

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030719\
 Data File : BF112919.D
 Acq On : 7 Mar 2019 14:18
 Operator : JU/SJ
 Sample : K1760-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 Z2-11

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-BF022719.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	5.334	548	552	571	rBV	2509385	2411195	70.13%	5.890%
2	6.363	723	727	734	rBV	2822302	2611979	75.97%	6.381%
3	6.498	746	750	753	rBV	3068337	2597493	75.55%	6.345%
4	6.728	786	789	793	rBV	1134841	916790	26.67%	2.240%
5	6.887	812	816	819	rBV	2509561	2021908	58.81%	4.939%
6	7.287	880	884	897	rBV	1836140	1630608	47.43%	3.983%
7	8.010	1004	1007	1014	rBV	1239864	1138707	33.12%	2.782%
8	9.086	1186	1190	1205	rBV	3394229	3121402	90.79%	7.625%
9	9.210	1209	1211	1221	rVB	109903	112996	3.29%	0.276%
10	9.480	1253	1257	1267	rBV	222837	198717	5.78%	0.485%
11	9.763	1301	1305	1315	rBV	1478268	1414856	41.15%	3.456%
12	9.975	1337	1341	1348	rBV3	21112	34784	1.01%	0.085%
13	10.545	1434	1438	1453	rBV	2276746	2264649	65.87%	5.532%
14	11.239	1552	1556	1563	rBV	1546985	1566118	45.55%	3.826%
