

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
 Data File : BF099582.D
 Acq On : 17 Oct 2017 15:48
 Operator : SJ/JU
 Sample : I5857-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-018

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-BF092317.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	5.046	500	503	517	rBV	216154	271822	13.83%	1.487%
2	5.451	568	572	591	rBV	1578059	1575017	80.16%	8.616%
3	6.463	739	744	759	rBV	1643594	1643042	83.62%	8.988%
4	6.598	763	767	770	rBV	1841645	1644358	83.69%	8.995%
5	6.822	802	805	812	rBV	545048	497100	25.30%	2.719%
6	6.981	828	832	835	rBV	1547752	1320009	67.18%	7.221%
7	7.392	897	902	905	rBV	1020011	993322	50.55%	5.434%
8	8.104	1019	1023	1027	rBV	820976	690781	35.16%	3.779%
9	8.663	1114	1118	1121	rBV	126134	108114	5.50%	0.591%
10	9.181	1200	1206	1209	rBV	2196729	1964840	100.00%	10.748%
11	9.575	1269	1273	1276	rBV	327046	254737	12.96%	1.394%
12	9.857	1317	1321	1325	rBV	809815	766131	38.99%	4.191%
13	10.057	1350	1355	1360	rBV3	16036	25022	1.27%	0.137%
14	10.569	1439	1442	1446	rVB	436763	394586	20.08%	2.159%
15	10.651	1452	1456	1459	rBV	1214842	1038014	52.83%	5.678%
16	11.345	1571	1574	1578	rBV	854410	773685	39.38%	4.232%
17	11.680	1615	1631	1632	rBV2	277191	618031	31.45%	3.381%
18	11.863	1658	1662	1671	rVB3	110213	145237	7.39%	0.795%
19	12.180	1706	1716	1725	rVB10	11766	45265	2.30%	0.248%
20	12.645	1789	1795	1804	rBV2	58002	86445	4.40%	0.473%
21	12.927	1839	1843	1846	rBV	1934161	1758982	89.52%	9.622%
22	13.127	1874	1877	1883	rVB3	15969	23726	1.21%	0.130%
