

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112219\
 Data File : BF117940.D
 Acq On : 23 Nov 2019 1:24
 Operator : JU
 Sample : K5840-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-SE-02

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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	2.216	15	22	28	rVB	596342	817421	16.69%	1.979%
2	5.122	506	516	524	rBV	544610	703856	14.37%	1.704%
3	5.522	578	584	587	rBV	3220476	3124016	63.79%	7.562%
4	6.528	749	755	759	rBV	3232313	3463544	70.73%	8.384%
5	6.669	775	779	783	rBV	3574713	3551384	72.52%	8.597%
6	6.904	815	819	822	rBV	1189495	1013888	20.70%	2.454%
7	7.057	841	845	849	rBV	3020601	2762742	56.42%	6.688%
8	7.463	909	914	917	rBV	2238052	2171741	44.35%	5.257%
9	8.187	1033	1037	1041	rBV	1425413	1343601	27.44%	3.252%
10	9.269	1216	1221	1224	rBV	4749343	4330111	88.42%	10.482%
11	9.663	1283	1288	1291	rBV	371403	330694	6.75%	0.801%
12	9.951	1332	1337	1341	rBV	1967882	1678472	34.27%	4.063%
13	10.745	1466	1472	1475	rBV	3327968	3113479	63.58%	7.537%
