

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
 Data File : BF094871.D
 Acq On : 4 May 2017 12:54
 Operator : SJ/MA
 Sample : I2916-04
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06-7.0-8.0

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	5.042	522	528	548	rBV	281782	581484	21.60%	2.601%
2	5.678	631	636	664	rBV	1758006	2479699	92.12%	11.093%
3	6.242	725	732	738	rBV2	21421	34456	1.28%	0.154%
4	7.272	901	907	921	rBV	1769453	2494616	92.68%	11.160%
5	7.389	921	927	938	rVB	2112450	2691739	100.00%	12.042%
6	7.725	980	984	995	rVB	478332	520259	19.33%	2.327%
7	7.966	1019	1025	1038	rBV	1628235	2221617	82.53%	9.938%
8	8.442	1101	1106	1113	rBV	30890	37388	1.39%	0.167%
9	8.625	1131	1137	1146	rBV	1277769	1606238	59.67%	7.186%
10	9.742	1322	1327	1340	rBV	575768	678476	25.21%	3.035%
11	11.518	1623	1629	1646	rBV	1833705	2217361	82.38%	9.919%
12	11.813	1674	1679	1686	rBV2	19531	27541	1.02%	0.123%
13	12.207	1741	1746	1754	rBV	212302	258321	9.60%	1.156%
14	12.571	1803	1808	1823	rBV2	512241	699780	26.00%	3.130%
15	13.418	1949	1952	1958	rVB	30536	33515	1.25%	0.150%
16	13.865	2023	2028	2042	rBV	873149	1194109	44.36%	5.342%
17	14.189	2079	2083	2086	rBV	36322	41852	1.55%	0.187%
18	14.924	2199	2208	2211	rBV2	23380	36302	1.35%	0.162%
19	14.971	2211	2216	2226	rVB2	470819	586577	21.79%	2.624%
20	15.195	2249	2254	2255	rBV3	27515	31340	1.16%	0.140%
21	15.942	2377	2381	2392	rBV3	133070	176543	6.56%	0.790%
22	17.030	2562	2566	2572	rBV2	19690	27579	1.02%	0.123%
23	17.295	2606	2611	2615	rBV	1250254	1292396	48.01%	5.782%