23	13.810	1990	1993	1996	rBV	120274	134945	6.87%	0.738%
24	13.845	1996	1999	2004	rVB2	51195	74764	3.81%	0.409%
25	13.986	2019	2023	2028	rVB	687142	590147	30.04%	3.228%
26	14.439	2096	2100	2106	rBV3	25961	38728	1.97%	0.212%
27	14.804	2158	2162	2173	rVB	102383	135145	6.88%	0.739%
28	14.927	2179	2183	2189	rVB3	27290	43988	2.24%	0.241%
29	14.992	2189	2194	2198	rVB4	12608	21846	1.11%	0.120%
30	15.063	2202	2206	2207	rBV3	27164	30014	1.53%	0.164%
31	15.451	2266	2272	2278	rBV	338381	430647	21.92%	2.356%
32	15.598	2295	2297	2306	rVB6	15684	33330	1.70%	0.182%
33	16.039	2365	2372	2373	rBV4	44951	73951	3.76%	0.405%
34	16.345	2418	2424	2431	rVB7	14766	34372	1.75%	0.188%

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

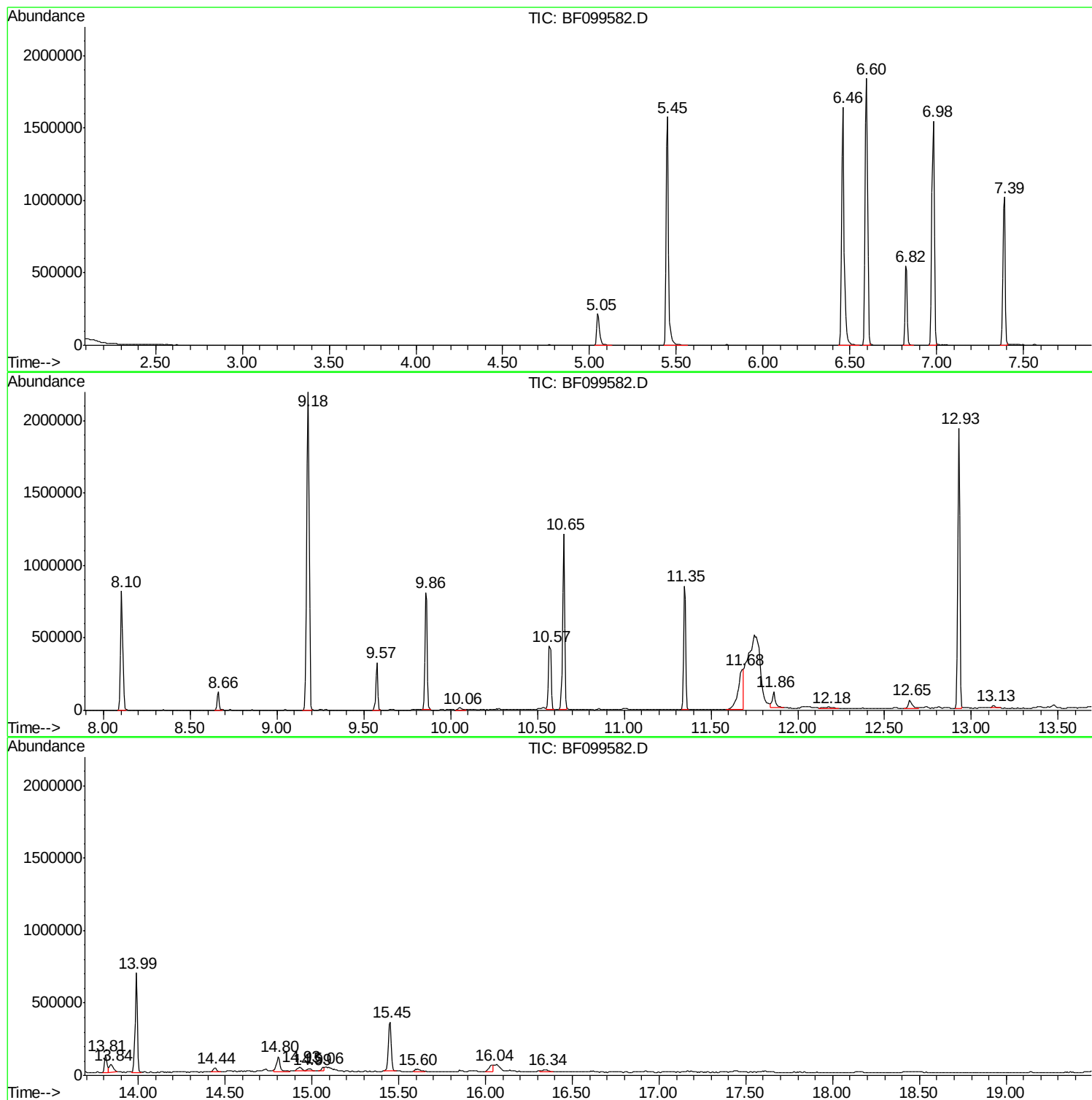
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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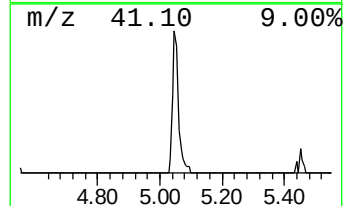
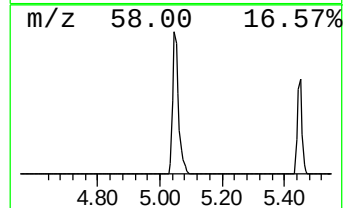
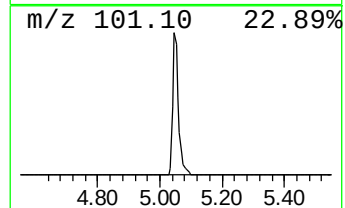
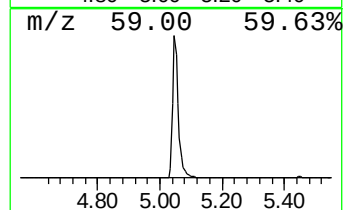
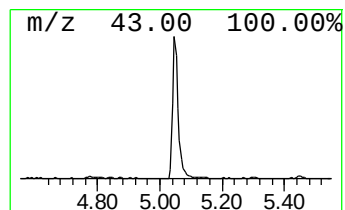
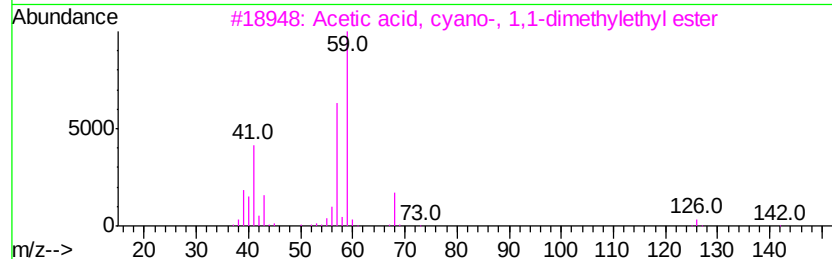
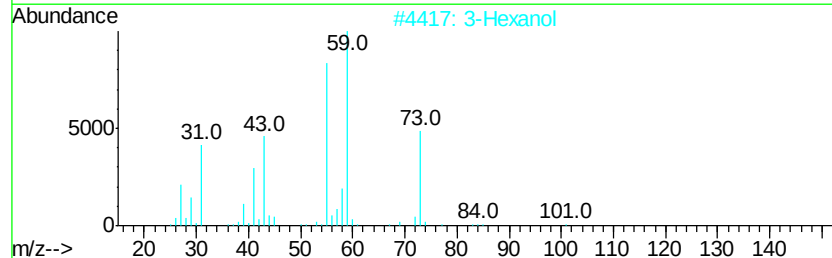
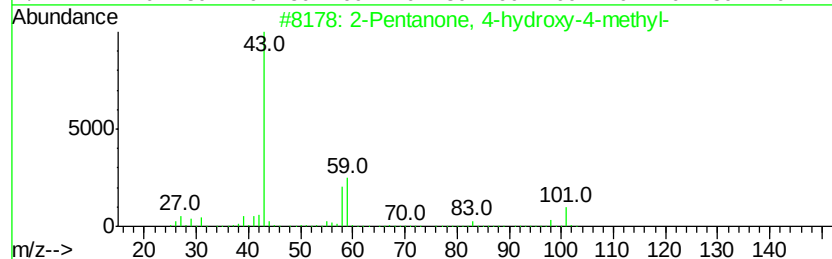
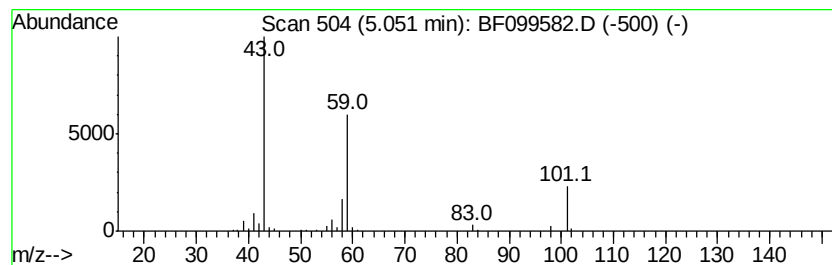
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	10.94 ng	271822	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol	102	C6H14O	000623-37-0	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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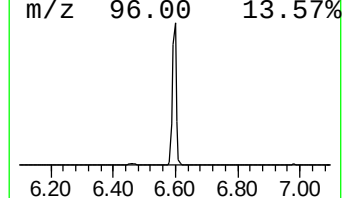
