

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
 Data File : BF121795.D
 Acq On : 2 Oct 2020 15:40
 Operator : JU/CG
 Sample : L4199-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 11940

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-BF091020.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	4.975	487	491	502	rBV	75760	105187	3.94%	0.457%
2	5.387	557	561	576	rBV	2396131	2239479	83.84%	9.727%
3	6.404	729	734	751	rBV	2327867	2299193	86.08%	9.987%
4	6.763	791	795	798	rBV	772276	661429	24.76%	2.873%
5	7.328	886	891	894	rBV	1622319	1594214	59.68%	6.925%
6	8.045	1009	1013	1021	rBV	924846	847338	31.72%	3.680%
7	9.122	1191	1196	1199	rBV	2932251	2671109	100.00%	11.602%
8	9.516	1259	1263	1270	rBV	210174	188116	7.04%	0.817%
9	9.798	1306	1311	1314	rBV	1023246	881183	32.99%	3.827%
10	10.586	1440	1445	1458	rBV	1468573	1380992	51.70%	5.998%
11	11.280	1559	1563	1565	rBV	918901	788280	29.51%	3.424%
12	11.304	1565	1567	1571	rVV	196014	156369	5.85%	0.679%
13	11.357	1573	1576	1579	rVB	35337	31814	1.19%	0.138%
14	11.810	1650	1653	1656	rBV	51236	38124	1.43%	0.166%
15	11.892	1663	1667	1669	rBV	43546	41047	1.54%	0.178%
16	12.492	1765	1769	1772	rBV	402007	339705	12.72%	1.476%
17	12.721	1800	1808	1811	rBV	313309	362058	13.55%	1.573%
18	12.863	1828	1832	1836	rVB	2425681	2196807	82.24%	9.542%
19	12.945	1840	1846	1848	rBV3	27914	43533	1.63%	0.189%
20	13.051	1861	1864	1867	rVB	51440	53951	2.02%	0.234%
21	13.092	1867	1871	1873	rBV	31111	40601	1.52%	0.176%
22	13.116	1873	1875	1877	rVB2	37830	29542	1.11%	0.128%
23	13.151	1877	1881	1883	rBV3	41251	40346	1.51%	0.175%
24	13.339	1910	1913	1920	rVB5	34936	44938	1.68%	0.195%
