

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
 Data File : BF095639.D
 Acq On : 2 Jun 2017 17:56
 Operator : SJ/MA
 Sample : I3420-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3-TP-4

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	4.798	526	529	554	rBV	68417	217228	7.47%	0.866%
2	5.451	636	640	671	rBV	1248957	2440793	83.90%	9.725%
3	7.092	914	919	932	rBV	1440026	2367432	81.38%	9.433%
4	7.192	932	936	952	rVB	1711848	2732298	93.92%	10.887%
5	7.533	991	994	1007	rBV	445027	610544	20.99%	2.433%
6	7.775	1030	1035	1052	rBV	1441341	1939719	66.68%	7.729%
7	8.451	1145	1150	1169	rBV	997021	1486387	51.10%	5.922%
8	9.569	1335	1340	1352	rBV	616755	885470	30.44%	3.528%
9	11.345	1636	1642	1654	rBV	2291502	2909034	100.00%	11.591%
10	11.557	1674	1678	1684	rVB3	20326	32315	1.11%	0.129%
11	12.033	1755	1759	1765	rBV	449102	586165	20.15%	2.336%
12	12.245	1790	1795	1801	rVB4	23446	39470	1.36%	0.157%
13	12.392	1815	1820	1840	rBV2	776298	1023360	35.18%	4.077%
14	13.239	1958	1964	1969	rBV	38384	42214	1.45%	0.168%
15	13.692	2036	2041	2056	rBV	894068	1391128	47.82%	5.543%
16	14.009	2090	2095	2105	rBV	37217	65113	2.24%	0.259%
17	14.739	2213	2219	2224	rBV2	24587	32010	1.10%	0.128%
18	14.798	2224	2229	2242	rVV	578041	836485	28.75%	3.333%
