

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031820\
 Data File : BF119432.D
 Acq On : 18 Mar 2020 23:22
 Operator : CG/JU
 Sample : L1913-18
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MK-031220-COMP-DP

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-BF031820.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	2.175	11	15	24	rVB	268488	357742	3.93%	0.471%
2	5.087	507	510	516	rVB	134468	160698	1.77%	0.212%
3	5.469	569	575	578	rBV	8177172	8889086	97.72%	11.708%
4	6.475	740	746	749	rBV	7556776	8830413	97.08%	11.631%
5	6.675	777	780	785	rVB	130832	104280	1.15%	0.137%
6	6.851	807	810	814	rBV	2610450	2211720	24.32%	2.913%
7	7.010	833	837	841	rVB	7187773	6951053	76.42%	9.155%
8	7.416	900	906	909	rBV	5660903	5846720	64.28%	7.701%
9	8.139	1024	1029	1032	rBV	3390916	2894220	31.82%	3.812%
10	9.222	1207	1213	1216	rBV	9560413	9096046	100.00%	11.981%
11	9.610	1275	1279	1282	rBV	1203272	925550	10.18%	1.219%
12	9.898	1322	1328	1332	rBV	3560726	3038360	33.40%	4.002%
13	10.686	1456	1462	1465	rBV	5658401	5350297	58.82%	7.047%
14	11.386	1577	1581	1583	rBV	3442879	2804773	30.84%	3.694%
15	11.404	1583	1584	1587	rVB	125572	94330	1.04%	0.124%
16	11.916	1667	1671	1681	rBV	955120	832765	9.16%	1.097%
17	12.598	1783	1787	1789	rBV	287452	247413	2.72%	0.326%
18	12.698	1801	1804	1812	rBV2	265988	302070	3.32%	0.398%
19	12.827	1819	1826	1828	rBV	215432	242932	2.67%	0.320%
20	12.974	1846	1851	1854	rBV	7210708	6696382	73.62%	8.820%
21	13.874	2000	2004	2014	rBV	1045195	1206954	13.27%	1.590%
22	14.021	2025	2029	2032	rBV	1907713	1947586	21.41%	2.565%