15	11.292	1563	1565	1570	rVB	31702	36165	1.05%	0.088%
16	11.710	1632	1636	1640	rBV2	34982	50424	1.47%	0.123%
17	11.774	1644	1647	1661	rVV2	592155	697306	20.28%	1.703%
18	12.280	1730	1733	1737	rBV	71274	61504	1.79%	0.150%
19	12.322	1737	1740	1746	rVB2	25540	35191	1.02%	0.086%
20	12.486	1762	1768	1777	rBV8	24725	69117	2.01%	0.169%
21	12.557	1777	1780	1788	rBV	276703	364596	10.60%	0.891%
22	12.816	1820	1824	1828	rBV	3524420	3438103	100.00%	8.399%
23	13.304	1901	1907	1911	rBV4	25269	43744	1.27%	0.107%
24	13.404	1921	1924	1926	rVB	53521	42786	1.24%	0.105%
25	13.727	1975	1979	1989	rBV2	314428	407980	11.87%	0.997%
26	13.863	1998	2002	2011	rVB	1820707	1775168	51.63%	4.336%
27	14.045	2029	2033	2038	rBV	455979	405194	11.79%	0.990%
28	14.345	2080	2084	2093	rVB	1039377	971051	28.24%	2.372%
29	14.645	2130	2135	2143	rBV	1619012	1769580	51.47%	4.323%
30	14.710	2143	2146	2150	rVB	157941	152867	4.45%	0.373%
31	14.839	2165	2168	2171	rVB	38342	39131	1.14%	0.096%
32	14.963	2184	2189	2193	rBV	1802281	2097144	61.00%	5.123%
33	15.174	2222	2225	2229	rBV	45580	52267	1.52%	0.128%
34	15.268	2235	2241	2244	rBV	1277840	1594576	46.38%	3.895%

