

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
 Data File : BF117356.D
 Acq On : 9 Oct 2019 15:45
 Operator : JU
 Sample : K5281-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-062

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-BF091319.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	5.004	493	496	511	rBV	25663	38428	3.52%	0.361%
2	5.428	564	568	590	rBV	685726	823218	75.49%	7.735%
3	6.445	737	741	759	rBV	811536	947777	86.91%	8.906%
4	6.575	759	763	776	rVB	1089353	974834	89.39%	9.160%
5	6.798	798	801	812	rBV	269483	247588	22.70%	2.326%
6	6.957	824	828	840	rBV	772137	730940	67.03%	6.868%
7	7.363	893	897	924	rBV	456665	583906	53.55%	5.487%
8	8.081	1015	1019	1026	rBV	256917	283818	26.03%	2.667%
9	9.157	1198	1202	1218	rBV	1068254	1090489	100.00%	10.246%
10	9.551	1265	1269	1280	rBV	170915	178265	16.35%	1.675%
11	9.833	1313	1317	1330	rBV	394064	368197	33.76%	3.460%
12	10.628	1448	1452	1465	rBV	546217	577098	52.92%	5.423%
13	11.322	1567	1570	1580	rBV2	281986	362827	33.27%	3.409%
14	11.845	1652	1659	1667	rBV2	115325	137195	12.58%	1.289%
15	11.945	1673	1676	1685	rVB3	8968	14201	1.30%	0.133%
16	12.539	1773	1777	1781	rBV	98838	98897	9.07%	0.929%
17	12.627	1790	1792	1801	rBV4	25501	37250	3.42%	0.350%
18	12.769	1811	1816	1819	rBV	76276	91275	8.37%	0.858%
19	12.904	1835	1839	1847	rBV	886583	784282	71.92%	7.369%
20	13.216	1886	1892	1893	rBV6	7132	13316	1.22%	0.125%
21	13.398	1921	1923	1928	rVB	16011	16307	1.50%	0.153%
22	13.469	1931	1935	1940	rBV5	16511	24290	2.23%	0.228%
23	13.798	1987	1991	2001	rVB4	114162	175826	16.12%	1.652%
24	13.968	2015	2020	2023	rBV2	261566	303029	27.79%	2.847%
