

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
 Data File : BF117486.D
 Acq On : 23 Oct 2019 16:45
 Operator : JU
 Sample : K5494-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP1-6FT

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-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	552	555	575	rBV	836531	888314	83.03%	8.262%
2	6.381	726	730	747	rBV	982388	1029539	96.23%	9.576%
3	6.504	747	751	762	rVB	1203432	1029366	96.21%	9.574%
4	6.728	787	789	802	rVB	266909	272676	25.49%	2.536%
5	6.887	812	816	827	rBV	833085	706990	66.08%	6.576%
6	7.298	882	886	907	rBV	585953	616389	57.61%	5.733%
7	8.010	1004	1007	1021	rBV	382029	364224	34.04%	3.388%
8	9.086	1186	1190	1201	rBV	1249029	1054994	98.61%	9.812%
9	9.204	1207	1210	1214	rVB	41109	33728	3.15%	0.314%
10	9.480	1254	1257	1271	rBV	252849	206584	19.31%	1.921%
11	9.763	1301	1305	1318	rBB	525640	441376	41.26%	4.105%
12	10.551	1436	1439	1451	rBV	692936	675834	63.17%	6.286%
13	11.245	1554	1557	1567	rBV	446603	456759	42.69%	4.248%
14	11.486	1595	1598	1604	rBV3	7148	12146	1.14%	0.113%
15	11.780	1640	1648	1656	rBV	107252	129956	12.15%	1.209%
16	12.298	1733	1736	1741	rBV3	26705	49249	4.60%	0.458%
17	12.463	1762	1764	1767	rBV	57153	56038	5.24%	0.521%
18	12.557	1778	1780	1787	rBV3	26307	30785	2.88%	0.286%
19	12.692	1798	1803	1809	rBV	56076	68685	6.42%	0.639%
20	12.833	1822	1827	1830	rBV	1111128	1069863	100.00%	9.951%
21	13.057	1861	1865	1869	rVB2	14008	13314	1.24%	0.124%
22	13.727	1975	1979	1993	rBV3	144310	239370	22.37%	2.226%
23	13.892	2002	2007	2019	rVB	394653	445426	41.63%	4.143%
24	14.045	2029	2033	2036	rBV	16075	18160	1.70%	0.169%
25	14.345	2081	2084	2087	rBV	28383	29928	2.80%	0.278%
26	14.645	2131	2135	2138	rVB	34723	32520	3.04%	0.302%
27	14.715	2143	2147	2150	rBV	20495	20076	1.88%	0.187%
28	14.921	2178	2182	2185	rBV	20330	27949	2.61%	0.260%
29	14.957	2185	2188	2192	rVB2	52145	57951	5.42%	0.539%
30	15.210	2228	2231	2235	rVB	12059	13236	1.24%	0.123%
31	15.268	2237	2241	2244	rBV	15874	15980	1.49%	0.149%
32	15.315	2244	2249	2259	rBV	275751	373298	34.89%	3.472%
33	15.715	2311	2317	2324	rBV	59522	88687	8.29%	0.825%
34	15.792	2324	2330	2335	rBV6	21527	54999	5.14%	0.512%

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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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35	16.186	2390	2397	2402	rBV2	30186	48814	4.56%	0.454%
36	16.727	2484	2489	2501	rVB7	17381	41028	3.83%	0.382%
37	16.868	2506	2513	2520	rBV10	6048	19047	1.78%	0.177%
38	17.386	2592	2601	2604	rBV5	8282	18454	1.72%	0.172%