23	14.051	2032	2034	2039	rVB	124703	112588	1.24%	0.148%
24	14.204	2056	2060	2064	rBV	314759	300388	3.30%	0.396%
25	14.504	2108	2111	2115	rBV	572316	554159	6.09%	0.730%
26	14.815	2160	2164	2171	rVB	659153	675084	7.42%	0.889%
27	15.063	2202	2206	2210	rBV	131064	195708	2.15%	0.258%
28	15.163	2219	2223	2230	rVB	652093	773558	8.50%	1.019%
29	15.368	2254	2258	2261	rBV	94767	125076	1.38%	0.165%
30	15.427	2265	2268	2274	rVV	109660	146954	1.62%	0.194%
31	15.498	2275	2280	2284	rVV	1518761	1872354	20.58%	2.466%
32	15.545	2284	2288	2295	rVB	549180	754898	8.30%	0.994%
33	15.992	2359	2364	2368	rBV	368025	556089	6.11%	0.732%
34	16.039	2368	2372	2380	rVB7	123262	232451	2.56%	0.306%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	16.509	2446	2452	2457	rBV	178064	337495	3.71%	0.445%
36	16.951	2524	2527	2535	rVB2	64168	120481	1.32%	0.159%
37	17.109	2550	2554	2563	rVB6	58546	134865	1.48%	0.178%

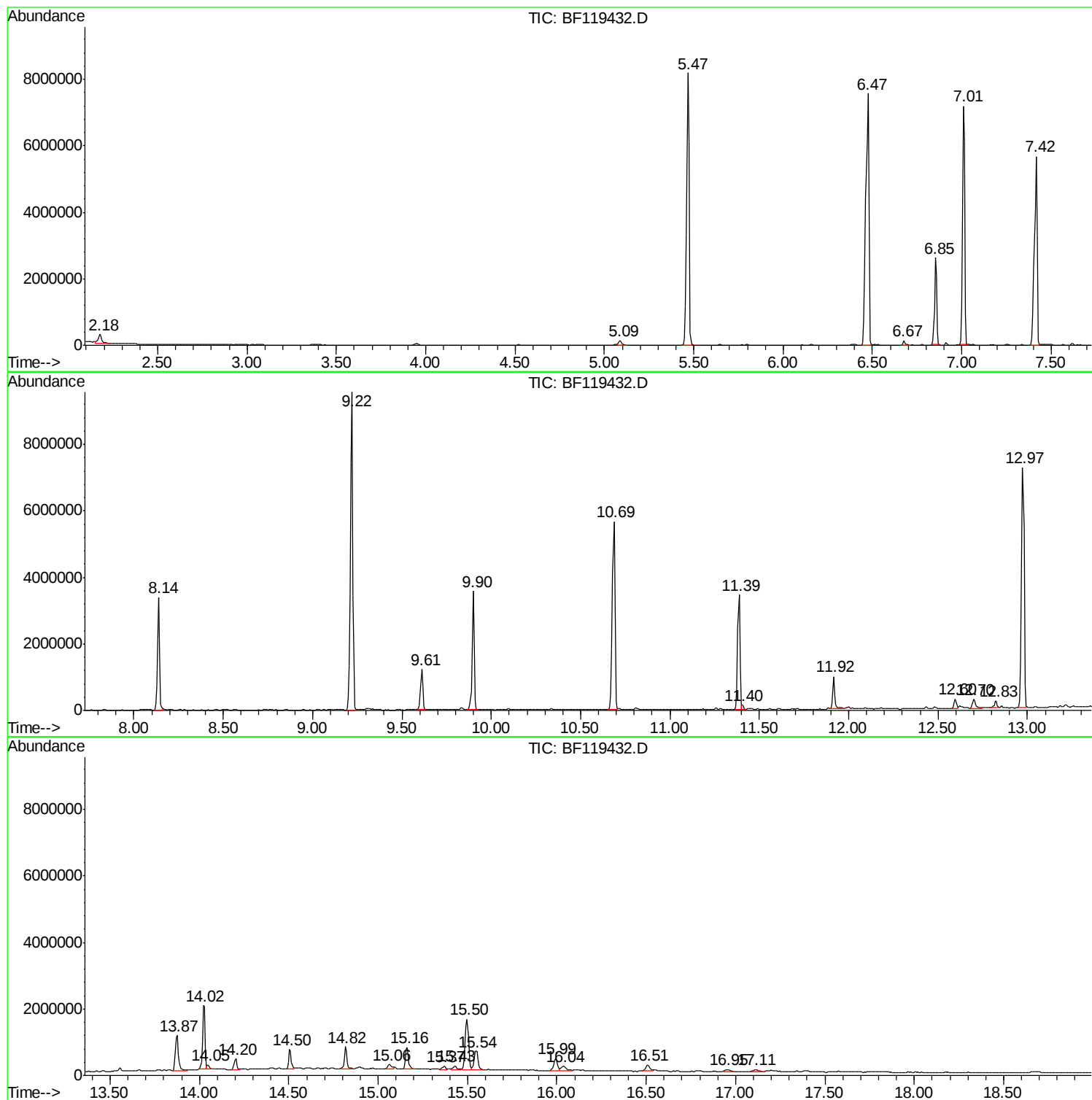
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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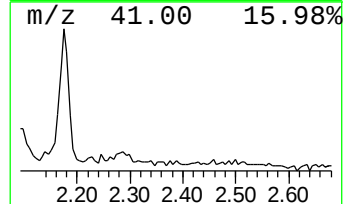
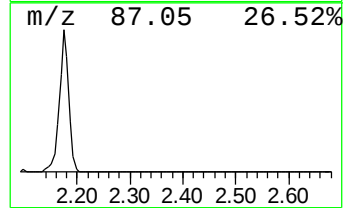
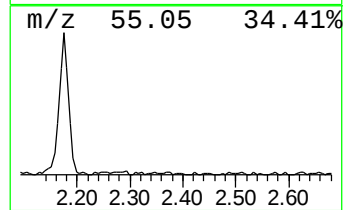
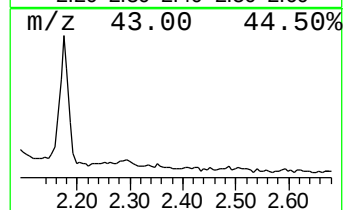
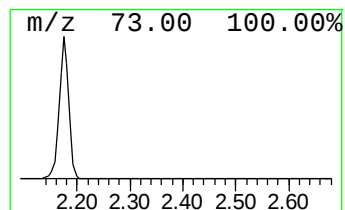
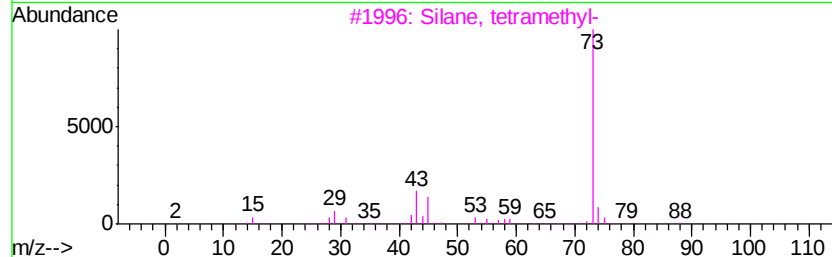
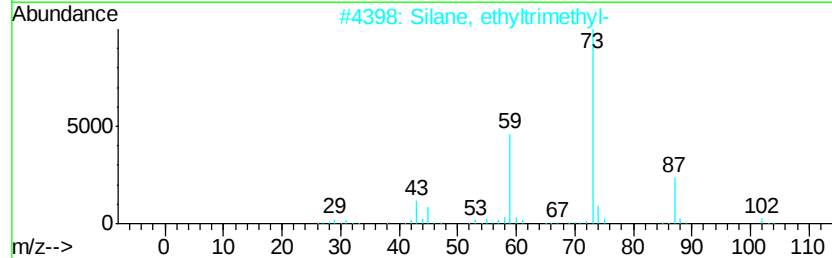
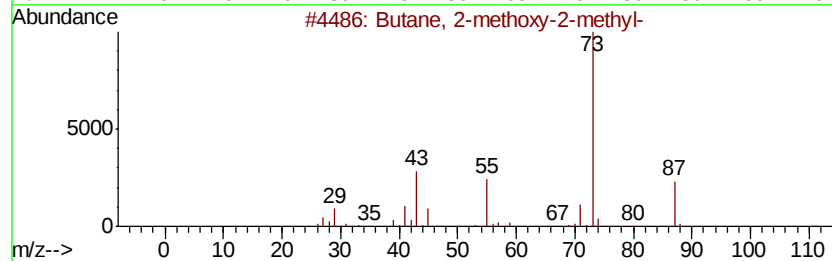
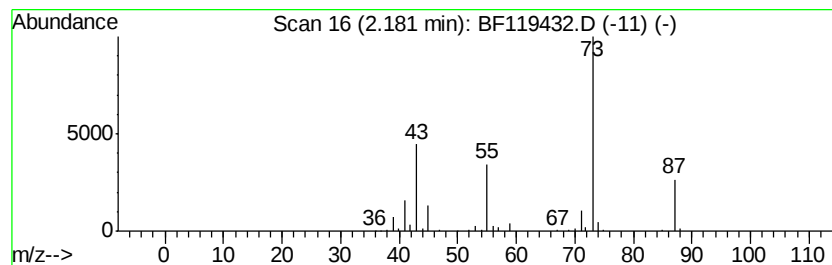
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	3.23 ng	357742	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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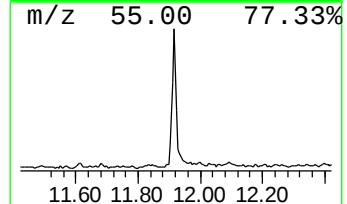