24	17.689	2669	2678	2681	rBV2	18688	32734	1.22%	0.146%
25	18.553	2820	2825	2835	rBV2	105201	271510	10.09%	1.215%
26	18.636	2835	2839	2847	rVV	472647	541252	20.11%	2.421%
27	19.365	2951	2963	2978	rBV7	109104	373598	13.88%	1.671%
28	19.665	3007	3014	3017	rBV3	44079	56108	2.08%	0.251%
29	19.777	3029	3033	3037	rVB	85639	93218	3.46%	0.417%
30	20.059	3077	3081	3085	rBV	103851	116094	4.31%	0.519%
31	20.112	3085	3090	3092	rBV3	35900	65614	2.44%	0.294%
32	20.300	3118	3122	3134	rBV	362792	436669	16.22%	1.953%
33	20.783	3199	3204	3211	rVB2	63806	87082	3.24%	0.390%
34	20.883	3213	3221	3225	rBV3	39634	89669	3.33%	0.401%

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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

35	21.847	3380	3385	3394	rVB7	25089	62597	2.33%	0.280%
36	22.112	3425	3430	3436	rVB6	24713	45190	1.68%	0.202%
37	22.353	3465	3471	3480	rBV6	25156	78186	2.90%	0.350%
38	22.918	3560	3567	3569	rBV6	15942	35136	1.31%	0.157%

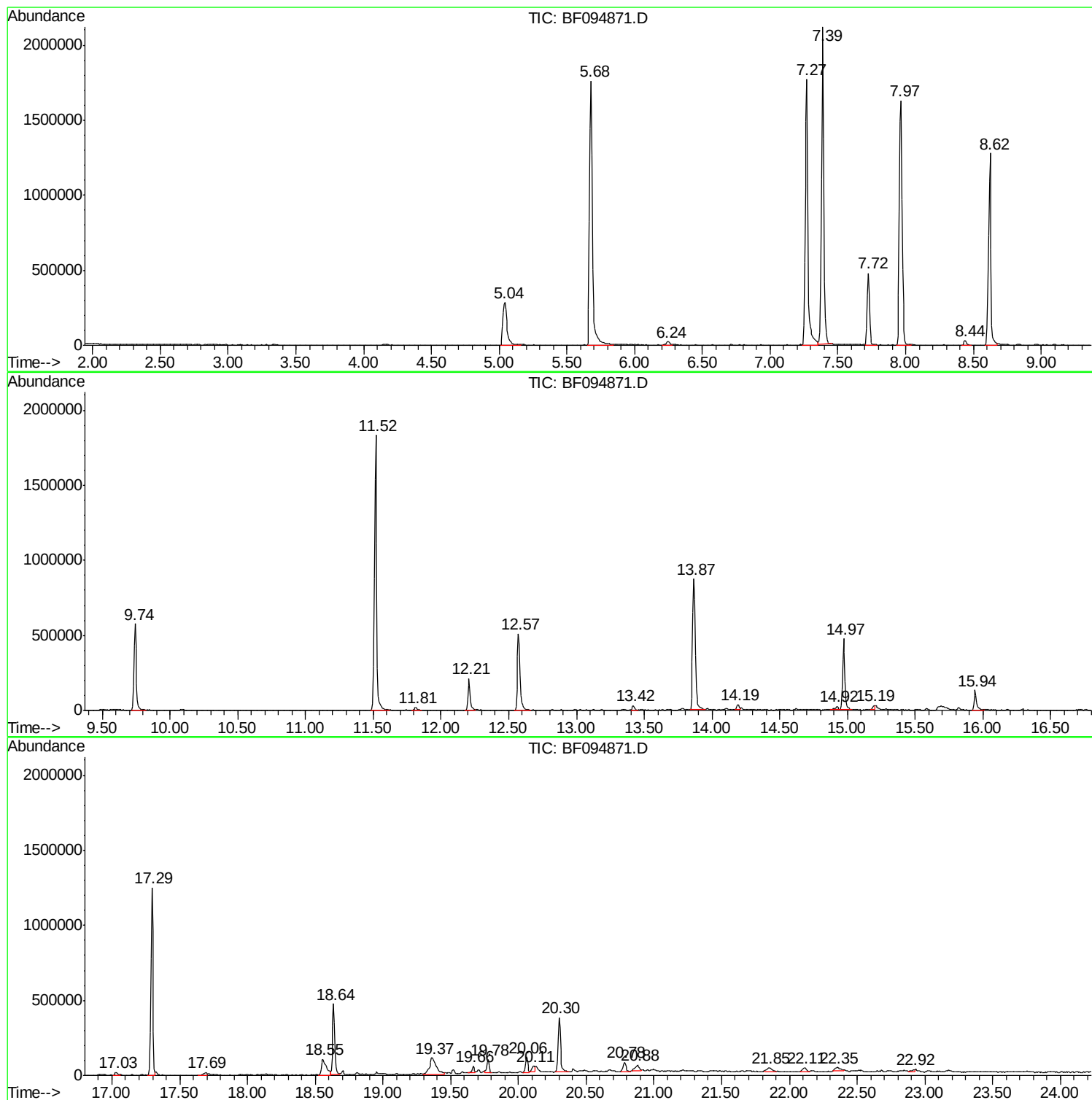
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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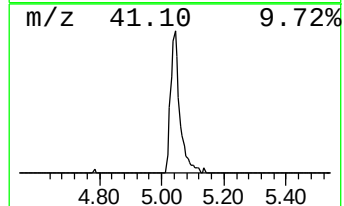
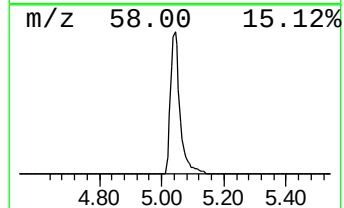
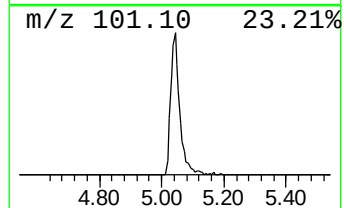
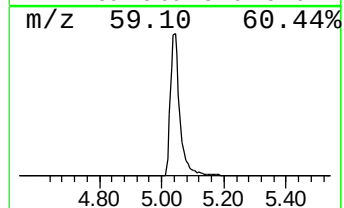
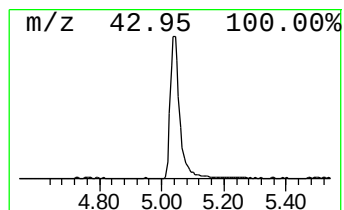
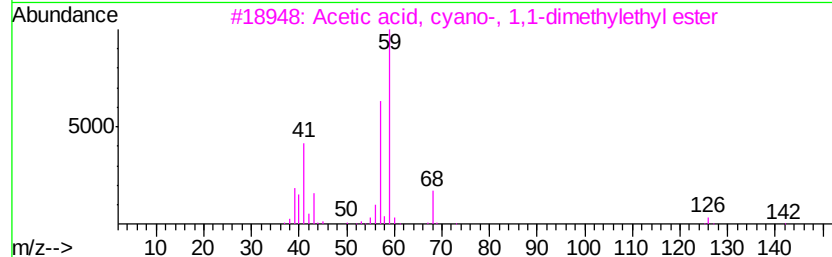
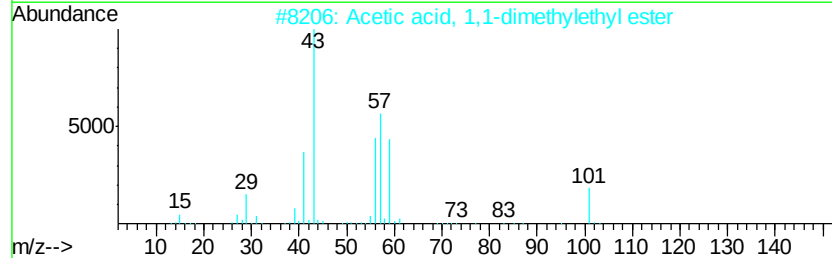
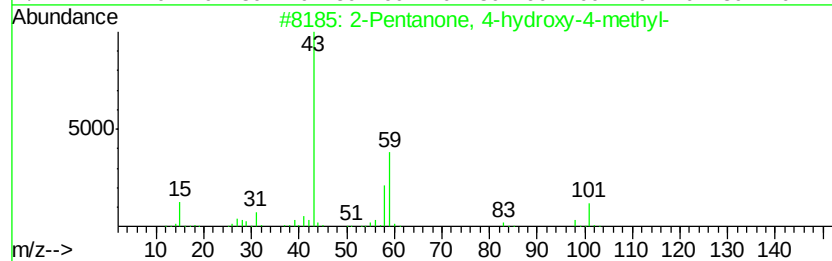
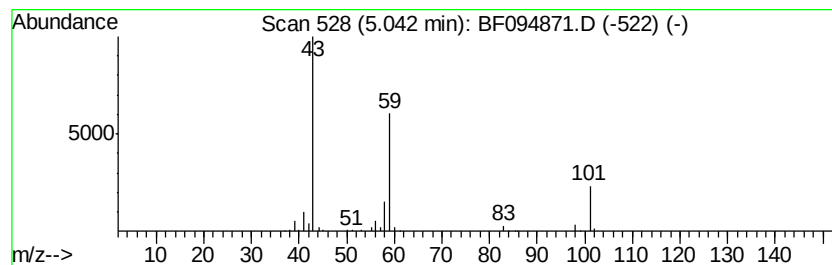
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	22.35 ng	581484	1,4-Dichlorobenzene-d4	7.72