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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 >
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35	15.315	2244	2249	2256	rVB	1570833	2049222	59.60%	5.006%
36	15.562	2288	2291	2295	rVB	51478	61603	1.79%	0.150%
37	15.610	2296	2299	2304	rVB2	32240	48667	1.42%	0.119%
38	15.721	2312	2318	2324	rBV	945787	1463686	42.57%	3.576%
39	16.186	2390	2397	2405	rBV	436346	783018	22.77%	1.913%
40	16.733	2484	2490	2497	rVB	124235	263408	7.66%	0.643%
41	17.374	2595	2599	2608	rVB3	54117	119864	3.49%	0.293%

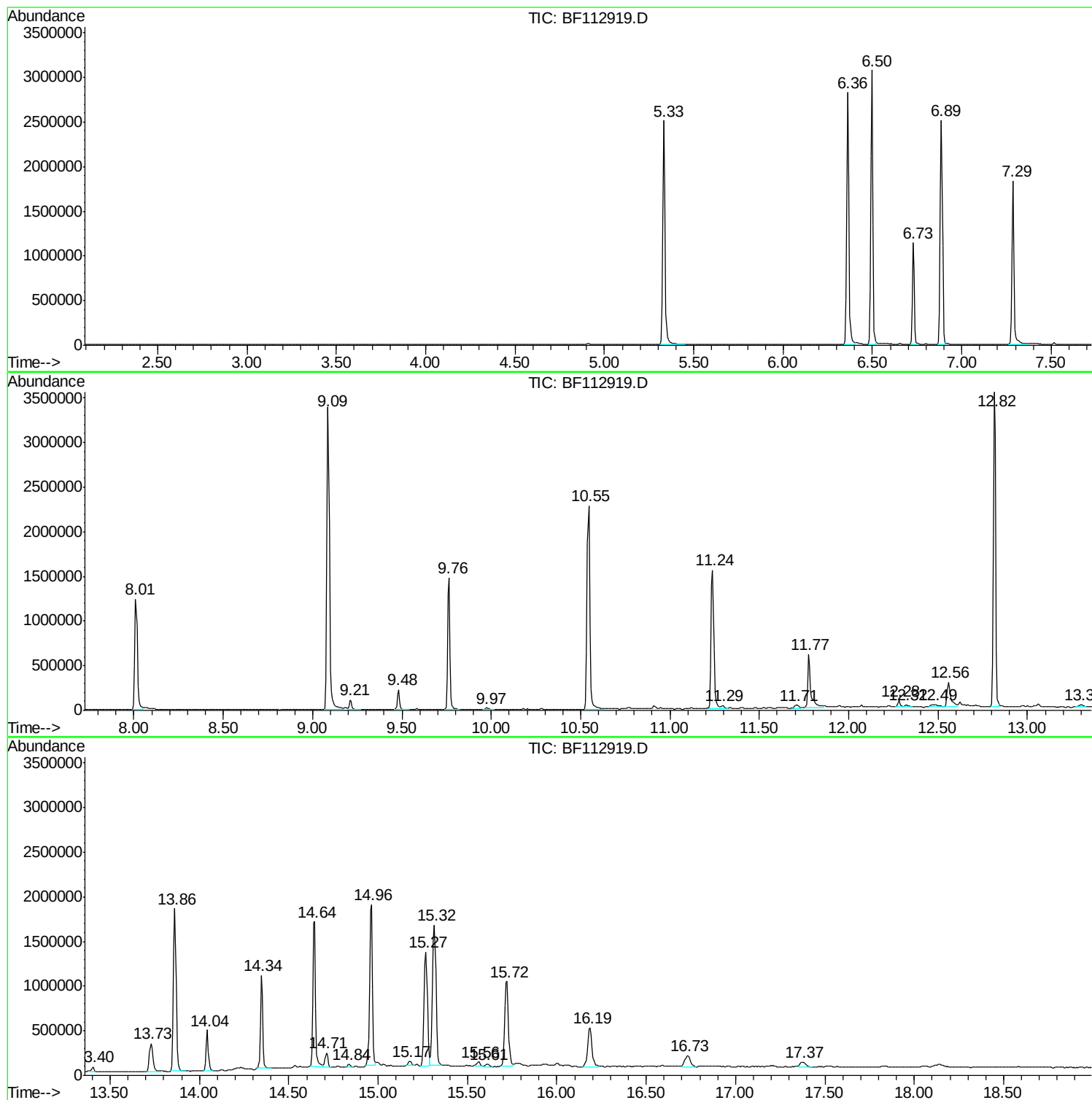
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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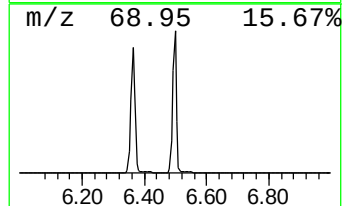
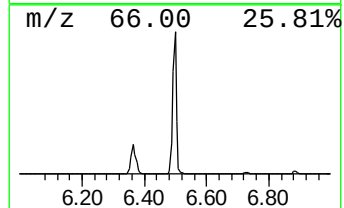
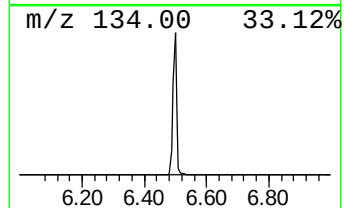
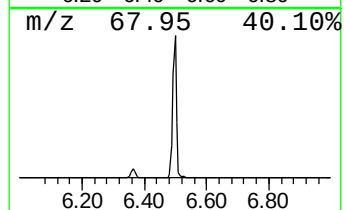
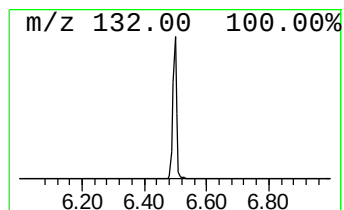
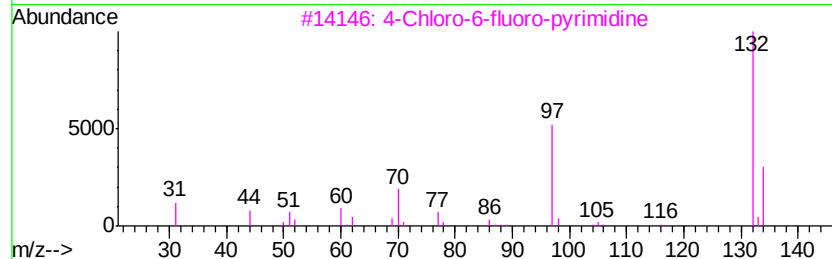
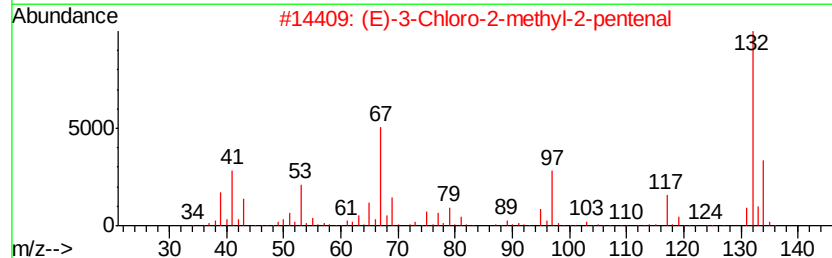
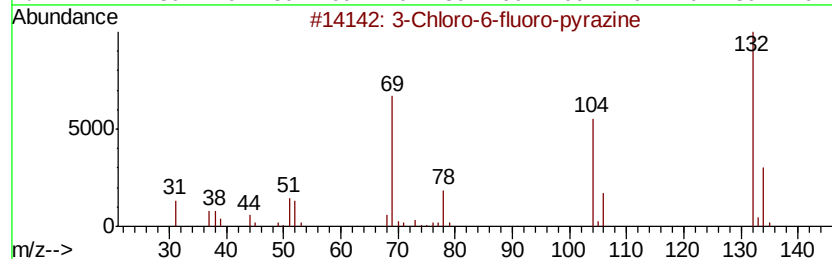
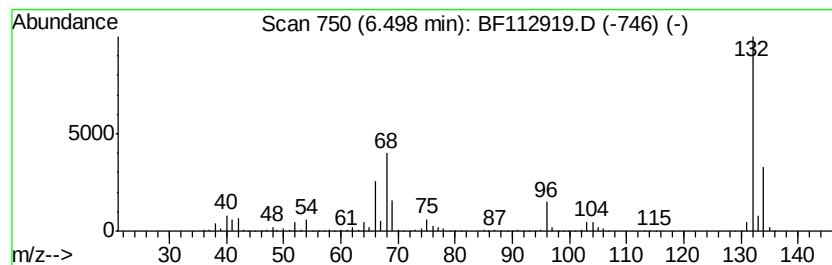
