

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071618\
 Data File : BF107412.D
 Acq On : 16 Jul 2018 19:45
 Operator : JU/SJ
 Sample : J3976-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-033

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-BF071618.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.213	485	489	494	rVB	328717	392920	10.26%	1.053%
2	5.596	549	554	557	rBV	3367321	3144021	82.10%	8.423%
3	6.595	718	724	728	rBV	3143118	3379326	88.24%	9.053%
4	6.743	745	749	753	rVB	3451467	3365429	87.88%	9.016%
5	6.795	755	758	761	rVB	46234	42672	1.11%	0.114%
6	6.978	785	789	792	rBV	1453030	1138958	29.74%	3.051%
7	7.131	811	815	819	rBV	2708240	2534453	66.18%	6.790%
8	7.537	879	884	887	rBV	2350176	2095661	54.72%	5.614%
9	8.260	1003	1007	1010	rBV	1639616	1430053	37.34%	3.831%
10	9.336	1185	1190	1193	rVB	4185647	3829528	100.00%	10.259%
11	9.725	1251	1256	1259	rBV	734272	572606	14.95%	1.534%
12	10.019	1302	1306	1310	rBV2	1950896	1671770	43.65%	4.479%
13	10.807	1434	1440	1443	rBV	2679414	2491630	65.06%	6.675%
14	10.919	1456	1459	1462	rVB5	36015	43033	1.12%	0.115%
15	11.507	1556	1559	1563	rBV	1815347	1757610	45.90%	4.709%
16	12.025	1642	1647	1655	rBV3	287375	383221	10.01%	1.027%
17	12.760	1769	1772	1776	rVB5	63468	68765	1.80%	0.184%
18	12.807	1777	1780	1787	rBV8	68559	97462	2.55%	0.261%
19	13.095	1825	1829	1833	rBV	3598808	3576987	93.41%	9.583%
20	13.524	1899	1902	1905	rBV4	95907	96932	2.53%	0.260%
21	13.783	1944	1946	1950	rBV5	35886	42419	1.11%	0.114%
22	13.977	1976	1979	1987	rBV2	264132	287988	7.52%	0.772%
23	14.154	2005	2009	2014	rVB	1415157	1342954	35.07%	3.598%
24	14.301	2032	2034	2037	rBV4	57596	64278	1.68%	0.172%
25	14.613	2084	2087	2092	rVB3	158717	216397	5.65%	0.580%