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			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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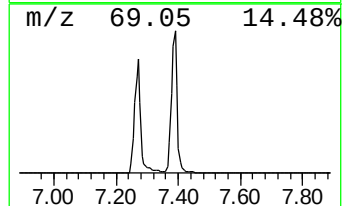
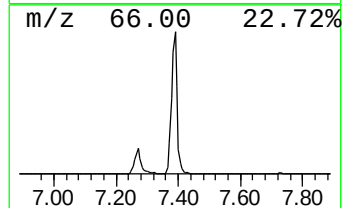
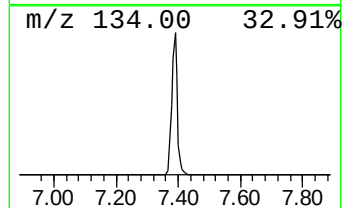
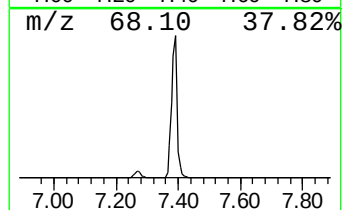
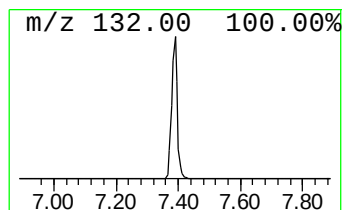
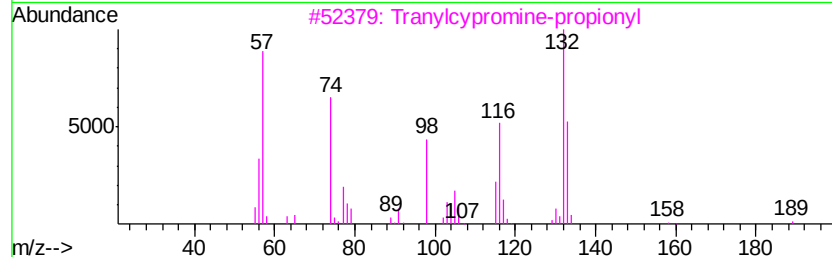
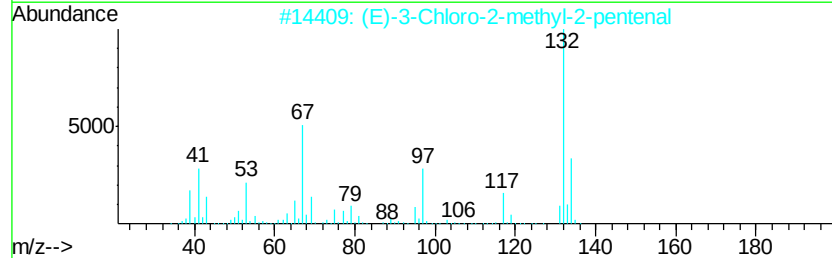
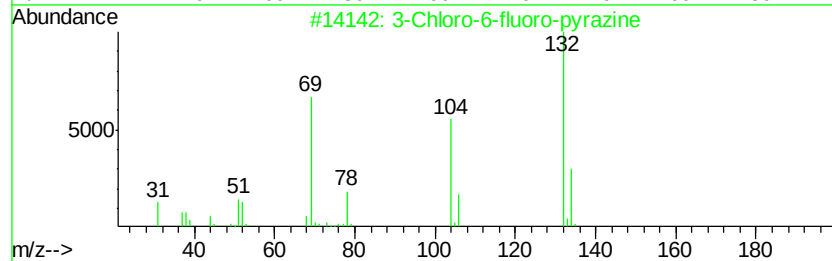
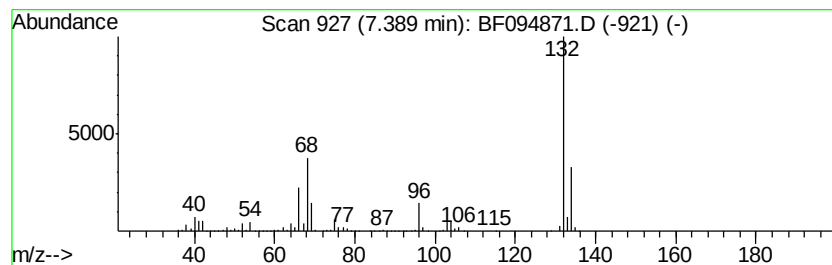
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Peak Number 2 unknown7.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.39	103.48 ng	2691740	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Xenon	132	Xe	007440-63-3	9



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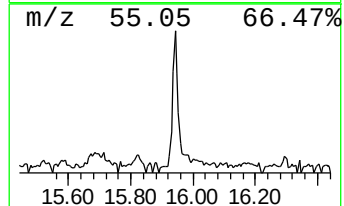
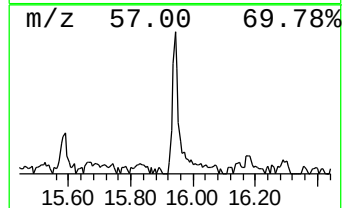
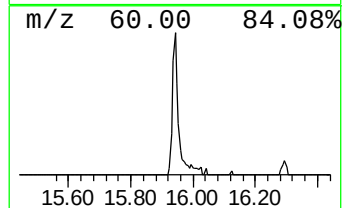
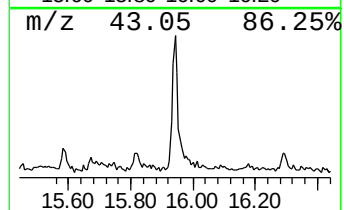
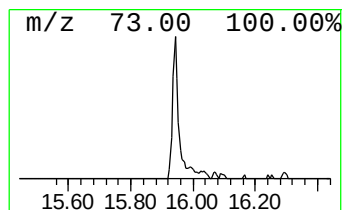
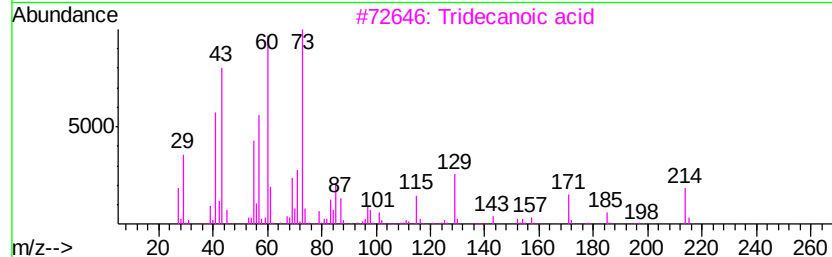
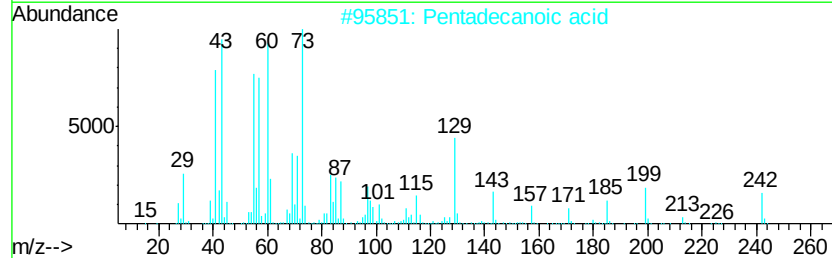
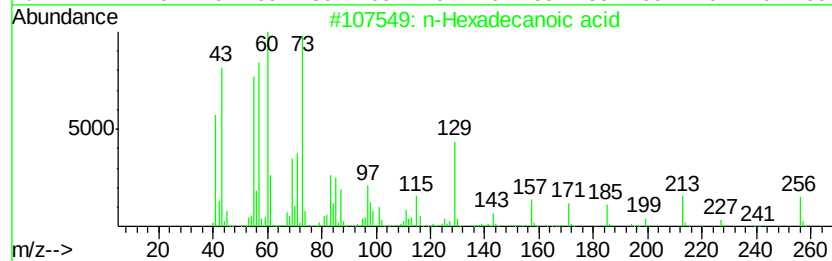
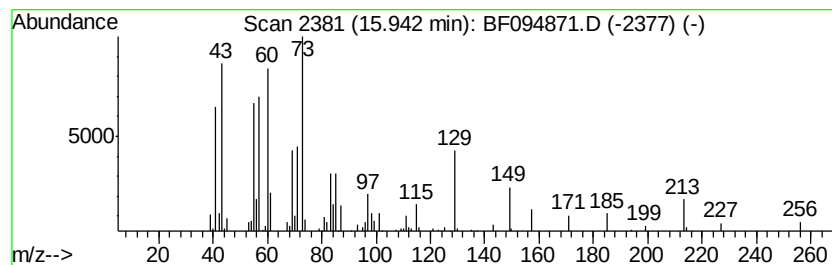
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.94	6.02 ng	176543	Phenanthrene-d10		14.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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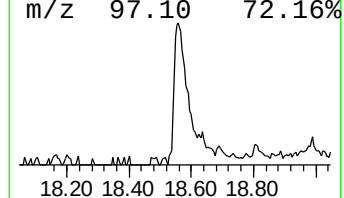
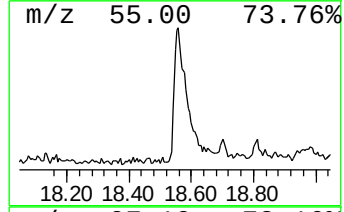
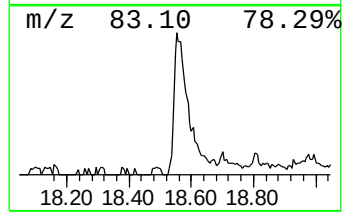