19	15.298	2309	2314	2327	rBV	115754	172826	5.94%	0.689%
20	15.780	2391	2396	2411	rBV2	95899	148273	5.10%	0.591%
21	16.486	2512	2516	2527	rBV	627782	829086	28.50%	3.303%
22	16.562	2527	2529	2535	rVV2	33974	41253	1.42%	0.164%
23	16.621	2535	2539	2545	rVB	26557	42306	1.45%	0.169%
24	16.880	2579	2583	2587	rBV2	44110	66967	2.30%	0.267%
25	16.915	2587	2589	2598	rVV	35697	53946	1.85%	0.215%
26	17.145	2623	2628	2636	rVB	1718078	1966777	67.61%	7.836%
27	17.792	2734	2738	2745	rBV	86484	107217	3.69%	0.427%
28	17.927	2756	2761	2764	rBV4	19058	31932	1.10%	0.127%
29	18.386	2835	2839	2848	rVB	90297	143075	4.92%	0.570%
30	18.492	2853	2857	2865	rBV	450378	611882	21.03%	2.438%
31	18.550	2865	2867	2870	rVB	35645	33139	1.14%	0.132%
32	19.515	3026	3031	3041	rBV	360036	447381	15.38%	1.783%
33	19.780	3072	3076	3079	rBV	34322	42048	1.45%	0.168%
34	20.062	3121	3124	3130	rBV	43382	50805	1.75%	0.202%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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

35	20.121	3131	3134	3138	rVV	45247	50747	1.74%	0.202%
36	20.168	3138	3142	3153	rVV	368879	533638	18.34%	2.126%
37	21.450	3355	3360	3366	rVB6	19161	45968	1.58%	0.183%
38	21.809	3416	3421	3426	rBV2	18199	41402	1.42%	0.165%

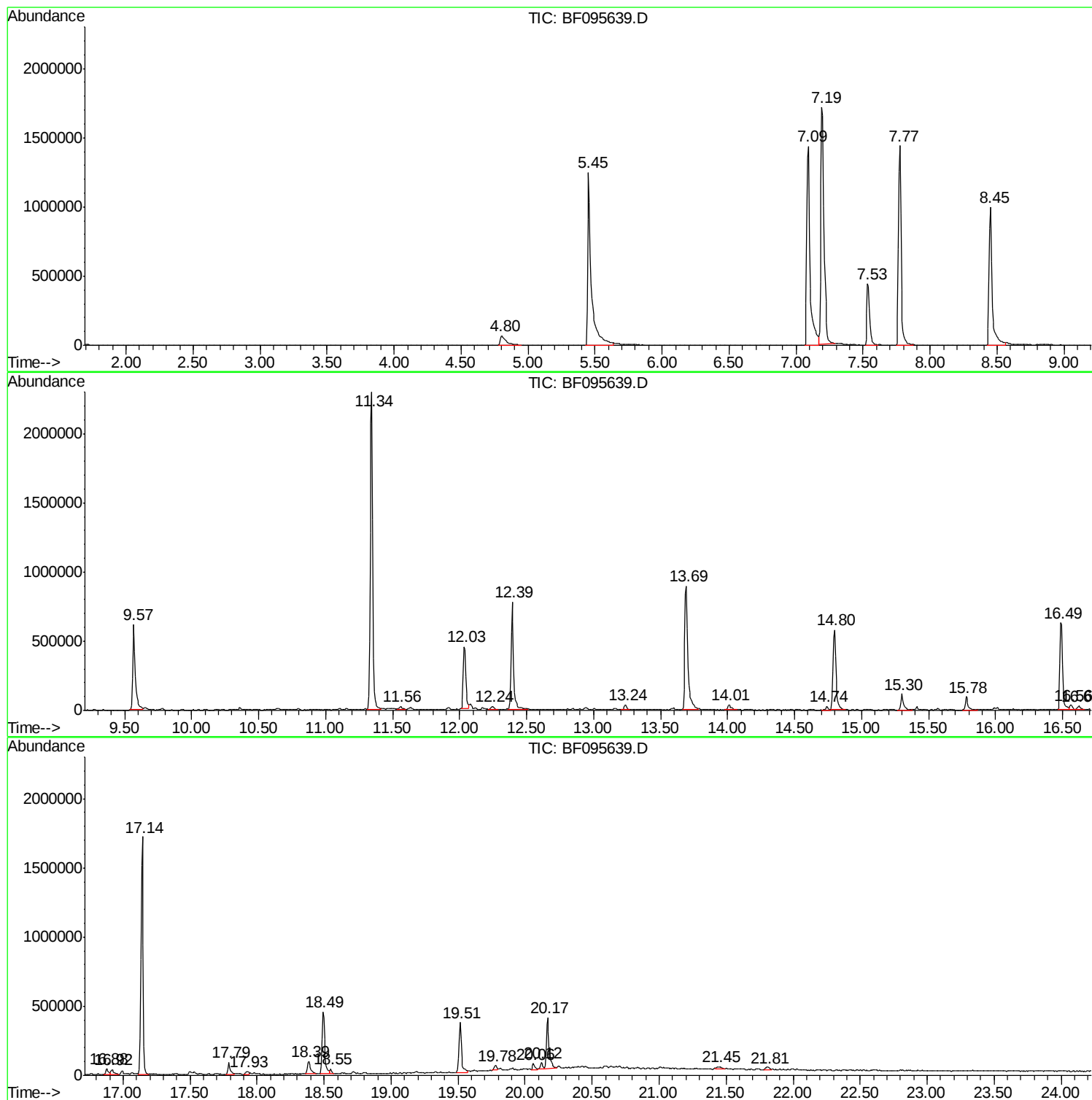