25	14.116	2041	2045	2048	rBV	71762	72230	6.62%	0.679%
26	14.421	2093	2097	2105	rVB	129239	157834	14.47%	1.483%
27	14.721	2142	2148	2152	rBV	168679	178335	16.35%	1.676%
28	14.792	2157	2160	2165	rVB	58962	58541	5.37%	0.550%
29	14.857	2168	2171	2173	rBV3	16359	20310	1.86%	0.191%
30	15.004	2193	2196	2199	rBV2	36311	49975	4.58%	0.470%
31	15.045	2199	2203	2208	rVB	169556	205097	18.81%	1.927%
32	15.304	2244	2247	2252	rVB2	28171	34949	3.20%	0.328%
33	15.368	2254	2258	2262	rVV	24982	36110	3.31%	0.339%
34	15.421	2262	2267	2277	rVB2	263666	444694	40.78%	4.178%

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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	15.610	2295	2299	2304	rBV6	14095	23710	2.17%	0.223%
36	15.833	2332	2337	2342	rVB	91702	138672	12.72%	1.303%
37	15.898	2344	2348	2349	rBV4	22300	27297	2.50%	0.256%
38	16.004	2364	2366	2370	rVB4	15105	17582	1.61%	0.165%
39	16.104	2380	2383	2390	rVB2	20460	39594	3.63%	0.372%
40	16.321	2415	2420	2425	rBV2	37490	67375	6.18%	0.633%
41	16.886	2511	2516	2523	rVB6	27923	58869	5.40%	0.553%
42	17.415	2601	2606	2614	rVB10	18685	52372	4.80%	0.492%
43	18.392	2768	2772	2781	rVB10	24298	55775	5.11%	0.524%

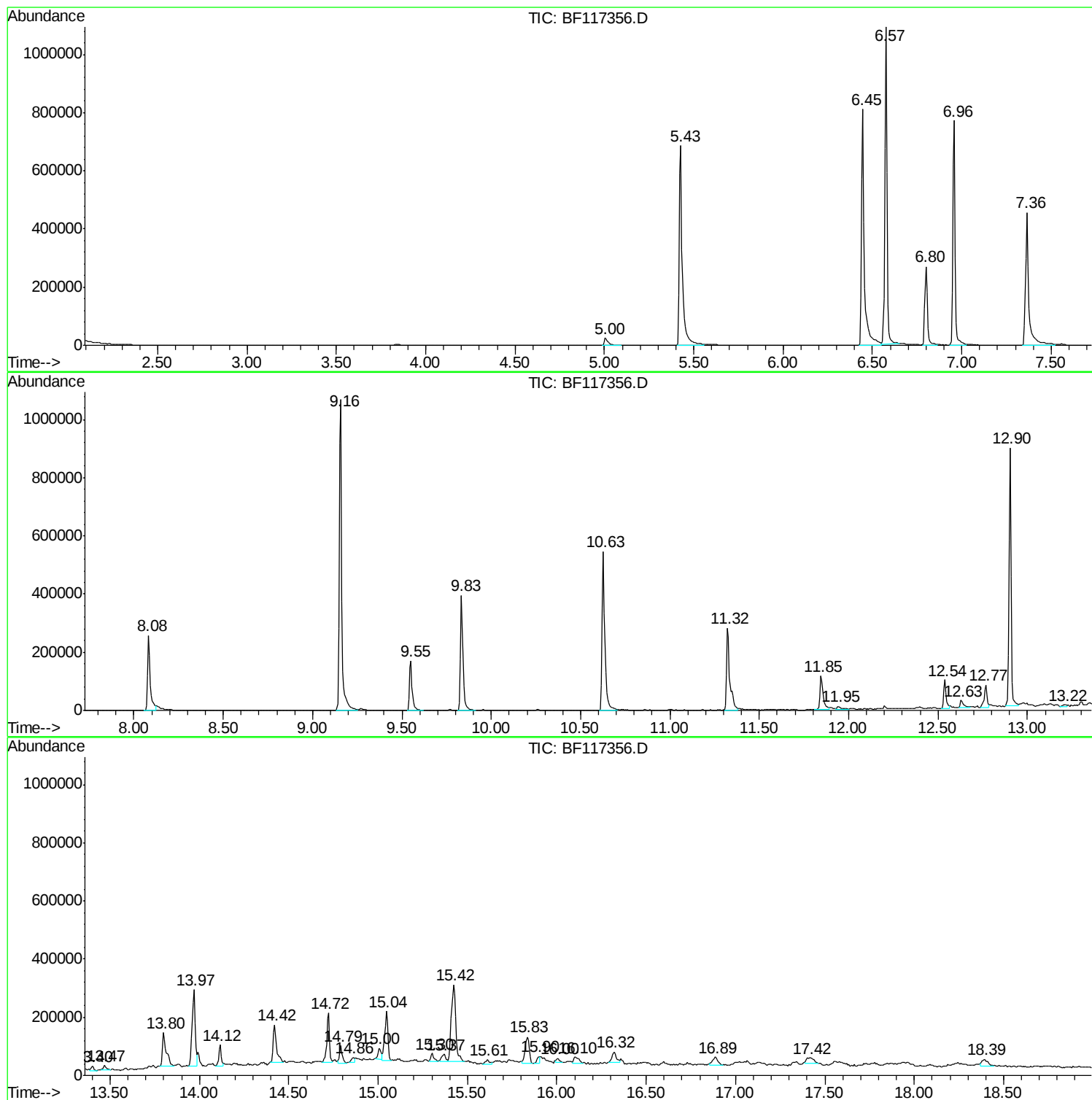
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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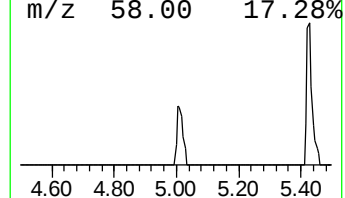
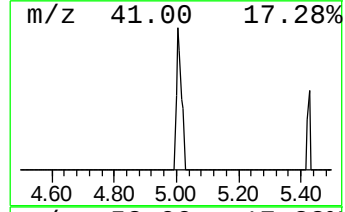
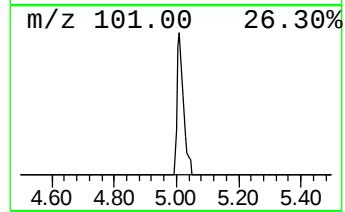
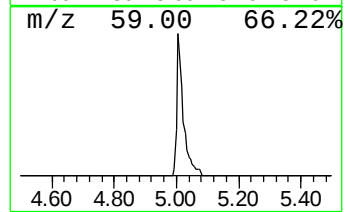
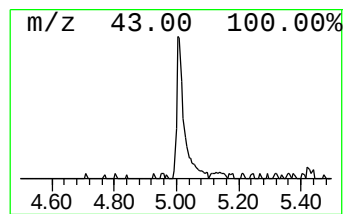
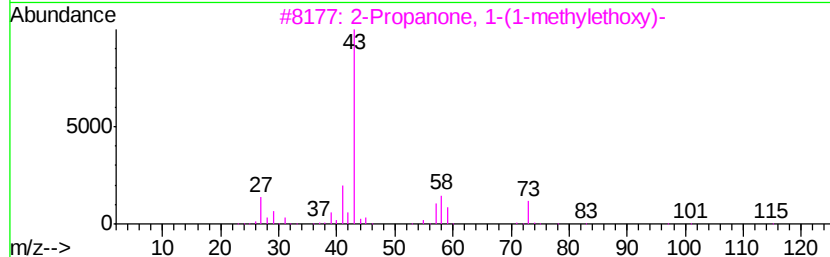
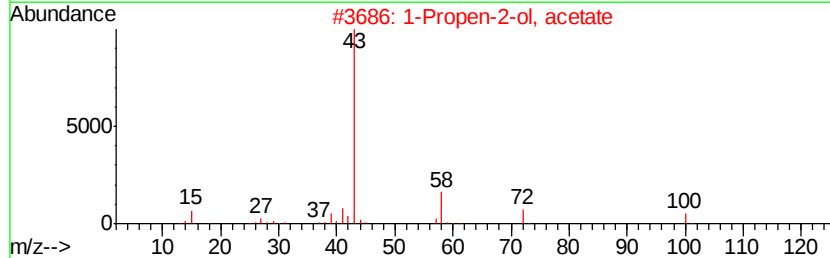
