

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082819\
 Data File : BF116637.D
 Acq On : 29 Aug 2019 1:29
 Operator : HP/JU
 Sample : K4576-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200034-RBR-200036

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-BF082819.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	2.146	3	10	15	rBV	1126545	1456606	69.39%	7.811%
2	5.487	573	578	581	rBV	2266022	2099179	100.00%	11.257%
3	6.492	744	749	754	rBV	1799657	1889067	89.99%	10.130%
4	6.634	769	773	777	rBV	2016107	1874615	89.30%	10.053%
5	6.863	809	812	816	rBB	507799	415025	19.77%	2.226%
6	7.022	835	839	842	rBV	1746362	1390414	66.24%	7.456%
7	7.422	902	907	910	rBV	1312087	1133846	54.01%	6.080%
8	8.145	1026	1030	1033	rBV	695049	551363	26.27%	2.957%
9	8.886	1152	1156	1166	rVB	12723	24502	1.17%	0.131%
10	9.216	1208	1212	1216	rBV	2353642	2070916	98.65%	11.105%
11	9.604	1275	1278	1282	rBV	266089	212628	10.13%	1.140%
12	9.898	1324	1328	1331	rVB	1050003	883046	42.07%	4.735%
13	10.680	1457	1461	1464	rBV	1375967	1140153	54.31%	6.114%
14	11.374	1576	1579	1582	rBV	496428	429230	20.45%	2.302%
15	11.398	1582	1583	1588	rVB	59891	35058	1.67%	0.188%
16	11.904	1665	1669	1673	rBV	176657	149641	7.13%	0.802%
17	12.586	1781	1785	1787	rBV	108481	92123	4.39%	0.494%
18	12.680	1799	1801	1809	rBV	49623	51716	2.46%	0.277%
19	12.810	1818	1823	1826	rBV	74686	72766	3.47%	0.390%
20	12.957	1844	1848	1851	rBV	1360247	1183896	56.40%	6.349%
21	13.851	1996	2000	2009	rBV	192195	219435	10.45%	1.177%
22	14.004	2019	2026	2029	rBV	347334	369867	17.62%	1.983%
23	14.027	2029	2030	2034	rVB	32384	25389	1.21%	0.136%
24	14.174	2052	2055	2060	rVB2	28091	26389	1.26%	0.142%
25	14.480	2104	2107	2112	rBV	53912	55758	2.66%	0.299%