14	11.445	1587	1591	1594	rBV	2084026	1811323	36.99%	4.385%
15	11.510	1598	1602	1605	rVB2	62836	56080	1.15%	0.136%
16	11.969	1676	1680	1695	rBV	956771	940072	19.20%	2.276%
17	12.675	1795	1800	1810	rBV2	68082	109276	2.23%	0.265%
18	12.757	1810	1814	1828	rVV	344020	404946	8.27%	0.980%
19	13.039	1857	1862	1865	rBV	4875407	4897129	100.00%	11.855%
20	13.927	2009	2013	2034	rBV	555684	795933	16.25%	1.927%
21	14.092	2037	2041	2044	rVB	1809479	1523169	31.10%	3.687%
22	14.251	2065	2068	2079	rBV	58815	64669	1.32%	0.157%
23	14.557	2116	2120	2132	rBV2	96156	140203	2.86%	0.339%
24	14.874	2171	2174	2180	rVB	99457	98298	2.01%	0.238%
25	14.951	2183	2187	2193	rVB	364241	374739	7.65%	0.907%
26	15.227	2229	2234	2238	rBV	96123	110588	2.26%	0.268%
27	15.598	2290	2297	2300	rBV	958512	1265226	25.84%	3.063%
28	15.621	2300	2301	2309	rVB	76974	83481	1.70%	0.202%
29	16.080	2374	2379	2385	rBV2	53028	81830	1.67%	0.198%
30	16.145	2385	2390	2406	rBV8	39550	148262	3.03%	0.359%

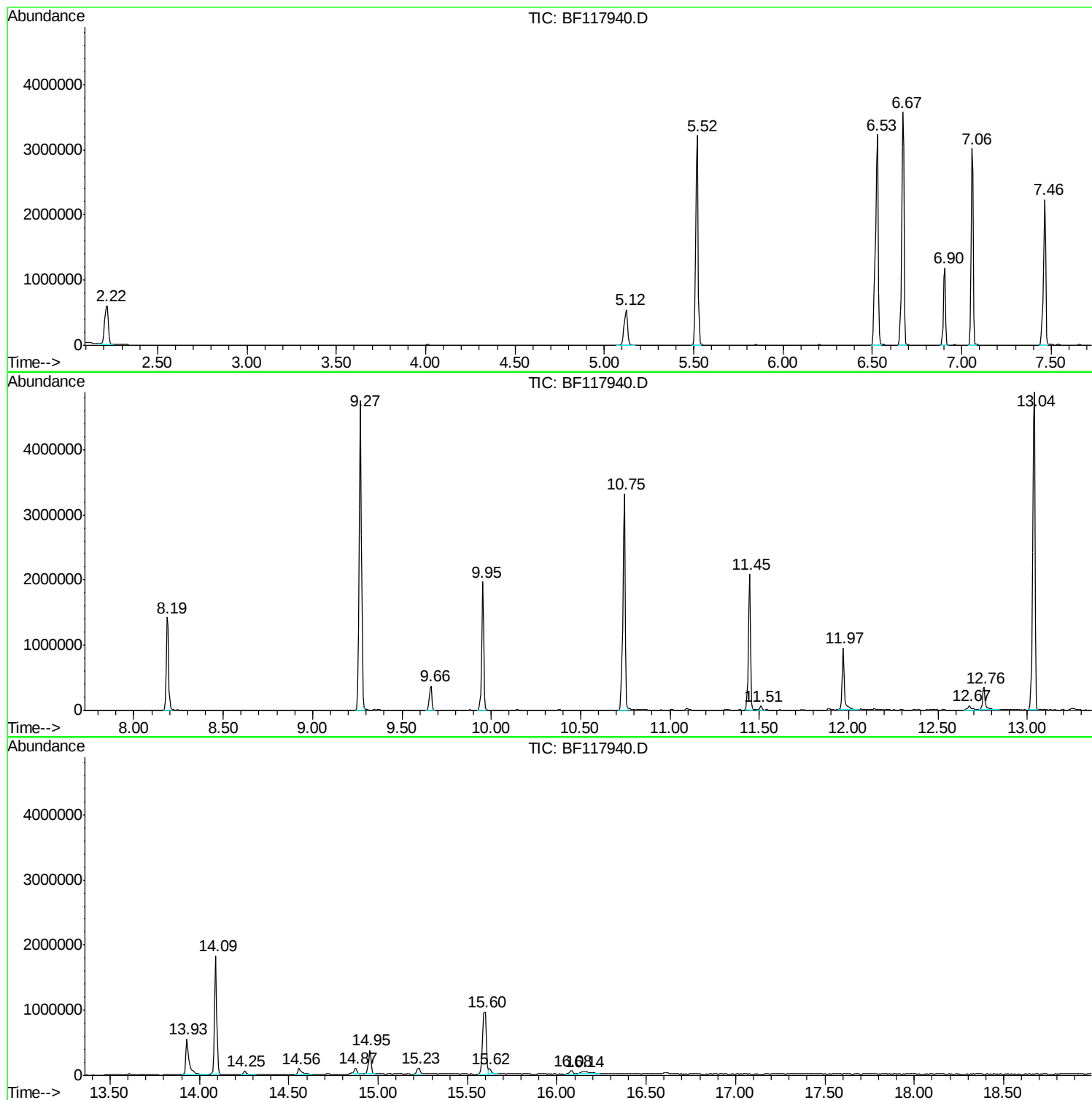
