

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
 Data File : BF121895.D
 Acq On : 8 Oct 2020 18:19
 Operator : JU/CG
 Sample : L4303-21
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IDW-20201006

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	4.963	485	489	497	rBV	34783	50918	1.97%	0.263%
2	5.381	556	560	577	rBV	2006650	2020329	78.21%	10.427%
3	6.404	730	734	741	rBV	1994577	2026879	78.46%	10.461%
4	6.757	791	794	803	rVB	736451	566522	21.93%	2.924%
5	7.322	886	890	903	rBV	1465668	1448796	56.09%	7.477%
6	8.039	1008	1012	1031	rBV	780271	755163	29.23%	3.898%
7	9.116	1191	1195	1207	rBV	2921562	2583176	100.00%	13.332%
8	9.516	1259	1263	1271	rBV	155583	160607	6.22%	0.829%
9	9.792	1306	1310	1322	rVB	965603	854294	33.07%	4.409%
10	10.586	1441	1445	1461	rVB	1572173	1506134	58.31%	7.773%
11	10.716	1465	1467	1472	rVB	46085	39535	1.53%	0.204%
12	10.763	1472	1475	1478	rBV	62640	66060	2.56%	0.341%
13	10.798	1478	1481	1484	rVV2	82432	105522	4.08%	0.545%
14	10.833	1484	1487	1489	rVV	79580	83562	3.23%	0.431%
15	10.857	1489	1491	1493	rVV	51887	45659	1.77%	0.236%
16	10.880	1493	1495	1499	rVV3	71478	84421	3.27%	0.436%
17	10.945	1503	1506	1510	rVV3	69946	90625	3.51%	0.468%
18	10.980	1510	1512	1514	rVV	67084	69689	2.70%	0.360%
19	11.021	1517	1519	1528	rVB	50675	52501	2.03%	0.271%
20	11.280	1559	1563	1570	rBV	935853	848222	32.84%	4.378%
21	12.757	1811	1814	1824	rVB	192503	233305	9.03%	1.204%
