

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
 Data File : BF117467.D
 Acq On : 22 Oct 2019 00:15
 Operator : JU
 Sample : K5453-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT1496

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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	5.351	551	555	574	rBV	1093178	1128492	68.86%	9.009%
2	6.381	726	730	747	rBV	1291969	1261666	76.98%	10.072%
3	6.504	747	751	757	rBV	1507652	1288720	78.63%	10.288%
4	6.734	786	790	804	rBV	247371	241659	14.75%	1.929%
5	6.887	812	816	831	rBV	1138538	972403	59.33%	7.763%
6	7.298	882	886	906	rBV	816961	777108	47.42%	6.204%
7	8.010	1004	1007	1031	rBV	299789	317430	19.37%	2.534%
8	9.086	1186	1190	1193	rBV	1854398	1510082	92.14%	12.055%
9	9.480	1254	1257	1267	rBV	188338	153322	9.36%	1.224%
10	9.763	1301	1305	1318	rBV	437391	373279	22.78%	2.980%
11	10.551	1436	1439	1454	rBV	890849	907197	55.35%	7.242%
12	11.251	1554	1558	1566	rBV	353363	400042	24.41%	3.194%
13	11.486	1593	1598	1603	rBV9	16410	36605	2.23%	0.292%
14	11.780	1645	1648	1654	rBV2	65602	72768	4.44%	0.581%
15	12.563	1778	1781	1787	rBV7	18051	33492	2.04%	0.267%
16	12.833	1822	1827	1830	rBV	1793645	1638899	100.00%	13.084%