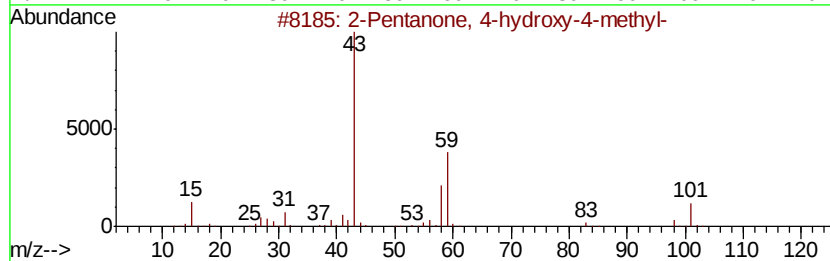
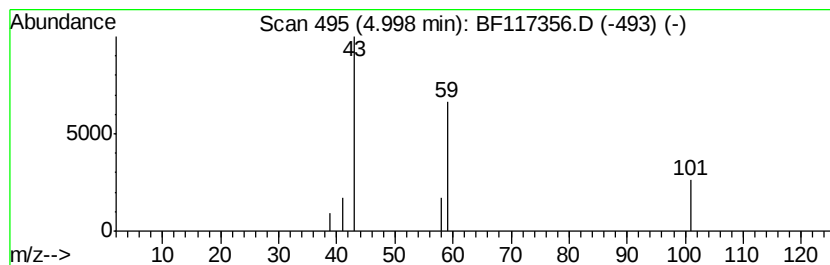
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.10 ng	38428	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7



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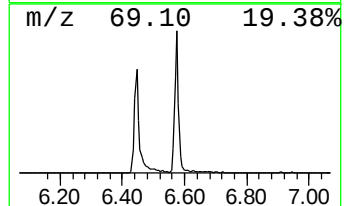
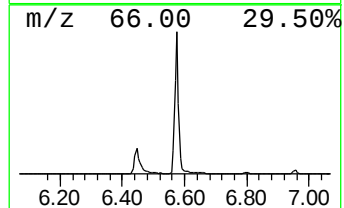
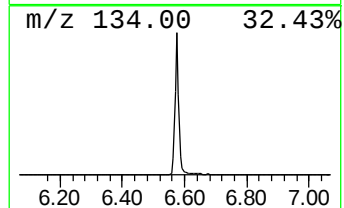
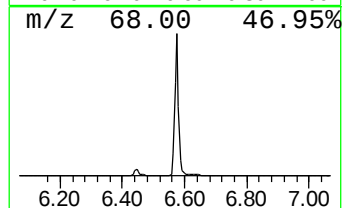
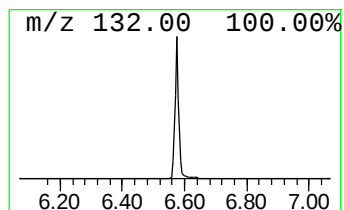
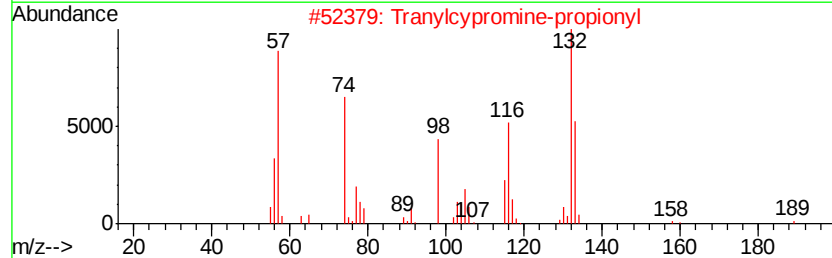
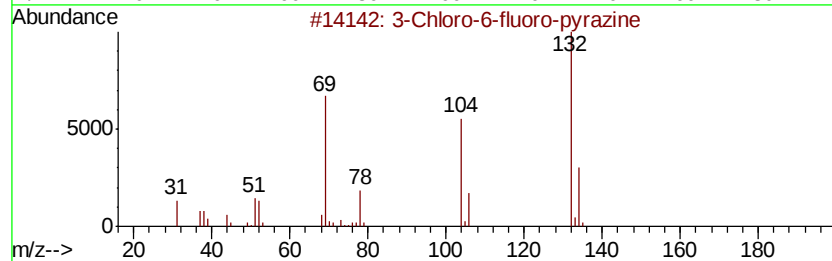
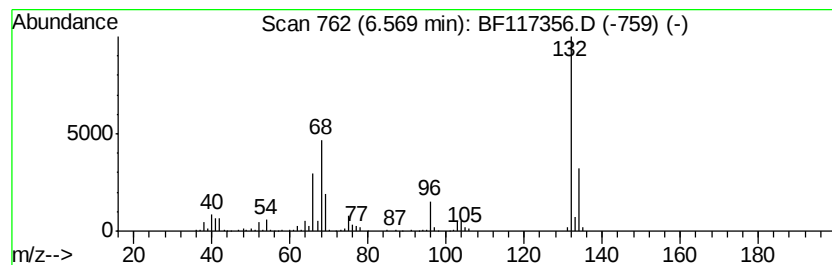
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.75 ng	974834	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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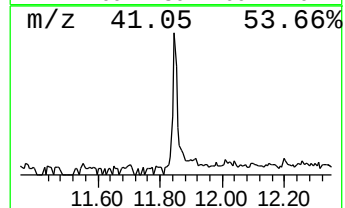
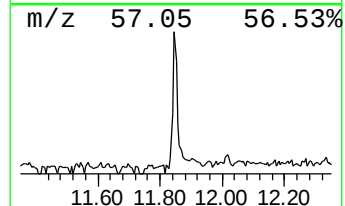
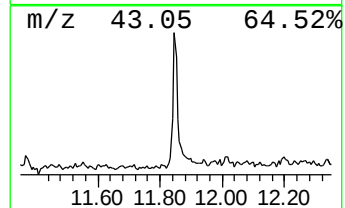
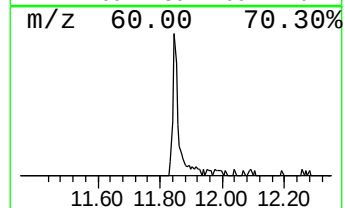
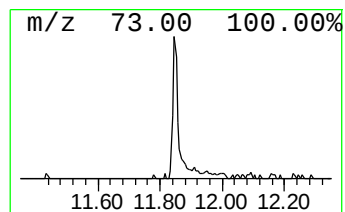
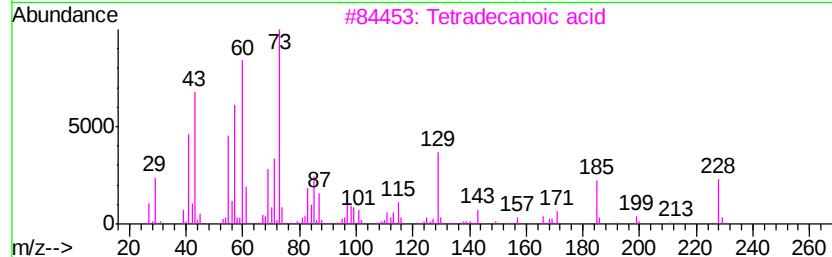
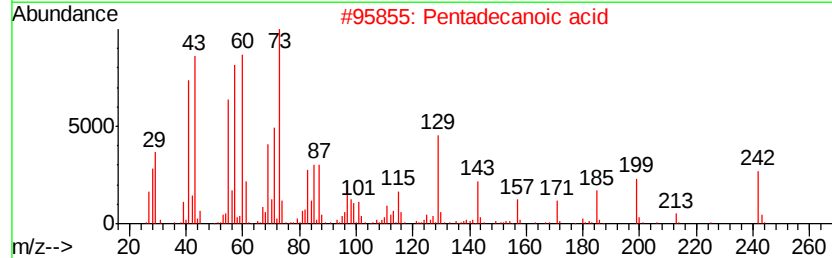
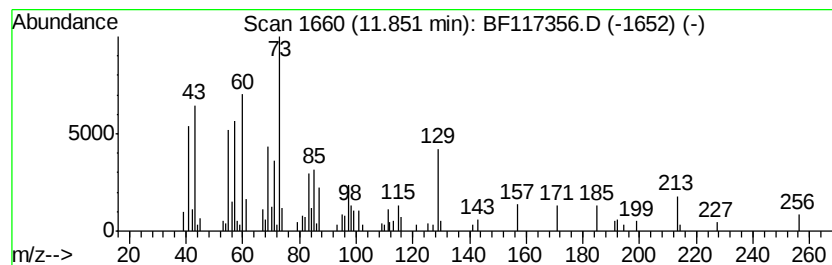
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	7.56 ng	137195	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	18
5		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	18



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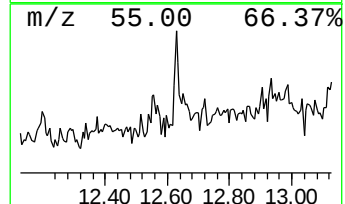
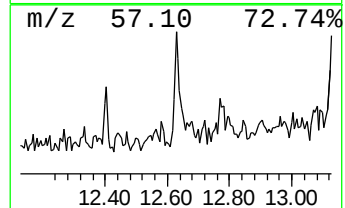
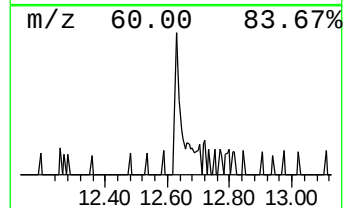
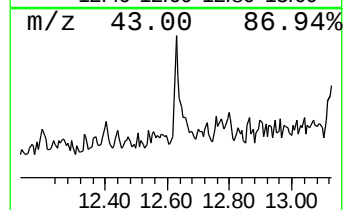
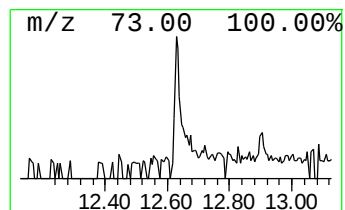
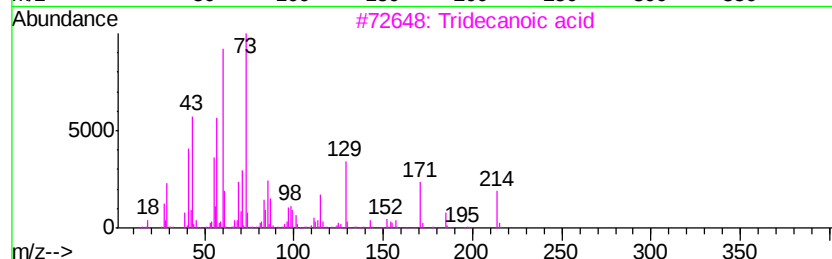