22	12.868	1828	1833	1836	rBV	2521545	2540402	98.34%	13.111%
23	13.092	1867	1871	1881	rBV2	33294	55137	2.13%	0.285%
24	13.345	1909	1914	1919	rVB4	21198	35886	1.39%	0.185%
25	13.774	1982	1987	1996	rBV	263905	514829	19.93%	2.657%
26	13.892	2004	2007	2008	rBV	41798	34361	1.33%	0.177%
27	13.915	2008	2011	2016	rVB	617406	616857	23.88%	3.184%
28	14.380	2086	2090	2093	rBV	53418	52250	2.02%	0.270%
29	14.421	2093	2097	2104	rVV4	49504	107054	4.14%	0.553%
30	14.680	2137	2141	2144	rBV	48635	53887	2.09%	0.278%
31	14.821	2162	2165	2167	rBV2	28077	34435	1.33%	0.178%
32	15.004	2192	2196	2201	rVB	77883	79775	3.09%	0.412%
33	15.074	2203	2208	2215	rVB7	26581	58045	2.25%	0.300%
34	15.356	2251	2256	2266	rBV	542454	724492	28.05%	3.739%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.786	2324	2329	2334	rVB	56746	87349	3.38%	0.451%
36	15.868	2336	2343	2354	rBV7	63733	236739	9.16%	1.222%
37	16.227	2399	2404	2407	rBV7	23757	52684	2.04%	0.272%
38	16.821	2501	2505	2513	rVB2	34059	68079	2.64%	0.351%
39	17.350	2588	2595	2606	rBV2	44454	154639	5.99%	0.798%
40	18.280	2745	2753	2765	rVB4	66041	176681	6.84%	0.912%

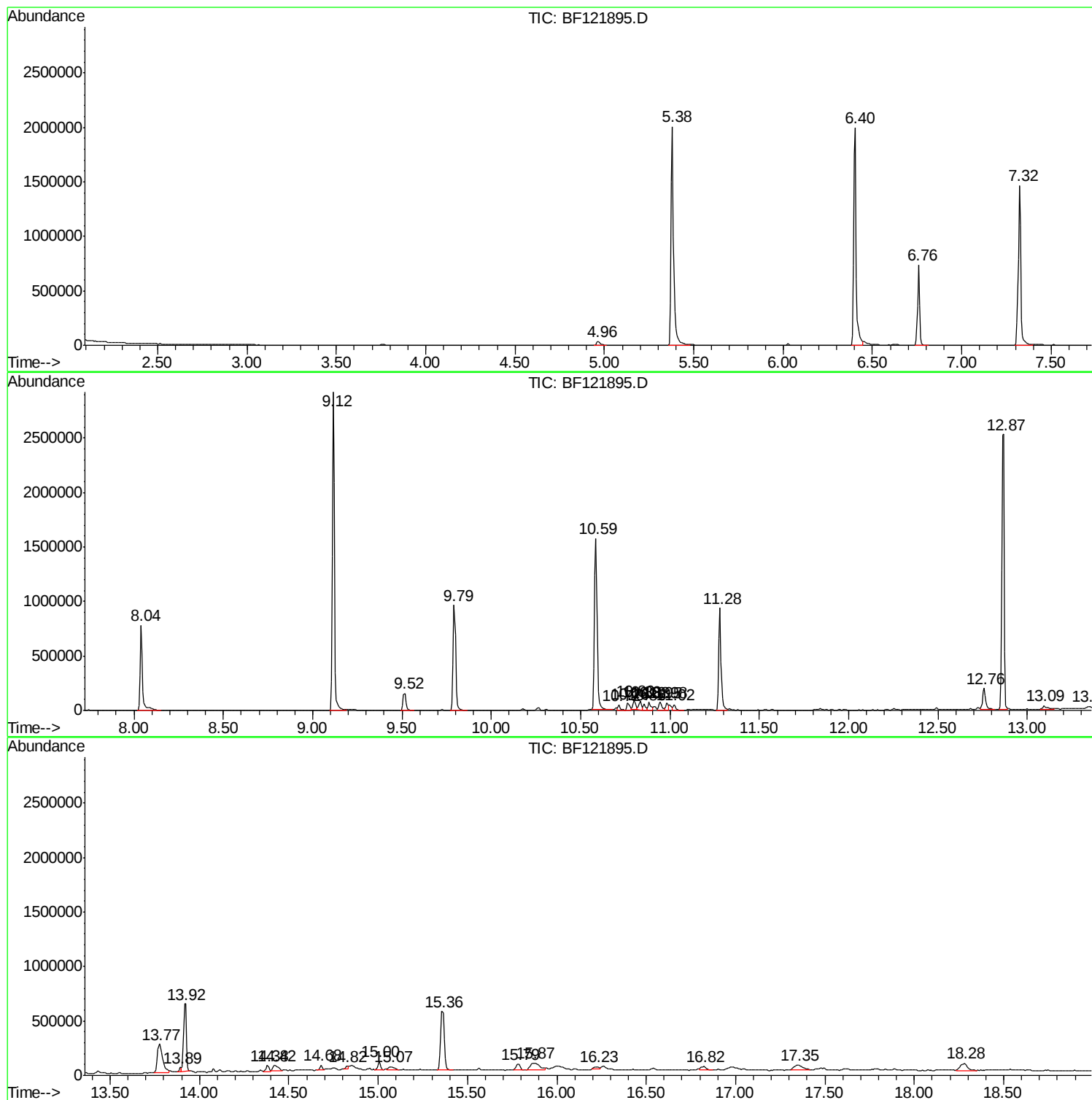
Sum of corrected areas: 19375500

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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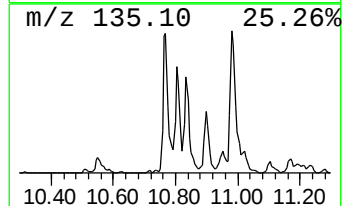
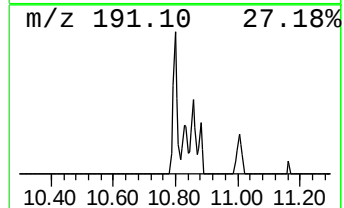