17	13.727	1975	1979	1997	rVB	146634	272700	16.64%	2.177%
18	13.892	2003	2007	2015	rBV	309681	336908	20.56%	2.690%
19	14.045	2029	2033	2036	rBV	33616	31810	1.94%	0.254%
20	14.345	2081	2084	2089	rBV	53987	57848	3.53%	0.462%
21	14.645	2131	2135	2139	rVB	73538	77246	4.71%	0.617%
22	14.957	2184	2188	2192	rBV	78133	80816	4.93%	0.645%
23	15.315	2244	2249	2262	rVB	272885	370183	22.59%	2.955%
24	15.721	2313	2318	2323	rVB2	45724	61508	3.75%	0.491%
25	15.780	2323	2328	2341	rBV8	18438	62041	3.79%	0.495%
26	16.186	2391	2397	2401	rBV	21366	38973	2.38%	0.311%
27	16.733	2481	2490	2499	rBV4	9446	23181	1.41%	0.185%

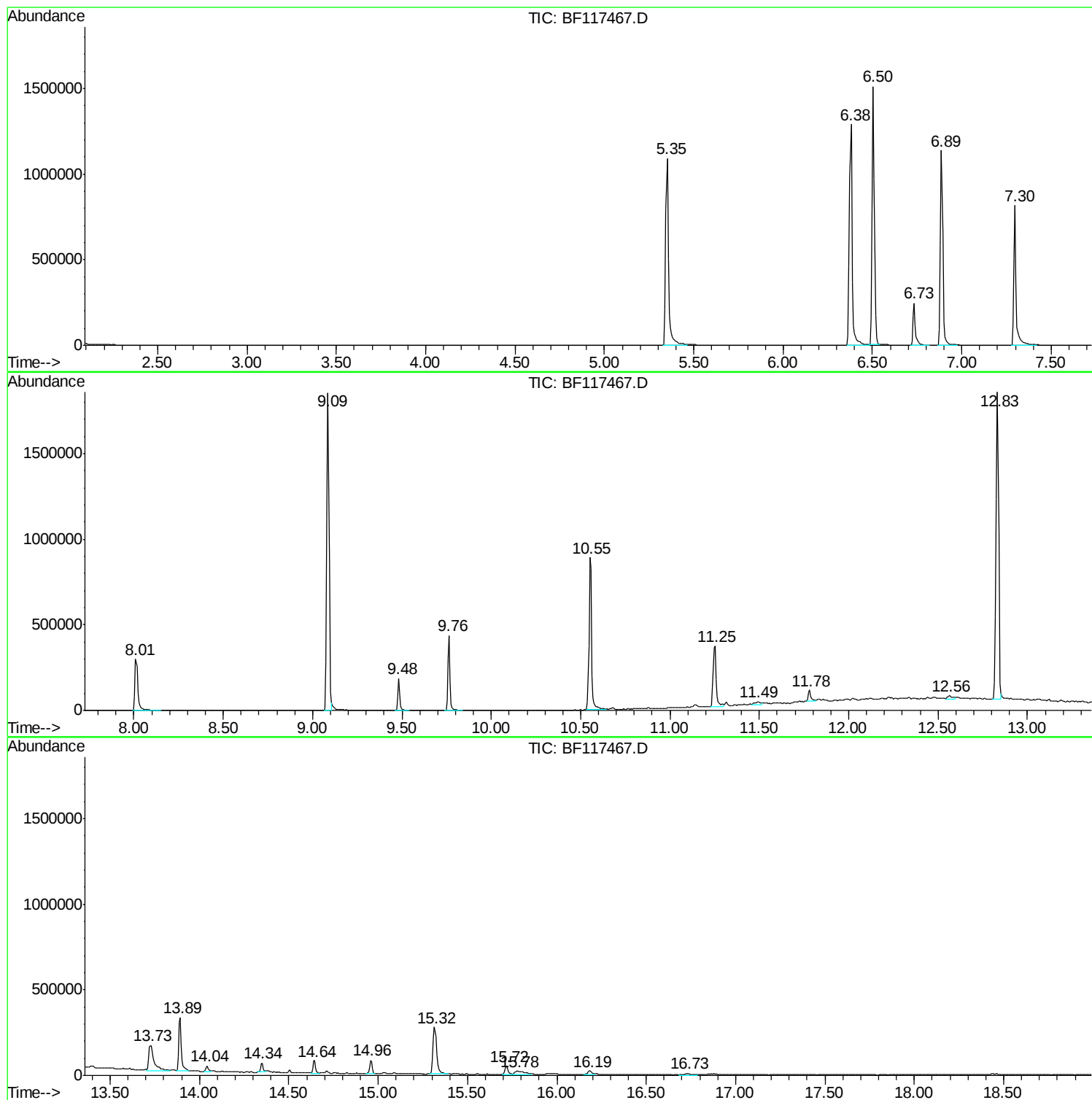
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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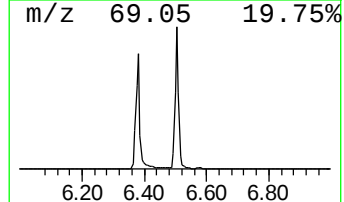
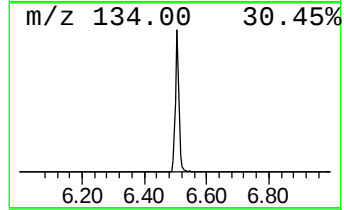
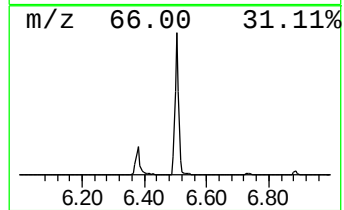
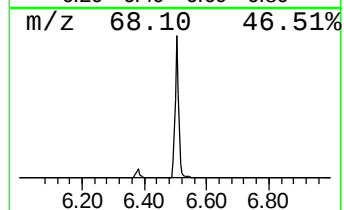
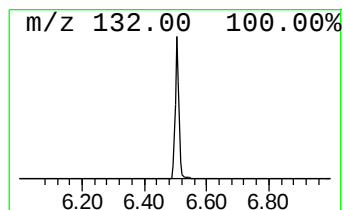
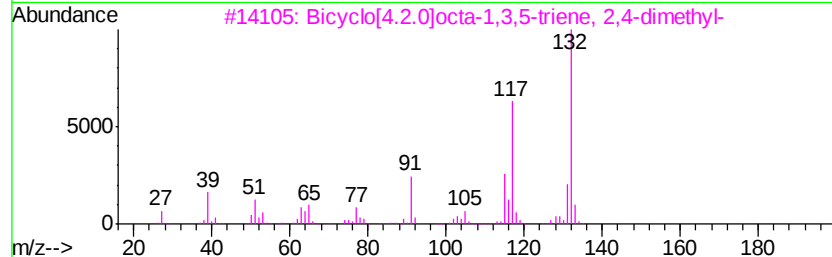
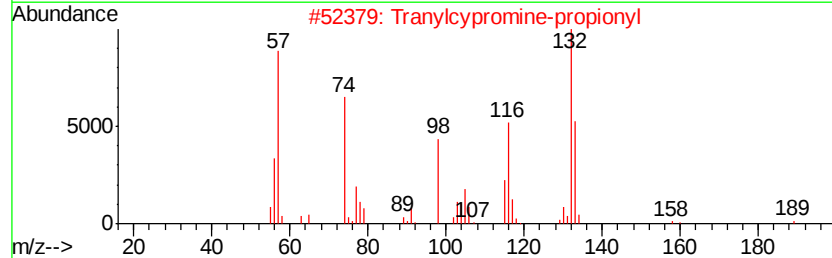
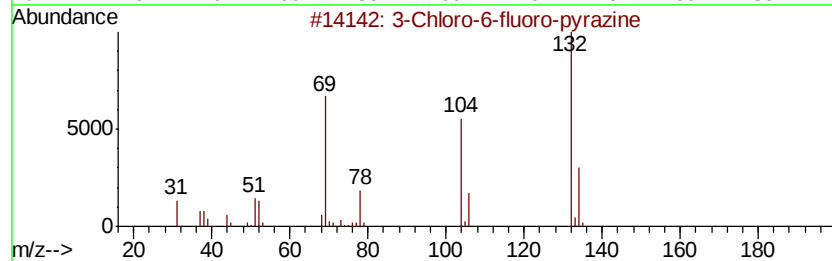
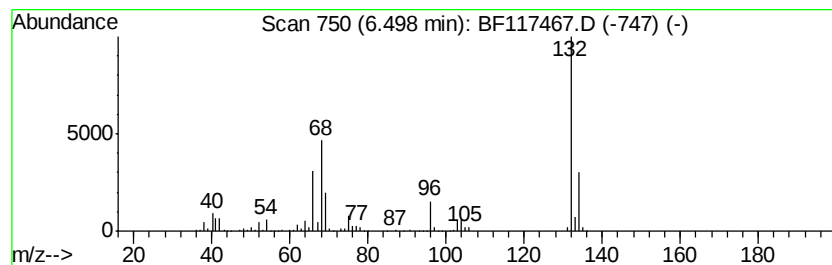