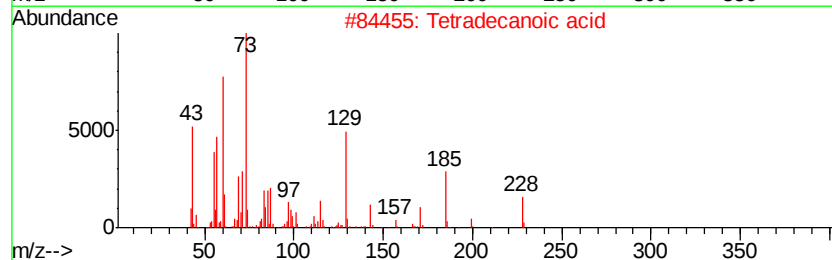
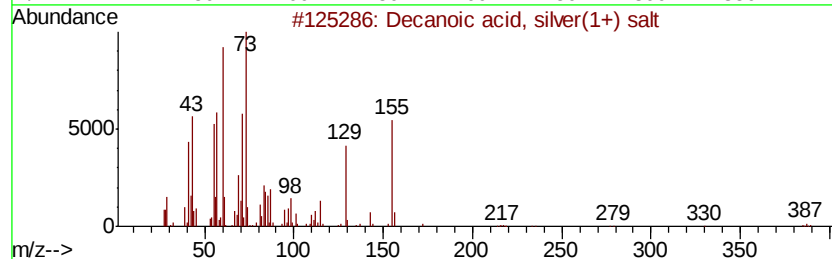
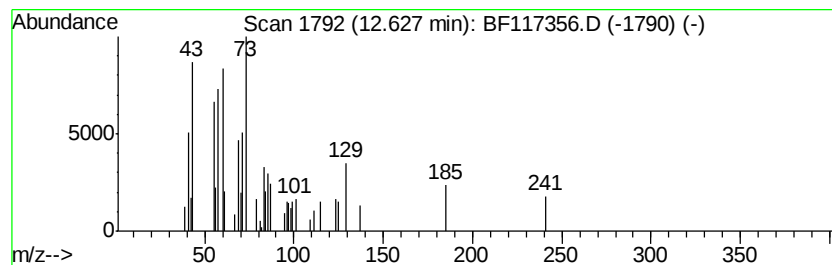
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	2.05 ng	37250	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	72
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3		Tridecanoic acid	214	C13H26O2	000638-53-9	59
4		Dodecanoic acid	200	C12H24O2	000143-07-7	53
5		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	47



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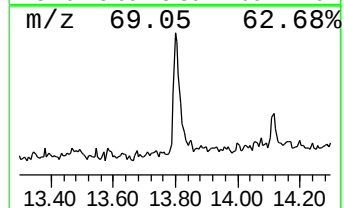
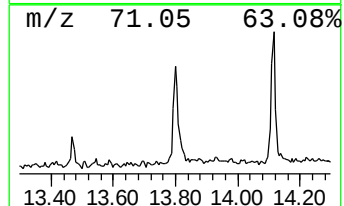
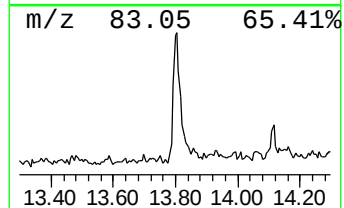
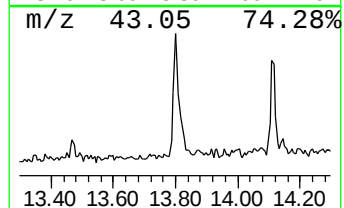
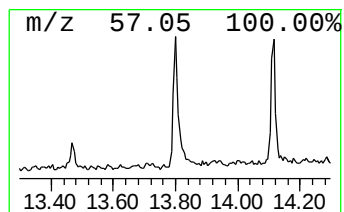
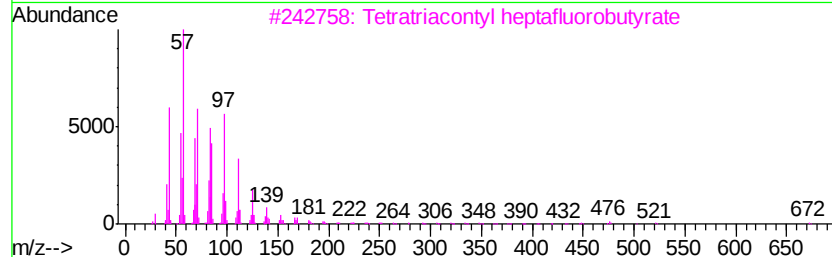
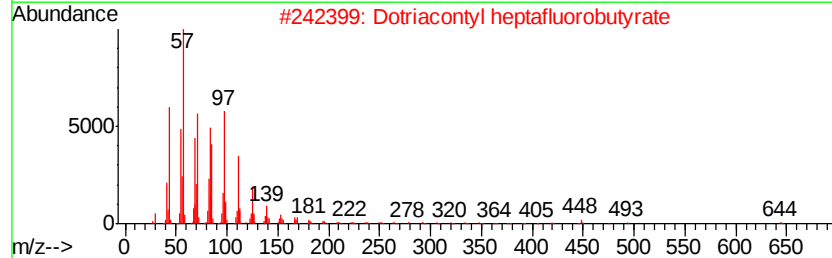
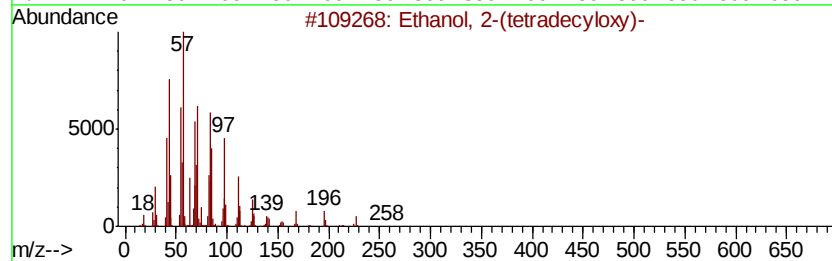
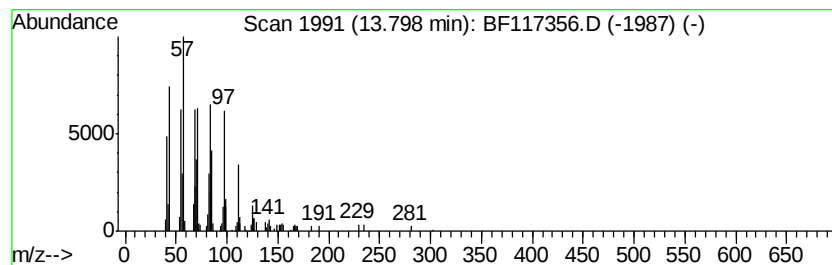
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	11.60 ng	175826	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	90
3		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	87
4		Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	87
5		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
Operator : JU
Sample : K5281-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-PS-01-062

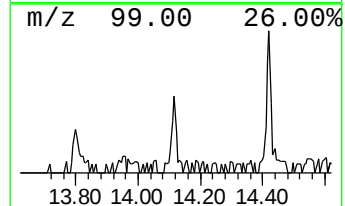
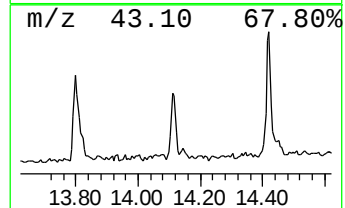
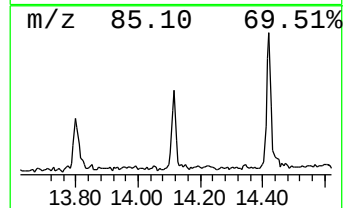
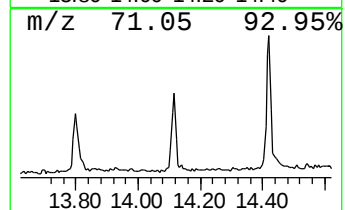
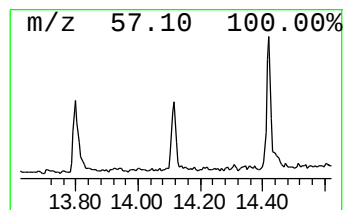
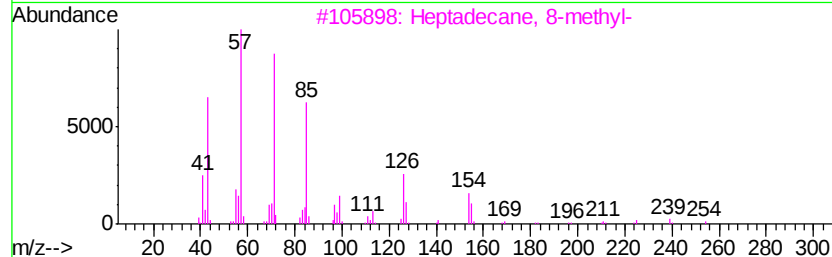
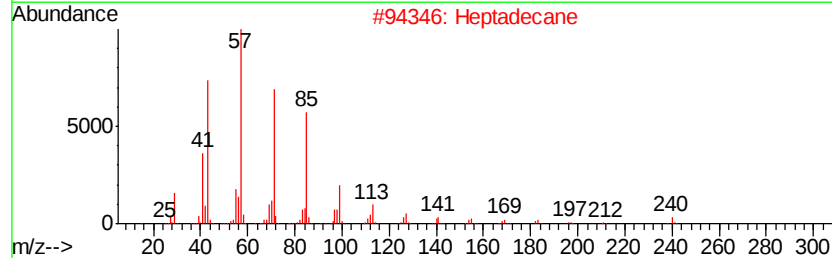
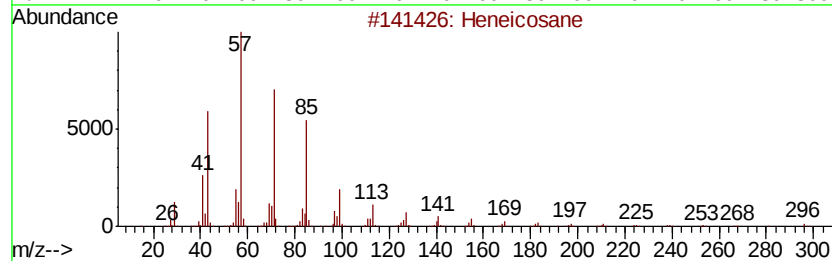