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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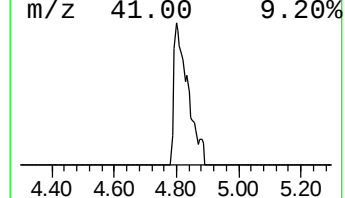
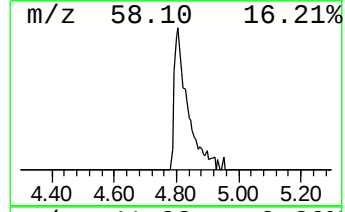
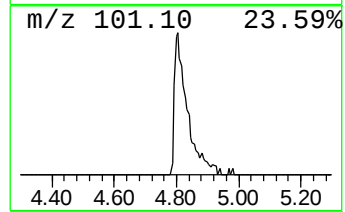
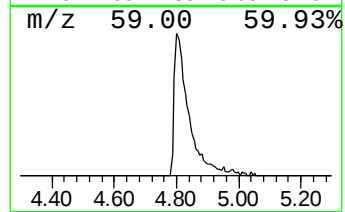
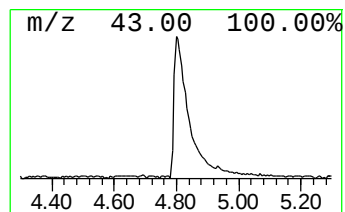
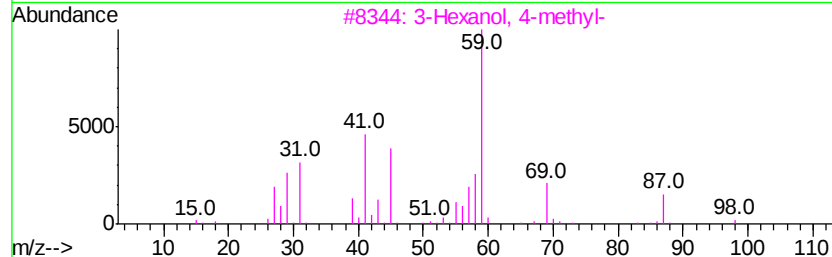
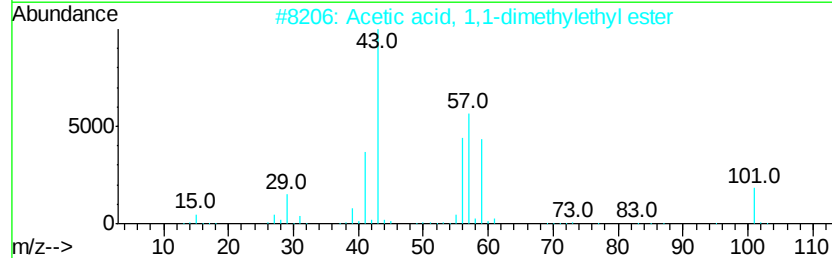
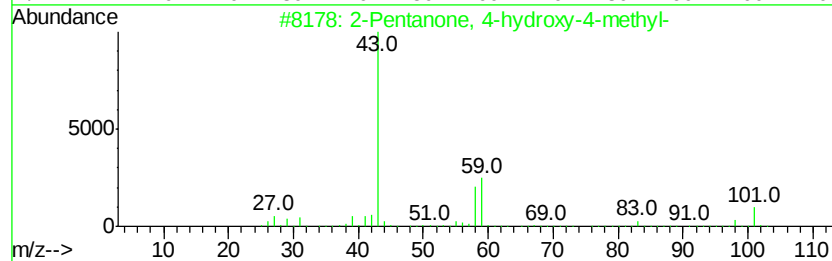
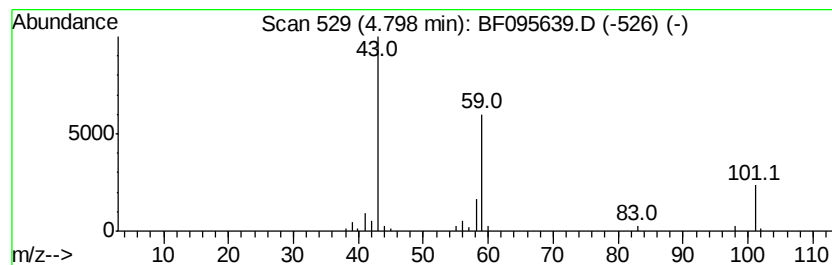
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.12 ng	217228	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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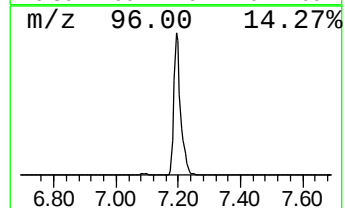
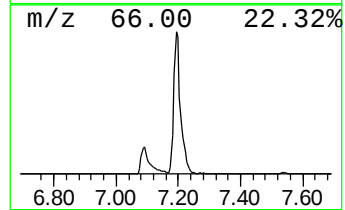
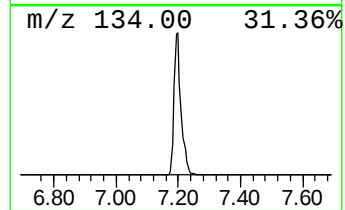
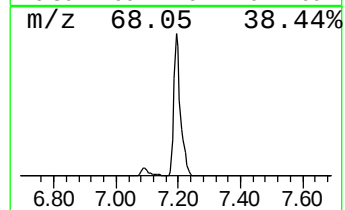
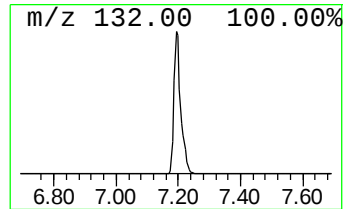
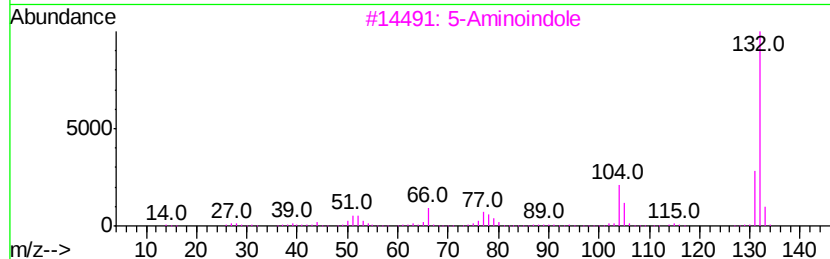
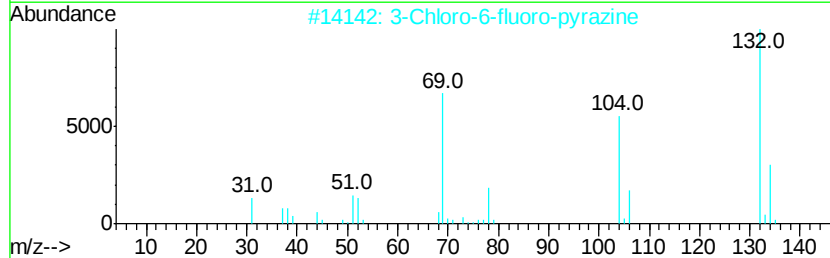
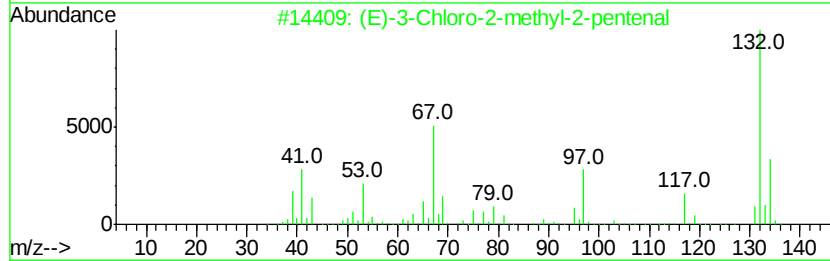
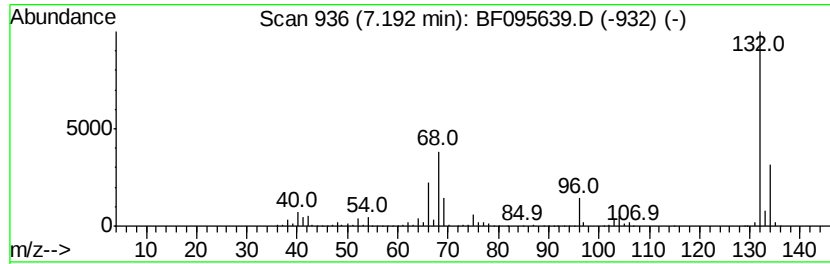
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	89.50 ng	2732300	1,4-Dichlorobenzene-d4	7.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16	
3	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9	