26	14.786	2156	2159	2162	rBV	26581	25237	1.20%	0.135%
27	15.033	2198	2201	2205	rBV	26957	39115	1.86%	0.210%
28	15.121	2212	2216	2219	rBV	44397	60669	2.89%	0.325%
29	15.333	2250	2252	2260	rVB2	23468	31281	1.49%	0.168%
30	15.462	2269	2274	2278	rBV	261792	307175	14.63%	1.647%
31	15.498	2278	2280	2288	rVB2	38518	47544	2.26%	0.255%
32	15.939	2350	2355	2359	rBV3	34390	56412	2.69%	0.303%
33	15.980	2359	2362	2371	rVB2	52299	93808	4.47%	0.503%
34	16.439	2435	2440	2445	rBV6	17270	32481	1.55%	0.174%

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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	17.039	2537	2542	2547	rBV5	11308	25838	1.23%	0.139%
36	17.515	2617	2623	2630	rBV9	21288	43901	2.09%	0.235%
37	18.545	2792	2798	2805	rVB6	13721	31787	1.51%	0.170%

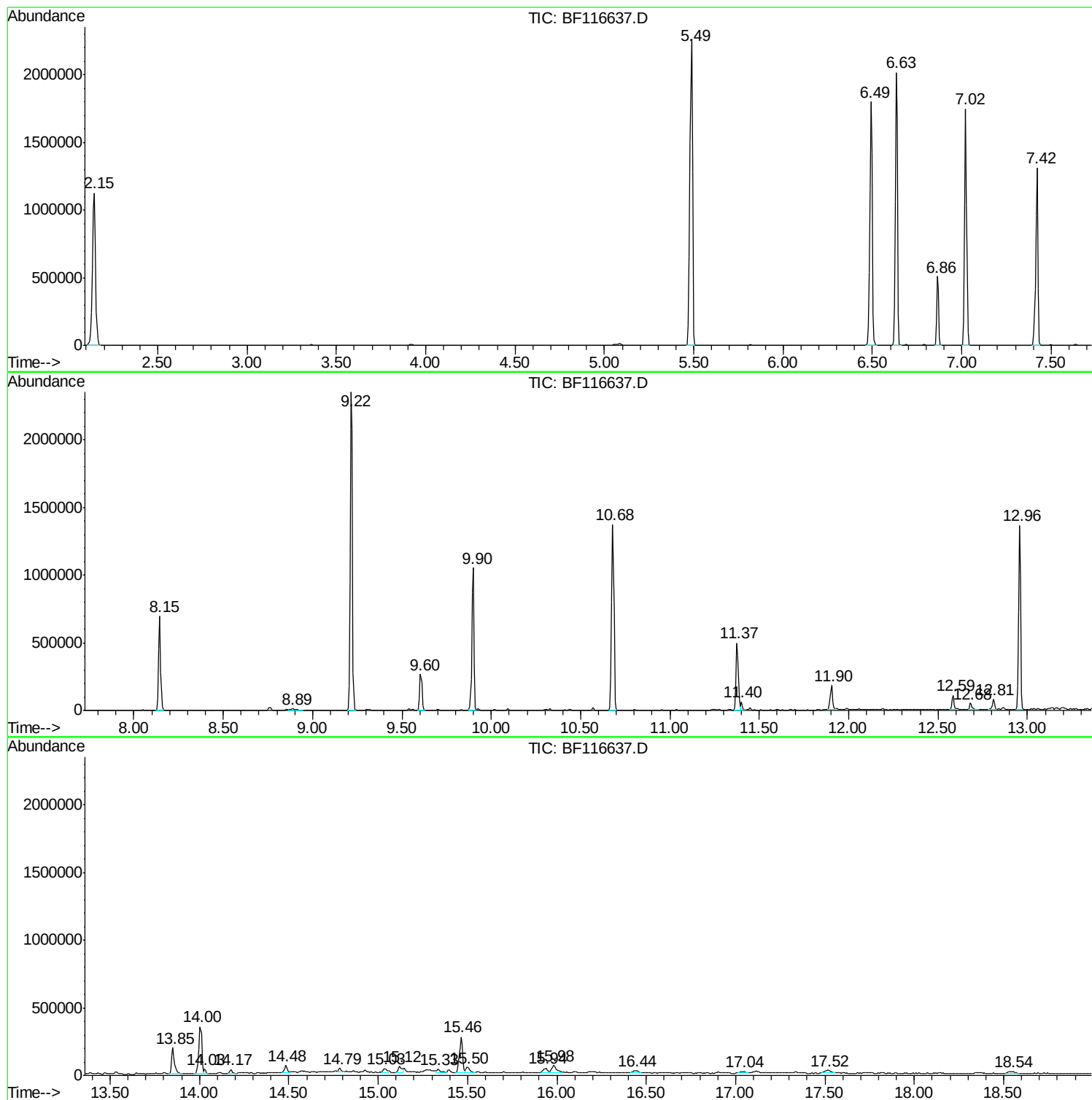
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF082819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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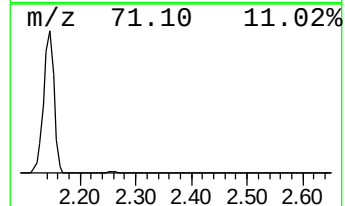
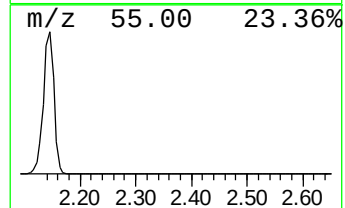
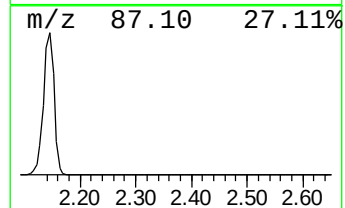
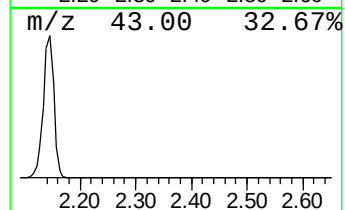
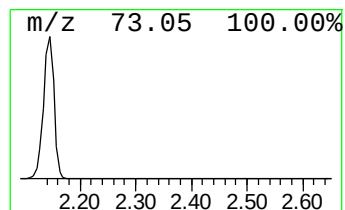
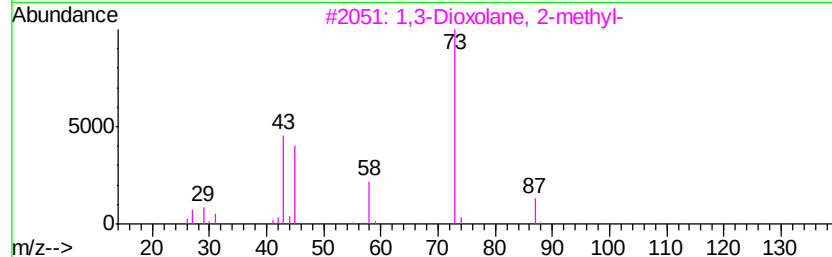
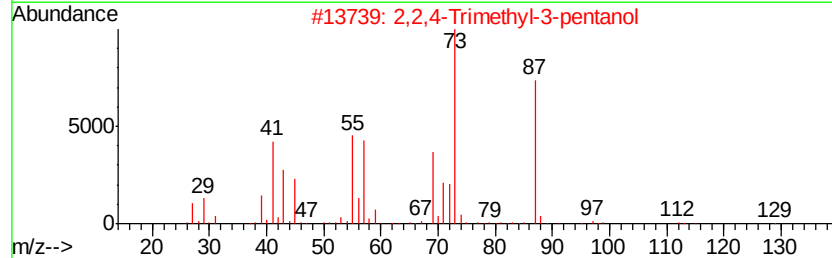
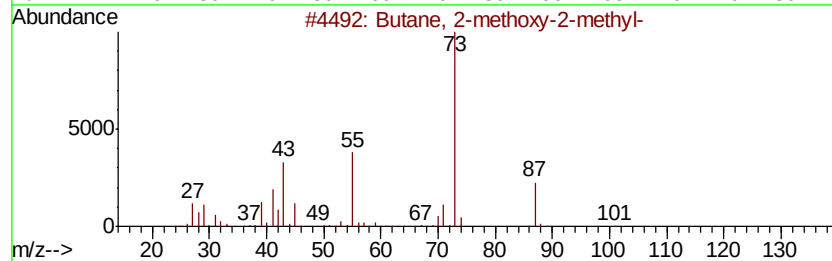
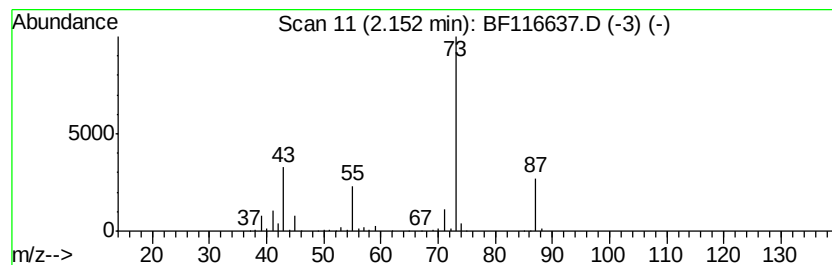
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	70.19 ng	1456610	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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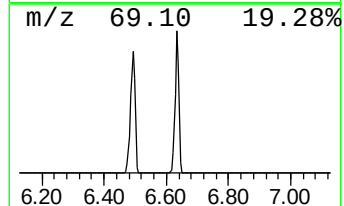
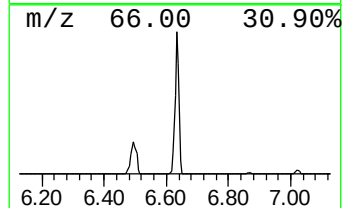
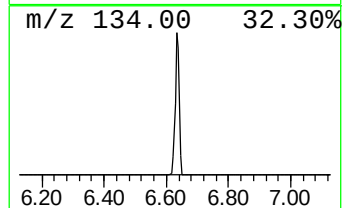
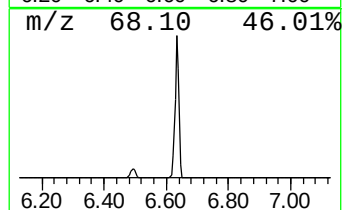
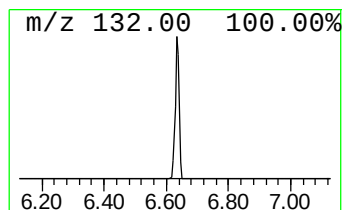
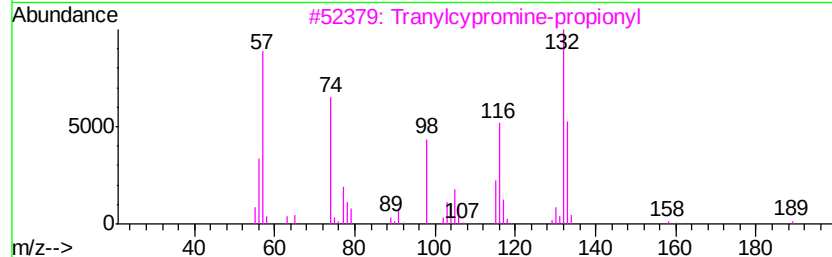