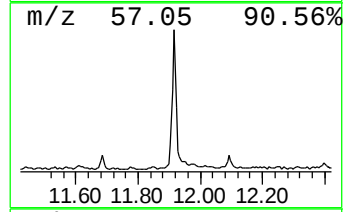
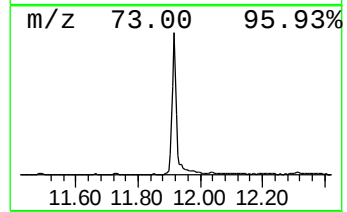
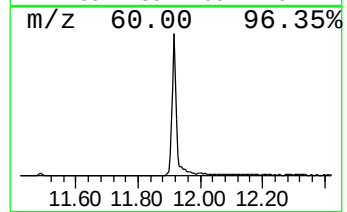
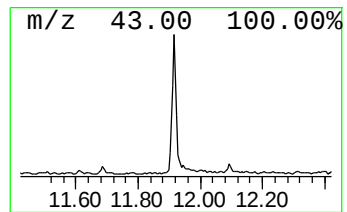
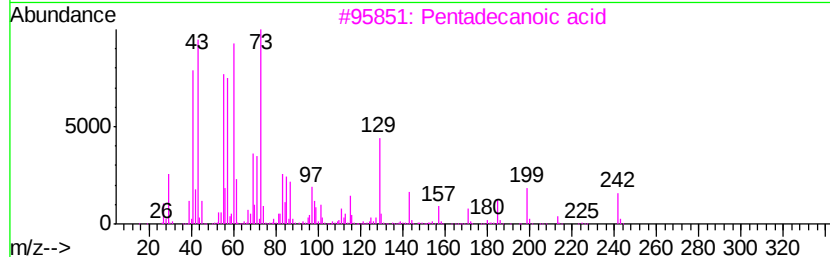
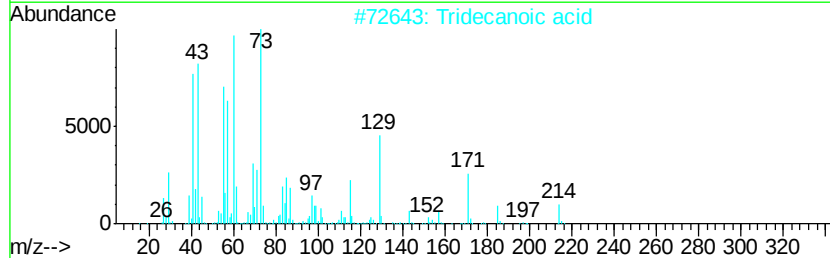
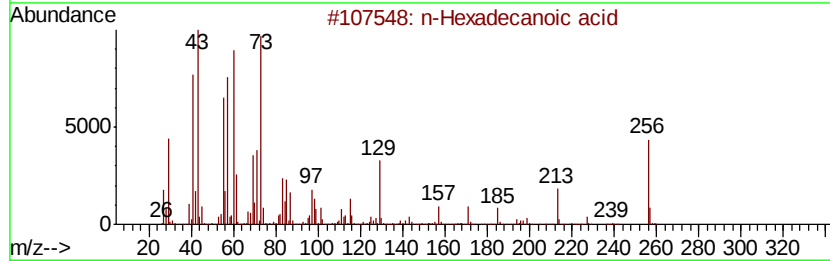
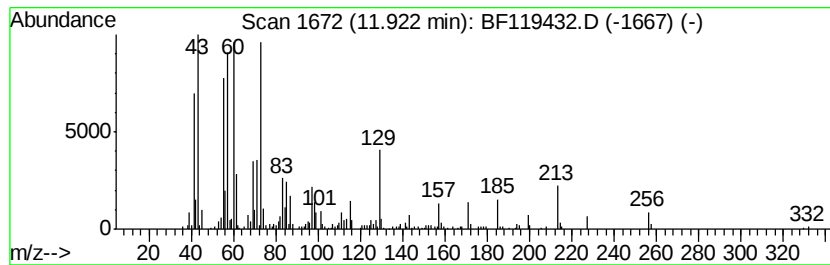
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	5.94 ng	832765	Phenanthrene-d10	11.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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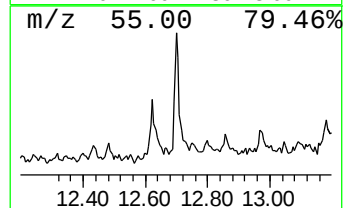
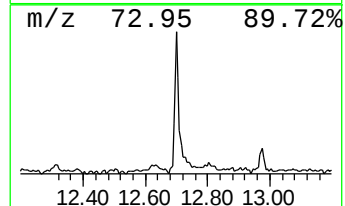
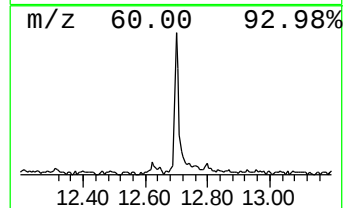
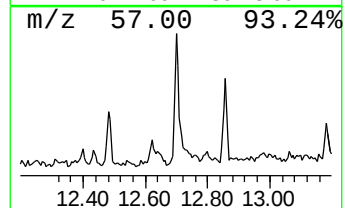
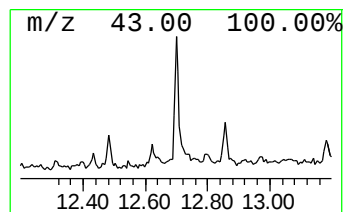
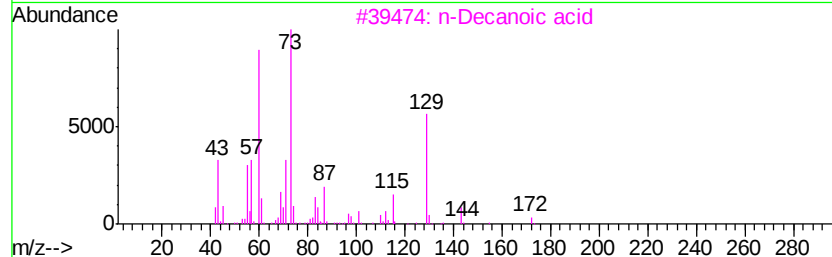
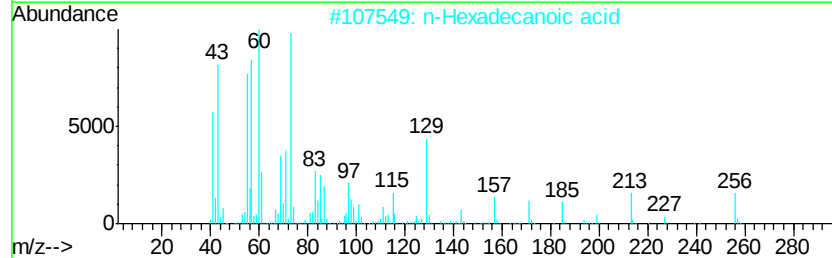
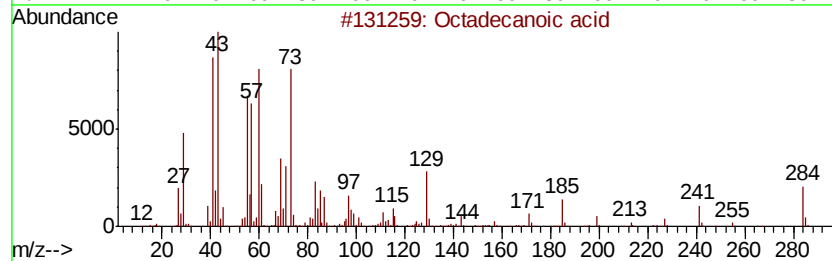
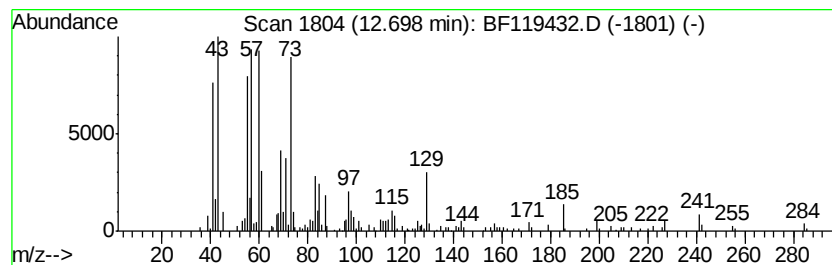
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.15 ng	302070	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3		n-Decanoic acid	172	C10H20O2	000334-48-5	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	74



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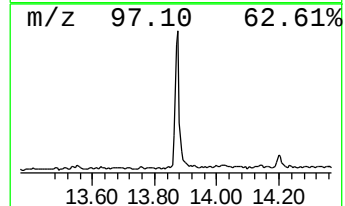
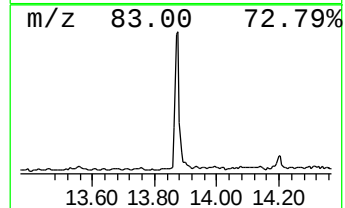
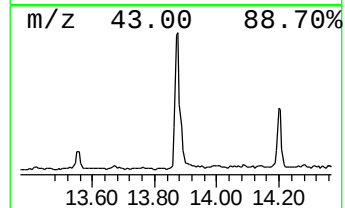
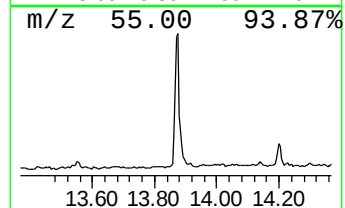
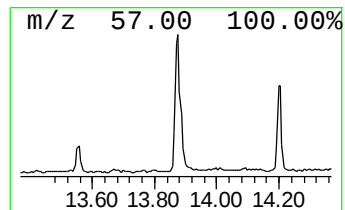
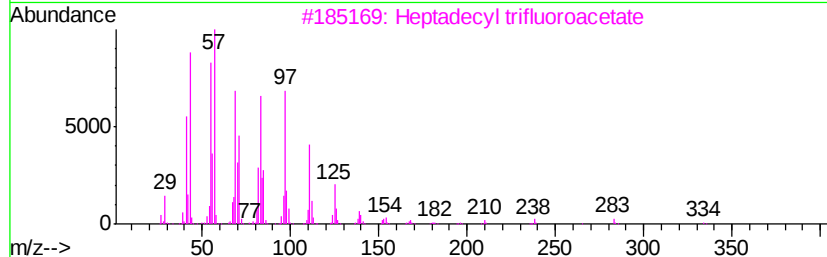
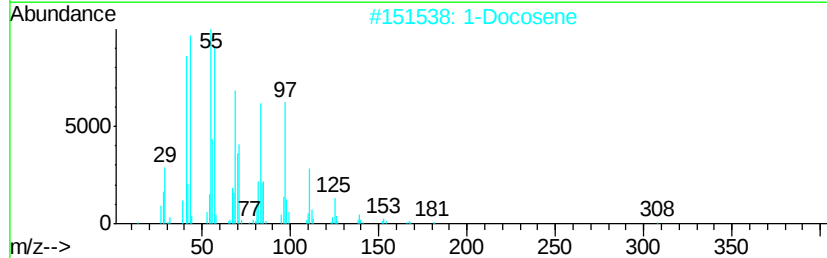
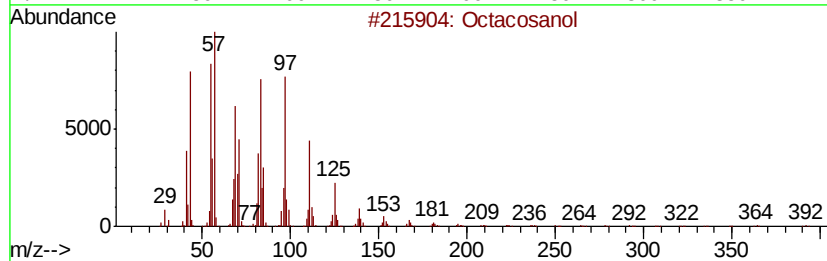
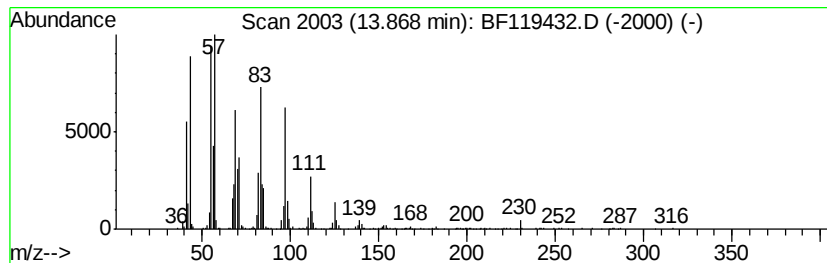