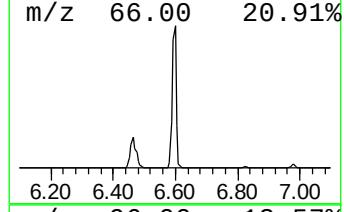
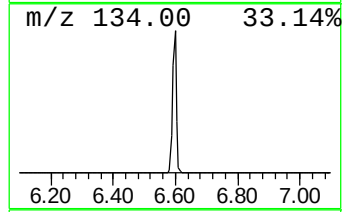
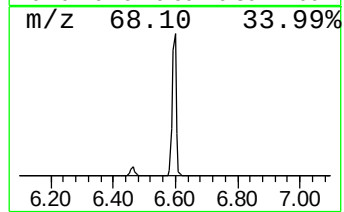
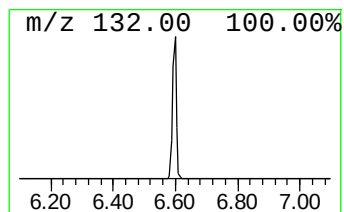
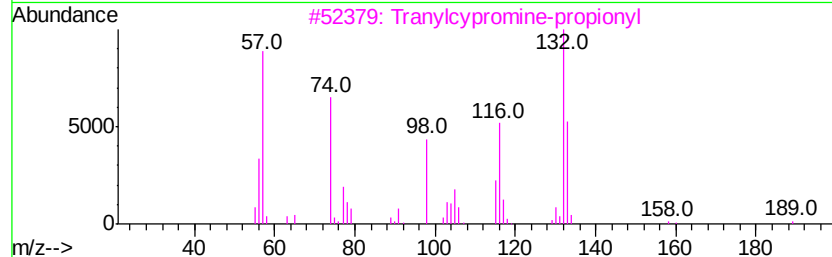
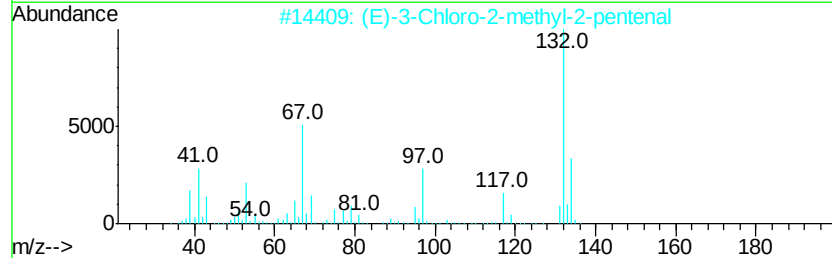
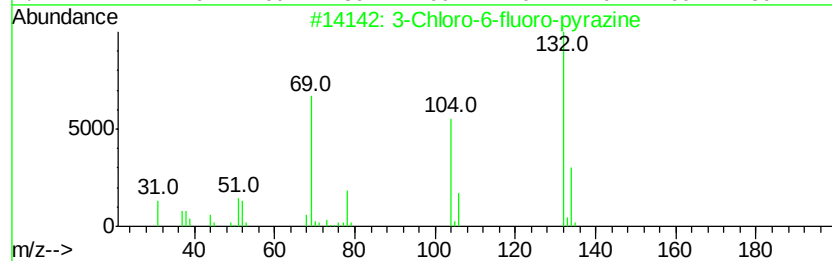
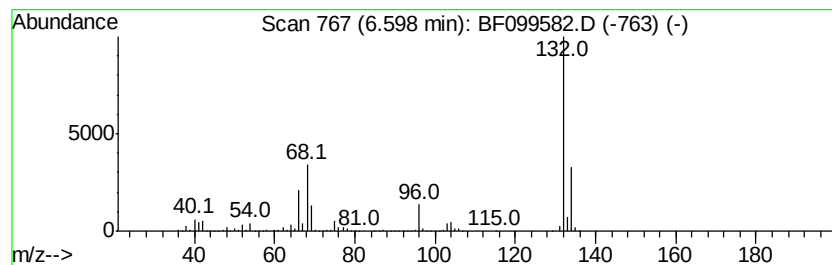
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	66.16 ng	1644360	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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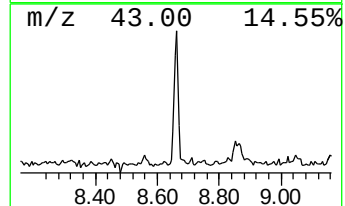
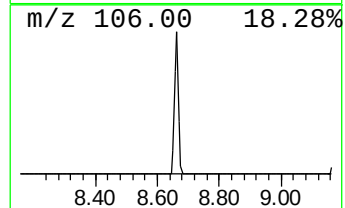
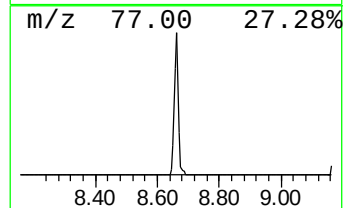
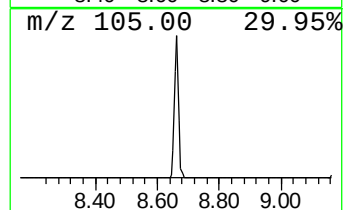
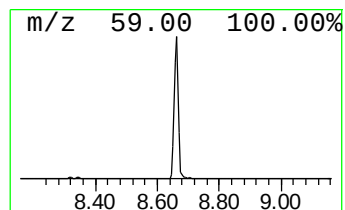
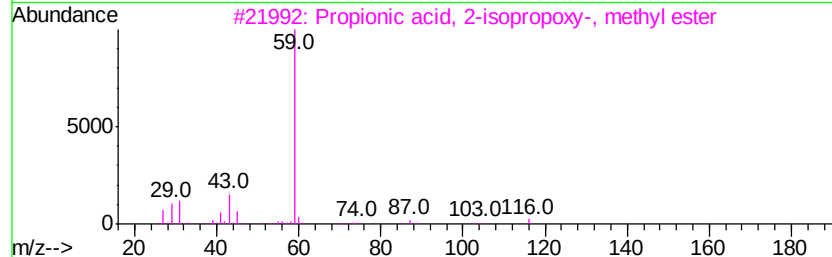
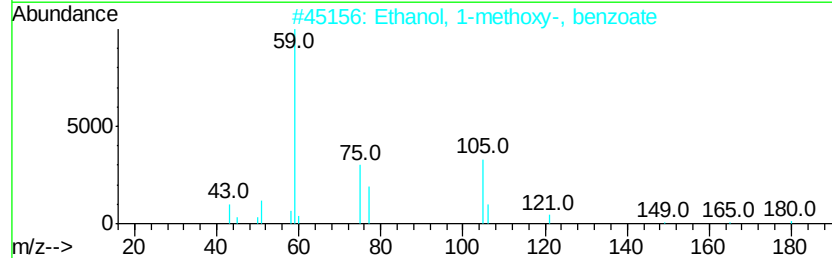
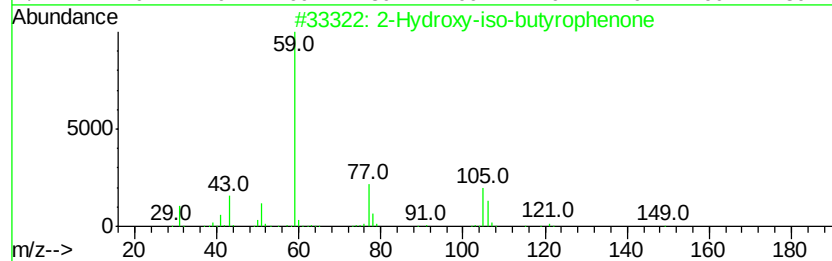
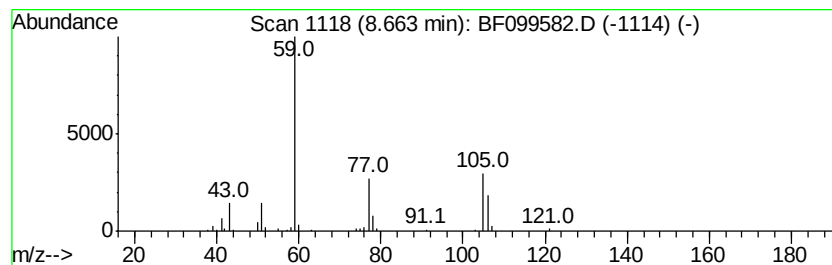
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	3.13 ng	108114	Napthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	78
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	23
4		Guanidine	59	CH5N3	000113-00-8	9
5		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	9



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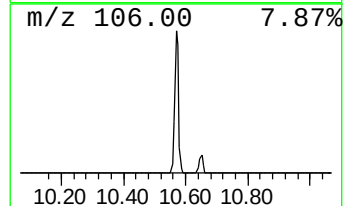
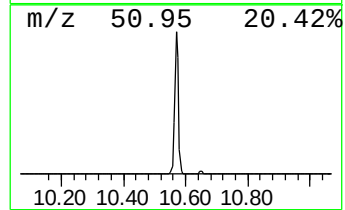
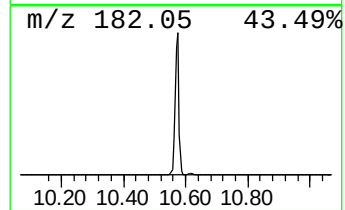
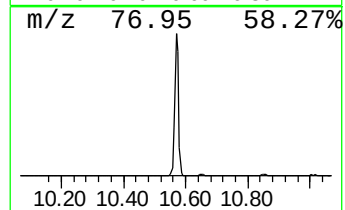
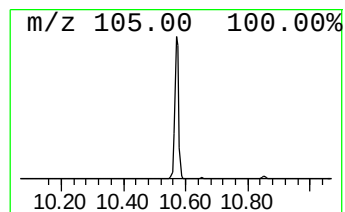
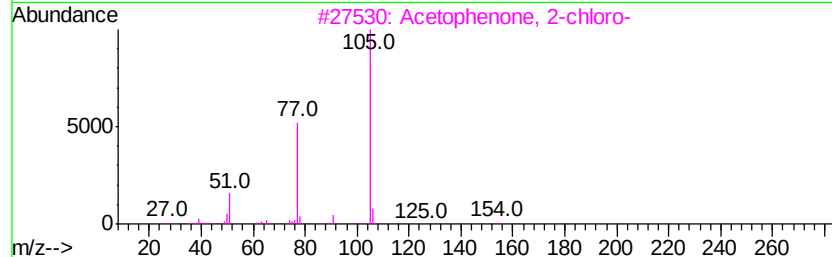