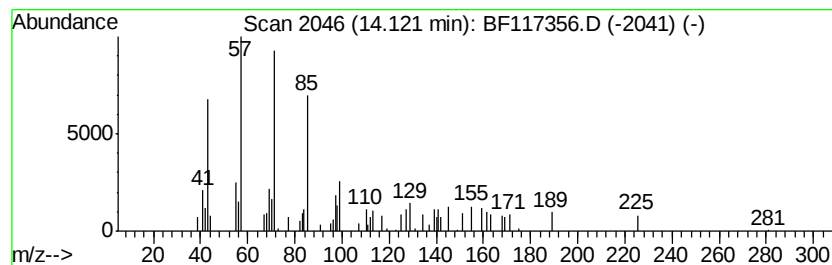
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	4.77 ng	72230	Chrysene-d12	13.97

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	Heptadecane, 8-methyl-		254	C18H38	013287-23-5	86
4	Octacosane		394	C28H58	000630-02-4	83
5	Hexacosane		366	C26H54	000630-01-3	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
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Misc :
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ClientSampleId :
FK-PS-01-062

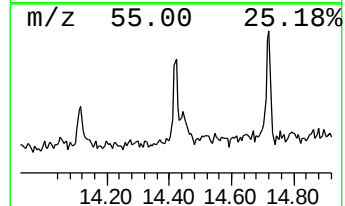
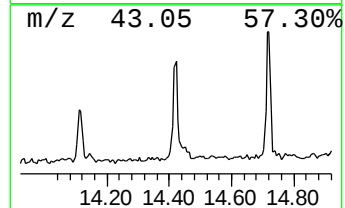
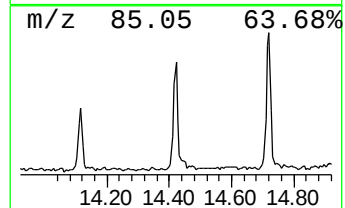
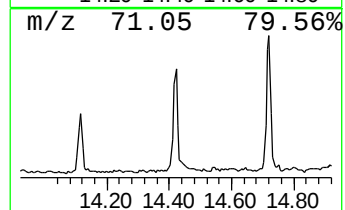
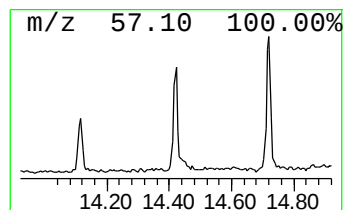
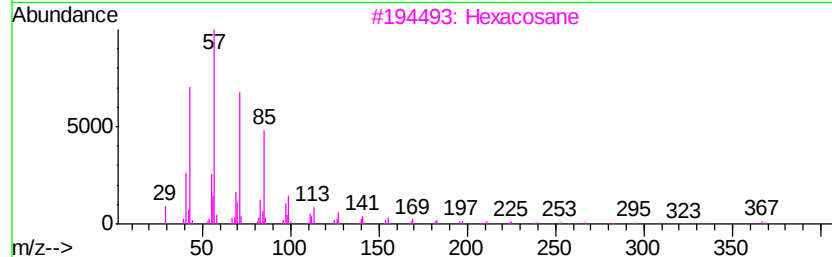
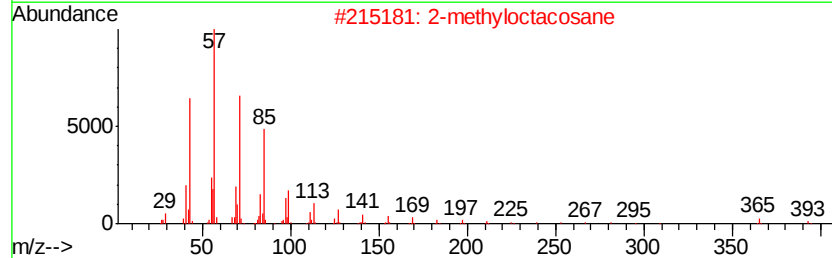
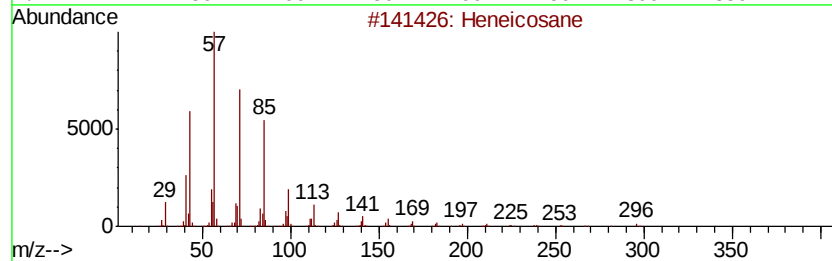
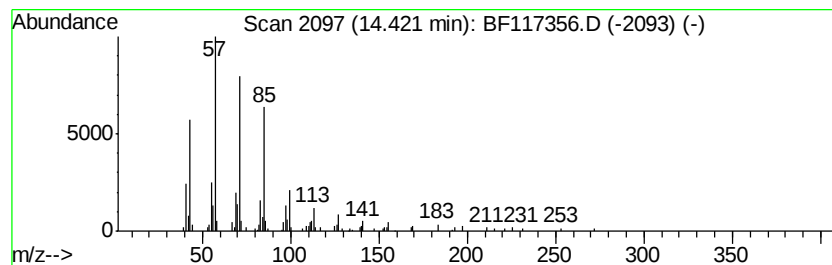
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	10.42 ng	157834	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptadecane	240	C17H36	000629-78-7	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
Operator : JU
Sample : K5281-01
Misc :
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Instrument :
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ClientSampleId :
FK-PS-01-062

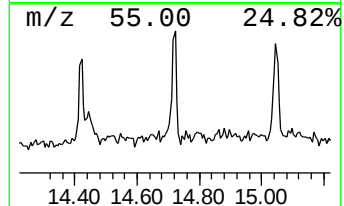
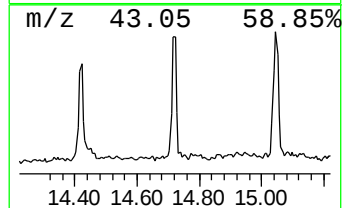
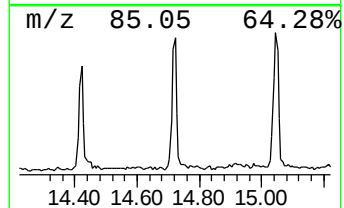
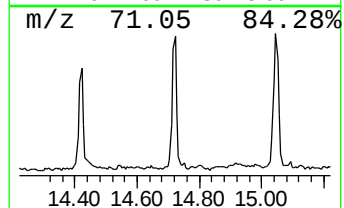
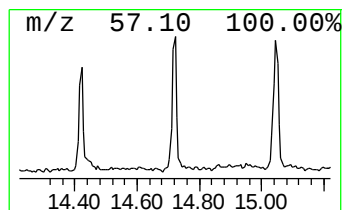
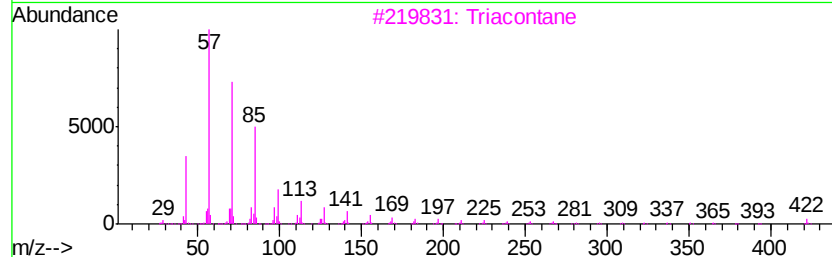
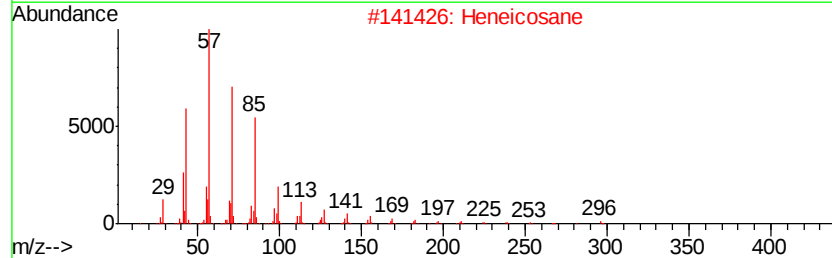
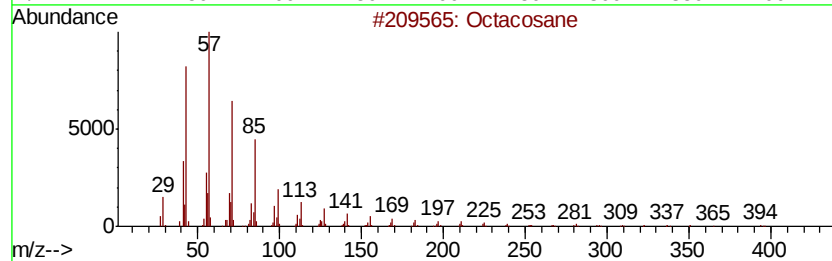