26	14.936	2140	2142	2146	rVB5	69413	64289	1.68%	0.172%
27	15.018	2153	2156	2160	rVB2	188099	192153	5.02%	0.515%
28	15.295	2200	2203	2208	rVB3	154016	172140	4.50%	0.461%
29	15.689	2265	2270	2279	rVB	985343	1347505	35.19%	3.610%
30	16.165	2348	2351	2356	rBV7	67020	103586	2.70%	0.278%
31	16.218	2356	2360	2366	rBV9	97839	164430	4.29%	0.440%
32	17.430	2563	2566	2568	rBV4	37296	48569	1.27%	0.130%
33	17.877	2635	2642	2649	rBV4	244949	534145	13.95%	1.431%
34	17.971	2655	2658	2665	rVB9	60266	144548	3.77%	0.387%

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ClientSampleId :
FK-PS-01-033

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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.242	2697	2704	2711	rBV9	93007	240253	6.27%	0.644%
36	18.389	2723	2729	2735	rBV9	75259	157937	4.12%	0.423%
37	18.759	2790	2792	2795	rBV4	36376	46318	1.21%	0.124%
38	18.912	2815	2818	2819	rBV3	49584	45122	1.18%	0.121%

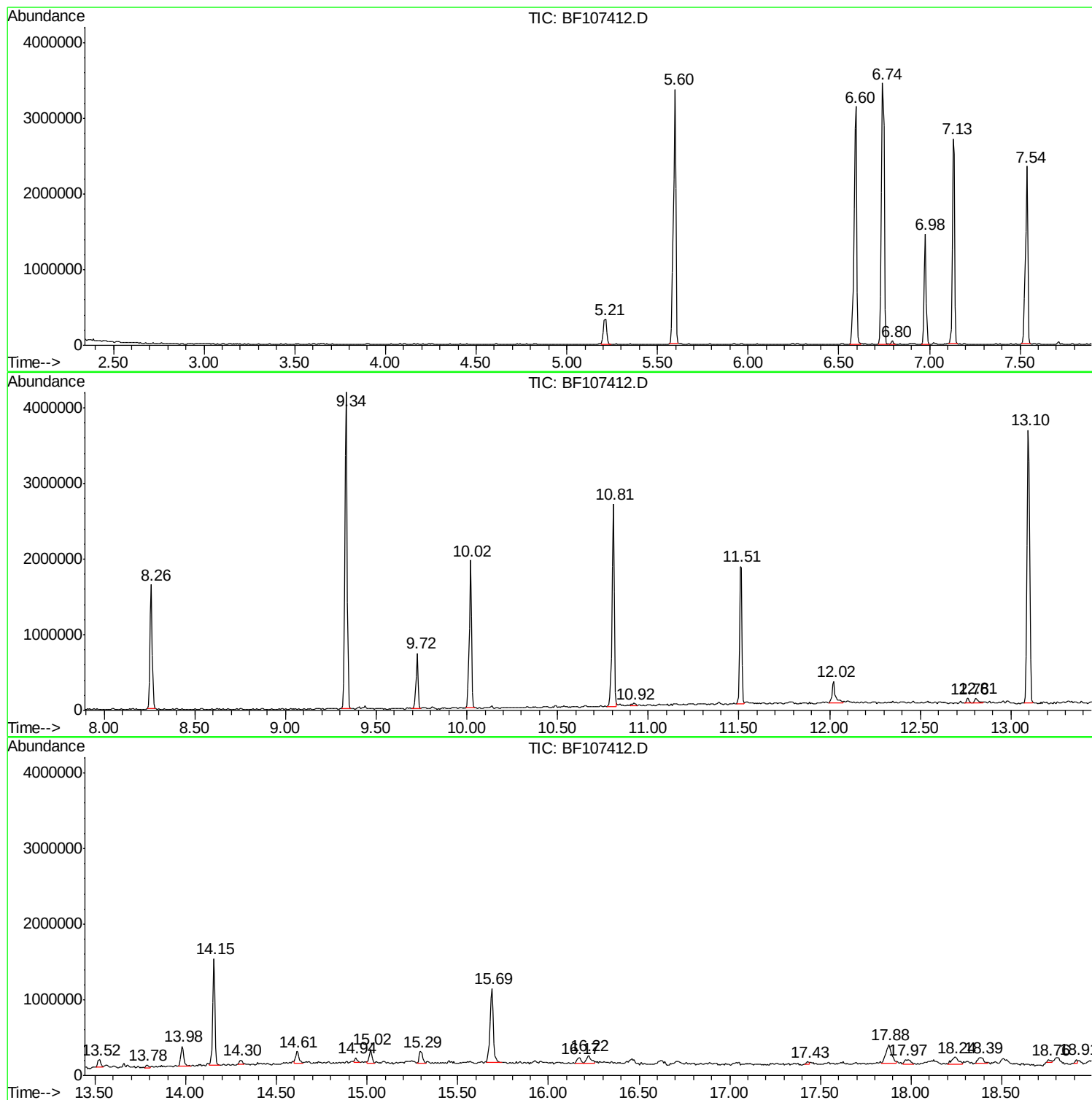
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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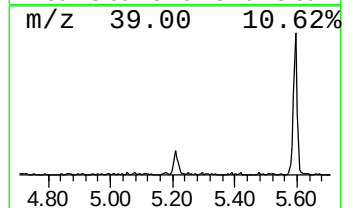
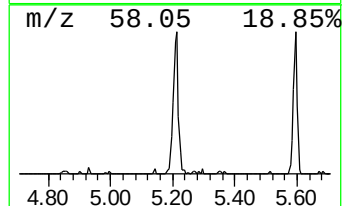
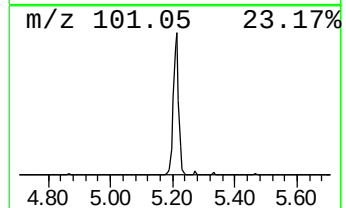
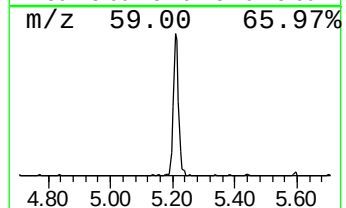
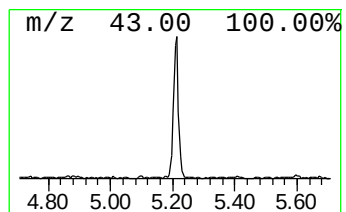
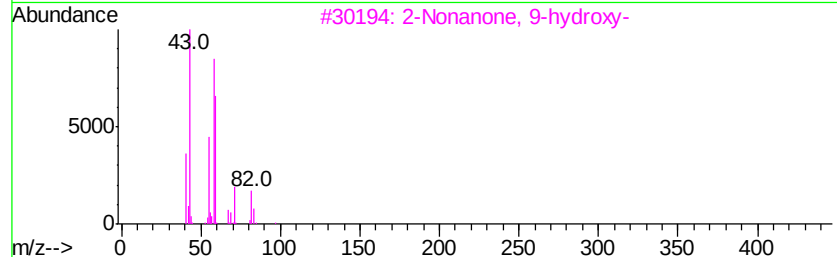
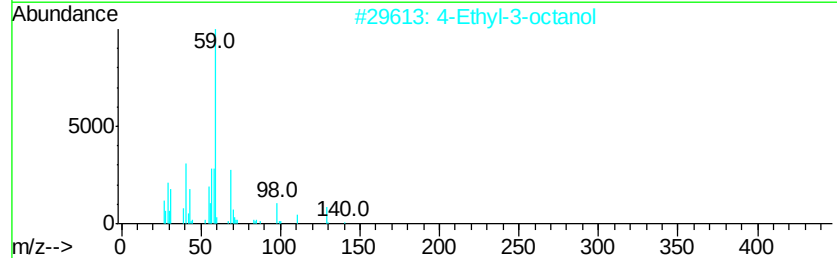
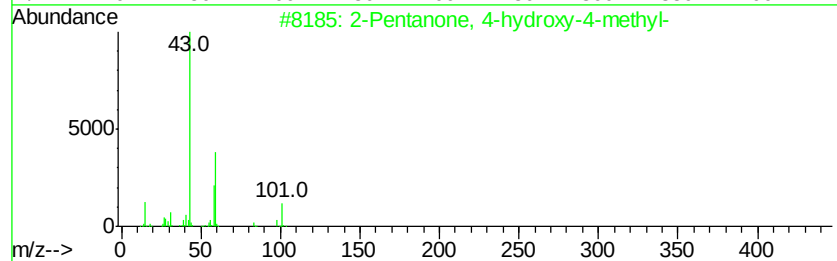
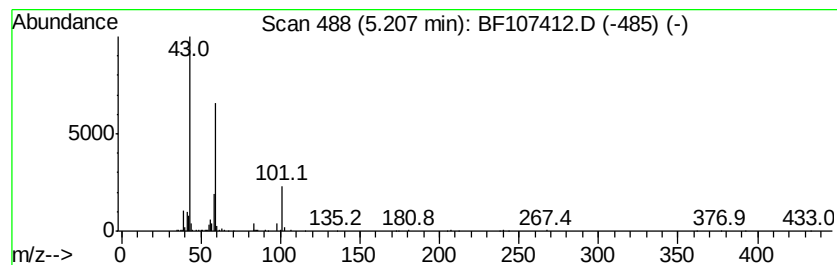
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	6.90 ng	392920	1,4-Dichlorobenzene-d4	6.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	23
4			Silane, dimethyl-	60	C2H8Si	001111-74-6	16
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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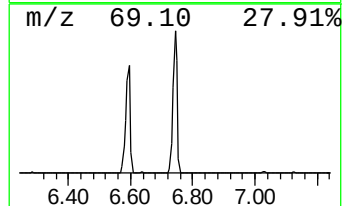