25	13.439	1925	1930	1933	rBV4	33126	37224	1.39%	0.162%
26	13.557	1947	1950	1953	rVB	38850	34626	1.30%	0.150%
27	13.663	1963	1968	1971	rBV2	39520	53738	2.01%	0.233%
28	13.768	1983	1986	1995	rVB2	282966	403462	15.10%	1.752%
29	13.898	2004	2008	2010	rBV	1406605	1488704	55.73%	6.466%
30	13.939	2014	2015	2023	rVB	191786	165177	6.18%	0.717%
31	14.021	2023	2029	2031	rBV2	37509	42641	1.60%	0.185%
32	14.080	2034	2039	2041	rBV2	51602	60586	2.27%	0.263%
33	14.304	2074	2077	2080	rVB	39108	34099	1.28%	0.148%
34	14.339	2080	2083	2086	rBV2	26612	27899	1.04%	0.121%

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35	14.386	2087	2091	2093	rBV	62976	72286	2.71%	0.314%
36	14.510	2109	2112	2114	rVV2	30701	29586	1.11%	0.129%
37	14.545	2114	2118	2123	rVB	247245	217373	8.14%	0.944%
38	14.686	2139	2142	2145	rVB	65578	66130	2.48%	0.287%
39	14.757	2152	2154	2161	rBV4	32395	46069	1.72%	0.200%
40	14.827	2163	2166	2168	rVB	44791	40696	1.52%	0.177%
41	14.939	2181	2185	2188	rBV	220388	320824	12.01%	1.394%
42	15.009	2194	2197	2200	rVB	95690	94684	3.54%	0.411%
43	15.051	2200	2204	2213	rVB2	78615	158828	5.95%	0.690%
44	15.233	2231	2235	2241	rVB	113315	138495	5.18%	0.602%
45	15.292	2241	2245	2250	rVB	181160	203049	7.60%	0.882%
46	15.351	2250	2255	2266	rBV	628488	888543	33.26%	3.859%
47	15.568	2288	2292	2296	rVB4	44467	62896	2.35%	0.273%
48	15.792	2325	2330	2336	rVB	103762	153246	5.74%	0.666%
49	15.862	2337	2342	2352	rBV6	59291	180015	6.74%	0.782%
50	16.268	2407	2411	2416	rVB3	41523	68917	2.58%	0.299%
51	16.545	2455	2458	2465	rBV4	36909	68684	2.57%	0.298%
52	16.756	2489	2494	2502	rBV2	105966	208258	7.80%	0.905%