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	56.67 ng	2597490	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		Xenon	132	Xe	007440-63-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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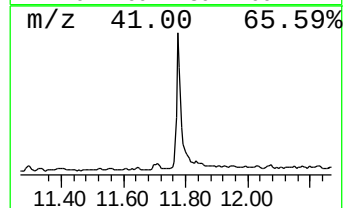
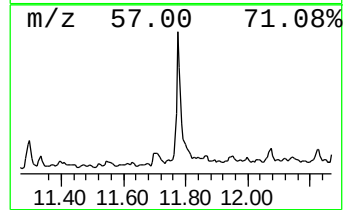
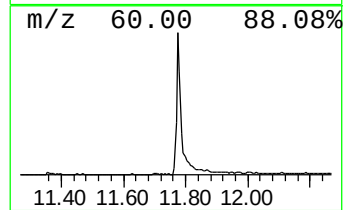
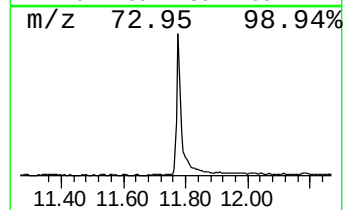
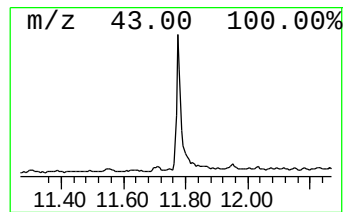
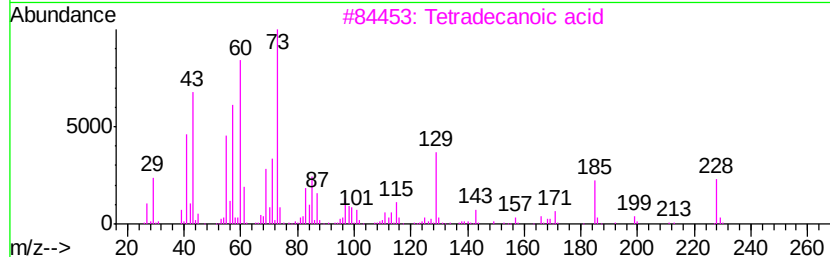
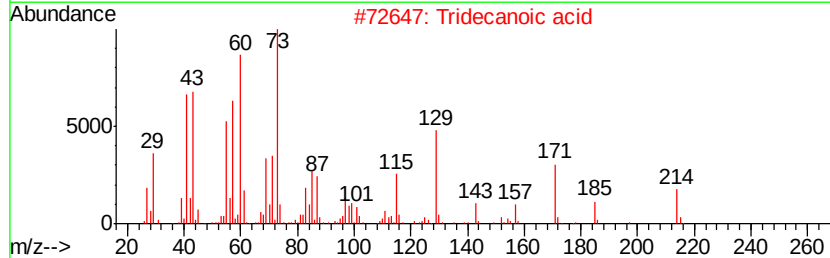
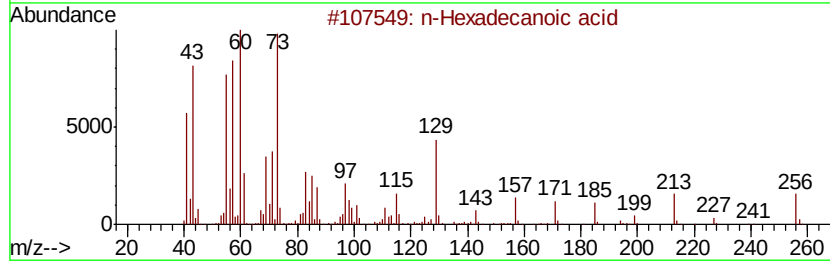
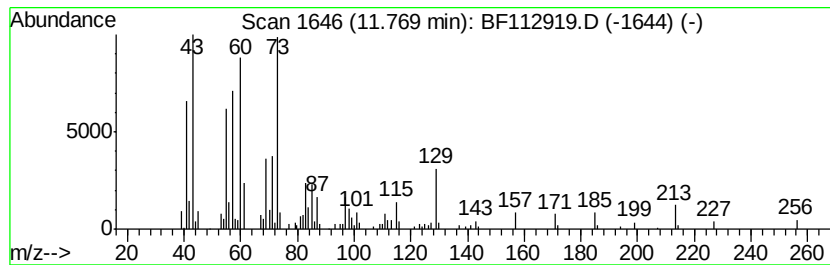
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	8.90 ng	697306	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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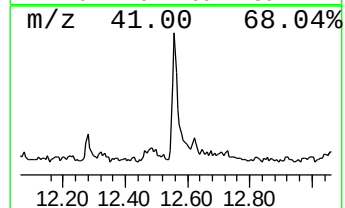
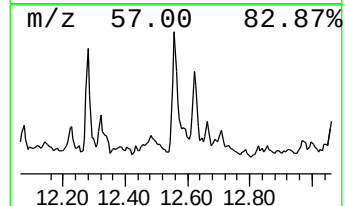
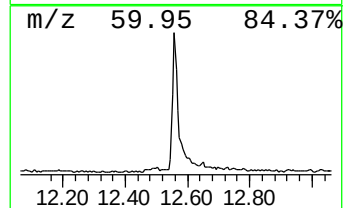
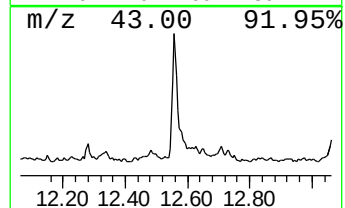
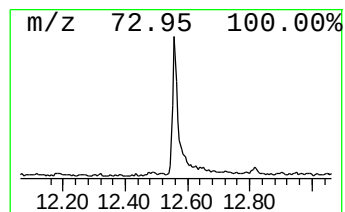
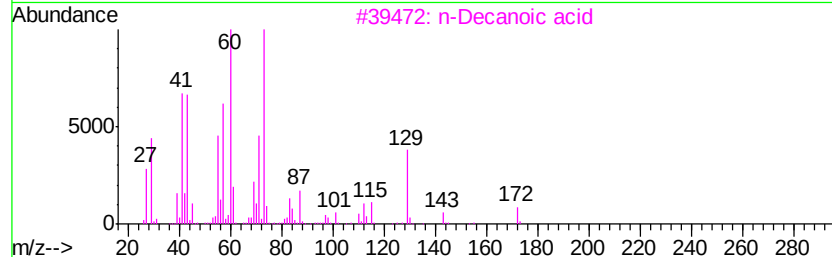
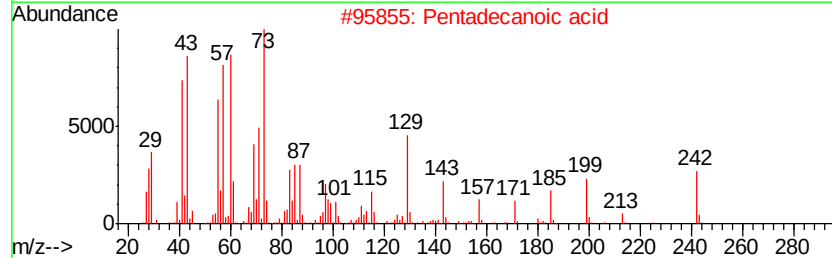
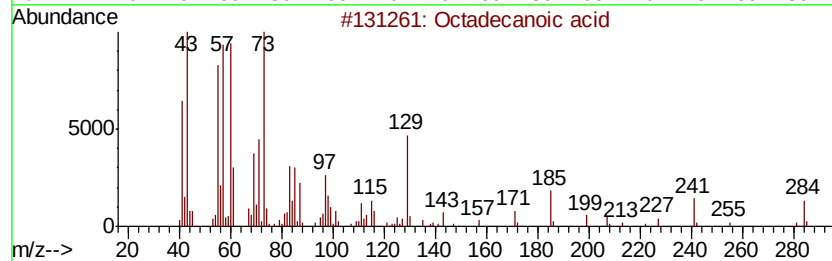
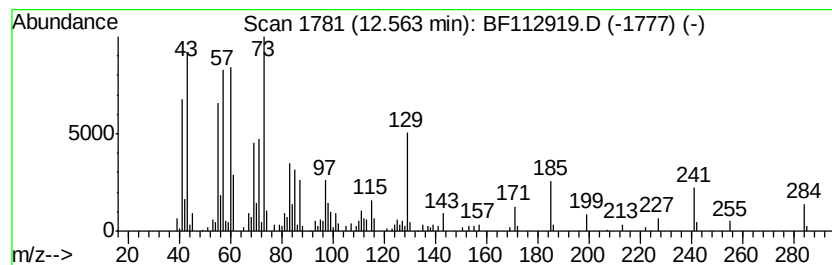