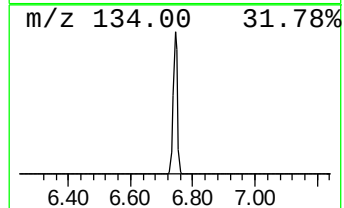
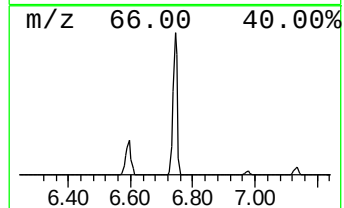
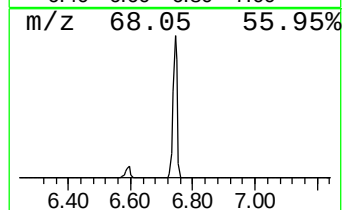
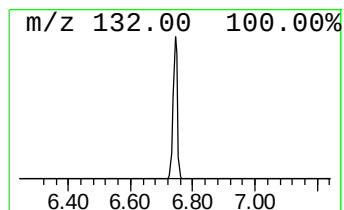
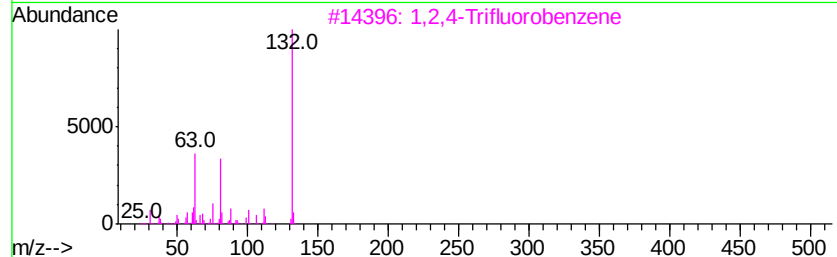
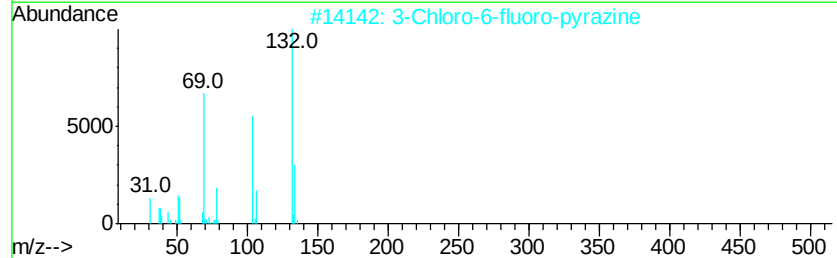
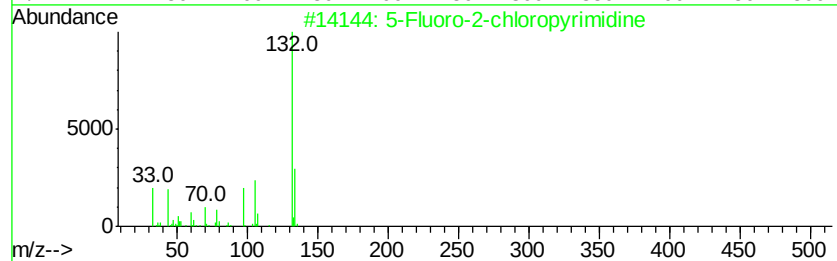
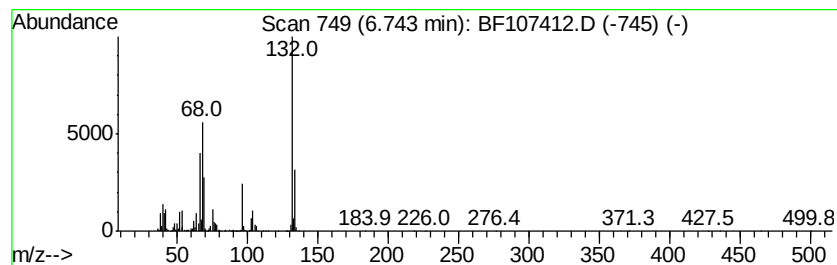
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	59.10 ng	3365430	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10



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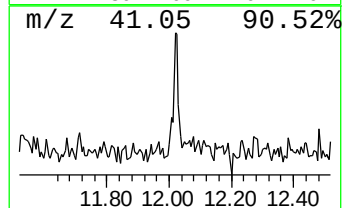
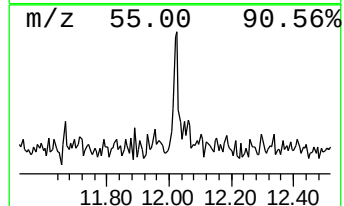
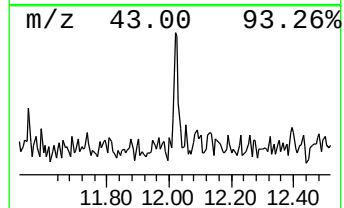
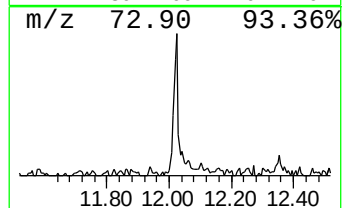
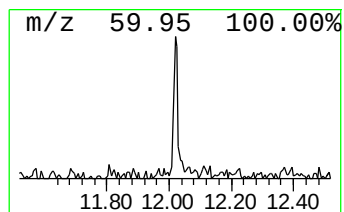
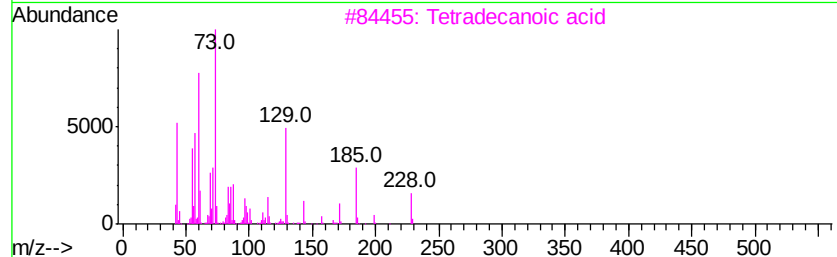
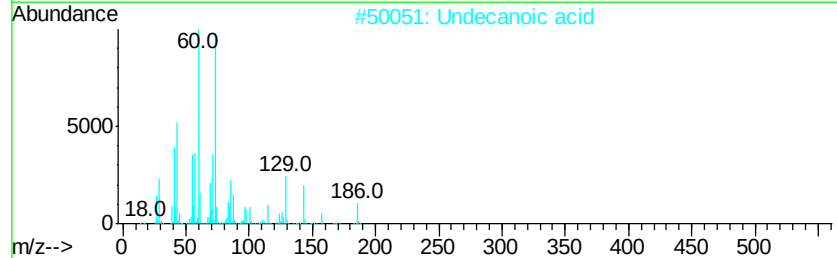
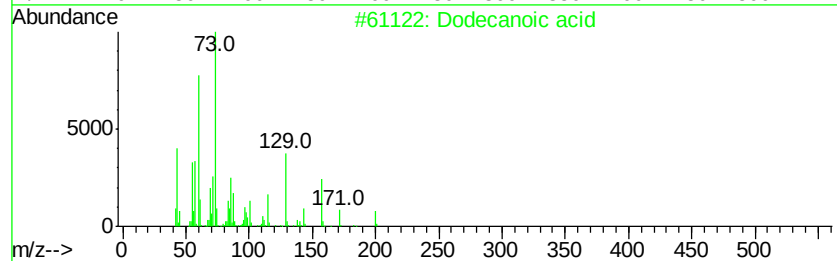
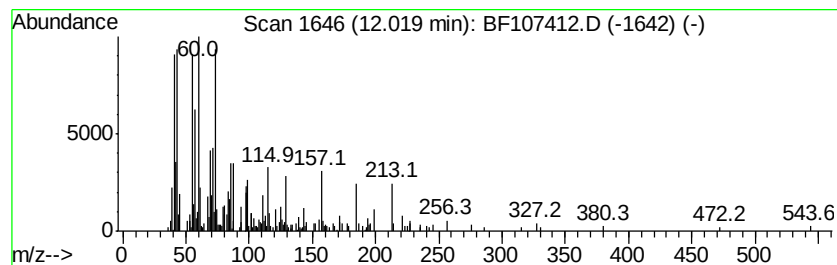
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	4.36 ng	383221	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	49
2	Undecanoic acid	186	C11H22O2	000112-37-8	49
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	27
5	n-Decanoic acid	172	C10H20O2	000334-48-5	27



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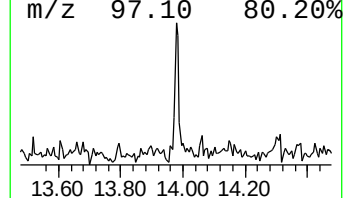
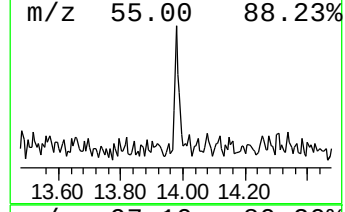
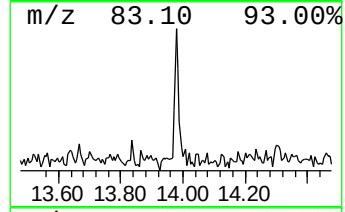
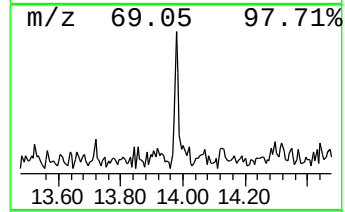
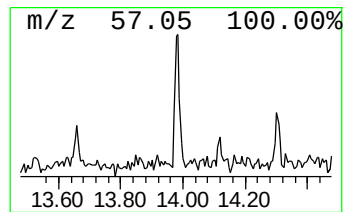
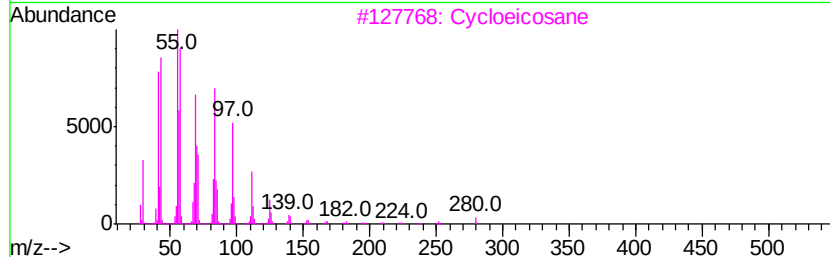
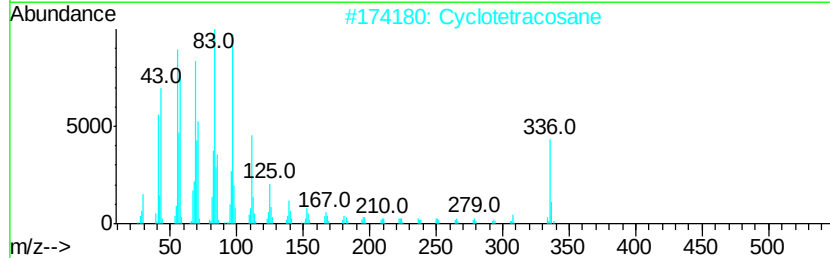
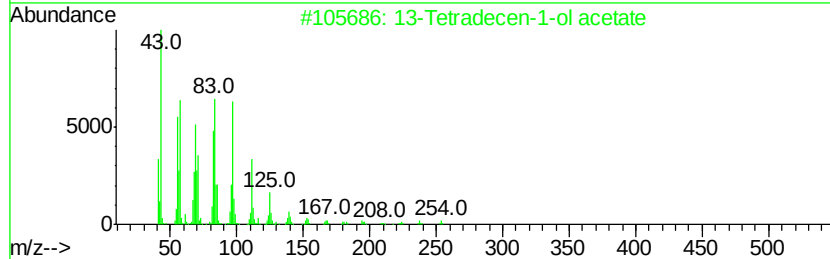
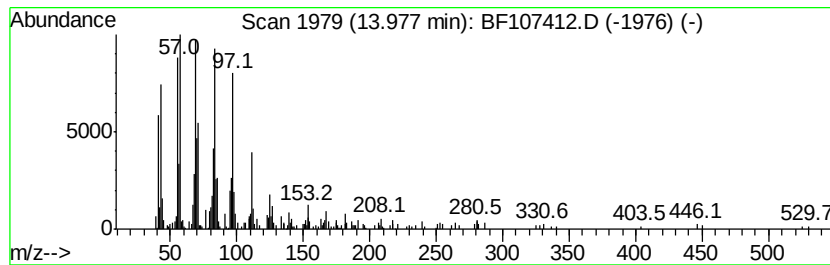
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 13-Tetradecen-1-ol acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.98	4.29 ng	287988	Chrysene-d12		14.15		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