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	106.66 ng	1288720	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



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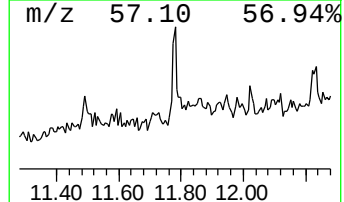
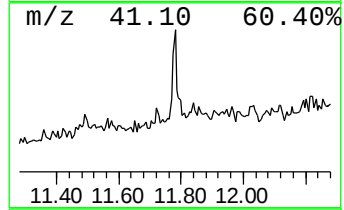
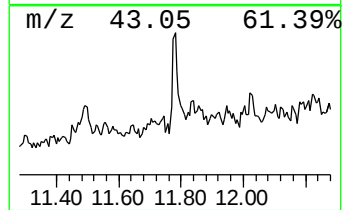
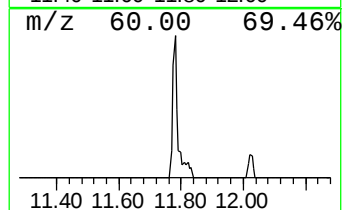
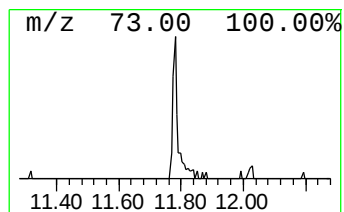
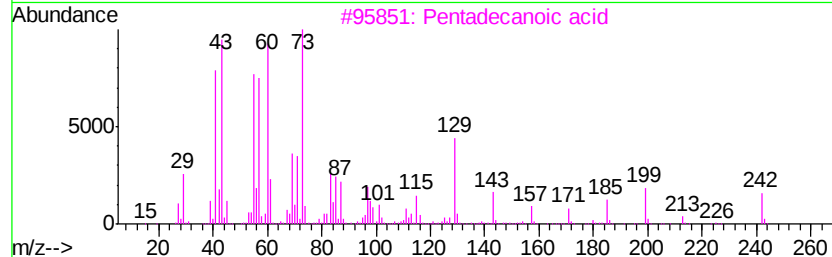
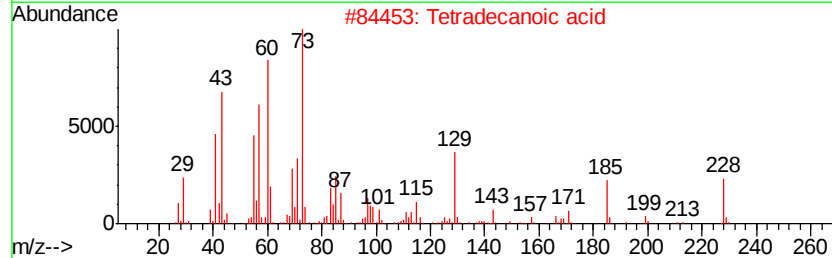
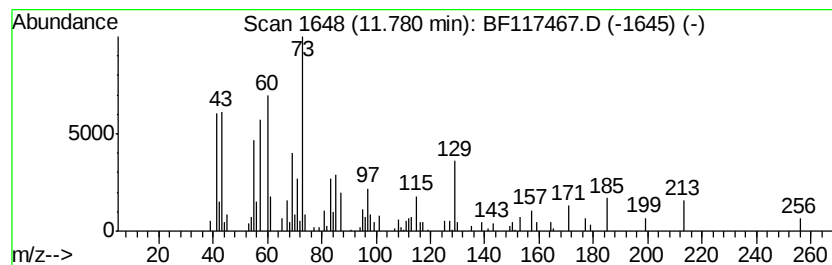
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	3.64 ng	72768	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43



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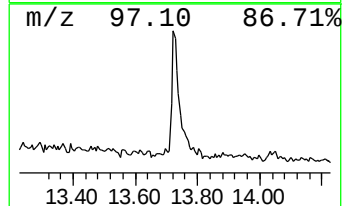
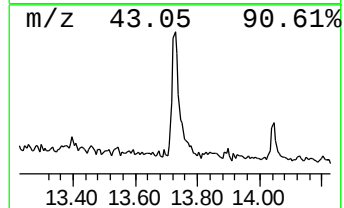
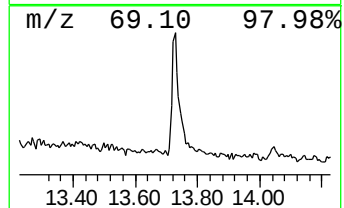
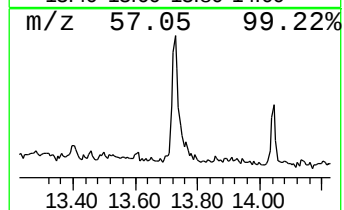
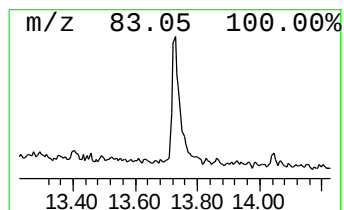
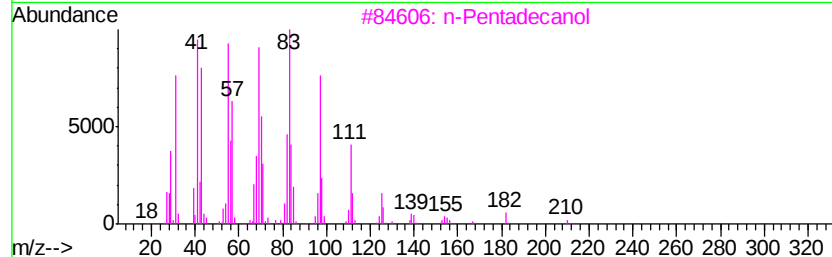
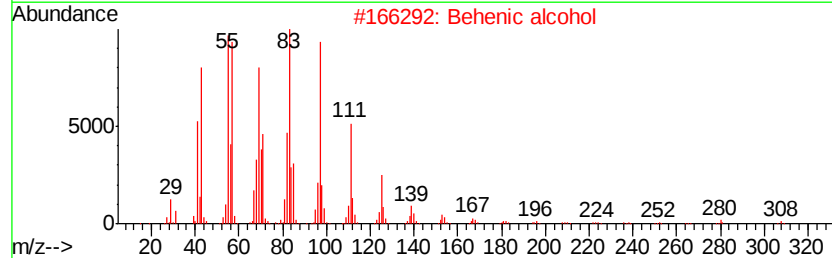
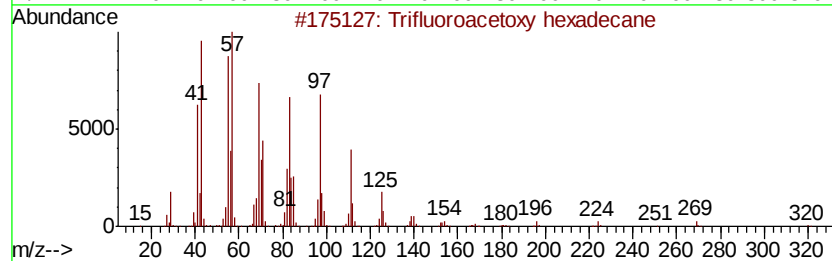
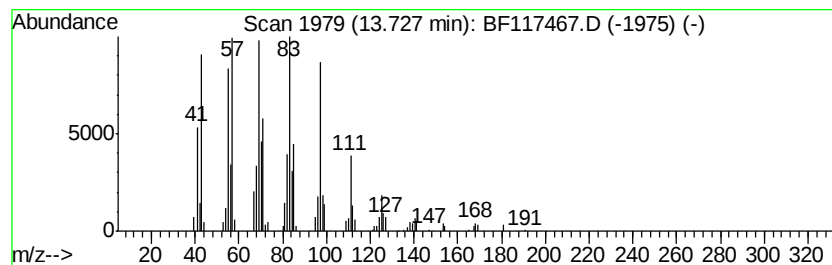
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	16.19 ng	272700	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		Behenic alcohol	326	C22H46O	000661-19-8	90
