

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
 Data File : BF115477.D
 Acq On : 11 Jul 2019 1:15
 Operator : HP/JU
 Sample : K3700-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-052

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-BF070519.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	2.187	9	17	29	rVB	1534139	2102179	54.70%	5.205%
2	3.404	221	224	240	rBV	14993	45371	1.18%	0.112%
3	5.516	577	583	586	rBV	3387975	3502966	91.16%	8.673%
4	6.522	748	754	757	rBV	3391471	3770677	98.12%	9.336%
5	6.663	773	778	782	rBV	3663543	3842864	100.00%	9.515%
6	6.892	814	817	821	rBV	1076476	859207	22.36%	2.127%
7	7.051	840	844	847	rBV	3126109	2696538	70.17%	6.677%
8	7.451	907	912	915	rBV	2354011	2438618	63.46%	6.038%
9	8.175	1031	1035	1039	rBV	1358004	1102478	28.69%	2.730%
10	9.251	1214	1218	1221	rBV	3863806	3411994	88.79%	8.448%
11	9.639	1281	1284	1288	rBV	791965	692468	18.02%	1.715%
12	9.933	1330	1334	1338	rBV	1596276	1338874	34.84%	3.315%
13	10.722	1463	1468	1471	rBV	3074264	2894914	75.33%	7.168%
14	11.416	1582	1586	1590	rBV	1723249	1461369	38.03%	3.618%
15	11.945	1672	1676	1686	rBV	710551	684024	17.80%	1.694%
16	12.121	1703	1706	1712	rVB3	37598	42271	1.10%	0.105%
17	12.727	1806	1809	1819	rBV	334920	362527	9.43%	0.898%
18	12.880	1832	1835	1841	rVB	74991	93410	2.43%	0.231%
19	13.004	1851	1856	1859	rBV	4114786	3797947	98.83%	9.404%
20	13.904	2005	2009	2016	rBV	367309	531252	13.82%	1.315%
21	14.057	2030	2035	2038	rBV	1259112	1236353	32.17%	3.061%
22	14.227	2061	2064	2067	rBV	54169	68299	1.78%	0.169%
23	14.533	2112	2116	2129	rVB2	223728	380655	9.91%	0.943%
24	14.839	2165	2168	2171	rBV	102757	91647	2.38%	0.227%
25	14.915	2179	2181	2184	rVB	51249	48722	1.27%	0.121%
26	15.186	2223	2227	2230	rBV	243054	277715	7.23%	0.688%
27	15.533	2281	2286	2290	rBV	915704	1109726	28.88%	2.748%
28	15.574	2290	2293	2299	rVB	117541	157024	4.09%	0.389%
29	16.021	2365	2369	2373	rVB	131778	190042	4.95%	0.471%
30	16.074	2374	2378	2388	rVB3	67935	153800	4.00%	0.381%
31	17.645	2638	2645	2655	rBV5	175273	561247	14.60%	1.390%
32	18.121	2721	2726	2736	rVB4	47067	120218	3.13%	0.298%
33	18.621	2806	2811	2817	rBV6	51392	124873	3.25%	0.309%
34	18.692	2818	2823	2833	rVB7	78016	194882	5.07%	0.483%

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ClientSampleId :
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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-BF070519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

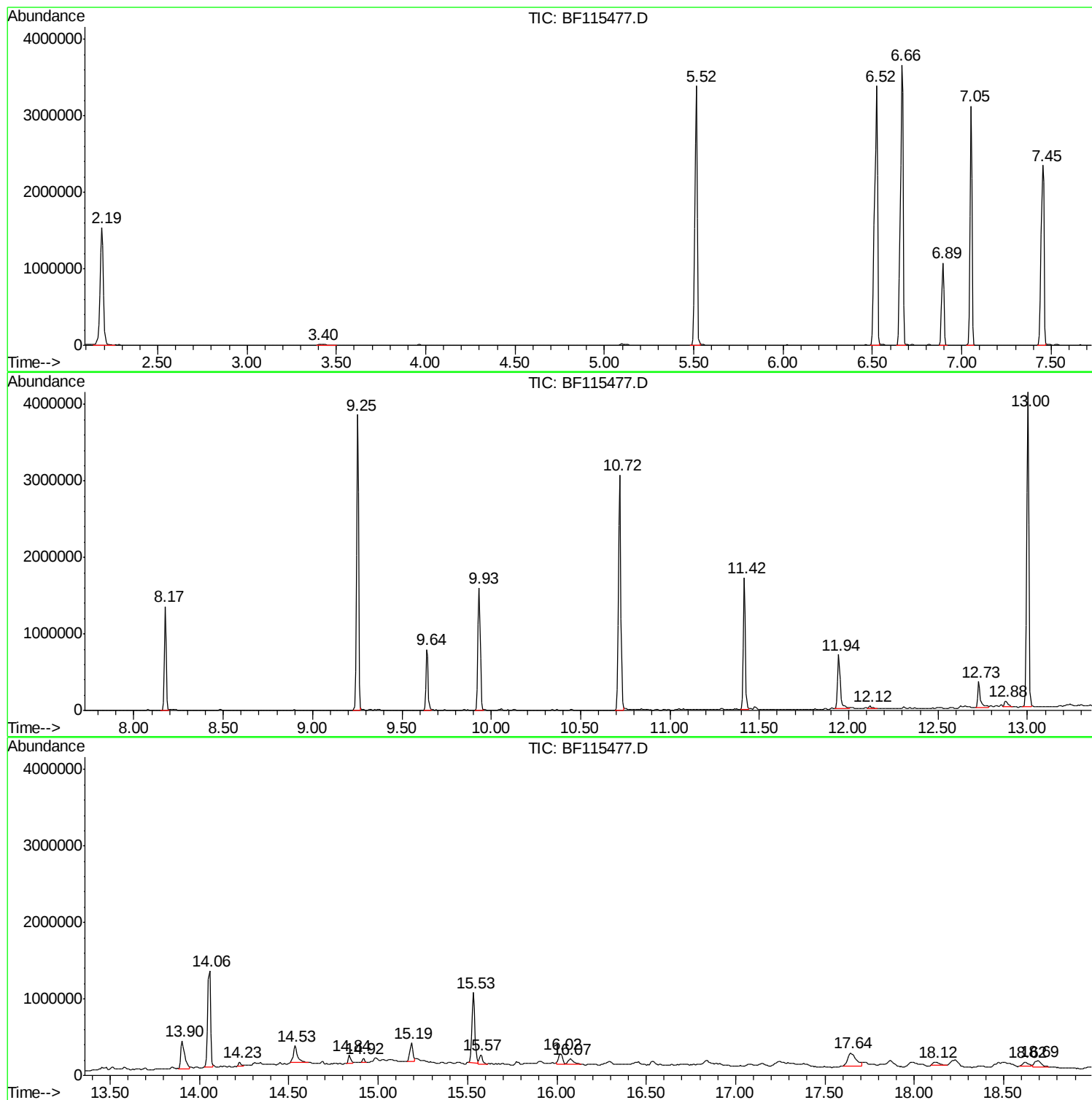
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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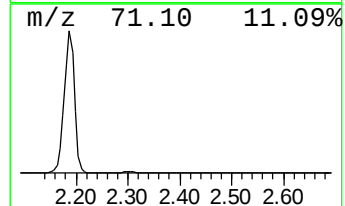
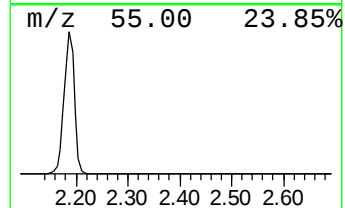
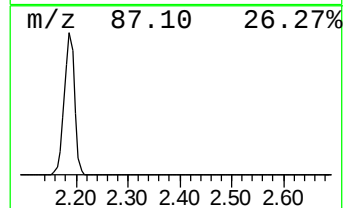
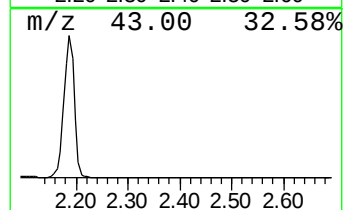
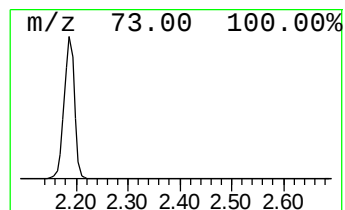
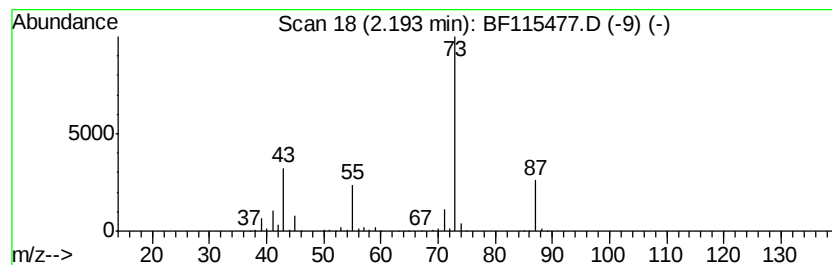
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	48.93 ng	2102180	1,4-Dichlorobenzene-d4	6.89