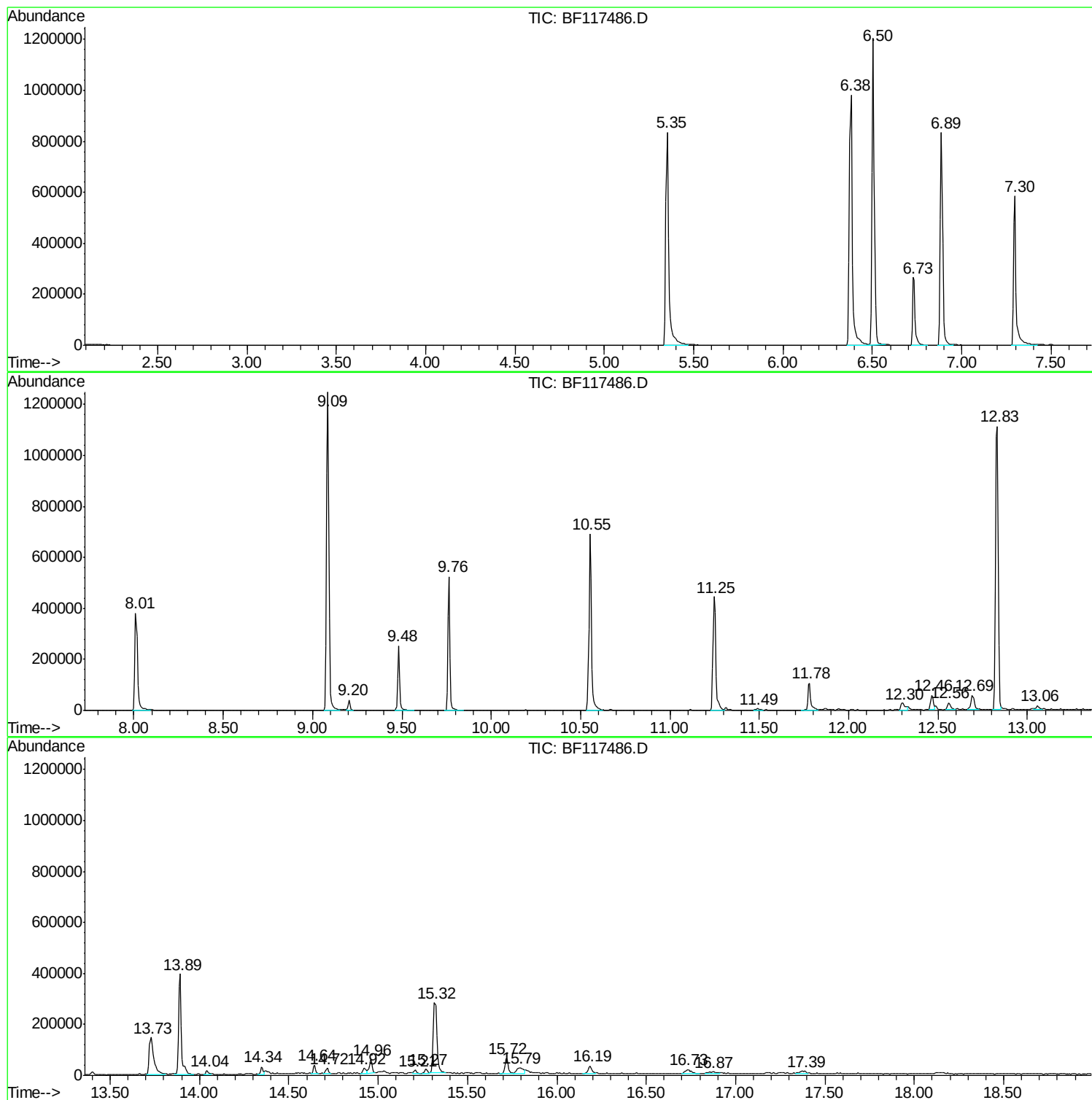
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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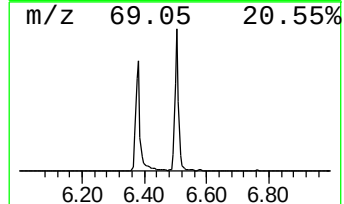
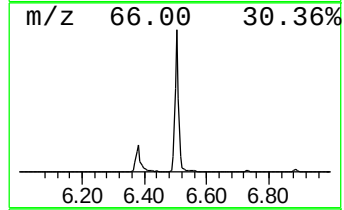
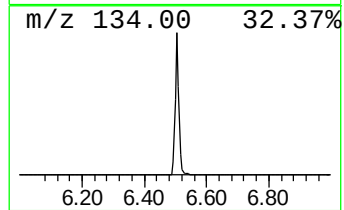
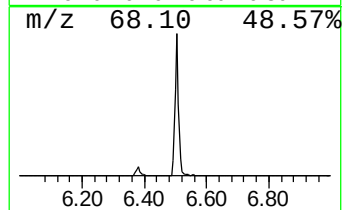
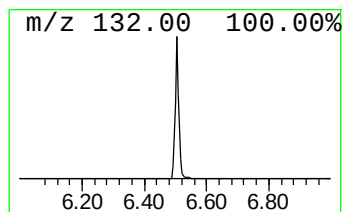
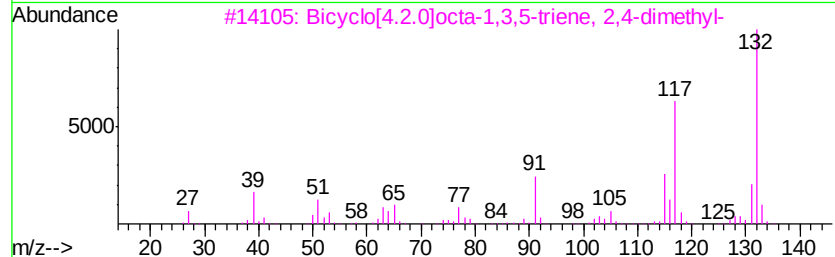
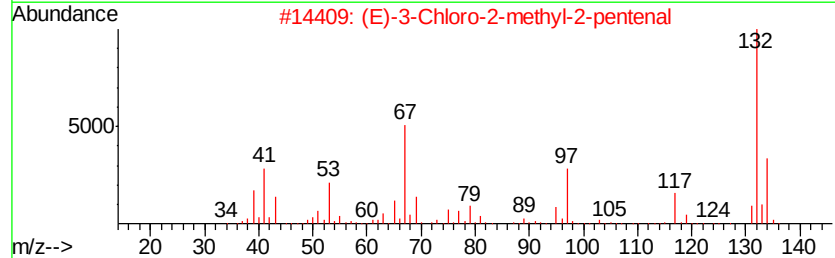
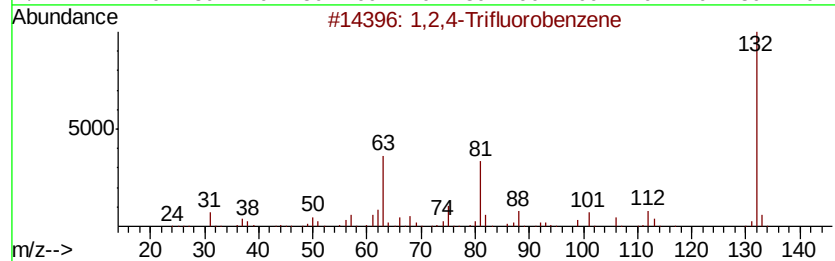
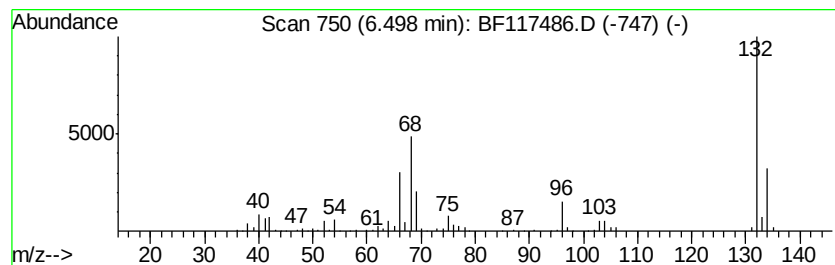
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	75.50 ng	1029370	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
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		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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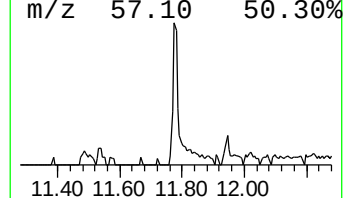
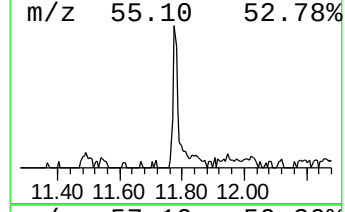
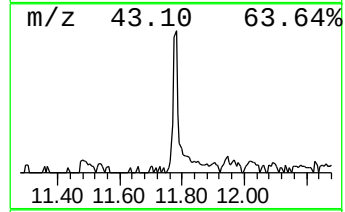
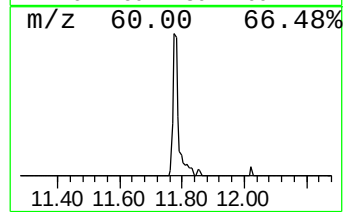
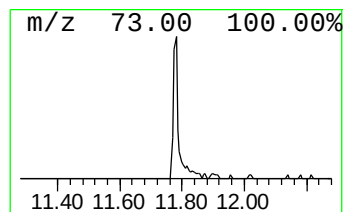
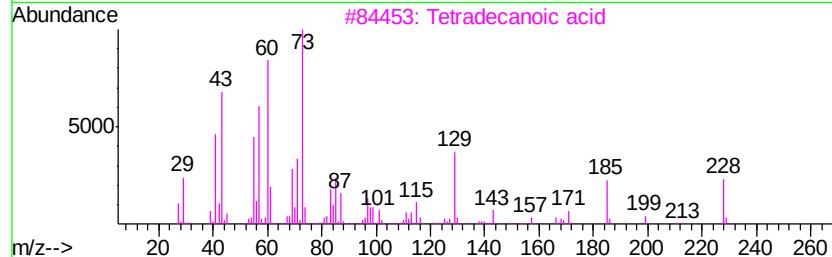
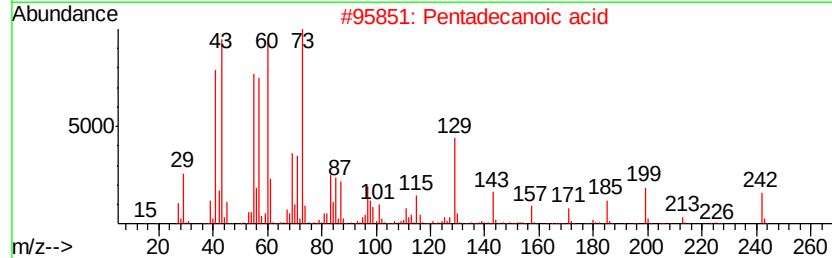