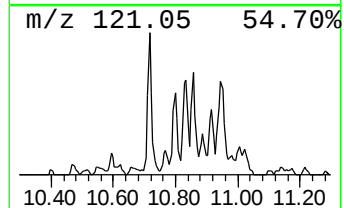
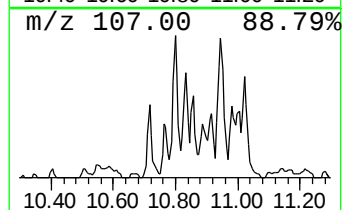
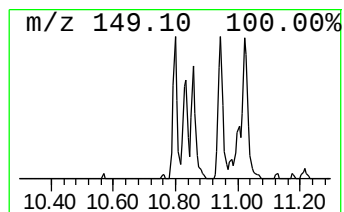
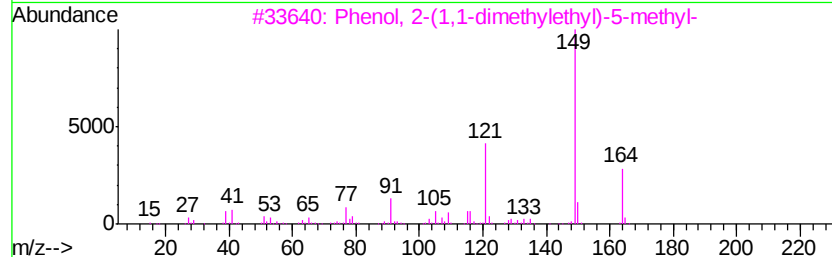
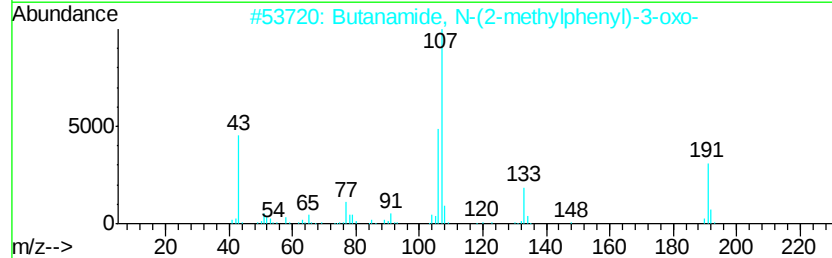
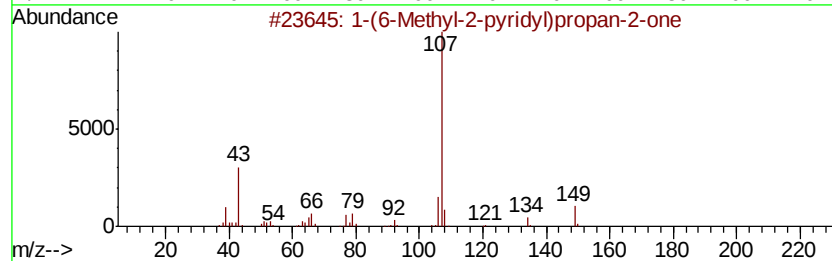
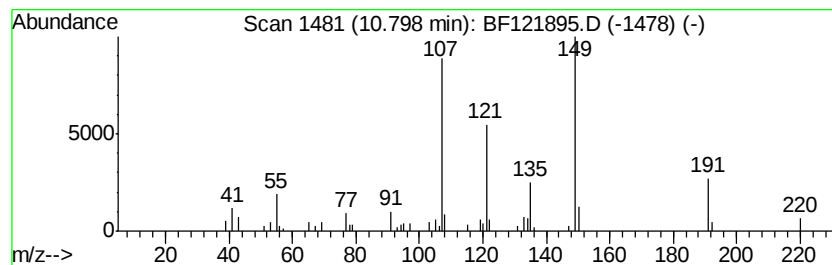
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-(6-Methyl-2-pyridyl)propan-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.80	2.49 ng	105522	Phenanthrene-d10	11.28		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	58
2		Butanamide, N-(2-methylphenyl)-3-oxo-	191	C11H13NO2	000093-68-5	35
3		Phenol, 2-(1,1-dimethylethyl)-5-methyl-	164	C11H16O	000088-60-8	35
4		Phenol, 2-methyl-4-(1,1,3,3-tetrachloro-2-propyl)-	220	C15H24O	002219-84-3	35
5		Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	30



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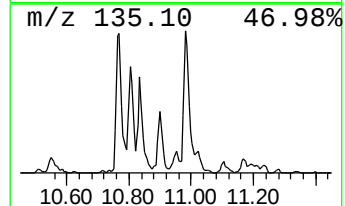
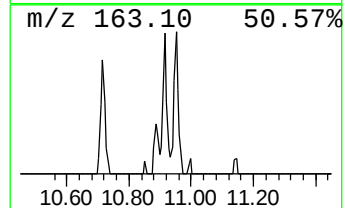
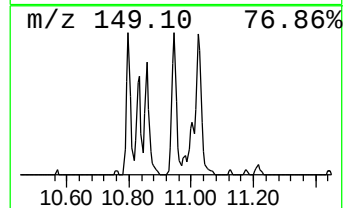
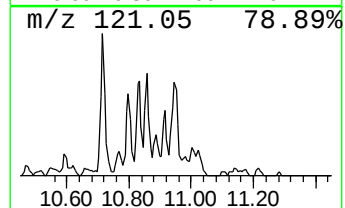
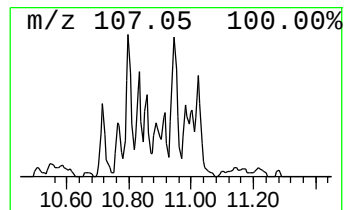
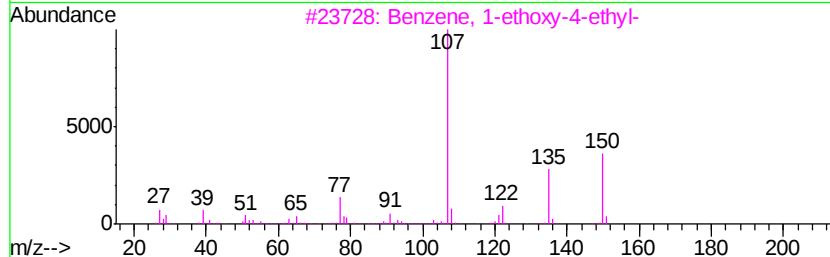
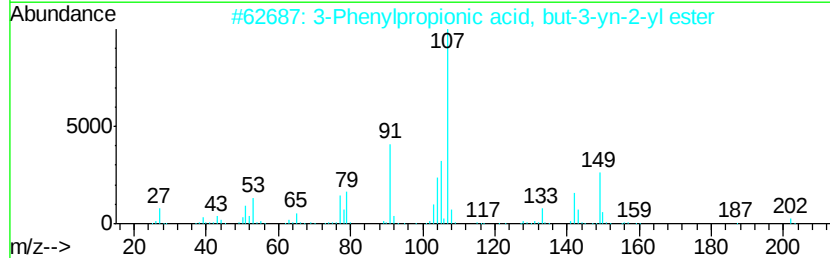
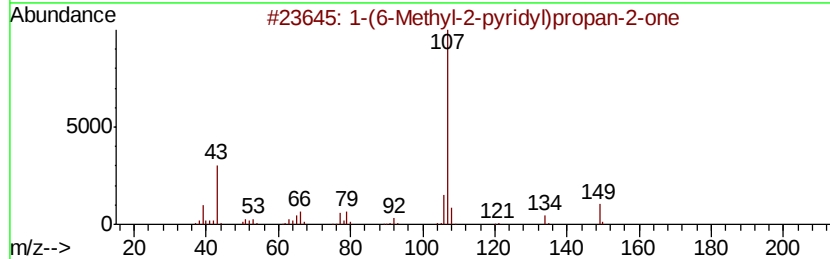
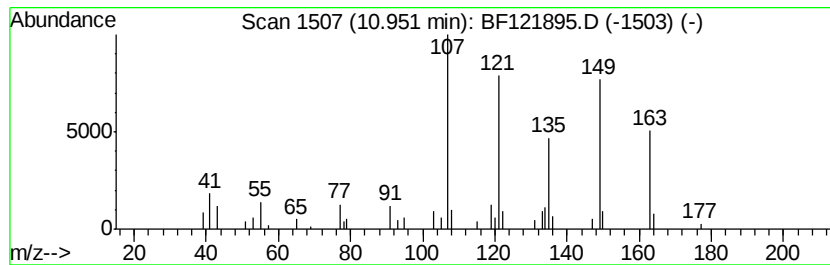
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown10.95 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.95	2.14 ng	90625	Phenanthrene-d10	11.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	42