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.56	4.11 ng	364596	Chrysene-d12		13.86	
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	89
3		n-Decanoic acid	172	C10H20O2	000334-48-5	70
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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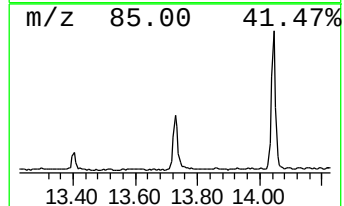
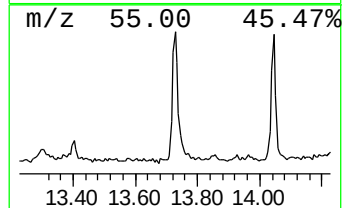
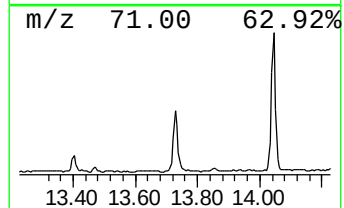
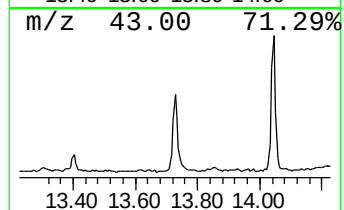
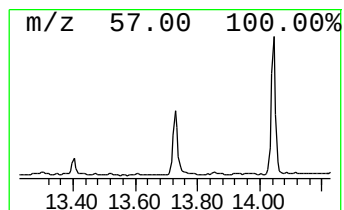
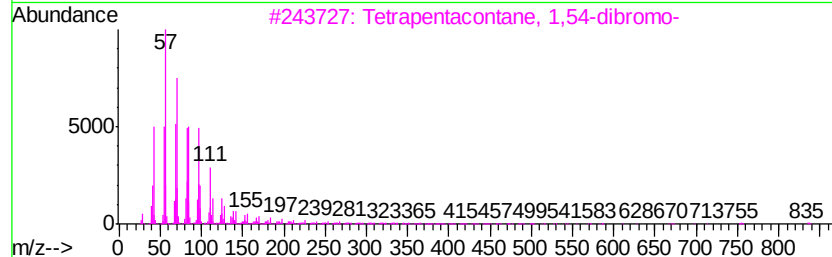
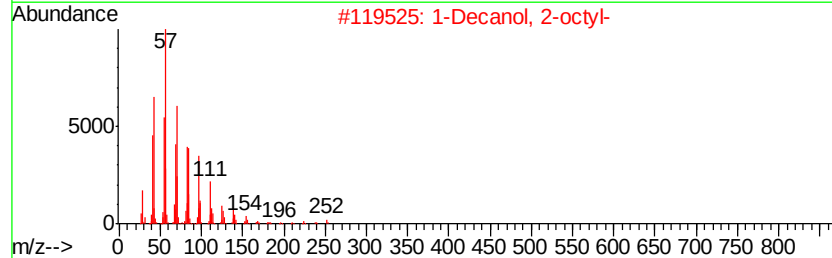
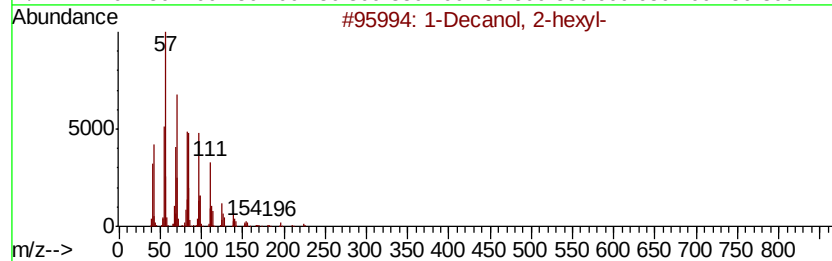
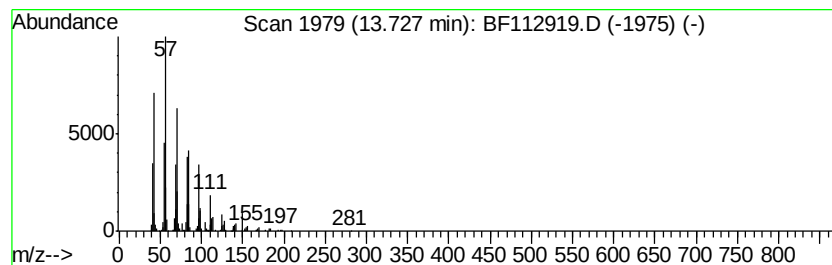
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.60 ng	407980	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	90
3		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	74
4		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	72
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	64



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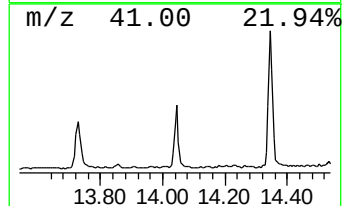
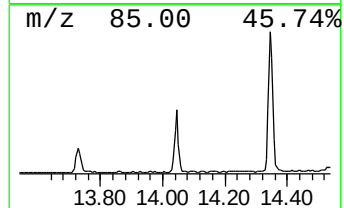