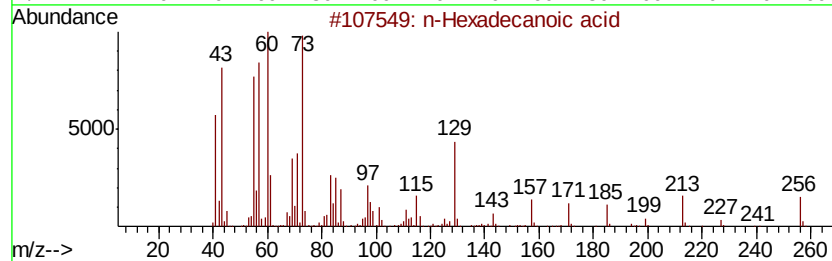
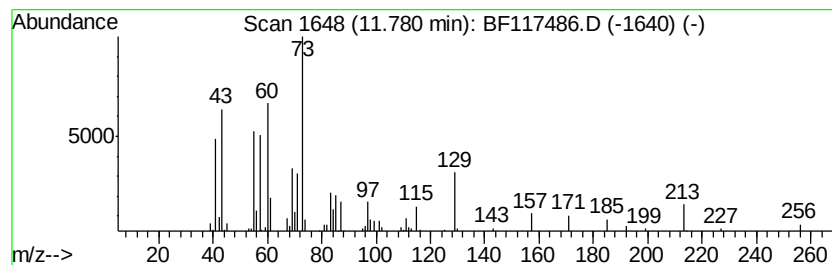
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	5.69 ng	129956	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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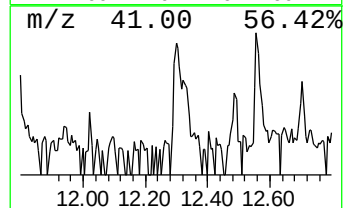
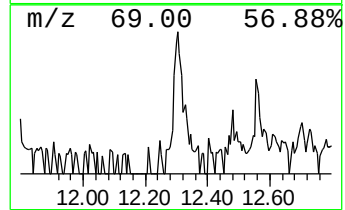
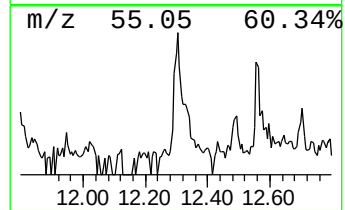
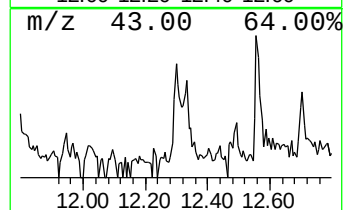
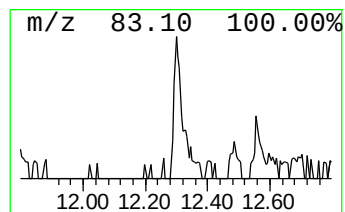
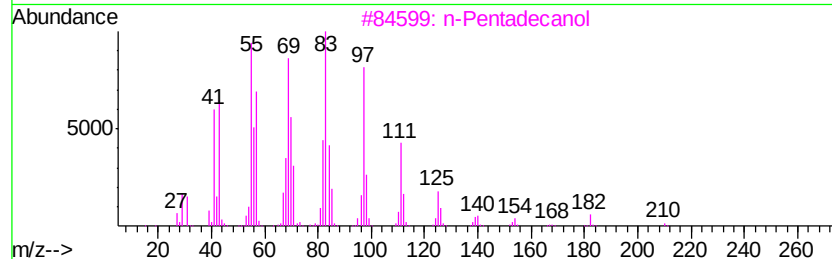
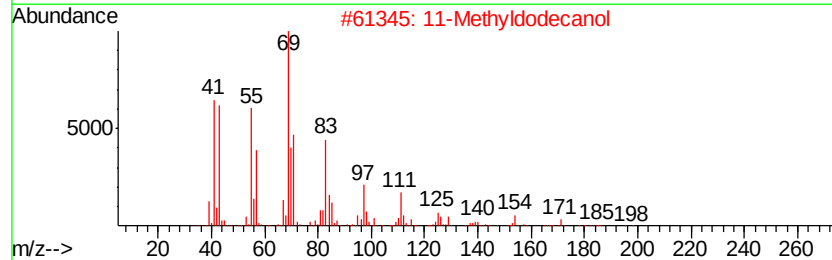
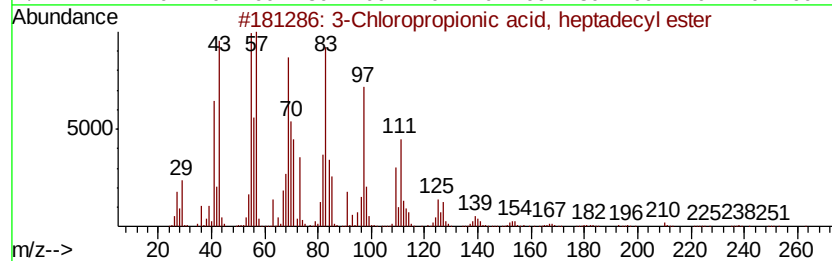
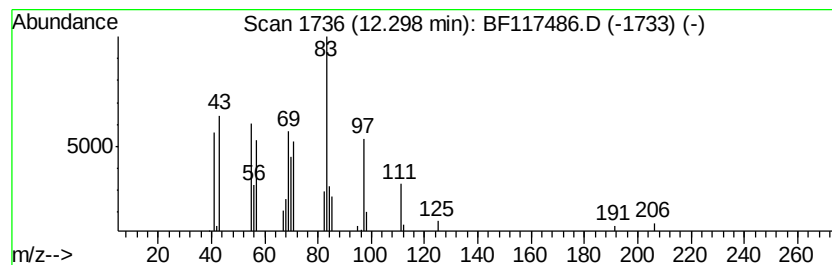
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 3-Chloropropionic acid, hep... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.30	2.16 ng	49249	Phenanthrene-d10	11.25		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	80
2		11-Methyldodecanol	200	C13H28O	085763-57-1	72
3		n-Pentadecanol	228	C15H32O	000629-76-5	70
4		Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	62
5		1-Hexadecanol	242	C16H34O	036653-82-4	62