2	3-Phenylpropionic acid, but-3-yn...	202	C13H14O2	1000299-17-2	40
3	Benzene, 1-ethoxy-4-ethyl-	150	C10H14O	001585-06-4	35
4	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	35
5	1,3-Cyclohexadiene-1-carboxaldeh...	150	C10H14O	000116-26-7	35



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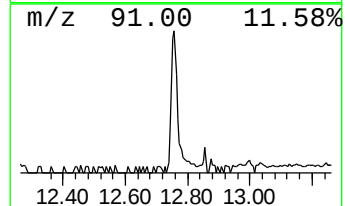
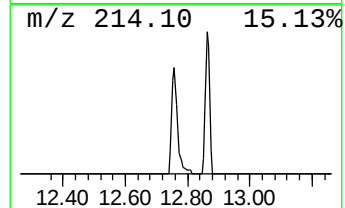
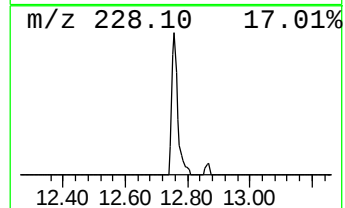
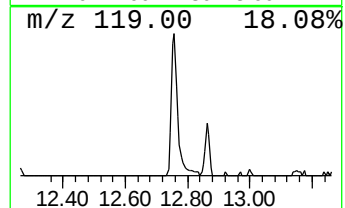
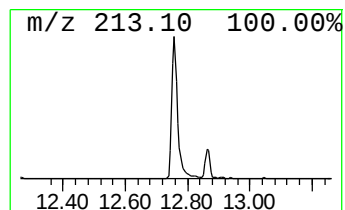
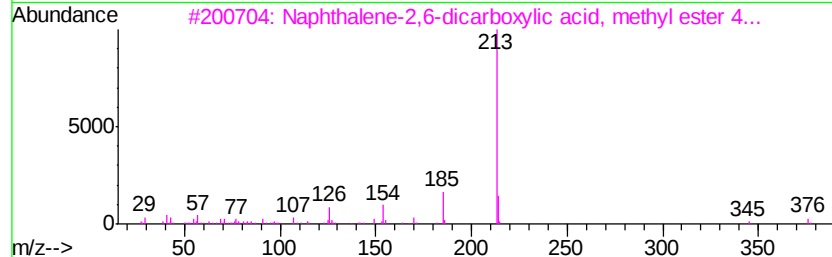
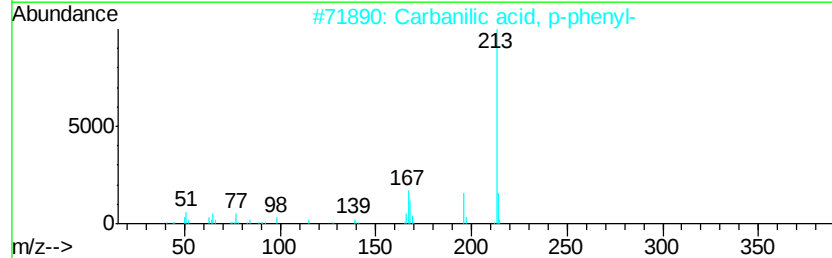
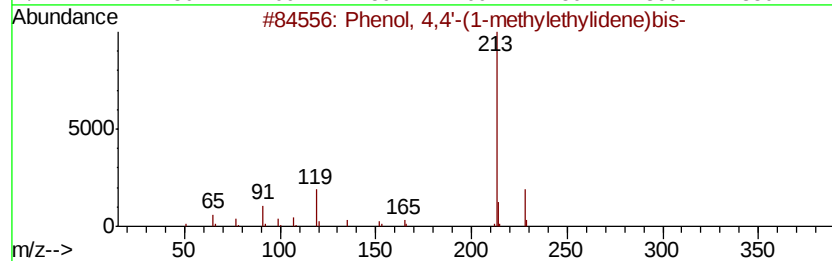
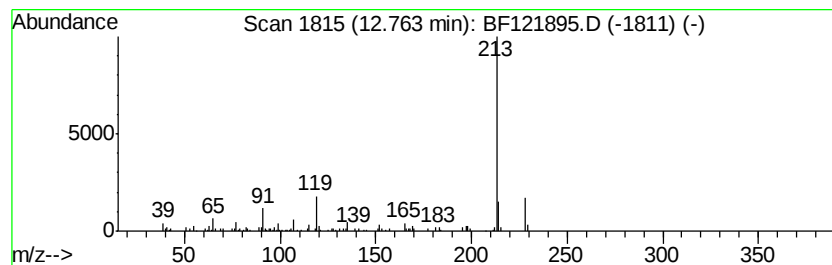
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.76	7.56 ng	233305	Chrysene-d12	13.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98	
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52	
3	Naphthalene-2,6-dicarboxylic aci...	376	C24H24O4	1000189-60-8	50	
4	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	50	
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	42	



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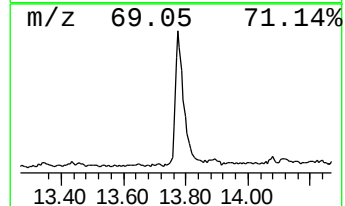
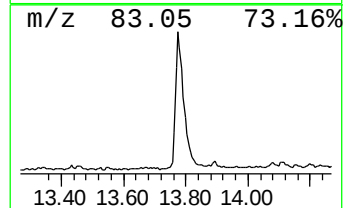
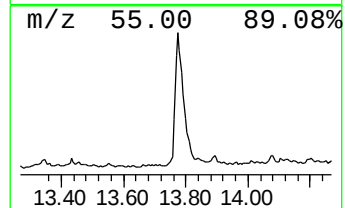
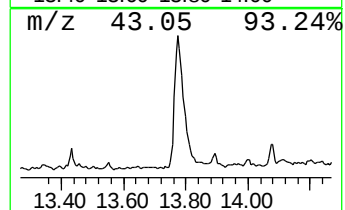
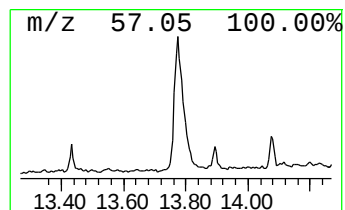
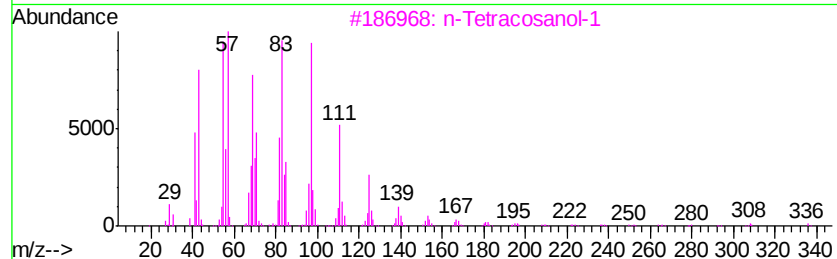