53	16.833	2503	2507	2515	rVB2	55823	104296	3.90%	0.453%
54	16.927	2519	2523	2524	rBV4	21703	30854	1.16%	0.134%
55	17.180	2561	2566	2574	rVB	87766	164154	6.15%	0.713%
56	17.333	2586	2592	2602	rBV10	48308	132532	4.96%	0.576%
57	18.280	2748	2753	2764	rVB8	55099	148724	5.57%	0.646%

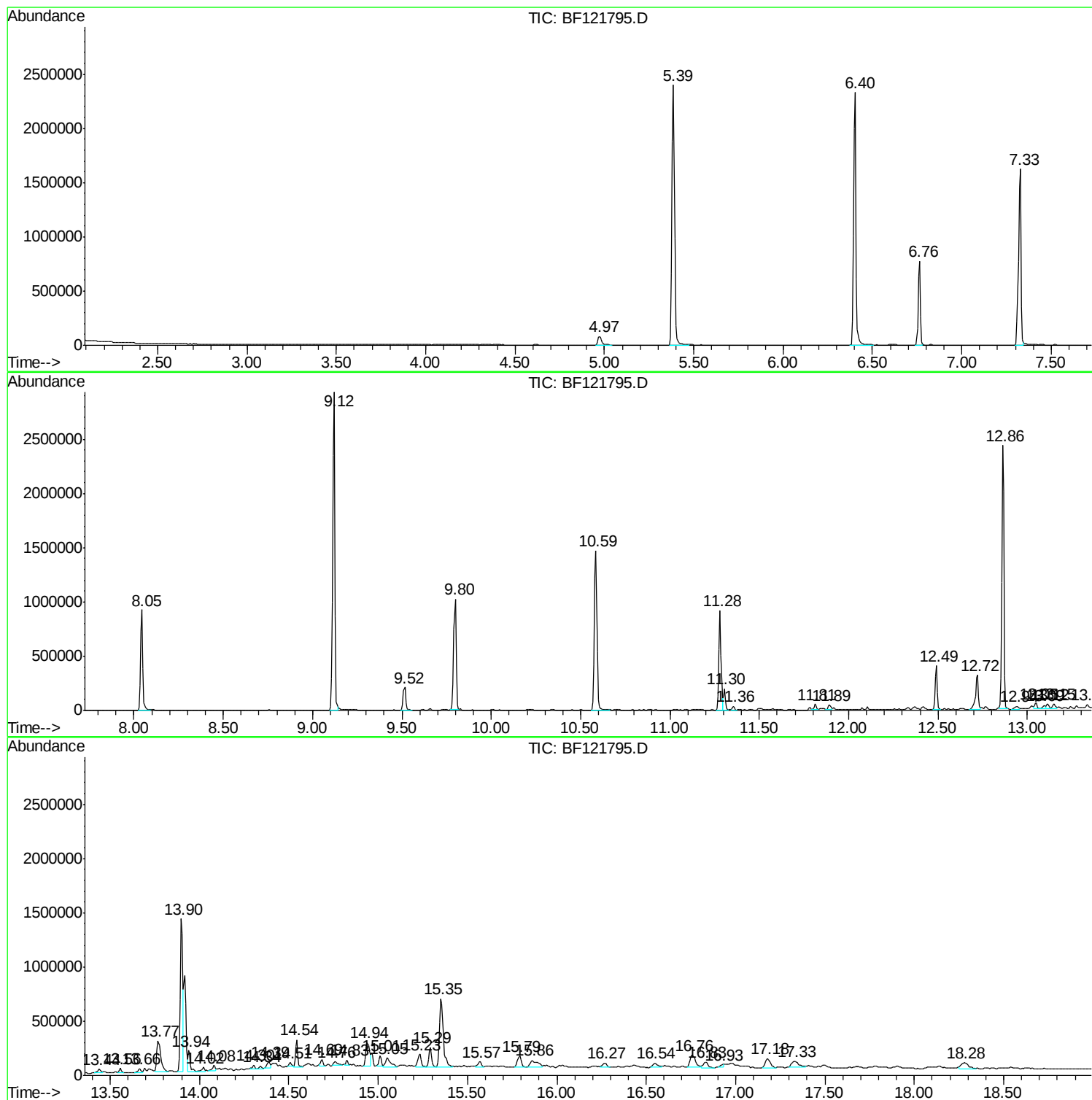
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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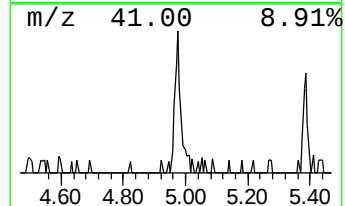
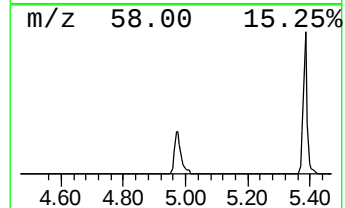
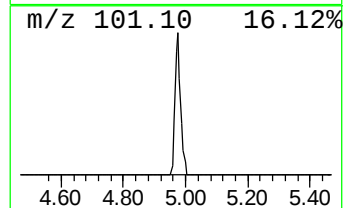
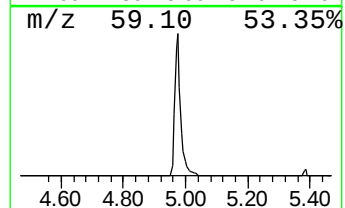
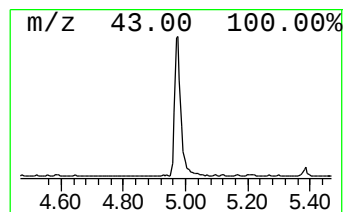
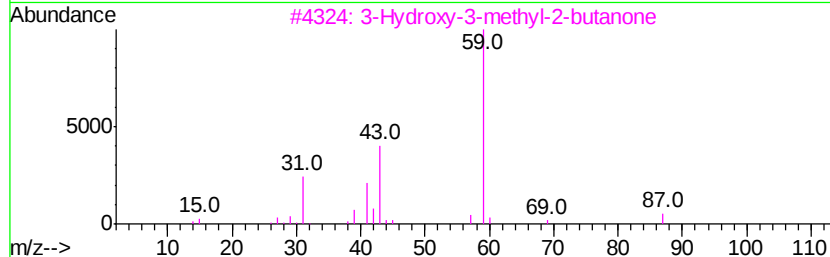
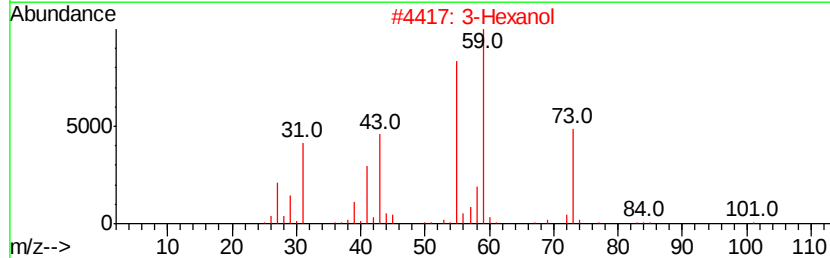
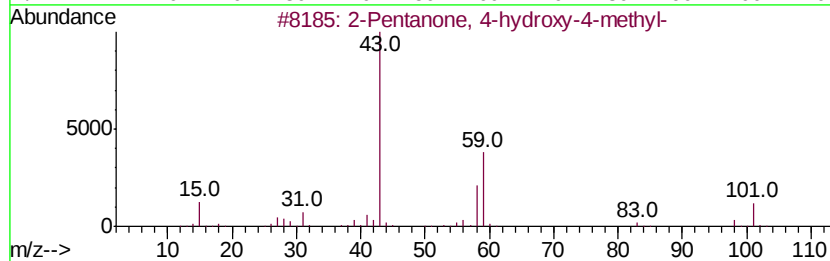
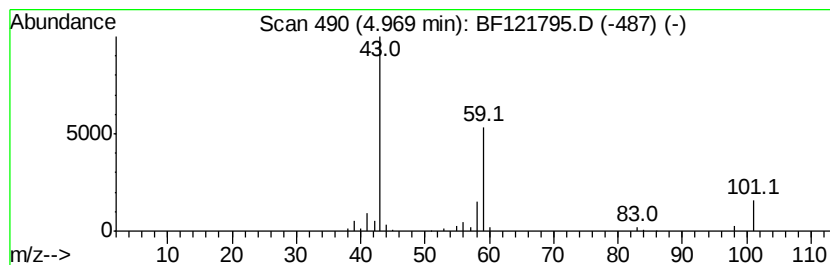
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	3.18 ng	105187	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol	102	C6H14O	000623-37-0	33		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9		



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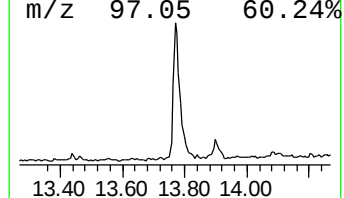
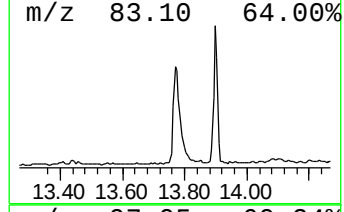
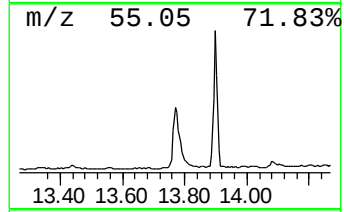
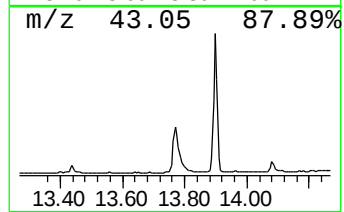
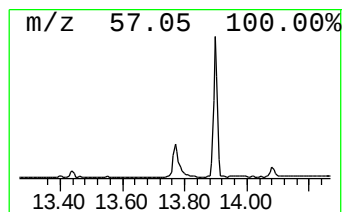
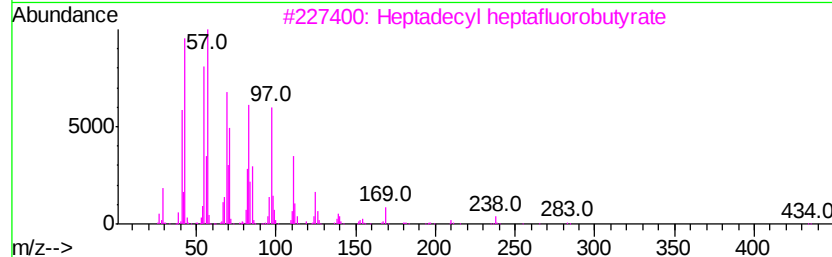
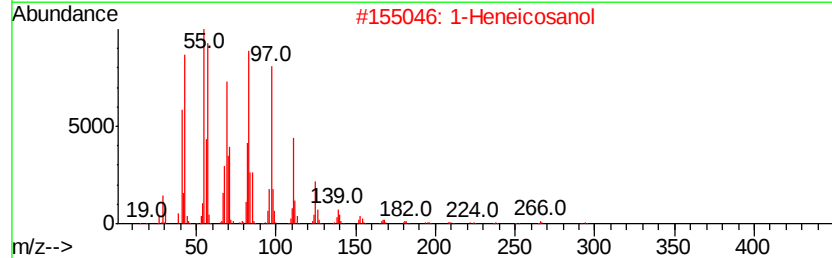
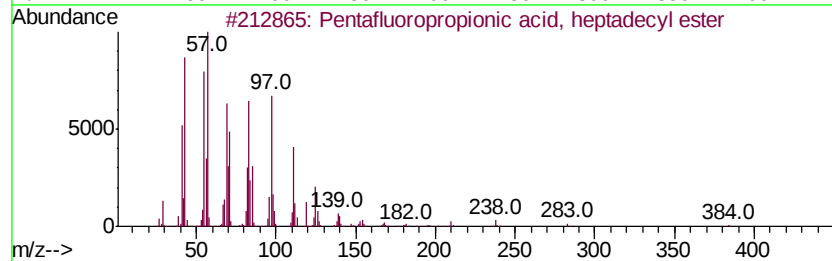
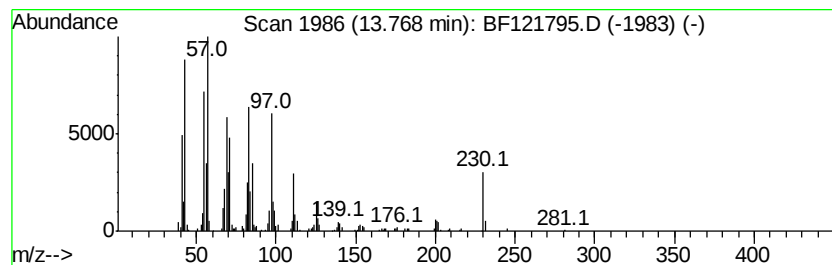
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	5.42 ng	403462	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
2		1-Heneicosanol	312	C21H44O	015594-90-8	92