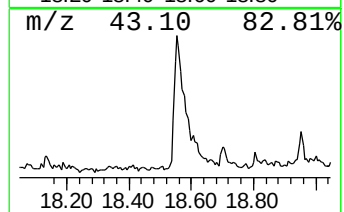
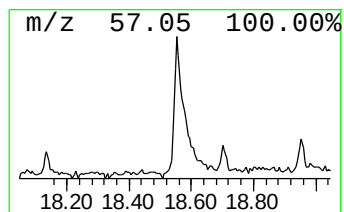
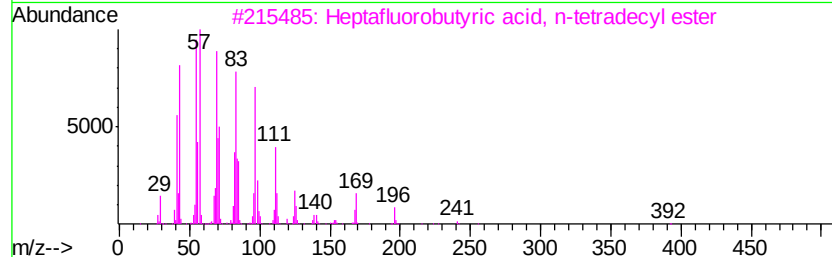
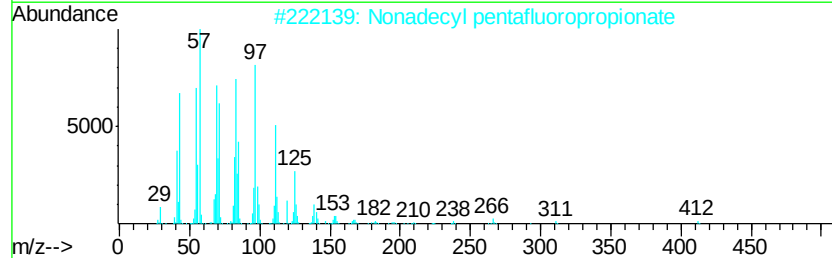
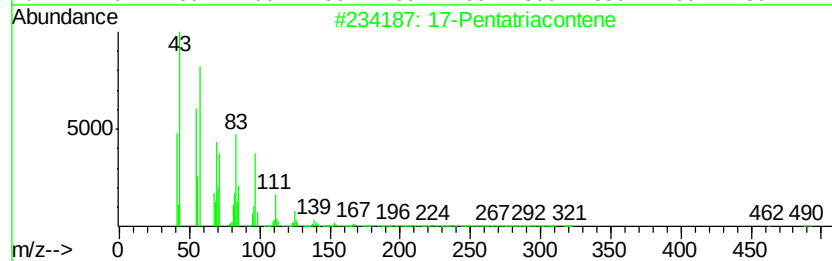
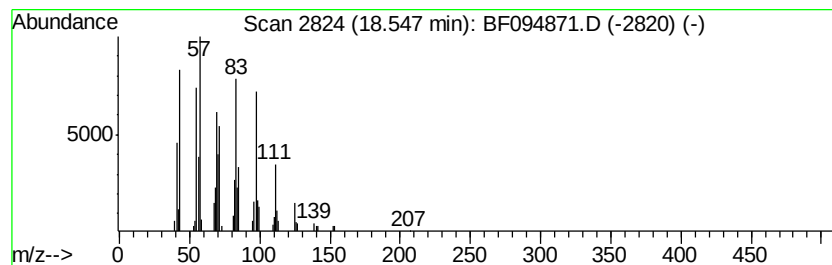
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.55	10.03 ng	271510	Chrysene-d12	18.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87



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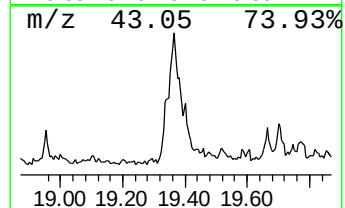
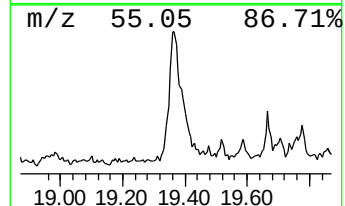
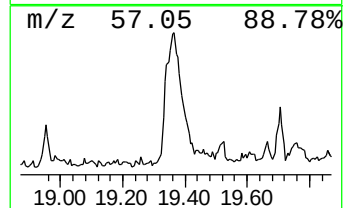
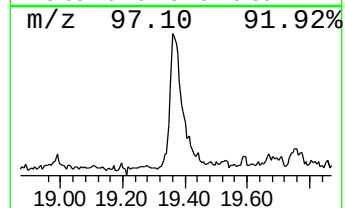
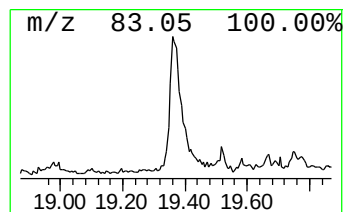
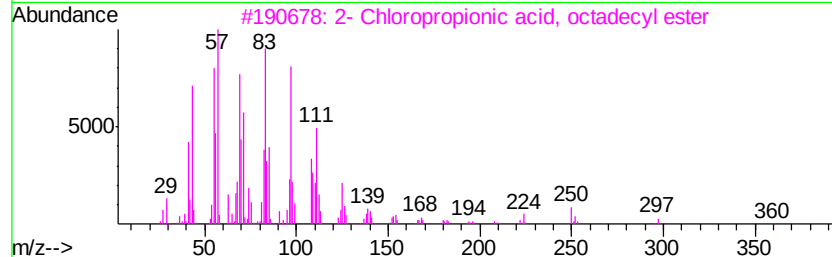
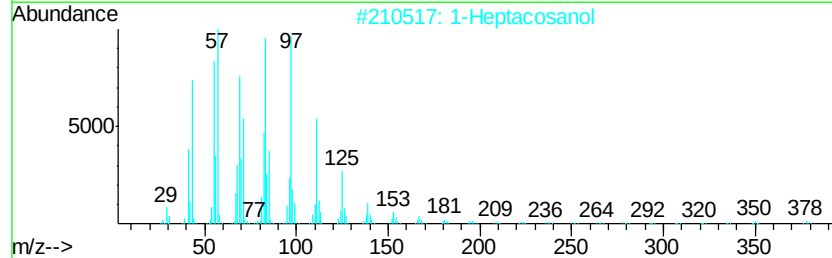
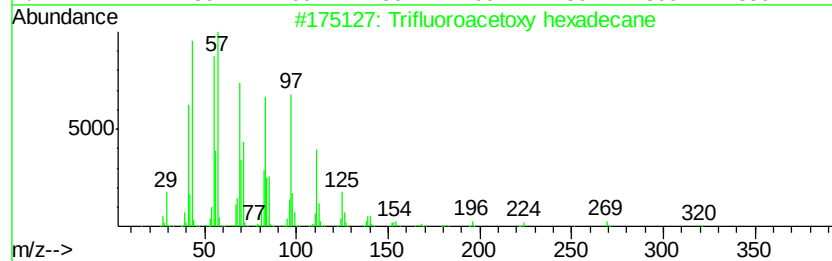
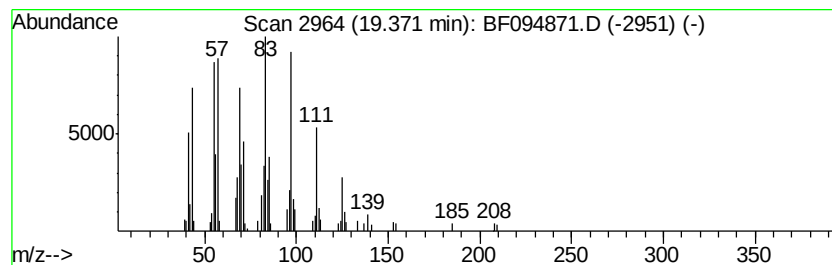
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	13.81 ng	373598	Chrysene-d12	18.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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Operator : SJ/MA
Sample : I2916-04
Misc :
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Instrument :
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ClientSampleId :
SB-06-7.0-8.0

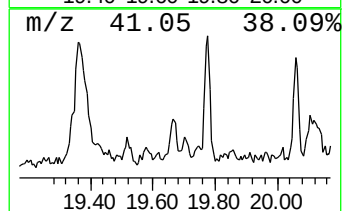
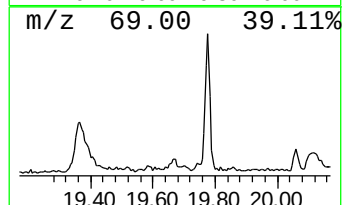
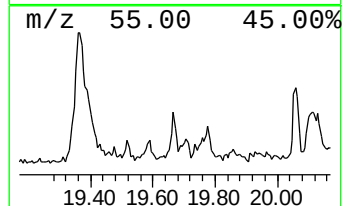
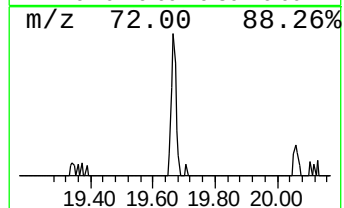
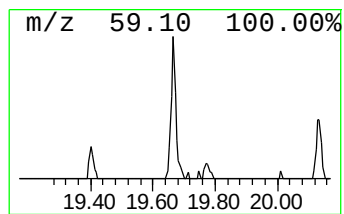
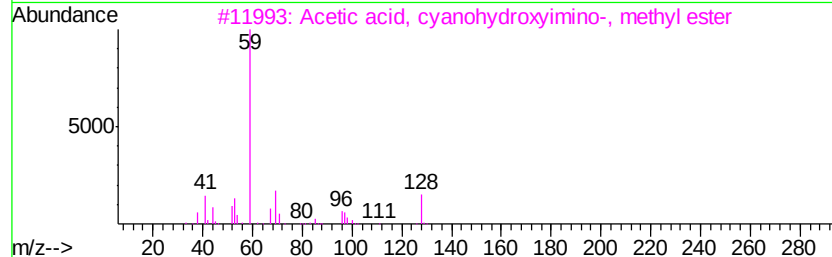
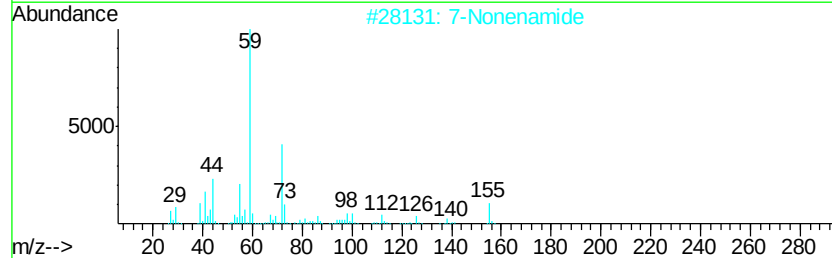
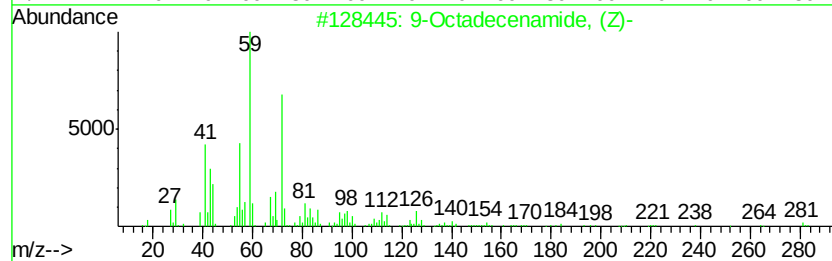