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	12.39 ng	1206950	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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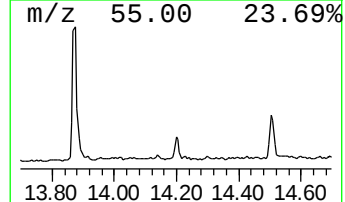
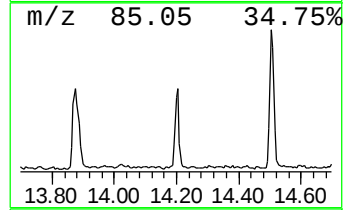
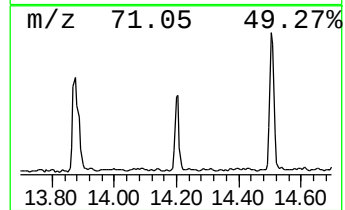
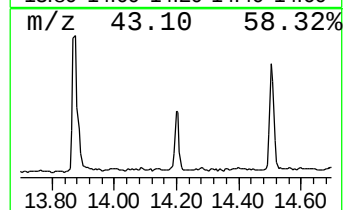
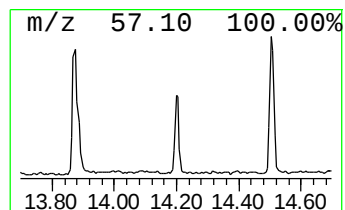
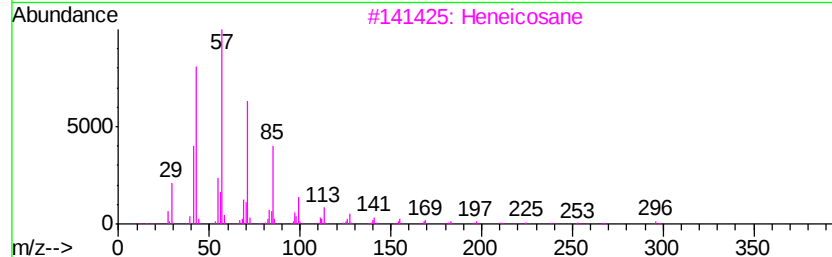
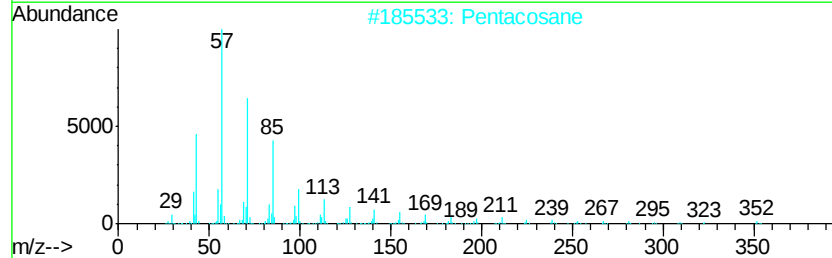
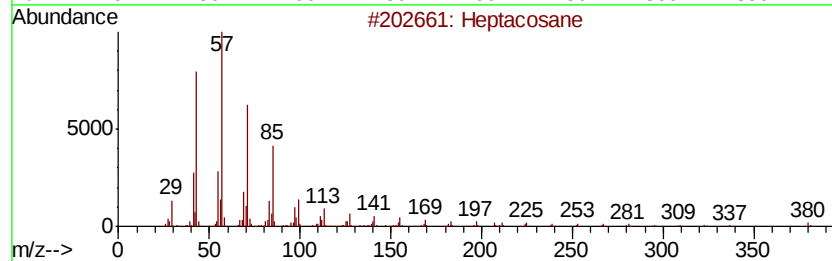
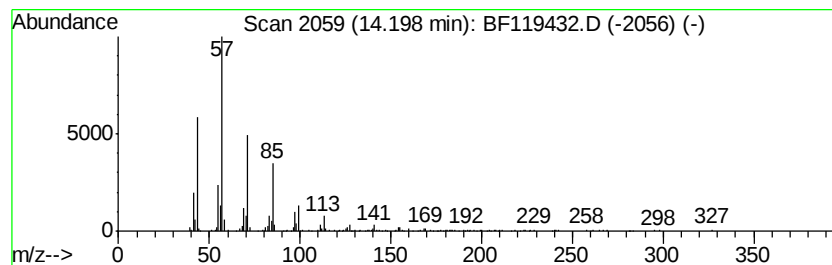
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.08 ng	300388	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Nonadecane	268	C19H40	000629-92-5	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
 Data File : BF119432.D
 Acq On : 18 Mar 2020 23:22
 Operator : CG/JU
 Sample : L1913-18
 Misc :
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Instrument :
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 ClientSampleId :
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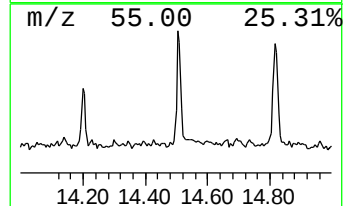
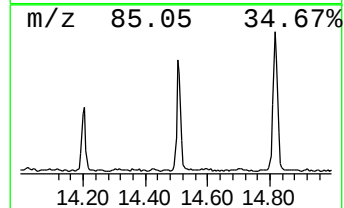
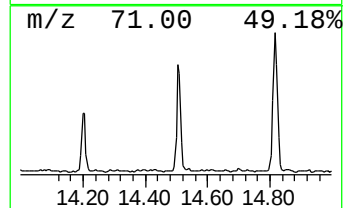
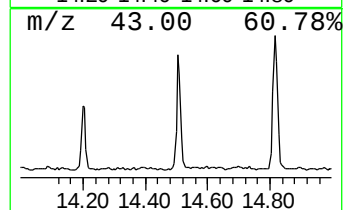
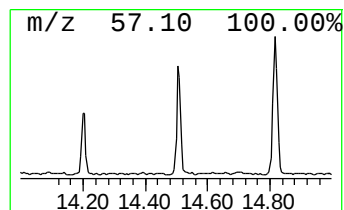
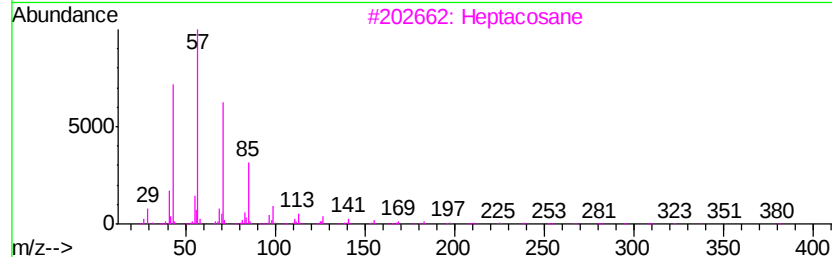
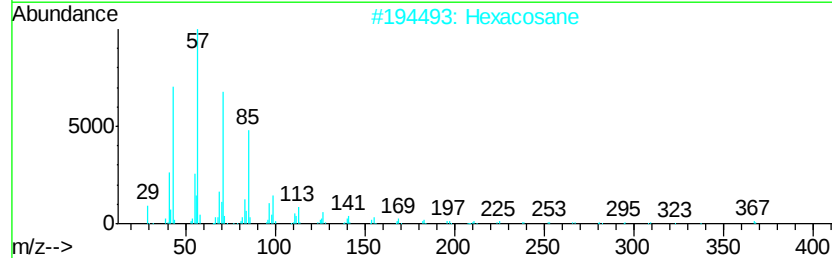
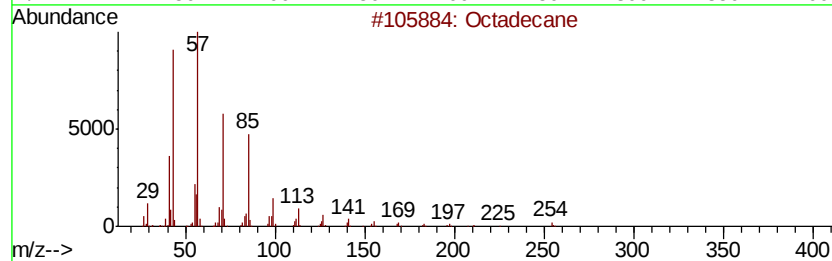
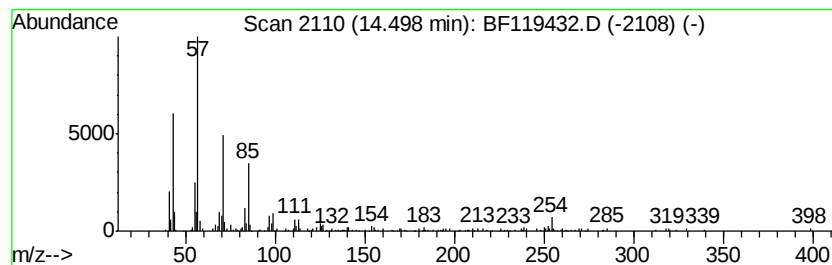
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	5.69 ng	554159	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	97
2	Hexacosane		366	C26H54	000630-01-3	90
3	Heptacosane		380	C27H56	000593-49-7	87