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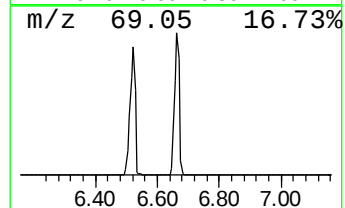
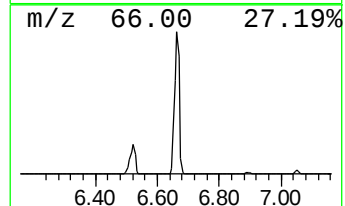
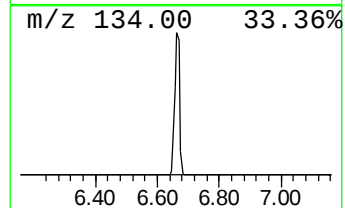
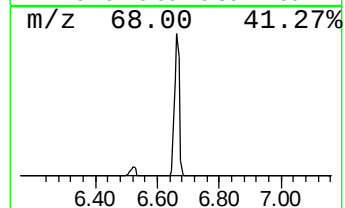
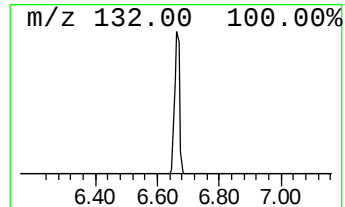
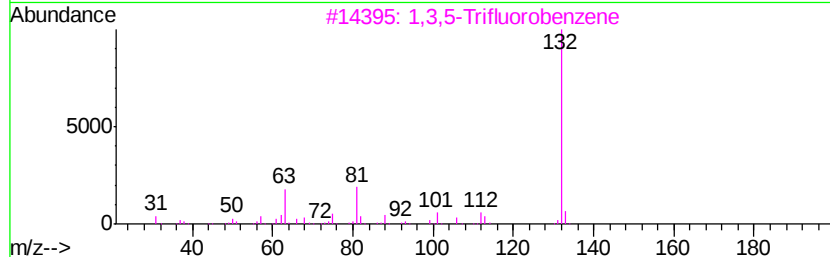
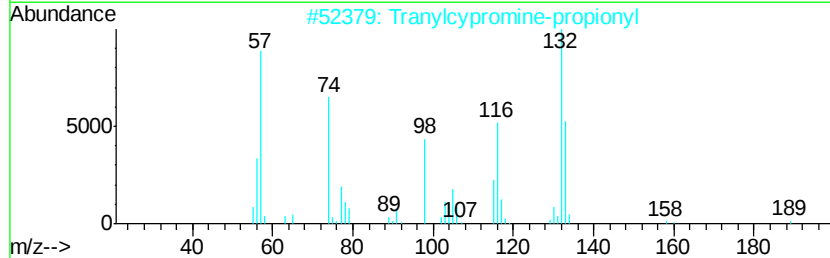
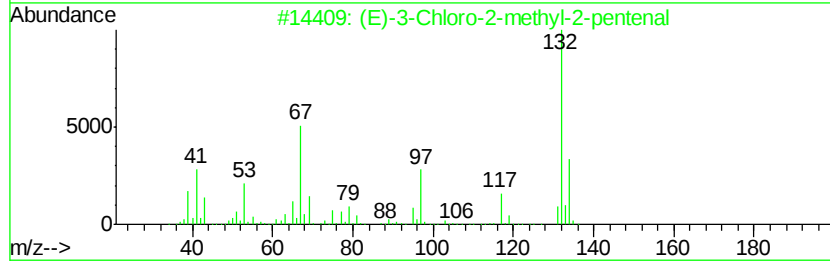
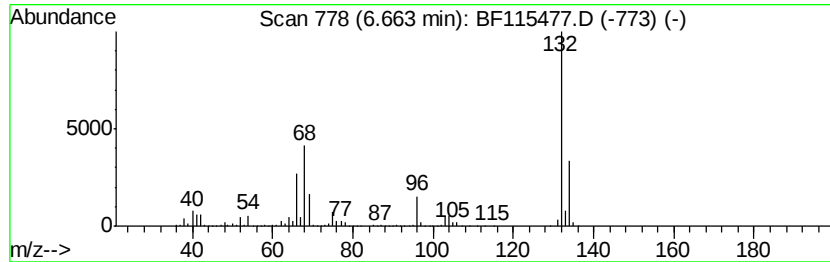
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	89.45 ng	3842860	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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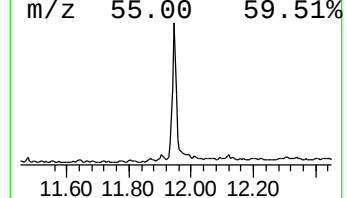
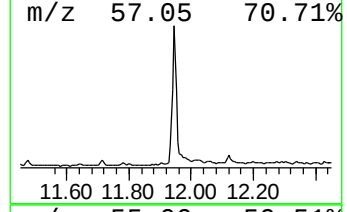
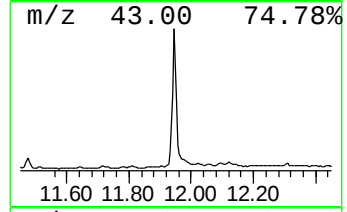
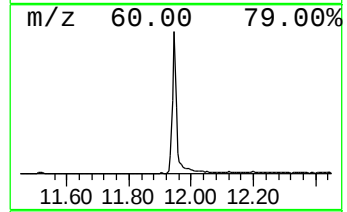
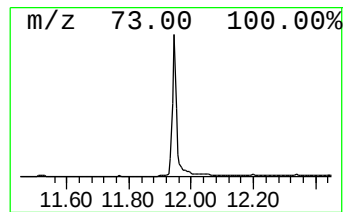
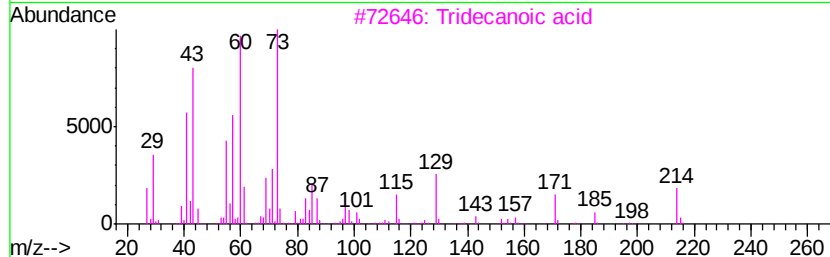
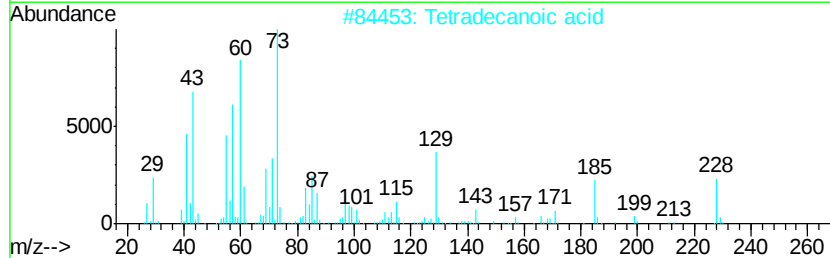
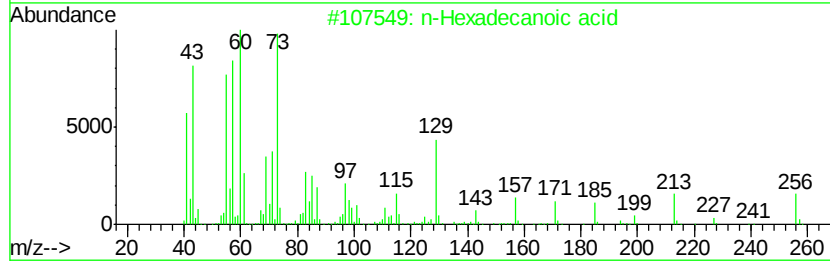