2			Cyclotetracosane	336	C24H48	000297-03-0	93
3			Cycloeicosane	280	C20H40	000296-56-0	92
4			Cyclotetradecane	196	C14H28	000295-17-0	91
5			Behenic alcohol	326	C22H46O	000661-19-8	90



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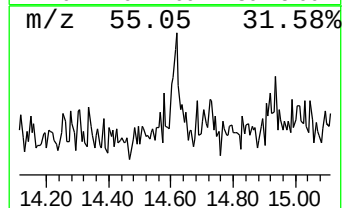
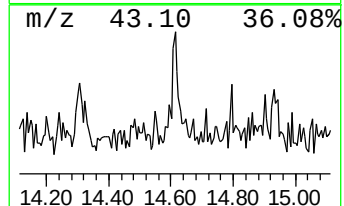
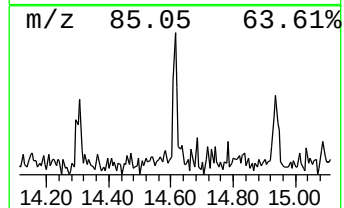
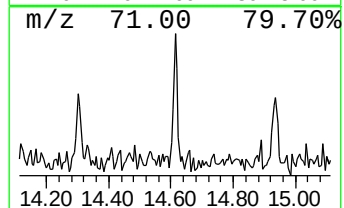
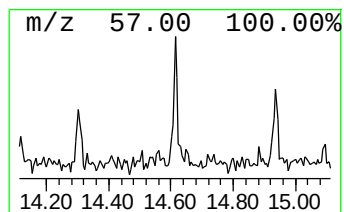
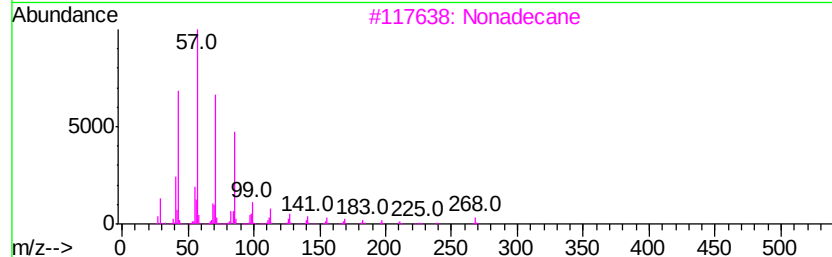
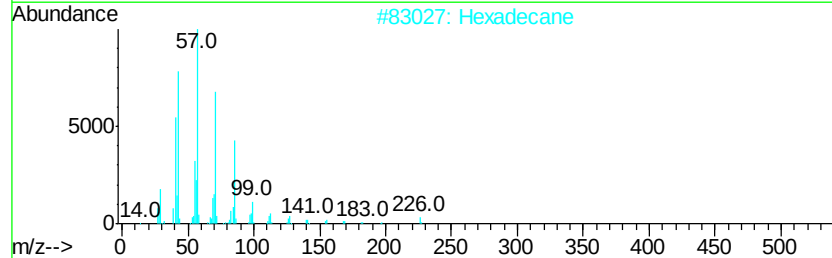
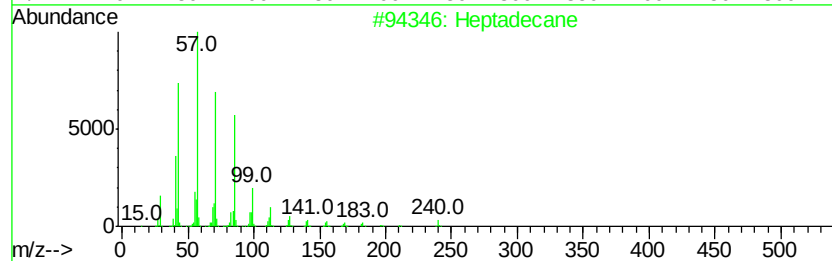
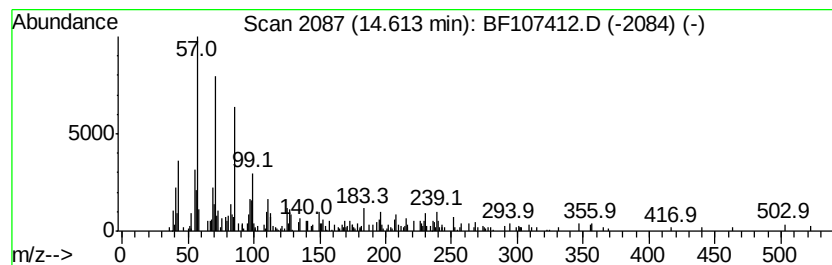
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	3.22 ng	216397	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Hexadecane		226	C16H34	000544-76-3	76
3	Nonadecane		268	C19H40	000629-92-5	76
4	Hentriacontane		437	C31H64	000630-04-6	72
5	Octadecane		254	C18H38	000593-45-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
Data File : BF107412.D
Acq On : 16 Jul 2018 19:45
Operator : JU/SJ
Sample : J3976-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-033

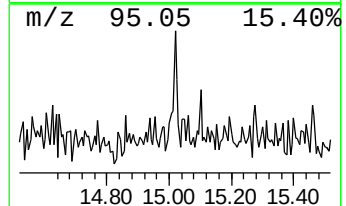
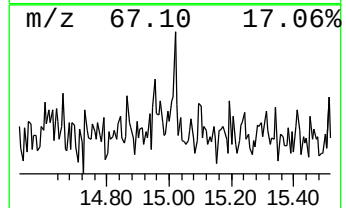
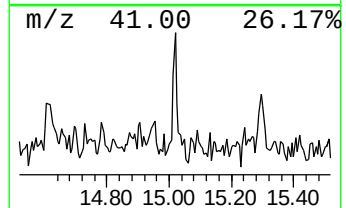
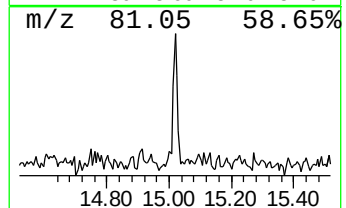
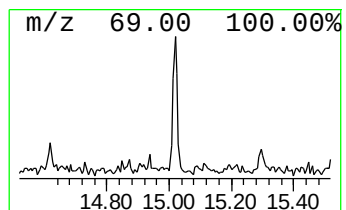
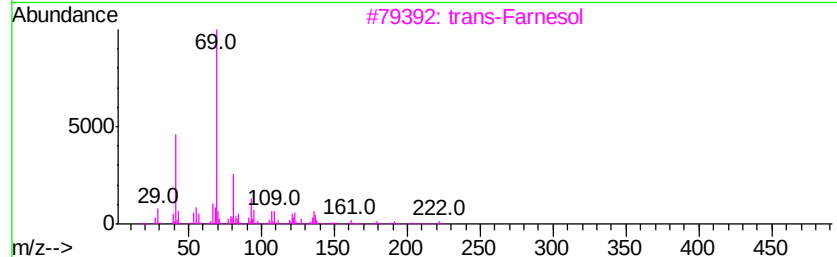
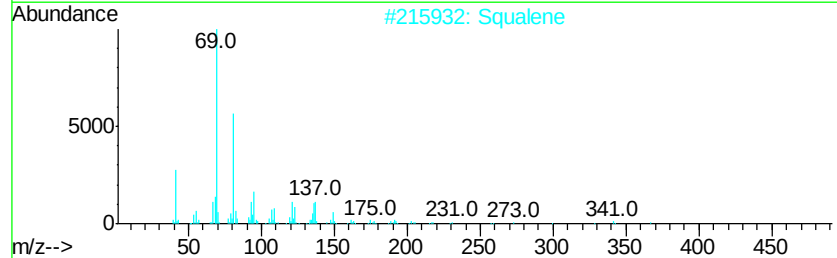
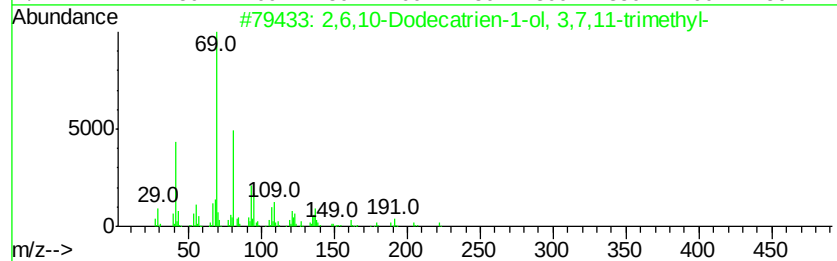
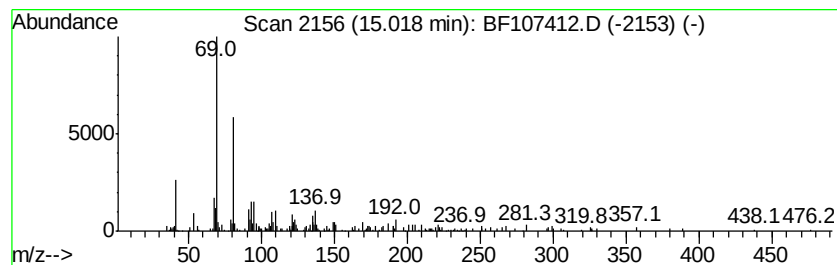
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.85 ng	192153	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	91		
2	Squalene	410	C30H50	000111-02-4	80		