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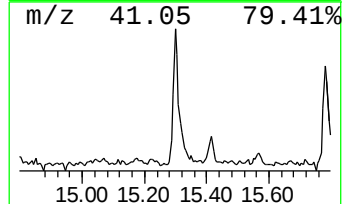
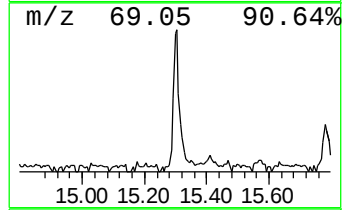
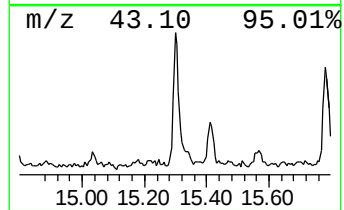
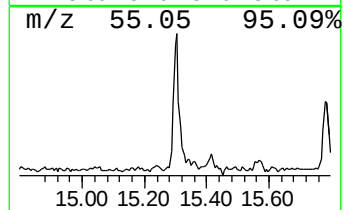
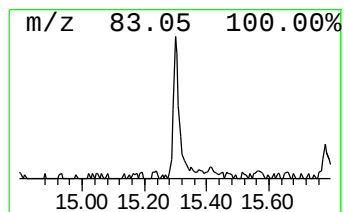
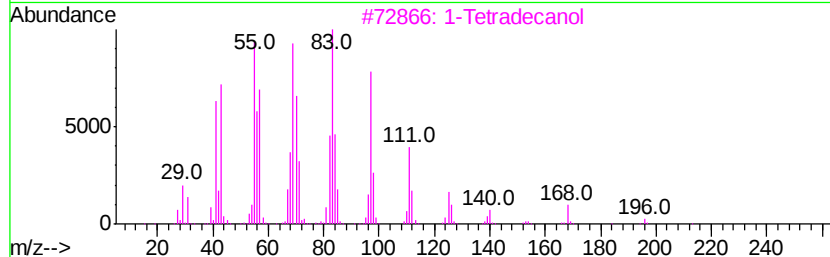
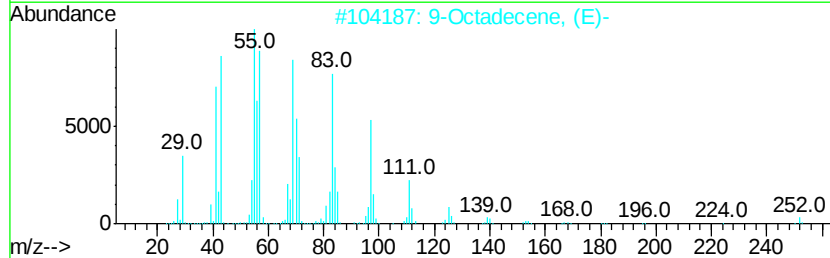
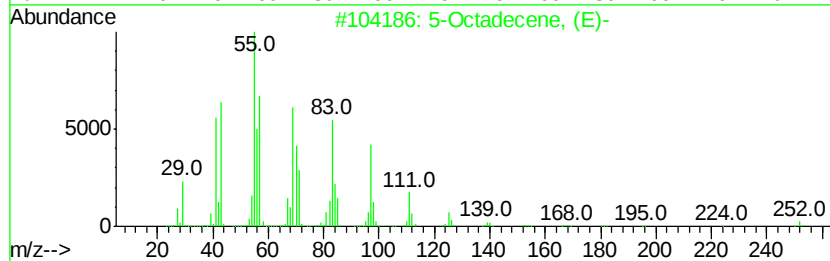
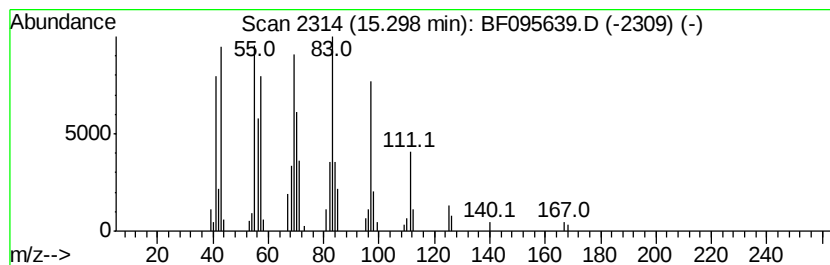
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	4.13 ng	172826	Phenanthrene-d10	14.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2		9-Octadecene, (E)-	252	C18H36	007206-25-9	91
3		1-Tetradecanol	214	C14H30O	000112-72-1	90
4		1-Hexadecanol	242	C16H34O	036653-82-4	87
5		Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	81



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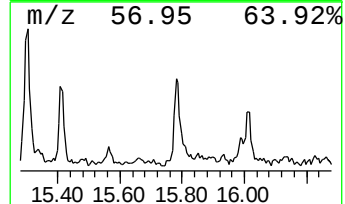
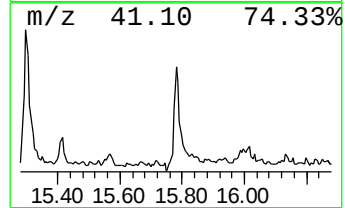
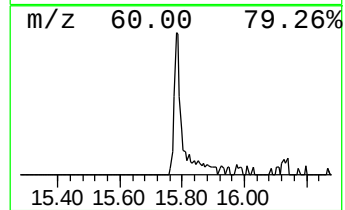
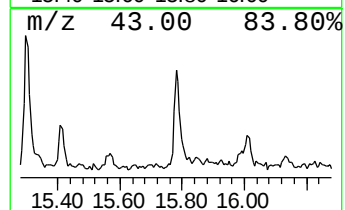
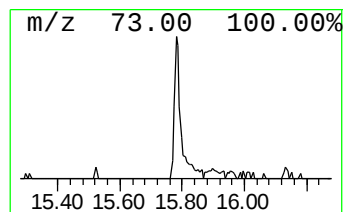
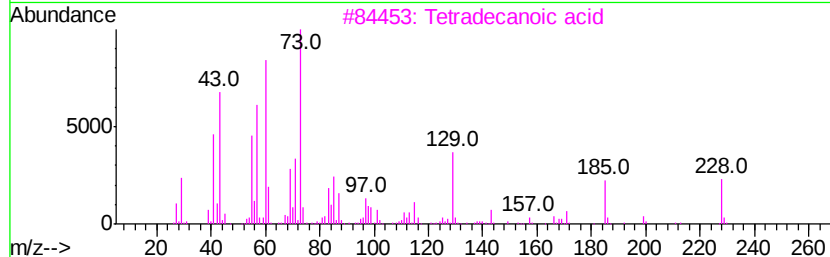
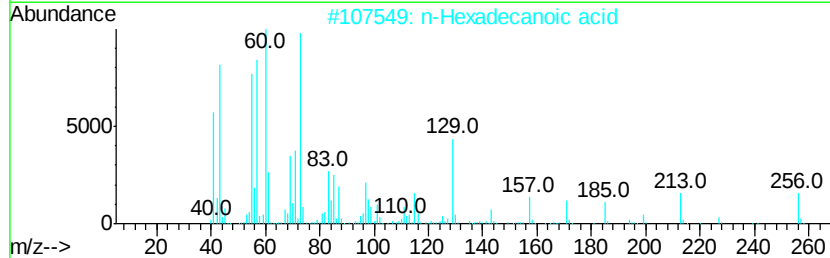
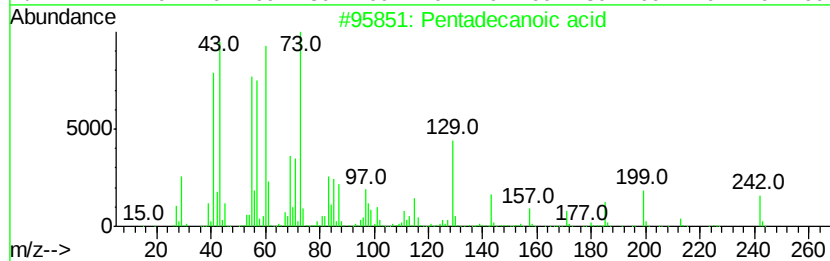
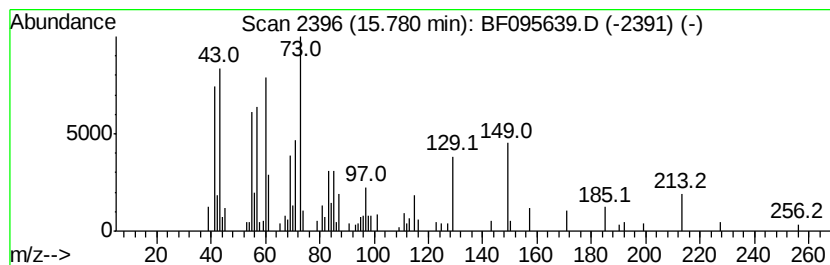
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	3.55 ng	148273	Phenanthrene-d10	14.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18