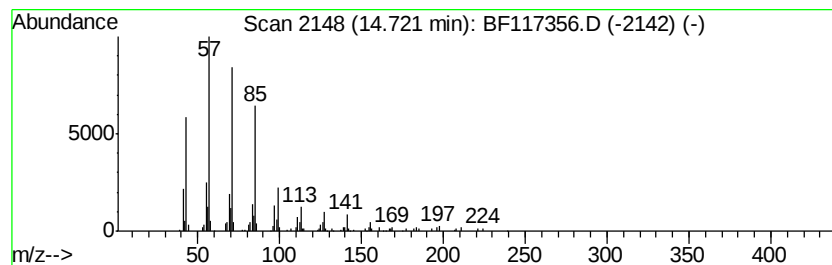
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	8.02 ng	178335	Perylene-d12	15.43

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		Triacontane	422	C30H62	000638-68-6	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
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Misc :
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Instrument :
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ClientSampleId :
FK-PS-01-062

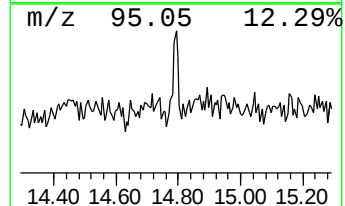
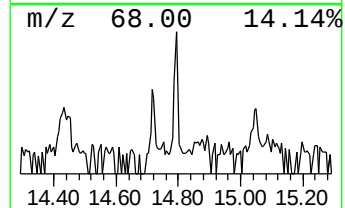
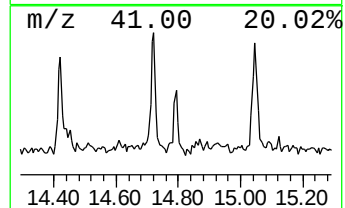
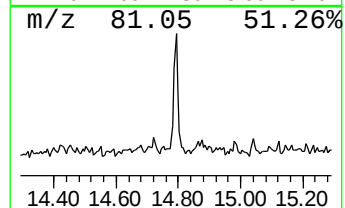
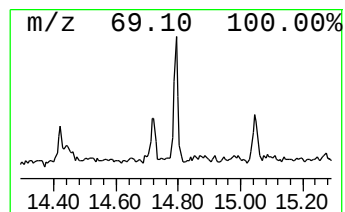
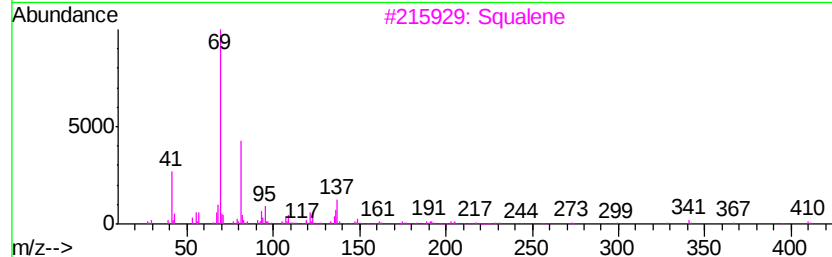
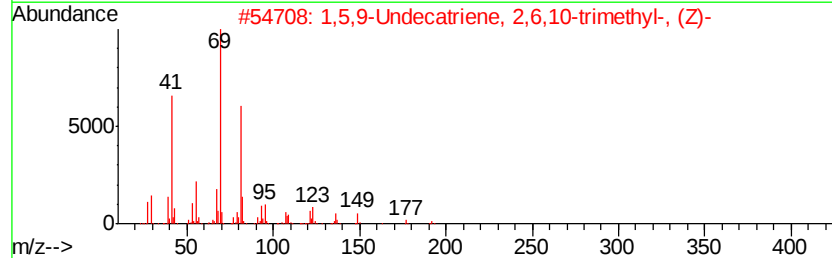
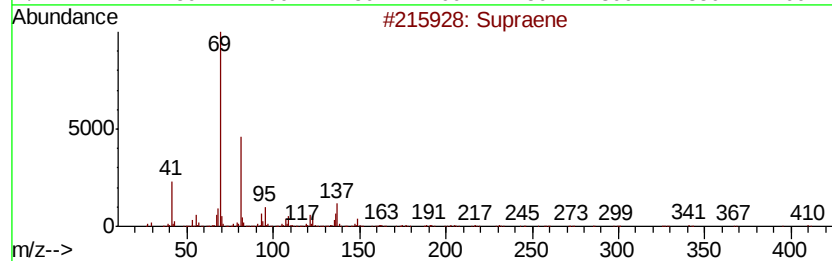
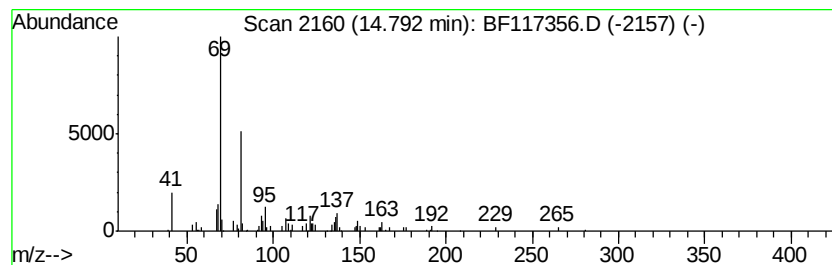
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.63 ng	58541	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	86
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
3		Squalene	410	C30H50	000111-02-4	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
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Misc :
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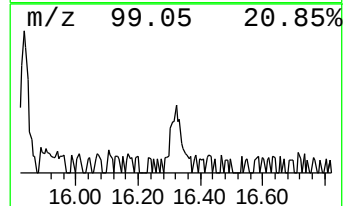
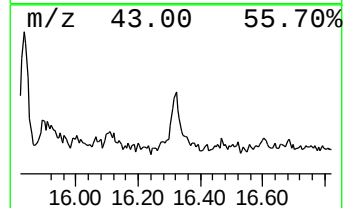
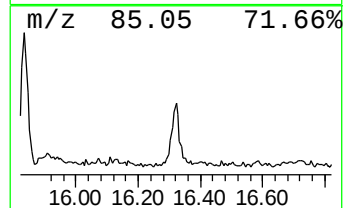
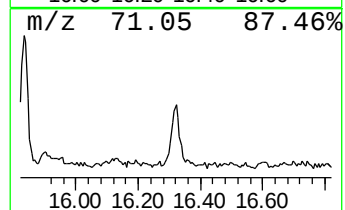
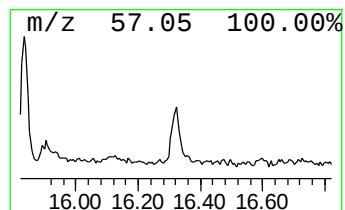
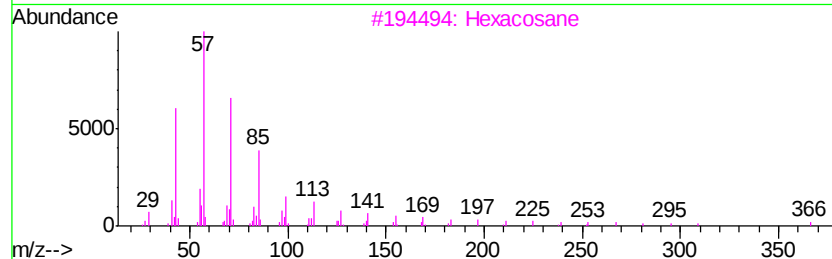
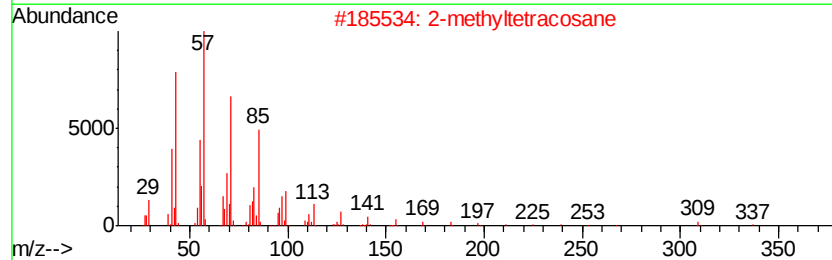
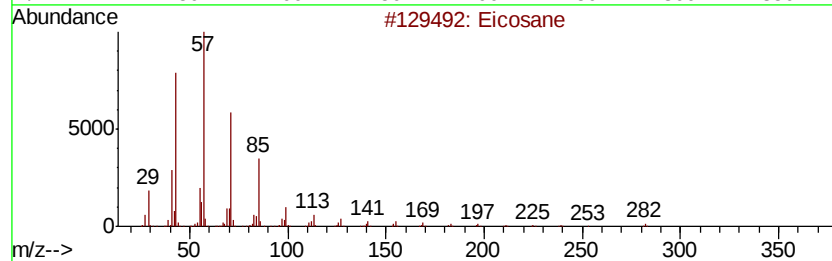
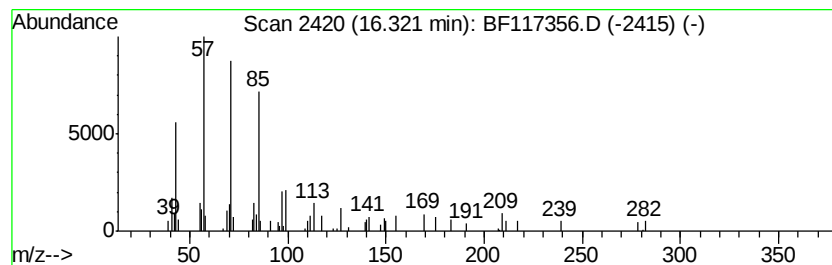
