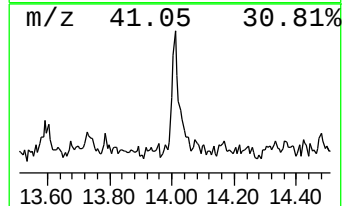
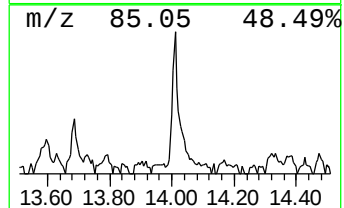
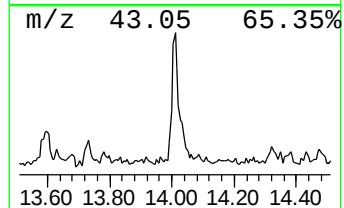
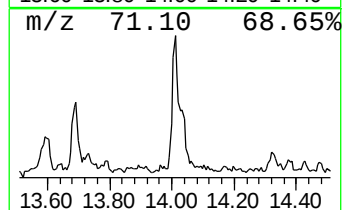
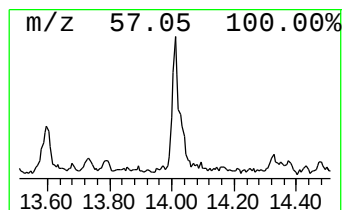
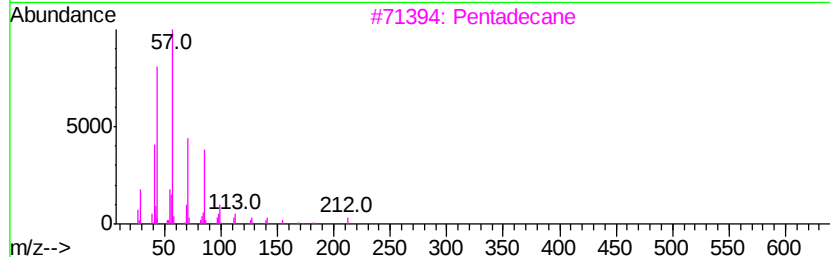
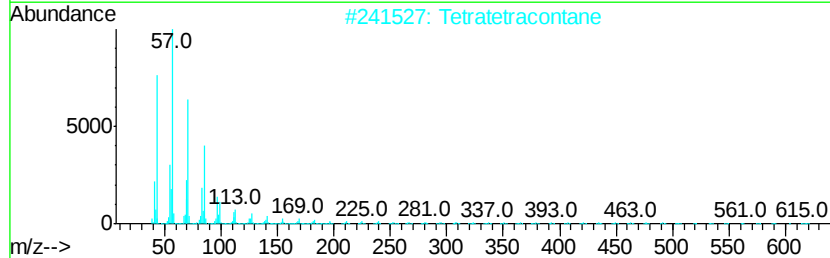
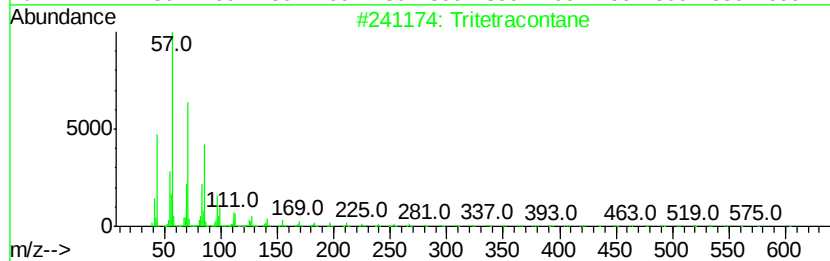
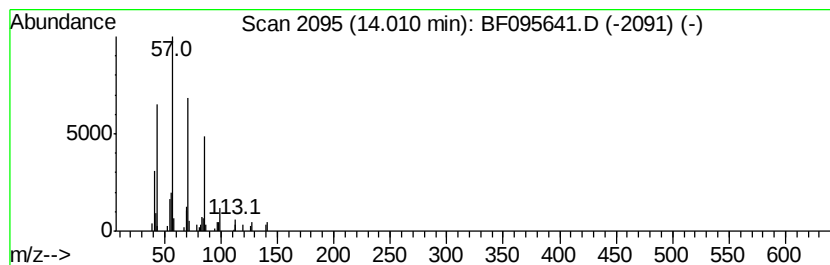
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tritetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	3.25 ng	101108	Phenanthrene-d10	14.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	90
2		Tetratetracontane	619	C44H90	007098-22-8	90
3		Pentadecane	212	C15H32	000629-62-9	90
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