3		n-Pentadecanol	228	C15H32O	000629-76-5	87
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	87
5		1-Hexadecanol	242	C16H34O	036653-82-4	83



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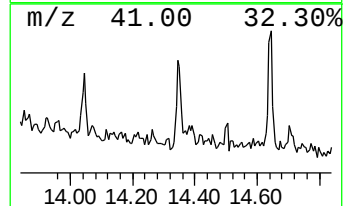
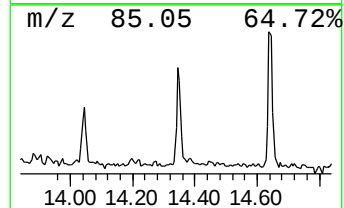
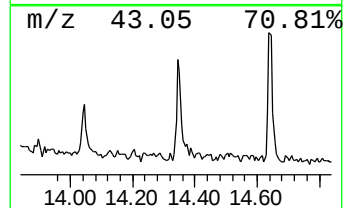
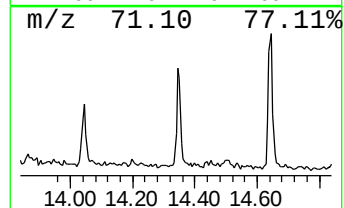
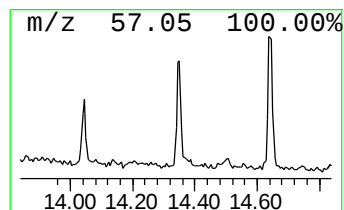
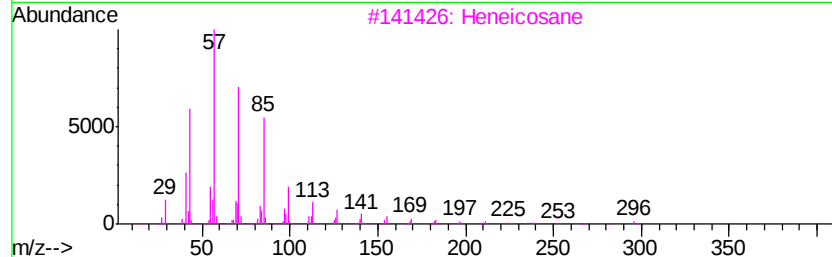
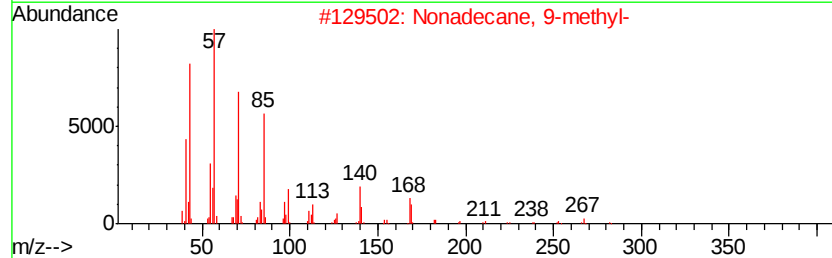
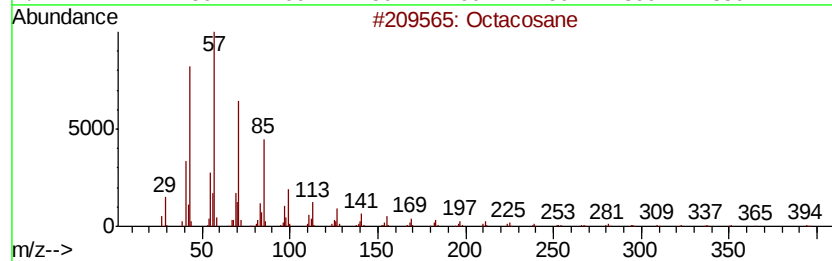
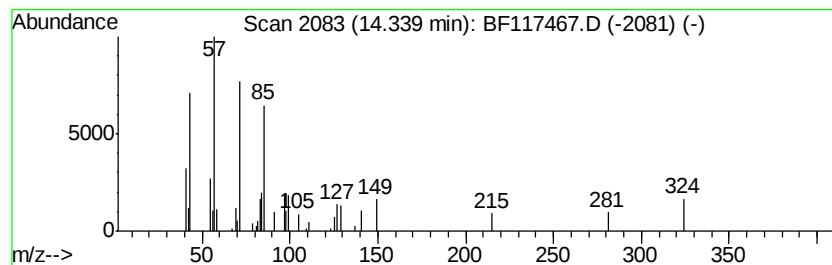
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Peak Number 5 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.43 ng	57848	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	86
3	Heneicosane		296	C21H44	000629-94-7	83
4	Heptadecane		240	C17H36	000629-78-7	83
5	Octadecane		254	C18H38	000593-45-3	80



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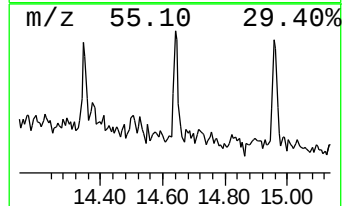
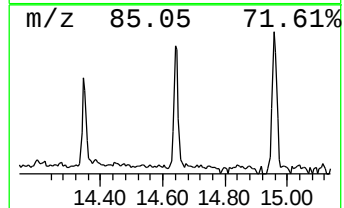
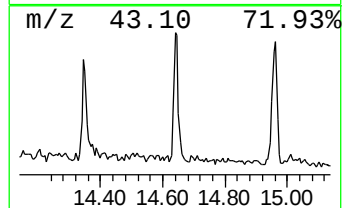
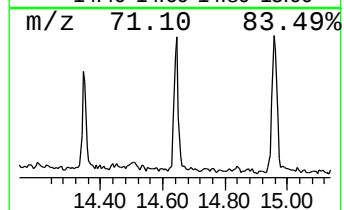