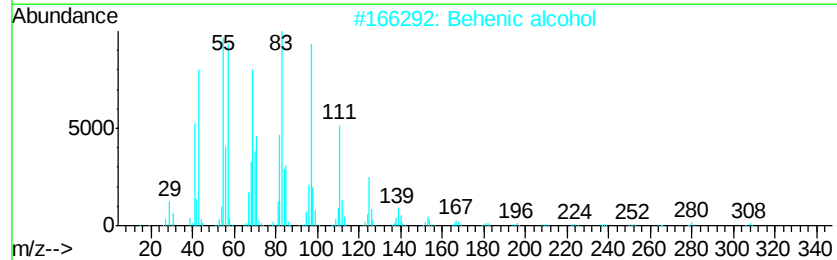
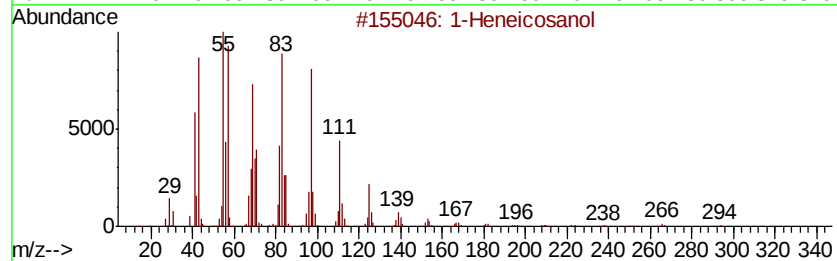
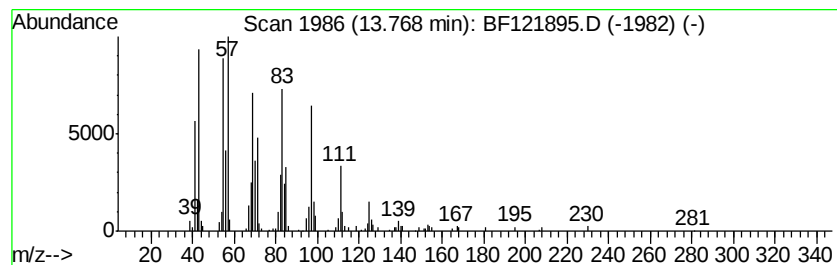
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.77	16.69 ng	514829	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91



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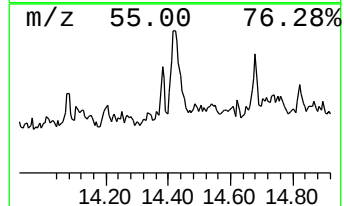
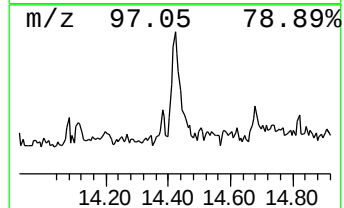
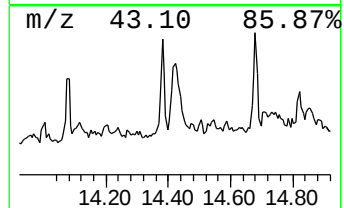
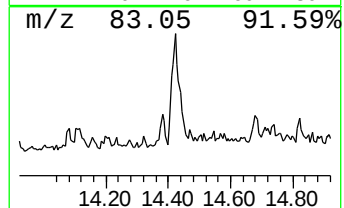
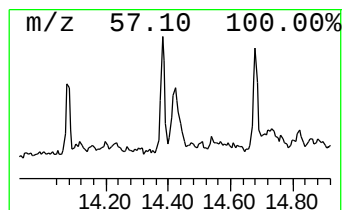
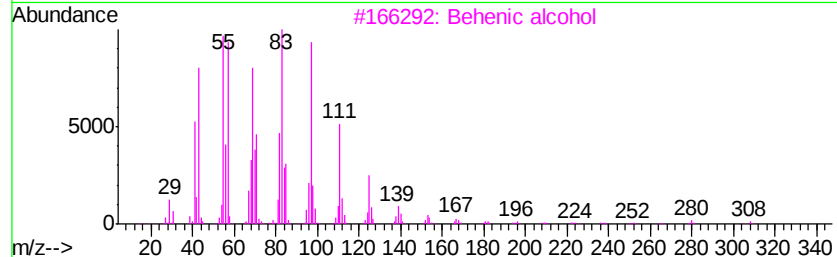
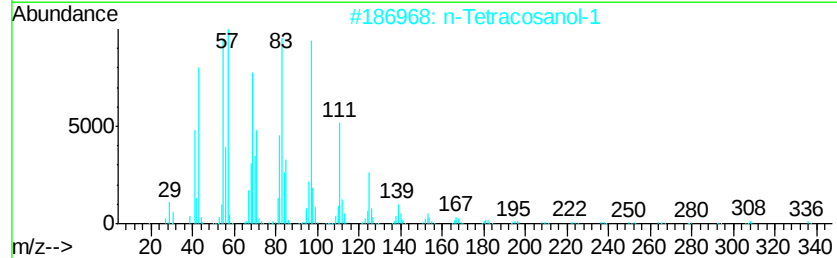
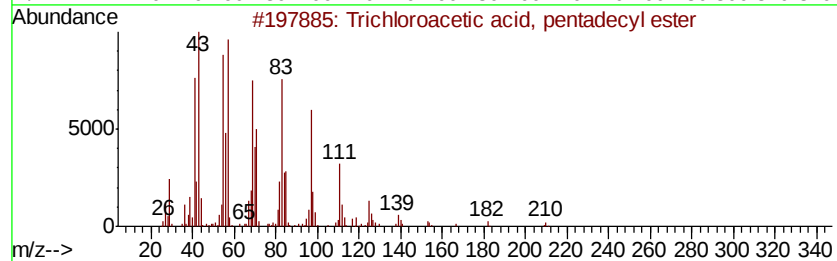
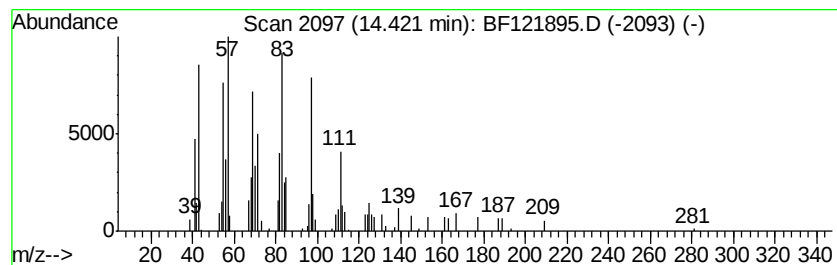
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	3.47 ng	107054	Chrysene-d12	13.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3		Behenic alcohol	326	C22H46O	000661-19-8	87
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121895.D
Acq On : 8 Oct 2020 18:19
Operator : JU/CG
Sample : L4303-21
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-20201006

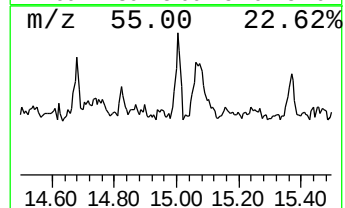
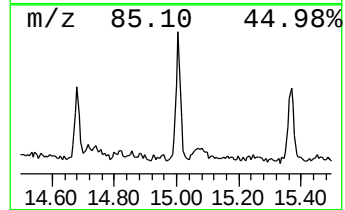
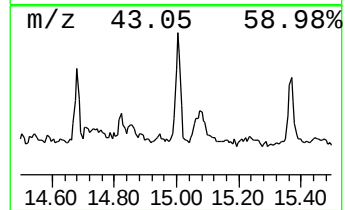
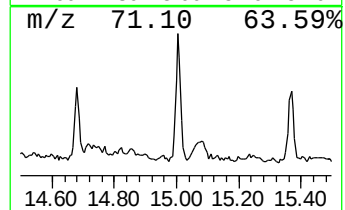
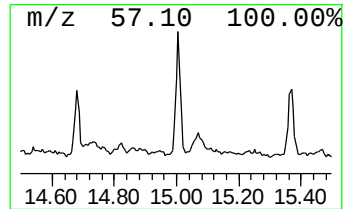
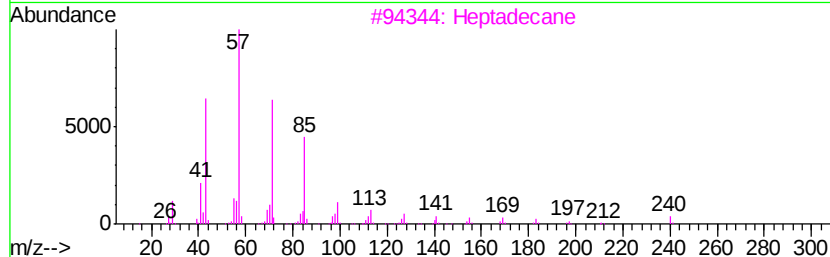
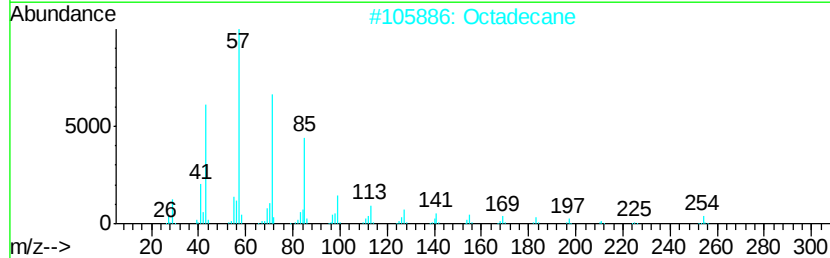
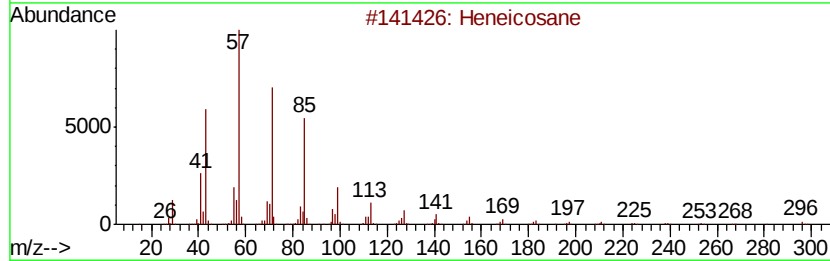
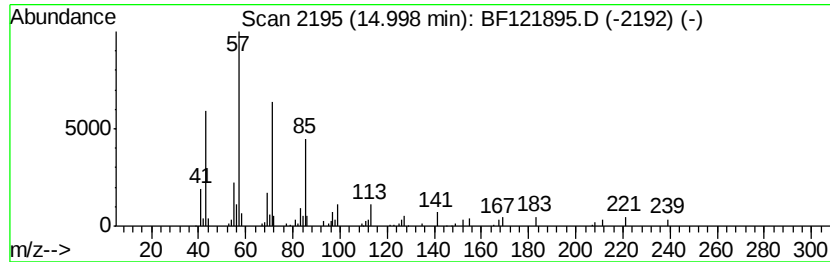