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-SE-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.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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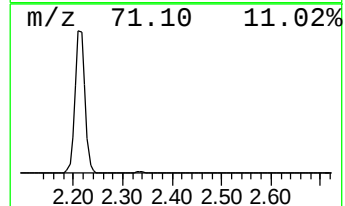
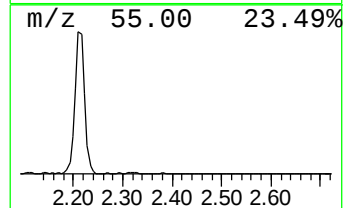
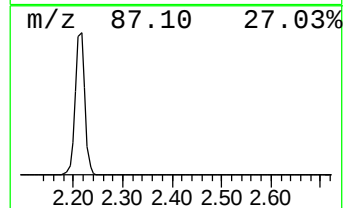
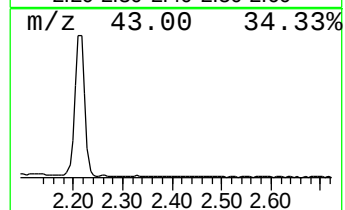
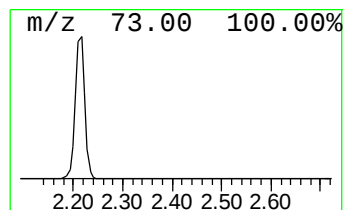
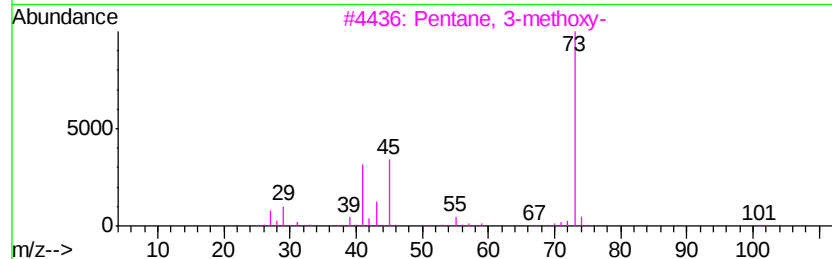
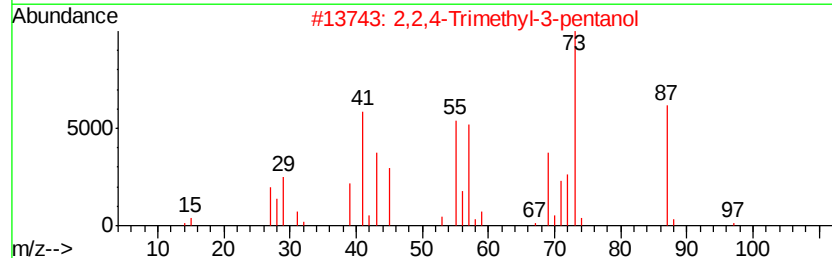
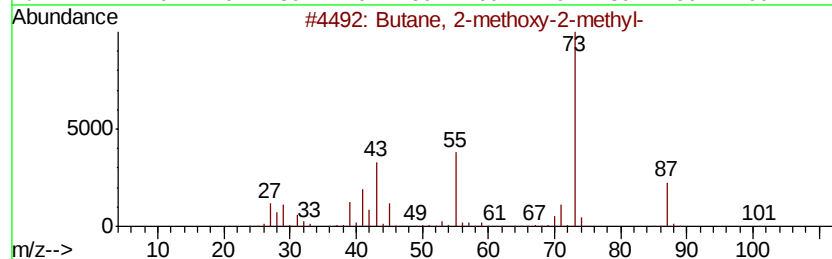
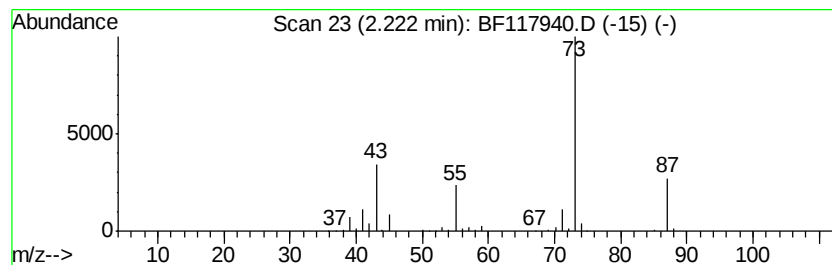
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	16.12 ng	817421	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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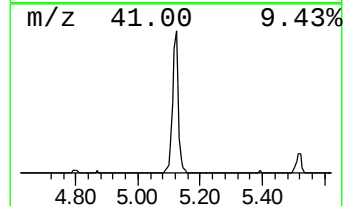
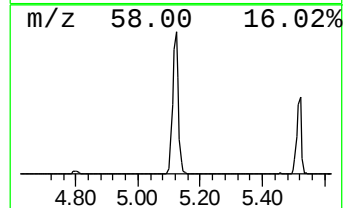
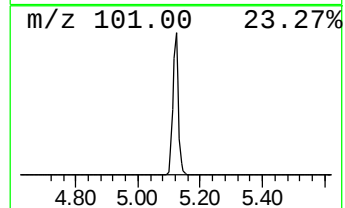
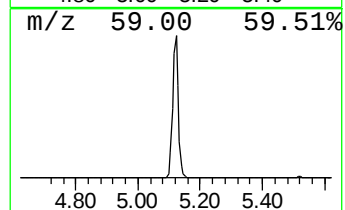
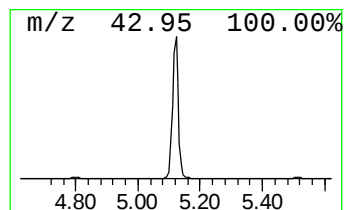
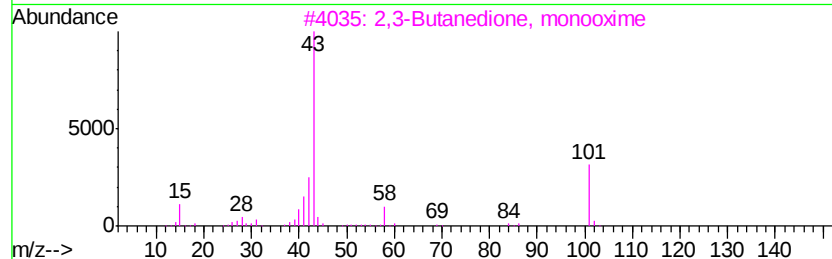
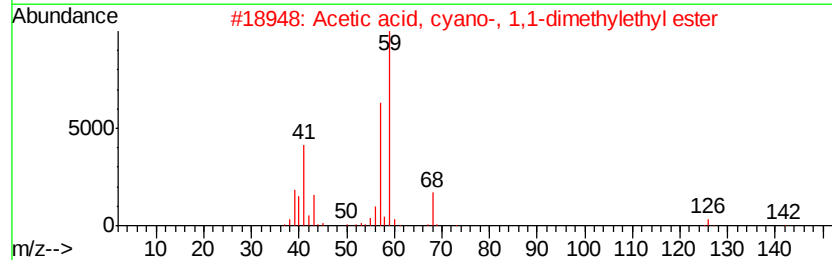