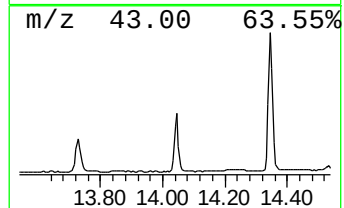
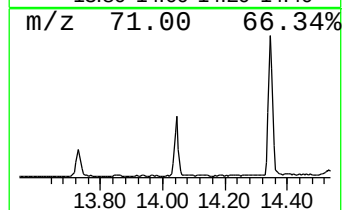
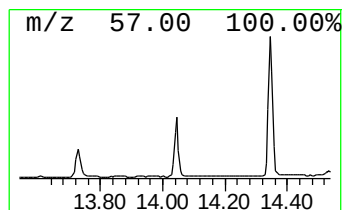
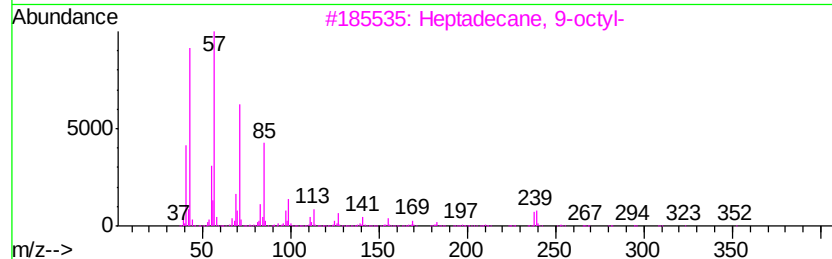
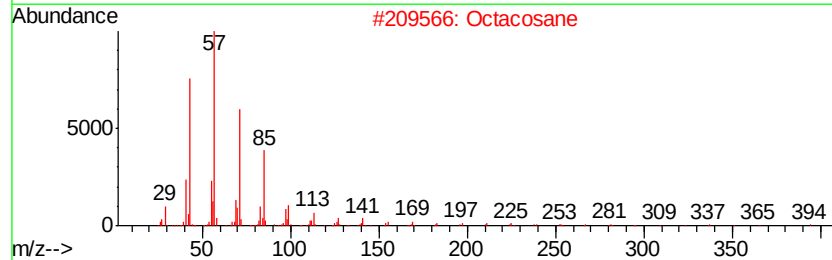
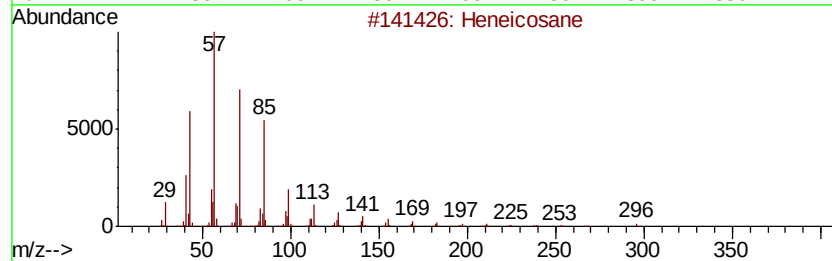
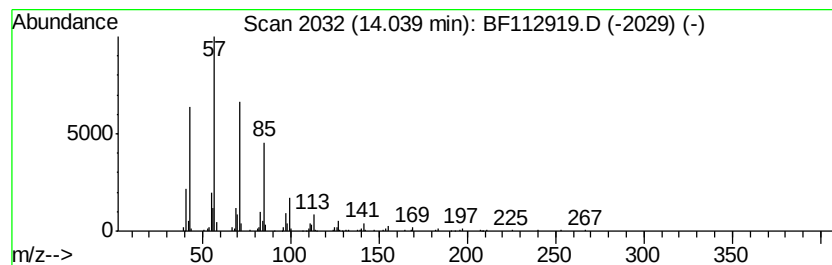
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	4.57 ng	405194	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Triacontane		422	C30H62	000638-68-6	90
5	Hexacosane		366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030719\
Data File : BF112919.D
Acq On : 7 Mar 2019 14:18
Operator : JU/SJ
Sample : K1760-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z2-11

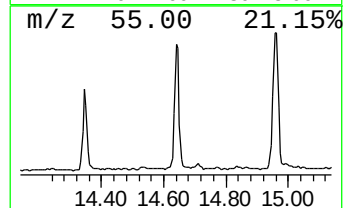
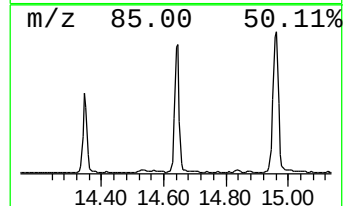
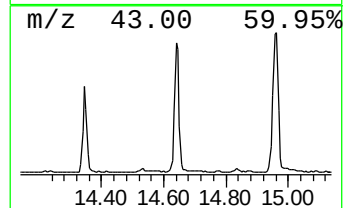
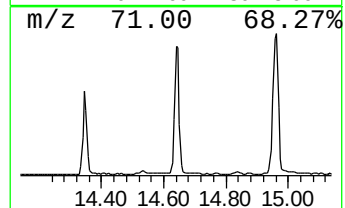
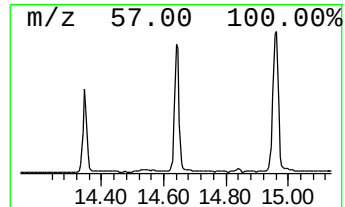
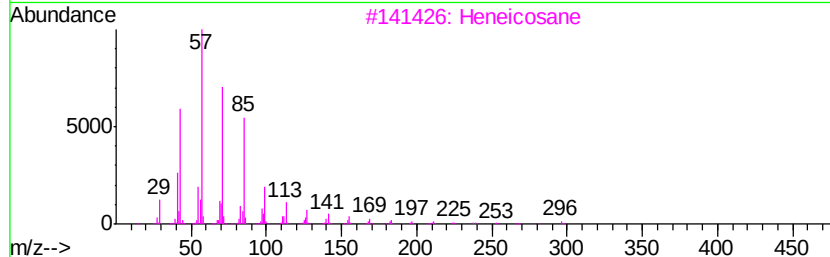
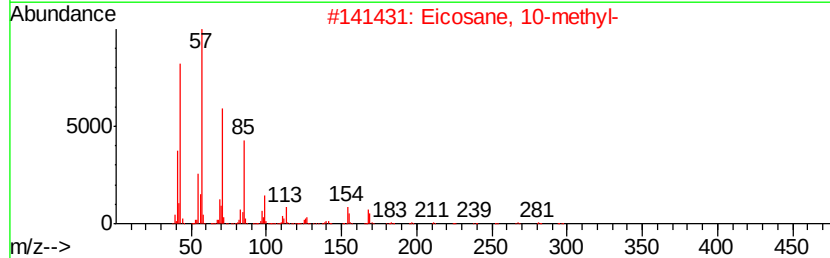
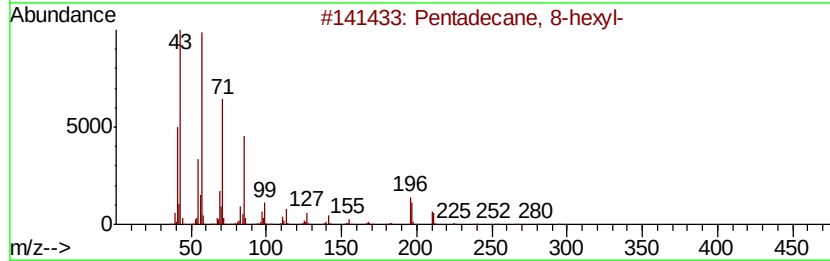
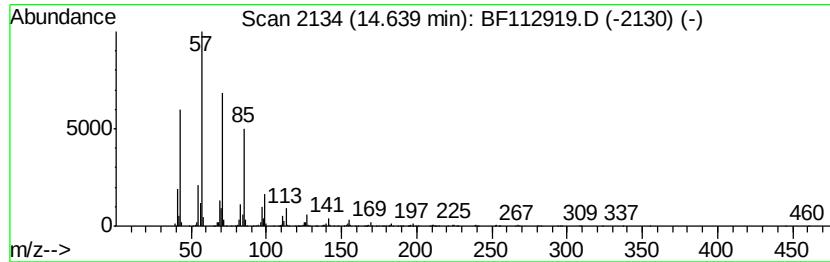
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	22.20 ng	1769580	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030719\