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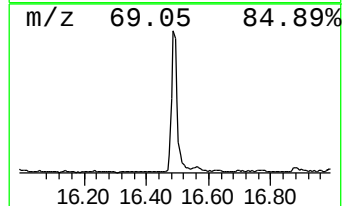
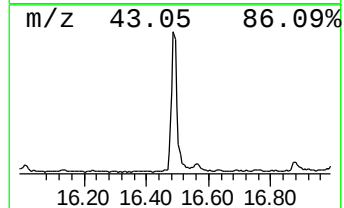
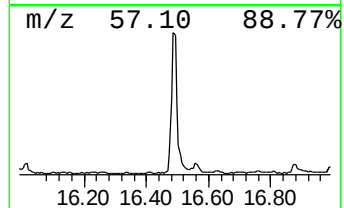
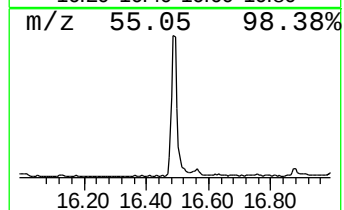
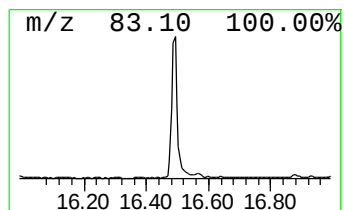
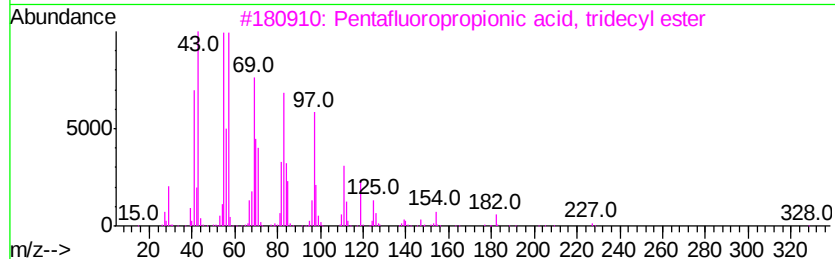
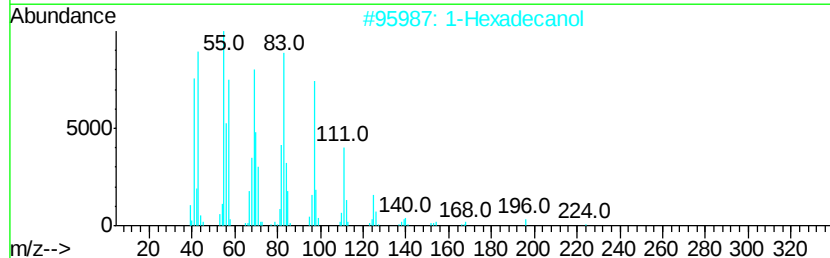
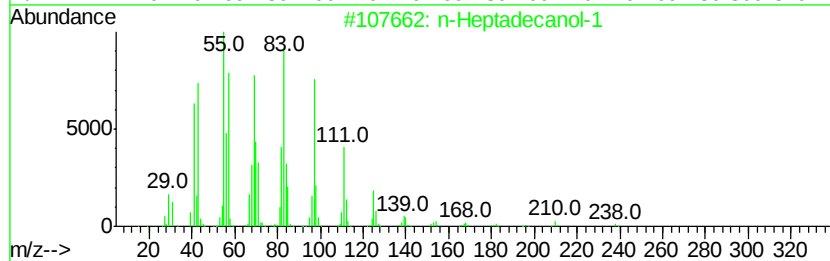
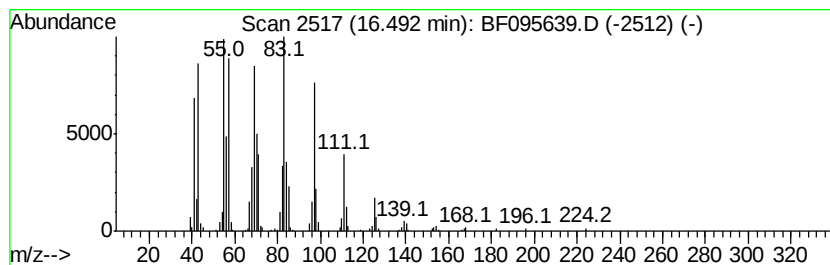
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Peak Number 6 n-Heptadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.49	19.82 ng	829086	Phenanthrene-d10		14.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2			1-Hexadecanol	242	C16H34O	036653-82-4	93
3			Pentafluoropropionic acid, tridecyl ester	346	C16H27F5O2	959261-22-4	93
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5			5-Octadecene, (E)-	252	C18H36	007206-21-5	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095639.D
Acq On : 2 Jun 2017 17:56
Operator : SJ/MA
Sample : I3420-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-TP-4

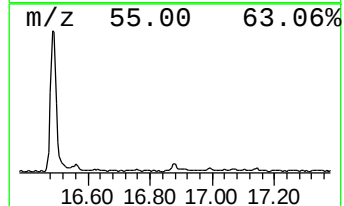
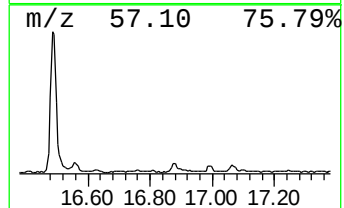
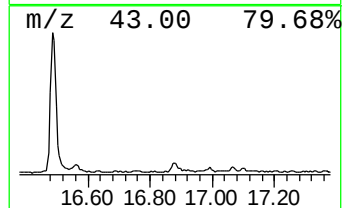
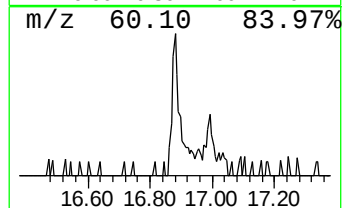
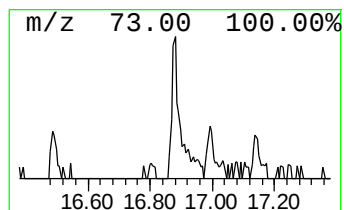