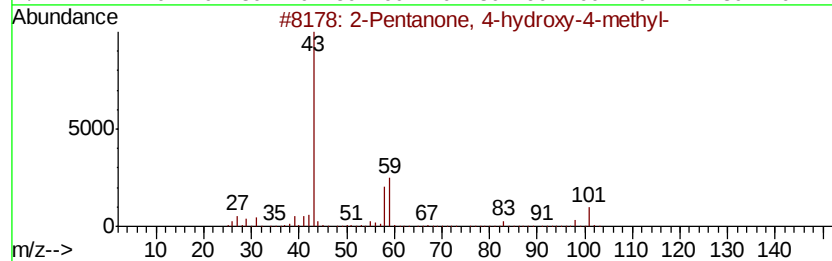
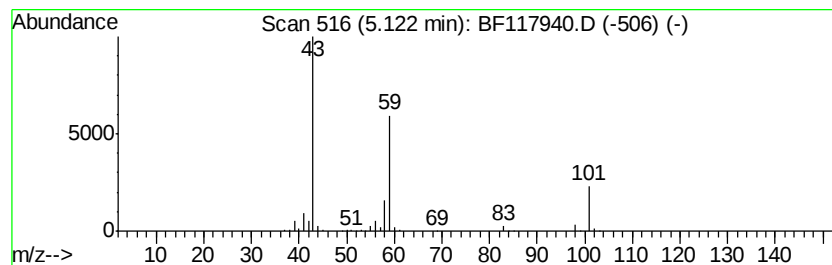
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.88 ng	703856	1,4-Dichlorobenzene-d4	6.90

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetone	58	C3H6O	000067-64-1	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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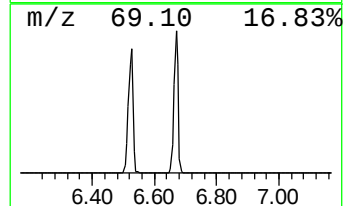
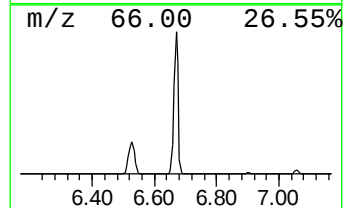
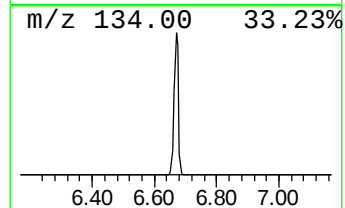
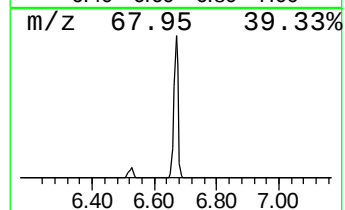
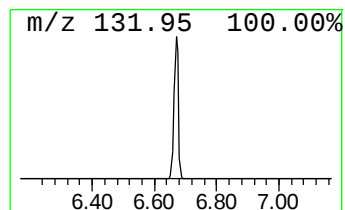
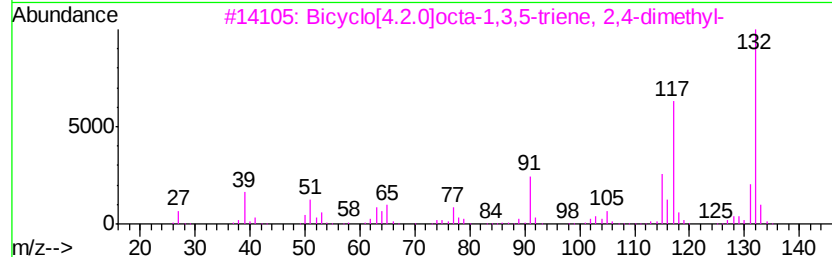
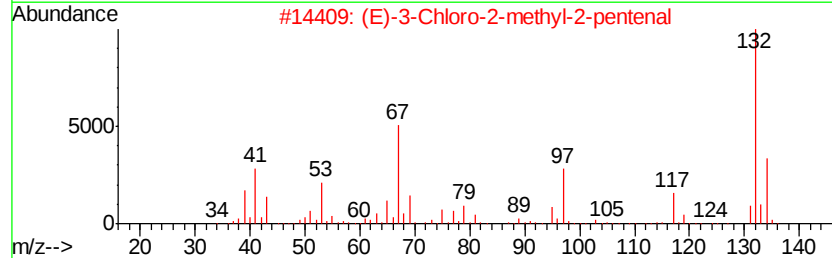
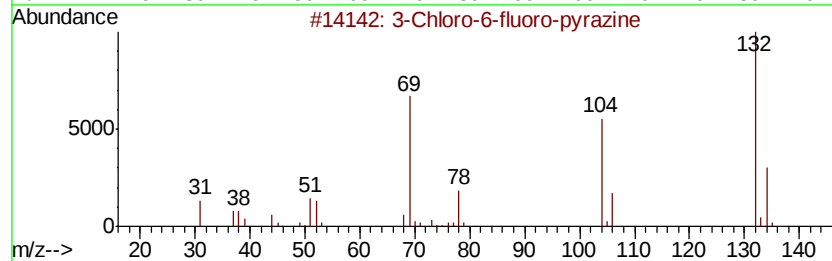
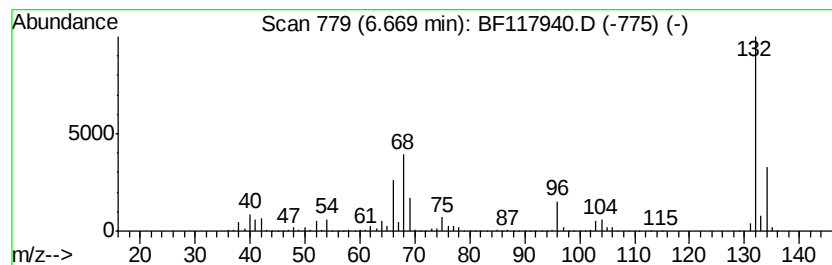
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	70.05 ng	3551380	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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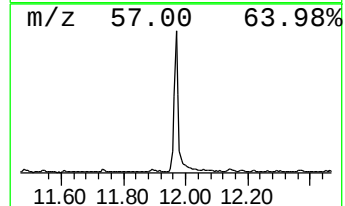
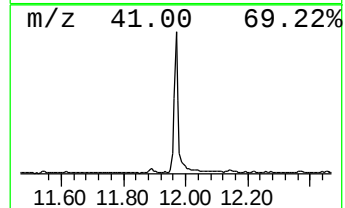
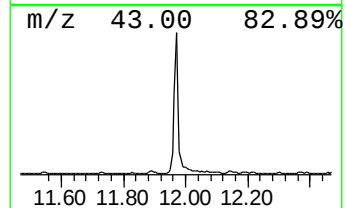