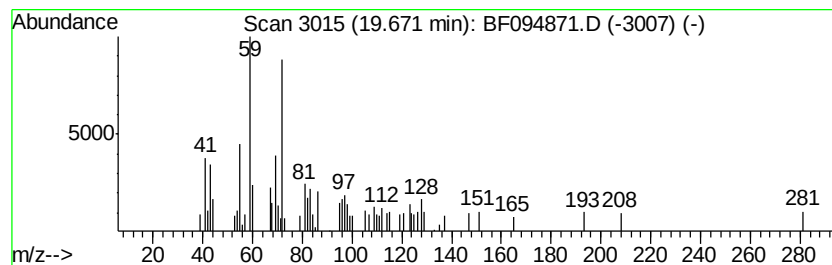
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.67	2.57 ng	56108	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		7-Nonenamide	155	C9H17NO	090949-53-4	64
3		Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	38
4		Dodecanamide	199	C12H25NO	001120-16-7	37
5		7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094871.D
Acq On : 4 May 2017 12:54
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Sample : I2916-04
Misc :
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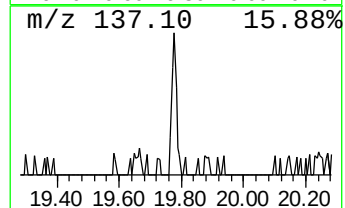
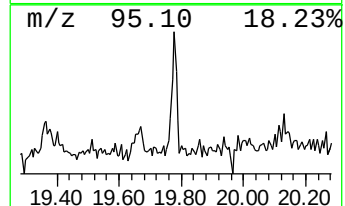
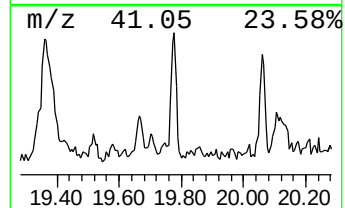
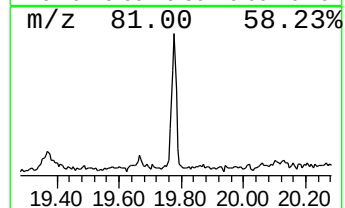
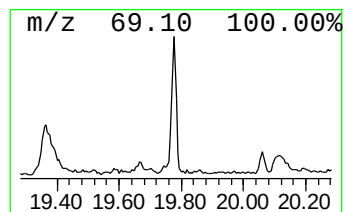
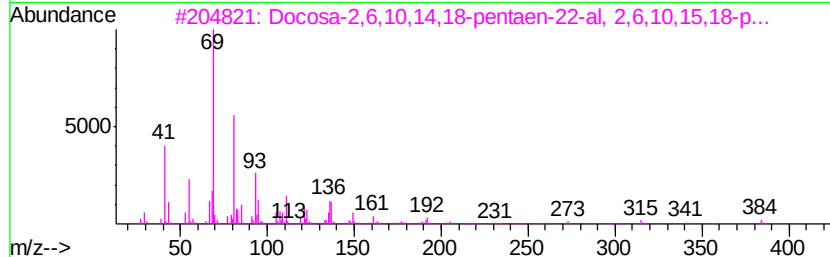
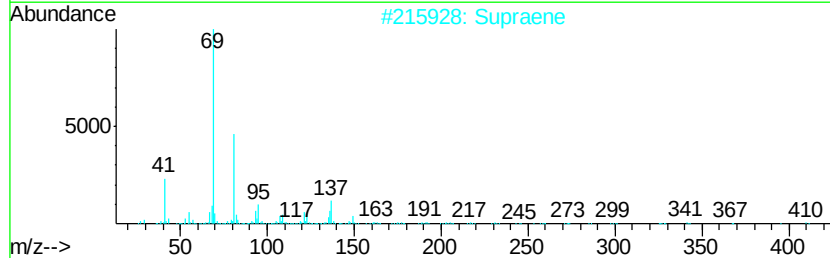
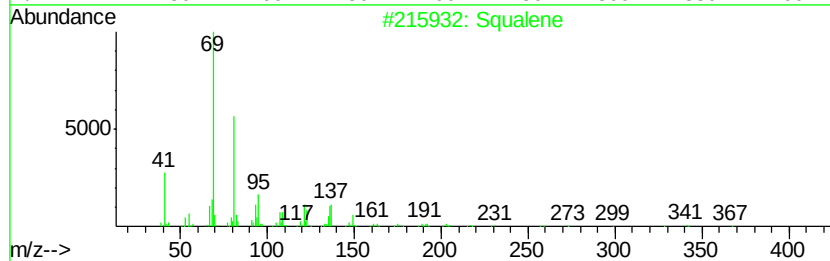
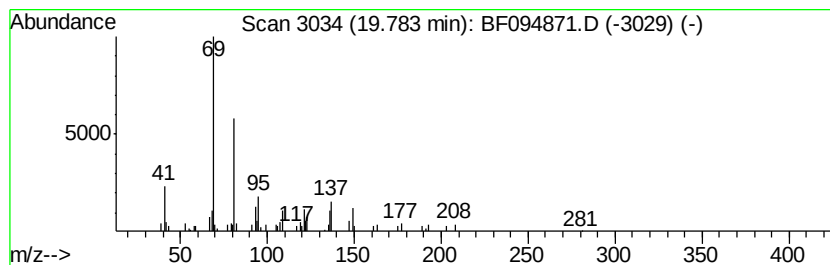
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	4.27 ng	93218	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	47
5		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094871.D
Acq On : 4 May 2017 12:54
Operator : SJ/MA
Sample : I2916-04
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ALS Vial : 32 Sample Multiplier: 1

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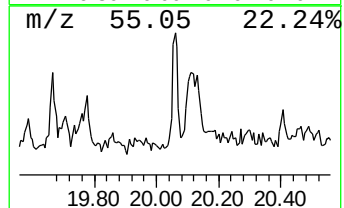
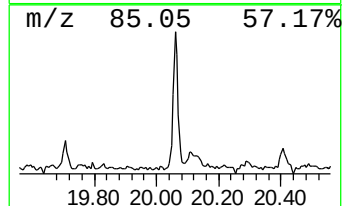
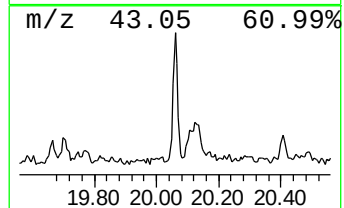
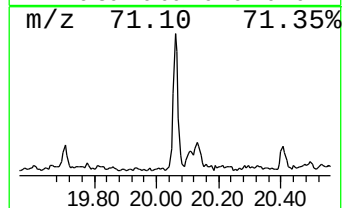
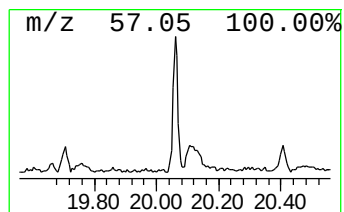
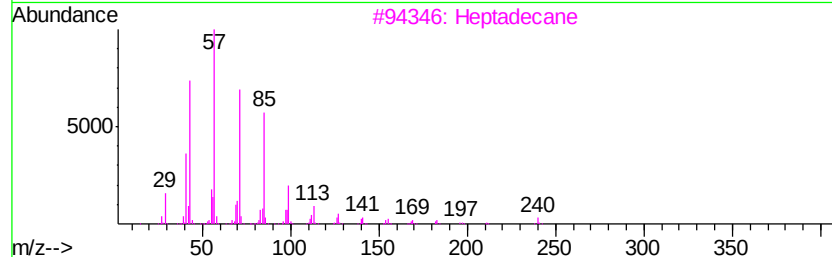