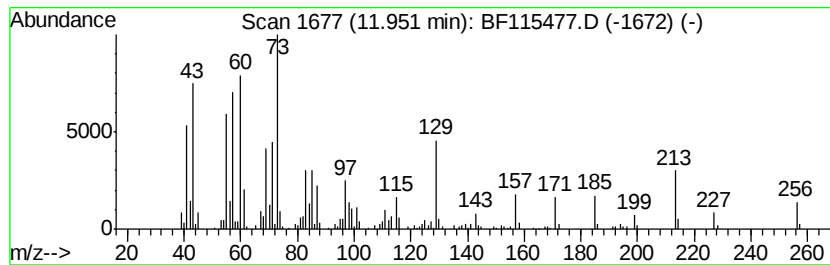
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	9.36 ng	684024	Phenanthrene-d10	11.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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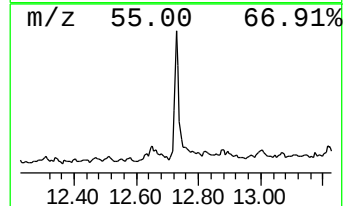
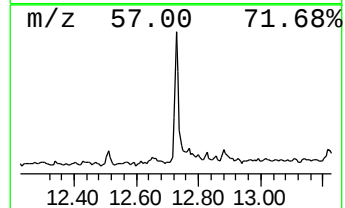
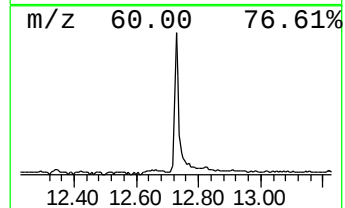
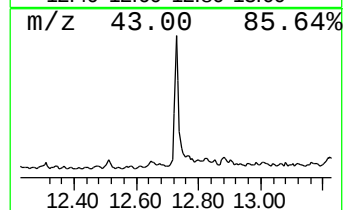
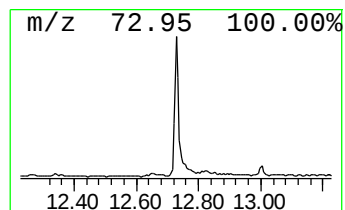
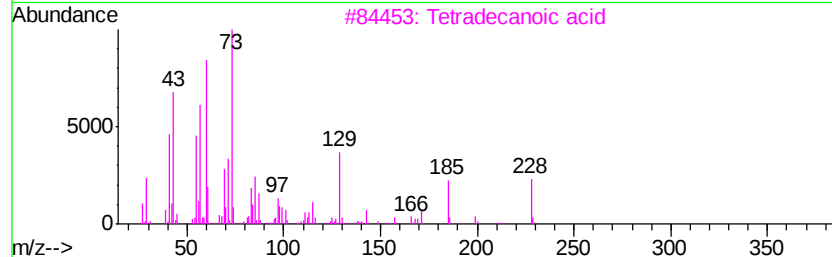
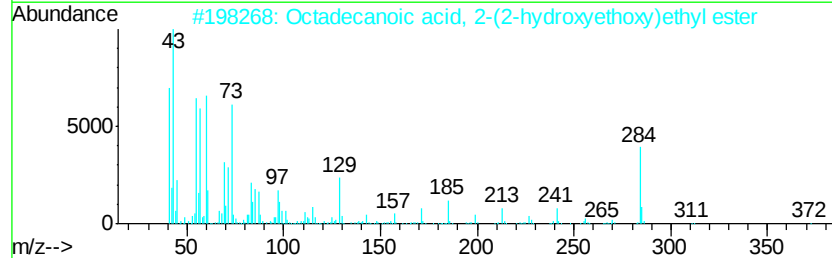
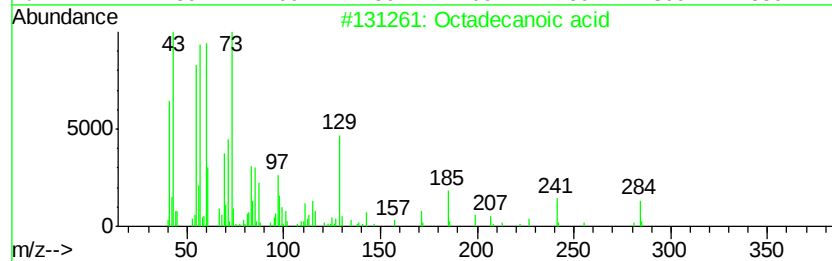
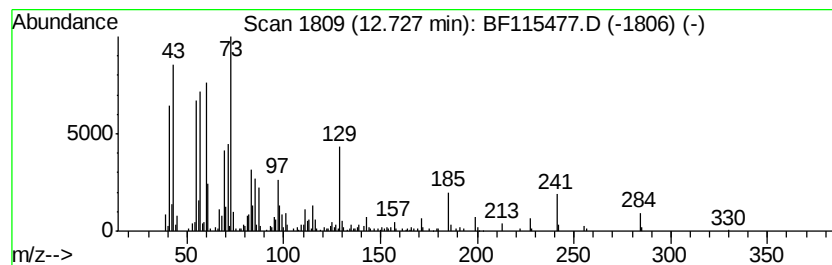
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	4.96 ng	362527	Phenanthrene-d10	11.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	87
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	76
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	68
5	n-Decanoic acid		172	C10H20O2	000334-48-5	68