3		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	91
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90



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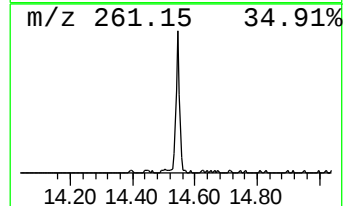
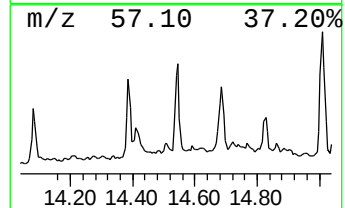
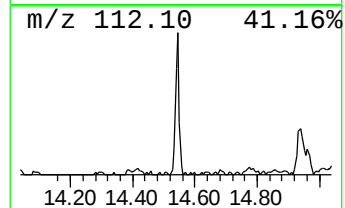
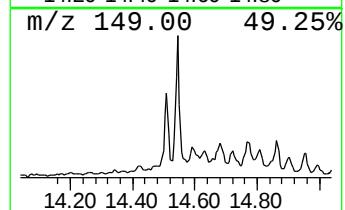
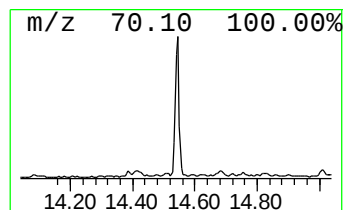
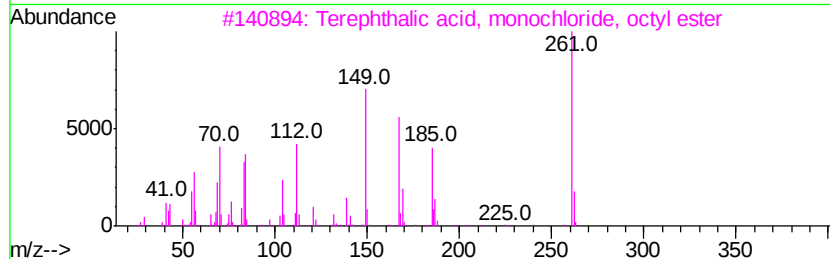
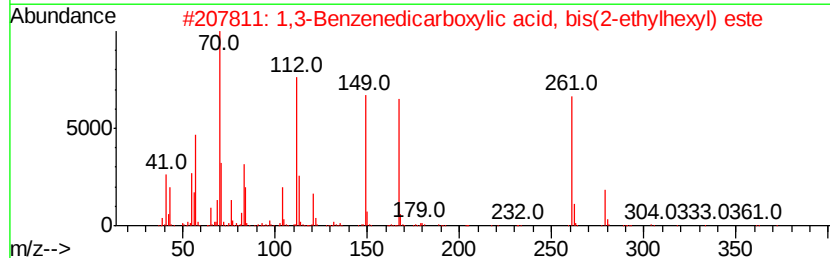
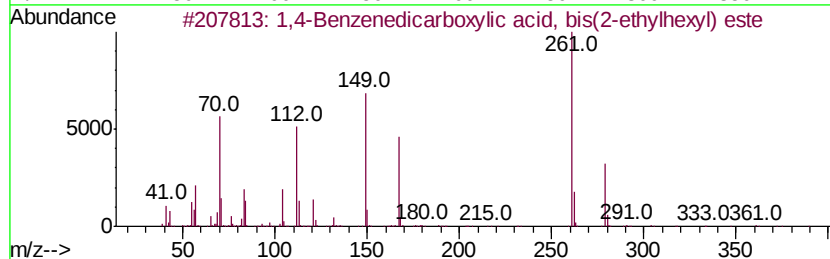
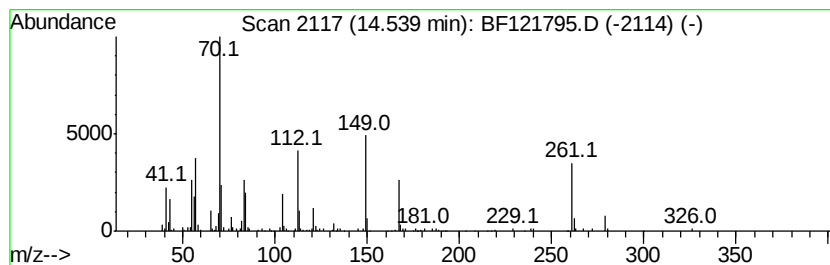
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1,4-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.92 ng	217373	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	91
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3		Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
4		Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	38
5		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	27



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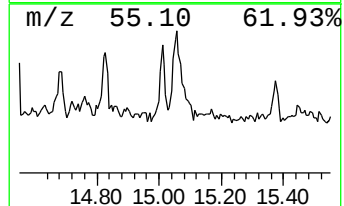
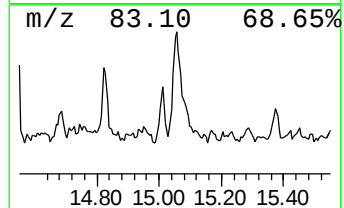
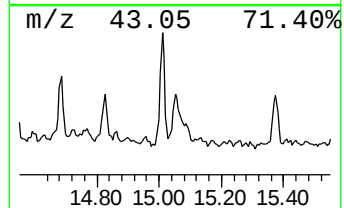
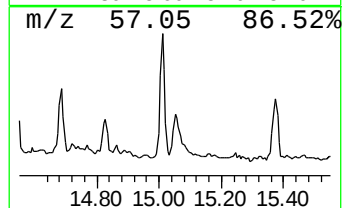
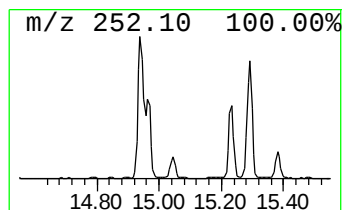
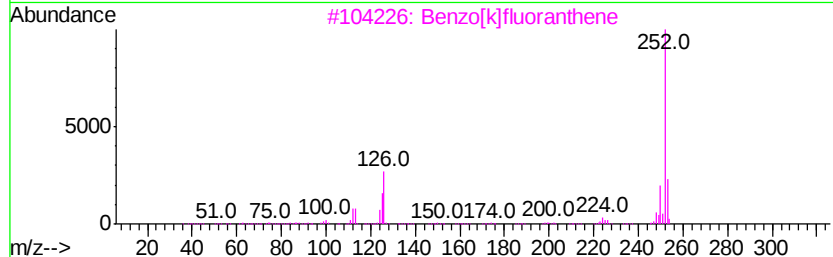
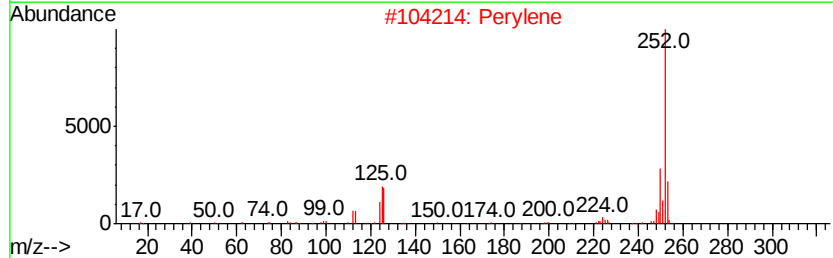
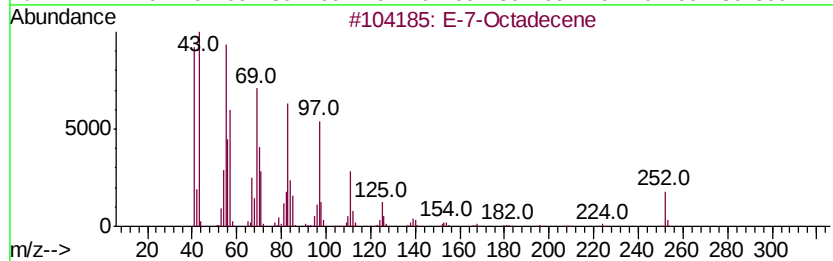
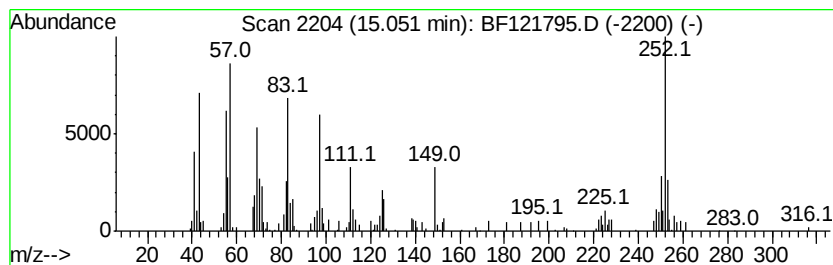
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Peak Number 4 E-7-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	3.58 ng	158828	Perylene-d12	15.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-7-Octadecene	252	C18H36	1000130-92-0	83	
2	Perylene	252	C20H12	000198-55-0	55	