Data File : BF112919.D
Acq On : 7 Mar 2019 14:18
Operator : JU/SJ
Sample : K1760-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z2-11

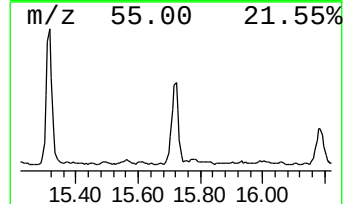
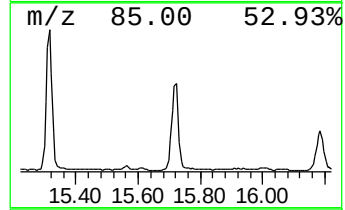
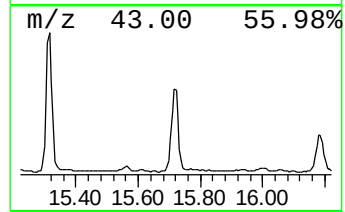
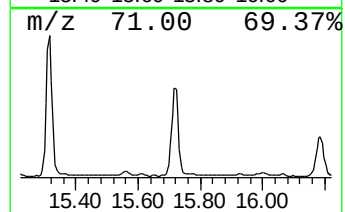
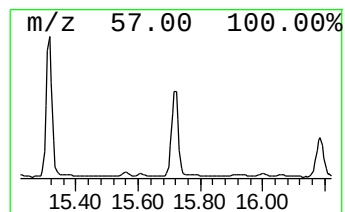
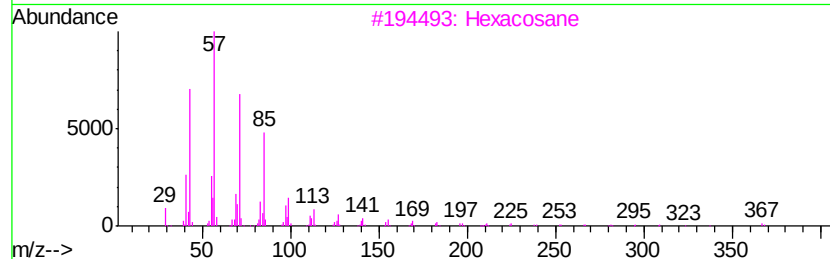
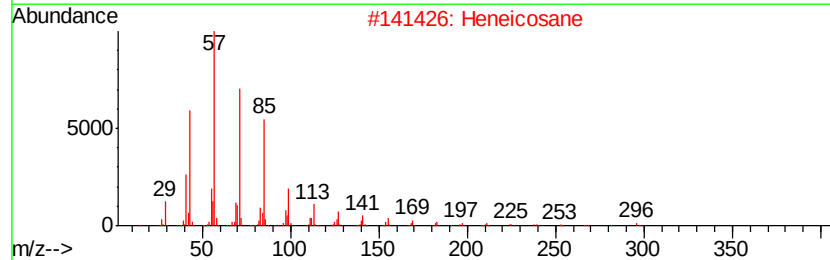
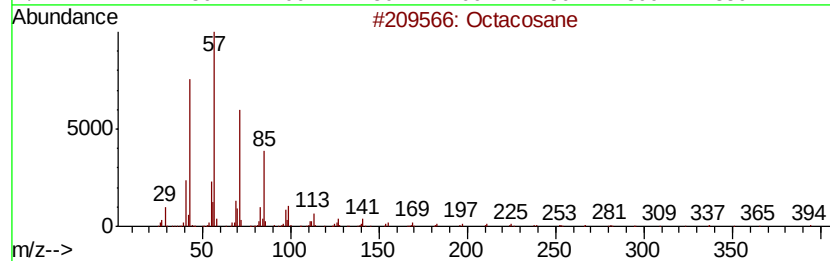
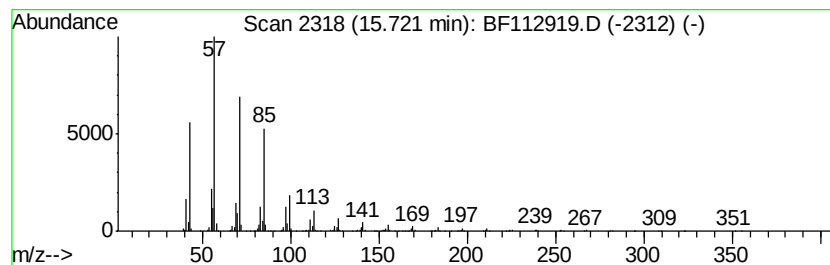
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	18.36 ng	1463690	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		2-Bromotetradecane	276	C14H29Br	074036-95-6	91
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030719\
Data File : BF112919.D
Acq On : 7 Mar 2019 14:18
Operator : JU/SJ
Sample : K1760-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z2-11

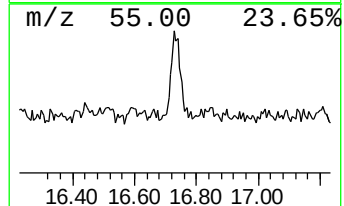
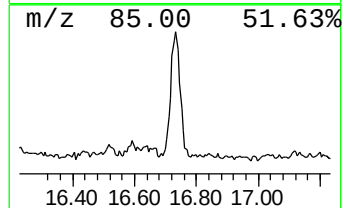
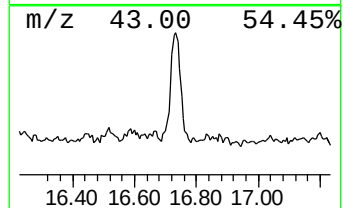
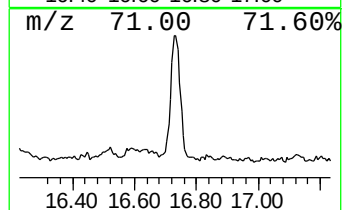