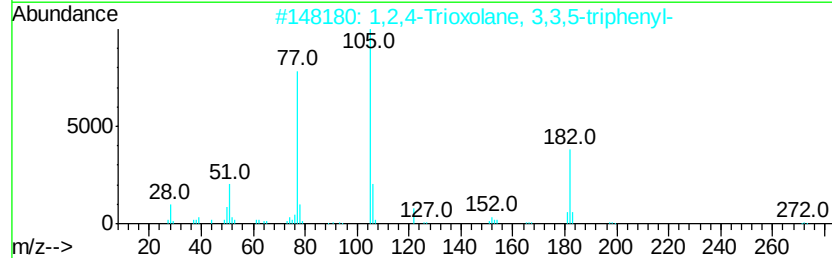
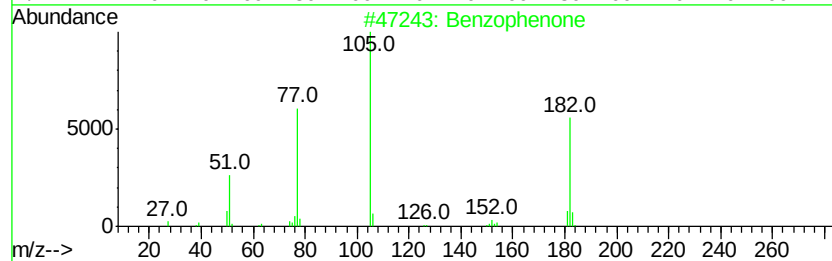
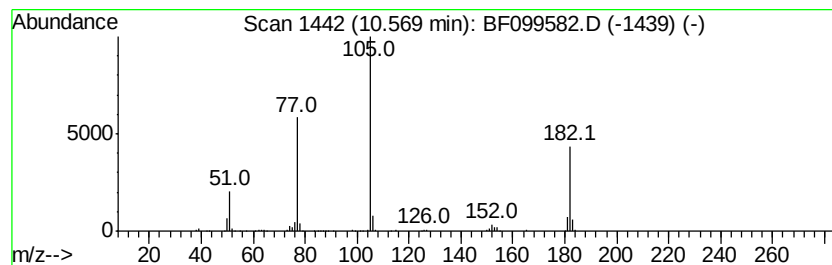
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	10.30 ng	394586	Acenaphthene-d10	9.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		1,2,4-Trioxolane, 3,3,5-triphenyl-	304 C20H16O3	023246-12-0 64
3		Acetophenone, 2-chloro-	154 C8H7ClO	000532-27-4 49
4		Benzenecarbothioic acid	138 C7H6OS	000098-91-9 47
5		Phenacyl thiocyanate	177 C9H7NOS	005399-30-4 47



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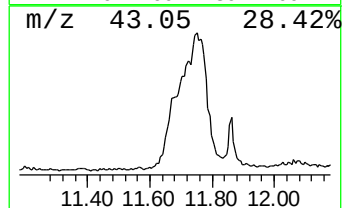
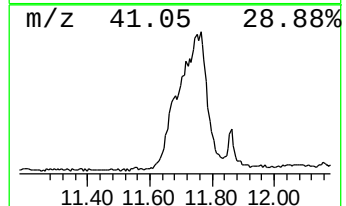
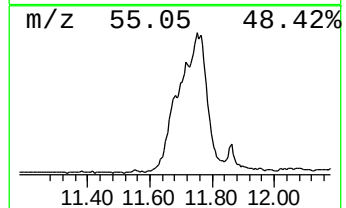
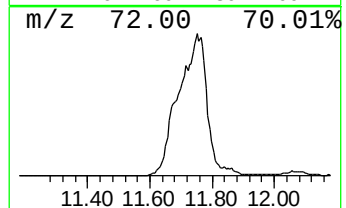
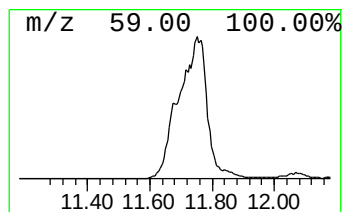
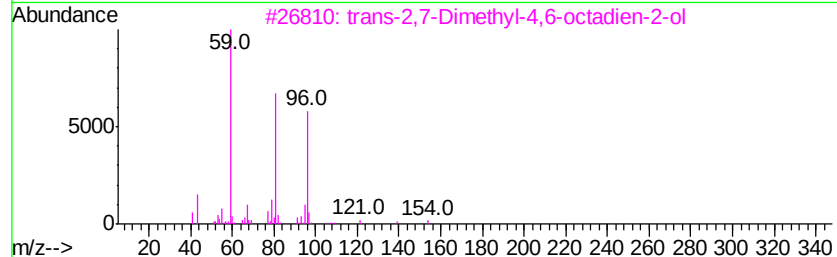
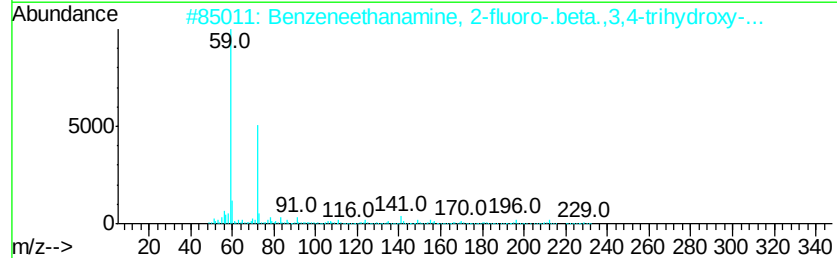
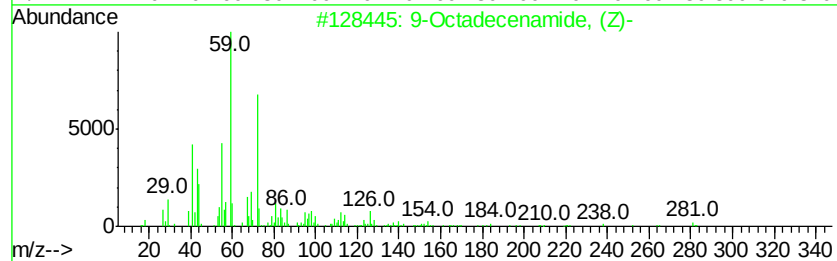
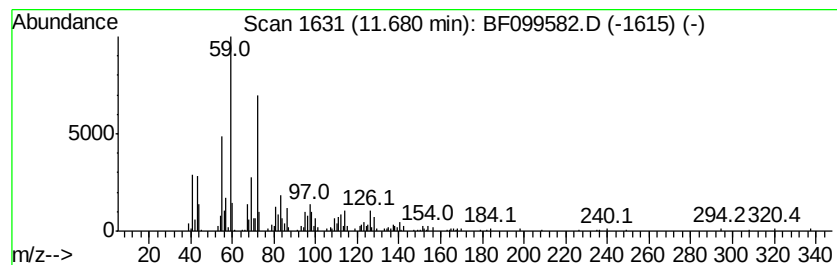
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.68	15.98 ng	618031	Phenanthrene-d10	11.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
3	trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	38
4	4.beta.H,5.alpha.H-Eudesman-11-ol	224	C15H28O	031756-53-3	35
5	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	35



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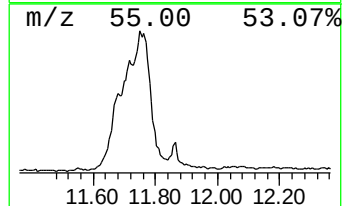
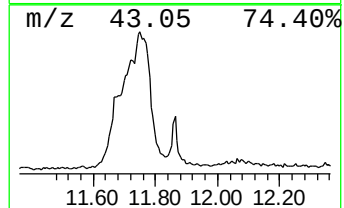
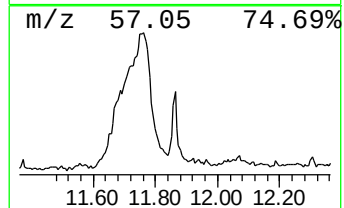
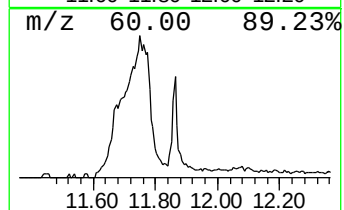
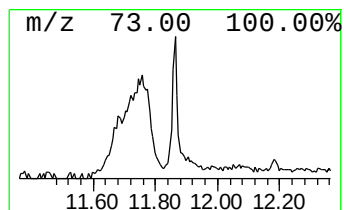