4	Octacosane		394	C28H58	000630-02-4	86
5	Hexadecane		226	C16H34	000544-76-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
Data File : BF119432.D
Acq On : 18 Mar 2020 23:22
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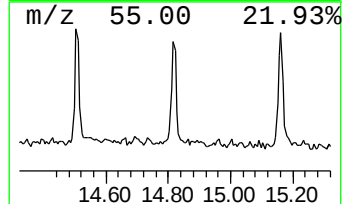
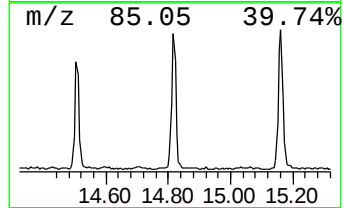
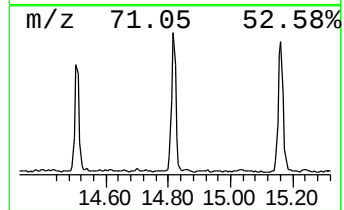
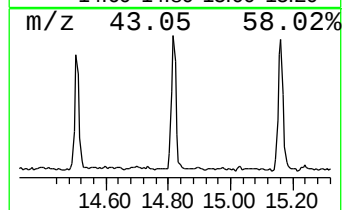
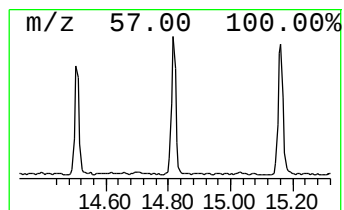
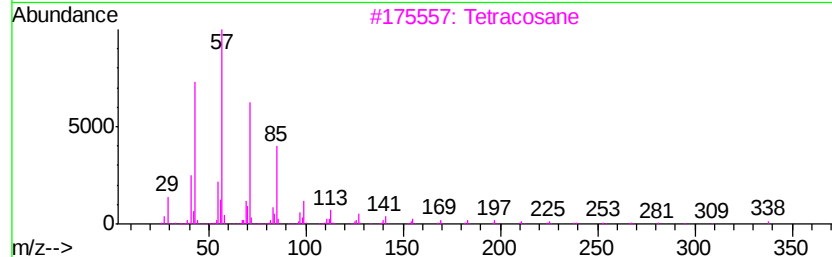
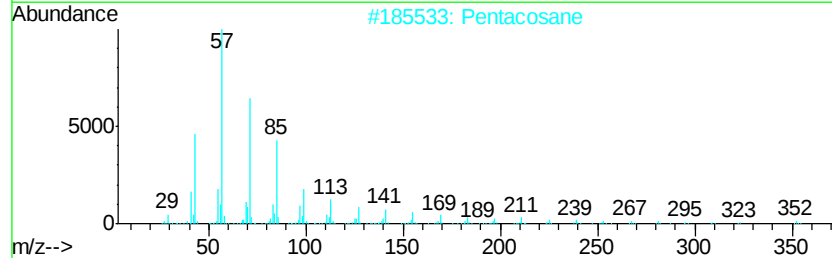
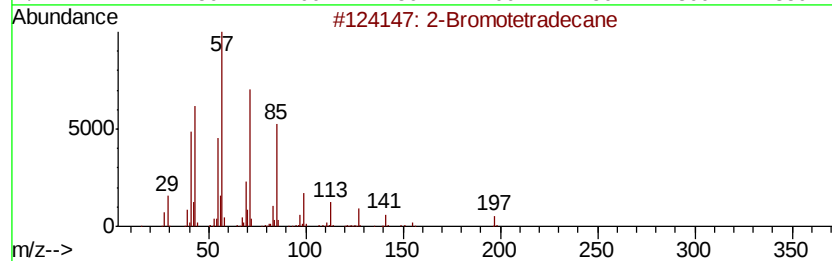
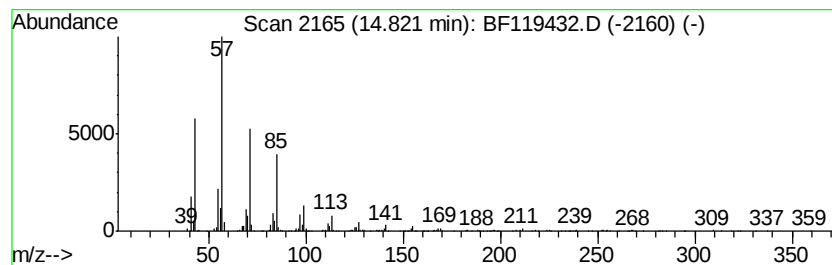
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Bromotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	7.21 ng	675084	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
2		Pentacosane	352	C25H52	000629-99-2	90
3		Tetracosane	338	C24H50	000646-31-1	87
4		Heptacosane	380	C27H56	000593-49-7	87
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
Data File : BF119432.D
Acq On : 18 Mar 2020 23:22
Operator : CG/JU
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Misc :
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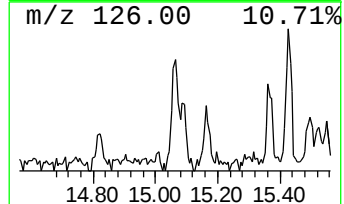
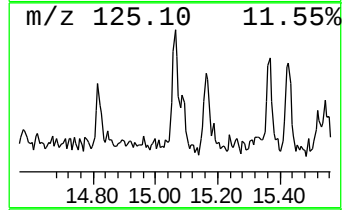
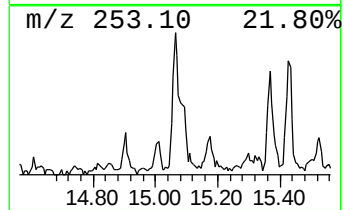
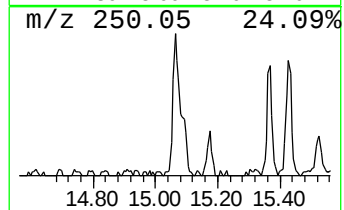
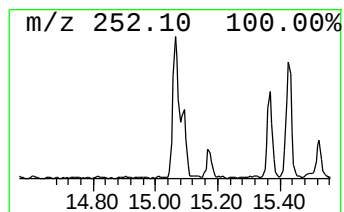
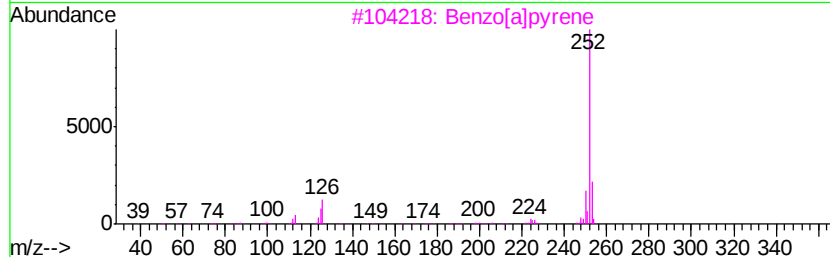
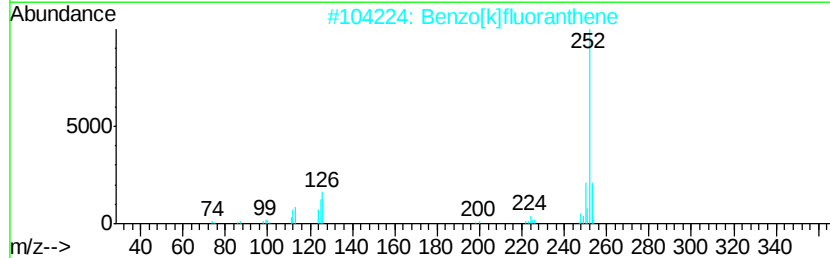
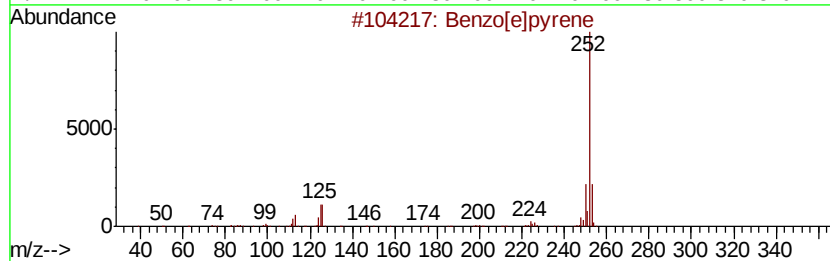
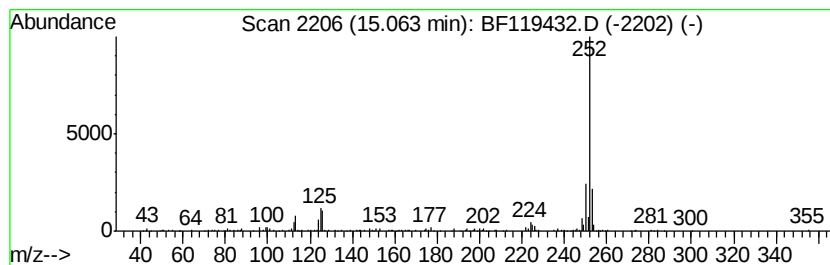