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	55	
4	1-Heneicosanol	312	C21H44O	015594-90-8	53	
5	Behenic alcohol	326	C22H46O	000661-19-8	53	



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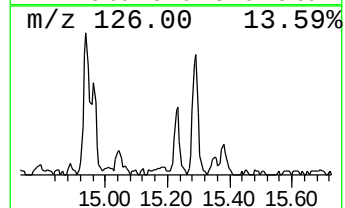
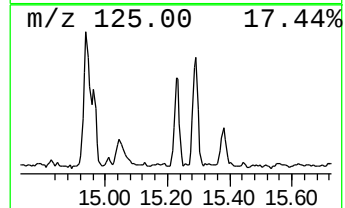
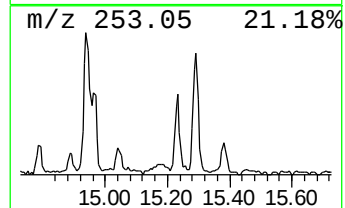
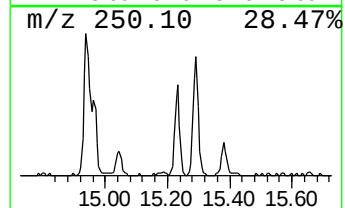
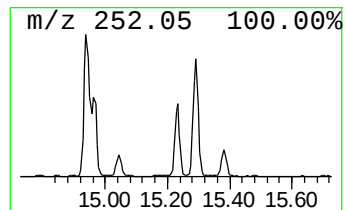
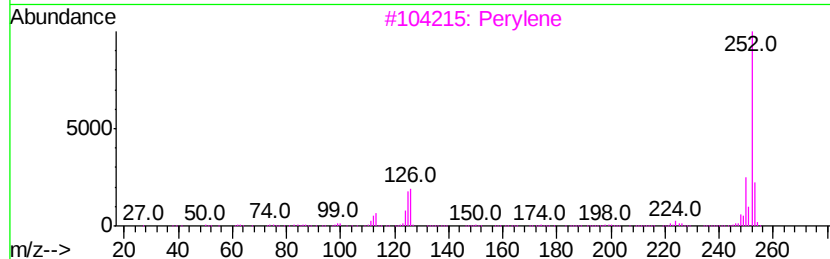
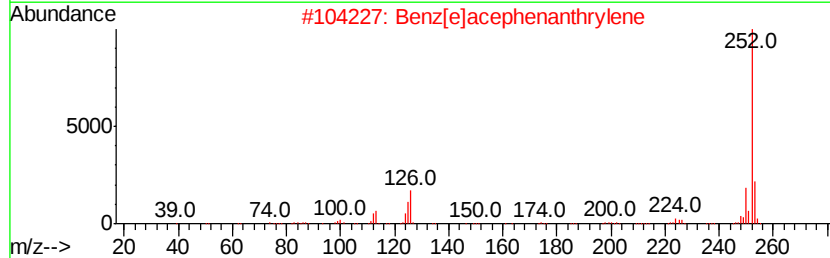
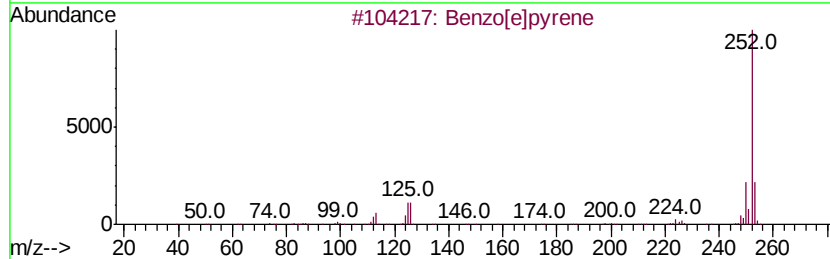
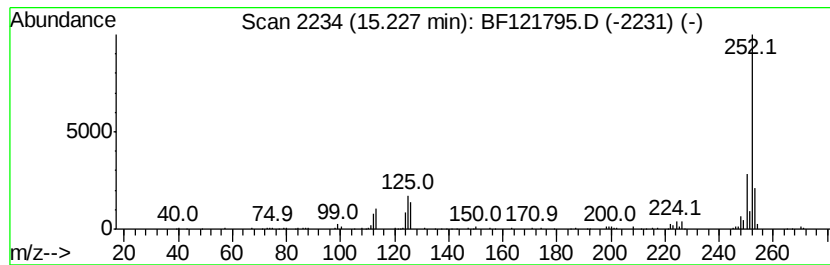
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.12 ng	138495	Perylene-d12	15.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3		Perylene	252	C20H12	000198-55-0	95
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121795.D
Acq On : 2 Oct 2020 15:40
Operator : JU/CG
Sample : L4199-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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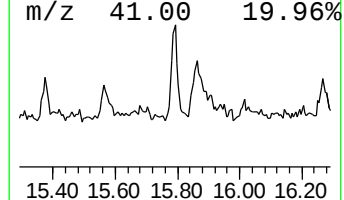
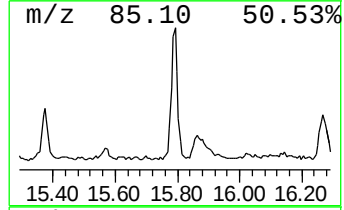
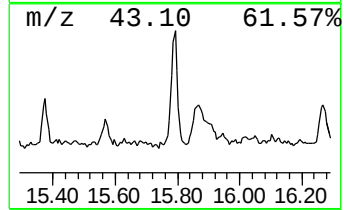
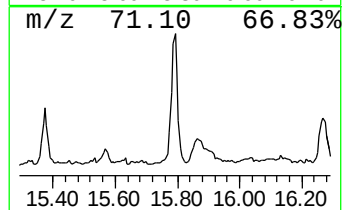
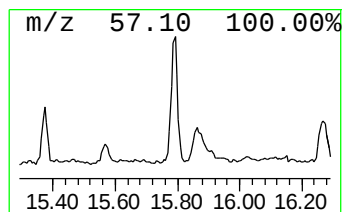
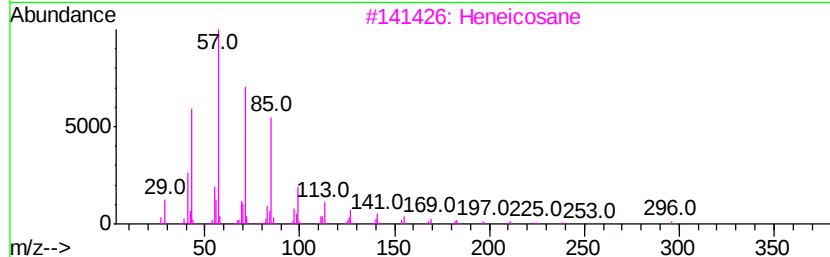
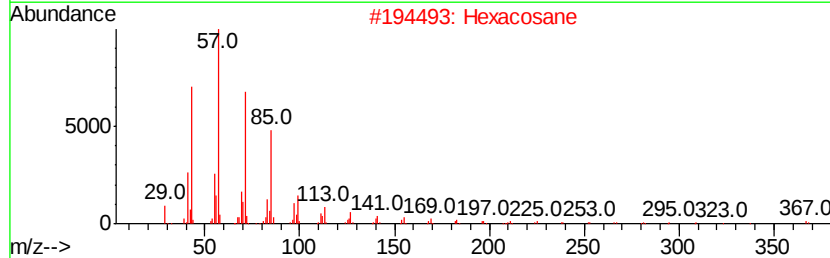
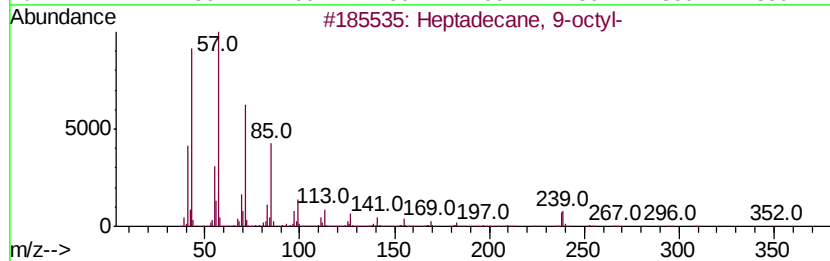
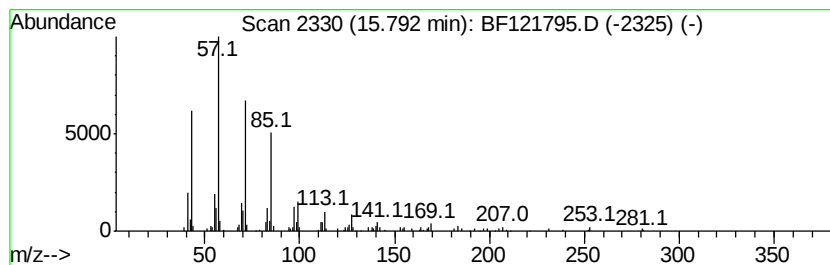
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.45 ng	153246	Perylene-d12	15.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heneicosane	296	C21H44	000629-94-7	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121795.D