3	trans-Farnesol	222	C15H26O	000106-28-5	72		
4	Butane, 1,2-dibromo-3-methyl-	228	C5H10Br2	010288-13-8	58		
5	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	58		



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
Data File : BF107412.D
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ALS Vial : 4 Sample Multiplier: 1

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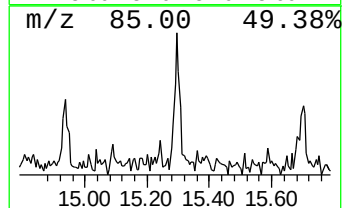
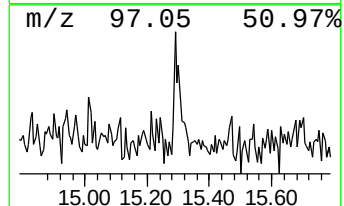
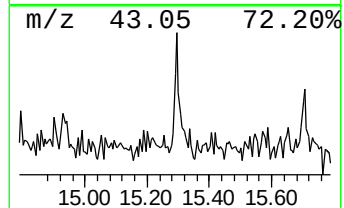
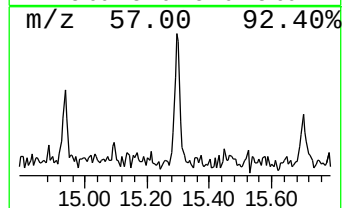
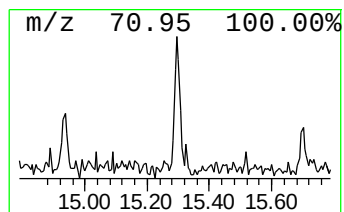
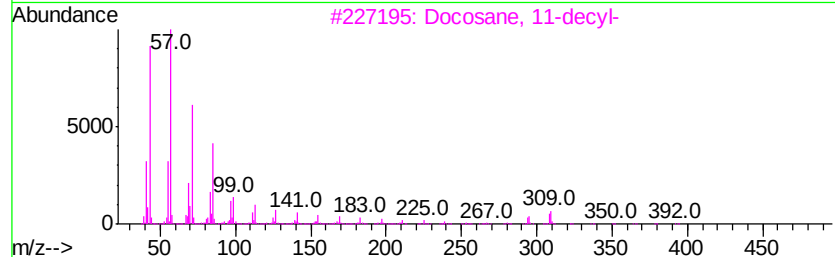
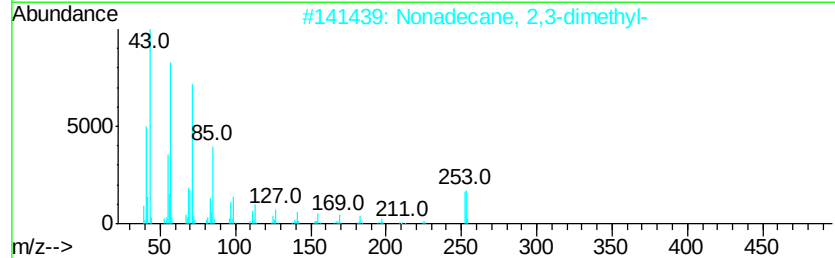
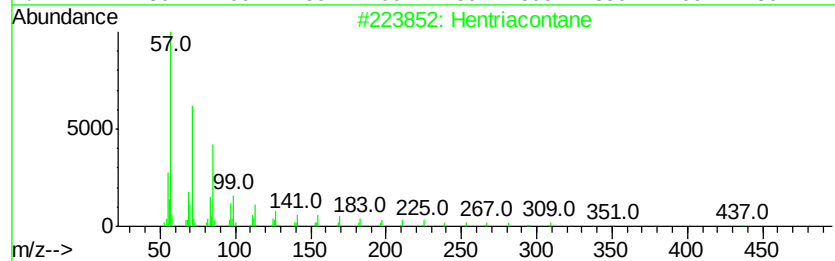
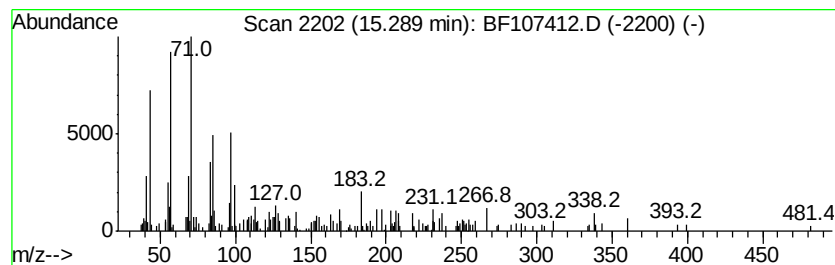
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.55 ng	172140	Perylene-d12	15.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	83
2		Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	72
3		Docosane, 11-decyl-	451	C32H66	055401-55-3	72
4		Eicosane	282	C20H42	000112-95-8	62
5		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
Data File : BF107412.D
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Sample : J3976-01
Misc :
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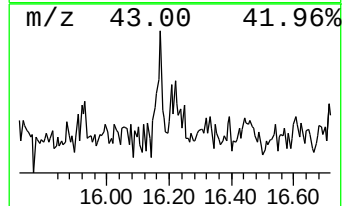
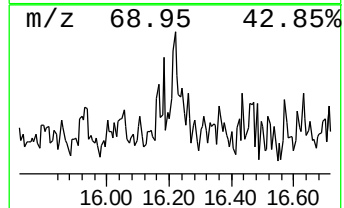
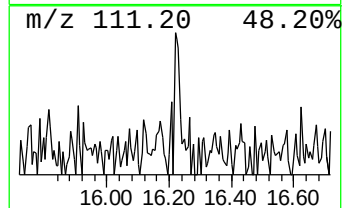
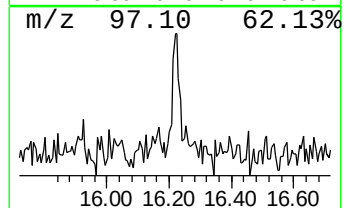
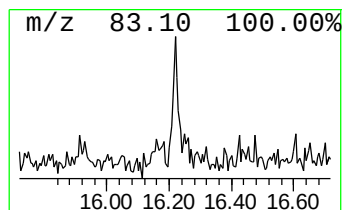
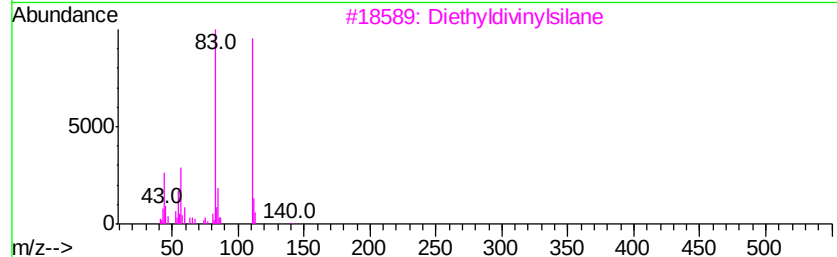
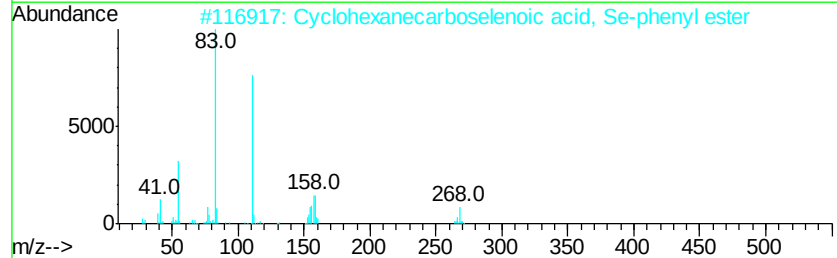
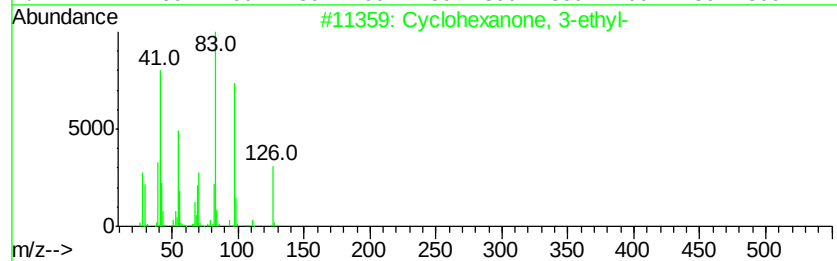
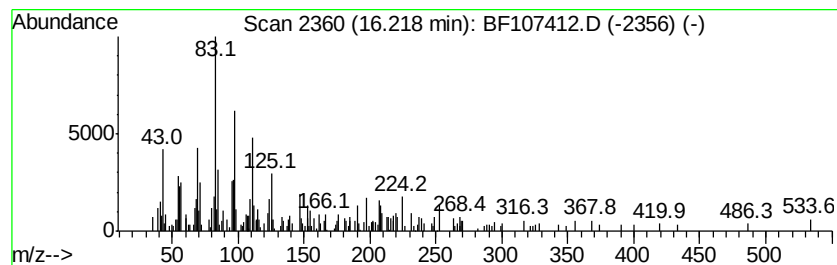
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexanone, 3-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.44 ng	164430	Perylene-d12	15.69