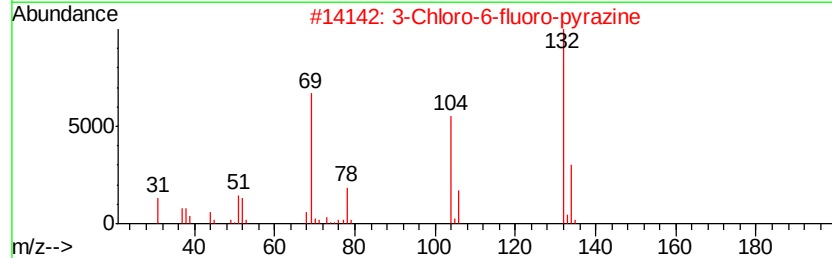
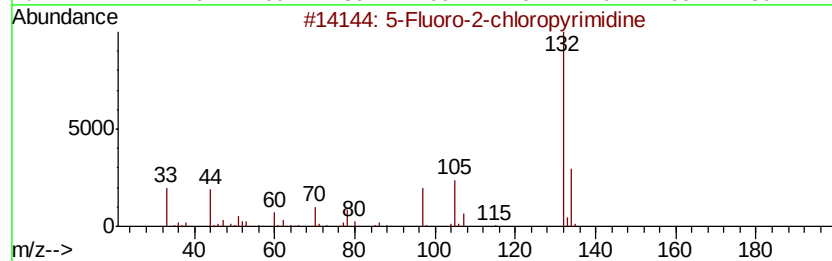
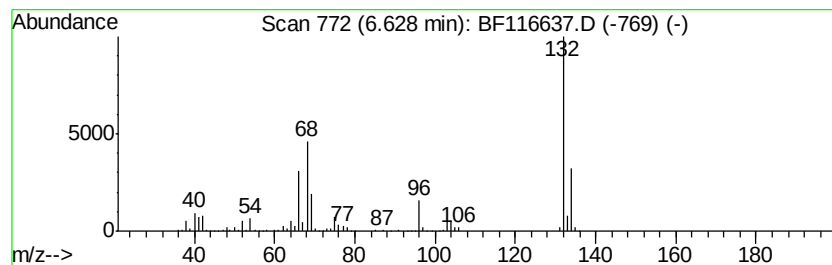
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	90.34 ng	1874620	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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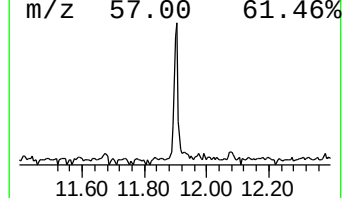
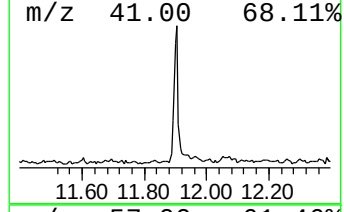
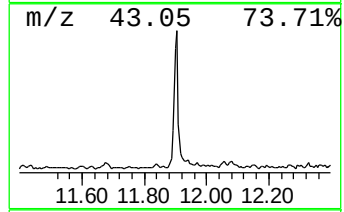
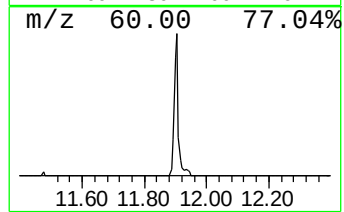
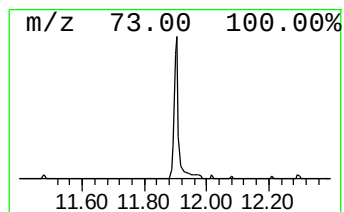
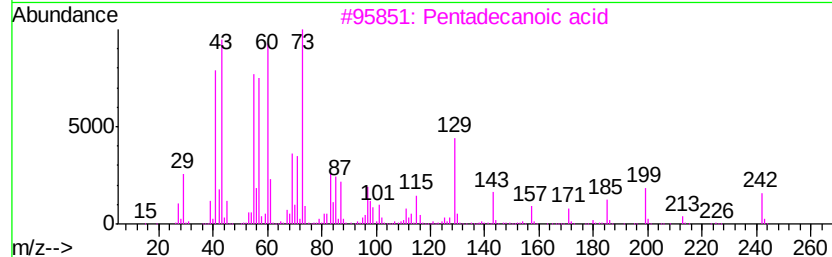
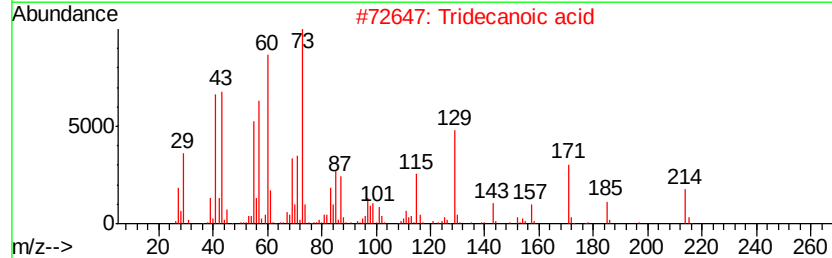
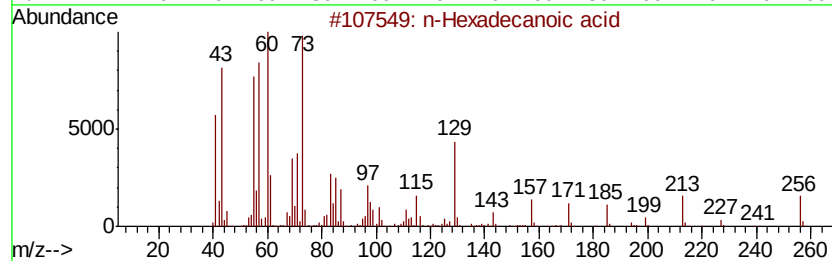
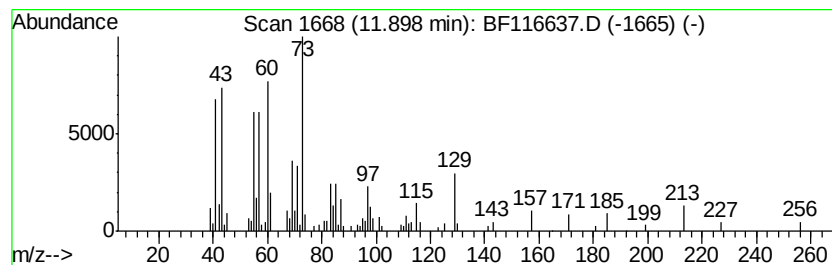
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	6.97 ng	149641	Phenanthrene-d10	11.37

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		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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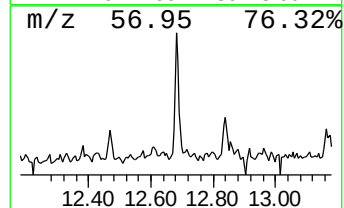
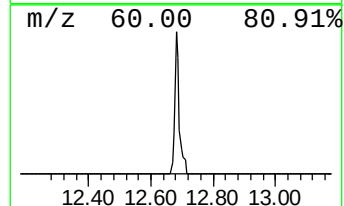
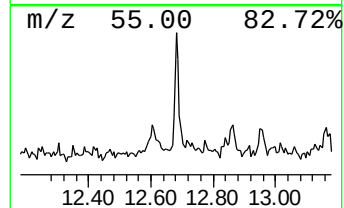
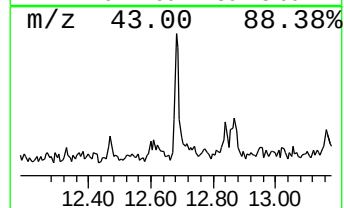
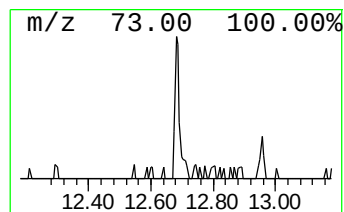
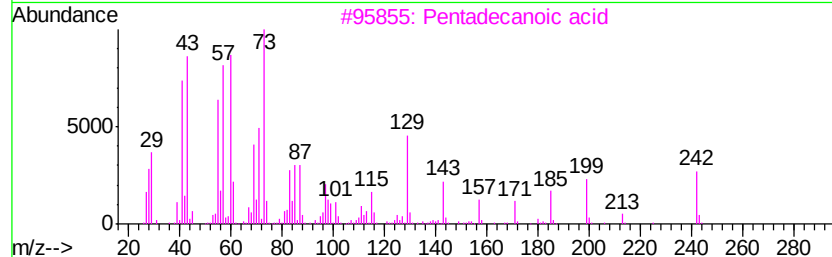
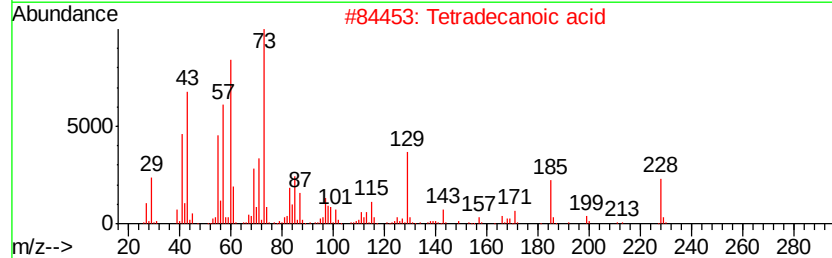
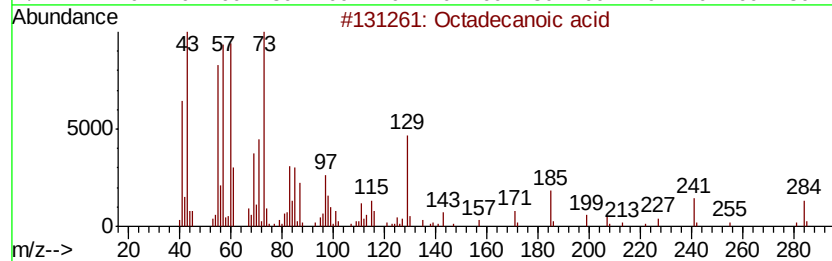
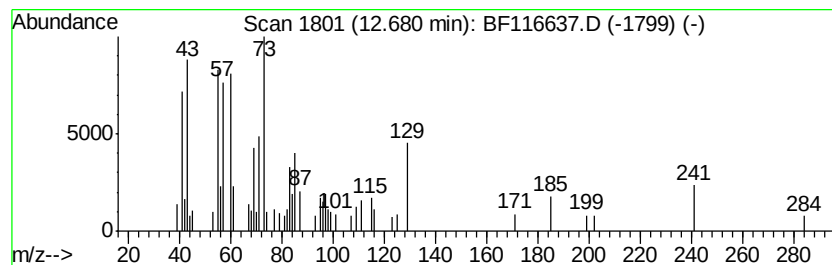
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.41 ng	51716	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



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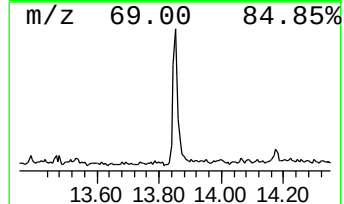
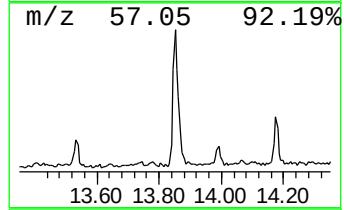
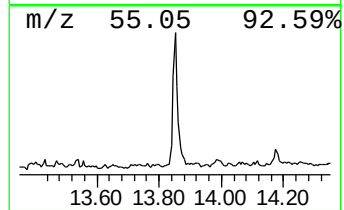
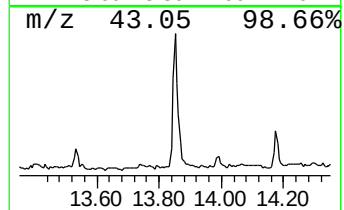
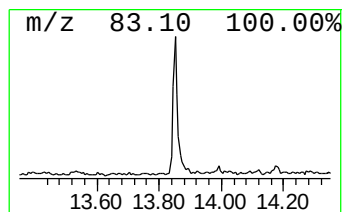
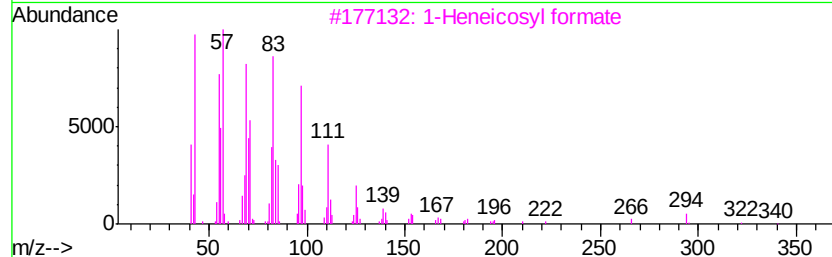