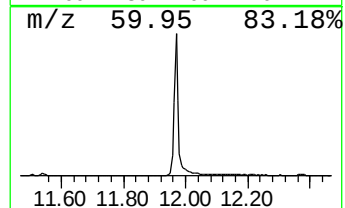
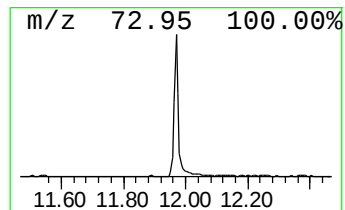
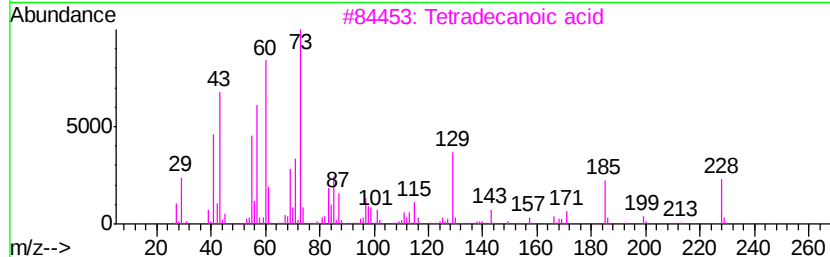
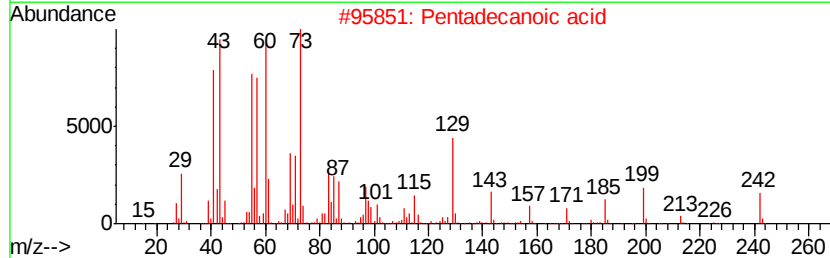
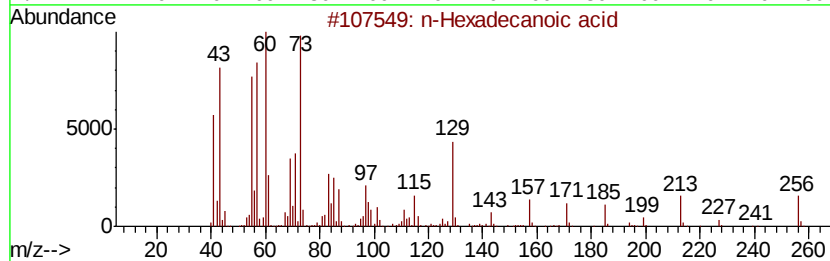
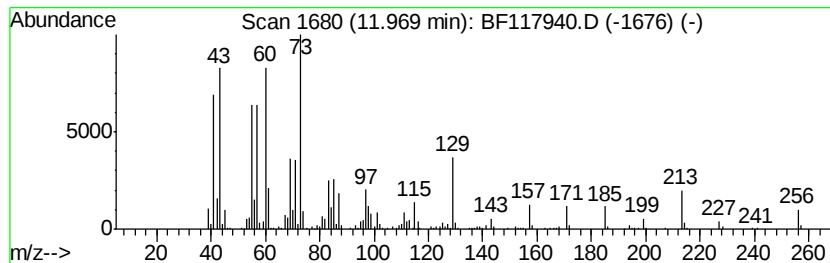
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	10.38 ng	940072	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	89
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



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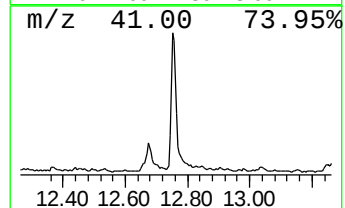
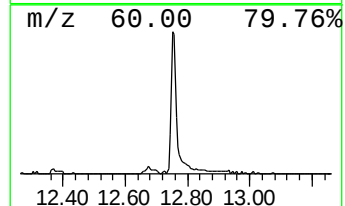
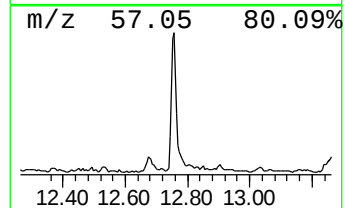
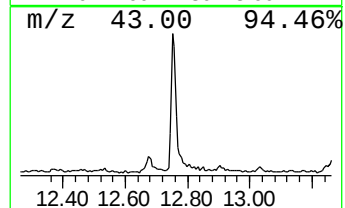
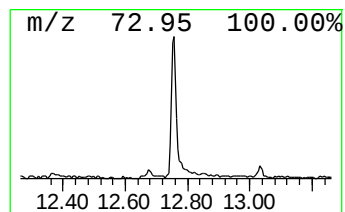
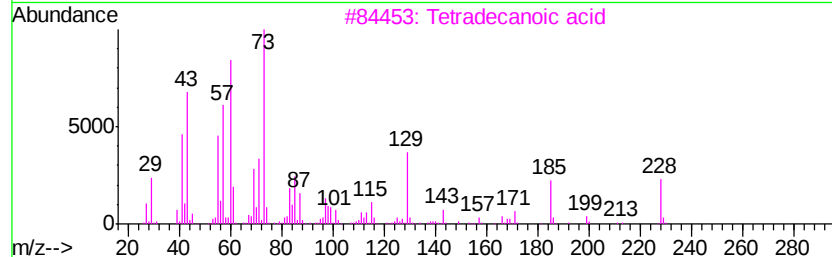
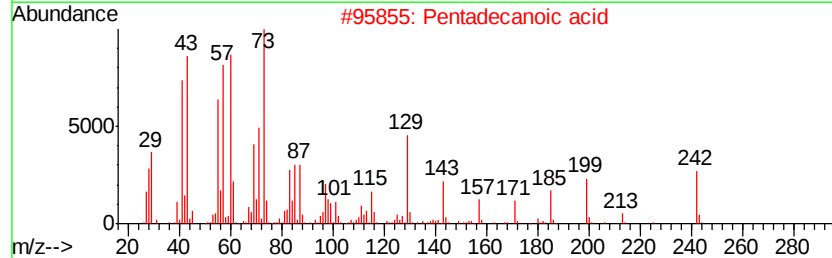
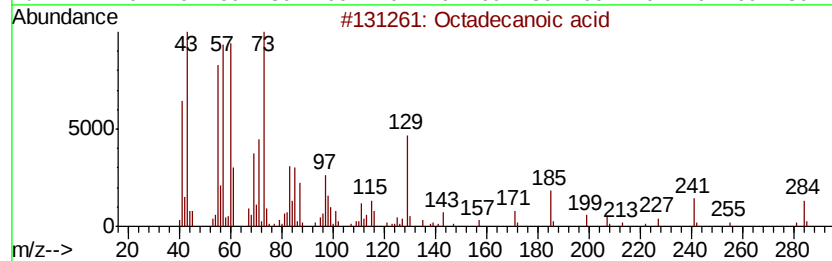
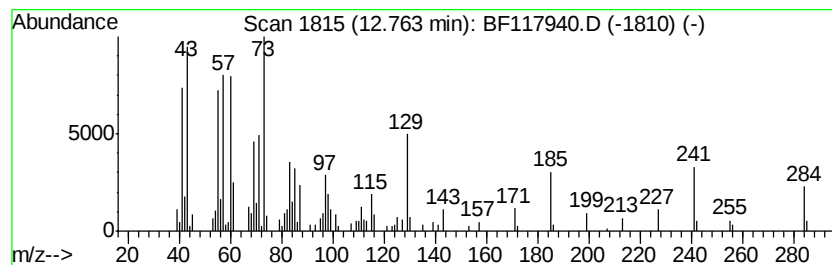
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.76	4.47 ng	404946	Phenanthrene-d10	11.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	20