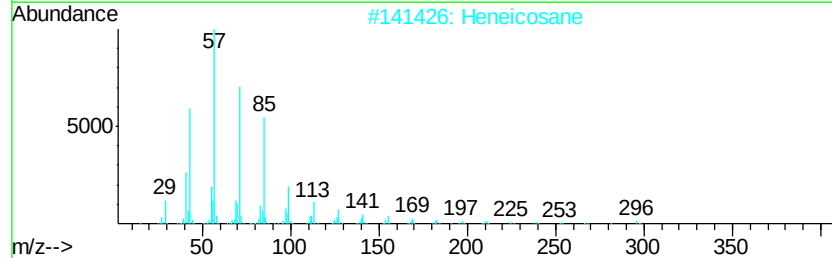
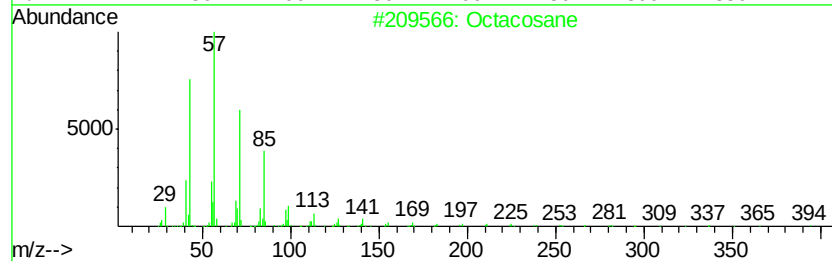
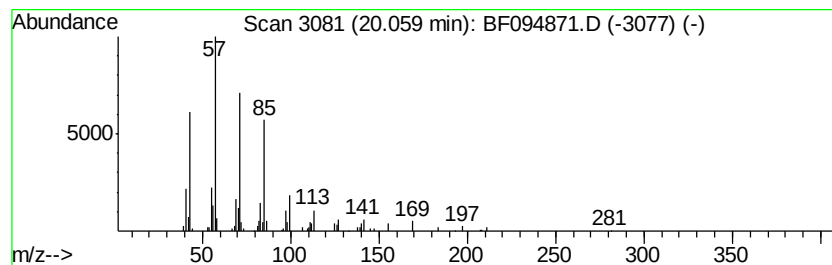
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.06	5.32 ng	116094	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptadecane	240	C17H36	000629-78-7	87
4		Octadecane	254	C18H38	000593-45-3	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094871.D
Acq On : 4 May 2017 12:54
Operator : SJ/MA
Sample : I2916-04
Misc :
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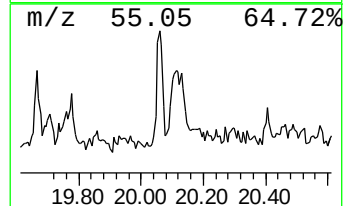
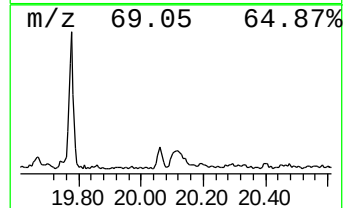
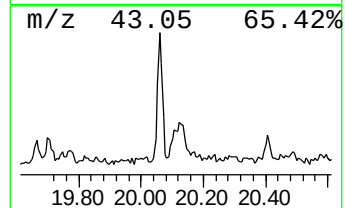
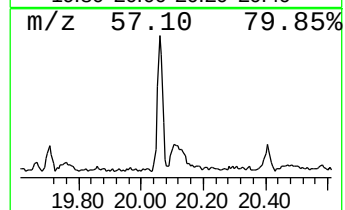
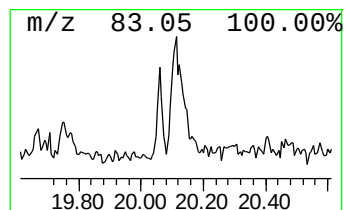
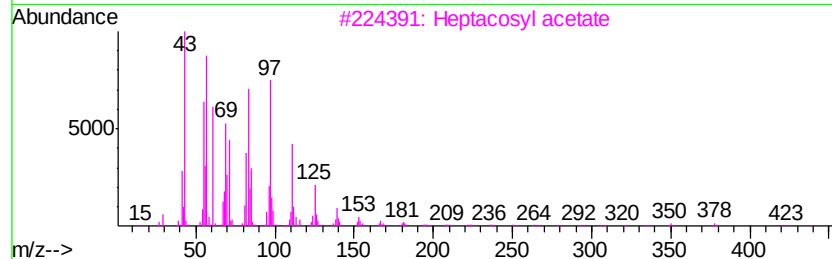
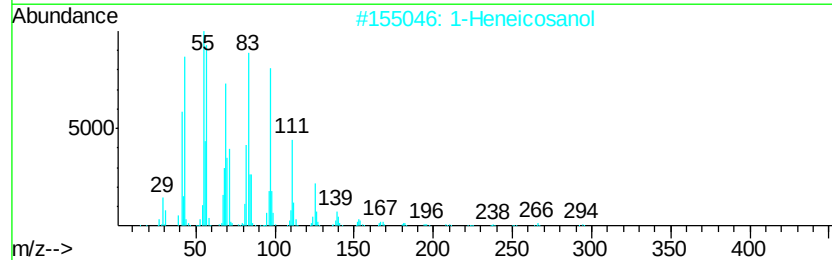
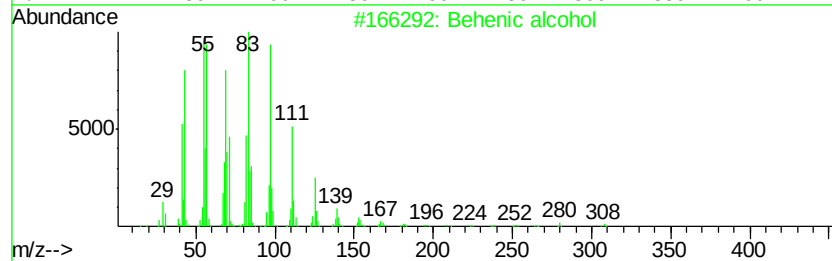
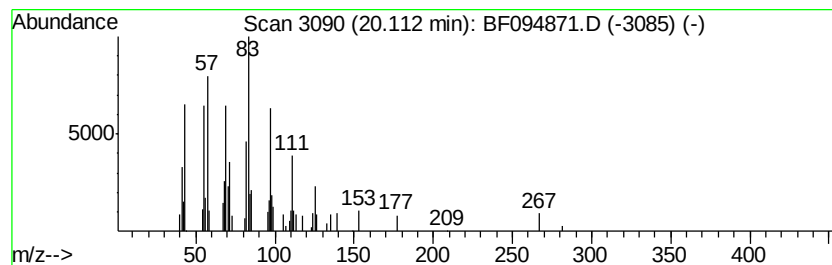
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Behenic alcohol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
20.11	3.01 ng	65614	Perylene-d12		20.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	70
3	Heptacosyl acetate	438	C29H58O2	1000351-78-2	64
4	Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	64
5	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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Acq On : 4 May 2017 12:54
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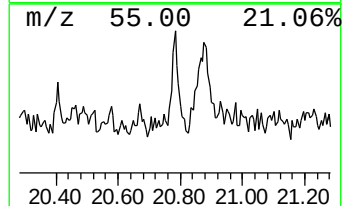
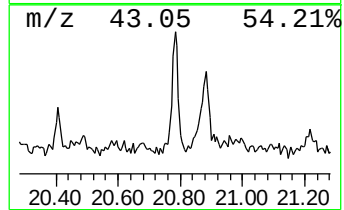
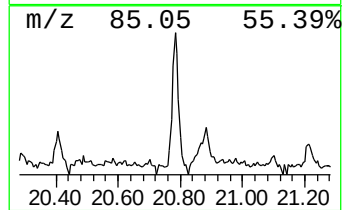