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Instrument :
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ClientSampleId :
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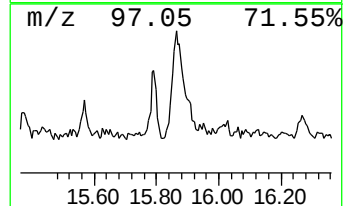
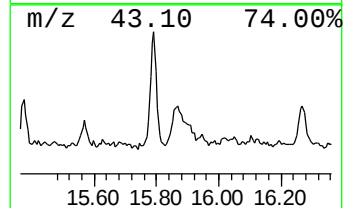
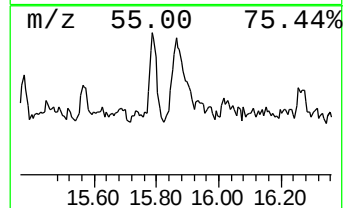
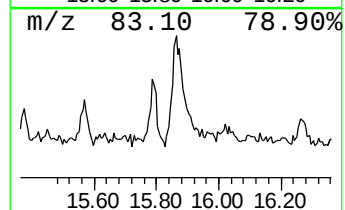
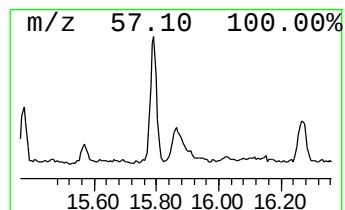
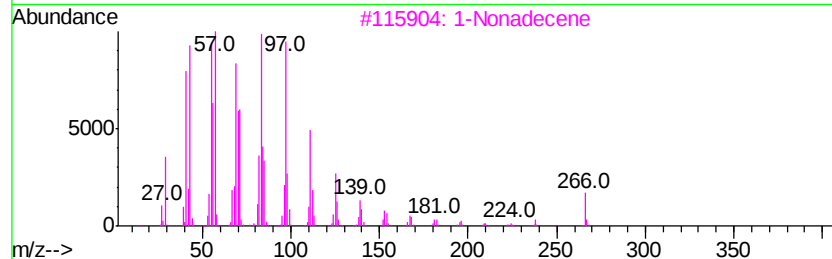
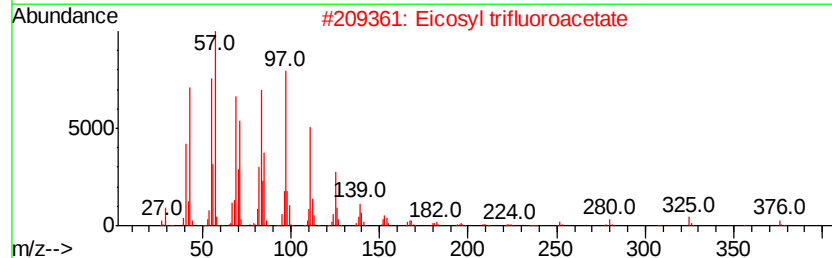
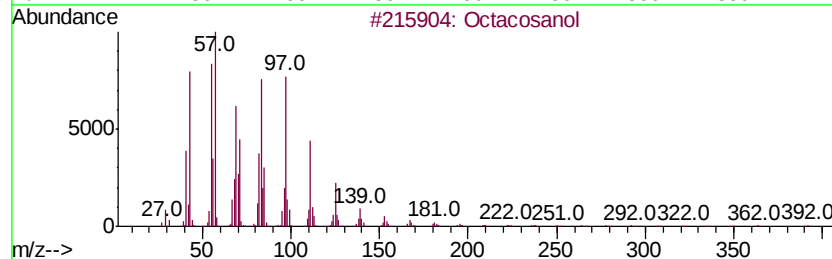
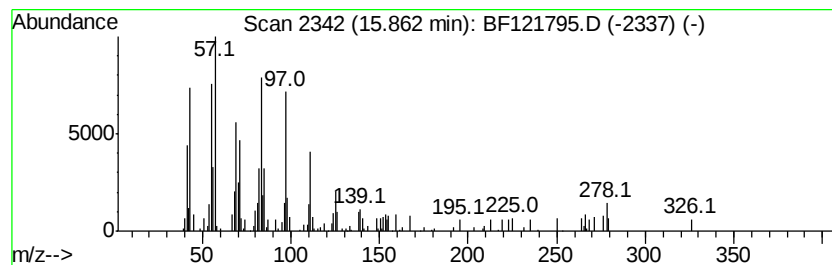
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	4.05 ng	180015	Perylene-d12	15.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosanol	410	C28H58O	000557-61-9	93
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	90
3		1-Nonadecene	266	C19H38	018435-45-5	87
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121795.D
Acq On : 2 Oct 2020 15:40
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Sample : L4199-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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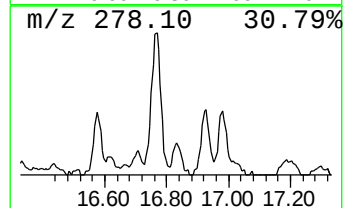
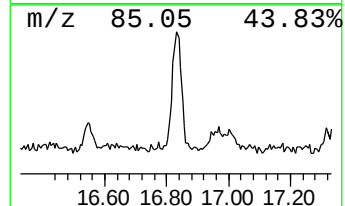
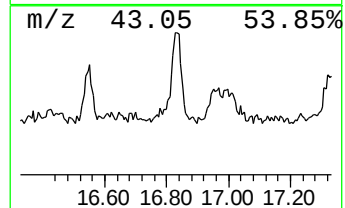
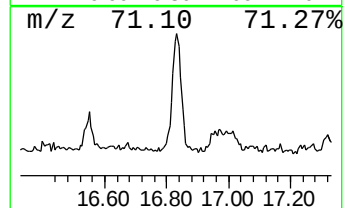
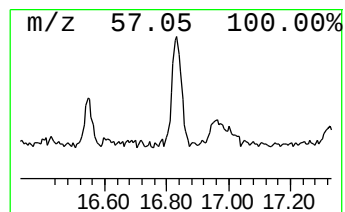
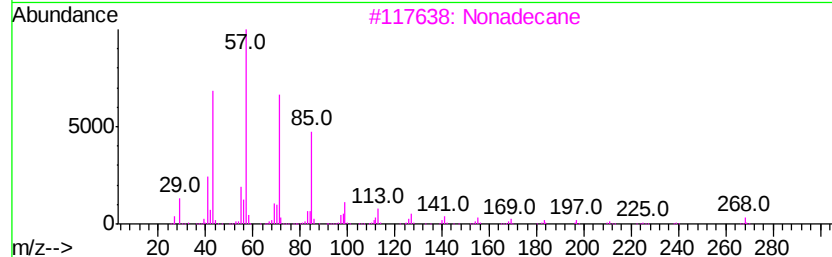
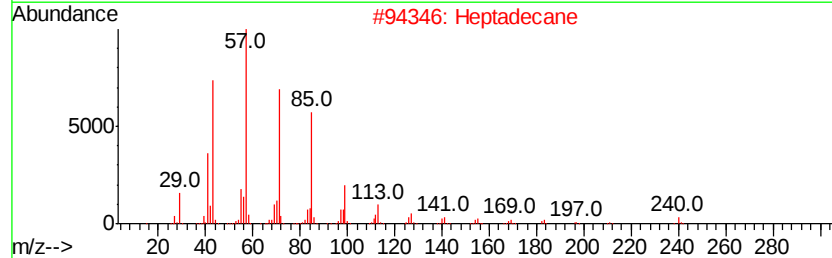
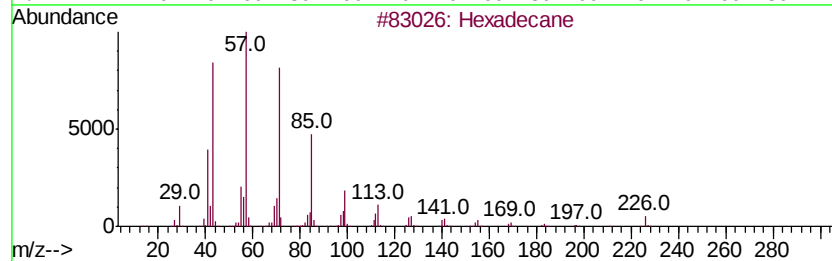
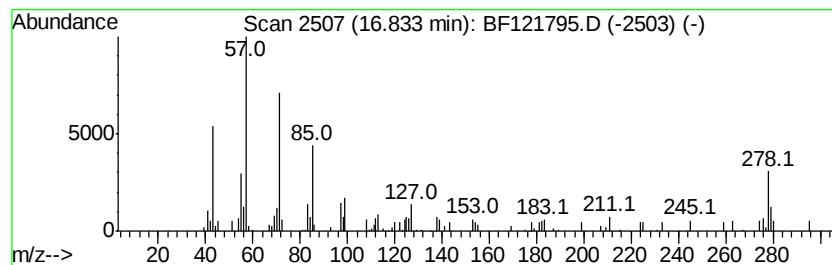
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.83 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	2.35 ng	104296	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	49