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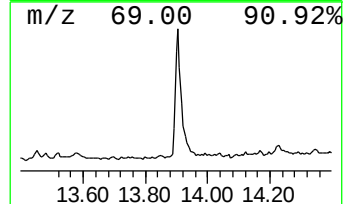
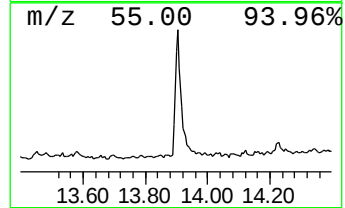
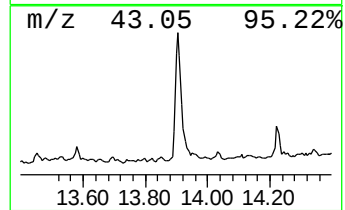
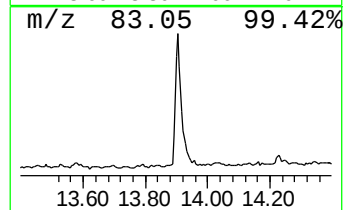
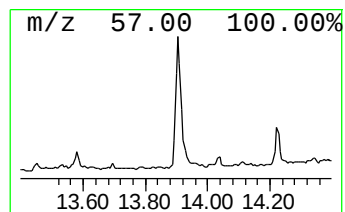
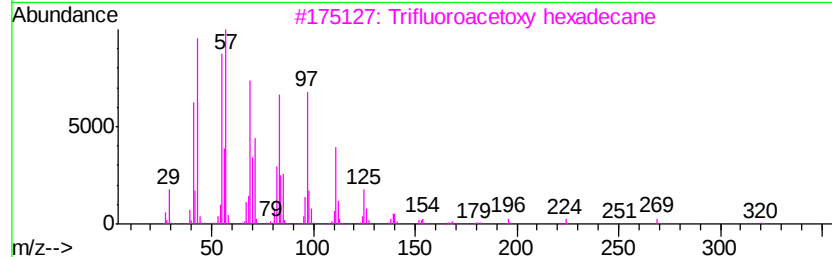
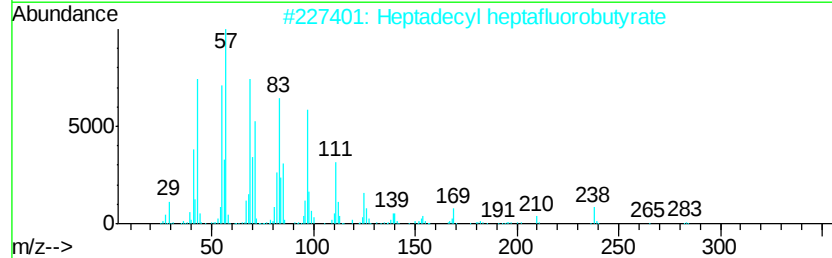
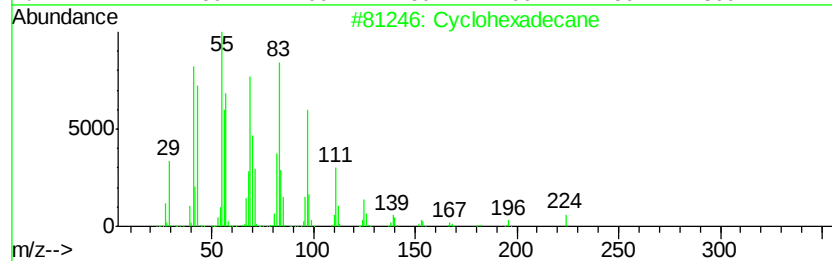
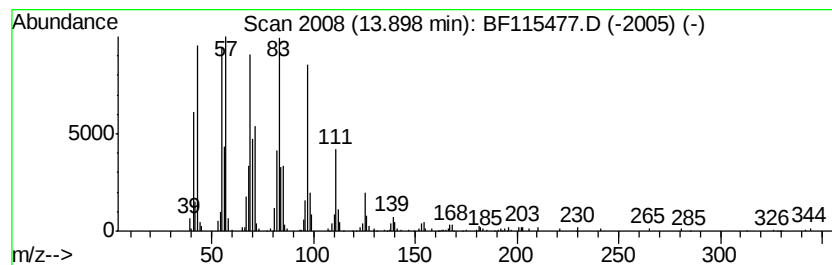
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	8.59 ng	531252	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexadecane	224	C16H32	000295-65-8	98
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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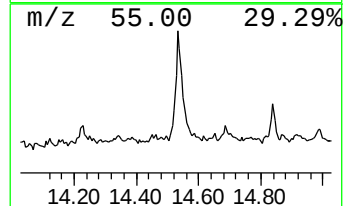
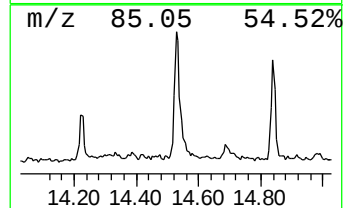
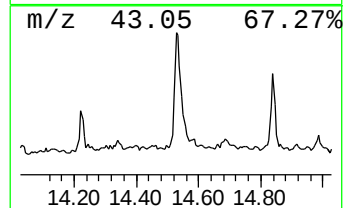
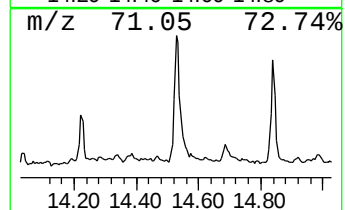
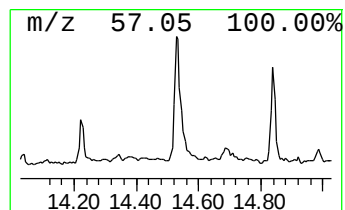
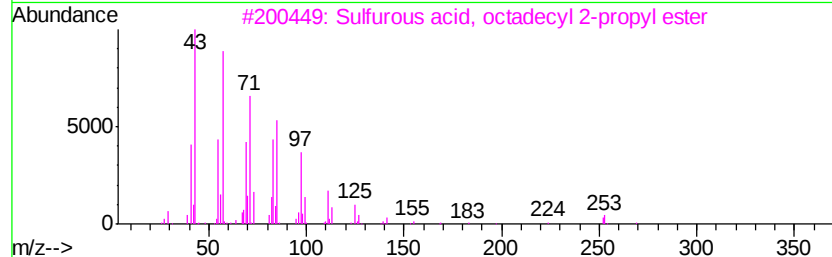
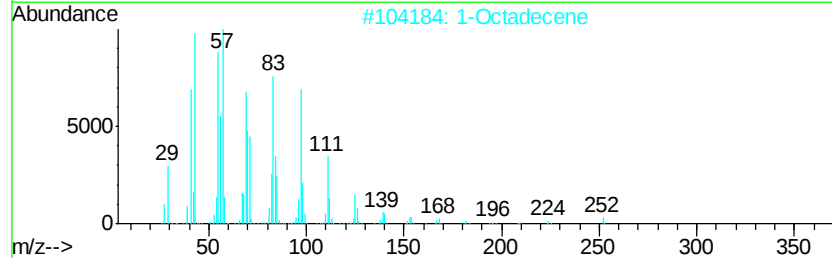
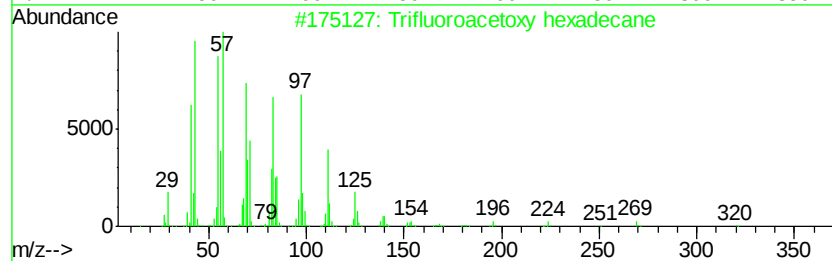
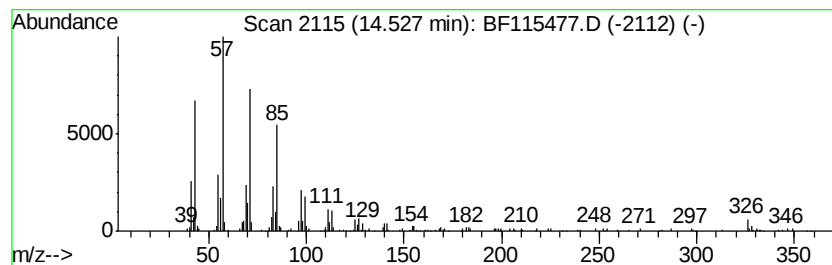
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ClientSampleId :
FK-PS-01-052