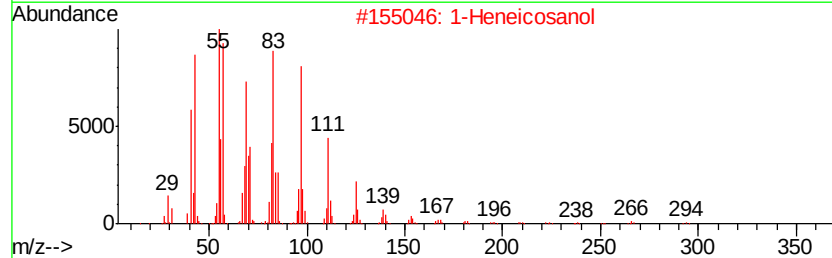
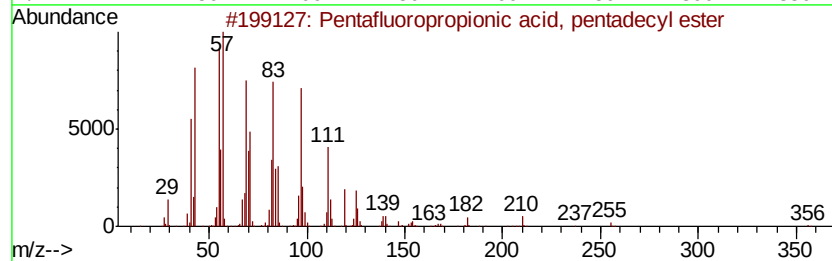
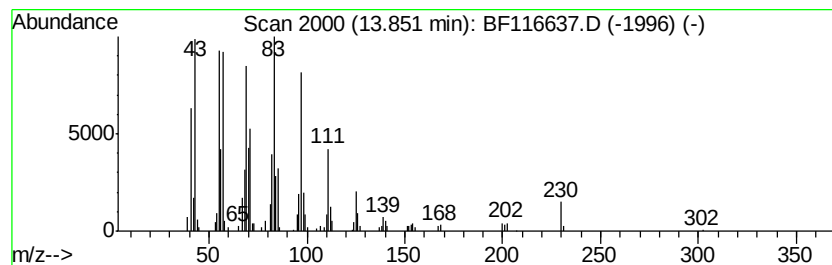
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	11.87 ng	219435	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5		Behenic alcohol	326	C22H46O	000661-19-8	95



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
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Acq On : 29 Aug 2019 1:29
Operator : HP/JU
Sample : K4576-02
Misc :
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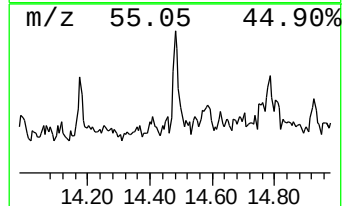
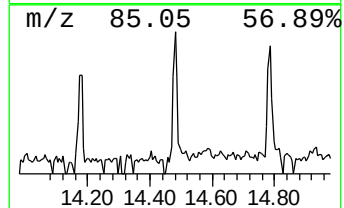
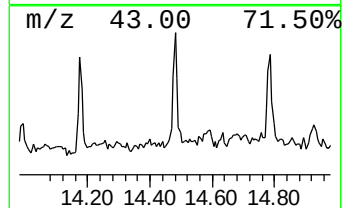
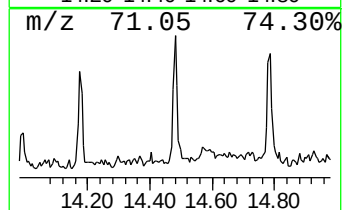
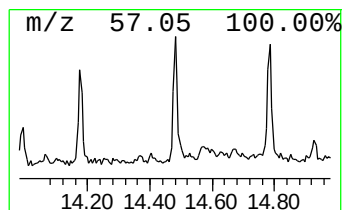
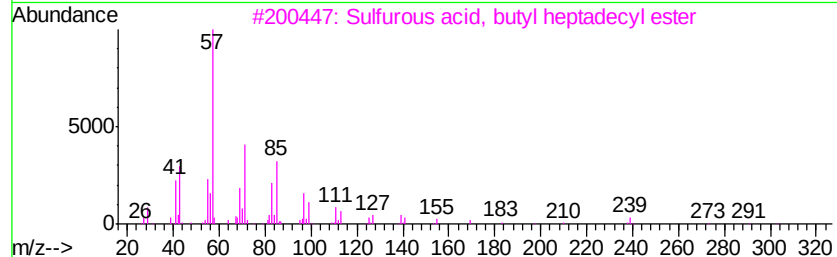
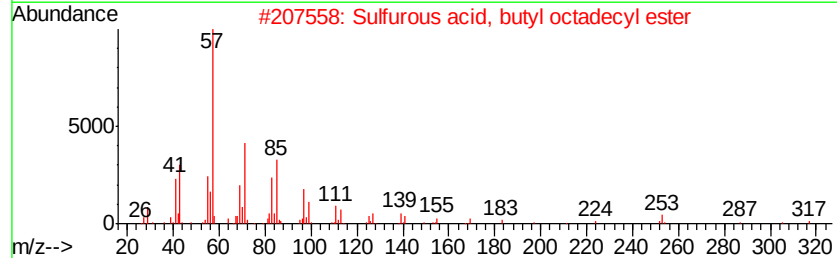
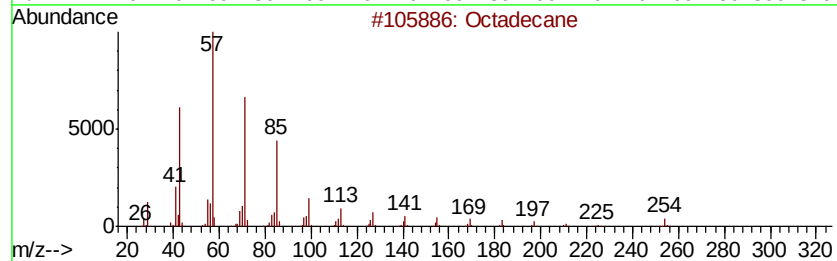
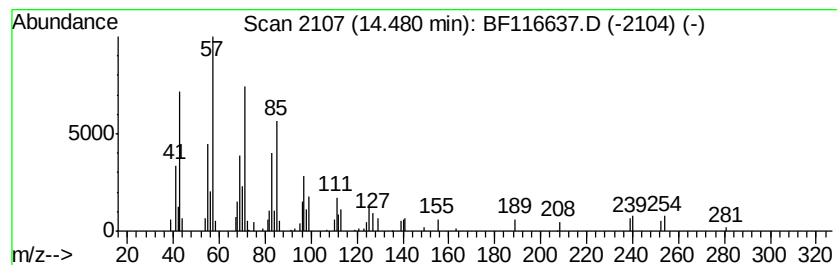
Instrument :
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ClientSampleId :
RBR-200034-RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF082819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	3.02 ng	55758	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	91
2	Sulfurous acid, butyl octadecyl ...	390 C22H46O3S	1000309-18-5	87
3	Sulfurous acid, butyl heptadecyl...	376 C21H44O3S	1000309-18-4	80
4	Sulfurous acid, octadecyl 2-prop...	376 C21H44O3S	1000309-12-7	80
5	Sulfurous acid, butyl hexadecyl ...	362 C20H42O3S	1000309-18-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
Data File : BF116637.D
Acq On : 29 Aug 2019 1:29
Operator : HP/JU
Sample : K4576-02
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Instrument :
BNA_F
ClientSampleId :
RBR-200034-RBR-200036

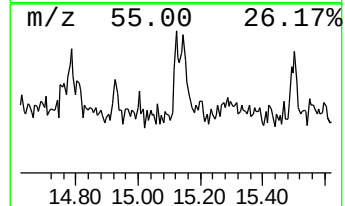