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.20 ng	79775	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Heptadecane		240	C17H36	000629-78-7	91
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	91
5	Hentriacontane		437	C31H64	000630-04-6	91



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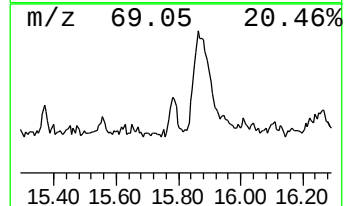
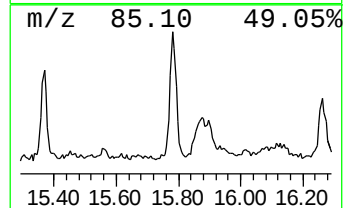
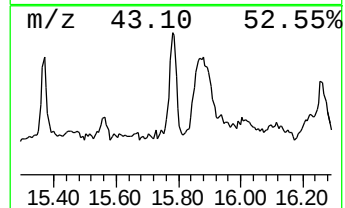
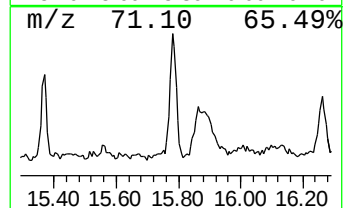
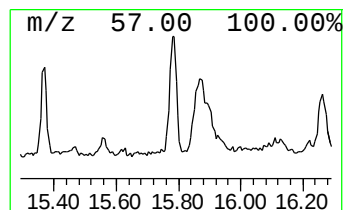
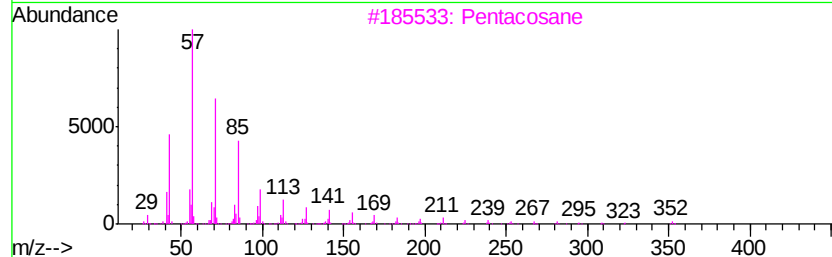
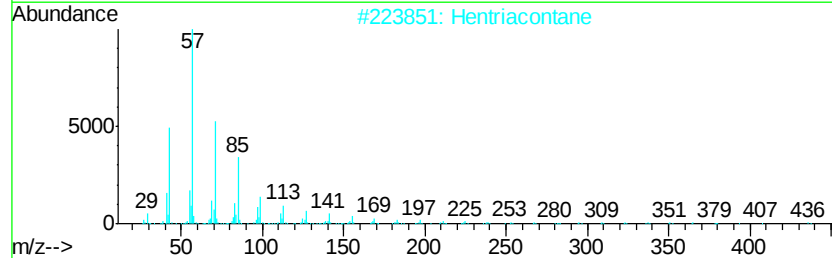
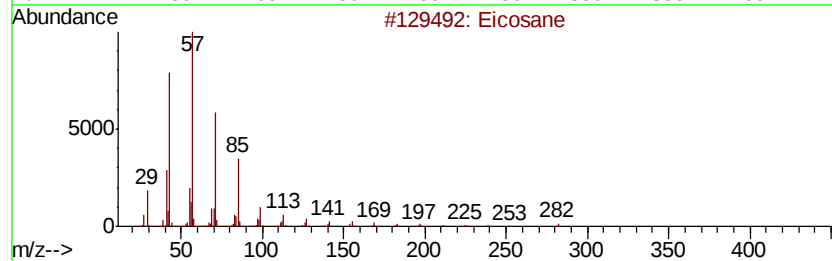
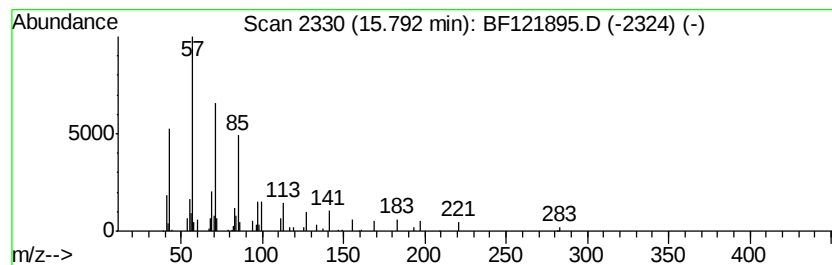
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.41 ng	87349	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121895.D
Acq On : 8 Oct 2020 18:19
Operator : JU/CG
Sample : L4303-21
Misc :
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ClientSampleId :
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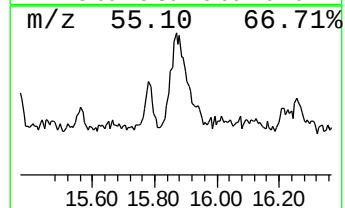
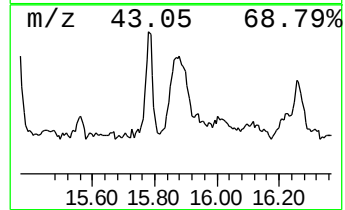
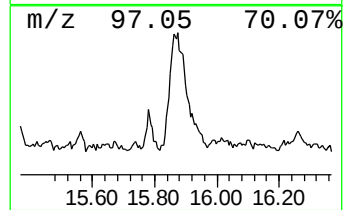
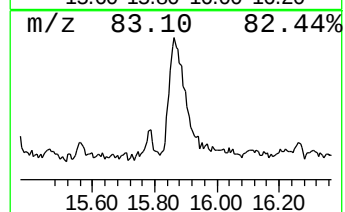
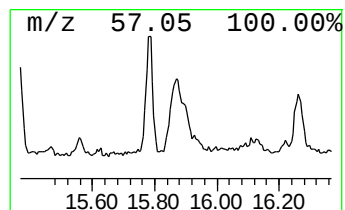
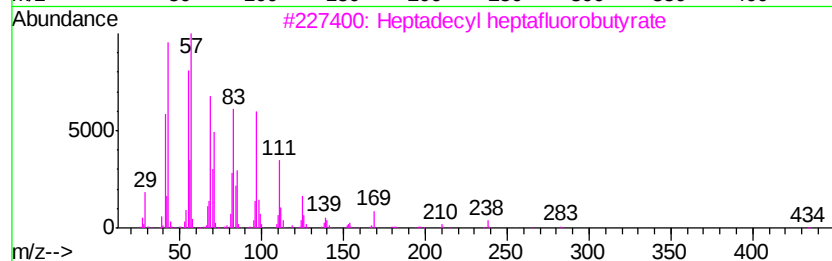
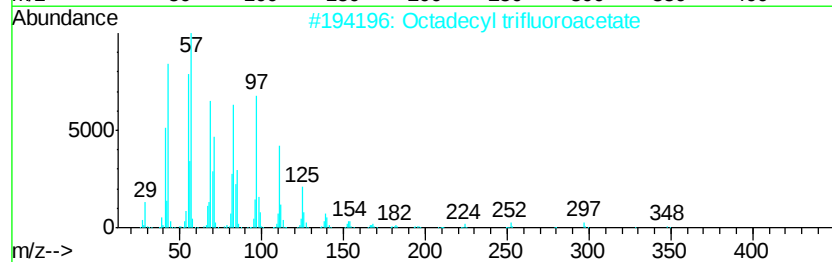
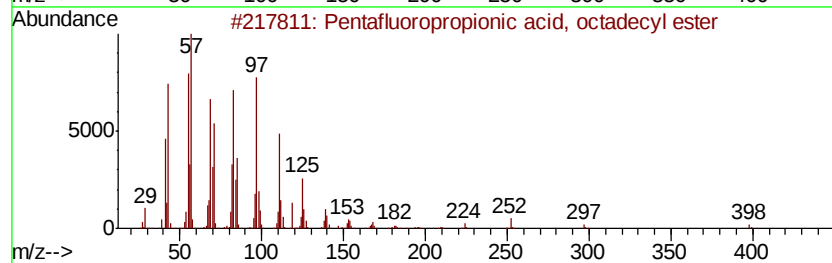
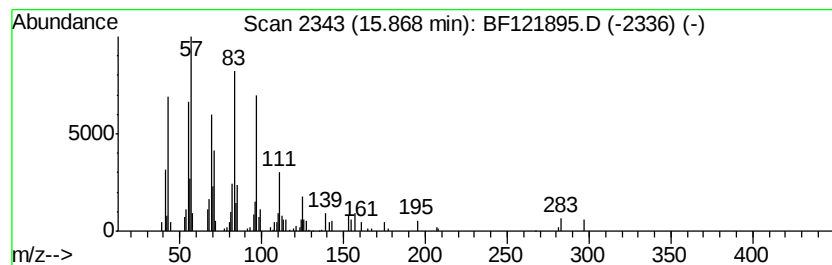