5		Heptadecane	240	C17H36	000629-78-7	86



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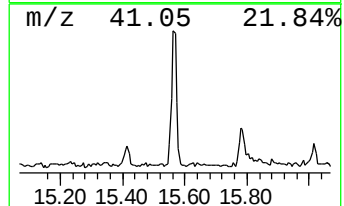
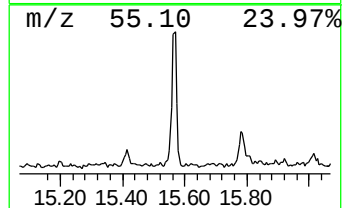
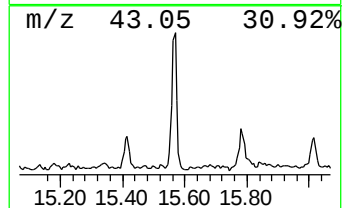
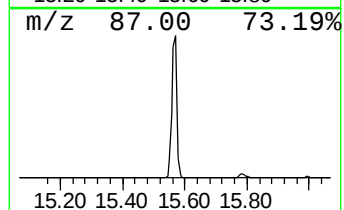
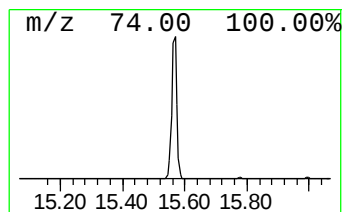
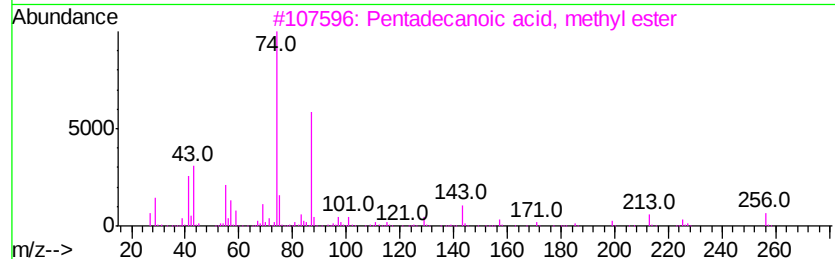
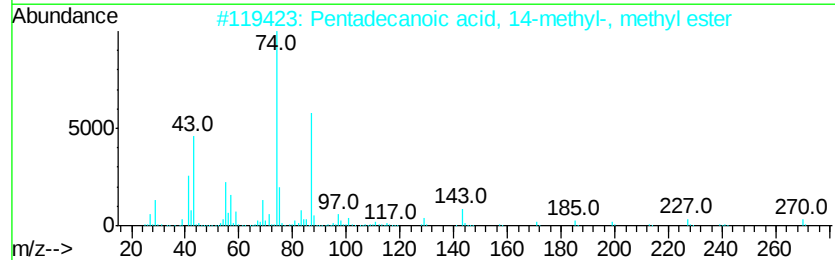
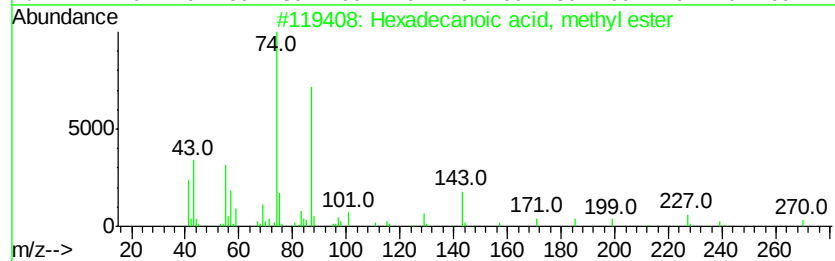
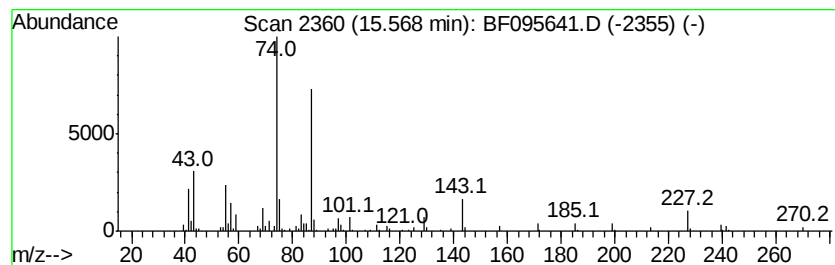
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	9.77 ng	303489	Phenanthrene-d10	14.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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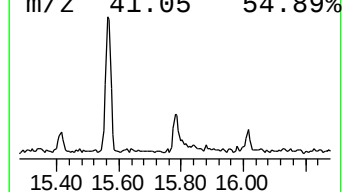
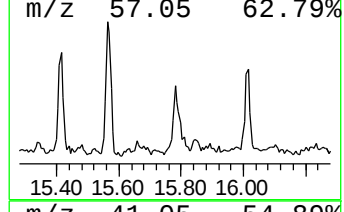