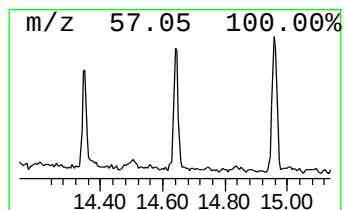
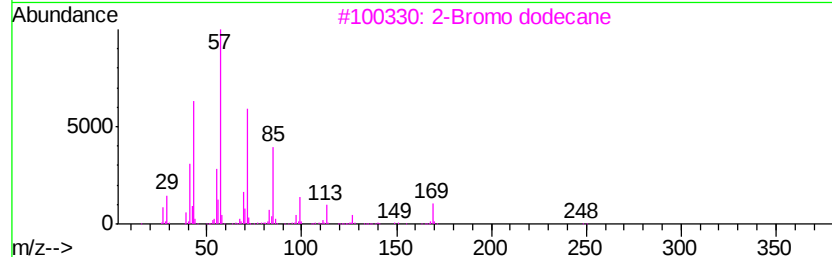
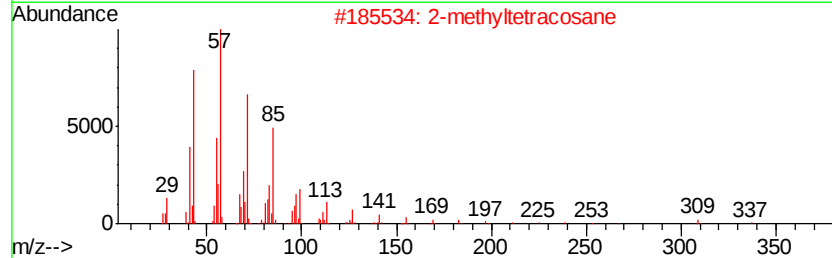
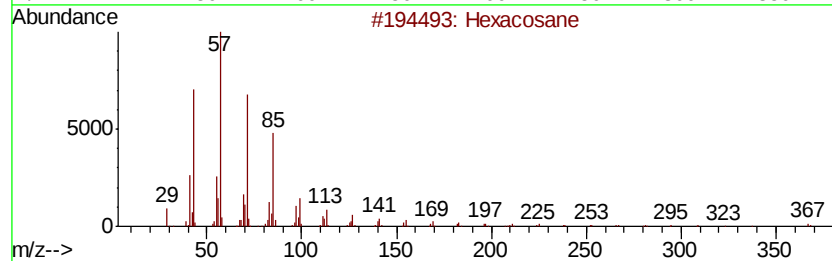
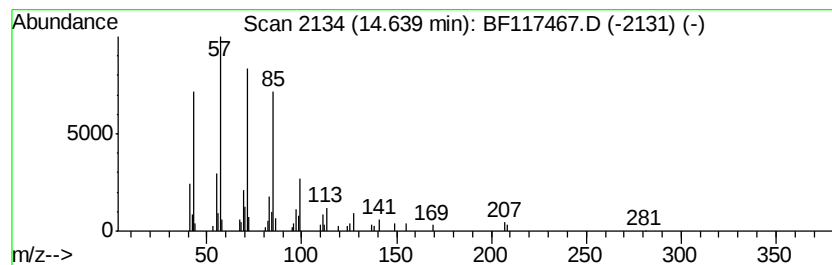
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.17 ng	77246	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	83
2	2-methyltetracosane		352	C25H52	1000376-72-6	80
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	80
4	triacontane		422	C30H62	000638-68-6	80
5	Heptacosane		380	C27H56	000593-49-7	80



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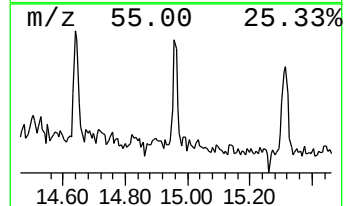
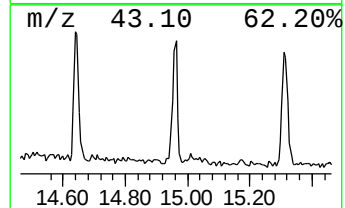
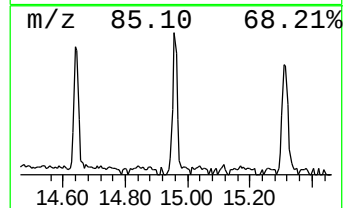
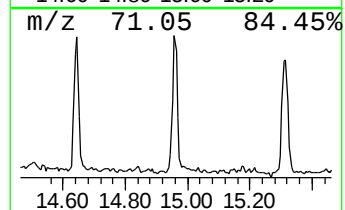
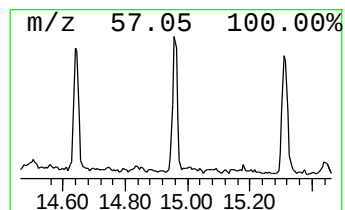
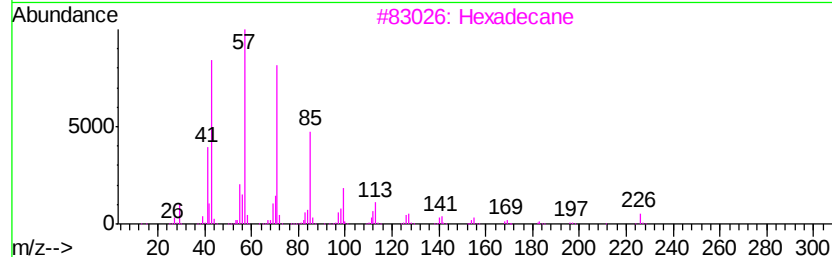
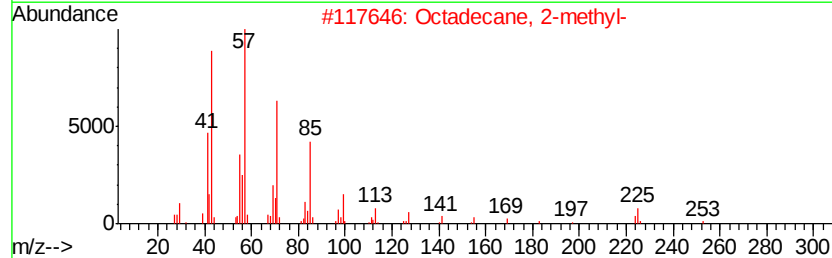
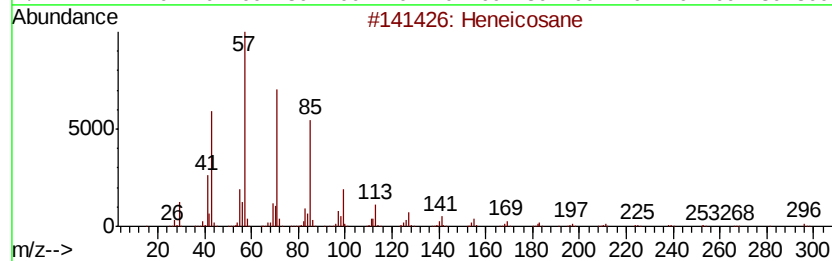
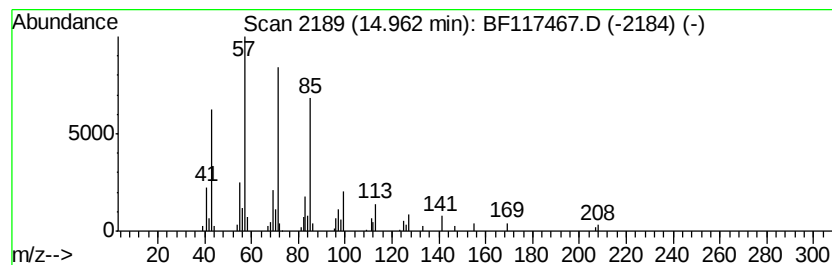
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	4.37 ng	80816	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octadecane, 2-methyl-		268	C19H40	001560-88-9	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	2-methyloctacosane		408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