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	6.54 ng	236739	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	74
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	68
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	64
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
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Acq On : 8 Oct 2020 18:19
Operator : JU/CG
Sample : L4303-21
Misc :
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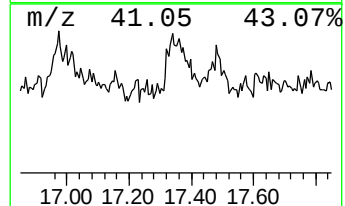
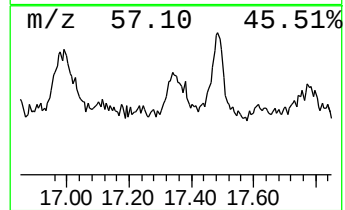
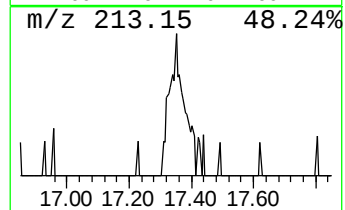
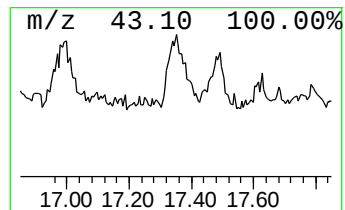
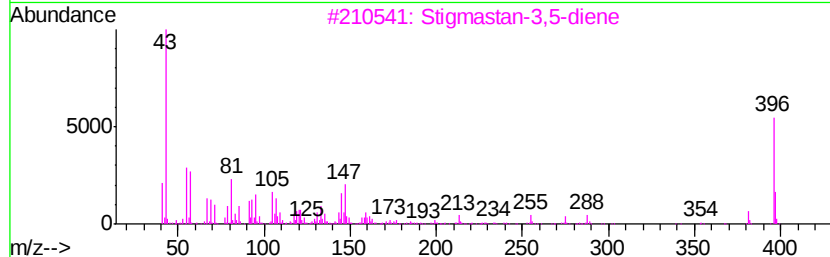
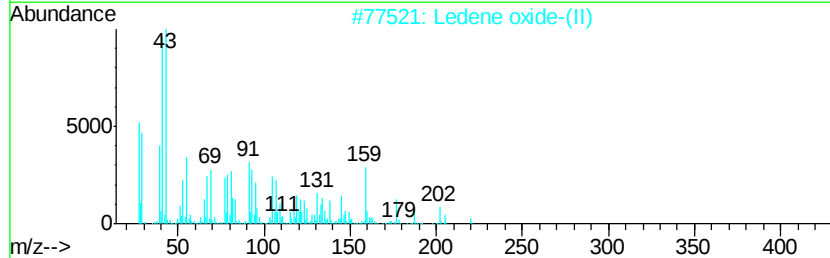
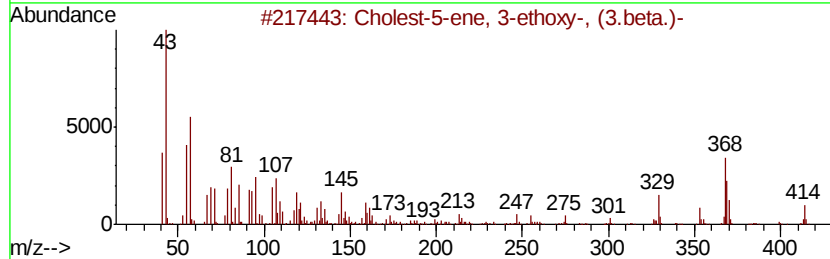
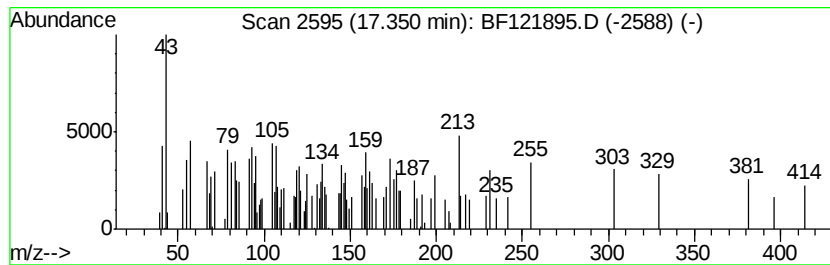
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.35 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.35	4.27 ng	154639	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H500	000986-19-6	38
2	Ledene oxide-(II)	220 C15H240	1000159-36-7	10
3	Stigmastan-3,5-diene	396 C29H48	1000214-16-4	9
4	.beta.-Sitosterol acetate	456 C31H5202	000915-05-9	9
5	Lanceol, cis	220 C15H240	010067-28-4	9



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Sample : L4303-21
Misc :
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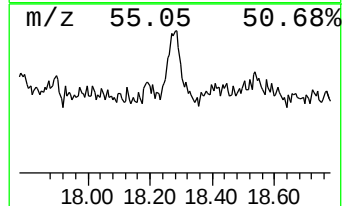
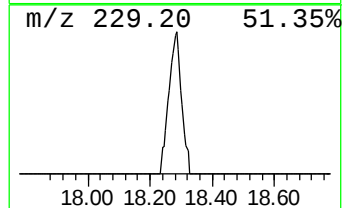
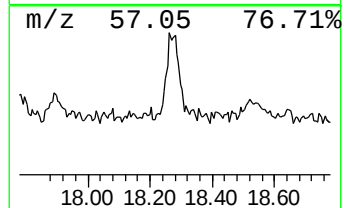