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexanone, 3-ethyl-	126 C8H14O	022461-89-8 55
2		Cyclohexanecarboselenoic acid, S...	268 C13H16OSe	060718-41-4 47
3		Diethyldivinylsilane	140 C8H16Si	018270-16-1 43
4		Cyclohexanecarboxylic acid, 4-pe...	292 C18H25FO2	079912-83-7 43
5		Cyclohexanehexanoic acid, .epsil...	212 C12H20O3	020606-25-1 43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
Data File : BF107412.D
Acq On : 16 Jul 2018 19:45
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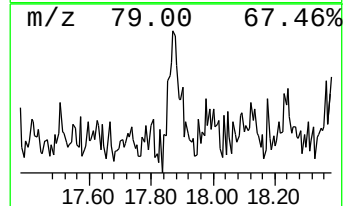
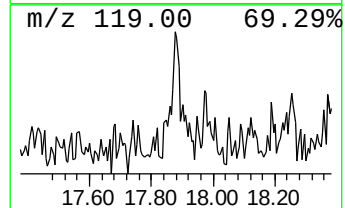
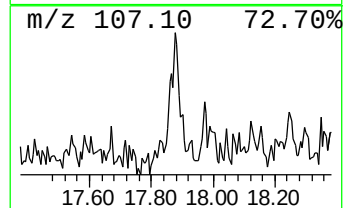
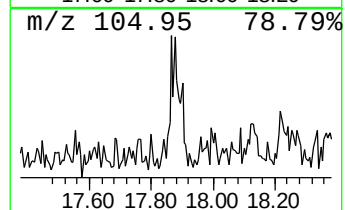
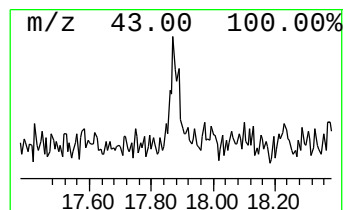
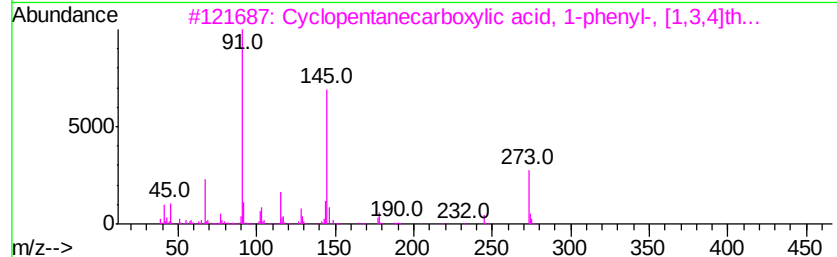
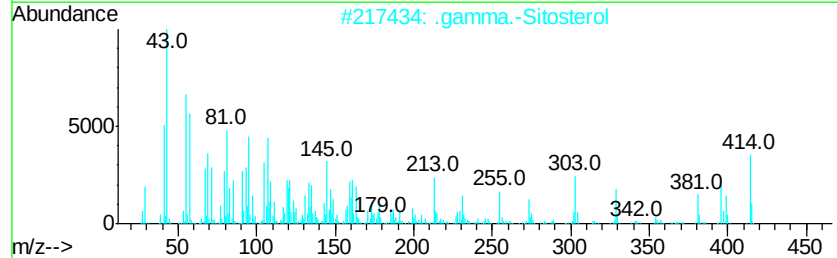
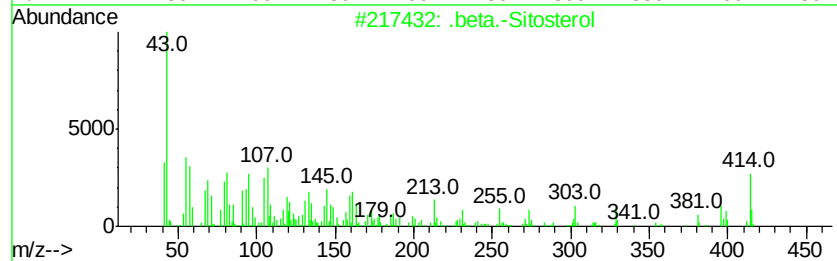
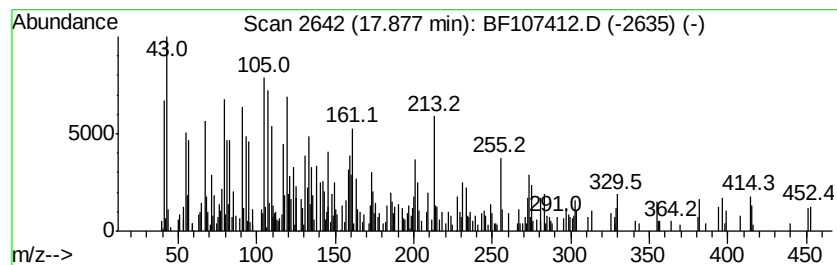
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	7.93 ng	534145	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	60
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	22
3			Cyclopentanecarboxylic acid, 1-phenyl-, [1,3,4]th...	273	C14H15N3OS	1000311-03-5	11
4			N-Acetyl-S-(2-oxocyclohexyl)-L-c...	273	C12H19N04S	077549-11-2	11
5			1-Oxaspiro[4.4]nonane-4-carboxam...	273	C16H19N03	1000319-97-0	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
Data File : BF107412.D
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Misc :
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Instrument :
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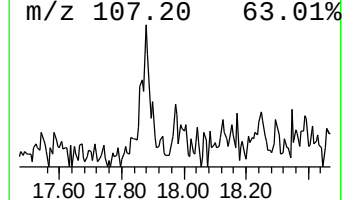
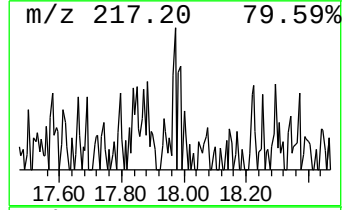
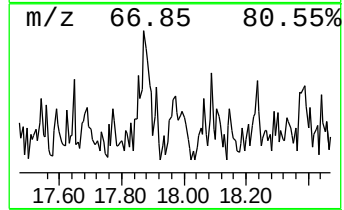
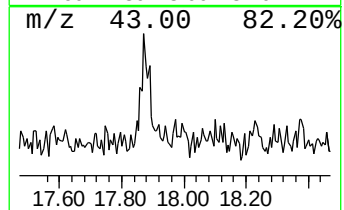