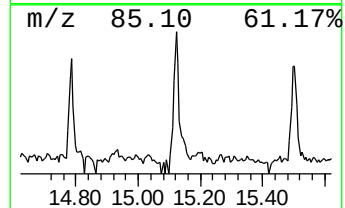
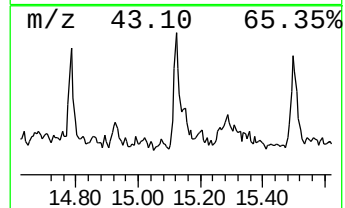
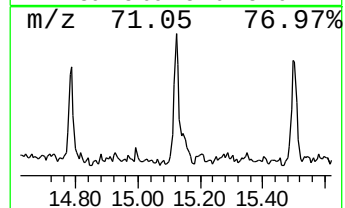
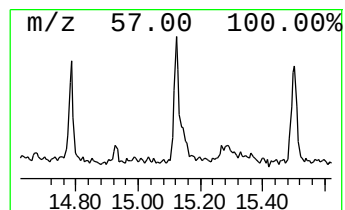
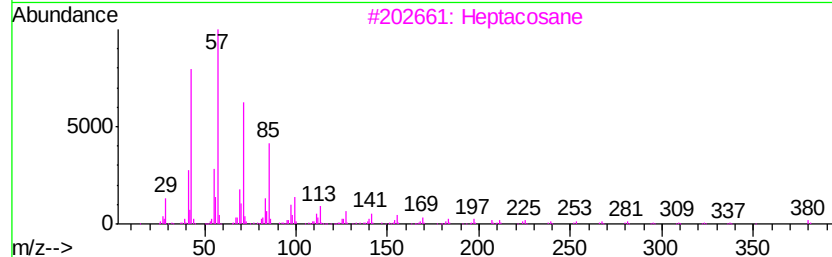
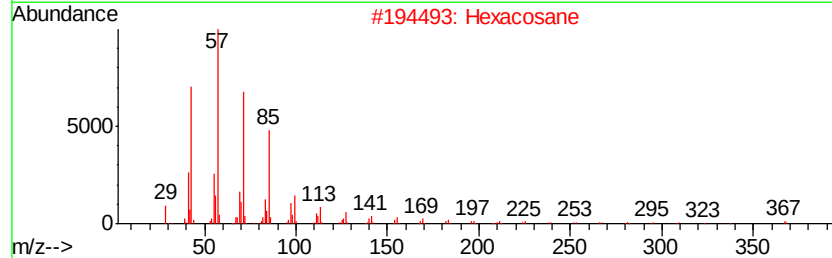
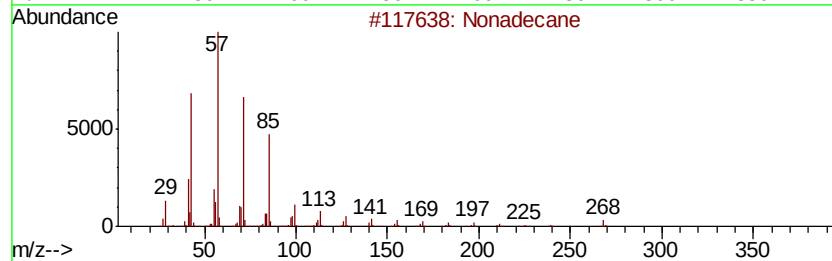
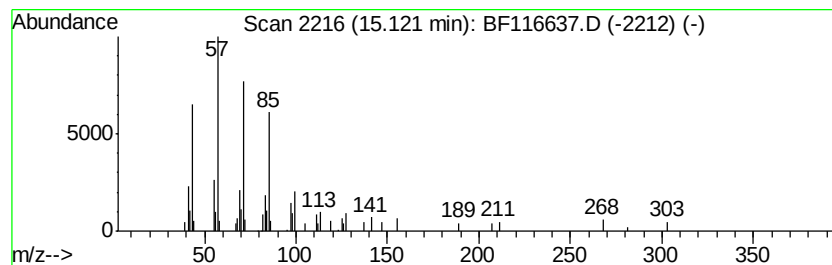
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.95 ng	60669	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	93
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Tetratetracontane		619	C44H90	007098-22-8	91
5	Hexatriacontane		507	C36H74	000630-06-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
Data File : BF116637.D
Acq On : 29 Aug 2019 1:29
Operator : HP/JU
Sample : K4576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RBR-200034-RBR-200036

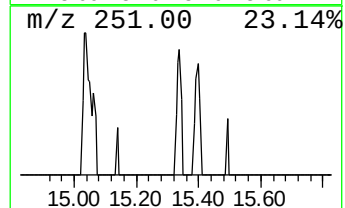
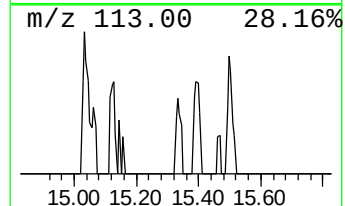
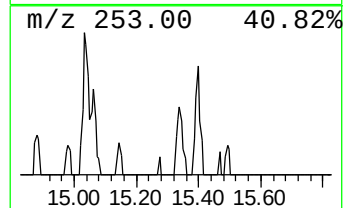
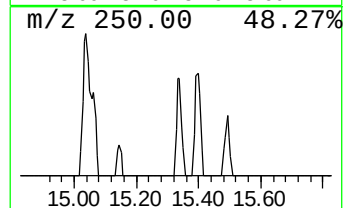
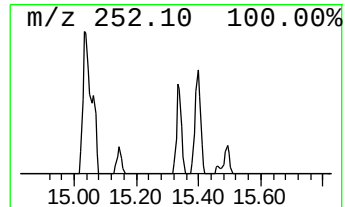
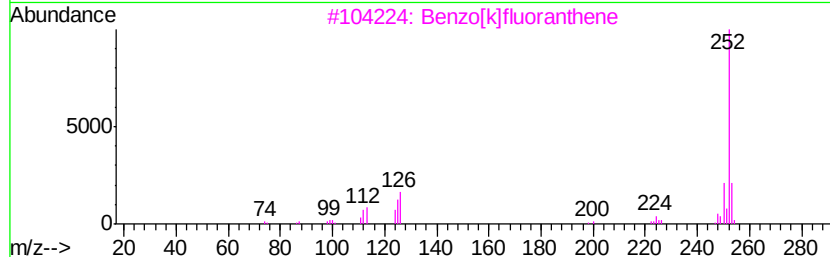
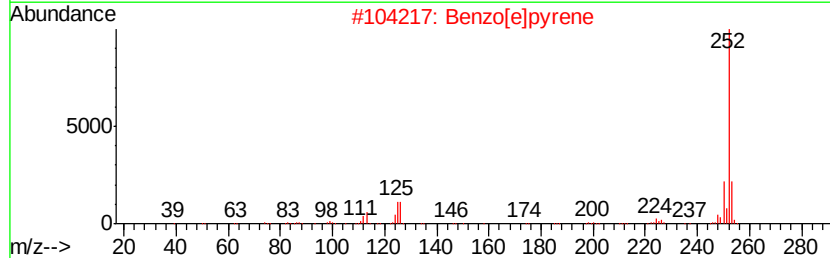
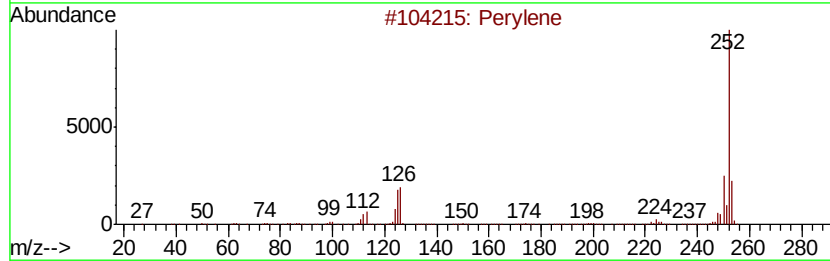
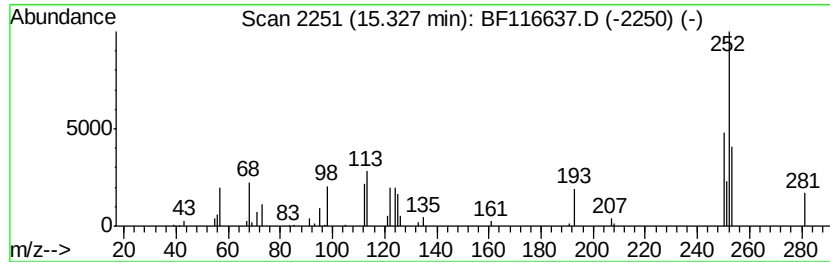
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	2.04 ng	31281	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	59
2		Benzo[e]pyrene	252	C20H12	000192-97-2	58
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	53
4		Benzo[a]pyrene	252	C20H12	000050-32-8	53
5		1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
Data File : BF116637.D
Acq On : 29 Aug 2019 1:29
Operator : HP/JU
Sample : K4576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

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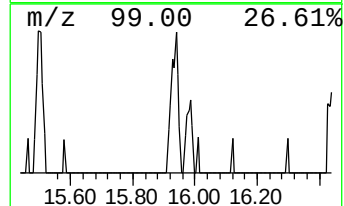