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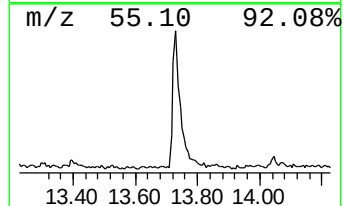
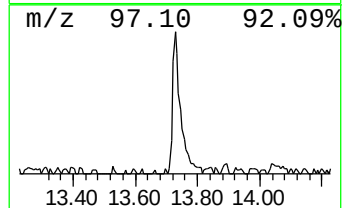
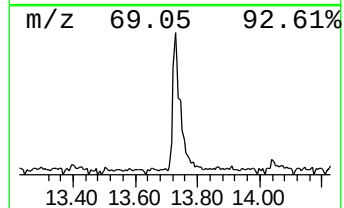
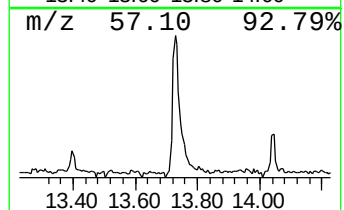
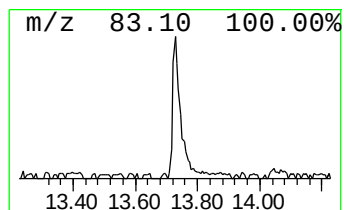
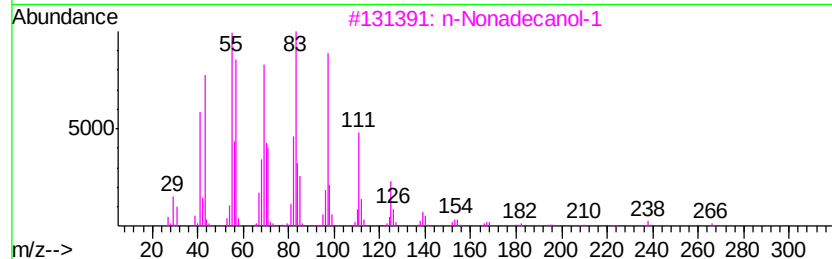
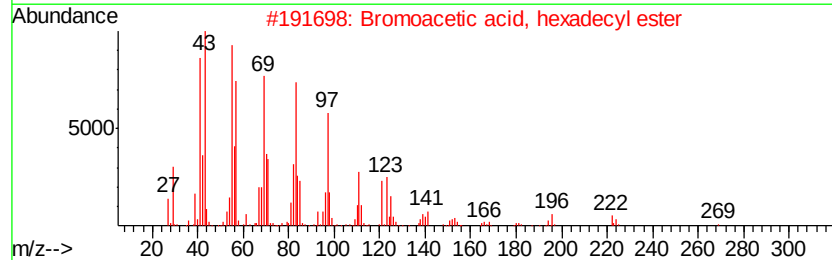
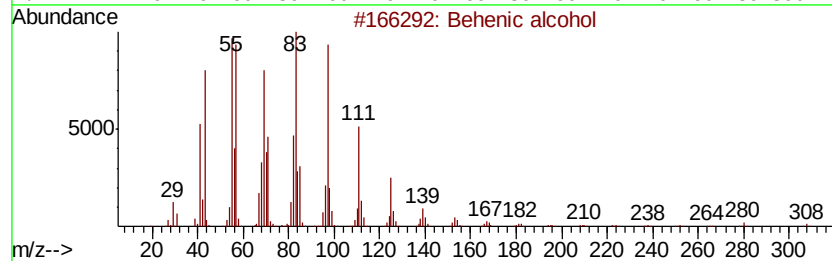
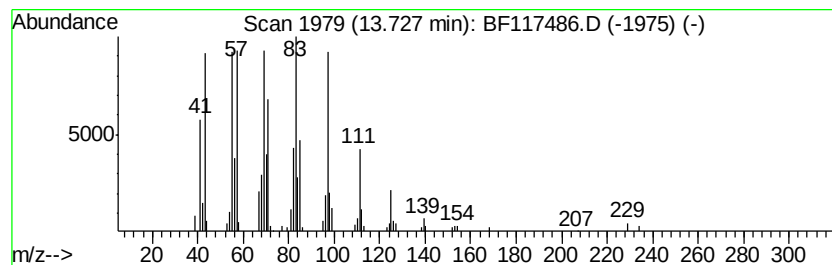
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	10.75 ng	239370	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4		1-Hexacosanol	382	C26H54O	000506-52-5	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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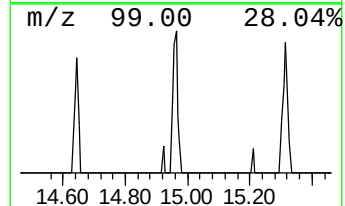
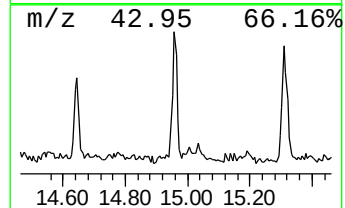
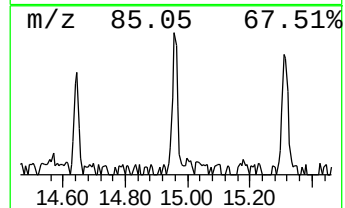
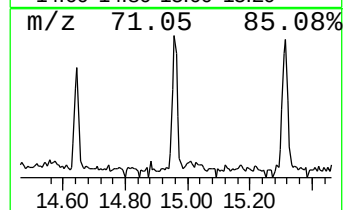
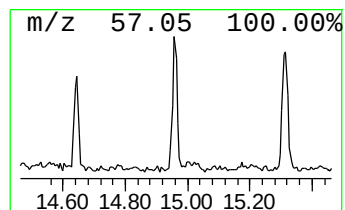
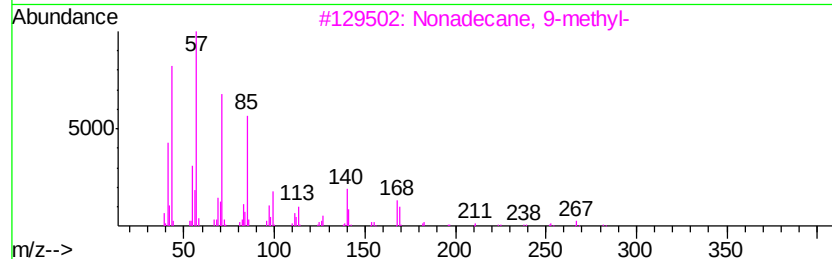
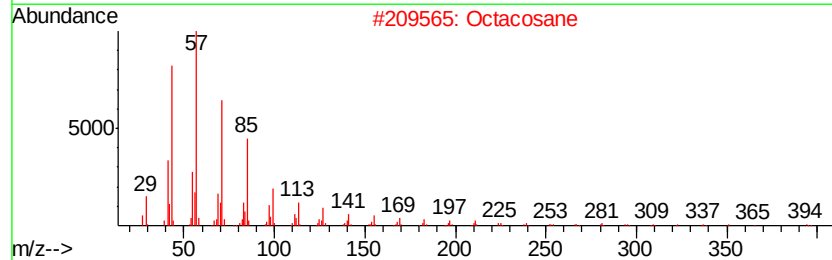
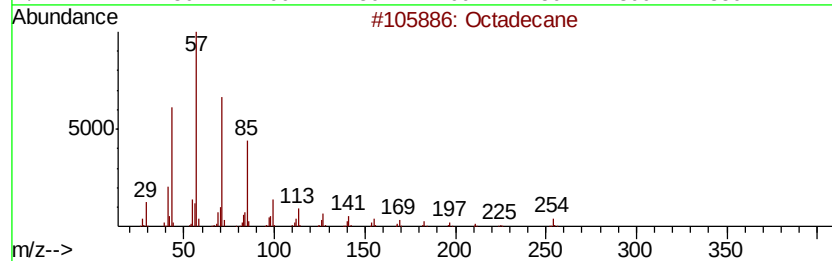
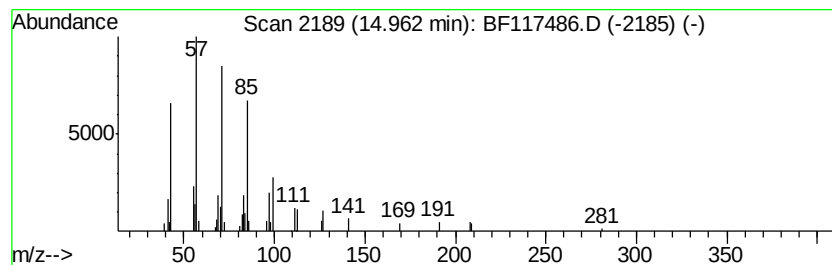
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Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.10 ng	57951	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Nonadecane, 9-methyl-	282 C20H42	013287-24-6	90
4	2-methyloctacosane	408 C29H60	1000376-72-8	90
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	90