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	3.03 ng	67375	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		2-methyltetracosane	352	C25H52	1000376-72-6	86
3		Hexacosane	366	C26H54	000630-01-3	83
4		Heneicosane	296	C21H44	000629-94-7	80
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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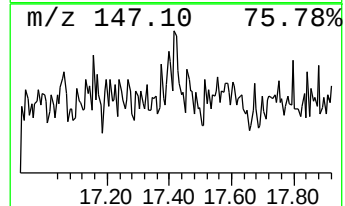
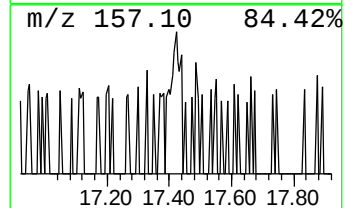
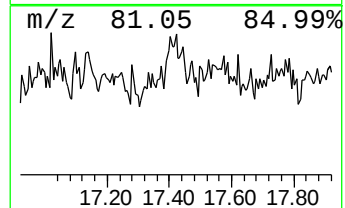
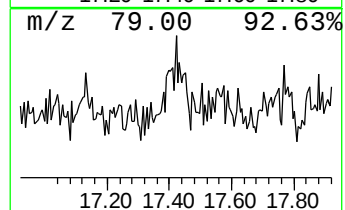
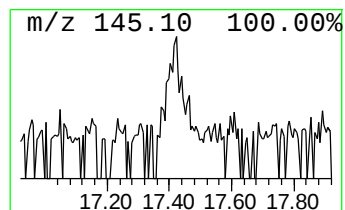
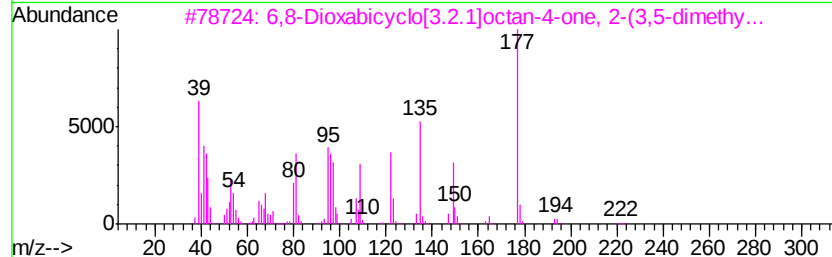
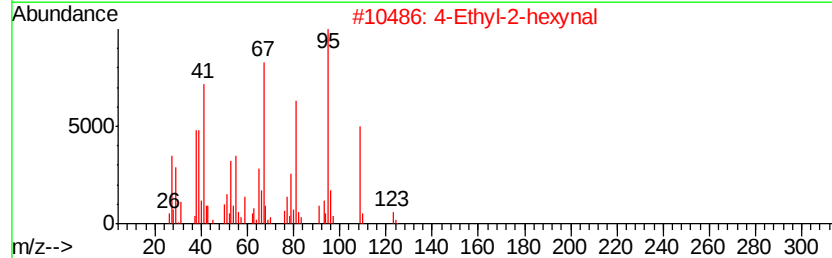
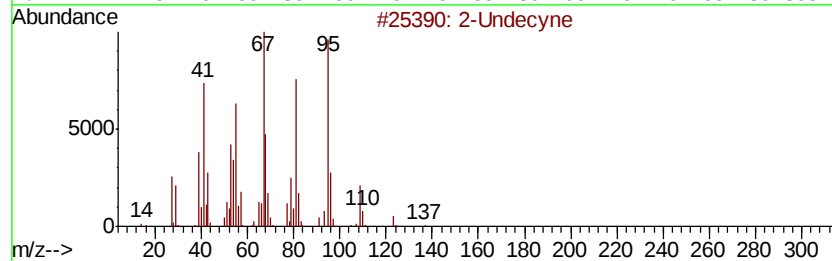
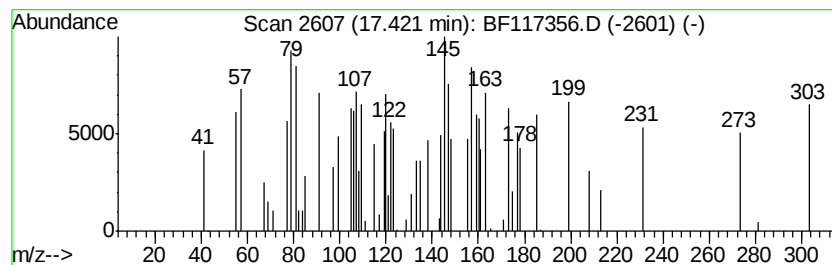
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.42 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	2.36 ng	52372	Perylene-d12	15.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		Undecyne	152	C11H20	060212-29-5	22
2	4		Ethyl-2-hexynal	124	C8H12O	071932-97-3	22
3	6,8		Dioxabicyclo[3.2.1]octan-4-one	222	C11H14N2O3	1000362-38-3	22
4	1		Cyclohexen, 1-cyano-4-isopropenyl-	147	C10H13N	1000126-45-8	12
5			Thiazolidin-4-one, 3-furfuryl-2-(1-methyl-1H-imidazol-2-ylmethyl)-	213	C8H7N2O2S2	004703-95-1	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100919\
Data File : BF117356.D
Acq On : 9 Oct 2019 15:45
Operator : JU
Sample : K5281-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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ClientSampleId :
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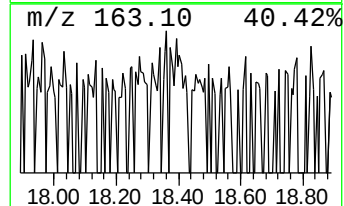
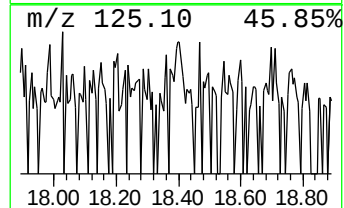