Data File : BF117467.D
Acq On : 22 Oct 2019 00:15
Operator : JU
Sample : K5453-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
RT1496

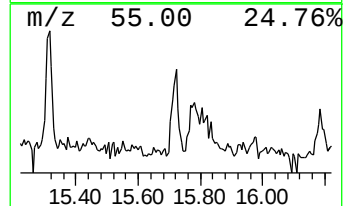
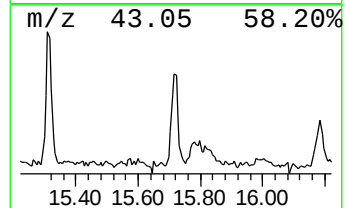
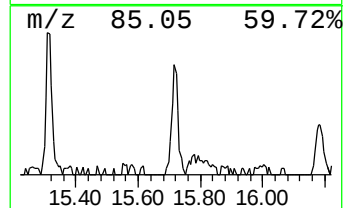
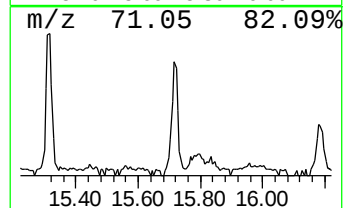
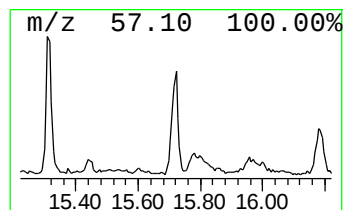
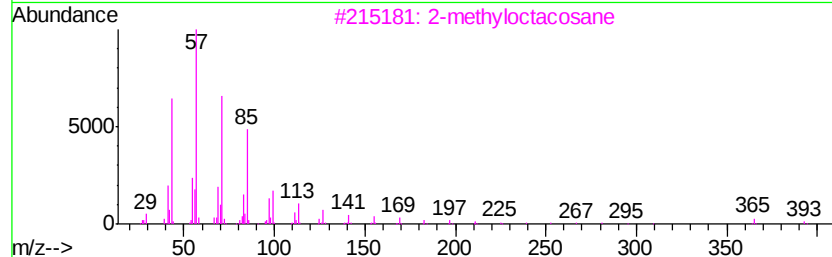
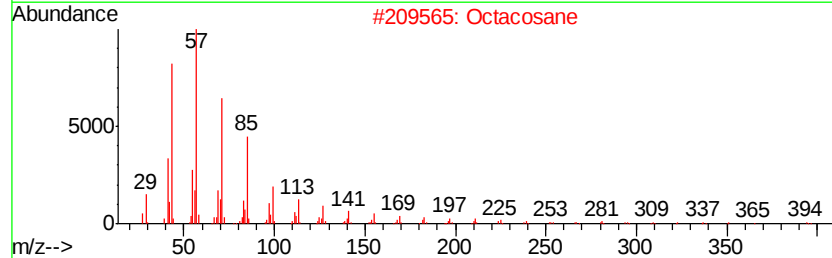
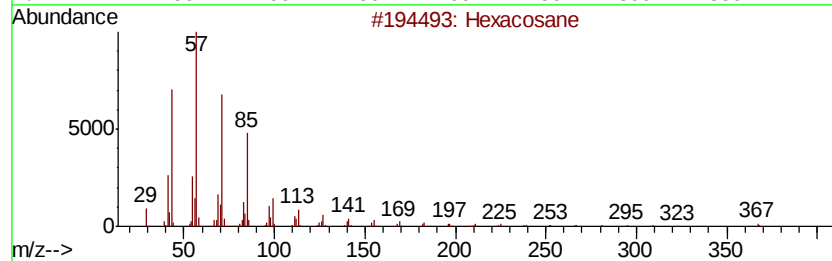
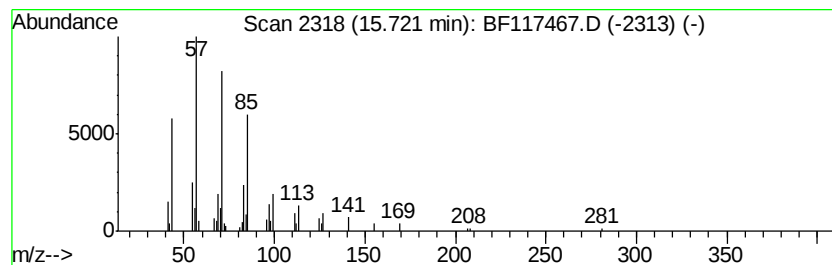
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.32 ng	61508	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Octacosane	394	C28H58	000630-02-4	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



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Data File : BF117467.D
Acq On : 22 Oct 2019 00:15
Operator : JU
Sample : K5453-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT1496

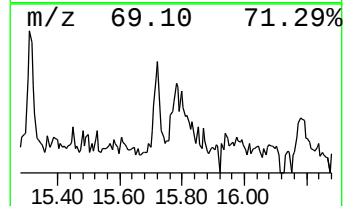
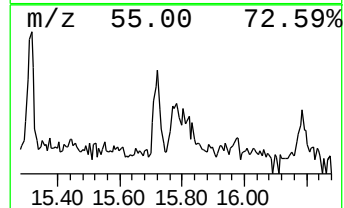
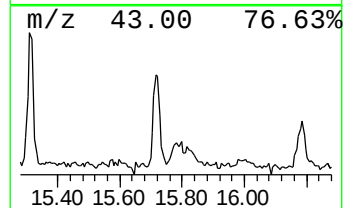
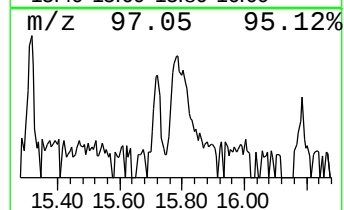