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.53	6.16 ng	380655	Chrysene-d12	14.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	92
2	1-Octadecene	252	C18H36	000112-88-9	92
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
5	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
Data File : BF115477.D
Acq On : 11 Jul 2019 1:15
Operator : HP/JU
Sample : K3700-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-052

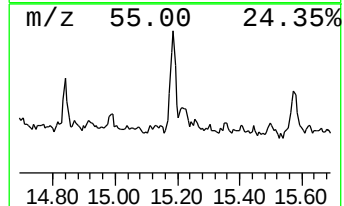
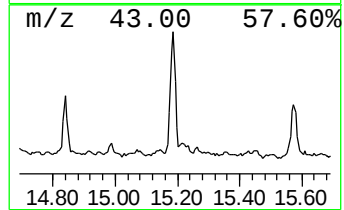
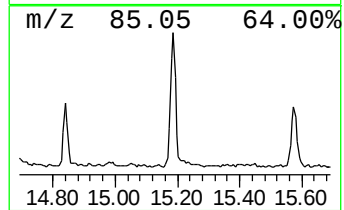
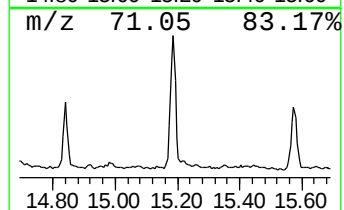
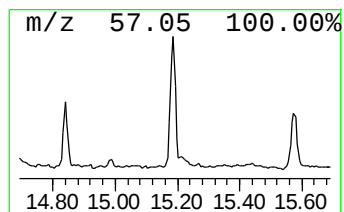
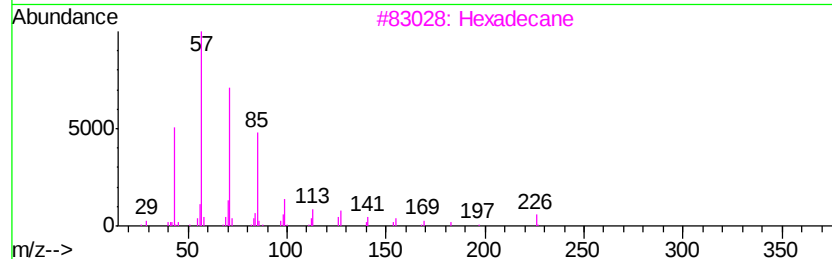
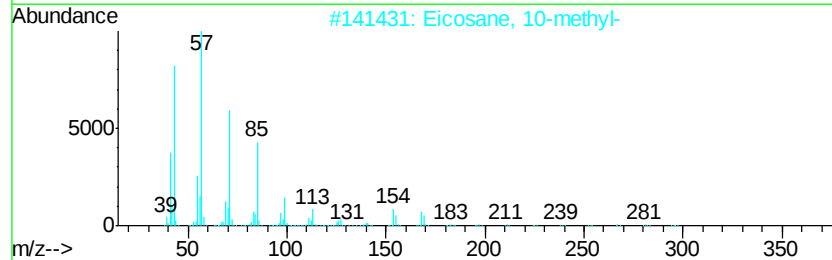
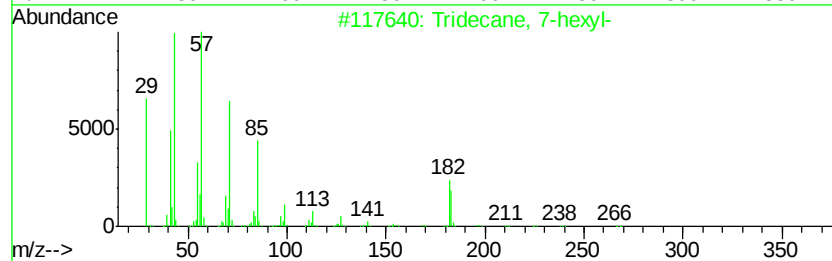
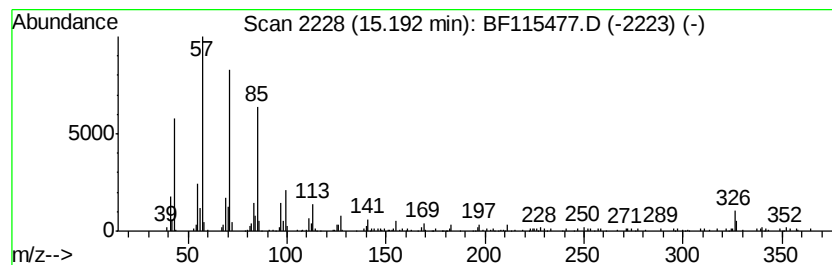
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 7-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	5.01 ng	277715	Perylene-d12	15.53

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 7-hexyl-	268	C19H40	007225-66-3	93
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3		Hexadecane	226	C16H34	000544-76-3	91
4		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
Data File : BF115477.D
Acq On : 11 Jul 2019 1:15
Operator : HP/JU
Sample : K3700-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-PS-01-052

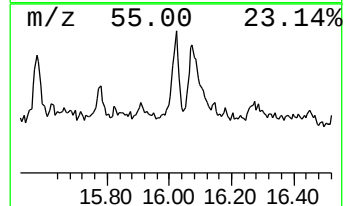
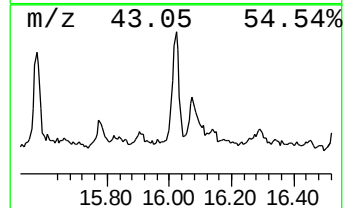
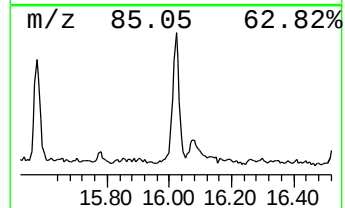
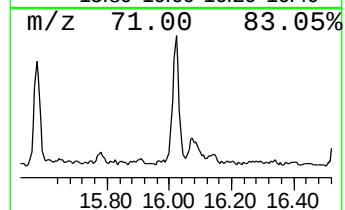
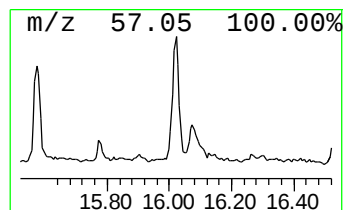
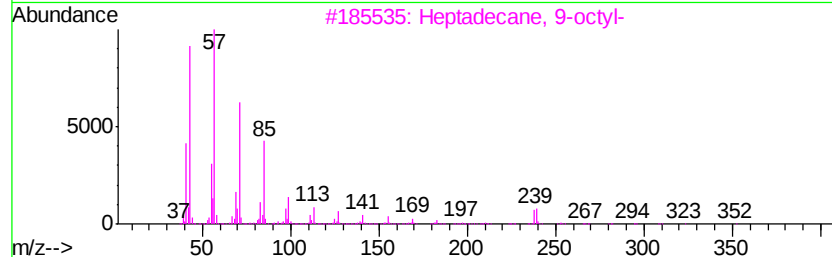
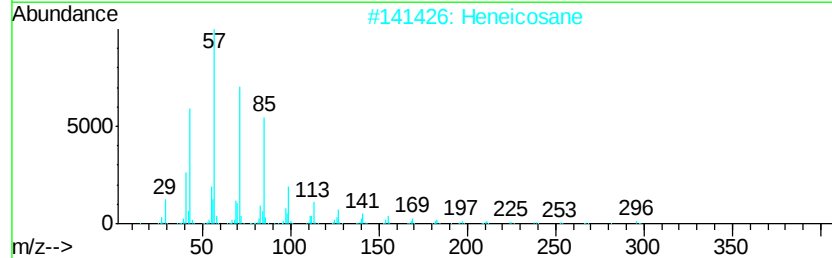
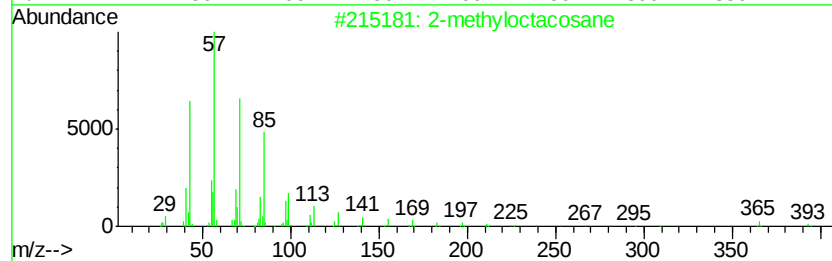
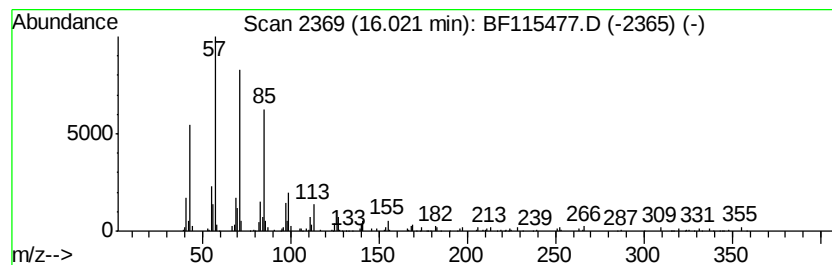
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	3.43 ng	190042	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
Data File : BF115477.D
Acq On : 11 Jul 2019 1:15
Operator : HP/JU
Sample : K3700-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