2		Heptadecane	240	C17H36	000629-78-7	46
3		Nonadecane	268	C19H40	000629-92-5	46
4		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	46
5		Tetradecane	198	C14H30	000629-59-4	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121795.D
Acq On : 2 Oct 2020 15:40
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Sample : L4199-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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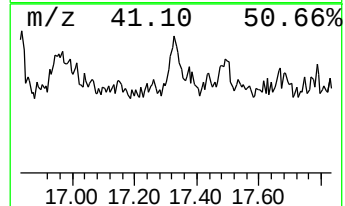
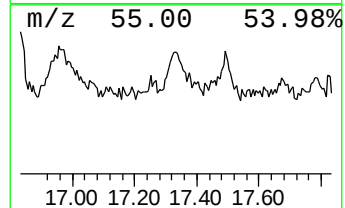
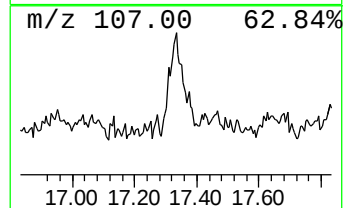
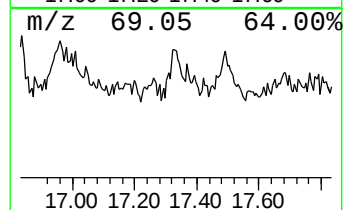
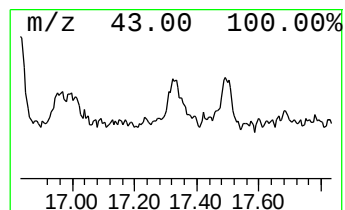
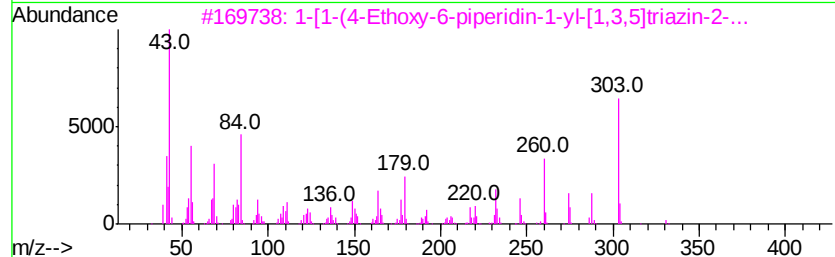
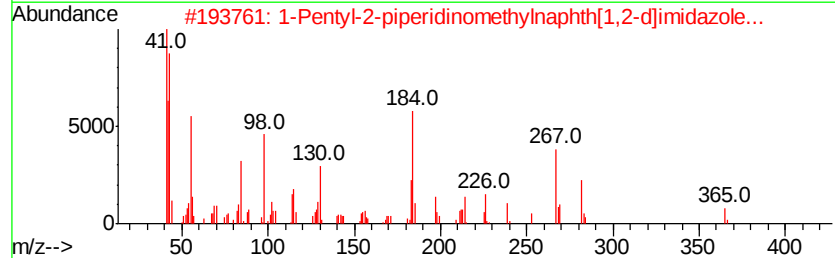
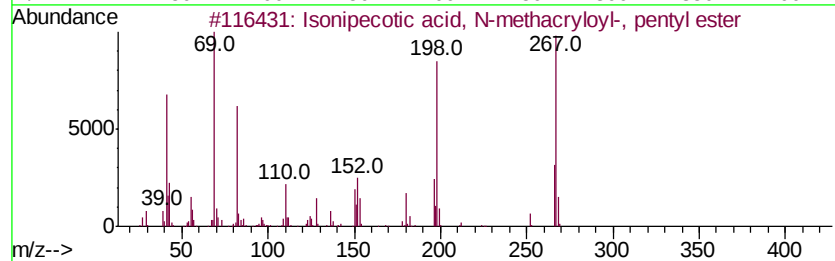
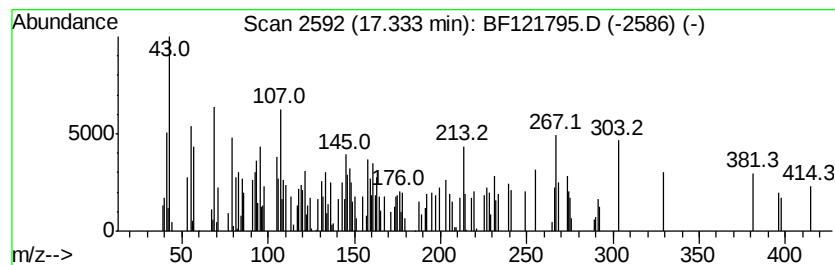
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.33 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	2.98 ng	132532	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isonipecotic acid, N-methacrylov...	267	C15H25N03	1000360-95-7	10
2		1-Pentyl-2-piperidinomethylnapht...	365	C22H27N302	027223-90-1	9
3		1-[1-(4-Ethoxy-6-piperidin-1-yl)-...	331	C15H21N702	1000300-82-4	9
4		Octadecanoic acid, 2-(acetyloxy)...	442	C25H4606	055401-62-2	9
5		2,4,6-Triisopropyl-benzenesulfon...	360	C21H2803S	082965-06-8	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121795.D
Acq On : 2 Oct 2020 15:40
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Sample : L4199-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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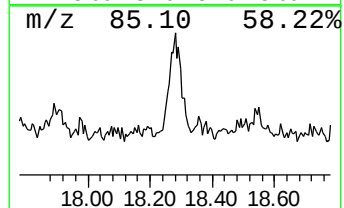