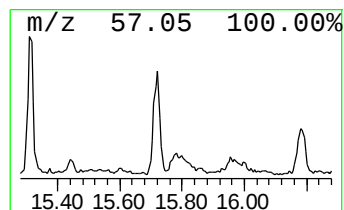
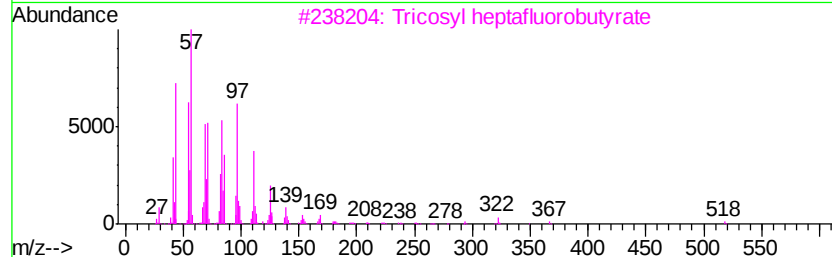
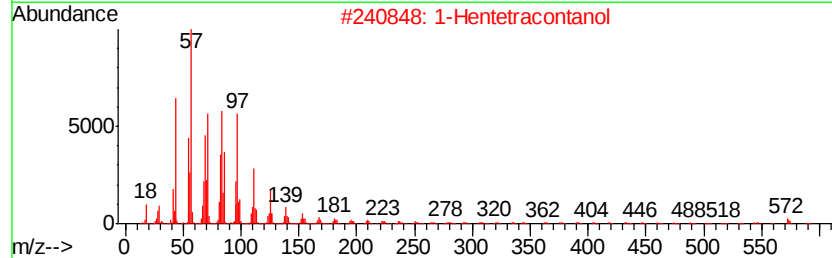
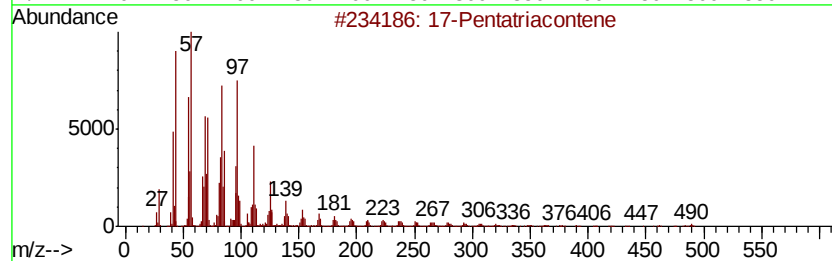
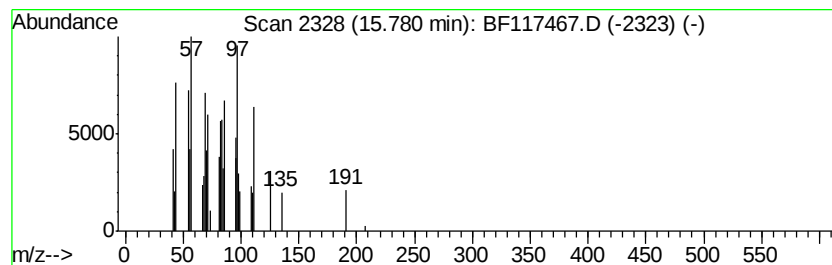
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	3.35 ng	62041	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene		491	C35H70	006971-40-0	80
2	1-Hentetracontanol		593	C41H84O	040710-42-7	64
3	Tricosyl heptafluorobutvrate		536	C27H47F7O2	1000351-83-4	50
4	1-Heptacosanol		396	C27H56O	002004-39-9	47
5	Octacosanol		410	C28H58O	000557-61-9	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
Data File : BF117467.D
Acq On : 22 Oct 2019 00:15
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Sample : K5453-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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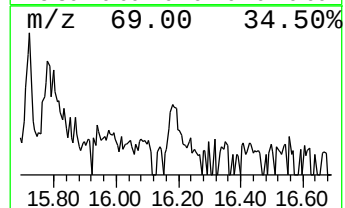
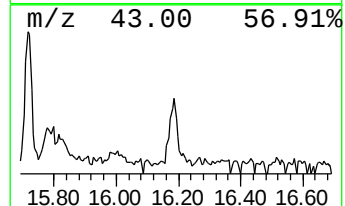
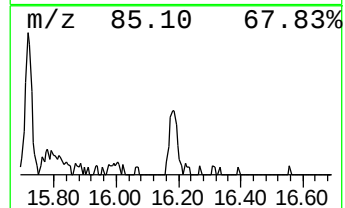
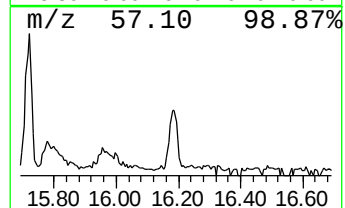
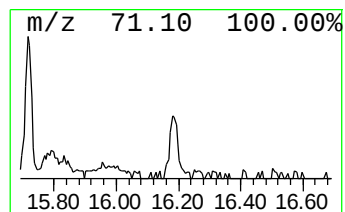
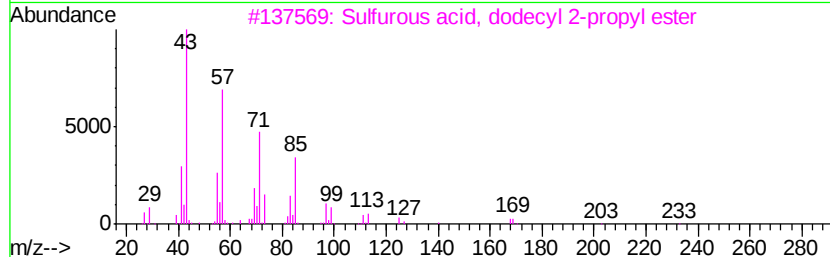
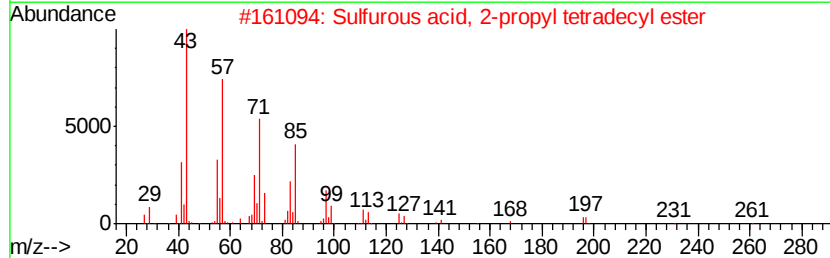
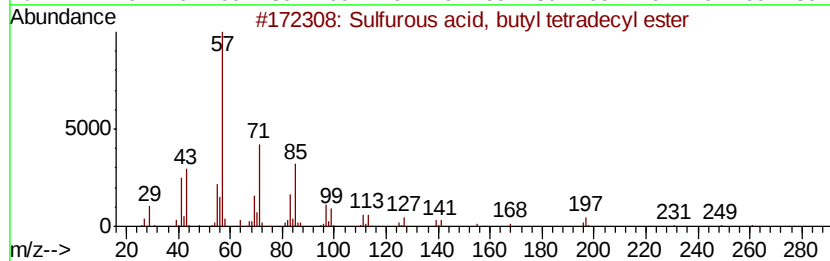