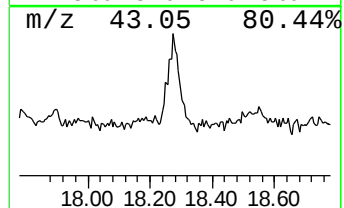
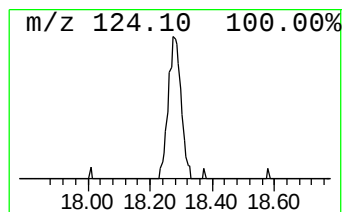
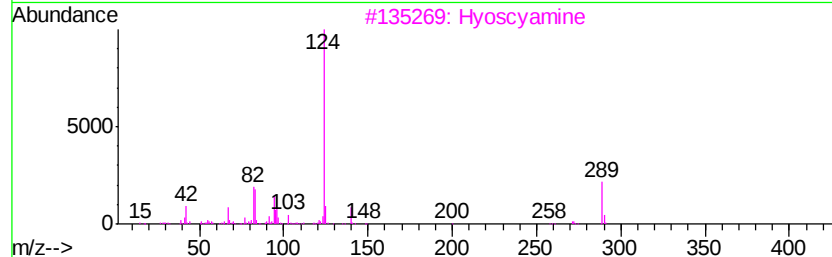
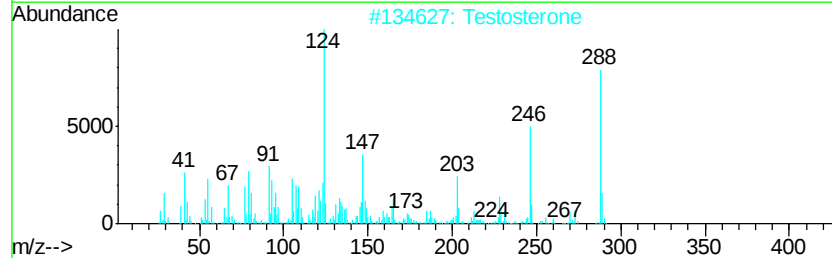
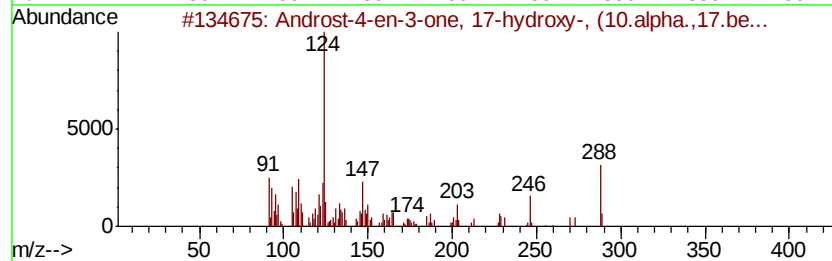
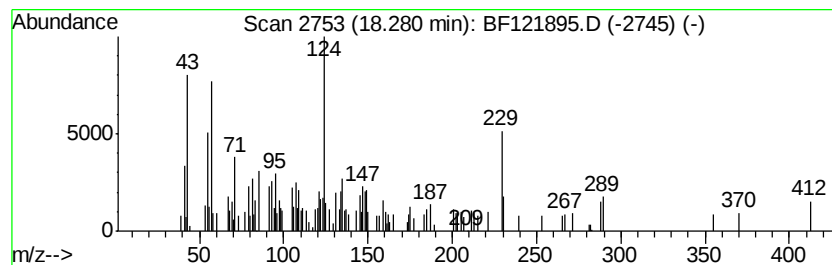
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Androst-4-en-3-one, 17-hydr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	4.88 ng	176681	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Androst-4-en-3-one, 17-hydroxy-, ...	288	C19H28O2	000604-39-7	89
2			Testosterone	288	C19H28O2	000058-22-0	50
3			Hyoscyamine	289	C17H23NO3	000101-31-5	30
4			3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	30
5			2,3-Diaminophenol	124	C6H8N2O	059649-56-8	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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
1-(6-Methyl-2-pyr...	10.80	2.5	ng	105522	4	11.28	848222	20.0
unknown10.95	10.95	2.1	ng	90625	4	11.28	848222	20.0
Phenol, 4,4'-(1-m...	12.76	7.6	ng	233305	5	13.92	616857	20.0
1-Heneicosanol	13.77	16.7	ng	514829	5	13.92	616857	20.0
Trichloroacetic a...	14.42	3.5	ng	107054	5	13.92	616857	20.0
Heneicosane	15.00	2.2	ng	79775	6	15.36	724492	20.0
Eicosane	15.79	2.4	ng	87349	6	15.36	724492	20.0
Pentafluoropropio...	15.87	6.5	ng	236739	6	15.36	724492	20.0
unknown17.35	17.35	4.3	ng	154639	6	15.36	724492	20.0
Androst-4-en-3-on...	18.28	4.9	ng	176681	6	15.36	724492	20.0