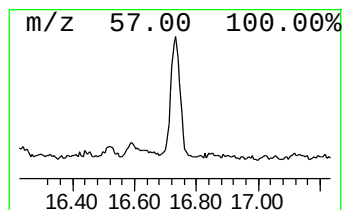
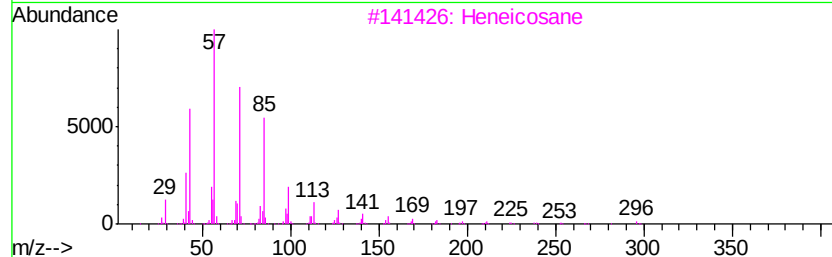
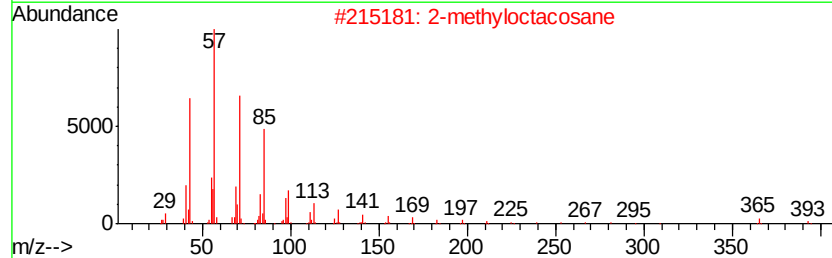
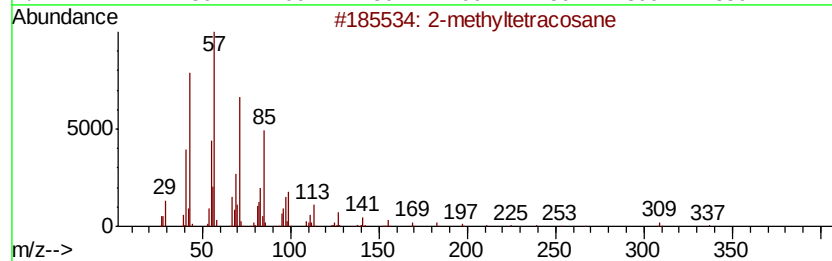
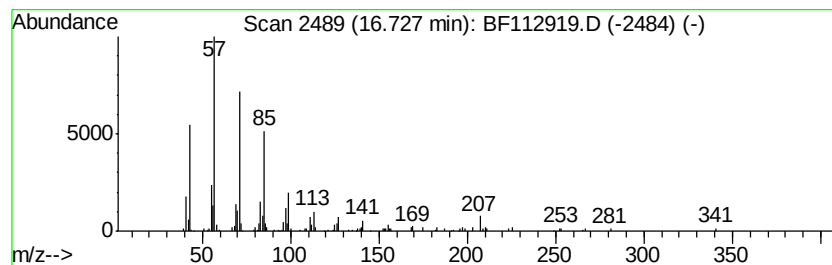
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyltetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	3.30 ng	263408	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyltetracosane	352	C25H52	1000376-72-6	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030719\
Data File : BF112919.D
Acq On : 7 Mar 2019 14:18
Operator : JU/SJ
Sample : K1760-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z2-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	56.7	ng	2597490	1	6.73	916790	20.0
n-Hexadecanoic acid	11.77	8.9	ng	697306	4	11.24	1566120	20.0
Octadecanoic acid	12.56	4.1	ng	364596	5	13.86	1775170	20.0
1-Decanol, 2-hexyl-	13.73	4.6	ng	407980	5	13.86	1775170	20.0
Heneicosane	14.04	4.6	ng	405194	5	13.86	1775170	20.0
Pentadecane, 8-he...	14.64	22.2	ng	1769580	6	15.27	1594580	20.0
Octacosane	15.72	18.4	ng	1463690	6	15.27	1594580	20.0
2-methyltetracosane	16.73	3.3	ng	263408	6	15.27	1594580	20.0