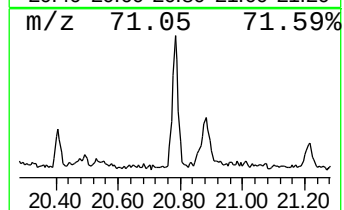
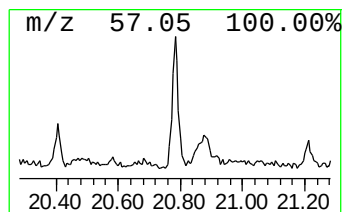
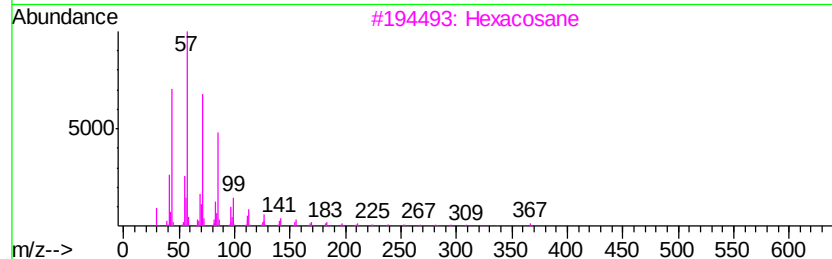
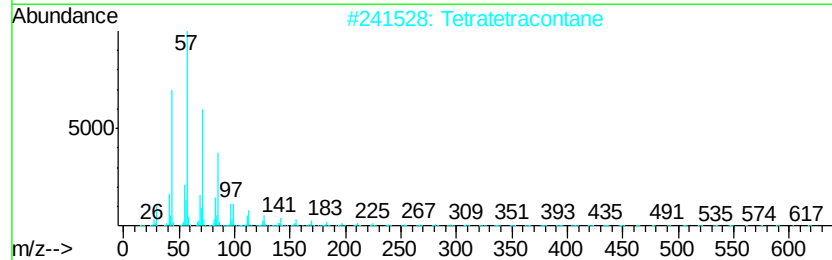
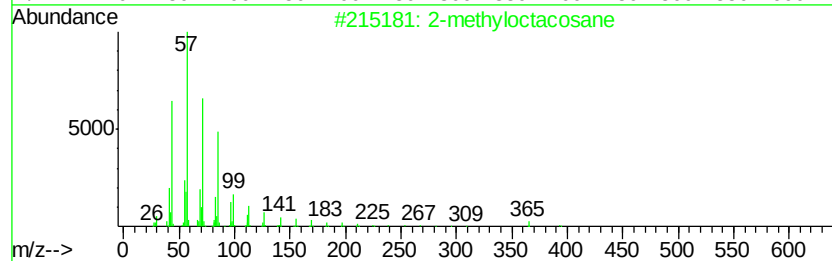
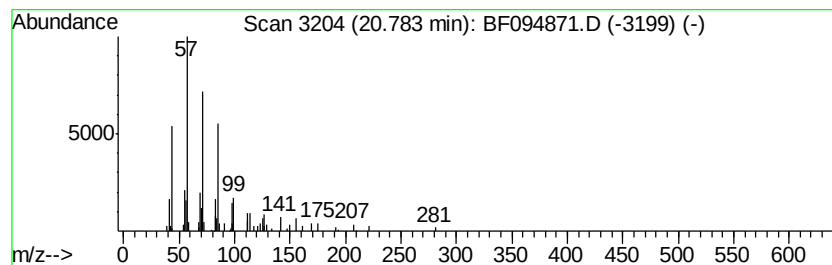
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	3.99 ng	87082	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			10-Methylnonadecane	282	C20H42	056862-62-5	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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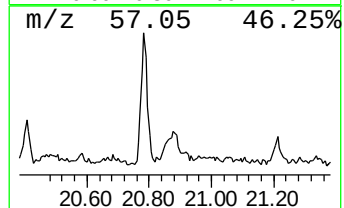
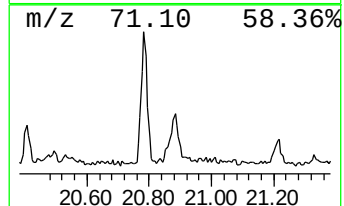
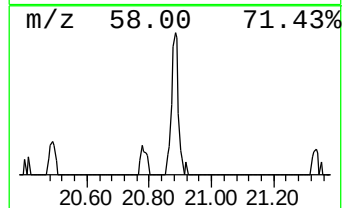
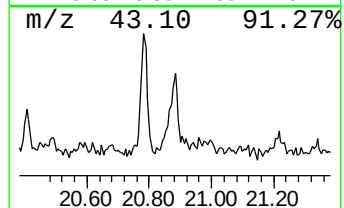
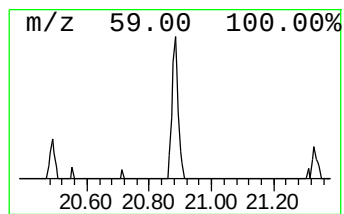
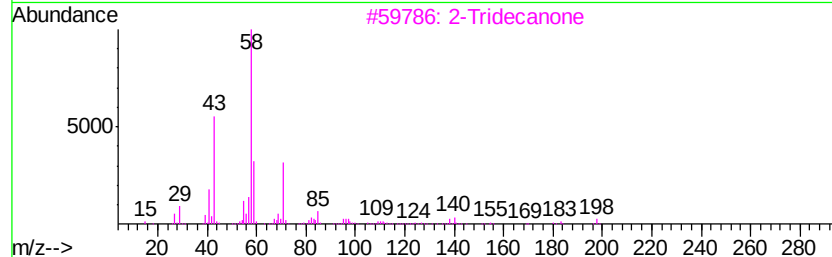
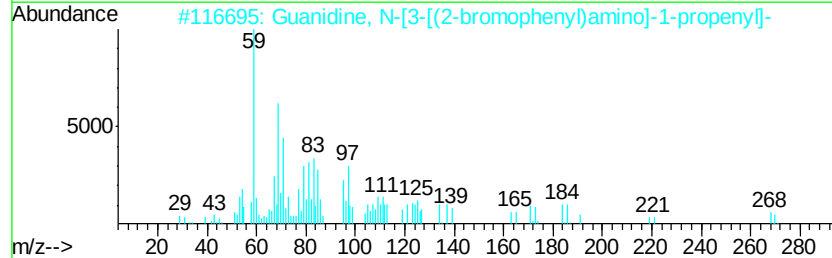
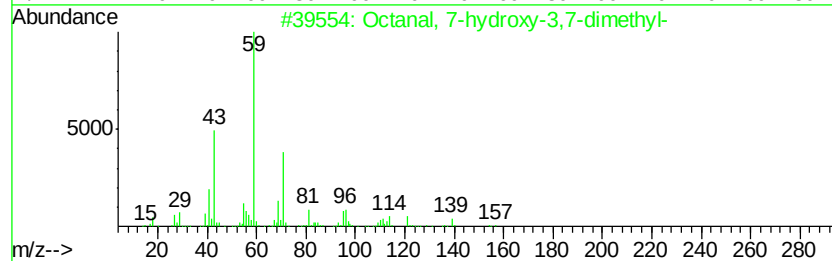
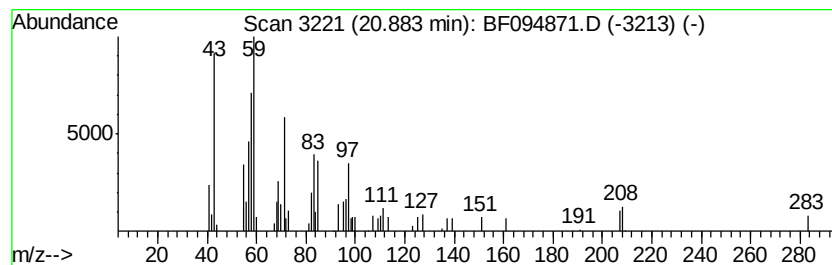
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown20.88 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.88	4.11 ng	89669	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	43
2			Guanidine, N-[3-[(2-bromophenyl)...]	268	C10H13BrN4	1000349-85-6	35
3			2-Tridecanone	198	C13H26O	000593-08-8	35
4			2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	27
5			Octacosyl acetate	452	C30H60O2	018206-97-8	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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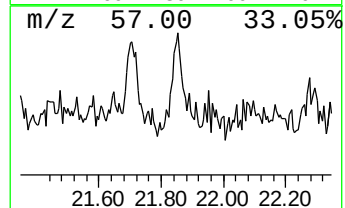
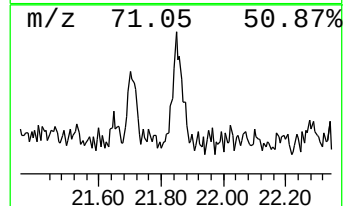
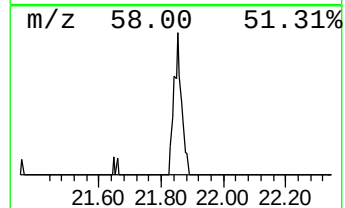