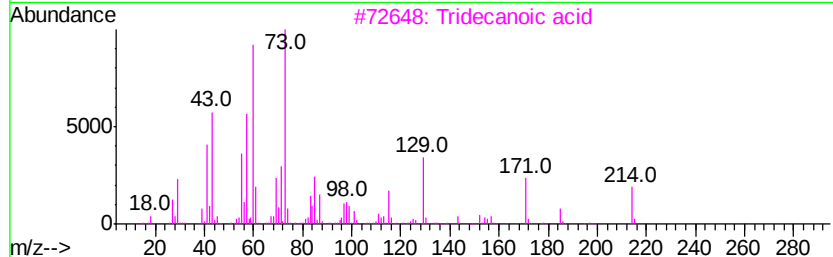
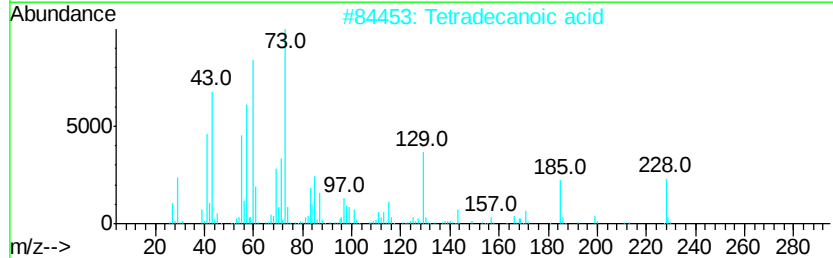
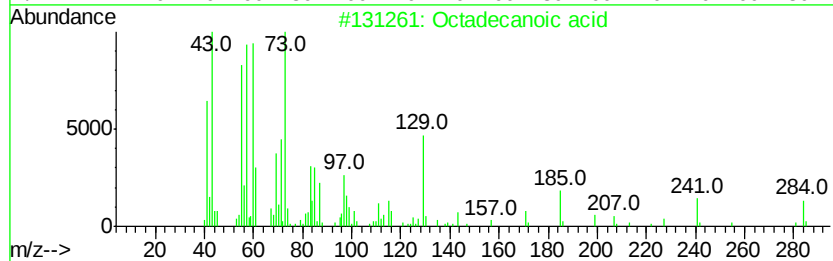
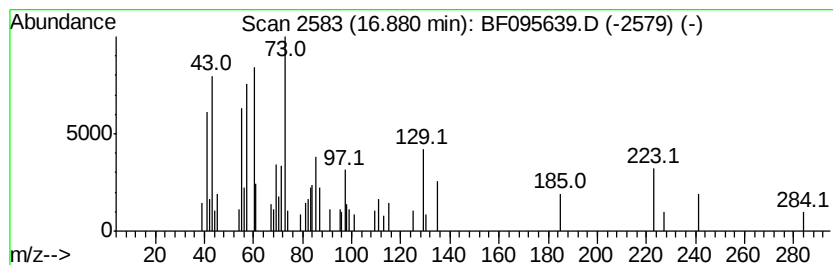
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	2.19 ng	66967	Chrysene-d12	18.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3		Tridecanoic acid	214	C13H26O2	000638-53-9	50
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095639.D
Acq On : 2 Jun 2017 17:56
Operator : SJ/MA
Sample : I3420-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-TP-4

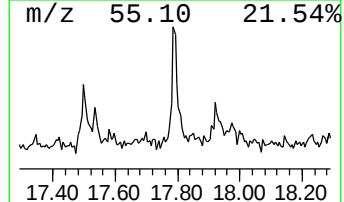
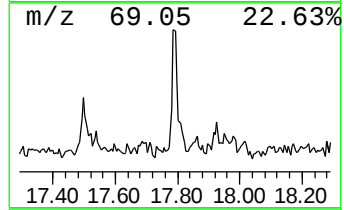
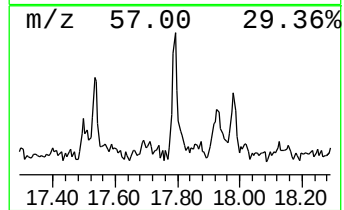
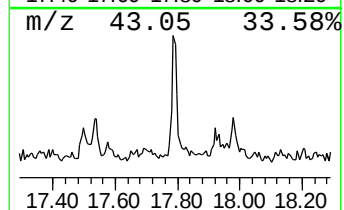
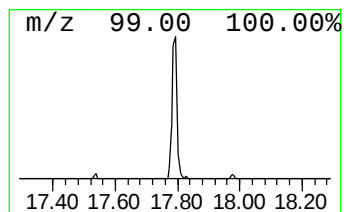
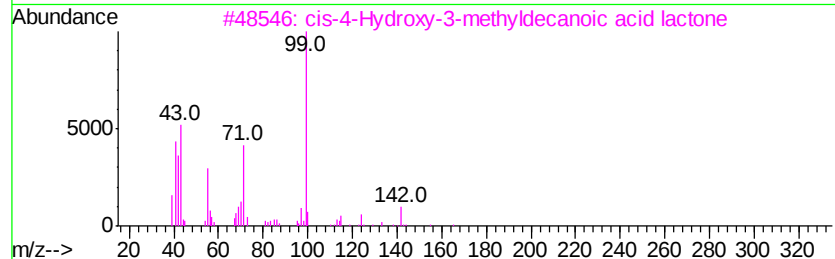
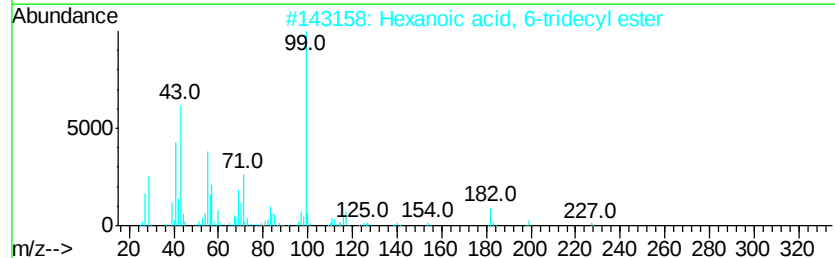
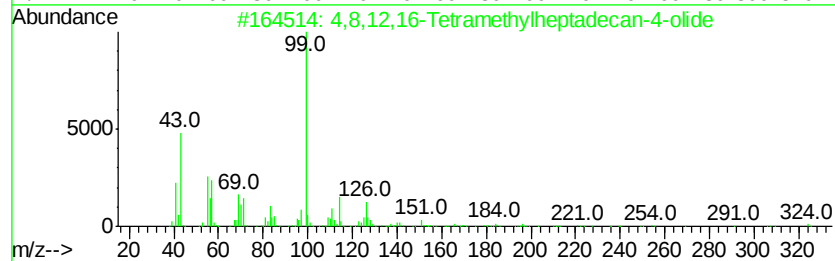
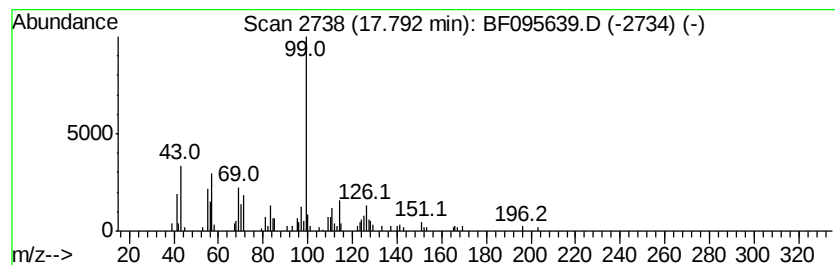
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,8,12,16-Tetramethylheptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	3.50 ng	107217	Chrysene-d12	18.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	90
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	50
3	cis-4-Hydroxy-3-methyldecanoic a...	184	C11H20O2	147254-32-8	50