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.09 ng	195708	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3		Benzo[a]pyrene	252	C20H12	000050-32-8	96
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
5		Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
Data File : BF119432.D
Acq On : 18 Mar 2020 23:22
Operator : CG/JU
Sample : L1913-18
Misc :
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ClientSampleId :
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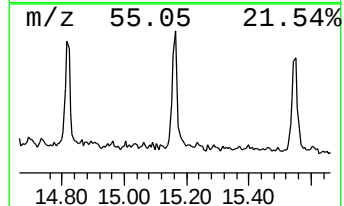
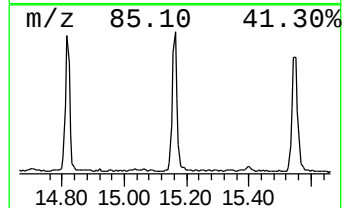
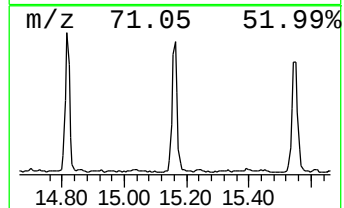
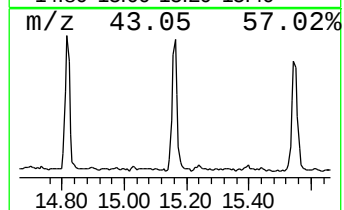
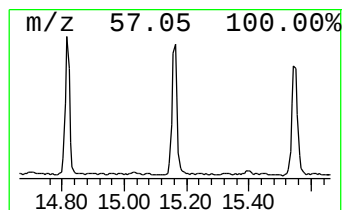
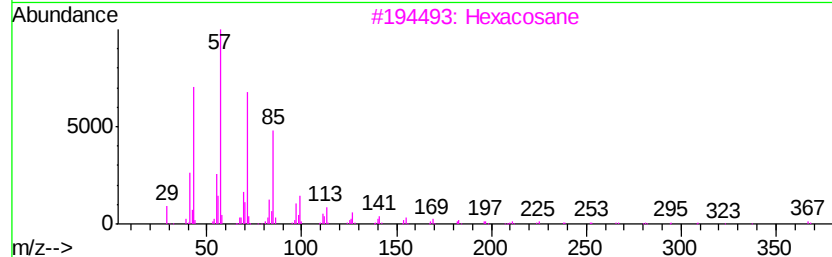
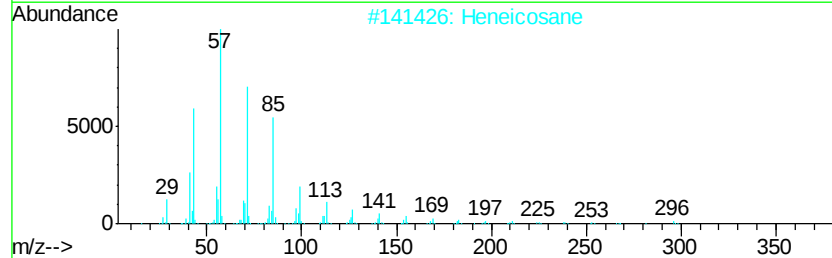
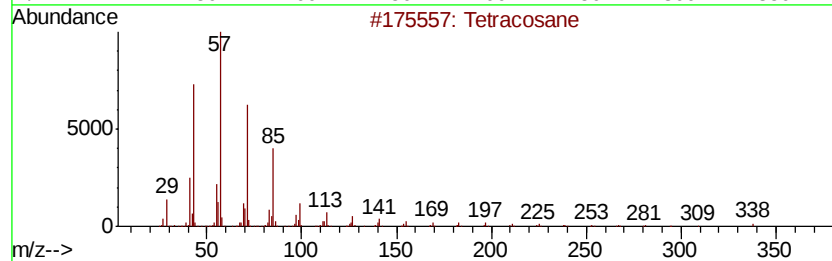
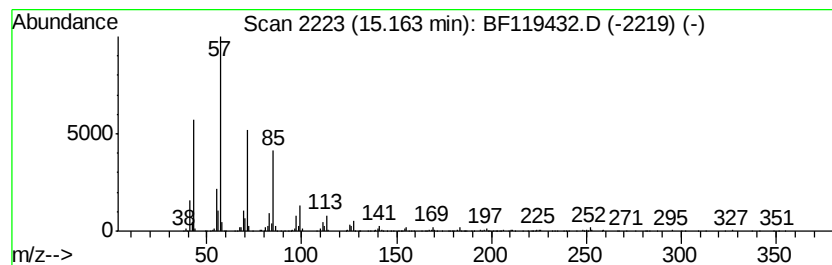
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	8.26 ng	773558	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			3,5-Dimethyldodecane	198	C14H30	107770-99-0	87
5			Tetratetracontane	619	C44H90	007098-22-8	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
Data File : BF119432.D
Acq On : 18 Mar 2020 23:22
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Sample : L1913-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

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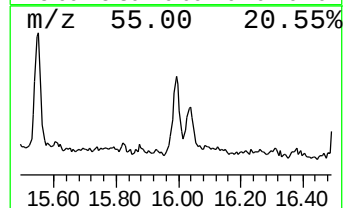
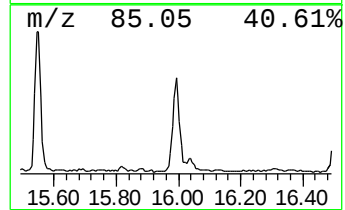
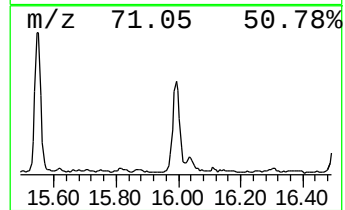
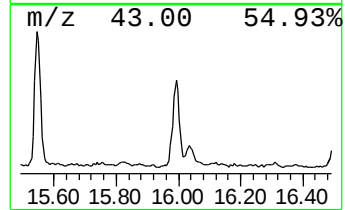
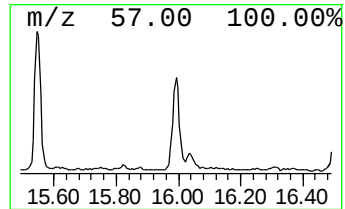
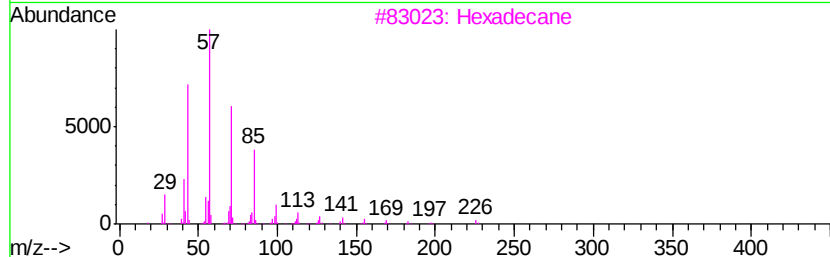
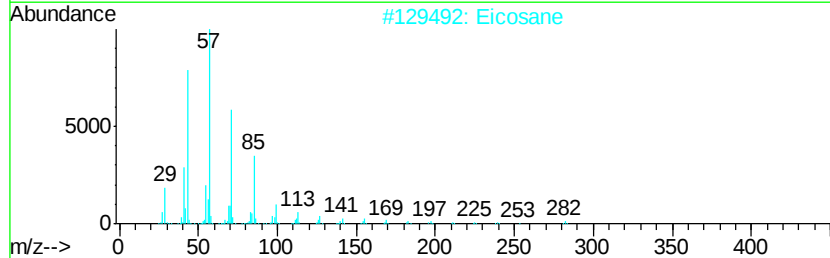