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Misc :
ALS Vial : 5 Sample Multiplier: 1

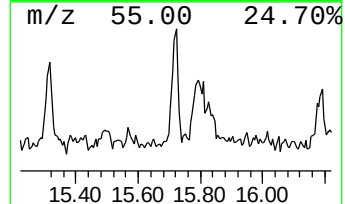
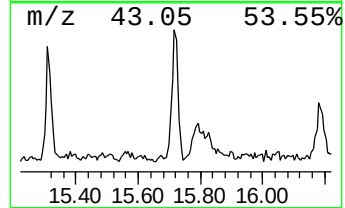
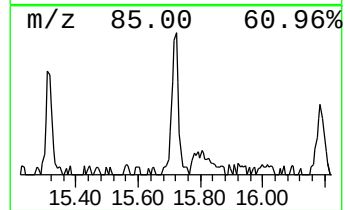
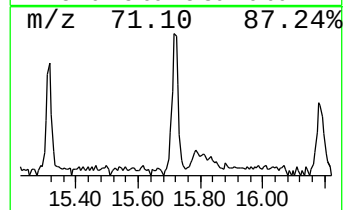
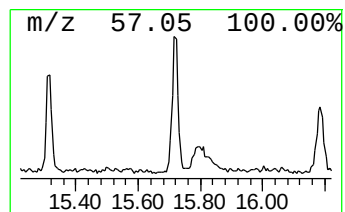
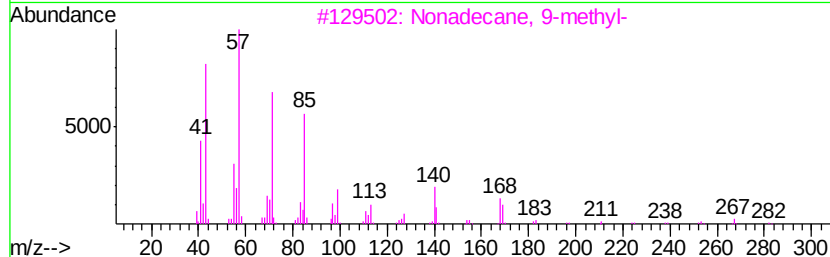
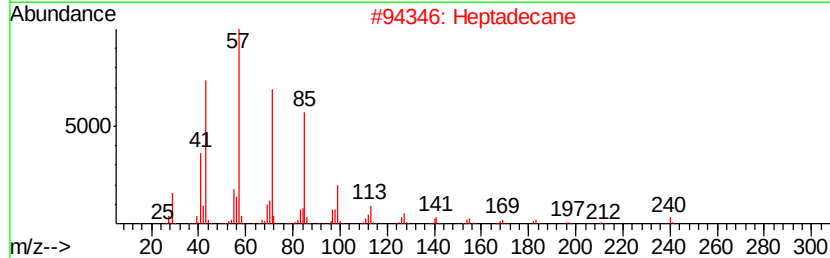
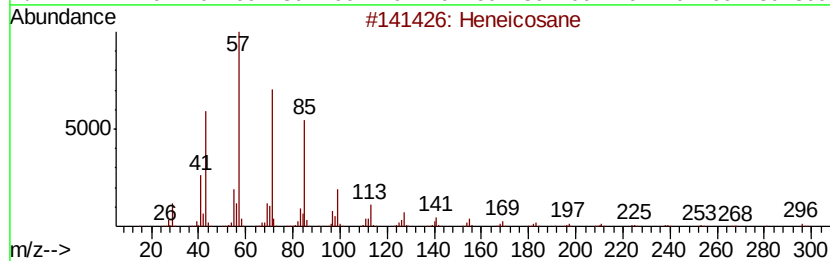
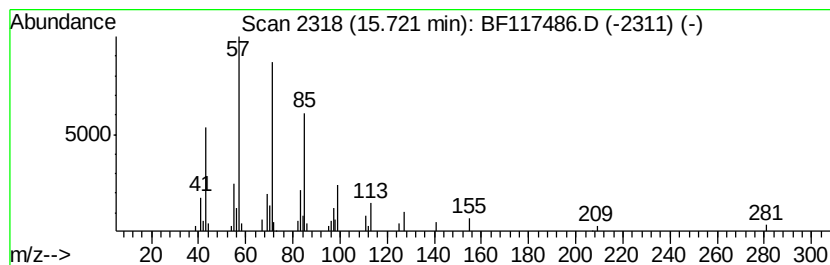
Instrument :
BNA_F
ClientSampleId :
TP1-6FT