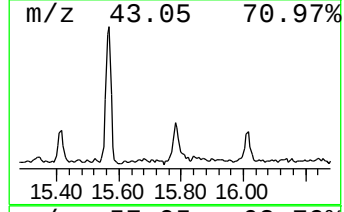
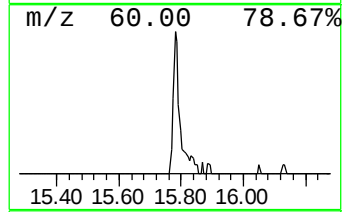
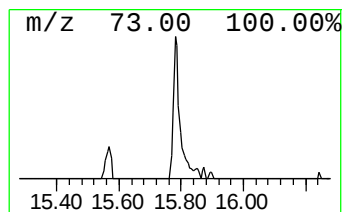
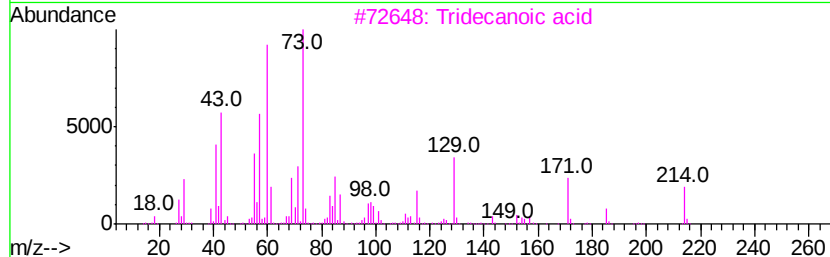
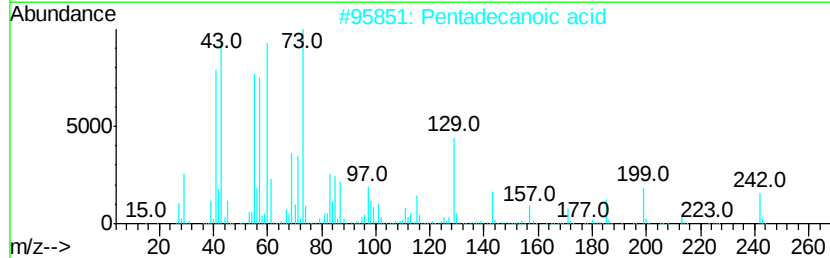
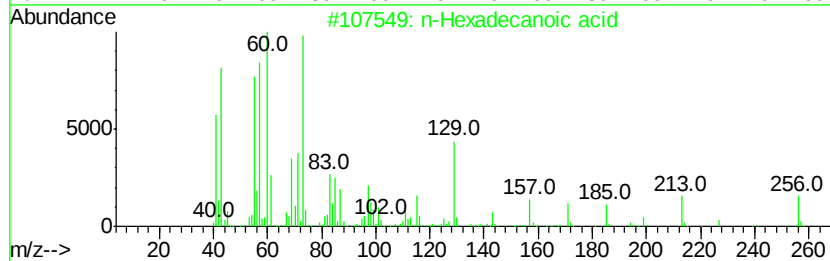
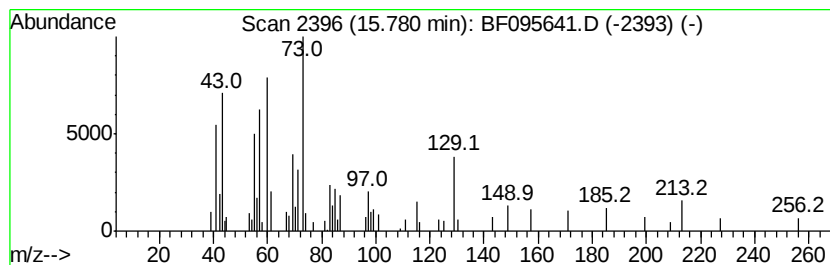
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	2.84 ng	88374	Phenanthrene-d10	14.79

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	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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SA-RO-6699AA-060117

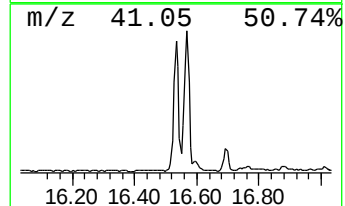
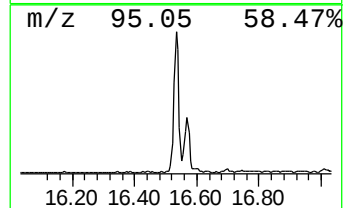
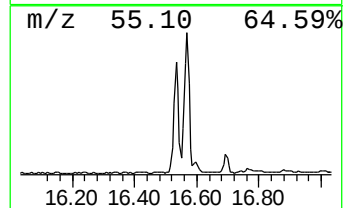
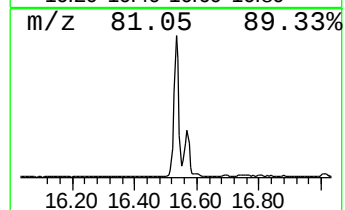