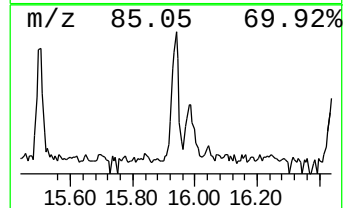
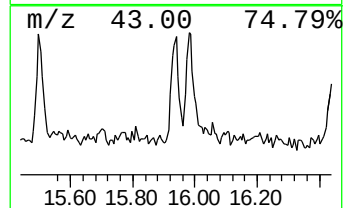
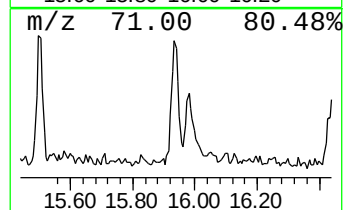
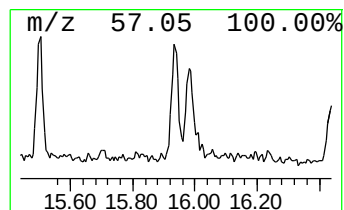
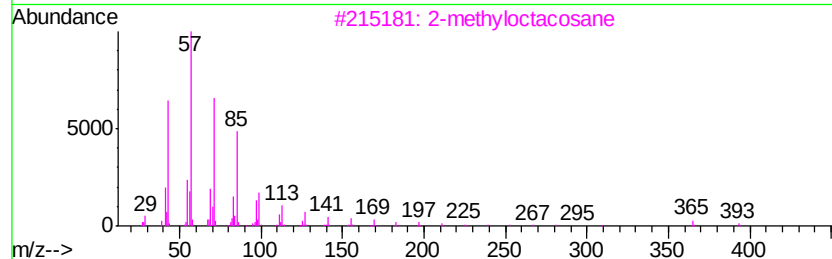
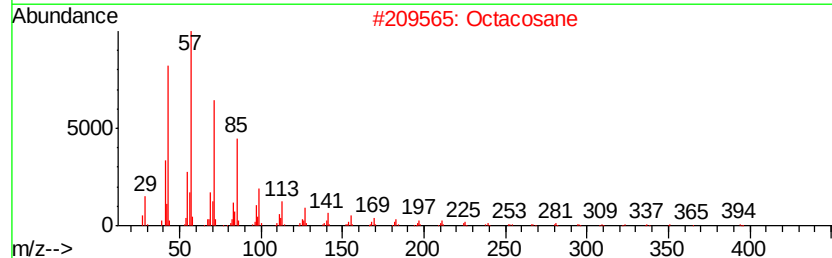
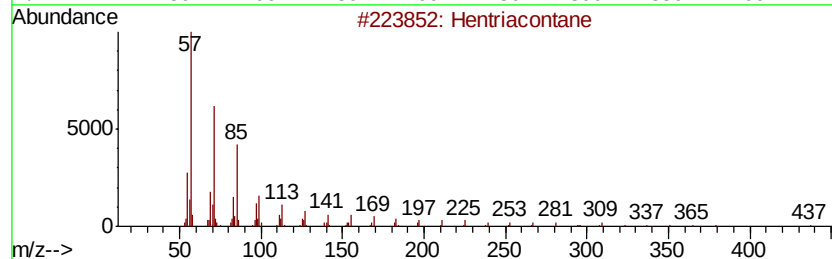
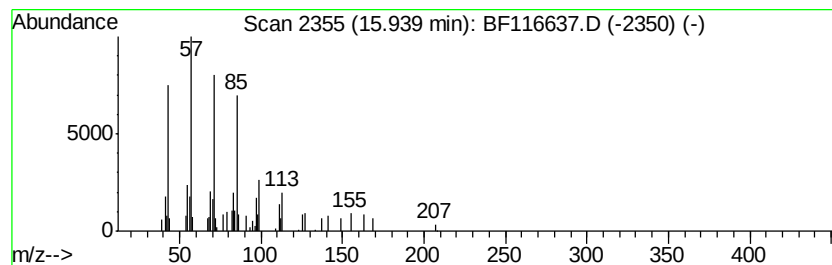
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.67 ng	56412	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Octacosane	394	C28H58	000630-02-4	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
Data File : BF116637.D
Acq On : 29 Aug 2019 1:29
Operator : HP/JU
Sample : K4576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

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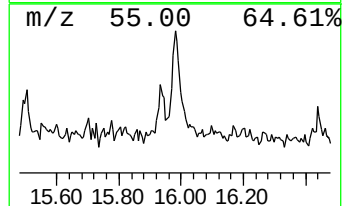
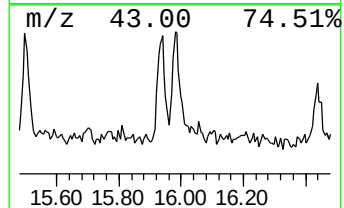
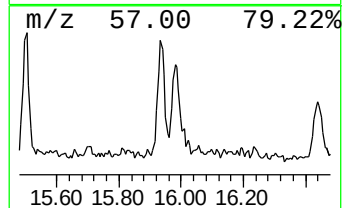
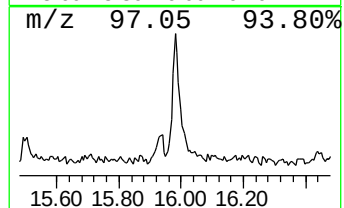
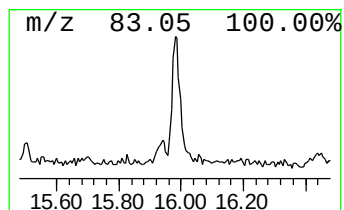
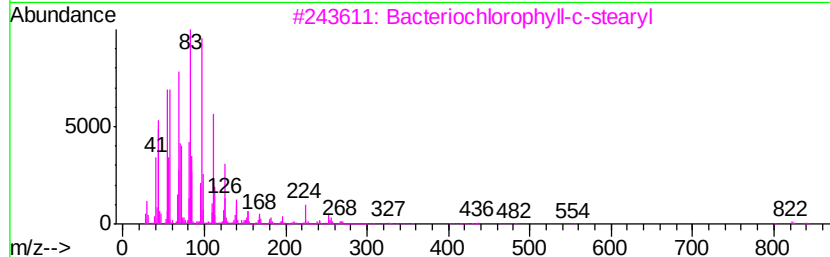
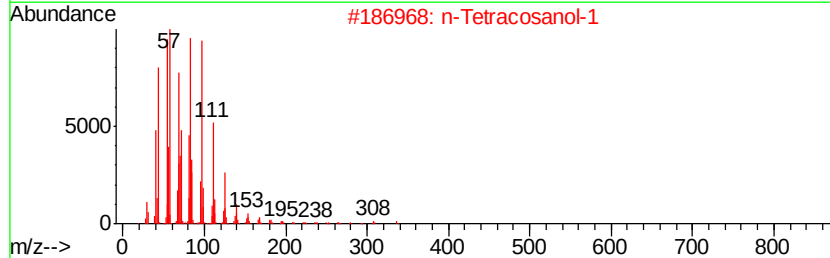
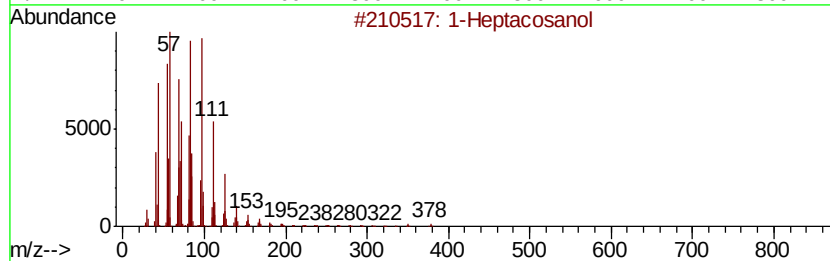
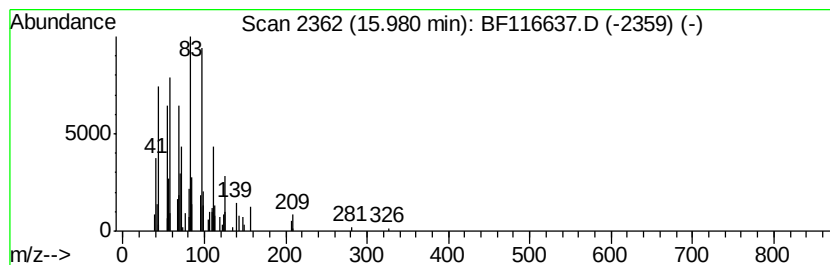
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	6.11 ng	93808	Perylene-d12	15.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	90
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	86
3			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	86
4			1-Nonadecene	266	C19H38	018435-45-5	86
5			1-Docosene	308	C22H44	001599-67-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
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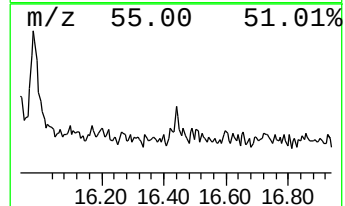
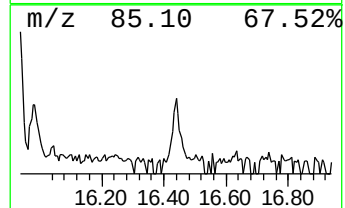
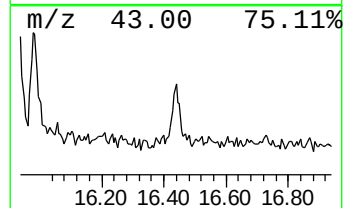
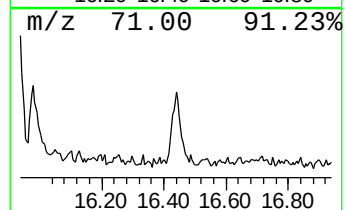
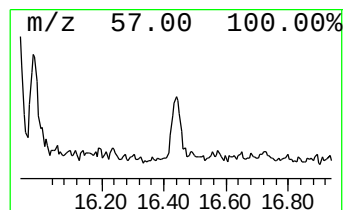