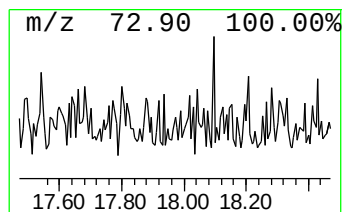
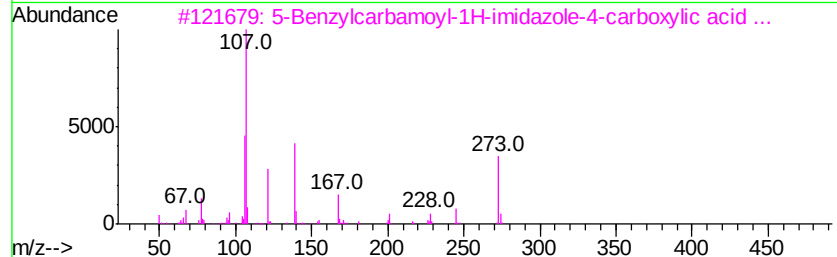
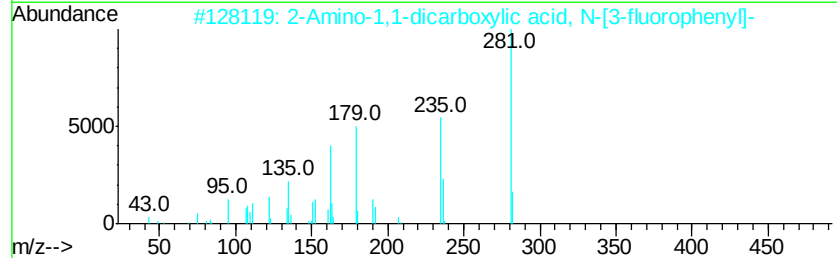
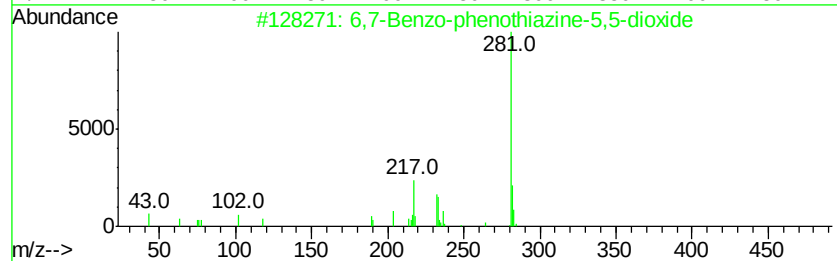
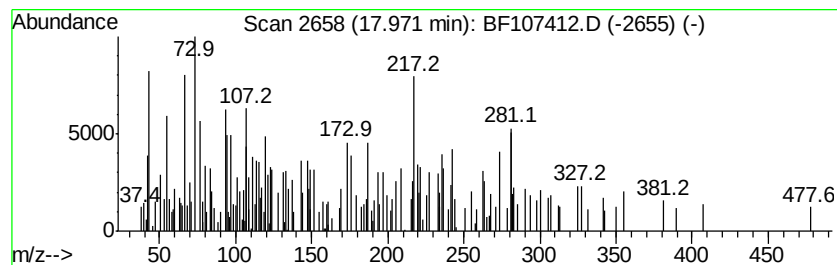
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.97 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	2.15 ng	144548	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6,7-Benzo-phenothiazine-5,5-dioxide	281	C16H11N02S	001225-11-2	14
2		2-Amino-1,1-dicarboxylic acid, N...	281	C14H16FN04	026832-95-1	14
3		5-Benzylcarbamoyl-1H-imidazole-4...	273	C14H15N3O3	312758-83-1	14
4		Phentolamine	281	C17H19N3O	000050-60-2	11
5		Quinoline-2-carboxylic acid (pyr...	263	C16H13N3O	1000302-58-7	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
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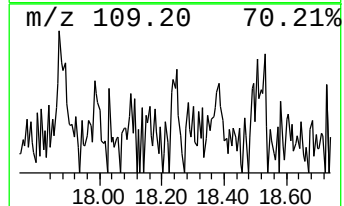
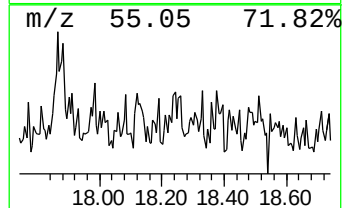
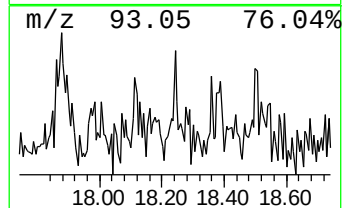
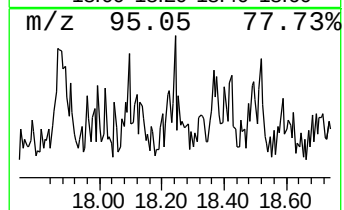
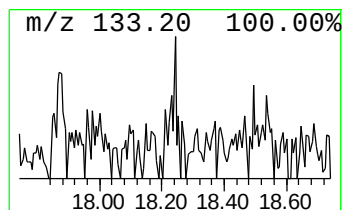
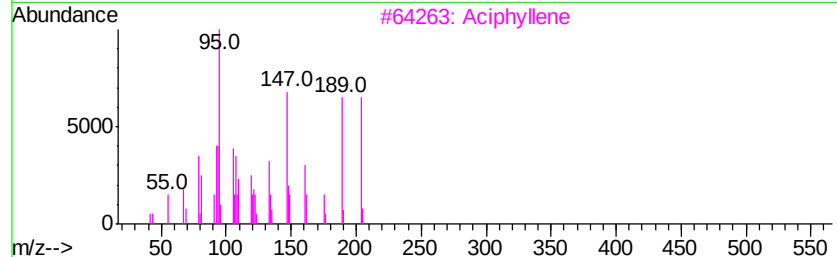
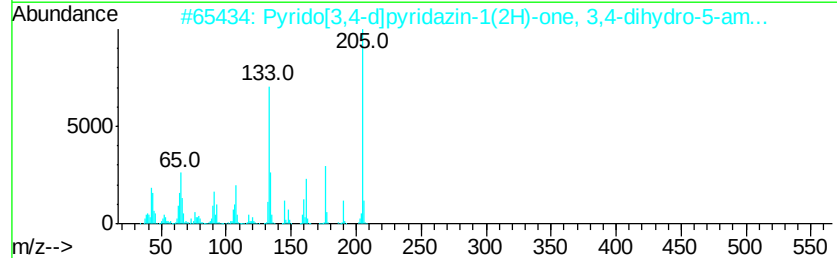
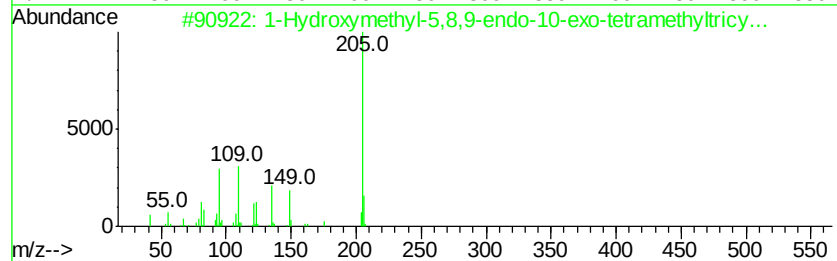
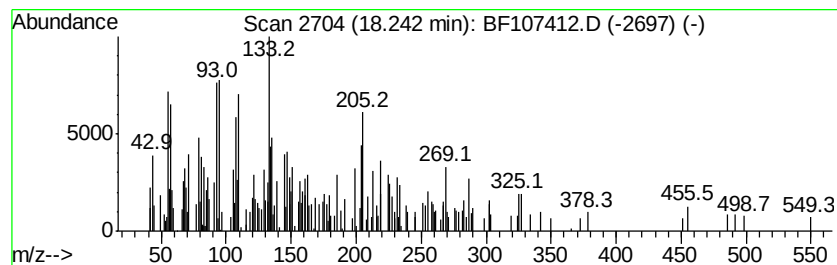
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.24 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	3.57 ng	240253	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	30
2		Pyrido[3,4-d]pyridazin-1(2H)-one...	205	C9H11N5O	1000271-08-5	27
3		Aciphyllene	204	C15H24	087745-31-1	18
4		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	16
5		9-Cedranone	220	C15H24O	1000156-23-2	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
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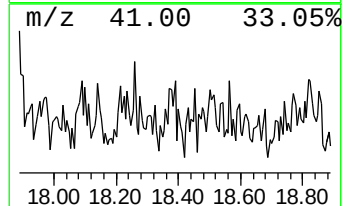
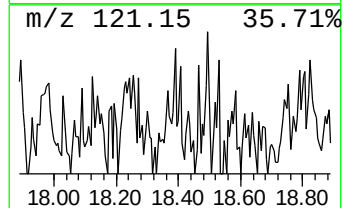