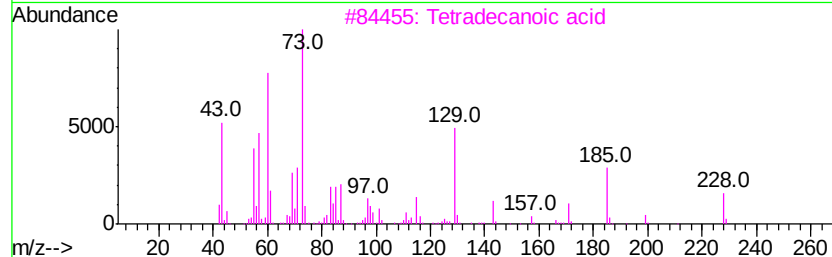
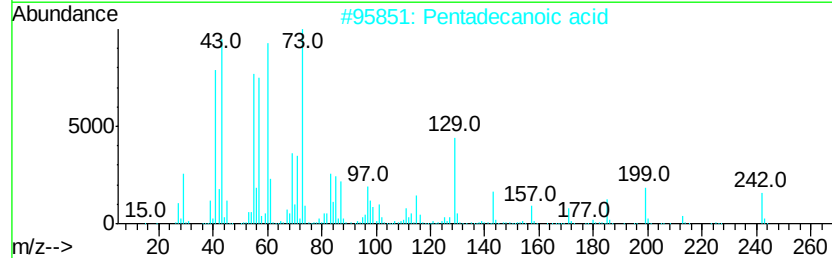
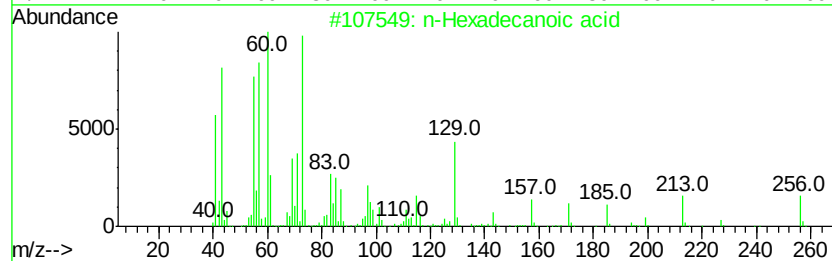
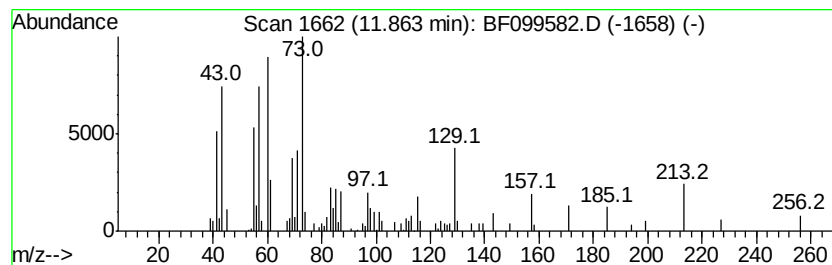
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	3.75 ng	145237	Phenanthrene-d10	11.35

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	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099582.D
Acq On : 17 Oct 2017 15:48
Operator : SJ/JU
Sample : I5857-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

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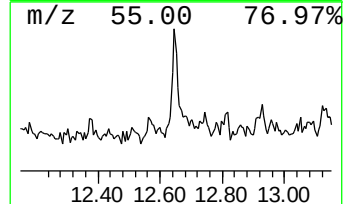
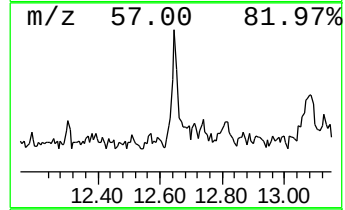
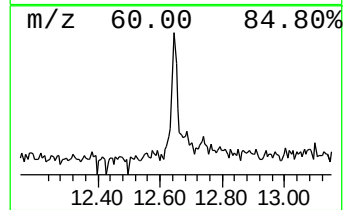
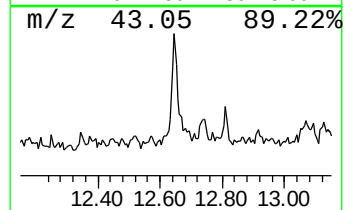
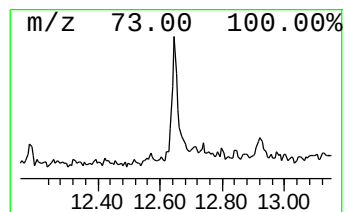
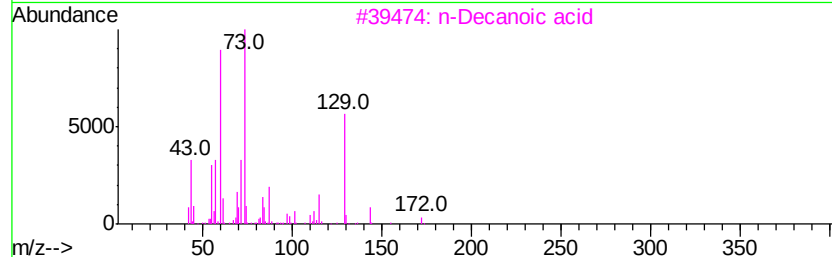
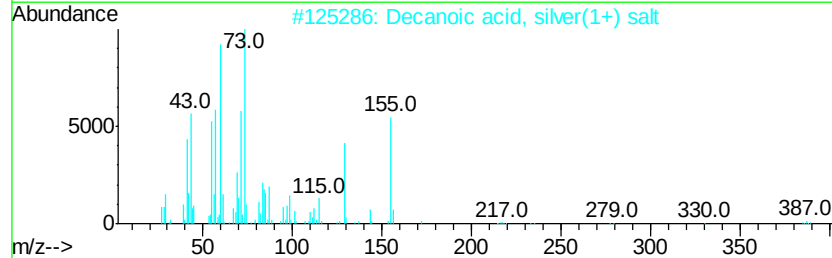
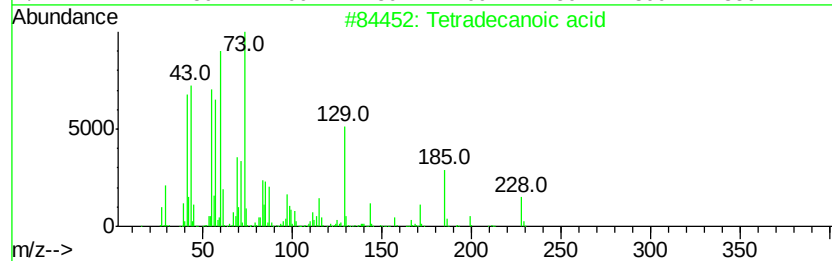
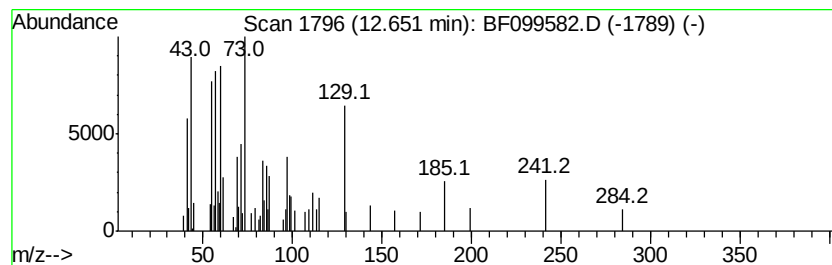
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.23 ng	86445	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	1-Hexacosanol	382	C26H54O	000506-52-5	30
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
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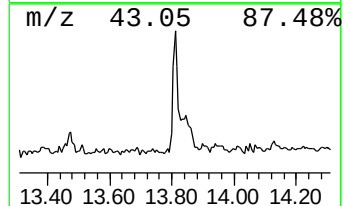
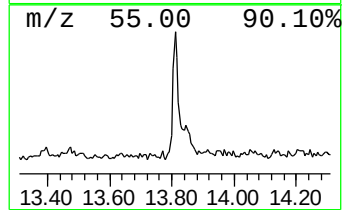
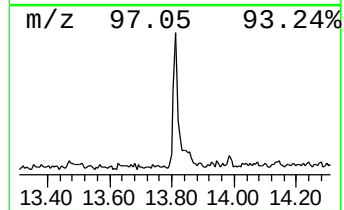
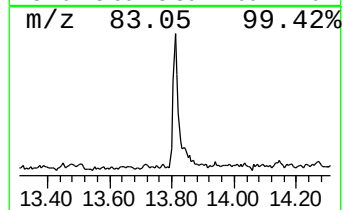
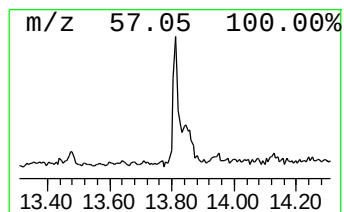
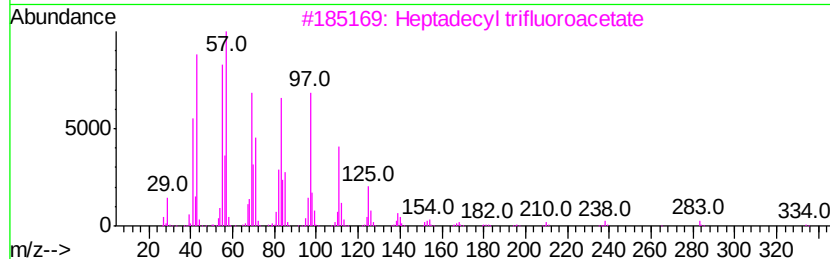
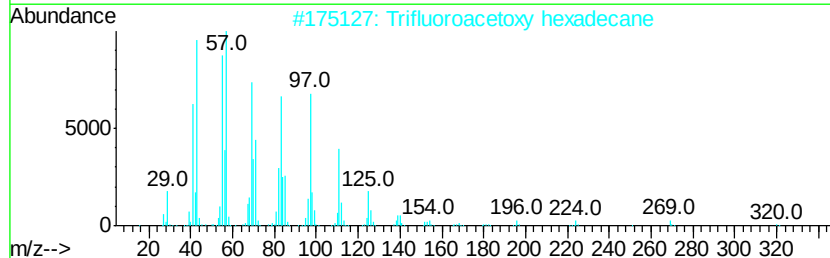
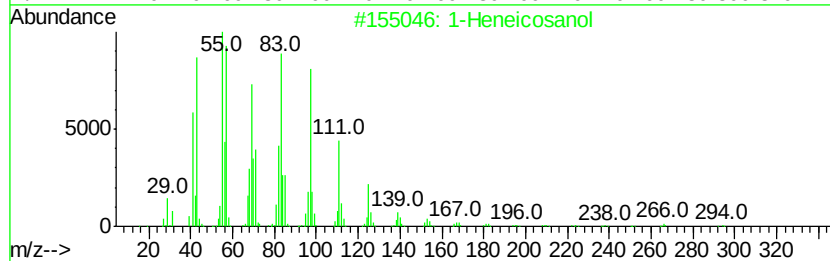
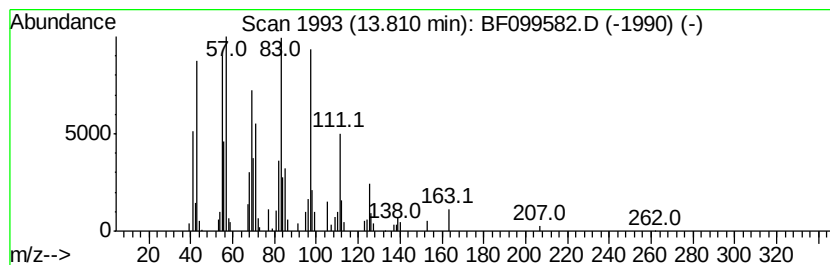