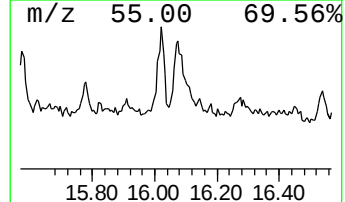
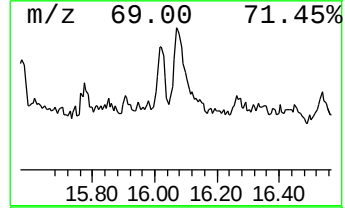
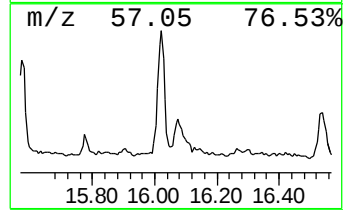
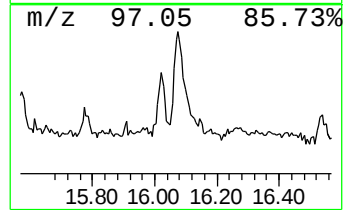
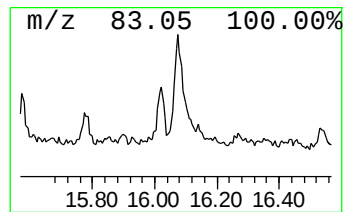
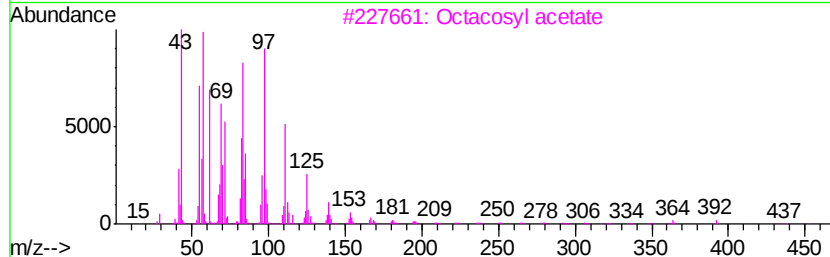
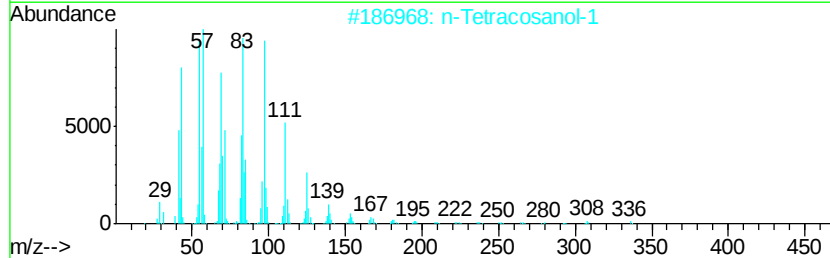
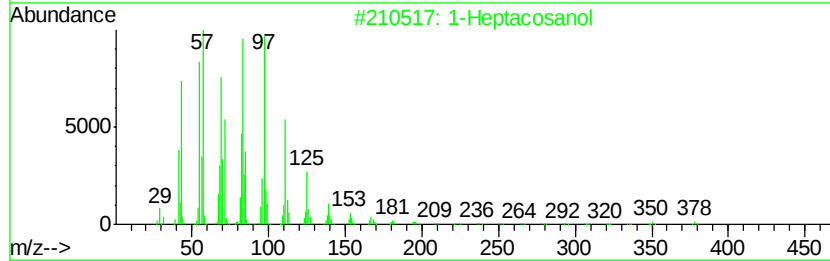
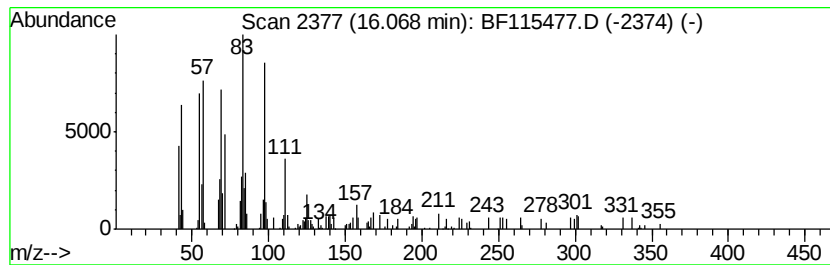
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptacosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.77 ng	153800	Perylene-d12	15.53
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heptacosanol	396 C27H56O	002004-39-9 89
2		n-Tetracosanol-1	354 C24H50O	000506-51-4 60
3		Octacosyl acetate	452 C30H60O2	018206-97-8 60
4		Heptadecyl heptafluorobutyrate	452 C21H35F7O2	959085-66-6 60
5		Heptafluorobutyric acid, n-octad...	466 C22H37F7O2	000400-57-7 60



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
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Operator : HP/JU
Sample : K3700-01
Misc :
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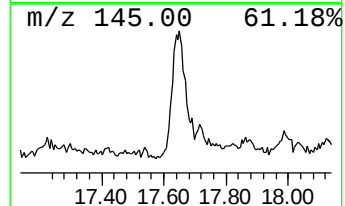
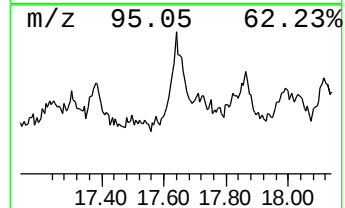
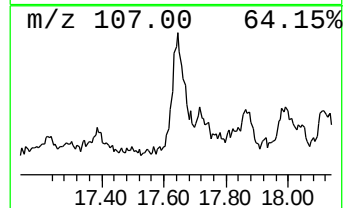
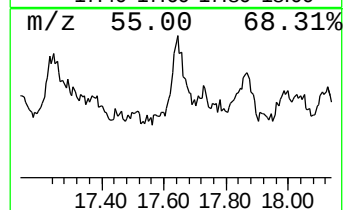
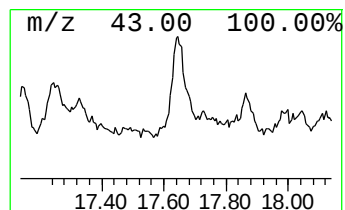
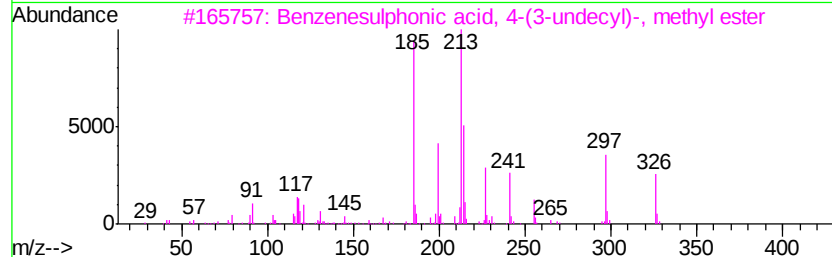
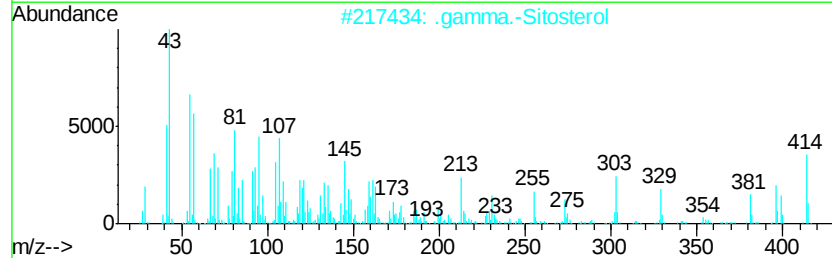
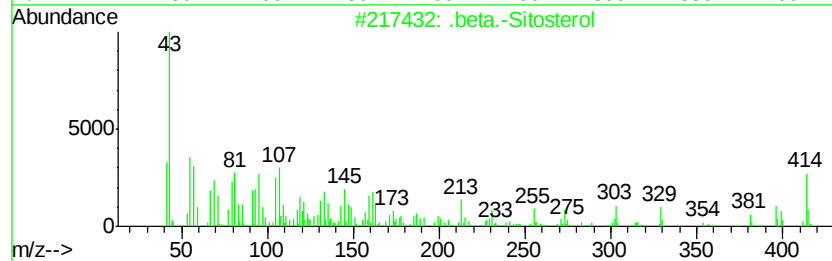
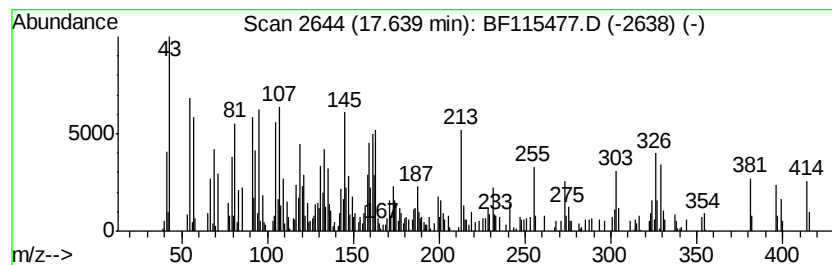
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .beta.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	10.12 ng	561247	Perylene-d12	15.53
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 96
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 46
3		Benzenesulphonic acid, 4-(3-unde...	326 C18H30O3S	1000376-68-2 14
4		As-Indacen-1(2H)-one, 3,6,7,8-te...	228 C16H20O	055591-18-9 11
5		4-(Acetyloxy)-.gamma.-[4-(acetyl...	370 C21H22O6	135439-71-3 11