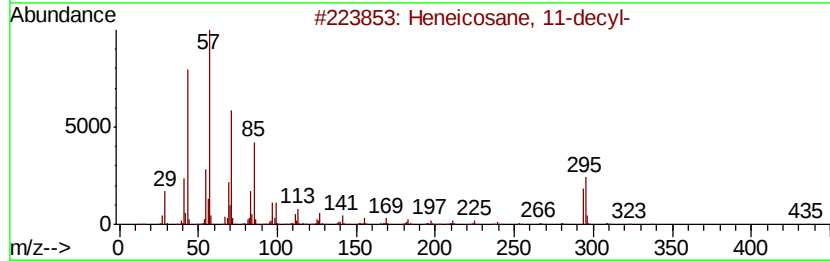
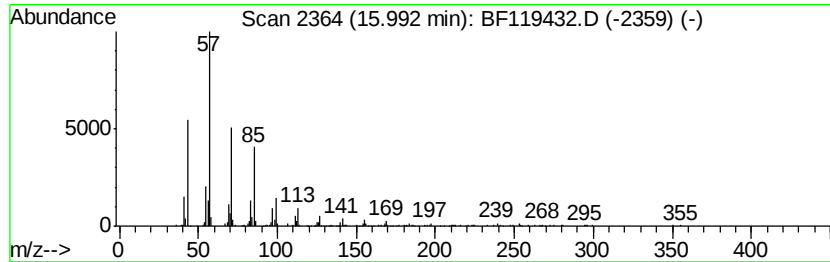
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane, 11-decyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	5.94 ng	556089	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Hexadecane	226	C16H34	000544-76-3	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
Data File : BF119432.D
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Sample : L1913-18
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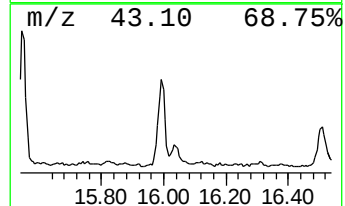
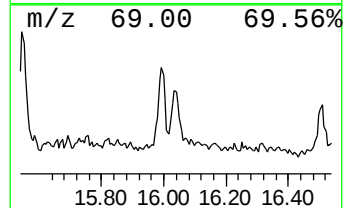
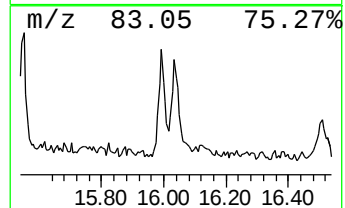
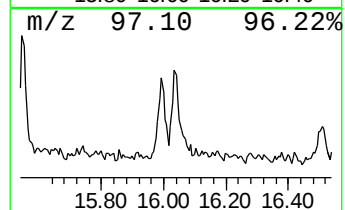
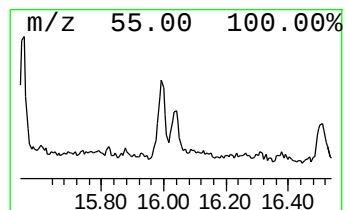
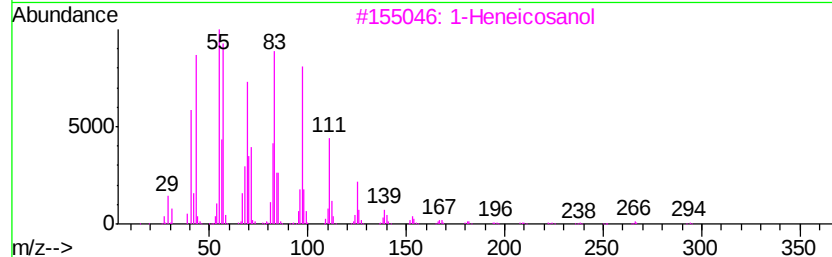
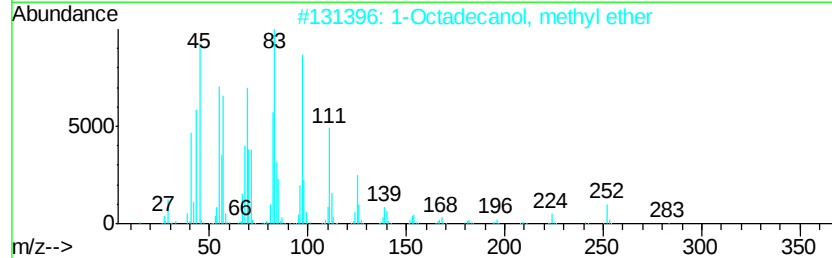
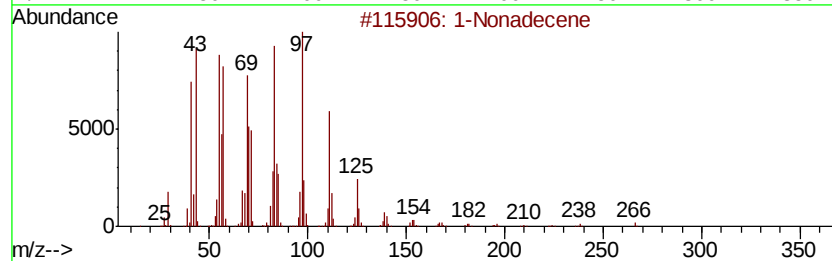
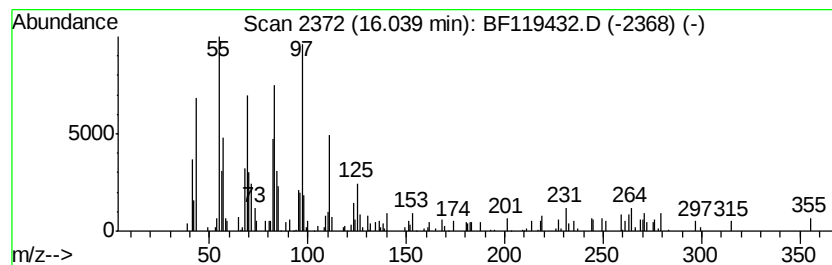
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Nonadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	2.48 ng	232451	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	83
2	1-Octadecanol, methyl ether	284 C19H40O	1000333-92-7	83
3	1-Heneicosanol	312 C21H44O	015594-90-8	80
4	Bacteriochlorophyll-c-stearyl	841 C52H72MnN4O4	1000164-49-7	62
5	7-Heptadecene, 1-chloro-	272 C17H33Cl	056554-78-0	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031820\
Data File : BF119432.D
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Sample : L1913-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
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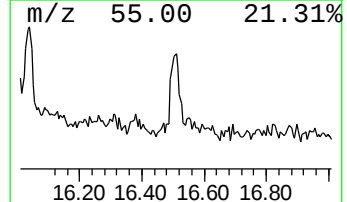