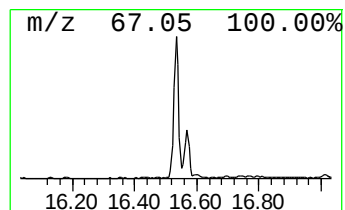
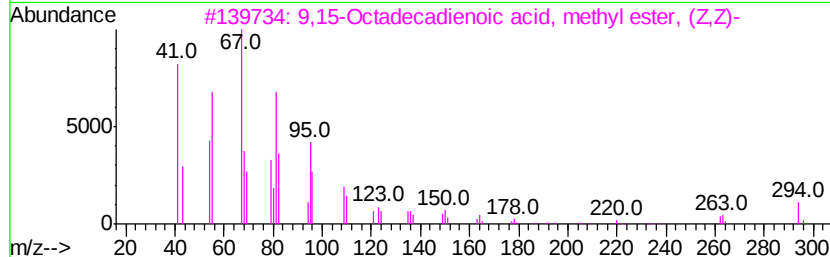
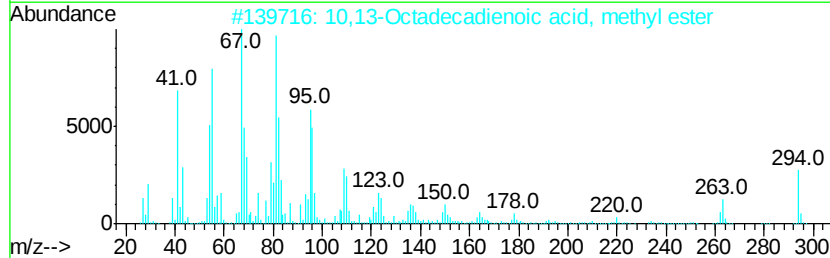
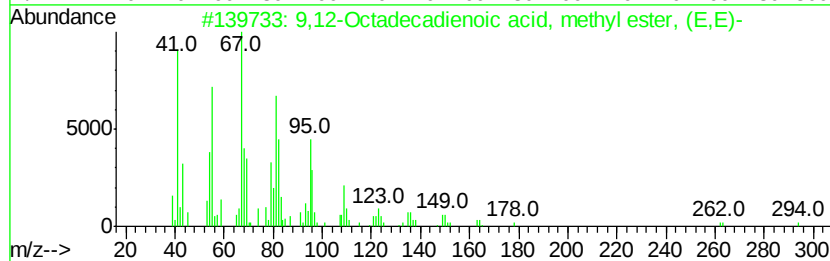
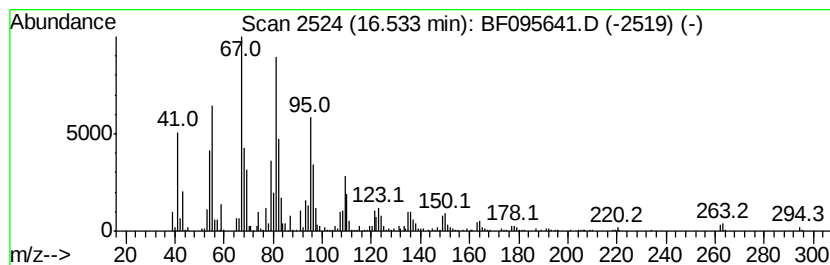
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	35.55 ng	1104430	Phenanthrene-d10	14.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3		9,15-Octadecadienoic acid, methv...	294	C19H34O2	017309-05-6	99
4		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095641.D
Acq On : 2 Jun 2017 19:00
Operator : SJ/MA
Sample : I3443-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-RO-6699AA-060117

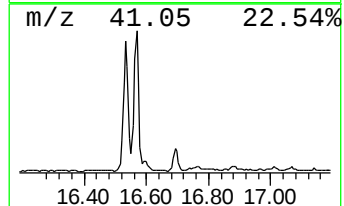
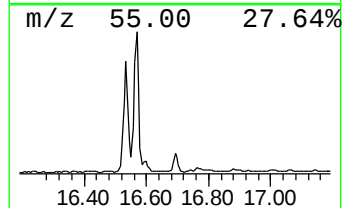
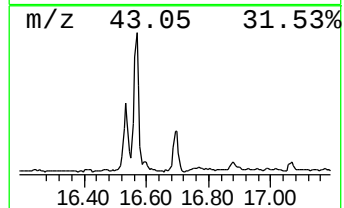