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.72	4.75 ng	88687	Perylene-d12	15.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117486.D
Acq On : 23 Oct 2019 16:45
Operator : JU
Sample : K5494-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

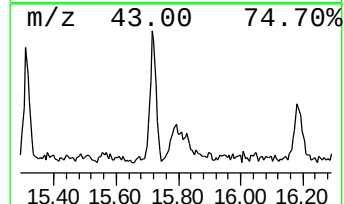
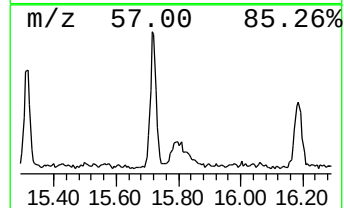
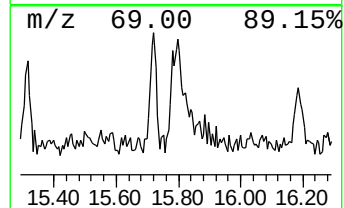
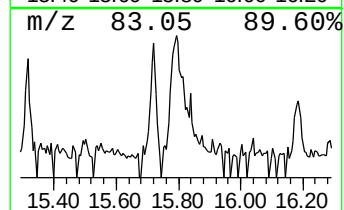
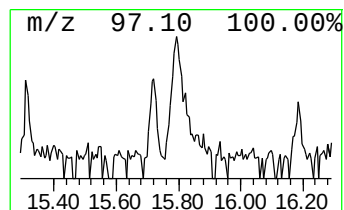
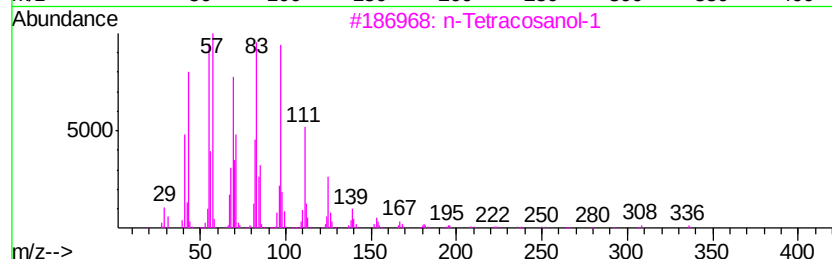
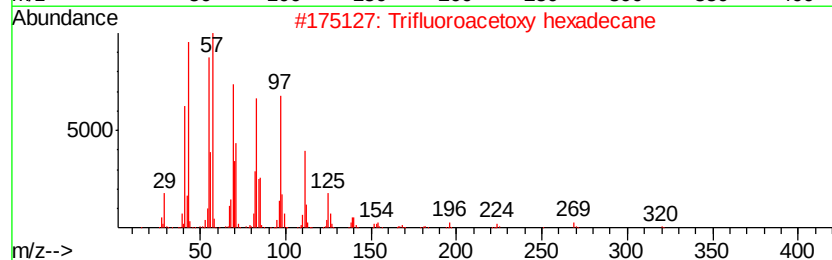
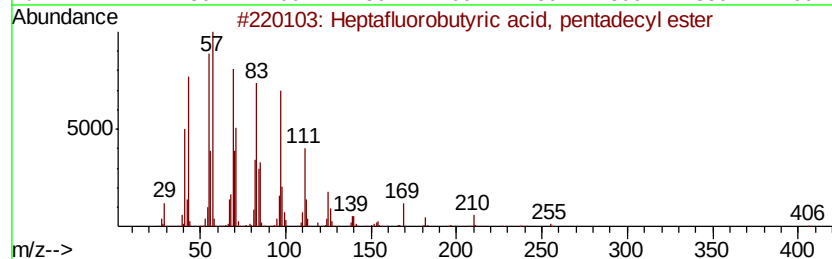
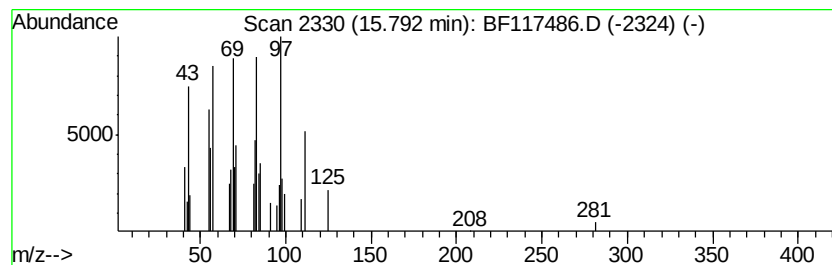
Instrument :
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ClientSampleId :
TP1-6FT