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	4.57 ng	134945	Chrysene-d12	13.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099582.D
Acq On : 17 Oct 2017 15:48
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Misc :
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Instrument :
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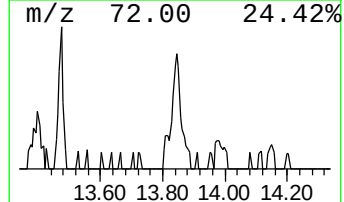
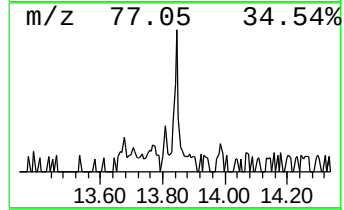
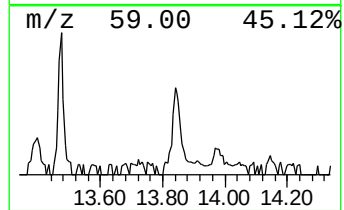
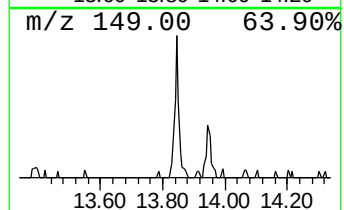
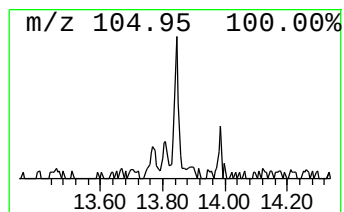
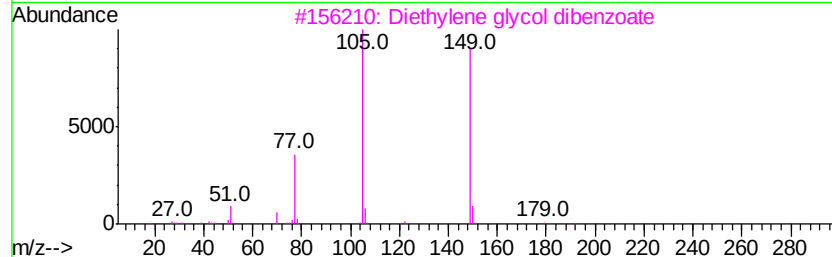
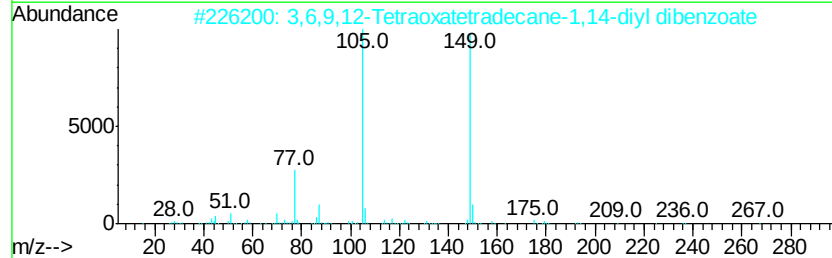
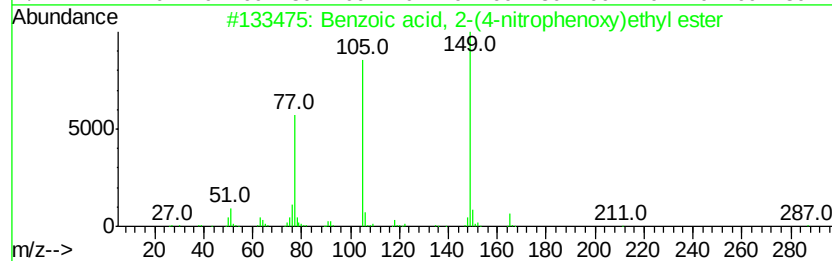
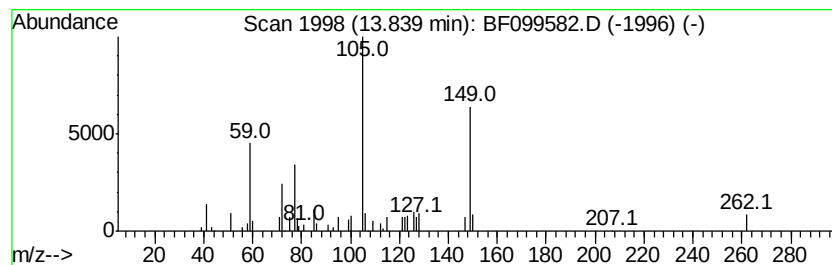
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzoic acid, 2-(4-nitrophe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	2.53 ng	74764	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13N05	1000368-92-7	53
2			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	42
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	42
4			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	42
5			2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	36



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
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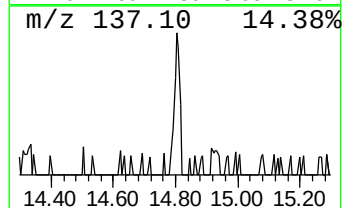
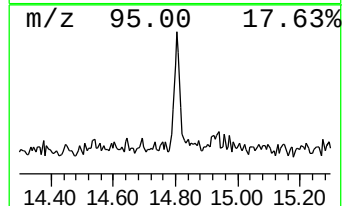
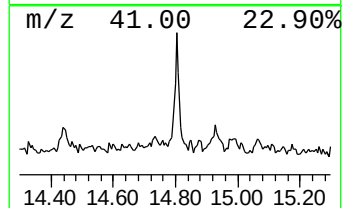
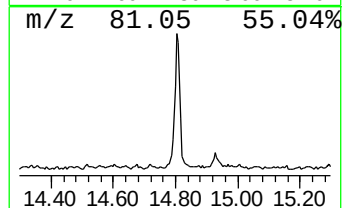
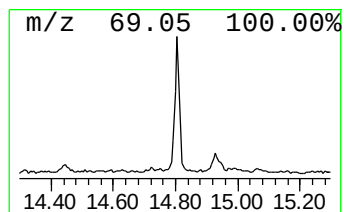