4	Hexanoic acid, 3-tetradecyl ester	312	C20H40O2	1000279-29-7	50
5	Hexanoic acid, 3-tridecyl ester	298	C19H38O2	1000279-29-2	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095639.D
Acq On : 2 Jun 2017 17:56
Operator : SJ/MA
Sample : I3420-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

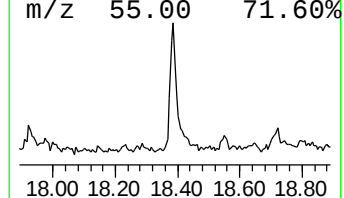
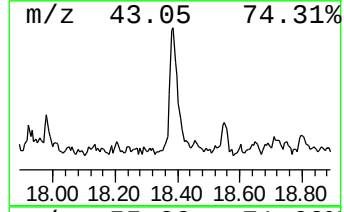
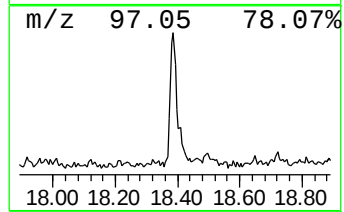
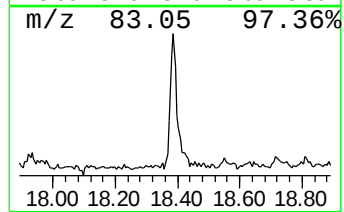
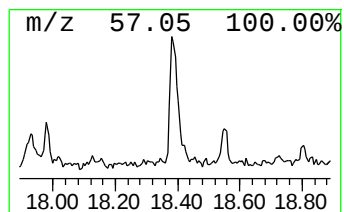
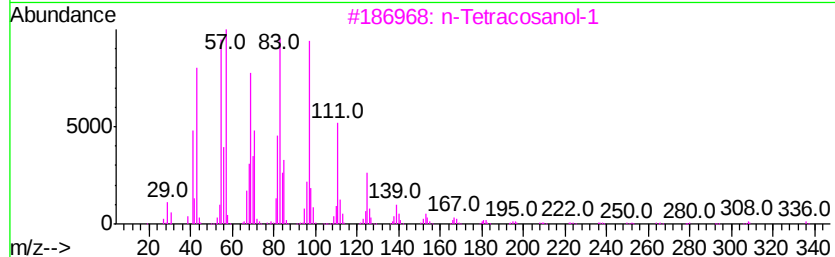
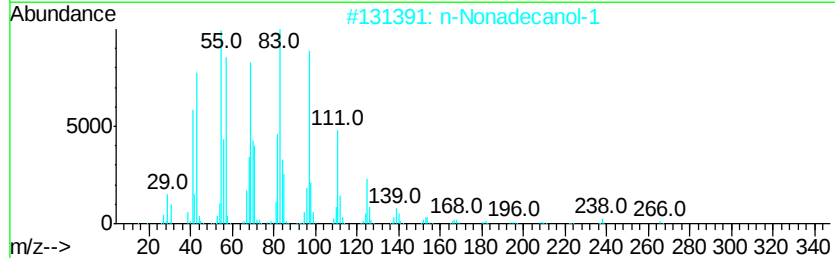
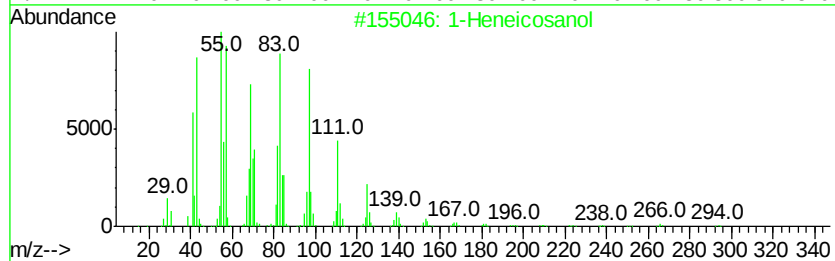
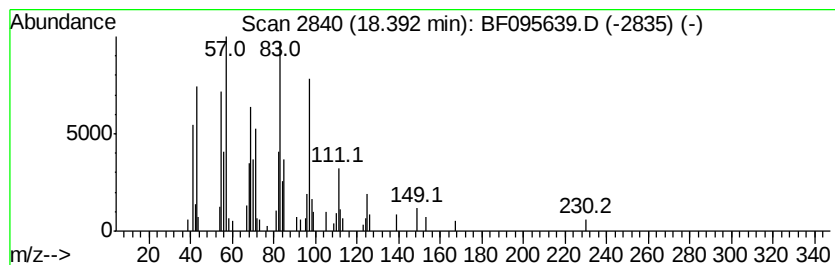
Instrument :
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ClientSampleId :
TP-3-TP-4

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 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.39	4.68 ng	143075	Chrysene-d12	18.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	1-Heptacosanol	396	C27H56O	002004-39-9	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060217\
Data File : BF095639.D
Acq On : 2 Jun 2017 17:56
Operator : SJ/MA
Sample : I3420-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-TP-4

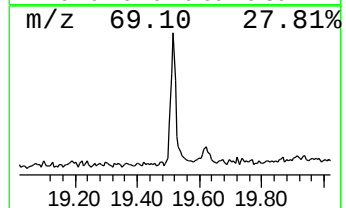
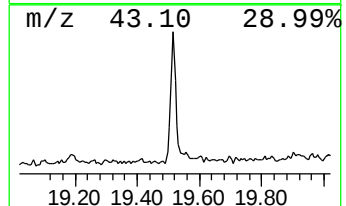