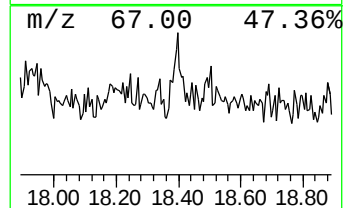
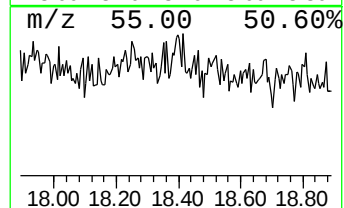
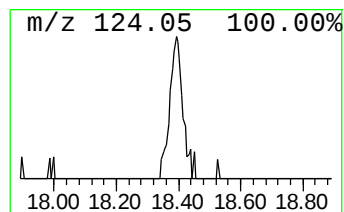
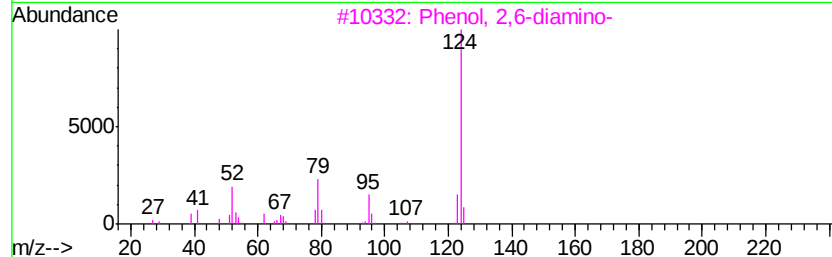
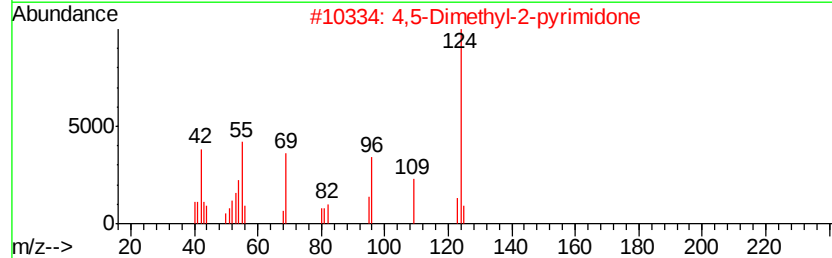
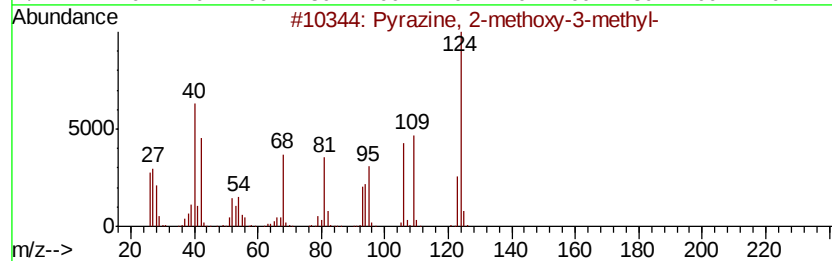
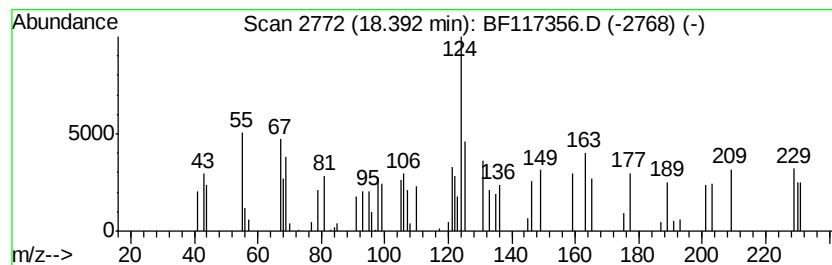
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.39 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.51 ng	55775	Perylene-d12	15.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	002847-30-5	11
2			4,5-Dimethyl-2-pyrimidone	124	C6H8N2O	034939-17-8	10
3			Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	10
4			2,3-Diaminophenol	124	C6H8N2O	059649-56-8	10
5			4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100919\
 Data File : BF117356.D
 Acq On : 9 Oct 2019 15:45
 Operator : JU
 Sample : K5281-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-062

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
2-Pentanone, 4-hy...	5.00	3.1 ng		38428	1	6.80	247588	20.0
unknown6.57	6.57	78.8 ng		974834	1	6.80	247588	20.0
n-Hexadecanoic acid	11.85	7.6 ng		137195	4	11.32	362827	20.0
Decanoic acid, si...	12.63	2.0 ng		37250	4	11.32	362827	20.0
Ethanol, 2-(tetra...	13.80	11.6 ng		175826	5	13.97	303029	20.0
Heneicosane	14.12	4.8 ng		72230	5	13.97	303029	20.0
2-methyloctacosane	14.42	10.4 ng		157834	5	13.97	303029	20.0
Octacosane	14.72	8.0 ng		178335	6	15.43	444694	20.0
Supraene	14.79	2.6 ng		58541	6	15.43	444694	20.0
Eicosane	16.32	3.0 ng		67375	6	15.43	444694	20.0
unknown17.42	17.42	2.4 ng		52372	6	15.43	444694	20.0
unknown18.39	18.39	2.5 ng		55775	6	15.43	444694	20.0