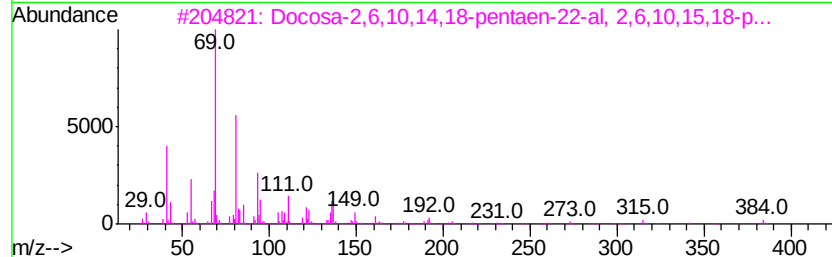
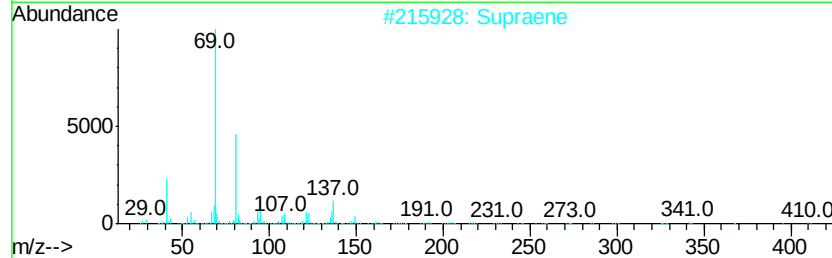
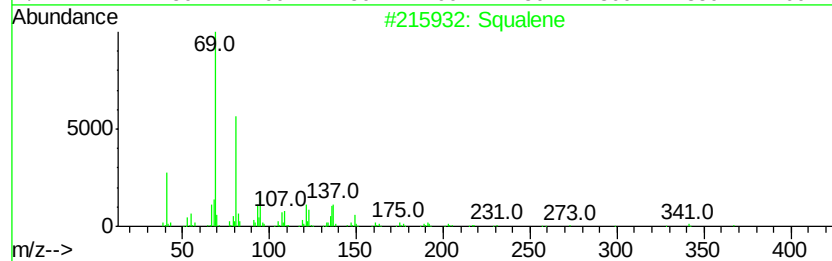
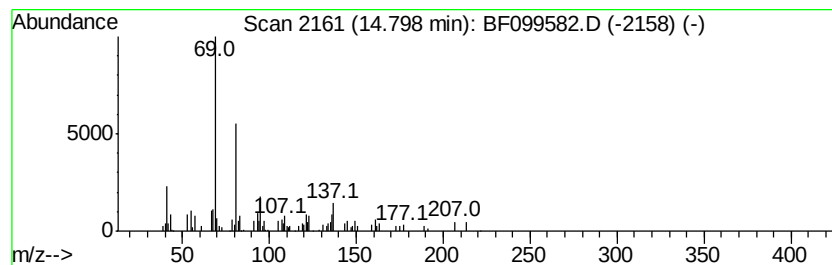
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	6.28 ng	135145	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Supraene	410	C30H50	007683-64-9	90
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
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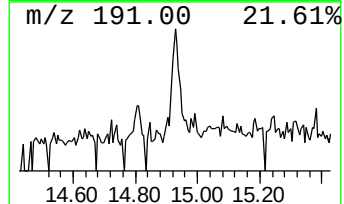
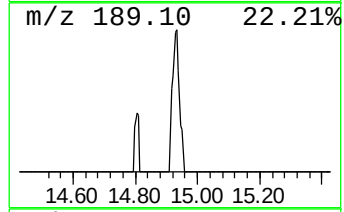
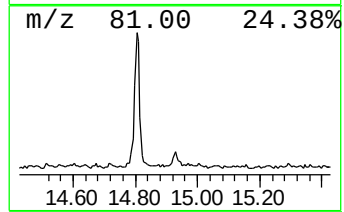
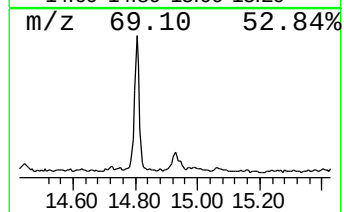
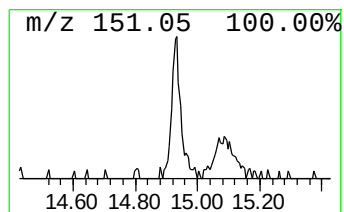
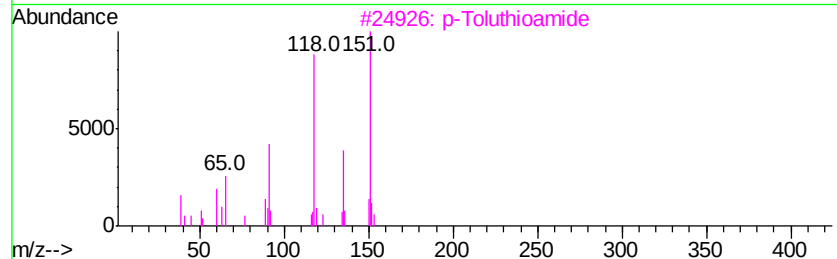
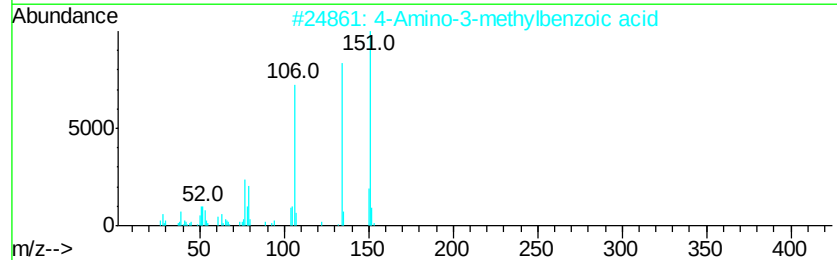
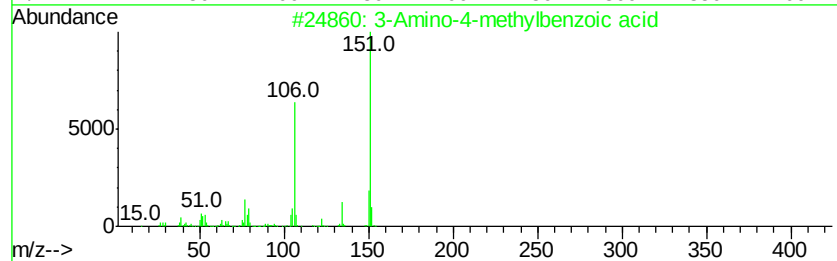
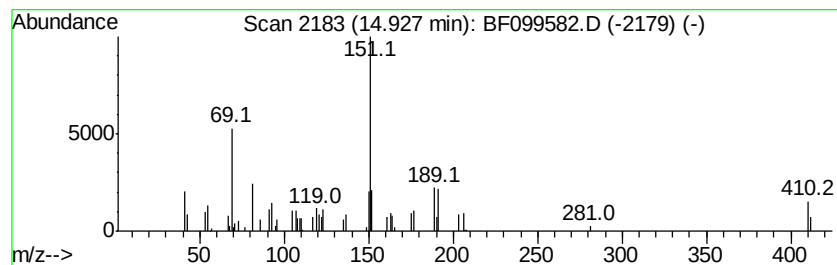
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.93 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.04 ng	43988	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Amino-4-methylbenzoic acid	151	C8H9NO2	002458-12-0	38
2		4-Amino-3-methylbenzoic acid	151	C8H9NO2	002486-70-6	38
3		p-Toluthioamide	151	C8H9NS	002362-62-1	37
4		Silane, 3-butenylmethoxymethylph...	206	C12H18OSi	076557-75-0	37
5		Benzene, 4-butyl-1,2-dimethoxy-	194	C12H18O2	059056-76-7	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
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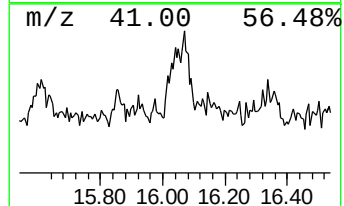
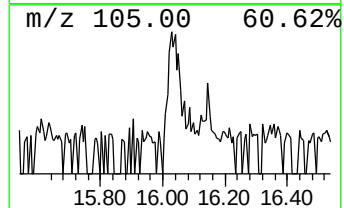
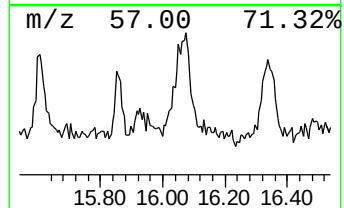
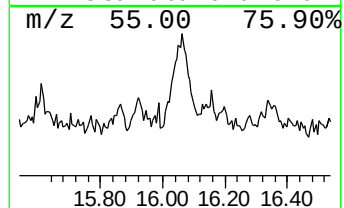