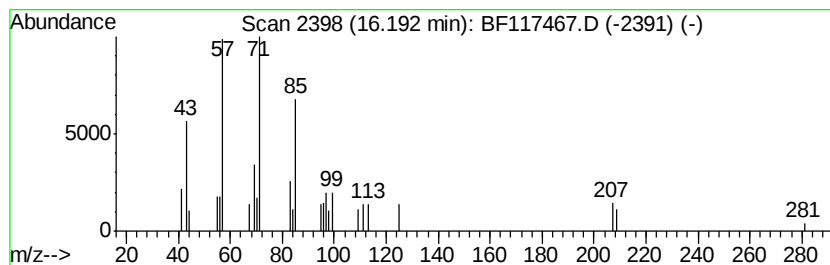
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, butyl tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.11 ng	38973	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	78
2			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	72
3			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	72
4			Hexatriacontane	507	C36H74	000630-06-8	72
5			Tetratetracontane	619	C44H90	007098-22-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102119\
Data File : BF117467.D
Acq On : 22 Oct 2019 00:15
Operator : JU
Sample : K5453-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT1496

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	106.7	ng	1288720	1	6.73	241659	20.0
n-Hexadecanoic acid	11.78	3.6	ng	72768	4	11.25	400042	20.0
Trifluoroacetoxy ...	13.73	16.2	ng	272700	5	13.89	336908	20.0
Octacosane	14.34	3.4	ng	57848	5	13.89	336908	20.0
Hexacosane	14.64	4.2	ng	77246	6	15.32	370183	20.0
Heneicosane	14.96	4.4	ng	80816	6	15.32	370183	20.0
2-methyloctacosane	15.72	3.3	ng	61508	6	15.32	370183	20.0
17-Pentatriacontene	15.78	3.4	ng	62041	6	15.32	370183	20.0
Sulfurous acid, b...	16.19	2.1	ng	38973	6	15.32	370183	20.0