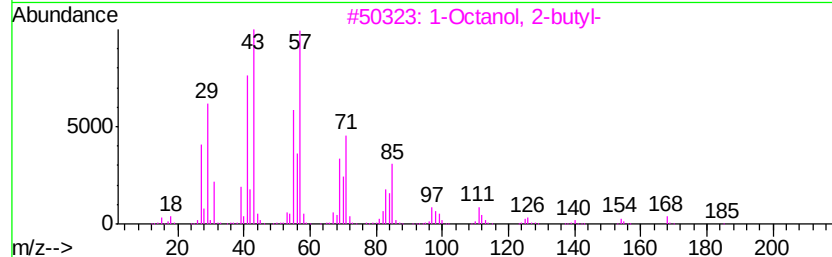
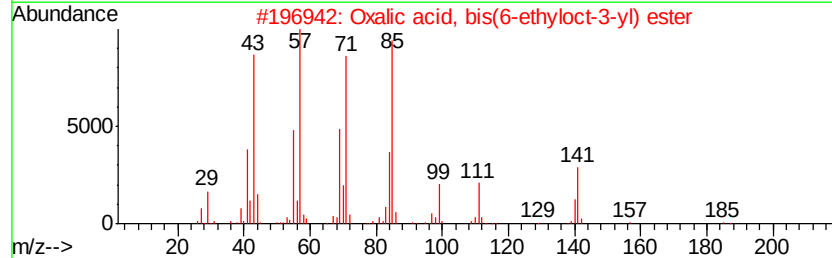
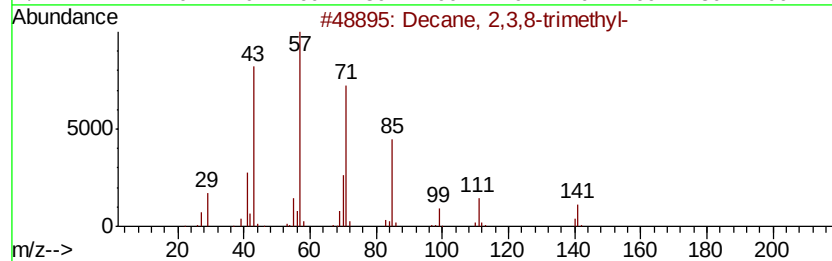
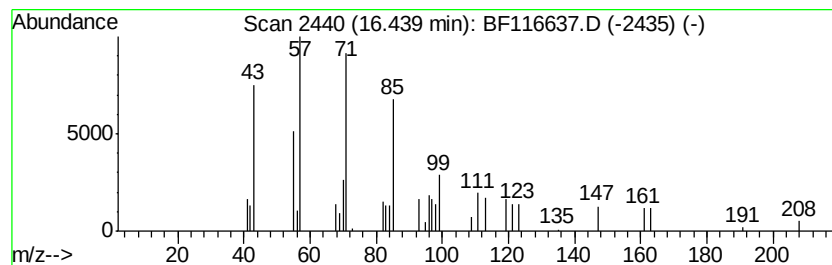
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Decane, 2,3,8-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.44	2.11 ng	32481	Perylene-d12	15.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	53
2	Oxalic acid, bis(6-ethyloct-3-yl...)	370	C22H42O4	1000309-34-6	53
3	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	53
4	Octacosane	394	C28H58	000630-02-4	50
5	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
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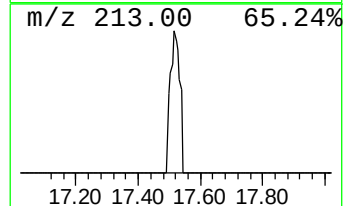
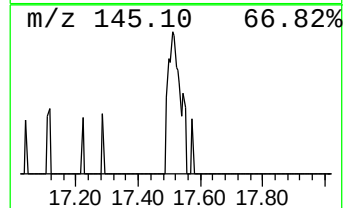
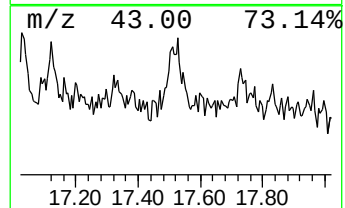
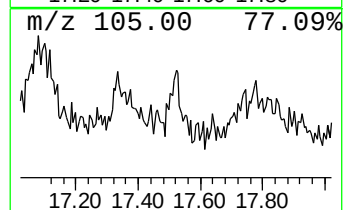
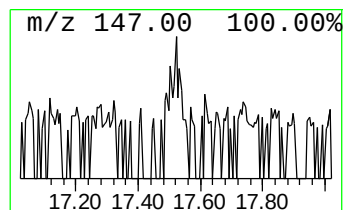
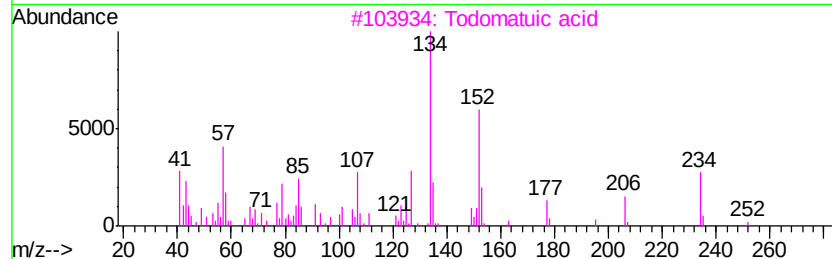
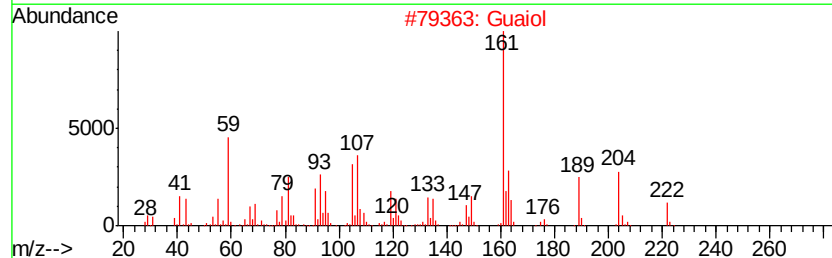
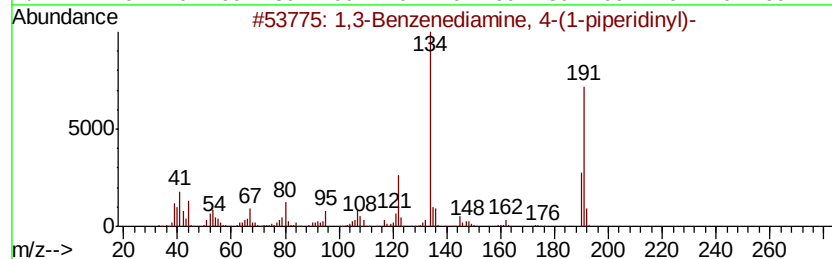
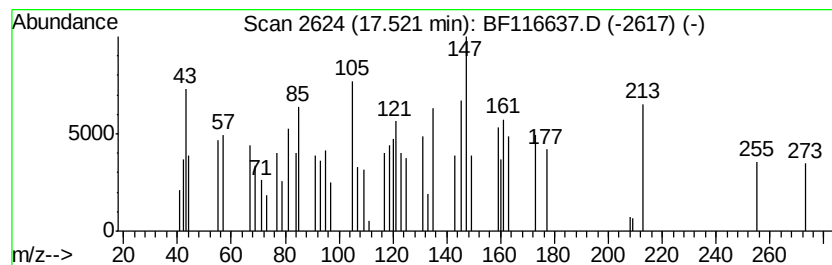
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.52 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.52	2.86 ng	43901	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenediamine, 4-(1-piperid...	191	C11H17N3	1000337-21-1	16
2		Guaiol	222	C15H26O	000489-86-1	12
3		Todomatuic acid	252	C15H24O3	017844-07-4	12
4		Ledene oxide-(II)	220	C15H24O	1000159-36-7	11
5		2,6,10-Dodecatrien-1-ol, 12-acet...	280	C17H28O3	093787-91-8	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082819\
Data File : BF116637.D
Acq On : 29 Aug 2019 1:29
Operator : HP/JU
Sample : K4576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200034-RBR-200036

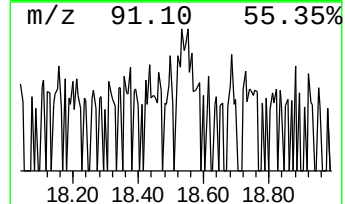