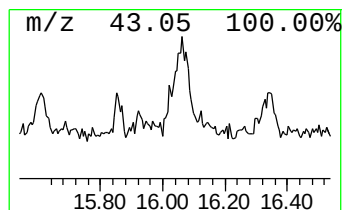
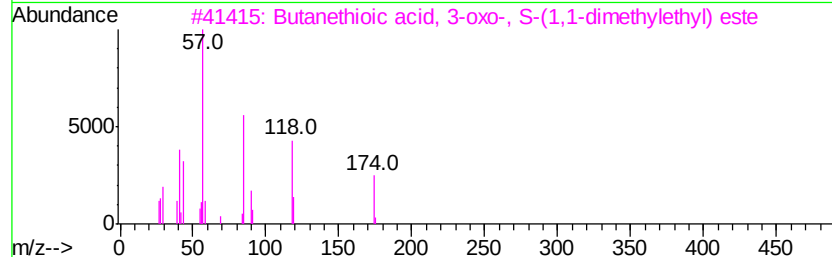
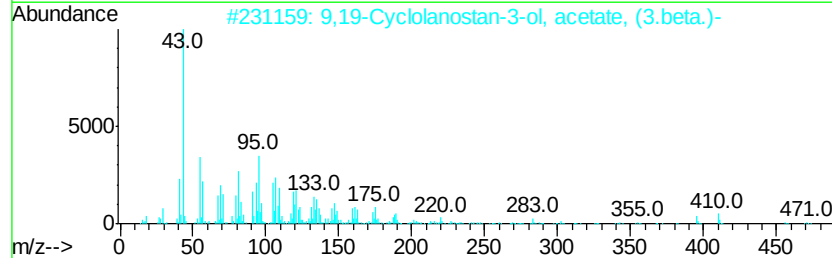
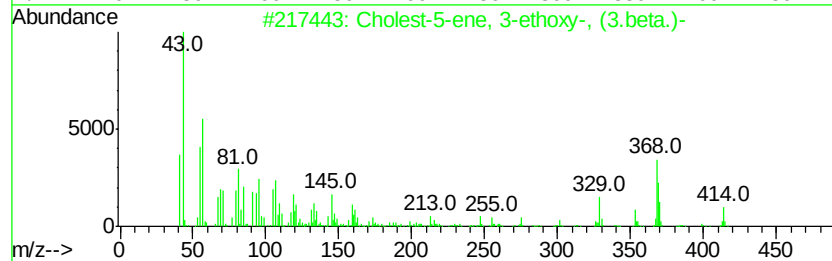
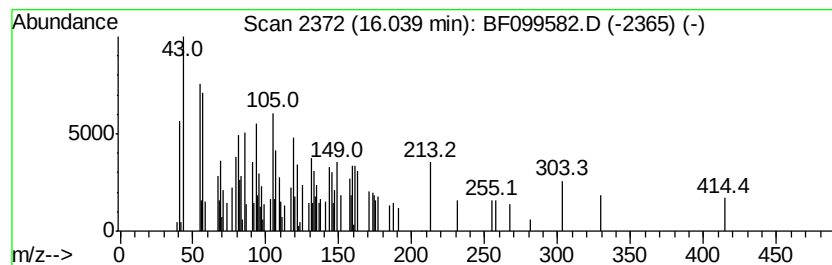
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.04 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	3.43 ng	73951	Perylene-d12	15.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H50O	000986-19-6 27
2		9,19-Cyclostan-3-ol, acetate...	470 C32H54O2	004575-74-0 14
3		Butanethioic acid, 3-oxo-, S-(1,...	174 C8H14O2S	015925-47-0 11
4		Methyl 10,12-pentacosadivnoate	388 C26H44O2	1000342-58-7 10
5		Tricyclo[5.1.0.0(2,4)]octane-5-c...	222 C14H22O2	074810-39-2 10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099582.D
Acq On : 17 Oct 2017 15:48
Operator : SJ/JU
Sample : I5857-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.05	10.9	ng	271822	1	6.83	497100	20.0
unknown6.60	6.60	66.2	ng	1644360	1	6.83	497100	20.0
2-Hydroxy-iso-but...	8.66	3.1	ng	108114	2	8.10	690781	20.0
Benzophenone	10.57	10.3	ng	394586	3	9.86	766131	20.0
9-Octadecenamide,...	11.68	16.0	ng	618031	4	11.35	773685	20.0
n-Hexadecanoic acid	11.86	3.8	ng	145237	4	11.35	773685	20.0
Tetradecanoic acid	12.65	2.2	ng	86445	4	11.35	773685	20.0
1-Heneicosanol	13.81	4.6	ng	134945	5	13.99	590147	20.0
Benzoic acid, 2-(...	13.84	2.5	ng	74764	5	13.99	590147	20.0
Squalene	14.80	6.3	ng	135145	6	15.45	430647	20.0
unknown14.93	14.93	2.0	ng	43988	6	15.45	430647	20.0
unknown16.04	16.04	3.4	ng	73951	6	15.45	430647	20.0