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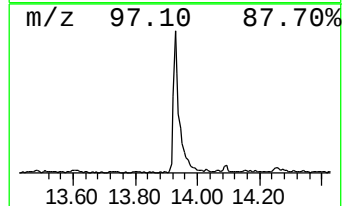
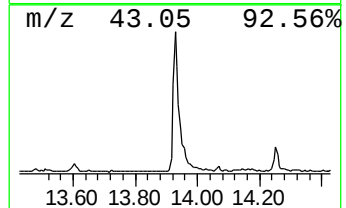
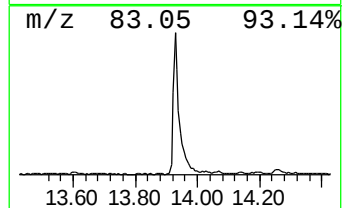
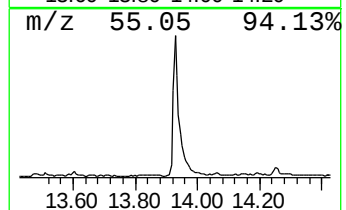
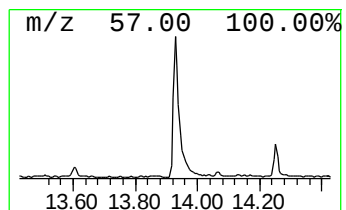
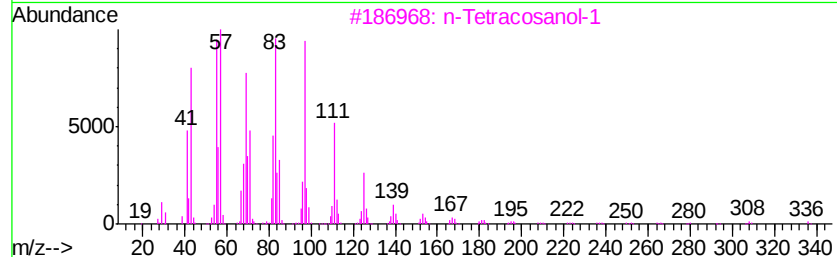
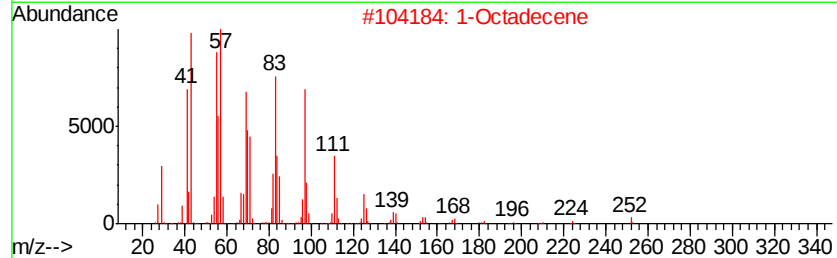
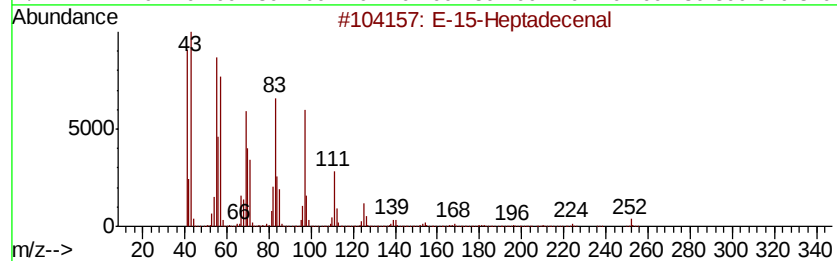
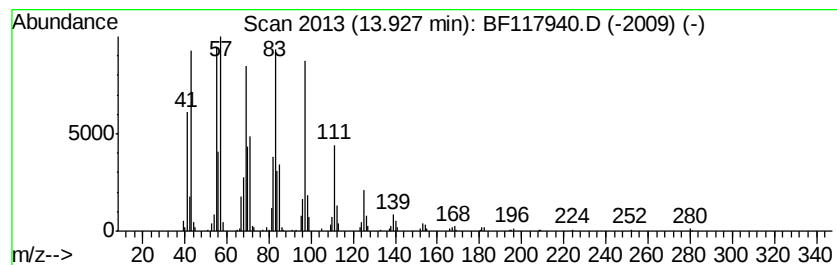
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.93	10.45 ng	795933	Chrysene-d12		14.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	99
2	1-Octadecene			252	C18H36	000112-88-9	97
3	n-Tetracosanol-1			354	C24H50O	000506-51-4	95
4	1-Heneicosanol			312	C21H44O	015594-90-8	95
5	n-Nonadecanol-1			284	C19H40O	001454-84-8	95



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117940.D
Acq On : 23 Nov 2019 1:24
Operator : JU
Sample : K5840-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-SE-02

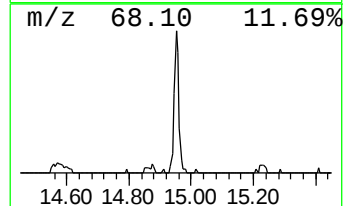
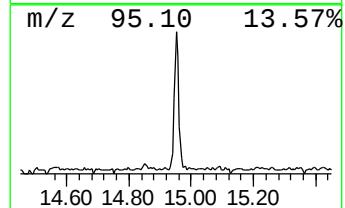
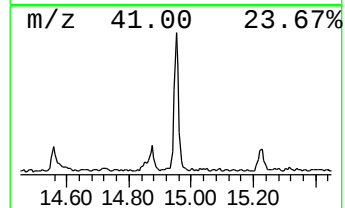