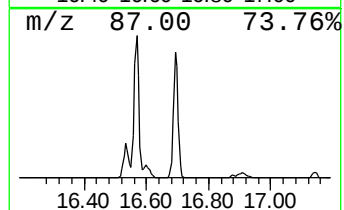
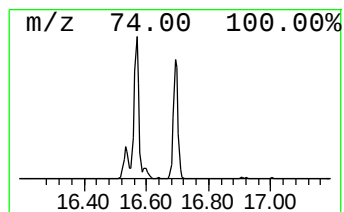
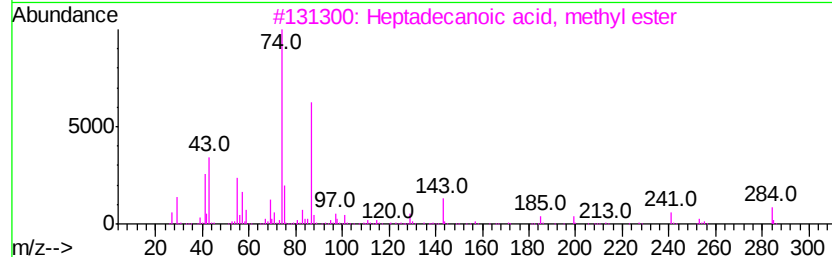
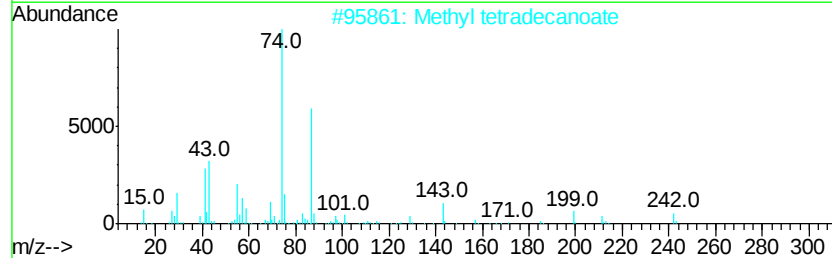
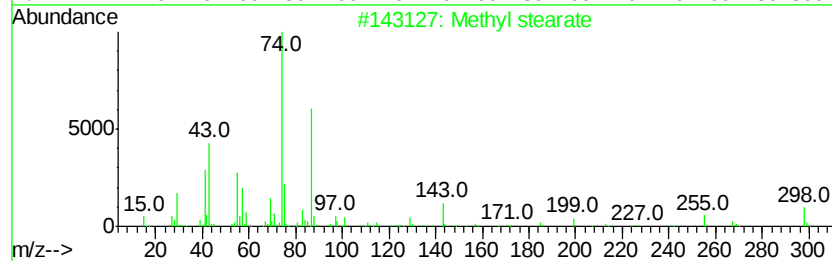
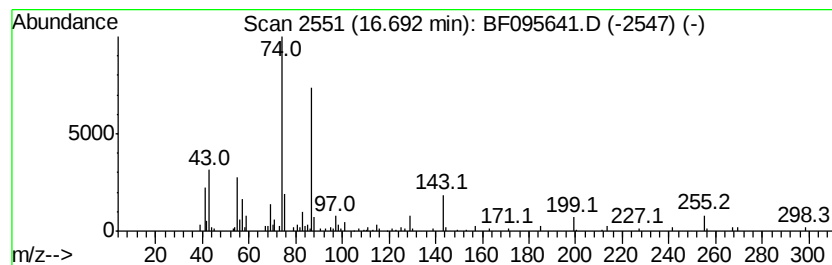
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	5.52 ng	188082	Chrysene-d12	18.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	97
2		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095641.D
Acq On : 2 Jun 2017 19:00
Operator : SJ/MA
Sample : I3443-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

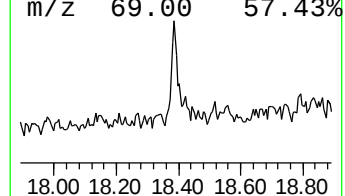
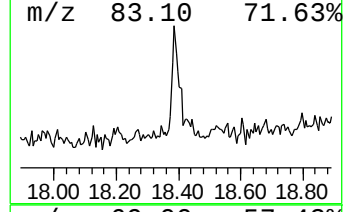
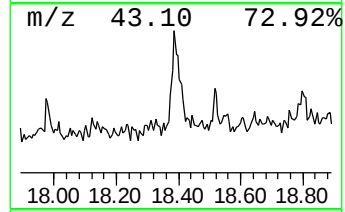
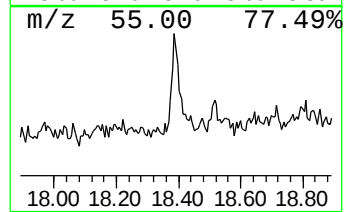