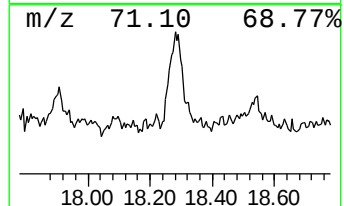
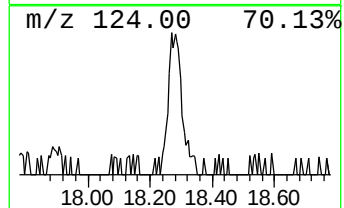
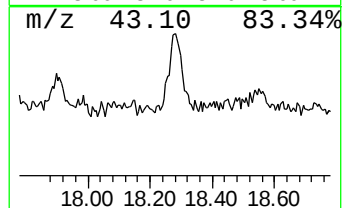
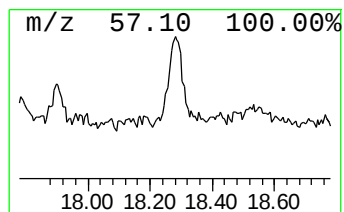
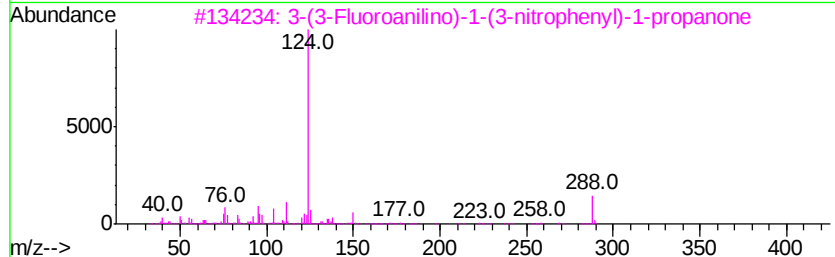
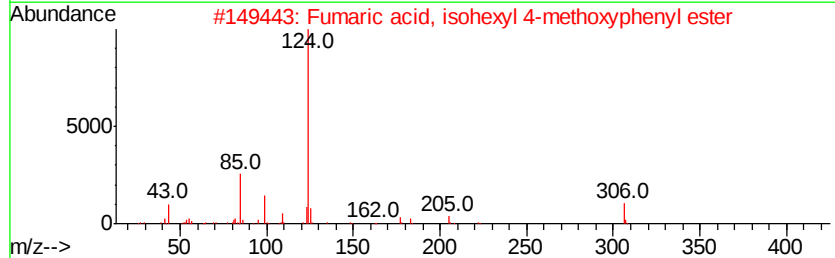
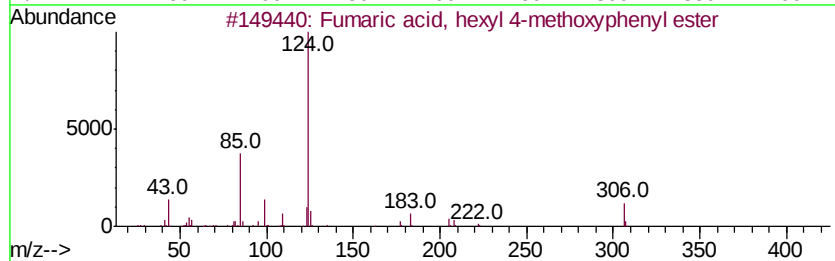
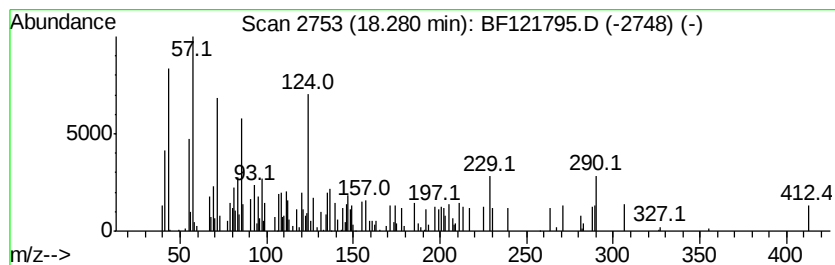
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.28 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	3.35 ng	148724	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, hexyl 4-methoxyvphe...	306	C17H22O5	1000344-74-4	25
2		Fumaric acid, isohexyl 4-methoxy...	306	C17H22O5	1000344-74-3	14
3		3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	14
4		3-(4-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	350039-84-8	14
5		N(5)-[[3,4-Dichlorophenyl]methyl...	283	C11H11Cl2N5	079318-71-1	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100220\
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Sample : L4199-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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
2-Pentanone, 4-hy...	4.97	3.2	ng	105187	1	6.76	661429	20.0
Pentafluoropropio...	13.77	5.4	ng	403462	5	13.92	1488700	20.0
1,4-Benzenedicarb...	14.54	2.9	ng	217373	5	13.92	1488700	20.0
E-7-Octadecene	15.05	3.6	ng	158828	6	15.35	888543	20.0
Benzo[e]pyrene	15.23	3.1	ng	138495	6	15.35	888543	20.0
Heptadecane, 9-oc...	15.79	3.5	ng	153246	6	15.35	888543	20.0
Octacosanol	15.86	4.0	ng	180015	6	15.35	888543	20.0
unknown16.83	16.83	2.4	ng	104296	6	15.35	888543	20.0
unknown17.33	17.33	3.0	ng	132532	6	15.35	888543	20.0
unknown18.28	18.28	3.4	ng	148724	6	15.35	888543	20.0