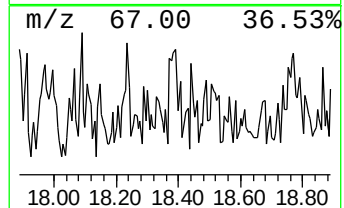
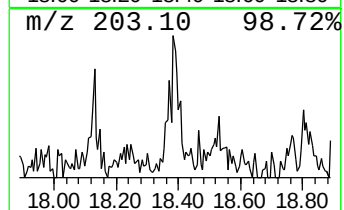
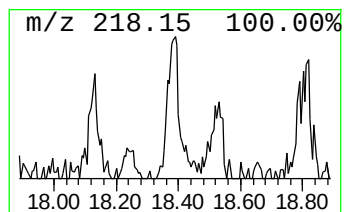
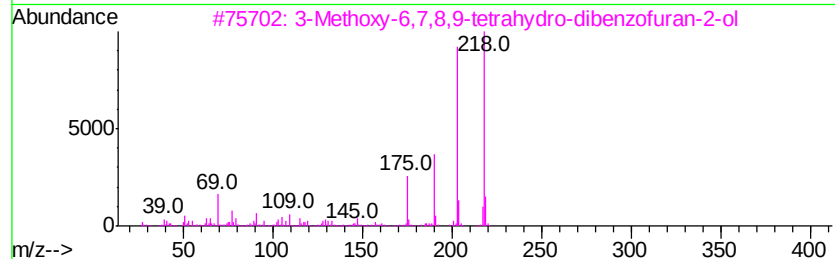
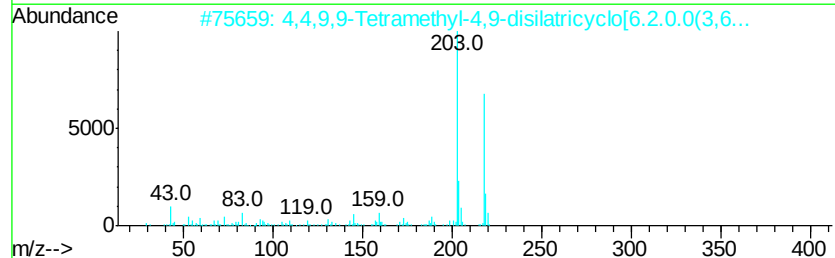
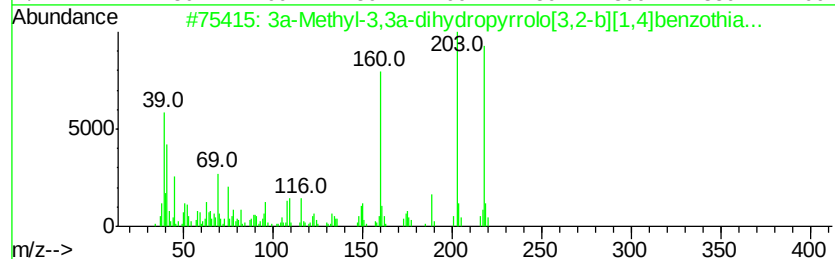
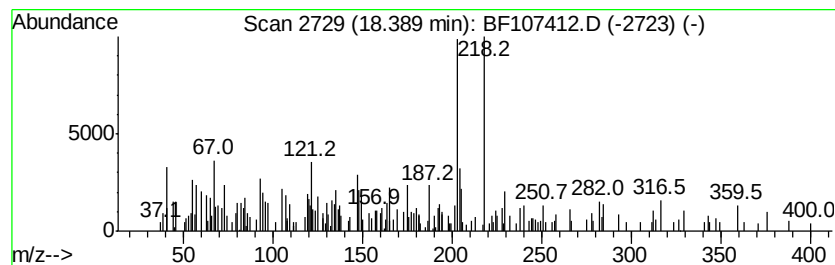
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 3a-Methyl-3,3a-dihydropyrro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.39	2.34 ng	157937	Perylene-d12	15.69		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	52
2		4,4,9,9-Tetramethyl-4,9-disilatr...	218	C12H18Si2	1000280-67-7	52
3		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	50
4		Quinolin-8-amine, 5,6-dimethoxy-...	218	C12H14N2O2	064992-95-6	50
5		5H-Oxazolo[3,2-a]pyridine-8-carb...	218	C12H14N2O2	1000337-58-3	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071618\
 Data File : BF107412.D
 Acq On : 16 Jul 2018 19:45
 Operator : JU/SJ
 Sample : J3976-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-033

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	6.9 ng		392920	1	6.98	1138960	20.0
unknown6.74	6.74	59.1 ng		3365430	1	6.98	1138960	20.0
unknown12.02	12.02	4.4 ng		383221	4	11.51	1757610	20.0
13-Tetradecen-1-o...	13.98	4.3 ng		287988	5	14.15	1342950	20.0
Heptadecane	14.61	3.2 ng		216397	5	14.15	1342950	20.0
2,6,10-Dodecatric...	15.02	2.9 ng		192153	6	15.69	1347510	20.0
Hentriacontane	15.29	2.5 ng		172140	6	15.69	1347510	20.0
Cyclohexanone, 3-...	16.22	2.4 ng		164430	6	15.69	1347510	20.0
.beta.-Sitosterol	17.88	7.9 ng		534145	6	15.69	1347510	20.0
unknown17.97	17.97	2.1 ng		144548	6	15.69	1347510	20.0
unknown18.24	18.24	3.6 ng		240253	6	15.69	1347510	20.0
3a-Methyl-3,3a-di...	18.39	2.3 ng		157937	6	15.69	1347510	20.0