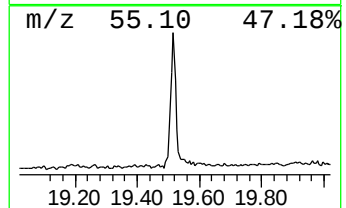
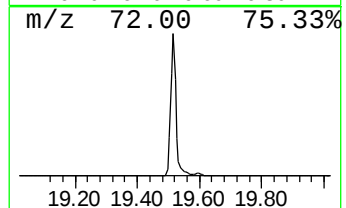
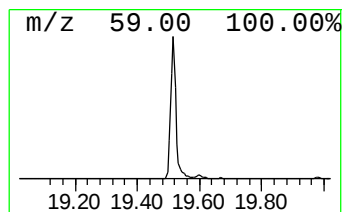
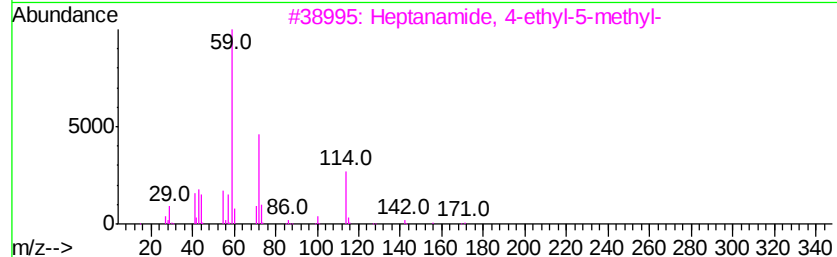
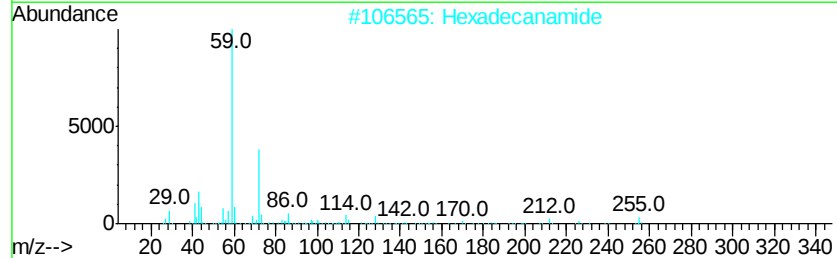
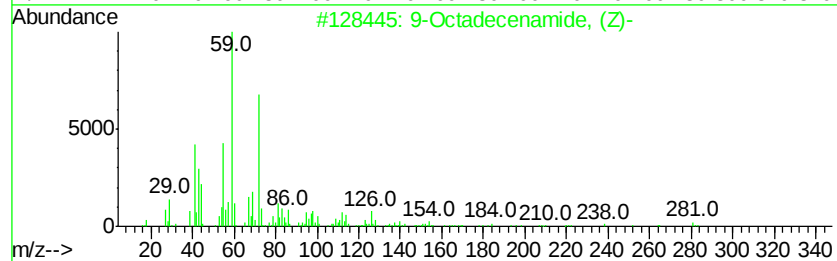
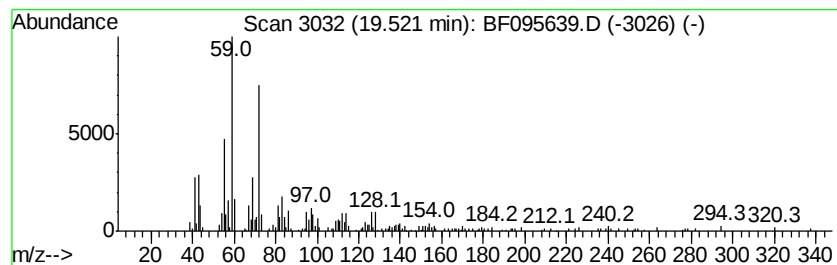
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	16.77 ng	447381	Perylene-d12	20.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	64
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	58
4		2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	43
5		trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060217\
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Sample : I3420-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	7.1 ng		217228	1	7.54	610544	20.0
unknown7.19	7.19	89.5 ng		2732300	1	7.54	610544	20.0
5-Octadecene, (E)-	15.30	4.1 ng		172826	4	14.80	836485	20.0
Pentadecanoic acid	15.78	3.5 ng		148273	4	14.80	836485	20.0
n-Heptadecanol-1	16.49	19.8 ng		829086	4	14.80	836485	20.0
Octadecanoic acid	16.88	2.2 ng		66967	5	18.49	611882	20.0
4,8,12,16-Tetrame...	17.79	3.5 ng		107217	5	18.49	611882	20.0
1-Heneicosanol	18.39	4.7 ng		143075	5	18.49	611882	20.0
9-Octadecenamide, ...	19.52	16.8 ng		447381	6	20.17	533638	20.0