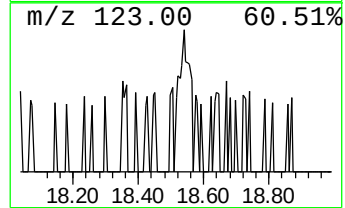
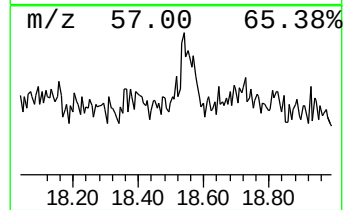
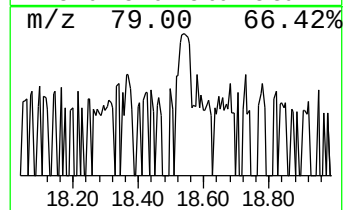
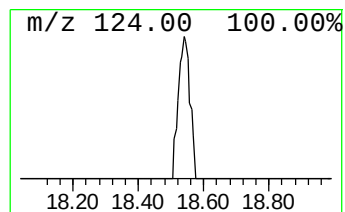
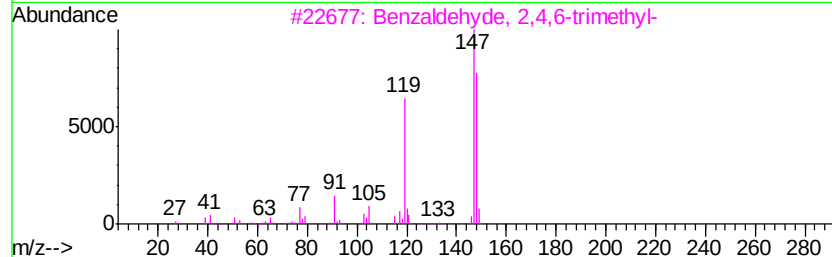
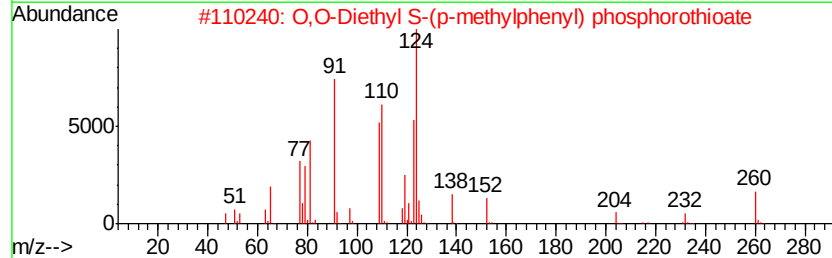
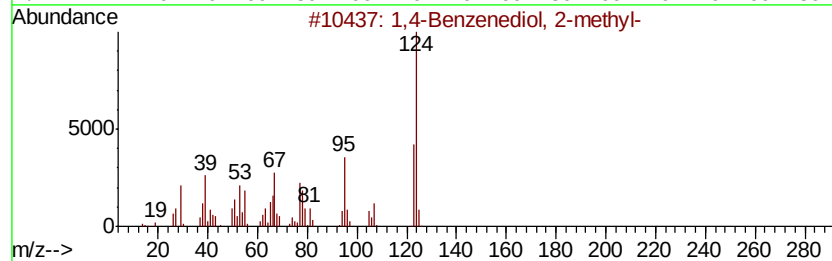
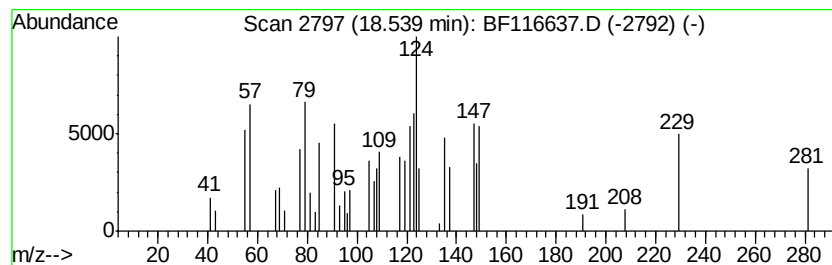
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.54 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	2.07 ng	31787	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	14
2		0,0-Diethyl S-(p-methylphenyl) p...	260	C11H17O3PS	1000306-08-0	14
3		Benzaldehyde, 2,4,6-trimethyl-	148	C10H12O	000487-68-3	14
4		1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	14
5		Orcinol	124	C7H8O2	000504-15-4	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082819\
 Data File : BF116637.D
 Acq On : 29 Aug 2019 1:29
 Operator : HP/JU
 Sample : K4576-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200034-RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082819.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...	2.15	70.2	ng	1456610	1	6.86	415025	20.0
unknown6.63	6.63	90.3	ng	1874620	1	6.86	415025	20.0
n-Hexadecanoic acid	11.90	7.0	ng	149641	4	11.37	429230	20.0
Octadecanoic acid	12.68	2.4	ng	51716	4	11.37	429230	20.0
Pentafluoropropio...	13.85	11.9	ng	219435	5	14.00	369867	20.0
Octadecane	14.48	3.0	ng	55758	5	14.00	369867	20.0
Nonadecane	15.12	4.0	ng	60669	6	15.46	307175	20.0
Perylene	15.33	2.0	ng	31281	6	15.46	307175	20.0
Hentriacontane	15.94	3.7	ng	56412	6	15.46	307175	20.0
1-Heptacosanol	15.98	6.1	ng	93808	6	15.46	307175	20.0
Decane, 2,3,8-tri...	16.44	2.1	ng	32481	6	15.46	307175	20.0
unknown17.52	17.52	2.9	ng	43901	6	15.46	307175	20.0
unknown18.54	18.54	2.1	ng	31787	6	15.46	307175	20.0