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

Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.79	2.95 ng	54999	Perylene-d12	15.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		1-Heneicosanol	312	C21H44O	015594-90-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117486.D
Acq On : 23 Oct 2019 16:45
Operator : JU
Sample : K5494-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

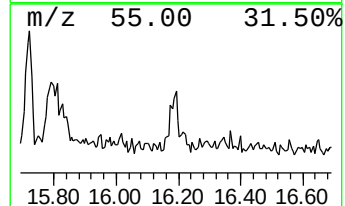
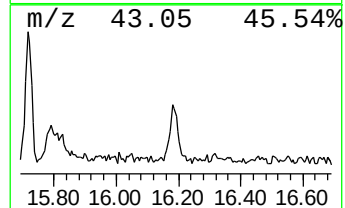
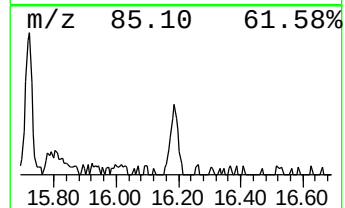
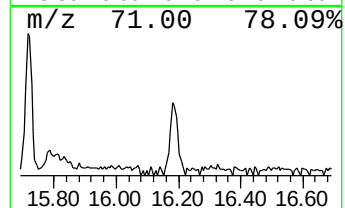
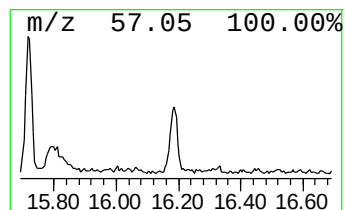
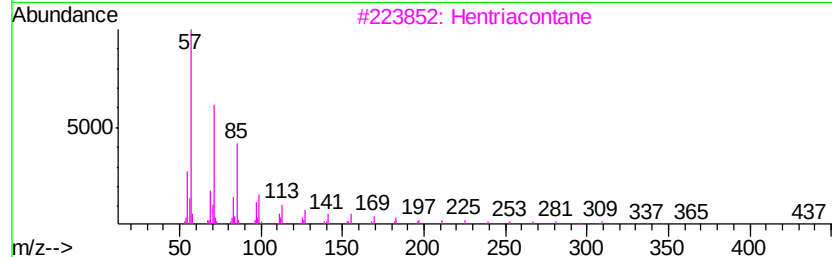
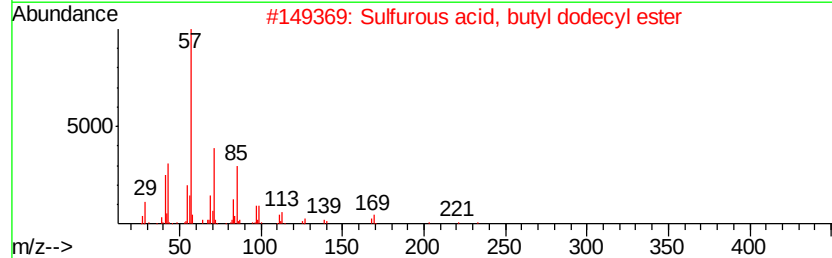
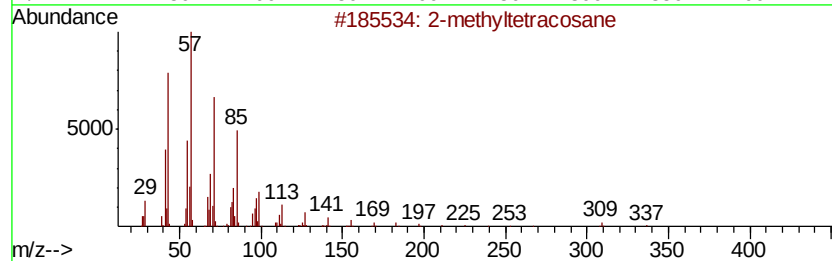
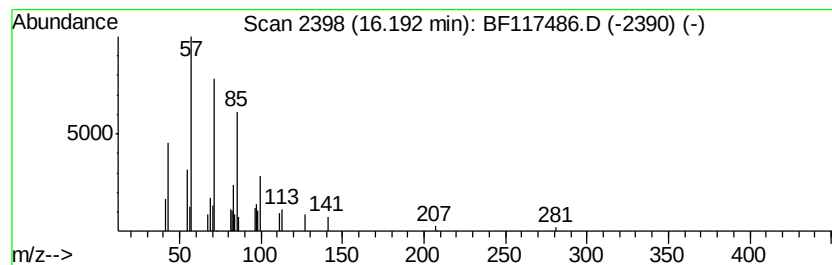
Instrument :
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ClientSampleId :
TP1-6FT