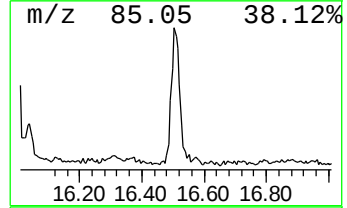
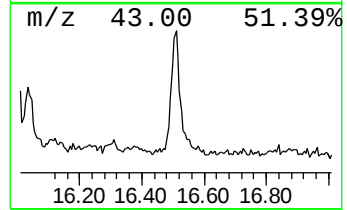
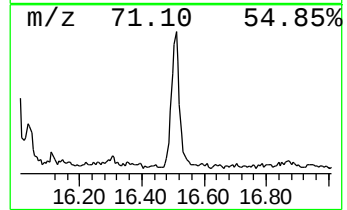
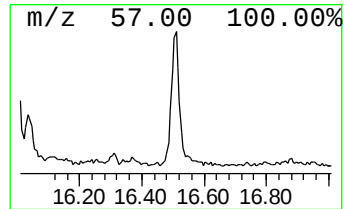
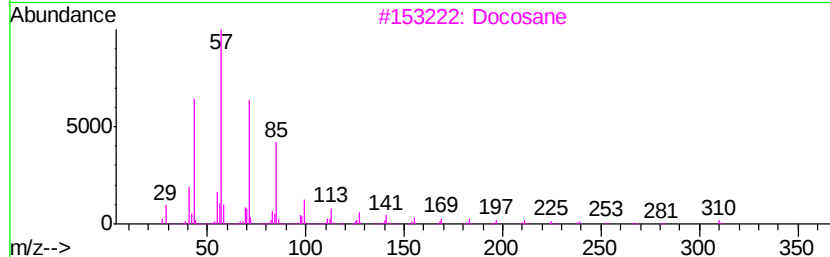
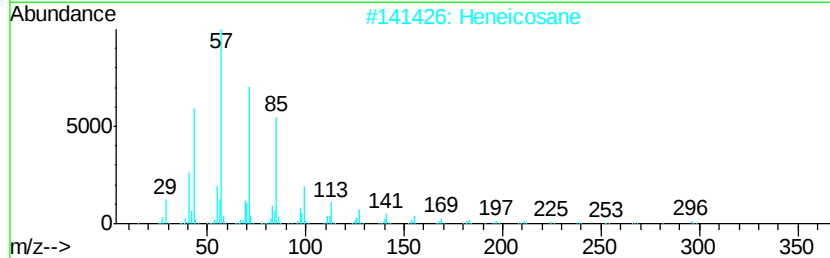
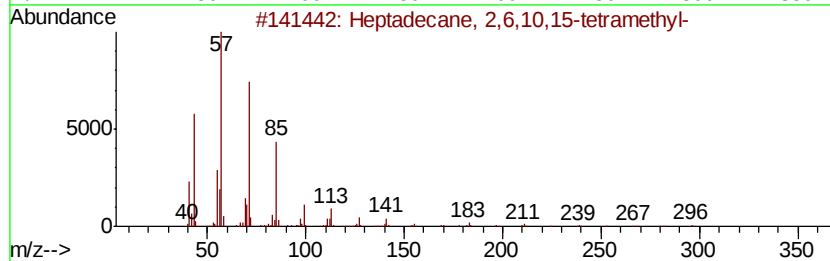
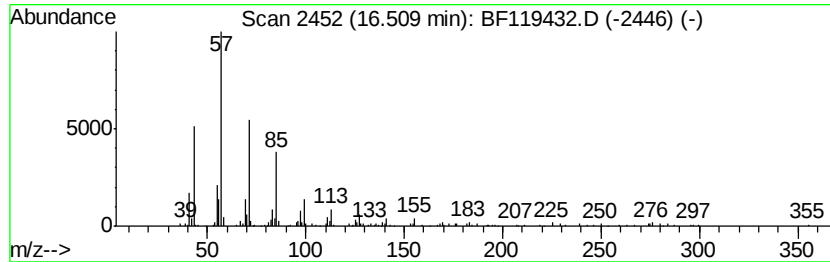
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.51	3.61 ng	337495	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2		Heneicosane	296	C21H44	000629-94-7	93
3		Docosane	310	C22H46	000629-97-0	83
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	83
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031820\
 Data File : BF119432.D
 Acq On : 18 Mar 2020 23:22
 Operator : CG/JU
 Sample : L1913-18
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MK-031220-COMP-DP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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...	2.18	3.2	ng	357742	1	6.85	2211720	20.0
n-Hexadecanoic acid	11.92	5.9	ng	832765	4	11.39	2804770	20.0
Octadecanoic acid	12.70	2.1	ng	302070	4	11.39	2804770	20.0
Octacosanol	13.87	12.4	ng	1206950	5	14.03	1947590	20.0
Heptacosane	14.20	3.1	ng	300388	5	14.03	1947590	20.0
Octadecane	14.50	5.7	ng	554159	5	14.03	1947590	20.0
2-Bromotetradecane	14.82	7.2	ng	675084	6	15.50	1872350	20.0
Benzo[e]pyrene	15.06	2.1	ng	195708	6	15.50	1872350	20.0
Tetracosane	15.16	8.3	ng	773558	6	15.50	1872350	20.0
Heneicosane, 11-d...	15.99	5.9	ng	556089	6	15.50	1872350	20.0
1-Nonadecene	16.04	2.5	ng	232451	6	15.50	1872350	20.0
Heptadecane, 2,6,...	16.51	3.6	ng	337495	6	15.50	1872350	20.0