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
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Sample : K3700-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

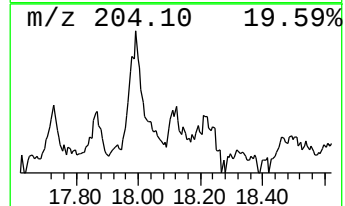
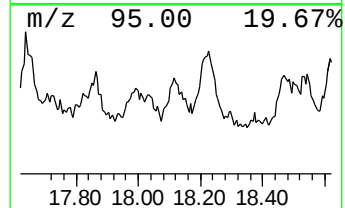
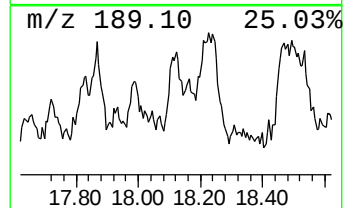
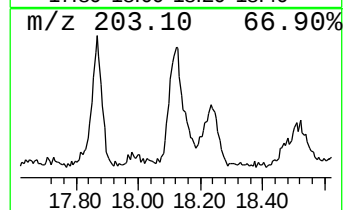
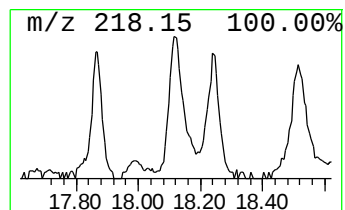
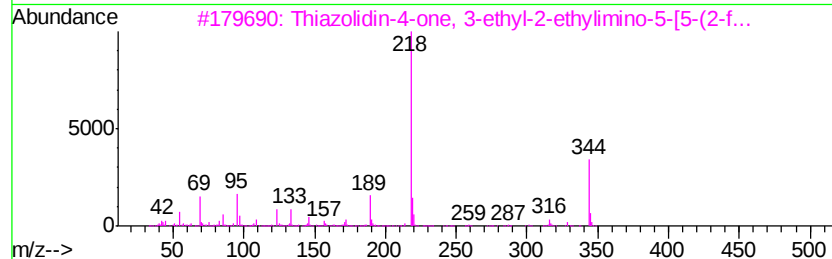
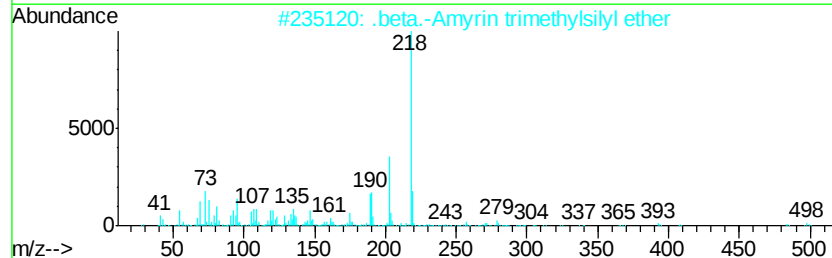
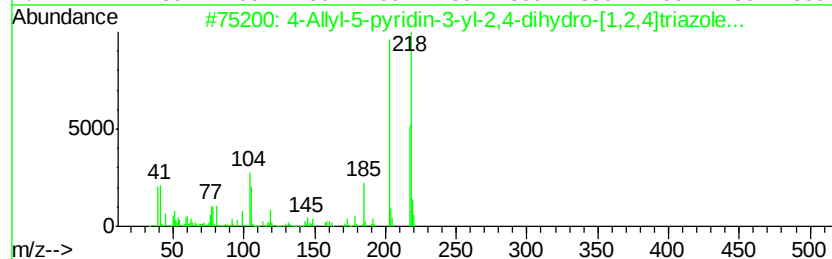
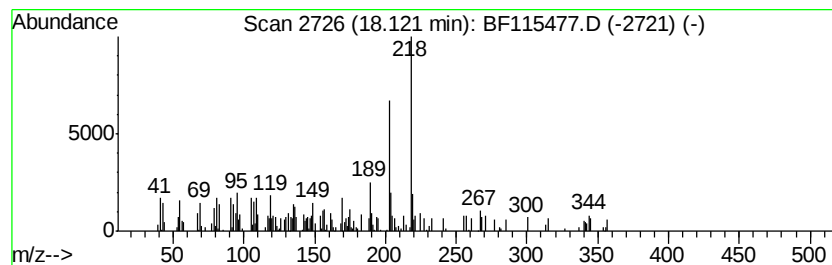
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 4-Allyl-5-pyridin-3-yl-2,4-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.12	2.17 ng	120218	Perylene-d12	15.53		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	53	
2	.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	50	
3	Thiazolidin-4-one, 3-ethyl-2-eth...	344	C18H17FN2O2S	1000272-54-5	47	
4	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	45	
5	D-Norandrostan-16-ol, (5.alpha.,...	262	C18H30O	035575-61-2	43	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
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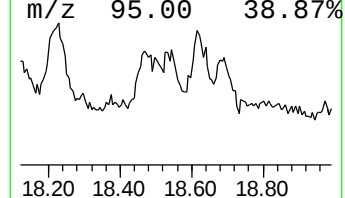
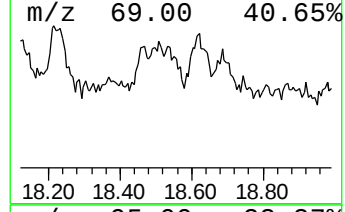
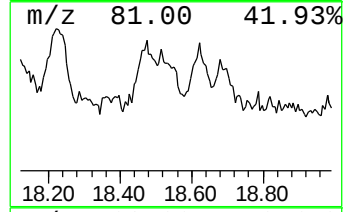
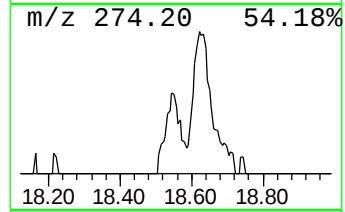
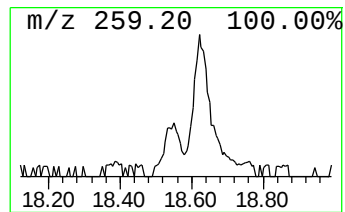
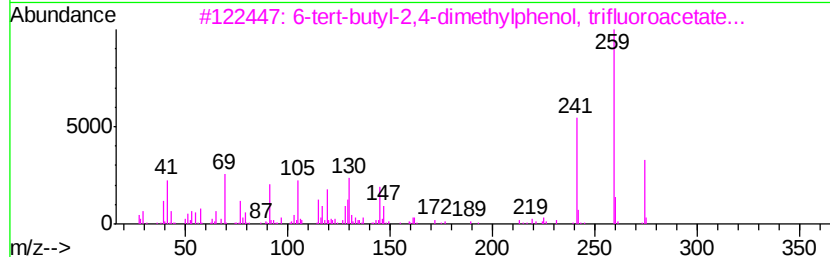
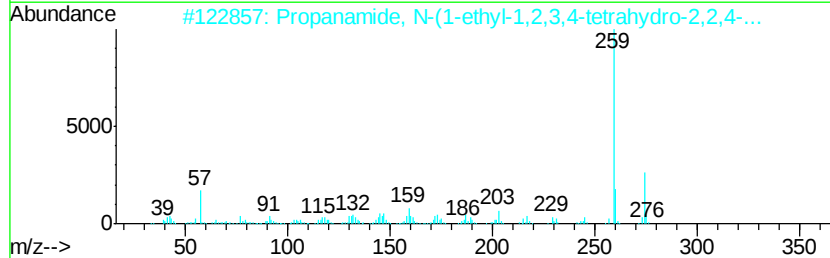
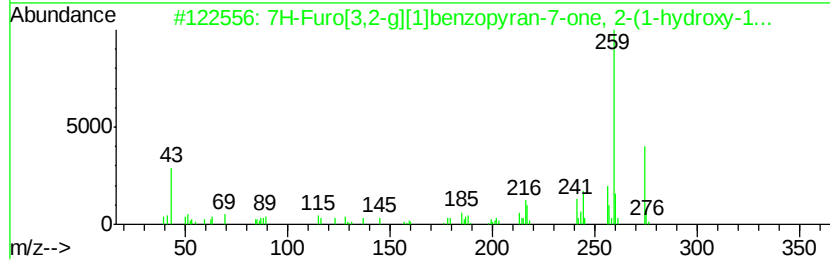
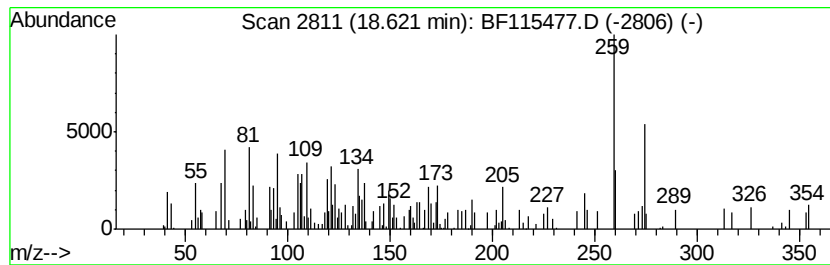
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.62 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.62	2.25 ng	124873	Perylene-d12	15.53
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	7H-Furo[3,2-g][1]benzopyran-7-on...	274 C15H14O5	054087-32-0	46
2	Propanamide, N-(1-ethyl-1,2,3,4-...	274 C17H26N2O	063134-09-8	43
3	6-tert-butyl-2,4-dimethylphenol,...	274 C14H17F3O2	1000376-41-4	37
4	Silane, diethyldiisohexyloxy-	288 C16H36O2Si	1000363-31-6	27
5	Dihydro-pretazettine	333 C18H23NO5	021850-86-2	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
Data File : BF115477.D
Acq On : 11 Jul 2019 1:15
Operator : HP/JU
Sample : K3700-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-052