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

Peak Number 9 2-methyltetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.62 ng	48814	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-methyltetracosane	352 C25H52	1000376-72-6	91
2	Sulfurous acid, butyl dodecyl ester	306 C16H34O3S	1000309-17-9	90
3	Hentriacontane	437 C31H64	000630-04-6	90
4	Octacosane	394 C28H58	000630-02-4	90
5	Tritetracontane	605 C43H88	007098-21-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117486.D
Acq On : 23 Oct 2019 16:45
Operator : JU
Sample : K5494-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-6FT

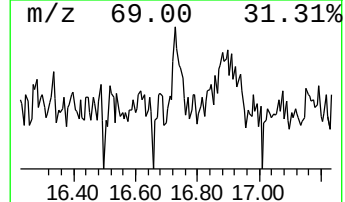
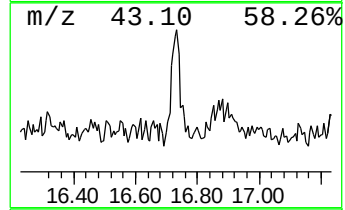
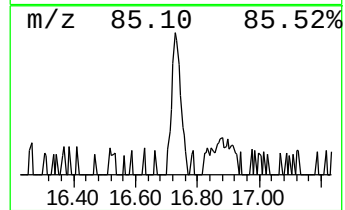
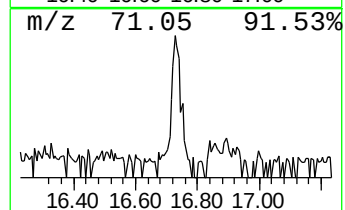
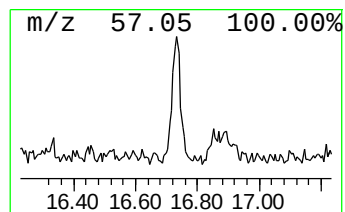
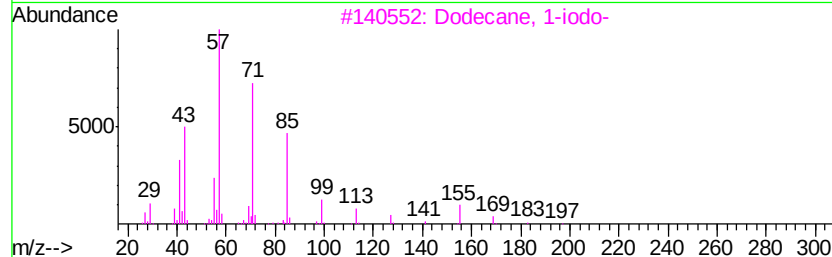
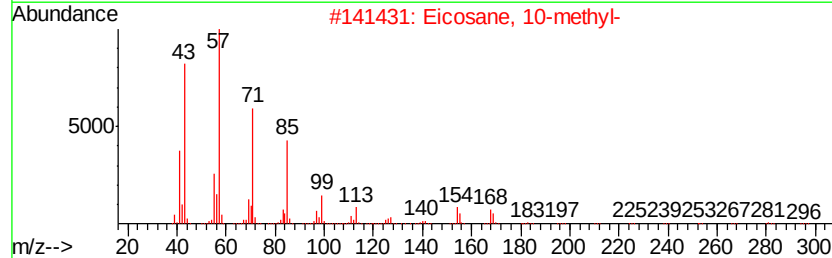
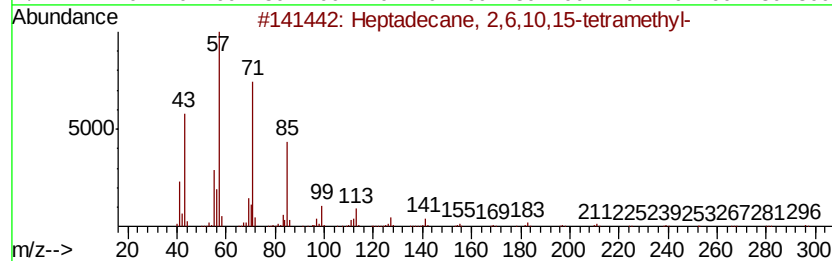
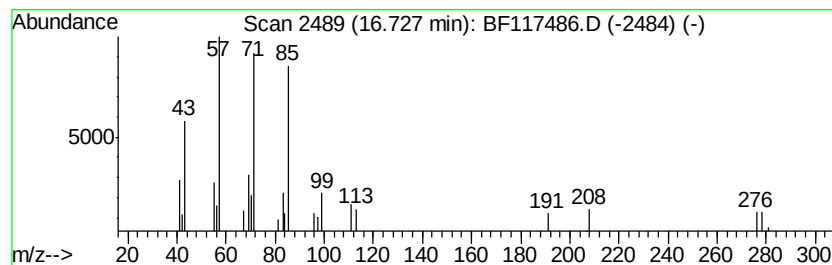
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.20 ng	41028	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59
4		Heptadecane	240	C17H36	000629-78-7	59
5		Dodecane, 2-methyl-	184	C13H28	001560-97-0	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102319\
Data File : BF117486.D
Acq On : 23 Oct 2019 16:45
Operator : JU
Sample : K5494-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	75.5	ng	1029370	1	6.73	272676	20.0
n-Hexadecanoic acid	11.78	5.7	ng	129956	4	11.25	456759	20.0
3-Chloropropionic...	12.30	2.2	ng	49249	4	11.25	456759	20.0
Behenic alcohol	13.73	10.8	ng	239370	5	13.89	445426	20.0
Octadecane	14.96	3.1	ng	57951	6	15.32	373298	20.0
Heneicosane	15.72	4.8	ng	88687	6	15.32	373298	20.0
Heptafluorobutyri...	15.79	3.0	ng	54999	6	15.32	373298	20.0
2-methyltetracosane	16.19	2.6	ng	48814	6	15.32	373298	20.0
Heptadecane, 2,6,...	16.73	2.2	ng	41028	6	15.32	373298	20.0