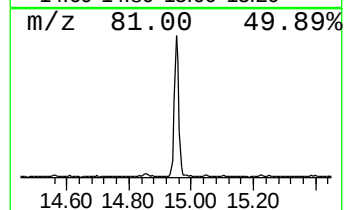
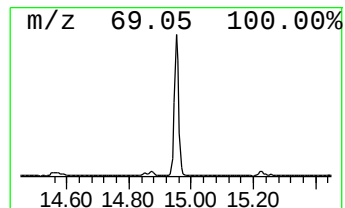
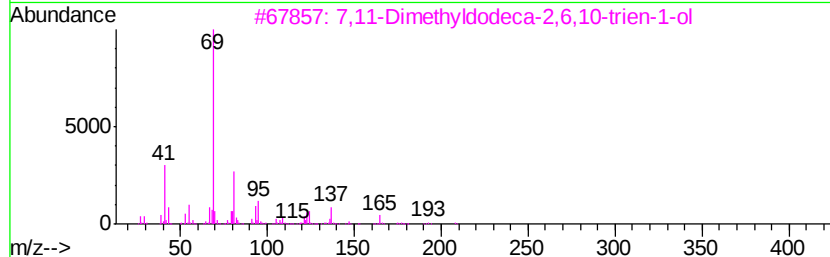
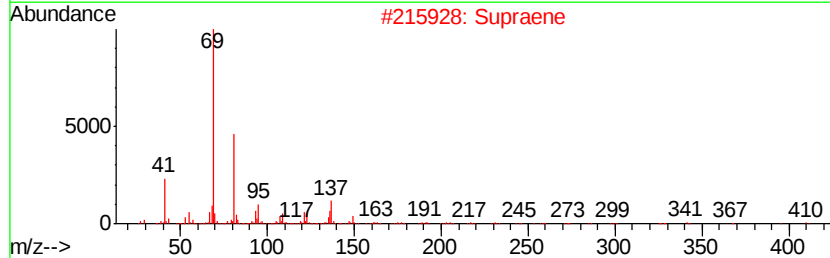
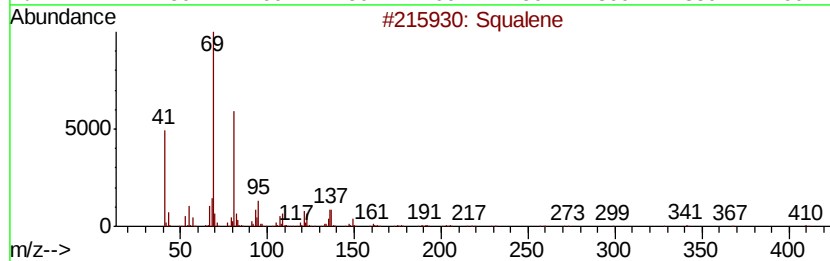
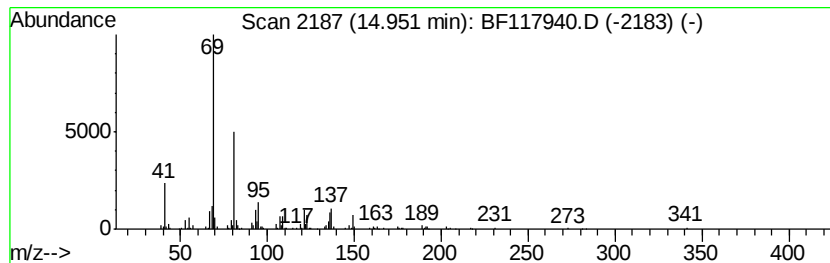
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	5.92 ng	374739	Perylene-d12	15.60

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		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		Farnesol isomer a	222	C15H26O	1000108-92-4	64
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117940.D
Acq On : 23 Nov 2019 1:24
Operator : JU
Sample : K5840-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-SE-02

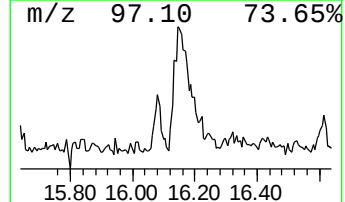
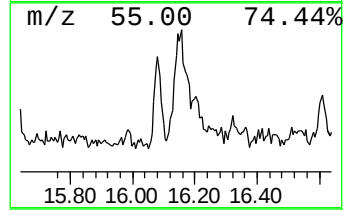
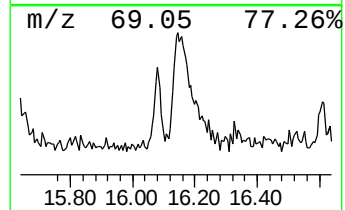
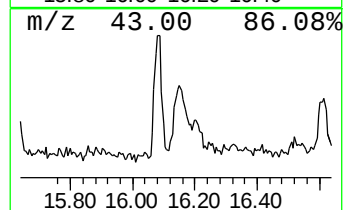
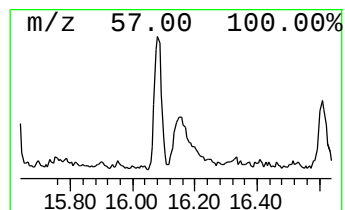
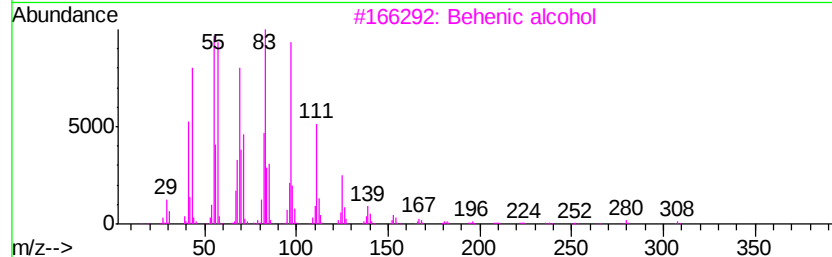
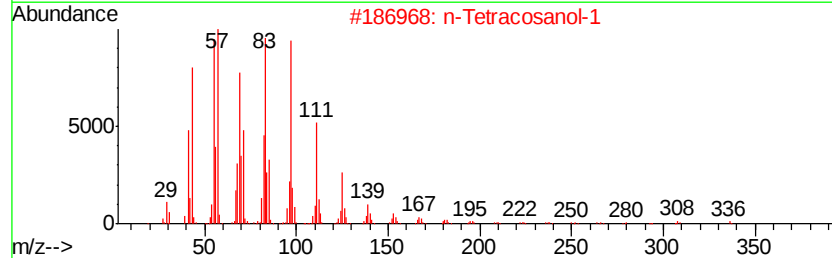
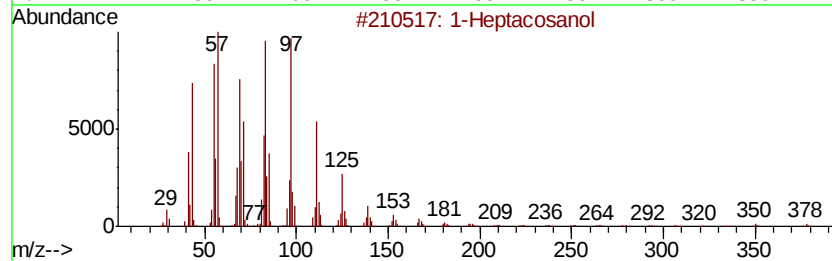
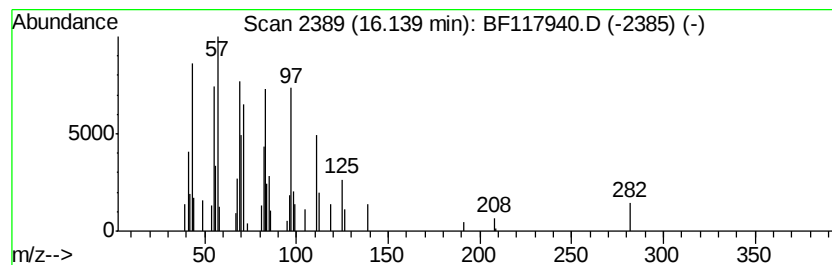
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.34 ng	148262	Perylene-d12	15.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	94
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	93
3	Behenic alcohol		326	C22H46O	000661-19-8	93
4	1-Heneicosanol		312	C21H44O	015594-90-8	87
5	n-Nonadecanol-1		284	C19H40O	001454-84-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112219\
Data File : BF117940.D
Acq On : 23 Nov 2019 1:24
Operator : JU
Sample : K5840-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-SE-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.22	16.1	ng	817421	1	6.90	1013890	20.0
2-Pentanone, 4-hy...	5.12	13.9	ng	703856	1	6.90	1013890	20.0
unknown6.67	6.67	70.0	ng	3551380	1	6.90	1013890	20.0
n-Hexadecanoic acid	11.97	10.4	ng	940072	4	11.45	1811320	20.0
Octadecanoic acid	12.76	4.5	ng	404946	4	11.45	1811320	20.0
E-15-Heptadecenal	13.93	10.4	ng	795933	5	14.09	1523170	20.0
Squalene	14.95	5.9	ng	374739	6	15.60	1265230	20.0
1-Heptacosanol	16.14	2.3	ng	148262	6	15.60	1265230	20.0