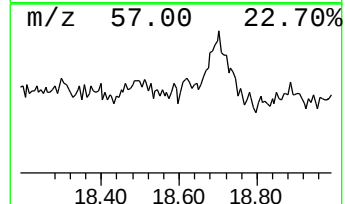
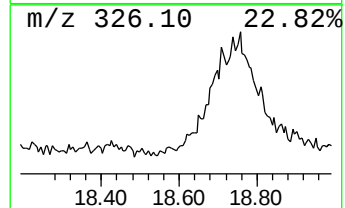
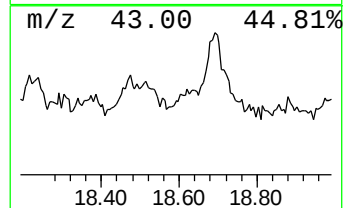
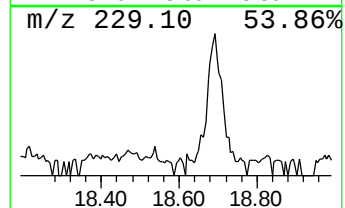
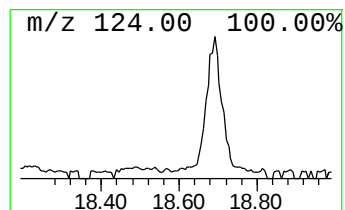
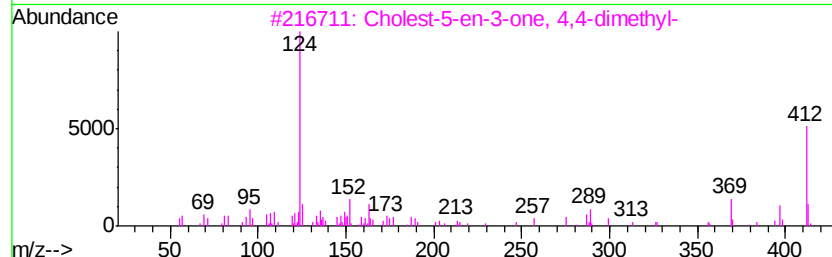
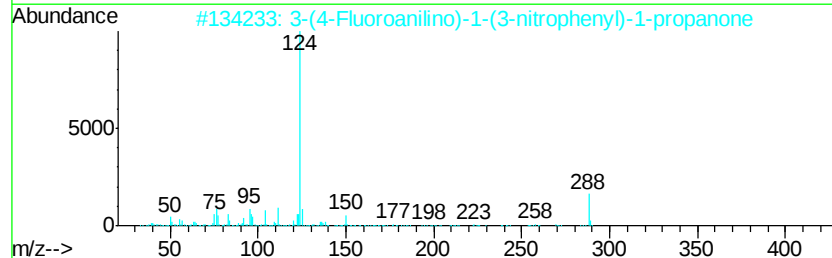
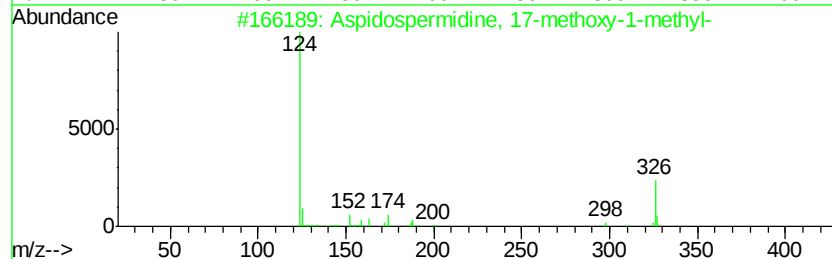
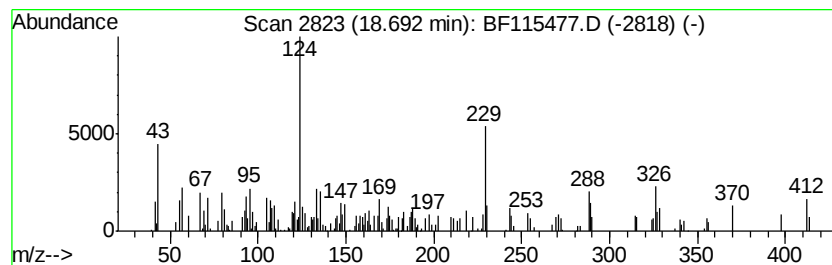
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.69 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.69	3.51 ng	194882	Perylene-d12	15.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aspidospermidine, 17-methoxy-1-m...	326	C21H30N2O	055400-14-1	45
2			3-(4-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	350039-84-8	38
3			Cholest-5-en-3-one, 4,4-dimethyl-	412	C29H48O	002220-42-0	35
4			Aspidospermidine-3-carboxylic ac...	340	C21H28N2O2	055700-36-2	30
5			1,3-Propanediol, 2-(3-ethylidene...	328	C20H28N2O2	001850-32-4	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071019\
 Data File : BF115477.D
 Acq On : 11 Jul 2019 1:15
 Operator : HP/JU
 Sample : K3700-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-052

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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...	2.19	48.9	ng	2102180	1	6.89	859207	20.0
unknown6.66	6.66	89.5	ng	3842860	1	6.89	859207	20.0
n-Hexadecanoic acid	11.95	9.4	ng	684024	4	11.42	1461370	20.0
Octadecanoic acid	12.73	5.0	ng	362527	4	11.42	1461370	20.0
Cyclohexadecane	13.90	8.6	ng	531252	5	14.06	1236350	20.0
Trifluoroacetoxy ...	14.53	6.2	ng	380655	5	14.06	1236350	20.0
Tridecane, 7-hexyl-	15.19	5.0	ng	277715	6	15.53	1109730	20.0
2-methyloctacosane	16.02	3.4	ng	190042	6	15.53	1109730	20.0
1-Heptacosanol	16.07	2.8	ng	153800	6	15.53	1109730	20.0
.beta.-Sitosterol	17.64	10.1	ng	561247	6	15.53	1109730	20.0
4-Allyl-5-pyridin...	18.12	2.2	ng	120218	6	15.53	1109730	20.0
unknown18.62	18.62	2.3	ng	124873	6	15.53	1109730	20.0
unknown18.69	18.69	3.5	ng	194882	6	15.53	1109730	20.0