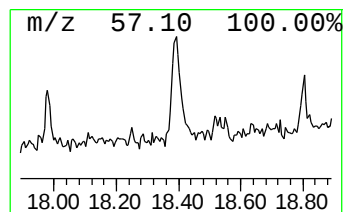
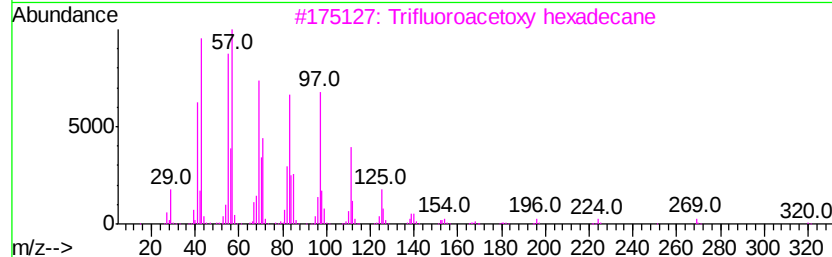
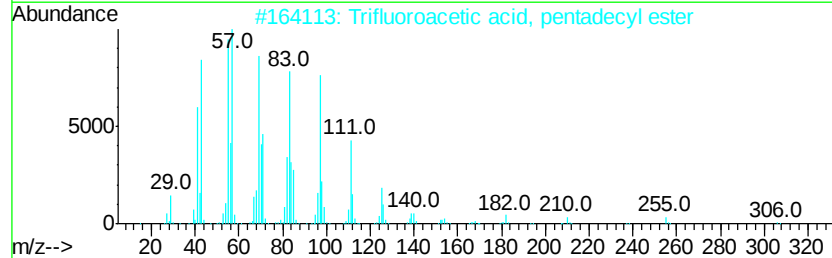
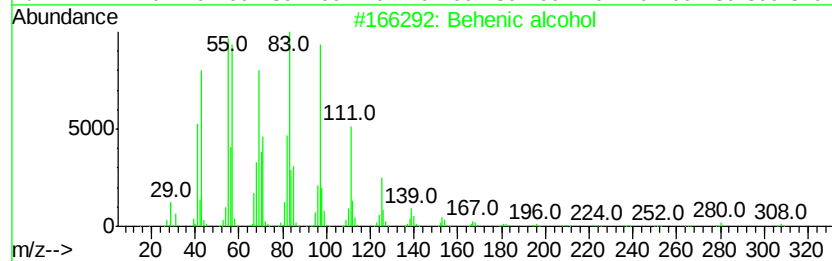
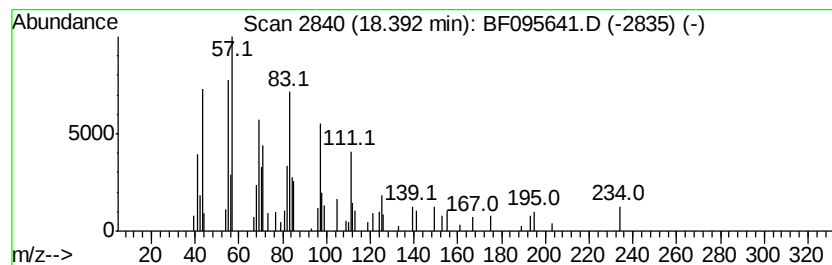
Instrument :
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ClientSampleId :
SA-RO-6699AA-060117

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Behenic alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.56 ng	87222	Chrysene-d12	18.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 90
2		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 83
3		Trifluoroacetoxv hexadecane	338 C18H33F3O2	006222-03-3 81
4		1-Hexadecanol	242 C16H34O	036653-82-4 74
5		1-Tetradecanol	214 C14H30O	000112-72-1 74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060217\
Data File : BF095641.D
Acq On : 2 Jun 2017 19:00
Operator : SJ/MA
Sample : I3443-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-RO-6699AA-060117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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...	4.79	6.3	ng	164037	1	7.54	524034	20.0
unknown7.19	7.19	87.6	ng	2294200	1	7.54	524034	20.0
Tritetracontane	14.01	3.3	ng	101108	4	14.79	621281	20.0
Hexadecanoic acid...	15.57	9.8	ng	303489	4	14.79	621281	20.0
n-Hexadecanoic acid	15.78	2.8	ng	88374	4	14.79	621281	20.0
9,12-Octadecadien...	16.53	35.5	ng	1104430	4	14.79	621281	20.0
Methyl stearate	16.69	5.5	ng	188082	5	18.49	681611	20.0
Behenic alcohol	18.39	2.6	ng	87222	5	18.49	681611	20.0