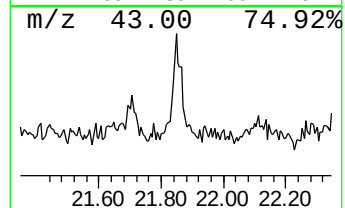
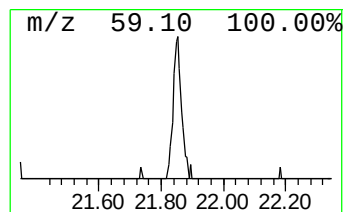
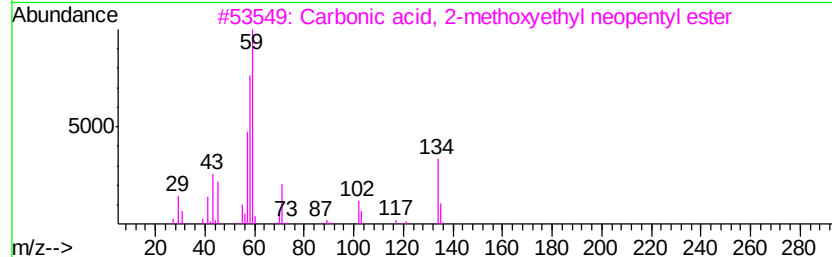
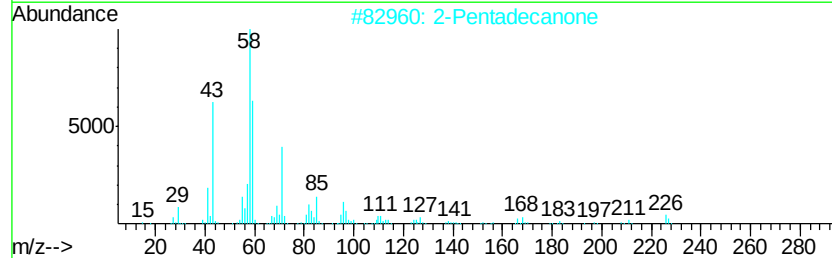
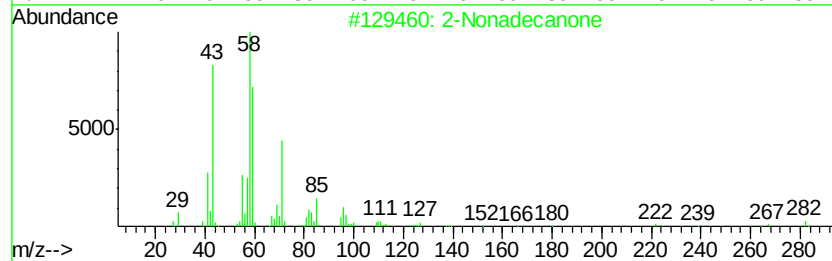
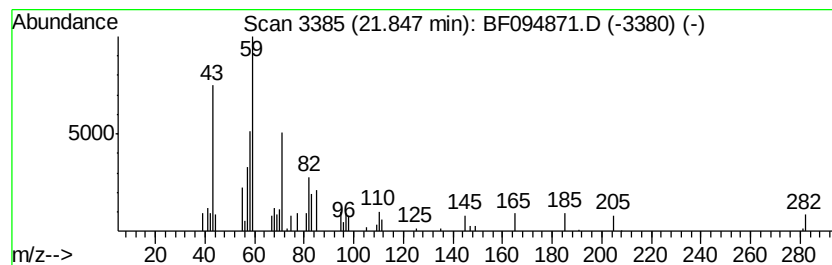
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown21.85 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.85	2.87 ng	62597	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonadecanone	282	C19H38O	000629-66-3	42
2			2-Pentadecanone	226	C15H30O	002345-28-0	42
3			Carbonic acid, 2-methoxyethyl ne...	190	C9H18O4	1000331-42-7	38
4			2,11-Dimethyl-2,11-dodecanediol	230	C14H30O2	022092-59-7	25
5			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094871.D
Acq On : 4 May 2017 12:54
Operator : SJ/MA
Sample : I2916-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-7.0-8.0

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...	5.04	22.4	ng	581484	1	7.72	520259	20.0
unknown7.39	7.39	103.5	ng	2691740	1	7.72	520259	20.0
n-Hexadecanoic acid	15.94	6.0	ng	176543	4	14.97	586577	20.0
17-Pentatriacontene	18.55	10.0	ng	271510	5	18.64	541252	20.0
Trifluoroacetoxy ...	19.37	13.8	ng	373598	5	18.64	541252	20.0
9-Octadecenamide,...	19.67	2.6	ng	56108	6	20.30	436669	20.0
Squalene	19.78	4.3	ng	93218	6	20.30	436669	20.0
Octacosane	20.06	5.3	ng	116094	6	20.30	436669	20.0
Behenic alcohol	20.11	3.0	ng	65614	6	20.30	436669	20.0
2-methyloctacosane	20.78	4.0	ng	87082	6	20.30	436669	20.0
unknown20.88	20.88	4.1	ng	89669	6	20.30	436669	20.0
unknown21.85	21.85	2.9	ng	62597	6	20.30	436669	20.0